BLACK LIQUOR GASIFICATION FOR CHEMICAL RECOVERY AND HYDROGEN GAS PRODUCTION IN SUPERCRITICAL WATER

Miss Yotwadee Hawangchu

จุฬาลงกรณ์มหาวิทยาลัย
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วิทยานิพนธ์นี้เป็นส่วนหนึ่งของการศึกษาตามหลักสูตรปริญญาวิทยาศาสตรดุษฎีบัณฑิต
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ยศวดี ฮะวังจู : การแก๊สซิฟิเคชั่นน้ำยางดำเพื่อนำกลับคืนสารเคมีและผลิตแก๊สไฮโดรเจนภายใต้สภาวะน้ำเหนือวิกฤติ (BLACK LIQUOR GASIFICATION FOR CHEMICAL RECOVERY AND HYDROGEN GAS PRODUCTION IN SUPERCRITICAL WATER) อ.ที่ปรึกษาวิทยานิพนธ์หลัก: รศ. ดร.วิบูลย์ ศรีเจริญชัยกุล, อ.ที่ปรึกษาวิทยานิพนธ์ร่วม: ดร.ดวงเดือน อาจองค์, 211 หน้า.

งานวิจัยนี้เป็นการศึกษาการแปรสภาพทางความร้อนของน้ำยางดำ โดยใช้น้ำยางดำจากกระบวนการผลิตที่ต่างกัน ได้แก่ กระบวนการคราฟท์ (KBL) และกระบวนการโซดา (SBL) และเพื่อการศึกษาองค์ประกอบลิกนิน ลิกนินจากคราฟท์ (KL) และลิกนินจากโซดา (SL) ถูกแยกออกมาจากน้ำยางดำเรียกรวมว่าเทคนิคอลลิกนิน งานวิจัยแบ่งออกเป็น 3 ส่วน โดยส่วนแรกจะทำการศึกษาผลของสารเคมีที่ใช้ในกระบวนการต่อลักษณะสมบัติของน้ำยางดำและเทคนิคอลลิกนิน ผลการศึกษาพบว่ากระบวนการย่อยเยื่อมีผลต่อลักษณะสมบัติของทั้งน้ำยางดำและเทคนิคอลลิกนิน โดย SBL จะมีของเสียทางเคมีเป็น Na_2CO_3 ในขณะที่ KBL มีทั้ง Na_2CO_3 และ Na_2SO_4 ผลการศึกษาโดย FTIR แสดงให้เห็นว่ากลุ่ม OH และ OCH_3 เป็นองค์ประกอบหลักในน้ำยางดำและเทคนิคอลลิกนิน KL มีสารประกอบอะโรมาติกเป็นองค์ประกอบหลัก ในขณะที่ SL มีสารประกอบอะลิฟาติกไฮโดรคาร์บอนมากกว่า เทคนิค TGA แสดงให้เห็นถึงความคล้ายคลึงกันของรูปแบบการสลายตัวทางความร้อนของ KL กับลิกนินสังเคราะห์ (lignin model compound) และของ SL กับสารประกอบเซลลูโลสสังเคราะห์ (cellulose model compound) ผลการทดลองชี้ให้เห็นว่าเทคนิคอลลิกนินมีโครงสร้างเฉพาะตัว โดยเฉพาะอย่างยิ่งเซลลูโลสที่หลงเหลืออยู่ใน SL ส่วนที่สองทำการศึกษาการแปรสภาพทางความร้อนของลิกนินด้วยเทคนิค Py-GC/MS ที่อุณหภูมิ 400-600 องศาเซลเซียส ผลการทดลองพบว่า KL เปลี่ยนแปลงได้น้อยมากต่ออุณหภูมิที่เพิ่มขึ้นและมีผลิตภัณฑ์หลักเป็นสารประกอบฟีนอลิก SL สลายตัวได้มากเมื่ออุณหภูมิสูงขึ้นและมีผลิตภัณฑ์หลักเป็นสารประกอบไฮโดรคาร์บอนที่มีออกซิเจน ผลการทดลองเหล่านี้แสดงให้เห็นว่า KL มีความคงทนต่อการความร้อนสูงตามธรรมชาติของลิกนิน ในขณะที่ปริมาณออกซิเจนส่วนใหญ่ใน SL แสดงให้เห็นถึงการผสมกันของเซลลูโลสและลิกนินในโครงสร้าง ตัวเร่งปฏิกิริยา Ni/ZrO_2 ช่วยเร่งให้เกิดสารประกอบพาราไฮดรอกซีฟีนิล แคททีคอล และ อะลิฟาติกไฮโดรคาร์บอนจาก KL ส่วนที่สามศึกษาการแก๊สซิฟิเคชั่นภายใต้สภาวะน้ำเหนือวิกฤตของ KBL และ SBL ที่อุณหภูมิ 400-600 องศาเซลเซียสและความดัน 250-400 บาร์ ผลการทดลองพบว่า สภาวะที่ดีที่สุดที่ให้แก๊สสังเคราะห์ที่มีไฮโดรเจนเป็นองค์ประกอบสูงคืออุณหภูมิ 600 องศาเซลเซียส ที่ความดัน 250 บาร์ โครงสร้างลิกนินที่ต่างกันมีผลอย่างมากต่อผลิตภัณฑ์แก๊สที่ได้คือผลิตภัณฑ์ไฮโดรเจน 38 และ 58 โมลต่อกิโลกรัมของ KBL และ SBL ตามลำดับ ตัวเร่งปฏิกิริยาเสริมโลหะนิกเกิลเป็นตัวเลือกที่เหมาะสมที่สุดทั้งด้านประสิทธิภาพและต้นทุนการดำเนินงาน

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สาขาวิชา การจัดการสิ่งแวดล้อม ลายมือชื่อนิสิต ....

ปีการศึกษา 2559 ลายมือชื่อ อ.ที่ปรึกษาหลัก ....

ลายมือชื่อ อ.ที่ปรึกษาร่วม ....

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YOTWADEE HAWANGCHU: BLACK LIQUOR GASIFICATION FOR CHEMICAL RECOVERY AND HYDROGEN GAS PRODUCTION IN SUPERCRITICAL WATER. ADVISOR: ASSOC. PROF. VIBOON SRICHAROENCHAIKUL, Ph.D., CO-ADVISOR: DUANGDUEN ATONG, Ph.D., 211 pp.

This study investigates the thermal conversion of industrial black liquors from the different pulping processes, including kraft process (KBL) and soda process (SBL). In order to study lignin content, kraft lignin (KL) and soda lignin (SL) were isolated from black liquor as the technical lignin. The research was divided into three parts. The first part was to study the effect of the pulping process on black liquors and technical lignins properties. The results showed the effect of the different pulping processes on black liquors and technical lignins composition. SBL mainly contained Na_2CO_3, which was the spent chemical while KBL contained both Na_2CO_3 and Na_2SO_4. The FTIR results presented the OH and OCH_3 group as the primary constituents in black liquors and technical lignins. Aromatic compounds were the main component of KL while SL contained more aliphatic HCs. TGA technique revealed the similarity in thermal decomposition pattern of KL and lignin model compound, and SL and cellulose model compound. These finding indicated the unique structure of the technical lignins, especially the cellulose residue in SL. The second part investigated the thermal conversion of lignin via Py-GC/MS technique at 400°C-600°C. The results showed that KL was slightly responded to increasing temperature with majority of phenolic compound production. With increasing temperature, SL was highly degraded and mainly produced the oxygenated HCs compounds. These results demonstrated high thermal stability of KL, corresponding to lignin nature while the large portion of oxygen content in SL exhibited the mixture of cellulose and lignin in structure. The catalytic of Ni/ZrO_2 can promote p-Hydroxyphenyl, catechol, and aliphatic HCs compounds from KL and enhance ether, aldehyde, ester, and aliphatic HCs compounds from SL. The third part investigated the SCWG of KBL and SBL at 400°C-600°C, 250-400 bar. The results showed that the most appropriate condition for H_2-rich syngas was 600°C at 250 bar. Different lignin structure strongly effected gas yield, 38 and 58 mol H_2 yielded per kg KBL and SBL, respectively. Nickel catalyst is the most promising option with regard to efficient and cost-effective provision.

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Field of Study: Environmental Management Student's Signature ....
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CHAPTER 1

INTRODUCTION

1.1 Statement of problem

According to the 12th National Economic and Social Development Plan (2017-2021), the renewable energy production and utilization have been encouraged and aims to have a 17.34% share of its gross final energy consumption from renewable sources by 2021. As the agricultural country, there are a lot of agricultural residues but they quite difficult to gather and seasonal produce. The continuous and sufficient amount of biomass source is essential to a large extent on the country' energy security. Therefore, the manufacturing sector with consistently process is promising option.

Pulping process generates fibers for further paper manufacture, while separated lignin and spent pulping chemical was together drained out as black liquor. In addition, this by-product spent pulping liquor also consists of residual inorganic chemicals, numerous organic extractives originally from the wood (Cardoso et al., 2009). High organic composition of this waste stream is comparable to those of animal manure, biodiesel by-product, food and beverages production wastes, etc. (Peterson et al., 2008). Therefore, black liquor could be considered as carbon source for energy recovery, especially for lignin in black liquor. The major source of commercial lignin is obtained from paper industry which is the black liquor from pulping process (Vishtal and Kraslawski, 2011). Over $4x10^8$ tons a year of lignin global generated are from pulp mill industry (Yu et al., 2013). The attractive properties of lignin in black liquor are the unique structure after pulping process which is different from native lignin in wood because the alkali chemical cleavage ether bond or β-O-4 linkage which is the highest linkage in lignin (Alekhina et al., 2015). Then lignin was broke into lower weight fraction and dissolved into black liquor. Therefore, its structure is highly condensed and contain greater phenolic hydroxyl group (Laurichesse and Avérous, 2014).

Many researches have dedicated to utilize lignin for application other than heat generation especially platform chemical, adhesives and resins, plastics, lubricants, pesticides, and cosmetics (Macfarlane et al., 2014). However, the different lignin properties in black liquor have many causes, especially wood species and delignification or pulping process (Doherty et al., 2011). Therefore, the lignin original including structure and functional groups is important variable in conversion and production process (Shen et al., 2010). The effect of chemical separation on lignins and their thermal behavior have been studied by pyrolysis reaction for determining the specific condition of high value product production (Lin et al., 2015). However, combustion for steam generation has been chosen as the mean of black liquor utilization in general. This method has relatively low energy recovery and may lead to a dangerous smelt-water explosion (Cao et al., 2017). In addition, due to an enormous amount of water in black liquor, the evaporation unit consumes a lot of energy for dewatering before firing in recovery boiler (Cao et al., 2011). In fact, pulping industry had been positioned as the forth of energy consumption manufacture (Kong et al., 2016). As a result, another possible alternative may be achieved by utilizing water in black liquor for supercritical water gasification (SCWG) reaction. In this case, water will act as oxidizing agent in the special state when its critical point (374°C and 221 bar) is overcome. In practical, this novel method would be added in parallel to the existing conventional system and not replacing it.

Supercritical water (SCW) condition induces water to act as an excellent solvent because of the distinctive properties (low viscosity, high diffusivity and low electric constant) of fluid state of water (Lu et al., 2006). In recent years, many researchers have investigated the SCW technique for treating industrial waste stream. However, most research has been focused on model compound, such as glucose, formic acid, and cellulose (Yoshida et al., 2004). The principal reactions in the SCWG are steam reforming, water-gas shift (WGS), and methanation. The mechanism involving these reactions is quite complex including competing generation and consumption of reactants and products from each individual step. Moreover, alkali inherent from pulping chemical was regarded as homogenous catalyst based on many researches (Peng et al., 2014). Hence, alkali in black liquor would have potential to act as catalyst for lignin decomposition reaction.

The major pulping manufacturers in Thailand utilize eucalyptus wood as raw material while employ different pulping processes. Therefore, it might be possible for lignin in black liquor to be affected in different way. The characteristic study on lignin may encourage the understanding of product distribution from black liquor thermal conversion. In conclusion, this research was divided into 3 parts: i) identify the effects of kraft and soda pulping process on black liquors and lignins properties ii) study thermal conversion of lignins via Py-GC/MS technique under non- and catalytic processes and iii) investigate the gasification of black liquors under supercritical water condition with non- and catalytic reactions. The expected knowledge from this research is to show the advanced thermal conversion that can efficiently convert organic in this hazardous waste steam without any dewatering and gain insight understanding of relation between feedstock properties and product distribution.

Waste steam from manufacturer is the promising source for biomass energy via thermal conversion. However, almost are impractical forms due to high water content. Therefore, the research to explore the biofuel production from this kind of biomass is necessary. Not only the most effective biomass utilization could be achieved, but also energy saving in the evaporation unit would be merited for paper making industry.

1.2 Objectives

The goals of this research are to identify the effects of different delignification process (kraft and soda pulping process) on lignin structure in kraft and soda black liquors. The product distribution of thermal conversion processes on black liquors and their technical lignins was studied. With high water content, industrial black liquors were carried out via advanced thermochemical conversion (supercritical water gasification) for rich-H_2 syngas production. The metal catalysts were added in thermal reaction to investigate the variation on products. To achieve these goals, several objectives are established as follows:

1) To identify the effects of kraft and soda pulping process on black liquors and lignins structure.
2) To study the product distribution of kraft and soda lignin using Py-GC/MS.
3) To obtain the appropriate condition for H_2-rich syngas production of black liquor via the SCWG reaction.
4) To study the effects of alkali compound as a catalyst under SCWG reaction and the effect of metal catalyst on product distribution under thermal conversion.

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1.3 Hypotheses

1) The variations in the pulping process can produce the black liquors with variety of lignins structure; therefore, the product distribution from their thermal conversions is dissimilar.

2) High water content in black liquor can be utilized as the oxidizing agent in the gasification reaction under supercritical water condition for H_2-rich syngas production.
3) Alkali content in black liquors acts as the homogeneous catalyst in SCWG reaction.
4) Metal catalysts play an important role in thermochemical conversion to promote the production.

1.4 Scopes of the Study

1) Kraft and soda black liquors were obtained from the local pulp mill. The position of black liquor collecting was after digestion or pulping process and before the evaporation unit.
2) Lignin extracted by acid precipitation from black liquor was the technical lignin.
3) Lignin model compound was the precursor.
4) The miniature fused quartz was used as the reactor to prevent other reactions due to catalytic wall effect.
5) Thermal conversion of the technical lignins was carried out in Py-GC/MS
6) Gas produced was analyzed by gas chromatography with TCD/FID.
7) Catalysts were prepared by wetness impregnation method.
8) All experiment in this research was carried out in laboratory scale at MTEC pilot plant and department of environmental engineering, faculty of engineering, Chulalongkorn University

1.5 Experimental framework

The conceptual framework of this study was to investigate thermal conversion for biofuel and biomaterial from black liquor which is a by-product of paper making industry. Particularly, direct gasified of black liquor for syngas production was conducted via its water under supercritical water condition. The catalytic reaction was applied for thermal conversion to study the upgrading ability of products. The experiment was divided into 3 parts (Fig 1.1).

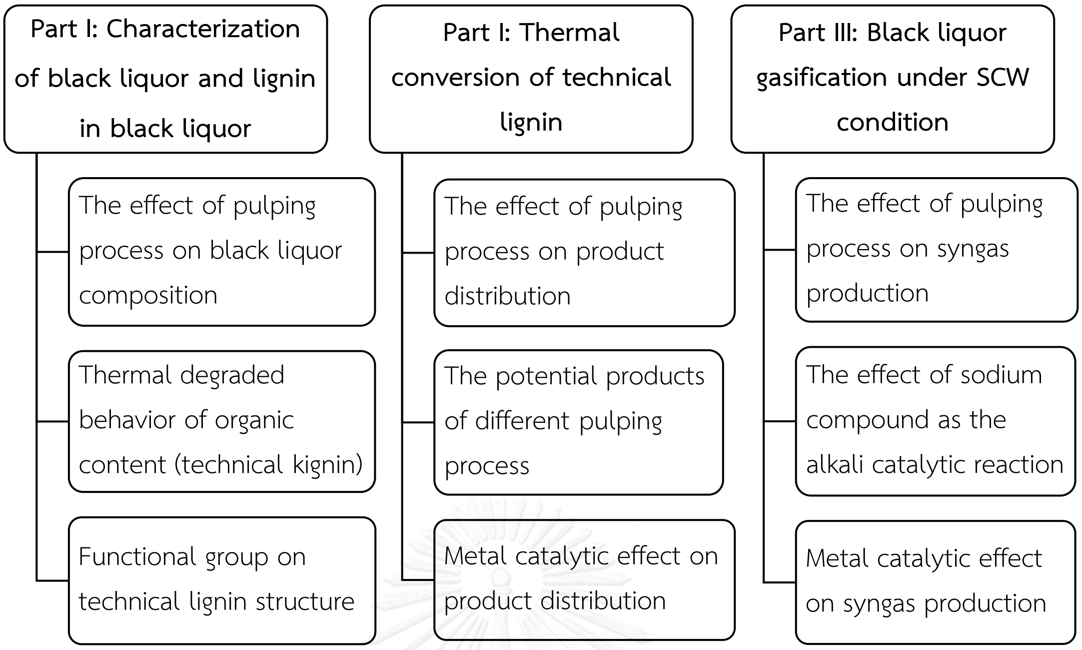

Figure 1.1 Flow chart of the research

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CHAPTER 2

THEORETICAL BACKGROUNDS AND LITERATURE REVIEWS

2.1 Backgrounds

This research aimed to utilize weak black liquor containing high water content from different pulp mill industry – kraft and soda pulping process. Organic in weak black liquor was the crucial substance of product distribution in thermal conversion method. Therefore, thermal degradation on lignin in black liquor was investigated by pyrolysis reaction for understanding the product distribution from lignin decomposition. In consequence of lignin thermal behavior, syngas production from lignin in black liquor by gasification might dissimilar.

2.1.1 Black liquor

The major waste steam of paper making generates from a digestion unit by the chemical pulping process (Naqvi et al., 2010). At this process wood chips are digested by pulping chemical for removing lignin and other organic compositions. After reaction, the spent chemical and dissolved organics e.g. polysaccharides, carboxylic acids and extractives, from wood are drained together named black liquor. Black liquor contains high water content as 85% which are dewatered to 25-30% and then be further combusted for cooking chemical (white liquor) and energy recovery (heat, steam) at recovery boiler (Cardoso et al., 2009).

2.1.1.1 Chemical pulping process

The chemical pulping methods can be classified into two major principles. The first pulping process is alkaline such as kraft process and soda process, and the other is sulfite pulping (Wool and Sun, 2005). However, the most popular method is kraft pulping which are applied to more than 90% of chemical pulps (Sixta and Schild, 2009).

Soda pulping is one of the simplest pulping processes and a source of sulfur-free lignin. In soda pulping lignocellulose is treated with aqueous NaOH at a temperature between 150 and 170°C. Under these conditions both lignin and carbohydrates are degraded. Therefore, the selectivity of soda pulping is low and it is currently limited to easily pulped materials like straw and some hardwoods. Soda lignin has been used as a biocide for wastewater treatment and as a dispersant (Gosselink 2004).

The kraft process (or sulfate process) is a modified soda process in that it uses NaOH and Na_2S as cooking chemical to fragment lignin until it is soluble in the alkaline medium. The pulping step is conducted at 140–180°C and lasts approximately 2 hours. The selectivity of kraft pulping is higher than soda pulping because hydrogen sulfite ions (HS^-) react with lignin (Gierer, 1985). As a result, a typical Kraft pulping process removes up to 80% of the lignin, 50% of the hemicellulose and less than 10% of the cellulose. Fig 2.1 showed the model of kraft lignin from pine wood composting of the diphenylmethane and vinyl aryl ether linkages (Zakzeski et al., 2010).

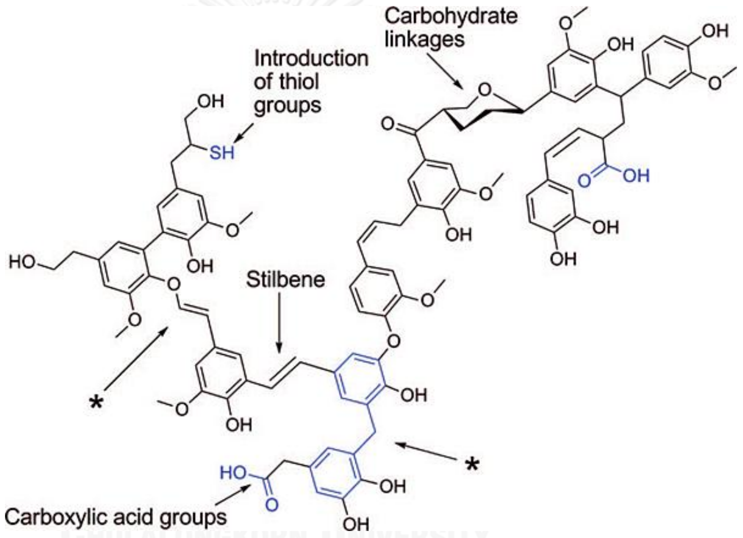

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Figure 2.1 Structural features of kraft pine lignin characteristic (Zakzeski et al., 2010).

2.1.1.2 Recovery cycle

The integrated units operate in black liquor treatment involving recovery boiler and causticizing plant. These processes is called recovery cycle which is the essential part of pulp mill because it can meet all internal steam and electricity demand for the processes (Naqvi et al., 2010). The important units are evaporators, recovery boiler (known as Tomlinson boiler), causticizing, and lime kiln. Particularly in recovery boiler, it plays the crucial role in energy and pulping chemical recovery.

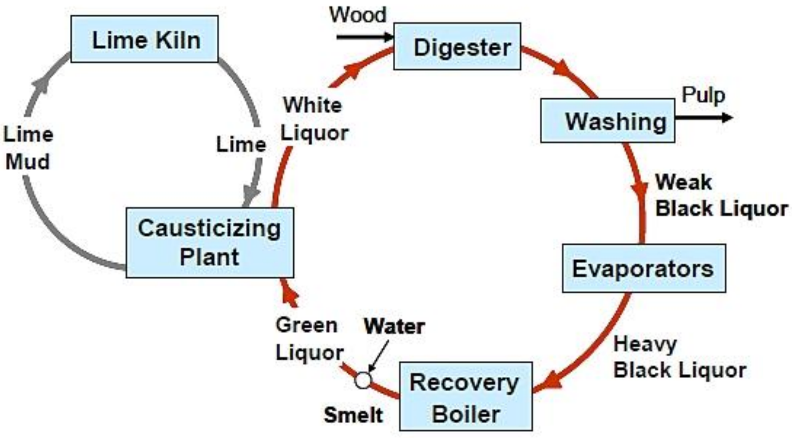

Figure 2.2 Schematic of pulping process (Tran and Vakkilainen, 2007)

Fig 2.2 displays treatment of black liquor from pulping process including two cycles. Weak black liquor from digestion stage is concentrated in the evaporation unit; in consequence, high solid content black liquor is burn in the recovery boiler. At this point, thermal conversion of solid black liquor provides power for pulp mill and recycles the cooking chemical (white liquor). The smelt is the solid inorganics which are dissolved in water to become green liquor and further processed in the causticizing plant. As a result, black liquor thermal conversion is the most important renewable bio-fuel production, especially in Sweden and Finland (Tran and Vakkilainen, 2007).

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2.1.1.3 Organic substance in black liquor

Waste organic and spent chemicals normally separated from raw materials such as hardwoods, softwoods or non-wood fiber during pulping process is called black liquor. These materials mainly composed of lignin and carbohydrates (cellulose and various hemicelluloses. During pulping, lignin is dissolved into the cooking chemical, resulting in simultaneous fiber separation. In conjunction with delignification, some polysaccharides degradation byproduct, including a significant proportion of hemicelluloses and a minor proportion of cellulose are also dissolved or degraded by the alkali-catalyzed cooking reactions. The proportions of organic and inorganic in BL vary from mill to mill due to natural variations in the organic constituents of wood species and the cooking conditions that are unique to each mill. The properties of BL therefore also vary depending on origin but also over with time within the same mill.

2.1.2 Lignin

2.1.2.1 Native lignin

The three major components of lignocellulosic biomass are cellulose, hemicelluloses and lignin. Lignin is the second large source of organic material which abundant natural aromatic polymer (Brebu and Vasile, 2009). In plant cell walls, lignin fills the spaces between cellulose and hemicellulose, and it acts as a resin that holds the lignocellulose matrix together. Crosslinking with the carbohydrate polymers encourages strength and rigidity to the system. However, lignin is considered involving the radical polymerization of three primary monomers: p-coumaryl, coniferyl, and sinapyl alcohols (Fig 2.3). Polymerization by random phenol radical-radical coupling reactions under chemical control leads to the formation of lignin vascular in plants (Zakzeski et al., 2010).

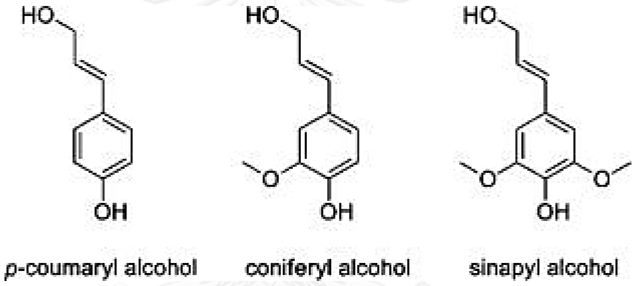

Figure 2.3 Three primary monomers in lignin (Zakzeski et al., 2010)

The composition of softwood and hardwood lignin (Fig 2.4) varies in the relative abundance of the p-coumaryl, coniferyl, and sinapyl alcohols (Zakzeski et al., 2010). While softwood lignin contains fewer sinapyl units and consists mainly of guaiacyl structures, hardwood lignin contains guaiacyl-syringyl structures (Brebu and Vasile, 2009).

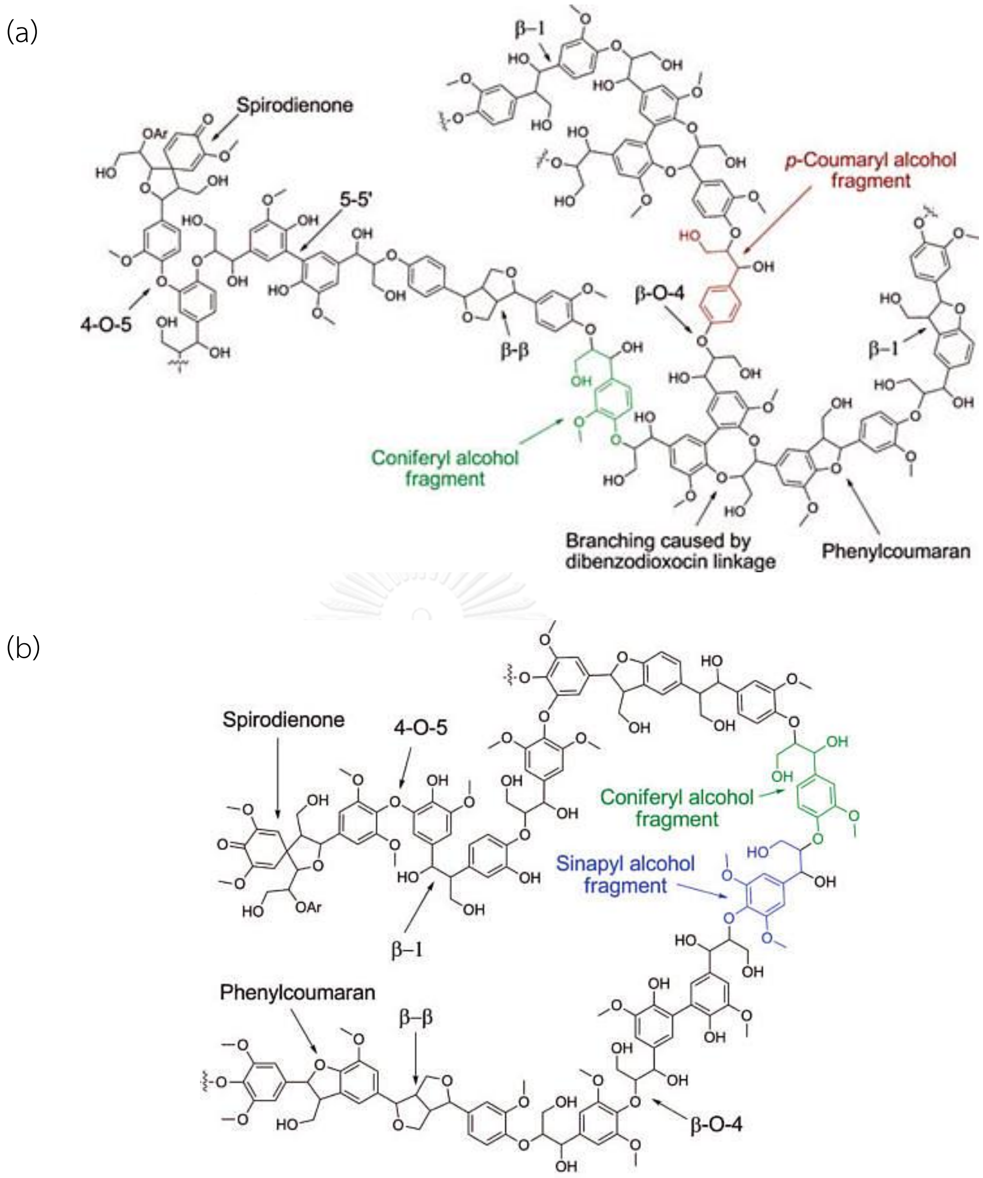

Figure 2.4 Lignin structure and linkages (a) softwood and (b) hardwood. (Zakzeski et al., 2010).

2.1.2.2 Technical lignin properties

Technical lignins are obtained from lignocellulosic biomass processing. Technical lignins differ from the native lignin as a result of a combination of multiple reactions including catalyzed biomass hydrolysis, condensation of lignin fragments, elimination of native lignin functional groups, formation of new functional groups, and others (Vishtal and Kraslawski, 2011). Technical lignins have a high variety of structural moieties present in rather small amounts (Balakshin et al., 2003, Liitiä et al., 2003).

During the lignification process and the processes applied to extract lignin from the plant material, several different types of linkages are formed between the monolignol building blocks. The most abundant linkage in lignin is the arylglycerol-β-aryl ether (β-O-4) linkage (Lochab et al., 2014). The β-O-4 ether bond is readily cleaved; indeed, the cleavage of these bonds during alkaline pretreatment constitutes the principle pathways in which the lignin is depolymerized (Chakar and Ragauskas, 2004). The fragmentation of these linkages tends to lead to the generation of more water-soluble compounds containing free phenolic groups. The carbon-carbon bonds in lignin are some of the most difficult bonds to break, and many of these linkages tend to survive the typical pretreatment processes. The development of catalysts capable of cleaving these more linkages is a considerable challenge (Dobele et al., 2011). Moreover, although carbon-carbon linkages are present in native lignin, extra carbon-carbon bonds can be formed during lignin pretreatment, such as in alkali-promoted condensation reactions during kraft pretreatment. The linkage in softwood such a spruce, and hardwood like a eucalyptus and birch, their dominant linkage is β-O-4. The β-O-4 consists of approximately 50% of spruce linkages and 60% of birch and eucalyptus linkages. The identification and quantification of the various structures and linkages in lignin is challenge, because of the complex and very sensitive to isolation technique of lignin. The composition of lignin softwood, hardwood and grasses varies also in the relative abundance of the p-coumaryl, coniferyl, and sinapyl alcohol monolignols (Capanema et al., 2004). Coniferyl alcohols constitute approximately 90% of softwood lignin, whereas roughly equal proportions of coniferyl alcohol and sinapyl alcohol appear in hardwood lignin, although many exceptions are known.

2.1.2.3 Lignin application

Nowadays, the major percentages of the lignin residues in industry, particularly in pulp and paper mills, is burned as a valuable fuel for energy recovery (Wiinikka et al., 2015). However, there is a growing interest and concern on exploring the potential of lignin and its derivatives as raw materials in the polymer industry and other chemicals (Laurichesse and Avérous, 2014).

Lignin is attractive for further utilization as raw material in the chemical based production:

- lignin is easily obtainable in industry and in large quantities
- reduction of its disposal as a pulp mill waste and the correspondent environmental problems
- interesting energetic value due to its high aromatic content
- compatible with important chemical products
- a large number of reactive points on its molecular skeleton where it can occur several kinds of reactions.

Technical applications of industrial lignins include the areas of thermoplastics, adhesive resins, carbon fibres, cement additives, sorption-active materials, medicinal antioxidants, automotive brakes, sealants, polyurethane foams, rubber fillers, surfactants, dispersants, electrical shielding, storage battery plates and many others.

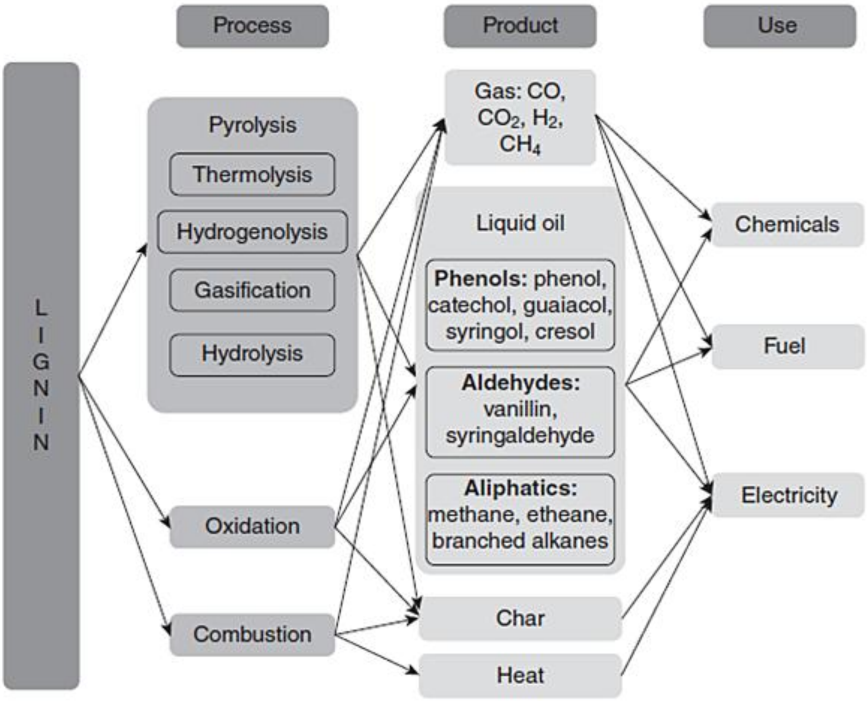

Figure 2.5 Thermal conversions of lignin and the potential products (Macfarlane et al., 2014).

Fig 2.5 presents the potential product from lignin degradation via thermochemical conversions. Pyrolysis, gasification, hydrogenolysis, chemical oxidation and hydrolysis under supercritical conditions are the major methods for generating the bio oil, syngas and phenols (Macfarlane et al., 2014). Therefore, thermal conversion method could be the attractive means for high-value products production from lignin.

2.1.3 Thermal conversion

Biomass could be converted into high-value products such as biofuel or biomaterials depended on the biomass properties and thermal process conditions (Goyal et al., 2008). Combustion, gasification, and pyrolysis are the promising methods in thermochemical conversion which are known as the major solution for the production of secondary production fuels (Parthasarathy and Narayanan, 2014). Particularly of gasification, this reaction is expected to be an important to convert biomass feed stocks into useful fuel gases and synthesis gases including hydrogen (Robbins et al., 2012). While pyrolysis reaction provide more varieties of product e.g. gas, bio-oil (liquid), and char (solid).

2.1.3.1 Gasification

In essence, gasification composes of the partial oxidation of combustible materials under high temperature in range of 800 and 1200°C with goal of valuable product gas (Robbins et al., 2012). The principal reactions of the gasification are endothermic (Molino et al., 2016) consisting of four main steps shown in Fig 2.6.

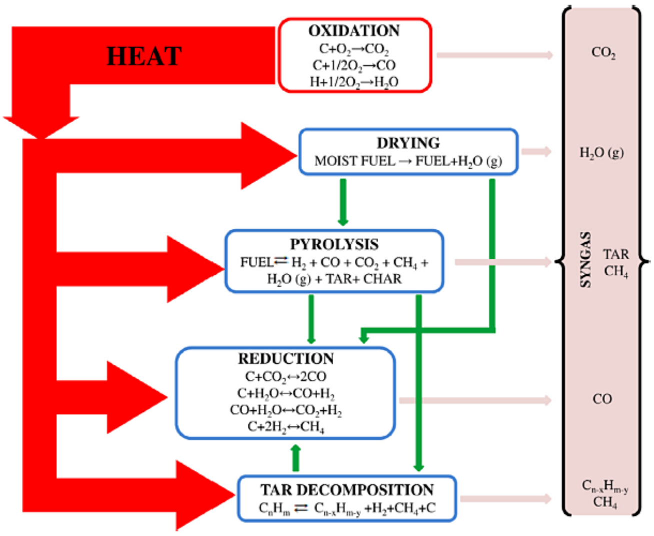

Figure 2.6 Major steps of the gasification process (Molino et al., 2016)

The oxidation is carried out in the absent oxygen in order to oxidize of raw material and provide thermal energy for the whole process. Drying step is the evaporation of moisture in biomass. The pyrolysis phase consists of several complex phenomena which are carried out for the cracking of chemical bonds of feedstock. The reduction step generates the final syngas via reaction of gas mixture and char from the pyrolysis and oxidation steps. Owing to the crucial role of temperature in gasification process, the various technological solutions have been developed which of each could generate the different syngas composition and different amount of solid residue (Molino et al., 2016).

However, the limitation of thermal conversion is moisture which could lower the efficiency of the system. Thermochemical decomposition can be utilized for the energy conversion of all of the categories of low moisture biomass materials (Ahmad et al., 2016). The moisture content in biomass must be below 30% (Robbins et al., 2012) for acceptable thermal processes. Therefore, in case of high moisture content need special solution to deal with. The supercritical water gasification is considered to be the promising technology because it does not require drying process (Yakaboylu et al., 2015).

2.1.3.2 Supercritical water properties

Under normal conditions, water has three states; ice, steam, and liquid. A new state of water is occurred when water temperature and pressure reach their critical point, at 374°C and 22.1 MPa (Fig 2.7), namely supercritical state (Guo et al., 2010). At that condition the physicochemical characteristics such as ion product, density, dielectric constant and viscosity of water are different from either extreme state, i.e. the gas phase or the liquid phase. The relation between water temperature and pressure on the dielectric constant has been reported.

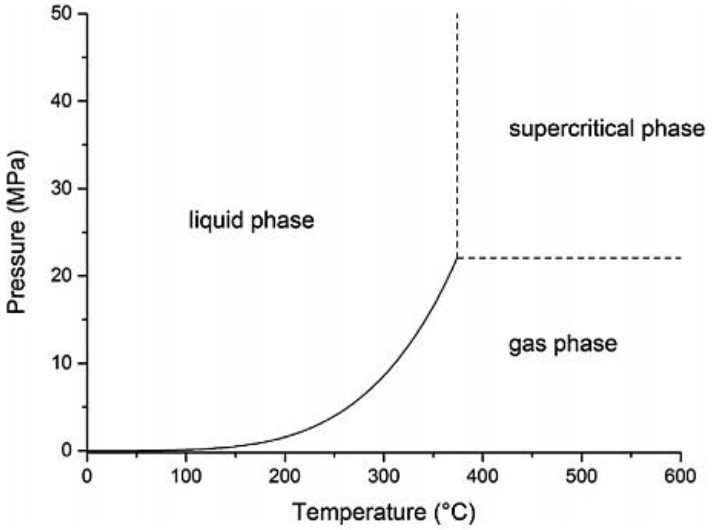

Figure 2.7 Schematic phase diagram of water (Yakaboylu et al., 2015).

Above the critical point, the dielectric constant of water drops sharply because decreased degree of hydrogen bonding as temperature is raised. At the critical point the degree of hydrogen bonding in water is half of what it is under ambient conditions (Gorbaty and Gupta, 1998). As the temperature of water increases from ambient to 200-300°C, its ion product K_w increases three orders of magnitude (Bandura and Lvov, 2006), allowing it to participate in acid and base catalyzed chemistry; (Ikushima et al., 2000, Watanabe et al., 2003)however, beyond the critical point the ion product falls drastically, making it a nonionic solvent (Fig 2.8).

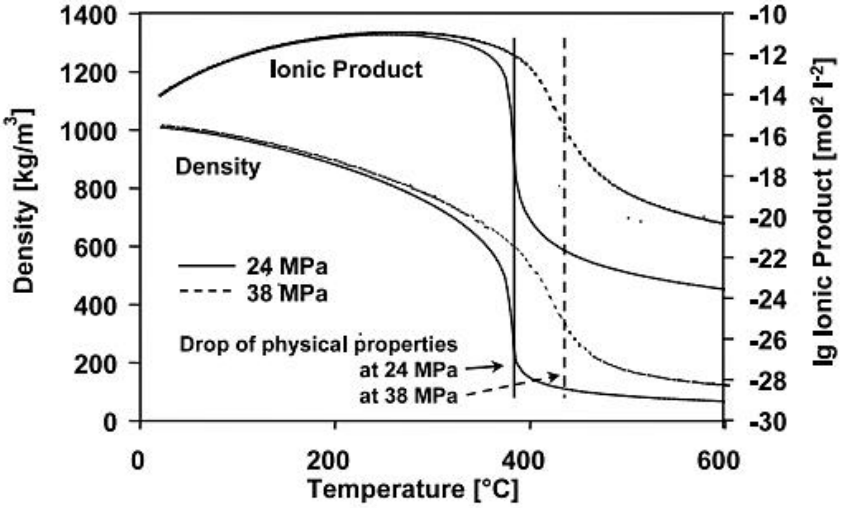

Figure 2.8 Drop of physical properties of high-temperature water at different pressures. (Kritzer, 2004).

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The transport properties of supercritical water have some gas-like characteristics as well as some liquid-like characteristics. The viscosity of supercritical water is an order of magnitude lower than that of liquid water, greatly enhancing mass transfer and diffusion controlled reactions (Bandura and Lvov, 2006). In particular, the low polarity of SCW makes it an ideal solvent for non-polar compounds and gases, which eliminates the mass transfer limitation between different phases in a reaction system. Therefore SCW can be employed as a suitable solvent or reactant for reactions, e.g., supercritical water gasification (SCWG) of biomass for renewable hydrogen generation.

2.1.3.3 Supercritical water gasification

SCW behaves like organic solvents so that many organic compounds have very high solubility in it. Moreover, gases are miscible in SCW. Thus, chemical reaction can be conducted in a single supercritical phase reaction media. High concentrations of reactants can often be attained and there are no inter phase mass transport processes to hinder reaction rates (Lu et al., 2007). Furthermore, as there is no limit of interphase mass transfer resistance the reactions proceed very rapidly and completely. SCWG is one of the hydrogen production methods with great potential. As a result, biomass gasification in SCW has a high reaction rate. In addition, biomass gasification in SCW has high gasification efficiency at much lower temperatures of approximately 673K compared with conventional gasification (Williams and Onwudili, 2005). Furthermore, biomass gasification in SCW produces higher concentration of hydrogen in product gas, because the high water excess favors the formation of H_2 and CO_2 instead of CO.

SCWG can enable shorter residence times and smaller reactor volumes. In the SCWG of biomass, many possible reaction pathways are possible. The overall chemical reaction for SCWG of biomass for H_2 production is endothermic (Guo et al., 2007). The principal reactions in the SCWG are steam reforming (eq.1), water-gas shift (eq.2), and methanation (eq.3-4). These reactions mainly produced CO, CO_2, CH_4 and H_2. The mechanism involving these reactions is quite complex including competing generation and consumption of reactants and products from each individual reacting step (Susanti et al., 2014).

Decomposition $C_xH_yO_z \longrightarrow CO + H_2 + CH_4 + CO_2 + \text{others}$ (1)

Steam reforming: $(CH_xO_y) + H_2O \longrightarrow CO_2 + CO + H_2$ (2)

Water gas shift: $CO + H_2O \longrightarrow CO_2 + H_2$ (3)

Methanation: $CO_2 + 4H_2 \longrightarrow CH_4 + 2H_2O$ (4)

Methanation: $CO + 3H_2 \longrightarrow CH_4 + H_2O$ (5)

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2.1.3.4 Pyrolysis

Pyrolysis is thermal degradation in the absence of air or oxygen which is the best solution for conversion of biomass to liquid fuel (Goyal et al., 2008). Moreover, it gives high yields and gas products including valuable chemicals, petrochemicals and fuels (Robbins et al., 2012). The production depends on thermal condition, particularly on the heating rate. Regarding the heating rate, pyrolysis can be classified into flash, fast, and slow pyrolysis process (Liu et al., 2017). Liu et al. (2017) suggested that at higher heating rate leads to higher volatile yield, less biochar, but no effect on bio-oil yield. Moreover, the higher temperature causes polycyclic aromatic hydrocarbons (PAHs) such as pyrene, and short vapor residence time influence on bio-oil.

2.2 Literature review

2.2.1 Lignin determination by Py-GC/MS

The main products produced in the pyrolysis of lignin include volatile compounds, mono-lignols, mono-phenols, and polysubstituted phenols (Liu et al., 2017). Lignin extracted from various types of biomass has also been studied using Py-GC/MS in order to understand its thermolysis structure, monomeric composition and the differences in these characteristics between the native and extracted lignin.. Lignin extracted using various techniques from different biomass sources was subjected to Py-GC/MS and thermogravimetric analysis in a study by Liang et al. (2015). Py-GC/MS data suggested that lignins from hardwood biomass types generated similar products even if the lignin extraction techniques were different. Kim et al. (2013) extracted lignin from poplar wood using assorted techniques and Py-GC/MS analysis indicated some differences in the product distributions of the lignins examined. Lignin isolated from industrial black liquor was analyzed by Py-GC/MS and bond dissociation energies were used to explain the formation of radicals that lead to the production observed (Hu et al., 2013). Lignin model monomers, dimers with β-O-4 linkages and various other synthesized lignin models have been analyzed by Py-GC/MS and other microscale pyrolysis-mass spectrometry techniques. (Shin et al., 2001, Kotake et al., 2013)

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2.2.2 Supercritical water gasification of biomass

Zhang et al. (2010) treated the secondary pulp/paper-mill sludge and sewage sludges for energy recovery. The experiments were carried out at 400°C and 550°C for 20–120 min under supercritical water condition. The results indicated that the heavy oil (HO) preferred lower temperature and short reaction time resulting for high gross calorific values (>36 MJ/kg) while syngas production was enhanced with increasing temperature not significantly affected by reaction time. The secondary pulp/paper-mill sludge presented a greater capability than sewage sludges for the production of HO and gases owing to its higher contents of volatiles and alkali metals. They concluded a prospective utilization potential for SPP as a source of bio-energy.

Williams and Onwudili (2005) conducted subcritical and supercritical water gasification of cellulose, starch, and glucose as representative biomass model compounds and biomass has been investigated in a heated batch reactor. The results showed the differences in chemical structures produce significantly different product yields.

Yanik et al. (2007) conducted studies on gasification of biomass feedstock in a batch autoclave at 500°C. They observed that the hydrogen yields ranging between 4.05 and 4.65 mol H_2/kg biomass) and composition of gases depend also on the organic materials other than cellulose and lignin contents of lignocellulosic material.

In conclusion, supercritical water gasification (SCWG) process has high reaction efficiency especially for H_2production. Because the reaction medium is water, so there is no need to dewatering process. Therefore, for wet biomass containing large amounts of water up to %90, SCWG appears to be a useful technology (Calzavara et al., 2005)

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Table 2.1 Lignin depolymerization methods (Davis et al., 2016)

Methods	Benefits	Challenges	Products
Pyrolysis	Simplest process	Selectivity for specific aromatic compounds is very low; char formation	Aromatic and non-aromatic molecules, char, and light gasses
Catalytic pyrolysis	Products are less Oxygenated and more stable	Coke deposits on catalysts	Aromatic hydrocarbon containing liquid, char, coke, light hydrocarbons, and oxygenate gasses
Supercritical water	Lower concentration of lignin means lower chance of condensation reactions	High cost for process heat; only one-third of lignin product is low molecular weight	Aromatic hydrocarbon containing liquid, char
Supercritical solvent	Products have a lower boiling point allowing for easier separation	Mid-high pressure High temperature	Primary product is monomeric substituted cyclohexyl derivatives, negligible aromatics, little to no char

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Table 2.2 Catalytic SCWG of lignin

Researchers	Condition	Results
Osada et al. (2004) (lignin and cellulose)	400°C, Ru/TiO_2	Higher decomposition of formaldehyde, higher CH_4
	400°C, Ni/TiO_2	Higher H_2 formation
Sato et al. (2006)	400°C, Ni/MgO	Highest gas production. Lignin was decomposed and reaction between intermediates was promoted.
Furasawa et al. (2007)	600°C, 10%wt Ni/MgO	30% carbon yield with optimal Ni particle size (the best catalytic performance)
Yamaguchi et al. (2008)	400°C 37.1 MPa ruthenium trivalent-salts on TiO_2 and charcoal support	The order of lignin gasification: $Ru/C \approx Ru(NO)(NO_3)_3/C \approx$ $Ru(NO)(NO_3)_3/TiO_2 >$ $RuCl_3/C \approx RuCl_3/TiO_2$
Yamaguchi et al. (2009)	Ni/C	The order of lignin gasification: Ru > Rh > Pt > Pd > Ni The order of H_2 production: Pd > Ru > Pt > Rh > Ni

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2.2.3 Black liquor gasification in supercritical water biomass

Cao et al. (2011) investigated the gasification of alkaline black liquor under supercritical water condition by a continuous flow system. The experiments were carried out at 400°C-600°C at pressure 250 bar, in temperature ranging from 4.94 to 13.71 s. The results showed that the gasification reaction was enhanced by temperature and residence time increase and feeding concentration decrease. High H_2 formation was 40.26-61.02%. The pH effluent decreased to the neutral region because the alkalis were precipitated in the reactor during the gasification. When reactor was cool down to about 360°C, the precipitated alkalis were dissolved in the water again led to higher pH in effluent.

Sricharoenchaikul (2009) carried out the gasification of black liquor gasification under supercritical water condition. The effect of temperature, pressure, reaction time and concentration of black liquor on conversion and energy was determined.

Weak black liquor, with a moisture content of 81.4%, was used for the experiments. The reaction took place in a quartz capillary with an inner diameter of 1 mm and a length of 15 cm. The heating was provided by a fluidized bed vessel which was preheated to a set temperature. When the desired temperature was reached, the quartz capillary was immersed into the vessel. After the reaction time was reached, the capillary was quenched to terminate the reaction. The obtained products were gas, char and tar. The char and tar separation was accomplished by solution in dichloromethane (DCM) and subsequent filtration. Tar was obtained after evaporation of the DCM. The product yields and carbon conversion did not show any dependence of pressure during the trials. For all studied operating conditions, higher yield of gas product were obtained for higher temperatures while the char and tar contents were reduced. The fraction of gaseous products also increased with reaction time. The amount of heavier carbon containing gases decreased at longer reaction times due to secondary decomposition. It was also concluded that higher energy efficiency was obtained for samples of lower black liquor concentration. The gas was found to have a maximum energy content of 9.4 MJ/m^3, which is satisfactory for use as a fuel gas.

Table 2.3 Black liquor gasification under supercritical condition

Condition	**Results**
Sricharoenchaikul (2009)	375°C-650°C, 220-400 bar Batch Max. %C conversion at 650°C
Cao et al. (2011)	400°C-600°C, 25 MPa Continuous Max COD removal eff. at 600°C
Blasio et al. (2016)	350°C-450°C, 25 MPa Catalytic effect of Nano-CeO_2 Conversion increased, coke formation suppressed Max. H_2 at 450°C
Hawangchu et al. (2017)	673-873 K, 250-400 bar batch Max. H_2 yield at 873K 250 bar

CHAPTER 3

EXPERIMENTAL SECTION

This chapter presented materials and methods for three parts. Kraft black liquor (KBL) and soda black liquor (SBL) from Eucalyptus wood pulping were used as feedstock for conversion process since they are the two most abundant liquors generated from Thai pulp and papermaking industry. The appearances of as received weak black liquor samples were dark-brown, odorous, and fluid due in part to high water content of more than 80%. The sample was collected at a point after digestion and before evaporation unit. It was kept under below 4°C for inhibiting any reaction. Lignin in black liquor was isolated from black liquor by acid precipitation called technical lignin. Lignin model compound (LMC) was used as the comparable substance for technical lignins in the first and second parts, and was used as a base case test for studying the effect of inorganic matter in black liquor in the third part. However, cellulose model compound obtained from Sigma-Aldrich was used only in the first part for comparing the thermal behavior result from TGA analysis of lignin from soda process. Details in each part were presented below.

3.1 Black liquor and technical lignin characterization (Part I)

3.1.1 Materials

For study on the properties of black liquor and lignin in black liquor from different pulping process, dried or solid samples were prepared by evaporation and crushing into solid powder (Fig 3.1) and sent out for analysis of compositions.

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3.1.1.1 Dried or solid black liquor

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Figure 3.1 Dried or solid black liquor preparation

3.1.1.2 Technical lignin from acid precipitation

Lignin in black liquor was isolated from black liquor by acid precipitation (Hu et al., 2013). 50%H_2SO_4 was added to black liquor until pH reached around 3. Then acidified black liquor was washed by distillation water via centrifugation until neutral pH. After that further dried at 60°C for 12 hrs (Fig 3.2).

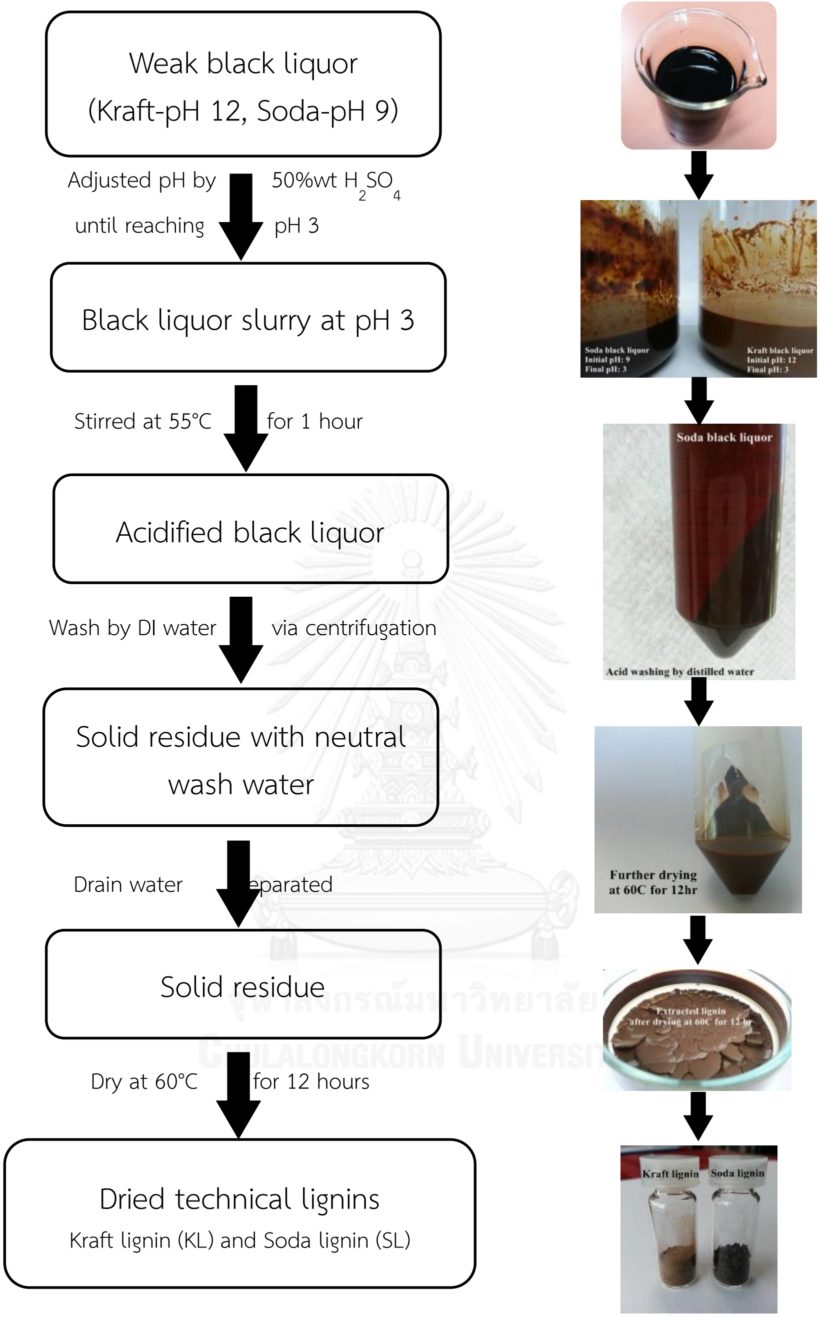

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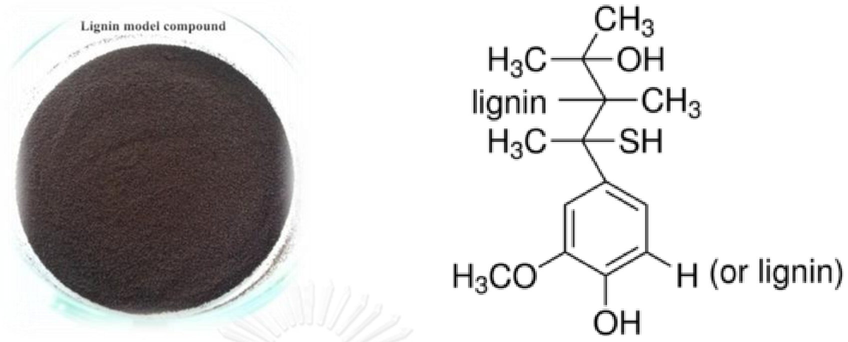
Figure 3.2 Acid precipitation for technical lignin from black liquor (adapted from Hu et al. (2013))

3.1.1.3 Lignin model compound

Lignin model compound (LMC) was alkali lignin with low sulfonate content obtained from Sigma-Aldrich (CAS no. 8068-05-1). LMC was used as the comparable substance for technical lignins (Fig 3.3).



http://www.sigmaaldrich.com

Figure 3.3 Lignin model compound from Sigma-Aldrich (CAS no. 8068-05-1)

However, cellulose model compound was used only for thermal degradation pattern which was compared with soda lignin degradation by TGA analysis. It was obtain from Sigma-Aldrich, cas no. 9004-34-6, in form of white power. Cellulose model compound was not carried out in any experiments excepted TGA analysis.

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3.2 Product distribution of technical lignin by Py-GC/MS (Part II)

The technical lignins from black liquors were studied in pyrolysis reaction via Py-GC/MS led to various product distributions. Metal catalysts were used to investigate the upgradable of the samples to other high value pyrolysis products. Materials and method of this part are presented.

3.2.1 Materials

Technical lignins (KL and SL) and LMC were the same as of those used in part I. Samples were used as 0.5 mg per run for non-catalytic reaction and with catalyst varied by metal species and ratio of sample to catalyst.

3.2.2 Catalyst preparation

Catalysts were prepared by impregnation method. For 5% active species on catalyst support, the calculated amount of metal catalyst precursor (nickel (II) nitrate hexahydrate ($Ni(NO_3)_2.6H_2O$), palladium (II) nitrate hydrate ($Pd(NO_3)_2.xH_2O$), and Ruthenium (III) chloride hydrate ($RuCl_3.xH_2O$)) was dissolved in distilled water for a metal catalyst solution. All metal precursors were obtained from Sigma-Aldrich and catalyst support from Alfa-Aesar (Table 3.1).

Table 3.1 Metal catalyst precursor and support

Active species (precursor of metal catalyst)	Ni	Nickel (II) nitrate hexahydrate (Yoshida et al., 2003)	Sigma-Aldrich
	Pd	Palladium (II) nitrate hydrate (Lu et al., 2012)	
	Ru	Ruthenium (III) chloride hydrate (Byrd et al., 2008)	
Catalyst support	ZrO_2	Zirconium (IV) oxide (Watanabe et al., 2003)	Alfa - Aesar

Zirconium support was impregnated in the solution and stirred at 80°C, 300 rpm for 3 hrs and then dried at 110°C for 24 hrs. The dried catalysts were calcined at 700°C for 4 hrs. Catalysts were reduced by H_2 flow (15 mL/min) at 800°C for 4 h before using in the reaction.

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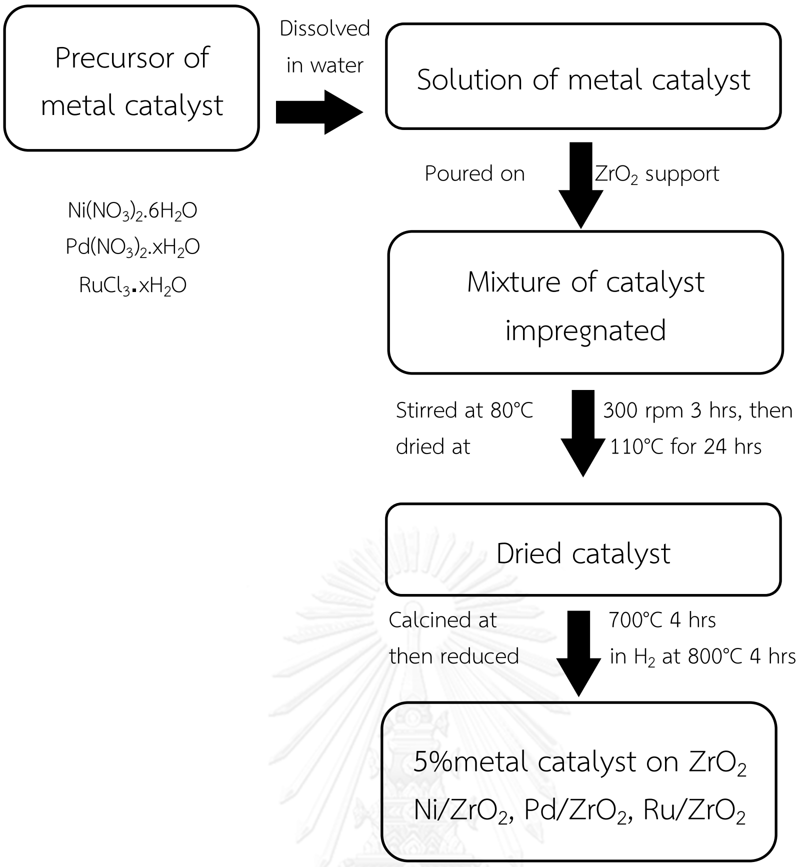

Figure 3.4 Catalyst preparations by wet impregnation

The procedures are exhibited in Fig. 3.4 and catalysts after each step are shown in Fig. 3.5. After H_2-reduced process, catalysts were kept in desiccator for using in the reaction.

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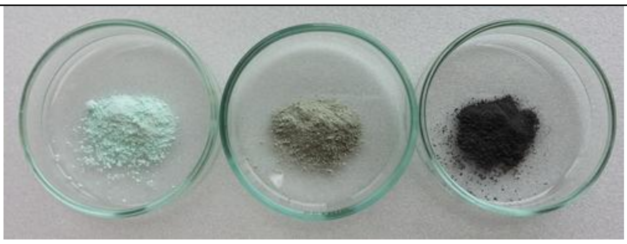
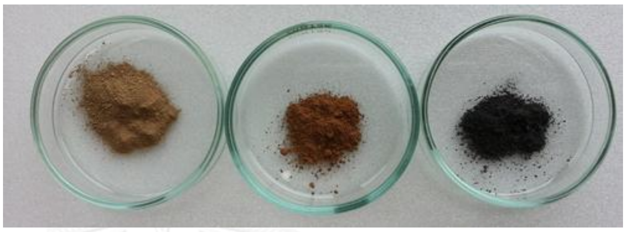
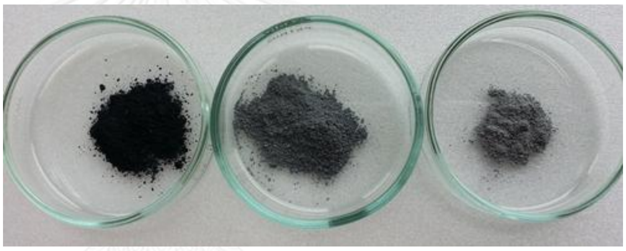
<table>
<tr><th>Catalyst</th><th>Dried
(110°C, 24 hrs)</th><th>Calcined
(700°C, 4 hrs)</th><th>H_2-reduced
(800°C, 4 hrs)</th></tr>
<tr><td>5%
Ni/ZrO_2</td><td colspan="3"></td></tr>
<tr><td>5%
Pd/ZrO_2</td><td colspan="3"></td></tr>
<tr><td>5%
Ru/ZrO_2</td><td colspan="3"></td></tr>
</table>

Figure 3.5 Metal catalyst after drying, calcination, and H_2-reduction

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3.2.3 Pyroprobe-GC/MS and experimental method

The multifunctional pyrolyzer (PY-2020iD, Frontier Lab) with autoshot sampler AS-1020E connected to a gas chromatograph coupled to a mass selective detector (GCMS- QP2010, Shimadzu) to decompose and detect the volatile products (Fig 3.6).

Figure 3.6 Pyroprobe GC/MS for pyrolysis reaction

The amount of technical lignin was 0.5 mg and with ratio of technical lignin tor catalyst varied at 1:1, 1:5 and 1:10. The sample was placed in a sample holder. For the catalytic reaction, the catalyst was placed over sample. After that the sample in holder was dropped into the heated zone of pyroprobe and hold for 0.50 min. Gas chromatography was conducted by an ultra-alloy capillary column (UA5-30M-0.25F, 30 m, 0.25 mm i.d., 0.25 lm film thickness). The carrier gas was 99.999% helium at flow rate 1.1 mL/min, and the split injector ratio of 1:50. The degraded compounds were then analyzed using a mass selective detector operating in electron impact mode (EI) at 70 eV from mass ions (m/z) of 20–800. The spectra identifying was carried out by matching the mass ion of each peak with the NIST mass spectral library.

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3.2.4 Experimental table

This part consisted of 48 runs including 22 tests of KL, 17 tests of SL, and 9 tests of LMC. The results were presented by qualitative of relative areas. All the experiments were in table 3.2.

Table 3.2 All experiments of non- and catalytic reaction of technical lignins and lignin model compound at 400°C-600°C.

Temp.	Kraft lignin	Soda lignin	Lignin model compound
400°C	Non-catalytic-KL	Non-catalytic-SL	Non-catalytic-LMC
Ratio of sample to catalyst	1-1_ZrO_2	1-1_ZrO_2	1-1_ZrO_2
	1-1_Ni/ZrO_2	1-1_Ni/ZrO_2	1-1_Ni/ZrO_2
	1-5_Ni/ZrO_2	1-5_Ni/ZrO_2	1-5_Ni/ZrO_2
	1-10_Ni/ZrO_2	1-10_Ni/ZrO_2	1-10_Ni/ZrO_2
	1-1_Pd/ZrO_2	1-1_Pd/ZrO_2	1-1_Pd/ZrO_2
	1-1_Ru/ZrO_2	1-1_Ru/ZrO_2	1-1_Ru/ZrO_2
500°C	Non-catalytic-KL	Non-catalytic-SL	Non-catalytic-LMC
Ratio of sample to catalyst	1-1_ZrO2	-	-
	1-1_Ni/ZrO_2	1-1_Ni/ZrO_2	-
	1-5_Ni/ZrO_2	1-5_Ni/ZrO_2	-
	1-10_Ni/ZrO_2	-	-
	1-1_Pd/ZrO_2	1-1_Pd/ZrO_2	-
	1-5_Pd/ZrO_2	1-5_Pd/ZrO_2	-
	1-1_Ru/ZrO_2	-	-
	1-5_Ru/ZrO_2	1-5_Ru/ZrO_2	-
600°C	Non-catalytic-KL	Non-catalytic-SL	Non-catalytic-LMC
Ratio of sample to catalyst	1-1_ZrO2	-	-
	1-1_Ni/ZrO_2	1-1_Ni/ZrO_2	1-1_Ni/ZrO_2
	1-5_Ni/ZrO_2	1-5_Ni/ZrO_2	1-1_Pd/ZrO_2
	1-10_Ni/ZrO_2	-	1-1_Ru/ZrO_2
	1-1_Pd/ZrO_2	1-1_Pd/ZrO_2	-
	1-5_Pd/ZrO_2	1-5_Pd/ZrO_2	-
	1-1_Ru/ZrO_2	1-1_Ru/ZrO_2	-
	1-5_Ru/ZrO_2	1-5_Ru/ZrO_2	-

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3.2.5 Categories of pyrolysis yield

The varieties of products evaluation were performed after pyrolysis reaction at 400°C-600°C. Compositions of the pyrolysis vapor were grouped the into four categories;

Chemical species

Guaiacyl
Syringyl
p-hydroxyphenyl
Catechol
Aromatic hydrocarbons
Aliphatic hydrocarbons
Furan
Oxygenated
Sterol
Other

Bond type	Bond energy (Petrucci et al., 2007; Carruth et al., 2002)	
Methoxy	O – CH_3	358
Hydroxyl	– OH	467
Cabonyl	C = O	745
Carbon	C – C	347
Other		

Chemical degraded compounds

Phenolic OH
Hydrocarbons
Ether
Alcohol
Ketone
Aldehyde
Ester
Carboxylic acid
Furan
Sugar
*N-Compound
Other

Chemical structure

Aliphatic hydrocarbons
Aromatic hydrocarbons
Phenol
Oxygenated
N-compound
Other

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Four main categories were used to discuss in detail of the degraded products from thermal conversion by Py-GC/MS. Regarding the chemical species and phenolic monomer of different lignin structure, the product distribution was split into two groups; the chemical species and bond type. On the subject of lignocellulosic bio-product, the third and fourth groups were termed chemical degraded compounds and chemical structure. N-compound species in the group of chemical degraded compounds is unexpected since nitrogen is not available in the technical lignin. This is probably due to mismatch of NIST library in which similarity among complex mass ion patterns is possible or the actual species data is not available in its database.

3.3 Supercritical water gasification of black liquor for H_2 production (Part III)

Weak black liquor contained high water content over 80% thus the intensive energy was used for concentrating of solid content to 75-80% before combustion in the recovery boiler (Cao et al., 2017). Direct gasified of weak black liquor was carried out in the part by supercritical water condition. Both kraft and soda weak black liquors were prepared for 10%solid content, LMC was set as the same. The inorganic contents in black liquor, alkali compounds, were investigated as the alkali catalytic reaction which LMC was conducted as the controlled experiment, without alkali compound.

3.3.1 Material

Samples were prepared from dried or solid black liquor (in part I) and LMC. Deionized water was used as solvent for weak black liquor in this part. Samples were filled in the miniature fused quartz reactor (Fig 3.7) and placed in sample holder for further reaction.

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Figure 3.7 Preparation of 10%solid weak black liquor

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3.3.2 Quartz reactor

Supercritical water gasification reaction of black liquor was carried out inside the miniature quartz tube which closed both side. This tube was 10 cm in length and inner diameter was 1 mm and outer diameter was varied 3-5 mm (Fig 3.8).

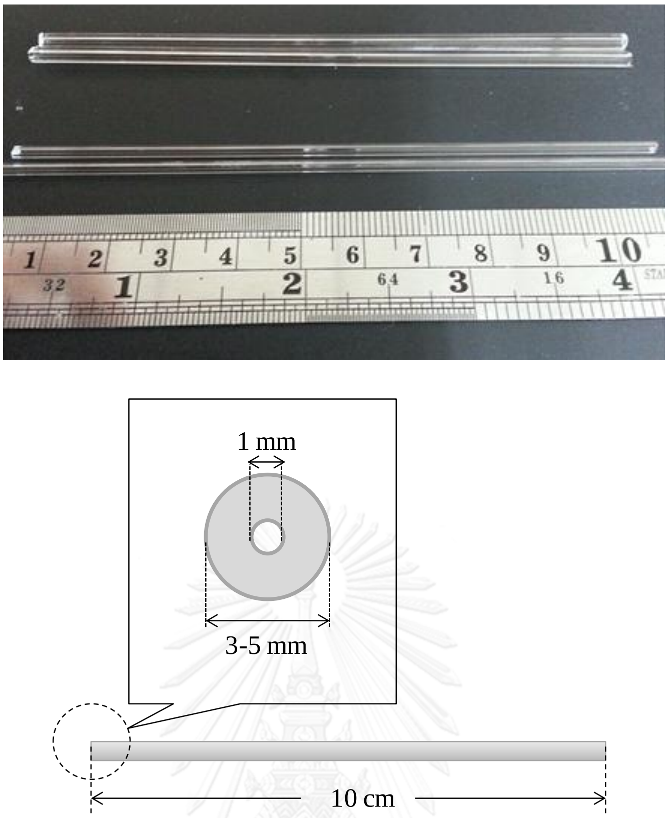

Figure 3.8 Miniature fused quartz tube for SCWG reactor

Fused quartz tubes were obtained from Technical Glass Products, Inc. USA. The varieties properties of fused quartz from manufacturer are permeability, extreme hardness, very low coefficient of thermal expansion, resistance to high temperature, high chemical purity, high corrosion resistance, extensive optical transmission from ultra-violet to infra-red, excellent electrical insulation qualities, remarkable stability under atomic bombardment. Examples of property and typical values are density (2.2 x 10^3 kg/m^3), hardness (5.5–6.5 Mohs' Scale), design tensile strength (4.8 x 10^7 Pa (N/m^2)), etc.

High temperature and pressure required to initiate SCW reaction of black liquor was achieved by placing a miniature quartz tube filled with black liquor sample into a temperature controlled hot fluidized bed which is similar to the work reported by Potic et al. (2004), Kersten et al. (2006), Sricharoenchaikul (2009), and Yamaguchi et al. (2009). Here, a quartz tube with 1 mm i.d., 3 mm o.d. and 100 mm long were used as a micro reactor. The tube was sealed by oxyacetylene welding at one end, injected with 10% black liquor solution feedstock and then quickly sealed at the other end before placing into the sample holder, ready to be heated (Fig 3.9).

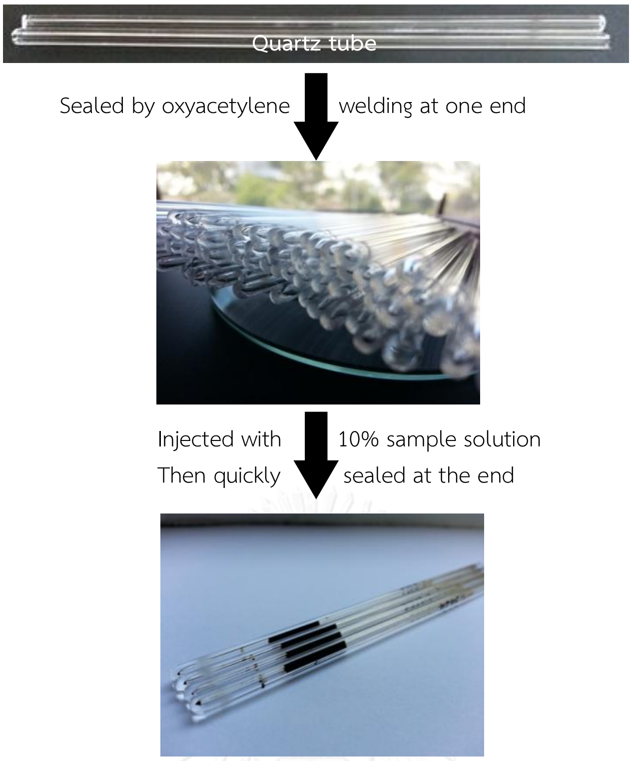

Figure 3.9 Preparation sample solution feedstock in quartz reactor

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3.3.3 Experimental setup

Fluidized bed vessel was setup with heating system (Fig. 3.10). Electrical tube furnace was controlled by PID temperature controller which responded to the temperature measurement via thermocouple type K placed in the bed material. As a bed medium, sand was fluidized by preheated nitrogen gas at steady flow rate regulated by a rotameter. Before carrying out the reaction, weak black liquor in miniature fused quartz tube was immersed in hot water at 90°C to match the pulping waste temperature prior to spraying into recovery boiler. Sample holder along with sample quartz tubes were then dropped into fluidized bed, initializing the reaction.

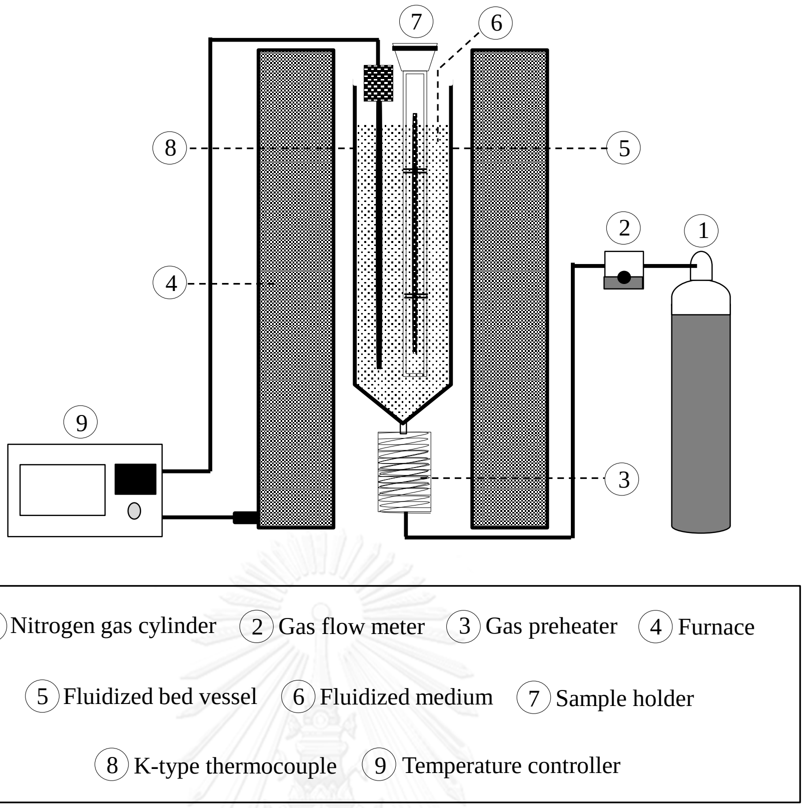

Figure 3.10 Experimental setup for SCWG experiment

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The experiments were carried out in the pressure rang of 250-400 bar which achieved by calculation. After 10 min reaction time, sample holder was pulled up and quickly soaked in water for quenching.

3.3.4 Yields collection

The capillary after reaction was broken inside the crusher for gas collection and then solid and liquid. Before breaking the capillary, purging of argon gas was carried out for a while to achieve the inert atmosphere inside the crusher. When shaking, ceramic balls inside the crusher would hit the tubes and break them into cullet. Then produced gas released and was kept in the crusher. Gas product was brought to gas chromatography analyzer by syringe and peristaltic pump while the rest of products were removed by acetone by filtering, dissolved tar was analyzed by GC/MS (Fig. 3.11).

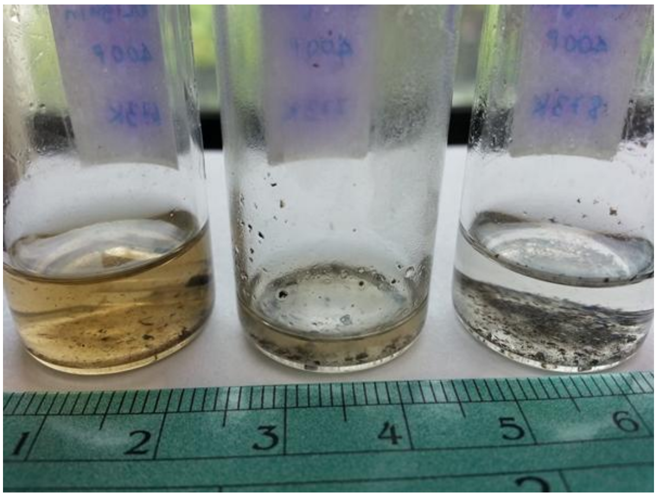

Figure 3.11 Liquid yield in acetone solution with cullet and solid residue

3.3.5 SCWG procedure and product analysis

Fig 3.12 exhibited the whole procedure of the experiment in this part. Start with sample preparation, the gasification was conducted in fluidized bed vessel for 10 min at 400°C-600°C and 250-400 bar. After reaction, gas product was released in the inert atmosphere chamber or crusher for further GC analyzer while liquid yield was removed by acetone solvent for GC/MS analysis.

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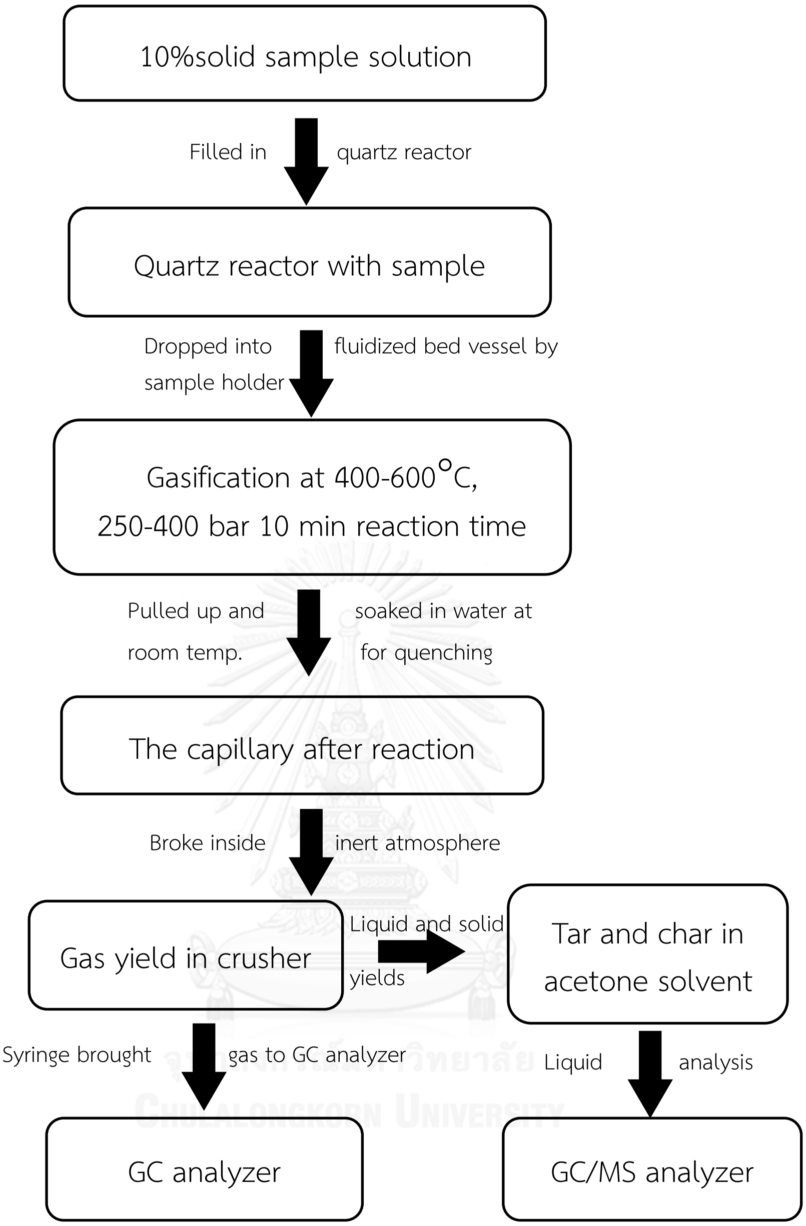

Figure 3.12 SCWG procedure and product analysis

3.4 Summary

The potential of lignin in black liquor was undermined by its high water content. Generally, pulp mill uses black liquor as fuel but intensive energy requirement for evaporation before combustion is required. Moreover, various and specific of lignin in black liquor due to wood species and pulping chemical are the essential issues about high effective utilization with appropriate condition (Doherty et al., 2012). Especially in biorefinery, alkaline lignin or lignin in black liquor is the major source of commercial lignin (Vishtal and Kraslawski, 2011).

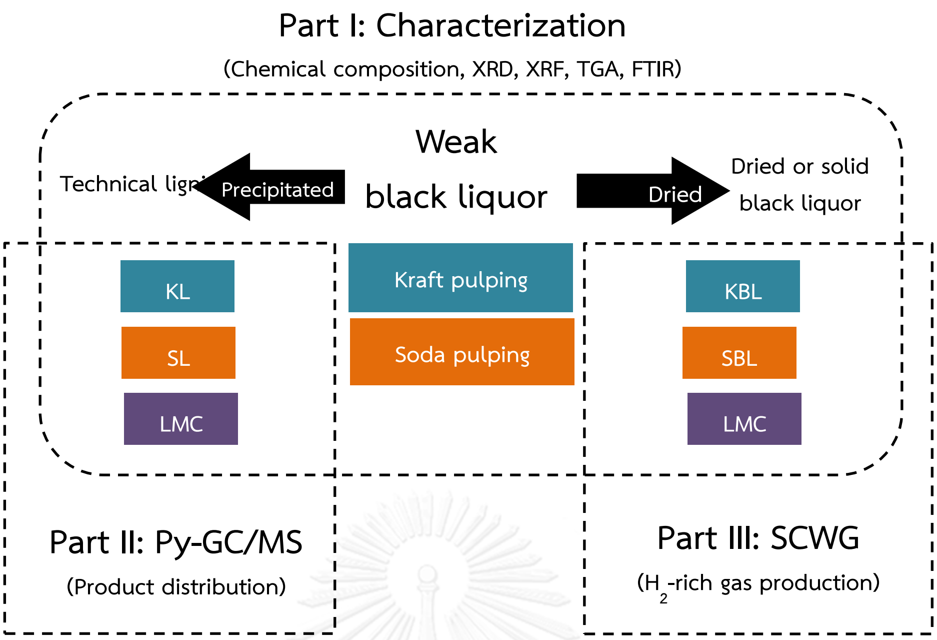

Figure 3.13 Summary of experimental tasks

Therefore, this research aimed to understand the different properties of lignin in black liquor from kraft and soda process for further gasification under supercritical water condition to produce H_2-rich syngas. The experiments were divided in 3 parts (Fig 3.13); the first part was characterization of black liquor and lignin in black liquor. Weak black liquor from paper making industry was evaporated to dried solid black liquor, whilst lignin in black liquor was isolated by acid precipitation in form of dried technical lignin. Lignin model compound was use as the precursor for technical lignin characters. The effect of different pulping chemical might cause differ specific properties among them. Then the second part focused on the product distribution from pyrolysis reaction of the technical lignins. Py-GC/MS technique was used for better understand the potential products from thermal reaction of technical lignin and, therefore, the different properties of lignin in black liquor was the evidence for the suitable useful production from these lignin in black liquor. Overall difference and specific properties of black liquor and lignin in black liquor could explain the H_2-rich syngas formation in the third part via gasification reaction under supercritical water condition. High water content in black liquor was use as the reactant in the reaction. LMC solution was used to investigate the alkali catalytic reaction of industrial black liquor. Thus black liquor could be converted into biofuel without

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dewatering process and along with the knowledge about the unique character of biomass from the promising internal source for alternative energy in the country

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CHAPTER 4

BLACK LIQUOR AND TECHNICAL LIGNIN CHARACTERISTICS

4.1 Introduction

Black liquor mainly composed of organic substance from wood and inorganic substance from spent chemical pulping. Regarding the thermal conversion process, lignin as a carbon source of the reaction is decomposed and then converted to new products. Meanwhile the alkali salt in biomass could play the role of homogeneous catalyst in several thermochemical reactions. Therefore, study into the fundamental properties of lignin, including chemical composition, thermal behavior, and function group might enhance our understanding about product distribution. The local pulp mills utilize the same kind of wood but different pulping chemicals, kraft (NaOH with Na_2S) and soda (NaOH). Thus, the technical lignin was obtained from the acid precipitation of black liquor. This chapter presents the characterization and thermal behavior of black liquors (kraft black liquor: KBL and soda black liquor: SBL) and technical lignins (kraft lignin: KL and soda lignin: SL). Lignin model compound was the major precursor and cellulose model compound in TGA analysis.

4.2 Results and discussion

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4.2.1 Elemental analysis

For identifying the core composition of feedstock, the elemental analysis was conducted on all materials including industrial black liquors (the origin of the technical lignins). The elemental contents are shown in Table 4.1. The predominant part was carbon which was the highest at KL as 60.40%, while the highest hydrogen content was SL as 5.63%. As the result, there were equal amount of carbon content in KBL and SBL around 33%. It could be found that the content of carbon of extracted lignins was rising amount comparing to the initial black liquors. For KL isolated from KBL, the carbon content increased for 1.8 times while 1.4 times for SL was larger than SBL. However, the carbon content of KL and SL were close to LMC which was the precursor for these experiments could be suggested the purity of extracted lignin from pulping process. The others analysis methods would be further revealed the similar properties of extracted lignins and lignin model compound.

Table 4.1 Chemical characterization of black liquor (wt.%, as received basis)

Materials	KBL	SBL	KL	SL	LMC
Proximate analysis (TGA)					
Moisture	80.2	81.4	4.4	5.5	12.5
Volatile matter	11.3	11.0	59.0	73.1	39.4
Fixed carbon	0.4	0.4	34.3	17.0	29.7
Ash	8.1	7.2	2.3	4.4	18.4
Ultimate analysis (CHNS/O Elemental analysis)					
C (%)	32.95	32.80	60.40	45.06	47.61
H (%)	3.35	2.97	5.16	5.63	4.74
N (%)	0.12	0.04	0.05	0.00	0.00
S (%)	5.12	0.25	4.39	0.15	4.02
O(a) (%)	58.46	63.94	30.0	49.2	43.6
Lower heating value (Bomb calorimeter)					
LHV (MJ/kg)	12.3	11.4	10.0	10.4	16.8
Lignin composition (TAPPI-T222-om-98)					
Lignin (wt.%)	27.8	24.0	n/a(b)	n/a(b)	n/a(b)

(a) By diff.

(b) Not available

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4.2.2 Inorganic component

To investigate the inorganic component of industrial black liquor from kraft and soda process, the sample was analyzed and showed the percentage of K, Cl, Ca, and Fe by the XRF technique. The results are in Table 4.2.

Table 4.2 XRF results of industrial black liquor, KBL and SBL

Industrial black liquor	**Elements (Wt%)**				
	Sodium	**Potassium**	**Chlorine**	**Calcium**	**Ferrous**
KBL	6.53	3.86	1.12	0.15	0.01
SBL	6.06	2.60	0.88	0.11	0.02
LMC	4.74	0.33	0.06	0.03	0.02

The content of sodium, potassium, chlorine, and calcium of KBL was higher than SBL. This conformed to the ash content in the proximate analysis; ash of KBL was larger than SBL 27.8%. However, the ferrous content could indicate the corrosion inside the digestion reactor, clearly illustrated in Fig 4.1. Form the XRD of black liquor showed that the $CaFe_4O_7$ compound in SBL was higher than KBL which could be confirmed from double Fe content in SBL higher than KBL (Table 4.2).

Furthermore, the XRD technique can illustrate the inorganic inform of crystallinity on structure of industrial black liquors and their technical lignins. As mentioned in the literature review, the spent chemical from pulping process was remained in black liquor which might impact on the organic structure. Therefore, the crystallinity of alkali salt was expected to appear.

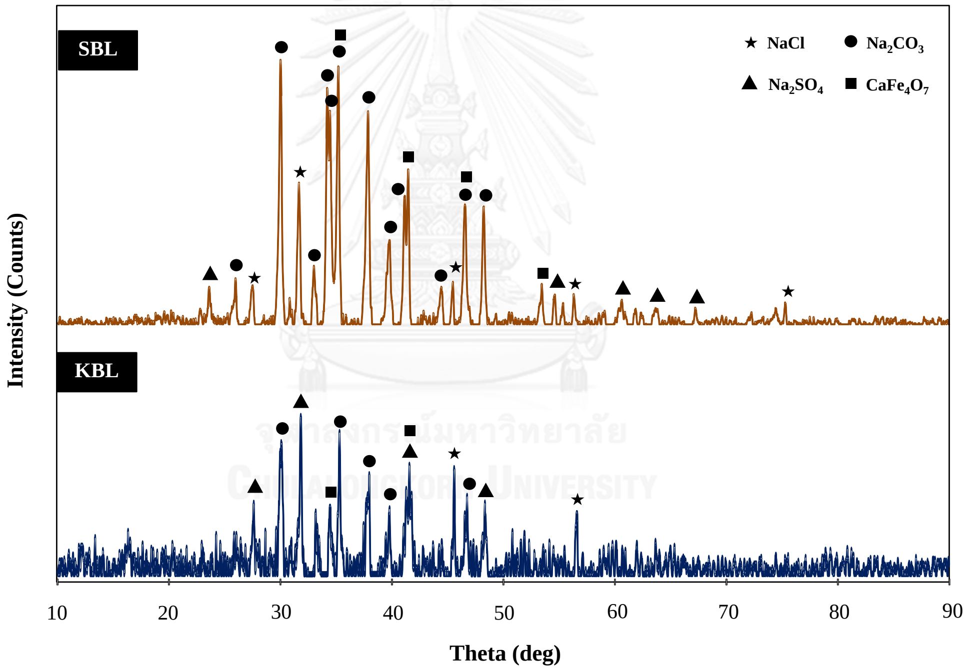

Figure 4.1 XRD pattern of industrial black liquor from kraft pulping (KBL) and soda pulping (SBL)

The results showed that the alkali compounds especially sodium were the majority content on the crytallinity of the residue salt in black liquors. These peaks were a resulting from the pulping process. In kraft pulping, Na_2S was added with NaOH, led to a coincidence of the spent alkali between Na_2SO_4, according to JCPDS: 37-1465 (Santo et al., 2014), and Na_2CO_3, according to JCPDS: 18-1208 (Fig. 4.1). Because soda process utilized only NaOH, so that the outstanding of Na_2CO_3 peaks were scattered over the SBL of XRD pattern which could be emphasized the catalytic properties of industrial black liquor (Guo et al., 2012). The different in carbonate and sulfate in black liquor was impacted on the S element in Table 4.1.

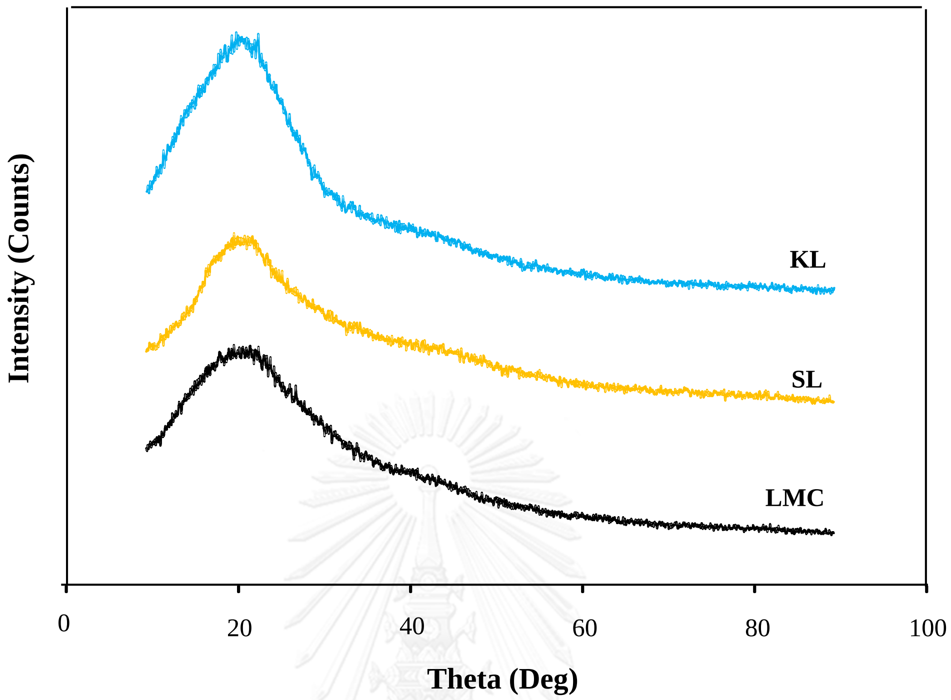

Figure 4.2 XRD patterns of technical lignin: kraft lignin (KL) and soda lignin (SL), and lignin model compound (LMC)

XRD patterns of three lignins are shown in the Fig. 4.2. The amorphous nature of lignin was be clearly illustrated the identical structure of all three lignin. However, this finding could be assumed that the acid precipitation method used for these experiments was effective. As a result of no crystalline phase appeared on XRD pattern of the technical lignins and performed in the similar form of LMC. Obviously, the spent chemicals left from pulping process were eliminated and created lignin substance which closed to synthesis lignin.

4.2.3 Thermal analysis

According to the hypothesis, the differences in chemical structure of lignins from kraft and soda pulping process leads to the varieties of thermal conversion products. TGA analysis can reveal the thermal behavior correlated with the different temperature in nitrogen condition. Relations between the percentage of weight loss and the raising temperature were presented in Fig. 4.3a for industrial black liquors and Fig. 4.3b for technical lignins and model compounds. Moreover, the rate of weight loss versus temperature of industrial black liquor (Fig. 4.3c) and technical lignins (Fig. 4.3d) are illustrated.

Table 4.3 The decomposition temperatures, %wt loss, and %residue of industrial black liquors, technical lignins and model compounds

Sample	Stage	1	2	3	4	5	% Residue
KBL	temp. (°C)	120	**270**	330	450	600-800	58.8
	%wt loss	2.5	**12.2**	7.7	5.8	13.0	
SBL	temp. (°C)	60	275	**345**	470	600-800	56.1
	%wt loss	4.0	9.8	**10.8**	8.2	11.1	
KL	temp. (°C)	70	250	**380**			54.2
	%wt loss	6.5	12.3	**27.0**			
SL	temp. (°C)	70	**300**	360			39.3
	%wt loss	14.0	**40.1**	6.6			
LMC	temp. (°C)	70	**330**	600-800			42.0
	%wt loss	15.7	**29.4**	12.9			
CL	temp. (°C)	60	**370**	600-800			4.3
	%wt loss	7.7	**70.9**	17.1			

In general, three main stages can be classified as dehydration, active pyrolysis, and passive pyrolysis (Liang et al., 2015). For this works, there are five stages of decomposition on industrial black liquors (Table 4.3). Normally, the active pyrolysis stage is the most important because it is the major decomposition phase. From Table 4.3, the active pyrolysis stage of the samples was different; stage 2-4 for industrial black liquors, stage 2-3 for technical lignins, and stage 2 for model compound. However, the maximum temperature for decomposition was different. This might be cause of dissimilar matter in feedstock.

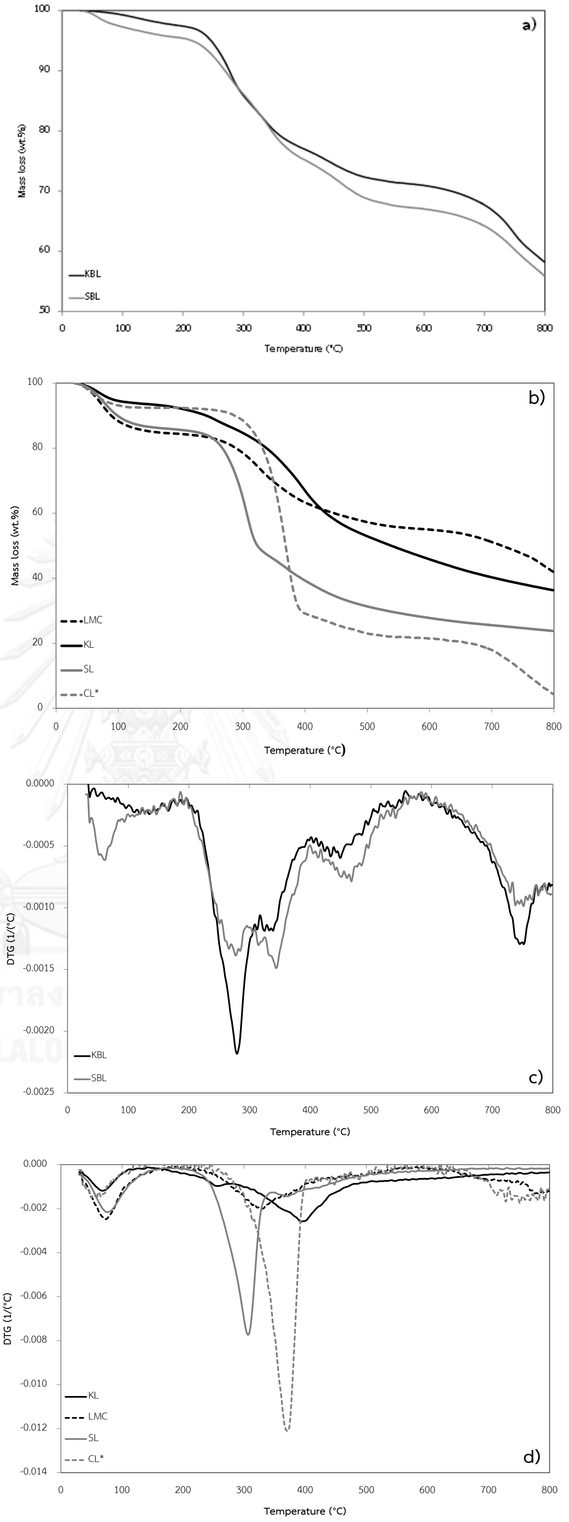

Figure 4.3 TGA and DTG curves of (a, b) industrial black liquors, and (c, d) technical lignins and model compounds.

The initial decomposition temperature was assigned for moisture and some low molecular weight gases volatilization (Zhang et al., 2012). The beginning degraded temperature of SBL stage was lower than KBL but higher in weight loss. This might indicate on the different water content in black liquor solid. The reason of the observed may be due to the cellulose mixed in SBL. Because the hygroscopic properties of cellulose was outstanding in water trapping inform of free water and bound wate (Célino et al., 2013). Therefore, soda process might extract not only lignin from wood, also cellulose. However, the rest volatile-elimination of SBL after 60 °C to the onset temperature at 200 °C might be the same as KBL. Moreover, the maximum decomposition temperatures were at 270 °C and 345 °C for KBL and SBL, respectively. The degradation in this range might describe as the decomposition of some weak linkages such as β-O-4’ which was the greatest amount in hardwood lignin (Wen et al., 2013; Guo et al., 2015). However, the percentage of weight loss at 275 °C of SBL was almost the same at 345 °C. This might indicate that the lowest temperature for thermolysis of industrial black liquor was at 270 °C. In the consequence, the decomposition in range of 450-470 °C might occur by demethoxylation which was the releasing of methoxyl group from aromatic rings (Sahoo et al., 2011). Therefore, the last decomposition in range of 600-800 °C was assigned for char formation form the residue aromatic ring compound. In addition, the final residue might be due to the approximate character of char (Table 4.3) and the other element in KBL (Table 4.1) (Constant et al., 2016) that encouraged the higher % residue than SBL. Moreover, the remaining percentages of them were very high (> 40wt.%) could suggest the predominate as lignin was the main part of all feedstock (Yang et al., 2007).

To prove the biopolymer material from the acid extraction, the model compound of lignin and cellulose were used for comparison with the technical lignins. The first decomposition stage of the technical lignins almost the same with model compounds. This indicated their components for volatilization were close. Moreover, the pattern of peak at the active pyrolysis stage looked the same KL as LMC, and SL as CL. This might confirm the polymer material from acid isolation of industrial black liquor. However, the maximum decomposition temperature of KL (Fig. 4.3b,c) was higher than LMC, whereas SL was lower CL. This may be because the influence of pulping and/or precipitation process which affecting the chemical structure of technical lignins (Constant et al., 2016). In the active pyrolysis stage, both of KL and SL included two DTG peaks which assigned for the degradation different contents. The maximum decomposition temperature of KL was at 380°C was described as lignin content which was the same degraded pattern of SL at 360°C. In addition, the greatest decomposed of SL at 300°C were assigned for cellulose material which KL appeared this pattern at 360°C. The concordance between KL and SL were containing the part of lignin and cellulose, in the meantime they contained in different amount. Lignin was the primary component in KL, meanwhile SL had the cellulose as the essential part. Therefore, the final residue of KL was larger than SL because of lignin's high thermal stability. As the feedstock for thermal conversion, SL was simply transformed into other products and the solid residue was less than others.

As the result of TGA analysis, thermal behavior of kraft black liquor and soda black liquor was slightly different which might due to the spent chemical from the pulping process. For gathering the lignin from the industrial black liquor, the acid precipitation was used and gained the technical lignin (KL from kraft black liquor and SL from soda black liquor). TGA analysis revealed the pulping process effect on chemical composition of those technical lignins in term of the biopolymer composition. As a consequence of different character, the utilization of the technical lignins from kraft and soda pulping process should rely on the proper of their chemical structure. Considerably more work about thermal conversion the processed lignocellulosic biomass, their structure need to be investigated for some varies from the chemical or physical process. The viable data can enhance the accurate direction for further study.

4.2.4 FTIR results

The FTIR spectra of the industrial black liquors, lignin model compound and technical lignins are shown in Fig. 4.4. Bands were assigned according to (Silverstein et al., 1981, Shen et al., 2010, Yuan et al., 2011). All of samples showed a broad band centered at 3400 cm^{-1}, attributed to the O-H stretching vibration in the phenolic and aliphatic structures. This is corresponding to alcohol and phenol as assigned to O-H stretching which indicated that all samples have a potential for being the initial substance of reaction in SCWG for fuel gas production.

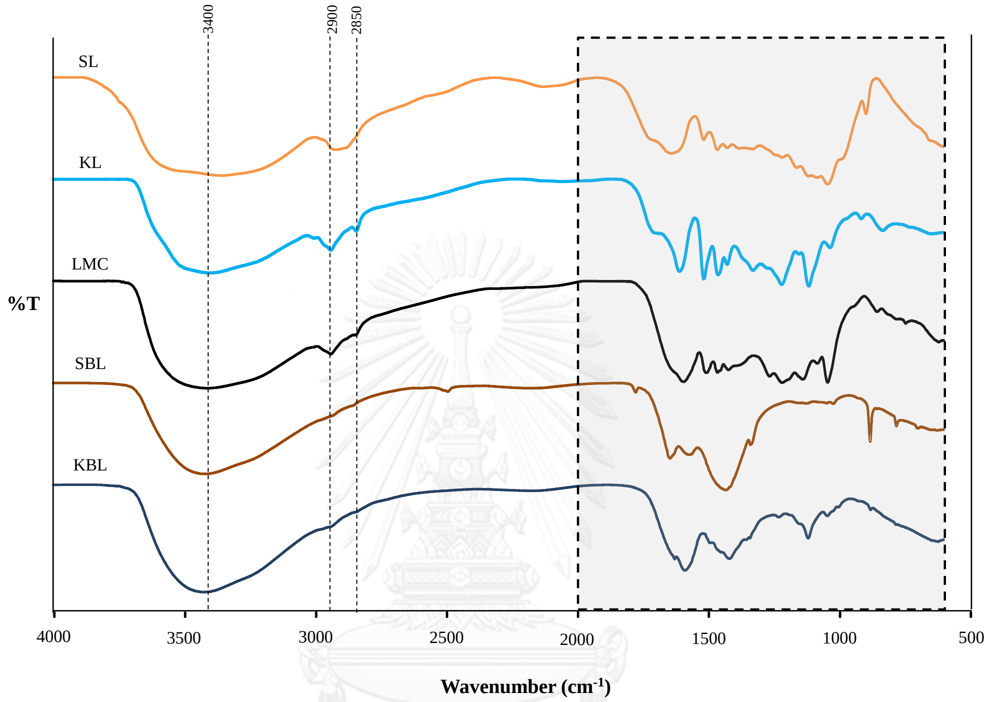

Figure 4.4 FTIR spectroscopy spectra of industrial black liquors, extracted lignins, and lignin model compound

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From Fig. 4.4, the spectrum of technical lignins performed a strong absorption at around 2900 cm^{-1} and 2850 cm^{-1} whereas of industrial black liquor almost not exhibited. At this region, the bands referred to C-H stretching vibration of the methoxyl group. This result might suggest the effects of acid precipitation. Moreover these bands can prove that the structure of technical lignins were nearly the same as lignin model compound. So this finding was the first unique character of isolated lignin or technical lignin from acid precipitation. It was remarkable that KL performed in stronger absorption than SL, thus KL might have the better lignin properties than SL.

As the precursor, LMC was utilized for the representative of lignin material. Therefore, some feedstock which showed the signals in the same range on the LMC band was indicated as the lignin material. For example, LMC the peak at 1050 – 1000 cm^{-1} corresponding to the stretching of O-CH_3 group, LMC and both of industrial black liquors and technical lignins responded signals in this range. Moreover, the industrial black liquors showed the signals at band 1430 – 1330 cm^{-1} corresponding to the existence of phenol. This finding might point out the potential of industrial black liquor for being the raw material for phenol chemical production. However, most of technical lignins more clearly illustrated the similar signals to LMC than industrial black liquors. For example, the carbonyl group in ketone at 1750 – 1680 cm^{-1} and in ester at 1123 – 1110 cm^{-1} specifically exhibited on the technical lignins. Moreover, lignins from the isolation process composed of carbonyl in guaiacol (1275 – 1266 cm^{-1}), and aliphatic hydrocarbon (1470 – 1460 cm^{-1}). These findings confirmed the effect of acid precipitation on lignin yields from industrial black liquor.

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Table 4.4 FTIR analysis results of three lignin samples (Silverstein et al., 1981, Shen et al., 2010, Yuan et al., 2011)

Wavelength (cm^{-1})	Band assignment	KBL	SBL	KL	SL	LMC
3500 – 3300	O –H stretching *(OH group)*	3431	3417	3402	3354	3414
3000 – 2850	C – H asym stretching in – CH_3 and =CH_2 group *(Aliphatic HC)*	2937	2937	2938	2918	2939
2850 – 2830	C – H sym stretching in – CH_3 and =CH_2 group *(Aliphatic HC)*	2839	2855	2842		2845
1750 – 1680	C = O stretching in ketone *(Carbonyl group)*			1688	1708	
1680 – 1620	C = C stretching in alkenes *(Aliphatic HC)*	1626	1644		1639	
1515 – 1505	Aromatic skeleton vibrations (G>S) *(Aromatic ring)*	1491		1515	1516	1505
1470 – 1460	C – H deformations (asym in – CH_3 and = CH_2) *(Aliphatic HC)*			1460	1464	1463
1430 – 1422	C – H in plane deformations with aromatic ring sketching *(OCH_3 gr.)*		1429	1425	1426	
1480 – 1350	C – H bending in alkane (– CH_3 and =CH_2 groups) *(Aliphatic HC)*	1451				1454
1430 – 1330	S rings and C – O stretching *(OCH_3 gr.)*	1339	1337		1330	1421
1275 – 1266	G ring and C – O stretching *(OCH_3 gr.)*			1274	1267	
1233 – 1214	C – O stretching in aromatic *(OCH_3 gr.))*	1229		1217	1216	1216
1123 - 1110	Aromatic C – H deformation in syringyl unit *(Aromatic)*			1114	1116	
1260 – 1000	C – O stretching in esters *(Carbonyl group)*	1188	1156	1152	1160	
1050 – 1000	C – O stretch for O – CH_3 *(OCH_3 group)*	1044	1046	1033	1043	1043
621	Sulphate O-S-O deformation	622	624			

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Due to the cleavage of core linkages, α-O-4 and β-O-4, alkali lignin structure could replace the ether bond with phenolic units so that the amount of phenolic hydroxyl groups was raised and higher amount of condense structure (Zhao et al., 2014). Nevertheless, the different pulping process led to the varied lignin structure especially kraft process which had higher potential to separate lignin from wood than soda process. The remaining cellulose blended in soda lignin, as evidenced by the band 1700 – 600 cm^{-1} (Fig. 4.4). The obvious existent of blending lignin (1600 – 1000 cm^{-1}) for KL and SL were considered that the former was a profile of lignin and the latter was of cellulose (Tran and Vakkilainen, 2007, Bajpai, 2015). Interestingly, this finding were relate to the origin of the technical lignins which generated from kraft and soda processes. Although the industrial black liquors similarly contained lignin from the digestion process, the ability of lignin separation was different. From Table 4.5, the spectra around 1800 – 800 cm^{-1} of industrial lignin compared to LMC was shown the specific properties of lignin cellulose and hemicellulose of feedstock in the Table 4.5 (Namane et al., 2016, Visakh and Lüftl, 2016)

Table 4.5 FTIR absorbance bands in industrial black liquors and lignin model compound

Component	**Wavenumber (cm^{-1})**		
	KBL	**SBL**	**LMC**
Lignin	1587, 1491, 1416	1587, 1572, 1429, 1077, 1054	1594, 1505, 1463, 1454, 1421, 1264, 1043
Cellulose	1337	1354	
Hemicellulose	1354, 1339	1644,1046, 1021, 880	

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Hence, the appropriate way for utilization of the technical lignins might not be the same. For example, the peak at 1639 cm^{-1}of SL showed the aliphatic structure while at 1608 cm^{-1} of KL displayed the aromatic form. The aromatic structure compounds played the key role as a feedstock for chemical production such as phenolic or aromatic products that substituted the petroleum-derived material, thus KL could be more appropriate for chemical production. On the other hand, aliphatic structure might favor for hydrocarbon compound production because of easier cleavage properties, so that SL would have more potential for bio-oil production. However, it depended on the desirable end products which could be planned and designed for suitable process.

4.2.5 SEM analysis

Referring to technical lignins structure analysis, the surface morphology of biopolymer from acid precipitation including the industrial black liquors were studied. The SEM micrographs of all samples are shown in Fig. 4.5 at different magnification (3kX and 300X). It can be observed that the particle of the technical lignin from different black liquor were not similar. Although various agglomeration along with granular particles were noticeable but the precise measurement of their original sizes was difficult because of the sintering phenomenon (Visakh and Lüftl, 2016). The appearance of the euhedral, pyramidal-shaped formation of industrial black liquors (Fig. 4.5 a – c) could indicate the existence of alkali salts and sulfur (Zhang et al., 2012), particularly on the surface. However, the structure of KBL was bigger and thicker bundling than SBL. This result indicated the effect of kraft and soda processes on the same wood. After acid precipitation, the technical lignin morphology was different from industrial black liquor because of the isolation process (Yang et al., 2007). The particle of KL was smaller than SL which was shrunk and formed as a large area. On the contrary, the morphology of KL had spherical shape like LMC but it had a tinny size. The particles of LMC which was the synthesis material were perfect round shape that might cause the production method. The surface porosities of LMC particle can be an evidence of structure changing from the regeneration and freeze-drying process (Chen et al., 1986) which might be the production process of the factory. Nevertheless, this kind of morphology was also occurred in the technical lignin char. These findings enhanced the understanding of the different pulping process on the lignin structure. In thermal conversion process for solid yield like char or biomaterial, this technique may yield interesting data for further study.

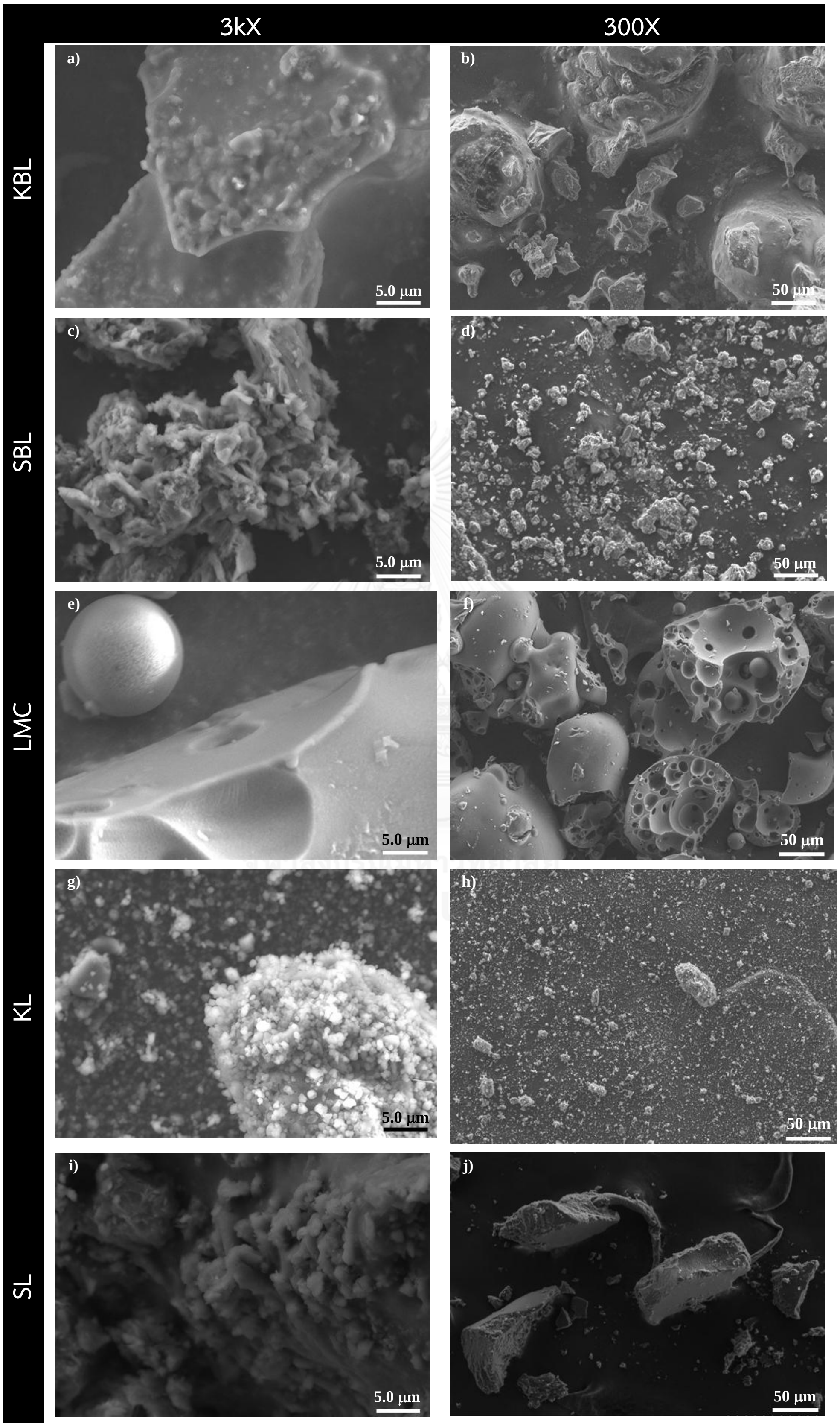
3kX
300X
KBL
SBL
LMC
KL
SL
a)
5.0 µm
b)
50 µm
c)
5.0 µm
d)
50 µm
e)
5.0 µm
f)
50 µm
g)
5.0 µm
h)
50 µm
i)
5.0 µm
j)
50 µm

Figure 4.5 SEM images of industrial black liquors (KBL; a, b and SBL; c, d), lignin model compound (LMC; e, f), and technical lignins (KL; g, h and SL; i, j) at magnification of 3kX and 300X

4.3 Conclusions

The major alkali compound in KBL was different form SBL which was Na_2SO_4 for KBL and Na_2CO_3 for SBL, according to their pulping chemicals. The organic waste from soda pulping process composed of higher oxygen whilst from kraft process contained greater carbon and sulfur. As the result of the organic characteristics, the technical lignins extracted from industrial black liquors exhibited different properties despite being the same amorphous structure. Relate to the specific composition, the degradation stage of KL was similar to lignin model compound while SL and cellulose model compound looked quite similar. The functional groups of technical lignins could be used to explain their unique thermal degradation. This result indicated the major proportion of kraft lignin was lignin material, while soda lignin was mainly composed of cellulose derivatives. This finding suggested the influence of pulping process on black liquors and their lignins characteristics which might impact on the different products from thermal conversion method. Therefore, further utilization of pulping byproducts should be based on their specific properties.

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CHAPTER 5

PRODUCT DISTRIBUTION OF TECHNICAL LIGNINS BY PY-GC/MS

5.1 Introduction

According to the hypothesis about the different lignin structure due to the pulping process, the results in chapter 4 showed the unique characters of the technical lignins (KL and SL) and lignin model compound (LMC). As a consequence, this chapter aimed to study the diversity of product distribution on the technical lignins due to their different basic structure via pyrolysis method. The pyrolysis products were analyzed by GC/MS and interpreted by NIST library. Moreover, the catalytic pyrolysis tests were carried out in lowest temperature for this research, 400°C, for study the effect of metal catalyst on products. However, some interested experiments were further conducted on higher temperature. For preparing some basic data about industrial black liquor under thermal conversion, the industrial black liquor was prepared in the solid powder for the pyrolysis reaction at 900°C. Therefore, this chapter will present the product distribution both from the technical lignins and solid industrial black liquors. LMC was conducted many investigation as the representative of lignin material.

5.2 Results and discussion

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The product distribution was presented by theses four groups for illustrating the several components in technical lignins. The experimental data was presented as the percentage of relative peak area. For this method, it was found that SL yielded the highest %relative peak area which due to its ability to be decomposed. The order of thermal stability from least to most stable was SL>KL>LMC so that SL produced the greatest and most variety of degraded compounds. The reason for high thermal stability of LMC might come from the factory production process. The production process might destroy aryl ether bond and left C-C bond which required high energy to break this bond. Moreover, SEM result of LMC (Fig. 4.5) illustrated the unique morphology which was dissimilar to the technical lignins. The sphere or round shape indicated the more stable form of material (Fierro et al., 2007). This finding was a clue to predict that the product distribution from thermal conversion of three samples might be different.

5.2.1 Product distribution of the technical lignins pyrolysis.

From the Figure 5.1, the key composition of KL was the phenolic chemical including the phenolic monomer such as guaiacyl and syringyl, methoxy bond, phenolic hydroxyl group, and phenol compound. These results demonstrated the organic composition from lignin pyrolysis (Rönnlund et al., 2012). With temperature increasing, the product yields were slightly decreased but more varieties of chemical derivatives were released. This finding indicated the degradation on lignin structure especially on methoxy group of phenolic monomers. From the Fig. 5.1a, higher temperature caused greater guaiacyl while smaller syringyl (dimethoxy phenol) because the O-CH_3 on syringyl was decomposed into guaiacyl (methoxy phenol). The organic compound with the functional group containing the methoxy group was the primary target to decompose in the pyrolysis (Lyu et al., 2015).

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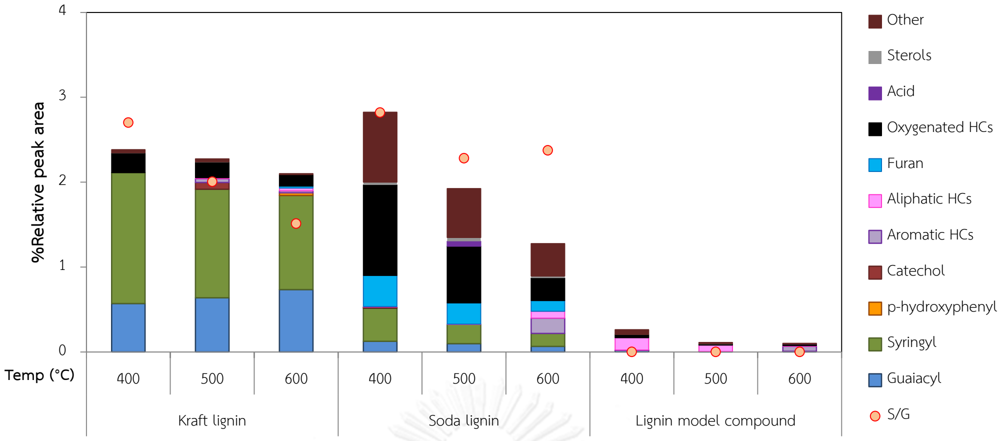

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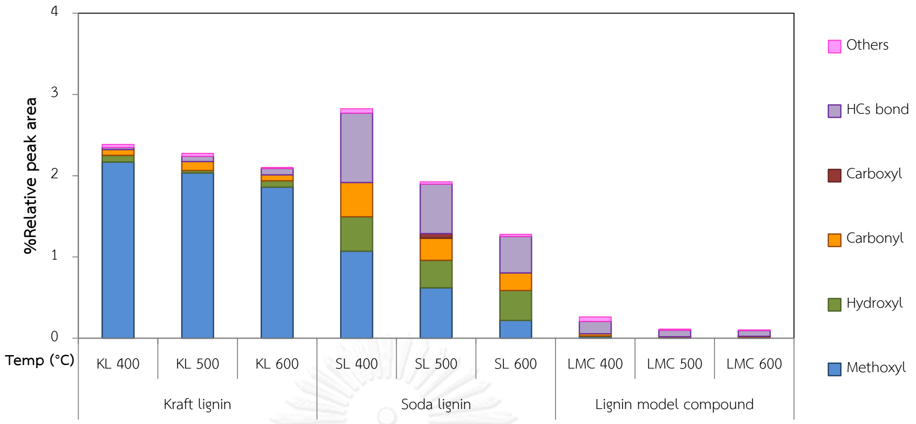

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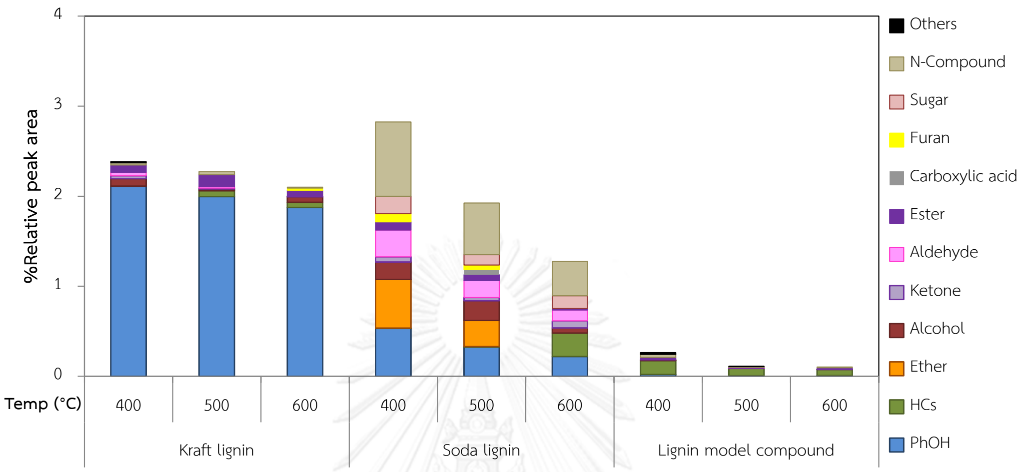

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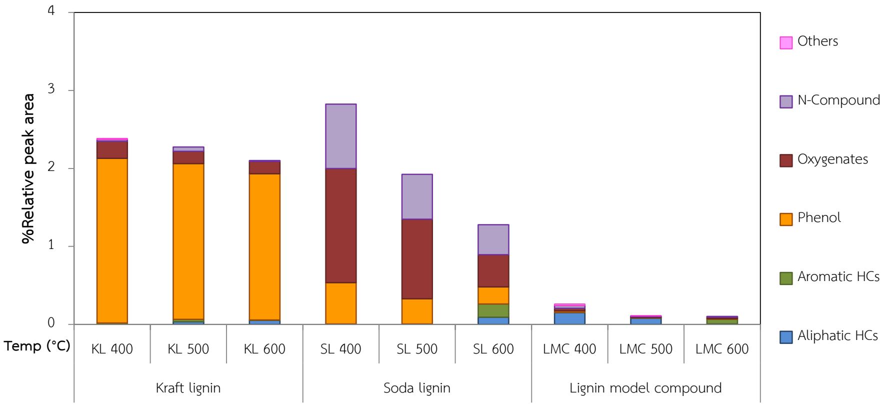

Figure 5.1 The relative distribution of pyrolysis products of the technical lignins and lignin model compound at 400°C-600°C (a) chemical species (b) bond type (c) chemical degraded compounds and (d) chemical structure

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The % area of syringyl (S) and guaiacyl (G) moieties were obtained from Py-GC/MS technique. To investigate the lignin structure, S/G ratio was used to determine the degrading characteristic of the interested lignin (Chen et al., 2015). The polymerization or cleavage of the macro molecule which mainly composted of the ether bond can enhance the formation of high stability product. Therefore, the whole %relative area and S/G ratio were decreased. Due to the condense polymer after depolymerizing O-CH_3, guaiacyl monomer contained more C–C linkage was difficult to decompose. Hence, lower ratio of S/G indicated harder degradation of material (Fig. 5.1a).

However, S/G ratio of SL showed conflicting results. At higher temperature, both guaiacyl and syringyl were decreased with no trend in S/G. The whole picture of product distribution was obviously decreased may be due to the influence of other competitive reaction on the SL pyrolysis. It was noticeable that most of degraded products continually decreased with temperature increased. In particular for the hydrocarbon products at 600°C, both of KL and SL behaved the similar way to generate the diversity of organic compounds, but SL yields were higher than KL. In addition, the chemical species of LS were primarily the oxygenated hydrocarbons instead of phenolic monomer as the case for KL.

This result may be together explained by TGA and FTIR analysis in the chapter 4. The appearance of cellulose in SL played a part of their thermal behavior. The products from lignin-cellulose mixture composed of hydrocarbons and other varieties of organic chemicals (Fig. 5.1c-d) which possibly further upgraded to high quality bio fuel (Lyu et al., 2015). Meanwhile, KL was suitable for being raw material used in the chemical production from petroleum or lignin based. As the comparable lignin material, LMC was pyrolyzed under comparable conditions to the technical lignins, but the results were not similar. Although its amorphous structure closely matched the technical lignins, only guaiacyl monomer was reported. LMC was highly stable in thermal condition, slight response to the raising temperature. Almost entire compound was hydrocarbon backbone including type of bond and aliphatic hydrocarbons compounds.

Furthermore, the interesting aspect of SL was the varieties of degraded compounds at higher temperature and lower product fraction. This finding may be due to the existence of cellulose which enhanced the concentration of oxygen in the reaction (Yoshida et al., 2014). According to the cellulose, it functioned as hydrogen donor and brought to higher degradation. In addition, C-O-C bond in cellulose was easy to cleavage. Therefore, the varieties of product were produced

(Fig. 5.1c,d). The co-process of cellulose and lignin produced the low molecular weight compounds; for example, ether, alcohol, ketone, aldehyde and ester (Wu et al., 2016). But for this research the formation of anhydrosugar especially the levoglucosan was not inhibited like the Wu et al., 2016. This discrepancy may be due to the different character of cellulose and lignin. The conducted the test on wood while the technical lignins of this research was processed and changed in origin structure. However, the present of sugar and furan in SL was the evidence of cellulose and hemicellulose (Lyu et al., 2015) which only small amount occurred in KL at 600°C according to Table 4.5. Nevertheless, the % fraction of these compounds was minute when compared to SL. This may suggest the relation and impact of cellulose and hemicellulose on degraded products. However, sugar of SL was slightly decreased with raising temperature, while furan disappeared. This result may be due to the easier degraded structure of furan than sugar. Nevertheless, sugar and furan detection showed the potential for further conversion into the raw material for pharmaceutical and chemical industries since they are suitable precursors to synthesize biological active products (Mendes et al., 2009, Vogelhuber et al., 2011).

Table 5.1 Major compounds of product yields (based on chemical species classified)

Temp. (°C)	Sample	Chemical species	Major compounds
400	KL	Syringol	Syringol 4-Methylsyringol 4-Ethylsyringol
	SL	Oxygenated HCs	Polypropylene glycol (Ether), Levoglucosan (Sugar), Pentanol (Alcohol)
	LMC	Aliphatics	4-Hexadecen-6-yne Squalene
500	KL	Syringol	Syringol 4-Methylsyringol 4-Ethylsyringol
	SL	Oxygenated HCs	Polypropylene glycol (Ether), Levoglucosan (Sugar),

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			Pentanol (Alcohol)
	LMC	Aliphatics	4-Hexadecen-6-yne Hexacosyne Squalene
600	KL	Syringol	Syringol 4-Methylsyringol 4-Ethylsyringol
	SL	Oxygenated HCs	Glucose (Sugar) Cyclohexanone (Ketone) Heptanol (Alcohol)
	LMC	Aromatic HCs	Toluene

Table 5.2 Major compounds of product yields (based on organic degraded compound classified)

Temp. (°C)	Sample	Organic compound type	Major compounds
400	KL	Phenolic OH (Phenol)	Syringol (S-phenol) 4-Methylsyringol (S-phenol) p-Ethylguaiacol (G-phenol)
	SL	Ether (Oxygenates)	Polypropylene glycol (Ether)
	LMC	Hydrocarbons	4-Hexadecen-6-yne (Aliphatic) Squalene (Aliphatic) Cholesta-3,5-diene (Sterol)
500	KL	Phenolic OH	Syringol (S-phenol) 4-Methylsyringol(S-phenol) Creosol (G-phenol)
	SL	Oxygenated HCs	Polypropylene glycol (Ether), Levoglucosan (Sugar), Pentanol (Alcohol)
	LMC	Hydrocarbons	4-Hexadecen-6-yne (Aliphatic) Cholesta-3,5-diene (Sterol)

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600	KL	Phenolic OH	Syringol (S-phenol) 4-Methylsyringol (S-phenol) p-Ethylguaiacol (G-phenol)
	SL	Hydrocarbons (Oxygenates)	1-Octene (Aliphatic) Toluene (Aromatic) 1-Octene (Aliphatic)
	LMC	Hydrocarbon (Aromatic)	Toluene

5.2.2 The effect of catalytic Py-GC/MS

Catalyst was generally uses for enhancing the desirable products or decreasing unwanted products. Besides that, catalyst can improve product quality at lower temperature and hence the catalytic experiments were focused at lower temperature (400°C). However, Ru and Pd based catalysts at 1-5 ratios were tested at 500°C-600°C. On account of the product distribution, this research aimed to investigate the degraded products from technical lignins thus the presentation was based on the reforming of products due to the varieties of catalysts. Moreover, the previous results showed the different products varied by type of technical lignin hence the outcomes of catalytic experiment were separately reported.

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5.2.2.1 The effect of catalyst on kraft technical lignin (KL)

As mentioned earlier, phenolic compounds were the main content in KL and S/G ratio was used for indicating their thermal stability. With raising temperature, S/G was small under non-catalytic condition but the catalyst could alter the outcome. Fig. 5.2a displayed the varieties pattern of S/G performed along the varied metal species and ratios. Although many experiments presented the higher value of S/G, the non-catalytic KL at 600°C showed the highest area% for the overall production. This finding illustrated the suitable temperature for β-O-4 cleavage was 400°C because of its lower bond association energy (Ben and Ragauskas, 2012) Moreover, there was not enough energy in the reaction for the intermediate product to be transformed into other species (Liu et al., 2016). Regarding the phenolic compounds, p-hydroxyphenol and catechol were interested because they have simple structure and tend to further process for products derived from phenol chemicals. The suitable condition for maximum p-hydroxyphenol was 1-1 Ni/ZrO_2 at 400°C which utilized lower temperature level and generated 3.4 times higher p-hydroxyphenol than non-catalytic at 600°C. Whereas the Ru catalyst played the role of increasing the p-hydroxyphenol but higher temperature was required.

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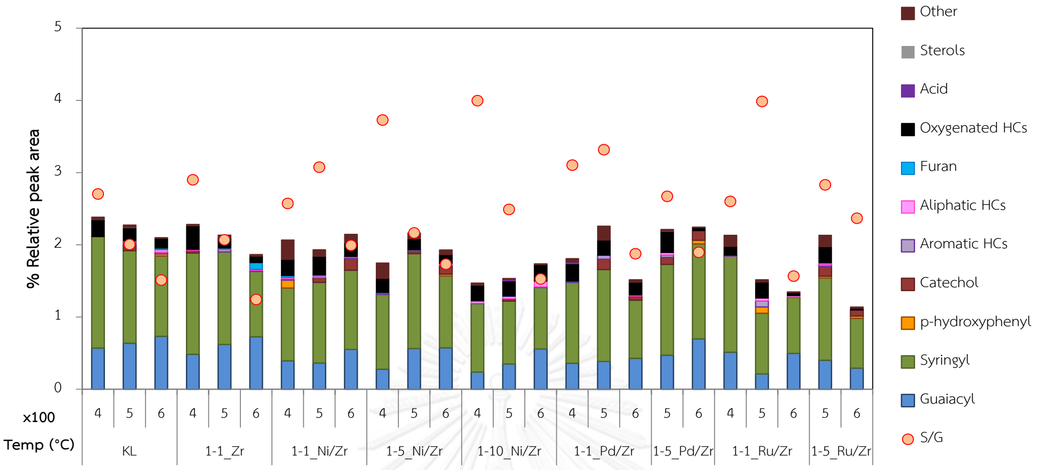

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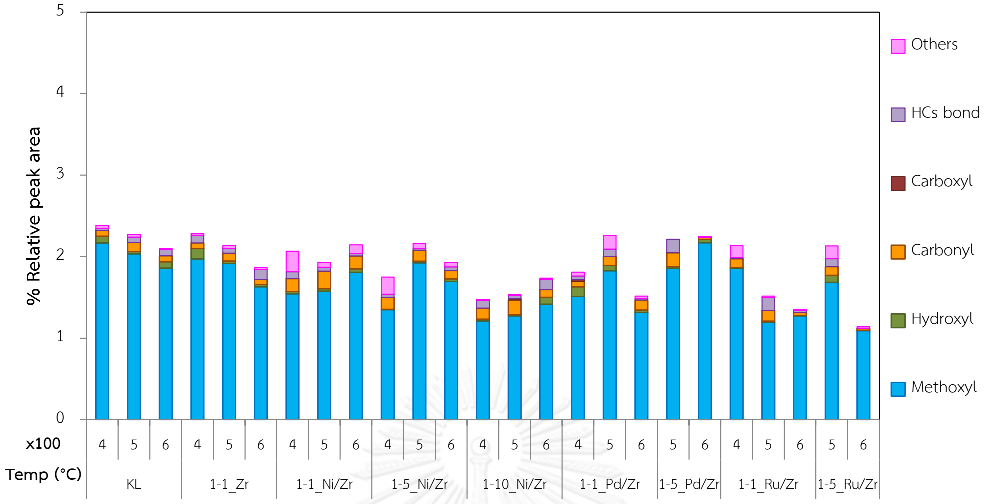

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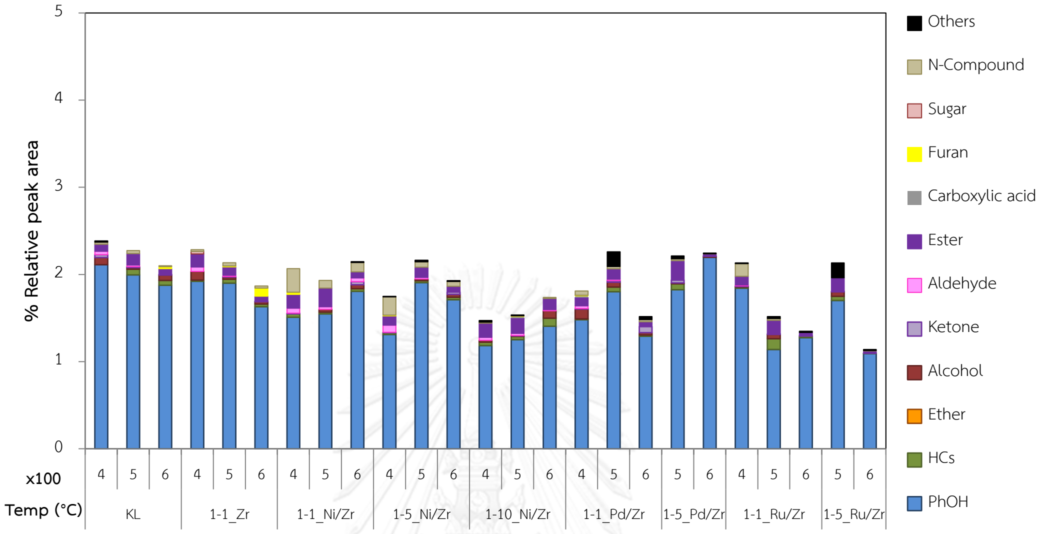

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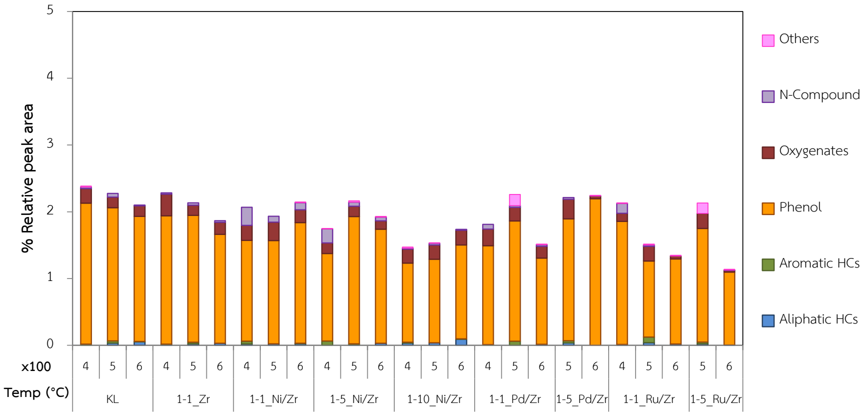

Figure 5.2 The relative distribution of catalytic pyrolysis products from kraft lignin at 400°C - 600°C (a) chemical species (b) bond type (c) chemical degraded compounds and (d) chemical structure

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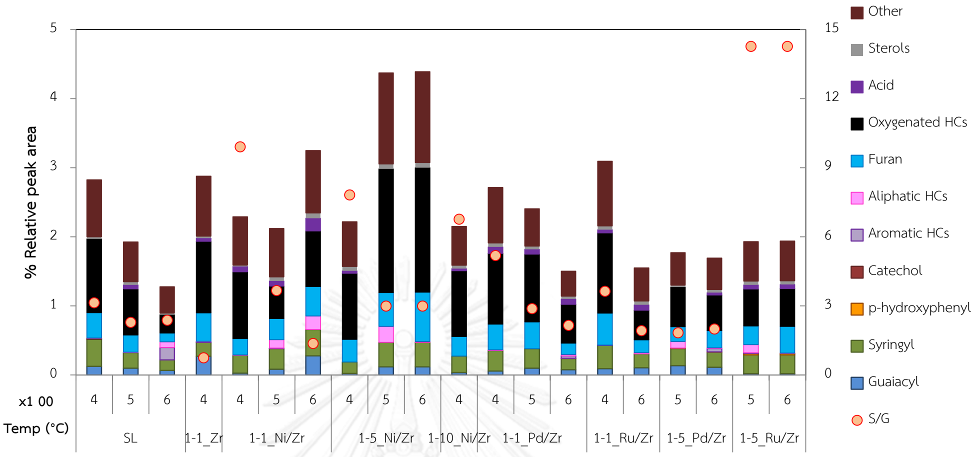
Another important phenolic compound was catechol which was highest at 600°C with 1-1 Ni/ZrO_2. Under non-catalytic, catechol occurred at 500°C but 2 times lower than the maximum yield of catalytic condition. However, not only the appropriate catalyst was used for a twofold catechol, the temperature was also raised from 400°C to 600°C. At the same temperature of highest catechol under non-catalytic reaction, 1-1 Pd/ZrO_2 and 1-5 Ru/ZrO_2 showed the interesting fractions but they were more expensive than nickel. Because the suitable condition for enhanced the phenolic product should not only be determined by the energy used but also the price of catalyst. Therefore, Ni catalyst was likely to be the most attractive choice.

In Fig. 5.2c clearly illustrated how catalyst effect on the phenolic hydroxyl group (PhOH) which was useful for any production based on the phenolic compound. Although the largest fraction of PhOH was %area of 2.20 at 1-5 Pd/ZrO_2 at 600°C, the non-catalytic at 400°C exhibited % area of 2.11. This result suggested that the non-catalytic at 400°C condition was more worthwhile than the catalytic condition with higher temperature, due to their % area of PhOH were almost equal. Another essential product of pyrolysis reaction, the aliphatic hydrocarbon responded to higher temperature as shown in Fig. 5.2d. Both of aromatic and aliphatic compounds scattered at 500°C-600°C and the greatest aliphatic hydrocarbon was at the highest temperature with 1-10 Ni/ZrO_2. However, hydrocarbon compound was relatively low amount compared to SL. This kind of technical lignin is appropriated for utilization in phenol chemical industries. Therefore, the future research should be done for upgrading the phenolic compound to high quality, valuable feedstock for chemical production.

5.2.2.2 The effect of catalyst on soda technical lignin (SL)

Although the soda technical lignin was referred as the residue lignin in industrial black liquor, the result of FTIR and TGA techniques including the product distribution in Fig. 5.1 revealed the distinctive characteristic of SL. The blending cellulose in SL had the strong influence on the degraded products not only the decomposition of lignin. From Fig. 5.3, the phenolic species such as guaiacyl and syringyl fraction were in small amount when compared to the cellulose derivative species like other oxygen containing compounds.

(a)



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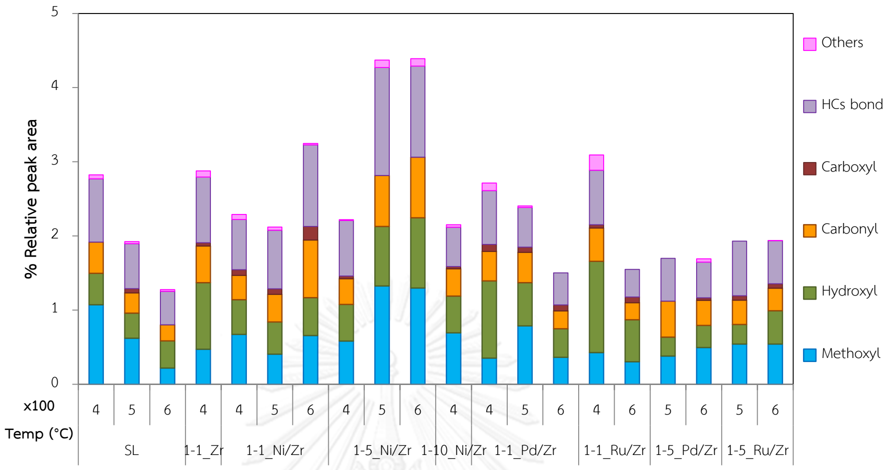

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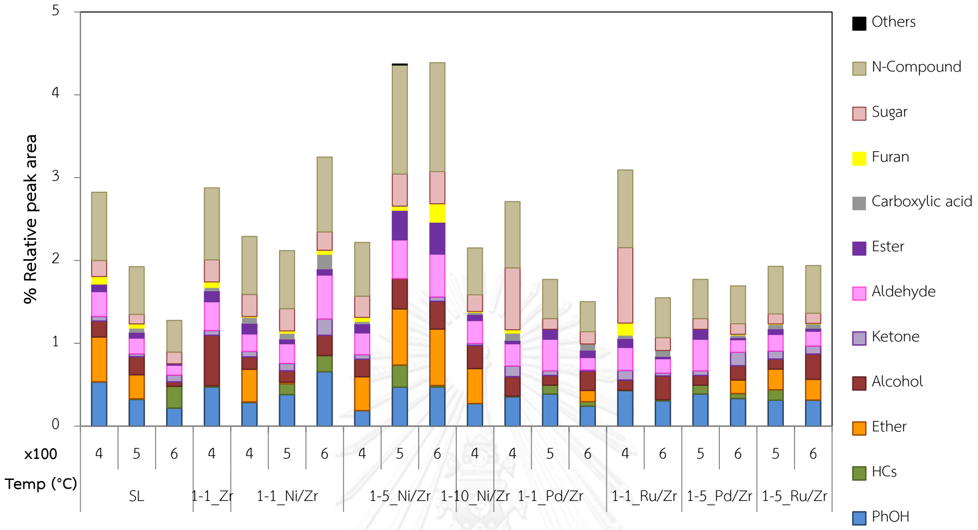

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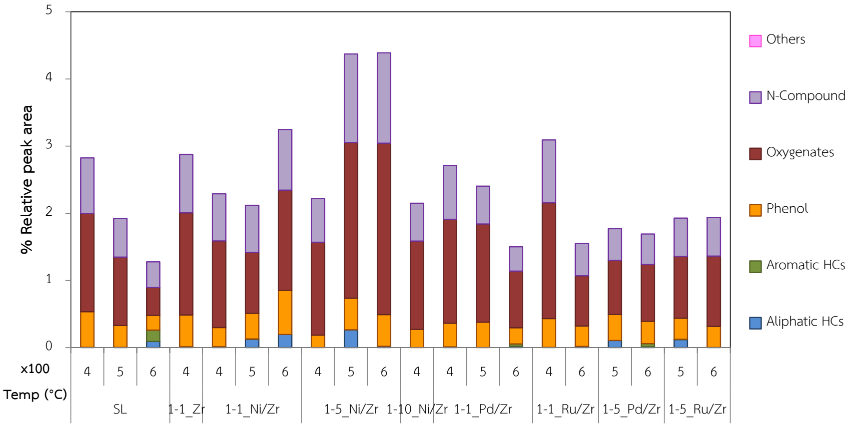

Figure 5.3 Relative distribution of catalytic pyrolysis products of the soda lignin at 400°C-600°C (a) chemical species (b) bond type (c) chemical degraded compounds and (d) chemical structure

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Relate to the phenolic compound as the unique character of lignin, only guaiacyl and syringyl species were produced (Fig. 5.3a). Under non-catalytic at 400°C, SL can produce guaiacyl and syringyl higher than those the catalytic experiments. With the exception of 1-1 Ni/ZrO_2 at 600°C, the guaiacyl was highest along with larger fraction of aliphatic hydrocarbons. The % area of aliphatic HCs from non-catalytic pyrolysis of SL at 600°C was 0.08, while 0.20 was of the catalytic reaction of 1-1 Ni/ZrO_2 at the same temperature. Therefore, 1-1Ni/ZrO_2 catalyst was suitable for applying in the upgrading of SL for valuable products. However, increasing Ni ratio to 1-5 and decreasing temperature to 500°C played an active part in raising the aliphatic HCs and furan up. By contrast, the oxygenated compound (Fig. 5.3d) was enhanced under that catalytic condition. Nonetheless for minimizing the oxygenated compound, the non-catalytic at 600°C condition was preferable, the catalytic condition was not required.

The degraded compositions derived from cellulose especially ether, ketone, aldehyde, and ester were outstandingly presented when compare to PhOH due to the effect of lignin-cellulose interaction (Wu et al., 2016). As the scientific fact, those organic components were the general ingredient of the bio-oil from thermochemical conversion of biomass (Lyu et al., 2015). This was the important issue for future research in upgrading the quality of bio-oil from SL thermal conversion. For this research, in Fig 5.3c, it seemed 1-5 Ni/ZrO_2 at 500°C and 600°C helped increased the ether, aldehyde and ester, while 1-1 ZrO_2 at 400°C produced the highest alcohol. From Fig. 5.3c, Pd and Ru of 1-1 ratios at 400°C yielded the highest sugar, especially for Ru catalyst which can highly improve the fraction of furan.

5.2.2.3 The effect of catalyst on lignin model compound (LMC)

As mentioned in the beginning of this topic, LMC has high stability might cause the factory production process. Regarding the phenolic compound, only guaiacyl was detected which implied that the wood origin for LMC process was softwood (Liu et al., 2008). According to the different in lignin nature, softwood was G-type wood which means the majority propane phynyl alcohol in their structure is guaiacyl. For hardwood, both of G and S type were the components at typical percentages of 40 and 60, respectively. Therefore, both of guaiacyl and syringyl were produced in this research because the eucalyptus is hardwood and is the feedstock of pulping process which generates industrial black liquors.

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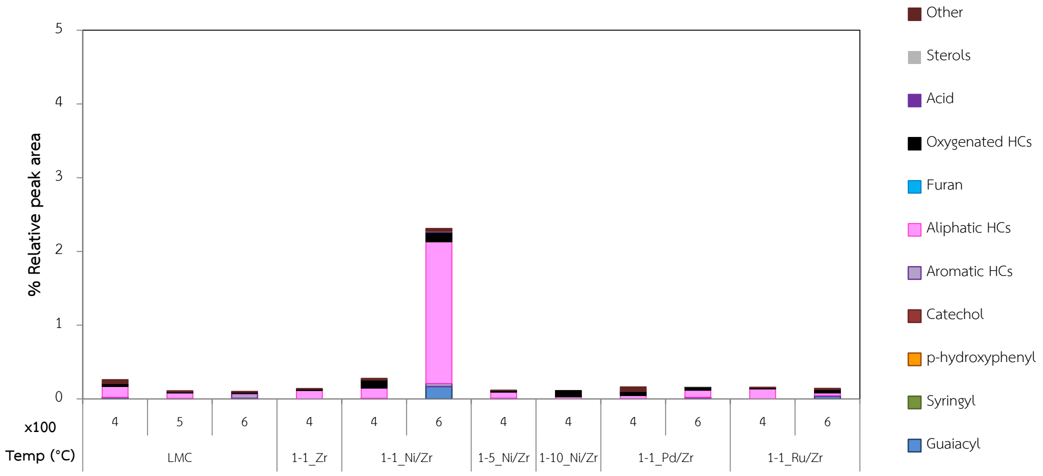
(a)



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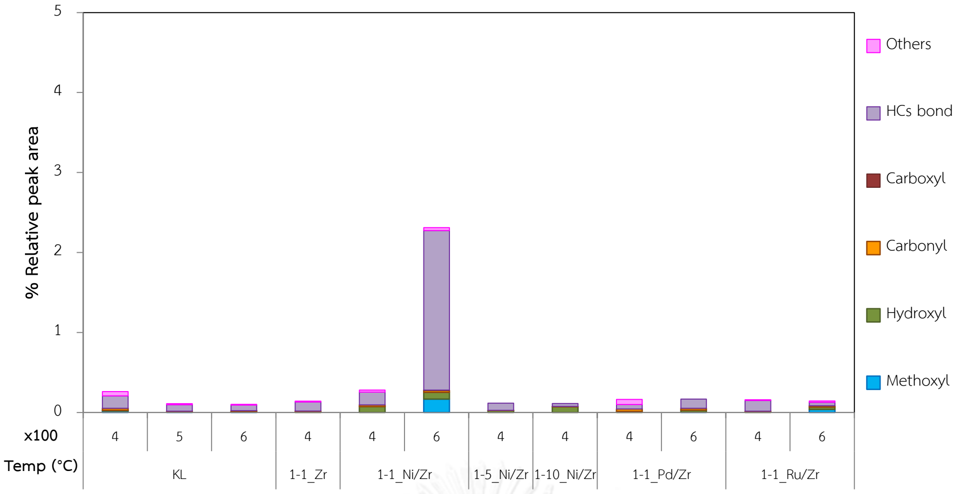

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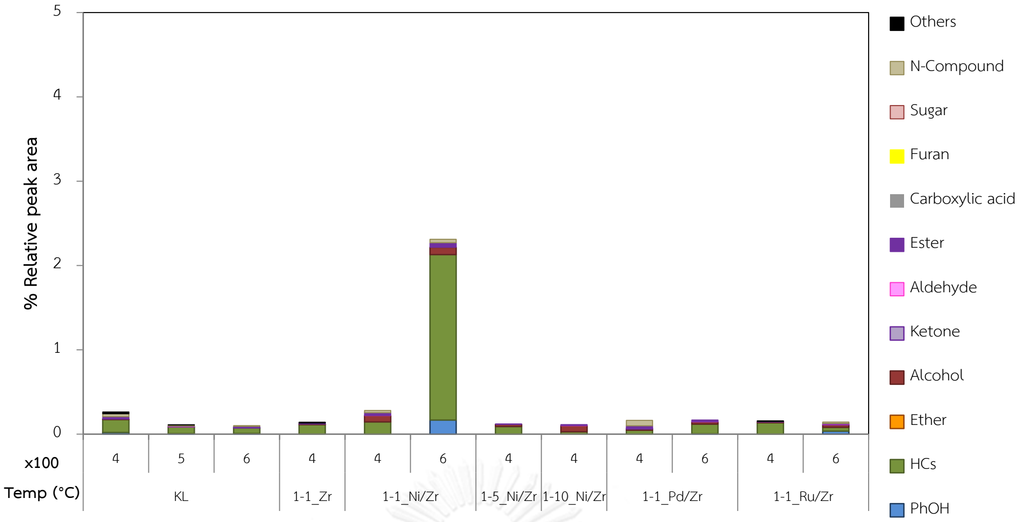

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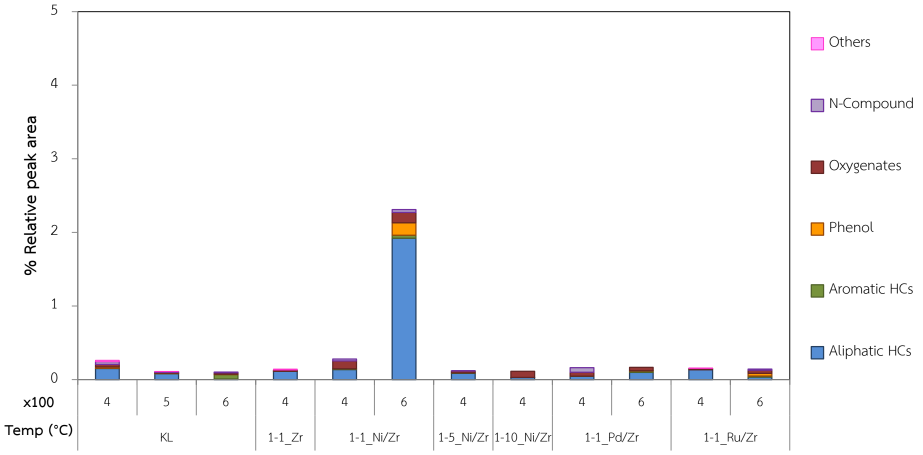

Figure 5.4 Relative distribution of catalytic pyrolysis products of the lignin model compound at 400°C - 600°C, (a) chemical species (b) bond type (c) chemical degraded compounds and (d) chemical structure

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Using 1-1 Ni/ZrO_2 catalyst at 600°C yielded superior products (Fig. 5.4a) including guaiacyl, aliphatic HCs, and oxygenated species. Hydrocarbon bond or C – C bond was the primary bonding of the product spread (Fig. 5.4b). The greatest hydrocarbons compound (Fig. 5.4c) was almost consisted of aliphatic type (Fig. 5.4d). This finding pointed out two facts that the most component in LMC was the hydrocarbons which were suitable for the production of high quality fuel. Despite the abundance of carbon and hydrogen, their thermal stability was the reason of high energy requirement to break and release of hydrocarbon products. The other fact was Ni catalyst played the essential role to enhance the lignin degradation similar to that of technical lignin experiments.

Table 5.3 Enhancement of specific compounds by catalytic reaction

Catalytic condition	Interest compounds	% relative area	
		Non-catalytic	Catalytic
Kraft technical lignin (KL)			
400°C 1-1 Ni/ZrO_2	p-Hydroxyphenyl	0.00	0.11
600°C 1-1 Ni/ZrO_2	Catechol	0.00	0.16
600°C 1-5 Pd/ZrO_2	Phenolic OH	2.11	2.20
500°C 1-10 Ni/ZrO_2	Aliphatic HCs	0.01	0.03
600°C 1-10 Ni/ZrO_2		0.03	0.08
Soda technical lignin (SL)			
400°C 1-1 ZrO_2	Alcohol	0.19	0.61
400°C 1-1 Pd/ZrO_2	Sugar	0.19	0.75
400°C 1-1 Ru/ZrO_2			0.91

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500°C 1-5 Ni/ZrO_2	Ether	0.29	0.68
	Aldehyde	0.19	0.47
	Ester	0.06	0.36
600°C 1-5 Ni/ZrO_2	Ether	0.00	0.68
	Aldehyde	0.53	0.52
	Ester	0.07	0.39
600°C 1-1 Ni/ZrO_2	Guaiacyl	0.06	0.28
	Aliphatic HCs	0.08	0.20
Lignin model compound (LMC)			
600°C 1-1 Ni/ZrO_2	Guaiacyl	0.01	0.17
	Aliphatic HCs	0.01	1.92
	Oxygenated HCs	0.02	0.13

5.3 Conclusion

The varieties of unique compounds from thermal conversion related to the composition in technical lignins. The majority of lignin material in KL resulted in phenolic structure, so the products mostly composed of hydroxyl phenols e.g. syringol, 4-Methylsyringol, and p-Ethylguaiacol. Whilst the main component in SL was cellulose and hemicellulose biopolymer, the various products of oxygenated hydrocarbons were predominated; for example, ether, sugar, and alcohol. According to the different nature in subunit and linkage of lignin, cellulose, and hemicellulose, the various amount of these biopolymers in KL and SL affected to the product distribution. This result indicated that the different pulping chemical was the important factor for generating the technical lignin with specific properties. As a result, the distinction between kraft and soda lignin would categorize in furtherance of utilization for high value products production. Obviously, KL might be appropriate for phenol production while SL is suitable for bio-oil production. Moreover, nickel based catalyst was the most effective for both of KL and SL in the quality upgrading via thermal conversion. Py-GC/MS technique can enhance the understanding of thermal degraded products which could lead to the optimal condition for thermochemical conversion of lignocellulosic biomass and lead to high effective production in the larger scale.

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CHAPTER 6

SUPERCRITICAL WATER GASIFICATION OF BLACK LIQUOR FOR SYNTHESIS GAS PRODUCTION

6.1 Introduction

According to chapter 5, technical lignins and lignin model compound (LMC) were studied on their thermal behavior under pyrolysis at the temperature of 400°C-600°C. Contrary to expectations, the product degradations were different even though their characteristic results in the chapter 5 were similar (Table 5.1). Kraft technical lignin mainly composed of phenolic compounds while the oxygenated compounds derived from cellulose residue were the primary content in soda technical lignin. For LMC, interestingly, the aliphatic HCs compounds were the principle products instead of the monomeric phenolic compound. In this chapter, all the technical lignins and LMC were converted under supercritical water (SCW) condition. The technical lignin of kraft and soda (KL and SL) is a portion of the kraft and soda black liquor (KBL and SBL), respectively. Both KBL and SBL contain two crucial parts that are lignin as the organic source and spent chemical as the alkali salt. Therefore, gasification yields of industrial black liquor might differ between KBL and SBL. Moreover, clear understanding of the relation between the specific characteristic of the organic part in black liquor and gas production can be achieved by the outcomes of chapters 4 and 5. Due to the complexities of hydrothermal reactions and the feedstock characteristics, especially the real biomass, many researches attempt to improve the gas yields and solve the technical and engineering obstacles (Pavlovič et al., 2013). Therefore, the result of this chapter leads a coherence of organic source structure and syngas production into further design the experiment for required gas production. Feedstock replaced in the reaction is mainly decomposed by the hydrolysis reaction first. The hydrolysis is the main reaction in the moderate-temperature region which generated the intermediates from the feedstock at sub- or near- critical water (Madenoğlu et al., 2012, Pavlovič et al., 2013). Therefore, the fundamental structure of feedstock is important for being the initial substance for the organic fragment production. At temperature of the supercritical water point, the free-radical reaction plays the crucial role of producing the gas products from the intermediates or the organic fragment generated by the hydrolysis reaction.

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The lignin in kraft black liquor (KBL) mainly composed of phenolic compound hence there were large portion of aromatic compounds and methoxyl groups. Moreover, the results of TGA and FTIR techniques (Fig. 4.3 and table 4.5) in chapter 4 and the degraded compound in chapter 5 (Fig. 5.1-5.2) illustrated the minute amount of cellulose and hemicellulose materials and their derivatives in kraft technical lignin structure. Therefore, not only oxygen content from the methoxyl and hydroxyl group in phenolic compounds, also the cellulose derivatives were another source of oxygen content in KBL. Hence, the decomposition reaction (eq. 1) could cooperate with the steam reforming reaction (eq. 2) to produce many fragments by breaking C–O and C–C bonds (Susanti et al., 2014). As a consequence of hydrolysis reaction, the intermediates generated might compose of the aromatic rings (C–C and C–H bonds) and low molecular weight fragments (formaldehyde, monomeric phenolic compounds; ether and ester bond). When the temperature reaches the SCW condition, the intermediates were degraded through many reactions such as dehydrogenation, decarboxylation, and dehydration, and hence H_2, CO_2 and CO formation, respectively. The CO yield was further involved in the WGS reaction for H_2 production. At this stage, the free-radical reaction was the dominant species to cleave those compound fragments.

There were cellulose, hemicellulose and lignin in SBL structure hence high concentration of oxygen influenced the overall reaction. In the similar manner, the KBL data from the previous chapters supported the understanding of the intermediates production by hydrolysis reaction. However, the oxygenated HCs structure of SBL can increase simple and small fragments than KBL. The main bonding of SBL were C=O, C–O and OH which appeared in cellulose and hemicellulose. Therefore, SBL tended to produce more syngas than KBL and LMC.

LMC was the precursor for comparative study into the technical lignins structure in chapter 4. Its thermal behavior was studied by Py-GC/MS in the chapter 5 for comparing with the technical lignins. In this chapter, LMC was gasified like KBL and SBL for studying the effect of the spent alkali in black liquor. However, the data from Py-GC/MS in chapter presented some unexpected results. There were minute amount of guaiacyl and small amount of aromatic HCs. The major portion of LMC was aliphatic HCs which is highly stable under thermal conversion.

Under hydrolysis condition, LMC might be degraded whenever the sufficient energy reached for bond dissociation. The decomposition and steam reforming reactions might be the initial process to degrade $C_xH_yO_z$ of LMC. After that the small pieces hydrocarbons further participated in the WGS and methanation reaction.

Therefore, LMC tended to produce the similar gas as KBL because of their aromatic structure but LMC consisted of lower oxygen content.

This chapter is categorized in four parts. The first part presents the effect of alkali in the industrial black liquor. The effect of temperature and pressure in range of 400°C-600°C and 250-400 bar, respectively are described in the second part. Some organic compounds in liquid yields from the non-catalytic SCWG reaction at 500°C, 250 and 400 bar is presented in the third part. The last is the study on catalytic SCWG reaction at 400°C and 250 bar using 5% metal based catalyst on ZrO_2 support and varying sample per catalyst as 1-1 and 1-10 ratios. The results of non-catalytic reaction at 400°C and 250 bar are compared as the base case scenario.

6.2 Results and discussion

After quenching, the appearance of product inside miniature fused quartz was in various form of liquid and solid residue according to the type of feedstock and experimental condition. Gas products was analyzed and calculated per kg of feedstock. The gaseous products were primary composed of H_2 and CH_4. The highest total gas production was achieved when using SBL as raw material at 250 bar with higher temperature. Although found in minute quantities, CO gas was a good indicator that may be used to understand the reaction mechanism involved here. LMC was carried out as the representative of lignin material without spent chemical or alkali salt like the industrial black liquors.

The crucial portion on industrial black liquor was the spent alkali which illustrated in XRD result in chapter 4. In general, the alkalis remaining in weak black liquor are recovered to regenerate the pulping chemical, white liquor. However, this research aims to convert the organic substance in waste steam without any dewatering process. For this reason, the organic substance in weak black liquor was process along with alkalis. Therefore, the extra role of the remained alkali was acting as the homogeneous catalyst (Rönnlund et al., 2011, Xu et al., 2013). The alkali presented the vital role in both the hydrolysis reaction and WGS reaction which cooperated in raising H_2 production. LMC, the representative organic substance, was gasified without alkalis under the same condition of the industrial black liquor.

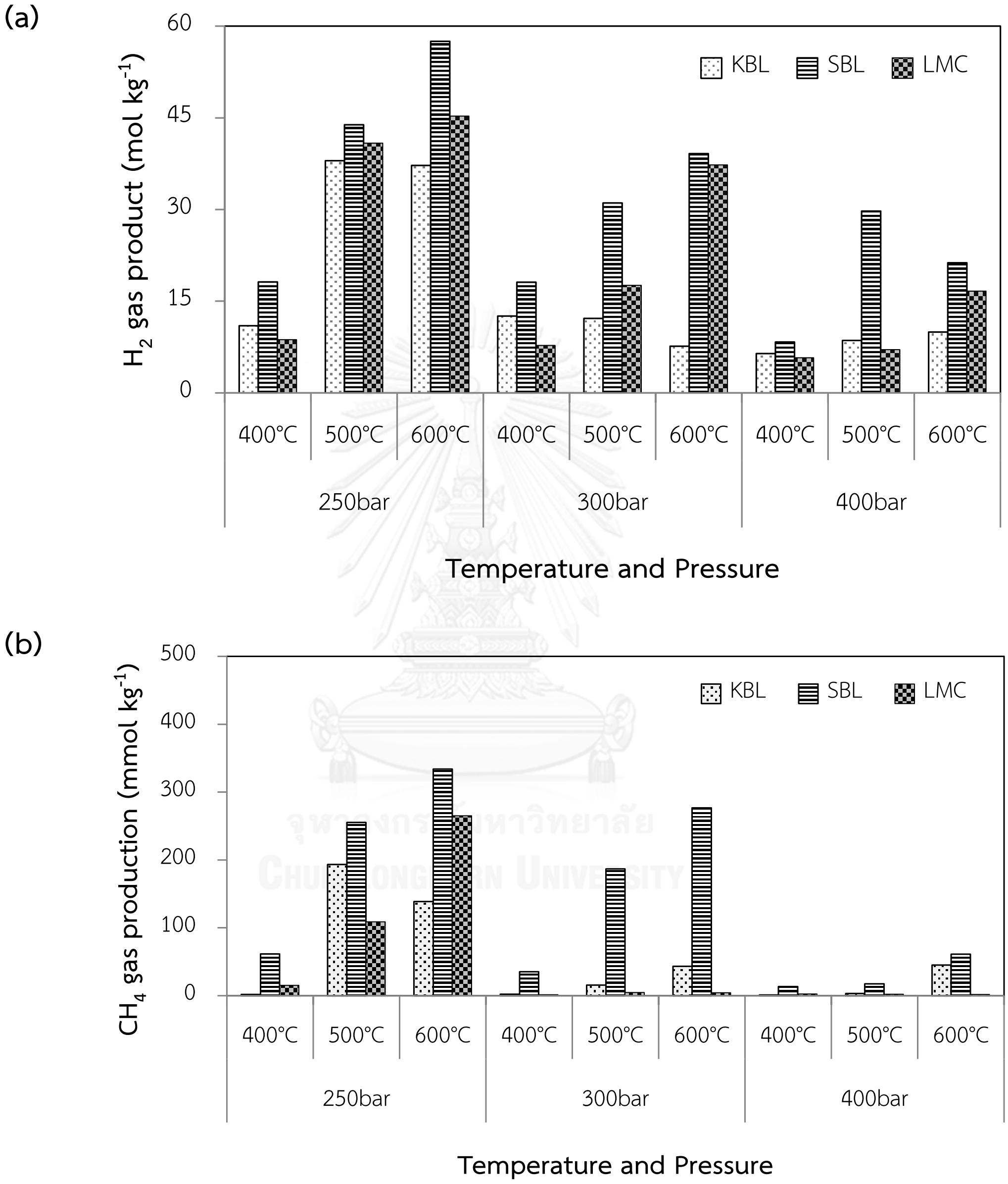
6.2.1 Effect of alkali in the industrial black liquors

The result of XRD analysis in the chapter 4 illustrated the alkali salt compound on the structure of the industrial black liquors. The different kind of alkali compound of KBL and SBL, Na_2SO_4 and Na_2CO_3 respectively, might play the key role in homogeneous catalytic reaction (Guo et al., 2012). Therefore, to study the effect of alkali salt on the technical lignins contained in the industrial black liquors, LMC was carried out to study of SCWG without alkalis..

Fig. 6.1 displayed gas production, the results are presented in mol unit per feedstock (kg). The maximum yield was obtained from conversion of SBL including H_2, CH_4 and CO. Hydrogen gas production from SBL was in range of 10-58 mol/kg SBL, whereas 6-38 mmol/kg and 6-45 mmol/kg were measured with KBL and LMC, respectively. About twofold greater H_2 products of SBL than LMC might illustrate the existing alkali catalytic effect. However, H_2 yield of KBL with alkali content was quite lower than that of LMC. This is probably due to higher percentages of carbon and hydrogen components in LMC when compared to KBL (Table 4.1). Here, steam reforming could generate CO gas from the available C and H which was further subjected to WGS and then resulting in higher H_2 yield from LMC. Although KBL was decomposed with the alkali catalytic reaction, which the hydrolysis of alkali solution was more efficient than that of acid and hydrothermal conditions (Rönnlund et al., 2011). As a result, syngas and organic/alcohol compounds from C–C and C–O bond cleavages were increased. Therefore, any $C_xH_yO_z$ materials could be effectively reacted under alkali solution of SCW condition for enhanced gas production reaction (eq.2-5). The result of LMC gas production might suggest that the higher original carbon and hydrogen contents could compensate for its lacking of the alkali when compared to KBL. Further research about mechanism of biomass thermal conversion should be emphasized on the initial carbon and hydrogen content of feedstock in the preparation process.

The main reaction in SCWG for H_2 production was WGS reaction (eq.3), which could be improved by alkali salt (Rönnlund et al., 2011, Nanda et al., 2016). Therefore, H_2 production was increased while CO decreased from its consumption under WGS reaction. In addition, alkali can promote the methanation reaction which normally preferred to proceed at lower temperature (Ondze et al., 2015). In Fig. 6.1b, CH_4 gas production was improved with temperature. CH_4 production from KBL and SBL were mostly higher than that of LMC as temperature increased. However, a moderate amount of CH_4 was produced from LMC at 250 bar and higher temperature even without alkali content which might due to the effect of intense temperature and pressure. Above the critical point, the intermediates were decomposed due to their hydrocarbon structure (Fig. 4.4) led to large amount of syngas production.

Therefore, these findings enhance the understanding of the excellent thermal conversion via the SCW condition and the effect of biomass structure, which may be more effective than the catalytic reaction by alkali salt.



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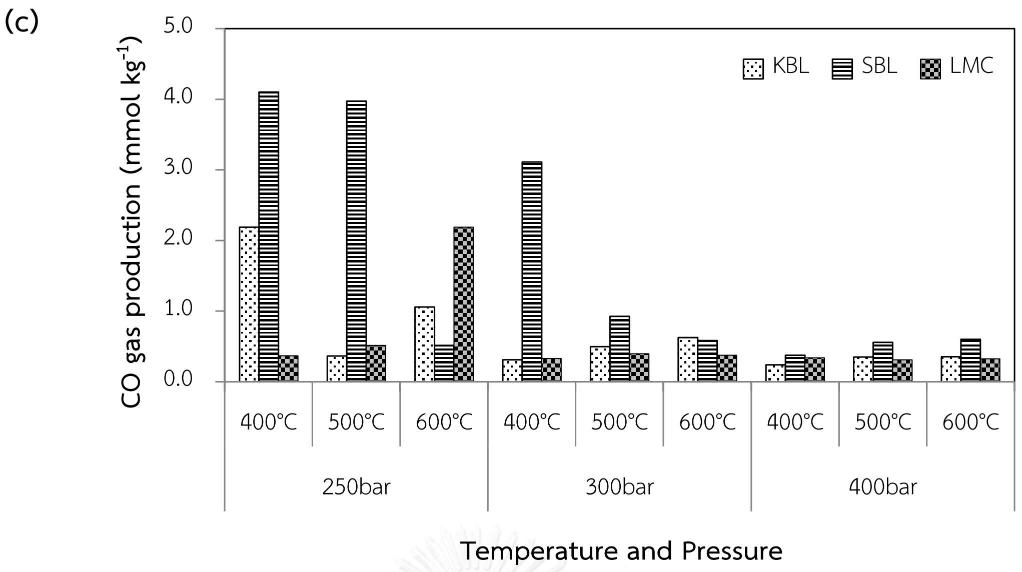

Figure 6.1 Gas production from conversion at various temperatures (400°C-600°C) and pressure (250-400 bar), (a) H_2, (b) CH_4, and (c) CO

.

In addition to distinctive properties of SCW on disintegration of biomass to syngas, the availability of alkali in the sample also play major role on gas generation, comparable to organic solvent. Although the bond scission was the major reforming reaction of $C_xH_yO_z$ component in biomass into radical forms, the alkali salt such as Na_2CO_3 may also act as catalyst for rapid splitting of C–C bond of organic substance to organic acid in water (Rönnlund et al., 2011, Guo et al., 2012, Susanti et al., 2014). Therefore, SBL, with its high Na_2CO_3, could yield higher gas production. In this case, XRD analysis was used to determine and compare inorganic (alkali or sodium) contents in the samples. From Fig 4.1, sodium compounds were dominant alkali in the spent chemical in black liquor. Regarding chemical pulping process, soda pulping used only NaOH while kraft pulping used both NaOH and Na_2S. Therefore, KBL contained more Na_2SO_4 whereas Na_2CO_3 was the major compound in SBL. However, the small amount of sodium sulfate (Na_2SO_4) presented in SBL, likely originated from intrinsic sulfur in eucalyptus wood (Pereira et al., 2013). Whereas the sulfur content of KBL was 20.5 times higher than SBL due to the chemical in digestion process. As the homogeneous catalytic properties, Na_2CO_3 played the crucial role in producing CO formation via eqs. 6-10 (Ibrahim et al., 2011)

$$Na_2CO_3 + C \longrightarrow \text{—}COONa + \text{—}CONa \tag{6}$$

$$\text{—}COONa + C \longrightarrow \text{—}CONa + CO \tag{7}$$

$$\text{—}CONa + C \longrightarrow \text{—}CNa + CO \tag{8}$$

$$\text{—}CNa + CO_2 \longrightarrow \text{—}CONa + CO \tag{9}$$

$$\text{—}CONa + CO_2 \longrightarrow \text{—}COONa + CO \tag{10}$$

From these reactions, Na_2CO_3 promotes formation of alkali ion and CO that further the WGS reaction (eq. 3) for formation of CO_2 and H_2 which would then result in enhanced methanation reactions (eqs. 3-4) and then CH_4 generation. These are possible added benefits of Na_2CO_3 in SBL besides aiding the dissolving of organic in water.

6.2.2 Effect of temperature

As mention above, WGS reaction was the main reaction controlled by radical reaction which was the function of temperature. Therefore, increasing temperature could promote the WGS via free radical reaction. Although both WGS and methanation reaction were exothermic reaction (Zhang et al., 2010), the excess water controlling free radical reaction reacted with the hydrolysis products from alkali solution can generate higher syngas at higher temperature. Moreover, the intermediates and gas products in hydrothermal process were affected by the structure of lignin in black liquor. Osada et al. (2004) studied the hydrolysis of lignin without catalyst and reported that the phenolic compound and aldehydes were formed and rapidly decomposed to gas e.g. CH_4, CO_2, H_2. Moreover, the H^+ and OH^- under SCW condition can cleavage the benzene ring and generate low-molecular weight compounds (Ding et al., 1996). Therefore, the amount of intermediates from lignin hydrolysis was the substrate for further WGS reaction. For these reasons, higher temperature increased gas production by WGS reaction. However, the obstacle to determine the ability of alkali catalytic was the different lignin structure in black liquor.

For the case of LMC which contains no additional alkali but with larger portion of C and H, CH_4 production was also higher with temperature at 250 bar. This probably resulted from the influence of temperature and pressure which can alter the ion and free radical reactions under SCW condition (Guo et al., 2010). Ion hydrolysis reaction can promote the bond cleavage of $C_xH_yO_z$ structure in LC for syngas productions and then enhanced steam reforming reaction, especially CO for methanation reaction. In consequence, the reaction for gas production under the free-radical controlled reaction (eqs. 1-4) further generated syngas from those produced gases, particularly for methanation reaction of LMC. Therefore, LMC can provide more CH_4 at high temperature even without alkali. However, further research with stricter control of the quantity of carbon and hydrogen fed in the SCWG reaction should be carried out in order to confirm this argument. However, at higher pressure region, the decomposition rate was lower because the free-radical reaction was inhibited due to favorable reaction direction toward lesser gas productions according to Le Châtelier's principle (Cantero et al., 2015).

Therefore, high temperature and moderate pressure of 600°C and 250 bar seemed to be the optimum for H_2 gas production. On the contrary to monomer products, alkali ion under SCW condition performed an excellent role of bond scission led to linkage-cleavage reaction. In consequence, smaller molecular compounds were promoted. A dilemma about high pressure on gas production and degraded compound should be carefully determined based on desired outcomes.

Although it was difficult to collect the solid yield from these experiments because most of them adhered to inner wall of the fused quartz tube and the retrievable amount was not enough quantity for further analysis in some tests. However, the liquid yield remaining in the reactor was analyzed for study the remaining organic and inorganic substance.

6.2.3 Liquid product from SCWG

In addition to gaseous (Fig. 6.1) and solid yields, the remaining in quartz reactor was liquid part which could be used to identify the extent of reaction. Organic compound in liquid indicated incomplete gasification. Rönnlund et al. (2011) carried out SCWG of black liquor at 250 bar, 773-923 K for five minutes and reported that organic compounds in liquid yield was higher molecular products from the interaction between the occurred intermediate substances. Once the reaction occurred, they found the sudden polymerization of phenolic compounds. By comparing the results from this study at 500°C, 250 and 400 bar with their works, it was found that longer time of 10 minutes affected the polymerization reaction. At the same temperature, reacting KBL and SBL at 250 and 400 bar generated the higher molecular weight polymers such as tributyl acetylcitrate than the end products of five-minute reaction time of Rönnlund. Moreover, they reported the effect of rising temperature that could cause replacing of the lower molecular weight compounds with the larger one, i.e. phenolics to phenanthrenes. Anyway, when pressure was increased in this study, there are no significant changes in molecular weight of varieties of organic compound products. Therefore, pressure has minimal effect on both gas yields and liquid yields while temperature has more profound influence on both quality and quantity of products when compared with Rönnlund.

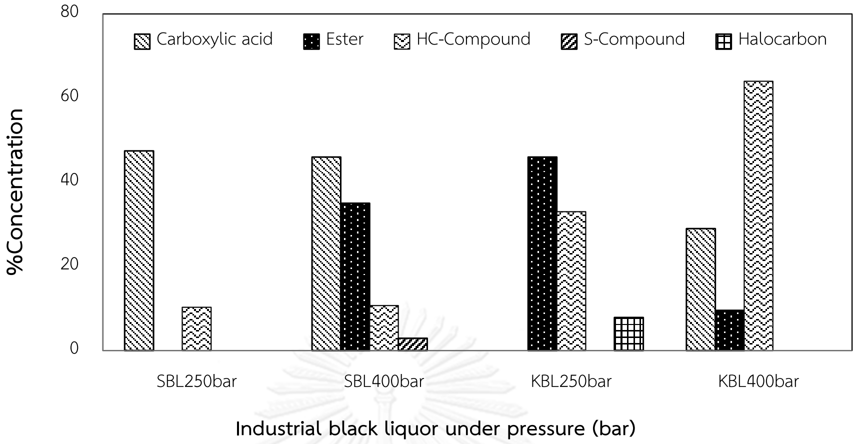

Figure 6.2 Organic compounds remained in the liquid yields from SCWG of industrial black liquors at 250 and 400 bar, 500°C for 10 min

Fig. 6.2 showed that HC-compounds, carboxylic acid and ester were dominant products appeared at all conditions. Aromatic compounds were affected by H and OH radicals generated via SCW ionization which caused instability of aromatic ring. These phenomena resulted in the ring cleavage reaction and led to generation of non-aromatic compounds (Cantero et al., 2015). Moreover, sodium ions from hydrolysis reaction under SCW condition of alkaline salt and proton from ionization of water behaved like scissors for the bond-cleavage of organic compound (Zhang et al., 2010). Therefore, the macromolecule of phenylpropane was separated into monomers via the special properties of water as medium and reactant at the SCW state. In consequence, HC-compound was generally produced as 40-60% for KBL and 10% for SBL. Remarkably, sodium content of SBL was higher than KBL (Table 4.2), but potassium of KBL was twice higher than SBL. A large difference (4-6 times) in HC-compound for KBL comparing to SBL might due to the potassium content (Table 4.2). Because of alkali properties, potassium is one element in heterogeneous catalytic reaction (Peng et al., 2014). While some trace element such as chlorine was found in form of halocarbon at 250 bar for KBL which was the highest chlorine content sample.

Alkali in black liquor played an important role on the homogeneous catalytic especially at the hydrolysis state. The intermediates generated were the raw material in the next reaction for syngas production by free-radical reaction. Although the low temperature study is required for any reactions to produce the energy or chemical via thermal conversion, the complete reaction at that condition is impossible (Pavlovič et al., 2013). Therefore, the metal catalysts have been utilized for upgrading the chemical or fuel production.

6.2.4 Catalytic SCWG by heterogeneous catalysts

The lowest temperature for this research was 400°C, and for comparison of results with the non-catalytic reaction, the conditions of catalytic SCWG were 400°C, 250 bar, 10 min reaction time. In Fig. 6.3, gas production is reported in the unit of mol per kg feedstock. The catalyst used was varied both of metal type and the ratio of feedstock to catalyst which were 1-1 and 1-10. The main gaseous products composed of H_2 and CH_4.

For the dominant gaseous products, the overall catalysts promote the formation of H_2. CH_4 yields of KBL increased compared to the base case. In contrast, CH_4 formation of LMC was all decreased in comparison to the base case. CO formation was not detected in SBL. The highest CO yield was 0.02 mmol/kg of 1-1 ZrO_2 of KBL, the remaining was varied around 0-0.01 mmol/kg.

Absence of CO detection in SBL trials suggested the effective of WGS reaction which was the main reaction that utilized CO for H_2 formation. The heterogeneous catalytic reaction of the metal base catalyst can enhance the reaction at that condition. The higher CH_4 formation in KBL indicated the better ability to cleavage some compounds like the aromatic rings than non-catalyst. Therefore, more initial gas products were generated and further consumed by the methanation reaction. In general, the methanation reaction refers to CH_4 formation from H_2 and CO or CO_2 but under the excess water the equilibrium position may reverse.

Referring to the Le Chatelier' principle, the excess water acts as the fixed concentration which is always sufficient for reacting with CH_4 and subsequently produce H_2 and CO. Rich in H_2 yield under SCWG proves the dominant of WGS reaction. Relate to the excess water condition, the initial substance of the WGS is infinite H_2O and CO which the latter is mainly generated from the methanation reaction. Therefore, greater H_2 formation in the catalytic condition may be suggested the availability of CO for WGS reaction which was generated from the effective methanation reaction. Therefore, catalyst can actively promote the CH_4 for the methanation and, inconsequence, the CO formation was increased to promote WGS reaction.

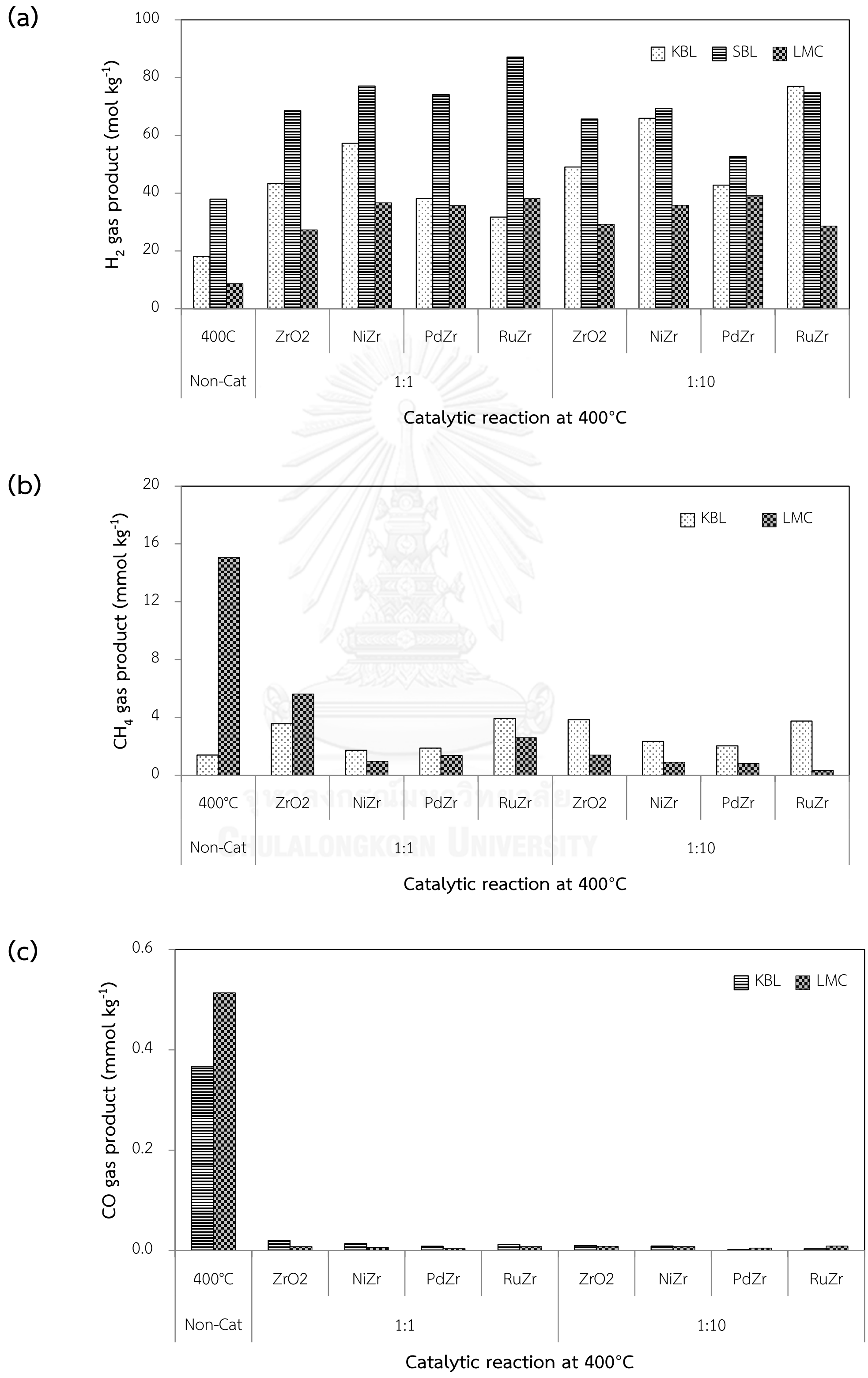

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Figure 6.3 Gas distributions of industrial black liquors and LMC under catalytic SCWG condition (a) H_2 yield and (b) CH_4 yield

Fig. 6.3 displayed, ruthenium and nickel based metal showed the effective H_2 formation in the overall ratios of SBL but some ratios for KBL and LMC that were 1-10 and 1-1, respectively. Increasing in the catalyst ratio, H_2 formation of KBL was also increased. On the contrary, H_2 yield from SBL was decreased. For LMC, the various in both of catalyst type and ratio slightly affected the H_2 formation. Noticeable H_2 production of KBL and LMC under non-catalytic condition, it seemed to be a function of temperature. With increasing temperature (from 400°C), H_2 formation from KBL and LMC were greatly increased but LMC was higher than KBL. At that condition, the reason may due to the greater carbon and hydrogen content of LMC. Moreover, the temperature might high enough for breaking some linkages in LMC structure. Under the catalytic condition, temperature was limited at 400°C, the additional H_2 generation might be the effect of catalyst. However, gas production of LMC was not significantly altered under the various catalysts. In contrast, the fluctuation in H_2 formation via catalyst was obvious in KBL. The possible explanation was the limitation of LMC structure. In the chapter 5, there were minute amount of guaiacyl and aromatic compound comparing to the aliphatic HCs compound. However, those components, especially the methoxy group and the aromatic compounds might be cleavage under the catalytic condition. As a consequence, the CH_4 formation of LMC was promoted because of their methoxy group and aromatic HCs. Although KBL composed of the methoxy group and aromatic compound like LMC, the structure of KBL composed of more varied chemical functional groups than LMC thus the consequential gas production of KLB was higher.

Despite the increasing ability in H_2 formation, the Ru base catalyst is relatively expensive compared to nickel. Table 6.1 displayed, 1-1 Ni/ZrO_2 yielded the second highest H_2 as 77.11 mol/kg feedstock which was 2.0 times higher than non-catalytic 400°C and 1.3 times higher than the maximum H_2 yield under non-catalytic reaction at 600°C. The results suggested the highest effective of Ru catalyst but the cost of Ni was cheaper and H_2 yield was almost equaled the Ru catalyst. Therefore, nickel might be better suit for large scale hydrogen production.

Table 6.1 Highest H2 production from non- and catalytic reactions

Condition		H_2 (mol/kg feedstock	Higher than (times)	
			Noncat 400°C	max. of Noncat
Non catalytic	400°C	11.0	KBL	
	Max. at 500°C	38.0		
Catalytic	**1-10 Ru/ZrO_2**	**77.0**	**7.0**	**2.2**
	1-10 Ni/ZrO_2	65.9	6.0	1.7
	1-1 Ni/ZrO_2	57.3	5.2	*1.5*
Non catalytic	400°C	38.0	SBL	
	Max. at 600°C	57.5		
Catalytic	**1-1 Ru/ZrO_2**	**87.1**	**2.3**	**1.5**
	1-1 Ni/ZrO_2	77.1	2.0	*1.3*
Non catalytic	400°C	8.7	LMC	
	Max. at 600°C	45.3		
Catalytic	**1-10 Pd/ZrO_2**	**39.2**	**4.5**	**0.9**
	1-1 Ni/ZrO_2	36.6	4.2	*0.8*

The different between H_2 production of the novel catalyst and Ni catalyst was considered for the most suitable large scale application. Moreover, the effective of the advantage of the catalytic case and higher energy (temperature) under the non-catalytic condition was compared. The result showed that adding the catalyst at lower temperature can better enhance H_2 yield than the higher temperature without catalyst as 1.5, 1.3, and 0.8 times for KBL, SBL, and LMC, respectively. The obtained results signify the important of the understanding about the chemical structure of the organic content in feedstock. Because the specific characters of feedstock should be processed by the suitable thermal conversion method for obtaining the favorable end products. Industrial black liquors contain the alkali catalyst with water and the organic lignin. The SCWG method can apply for conversion the organic material to H_2-rich syngas. Not only the waste steam from the pulp mill industry, any production based on the organic composition as the raw material can generate the organic waste in water and subsequently become wastewater. This waste steam could effectively be used as the feedstock for syngas production by SCWG reaction.

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6.3 Conclusion

Due to the excellent solvent property of supercritical water condition, H_2 gas production could be obtained from black liquors via their high water content using this process. The most appropriate condition for H_2-rich syngas was 600°C at 250 bar, in fact the higher temperature led to greater syngas production. The effect of temperature was obvious and dominant for this reaction. Regarding the organic structure, cellulose and hemicellulose contents in SBL enhanced the reaction because of the abundance of hydroxyl group, resulted in the greatest H_2 gas formation. Thus, the different properties of organic composition in black liquor caused by the pulping process effect gas production. Relate to alkali catalytic of spent chemical in black liquor, it is difficult to determine that the lower H_2 formation of KBL was affected by the smaller Na_2CO_3 compound or due to the chemical structure. The metal catalyst exhibited the potential to catalyze the aromatic structure of KBL, particularly for ruthenium and nickel. This result showed that the excess water in black liquor could be applied for the practical agent to oxidize lignin for syngas production. The major gas production was H_2 and CO_2 from the water-gas shift reaction, while the minute amount of CH_4 and CO formation was detected. Therefore, SCWG reaction could be the alternative treatment solution for high water content biomass which would be another source for biofuel.

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CHAPTER 7

CONCLUSIONS AND RECOMMENDATIONS

7.1 Conclusions

The industrial black liquors in this research were obtained from the same wood, eucalyptus wood, but pulping processes were different. The chemical in pulping directly affected the inorganic portion in black liquor which was the alkali compound. Relate to the chemical in pulping, kraft process utilized NaOH and Na_2S and then the spent chemical was mainly generated as Na_2CO_3 and Na_2SO_4 presented in XRD results. Soda process used only NaOH thus Na_2CO_3 was the primary spent chemical compound displayed in the XRD results. The different pulping chemical had an influence on lignin separated from wood. This organic portion in black liquor showed the carbon content as 33% for both KBL and SBL. Oxygen content in SBL was slightly higher than KBL, but sulfur content of KBL was 20.5 times higher than SBL due to the chemical in pulping process. Lignin in black liquor was isolate by acid precipitation for further study in chemical structure. TGA revealed the thermal behavior of KL and SL which were similar to lignin and cellulose model compounds, respectively. This finding suggested the primary component in the technical lignins. However, the minor degradation peak of cellulose presented in KL while minor lignin was presented in SL. These results indicated that thermal behavior of KL was controlled by lignin while cellulose residue had an influence on SL thermal degradation. Regarding to the mixture of lignin and cellulose, FTIR results can confirm the cellulose residue on KL and SL. About the chemical structure of the industrial black liquors and technical lignins, the OH group was in the majority which referred to alcohol and phenol. The methoxy group (OCH_3), the unique functional group which particularly detected in lignin exhibited in the technical lignins and LMC. Moreover, the unique patterns of signal in the fingerprint region suggested the different functional groups in lignin structure. The C–O bond in carbonyl and methoxy groups indicated the oxygen compounds in the structure, while C–C and C–H bond presented the aliphatic HCs compounds. However, the structure of KL mainly composed of lignin so the aromatic ring and methoxy group may be the primary. Regarding to thermal degradation, these functional groups were the important role in the reactions.

For investigating the effects of varied lignin chemical properties on thermal conversion products, Py-GC/MS technique was used to decompose the technical lignin at 400°C-600°C. The KL was the phenolic structure, so the products mostly composted of hydroxyl phenols. Cellulose and hemicellulose remaining in SL affected the various products led to larger oxygenated hydrocarbons production. Note that guaiacyl and syringyl were minor content in SL which may due to high degradation since enough oxygen concentration. LMC was highly stable in thermal conversion which may be due to the specific structure caused by the manufacturing process. Although the structure characterizations seemed to be similar, but thermal behavior were differed. These results suggested the selectivity of thermal degradation may depend on the linkages or bonding within their structure. The weakest and simplest bond was ether bond which can be destroyed at lower temperature. Therefore, the lignin holding large portion of ether and ester bond tended to generate more phenolic compound. In contrast, C-C bond which was the remaining bond after cleavage of ether bond poses high thermal stability. Hence, not only higher energy from raising temperature, also the remaining of the strong bonding was the major reason to lower overall product generation. These findings supported the first hypothesis about the differences in product distribution due to dissimilar structure of the technical lignin from kraft and soda pulping process. The end-production of technical lignins was revealed according to their specific character under thermal conversion. KL might be appropriate for phenol production while SL is suitable for bio-oil production. Nickel based catalyst was the most effective for both of KL and SL in the quality upgrading via thermal conversion method.

Chemical composition in lignin structure was differed between the kraft and soda pulping processes. As a consequence, the degraded compounds from thermal conversion were difference. However, the technical lignins might be classified as phenolic compound for kraft lignin and oxygenated compound for soda kraft based on the majority of degraded products under thermal conversion. To study the gas production from those technical lignin in form of weak black liquor, 10% solid of kraft and soda black liquor (KBL and SBL) were gasified under supercritical water (SCW) condition at 400°C-600°C and 250-400 bar for 10 minute residence time. The results showed that syngas production increased with higher temperature. The most appropriate condition for H_2-rich syngas was 600°C at 250 bar. Different lignin structure strongly effects gas yield, i.e., SBL with oxygenated compound in the structure generated the maximum H_2 which H_2 yield from KBL with mostly phenolic structure was lower. The greatest gasification yield was produced by soda black liquor which not only because the structure of SBL, but due to the alkali salt in black liquor. The alkali catalytic reaction under SCW condition enhanced hydrolysis reaction in hydrothermal condition and in the organic carbon gasification by CO_2 with alkali carbonates (Na_2CO_3) (eq. 6-10). As the result of organic intermediates and syngas formation, the overall products were further acted as precursors for gasification reaction dominating by the WGS and methanation reactions. Therefore, the synergy between the Na_2CO_3 predominance and the oxygenated structure of SBL caused the greatest H_2 formation. However, it is difficult to determine that the lower H_2 formation of KBL was affected by the smaller Na_2CO_3 compound due to the issue of the chemical structure. Including the higher gas products of SBL over LMC despite of the highest C and H in LMC. Thus, further research for proving the hypothesis about the effect of the alkali catalytic on SCWG yields should be carried out on the technical lignin from the industrial black liquor instead of LMC. Positive influence of metal catalyst on H_2 generation during gasification reaction including WGS and methanation was obvious. The oxygen compounds in the organic structure of feedstock resulted in the different syngas products. Absent of CO and CH_4 yields in SBL indicated high oxygen concentration in the reaction due to its structure. Though the fluctuation in H_2 production among the various catalysts of KBL and SBL may point out the varieties of organic composition in lignin. The results suggest nickel catalyst as the most promising option with regard to efficient and cost-effective provision. The overall hydrogen conversion of every test was over 100% due to excess H_2O availability under SCW condition. Therefore, the gasification of weak black liquor under high temperature and pressure was appropriate for industrial black liquor due to the need for the evaporator unit with the current legacy process.

7.2 Recommendations

7.2.1 Recommendations from this work

1) To investigate the effect of alkali salt in BL on lignin degradation under SCWG, one should extract the lignin from BL and use it as controlled.

2) Because the precipitation method affect the structure of the technical lignin (Zhu et al., 2014), further work should be carried out to investigate the suitable preparation methods and their effects on technical lignin structure.

3) Regarding large portion of phenolic compound in technical lignin from kraft process, the future researches on the production and upgrading the phenolic chemical from kraft black liquor are recommended.

7.2.2 Recommendation for the estimate amount of weak black liquor

Several points should be addressed on implementation of black liquor SCWG to the actual industrial scale beside the anticipated high capital cost. Since it is unlikely that this proposed SCWG would replace the conventional recovery boiler (RB) cycle but be installed in parallel, one major concern is about the amount of WBL that may be diverted to this process without effecting the overall operation. Here, one needs to consider the key factors in variety of black liquor properties which are wood species feedstock and the pulping methods (Hamaguchi et al., 2012, Bajpai, 2015). Hence, the estimated proportion of WBL that can be separated after digestion process and fed to SCWG may not equal among the manufacturers. Waste management policy or byproduct utilization of each plant would also play a major role on the implementation. Therefore, the possible scenario for this utilization may be categorized based on the RB operation and black liquor management which are 1) non-RB, 2) electricity or energy surplus from RB, and 3) debottleneck at RB. Calculations for estimating the availability of WBL for each case may be based on proportion of pulp production to WBL to black liquor solid (BLs) of about 1:10:1.5 (Tran and Vakkilainen, 2007). For the case of plant with no RB system, all WBL generated may be utilized which is estimated by multiply the pulp production by 10. In second scenario, estimation may be carried out by reversing the electricity and energy surplus into available WBL. After obtaining the electricity production per unit (ton) of BLs, available WBL can be determined from the ratio of WBL to BLs. Note that pulping chemical (white liquor) recovery utilizes alkali in black liquor as raw materials. Total titratable alkali (TTA) in black liquor is an important factor to control the causticizing process. Once the amount of black liquor is reduced, the TTA may be of poor balance. Therefore, the addition of stabilization tank could help adjusting TTA before feeding to lime slaker and further reaction for white liquor generation (Sanchez, D.R., 2007). For the debottlenecking at RB option, many researches focused on lignin removal from black liquor in order to decrease heat load in RB and increase throughput (Axelsson et al., 2006, Olsson et al., 2006, Vakkilainen and Välimäki, 2009, Ghezzaz et al., 2012, Pettersson et al., 2012). Similarly, in this case, WBL withdrawal to SCWG could help increase the pulp production capacity. Here, the estimated amount of WBL for further SCWG reaction could be based on the ratio of pulp production to WBL of 1:10. Assuming pulp production of X tons, the surplus WBL would equal to 9X which may be available to SCWG without effecting existing RB cycle. In addition, TTA in molten smelt is of no concern because the amount of WBL in the process is stable.

7.2.3 Recommendation for CO_2 utilization

Not only H_2 rich gas which is the major production from SCWG process (Fig 7.1), but CO_2 is also abundance and must be eliminated from the process (Fig 7.2). In fact, CO_2 must be captured and either stored or converted into global warming neutral impact compounds (Hu et al., 2013). There are many research teams who dedicate to investigate the solution of CO_2 utilization.

Figure 7.1 Water gas shift reaction

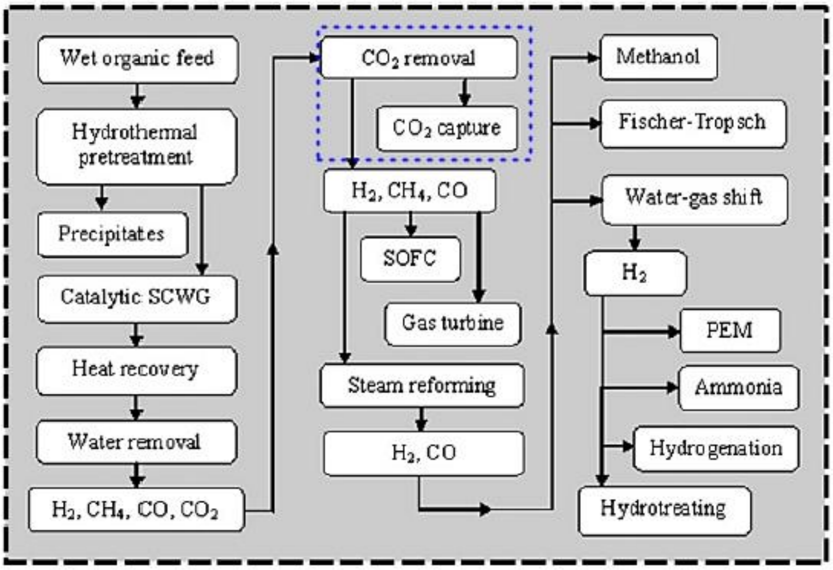

Figure 7.2 Process flow diagram of SCWG and its subsequent applications (Azadi and Farnood, 2011).

General classification in CO_2 utilization is of two categories, direct use of CO_2 and conversion of CO_2 to chemicals (Huanh and Tan, 2014). Table 7.1 exhibits the CO_2 utilization from many publications.

Table 7.1 CO_2 utilization

Authors	CO_2 utilization
Whipple and Kenis (2010)	The heterogeneous electrochemical conversion of carbon dioxide to produce a variety of organic compounds such as formic acid, carbon monoxide, methane, and ethylene. These products are feedstock for chemical synthesis or hydrocarbon fuel production.
Jiang et al. (2010)	Recycling of CO_2 to energy fuels by photosynthesis using sunlight as the primary energy source.
Hu et al. (2013)	- Conversion CO_2 to CO by plasma, electrocatalysis, and reduction of CO_2 - Conversion CO_2 to formic acid (HCOOH) and formaldehyde (HCHO) - Conversion CO_2 to methanol (CH_3OH) - Conversion CO_2 to long chain hydrocarbons and oxygenates. - CO_2 as building blocks for oxygen-rich compounds and polymers
Huanh and Tan (2014)	- Chemical production such as urea and cyclic carbonates. - Energy production such as DMC and DME - As a carbon source for H_2 production via biomass decomposition or water splitting by thermolysis, solar energy and biological process.
Ravanchi and Sahebdelfar (2014)	- fixation as valuable petrochemical commodities or fuels such as salicylic acid, urea, inorganic carbonates, and methanol (as feed additive) - Conversion of CO_2 by catalyst for formic acid, methane, and CO - Potential source for H_2 production - Potential process for convert to CO, oxidative dehydrogenation of hydrocarbon, hydrogenation, and polymerization.
Alper and Orhan	Conventional heterogeneous catalysis

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(2017)	- CO$_2$ reforming of methane - Hydrogenation of CO$_2$ to methanol - Dimethyl carbonate from CO$_2$ and methanol - Cyclic carbonate from CO$_2$ and epoxide Electro- and photochemical conversion of CO$_2$ - Electrochemical activation of carbon dioxide - Photocatalytic activation of carbon dioxide Polymer and fine chemical production Inorganic production Utilization in petrochemical plants - Acrylic acid - Ethylene - Mono-ethylene glycol - Monomers of polyurethanes (polyols and isocyanate)

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APPENDIX A

จุฬาลงกรณ์มหาวิทยาลัย
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MATERIALS AND EQUIPMENT

Chemical/Material	Manufacturer
Sulfuric acid	Merck
Acetone	RCI Lacscan
Lignin low sulfonate content	Sigma-Aldrich (CAS no. 8068-05-1)
Cellulose micro crystalline	Sigma-Aldrich, cas no. 9004-34-6
Nickel (II) nitrate hexahydrate	Sigma-Aldrich
Palladium (II) nitrate hydrate	Sigma-Aldrich
Ruthenium (III) chloride hydrate	Sigma-Aldrich
Zirconium (IV) oxide	Alfa - Aesar
Oxygen 99.8%	Bangkok industrial gas (BIG)
Acetylene 99.6%	Bangkok industrial gas (BIG)
Nitrogen 99.99%	Bangkok industrial gas (BIG)
Helium99.999%	Bangkok industrial gas (BIG)
Argon 99.99%	Bangkok industrial gas (BIG)
Hydrogen 99.99%	Bangkok industrial gas (BIG)

Equipment	Manufacturer
pH meter	DELTA 320 pH meter, METTLER TOLEDO
Centrifugation equipment	Hettich Universal 320
Heating oven	Memmert GmbH
Multifunctional pyrolyzer	PY-2020iD, Frontier Lab
Gas Chromatograph – Mass Selective	QP2010, Shimadzu
Fused quartz tube	Technical Glass Products, Inc. USA.
Tube (cylinder) furnace	CRFC Series, OMEGA Engineering, USA
Gas Chromatograph	SRI 8610C
Thermocouple type-K	OMEGA Engineering
Temperature controller	MAC3A, SHIMAX
Hot plate and stirrer	HP 220 Hot Plate/Stirrer

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The property and typical values of fused quartz form manufacturer

Property	Typical value	Unit
Density	2.2 x 10^{3}	kg/m^{3}
Hardness	5.5–6.5	Mohs' Scale
Design Tensile Strength	4.8 x 10^{7}	Pa (N/m^{2}) (7,000 psi)
Design Compressive Strength	>1.1 x 10^{9}	Pa (160,000 psi)
Bulk Modulus	3.7 x 10^{10}	Pa (5.3 x 106 psi)
Rigidity Modulus	3.1 x 10^{10}	Pa (4.5 x 106psi)
Young's Modulus	7.2 x 10^{10}	Pa (10.5 x 106 psi)
Poisson's Ratio	0.17	-
Coefficient of Thermal Expansion	5.5 x 10^{-7}	cm/cm °C
Thermal Conductivity (20°C)	670	J/kg °C
Softening Point	1683	°C
Annealing Point	1215°C	
Strain Point	1120°C	
Electrical Resistivity (350°C)	7 x 10^{7}	ohm cm
Dielectric Properties (20°C, 1 MHz)		
Constant	3.75	
Strength	5 x 10^{7}	
Loss Factor	>4 x 10^{-4}	
Dissipation Factor	>1 x 10^{-4}	
Index of Refraction	1.4585	
Constringence (Nu value)	67.56	
Velocity of Sound-Shear Wave	3.75 x 10^{3}	
Velocity of Sound/Compressional	5.90 x 10^{3} m/s	
Sonic Attentuation	<11	dB/m MHz
Permeability Constants (700°C) (cm^{3} mm/cm^{2} sec cm Hg)		
Helium	210 x 10^{-10}	
Hydrogen	21 x 10^{-10}	
Deutrium	17 x 10^{-10}	
Neon	9.5 x 10^{-10}	

(https://www.technicalglass.com/technical_properties.html)

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APPENDIX B

จุฬาลงกรณ์มหาวิทยาลัย
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NMR RESULT

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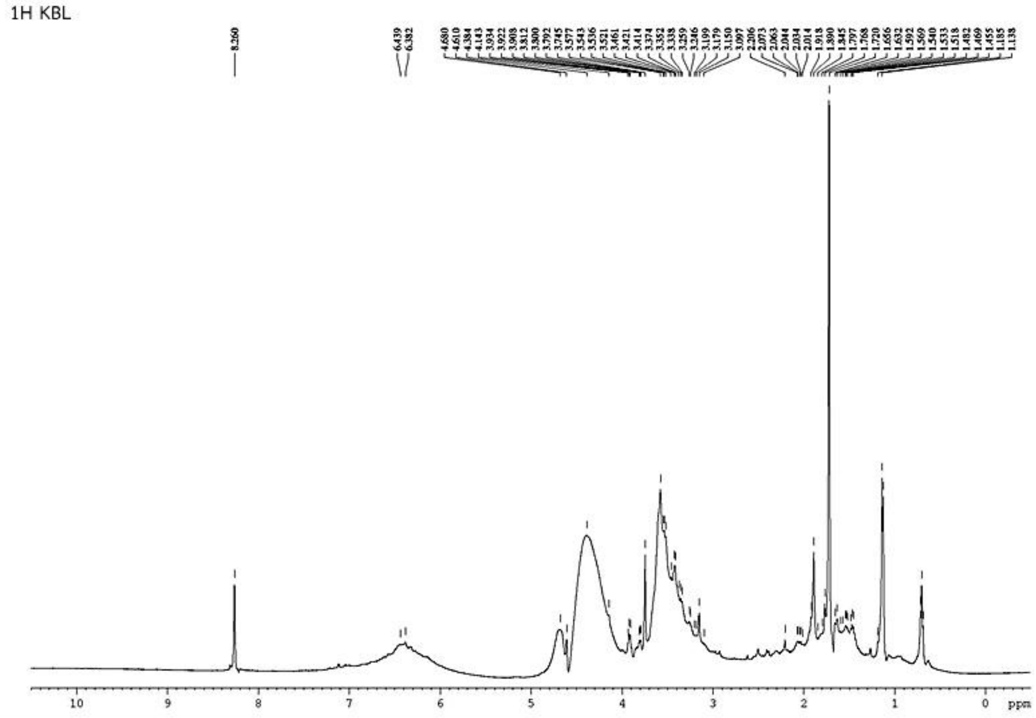

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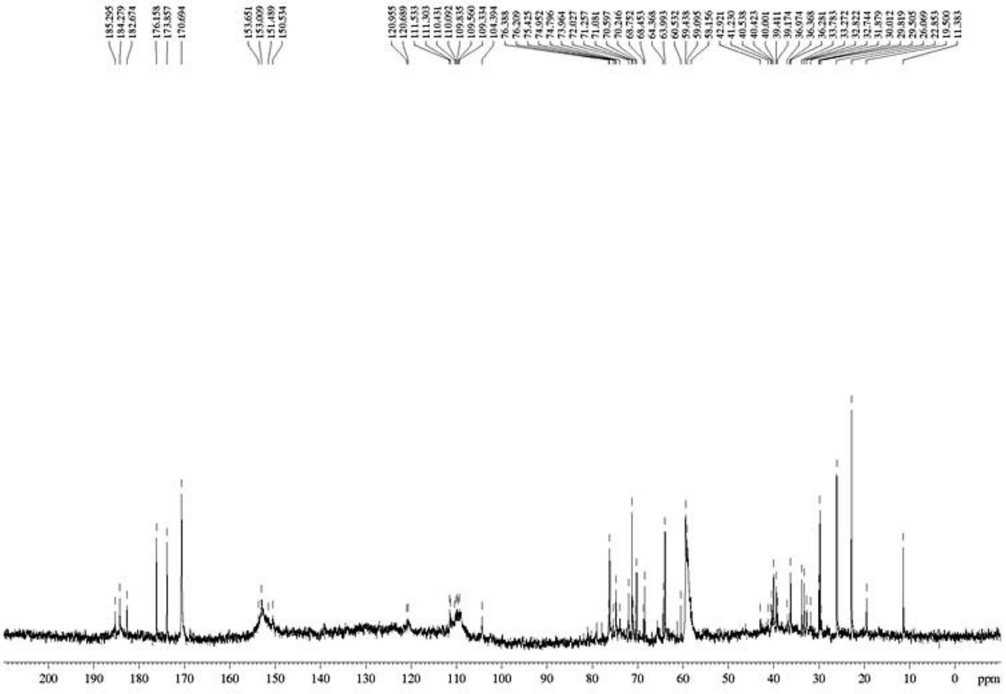
13C KBL



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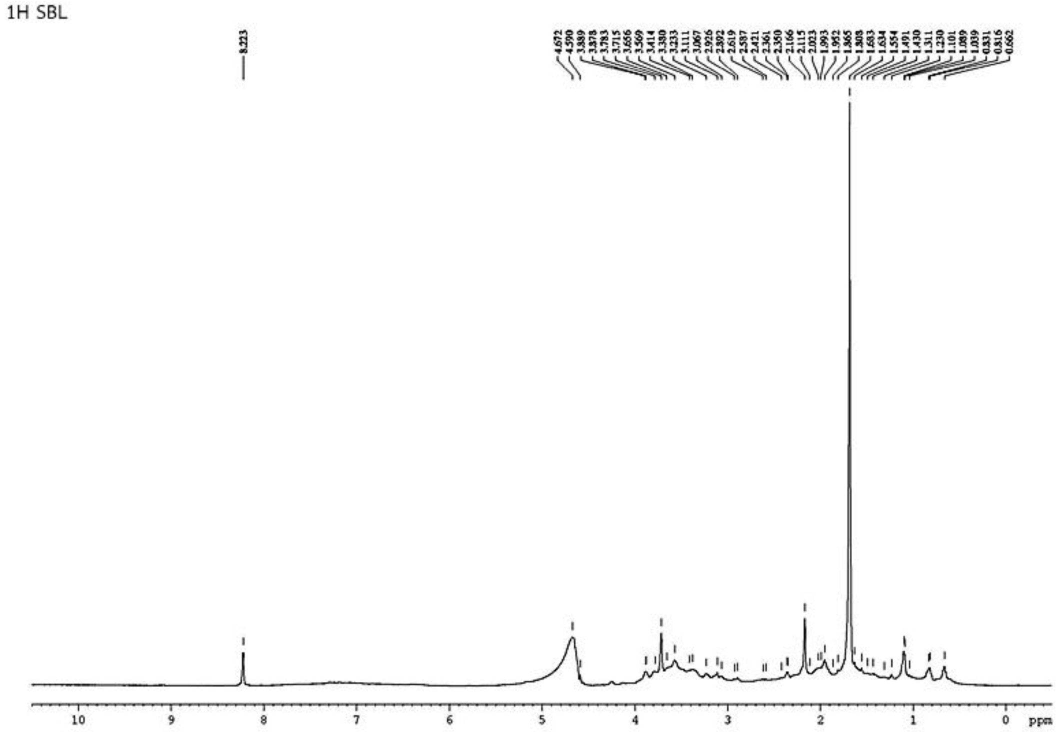

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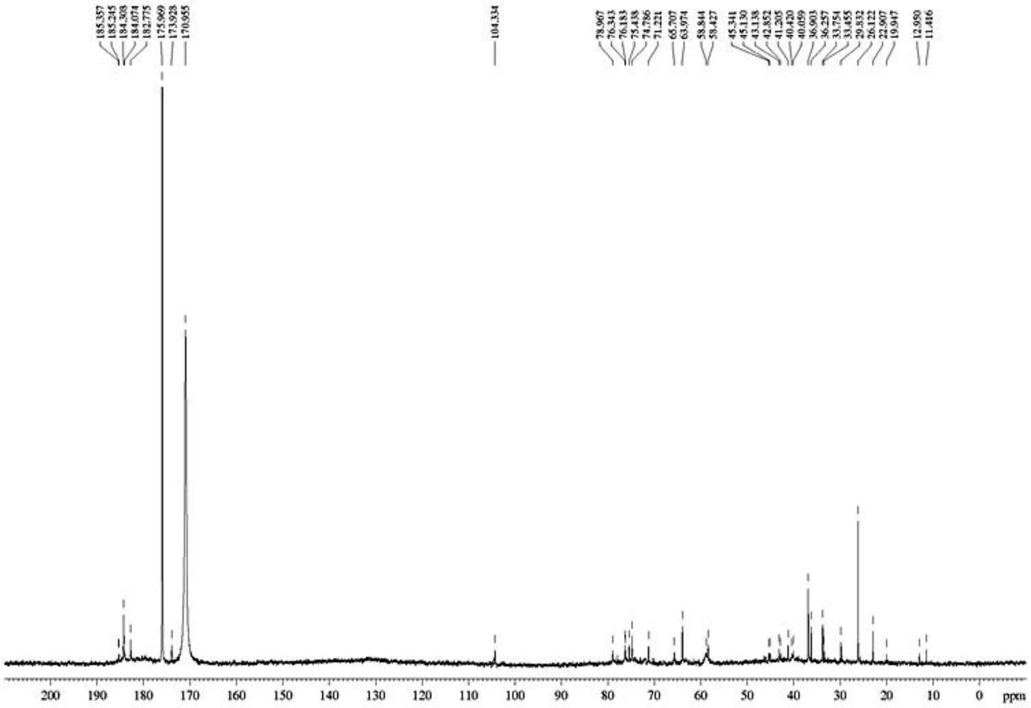

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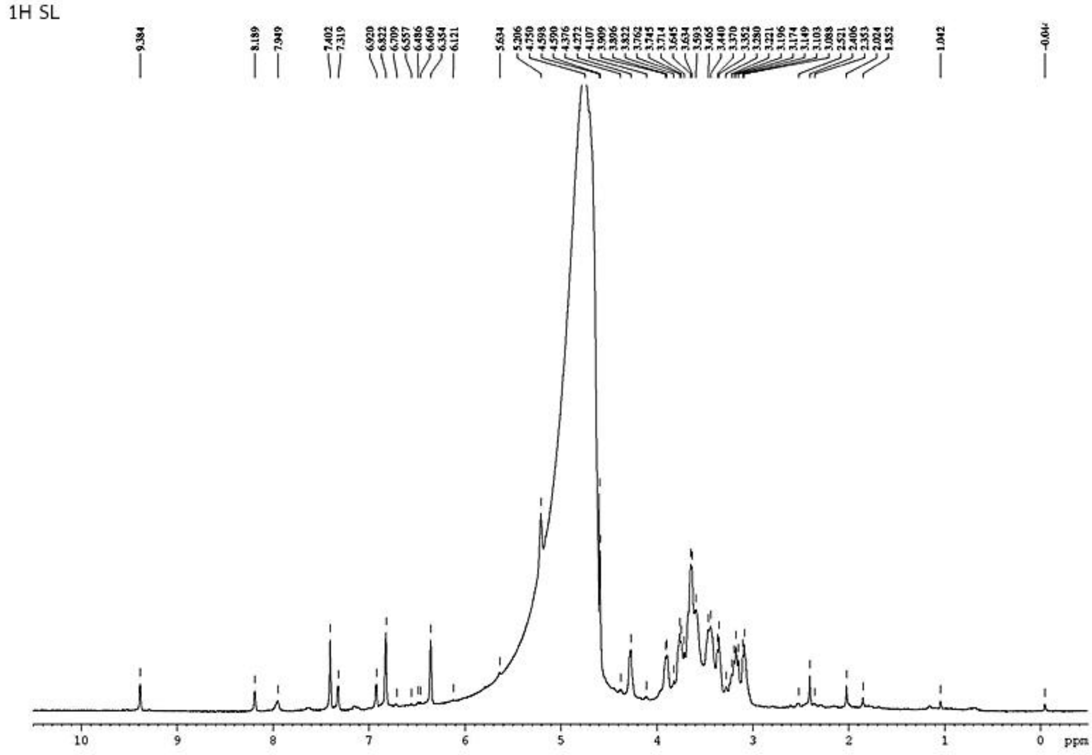

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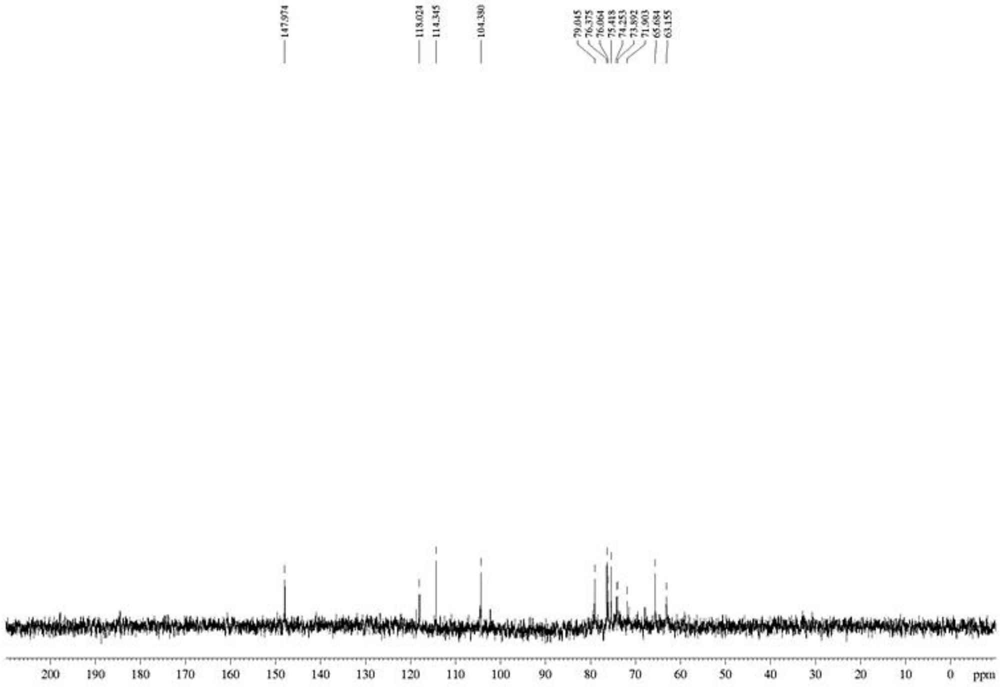
13C SL



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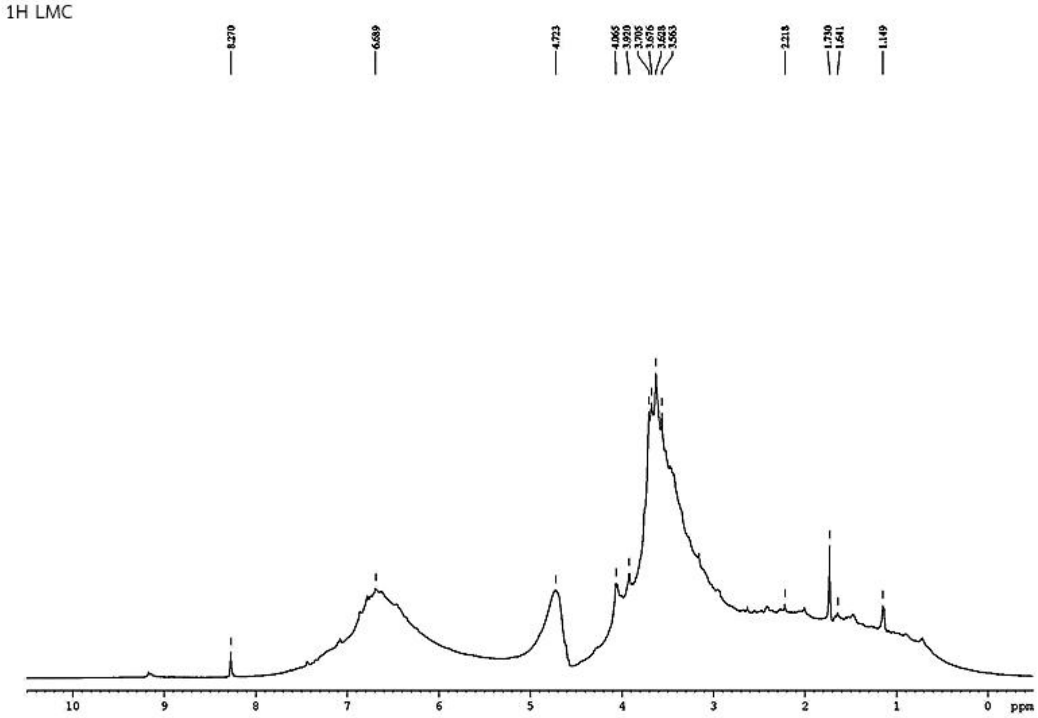

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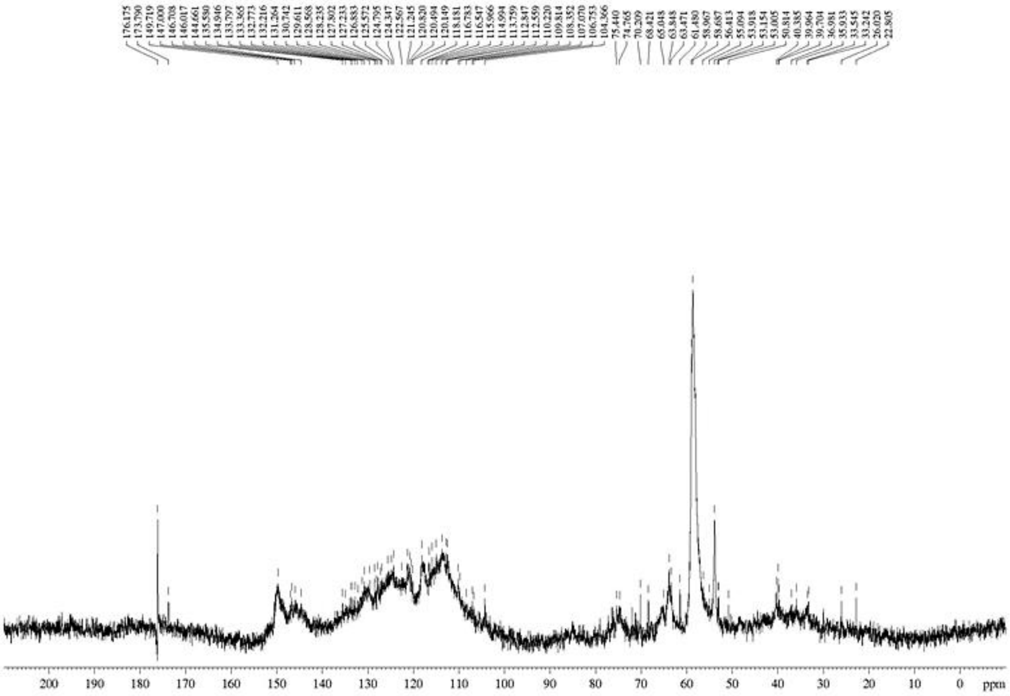
13C LMC



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APPENDIX C

จุฬาลงกรณ์มหาวิทยาลัย
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TGA RESULT

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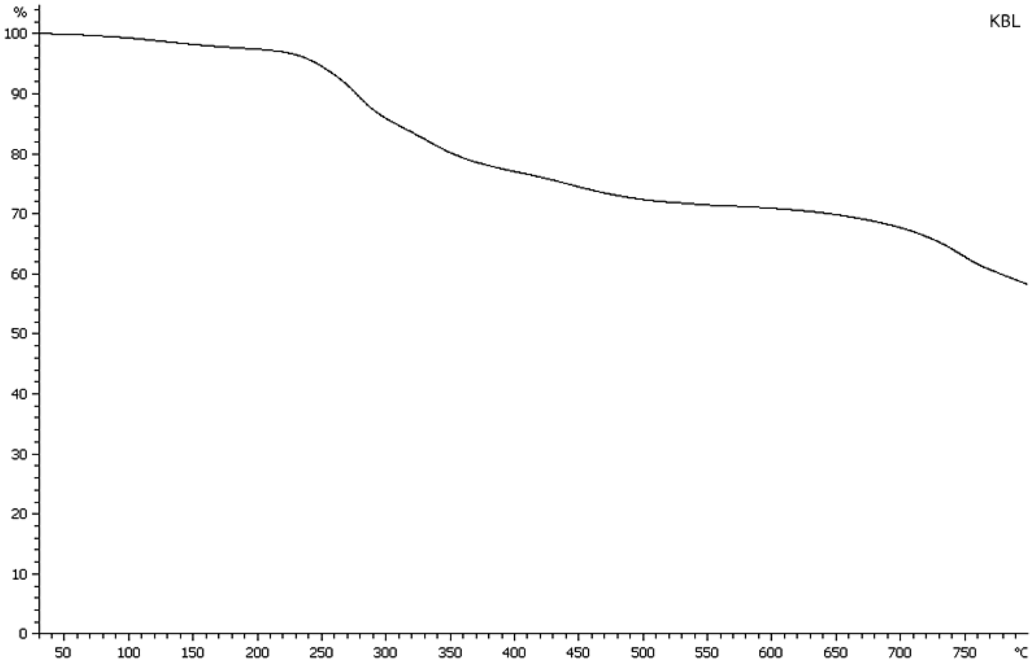

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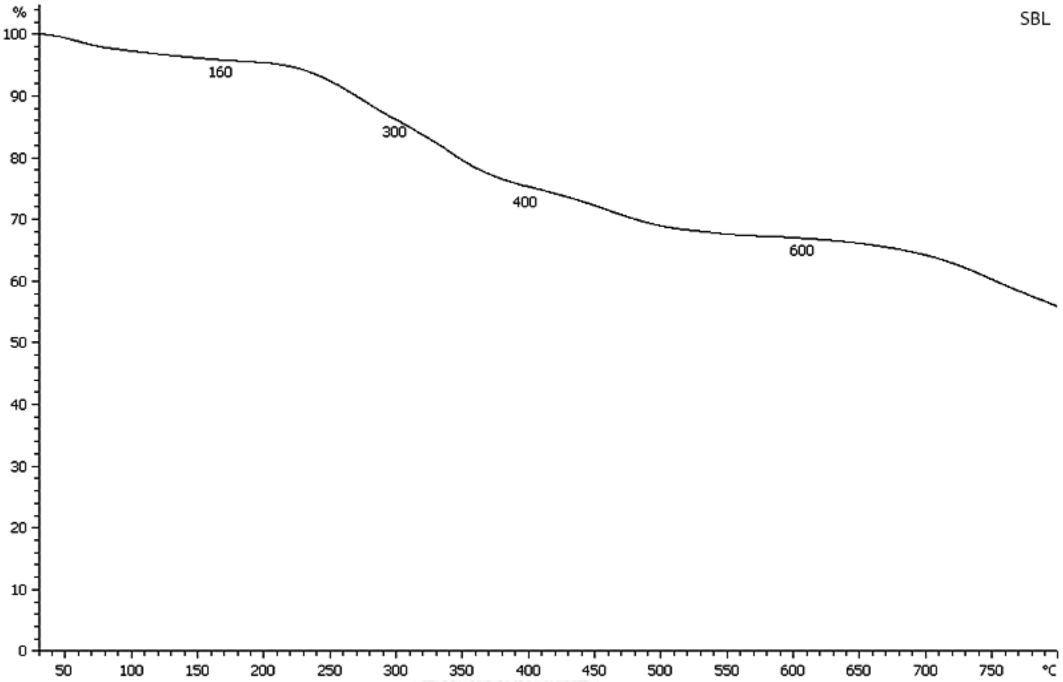

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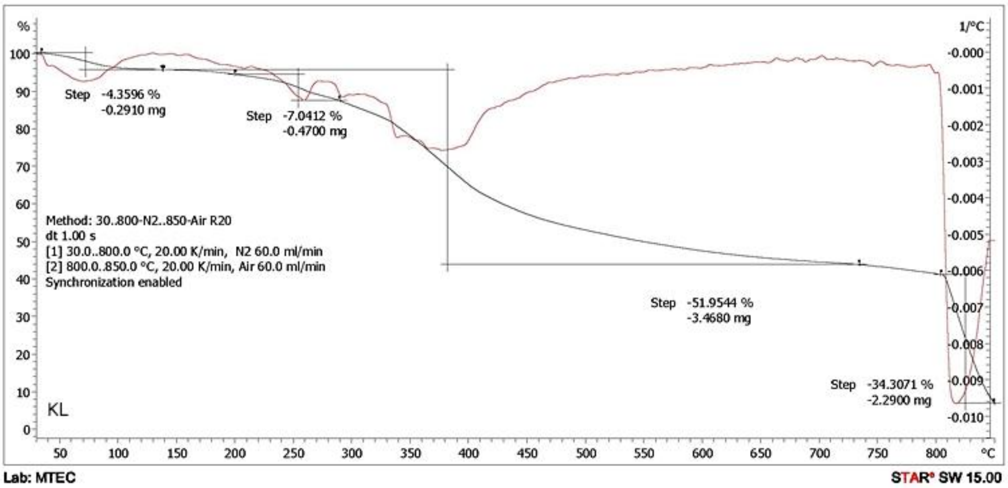

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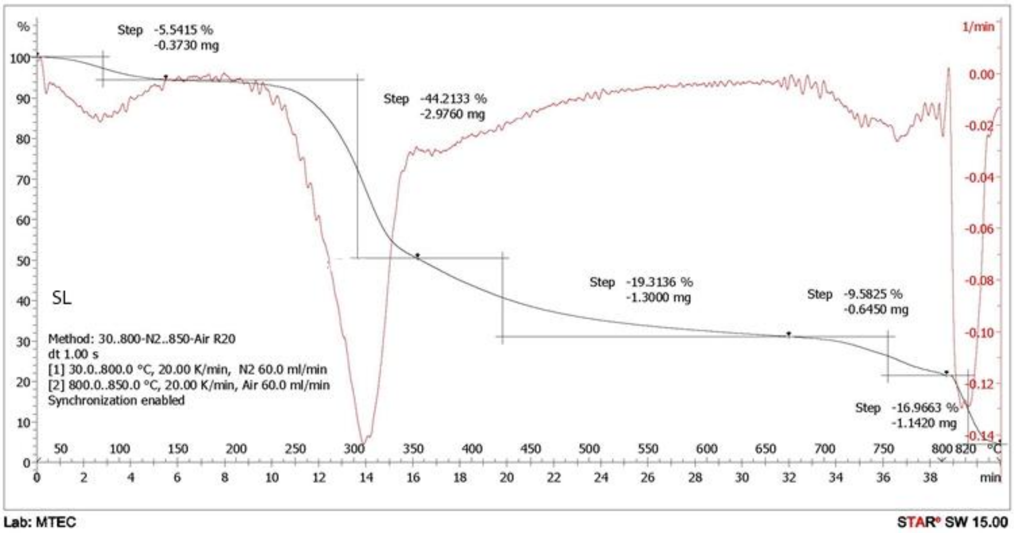

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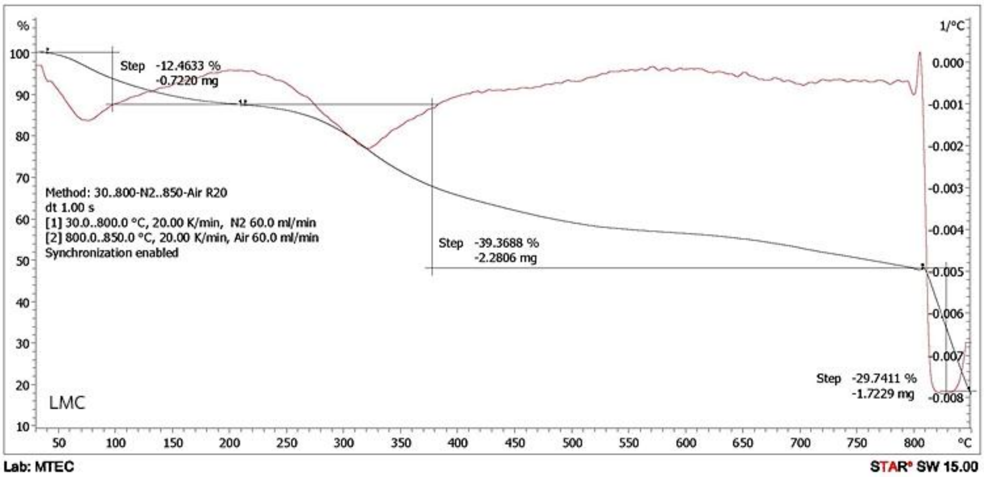

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APPENDIX D

จุฬาลงกรณ์มหาวิทยาลัย
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PYROPROBE GC/MS LIBRARY

Abbreviation of pyrolysis compound in the library.

i) Chemical species		ii) Bond type	
G	Guaiacyl	Met	Methoxyl
S	Syringyl	Hydx	Hydroxyl
H	p-hydroxyphenyl	Cbn	Carbonyl
C	Catechol	Car	Carboxyl
B	Aromatic HCs	HC	HCs bond
A	Aliphatic HCs	O	Others
F	Furan		
Oxy	Oxygenated HCs		
Acd	Acid		
ST	Sterols		
O	Other		

iii) Chemical degraded compounds		iv) Chemical structure	
PhOH	Phenolic hydroxyl group	A	Aliphatic HCs (AHCs)
HCs	Hydrocarbons	Ar	Aromatic HCs (ArHCs)
Eth	Ether	Ph	Phenol
Alc	Alcohol	Oxy	Oxygenates
Ket	Ketone	N	N-Compound
Aldh	Aldehyde	O	Others
Es	Ester		
Cabox	Carboxylic acid		
Fu	Furan		
Su	Sugar		
N	N-Compound		
O	Others		

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Formula	Compound	i	ii	iii	iv
		Chemical	Bond	Chemical	Chemical
$C_2H_4S_5$	Lenthionine	O	O	O	O
C_2H_6O	Ethanol	Oxy	Hydx	Alc	Oxy
$C_2H_6S_2$	Dimethyl disulfide	O	O	O	O
C_3H_4O	Acrolein	Oxy	Cbn	Aldh	Oxy
$C_3H_4O_2$	Acroleic acid	Acd	Car	Cabox	Oxy
$C_3H_4O_3$	Pyruvic acid	Acd	Car	Cabox	Oxy
$C_3H_6O_2$	Propionic acid	Acd	Car	Cabox	Oxy
$C_3H_6O_3$	Lactic acid	Acd	Car	Cabox	Oxy
$C_3H_8O_3$	Glycerol	Oxy	Hydx	Alc	Oxy
C_4H_4O	Furan	F	HC	Fu	Oxy
$C_4H_4O_2$	Furanone	F	Cbn	Ket	Oxy
$C_4H_6O_2$	2(3H)-Furanone, dihydro-	F	Cbn	Ket	Oxy
$C_4H_6O_3$	Methyl pyruvate	Oxy	Cbn	Es	Oxy
C_4H_8O	Tetrahydrofuran	F	HC	Fu	Oxy
$C_4H_8O_2$	Acetoin	Oxy	Hydx	Ket	Oxy
$C_4H_8O_3$	Methyl methoxyacetate	Oxy	Met	Es	Oxy
$C_5H_4N_4O$	Hypoxanthine	O	Hydx	Alc	N
$C_5H_4O_2$	Furfural	F	Cbn	Aldh	Oxy
C_5H_6O	2-Methylfuran	F	HC	Fu	Oxy
$C_5H_6O_2$	Furfuranol	F	Hydx	Alc	Oxy
C_5H_8O	Cyclopentanone	Oxy	Cbn	Ket	Oxy
$C_5H_8O_2$	Methyl methacrylate	F	Cbn	Ket	Oxy
$C_5H_8O_3$	Levulinic acid	Acd	Car	Cabox	Oxy
$C_5H_{10}O$	3-Methylbutanal	Oxy	Cbn	Aldh	Oxy
$C_5H_{10}O_2$	Tetrahydrofurfuryl alcohol	F	Hydx	Alc	Oxy
$C_5H_{10}O_4$	Deoxyribose	Oxy	Hydx	Su	Oxy
$C_5H_{10}O_5$	Ribose	Oxy	Hydx	Su	Oxy
$C_5H_{12}O$	Pentanol	Oxy	Hydx	Alc	Oxy
C_6H_6	Benzene	B	HC	HCs	Ar
C_6H_6O	Phenol	H	Hydx	PhOH	Ph
$C_6H_6O_2$	Pyrocatechol	C	Hydx	PhOH	Ph
$C_6H_6O_4$	3(2H)-Furanone, 2-acetyl-4-	F	Hydx	Fu	Oxy
$C_6H_6N_2O_3$	3-Hydroxy-6-methyl-2-	O	Hydx	N	N
C_6H_8O	2,5-Dimethylfuran	F	HC	Fu	Oxy
$C_6H_8O_3$	Furaneol	F	Hydx	Fu	Oxy
$C_6H_8O_4$	Dimethyl fumarate	Oxy	Met	Es	Oxy
$C_6H_{10}O$	Cyclohexanone	Oxy	Cbn	Ket	Oxy
$C_6H_{10}O_2$	Allyl propionate	Oxy	Cbn	Es	Oxy
$C_6H_{10}O_5$	Levoglucosan	Oxy	Hydx	Su	Oxy
$C_6H_{12}O_2$	Ethyl butanoate	Oxy	Cbn	Es	Oxy
$C_6H_{12}O_5$	2-Deoxy-D-glucose	Oxy	Hydx	Su	Oxy
$C_6H_{12}O_6$	Glucose	Oxy	Hydx	Su	Oxy
$C_6H_{14}O$	2-Hexanol	Oxy	Hydx	Alc	Oxy
$C_6H_{14}O_3$	Diethylene glycol dimethyl ether	Oxy	Met	Eth	Oxy

C_7H_8	Toluene	B	HC	HCs	Ar
C_7H_8O	Cresol	H	HC	PhOH	Ph
$C_7H_8O_2$	Guaiacol	G	Met	PhOH	Ph
$C_7H_8O_3$	3-Methoxycatechol	C	Met	PhOH	Ph
$C_7H_{12}O_2$	Ethyl 4-pentenoate	Oxy	Methx	Es	Oxy
$C_7H_{12}O_3$	Ethyl 3-acetylpropionate	Oxy	Cbn	Es	Oxy
C_7H_{14}	1-Heptene	A	HC	HCs	A
$C_7H_{14}O$	Heptanal	Oxy	Cbn	Aldh	Oxy
$C_7H_{15}NO_2$	L-Valine, ethyl ester	Oxy	HC	Es	N
$C_7H_{16}O$	Heptanol	Oxy	Hydx	Alc	Oxy
$C_8H_5NO_6$	m-Nitrophthalic acid	Acd	Car	Cabox	N
$C_8H_7NO_4$	methyl 4-nitrobenzoate	Oxy	Met	Es	N
C_8H_8	Styrene	B	HC	HCs	Ar
C_8H_8O	p-vinylphenol	C	HC	PhOH	Ph
$C_8H_8O_3$	Vanillin	G	Met	PhOH	Ph
$C_8H_8O_4$	p-Vanillic acid	G	Met	PhOH	Ph
C_8H_{10}	Xylene	B	HC	HCs	Ar
$C_8H_{10}O$	4-Ethylphenol	H	HC	PhOH	Ph
$C_8H_{10}O_2$	Creosol	G	Met	PhOH	Ph
$C_8H_{10}O_3$	Syringol	S	Met	PhOH	Ph
$C_8H_{12}O_2$	1-Oxetan-2-one, 4,4-diethyl-3-	Oxy	Cbn	Ket	Oxy
$C_8H_{15}NO_2$	Ethyl pipecolinate	Oxy	Cbn	Es	N
C_8H_{16}	1-Octene	A	HC	HCs	A
$C_8H_{16}O$	Octanal	Oxy	Cbn	Aldh	Oxy
$C_8H_{16}O_2$	Ethyl hexanoate	Oxy	HC	Es	Oxy
$C_8H_{16}O_4$	2-(2-Ethoxyethoxy)ethyl acetate	Oxy	HC	Es	Oxy
$C_8H_{18}O$	1-Octanol	Oxy	Hydx	Alc	Oxy
$C_8H_{19}N$	Octylamine	O	HC	N	N
C_9H_8O	Cinnamaldehyde	Oxy	Cbn	Aldh	Oxy
$C_9H_{10}O_2$	Vinylguaiacol	G	Met	PhOH	Ph
$C_9H_{10}O_3$	Ethylvanillin	G	Met	PhOH	Ph
$C_9H_{10}O_4$	Syringaldehyde	S	Met	PhOH	Ph
C_9H_{12}	1,2,3-trimethylbenzene	B	HC	HCs	Ar
$C_9H_{12}O$	4-Propylphenol	H	HC	PhOH	Ph
$C_9H_{12}O_2$	p-Ethylguaiacol	G	Met	PhOH	Ph
$C_9H_{12}O_3$	4-Methylsyringol	S	Met	PhOH	Ph
$C_9H_{14}O_5$	Diethyl acetylmalonate	Oxy	HC	Es	Oxy
C_9H_{18}	1-Nonene	B	HC	HCs	A
$C_9H_{18}O$	Nonaldehyde	Oxy	Cbn	Aldh	Oxy
$C_9H_{19}NO$	Nonamide	O	HC	N	N
$C_9H_{20}O$	Nonanol	Oxy	Hydx	Alc	Oxy
$C_9H_{20}O_4$	Tripropylene glycol	Oxy	Hydx	Alc	Oxy
$C_{10}H_{10}O_3$	Coniferyl aldehyde	G	Met	PhOH	Ph
$C_{10}H_{12}$	4-Ethylstyrene	B	HC	HCs	Ar
$C_{10}H_{12}O_2$	Eugenol	G	Met	PhOH	Ph
$C_{10}H_{12}O_3$	4-Vinylsyringol	S	Met	PhOH	Ph

$C_{10}H_{12}O_4$	Acetosyringone	S	Met	PhOH	Ph
$C_{10}H_{12}O_5$	Methyl syringate	S	Met	PhOH	Ph
$C_{10}H_{13}N_5O_5$	Guanosine	O	Hydx	N	N
$C_{10}H_{14}O$	Thymol	H	Hydx	PhOH	Ph
$C_{10}H_{14}O_2$	Propylguaiacol	G	Met	PhOH	Ph
$C_{10}H_{14}O_3$	4-Ethylsyringol	S	Met	PhOH	Ph
$C_{10}H_{14}OS_2$	2,4-Bis(allylthio)but-2-enal	O	Cbn	O	O
$C_{10}H_{16}$	Limonene	A	HC	HCs	A
$C_{10}H_{16}O$	2-Hexylfuran	F	HC	Fu	Oxy
$C_{10}H_{16}O_2$	Geranic acid	Acd	Car	Cabox	Oxy
$C_{10}H_{18}O$	Eucalyptol	Oxy	HC	Eth	Oxy
$C_{10}H_{20}$	1-Decene	A	HC	HCs	A
$C_{10}H_{20}O_2$	Ethyl octanoate	Oxy	HC	Es	Oxy
$C_{10}H_{20}O_3$	Ethyl 3-hydroxyoctanoate	Oxy	HC	Es	Oxy
$C_{10}H_{21}Cl$	1-Chlorodecane	O	O	O	O
$C_{10}H_{21}NO$	Decanamide	O	Cbn	N	N
$C_{10}H_{22}O$	4-Decanol	Oxy	Hydx	Alc	Oxy
$C_{10}H_{22}O_2$	Decamethylenediol	Oxy	Hydx	Alc	Oxy
$C_{10}H_{22}O_3$	Ethanol, 2-[2-(hexyloxy)ethoxy]-	Oxy	Hydx	Eth	Oxy
$C_{11}H_{12}O_3$	Cinnamaldehyde, 3,4-dimethoxy-	Oxy	Met	Aldh	Oxy
$C_{11}H_{12}O_4$	Sinapinaldehyde	S	Met	Aldh	Ph
$C_{11}H_{14}O_3$	4-Allylsyringol	S	Met	PhOH	Ph
$C_{11}H_{14}O_4$	Sinapyl alcohol	S	Met	PhOH	Ph
$C_{11}H1_6O_2$	Phenol, 3-tert-butyl-4-methoxy	H	Met	PhOH	Ph
$C_{11}H_{16}O_3$	4-Propylsyringol	S	Met	PhOH	Ph
$C_{11}H_{16}O_4$	5-(3-Hydroxypropyl)-2,3-	S	Met	PhOH	Ph
$C_{11}H_{20}O_2$	2-Propenoic acid, octyl ester	Oxy	Cbn	Es	Oxy
$C_{11}H_{21}N$	1-Cyanodecane	O	O	N	N
$C_{11}H_{22}O_3$	Methyl 10-hydroxydecanoate	Oxy	Cbn	Es	Oxy
$C_{11}H_{23}Cl$	1-Chloroundecane	O	O	O	O
$C_{11}H_{24}O$	1-Undecanol	Oxy	Hydx	Alc	Oxy
$C_{11}H_{24}O_2$	Heptanal, diethyl acetal	Oxy	Hydx	Alc	Oxy
$C_{12}H_{10}$	Biphenyl	B	O	HCs	Ar
$C_{12}H_{12}O_5$	5,7,8-trimethoxycoumarin	Oxy	Met	Ket	Oxy
$C_{12}H_{14}N_2O_4$	Benzamide, N-tetrahydrofurfuryl-	O	O	N	N
$C_{12}H_{16}O$	p-Cyclohexylphenol	Oxy	Hydx	PhOH	Ph
$C_{12}H_{16}O_2$	Isopentyl benzoate	Oxy	Cbn	Es	Oxy
$C_{12}H_{18}O$	p-Hexylphenol	H	HC	PhOH	Ph
$C_{12}H_{18}O_3$	1-(4,6-Dimethoxy-2,3-	Oxy	Met	Alc	Oxy
$C_{12}H_{18}O_4$	Hexamethylene diacrylate	Oxy	Cbn	Es	Oxy
$C_{12}H_{20}O$	Furan, 2,5-dibutyl-	F	HC	Fu	Oxy
$C_{12}H_{22}O_{11}$	Maltose	Oxy	Hydx	Su	Oxy
$C_{12}H_{24}$	cis-5-Dodecene	A	HC	HCs	A
$C_{12}H_{24}O_3$	2-Ethyl-3-hydroxyhexyl 2-	Oxy	Cbn	Es	Oxy
$C_{12}H_{24}O_6$	1,4,7,10,13,16-	Oxy	Met	O	Oxy
$C_{12}H_{26}$	Dodecane	A	HC	HCs	A

$C_{12}H_{26}O$	6-Dodecanol	Oxy	Hydx	Alc	Oxy
$C_{13}H_{12}$	4-Methylbiphenyl	B	HC	HCs	Ar
$C_{13}H_{12}N_2O_3$	Propanedinitrile, 2-[(3,4,5-	O	O	N	N
$C_{13}H_{18}O_3$	Hexyl salicylate	Oxy	Cbn	Es	Oxy
$C_{13}H_{18}O_4$	Methyl 7-(2-furoyl)heptanoate	F	Cbn	Es	Oxy
$C_{13}H_{20}O_3$	furfuryl octanoate	F	Cbn	Es	Oxy
$C_{13}H_{26}$	1-Tridecene	A	HC	HCs	A
$C_{13}H_{26}O$	Tridecanal	Oxy	Cbn	Aldh	Oxy
$C_{13}H_{28}$	3-Ethylundecane	A	HC	HCs	A
$C_{13}H_{28}O$	1-Tridecanol	Oxy	Hydx	Alc	Oxy
$C_{14}H_{18}N_4O_3$	Trimethoprim	O	O	N	N
$C_{14}H_{22}$	Octylbenzene	B	HC	HCs	Ar
$C_{14}H_{22}O$	Phenol, 2,4-bis(1,1-dimethylethyl)-	H	Hydx	PhOH	Ph
$C_{14}H_{22}O_2$	3,5-Di-tert-butyl pyrocatechol	C	Hydx	PhOH	Ph
$C_{14}H_{24}S$	2-decylthiophene	O	O	O	O
$C_{14}H_{28}$	1-Tetradecene	A	HC	HCs	A
$C_{14}H_{28}O$	Tetradecanal	Oxy	Cbn	Aldh	Oxy
$C_{14}H_{28}O_2$	Methyl tridecanoate	Oxy	Cbn	Es	Oxy
$C_{14}H_{28}O_3$	Ethyl 3-hydroxydodecanoate	Oxy	Cbn	Es	Oxy
$C_{14}H_{30}O$	Tetradecanol	Oxy	Hydx	Alc	Oxy
$C_{14}H_{30}O_6$	Pentaethylene glycol monobutyl	Oxy	Hydx	Alc	Oxy
$C_{15}H_{18}$	1,6-Dimethyl-4-	B	HC	HCs	Ar
$C_{15}H_{30}O$	2-Pentadecanone	Oxy	Cbn	Ket	Oxy
$C_{15}H_{30}O_2$	Methyl tetradecanoate	Oxy	Cbn	Es	Oxy
$C_{16}H_{18}O_4$	Dibut-3-enyl phthalate	Oxy	Cbn	Es	Oxy
$C_{16}H_{19}NO_2$	2-Methoxy-4-(phenethylamino-	G	Met	PhOH	Ph
$C_{16}H_{22}O_4$	Dibutyl phthalate	Oxy	Cbn	Es	Oxy
$C_{16}H_{26}O_3$	3-dodecylfuran-2,5-dione	F	Cbny	Ket	Oxy
$C_{16}H_{28}$	4-Hexadecen-6-yne	A	HC	HCs	A
$C_{16}H_{30}O$	cis-9-Hexadecenal	Oxy	Cbn	Aldh	Ar
$C_{16}H_{30}O_4$	Dihexyl succinate	Oxy	Cbn	Es	Oxy
$C_{16}H_{31}N$	Palmitonitrile	O	O	N	N
$C_{16}H_{32}O_2$	Hexadecanoic acid	Acd	Car	Cabox	Oxy
$C_{16}H_{33}NO$	Palmiticamide	O	O	N	N
$C_{16}H_{34}$	Hexadecane	A	HC	HCs	A
$C_{16}H_{34}O$	Hexadecanol	Oxy	Hydx	Alc	Oxy
$C_{16}H_{34}O_3$	3-(Tridecyloxy)-1,2-propanediol	Oxy	Hydx	Alc	Oxy
$C_{17}H_{16}O$	1,4-diphenyl-4-penten-1-one	Oxy	Cbn	Ket	Oxy
$C_{17}H_{18}O$	1,4-diphenyl-1-pentanone	Oxy	Cbn	Ket	Oxy
$C_{17}H_{18}O_2$	3-(4-Tert-	Oxy	Cbn	Es	Oxy
$C_{17}H_{20}O_6$	Fumaric acid, 2,6-	Oxy	Cbn	Es	Oxy
$C_{17}H_{28}$	Undecylbenzene	B	HC	HCs	Ar
$C_{17}H_{33}N$	Heptadecanenitrile	O	O	N	N
$C_{17}H_{34}O_2$	Methyl hexadecanoate	Oxy	Cbn	Es	Oxy
$C_{17}H_{34}O_3$	tetradecyl lactate	Oxy	Cbn	Es	Oxy
$C_{17}H_{36}O$	2-Methyl-1-hexadecanol	Oxy	Hydx	Alc	Oxy

$C_{18}H_{18}$	3,4,5,6-Tetramethylphenanthrene	B	HC	HCs	Ar
$C_{18}H_{22}O$	4-tert-butyl-2-(1-	H	Hydx	PhOH	Ph
$C_{18}H_{26}O_3$	2-Propenoic acid, 3-(4-	Oxy	Met	Es	Oxy
$C_{18}H_{30}$	n-dodecylbenzene	B	HC	HCs	Ar
$C_{18}H_{31}N$	N-Dodecylaniline	O	O	N	N
$C_{18}H_{33}N$	Tricyclohexylamine	O	O	N	N
$C_{18}H_{34}O_2$	Vinyl palmitate	Oxy	Cbn	Es	Oxy
$C_{18}H_{35}NO$	9-Octadecenamide	O	O	N	N
$C_{18}H_{36}$	1-Octadecene	A	HC	HCs	A
$C_{18}H_{37}NO$	Octadecanamide	O	O	N	N
$C_{18}H_{38}$	8-Methylheptadecane	A	HC	HCs	A
$C_{18}H_{38}O_4$	Triethylene glycol monododecyl	Oxy	Hydx	Alc	Oxy
$C_{18}H_{38}O_5$	Tetraethylene glycol, decyl ether	Oxy	Hydx	Alc	Oxy
$C_{19}H_{24}$	1,1-Diphenylheptane	B	HC	HCs	Ar
$C_{19}H_{34}O_2$	Methyl linoleate	Oxy	Cbn	Es	Oxy
$C_{19}H_{36}O_2$	Methyloleate	Oxy	Cbn	Es	Oxy
$C_{19}H_{37}N$	Nonadecanenitrile	O	O	N	N
$C_{19}H_{38}O_2$	Methyl stearate	Oxy	Cbn	Es	Oxy
$C_{19}H_{40}$	Nonadecane	A	HC	HCs	A
$C_{20}H_{14}O_5$	Helenaquinol	Oxy	Hydx	Ket	Oxy
$C_{20}H_{22}O_7$	Flavanone, 4',5,6,7,8-	Oxy	Met	Ket	Ar
$C_{20}H_{22}N_2$	3H-Indole, 3,3-dimethyl-2-[2-(4-	O	HC	N	N
$C_{20}H_{38}O_2$	Octadecanoic acid, ethenyl ester	Oxy	Cbn	Es	Oxy
$C_{20}H_{42}$	Icosane	A	HC	HCs	A
$C_{20}H_{42}O$	1-Icosanol	Oxy	Hydx	Alc	Oxy
$C_{21}H_{24}O_6$	Phenol, 2,6-dimethoxy-4-[[2-	G	Met	PhOH	Ph
$C_{21}H_{24}O_8$	Glutaric acid, di(2,6-	Oxy	Cbn	Es	Oxy
$C_{21}H_{30}O_2$	Methyl dehydroabietate	Oxy	Cbn	Es	Oxy
$C_{21}H_{32}O_2$	Methyl pimarate	Oxy	Cbn	Es	Oxy
$C_{22}H_{43}NO$	Erucylamide	O	O	N	N
$C_{22}H_{44}O_2$	Octadecyl butyrate	Oxy	Cbn	Es	Oxy
$C_{22}H_{46}O$	1-Docosanol	Oxy	Hydx	Alc	Oxy
$C_{22}H_{46}O_6$	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy
$C_{23}H_{46}$	1-Tricosene	A	HC	HCs	A
$C_{23}H_{46}O_2$	Methyl docosanoate	Oxy	Cbn	Es	Oxy
$C_{24}H_{20}$	2,6-Dibenzylnaphthalene	B	HC	HCs	Ar
$C_{24}H_{38}O_4$	Bis(2-ethylhexyl) phthalate	Oxy	Cbn	Es	Oxy
$C_{25}H_{38}O_7$	Androstane-17-carboxylic acid,	HC	Cbny	Cabox	Cyclo
$C_{25}H_{42}O_2$	Octadecyl benzoate	Oxy	Cbn	Es	Oxy
$C_{25}H_{48}$	6,9-Pentacosadiene	A	HC	HCs	A
$C_{26}H_{20}$	Tetraphenylethene	B	HC	HCs	Ar
$C_{26}H_{22}$	Bibenzhydryl	B	HC	HCs	Ar
$C_{26}H_{50}$	Cyclohexane, 1,1'-	A	HC	HCs	A
$C_{26}H_{54}O_8$	Heptaethylene glycol	Oxy	Hydx	Alc	Oxy
$C_{27}H_{44}$	Cholesta-3,5-diene	ST	HC	HCs	A
$C_{27}H_{44}O$	4,6-Cholestadien-3-β-ol	ST	Hydx	Alc	Oxy

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$C_{27}H_{46}O$	Epicholesterol	ST	Hydx	Alc	Oxy
$C_{27}H_{48}O$	Dihydrocholesterol	ST	Hydx	Alc	Oxy
$C_{28}H_{26}$	BUTANE, 1,2,3,4-TETRAPHENYL-	B	HC	HCs	Ar
$C_{28}H_{42}O_4$	Phthalic acid, di-(-)-menthyl ester	Oxy	Cbn	Es	Oxy
$C_{28}H_{44}O$	Ergosterol	ST	Hydx	Alc	Oxy
$C_{29}H_{50}O$	β-Sitosterol	ST	Hydx	Alc	Oxy
$C_{30}H_{30}$	1,3,4,6-tetraphenylhexane	B	HC	HCs	Ar
$C_{30}H_{50}$	Squalene	A	HC	HCs	A
$C_{31}H_{62}O$	16-Hentriacontanone	Oxy	Cbn	Ket	Oxy

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APPENDIX E

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PYROPROBE GC/MS DATA

Temp.	Kraft lignin	Soda lignin	Lignin model compound
400°C	Non-catalytic-KL	Non-catalytic-SL	Non-catalytic-LMC
Ratio of sample to catalyst	1-1_ZrO$_2$	1-1_ZrO$_2$	1-1_ZrO$_2$
	1-1_Ni/ZrO$_2$	1-1_Ni/ZrO$_2$	1-1_Ni/ZrO$_2$
	1-5_Ni/ZrO$_2$	1-5_Ni/ZrO$_2$	1-5_Ni/ZrO$_2$
	1-10_Ni/ZrO$_2$	1-10_Ni/ZrO$_2$	1-10_Ni/ZrO$_2$
	1-1_Pd/ZrO$_2$	1-1_Pd/ZrO$_2$	1-1_Pd/ZrO$_2$
	1-1_Ru/ZrO$_2$	1-1_Ru/ZrO$_2$	1-1_Ru/ZrO$_2$
500°C	Non-catalytic-KL	Non-catalytic-SL	Non-catalytic-LMC
Ratio of sample to catalyst	1-1_ZrO2	-	-
	1-1_Ni/ZrO$_2$	1-1_Ni/ZrO$_2$	-
	1-5_Ni/ZrO$_2$	1-5_Ni/ZrO$_2$	-
	1-10_Ni/ZrO$_2$	-	-
	1-1_Pd/ZrO$_2$	1-1_Pd/ZrO$_2$	-
	1-5_Pd/ZrO$_2$	1-5_Pd/ZrO$_2$	-
	1-1_Ru/ZrO$_2$	-	-
	1-5_Ru/ZrO$_2$	1-5_Ru/ZrO$_2$	-
600°C	Non-catalytic-KL	Non-catalytic-SL	Non-catalytic-LMC
Ratio of sample to catalyst	1-1_ZrO2	-	-
	1-1_Ni/ZrO$_2$	1-1_Ni/ZrO$_2$	1-1_Ni/ZrO$_2$
	1-5_Ni/ZrO$_2$	1-5_Ni/ZrO$_2$	1-1_Pd/ZrO$_2$
	1-10_Ni/ZrO$_2$	-	1-1_Ru/ZrO$_2$
	1-1_Pd/ZrO$_2$	1-1_Pd/ZrO$_2$	-
	1-5_Pd/ZrO$_2$	1-5_Pd/ZrO$_2$	-
	1-1_Ru/ZrO$_2$	1-1_Ru/ZrO$_2$	-
	1-5_Ru/ZrO$_2$	1-5_Ru/ZrO$_2$	-

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KL400C

Peak	RT	Mol.Form	Name	i	ii	iii	iv	Run	Tot
1	12.198	C7H8O2	Guaiacol	G	Met	PhOH	Ph	3.90	0.09
2	15	C8H10O2	Creosol	G	Met	PhOH	Ph	0.47	0.01
3	15.235	C8H10O2	Creosol	G	Met	PhOH	Ph	5.73	0.14
4	17.685	C9H12O2	p-Ethylguaiacol	G	Met	PhOH	Ph	10.78	0.26
5	18.717	C9H10O2	Vinylguaiacol	G	Met	PhOH	Ph	2.88	0.07
6	19.644	C8H10O3	Syringol	S	Met	PhOH	Ph	20.38	0.49
7	20.133	C10H14O2	Propylguaiacol	G	Met	PhOH	Ph	0.16	0.00
8	20.421	C8H10O3	Syringol	S	Met	PhOH	Ph	0.78	0.02
9	21.12	C10H14O3	4-Ethylsyringol	S	Met	PhOH	Ph	0.33	0.01
10	22.226	C9H12O3	4-Methylsyringol	S	Met	PhOH	Ph	14.54	0.35
11	24.083	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	0.25	0.01
12	24.275	C10H14O3	4-Ethylsyringol	S	Met	PhOH	Ph	7.93	0.19
13	24.808	C10H12O3	4-Vinylsyringol	S	Met	PhOH	Ph	0.92	0.02
14	25.301	C10H12O3	4-Vinylsyringol	S	Met	PhOH	Ph	6.00	0.14
15	26.286	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	0.59	0.01
16	26.372	C10H12O5	Methyl syringate	S	Met	PhOH	Ph	1.31	0.03
17	27.086	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	0.65	0.02
18	27.468	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	0.78	0.02
19	27.903	C9H10O4	Syringaldehyde	S	Met	PhOH	Ph	1.51	0.04
20	28.048	C11H12O3	Cinnamaldehyde, 3,4-	Oxy	Met	Aldh	Oxy	1.12	0.03
21	28.218	C11H12O3	Cinnamaldehyde, 3,4-	Oxy	Met	Aldh	Oxy	0.52	0.01
22	28.522	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	4.29	0.10
23	28.867	C12H26O	6-Dodecanol	Oxy	Hydx	Alc	Oxy	0.16	0.00
24	29.29	C14H30O	Tetradecanol	Oxy	Hydx	Alc	Oxy	0.16	0.00
25	29.474	C10H12O4	Acetosyringone	S	Met	PhOH	Ph	1.69	0.04
26	29.633	C10H20O3	Ethyl 3-	Oxy	HC	Es	Oxy	0.75	0.02
27	30.275	C10H12O5	Methyl syringate	S	Met	PhOH	Ph	1.54	0.04
28	30.745	C14H30O	Tetradecanol	Oxy	Hydx	Alc	Oxy	0.34	0.01
29	31.501	C10H12O4	Acetosyringone	S	Met	PhOH	Ph	1.17	0.03
30	31.835	C10H20O3	Ethyl 3-	Oxy	HC	Es	Oxy	0.27	0.01
31	31.98	C18H38O5	Tetraethylene glycol,	Oxy	Hydx	Alc	Oxy	0.33	0.01
32	32.067	C6H14O	2-Hexanol	Oxy	Hydx	Alc	Oxy	0.21	0.01
33	33.96	C16H22O4	Dibutyl phthalate	Oxy	Cbn	Es	Oxy	0.90	0.02
34	34.061	C6H14O	2-Hexanol	Oxy	Hydx	Alc	Oxy	0.44	0.01
35	34.283	C22H46O6	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy	0.68	0.02
36	34.715	C22H46O6	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy	0.66	0.02
37	35.087	C22H46O6	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy	0.23	0.01
38	36.42	C17H16O	1,4-diphenyl-4-penten-	Oxy	Cbn	Ket	Oxy	0.24	0.01
39	36.689	C17H16O	1,4-diphenyl-4-penten-	Oxy	Cbn	Ket	Oxy	0.40	0.01
42	39.432	C20H22O7	Flavanone, 4',5,6,7,8-	Oxy	Met	Ket	Ar	0.45	0.01
43	39.617	C20H22O7	Flavanone, 4',5,6,7,8-	Oxy	Met	Ket	Ar	0.29	0.01
44	39.731	C22H43NO	Erucylamide	O	O	N	N	0.38	0.01
46	41.249	C24H38O4	Bis(2-ethylhexyl)	Oxy	Cbn	Es	Oxy	1.19	0.03

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47	41.694	C14H24S	2-decylthiophene	O	O	O	O	0.61	0.01
48	43.053	C17H20O6	Fumaric acid, 2,6-	Oxy	Cbn	Es	Oxy	0.28	0.01
49	43.391	C18H35NO	9-Octadecenamide	O	O	N	N	0.58	0.01
50	45.766	C29H50O	β-Sitosterol	ST	Hydx	Alc	Oxy	0.23	0.01
Sum								100.0	2.38

1-1KL400C_ZrO2

Peak	RT	Mol.Form	Name	i	ii	iii	iv	Run	Tot
1	12.292	C7H8O2	Guaiacol	G	Met	PhOH	Ph	3.31	0.08
2	15.067	C8H10O2	Creosol	G	Met	PhOH	Ph	0.37	0.01
3	15.279	C8H10O2	Creosol	G	Met	PhOH	Ph	5.34	0.12
4	17.704	C9H12O2	p-Ethylguaiacol	G	Met	PhOH	Ph	8.27	0.19
5	18.033	C7H8O3	3-Methoxycatechol	C	Met	PhOH	Ph	1.62	0.04
6	18.25	C12H26	Dodecane	A	HC	HCs	A	0.63	0.01
7	18.735	C9H10O2	Vinylguaiacol	G	Met	PhOH	Ph	3.45	0.08
9	19.634	C8H10O3	Syringol	S	Met	PhOH	Ph	19.45	0.44
10	20.448	C8H10O3	Syringol	S	Met	PhOH	Ph	0.54	0.01
11	21.13	C10H14O3	4-Ethylsyringol	S	Met	PhOH	Ph	0.24	0.01
12	22.216	C9H12O3	4-Methylsyringol	S	Met	PhOH	Ph	14.32	0.33
13	24.1	C9H10O3	Ethylvanillin	G	Met	PhOH	Ph	0.43	0.01
14	24.284	C10H14O3	4-Ethylsyringol	S	Met	PhOH	Ph	5.47	0.12
15	24.883	C6H10O5	Levoglucosan	Oxy	Hydx	Su	Oxy	1.31	0.03
16	25.304	C10H12O3	4-Vinylsyringol	S	Met	PhOH	Ph	5.94	0.14
17	26.3	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	0.55	0.01
18	26.389	C10H12O5	Methyl syringate	S	Met	PhOH	Ph	1.36	0.03
19	27.118	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	0.63	0.01
20	27.5	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	0.96	0.02
21	27.983	C9H10O4	Syringaldehyde	S	Met	PhOH	Ph	0.93	0.02
22	28.088	C11H12O3	Cinnamaldehyde, 3,4-	Oxy	Met	Aldh	Oxy	1.34	0.03
23	28.25	C11H12O3	Cinnamaldehyde, 3,4-	Oxy	Met	Aldh	Oxy	0.82	0.02
24	28.532	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	5.36	0.12
25	28.864	C9H20O	Nonanol	Oxy	Hydx	Alc	Oxy	0.67	0.02
27	29.285	C17H36O	2-Methyl-1-	Oxy	Hydx	Alc	Oxy	0.66	0.01
28	29.522	C10H12O4	Acetosyringone	S	Met	PhOH	Ph	1.29	0.03
29	29.636	C10H20O3	Ethyl 3-	Oxy	HC	Es	Oxy	2.24	0.05
30	30.319	C10H12O5	Methyl syringate	S	Met	PhOH	Ph	2.30	0.05
31	30.73	C12H26O	6-Dodecanol	Oxy	Hydx	Alc	Oxy	0.99	0.02
32	30.867	C11H24O2	Heptanal, diethyl	Oxy	Hydx	Alc	Oxy	0.42	0.01
33	31.085	C12H26O	6-Dodecanol	Oxy	Hydx	Alc	Oxy	0.55	0.01
34	31.548	C10H12O4	Acetosyringone	S	Met	PhOH	Ph	1.52	0.03
35	31.852	C10H20O3	Ethyl 3-	Oxy	HC	Es	Oxy	0.44	0.01
36	32.056	C16H22O4	Dibutyl phthalate	Oxy	Cbn	Es	Oxy	0.81	0.02
37	32.34	C18H38O5	Tetraethylene glycol,	Oxy	Hydx	Alc	Oxy	0.20	0.00
38	33.291	C17H34O2	Methyl	Oxy	Cbn	Es	Oxy	0.17	0.00

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39	33.964	C16H22O4	Dibutyl phthalate	Oxy	Cbn	Es	Oxy	1.02	0.02
40	34.068	C8H16O4	2-(2-	Oxy	HC	Es	Oxy	0.38	0.01
42	34.305	C10H20O3	Ethyl 3-	Oxy	HC	Es	Oxy	0.49	0.01
43	34.744	C18H38O5	Tetraethylene glycol,	Oxy	Hydx	Alc	Oxy	0.58	0.01
44	39.483	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	0.49	0.01
45	39.773	C18H35NO	9-Octadecenamide	O	O	N	N	0.24	0.01
46	40.764	C16H30O	cis-9-Hexadecenal	Oxy	Cbn	Aldh	Ar	0.14	0.00
48	41.249	C16H22O4	Dibutyl phthalate	Oxy	Cbn	Es	Oxy	0.95	0.02
49	43.386	C18H35NO	9-Octadecenamide	O	O	N	N	0.62	0.01
50	45.766	C29H50O	β-Sitosterol	ST	Hydx	Alc	Oxy	0.22	0.00
Sum								100.0	2.28

1-1_KL400C_NiZrO2

Peak	RT	Mol.Form	Name	i	ii	iii	iv	Run	Tot
1	12.022	C7H8O2	Guaiacol	G	Met	PhOH	Ph	3.38	0.07
2	15.1	C8H10O2	Creosol	G	Met	PhOH	Ph	4.97	0.10
3	17.586	C9H12O2	p-Ethylguaiacol	G	Met	PhOH	Ph	8.70	0.18
4	17.917	C13H26	1-Tridecene	A	HC	HCs	A	0.90	0.02
5	18.602	C9H10O2	Vinylguaiacol	G	Met	PhOH	Ph	1.92	0.04
6	19.56	C8H10O3	Syringol	S	Met	PhOH	Ph	17.49	0.36
7	20.313	C8H10O3	Syringol	S	Met	PhOH	Ph	0.72	0.01
8	22.142	C9H12O3	4-Methylsyringol	S	Met	PhOH	Ph	12.55	0.26
9	24.184	C10H14O3	4-Ethylsyringol	S	Met	PhOH	Ph	5.48	0.11
10	25.199	C11H16O2	Phenol, 3-tert-butyl-	H	Met	PhOH	Ph	5.25	0.11
11	26.16	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	0.87	0.02
12	26.264	C12H18O4	Hexamethylene	Oxy	Cbn	Es	Oxy	1.32	0.03
13	26.97	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	0.70	0.01
14	27.352	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	0.83	0.02
15	27.8	C9H10O4	Syringaldehyde	S	Met	PhOH	Ph	1.25	0.03
16	27.937	C11H12O3	Cinnamaldehyde,	Oxy	Met	Aldh	Oxy	1.14	0.02
17	28.117	C11H12O3	Cinnamaldehyde,	Oxy	Met	Aldh	Oxy	0.49	0.01
18	28.432	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	3.44	0.07
19	29.355	C10H12O4	Acetosyringone	S	Met	PhOH	Ph	1.65	0.03
21	30.139	C10H12O5	Methyl syringate	S	Met	PhOH	Ph	1.87	0.04
22	31.374	C10H12O4	Acetosyringone	S	Met	PhOH	Ph	1.04	0.02
23	33.846	C10H12O5	Methyl syringate	S	Met	PhOH	Ph	0.57	0.01
24	33.967	C10H12O4	Acetosyringone	S	Met	PhOH	Ph	0.34	0.01
25	34.174	C8H16O4	2-(2-	Oxy	HC	Es	Oxy	0.60	0.01
26	34.601	C8H16O4	2-(2-	Oxy	HC	Es	Oxy	0.42	0.01
27	35.889	C16H30O	cis-9-Hexadecenal	Oxy	Cbn	Aldh	Ar	0.71	0.01
28	35.971	C16H30O	cis-9-Hexadecenal	Oxy	Cbn	Aldh	Ar	0.46	0.01
29	36.29	C19H37N	Nonadecanenitrile	O	O	N	N	0.47	0.01
31	37.193	C18H35NO	9-Octadecenamide	O	O	N	N	0.89	0.02
32	37.448	C16H33NO	Palmiticamide	O	O	N	N	2.17	0.04

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35	38.651	C6H6N2O3	3-Hydroxy-6-methyl-	O	Hydx	N	N	0.49	0.01
36	39.267	C16H18O4	Dibut-3-enyl	Oxy	Cbn	Es	Oxy	0.49	0.01
37	39.462	C18H35NO	9-Octadecenamide	O	O	N	N	4.62	0.10
38	39.55	C18H35NO	9-Octadecenamide	O	O	N	N	2.98	0.06
39	39.783	C16H33NO	Palmiticamide	O	O	N	N	1.09	0.02
40	40.055	C10H16O	2-Hexylfuran	F	HC	Fu	Oxy	1.22	0.03
41	40.521	C19H34O2	Methyl linoleate	Oxy	Cbn	Es	Oxy	0.79	0.02
43	41.1	C6H6N2O3	3-Hydroxy-6-methyl-	O	Hydx	N	N	0.43	0.01
44	41.185	C16H22O4	Dibutyl phthalate	Oxy	Cbn	Es	Oxy	1.17	0.02
45	41.519	C12H18O4	Hexamethylene	Oxy	Cbn	Es	Oxy	0.72	0.01
46	41.754	C12H18O4	Hexamethylene	Oxy	Cbn	Es	Oxy	0.42	0.01
47	42.183	C26H22	Bibenzhydryl	B	HC	HCs	Ar	0.24	0.00
48	42.767	C20H14O5	Helenaquinol	Oxy	Hydx	Ket	Oxy	0.43	0.01
49	42.843	C17H20O6	Fumaric acid, 2,6-	Oxy	Cbn	Es	Oxy	1.62	0.03
50	43.344	C13H12	4-Methylbiphenyl	B	HC	HCs	Ar	0.70	0.01
Sum								100.0	2.07

1-5_KL400C_NiZrO2

Peak	RT	Mol.Form	Name	i	ii	iii	iv	Run	Tot
1	15.124	C8H10O2	Creosol	G	Met	PhOH	Ph	5.32	0.09
2	17.606	C9H12O2	p-Ethylguaiacol	G	Met	PhOH	Ph	6.73	0.12
3	18.605	C9H10O2	Vinylguaiacol	G	Met	PhOH	Ph	2.86	0.05
4	19.566	C8H10O3	Syringol	S	Met	PhOH	Ph	18.45	0.32
5	20.05	C10H14O2	Propylguaiacol	G	Met	PhOH	Ph	0.21	0.00
6	21.018	C10H14O3	4-Ethylsyringol	S	Met	PhOH	Ph	0.36	0.01
7	22.142	C9H12O3	4-Methylsyringol	S	Met	PhOH	Ph	14.74	0.26
8	24.189	C10H14O3	4-Ethylsyringol	S	Met	PhOH	Ph	6.27	0.11
9	24.683	C13H18O3	Hexyl salicylate	Oxy	Cbn	Es	Oxy	0.58	0.01
10	25.196	C10H12O3	4-Vinylsyringol	S	Met	PhOH	Ph	7.07	0.12
11	26.173	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	1.08	0.02
12	26.283	C12H18O4	Hexamethylene diacrylate	Oxy	Cbn	Es	Oxy	1.35	0.02
13	26.981	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	0.90	0.02
14	27.368	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	1.11	0.02
16	27.957	C11H12O3	Cinnamaldehyde, 3,4-	Oxy	Met	Aldh	Oxy	1.47	0.03
17	28.15	C11H12O3	Cinnamaldehyde, 3,4-	Oxy	Met	Aldh	Oxy	0.67	0.01
18	28.448	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	4.27	0.07
19	29.382	C10H12O4	Acetosyringone	S	Met	PhOH	Ph	1.63	0.03
21	30.158	C10H12O5	Methyl syringate	S	Met	PhOH	Ph	2.34	0.04
22	31.395	C10H12O4	Acetosyringone	S	Met	PhOH	Ph	0.88	0.02
23	32.681	C16H31N	Palmitonitrile	O	O	N	N	0.42	0.01
24	33.187	C17H34O2	Methyl hexadecanoate	Oxy	Cbn	Es	Oxy	0.24	0.00
25	33.85	C8H16O4	2-(2-Ethoxyethoxy)ethyl	Oxy	HC	Es	Oxy	0.23	0.00
26	34.614	C8H16O4	2-(2-Ethoxyethoxy)ethyl	Oxy	HC	Es	Oxy	0.26	0.00
27	35.893	C16H30O	cis-9-Hexadecenal	Oxy	Cbn	Aldh	Ar	1.13	0.02

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28	35.971	C16H30O	cis-9-Hexadecenal	Oxy	Cbn	Aldh	Ar	1.38	0.02
29	36.294	C17H33N	Heptadecanenitrile	O	O	N	N	0.78	0.01
31	37.216	C18H35NO	9-Octadecenamide	O	O	N	N	0.71	0.01
32	37.47	C16H33NO	Palmiticamide	O	O	N	N	1.77	0.03
34	39.471	C18H35NO	9-Octadecenamide	O	O	N	N	4.87	0.09
35	39.566	C18H35NO	9-Octadecenamide	O	O	N	N	2.52	0.04
36	39.8	C18H37NO	Octadecanamide	O	O	N	N	0.71	0.01
37	40.072	C10H16O	2-Hexylfuran	F	HC	Fu	Oxy	0.52	0.01
38	40.687	C25H42O2	Octadecyl benzoate	Oxy	Cbn	Es	Oxy	0.19	0.00
41	41.189	C16H22O4	Dibutyl phthalate	Oxy	Cbn	Es	Oxy	1.01	0.02
43	41.531	C21H24O6	Phenol, 2,6-dimethoxy-4-	G	Met	PhOH	Ph	0.74	0.01
44	41.766	C12H18O4	Hexamethylene diacrylate	Oxy	Cbn	Es	Oxy	0.76	0.01
45	41.992	C10H14OS2	2,4-Bis(allylthio)but-2-enal	O	Cbn	O	O	0.37	0.01
46	42.196	C19H24	1,1-Diphenylheptane	B	HC	HCs	Ar	0.59	0.01
47	42.767	C20H14O5	Helenaquinol	Oxy	Hydx	Ket	Oxy	0.29	0.00
48	42.842	C17H20O6	Fumaric acid, 2,6-	Oxy	Cbn	Es	Oxy	1.47	0.03
49	43.233	C18H35NO	9-Octadecenamide	O	O	N	N	0.18	0.00
50	43.347	C26H22	Bibenzhydryl	B	HC	HCs	Ar	0.58	0.01
Sum								100.0	1.75

1-10_KL400C_NiZrO2

Peak	RT	Mol.Form	Name	i	ii	iii	iv	Run	Tot
1	15.189	C8H10O2	Creosol	G	Met	PhOH	Ph	6.01	0.09
2	17.706	C9H12O2	p-Ethylguaiacol	G	Met	PhOH	Ph	4.60	0.07
3	17.933	C13H26	1-Tridecene	A	HC	HCs	A	1.62	0.02
4	18.673	C9H10O2	Vinylguaiacol	G	Met	PhOH	Ph	2.48	0.04
5	19.583	C8H10O3	Syringol	S	Met	PhOH	Ph	19.65	0.29
6	20.067	C10H14O2	Propylguaiacol	G	Met	PhOH	Ph	2.00	0.03
7	20.385	C9H12O3	4-Methylsyringol	S	Met	PhOH	Ph	1.62	0.02
8	20.683	C13H26	1-Tridecene	A	HC	HCs	A	0.64	0.01
9	21.038	C10H14O3	4-Ethylsyringol	S	Met	PhOH	Ph	1.04	0.02
10	22.15	C9H12O3	4-Methylsyringol	S	Met	PhOH	Ph	17.06	0.25
11	24.219	C10H14O3	4-Ethylsyringol	S	Met	PhOH	Ph	6.55	0.10
12	25.237	C10H12O3	4-Vinylsyringol	S	Met	PhOH	Ph	7.05	0.10
13	26.233	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	0.75	0.01
14	26.321	C12H18O4	Hexamethylene diacrylate	Oxy	Cbn	Es	Oxy	1.19	0.02
15	27.035	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	0.83	0.01
16	27.444	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	0.88	0.01
17	28.099	C11H12O3	Cinnamaldehyde, 3,4-	Oxy	Met	Aldh	Oxy	0.98	0.01
18	28.217	C11H12O3	Cinnamaldehyde, 3,4-	Oxy	Met	Aldh	Oxy	0.82	0.01
19	28.519	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	4.90	0.07
20	28.817	C13H28O	1-Tridecanol	Oxy	Hydx	Alc	Oxy	0.38	0.01
21	29.5	C10H12O4	Acetosyringone	S	Met	PhOH	Ph	0.95	0.01
23	30.268	C10H12O5	Methyl syringate	S	Met	PhOH	Ph	2.28	0.03

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24	30.627	C14H30O	Tetradecanol	Oxy	Hydx	Alc	Oxy	0.81	0.01
25	31.552	C10H12O4	Acetosyringone	S	Met	PhOH	Ph	0.83	0.01
26	31.91	C10H20O3	Ethyl 3-hydroxyoctanoate	Oxy	HC	Es	Oxy	0.55	0.01
28	32.738	C14H28O3	Ethyl 3-	Oxy	Cbn	Es	Oxy	0.34	0.01
29	33.202	C17H34O2	Methyl hexadecanoate	Oxy	Cbn	Es	Oxy	0.72	0.01
30	33.869	C10H20O3	Ethyl 3-hydroxyoctanoate	Oxy	HC	Es	Oxy	0.88	0.01
31	33.994	C10H20O3	Ethyl 3-hydroxyoctanoate	Oxy	HC	Es	Oxy	0.63	0.01
32	34.22	C10H20O3	Ethyl 3-hydroxyoctanoate	Oxy	HC	Es	Oxy	0.81	0.01
33	34.663	C10H20O3	Ethyl 3-hydroxyoctanoate	Oxy	HC	Es	Oxy	0.62	0.01
34	35.935	C16H30O	cis-9-Hexadecenal	Oxy	Cbn	Aldh	Ar	0.52	0.01
35	36.59	C19H38O2	Methyl stearate	Oxy	Cbn	Es	Oxy	0.38	0.01
37	39.391	C10H14O2	Propylguaiacol	G	Met	PhOH	Ph	0.33	0.00
38	39.626	C18H35NO	9-Octadecenamide	O	O	N	N	0.88	0.01
40	41.201	C16H22O4	Dibutyl phthalate	Oxy	Cbn	Es	Oxy	1.28	0.02
42	41.56	C21H24O6	Phenol, 2,6-dimethoxy-4-	G	Met	PhOH	Ph	0.69	0.01
44	41.802	C12H18O4	Hexamethylene diacrylate	Oxy	Cbn	Es	Oxy	0.42	0.01
47	42.219	C19H24	1,1-Diphenylheptane	B	HC	HCs	Ar	0.32	0.00
48	42.858	C17H20O6	Fumaric acid, 2,6-	Oxy	Cbn	Es	Oxy	3.22	0.05
49	43.366	C10H14OS2	2,4-Bis(allylthio)but-2-enal	O	Cbn	O	O	1.21	0.02
50	45.685	C28H44O	Ergosterol	ST	Hydx	Alc	Oxy	0.32	0.00
Sum								100.0	1.47

1-1_KL400C_PdZrO2

Peak	RT	Mol.Form	Name	i	ii	iii	iv	Run	Tot
1	12.031	C7H8O2	Guaiacol	G	Met	PhOH	Ph	4.76	0.09
2	15.112	C8H10O2	Creosol	G	Met	PhOH	Ph	6.06	0.11
3	17.601	C9H12O2	p-Ethylguaiacol	G	Met	PhOH	Ph	6.68	0.12
4	18.61	C9H10O2	Vinylguaiacol	G	Met	PhOH	Ph	2.12	0.04
5	19.562	C8H10O3	Syringol	S	Met	PhOH	Ph	20.82	0.38
6	20.018	C10H14O2	Propylguaiacol	G	Met	PhOH	Ph	0.30	0.01
7	20.318	C8H10O3	Syringol	S	Met	PhOH	Ph	0.68	0.01
8	21.014	C10H14O3	4-Ethylsyringol	S	Met	PhOH	Ph	0.37	0.01
9	22.141	C9H12O3	4-Methylsyringol	S	Met	PhOH	Ph	14.47	0.26
10	24.185	C10H14O3	4-Ethylsyringol	S	Met	PhOH	Ph	6.48	0.12
11	24.65	C13H18O3	Hexyl salicylate	Oxy	Cbn	Es	Oxy	0.62	0.01
12	25.203	C10H12O3	4-Vinylsyringol	S	Met	PhOH	Ph	5.79	0.10
13	26.163	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	0.95	0.02
14	26.264	C12H18O4	Hexamethylene	Oxy	Cbn	Es	Oxy	1.43	0.03
15	26.968	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	0.76	0.01
16	27.351	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	0.93	0.02
17	27.783	C9H10O4	Syringaldehyde	S	Met	PhOH	Ph	1.65	0.03
18	27.935	C11H12O3	Cinnamaldehyde,	Oxy	Met	Aldh	Oxy	1.25	0.02
19	28.117	C11H12O3	Cinnamaldehyde,	Oxy	Met	Aldh	Oxy	0.50	0.01
20	28.431	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	3.89	0.07

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21	29.353	C10H12O4	Acetosyringone	S	Met	PhOH	Ph	1.82	0.03
23	30.139	C10H12O5	Methyl syringate	S	Met	PhOH	Ph	2.03	0.04
24	31.367	C10H12O4	Acetosyringone	S	Met	PhOH	Ph	1.16	0.02
26	31.95	C6H14O	2-Hexanol	Oxy	Hydx	Alc	Oxy	0.27	0.00
27	32.185	C8H16O4	2-(2-	Oxy	HC	Es	Oxy	0.26	0.00
28	33.816	C6H14O	2-Hexanol	Oxy	Hydx	Alc	Oxy	1.78	0.03
29	33.937	C6H14O	2-Hexanol	Oxy	Hydx	Alc	Oxy	1.48	0.03
30	34.16	C10H20O3	Ethyl 3-	Oxy	HC	Es	Oxy	1.21	0.02
31	34.591	C10H22O2	Decamethylenediol	Oxy	Hydx	Alc	Oxy	1.45	0.03
32	34.958	C22H46O6	Pentaethylene	Oxy	Hydx	Alc	Oxy	0.57	0.01
33	35.49	C6H14O	2-Hexanol	Oxy	Hydx	Alc	Oxy	0.40	0.01
35	37.479	C16H33NO	Palmiticamide	O	O	N	N	0.93	0.02
37	39.522	C18H35NO	9-Octadecenamide	O	O	N	N	1.07	0.02
38	39.617	C18H35NO	9-Octadecenamide	O	O	N	N	0.35	0.01
39	39.815	C16H33NO	Palmiticamide	O	O	N	N	0.33	0.01
40	40.071	C10H16O	2-Hexylfuran	F	HC	Fu	Oxy	0.43	0.01
43	41.192	C8H5NO6	m-Nitrophthalic acid	Acd	Car	Cabox	N	1.13	0.02
45	41.766	C12H18O4	Hexamethylene	Oxy	Cbn	Es	Oxy	0.41	0.01
46	42.197	C19H24	1,1-Diphenylheptane	B	HC	HCs	Ar	0.21	0.00
47	42.767	C20H14O5	Helenaquinol	Oxy	Hydx	Ket	Oxy	0.33	0.01
48	42.859	C17H20O6	Fumaric acid, 2,6-	Oxy	Cbn	Es	Oxy	1.22	0.02
49	43.357	C13H12	4-Methylbiphenyl	B	HC	HCs	Ar	0.41	0.01
50	45.694	C29H50O	β-Sitosterol	ST	Hydx	Alc	Oxy	0.27	0.00
Sum								100.0	1.81

1-1KL400C_RuZrO2

Peak	RT	Mol.Form	Name	i	ii	iii	iv	Run	Tot
1	12.029	C7H8O2	Guaiacol	G	Met	PhOH	Ph	4.09	0.09
2	14.833	C8H10O2	Creosol	G	Met	PhOH	Ph	0.54	0.01
3	15.118	C8H10O2	Creosol	G	Met	PhOH	Ph	5.30	0.11
4	17.587	C9H12O2	p-Ethylguaiacol	G	Met	PhOH	Ph	10.79	0.23
5	18.604	C9H10O2	Vinylguaiacol	G	Met	PhOH	Ph	2.60	0.06
6	19.565	C8H10O3	Syringol	S	Met	PhOH	Ph	20.85	0.44
7	20.033	C10H14O2	Propylguaiacol	G	Met	PhOH	Ph	0.20	0.00
8	20.311	C8H10O3	Syringol	S	Met	PhOH	Ph	0.75	0.02
9	21.019	C10H14O3	4-Ethylsyringol	S	Met	PhOH	Ph	0.26	0.01
10	22.144	C9H12O3	4-Methylsyringol	S	Met	PhOH	Ph	13.91	0.30
11	24.186	C10H14O3	4-Ethylsyringol	S	Met	PhOH	Ph	6.52	0.14
12	24.65	C9H12O3	4-Methylsyringol	S	Met	PhOH	Ph	0.59	0.01
13	25.202	C10H12O3	4-Vinylsyringol	S	Met	PhOH	Ph	5.61	0.12
14	26.171	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	0.77	0.02
15	26.269	C12H18O4	Hexamethylene diacrylate	Oxy	Cbn	Es	Oxy	1.36	0.03
16	26.971	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	0.70	0.01
17	27.353	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	0.83	0.02

18	27.79	C9H10O4	Syringaldehyde	S	Met	PhOH	Ph	2.67	0.06
19	28.117	C11H12O3	Cinnamaldehyde, 3,4-	Oxy	Met	Aldh	Oxy	0.42	0.01
20	28.426	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	3.77	0.08
21	29.357	C10H12O4	Acetosyringone	S	Met	PhOH	Ph	2.37	0.05
22	30.157	C10H12O5	Methyl syringate	S	Met	PhOH	Ph	1.69	0.04
23	31.375	C10H12O4	Acetosyringone	S	Met	PhOH	Ph	0.93	0.02
25	36.303	C12H12O5	5,7,8-trimethoxycoumarin	Oxy	Met	Ket	Oxy	0.18	0.00
27	37.4	C13H12N2O3	Propanedinitrile, 2-[(3,4,5-	O	O	N	N	0.20	0.00
28	37.487	C16H33NO	Palmiticamide	O	O	N	N	0.89	0.02
30	37.94	C12H14N2O4	Benzamide, N-	O	O	N	N	0.47	0.01
32	39.298	C11H14O4	Sinapyl alcohol	S	Met	PhOH	Ph	0.20	0.00
33	39.491	C18H35NO	9-Octadecenamide	O	O	N	N	2.17	0.05
34	39.585	C18H35NO	9-Octadecenamide	O	O	N	N	1.08	0.02
35	39.801	C16H33NO	Palmiticamide	O	O	N	N	0.66	0.01
36	40.069	C9H12O2	p-Ethylguaiacol	G	Met	PhOH	Ph	0.48	0.01
37	40.684	C25H48	6,9-Pentacosadiene	A	HC	HCs	A	0.16	0.00
40	41.189	C16H22O4	Dibutyl phthalate	Oxy	Cbn	Es	Oxy	1.05	0.02
41	41.532	C12H18O4	Hexamethylene diacrylate	Oxy	Cbn	Es	Oxy	0.67	0.01
43	41.767	C12H18O4	Hexamethylene diacrylate	Oxy	Cbn	Es	Oxy	0.47	0.01
45	42.197	C10H14OS2	2,4-Bis(allylthio)but-2-enal	O	Cbn	O	O	0.41	0.01
46	42.767	C20H14O5	Helenaquinol	Oxy	Hydx	Ket	Oxy	0.27	0.01
47	42.862	C17H20O6	Fumaric acid, 2,6-	Oxy	Cbn	Es	Oxy	1.08	0.02
48	43.22	C18H35NO	9-Octadecenamide	O	O	N	N	1.39	0.03
49	43.357	C26H22	Bibenzhydryl	B	HC	HCs	Ar	0.41	0.01
50	45.691	C29H50O	β-Sitosterol	ST	Hydx	Alc	Oxy	0.23	0.01
Sum								100.0	2.13

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Peak	RT	Mol.Form	Name	i	ii	iii	iv	Run	Tot
1	4.678	C9H18	1-Nonene	B	HC	HCs	A	0.49	0.01
2	12.018	C7H8O2	Guaiacol	G	Met	PhOH	Ph	4.21	0.10
3	14.8	C8H10O2	Creosol	G	Met	PhOH	Ph	0.90	0.02
4	15.19	C8H10O2	Creosol	G	Met	PhOH	Ph	6.85	0.16
5	17.546	C7H8O3	3-Methoxycatechol	C	Met	PhOH	Ph	3.44	0.08
6	17.76	C9H12O2	p-Ethylguaiacol	G	Met	PhOH	Ph	6.59	0.15
7	18.782	C9H10O2	Vinylguaiacol	G	Met	PhOH	Ph	2.50	0.06
8	19.799	C8H10O3	Syringol	S	Met	PhOH	Ph	13.56	0.31
9	19.983	C10H12O2	Eugenol	G	Met	PhOH	Ph	2.13	0.05
10	20.233	C10H14O2	Propylguaiacol	G	Met	PhOH	Ph	0.60	0.01
11	20.32	C8H10O3	Syringol	S	Met	PhOH	Ph	1.78	0.04
12	20.517	C9H12O3	4-Methylsyringol	S	Met	PhOH	Ph	0.55	0.01
13	21.228	C10H14O3	4-Ethylsyringol	S	Met	PhOH	Ph	0.28	0.01
14	21.407	C10H12O2	Eugenol	G	Met	PhOH	Ph	0.26	0.01
15	22.402	C9H12O3	4-Methylsyringol	S	Met	PhOH	Ph	11.16	0.25

16	22.499	C10H12O2	Eugenol	G	Met	PhOH	Ph	2.81	0.06
17	24.417	C10H14O3	4-Ethylsyringol	S	Met	PhOH	Ph	6.77	0.15
18	24.789	C10H12O3	4-Vinylsyringol	S	Met	PhOH	Ph	0.60	0.01
19	25.417	C10H12O3	4-Vinylsyringol	S	Met	PhOH	Ph	5.85	0.13
20	26.356	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	1.32	0.03
21	26.486	C10H12O5	Methyl syringate	S	Met	PhOH	Ph	1.30	0.03
22	27.167	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	0.66	0.02
23	27.535	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	1.17	0.03
24	27.952	C9H10O4	Syringaldehyde	S	Met	PhOH	Ph	2.21	0.05
25	28.15	C11H12O3	Cinnamaldehyde, 3,4-	Oxy	Met	Aldh	Oxy	0.81	0.02
26	28.653	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	4.38	0.10
27	28.783	C11H24O2	Heptanal, diethyl acetal	Oxy	Hydx	Alc	Oxy	0.54	0.01
28	29.419	C12H26O	6-Dodecanol	Oxy	Hydx	Alc	Oxy	0.28	0.01
29	29.549	C10H12O4	Acetosyringone	S	Met	PhOH	Ph	1.99	0.05
30	29.739	C8H7NO4	methyl 4-nitrobenzoate	Oxy	Met	Es	N	0.88	0.02
31	30.358	C10H12O5	Methyl syringate	S	Met	PhOH	Ph	1.50	0.03
32	30.845	C14H28	1-Tetradecene	A	HC	HCs	A	0.58	0.01
33	31.552	C10H12O4	Acetosyringone	S	Met	PhOH	Ph	1.20	0.03
34	34.099	C16H22O4	Dibutyl phthalate	Oxy	Cbn	Es	Oxy	0.55	0.01
36	37.538	C13H12N2O3	Propanedinitrile, 2-[(3,4,5-	O	O	N	N	0.30	0.01
38	39.595	C9H12O2	p-Ethylguaiacol	G	Met	PhOH	Ph	0.83	0.02
39	40.198	C9H12O2	p-Ethylguaiacol	G	Met	PhOH	Ph	0.38	0.01
40	41.023	C14H18N4O3	Trimethoprim	O	O	N	N	1.24	0.03
41	41.329	C16H22O4	Dibutyl phthalate	Oxy	Cbn	Es	Oxy	1.15	0.03
43	41.622	C12H18O4	Hexamethylene diacrylate	Oxy	Cbn	Es	Oxy	0.57	0.01
44	41.865	C12H18O4	Hexamethylene diacrylate	Oxy	Cbn	Es	Oxy	0.35	0.01
45	42.295	C19H24	1,1-Diphenylheptane	B	HC	HCs	Ar	0.38	0.01
46	42.867	C20H14O5	Helenaquinol	Oxy	Hydx	Ket	Oxy	0.46	0.01
47	42.945	C17H20O6	Fumaric acid, 2,6-	Oxy	Cbn	Es	Oxy	2.24	0.05
48	43.443	C13H12	4-Methylbiphenyl	B	HC	HCs	Ar	1.09	0.02
50	45.83	C27H44	Cholesta-3,5-diene	ST	HC	HCs	A	0.34	0.01
Sum								100.0	2.27

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Peak	RT	Mol.Form	Name	i	ii	iii	iv	Run	Tot
1	4.311	C9H18	1-Nonene	B	HC	HCs	A	0.49	0.01
2	11.555	C7H8O2	Guaiacol	G	Met	PhOH	Ph	4.27	0.09
3	14.283	C8H10O2	Creosol	G	Met	PhOH	Ph	1.00	0.02
4	14.633	C8H10O2	Creosol	G	Met	PhOH	Ph	6.37	0.14
5	17.148	C9H12O2	p-Ethylguaiacol	G	Met	PhOH	Ph	10.09	0.22
6	17.783	C11H24O	1-Undecanol	Oxy	Hydx	Alc	Oxy	0.94	0.02
7	18.167	C9H10O2	Vinylguaiacol	G	Met	PhOH	Ph	4.49	0.10
8	18.769	C17H18O2	3-(4-Tert-	Oxy	Cbn	Es	Oxy	1.12	0.02
9	19.086	C8H10O3	Syringol	S	Met	PhOH	Ph	18.10	0.39

10	19.525	C10H14O2	Propylguaiacol	G	Met	PhOH	Ph	1.62	0.03
11	19.834	C8H10O3	Syringol	S	Met	PhOH	Ph	2.59	0.06
12	20.217	C9H12O2	p-Ethylguaiacol	G	Met	PhOH	Ph	0.72	0.02
13	20.533	C10H14O3	4-Ethylsyringol	S	Met	PhOH	Ph	0.68	0.01
14	21.649	C9H12O3	4-Methylsyringol	S	Met	PhOH	Ph	14.12	0.30
15	23.483	C9H10O3	Ethylvanillin	G	Met	PhOH	Ph	0.50	0.01
16	23.684	C10H14O3	4-Ethylsyringol	S	Met	PhOH	Ph	6.16	0.13
17	24.716	C10H12O3	4-Vinylsyringol	S	Met	PhOH	Ph	5.23	0.11
18	25.683	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	0.55	0.01
19	25.757	C10H12O5	Methyl syringate	S	Met	PhOH	Ph	1.22	0.03
20	26.486	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	0.70	0.01
21	26.868	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	1.13	0.02
22	27.462	C9H10O4	Syringaldehyde	S	Met	PhOH	Ph	2.22	0.05
23	27.633	C11H12O3	Cinnamaldehyde, 3,4-	Oxy	Met	Aldh	Oxy	0.67	0.01
24	27.93	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	4.23	0.09
25	28.905	C10H12O4	Acetosyringone	S	Met	PhOH	Ph	1.17	0.02
27	29.682	C10H12O5	Methyl syringate	S	Met	PhOH	Ph	1.34	0.03
28	30.902	C10H12O4	Acetosyringone	S	Met	PhOH	Ph	0.63	0.01
29	37.15	C16H33NO	Palmiticamide	O	O	N	N	0.52	0.01
30	37.641	C14H28	1-Tetradecene	A	HC	HCs	A	0.26	0.01
33	39.179	C18H35NO	9-Octadecenamide	O	O	N	N	0.37	0.01
34	39.471	C18H37NO	Octadecanamide	O	O	N	N	0.26	0.01
35	39.661	C12H20O	Furan, 2,5-dibutyl-	F	HC	Fu	Oxy	0.42	0.01
36	40.267	C25H48	6,9-Pentacosadiene	A	HC	HCs	A	0.23	0.00
38	40.764	C24H38O4	Bis(2-ethylhexyl) phthalate	Oxy	Cbn	Es	Oxy	1.35	0.03
42	41.351	C12H18O4	Hexamethylene diacrylate	Oxy	Cbn	Es	Oxy	0.40	0.01
44	41.779	C19H24	1,1-Diphenylheptane	B	HC	HCs	Ar	0.44	0.01
45	42.352	C20H14O5	Helenaquinol	Oxy	Hydx	Ket	Oxy	0.32	0.01
46	42.434	C17H20O6	Fumaric acid, 2,6-	Oxy	Cbn	Es	Oxy	1.66	0.04
47	42.833	C18H35NO	9-Octadecenamide	O	O	N	N	0.57	0.01
48	42.931	C26H22	Bibenzhydryl	B	HC	HCs	Ar	0.69	0.01
49	45.233	C29H50O	β-Sitosterol	ST	Hydx	Alc	Oxy	0.18	0.00
Sum								100.0	2.13

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1-1_KL500_NiZrO2

Peak	RT	Mol.Form	Name	i	ii	iii	iv	Run	Tot
1	11.446	C7H8O2	Guaiacol	G	Met	PhOH	Ph	0.82	0.02
2	14.183	C8H10O2	Creosol	G	Met	PhOH	Ph	0.85	0.02
3	14.484	C8H10O2	Creosol	G	Met	PhOH	Ph	6.45	0.12
4	16.951	C9H12O2	p-Ethylguaiacol	G	Met	PhOH	Ph	5.55	0.11
5	17.2	C7H8O3	3-Methoxycatechol	C	Met	PhOH	Ph	3.52	0.07
6	17.433	C13H28	3-Ethylundecane	A	HC	HCs	A	0.84	0.02
7	17.55	C11H24O	1-Undecanol	Oxy	Hydx	Alc	Oxy	1.32	0.03
8	17.987	C9H10O2	Vinylguaiacol	G	Met	PhOH	Ph	3.96	0.08

9	18.333	C9H10O3	Ethylvanillin	G	Met	PhOH	Ph	0.60	0.01
10	18.854	C8H10O3	Syringol	S	Met	PhOH	Ph	18.76	0.36
11	19.3	C9H19NO	Nonamide	O	HC	N	N	1.37	0.03
12	19.483	C9H12O3	4-Methylsyringol	S	Met	PhOH	Ph	0.46	0.01
13	19.634	C10H14O3	4-Ethylsyringol	S	Met	PhOH	Ph	1.06	0.02
14	20.317	C9H12O3	4-Methylsyringol	S	Met	PhOH	Ph	0.47	0.01
15	21.402	C9H12O3	4-Methylsyringol	S	Met	PhOH	Ph	15.40	0.30
17	23.296	C10H14O3	4-Ethylsyringol	S	Met	PhOH	Ph	0.18	0.00
18	23.452	C10H12O3	4-Vinylsyringol	S	Met	PhOH	Ph	7.28	0.14
19	24.133	C10H12O3	4-Vinylsyringol	S	Met	PhOH	Ph	1.35	0.03
20	24.485	C12H18O4	Hexamethylene	Oxy	Cbn	Es	Oxy	6.76	0.13
21	25.531	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	2.22	0.04
22	26.285	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	0.74	0.01
23	26.672	C12H16O2	Isopentyl benzoate	Oxy	Cbn	Es	Oxy	1.22	0.02
24	27.303	C11H12O3	Cinnamaldehyde, 3,4-	Oxy	Met	Aldh	Oxy	1.52	0.03
25	27.417	C11H21N	1-Cyanodecane	O	O	N	N	0.96	0.02
26	27.567	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	0.50	0.01
27	27.715	C10H12O4	Acetosyringone	S	Met	PhOH	Ph	4.87	0.09
28	28.811	C10H12O5	Methyl syringate	S	Met	PhOH	Ph	2.22	0.04
29	29.505	C10H12O4	Acetosyringone	S	Met	PhOH	Ph	2.25	0.04
30	30.748	C16H31N	Palmitonitrile	O	O	N	N	0.67	0.01
31	31.919	C18H33N	Tricyclohexylamine	O	O	N	N	0.26	0.01
32	35.217	C18H36	1-Octadecene	A	HC	HCs	A	0.29	0.01
33	35.304	C16H33NO	Palmiticamide	O	O	N	N	0.22	0.00
36	37.009	C13H20O3	furfuryl octanoate	F	Cbn	Es	Oxy	0.78	0.02
37	38.017	C18H35NO	9-Octadecenamide	O	O	N	N	0.65	0.01
38	38.383	C18H35NO	9-Octadecenamide	O	O	N	N	0.45	0.01
40	38.796	C9H12O2	p-Ethylguaiacol	G	Met	PhOH	Ph	0.56	0.01
42	39.009	C16H22O4	Dibutyl phthalate	Oxy	Cbn	Es	Oxy	1.26	0.02
48	39.127	C17H20O6	Fumaric acid, 2,6-	Oxy	Cbn	Es	Oxy	0.60	0.01
49	39.35	C12H18O4	Hexamethylene	Oxy	Cbn	Es	Oxy	0.46	0.01
50	39.539	C29H50O	β-Sitosterol	ST	Hydx	Alc	Oxy	0.29	0.01
Sum								100.0	1.93

1-5_KL500_NiZrO2

Peak	RT	Mol.Form	Name	i	ii	iii	iv	Run	Tot
1	4.217	C9H18	1-Nonene	B	HC	HCs	A	0.38	0.01
2	11.422	C7H8O2	Guaiacol	G	Met	PhOH	Ph	4.35	0.09
3	14.15	C8H10O2	Creosol	G	Met	PhOH	Ph	0.86	0.02
4	14.461	C8H10O2	Creosol	G	Met	PhOH	Ph	6.31	0.14
5	16.913	C9H12O2	p-Ethylguaiacol	G	Met	PhOH	Ph	8.72	0.19
6	17.367	C7H8O3	3-Methoxycatechol	C	Met	PhOH	Ph	1.40	0.03
7	17.55	C11H24O	1-Undecanol	Oxy	Hydx	Alc	Oxy	0.70	0.02
8	17.953	C9H10O2	Vinylguaiacol	G	Met	PhOH	Ph	4.08	0.09

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9	18.317	C9H10O3	Ethylvanillin	G	Met	PhOH	Ph	0.47	0.01
10	18.854	C8H10O3	Syringol	S	Met	PhOH	Ph	16.53	0.36
11	19.3	C10H14O2	Propylguaiacol	G	Met	PhOH	Ph	1.20	0.03
12	19.595	C8H10O3	Syringol	S	Met	PhOH	Ph	1.45	0.03
13	20.32	C10H14O3	4-Ethylsyringol	S	Met	PhOH	Ph	0.29	0.01
14	21.402	C9H12O3	4-Methylsyringol	S	Met	PhOH	Ph	14.97	0.32
16	23.441	C10H14O3	4-Ethylsyringol	S	Met	PhOH	Ph	6.63	0.14
17	24.067	C10H12O3	4-Vinylsyringol	S	Met	PhOH	Ph	1.31	0.03
18	24.469	C10H12O3	4-Vinylsyringol	S	Met	PhOH	Ph	6.48	0.14
19	25.519	C12H18O4	Hexamethylene	Oxy	Cbn	Es	Oxy	2.01	0.04
20	26.257	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	0.80	0.02
21	26.648	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	1.31	0.03
22	27.249	C9H10O4	Syringaldehyde	S	Met	PhOH	Ph	2.02	0.04
23	27.383	C11H12O3	Cinnamaldehyde,	Oxy	Met	Aldh	Oxy	0.85	0.02
24	27.696	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	4.44	0.10
25	28.703	C10H12O4	Acetosyringone	S	Met	PhOH	Ph	2.07	0.04
27	29.456	C10H12O5	Methyl syringate	S	Met	PhOH	Ph	1.51	0.03
28	30.705	C10H12O4	Acetosyringone	S	Met	PhOH	Ph	0.91	0.02
29	37.011	C18H37NO	Octadecanamide	O	O	N	N	0.78	0.02
30	39.002	C18H35NO	9-Octadecenamide	O	O	N	N	1.04	0.02
33	39.117	C18H35NO	9-Octadecenamide	O	O	N	N	0.43	0.01
34	39.332	C18H37NO	Octadecanamide	O	O	N	N	0.23	0.01
35	39.525	C13H18O3	Hexyl salicylate	Oxy	Cbn	Es	Oxy	0.29	0.01
36	40.599	C16H22O4	Dibutyl phthalate	Oxy	Cbn	Es	Oxy	1.18	0.03
38	41.24	C12H18O4	Hexamethylene	Oxy	Cbn	Es	Oxy	0.37	0.01
42	41.421	C10H14OS2	2,4-Bis(allylthio)but-	O	Cbn	O	O	0.23	0.01
44	41.635	C10H14OS2	2,4-Bis(allylthio)but-	O	Cbn	O	O	0.36	0.01
45	42.2	C10H14OS2	2,4-Bis(allylthio)but-	O	Cbn	O	O	0.32	0.01
46	42.298	C17H20O6	Fumaric acid, 2,6-	Oxy	Cbn	Es	Oxy	1.54	0.03
47	42.717	C18H35NO	9-Octadecenamide	O	O	N	N	0.39	0.01
48	42.791	C26H22	Bibenzhydryl	B	HC	HCs	Ar	0.61	0.01
49	45.079	C29H50O	β-Sitosterol	ST	Hydx	Alc	Oxy	0.16	0.00
Sum								100.0	2.16

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1-10_KL500_NiZrO2

Peak	RT	Mol.Form	Name	i	ii	iii	iv	Run	Tot
1	11.66	C7H8O2	Guaiacol	G	Met	PhOH	Ph	4.18	0.06
2	14.267	C8H10O2	Creosol	G	Met	PhOH	Ph	0.78	0.01
3	14.555	C8H10O2	Creosol	G	Met	PhOH	Ph	6.61	0.10
4	17.057	C9H12O2	p-Ethylguaiacol	G	Met	PhOH	Ph	3.51	0.05
5	17.233	C7H8O3	3-Methoxycatechol	C	Met	PhOH	Ph	2.00	0.03
6	17.555	C11H24O	1-Undecanol	Oxy	Hydx	Alc	Oxy	0.47	0.01
7	18.066	C9H10O2	Vinylguaiacol	G	Met	PhOH	Ph	1.24	0.02
8	18.367	C9H10O3	Ethylvanillin	G	Met	PhOH	Ph	0.22	0.00

9	18.893	C8H10O3	Syringol	S	Met	PhOH	Ph	12.85	0.20
10	19.067	C10H14O2	Propylguaiacol	G	Met	PhOH	Ph	6.24	0.10
11	19.317	C8H10O3	Syringol	S	Met	PhOH	Ph	3.03	0.05
12	19.751	C18H36	1-Octadecene	A	HC	HCs	A	2.23	0.03
13	19.933	C10H14O3	4-Ethylsyringol	S	Met	PhOH	Ph	0.56	0.01
14	20.345	C9H12O3	4-Methylsyringol	S	Met	PhOH	Ph	1.18	0.02
15	21.421	C10H12O4	Acetosyringone	S	Met	PhOH	Ph	20.45	0.31
16	22.268	C10H12O4	Acetosyringone	S	Met	PhOH	Ph	0.18	0.00
17	22.532	C10H14O3	4-Ethylsyringol	S	Met	PhOH	Ph	0.13	0.00
18	23.488	C10H12O3	4-Vinylsyringol	S	Met	PhOH	Ph	8.58	0.13
19	24.566	C12H18O4	Hexamethylene	Oxy	Cbn	Es	Oxy	6.40	0.10
20	25.59	C12H18O4	Hexamethylene	Oxy	Cbn	Es	Oxy	2.14	0.03
21	26.354	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	0.69	0.01
22	26.754	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	0.74	0.01
23	27.516	C11H12O3	Cinnamaldehyde,	Oxy	Met	Aldh	Oxy	1.54	0.02
24	27.806	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	4.72	0.07
25	28.873	C10H12O4	Acetosyringone	S	Met	PhOH	Ph	2.33	0.04
27	29.625	C10H12O5	Methyl syringate	S	Met	PhOH	Ph	1.26	0.02
28	32.414	C14H28O2	Methyl tridecanoate	Oxy	Cbn	Es	Oxy	0.22	0.00
29	35.922	C19H38O2	Methyl stearate	Oxy	Cbn	Es	Oxy	0.25	0.00
30	37.346	C12H14N2O4	Benzamide, N-	O	O	N	N	0.40	0.01
33	38.833	C12H20O	Furan, 2,5-dibutyl-	F	HC	Fu	Oxy	0.24	0.00
34	39.165	C18H35NO	9-Octadecenamide	O	O	N	N	0.10	0.00
35	40.188	C14H22O2	3,5-Di-tert-butyl	C	Hydx	PhOH	Ph	0.13	0.00
36	40.618	C8H5NO6	m-Nitrophthalic acid	Acd	Car	Cabox	N	1.14	0.02
38	41.693	C10H14OS2	2,4-Bis(allylthio)but-	O	Cbn	O	O	0.43	0.01
42	42.248	C20H14O5	Helenaquinol	Oxy	Hydx	Ket	Oxy	0.23	0.00
44	42.34	C17H20O6	Fumaric acid, 2,6-	Oxy	Cbn	Es	Oxy	1.51	0.02
45	42.829	C12H18O4	Hexamethylene	Oxy	Cbn	Es	Oxy	0.92	0.01
46	45.098	C27H44	Cholesta-3,5-diene	ST	HC	HCs	A	0.17	0.00
Sum								100.0	1.53

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Peak	RT	Mol.Form	Name	i	ii	iii	iv	Run	Tot
1	11.833	C7H8O2	Guaiacol	G	Met	PhOH	Ph	1.68	0.04
2	12.054	C7H8O2	Guaiacol	G	Met	PhOH	Ph	2.13	0.05
3	14.714	C8H10O2	Creosol	G	Met	PhOH	Ph	6.67	0.15
4	17.033	C9H12O2	p-Ethylguaiacol	G	Met	PhOH	Ph	3.52	0.08
5	17.283	C7H8O3	3-Methoxycatechol	C	Met	PhOH	Ph	2.59	0.06
6	17.5	C7H8O3	3-Methoxycatechol	C	Met	PhOH	Ph	2.42	0.05
7	17.75	C7H8O3	3-Methoxycatechol	C	Met	PhOH	Ph	1.38	0.03
8	18.122	C9H10O2	Vinylguaiacol	G	Met	PhOH	Ph	2.00	0.05
9	18.4	C9H10O3	Ethylvanillin	G	Met	PhOH	Ph	0.42	0.01
10	18.912	C8H10O3	Syringol	S	Met	PhOH	Ph	16.67	0.38

11	19.467	C8H10O3	Syringol	S	Met	PhOH	Ph	0.53	0.01
12	21.455	C9H12O3	4-Methylsyringol	S	Met	PhOH	Ph	16.33	0.37
13	23.555	C10H14O3	4-Ethylsyringol	S	Met	PhOH	Ph	6.39	0.14
14	24.653	C10H12O3	4-Vinylsyringol	S	Met	PhOH	Ph	5.72	0.13
15	25.67	C12H18O4	Hexamethylene diacrylate	Oxy	Cbn	Es	Oxy	1.85	0.04
16	26.455	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	0.46	0.01
17	26.83	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	0.72	0.02
19	27.567	C11H12O3	Cinnamaldehyde, 3,4-	Oxy	Met	Aldh	Oxy	0.78	0.02
20	27.795	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	3.68	0.08
21	28.917	C10H12O4	Acetosyringone	S	Met	PhOH	Ph	1.55	0.03
22	29.713	C10H12O5	Methyl syringate	S	Met	PhOH	Ph	1.33	0.03
23	30.917	C10H12O4	Acetosyringone	S	Met	PhOH	Ph	2.99	0.07
25	32.066	S8	Cyclooctasulfur	O	O	O	O	7.41	0.17
26	33.142	C10H20O3	Ethyl 3-hydroxyoctanoate	Oxy	HC	Es	Oxy	0.41	0.01
27	33.285	C14H30O6	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy	0.33	0.01
30	37.297	C22H46O6	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy	0.80	0.02
31	37.404	C22H46O6	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy	0.73	0.02
32	37.567	C22H46O6	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy	0.60	0.01
36	39.729	C16H19NO2	2-Methoxy-4-(phenethylamino-	G	Met	PhOH	Ph	0.59	0.01
37	40.464	C20H22N2	3H-Indole, 3,3-dimethyl-2-[2-(4-	O	HC	N	N	1.17	0.03
38	40.641	C16H22O4	Dibutyl phthalate	Oxy	Cbn	Es	Oxy	0.81	0.02
42	41.314	C26H22	Bibenzhydryl	B	HC	HCs	Ar	0.44	0.01
43	41.723	C26H22	Bibenzhydryl	B	HC	HCs	Ar	0.40	0.01
45	42.252	C20H14O5	Helenaquinol	Oxy	Hydx	Ket	Oxy	0.47	0.01
46	42.336	C17H20O6	Fumaric acid, 2,6-	Oxy	Cbn	Es	Oxy	2.22	0.05
47	42.533	C20H22O7	Flavanone, 4',5,6,7,8-	Oxy	Met	Ket	Ar	0.31	0.01
48	42.837	C26H22	Bibenzhydryl	B	HC	HCs	Ar	1.56	0.04
Sum								100.0	2.26

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Peak	RT	Mol.Form	Name	i	ii	iii	iv	Run	Tot
1	11.775	C7H8O2	Guaiacol	G	Met	PhOH	Ph	3.44	0.08
2	14.417	C8H10O2	Creosol	G	Met	PhOH	Ph	0.69	0.02
3	14.691	C8H10O2	Creosol	G	Met	PhOH	Ph	5.81	0.13
4	17.054	C9H12O2	p-Ethylguaiacol	G	Met	PhOH	Ph	3.48	0.08
5	17.241	C7H8O3	3-Methoxycatechol	C	Met	PhOH	Ph	1.64	0.04
6	17.383	C12H24	cis-5-Dodecene	A	HC	HCs	A	0.97	0.02
7	17.567	C7H8O3	3-Methoxycatechol	C	Met	PhOH	Ph	2.67	0.06
8	17.874	C8H12O2	1-Oxetan-2-one, 4,4-diethyl-3-	Oxy	Cbn	Ket	Oxy	1.08	0.02
9	18.091	C9H10O2	Vinylguaiacol	G	Met	PhOH	Ph	3.22	0.07
10	18.367	C9H10O3	Ethylvanillin	G	Met	PhOH	Ph	0.73	0.02
11	18.52	C17H18O2	3-(4-Tert-	Oxy	Cbn	Es	Oxy	0.80	0.02
12	18.916	C8H10O3	Syringol	S	Met	PhOH	Ph	16.79	0.37
13	19.333	C10H14O2	Propylguaiacol	G	Met	PhOH	Ph	3.38	0.07

14	19.683	C9H12O3	4-Methylsyringol	S	Met	PhOH	Ph	0.63	0.01
15	19.897	C8H10O3	Syringol	S	Met	PhOH	Ph	2.05	0.05
16	20.15	C12H26	Dodecane	A	HC	HCs	A	0.60	0.01
17	20.38	C10H12O2	Eugenol	G	Met	PhOH	Ph	0.53	0.01
18	21.453	C9H12O3	4-Methylsyringol	S	Met	PhOH	Ph	15.68	0.35
19	23.539	C10H14O3	4-Ethylsyringol	S	Met	PhOH	Ph	6.06	0.13
20	24.62	C10H12O3	4-Vinylsyringol	S	Met	PhOH	Ph	5.15	0.11
21	25.639	C12H18O4	Hexamethylene diacrylate	Oxy	Cbn	Es	Oxy	1.55	0.03
22	26.433	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	0.54	0.01
23	26.819	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	0.96	0.02
24	27.586	C12H16O2	Isopentyl benzoate	Oxy	Cbn	Es	Oxy	1.30	0.03
25	27.837	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	4.18	0.09
26	28.95	C10H12O4	Acetosyringone	S	Met	PhOH	Ph	2.56	0.06
27	29.714	C10H12O5	Methyl syringate	S	Met	PhOH	Ph	1.28	0.03
28	30.929	C10H12O4	Acetosyringone	S	Met	PhOH	Ph	0.98	0.02
30	31.283	C12H24O6	1,4,7,10,13,16-	Oxy	Met	O	Oxy	0.87	0.02
31	31.529	C8H16O4	2-(2-Ethoxyethoxy)ethyl	Oxy	HC	Es	Oxy	0.49	0.01
32	33.105	C10H20O3	Ethyl 3-hydroxyoctanoate	Oxy	HC	Es	Oxy	0.78	0.02
33	33.25	C10H20O3	Ethyl 3-hydroxyoctanoate	Oxy	HC	Es	Oxy	0.57	0.01
34	33.498	C10H20O3	Ethyl 3-hydroxyoctanoate	Oxy	HC	Es	Oxy	0.40	0.01
35	33.953	C10H20O3	Ethyl 3-hydroxyoctanoate	Oxy	HC	Es	Oxy	0.43	0.01
36	34.334	C10H20O3	Ethyl 3-hydroxyoctanoate	Oxy	HC	Es	Oxy	0.52	0.01
39	37.302	C12H24O6	1,4,7,10,13,16-	Oxy	Met	O	Oxy	0.63	0.01
41	37.583	C18H38O5	Tetraethylene glycol, decyl	Oxy	Hydx	Alc	Oxy	0.42	0.01
42	40.466	C20H22N2	3H-Indole, 3,3-dimethyl-2-[2-(4-	O	HC	N	N	0.92	0.02
43	40.638	C16H22O4	Dibutyl phthalate	Oxy	Cbn	Es	Oxy	0.66	0.01
45	41.724	C8H5NO6	m-Nitrophthalic acid	Acd	Car	Cabox	N	0.31	0.01
46	42.252	C20H14O5	Helenaquinol	Oxy	Hydx	Ket	Oxy	0.42	0.01
47	42.336	C17H20O6	Fumaric acid, 2,6-	Oxy	Cbn	Es	Oxy	2.05	0.05
48	42.533	C17H20O6	Fumaric acid, 2,6-	Oxy	Cbn	Es	Oxy	0.29	0.01
49	42.836	C26H22	Bibenzhydryl	B	HC	HCs	Ar	1.49	0.03
Sum								100.0	2.21

1-1_KL500C_RuZrO2

Peak	RT	Mol.Form	Name	i	ii	iii	iv	Run	Tot
1	14.417	C8H10O2	Creosol	G	Met	PhOH	Ph	0.83	0.01
2	14.69	C8H10O2	Creosol	G	Met	PhOH	Ph	7.46	0.11
4	17.046	C9H12O2	p-Ethylguaiacol	G	Met	PhOH	Ph	2.75	0.04
5	18.1	C9H10O2	Vinylguaiacol	G	Met	PhOH	Ph	0.93	0.01
6	18.513	C17H18O2	3-(4-Tert-	Oxy	Cbn	Es	Oxy	0.18	0.00
7	18.916	C8H10O3	Syringol	S	Met	PhOH	Ph	19.63	0.30
8	19.35	C10H14O2	Propylguaiacol	G	Met	PhOH	Ph	1.95	0.03
9	21.454	C9H12O3	4-Methylsyringol	S	Met	PhOH	Ph	19.21	0.29
10	23.543	C10H14O3	4-Ethylsyringol	S	Met	PhOH	Ph	7.97	0.12

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11	24.638	C11H16O2	Phenol, 3-tert-butyl-4-	H	Met	PhOH	Ph	5.73	0.09
12	25.655	C12H18O4	Hexamethylene diacrylate	Oxy	Cbn	Es	Oxy	1.62	0.02
13	26.417	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	0.38	0.01
14	27.5	C12H18O3	1-(4,6-Dimethoxy-2,3-	Oxy	Met	Alc	Oxy	2.18	0.03
15	27.812	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	4.81	0.07
16	28.05	C10H12	4-Ethylstyrene	B	HC	HCs	Ar	0.85	0.01
17	28.935	C10H12O4	Acetosyringone	S	Met	PhOH	Ph	2.76	0.04
18	29.699	C10H12O5	Methyl syringate	S	Met	PhOH	Ph	0.71	0.01
19	33.11	C10H20O3	Ethyl 3-hydroxyoctanoate	Oxy	HC	Es	Oxy	0.77	0.01
20	33.25	C10H20O3	Ethyl 3-hydroxyoctanoate	Oxy	HC	Es	Oxy	0.55	0.01
21	33.486	C10H20O3	Ethyl 3-hydroxyoctanoate	Oxy	HC	Es	Oxy	0.30	0.00
22	33.935	C10H20O3	Ethyl 3-hydroxyoctanoate	Oxy	HC	Es	Oxy	0.36	0.01
23	34.316	C18H38O5	Tetraethylene glycol, decyl	Oxy	Hydx	Alc	Oxy	0.49	0.01
24	34.886	C10H20O3	Ethyl 3-hydroxyoctanoate	Oxy	HC	Es	Oxy	0.32	0.00
25	35.329	C16H34O	Hexadecanol	Oxy	Hydx	Alc	Oxy	0.26	0.00
27	36.14	C12H12O5	5,7,8-trimethoxycoumarin	Oxy	Met	Ket	Oxy	0.35	0.01
28	37.287	C12H24O6	1,4,7,10,13,16-	Oxy	Met	O	Oxy	0.59	0.01
30	37.553	C18H38O5	Tetraethylene glycol, decyl	Oxy	Hydx	Alc	Oxy	0.40	0.01
31	38.595	C18H26O3	2-Propenoic acid, 3-(4-	Oxy	Met	Es	Oxy	0.34	0.01
34	39.689	C30H30	1,3,4,6-tetraphenylhexane	B	HC	HCs	Ar	1.48	0.02
35	40.454	C14H18N4O3	Trimethoprim	O	O	N	N	1.28	0.02
36	40.622	C16H22O4	Dibutyl phthalate	Oxy	Cbn	Es	Oxy	1.24	0.02
39	41.133	C24H20	2,6-Dibenzylnaphthalene	B	HC	HCs	Ar	0.27	0.00
40	41.518	C20H42	Icosane	A	HC	HCs	A	1.15	0.02
41	41.708	C10H14OS2	2,4-Bis(allylthio)but-2-enal	O	Cbn	O	O	0.89	0.01
42	42.316	C24H38O4	Bis(2-ethylhexyl) phthalate	Oxy	Cbn	Es	Oxy	4.66	0.07
44	42.833	C26H22	Bibenzhydryl	B	HC	HCs	Ar	1.60	0.02
45	42.9	C30H50	Squalene	A	HC	HCs	A	1.43	0.02
49	45.571	C26H20	Tetraphenylethene	B	HC	HCs	Ar	1.32	0.02
Sum								100.0	1.52

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1-5_KL500C_RuZrO2

Peak	RT	Mol.Form	Name	i	ii	iii	iv	Run	Tot
1	11.922	C7H8O2	Guaiacol	G	Met	PhOH	Ph	3.77	0.08
2	14.4	C8H10O2	Creosol	G	Met	PhOH	Ph	0.62	0.01
3	14.689	C8H10O2	Creosol	G	Met	PhOH	Ph	5.28	0.11
5	17.062	C9H12O2	p-Ethylguaiacol	G	Met	PhOH	Ph	3.15	0.07
6	17.253	C7H8O3	3-Methoxycatechol	C	Met	PhOH	Ph	4.91	0.10
7	17.812	C7H8O3	3-Methoxycatechol	C	Met	PhOH	Ph	1.44	0.03
8	18.105	C9H10O2	Vinylguaiacol	G	Met	PhOH	Ph	2.91	0.06
10	18.501	C18H22O	4-tert-butyl-2-(1-	H	Hydx	PhOH	Ph	1.27	0.03
11	18.907	C8H10O3	Syringol	S	Met	PhOH	Ph	17.60	0.38
12	19.333	C10H14O2	Propylguaiacol	G	Met	PhOH	Ph	3.10	0.07
13	19.667	C9H12O3	4-Methylsyringol	S	Met	PhOH	Ph	0.98	0.02

14	19.899	C8H10O3	Syringol	S	Met	PhOH	Ph	1.93	0.04
15	20.133	C13H28	3-Ethylundecane	A	HC	HCs	A	0.68	0.01
16	20.371	C10H14O3	4-Ethylsyringol	S	Met	PhOH	Ph	0.83	0.02
17	21.456	C9H12O3	4-Methylsyringol	S	Met	PhOH	Ph	14.19	0.30
18	23.563	C10H14O3	4-Ethylsyringol	S	Met	PhOH	Ph	4.86	0.10
19	24.641	C10H12O3	4-Vinylsyringol	S	Met	PhOH	Ph	5.01	0.11
20	25.666	C12H18O4	Hexamethylene	Oxy	Cbn	Es	Oxy	1.13	0.02
21	26.422	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	0.41	0.01
22	26.805	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	0.79	0.02
23	27.565	C12H16O2	Isopentyl benzoate	Oxy	Cbn	Es	Oxy	1.14	0.02
24	27.816	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	3.76	0.08
25	28.93	C10H12O4	Acetosyringone	S	Met	PhOH	Ph	2.02	0.04
26	29.722	C10H12O5	Methyl syringate	S	Met	PhOH	Ph	0.93	0.02
27	29.917	C12H24	cis-5-Dodecene	A	HC	HCs	A	0.36	0.01
29	31.188	C10H20O3	Ethyl 3-	Oxy	HC	Es	Oxy	0.82	0.02
30	31.6	C16H34O	Hexadecanol	Oxy	Hydx	Alc	Oxy	2.45	0.05
31	31.883	S8	Cyclooctasulfur	O	O	O	O	2.74	0.06
32	31.975	S8	Cyclooctasulfur	O	O	O	O	4.68	0.10
33	33.113	C10H20O3	Ethyl 3-	Oxy	HC	Es	Oxy	0.56	0.01
34	33.251	C10H20O3	Ethyl 3-	Oxy	HC	Es	Oxy	0.32	0.01
35	33.497	C10H20O3	Ethyl 3-	Oxy	HC	Es	Oxy	0.29	0.01
36	33.95	C10H20O3	Ethyl 3-	Oxy	HC	Es	Oxy	0.32	0.01
37	37.291	C12H24O6	1,4,7,10,13,16-	Oxy	Met	O	Oxy	0.53	0.01
42	40.625	C16H22O4	Dibutyl phthalate	Oxy	Cbn	Es	Oxy	0.85	0.02
45	42.249	C20H14O5	Helenaquinol	Oxy	Hydx	Ket	Oxy	0.34	0.01
46	42.333	C17H20O6	Fumaric acid, 2,6-	Oxy	Cbn	Es	Oxy	1.81	0.04
47	42.833	C13H12	4-Methylbiphenyl	B	HC	HCs	Ar	1.20	0.03
Sum								100.0	2.13

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Peak	RT	Mol.Form	Name	i	ii	iii	iv	Run	Tot
1	4.214	C9H18	1-Nonene	B	HC	HCs	A	0.79	0.02
2	11.489	C7H8O2	Guaiacol	G	Met	PhOH	Ph	3.70	0.08
3	14.225	C8H10O2	Creosol	G	Met	PhOH	Ph	1.26	0.03
4	14.5	C12H24	cis-5-Dodecene	A	HC	HCs	A	0.23	0.00
5	14.605	C8H10O2	Creosol	G	Met	PhOH	Ph	5.07	0.11
7	16.817	C9H12O2	p-Ethylguaiacol	G	Met	PhOH	Ph	0.65	0.01
8	17.097	C9H12O2	p-Ethylguaiacol	G	Met	PhOH	Ph	10.50	0.22
9	17.4	C14H28	1-Tetradecene	A	HC	HCs	A	1.01	0.02
10	17.567	C10H14O	Thymol	H	Hydx	PhOH	Ph	0.74	0.02
11	17.778	C11H24O	1-Undecanol	Oxy	Hydx	Alc	Oxy	1.12	0.02
12	18.121	C9H10O2	Vinylguaiacol	G	Met	PhOH	Ph	5.54	0.12
13	18.533	C9H10O3	Ethylvanillin	G	Met	PhOH	Ph	0.62	0.01
14	18.764	C17H18O2	3-(4-Tert-	Oxy	Cbn	Es	Oxy	0.64	0.01

15	19.1	C8H10O3	Syringol	S	Met	PhOH	Ph	11.84	0.25
16	19.283	C10H14O2	Propylguaiacol	G	Met	PhOH	Ph	3.97	0.08
17	19.533	C10H14O2	Propylguaiacol	G	Met	PhOH	Ph	1.08	0.02
18	19.71	C8H10O3	Syringol	S	Met	PhOH	Ph	5.04	0.11
19	20.133	C10H16O	2-Hexylfuran	F	HC	Fu	Oxy	1.08	0.02
20	20.39	C10H12O2	Eugenol	G	Met	PhOH	Ph	0.46	0.01
21	20.527	C10H14O3	4-Ethylsyringol	S	Met	PhOH	Ph	0.64	0.01
22	20.719	C10H12O2	Eugenol	G	Met	PhOH	Ph	0.63	0.01
23	21.217	C11H16O2	Phenol, 3-tert-butyl-4-	H	Met	PhOH	Ph	0.76	0.02
24	21.657	C9H12O3	4-Methylsyringol	S	Met	PhOH	Ph	11.76	0.25
25	22.217	C8H8O4	p-Vanillic acid	G	Met	PhOH	Ph	0.98	0.02
26	23.339	C9H10O3	Ethylvanillin	G	Met	PhOH	Ph	0.49	0.01
27	23.55	C13H26	1-Tridecene	A	HC	HCs	A	0.40	0.01
28	23.69	C10H14O3	4-Ethylsyringol	S	Met	PhOH	Ph	5.83	0.12
29	24.2	C10H12O3	4-Vinylsyringol	S	Met	PhOH	Ph	0.59	0.01
30	24.702	C10H12O3	4-Vinylsyringol	S	Met	PhOH	Ph	5.17	0.11
31	25.673	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	0.68	0.01
32	25.76	C12H18O4	Hexamethylene diacrylate	Oxy	Cbn	Es	Oxy	1.01	0.02
33	26.474	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	0.51	0.01
34	26.837	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	0.91	0.02
35	27.39	C9H10O4	Syringaldehyde	S	Met	PhOH	Ph	2.40	0.05
36	27.933	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	3.10	0.07
37	28.905	C10H12O4	Acetosyringone	S	Met	PhOH	Ph	2.14	0.04
38	29.688	C10H12O5	Methyl syringate	S	Met	PhOH	Ph	1.27	0.03
39	30.904	C10H12O4	Acetosyringone	S	Met	PhOH	Ph	0.93	0.02
40	33.31	C22H46O6	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy	0.33	0.01
41	33.433	C22H46O6	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy	0.19	0.00
42	33.65	C22H46O6	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy	0.92	0.02
43	34.103	C22H46O6	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy	0.40	0.01
44	37.647	C15H30O	2-Pentadecanone	Oxy	Cbn	Ket	Oxy	0.33	0.01
46	40.54	C18H35NO	9-Octadecenamide	O	O	N	N	0.53	0.01
47	40.77	C16H22O4	Dibutyl phthalate	Oxy	Cbn	Es	Oxy	0.79	0.02
49	42.451	C17H20O6	Fumaric acid, 2,6-	Oxy	Cbn	Es	Oxy	0.72	0.02
50	42.949	C26H22	Bibenzhydryl	B	HC	HCs	Ar	0.26	0.01
Sum								100.0	2.10

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1-1_KL600_ZrO2

Peak	RT	Mol.Form	Name	i	ii	iii	iv	Run	Tot
1	4.214	C9H18	1-Nonene	B	HC	HCs	A	0.78	0.01
2	11.557	C7H8O2	Guaiacol	G	Met	PhOH	Ph	3.22	0.06
3	14.282	C8H10O2	Creosol	G	Met	PhOH	Ph	1.12	0.02
4	14.5	C12H24	cis-5-Dodecene	A	HC	HCs	A	0.37	0.01
5	14.64	C8H10O2	Creosol	G	Met	PhOH	Ph	5.22	0.10
7	16.867	C9H12O2	p-Ethylguaiacol	G	Met	PhOH	Ph	0.64	0.01

8	17.128	C9H12O2	p-Ethylguaiacol	G	Met	PhOH	Ph	12.06	0.23
9	17.78	C11H24O	1-Undecanol	Oxy	Hydx	Alc	Oxy	0.89	0.02
10	18.149	C9H10O2	Vinylguaiacol	G	Met	PhOH	Ph	5.98	0.11
11	18.533	C9H10O3	Ethylvanillin	G	Met	PhOH	Ph	0.71	0.01
12	18.763	C17H18O2	3-(4-Tert-	Oxy	Cbn	Es	Oxy	0.84	0.02
13	19.101	C8H10O3	Syringol	S	Met	PhOH	Ph	12.03	0.22
14	19.283	C10H12O2	Eugenol	G	Met	PhOH	Ph	4.58	0.09
15	19.533	C10H14O2	Propylguaiacol	G	Met	PhOH	Ph	1.21	0.02
16	19.736	C12H20O	Furan, 2,5-dibutyl-	F	HC	Fu	Oxy	4.90	0.09
17	20.137	C10H12O2	Eugenol	G	Met	PhOH	Ph	1.25	0.02
18	20.413	C10H12O2	Eugenol	G	Met	PhOH	Ph	0.50	0.01
19	20.538	C10H12O2	Eugenol	G	Met	PhOH	Ph	0.65	0.01
20	20.739	C10H12O2	Eugenol	G	Met	PhOH	Ph	0.64	0.01
21	21.656	C9H12O3	4-Methylsyringol	S	Met	PhOH	Ph	11.68	0.22
23	23.702	C10H14O3	4-Ethylsyringol	S	Met	PhOH	Ph	5.01	0.09
24	24.25	C10H14O2	Propylguaiacol	G	Met	PhOH	Ph	1.14	0.02
25	24.707	C10H12O3	4-Vinylsyringol	S	Met	PhOH	Ph	5.80	0.11
26	25.683	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	0.63	0.01
27	25.77	C12H18O4	Hexamethylene diacrylate	Oxy	Cbn	Es	Oxy	0.94	0.02
28	26.487	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	0.62	0.01
29	26.859	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	1.17	0.02
30	27.469	C9H10O4	Syringaldehyde	S	Met	PhOH	Ph	3.06	0.06
31	27.947	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	3.93	0.07
32	28.938	C10H12O4	Acetosyringone	S	Met	PhOH	Ph	2.51	0.05
33	29.722	C10H12O5	Methyl syringate	S	Met	PhOH	Ph	1.26	0.02
34	30.936	C10H12O4	Acetosyringone	S	Met	PhOH	Ph	0.73	0.01
35	33.314	C22H46O6	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy	0.36	0.01
36	33.433	C22H46O6	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy	0.20	0.00
37	34.538	C15H30O	2-Pentadecanone	Oxy	Cbn	Ket	Oxy	0.37	0.01
39	37.202	C18H37NO	Octadecanamide	O	O	N	N	0.32	0.01
44	40.767	C16H22O4	Dibutyl phthalate	Oxy	Cbn	Es	Oxy	1.07	0.02
46	41.133	C17H20O6	Fumaric acid, 2,6-	Oxy	Cbn	Es	Oxy	0.23	0.00
47	42.449	C18H35NO	9-Octadecenamide	O	O	N	N	0.97	0.02
49	42.944	C18H36	1-Octadecene	A	HC	HCs	A	0.44	0.01
Sum								100.0	1.87

1-1_KL600C_NiZrO2

Peak	RT	Mol.Form	Name	i	ii	iii	iv	Run	Tot
1	4.428	C9H18	1-Nonene	B	HC	HCs	A	0.62	0.01
2	5.619	C9H8O	Cinnamaldehyde	Oxy	Cbn	Aldh	Oxy	1.93	0.04
3	11.736	C7H8O2	Guaiacol	G	Met	PhOH	Ph	3.64	0.08
4	14.518	C8H10O2	Creosol	G	Met	PhOH	Ph	0.89	0.02
5	14.916	C8H10O2	Creosol	G	Met	PhOH	Ph	5.74	0.12
7	17.241	C7H8O3	3-Methoxycatechol	C	Met	PhOH	Ph	5.01	0.11

8	17.454	$C_9H_{12}O_2$	p-Ethylguaiacol	G	Met	PhOH	Ph	6.72	0.14
9	17.983	$C_7H_8O_3$	3-Methoxycatechol	C	Met	PhOH	Ph	2.35	0.05
10	18.27	$C_{11}H_{24}O$	1-Undecanol	Oxy	Hydx	Alc	Oxy	0.66	0.01
11	18.498	$C_9H_{10}O_2$	Vinylguaiacol	G	Met	PhOH	Ph	3.81	0.08
12	18.75	$C_{11}H_{24}O$	1-Undecanol	Oxy	Hydx	Alc	Oxy	0.68	0.01
13	19.266	$C_{17}H_{18}O_2$	3-(4-Tert-	Oxy	Cbn	Es	Oxy	0.87	0.02
14	19.51	$C_8H_{10}O_3$	Syringol	S	Met	PhOH	Ph	14.59	0.31
15	19.976	$C_8H_{10}O_3$	Syringol	S	Met	PhOH	Ph	4.29	0.09
16	20.233	$C_{15}H_{30}O$	2-Pentadecanone	Oxy	Cbn	Ket	Oxy	1.32	0.03
17	20.465	$C_9H_{12}O_2$	p-Ethylguaiacol	G	Met	PhOH	Ph	0.69	0.01
18	20.65	$C_{14}H_{28}$	1-Tetradecene	A	HC	HCs	A	0.44	0.01
19	20.78	$C_{10}H_{12}O_2$	Eugenol	G	Met	PhOH	Ph	0.43	0.01
20	20.937	$C_{10}H_{12}O_2$	Eugenol	G	Met	PhOH	Ph	0.51	0.01
21	21.103	$C_{10}H_{12}O_2$	Eugenol	G	Met	PhOH	Ph	0.67	0.01
22	21.427	$C_8H_8O_3$	Vanillin	G	Met	PhOH	Ph	1.08	0.02
23	22.098	$C_9H_{12}O_3$	4-Methylsyringol	S	Met	PhOH	Ph	11.80	0.25
24	22.389	$C_8H_8O_4$	p-Vanillic acid	G	Met	PhOH	Ph	1.49	0.03
25	22.668	$C_{10}H_{21}CL$	1-Chlorodecane	O	O	O	O	0.46	0.01
26	24.133	$C_{10}H_{14}O_3$	4-Ethylsyringol	S	Met	PhOH	Ph	4.31	0.09
27	24.461	$C_{10}H_{12}O_3$	4-Vinylsyringol	S	Met	PhOH	Ph	0.46	0.01
28	25.141	$C_{10}H_{12}O_3$	4-Vinylsyringol	S	Met	PhOH	Ph	5.10	0.11
29	26.072	$C_{11}H_{14}O_3$	4-Allylsyringol	S	Met	PhOH	Ph	1.21	0.03
30	26.215	$C_{12}H_{18}O_4$	Hexamethylene diacrylate	Oxy	Cbn	Es	Oxy	0.80	0.02
31	26.878	$C_{11}H_{14}O_3$	4-Allylsyringol	S	Met	PhOH	Ph	0.52	0.01
32	27.247	$C_{11}H_{14}O_3$	4-Allylsyringol	S	Met	PhOH	Ph	0.93	0.02
33	27.714	$C_9H_{10}O_4$	Syringaldehyde	S	Met	PhOH	Ph	1.71	0.04
34	28.402	$C_{11}H_{14}O_3$	4-Allylsyringol	S	Met	PhOH	Ph	3.11	0.07
35	29.182	$C_{22}H_{46}O$	1-Docosanol	Oxy	Hydx	Alc	Oxy	0.42	0.01
36	29.326	$C_{10}H_{12}O_4$	Acetosyringone	S	Met	PhOH	Ph	1.70	0.04
37	30.12	$C_{10}H_{12}O_5$	Methyl syringate	S	Met	PhOH	Ph	0.86	0.02
38	31.324	$C_{10}H_{12}O_4$	Acetosyringone	S	Met	PhOH	Ph	0.56	0.01
39	34.15	$C_{15}H_{30}O_2$	Methyl tetradecanoate	Oxy	Cbn	Es	Oxy	0.58	0.01
40	37.473	$C_{16}H_{33}NO$	Palmiticamide	O	O	N	N	0.81	0.02
41	39.49	$C_{18}H_{35}NO$	9-Octadecenamide	O	O	N	N	2.08	0.04
42	39.579	$C_{18}H_{35}NO$	9-Octadecenamide	O	O	N	N	1.19	0.03
43	39.805	$C_{10}H_{21}NO$	Decanamide	O	Cbn	N	N	0.37	0.01
44	40.287	$C_{10}H_{12}$	4-Ethylstyrene	B	HC	HCs	Ar	0.35	0.01
46	41.184	$C_{16}H_{22}O_4$	Dibutyl phthalate	Oxy	Cbn	Es	Oxy	0.60	0.01
47	42.846	$C_{17}H_{20}O_6$	Fumaric acid, 2,6-	Oxy	Cbn	Es	Oxy	0.46	0.01
48	43.221	$C_{18}H_{35}NO$	9-Octadecenamide	O	O	N	N	0.49	0.01
49	45.541	$C_{15}H_{30}O$	2-Pentadecanone	Oxy	Cbn	Ket	Oxy	0.39	0.01
50	45.678	$C_{29}H_{50}O$	β-Sitosterol	ST	Hydx	Alc	Oxy	0.29	0.01
Sum								100.0	2.15

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1-5_KL600C_NiZrO2

Peak	RT	Mol.Form	Name	i	ii	iii	iv	Run	Tot
1	4.429	C9H18	1-Nonene	B	HC	HCs	A	0.63	0.01
2	11.755	C7H8O2	Guaiacol	G	Met	PhOH	Ph	3.63	0.07
3	14.524	C8H10O2	Creosol	G	Met	PhOH	Ph	1.17	0.02
4	14.928	C8H10O2	Creosol	G	Met	PhOH	Ph	5.87	0.11
6	17.273	C7H8O3	3-Methoxycatechol	C	Met	PhOH	Ph	4.22	0.08
7	17.465	C9H12O2	p-Ethylguaiacol	G	Met	PhOH	Ph	7.35	0.14
8	17.867	C14H28	1-Tetradecene	A	HC	HCs	A	0.41	0.01
9	18	C7H8O3	3-Methoxycatechol	C	Met	PhOH	Ph	1.83	0.04
10	18.265	C11H24O	1-Undecanol	Oxy	Hydx	Alc	Oxy	0.64	0.01
11	18.5	C9H10O2	Vinylguaiacol	G	Met	PhOH	Ph	3.95	0.08
12	18.75	C11H24O	1-Undecanol	Oxy	Hydx	Alc	Oxy	0.66	0.01
13	19.265	C17H18O2	3-(4-Tert-	Oxy	Cbn	Es	Oxy	0.81	0.02
14	19.512	C8H10O3	Syringol	S	Met	PhOH	Ph	13.85	0.27
15	19.733	C9H10O3	Ethylvanillin	G	Met	PhOH	Ph	1.72	0.03
16	19.984	C8H10O3	Syringol	S	Met	PhOH	Ph	4.89	0.09
17	20.233	C15H30O	2-Pentadecanone	Oxy	Cbn	Ket	Oxy	1.35	0.03
18	20.464	C9H12O2	p-Ethylguaiacol	G	Met	PhOH	Ph	0.81	0.02
19	20.65	C14H28	1-Tetradecene	A	HC	HCs	A	0.51	0.01
20	20.779	C10H12O2	Eugenol	G	Met	PhOH	Ph	0.49	0.01
21	20.932	C10H12O2	Eugenol	G	Met	PhOH	Ph	0.64	0.01
22	21.107	C10H12O2	Eugenol	G	Met	PhOH	Ph	0.63	0.01
23	21.425	C8H8O3	Vanillin	G	Met	PhOH	Ph	0.95	0.02
24	21.678	C11H16O2	Phenol, 3-tert-butyl-4-	H	Met	PhOH	Ph	0.60	0.01
25	22.099	C9H12O3	4-Methylsyringol	S	Met	PhOH	Ph	11.78	0.23
26	22.385	C8H8O4	p-Vanillic acid	G	Met	PhOH	Ph	1.79	0.03
27	22.667	C11H23Cl	1-Chloroundecane	O	O	O	O	0.52	0.01
28	22.92	C12H18O	p-Hexylphenol	H	HC	PhOH	Ph	0.71	0.01
29	23.495	C9H10O3	Ethylvanillin	G	Met	PhOH	Ph	0.71	0.01
30	24.135	C10H14O3	4-Ethylsyringol	S	Met	PhOH	Ph	4.43	0.09
31	24.455	C10H12O3	4-Vinylsyringol	S	Met	PhOH	Ph	0.56	0.01
32	25.139	C10H12O3	4-Vinylsyringol	S	Met	PhOH	Ph	5.20	0.10
33	26.071	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	1.00	0.02
34	26.216	C12H18O4	Hexamethylene diacrylate	Oxy	Cbn	Es	Oxy	0.76	0.01
35	26.874	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	0.54	0.01
36	27.245	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	0.87	0.02
37	27.723	C9H10O4	Syringaldehyde	S	Met	PhOH	Ph	1.88	0.04
38	28.399	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	3.06	0.06
39	29.18	C20H42O	1-Icosanol	Oxy	Hydx	Alc	Oxy	0.38	0.01
40	29.323	C10H12O4	Acetosyringone	S	Met	PhOH	Ph	1.81	0.03
41	30.119	C10H12O5	Methyl syringate	S	Met	PhOH	Ph	0.95	0.02
42	31.322	C10H12O4	Acetosyringone	S	Met	PhOH	Ph	0.66	0.01
43	34.15	C15H30O2	Methyl tetradecanoate	Oxy	Cbn	Es	Oxy	0.57	0.01
44	34.545	C19H38O2	Methyl stearate	Oxy	Cbn	Es	Oxy	0.27	0.01
45	37.513	C10H21NO	Decanamide	O	Cbn	N	N	0.48	0.01

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46	39.514	C18H35NO	9-Octadecenamide	O	O	N	N	1.17	0.02
47	39.608	C18H35NO	9-Octadecenamide	O	O	N	N	0.82	0.02
48	40.922	C14H18N4O3	Trimethoprim	O	O	N	N	0.38	0.01
49	41.184	C16H22O4	Dibutyl phthalate	Oxy	Cbn	Es	Oxy	0.53	0.01
50	42.844	C17H20O6	Fumaric acid, 2,6-	Oxy	Cbn	Es	Oxy	0.52	0.01
Sum								100.0	1.93

1-10_KL600C_NiZrO2

Peak	RT	Mol.Form	Name	i	ii	iii	iv	Run	Tot
1	4.527	C9H18	1-Nonene	B	HC	HCs	A	0.61	0.01
2	12.031	C7H8O2	Guaiacol	G	Met	PhOH	Ph	3.44	0.06
3	14.783	C8H10O2	Creosol	G	Met	PhOH	Ph	1.24	0.02
4	15.154	C8H10O2	Creosol	G	Met	PhOH	Ph	5.07	0.09
6	17.383	C9H12O2	p-Ethylguaiacol	G	Met	PhOH	Ph	1.11	0.02
7	17.645	C9H12O2	p-Ethylguaiacol	G	Met	PhOH	Ph	9.05	0.16
8	17.95	C14H28	1-Tetradecene	A	HC	HCs	A	1.24	0.02
9	18.117	C13H26	1-Tridecene	A	HC	HCs	A	0.95	0.02
10	18.342	C11H24O	1-Undecanol	Oxy	Hydx	Alc	Oxy	1.66	0.03
11	18.666	C9H10O2	Vinylguaiacol	G	Met	PhOH	Ph	4.25	0.07
12	18.8	C11H24O	1-Undecanol	Oxy	Hydx	Alc	Oxy	1.66	0.03
13	18.983	C10H12O2	Eugenol	G	Met	PhOH	Ph	0.65	0.01
14	19.1	C10H14O2	Propylguaiacol	G	Met	PhOH	Ph	0.76	0.01
15	19.328	C17H18O2	3-(4-Tert-	Oxy	Cbn	Es	Oxy	0.70	0.01
16	19.607	C8H10O3	Syringol	S	Met	PhOH	Ph	12.21	0.21
17	19.817	C10H12O2	Eugenol	G	Met	PhOH	Ph	4.19	0.07
18	20.1	C10H14O2	Propylguaiacol	G	Met	PhOH	Ph	0.92	0.02
19	20.254	C10H12O4	Acetosyringone	S	Met	PhOH	Ph	4.29	0.07
20	20.717	C14H28	1-Tetradecene	A	HC	HCs	A	1.62	0.03
21	20.95	C13H28	3-Ethylundecane	A	HC	HCs	A	0.81	0.01
22	21.08	C10H12O2	Eugenol	G	Met	PhOH	Ph	0.75	0.01
23	21.304	C10H12O2	Eugenol	G	Met	PhOH	Ph	0.62	0.01
24	22.187	C9H12O3	4-Methylsyringol	S	Met	PhOH	Ph	10.04	0.17
25	24.253	C10H14O3	4-Ethylsyringol	S	Met	PhOH	Ph	4.22	0.07
26	25.253	C10H12O3	4-Vinylsyringol	S	Met	PhOH	Ph	5.40	0.09
27	26.25	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	0.63	0.01
28	26.347	C12H18O4	Hexamethylene diacrylate	Oxy	Cbn	Es	Oxy	0.77	0.01
29	27.05	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	0.57	0.01
30	27.42	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	1.06	0.02
31	28.027	C9H10O4	Syringaldehyde	S	Met	PhOH	Ph	2.35	0.04
32	28.2	C11H12O3	Cinnamaldehyde, 3,4-	Oxy	Met	Aldh	Oxy	0.52	0.01
33	28.503	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	4.47	0.08
34	28.817	C23H46O2	Methyl docosanoate	Oxy	Cbn	Es	Oxy	0.65	0.01
35	29.236	C11H22O3	Methyl 10-	Oxy	Cbn	Es	Oxy	0.59	0.01
36	29.489	C10H12O4	Acetosyringone	S	Met	PhOH	Ph	0.95	0.02

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37	29.59	C10H20O3	Ethyl 3-hydroxyoctanoate	Oxy	HC	Es	Oxy	1.67	0.03
38	30.303	C10H12O5	Methyl syringate	S	Met	PhOH	Ph	1.31	0.02
39	30.687	C13H28O	1-Tridecanol	Oxy	Hydx	Alc	Oxy	1.03	0.02
40	30.816	C14H30O	Tetradecanol	Oxy	Hydx	Alc	Oxy	0.53	0.01
41	31.041	C23H46O2	Methyl docosanoate	Oxy	Cbn	Es	Oxy	0.35	0.01
42	31.527	C10H12O4	Acetosyringone	S	Met	PhOH	Ph	1.22	0.02
43	31.807	C10H20O3	Ethyl 3-hydroxyoctanoate	Oxy	HC	Es	Oxy	0.42	0.01
44	33.93	C16H22O4	Dibutyl phthalate	Oxy	Cbn	Es	Oxy	0.97	0.02
45	40.733	C16H30O	cis-9-Hexadecenal	Oxy	Cbn	Aldh	Ar	0.31	0.01
47	41.221	C16H22O4	Dibutyl phthalate	Oxy	Cbn	Es	Oxy	0.50	0.01
48	42.903	C17H20O6	Fumaric acid, 2,6-	Oxy	Cbn	Es	Oxy	0.68	0.01
49	43.273	C18H35NO	9-Octadecenamide	O	O	N	N	0.77	0.01
50	43.417	C9H10O4	Syringaldehyde	S	Met	PhOH	Ph	0.23	0.00
Sum								100.0	1.74

1-1_KL600C_PdZr

Peak	RT	Mol.Form	Name	i	ii	iii	iv	Run	Tot
1	11.523	C7H8O2	Guaiacol	G	Met	PhOH	Ph	3.38	0.05
2	14.167	C8H10O2	Creosol	G	Met	PhOH	Ph	1.20	0.02
3	14.455	C8H10O2	Creosol	G	Met	PhOH	Ph	6.33	0.10
4	16.932	C9H12O2	p-Ethylguaiacol	G	Met	PhOH	Ph	4.08	0.06
5	17.133	C7H8O3	3-Methoxycatechol	C	Met	PhOH	Ph	3.83	0.06
6	17.283	C8H12O2	1-Oxetan-2-one, 4,4-diethyl-	Oxy	Cbn	Ket	Oxy	4.50	0.07
7	17.958	C9H10O2	Vinylguaiacol	G	Met	PhOH	Ph	6.27	0.10
8	18.3	C10H14O2	Propylguaiacol	G	Met	PhOH	Ph	1.14	0.02
9	18.469	C17H18O2	3-(4-Tert-	Oxy	Cbn	Es	Oxy	0.74	0.01
10	18.75	C10H14O2	Propylguaiacol	G	Met	PhOH	Ph	1.06	0.02
11	18.874	C8H10O3	Syringol	S	Met	PhOH	Ph	16.60	0.25
12	19.283	C10H14O2	Propylguaiacol	G	Met	PhOH	Ph	2.42	0.04
13	19.601	C10H12O4	Acetosyringone	S	Met	PhOH	Ph	3.81	0.06
14	19.867	C12H24	cis-5-Dodecene	A	HC	HCs	A	0.97	0.01
15	19.983	C9H12O2	p-Ethylguaiacol	G	Met	PhOH	Ph	0.94	0.01
16	20.2	C10H12O2	Eugenol	G	Met	PhOH	Ph	0.37	0.01
17	20.302	C10H12O2	Eugenol	G	Met	PhOH	Ph	0.59	0.01
18	20.532	C10H12O2	Eugenol	G	Met	PhOH	Ph	0.50	0.01
19	21.408	C9H12O3	4-Methylsyringol	S	Met	PhOH	Ph	13.72	0.21
20	23.471	C10H14O3	4-Ethylsyringol	S	Met	PhOH	Ph	5.29	0.08
21	24.55	C10H12O3	4-Vinylsyringol	S	Met	PhOH	Ph	5.11	0.08
22	25.55	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	1.32	0.02
23	25.717	C2H4S5	Lenthionine	O	O	O	O	0.54	0.01
24	26.335	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	0.41	0.01
25	26.707	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	0.93	0.01
26	27.533	C9H10O4	Syringaldehyde	S	Met	PhOH	Ph	0.82	0.01
27	27.84	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	3.29	0.05

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28	29.002	C10H12O4	Acetosyringone	S	Met	PhOH	Ph	1.16	0.02
29	29.8	C11H14O4	Sinapyl alcohol	S	Met	PhOH	Ph	0.56	0.01
30	37.3	C12H24O6	1,4,7,10,13,16-	Oxy	Met	O	Oxy	1.14	0.02
31	37.405	C14H30O6	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy	0.73	0.01
32	37.581	C14H30O6	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy	0.54	0.01
33	37.909	C14H30O6	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy	0.43	0.01
34	38.188	C12H24O6	1,4,7,10,13,16-	Oxy	Met	O	Oxy	0.51	0.01
36	39.203	C18H35NO	9-Octadecenamide	O	O	N	N	0.31	0.00
37	39.29	C18H35NO	9-Octadecenamide	O	O	N	N	0.64	0.01
38	39.485	C18H35NO	9-Octadecenamide	O	O	N	N	0.47	0.01
40	40.636	C16H22O4	Dibutyl phthalate	Oxy	Cbn	Es	Oxy	0.66	0.01
42	41.665	C16H33NO	Palmiticamide	O	O	N	N	0.23	0.00
44	42.283	C20H14O5	Helenaquinol	Oxy	Hydx	Ket	Oxy	0.21	0.00
45	42.382	C17H20O6	Fumaric acid, 2,6-	Oxy	Cbn	Es	Oxy	1.29	0.02
46	42.879	C12H18O4	Hexamethylene diacrylate	Oxy	Cbn	Es	Oxy	0.96	0.01
Sum								100.0	1.52

1-5_KL600C_PdZr

Peak	RT	Mol.Form	Name	i	ii	iii	iv	Run	Tot
1	11.684	C7H8O2	Guaiacol	G	Met	PhOH	Ph	3.71	0.08
2	14.33	C8H10O2	Creosol	G	Met	PhOH	Ph	1.15	0.03
3	14.556	C8H10O2	Creosol	G	Met	PhOH	Ph	6.42	0.14
5	16.75	C9H10O2	Vinylguaiacol	G	Met	PhOH	Ph	0.69	0.02
6	17.037	C9H12O2	p-Ethylguaiacol	G	Met	PhOH	Ph	4.73	0.11
7	17.294	C7H8O3	3-Methoxycatechol	C	Met	PhOH	Ph	2.69	0.06
8	17.417	C10H14O	Thymol	H	Hydx	PhOH	Ph	1.07	0.02
9	17.567	C7H8O3	3-Methoxycatechol	C	Met	PhOH	Ph	3.22	0.07
10	18.018	C9H10O2	Vinylguaiacol	G	Met	PhOH	Ph	5.35	0.12
11	18.317	C10H14O2	Propylguaiacol	G	Met	PhOH	Ph	2.35	0.05
13	18.767	C10H14O2	Propylguaiacol	G	Met	PhOH	Ph	1.49	0.03
14	18.913	C8H10O3	Syringol	S	Met	PhOH	Ph	20.50	0.46
15	19.713	C8H10O3	Syringol	S	Met	PhOH	Ph	5.37	0.12
16	20.083	C9H12O2	p-Ethylguaiacol	G	Met	PhOH	Ph	1.59	0.04
17	20.32	C10H12O2	Eugenol	G	Met	PhOH	Ph	2.21	0.05
18	20.597	C10H12O2	Eugenol	G	Met	PhOH	Ph	1.15	0.03
19	20.975	C11H16O2	Phenol, 3-tert-butyl-	H	Met	PhOH	Ph	1.15	0.03
20	21.439	C9H12O3	4-Methylsyringol	S	Met	PhOH	Ph	16.16	0.36
21	22.233	C10H12O4	Acetosyringone	S	Met	PhOH	Ph	1.12	0.03
23	23.522	C10H14O3	4-Ethylsyringol	S	Met	PhOH	Ph	5.48	0.12
24	24.619	C10H12O3	4-Vinylsyringol	S	Met	PhOH	Ph	4.74	0.11
25	25.676	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	1.14	0.03
26	25.8	C2H4S5	Lenthionine	O	O	O	O	0.39	0.01
27	26.445	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	0.20	0.00
28	26.717	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	0.15	0.00

29	26.837	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	0.48	0.01
30	27.958	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	3.32	0.07
32	37.406	C26H54O8	Heptaethylene	Oxy	Hydx	Alc	Oxy	0.54	0.01
33	39.072	C9H12O2	p-Ethylguaiacol	G	Met	PhOH	Ph	0.12	0.00
34	40.198	C18H33N	Tricyclohexylamine	O	O	N	N	0.06	0.00
36	40.65	C16H22O4	Dibutyl phthalate	Oxy	Cbn	Es	Oxy	0.12	0.00
41	42.3	C20H14O5	Helenaquinol	Oxy	Hydx	Ket	Oxy	0.17	0.00
42	42.398	C17H20O6	Fumaric acid, 2,6-	Oxy	Cbn	Es	Oxy	0.97	0.02
Sum								100.0	2.25

1-1_KL600C_RuZrO2

Peak	RT	Mol.Form	Name	i	ii	iii	iv	Run	Tot
1	11.471	C7H8O2	Guaiacol	G	Met	PhOH	Ph	3.54	0.05
2	14.106	C8H10O2	Creosol	G	Met	PhOH	Ph	1.14	0.02
3	14.439	C8H10O2	Creosol	G	Met	PhOH	Ph	6.22	0.08
4	16.902	C9H12O2	p-Ethylguaiacol	G	Met	PhOH	Ph	12.55	0.17
5	17.934	C9H10O2	Vinylguaiacol	G	Met	PhOH	Ph	7.39	0.10
6	18.467	C17H18O2	3-(4-Tert-	Oxy	Cbn	Es	Oxy	0.54	0.01
7	18.733	C10H14O2	Propylguaiacol	G	Met	PhOH	Ph	0.96	0.01
8	18.855	C8H10O3	Syringol	S	Met	PhOH	Ph	17.15	0.23
9	19.267	C10H14O2	Propylguaiacol	G	Met	PhOH	Ph	1.80	0.02
10	19.559	C8H10O3	Syringol	S	Met	PhOH	Ph	5.36	0.07
11	19.95	C9H12O2	p-Ethylguaiacol	G	Met	PhOH	Ph	0.98	0.01
12	20.281	C10H12O2	Eugenol	G	Met	PhOH	Ph	0.88	0.01
13	20.499	C10H12O2	Eugenol	G	Met	PhOH	Ph	0.61	0.01
14	21.403	C9H12O3	4-Methylsyringol	S	Met	PhOH	Ph	14.10	0.19
15	22.067	C9H12O3	4-Methylsyringol	S	Met	PhOH	Ph	0.97	0.01
16	22.217	C12H18O	p-Hexylphenol	H	HC	PhOH	Ph	0.24	0.00
17	23.317	C10H14O2	Propylguaiacol	G	Met	PhOH	Ph	0.64	0.01
18	23.461	C10H14O3	4-Ethylsyringol	S	Met	PhOH	Ph	5.21	0.07
19	24.518	C10H12O3	4-Vinylsyringol	S	Met	PhOH	Ph	5.66	0.08
20	25.522	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	1.30	0.02
21	25.677	C2H4S5	Lenthionine	O	O	O	O	0.82	0.01
23	26.297	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	0.46	0.01
24	26.666	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	0.97	0.01
25	27.483	C9H10O4	Syringaldehyde	S	Met	PhOH	Ph	1.54	0.02
26	27.8	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	3.41	0.05
27	28.986	C10H12O4	Acetosyringone	S	Met	PhOH	Ph	1.02	0.01
28	29.804	C10H12O5	Methyl syringate	S	Met	PhOH	Ph	0.32	0.00
30	37.345	C12H24O6	1,4,7,10,13,16-	Oxy	Met	O	Oxy	0.25	0.00
33	40.65	C16H22O4	Dibutyl phthalate	Oxy	Cbn	Es	Oxy	0.32	0.00
37	42.283	C20H14O5	Helenaquinol	Oxy	Hydx	Ket	Oxy	0.24	0.00
38	42.381	C17H20O6	Fumaric acid, 2,6-	Oxy	Cbn	Es	Oxy	1.18	0.02
39	42.88	C12H18O4	Hexamethylene diacrylate	Oxy	Cbn	Es	Oxy	0.77	0.01

48	50.292	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	0.26	0.00
49	52.273	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	0.88	0.01
50	55.046	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	0.33	0.00
Sum								100.0	1.35

1-5_KL600C_RuZrO2

Peak	RT	Mol.Form	Name	i	ii	iii	iv	Run	Tot
1	11.569	C7H8O2	Guaiacol	G	Met	PhOH	Ph	3.16	0.04
2	14.218	C8H10O2	Creosol	G	Met	PhOH	Ph	1.05	0.01
3	14.507	C8H10O2	Creosol	G	Met	PhOH	Ph	6.80	0.08
4	16.633	C9H12O2	p-Ethylguaiacol	G	Met	PhOH	Ph	0.49	0.01
5	16.999	C9H12O2	p-Ethylguaiacol	G	Met	PhOH	Ph	4.38	0.05
6	17.189	C7H8O3	3-Methoxycatechol	C	Met	PhOH	Ph	3.05	0.03
7	17.389	C7H8O3	3-Methoxycatechol	C	Met	PhOH	Ph	4.06	0.05
8	17.989	C9H10O2	Vinylguaiacol	G	Met	PhOH	Ph	5.84	0.07
9	18.283	C11H16O2	Phenol, 3-tert-butyl-	H	Met	PhOH	Ph	2.58	0.03
11	18.75	C10H14O2	Propylguaiacol	G	Met	PhOH	Ph	1.18	0.01
12	18.9	C8H10O3	Syringol	S	Met	PhOH	Ph	20.73	0.24
13	19.657	C8H10O3	Syringol	S	Met	PhOH	Ph	4.14	0.05
14	20	C9H12O2	p-Ethylguaiacol	G	Met	PhOH	Ph	1.18	0.01
15	20.31	C10H12O2	Eugenol	G	Met	PhOH	Ph	1.12	0.01
16	20.566	C10H12O2	Eugenol	G	Met	PhOH	Ph	0.43	0.00
17	21.438	C9H12O3	4-Methylsyringol	S	Met	PhOH	Ph	16.92	0.19
18	22.233	C10H12O4	Acetosyringone	S	Met	PhOH	Ph	0.16	0.00
19	23.505	C10H14O3	4-Ethylsyringol	S	Met	PhOH	Ph	5.76	0.07
20	24.578	C10H12O3	4-Vinylsyringol	S	Met	PhOH	Ph	5.50	0.06
21	25.583	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	0.83	0.01
22	25.7	C2H4S5	Lenthionine	O	O	O	O	1.07	0.01
23	25.95	C10H12O3	4-Vinylsyringol	S	Met	PhOH	Ph	0.31	0.00
24	26.375	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	0.16	0.00
25	26.761	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	0.88	0.01
26	27.633	C9H10O4	Syringaldehyde	S	Met	PhOH	Ph	0.64	0.01
27	27.894	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	3.25	0.04
28	29.08	C10H12O4	Acetosyringone	S	Met	PhOH	Ph	1.38	0.02
34	39.525	C18H37NO	Octadecanamide	O	O	N	N	0.39	0.00
36	40.642	C16H22O4	Dibutyl phthalate	Oxy	Cbn	Es	Oxy	0.34	0.00
40	42.3	C20H14O5	Helenaquinol	Oxy	Hydx	Ket	Oxy	0.24	0.00
41	42.405	C17H20O6	Fumaric acid, 2,6-	Oxy	Cbn	Es	Oxy	1.13	0.01
42	42.905	C12H18O4	Hexamethylene	Oxy	Cbn	Es	Oxy	0.58	0.01
50	55.191	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	0.28	0.00
Sum								100.0	1.14

SL400C

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Peak	RT	Mol.Form	Name	i	ii	iii	iv	Run	Tot
1	2.268	C5H12O	Pentanol	Oxy	Hydx	Alc	Oxy	3.87	0.11
2	2.624	C8H19N	Octylamine	O	HC	N	N	27.29	0.77
3	3.114	C6H8O3	Furaneol	F	Hydx	Fu	Oxy	0.53	0.02
4	3.3	C7H8O2	Guaiacol	G	Met	PhOH	Ph	1.94	0.05
5	3.525	C7H14O	Heptanal	Oxy	Cbn	Aldh	Oxy	1.04	0.03
6	3.754	C8H10O2	Creosol	G	Met	PhOH	Ph	0.73	0.02
7	4.316	C8H18O	1-Octanol	Oxy	Hydx	Alc	Oxy	0.18	0.01
8	7.581	C9H12O2	p-Ethylguaiacol	G	Met	PhOH	Ph	0.33	0.01
9	7.905	C7H8O3	3-Methoxycatechol	C	Met	PhOH	Ph	0.47	0.01
10	9.045	C6H14O3	Diethylene glycol	Oxy	Met	Eth	Oxy	19.16	0.54
11	11.917	C8H10O3	Syringol	S	Met	PhOH	Ph	2.59	0.07
12	12.363	C9H14O5	Diethyl	Oxy	HC	Es	Oxy	0.65	0.02
13	14.905	C9H12O3	4-Methylsyringol	S	Met	PhOH	Ph	2.42	0.07
14	15.27	C9H10O3	Ethylvanillin	G	Met	PhOH	Ph	1.42	0.04
15	15.983	C10H14O3	4-Ethylsyringol	S	Met	PhOH	Ph	1.58	0.04
16	17.817	C6H10O5	Levoglucosan	Oxy	Hydx	Su	Oxy	6.86	0.19
17	18.05	C10H12O3	4-Vinylsyringol	S	Met	PhOH	Ph	5.08	0.14
18	18.725	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	0.25	0.01
19	19.77	C12H16O2	Isopentyl benzoate	Oxy	Cbn	Es	Oxy	0.63	0.02
20	21.14	C14H28	1-Tetradecene	A	HC	HCs	A	0.16	0.00
21	22.319	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	0.90	0.03
22	23.967	C10H12O4	Acetosyringone	S	Met	PhOH	Ph	0.50	0.01
23	24.388	C10H12O5	Methyl syringate	S	Met	PhOH	Ph	0.55	0.02
24	25.25	C12H26O	6-Dodecanol	Oxy	Hydx	Alc	Oxy	0.32	0.01
25	25.354	C22H46O6	Pentaethylene	Oxy	Hydx	Alc	Oxy	0.15	0.00
26	26.314	C8H16O4	2-(2-	Oxy	HC	Es	Oxy	0.21	0.01
27	28.15	C16H22O4	Dibutyl phthalate	Oxy	Cbn	Es	Oxy	0.37	0.01
28	28.542	C22H46O6	Pentaethylene	Oxy	Hydx	Alc	Oxy	0.14	0.00
29	28.656	C22H46O6	Pentaethylene	Oxy	Hydx	Alc	Oxy	0.10	0.00
30	29.639	C16H33NO	Palmiticamide	O	O	N	N	0.15	0.00
31	30.383	C18H35NO	9-Octadecenamide	O	O	N	N	1.32	0.04
32	30.728	C18H37NO	Octadecanamide	O	O	N	N	0.26	0.01
33	31.98	C16H22O4	Dibutyl phthalate	Oxy	Cbn	Es	Oxy	1.09	0.03
34	32.083	C17H20O6	Fumaric acid, 2,6-	Oxy	Cbn	Es	Oxy	0.27	0.01
35	33.973	C18H35NO	9-Octadecenamide	O	O	N	N	0.16	0.00
36	34.07	C29H50O	β-Sitosterol	ST	Hydx	Alc	Oxy	0.12	0.00
37	34.297	C27H48O	Dihydrocholesterol	ST	Hydx	Alc	Oxy	0.11	0.00
38	37.716	C29H50O	β-Sitosterol	ST	Hydx	Alc	Oxy	0.12	0.00
39	39.668	C27H44O	4,6-Cholestadien-	ST	Hydx	Alc	Oxy	0.12	0.00
40	39.997	C29H50O	β-Sitosterol	ST	Hydx	Alc	Oxy	0.55	0.02
42	41.251	C29H50O	β-Sitosterol	ST	Hydx	Alc	Oxy	0.11	0.00
43	43.043	C5H12O	Pentanol	Oxy	Hydx	Alc	Oxy	3.87	0.11
44	43.375	C8H19N	Octylamine	O	HC	N	N	27.29	0.77
45	44.75	C6H8O3	Furaneol	F	Hydx	Fu	Oxy	0.53	0.02
46	45.396	C7H8O2	Guaiacol	G	Met	PhOH	Ph	1.94	0.05

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47	45.501	C7H14O	Heptanal	Oxy	Cbn	Aldh	Oxy	1.04	0.03
48	45.622	C8H10O2	Creosol	G	Met	PhOH	Ph	0.73	0.02
49	45.758	C8H18O	1-Octanol	Oxy	Hydx	Alc	Oxy	0.18	0.01
50	47.329	C9H12O2	p-Ethylguaiacol	G	Met	PhOH	Ph	0.33	0.01
Sum								100.0	2.82

1-1_SL400C_ZrO2

Peak	RT	Mol.Form	Name	i	ii	iii	iv	Run	Tot
1	2.267	C3H6O2	Propionic acid	Acd	Car	Cabox	Oxy	1.56	0.04
2	3.141	C4H6O2	2(3H)-Furanone,	F	Cbn	Ket	Oxy	0.69	0.02
3	3.333	C5H8O	Cyclopentanone	Oxy	Cbn	Ket	Oxy	0.51	0.01
4	3.534	C4H8O	Tetrahydrofuran	F	HC	Fu	Oxy	1.59	0.05
5	3.738	C4H4O2	Furanone	F	Cbn	Ket	Oxy	0.90	0.03
6	4.285	C5H4O2	Furfural	F	Cbn	Aldh	Oxy	10.10	0.29
7	7.559	C7H16O	Heptanol	Oxy	Hydx	Alc	Oxy	1.15	0.03
8	7.901	C5H12O	Pentanol	Oxy	Hydx	Alc	Oxy	3.71	0.11
9	9.045	C8H19N	Octylamine	O	HC	N	N	27.30	0.79
10	11.909	C6H8O3	Furaneol	F	Hydx	Fu	Oxy	0.74	0.02
11	12.117	C7H8O2	Guaiacol	G	Met	PhOH	Ph	0.67	0.02
12	12.288	C5H10O	3-Methylbutanal	Oxy	Cbn	Aldh	Oxy	1.00	0.03
13	12.606	C5H6O2	Furfuranol	F	Hydx	Alc	Oxy	0.30	0.01
14	14.887	C9H18O	Nonaldehyde	Oxy	Cbn	Aldh	Oxy	0.87	0.02
15	15.239	C8H10O2	Creosol	G	Met	PhOH	Ph	0.75	0.02
16	15.956	C8H18O	1-Octanol	Oxy	Hydx	Alc	Oxy	0.30	0.01
17	18.667	C6H14O	2-Hexanol	Oxy	Hydx	Alc	Oxy	9.42	0.27
18	18.791	C9H10O2	Vinylguaiacol	G	Met	PhOH	Ph	8.00	0.23
19	19.756	C8H10O3	Syringol	S	Met	PhOH	Ph	2.30	0.07
20	22.303	C9H12O3	4-Methylsyringol	S	Met	PhOH	Ph	2.27	0.07
21	24.379	C10H14O3	4-Ethylsyringol	S	Met	PhOH	Ph	0.98	0.03
22	24.583	C9H20O4	Tripropylene glycol	Oxy	Hydx	Alc	Oxy	0.32	0.01
23	24.75	C13H18O3	Hexyl salicylate	Oxy	Cbn	Es	Oxy	0.48	0.01
24	25.347	C6H10O5	Levoglucosan	Oxy	Hydx	Su	Oxy	9.28	0.27
25	26.293	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	0.22	0.01
26	28.133	C9H10O4	Syringaldehyde	S	Met	PhOH	Ph	0.61	0.02
27	28.499	C12H26O	6-Dodecanol	Oxy	Hydx	Alc	Oxy	0.82	0.02
28	28.626	C11H24O2	Heptanal, diethyl	Oxy	Hydx	Alc	Oxy	1.23	0.04
29	28.831	C13H28O	1-Tridecanol	Oxy	Hydx	Alc	Oxy	0.71	0.02
30	29.251	C11H22O3	Methyl 10-	Oxy	Cbn	Es	Oxy	0.51	0.01
31	29.606	C10H20O3	Ethyl 3-	Oxy	HC	Es	Oxy	1.07	0.03
32	30.36	C10H12O5	Methyl syringate	S	Met	PhOH	Ph	0.61	0.02
33	30.714	C12H26O	6-Dodecanol	Oxy	Hydx	Alc	Oxy	0.96	0.03
34	30.837	C11H24O2	Heptanal, diethyl	Oxy	Hydx	Alc	Oxy	0.50	0.01
35	31.063	C12H26O	6-Dodecanol	Oxy	Hydx	Alc	Oxy	0.44	0.01
36	31.479	C12H26O	6-Dodecanol	Oxy	Hydx	Alc	Oxy	0.31	0.01

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37	31.822	$C_{10}H_{20}O_3$	Ethyl 3-	Oxy	HC	Es	Oxy	0.25	0.01
38	33.95	$C_{16}H_{22}O_4$	Dibutyl phthalate	Oxy	Cbn	Es	Oxy	0.76	0.02
39	40.751	$C_{18}H_{33}N$	Tricyclohexylamine	O	O	N	N	0.12	0.00
41	41.245	$C_{16}H_{22}O_4$	Dibutyl phthalate	Oxy	Cbn	Es	Oxy	0.79	0.02
42	41.635	$C_{18}H_{35}NO$	9-Octadecenamide	O	O	N	N	0.25	0.01
43	42.943	$C_{17}H_{20}O_6$	Fumaric acid, 2,6-	Oxy	Cbn	Es	Oxy	0.59	0.02
44	43.257	$C_{18}H_{35}NO$	9-Octadecenamide	O	O	N	N	2.54	0.07
45	43.467	$C_{13}H_{12}$	4-Methylbiphenyl	B	HC	HCs	Ar	0.36	0.01
46	43.55	$C_{30}H_{50}$	Squalene	A	HC	HCs	A	0.15	0.00
47	44.738	$C_{29}H_{50}O$	β-Sitosterol	ST	Hydx	Alc	Oxy	0.16	0.00
48	45.383	$C_{27}H_{48}O$	Dihydrocholesterol	ST	Hydx	Alc	Oxy	0.12	0.00
49	45.602	$C_{27}H_{44}O$	4,6-Cholestadien-3β-	ST	Hydx	Alc	Oxy	0.14	0.00
50	45.74	$C_{29}H_{50}O$	β-Sitosterol	ST	Hydx	Alc	Oxy	0.60	0.02
Sum								100.0	2.88

1-1_SL400C_NiZrO2

Peak	RT	Mol.Form	Name	i	ii	iii	iv	Run	Tot
1	2.248	$C_3H_6O_2$	Propionic acid	Acd	Car	Cabox	Oxy	1.79	0.04
2	2.582	$C_5H_{10}O$	3-Methylbutanal	Oxy	Cbn	Aldh	Oxy	0.54	0.01
3	3.069	$C_4H_6O_2$	2(3H)-Furanone,	F	Cbn	Ket	Oxy	0.90	0.02
4	3.233	$C_4H_8O_2$	Acetoin	Oxy	Hydx	Ket	Oxy	0.37	0.01
5	3.471	$C_3H_6O_2$	Propionic acid	Acd	Car	Cabox	Oxy	1.51	0.03
6	3.717	$C_4H_4O_2$	Furanone	F	Cbn	Ket	Oxy	0.51	0.01
7	4.265	$C_5H_4O_2$	Furfural	F	Cbn	Aldh	Oxy	8.37	0.19
8	7.485	$C_4H_8O_2$	Acetoin	Oxy	Hydx	Ket	Oxy	1.11	0.03
9	7.817	$C_6H_{14}O_2$	2-Butoxyethanol	Oxy	Hydx	Alc	Oxy	4.19	0.10
10	8.979	$C_8H_{19}N$	Octylamine	O	HC	N	N	27.57	0.63
11	11.786	$C_6H_8O_3$	Furaneol	F	Hydx	Fu	Oxy	0.51	0.01
12	14.801	$C_8H_{18}O$	1-Octanol	Oxy	Hydx	Alc	Oxy	0.90	0.02
13	15.123	$C_8H_{10}O_2$	Creosol	G	Met	PhOH	Ph	1.14	0.03
14	18.693	$C_6H_{14}O_3$	Diethylene glycol	Oxy	Met	Eth	Oxy	16.91	0.39
15	19.669	$C_8H_{10}O_3$	Syringol	S	Met	PhOH	Ph	3.24	0.07
16	22.221	$C_9H_{12}O_3$	4-Methylsyringol	S	Met	PhOH	Ph	2.96	0.07
17	24.284	$C_{10}H_{14}O_3$	4-Ethylsyringol	S	Met	PhOH	Ph	0.77	0.02
18	24.617	$C_{13}H_{18}O_3$	Hexyl salicylate	Oxy	Cbn	Es	Oxy	0.48	0.01
19	25.255	$C_6H_{10}O_5$	Levoglucosan	Oxy	Hydx	Su	Oxy	11.62	0.27
20	26.196	$C_{11}H_{14}O_3$	4-Allylsyringol	S	Met	PhOH	Ph	0.22	0.00
21	27.983	$C_9H_{10}O_4$	Syringaldehyde	S	Met	PhOH	Ph	1.09	0.02
22	28.444	$C_{14}H_{28}$	1-Tetradecene	A	HC	HCs	A	0.21	0.00
23	28.54	$C_{11}H_{14}O_3$	4-Allylsyringol	S	Met	PhOH	Ph	1.12	0.03
24	28.771	$C_{23}H_{46}O_2$	Methyl docosanoate	Oxy	Cbn	Es	Oxy	0.59	0.01
25	29.522	$C_{10}H_{12}O_4$	Acetosyringone	S	Met	PhOH	Ph	0.83	0.02
26	30.217	$C_{10}H_{12}O_5$	Methyl syringate	S	Met	PhOH	Ph	1.04	0.02
27	30.643	$C_{14}H_{30}O$	Tetradecanol	Oxy	Hydx	Alc	Oxy	0.52	0.01

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28	31.875	C6H14O	2-Hexanol	Oxy	Hydx	Alc	Oxy	0.19	0.00
29	31.968	C8H16O4	2-(2-	Oxy	HC	Es	Oxy	0.31	0.01
30	32.2	C10H20O3	Ethyl 3-	Oxy	HC	Es	Oxy	0.53	0.01
31	32.676	C14H28O3	Ethyl 3-	Oxy	Cbn	Es	Oxy	0.21	0.00
32	33.871	C16H22O4	Dibutyl phthalate	Oxy	Cbn	Es	Oxy	0.62	0.01
33	33.983	C10H20O3	Ethyl 3-	Oxy	HC	Es	Oxy	0.26	0.01
34	34.183	C8H16O4	2-(2-	Oxy	HC	Es	Oxy	0.49	0.01
35	34.612	C10H22O3	Ethanol, 2-[2-	Oxy	Hydx	Eth	Oxy	0.30	0.01
36	37.552	C16H33NO	Palmiticamide	O	O	N	N	0.41	0.01
37	39.54	C18H35NO	9-Octadecenamide	O	O	N	N	2.10	0.05
38	40.695	C16H30O	cis-9-Hexadecenal	Oxy	Cbn	Aldh	Ar	0.22	0.01
40	41.2	C24H38O4	Bis(2-ethylhexyl)	Oxy	Cbn	Es	Oxy	1.32	0.03
41	42.889	C17H20O6	Fumaric acid, 2,6-	Oxy	Cbn	Es	Oxy	0.62	0.01
42	43.237	C18H35NO	9-Octadecenamide	O	O	N	N	0.51	0.01
43	44.702	C29H50O	β-Sitosterol	ST	Hydx	Alc	Oxy	0.22	0.01
44	45.25	C27H44	Cholesta-3,5-diene	ST	HC	HCs	A	0.18	0.00
45	45.342	C27H48O	Dihydrocholesterol	ST	Hydx	Alc	Oxy	0.20	0.00
46	45.448	C13H12	4-Methylbiphenyl	B	HC	HCs	Ar	0.36	0.01
Sum								100.0	2.29

1-5_SL400C_NiZrO2

Peak	RT	Mol.Form	Name	i	ii	iii	iv	Run	Tot
1	2.256	C3H6O2	Propionic acid	Acd	Car	Cabox	Oxy	1.62	0.04
2	3.1	C5H8O	Cyclopentanone	Oxy	Cbn	Ket	Oxy	1.31	0.03
3	3.491	C4H8O	Tetrahydrofuran	F	HC	Fu	Oxy	1.61	0.04
4	3.695	C4H4O2	Furanone	F	Cbn	Ket	Oxy	1.09	0.02
5	4.249	C5H4O2	Furfural	F	Cbn	Aldh	Oxy	11.56	0.26
6	7.485	C7H16O	Heptanol	Oxy	Hydx	Alc	Oxy	1.33	0.03
7	7.834	C5H12O	Pentanol	Oxy	Hydx	Alc	Oxy	3.37	0.07
8	8.995	C8H19N	Octylamine	O	HC	N	N	28.83	0.64
9	11.821	C6H8O3	Furaneol	F	Hydx	Fu	Oxy	0.54	0.01
10	14.817	C10H22O	4-Decanol	Oxy	Hydx	Alc	Oxy	0.87	0.02
11	15.154	C8H10O2	Creosol	G	Met	PhOH	Ph	0.96	0.02
12	18.733	C6H14O3	Diethylene glycol	Oxy	Met	Eth	Oxy	17.80	0.39
13	19.705	C8H10O3	Syringol	S	Met	PhOH	Ph	2.52	0.06
14	22.251	C9H12O3	4-Methylsyringol	S	Met	PhOH	Ph	2.36	0.05
15	24.305	C10H14O3	4-Ethylsyringol	S	Met	PhOH	Ph	0.46	0.01
16	25.289	C6H10O5	Levoglucosan	Oxy	Hydx	Su	Oxy	11.39	0.25
18	28.452	C12H26O	6-Dodecanol	Oxy	Hydx	Alc	Oxy	0.14	0.00
19	28.567	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	0.70	0.02
20	29.183	C12H26O	6-Dodecanol	Oxy	Hydx	Alc	Oxy	0.11	0.00
21	29.536	C10H12O4	Acetosyringone	S	Met	PhOH	Ph	0.63	0.01
22	30.255	C10H12O5	Methyl syringate	S	Met	PhOH	Ph	0.83	0.02
23	30.667	C12H26O	6-Dodecanol	Oxy	Hydx	Alc	Oxy	0.53	0.01

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24	30.783	$C_{11}H_{24}O_2$	Heptanal, diethyl acetal	Oxy	Hydx	Alc	Oxy	0.13	0.00
25	31.4	$C_{14}H_{28}O_2$	Methyl tridecanoate	Oxy	Cbn	Es	Oxy	0.40	0.01
26	31.878	$C_6H_{14}O$	2-Hexanol	Oxy	Hydx	Alc	Oxy	0.25	0.01
27	31.974	$C_8H_{16}O_4$	2-(2-Ethoxyethoxy)ethyl	Oxy	HC	Es	Oxy	0.36	0.01
28	32.21	$C_5H_{10}O_4$	Deoxyribose	Oxy	Hydx	Su	Oxy	0.17	0.00
29	32.68	$C_{10}H_{20}O_3$	Ethyl 3-	Oxy	HC	Es	Oxy	0.25	0.01
30	33.85	$C_{10}H_{20}O_3$	Ethyl 3-	Oxy	HC	Es	Oxy	0.95	0.02
31	33.968	$C_{10}H_{20}O_3$	Ethyl 3-	Oxy	HC	Es	Oxy	0.64	0.01
32	34.192	$C_{10}H_{22}O_3$	Ethanol, 2-[2-	Oxy	Hydx	Eth	Oxy	0.60	0.01
33	34.62	$C_{10}H_{20}O_3$	Ethyl 3-	Oxy	HC	Es	Oxy	0.85	0.02
34	34.995	$C_{10}H_{20}O_3$	Ethyl 3-	Oxy	HC	Es	Oxy	0.26	0.01
35	39.617	$C_{18}H_{35}NO$	9-Octadecenamide	O	O	N	N	0.27	0.01
37	41.034	$C_{13}H_{26}O$	Tridecanal	Oxy	Cbn	Aldh	Oxy	0.20	0.00
38	41.206	$C_{16}H_{22}O_4$	Dibutyl phthalate	Oxy	Cbn	Es	Oxy	0.94	0.02
39	42.95	$C_{17}H_{20}O_6$	Fumaric acid, 2,6-	Oxy	Cbn	Es	Oxy	0.09	0.00
40	43.271	$C_{18}H_{35}NO$	9-Octadecenamide	O	O	N	N	0.16	0.00
41	44.703	$C_{29}H_{50}O$	β-Sitosterol	ST	Hydx	Alc	Oxy	0.23	0.01
42	45.25	$C_{29}H_{50}O$	β-Sitosterol	ST	Hydx	Alc	Oxy	0.13	0.00
43	45.345	$C_{27}H_{48}O$	Dihydrocholesterol	ST	Hydx	Alc	Oxy	0.21	0.00
44	45.451	$C_{29}H_{50}O$	β-Sitosterol	ST	Hydx	Alc	Oxy	0.23	0.01
45	45.566	$C_{27}H_{44}O$	4,6-Cholestadien-3β-ol	ST	Hydx	Alc	Oxy	0.20	0.00
46	45.705	$C_{29}H_{50}O$	β-Sitosterol	ST	Hydx	Alc	Oxy	0.96	0.02
47	47.249	$C_{29}H_{50}O$	β-Sitosterol	ST	Hydx	Alc	Oxy	0.51	0.01
48	47.35	$C_{27}H_{48}O$	Dihydrocholesterol	ST	Hydx	Alc	Oxy	0.23	0.01
49	47.65	$C_{27}H_{46}O$	Epicholesterol	ST	Hydx	Alc	Oxy	0.11	0.00
50	47.952	$C_{31}H_{62}O$	16-Hentriacontanone	Oxy	Cbn	Ket	Oxy	0.12	0.00
Sum								100.0	2.22

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1-10_SL400C_NiZrO2

Peak	RT	Mol.Form	Name	i	ii	iii	iv	Run	Tot
1	2.27	$C_3H_4O_3$	Pyruvic acid	Acd	Car	Cabox	Oxy	1.34	0.03
2	3.298	C_3H_4O	Acrolein	Oxy	Cbn	Aldh	Oxy	0.59	0.01
3	3.522	$C_6H_{14}O$	2-Hexanol	Oxy	Hydx	Alc	Oxy	1.47	0.03
4	3.719	$C_4H_4O_2$	Furanone	F	Cbn	Ket	Oxy	1.13	0.02
5	4.269	$C_5H_4O_2$	Furfural	F	Cbn	Aldh	Oxy	10.87	0.23
6	7.499	$C_7H_{16}O$	Heptanol	Oxy	Hydx	Alc	Oxy	1.24	0.03
7	7.883	$C_5H_{12}O$	Pentanol	Oxy	Hydx	Alc	Oxy	2.81	0.06
8	8.963	$C_8H_{19}N$	Octylamine	O	HC	N	N	24.66	0.53
9	11.826	$C_6H_8O_3$	Furaneol	F	Hydx	Fu	Oxy	0.53	0.01
10	12.1	$C_7H_8O_2$	Guaiacol	G	Met	PhOH	Ph	0.81	0.02
11	12.238	$C_6H_{10}O_2$	Allyl propionate	Oxy	Cbn	Es	Oxy	1.11	0.02
12	12.542	$C_5H_6O_2$	Furfuranol	F	Hydx	Alc	Oxy	0.42	0.01
13	14.813	$C_7H_{14}O$	Heptanal	Oxy	Cbn	Aldh	Oxy	1.37	0.03
14	15.199	$C_8H_{10}O_2$	Creosol	G	Met	PhOH	Ph	0.82	0.02

15	15.899	C8H18O	1-Octanol	Oxy	Hydx	Alc	Oxy	0.39	0.01
16	16.05	C5H10O2	Tetrahydrofurfuryl	F	Hydx	Alc	Oxy	0.27	0.01
17	18.676	C6H14O3	Diethylene glycol	Oxy	Met	Eth	Oxy	18.32	0.39
18	19.758	C8H10O3	Syringol	S	Met	PhOH	Ph	2.02	0.04
19	22.287	C9H12O3	4-Methylsyringol	S	Met	PhOH	Ph	1.78	0.04
20	24.344	C10H14O3	4-Ethylsyringol	S	Met	PhOH	Ph	0.48	0.01
21	25.2	C6H10O5	Levoglucosan	Oxy	Hydx	Su	Oxy	9.41	0.20
22	25.315	C10H12O3	4-Vinylsyringol	S	Met	PhOH	Ph	4.35	0.09
23	26.248	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	0.27	0.01
24	28.135	C12H16O2	Isopentyl benzoate	Oxy	Cbn	Es	Oxy	0.33	0.01
25	28.236	C11H21N	1-Cyanodecane	O	O	N	N	0.40	0.01
26	28.604	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	0.82	0.02
27	29.003	C11H24O	1-Undecanol	Oxy	Hydx	Alc	Oxy	0.24	0.01
28	29.59	C10H12O4	Acetosyringone	S	Met	PhOH	Ph	0.55	0.01
29	30.307	C11H14O4	Sinapyl alcohol	S	Met	PhOH	Ph	0.73	0.02
30	31.888	C6H14O3	Diethylene glycol	Oxy	Met	Eth	Oxy	0.25	0.01
31	31.984	C6H14O	2-Hexanol	Oxy	Hydx	Alc	Oxy	0.35	0.01
32	32.231	C11H24O	1-Undecanol	Oxy	Hydx	Alc	Oxy	0.47	0.01
33	32.689	C16H34O3	3-(Tridecyloxy)-1,2-	Oxy	Hydx	Alc	Oxy	0.45	0.01
34	33.846	C6H14O3	Diethylene glycol	Oxy	Met	Eth	Oxy	1.08	0.02
35	33.97	C14H30O6	Pentaethylene	Oxy	Hydx	Alc	Oxy	0.84	0.02
36	34.197	C12H24O3	2-Ethyl-3-	Oxy	Cbn	Es	Oxy	0.83	0.02
37	34.626	C18H38O5	Tetraethylene	Oxy	Hydx	Alc	Oxy	0.85	0.02
38	34.998	C18H38O5	Tetraethylene	Oxy	Hydx	Alc	Oxy	0.41	0.01
39	35.57	C22H46O6	Pentaethylene	Oxy	Hydx	Alc	Oxy	0.35	0.01
40	35.683	C22H46O6	Pentaethylene	Oxy	Hydx	Alc	Oxy	0.20	0.00
41	35.914	C18H33N	Tricyclohexylamine	O	O	N	N	0.59	0.01
42	39.655	C18H35NO	9-Octadecenamide	O	O	N	N	0.57	0.01
43	41.053	C18H34O2	Vinyl palmitate	Oxy	Cbn	Es	Oxy	0.26	0.01
44	41.212	C24H38O4	Bis(2-ethylhexyl)	Oxy	Cbn	Es	Oxy	0.69	0.01
45	44.703	C29H50O	β-Sitosterol	ST	Hydx	Alc	Oxy	0.26	0.01
46	45.346	C27H48O	Dihydrocholesterol	ST	Hydx	Alc	Oxy	0.23	0.00
47	45.453	C29H50O	β-Sitosterol	ST	Hydx	Alc	Oxy	0.24	0.01
48	45.569	C27H44O	4,6-Cholestadien-	ST	Hydx	Alc	Oxy	0.23	0.01
49	45.706	C29H50O	β-Sitosterol	ST	Hydx	Alc	Oxy	0.99	0.02
50	47.255	C29H50O	β-Sitosterol	ST	Hydx	Alc	Oxy	0.33	0.01
Sum								100.0	2.20

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1-1_SL400C_PdZrO2

Peak	RT	Mol.Form	Name	i	ii	iii	iv	Run	Tot
1	2.244	C3H6O2	Propionic acid	Acd	Car	Cabox	Oxy	1.57	0.04
2	2.574	C4H6O2	2(3H)-Furanone,	F	Cbn	Ket	Oxy	0.17	0.00
3	3.058	C4H6O2	2(3H)-Furanone,	F	Cbn	Ket	Oxy	1.25	0.03
4	3.217	C4H6O2	2(3H)-Furanone,	F	Cbn	Ket	Oxy	0.88	0.02

5	3.457	C3H6O2	Propionic acid	Acd	Car	Cabox	Oxy	1.86	0.05
6	3.676	C4H4O2	Furanone	F	Cbn	Ket	Oxy	0.93	0.03
7	4.248	C5H4O2	Furfural	F	Cbn	Aldh	Oxy	8.55	0.23
8	7.46	C4H8O2	Acetoin	Oxy	Hydx	Ket	Oxy	1.22	0.03
9	7.797	C5H12O	Pentanol	Oxy	Hydx	Alc	Oxy	4.16	0.11
10	8.978	C8H19N	Octylamine	O	HC	N	N	25.80	0.70
11	10.622	C5H10O2	Tetrahydrofurfuryl	F	Hydx	Alc	Oxy	0.24	0.01
12	11.72	C6H8O3	Furaneol	F	Hydx	Fu	Oxy	0.99	0.03
13	11.95	C7H8O2	Guaiacol	G	Met	PhOH	Ph	0.80	0.02
14	12.108	C7H14O	Heptanal	Oxy	Cbn	Aldh	Oxy	1.35	0.04
15	12.493	C5H6O2	Furfuranol	F	Hydx	Alc	Oxy	0.20	0.01
16	14.784	C7H16O	Heptanol	Oxy	Hydx	Alc	Oxy	0.94	0.03
17	15.101	C8H10O2	Creosol	G	Met	PhOH	Ph	0.99	0.03
18	15.843	C8H18O	1-Octanol	Oxy	Hydx	Alc	Oxy	0.33	0.01
19	16.002	C8H18O	1-Octanol	Oxy	Hydx	Alc	Oxy	0.22	0.01
20	17.653	C9H12O2	p-Ethylguaiacol	G	Met	PhOH	Ph	0.31	0.01
21	18.67	C5H10O5	Ribose	Oxy	Hydx	Su	Oxy	16.55	0.45
22	19.639	C8H10O3	Syringol	S	Met	PhOH	Ph	3.01	0.08
23	20.8	C9H20O	Nonanol	Oxy	Hydx	Alc	Oxy	0.36	0.01
24	21.028	C10H14O3	4-Ethylsyringol	S	Met	PhOH	Ph	0.20	0.01
25	22.204	C9H12O3	4-Methylsyringol	S	Met	PhOH	Ph	2.47	0.07
26	23.967	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	0.61	0.02
27	24.257	C10H14O3	4-Ethylsyringol	S	Met	PhOH	Ph	1.27	0.03
28	24.583	C12H20O	Furan, 2,5-dibutyl-	F	HC	Fu	Oxy	0.49	0.01
29	25.234	C6H10O5	Levoglucosan	Oxy	Hydx	Su	Oxy	11.00	0.30
30	26.17	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	0.39	0.01
31	27.956	C9H10O4	Syringaldehyde	S	Met	PhOH	Ph	0.53	0.01
32	28.512	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	0.78	0.02
33	29.441	C10H12O4	Acetosyringone	S	Met	PhOH	Ph	0.73	0.02
34	30.181	C10H12O5	Methyl syringate	S	Met	PhOH	Ph	0.71	0.02
35	31.473	C10H12O4	Acetosyringone	S	Met	PhOH	Ph	0.19	0.01
36	37.497	C18H35NO	9-Octadecenamide	O	O	N	N	0.48	0.01
37	39.5	C18H35NO	9-Octadecenamide	O	O	N	N	2.71	0.07
38	39.817	C18H37NO	Octadecanamide	O	O	N	N	0.34	0.01
39	41.016	C15H30O	2-Pentadecanone	Oxy	Cbn	Ket	Oxy	0.17	0.00
40	41.191	C24H38O4	Bis(2-ethylhexyl)	Oxy	Cbn	Es	Oxy	1.00	0.03
41	42.887	C17H20O6	Fumaric acid, 2,6-	Oxy	Cbn	Es	Oxy	0.31	0.01
42	43.234	C18H35NO	9-Octadecenamide	O	O	N	N	0.24	0.01
43	43.517	C30H50	Squalene	A	HC	HCs	A	0.44	0.01
44	44.683	C29H50O	β-Sitosterol	ST	Hydx	Alc	Oxy	0.24	0.01
45	45.333	C27H48O	Dihydrocholesterol	ST	Hydx	Alc	Oxy	0.20	0.01
46	45.433	C29H50O	β-Sitosterol	ST	Hydx	Alc	Oxy	0.18	0.00
47	45.551	C27H44O	4,6-Cholestadien-3β-ol	ST	Hydx	Alc	Oxy	0.18	0.00
48	45.692	C29H50O	β-Sitosterol	ST	Hydx	Alc	Oxy	0.71	0.02
49	46.686	C31H62O	16-Hentriacontanone	Oxy	Cbn	Ket	Oxy	0.10	0.00
50	47.235	C29H50O	β-Sitosterol	ST	Hydx	Alc	Oxy	0.63	0.02

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Sum								100.0	2.71

1-1_SL400C_RuZrO2

Peak	RT	Mol.Form	Name	i	ii	iii	iv	Run	Tot
1	2.248	C3H6O2	Propionic acid	Acd	Car	Cabox	Oxy	1.47	0.05
2	2.591	C5H10O	3-Methylbutanal	Oxy	Cbn	Aldh	Oxy	0.14	0.00
3	3.076	C4H6O2	2(3H)-Furanone,	F	Cbn	Ket	Oxy	0.90	0.03
4	3.25	C4H6O2	2(3H)-Furanone,	F	Cbn	Ket	Oxy	0.63	0.02
5	3.472	C4H8O2	Acetoin	Oxy	Hydx	Ket	Oxy	1.51	0.05
6	3.688	C4H4O2	Furanone	F	Cbn	Ket	Oxy	0.74	0.02
7	4.247	C5H4O2	Furfural	F	Cbn	Aldh	Oxy	7.76	0.24
8	7.468	C6H14O	2-Hexanol	Oxy	Hydx	Alc	Oxy	1.17	0.04
9	7.799	C6H8O3	Furaneol	F	Hydx	Fu	Oxy	3.96	0.12
10	8.979	C8H19N	Octylamine	O	HC	N	N	23.62	0.73
11	10.651	C6H12O5	2-Deoxy-D-glucose	Oxy	Hydx	Su	Oxy	0.22	0.01
12	11.758	C6H8O3	Furaneol	F	Hydx	Fu	Oxy	0.76	0.02
13	11.983	C7H8O2	Guaiacol	G	Met	PhOH	Ph	0.78	0.02
14	12.143	C5H10O	3-Methylbutanal	Oxy	Cbn	Aldh	Oxy	1.00	0.03
15	12.513	C5H6O2	Furfuranol	F	Hydx	Alc	Oxy	0.23	0.01
16	14.8	C10H22O	4-Decanol	Oxy	Hydx	Alc	Oxy	0.59	0.02
17	15.124	C8H10O2	Creosol	G	Met	PhOH	Ph	0.75	0.02
18	15.858	C8H18O	1-Octanol	Oxy	Hydx	Alc	Oxy	0.29	0.01
19	16.016	C6H10O5	Levoglucosan	Oxy	Hydx	Su	Oxy	0.20	0.01
20	17.667	C9H12O2	p-Ethylguaiacol	G	Met	PhOH	Ph	0.28	0.01
21	18.687	C5H10O5	Ribose	Oxy	Hydx	Su	Oxy	15.91	0.49
22	19.658	C8H10O3	Syringol	S	Met	PhOH	Ph	2.36	0.07
23	21.033	C10H14O3	4-Ethylsyringol	S	Met	PhOH	Ph	0.16	0.00
24	22.218	C9H12O3	4-Methylsyringol	S	Met	PhOH	Ph	1.87	0.06
25	23.8	C9H10O3	Ethylvanillin	G	Met	PhOH	Ph	1.18	0.04
26	23.983	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	1.45	0.04
27	24.273	C10H14O3	4-Ethylsyringol	S	Met	PhOH	Ph	2.02	0.06
28	24.617	C13H18O3	Hexyl salicylate	Oxy	Cbn	Es	Oxy	1.81	0.06
29	25.251	C6H10O5	Levoglucosan	Oxy	Hydx	Su	Oxy	13.14	0.41
30	26.185	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	0.67	0.02
31	27.983	C9H10O4	Syringaldehyde	S	Met	PhOH	Ph	0.65	0.02
32	28.534	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	0.57	0.02
33	29.492	C10H12O4	Acetosyringone	S	Met	PhOH	Ph	0.61	0.02
34	30.223	C10H12O5	Methyl syringate	S	Met	PhOH	Ph	0.52	0.02
35	37.235	C18H35NO	9-Octadecenamide	O	O	N	N	0.25	0.01
36	37.483	C16H33NO	Palmiticamide	O	O	N	N	0.71	0.02
38	39.483	C16H33NO	Palmiticamide	O	O	N	N	4.09	0.13
39	39.817	C16H33NO	Palmiticamide	O	O	N	N	0.40	0.01
41	41.188	C16H22O4	Dibutyl phthalate	Oxy	Cbn	Es	Oxy	1.08	0.03
42	42.887	C17H20O6	Fumaric acid, 2,6-	Oxy	Cbn	Es	Oxy	0.47	0.01

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43	43.208	C18H35NO	9-Octadecenamide	O	O	N	N	1.23	0.04
44	43.383	C13H12	4-Methylbiphenyl	B	HC	HCs	Ar	0.14	0.00
45	44.688	C29H50O	β-Sitosterol	ST	Hydx	Alc	Oxy	0.14	0.00
46	45.333	C27H48O	Dihydrocholesterol	ST	Hydx	Alc	Oxy	0.14	0.00
47	45.434	C29H50O	β-Sitosterol	ST	Hydx	Alc	Oxy	0.17	0.01
48	45.55	C27H44O	4,6-Cholestadien-3β-	ST	Hydx	Alc	Oxy	0.11	0.00
49	45.689	C29H50O	β-Sitosterol	ST	Hydx	Alc	Oxy	0.65	0.02
50	47.234	C29H50O	β-Sitosterol	ST	Hydx	Alc	Oxy	0.52	0.02
Sum								100.0	3.09

SL500C

Peak	RT	Mol.Form	Name	i	ii	iii	iv	Run	Tot
1	2.238	C3H6O2	Propionic acid	Acd	Car	Cabox	Oxy	2.98	0.06
2	3.15	C4H6O2	2(3H)-Furanone,	F	Cbn	Ket	Oxy	0.80	0.02
3	3.297	C7H16O	Heptanol	Oxy	Hydx	Alc	Oxy	1.18	0.02
4	3.534	C4H8O	Tetrahydrofuran	F	HC	Fu	Oxy	2.32	0.04
5	3.769	C4H4O2	Furanone	F	Cbn	Ket	Oxy	1.02	0.02
6	4.38	C5H4O2	Furfural	F	Cbn	Aldh	Oxy	8.43	0.16
7	5.416	C7H14O	Heptanal	Oxy	Cbn	Aldh	Oxy	0.52	0.01
8	7.667	C7H16O	Heptanol	Oxy	Hydx	Alc	Oxy	1.41	0.03
9	7.995	C5H12O	Pentanol	Oxy	Hydx	Alc	Oxy	5.22	0.10
10	9.162	C8H19N	Octylamine	O	HC	N	N	28.44	0.55
11	9.995	C10H16	Limonene	A	HC	HCs	A	0.28	0.01
12	11.967	C6H8O3	Furaneol	F	Hydx	Fu	Oxy	0.36	0.01
13	12.102	C7H8O2	Guaiacol	G	Met	PhOH	Ph	0.87	0.02
14	14.883	C8H10O2	Creosol	G	Met	PhOH	Ph	0.26	0.00
15	15.017	C7H14O	Heptanal	Oxy	Cbn	Aldh	Oxy	0.88	0.02
16	15.304	C8H10O2	Creosol	G	Met	PhOH	Ph	1.23	0.02
17	16.088	C6H8O4	Dimethyl fumarate	Oxy	Met	Es	Oxy	0.26	0.00
18	17.881	C9H12O2	p-Ethylguaiacol	G	Met	PhOH	Ph	0.39	0.01
19	18.632	C6H14O3	Diethylene glycol	Oxy	Met	Eth	Oxy	15.13	0.29
20	18.913	C9H10O2	Vinylguaiacol	G	Met	PhOH	Ph	2.39	0.05
22	19.871	C8H10O3	Syringol	S	Met	PhOH	Ph	3.37	0.06
23	22.443	C9H12O3	4-Methylsyringol	S	Met	PhOH	Ph	2.91	0.06
24	24.502	C10H14O3	4-Ethylsyringol	S	Met	PhOH	Ph	0.64	0.01
25	24.875	C6H10O5	Levoglucosan	Oxy	Hydx	Su	Oxy	5.91	0.11
26	25.488	C10H12O3	4-Vinylsyringol	S	Met	PhOH	Ph	2.00	0.04
27	26.408	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	0.20	0.00
28	28.213	C9H10O4	Syringaldehyde	S	Met	PhOH	Ph	0.41	0.01
29	28.667	C9H20O	Nonanol	Oxy	Hydx	Alc	Oxy	0.33	0.01
30	28.77	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	1.29	0.02
31	29.003	C13H28O	1-Tridecanol	Oxy	Hydx	Alc	Oxy	0.36	0.01
32	29.421	C11H22O3	Methyl 10-	Oxy	Cbn	Es	Oxy	0.24	0.00
33	29.683	C10H12O4	Acetosyringone	S	Met	PhOH	Ph	0.21	0.00

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34	29.766	C10H20O3	Ethyl 3-	Oxy	HC	Es	Oxy	0.57	0.01
35	30.447	C10H12O5	Methyl syringate	S	Met	PhOH	Ph	0.66	0.01
36	30.89	C12H26O	6-Dodecanol	Oxy	Hydx	Alc	Oxy	0.45	0.01
37	34.106	C16H22O4	Dibutyl phthalate	Oxy	Cbn	Es	Oxy	0.55	0.01
38	37.708	C18H37NO	Octadecanamide	O	O	N	N	0.29	0.01
39	39.702	C18H35NO	9-Octadecenamide	O	O	N	N	0.45	0.01
40	39.965	C18H37NO	Octadecanamide	O	O	N	N	0.40	0.01
42	41.331	C16H22O4	Dibutyl phthalate	Oxy	Cbn	Es	Oxy	1.45	0.03
43	43.019	C17H20O6	Fumaric acid, 2,6-	Oxy	Cbn	Es	Oxy	0.25	0.00
44	43.352	C18H35NO	9-Octadecenamide	O	O	N	N	0.33	0.01
45	44.845	C29H50O	β-Sitosterol	ST	Hydx	Alc	Oxy	0.16	0.00
46	45.585	C29H50O	β-Sitosterol	ST	Hydx	Alc	Oxy	0.19	0.00
47	45.698	C27H44O	4,6-Cholestadien-3β-	ST	Hydx	Alc	Oxy	0.13	0.00
48	45.837	C29H50O	β-Sitosterol	ST	Hydx	Alc	Oxy	0.81	0.02
49	47.37	C29H50O	β-Sitosterol	ST	Hydx	Alc	Oxy	0.79	0.02
50	47.45	C29H50O	β-Sitosterol	ST	Hydx	Alc	Oxy	0.29	0.01
Sum								100.0	1.92

1-1_SL500C_NiZrO2

Peak	RT	Mol.Form	Name	i	ii	iii	iv	Run	Tot
1	2.125	C3H6O2	Propionic acid	Acd	Car	Cabox	Oxy	3.53	0.07
2	2.863	C4H6O2	2(3H)-Furanone,	F	Cbn	Ket	Oxy	0.45	0.01
3	3.014	C6H8O3	Furaneol	F	Hydx	Fu	Oxy	1.37	0.03
4	3.215	C6H10O	Cyclohexanone	Oxy	Cbn	Ket	Oxy	2.86	0.06
5	3.45	C4H4O2	Furanone	F	Cbn	Ket	Oxy	0.93	0.02
6	3.918	C5H4O2	Furfural	F	Cbn	Aldh	Oxy	11.14	0.24
7	6.75	C5H6O2	Furfuranol	F	Hydx	Alc	Oxy	0.46	0.01
8	6.945	C6H14O	2-Hexanol	Oxy	Hydx	Alc	Oxy	2.14	0.05
9	7.333	C7H14	1-Heptene	A	HC	HCs	A	5.37	0.11
10	8.466	C8H19N	Octylamine	O	HC	N	N	31.12	0.66
11	11.372	C7H8O2	Guaiacol	G	Met	PhOH	Ph	1.47	0.03
12	14.183	C8H10O2	Creosol	G	Met	PhOH	Ph	0.30	0.01
13	14.323	C8H18O	1-Octanol	Oxy	Hydx	Alc	Oxy	0.91	0.02
14	14.539	C8H10O2	Creosol	G	Met	PhOH	Ph	1.72	0.04
15	15.524	C6H8O4	Dimethyl fumarate	Oxy	Met	Es	Oxy	0.24	0.01
16	17.102	C9H12O2	p-Ethylguaiacol	G	Met	PhOH	Ph	0.36	0.01
17	18.156	C6H14O3	Diethylene glycol	Oxy	Met	Eth	Oxy	0.96	0.02
18	19.105	C8H10O3	Syringol	S	Met	PhOH	Ph	3.76	0.08
19	21.621	C9H12O3	4-Methylsyringol	S	Met	PhOH	Ph	3.36	0.07
20	23.642	C10H14O3	4-Ethylsyringol	S	Met	PhOH	Ph	2.28	0.05
21	24.233	C10H12O4	Acetosyringone	S	Met	PhOH	Ph	1.59	0.03
22	24.666	C6H10O5	Levoglucosan	Oxy	Hydx	Su	Oxy	12.68	0.27
23	25.569	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	1.02	0.02
24	27.938	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	0.94	0.02

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25	28.133	C20H42O	1-Icosanol	Oxy	Hydx	Alc	Oxy	0.23	0.00
26	29.084	C10H12O4	Acetosyringone	S	Met	PhOH	Ph	0.53	0.01
27	33.119	C16H22O4	Dibutyl phthalate	Oxy	Cbn	Es	Oxy	0.25	0.01
28	37.244	C18H37NO	Octadecanamide	O	O	N	N	0.23	0.00
29	39.164	C18H35NO	9-Octadecenamide	O	O	N	N	0.54	0.01
30	39.478	C18H35NO	9-Octadecenamide	O	O	N	N	0.29	0.01
31	39.724	C30H30	1,3,4,6-	B	HC	HCs	Ar	0.33	0.01
32	39.967	C10H14O3	4-Ethylsyringol	S	Met	PhOH	Ph	0.64	0.01
33	40.127	C18H33N	Tricyclohexylamine	O	O	N	N	0.46	0.01
35	40.616	C24H38O4	Bis(2-ethylhexyl)	Oxy	Cbn	Es	Oxy	1.35	0.03
36	42.328	C24H38O4	Bis(2-ethylhexyl)	Oxy	Cbn	Es	Oxy	0.25	0.01
37	42.483	C17H20O6	Fumaric acid, 2,6-	Oxy	Cbn	Es	Oxy	0.32	0.01
38	42.771	C22H43NO	Erucylamide	O	O	N	N	0.47	0.01
39	44.059	C29H50O	β-Sitosterol	ST	Hydx	Alc	Oxy	0.21	0.00
40	44.619	C29H50O	β-Sitosterol	ST	Hydx	Alc	Oxy	0.15	0.00
42	44.821	C29H50O	β-Sitosterol	ST	Hydx	Alc	Oxy	0.20	0.00
43	44.947	C27H44O	4,6-Cholestadien-	ST	Hydx	Alc	Oxy	0.19	0.00
44	45.081	C29H50O	β-Sitosterol	ST	Hydx	Alc	Oxy	0.89	0.02
45	46.635	C29H50O	β-Sitosterol	ST	Hydx	Alc	Oxy	0.61	0.01
46	46.723	C27H48O	Dihydrocholesterol	ST	Hydx	Alc	Oxy	0.47	0.01
47	48.676	C16H28	4-Hexadecen-6-	A	HC	HCs	A	0.16	0.00
48	48.879	C16H28	4-Hexadecen-6-	A	HC	HCs	A	0.20	0.00
49	48.967	C16H28	4-Hexadecen-6-	A	HC	HCs	A	0.09	0.00
Sum								100.0	2.12

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Peak	RT	Mol.Form	Name	i	ii	iii	iv	Run	Tot
1	2.136	C4H8O3	Methyl methoxyacetate	Oxy	Met	Es	Oxy	3.36	0.15
3	3.044	C6H8O3	Furaneol	F	Hydx	Fu	Oxy	1.18	0.05
4	3.23	C6H12O2	Ethyl butanoate	Oxy	Cbn	Es	Oxy	3.28	0.14
6	3.951	C5H4O2	Furfural	F	Cbn	Aldh	Oxy	10.00	0.44
7	6.733	C8H16O	Octanal	Oxy	Cbn	Aldh	Oxy	0.69	0.03
8	6.915	C6H14O	2-Hexanol	Oxy	Hydx	Alc	Oxy	2.47	0.11
9	7.352	C7H14	1-Heptene	A	HC	HCs	A	5.12	0.22
10	8.394	C8H19N	Octylamine	O	HC	N	N	27.19	1.19
11	9.05	C10H16	Limonene	A	HC	HCs	A	0.18	0.01
12	11.406	C7H8O2	Guaiacol	G	Met	PhOH	Ph	1.13	0.05
13	14.255	C10H22O	4-Decanol	Oxy	Hydx	Alc	Oxy	1.13	0.05
14	14.555	C8H10O2	Creosol	G	Met	PhOH	Ph	1.06	0.05
15	15.477	C6H8O4	Dimethyl fumarate	Oxy	Met	Es	Oxy	0.40	0.02
16	17.119	C9H12O2	p-Ethylguaiacol	G	Met	PhOH	Ph	0.25	0.01
17	18.179	C6H14O3	Diethylene glycol	Oxy	Met	Eth	Oxy	15.55	0.68
18	19.151	C8H10O3	Syringol	S	Met	PhOH	Ph	4.63	0.20
19	21.615	C9H12O3	4-Methylsyringol	S	Met	PhOH	Ph	2.20	0.10

20	21.9	$C_{10}H_{12}O_2$	Eugenol	G	Met	PhOH	Ph	0.26	0.01
21	23.622	$C_{10}H_{14}O_3$	4-Ethylsyringol	S	Met	PhOH	Ph	0.58	0.03
22	24.643	$C_6H_{10}O_5$	Levoglucosan	Oxy	Hydx	Su	Oxy	8.85	0.39
23	27.921	$C_{11}H_{14}O_3$	4-Allylsyringol	S	Met	PhOH	Ph	0.65	0.03
24	28.1	$C_{20}H_{42}O$	1-Icosanol	Oxy	Hydx	Alc	Oxy	0.19	0.01
25	36.768	$C_{20}H_{42}O$	1-Icosanol	Oxy	Hydx	Alc	Oxy	0.17	0.01
26	37.1	$C_{10}H_{21}NO$	Decanamide	O	Cbn	N	N	0.64	0.03
27	37.219	$C_{22}H_{46}O_6$	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy	0.59	0.03
28	37.313	$C_{22}H_{46}O_6$	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy	0.37	0.02
29	37.491	$C_{22}H_{46}O_6$	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy	0.38	0.02
30	37.828	$C_{22}H_{46}O_6$	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy	0.44	0.02
31	38.102	$C_{22}H_{46}O_6$	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy	0.44	0.02
32	38.389	$C_{22}H_{46}O_6$	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy	0.32	0.01
34	39.085	$C_{18}H_{35}NO$	9-Octadecenamide	O	O	N	N	0.66	0.03
35	39.217	$C_{22}H_{46}O_6$	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy	0.55	0.02
36	39.385	$C_{18}H_{37}NO$	Octadecanamide	O	O	N	N	0.69	0.03
39	40.113	$C_{18}H_{38}O_4$	Triethylene glycol	Oxy	Hydx	Alc	Oxy	0.43	0.02
40	40.217	$C_{12}H_{24}O_6$	1,4,7,10,13,16-	Oxy	Met	O	Oxy	0.25	0.01
41	40.583	$C_{16}H_{22}O_4$	Dibutyl phthalate	Oxy	Cbn	Es	Oxy	1.12	0.05
42	42.719	$C_{18}H_{35}NO$	9-Octadecenamide	O	O	N	N	0.93	0.04
43	44.021	$C_{27}H_{44}$	Cholesta-3,5-diene	ST	HC	HCs	A	0.16	0.01
45	44.917	$C_{27}H_{44}O$	4,6-Cholestadien-3β-ol	ST	Hydx	Alc	Oxy	0.15	0.01
46	45.05	$C_{27}H_{44}$	Cholesta-3,5-diene	ST	HC	HCs	A	0.64	0.03
47	46.62	$C_{29}H_{50}O$	β-Sitosterol	ST	Hydx	Alc	Oxy	0.48	0.02
48	46.733	$C_{27}H_{48}O$	Dihydrocholesterol	ST	Hydx	Alc	Oxy	0.24	0.01
Sum								100.0	4.37

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Peak	RT	Mol.Form	Name	i	ii	iii	iv	Run	Tot
1	2.142	$C_3H_6O_2$	Propionic acid	Acd	Car	Cabox	Oxy	2.95	0.07
2	2.877	$C_4H_6O_2$	2(3H)-Furanone,	F	Cbn	Ket	Oxy	0.45	0.01
3	3.021	$C_6H_8O_3$	Furaneol	F	Hydx	Fu	Oxy	1.48	0.04
4	3.221	$C_6H_{12}O_2$	Ethyl butanoate	Oxy	Cbn	Es	Oxy	2.75	0.07
5	3.464	$C_8H_{15}NO_2$	Ethyl pipecolinate	Oxy	Cbn	Es	N	0.86	0.02
6	3.934	$C_5H_4O_2$	Furfural	F	Cbn	Aldh	Oxy	9.62	0.23
7	4.947	$C_6H_{10}O_2$	Allyl propionate	Oxy	Cbn	Es	Oxy	0.41	0.01
8	6.683	$C_8H_{16}O$	Octanal	Oxy	Cbn	Aldh	Oxy	0.95	0.02
9	6.948	$C_6H_{14}O$	2-Hexanol	Oxy	Hydx	Alc	Oxy	1.82	0.04
10	7.346	$C_6H_8O_3$	Furaneol	F	Hydx	Fu	Oxy	4.21	0.10
11	8.454	$C_8H_{19}N$	Octylamine	O	HC	N	N	21.62	0.52
12	11.38	$C_7H_8O_2$	Guaiacol	G	Met	PhOH	Ph	1.81	0.04
13	14.2	$C_8H_{10}O_2$	Creosol	G	Met	PhOH	Ph	0.27	0.01
14	14.304	$C_7H_{14}O$	Heptanal	Oxy	Cbn	Aldh	Oxy	0.99	0.02
15	14.552	$C_8H_{10}O_2$	Creosol	G	Met	PhOH	Ph	1.53	0.04

16	15.527	C10H20O3	Ethyl 3-	Oxy	HC	Es	Oxy	0.21	0.01
17	17.017	C9H12O2	p-Ethylguaiacol	G	Met	PhOH	Ph	0.16	0.00
18	17.117	C10H16O	2-Hexylfuran	F	HC	Fu	Oxy	0.37	0.01
19	18.15	C6H14O3	Diethylene glycol	Oxy	Met	Eth	Oxy	8.10	0.19
20	18.409	C6H14O3	Diethylene glycol	Oxy	Met	Eth	Oxy	8.86	0.21
21	19.11	C8H10O3	Syringol	S	Met	PhOH	Ph	4.94	0.12
22	21.05	C12H22O11	Maltose	Oxy	Hydx	Su	Oxy	0.57	0.01
23	21.622	C9H12O3	4-Methylsyringol	S	Met	PhOH	Ph	3.71	0.09
24	22.083	C10H12O2	Eugenol	G	Met	PhOH	Ph	0.29	0.01
25	23.654	C10H14O3	4-Ethylsyringol	S	Met	PhOH	Ph	1.63	0.04
26	24.658	C6H10O5	Levoglucosan	Oxy	Hydx	Su	Oxy	12.46	0.30
27	25.576	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	0.72	0.02
28	27.953	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	0.72	0.02
29	28.133	C10H22O	4-Decanol	Oxy	Hydx	Alc	Oxy	0.21	0.01
30	35.257	C18H33N	Tricyclohexylamine	O	O	N	N	0.17	0.00
32	37.29	C18H38O5	Tetraethylene	Oxy	Hydx	Alc	Oxy	0.28	0.01
33	37.4	C22H46O6	Pentaethylene	Oxy	Hydx	Alc	Oxy	0.21	0.01
34	37.56	C22H46O6	Pentaethylene	Oxy	Hydx	Alc	Oxy	0.18	0.00
35	37.876	C22H46O6	Pentaethylene	Oxy	Hydx	Alc	Oxy	0.29	0.01
36	39.132	C18H35NO	9-Octadecenamide	O	O	N	N	0.53	0.01
37	39.254	C22H46O6	Pentaethylene	Oxy	Hydx	Alc	Oxy	0.34	0.01
40	40.138	C18H38O4	Triethylene glycol	Oxy	Hydx	Alc	Oxy	0.31	0.01
42	40.617	C16H22O4	Dibutyl phthalate	Oxy	Cbn	Es	Oxy	0.96	0.02
44	42.798	C18H35NO	9-Octadecenamide	O	O	N	N	0.22	0.01
46	44.722	C27H48O	Dihydrocholesterol	ST	Hydx	Alc	Oxy	0.17	0.00
47	44.952	C27H44O	4,6-Cholestadien-	ST	Hydx	Alc	Oxy	0.18	0.00
48	45.088	C29H50O	β-Sitosterol	ST	Hydx	Alc	Oxy	0.62	0.01
49	46.647	C29H50O	β-Sitosterol	ST	Hydx	Alc	Oxy	0.48	0.01
50	46.734	C27H48O	Dihydrocholesterol	ST	Hydx	Alc	Oxy	0.37	0.01
Sum								100.0	2.41

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Peak	RT	Mol.Form	Name	i	ii	iii	iv	Run	Tot
1	2.154	C5H10O	3-Methylbutanal	Oxy	Cbn	Aldh	Oxy	3.48	0.06
2	2.917	C4H6O2	2(3H)-Furanone,	F	Cbn	Ket	Oxy	0.85	0.01
3	3.272	C7H12O2	Ethyl 4-pentenoate	Oxy	Methx	Es	Oxy	3.43	0.06
4	3.467	C4H4O2	Furanone	F	Cbn	Ket	Oxy	1.48	0.03
5	4.008	C5H4O2	Furfural	F	Cbn	Aldh	Oxy	8.75	0.15
6	6.783	C5H6O2	Furfuranol	F	Hydx	Alc	Oxy	0.40	0.01
7	6.933	C7H16O	Heptanol	Oxy	Hydx	Alc	Oxy	1.97	0.03
8	7.382	C7H14	1-Heptene	A	HC	HCs	A	3.87	0.07
9	8.35	C8H19N	Octylamine	O	HC	N	N	26.62	0.47
10	14.274	C10H22O	4-Decanol	Oxy	Hydx	Alc	Oxy	1.47	0.03
11	14.467	C13H28	3-Ethylundecane	A	HC	HCs	A	0.42	0.01

12	14.624	C8H10O2	Creosol	G	Met	PhOH	Ph	1.55	0.03
13	14.9	C12H24	cis-5-Dodecene	A	HC	HCs	A	0.29	0.01
15	18.091	C5H10O	3-Methylbutanal	Oxy	Cbn	Aldh	Oxy	9.24	0.16
16	18.25	C9H10O2	Vinylguaiacol	G	Met	PhOH	Ph	6.05	0.11
17	19.212	C8H10O3	Syringol	S	Met	PhOH	Ph	2.93	0.05
18	19.879	C18H36	1-Octadecene	A	HC	HCs	A	0.10	0.00
19	21.656	C9H12O3	4-Methylsyringol	S	Met	PhOH	Ph	2.69	0.05
21	23.114	C14H22O	Phenol, 2,4-bis(1,1-	H	Hydx	PhOH	Ph	0.40	0.01
22	23.657	C10H14O3	4-Ethylsyringol	S	Met	PhOH	Ph	1.25	0.02
23	24.4	C6H10O5	Levoglucosan	Oxy	Hydx	Su	Oxy	7.35	0.13
24	24.706	C10H12O3	4-Vinylsyringol	S	Met	PhOH	Ph	4.72	0.08
25	25.133	C20H42	Icosane	A	HC	HCs	A	0.39	0.01
26	25.648	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	0.49	0.01
27	28	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	0.85	0.02
28	28.121	C20H42O	1-Icosanol	Oxy	Hydx	Alc	Oxy	0.93	0.02
29	29.158	C20H38O2	Octadecanoic acid,	Oxy	Cbn	Es	Oxy	0.83	0.01
30	29.871	C10H12O5	Methyl syringate	S	Met	PhOH	Ph	0.98	0.02
31	31.123	C16H22O4	Dibutyl phthalate	Oxy	Cbn	Es	Oxy	1.12	0.02
33	36.815	C18H36	1-Octadecene	A	HC	HCs	A	0.18	0.00
34	36.888	C16H34	Hexadecane	A	HC	HCs	A	0.14	0.00
35	37.311	C22H46O6	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy	0.32	0.01
36	37.416	C22H46O6	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy	0.34	0.01
37	37.589	C22H46O6	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy	0.23	0.00
38	40.154	C16H26O3	3-dodecylfuran-2,5-	F	Cbny	Ket	Oxy	0.65	0.01
39	40.48	C15H30O	2-Pentadecanone	Oxy	Cbn	Ket	Oxy	0.23	0.00
40	40.631	C16H22O4	Dibutyl phthalate	Oxy	Cbn	Es	Oxy	1.20	0.02
41	42.488	C17H20O6	Fumaric acid, 2,6-	Oxy	Cbn	Es	Oxy	0.27	0.00
42	44.725	C27H48O	Dihydrocholesterol	ST	Hydx	Alc	Oxy	0.15	0.00
43	44.961	C27H44O	4,6-Cholestadien-3β-	ST	Hydx	Alc	Oxy	0.19	0.00
44	45.095	C27H44	Cholesta-3,5-diene	ST	HC	HCs	A	0.58	0.01
45	46.651	C29H50O	β-Sitosterol	ST	Hydx	Alc	Oxy	0.26	0.00
46	46.749	C27H48O	Dihydrocholesterol	ST	Hydx	Alc	Oxy	0.25	0.00
48	47.603	C27H44O	4,6-Cholestadien-3β-	ST	Hydx	Alc	Oxy	0.13	0.00
Sum								100.0	1.17

1-5_SL500C_RuZrO2

Peak	RT	Mol.Form	Name	i	ii	iii	iv	Run	Tot
1	2.147	C3H6O2	Propionic acid	Acd	Car	Cabox	Oxy	3.06	0.06
2	2.917	C4H6O2	2(3H)-Furanone,	F	Cbn	Ket	Oxy	0.50	0.01
3	3.28	C5H8O2	Methyl	F	Cbn	Ket	Oxy	3.32	0.06
4	3.5	C4H4O2	Furanone	F	Cbn	Ket	Oxy	0.72	0.01
5	4	C5H4O2	Furfural	F	Cbn	Aldh	Oxy	9.25	0.18
6	6.946	C7H16O	Heptanol	Oxy	Hydx	Alc	Oxy	2.14	0.04
7	7.355	C7H14	1-Heptene	A	HC	HCs	A	6.01	0.12

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8	8.38	C8H19N	Octylamine	O	HC	N	N	29.71	0.57
9	9.068	C10H16	Limonene	A	HC	HCs	A	0.12	0.00
10	14.303	C7H14O	Heptanal	Oxy	Cbn	Aldh	Oxy	1.15	0.02
11	14.652	C8H10O2	Creosol	G	Met	PhOH	Ph	0.99	0.02
12	17.181	C10H16O	2-Hexylfuran	F	HC	Fu	Oxy	0.28	0.01
13	18.242	C6H14O3	Diethylene glycol	Oxy	Met	Eth	Oxy	13.01	0.25
14	19.236	C8H10O3	Syringol	S	Met	PhOH	Ph	2.63	0.05
15	21.677	C9H12O3	4-Methylsyringol	S	Met	PhOH	Ph	2.81	0.05
16	23.133	C14H22O	Phenol, 2,4-bis(1,1-	H	Hydx	PhOH	Ph	1.14	0.02
17	23.683	C10H14O3	4-Ethylsyringol	S	Met	PhOH	Ph	1.93	0.04
18	24.524	C6H10O5	Levoglucosan	Oxy	Hydx	Su	Oxy	6.33	0.12
19	24.705	C10H12O3	4-Vinylsyringol	S	Met	PhOH	Ph	5.63	0.11
20	25.622	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	0.38	0.01
21	27.973	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	0.72	0.01
23	33.099	C10H20O3	Ethyl 3-	Oxy	HC	Es	Oxy	0.49	0.01
24	33.236	C8H16O4	2-(2-	Oxy	HC	Es	Oxy	0.31	0.01
25	33.49	C10H20O3	Ethyl 3-	Oxy	HC	Es	Oxy	0.16	0.00
26	33.943	C10H20O3	Ethyl 3-	Oxy	HC	Es	Oxy	0.25	0.00
27	34.334	C18H38O5	Tetraethylene	Oxy	Hydx	Alc	Oxy	0.18	0.00
28	34.897	C10H20O3	Ethyl 3-	Oxy	HC	Es	Oxy	0.27	0.01
29	35.02	C10H20O3	Ethyl 3-	Oxy	HC	Es	Oxy	0.14	0.00
30	37.289	C18H38O5	Tetraethylene	Oxy	Hydx	Alc	Oxy	0.41	0.01
31	37.4	C18H38O5	Tetraethylene	Oxy	Hydx	Alc	Oxy	0.43	0.01
32	37.566	C18H38O5	Tetraethylene	Oxy	Hydx	Alc	Oxy	0.34	0.01
36	39.507	C15H30O	2-Pentadecanone	Oxy	Cbn	Ket	Oxy	0.21	0.00
37	39.727	C30H30	1,3,4,6-	B	HC	HCs	Ar	0.39	0.01
39	40.471	C15H30O	2-Pentadecanone	Oxy	Cbn	Ket	Oxy	0.25	0.00
40	40.623	C16H22O4	Dibutyl phthalate	Oxy	Cbn	Es	Oxy	1.39	0.03
41	42.499	C17H20O6	Fumaric acid, 2,6-	Oxy	Cbn	Es	Oxy	0.19	0.00
42	44.053	C29H50O	β-Sitosterol	ST	Hydx	Alc	Oxy	0.17	0.00
43	44.618	C29H50O	β-Sitosterol	ST	Hydx	Alc	Oxy	0.14	0.00
44	44.715	C27H48O	Dihydrocholesterol	ST	Hydx	Alc	Oxy	0.25	0.00
45	44.951	C27H44O	4,6-Cholestadien-	ST	Hydx	Alc	Oxy	0.22	0.00
46	45.082	C29H50O	β-Sitosterol	ST	Hydx	Alc	Oxy	1.02	0.02
47	46.643	C29H50O	β-Sitosterol	ST	Hydx	Alc	Oxy	0.60	0.01
48	46.75	C27H48O	Dihydrocholesterol	ST	Hydx	Alc	Oxy	0.35	0.01
Sum								100.0	1.93

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Peak	RT	Mol.Form	Name	i	ii	iii	iv	Run	Tot
1	2.155	C6H10O	Cyclohexanone	Oxy	Cbn	Ket	Oxy	4.61	0.06
2	2.294	C8H16	1-Octene	A	HC	HCs	A	1.63	0.02
3	2.448	C5H8O2	Methyl	F	Cbn	Ket	Oxy	0.84	0.01
4	3.041	C7H8	Toluene	B	HC	HCs	Ar	2.14	0.03

5	3.333	C8H16	1-Octene	A	HC	HCs	A	4.13	0.05
6	3.483	C8H16O	Octanal	Oxy	Cbn	Aldh	Oxy	1.19	0.02
7	3.633	C4H4O2	Furanone	F	Cbn	Ket	Oxy	0.79	0.01
8	4.165	C5H4O2	Furfural	F	Cbn	Aldh	Oxy	8.21	0.10
9	4.703	C8H10	Xylene	B	HC	HCs	Ar	0.27	0.00
10	5.444	C9H18	1-Nonene	B	HC	HCs	A	0.77	0.01
11	7.224	C7H16O	Heptanol	Oxy	Hydx	Alc	Oxy	1.48	0.02
12	8.347	C12H24	cis-5-Dodecene	A	HC	HCs	A	0.38	0.00
13	8.595	C8H19N	Octylamine	O	HC	N	N	15.70	0.20
14	14.606	C10H22O	4-Decanol	Oxy	Hydx	Alc	Oxy	0.88	0.01
15	18.278	C10H13N5O5	Guanosine	O	Hydx	N	N	13.33	0.17
16	18.533	C9H10O2	Vinylguaiacol	G	Met	PhOH	Ph	5.07	0.06
17	19.442	C8H10O3	Syringol	S	Met	PhOH	Ph	3.54	0.05
18	19.915	C12H10	Biphenyl	B	O	HCs	Ar	0.98	0.01
19	20.258	C14H28	1-Tetradecene	A	HC	HCs	A	0.31	0.00
20	21.939	C9H12O3	4-Methylsyringol	S	Met	PhOH	Ph	2.55	0.03
21	22.183	C14H22	Octylbenzene	B	HC	HCs	Ar	0.24	0.00
22	23.989	C10H14O3	4-Ethylsyringol	S	Met	PhOH	Ph	0.82	0.01
23	24.517	C6H12O6	Glucose	Oxy	Hydx	Su	Oxy	11.06	0.14
24	24.984	C10H12O3	4-Vinylsyringol	S	Met	PhOH	Ph	3.06	0.04
25	25.883	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	0.70	0.01
26	26.217	C17H28	Undecylbenzene	B	HC	HCs	Ar	0.20	0.00
27	26.307	C17H28	Undecylbenzene	B	HC	HCs	Ar	0.37	0.00
28	26.544	C17H28	Undecylbenzene	B	HC	HCs	Ar	0.32	0.00
29	27.02	C17H28	Undecylbenzene	B	HC	HCs	Ar	0.35	0.00
30	27.483	C13H28O	1-Tridecanol	Oxy	Hydx	Alc	Oxy	0.17	0.00
31	27.873	C17H28	Undecylbenzene	B	HC	HCs	Ar	0.45	0.01
32	28.283	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	0.84	0.01
33	28.468	C18H30	n-dodecylbenzene	B	HC	HCs	Ar	1.21	0.02
34	28.574	C18H30	n-dodecylbenzene	B	HC	HCs	Ar	1.00	0.01
35	28.846	C18H30	n-dodecylbenzene	B	HC	HCs	Ar	0.68	0.01
36	29.322	C18H30	n-dodecylbenzene	B	HC	HCs	Ar	0.85	0.01
37	30	C11H14O4	Sinapyl alcohol	S	Met	PhOH	Ph	0.52	0.01
38	30.161	C18H30	n-dodecylbenzene	B	HC	HCs	Ar	0.81	0.01
39	30.627	C18H30	n-dodecylbenzene	B	HC	HCs	Ar	1.33	0.02
40	30.776	C18H30	n-dodecylbenzene	B	HC	HCs	Ar	0.67	0.01
41	31.046	C18H30	n-dodecylbenzene	B	HC	HCs	Ar	0.55	0.01
42	31.532	C18H30	n-dodecylbenzene	B	HC	HCs	Ar	0.42	0.01
43	32.348	C18H30	n-dodecylbenzene	B	HC	HCs	Ar	0.44	0.01
44	40.356	C18H33N	Tricyclohexylamine	O	O	N	N	0.43	0.01
45	40.853	C16H22O4	Dibutyl phthalate	Oxy	Cbn	Es	Oxy	1.32	0.02
46	42.966	C18H35NO	9-Octadecenamide	O	O	N	N	0.53	0.01
47	44.317	C29H50O	β-Sitosterol	ST	Hydx	Alc	Oxy	0.16	0.00
48	45.191	C29H50O	β-Sitosterol	ST	Hydx	Alc	Oxy	0.42	0.01
49	45.329	C29H50O	β-Sitosterol	ST	Hydx	Alc	Oxy	0.91	0.01
50	46.883	C29H50O	β-Sitosterol	ST	Hydx	Alc	Oxy	0.37	0.00

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Sum								100.0	1.28

1-1_SL600C_NiZrO2

Peak	RT	Mol.Form	Name	i	ii	iii	iv	Run	Tot
1	2.11	C3H6O2	Propionic acid	Acd	Car	Cabox	Oxy	5.29	0.17
2	2.869	C4H6O2	2(3H)-Furanone,	F	Cbn	Ket	Oxy	1.30	0.04
3	3.032	C6H8O3	Furaneol	F	Hydx	Fu	Oxy	1.49	0.05
4	3.185	C5H8O	Cyclopentanone	Oxy	Cbn	Ket	Oxy	4.04	0.13
5	3.517	C4H4O2	Furanone	F	Cbn	Ket	Oxy	0.75	0.02
6	4.009	C5H4O2	Furfural	F	Cbn	Aldh	Oxy	8.39	0.27
7	6.45	C5H8O3	Levulinic acid	Acd	Car	Cabox	Oxy	0.34	0.01
8	6.683	C5H6O2	Furfuranol	F	Hydx	Alc	Oxy	1.21	0.04
9	6.913	C6H14O	2-Hexanol	Oxy	Hydx	Alc	Oxy	2.61	0.08
10	7.37	C7H14	1-Heptene	A	HC	HCs	A	5.55	0.18
11	8.347	C8H19N	Octylamine	O	HC	N	N	27.21	0.88
12	9.038	C10H16	Limonene	A	HC	HCs	A	0.16	0.01
13	11.53	C7H8O2	Guaiacol	G	Met	PhOH	Ph	1.94	0.06
14	14.337	C14H28O	Tetradecanal	Oxy	Cbn	Aldh	Oxy	1.22	0.04
15	14.73	C8H10O2	Creosol	G	Met	PhOH	Ph	0.96	0.03
16	18.044	C5H10O	3-Methylbutanal	Oxy	Cbn	Aldh	Oxy	6.73	0.22
17	18.183	C9H10O2	Vinylguaiacol	G	Met	PhOH	Ph	5.65	0.18
18	19.205	C8H10O3	Syringol	S	Met	PhOH	Ph	2.67	0.09
19	21.686	C9H12O3	4-Methylsyringol	S	Met	PhOH	Ph	2.12	0.07
20	23.67	C10H14O3	4-Ethylsyringol	S	Met	PhOH	Ph	1.09	0.04
21	24.357	C6H10O5	Levoglucosan	Oxy	Hydx	Su	Oxy	6.79	0.22
22	24.688	C10H12O3	4-Vinylsyringol	S	Met	PhOH	Ph	4.14	0.13
23	25.601	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	0.46	0.01
24	27.972	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	0.60	0.02
25	28.096	C22H44O2	Octadecyl butyrate	Oxy	Cbn	Es	Oxy	0.40	0.01
26	29.155	C10H12O4	Acetosyringone	S	Met	PhOH	Ph	0.60	0.02
27	33.086	C10H20O3	Ethyl 3-	Oxy	HC	Es	Oxy	0.30	0.01
28	33.22	C8H16O4	2-(2-	Oxy	HC	Es	Oxy	0.18	0.01
29	33.471	C10H20O3	Ethyl 3-	Oxy	HC	Es	Oxy	0.13	0.00
30	33.617	C23H46	1-Tricosene	A	HC	HCs	A	0.33	0.01
31	33.914	C22H46O6	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy	0.32	0.01
32	34.298	C22H46O6	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy	0.20	0.01
33	34.859	C22H46O6	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy	0.20	0.01
34	37.27	C22H46O6	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy	0.34	0.01
35	37.367	C22H46O6	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy	0.22	0.01
36	39.227	C18H35NO	9-Octadecenamide	O	O	N	N	0.25	0.01
39	40.603	C16H22O4	Dibutyl phthalate	Oxy	Cbn	Es	Oxy	1.08	0.04
40	42.763	C18H35NO	9-Octadecenamide	O	O	N	N	0.36	0.01
41	44.032	C29H50O	β-Sitosterol	ST	Hydx	Alc	Oxy	0.12	0.00
43	44.797	C29H50O	β-Sitosterol	ST	Hydx	Alc	Oxy	0.12	0.00

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44	44.917	C27H44O	4,6-Cholestadien-3β-	ST	Hydx	Alc	Oxy	0.18	0.01
45	45.056	C29H50O	β-Sitosterol	ST	Hydx	Alc	Oxy	0.68	0.02
46	46.605	C29H50O	β-Sitosterol	ST	Hydx	Alc	Oxy	0.83	0.03
47	46.7	C27H48O	Dihydrocholesterol	ST	Hydx	Alc	Oxy	0.45	0.01
Sum								100.0	3.25

1-5_SL600C_NiZrO2

Peak	RT	Mol.Form	Name	i	ii	iii	iv	Run	Tot
1	2.136	C4H8O3	Methyl	Oxy	Met	Es	Oxy	3.34	0.15
3	3.044	C4H6O2	2(3H)-Furanone,	F	Cbn	Ket	Oxy	1.17	0.05
4	3.23	C6H12O2	Ethyl butanoate	Oxy	Cbn	Es	Oxy	3.27	0.14
5	3.483	C8H15NO2	Ethyl pipecolinate	Oxy	Cbn	Es	N	0.66	0.03
6	3.951	C5H4O2	Furfural	F	Cbn	Aldh	Oxy	9.96	0.44
7	6.733	C8H16O	Octanal	Oxy	Cbn	Aldh	Oxy	0.69	0.03
8	6.915	C6H14O	2-Hexanol	Oxy	Hydx	Alc	Oxy	2.46	0.11
9	7.352	C6H8O3	Furaneol	F	Hydx	Fu	Oxy	5.10	0.22
10	8.394	C8H19N	Octylamine	O	HC	N	N	27.08	1.19
11	9.05	C10H16	Limonene	A	HC	HCs	A	0.17	0.01
12	11.406	C7H8O2	Guaiacol	G	Met	PhOH	Ph	1.13	0.05
13	14.255	C7H14O	Heptanal	Oxy	Cbn	Aldh	Oxy	1.12	0.05
14	14.555	C8H10O2	Creosol	G	Met	PhOH	Ph	1.06	0.05
15	15.477	C10H20O3	Ethyl 3-	Oxy	HC	Es	Oxy	0.39	0.02
16	17.119	C9H12O2	p-Ethylguaiacol	G	Met	PhOH	Ph	0.24	0.01
17	18.179	C6H14O3	Diethylene glycol	Oxy	Met	Eth	Oxy	15.49	0.68
18	19.151	C8H10O3	Syringol	S	Met	PhOH	Ph	4.61	0.20
19	21.615	C9H12O3	4-Methylsyringol	S	Met	PhOH	Ph	2.19	0.10
20	21.9	C10H12O2	Eugenol	G	Met	PhOH	Ph	0.26	0.01
21	23.622	C10H14O3	4-Ethylsyringol	S	Met	PhOH	Ph	0.58	0.03
22	24.643	C6H10O5	Levoglucosan	Oxy	Hydx	Su	Oxy	8.81	0.39
23	27.921	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	0.64	0.03
24	28.1	C11H24O	1-Undecanol	Oxy	Hydx	Alc	Oxy	0.18	0.01
25	36.768	C18H36	1-Octadecene	A	HC	HCs	A	0.16	0.01
26	37.1	C10H21NO	Decanamide	O	Cbn	N	N	0.63	0.03
27	37.219	C22H46O6	Pentaethylene	Oxy	Hydx	Alc	Oxy	0.59	0.03
28	37.313	C22H46O6	Pentaethylene	Oxy	Hydx	Alc	Oxy	0.37	0.02
29	37.491	C22H46O6	Pentaethylene	Oxy	Hydx	Alc	Oxy	0.37	0.02
30	37.828	C22H46O6	Pentaethylene	Oxy	Hydx	Alc	Oxy	0.44	0.02
31	38.102	C22H46O6	Pentaethylene	Oxy	Hydx	Alc	Oxy	0.44	0.02
32	38.389	C22H46O6	Pentaethylene	Oxy	Hydx	Alc	Oxy	0.32	0.01
34	39.085	C18H35NO	9-Octadecenamide	O	O	N	N	0.66	0.03
35	39.217	C22H46O6	Pentaethylene	Oxy	Hydx	Alc	Oxy	0.55	0.02
36	39.385	C18H37NO	Octadecanamide	O	O	N	N	0.69	0.03
39	40.113	C22H46O6	Pentaethylene	Oxy	Hydx	Alc	Oxy	0.42	0.02
41	40.583	C16H22O4	Dibutyl phthalate	Oxy	Cbn	Es	Oxy	1.12	0.05

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42	42.719	C18H35NO	9-Octadecenamide	O	O	N	N	0.93	0.04
43	44.021	C29H50O	β-Sitosterol	ST	Hydx	Alc	Oxy	0.16	0.01
45	44.917	C27H44	Cholesta-3,5-diene	ST	HC	HCs	A	0.15	0.01
46	45.05	C29H50O	β-Sitosterol	ST	Hydx	Alc	Oxy	0.64	0.03
47	46.62	C29H50O	β-Sitosterol	ST	Hydx	Alc	Oxy	0.47	0.02
48	46.733	C27H48O	Dihydrocholesterol	ST	Hydx	Alc	Oxy	0.24	0.01
Sum								100.0	4.39

1-1_SL600C_PdZrO2

Peak	RT	Mol.Form	Name	i	ii	iii	iv	Run	Tot
1	2.123	C3H4O3	Pyruvic acid	Acd	Car	Cabox	Oxy	5.31	0.08
2	2.917	C7H8	Toluene	B	HC	HCs	Ar	1.57	0.02
3	3.083	C7H16O	Heptanol	Oxy	Hydx	Alc	Oxy	1.09	0.02
4	3.189	C11H20O2	2-Propenoic acid,	Oxy	Cbn	Es	Oxy	3.75	0.06
5	3.517	C4H4O2	Furanone	F	Cbn	Ket	Oxy	0.93	0.01
6	4.005	C5H4O2	Furfural	F	Cbn	Aldh	Oxy	9.96	0.15
7	5.232	C8H8	Styrene	B	HC	HCs	Ar	0.80	0.01
8	6.947	C6H14O	2-Hexanol	Oxy	Hydx	Alc	Oxy	1.68	0.03
9	8.336	C8H19N	Octylamine	O	HC	N	N	24.12	0.36
10	14.242	C14H28	1-Tetradecene	A	HC	HCs	A	0.29	0.00
11	14.378	C10H22O	4-Decanol	Oxy	Hydx	Alc	Oxy	1.33	0.02
12	14.767	C8H10O2	Creosol	G	Met	PhOH	Ph	1.15	0.02
13	16.933	C10H18O	Eucalyptol	Oxy	HC	Eth	Oxy	0.65	0.01
14	17.144	C14H28	1-Tetradecene	A	HC	HCs	A	0.47	0.01
15	17.287	C13H26	1-Tridecene	A	HC	HCs	A	0.36	0.01
16	17.956	C6H14O3	Diethylene glycol	Oxy	Met	Eth	Oxy	8.40	0.13
17	18.29	C9H10O2	Vinylguaiacol	G	Met	PhOH	Ph	3.87	0.06
18	19.277	C8H10O3	Syringol	S	Met	PhOH	Ph	3.14	0.05
19	19.896	C18H36	1-Octadecene	A	HC	HCs	A	0.22	0.00
20	21.722	C9H12O3	4-Methylsyringol	S	Met	PhOH	Ph	2.33	0.03
21	23.148	C14H22O	Phenol, 2,4-bis(1,1-	H	Hydx	PhOH	Ph	0.17	0.00
22	23.75	C10H14O3	4-Ethylsyringol	S	Met	PhOH	Ph	0.96	0.01
23	24.159	C6H10O5	Levoglucosan	Oxy	Hydx	Su	Oxy	9.90	0.15
24	24.772	C10H12O3	4-Vinylsyringol	S	Met	PhOH	Ph	2.70	0.04
25	28.133	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	1.67	0.03
26	33.12	C22H46O6	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy	0.50	0.01
27	33.261	C22H46O6	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy	0.45	0.01
28	33.982	C22H46O6	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy	0.53	0.01
29	34.36	C22H46O6	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy	0.37	0.01
30	34.917	C10H20O3	Ethyl 3-	Oxy	HC	Es	Oxy	0.36	0.01
31	37.279	C22H46O6	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy	1.12	0.02
32	37.382	C22H46O6	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy	1.17	0.02
33	37.563	C22H46O6	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy	0.85	0.01
34	37.894	C22H46O6	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy	0.92	0.01

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35	38.05	C20H42O	1-Icosanol	Oxy	Hydx	Alc	Oxy	0.33	0.00
36	38.179	C22H46O6	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy	0.79	0.01
37	38.449	C22H46O6	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy	0.74	0.01
38	38.567	C22H46O6	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy	0.41	0.01
39	38.728	C22H46O6	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy	0.28	0.00
40	39.321	C22H46O6	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy	0.35	0.01
42	40.64	C16H22O4	Dibutyl phthalate	Oxy	Cbn	Es	Oxy	1.39	0.02
43	44.067	C29H50O	β-Sitosterol	ST	Hydx	Alc	Oxy	0.15	0.00
44	44.729	C27H48O	Dihydrocholesterol	ST	Hydx	Alc	Oxy	0.28	0.00
45	44.965	C27H44O	4,6-Cholestadien-3β-	ST	Hydx	Alc	Oxy	0.27	0.00
46	45.102	C29H50O	β-Sitosterol	ST	Hydx	Alc	Oxy	1.01	0.02
47	46.661	C29H50O	β-Sitosterol	ST	Hydx	Alc	Oxy	0.57	0.01
48	46.767	C27H48O	Dihydrocholesterol	ST	Hydx	Alc	Oxy	0.34	0.01
Sum								100.0	1.50

1-5_SL600C_PdZrO2

Peak	RT	Mol.Form	Name	i	ii	iii	iv	Run	Tot
1	2.124	C6H10O	Cyclohexanone	Oxy	Cbn	Ket	Oxy	4.35	0.07
2	2.25	C6H10O	Cyclohexanone	Oxy	Cbn	Ket	Oxy	1.08	0.02
3	2.913	C7H8	Toluene	B	HC	HCs	Ar	1.72	0.03
4	3.182	C5H8O	Cyclopentanone	Oxy	Cbn	Ket	Oxy	2.68	0.05
5	3.283	C3H6O2	Propionic acid	Acd	Car	Cabox	Oxy	2.08	0.04
6	3.451	C4H4O2	Furanone	F	Cbn	Ket	Oxy	1.63	0.03
7	4.022	C5H4O2	Furfural	F	Cbn	Aldh	Oxy	7.61	0.13
8	4.433	C8H10	Xylene	B	HC	HCs	Ar	0.58	0.01
9	6.671	C5H6O2	Furfuranol	F	Hydx	Alc	Oxy	1.16	0.02
10	6.936	C7H16O	Heptanol	Oxy	Hydx	Alc	Oxy	2.07	0.04
11	7.39	C5H6O2	Furfuranol	F	Hydx	Alc	Oxy	3.71	0.06
12	8.336	C8H19N	Octylamine	O	HC	N	N	24.35	0.41
13	14.336	C8H16O	Octanal	Oxy	Cbn	Aldh	Oxy	1.15	0.02
14	14.483	C13H28	3-Ethylundecane	A	HC	HCs	A	0.51	0.01
15	14.737	C8H10O2	Creosol	G	Met	PhOH	Ph	1.45	0.02
16	17.2	C10H16O	2-Hexylfuran	F	HC	Fu	Oxy	0.52	0.01
17	18.065	C6H14O3	Diethylene glycol	Oxy	Met	Eth	Oxy	9.72	0.16
18	18.267	C9H10O2	Vinylguaiacol	G	Met	PhOH	Ph	5.06	0.09
19	19.279	C8H10O3	Syringol	S	Met	PhOH	Ph	2.96	0.05
20	21.72	C9H12O3	4-Methylsyringol	S	Met	PhOH	Ph	1.88	0.03
21	23.169	C14H22O	Phenol, 2,4-bis(1,1-	H	Hydx	PhOH	Ph	0.19	0.00
22	23.69	C10H14O3	4-Ethylsyringol	S	Met	PhOH	Ph	1.24	0.02
23	24.404	C6H10O5	Levoglucosan	Oxy	Hydx	Su	Oxy	7.46	0.13
24	24.759	C10H12O3	4-Vinylsyringol	S	Met	PhOH	Ph	4.52	0.08
25	25.684	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	0.62	0.01
26	28.142	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	1.15	0.02
27	29.251	C10H12O4	Acetosyringone	S	Met	PhOH	Ph	0.61	0.01

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28	35.315	C18H33N	Tricyclohexylamine	O	O	N	N	0.15	0.00
29	35.398	C18H36	1-Octadecene	A	HC	HCs	A	0.19	0.00
30	37.309	C18H37NO	Octadecanamide	O	O	N	N	0.24	0.00
31	39.168	C18H35NO	9-Octadecenamide	O	O	N	N	0.79	0.01
32	39.3	C18H35NO	9-Octadecenamide	O	O	N	N	0.53	0.01
33	39.474	C18H37NO	Octadecanamide	O	O	N	N	0.46	0.01
34	39.75	C28H26	BUTANE, 1,2,3,4-	B	HC	HCs	Ar	0.56	0.01
36	40.159	C16H34O	Hexadecanol	Oxy	Hydx	Alc	Oxy	0.47	0.01
39	40.63	C16H22O4	Dibutyl phthalate	Oxy	Cbn	Es	Oxy	1.42	0.02
41	42.789	C18H35NO	9-Octadecenamide	O	O	N	N	0.45	0.01
43	44.732	C27H48O	Dihydrocholesterol	ST	Hydx	Alc	Oxy	0.24	0.00
44	44.966	C27H44O	4,6-Cholestadien-3β-	ST	Hydx	Alc	Oxy	0.25	0.00
45	45.1	C29H50O	β-Sitosterol	ST	Hydx	Alc	Oxy	0.68	0.01
46	46.653	C29H50O	β-Sitosterol	ST	Hydx	Alc	Oxy	0.49	0.01
47	46.748	C27H48O	Dihydrocholesterol	ST	Hydx	Alc	Oxy	0.37	0.01
49	47.608	C27H44O	4,6-Cholestadien-3β-	ST	Hydx	Alc	Oxy	0.22	0.00
50	47.876	C27H46O	Epicholesterol	ST	Hydx	Alc	Oxy	0.41	0.01
Sum								100.0	1.69

1-1_SL600C_RuZrO2

Peak	RT	Mol.Form	Name	i	ii	iii	iv	Run	Tot
1	2.124	C3H4O3	Pyruvic acid	Acd	Car	Cabox	Oxy	5.01	0.08
2	2.912	C10H12O2	Eugenol	G	Met	PhOH	Ph	1.24	0.02
3	3.083	C5H8O2	Methyl methacrylate	F	Cbn	Ket	Oxy	0.92	0.01
4	3.232	C6H14O2	2-Butoxyethanol	Oxy	Hydx	Alc	Oxy	3.26	0.05
5	3.517	C4H4O2	Furanone	F	Cbn	Ket	Oxy	1.01	0.02
6	3.995	C5H4O2	Furfural	F	Cbn	Aldh	Oxy	9.70	0.15
7	6.667	C5H6O2	Furfuranol	F	Hydx	Alc	Oxy	0.43	0.01
8	6.941	C7H16O	Heptanol	Oxy	Hydx	Alc	Oxy	1.61	0.02
9	7.41	C5H12O	Pentanol	Oxy	Hydx	Alc	Oxy	3.19	0.05
10	8.348	C8H19N	Octylamine	O	HC	N	N	22.88	0.35
11	14.334	C8H16O	Octanal	Oxy	Cbn	Aldh	Oxy	1.47	0.02
12	17.133	C14H28	1-Tetradecene	A	HC	HCs	A	0.46	0.01
13	17.283	C14H28	1-Tetradecene	A	HC	HCs	A	0.21	0.00
14	17.783	C14H28	1-Tetradecene	A	HC	HCs	A	0.33	0.01
15	17.959	C10H13N5O5	Guanosine	O	Hydx	N	N	8.09	0.13
16	18.217	C9H10O2	Vinylguaiacol	G	Met	PhOH	Ph	5.50	0.09
17	19.207	C8H10O3	Syringol	S	Met	PhOH	Ph	3.46	0.05
18	19.894	C18H36	1-Octadecene	A	HC	HCs	A	0.13	0.00
19	21.679	C9H12O3	4-Methylsyringol	S	Met	PhOH	Ph	3.00	0.05
20	23.688	C10H14O3	4-Ethylsyringol	S	Met	PhOH	Ph	0.93	0.01
21	24.316	C6H10O5	Levoglucosan	Oxy	Hydx	Su	Oxy	10.07	0.16
22	24.718	C10H12O3	4-Vinylsyringol	S	Met	PhOH	Ph	3.68	0.06
23	25.613	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	0.75	0.01

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24	28.008	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	1.09	0.02
25	33.099	C22H46O6	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy	0.60	0.01
26	33.237	C22H46O6	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy	0.42	0.01
27	33.488	C22H46O6	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy	0.26	0.00
28	33.948	C22H46O6	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy	0.38	0.01
29	34.336	C22H46O6	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy	0.27	0.00
30	34.901	C22H46O6	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy	0.43	0.01
31	35.033	C22H46O6	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy	0.20	0.00
32	37.284	C22H46O6	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy	0.75	0.01
33	37.386	C22H46O6	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy	0.80	0.01
34	37.565	C22H46O6	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy	0.65	0.01
35	37.894	C22H46O6	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy	0.64	0.01
36	38.05	C20H42O	1-Icosanol	Oxy	Hydx	Alc	Oxy	0.15	0.00
37	38.178	C22H46O6	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy	0.33	0.01
38	38.452	C22H46O6	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy	0.41	0.01
39	39.516	C15H30O	2-Pentadecanone	Oxy	Cbn	Ket	Oxy	0.20	0.00
40	40.485	C15H30O	2-Pentadecanone	Oxy	Cbn	Ket	Oxy	0.18	0.00
41	40.635	C16H22O4	Dibutyl phthalate	Oxy	Cbn	Es	Oxy	1.35	0.02
42	44.067	C29H50O	β-Sitosterol	ST	Hydx	Alc	Oxy	0.21	0.00
43	44.728	C27H48O	Dihydrocholesterol	ST	Hydx	Alc	Oxy	0.31	0.00
44	44.833	C29H50O	β-Sitosterol	ST	Hydx	Alc	Oxy	0.23	0.00
45	44.963	C27H44O	4,6-Cholestadien-3β-	ST	Hydx	Alc	Oxy	0.32	0.00
46	45.096	C29H50O	β-Sitosterol	ST	Hydx	Alc	Oxy	1.24	0.02
47	46.651	C29H50O	β-Sitosterol	ST	Hydx	Alc	Oxy	0.85	0.01
48	46.75	C27H48O	Dihydrocholesterol	ST	Hydx	Alc	Oxy	0.42	0.01
Sum								100.0	1.55

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1-5_SL600C_RuZrO2

Peak	RT	Mol.Form	Name	i	ii	iii	iv	Run	Tot
1	2.147	C3H6O2	Propionic acid	Acd	Car	Cabox	Oxy	3.05	0.06
2	2.917	C4H6O2	2(3H)-Furanone,	F	Cbn	Ket	Oxy	0.50	0.01
3	3.28	C5H8O2	Methyl methacrylate	F	Cbn	Ket	Oxy	3.31	0.06
4	3.5	C4H4O2	Furanone	F	Cbn	Ket	Oxy	0.71	0.01
5	4	C5H4O2	Furfural	F	Cbn	Aldh	Oxy	9.21	0.18
6	6.946	C7H16O	Heptanol	Oxy	Hydx	Alc	Oxy	2.13	0.04
7	7.355	C5H6O2	Furfuranol	F	Hydx	Alc	Oxy	5.98	0.12
8	8.38	C8H19N	Octylamine	O	HC	N	N	29.56	0.57
9	9.068	C10H16	Limonene	A	HC	HCs	A	0.12	0.00
10	14.303	C12H26O	6-Dodecanol	Oxy	Hydx	Alc	Oxy	1.15	0.02
11	14.652	C8H10O2	Creosol	G	Met	PhOH	Ph	0.98	0.02
12	17.181	C10H16O	2-Hexylfuran	F	HC	Fu	Oxy	0.27	0.01
13	18.242	C6H14O3	Diethylene glycol	Oxy	Met	Eth	Oxy	12.95	0.25
14	19.236	C8H10O3	Syringol	S	Met	PhOH	Ph	2.61	0.05
15	21.677	C9H12O3	4-Methylsyringol	S	Met	PhOH	Ph	2.79	0.05

16	23.133	C14H22O	Phenol, 2,4-bis(1,1-	H	Hydx	PhOH	Ph	1.13	0.02
17	23.683	C10H14O3	4-Ethylsyringol	S	Met	PhOH	Ph	1.92	0.04
18	24.524	C6H10O5	Levoglucosan	Oxy	Hydx	Su	Oxy	6.30	0.12
19	24.705	C10H12O3	4-Vinylsyringol	S	Met	PhOH	Ph	5.60	0.11
20	25.622	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	0.38	0.01
21	27.973	C11H14O3	4-Allylsyringol	S	Met	PhOH	Ph	0.71	0.01
22	28.133	C11H24O	1-Undecanol	Oxy	Hydx	Alc	Oxy	0.18	0.00
23	33.099	C22H46O6	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy	0.49	0.01
24	33.236	C22H46O6	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy	0.31	0.01
25	33.49	C22H46O6	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy	0.16	0.00
26	33.943	C22H46O6	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy	0.25	0.00
27	34.334	C22H46O6	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy	0.18	0.00
28	34.897	C22H46O6	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy	0.27	0.01
29	35.02	C22H46O6	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy	0.14	0.00
30	37.289	C22H46O6	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy	0.41	0.01
31	37.4	C22H46O6	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy	0.43	0.01
32	37.566	C22H46O6	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy	0.34	0.01
33	37.9	C22H46O6	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy	0.41	0.01
34	38.032	C20H42O	1-Icosanol	Oxy	Hydx	Alc	Oxy	0.13	0.00
35	39.278	C18H35NO	9-Octadecenamide	O	O	N	N	0.16	0.00
36	39.507	C15H30O	2-Pentadecanone	Oxy	Cbn	Ket	Oxy	0.21	0.00
39	40.471	C15H30O	2-Pentadecanone	Oxy	Cbn	Ket	Oxy	0.24	0.00
40	40.623	C16H22O4	Dibutyl phthalate	Oxy	Cbn	Es	Oxy	1.39	0.03
41	42.499	C17H20O6	Fumaric acid, 2,6-	Oxy	Cbn	Es	Oxy	0.19	0.00
42	44.053	C29H50O	β-Sitosterol	ST	Hydx	Alc	Oxy	0.17	0.00
43	44.618	C29H50O	β-Sitosterol	ST	Hydx	Alc	Oxy	0.14	0.00
44	44.715	C27H48O	Dihydrocholesterol	ST	Hydx	Alc	Oxy	0.25	0.00
45	44.951	C27H44O	4,6-Cholestadien-3β-	ST	Hydx	Alc	Oxy	0.22	0.00
46	45.082	C29H50O	β-Sitosterol	ST	Hydx	Alc	Oxy	1.02	0.02
47	46.643	C29H50O	β-Sitosterol	ST	Hydx	Alc	Oxy	0.60	0.01
48	46.75	C27H48O	Dihydrocholesterol	ST	Hydx	Alc	Oxy	0.35	0.01
Sum								100.0	1.94

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LMC400C

Peak	RT	Mol.Form	Name	i	ii	iii	iv	Run	Tot
1	3.036	C2H6S2	Dimethyl disulfide	O	O	O	O	7.62	0.02
2	12.835	C7H8O2	Guaiacol	G	Met	PhOH	Ph	7.33	0.02
3	34.094	C18H38O5	Tetraethylene glycol,	Oxy	Hydx	Alc	Oxy	1.22	0.00
4	34.224	C16H22O4	Dibutyl phthalate	Oxy	Cbn	Es	Oxy	2.52	0.01
5	34.487	C22H46O6	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy	1.01	0.00
6	34.92	C22H46O6	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy	0.73	0.00
7	35.733	C19H24	1,1-Diphenylheptane	B	HC	HCs	Ar	1.02	0.00
8	36.35	C19H36O2	Methyloleate	Oxy	Cbn	Es	Oxy	0.32	0.00
10	38.074	C18H35NO	9-Octadecenamide	O	O	N	N	1.77	0.00

11	39.347	C21H30O2	Methyl	Oxy	Cbn	Es	Oxy	0.48	0.00
12	39.941	C18H35NO	9-Octadecenamide	O	O	N	N	4.51	0.01
13	40.207	C18H37NO	Octadecanamide	O	O	N	N	1.96	0.01
14	41.304	C24H38O4	Bis(2-ethylhexyl)	Oxy	Cbn	Es	Oxy	5.98	0.02
15	41.929	C11H22O3	Methyl 10-	Oxy	Cbn	Es	Oxy	0.45	0.00
16	43.038	C24H38O4	Bis(2-ethylhexyl)	Oxy	Cbn	Es	Oxy	0.38	0.00
17	43.265	C27H44	Cholesta-3,5-diene	ST	HC	HCs	A	0.51	0.00
18	43.441	C22H43NO	Erucylamide	O	O	N	N	5.03	0.01
19	43.579	C30H50	Squalene	A	HC	HCs	A	4.50	0.01
20	44.37	C27H44	Cholesta-3,5-diene	ST	HC	HCs	A	1.28	0.00
21	45.828	C25H38O7	Androstane-17-	HC	Cbny	Cabox	Cyclo	0.45	0.00
24	47.769	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	1.93	0.01
25	47.897	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	1.20	0.00
26	48.033	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	1.78	0.00
27	48.414	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	8.78	0.02
28	48.629	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	4.29	0.01
29	48.747	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	3.45	0.01
32	49.185	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	1.85	0.00
34	49.381	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	1.85	0.00
35	50.304	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	0.51	0.00
36	52.835	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	0.26	0.00
37	53.116	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	0.88	0.00
38	53.192	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	4.84	0.01
39	53.722	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	6.13	0.02
40	54.272	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	5.13	0.01
41	54.739	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	1.29	0.00
44	55.108	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	0.43	0.00
47	57.18	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	2.02	0.01
48	57.283	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	0.41	0.00
49	57.403	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	1.41	0.00
Sum								100.0	0.26

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1-1_LMC400C_ZrO2

Peak	RT	Mol.Form	Name	i	ii	iii	iv	Run	Tot
1	3.125	C12H26O	6-Dodecanol	Oxy	Hydx	Alc	Oxy	1.64	0.00
2	28.95	C11H24O2	Heptanal, diethyl acetal	Oxy	Hydx	Alc	Oxy	2.75	0.00
3	29.1	C12H26O	6-Dodecanol	Oxy	Hydx	Alc	Oxy	2.00	0.00
4	29.383	C16H22O4	Dibutyl phthalate	Oxy	Cbn	Es	Oxy	2.80	0.00
5	34.501	C19H24	1,1-Diphenylheptane	B	HC	HCs	Ar	0.19	0.00
6	35.85	C21H30O2	Methyl	Oxy	Cbn	Es	Oxy	0.66	0.00
7	39.483	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	4.74	0.01
11	47.64	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	1.00	0.00
19	48.75	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	2.94	0.00
20	48.98	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	0.30	0.00

21	49.6	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	1.65	0.00
22	50.5	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	5.42	0.01
23	50.567	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	5.92	0.01
25	50.85	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	2.45	0.00
26	51.246	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	1.34	0.00
27	51.352	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	0.69	0.00
28	52.006	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	1.51	0.00
29	52.1	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	0.78	0.00
30	52.233	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	0.97	0.00
31	52.317	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	2.32	0.00
32	52.715	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	0.48	0.00
33	52.98	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	2.88	0.00
34	53.548	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	2.09	0.00
35	53.667	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	2.92	0.00
37	53.821	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	0.62	0.00
38	54.1	C21H30O2	Methyl	Oxy	Cbn	Es	Oxy	2.72	0.00
39	54.2	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	1.16	0.00
40	54.334	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	2.14	0.00
41	54.517	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	0.33	0.00
42	55.296	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	8.58	0.01
43	55.45	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	5.40	0.01
44	56.081	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	2.35	0.00
45	56.233	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	8.68	0.01
46	56.398	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	4.79	0.01
47	56.852	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	0.85	0.00
48	57.366	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	3.44	0.00
49	57.585	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	0.39	0.00
50	57.717	C16H22O4	Dibutyl phthalate	Oxy	Cbn	Es	Oxy	0.76	0.02
Sum								100.0	0.14

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1-1_LMC400C_NiZrO2

Peak	RT	Mol.Form	Name	i	ii	iii	iv	Run	Tot
1	15.274	C14H28	1-Tetradecene	A	HC	HCs	A	1.21	0.00
2	18.105	C14H28	1-Tetradecene	A	HC	HCs	A	3.62	0.01
3	18.283	C14H28	1-Tetradecene	A	HC	HCs	A	2.28	0.01
4	18.667	C12H24	cis-5-Dodecene	A	HC	HCs	A	0.58	0.00
5	18.844	C12H24	cis-5-Dodecene	A	HC	HCs	A	0.69	0.00
6	20.948	C14H28	1-Tetradecene	A	HC	HCs	A	1.40	0.00
7	21.133	C14H28	1-Tetradecene	A	HC	HCs	A	0.54	0.00
8	23.779	C15H30O2	Methyl tetradecanoate	Oxy	Cbn	Es	Oxy	0.47	0.00
9	28.98	C16H34O	Hexadecanol	Oxy	Hydx	Alc	Oxy	1.31	0.00
10	29.272	C19H38O2	Methyl stearate	Oxy	Cbn	Es	Oxy	0.86	0.00
11	29.7	C18H38O4	Triethylene glycol	Oxy	Hydx	Alc	Oxy	0.34	0.00
12	31.019	C13H28O	1-Tridecanol	Oxy	Hydx	Alc	Oxy	0.51	0.00

13	31.141	C11H24O2	Heptanal, diethyl acetal	Oxy	Hydx	Alc	Oxy	0.43	0.00
14	31.388	C23H46O2	Methyl docosanoate	Oxy	Cbn	Es	Oxy	0.36	0.00
15	32.206	C22H46O6	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy	0.86	0.00
16	32.338	C18H38O5	Tetraethylene glycol,	Oxy	Hydx	Alc	Oxy	1.29	0.00
17	32.678	C10H20O2	Ethyl octanoate	Oxy	HC	Es	Oxy	2.30	0.01
18	33.095	C16H31N	Palmitonitrile	O	O	N	N	2.34	0.01
19	33.406	C17H34O2	Methyl hexadecanoate	Oxy	Cbn	Es	Oxy	0.61	0.00
20	33.633	C18H38O5	Tetraethylene glycol,	Oxy	Hydx	Alc	Oxy	0.73	0.00
21	34.068	C18H38O5	Tetraethylene glycol,	Oxy	Hydx	Alc	Oxy	4.17	0.01
22	34.223	C18H38O5	Tetraethylene glycol,	Oxy	Hydx	Alc	Oxy	4.84	0.01
23	34.507	C22H46O6	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy	4.33	0.01
24	34.983	C22H46O6	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy	2.42	0.01
25	35.477	C22H46O6	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy	1.50	0.00
26	35.687	C19H24	1,1-Diphenylheptane	B	HC	HCs	Ar	0.67	0.00
27	35.843	C22H46O6	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy	1.77	0.00
29	36.171	C18H33N	Tricyclohexylamine	O	O	N	N	5.60	0.02
30	36.35	C19H36O2	Methyloleate	Oxy	Cbn	Es	Oxy	2.70	0.01
31	36.712	C10H20O2	Ethyl octanoate	Oxy	HC	Es	Oxy	2.41	0.01
32	37.123	C26H54O8	Heptaethylene glycol	Oxy	Hydx	Alc	Oxy	1.55	0.00
35	38.3	C26H54O8	Heptaethylene glycol	Oxy	Hydx	Alc	Oxy	0.36	0.00
37	38.499	C18H18	3,4,5,6-	B	HC	HCs	Ar	2.52	0.01
39	39.364	C21H30O2	Methyl dehydroabietate	Oxy	Cbn	Es	Oxy	0.58	0.00
40	40.217	C18H35NO	9-Octadecenamide	O	O	N	N	1.19	0.00
44	40.937	C16H30O	cis-9-Hexadecenal	Oxy	Cbn	Aldh	Ar	0.83	0.00
45	41.365	C16H22O4	Dibutyl phthalate	Oxy	Cbn	Es	Oxy	1.41	0.00
48	49.55	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	35.98	0.10
49	49.733	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	1.66	0.00
50	49.983								
Sum								100.0	0.28

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1-5_LMC400C_NiZrO2

Peak	RT	Mol.Form	Name	i	ii	iii	iv	Run	Tot
1	15.881	C14H28	1-Tetradecene	A	HC	HCs	A	3.15	0.00
2	18.391	C14H28	1-Tetradecene	A	HC	HCs	A	3.45	0.00
3	18.578	C14H28	1-Tetradecene	A	HC	HCs	A	6.66	0.01
4	19.216	C9H18	1-Nonene	B	HC	HCs	A	2.49	0.00
5	19.467	C5H4N4O	Hypoxanthine	O	Hydx	Alc	N	0.69	0.00
6	21.568	C18H36	1-Octadecene	A	HC	HCs	A	3.34	0.00
8	31.454	C14H28	1-Tetradecene	A	HC	HCs	A	0.85	0.00
9	32.617	C6H14O	2-Hexanol	Oxy	Hydx	Alc	Oxy	0.64	0.00
10	32.786	C6H14O	2-Hexanol	Oxy	Hydx	Alc	Oxy	0.78	0.00
11	34.393	C18H38O5	Tetraethylene glycol,	Oxy	Hydx	Alc	Oxy	3.92	0.00
12	34.609	C18H38O5	Tetraethylene glycol,	Oxy	Hydx	Alc	Oxy	6.26	0.01
13	34.965	C18H38O5	Tetraethylene glycol,	Oxy	Hydx	Alc	Oxy	4.99	0.01

14	35.529	C18H38O5	Tetraethylene glycol,	Oxy	Hydx	Alc	Oxy	1.77	0.00
16	35.883	C19H24	1,1-Diphenylheptane	B	HC	HCs	Ar	0.35	0.00
17	36.445	C18H38O5	Tetraethylene glycol,	Oxy	Hydx	Alc	Oxy	2.59	0.00
18	38.907	C18H18	3,4,5,6-	B	HC	HCs	Ar	1.12	0.00
19	40.663	C10H12	4-Ethylstyrene	B	HC	HCs	Ar	4.42	0.01
22	41.572	C16H22O4	Dibutyl phthalate	Oxy	Cbn	Es	Oxy	0.93	0.00
23	42.3	C19H40	Nonadecane	A	HC	HCs	A	0.63	0.00
25	43.6	C19H40	Nonadecane	A	HC	HCs	A	0.51	0.00
31	50.862	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	29.71	0.03
34	51.314	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	13.80	0.02
38	52.054	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	6.20	0.01
50	57.735	C6H10O5	Levoglucosan	Oxy	Hydx	Su	Oxy	9.28	0.27
Sum								100.0	0.12

1-10_LMC400C_NiZrO2

Pea	RT	Mol.Form	Name	i	ii	iii	iv	Run	Tot
1	18.42	C12H24	cis-5-Dodecene	A	HC	HCs	A	10.4	0.0
2	31.16	C12H24	cis-5-Dodecene	A	HC	HCs	A	1.11	0.0
3	32.30	C22H46O	Dodecylpentaglycol	Ox	Hyd	Alc	Ox	1.13	0.0
4	32.44	C22H46O	Dodecylpentaglycol	Ox	Hyd	Alc	Ox	2.31	0.0
5	32.74	C22H46O	Dodecylpentaglycol	Ox	Hyd	Alc	Ox	1.08	0.0
6	33.86	C18H38O	Decyltetraglycol	Ox	Hyd	Alc	Ox	0.63	0.0
7	34.10	C18H38O	Decyltetraglycol	Ox	Hyd	Alc	Ox	10.7	0.0
8	34.29	C18H38O	Decyltetraglycol	Ox	Hyd	Alc	Ox	13.5	0.0
9	34.59	C18H38O	Decyltetraglycol	Ox	Hyd	Alc	Ox	12.1	0.0
10	35.12	C18H38O	Decyltetraglycol	Ox	Hyd	Alc	Ox	7.24	0.0
11	35.65	C18H38O	Decyltetraglycol	Ox	Hyd	Alc	Ox	1.10	0.0
13	35.93	C18H38O	Decyltetraglycol	Ox	Hyd	Alc	Ox	6.33	0.0
14	36.13	C18H38O	Decyltetraglycol	Ox	Hyd	Alc	Ox	5.10	0.0
15	36.45	C10H20O	8-Methyl-8-nonene-2,4-diol	Ox	HC	Es	Ox	7.47	0.0
16	37.01	C22H46O	Dodecylpentaglycol	Ox	Hyd	Alc	Ox	2.39	0.0
19	41.23	C16H30O	cis-9-Hexadecenal	Ox	Cbn	Ald	Ar	1.01	0.0
20	41.50	C16H22O	1,2-Benzenedicarboxylic acid,	Ox	Cbn	Es	Ox	2.05	0.0
22	42.26	C13H28	3-Ethylundecane	A	HC	HCs	A	0.17	0.0
37	45.73	C16H28	4,5-	A	HC	HCs	A	0.26	0.0
43	47.56	C16H28	4,5-	A	HC	HCs	A	2.11	0.0
44	47.92	C16H28	4,5-	A	HC	HCs	A	8.11	0.0
46	48.16	C9H20O4	Tripropylene glycol	Ox	Hyd	Alc	Ox	0.32	0.0
Sum								100.	0.1

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1-1_LMC400C_PdZrO2

Peak	RT	Mol.Form	Name	i	ii	iii	iv	Run	Tot

1	32.567	C10H20O2	Ethyl octanoate	Oxy	HC	Es	Oxy	2.32	0.00
2	32.989	C11H21N	1-Cyanodecane	O	O	N	N	1.86	0.00
3	33.34	C17H34O2	Methyl	Oxy	Cbn	Es	Oxy	1.05	0.00
4	34.033	C10H20O3	Ethyl 3-	Oxy	HC	Es	Oxy	1.39	0.00
5	34.169	C16H22O4	Dibutyl phthalate	Oxy	Cbn	Es	Oxy	3.57	0.01
6	34.45	C12H24O3	2-Ethyl-3-	Oxy	Cbn	Es	Oxy	2.59	0.00
7	34.867	C10H20O3	Ethyl 3-	Oxy	HC	Es	Oxy	0.75	0.00
8	35.283	C11H24O2	Heptanal, diethyl	Oxy	Hyd	Alc	Oxy	0.98	0.00
9	35.65	C19H24	1,1-	B	HC	HCs	Ar	0.87	0.00
11	36.048	C18H33N	Tricyclohexylamine	O	O	N	N	8.02	0.01
12	36.15	C16H34O	Hexadecanol	Oxy	Hyd	Alc	Oxy	3.92	0.01
13	36.283	C19H36O2	Methyloleate	Oxy	Cbn	Es	Oxy	1.14	0.00
14	36.437	C17H33N	Heptadecanenitrile	O	O	N	N	1.78	0.00
15	36.649	C15H30O2	Methyl	Oxy	Cbn	Es	Oxy	0.58	0.00
16	37.467	C18H31N	N-Dodecylaniline	O	O	N	N	0.59	0.00
17	37.65	C18H35NO	9-Octadecenamide	O	O	N	N	1.63	0.00
18	37.93	C18H35NO	9-Octadecenamide	O	O	N	N	4.45	0.01
19	39.29	C21H30O2	Methyl	Oxy	Cbn	Es	Oxy	0.62	0.00
21	39.785	C18H35NO	9-Octadecenamide	O	O	N	N	19.91	0.03
22	40.083	C9H20O4	Tripropylene glycol	Oxy	Hyd	Alc	Oxy	4.11	0.01
23	40.788	C18H33N	Tricyclohexylamine	O	O	N	N	0.73	0.00
24	41.255	C16H22O4	Dibutyl phthalate	Oxy	Cbn	Es	Oxy	3.92	0.01
27	44.317	C27H44	Cholesta-3,5-diene	ST	HC	HCs	A	0.43	0.00
33	46.71	C31H62O	16-	Oxy	Cbn	Ket	Oxy	2.25	0.00
36	47.967	C31H62O	16-	Oxy	Cbn	Ket	Oxy	2.94	0.00
37	48.314	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	6.69	0.01
40	50.115	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	3.42	0.01
41	50.233	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	0.84	0.00
42	50.444	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	7.81	0.01
43	51.783	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	0.31	0.00
47	57.333	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	4.80	0.01
48	57.418	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	0.42	0.00
49	57.612	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	1.70	0.00
50	57.839	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	1.60	0.00
Sum								100.0	0.16

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1-1_LMC400C_RuZrO2

Peak	RT	Mol.Form	Name	i	ii	iii	iv	Run	Tot
1	3.19	C2H6S2	Dimethyl disulfide	O	O	O	O	4.55	0.01
2	28.933	C12H26O	6-Dodecanol	Oxy	Hyd	Alc	Oxy	1.67	0.00
3	29.067	C11H24O2	Heptanal, diethyl	Oxy	Hyd	Alc	Oxy	2.61	0.00
4	29.367	C10H22O	4-Decanol	Oxy	Hyd	Alc	Oxy	2.00	0.00
5	34.482	C16H22O4	Dibutyl phthalate	Oxy	Cbn	Es	Oxy	3.19	0.01
6	39.48	C21H30O2	Methyl	Oxy	Cbn	Es	Oxy	0.48	0.00
7	41.493	C24H38O4	Bis(2-ethylhexyl)	Oxy	Cbn	Es	Oxy	0.60	0.00

8	46.167	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	2.04	0.00
9	46.417	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	1.30	0.00
13	48.267	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	6.78	0.01
16	48.727	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	10.41	0.02
18	49.129	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	5.66	0.01
19	49.217	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	21.14	0.03
20	49.533	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	6.32	0.01
25	50.205	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	5.92	0.01
27	50.59	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	2.28	0.00
28	51.472	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	2.25	0.00
29	51.785	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	0.60	0.00
30	52.732	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	0.21	0.00
32	53.55	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	1.35	0.00
36	54.206	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	0.95	0.00
37	54.315	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	1.46	0.00
38	54.49	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	2.59	0.00
39	54.69	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	0.47	0.00
41	55.28	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	4.65	0.01
43	55.696	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	0.86	0.00
44	55.829	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	0.67	0.00
45	55.903	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	0.34	0.00
46	56.615	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	2.39	0.00
47	56.887	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	0.37	0.00
48	56.988	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	2.49	0.00
50	57.608	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	1.39	0.00
Sum								100.0	0.16

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LMC500C

Peak	RT	Mol.Form	Name	i	ii	iii	iv	Run	Tot
1	3.135	C2H6S2	Dimethyl disulfide	O	O	O	O	2.19	0.00
2	32.69	C17H34O2	Methyl hexadecanoate	Oxy	Cbn	Es	Oxy	1.09	0.00
4	35.535	C18H33N	Tricyclohexylamine	O	O	N	N	6.56	0.01
5	35.7	C19H36O2	Methyloleate	Oxy	Cbn	Es	Oxy	2.96	0.00
6	35.908	C16H31N	Palmitonitrile	O	O	N	N	3.37	0.00
7	36.07	C19H38O2	Methyl stearate	Oxy	Cbn	Es	Oxy	1.03	0.00
10	40.334	C10H12O2	Eugenol	G	Met	PhOH	Ph	5.79	0.01
11	40.467	C16H30O	cis-9-Hexadecenal	Oxy	Cbn	Aldh	Ar	1.31	0.00
13	41.332	C16H22O4	Dibutyl phthalate	Oxy	Cbn	Es	Oxy	1.05	0.00
14	42.982	C15H30O	2-Pentadecanone	Oxy	Cbn	Ket	Oxy	1.86	0.00
15	45.187	C30H50	Squalene	A	HC	HCs	A	0.88	0.00
16	46.183	C27H44	Cholesta-3,5-diene	ST	HC	HCs	A	5.90	0.01
20	47.083	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	2.30	0.00
29	48.55	C26H50	Cyclohexane, 1,1'-	A	HC	HCs	A	9.33	0.01
34	49.317	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	8.11	0.01

35	49.417	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	5.72	0.01
38	49.82	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	12.17	0.01
39	50.084	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	16.41	0.02
40	50.2	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	5.37	0.01
42	50.633	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	2.27	0.00
46	53.439	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	2.12	0.00
47	54.603	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	0.74	0.00
49	55.979	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	1.46	0.00
Sum								100.0	0.11

LMC600C

Peak	RT	Mol.Form	Name	i	ii	iii	iv	Run	Tot
1	2.231	C7H8O2	Guaiacol	G	Met	PhOH	Ph	5.18	0.01
2	3.291	C6H6	Benzene	B	HC	HCs	Ar	4.33	0.00
3	5.791	C7H8	Toluene	B	HC	HCs	Ar	29.83	0.03
4	20.685	C8H8	Styrene	B	HC	HCs	Ar	2.13	0.00
5	23.247	C18H36	1-Octadecene	A	HC	HCs	A	0.66	0.00
6	26.578	C18H36	1-Octadecene	A	HC	HCs	A	1.80	0.00
7	26.854	C17H28	Undecylbenzene	B	HC	HCs	Ar	0.72	0.00
8	27.938	C18H30	n-dodecylbenzene	B	HC	HCs	Ar	0.43	0.00
9	28.667	C18H36	1-Octadecene	A	HC	HCs	A	2.22	0.00
10	28.787	C18H30	n-dodecylbenzene	B	HC	HCs	Ar	2.72	0.00
11	28.983	C18H30	n-dodecylbenzene	B	HC	HCs	Ar	2.11	0.00
12	29.081	C10H20O2	Ethyl octanoate	Oxy	HC	Es	Oxy	4.12	0.00
13	29.572	C18H30	n-dodecylbenzene	B	HC	HCs	Ar	1.62	0.00
14	30.13	C18H30	n-dodecylbenzene	B	HC	HCs	Ar	0.54	0.00
15	30.426	C18H36	1-Octadecene	A	HC	HCs	A	1.42	0.00
16	30.793	C18H30	n-dodecylbenzene	B	HC	HCs	Ar	3.69	0.00
17	30.962	C18H30	n-dodecylbenzene	B	HC	HCs	Ar	2.15	0.00
18	31.258	C18H30	n-dodecylbenzene	B	HC	HCs	Ar	1.97	0.00
19	31.767	C18H30	n-dodecylbenzene	B	HC	HCs	Ar	0.96	0.00
20	32.619	C18H30	n-dodecylbenzene	B	HC	HCs	Ar	0.81	0.00
21	32.817	C18H30	n-dodecylbenzene	B	HC	HCs	Ar	1.38	0.00
22	33.057	C16H31N	Palmitonitrile	O	O	N	N	1.36	0.00
23	34.337	C16H32O2	Hexadecanoic acid	Acd	Car	Cabox	Oxy	0.59	0.00
25	35.317	C21H30O2	Methyl dehydroabietate	Oxy	Cbn	Es	Oxy	0.52	0.00
26	35.583	C19H24	1,1-Diphenylheptane	B	HC	HCs	Ar	0.75	0.00
28	36.016	C18H33N	Tricyclohexylamine	O	O	N	N	3.61	0.00
29	36.133	C19H36O2	Methyloleate	Oxy	Cbn	Es	Oxy	1.00	0.00
31	36.367	C17H33N	Heptadecanenitrile	O	O	N	N	1.28	0.00
32	36.55	C19H38O2	Methyl stearate	Oxy	Cbn	Es	Oxy	2.97	0.00
34	37.217	C17H16O	1,4-diphenyl-4-penten-1-	Oxy	Cbn	Ket	Oxy	1.65	0.00
36	38.038	C14H22O2	3,5-Di-tert-butyl	C	Hydx	PhOH	Ph	2.75	0.00
37	38.973	C18H18	3,4,5,6-	B	HC	HCs	Ar	1.78	0.00

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38	39.228	$C_{21}H_{30}O_2$	Methyl dehydroabietate	Oxy	Cbn	Es	Oxy	5.58	0.01
43	41.039	$C_{18}H_{33}N$	Tricyclohexylamine	O	O	N	N	1.43	0.00
44	41.843	$C_{16}H_{22}O_4$	Dibutyl phthalate	Oxy	Cbn	Es	Oxy	0.84	0.00
45	42.517	$C_{18}H_{38}$	8-Methylheptadecane	A	HC	HCs	A	1.73	0.00
47	44.046	$C_{24}H_{38}O_4$	Bis(2-ethylhexyl)	Oxy	Cbn	Es	Oxy	0.74	0.00
50	53.913	$C_{29}H_{50}O$	β-Sitosterol	ST	Hydx	Alc	Oxy	0.62	0.00
Sum								100.0	0.10

1-1_LMC600C_NiZrO2

Peak	RT	Mol.Form	Name	i	ii	iii	iv	Run	Tot
1	2.279	C_6H_6	Benzene	B	HC	HCs	Ar	0.42	0.01
2	3.453	C_7H_8	Toluene	B	HC	HCs	Ar	0.51	0.01
4	12.3	$C_7H_8O_2$	Guaiacol	G	Met	PhOH	Ph	2.36	0.05
5	12.599	$C_7H_8O_2$	Guaiacol	G	Met	PhOH	Ph	3.53	0.08
6	16.153	$C_8H_{10}O_2$	Creosol	G	Met	PhOH	Ph	0.39	0.01
7	17.668	$C_{14}H_{28}$	1-Tetradecene	A	HC	HCs	A	0.38	0.01
8	20.464	$C_9H_{10}O_2$	Vinylguaiacol	G	Met	PhOH	Ph	0.62	0.01
9	23.589	$C_{10}H_{12}O_2$	Eugenol	G	Met	PhOH	Ph	0.34	0.01
10	33.436	$C_{10}H_{20}O_3$	Ethyl 3-hydroxyoctanoate	Oxy	HC	Es	Oxy	0.40	0.01
11	33.604	$C_8H_{16}O_4$	2-(2-Ethoxyethoxy)ethyl	Oxy	HC	Es	Oxy	0.59	0.01
12	33.897	$C_{10}H_{20}O_3$	Ethyl 3-hydroxyoctanoate	Oxy	HC	Es	Oxy	0.45	0.01
13	34.355	$C_{22}H_{46}O_6$	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy	0.28	0.01
14	34.757	$C_{22}H_{46}O_6$	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy	0.20	0.00
15	35.152	$C_{22}H_{46}O_6$	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy	0.28	0.01
18	35.611	$C_{14}H_{30}O$	Tetradecanol	Oxy	Hydx	Alc	Oxy	0.16	0.00
19	35.731	$C_{19}H_{36}O_2$	Methyloleate	Oxy	Cbn	Es	Oxy	0.17	0.00
20	36.087	$C_{16}H_{32}O_2$	Hexadecanoic acid	Acd	Car	Cabox	Oxy	0.18	0.00
21	36.353	$C_{22}H_{46}O_6$	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy	0.23	0.01
22	36.451	$C_{22}H_{46}O_6$	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy	0.29	0.01
23	36.663	$C_{22}H_{46}O_6$	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy	0.13	0.00
25	37.507	$C_{22}H_{46}O_6$	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy	0.60	0.01
26	37.617	$C_{22}H_{46}O_6$	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy	0.63	0.01
27	37.857	$C_{18}H_{18}$	3,4,5,6-	B	HC	HCs	Ar	0.91	0.02
28	38.067	$C_{16}H_{33}NO$	Palmiticamide	O	O	N	N	0.40	0.01
29	38.296	$C_{22}H_{46}O_6$	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy	0.55	0.01
30	38.689	$C_{21}H_{30}O_2$	Methyl dehydroabietate	Oxy	Cbn	Es	Oxy	0.25	0.01
31	40.019	$C_{18}H_{35}NO$	9-Octadecenamide	O	O	N	N	0.41	0.01
32	40.223	$C_{18}H_{35}NO$	9-Octadecenamide	O	O	N	N	0.49	0.01
33	40.856	$C_{16}H_{22}O_4$	Dibutyl phthalate	Oxy	Cbn	Es	Oxy	0.34	0.01
34	43.35	$C_{18}H_{35}NO$	9-Octadecenamide	O	O	N	N	0.23	0.01
35	43.52	$C_{10}H_{21}NO$	Decanamide	O	Cbn	N	N	0.17	0.00
36	45.267	$C_{29}H_{50}O$	β-Sitosterol	ST	Hydx	Alc	Oxy	0.39	0.01
37	45.517	$C_{16}H_{28}$	4-Hexadecen-6-yne	A	HC	HCs	A	0.43	0.01
39	46.165	$C_{16}H_{28}$	4-Hexadecen-6-yne	A	HC	HCs	A	1.55	0.04

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40	46.9	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	5.51	0.13
43	49.383	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	21.61	0.50
44	49.583	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	6.46	0.15
45	50.095	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	23.17	0.54
46	51.779	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	12.56	0.29
47	52.233	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	3.97	0.09
48	52.633	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	3.92	0.09
50	53.633	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	3.53	0.08
Sum								100.0	2.31

1-1_LMC600C_PdZrO2

Peak	RT	Mol.Form	Name	i	ii	iii	iv	Run	Tot
1	2.304	C6H6	Benzene	B	HC	HCs	Ar	2.05	0.00
3	12.967	C7H8O2	Guaiacol	G	Met	PhOH	Ph	2.31	0.00
5	35.698	C16H30O	cis-9-Hexadecenal	Oxy	Cbn	Aldh	Ar	1.14	0.00
6	35.831	C18H34O2	Vinyl palmitate	Oxy	Cbn	Es	Oxy	0.64	0.00
7	37.71	C22H46O6	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy	6.66	0.01
8	38.035	C18H18	3,4,5,6-	B	HC	HCs	Ar	8.19	0.01
9	38.31	C22H46O6	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy	3.87	0.01
10	38.771	C21H30O2	Methyl dehydroabietate	Oxy	Cbn	Es	Oxy	2.35	0.00
12	40.441	C16H30O	cis-9-Hexadecenal	Oxy	Cbn	Aldh	Ar	0.94	0.00
13	40.826	C16H22O4	Dibutyl phthalate	Oxy	Cbn	Es	Oxy	7.13	0.01
14	42.6	C24H38O4	Bis(2-ethylhexyl)	Oxy	Cbn	Es	Oxy	1.40	0.00
21	46.867	C29H50O	β-Sitosterol	ST	Hydx	Alc	Oxy	5.16	0.01
31	48.55	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	15.21	0.03
37	49.503	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	8.90	0.01
39	49.75	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	10.37	0.02
41	50.442	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	8.86	0.01
44	50.832	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	6.57	0.01
45	51.05	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	0.84	0.00
46	51.614	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	0.26	0.00
47	52.75	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	3.57	0.01
48	53.078	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	2.28	0.00
49	53.167	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	0.41	0.00
50	53.573	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	0.92	0.00
Sum								100.0	0.17

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1-1_LMC600C_RuZrO2

Peak	RT	Mol.Form	Name	i	ii	iii	iv	Run	Tot
1	12.933	C7H8O2	Guaiacol	G	Met	PhOH	Ph	10.99	0.02
2	13.104	C7H8O2	Guaiacol	G	Met	PhOH	Ph	14.85	0.02
5	35.918	C16H30O	cis-9-Hexadecenal	Oxy	Cbn	Aldh	Ar	3.77	0.01
7	36.661	C22H46O6	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy	2.16	0.00

8	36.993	C17H16O	1,4-diphenyl-4-penten-1-	Oxy	Cbn	Ket	Oxy	2.17	0.00
9	37.686	C22H46O6	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy	4.16	0.01
10	37.848	C22H46O6	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy	6.32	0.01
11	38.075	C18H18	3,4,5,6-	B	HC	HCs	Ar	6.12	0.01
12	38.267	C16H33NO	Palmiticamide	O	O	N	N	2.79	0.00
13	38.456	C22H46O6	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy	6.16	0.01
14	38.778	C21H30O2	Methyl dehydroabietate	Oxy	Cbn	Es	Oxy	2.94	0.00
15	38.967	C22H46O6	Pentaethylene glycol	Oxy	Hydx	Alc	Oxy	2.63	0.00
18	40.133	C18H35NO	9-Octadecenamide	O	O	N	N	3.32	0.00
19	40.294	C18H37NO	Octadecanamide	O	O	N	N	5.45	0.01
20	40.95	C16H22O4	Dibutyl phthalate	Oxy	Cbn	Es	Oxy	2.34	0.00
25	49.133	C16H28	4-Hexadecen-6-yne	A	HC	HCs	A	23.85	0.03
Sum								100.0	0.14

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APPENDIX F

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GAS PRODUCTION DATA

Non-catalytic reaction

H_2	250bar			300bar			400bar		
mol kg$^-$	400°C	500°C	600°C	400°C	500°C	600°C	400°C	500°C	600°C
KBL	11.0	38.0	37.2	12.5	12.2	7.6	6.4	8.6	9.9
SBL	18.1	43.9	57.50	18.1	31.1	39.1	8.3	29.7	21.3
LMC	8.7	40.8	45.3	7.7	17.6	37.3	5.7	7.1	16.6

CH_4	250bar			300bar			400bar		
mmol	400°C	500°C	600°C	400°C	500°C	600°C	400°C	500°C	600°C
KBL	1.41	193.38	138.56	2.12	15.29	43.12	0.70	3.04	44.86
SBL	61.34	255.27	334.03	34.93	186.79	276.74	13.05	17.36	60.84
LMC	15.08	108.61	265.14	1.13	4.61	4.24	2.207	2.033	1.676

CO	250bar			300bar			400bar		
mmol	400°C	500°C	600°C	400°C	500°C	600°C	400°C	500°C	600°C
KBL	2.19	0.36	1.06	0.31	0.50	0.62	0.24	0.35	0.35
SBL	4.10	3.97	0.51	3.11	0.92	0.58	0.37	0.56	0.60
LMC	0.37	0.51	2.19	0.33	0.39	0.37	0.34	0.31	0.32

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Catalytic reaction

H_2	1:1				1:10			
mol kg$^-$	ZrO_2	Ni/ZrO_2	Pd/ZrO_2	Ru/ZrO_2	ZrO_2	Ni/ZrO_2	Pd/ZrO_2	Ru/ZrO_2
KBL	43.35	57.27	38.10	31.71	49.05	65.94	42.78	77.00
SBL	68.55	77.11	74.14	87.11	65.69	69.38	52.72	74.73
LMC	27.30	36.64	35.67	38.22	29.24	35.79	39.16	28.63

CH_4	1:1				1:10			
mmol kg$^-$	ZrO_2	Ni/ZrO_2	Pd/ZrO_2	Ru/ZrO_2	ZrO_2	Ni/ZrO_2	Pd/ZrO_2	Ru/ZrO_2
KBL	3.57	1.73	1.89	3.94	3.86	2.35	2.04	3.76
LMC	5.63	0.97	1.37	2.62	1.41	0.92	0.82	0.35

CO	1:1				1:10			
mmol	ZrO_2	Ni/ZrO_2	Pd/ZrO_2	Ru/ZrO_2	ZrO_2	Ni/ZrO_2	Pd/ZrO_2	Ru/ZrO_2
KBL	0.02	0.01	0.01	0.01	0.01	0.01	0.00	0.00
LMC	0.01	0.01	0.00	0.01	0.01	0.01	0.00	0.01

VITA

Miss Yotwadee Hawangchu was born on March 31, 1983 in Samut Sakhon, Thailand. She graduated with a Bachelor of Science in Environmental Science and Technology from Faculty of Environmetal and Resource Studies of Mahidol university, Thailand. Later, she pursued her master's degree study in the Environmental engineering, Faculty of Engineering, Chulalongkorn university, Thailand since 2010 and complete her Doctoral degree in Environental Management in 2016.

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