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AROMATIC BIOMARKER FROM BROWN COAL, SANGATTA COALFIELD, EAST BORNEO OF MIDDLE MIOCENE TO LATE MIOCENE AGE

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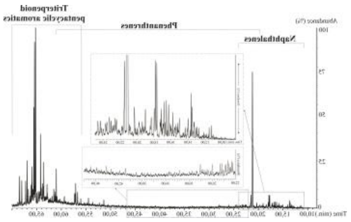
Graphical abstract



Abstract

A section of the Sangatta coalfield in the Balikpapan formation located in Kutai Basin, East Borneo, Indonesia, is the Inul area, located North of Pinang Dome. This section of the coalmine has coals with low calories (ca. 4379 cal/g), which is why they cannot be used optimally yet. The reasons of using low calorie coals are besides from being used as a mixing ingredient for the blending process of high calorie coals, they are also used to diversify the coals through the process of coal liquefaction (coal to liquid). In order for the coal liquefaction to be processed correctly, there needs to be a study on the geochemistry organics through coal biomarker analysis, particularly on the hydrocarbon aromatic fractions, so that the origins of the coal organic compounds could be known. Biomarker analysis on the aromatic hydrocarbon fraction shows the existence of naphthalene compound groups with sesquiterpenoids skeleton, phenanthrene with diterpenoids, sesterpenoids skeleton and triterpenoids aromatic pentacyclic. The existence of cadalene compound, triterpene pentacyclic monoaromatic, -triaromatic, -tetraaromatic, -pentaaromatic and triterpenoid C-ring cleaved hydrocarbon with oleanane, ursane and lupane skeletons indicated that the source of coal organic compounds were derived from β-amyrin which were produced by Angiospermae plants. The coal biomarkers distribution, particularly the high abundance of triterpenoid pentacyclic triaromatic compound, confirmed the low maturity of the coals which is predicted to profit from the process of liquefaction due to the high contents of their aromatic fractions.

Keywords: Brown coal, Inul area, Sangatta coalfield, pentacyclic aromatic triterpenoids, GCMS

1.0 INTRODUCTION

The KPC Sangatta coalfield which is a part of the Balikpapan formation in Kutai Basin, East Borneo, Indonesia, is generally made up of high calorie coals (around 5800-7100 cal/g) all of which have been used optimally. Some of the layers of coal obtained from the KPC Sangatta coalfield, which is located within the Inul area, is predicted to be aged as old as Middle Miocene to Late Miocene, and have a low calorie value, hence making them less economical. Using low calorie coals in increasing energy efficiency and reducing carbon emissions during the process of energy conversion is being advised that diversification should be done; and one of them is by coal liquefaction. The Indonesian Government, in the Outlook Energy 2014, projected that there should be an increase in the coal consumption to power the electric power stations from 53 million tons in 2012 to 321 million tons in 2035. The other needs for coal is to be used as raw materials to produce CTL (coal to liquid) by as much as 4,5 million tons per year, starting from 2030 [1]. Choosing the suitable types of coals to be used for CTL needs accurate criteria. The studies on biomarkers, particularly aromatic hydrocarbon fractions, is an analysis chosen to prepare the productions of CTL.

Aromatic hydrocarbons is an important fraction and richer than saturated hydrocarbon fraction in the coal extract bitumens. The aim of the analysis on biomarkers aromatic hydrocarbon fractions is to find out the origins of the coal organic compounds, the sedimentation environments and the coal maturity, particularly for brown coals or lignite. This information can be translated as an estimation of the types of coals with more economic values for the CTL process. Biomarkers in low grade coals has been interesting in the past recent years [2, 3, 4] because they contain intermediate components in the coalification process and lipid precursors which have not been altered during the diagenesis and catagenesis pathways.

Some studies have been done to identify the components of aromatics as polynuclear aromatic hydrocarbons (PAH) in coals and derived products. In general, the PAH in subbituminous and bituminous coals contain naphthalene, biphenyl, phenanthrene, fluorene, fluoranthene, pyrene, chrysene, picene, and coronene compounds, and their C_1-C_3 alkyl substituted homologues [3]. The constituent PAH compounds are such as mono-, tri- and tetraaromatic pentacyclic compounds, alkylated benzenes, naphthalenes and phenanthrenes as the main components, whilst the aromatic diterpenoid and steroid hydrocarbons as the minor components [3]. The discovery of these biomarker compounds suggested that the origins of the coal organic compounds are from the Angiospermae higher plants. These coals can be classified as immature coals which are less economical if being used directly and is the perfect coal when being prepared for processed coals (CTL).

In the present study, we will report the characteristics of the aromatic hydrocarbon fractions of brown coals taken from the Inul area in the Sangatta coalfield, Kutai Basin, East Borneo, as the first step to design immature coals liquefaction. The study on coal macromolecule structures is expected to give the understanding to the reactions that took place during the process of liquefaction so that it can be developed as an accuracy standard of brown coals when being processed into liquid coals.

2.0 EXPERIMENTAL

2.1 Samples

The samples used in this research is taken from the Inul area located in the Sangatta coalmine, East Borneo, Indonesia, which is a part of the Kutai Basin in the Balikpapan Formation and aged Middle to Late Miocene. The location of where the samples were taken was in the North of Pinang Dome. Geographically, the location of Inul area is in the co-ordinates of 117° 27" 7.40"- 117° 40' 43.40" BT and 0° 31' 20.52" - 0° 52' 4.60" North. The samples were taken at an interval of 74,80 meters; base interval 76,12 meters; and thickness of 1,32 meters.

2.2 Methodology

Coal powder (ca. 100 g) was extracted in a Soxhlet apparatus for 48 hours using an azeotropic mixture of acetone (47%), methanol (23%) and chloroform (30%). The solvent was removed with a rotary evaporator. The extracts were separated using column chromatography over activated silica gel GF_{254}, with KOH/isopropylalcohol and eluted repeatedly into three fractions which were the neutral fraction, the acid fraction and the polar fraction. Neutral fractions were eluted using eluent diethylether, acid fractions were eluted using formic acid/diethylether (2%) and polar fractions were eluted with $CH_2Cl_2/MeOH/H_2O$ (60:25:4). Neutral fractions were separated into hydrocarbons fractions, cetone fractions and alcools fractions using thin layer chromatography (TLC) over activated silica gel in dichloromethanes used as eluents. Next, the process of separating the hydrocarbon fractions was done by using thin layer chromatography (TLC) over activated silica gel, separated into two fractions, which were aliphatic hydrocarbon fractions and aromatic hydrocarbon fractions using *n*-hexane. In this study, only the aromatic hydrocarbons that were analyzed.

The gas chromatography - mass spectrometry analysis was done by using the GC-MS Agilent 122-5561, DB-5 MS column, 60 m × 0,25 m x 0,1 μm. The spectrometer was operated by an electron energy of 70 eV. The operational condition was set by using Helium carrier gas with a flow rate of 1,2 mL/min; isothermal oven temperature of 70 °C for 1 minute; increase in temperature from 70-150 °C with a rate of 10°C/min., from 150°C to 180°C with a rate of 1°C/menit and from 180°C to 315°C with a rate of 5°C/menit, and isothermal temperature for 7 minutes.

3.0 RESULTS AND DISCUSSION

The aromatic hydrocarbon biomarkers were identified based on the interpretations on the given mass spectra data and by comparing them with mass spectra which were already published previously [5, 6, 7]. The structure identification, presented the total ion chromatogram (TIC) as shown in Figure 1.

The chromatogram shows that there were 3 groups of compounds, which were, the naphthalene derivative with sesquiterpenoids skeleton, phenanthrene derivative with diterpenoids, sesterterpenoids skeletons and triterpenoid pentacyclic aromatic compounds as shown on the TIC in Figure 1. The distributions of the biomarkers compounds can be seen in Table 1.

3.1 Naphthalene with Sesquiterpenoids Skeleton

Structure identification on the naphthalene derivative based on the mass fragmentation that specifically used the base peak (m/z = 142 + 156 + 170 + 184 + 183 + 174 + 202) and from the previous publications [8,9] showed the presence of methylnaphthalene (MN); dimethylnaphthalene (DMN); trimethylnaphthalene (TMN); tetramethylnaphthalene (TeMN), cadalene, isocadalene, ionene, calamene and 5,6,7,8-tetrahydrocadalene compounds. The cadalene compound with a base peak on m/z 183 showed a dominant abundance in the aromatic hydrocarbon fraction compared to the alkylnaphthalene as shown on the TIC in Figure 1.

The presence of alkylnaphthalene in the coal samples indicated that the organic compounds originated from terrestrial higher plants, where the β-amyrin compound produced by the Angiospermae higher plants functioned as a precursor during the process of forming alkylnaphthalene compound [10]. The presence of unsubstituted naphthalene compound (base peak m/z 128) was not detected in the aromatic hydrocarbon fraction. The methylnaphthalene (MN) compound with base peak of m/z 142 was identified as 2-methylnaphthalene (2-MN) and 1-methylnaphthalene (1-MN), where the abundance of 2-MN is higher compared to 1-MN as shown in Figure 2.

The intensity difference in 2-MN compared to 1-MN have correlations to their isomer structure stability [10]. The isomer structure stability of 2-MN is lower compared to 1-MN. However, the fragmentogram data showed the intensity peak of 2-MN is higher than 1-MN. The high intensity peak of 2-MN, which had better isomer structure stability than 1-MN, showed the low maturity level of the analysed coal sample. The low maturity level of the analysed coal also has correlations to the presence of other derivatives of naphthalenes such as (DMN), trimethylnaphthalene (TMN) and tetramethylnaphthalene (TeMN).

The dimethylnaphthalene (DMN) compound which was identified based on the m/z 156 fragmentogram showed that there was a presence of 2,6-DMN; 2,7-DMN; (1,3+1,7-DMN); 1,6-DMN; (1,4+2,3)-DMN; 1,5-DMN and 1,2-DMN isomers as shown on the fragmentogram in Figure 2, where the peak intensity of 1,6-DMN was higher compared to 2,6-DMN dan 2,7-DMN. Based on their structures, the 1,6-DMN compound had a lower structure stability compared to the 2,6-DMN and 2,7-DMN compounds. Hence, the high intensity peak of 1,6-DMN compared to the 2,6-DMN and 2,7-DMN could indicate the low maturity level of the analyzed coal samples [10,11]. The existence of trimethylnaphthalene compound which was identified based on the m/z 170 fragmentogram showed the presence of other compounds such as 1,3,7-TMN; 1,3,6-TMN; (1,3,5+1,4,6-TMN); 2,3,6-TMN; 1,2,7-TMN; 1,6,7-TMN; 1,2,6-TMN; 1,2,4-TMN and 1,2,5-TMN (shown in Figure 2). The structure stability of 1,2,7-TMN is lower compared to 1,2,5-TMN, therefore the high intensity peak of 1,2,7-TMN compared to 1,2,5-TMN indicated the low maturity level of the analyzed coal (10).

The presence of tetramethylnaphthalene compound which was identified based on the m/z 184 fragmentogram showed the existence of 1,3,5,7-TeMN; 1,3,6,7-TeMN; 1,2,4,7-TeMN; 1,2,5,7-TeMN; 2,3,6,7-TeMN; 1,2,6,7-TeMN; 1,2,3,7-TeMN; 1,2,3,6-TeMN and 1,2,5,6-TeMN (Figure 2). The discovery of 1,2,5,6-TeMN compound along with 1,2,5-TMN and 1,2,7-TMN compounds indicated that these compounds originated from the aromatized β–amyrin produced by the Angiospermae higher plants. Therefore, the existence of these compounds can be potentially used as an indicator of organic compounds that originated from Angiospermae higher plants and also as an indicator of immature coals [10].

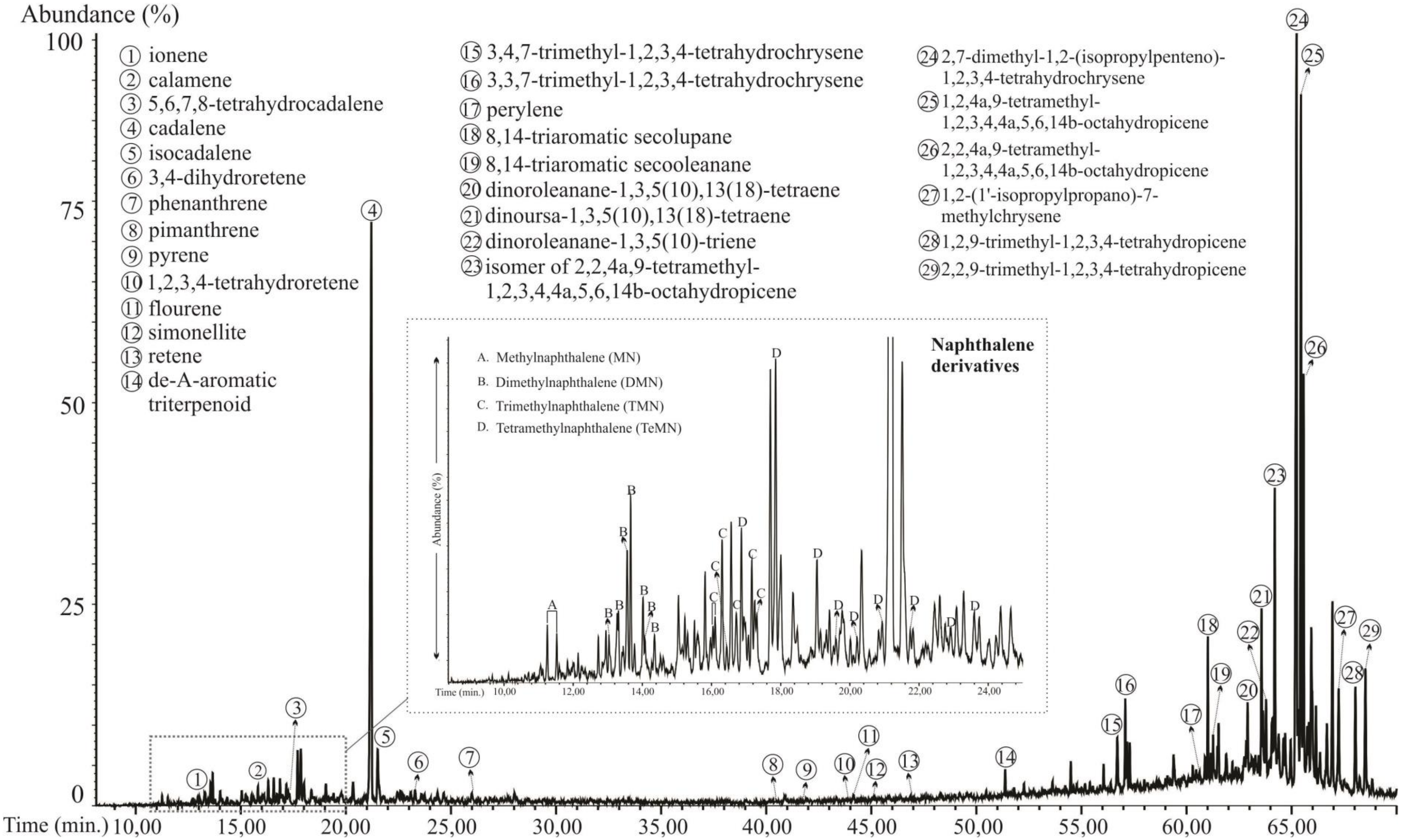


Figure 1 Total ion chromatograms (TIC) of the aromatic hydrocarbon fractions showing the distributions of aromatic hydrocarbons

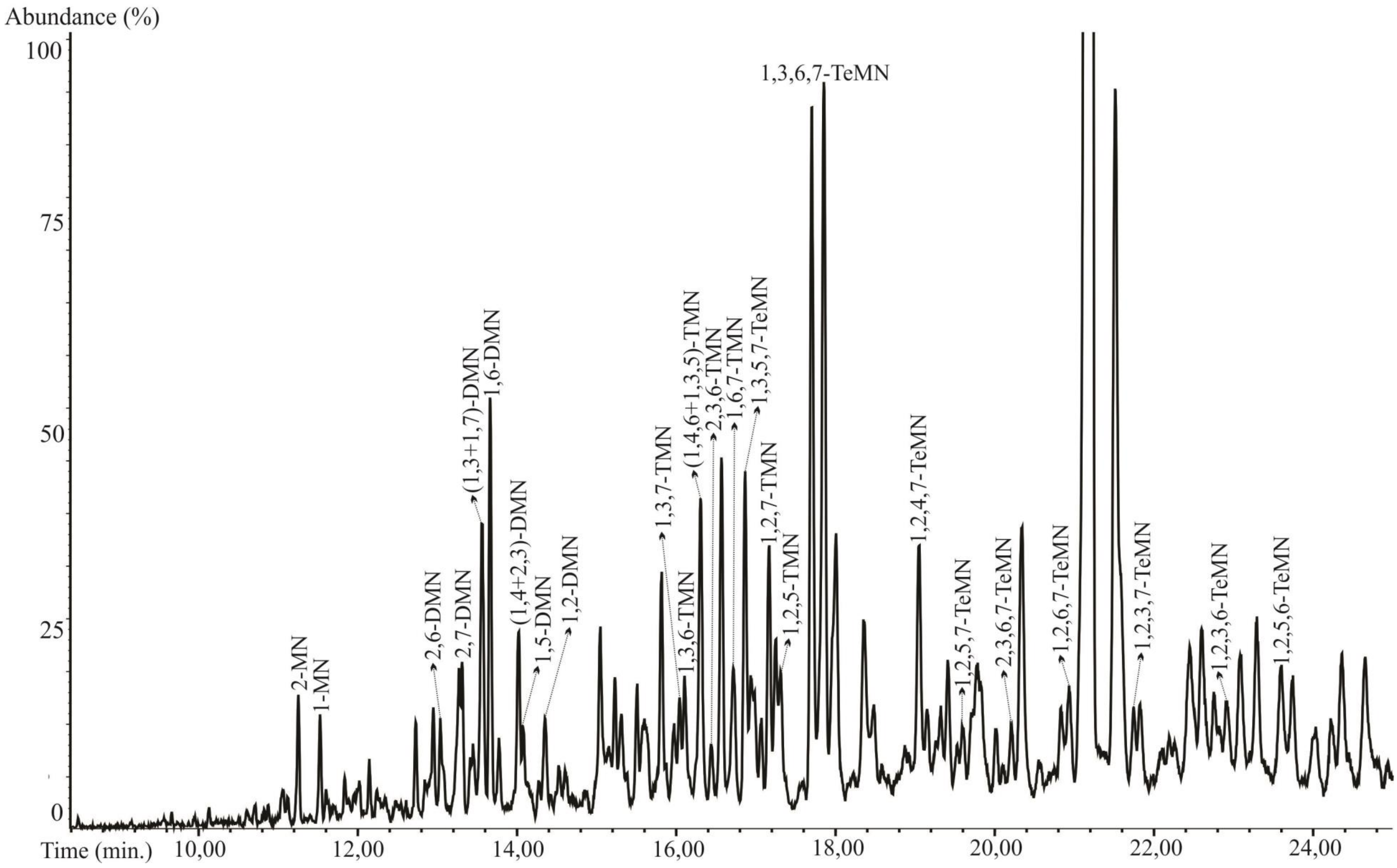


Figure 2 Chromatogram of the alkylnaphthalene derivatives

Table 1 Aromatic hydrocarbon biomarkers

Peak	m/z (M^+)/base peak	Compound(a), (b)	Molecular formula
1	174/159	ionene	$C_{13}H_{18}$
2	202/159	calamene	$C_{15}H_{22}$
3	202/187	5,6,7,8-tetrahydrocadalene	$C_{15}H_{22}$
4	198/183	cadalene	$C_{15}H_{18}$
5	198/183	isocadalene	$C_{15}H_{18}$
A	142/142	Methylnaphthalene (MN)	$C_{11}H_{10}$
B	156/156	Dimethylnaphthalene (DMN	$C_{12}H_{22}$
C	170/170	Trimethylnaphthalene (TMN)	$C_{13}H_{14}$
D	184/169	Tetramethylnaphthalene (TeMN)	$C_{14}H_{16}$
6	236/221	3,4-Dihydroretene	$C_{18}H_{20}$
7	178/178	Phenanthrene	$C_{14}H_{10}$
8	206/206	Pimanthrene	$C_{16}H_{14}$
9	202/202	Pyrene	$C_{16}H_{10}$
10	238/223	1,2,3,4-tetrahydroretene	$C_{18}H_{22}$
11	202/202	Fluorene	$C_{16}H_{10}$
12	252/237	Simonellite	$C_{19}H_{24}$
13	234/219	Retene	$C_{18}H_{18}$
14	306/187	De-A-aromatic triterpenoid	$C_{24}H_{18}$
15	274/259	3,4,7- trimethyl-1,2,3,4-tetrahydrochrysene	$C_{21}H_{22}$
16	274/218	3,3,7-trimethyl-1,2,3,4-tetrahydrochrysene	$C_{21}H_{22}$
17	252/252	Perylene	$C_{20}H_{12}$
18	356/169	8,14-triaromatic secolupane	$C_{27}H_{32}$
19	356/169	8,14-triaromatic secooleanane	$C_{27}H_{32}$
20	376/145	Dinoroleane-1,3,5(10),13(18)-tetraene	$C_{28}H_{40}$
21	376/145	Dinorursa-1,3,5(10),13(18)-tetraene	$C_{28}H_{40}$
22	378/145	Dinoroleane-1,3,5(10)-triene	$C_{28}H_{42}$
23	342/342	isomer de 2,2,4a,9-tetramethyl-1,2,3,4,4a,5,6,14b-octahydropicene	$C_{26}H_{30}$
24	342/342	2,7-dimethyl-1,2-(isopropylpenteno)-1,2,3,4-tetrahydrochrysene	$C_{26}H_{30}$
25	342/342	1,2,4a,9-tetramethyl-1,2,3,4,4a,5,6,14b-octahydropicene	$C_{26}H_{30}$
26	342/342	2,2,4a,9-tetramethyl-1,2,3,4,4a,5,6,14b-octahydropicene	$C_{26}H_{30}$
27	324/281	1,2-(1'-isopropilpropano)-7-methylchrisene	$C_{25}H_{24}$
28	324/324	1,2,9-trimethyl-1,2,3,4-tetrahydropicene	$C_{25}H_{24}$
29	324/324	2,2,9-trimethyl-1,2,3,4-tetrahydropicene	$C_{25}H_{24}$

(a) Base on: reff.[3,5,6,7,8,9,23], (b)structure in appendix

The cadalene biormarker compound which was identified based on the m/z 183 fragmentogram, showed a peak with very dominant intensities in the naphthalene derivatives with sesquiterpenoid skeleton as shown by the total ion chromatogram (TIC, Figure 1). This compound was produced by the polycadinenes as abundant precursors in the Angiospermae higher plants resins [3, 12]. The polycadinene depolymerisation reaction which was followed by the aromatization reaction that occurred during the catagenesis stage, lead to the process of forming 5,6,7,8-tetrahydrocadalene and calamene, which were partially aromatized, and cadalene, which was perfectly aromatized [8,12,13]. Therefore, the simultaneous discovery of this compound in the geology samples was often used as an indicator of coal maturity.

The high abundance of cadalene in the brown coal obtained from Inul area in the Sangatta coalmine, East Borneo, showed the dominance of Dipterocarpaceae vegetation plant during the Miocene age [14,15]. The Angiospermae plant is an input towards the coal formation and sediments in South East Asia such as Indonesia and India which have tropical climates, hence the abundance of cadalene compound in Miocene coal can be potentially used as an Angiospermae indicator [8, 16, 17].

3.2 Phenanthrene with Diterpenoid and Sesterterpenoid Skeletons

Identifying phenanthrene derivatives based on their specific fragmentogram, and by comparing them with the previously published research [3,5,6,8] showed the presence of these compounds: phenanthrene (m/z = 178); fluorene, pyrene (m/z = 202); 3,4-dihydroretene (m/z 221); 1,2,3,4-tetrahydroretene (m/z 223); pimanthrene (m/z 192); perylene, (m/z 252); retene (m/z = 219) and simonellite (m/z = 237). The presence of the phenanthrene derivative biomarkers with tricyclic diterpenoid skeleton can be seen on the chromatogram in Figure 3.

The aromatic hydrocarbon compounds with relatively small molecule mass such as retene, phenanthrene and simonellite were derived from non-aromatic hydrocarbon precursors that underwent an aromatization during the process of coalification [5]. The tricyclic diterpenoid compound is a chemical component mostly found in higher plants resin, mainly Gymnospermae [13, 18]. The low abundance of phenanthrene derivatives with diterpenoid skeletons in the Miocene coals obtained from the Sangatta coalmine is possibly caused by the absence or the low presence of the Gymnospermae plant vegetations and the dominance of Angiospermae vegetations during the Tertiary coal deposition in Malay-Indonesia [19]. Therefore, retene, tetrahydroretene and simonellite, and other tricyclic diterpenoid compounds were considered as a terrestrial organic compound indicator which was derived from a conifer resin precursor known as Gymnospermae [17, 20]. By diagenesis, the retene and simonellite compounds, of which many are found in the conifer resin, were produced through the aromatization abietic acid reaction. The aromatization abietic acid reaction will gradually produce partly aromatized dehydroabietane and simonellite compounds and ends with the process of forming fully aromatized retene [9].

The identification of perylene compound based on the m/z 252 fragmentograms suggested a low abundance in the analyzed coal samples of the Inul area in the KPC-Sangatta coalmine. The aromatic biomarker compound is generally found in the coal samples with low maturity and originated from terrestrial environments [21, 22]. The existence of perylene could also possibly indicate a direct peat formation due to the presence of microbe activities under an oxic environment condition [22].

The phenanthrene compound with sesterterpenoid aromatic hydrocarbon skeleton that were identified in the coal samples of Inul area is a compound with triaromatic de-A-ursane and triaromatic de-A-oleanane structures. Based on the m/z 274 fragmentogram and the published literatures [5,7,23], the compound with triaromatic de-A-ursane structure was identified as 3,4,7-trimethyl-1,2,3,4-tetrahydrochrysene and the compound with triaromatic de-A-oleanane structure was identified as 3,3,7- trimethyl-1,2,3,4-tetrahydrochrysene (TIC, Figure 1). The abundance of 3,3,7- trimethyl-1,2,3,4-tetrahydrochrysene were more dominant compared to 3,4,7-trimethyl-1,2,3,4-tetrahydrochrysene. The presence of trimethyl tetrahydrochrysene compound in the Miocene coal samples that were taken from the Inul area in the KPC-Sangatta coalmine, showed a contribution of the Angiospermae plant vegetations during the process of coal formation [24, 25]. Even though both of these compounds originated from the same isomers, however, both were produced from the different biogenic precursors. The 3,4,7-trimethyl-1,2,3,4-tetrahydrochrysene compound was derived from ursane type triterpenoid, whilst 3,3,7-trimethyl-1,2,3,4-tetrahydrochrysene compound was derived from β-amyrin or other oleanane type precursors. This process took place through biodegradation or geodegradation which caused the disappearance of ring-A during the early stage of diagenesis. Therefore, the existence of these two biomarkers indicated the low maturity level of the analysed coal samples [3, 5, 26].

3.3 Aromatic Pentacyclic Triterpenoid

Structure identification based on the fragmentogram and mass spectra which had been published by the previous researchers [3,5,8,23] showed the presence of triterpene pentacyclic monoaromatic, triaromatic, tetraaromatic, pentaaromatic and triterpenoid triaromatic C-ring cleaved hydrocarbon compound groups. The presence of these compounds in the geology samples is an indicator of higher plants [23] because diagenetically, these samples were derived from triterpenoid with oleanane, ursane and lupane skeletons. The existence of polycyclic aromatic hydrocarbon (PAHs) compound also indicated the low maturity of the coals [27].

Triterpenoid Pentacyclic Monoaromatic

Structure identification based on the m/z 145 fragmentogram showed the presence of three triterpenoid pentacyclic monoaromatic compounds which are dinoroleane-1,3,5(10),13(18)-tetraene, dinoroleane-1,3,5(10)-triene and dinorursa-1,3,5(10),13(18)-tetraene (TIC, Figure 1). By *palaeoecology, the* triterpene pentacyclic monoaromatic compound with oleanane and ursane skeletons was derived from α-amyrin and β-amyrin which is commonly produced by dicotyledoneae plants, such as Angiospermae. Only a small fraction of Gymnospermae plants that can produce the same compound [18,24,28,29], therefore this compound can be potentially used as an indicator of dicotyledoneae plants, mainly Angiospermae.

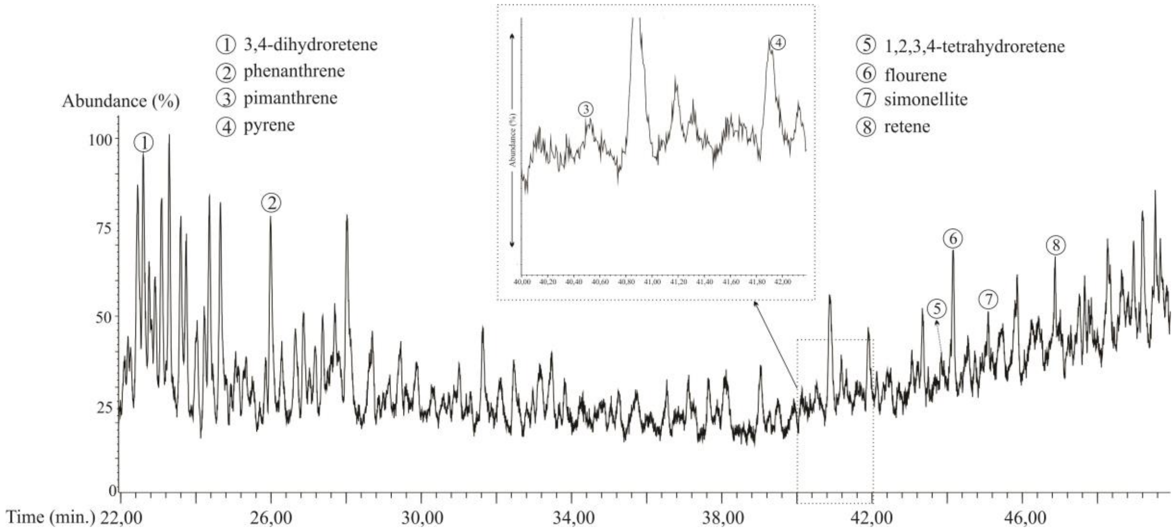


Figure 3 The chromatogram of a combined phenanthrene derivative biomarkers: 3,4-dihydroretene; phenanthrene; pimanthrene; pyrene; 1,2,3,4-tetrahydroretene; fluorene; simonellite and retene

Triterpenoid Pentacyclic Triaromatic

The domination of triterpenoid pentacyclic triaromatic compound in the coal samples taken from the Inul area, were identified based on the m/z 257 fragmentogram, and showed the presence of four triaromatic hydrocarbon compounds (TIC, Figure 1) with ion M^+ peak at m/z 342 and the base peaks at m/z 257 and m/z 342. The four compounds were shown by peak 23 as isomers of 2,2,4a,9-tetramethyl-1,2,3,4,4a,5,6,14b-octahydropicene; peak 24 as 2,7-dimethyl-1,2-(isopropylpenteno)-1,2,3,4-tetrahydrochrysene with triaromatic lupane skeleton; peak 25 as 1,2,4a,9-tetramethyl-1,2,3,4,4a,5,6,14b-octahydropicene with triaromatic ursane skeleton and peak 26 as 2,2,4a,9-tetramethyl-1,2,3,4,4a,5,6,14b-octahydropicene with triaromatic oleanane skeleton [5]. In a biosynthesis manner, the triterpene pentacyclic triaromatic compound was derived from Angiospermae higher plants [30] where the α-amyrin dan β-amyrin compounds functioned as precursors during the process of forming triterpene pentacyclic triaromatic compounds [3]. Therefore, the domination of triterpene pentacyclic triaromatic compound in the analyzed coal samples indicated the dominance of Angiospermae plant vegetations in the Borneo forest during the Middle Miocene to Late Miocene periode.

Triterpenoid Pentacyclic Tetraaromatic, Pentaaromatic

The identification of triterpenoid pentacyclic tetraaromatic compound based on the m/z 324 fragmentogram and the compound mass spectra was already been published previously [3, 5, 8, 23]. Identification based on the m/z 324 fragmentogram, showed the presence of these compounds: 1,2-(1'-isopropylpropano)-7-methylchrysene; 1,2,9-trimethyl-1,2,3,4-tetrahydropicene which is a tetraaromatic ursane and 2,2,9-trimethyl-1,2,3,4-tetrahydropicene which is a tetraaromatic oleanane (TIC, Figure 1). The existence of triterpenoid pentacyclic tetraaromatic compound indicated that there was an Angiospermae plant vegetation input into the formation of coal organic compounds [23]. The triterpenoid compound with picene structure was also found in the coals that were obtained from Lower Suban in South Sumatra, which were aged from Late Miocene to Early Pliocene [13]. The same compound which were also identified in the peat deposits in Indonesia, may also been produced from microbial aromatized triterpenoid compound, which indicated that dehydrogenation of triterpenoid compound that produced aromatic polycyclic hydrocarbon did not need a long period of time and high temperatures [31].

The triterpenoid pentacyclic pentaaromatic compound was identified based on the m/z 306 fragmentogram (TIC, Figure 1). The identifications showed the presence of de-*A* aromatic-triterpenoid compound which was proved by the m/z 187 and 119 fragmentations on the given mass spectra. The de-A aromatic-triterpenoid compound is a triterpene pentacyclic pentaaromatic which underwent a removal of ring-A and dearomatization reaction [13, 23, 32].

Identifications based on the m/z 145 fragmentogram showed the presence of two compounds with triaromatic C-ring cleaved hydrocarbon skeleton structure (ion M^+ on m/z 356), which were identified as 8,14-triaromatic secolupane and 8,14-triaromatic secooleanane (TIC, Figure 1). Both of these compounds were identified by comparing the mass spectra of both compounds with the mass spectra from the previously published researches [3, 5]. Both of these compounds have mass spectrum that are similar to one another. The difference between the two mass spectra can only be seen from the m/z 145 fragment intensity, which showed a higher mass spectrum for 8,14-triaromatic secooleanane compound compared to the mass spectrum for 8,14-triaromatic secolupane compound. The m/z 145 fragment is related to the removal of C_3H_6 groups from the m/z 187 ions (the tetrahydronaphthalene fragment which was substituted by tetramethyl). This characteristic showed that both of these compounds were an isomer of one another and originated from β-amyrin or the same oleanane type precursor. Therefore, both of these compounds can be considered as an indicator of Angiospermae plants [5, 26, 33, 34].

The compounds that were found in the coal samples of Inul area in the KPC-Sangatta coalmine in East Borneo that aged Middle Miocene to Late Miocene can be considered as a form of alteration, followed by the triterpenoid aromatization reaction which occurred during the stage of diagenesis. Therefore the existence of these compounds indicated the low maturity of the coals [35, 36].

4.0 CONCLUSION

The organic geochemistry studies on the brown coals of Inul area located in the Sangatta coalfield indicated a low maturity of the coals. The low maturity of the coals is shown by the existence of some biomarkers which are the derivatives of naphthalene with sesquiterpenoid skeletons and aromatic pentacyclic triterpenoid compound. The low maturity of the coals is mainly shown by the domination of triaromatic pentacyclic triterpenoid biomarkers compounds such as 2,7-dimethyl-1,2-(isopropylpenteno)-1,2,3,4 te-trahydrocrysene with triaromatic lupane skeleton; 1,2,4a,9-tetramethyl-1,2,3,4,4a,5,6,14b -octahydropicene with triaromatic ursane skeleton and 2,2,4a,9-tetramethyl-1,2,3,4,4a,5,6,14b octahydropicene with triaromatic oleanane skeleton. The existence of the biomarkers compounds also indicated that the coal organic compounds originated from Angiospermae higher plants which are very dominant in the forests of Borneo during the Tertiary era. In an organic geochemistry manner, the biomarkers compounds which were found in the brown coals of Inul area showed that these coals are coals with low maturity level, which is identic to their low calorie values. Low grade coals have low economic values, therefore the discovery of the aromatic biomarkers compounds which had been explained previously can be used as a reference if low grade coals should be used as raw materials in the production of CTL on the subsequent planning.

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