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Origin, Distribution and Geochemical Significance of Isopropyltoluene Isomers in Crude Oil

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ABSTRACT: With comprehensive two-dimensional gas chromatography linked to time-of-flight mass spectrometry (GC × GC-TOFMS), ten light hydrocarbon (LH) compounds were qualitatively and quantitatively studied in light hydrocarbons (LHs) components of crude oils. For significant differences in the concentrations of 3-isoproyltoluene (3-iPT), 4-isoproyltoluene (4-iPT) and 2-isoproyltoluene (2-iPT) in crude oils, and the 2-iPT probably derived mainly from similar skeleton monocyclic terpenoids via dehydrogenation and aromatization, the ratios of (3+4)-/2-iPT (iPTr), 3-/2-iPT (iPTr1) and 4-/2-iPT (iPTr2) are proposed to distinguish the organic matter origin of crude oils. Relatively higher iPTr (>8.0), iPTr1 (>7.0) and iPTr2 (>4.0) values indicate that crude oils are sourced from the co-contribution of lower aquatic organisms, bacteria, algae, and terrestrial higher plants, whereas lower iPTr (<5.0), iPTr1 (<3.0), iPTr2 (<2.0) values suggest that crude oils originated from terrestrial higher plants. The iPTr, iPTr1, and iPTr2 values show notable distinction which is mainly controlled by 2-iPT concentrations, while the concentrations of 3-iPT and 4-iPT have similar distribution range in all studied oils. The 2-iPT depleted in marine oils from the Tarim Basin and lacustrine oils from the Beibuwan Basin is less than 0.30 mg/g LHs, whereas 2-iPT enriched in swamp oils from the Tarim Basin is greater than 0.50 mg/g LHs. The iPTr, iPTr1, and iPTr2 ratios and 2-iPT concentrations can be used to distinguish the organic matter origin of crude oils, especially for light oils and condensates with low concentrations of biomarkers.

KEY WORDS: organic carbon, GC × GC-TOFMS, light oils and condensates, organic matter origin.

0 INTRODUCTION

Due to heavy molecular weight biomarkers absent or present only in trace amounts in high to over mature light oils and condensates, it is extremely difficult to recognize the organic matter origin of light oils and condensates through conventional geochemical indicators. The light hydrocarbons (LHs) components can account for more than 90% in light oils and condensates (Hunt et al., 1980). Therefore, the LHs components can better represent the composition characteristics of light oils and condensates. One of the most important components of LHs are monocyclic aromatic hydrocarbons (alkylbenzenes). Alkylbenzenes composition and distribution were usually used in petroleum geochemistry to indicate the origin of organic matter (Jia et al., 2008, 2007; Pedentchouk et al., 2004; Sun et al., 2003; Hartgers et al., 1994a, b; Douglas et al., 1991), depositional environment (Cheng et al., 2015a, b; Sinninghe Damsté et al., 1993), thermal maturity (Zhang et al., 2014a; Lis et al., 2008; Sinninghe Damsté et al., 1991) and secondary alteration (Thompson, 1988, 1987; Connan, 1984; Volkman et al., 1984).

Isopropyltoluene with three isomers (3-isoproyltoluene (3-iPT), 4-isoproyltoluene (4-iPT) and 2-isoproyltoluene (2-iPT)) have been detected in kerogens, crude oils, coals, and asphaltenes (Cheng et al., 2015a, b; Zhang et al., 2014a; Hartgers et al., 1994c). The 4-iPT, 3-iPT and 2-iPT can produced by the α-, β-cleavage of the side chain of the macromolecular structure (e.g., kerogen). The 4-iPT is condisered to be linked to macromolecular structure through a single C-C bond or heteroatom (oxygen) (Hartgers et al., 1994c). The 4-iPT and 3-iPT are readily obtained from structrues corresponding to monocyclic terpenoids by dehydrogenation and the 4-iPT and 3-iPT concentrations are significantly larger than 2-iPT in petroleum (Grayson, 2000; Mair, 1964). The corresponding terpenoid structure of 2-iPT formed by dehydrogenation is unknown (Mair, 1964).

Generally, when light oils and condensates were analyzed using gas chromatography-mass spectrometry (GC-MS), a large number of LHs components have similar polarity and boiling leading to the co-elution of low molecular weight hydrocarbons (e.g., alkylbenzenes). Fortunately, comprehensive two-dimensional gas chromatography linked to time-of-flight

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mass spectrometry (GC × GC-TOFMS) can well separate alkylbenzene compounds from other LHs components. The main reasons that the GC is equipped with two reversed-phase columns. The compounds can be separated by compounds boiling points in first dimension with a non-polar column and compounds can be separated by compounds polarity in second dimension with a polar column (Cheng et al., 2015a, b; Wang et al., 2014).

Although the geochemical significance of isopropyltoluene isomers have been reported in many previous studies, they have mainly focused on their identification and possible biological origins (Cheng et al., 2015a; Zhang et al., 2014a; Grayson, 2000; Hartgers et al., 1994c; Mair, 1964). The distribution, potential applications, and other geochemical characteristics of isopropyltoluene isomers have not been thoroughly investigated. By comparison of the mass spectra, retention indices and relative retention time with the pertinent works of literatures and documents, ten LH compounds were identified in crude oils and condensates from the Tarim Basin and Beibuwan Basin (Wang et al., 2014; Hartgers et al., 1992). By analyzing the isoproyltoluene isomers distribution of crude oils from different basins, the potential indicators of sedimentary environment, organic matter source, and maturity in crude oils will be sought.

1 GEOLOGICAL SETTING

With an area of about 560 000 km^2, the Tarim Basin is a cratonic foreland superimposed basin, including three uplifts and four depressions (Fig. 1a) (Ngia et al., 2019; Song et al., 2015; Li et al., 2012). There are mainly three sets of source rock series in the Tarim Basin, containing the Cambrian–Ordovician marine source rocks, Carboniferous–Permian and Triassic–Jurassic terrestrial source rocks (Zhu et al., 2012; Liang et al., 2003; Kang and Kang, 1996). A large amount of crude oils, gases and condensates derived from Cambrian–Ordovician marine source rocks have been found in the Tabei uplift (Kang and Kang, 1996). The Cambrian–Ordovician marine source rocks are mainly composed of marls, mudstones, carbonates, dolomite, and argillaceous limestones (Zhang and Huang, 2005) deposited in strongly reducing sedimentary environments (Chang et al., 2013; Sun et al., 2003; Zhang et al., 2002, 2000; Hanson et al., 2000). Besides, a large number of swamp crude oils and condensates from the Kuqa depression and the Tabei uplift (Lutai sub-uplift) have been reported in previous studies (Zhu et al., 2012; Xiao et al., 2004). These swamp oils originated from thick Jurassic limnetic coal measures deposited in sub-oxic conditions (Cheng et al., 2015b; Zhu et al., 2012; Zhang et al., 2011; Fan et al., 2009; Liang et al., 2003).

Situated in the south margin of the Beibuwan Basin, the Fushan depression is a Mesozoic–Cenozoic fault basin, which developed from the Late Cretaceous with Paleozoic strata and Mesozoic intermediate to acid igneous rocks as the basement (Fig. 1b) (Li et al., 2009, 2008, 2007). A large amount of lacustrine oils and condensates have been found in the Fushan depression (Li et al., 2009, 2008, 2007). The main source rocks of the Fushan depression are the dark mudstone and shale of the Liushagang Formation (E_2l), with type II–III kerogen and high organic matter abundance (Li et al., 2008). The lacustrine oils and condensates from the Fushan depression originated from the Liushagang Formation (E_2l) mudstone deposited under oxic conditions (Li et al., 2009, 2007).

2 SAMPLES AND METHODS

2.1 Samples

In this study, 32 crude oils and condensates were sampled from the Tarim Basin and the Beibuwan Basin, including 15 marine oils derived from the Tabei uplift, one marine oil and three swamp oils derived from the Luntai sub-uplift of the Tabei uplift, 5 swamp oils derived from the Kuqa depression in the Tarim Basin, respectively, and 8 lacustrine oils derived from the Fushan depression of the Beibuwan Basin. Detailed descriptions of these oils are shown in Table 1.

Previous research results showed that complete *n*-alkanes and acyclic isoprenoids coexisted with 25-norhopanes in the Tarim marine oils and condensates demonstrated that these oils have experienced the process of mixing and multiple charges (Zhang et al, 2014b; Cheng et al., 2013; Wang et al., 2008). Therefore, the LHs components of the Tarim marine oils and condensates were derived from later charge when the process of biodegradation of crude oils has ceased in early charge (Zhang et al., 2014b; Cheng et al., 2013). Considering above observations, the concentrations of isopropyltoluene isomers in LHs (including all C_6–C_{13} hydrocarbons) indicate the concentrations of 3-iPT, 4-iPT, and 2-iPT. Only by doing so can we believe that the influence of mixing and multiple charges on the quantitative error of 3-iPT, 4-iPT and 2-iPT in crude oils can be minimized as far as possible.

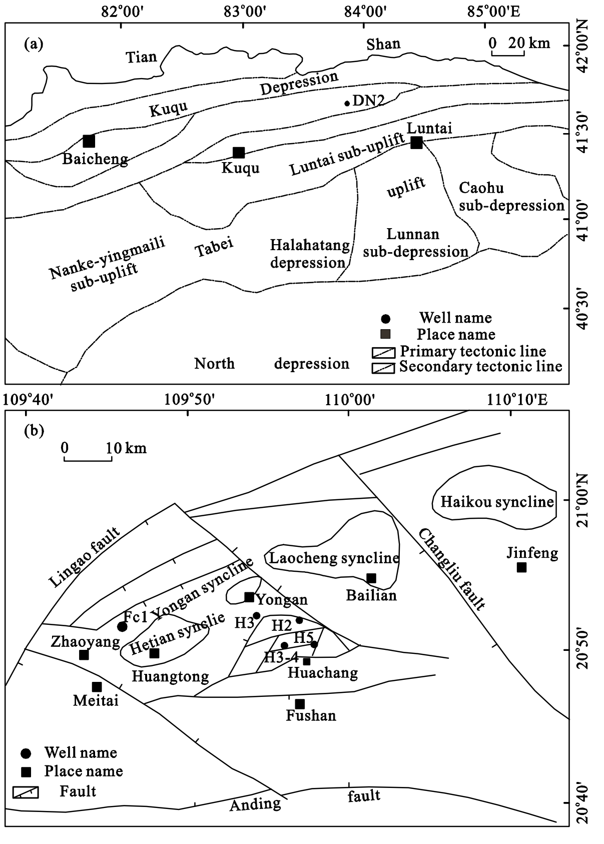

Figure 1. Geological structure distribution map of (a) the Northern Tarim Basin and (b) the Fushan depression of the Beibuwan Basin.

2.2 Methods

2.2.1 Gas chromatography (GC) and gas chromatography-mass spectrometry (GC-MS)

All whole oils were analyzed by Agilent 6890A GC equipped with HP-PONA (50 m × 0.2 mm × 0.5 μm). The injector temperature of the GC was set at 300 ºC. The GC oven temperature initially was set at 35 ºC and maintained 5 min, then programmed at 3 ºC/min to 70 ºC, and finally programmed at 4.5 ºC/min to 300 ºC and hold on 35 min. The carrier gas is helium. The hydrogen generator and air pump were installed on Agilent 6890A GC to provide hydrogen and oxygen.

All studied oils were deasphalted by petroleum ether and separated into saturated, aromatic hydrocarbons and other components by chromatography column, eluting with petroleum ether, petroleum ether/dichloromethane (1 : 2, *v* : *v*) and methanol/dichloromethane (7 : 93, *v* : *v*). Saturated and aromatic hydrocarbons were tested by Agilent 6890 GC coupled with Agilent 5979i MS. The GC was equipped with an HP-5MS (60 m × 0.25 μm × 0.25 μm). The GC oven temperature initially was set at 80 ºC and maintained 1 min, then increased at 3 ºC/min to 310 ºC, and finally maintained 20 min. The carrier gas is helium. The voltage of ion source is 70 eV.

2.2.2 Comprehensive two-dimensional gas chromatography linked to time-of-flight mass spectrometry (GC × GC-TOFMS)

Before crude oils were analyzed, internal standard (1-hexene) was added into the crude oils of known weight. The Agilent 7890 GC was equipped with the non-polar capillary

Table 1 The basic geological information of all studied oils

No.	Well	Location	Source age	Type of source rocks	Depositional environment of source rocks	References
1	RP14-5X	Tabei uplift	O–Є	Marls	Marine	Hanson et al. (2000), Zhang and Huang (2005)
2	RP8-1	Tabei uplift	O–Є	Marls	Marine	As above
3	RP8001	Tabei uplift	O–Є	Marls	Marine	As above
4	XK501C	Tabei uplift	O–Є	Marls	Marine	As above
5	XK8-1	Tabei uplift	O–Є	Marls	Marine	As above
6	JY103C	Tabei uplift	O–Є	Marls	Marine	As above
7	JY5H	Tabei uplift	O–Є	Marls	Marine	As above
8	YM1	Tabei uplift	O–Є	Marls	Marine	As above
9	YM2	Tabei uplift	O–Є	Marls	Marine	As above
10	YM3	Tabei uplift	O–Є	Marls	Marine	As above
11	YM4	Tabei uplift	O–Є	Marls	Marine	As above
12	YM5	Tabei uplift	O–Є	Marls	Marine	As above
13	YM102	Tabei uplift	O–Є	Marls	Marine	As above
14	YJ1X	Tabei uplift	O–Є	Marls	Marine	As above
15	YJ2X	Tabei uplift	O–Є	Marls	Marine	As above
16	YK11	Luntai uplift	O	Marls	Marine	Song et al. (2015)
17	S3-1	Luntai uplift	J	Coal	Swamp	Cheng et al. (2015b)
18	YL2-2	Luntai uplift	J	Coal	Swamp	As above
19	YD2-2	Luntai uplift	J	Coal	Swamp	As above
20	KU1	Kuqa depression	J	Coal	Swamp	Fan et al. (2009)
21	DW105	Kuqa depression	J	Coal	Swamp	Zhang et al. (2011)
22	DN201-E	Kuqa depression	J	Coal	Swamp	Zhu et al. (2012)
23	DB2	Kuqa depression	J	Coal	Swamp	Zhang et al. (2011)
24	DN202	Kuqa depression	J	Coal	Swamp	Zhang et al. (2011)
25	H1-01	Beibuwan Basin	E	Mudstone	Lacustrine	Li et al. (2009, 2007)
26	H1-02	Beibuwan Basin	E	Mudstone	Lacustrine	As above
27	H2	Beibuwan Basin	E	Mudstone	Lacustrine	As above
28	H2-3	Beibuwan Basin	E	Mudstone	Lacustrine	As above
29	H3	Beibuwan Basin	E	Mudstone	Lacustrine	As above
30	HX4-01	Beibuwan Basin	E	Mudstone	Lacustrine	As above
31	FCl-02	Beibuwan Basin	E	Mudstone	Lacustrine	As above
32	HD-1-1	Beibuwan Basin	E	Mudstone	Lacustrine	As above

Note: Є. Cambrian; O. Ordovician; J. Jurassic; E. Eocene.

column HP-PONA phase (50 m × 0.20 mm × 0.50 μm) in first dimension and the polar capillary column Rxi-17 phase (1.7 m × 0.1 m × 0.1 μm) in second dimension. The first and second GC oven temperature were set as follows: the originally first GC oven temperature was set at 35 ºC and maintained 5 min, then increased at 2 ºC/min to 295 ºC, and finally maintained 30 min. The second GC oven temperature was set at 40 ºC and held on 5 min, then increased at 2 ºC/min to 280 ºC, and finally maintained 30 min. The injector temperature of the GC is 300 ºC with a split mode (100 : 1), and carrier gas is helium. The modulator temperature offset 15 ºC higher than the first GC oven and modulation period was set as 6 s with 4.8 s cold pulse time. The MS transfer and ion source temperature were set as 280 and 250 ºC, respectively. The detector and ion source voltage were set as 1 350 V and 70 eV, respectively.

3 RESULTS AND DISCUSSION

3.1 Identification and Distribution of Ten LH Compounds in Crude Oils and Condensates

Ten LH compounds were identified by comparing their mass spectra, retention indices and relative retention time with the pertinent works of literatures and documents (Table 2) (Wang et al., 2014; Hartgers et al., 1992). Figure 2 showed that ten LH compounds were displayed between *n*-nonane (*n*C_9) and *n*-dodecane (*n*C_{12}).

Figure 3 shows that the molecular structure and mass spectra of ten LH compounds. The mass spectra of 2,6-dimethyloctane (2,6-DMO), 3-methylnonane (3-MN) and 2-methyl-3-ethylheptane (2-M-3-EH) all display same base peak and parent ion (*m*/*z* 57 and 142, respectively), and $C_{10}H_{22}$ molecular formula. The 2,6-DMO and 3-MN all have two higher peaks (*m*/*z* 71 and 113), and a lower peak (*m*/*z* 98), which differs from 2-M-3-EH. The mass spectra of propylcyclohexane (PCyC_6) shows a base and higher peak (*m*/*z* 83 and 67, respectively), and C_9H_{18} molecular formula, whereas 1,1,2,3-tetramethylcyclohexane (1,1,2,3-TeMCHx) mass spectra have a base peak (*m*/*z* 69), three higher peaks (*m*/*z* 97, 111 and 125) and $C_{10}H_{20}$ molecular formula. PCyC_6 parent ion (*m*/*z* 126) is different from 1,1,2,3-TeMCHx parent ion (*m*/*z* 140). The 3-iPT, 4-iPT, 2-iPT, 1,2,3,5-tetramethylbenzene (TeMB) and 1,2,3,4-TeMB mass spectra all have a higher peak (*m*/*z* 91), a base peak (*m*/*z* 119), and parent ion (*m*/*z* 134) with $C_{10}H_{14}$ molecular formula.

Ten LH compounds concentrations quantitative results are showed in Table 3. The results indicated that the concentrations of ten LH compounds follow trends of 2,6-DMO > 2-M-3-EH> 3-MN > 1,1,2,3-TeMCHx > PCyC6 > 1,2,3,4-TeMB > 1,2,3,5-TeMB > 3-iPT > 4-iPT > 2-iPT in swamp oils from the Tarim Basin, and 1,2,3,5-TeMB > 3-MN > 2,6-DMO > PCyC6 >1,2,3,4-TeMB > 3-iPT > 2-M-3-EH > 4-iPT > 1,1,2,3-TeMCHx > 2-iPT in lacustrine oils from

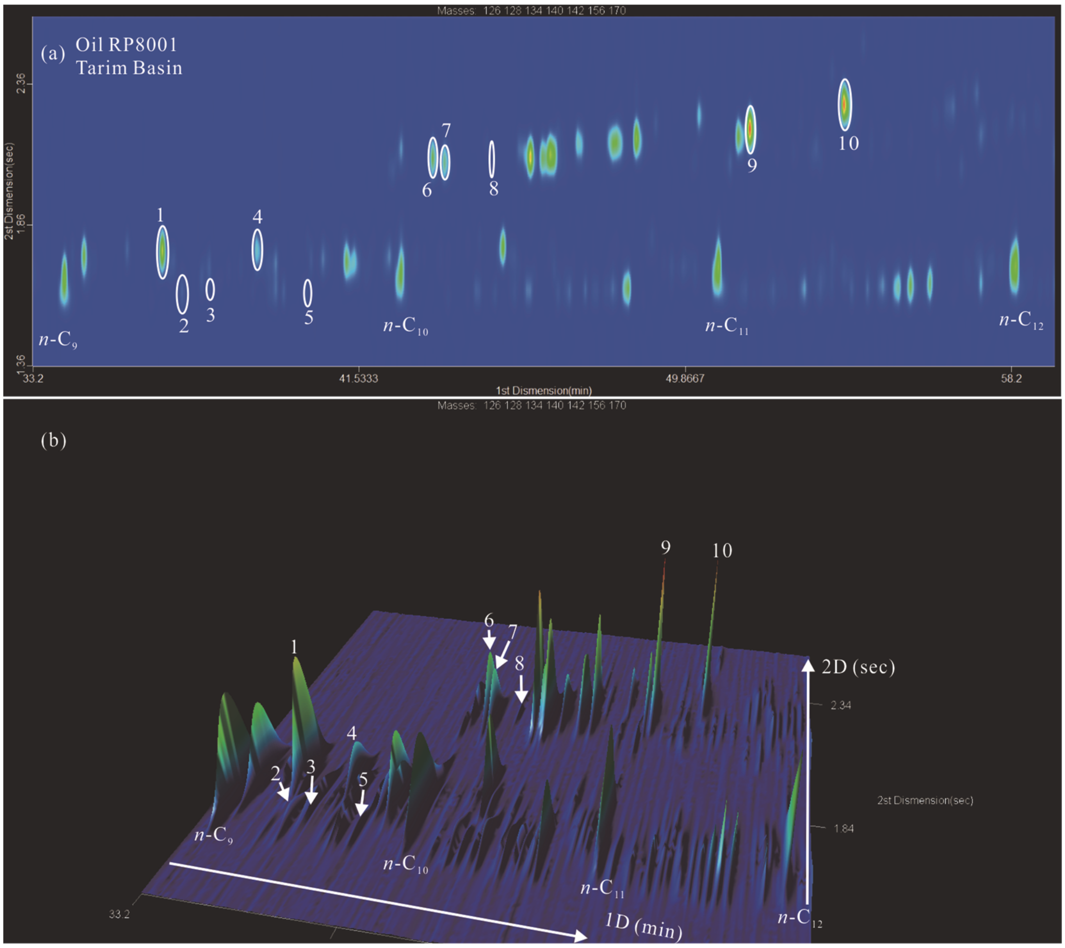

Figure 2. Ten LH compounds in RP8001 oil are shown on (a) the planar graph and (b) three-dimensional picture of GC × GC-TOFMS. The compound names corresponding to the peak numbers are shown in Table 2.

Table 2 Ten LH compounds were identified in all studied oils. Peak numbers refer to Fig. 2

Peak No.	Compound	1D retention time (min)	1D retention index	2D retention time (s)	Molecular weight	Base peak	Abbreviation
1	propylcyclohexane	36.5	929.1	1.8	126	83	$PCyC_6$
2	2,6-dimethyloctane	37.0	934.9	1.6	142	57	2,6-DMO
3	2-methyl-3-ethylheptane	37.7	943.0	1.6	142	57	2-M-3-EH
4	1,1,2,3-tetramethylcyclohexane	38.9	957.0	1.8	140	69	1,1,2,3-TeMCHx
5	3-methylnonane	40.2	972.1	1.6	142	57	3-MN
6	3-isopropyltoluene	43.4	1 009.9	2.1	134	119	3-iPT
7	4-isopropyltoluene	43.7	1 013.6	2.1	134	119	4-iPT
8	2-isopropyltoluene	44.8	1 027.2	2.2	134	119	2-iPT
9	1,2,3,5-tetramethylbenzene	51.5	1 110.5	2.2	134	119	1,2,3,5-TeMB
10	1,2,3,4-tetramethylbenzene	53.9	1 142.1	2.3	134	119	1,2,3,4-TeMB

the Beibuwan Basin (Table 3). The 2-M-3-EH, 1,1,2,3-TeMCHx and 2-iPT concentrations display significant differences in all studied oils. The 2-M-3-EH and 1,1,2,3-TeMCHx concentrations are enriched in marine oils from the Tarim Basin, ranging from 6.07 to 9.52 mg/g LHs, from 2.27 to 4.15 mg/g LHs, respectively, while depleted in swamp oils from the Tarim Basin (ranging from 1.35 to 3.12 mg/g LHs, from 1.06 to 2.21 mg/g LHs, respectively) and lacustrine oils from the Beibuwan Basin (ranging from 0.97 to 2.06 mg/g LHs, from 0.40 to 1.22 mg/g LHs, respectively) (Table 3). The 2-iPT is depleted in marine oils from the Tarim Basin and lacustrine oils from the Beibuwan Basin, varying from 0.11 to 0.21 mg/g LHs and from 0.08 to 0.29 mg/g LHs, respectively, but is enriched in swamp oils from the Tarim Basin, ranging from 0.50 to 1.11 mg/g LHs (Table 3). Other seven LH compounds concentrations show no significant differences in all studied oils.

3.2 Origin of 3-iPT, 4-iPT, and 2-iPT in Crude Oils and Condensates

As we all know, monoterpenoids are terpenes and their derivatives containing two isoprene units in a molecule, which are an important source of alkylbenzenes (Yassaa et al., 2008; Grayson, 2000; Buhl et al., 1998; Banthorpe et al., 1972; Mair, 1964). The 4-iPT probably originated from monocyclic terpenoids (e.g., limonene, terpinolene and phellandrene) during the diagenesis of organic matter as they share similar carbon skeleton (Yassaa et al., 2008; Grayson, 2000; Buhl et al., 1998; Banthorpe et al., 1972; Mair, 1964). Additionally, 4-iPT also emerged in six essential oils derived from terrestrial higher plants, including pennyroyal, cypress oil, lavender oil, lemon oil, citronella oil, and camphor oil, which are primarily composed of monoterpenoids (Cheng, 2016). To understand the above discussions, 4-iPT seemingly can indicate the contribution of terrestrial higher plants. However, it is noteworthy that 4-iPT was identified in the marine oils, swamp oils, and lacustrine oils from Cambrian–Ordovician, Jurassic, and Eocene source rocks in this study, respectively, which imply that 4-iPT exist in another formation pathway. For example, the 4-iPT is probably derived from the α-terpineol which is linked to macromolecular substances (e.g., kerogen) via ether linkages during the diagenesis of organic matter (Hartgers et al., 1994c). Thus, the precursors of 4-iPT or itself can be produced by α-, β-cleavages of the side chain via either a heteroatom or a single C-C bond to macromolecular structure during the diagenesis of organic matter.

In this study, 3-iPT and 4-iPT have similar distribution range in marine oils from the Tarim Basin (0.97–2.25 mg/g LHs and 0.64–1.36 mg/g LHs, respectively), swamp oils from the Tarim Basin (0.26–1.52 mg/g LHs and 0.16–1.17 mg/g LHs, respectively), and lacustrine oils from the Beibuwan Basin (0.66–3.29 mg/g LHs and 0.07–1.77 mg/g LHs, respectively) (Figs. 4a and 4b, Table 3). Therefore, 3-iPT also probably could have existed in two formation pathways during the diagenesis of organic matter. The 3-iPT not only could be derived from structures corresponding to monocyclic terpenoids by dehydrogenation but also can be produced by α-, β-cleavages of the side chain via either a heteroatom or a single C-C bond to macromolecular structure during the diagenesis of organic matter.

Interestingly, the concentrations of 2-iPT in swamp oils from the Tarim Basin (0.50–1.11 mg/g LHs) are higher than marine oils from the Tarim Basin (0.11–0.21 mg/g LHs) and lacustrine oils from the Beibuwan Basin (0.08–0.29 mg/g LHs) (Fig. 4c, Table 3). It is proved that 2-iPT probably originated from terrestrial higher plants. Furthermore, monoterpenoids were widely found in secretory tissues of terrestrial higher plants, especially in essential oils of terrestrial higher plants (Tissot and Welte, 1984). Therefore, 2-iPT is probably derived mainly from similar skeleton monocyclic terpenoids. The high contents of 2-iPT can be used as an important indicator of the contribution of terrestrial higher plants.

Based on above discussion, the ratios of (3+4)-/2-iPT (iPTr), 3-/2-iPT (iPTr1) and 4-/2-iPT (iPTr2) are proposed to distinguish the origin of organic matter of crude oils. Variations in compound ratios can arise from multiple causes, such as an increase in the numerator, a decrease in the denominator or combination of both. The compound concentrations can more accurately reflect the underlying controls. Based on the distribution of 3-iPT, 4-iPT, and 2-iPT in all studied oils (Fig. 4, Table 3), the variations of iPTr1, iPTr2 and iPTr values are mainly caused by fluctuation in the 2-iPT concentrations. Whether the distribution of 3-iPT, 4-iPT, and 2-iPT is affected by secondary alteration processes, thermal maturity and depositional environment will be discussed as follows.

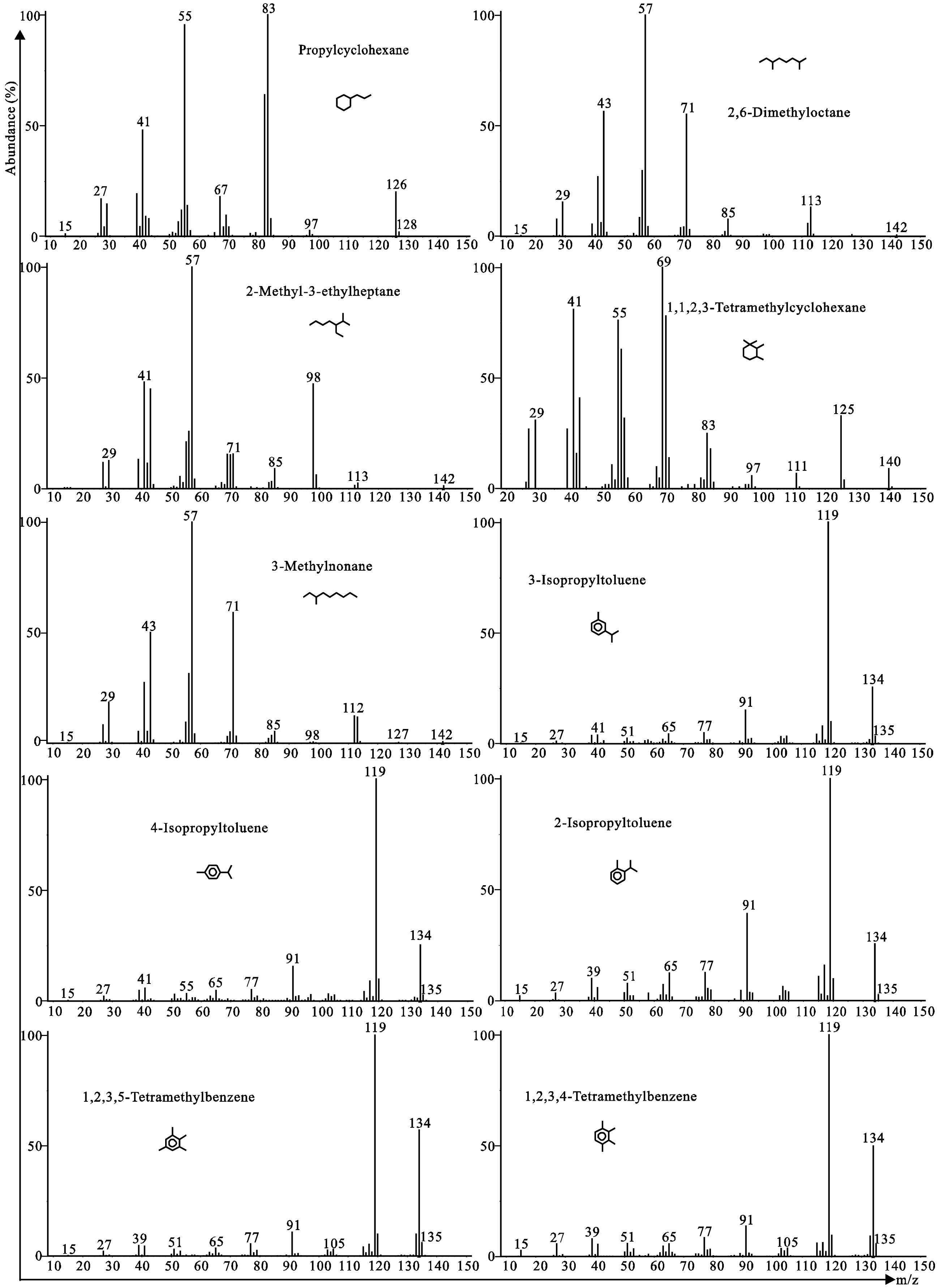

Figure 3. The mass spectra and molecular structures of ten LH compounds.

Table 3 The concentrations of ten LH compounds for all studied oils

No.	Well	Concentration (in mg/g LHs)									
		a	b	c	d	e	f	g	h	i	k
1	RP14-5X	3.36	9.44	8.47	4.15	5.88	1.12	1.36	0.16	2.03	2.37
2	RP8-1	3.62	10.32	6.85	3.17	5.73	1.34	1.03	0.12	1.83	2.34
3	RP8001	2.35	11.00	8.75	3.50	6.35	1.44	1.08	0.14	1.91	2.46
4	XK501C	3.37	8.90	9.52	2.72	5.02	0.97	1.02	0.14	1.85	2.96
5	XK8-1	3.79	9.86	9.43	3.86	5.72	1.15	1.14	0.14	1.94	1.84
6	JY103C	4.07	10.14	9.10	3.67	5.02	1.60	1.32	0.17	2.55	3.62
7	JY5H	2.92	9.76	8.74	3.62	4.69	1.40	1.26	0.11	2.02	4.03
8	YM1	3.64	10.48	7.07	3.89	5.42	1.30	1.13	0.15	1.84	1.82
9	YM2	3.55	9.98	8.98	4.03	5.49	1.66	1.36	0.15	2.22	3.80
10	YM3	4.02	10.01	7.71	3.52	5.56	1.62	1.27	0.16	2.09	2.02
11	YM4	1.18	9.65	6.79	3.87	5.34	1.64	1.25	0.14	2.30	3.29
12	YM5	3.29	10.02	6.07	3.37	5.76	1.01	1.22	0.12	1.85	1.79
13	YM102	2.59	9.93	7.49	3.77	5.14	1.59	1.26	0.12	2.25	3.26
14	YJ1X	3.55	9.49	7.24	3.45	5.59	1.64	0.86	0.14	2.24	3.14
15	YJ2X	3.99	9.78	9.07	2.93	5.41	1.52	0.64	0.14	1.91	1.77
16	YK11	3.48	8.91	6.86	3.30	5.64	2.25	1.03	0.21	3.50	3.87
17	S3-1	3.95	6.82	2.78	2.01	5.32	1.49	0.71	0.50	3.00	1.43
18	YL2-2	5.89	6.23	2.13	2.04	6.50	0.65	0.16	0.53	0.95	0.50
19	YD2-2	3.16	6.37	2.66	1.51	6.09	0.52	1.17	0.62	1.63	0.79
20	KU1	5.15	12.42	3.22	2.21	10.00	0.79	0.23	0.50	2.64	2.19
21	DW105	3.77	5.34	2.93	1.36	5.30	1.31	0.80	0.73	2.69	1.69
22	DN201-E	4.28	7.18	1.35	1.70	9.30	0.26	0.27	0.76	1.86	0.96
23	DB2	3.78	6.96	3.11	1.59	6.82	1.30	0.64	1.11	1.86	1.52
24	DB202	3.41	6.00	2.10	1.06	9.06	1.52	0.46	0.96	2.13	1.56
25	H1-01	4.36	7.38	2.02	1.22	6.87	3.29	1.77	0.29	5.45	3.18
26	H1-02	3.92	4.53	1.60	0.97	5.22	2.29	1.37	0.21	4.09	2.38
27	H2	1.40	4.34	1.81	0.77	5.42	2.40	1.11	0.22	8.35	5.02
28	H2-3	0.59	2.28	0.97	0.40	1.49	1.39	1.03	0.18	8.36	5.09
29	H3	4.42	6.38	2.61	1.12	6.31	2.36	1.65	0.25	5.74	3.40
30	HX4-01	4.12	5.44	0.99	0.89	5.53	2.12	1.24	0.13	4.99	2.45
31	FCl-02	3.70	5.37	2.10	0.83	4.41	2.02	0.82	0.11	5.96	3.25
32	HD-1-1	4.72	5.03	1.97	0.78	7.04	0.66	0.07	0.08	6.03	2.15

Note: a. Propylcyclohexane; b. 2,6-dimethyloctane; c. 2-methyl-3-ethylheptane; d. 1,1,2,3-tetramethylcyclohexane; e. 3-methylnonane; f. 3-isopropyltoluene; g. 4-isopropyltoluene; h. 2-isopropyltoluene; i. 1,2,3,5-tetramethylbenzene; j. 1,2,3,4-tetramethylbenzene.

3.3 Secondary Alteration Influence on the Distribution of 3-iPT, 4-iPT, and 2-iPT in Crude Oils and Condensates

Biodegradation can prominently alter the composition of crude oils, especially in shallow reservoirs (Peters and Fowler, 2002; Evans et al., 1971). The previous studies showed that the LHs components of marine oils from the Tarim Basin are derived from the later charge and did not undergo the process of biodegradation (Zhang et al., 2014b; Cheng et al., 2013). The 25-norhopanes and unresolved complex mixture (UCM) are not detected in lacustrine oils from the Beibuwan Basin and swamp oils from the Tarim Basin, indicating that these crude oils did not undergo biodegradation process. For aromatic compounds, biodegradation rate is discovered to decrease with the amount of aromatic rings and increase with the amount of alkyl substituents (Volkman et al., 1984). Due to 3-iPT, 4-iPT and 2-iPT have similar molecular structures and same molecular weight, therefore, 3-iPT, 4-iPT, and 2-iPT may have similar susceptibility to biodegradation. In addition, if crude oils undergo the process of biodegradation, 3-iPT, 4-iPT, and 2-iPT will not be selectively biodegraded. Thus, iPTr, iPTr1, and iPTr2 ratios may not be affected by the process of biodegradation.

The evaporative fractionation will transform low molecular

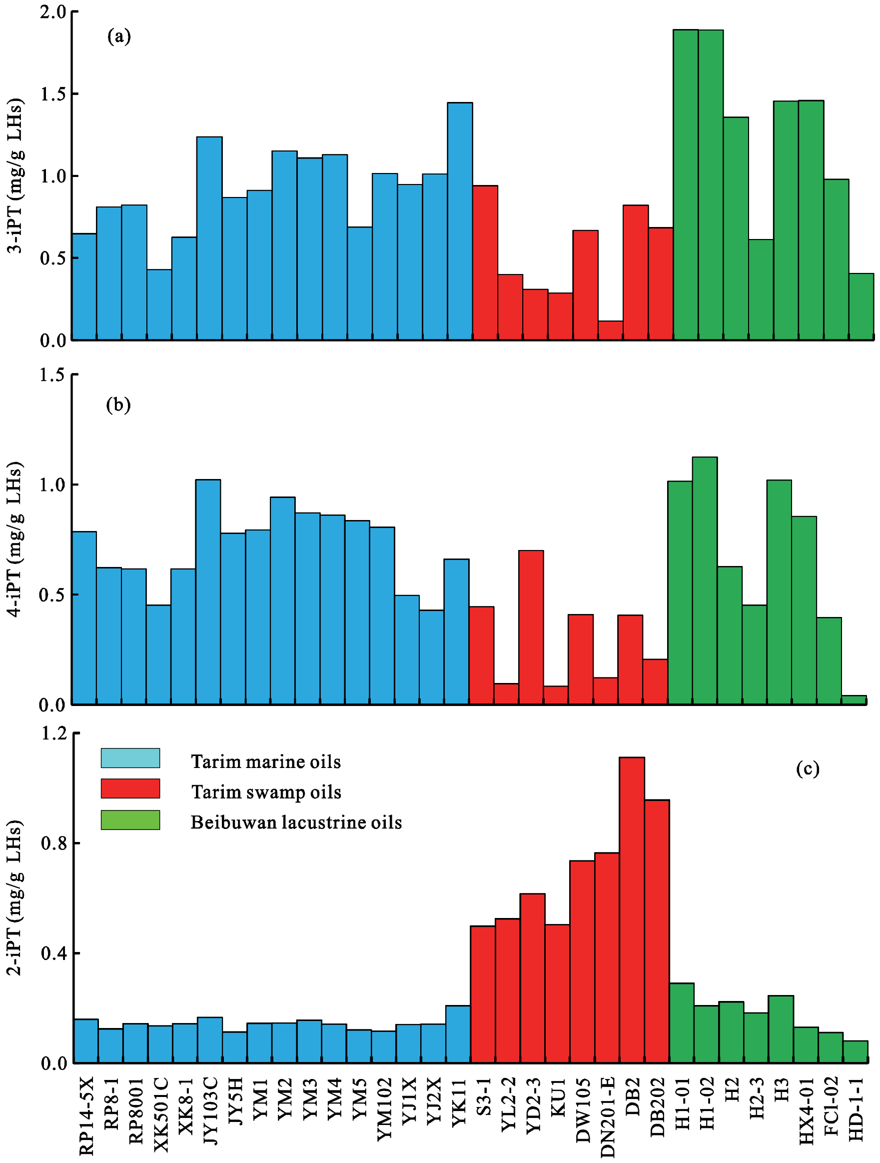

Figure 4. The histogram of the concentrations of (a) 3-isopropyltoluene (3-iPT), (b) 4-isopropyltoluene (4-iPT), and (c) 2-isopropyltoluene (2-iPT) for all studied oils.

weight hydrocarbons to gas phase (Thompson, 1988, 1987). It is generally known that both Tol/nC$_7$ (B) and nC$_7$/MCyCC$_6$ (F) were usually used to recognize the process of evaporative fraction (Thompson, 1988, 1987). Thompson (1987) suggested that crude oils that experienced evaporative fraction will deviate from the normal oil with decreasing F values (<0.5) and increasing B values (>1.0). In the present study, the marine oils from the Tarim Basin have low B values (0.08–0.45) and high F values (1.64–2.04) (Table 4), suggesting that marine oils from the Tarim Basin did not undergo the process of evaporative fractionation. However, swamp oils from the Tarim Basin and lacustrine oils from the Beibuwan Basin have higher B values (0.49–3.55 and 0.61–2.66, respectively) and lower F values (0.19–0.69 and 0.18–0.53, respectively) relative to marine oils from the Tarim Basin (Table 4). The F values are determined by both organic matter source and maturity, and low F values for lacustrine oils from the Beibuwan Basin and swamp oils from the Tarim Basin probably reflect terrestrial organic matter contribution. The difference of B values among marine oils from the Tarim Basin, lacustrine oils from the Beibuwan Basin, and swamp oils from the Tarim Basin are consistent with the previous works, which the benzene and toluene contents in terrestrial source rocks were higher than in marine source rocks (Leythaeuser et al., 1979a, b). Also, whether a compound easily enters vapor phase mainly depends on the molecular weight and molecular structure of the compounds (Thompson, 1988, 1987). Because 4-iPT, 3-iPT and 2-iPT share equal molecular weight and analogous molecular skeleton, iPTr, iPTr1, and iPTr2 ratios may not be affected by evaporative fractionation process. In addition, whether the distribution of 4-iPT, 3-iPT and 2-iPT in crude oils affected by biodegradation and evaporative fractionation need more investigations.

3.4 Thermal Maturity Effects on the Distribution of 3-iPT, 4-iPT, and 2-iPT in Crude Oils and Condensates

Because the thermodynamic stability of both the

Table 4 Geochemical parameters for all studied oils

No.	Well	iPTr	iPTr1	iPTr2	Pr/Ph	B	F	MDR	MDR'	EDR	EDR'	MTR	MT1	MT2	TeMBr
1	RP14-5X	15.53	7.02	8.51	0.98	0.17	1.71	9.72	0.91	9.78	0.91	0.90	1.44	1.24	0.86
2	RP8-1	19.00	10.74	8.26	0.88	0.20	1.75	7.44	0.88	9.12	0.90	0.66	1.20	0.88	0.78
3	RP8001	17.49	9.99	7.50	1.05	0.21	1.72	7.90	0.89	9.21	0.90	0.79	1.38	2.53	0.78
4	XK501C	14.58	7.09	7.48	0.85	0.19	1.64	6.13	0.86	6.44	0.87	1.07	1.90	0.81	0.63
5	XK8-1	15.99	8.05	7.93	0.94	0.22	1.73	13.98	0.93	12.11	0.92	0.96	1.65	1.02	1.05
6	JY103C	17.48	9.57	7.91	0.89	0.14	1.75	6.43	0.87	7.20	0.88	0.90	1.81	0.90	0.70
7	JY5H	23.37	12.32	11.04	0.82	0.14	1.79	5.28	0.84	7.15	0.88	0.90	1.86	1.24	0.50
8	YM1	16.63	8.89	7.74	0.98	0.23	1.72	15.57	0.94	12.56	0.93	0.67	1.30	1.07	1.02
9	YM2	20.67	11.37	9.30	0.91	0.08	2.04	5.99	0.86	7.14	0.88	0.90	1.63	1.13	0.58
10	YM3	18.38	10.29	8.09	0.93	0.26	1.74	15.28	0.94	12.65	0.93	0.77	1.39	0.87	1.03
11	YM4	20.34	11.54	8.80	0.97	0.17	1.98	8.72	0.90	8.52	0.89	0.70	1.27	3.29	0.70
12	YM5	18.35	8.29	10.06	0.87	0.25	1.75	16.46	0.94	13.19	0.93	0.61	1.05	1.02	1.03
13	YM102	24.35	13.56	10.78	0.92	0.11	1.98	8.02	0.89	7.92	0.89	0.75	1.46	1.46	0.69
14	YJ1X	17.77	11.67	6.11	0.90	0.26	1.86	7.85	0.89	8.78	0.90	0.76	1.30	0.97	0.71
15	YJ2X	15.17	10.66	4.51	0.95	0.31	1.77	13.82	0.93	12.47	0.93	0.93	1.68	0.73	1.08
16	YK11	15.70	10.77	4.93	1.06	0.45	1.82	9.32	0.90	7.99	0.89	0.77	1.22	0.95	0.90
17	S3-1	4.40	2.98	1.42	2.22	1.96	0.19	28.94	0.97	34.27	0.97	0.41	0.52	0.51	2.13
18	YL2-2	1.53	1.23	0.30	1.86	0.49	0.35	15.05	0.94	24.81	0.96	0.34	0.33	0.35	1.88
19	YD2-3	2.74	0.84	1.90	2.08	1.39	0.56	9.13	0.90	13.32	0.93	0.42	0.44	0.48	2.05
20	KU1	2.04	1.57	0.47	1.68	3.55	0.34	9.45	0.90	12.09	0.92	0.26	0.32	0.43	1.21
21	DW105	2.87	1.78	1.09	2.20	/	/	/	/	/	/	0.55	0.55	0.36	1.59
22	DN201-E	0.70	0.34	0.36	2.24	/	/	/	/	/	/	0.19	0.15	0.40	1.93
23	DB2	1.74	1.17	0.58	2.46	2.32	0.69	/	/	/	/	0.45	0.46	0.42	1.22
24	DB202	2.07	1.59	0.48	2.72	2.71	0.51	/	/	/	/	0.35	0.23	0.31	1.37
25	H1-01	17.40	11.32	6.08	3.81	1.38	0.22	6.98	0.87	6.12	0.86	0.27	0.29	0.28	1.71
26	H1-02	17.45	10.93	6.52	3.73	0.80	0.40	6.26	0.86	5.50	0.85	0.35	0.31	0.25	1.71
27	H2	15.69	10.73	4.96	4.30	0.89	0.44	5.65	0.85	6.00	0.86	0.42	0.33	0.55	1.66
28	H2-3	13.20	7.59	5.61	4.26	0.94	0.53	6.54	0.87	5.75	0.85	0.43	0.66	0.67	1.64
29	H3	16.35	9.61	6.74	3.89	0.86	0.18	5.38	0.84	5.20	0.84	0.41	0.41	0.25	1.69
30	HX4-01	25.74	16.23	9.52	4.46	0.61	0.48	5.71	0.85	6.17	0.86	0.18	0.18	0.22	2.04
31	FCl-02	25.29	18.00	7.29	2.93	0.61	0.26	3.73	0.79	4.84	0.83	0.39	0.48	0.22	1.84
32	HD-1-1	8.89	8.06	0.83	3.65	2.66	0.35	11.44	0.92	7.42	0.88	0.39	0.28	0.16	2.80

Note: iPTr. (3+4)-/2-iPT; iPTr1. 3-/2-iPT; iPTr2. 4-/2-iPT; Pr/Ph. pristane/phytane; B. toluene/*n*-heptane; F. $n\mathrm{C}_7$/MCyCC$_6$; MDR. 4-/1-MDBT; MDR'. 4-/(4+1)-MDBT; EDR. 4,6-DMDBT/4-EDBT; EDR'. 4,6-DMDBT/(4,6-DMDBT+4-EDBT); MT1. 2-methyl-3-ethylheptane/3-methylnonane; MT2. 1,1,2,3-tetramethylcyclohexane/propylcyclohexane; MTR. 2-methyl-3-ethylheptane/2,6-dimethyloctane; TeMBr. 1,2,3,5-/1,2,3,4-tetramethylbenzene; 3-iPT. 3-isopropyltoluene; 4-iPT. 4-isopropyltoluene; 2-iPT. 2-isopropyltoluene; MDBT. methyldibenzothiophene; DMDBT. dimethyldibenzothiophene; EDBT. ethyldibenzothiophene; /. not detected.

4-methyldibenzothiophene (4-MDBT) is higher than 1-methyldibenzothiophene (1-MDBT) and the 4,6-dimethyldibenzothiophene (4,6-DMDBT) is higher than 4-ethydibenzothiophene (4-EDBT), therefore, MDBT ratios (MDR = 4-MDBT/1-MDBT and MDR' = 4-/(4- + 1-MDBT), and the ratios of DMDBT to EDBT (EDR = 4,6-DMDBT/4-EDBT and (EDR' = 4,6-DMDBT/(4,6-DMDBT + 4-EDBT) usually are used for maturity assessment (Radke and Willsch, 1994). In this study, marine oils from the Tarim Basin, swamp oils from the Tarim Basin, and lacustrine oils from the Beibuwan Basin have MDR values (5.28–16.46, 9.13–28.94 and 3.73–11.44, respectively), and EDR values (6.44–13.19, 12.09–34.27, 4.84–7.42, respectively) (Table 4), indicating a relatively wider maturity range, and a positive correlation for all studied oils (Fig. 5). In addition, all crude oil samples have higher iPTr, iPTr1 and iPTr2 values corresponding to higher MDR, MDR', EDR and EDR' values (Table 4), suggesting that the relative abundance of 3-iPT, 4-iPT and 2-iPT with the influence of thermal evolution cannot be eliminated. The large difference in MDR, MDR', EDR and EDR' values between marine oils from the Tarim Basin and lacustrine oils from the Beibuwan Basin, but the iPTr, iPTr1 and iPTr2 values have similar distribution range (Table 4). Thus, it is considered that iPTr, iPTr1 and iPTr2 values are not or slightly affected by thermal maturity.

3.5 The 3-iPT, 4-iPT, and 2-iPT Values as Indicators of Organic Matter Source in Crude Oils and Condensates

According to previous studies, the depositional environments of sedimentary organic matter can be indicated by Pr/Ph ratio (pristine/phytane) (Didyk et al., 1978). It is generally known that crude oils have high Pr/Ph values (>3.0) indicating oxic/sub-oxic depositional conditions, while crude oils have lower Pr/Ph values (<0.8) suggesting reducing/anoxic depositional environments (Didyk et al., 1978). In Figs. 6 and 7, marine oils from the Tarim Basin derived from lower hydrobiont, bacterium, and algae (Song et al., 2015; Zhang and Huang, 2005; Hanson et al., 2000) (with Pr/Ph values of 0.82–1.06) and lacustrine oils from the Beibuwan Basin derived from the co-contribution of terrestrial higher plants and lower hydrobiont, bacterium, and algae (Li et al., 2009, 2007) (with Pr/Ph values of 2.93–4.46) all have high iPTr (>8.0), iPTr1 (>7.0) and iPTr2 (>4.0, except HD-1-1 oil) values, while swamp oils from the Tarim Basin derived from terrestrial higher plants (Cheng et al., 2015b; Zhu et al., 2012; Zhang et al., 2011; Fan et al., 2009) (with Pr/Ph values of 0.70–4.40) have lower iPTr (<5.0), iPTr1 (<3.0), iPTr2 (<2.0) values (Table 4). Based on the distribution of 3-iPT, 4-iPT, and 2-iPT in all studied oils (Fig. 4, Table 3), iPTr2 (4-/2-iPT) value less than 4.0 in HD-1-1 oil probably accused by the increase of 2-iPT concentrations. The high contents of 2-iPT probably controlled by terrestrial higher plants contribution is deemed in Section 3.2. The HD-1-1 oil is derived from the Liushagang Formation (E_2l) lacustrine mudstone of the Beibuwan Basin (Li et al., 2009, 2007). Thus, HD-1-1 oil could have higher terrestrial high plants contribution.

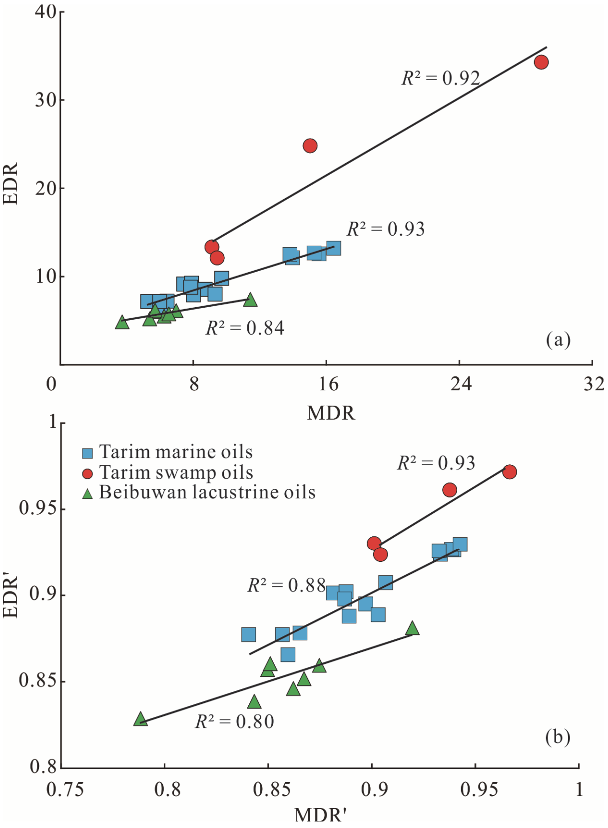

Figure 5. Cross-plots of (a) MDR vs. EDR, and (b) MDR' vs. EDR' for all studied oils.

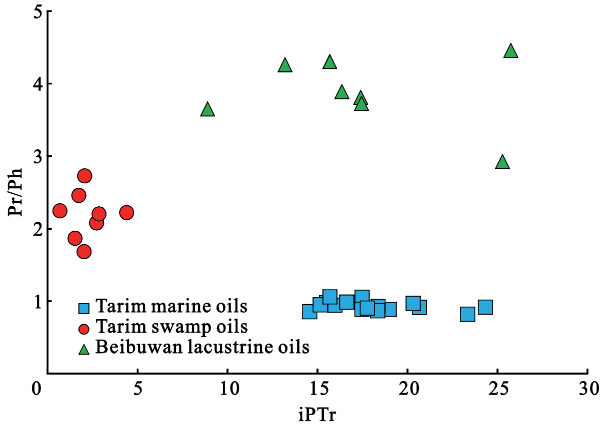

Figure 6. Cross-plots of (3+4)-/2-isopropyltoluene (iPTr) vs. pristine/phytane (Pr/Ph) for all studied oils.

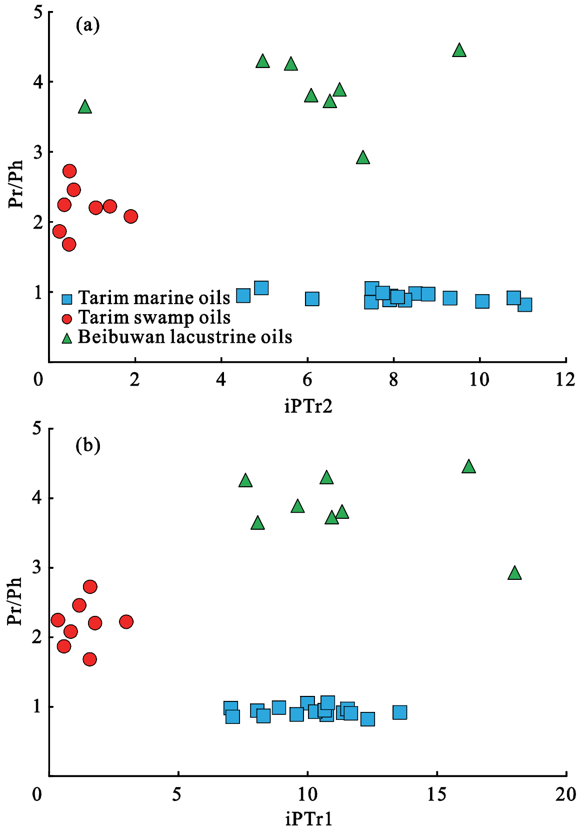

Figure 7. Cross-plots of (a) 3-/2-isopropyltoluene (iPTr1) vs. pristine/phytane (Pr/Ph), and (b) 4-/2-isopropyltoluene (iPTr2) vs. pristine/phytane (Pr/Ph) for all studied oils.

The 2-M-3EH/3-MN (MT1) ratio linked to 1,1,2,3-TeMCHx/$PCyC_6$ (MT2) ratio are useful parameters for inferring depositional environments (Wang et al., 2014). Furthermore, MTR and 1,2,3,5-/1,2,3,4-TeMB (TeMBr) ratios were proposed to infer depositional environments (Cheng et al., 2015a, b). In Figs. 8–10, although marine oils from the Tarim Basin with low TeMBr (0.50–1.08), high MTR (0.61–1.07), MT1 (1.05–1.90) and MT2 (0.73–3.29) values and lacustrine oils from the Beibuwan Basin with higher TeMBr (1.64–2.80) and lower MTR (0.18–0.43), MT1 (0.18–0.66) and MT2 (0.16–0.67) values, marine oils from the Tarim Basin and lacustrine oils from the Beibuwan Basin all have high iPTr (>8.0), iPTr1 (>7.0) and iPTr2 values (>4.0, except HD-1-1 oil). In addition, with higher TeMBr (1.23–2.13) and lower MTR

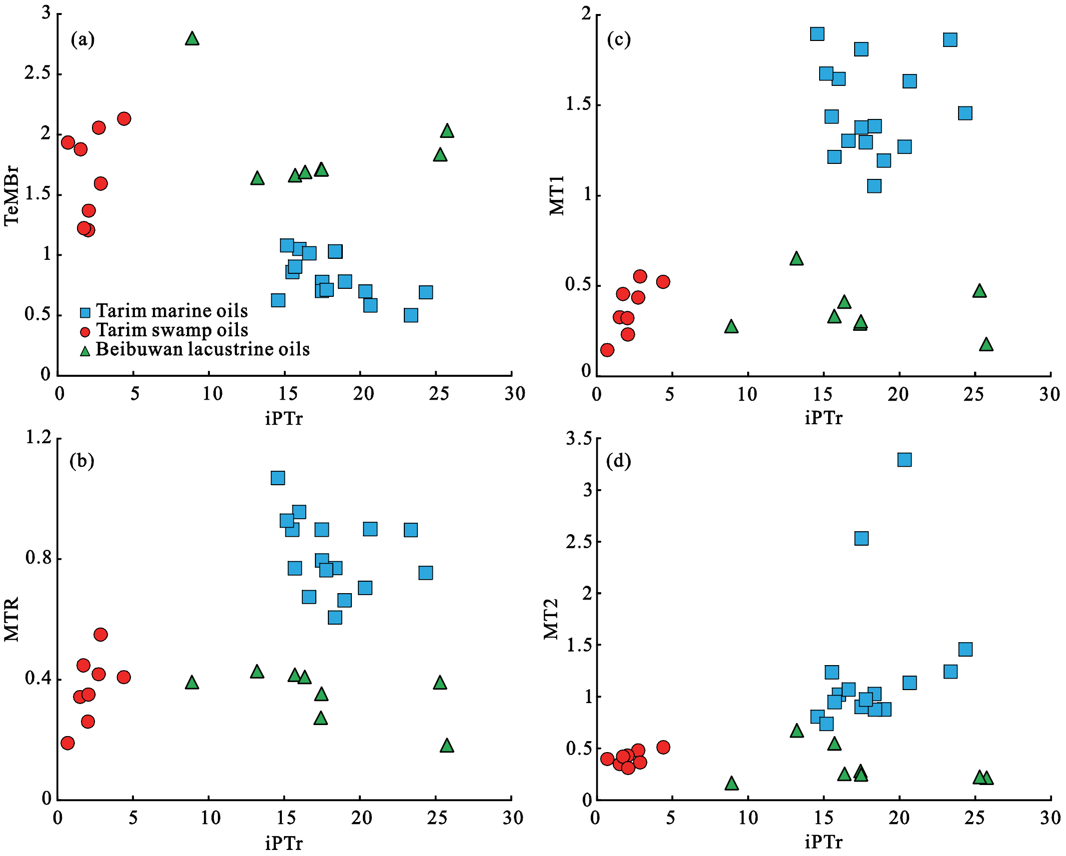

Figure 8. Cross-plots of (3+4)-/2-isopropyltoluene (iPTr) vs. (a) TeMBr, (b) MTR, (c) MT1, and (d) MT2 for all studied oils.

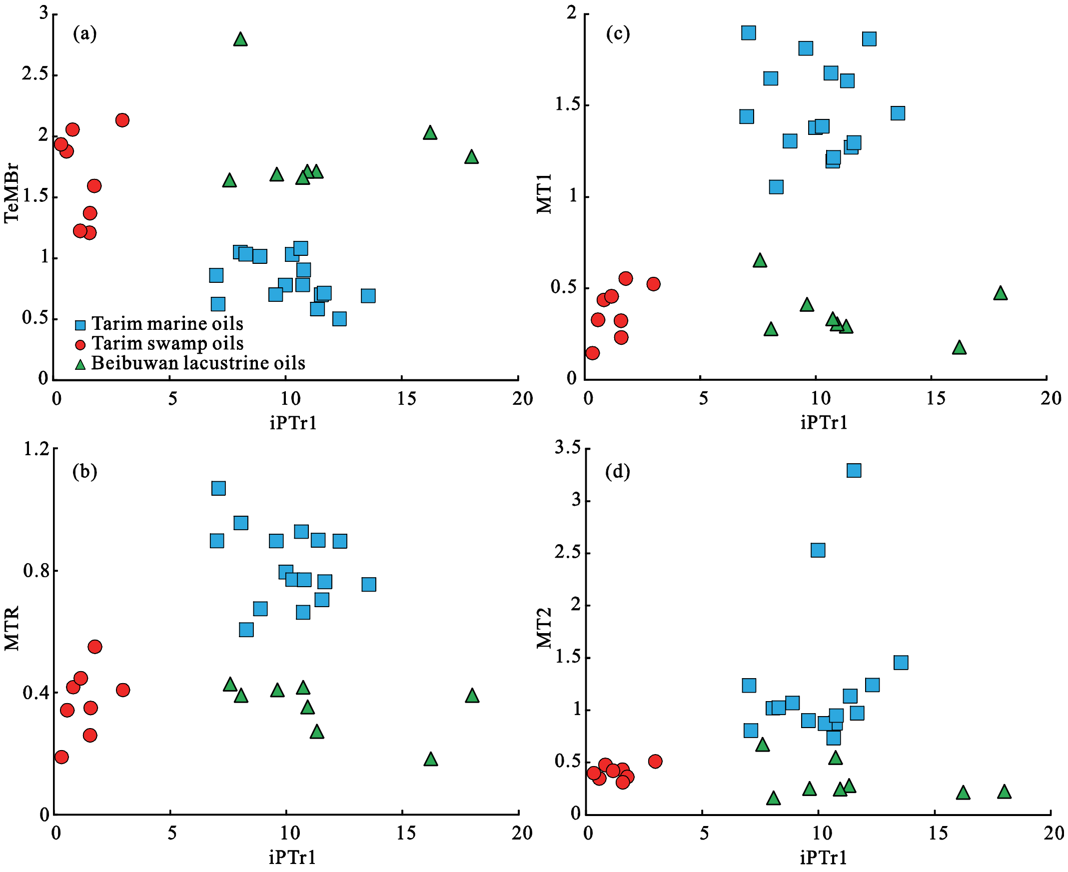

Figure 9. Cross-plots of 3-/2-isopropyltoluene (iPTr1) vs. (a) TeMBr, (b) MTR, (c) MT1, and (d) MT2 for all studied oils.

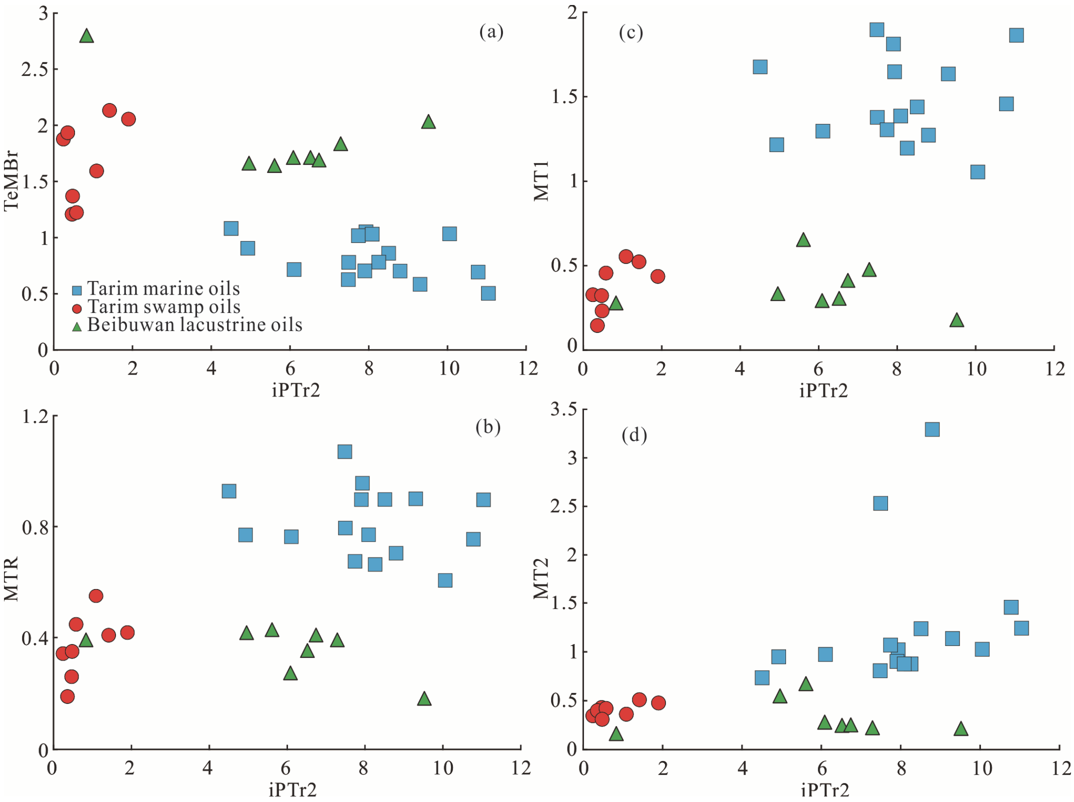

Figure 10. Cross-plots of 4-/2-isopropyltoluene (iPTr2) vs. (a) TeMBr, (b) MTR, (c) MT1, and (d) MT2 for all studied oils.

(0.19–0.55), MT1 (0.15–0.55) and MT2 (0.31–0.51) values, swamp oils from the Tarim Basin have lower iPTr (<5.0), iPTr1 (<3.0), iPTr2 (<2.0) values (Table 4). According to the above discussion, it should be pointed out that iPTr, iPTr1 and iPTr2 ratios are not controlled mainly by depositional redox conditions.

In conclusion, iPTr, iPTr1 and iPTr2 ratios in crude oils basically are not or slightly affected by the secondary alteration process, thermal maturity and depositional environment, while the iPTr, iPTr1 and iPTr2 ratios probably are mainly affected by the organic matter origins. In this study, high iPTr (>8.0), iPTr1 (>7.0) and iPTr2 (>4.0) values indicate that crude oils are derived from the co-contribution of lower aquatic organisms, bacteria, algae, and terrestrial higher plants, whereas lower iPTr (<5.0), iPTr1 (<3.0), iPTr2 (<2.0) values indicate that crude oils are derived from terrestrial higher plants.

4 CONCLUSIONS

Isopropyltoluene with three isomers (4-iPT, 3-iPT, and 2-iPT) were detected in crude oils from the Tarim Basin and Beibuwan Basin by GC × GC-TOFMS. Based on the striking differences in the concentrations of 4-iPT, 3-iPT and 2-iPT in crude oils, and 2-iPT probably derived mainly from similar skeleton monocyclic terpenoids via dehydrogenation and aromatization, the ratios of (3+4)-/2-iPT (iPTr), 3-/2-iPT (iPTr1) and 4-/2-iPT (iPTr2) are proposed to infer the organic matter origin of crude oils. Relatively higher iPTr (>8.0), iPTr1 (>7.0) and iPTr2 (>4.0) values imply that crude oils are sourced from co-contribution of lower aquatic organisms, bacteria, algae, and terrestrial higher plants, while lower iPTr (<5.0), iPTr1 (<3.0), iPTr2 (<2.0) values indicate that crude oils originated from terrestrial higher plants. The significant differences in iPTr, iPTr1 and iPTr2 ratios are mainly controlled by the concentrations of 2-iPT, while the concentrations of 3-iPT and 4-iPT show similar distribution range in all studied oils. The 2-iPT is depleted in marine oils from the Tarim Basin and lacustrine oils from the Beibuwan Basin at less than 0.30 mg/g LHs, but is enriched in swamp oils from the Tarim Basin at greater than 0.50 mg/g LHs. The iPTr, iPTr1 and iPTr2 ratios and 2-iPT contents are useful for inferring organic matter origin, especially for light oils and condensates. The iPTr, iPTr1 and iPTr2 ratios in crude oils basically are not or slightly affected by the biodegradation, evaporative fractionation, thermal maturity and depositional environment and the distribution of 4-iPT, 3-iPT and 2-iPT in crude oils affected by other secondary alteration need more investigations.

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