Datashare 169

Novel diamondoid-based maturity models using naturally occurring petroleum fluids

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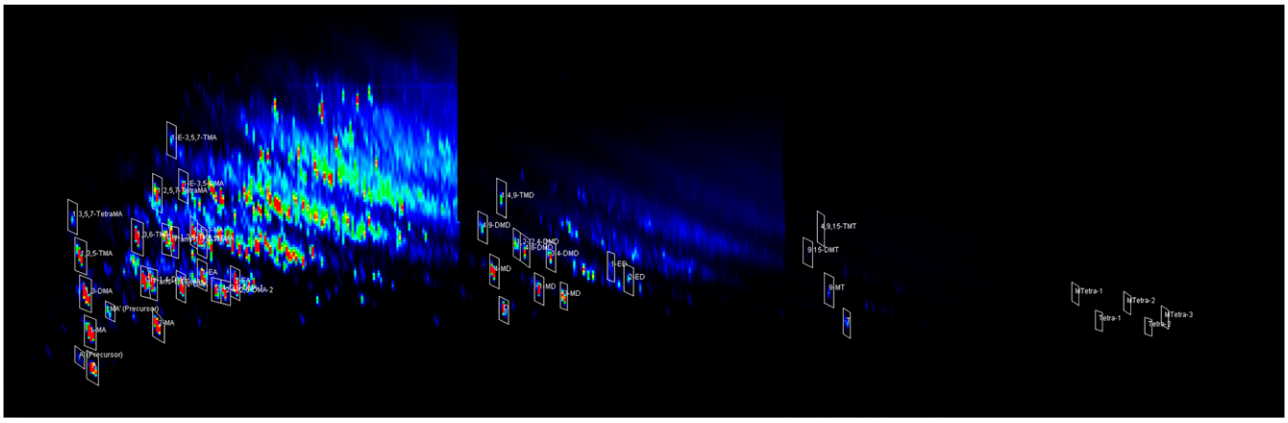

Figure S1. Representative two-dimensional gas chromatography trace of a crude oil sample used in-house for monitoring of analytical reproducibility, showing the occurrence of all diamondoid compounds quantified in this study. Warmer colors indicate higher peak areas. See Table S1 for abbreviated names.

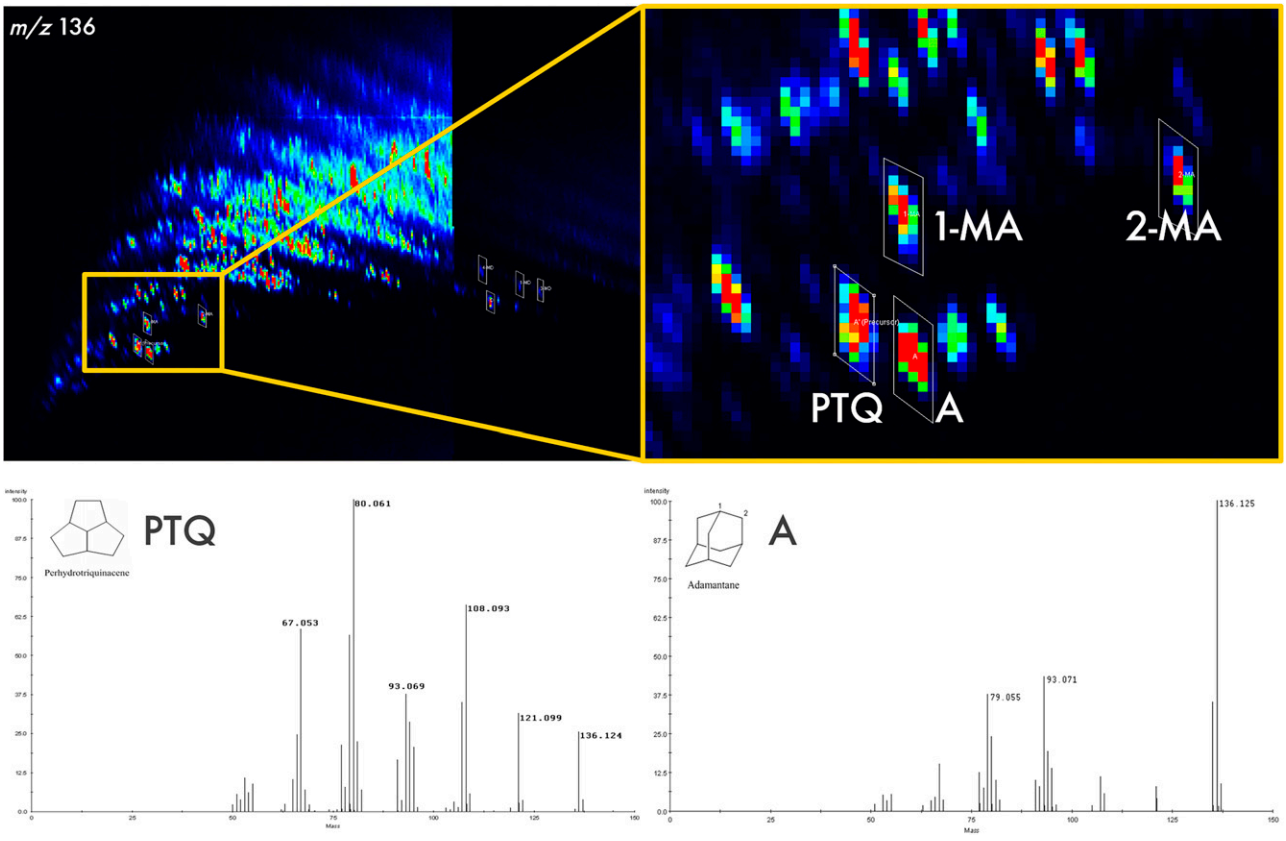

Figure S2. Two-dimensional gas chromatography (GC × GC) trace of a crude oil sample showing the position of perhydrotriquinacene (PTQ) relative to adamantane (A), along with their representative mass spectra obtained using full scan GC × GC-mass spectrometry. See Table S1 for abbreviated names.

Table S1. List of Diamondoid Compounds Identified and Their Mass-to-Charge Ratio for Quantification

Abbreviated Name	Full Name	Filter	Quantifiers, *m/z*
D16-adamantane	Perdeuteroadamantane (internal standard)	D16-A	152.1
A	Adamantane	A	136.1
PTQ	Perhydrotriquinacene	A	136.1
1-MA	1-methyladamantane	MA	135.1
2-MA	2-methyladamantane	MA	135.1
1,3-DMA	1,3-dimethyladamantane	DMA	149.1
Cis-1,4-DMA	*Cis*-1,4-dimethyladamantane	DMA	149.1
Trans-1,4-DMA	*Trans*-1,4-dimethyladamantane	DMA	149.1
1,2-DMA	1,2-dimethyladamantane	DMA	149.1
2,4-/2,6-DMA-1	2,4-/2,6-dimethyladamantane-1	DMA	149.1
2,4-/2,6-DMA-2	2,4-/2,6-dimethyladamantane-2	DMA	149.1
1-EA	1-ethyladamantane	MA	135.1
2-EA	2-ethyladamantane	MA	135.1
1,3,5-TMA	1,3,5-trimethyladamantane	TMA	163.1
1,3,6-TMA	1,3,6-trimethyladamantane	TMA	163.1
Cis-1,3,4-TMA	*Cis*-1,3,4-trimethyladamantane	TMA	163.1
Trans-1,3,4-TMA	*Trans*-1,3,4-trimethyladamantane	TMA	163.1
1,2,3-TMA	1,2,3-trimethyladamantane	TMA	163.1

(*continued*)

Table S1. Continued

Abbreviated Name	Full Name	Filter	Quantifiers, *m/z*
1-E-3-MA	1-ethyl-3-methyladamantane	DMA	149.1
1,3,5,7-TetraMA	1,3,5,7-tetramethyladamantane	TetraMA	177.1
1,3,5,6-TetraMA	1,3,5,6-tetramethyladamantane	TetraMA	177.1
1-E-3,5-DMA	1-ethyl-3,5-dimethyladamantane	TMA	163.1
1-E-3,5,7-TMA	1-ethyl-3,5,7-trimethyladamantane	TetraMA	177.1
D	Diamantane	D	188.2
4-MD	4-methyldiamantane	MD	187.2
1-MD	1-methyldiamantane	MD	187.2
3-MD	3-methyldiamantane	MD	187.2
4,9-DMD	4,9-dimethyldiamantane	DMD	201.2
1,2-/2,4-DMD	1,2-/2,4-dimethyldiamantane	DMD	201.2
4,8-DMD	4,8-dimethyldiamantane	DMD	201.2
3,4-DMD	3,4-dimethyldiamantane	DMD	201.2
1-ED	1-ethyldiamantane	MD	187.2
2-ED	2-ethyldiamantane	MD	187.2
1,4,9-TMD	1,4,9-trimethyldiamantane	TMD	215.2
T	Triamantane	T	240.2
9-MT	9-methyltriamantane	MT	239.2
9,15-DMT	9,15-dimethyltriamantane	DMT	253.2
4,9,15-TMT	4,9,15-trimethyltriamantane	TMT	267.2
Tetra-1	Tetramantane-1	Tetra	292.3
Tetra-2	Tetramantane-2	Tetra	292.3
Tetra-3	Tetramantane-3	Tetra	292.3
MTetra-1	Methyltetramantane-1	MTetra	291.3
MTetra-2	Methyltetramantane-2	MTetra	291.3
MTetra-3	Methyltetramantane-3	MTetra	291.3
Adamantanes	Adamantanes	A: adamantanes	136.1, 135.1, 149.1, 163.1, 177.1
C1-adamantanes	C1-adamantanes	MA	135.1
C2-adamantanes	C2-adamantanes	DMA	149.1
C3-adamantanes	C3-adamantanes	TMA	163.1
C4-adamantanes	C4-adamantanes	TetraMA	177.1
Diamantanes	Diamantanes	D: diamantanes	188.2, 187.2, 201.2, 215.2
C1-diamantanes	C1-diamantanes	MD	187.2
C2-diamantanes	C2-diamantanes	DMD	201.2
C3-diamantanes	C3-diamantanes	TMD	215.2
C4-diamantanes	C4-diamantanes	TetraMD	229.2
Triamantanes	Triamantanes	T: triamantanes	240.2, 239.2, 253.2, 267.2, 281.2
C1-triamantanes	C1-triamantanes	MT	239.2
C2-triamantanes	C2-triamantanes	DMT	253.2
C3-triamantanes	C3-triamantanes	TMT	267.2
C4-triamantanes	C4-triamantanes	TetraMT	281.2
Tetramantanes	Tetramantanes	Tetra: tetramantanes	292.3, 291.3, 305.3, 319.3, 333.3
C1-tetramantanes	C1-tetramantanes	MTetra	291.3
C2-tetramantanes	C2-tetramantanes	DMTetra	305.3
C3-tetramantanes	C3-tetramantanes	TMTetra	319.3
C4-tetramantanes	C4-tetramantanes	TetraMTetra	333.3

Abbreviation: *m/z* = mass-to charge ratio.

Table S2. List of Diamondoid Parameters and Their Definitions

Parameter Name	Full Name	Definition*	Reference and Comments
MAI	Methyladamantane index	1-MA/(1-MA + 2-MA)	Chen et al. (1996)
EAI	Ethyladamantane index	1-EA/(1-EA + 2-EA)	Schulz et al. (2001), reformulated as in Zhang et al. (2005)
DMAI-1	Dimethyladamantane index 1	1,3-DMA/(1,3-DMA + 1,2-DMA)	Zhang et al. (2005)
DMAI-2	Dimethyladamantane index 2	1,3-DMA/(1,3-DMA + *cis*-1,4-DMA + *trans*-1,4-DMA)	Zhang et al. (2005)
TMAI-1	Trimethyladamantane index 1	1,3,5-TMA/(1,3,5-TMA + 1,3,6-TMA)	Zhang et al. (2005)
TMAI-2	Trimethyladamantane index 2	1,3,5-TMA/(1,3,5-TMA + *cis*-1,3,4-TMA + *trans*-1,3,4-TMA)	Zhang et al. (2005)
MDI	Methyldiamantane index	4-MD/(4-MD + 1-MD + 3-MD)	Chen et al. (1996)
DMDI-1	Dimethyldiamantane index 1	4,9-DMD/(4,9-DMD + 3,4-DMD)	Schulz et al. (2001), reformulated as in Zhang et al. (2005)
DMDI-2	Dimethyldiamantane index 2	4,9-DMD/(4,9-DMD + 4,8-DMD)	Schulz et al. (2001), reformulated as in Zhang et al. (2005)
MA/A	Methyladamantane to adamantane ratio	(1-MA + 2-MA)/A	Grice et al. (2000)
MD/D	Methyldiamantane to diamantane ratio	(4-MD + 1-MD + 3-MD)/D	Grice et al. (2000)
BTS-1	Bridgehead-to-secondary carbon ratio of single-caged adamantanes	(1-MA + 1,3-DMA + 1,3,5-TMA + 1,3,5,7-TetraMA)/(2-MA + 1,2-DMA + 1,3,6-TMA + 1,3,5,6-TetraMA)	Mankiewicz et al. (2009)
BTS-2	Bridgehead-to-secondary carbon ratio of dual-caged diamantanes	(4-MD + 4,9-DMD)/(3-MD + 3,4-MD)	Mankiewicz et al. (2009)
E-DMAI	Ethyl-dimethyladamantane index	1,3-DMA/(1,3-DMA + 1-EA)	This study
E-TMAI	Ethyl-trimethyladamantane index	1,3,5-TMA/(1,3,5-TMA + 1-E-3-MA)	This study
E-TeMAI	Ethyl-tetramethyladamantane index	1,3,5,7-TetraMA/(1,3,5,7-TetraMA + 1-E-3,5-DMA)	This study
AI	Adamantane index	A/(A + PTQ)	This study

*Equations are based on the abbreviated names as in Table S1.

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