Supplemental material:

REGIOSPECIFIC SYNTHESIS OF DIMETHYLPHENANTHRENES

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¹H-NMR was recorded at a Bruker 400 MHz instrument.

GC-FID were performed on a Agilent 6890N GC-FID with a 30m×0.25mm Agilent DB-225MS column with 21 cm/s He-flow. The sample was dissolved in acetone and injected as 1 µL split(10:1) injection at 250 °C. The temperature program was 80 °C/1 min, 10 °C/min to 200 °C, 3 °C/min to 230 °C, and 230 °C/11 min.

4a

Current Data Parameters
NAME 4a
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160226
Time 11.46
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 63.41
DW 62.400 usec
DE 6.50 usec
TE 296.4 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SF01 400.1324710 MHz
NUC1 1H
P1 8.60 usec
PLW1 18.10000038 W

F2 - Processing parameters
SI 65536
SF 400.1300139 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Current Data Parameters
 NAME 4b
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20160226
 Time 11.51
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 78.54
 DW 62.400 usec
 DE 6.50 usec
 TE 296.4 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SF01 400.1324710 MHz
 NUC1 1H
 P1 8.60 usec
 PLW1 18.10000038 W

F2 - Processing parameters
 SI 65536
 SF 400.1300139 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Current Data Parameters
 NAME 4c
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20160226
 Time 11.55
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 71.31
 DW 62.400 usec
 DE 6.50 usec
 TE 296.4 K
 D1 1.0000000 sec
 TD0 1

===== CHANNEL f1 =====
 SF01 400.1324710 MHz
 NUC1 1H
 P1 8.60 usec
 PLW1 18.10000038 W

F2 - Processing parameters
 SI 65536
 SF 400.1300139 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Current Data Parameters
NAME K-154 Thomas 7D recryst
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

Date_ 20151127
Time 12.53
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 78.54
DW 62.400 usec
DE 6.50 usec
TE 296.2 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====

SFO1 400.1324710 MHz
NUC1 1H
P1 8.60 usec
PLW1 18.10000038 W

F2 - Processing parameters

SI 65536
SF 400.1300097 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

File :C:\MassHunter\GCMS\1\data\Kåre\20160229\blank.D
Operator :
Acquired : 29 Feb 2016 20:04 using AcqMethod Kaare_Phenanthrene.M
Instrument : GCMS
Sample Name:
Misc Info :
Vial Number: 29

Data Path : C:\MassHunter\GCMS\1\data\Kåre\20160229\
Data File : 4a.D
Signal(s) : FID1A.ch
Acq On : 29 Feb 2016 17:16
Sample :
Misc :
ALS Vial : 30 Sample Multiplier: 1

Integration File: autoint1.e

Method : C:\MassHunter\GCMS\1\methods\FAME extracts Dmitry latest 9 dec FID.M
Title : 37 comp mix

Signal : FID1A.ch

peak #	R.T. min	Start min	End min	PK TY	peak height	peak area	peak % max.	% of total
1	22.017	21.584	22.090	BB	3030	88821	0.22%	0.223%
2	23.241	22.124	23.357	BB	2841	186139	0.47%	0.467%
3	27.015	26.710	27.164	BB	727186	39546658	100.00%	99.310%
Sum of corrected areas:						39821618		

Data Path : C:\MassHunter\GCMS\1\data\Kåre\20160229\
Data File : 4a.D
Signal(s) : FID1A.ch
Acq On : 29 Feb 2016 17:16
Sample :
Misc :
ALS Vial : 30 Sample Multiplier: 1

Integration File: autoint1.e

Method : C:\MassHunter\GCMS\1\methods\FAME extracts Dmitry latest 9 dec FID.M
Title : 37 comp mix

Data Path : C:\MassHunter\GCMS\1\data\Kåre\20160229\
Data File : 4b.D
Signal(s) : FID1A.ch
Acq On : 29 Feb 2016 18:02
Sample :
Misc :
ALS Vial : 31 Sample Multiplier: 1

Integration File: autoint1.e

Method : C:\MassHunter\GCMS\1\methods\FAME extracts Dmitry latest 9 dec FID.M
Title : 37 comp mix

Signal : FID1A.ch

peak #	R.T. min	Start min	End min	PK TY	peak height	peak area	peak % max.	% of total
1	21.196	21.017	21.277	BB	6990	234696	0.71%	0.701%
2	23.063	21.563	23.150	BB	1145	-123266	-0.37%	-0.368%
3	25.388	23.670	25.537	BB	694472	32943162	100.00%	98.368%
4	26.086	25.843	26.270	BB	8717	435056	1.32%	1.299%
Sum of corrected areas:						33489647		

Data Path : C:\MassHunter\GCMS\1\data\Kåre\20160229\
Data File : 4b.D
Signal(s) : FID1A.ch
Acq On : 29 Feb 2016 18:02
Sample :
Misc :
ALS Vial : 31 Sample Multiplier: 1

Integration File: autoint1.e

Method : C:\MassHunter\GCMS\1\methods\FAME extracts Dmitry latest 9 dec FID.M
Title : 37 comp mix

Data Path : C:\MassHunter\GCMS\1\data\Kåre\20160229\
Data File : 4c.D
Signal(s) : FID1A.ch
Acq On : 29 Feb 2016 18:40
Sample :
Misc :
ALS Vial : 32 Sample Multiplier: 1

Integration File: autoint1.e

Method : C:\MassHunter\GCMS\1\methods\FAME extracts Dmitry latest 9 dec FID.M
Title : 37 comp mix

Signal : FID1A.ch

peak #	R.T. min	Start min	End min	PK TY	peak height	peak area	peak % max.	% of total
1	13.488	13.310	13.597	BB	11333	238318	1.93%	1.725%
2	19.622	19.184	19.890	BB	4387	545905	4.43%	3.951%
3	22.945	21.570	23.010	BB	990	-30005	-0.24%	-0.217%
4	23.286	23.050	23.357	BB	4009	128961	1.05%	0.933%
5	25.214	23.644	25.337	BB	271334	12332761	100.00%	89.249%
6	28.413	28.164	28.550	BB	9802	602480	4.89%	4.360%
Sum of corrected areas:						13818420		

Method : C:\MassHunter\GCMS\1\methods\FAME extracts Dmitry latest 9 dec FID.M
Title : 37 comp mix

Data Path : C:\MassHunter\GCMS\1\data\Kåre\20160229\
Data File : 4d.D
Signal(s) : FID1A.ch
Acq On : 29 Feb 2016 19:20
Sample :
Misc :
ALS Vial : 33 Sample Multiplier: 1

Integration File: autoint1.e

Method : C:\MassHunter\GCMS\1\methods\FAME extracts Dmitry latest 9 dec FID.M
Title : 37 comp mix

Signal : FID1A.ch

peak #	R.T. min	Start min	End min	PK TY	peak height	peak area	peak % max.	% of total
1	23.969	21.630	24.103	BB	7673	737879	2.86%	2.770%
2	25.404	24.143	25.483	BB	692	145079	0.56%	0.545%
3	26.391	25.983	26.557	BB	496493	25756490	100.00%	96.686%
Sum of corrected areas:						26639449		

```
Data Path : C:\MassHunter\GCMS\1\data\Kåre\20160229\
Data File : 4d.D
Signal(s) : FID1A.ch
Acq On    : 29 Feb 2016   19:20
Sample    :
Misc      :
ALS Vial  : 33    Sample Multiplier: 1
```

Method : C:\MassHunter\GCMS\1\methods\FAME extracts Dmitry latest 9 dec FID.M
Title : 37 comp mix