SUPPORTING INFORMATION

Supporting Information

Evaluation of P-bridged biaryl phosphine ligands in palladium-catalysed Suzuki-Miyaura cross-coupling reactions

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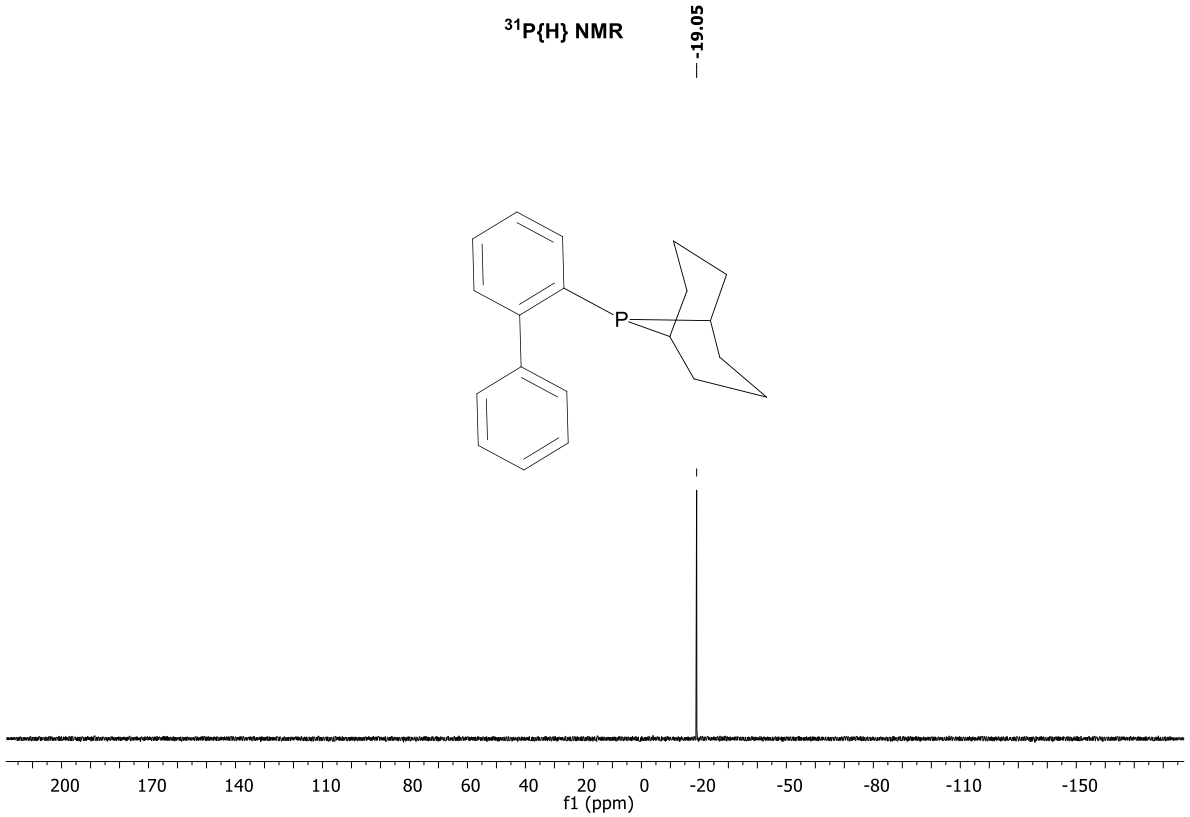
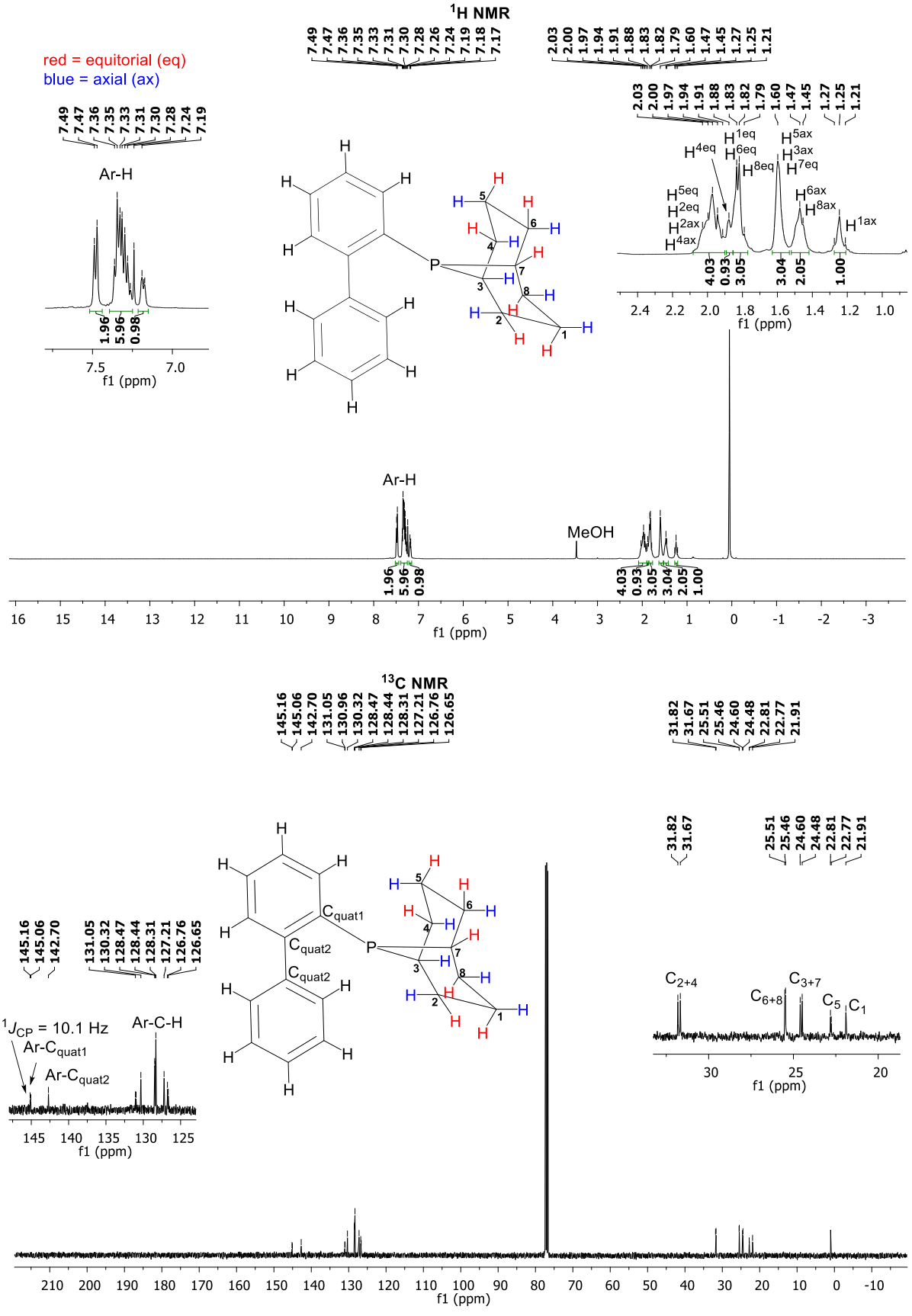
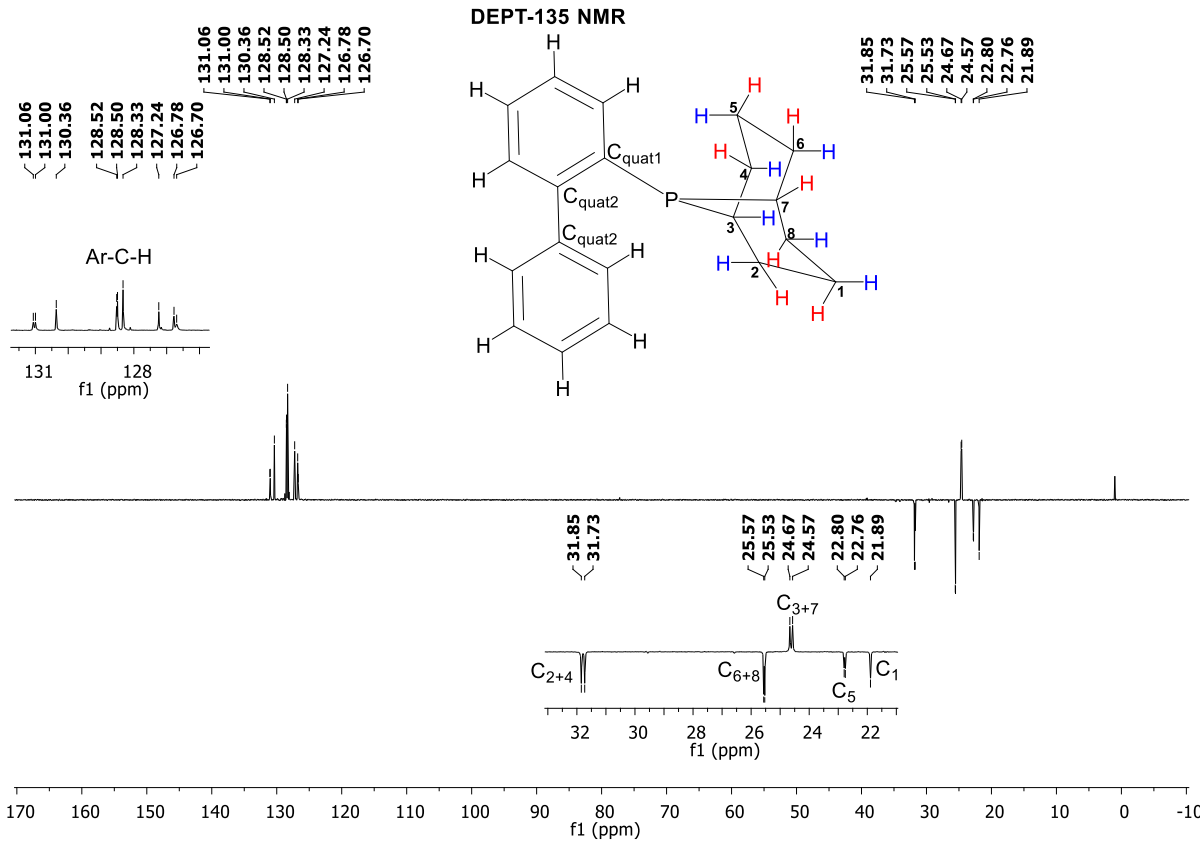
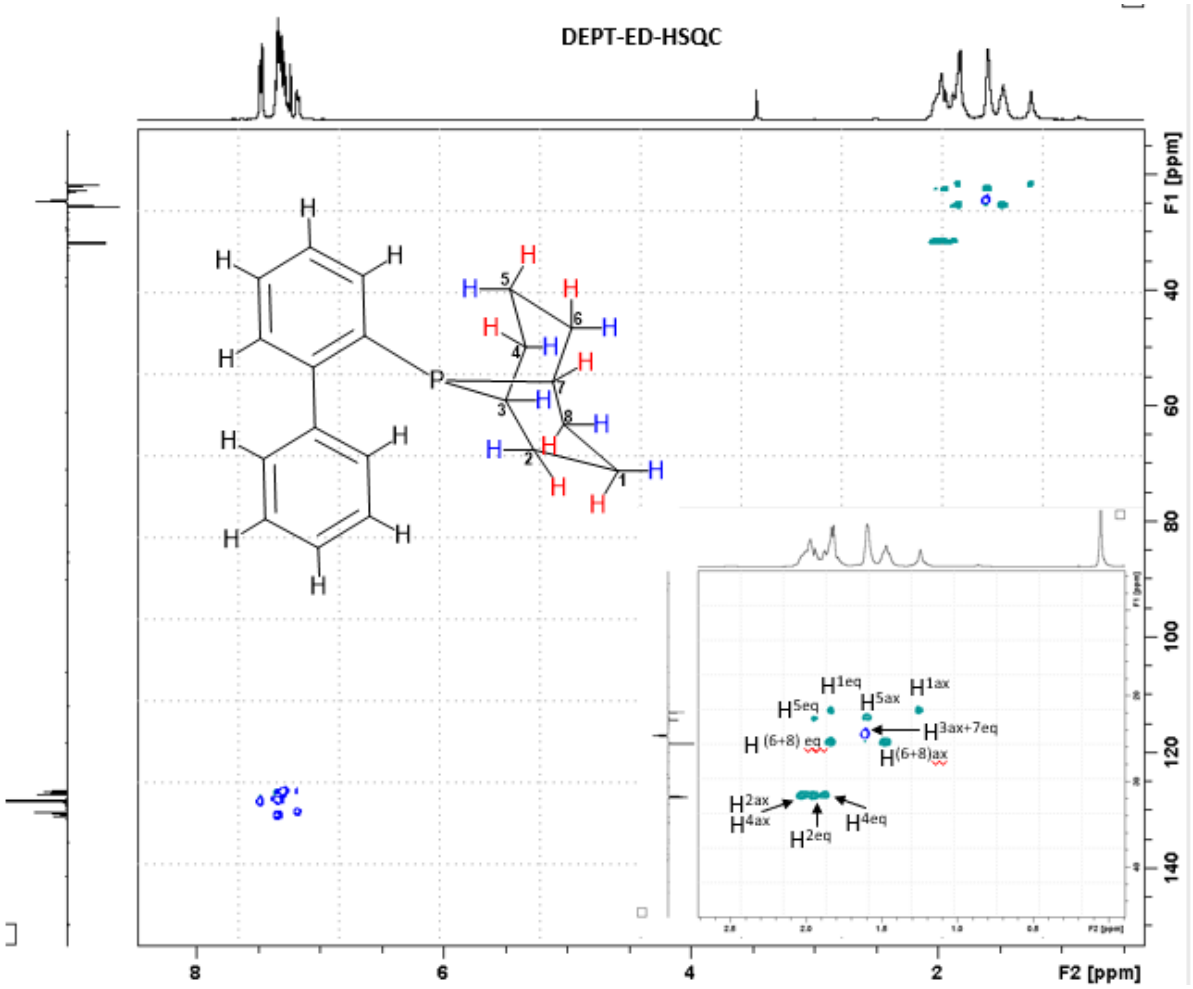
NMR and HRMS spectra: Ligands and precursors

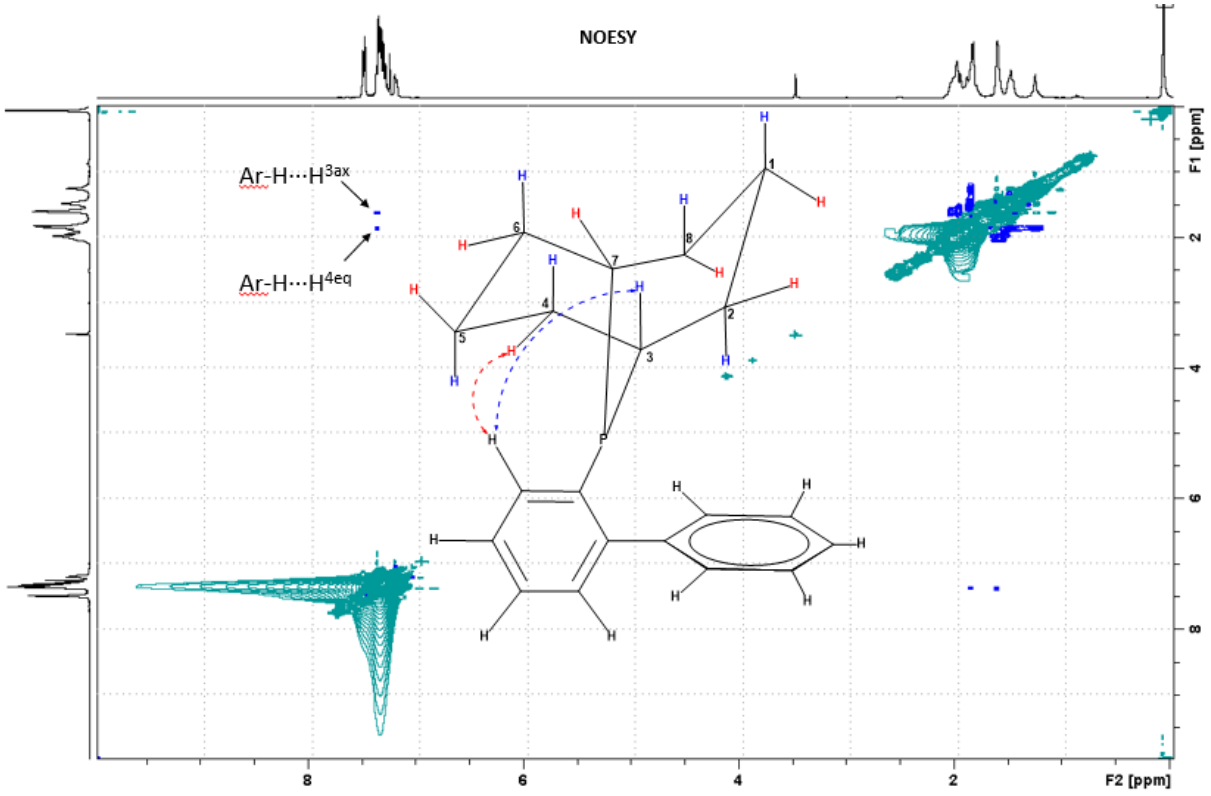
Ligand 1 (NMR experiments carried out in $CDCl_3$)

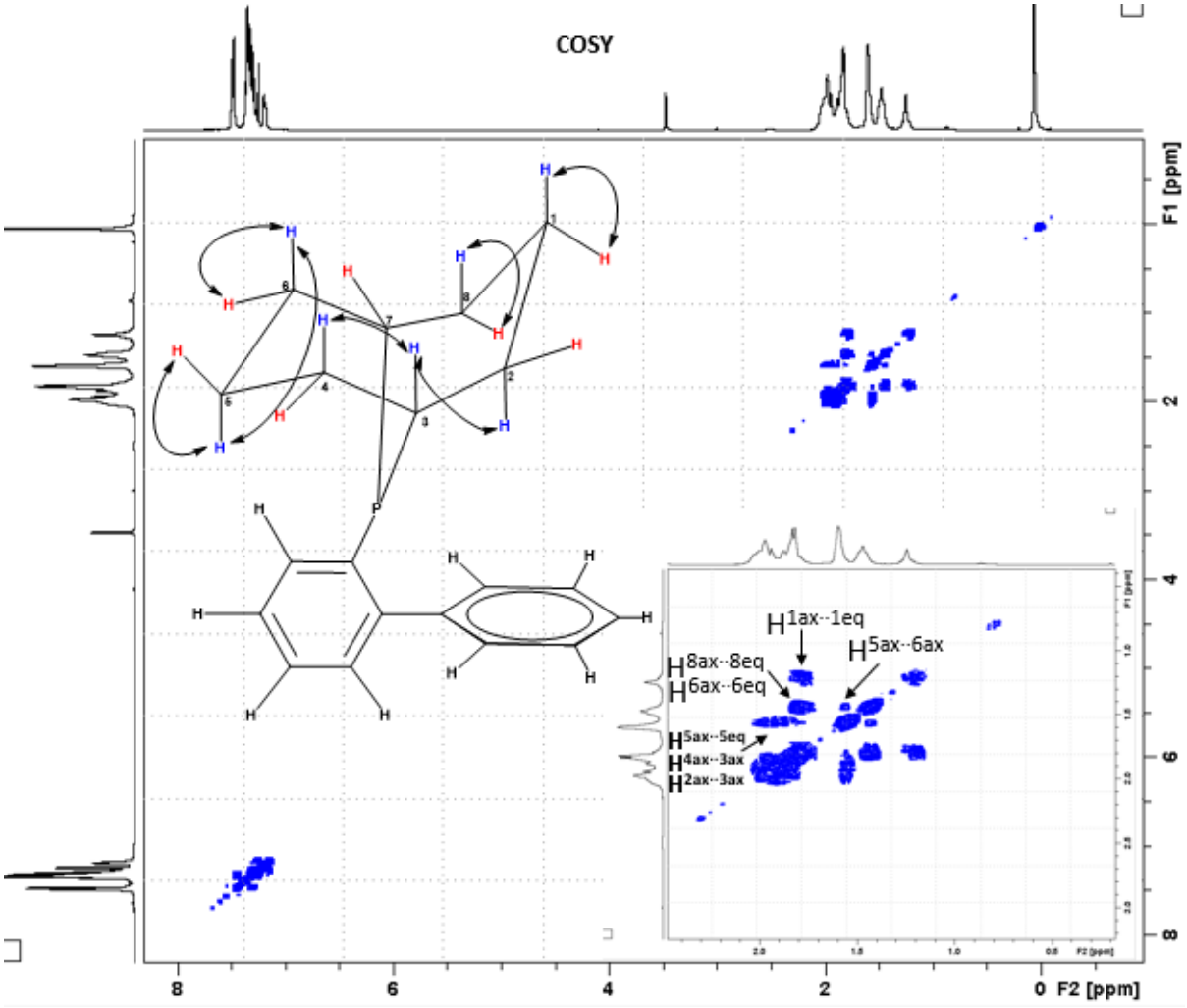


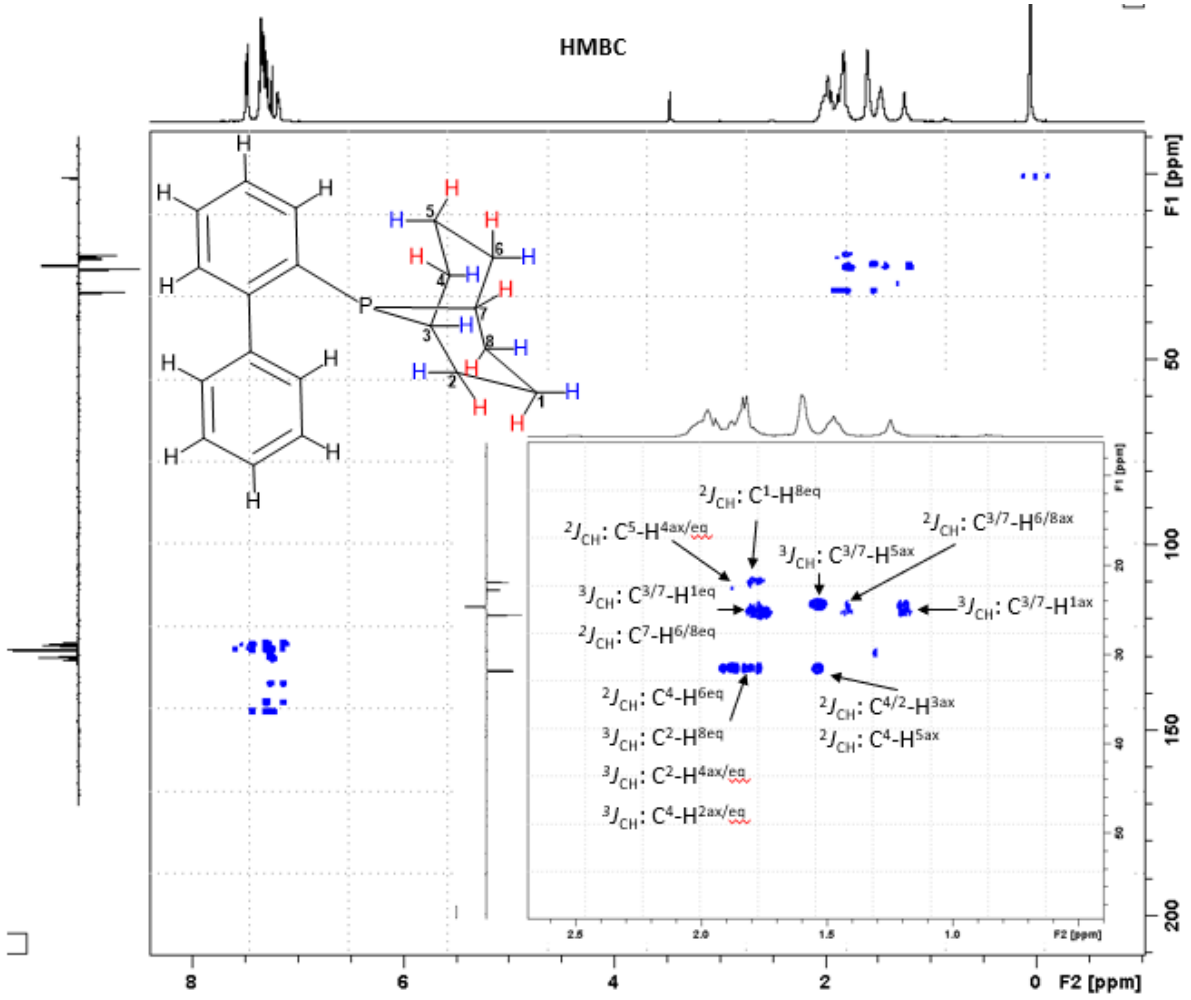

^{1}H NMR
red = equitorial (eq)
blue = axial (ax)
Ar-H
MeOH
f1 (ppm)
^{13}C NMR
$^{1}J_{CP}$ = 10.1 Hz
Ar-C-H
Ar-C$_{quat1}$
Ar-C$_{quat2}$
C$_{quat1}$
C$_{quat2}$
C$_{2+4}$
C$_{3+7}$
C$_{6+8}$
C$_5$
C$_1$

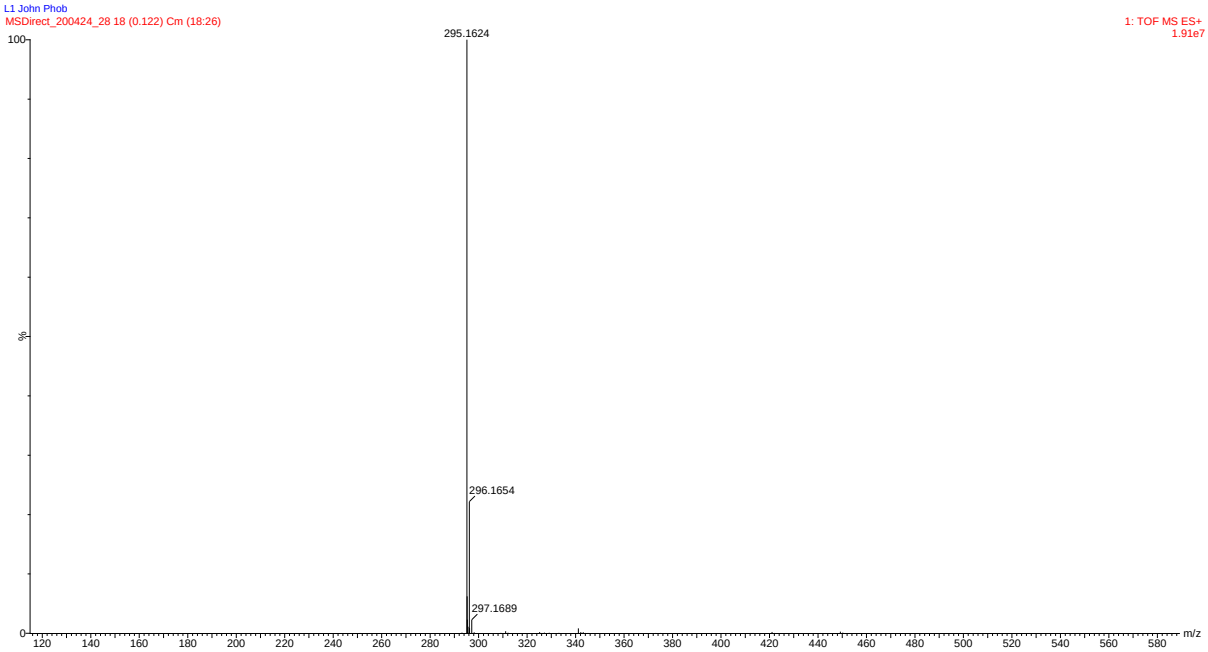

DEPT-135 NMR
131.06
131.00
130.36
128.52
128.50
128.33
127.24
126.78
126.70
31.85
31.73
25.57
25.53
24.67
24.57
22.80
22.76
21.89
Ar-C-H
131
128
f1 (ppm)
Cquat1
Cquat2
Cquat2
P
C3+7
C2+4
C6+8
C5
C1
32
30
28
26
24
22
f1 (ppm)
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


DEPT-ED-HSQC
F1 [ppm]
F2 [ppm]
H1eq
H1ax
H5eq
H5ax
H3ax+7eq
H(6+8) eq
H(6+8)ax
H2ax
H4ax
H2eq
H4eq

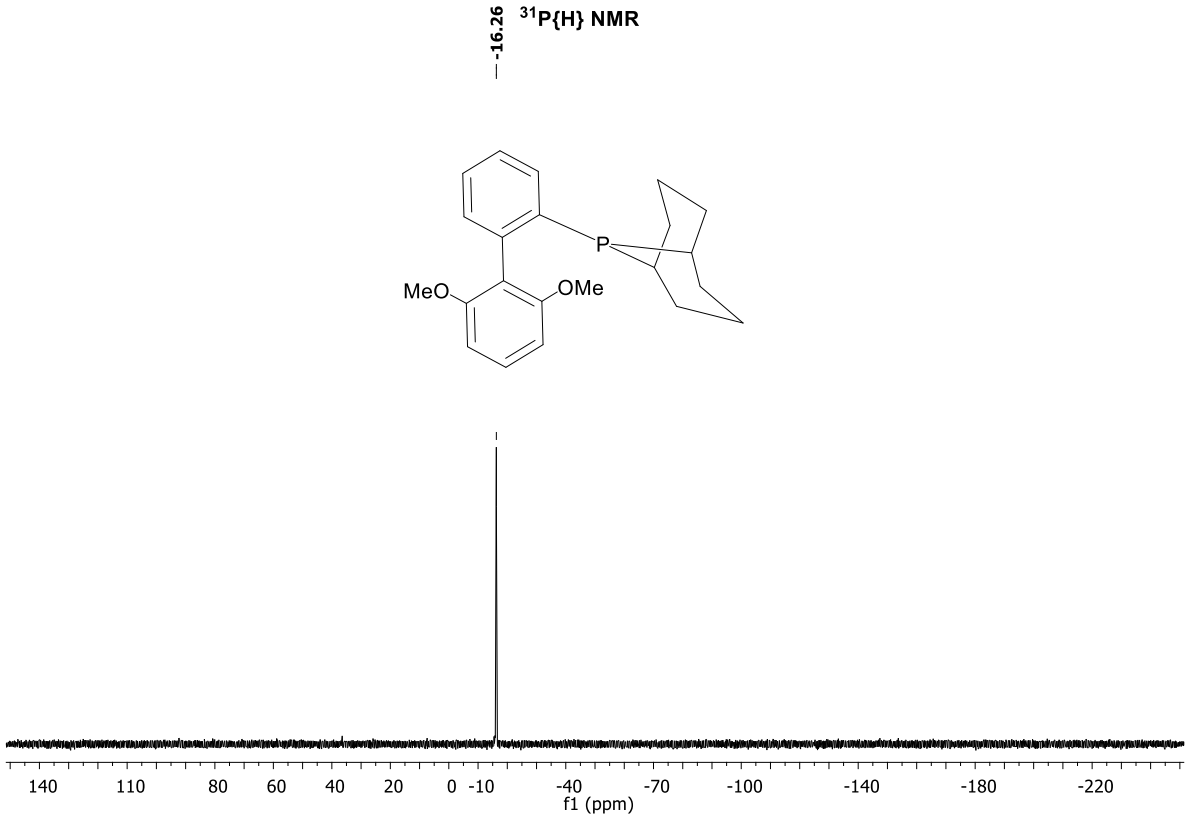

NOESY
Ar-H···H3ax
Ar-H···H4eq
F1 [ppm]
F2 [ppm]
8
6
4
2

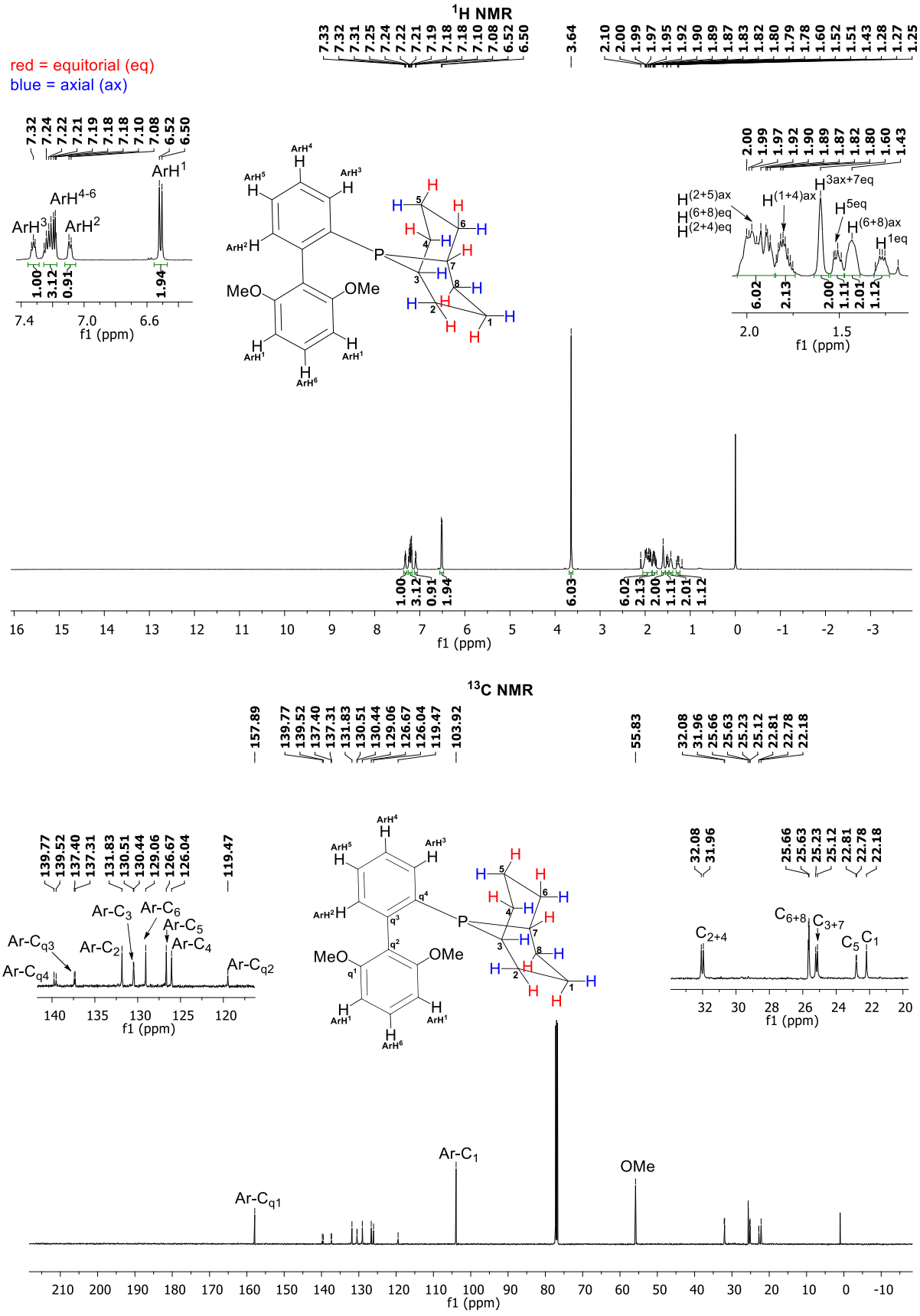

COSY
F1 [ppm]
F2 [ppm]
H1ax--1eq
H5ax--6ax
H8ax--8eq
H6ax--6eq
H5ax--5eq
H4ax--3ax
H2ax--3ax

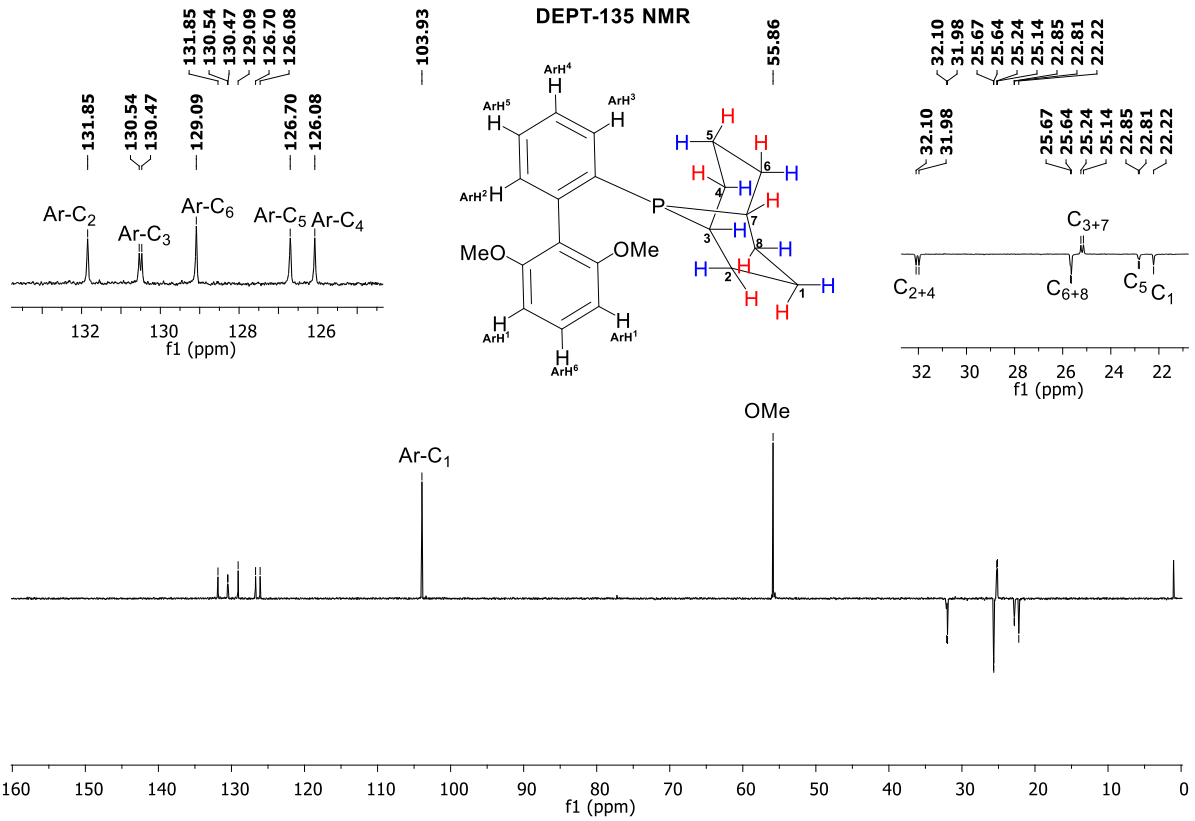

HMBC
F1 [ppm]
F2 [ppm]
$^{2}J_{CH}$: C^{1}-H^{8eq}
$^{2}J_{CH}$: C^{5}-H$^{4ax/eq}$
$^{2}J_{CH}$: C$^{3/7}$-H$^{6/8ax}$
$^{3}J_{CH}$: C$^{3/7}$-H^{5ax}
$^{3}J_{CH}$: C$^{3/7}$-H^{1eq}
$^{3}J_{CH}$: C$^{3/7}$-H^{1ax}
$^{2}J_{CH}$: C^{7}-H$^{6/8eq}$
$^{2}J_{CH}$: C^{4}-H^{6eq}
$^{2}J_{CH}$: C$^{4/2}$-H^{3ax}
$^{3}J_{CH}$: C^{2}-H^{8eq}
$^{2}J_{CH}$: C^{4}-H^{5ax}
$^{3}J_{CH}$: C^{2}-H$^{4ax/eq}$
$^{3}J_{CH}$: C^{4}-H$^{2ax/eq}$

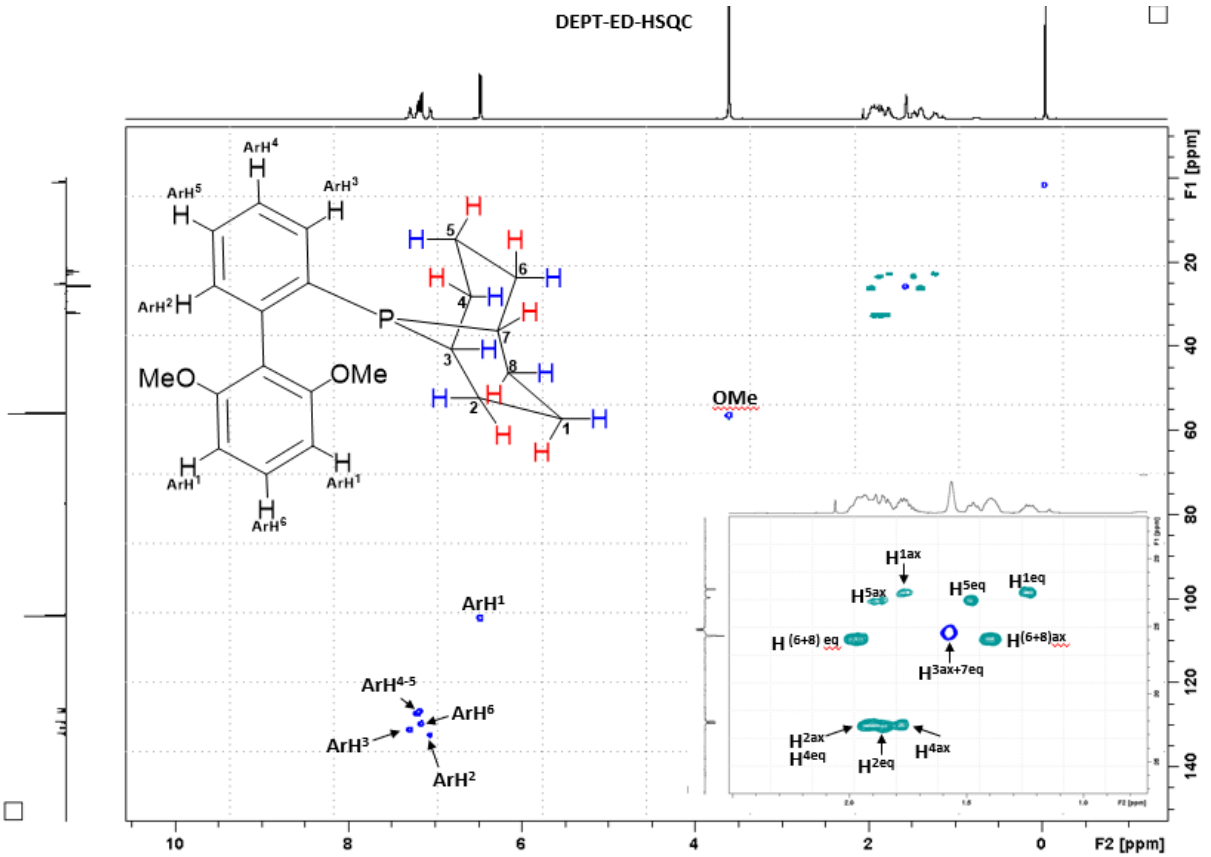

L1 John Phob
MSDirect_200424_28 18 (0.122) Cm (18:26)
1: TOF MS ES+
1.91e7
295.1624
296.1654
297.1689
%
m/z

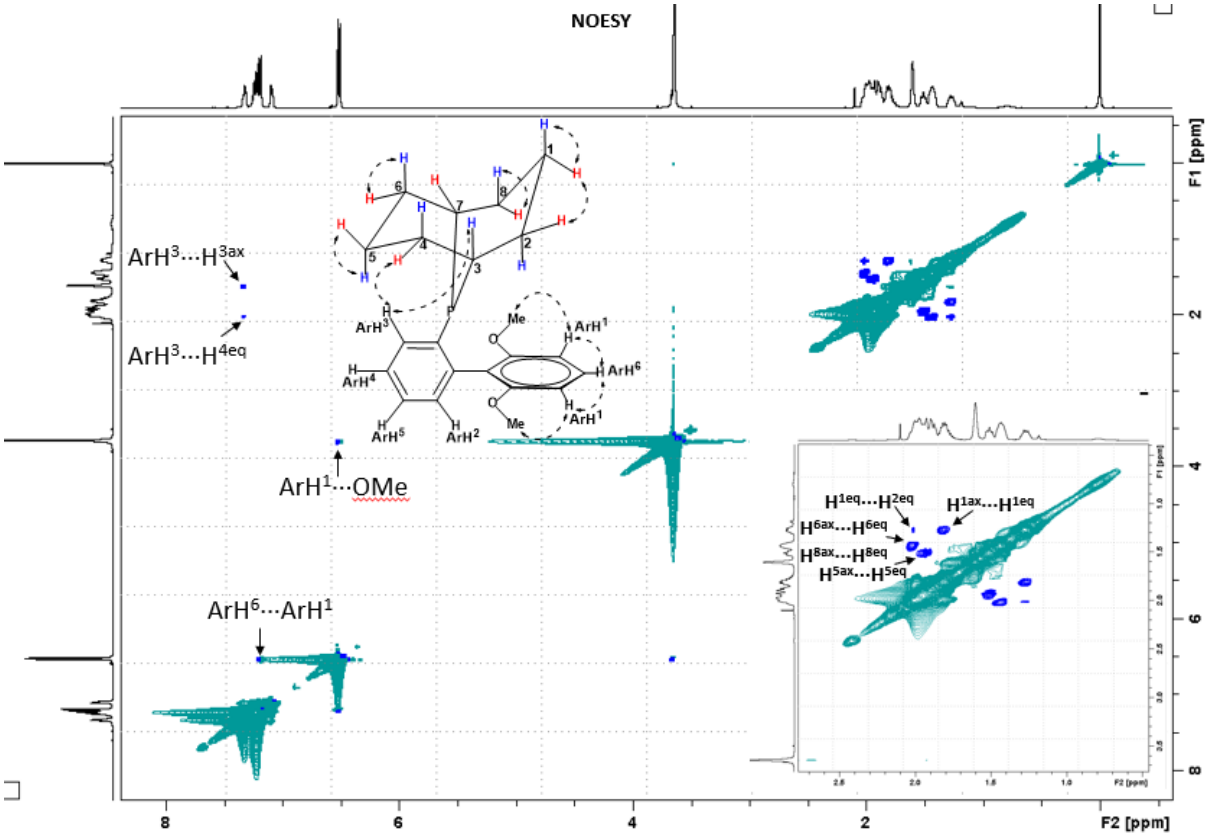
Ligand 2 (NMR experiments carried out in $CDCl_3$)

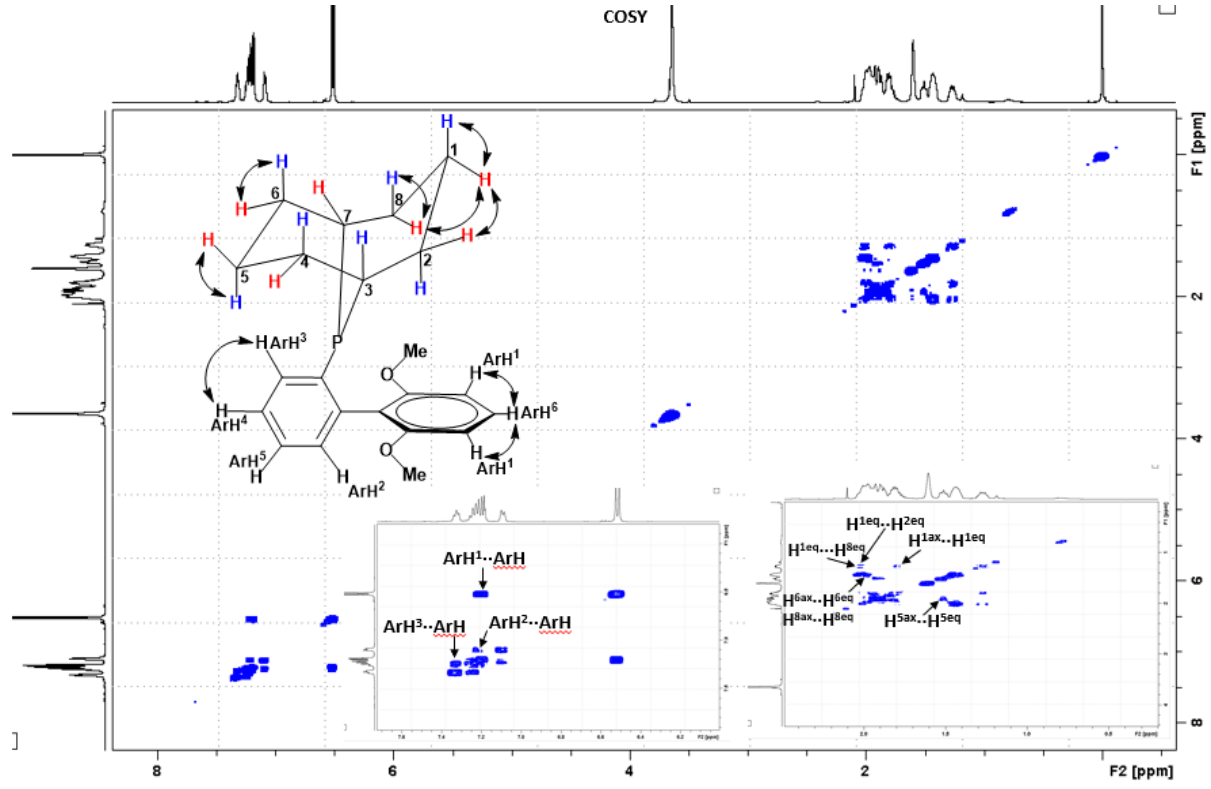


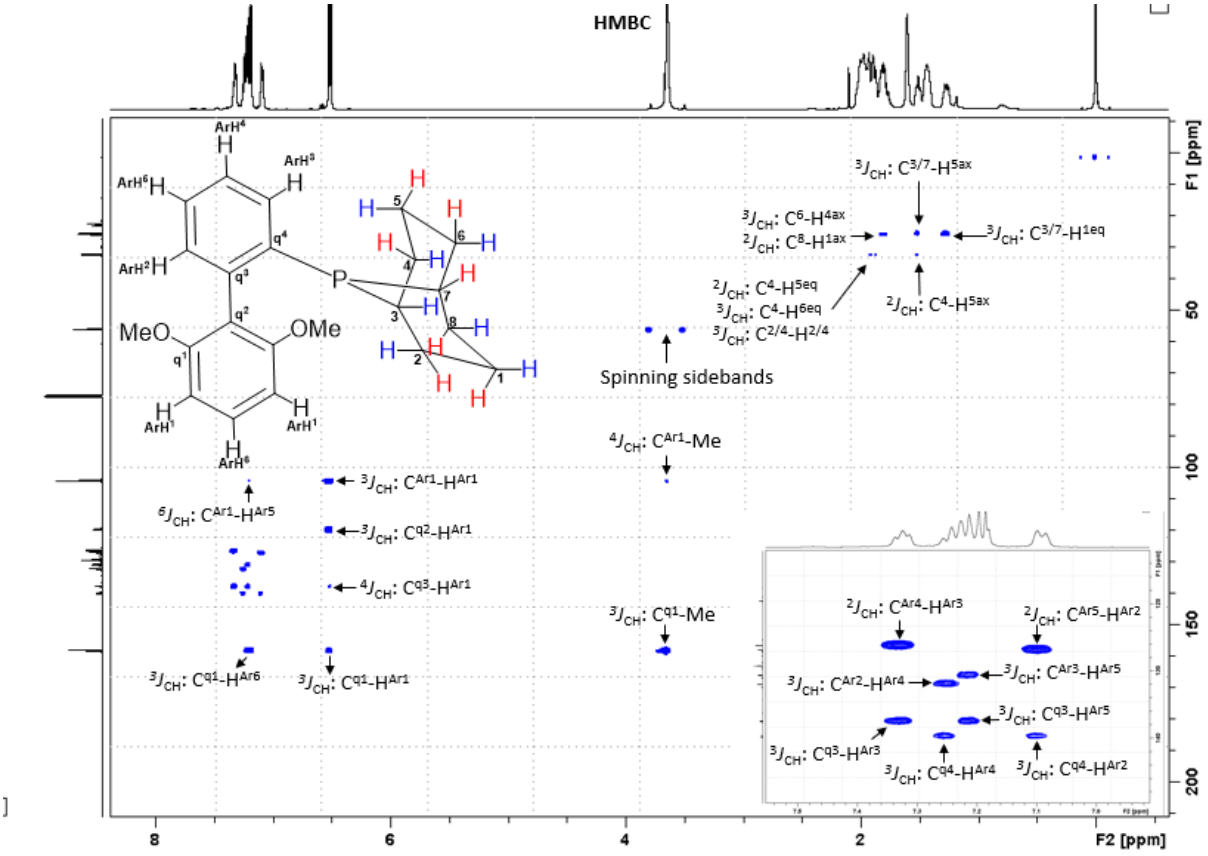

^{1}H NMR
red = equitorial (eq)
blue = axial (ax)
f1 (ppm)
^{13}C NMR
Ar-C$_{q1}$
Ar-C$_1$
OMe
f1 (ppm)

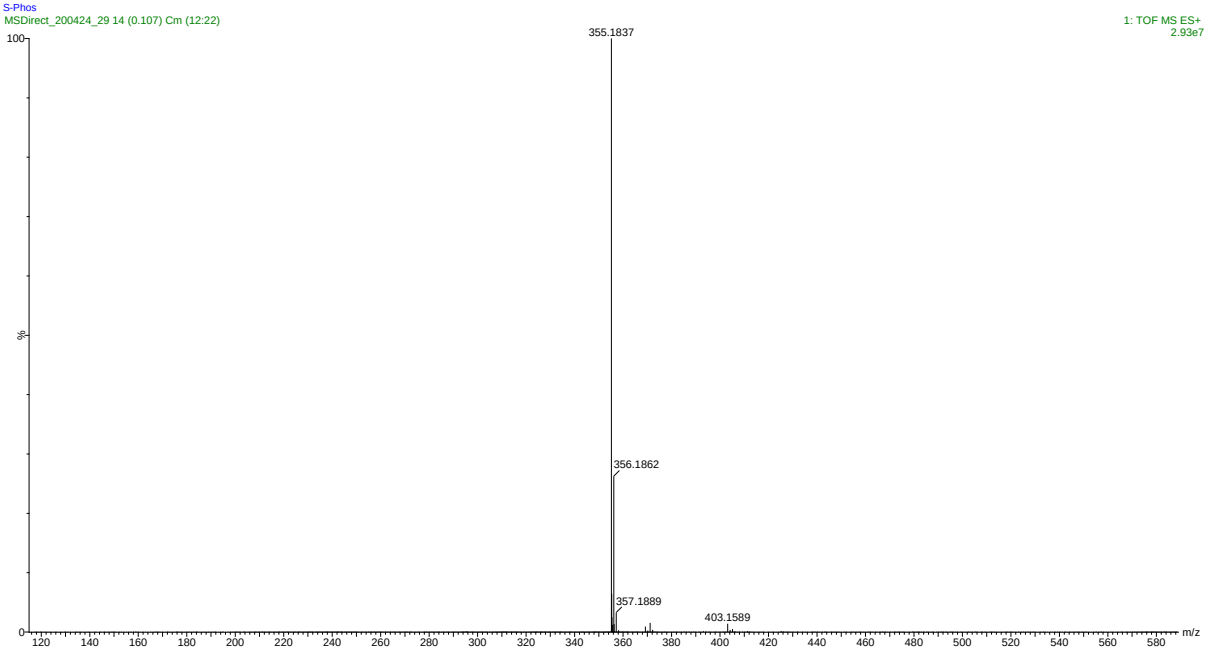

DEPT-135 NMR
131.85
130.54
130.47
129.09
126.70
126.08
103.93
55.86
32.10
31.98
25.67
25.64
25.24
25.14
22.85
22.81
22.22
Ar-C2
Ar-C3
Ar-C6
Ar-C5
Ar-C4
MeO
OMe
C3+7
C2+4
C6+8
C5
C1
Ar-C1
OMe
f1 (ppm)


DEPT-ED-HSQC
MeO
OMe
ArH1
ArH4-5
ArH6
ArH3
ArH2
H1ax
H5ax
H5eq
H1eq
H (6+8) eq
H(6+8)ax
H3ax+7eq
H2ax
H4eq
H2eq
H4ax
F1 [ppm]
F2 [ppm]

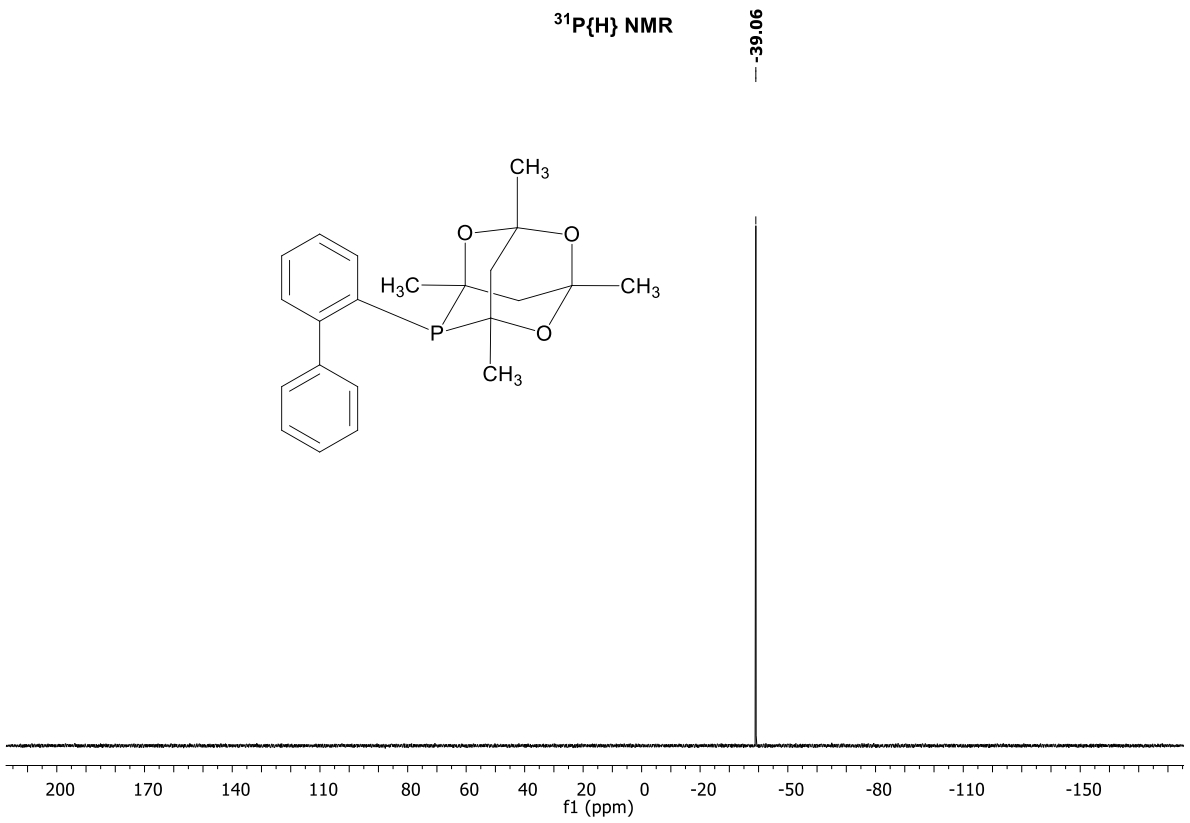

NOESY
ArH3···H3ax
ArH3···H4eq
ArH1···OMe
ArH6···ArH1
H1eq···H2eq
H1ax···H1eq
H6ax···H6eq
H8ax···H8eq
H5ax···H5eq
F1 [ppm]
F2 [ppm]

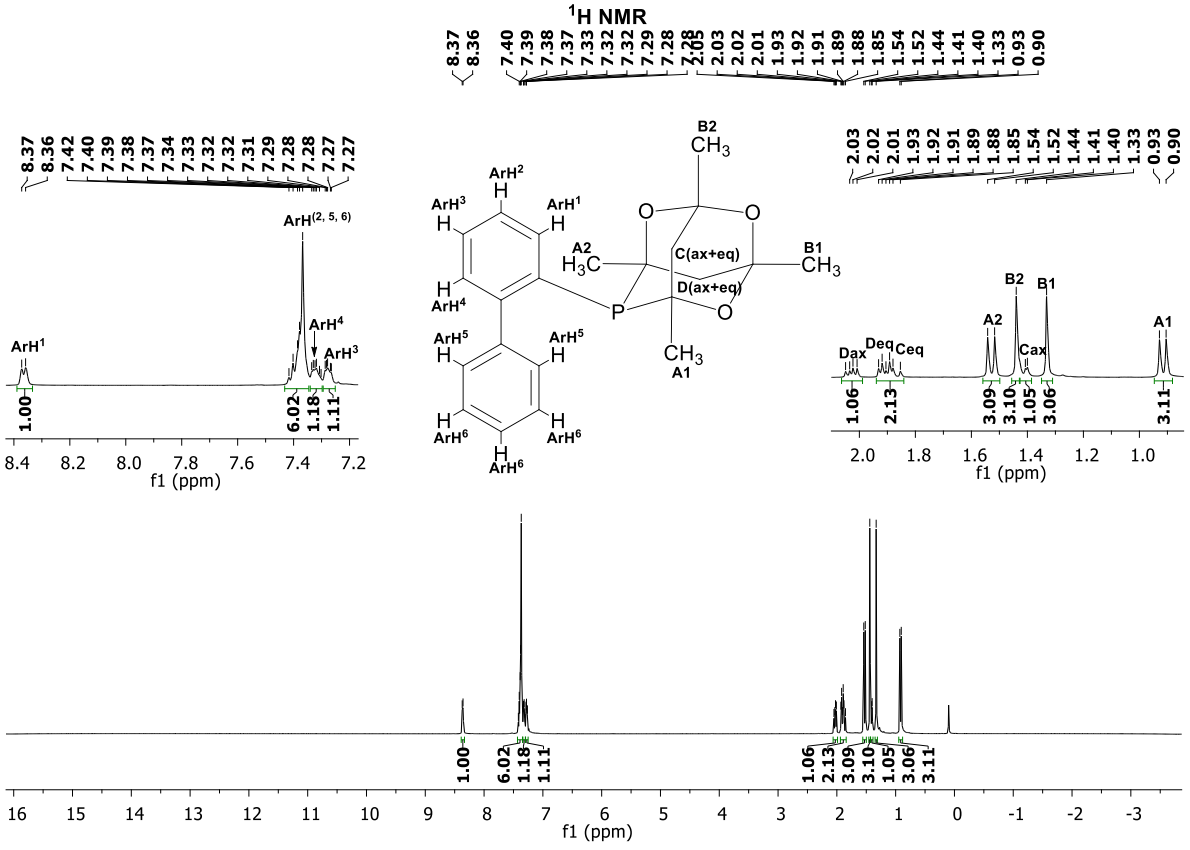

COSY
ArH1··ArH
ArH3··ArH
ArH2··ArH
H1eq··H2eq
H1ax··H1eq
H1eq···H8eq
H6ax··H6eq
H8ax··H8eq
H5ax··H5eq
F1 [ppm]
F2 [ppm]

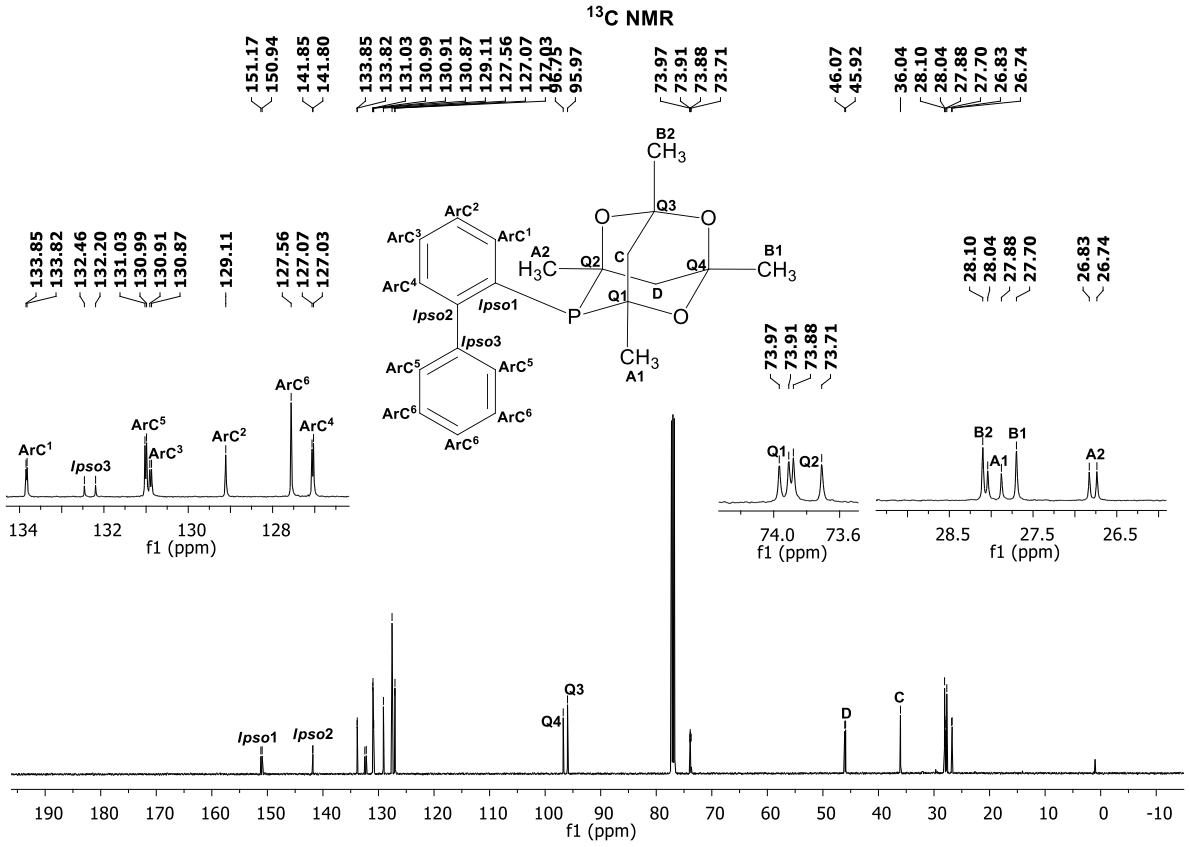


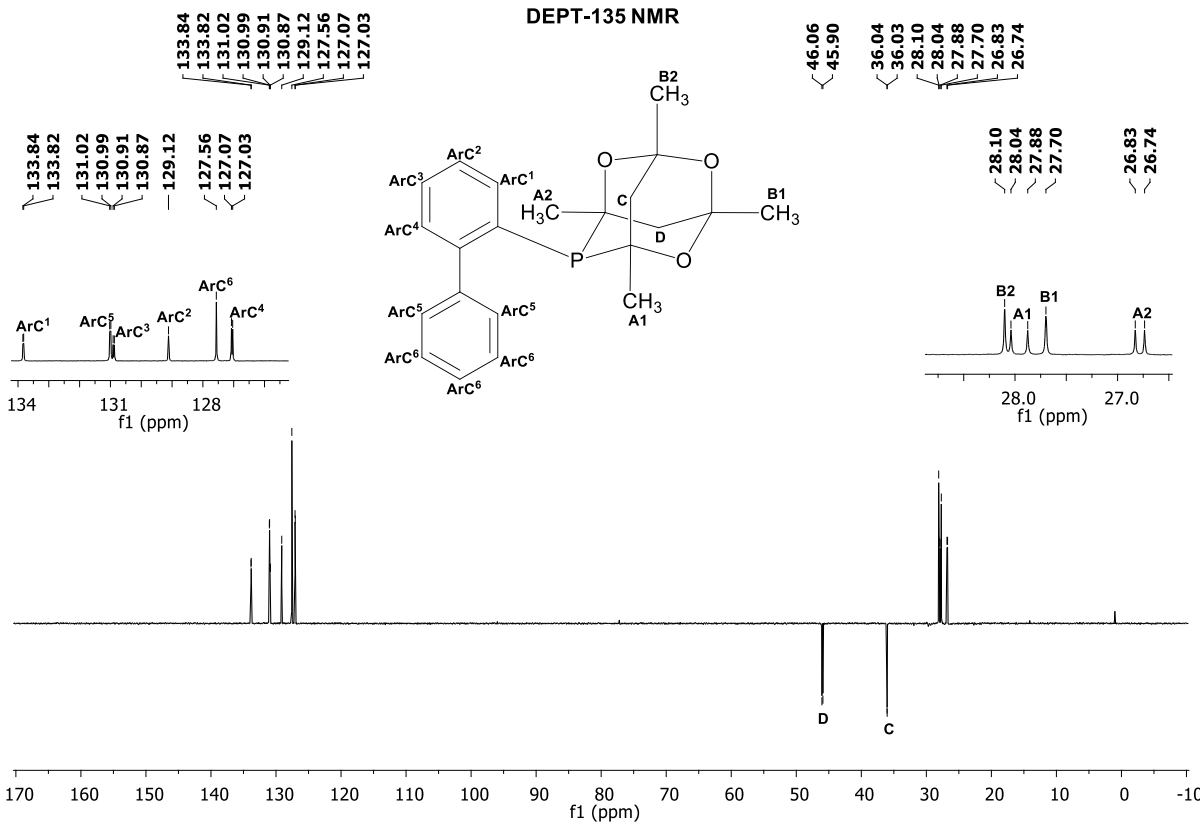


Ligand 3 (NMR experiments carried out in $CDCl_3$)


31P{H} NMR
-39.06
CH3
O
O
H3C
CH3
P
O
CH3
200
170
140
110
80
60
40
20
0
-20
-50
-80
-110
-150
f1 (ppm)


1H NMR
8.37
8.36
7.40
7.39
7.38
7.37
7.33
7.32
7.32
7.29
7.28
2.03
2.02
2.01
1.93
1.92
1.91
1.89
1.88
1.85
1.54
1.52
1.44
1.41
1.40
1.33
0.93
0.90
ArH(2, 5, 6)
ArH1
ArH4
ArH3
1.00
6.02
1.18
1.11
8.4
8.2
8.0
7.8
7.6
7.4
7.2
f1 (ppm)
B2
CH3
ArH2
ArH3
ArH1
O
O
A2
H3C
C(ax+eq)
B1
CH3
D(ax+eq)
P
O
ArH4
CH3
A1
ArH5
ArH5
ArH6
ArH6
ArH6
Dax
Deq
Ceq
A2
B2
B1
Cax
A1
1.06
2.13
3.09
3.10
1.05
3.06
3.11
2.0
1.8
1.6
1.4
1.2
1.0
f1 (ppm)
1.00
6.02
1.18
1.11
1.06
2.13
3.09
3.10
1.05
3.06
3.11
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
f1 (ppm)


13C NMR
151.17
150.94
141.85
141.80
133.85
133.82
131.03
130.99
130.91
130.87
129.11
127.56
127.07
127.03
95.97
73.97
73.91
73.88
73.71
46.07
45.92
36.04
28.10
28.04
27.88
27.70
26.83
26.74
B2
CH3
Q3
O
O
ArC2
ArC3
ArC1
A2
H3C
Q2
C
Q4
B1
CH3
ArC4
Ipso1
Q1
D
P
O
Ipso2
Ipso3
CH3
A1
ArC5
ArC5
ArC6
ArC6
ArC6
ArC1
Ipso3
ArC5
ArC3
ArC2
ArC6
ArC4
134
132
130
128
f1 (ppm)
Q1
Q2
74.0
73.6
f1 (ppm)
B2
B1
A1
A2
28.5
27.5
26.5
f1 (ppm)
Ipso1
Ipso2
Q4
Q3
D
C
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


DEPT-135 NMR
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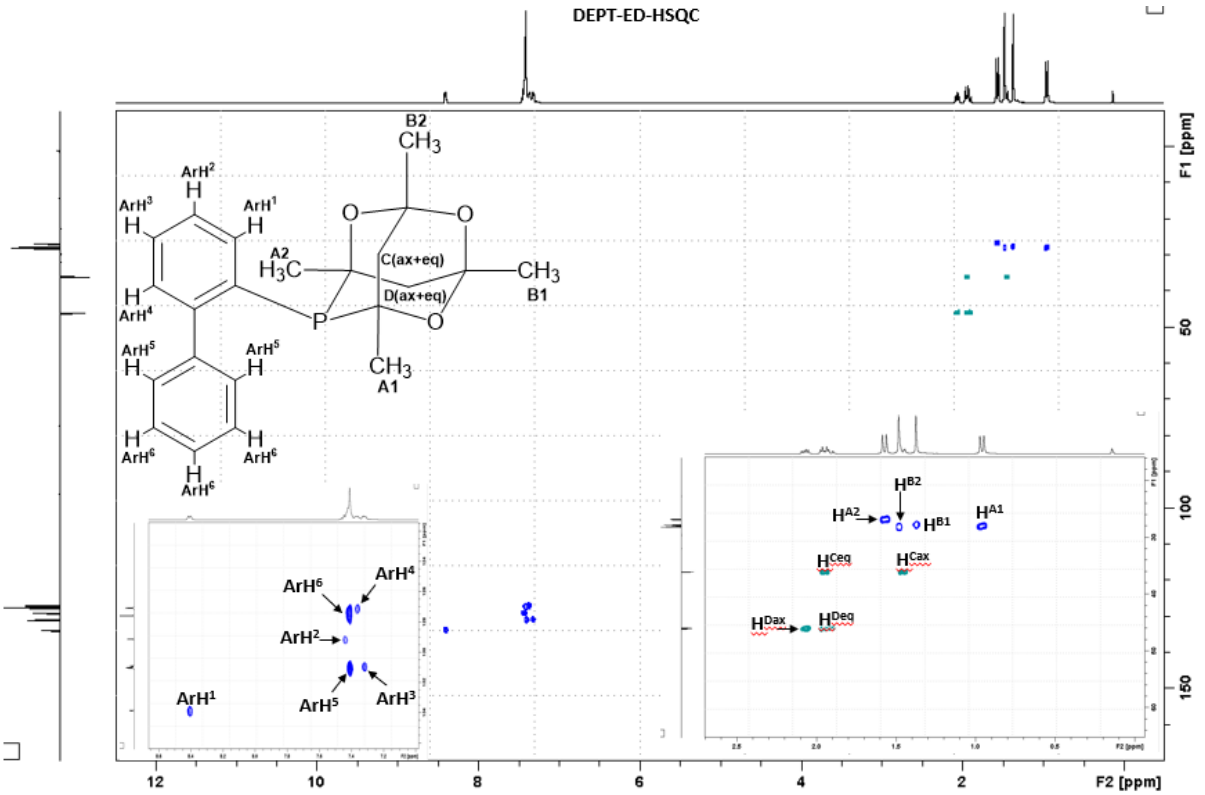
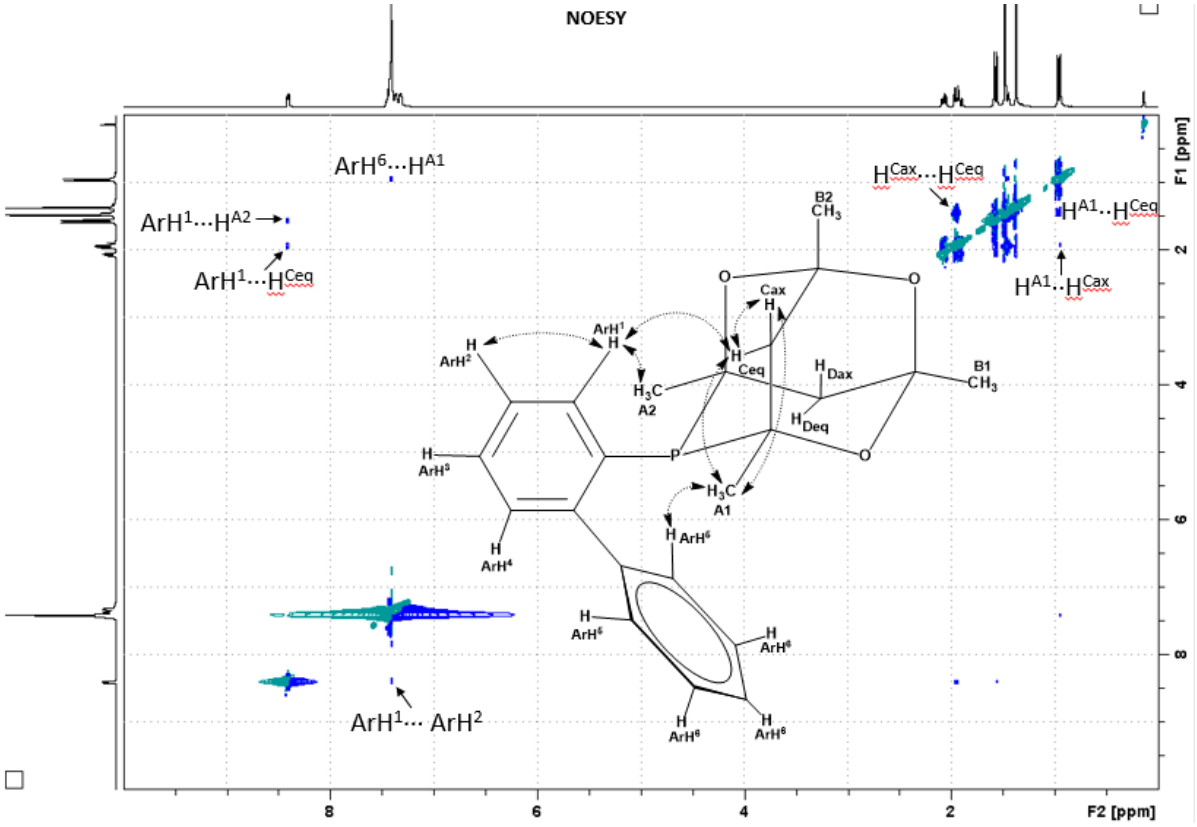
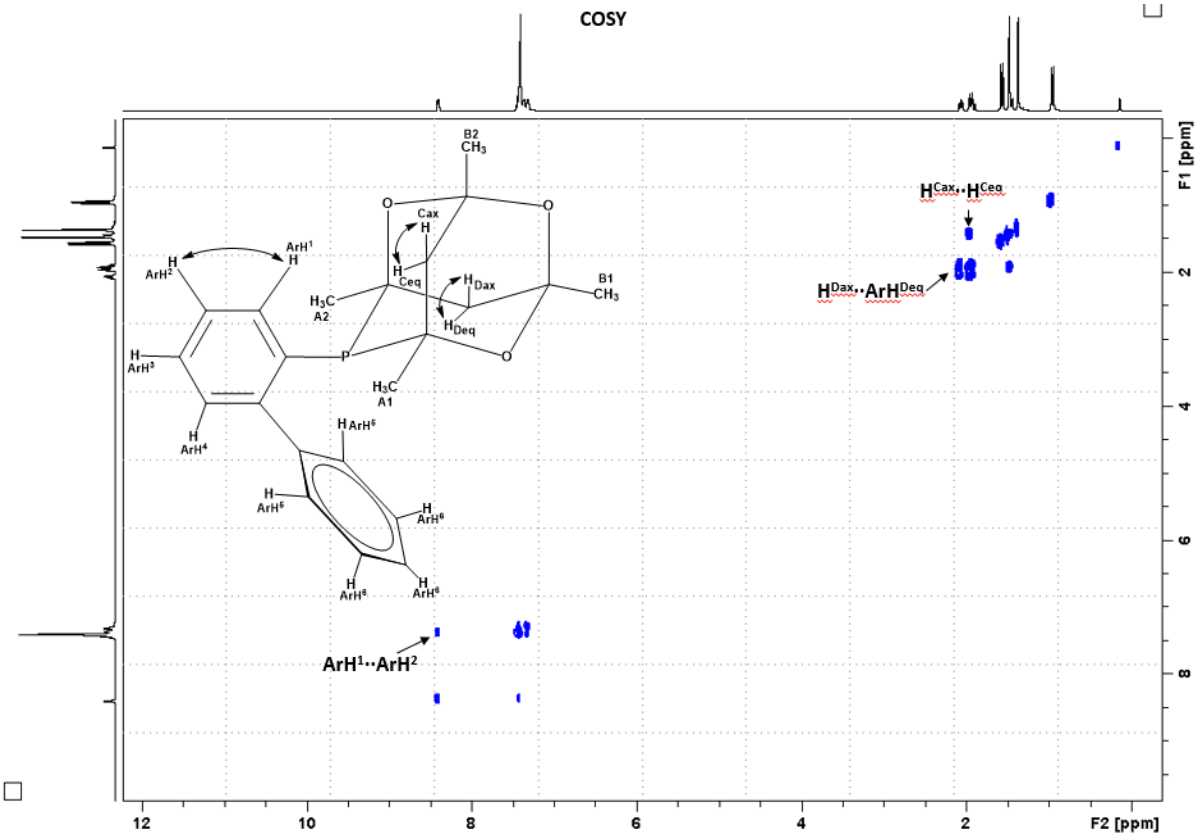
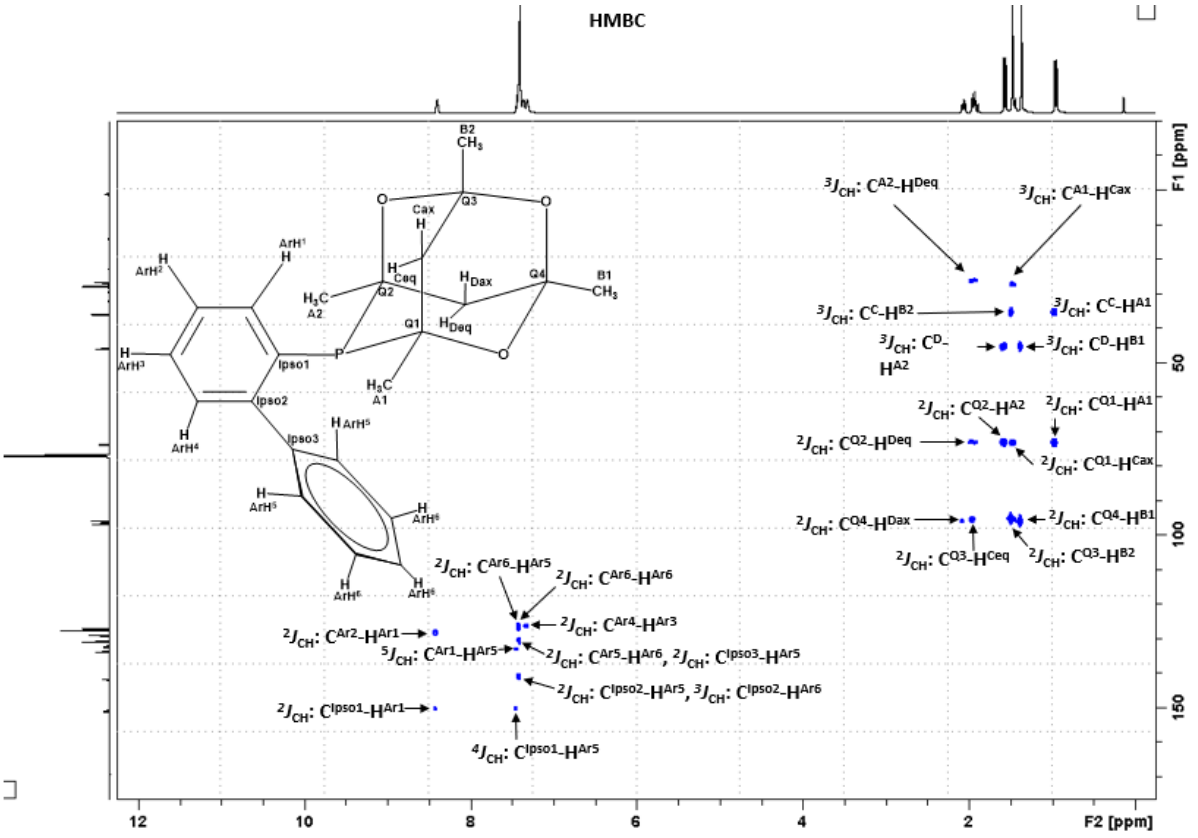
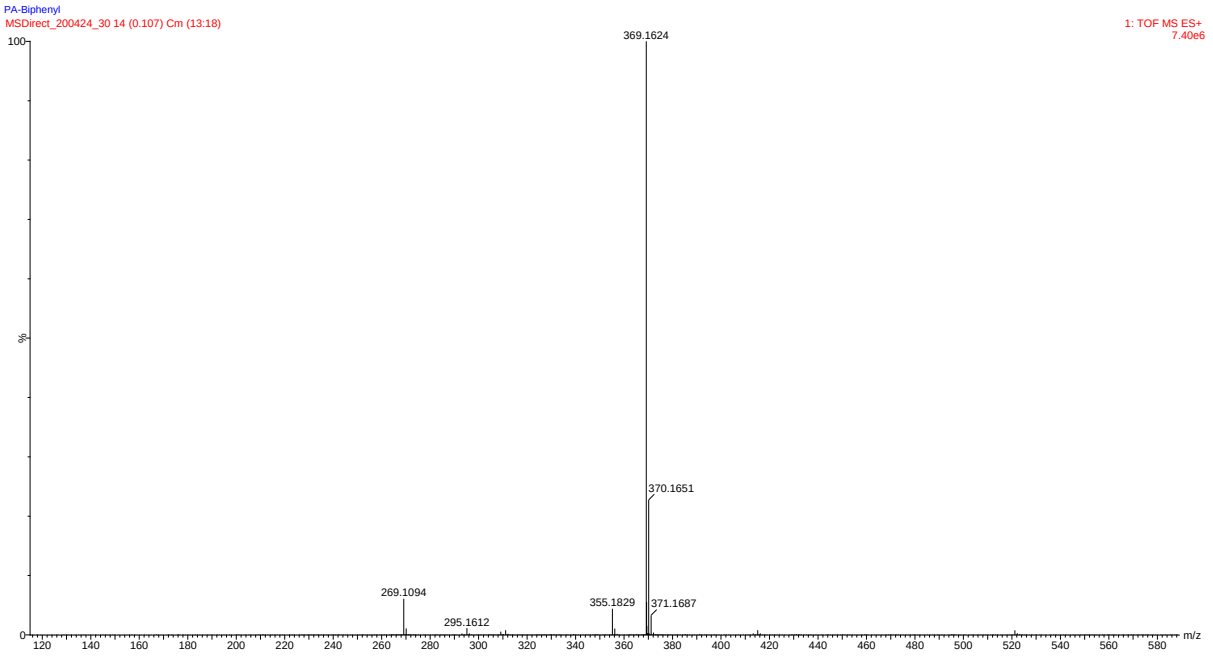
133.82
131.02
130.99
130.91
130.87
129.12
127.56
127.07
127.03
46.06
45.90
36.04
36.03
28.10
28.04
27.88
27.70
26.83
26.74
B2
CH3
ArC2
ArC1
ArC3
ArC4
A2
H3C
C
B1
CH3
D
P
O
CH3
A1
ArC5
ArC6
ArC1
ArC5
ArC3
ArC2
ArC6
ArC4
134
131
128
f1 (ppm)
B2
A1
B1
A2
28.0
27.0
f1 (ppm)
D
C
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


DEPT-ED-HSQC
B2
CH3
ArH2
ArH3
ArH1
A2
H3C
C(ax+eq)
CH3
B1
D(ax+eq)
P
O
CH3
A1
ArH4
ArH5
ArH5
ArH6
ArH6
ArH6
ArH6
ArH4
ArH2
ArH1
ArH5
ArH3
HB2
HA2
HB1
HA1
HCeq
HCax
HDax
HDeq
F1 [ppm]
50
100
150
12
10
8
6
4
2
F2 [ppm]

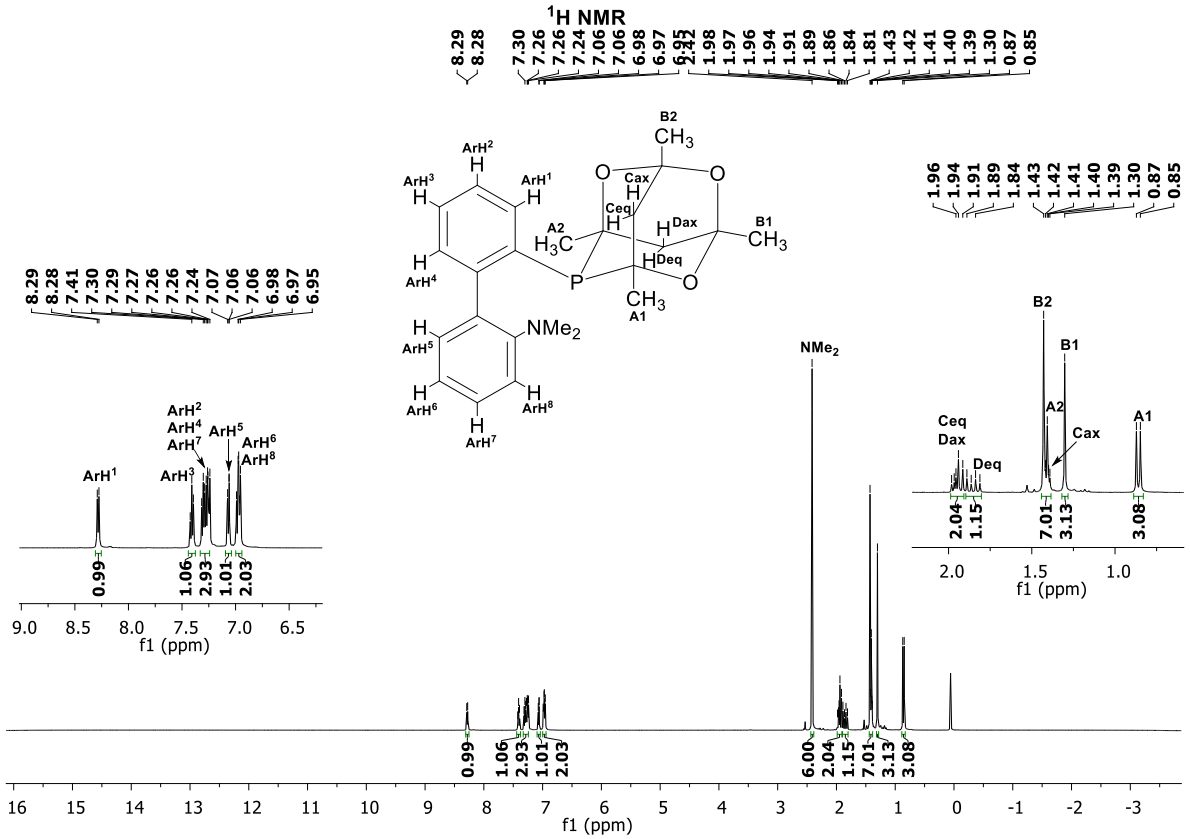

NOESY
ArH6···HA1
ArH1···HA2
ArH1···HCeq
HCax···HCeq
HA1··HCeq
HA1··HCax
ArH1··· ArH2
F1 [ppm]
F2 [ppm]

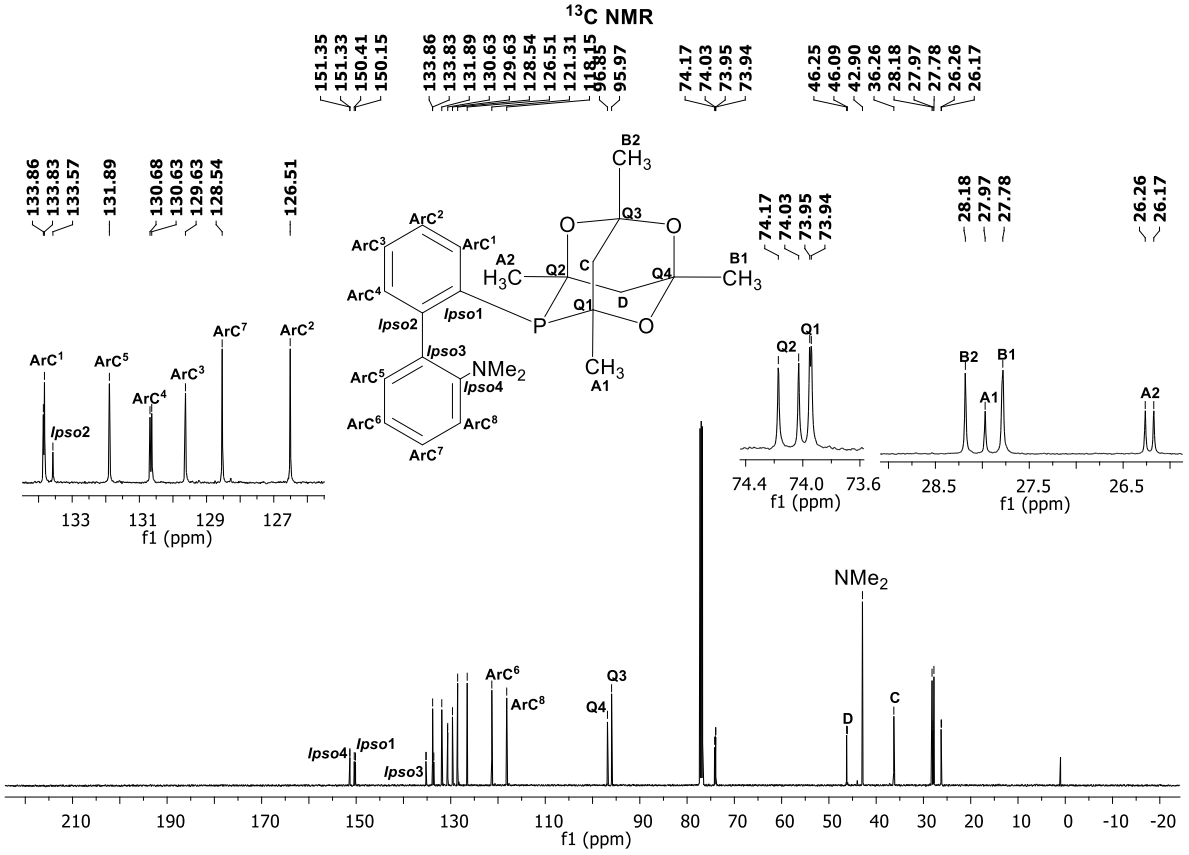

COSY
HCax··HCeq
HDax··ArHDeq
ArH1··ArH2
F1 [ppm]
F2 [ppm]

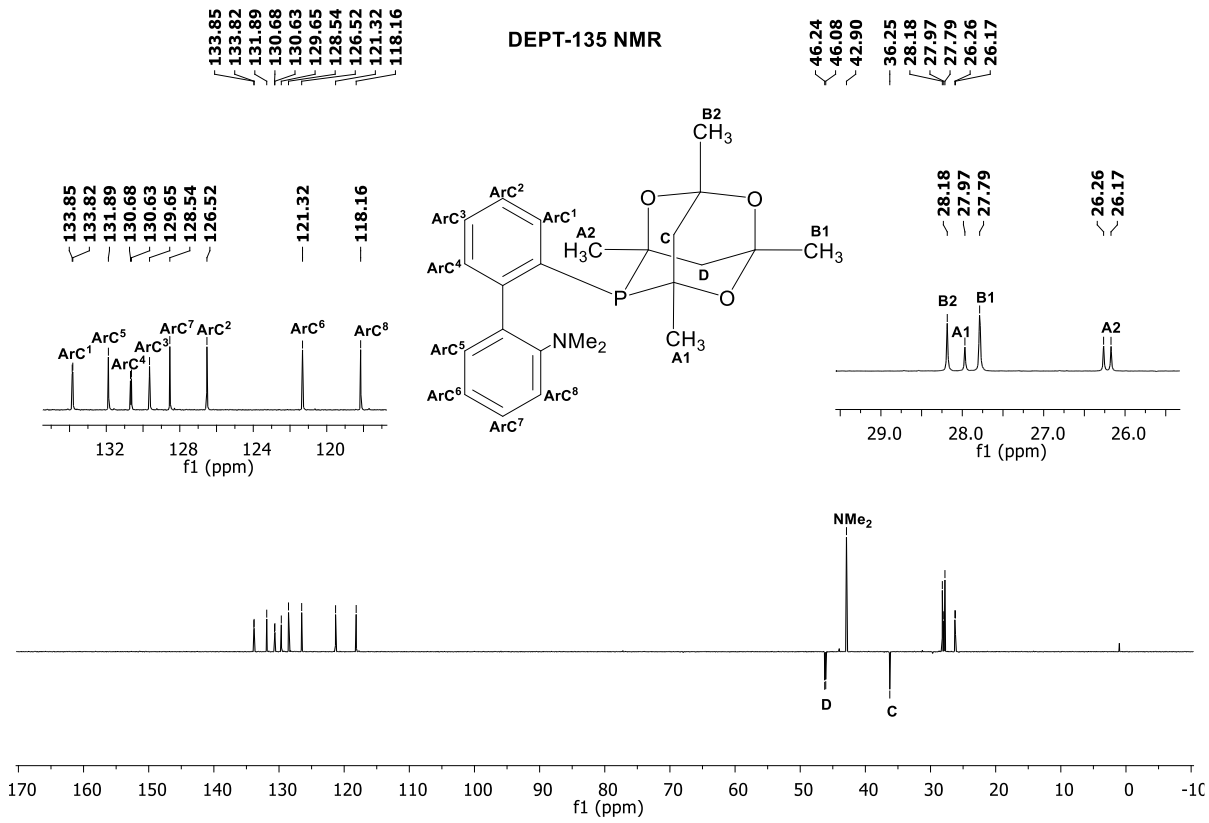


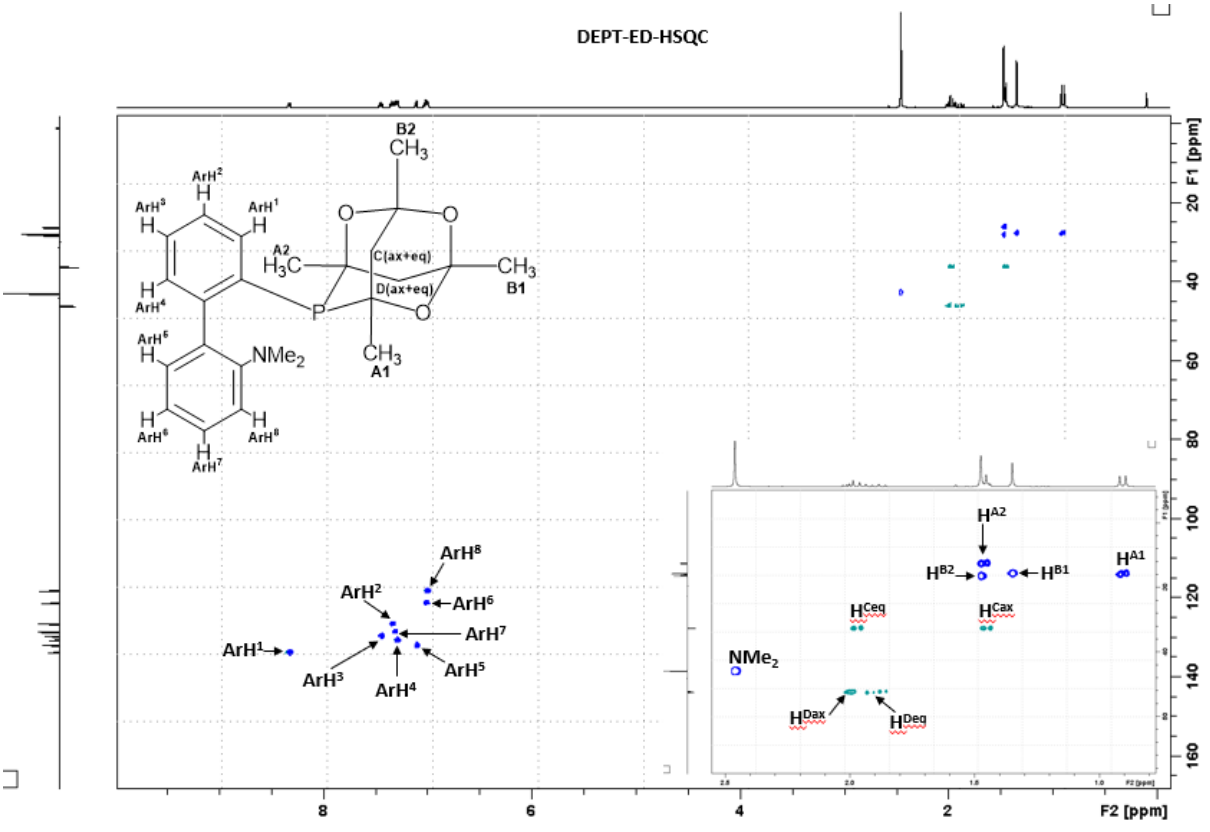


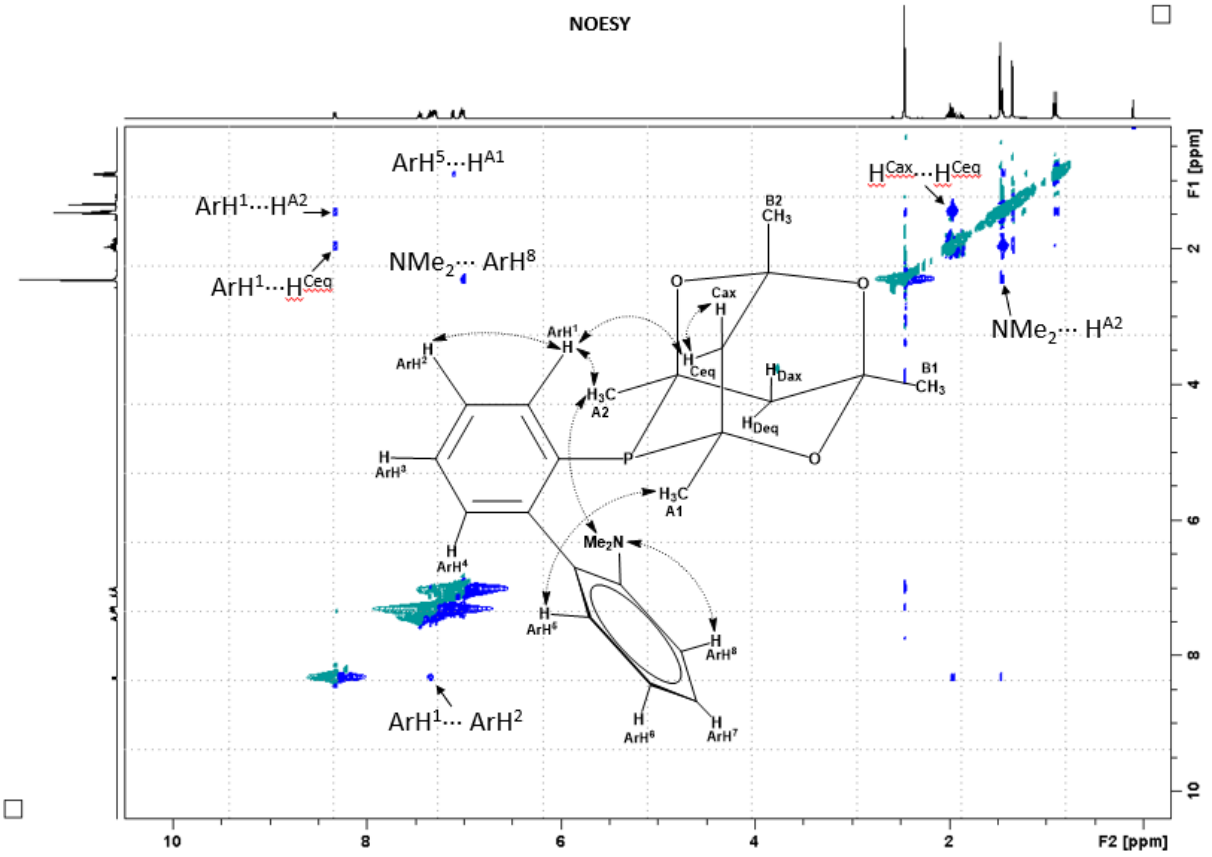
Ligand 4 (NMR experiments carried out in $CDCl_3$)

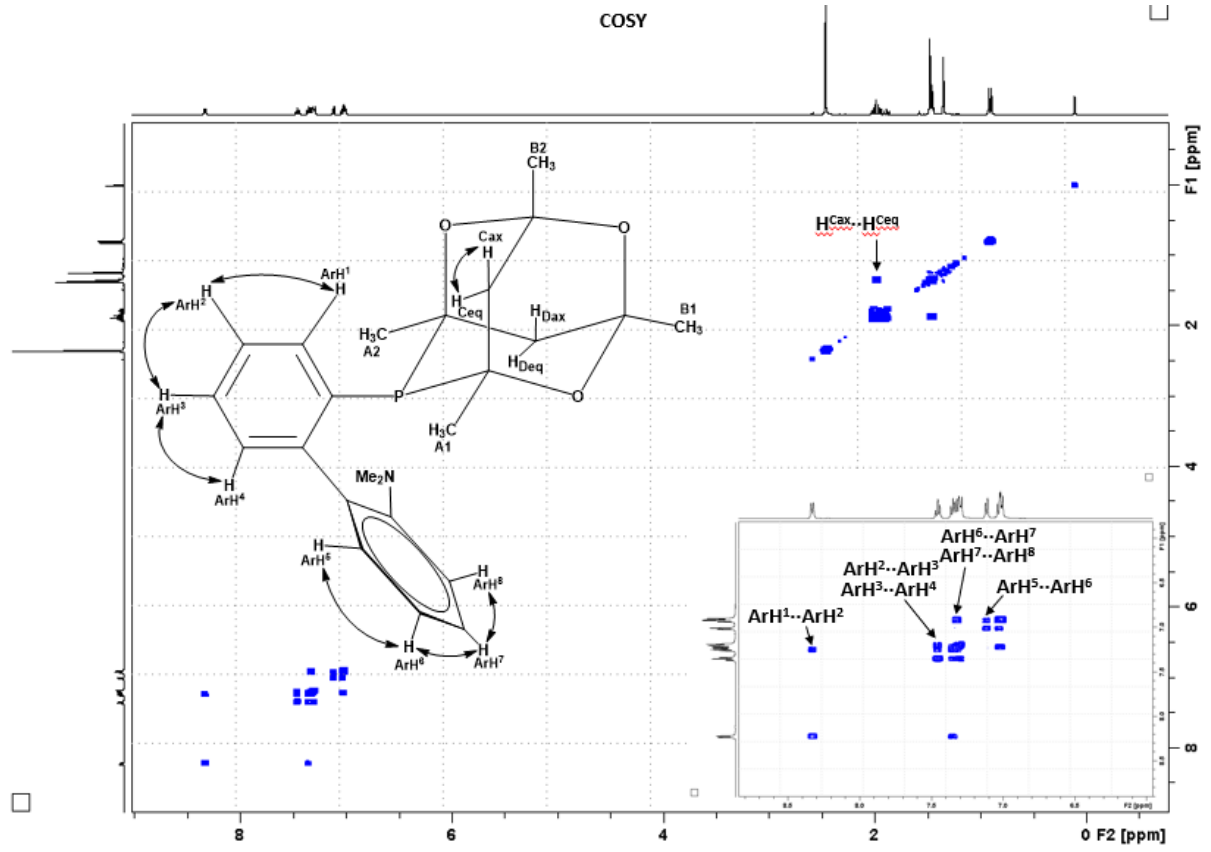

1H NMR
8.29 8.28 7.30 7.26 7.26 7.24 7.06 7.06 6.98 6.97 6.95 2.42 1.98 1.97 1.96 1.94 1.91 1.89 1.86 1.84 1.81 1.43 1.42 1.41 1.40 1.39 1.30 0.87 0.85
B2
CH3
ArH2
ArH3
ArH1
Cax
Ceq
A2
H3C
HDax
B1
CH3
HDeq
P
O
CH3
A1
ArH4
ArH5
NMe2
ArH6
ArH8
ArH7
NMe2
ArH1
ArH2 ArH4 ArH7
ArH3
ArH5
ArH6 ArH8
0.99 1.06 2.93 1.01 2.03
9.0 8.5 8.0 7.5 7.0 6.5
f1 (ppm)
B2
B1
A2
A1
Ceq Dax
Deq
Cax
2.04 1.15 7.01 3.13 3.08
2.0 1.5 1.0
f1 (ppm)
0.99 1.06 2.93 1.01 2.03 6.00 2.04 1.15 7.01 3.13 3.08
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)

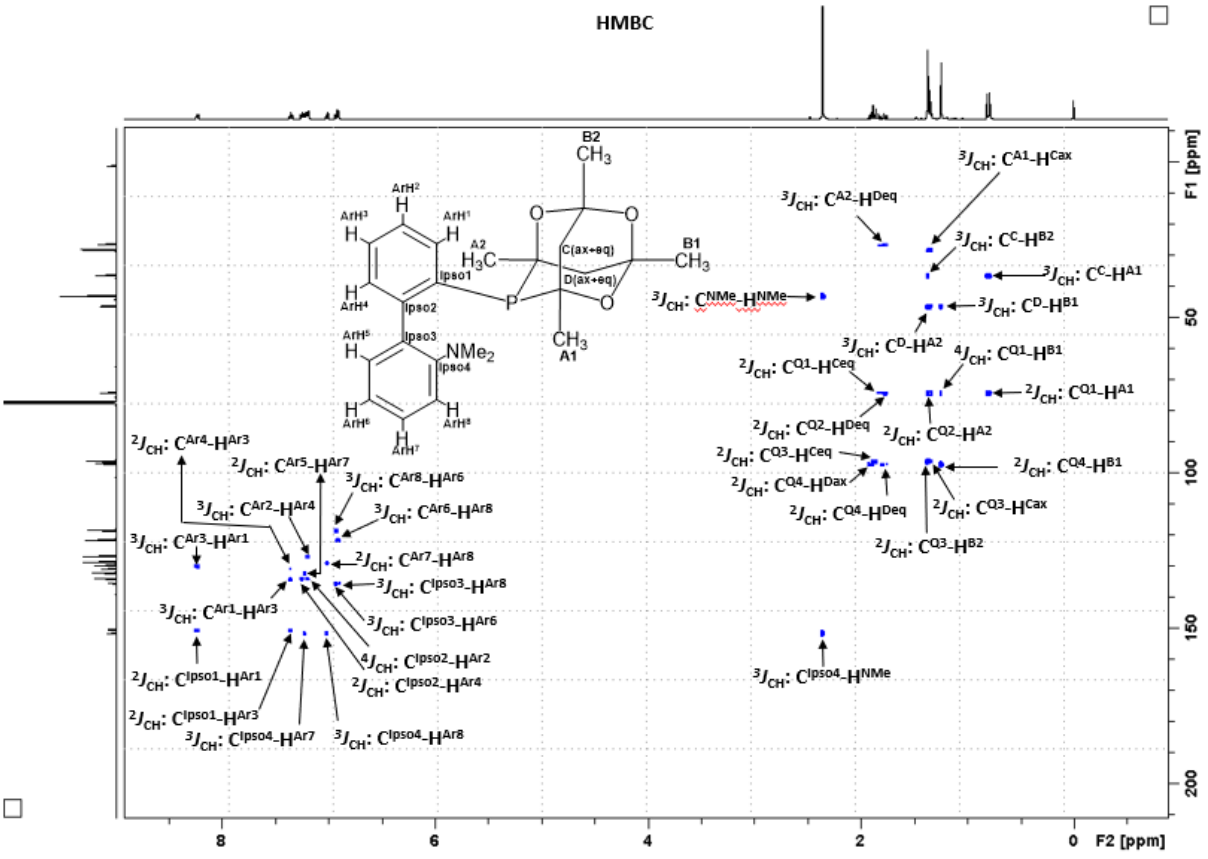

13C NMR
151.35 151.33 150.41 150.15
133.86 133.83 131.89 130.63 129.63 128.54 126.51 121.31 118.15
96.85 95.97
74.17 74.03 73.95 73.94
46.25 46.09 42.90
36.26 28.18 27.97 27.78 26.26 26.17
133.86 133.83 133.57 131.89 130.68 130.63 129.63 128.54 126.51
74.17 74.03 73.95 73.94
28.18 27.97 27.78
26.26 26.17
ArC1 ArC5 ArC4 ArC3 ArC7 ArC2 Ipso2
133 131 129 127 f1 (ppm)
Q2 Q1
74.4 74.0 73.6 f1 (ppm)
B2 A1 B1 A2
28.5 27.5 26.5 f1 (ppm)
B2 CH3 Q3 O O C Q4 B1 CH3
A2 H3C Q2 Q1 D P O CH3 A1
ArC2 ArC3 ArC1 ArC4 Ipso2 Ipso1 Ipso3 NMe2 Ipso4 ArC5 ArC6 ArC8 ArC7
NMe2 ArC6 Q3 ArC8 Q4 D C Ipso4 Ipso1 Ipso3
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)

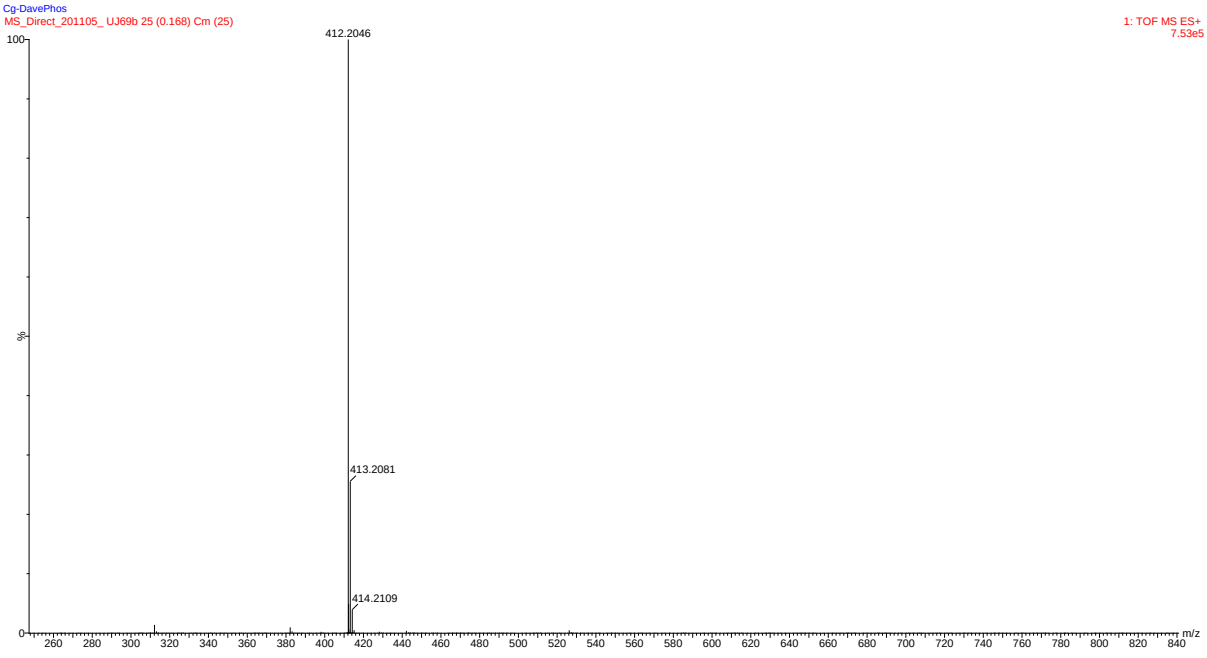

DEPT-135 NMR
133.85
133.82
131.89
130.68
130.63
129.65
128.54
126.52
121.32
118.16
46.24
46.08
42.90
36.25
28.18
27.97
27.79
26.26
26.17
f1 (ppm)
NMe2
D
C


DEPT-ED-HSQC
F1 [ppm]
F2 [ppm]
NMe2

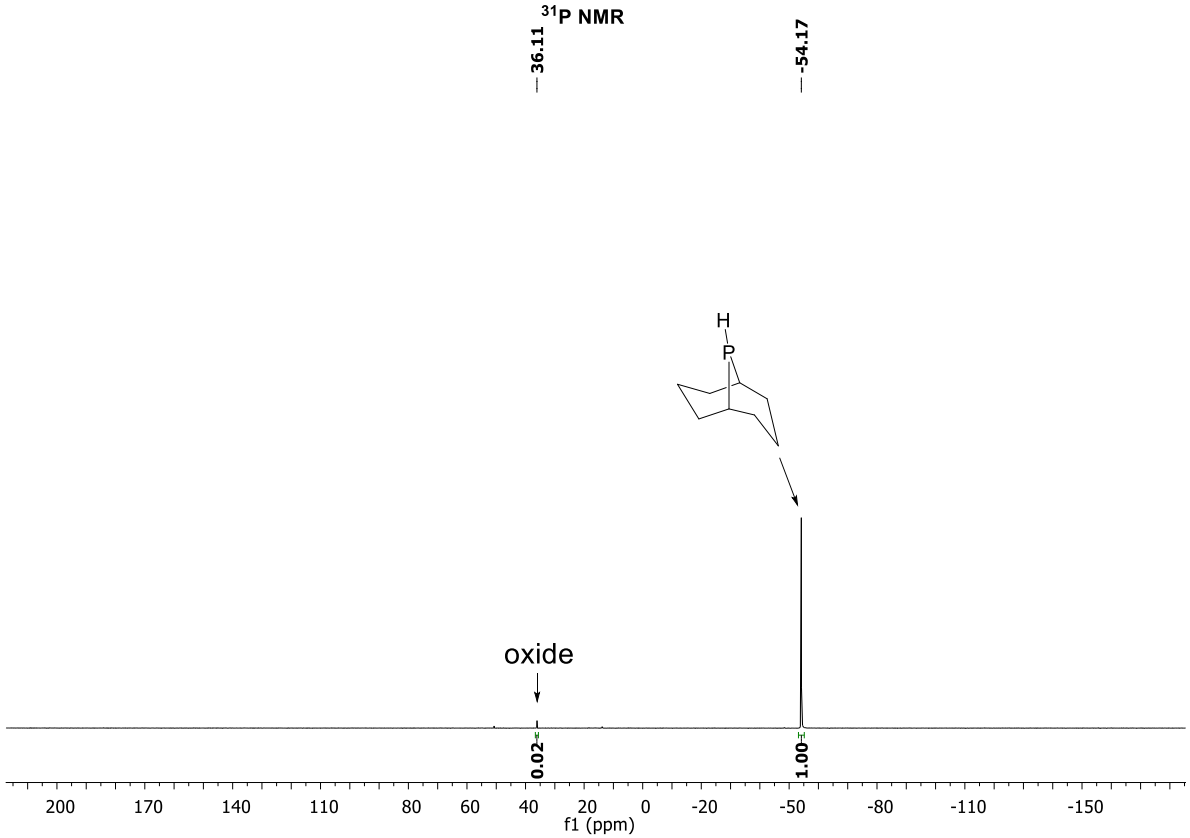

NOESY
ArH5···HA1
ArH1···HA2
ArH1···HCeq
NMe2··· ArH8
HCax···HCeq
NMe2··· HA2
ArH1··· ArH2
F1 [ppm]
F2 [ppm]


COSY
HCax··HCeq
ArH1··ArH2
ArH2··ArH3
ArH3··ArH4
ArH5··ArH6
ArH6··ArH7
ArH7··ArH8
F1 [ppm]
F2 [ppm]

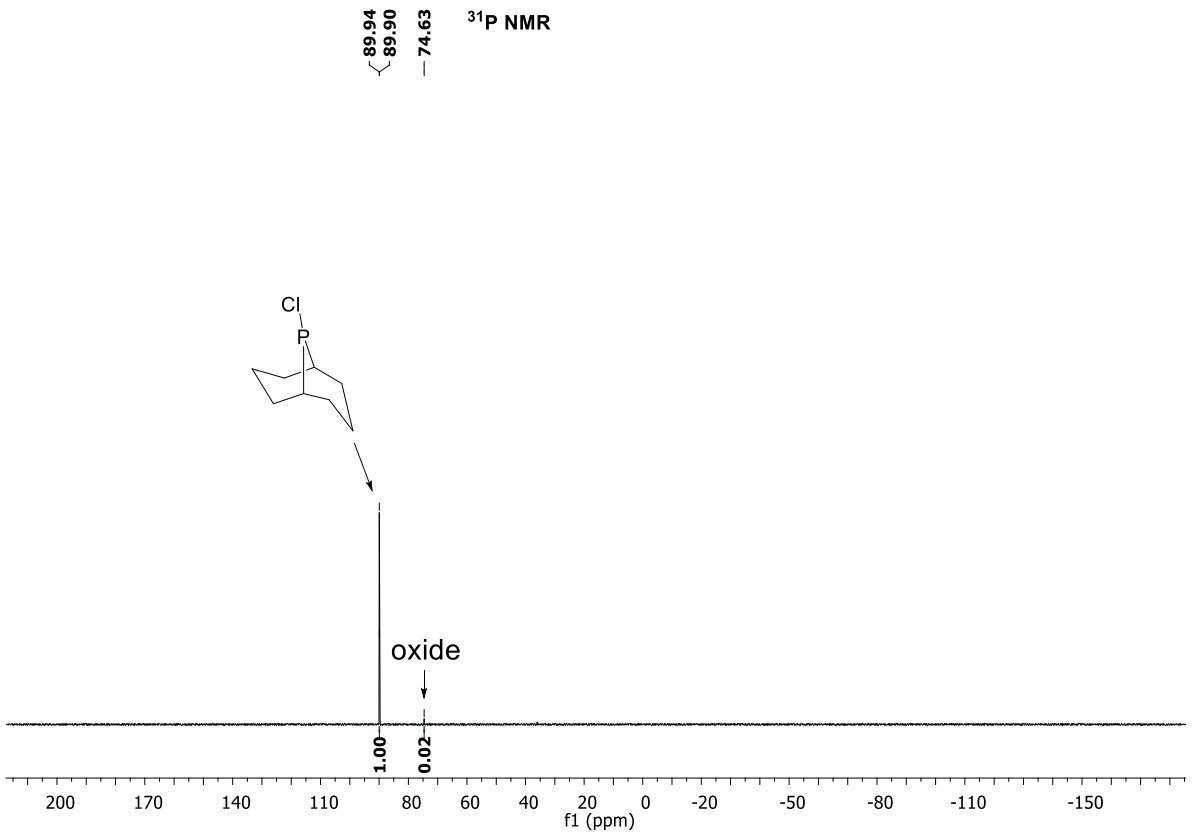

HMBC
F1 [ppm]
F2 [ppm]
B2
B1
A1
A2
C(ax+eq)
D(ax+eq)
NMe2
ArH1
ArH2
ArH3
ArH4
ArH5
ArH6
ArH7
ArH8
Ipso1
Ipso2
Ipso3
Ipso4
3JCH: CA1-HCax
3JCH: CA2-HDeq
3JCH: CC-HB2
3JCH: CC-HA1
3JCH: CNMe-HNMe
3JCH: CD-HB1
3JCH: CD-HA2
4JCH: CQ1-HB1
2JCH: CQ1-HCeq
2JCH: CQ1-HA1
2JCH: CQ2-HDeq
2JCH: CQ2-HA2
2JCH: CQ4-HB1
2JCH: CQ3-HCeq
2JCH: CQ4-HDax
2JCH: CQ4-HDeq
2JCH: CQ3-HCax
2JCH: CQ3-HB2
2JCH: CAr4-HAr3
2JCH: CAr5-HAr7
3JCH: CAr8-HAr6
3JCH: CAr2-HAr4
3JCH: CAr6-HAr8
3JCH: CAr3-HAr1
2JCH: CAr7-HAr8
3JCH: Cipso3-HAr8
3JCH: CAr1-HAr3
3JCH: Cipso3-HAr6
4JCH: Cipso2-HAr2
2JCH: Cipso1-HAr1
2JCH: Cipso2-HAr4
2JCH: Cipso1-HAr3
3JCH: Cipso4-HAr7
3JCH: Cipso4-HAr8
3JCH: Cipso4-HNMe

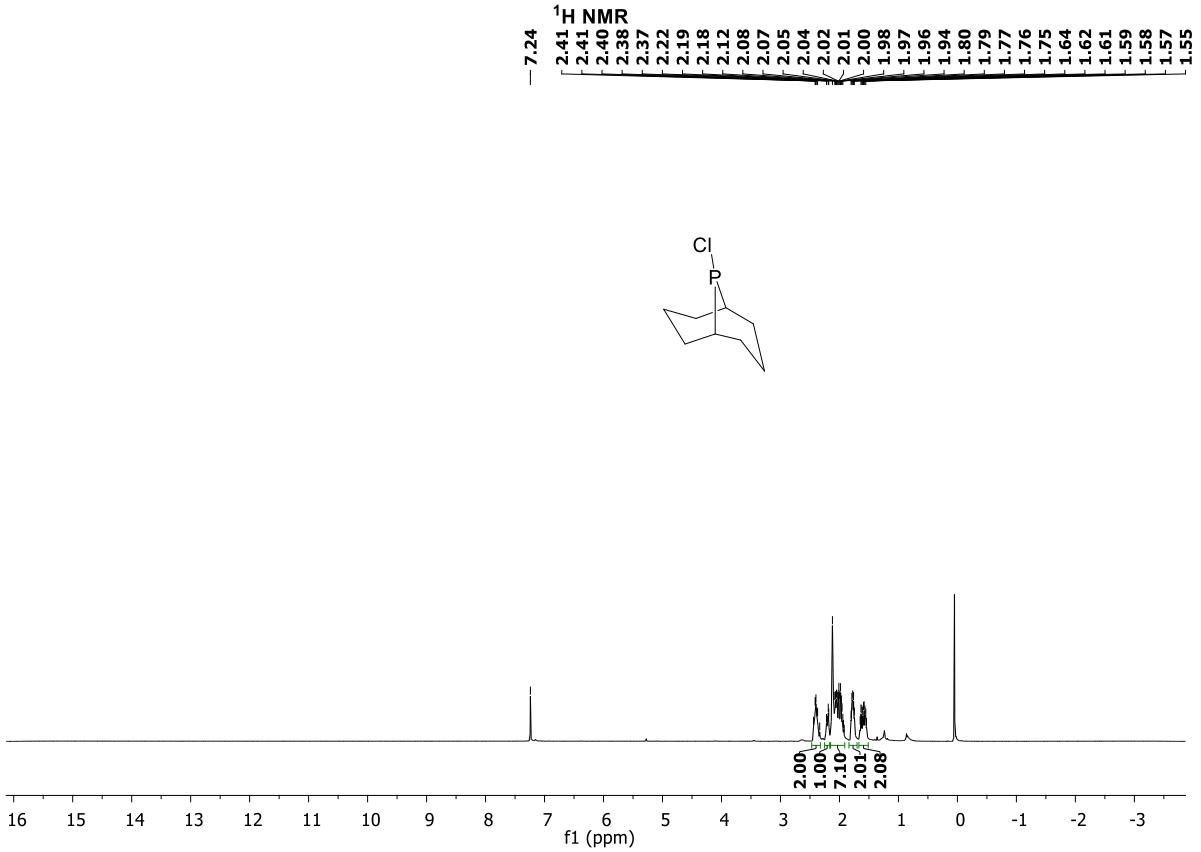

Cg-DavePhos
MS_Direct_201105_ UJ69b 25 (0.168) Cm (25)
1: TOF MS ES+
7.53e5
412.2046
413.2081
414.2109
%
m/z

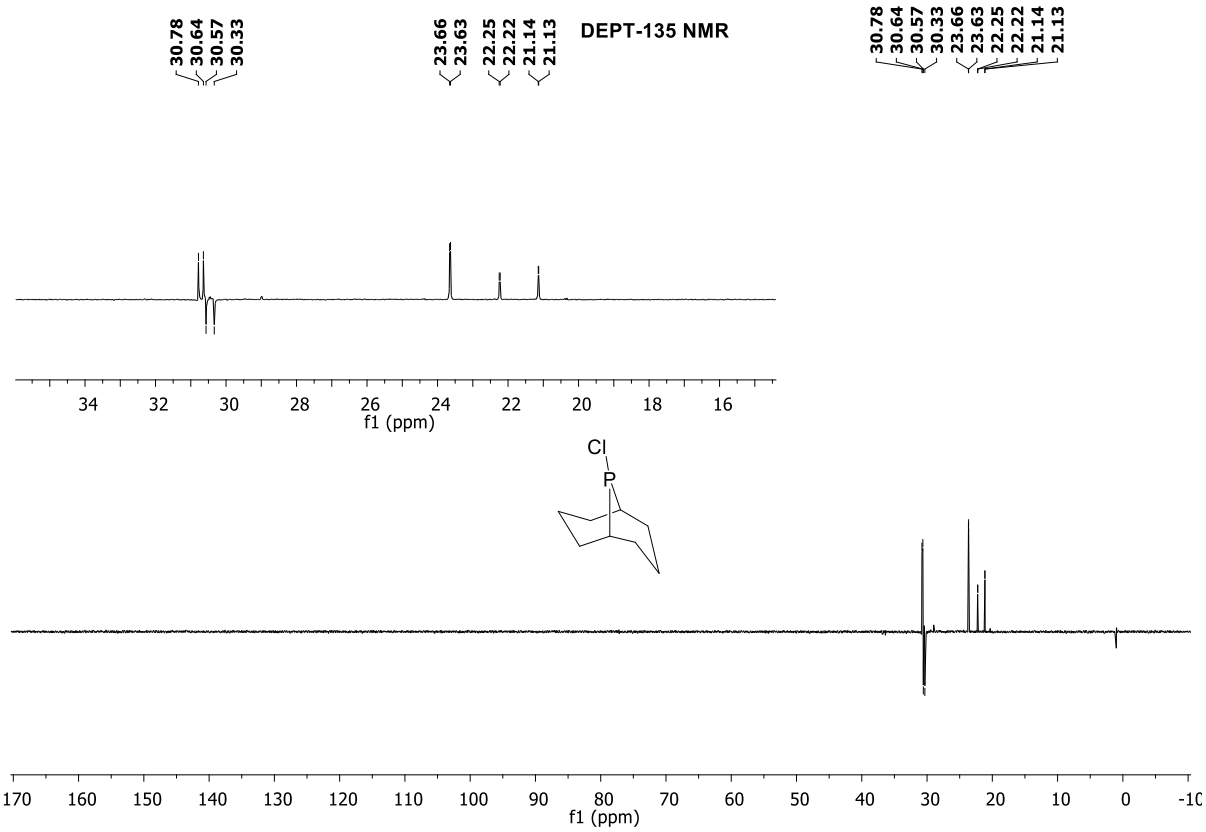
***s*-Phob-H [3.3.1]**


31P NMR
36.11
-54.17
H
P
oxide
0.02
1.00
200
170
140
110
80
60
40
20
0
-20
-50
-80
-110
-150
f1 (ppm)

***s*-Phob-Cl**

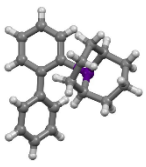
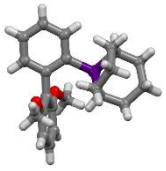
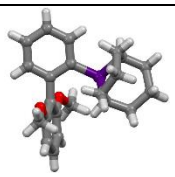
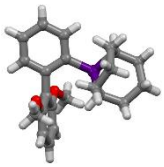

89.94
89.90
74.63
31P NMR
Cl
P
oxide
1.00
0.02
200 170 140 110 80 60 40 20 0 -20 -50 -80 -110 -150
f1 (ppm)


1H NMR
7.24
2.41 2.41 2.40 2.38 2.37 2.22 2.19 2.18 2.12 2.08 2.07 2.05 2.04 2.02 2.01 2.00 1.98 1.97 1.96 1.94 1.80 1.79 1.77 1.76 1.75 1.64 1.62 1.61 1.59 1.58 1.57 1.55
Cl
P
2.00
1.00
7.10
2.01
2.08
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)



Crystallographic Data

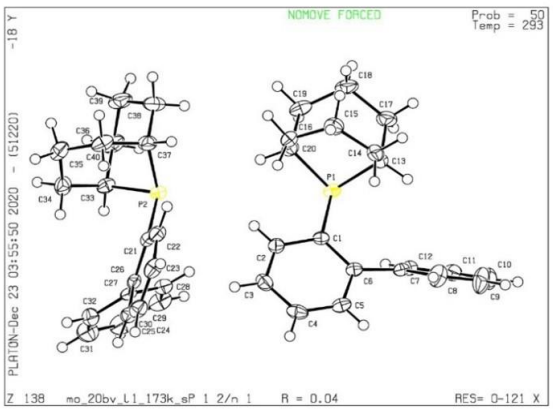
Table S1: Crystal data and refinement parameters for biaryl phosphacyles **1** – **4**.

Crystal structure				
Ligand	**Ligand 1**	**Ligand 2**	**Ligand 3**	**Ligand 4**
CCDC no.	2051924	2051881	2051950	2051945
Empirical formula	$C_{20}H_{23}P$	$C_{44}H_{54}O_4P_2$	$C_{22}H_{25}O_3P$	$C_{24}H_{30}NO_3P$
Formula weight	294.35	354.41	368.39	411.46
Temperature/K	293(2)	149.99(10)	293(2)	296.15
Crystal system	monoclinic	triclinic	triclinic	monoclinic
Space group	*P*2/*n*	*P*-1	*P*-1	*C*2/*c*
a/Å	14.554(2)	10.80490(10)	8.0873(7)	23.219(2)
b/Å	7.2220(11)	13.8758(2)	9.4963(9)	8.4649(8)

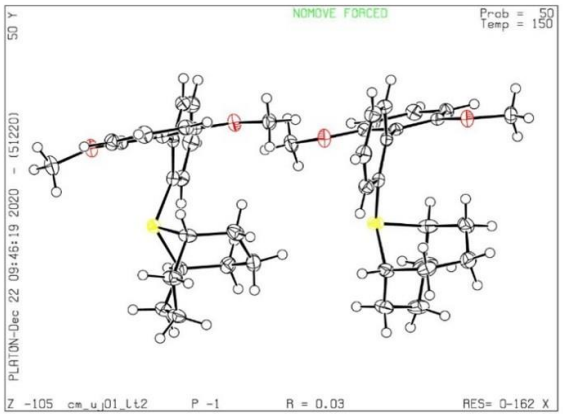
c/Å	31.176(4)	14.4304(2)	13.1468(12)	24.795(2)
α/°	90	62.5460(10)	92.553(4)	90
β/°	97.878(5)	81.2320(10)	105.035(4)	110.975(2)
γ/°	90	88.0550(10)	95.537(4)	90
Volume/Å^3	3246.0(8)	1895.79(4)	968.01(15)	4550.3(8)
Z	8	4	2	8
ρ_{calc}g/cm^3	1.205	1.242	1.264	1.201
μ/mm^{-1}	0.161	1.368	0.160	0.144
F(000)	1264.0	760.0	392.0	1760.0
Crystal size/mm^3	0.225 × 0.212 × 0.096	0.241 × 0.110 × 0.091	0.321 × 0.285 × 0.240	0.465 × 0.346 × 0.281
Radiation	MoKα (λ = 0.71073)	CuKα (λ = 1.54184)	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.168 to 52.176	6.986 to 144.258	3.216 to 52.166	3.518 to 52.518
Index ranges	-18 ≤ h ≤ 17, -8 ≤ k ≤ 8, -38 ≤ l ≤ 38	-13 ≤ h ≤ 12, -17 ≤ k ≤ 17, -17 ≤ l ≤ 17	-9 ≤ h ≤ 9, -11 ≤ k ≤ 11, -16 ≤ l ≤ 16	-28 ≤ h ≤ 28, -10 ≤ k ≤ 10, -30 ≤ l ≤ 30
Reflections collected	37990	44733	35452	91270
Independent reflections	6384 [R_{int} = 0.0476, R_{sigma} = 0.0342]	7445 [R_{int} = 0.0406, R_{sigma} = 0.0218]	3831 [R_{int} = 0.1041, R_{sigma} = 0.0664]	4612 [R_{int} = 0.0480, R_{sigma} = 0.0164]
Data/restraints/parameters	6384/0/379	7445/0/455	3831/0/239	4612/0/268
Goodness-of-fit on F^2	1.062	1.078	1.058	1.038
Final R indexes [I>=2σ (I)]	R_1 = 0.0413, wR_2 = 0.0941	R_1 = 0.0344, wR_2 = 0.0914	R_1 = 0.0446, wR_2 = 0.1056	R_1 = 0.0358, wR_2 = 0.0910
Final R indexes [all data]	R_1 = 0.0495, wR_2 = 0.0980	R_1 = 0.0366, wR_2 = 0.0932	R_1 = 0.0624, wR_2 = 0.1138	R_1 = 0.0438, wR_2 = 0.0971
Largest diff. peak/hole / e Å^{-3}	0.63/-0.22	0.33/-0.34	0.45/-0.29	0.17/-0.24

Table S2: Ellipsoid plots for ligadds **1** – **4**, from checkCIF/PLATON (50% probability displacement ellipsoids).

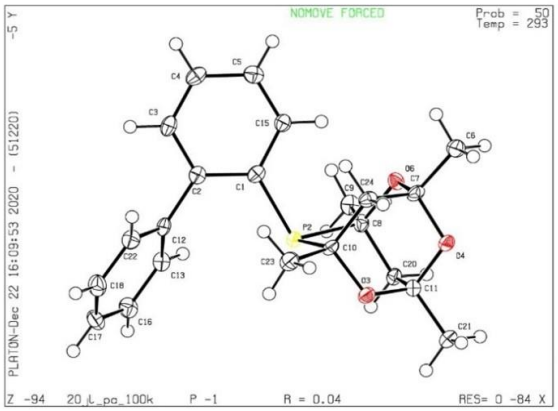
Ligand 1



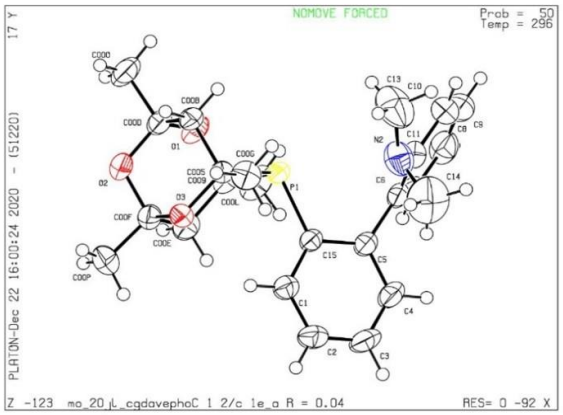
Ligand 2



Ligand 3



Ligand 4



Ligand 1

Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for mo_20bv_L1_173K_solve_a. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
P1	16.8(3)	4603.2(6)	3623.4(2)	22.32(11)
P2	2510.6(3)	9507.9(6)	4239.7(2)	23.60(11)
C13	-1270.4(12)	4619(2)	3509.3(5)	26.2(4)

C6	174.7(11)	5123(2)	2721.9(5)	19.8(3)
C12	-204.5(11)	1760(2)	2782.0(5)	22.9(3)
C1	431.5(11)	5718(2)	3154.7(5)	19.5(3)
C26	3700.0(11)	10119(2)	3588.7(5)	20.9(3)
C7	-420.1(11)	3483(2)	2593.9(5)	20.6(3)
C21	2901.2(11)	10659(2)	3769.7(5)	20.8(3)
C2	1109.7(11)	7104(2)	3234.6(6)	24.9(4)
C28	3914.8(12)	6767(2)	3785.8(5)	26.3(4)
C3	1507.8(12)	7924(2)	2903.3(6)	28.9(4)
C25	3917.0(12)	11040(2)	3220.1(5)	25.0(4)
C32	5267.7(12)	8683(3)	3814.4(6)	31.3(4)
C5	563.5(12)	6028(2)	2391.8(5)	24.7(4)
C33	3510.2(12)	9597(2)	4680.8(5)	26.2(4)
C29	4472.9(14)	5238(3)	3895.3(6)	35.4(4)
C24	3341.2(13)	12388(2)	3012.5(5)	29.0(4)
C23	2540.0(13)	12870(2)	3178.2(6)	29.9(4)
C4	1224.3(12)	7395(2)	2479.0(6)	28.5(4)
C27	4301.1(11)	8518(2)	3746.2(5)	21.8(3)
C14	-1675.1(12)	6506(3)	3354.4(6)	30.1(4)
C20	61.0(12)	6470(2)	4036.8(5)	25.9(4)
C17	-1612.8(14)	3851(3)	3922.3(6)	36.6(5)
C22	2329.5(12)	12028(2)	3551.5(5)	26.9(4)
C16	-424.8(12)	8276(2)	3875.4(6)	28.0(4)
C8	-1145.5(13)	3582(3)	2250.0(6)	35.1(4)
C34	3957.7(12)	11519(3)	4738.3(6)	31.2(4)
C37	1848.1(12)	11328(3)	4488.0(6)	30.7(4)
C11	-697.0(12)	190(2)	2634.6(6)	28.7(4)

C38	1556.2(14)	10402(3)	4895.5(7)	41.8(5)
C18	-1338.8(15)	4955(3)	4342.0(6)	37.8(5)
C10	-1413.9(13)	312(3)	2295.2(7)	38.9(5)
C36	2358.2(13)	13177(3)	4572.2(6)	33.3(4)
C19	-318.9(14)	5559(3)	4424.1(6)	34.9(4)
C39	2353.6(16)	9877(3)	5248.1(6)	41.4(5)
C15	-1441.9(12)	8143(3)	3664.3(6)	31.6(4)
C30	5428.2(15)	5425(3)	3965.4(7)	42.8(5)
C31	5822.8(14)	7136(3)	3923.5(7)	42.3(5)
C35	3330.5(14)	13123(3)	4837.7(6)	33.7(4)
C40	3151.1(15)	8809(3)	5088.6(6)	37.4(5)
C9	-1635.2(14)	2009(3)	2103.4(7)	46.4(5)

Anisotropic Displacement Parameters ($Å^2×10^3$) for mo_20bv_L1_173K_solve_a. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
P1	27.4(2)	23.3(2)	17.1(2)	0.55(17)	5.86(16)	2.18(18)
P2	24.5(2)	27.1(2)	20.2(2)	-3.27(18)	6.48(17)	-1.29(18)
C13	27.8(9)	28.7(9)	23.5(8)	-6.9(7)	8.8(7)	-8.3(7)
C6	22.5(8)	16.7(8)	20.7(8)	0.8(6)	4.9(6)	4.7(6)
C12	24.5(8)	24.2(8)	20.4(8)	-0.5(7)	4.1(6)	1.2(7)
C1	20.5(8)	19.4(8)	19.5(8)	0.3(6)	5.4(6)	3.7(6)
C26	23.6(8)	18.7(8)	20.2(8)	-4.5(6)	1.9(6)	-2.7(6)
C7	22.1(8)	23.3(8)	16.9(7)	-1.9(6)	4.7(6)	2.9(6)
C21	22.6(8)	21.4(8)	17.8(8)	-3.7(6)	1.4(6)	-1.1(6)
C2	21.8(8)	25.8(9)	27.4(9)	-5.7(7)	4.6(7)	1.4(7)
C28	31.1(9)	25.7(9)	22.8(8)	-0.7(7)	6.3(7)	1.7(7)
C3	24.6(9)	23.8(9)	39.9(10)	-3.0(8)	10.6(8)	-2.9(7)

C25	28.5(9)	23.4(8)	24.1(8)	-2.6(7)	6.7(7)	-3.6(7)
C32	26.5(9)	35.6(10)	31.2(9)	-3.6(8)	2.3(7)	-0.4(8)
C5	32.8(9)	22.9(8)	19.1(8)	1.8(7)	6.4(7)	5.9(7)
C33	31.6(9)	28.6(9)	18.2(8)	-0.4(7)	2.5(7)	4.3(7)
C29	52.2(12)	26.1(9)	28.3(9)	2.4(8)	6.7(9)	7.3(9)
C24	41.8(10)	24.2(9)	20.9(8)	2.3(7)	3.4(7)	-4.8(8)
C23	38.1(10)	24.5(9)	24.5(9)	0.2(7)	-5.6(7)	5.3(8)
C4	33.8(9)	23.4(9)	31.7(9)	6.8(7)	16.4(8)	3.3(7)
C27	25.0(8)	25.6(8)	15.2(7)	-3.6(6)	4.6(6)	3.1(7)
C14	21.4(8)	39.6(10)	29.0(9)	-1.9(8)	2.7(7)	-0.6(8)
C20	27.0(9)	31.3(9)	19.2(8)	-4.5(7)	2.6(7)	0.9(7)
C17	44.9(11)	34.0(10)	35.6(10)	-4.1(8)	21.8(9)	-10.7(9)
C22	26.1(9)	29.6(9)	23.8(8)	-5.9(7)	-1.0(7)	5.1(7)
C16	30.8(9)	26.7(9)	27.2(9)	-7.4(7)	6.3(7)	-1.5(7)
C8	35.7(10)	30.1(10)	35.8(10)	0.9(8)	-8.0(8)	5.8(8)
C34	29.9(9)	35.9(10)	25.9(9)	0.7(8)	-3.0(7)	-2.7(8)
C37	26.2(9)	38.8(10)	28.1(9)	-5.9(8)	7.3(7)	5.4(8)
C11	31.8(9)	22.6(9)	33.6(10)	-1.6(7)	10.7(8)	-0.7(7)
C38	43.7(12)	47.9(12)	39.1(11)	-10.0(10)	24.1(9)	-3.8(10)
C18	54.0(12)	37.6(11)	26.4(9)	-0.9(8)	21.7(9)	-3.6(9)
C10	30.8(10)	34.8(10)	49.7(12)	-12.6(9)	0.5(9)	-5.9(8)
C36	44.1(11)	29.9(10)	26.7(9)	-4.8(8)	7.1(8)	9.5(8)
C19	47.5(11)	39.9(11)	18.3(8)	-1.2(8)	8.5(8)	5.4(9)
C39	63.8(14)	39.5(11)	25.1(10)	-1.8(8)	21.4(9)	-7.0(10)
C15	30.2(9)	29.9(9)	35.2(10)	-1.3(8)	6.9(8)	5.3(8)
C30	50.4(13)	40.8(12)	35.6(11)	1.7(9)	-0.3(9)	21.8(10)
C31	27.2(10)	57.4(14)	40.4(11)	-4.9(10)	-1.5(8)	14.0(9)

C35	46.2(11)	27.9(9)	26.6(9)	-4.6(8)	3.6(8)	-3.9(8)
C40	58.0(13)	31.9(10)	22.9(9)	3.2(8)	8.0(9)	1.3(9)
C9	34.9(11)	47.2(12)	50.6(13)	-9.5(10)	-18.3(9)	1.7(10)

Bond Lengths for mo_20bv_L1_173K_solve_a.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
P1	C13	1.8583(18)	C32	C27	1.399(2)
P1	C1	1.8410(16)	C32	C31	1.393(3)
P1	C20	1.8600(17)	C5	C4	1.379(2)
P2	C21	1.8411(17)	C33	C34	1.533(2)
P2	C33	1.8611(17)	C33	C40	1.548(2)
P2	C37	1.8604(18)	C29	C30	1.384(3)
C13	C14	1.536(3)	C24	C23	1.383(3)
C13	C17	1.546(2)	C23	C22	1.384(2)
C6	C1	1.417(2)	C14	C15	1.535(3)
C6	C7	1.489(2)	C20	C16	1.535(2)
C6	C5	1.402(2)	C20	C19	1.543(2)
C12	C7	1.393(2)	C17	C18	1.537(3)
C12	C11	1.386(2)	C16	C15	1.538(2)
C1	C2	1.404(2)	C8	C9	1.384(3)
C26	C21	1.415(2)	C34	C35	1.533(3)
C26	C25	1.401(2)	C37	C38	1.546(3)
C26	C27	1.492(2)	C37	C36	1.533(3)
C7	C8	1.400(2)	C11	C10	1.383(3)
C21	C22	1.406(2)	C38	C39	1.533(3)
C2	C3	1.384(2)	C18	C19	1.535(3)
C28	C29	1.386(2)	C10	C9	1.383(3)

C28	C27	1.397(2)	C36	C35	1.539(3)
C3	C4	1.384(3)	C39	C40	1.532(3)
C25	C24	1.386(2)	C30	C31	1.376(3)

Bond Angles for mo_20bv_L1_173K_solve_a.

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
C13	P1	C20	93.81(8)	C40	C33	P2	106.05(13)
C1	P1	C13	106.08(7)	C30	C29	C28	120.22(19)
C1	P1	C20	104.42(8)	C23	C24	C25	119.28(16)
C21	P2	C33	106.08(8)	C24	C23	C22	119.92(16)
C21	P2	C37	104.25(8)	C5	C4	C3	119.64(16)
C37	P2	C33	93.74(8)	C28	C27	C26	120.39(15)
C14	C13	P1	113.50(12)	C28	C27	C32	118.18(16)
C14	C13	C17	115.26(15)	C32	C27	C26	121.10(15)
C17	C13	P1	105.66(13)	C15	C14	C13	116.31(14)
C1	C6	C7	124.34(14)	C16	C20	P1	114.72(11)
C5	C6	C1	118.51(15)	C16	C20	C19	114.87(14)
C5	C6	C7	116.92(14)	C19	C20	P1	104.54(12)
C11	C12	C7	121.00(15)	C18	C17	C13	116.57(15)
C6	C1	P1	123.44(12)	C23	C22	C21	122.08(16)
C2	C1	P1	118.04(12)	C20	C16	C15	117.37(15)
C2	C1	C6	118.19(14)	C9	C8	C7	120.76(18)
C21	C26	C27	124.02(14)	C35	C34	C33	116.92(15)
C25	C26	C21	119.09(15)	C38	C37	P2	104.65(13)
C25	C26	C27	116.74(14)	C36	C37	P2	114.86(12)
C12	C7	C6	120.58(14)	C36	C37	C38	114.66(15)
C12	C7	C8	118.07(16)	C10	C11	C12	120.20(17)

C8	C7	C6	120.98(15)	C39	C38	C37	115.47(16)
C26	C21	P2	123.57(12)	C19	C18	C17	114.94(15)
C22	C21	P2	118.41(12)	C9	C10	C11	119.59(18)
C22	C21	C26	117.71(15)	C37	C36	C35	117.26(15)
C3	C2	C1	121.92(16)	C18	C19	C20	115.65(15)
C29	C28	C27	120.94(17)	C40	C39	C38	115.13(16)
C2	C3	C4	119.63(16)	C14	C15	C16	115.74(14)
C24	C25	C26	121.79(16)	C31	C30	C29	119.73(18)
C31	C32	C27	120.43(18)	C30	C31	C32	120.50(18)
C4	C5	C6	121.98(16)	C34	C35	C36	116.08(15)
C34	C33	P2	113.22(12)	C39	C40	C33	115.95(16)
C34	C33	C40	115.00(15)	C10	C9	C8	120.37(18)

Torsion Angles for mo_20bv_L1_173K_solve_a.

A	B	C	D	Angle/˚	A	B	C	D	Angle/˚
P1	C13	C14	C15	-59.07(18)	C25	C26	C27	C28	-122.49(17)
P1	C13	C17	C18	61.0(2)	C25	C26	C27	C32	50.8(2)
P1	C1	C2	C3	175.40(13)	C25	C24	C23	C22	1.1(3)
P1	C20	C16	C15	54.01(18)	C5	C6	C1	P1	-177.40(12)
P1	C20	C19	C18	-64.81(18)	C5	C6	C1	C2	-4.1(2)
P2	C21	C22	C23	-175.47(13)	C5	C6	C7	C12	121.83(17)
P2	C33	C34	C35	58.36(18)	C5	C6	C7	C8	-51.0(2)
P2	C33	C40	C39	-61.37(19)	C33	P2	C21	C26	55.74(15)
P2	C37	C38	C39	64.95(19)	C33	P2	C21	C22	-130.80(13)
P2	C37	C36	C35	-53.7(2)	C33	P2	C37	C38	-69.78(13)
C13	P1	C1	C6	-54.94(15)	C33	P2	C37	C36	56.84(14)
C13	P1	C1	C2	131.79(13)	C33	C34	C35	C36	-43.2(2)

C13 P1 C20 C16 -56.32(13)
C13 P1 C20 C19 70.38(13)
C13 C14 C15 C16 44.5(2)
C13 C17 C18 C19 -45.7(3)
C6 C1 C2 C3 1.8(2)
C6 C7 C8 C9 173.29(18)
C6 C5 C4 C3 -1.1(3)
C12 C7 C8 C9 0.3(3)
C12 C11 C10 C9 0.1(3)
C1 P1 C13 C14 -47.57(13)
C1 P1 C13 C17 -174.80(11)
C1 P1 C20 C16 51.36(14)
C1 P1 C20 C19 178.07(11)
C1 C6 C7 C12 -52.6(2)
C1 C6 C7 C8 134.56(18)
C1 C6 C5 C4 3.9(2)
C1 C2 C3 C4 1.1(3)
C26 C21 C22 C23 -1.6(2)
C26 C25 C24 C23 1.4(3)
C7 C6 C1 P1 -3.1(2)
C7 C6 C1 C2 170.20(14)
C7 C6 C5 C4 -170.87(15)
C7 C12 C11 C10 0.2(3)
C7 C8 C9 C10 0.0(3)
C21 P2 C33 C34 47.41(14)
C21 P2 C33 C40 174.43(12)
C21 P2 C37 C38 -177.41(12)
C29 C28 C27 C26 174.34(15)
C29 C28 C27 C32 0.8(2)
C29 C30 C31 C32 0.5(3)
C24 C23 C22 C21 -0.9(3)
C27 C26 C21 P2 2.2(2)
C27 C26 C21 C22 -171.31(15)
C27 C26 C25 C24 171.64(15)
C27 C28 C29 C30 -0.3(3)
C27 C32 C31 C30 0.0(3)
C14 C13 C17 C18 -65.2(2)
C20 P1 C13 C14 58.63(13)
C20 P1 C13 C17 -68.61(13)
C20 P1 C1 C6 -153.31(13)
C20 P1 C1 C2 33.42(14)
C20 C16 C15 C14 -41.9(2)
C17 C13 C14 C15 63.0(2)
C17 C18 C19 C20 47.8(2)
C16 C20 C19 C18 61.8(2)
C34 C33 C40 C39 64.6(2)
C37 P2 C21 C26 153.98(14)
C37 P2 C21 C22 -32.56(15)
C37 P2 C33 C34 -58.59(14)
C37 P2 C33 C40 68.43(13)
C37 C38 C39 C40 -48.9(2)
C37 C36 C35 C34 40.5(2)
C11 C12 C7 C6 -173.40(15)
C11 C12 C7 C8 -0.3(2)

C21 P2 C37 C36 -50.80(15)		C11 C10 C9 C8 -0.2(3)	
C21 C26 C25 C24 -4.0(2)		C38 C37 C36 C35 67.6(2)	
C21 C26 C27 C28 52.9(2)		C38 C39 C40 C33 46.7(2)	
C21 C26 C27 C32 -133.79(17)		C36 C37 C38 C39 -61.8(2)	
C2 C3 C4 C5 -1.5(3)		C19 C20 C16 C15 -67.2(2)	
C28 C29 C30 C31 -0.4(3)		C31 C32 C27 C26 -174.15(16)	
C25 C26 C21 P2 177.49(12)		C31 C32 C27 C28 -0.7(3)	
C25 C26 C21 C22 4.0(2)		C40 C33 C34 C35 -63.8(2)	

Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for mo_20bv_L1_173K_solve_a.

Atom	*x*	*y*	*z*	U(eq)
H13	-1450.43	3726.57	3276.09	31
H12	277.21	1662.15	3009.96	28
H2	1296.96	7482.43	3518.21	30
H28	3273.82	6624.68	3737.98	32
H3	1963.24	8824.41	2965.55	35
H25	4462.35	10738.71	3111.78	30
H32	5541.65	9832.21	3786.7	38
H5	369.94	5696.9	2105.37	30
H33	3982.74	8740.89	4602.88	31
H29	4204.75	4081.74	3921.75	42
H24	3491.9	12963.04	2764.49	35
H23	2143.05	13757.78	3038.92	36
H4	1478.03	7958.49	2254.08	34
H14A	-1457.83	6799.58	3081.76	36
H14B	-2344.63	6388.61	3297.3	36
H20	715.77	6761.45	4129.3	31

H17A	-2284.23	3774.7	3869.57	44
H17B	-1378.5	2599.27	3968.67	44
H22	1792.95	12378.66	3661.48	32
H16A	-70.47	8833.16	3667.14	34
H16B	-397.41	9118.51	4119.21	34
H8	-1300.39	4716.16	2118.51	42
H34A	4472.15	11446.14	4971.05	37
H34B	4213.92	11819.89	4475.6	37
H37	1281.37	11569.67	4287.43	37
H11	-545.02	-949.68	2764.34	34
H38A	1143.47	11237.79	5020.36	50
H38B	1206.65	9290.7	4806.66	50
H18A	-1726.31	6050.39	4333.55	45
H18B	-1469.9	4204.35	4584.46	45
H10	-1745.07	-741.92	2196.62	47
H36A	1972.59	13987.44	4720.18	40
H36B	2413.08	13739.39	4294.28	40
H19A	57.71	4481.14	4512.39	42
H19B	-244.64	6425.08	4664.22	42
H39A	2601.98	11001.09	5389.49	50
H39B	2104.85	9130.83	5463.95	50
H15A	-1831.35	8063.13	3892.41	38
H15B	-1602.15	9280.04	3505.96	38
H30	5801.86	4398.78	4040.48	51
H31	6464.81	7260.58	3968.36	51
H35A	3643.51	14276.65	4790.75	40
H35B	3258.99	13068.05	5142.25	40

H40A	2948.99	7544.52	5028.09	45
H40B	3665.66	8767.48	5321.78	45
H9	-2115.62	2095.81	1874.57	56

Ligand 2

Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for CM_UJ01_LT2. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
P1	2729.6(3)	2226.1(3)	1955.5(2)	21.83(9)
P26	2187.1(3)	7194.9(3)	2178.9(3)	24.27(9)
O21	4915.5(8)	492.8(7)	2938.1(7)	25.5(2)
O44	2901.0(8)	4922.2(7)	4261.1(7)	25.5(2)
O46	3150.2(8)	8123.3(7)	4551.6(7)	24.00(19)
O19	5142.5(8)	3590.3(7)	3413.6(7)	24.21(19)
C14	5711.8(11)	3014.4(10)	2927.0(9)	20.4(2)
C38	2972.3(11)	6521.8(10)	4415.5(9)	19.2(2)
C32	4007.3(11)	6948.7(9)	3496.6(10)	19.6(2)
C13	5046.0(11)	2071.6(10)	3125.7(9)	19.9(2)
C39	2401.5(11)	5494.5(10)	4774.8(10)	20.3(2)
C18	5582.5(11)	1430.6(10)	2664.4(10)	21.3(2)
C12	2683.3(11)	1873.1(9)	3359.0(10)	20.7(2)
C7	3787.9(11)	1771.2(9)	3799.8(10)	20.2(2)
C43	2543.9(11)	7138.0(10)	4936.4(9)	19.8(2)
C11	1542.4(12)	1536.8(10)	4051.1(10)	24.9(3)
C37	3770.8(11)	7310.1(10)	2457.2(10)	20.4(2)
C36	4799.7(12)	7616.6(11)	1646.1(10)	25.3(3)
C17	6723.6(12)	1742.0(11)	1987.4(10)	25.8(3)
C42	1556.7(12)	6749.2(10)	5777.5(10)	23.1(3)
C8	3720.7(12)	1376.9(10)	4889.3(10)	24.0(3)

C35	6016.9(12)	7599.9(11)	1844.2(11)	28.2(3)
C40	1407.3(12)	5103.0(10)	5604.7(10)	24.1(3)
C33	5235.8(12)	6953.1(10)	3685.5(10)	24.6(3)
C2	3565.0(12)	3576.7(11)	1139.0(10)	24.9(3)
C41	1002.2(12)	5734.7(11)	6098.6(10)	25.0(3)
C10	1487.9(13)	1137.0(11)	5134.7(11)	28.5(3)
C34	6235.2(12)	7277.0(11)	2866.0(11)	28.1(3)
C15	6859.4(12)	3327.4(10)	2262.6(10)	24.2(3)
C9	2576.7(13)	1058.8(11)	5555.2(10)	28.2(3)
C31	2225.0(13)	8232.7(11)	774.9(10)	27.0(3)
C6	1166.7(12)	2784.6(10)	1653.8(10)	23.8(3)
C20	5656.8(12)	4654.8(10)	3094.5(11)	25.6(3)
C25	3472.4(13)	3861.4(13)	-17.5(10)	30.8(3)
C5	821.0(12)	3717.1(11)	1928.2(11)	27.3(3)
C16	7345.2(12)	2690.2(11)	1794.4(11)	27.6(3)
C45	2272.7(13)	3922.0(11)	4518.2(11)	27.7(3)
C47	2623.4(13)	8857.1(11)	4935.9(11)	27.5(3)
C30	2664.6(13)	9382.8(11)	514.8(11)	30.4(3)
C3	3109.1(13)	4447.2(11)	1466.6(11)	29.3(3)
C23	1175.5(13)	3073.7(11)	485.3(11)	28.9(3)
C24	2145.8(13)	3959.9(12)	-314.3(10)	29.6(3)
C4	1729.3(13)	4714.5(11)	1417.9(11)	29.6(3)
C27	1137.3(12)	7992.8(12)	2687.9(10)	29.5(3)
C22	5207.1(14)	-27.6(12)	2285.1(12)	32.1(3)
C49	-172.9(13)	8456.9(13)	1155.3(12)	34.6(3)
C28	1668.0(14)	9133.5(12)	2359.4(12)	33.2(3)
C29	1952.0(14)	9890.6(11)	1173.1(12)	32.1(3)

C50	903.5(15)	8155.4(13)	528.0(12)	35.6(3)
C48	-143.6(13)	7954.5(14)	2347.4(12)	38.3(4)

Anisotropic Displacement Parameters ($Å^2×10^3$) for CM_UJ01_LT2. The Anisotropic displacement factor exponent takes the form: $-2π^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+…]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
P1	22.63(16)	24.32(17)	22.29(16)	-13.72(13)	-4.65(12)	3.26(12)
P26	24.52(17)	22.87(17)	24.61(17)	-8.93(13)	-7.76(13)	-1.66(12)
O21	27.8(5)	21.9(4)	29.5(5)	-15.5(4)	0.3(4)	-1.3(4)
O44	28.8(5)	20.4(4)	28.6(5)	-14.2(4)	2.1(4)	-0.5(3)
O46	26.7(4)	20.2(4)	27.5(5)	-13.9(4)	-0.8(4)	0.1(3)
O19	25.4(4)	21.8(4)	28.0(5)	-14.7(4)	0.1(4)	-1.7(3)
C14	21.3(6)	21.4(6)	19.8(6)	-10.0(5)	-6.2(5)	3.4(5)
C38	18.1(5)	20.7(6)	19.3(6)	-9.1(5)	-5.4(5)	2.8(4)
C32	21.0(6)	16.7(5)	22.5(6)	-10.3(5)	-3.4(5)	2.0(4)
C13	20.6(6)	20.0(6)	19.2(6)	-8.5(5)	-5.5(5)	2.3(4)
C39	21.4(6)	21.0(6)	21.3(6)	-11.4(5)	-6.1(5)	4.5(5)
C18	22.8(6)	20.0(6)	21.2(6)	-9.1(5)	-5.3(5)	1.3(5)
C12	22.2(6)	17.2(5)	22.9(6)	-9.9(5)	-2.6(5)	1.2(4)
C7	23.0(6)	16.1(5)	22.2(6)	-10.0(5)	-2.2(5)	0.9(4)
C43	20.4(6)	19.8(6)	20.7(6)	-9.4(5)	-7.1(5)	2.7(4)
C11	21.4(6)	24.6(6)	27.4(6)	-11.4(5)	-2.0(5)	0.6(5)
C37	21.4(6)	18.0(6)	23.1(6)	-10.8(5)	-3.0(5)	2.3(4)
C36	28.2(6)	25.7(6)	22.0(6)	-11.6(5)	-2.1(5)	2.6(5)
C17	25.8(6)	27.4(7)	25.7(6)	-14.6(5)	-0.9(5)	3.1(5)
C42	23.2(6)	27.0(6)	23.2(6)	-15.1(5)	-4.1(5)	3.8(5)
C8	26.9(6)	22.9(6)	23.0(6)	-10.9(5)	-4.7(5)	1.6(5)
C35	23.4(6)	28.9(7)	29.8(7)	-13.9(6)	4.2(5)	0.4(5)

C40	24.2(6)	21.7(6)	25.5(6)	-10.4(5)	-2.3(5)	-1.7(5)
C33	23.8(6)	25.5(6)	26.0(6)	-12.4(5)	-7.0(5)	3.3(5)
C2	19.6(6)	32.9(7)	20.0(6)	-10.4(5)	-2.7(5)	-0.8(5)
C41	20.9(6)	29.5(7)	23.6(6)	-12.5(5)	1.1(5)	-1.3(5)
C10	26.0(6)	27.6(7)	26.4(7)	-10.4(5)	5.0(5)	-1.3(5)
C34	18.4(6)	31.0(7)	34.8(7)	-15.1(6)	-3.8(5)	1.8(5)
C15	23.0(6)	23.4(6)	25.0(6)	-9.9(5)	-3.8(5)	-2.3(5)
C9	34.1(7)	27.2(7)	20.2(6)	-9.5(5)	-0.4(5)	1.3(5)
C31	30.5(7)	31.9(7)	21.8(6)	-14.4(6)	-6.9(5)	4.2(5)
C6	21.7(6)	24.1(6)	26.1(6)	-11.4(5)	-4.7(5)	-2.0(5)
C20	28.1(6)	20.9(6)	30.2(7)	-13.7(5)	-4.6(5)	0.1(5)
C25	27.0(7)	43.1(8)	20.8(6)	-14.0(6)	-2.1(5)	2.8(6)
C5	23.2(6)	28.9(7)	29.6(7)	-14.3(6)	-1.9(5)	4.6(5)
C16	22.8(6)	30.8(7)	27.3(7)	-13.3(6)	1.9(5)	-1.7(5)
C45	28.8(7)	26.2(7)	34.8(7)	-19.7(6)	-4.9(6)	0.0(5)
C47	32.7(7)	22.1(6)	31.7(7)	-16.2(6)	-4.1(6)	3.6(5)
C30	29.1(7)	28.5(7)	25.2(7)	-5.5(6)	-3.1(5)	-0.6(5)
C3	33.7(7)	27.3(7)	26.9(7)	-12.0(6)	-4.5(6)	-8.1(5)
C23	30.5(7)	30.8(7)	30.4(7)	-16.2(6)	-12.2(6)	1.3(5)
C24	32.1(7)	37.5(8)	21.7(6)	-14.9(6)	-7.4(5)	2.7(6)
C4	36.7(7)	25.1(7)	29.6(7)	-15.5(6)	-3.0(6)	2.2(5)
C27	22.3(6)	41.2(8)	20.0(6)	-9.8(6)	-4.5(5)	4.4(5)
C22	34.5(7)	32.2(7)	39.0(8)	-25.3(6)	-1.7(6)	-0.1(6)
C49	26.2(7)	38.6(8)	33.8(8)	-9.3(6)	-13.7(6)	-2.3(6)
C28	33.1(7)	43.5(8)	36.1(8)	-27.9(7)	-13.1(6)	13.6(6)
C29	32.9(7)	26.4(7)	40.7(8)	-16.4(6)	-13.0(6)	2.6(5)
C50	42.9(8)	37.5(8)	32.5(7)	-17.5(6)	-19.0(6)	3.1(6)

C48	22.0(7)	46.0(9)	31.4(8)	-4.1(7)	-5.8(6)	-0.8(6)

Bond Lengths for CM_UJ01_LT2.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
P1	C12	1.8439(13)	C43	C42	1.3937(18)
P1	C2	1.8627(13)	C11	C10	1.3895(19)
P1	C6	1.8617(13)	C37	C36	1.4012(17)
P26	C37	1.8445(12)	C36	C35	1.3850(19)
P26	C31	1.8624(14)	C17	C16	1.3873(19)
P26	C27	1.8608(14)	C42	C41	1.3879(18)
O21	C18	1.3681(15)	C8	C9	1.3891(19)
O21	C22	1.4249(15)	C35	C34	1.386(2)
O44	C39	1.3650(14)	C40	C41	1.3866(18)
O44	C45	1.4273(15)	C33	C34	1.3857(19)
O46	C43	1.3625(14)	C2	C25	1.5464(17)
O46	C47	1.4328(15)	C2	C3	1.5298(19)
O19	C14	1.3645(14)	C10	C9	1.383(2)
O19	C20	1.4329(14)	C15	C16	1.3874(18)
C14	C13	1.4023(17)	C31	C30	1.5356(19)
C14	C15	1.3913(18)	C31	C50	1.5420(19)
C38	C32	1.4927(17)	C6	C5	1.5378(18)
C38	C39	1.4006(17)	C6	C23	1.5414(18)
C38	C43	1.4037(16)	C25	C24	1.5417(19)
C32	C37	1.4075(17)	C5	C4	1.5340(19)
C32	C33	1.3959(17)	C30	C29	1.533(2)
C13	C18	1.4012(17)	C3	C4	1.528(2)
C13	C7	1.4932(17)	C23	C24	1.5340(19)

C39	C40	1.3895(18)	C27	C28	1.532(2)
C18	C17	1.3932(18)	C27	C48	1.5480(19)
C12	C7	1.4094(17)	C49	C50	1.530(2)
C12	C11	1.4031(17)	C49	C48	1.535(2)
C7	C8	1.3968(17)	C28	C29	1.527(2)

Bond Angles for CM_UJ01_LT2.

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
C12	P1	C2	108.05(5)	C36	C37	P26	119.84(9)
C12	P1	C6	104.27(6)	C36	C37	C32	118.03(11)
C6	P1	C2	93.25(6)	C35	C36	C37	121.64(12)
C37	P26	C31	104.13(6)	C16	C17	C18	118.88(12)
C37	P26	C27	107.45(6)	C41	C42	C43	118.86(11)
C27	P26	C31	93.07(6)	C9	C8	C7	120.91(12)
C18	O21	C22	117.51(10)	C36	C35	C34	119.77(12)
C39	O44	C45	117.49(10)	C41	C40	C39	118.95(12)
C43	O46	C47	117.45(10)	C34	C33	C32	120.88(12)
C14	O19	C20	117.76(10)	C25	C2	P1	105.18(9)
O19	C14	C13	115.23(10)	C3	C2	P1	114.31(9)
O19	C14	C15	123.74(11)	C3	C2	C25	114.96(11)
C15	C14	C13	121.02(11)	C40	C41	C42	121.64(12)
C39	C38	C32	120.53(10)	C9	C10	C11	119.95(12)
C39	C38	C43	118.43(11)	C33	C34	C35	119.77(12)
C43	C38	C32	121.04(11)	C16	C15	C14	119.02(12)
C37	C32	C38	121.37(10)	C10	C9	C8	119.64(12)
C33	C32	C38	118.75(11)	C30	C31	P26	115.13(9)
C33	C32	C37	119.85(11)	C30	C31	C50	114.51(11)

C14	C13	C7	120.56(10)	C50	C31	P26	104.96(9)
C18	C13	C14	118.39(11)	C5	C6	P1	114.38(9)
C18	C13	C7	121.05(11)	C5	C6	C23	114.76(11)
O44	C39	C38	115.23(11)	C23	C6	P1	105.29(9)
O44	C39	C40	123.62(11)	C24	C25	C2	116.95(11)
C40	C39	C38	121.15(11)	C4	C5	C6	117.04(11)
O21	C18	C13	115.27(11)	C17	C16	C15	121.54(12)
O21	C18	C17	123.63(11)	C29	C30	C31	116.81(11)
C17	C18	C13	121.10(11)	C4	C3	C2	115.91(11)
C7	C12	P1	121.72(9)	C24	C23	C6	115.63(11)
C11	C12	P1	119.77(9)	C23	C24	C25	115.75(11)
C11	C12	C7	117.81(11)	C3	C4	C5	114.44(11)
C12	C7	C13	121.37(11)	C28	C27	P26	113.90(9)
C8	C7	C13	118.60(11)	C28	C27	C48	115.22(12)
C8	C7	C12	120.03(11)	C48	C27	P26	105.32(10)
O46	C43	C38	115.23(10)	C50	C49	C48	115.11(12)
O46	C43	C42	123.83(11)	C29	C28	C27	116.31(11)
C42	C43	C38	120.94(11)	C28	C29	C30	115.10(11)
C10	C11	C12	121.64(12)	C49	C50	C31	115.87(11)
C32	C37	P26	121.50(9)	C49	C48	C27	116.74(11)

Torsion Angles for CM_UJ01_LT2.

A	**B**	**C**	**D**	**Angle/˚**	**A**	**B**	**C**	**D**	**Angle/˚**
P1	C12	C7	C13	7.33(16)	C43	C38	C39	O44	-177.29(10)
P1	C12	C7	C8	-172.32(9)	C43	C38	C39	C40	2.04(17)
P1	C12	C11	C10	171.98(10)	C43	C42	C41	C40	0.06(19)
P1	C2	C25	C24	60.76(14)	C11	C12	C7	C13	177.76(11)
P1	C2	C3	C4	-59.98(14)	C11	C12	C7	C8	-1.88(17)

P1	C6	C5	C4	56.75(14)	C11	C10	C9	C8	-0.3(2)
P1	C6	C23	C24	-63.31(13)	C37	P26	C31	C30	-52.76(11)
P26	C37	C36	C35	-172.95(10)	C37	P26	C31	C50	-179.60(9)
P26	C31	C30	C29	-55.44(15)	C37	P26	C27	C28	47.90(11)
P26	C31	C50	C49	64.12(14)	C37	P26	C27	C48	175.10(9)
P26	C27	C28	C29	59.86(14)	C37	C32	C33	C34	-2.06(18)
P26	C27	C48	C49	-61.56(16)	C37	C36	C35	C34	-0.2(2)
O21	C18	C17	C16	-177.57(12)	C36	C35	C34	C33	1.2(2)
O44	C39	C40	C41	177.56(11)	C33	C32	C37	P26	173.89(9)
O46	C43	C42	C41	179.55(11)	C33	C32	C37	C36	3.01(17)
O19	C14	C13	C18	-179.07(10)	C2	P1	C12	C7	-60.00(11)
O19	C14	C13	C7	1.83(16)	C2	P1	C12	C11	129.75(10)
O19	C14	C15	C16	-178.97(11)	C2	P1	C6	C5	-55.79(10)
C14	C13	C18	O21	176.53(10)	C2	P1	C6	C23	71.13(9)
C14	C13	C18	C17	-2.75(18)	C2	C25	C24	C23	-43.65(18)
C14	C13	C7	C12	107.54(13)	C2	C3	C4	C5	47.48(16)
C14	C13	C7	C8	-72.81(15)	C15	C14	C13	C18	1.96(17)
C14	C15	C16	C17	-1.1(2)	C15	C14	C13	C7	-177.14(11)
C38	C32	C37	P26	-4.02(15)	C31	P26	C37	C32	158.00(10)
C38	C32	C37	C36	-174.91(11)	C31	P26	C37	C36	-31.27(11)
C38	C32	C33	C34	175.90(12)	C31	P26	C27	C28	-57.94(10)
C38	C39	C40	C41	-1.72(18)	C31	P26	C27	C48	69.26(10)
C38	C43	C42	C41	0.29(18)	C31	C30	C29	C28	43.95(17)
C32	C38	C39	O44	3.00(16)	C6	P1	C12	C7	-158.30(10)

C32	C38	C39	C40	-177.67(11)	C6	P1	C12	C11	31.45(11)
C32	C38	C43	O46	-0.93(16)	C6	P1	C2	C25	-69.32(9)
C32	C38	C43	C42	178.39(11)	C6	P1	C2	C3	57.72(10)
C32	C37	C36	C35	-1.91(18)	C6	C5	C4	C3	-46.13(16)
C32	C33	C34	C35	-0.1(2)	C6	C23	C24	C25	44.64(17)
C13	C14	C15	C16	-0.09(18)	C20	O19	C14	C13	-168.88(10)
C13	C18	C17	C16	1.65(19)	C20	O19	C14	C15	10.05(17)
C13	C7	C8	C9	-178.28(11)	C25	C2	C3	C4	61.84(15)
C39	C38	C32	C37	73.37(15)	C5	C6	C23	C24	63.37(15)
C39	C38	C32	C33	-104.56(13)	C45	O44	C39	C38	-173.48(11)
C39	C38	C43	O46	179.36(10)	C45	O44	C39	C40	7.20(17)
C39	C38	C43	C42	-1.32(17)	C47	O46	C43	C38	170.06(10)
C39	C40	C41	C42	0.64(19)	C47	O46	C43	C42	-9.24(17)
C18	C13	C7	C12	-71.54(15)	C30	C31	C50	C49	-63.10(16)
C18	C13	C7	C8	108.11(13)	C3	C2	C25	C24	-65.88(16)
C18	C17	C16	C15	0.3(2)	C23	C6	C5	C4	-65.11(15)
C12	P1	C2	C25	-175.47(8)	C27	P26	C37	C32	60.13(11)
C12	P1	C2	C3	-48.43(10)	C27	P26	C37	C36	-129.15(10)
C12	P1	C6	C5	53.76(10)	C27	P26	C31	C30	56.11(11)
C12	P1	C6	C23	-179.32(8)	C27	P26	C31	C50	-70.74(10)
C12	C7	C8	C9	1.38(18)	C27	C28	C29	C30	-46.35(17)
C12	C11	C10	C9	-0.3(2)	C22	O21	C18	C13	162.54(11)
C7	C13	C18	O21	-4.37(16)	C22	O21	C18	C17	-18.20(18)
C7	C13	C18	C17	176.34(11)	C28	C27	C48	C49	64.83(18)
C7	C12	C11	C10	1.35(18)	C50	C31	C30	C29	66.39(16)

C7	C8	C9	C10	-0.26(19)	C50	C49	C48	C27	44.9(2)
C43	C38	C32	C37	-106.33(13)	C48	C27	C28	C29	-62.02(16)
C43	C38	C32	C33	75.74(15)	C48	C49	C50	C31	-46.20(18)

Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for CM_UJ01_LT2.

Atom	*x*	*y*	*z*	U(eq)
H11	804.33	1582.75	3777.7	30
H36	4661.92	7836.65	957.55	30
H17	7062.83	1321.46	1670.34	31
H42	1274.33	7162.48	6117.63	28
H8	4451.85	1326.72	5172.86	29
H35	6685.33	7804.68	1293.37	34
H40	1019.8	4428.03	5825.43	29
H33	5385.49	6735.79	4370.59	29
H2	4451.25	3476.74	1220.66	30
H41	342.62	5472.1	6659	30
H10	719.7	922.07	5576.87	34
H34	7049.53	7277.66	3001.2	34
H15	7294.49	3954.47	2134.13	29
H9	2543.31	794.64	6279.74	34
H31	2813.28	7994.44	341.15	32
H6	537.96	2191.44	2078.13	29
H20A	5692.46	5086.02	2344.95	38
H20B	6486.45	4598.89	3271.51	38
H20C	5136.09	4992.65	3453.37	38
H25A	3934.52	4545.75	-476.06	37

H25B	3890.96	3309.36	-169.67	37
H5A	4.57	3959.22	1730.02	33
H5B	737.41	3426.66	2689.24	33
H16	8105.36	2903.68	1340.48	33
H45A	2700.25	3609.18	4094.05	42
H45B	1425.33	4055.61	4381.08	42
H45C	2269.74	3428.41	5252.39	42
H47A	3079.96	9544.64	4554.11	41
H47B	2676.1	8561.3	5674.6	41
H47C	1761.05	8956.84	4836.35	41
H30A	3541.28	9365.27	595.67	37
H30B	2612.5	9858.7	-223.25	37
H3A	3258.39	4211.17	2184.44	35
H3B	3614.27	5109.68	1015.01	35
H23A	1326.01	2419.61	407.65	35
H23B	349.37	3307.26	307.77	35
H24A	1838.62	4660.02	-410.6	36
H24B	2206.86	3952.43	-988.59	36
H4A	1623.49	5139.1	683.04	35
H4B	1506.36	5162.99	1766.9	35
H27	1023.42	7596.01	3461.5	35
H22A	5124.54	474.96	1568.94	48
H22B	4641.31	-644.41	2530.63	48
H22C	6052.02	-264.1	2315.68	48
H49A	-958.52	8232.76	1050.27	42
H49B	-159.52	9241.71	868.1	42
H28A	1075.35	9478.49	2676.78	40

H28B	2435.38	9059.59	2654.46	40
H29A	2439.5	10519.52	1061.78	39
H29B	1166.39	10145.84	913.19	39
H50A	898.84	8626.84	-218.87	43
H50B	741.94	7416.67	658.41	43
H48A	-435.74	7200.02	2668.05	46
H48B	-737.61	8322.87	2636.98	46

Ligand 3

Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 20jl_PA_100K. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
P2	3768.0(7)	1821.1(5)	6987.9(4)	15.53(15)
C1	5579(3)	2178.8(19)	6396.8(15)	16.1(4)
C2	5215(3)	2411.1(19)	5309.6(15)	15.3(4)
C3	6576(3)	2720.9(19)	4860.5(16)	18.3(4)
C8	4617(3)	852(2)	8192.9(15)	16.9(4)
C7	5938(3)	2898(2)	9411.7(15)	17.6(4)
C5	8643(3)	2532(2)	6504.4(16)	20.1(5)
C6	7571(3)	3351(2)	10262.1(16)	21.9(5)
C9	5058(3)	-596(2)	7898.7(16)	21.0(5)
C4	8273(3)	2789(2)	5442.9(16)	20.2(5)
O6	6140.4(17)	1552.2(13)	8957.9(10)	16.5(3)
O3	2514.4(17)	3197.6(14)	8379.7(10)	17.4(3)
O4	4570.9(17)	2752.8(14)	9915.3(10)	17.6(3)
C15	7310(3)	2232(2)	6964.0(16)	17.8(4)
C10	3794(2)	3518(2)	7796.7(15)	16.5(4)
C12	3423(3)	2349(2)	4602.9(15)	16.1(4)

C13	2286(3)	1105(2)	4421.1(15)	19.1(4)
C22	2886(3)	3524(2)	4064.9(15)	20.2(5)
C20	3155(3)	769(2)	8735.1(15)	17.4(4)
C11	2970(3)	2231(2)	9186.0(15)	18.1(4)
C24	5515(2)	3975(2)	8589.1(15)	17.3(4)
C17	151(3)	2224(2)	3198.6(16)	23.0(5)
C18	1271(3)	3463(2)	3366.4(16)	24.0(5)
C16	668(3)	1049(2)	3731.5(15)	21.9(5)
C21	1599(3)	2212(2)	9777.2(16)	23.0(5)
C23	3172(3)	4677(2)	7094.3(16)	22.1(5)

Anisotropic Displacement Parameters ($Å^2×10^3$) for 20jl_PA_100K. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
P2	15.2(3)	19.0(3)	12.5(3)	0.8(2)	4.3(2)	0.9(2)
C1	19.8(11)	12.0(10)	18.4(10)	-1.2(8)	8.4(8)	2.2(8)
C2	20.0(10)	9.2(9)	16.3(10)	-2.9(8)	5.3(8)	0.4(8)
C3	27.0(12)	13.7(10)	16.3(10)	0.6(8)	9.5(9)	1.6(8)
C8	19.7(11)	16.7(10)	13.5(10)	-0.6(8)	4.1(8)	0.0(8)
C7	17.6(11)	19.3(10)	18.4(10)	-3.5(8)	9.5(9)	3.3(8)
C5	19.0(11)	17.5(10)	22.4(11)	-3.5(8)	4.1(9)	1.4(8)
C6	19.4(11)	26.9(12)	19.2(11)	-4.7(9)	5.4(9)	3.3(9)
C9	25.3(12)	17.5(11)	20.2(11)	-0.2(8)	6.1(9)	2.0(9)
C4	23.5(11)	15.3(10)	24.9(11)	-1.9(8)	13.1(9)	0.4(8)
O6	17.5(7)	16.6(7)	14.2(7)	-1.9(5)	2.1(6)	3.1(6)
O3	17.0(7)	20.0(7)	17.5(7)	3.1(6)	7.5(6)	4.5(6)
O4	16.9(7)	22.2(8)	14.7(7)	-2.2(6)	6.7(6)	1.5(6)
C15	19.5(11)	18.5(10)	15.8(10)	-1.7(8)	5.7(8)	2.9(8)

C10	16.2(10)	19.4(10)	16.7(10)	1.2(8)	9.2(8)	3.0(8)
C12	21.1(11)	16.7(10)	11.6(9)	-2.7(8)	6.7(8)	3.0(8)
C13	22.7(11)	17.5(10)	17.1(10)	1.4(8)	5.3(9)	2.3(8)
C22	23.2(11)	17.4(10)	19.9(11)	0.4(8)	6.8(9)	-0.7(8)
C20	18.3(11)	20.3(11)	13.8(10)	3.2(8)	5.3(8)	-0.1(8)
C11	16.7(10)	23.3(11)	14.0(10)	1.9(8)	3.9(8)	2.0(8)
C24	17.1(10)	16.1(10)	20.0(10)	-2.6(8)	7.9(9)	1.2(8)
C17	21.2(11)	27.5(12)	16.9(11)	-0.8(9)	-1.2(9)	4.6(9)
C18	28.9(12)	24.1(11)	19.9(11)	5.5(9)	5.3(10)	8.3(9)
C16	24.9(12)	18.6(11)	19.6(11)	-4.2(9)	3.8(9)	-1.7(9)
C21	20.4(11)	32.3(12)	18.8(11)	1.2(9)	9.6(9)	3.1(9)
C23	23.3(11)	22.7(11)	23.2(11)	5.8(9)	8.9(9)	6.6(9)

Bond Lengths for 20jl_PA_100K.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
P2	C1	1.839(2)	C5	C4	1.387(3)
P2	C8	1.875(2)	C5	C15	1.379(3)
P2	C10	1.886(2)	O3	C10	1.457(2)
C1	C2	1.414(3)	O3	C11	1.433(2)
C1	C15	1.400(3)	O4	C11	1.425(2)
C2	C3	1.391(3)	C10	C24	1.517(3)
C2	C12	1.499(3)	C10	C23	1.508(3)
C3	C4	1.381(3)	C12	C13	1.396(3)
C8	C9	1.512(3)	C12	C22	1.392(3)
C8	O6	1.453(2)	C13	C16	1.380(3)
C8	C20	1.529(3)	C22	C18	1.383(3)
C7	C6	1.503(3)	C20	C11	1.520(3)

C7	O6	1.428(2)	C11	C21	1.510(3)
C7	O4	1.428(2)	C17	C18	1.386(3)
C7	C24	1.519(3)	C17	C16	1.385(3)

Bond Angles for 20jl_PA_100K.

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
C1	P2	C8	106.00(9)	C11	O3	C10	115.15(14)
C1	P2	C10	103.94(9)	C11	O4	C7	111.66(14)
C8	P2	C10	92.54(9)	C5	C15	C1	122.31(18)
C2	C1	P2	118.61(15)	O3	C10	P2	104.84(12)
C15	C1	P2	123.59(15)	O3	C10	C24	108.12(15)
C15	C1	C2	117.80(17)	O3	C10	C23	106.52(15)
C1	C2	C12	123.43(17)	C24	C10	P2	113.37(13)
C3	C2	C1	119.10(18)	C23	C10	P2	110.92(14)
C3	C2	C12	117.48(17)	C23	C10	C24	112.51(16)
C4	C3	C2	121.88(18)	C13	C12	C2	121.45(17)
C9	C8	P2	111.16(13)	C22	C12	C2	120.15(17)
C9	C8	C20	112.51(16)	C22	C12	C13	118.31(18)
O6	C8	P2	116.19(12)	C16	C13	C12	120.65(19)
O6	C8	C9	106.37(15)	C18	C22	C12	121.00(19)
O6	C8	C20	106.87(15)	C11	C20	C8	110.51(16)
C20	C8	P2	103.81(13)	O3	C11	C20	112.12(15)
C6	C7	C24	113.16(16)	O3	C11	C21	106.02(16)
O6	C7	C6	106.56(15)	O4	C11	O3	110.14(15)
O6	C7	C24	112.15(15)	O4	C11	C20	107.80(15)
O4	C7	C6	107.00(15)	O4	C11	C21	107.46(15)
O4	C7	O6	110.05(15)	C21	C11	C20	113.19(17)

O4	C7	C24	107.79(15)	C10	C24	C7	111.00(16)
C15	C5	C4	119.47(19)	C16	C17	C18	119.44(19)
C3	C4	C5	119.42(19)	C22	C18	C17	120.09(19)
C7	O6	C8	115.19(14)	C13	C16	C17	120.50(19)

Torsion Angles for 20jl_PA_100K.

A	B	C	D	Angle/˚	A	B	C	D	Angle/˚
P2	C1	C2	C3	178.27(14)	C9	C8	O6	C7	-174.56(15)
P2	C1	C2	C12	-1.4(3)	C9	C8	C20	C11	170.05(16)
P2	C1	C15	C5	-178.64(15)	C4	C5	C15	C1	-0.1(3)
P2	C8	O6	C7	61.13(18)	O6	C8	C20	C11	53.67(19)
P2	C8	C20	C11	-69.66(17)	O6	C7	O4	C11	-60.60(19)
P2	C10	C24	C7	-63.92(18)	O6	C7	C24	C10	63.5(2)
C1	P2	C8	C9	-66.55(15)	O3	C10	C24	C7	51.9(2)
C1	P2	C8	O6	55.25(15)	O4	C7	O6	C8	57.77(19)
C1	P2	C8	C20	172.25(12)	O4	C7	C24	C10	-57.75(19)
C1	P2	C10	O3	-172.89(11)	C15	C1	C2	C3	-1.9(3)
C1	P2	C10	C24	-55.18(15)	C15	C1	C2	C12	178.45(17)
C1	P2	C10	C23	72.53(15)	C15	C5	C4	C3	-0.9(3)
C1	C2	C3	C4	0.9(3)	C10	P2	C1	C2	-106.24(16)
C1	C2	C12	C13	-61.9(3)	C10	P2	C1	C15	73.88(17)
C1	C2	C12	C22	121.6(2)	C10	P2	C8	C9	-171.84(14)
C2	C1	C15	C5	1.5(3)	C10	P2	C8	O6	-50.03(14)
C2	C3	C4	C5	0.5(3)	C10	P2	C8	C20	66.96(13)
C2	C12	C13	C16	-177.09(18)	C10	O3	C11	O4	56.40(19)
C2	C12	C22	C18	176.51(18)	C10	O3	C11	C20	-63.6(2)
C3	C2	C12	C13	118.4(2)	C10	O3	C11	C21	172.36(15)

C3	C2	C12	C22	-58.1(2)	C12	C2	C3	C4	-179.37(17)
C8	P2	C1	C2	156.94(15)	C12	C13	C16	C17	0.7(3)
C8	P2	C1	C15	-22.93(18)	C12	C22	C18	C17	0.5(3)
C8	P2	C10	O3	-65.71(13)	C13	C12	C22	C18	-0.1(3)
C8	P2	C10	C24	51.99(14)	C22	C12	C13	C16	-0.5(3)
C8	P2	C10	C23	179.70(14)	C20	C8	O6	C7	-54.15(19)
C8	C20	C11	O3	62.8(2)	C11	O3	C10	P2	69.32(16)
C8	C20	C11	O4	-58.63(19)	C11	O3	C10	C24	-51.9(2)
C8	C20	C11	C21	-177.35(16)	C11	O3	C10	C23	-173.05(15)
C7	O4	C11	O3	-61.09(19)	C24	C7	O6	C8	-62.2(2)
C7	O4	C11	C20	61.53(18)	C24	C7	O4	C11	61.99(19)
C7	O4	C11	C21	-176.15(15)	C18	C17	C16	C13	-0.3(3)
C6	C7	O6	C8	173.45(15)	C16	C17	C18	C22	-0.4(3)
C6	C7	O4	C11	-176.00(15)	C23	C10	C24	C7	169.21(16)
C6	C7	C24	C10	-175.86(16)					

Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 20jl_PA_100K.

Atom	*x*	*y*	*z*	U(eq)
H3	6335.31	2886.92	4147.89	22
H5	9779.84	2560.92	6902.89	24
H6A	7791.48	2619.04	10744.68	33
H6B	7449.5	4209.6	10636.25	33
H6C	8513.67	3512.29	9948.3	33
H9A	4088.87	-1097.85	7385.22	32
H9B	5332.99	-1119.61	8517.26	32
H9C	6030.89	-489.73	7606.97	32
H4	9160.61	3004.86	5126.08	24

H15	7570.24	2059.72	7675.82	21
H13	2623.39	305.64	4768.2	23
H22	3625.33	4362.44	4176.96	24
H20A	2083.66	391.9	8229.26	21
H20B	3391.26	132.31	9298.96	21
H24A	5477.82	4890.32	8936.26	21
H24B	6412.9	4077.06	8222.76	21
H17	-938.92	2181.88	2732.2	28
H18	935.41	4255.19	3008.49	29
H16	-80.32	216.94	3623.78	26
H21A	1596.96	3147.66	10085.68	35
H21B	1834.57	1566.08	10324.45	35
H21C	492.38	1912.25	9297.35	35
H23A	3952.1	4894.38	6668.91	33
H23B	3122.9	5510.27	7522.16	33
H23C	2044.21	4365.2	6644.55	33

Ligand 4

Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for mo_20jl_CGdavePhos_RT_solve_a. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
P1	6417.3(2)	6877.0(4)	6259.9(2)	33.53(11)
O1	6879.6(5)	4575.1(12)	5806.3(5)	46.5(3)
O2	6780.2(5)	5817.9(13)	4932.9(4)	46.2(3)
N2	6495.0(7)	8984.1(18)	7368.1(6)	60.7(4)
O3	6297.2(4)	8021.3(11)	5154.1(4)	36.8(2)
C1	5237.1(6)	8328.6(18)	5650.5(6)	42.5(3)

C00B	7297.4(6)	7222.3(18)	5802.4(6)	39.0(3)
C00D	7166.1(6)	5605.2(18)	5522.1(6)	42.8(3)
C00E	5879.5(7)	5389.3(18)	5161.0(7)	45.2(3)
C00F	6202.8(6)	6510.0(18)	4884.9(6)	41.9(3)
C00G	6776.9(7)	9757.9(18)	5928.9(7)	49.0(4)
C00L	6025.3(9)	3737(2)	6044.4(9)	61.3(5)
C00O	7741.2(8)	4760(2)	5527.3(8)	61.4(5)
C00P	5852.8(8)	6802(3)	4250.7(7)	61.4(5)
C2	4645.6(7)	8750(2)	5596.6(7)	54.1(4)
C3	4432.5(8)	8405(2)	6034.7(8)	63.5(5)
C4	4816.8(7)	7711(2)	6533.2(7)	54.9(4)
C5	5424.7(6)	7335.7(17)	6605.9(6)	38.3(3)
C005	6695.0(6)	8037.1(16)	5759.0(5)	33.5(3)
C6	5828.2(6)	6674.9(17)	7173.3(6)	39.4(3)
C7	5683.9(8)	5221(2)	7346.6(7)	50.1(4)
C8	6035.9(9)	4564(2)	7872.5(8)	63.3(5)
C9	6537.6(9)	5371(3)	8230.0(8)	68.5(6)
C009	6272.4(6)	5074.8(17)	5785.8(7)	41.1(3)
C10	6693.4(8)	6813(3)	8069.1(7)	61.3(5)
C11	6342.5(7)	7503(2)	7542.9(6)	46.4(4)
C13	7144.1(11)	9442(3)	7621.1(10)	96.3(8)
C15	5635.1(6)	7591.1(16)	6148.2(6)	34.0(3)
C14	6079.0(14)	10249(3)	7368.7(13)	105.2(9)

Anisotropic Displacement Parameters ($Å^2×10^3$) for mo_20jl_CGdavePhos_RT_solve_a. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
P1	29.12(18)	40.7(2)	33.13(18)	4.40(14)	14.00(14)	5.86(14)

O1	45.4(6)	41.8(6)	63.4(7)	7.6(5)	33.1(5)	11.9(4)
O2	42.6(5)	59.0(7)	42.9(6)	-7.0(5)	22.6(5)	3.6(5)
N2	72.6(10)	58.2(9)	50.8(8)	-8.8(7)	21.4(7)	-13.0(7)
O3	34.6(5)	43.4(5)	31.6(5)	2.2(4)	10.7(4)	1.4(4)
C1	39.2(7)	48.7(8)	41.5(8)	6.9(6)	16.8(6)	8.3(6)
C00B	28.4(6)	51.9(8)	38.7(7)	3.4(6)	14.6(5)	-0.5(6)
C00D	37.3(7)	51.1(8)	46.8(8)	4.3(7)	23.3(6)	7.6(6)
C00E	38.9(7)	46.0(8)	52.6(9)	-14.3(7)	18.9(7)	-8.1(6)
C00F	35.9(7)	52.8(9)	38.0(7)	-8.8(6)	14.3(6)	-1.7(6)
C00G	50.8(9)	42.4(8)	53.6(9)	-4.8(7)	18.3(7)	-7.6(7)
C00L	68.0(11)	39.7(8)	93.6(14)	6.4(9)	50.1(10)	-0.3(8)
C00O	52.1(9)	72.7(12)	72.7(12)	8.7(9)	38.5(9)	20.4(9)
C00P	55.2(10)	87.6(13)	37.5(8)	-9.7(8)	11.7(7)	-2.4(9)
C2	42.3(8)	63.5(10)	52.8(9)	13.5(8)	12.7(7)	19.4(8)
C3	37.4(8)	88.2(13)	69.3(11)	16.0(10)	24.5(8)	24.2(9)
C4	42.4(8)	75.9(12)	56.4(10)	11.6(8)	29.9(7)	14.7(8)
C5	35.7(7)	43.1(8)	40.2(7)	2.4(6)	18.5(6)	5.7(6)
C005	29.7(6)	39.4(7)	31.0(6)	-0.6(5)	10.5(5)	-1.1(5)
C6	39.6(7)	48.7(8)	37.1(7)	4.5(6)	22.3(6)	10.3(6)
C7	52.9(9)	55.6(9)	51.5(9)	7.7(7)	30.6(7)	6.4(7)
C8	78.0(13)	62.2(11)	63.6(11)	24.2(9)	42.0(10)	22.1(10)
C9	63.3(11)	93.9(15)	51.1(10)	26.8(10)	23.7(9)	30.2(11)
C009	38.8(7)	35.9(7)	57.0(9)	0.6(6)	27.6(7)	2.8(6)
C10	50.3(9)	89.5(14)	41.4(9)	1.3(9)	13.0(7)	10.3(9)
C11	47.8(8)	57.5(9)	37.8(7)	-1.5(7)	20.1(6)	5.8(7)
C13	96.2(17)	114(2)	70.0(14)	-18.1(13)	19.2(12)	-51.9(15)
C15	31.7(6)	36.8(7)	35.9(7)	2.3(5)	15.0(5)	4.7(5)

C14	146(2)	52.3(12)	125(2)	-8.2(13)	57.2(19)	3.7(14)

Bond Lengths for mo_20jl_CGdavePhos_RT_solve_a.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
P1	C005	1.8698(14)	C00E	C00F	1.517(2)
P1	C009	1.8813(15)	C00E	C009	1.514(2)
P1	C15	1.8385(13)	C00F	C00P	1.510(2)
O1	C00D	1.4266(18)	C00G	C005	1.509(2)
O1	C009	1.4553(16)	C00L	C009	1.512(2)
O2	C00D	1.4256(18)	C2	C3	1.377(2)
O2	C00F	1.4285(17)	C3	C4	1.371(2)
N2	C11	1.413(2)	C4	C5	1.3942(19)
N2	C13	1.462(3)	C5	C6	1.4921(19)
N2	C14	1.443(3)	C5	C15	1.4036(18)
O3	C00F	1.4231(17)	C6	C7	1.384(2)
O3	C005	1.4530(15)	C6	C11	1.405(2)
C1	C2	1.378(2)	C7	C8	1.384(2)
C1	C15	1.3964(19)	C8	C9	1.367(3)
C00B	C00D	1.516(2)	C9	C10	1.373(3)
C00B	C005	1.5282(18)	C10	C11	1.395(2)
C00D	C00O	1.511(2)			

Bond Angles for mo_20jl_CGdavePhos_RT_solve_a.

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
C005	P1	C009	92.17(6)	C4	C5	C15	119.31(13)
C15	P1	C005	106.51(6)	C15	C5	C6	122.50(12)
C15	P1	C009	103.09(6)	O3	C005	P1	115.97(8)

C00D	O1	C009	114.98(10)	O3	C005	C00B	107.23(10)
C00D	O2	C00F	111.34(10)	O3	C005	C00G	105.49(11)
C11	N2	C13	115.90(17)	C00B	C005	P1	103.93(9)
C11	N2	C14	114.67(17)	C00G	C005	P1	111.12(10)
C14	N2	C13	113.0(2)	C00G	C005	C00B	113.28(12)
C00F	O3	C005	115.25(10)	C7	C6	C5	119.08(14)
C2	C1	C15	121.51(14)	C7	C6	C11	119.01(14)
C00D	C00B	C005	110.27(11)	C11	C6	C5	121.89(13)
O1	C00D	C00B	112.23(11)	C8	C7	C6	121.53(17)
O1	C00D	C00O	105.85(13)	C9	C8	C7	119.28(18)
O2	C00D	O1	110.50(12)	C8	C9	C10	120.51(17)
O2	C00D	C00B	107.77(12)	O1	C009	P1	105.05(9)
O2	C00D	C00O	107.33(12)	O1	C009	C00E	107.96(11)
C00O	C00D	C00B	113.07(13)	O1	C009	C00L	106.10(12)
C009	C00E	C00F	110.95(11)	C00E	C009	P1	113.84(10)
O2	C00F	C00E	107.90(12)	C00L	C009	P1	110.65(11)
O2	C00F	C00P	107.04(12)	C00L	C009	C00E	112.62(14)
O3	C00F	O2	110.32(11)	C9	C10	C11	121.17(18)
O3	C00F	C00E	111.63(11)	C6	C11	N2	119.38(14)
O3	C00F	C00P	106.05(13)	C10	C11	N2	122.12(16)
C00P	C00F	C00E	113.81(13)	C10	C11	C6	118.49(16)
C3	C2	C1	119.72(15)	C1	C15	P1	125.85(10)
C4	C3	C2	120.03(14)	C1	C15	C5	118.14(12)
C3	C4	C5	121.09(14)	C5	C15	P1	116.00(10)
C4	C5	C6	118.18(13)				

Torsion Angles for mo_20jl_CGdavePhos_RT_solve_a.

A	B	C	D	Angle/˚	A	B	C	D	Angle/˚
C1	C2	C3	C4	3.0(3)	C005	O3	C00F	C00P	-172.62(11)
C00D	O1	C009	P1	-69.44(13)	C005	C00B	C00D	O1	-62.77(15)
C00D	O1	C009	C00E	52.37(16)	C005	C00B	C00D	O2	59.12(14)
C00D	O1	C009	C00L	173.32(13)	C005	C00B	C00D	C00O	177.57(12)
C00D	O2	C00F	O3	60.65(15)	C6	C5	C15	P1	5.98(19)
C00D	O2	C00F	C00E	-61.54(14)	C6	C5	C15	C1	-175.07(14)
C00D	O2	C00F	C00P	175.59(13)	C6	C7	C8	C9	0.1(2)
C00D	C00B	C005	P1	69.85(12)	C7	C6	C11	N2	179.69(14)
C00D	C00B	C005	O3	-53.47(14)	C7	C6	C11	C10	0.8(2)
C00D	C00B	C005	C00G	-169.43(12)	C7	C8	C9	C10	-0.3(3)
C00F	O2	C00D	O1	60.82(15)	C8	C9	C10	C11	0.8(3)
C00F	O2	C00D	C00B	-62.14(14)	C9	C10	C11	N2	-179.88(16)
C00F	O2	C00D	C00O	175.79(13)	C9	C10	C11	C6	-1.1(2)
C00F	O3	C005	P1	-62.20(12)	C009	P1	C005	O3	50.25(10)
C00F	O3	C005	C00B	53.35(14)	C009	P1	C005	C00B	-67.15(9)
C00F	O3	C005	C00G	174.37(11)	C009	P1	C005	C00G	170.69(10)
C00F	C00E	C009	P1	63.85(14)	C009	P1	C15	C1	-72.61(14)
C00F	C00E	C009	O1	-52.36(15)	C009	P1	C15	C5	106.24(12)
C00F	C00E	C009	C00L	-169.15(12)	C009	O1	C00D	O2	-56.71(15)
C2	C1	C15	P1	176.58(13)	C009	O1	C00D	C00B	63.61(16)
C2	C1	C15	C5	-2.3(2)	C009	O1	C00D	C00O	-172.61(13)
C2	C3	C4	C5	-0.3(3)	C009	C00E	C00F	O2	57.99(15)
C3	C4	C5	C6	176.27(17)	C009	C00E	C00F	O3	-63.39(15)
C3	C4	C5	C15	-3.6(3)	C009	C00E	C00F	C00P	176.61(13)
C4	C5	C6	C7	64.36(19)	C11	C6	C7	C8	-0.4(2)
C4	C5	C6	C11	-114.14(17)	C13	N2	C11	C6	-153.70(16)

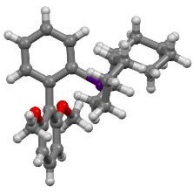
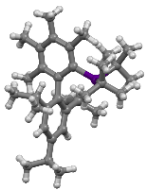
C4	C5	C15	P1	-174.11(13)	C13	N2	C11	C10	25.1(2)
C4	C5	C15	C1	4.8(2)	C15	P1	C005	O3	-54.08(11)
C5	C6	C7	C8	-178.92(14)	C15	P1	C005	C00B	-171.48(9)
C5	C6	C11	N2	-1.8(2)	C15	P1	C005	C00G	66.35(11)
C5	C6	C11	C10	179.33(13)	C15	P1	C009	O1	173.40(9)
C005	P1	C009	O1	65.89(9)	C15	P1	C009	C00E	55.51(11)
C005	P1	C009	C00E	-52.00(10)	C15	P1	C009	C00L	-72.51(12)
C005	P1	C009	C00L	179.98(11)	C15	C1	C2	C3	-1.7(3)
C005	P1	C15	C1	23.67(15)	C15	C5	C6	C7	-115.73(16)
C005	P1	C15	C5	-157.47(11)	C15	C5	C6	C11	65.8(2)
C005	O3	C00F	O2	-57.06(14)	C14	N2	C11	C6	71.8(2)
C005	O3	C00F	C00E	62.91(14)	C14	N2	C11	C10	-109.4(2)

Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for mo_20jl_CGdavePhos_RT_solve_a.

Atom	*x*	*y*	*z*	U(eq)
H1	5374.26	8540.58	5348.58	51
H00A	7514.42	7862.34	5611.94	47
H00B	7559.04	7113.6	6205.24	47
H00C	5488.79	5844.21	5140.63	54
H00D	5794.81	4400.34	4949.42	54
H00E	6385.05	10202.7	5894.85	74
H00F	6941	10315.14	5678.76	74
H00G	7056.61	9850.24	6321.12	74
H00H	6309.11	3518.13	6427.19	92
H00I	5977.13	2810.31	5808.86	92
H00J	5632.93	4032.02	6061.19	92
H00K	8008.87	4580.54	5919.37	92

H00L	7950.5	5396.07	5334.44	92
H00M	7629.57	3765.06	5331.52	92
H00N	6095.94	7453.71	4097.21	92
H00O	5471	7326.03	4202.79	92
H00P	5769.06	5811.51	4048.75	92
H2	4391.57	9264.56	5265.64	65
H3	4027.53	8642.11	5992.45	76
H4	4669.54	7487.22	6827.72	66
H7	5342.25	4672.87	7103.96	60
H8	5932.46	3584.82	7981.55	76
H9	6775.06	4938.84	8584.92	82
H10	7039.17	7339.73	8315.19	74
H13A	7248.17	9655.22	8025.21	145
H13B	7212.42	10373.41	7431.28	145
H13C	7397.71	8598.47	7572.85	145
H14A	5661.56	9916.5	7167.41	158
H14B	6167.35	11156.91	7179.38	158
H14C	6131.28	10516.58	7759.71	158

Table S3: Crystal data and refinement parameters for SPhos[1] (**5**) and tetramethyl-^{t}BuXPhos[2] (**11**).[a]

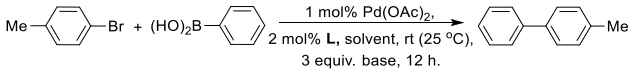
Crystal structure		
Ligand	SPhos	tetramethyl-^{t}BuXPhos
CCDC code	IYUREB	YUTZOD
Empirical formula	$C_{26}H_{35}O_2P$	$C_{33}H_{53}P$
Formula weight	410.51	480.72
Temperature/K	100	100(2)

Crystal system	orthorhombic	N/A
Space group	*Pbca*	*P*-1
a/Å	16.2168(15)	11.2779(5)
b/Å	15.5468(12)	15.8314(7)
c/Å	17.9870(15)	17.6683(8)
α/°	90	76.5310(10)
β/°	90	83.3630(10)
γ/°	90	79.6560(10)
Volume/Å^3	4534.9(7)	3009.0(2)
Z	8	4
ρ_{calc}g/cm^3	1.203	1.061
μ/mm^{-1}	0.140	0.109
F(000)	1776.0	1064.0
Crystal size/mm^3	0.33 × 0.3 × 0.29	0.40 × 0.33 × 0.20
Radiation	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.53 to 54.238	2.38 to 41.62
Index ranges	-20 ≤ h ≤ 20, -18 ≤ k ≤ 19, -22 ≤ l ≤ 22	-11 ≤ h ≤ 5, -15 ≤ k ≤ 15, -17 ≤ l ≤ 17
Reflections collected	23770	10069
Independent reflections	5001 [R_{int} = 0.0587, R_{sigma} = 0.0523]	5990 [R_{int} = 0.0216, R_{sigma} = N/A]
Data/restraints/parameters	5001/0/264	5990/0/645
Goodness-of-fit on F^2	1.010	1.030
Final R indexes [I>=2σ (I)]	R_1 = 0.0436, wR_2 = 0.0897	R_1 = 0.0602, wR_2 = 0.1657
Final R indexes [all data]	R_1 = 0.0741, wR_2 = 0.1035	R_1 = 0.0667, wR_2 = 0.1740
Largest diff. peak/hole / e Å^{-3}	0.35/-0.30	1.08/-0.34

[a]The CIF files were retrieved from CCDC as per references.

Catalytic evaluation

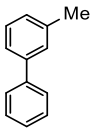
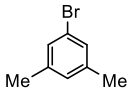
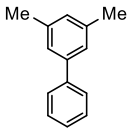
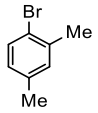
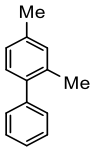
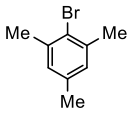
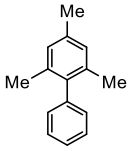
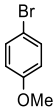
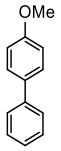
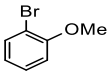
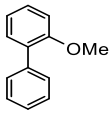
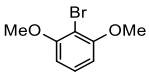
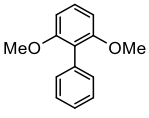
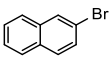
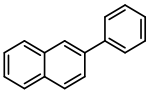
Table S4: Determination of suitable conditions for room temperature coupling reactions.[a]

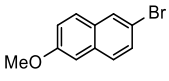
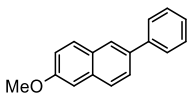
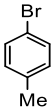
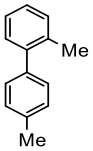
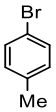
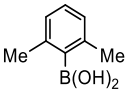
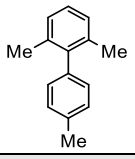
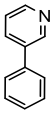
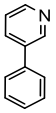
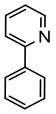


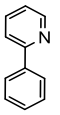
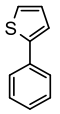
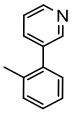
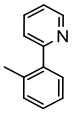
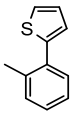
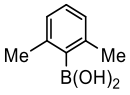
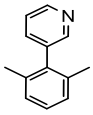
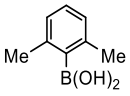
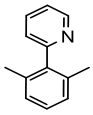
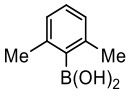
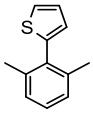
Entry	Pd source	ligand	Base	solvent	Yield (%)[b]
1	$Pd(OAc)_2$	**1**	KF	THF	69
2	$Pd(OAc)_2$	**3**	KF	THF	91
3	$Pd(OAc)_2$	**1**	CsF	THF	32
4	$Pd(OAc)_2$	**3**	CsF	THF	57
5	$Pd(OAc)_2$	**1**	TBAF	THF	40
6	$Pd(OAc)_2$	**3**	TBAF	THF	42
7	$Pd(OAc)_2$	**1**	K_3PO_4	THF	62
8	$Pd(OAc)_2$	**3**	K_3PO_4	THF	90
9	$Pd(OAc)_2$	**1**	K_2CO_3	THF	71
10	$Pd(OAc)_2$	**3**	K_2CO_3	THF	40
11	$Pd(OAc)_2$	**1**	Cs_2CO_3	THF	37
12	$Pd(OAc)_2$	**3**	Cs_2CO_3	THF	41
13	$Pd(OAc)_2$	**1**	Cy_2NMe	THF	49
14	$Pd(OAc)_2$	**3**	Cy_2NMe	THF	31
15	**$Pd(OAc)_2$**	**1**	**KOH**	**THF**	**100**
16	**$Pd(OAc)_2$**	**3**	**KOH**	**THF**	**100**
17	$Pd(OAc)_2$	**1**	KOH	Toluene	99
18	$Pd(OAc)_2$	**3**	KOH	Toluene	89
19	$Pd(OAc)_2$	**1**	K_3PO_4	Toluene	76
20	$Pd(OAc)_2$	**3**	K_3PO_4	Toluene	72
21	$Pd(OAc)_2$	**1**	K_2CO_3	Toluene	48
22	$Pd(OAc)_2$	**3**	K_2CO_3	Toluene	61
23	$Pd(OAc)_2$	**1**	KOH	Dioxane	86
24	$Pd(OAc)_2$	**3**	KOH	Dioxane	88
25	$Pd(OAc)_2$	**1**	K_3PO_4	Dioxane	83
26	$Pd(OAc)_2$	**3**	K_3PO_4	Dioxane	85
27	$Pd(OAc)_2$	**1**	K_2CO_3	Dioxane	2
28	$Pd(OAc)_2$	**3**	K_2CO_3	Dioxane	7
29	$Pd(OAc)_2$	**1**	KOH	DMA	71
30	$Pd(OAc)_2$	**3**	KOH	DMA	95
31	$Pd(OAc)_2$	**1**	K_3PO_4	DMA	0
32	$Pd(OAc)_2$	**3**	K_3PO_4	DMA	28
33	$Pd(OAc)_2$	**1**	K_2CO_3	DMA	21
34	$Pd(OAc)_2$	**3**	K_2CO_3	DMA	6
35	$Pd(OAc)_2$	**1**	KOH	DMF	72
36	$Pd(OAc)_2$	**3**	KOH	DMF	78
19	$Pd(OAc)_2$	**1**	K_3PO_4	DMF	17
20	$Pd(OAc)_2$	**3**	K_3PO_4	DMF	49
21	$Pd(OAc)_2$	**1**	K_2CO_3	DMF	11
22	$Pd(OAc)_2$	**3**	K_2CO_3	DMF	23

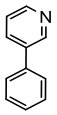
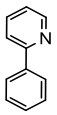
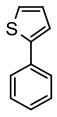
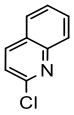
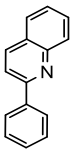
Reaction conditions: aryl bromide (1 equiv.), arylboronic acid (1.5 equiv.), base (3 equiv.), 1 mol% $Pd(OAc)_2$, 2 mol% **L**, Ar, 12 h, rt. KOH was dissolved in MeOH (2M base solution). [b]GC yield from an average of two runs with <5% deviation. In all cases coupling was selective to the desired product. Thus, conversion = GC yield

Table S5: Substrate screening

Entry	ArX	$ArB(OH)_2$	Product	Ligand	Conversion (%)	Selectivity (%)[a]	GC Yield (%)
1				**1**	100	100	100
				2	100	96	96
				3	100	97	97
				4	51	96	49
2				**1**	100	100	100
				2	87	85	74
				3	100	97	97
				4	14	80	11
				PPh_3	26	44	11
3				**1**	100	98	98
				2	22	40	9
				3	100	93	93
				4	37	87	32
				PPh_3	32	28	9
4				**1**	100	76	76
				2	41	11	4
				3	82	65	53
				4	31	46	14
				PPh_3	11	46	5
5				**1**	97	90	87
				2	100	91	91
				3	100	96	96
				4	57	94	54
6				**1**	100	98	98
				2	27	49	14
				3	100	95	95
				4	32	70	22
				PPh_3	45	27	28
7				**1**	100	97	97
				2	48	20	10
				3	100	94	94
				4	15	49	7
				PPh_3	12	13	2
8				**1**	100	100	100
				2	100	75	75
				3	100	95	95

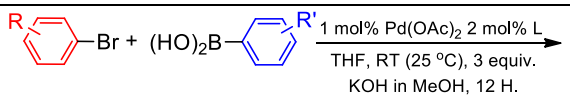
				4	90	80	72
9[b]				**1**	100	-	-
				2	100	-	-
				3	100	-	-
				4	70	-	-
10				**1**	100	93	93
				2	100	88	88
				3	100	91	91
				4	95	76	72
11				**1**	76	85	64
				2	19	40	11
				3	81	93	76
				4	40	60	24
12				**1**	89	97	86
				2	79	0	0
				3	74	0	0
				4	67	0	0
				5	82	0	0
				6	75	0	0
				7	75	0	0
				8	67	0	0
13[c]				**1**	43	100	20
				2	88	100	88
				3	91	100	91
				4	94	100	94
				5	89	100	89
				6	87	100	87
				7	100	100	100
				8	74	100	74
14				**1**	100	100	100
				2	84	91	76
				3	73	34	25
				4	100	34	34
				5	61	87	53
				6	30	92	28
				7	100	0	0
				8	100	0	0
				PPh_3	24	83	20
15[c]				**1**	43	100	43
				2	15	100	15

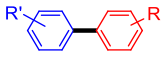
				**3**	88	100	88
				4	85	100	85
				5	22	100	22
				6	18	100	18
				7	90	100	90
				8	35	100	35
				PPh_3	11	100	11
16[c]				**1**	59	100	59
				2	100	100	100
				3	91	100	91
				4	85	100	85
				5	96	100	96
				6	88	100	88
				7	91	100	91
				8	65	100	65
17				**2**	78	100	78
				4	100	100	100
				5	93	100	93
				7	75	100	75
18				**1**	100	100	100
				3	84	100	84
				5	84	92	78
				7	37	100	37
19				**2**	95	100	95
				3	12	100	12
				5	30	100	30
				7	67	100	67
20				**2**	20	100	20
				4	0	0	0
				5	0	0	0
				7	14	0	0
21				**1**	100	100	100
				3	0	0	0
				5	15	0	0
				7	100	0	0
22				**2**	53	100	53
				3	0	0	0
				5	9	36	3
				7	10	57	6

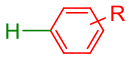
23				**1**	100	100	100
				2	100	100	100
				3	100	100	100
				5	100	100	100
				6	100	100	100
				7	100	100	100
				PPh_3	0	0	0
24				**1**	100	100	100
				2	100	100	100
				3	100	100	100
				5	100	100	100
				6	100	100	100
				7	0	0	0
25				**1**	88	100	88
				2	91	100	91
				3	90	100	90
				5	98	100	98
				6	99	100	99
				7	53	100	53
				PPh_3	0	0	0
26				**1**	100	100	100
				2	100	100	100
				3	100	100	100
				5	100	100	100
				6	100	100	100
				7	0	0	0

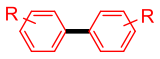
[a]Selectivity was calculated from side product(s) derived from the aryl halide. Identified side reactions include dehalogenation, dehalomethoxylation and homo-coupling. [b]Product peak unidentified from GC-FID. [c]KF used as a base.

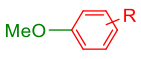
Table S6: Product distributions for room temperature cross-coupling reactions.[a]



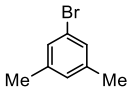
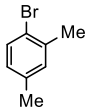
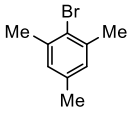
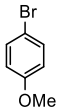


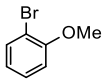
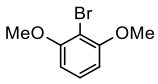
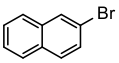
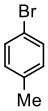
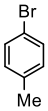
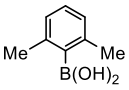


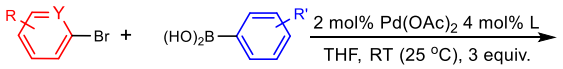




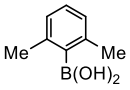
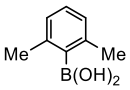
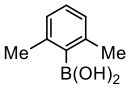
Entry	ArBr	$ArB(OH)_2$	Ligand	Desired product (%)	Dehalogen-ation (%)	Homo-coupling (%)	Dehalomet hoxylation (%)
1			**1**	100	0	0	0
			2	96	4	0	0
			3	97	3	0	0

			4	49	2	0	0
			PPh_3	45	12	7	0
2			**1**	100	0	0	0
			2	74	13	0	0
			3	97	3	0	0
			4	11	3	0	0
			PPh_3	11	9	5	0
3			**1**	98	2	0	0
			2	9	6	0	7
			3	93	7	0	0
			4	32	5	0	0
			PPh_3	9	20	3	0
4			**1**	76	24	0	0
			2	4	9	0	27
			3	53	29	0	0
			4	5	16	0	0
			PPh_3	5	6	0	0
5			**1**	87	10	0	0
			2	91	9	0	0
			3	96	4	0	0
			4	54	4	0	0
			PPh_3	25	18	11	0
6			**1**	98	2	0	0

			**2**	13	14	0	0
			3	95	5	0	0
			4	22	10	0	0
			PPh_3	12	28	5	0
7			**1**	97	3	0	0
			2	10	38	0	0
			3	94	6	0	0
			4	7	8	0	0
			PPh_3	2	11	0	0
8			**1**	100	0	0	0
			2	75	7	0	18
			3	95	5	0	0
			4	72	18	0	0
			PPh_3	32	57	0	0
10			**1**	93	7	0	0
			2	88	12	0	0
			3	91	9	0	0
			4	72	23	0	0
			PPh_3	30	28	3	0
11			**1**	64	6	6	0
			2	8	11	0	0
			3	76	6	0	0
			4	24	9	7	0
			PPh_3	38	9	5	0

							
12			**1**	86	3	0	0
			2	10	5	0	0
			3	0	7	0	0
			4	0	6	0	0
			5	9	5	0	0
			6	9	6	0	0
			7	0	5	0	0
			8	0	6	8	0
13			**1**	100	0	0	0
			2	76	3	0	5
			3	25	0	0	48
			4	34	0	0	66
			5	51	2	0	8
			6	27	1	0	2
			7	0	0	0	100
			8	0	0	0	100
			PPh_3	20	0	0	4
14[b]			**1**	43	0	0	0
			2	88	0	0	0
			3	91	0	0	0
			4	94	0	0	0
			5	89	0	0	0
			6	87	0	0	0
			7	100	0	0	0

			8	74	0	0	0
15[b]			**1**	43	0	0	0
			2	15	0	0	0
			3	88	0	0	0
			4	85	0	0	0
			5	22	0	0	0
			6	18	0	0	0
			7	90	0	0	0
			8	35	0	0	0
			PPh_3	11	0	0	0
16[cd]			**1**	59	0	0	0
			2	100	0	0	0
			3	91	0	0	0
			4	85	0	0	0
			5	96	0	0	0
			6	88	0	0	0
			7	90	0	0	0
			8	65	0	0	0
17			**2**	78	0	0	0
			4	100	0	0	0
			5	93	0	0	0
			7	75	0	0	0
18			**1**	100	0	0	0
			3	84	0	0	0

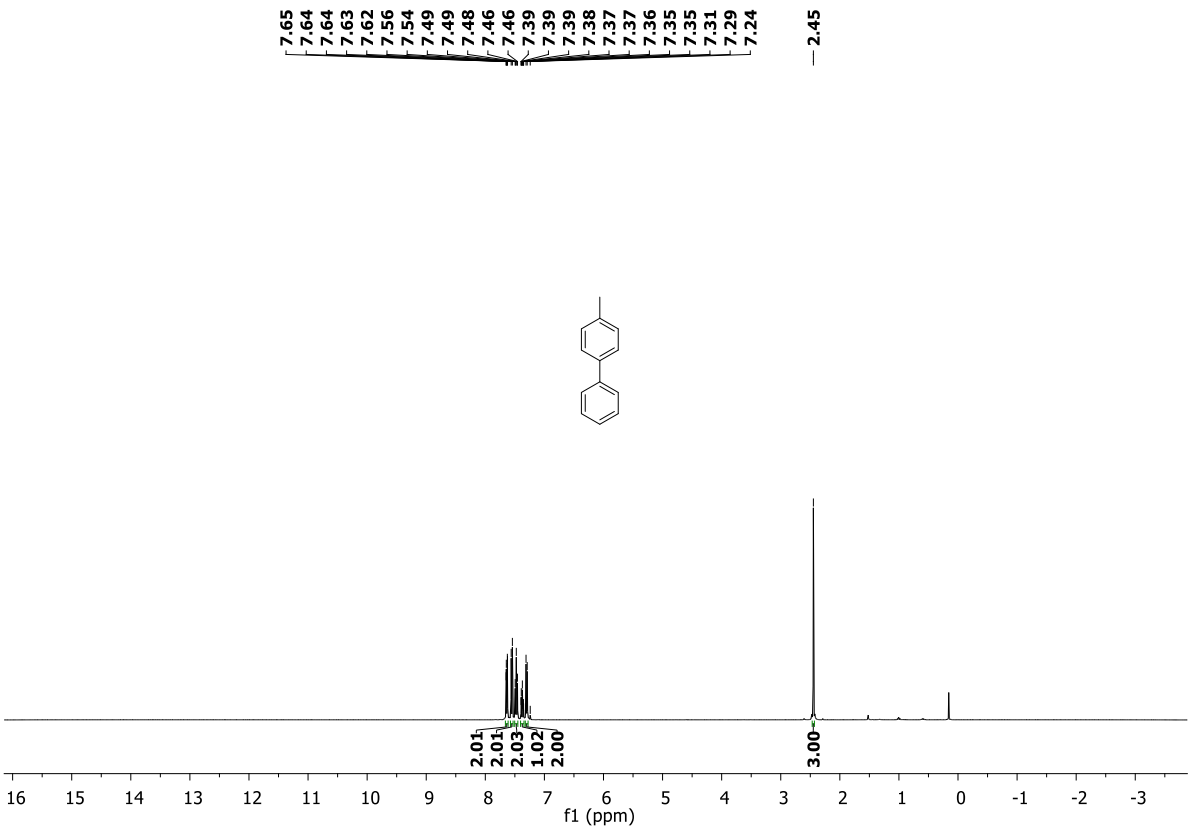
			5	78	0	6	0
			7	37	0	0	0
19			**2**	95	0	0	0
			3	12	0	0	0
			5	30	0	0	0
			7	67	0	0	0
20			**2**	20	0	0	0
			4	0	28	0	0
			5	0	27	0	0
			7	0	12	2	0
21			**1**	100	0	0	0
			3	0	0	0	0
			5	0	0	0	0
			7	0	0	0	0
22			**2**	53	0	0	0
			3	0	0	0	0
			5	3	0	6	0
			7	6	0	4	0

[a]GC yields (%) of identified side products derived from the aryl halide. The mechanism of dehalogenation, homo-coupling, and dehalomethoxylation can be retrieved from the provided references.[3–8] [b]KF used as the base. [c]Yields were lower/moderate with KOH as the base, ligand **1** (42%) and **3** (63%). Reactions with aryl chlorides were selective towards the desired product, i.e no side reaction(s). Also see attached GC chromatograms.

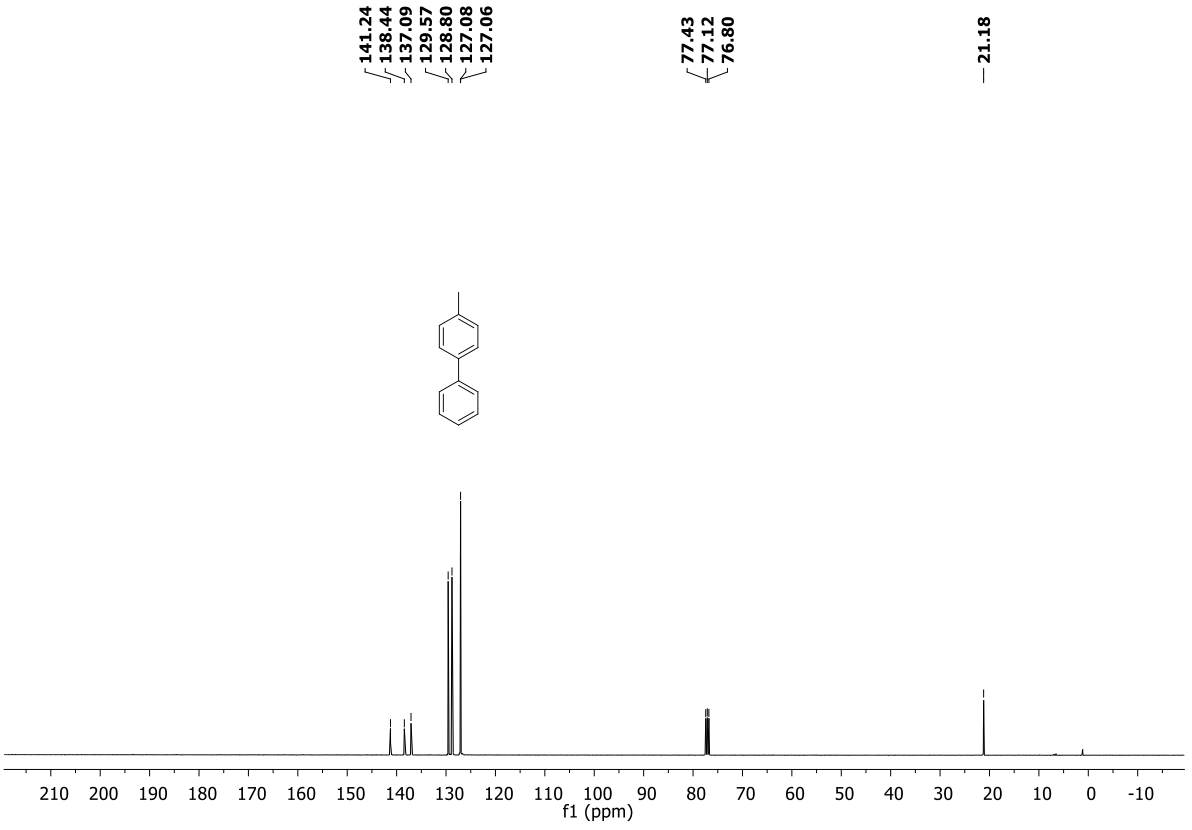
NMR spectra: Suzuki products

4-Methyl-biphenyl

^{1}H-NMR ($CDCl_3$)

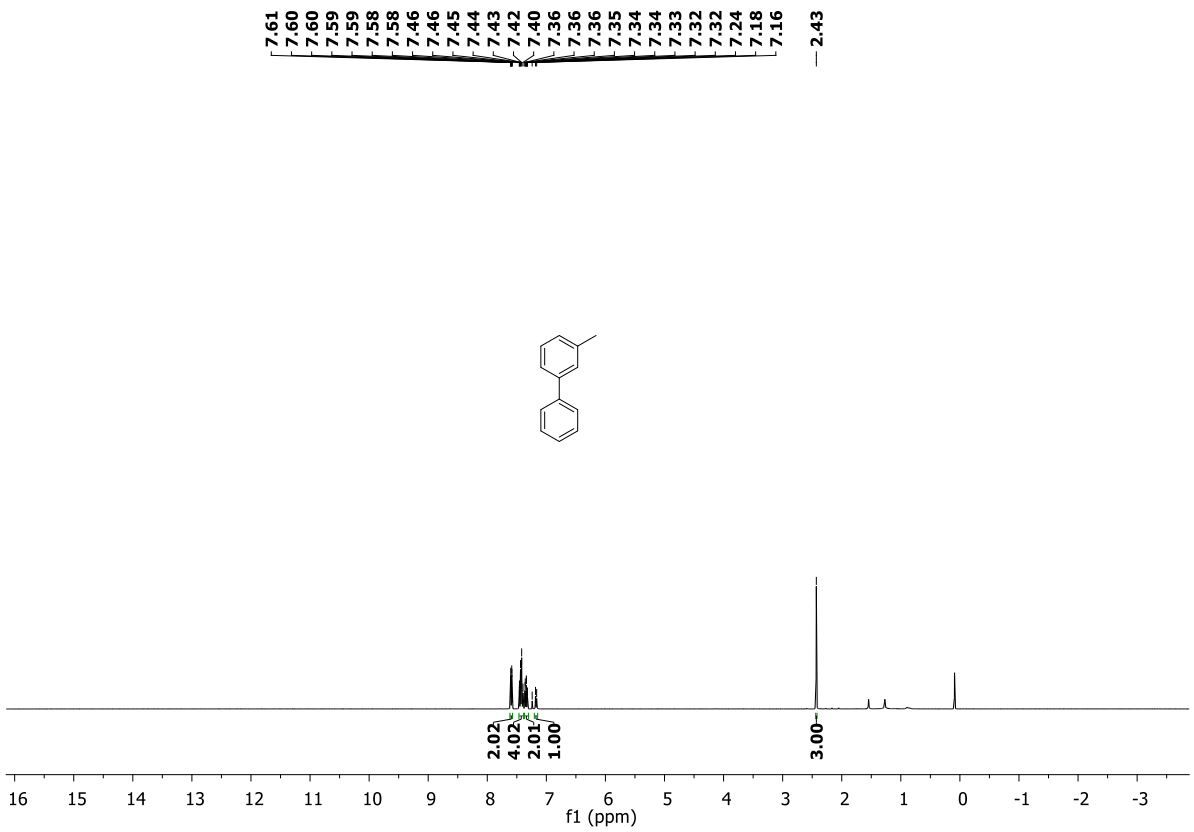


^{13}C-NMR ($CDCl_3$)

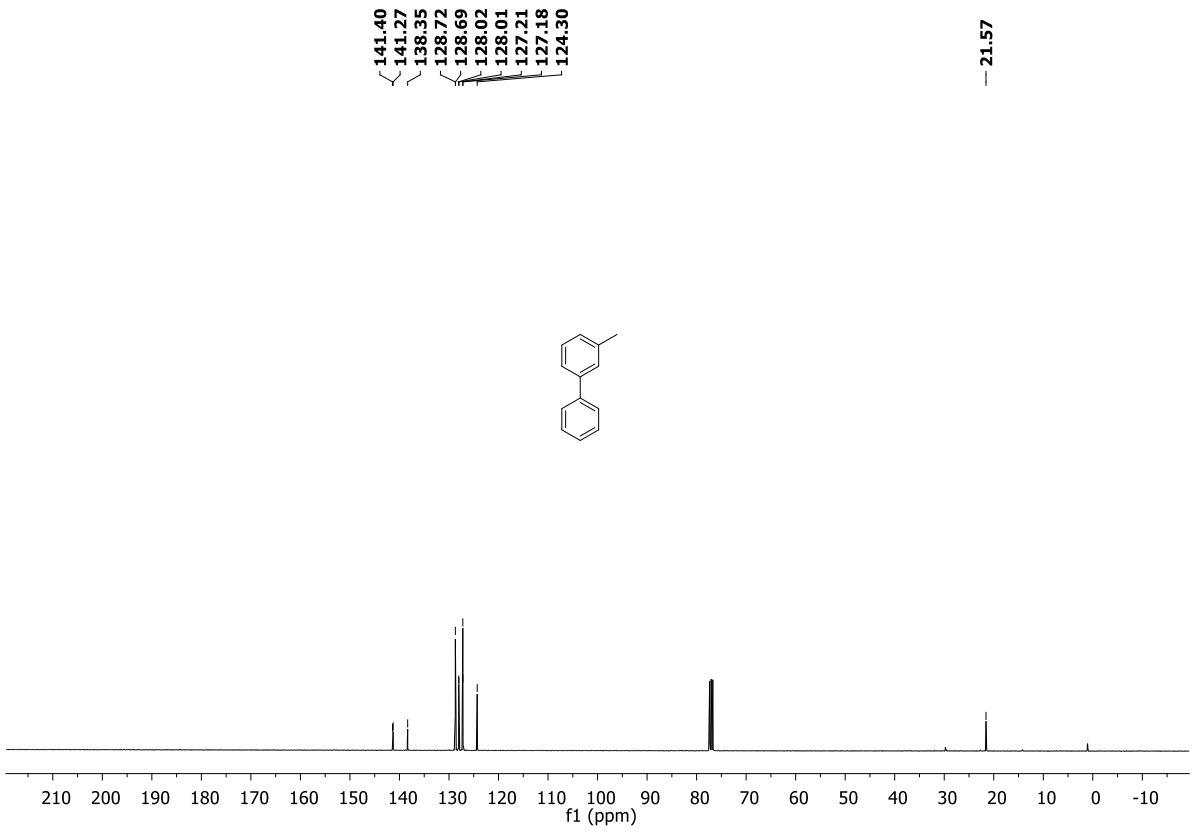


3-Methyl-biphenyl

^{1}H-NMR ($CDCl_3$)

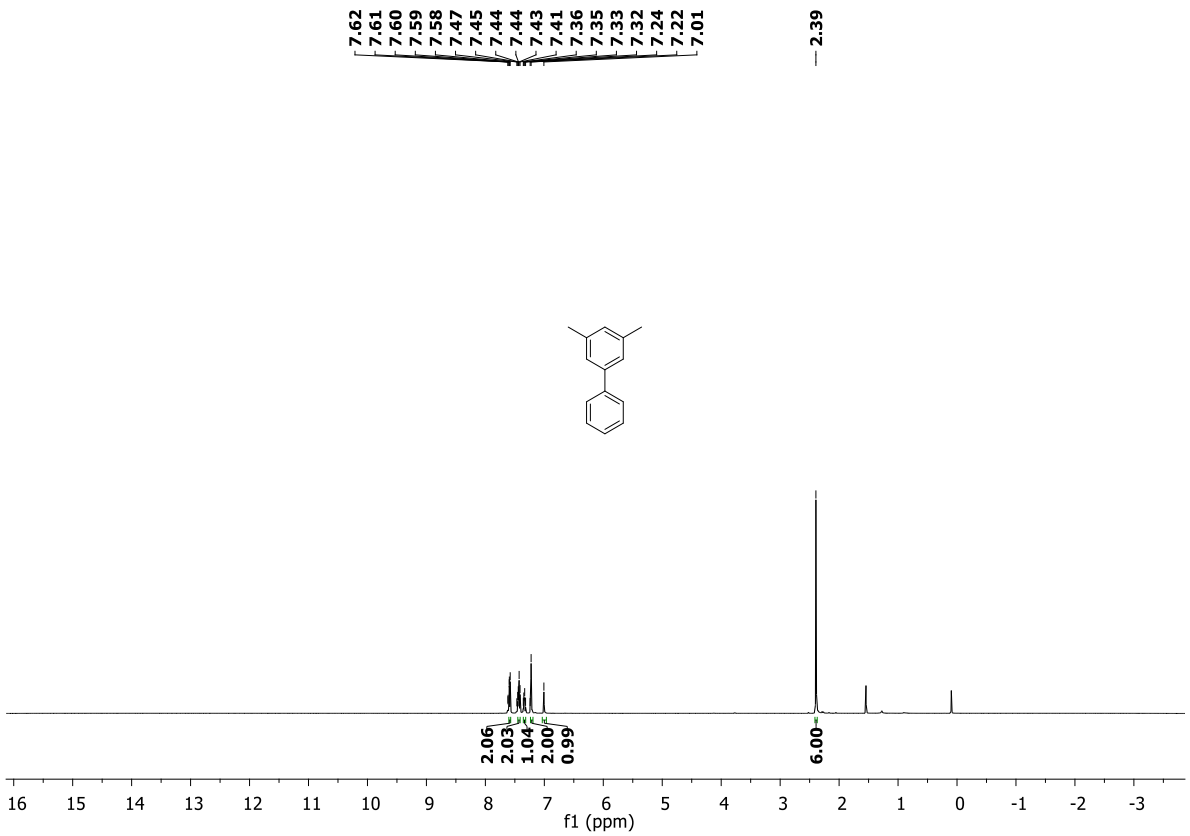


^{13}C-NMR ($CDCl_3$)

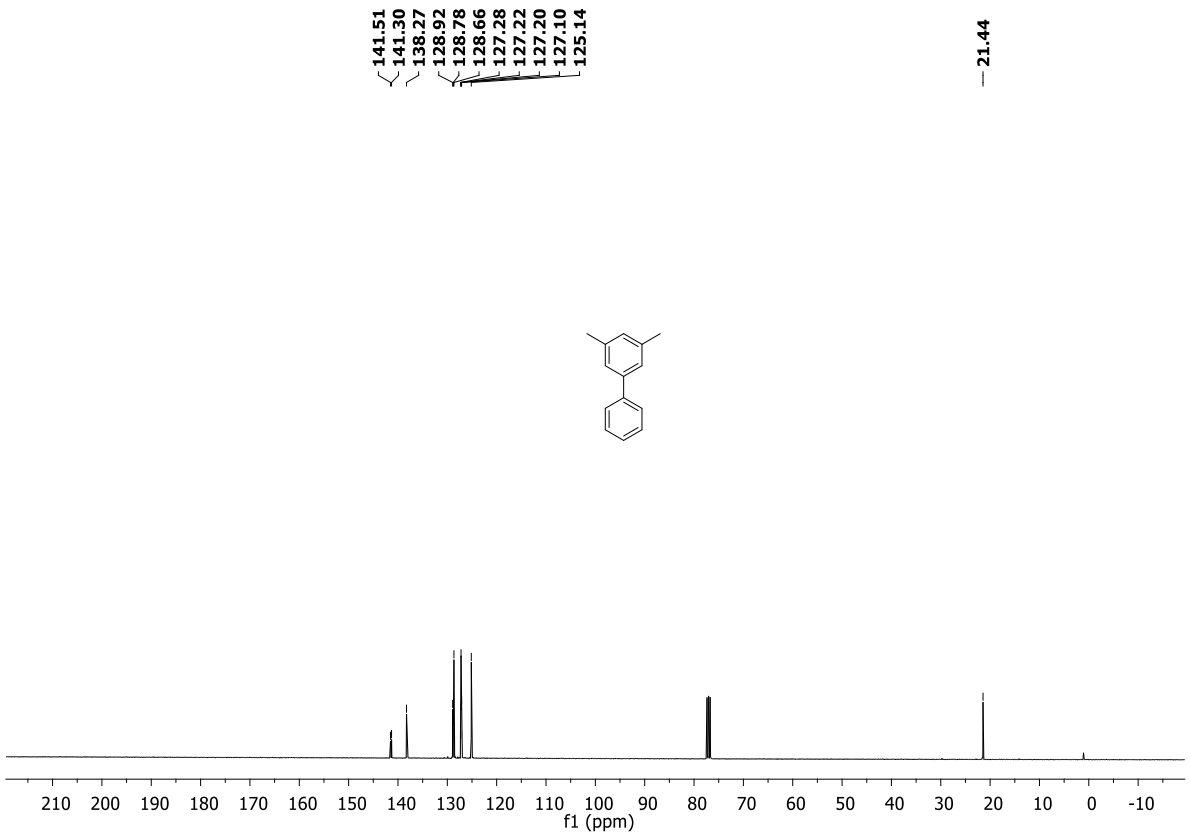


3,5-Dimethyl-1,1'-biphenyl

^{1}H-NMR ($CDCl_3$)

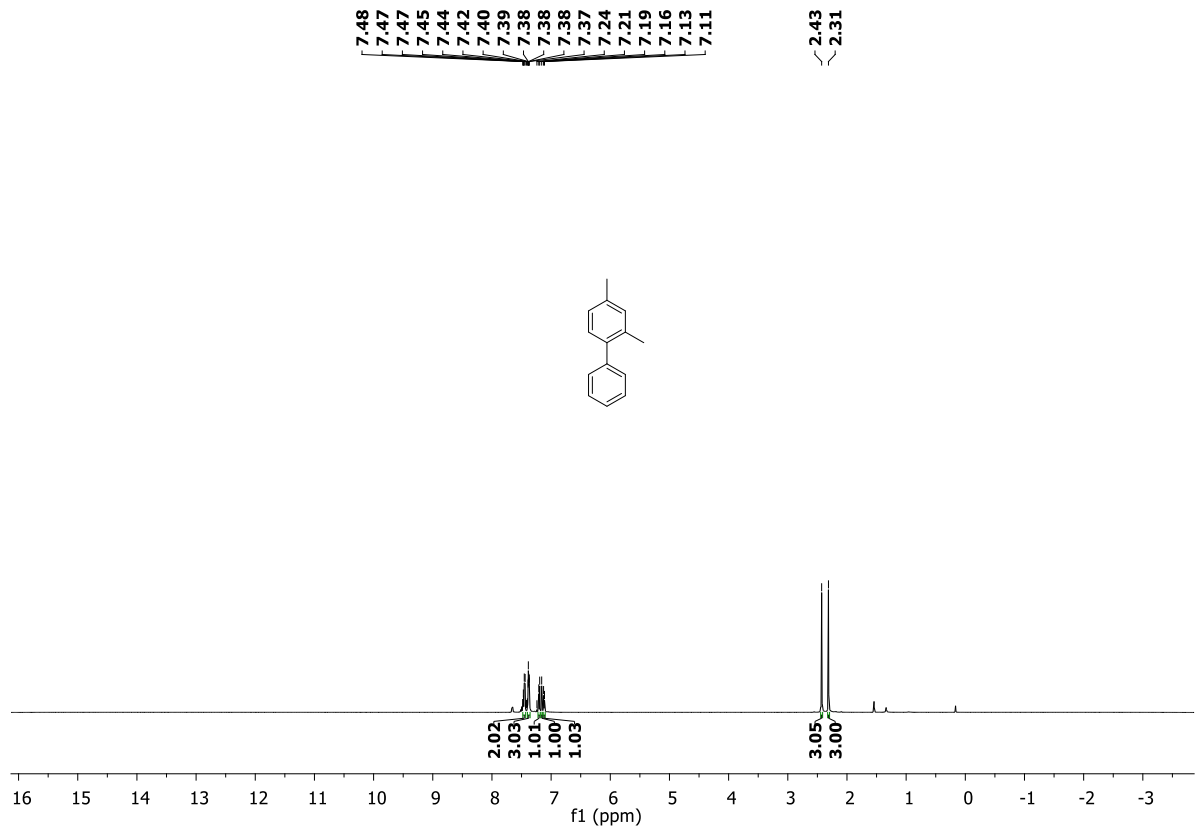


^{13}C-NMR ($CDCl_3$)

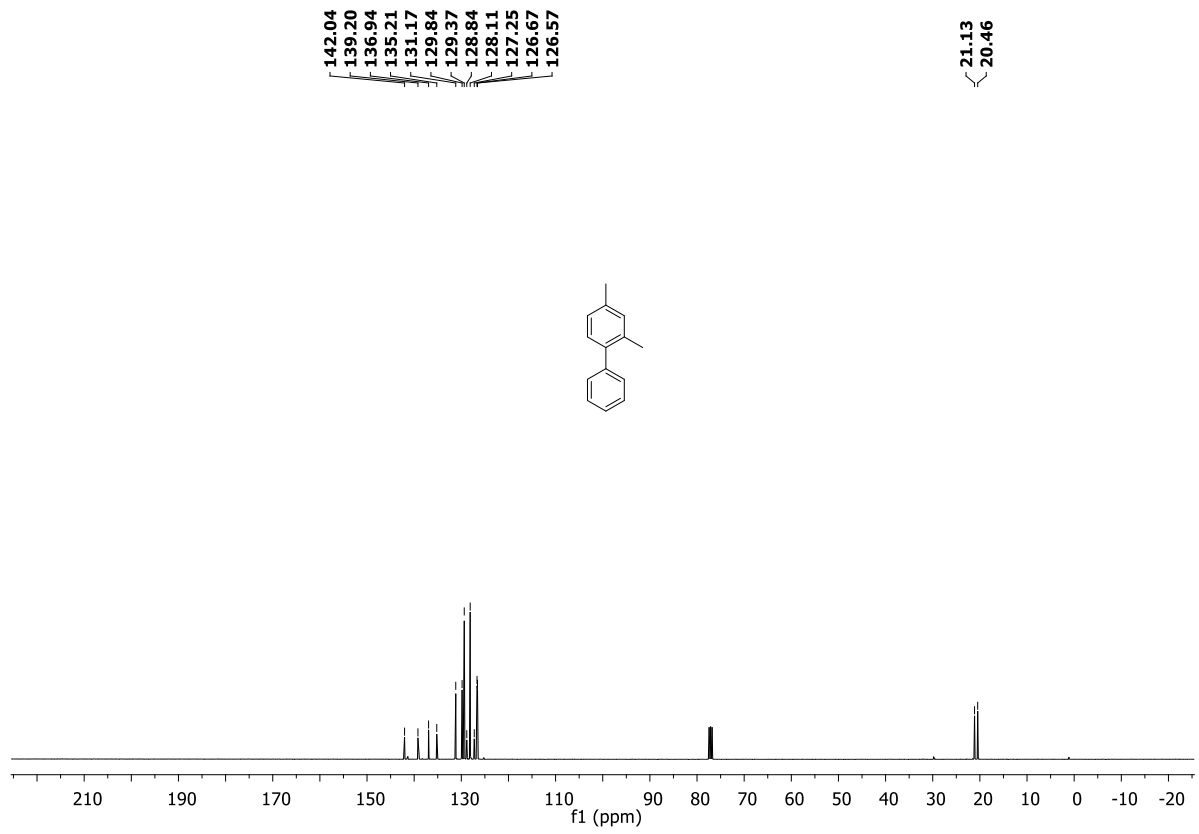


2,4-Dimethyl-1,1'-biphenyl

^{1}H-NMR ($CDCl_3$)

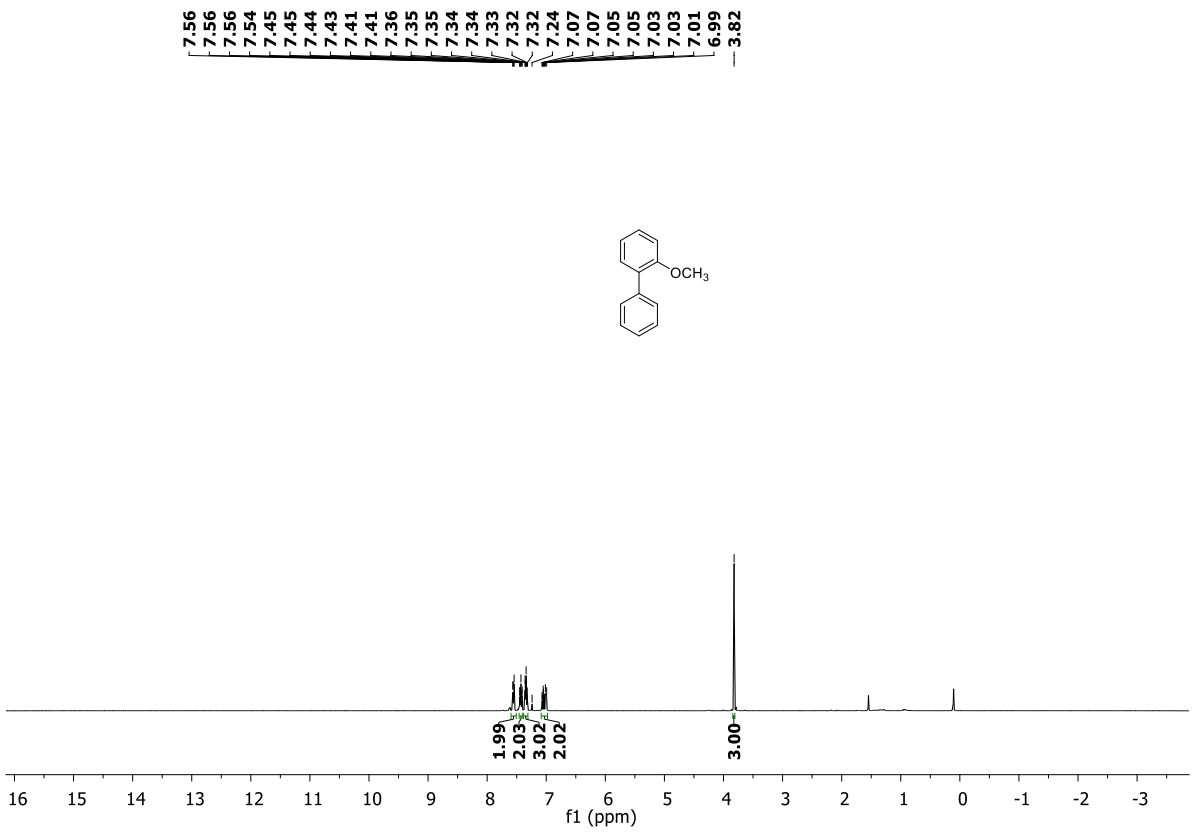


^{13}C-NMR ($CDCl_3$)

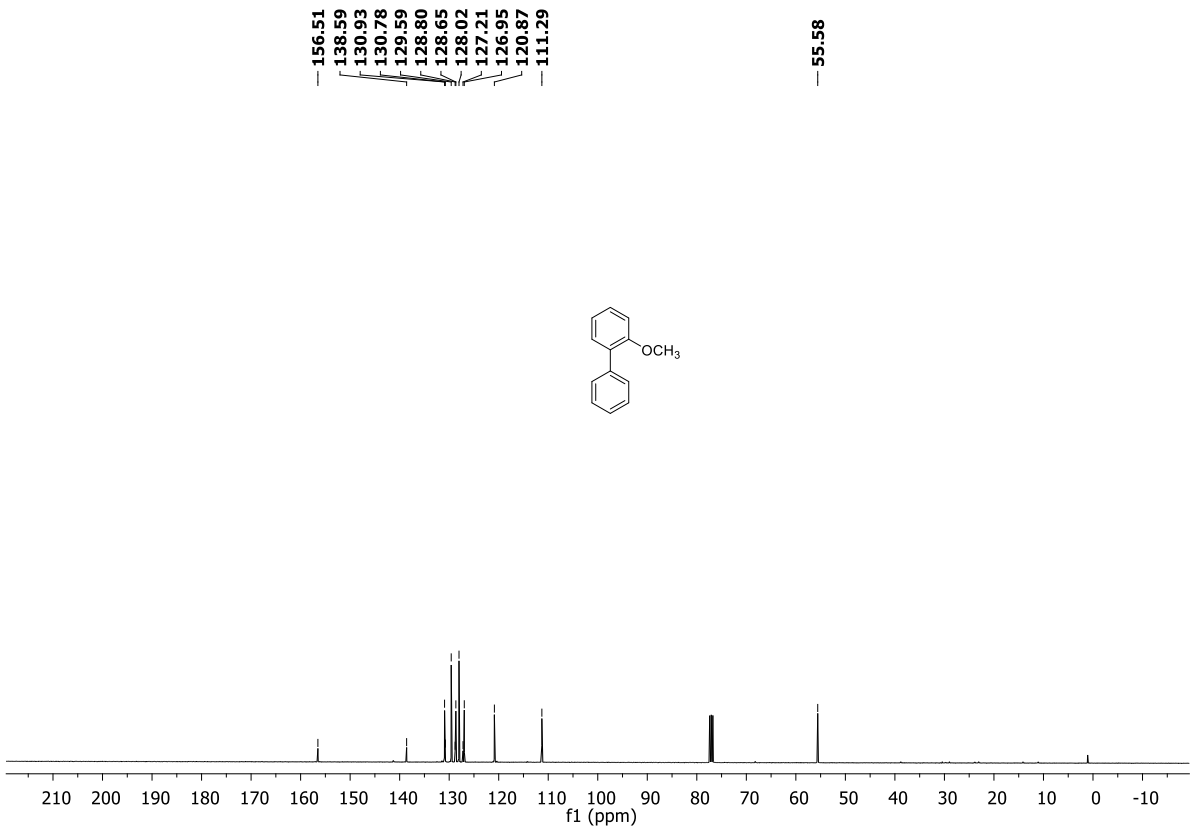


2-Methoxy-biphenyl

^{1}H-NMR ($CDCl_3$)

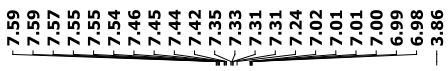


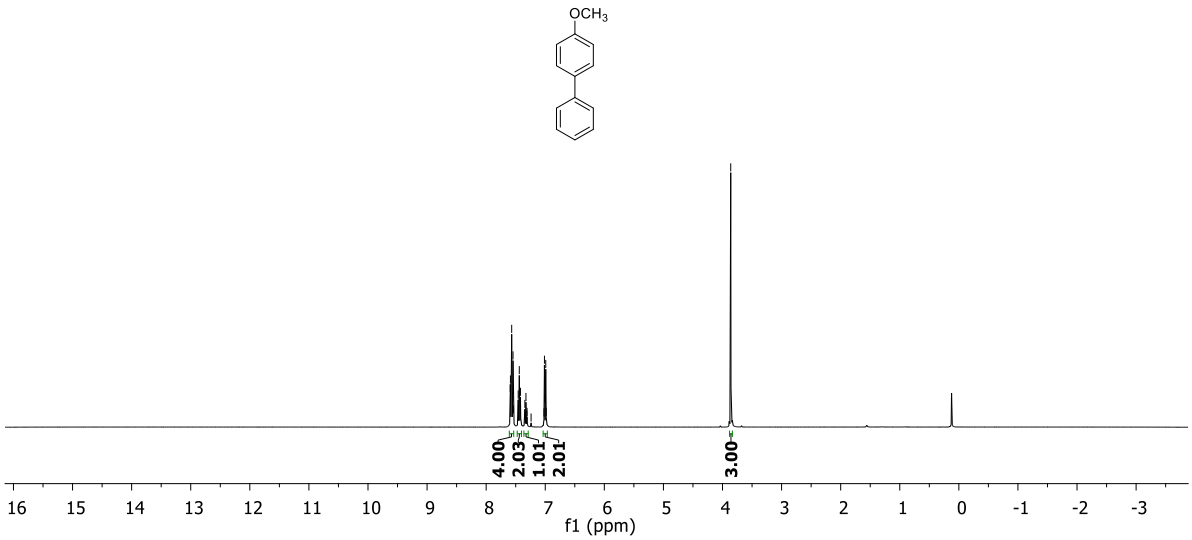
^{13}C-NMR ($CDCl_3$)



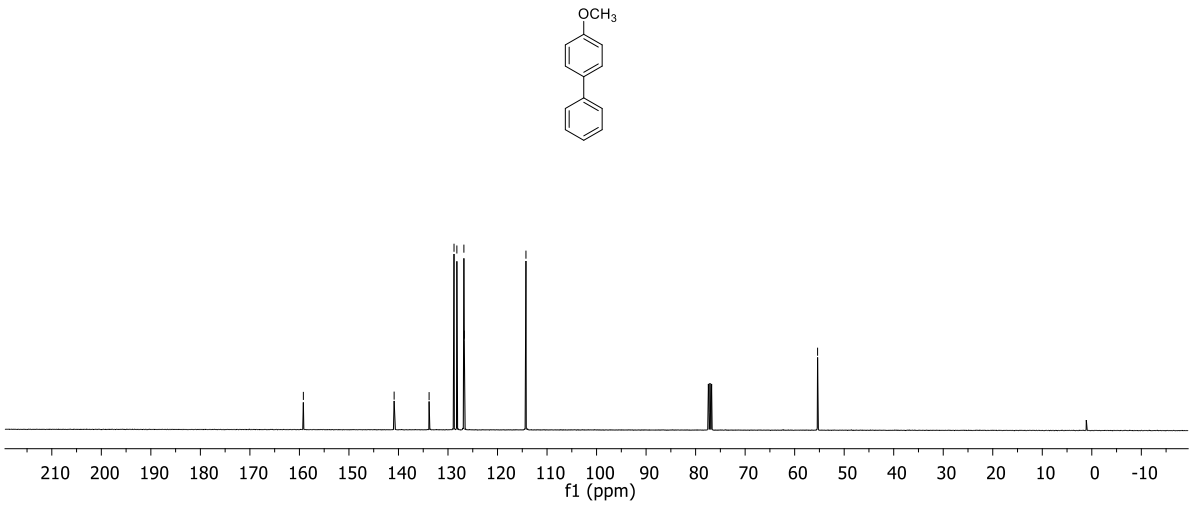
4-Methoxy-biphenyl

^{1}H-NMR ($CDCl_3$)



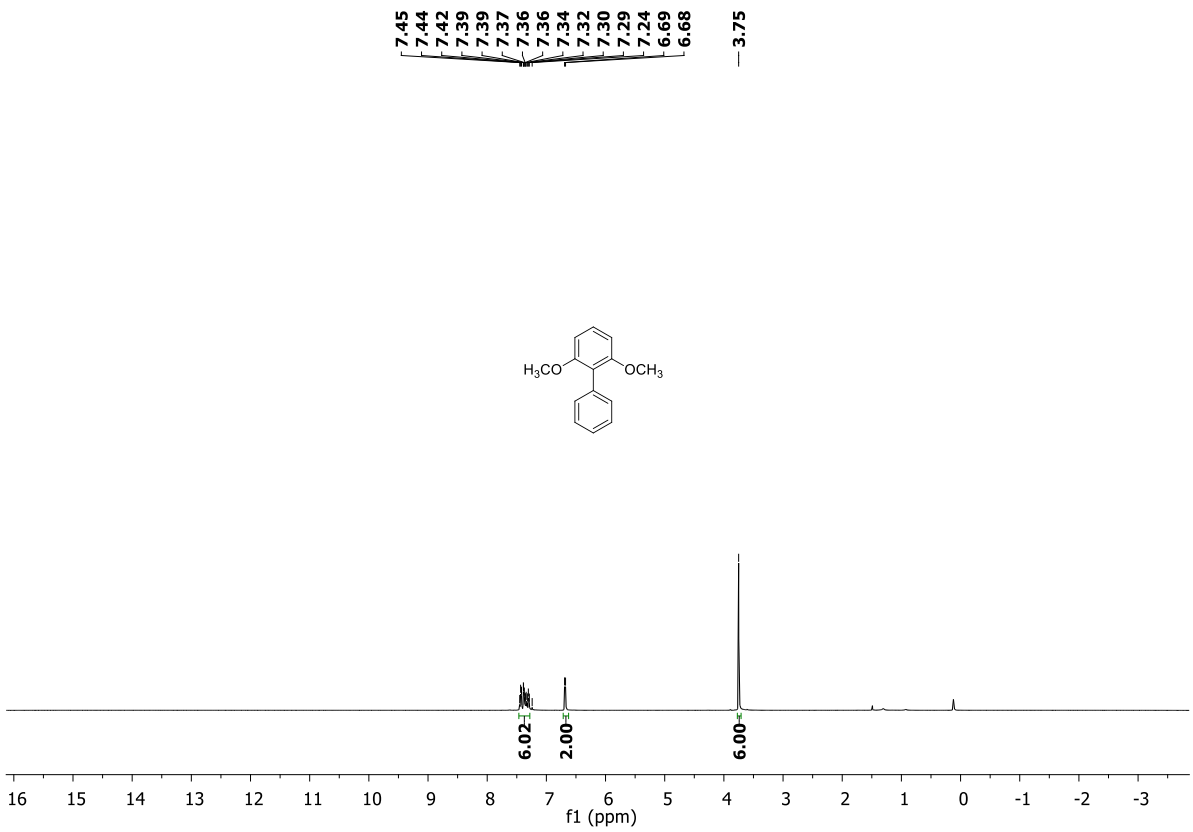


^{13}C-NMR ($CDCl_3$)

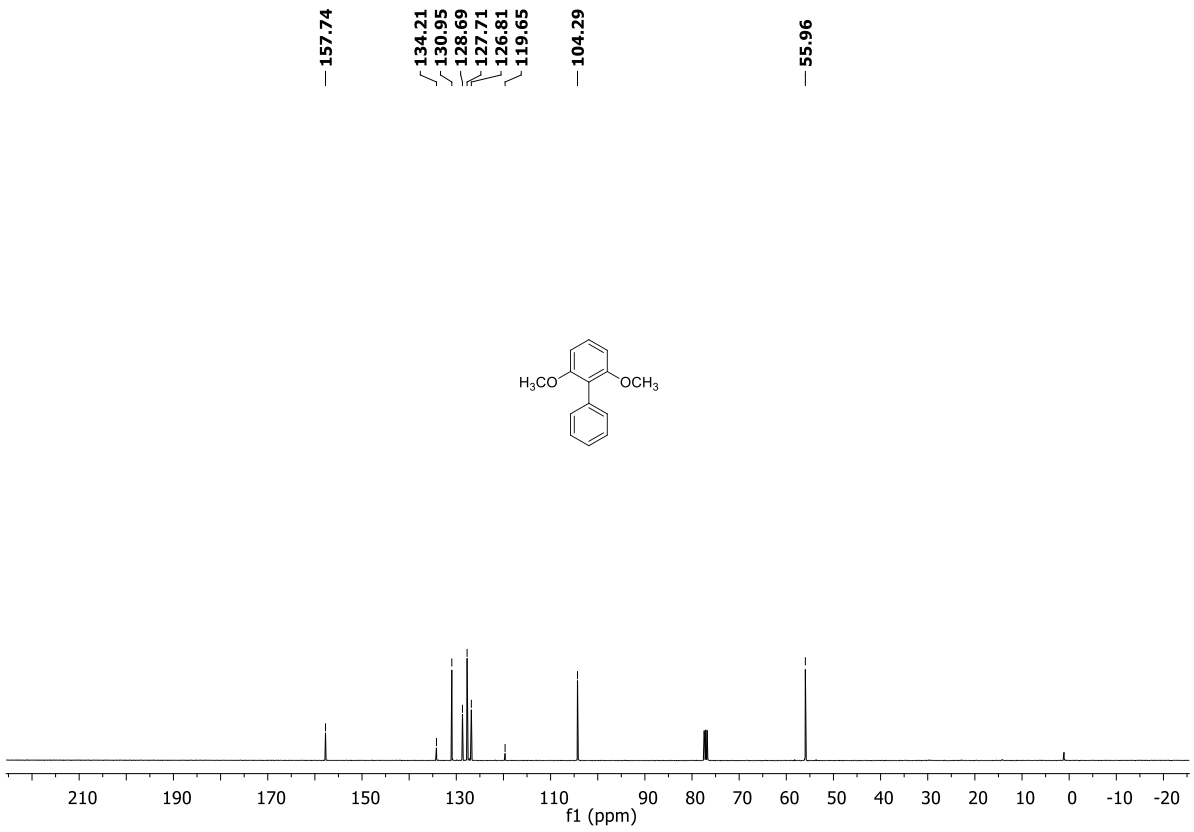


2,6-Dimethoxy-1,1'-biphenyl

^{1}H-NMR ($CDCl_3$)

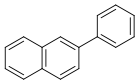


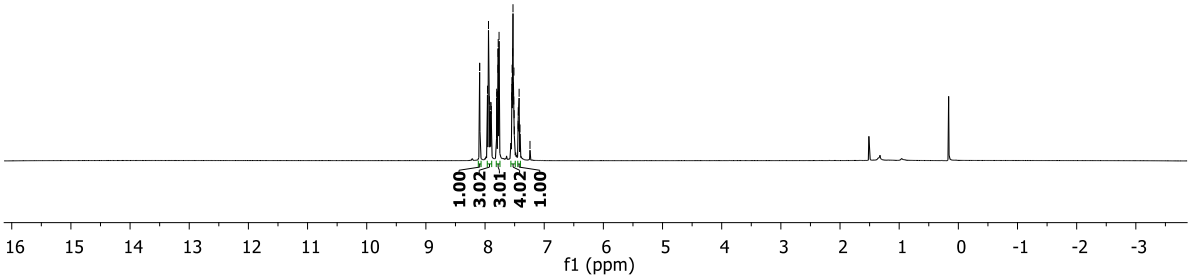
^{13}C-NMR ($CDCl_3$)



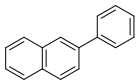
2-Phenylnaphthalene

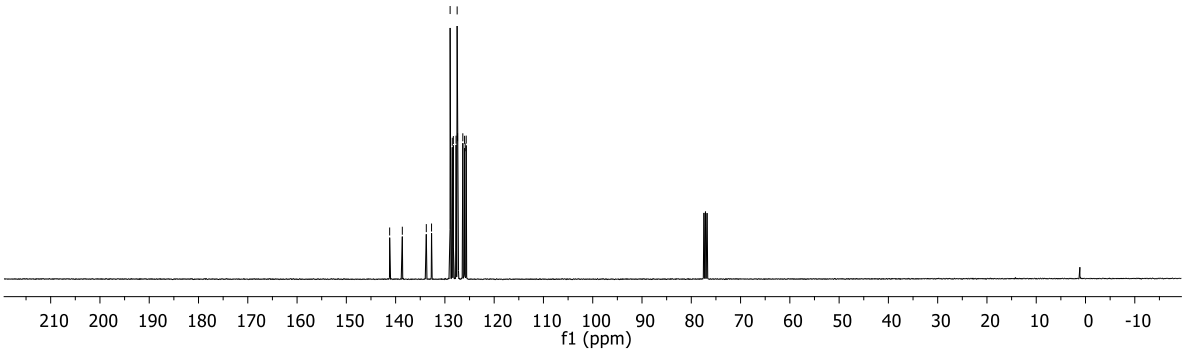
^{1}H-NMR ($CDCl_3$)





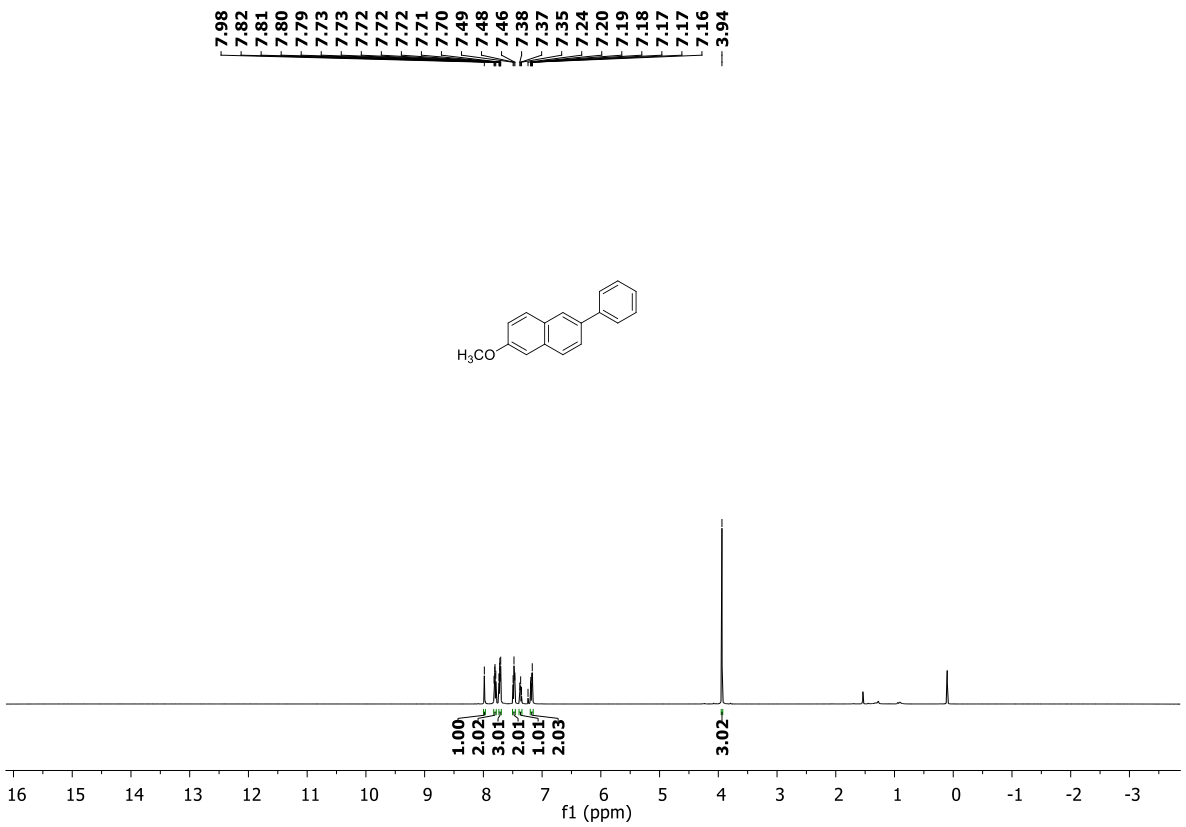
^{13}C-NMR ($CDCl_3$)



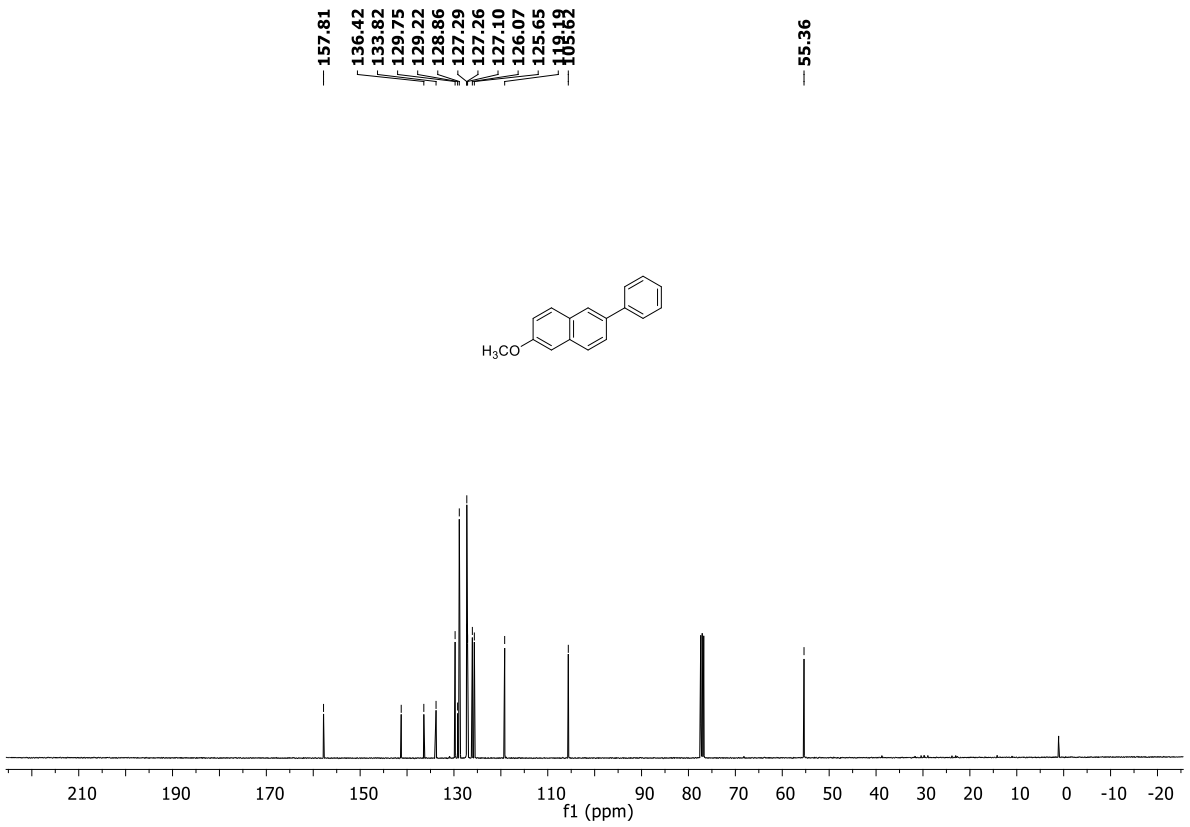


2-Methoxy-6-phenylnaphthalene

^{1}H-NMR ($CDCl_3$)

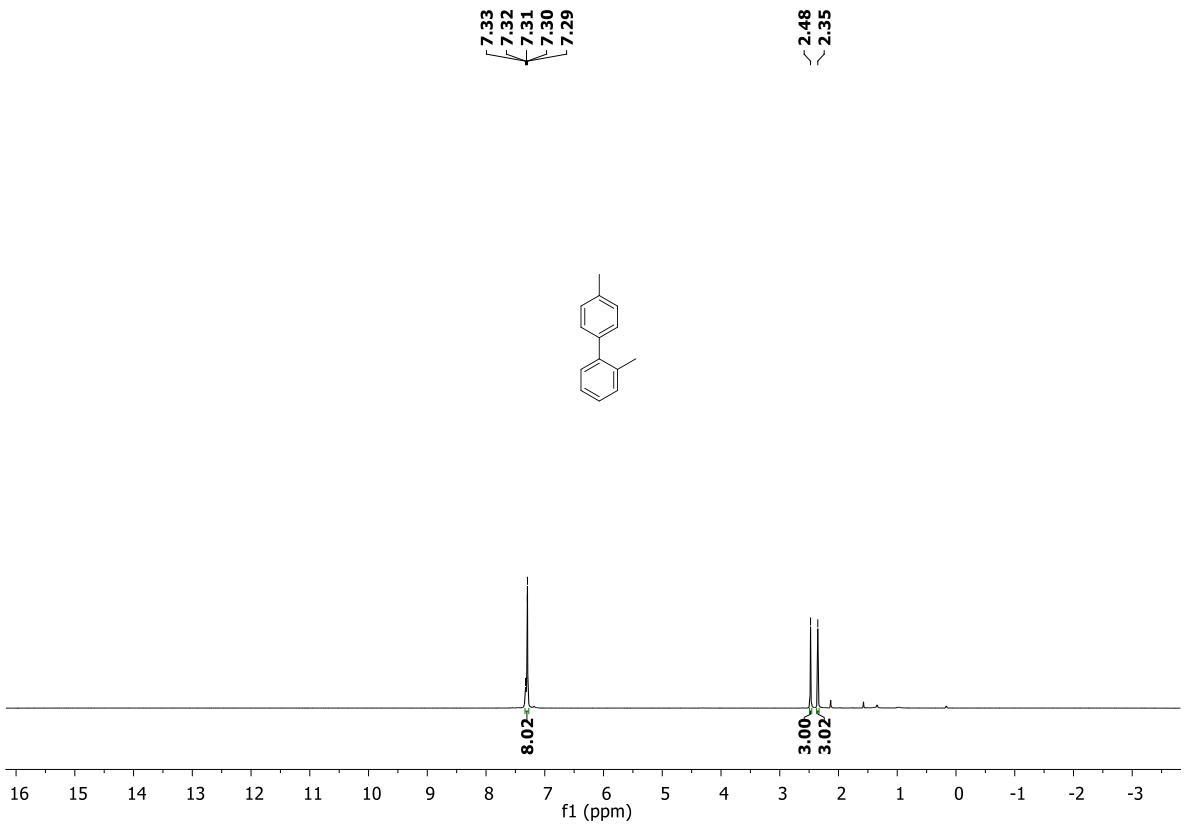


^{13}C-NMR ($CDCl_3$)

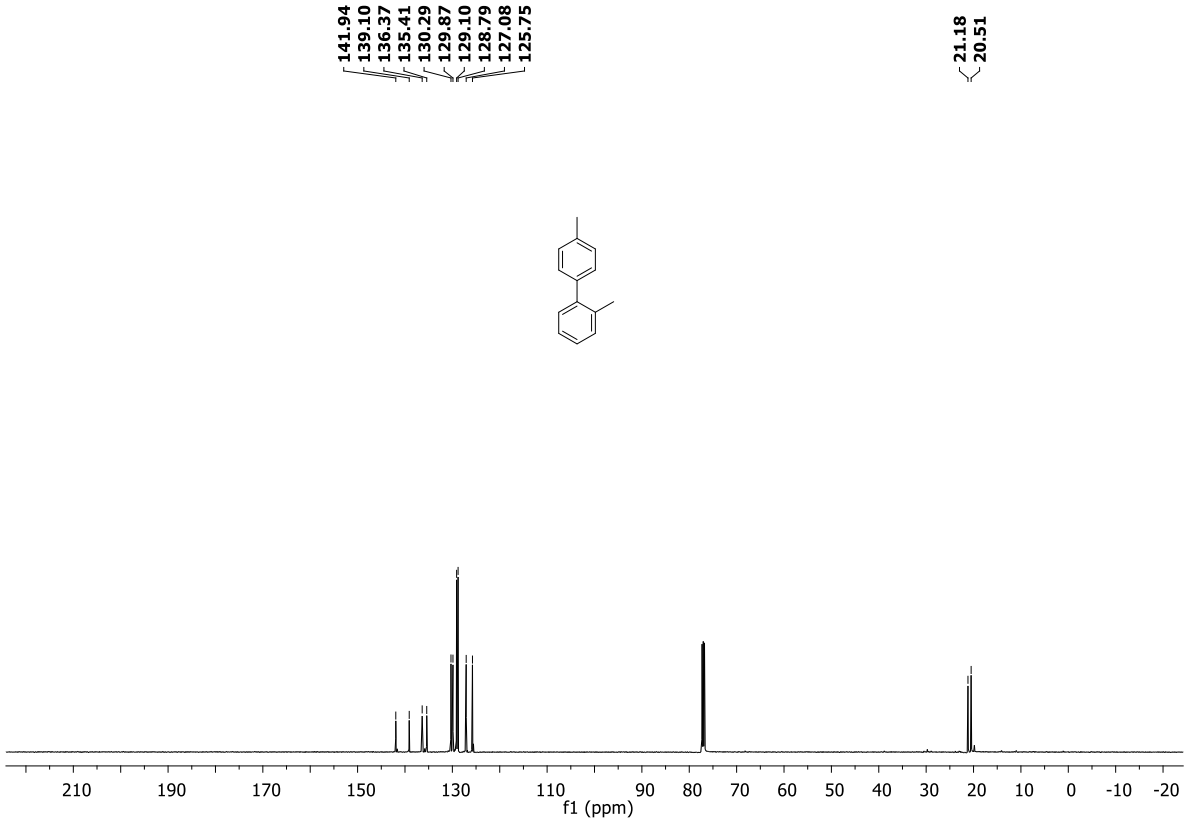


2,4'-Dimethyl-1,1'-biphenyl

^{1}H-NMR ($CDCl_3$)

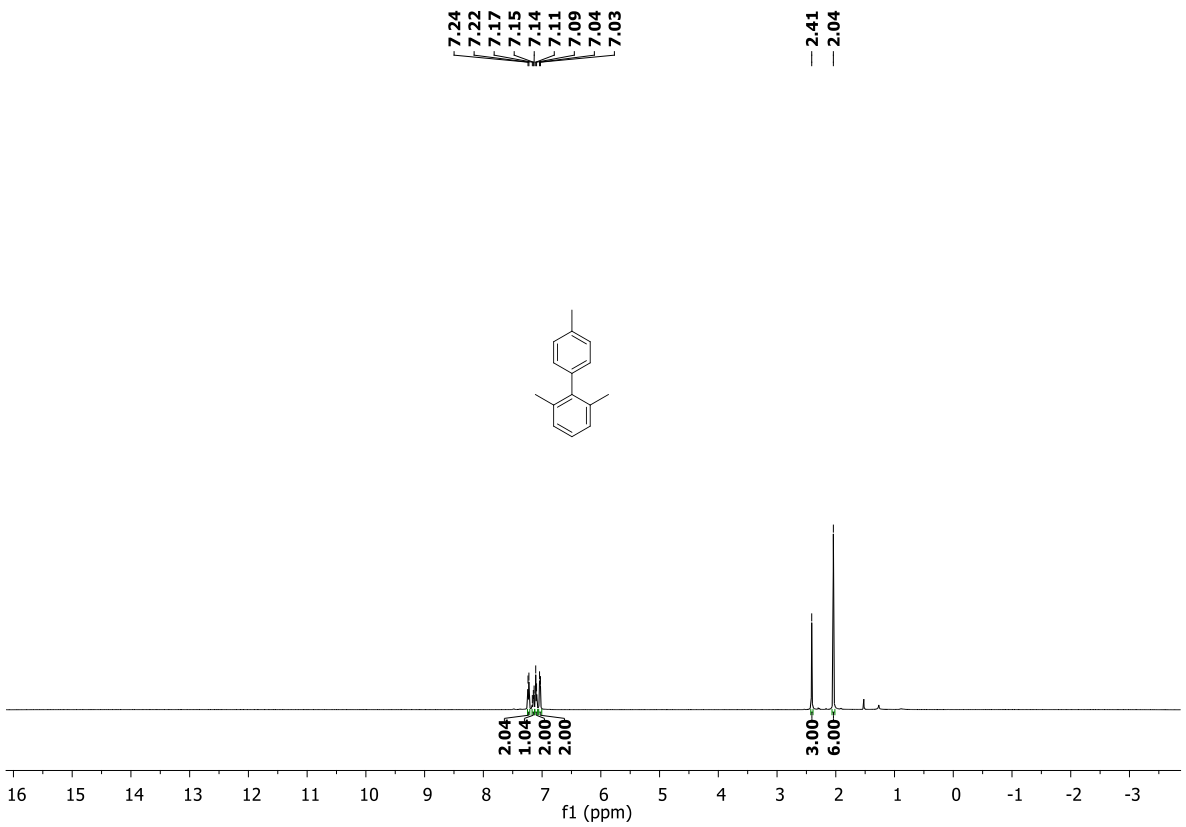


^{13}C-NMR ($CDCl_3$)

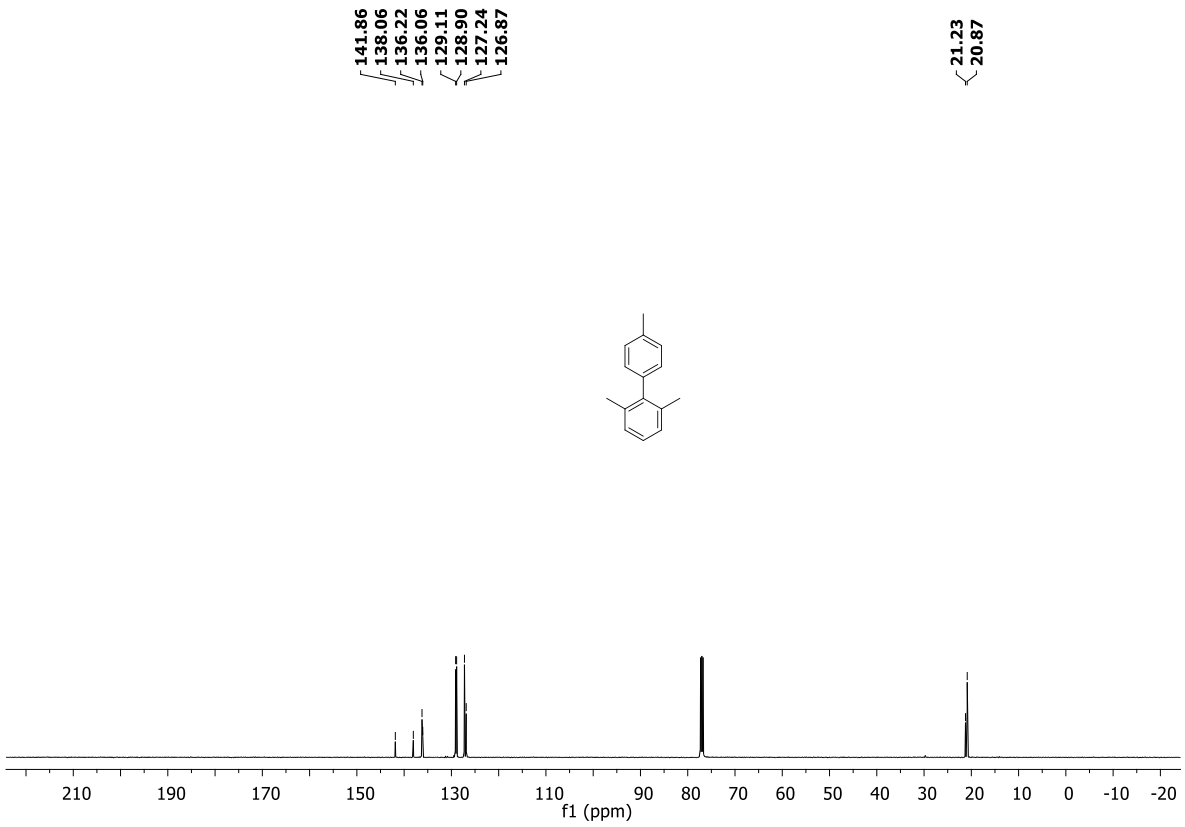


2,4',6-Trimethyl-1,1'-biphenyl.

^{1}H-NMR ($CDCl_3$)

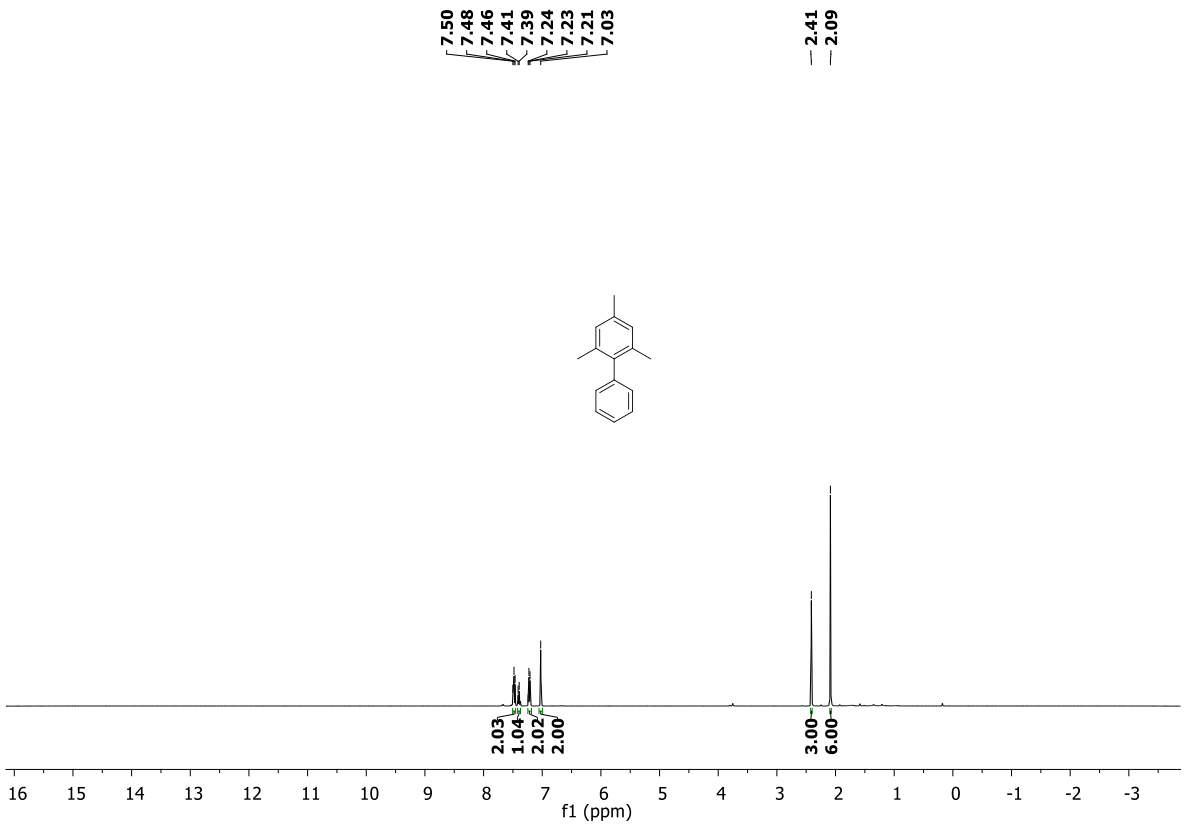


^{13}C-NMR ($CDCl_3$)

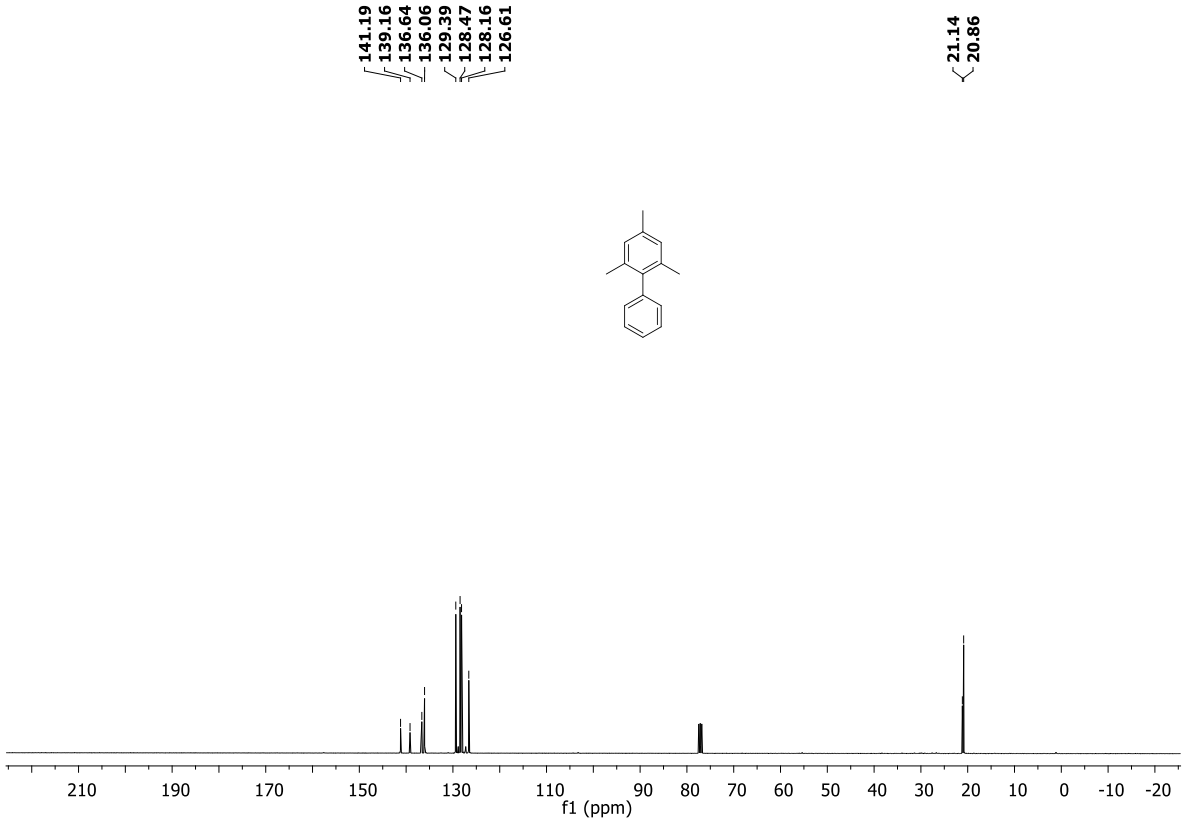


2,4,6-trimethyl-1,1'-biphenyl

^{1}H-NMR ($CDCl_3$)

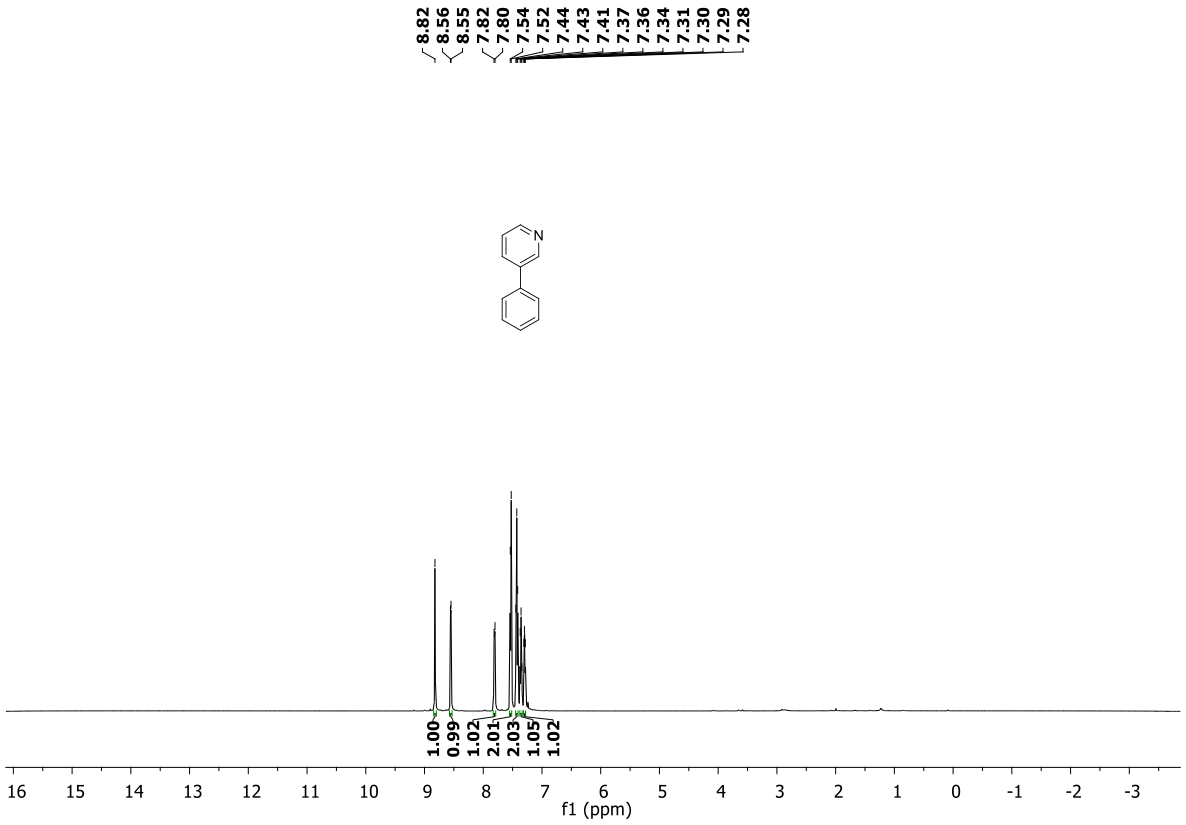


^{13}C-NMR ($CDCl_3$)

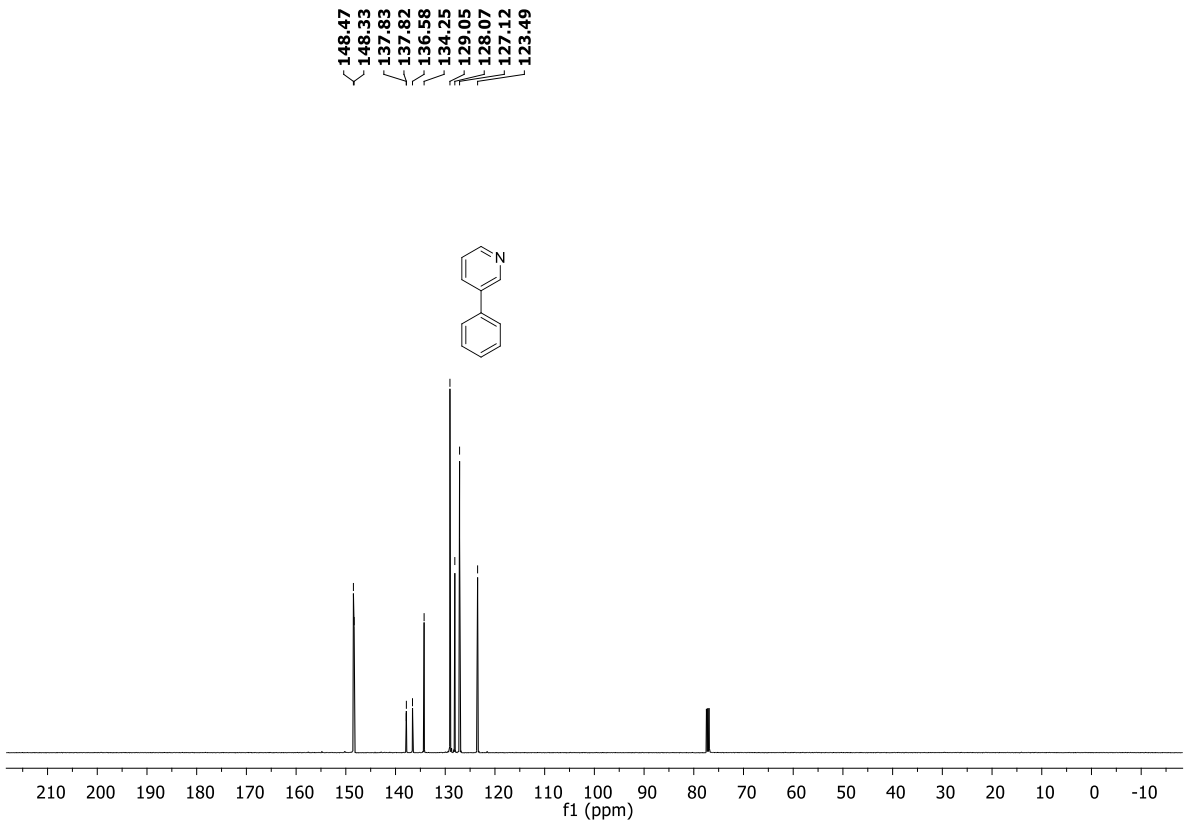


3-Phenyl-pyridine

^{1}H-NMR ($CDCl_3$)

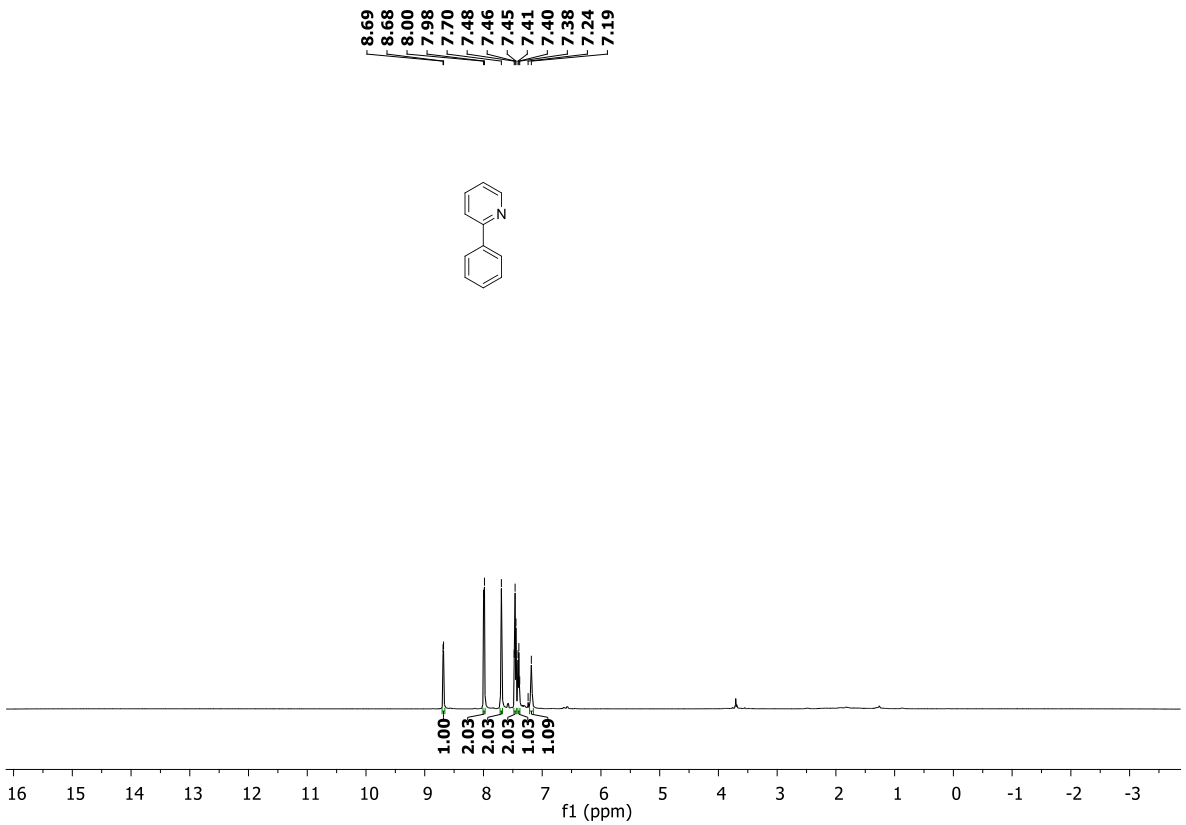


^{13}C-NMR ($CDCl_3$)

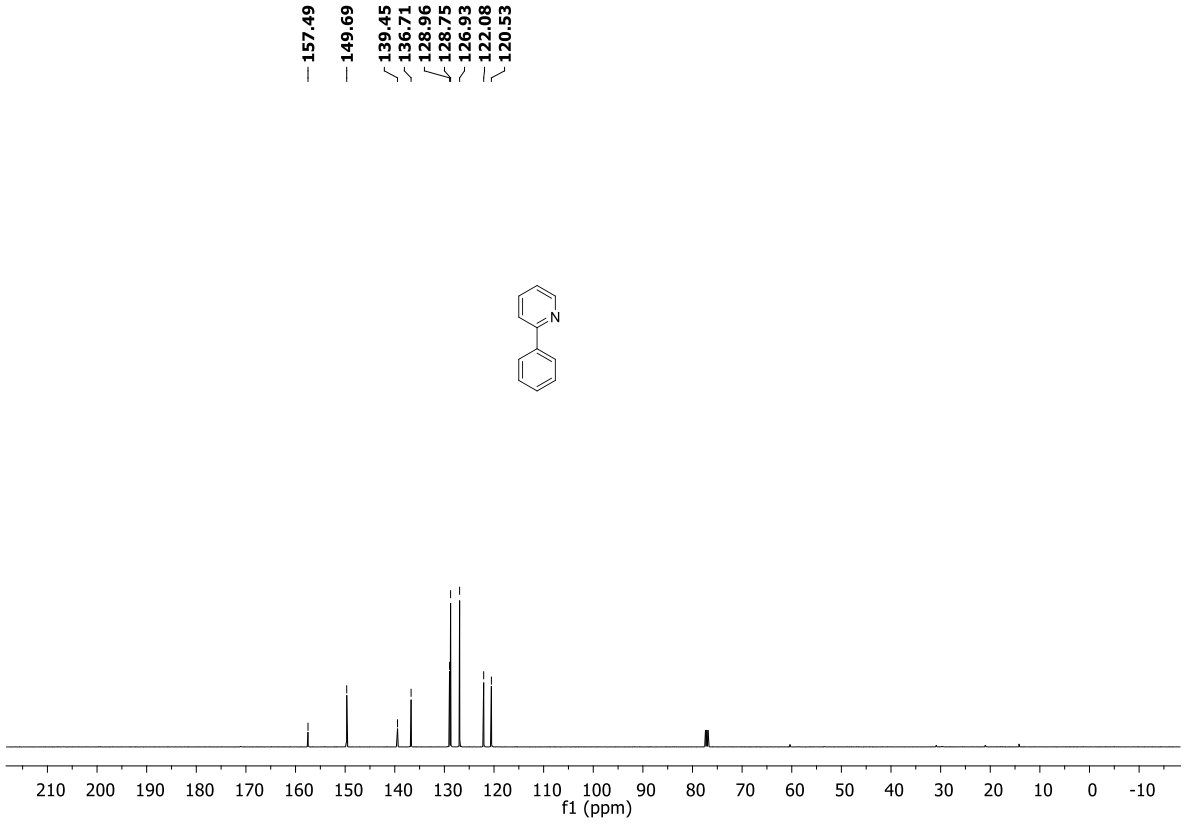


2-Phenyl-pyridine

^{1}H-NMR ($CDCl_3$)

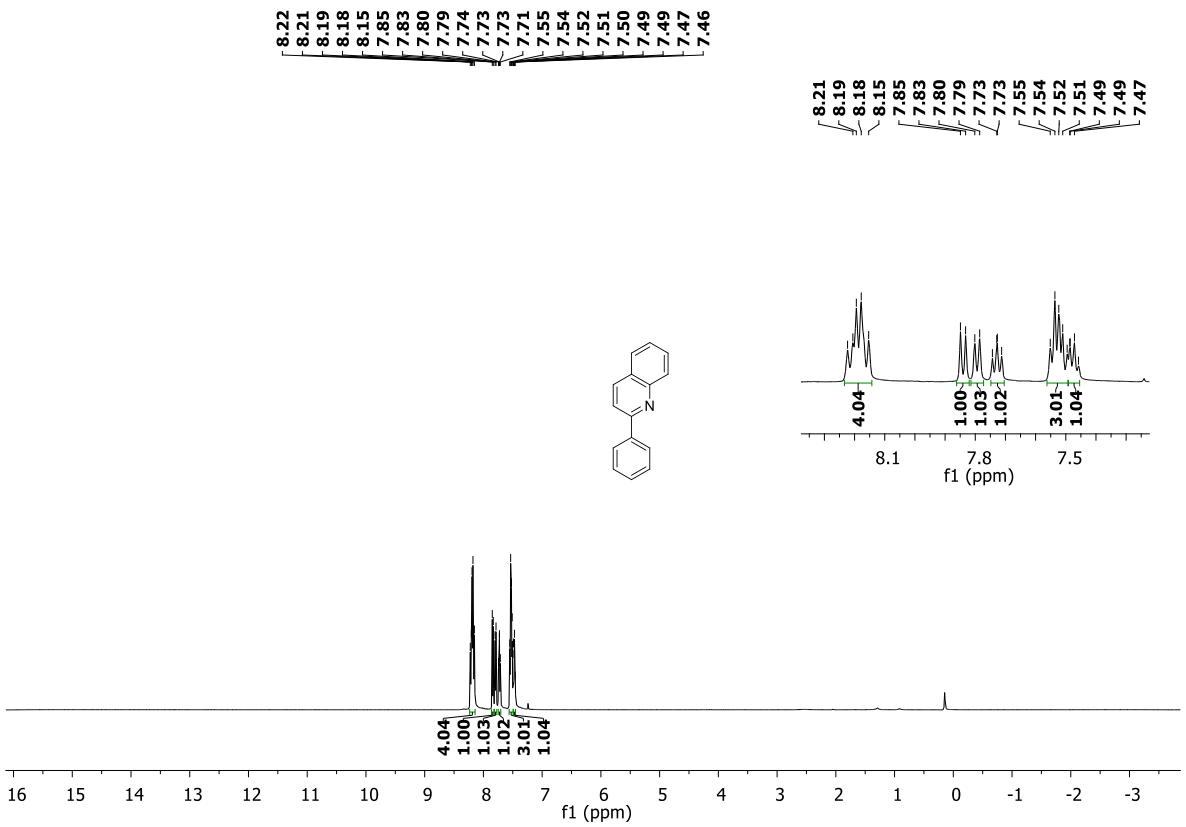


^{13}C-NMR ($CDCl_3$)

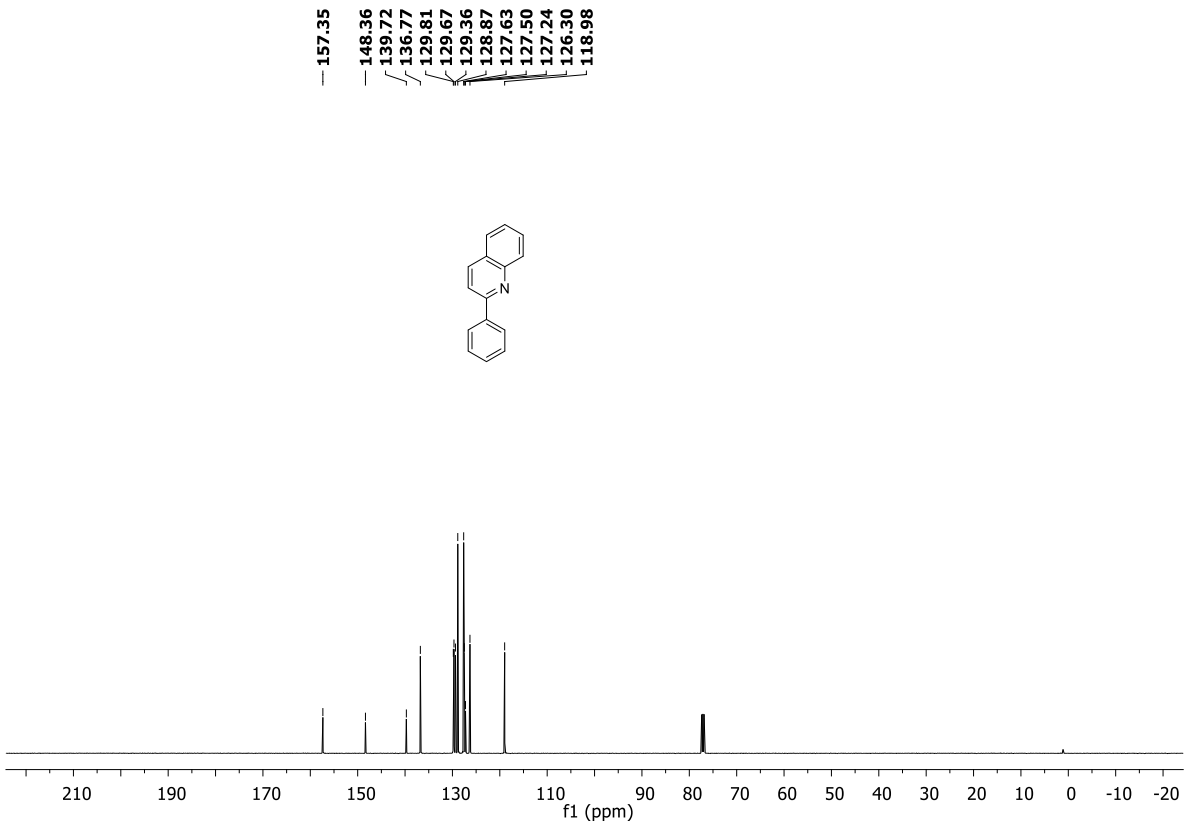


2-Phenyl-quinoline

^{1}H-NMR ($CDCl_3$)

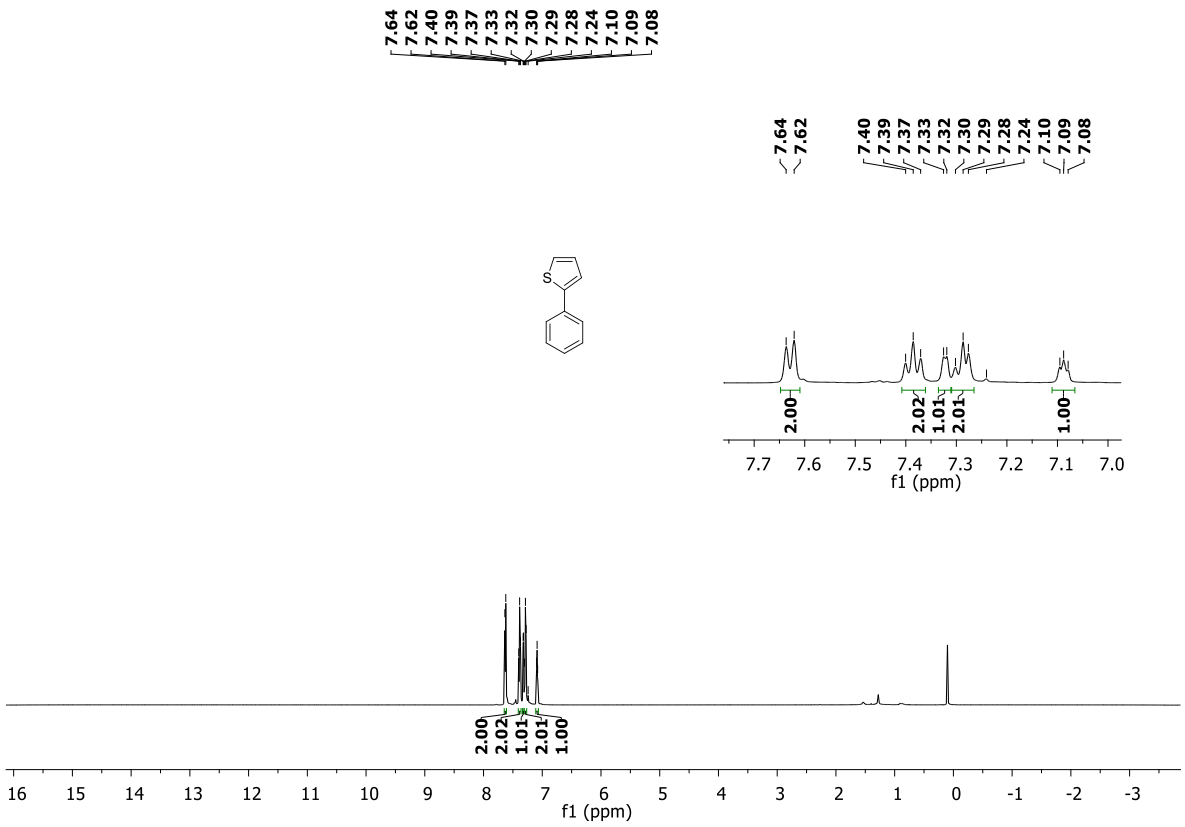


^{13}C-NMR ($CDCl_3$)

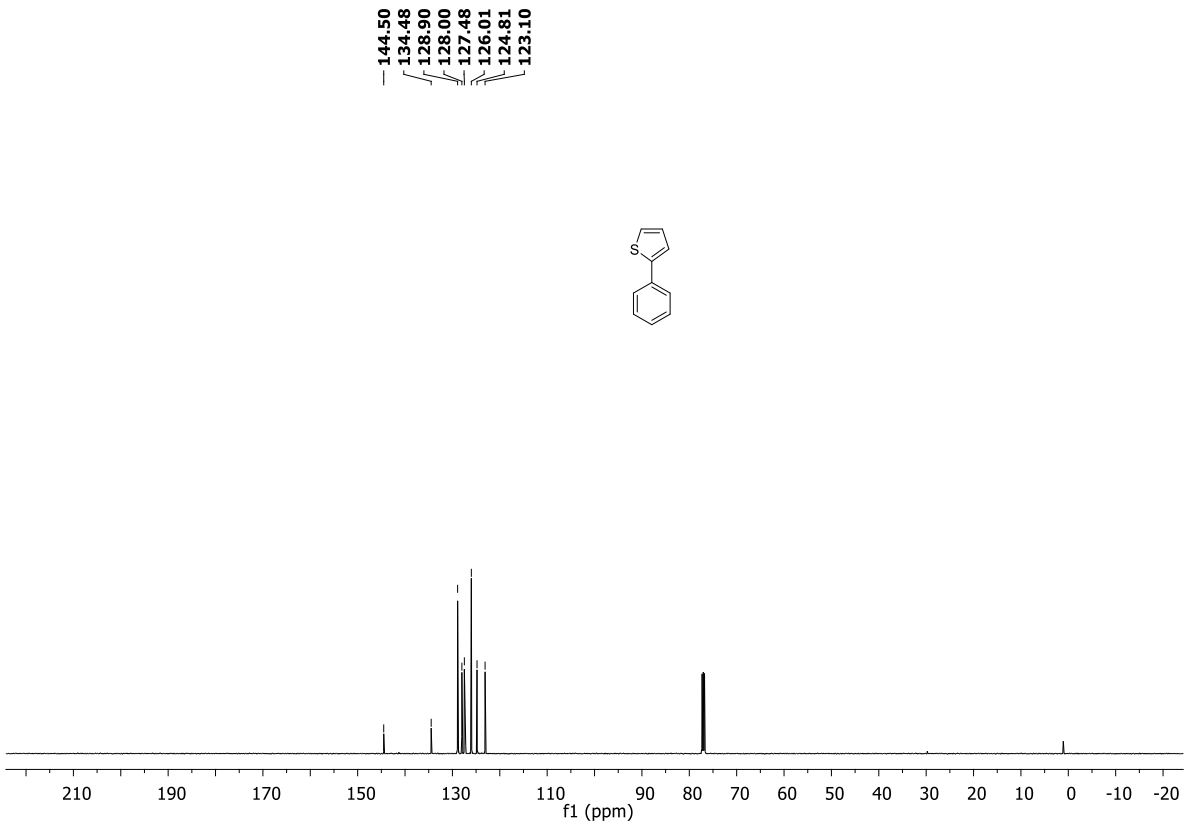


2-Phenyl-thiophene

^{1}H-NMR ($CDCl_3$)

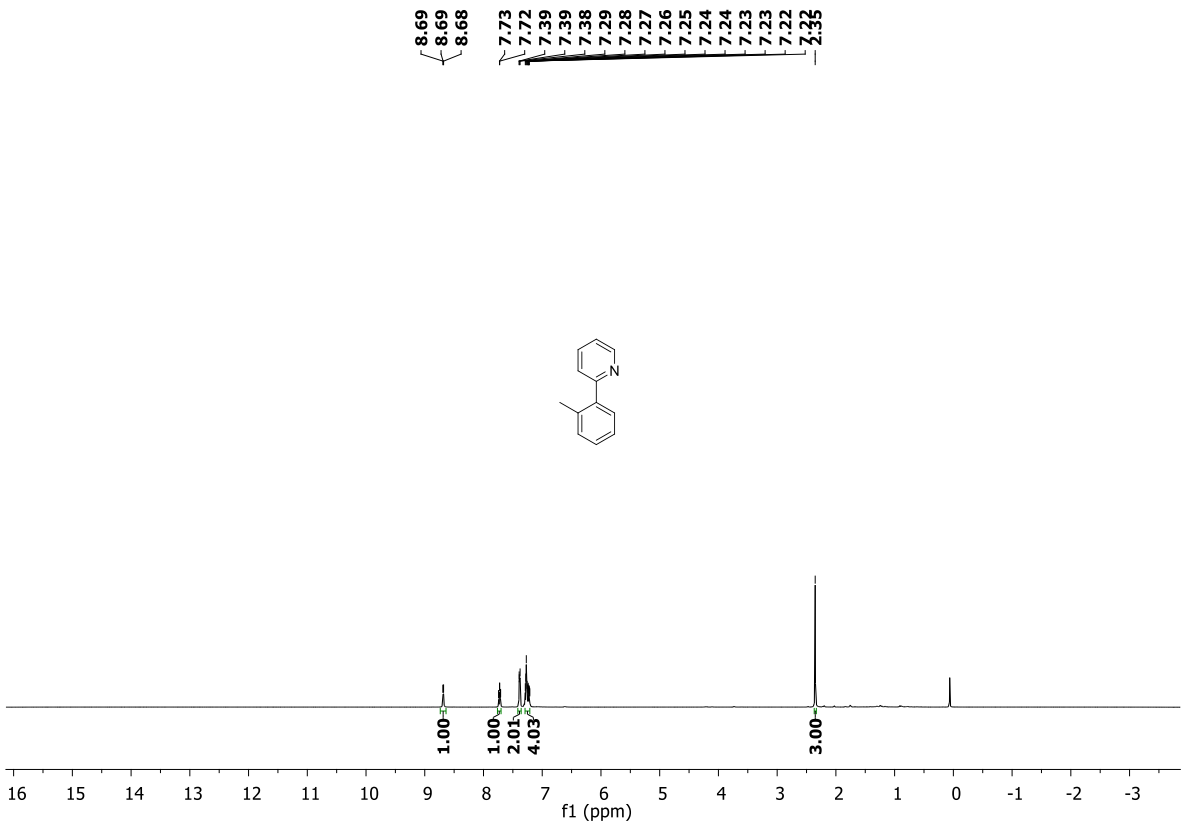


^{13}C-NMR ($CDCl_3$)

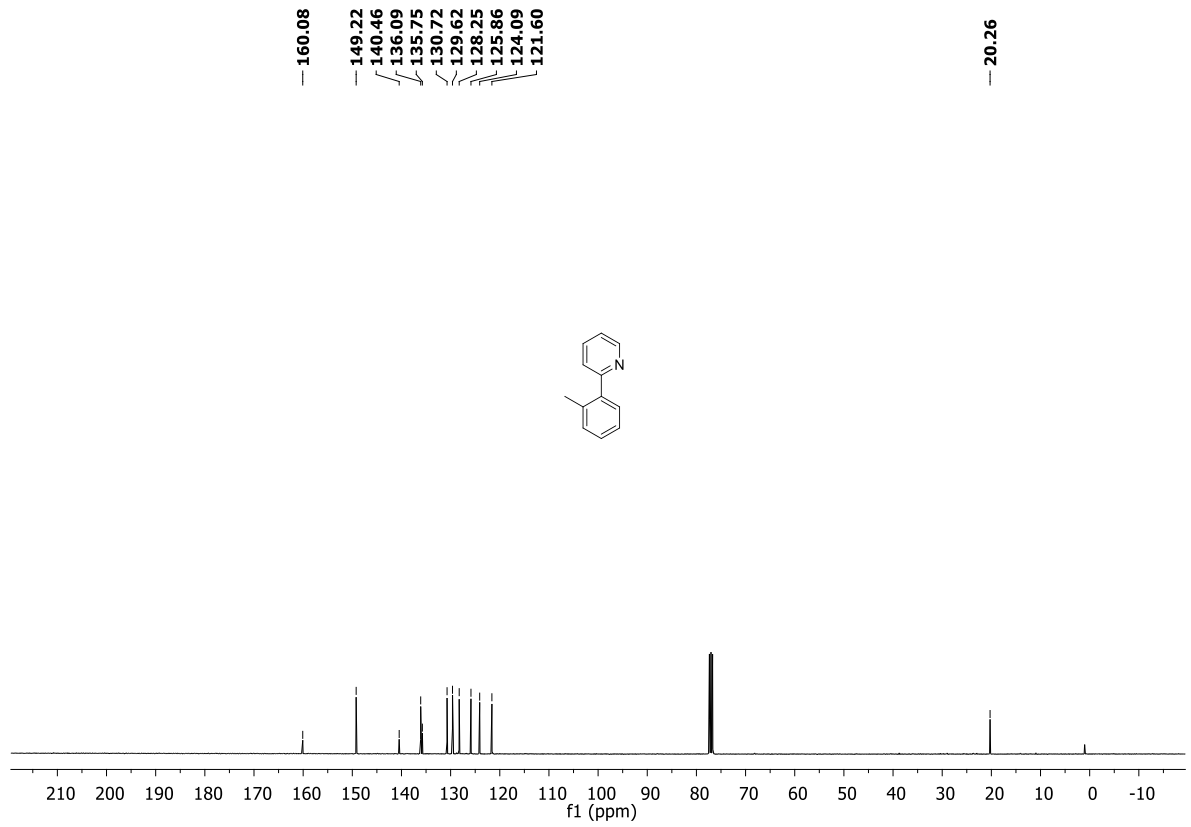


2-(*o*-Tolyl)pyridine

^{1}H-NMR ($CDCl_3$)

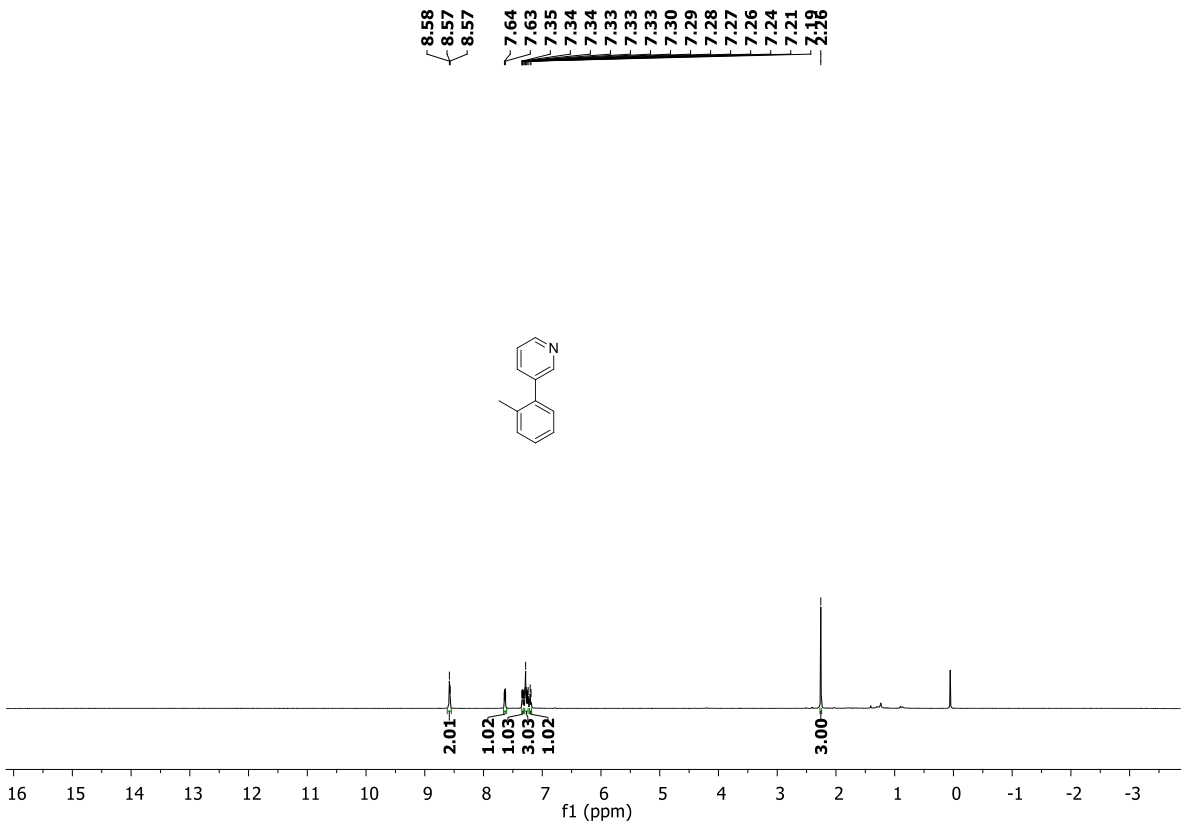


^{13}C-NMR ($CDCl_3$)

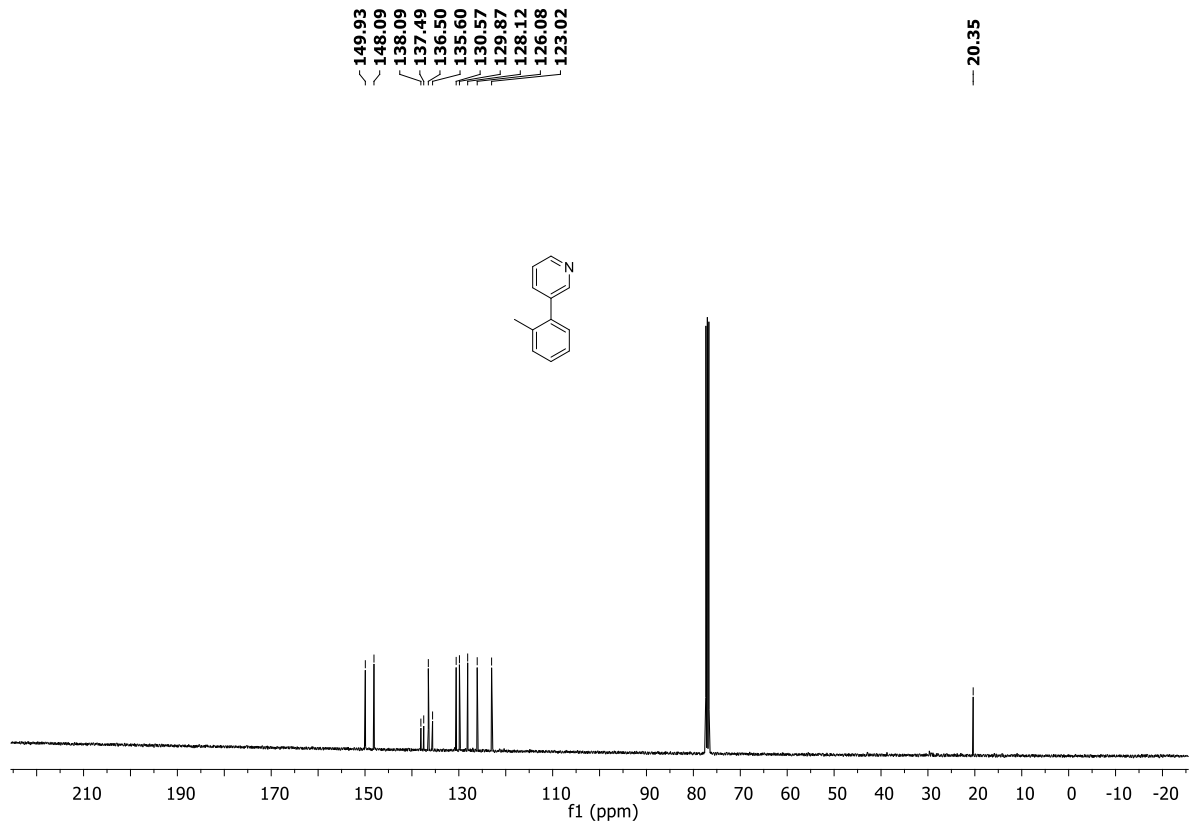


3-(*o*-Tolyl)pyridine

^{1}H-NMR ($CDCl_3$)

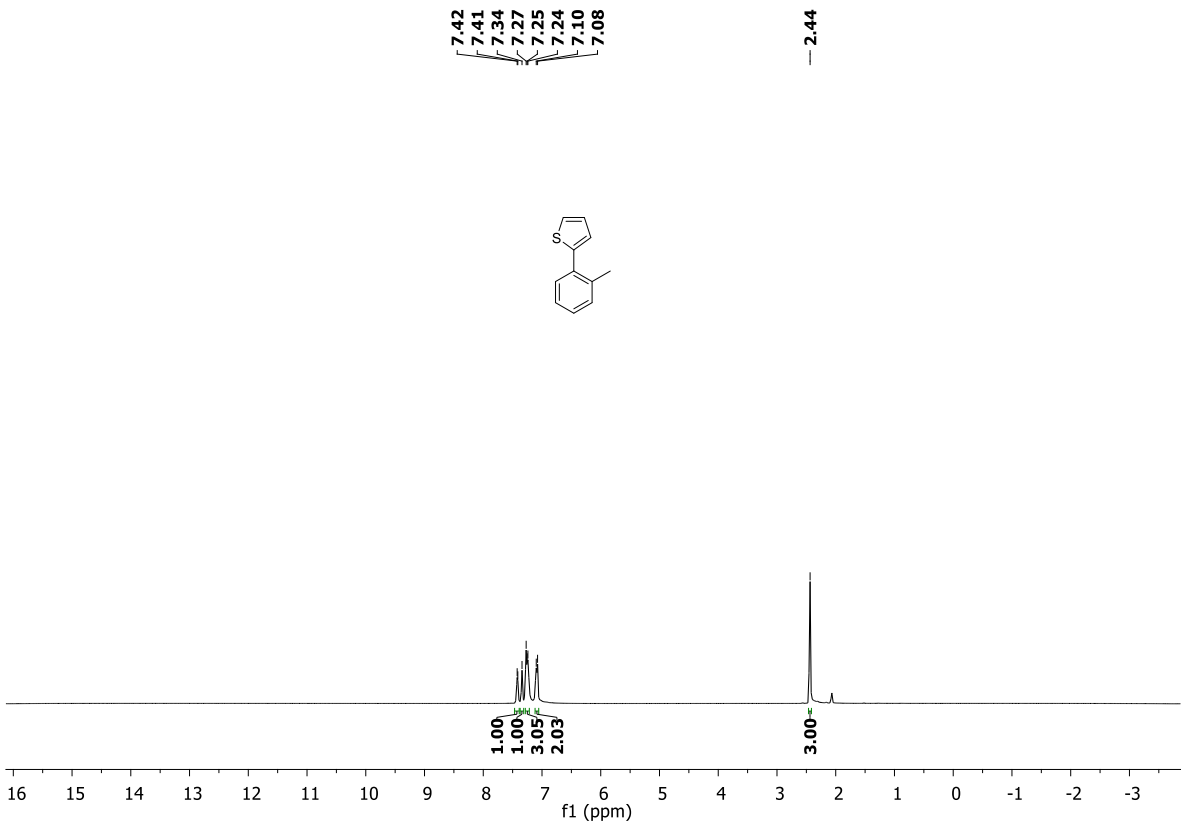


^{13}C-NMR ($CDCl_3$)

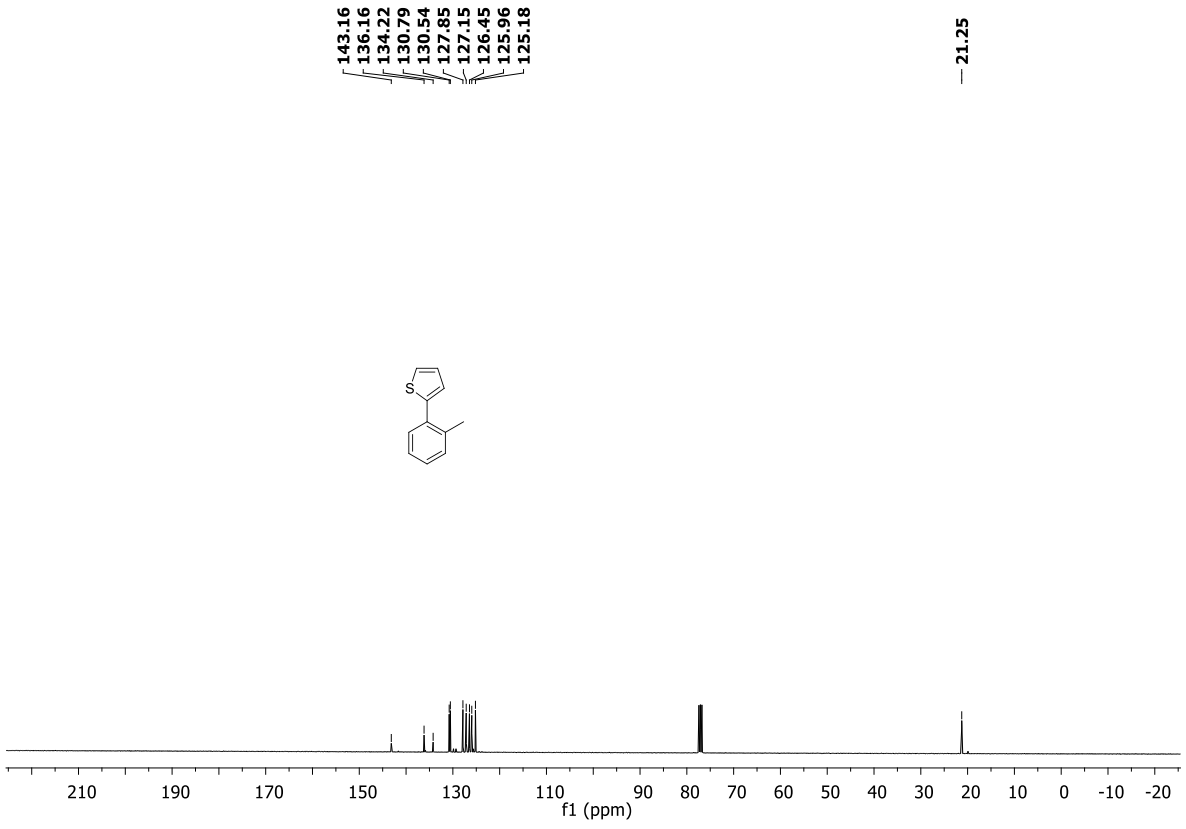


2-(*o*-Tolyl)-thiophene

^{1}H-NMR ($CDCl_3$)

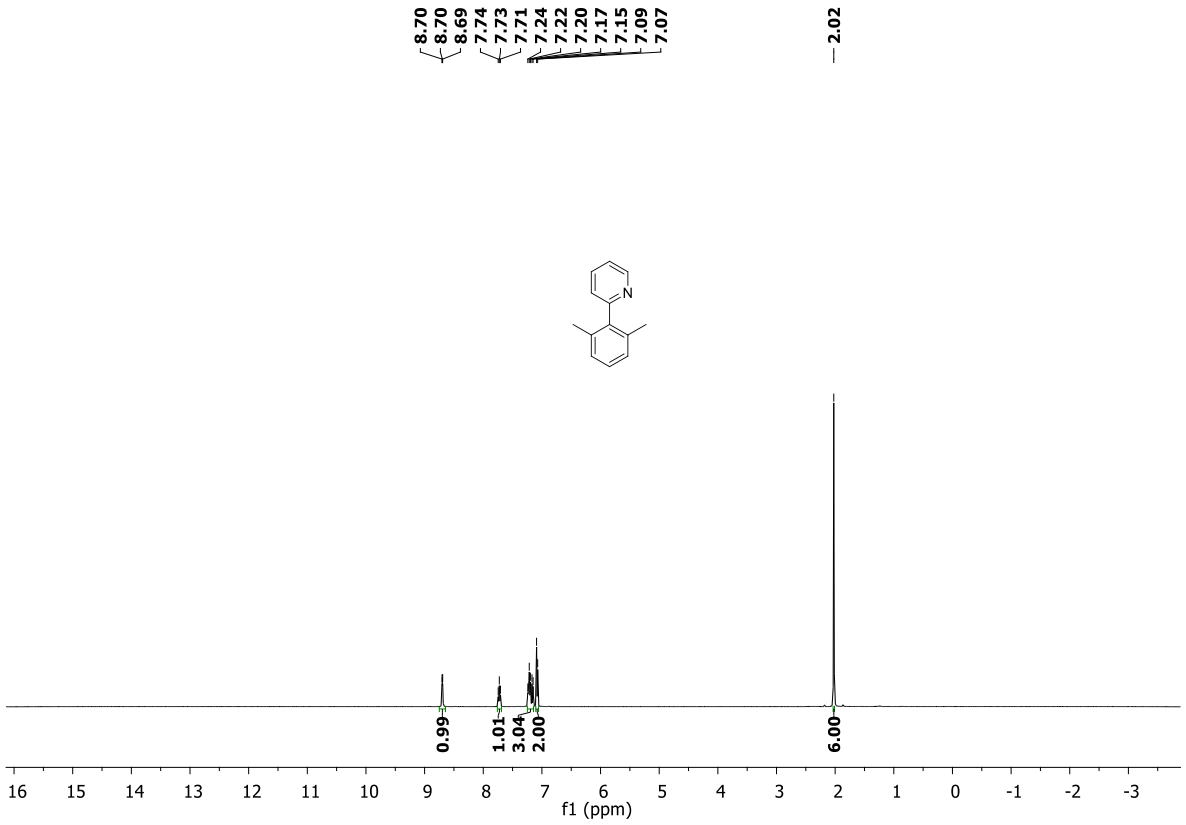


^{13}C-NMR ($CDCl_3$)

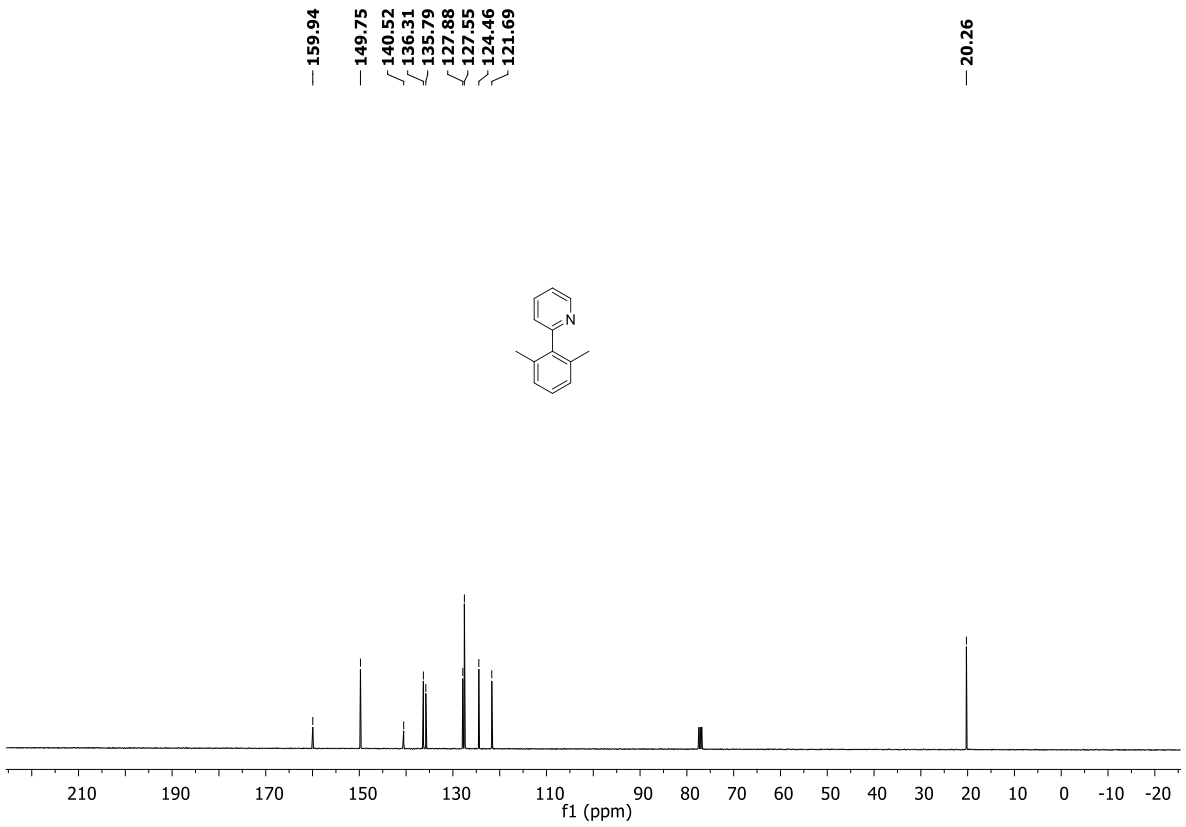


2-(2,6-Dimethylphenyl)pyridine

^{1}H-NMR ($CDCl_3$)

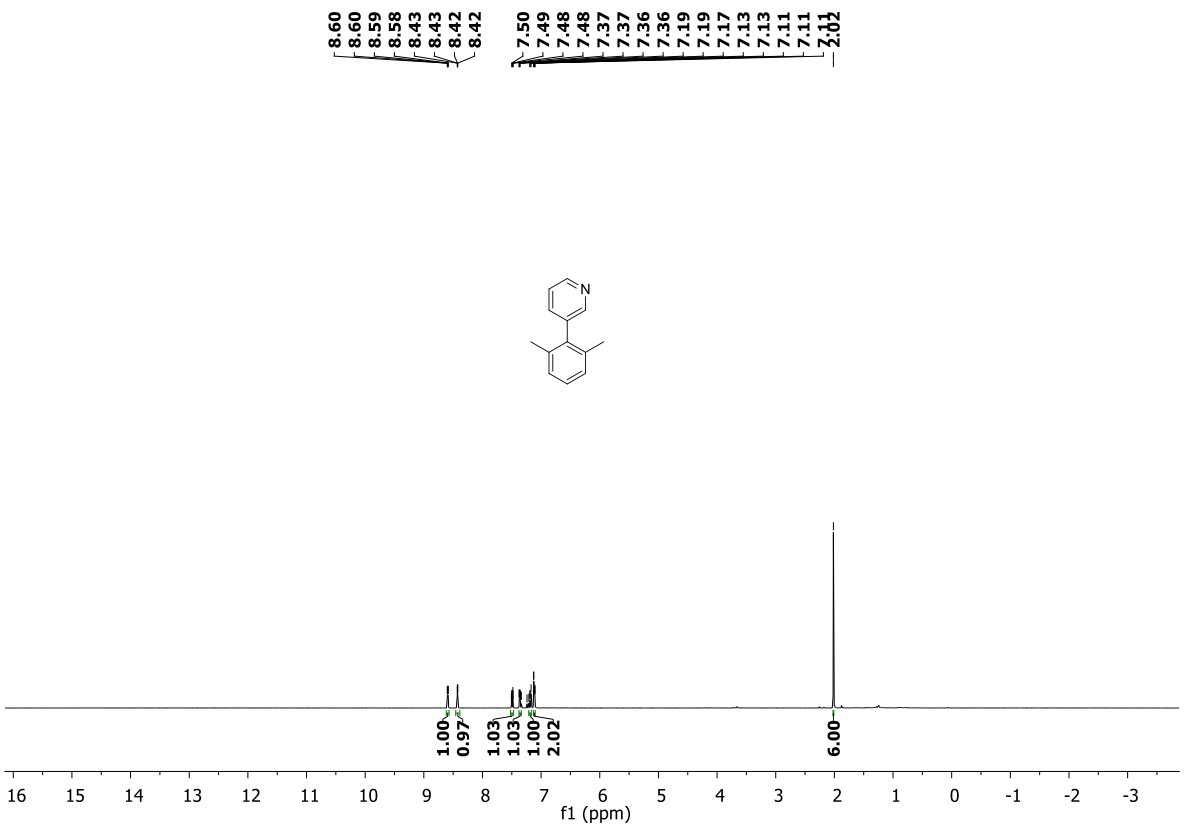


^{13}C-NMR ($CDCl_3$)

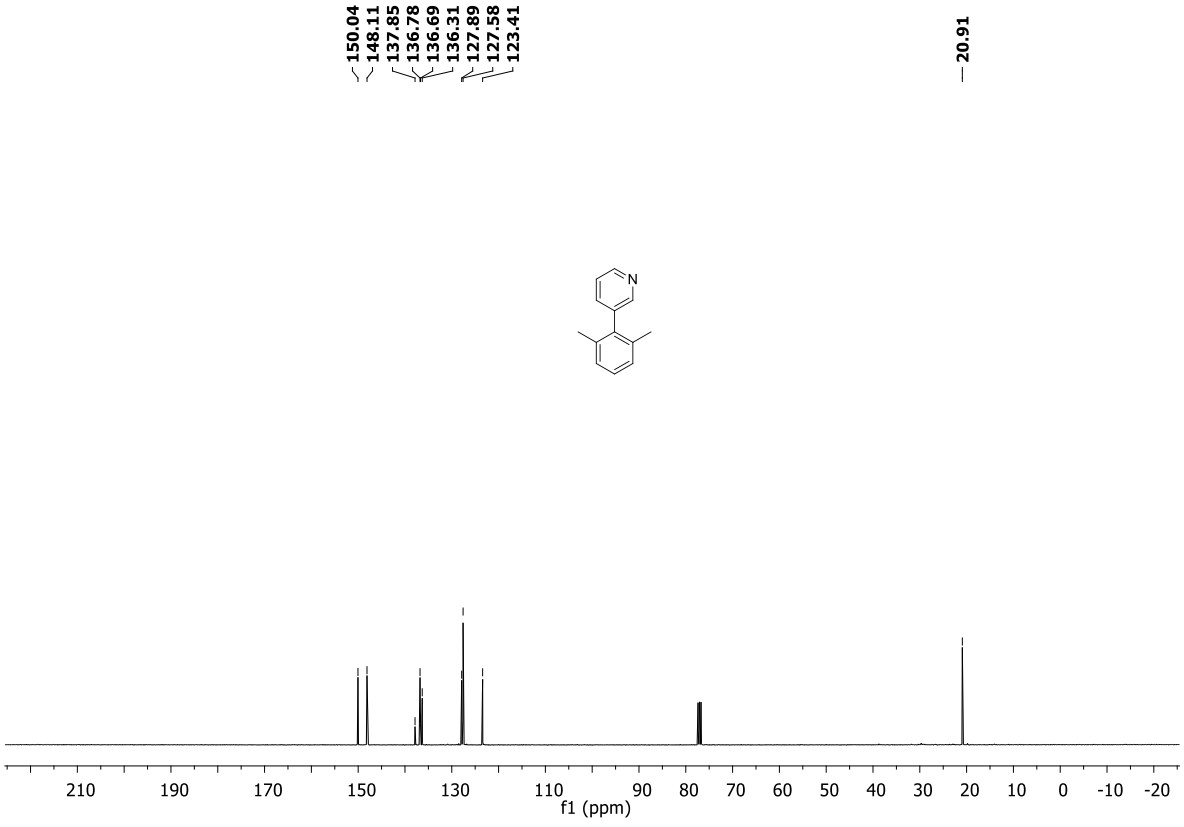


3-(2,6-Dimethylphenyl)pyridine

^{1}H-NMR ($CDCl_3$)

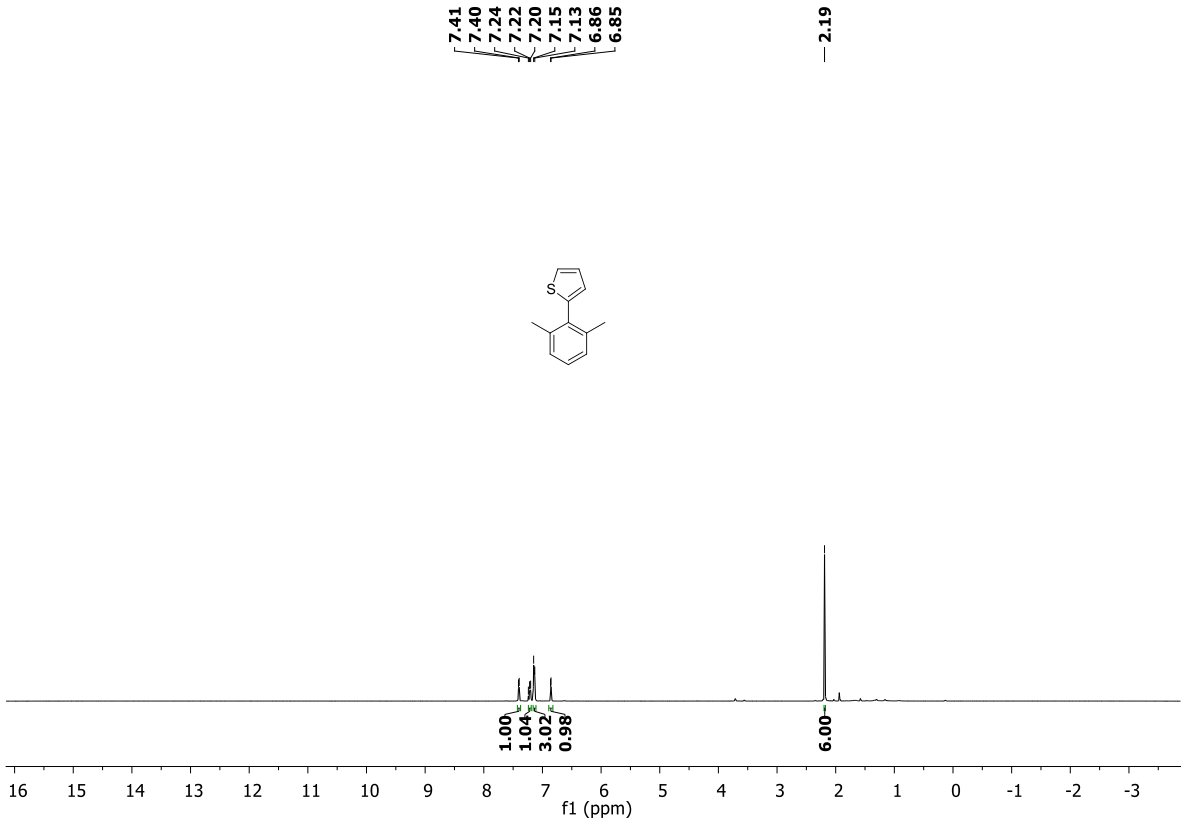


^{13}C-NMR ($CDCl_3$)

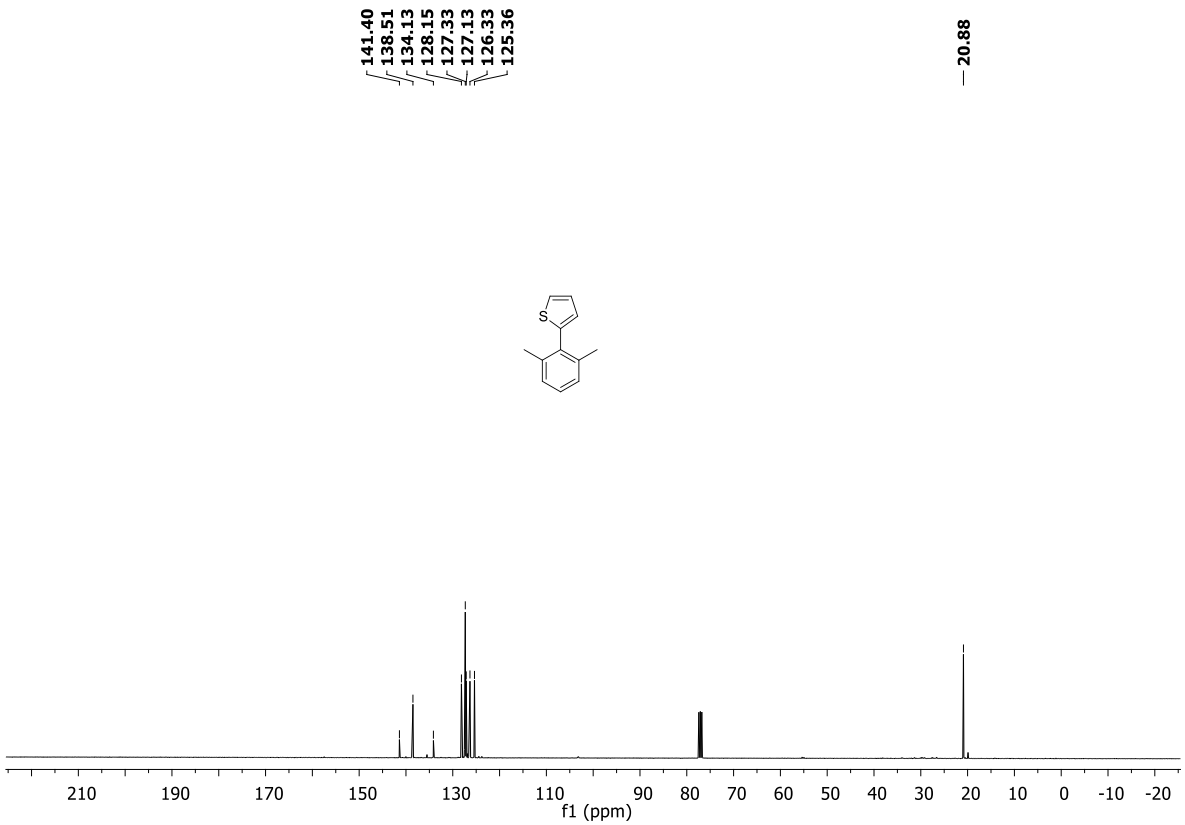


2-(2,6-dimethylphenyl)-thiophene

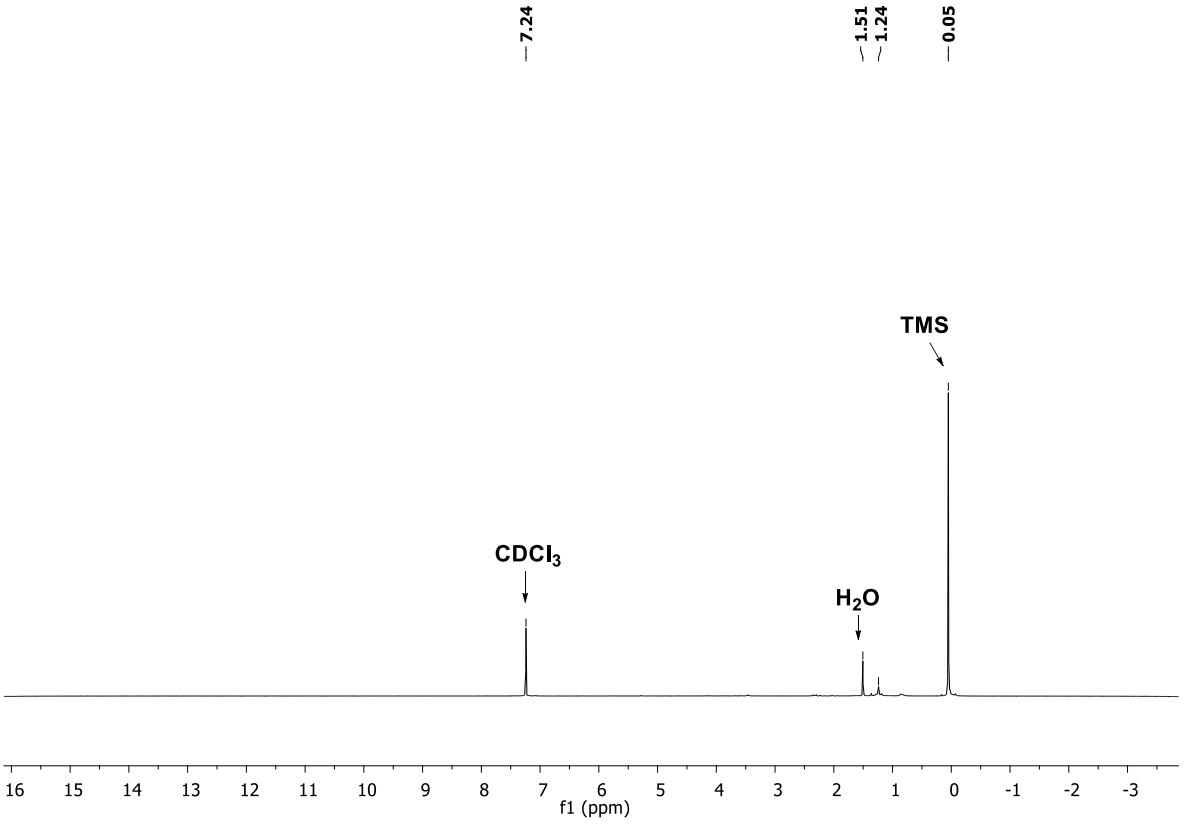
^{1}H-NMR ($CDCl_3$)



^{13}C-NMR ($CDCl_3$)



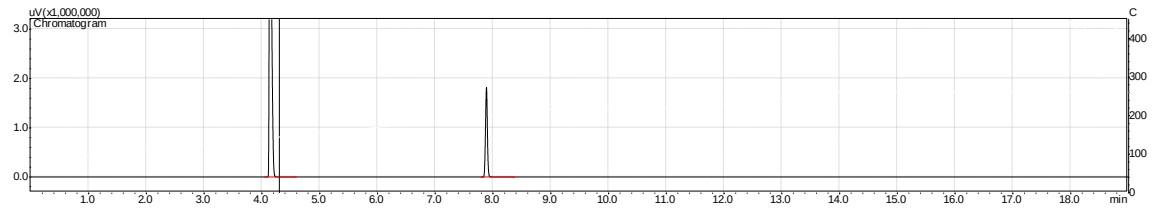
$CDCl_3$ commercial



GC Data

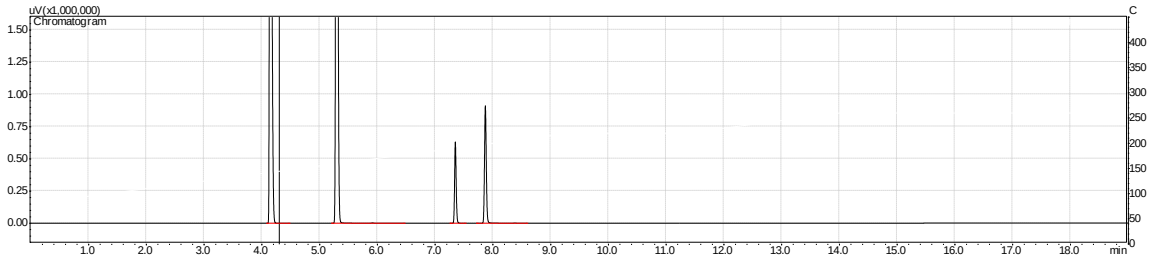
Room temperature optimisation

4-Bromotoluene



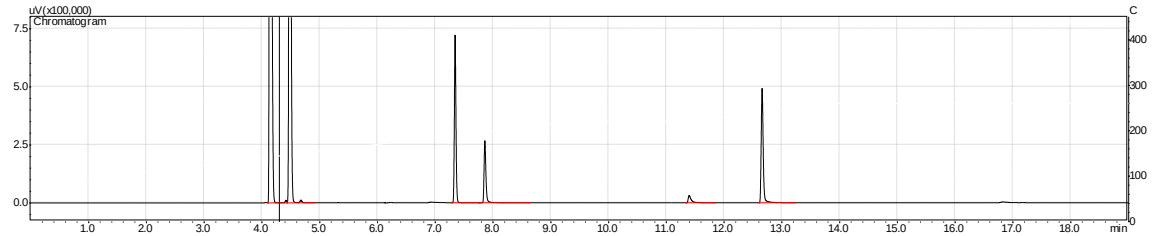
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.140	18938967.5	6707569.1	0.00000	ppm	S	1	DCM
2	7.887	4147843.9	1799980.9	0.00000				

To



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.145	14105421.0	5440319.4	0.00000	ppm	SV	1	DCM
2	5.295	19478270.1	9264369.6	0.00000		S		
3	7.350	1180742.5	621261.6	0.00000				
4	7.870	1958450.5	901354.8	0.00000		SV		

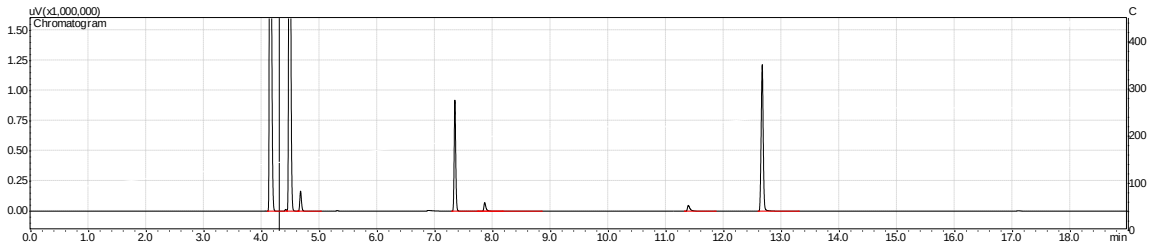
L1 RT THF_KF_



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.142	11944536.4	5042639.2	0.00000	ppm	SV	1	
2	4.481	8729420.3	4212115.2	0.00000	ppm	SV	1	
3	7.344	1355114.2	716902.9	0.00000	ppm	SV	3	

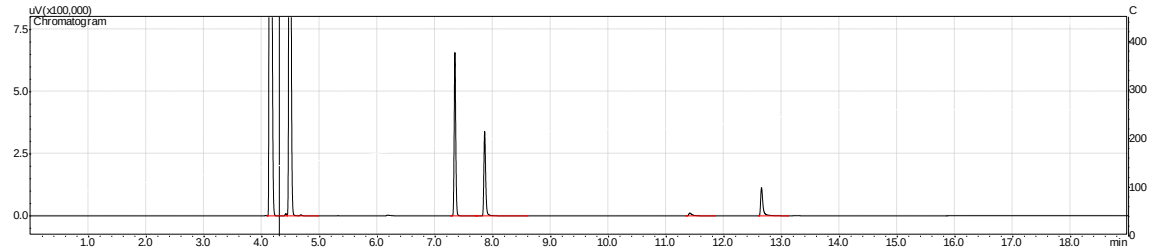
4	7.859	597954.0	264028.3	0.00000		SV		
5	11.396	118645.0	31735.6	0.00000				
6	12.658	1184853.0	488499.5	0.00000				

L3 RT THF_KF_



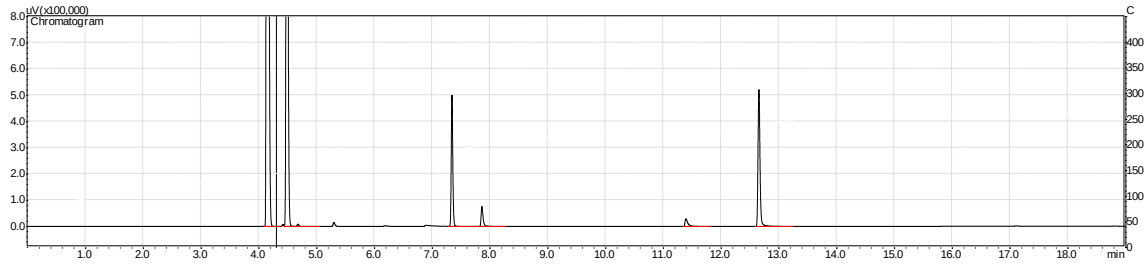
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.143	10816497.8	4647633.0	0.00000	ppm	SV	1	
2	4.479	11416156.2	5498279.9	0.00000	ppm	V	1	
3	4.670	344889.7	166367.3	0.00000		V		
4	7.343	1739482.5	915115.0	0.00000	ppm	SV	3	
5	7.859	185350.0	71155.6	0.00000		T		
6	11.385	164534.6	48528.8	0.00000				
7	12.664	3037158.4	1211137.2	0.00000		V		

L1 RT THF_K3PO4_



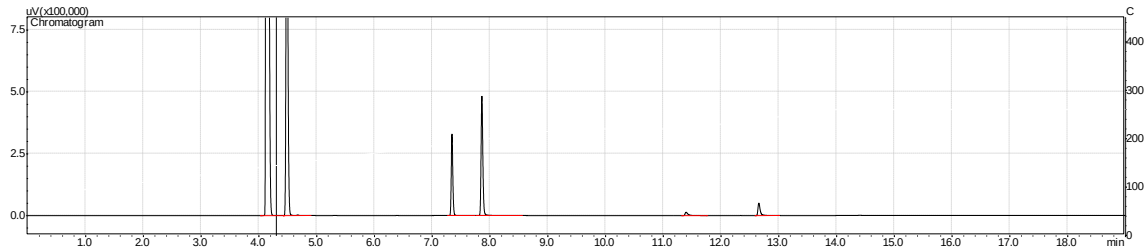
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.141	12809670.2	5283748.3	0.00000	ppm	SV	1	
2	4.481	8189442.2	3945931.5	0.00000	ppm	SV	1	
3	7.341	1231101.7	644556.2	0.00000	ppm	SV	3	
4	7.856	747316.8	337816.7	0.00000		SV		
5	11.408	50401.9	11558.8	0.00000		S		
6	12.649	320952.9	113368.1	0.00000		V		

L3 RT THF_ K3PO4_



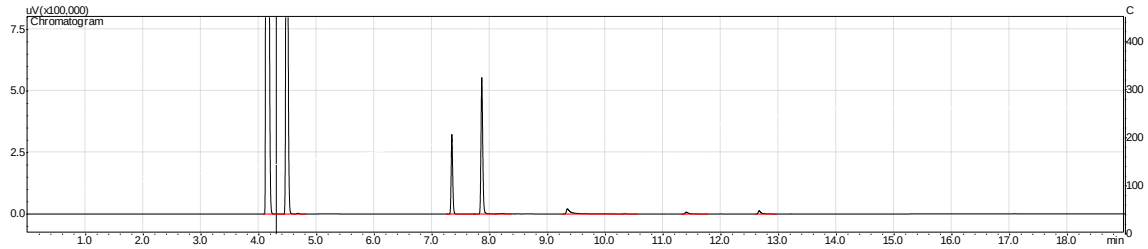
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.140	13388163.8	5487867.3	0.00000	ppm	V	1	
2	4.483	6470805.1	3173267.5	0.00000	ppm	SV	1	
3	7.340	934011.2	496557.1	0.00000	ppm	SV	3	
4	7.858	186707.1	75743.2	0.00000		SV		
5	11.390	107891.4	29827.1	0.00000				
6	12.653	1253214.2	517106.0	0.00000				

L1 CsF T12



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.134	18192068.6	6720802.1	0.00000	ppm	SV	1	
2	4.483	3684036.5	1715451.4	0.00000	ppm	SV	1	
3	7.342	611408.3	321847.2	0.00000	ppm	S	3	
4	7.860	1025000.9	472633.7	0.00000		S		
5	11.395	48847.1	13491.2	0.00000				
6	12.654	139147.7	50283.7	0.00000				

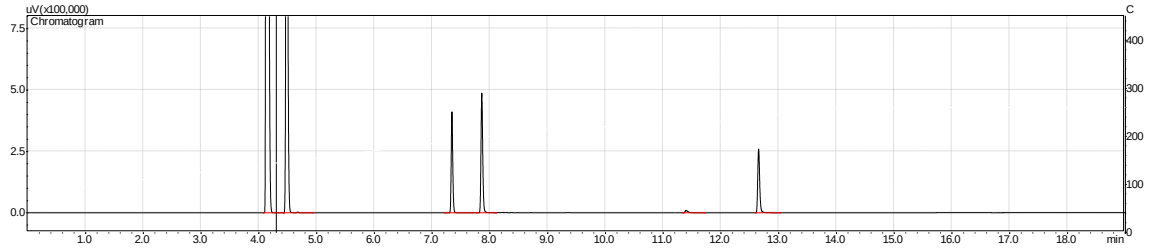
L1 TBAF T12



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name

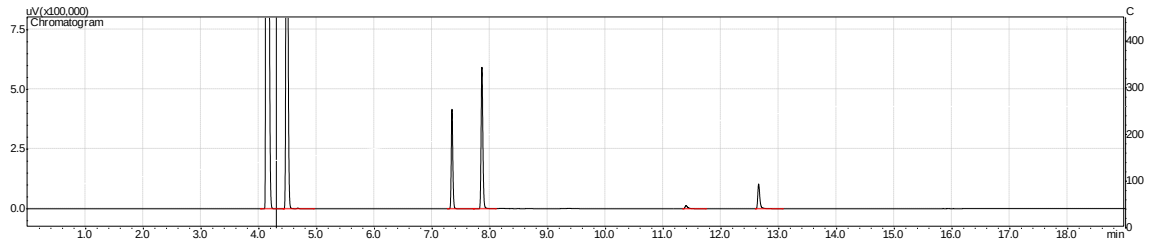
1	4.135	17370489.5	6422791.3	0.00000	ppm	SV	1	
2	4.483	5564450.9	2552664.6	0.00000	ppm	S	1	
3	7.341	600851.0	315857.9	0.00000	ppm	S	3	
4	7.860	1178963.8	543304.7	0.00000		V		
5	8.207	20019.0	2058.1	0.00000	ppm	V	4	
6	9.342	143024.1	21727.3	0.00000	ppm	S	5	
7	11.400	32276.4	7892.4	0.00000				
8	12.663	46073.0	13794.4	0.00000				

L1 K3PO4 T12



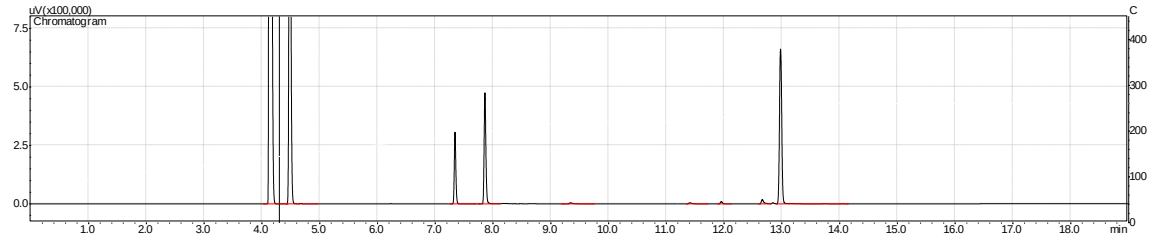
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.135	16362197.6	6208594.1	0.00000	ppm	SV	1	
2	4.481	5257455.5	2441932.3	0.00000	ppm	SV	1	
3	7.342	767187.7	404069.3	0.00000	ppm	SV	3	
4	7.859	1031717.1	480861.2	0.00000				
5	11.397	36367.3	9753.6	0.00000				
6	12.652	614233.4	256121.6	0.00000				

L1 CsCO3



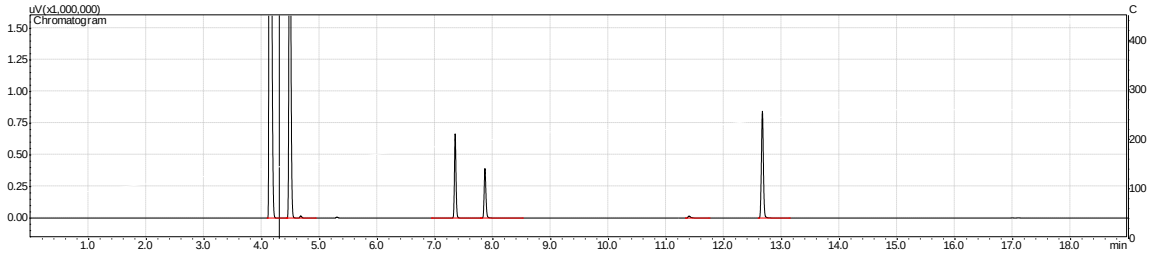
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.135	17586057.9	6483013.0	0.00000	ppm	SV	1	
2	4.483	5310398.9	2440835.8	0.00000	ppm	SV	1	
3	7.342	777246.7	411142.1	0.00000	ppm	SV	3	
4	7.860	1260616.6	587063.6	0.00000		V		
5	11.394	46868.2	13426.7	0.00000				
6	12.651	262046.1	102861.9	0.00000				

L1 Cy2NMe T12



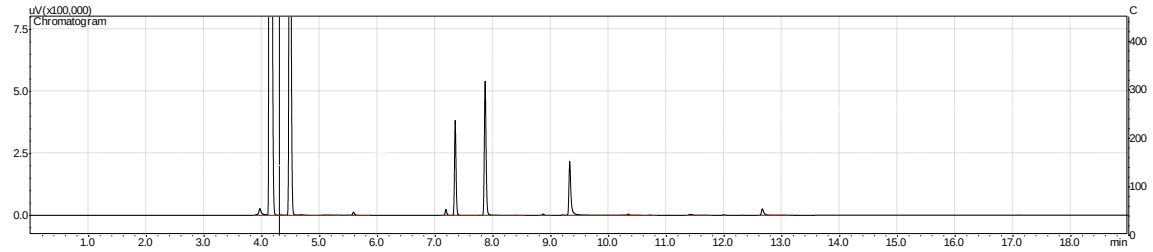
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.135	16292430.9	6159534.2	0.00000	ppm	SV	1	
2	4.482	5059191.6	2366068.9	0.00000	ppm	SV	1	
3	7.342	569747.5	301707.2	0.00000	ppm	S	3	
4	7.860	1006471.5	467850.0	0.00000				
5	9.340	22084.0	4651.1	0.00000	ppm		5	
6	11.408	20106.3	4845.4	0.00000				
7	11.951	25508.2	10077.2	0.00000				
8	12.660	56606.9	18680.6	0.00000				
9	12.977	1813212.4	660606.3	0.00000		SV		

L3 CsF T12



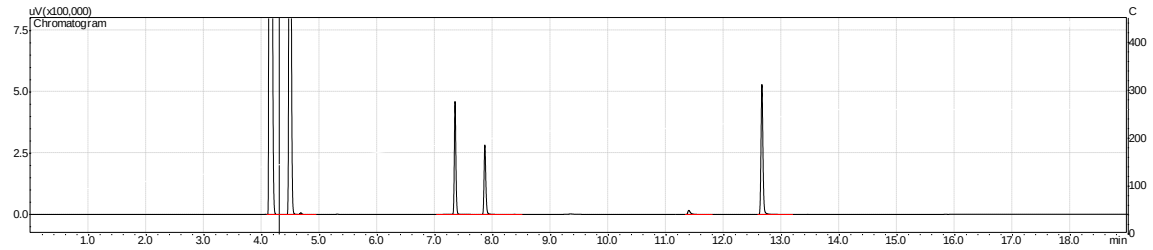
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.138	16237513.2	6157085.5	0.00000	ppm	SV	1	
2	4.483	7244571.5	3344451.2	0.00000	ppm	SV	1	
3	7.346	1267162.6	651028.7	0.00000	ppm	S	3	
4	7.862	846343.1	391365.4	0.00000		SV		
5	11.395	55664.5	16484.4	0.00000				
6	12.665	2016324.0	836639.5	0.00000				

L3 TBAF T12



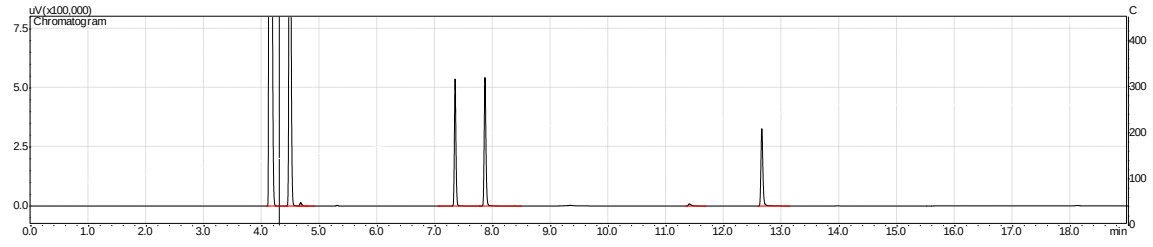
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	3.963	108005.2	27828.8	0.00000		V		
2	4.137	16220993.5	6166981.2	0.00000	ppm	SV	1	
3	4.483	5834574.4	2727308.5	0.00000	ppm	V	1	
4	4.676	26287.8	3290.6	0.00000		V		
5	5.091	18494.1	1411.0	0.00000		V		
6	5.584	31715.2	13153.0	0.00000		SV		
7	7.183	46465.3	23394.8	0.00000	ppm	V	3	
8	7.345	713825.3	379684.2	0.00000	ppm	SV	3	
9	7.863	1146047.0	535960.3	0.00000		S		
10	8.866	10568.8	5408.2	0.00000				
11	9.327	563596.9	215874.9	0.00000	ppm	SV	5	
12	10.339	11773.6	4872.7	0.00000		T		
13	11.414	19083.7	4218.0	0.00000				
14	12.661	77321.1	25250.1	0.00000		S		

L3 K3PO4 T12



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.139	17130818.0	6329858.3	0.00000	ppm	SV	1	
2	4.485	7401203.4	3333914.0	0.00000	ppm	SV	1	
3	7.346	883351.8	451454.6	0.00000	ppm	SV	3	
4	7.862	610876.8	281979.3	0.00000		SV		
5	11.394	56848.8	16952.8	0.00000				
6	12.660	1236680.0	527551.4	0.00000				

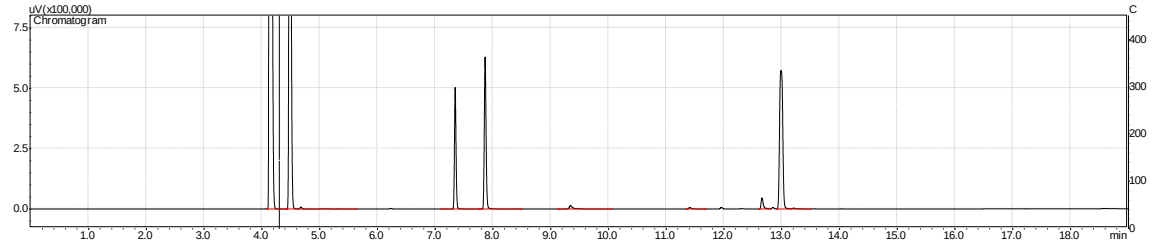
L3 CsCO3



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name

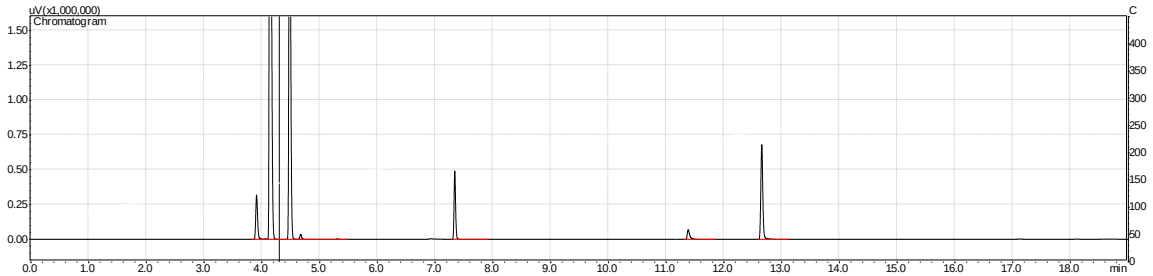
1	4.137	17248925.5	6432912.0	0.00000	ppm	SV	1	
2	4.484	5248451.1	2425953.9	0.00000	ppm	SV	1	
3	4.673	32190.2	14596.4	0.00000		T		
4	7.346	1009120.5	525123.8	0.00000	ppm	SV	3	
5	7.863	1149304.6	536562.2	0.00000		SV		
6	11.402	33762.0	9231.9	0.00000				
7	12.656	772320.0	323087.1	0.00000		S		

L3 Cy2NMe T12



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.139	16427903.9	6167123.7	0.00000	ppm	SV	1	
2	4.484	7221468.7	3303704.3	0.00000	ppm	SV	1	
3	7.346	946343.8	491987.8	0.00000	ppm	SV	3	
4	7.865	1342543.1	620163.7	0.00000		SV		
5	9.341	63667.8	14249.5	0.00000	ppm	S	5	
6	11.407	22982.7	5931.6	0.00000				
7	12.658	123889.8	46048.6	0.00000				
8	12.987	2216486.7	573761.8	0.00000		V		
9	13.208	20036.4	3595.1	0.00000		V		

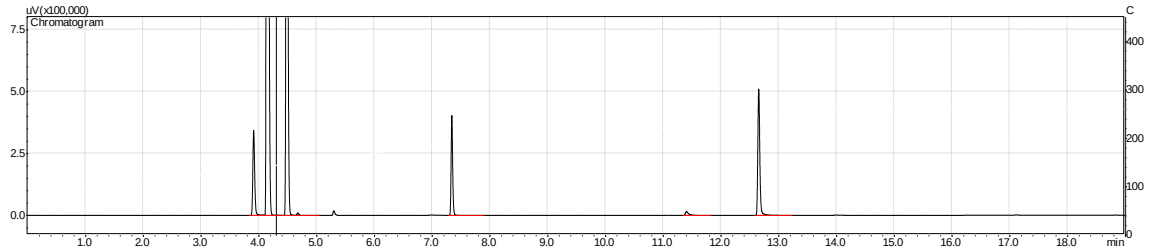
L1 RT_THF_KOH_



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	3.908	724841.5	318070.0	0.00000		SV		
2	4.141	12110624.8	5074461.6	0.00000	ppm	SV	1	
3	4.481	7197512.1	3500147.2	0.00000	ppm	SV	1	
4	4.671	76247.4	36275.8	0.00000		T		
5	7.340	922137.8	485746.8	0.00000	ppm	SV	3	

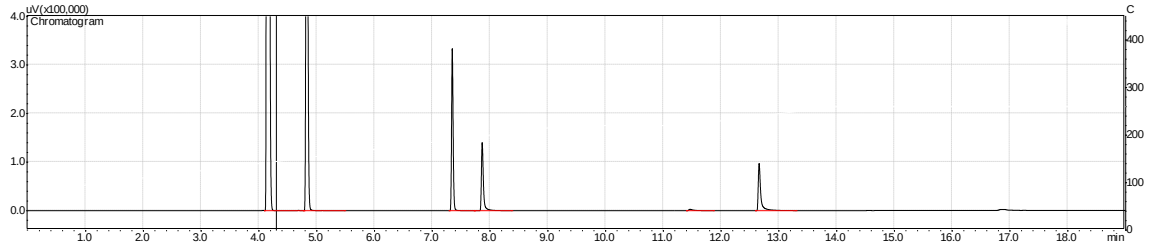
6	11.382	79578.2	69397.9	0.00000				
7	12.656	1636017.5	672532.7	0.00000				

L3 RT_THF_KOH_



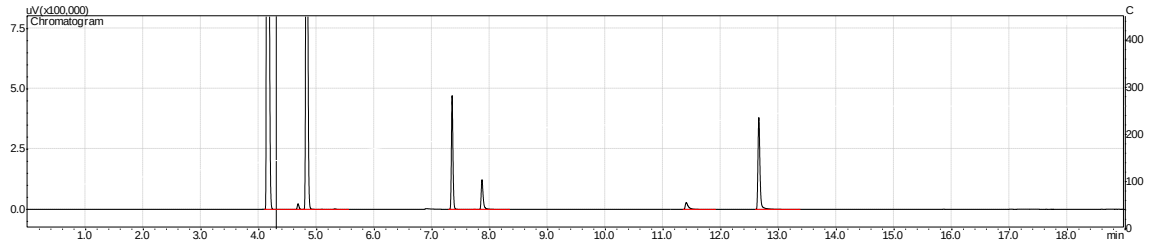
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	3.909	777136.3	342264.9	0.00000		SV		
2	4.140	12677924.9	5230094.5	0.00000	ppm	SV	1	
3	4.482	6659770.0	3251311.0	0.00000	ppm	SV	1	
4	7.339	761469.3	401384.0	0.00000	ppm	SV	3	
5	11.402	66680.7	15860.1	0.00000				
6	12.652	1230300.3	502719.0	0.00000				

L1 RT DIOXANE_K3PO4_



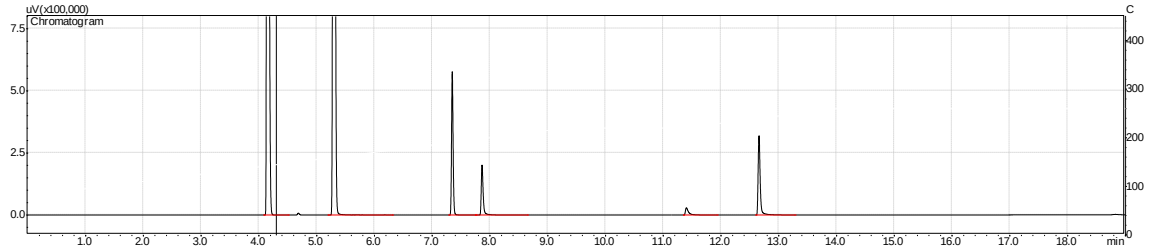
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.145	13502683.2	5510217.2	0.00000	ppm	SV	1	
2	4.827	2952194.4	1459853.5	0.00000		SV		
3	7.347	626812.9	326798.2	0.00000	ppm	SV	3	
4	7.864	340236.1	137951.8	0.00000		V		
5	11.463	18188.1	3049.5	0.00000				
6	12.658	296378.1	96199.4	0.00000				

L3 RT DIOXANE_K3PO4_



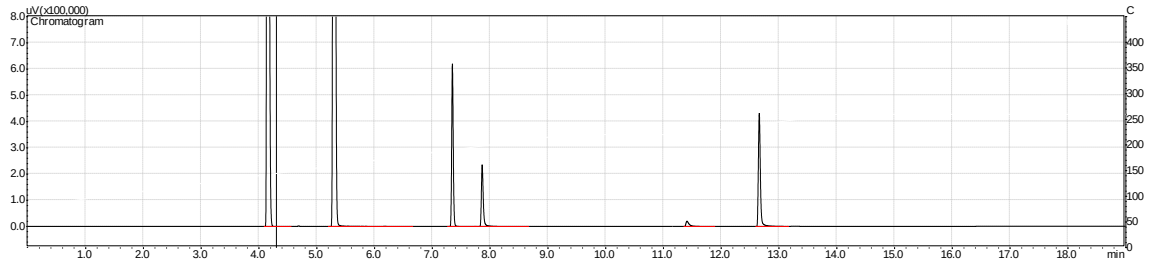
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.147	12123367.3	5090233.5	0.00000	ppm	SV	1	
2	4.827	5919447.5	2878865.3	0.00000		SV		
3	7.346	880265.8	461082.8	0.00000	ppm	SV	3	
4	7.864	298864.9	122068.7	0.00000		SV		
5	11.401	111690.1	28489.6	0.00000				
6	12.658	938724.2	376243.1	0.00000				

L1_RT TOLUENE_K3PO4_



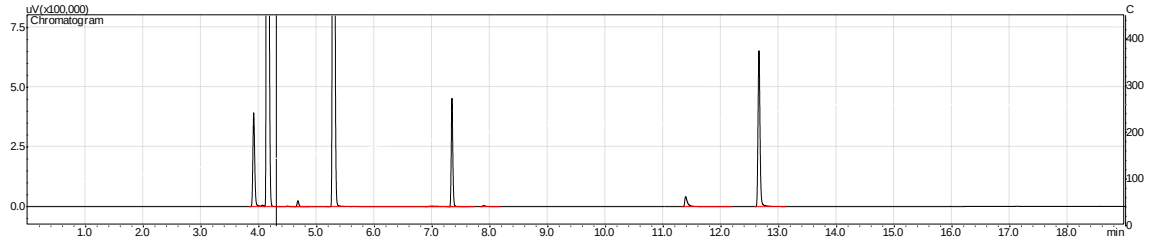
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.147	12384790.0	5181617.7	0.00000	ppm	SV	1	
2	5.296	19348770.9	9322889.9	0.00000		SV		
3	7.347	1077437.0	567905.4	0.00000	ppm	SV	3	
4	7.863	467011.5	199190.0	0.00000		SV		
5	11.401	115162.4	29164.0	0.00000				
6	12.658	800004.1	316540.5	0.00000		V		

L3_RT TOLUENE_K3PO4_



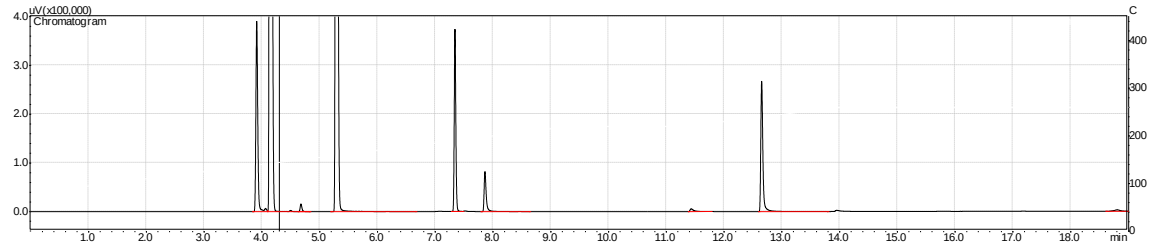
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.148	12183969.1	5107041.2	0.00000	ppm	SV	1	
2	5.297	22817139.4	10789879.6	0.00000		SV		
3	7.348	1160102.2	614239.7	0.00000	ppm	S	3	
4	7.863	542849.1	233831.5	0.00000		SV		
5	11.408	85373.8	20528.9	0.00000				
6	12.659	1050371.6	428293.5	0.00000				

L1 RT TOLUENE KOH



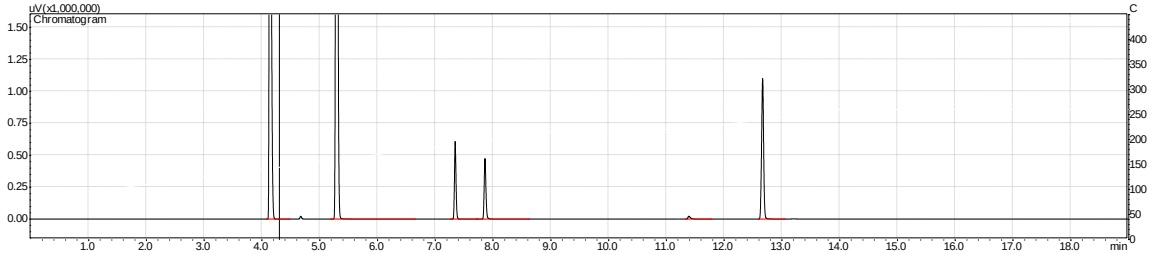
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	3.910	887116.7	390708.5	0.00000		SV		
2	4.143	12386709.7	5168522.4	0.00000	ppm	SV	1	
3	4.675	54423.5	25042.1	0.00000		T		
4	5.290	14249310.5	6997260.1	0.00000		S		
5	7.004	27653.9	2055.2	0.00000	ppm	T	3	
6	7.342	847038.0	444194.6	0.00000	ppm	TV	3	
7	7.888	16226.3	4187.8	0.00000				
8	11.388	148627.2	41913.7	0.00000		SV		
9	12.656	1576461.6	645009.9	0.00000				

L3 RT TOLUENE KOH



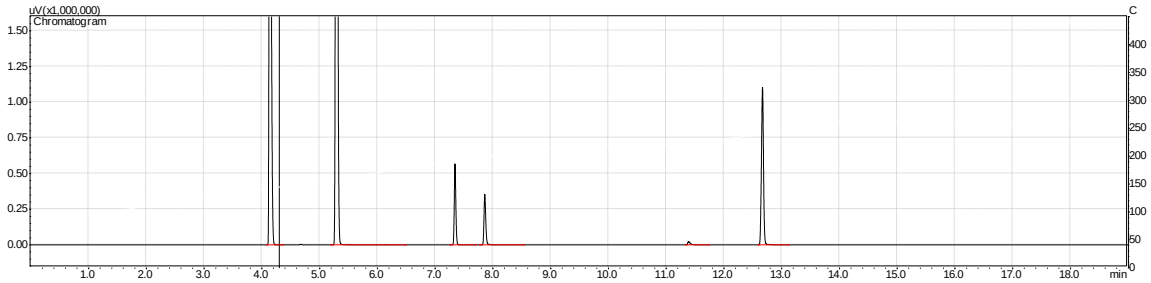
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	3.910	887214.7	388577.5	0.00000		SV		
2	4.142	12742468.1	5283333.0	0.00000	ppm	SV	1	
3	4.675	33811.3	15609.9	0.00000		T		
4	5.290	12606460.1	6210109.8	0.00000		S		
5	7.341	694271.6	364732.2	0.00000	ppm		3	
6	7.860	209377.2	81455.7	0.00000		SV		
7	11.431	27586.6	5789.1	0.00000				
8	12.651	672869.7	265862.0	0.00000		SV		
9	18.805	22993.6	2985.9	0.00000	ppm		8	

L1 RT TOLUENE K2CO3



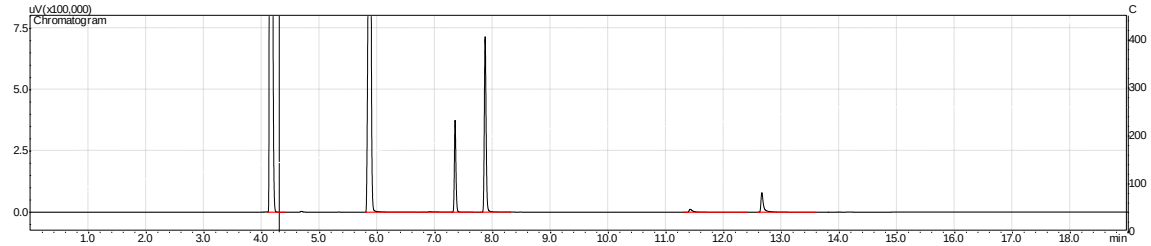
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.138	11536875.2	4886854.7	0.00000	ppm	V	1	
2	5.291	20925943.2	10009744.5	0.00000		SV		
3	7.344	1127325.4	601772.8	0.00000	ppm	S	3	
4	7.860	1009939.2	466157.3	0.00000		SV		
5	11.390	76200.3	22912.8	0.00000				
6	12.666	2717608.8	1085679.3	0.00000		V		

L3 RT TOLUENE K2CO3



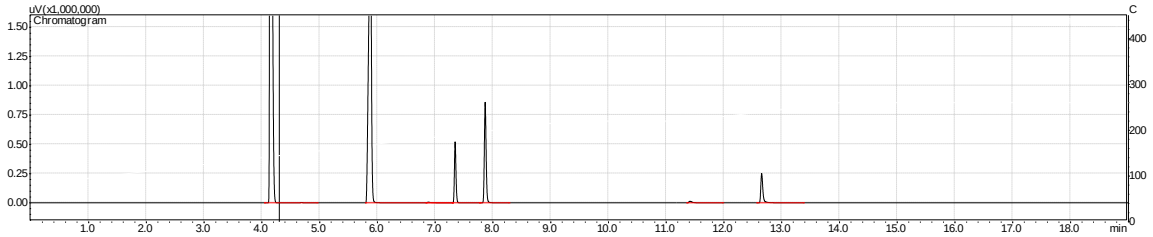
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.138	11589447.2	4902433.3	0.00000	ppm	V	1	
2	5.291	21292447.7	10180164.1	0.00000		SV		
3	7.344	1053197.3	562658.8	0.00000	ppm	S	3	
4	7.859	760809.3	349811.6	0.00000		S		
5	11.390	76090.5	23246.2	0.00000				
6	12.668	2739811.8	1098930.7	0.00000		S		

L1 RT DMA K2CO3



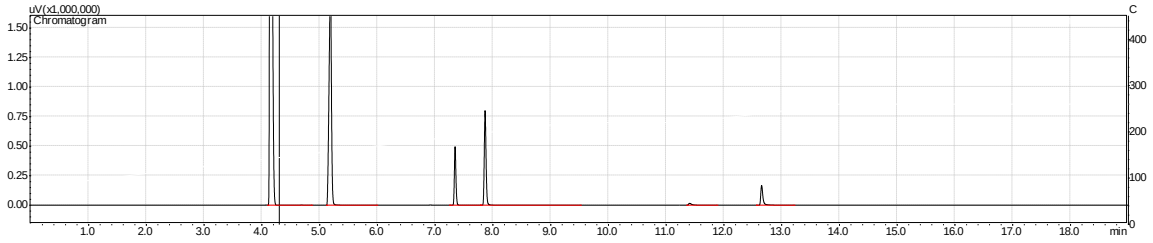
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.147	14859921.5	5632825.6	0.00000	ppm	V	1	
2	5.872	6716732.9	2167832.7	0.00000		SV		
3	7.346	701521.4	365071.3	0.00000	ppm	SV	3	
4	7.867	1538366.8	712169.7	0.00000				
5	11.418	57834.7	12241.3	0.00000		SV		
6	12.659	250091.7	79429.8	0.00000		S		

L3 RT DMA K2CO3



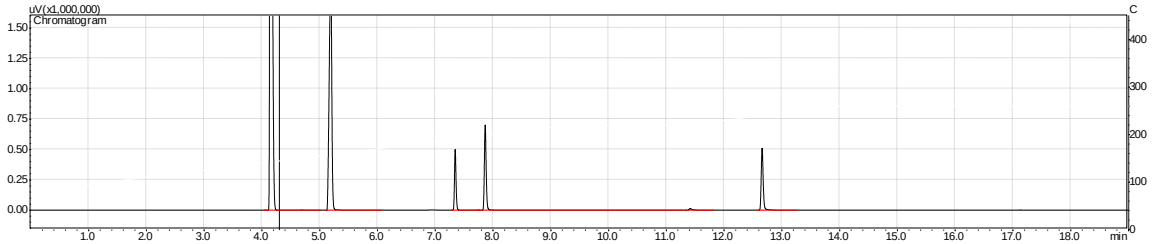
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.150	15538969.4	5656629.8	0.00000	ppm	SV	1	
2	5.878	8310680.9	2478483.3	0.00000		SV		
3	6.882	41385.5	6637.0	0.00000	ppm	T	3	
4	7.346	974436.3	509889.8	0.00000	ppm	SV	3	
5	7.866	1841346.4	854824.8	0.00000		V		
6	11.412	65978.0	14293.5	0.00000		SV		
7	12.653	646657.1	248241.4	0.00000		S		

L1 RT DMF K2CO3



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.149	16288686.3	5877196.7	0.00000	ppm	SV	1	
2	5.187	5366605.4	1849458.3	0.00000		SV		
3	7.345	936001.4	488954.4	0.00000	ppm	SV	3	
4	7.865	1735730.2	792983.6	0.00000		SV		
5	11.406	70474.5	16689.2	0.00000		SV		
6	12.653	455789.1	165775.8	0.00000		SV		

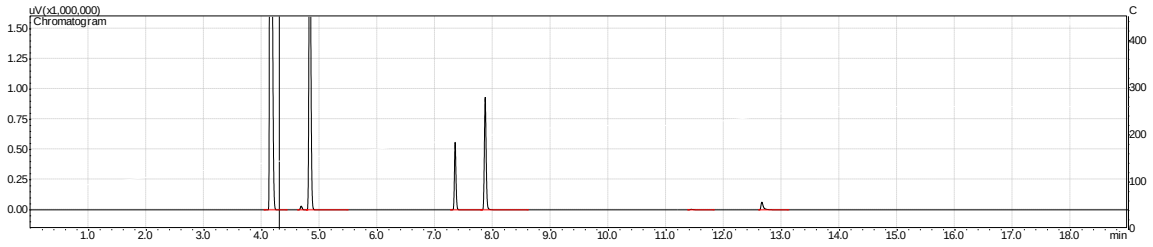
L3 RT DMF K2CO3



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name

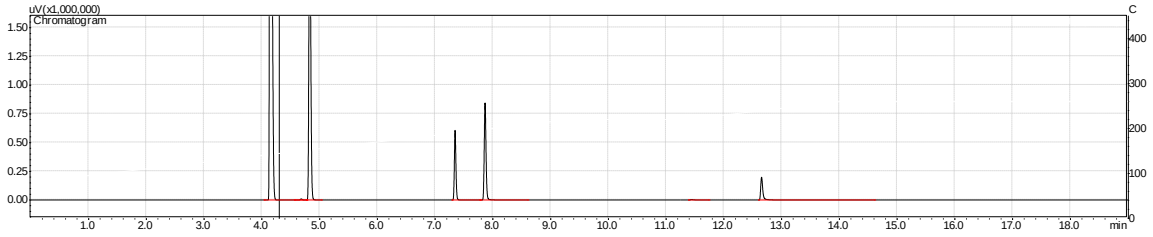
1	4.150	15504551.6	5614423.4	0.00000	ppm	SV	1	
2	5.191	6119656.0	2007372.9	0.00000		S		
3	7.345	941039.4	496730.6	0.00000	ppm	SV	3	
4	7.864	1514023.0	688854.0	0.00000		SV		
5	11.412	57446.4	13040.3	0.00000		S		
6	12.658	1227983.6	504578.1	0.00000		SV		

L1 RT DIOXANE K2CO3



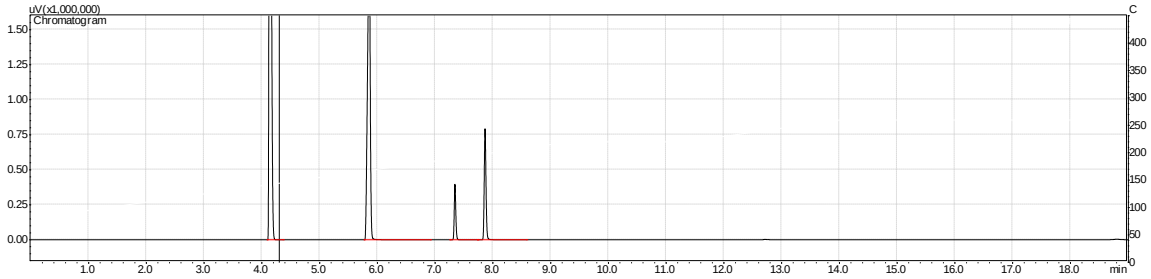
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.148	16156130.7	5992274.9	0.00000	ppm	V	1	
2	4.680	72075.9	32001.2	0.00000				
3	4.829	6439221.5	2965025.8	0.00000		SV		
4	7.346	1046971.0	549634.2	0.00000	ppm	SV	3	
5	7.866	2024032.8	927652.7	0.00000		SV		
6	11.435	25545.8	4930.3	0.00000				
7	12.656	201077.0	63445.6	0.00000		V		

L3 RT DIOXANE K2CO3



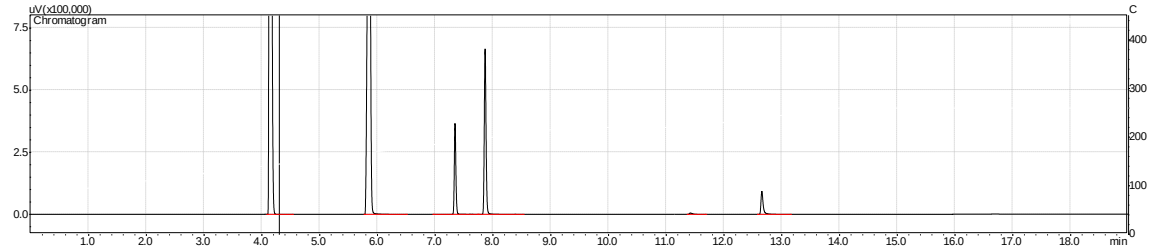
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.147	16203865.4	6016681.6	0.00000	ppm	SV	1	
2	4.681	22945.4	9870.5	0.00000		T		
3	4.829	6245004.6	2887544.1	0.00000		V		
4	7.346	1139371.2	595768.1	0.00000	ppm	SV	3	
5	7.865	1826969.6	834562.2	0.00000		SV		
6	11.441	18214.0	3527.2	0.00000		S		
7	12.653	499122.6	196670.5	0.00000		SV		

L1 RT DMA K3PO4



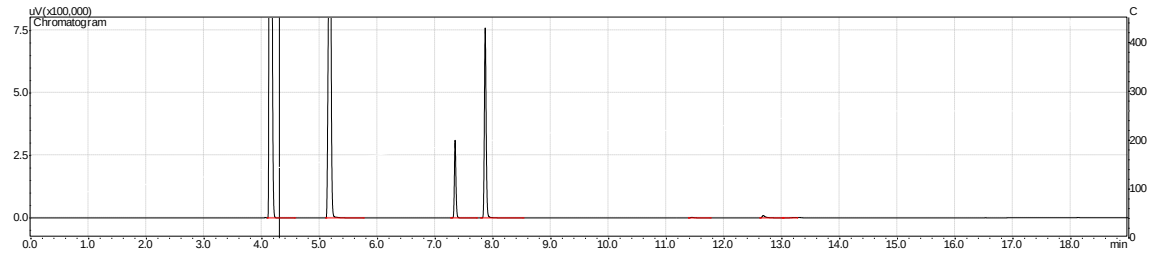
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.138	13722717.1	5527632.7	0.00000	ppm	V	1	
2	5.858	6999051.8	2188345.5	0.00000		S		
3	7.343	736928.5	393903.6	0.00000	ppm	S	3	
4	7.864	1693252.2	781781.7	0.00000		SV		

L3 RT DMA K3PO4



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.138	13050133.0	5333303.6	0.00000	ppm	SV	1	
2	5.860	7158175.1	2228700.8	0.00000		S		
3	7.343	694975.5	363631.3	0.00000	ppm	S	3	
4	7.864	1412630.5	654243.6	0.00000		SV		
5	11.419	22664.8	5485.2	0.00000				
6	12.655	250317.4	91900.2	0.00000				

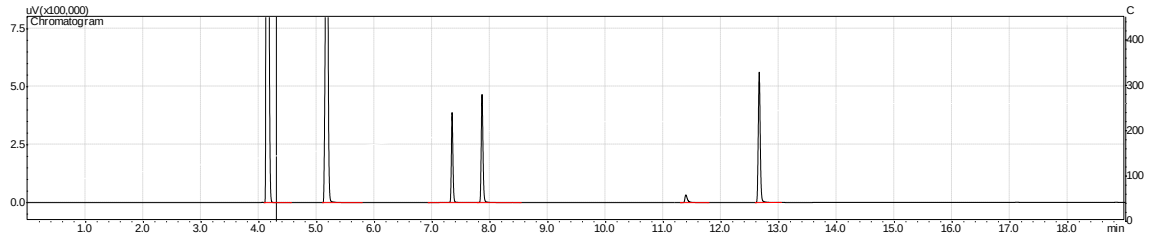
L1 RT DMF K3PO4



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name

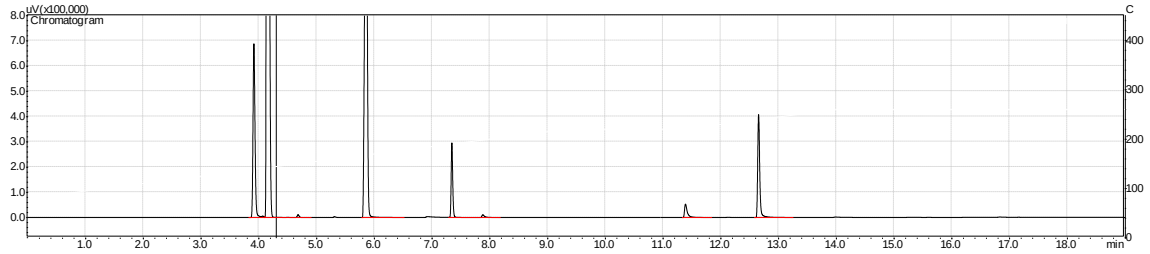
1	4.138	13706364.3	5509237.4	0.00000	ppm	SV	1	
2	5.177	5136249.9	1785497.7	0.00000		S		
3	7.343	578980.3	308609.3	0.00000	ppm	S	3	
4	7.864	1624660.8	747303.9	0.00000		S		
5	11.441	11602.1	2223.9	0.00000				
6	12.676	41076.6	9649.2	0.00000		V		
7	13.237	11026.5	1652.9	0.00000		V		

L3 RT DMF K3PO4



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.138	13033785.5	5329082.0	0.00000	ppm	SV	1	
2	5.177	5293679.0	1822547.1	0.00000				
3	7.343	759216.4	384961.0	0.00000	ppm	S	3	
4	7.861	1003392.5	463590.7	0.00000		SV		
5	11.390	106382.7	33458.6	0.00000				
6	12.659	1338478.0	560051.0	0.00000				

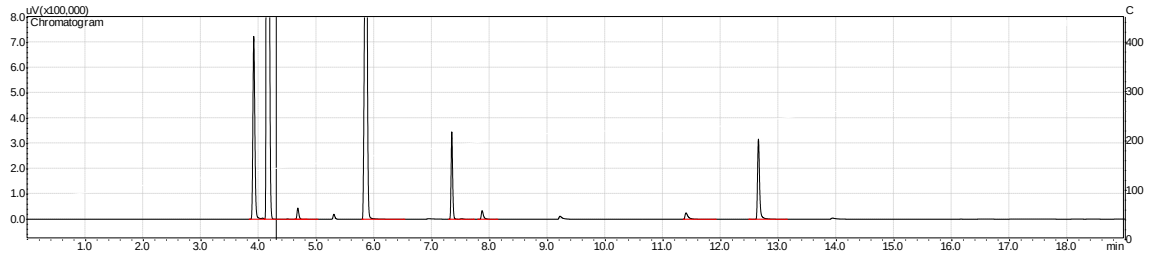
L1 RT DMA KOH



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	3.914	1668829.8	685238.7	0.00000		SV		
2	4.145	15415119.3	5765699.6	0.00000	ppm	SV	1	
3	5.859	5489125.7	1879928.6	0.00000		S		
4	7.342	559124.3	291300.2	0.00000	ppm	SV	3	
5	11.387	181300.5	52830.0	0.00000				

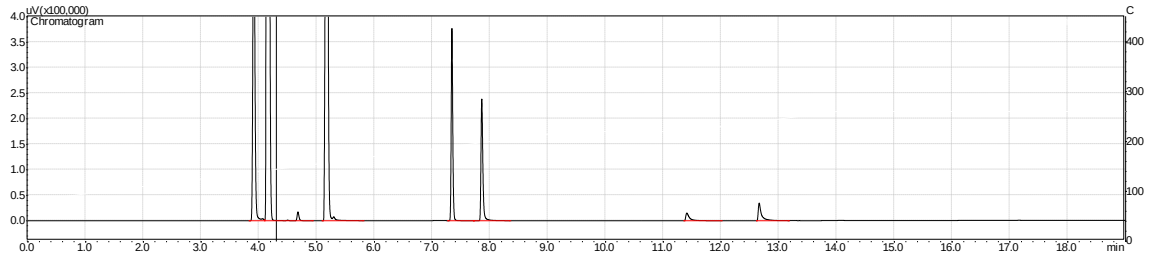
6	12.654	997841.2	405444.0	0.00000		S		

L3 RT DMA KOH



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	3.912	1718711.0	715597.0	0.00000		SV		
2	4.144	14261447.4	5513068.5	0.00000	ppm	SV	1	
3	4.675	100018.2	44823.0	0.00000		T		
4	5.858	5421448.3	1851105.7	0.00000		S		
5	7.341	651029.8	340165.7	0.00000	ppm	SV	3	
6	7.866	93124.4	34326.9	0.00000				
7	11.397	102777.8	25363.0	0.00000				
8	12.651	789138.6	316462.3	0.00000				

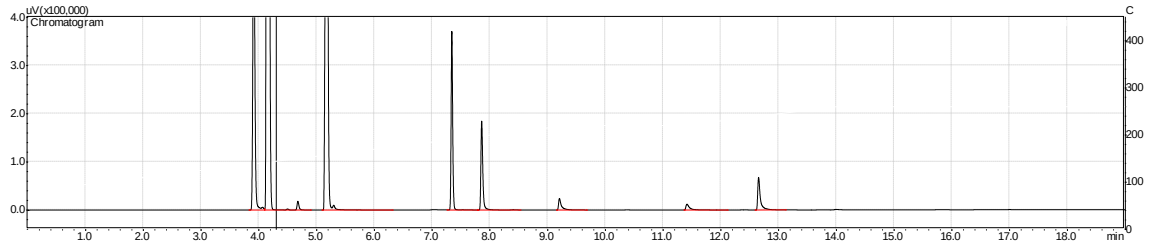
L1 RT DMF KOH



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	3.910	1695872.9	719179.2	0.00000		SV		
2	4.143	13039676.3	5176624.1	0.00000	ppm	SV	1	
3	5.175	4179208.3	1544733.6	0.00000		S		

4	7.341	705526.9	369123.4	0.00000	ppm	SV	3	
5	7.858	544396.3	237337.5	0.00000				
6	11.408	69719.2	15254.2	0.00000		SV		
7	12.660	137244.2	34377.9	0.00000		V		

L3 RT DMF KOH

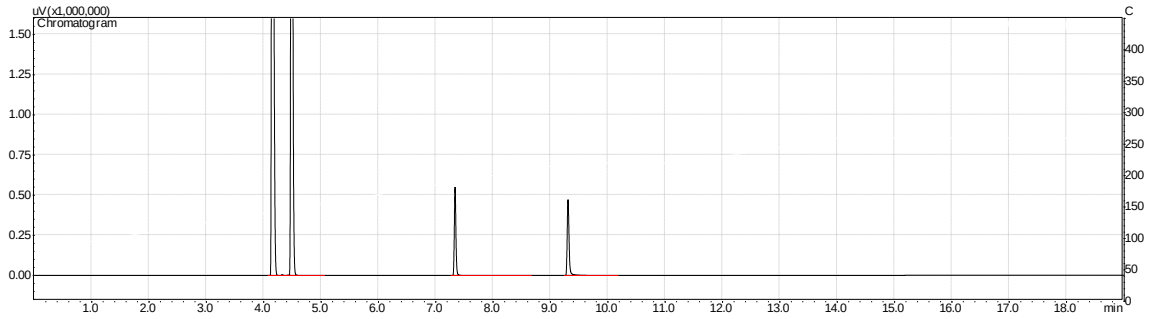


Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	3.911	1613042.5	675118.7	0.00000		SV		
2	4.144	13446996.1	5296670.0	0.00000	ppm	SV	1	
3	5.175	4095356.1	1522510.6	0.00000		S		
4	7.341	694788.4	361299.7	0.00000	ppm	SV	3	
5	7.858	421928.5	182947.8	0.00000		SV		
6	9.205	85914.2	23871.1	0.00000	ppm	SV	5	
7	11.413	58915.1	12159.6	0.00000		SV		
8	12.654	215359.4	67085.3	0.00000				

<u>Room temperature substrate screening</u>

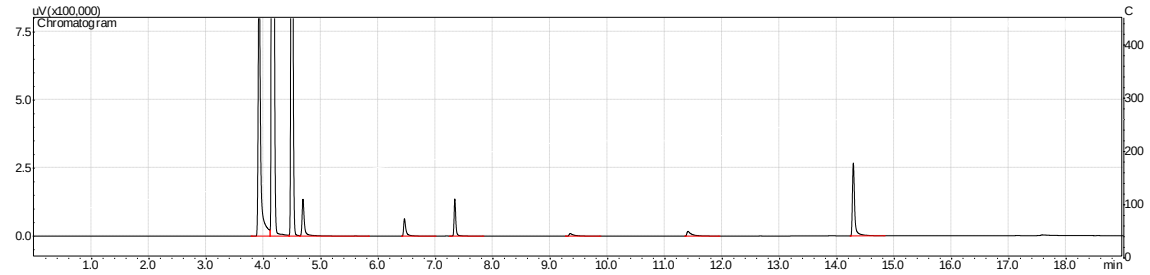
4-Methoxy-biphenyl

Ar_Br_1_RT_ To



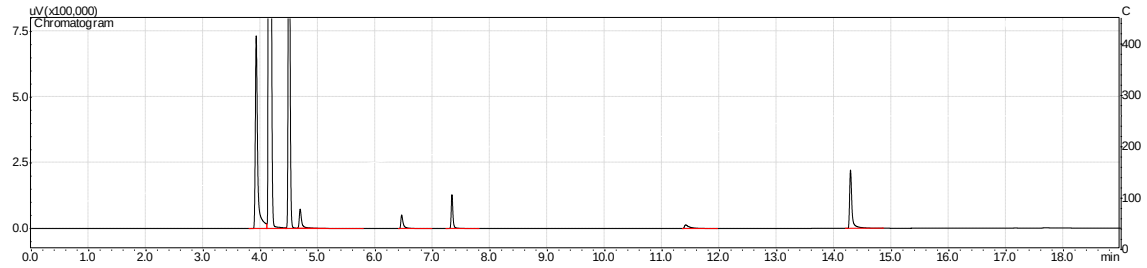
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.149	12798233.3	5286538.8	0.00000	ppm	SV	1	
2	4.485	12196844.3	5776622.4	0.00000	ppm	V	1	
3	7.336	1053454.2	542515.1	0.00000	ppm	SV	3	
4	9.306	1103305.7	465699.3	0.00000	ppm		5	

L1_Ar_Br_1_RT _12H:



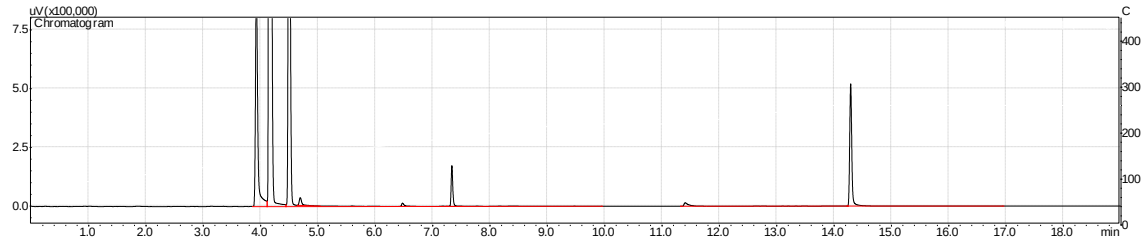
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	3.920	2936038.3	1026098.7	0.00000				
2	4.149	13127892.5	5318978.7	0.00000	ppm	SV	1	
3	4.490	6773409.9	3250833.1	0.00000	ppm	V	1	
4	4.686	417478.0	134353.6	0.00000		SV		
5	6.456	84461.2	63794.7	0.00000	ppm		2	
6	7.334	287321.2	136169.9	0.00000	ppm	V	3	
7	9.348	37217.8	9520.0	0.00000	ppm		5	
8	11.401	104817.0	17622.5	0.00000		V		
9	14.285	742659.5	263896.4	0.00000	ppm		6	

L3_Ar_Br_1_RT_ 12H:



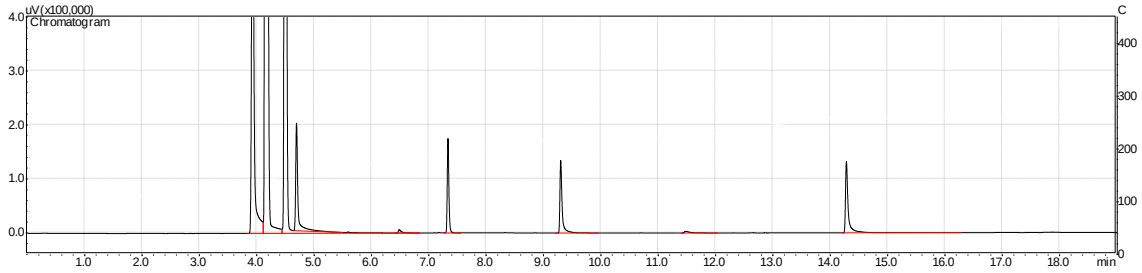
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	3.921	2086796.3	727118.4	0.00000				
2	4.147	15126787.6	5976183.5	0.00000	ppm	V	1	
3	4.493	3706066.9	1768612.0	0.00000	ppm	SV	1	
4	4.688	217447.1	72808.7	0.00000		T		
5	6.458	156224.8	51694.9	0.00000	ppm		2	
6	7.334	275518.4	128572.1	0.00000	ppm	V	3	
7	11.410	89890.8	14133.6	0.00000				
8	14.285	633543.8	219038.7	0.00000	ppm		6	

CyJohnPhos_Ar_Br_1_RT _12H:



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	3.925	2608259.1	917695.5	0.00000		V		
2	4.152	20006847.1	7756672.9	0.00000	ppm	V	1	
3	4.495	6536418.1	2844949.3	0.00000	ppm	SV	1	
4	4.690	105829.6	32858.9	0.00000		T		
5	6.473	57070.0	14825.2	0.00000	ppm	T	2	
6	7.334	358824.2	173236.8	0.00000	ppm	TV	3	
7	11.403	74028.7	15619.8	0.00000		SV		
8	14.289	1360420.9	516776.1	0.00000	ppm	SV	6	

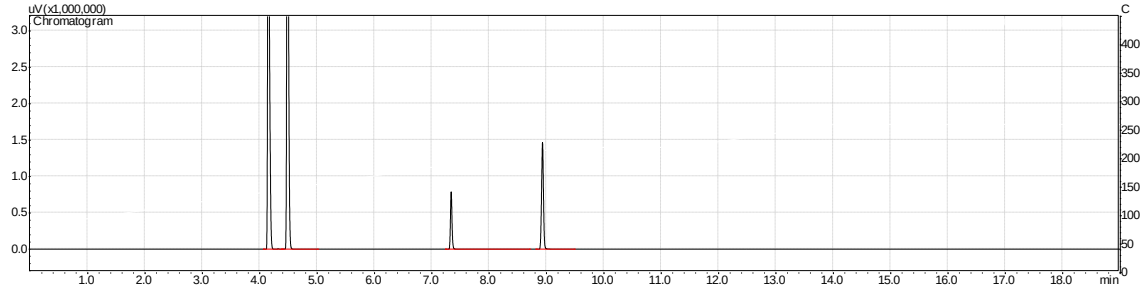
JohnPhos_Ar_Br_1_RT _12H:



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	3.926	2416539.2	845193.4	0.00000				
2	4.153	17974753.1	6881425.8	0.00000	ppm	V	1	
3	4.495	6824195.5	2934644.4	0.00000	ppm	SV	1	
4	4.693	546079.4	198386.3	0.00000		T		
5	6.486	29303.3	6542.1	0.00000	ppm	TV	2	
6	7.334	350723.1	174385.6	0.00000	ppm	V	3	
7	9.300	372700.9	134090.8	0.00000	ppm	SV	5	
8	11.482	28130.7	3460.5	0.00000		S		
9	14.282	440958.3	131369.1	0.00000	ppm	SV	6	

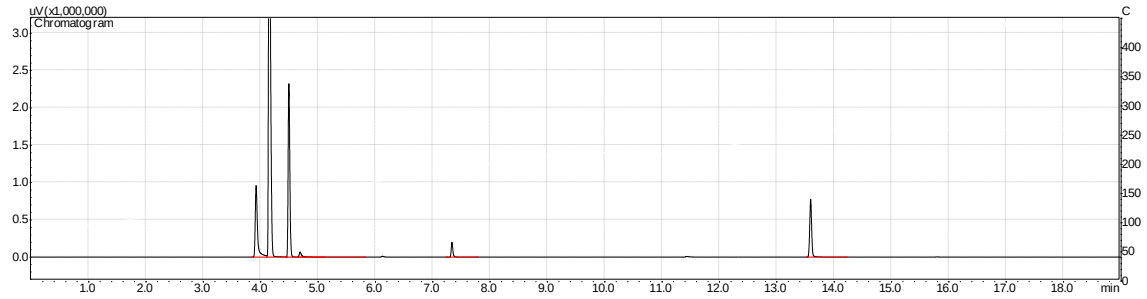
3,5-Dimethyl-1,1'-biphenyl

Ar_Br_2_RT_ To



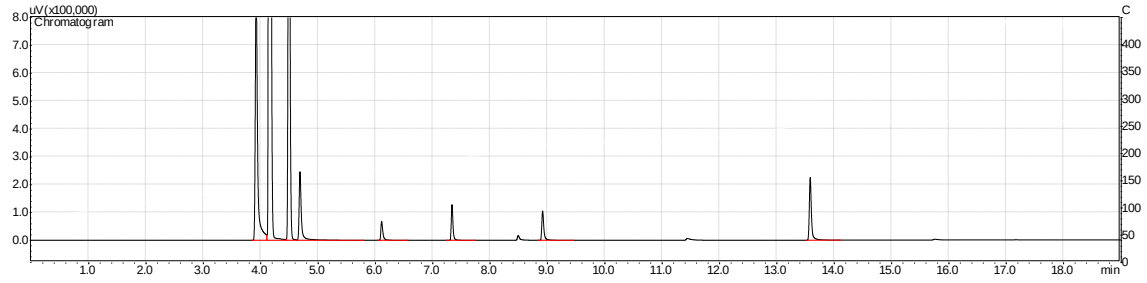
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.149	12083239.4	5028464.4	0.00000	ppm	SV	1	
2	4.483	14497131.7	6812399.3	0.00000	ppm	V	1	
3	7.337	1500159.6	771529.8	0.00000	ppm	SV	3	
4	8.930	3393013.0	1456478.6	0.00000				

L1_Ar_Br_2_RT _12H:



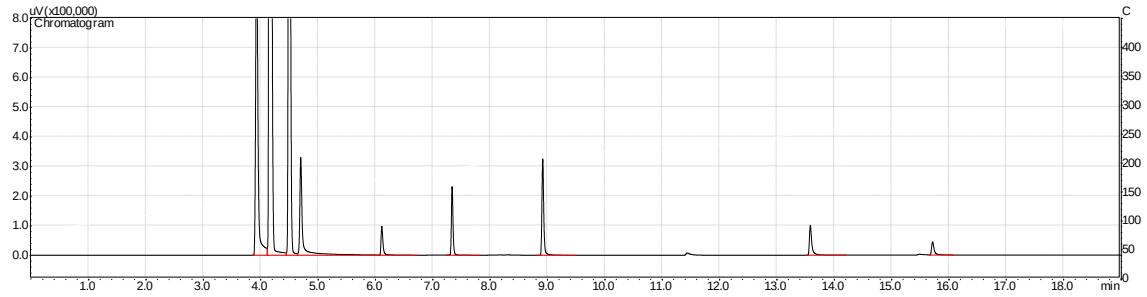
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	3.920	2674872.9	954795.1	0.00000		V		
2	4.148	13405195.1	5436174.9	0.00000	ppm	V	1	
3	4.491	4807114.5	2291566.8	0.00000	ppm	SV	1	
4	4.686	203601.8	64463.4	0.00000		T		
5	7.334	404573.7	198436.4	0.00000	ppm	V	3	
6	13.590	1853648.4	765044.6	0.00000		S		

L3_Ar_Br_2_RT_ 12H:



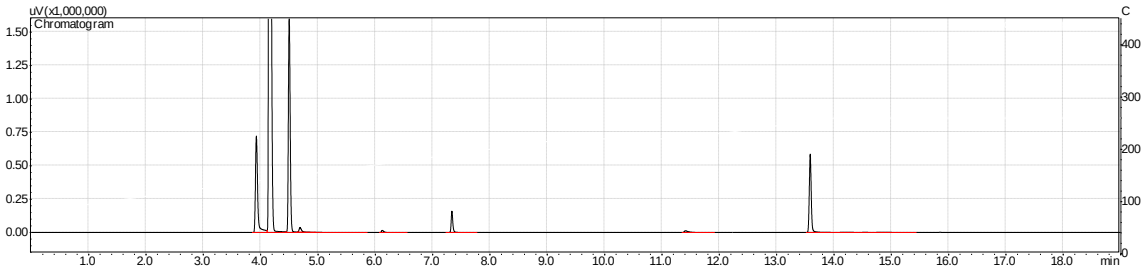
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	3.920	2550991.1	904724.6	0.00000		V		
2	4.149	13190995.1	5356703.0	0.00000	ppm	V	1	
3	4.491	4963602.5	2394041.9	0.00000	ppm	V	1	
4	4.684	702707.5	245541.5	0.00000		SV		
5	6.108	101881.3	67990.2	0.00000		S		
6	7.335	266162.4	127388.3	0.00000	ppm	V	3	
7	8.915	454780.2	104323.8	0.00000		SV		
8	13.581	585572.0	221461.4	0.00000				

PPh3_Ar_Br_2_RT _12H:



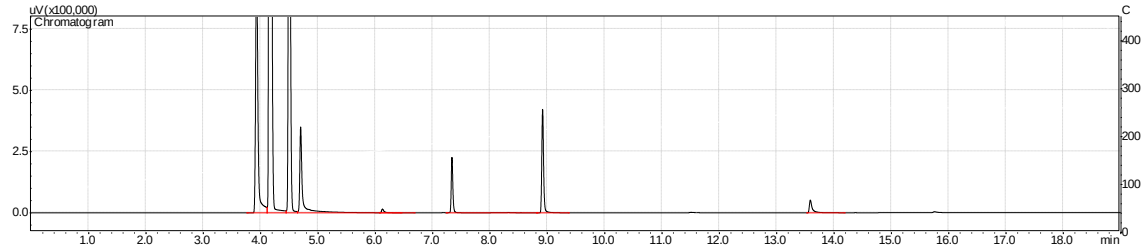
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	3.928	3030547.0	1057558.7	0.00000		V		
2	4.155	16501085.4	6183956.7	0.00000	ppm	V	1	
3	4.496	7168854.6	3180089.4	0.00000	ppm	V	1	
4	4.697	1167706.1	328433.7	0.00000		SV		
5	6.110	244536.6	97050.9	0.00000		SV		
6	7.336	459707.1	229393.4	0.00000	ppm	SV	3	
7	8.916	727099.2	323849.4	0.00000				
8	13.582	302904.3	100552.6	0.00000		S		
9	15.713	146021.4	44218.7	0.00000	ppm	V	6	

CyJohnPhos_Ar_Br_2_RT _12H:



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	3.925	1968250.9	717269.4	0.00000				
2	4.152	18199956.5	6881091.7	0.00000	ppm	V	1	
3	4.498	3632886.2	1607024.6	0.00000	ppm	SV	1	
4	4.687	100071.7	34169.3	0.00000		T		
5	6.121	50513.1	16705.7	0.00000				
6	7.335	328422.3	158380.9	0.00000	ppm	V	3	
7	11.410	77853.2	13453.6	0.00000				
8	13.585	1420908.8	579071.0	0.00000		SV		

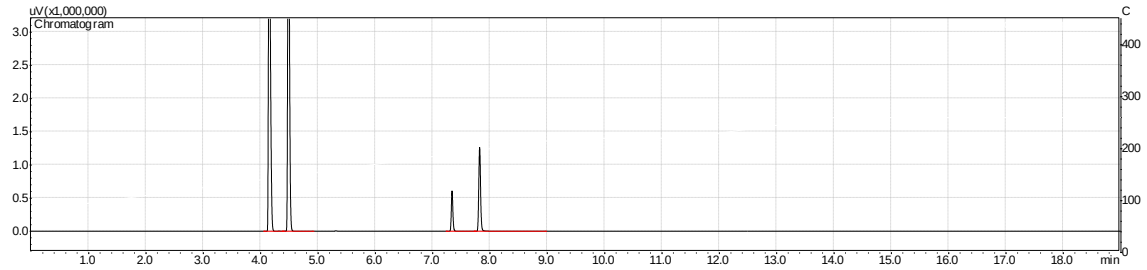
JohnPhos_Ar_Br_2_RT _12H:



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	3.928	2928920.9	1014625.4	0.00000				
2	4.154	17532575.0	6480499.3	0.00000	ppm	V	1	
3	4.498	5836239.4	2581508.1	0.00000	ppm	V	1	
4	4.697	1218075.3	349182.3	0.00000		SV		
5	6.123	47660.1	15181.1	0.00000		T		
6	7.336	450128.3	223744.8	0.00000	ppm	SV	3	
7	8.917	927969.9	420877.7	0.00000				
8	13.586	187993.0	51902.7	0.00000				

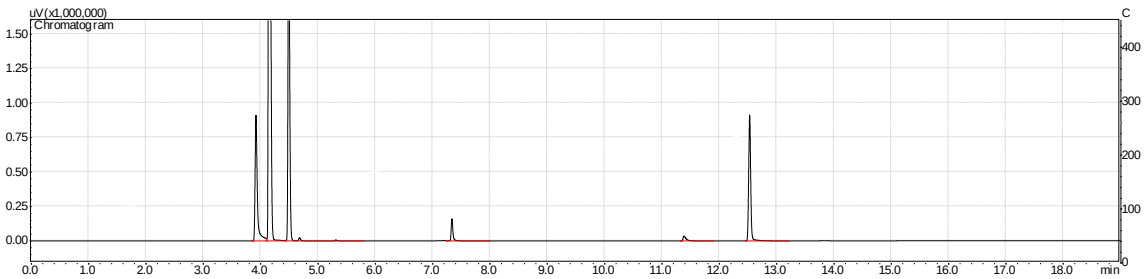
3-Methyl-biphenyl

Ar_Br_3_RT_ To



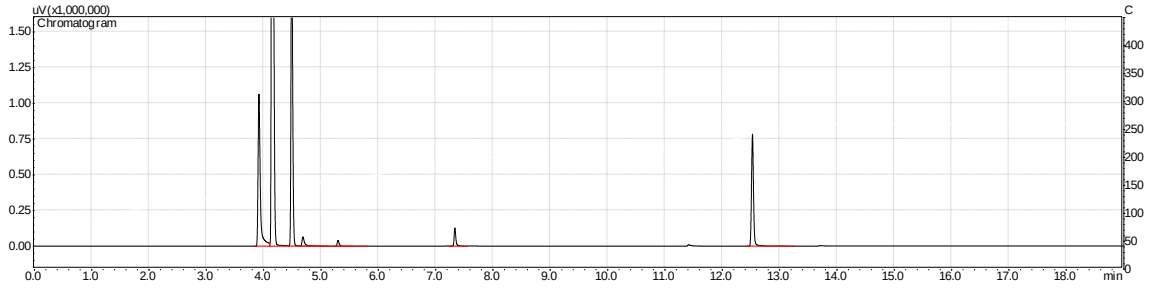
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.148	12508966.0	5204094.2	0.00000	ppm	SV	1	
2	4.484	12561854.5	5981187.9	0.00000	ppm	V	1	
3	7.337	1152613.7	596712.8	0.00000	ppm	SV	3	
4	7.819	2797176.3	1251694.9	0.00000		SV		

L1_Ar_Br_3_RT _12H:



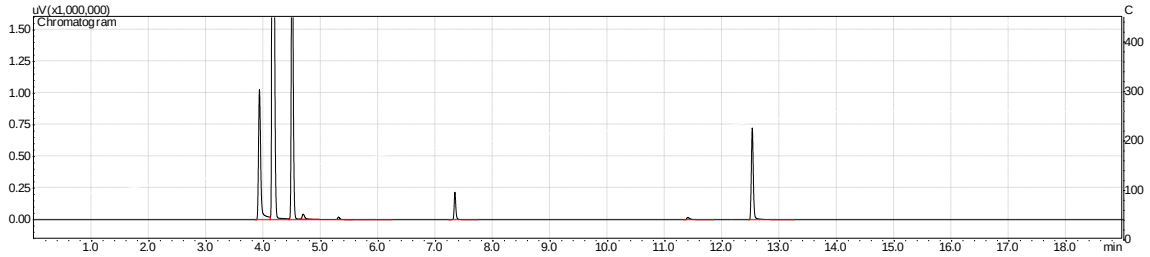
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	3.918	2489593.5	908256.8	0.00000		V		
2	4.147	13187189.2	5378284.2	0.00000	ppm	SV	1	
3	4.490	5061647.5	2427317.2	0.00000	ppm	SV	1	
4	7.335	356604.0	159847.7	0.00000	ppm	SV	3	
5	11.385	139697.7	35741.5	0.00000		S		
6	12.529	2252119.0	908782.0	0.00000		S		

L3_Ar_Br_3_RT_ 12H:



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	3.918	2905603.2	1059644.3	0.00000		V		
2	4.148	12809088.7	5245219.6	0.00000	ppm	V	1	
3	4.490	4595002.3	2186214.8	0.00000	ppm	SV	1	
4	4.685	200968.1	63268.7	0.00000		T		
5	5.297	77144.3	40477.7	0.00000		T		
6	7.335	272061.6	126858.1	0.00000	ppm	V	3	
7	12.526	1930096.7	773000.6	0.00000		S		

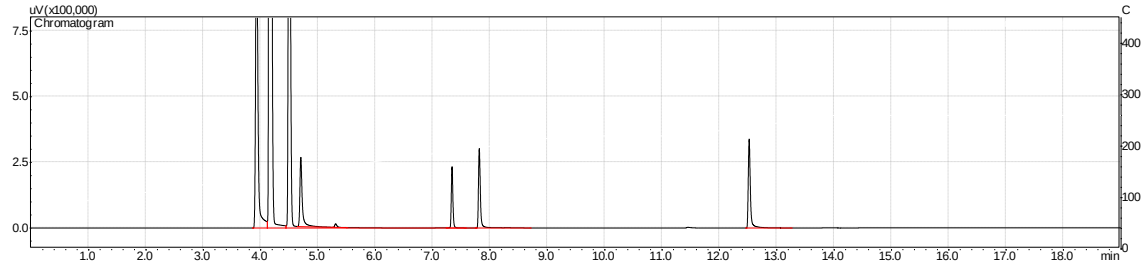
CyJohnPhos_Ar_Br_3_RT _12H:



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	3.927	2844176.7	1021498.6	0.00000		V		
2	4.157	14939673.0	5743196.4	0.00000	ppm	V	1	
3	4.497	5962750.6	2620227.9	0.00000	ppm	SV	1	
4	4.690	125838.8	39676.6	0.00000		T		
5	5.306	53019.2	20245.9	0.00000		T		

6	7.336	439061.3	215360.1	0.00000	ppm	V	3	
7	11.398	78826.4	18130.1	0.00000		S		
8	12.523	1775952.8	721435.5	0.00000		S		

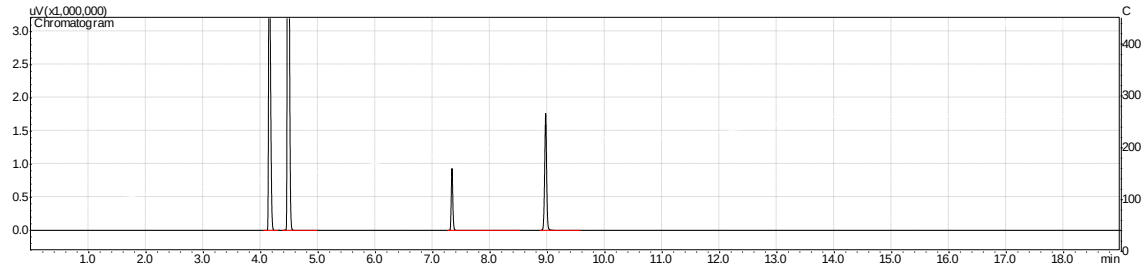
JohnPhos_Ar_Br_3_RT _12H:



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	3.928	3439155.9	1194170.4	0.00000		V		
2	4.156	16240344.2	6070235.3	0.00000	ppm	V	1	
3	4.497	6742841.7	2852420.9	0.00000	ppm	SV	1	
4	4.699	759046.1	261158.7	0.00000		T		
5	5.307	35686.6	13466.5	0.00000		T		
6	7.336	452285.1	229778.3	0.00000	ppm	TV	3	
7	7.811	1359058.6	300265.8	0.00000		SV		
8	12.518	886056.7	336718.5	0.00000				

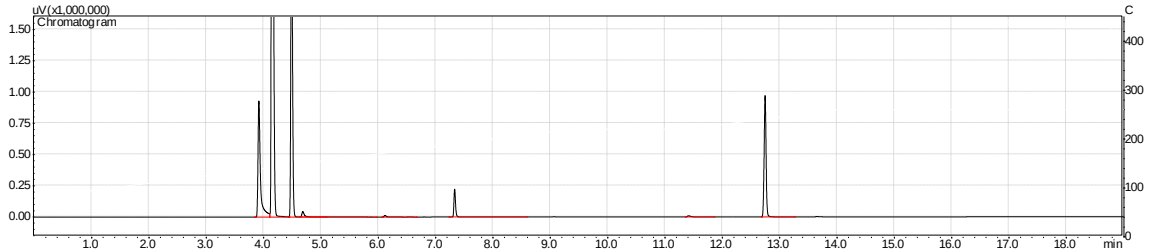
2,4-Dimethyl-1,1'-biphenyl

Ar_Br_4_RT_ To



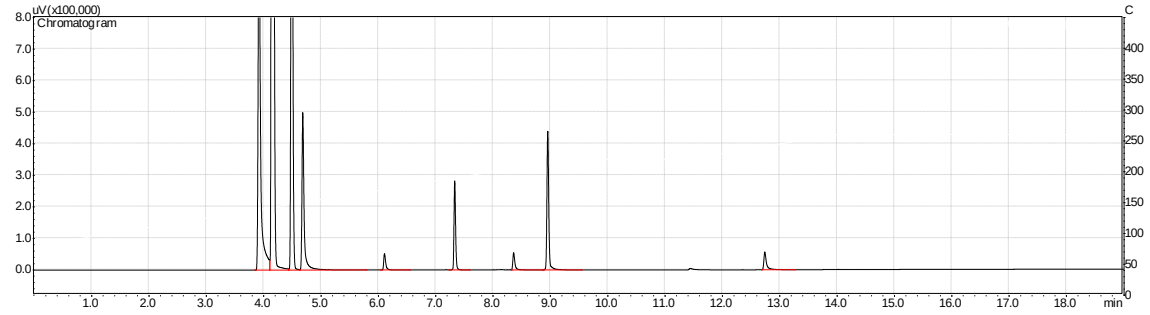
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.149	10376768.1	4437065.4	0.00000	ppm	V	1	
2	4.475	19922481.6	9076037.2	0.00000	ppm	V	1	
3	7.334	1774688.2	927456.9	0.00000	ppm	SV	3	
4	8.968	4232201.0	1759051.1	0.00000		V		

L1_Ar_Br_4_RT _12H:



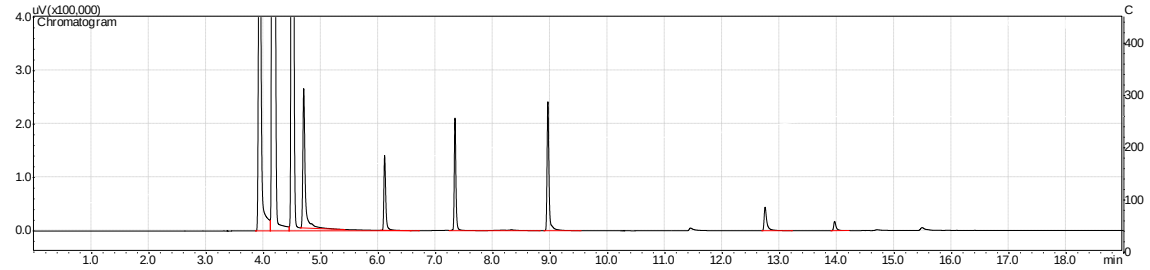
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	3.916	2776210.7	918830.3	0.00000		V		
2	4.146	12285980.9	5076474.7	0.00000	ppm	V	1	
3	4.486	5333404.8	2572563.9	0.00000	ppm	SV	1	
4	4.682	149082.4	44566.3	0.00000		T		
5	6.115	46158.4	14632.5	0.00000		S		
6	7.330	452824.4	223505.0	0.00000	ppm	SV	3	
7	11.411	55451.0	10655.7	0.00000				
8	12.746	2307149.3	956916.8	0.00000		SV		

L3_Ar_Br_4_RT_ 12H:



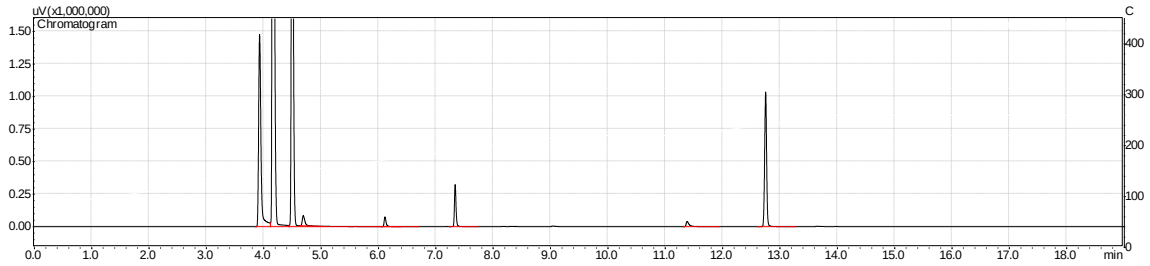
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	3.918	3443175.4	1152427.4	0.00000		V		
2	4.146	13918371.0	5548981.5	0.00000	ppm	V	1	
3	4.488	4859878.8	2352755.4	0.00000	ppm	V	1	
4	4.681	1319466.3	491871.3	0.00000		SV		
5	6.107	133823.6	51989.6	0.00000				
6	7.331	548041.1	280069.1	0.00000	ppm	V	3	
7	8.359	142023.7	54228.2	0.00000	ppm	SV	4	
8	8.953	987485.6	436698.9	0.00000		SV		
9	12.739	184833.2	55792.2	0.00000		SV		

PPh3_Ar_Br_4_RT _12H:



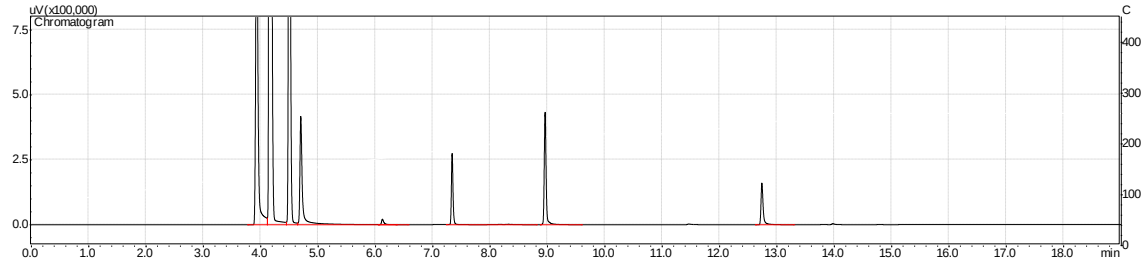
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	3.928	2772004.0	975061.9	0.00000		V		
2	4.156	16266744.0	6036759.5	0.00000	ppm	V	1	
3	4.497	7535612.1	3217339.0	0.00000	ppm	SV	1	
4	4.699	755184.1	258995.0	0.00000		T		
5	6.110	322318.0	137936.8	0.00000		T		
6	7.337	428154.2	206074.3	0.00000	ppm	SV	3	
7	8.957	574413.9	238682.0	0.00000				
8	12.746	148351.3	43789.9	0.00000		V		
9	13.959	51121.3	17127.7	0.00000		V		

CyJohnPhos_Ar_Br_4_RT _12H:



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	3.927	4200061.2	1472141.2	0.00000		V		
2	4.158	14122868.6	5317643.8	0.00000	ppm	V	1	
3	4.495	9817815.4	4168017.1	0.00000	ppm	SV	1	
4	4.689	253745.4	76840.5	0.00000		T		
5	6.112	181269.2	75125.1	0.00000		T		
6	7.337	635468.7	317228.1	0.00000	ppm	SV	3	
7	11.381	162265.3	40956.6	0.00000				
8	12.750	2480096.5	1024229.0	0.00000		V		

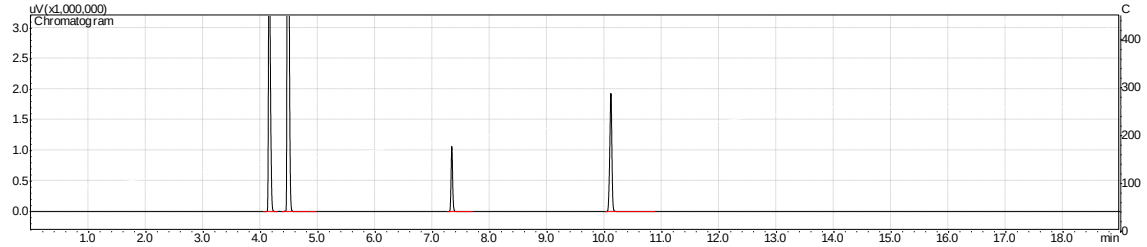
JohnPhos_Ar_Br_4_RT _12H:



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	3.928	3662711.3	1281815.7	0.00000				
2	4.155	16221730.8	6049298.2	0.00000	ppm	V	1	
3	4.498	5265432.5	2331319.2	0.00000	ppm	V	1	
4	4.698	1329977.6	415312.9	0.00000		SV		
5	6.121	61373.5	21037.1	0.00000		T		
6	7.336	545394.6	268603.0	0.00000	ppm	SV	3	
7	8.957	982904.0	430061.7	0.00000				
8	12.738	425321.6	159722.0	0.00000		S		

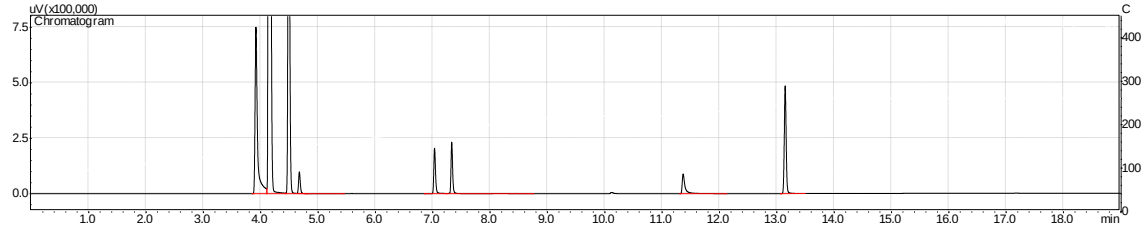
2,4,6-trimethyl-1,1'-biphenyl

Ar_Br_5_RT_ To



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.149	10185532.8	4385318.6	0.00000	ppm	V	1	
2	4.475	20446250.9	9344811.8	0.00000	ppm	V	1	
3	7.335	2029652.7	1054788.5	0.00000	ppm	SV	3	
4	10.110	4964057.7	1922839.7	0.00000	ppm	S	5	

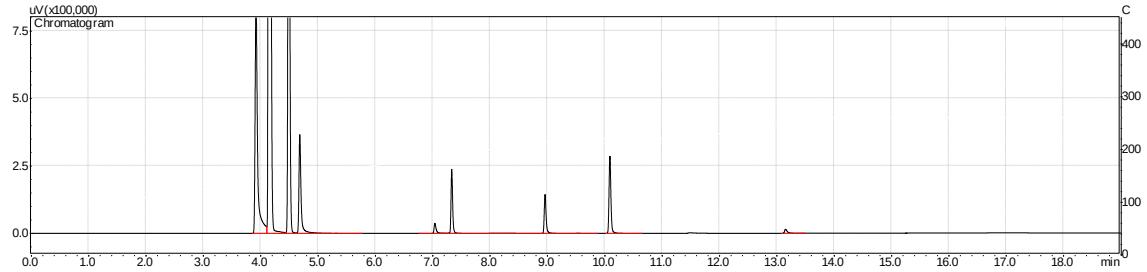
L1_Ar_Br_5_RT _12H:



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name

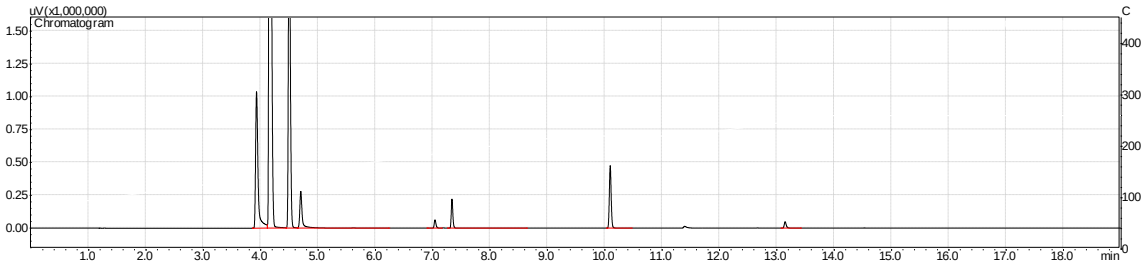
1	3.917	2218199.0	742560.6	0.00000		V		
2	4.144	14250430.7	5704125.9	0.00000	ppm	V	1	
3	4.488	4302172.0	2089866.2	0.00000	ppm	SV	1	
4	4.673	201041.5	96537.9	0.00000		T		
5	7.031	340197.9	204639.5	0.00000	ppm	SV	3	
6	7.331	475140.1	230575.0	0.00000	ppm	SV	3	
7	11.367	312171.5	88498.6	0.00000		S		
8	13.146	1094546.6	480854.6	0.00000				

L3_Ar_Br_5_RT_ 12H:



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	3.918	2611702.8	882780.6	0.00000		V		
2	4.144	14435876.7	5715114.8	0.00000	ppm	V	1	
3	4.488	4981556.2	2420044.3	0.00000	ppm	V	1	
4	4.681	964823.8	362302.1	0.00000		SV		
5	7.037	105815.8	37526.8	0.00000	ppm	SV	3	
6	7.330	485901.0	235817.9	0.00000	ppm	SV	3	
7	8.957	324439.6	142970.8	0.00000		SV		
8	10.088	2953055.7	283973.5	0.00000	ppm	S	5	
9	13.152	52588.4	15152.3	0.00000				

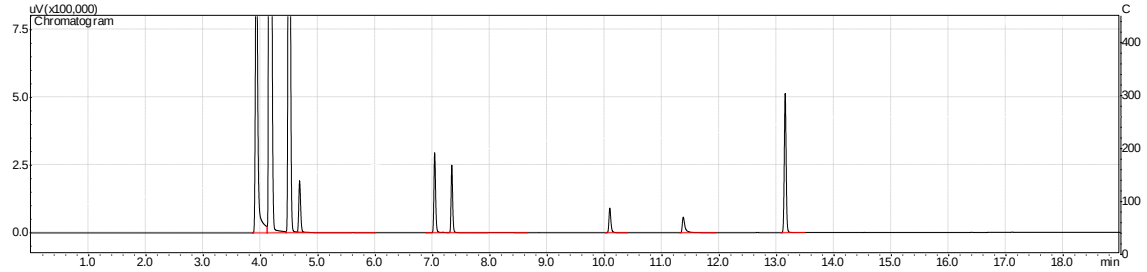
PPh3_Ar_Br_5_RT _12H:



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	3.927	3113944.3	1034006.0	0.00000		V		
2	4.155	16125156.5	5773740.0	0.00000	ppm	V	1	
3	4.497	6170530.6	2644322.1	0.00000	ppm	V	1	
4	4.698	907693.6	279182.3	0.00000		SV		

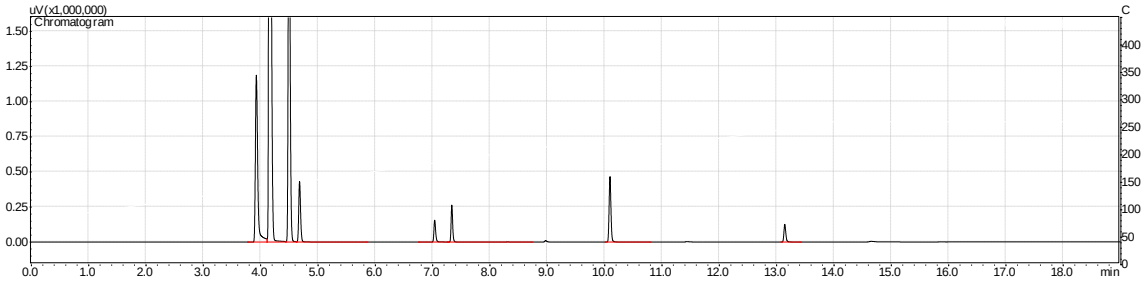
5	7.039	142383.4	62413.6	0.00000	ppm	V	3	
6	7.335	438806.8	220982.2	0.00000	ppm	SV	3	
7	10.094	4436527.4	470579.8	0.00000	ppm	S	5	
8	13.145	120643.9	48086.4	0.00000		V		

CyJohnPhos_Ar_Br_5_RT _12H:



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	3.925	3437159.4	1188967.1	0.00000		V		
2	4.154	15123871.7	5506904.2	0.00000	ppm	V	1	
3	4.494	7507864.0	3231288.7	0.00000	ppm	SV	1	
4	4.679	423254.3	188666.5	0.00000		T		
5	7.035	622658.5	293543.6	0.00000	ppm	SV	3	
6	7.333	493176.2	246821.8	0.00000	ppm	SV	3	
7	10.089	918174.9	90564.5	0.00000	ppm		5	
8	11.371	196494.3	57697.4	0.00000				
9	13.148	1157849.8	510696.0	0.00000				

JohnPhos_Ar_Br_5_RT _12H:

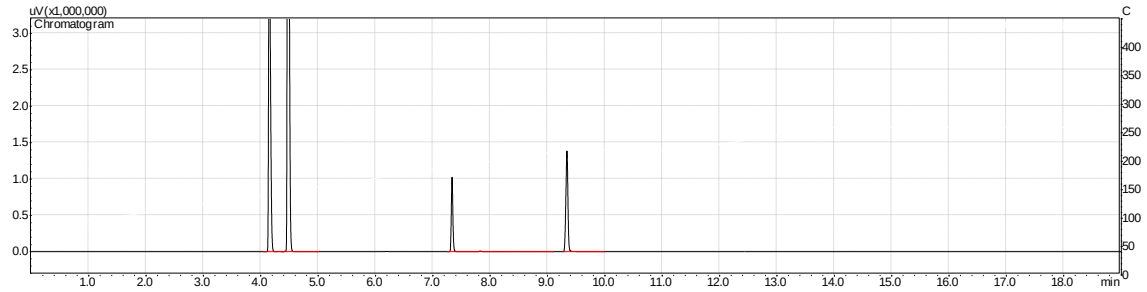


Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	3.925	3421247.7	1176924.7	0.00000				
2	4.154	15458552.8	5608169.3	0.00000	ppm	V	1	
3	4.494	6616093.3	2849006.9	0.00000	ppm	V	1	
4	4.678	1009283.2	430481.0	0.00000		SV		
5	7.035	344664.1	155804.2	0.00000	ppm	SV	3	
6	7.334	517728.7	261555.6	0.00000	ppm	SV	3	
7	10.093	3448786.1	463527.6	0.00000	ppm	S	5	

8	13.142	293102.2	124062.8	0.00000				

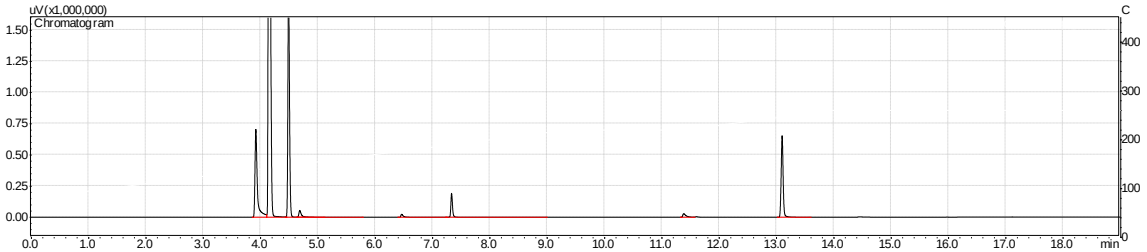
2-Methoxy-biphenyl

Ar_Br_6_RT_ To



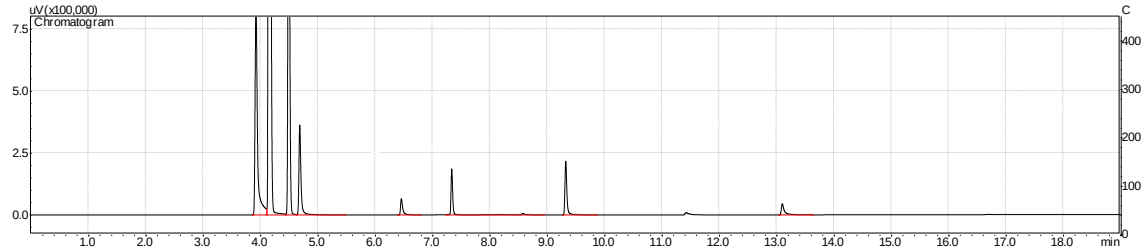
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.149	10164641.1	4365003.6	0.00000	ppm	SV	1	
2	4.474	21218423.1	9652291.5	0.00000	ppm	V	1	
3	7.335	1938495.0	1011905.5	0.00000	ppm	SV	3	
4	9.338	3465831.9	1369660.0	0.00000	ppm	V	5	

L1_Ar_Br_6_RT _12H:



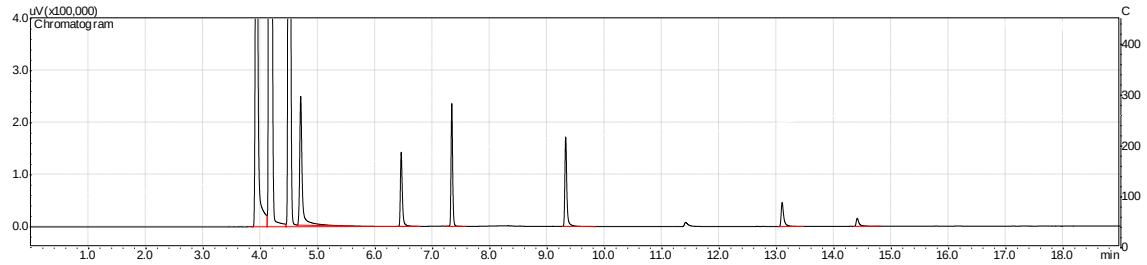
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	3.917	2057239.7	697907.3	0.00000		V		
2	4.146	12373237.3	5109163.6	0.00000	ppm	V	1	
3	4.488	3631220.6	1757309.4	0.00000	ppm	SV	1	
4	4.683	170705.6	53762.5	0.00000		T		
5	6.461	31465.6	24910.6	0.00000	ppm	SV	2	
6	7.331	405706.6	190240.7	0.00000	ppm	SV	3	
7	11.382	124468.5	29513.2	0.00000				
8	13.097	1572789.1	649858.0	0.00000				

L3_Ar_Br_6_RT_ 12H:



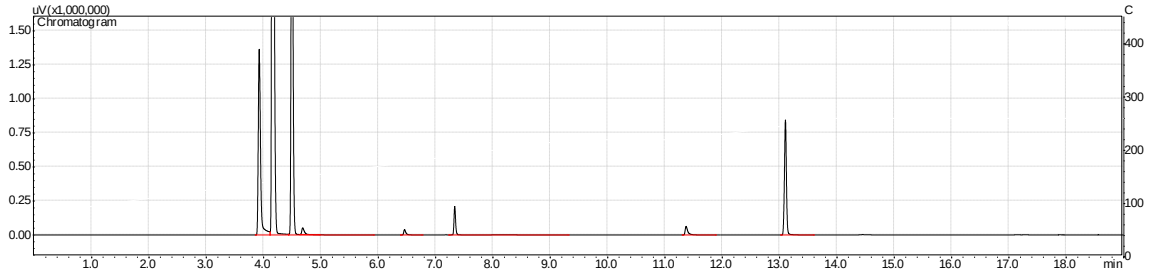
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	3.917	2582219.5	881732.2	0.00000		V		
2	4.144	13839352.1	5564829.0	0.00000	ppm	V	1	
3	4.488	4224617.3	2065984.0	0.00000	ppm	V	1	
4	4.680	920912.2	361623.1	0.00000		SV		
5	6.452	185563.9	65783.4	0.00000	ppm	V	2	
6	7.331	388759.9	185182.6	0.00000	ppm	SV	3	
7	9.319	2521232	215802.6	0.00000	ppm	V	5	
8	13.095	176259.4	44870.6	0.00000		S		

PPh3_Ar_Br_6_RT _12H:



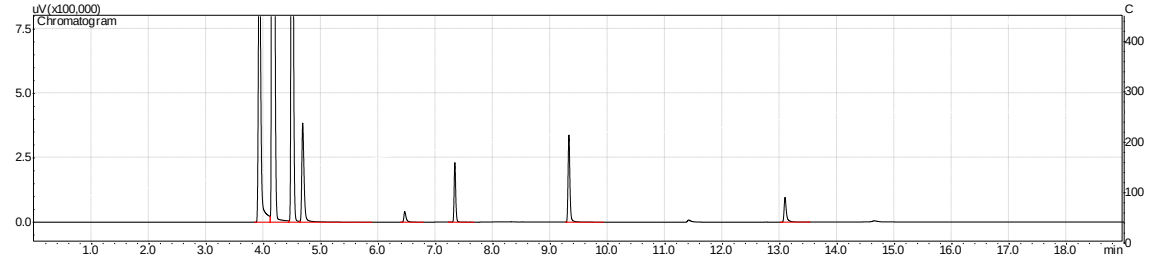
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	3.925	3101296.1	1066655.8	0.00000		V		
2	4.155	14652983.1	5406725.2	0.00000	ppm	V	1	
3	4.495	6602516.7	2781679.3	0.00000	ppm	SV	1	
4	4.698	768762.9	245978.7	0.00000		T		
5	6.451	337685.5	141420.8	0.00000	ppm	T	2	
6	7.333	456857.7	233464.1	0.00000	ppm	V	3	
7	9.320	1914389	168976.2	0.00000	ppm	V	5	
8	13.095	146028.2	45641.3	0.00000				
9	14.405	57137.2	15634.9	0.00000	ppm	V	6	

CyJohnPhos_Ar_Br_6_RT _12H:



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	3.922	3800493.7	1357670.6	0.00000		V		
2	4.153	14848827.7	5505807.2	0.00000	ppm	V	1	
3	4.492	7538563.8	3272810.2	0.00000	ppm	SV	1	
4	4.681	155614.5	49373.3	0.00000		T		
5	6.458	113566.6	39853.5	0.00000	ppm	V	2	
6	7.333	443872.1	205672.5	0.00000	ppm	SV	3	
7	11.369	211723.7	62658.2	0.00000		S		
8	13.101	2035719.4	838148.8	0.00000				

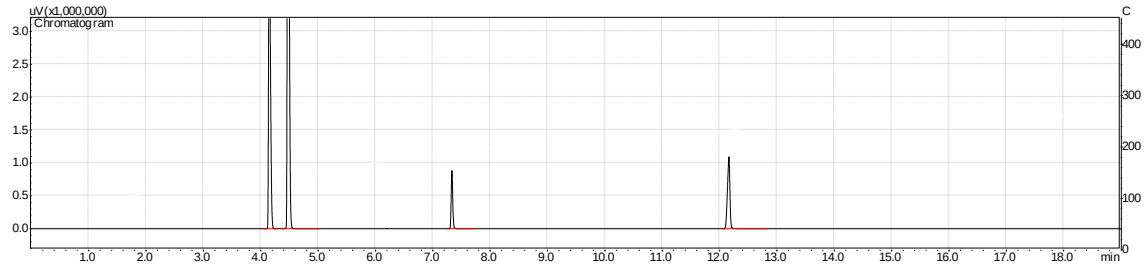
JohnPhos_Ar_Br_6_RT _12H:



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	3.924	3685972.4	1278127.7	0.00000		V		
2	4.153	15304740.1	5637033.8	0.00000	ppm	V	1	
3	4.493	7290058.9	3184302.5	0.00000	ppm	V	1	
4	4.680	1111168.4	384157.8	0.00000		SV		
5	6.459	118850.4	41623.1	0.00000	ppm		2	
6	7.333	447874.4	227396.6	0.00000	ppm	SV	3	
7	9.321	2372664.8	335865.2	0.00000	ppm	V	5	
8	13.090	274121.8	95496.7	0.00000				

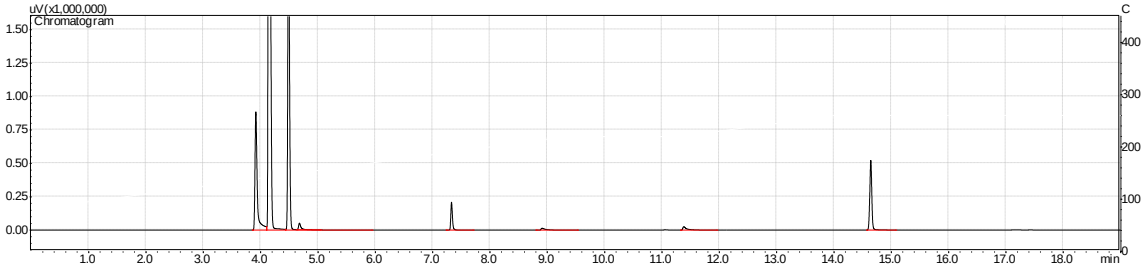
2,6-Dimethoxy-1,1'-biphenyl

Ar_Br_7_RT_ To



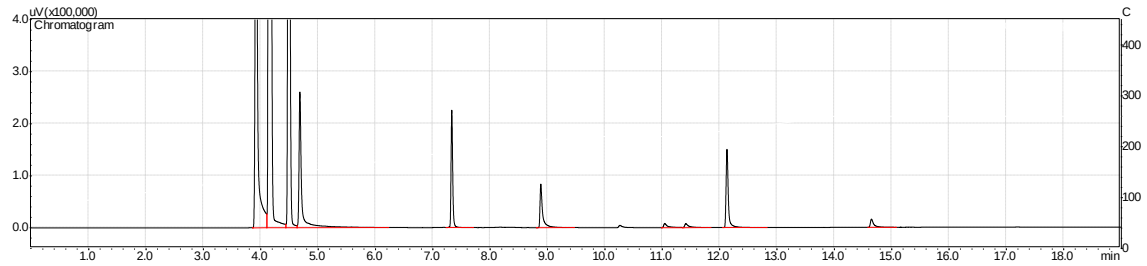
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.149	10382835.0	4449320.3	0.00000	ppm	V	1	
2	4.475	20290124.9	9270132.7	0.00000	ppm	SV	1	
3	7.332	1673390.4	867703.8	0.00000	ppm	SV	3	
4	12.162	3279090.1	1080812.7	0.00000		S		

L1_Ar_Br_7_RT _12H:



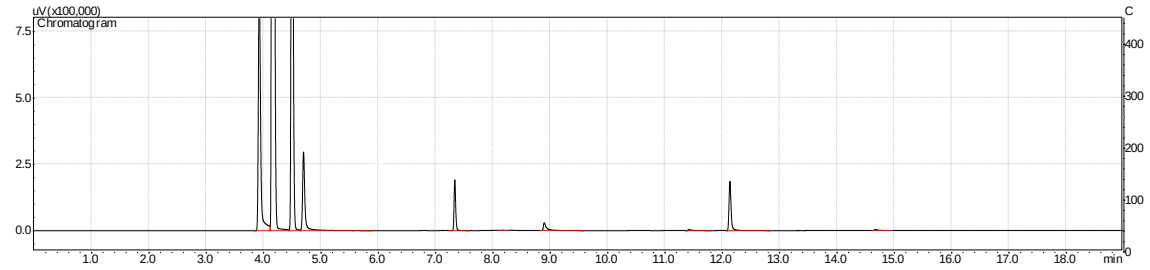
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	3.916	2471582.0	874623.8	0.00000		V		
2	4.144	13893369.6	5563501.6	0.00000	ppm	V	1	
3	4.486	5224971.7	2463232.8	0.00000	ppm	SV	1	
4	4.676	145198.3	49397.3	0.00000		T		
5	7.329	417416.2	206086.5	0.00000	ppm	SV	3	
6	8.909	45107.2	14375.8	0.00000				
7	11.381	134599.6	25797.8	0.00000		V		
8	14.642	1283997.1	518215.5	0.00000	ppm		6	

L3_Ar_Br_7_RT_ 12H:



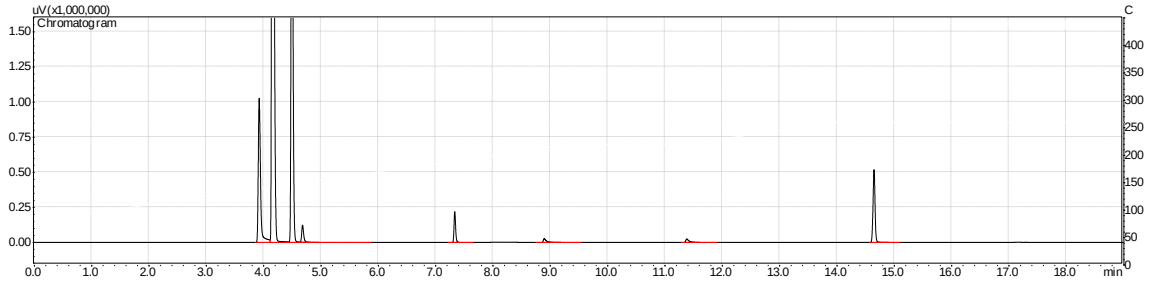
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	3.917	2599615.1	917727.9	0.00000		V		
2	4.145	14017958.0	5564051.1	0.00000	ppm	V	1	
3	4.487	5195686.7	2504359.3	0.00000	ppm	V	1	
4	4.682	850439.1	257675.7	0.00000		SV		
5	7.330	447871.3	224262.8	0.00000	ppm	SV	3	
6	8.883	264284.5	83013.7	0.00000				
7	11.043	42124.7	8096.0	0.00000				
8	11.411	40136.4	7579.2	0.00000		V		
9	12.128	1708242.7	149553.0	0.00000		S		
10	14.648	67866.3	15975.5	0.00000	ppm		6	

PPh3_Ar_Br_7_RT _12H:



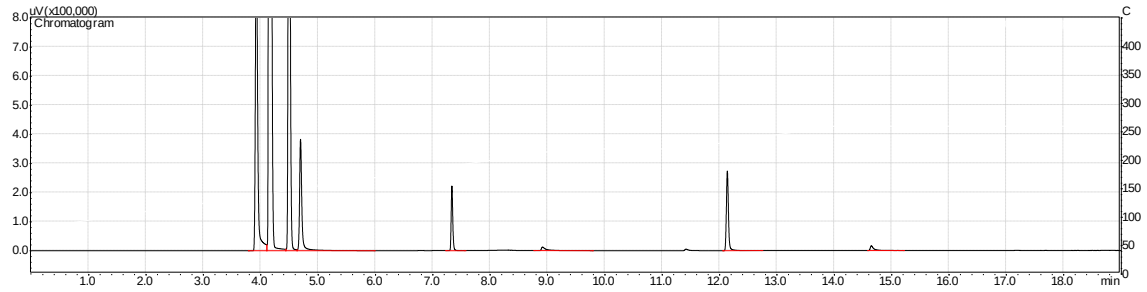
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	3.923	2562620.8	913840.1	0.00000		V		
2	4.151	16483698.3	6017166.9	0.00000	ppm	V	1	
3	4.494	5868890.2	2590994.8	0.00000	ppm	V	1	
4	4.695	871920.4	293017.8	0.00000		SV		
5	7.333	374035.2	189259.9	0.00000	ppm	V	3	
6	8.183	10801.6	1412.0	0.00000	ppm	V	4	
7	8.894	125248.3	29352.3	0.00000		S		
8	11.422	22069.7	4255.9	0.00000		V		
9	12.132	2879630.8	184866.8	0.00000		SV		
10	14.671	19096.8	3978.1	0.00000	ppm		6	

CyJohnPhos_Ar_Br_7_RT _12H:



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	3.922	2843351.5	1023290.4	0.00000		V		
2	4.152	15687202.7	5770111.1	0.00000	ppm	V	1	
3	4.492	7763484.1	3377418.7	0.00000	ppm	SV	1	
4	4.678	279962.2	120243.8	0.00000		T		
5	7.333	422970.5	216573.4	0.00000	ppm	SV	3	
6	8.894	77420.1	27389.4	0.00000		SV		
7	11.381	113169.6	25028.7	0.00000				
8	14.647	1268155.6	514070.1	0.00000	ppm		6	

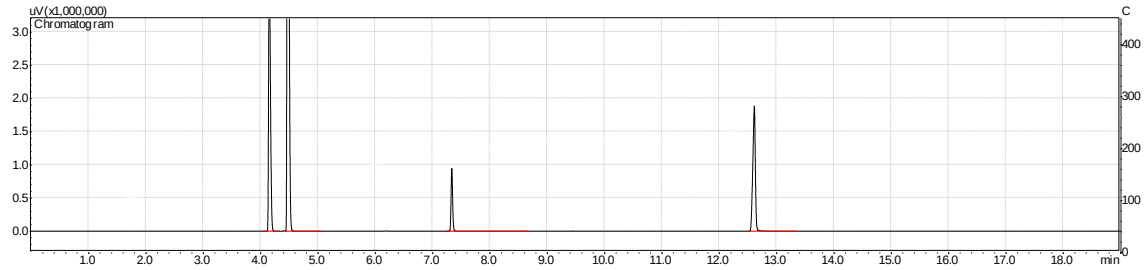
JohnPhos_Ar_Br_7_RT _12H:



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	3.922	3079309.8	1103842.4	0.00000				
2	4.150	15937700.3	5860617.1	0.00000	ppm	V	1	
3	4.493	5667063.3	2525898.7	0.00000	ppm	V	1	
4	4.693	1085227.4	381922.0	0.00000		SV		
5	7.332	429675.1	216866.9	0.00000	ppm	V	3	
6	8.912	79912.3	12570.0	0.00000		SV		
7	12.135	2789707.9	270661.0	0.00000		S		
8	14.646	77726.2	16467.4	0.00000	ppm	S	6	

2-Phenylnaphthalene

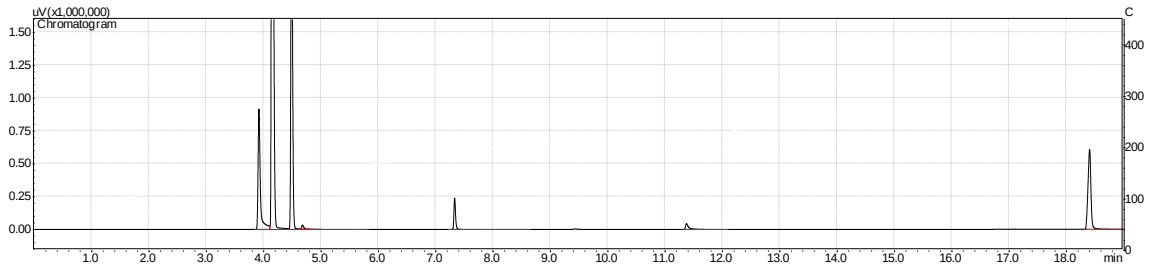
Ar_Br_8_RT_ To



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name

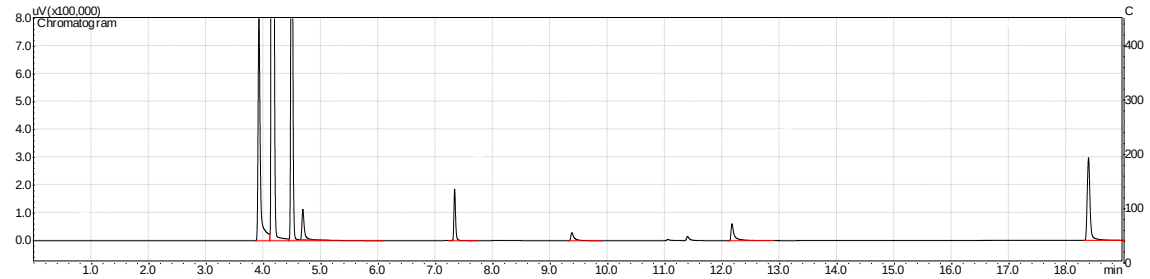
1	4.151	9007669.2	3961869.9	0.00000	ppm	V	1	
2	4.472	23041119.4	10326071.9	0.00000	ppm	SV	1	
3	7.333	1798784.5	928800.7	0.00000	ppm	SV	3	
4	12.609	5811076.1	1873679.4	0.00000				

L1_Ar_Br_8_RT _12H:



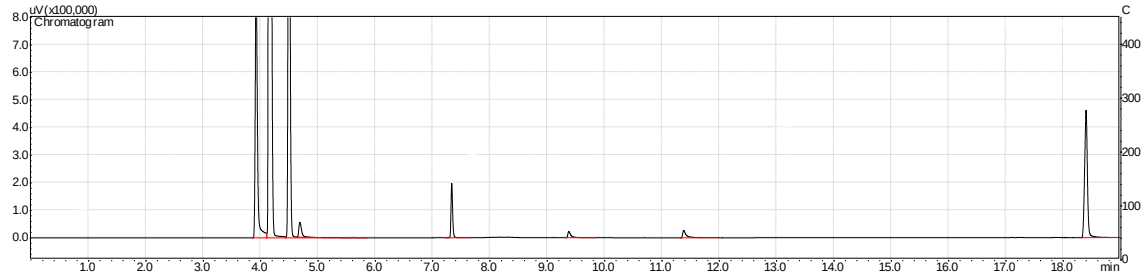
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	3.916	2549295.1	906565.7	0.00000		V		
2	4.146	13078365.2	5303977.1	0.00000	ppm	V	1	
3	4.486	5689663.1	2694061.8	0.00000	ppm	SV	1	
4	4.676	80077.4	31227.1	0.00000		T		
5	7.329	493423.0	238249.8	0.00000	ppm	SV	3	
6	11.372	197406.3	44686.8	0.00000		V		
7	18.401	2199825.1	606511.0	0.00000	ppm		8	

L3_Ar_Br_8_RT_ 12H:



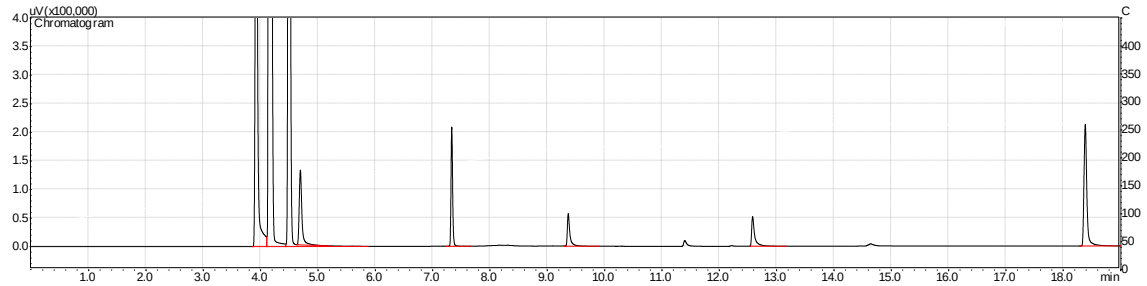
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	3.917	2245650.5	799086.4	0.00000		V		
2	4.145	13852437.4	5524107.5	0.00000	ppm	V	1	
3	4.487	4651225.9	2192271.1	0.00000	ppm	SV	1	
4	4.683	322429.1	108673.5	0.00000		T		
5	7.330	376013.6	184621.5	0.00000	ppm	SV	3	
6	9.373	89901.1	28786.4	0.00000	ppm		5	
7	12.166	253104.6	60467.7	0.00000		S		
8	18.384	1038551.5	296871.9	0.00000	ppm		8	

CyJohnPhos_Ar_Br_8_RT _12H:



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	3.921	2511955.8	918006.9	0.00000		V		
2	4.150	16497388.3	6005278.7	0.00000	ppm	V	1	
3	4.493	5072144.2	2222363.7	0.00000	ppm	SV	1	
4	4.683	180859.5	53978.7	0.00000		T		
5	7.332	386525.7	193039.7	0.00000	ppm	SV	3	
6	9.375	85550.6	23081.2	0.00000	ppm		5	
7	11.379	121720.8	26941.1	0.00000				
8	18.396	1561941.9	457420.9	0.00000	ppm		8	

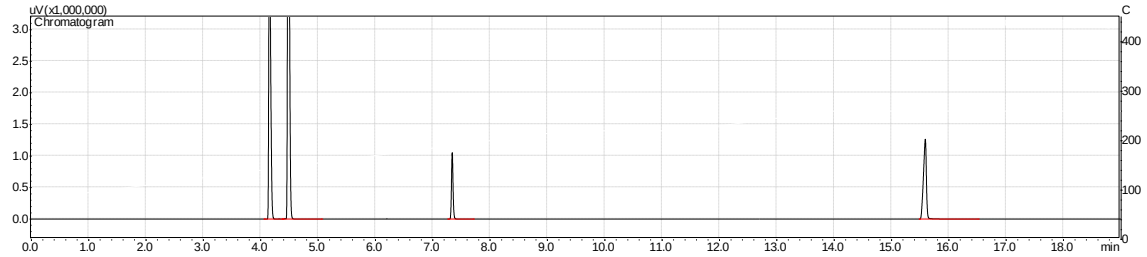
JohnPhos_Ar_Br_8_RT _12H:



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	3.921	2549485.6	921362.4	0.00000		V		
2	4.150	16422252.4	5961486.2	0.00000	ppm	V	1	
3	4.493	5548850.1	2413766.9	0.00000	ppm	SV	1	
4	4.693	425431.8	130481.0	0.00000		T		
5	7.333	405587.2	204224.3	0.00000	ppm	SV	3	
6	9.365	179131.8	57064.3	0.00000	ppm	V	5	
7	12.581	593155.5	51748.5	0.00000				
8	18.383	737498.7	210284.5	0.00000	ppm		8	

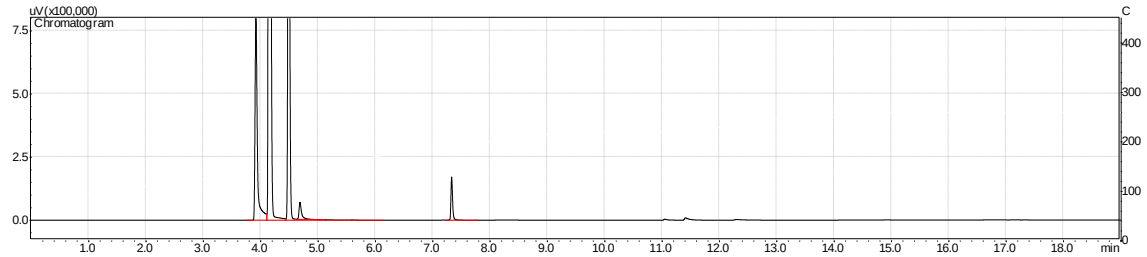
2-Methoxy-6-phenylnaphthalene

Ar_Br_9_RT_ To



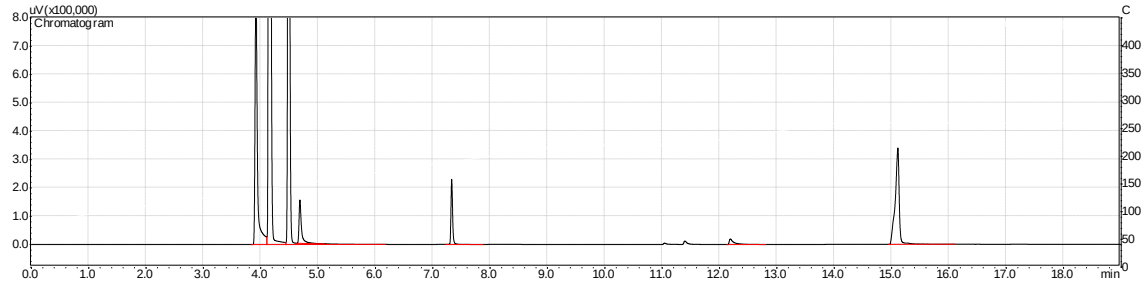
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.153	10698300.9	4582010.0	0.00000	ppm	SV	1	
2	4.480	18822564.3	8620170.7	0.00000	ppm	V	1	
3	7.339	2014845.0	1046882.8	0.00000	ppm	SV	3	
4	15.589	4525015.0	1260569.8	0.00000	ppm	S	6	

L1_Ar_Br_9_RT _12H:



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	3.916	2351326.1	835155.9	0.00000				
2	4.146	13152263.9	5317185.1	0.00000	ppm	V	1	
3	4.486	5073611.0	2381895.0	0.00000	ppm	SV	1	
4	4.684	215912.9	67511.1	0.00000		T		
5	7.329	350083.9	168989.7	0.00000	ppm	V	3	

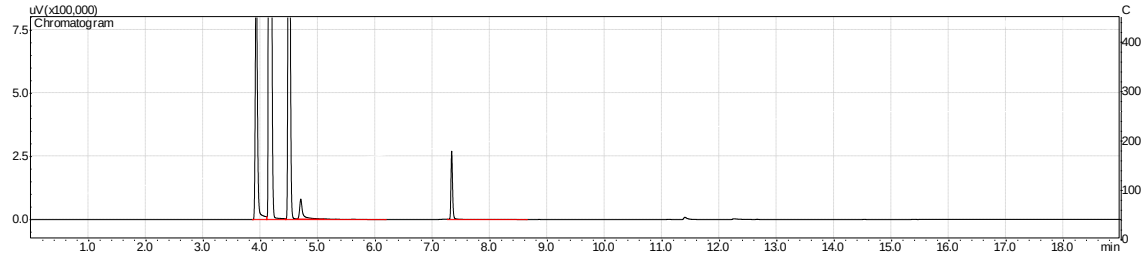
L3_Ar_Br_9_RT_ 12H:



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	3.916	2645976.9	941640.3	0.00000		V		
2	4.146	12371332.4	5086380.5	0.00000	ppm	V	1	

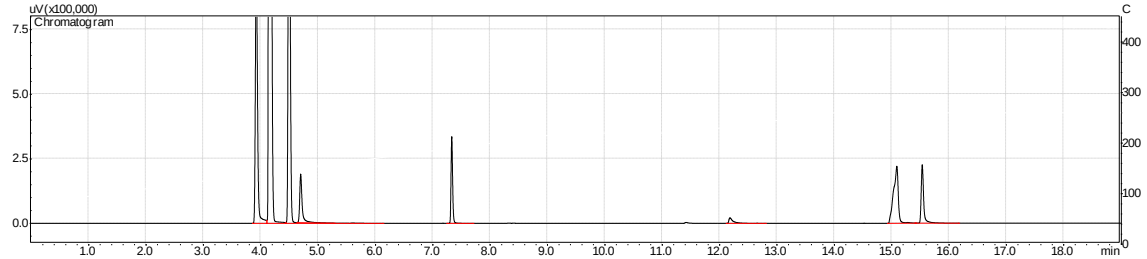
3	4.485	7030724.2	3293094.7	0.00000	ppm	SV	1	
4	4.683	449515.9	151437.1	0.00000		T		
5	7.329	459548.8	228372.8	0.00000	ppm	SV	3	
6	12.189	116533.9	19840.2	0.00000		S		
7	15.109	1664022.5	339446.0	0.00000	ppm	S	6	

CyJohnPhos_Ar_Br_9_RT _12H:



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	3.921	2646147.4	1004117.8	0.00000		V		
2	4.150	15754340.7	5822421.6	0.00000	ppm	V	1	
3	4.491	6645622.5	2887385.2	0.00000	ppm	SV	1	
4	4.698	310295.2	79086.2	0.00000		T		
5	7.329	567587.9	269363.1	0.00000	ppm	SV	3	

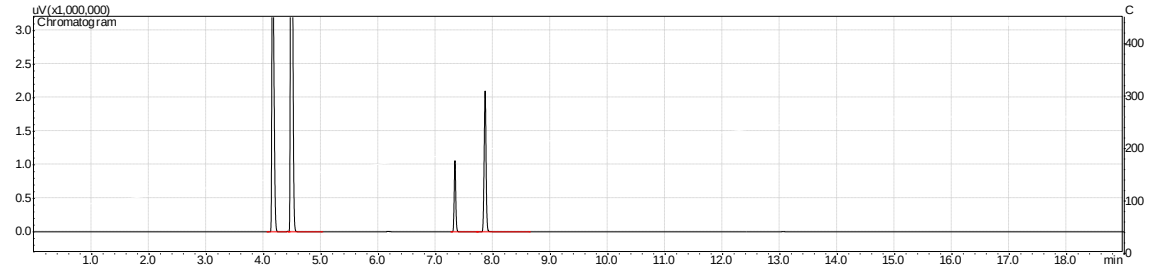
JohnPhos_Ar_Br_9_RT _12H:



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	3.922	2668589.4	997908.9	0.00000		V		
2	4.150	15905333.4	5852832.7	0.00000	ppm	V	1	
3	4.492	5339040.5	2322446.8	0.00000	ppm	SV	1	
4	4.696	563269.6	185345.4	0.00000		T		
5	7.329	646209.1	333694.6	0.00000	ppm	SV	3	
6	12.180	115823.0	21831.5	0.00000		S		
7	15.089	1273396.2	220789.5	0.00000	ppm	S	6	
8	15.533	679665.0	225184.7	0.00000	ppm	V	6	

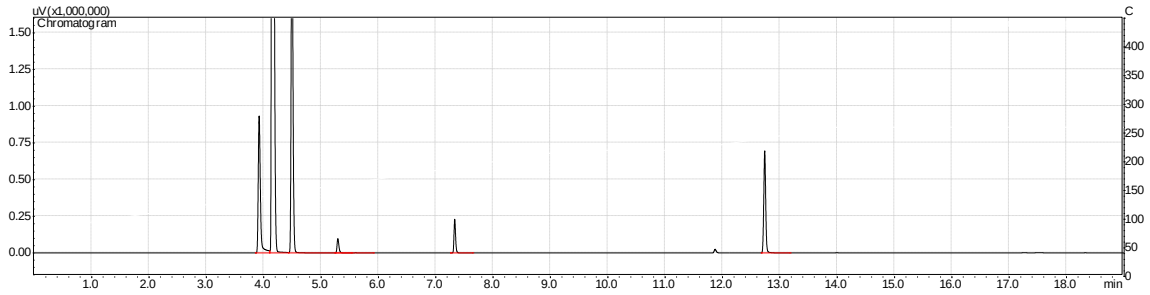
2,4'-Dimethyl-1,1'-biphenyl

Ar_Br_10_RT_ To



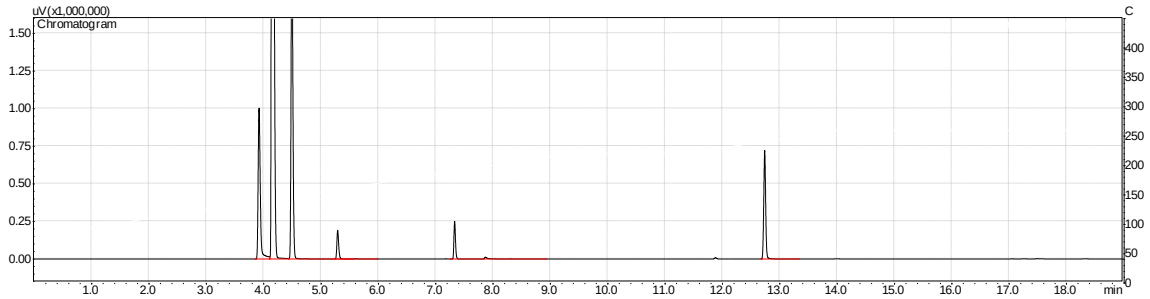
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.154	11240263.0	4435319.0	0.00000	ppm	SV	1	
2	4.479	22748401.1	9603548.3	0.00000	ppm	V	1	
3	7.333	2017808.1	1048190.0	0.00000	ppm	SV	3	
4	7.859	4897215.1	2066624.7	0.00000		S		

L1_Ar_Br_10_RT _12H:



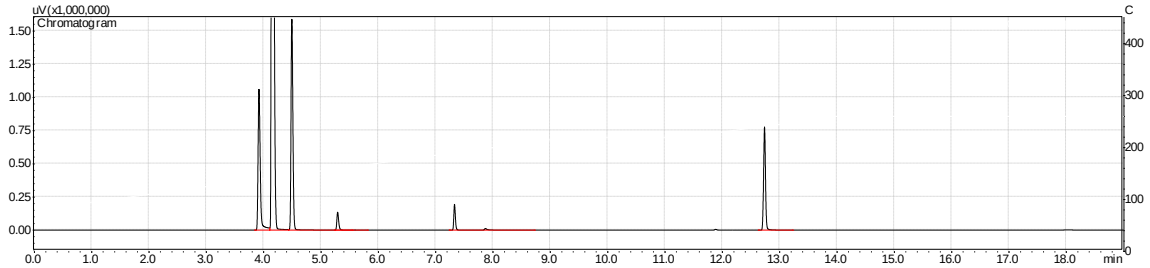
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	3.920	2477747.7	925844.8	0.00000		V		
2	4.149	16526807.5	6019481.6	0.00000	ppm	V	1	
3	4.492	5326914.5	2343954.5	0.00000	ppm	SV	1	
4	5.292	127630.7	97547.4	0.00000		T		
5	7.330	444979.7	228464.1	0.00000	ppm	SV	3	
6	12.736	1629267.6	685405.9	0.00000		SV		

L3_Ar_Br_10_RT_ 12H:



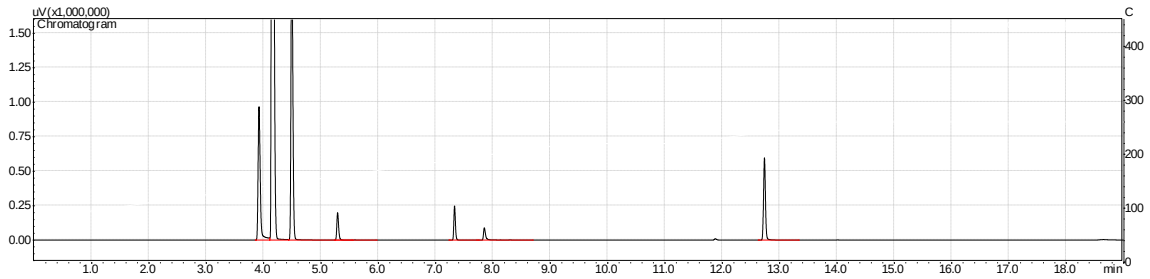
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	3.918	2671598.3	1002006.8	0.00000		V		
2	4.148	16509509.4	6024115.1	0.00000	ppm	V	1	
3	4.491	4794317.9	2083353.7	0.00000	ppm	SV	1	
4	5.289	227483.8	190247.5	0.00000		T		
5	7.329	477478.4	248958.6	0.00000	ppm	SV	3	
6	12.736	1681492.0	711678.3	0.00000		SV		

CyJohnPhos_Ar_Br_10_RT _12H:



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	3.918	2834001.1	1056064.2	0.00000		V		
2	4.147	16915247.6	6135430.1	0.00000	ppm	V	1	
3	4.491	3634435.3	1579860.8	0.00000	ppm	SV	1	
4	5.290	189190.3	134839.5	0.00000		T		
5	7.328	371229.9	192416.3	0.00000	ppm	SV	3	
6	12.735	1812292.8	764277.3	0.00000		V		

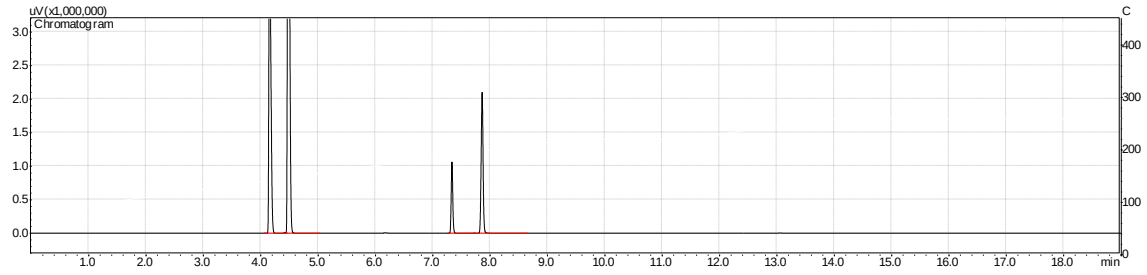
JohnPhos_Ar_Br_10_RT _12H:



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	3.919	2592727.1	964491.3	0.00000		V		
2	4.148	16486942.0	6013652.1	0.00000	ppm	V	1	
3	4.490	5088352.2	2197714.3	0.00000	ppm	SV	1	
4	5.289	441166.0	196941.8	0.00000		T		
5	7.329	471893.8	246539.4	0.00000	ppm	SV	3	
6	7.848	254336.5	89113.7	0.00000		S		
7	12.735	1391576.3	594068.4	0.00000		SV		

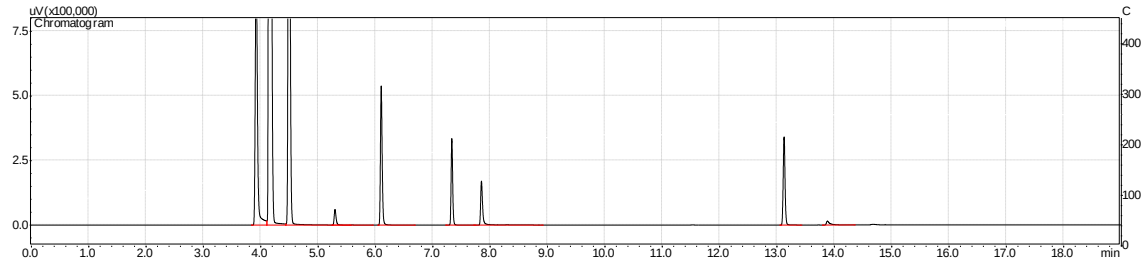
2,4',6-Trimethyl-1,1'-biphenyl

Ar_Br_11_RT_ To



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.154	11240263.0	4435319.0	0.00000	ppm	SV	1	
2	4.479	22748401.1	9603548.3	0.00000	ppm	V	1	
3	7.333	2017808.1	1048190.0	0.00000	ppm	SV	3	
4	7.859	4897215.1	2066624.7	0.00000		S		

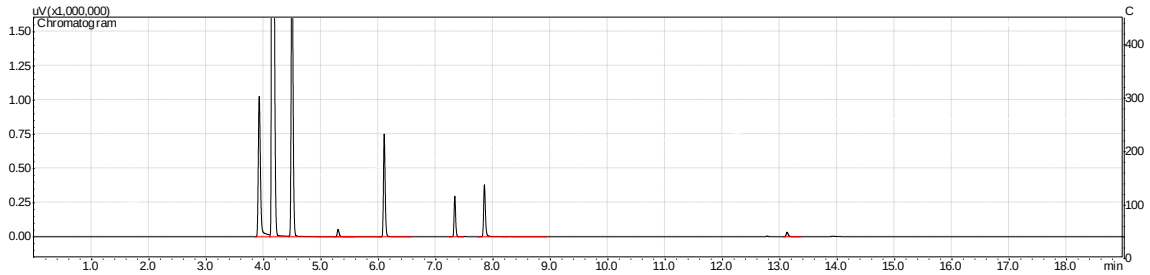
L1_Ar_Br_11_RT _12H:



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	3.920	2769350.6	1023325.8	0.00000		V		
2	4.149	16003763.0	5828033.2	0.00000	ppm	V	1	
3	4.491	5680355.1	2473847.5	0.00000	ppm	SV	1	
4	5.294	68286.5	58954.5	0.00000		T		
5	6.100	1129205.3	529098.2	0.00000		S		
6	7.331	633825.2	330681.6	0.00000	ppm	SV	3	

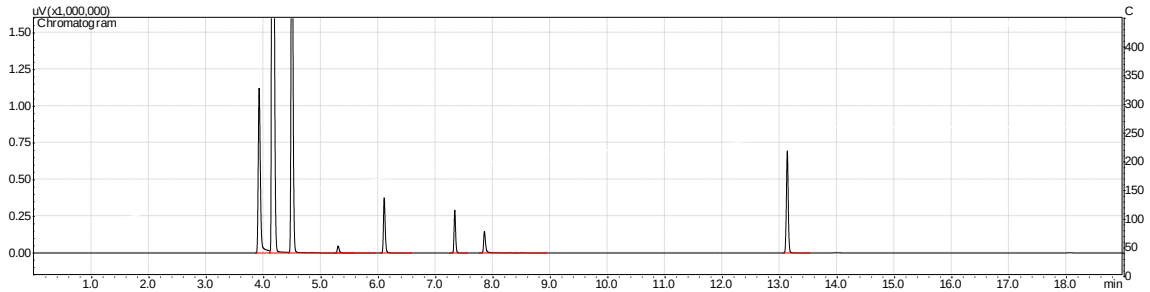
7	7.847	1199615.9	169733.6	0.00000		S		
8	13.124	764825.3	338240.3	0.00000				
9	13.880	69188.9	15130.9	0.00000				

L3_Ar_Br_11_RT_ 12H:



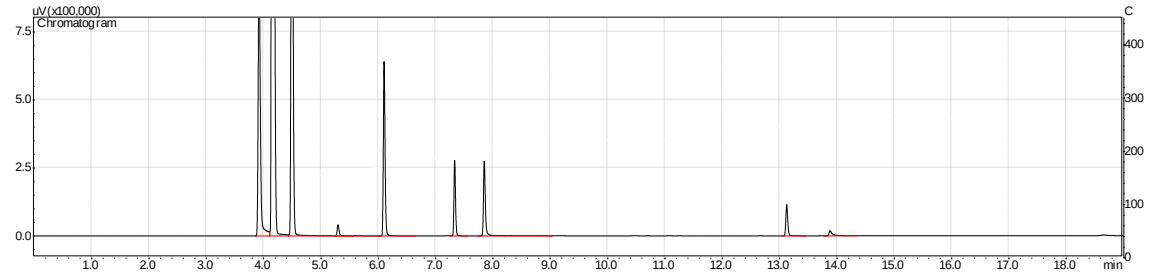
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	3.921	2784101.9	1013276.6	0.00000		V		
2	4.150	16213816.7	5881198.7	0.00000	ppm	V	1	
3	4.492	5023760.6	2176234.2	0.00000	ppm	SV	1	
4	5.296	129259.4	54043.4	0.00000		T		
5	6.100	1558631.9	740463.6	0.00000		SV		
6	7.331	561404.3	295107.7	0.00000	ppm	V	3	
7	7.847	3958885.4	377043.1	0.00000		S		
8	13.125	87664.1	34283.5	0.00000				

CyJohnPhos_Ar_Br_11_RT _12H:



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	3.920	3014352.4	1114500.9	0.00000		V		
2	4.151	14703707.8	5472727.9	0.00000	ppm	V	1	
3	4.491	6736369.4	2920557.2	0.00000	ppm	SV	1	
4	5.297	114930.8	47273.9	0.00000		T		
5	6.101	798967.6	372278.8	0.00000		S		
6	7.331	548295.2	287656.2	0.00000	ppm	V	3	
7	7.848	909160.5	145942.8	0.00000		S		
8	13.130	1569071.6	692517.5	0.00000				

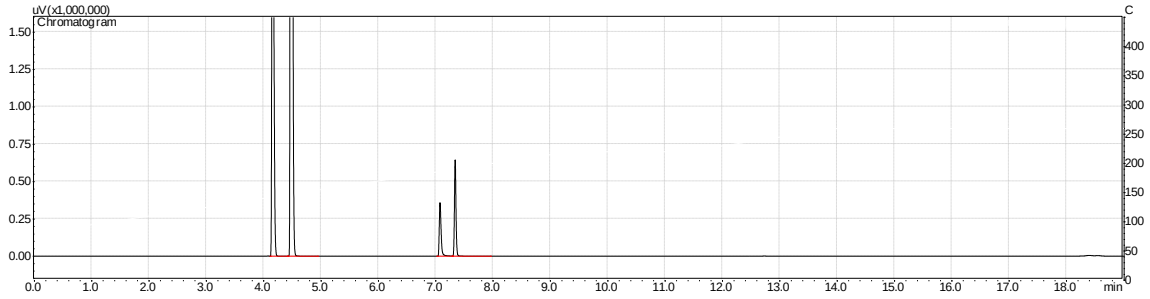
JohnPhos_Ar_Br_11_RT _12H:



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	3.921	2665665.2	983338.3	0.00000		V		
2	4.150	16055419.3	5850855.4	0.00000	ppm	V	1	
3	4.492	5233954.1	2279559.4	0.00000	ppm	SV	1	
4	5.296	97168.3	40877.2	0.00000		T		
5	6.101	1335849.3	633635.5	0.00000		SV		
6	7.332	525750.0	271822.7	0.00000	ppm	V	3	
7	7.848	2949200.4	273503.2	0.00000		S		
8	13.123	267316.3	113369.7	0.00000				
9	13.879	80404.1	18566.9	0.00000		V		

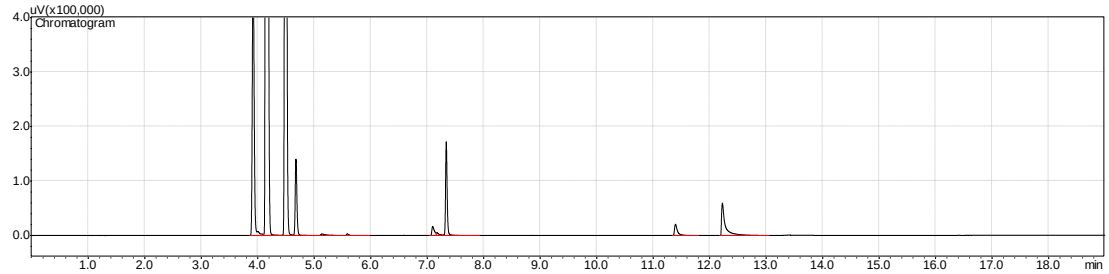
3-Phenyl-pyridine: KOH in MeOH

Ar_Br_52_RT_To



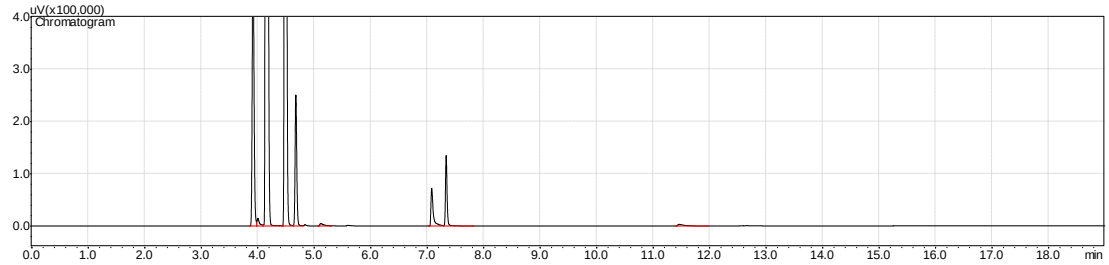
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.155	8378818.4	3742545.8	0.00000	ppm	SV	1	
2	4.476	23303114.4	10461192.8	0.00000	ppm		1	
3	7.074	816951.0	355151.1	0.00000	ppm		3	
4	7.338	1216411.6	638908.6	0.00000	ppm	SV	3	

L1_Br_52_RT _24H:



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	3.918	1167376.3	514580.9	0.00000		SV		
2	4.149	12954926.7	5371540.3	0.00000	ppm	SV	1	
3	4.489	5817923.2	2843343.0	0.00000	ppm	V	1	
4	4.676	304132.5	138317.6	0.00000		SV		
5	5.136	9182.6	2817.8	0.00000		T		
6	7.097	89496.3	16946.7	0.00000	ppm		3	
7	7.171	21217.6	5641.7	0.00000	ppm	V	3	
8	7.337	338696.8	168028.4	0.00000	ppm	SV	3	
9	11.395	78468.6	20883.7	0.00000				
10	12.225	274724.5	59573.0	0.00000				

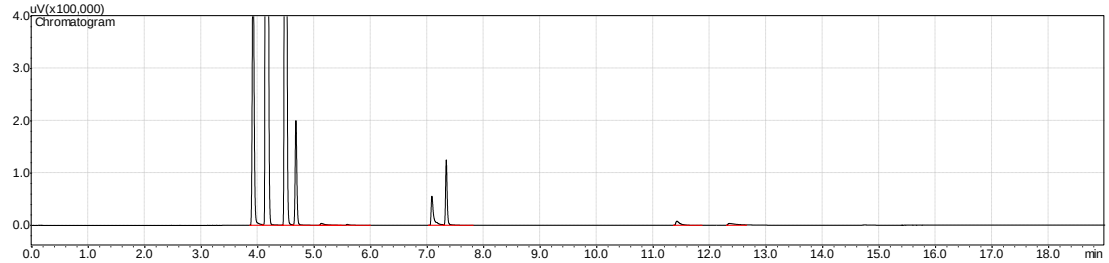
L3_ Ar_ Br _52_RT _ 24H:



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	3.916	1200715.6	539952.1	0.00000		V		
2	4.003	46907.7	15067.7	0.00000		V		
3	4.148	12251136.4	5148276.9	0.00000	ppm	SV	1	

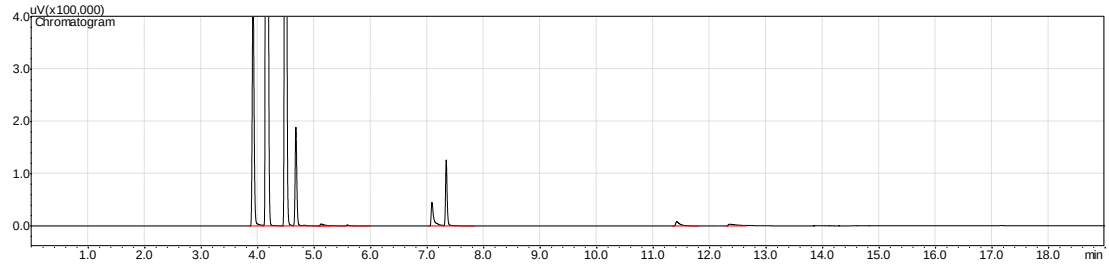
4	4.487	7194563.2	3524313.8	0.00000	ppm	V	1	
5	4.674	510137.9	249586.9	0.00000		V		
6	5.115	28821.4	5093.6	0.00000		V		
7	7.079	758797.5	71910.4	0.00000	ppm		3	
8	7.335	870374.1	134021.0	0.00000	ppm	V	3	
9	11.462	29763.1	3390.9	0.00000		S		

L2 Ar_ Br _52_RT _24H:



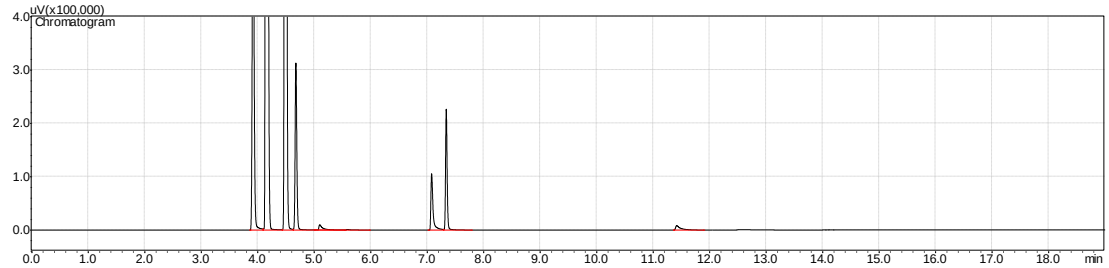
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	3.917	1258045.3	554908.2	0.00000		V		
2	4.148	12562925.5	5221153.1	0.00000	ppm	V	1	
3	4.488	6881137.8	3366767.3	0.00000	ppm	V	1	
4	4.675	432217.0	199195.1	0.00000		SV		
5	5.126	22664.6	3572.5	0.00000		T		
6	7.083	692071.7	55597.8	0.00000	ppm		3	
7	7.337	852928.7	122599.9	0.00000	ppm	V	3	
8	11.420	45625.7	8189.4	0.00000				
9	12.352	41812.0	3641.1	0.00000				

CyJohnPhos_ Br _52_RT _24H:



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	3.917	1066355.2	469860.6	0.00000		V		
2	4.151	10125575.8	4403750.9	0.00000	ppm	V	1	
3	4.488	5336982.9	2639322.7	0.00000	ppm	V	1	
4	4.675	405789.2	188067.3	0.00000		SV		
5	5.123	20450.2	3745.0	0.00000		T		
6	7.084	705551.8	45145.7	0.00000	ppm		3	
7	7.336	854574.7	124371.0	0.00000	ppm	V	3	
8	11.418	45723.2	8394.7	0.00000				
9	12.357	39192.3	3418.7	0.00000				

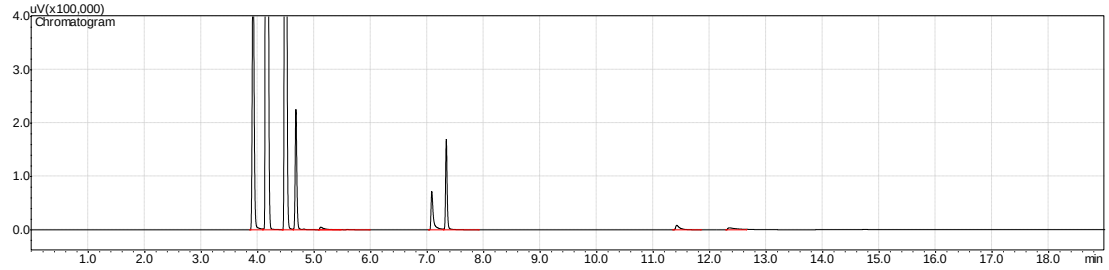
JohnPhos_ Br _52_RT _24H:



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	3.917	1653409.2	726977.4	0.00000		V		
2	4.149	11823604.3	4949835.9	0.00000	ppm	V	1	
3	4.487	8039480.3	3908172.9	0.00000	ppm	V	1	
4	4.675	660353.8	311698.3	0.00000		SV		
5	5.097	45241.0	9798.6	0.00000		T		

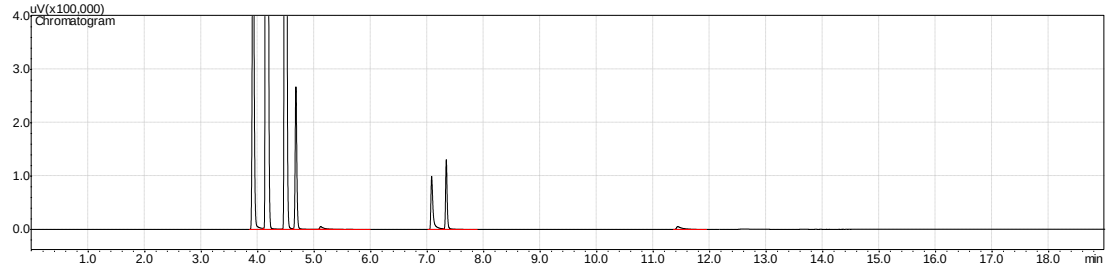
6	7.078	772018.7	105551.7	0.00000	ppm		3	
7	7.337	942093.6	221669.1	0.00000	ppm	V	3	
8	11.418	55072.1	8510.4	0.00000				

SPhos_ Br _52_RT _24H:



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	3.917	1230241.3	544212.3	0.00000		V		
2	4.151	10885258.1	4664928.8	0.00000	ppm	V	1	
3	4.488	6478740.9	3192438.6	0.00000	ppm	V	1	
4	4.675	479467.8	224451.8	0.00000		SV		
5	5.115	28293.4	5019.3	0.00000		T		
6	7.081	697405.6	71155.1	0.00000	ppm		3	
7	7.337	938128.9	165769.1	0.00000	ppm	SV	3	
8	11.418	46453.4	8633.1	0.00000				
9	12.347	41161.2	3729.6	0.00000				

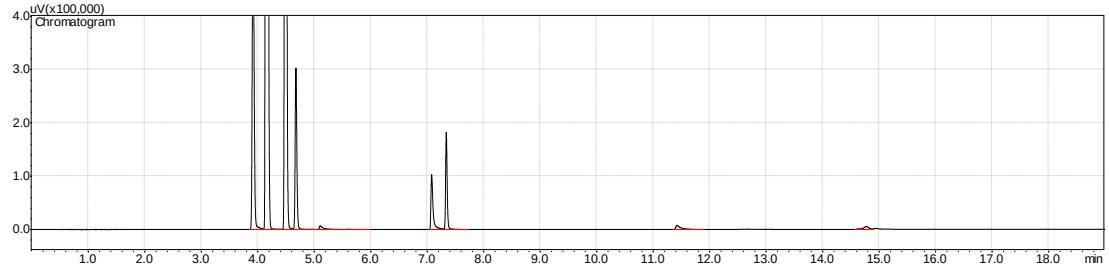
L4_ Br _52_RT _24H:



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name

1	3.917	1576214.7	694445.8	0.00000		V		
2	4.150	11616915.9	4882032.3	0.00000	ppm	SV	1	
3	4.486	8702391.0	4207801.0	0.00000	ppm	V	1	
4	4.675	566495.7	266024.9	0.00000		SV		
5	5.113	28888.9	5211.7	0.00000		T		
6	7.078	768193.6	99006.4	0.00000	ppm		3	
7	7.337	862930.4	127476.3	0.00000	ppm	SV	3	
8	11.435	40908.4	5519.1	0.00000				

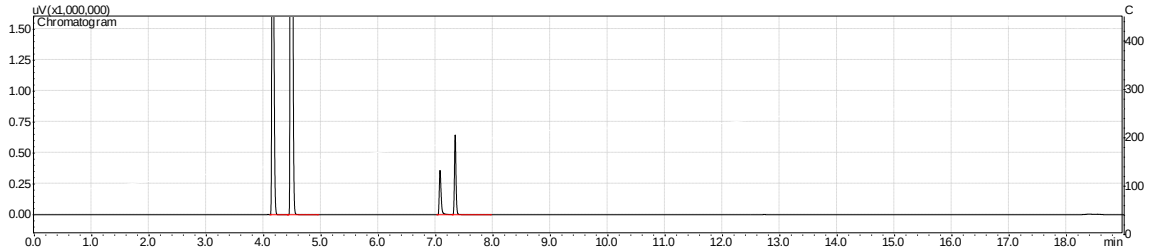
tBuDavePhos_ Br _52_RT _24H:



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	3.917	1430586.6	630720.4	0.00000		V		
2	4.149	12518593.5	5204336.8	0.00000	ppm	V	1	
3	4.489	6398048.6	3135363.1	0.00000	ppm	V	1	
4	4.675	636464.0	300765.7	0.00000		SV		
5	5.106	34256.4	6772.8	0.00000		T		
6	7.079	703498.6	102012.4	0.00000	ppm		3	
7	7.338	855001.7	179719.5	0.00000	ppm	V	3	
8	11.421	53125.9	7907.0	0.00000				
9	14.775	41261.4	5752.5	0.00000	ppm	V	6	

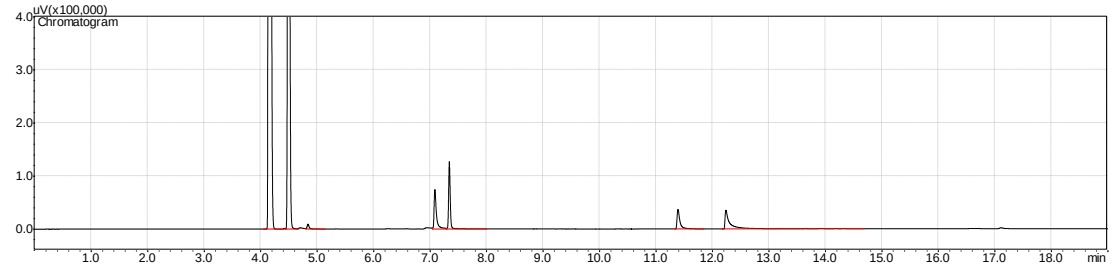
3-Phenyl-pyridine: KF

Ar_Br_52_RT_To



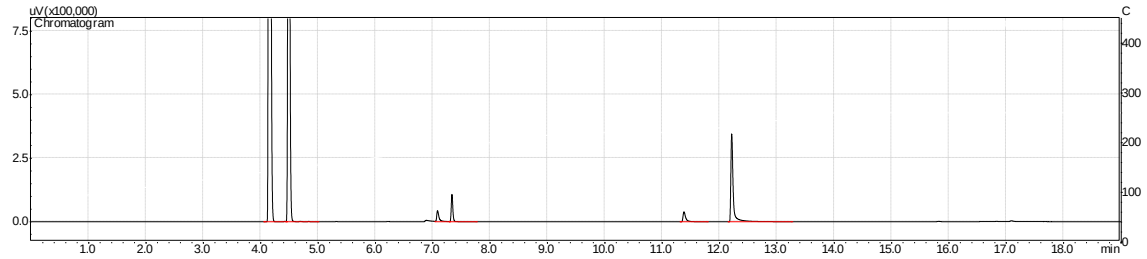
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.155	8378818.4	3742545.8	0.00000	ppm	SV	1	
2	4.476	23303114.4	10461192.8	0.00000	ppm		1	
3	7.074	816951.0	355151.1	0.00000	ppm		3	
4	7.338	1216411.6	638908.6	0.00000	ppm	SV	3	

L1_Br_52_RT _24H:



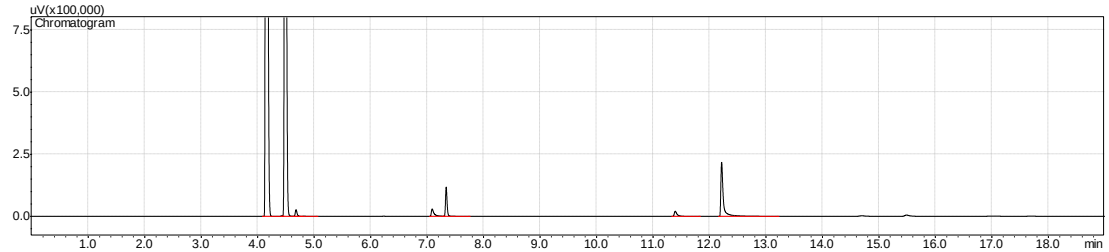
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.148	13863301.7	5687531.2	0.00000	ppm	SV	1	
2	4.492	4769558.0	2355502.0	0.00000	ppm	V	1	
3	4.837	20322.0	9126.5	0.00000		V		
4	7.084	469438.1	74012.8	0.00000	ppm	V	3	
5	7.340	254399.5	125718.1	0.00000	ppm	SV	3	
6	11.389	131308.0	36695.4	0.00000				
7	12.238	421705.2	35052.7	0.00000		S		

L3_ Ar_ Br _52_RT _ 24H:



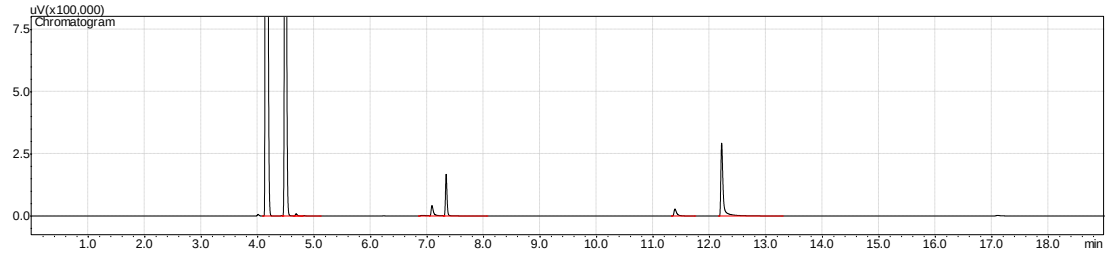
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.147	12091895.8	5109311.7	0.00000	ppm	SV	1	
2	4.486	6834493.8	3311921.0	0.00000	ppm	SV	1	
3	7.083	72934.8	43644.7	0.00000	ppm	V	3	
4	7.334	215595.3	107250.9	0.00000	ppm	V	3	
5	11.380	130791.9	39071.2	0.00000				
6	12.212	985128.5	343471.9	0.00000				

L2 Ar_ Br _52_RT _24H:



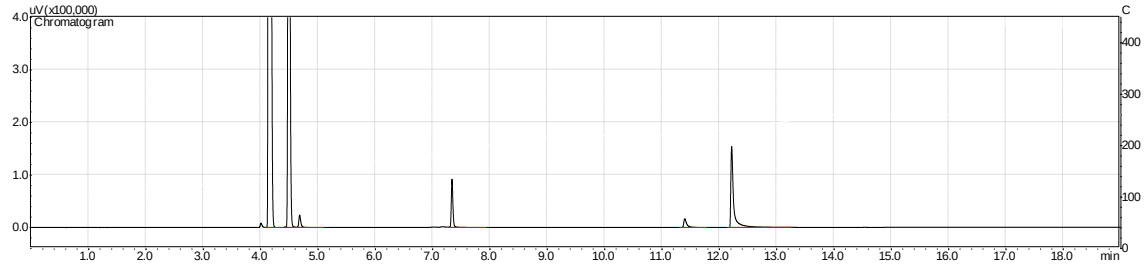
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.146	14202964.4	5794945.3	0.00000	ppm	V	1	
2	4.490	4709529.0	2295312.9	0.00000	ppm	SV	1	
3	7.093	99251.7	23072.5	0.00000	ppm		3	
4	7.338	192257.5	91970.1	0.00000	ppm	V	3	
5	12.224	283656.9	58366.2	0.00000		S		

CyJohnPhos_ Br _52_RT _24H:



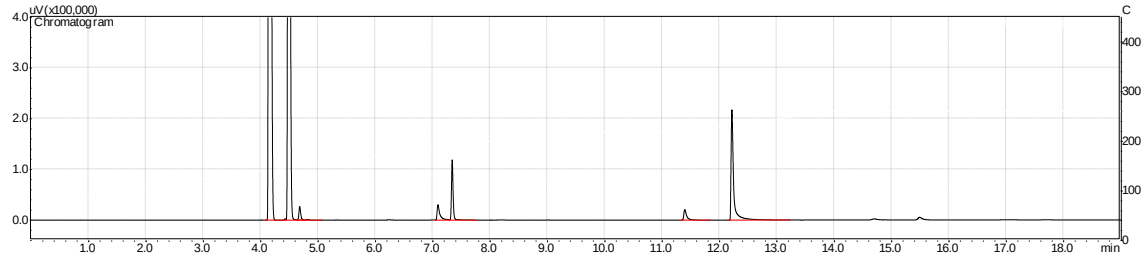
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.148	13290404.1	5494390.8	0.00000	ppm	SV	1	
2	4.489	6843114.2	3349648.2	0.00000	ppm	SV	1	
3	4.681	21068.8	8675.9	0.00000		T		
4	6.914	22497.8	2699.9	0.00000	ppm		3	
5	7.086	87717.6	42222.3	0.00000	ppm	V	3	
6	7.337	334850.7	164001.0	0.00000	ppm	SV	3	
7	11.388	99791.2	28101.3	0.00000				
8	12.215	857816.9	291700.9	0.00000		S		

JohnPhos_ Br _52_RT _24H:



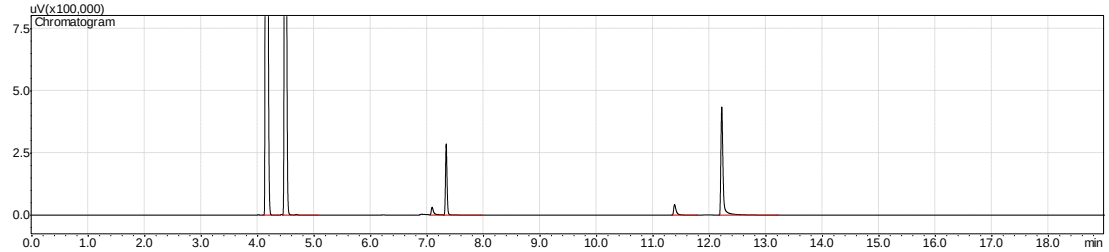
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.147	14092734.2	5753893.4	0.00000	ppm	V	1	
2	4.490	4108832.9	2013154.6	0.00000	ppm	V	1	
3	4.680	62263.6	23990.5	0.00000		SV		
4	7.337	187863.9	90654.3	0.00000	ppm	SV	3	
5	11.397	63244.9	16613.3	0.00000				
6	12.215	626989.9	153557.2	0.00000		S		

SPhos_ Br _52_RT _24H:



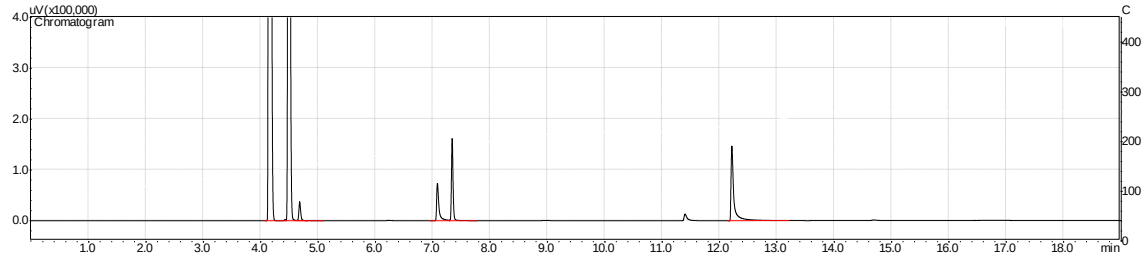
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.149	12854948.4	5327716.6	0.00000	ppm	SV	1	
2	4.487	9273548.9	4494399.9	0.00000	ppm	SV	1	
3	4.679	56987.9	26171.0	0.00000		T		
4	7.089	106666.6	30084.3	0.00000	ppm	V	3	
5	7.338	235573.7	116720.5	0.00000	ppm	V	3	
6	11.393	75426.8	20698.3	0.00000				
7	12.215	669766.0	215873.2	0.00000		SV		

Cg_Dave_Phos_(L4)_Br _52_RT _24H:



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.149	12782958.9	5289604.8	0.00000	ppm	V	1	
2	4.487	9100642.8	4420269.8	0.00000	ppm	SV	1	
3	7.088	48111.3	32569.0	0.00000	ppm	V	3	
4	7.337	553481.4	283607.6	0.00000	ppm	SV	3	
5	11.381	138842.1	42590.0	0.00000				
6	12.217	1188254.5	431571.3	0.00000		SV		

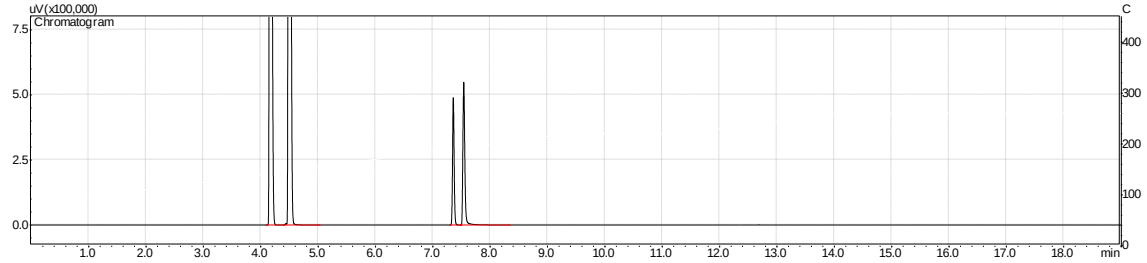
tBuDavePhos_ Br _52_RT _24H:



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.148	13581103.0	5586843.9	0.00000	ppm	SV	1	
2	4.488	7663607.2	3743538.6	0.00000	ppm	SV	1	
3	4.679	77823.9	36487.5	0.00000		T		
4	7.081	208425.2	72758.8	0.00000	ppm		3	
5	7.338	315288.0	159726.8	0.00000	ppm	SV	3	
6	12.215	704795.5	145862.6	0.00000		S		

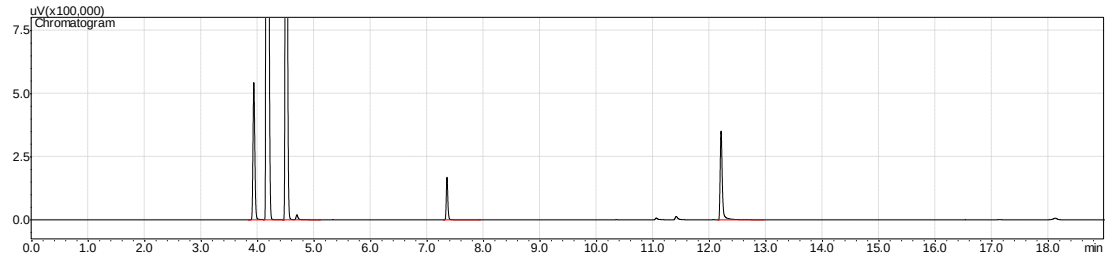
2-Phenyl-pyridine: KOH in MeOH

Ar_Br_50_RT_To



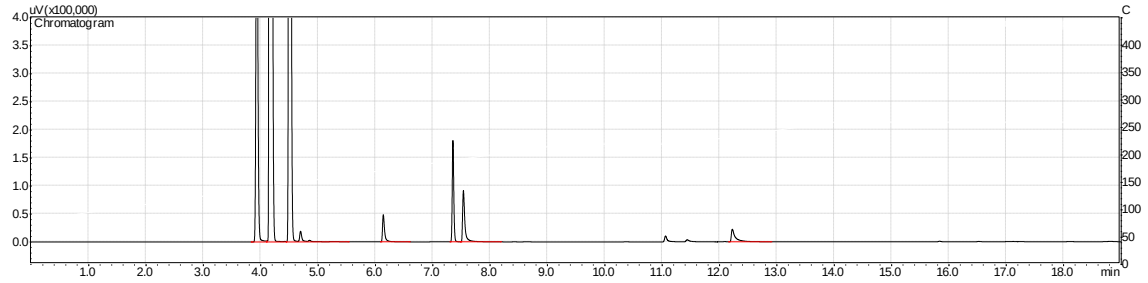
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.164	12749509.2	5138847.4	0.00000	ppm	SV	1	
2	4.494	22075436.0	9730688.5	0.00000	ppm	V	1	
3	7.356	934864.6	480970.6	0.00000		V		
4	7.539	1298336.5	543467.1	0.00000		SV		

L1_Br_50_RT _24H:



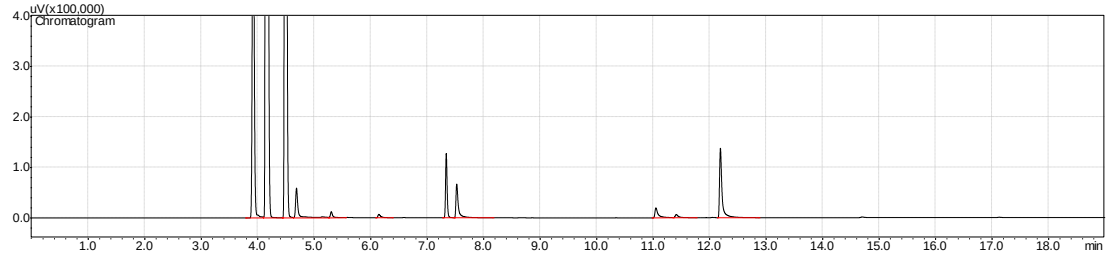
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	3.932	1237031.1	540822.3	0.00000				
2	4.160	16150780.6	6269489.0	0.00000	ppm	SV		
3	4.503	8736798.5	4099498.5	0.00000	ppm	SV		
4	7.351	329617.5	166602.6	0.00000		SV		
5	12.204	934425.7	348423.8	0.00000		SV		

L3_ Ar_ Br _50_RT _ 24H:



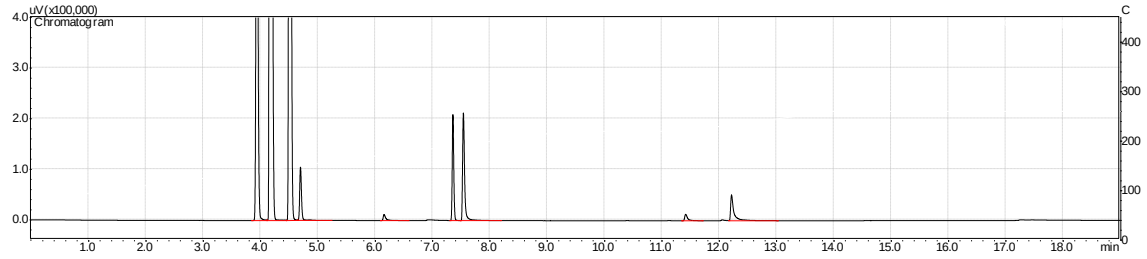
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	3.931	1664772.6	724038.3	0.00000				
2	4.161	15899245.0	6187489.5	0.00000	ppm	SV	1	
3	4.503	8453083.5	3957020.2	0.00000	ppm	SV	1	
4	6.137	223784	47846.6	0.00000		S		
5	7.351	334255.3	176805.2	0.00000				
6	7.534	350960.2	90320.5	0.00000		V		
7	12.223	114726.3	22339.7	0.00000		SV		

L2 Ar_ Br _50_RT _24H:



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	3.918	1868288.9	810102.3	0.00000				
2	4.149	13339191.9	5419793.9	0.00000	ppm	SV	1	
3	4.489	7877255.7	3760375.7	0.00000	ppm	V	1	
4	4.685	192800.5	58358.2	0.00000		SV		
5	5.301	14799.7	12118.0	0.00000		V		
6	6.143	24799.7	6776.0	0.00000				
7	7.337	242725.3	124230.1	0.00000	ppm		3	
8	7.522	203327.1	66429.9	0.00000		V		
9	11.048	83700.2	19869.1	0.00000				
10	11.408	28947.1	6431.1	0.00000		V		
11	12.190	426545.6	135963.3	0.00000		SV		

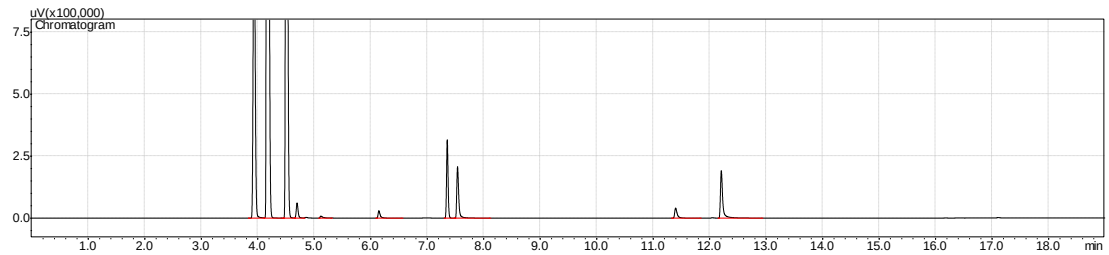
PPh3_Ar_ Br _50_RT _24H:



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	3.934	2340978.3	1009462.0	0.00000				
2	4.165	14809355.8	5858812.0	0.00000	ppm	SV	1	

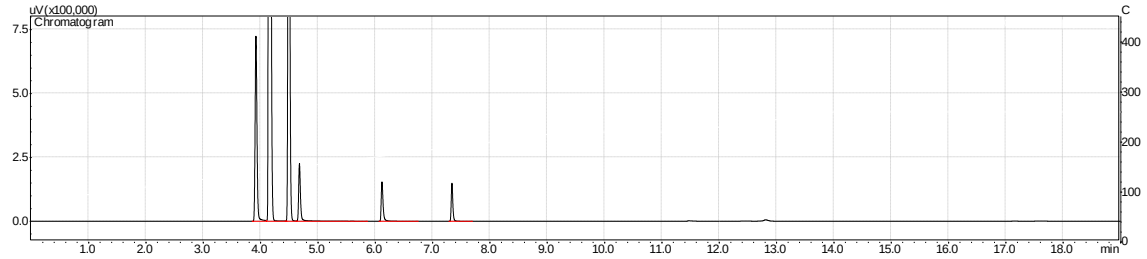
3	4.507	9327458.2	4388963.5	0.00000	ppm	V	1	
4	4.695	238355.4	104357.0	0.00000		SV		
5	6.153	41440.7	12248.8	0.00000		S		
6	7.354	390811.0	207736.7	0.00000		V		
7	7.536	522731.3	211249.6	0.00000		V		
8	11.414	47458.5	13160.8	0.00000				
9	12.214	209278.4	50785.7	0.00000		SV		

CyJohnPhos_ Br _50_RT _24H:



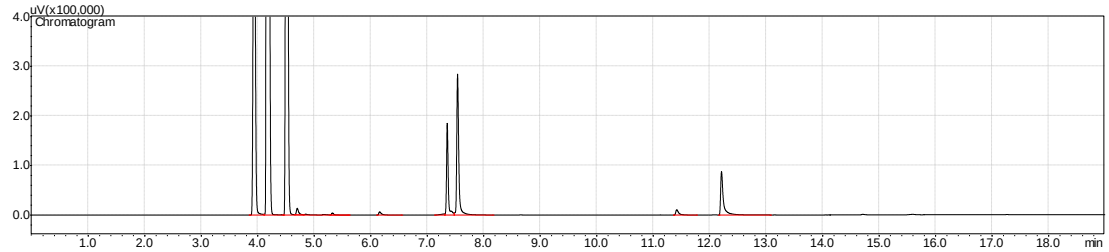
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	3.934	3528602.0	1506177.0	0.00000				
2	4.167	13789579.9	5505525.6	0.00000	ppm	SV	1	
3	4.507	9663513.2	4519423.2	0.00000	ppm	V	1	
4	4.695	144586.1	60986.1	0.00000		V		
5	5.117	33708.3	8429.0	0.00000		V		
6	6.144	82236.9	29712.3	0.00000		S		
7	7.354	589074.7	312758.7	0.00000		V		
8	7.537	503835.1	205863.4	0.00000		V		
9	11.397	130481.2	40747.7	0.00000		S		
10	12.206	552477.9	190449.1	0.00000		V		

JohnPhos_ Br _50_RT _24H:



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	3.918	1660098.6	719882.7	0.00000		V		
2	4.149	12988701.4	5360033.4	0.00000	ppm	SV	1	
3	4.490	5384433.9	2631220.1	0.00000	ppm	V	1	
4	4.676	552172.2	223501.4	0.00000		SV		
5	6.116	353086.4	153048.5	0.00000		S		
6	7.337	293423.2	146991.3	0.00000	ppm	S	3	

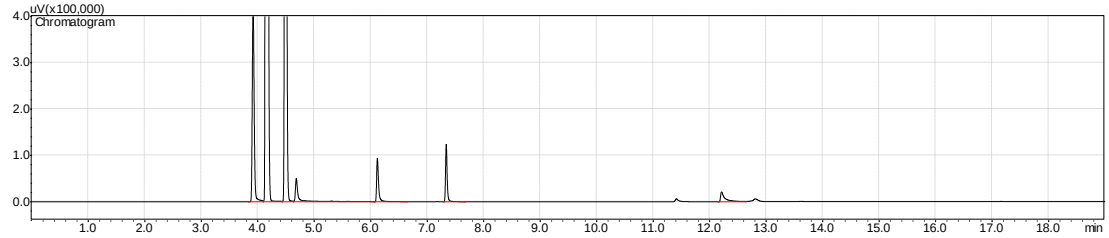
SPhos_ Br _50_RT _24H:



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	3.935	2615806.0	1123943.0	0.00000				
2	4.165	15120229.8	5945167.2	0.00000	ppm	SV	1	
3	4.508	7790861.4	3652017.8	0.00000	ppm	SV	1	
4	4.699	35845.4	12962.0	0.00000		T		
5	5.322	12258.0	4229.7	0.00000		TV		
6	6.158	24348.7	6708.5	0.00000		S		
7	7.293	12941.8	2302.6	0.00000	ppm	V	3	
8	7.354	383184.6	183001.0	0.00000		SV		

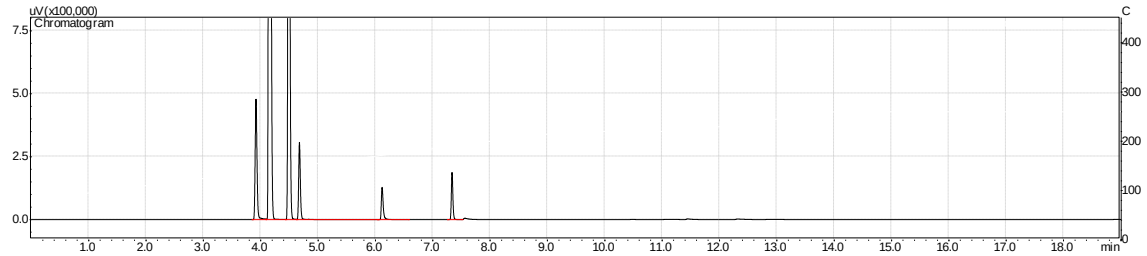
9	7.537	707498.9	280415.8	0.00000		V		
10	11.418	41319.6	10961.8	0.00000		S		
11	12.209	300287.2	86737.2	0.00000		SV		

L4_Br _50_RT _24H:



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	3.918	1003120.7	433680.2	0.00000				
2	4.148	13297316.3	5487253.7	0.00000	ppm	SV	1	
3	4.489	5790556.3	2839028.1	0.00000	ppm	V	1	
4	4.682	210504.1	50500.9	0.00000		SV		
5	6.117	226859.0	93127.2	0.00000		SV		
6	7.336	246676.2	121646.7	0.00000	ppm	S	3	
7	12.211	116735.0	21164.5	0.00000				

tBuDavePhos_ Br _50_RT _24H:

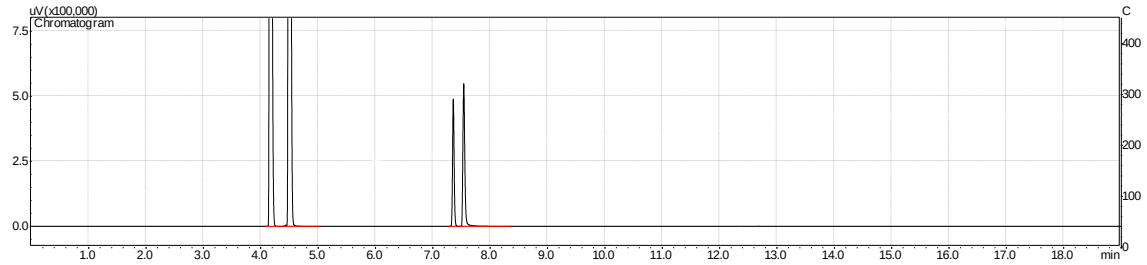


Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	3.917	1090132.8	473588.4	0.00000				
2	4.148	12938947.1	5368811.9	0.00000	ppm	SV	1	

3	4.488	6645564.7	3257025.8	0.00000	ppm	V	1	
4	4.675	656338.9	305165.5	0.00000		SV		
5	6.116	295784.7	127851.6	0.00000		SV		
6	7.336	350804.7	185294.5	0.00000	ppm	V	3	

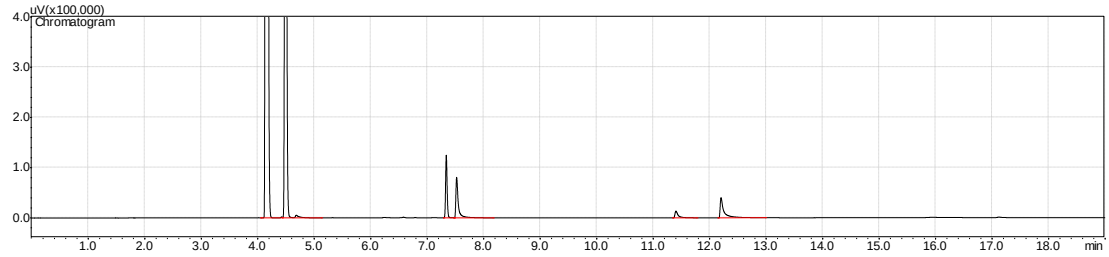
2-Phenyl-pyridine: KF

Ar_Br_50_RT_To



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.164	12749509.2	5138847.4	0.00000	ppm	SV	1	
2	4.494	22075436.0	9730688.5	0.00000	ppm	V	1	
3	7.356	934864.6	480970.6	0.00000		V		
4	7.539	1298336.5	543467.1	0.00000		SV		

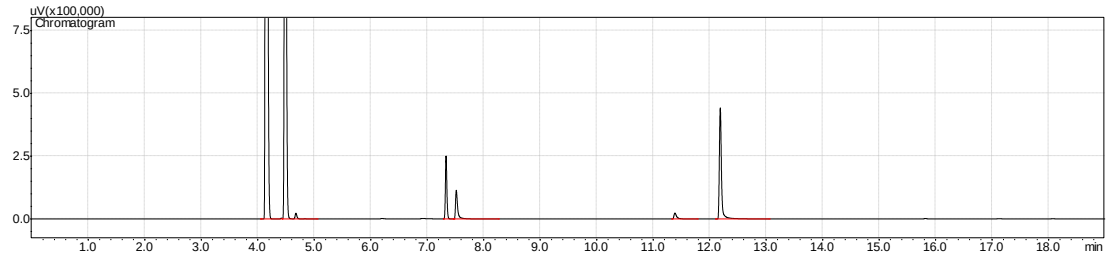
L1_Br_50_RT _24H:



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.146	13816055.8	5664674.5	0.00000	ppm	SV	1	
2	4.490	4331390.3	2129564.7	0.00000	ppm	SV	1	
3	7.337	230553.2	121432.5	0.00000	ppm		3	

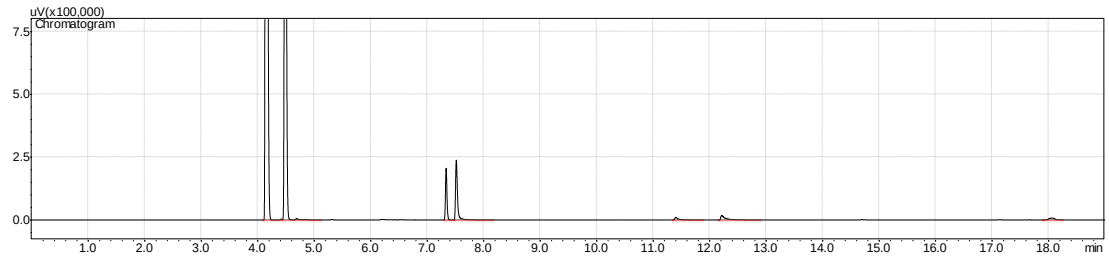
4	7.521	737973.6	80158.8	0.00000		V		
5	12.202	187856.7	39842.0	0.00000				

L3_ Ar_ Br _50_RT _ 24H:



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.145	13075431.5	5396376.2	0.00000	ppm	SV	1	
2	4.484	7869206.7	3828369.2	0.00000	ppm	SV	1	
3	7.333	462657.7	247637.3	0.00000	ppm	V	3	
4	7.514	310892.8	113392.1	0.00000		SV		
5	11.384	82785.4	23891.9	0.00000				
6	12.187	1159288.4	440695.1	0.00000				

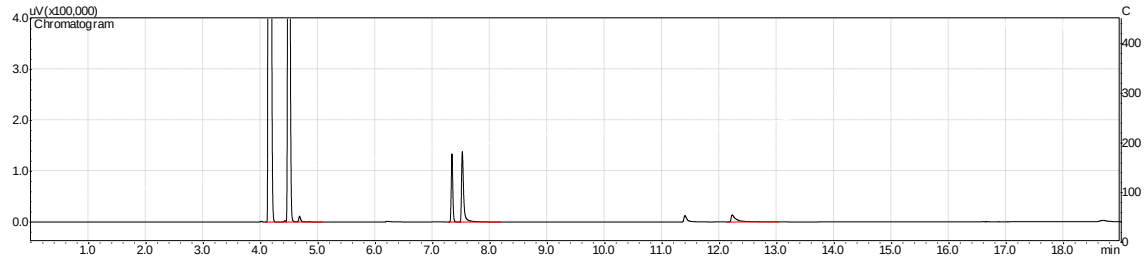
L2 Ar_ Br _50_RT _24H:



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.145	13283579.2	5467026.7	0.00000	ppm	SV	1	
2	4.485	8155487.6	3962491.7	0.00000	ppm	SV	1	
3	7.335	379466.3	204795.6	0.00000	ppm		3	
4	7.515	576678.1	235011.9	0.00000		V		

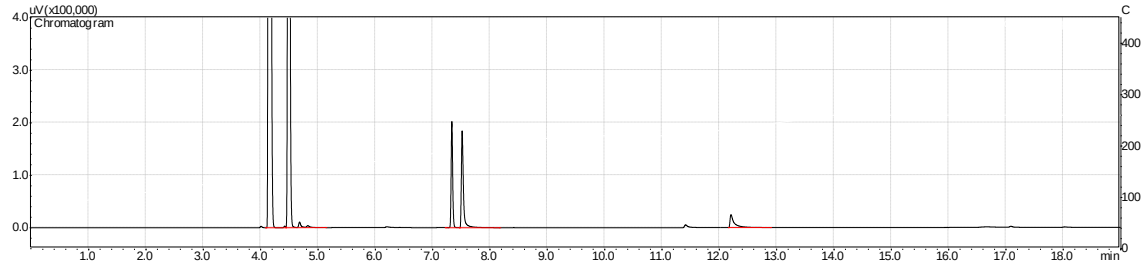
5	11.401	50832.3	10757.0	0.00000				
6	12.213	107819.3	17897.6	0.00000				
7	18.063	51004.5	7494.3	0.00000	ppm		8	

PPh3_Ar_ Br _50_RT _24H:



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.145	13695550.9	5591132.8	0.00000	ppm	SV	1	
2	4.487	5633231.0	2765452.8	0.00000	ppm	SV	1	
3	7.334	249318.4	132962.8	0.00000	ppm	V	3	
4	7.515	1161951.1	136312.9	0.00000		V		
5	12.221	91397.8	13711.5	0.00000		S		

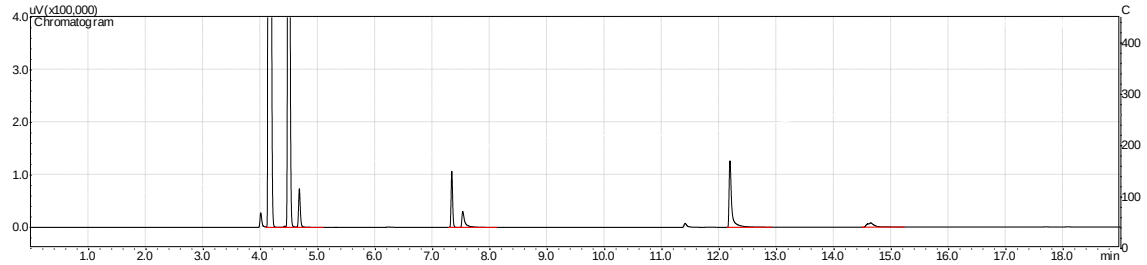
CyJohnPhos_ Br _50_RT _24H:



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.145	13543283.2	5530185.3	0.00000	ppm	SV	1	
2	4.486	6519466.5	3167064.6	0.00000	ppm	SV	1	
3	7.334	373807.6	200408.3	0.00000	ppm	V	3	

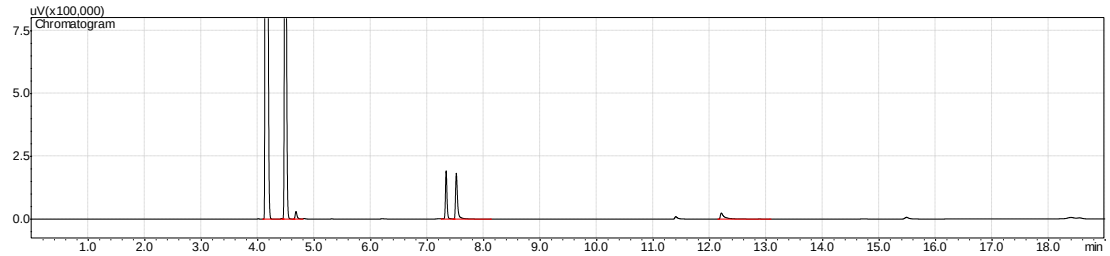
4	7.514	1008426.6	181389.1	0.00000		V		
5	12.204	131024.6	24720.2	0.00000		SV		

JohnPhos_ Br _50_RT _24H:



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.145	14138157.3	5738984.6	0.00000	ppm	SV	1	
2	4.487	5114803.8	2526992.3	0.00000	ppm	V	1	
3	4.675	131442.8	73540.0	0.00000		SV		
4	7.334	199426.4	105897.6	0.00000	ppm	V	3	
5	7.525	134317.2	30411.2	0.00000		SV		
6	12.185	405313.4	124965.1	0.00000		S		
7	14.639	73910.7	8332.1	0.00000	ppm	S	6	

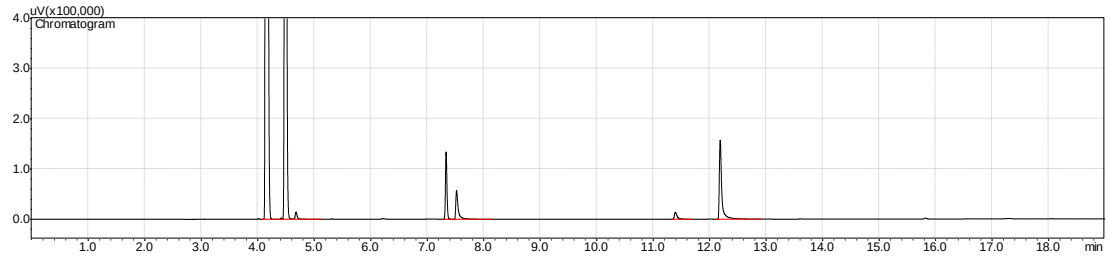
SPhos_ Br _50_RT _24H:



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.145	13820169.8	5619015.1	0.00000	ppm	SV	1	
2	4.488	5180878.9	2556052.2	0.00000	ppm	V	1	
3	4.676	75068.1	30433.6	0.00000		V		

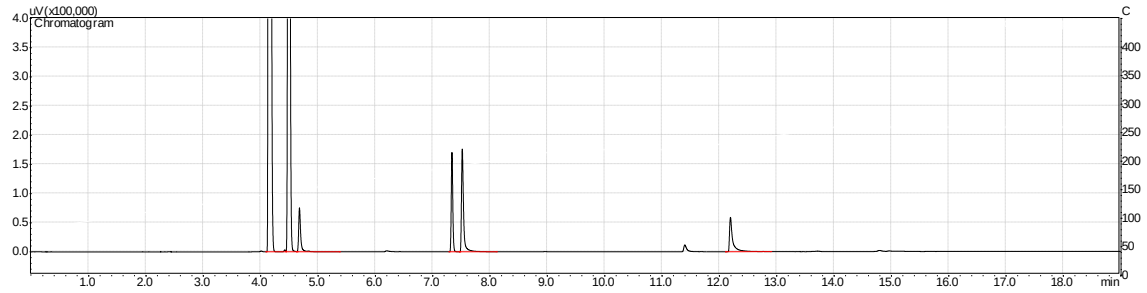
4	7.335	373904.0	191643.5	0.00000	ppm	V	3	
5	7.515	1059808.9	180030.2	0.00000		V		
6	12.206	128773.1	24051.4	0.00000		S		

L4_ Br _50_RT _24H:



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.148	12337159.9	5190833.4	0.00000	ppm	SV	1	
2	4.487	6229033.3	3061932.9	0.00000	ppm	SV	1	
3	7.334	246794.6	132846.7	0.00000	ppm		3	
4	7.520	119795.7	56956.3	0.00000				
5	12.186	472042.2	156118.8	0.00000		V		

tBuDavePhos_ Br _50_RT _24H:

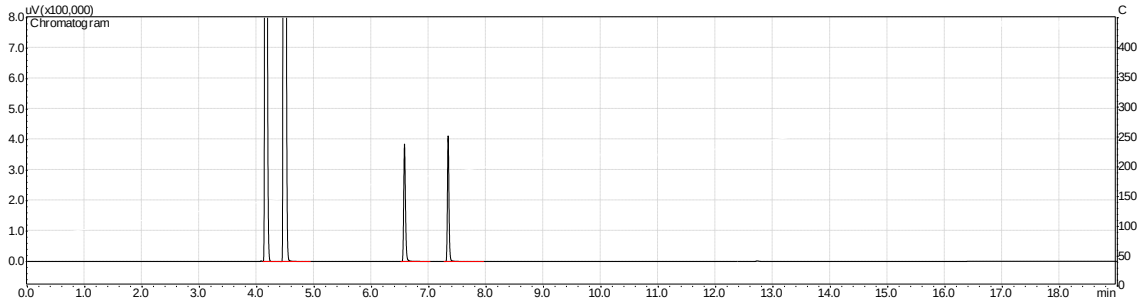


Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.147	13077859.3	5427697.3	0.00000	ppm	SV	1	
2	4.487	6855067.4	3356100.9	0.00000	ppm	V	1	
3	4.676	157405.8	74744.4	0.00000		SV		

4	7.335	513272.6	168675.3	0.00000	ppm		3	
5	7.516	528699.5	174550.6	0.00000		SV		
6	12.193	329215.2	58755.7	0.00000		S		

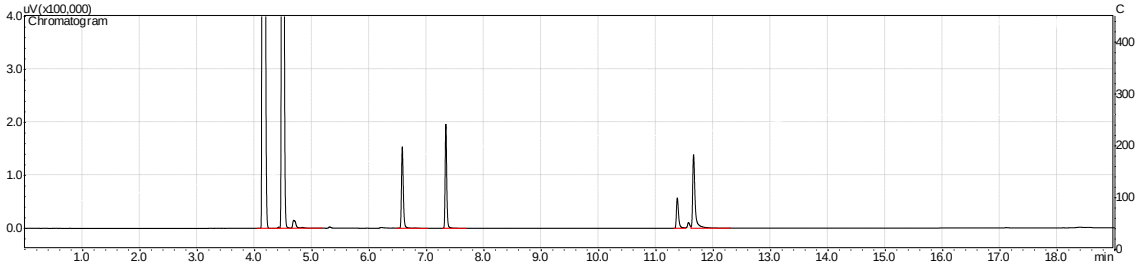
2-Phenyl-thiophene: KF

Ar_Br_54_RT_To



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.153	9063126.1	3996843.0	0.00000	ppm	SV	1	
2	4.476	22355698.7	10097663.1	0.00000	ppm		1	
3	6.575	830177.4	380211.2	0.00000	ppm	S	2	
4	7.336	779748.6	403588.9	0.00000	ppm	SV	3	

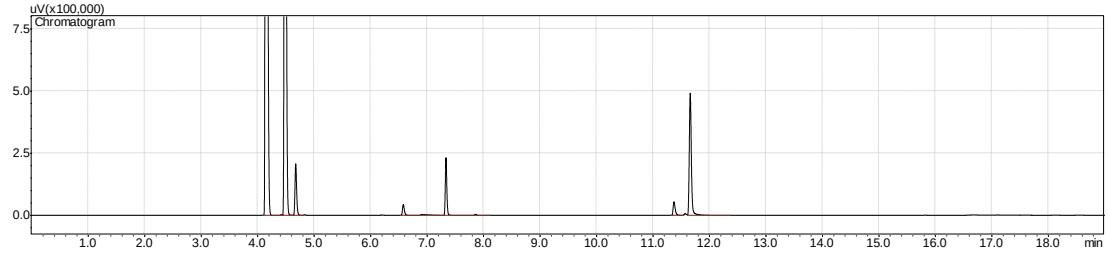
L1_Br_54_RT _24H:



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.145	13915423.0	5659448.8	0.00000	ppm	SV	1	
2	4.485	8212447.3	3970692.2	0.00000	ppm	SV	1	
3	6.574	341674.7	152701.9	0.00000	ppm	SV	2	

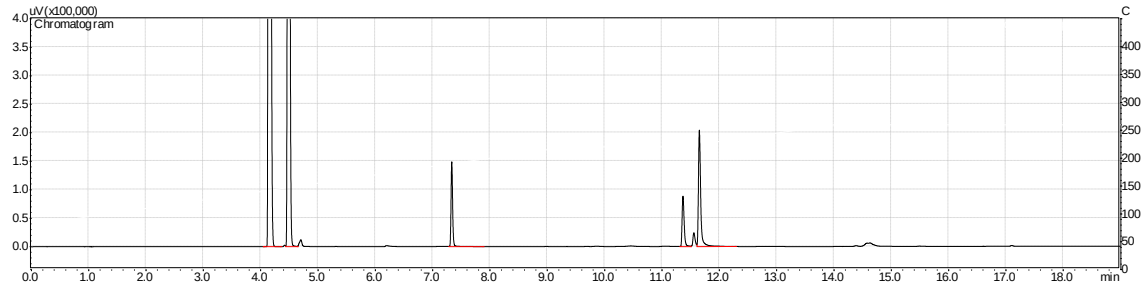
4	7.334	377913.2	194322.9	0.00000	ppm	SV	3	
5	11.371	151118.2	57171.0	0.00000				
6	11.655	412984.6	138126.7	0.00000		V		

L3_ Ar_ Br _54_RT _ 24H:



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.146	13128864.3	5405540.7	0.00000	ppm	SV	1	
2	4.484	9452947.5	4569745.5	0.00000	ppm	V	1	
3	4.673	108175.4	204158.4	0.00000		V		
4	6.578	71250.0	43891.5	0.00000	ppm	SV	2	
5	7.334	441243.3	229123.9	0.00000	ppm	SV	3	
6	11.371	142363.0	54422.4	0.00000				
7	11.658	1254178.8	485429.9	0.00000		V		

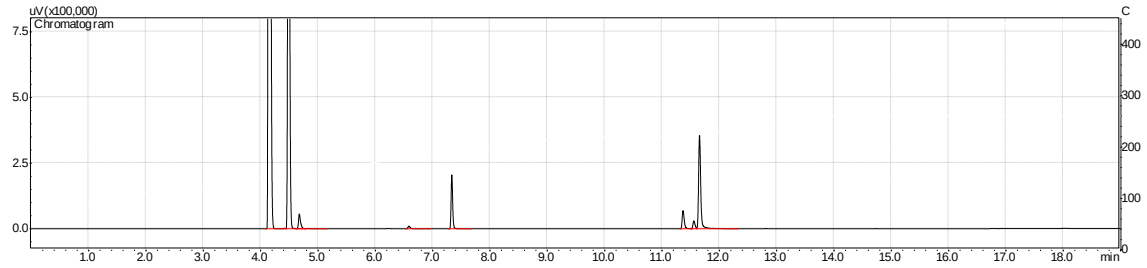
L2 Ar_ Br _54_RT _24H:



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.146	12044168.2	5068029.6	0.00000	ppm	V	1	
2	4.483	8559607.6	4179788.7	0.00000	ppm	V	1	

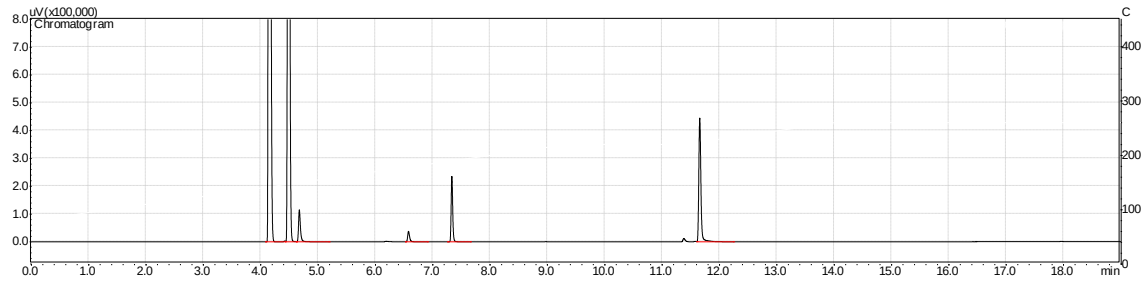
3	7.333	291214.8	147317.4	0.00000	ppm	SV	3	
4	11.366	222447.3	88219.8	0.00000		V		
5	11.652	563154.8	202812.8	0.00000		V		

CyJohnPhos_ Br _54_RT _24H:



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.144	13359887.0	5487310.0	0.00000	ppm	SV	1	
2	4.485	6014261.0	2922409.8	0.00000	ppm	SV	1	
3	4.674	136506.5	55603.7	0.00000		T		
4	6.585	29075.0	10463.5	0.00000	ppm	SV	2	
5	7.334	389562.1	202652.8	0.00000	ppm	S	3	
6	11.367	175161.1	69203.5	0.00000				
7	11.555	76123.5	29523.1	0.00000		V		
8	11.655	924604.5	352305.3	0.00000		V		

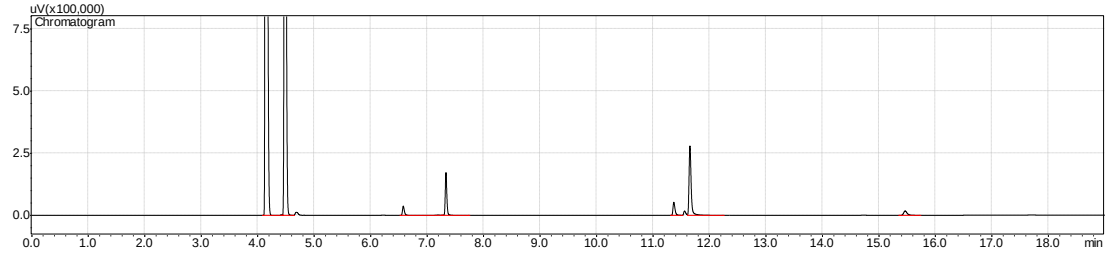
JohnPhos_ Br _54_RT _24H:



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name

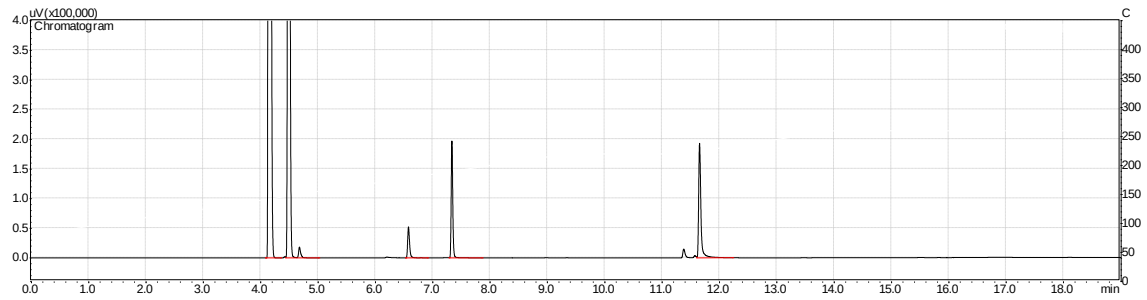
1	4.146	11730229.9	4965669.5	0.00000	ppm	SV	1	
2	4.482	10144763.8	4901087.8	0.00000	ppm	V	1	
3	4.673	90242.3	114641.8	0.00000		SV		
4	6.577	78345	37874.2	0.00000	ppm	SV	2	
5	7.332	445190.9	231682.6	0.00000	ppm	S	3	
6	11.655	1138959.2	443638.7	0.00000		V		

SPhos_ Br _54_RT _24H:



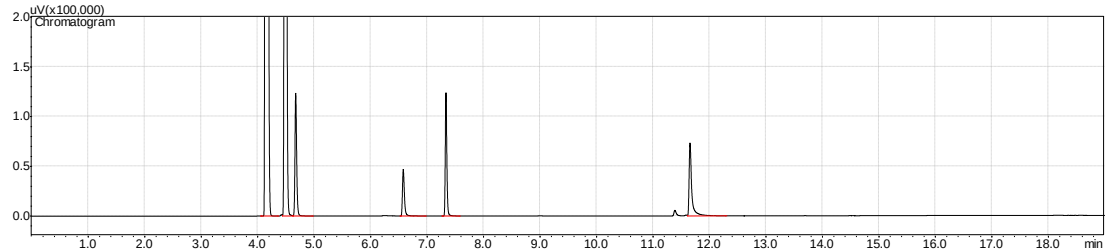
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.145	12582681.5	5227104.3	0.00000	ppm	SV	1	
2	4.483	8147708.4	3985522.2	0.00000	ppm	V	1	
3	6.578	98452.9	37291.2	0.00000	ppm	SV	2	
4	7.333	335759.3	170262.1	0.00000	ppm	V	3	
5	11.368	135017.6	52127.4	0.00000				
6	11.653	728416.9	275997.1	0.00000		V		
7	15.464	76126.5	17735.4	0.00000	ppm		6	

L4_Br _54_RT _24H:



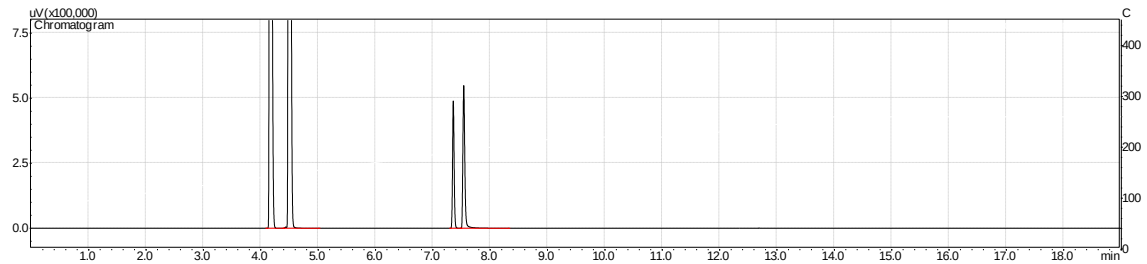
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.145	12850739.1	5298921.2	0.00000	ppm	V	1	
2	4.484	6946671.7	3374859.6	0.00000	ppm	SV	1	
3	6.576	124106.3	51903.9	0.00000	ppm	SV	2	
4	7.333	377063.1	195548.0	0.00000	ppm	SV	3	
5	11.652	528637.1	191218.9	0.00000		V		

tBuDavePhos_ Br _54_RT _24H:



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.144	13593053.8	5545587.9	0.00000	ppm	V	1	
2	4.486	5137668.0	2524355.8	0.00000	ppm	V	1	
3	4.673	258168.0	122076.2	0.00000		V		
4	6.577	173801.8	46549.9	0.00000	ppm	SV	2	
5	7.334	238237.2	122739.7	0.00000	ppm		3	
6	11.655	239290.2	73043.7	0.00000		SV		

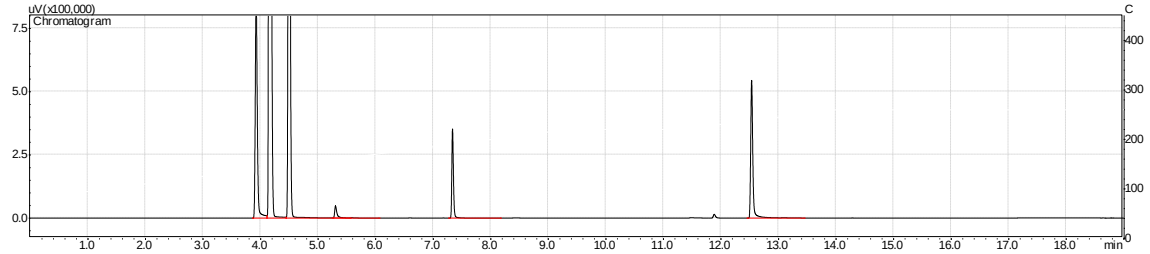
Ar_Br_50_A_RT_To



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name

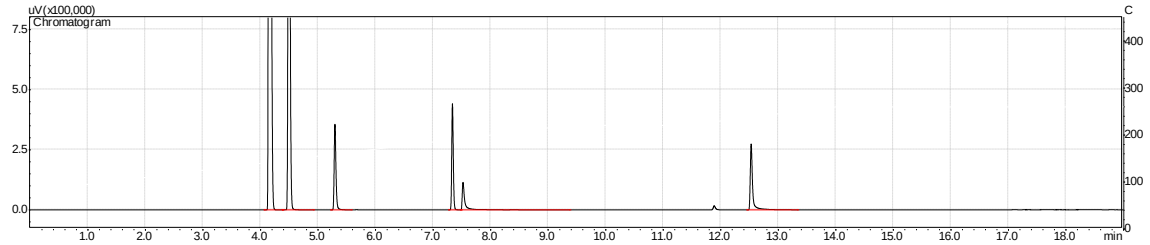
1	4.164	12749509.2	5138847.4	0.00000	ppm	SV	1	
2	4.494	22075436.0	9730688.5	0.00000	ppm	V	1	
3	7.356	934864.6	480970.6	0.00000		V		
4	7.539	1298336.5	543467.1	0.00000		SV		

L1_Br_50_A_RT _24H:



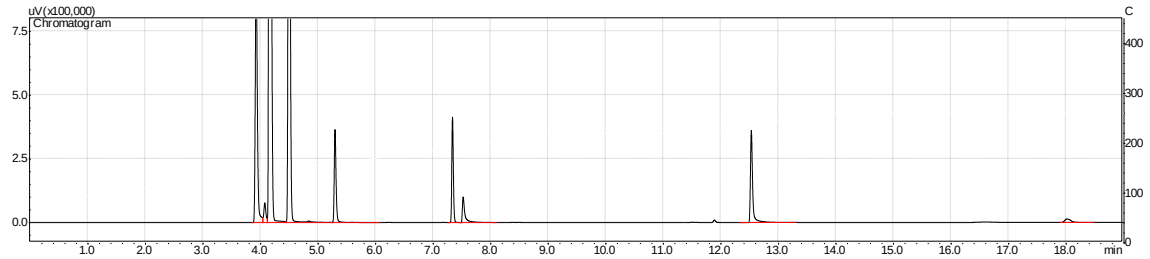
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	3.923	2172025.4	863129.4	0.00000		V		
2	4.154	13514039.0	5283618.4	0.00000	ppm	V	1	
3	4.492	7085670.7	3239634.8	0.00000	ppm	SV	1	
4	5.301	136528.1	47339.5	0.00000		T		toluene
5	7.335	686224.0	350398.3	0.00000	ppm	S	3	
6	12.532	1426439.5	541521.8	0.00000		S		

L3_ Ar_ Br _50_A_RT _ 24H:



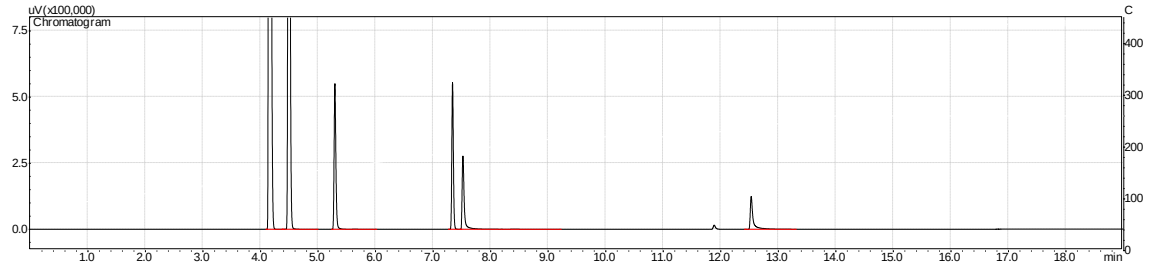
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.152	15171250.1	5885437.5	0.00000	ppm	V	1	
2	4.493	6283252.2	2954642.1	0.00000	ppm	V	1	
3	5.293	770209.0	350573.5	0.00000				toluene
4	7.336	818724.0	437448.0	0.00000	ppm	V	3	
5	7.520	210524.5	112972.9	0.00000		SV		
6	12.528	779244.0	272799.0	0.00000				

CyJohnPhos_Ar_ Br _50_A_RT _24H:



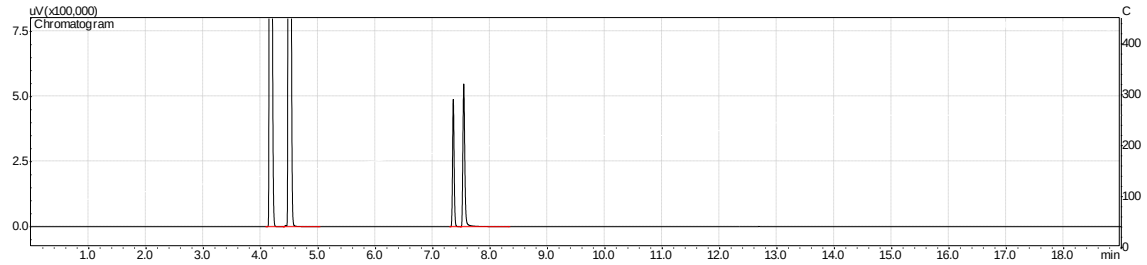
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	3.923	2487588.6	987350.9	0.00000		V		
2	4.073	199325.8	77304.2	0.00000	ppm	V	1	
3	4.155	12886853.1	5047157.0	0.00000	ppm	V	1	
4	4.493	7274611.6	3295404.8	0.00000	ppm	SV	1	
5	5.294	811719.1	360113.4	0.00000		SV		toluene
6	7.335	768624.5	410483.8	0.00000	ppm		3	
7	7.520	204268.5	99993.7	0.00000		V		
8	12.528	1203089.5	359602.3	0.00000				
9	18.014	102013.3	13638.5	0.00000	ppm		7	

JohnPhos_Ar_ Br _50_A_RT _24H:



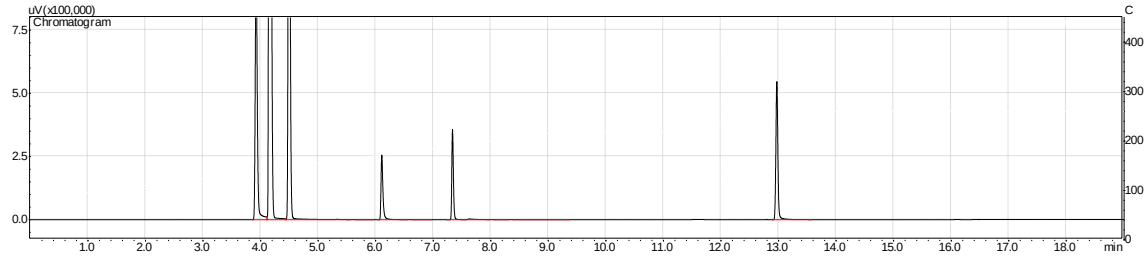
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.153	13934795.6	5497121.7	0.00000	ppm	V	1	
2	4.491	8399473.8	3890080.1	0.00000	ppm	V	1	
3	5.292	1168447.9	542263.8	0.00000		S		toluene
4	7.337	1035941.9	544262.2	0.00000	ppm	V	3	
5	7.518	816905.7	274106.8	0.00000		SV		
6	12.528	427955.3	124287.4	0.00000				

Ar_Br_50_B_RT_To



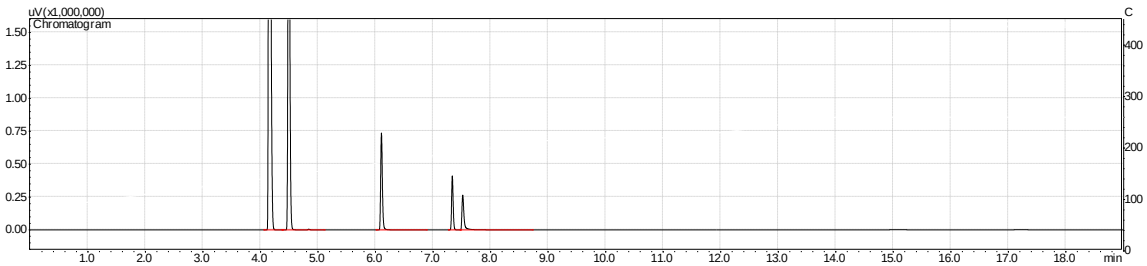
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.164	12749509.2	5138847.4	0.00000	ppm	SV	1	
2	4.494	22075436.0	9730688.5	0.00000	ppm	V	1	
3	7.356	934864.6	480970.6	0.00000		V		
4	7.539	1298336.5	543467.1	0.00000		SV		

L1_Br_50_B_RT _24H:



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	3.922	2556081.5	1014459.6	0.00000		V		
2	4.154	13151120.2	5123544.0	0.00000	ppm	V	1	
3	4.493	5732916.5	2611967.6	0.00000	ppm	SV	1	
4	6.106	610331.2	253476.6	0.00000		S		m-xylene
5	7.335	686487.7	353850.8	0.00000	ppm	S	3	
6	12.970	1330824.0	541083.3	0.00000		V		

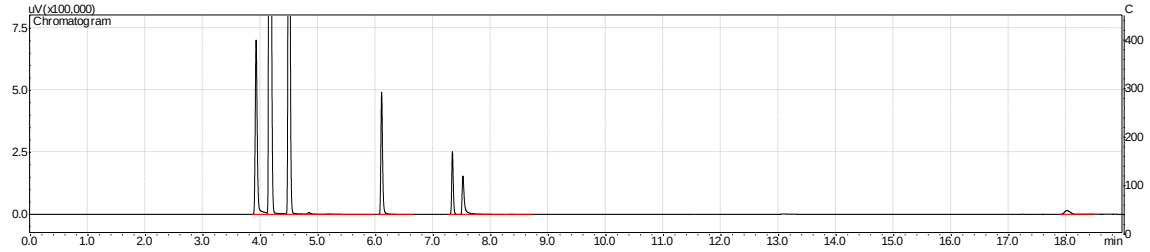
L3_ Ar_ Br _50_B_RT _ 24H:



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.151	14355453.9	5617280.3	0.00000	ppm	V	1	

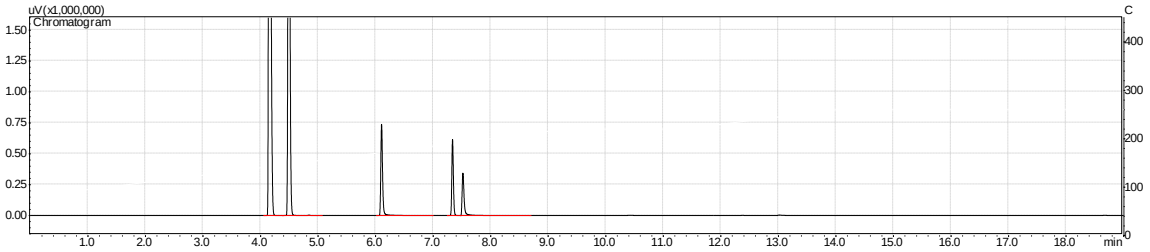
2	4.490	7448111.2	3435262.7	0.00000	ppm	SV	1	
3	6.102	1523838.8	732024.8	0.00000		S		m-xylene
4	7.334	760727.4	406397.5	0.00000	ppm	V	3	
5	7.515	689139.7	262599.9	0.00000		SV		

CyJohnPhos_Ar_ Br _50_B_RT _24H:



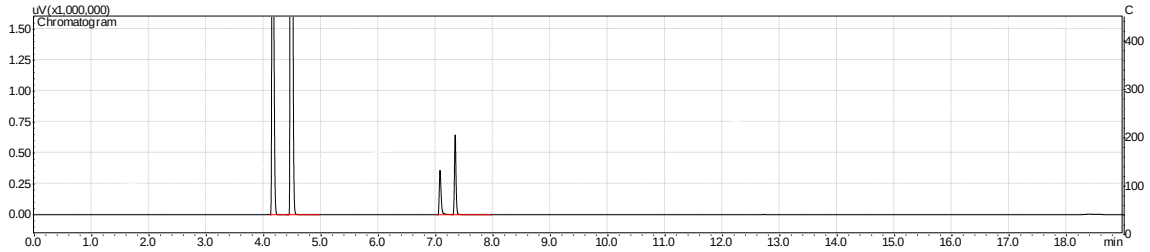
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	3.922	1723215.0	697248.0	0.00000		V		
2	4.154	11501247.1	4688996.6	0.00000	ppm	V	1	
3	4.491	5873561.9	2745473.3	0.00000	ppm	SV	1	
4	6.102	1031539.9	490584.3	0.00000				m-xylene
5	7.332	469608.0	248696.2	0.00000	ppm		3	
6	7.515	443738.7	152833.7	0.00000		SV		
7	18.009	106258.2	15053.6	0.00000	ppm		7	

JohnPhos_Ar_ Br _50_B_RT _24H:



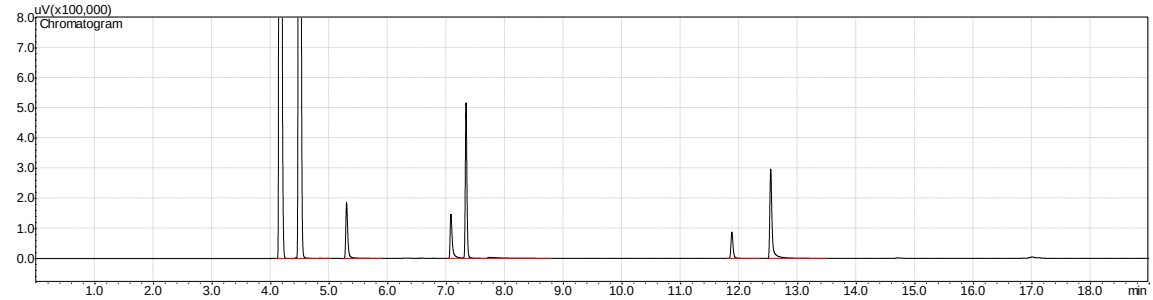
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.152	14436647.6	5594525.6	0.00000	ppm	V	1	
2	4.489	9914143.1	4514933.0	0.00000	ppm	SV	1	
3	6.103	1601555.7	733045.7	0.00000		S		m-xylene
4	7.337	1154987.5	602501.4	0.00000	ppm		3	
5	7.517	847640.0	341784.4	0.00000		SV		

Ar_Br_52_A_RT_To



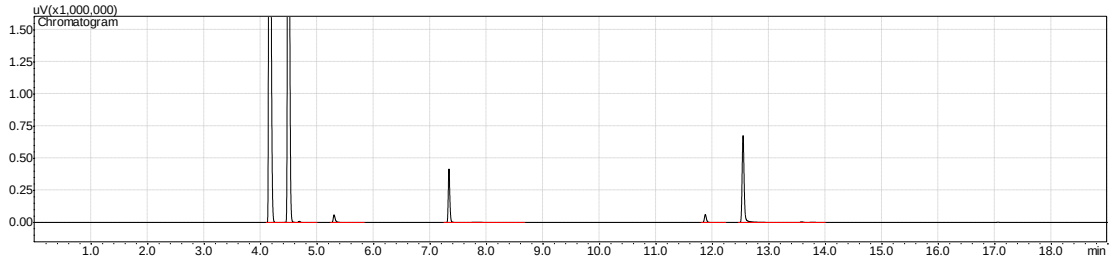
Peak #	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.155	8378818.4	3742545.8	0.00000	ppm	SV	1	
2	4.476	23303114.4	10461192.8	0.00000	ppm		1	
3	7.074	816951.0	355151.1	0.00000	ppm		3	
4	7.338	1216411.6	638908.6	0.00000	ppm	SV	3	

L2_Br_52_A_RT _24H_KF:



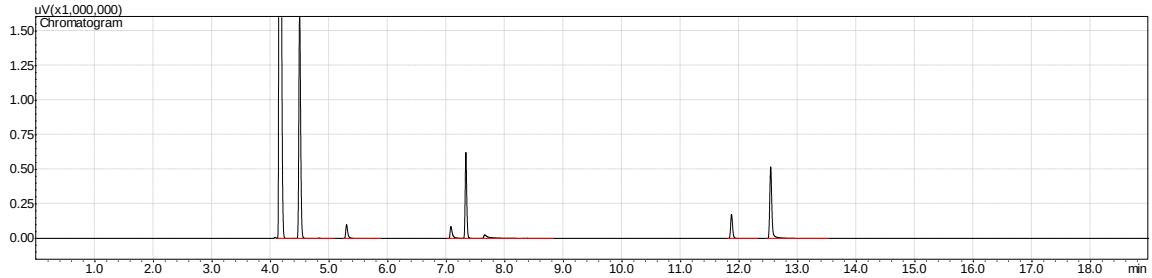
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.157	13237232.1	5224483.6	0.00000	ppm	SV	1	
2	4.489	14166751.6	6339253.6	0.00000	ppm	SV	1	
3	5.296	450389.8	185338.6	0.00000				toluene
4	7.078	181612.0	145516.2	0.00000	ppm		3	
5	7.336	992683.4	509797.5	0.00000	ppm	SV	3	
6	11.875	220483.5	87446.0	0.00000		S		
7	12.538	833557.6	295432.9	0.00000		S		

L4_ Ar_ Br _52_A_RT _ 24H_KF:



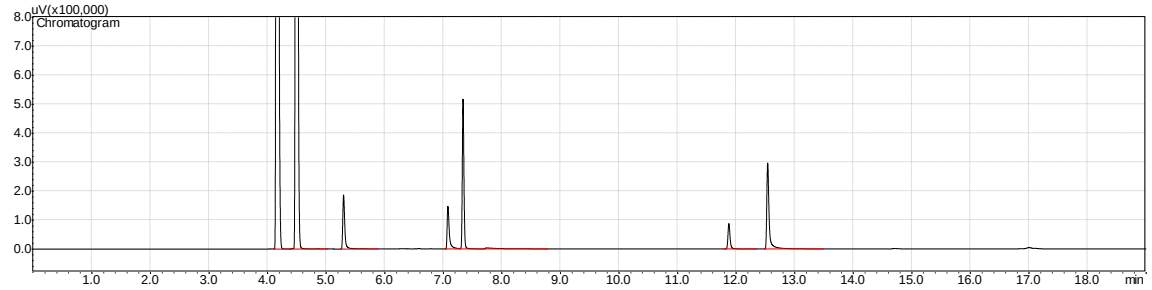
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.155	13536573.5	5292861.8	0.00000	ppm	SV	1	
2	4.489	12137058.0	5504777.9	0.00000	ppm	SV	1	
3	5.298	158160.0	59269.5	0.00000		S		toluene
4	7.333	798783.1	410536.6	0.00000	ppm	S	3	
5	11.872	154947.2	61916.6	0.00000		S		
6	12.541	1730317.8	670143.3	0.00000		S		

CyJohnPhos_Ar_ Br _52_A_RT _24H:



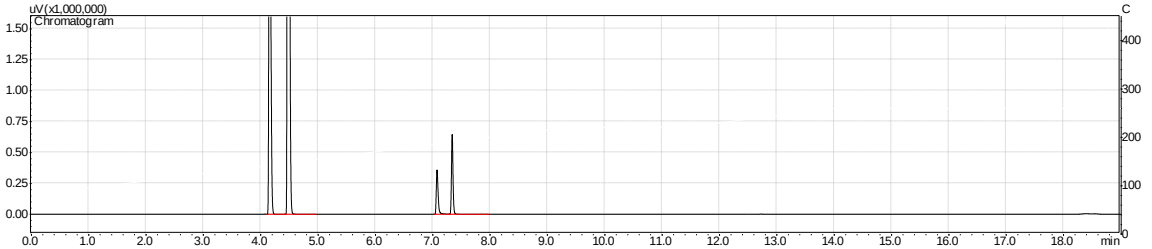
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.155	13237869.0	5257926.9	0.00000	ppm	V	1	
2	4.495	3481225.7	1614922.6	0.00000	ppm	SV	1	
3	5.296	249565.6	100362.0	0.00000		S		toluene
4	7.078	59790.5	85801.4	0.00000	ppm		3	
5	7.334	1171767.7	615799.7	0.00000	ppm	V	3	
6	7.656	195603.6	26100.6	0.00000		SV		
7	11.870	407337.9	172539.0	0.00000		SV		
8	12.538	1336102.3	513460.1	0.00000				

JohnPhos_Ar_ Br _52_A_RT _24H:



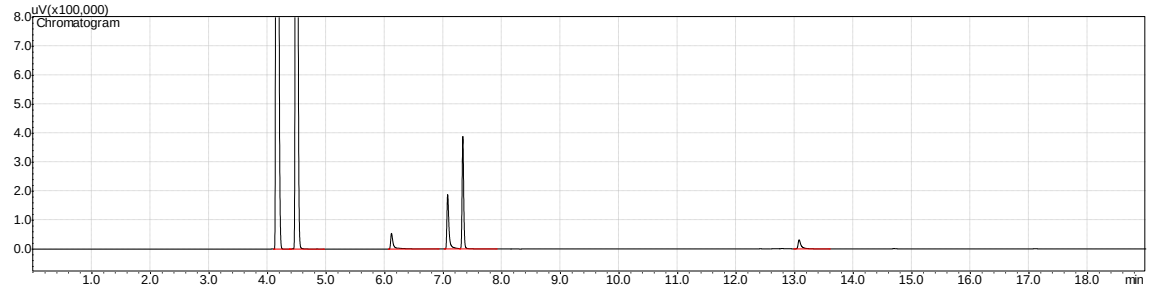
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.157	13237232.1	5224483.6	0.00000	ppm	SV	1	
2	4.489	14166751.6	6339253.6	0.00000	ppm	SV	1	
3	5.296	450389.8	185338.6	0.00000				toluene
4	7.078	201612	145516.2	0.00000	ppm		3	
5	7.336	992683.4	509797.5	0.00000	ppm	SV	3	
6	11.875	220483.5	87446.0	0.00000		S		
7	12.538	833557.6	295432.9	0.00000		S		

Ar_Br_52_B_RT_To



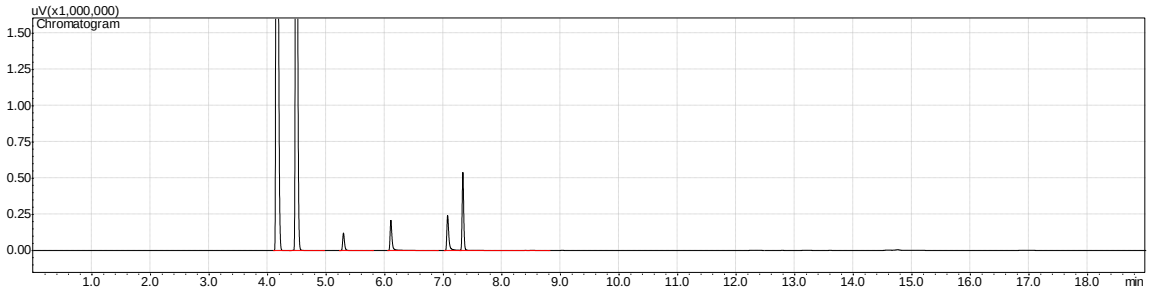
Peak #	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.155	8378818.4	3742545.8	0.00000	ppm	SV	1	
2	4.476	23303114.4	10461192.8	0.00000	ppm		1	
3	7.074	816951.0	355151.1	0.00000	ppm		3	
4	7.338	1216411.6	638908.6	0.00000	ppm	SV	3	

L2_Br_52_B_RT _24H_KF:



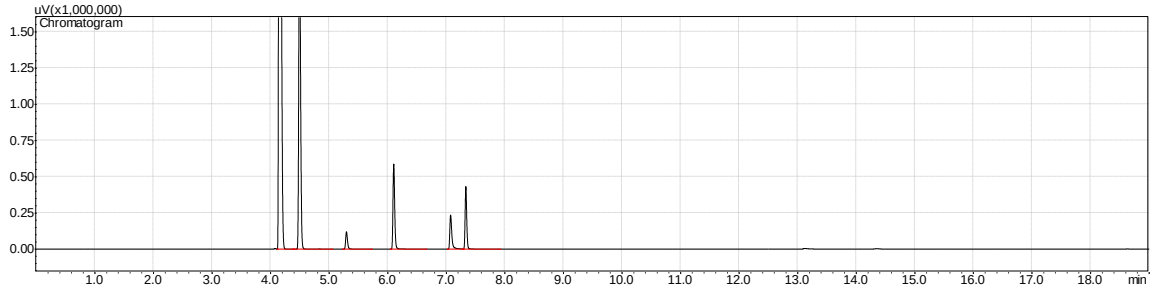
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.154	13823053.7	5396472.2	0.00000	ppm	V	1	
2	4.489	11817732.7	5351163.2	0.00000	ppm	SV	1	
3	6.115	195434.2	54123.7	0.00000		S		m-xylene
4	7.074	652955.6	187147.0	0.00000	ppm		3	
5	7.332	745507.3	379741.9	0.00000	ppm	SV	3	
6	13.075	118442.1	31505.0	0.00000		SV		

L4_ Ar_ Br _52_B_RT _ 24H_KF:



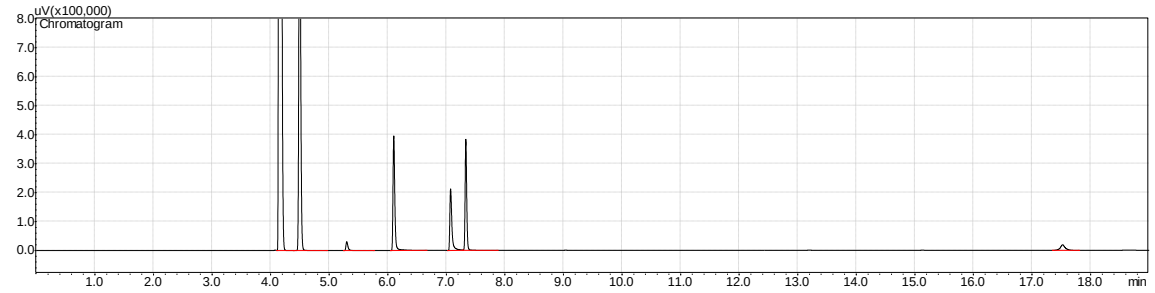
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.154	13612575.3	5310458.5	0.00000	ppm	SV	1	
2	4.488	12407637.3	5614667.5	0.00000	ppm	SV	1	
3	5.294	273311.6	120739.8	0.00000		S		
4	6.104	512888.6	205888.3	0.00000		S		m-xylene
5	7.073	587878.6	240158.2	0.00000	ppm		3	
6	7.333	1029077.1	531089.5	0.00000	ppm	SV	3	

CyJohnPhos_Ar_ Br _52_B_RT _24H:



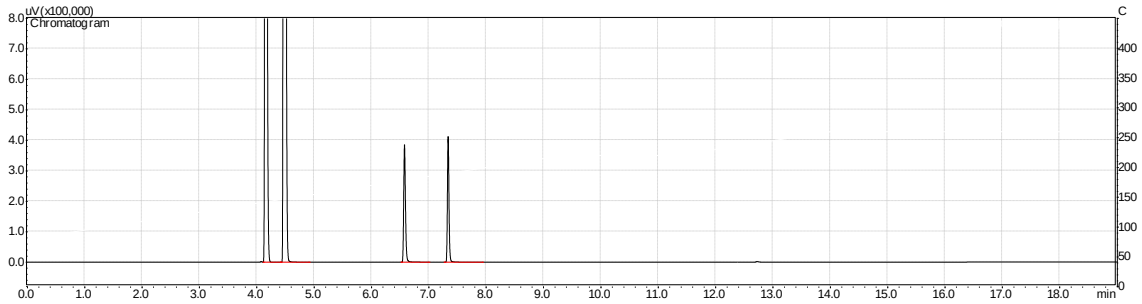
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.151	15837782.6	6038324.6	0.00000	ppm	V	1	
2	4.493	4799139.7	2236927.2	0.00000	ppm	SV	1	
3	5.294	268600.1	119581.2	0.00000		S		
4	6.102	1215891.7	582272.7	0.00000		S		m-xylene
5	7.073	593976.4	233856.6	0.00000	ppm		3	
6	7.333	831459.4	424873.5	0.00000	ppm	SV	3	

JohnPhos_Ar_ Br _52_B_RT _24H:



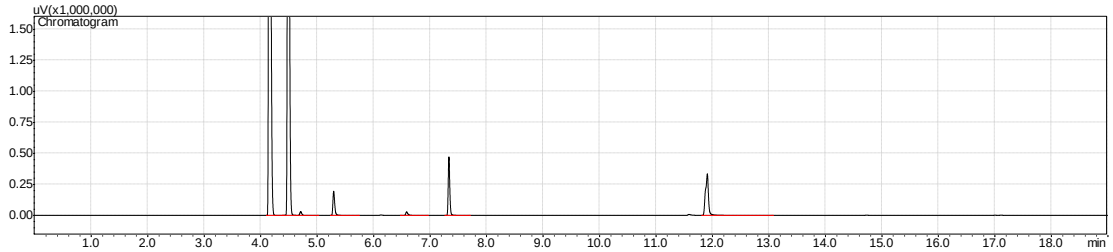
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.151	16013780.0	6103904.7	0.00000	ppm	SV	1	
2	4.495	3126958.3	1448629.2	0.00000	ppm	SV	1	
3	5.300	77529.7	30904.0	0.00000		S		
4	6.102	859521.7	393268.5	0.00000				m-xylene
5	7.073	705239.5	211180.4	0.00000	ppm		3	
6	7.333	735408.1	378435.5	0.00000	ppm	SV	3	
7	17.522	111527.6	19022.8	0.00000	ppm		7	

Ar_Br_54_A_RT_To



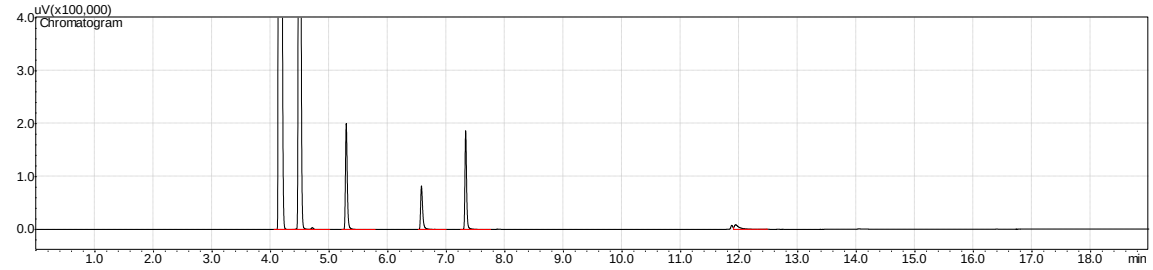
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.153	9063126.1	3996843.0	0.00000	ppm	SV	1	
2	4.476	22355698.7	10097663.1	0.00000	ppm		1	
3	6.575	830177.4	380211.2	0.00000	ppm	S	2	
4	7.336	779748.6	403588.9	0.00000	ppm	SV	3	

L2_Br_54_A_RT _24H:



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.153	13667509.2	5386430.1	0.00000	ppm	SV	1	
2	4.487	12740693.8	5741663.8	0.00000	ppm	SV	1	
3	5.292	436200.5	194541.2	0.00000		S		toluene
4	6.583	40123.3	28817.3	0.00000	ppm	SV	2	
5	7.333	898210.0	461482.4	0.00000	ppm	S	3	
6	11.908	1225416.1	332362.1	0.00000		SV		

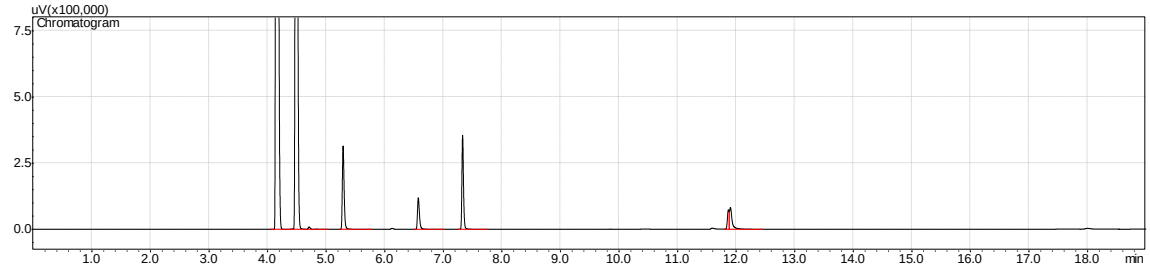
L3_ Ar_A_ Br _54_RT _ 24H:



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name

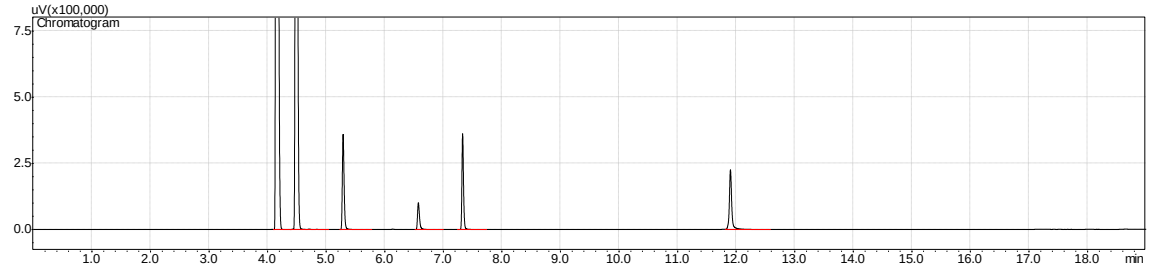
1	4.149	16485417.1	6247488.7	0.00000	ppm	V	1	
2	4.491	5907424.3	2737454.0	0.00000	ppm	SV	1	
3	5.291	435609.9	199137.3	0.00000		S		toluene
4	6.575	733558.9	81971.3	0.00000	ppm	SV	2	
5	7.330	368153.8	184953.0	0.00000	ppm		3	
6	11.940	56500.4	8952.3	0.00000		V		

CyJohnPhos_Ar_ Br _54_A_RT _24H:



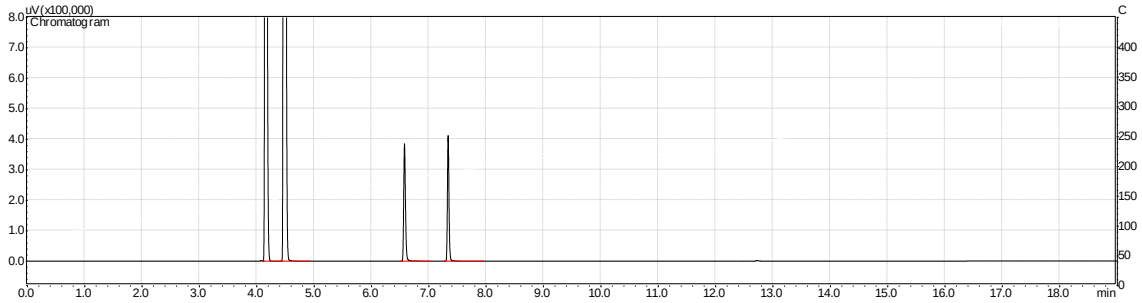
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.151	14252315.8	5572666.4	0.00000	ppm	SV	1	
2	4.486	11300227.9	5131135.8	0.00000	ppm	SV	1	
3	5.289	672469.5	310287.7	0.00000		S		toluene
4	6.572	583678.6	118713.7	0.00000	ppm	SV	2	
5	7.329	682146.6	352734.2	0.00000	ppm	S	3	
6	11.867	147518.7	73316.4	0.00000		V		
7	11.901	263828.0	82007.0	0.00000		V		

JohnPhos_Ar_ Br _54_A_RT _24H:



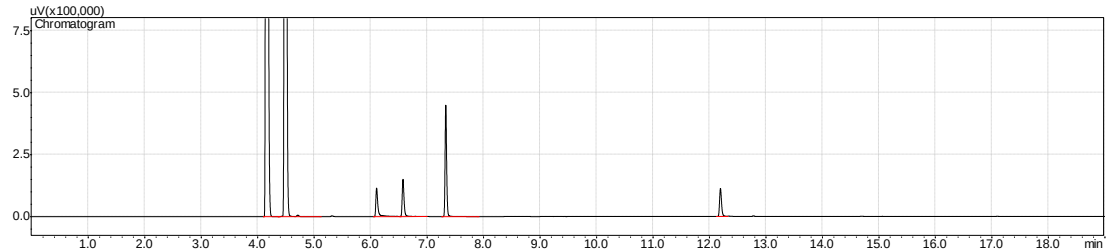
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.151	14003058.7	5503664.7	0.00000	ppm	SV	1	
2	4.486	11180184.2	5100033.7	0.00000	ppm	SV	1	
3	5.289	762891.8	353895.9	0.00000		S		toluene
4	6.573	272446.2	100983.8	0.00000	ppm	SV	2	
5	7.329	692669.2	359903.4	0.00000	ppm	S	3	
6	11.902	637822.4	224525.9	0.00000		V		

Ar_Br_54_B_RT_To



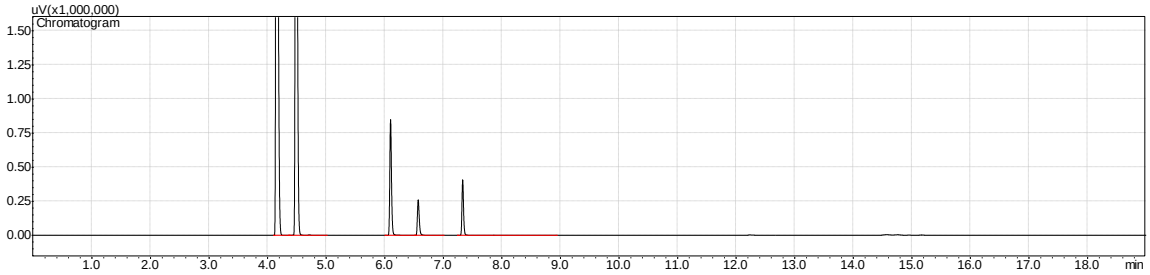
Peak #	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.153	9063126.1	3996843.0	0.00000	ppm	SV	1	
2	4.476	22355698.7	10097663.1	0.00000	ppm		1	
3	6.575	830177.4	380211.2	0.00000	ppm	S	2	
4	7.336	779748.6	403588.9	0.00000	ppm	SV	3	

L2_Br_54_B_RT _24H:



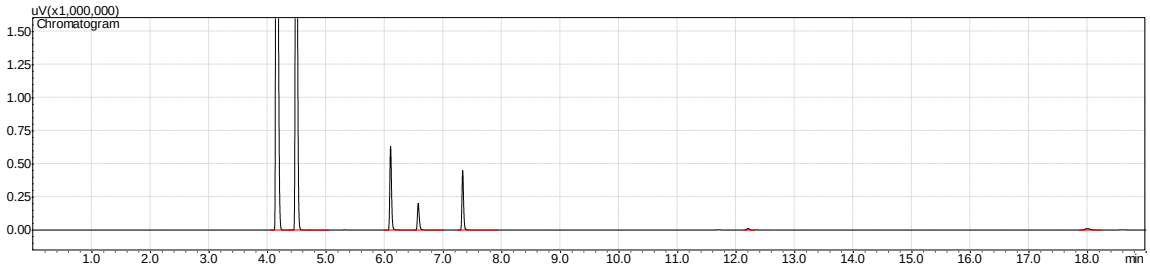
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.153	13247857.1	5236773.0	0.00000	ppm	V	1	
2	4.485	13994258.1	6246508.2	0.00000	ppm	SV	1	
3	6.105	322058.1	113767.6	0.00000		S		m-xylene
4	6.572	393746.2	148577.5	0.00000	ppm	SV	2	
5	7.330	851760.5	445937.9	0.00000	ppm	S	3	
6	12.194	275383.4	112804.4	0.00000				

L3_ Ar_ Br _54_B_RT _ 24H:



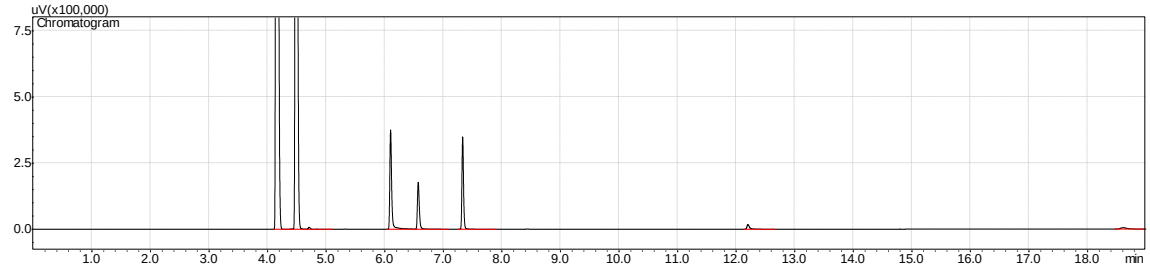
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.152	13185244.6	5240434.2	0.00000	ppm	V	1	
2	4.485	13293070.5	5994292.0	0.00000	ppm	SV	1	
3	6.099	1725657.7	843086.8	0.00000		S		m-xylene
4	6.571	574068.7	255825.7	0.00000	ppm	SV	2	
5	7.330	772288.6	403381.4	0.00000	ppm	S	3	

CyJohnPhos_Ar_ Br _54_B_RT _24H:



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.151	13922743.1	5474093.3	0.00000	ppm	V	1	
2	4.487	10849552.1	4944175.4	0.00000	ppm	SV	1	
3	6.099	1293522.6	628165.9	0.00000		S		
4	6.571	456514.9	198957.7	0.00000	ppm	SV	2	m-xylene
5	7.330	853609.2	445527.6	0.00000	ppm	S	3	
6	12.203	36544.5	12920.6	0.00000		V		
7	17.994	64095.2	10734.5	0.00000	ppm		7	

JohnPhos_Ar_ Br _54_B_RT _24H:

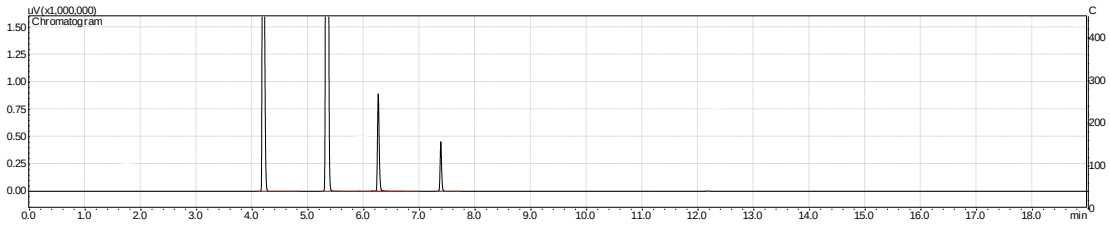


Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.151	13773870.0	5416126.1	0.00000	ppm	V	1	
2	4.485	11961240.9	5386185.1	0.00000	ppm	SV	1	
3	6.099	856620.7	372226.5	0.00000				
4	6.571	749365.4	174547.8	0.00000	ppm	SV	2	m-xylene
5	7.330	662937.6	345925.9	0.00000	ppm	S	3	
6	12.200	57175.1	17780.7	0.00000		S		
7	18.608	43820.9	5535.3	0.00000	ppm		8	

ArCl 100 °C

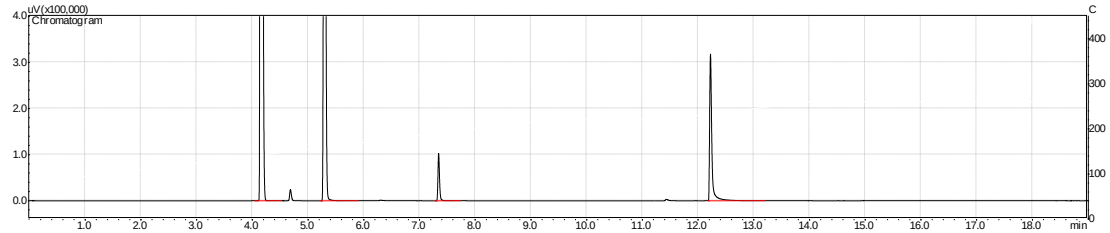
3-Phenyl-pyridine

Ar_Cl_26.1_100oC_3_pyridine_Tol_ To



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.191	11039719.4	4417633.9	0.00000	ppm	SV	1	DCM
2	5.336	38237661.7	16980543.7	0.00000		SV		Toluene
3	6.260	1928722.3	885425.8	0.00000		TV		3-chloropyridine
4	7.382	850484.3	446759.9	0.00000		S		*n*-decane IS

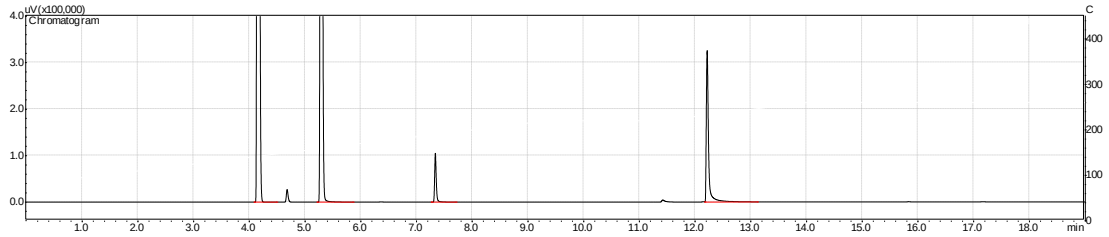
Ar_Cl_26.1_L1_100oC_12H:



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.154	11825670.8	4877005.1	0.00000	ppm	SV	1	

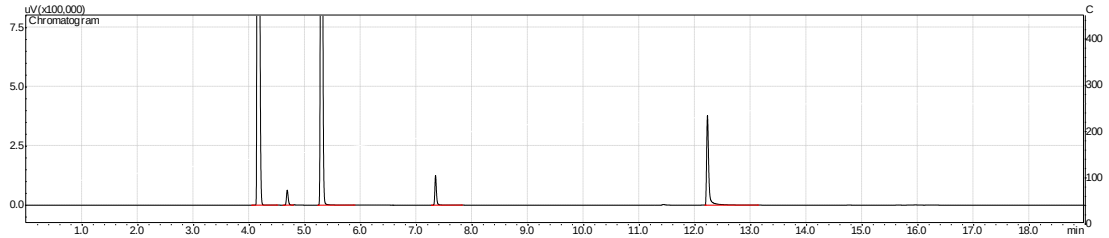
2	5.294	6634961.2	3259328.5	0.00000				
3	7.343	208339.8	102602.9	0.00000	ppm		3	
4	12.223	892932.2	314951.1	0.00000		V		

Ar_Cl_26.1_L3_100oC_12H:



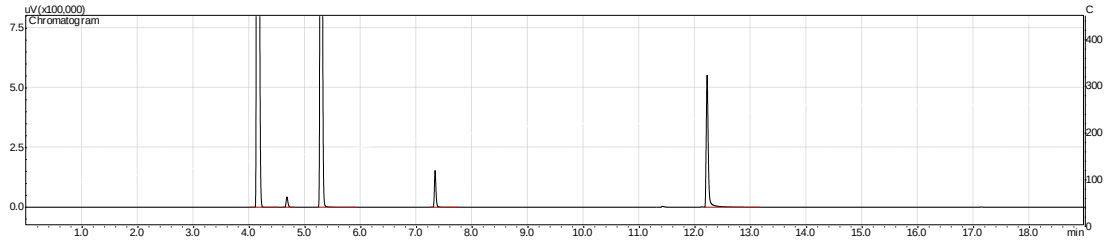
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.149	11689753.5	4809300.3	0.00000	ppm	SV	1	
2	5.289	9041540.2	4416504.7	0.00000				
3	7.338	211744.4	103893.6	0.00000	ppm	S	3	
4	12.217	916760.0	324363.4	0.00000		V		

Ar_Cl_26.1_L2_100oC_12H:



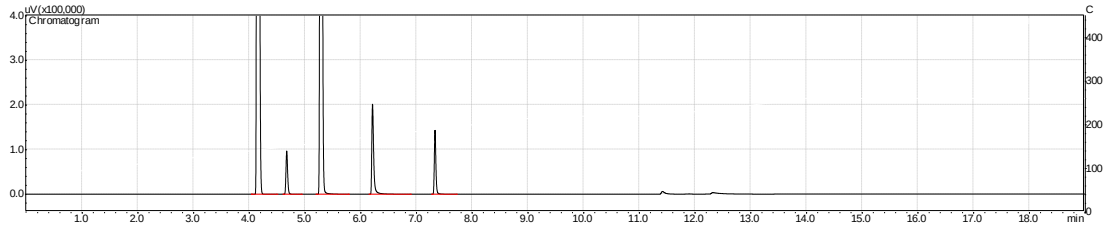
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.153	11767746.5	4829202.9	0.00000	ppm	SV	1	
2	4.680	138934.4	63249.4	0.00000				
3	5.293	9732018.2	4709539.7	0.00000				
4	7.342	250095.5	123484.1	0.00000	ppm	S	3	
5	12.222	1033532.8	374804.8	0.00000		V		

Ar_Cl_26.1_CyJohnPhos_100oC_12H:



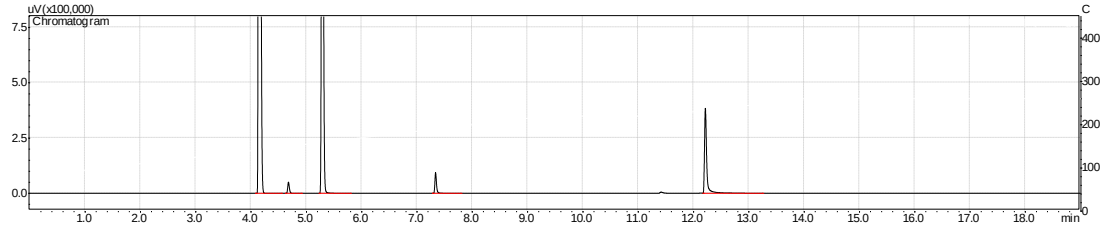
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.143	15362394.2	5981098.1	0.00000	ppm	SV	1	
2	4.674	99815.7	43646.7	0.00000				
3	5.286	12508931.5	6078581.6	0.00000				
4	7.334	304680.9	153513.5	0.00000	ppm	S	3	
5	12.216	1445744.0	549515.7	0.00000		V		

Ar_Cl_26.1_PPh3_100oC_12H:



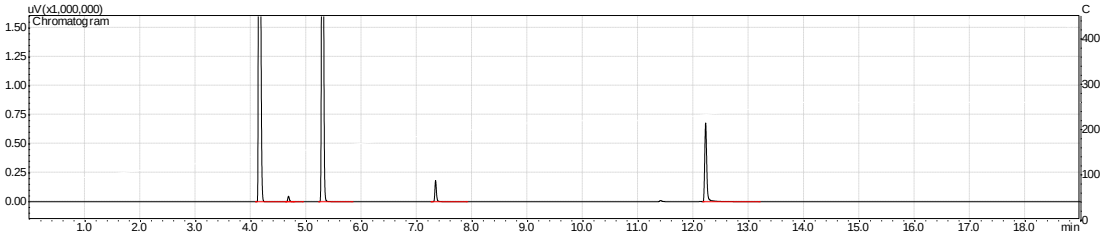
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.146	11546439.0	4750217.9	0.00000	ppm	SV	1	
2	4.671	204939.8	96523.8	0.00000				
3	5.284	10501716.5	5120604.0	0.00000				
4	6.211	480596.6	200817.0	0.00000		V		
5	7.332	279433.6	140085.9	0.00000	ppm	S	3	

Ar_Cl_26.1_JohnPhos_100oC_12H:



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.144	13721179.4	5613706.3	0.00000	ppm	SV	1	
2	4.676	107447.1	50976.2	0.00000				
3	5.288	8191981.9	4061934.9	0.00000				
4	7.336	194154.6	92147.3	0.00000	ppm	V	3	
5	12.214	1072533.9	379162.1	0.00000		SV		

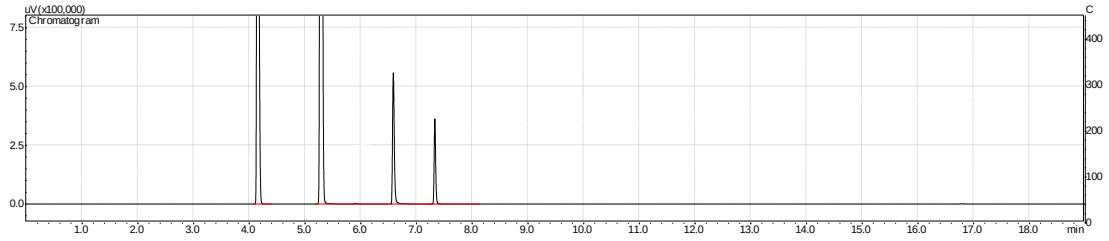
Ar_Cl_26.1_SPhos_100oC_12H:



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.146	13014778.6	5403624.3	0.00000	ppm	SV	1	
2	4.676	101049.0	47627.1	0.00000		T		
3	5.290	12950760.8	6379061.7	0.00000		S		
4	7.336	370822.0	181037.4	0.00000	ppm	SV	3	
5	12.219	1800012.8	671415.5	0.00000		SV		

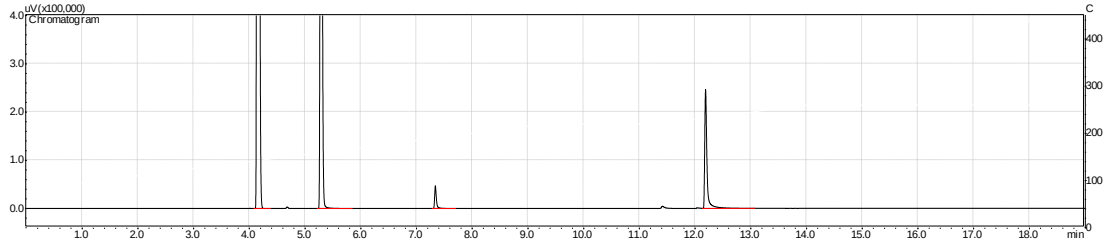
2-Phenyl-pyridine

Ar_Cl_30.1_100oC_2_pyridine_Tol_ To



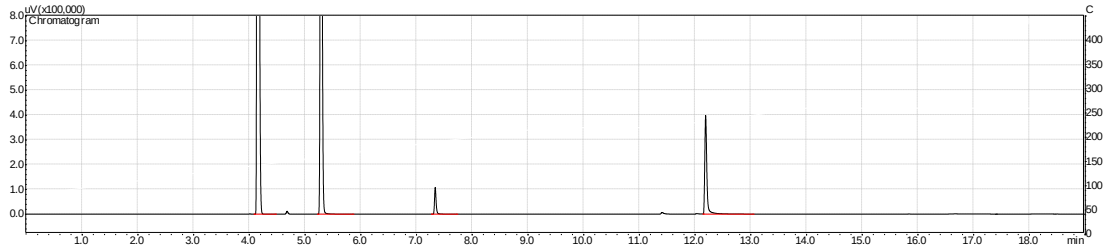
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.147	8990469.1	3848185.9	0.00000	ppm	V	1	DCM
2	5.284	26343487.9	12270770.1	0.00000		SV		Toluene
3	6.584	1240265.4	554547.3	0.00000	ppm		2	2-chloropyridine
4	7.329	679307.9	358683.8	0.00000	ppm	SV	3	*n*-decane

Ar_Cl_30.1_L1_100oC_12H:



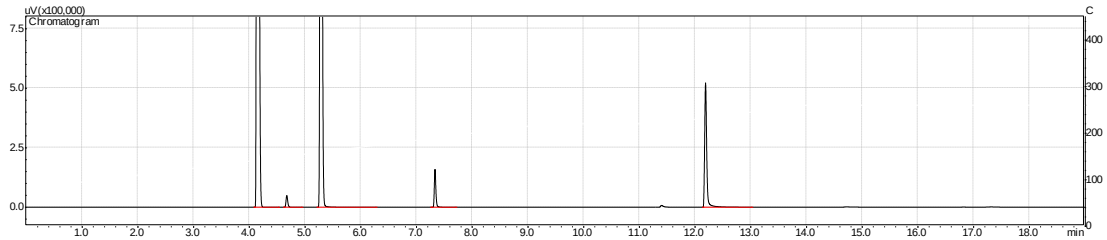
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.147	12348438.2	5068966.4	0.00000	ppm	V	1	
2	5.287	5380124.7	2650662.2	0.00000				
3	7.338	103085.8	46277.2	0.00000	ppm		3	
4	12.188	695124.3	245505.6	0.00000		SV		

Ar_Cl_30.1_L3_100oC_12H:



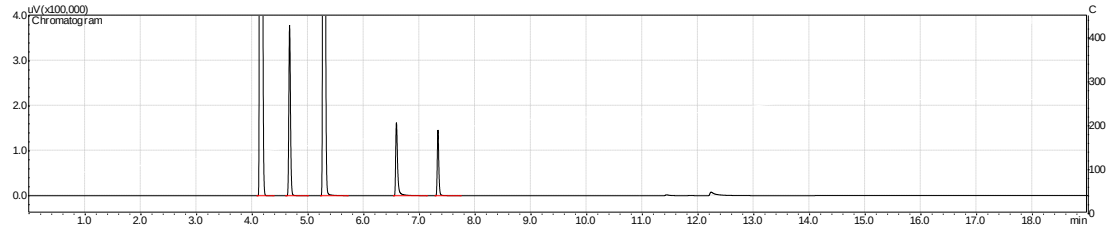
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.148	11753908.3	4853412.5	0.00000	ppm	SV	1	
2	5.287	7547741.3	3707106.6	0.00000				
3	7.336	219597.6	107392.8	0.00000	ppm		3	
4	12.189	1053791.7	395283.1	0.00000		V		

Ar_Cl_30.1_L2_100oC_12H:



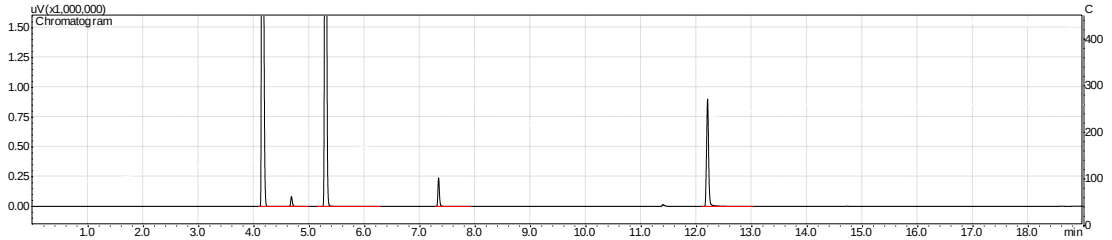
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.141	15400379.9	5953124.5	0.00000	ppm	SV	1	
2	4.672	108384.1	48873.2	0.00000		S		
3	5.285	13953794.4	6719422.4	0.00000		S		
4	7.332	310025.5	155300.2	0.00000	ppm	S	3	
5	12.188	1349421.9	520222.2	0.00000		V		

Ar_Cl_30.1_JohnPhos_100oC_12H:



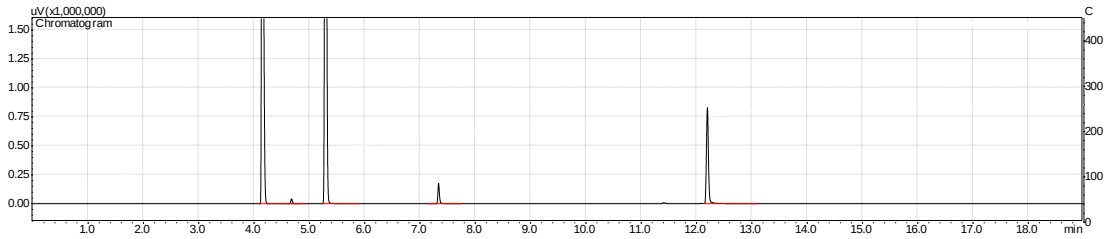
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.145	11677076.5	4786424.0	0.00000	ppm	V	1	
2	4.668	782494.2	374761.9	0.00000				
3	5.283	9839776.2	4765660.0	0.00000				
4	6.586	402537.3	160203.4	0.00000	ppm		2	
5	7.331	280776.8	143752.8	0.00000	ppm	S	3	

Ar_Cl_30.1_SPhos_100oC_12H:



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.147	12695457.9	5303325.7	0.00000	ppm	SV	1	
2	4.676	171727.7	83206.0	0.00000		T		
3	5.290	15025541.6	7372664.0	0.00000		S		
4	7.336	466129.2	238517.2	0.00000	ppm	SV	3	
5	12.199	2374982.6	892680.6	0.00000		S		

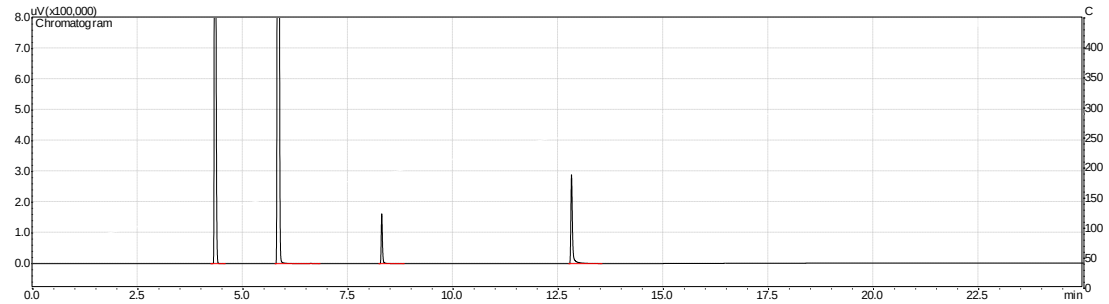
Ar_Cl_30.1_CyJohnPhos_100oC_12H:



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.148	12191598.5	5144028.0	0.00000	ppm	SV	1	
2	4.677	88780.0	41740.8	0.00000		T		
3	5.291	16970853.4	8262172.9	0.00000				
4	7.335	346384.4	173891.8	0.00000	ppm		3	
5	12.196	2152950.3	824073.6	0.00000		SV		

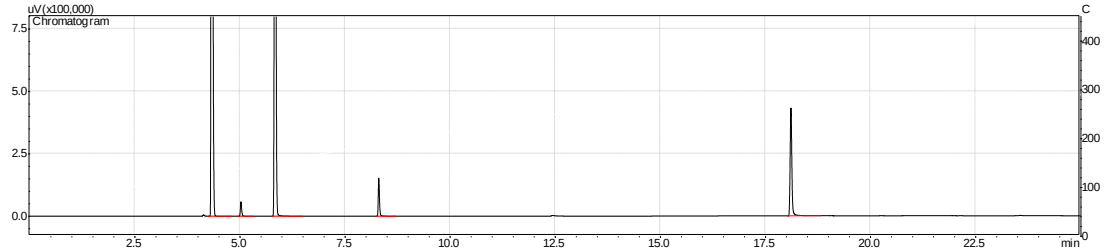
2-Phenyl-quinoline

Ar_Cl_48_100oC_ Chloroquinoline_To



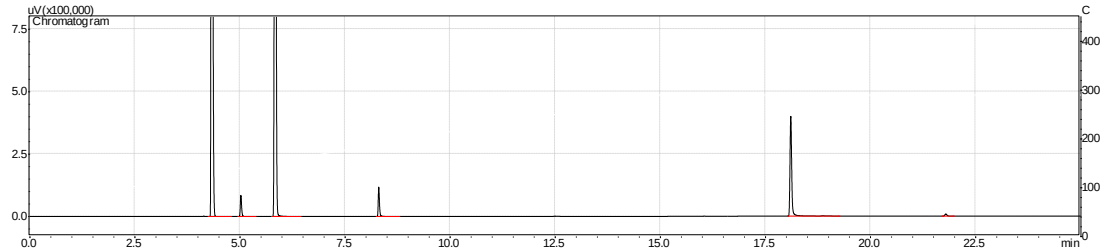
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.332	6240701.7	2776323.1	0.00000		V		DCM
2	5.836	16052460.8	7254581.6	0.00000	ppm	S	2	Toluene
3	8.300	336755.7	161675.0	0.00000				*n*-decane
4	12.815	796669.5	285790.0	0.00000				2-chloroquinoline

L1_Cl_48_100oC _12H:



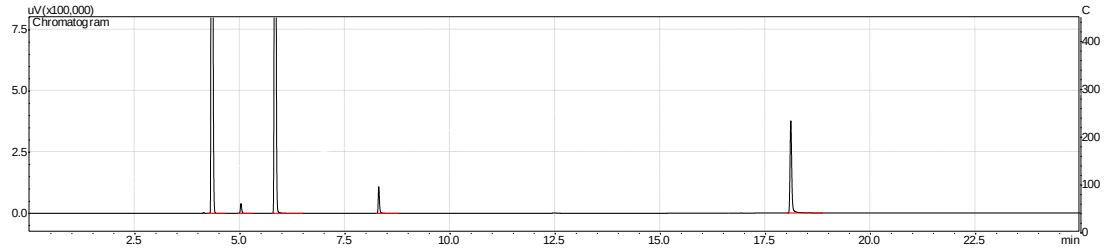
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.324	10453473.0	4311027.9	0.00000		SV		
2	5.022	124399.9	56044.8	0.00000				
3	5.833	9506672.2	4466531.1	0.00000	ppm		2	
4	8.301	311108.9	151723.5	0.00000		S		
5	18.106	1231473.2	428887.2	0.00000	ppm		13	

L3_ Ar_Cl_48_100oC_ 12H:



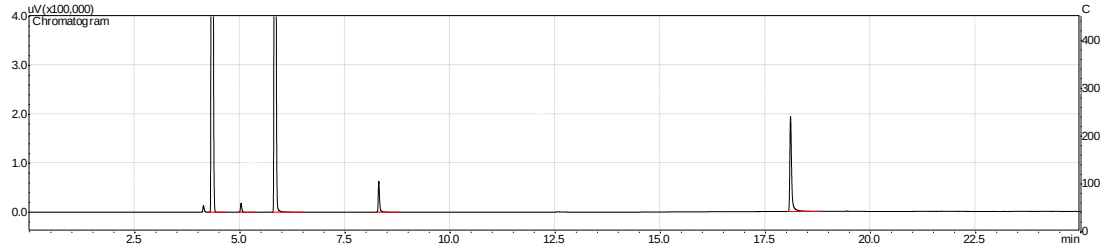
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.324	9892997.2	4123602.5	0.00000		SV		
2	5.021	183266.0	84103.1	0.00000				
3	5.834	12470171.8	5721271.8	0.00000	ppm		2	
4	8.300	247564.4	117355.5	0.00000				
5	18.102	1148064.8	395164.0	0.00000	ppm	S	13	
6	21.792	29678.9	8926.6	0.00000	ppm		14	

L2 Ar_Cl_48_100oC _12H:



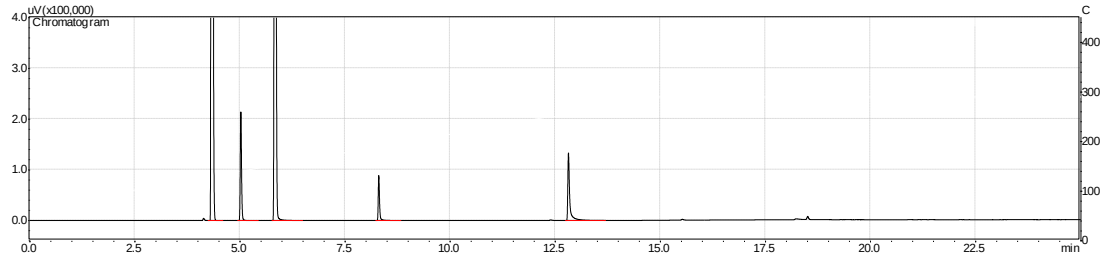
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.325	9582109.5	4023679.0	0.00000		V		
2	5.022	89052.6	39496.1	0.00000				
3	5.833	10843873.2	5029210.7	0.00000	ppm	S	2	
4	8.301	231285.8	108766.0	0.00000				
5	18.103	1086977.9	374332.5	0.00000	ppm		13	

CyJohnPhos_Cl_48_100oC _12H:



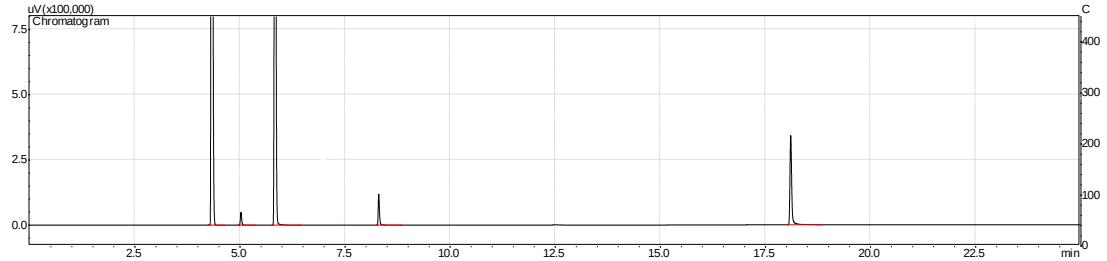
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.328	8019770.6	3456640.8	0.00000		V		
2	5.025	43474.7	18582.6	0.00000		S		
3	5.831	7316237.5	3473794.8	0.00000	ppm		2	
4	8.301	143183.7	63221.2	0.00000				
5	18.097	592033.7	192817.8	0.00000	ppm		13	

JohnPhos_Cl_48_100oC _12H:



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.324	10248078.1	4248594.6	0.00000		V		
2	5.019	450736.2	213042.1	0.00000		S		
3	5.832	9440277.0	4447060.6	0.00000	ppm		2	
4	8.301	194120.1	88047.2	0.00000				
5	12.813	429556.8	132759.8	0.00000		S		

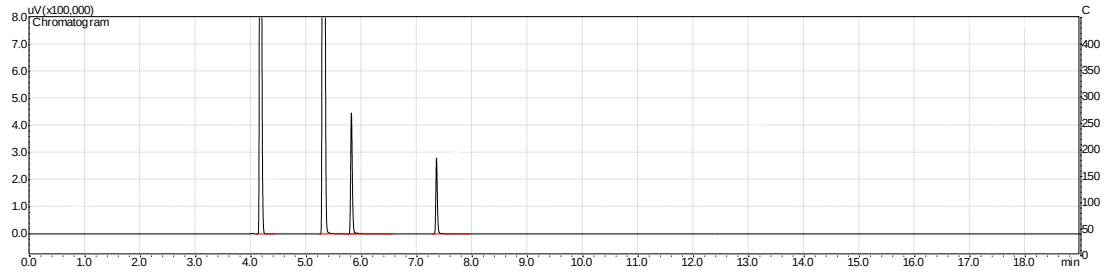
SPhos_Cl_48_100oC _12H:



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.324	10419027.8	4288777.7	0.00000		V		
2	5.022	107581.5	47532.4	0.00000		S		
3	5.832	9696839.6	4554054.5	0.00000	ppm		2	
4	8.300	252609.1	118389.7	0.00000				
5	18.101	994516.0	339292.5	0.00000	ppm		13	

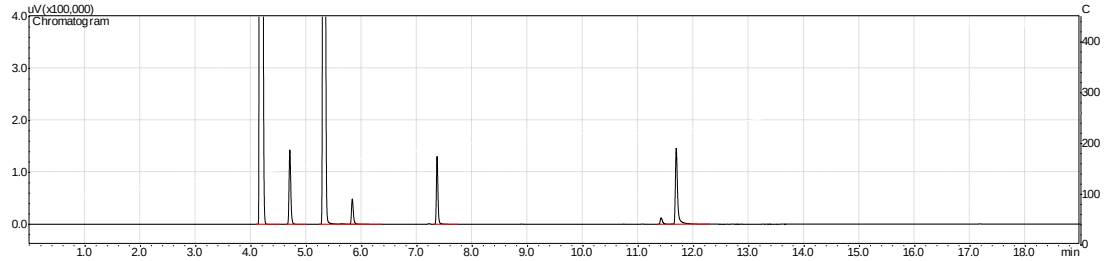
2-Phenyl-thiophene

Ar_Cl_49_100oC_To



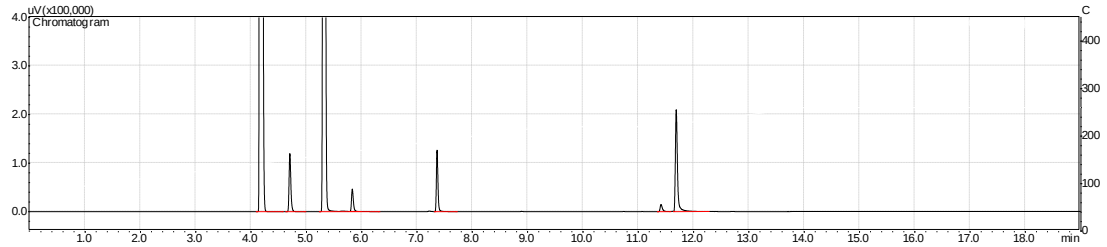
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.166	7172632.1	3288232.5	0.00000	ppm	V	1	DCM
2	5.308	23182824.3	10939671.4	0.00000		S		Toluene
3	5.813	933589.9	444096.0	0.00000		T		2-chlorothiophene
4	7.352	541549.4	278700.3	0.00000		S		n-decane (IS)

L1_Cl_49_100oC _12H:



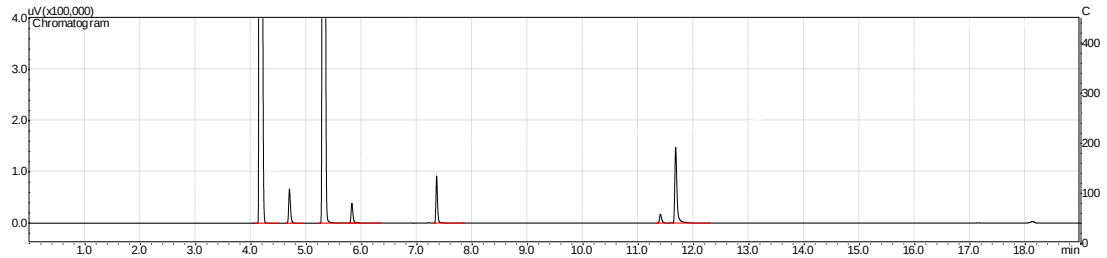
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.166	18252199.5	6860769.7	0.00000	ppm	SV	1	
2	4.701	311900.5	141314.5	0.00000				
3	5.315	11839791.3	5692233.7	0.00000		S		
4	5.829	112210.4	47744.0	0.00000		T		
5	7.363	257089.3	130008.3	0.00000		SV		
6	11.414	37397.8	12423.1	0.00000		S		
7	11.687	413945.7	144619.2	0.00000		V		

L3_ Ar_Cl_49_100oC_ 12H:



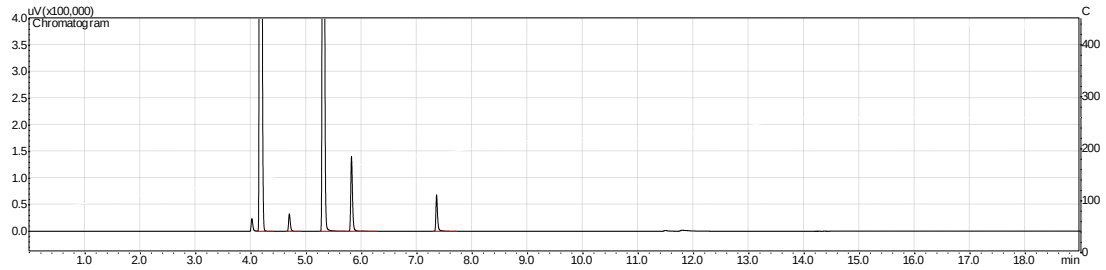
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.167	17696207.0	6696974.2	0.00000	ppm	SV	1	
2	4.701	265710.2	118526.6	0.00000				
3	5.316	14153727.5	6727654.4	0.00000		S		
4	5.830	106647.4	45492.3	0.00000		TV		
5	7.362	250540.5	125804.2	0.00000		SV		
6	11.412	42062.0	14418.3	0.00000				
7	11.687	562891.8	207140.2	0.00000		V		

L2 Ar_Cl_49_100oC _12H:



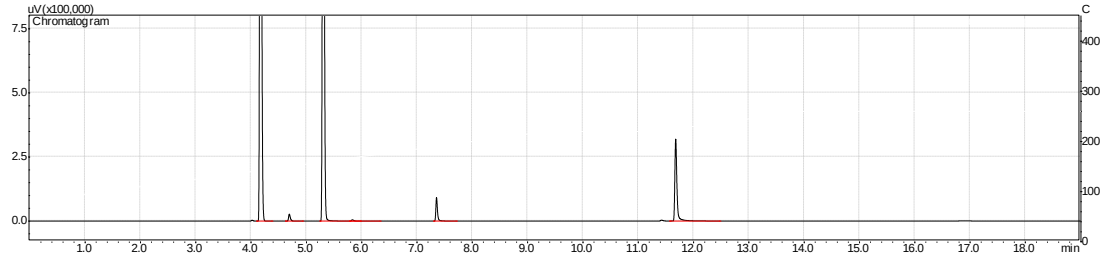
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.161	16332761.3	6296376.8	0.00000	ppm	SV	1	DCM
2	4.694	153810.2	67036.8	0.00000				
3	5.309	22151461.5	10451673.2	0.00000		S		
4	5.822	89627.8	38481.3	0.00000		T		
5	7.355	190891.7	91422.0	0.00000		V		
6	11.400	51012.2	17870.0	0.00000				
7	11.676	417983.7	147217.9	0.00000		V		

PPh3_Ar_Cl_49_100oC _12H:



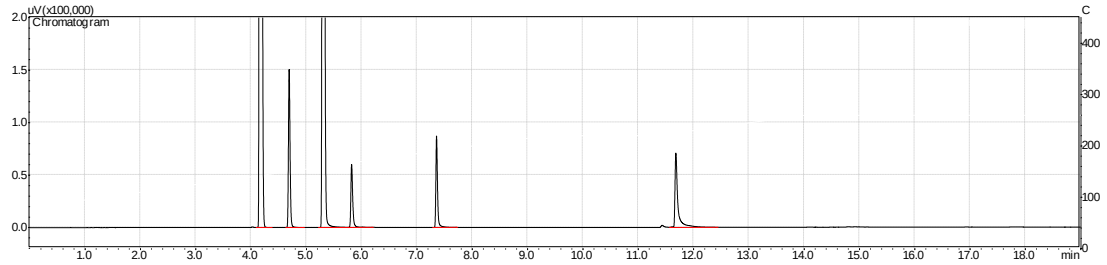
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.165	9027123.7	3989634.0	0.00000	ppm	V	1	
2	4.692	71452.4	32492.3	0.00000				
3	5.304	6249984.7	3121762.0	0.00000				
4	5.815	312888.8	137915.7	0.00000		SV		
5	7.354	146539.7	68207.9	0.00000				

CyJohnPhos_Cl_49_100oC _12H:



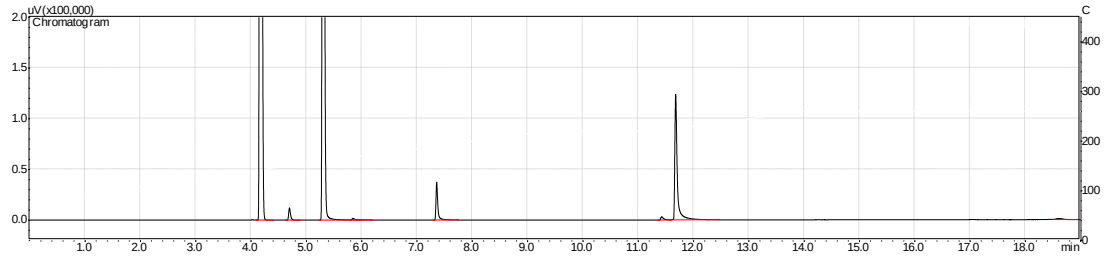
Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.167	7267696.3	3300123.9	0.00000	ppm	V	1	DCM
2	4.691	62490.7	27018.1	0.00000				
3	5.303	7662202.6	3806112.5	0.00000		S		
4	5.831	14399.8	5220.0	0.00000		T		
5	7.353	191201.6	91342.3	0.00000				
6	11.677	858927.6	315988.8	0.00000		SV		

JohnPhos_Cl_49_100oC _12H:



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.165	8707477.1	3861784.2	0.00000	ppm	V	1	
2	4.688	307077.6	149805.8	0.00000				
3	5.303	6556199.8	3265192.0	0.00000				
4	5.818	141885.6	59761.9	0.00000		SV		
5	7.353	182073.6	86597.6	0.00000				
6	11.680	257016.5	70531.5	0.00000		V		

SPhos_Cl_49_100oC _12H:



Peak#	Ret.Time	Area	Height	Conc.	Units	Mark	Compound ID#	Compound Name
1	4.167	7712414.9	3491763.0	0.00000	ppm	V	1	
2	4.693	28371.2	12128.8	0.00000				
3	5.303	4560092.4	2263536.8	0.00000		S		
4	5.843	4861.9	1581.6	0.00000		T		
5	7.355	87587.6	36735.0	0.00000				
6	11.424	11466.0	3111.5	0.00000				
7	11.677	386888.3	122571.6	0.00000		V		

8	18.605	10172.6	1160.6	0.00000	ppm	SV	8	

General formular for GC calculations

$$Conversion = \frac{Area\ (Aryl\ halide\ initial) - Area\ (Aryl\ halide\ final)}{Area\ (Aryl\ halide\ initial)} \times 100\ \%$$

$$Selectivity = \frac{Area\ (Desired\ product)}{Area\ (Sum\ of\ products)} \times 100\ \%$$

$$GC\ yield = \left[\frac{Conversion}{100}\right] \times \left[\frac{Selectivity}{100}\right] \times 100\ \%$$

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