SUPPLEMENTARY MATERIAL

Syntheses and study of a pyrroline nitroxide condensed phospholene oxide and a pyrroline nitroxide attached diphenylphosphine

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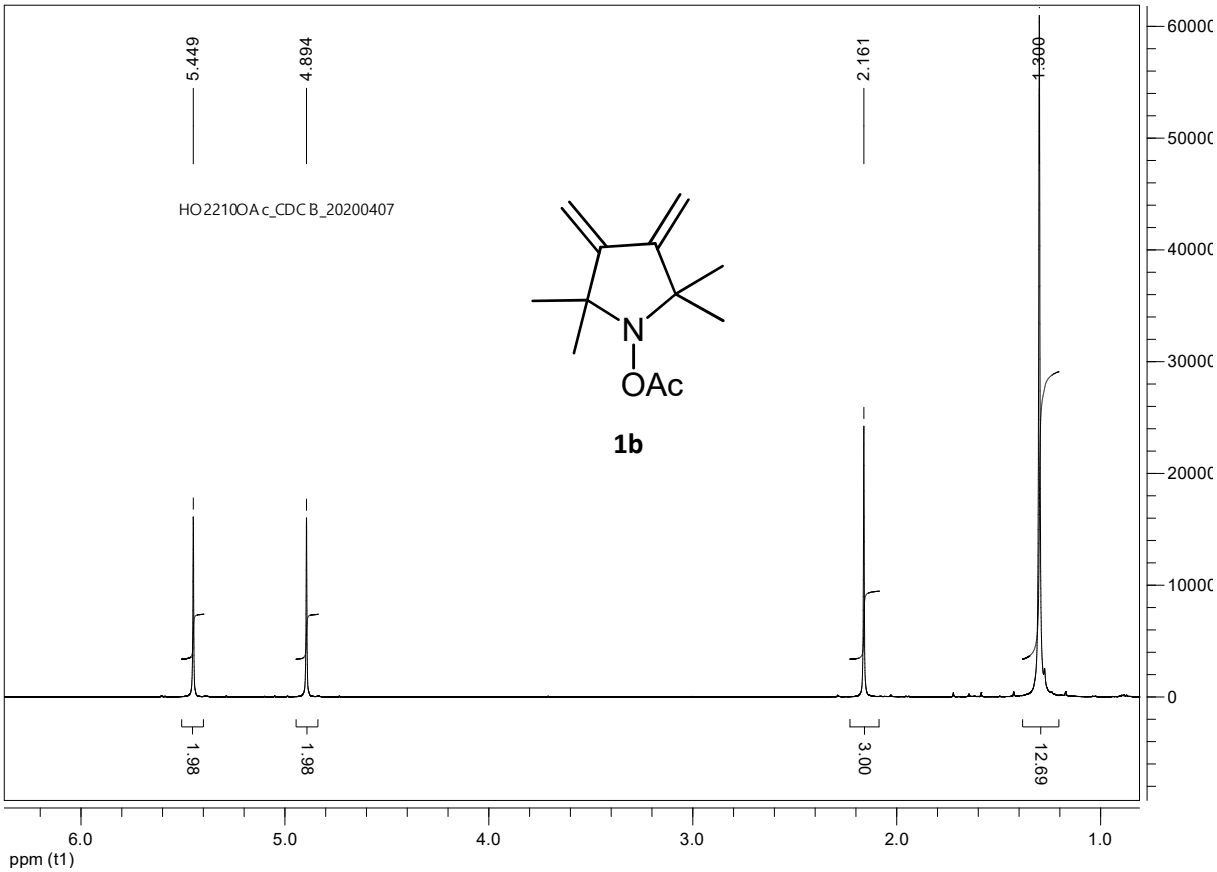
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1.300
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N
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1b
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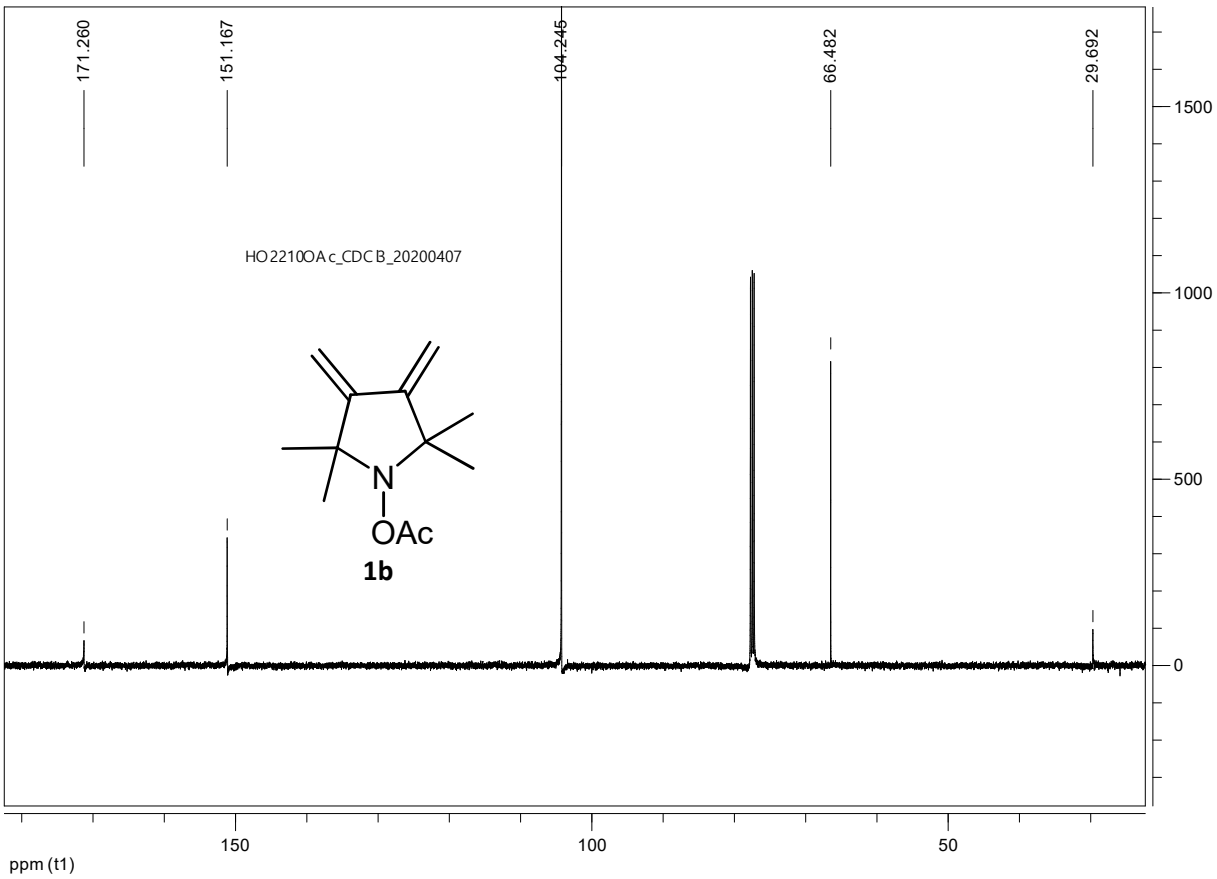
3.00
12.69
6.0
5.0
4.0
3.0
2.0
1.0
ppm (t1)


171.260
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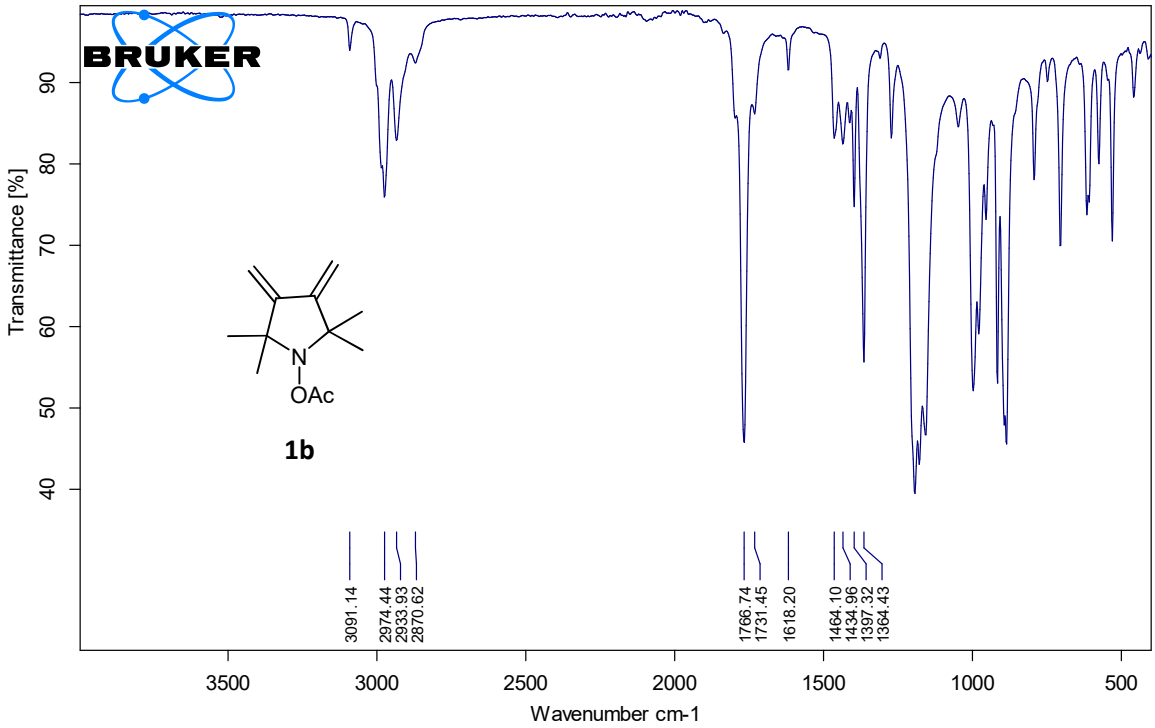
104.245
66.482
29.692
HO2210OAc_CDCB_20200407
N
OAc
1b
150
100
50
ppm (t1)



C:\OPUS_7.2.139.1294\Measure\ATR_Di\HO-2210-OAc.0	HO-2210-OAc	Instrument type and / or accessory	2021.04.01

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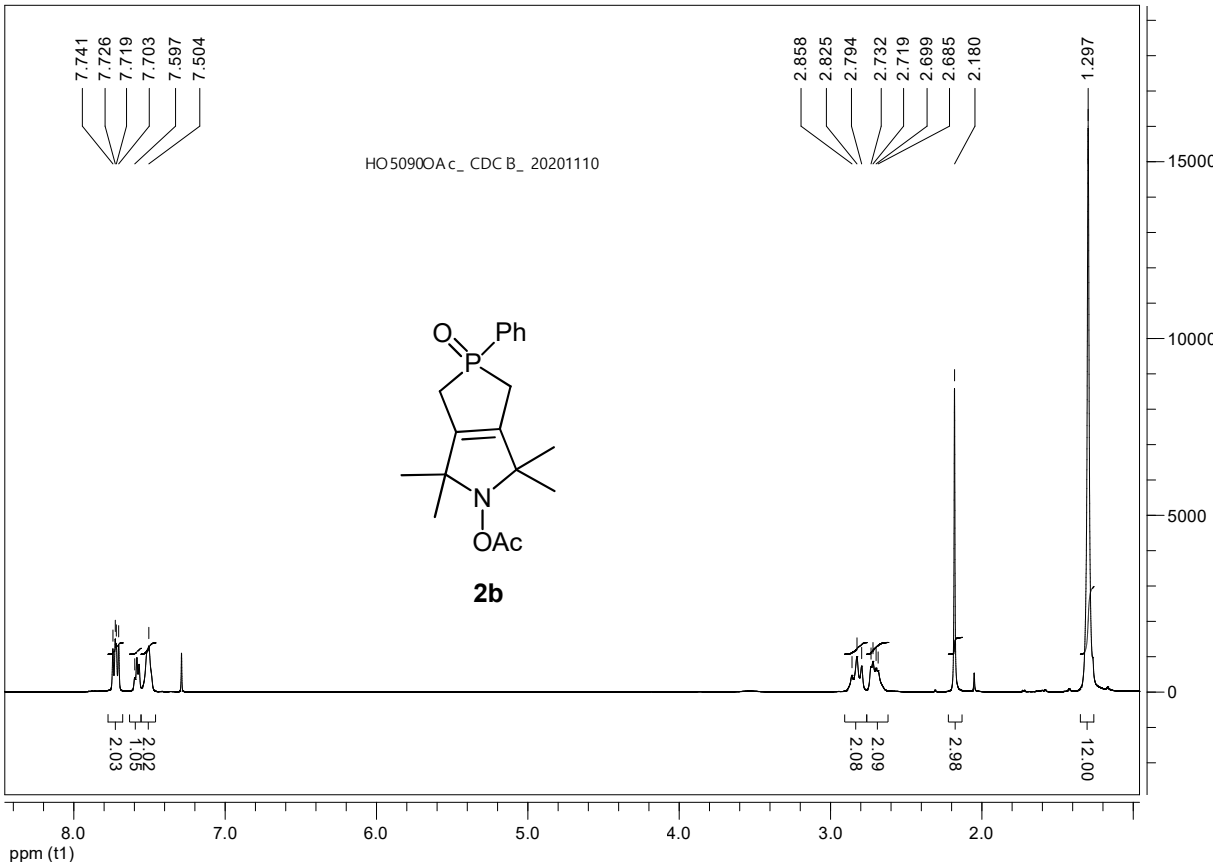
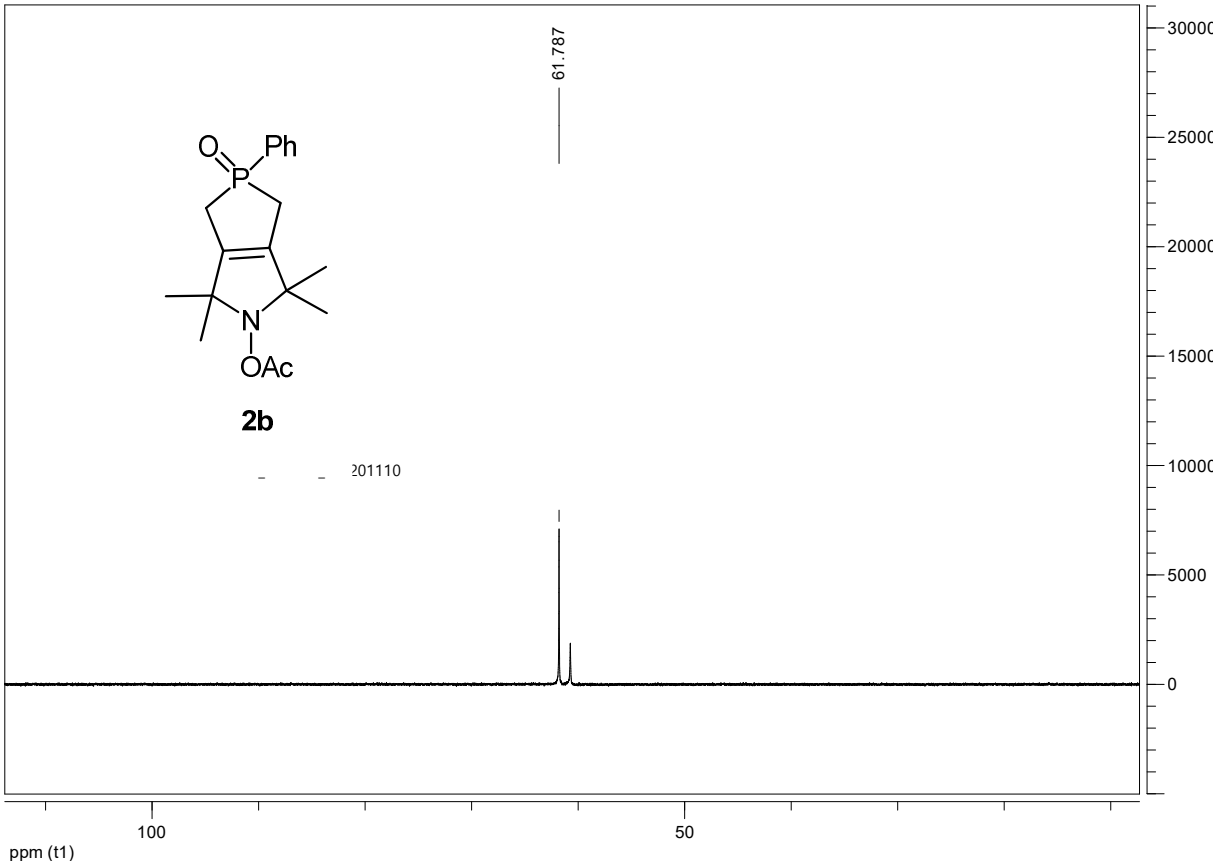
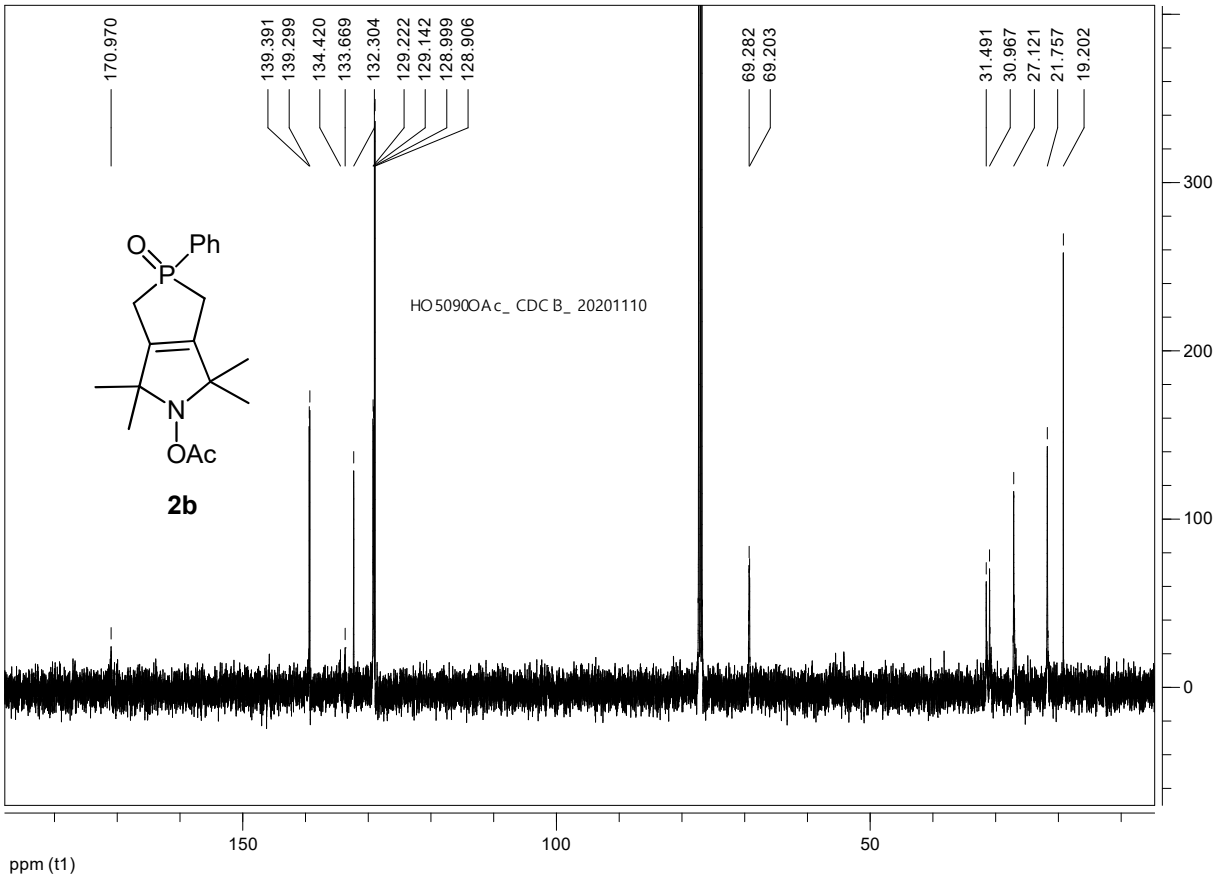
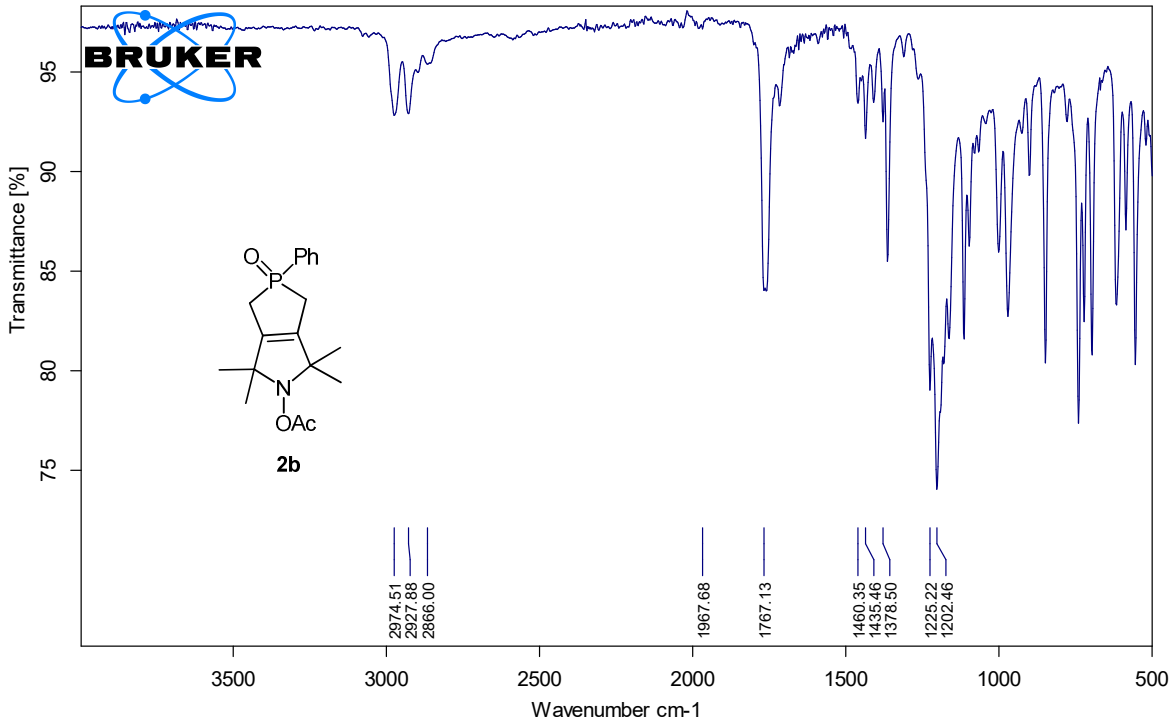

7.741
7.726
7.719
7.703
7.597
7.504
2.858
2.825
2.794
2.732
2.719
2.699
2.685
2.180
1.297
HO5090OAc_ CDC B_ 20201110
O
Ph
P
N
OAc
2b
2.03
1.05
2.02
2.08
2.09
2.98
12.00
15000
10000
5000
0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
ppm (t1)


61.787
O
Ph
P
N
OAc
2b
201110
30000
25000
20000
15000
10000
5000
0
100
50
ppm (t1)





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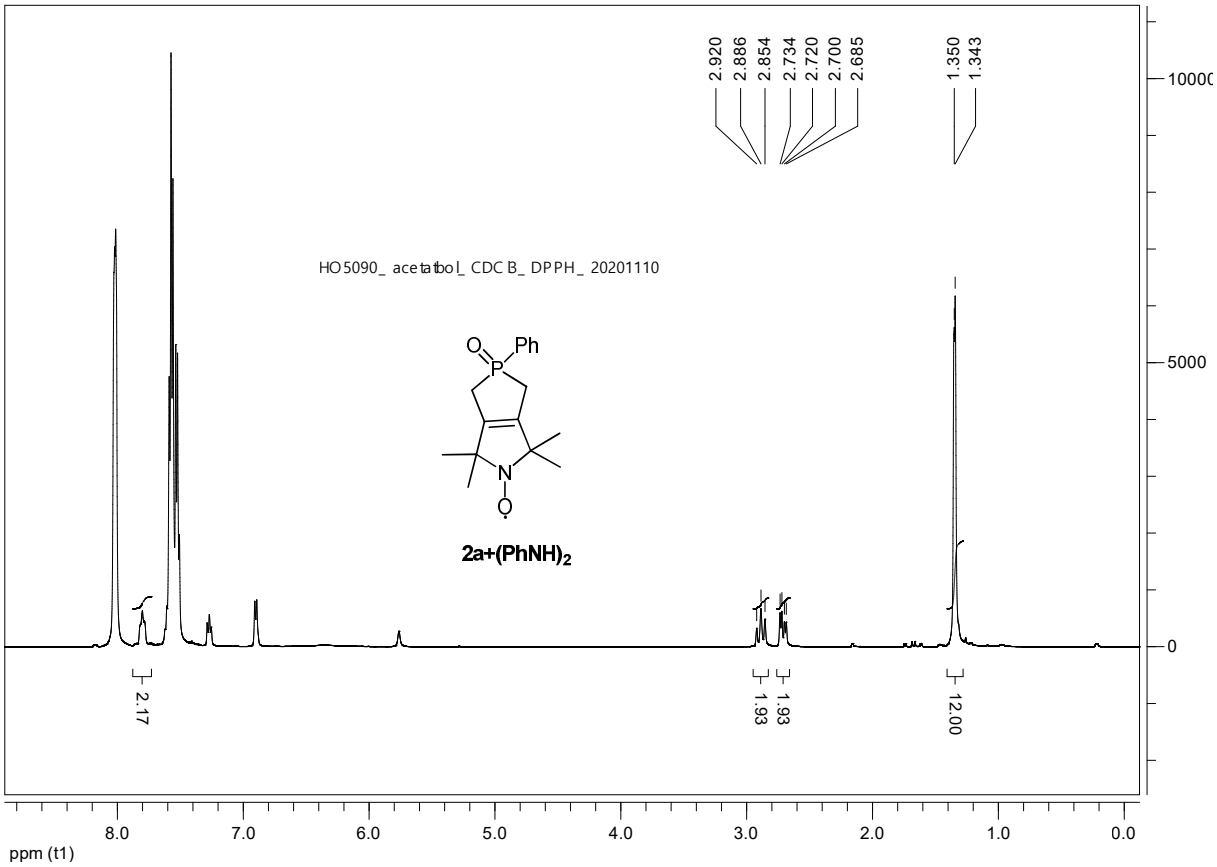
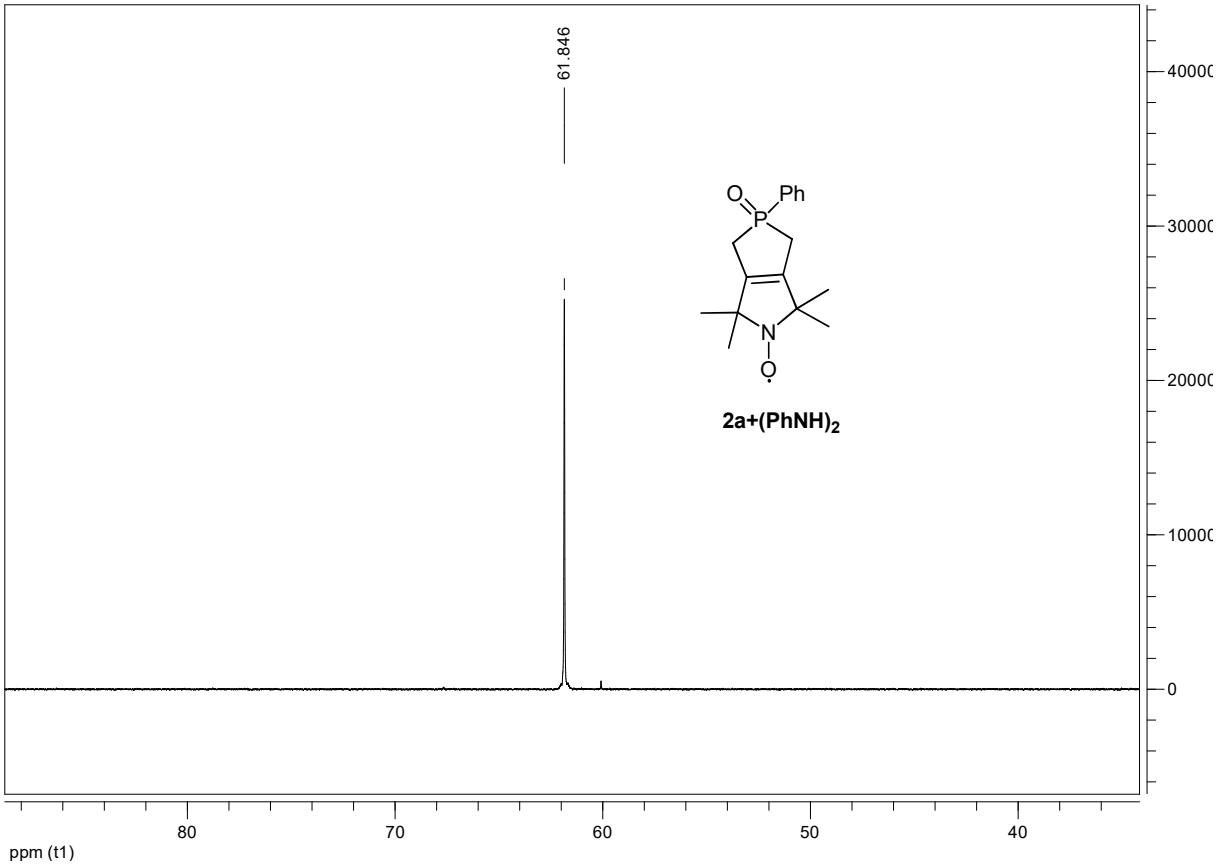
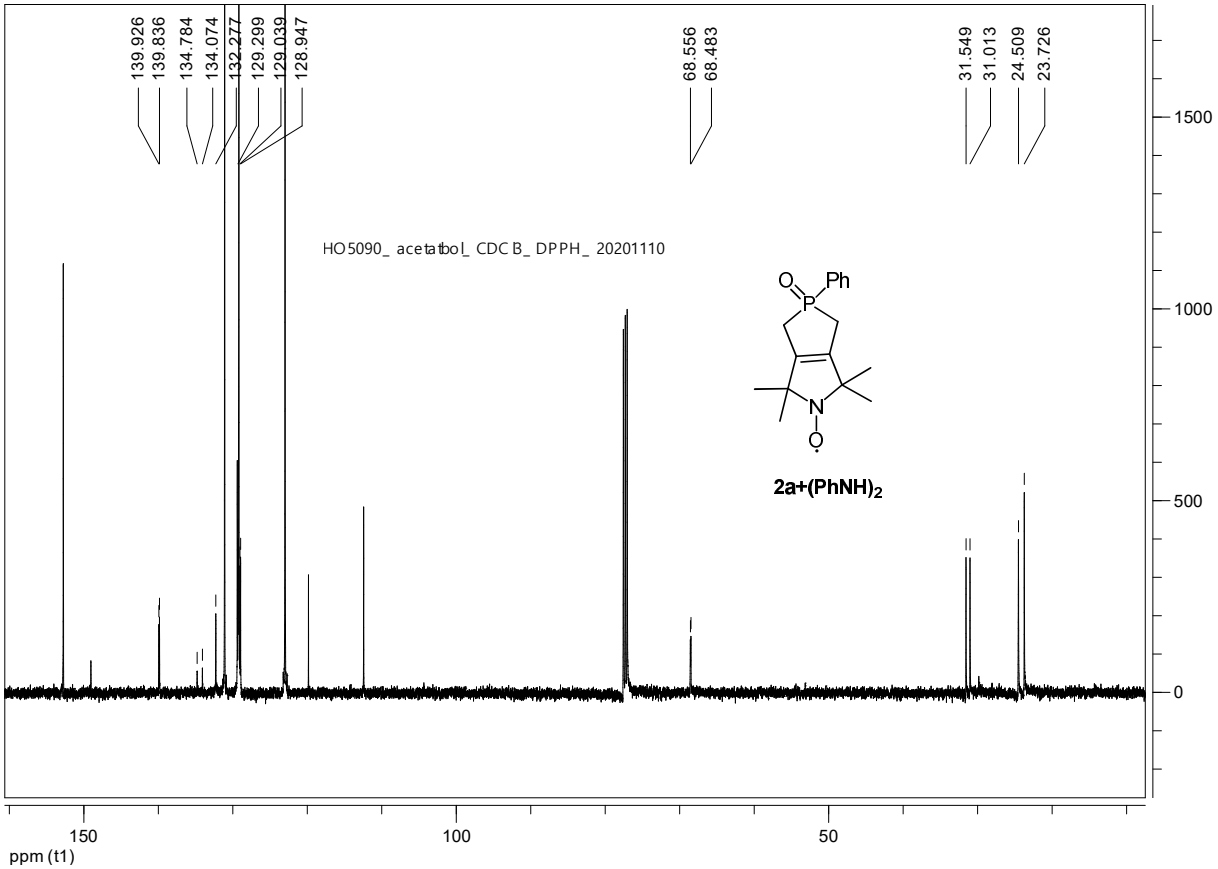
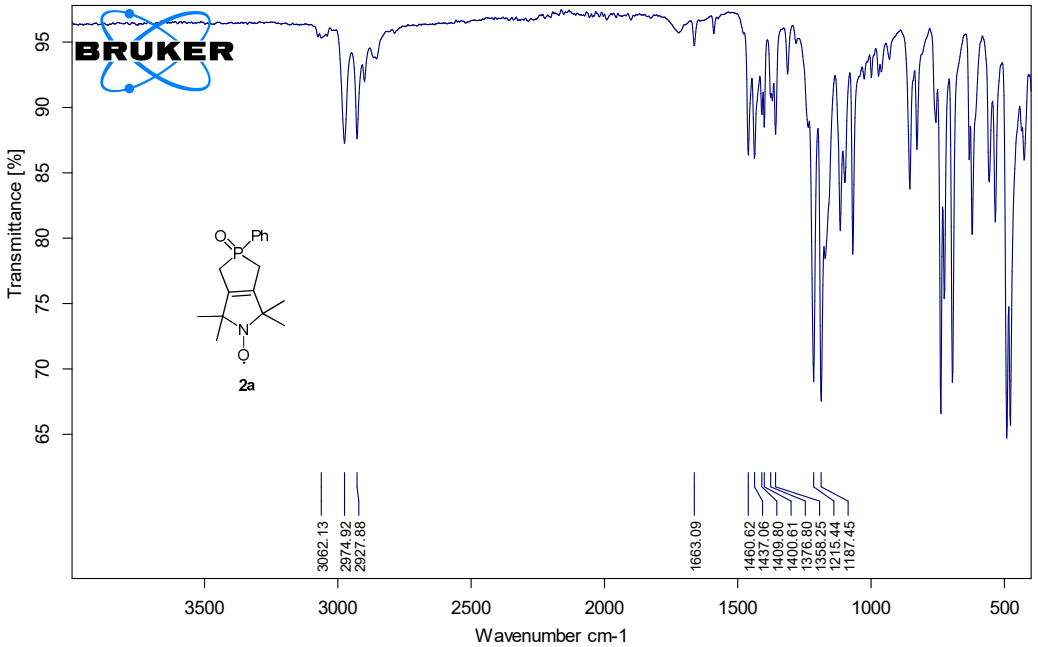

2.920
2.886
2.854
2.734
2.720
2.700
2.685
1.350
1.343
HO5090_ acetatbol_ CDCB_ DPPH_ 20201110
O
Ph
P
N
O
2a+(PhNH)2
2.17
1.93
1.93
12.00
10000
5000
0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)


61.846
O
Ph
P
N
O
2a+(PhNH)2
40000
30000
20000
10000
0
80
70
60
50
40
ppm (t1)





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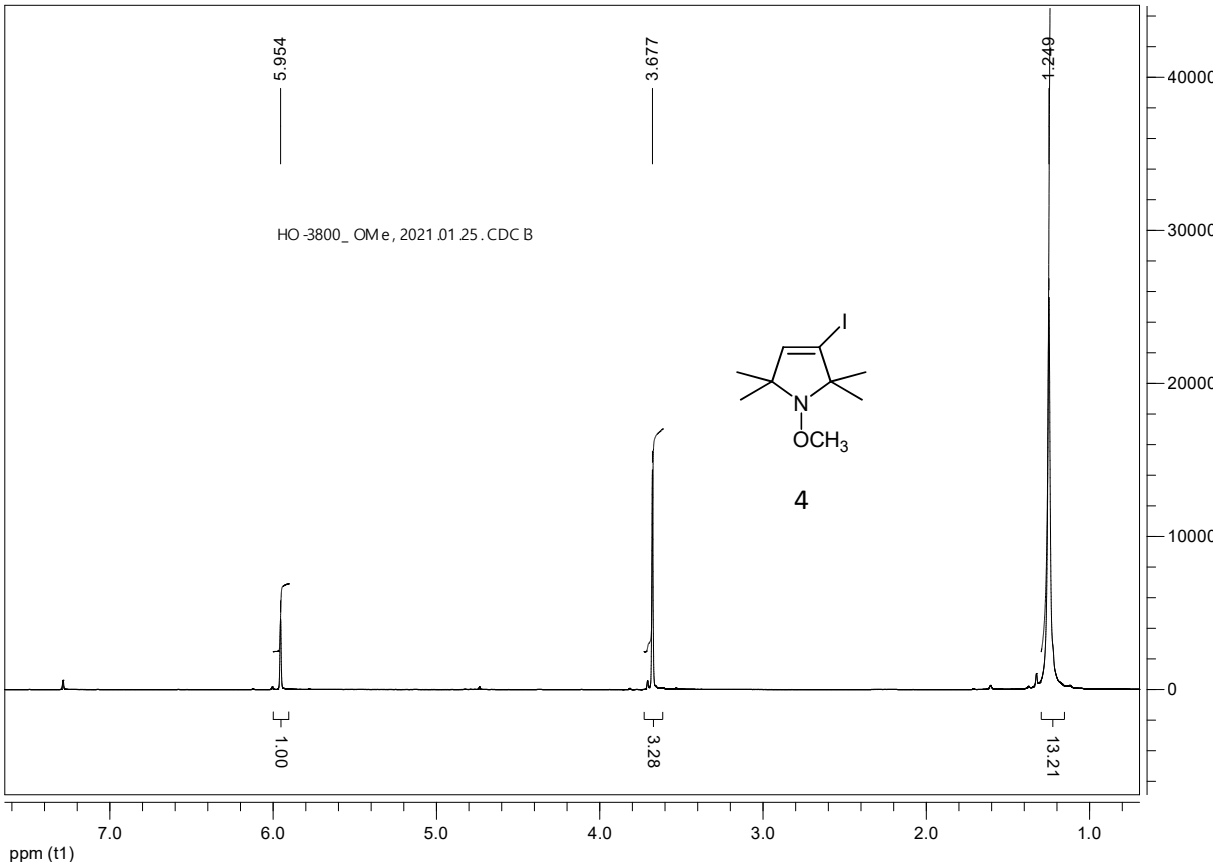
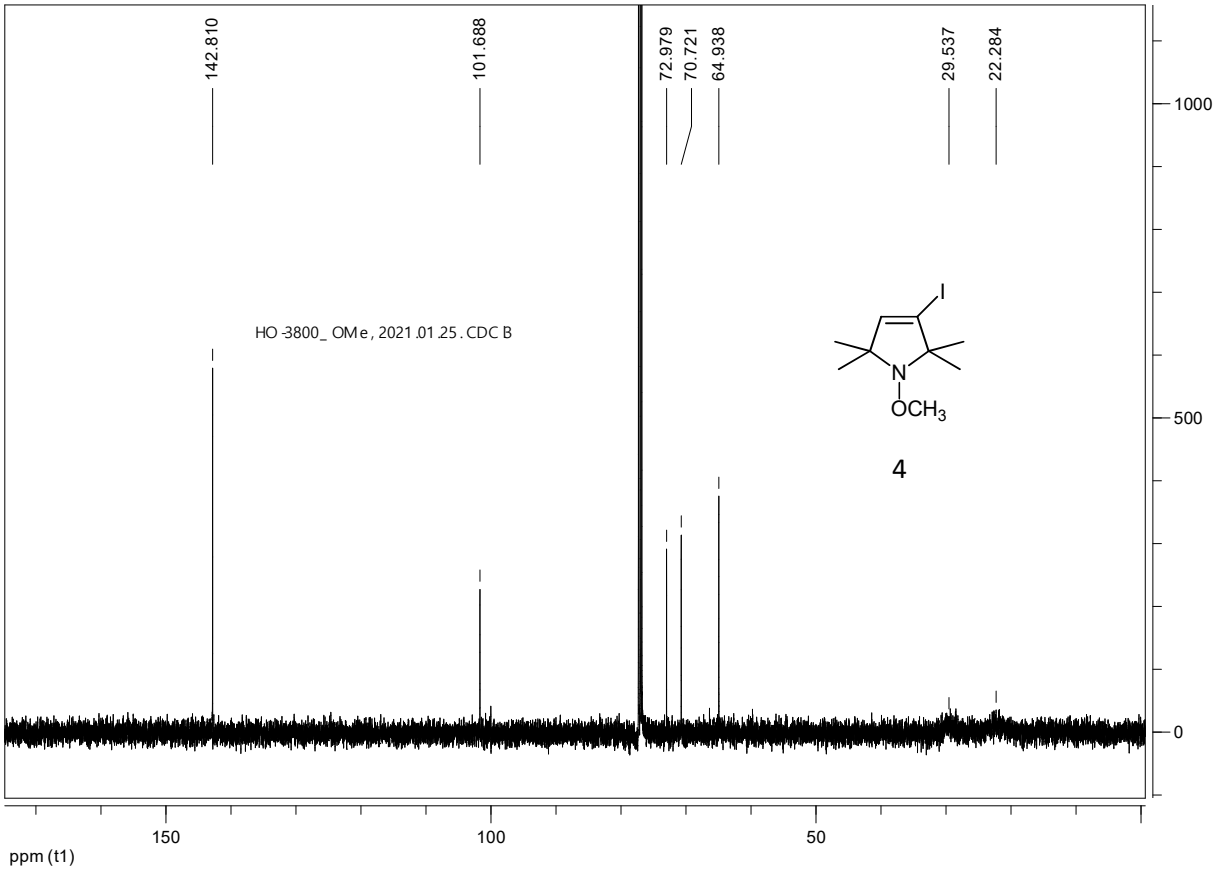
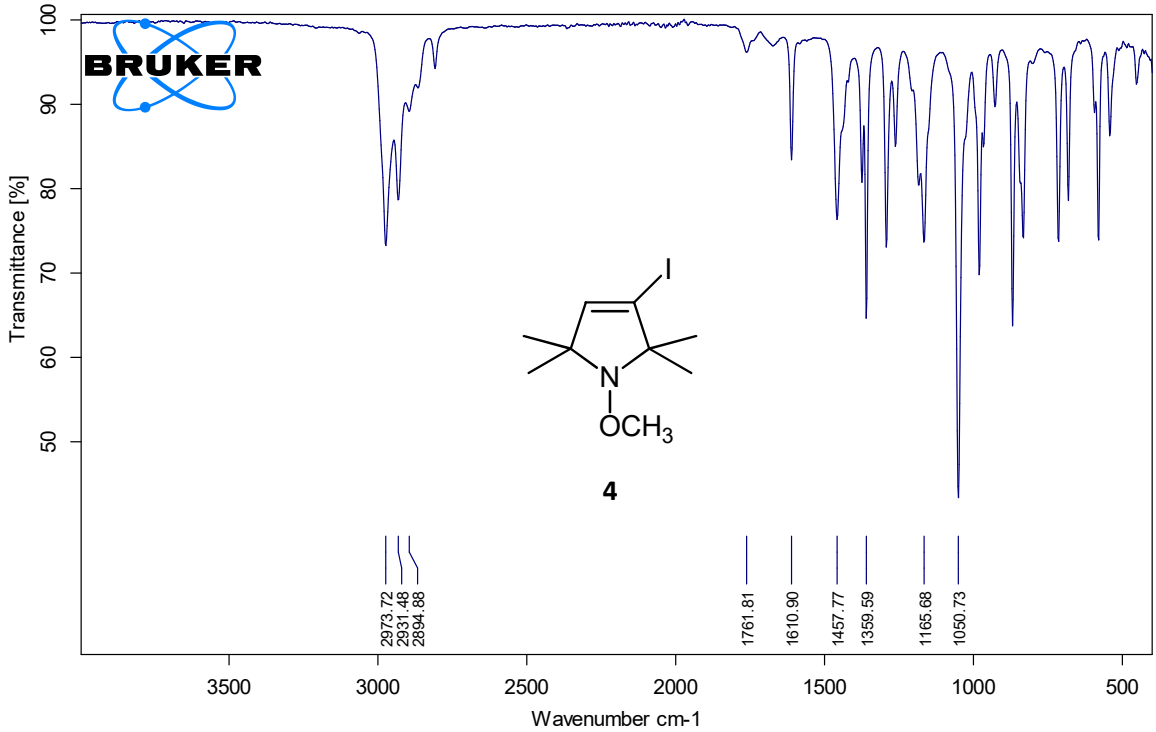

5.954
3.677
1.249
HO-3800_OMe, 2021.01.25. CDC B
I
N
OCH3
4
1.00
3.28
13.21
ppm (t1)


142.810
101.688
72.979
70.721
64.938
29.537
22.284
HO-3800_OMe, 2021.01.25. CDC B
I
N
OCH3
4
ppm (t1)



C:\OPUS_7.2.139.1294\Measure\ATR_Di\HO-3800-OMe.0	HO-3800-OMe	Instrument type and / or accessory	2021.03.26

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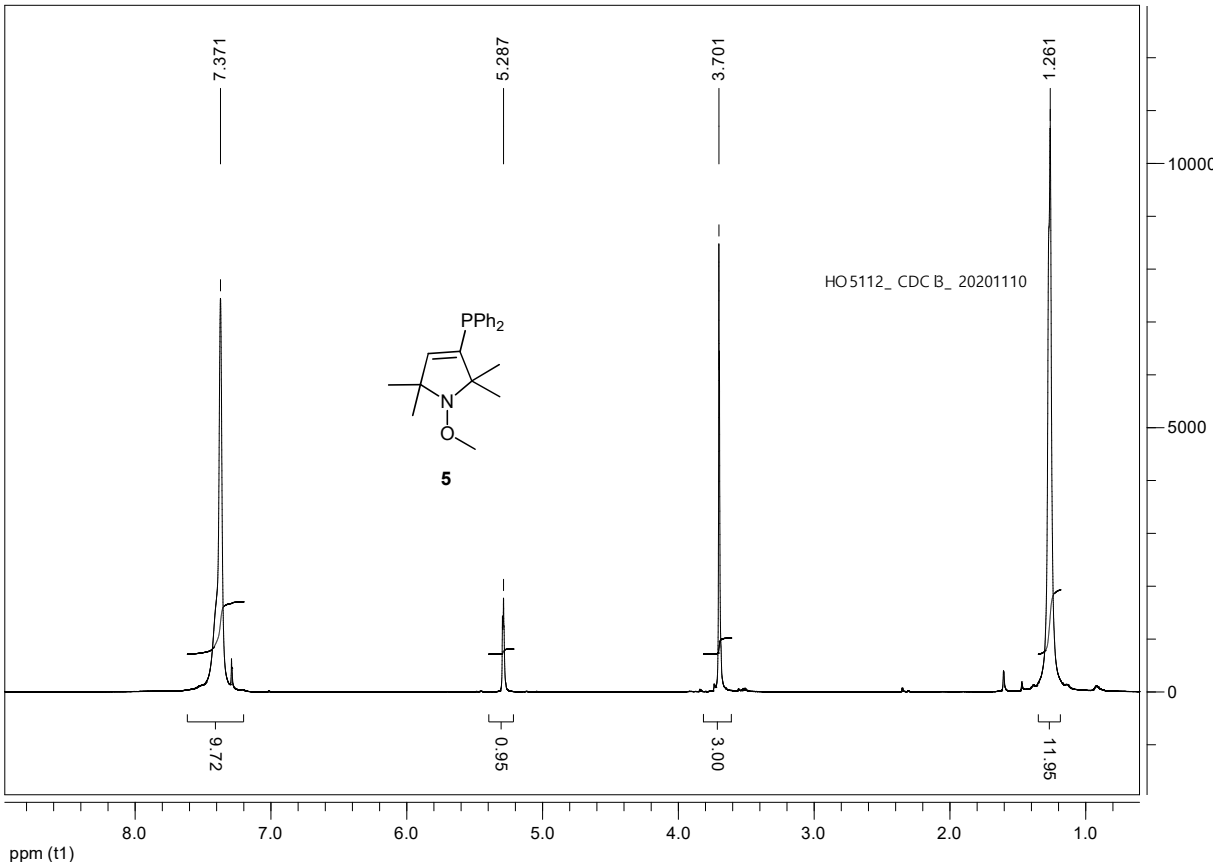
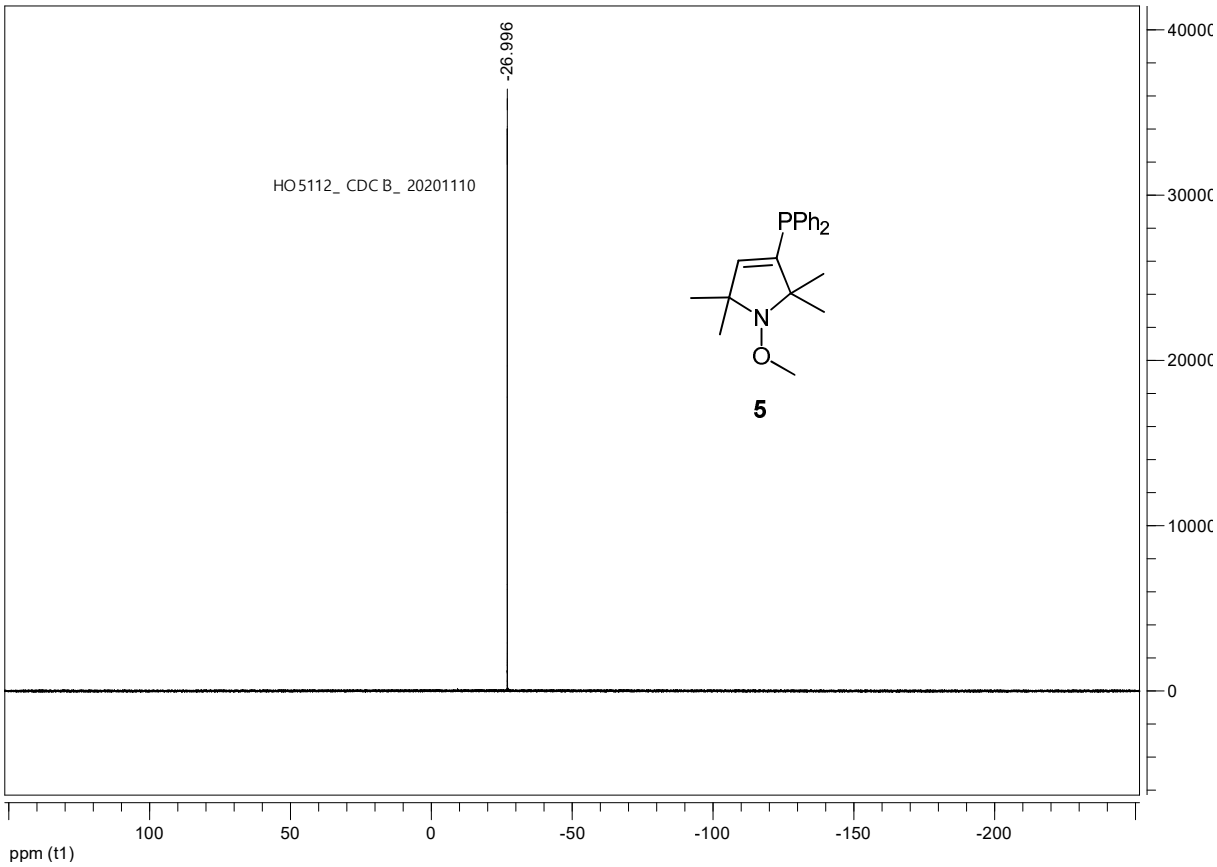
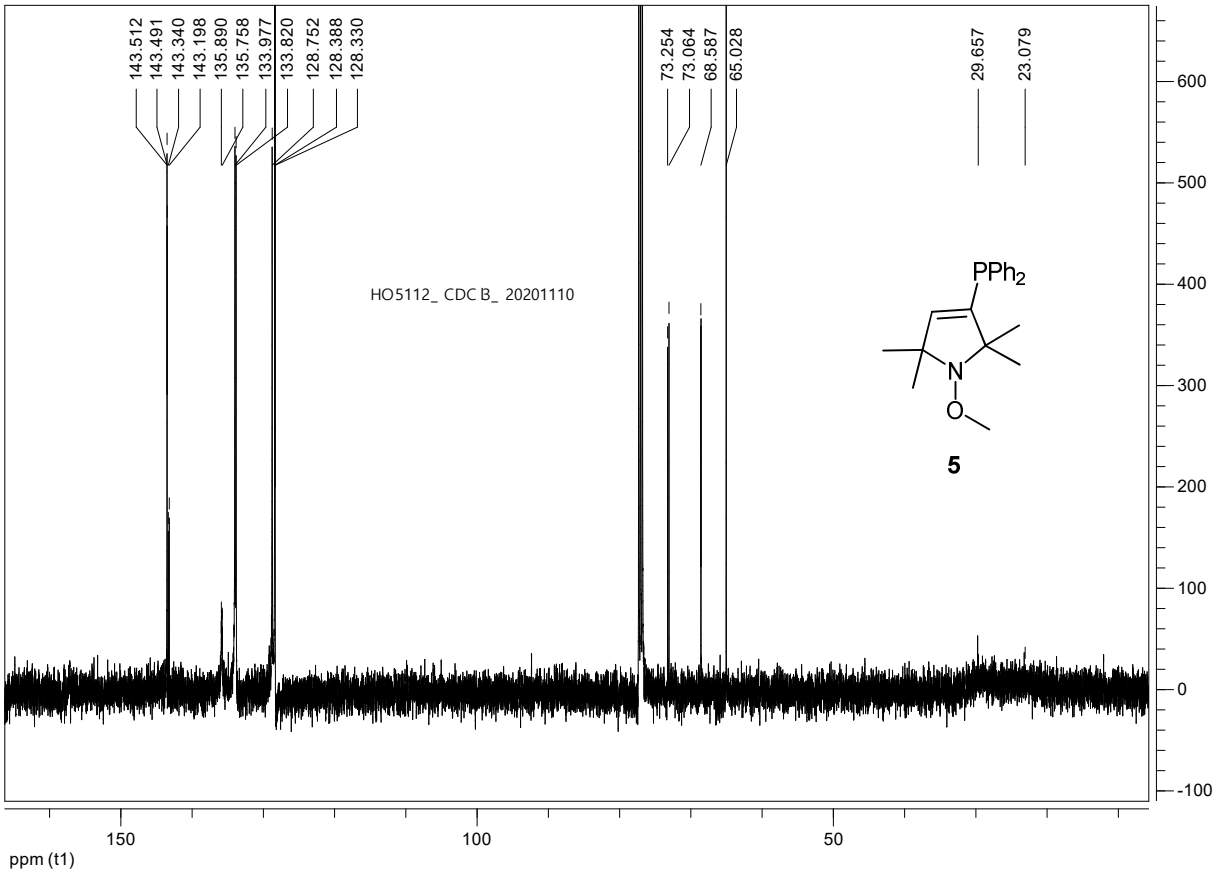
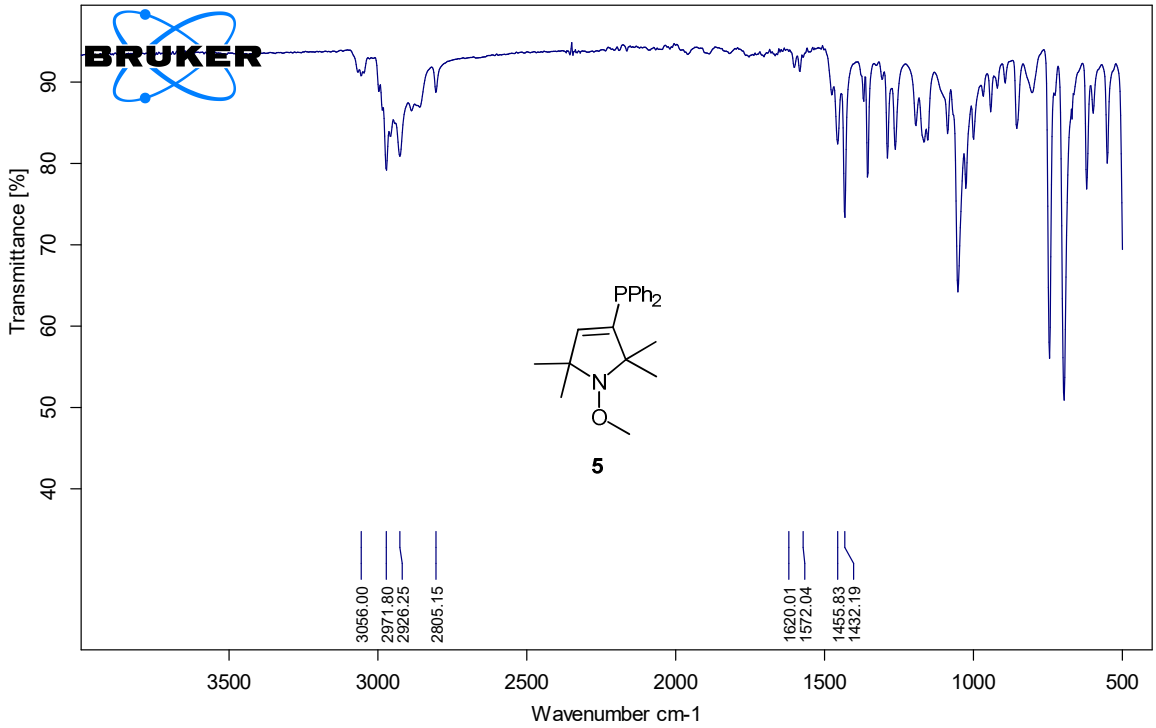

7.371
5.287
3.701
1.261
HO5112_ CDC B_ 20201110
PPh2
N
O
5
9.72
0.95
3.00
11.95
10000
5000
0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
ppm (t1)


-26.996
HO5112_ CDC B_ 20201110
PPh2
N
O
5
40000
30000
20000
10000
0
100
50
0
-50
-100
-150
-200
ppm (t1)





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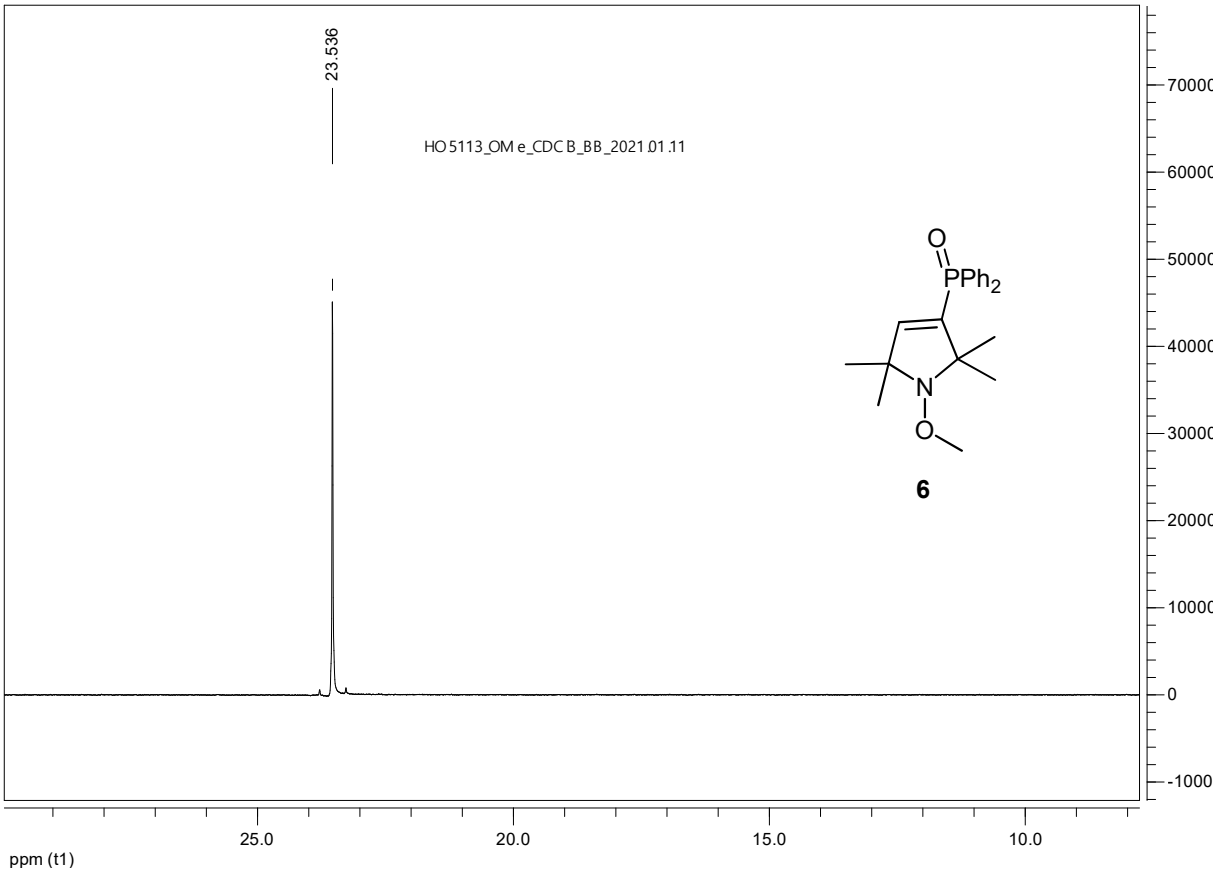
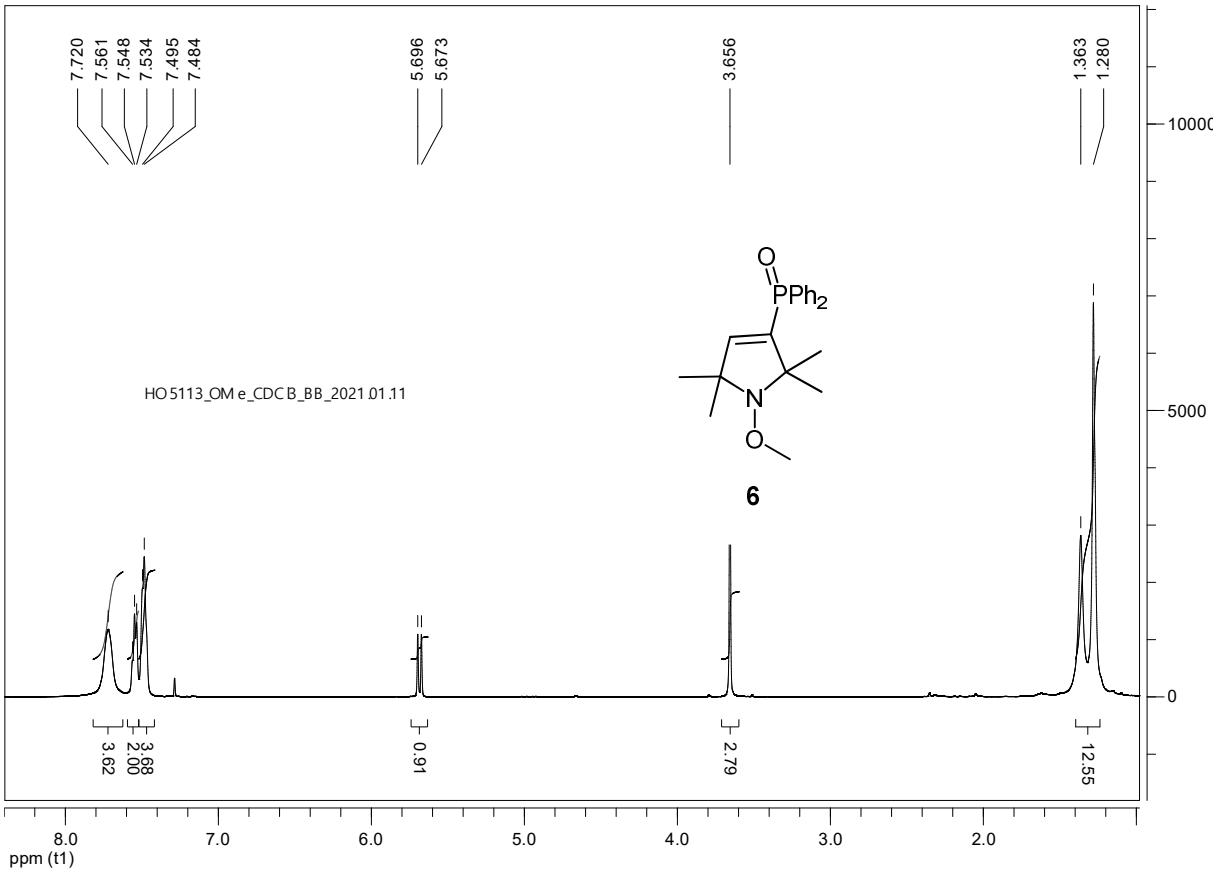
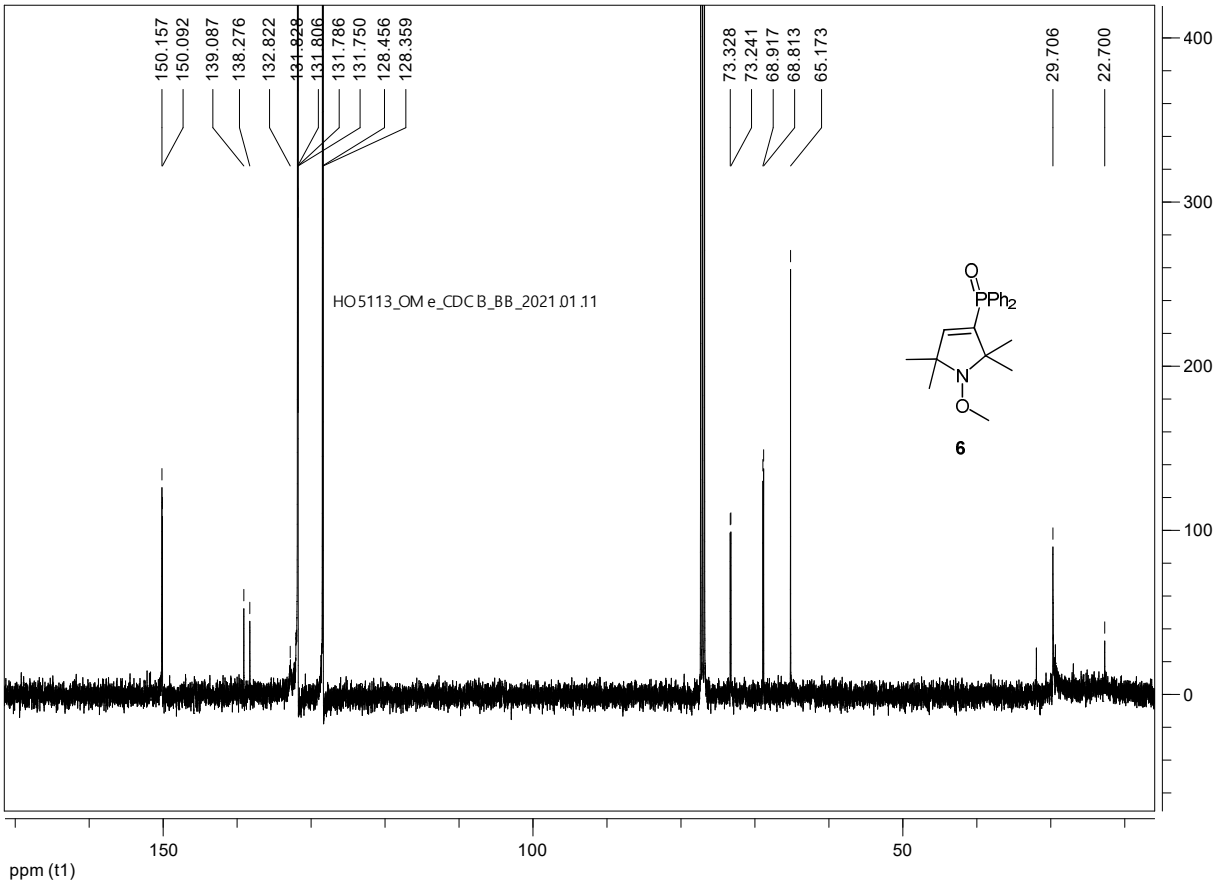
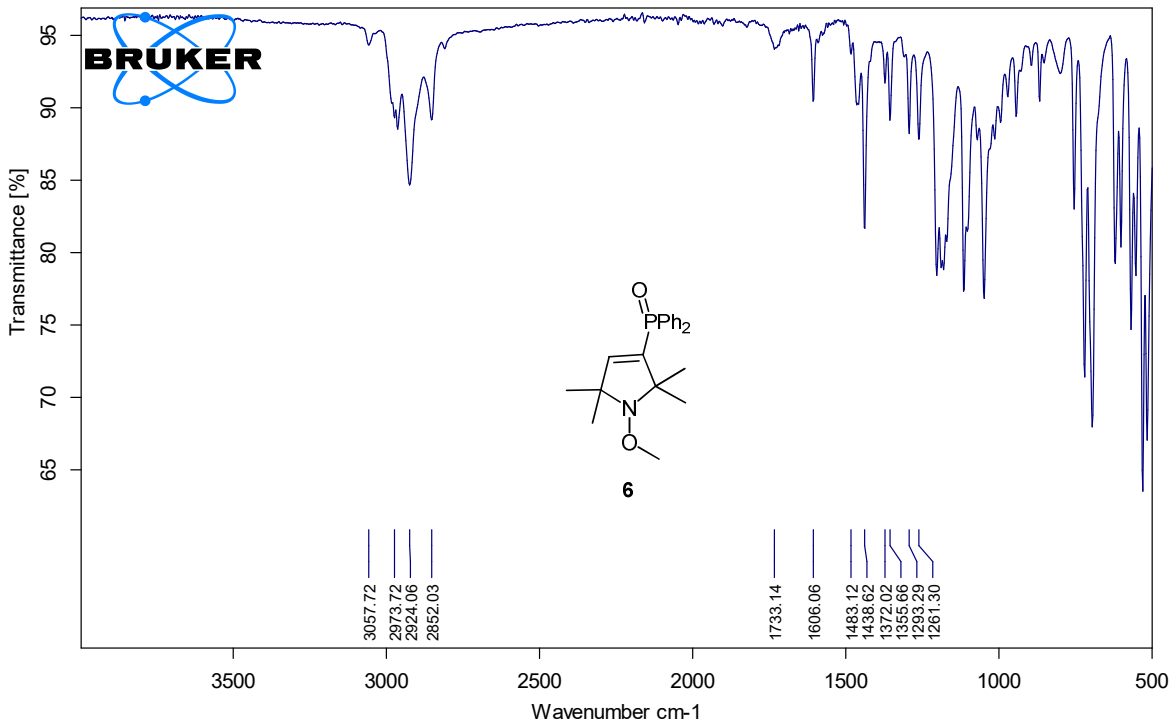

23.536
HO5113_OM e_CDCB_BB_2021.01.11
O
PPh2
N
O
6
ppm (t1)


7.720
7.561
7.548
7.534
7.495
7.484
5.696
5.673
3.656
1.363
1.280
HO5113_OM e_CDCB_BB_2021.01.11
O
PPh2
N
O
6
3.62
2.00
3.68
0.91
2.79
12.55
ppm (t1)





C:\OPUS_7.2.139.1294\Measure\HO-5113-OMe.0	HO-5113-OMe	Instrument type and / or accessory	2021.01.25

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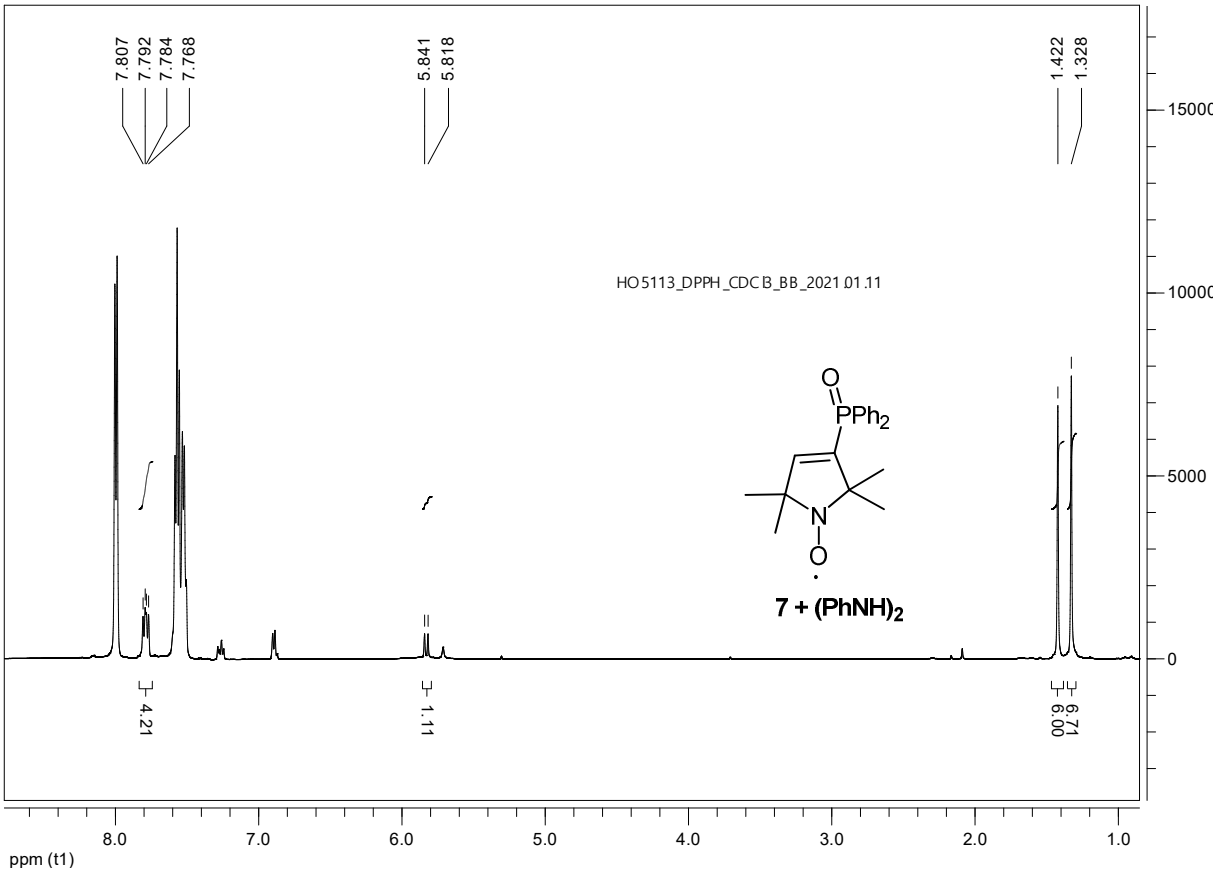
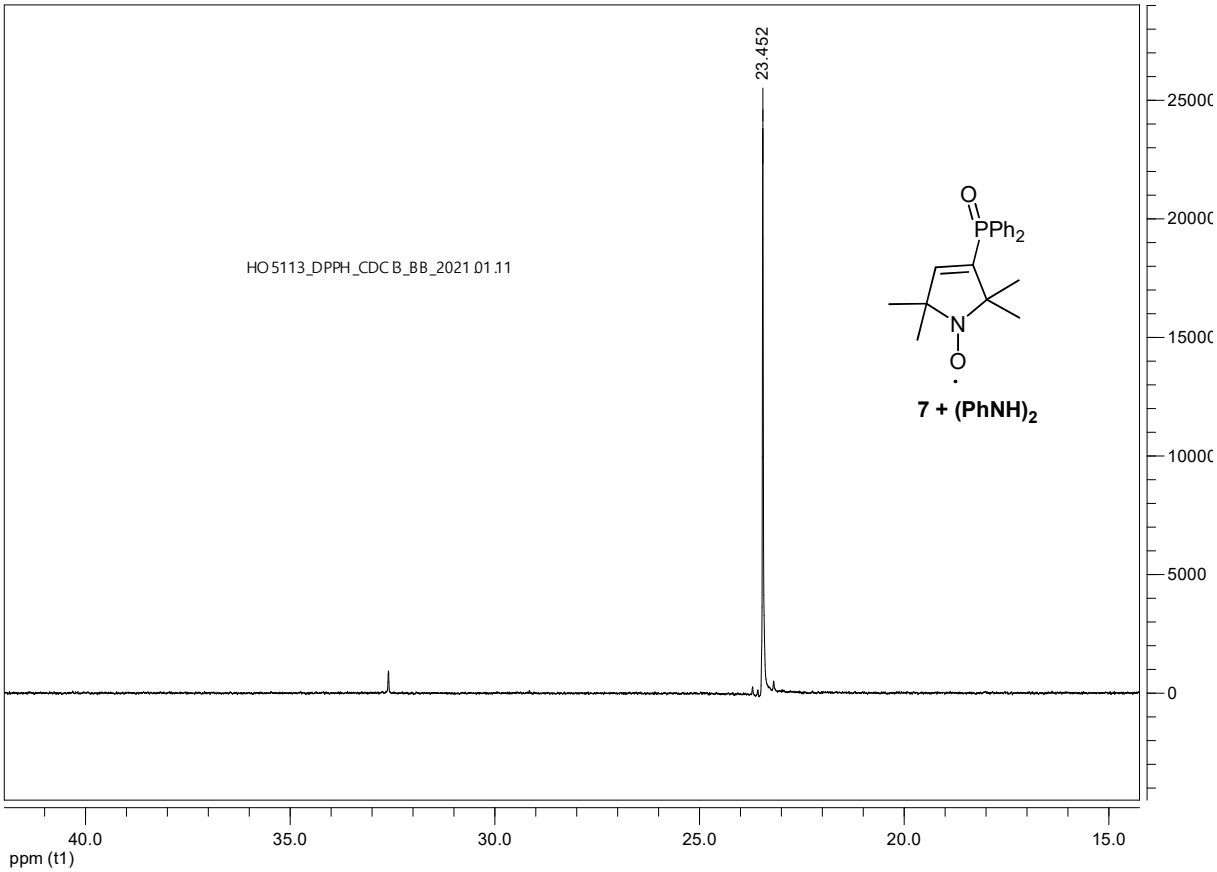
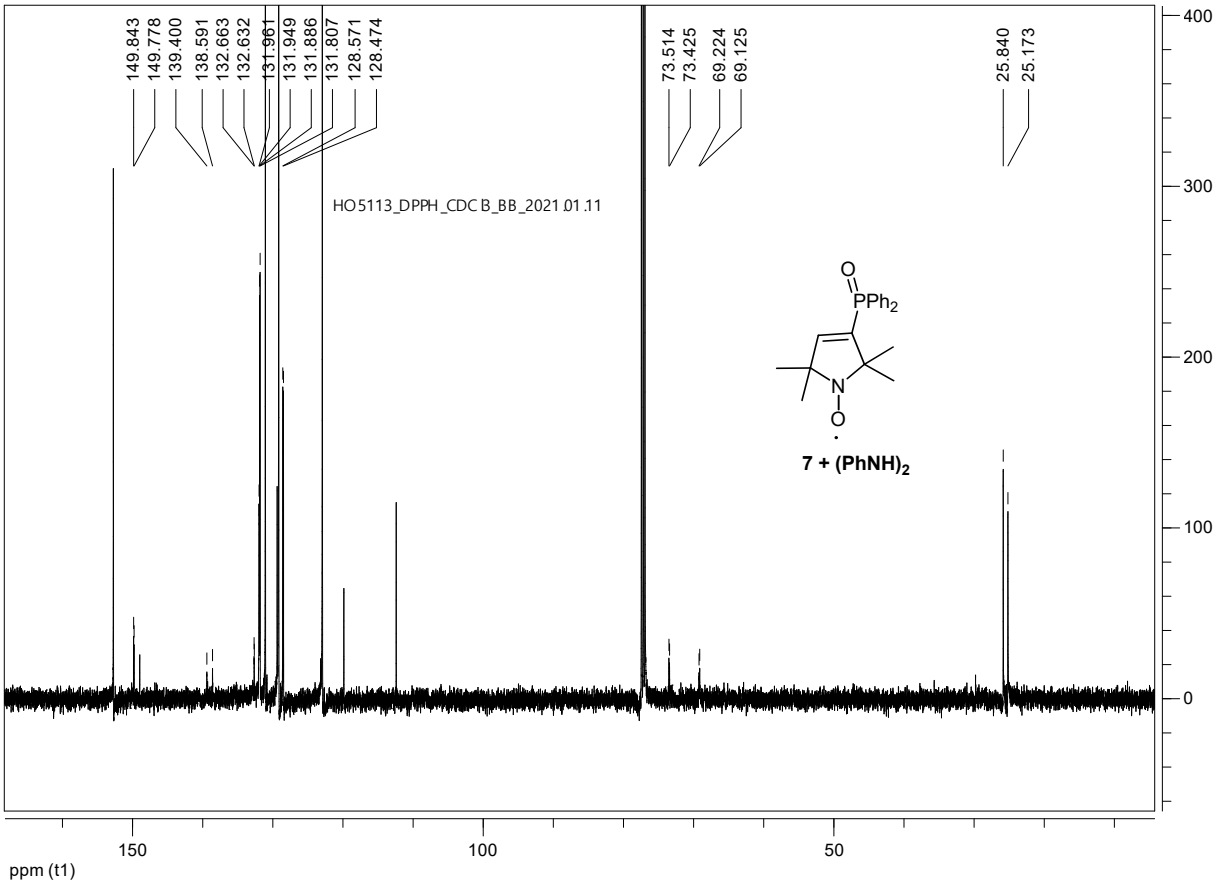
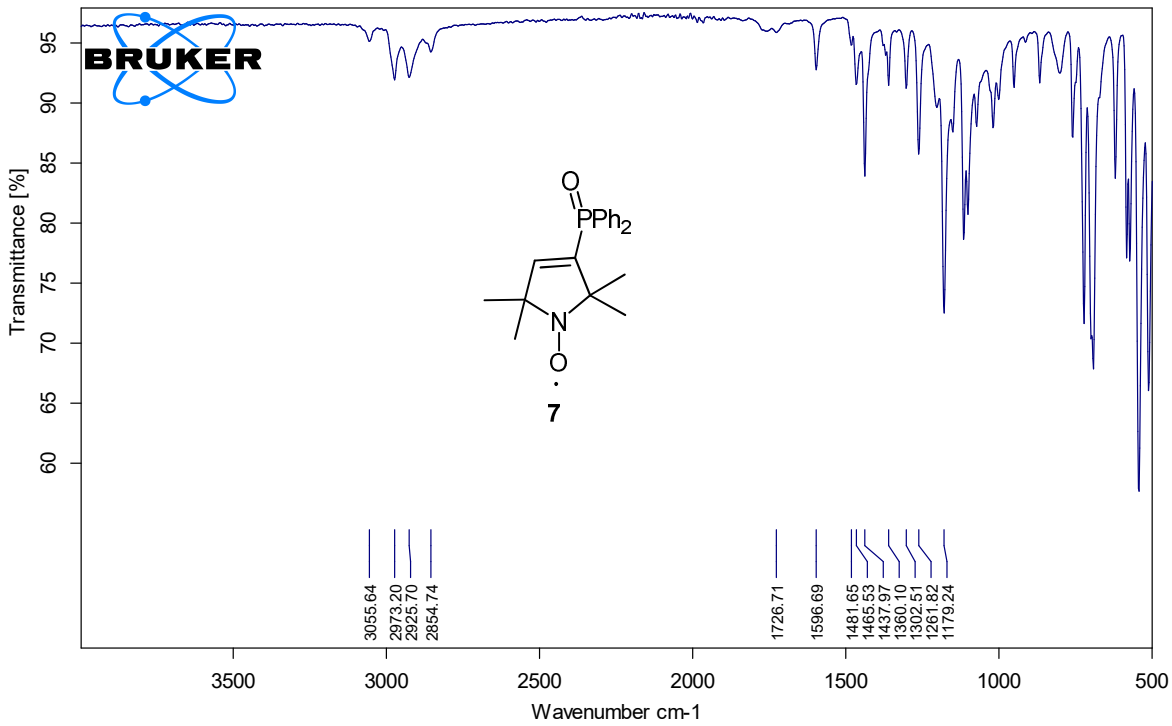

7.807
7.792
7.784
7.768
5.841
5.818
1.422
1.328
HO5113_DPPH_CDCB_BB_2021.01.11
PPh2
N
O
7 + (PhNH)2
4.21
1.11
6.00
6.71
15000
10000
5000
0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
ppm (t1)


23.452
HO5113_DPPH_CDCB_BB_2021.01.11
PPh2
N
O
7 + (PhNH)2
25000
20000
15000
10000
5000
0
40.0
35.0
30.0
25.0
20.0
15.0
ppm (t1)





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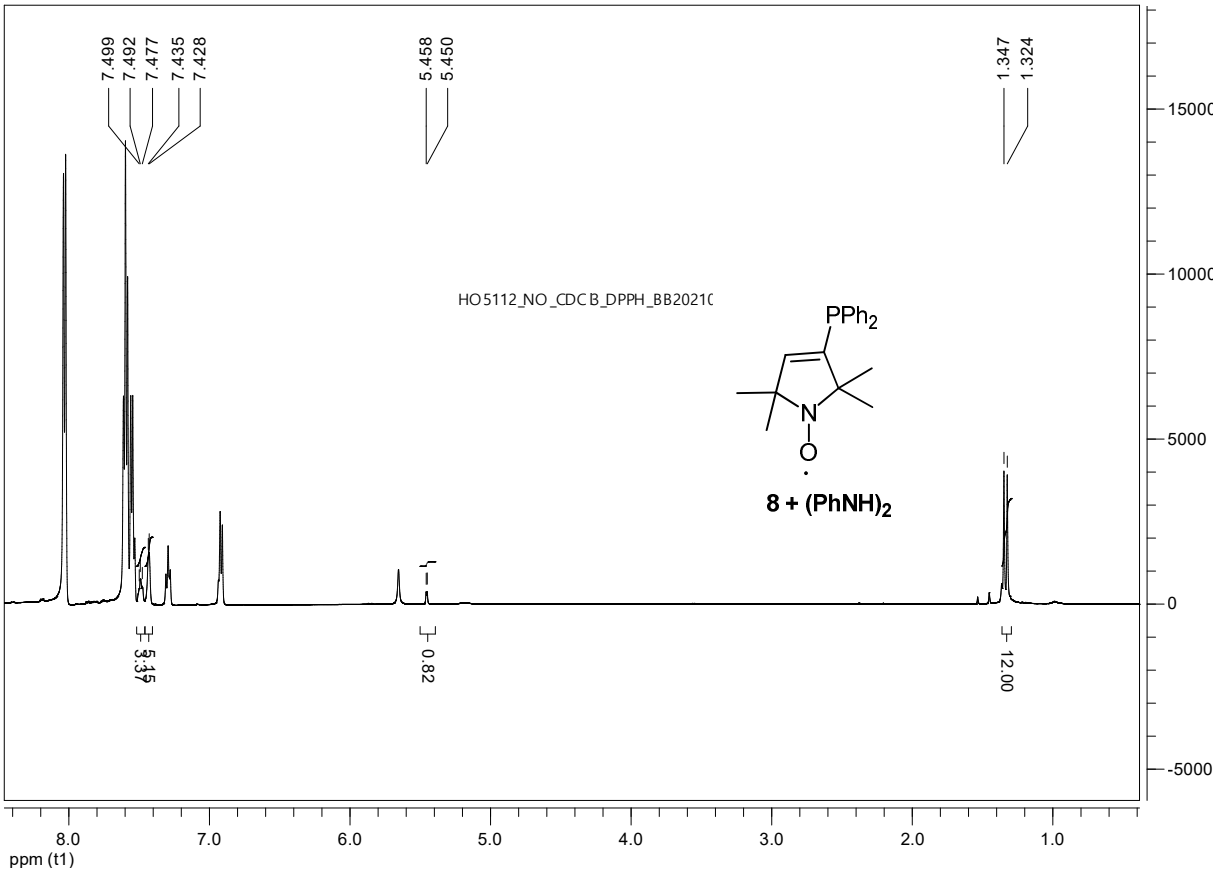
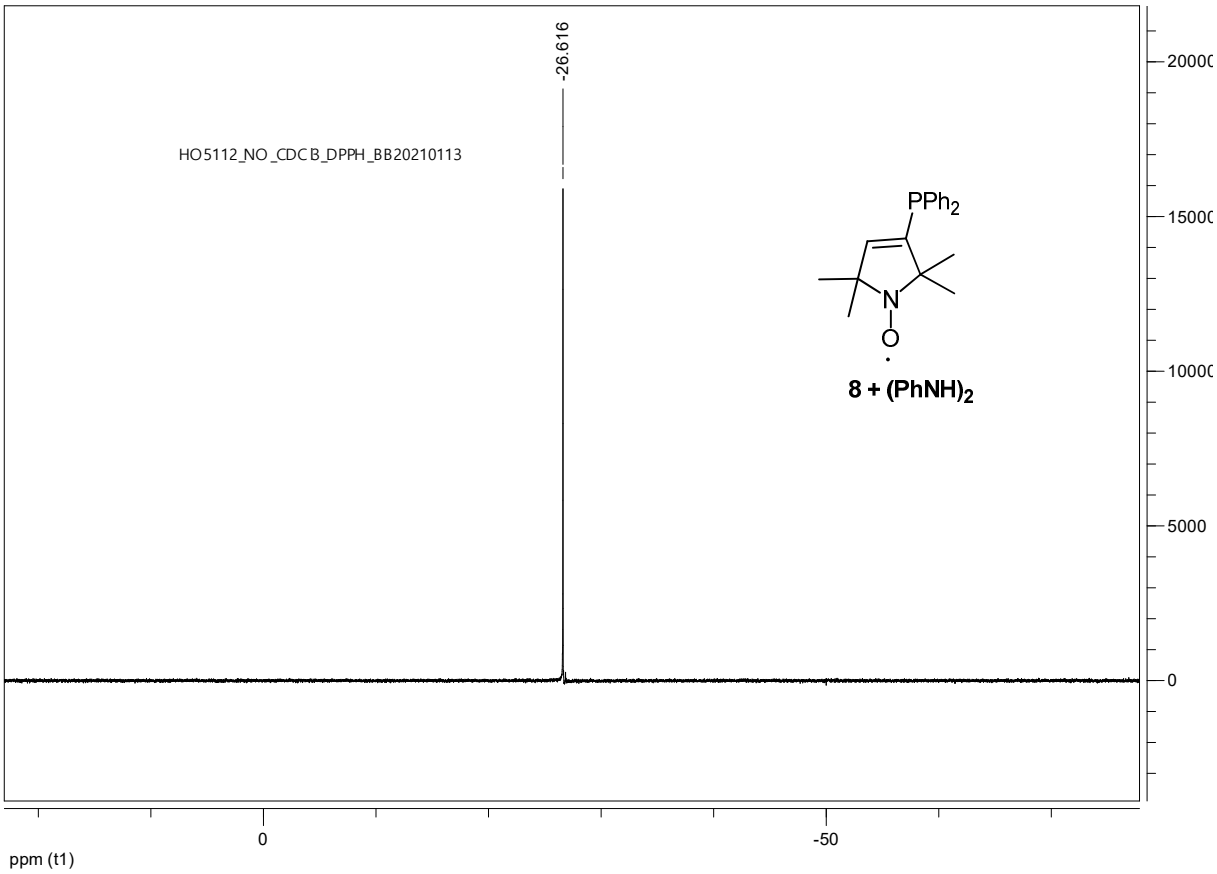
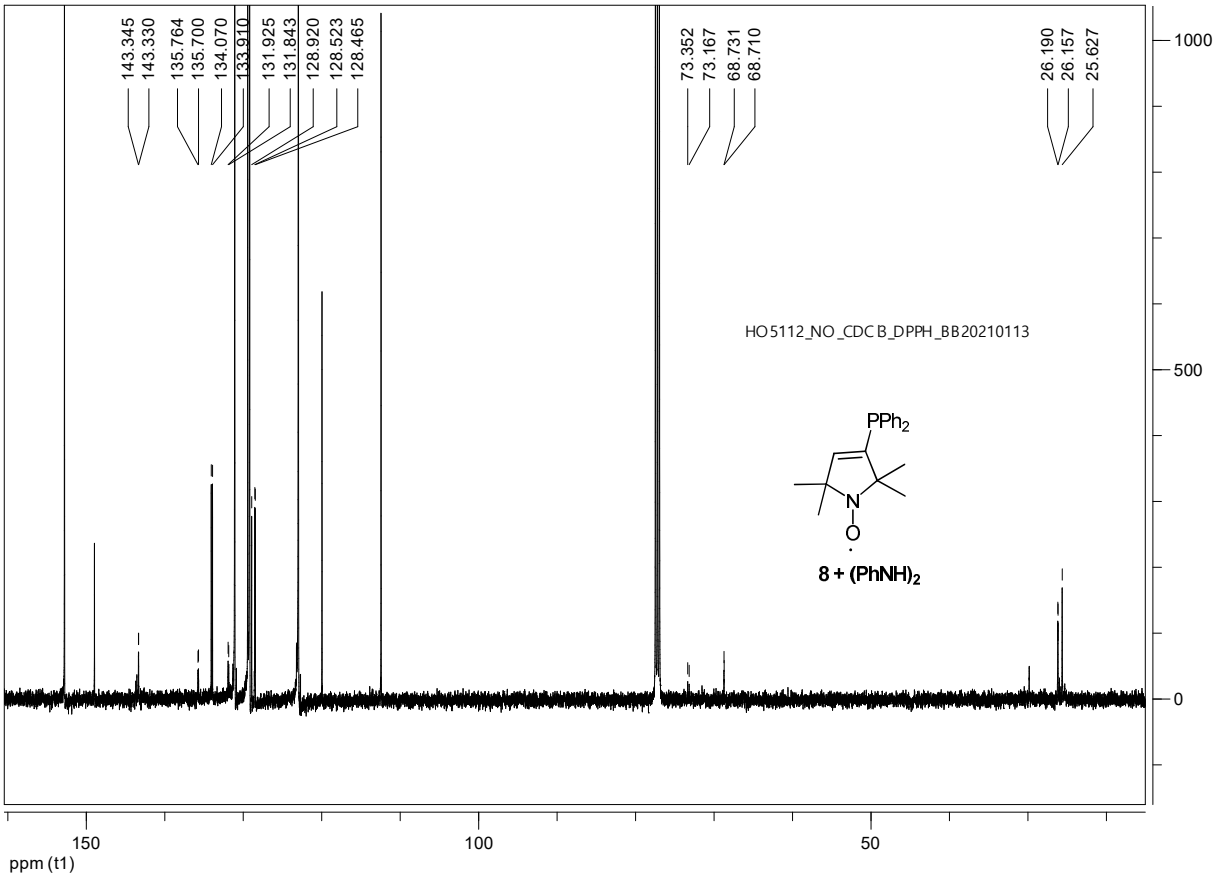
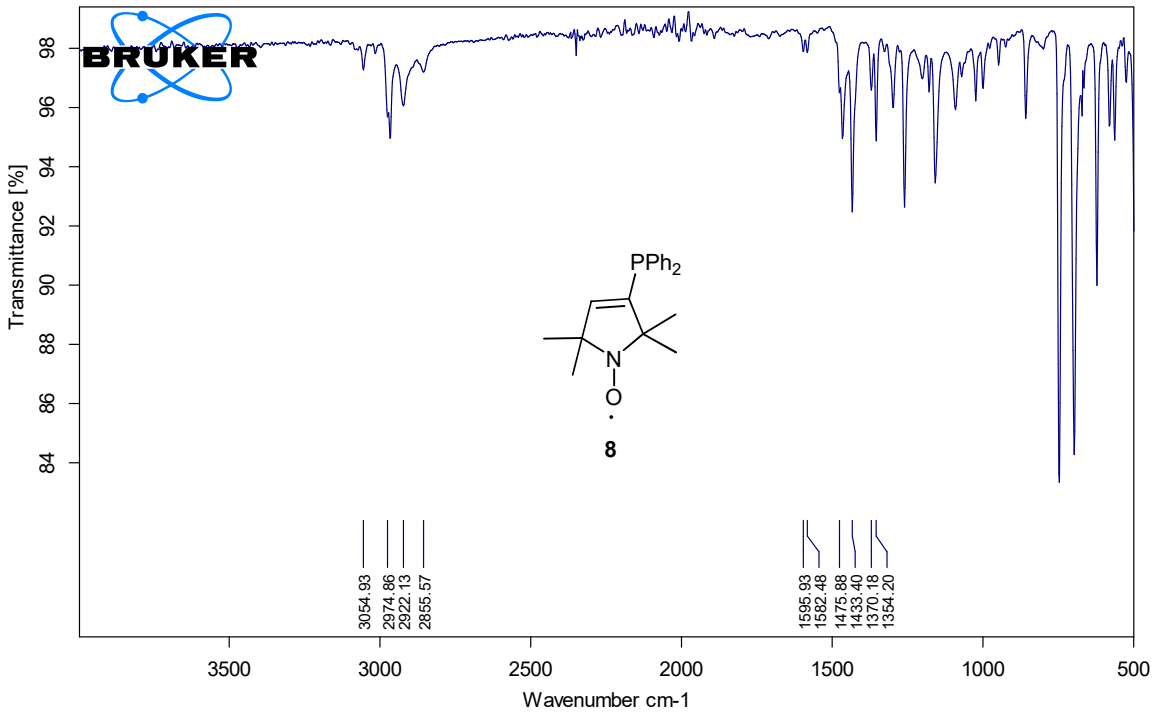

7.499
7.492
7.477
7.435
7.428
5.458
5.450
1.347
1.324
HO5112_NO_CDCB_DPPH_BB2021C
PPh2
N
O
8 + (PhNH)2
5.15
3.37
0.82
12.00
15000
10000
5000
0
-5000
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
ppm (t1)


-26.616
HO5112_NO_CDCB_DPPH_BB20210113
PPh2
N
O
8 + (PhNH)2
20000
15000
10000
5000
0
0
-50
ppm (t1)





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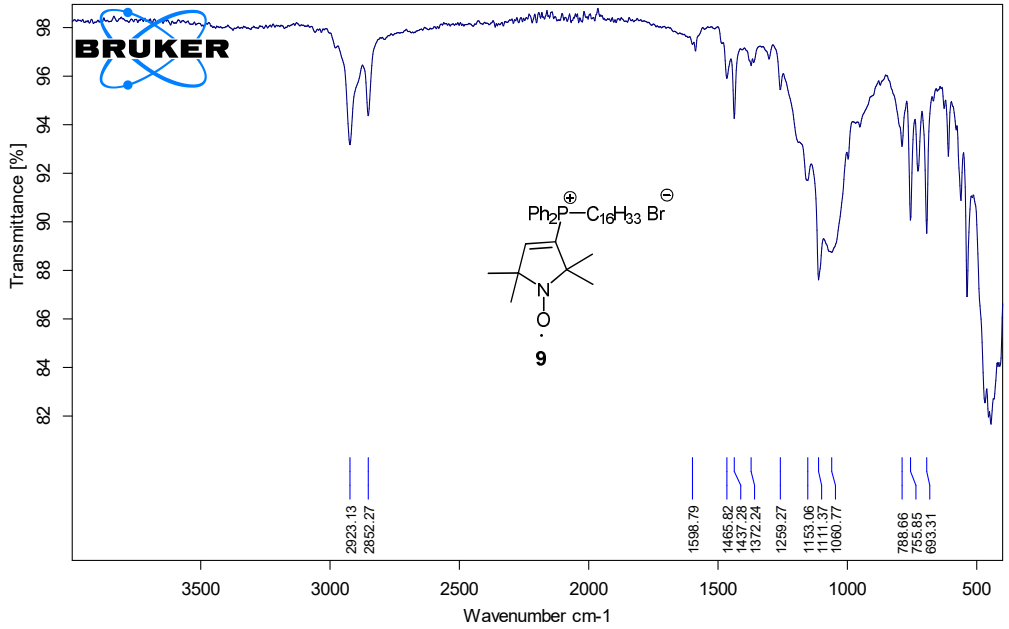

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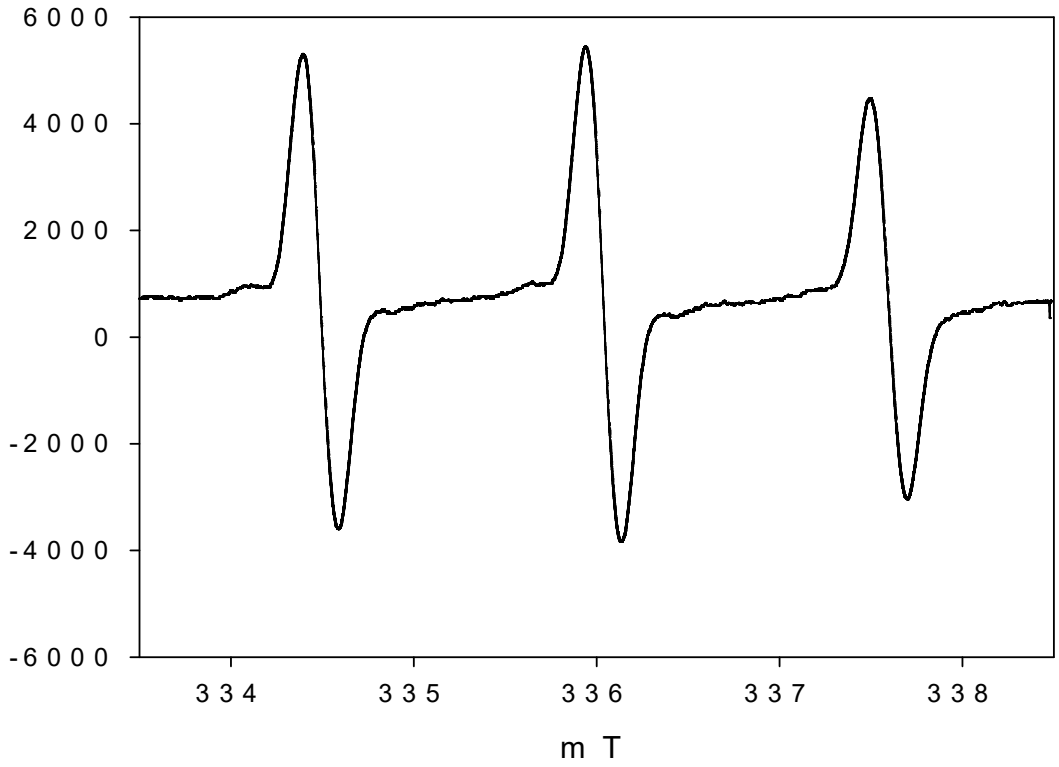
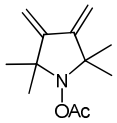
E P R o f c o m p o u n d **9**

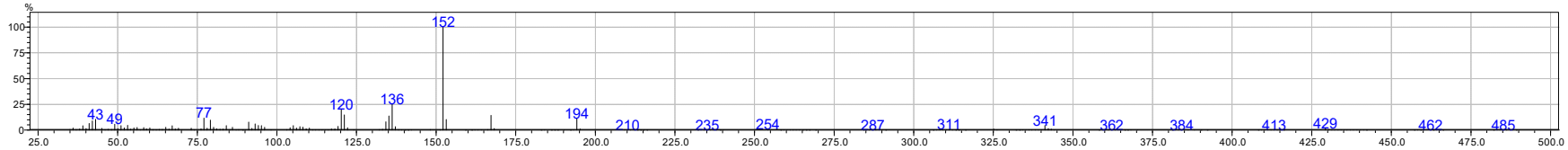


Thee EPR spectra of compound **9** (1 ×10^{-4} M) in water/dioxane 9:1.

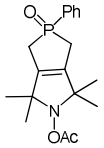
EI-MS spectra of compound **1b:**



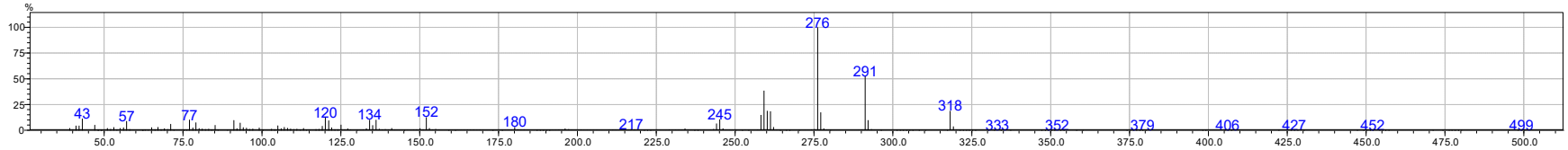
1b



EI-MS spectra of compound **2b:**



2b



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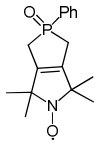
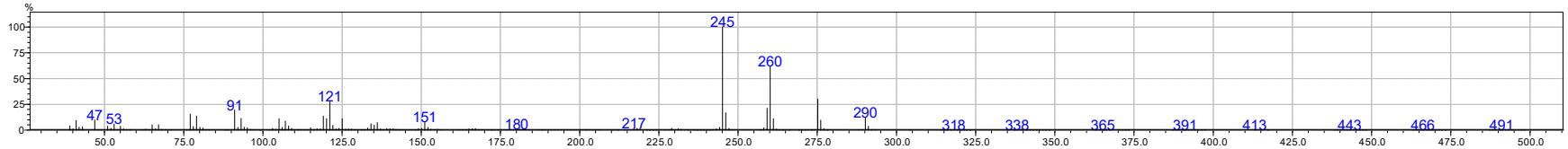


2a



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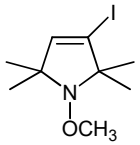
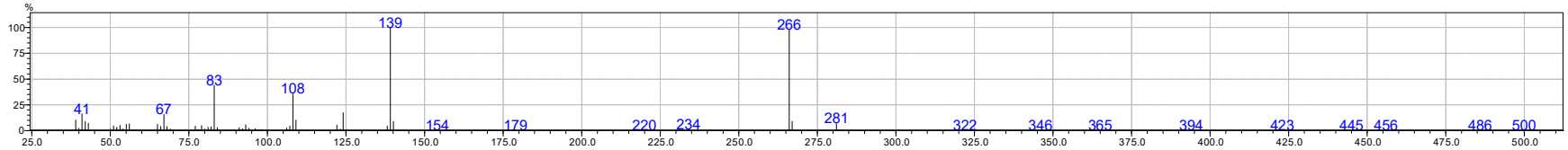
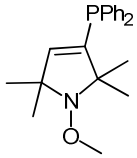


4



EI-MS spectra of compound **5**:



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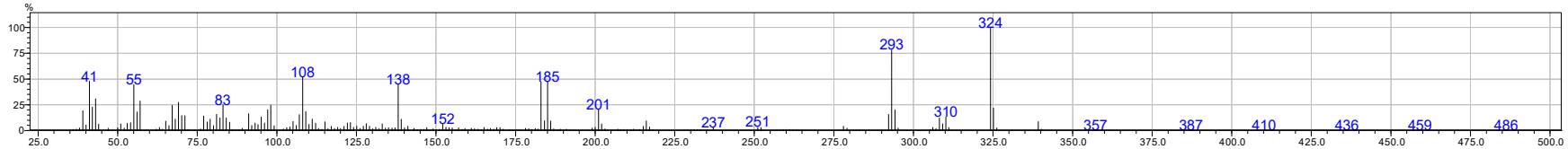

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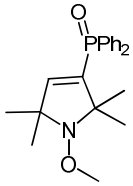

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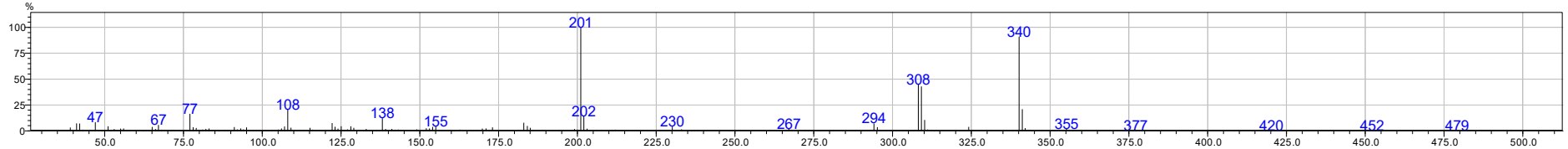

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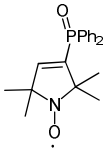

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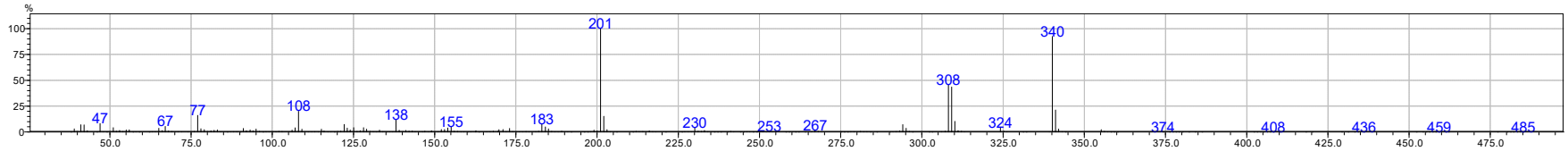
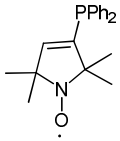


EI-MS spectra of compound **8:**



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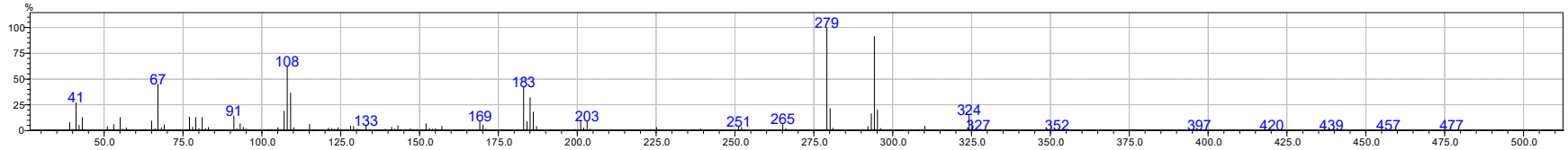


ESI-MS spectra of compound **9**:

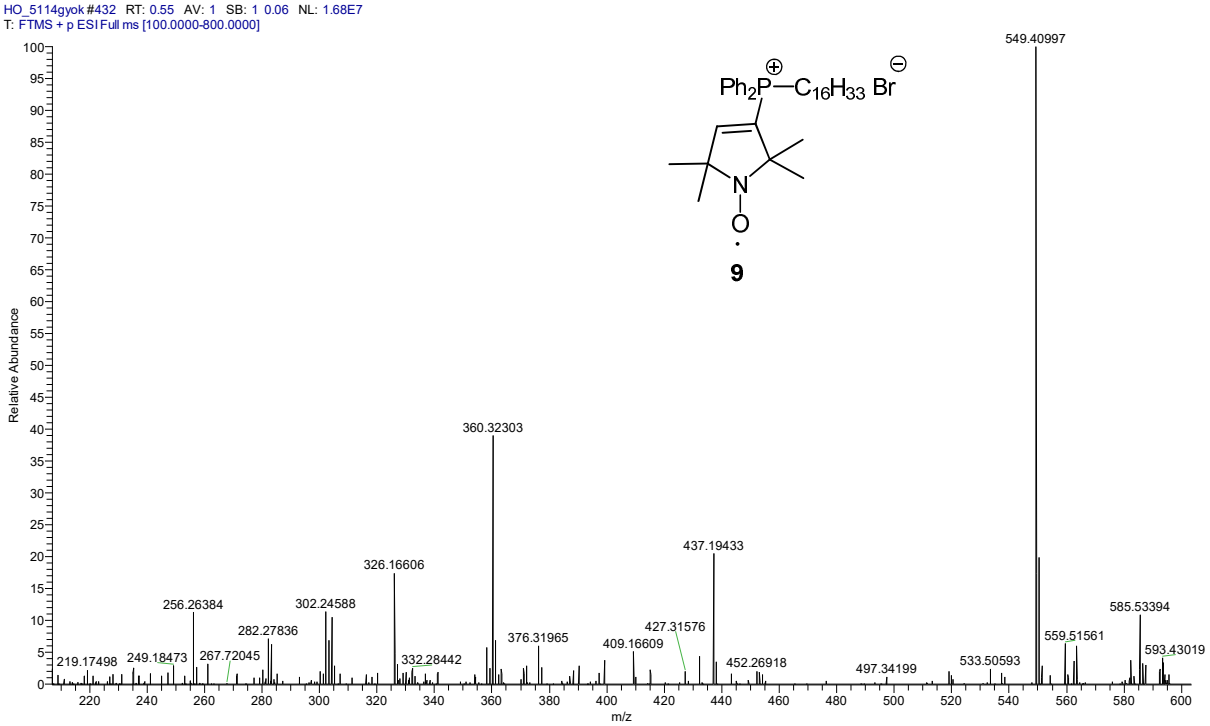
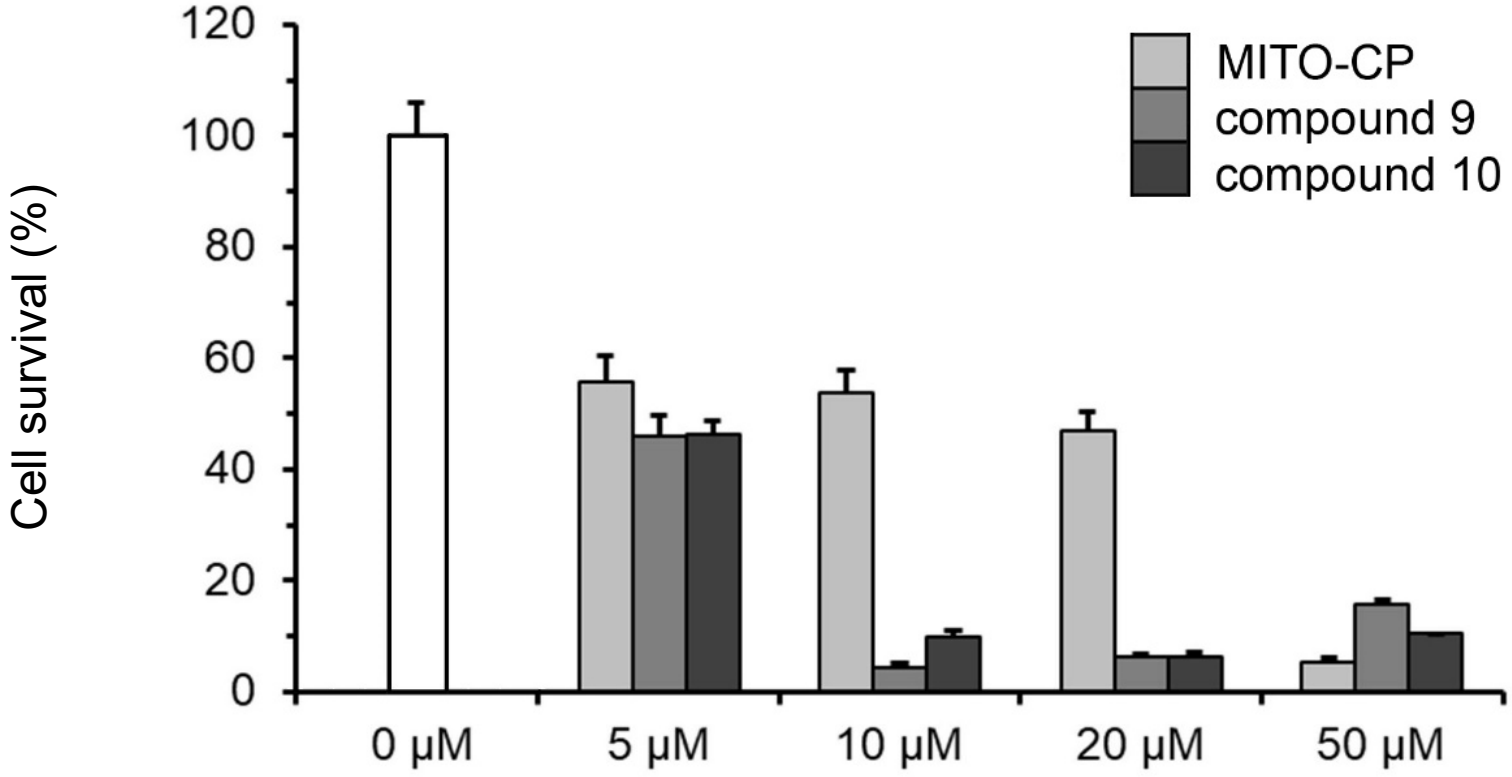


Table S1: Elememtal analysis of new compounds synthesized

Compound	Formula	Calculated %			Found %		
		C	H	N	C	H	N
1b	$C_{12}H_{19}NO_2$	68.87	9.15	6.69	68.75	8.95	6.59
2a	$C_{16}H_{21}NO_2P$	66.19	7.29	4.82	66.05	7.15	4.84
2b	$C_{18}H_{24}NO_3P$	64.85	7.26	4.20	64.65	7.15	4.17
4	$C_9H_{16}INO$	38.45	5.74	4.98	38.36	5.65	4.99
5	$C_{21}H_{26}NOP$	74.31	7.72	4.13	74.21	7.66	4.11
6	$C_{21}H_{26}NO_2P$	70.97	7.37	3.94	71.07	7.41	3.87
7	$C_{20}H_{23}NO_2P$	70.57	6.81	4.12	70.71	6.77	4.01
8	$C_{20}H_{23}NOP$	74.05	7.15	4.32	74.21	6.94	4.46
9	$C_{36}H_{56}BrNOP$	68.66	8.96	2.22	68.47	8.89	2.13

Figure S1: Preliminary biological data of compound 9 and cetyltriphenylphosphonium bromide (compound 10) compared to MITO-CP.



Supplementary Figure S1. Cytostatic effect of the substances on the MCF-7 human breast cancer line. The cells were treated with MITO-CP (light gray bars), compound **9** (gray bars) or compound **10** (dark gray bars) at the indicated concentrations for 24 h. Survival rate was is presented as the % of the untreated cells (empty bar) mean + standard error of the mean (SEM)of three independent experiments each running in at least four parallels (n=12).