Supporting Information for High-Efficiency, Visible-Light-Induced Direct Dehydrogenative Phosphonylation by Bismuth Quantum Dots under Ambient Conditions

You Zi,[a]† Songrui Wei,[b]† Zhihui Huang,[a] Jun Zhu,[a] Yi Hu,[a] Mengke Wang,*[a] Han Zhang [b] and Weichun Huang*[a]

[a]*School of Chemistry and Chemical Engineering, Nantong University, Nantong 226019, Jiangsu, P. R. China*

[b]*Collaborative Innovation Center for Optoelectronic Science & Technology, International Collaborative Laboratory of 2D Materials for Optoelectronics Science and Technology of Ministry of Education, Institute of Microscale Optoelectronics, Shenzhen University, Shenzhen 518060, P. R. China*

E-mail address: mengkewang@ntu.edu.cn (M. Wang); huangweichun@ntu.edu.cn (W. Huang)

†The authors contributed equally to this work.

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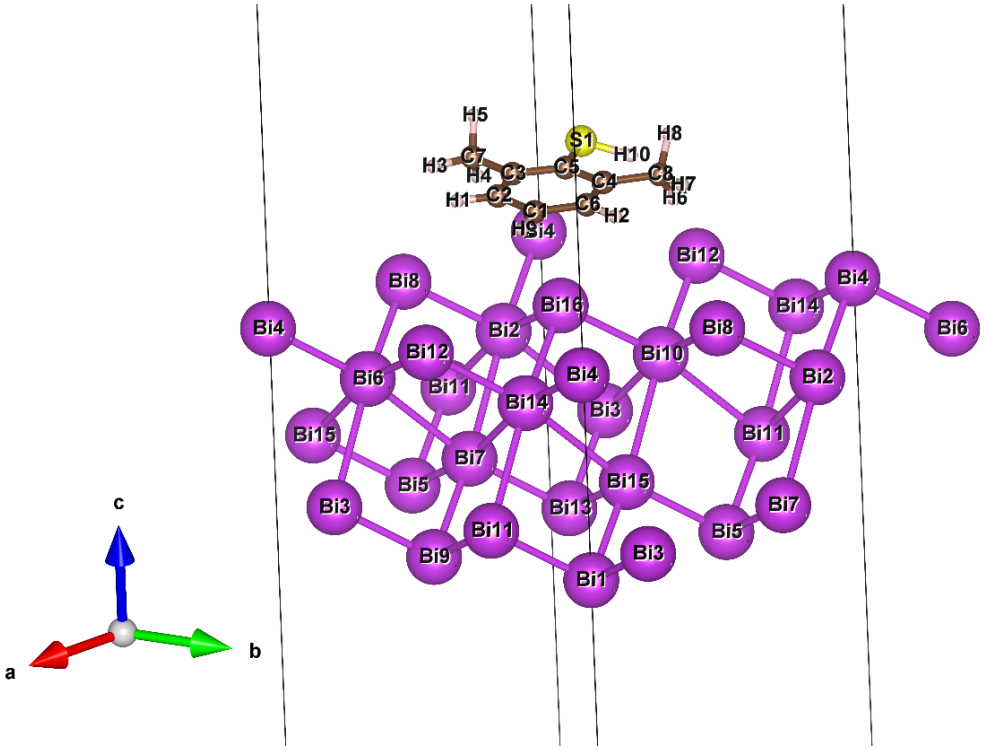
Table S1. The partial electron transfer property of 0D Bi QDs to substrate **1n** and its schematic diagram.

Specimen	Elements	Charge transfer	Specimen	Elements	Charge transfer	Gain (+) and loss (-) electron level
0D Bi QDs	Bi1	14.617	**0D Bi QD@1n**	Bi1	14.080	-0.537
	Bi2	14.784		Bi2	14.700	-0.084
	Bi3	15.423		Bi3	16.805	1.382
	Bi4	15.176		Bi4	14.800	-0.376
	Bi5	14.617		Bi5	14.082	-0.535
	Bi6	14.784		Bi6	15.144	0.360
	Bi7	15.423		Bi7	16.200	0.777
	Bi8	15.176		Bi8	14.925	-0.251
	Bi9	14.617		Bi9	14.062	-0.555
	Bi10	14.784		Bi10	14.041	-0.743
	Bi11	15.423		Bi11	17.110	1.687
	Bi12	15.176		Bi12	14.447	-0.729
	Bi13	14.617		Bi13	14.037	-0.580
	Bi14	14.783		Bi14	14.368	-0.415
	Bi15	15.423		Bi15	16.320	0.897
	Bi16	15.176		Bi16	14.978	-0.198
1n	S1	6.000		S1	6.351	0.351
	C1	4.043		C1	3.586	-0.457
	C2	4.040		C2	3.972	-0.068
	C3	3.990		C3	3.878	-0.112
	C4	3.991		C4	3.919	-0.072
	C5	4.167		C5	4.207	0.040
	C6	4.020		C6	3.474	-0.546
	C7	4.075		C7	3.426	-0.649
	C8	4.037		C8	3.675	-0.362
	H1	0.950		H1	1.299	0.349
	H2	0.975		H2	1.570	0.595
	H3	0.969		H3	1.374	0.405
	H4	0.981		H4	0.993	0.012
	H5	0.925		H5	0.960	0.035
	H6	0.963		H6	1.010	0.047
	H7	0.971		H7	1.057	0.086
	H8	0.993		H8	0.942	-0.051
	H9	0.950		H9	1.356	0.406
	H10	0.960		H10	0.853	-0.107


H5
S1
H8
H3
C7
H10
H4
C3
C5
C8
C4
H7
H1
C2
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H6
C1
H2
H9
Si4
Bi12
Bi8
Bi4
Bi16
Bi14
Bi4
Bi2
Bi8
Bi6
Bi12
Bi10
Bi6
Bi11
Bi4
Bi2
Bi14
Bi3
Bi15
Bi11
Bi7
Bi15
Bi5
Bi7
Bi3
Bi13
Bi5
Bi11
Bi3
Bi9
Bi1
c
b
a

Table S2. The partial electron transfer property of 2D Bi NSs to substrate **1n** and its schematic diagram.

Specimen	Elements	Charge transfer	Specimen	Elements	Charge transfer	Gain (+) and loss (-) electron level
2D Bi NSs	Bi1	14.734	**2D Bi NS@1n**	Bi1	14.909	0.175
	Bi2	15.266		Bi2	15.077	-0.189
	Bi3	14.734		Bi3	14.905	0.171
	Bi4	15.266		Bi4	15.099	-0.167
	Bi5	14.734		Bi5	14.916	0.182
	Bi6	15.266		Bi6	15.095	-0.171
	Bi7	14.734		Bi7	14.921	0.187
	Bi8	15.266		Bi8	15.096	-0.174
	Bi9	14.734		Bi9	14.909	0.175
	Bi10	15.266		Bi10	15.084	-0.182
	Bi11	14.734		Bi11	14.966	0.232
	Bi12	15.267		Bi12	15.052	-0.215
	Bi13	14.734		Bi13	14.819	0.086
	Bi14	15.266		Bi14	15.050	-0.216
	Bi15	14.734		Bi15	14.925	0.191
	Bi16	15.266		Bi16	15.101	-0.165
	Bi17	14.733		Bi17	14.919	0.186
	Bi18	15.266		Bi18	15.088	-0.178
	Bi19	14.733		Bi19	14.918	0.185
	Bi20	15.266		Bi20	15.072	-0.194
	Bi21	14.733		Bi21	14.956	0.223
	Bi22	15.266		Bi22	15.085	-0.181
	Bi23	14.733		Bi23	14.944	0.211
	Bi24	15.266		Bi24	15.072	-0.194
	Bi25	14.733		Bi25	14.944	0.211
	Bi26	15.266		Bi26	15.084	-0.182
	Bi27	14.733		Bi27	14.905	0.172
	Bi28	15.266		Bi28	15.095	-0.171
	Bi29	14.733		Bi29	14.908	0.175
	Bi30	15.266		Bi30	15.081	-0.185
	Bi31	14.733		Bi31	14.910	0.177
	Bi32	15.266		Bi32	15.077	-0.189
1n	S1	6.000		S1	5.913	-0.087
	C1	4.043		C1	3.859	-0.184
	C2	4.040		C2	3.948	-0.092
	C3	3.990		C3	3.886	-0.104
	C4	3.990		C4	3.970	-0.020
	C5	4.166		C5	4.174	0.008
	C6	4.019		C6	4.076	0.057
	C7	4.075		C7	4.072	-0.003
	C8	4.037		C8	3.961	-0.076
	H1	0.951		H1	1.021	0.070
	H2	0.975		H2	0.994	0.019
	H3	0.969		H3	0.990	0.021
	H4	0.981		H4	1.001	0.020
	H5	0.925		H5	0.940	0.015
	H6	0.963		H6	0.977	0.014
	H7	0.970		H7	1.006	0.036
	H8	0.993		H8	1.005	0.012
	H9	0.950		H9	1.205	0.255
	H10	0.960		H10	1.012	0.052

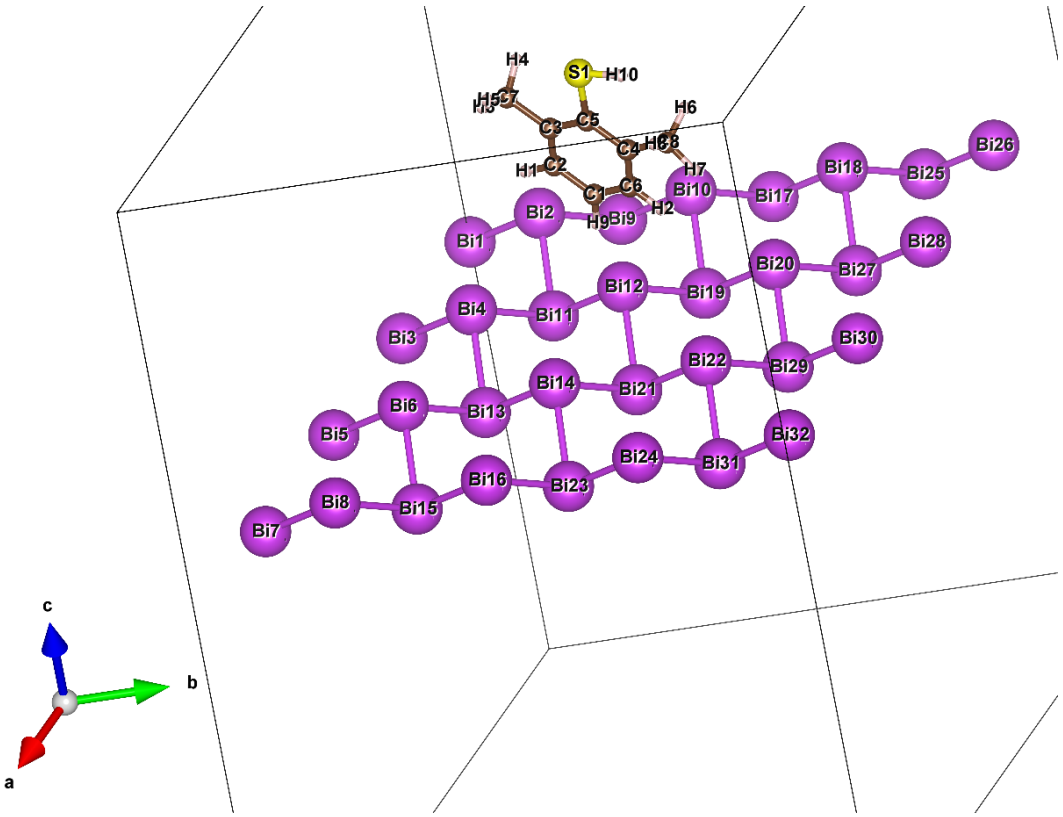
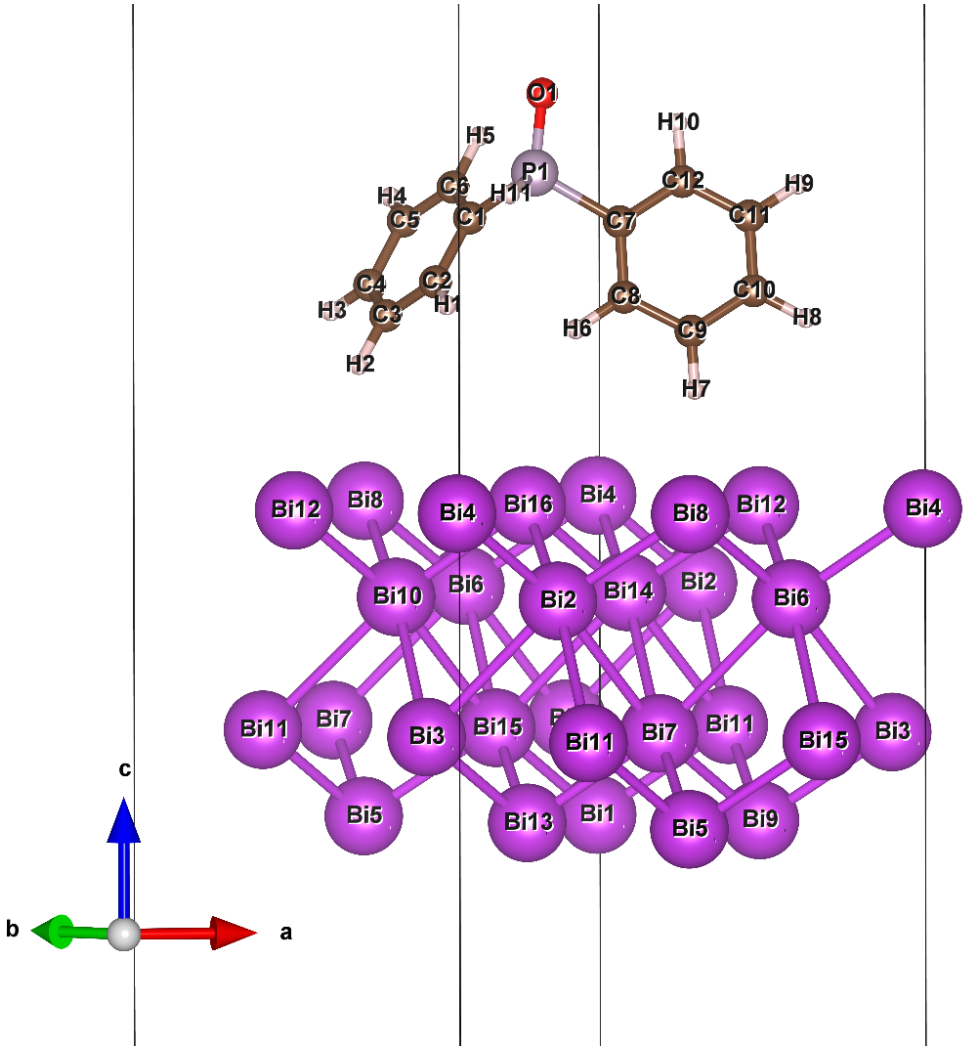

H4
S1
H10
H5
C3
C5
H6
C4
H8
H7
H1
C2
C1
C6
Bi10
H2
H9
Bi9
Bi2
Bi1
Bi17
Bi18
Bi25
Bi26
Bi20
Bi27
Bi28
Bi12
Bi19
Bi4
Bi11
Bi3
Bi30
Bi22
Bi29
Bi14
Bi21
Bi6
Bi13
Bi5
Bi32
Bi24
Bi31
Bi16
Bi23
Bi8
Bi15
Bi7
c
b
a

Table S3. The partial electron transfer property of 0D Bi QDs to substrate **2a** and its schematic diagram.

Specimen	Elements	Charge transfer	Specimen	Elements	Charge transfer	Gain (+) and loss (-) electron level
0D Bi QDs	Bi1	14.617	**0D Bi QD@2a**	Bi1	15.493	0.876
	Bi2	14.784		Bi2	14.507	-0.277
	Bi3	15.423		Bi3	16.455	1.032
	Bi4	15.176		Bi4	14.711	-0.465
	Bi5	14.617		Bi5	15.311	0.694
	Bi6	14.783		Bi6	14.327	-0.456
	Bi7	15.423		Bi7	14.775	-0.648
	Bi8	15.176		Bi8	15.425	0.249
	Bi9	14.617		Bi9	14.433	-0.184
	Bi10	14.783		Bi10	15.061	0.278
	Bi11	15.423		Bi11	15.256	-0.167
	Bi12	15.176		Bi12	15.595	0.419
	Bi13	14.617		Bi13	15.022	0.405
	Bi14	14.783		Bi14	14.125	-0.658
	Bi15	15.423		Bi15	14.722	-0.701
	Bi16	15.176		Bi16	14.720	-0.456
2a	P1	2.287		P1	3.102	0.815
	O1	7.423		O1	7.087	-0.336
	C1	4.608		C1	4.023	-0.585
	C2	3.968		C2	3.812	-0.156
	C3	4.100		C3	4.072	-0.028
	C4	4.053		C4	3.758	-0.295
	C5	3.926		C5	3.632	-0.294
	C6	4.056		C6	4.171	0.115
	C7	4.519		C7	3.850	-0.669
	C8	4.004		C8	3.589	-0.415
	C9	4.095		C9	4.035	-0.060
	C10	4.056		C10	3.938	-0.118
	C11	3.976		C11	3.994	0.018
	C12	4.114		C12	3.955	-0.159
	H1	0.960		H1	1.220	0.260
	H2	0.957		H2	1.174	0.217
	H3	0.934		H3	1.220	0.286
	H4	0.949		H4	1.394	0.445
	H5	0.928		H5	0.949	0.021
	H6	0.952		H6	1.231	0.279
	H7	0.948		H7	1.290	0.342
	H8	0.930		H8	0.899	-0.031
	H9	0.908		H9	1.018	0.110
	H10	0.891		H10	1.190	0.299
	H11	1.455		H11	1.455	-0.000


O1
H5
H10
P1
C12
H9
H4
C6
H11
C5
C1
C7
C11
C4
C2
C10
H3
C3
H1
C8
H8
H6
C9
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H7
Bi12
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Bi14
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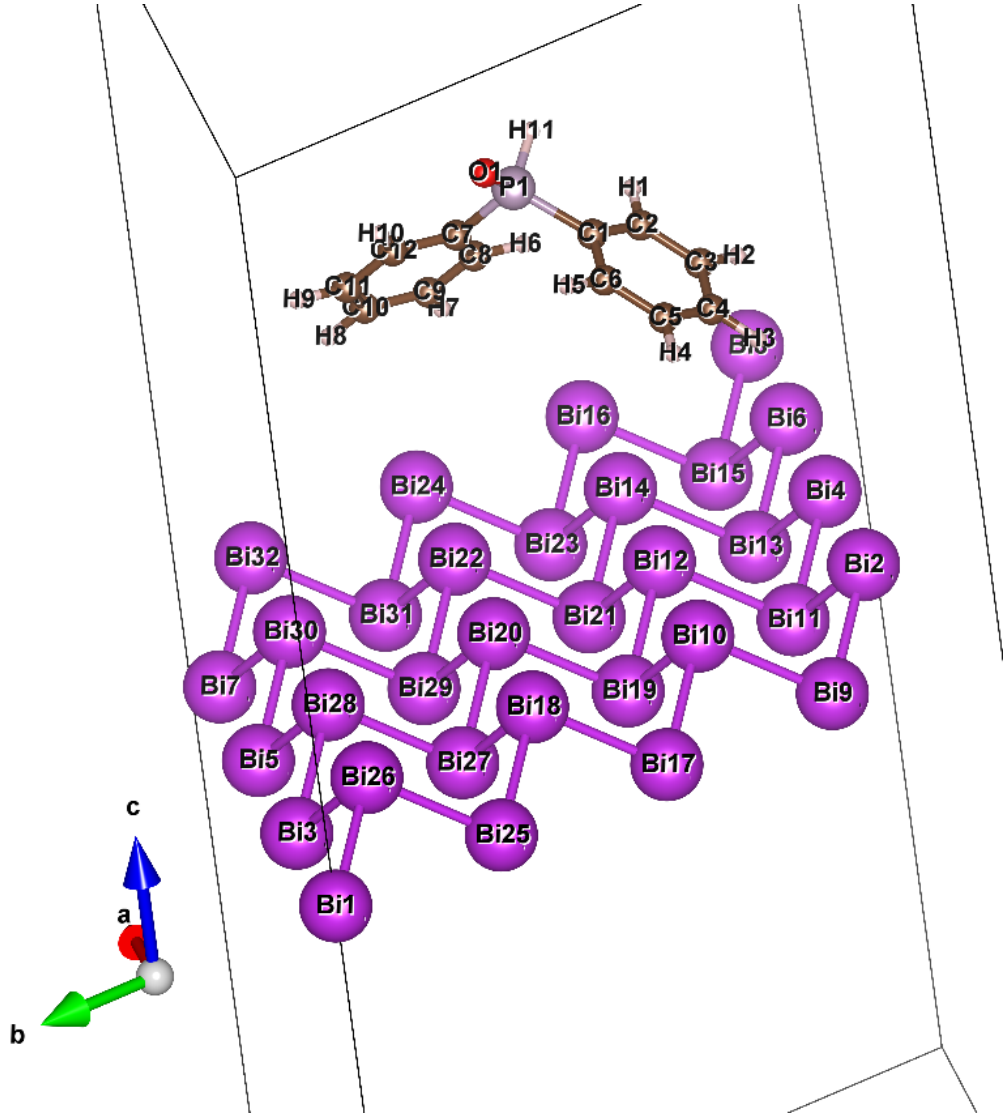
Bi6
Bi11
Bi7
Bi3
Bi15
Bi11
Bi7
Bi11
Bi15
Bi3
Bi5
Bi13
Bi1
Bi5
Bi9
c
b
a

Table S4. The partial electron transfer property of 2D Bi NSs to substrate **2a** and its schematic diagram.

Specimen	Elements	Charge transfer	Specimen	Elements	Charge transfer	Gain (+) and loss (-) electron level
2D Bi NSs	Bi1	14.734	**2D Bi NS@2a**	Bi1	15.087	0.353
	Bi2	15.266		Bi2	14.820	-0.446
	Bi3	14.733		Bi3	15.217	0.484
	Bi4	15.266		Bi4	15.034	-0.232
	Bi5	14.733		Bi5	15.285	0.552
	Bi6	15.266		Bi6	14.748	-0.518
	Bi7	14.734		Bi7	15.220	0.486
	Bi8	15.266		Bi8	14.683	-0.583
	Bi9	14.734		Bi9	15.280	0.546
	Bi10	15.266		Bi10	14.784	-0.482
	Bi11	14.734		Bi11	15.066	0.332
	Bi12	15.266		Bi12	15.239	-0.027
	Bi13	14.733		Bi13	14.980	0.247
	Bi14	15.266		Bi14	15.222	-0.044
	Bi15	14.734		Bi15	15.428	0.694
	Bi16	15.266		Bi16	14.742	-0.524
	Bi17	14.733		Bi17	15.360	0.627
	Bi18	15.266		Bi18	14.733	-0.533
	Bi19	14.733		Bi19	14.843	0.110
	Bi20	15.266		Bi20	14.790	-0.476
	Bi21	14.733		Bi21	14.791	0.058
	Bi22	15.266		Bi22	15.458	0.192
	Bi23	14.733		Bi23	14.929	0.196
	Bi24	15.266		Bi24	15.003	-0.263
	Bi25	14.733		Bi25	15.060	0.327
	Bi26	15.266		Bi26	14.765	-0.501
	Bi27	14.733		Bi27	15.267	0.534
	Bi28	15.266		Bi28	14.726	-0.540
	Bi29	14.734		Bi29	14.880	0.146
	Bi30	15.266		Bi30	14.755	-0.511
	Bi31	14.733		Bi31	14.862	0.129
	Bi32	15.266		Bi32	14.891	-0.375
2a	P1	2.287		P1	3.317	1.030
	O1	7.423		O1	6.888	-0.535
	C1	4.607		C1	4.370	-0.237
	C2	3.968		C2	4.023	0.055
	C3	4.100		C3	3.775	-0.325
	C4	4.053		C4	4.072	0.019
	C5	3.926		C5	3.593	-0.333
	C6	4.056		C6	4.064	0.008
	C7	4.519		C7	4.392	-0.127
	C8	4.004		C8	3.982	-0.022
	C9	4.096		C9	3.890	-0.206
	C10	4.057		C10	3.896	-0.161
	C11	3.976		C11	3.861	-0.115
	C12	4.114		C12	3.927	-0.187
	H1	0.960		H1	0.949	-0.011
	H2	0.957		H2	1.174	0.217
	H3	0.934		H3	1.069	0.135
	H4	0.949		H4	1.051	0.102
	H5	0.928		H5	1.115	0.187
	H6	0.952		H6	1.013	0.061
	H7	0.948		H7	1.059	0.111
	H8	0.930		H8	1.116	0.186
	H9	0.909		H9	1.108	0.199
	H10	0.891		H10	1.078	0.187
	H11	1.455		H11	1.258	-0.197


H11
O1
P1
H1
C1
C2
C3
H2
H10
C7
C12
C8
H6
H9
C11
C9
H5
C6
C10
H7
C5
C4
H8
H4
H3
Bi16
Bi6
Bi15
Bi24
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Bi10
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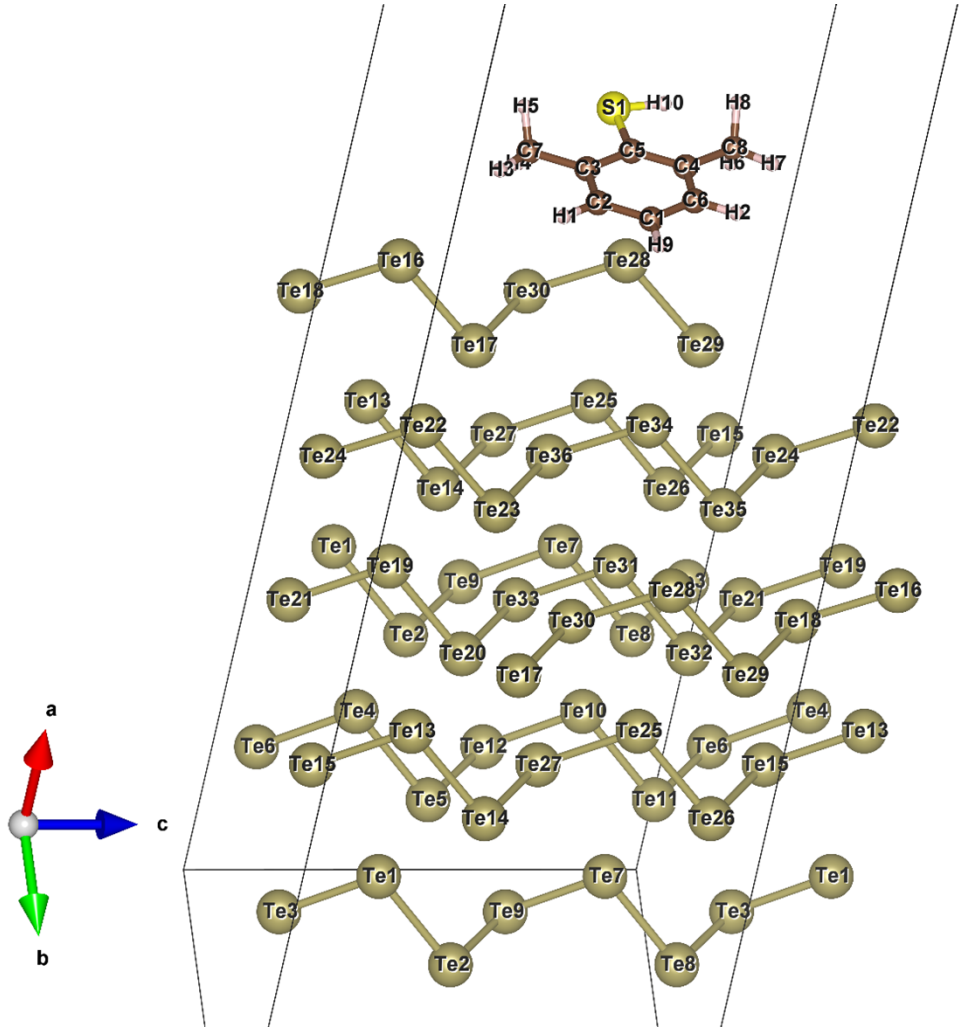
Bi28
Bi18
Bi5
Bi27
Bi17
Bi26
Bi3
Bi25
Bi1
c
a
b

Table S5. The partial electron transfer property of 0D Te QDs to substrate **1n** and its schematic diagram.

Specimen	Elements	Charge transfer	Specimen	Elements	Charge transfer	Gain (+) and loss (-) electron level
0D Te QDs	Te1	5.969	**0D Te QD@1n**	Te1	5.964	-0.005
	Te2	5.956		Te2	5.959	0.003
	Te3	6.082		Te3	6.084	0.002
	Te4	5.969		Te4	5.964	-0.005
	Te5	5.956		Te5	5.959	0.003
	Te6	6.081		Te6	6.083	0.002
	Te7	5.969		Te7	5.963	-0.006
	Te8	5.956		Te8	5.959	0.003
	Te9	6.081		Te9	6.083	0.002
	Te10	5.969		Te10	5.963	-0.006
	Te11	5.956		Te11	5.959	0.003
	Te12	6.082		Te12	6.083	0.001
	Te13	6.006		Te13	6.000	-0.006
	Te14	5.982		Te14	5.990	0.008
	Te15	5.997		Te15	5.998	0.001
	Te16	6.090		Te16	6.090	0.000
	Te17	5.949		Te17	5.937	-0.012
	Te18	5.968		Te18	5.979	0.011
	Te19	6.006		Te19	6.000	-0.006
	Te20	5.981		Te20	5.990	0.009
	Te21	5.997		Te21	5.998	0.001
	Te22	6.091		Te22	6.088	-0.003
	Te23	5.949		Te23	5.937	-0.012
	Te24	5.968		Te24	5.980	0.012
	Te25	6.006		Te25	6.000	-0.006
	Te26	5.982		Te26	5.990	0.008
	Te27	5.997		Te27	5.998	0.001
	Te28	6.091		Te28	6.085	-0.006
	Te29	5.949		Te29	5.941	-0.008
	Te30	5.968		Te30	5.978	0.010
	Te31	6.006		Te31	6.000	-0.006
	Te32	5.981		Te32	5.990	0.009
	Te33	5.997		Te33	5.998	0.001
	Te34	6.091		Te34	6.086	-0.004
	Te35	5.949		Te35	5.941	-0.008
	Te36	5.968		Te36	5.979	0.011
1n	S1	6.000		S1	5.977	-0.023
	C1	4.043		C1	4.013	-0.030
	C2	4.040		C2	4.099	0.059
	C3	3.990		C3	3.927	-0.063
	C4	3.991		C4	3.928	-0.063
	C5	4.167		C5	4.227	0.060
	C6	4.020		C6	4.108	0.088
	C7	4.074		C7	4.088	0.014
	C8	4.037		C8	4.079	0.042
	H1	0.951		H1	0.953	0.002
	H2	0.975		H2	0.958	-0.017
	H3	0.969		H3	0.973	0.004
	H4	0.981		H4	0.927	-0.054
	H5	0.925		H5	0.953	0.028
	H6	0.963		H6	0.965	0.002
	H7	0.970		H7	0.963	-0.007
	H8	0.993		H8	0.964	-0.029
	H9	0.950		H9	0.911	-0.039
	H10	0.960		H10	0.986	0.026


a
c
b
S1
H5
H10
H8
C7
C5
C8
H3
C3
C4
H6
H7
C2
C6
H1
C1
H2
H9
Te16
Te28
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Te6
Te13
Te15
Te27
Te15
Te5
Te11
Te14
Te26
Te1
Te7
Te1
Te3
Te9
Te3
Te2
Te8

Table S6. The partial electron transfer property of 0D Sb QDs to substrate **1n** and its schematic diagram.

Specimen	Elements	Charge transfer	Specimen	Elements	Charge transfer	Gain (+) and loss (-) electron level
0D Sb QDs	Sb1	5.016	**0D Sb QD@1n**	Sb1	5.020	0.004
	Sb2	4.980		Sb2	4.980	0.000
	Sb3	4.990		Sb3	4.986	-0.004
	Sb4	5.014		Sb4	5.008	-0.006
	Sb5	5.016		Sb5	5.019	0.003
	Sb6	4.980		Sb6	4.980	0.000
	Sb7	4.989		Sb7	4.982	-0.007
	Sb8	5.014		Sb8	5.016	0.002
	Sb9	5.016		Sb9	5.019	0.003
	Sb10	4.980		Sb10	4.978	-0.002
	Sb11	4.990		Sb11	4.983	-0.007
	Sb12	5.014		Sb12	5.031	0.017
	Sb13	5.016		Sb13	5.018	0.002
	Sb14	4.980		Sb14	4.982	0.002
	Sb15	4.990		Sb15	4.980	-0.010
	Sb16	5.014		Sb16	4.970	-0.044
1n	S1	6.000		S1	5.990	-0.010
	C1	4.042		C1	4.021	-0.021
	C2	4.040		C2	4.028	-0.012
	C3	3.990		C3	3.957	-0.033
	C4	3.991		C4	3.946	-0.045
	C5	4.166		C5	4.216	0.050
	C6	4.020		C6	4.102	0.082
	C7	4.075		C7	4.077	0.002
	C8	4.037		C8	4.092	0.055
	H1	0.951		H1	0.964	0.013
	H2	0.975		H2	0.960	-0.015
	H3	0.969		H3	1.006	0.037
	H4	0.981		H4	0.943	-0.038
	H5	0.925		H5	0.935	0.010
	H6	0.963		H6	0.953	-0.010
	H7	0.971		H7	0.967	-0.004
	H8	0.993		H8	0.956	-0.037
	H9	0.950		H9	0.954	0.004
	H10	0.960		H10	0.978	0.018
	Sb1	5.016		Sb1	5.020	0.004
	Sb2	4.980		Sb2	4.980	0.000
	Sb3	4.990		Sb3	4.986	-0.004
	Sb4	5.014		Sb4	5.008	-0.006
	Sb5	5.016		Sb5	5.019	0.003
	Sb6	4.980		Sb6	4.980	0.000

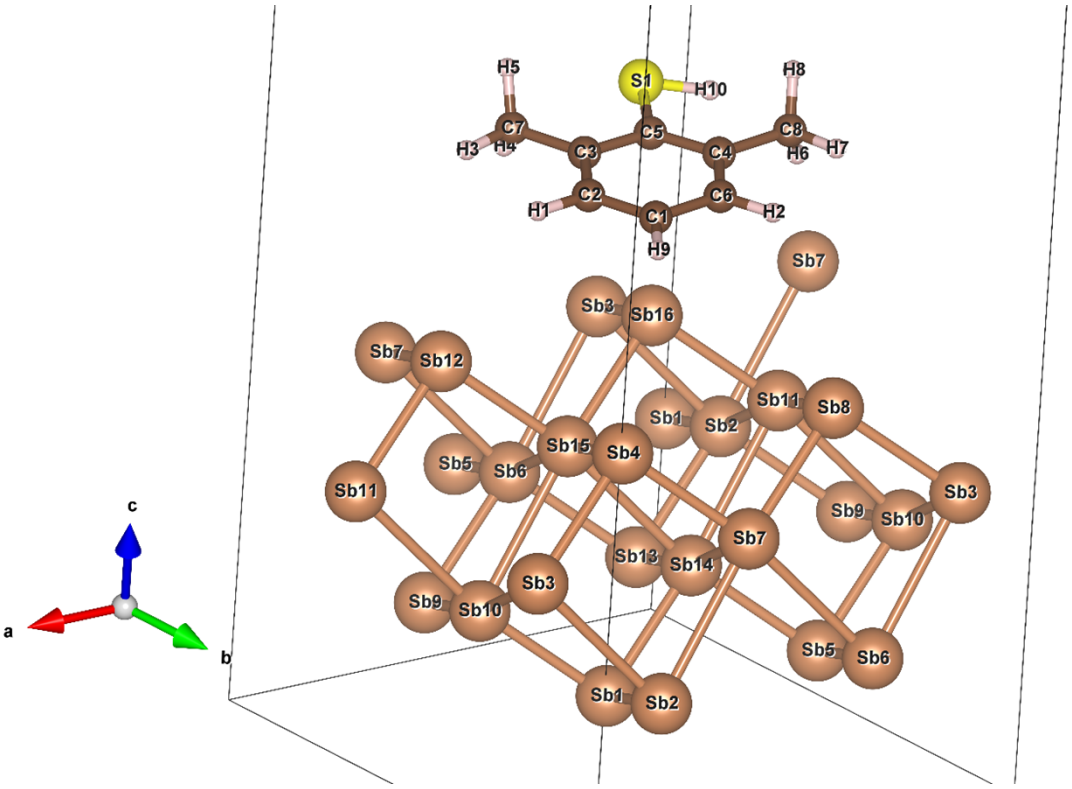

c
a
b
H5
S1
H10
H8
C7
C5
C8
H3
H4
C3
C4
H6
H7
C2
C6
H1
C1
H2
H9
Sb7
Sb3
Sb16
Sb7
Sb12
Sb1
Sb2
Sb11
Sb8
Sb15
Sb4
Sb5
Sb6
Sb11
Sb3
Sb9
Sb10
Sb7
Sb13
Sb14
Sb3
Sb9
Sb10
Sb5
Sb6
Sb1
Sb2

Table S7. The partial electron transfer property of 0D Se QDs to substrate **1n** and its schematic diagram.

Specimen	Elements	Charge transfer	Specimen	Elements	Charge transfer	Gain (+) and loss (-) electron level
0D Se QDs	Se1	5.995	**0D Se QD@1n**	Se1	5.984	-0.011
	Se2	5.972		Se2	5.985	0.013
	Se3	6.035		Se3	6.032	-0.003
	Se4	5.995		Se4	5.984	-0.011
	Se5	5.972		Se5	5.9857	0.013
	Se6	6.035		Se6	6.032	-0.003
	Se7	5.995		Se7	5.984	-0.011
	Se8	5.972		Se8	5.985	0.013
	Se9	6.035		Se9	6.032	-0.003
	Se10	5.995		Se10	5.984	-0.011
	Se11	5.972		Se11	5.985	0.013
	Se12	6.035		Se12	6.032	-0.003
	Se13	6.012		Se13	6.010	-0.002
	Se14	5.993		Se14	5.992	-0.001
	Se15	5.989		Se15	5.993	0.004
	Se16	6.035		Se16	6.043	0.008
	Se17	5.969		Se17	5.970	0.001
	Se18	5.999		Se18	5.987	-0.012
	Se19	6.012		Se19	6.010	-0.002
	Se20	5.993		Se20	5.992	-0.001
	Se21	5.989		Se21	5.993	0.004
	Se22	6.035		Se22	6.043	0.008
	Se23	5.969		Se23	5.969	0.000
	Se24	5.998		Se24	5.987	-0.011
	Se25	6.012		Se25	6.010	-0.002
	Se26	5.993		Se26	5.992	-0.001
	Se27	5.989		Se27	5.993	0.004
	Se28	6.035		Se28	6.043	0.008
	Se29	5.969		Se29	5.974	0.005
	Se30	5.999		Se30	5.987	-0.012
	Se31	6.012		Se31	6.010	-0.002
	Se32	5.993		Se32	5.992	-0.001
	Se33	5.989		Se33	5.993	0.004
	Se34	6.035		Se34	6.047	0.008
	Se35	5.969		Se35	5.974	0.005
	Se36	5.998		Se36	5.987	-0.011
1n	S1	6.000		S1	5.956	-0.044
	C1	4.042		C1	4.073	0.031
	C2	4.040		C2	4.024	-0.016
	C3	3.990		C3	4.007	0.017
	C4	3.990		C4	3.968	-0.022
	C5	4.166		C5	4.178	0.012
	C6	4.019		C6	4.031	0.012
	C7	4.074		C7	4.106	0.032
	C8	4.037		C8	4.034	-0.003
	H1	0.950		H1	0.948	-0.002
	H2	0.975		H2	0.943	-0.032
	H3	0.969		H3	0.947	-0.022
	H4	0.981		H4	0.943	-0.038
	H5	0.925		H5	0.959	0.034
	H6	0.963		H6	0.959	-0.004
	H7	0.970		H7	0.992	0.022
	H8	0.993		H8	0.975	-0.018
	H9	0.950		H9	0.950	0.000
	H10	0.959		H10	1.000	0.041

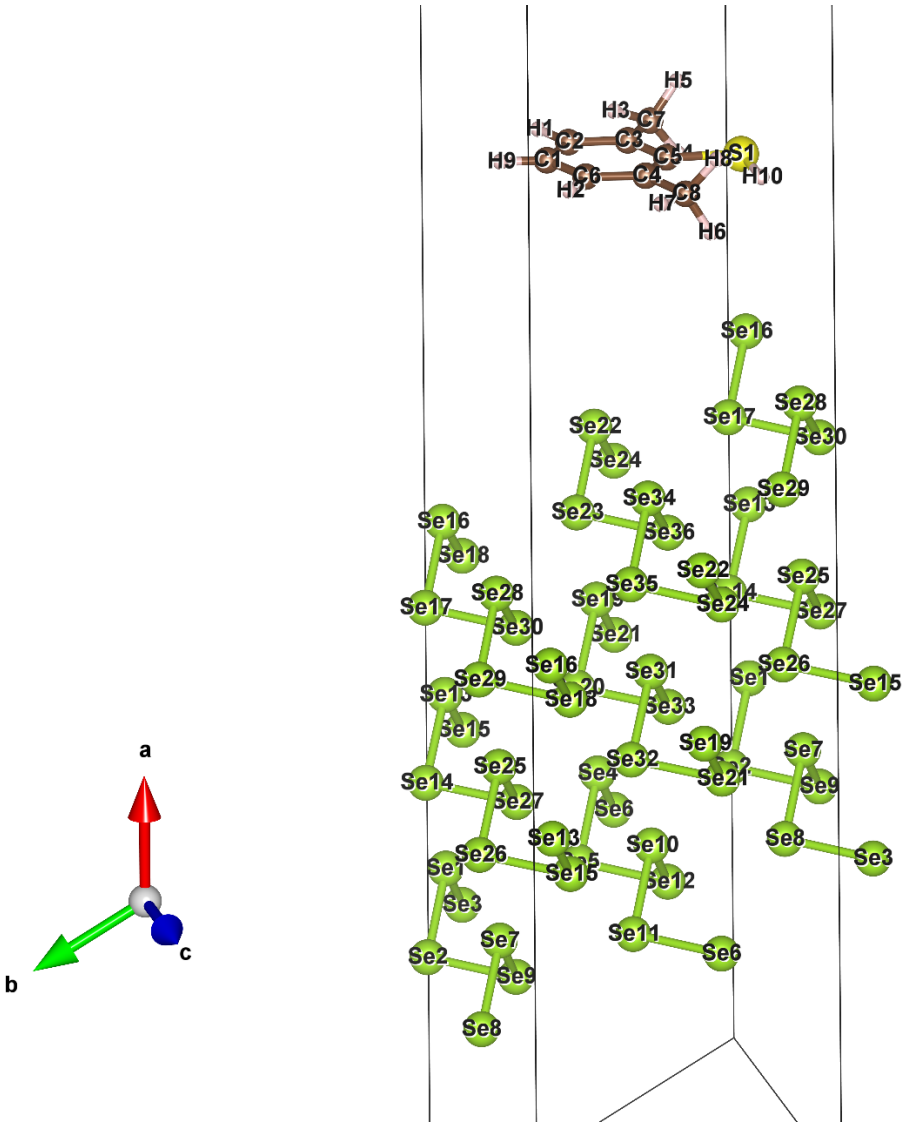
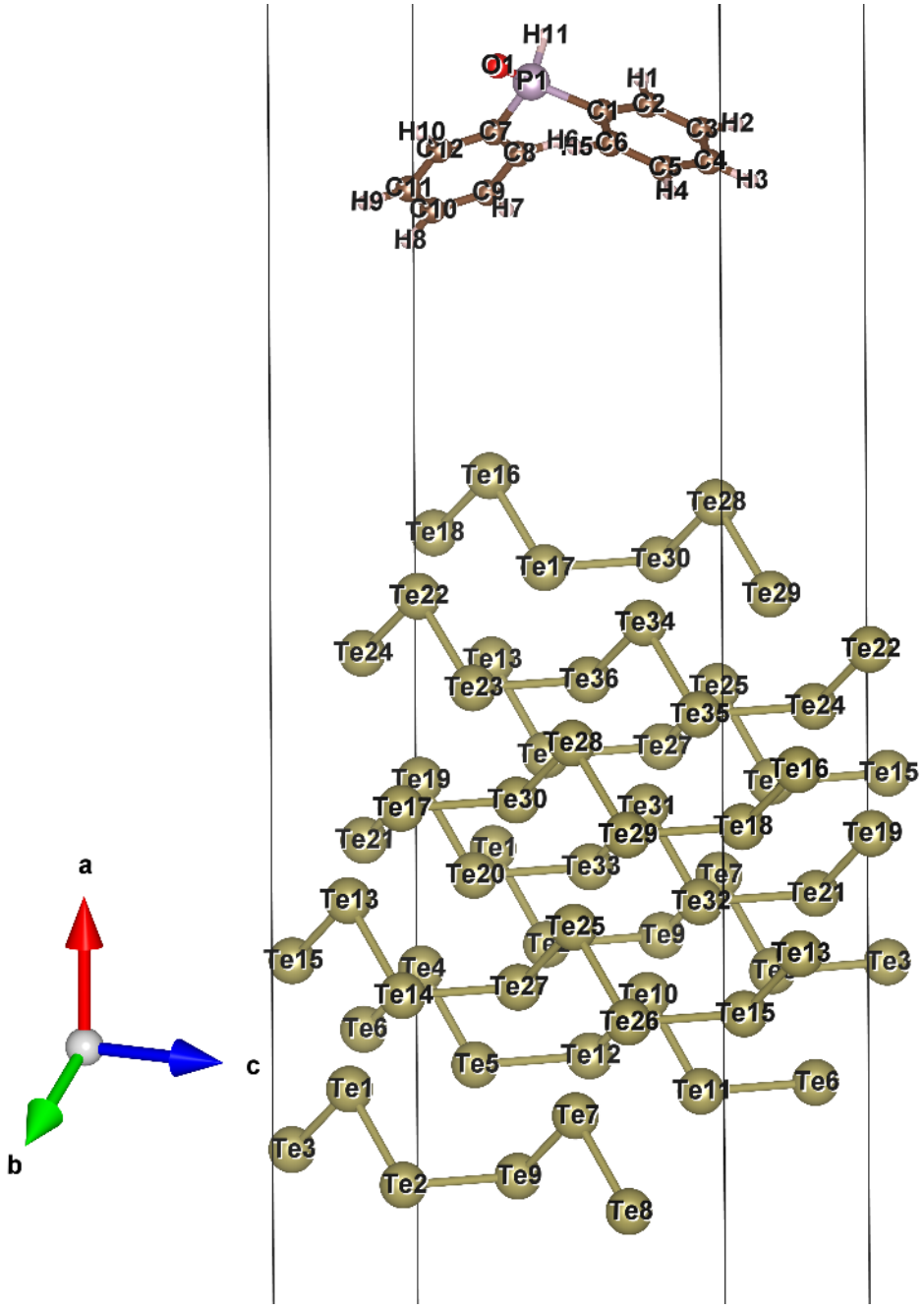

H5
H3
C7
H1
C2
C3
C5
H8
S1
H9
C1
C6
C4
H10
H2
H7
C8
H6
Se16
Se17
Se28
Se30
Se22
Se24
Se29
Se23
Se34
Se36
Se16
Se18
Se22
Se25
Se28
Se35
Se24
Se27
Se17
Se30
Se21
Se16
Se31
Se26
Se29
Se33
Se15
Se19
Se7
Se25
Se32
Se14
Se21
Se9
Se27
Se6
Se13
Se10
Se8
Se3
Se26
Se12
Se3
Se11
Se7
Se6
Se2
Se9
Se8
a
b
c

Table S8. The partial electron transfer property of 0D Te QDs to substrate **2a** and its schematic diagram.

Specimen	Elements	Charge transfer	Specimen	Elements	Charge transfer	Gain (+) and loss (-) electron level
0D Te QDs	Te1	5.969	**0D Te QD@2a**	Te1	5.981	0.012
	Te2	5.956		Te2	5.949	-0.007
	Te3	6.082		Te3	6.070	-0.012
	Te4	5.969		Te4	5.981	0.012
	Te5	5.956		Te5	5.949	-0.007
	Te6	6.081		Te6	6.069	-0.012
	Te7	5.969		Te7	5.981	0.012
	Te8	5.956		Te8	5.949	-0.007
	Te9	6.082		Te9	6.070	-0.012
	Te10	5.969		Te10	5.981	0.012
	Te11	5.956		Te11	5.949	-0.007
	Te12	6.081		Te12	6.069	-0.012
	Te13	6.006		Te13	6.003	-0.003
	Te14	5.981		Te14	5.981	0.000
	Te15	5.997		Te15	6.002	0.005
	Te16	6.090		Te16	6.100	0.010
	Te17	5.949		Te17	5.953	0.004
	Te18	5.968		Te18	5.960	-0.008
	Te19	6.006		Te19	6.003	-0.003
	Te20	5.982		Te20	5.982	0.000
	Te21	5.996		Te21	6.002	0.006
	Te22	6.091		Te22	6.100	0.009
	Te23	5.949		Te23	5.953	0.004
	Te24	5.968		Te24	5.960	-0.008
	Te25	6.006		Te25	6.003	-0.003
	Te26	5.982		Te26	5.982	0.000
	Te27	5.996		Te27	6.002	0.006
	Te28	6.091		Te28	6.099	0.008
	Te29	5.949		Te29	5.953	0.004
	Te30	5.968		Te30	5.959	-0.008
	Te31	6.006		Te31	6.003	-0.003
	Te32	5.982		Te32	5.982	0.000
	Te33	5.996		Te33	6.002	0.006
	Te34	6.091		Te34	6.099	0.008
	Te35	5.948		Te35	5.952	0.004
	Te36	5.968		Te36	5.959	-0.008
2a	S1	2.286		S1	2.275	-0.011
	C1	7.423		C1	7.415	-0.008
	C2	4.607		C2	4.566	-0.041
	C3	3.968		C3	4.041	0.073
	C4	4.100		C4	4.070	-0.030
	C5	4.052		C5	4.082	0.030
	C6	3.926		C6	4.026	0.100
	C7	4.056		C7	4.017	-0.039
	C8	4.519		C8	4.547	0.028
	H1	4.005		H1	4.079	0.074
	H2	4.096		H2	4.030	-0.066
	H3	4.057		H3	4.043	-0.014
	H4	3.976		H4	4.074	0.098
	H5	4.114		H5	4.040	-0.074
	H6	0.960		H6	0.971	0.011
	H7	0.957		H7	0.918	-0.039
	H8	0.933		H8	0.918	-0.015
	H9	0.949		H9	0.940	-0.009
	H10	0.928		H10	0.890	-0.038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O1
P1
H1
C1
C2
C3
H2
H10
C7
H6
C12
C8
H5
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C4
H3
H4
C11
C9
H9
C10
H7
H8
Te16
Te28
Te18
Te17
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Te33
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Te32
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Te9
Te15
Te4
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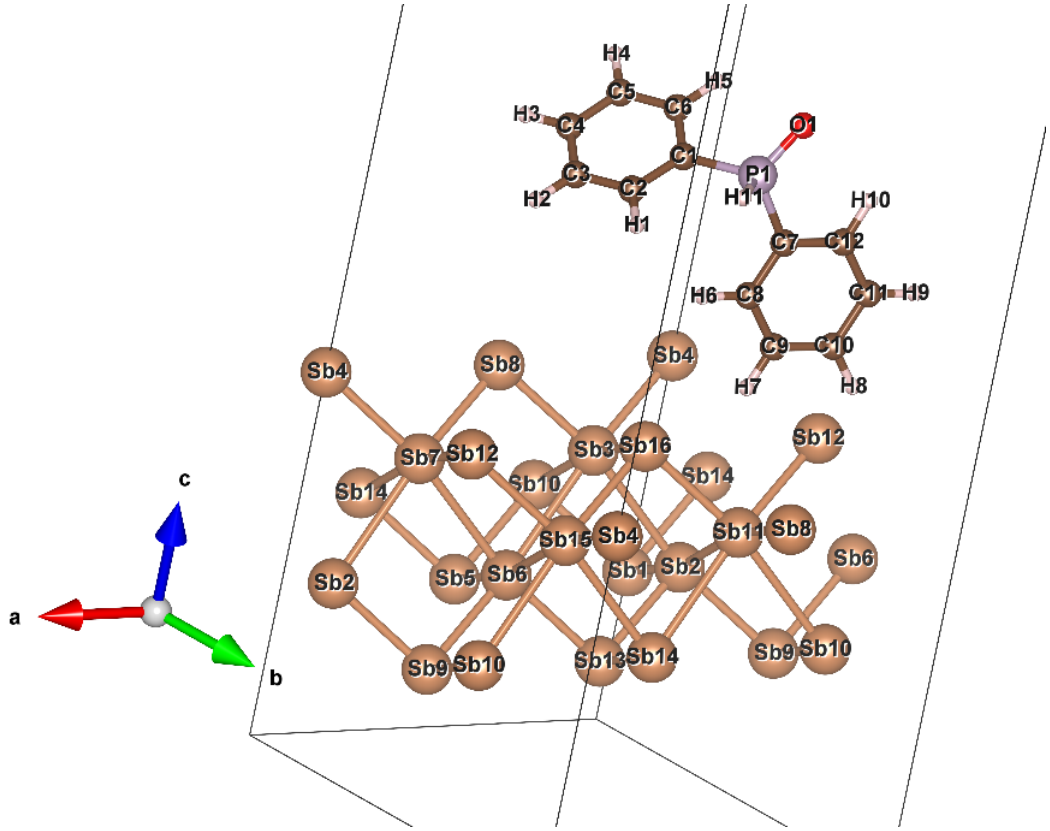
Te3
Te14
Te27
Te10
Te26
Te15
Te6
Te5
Te12
Te11
Te6
Te1
Te7
Te3
Te2
Te9
Te8
a
b
c

Table S9. The partial electron transfer property of 0D Sb QDs to substrate **2a** and its schematic diagram.

Specimen	Elements	Charge transfer	Specimen	Elements	Charge transfer	Gain (+) and loss (-) electron level
0D Sb QDs	Sb1	5.015	**0D Sb QD@2a**	Sb1	5.011	-0.004
	Sb2	4.980		Sb2	4.985	0.005
	Sb3	4.990		Sb3	4.975	-0.015
	Sb4	5.014		Sb4	5.028	0.014
	Sb5	5.016		Sb5	5.011	-0.005
	Sb6	4.980		Sb6	4.985	0.005
	Sb7	4.990		Sb7	4.977	-0.013
	Sb8	5.014		Sb8	5.022	0.008
	Sb9	5.016		Sb9	5.009	-0.007
	Sb10	4.980		Sb10	4.984	0.004
	Sb11	4.990		Sb11	4.980	-0.010
	Sb12	5.014		Sb12	5.014	0.000
	Sb13	5.015		Sb13	5.009	-0.006
	Sb14	4.980		Sb14	4.985	0.005
	Sb15	4.990		Sb15	4.980	-0.010
	Sb16	5.014		Sb16	5.016	0.002
2a	S1	2.287		S1	2.294	0.007
	C1	7.423		C1	7.411	-0.012
	C2	4.608		C2	4.603	-0.005
	C3	3.968		C3	4.015	0.047
	C4	4.100		C4	4.059	-0.041
	C5	4.053		C5	4.036	-0.017
	C6	3.926		C6	4.048	0.122
	C7	4.056		C7	4.038	-0.018
	C8	4.519		C8	4.560	0.041
	H1	4.005		H1	4.060	0.055
	H2	4.096		H2	4.015	-0.081
	H3	4.057		H3	4.036	-0.021
	H4	3.976		H4	4.069	0.093
	H5	4.114		H5	4.012	-0.102
	H6	0.960		H6	0.942	-0.018
	H7	0.957		H7	0.948	-0.009
	H8	0.933		H8	0.940	0.007
	H9	0.949		H9	0.913	-0.036
	H10	0.928		H10	0.895	-0.033
	Sb1	0.952		Sb1	0.935	-0.017
	Sb2	0.948		Sb2	0.968	0.020
	Sb3	0.930		Sb3	0.941	0.011
	Sb4	0.909		Sb4	0.939	0.030
	Sb5	0.890		Sb5	0.922	0.032
	Sb6	1.455		Sb6	1.427	-0.028


H4
H5
C5
C6
H3
C4
O1
C1
P1
C3
C2
H11
H10
H2
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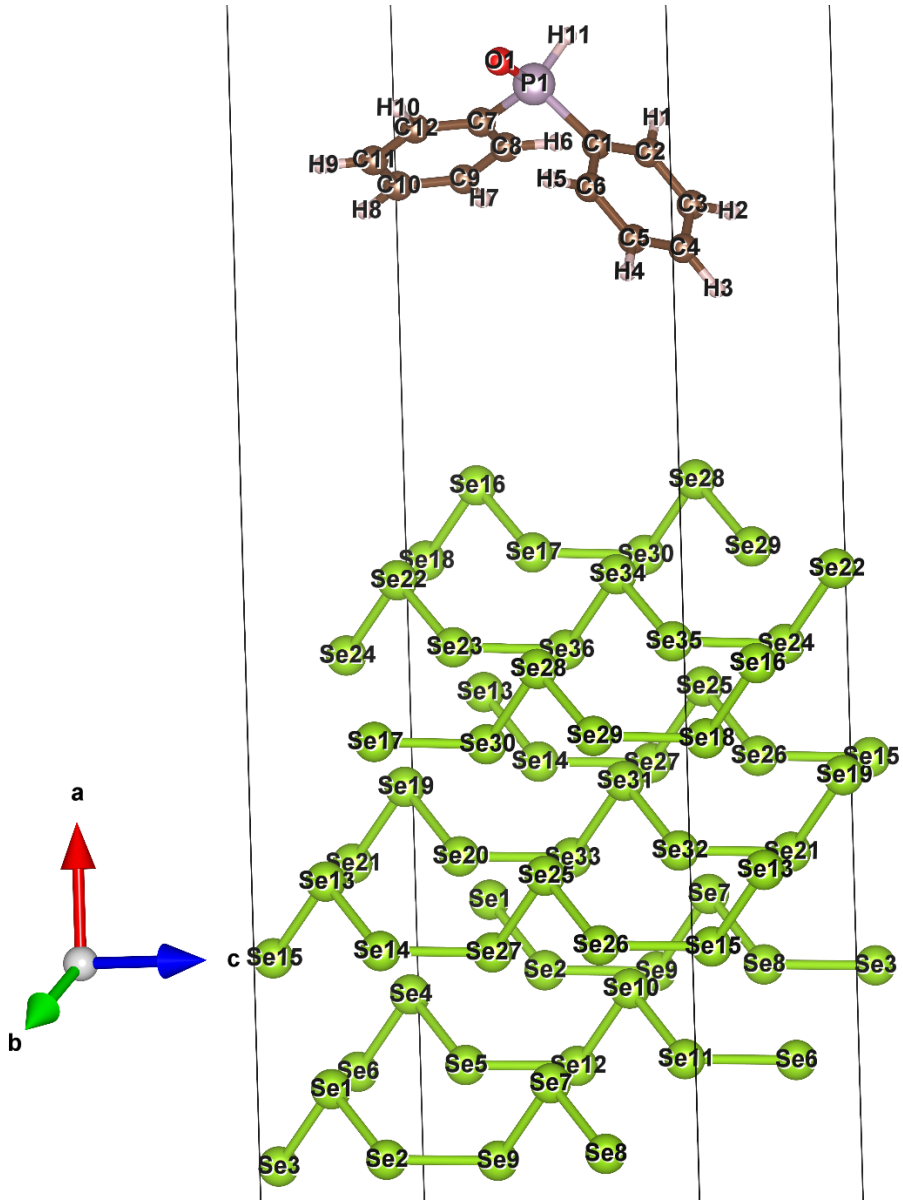
C12
H6
C8
C11
H9
C9
C10
H7
H8
Sb4
Sb8
Sb4
Sb12
Sb7
Sb12
Sb3
Sb16
Sb14
Sb10
Sb14
Sb15
Sb4
Sb11
Sb8
Sb6
Sb2
Sb5
Sb6
Sb1
Sb2
Sb9
Sb10
Sb13
Sb14
Sb9
Sb10
c
a
b

Table S10. The partial electron transfer property of 0D Se QDs to substrate **2a** and its schematic diagram.

Specimen	Elements	Charge transfer	Specimen	Elements	Charge transfer	Gain (+) and loss (-) electron level
0D Se QDs	Se1	5.995	**0D Se QD@2a**	Se1	5.982	-0.013
	Se2	5.972		Se2	5.981	0.009
	Se3	6.035		Se3	6.033	-0.002
	Se4	5.995		Se4	5.983	-0.012
	Se5	5.972		Se5	5.981	0.009
	Se6	6.035		Se6	6.032	-0.003
	Se7	5.995		Se7	5.982	-0.013
	Se8	5.972		Se8	5.981	0.009
	Se9	6.035		Se9	6.033	-0.002
	Se10	5.995		Se10	5.982	-0.013
	Se11	5.972		Se11	5.981	0.009
	Se12	6.035		Se12	6.033	-0.002
	Se13	6.012		Se13	6.004	-0.008
	Se14	5.993		Se14	5.997	0.004
	Se15	5.989		Se15	5.995	0.006
	Se16	6.035		Se16	6.035	0.000
	Se17	5.969		Se17	5.980	0.011
	Se18	5.998		Se18	5.991	-0.007
	Se19	6.012		Se19	6.004	-0.008
	Se20	5.993		Se20	5.997	0.004
	Se21	5.989		Se21	5.995	0.006
	Se22	6.035		Se22	6.035	0.000
	Se23	5.968		Se23	5.980	0.012
	Se24	5.998		Se24	5.990	-0.008
	Se25	6.012		Se25	6.004	-0.008
	Se26	5.993		Se26	5.997	0.004
	Se27	5.989		Se27	5.995	0.006
	Se28	6.035		Se28	6.033	-0.002
	Se29	5.968		Se29	5.981	0.013
	Se30	5.998		Se30	5.990	-0.008
	Se31	6.012		Se31	6.004	-0.008
	Se32	5.993		Se32	5.997	0.004
	Se33	5.989		Se33	5.995	0.006
	Se34	6.035		Se34	6.033	-0.002
	Se35	5.968		Se35	5.982	0.014
	Se36	5.998		Se36	5.990	-0.008
2a	S1	2.287		S1	2.275	-0.012
	C1	7.423		C1	7.420	-0.003
	C2	4.607		C2	4.476	-0.131
	C3	3.967		C3	4.147	0.180
	C4	4.100		C4	4.059	-0.041
	C5	4.052		C5	4.057	0.005
	C6	3.926		C6	4.034	0.108
	C7	4.056		C7	4.025	-0.031
	C8	4.519		C8	4.598	0.079
	H1	4.004		H1	4.046	0.042
	H2	4.095		H2	4.071	-0.024
	H3	4.056		H3	4.029	-0.027
	H4	3.975		H4	4.028	0.053
	H5	4.114		H5	4.028	-0.086
	H6	0.960		H6	0.919	-0.041
	H7	0.957		H7	0.952	-0.005
	H8	0.934		H8	0.930	-0.004
	H9	0.949		H9	0.954	0.005
	H10	0.928		H10	0.895	-0.033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H9
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C8
H6
C1
C2
C10
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H5
C6
C3
H2
H8
H7
C5
C4
H4
H3
Se16
Se28
Se18
Se17
Se30
Se29
Se22
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Se25
Se13
Se1
Se7
a
c Se15
Se14
Se27
Se26
Se15
Se8
Se3
Se2
Se9
Se10
b
Se4
Se6
Se5
Se12
Se11
Se6
Se1
Se7
Se3
Se2
Se9
Se8

Table S11. The average of the five biggest absolute change differences ($|\Delta q|$) between the photocatalyst surface and substrate.

Sample	$\|\Delta q\|/e^-$
0D Bi QD@1n	1.097
2D Bi QD@1n	0.228
0D Bi QD@2a	0.824
2D Bi QD@2a	0.697
0D Te QD@1n	0.067
0D Sb QD@1n	0.055
0D Se QD@1n	0.037
0D Te QD@2a	0.084
0D Sb QD@2a	0.089
0D Se QD@2a	0.117

The TEM images of all the obtained QDs (Sb QDs, Te QDs and Se QDs) exhibit a very uniform distribution with a narrow size of 3-5 nm (**Figure S1a**, **Figure S2a** and **Figure S3a**). The atomic arrangements of the obtained QDs are also confirmed by HRTEM image (**Figure S1b**, **Figure S2b** and **Figure S3b**). In addition, all the obtained QDs show strong adsorption in the UV-Vis region (**Figure S1c**, **Figure S2c** and **Figure S3c**).

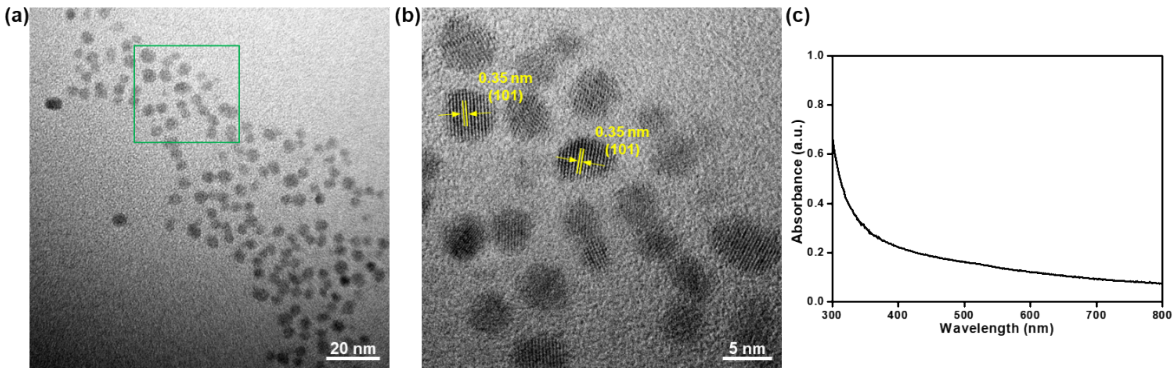


Fig. S1. Structural characterization of 0D Sb QDs. (a) TEM image, (b) HRTEM image, and (c) UV-Vis spectrum.

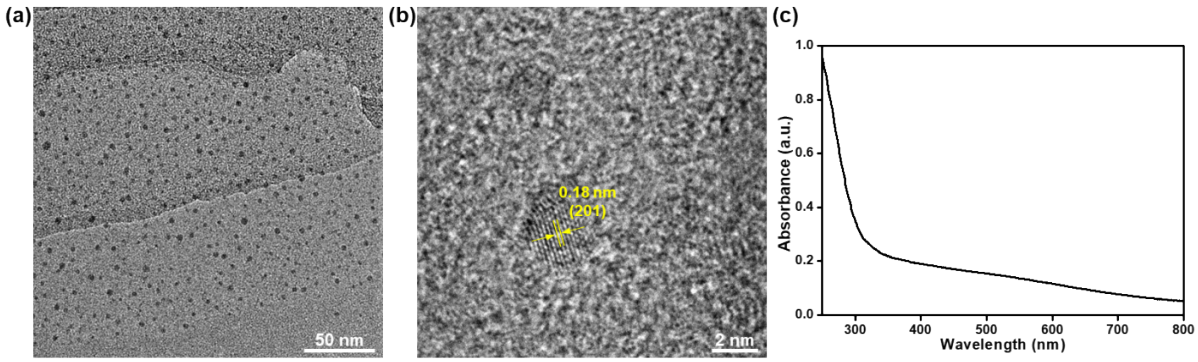


Fig. S2. Structural characterization of 0D Te QDs. (a) TEM image, (b) HRTEM image, and (c) UV-Vis spectrum.

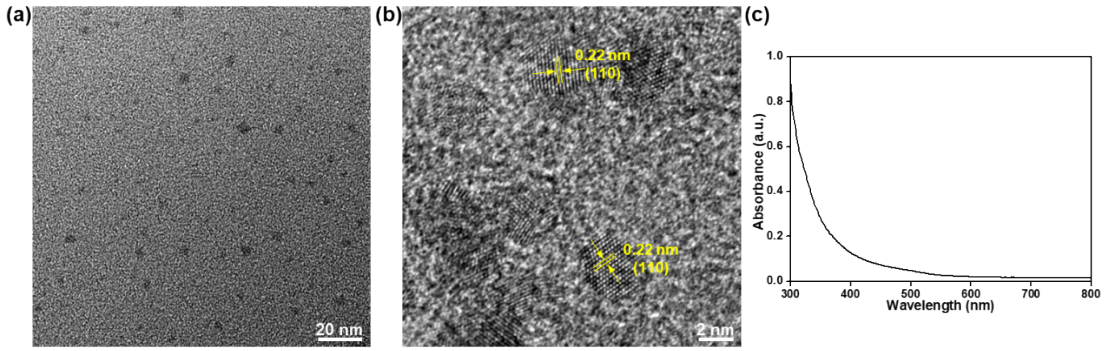


Fig. S3. Structural characterization of 0D Se QDs. (a) TEM image, (b) HRTEM image, and (c) UV-Vis spectrum.

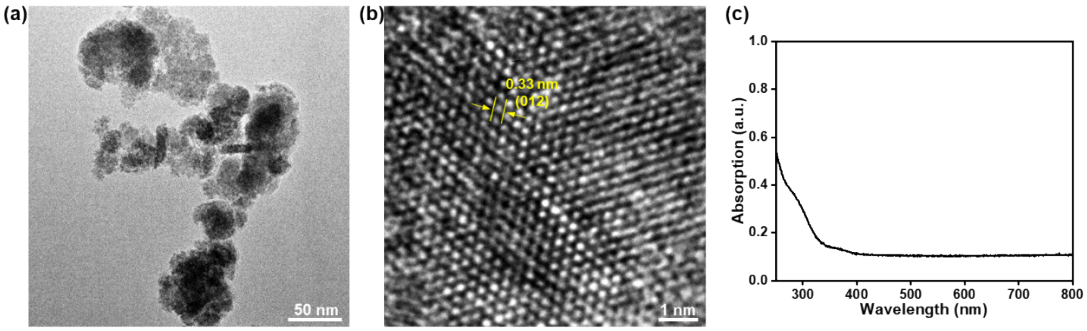
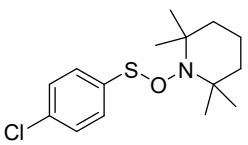


Fig. S4. Structural characterization of 2D Bi NSs. (a) TEM image, (b) HRTEM image, and (c) UV-Vis spectrum.

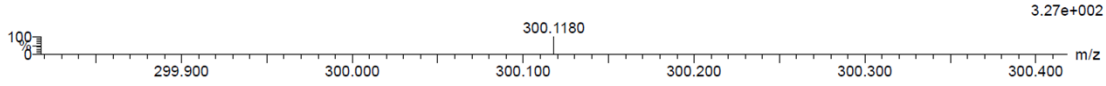
Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
83 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 14-15 H: 20-28 N: 0-2 O: 0-4 S: 0-2 Cl: 0-2



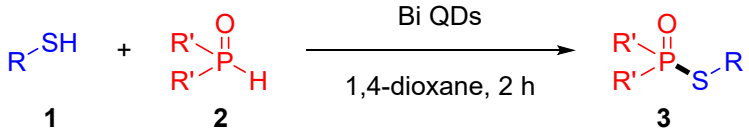
HZH-383 51 (0.383)
1: TOF MS ES+



Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
300.1180	300.1189	-0.9	-3.0	4.5	21.3	n/a	n/a	C15 H23 N O S Cl

Fig. S5. HRMS of radical quenching intermediate. (**HRMS [ESI]**: m/z calculated for $C_{15}H_{22}ClNOS$ $[M+H]^+$ 300.1183, found 300.1180.)

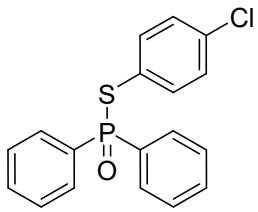
Synthesis of thiophosphinates:



1 **2** **3**

To an oven dried reaction vessel equipped with a stirring bar was charged with phosphine oxide (0.4 mmol), 1,4-dioxane solution of Bi QDs (1 M, 1 ml) was added followed by the addition of thiol (0.2 mmol). The reaction vessel was then sealed and stirred at ambient temperature under blue light irradiation for 2 hours. The reaction was stopped when it completed, monitored by TLC. The crude product was purified by column chromatography using silica gel with ethyl acetate in petroleum ether as the eluent.

S-(4-chlorophenyl) diphenylphosphinothioate (3a)[1]



Yield: 87%, white solid.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.83-7.72 (m, 4H), 7.49-7.43 (m, 2H), 7.42-7.36 (m, 4H), 7.32-7.27 (m, 2H), 7.14-7.07 (m, 2H).

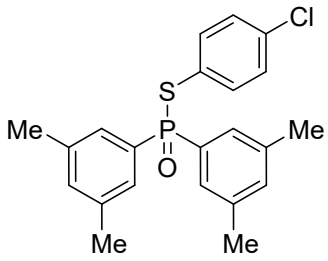
^{13}C NMR (101 MHz, $CDCl_3$) δ 136.57, 136.53, 135.58, 135.55, 132.67, 132.55, 132.52, 131.66, 131.60, 131.56, 129.36, 129.34, 128.73, 128.60, 124.67, 124.62.

^{31}P NMR (162 MHz, $CDCl_3$) δ 41.68.

IR (ATR): $\tilde{\nu}$= 2922, 1674, 1588, 1438, 1129, 960, 728, 551 cm^{-1}.

HRMS [ESI]: m/z calculated for $C_{18}H_{14}ClOPS$ $[M+H]^+$ 345.0264, found 345.0266.

S-(4-chlorophenyl) bis(3,5-dimethylphenyl)phosphinothioate (3b)



Yield: 78%, white solid.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.35 (d, *J* = 13.3 Hz, 4H), 7.32-7.28 (m, 2H), 7.13-7.09 (m, 2H), 7.06 (s, 2H), 2.25 (s, 12H).

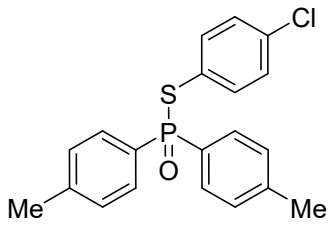
^{13}C NMR (101 MHz, $CDCl_3$) δ 138.44, 138.31, 136.56, 136.52, 135.40, 135.37, 134.24, 134.21, 132.44, 131.38, 129.28, 129.26, 129.16, 129.05, 125.16, 125.11, 21.32.

^{31}P NMR (162 MHz, $CDCl_3$) δ 43.07.

IR (ATR): $\tilde{\nu}$= 3433, 2920, 1598, 1471, 1385, 1202, 1085, 819, 692, 586 cm^{-1}.

HRMS [ESI]: m/z calculated for $C_{22}H_{22}ClOPS$ $[M+H]^+$ 401.0890, found 401.0897.

S-(4-chlorophenyl) di-p-tolylphosphinothioate (3c)[2]



Yield: 73%, white solid.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.68-7.60 (m, 4H), 7.33-7.28 (m, 2H), 7.20-7.16 (m, 4H), 7.13-7.08 (m, 2H), 2.32 (s, 6H).

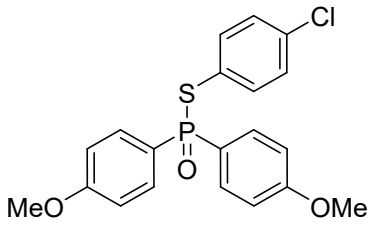
^{13}C NMR (101 MHz, $CDCl_3$) δ 143.12, 143.09, 136.42, 136.38, 135.35, 135.33, 131.67, 131.56, 129.62, 129.44, 129.30, 129.28, 128.53, 125.21, 125.16, 21.67, 21.66.

^{31}P NMR (162 MHz, $CDCl_3$) δ 42.26.

IR (ATR): $\tilde{\nu}$= 3423, 2920, 1600, 1474, 1397, 1201, 1113, 964, 808, 661, 532 cm^{-1}.

HRMS [ESI]: m/z calculated for $C_{20}H_{18}ClOPS$ $[M+H]^+$ 373.0577, found 373.0580.

S-(4-chlorophenyl) bis(4-methoxyphenyl)phosphinothioate (3d)



Yield: 83%, white solid.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.80-7.72 (m, 4H), 7.41-7.36 (m, 2H), 7.21-7.15 (m, 2H), 6.99-6.92 (m, 4H), 3.84 (s, 6H).

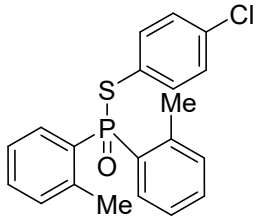
^{13}C NMR (101 MHz, $CDCl_3$) δ 162.83, 162.80, 136.35, 136.31, 135.27, 135.24, 133.60, 133.48, 129.27, 129.25, 125.54, 125.49, 124.10, 122.96, 114.21, 114.07, 55.41.

^{31}P NMR (162 MHz, $CDCl_3$) δ 41.86.

IR (ATR): $\tilde{\nu}$= 3404, 2925, 2838, 2308, 1595, 1501, 1439, 1255, 1116, 952, 817, 668, 546 cm^{-1}.

HRMS [ESI]: m/z calculated for $C_{20}H_{18}ClO_3PS$ $[M+H]^+$ 405.0476, found 405.0475.

S-(4-chlorophenyl) di-o-tolylphosphinothioate (3e)



Yield: 81%, white solid.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.78 (ddd, *J* = 15.2, 7.7, 1.3 Hz, 2H), 7.47-7.39 (m, 4H), 7.29-7.19 (m, 6H), 2.42 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 142.01, 141.91, 136.88, 136.85, 135.47, 135.44, 132.71, 132.59,

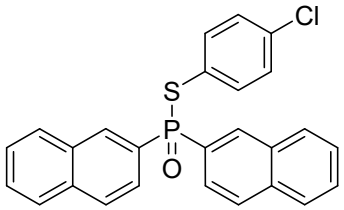
132.48, 132.45, 132.04, 131.92, 131.61, 130.59, 129.23, 129.21, 125.71, 125.58, 124.86, 124.81, 21.50, 21.46.

^{31}P NMR (162 MHz, $CDCl_3$) δ 44.04.

IR (ATR): $\tilde{\nu}$= 3429, 3056, 2924, 2852, 1590, 1473, 1385, 1192, 1087, 1012, 748, 559 cm^{-1}.

HRMS [ESI]: m/z calculated for $C_{20}H_{18}ClOPS$ $[M+H]^+$ 373.0577, found 373.0579.

S-(4-chlorophenyl) di(naphthalen-2-yl)phosphinothioate (3f)



Yield: 92%, white solid.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.36 (dd, *J* = 15.0, 1.3 Hz, 2H), 7.86-7.70 (m, 8H), 7.51-7.39 (m, 4H), 7.35-7.29 (m, 2H), 7.05-6.98 (m, 2H).

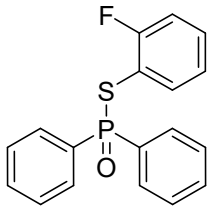
^{13}C NMR (101 MHz, $CDCl_3$) δ 136.60, 136.56, 135.65, 135.62, 134.93, 134.91, 134.13, 134.03, 132.49, 132.34, 129.75, 129.45, 129.43, 129.12, 128.69, 128.67, 128.56, 127.88, 127.87, 127.19, 127.18, 126.15, 126.03, 124.66, 124.61.

^{31}P NMR (162 MHz, $CDCl_3$) δ 41.78.

IR (ATR): $\tilde{\nu}$= 3435, 3053, 2924, 2853, 1587, 1473, 1199, 1089, 819, 753, 643, 546 cm^{-1}.

HRMS [ESI]: m/z calculated for $C_{26}H_{18}ClOPS$ $[M+H]^+$ 445.0577, found 445.0580.

S-(2-fluorophenyl) diphenylphosphinothioate (3g)[3]



Yield: 61%, white solid.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.84-7.76 (m, 4H), 7.64-7.58 (m, 1H), 7.48-7.41 (m, 2H), 7.39-7.34 (m, 4H), 7.19-7.11 (m, 1H), 6.99-6.82 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 163.84, 163.80, 161.37, 161.33, 137.88, 137.84, 132.78, 132.54, 132.51, 131.71, 131.67, 131.62, 131.56, 131.36, 131.34, 131.28, 131.26, 131.18, 128.64, 128.51, 128.34, 128.20, 124.74, 124.72, 124.70, 124.68, 116.09, 116.08, 115.87, 115.85, 113.57, 113.52, 113.39, 113.34.

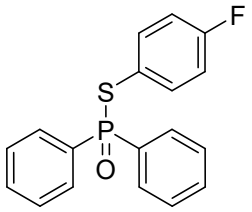
^{31}P NMR (162 MHz, $CDCl_3$) δ 42.14, 42.12.

^{19}F NMR (376 MHz, $CDCl_3$) δ -111.31, -111.32.

IR (ATR): $\tilde{\nu}$= 3478, 2923, 1646, 1438, 1129, 959, 692, 551 cm^{-1}.

HRMS [ESI]: m/z calculated for $C_{18}H_{14}FOPS$ $[M+H]^+$ 329.0560, found 329.0556.

S-(4-fluorophenyl) diphenylphosphinothioate (3h)[4]



Yield: 88%, white solid.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.83-7.70 (m, 4H), 7.48-7.41 (m, 2H), 7.40-7.29 (m, 6H), 6.86-6.77 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 164.66, 164.63, 162.17, 162.15, 137.51, 137.47, 137.42, 137.39, 132.48, 132.45, 131.66, 131.64, 131.59, 131.54, 128.69, 128.56, 121.16, 121.13, 121.11, 121.08, 116.48, 116.46, 116.26, 116.24.

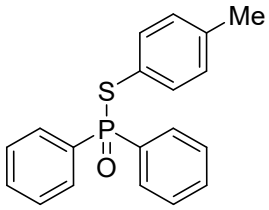
^{31}P NMR (162 MHz, $CDCl_3$) δ 41.69, 41.67.

^{19}F NMR (376 MHz, $CDCl_3$) δ -111.64, -111.65.

IR (ATR): $\tilde{\nu}$= 3061, 2922, 1585, 1487, 1397, 1206, 1094, 961, 836, 695, 558 cm^{-1}.

HRMS [ESI]: m/z calculated for $C_{18}H_{14}FOPS$ $[M+H]^+$ 329.0560, found 329.0566.

S-(p-tolyl) diphenylphosphinothioate (3i)[4]



Yield: 80%, white solid.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.83-7.72 (m, 4H), 7.47-7.40 (m, 2H), 7.40-7.33 (m, 4H), 7.28-7.21 (m, 2H), 6.93 (d, *J* = 7.9 Hz, 2H), 2.17 (s, 3H).

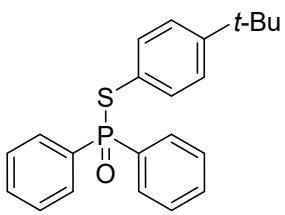
^{13}C NMR (101 MHz, $CDCl_3$) δ 139.23, 139.21, 135.40, 135.37, 133.14, 132.29, 132.26, 132.08, 131.70, 131.60, 129.99, 129.97, 128.59, 128.46, 122.22, 122.17, 21.19.

^{31}P NMR (162 MHz, $CDCl_3$) δ 41.46.

IR (ATR): $\tilde{\nu}$= 3445, 3049, 1645, 1437, 1209, 996, 810, 695, 557 cm^{-1}.

HRMS [ESI]: m/z calculated for $C_{19}H_{17}OPS$ $[M+H]^+$ 325.0810, found 325.0811.

S-(4-(tert-butyl)phenyl) diphenylphosphinothioate (3j)[4]



Yield: 79%, white solid.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.81-7.73 (m, 4H), 7.47-7.41 (m, 2H), 7.40-7.34 (m, 4H), 7.30-7.25 (m, 2H), 7.17-7.12 (m, 2H), 1.16 (s, 9H).

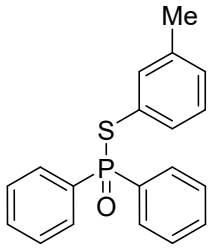
^{13}C NMR (101 MHz, $CDCl_3$) δ 152.30, 152.27, 135.25, 135.22, 133.17, 132.27, 132.24, 132.11, 131.70, 131.60, 128.57, 128.43, 126.33, 126.31, 122.24, 122.19, 34.61, 31.15.

^{31}P NMR (162 MHz, $CDCl_3$) δ 41.71.

IR (ATR): $\tilde{\nu}$= 3444, 2950, 1586, 1436, 1208, 1112, 828, 695, 524 cm^{-1}.

HRMS [ESI]: m/z calculated for $C_{22}H_{23}OPS$ $[M+H]^+$ 367.1280, found 367.1279.

S-(m-tolyl) diphenylphosphinothioate (3k)[1]



Yield: 80%, white solid.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.82-7.72 (m, 4H), 7.47-7.40 (m, 2H), 7.40-7.33 (m, 4H), 7.19-7.13 (m, 2H), 7.04-6.94 (m, 2H), 2.14 (s, 3H).

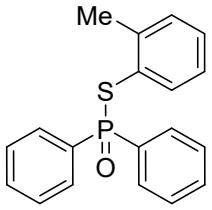
^{13}C NMR (101 MHz, $CDCl_3$) δ 138.99, 138.97, 136.10, 136.06, 133.16, 132.39, 132.35, 132.28, 132.25, 132.10, 131.71, 131.61, 129.82, 129.80, 128.90, 128.88, 128.56, 128.43, 125.70, 125.65, 21.20.

^{31}P NMR (162 MHz, $CDCl_3$) δ 41.32.

IR (ATR): $\tilde{\nu}$= 3440, 3057, 2921, 1590, 1436, 1207, 1112, 781, 695, 568 cm^{-1}.

HRMS [ESI]: m/z calculated for $C_{19}H_{17}OPS$ $[M+H]^+$ 325.0810, found 325.0806.

S-(o-tolyl) diphenylphosphinothioate (3l)[4]



Yield: 75%, white solid.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.90-7.79 (m, 4H), 7.58-7.50 (m, 2H), 7.50-7.42 (m, 5H), 7.23-7.13 (m, 2H), 7.03 (td, *J* = 7.4, 1.9 Hz, 1H), 2.36 (s, 3H).

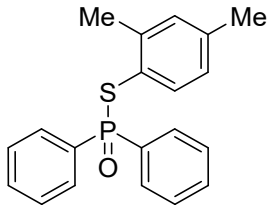
^{13}C NMR (101 MHz, $CDCl_3$) δ 142.93, 142.89, 136.81, 136.77, 133.28, 132.32, 132.29, 132.22, 131.55, 131.45, 130.73, 130.71, 129.33, 129.30, 128.55, 128.42, 126.49, 126.47, 125.38, 125.33, 21.45.

^{31}P NMR (162 MHz, $CDCl_3$) δ 41.13.

IR (ATR): $\tilde{\nu}$= 3435, 3076, 2923, 1644, 1588, 1438, 1129, 959, 692, 525 cm^{-1}.

HRMS [ESI]: m/z calculated for $C_{19}H_{17}OPS$ $[M+H]^+$ 325.0810, found 325.0811.

S-(2,4-dimethylphenyl) diphenylphosphinothioate (3m)[5]



Yield: 95%, pale yellow solid.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.89-7.81 (m, 4H), 7.55-7.50 (m, 2H), 7.48-7.42 (m, 4H), 7.34-7.30 (m, 1H), 6.98 (s, 1H), 6.84 (dd, *J* = 8.0, 1.9 Hz, 1H), 2.33 (s, 3H), 2.25 (s, 3H).

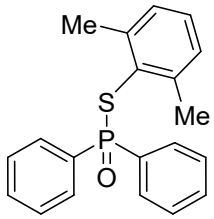
^{13}C NMR (101 MHz, $CDCl_3$) δ 142.78, 142.75, 139.52, 139.49, 136.77, 136.74, 133.45, 132.39, 132.26, 132.23, 131.67, 131.65, 131.58, 131.48, 128.52, 128.39, 127.36, 127.34, 121.52, 121.47, 21.39, 21.12.

^{31}P NMR (162 MHz, $CDCl_3$) δ 40.95.

IR (ATR): $\tilde{\nu}$= 3075, 2920, 1587, 1436, 1276, 1198, 1109, 961, 832, 695, 546 cm^{-1}.

HRMS [ESI]: m/z calculated for $C_{20}H_{19}OPS$ $[M+H]^+$ 339.0967, found 339.0969.

S-(2,6-dimethylphenyl) diphenylphosphinothioate (3n)[6]



Yield: 89%, white solid.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.83-7.73 (m, 4H), 7.59-7.52 (m, 2H), 7.49-7.41 (m, 4H), 7.17-7.11 (m, 1H), 7.07-7.01 (m, 2H), 2.31 (s, 6H).

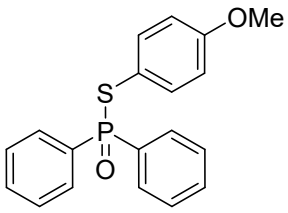
^{13}C NMR (101 MHz, $CDCl_3$) δ 145.15, 145.12, 133.64, 132.59, 132.29, 132.26, 131.38, 131.27, 129.32, 129.29, 128.48, 128.40, 128.38, 128.35, 124.49, 124.43, 22.57.

^{31}P NMR (162 MHz, $CDCl_3$) δ 39.89.

IR (ATR): $\tilde{\nu}$= 3445, 3050, 2923, 1581, 1437, 1191, 1111, 777, 698, 567 cm^{-1}.

HRMS [ESI]: m/z calculated for $C_{20}H_{19}OPS$ $[M+H]^+$ 339.0967, found 339.0964.

S-(4-methoxyphenyl) diphenylphosphinothioate (3o)[1]



Yield: 74%, white solid.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.91-7.82 (m, 4H), 7.56-7.50 (m, 2H), 7.49-7.43 (m, 4H), 7.39-7.32 (m, 2H), 6.78-6.72 (m, 2H), 3.75 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 160.46, 160.44, 137.09, 137.05, 133.13, 132.26, 132.23, 132.07,

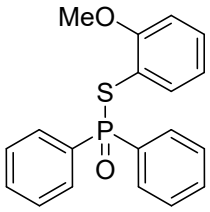
131.69, 131.59, 128.58, 128.45, 116.00, 115.94, 114.81, 114.80, 55.29.

^{31}P NMR (162 MHz, $CDCl_3$) δ 41.41.

IR (ATR): $\tilde{\nu}$= 3431, 2930, 1590, 1494, 1437, 1249, 1197, 1025, 827, 698, 566 cm^{-1}.

HRMS [ESI]: m/z calculated for $C_{19}H_{17}O_2PS$ $[M+H]^+$ 341.0760, found 341.0761.

S-(2-methoxyphenyl) diphenylphosphinothioate (3p)[1]



Yield: 63%, white solid.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.95-7.85 (m, 4H), 7.71 (dt, *J* = 7.7, 1.7 Hz, 1H), 7.55-7.48 (m, 2H), 7.47-7.40 (m, 4H), 7.25 (ddt, *J* = 8.9, 7.7, 1.6 Hz, 1H), 6.89 (td, *J* = 7.6, 1.2 Hz, 1H), 6.73 (dd, *J* = 8.3, 1.1 Hz, 1H), 3.65 (s, 3H).

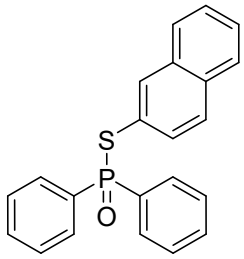
^{13}C NMR (101 MHz, $CDCl_3$) δ 159.43, 159.39, 137.66, 137.62, 133.55, 132.48, 132.15, 132.12, 131.70, 131.60, 130.73, 130.71, 128.36, 128.23, 121.22, 121.20, 114.09, 114.04, 111.10, 111.08, 55.51.

^{31}P NMR (162 MHz, $CDCl_3$) δ 41.56.

IR (ATR): $\tilde{\nu}$= 3450, 3057, 2923, 1581, 1479, 1436, 1201, 1114, 1023, 750, 696, 563, 524 cm^{-1}.

HRMS [ESI]: m/z calculated for $C_{19}H_{17}O_2PS$ $[M+H]^+$ 341.0760, found 341.0762.

S-(naphthalen-2-yl) diphenylphosphinothioate (3q)[4]



Yield: 85%, white solid.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.04-8.00 (m, 1H), 7.94-7.86 (m, 4H), 7.78-7.71 (m, 2H), 7.68 (d, *J* = 8.6 Hz, 1H), 7.55-7.42 (m, 9H).

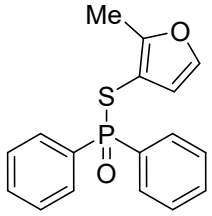
^{13}C NMR (101 MHz, $CDCl_3$) δ 135.46, 135.41, 133.52, 133.50, 133.02, 133.02, 133.00, 132.99, 132.40, 132.37, 131.72, 131.61, 131.58, 131.55, 128.71, 128.70, 128.65, 128.52, 127.83, 127.62, 126.91, 126.46, 123.47, 123.41.

^{31}P NMR (162 MHz, $CDCl_3$) δ 41.62.

IR (ATR): $\tilde{\nu}$= 3423, 3053, 2921, 1586, 1438, 1353, 1203, 1108, 817, 694, 558 cm^{-1}.

HRMS [ESI]: m/z calculated for $C_{22}H_{17}OPS$ $[M+H]^+$ 361.0810, found 361.0816.

S-(2-methylfuran-3-yl) diphenylphosphinothioate (3r)



Yield: 66%, brown solid.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.91-7.84 (m, 4H), 7.59-7.53 (m, 2H), 7.52-7.46 (m, 4H), 7.18 (d, *J* = 1.9 Hz, 1H), 6.19 (d, *J* = 1.9 Hz, 1H), 2.18 (d, *J* = 2.6 Hz, 3H).

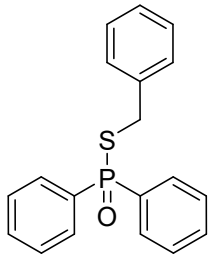
^{13}C NMR (101 MHz, $CDCl_3$) δ 157.76, 157.70, 140.70, 133.12, 132.40, 132.37, 132.08, 131.61, 131.50, 128.60, 128.47, 115.62, 115.61, 100.97, 100.92, 11.85, 11.83.

^{31}P NMR (162 MHz, $CDCl_3$) δ 41.59.

IR (ATR): $\tilde{\nu}$= 3444, 3052, 2916, 1587, 1439, 1193, 1115, 943, 697, 560 cm^{-1}.

HRMS [ESI]: m/z calculated for $C_{17}H_{15}O_2PS$ $[M+H]^+$ 315.0603, found 315.0605.

S-benzyl diphenylphosphinothioate (3s)[4]



Yield: 21%, white solid.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.94-7.84 (m, 4H), 7.59-7.52 (m, 2H), 7.52-7.45 (m, 4H), 7.24 (d, *J* = 4.1 Hz, 4H), 4.05 (d, *J* = 9.1 Hz, 2H).

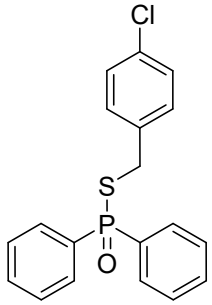
^{13}C NMR (101 MHz, $CDCl_3$) δ 136.82, 136.76, 133.53, 132.47, 132.36, 132.33, 131.60, 131.50, 129.04, 128.74, 128.61, 128.59, 127.45, 127.45, 33.20, 33.18.

^{31}P NMR (162 MHz, $CDCl_3$) δ 42.80.

IR (ATR): $\tilde{\nu}$= 3433, 2923, 1437, 1195, 1092, 994, 693, 570, 486 cm^{-1}.

HRMS [ESI]: m/z calculated for $C_{19}H_{17}OPS$ $[M+H]^+$ 325.0810, found 325.0808.

S-(4-chlorobenzyl) diphenylphosphinothioate (3t)[7]



Yield: 21%, white solid.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.81-7.72 (m, 4H), 7.51-7.44 (m, 2H), 7.42-7.35 (m, 4H), 7.11-

7.02 (m, 4H), 3.92 (d, *J* = 10.1 Hz, 2H).

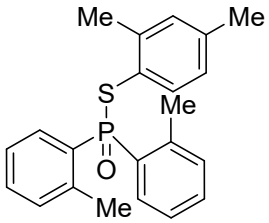
^{13}C NMR (101 MHz, $CDCl_3$) δ 135.49, 135.45, 133.36, 133.25, 132.42, 132.39, 131.58, 131.47, 130.42, 128.76, 128.64, 128.64, 32.55, 32.53.

^{31}P NMR (162 MHz, $CDCl_3$) δ 42.84.

IR (ATR): $\tilde{\nu}$= 3434, 2923, 1489, 1436, 1246, 1191, 1089, 818, 568 cm^{-1}.

HRMS [ESI]: m/z calculated for $C_{19}H_{16}ClOPS$ $[M+H]^+$ 359.0421, found 359.0426.

S-(2,4-dimethylphenyl) di-o-tolylphosphinothioate (3y)



Yield: 64%, white solid.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.90-7.77 (m, 2H), 7.47-7.38 (m, 2H), 7.30-7.17 (m, 5H), 7.01 (s, 1H), 6.84 (d, *J* = 7.8 Hz, 1H), 2.33 (s, 6H), 2.31 (s, 3H), 2.27 (s, 3H).

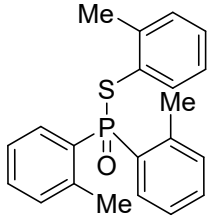
^{13}C NMR (101 MHz, $CDCl_3$) δ 143.35, 143.32, 141.77, 141.67, 139.43, 139.40, 137.32, 137.29, 132.58, 132.53, 132.47, 132.16, 132.13, 131.83, 131.71, 131.58, 131.56, 131.51, 127.22, 127.20, 125.61, 125.47, 121.18, 121.13, 21.35, 21.31, 21.13.

^{31}P NMR (162 MHz, $CDCl_3$) δ 42.51.

IR (ATR): $\tilde{\nu}$= 3418, 3054, 2920, 2852, 1943, 1591, 1453, 1275, 1190, 1081, 759, 553 cm^{-1}.

HRMS [ESI]: m/z calculated for $C_{22}H_{23}OPS$ $[M+H]^+$ 367.1280, found 367.1273.

S-(o-tolyl) di-o-tolylphosphinothioate (3z)[8]



Yield: 57%, white solid.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.86-7.77 (m, 2H), 7.45-7.36 (m, 3H), 7.28-7.18 (m, 6H), 7.05-7.00 (m, 1H), 2.34 (s, 3H), 2.33 (s, 6H).

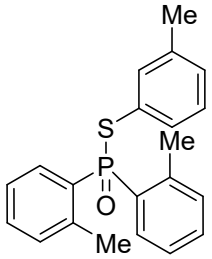
^{13}C NMR (101 MHz, $CDCl_3$) δ 143.51, 143.48, 141.78, 141.68, 137.36, 137.32, 132.52, 132.40, 132.38, 132.23, 132.20, 131.85, 131.73, 131.36, 130.64, 130.62, 129.23, 129.21, 126.33, 126.31, 125.64, 125.51, 125.06, 125.01, 21.39, 21.33, 21.29.

^{31}P NMR (162 MHz, $CDCl_3$) δ 42.84.

IR (ATR): $\tilde{\nu}$= 3436, 3058, 2920, 1940, 1589, 1454, 1188, 1079, 755, 713, 553 cm^{-1}.

HRMS [ESI]: m/z calculated for $C_{21}H_{21}OPS$ $[M+H]^+$ 353.1123, found 353.1119.

S-(m-tolyl) di-o-tolylphosphinothioate (3aa)



Yield: 56%, white solid.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.82 (dd, *J* = 15.0, 7.7 Hz, 2H), 7.45-7.37 (m, 2H), 7.31-7.19 (m, 6H), 7.15-7.06 (m, 2H), 2.41 (s, 6H), 2.25 (s, 3H).

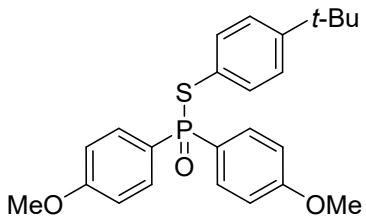
^{13}C NMR (101 MHz, $CDCl_3$) δ 141.97, 141.87, 138.86, 138.84, 136.37, 136.33, 132.76, 132.71, 132.64, 132.24, 132.21, 132.05, 131.88, 131.76, 131.03, 129.74, 129.72, 128.80, 128.78, 125.80, 125.75, 125.58, 125.45, 21.49, 21.45, 21.25.

^{31}P NMR (162 MHz, $CDCl_3$) δ 43.81.

IR (ATR): $\tilde{\nu}$= 3443, 3058, 2921, 2852, 1590, 1448, 1190, 1074, 917, 764, 688, 571 cm^{-1}.

HRMS [ESI]: m/z calculated for $C_{21}H_{21}OPS$ $[M+H]^+$ 353.1123, found 353.1122.

S-(4-(tert-butyl)phenyl) bis(4-methoxyphenyl)phosphinothioate (3ab)



Yield: 92%, white solid.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.82-7.71 (m, 4H), 7.39-7.33 (m, 2H), 7.23 (d, *J* = 8.2 Hz, 2H), 6.93 (dd, *J* = 8.8, 2.7 Hz, 4H), 3.82 (s, 6H), 1.24 (s, 9H).

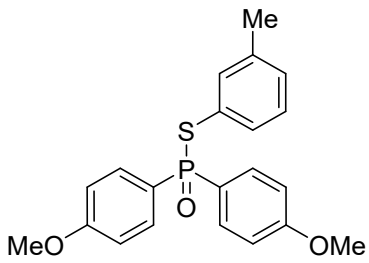
^{13}C NMR (101 MHz, $CDCl_3$) δ 162.65, 162.62, 152.00, 151.97, 135.06, 135.02, 133.62, 133.50, 126.25, 126.23, 124.69, 123.56, 123.11, 123.05, 114.05, 113.91, 55.37, 34.59, 31.17.

^{31}P NMR (162 MHz, $CDCl_3$) δ 41.79.

IR (ATR): $\tilde{\nu}$= 3437, 3055, 2963, 2557, 1913, 1593, 1442, 1251, 1179, 1113, 1021, 826, 528 cm^{-1}.

HRMS [ESI]: m/z calculated for $C_{24}H_{27}O_3PS$ $[M+H]^+$ 427.1491, found 427.1492.

S-(m-tolyl) bis(4-methoxyphenyl)phosphinothioate (3ac)



Yield: 56%, white solid.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.73-7.63 (m, 4H), 7.20-7.12 (m, 2H), 7.03-6.95 (m, 2H), 6.86

(dd, *J* = 8.8, 2.8 Hz, 4H), 3.75 (s, 6H), 2.15 (s, 3H).

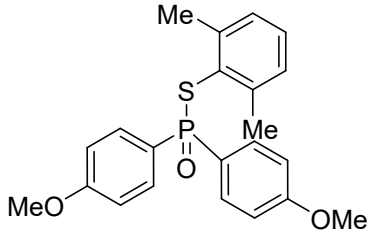
^{13}C NMR (101 MHz, $CDCl_3$) δ 162.67, 162.64, 138.89, 138.87, 135.92, 135.88, 133.63, 133.51, 132.17, 132.13, 129.63, 129.61, 128.84, 128.82, 126.48, 126.43, 124.61, 123.47, 114.07, 113.93, 55.39, 21.23.

^{31}P NMR (162 MHz, $CDCl_3$) δ 41.64.

IR (ATR): $\tilde{\nu}$= 3441, 3055, 2923, 2839, 1594, 1568, 1499, 1256, 1115, 1025, 829, 559 cm^{-1}.

HRMS [ESI]: m/z calculated for $C_{21}H_{21}O_3PS$ $[M+H]^+$ 385.1022, found 385.1016.

S-(2,6-dimethylphenyl) bis(4-methoxyphenyl)phosphinothioate (3ad)



Yield: 98%, white solid.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.73-7.64 (m, 4H), 7.14-7.09 (m, 1H), 7.02 (d, *J* = 7.5 Hz, 2H), 6.93 (dd, *J* = 8.9, 2.7 Hz, 4H), 3.84 (s, 6H), 2.33 (s, 6H).

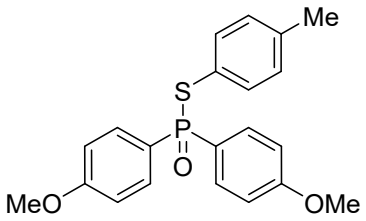
^{13}C NMR (101 MHz, $CDCl_3$) δ 162.68, 162.64, 145.03, 144.99, 133.31, 133.20, 129.15, 129.13, 128.33, 128.31, 125.23, 125.20, 125.14, 124.10, 113.93, 113.79, 55.41, 22.66.

^{31}P NMR (162 MHz, $CDCl_3$) δ 40.15.

IR (ATR): $\tilde{\nu}$= 3430, 3053, 2930, 2837, 2554, 1591, 1463, 1293, 1119, 827, 664, 558 cm^{-1}.

HRMS [ESI]: m/z calculated for $C_{22}H_{23}O_3PS$ $[M+H]^+$ 399.1178, found 399.1182.

S-(p-tolyl) bis(4-methoxyphenyl)phosphinothioate (3ae)[5]



Yield: 60%, white solid.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.81-7.73 (m, 4H), 7.33 (dd, *J* = 8.1, 1.7 Hz, 2H), 7.03 (d, *J* = 7.9 Hz, 2H), 6.95 (dd, *J* = 8.8, 2.7 Hz, 4H), 3.84 (s, 6H), 2.27 (s, 3H).

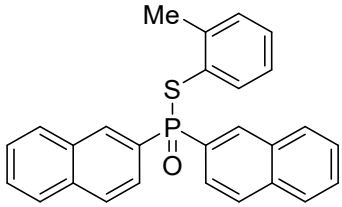
^{13}C NMR (101 MHz, $CDCl_3$) δ 162.65, 162.62, 138.96, 138.93, 135.20, 135.17, 133.63, 133.52, 129.93, 129.91, 124.65, 123.51, 123.05, 123.00, 114.08, 113.94, 55.38, 21.19.

^{31}P NMR (162 MHz, $CDCl_3$) δ 41.61.

IR (ATR): $\tilde{\nu}$= 3445, 2924, 1594, 1499, 1257, 1116, 807, 558 cm^{-1}.

HRMS [ESI]: m/z calculated for $C_{21}H_{21}O_3PS$ $[M+H]^+$ 385.1022, found 385.1023.

S-(o-tolyl) di(naphthalen-2-yl)phosphinothioate (3af)



Yield: 74%, white solid.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.46 (d, *J* = 14.8 Hz, 2H), 7.99-7.84 (m, 8H), 7.68-7.48 (m, 5H), 7.21-7.09 (m, 2H), 6.99 (td, *J* = 7.2, 6.7, 2.4 Hz, 1H), 2.43 (s, 3H).

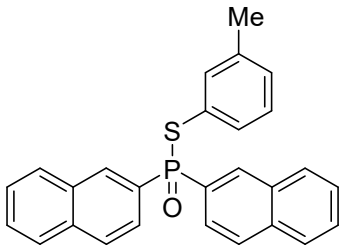
^{13}C NMR (101 MHz, $CDCl_3$) δ 142.95, 142.91, 136.79, 136.75, 134.87, 134.84, 133.88, 133.79, 132.46, 132.32, 130.82, 130.80, 130.42, 129.37, 129.35, 129.11, 128.46, 128.44, 128.31, 127.84, 127.03, 126.56, 126.55, 126.25, 126.14, 125.41, 125.36, 21.58.

^{31}P NMR (162 MHz, $CDCl_3$) δ 41.22.

IR (ATR): $\tilde{\nu}$= 3444, 3052, 2920, 1621, 1457, 1193, 1089, 750, 645, 545 cm^{-1}.

HRMS [ESI]: m/z calculated for $C_{27}H_{21}OPS$ $[M+H]^+$ 425.1123, found 425.1121.

S-(m-tolyl) di(naphthalen-2-yl)phosphinothioate (3ag)



Yield: 82%, white solid.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.51 (d, *J* = 14.8 Hz, 2H), 8.00-7.82 (m, 8H), 7.64-7.50 (m, 4H), 7.33 (s, 2H), 7.10-6.98 (m, 2H), 2.15 (s, 3H).

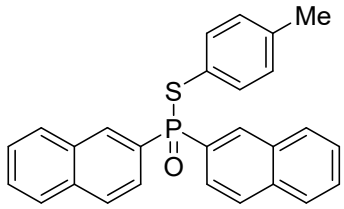
^{13}C NMR (101 MHz, $CDCl_3$) δ 139.08, 139.06, 136.19, 136.15, 134.87, 134.84, 134.07, 133.97, 132.49, 132.44, 132.40, 132.35, 130.21, 129.94, 129.92, 129.14, 129.09, 129.00, 128.98, 128.51, 128.49, 128.38, 127.84, 127.04, 126.34, 126.23, 125.68, 125.62, 21.15.

^{31}P NMR (162 MHz, $CDCl_3$) δ 41.60.

IR (ATR): $\tilde{\nu}$= 3446, 3055, 2920, 1587, 1357, 1211, 1087, 827, 653, 533 cm^{-1}.

HRMS [ESI]: m/z calculated for $C_{27}H_{21}OPS$ $[M+H]^+$ 425.1123, found425.1129.

S-(p-tolyl) di(naphthalen-2-yl)phosphinothioate (3ah)[5]



Yield: 94%, white solid.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.50 (d, *J* = 14.8 Hz, 2H), 7.98-7.85 (m, 8H), 7.64-7.51 (m, 4H),

7.41 (d, *J* = 7.7 Hz, 2H), 6.99 (d, *J* = 8.0 Hz, 2H), 2.22 (s, 3H).

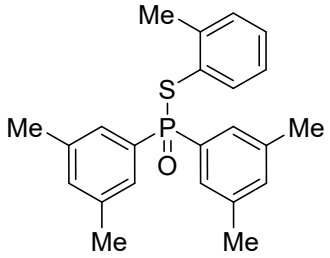
^{13}C NMR (101 MHz, $CDCl_3$) δ 139.31, 139.29, 135.43, 135.39, 134.87, 134.84, 134.06, 133.96, 132.51, 132.37, 130.26, 130.10, 130.08, 129.19, 129.11, 128.51, 128.46, 128.38, 127.84, 127.01, 126.37, 126.25, 122.22, 122.17, 21.16.

^{31}P NMR (162 MHz, $CDCl_3$) δ 41.58.

IR (ATR): $\tilde{\nu}$= 3448, 3052, 1624, 1490, 1339, 1204, 1086, 808, 646, 546 cm^{-1}.

HRMS [ESI]: m/z calculated for $C_{27}H_{21}OPS$ $[M+H]^+$ 425.1123, found 425.1129.

S-(o-tolyl) bis(3,5-dimethylphenyl)phosphinothioate (3ai)



Yield: 91%, white solid.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.49 (d, *J* = 7.8 Hz, 1H), 7.43 (d, *J* = 13.2 Hz, 4H), 7.22-7.12 (m, 4H), 7.05 (td, *J* = 7.2, 2.2 Hz, 1H), 2.38 (s, 3H), 2.33 (s, 12H).

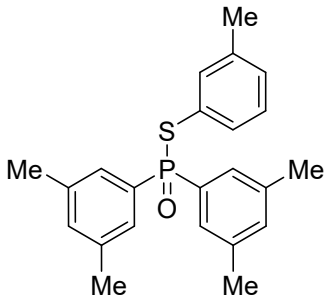
^{13}C NMR (101 MHz, $CDCl_3$) δ 142.87, 142.83, 138.22, 138.08, 136.84, 136.81, 133.99, 133.96, 133.06, 132.01, 130.63, 130.61, 129.17, 129.14, 129.06, 128.96, 126.43, 126.41, 125.85, 125.80, 21.44, 21.30.

^{31}P NMR (162 MHz, $CDCl_3$) δ 42.45.

IR (ATR): $\tilde{\nu}$= 3451, 2918, 2855, 1472, 1193, 875, 761, 690, 582 cm^{-1}.

HRMS [ESI]: m/z calculated for $C_{23}H_{25}OPS$ $[M+H]^+$ 381.1436, found 381.1432.

S-(m-tolyl) bis(3,5-dimethylphenyl)phosphinothioate (3aj)



Yield: 70%, white solid.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.47 (d, *J* = 13.2 Hz, 4H), 7.27 (d, *J* = 10.4 Hz, 2H), 7.16-7.04 (m, 4H), 2.34 (s, 12H), 2.25 (s, 3H).

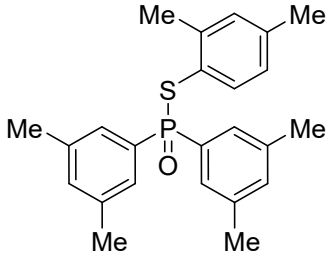
^{13}C NMR (101 MHz, $CDCl_3$) δ 138.87, 138.85, 138.26, 138.12, 136.19, 136.15, 133.98, 133.95, 132.91, 132.40, 132.37, 131.86, 129.70, 129.68, 129.22, 129.12, 128.83, 128.81, 126.13, 126.08, 21.30, 21.21.

^{31}P NMR (162 MHz, $CDCl_3$) δ 42.63.

IR (ATR): $\tilde{\nu}$= 3441, 2918, 1590, 1468, 1208, 1119, 846, 687, 572 cm^{-1}.

HRMS [ESI]: m/z calculated for $C_{23}H_{25}OPS$ $[M+H]^+$ 381.1436, found 381.1439.

S-(2,4-dimethylphenyl) bis(3,5-dimethylphenyl)phosphinothioate (3ak)



Yield: 85%, white solid.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.43 (d, *J* = 13.1 Hz, 4H), 7.35 (dd, *J* = 7.9, 1.6 Hz, 1H), 7.14 (s, 2H), 6.98 (s, 1H), 6.86 (d, *J* = 7.9 Hz, 1H), 2.33 (s, 15H), 2.25 (s, 3H).

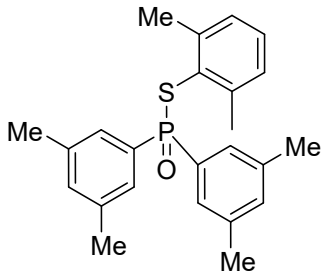
^{13}C NMR (101 MHz, $CDCl_3$) δ 142.77, 142.73, 139.30, 139.27, 138.16, 138.03, 136.84, 136.81, 133.92, 133.89, 133.20, 132.16, 131.56, 131.54, 129.09, 128.98, 127.30, 127.28, 122.02, 121.97, 21.37, 21.30, 21.07.

^{31}P NMR (162 MHz, $CDCl_3$) δ 42.38.

IR (ATR): $\tilde{\nu}$= 3443, 2916, 1599, 1448, 1211, 1045, 818, 693, 579 cm^{-1}.

HRMS [ESI]: m/z calculated for $C_{24}H_{27}OPS$ $[M+H]^+$ 395.1593, found 395.1594.

S-(2,6-dimethylphenyl) bis(3,5-dimethylphenyl)phosphinothioate (3al)



Yield: 97%, white solid.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.34 (d, *J* = 13.0 Hz, 4H), 7.18-7.10 (m, 3H), 7.04 (d, *J* = 7.7 Hz, 2H), 2.32 (s, 18H).

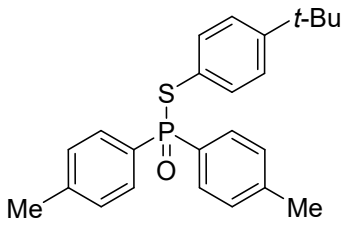
^{13}C NMR (101 MHz, $CDCl_3$) δ 145.22, 145.18, 138.13, 137.99, 133.90, 133.87, 133.30, 132.26, 129.14, 129.11, 128.86, 128.75, 128.29, 128.27, 124.95, 124.89, 77.47, 77.15, 76.84, 22.54, 22.54, 22.53, 21.29.

^{31}P NMR (162 MHz, $CDCl_3$) δ 41.25.

IR (ATR): $\tilde{\nu}$= 3435, 2914, 2855, 1598, 1458, 1199, 846, 686, 577 cm^{-1}.

HRMS [ESI]: m/z calculated for $C_{24}H_{27}OPS$ $[M+H]^+$ 395.1593, found 395.1595.

S-(4-(tert-butyl)phenyl) di-p-tolylphosphinothioate (3am)[9]



Yield: 88%, white solid.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.74 (dd, *J* = 12.7, 8.0 Hz, 4H), 7.37 (d, *J* = 7.1 Hz, 2H), 7.28-7.21 (m, 6H), 2.40 (s, 6H), 1.26 (s, 9H).

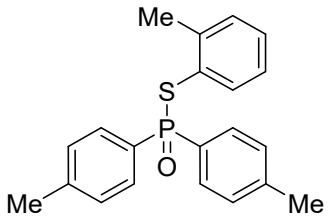
^{13}C NMR (101 MHz, $CDCl_3$) δ 152.05, 152.02, 142.75, 142.72, 135.13, 135.09, 131.71, 131.60, 130.20, 129.28, 129.14, 129.11, 126.27, 126.25, 122.80, 122.75, 34.59, 31.16, 21.66, 21.64.

^{31}P NMR (162 MHz, $CDCl_3$) δ 42.17.

IR (ATR): $\tilde{\nu}$= 3442, 3050, 2965, 1598, 1392, 1201, 1010, 804, 659, 550 cm^{-1}.

HRMS [ESI]: m/z calculated for $C_{24}H_{27}OPS$ $[M+H]^+$ 395.1593, found 395.1588.

S-(o-tolyl) di-p-tolylphosphinothioate (3an)



Yield: 95%, white solid.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.72 (dd, *J* = 12.7, 8.1 Hz, 4H), 7.50 (d, *J* = 7.8 Hz, 1H), 7.25 (dd, *J* = 7.9, 3.3 Hz, 4H), 7.20-7.12 (m, 2H), 7.07-6.99 (m, 1H), 2.39 (s, 6H), 2.38 (s, 3H).

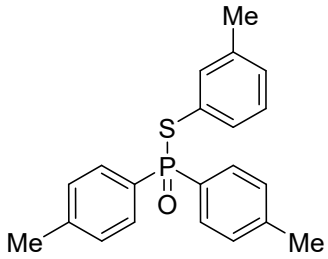
^{13}C NMR (101 MHz, $CDCl_3$) δ 142.82, 142.79, 142.73, 142.69, 136.62, 136.58, 131.56, 131.46, 130.67, 130.65, 130.30, 129.26, 129.21, 129.13, 129.10, 126.44, 126.43, 125.94, 125.89, 21.67, 21.65, 21.50.

^{31}P NMR (162 MHz, $CDCl_3$) δ 41.65.

IR (ATR): $\tilde{\nu}$= 3443, 3035, 2961, 2918, 1598, 1460, 1187, 885, 747, 657, 556 cm^{-1}.

HRMS [ESI]: m/z calculated for $C_{21}H_{21}OPS$ $[M+H]^+$ 353.1123, found 353.1128.

S-(m-tolyl) di-p-tolylphosphinothioate (3ao)



Yield: 90%, white solid.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.74 (dd, *J* = 12.7, 8.1 Hz, 4H), 7.25 (dd, *J* = 8.0, 3.2 Hz, 6H), 7.13 – 7.02 (m, 2H), 2.39 (s, 6H), 2.24 (s, 3H).

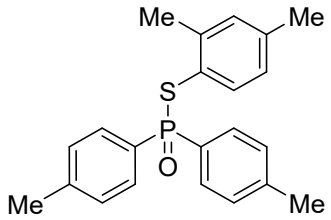
^{13}C NMR (101 MHz, $CDCl_3$) δ 142.81, 142.78, 138.89, 138.87, 136.00, 135.96, 132.25, 132.21, 131.70, 131.59, 130.09, 129.67, 129.65, 129.30, 129.16, 129.00, 128.85, 128.83, 126.18, 126.13, 21.65, 21.63, 21.20.

^{31}P NMR (162 MHz, $CDCl_3$) δ 42.02.

IR (ATR): $\tilde{\nu}$= 3457, 3052, 3021, 2920, 1599, 1474, 1200, 1019, 807, 659, 555 cm^{-1}.

HRMS [ESI]: m/z calculated for $C_{21}H_{21}OPS$ $[M+H]^+$ 353.1123, found 353.1121.

S-(2,4-dimethylphenyl) di-p-tolylphosphinothioate (3ap)



Yield: 89%, white solid.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.72 (dd, *J* = 12.6, 8.1 Hz, 4H), 7.34 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.25 (dd, *J* = 7.9, 3.2 Hz, 4H), 6.98 (s, 1H), 6.84 (d, *J* = 7.9 Hz, 1H), 2.39 (s, 6H), 2.34 (s, 3H), 2.24 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 142.73, 142.70, 142.62, 142.58, 139.28, 139.25, 136.62, 136.58, 131.59, 131.49, 130.45, 129.37, 129.28, 129.24, 129.15, 129.10, 127.32, 127.30, 122.06, 122.00, 21.66, 21.65, 21.42, 21.11. [3]

^{1}P NMR (162 MHz, $CDCl_3$) δ 41.51.

IR (ATR): $\tilde{\nu}$= 3469, 3021, 2919, 2862, 1915, 1599, 1396, 1200, 807, 658, 540 cm^{-1}.

HRMS [ESI]: m/z calculated for $C_{22}H_{23}OPS$ $[M+H]^+$ 367.1280, found 367.1278.

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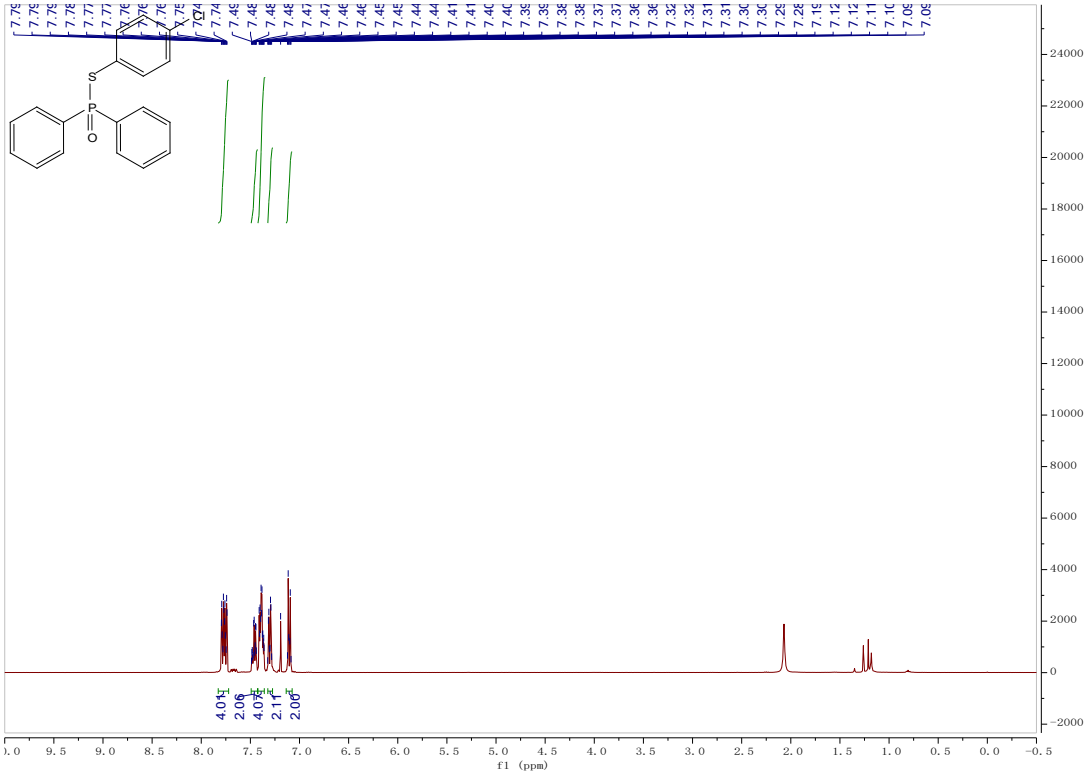
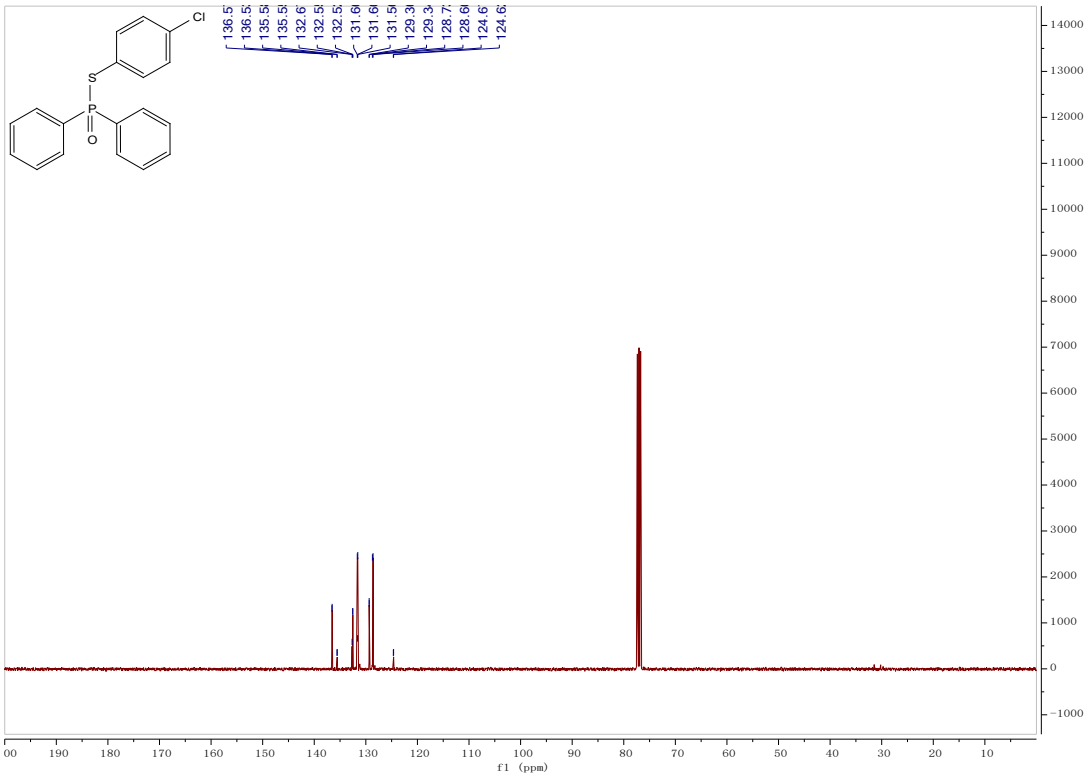
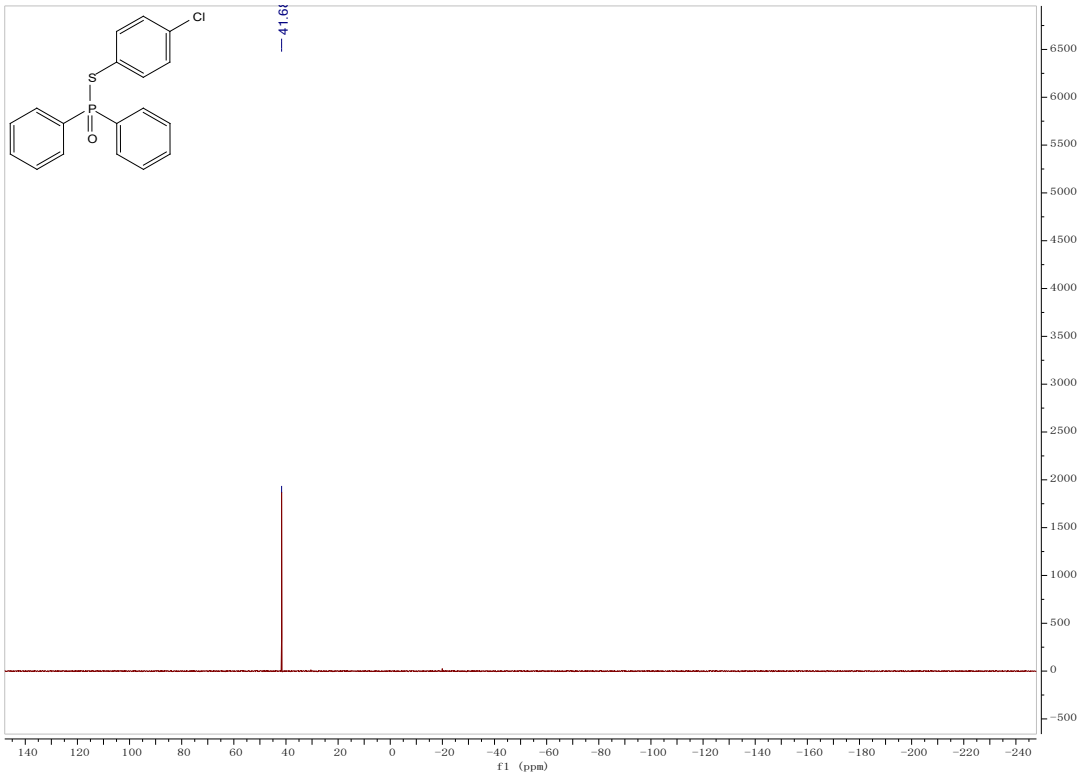
Copies of NMR spectra

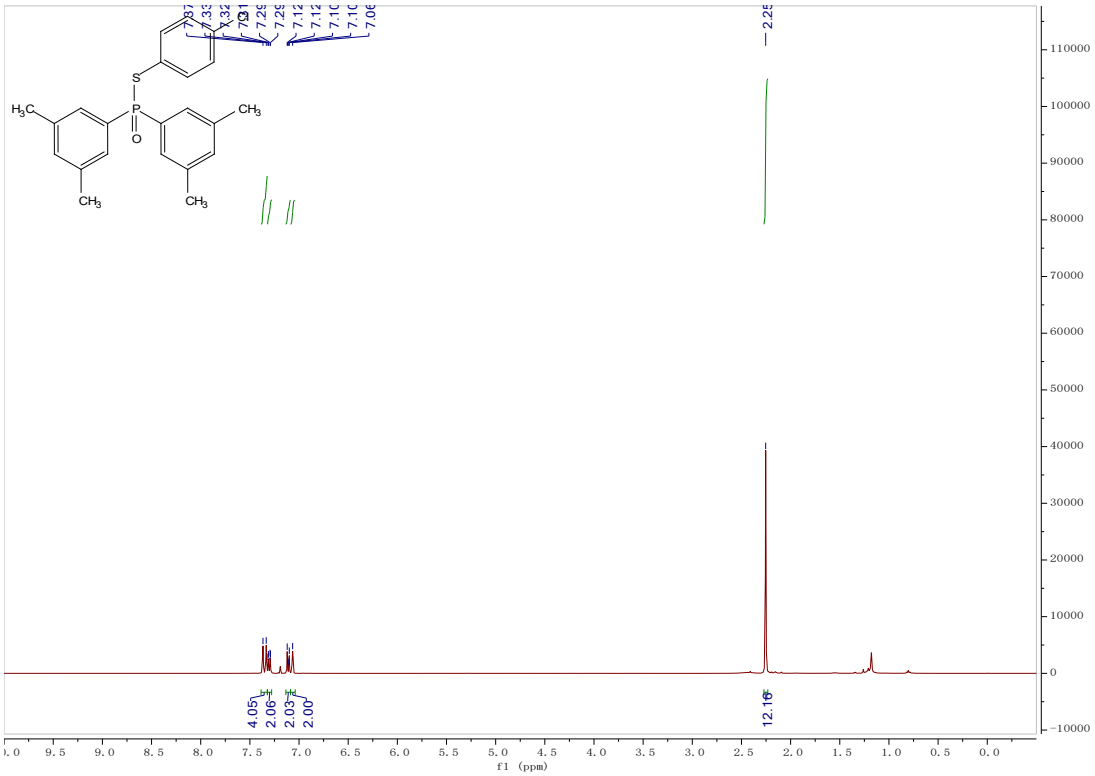
S-(4-chlorophenyl) diphenylphosphinothioate (3a)

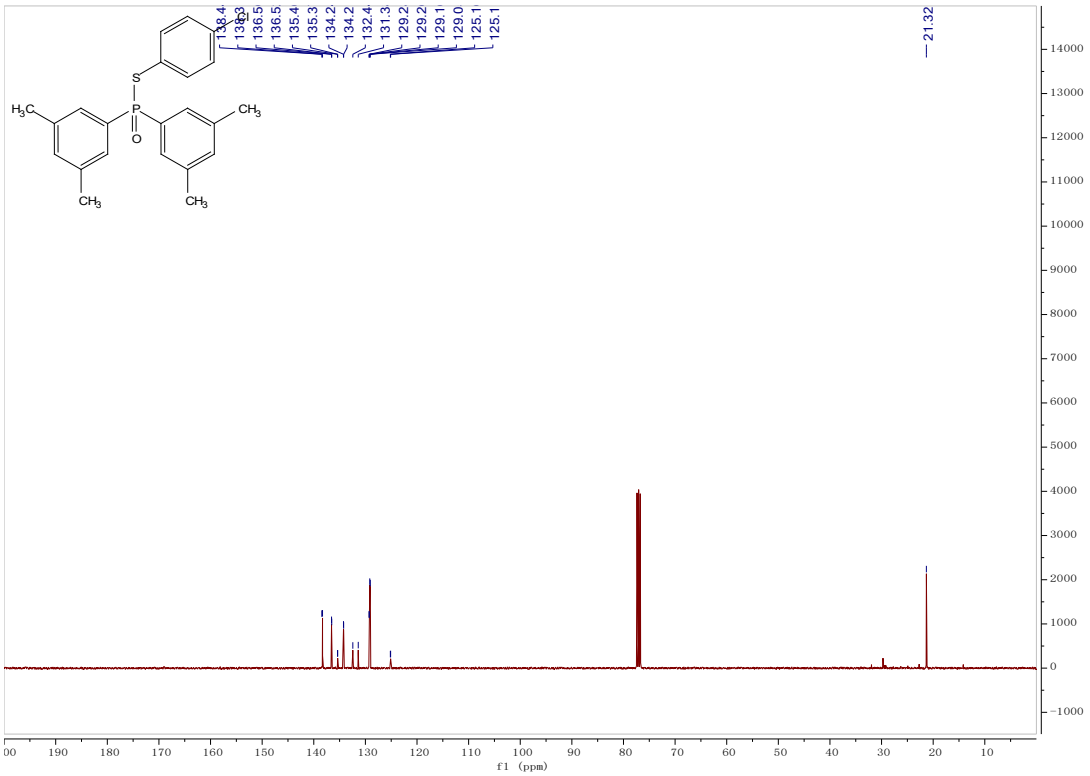


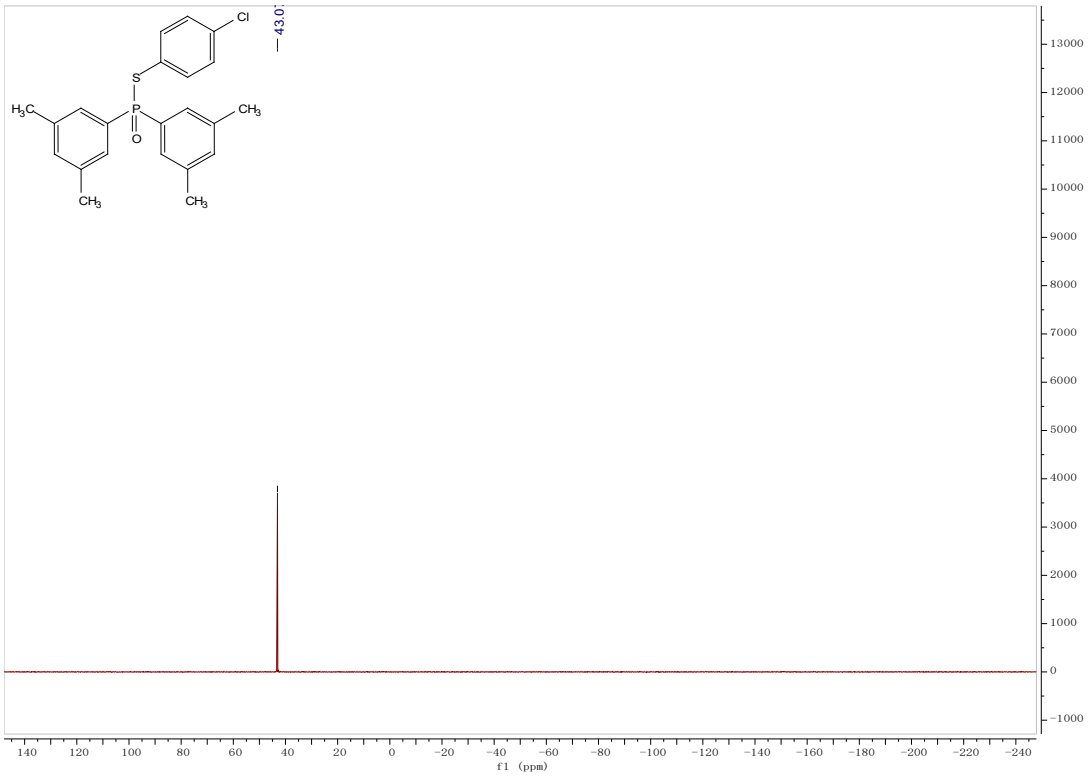




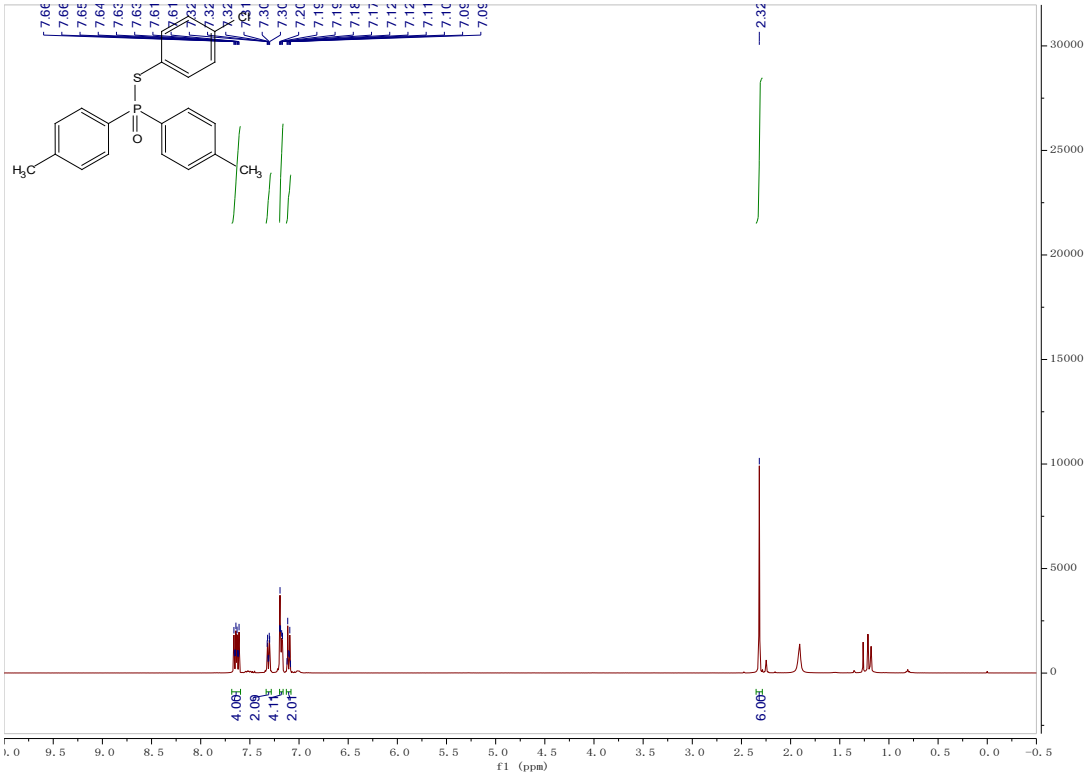
S-(4-chlorophenyl) bis(3,5-dimethylphenyl)phosphinothioate (3b)

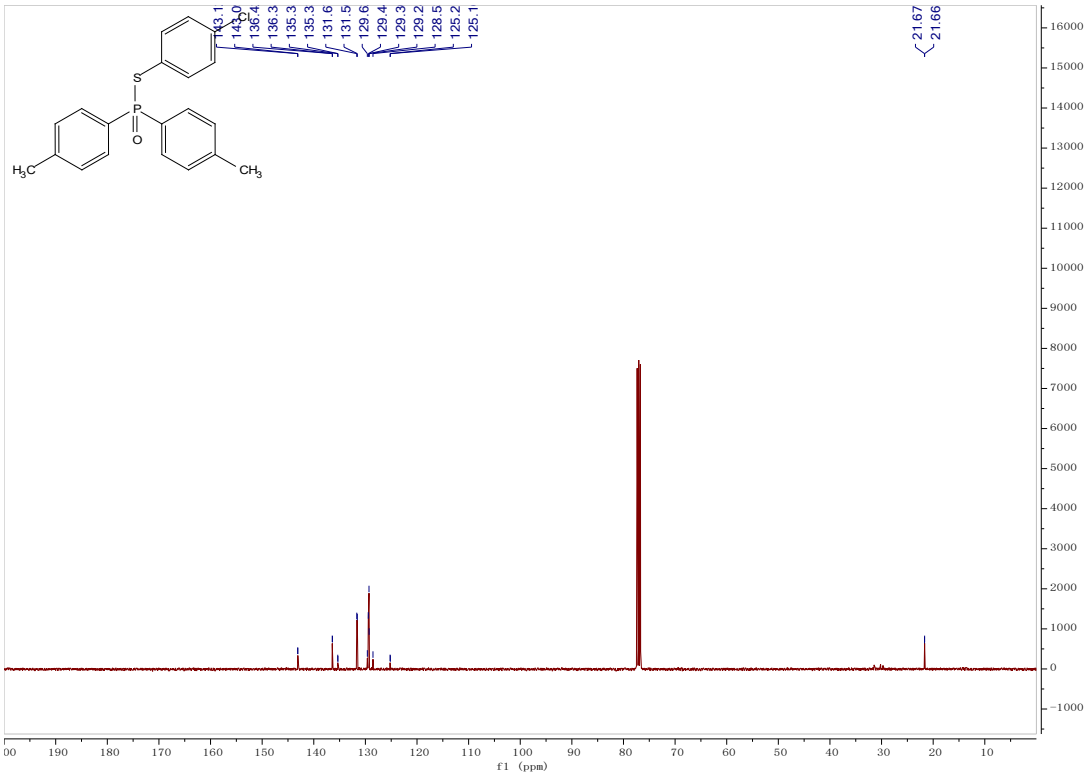


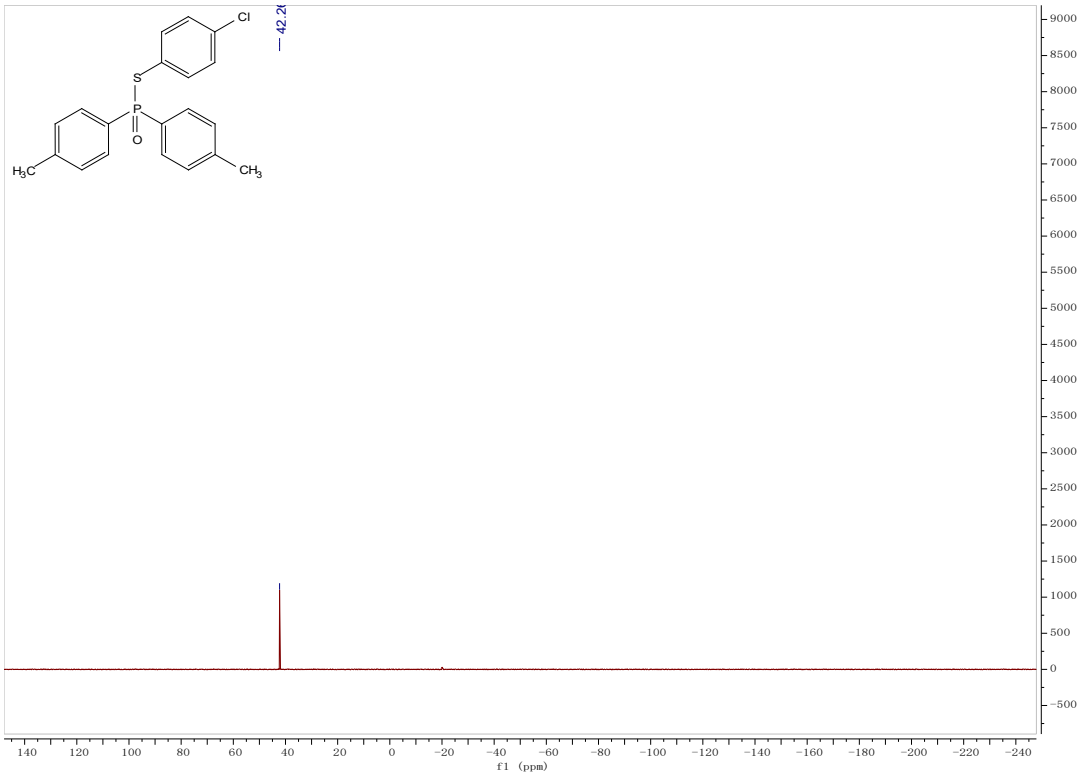

138.4
136.5
136.5
135.4
135.3
134.2
134.2
132.4
131.3
129.2
129.2
129.1
129.0
125.1
125.1
21.32
Cl
S
P
O
H3C
CH3
CH3
CH3
f1 (ppm)


43.0
Cl
S
P
O
H3C
CH3
CH3
CH3
f1 (ppm)

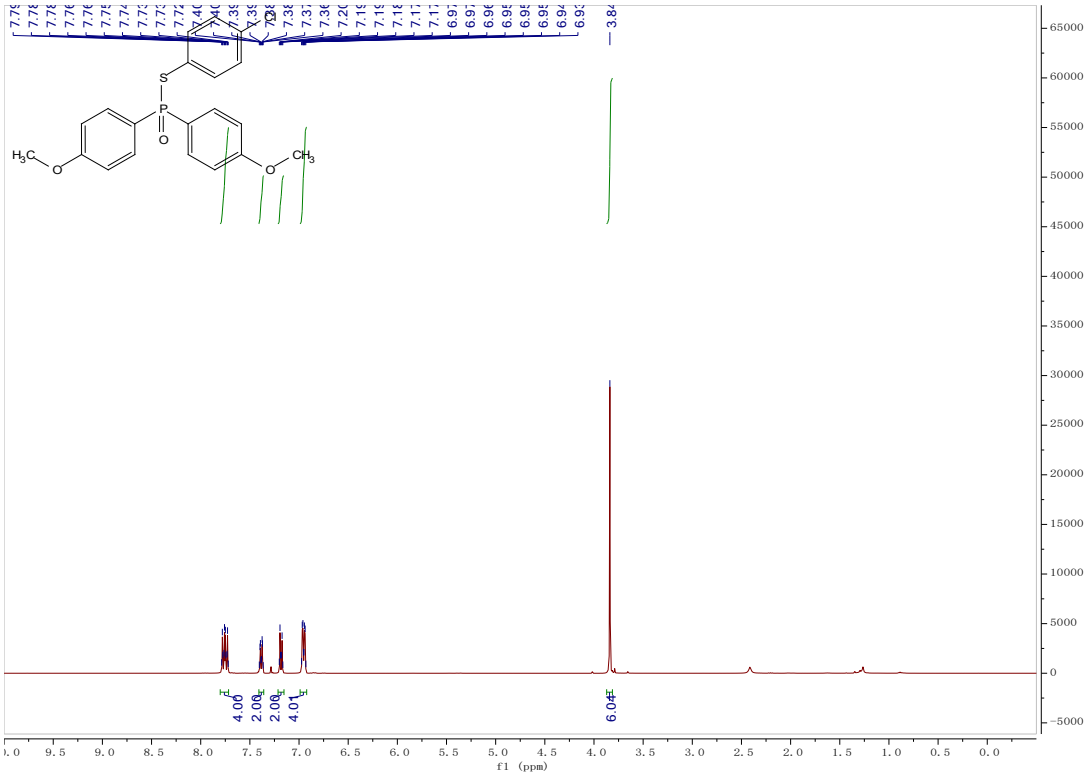
S-(4-chlorophenyl) di-p-tolylphosphinothioate (3c)

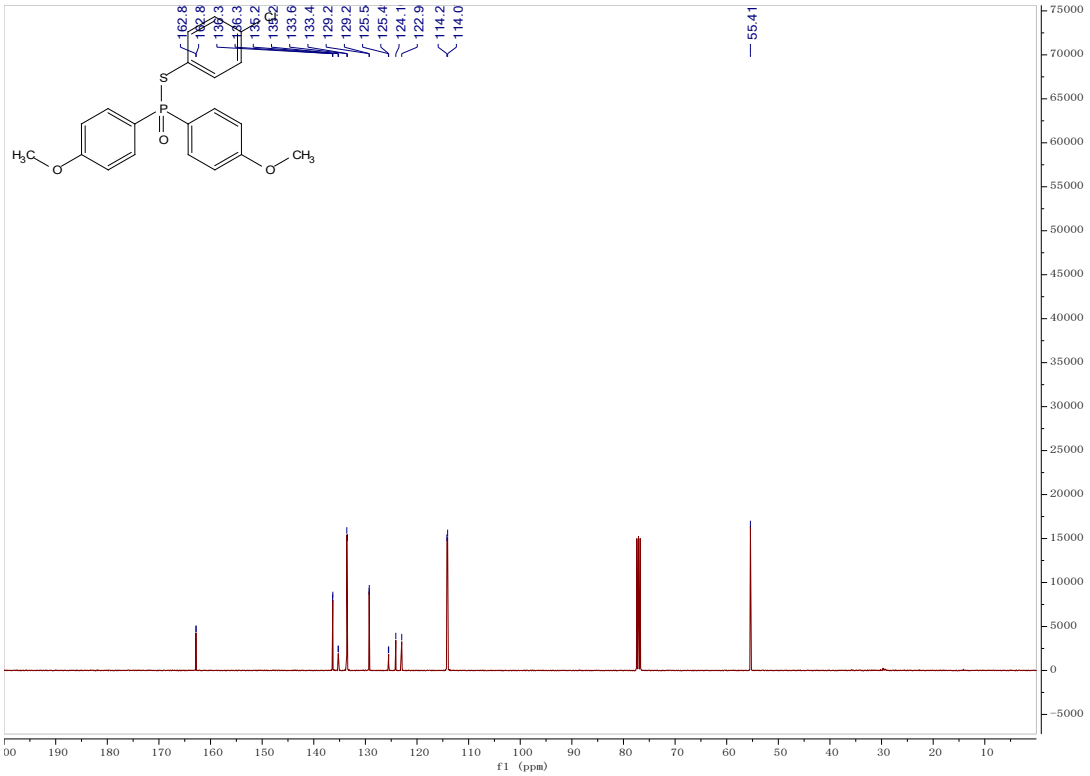


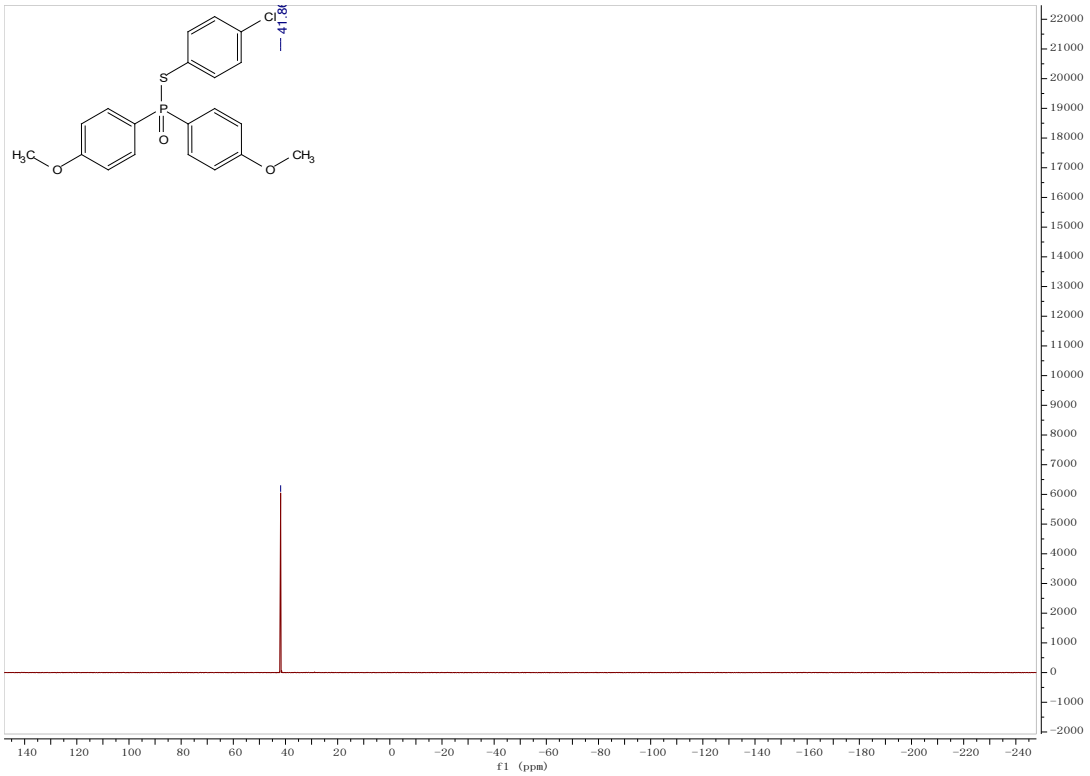




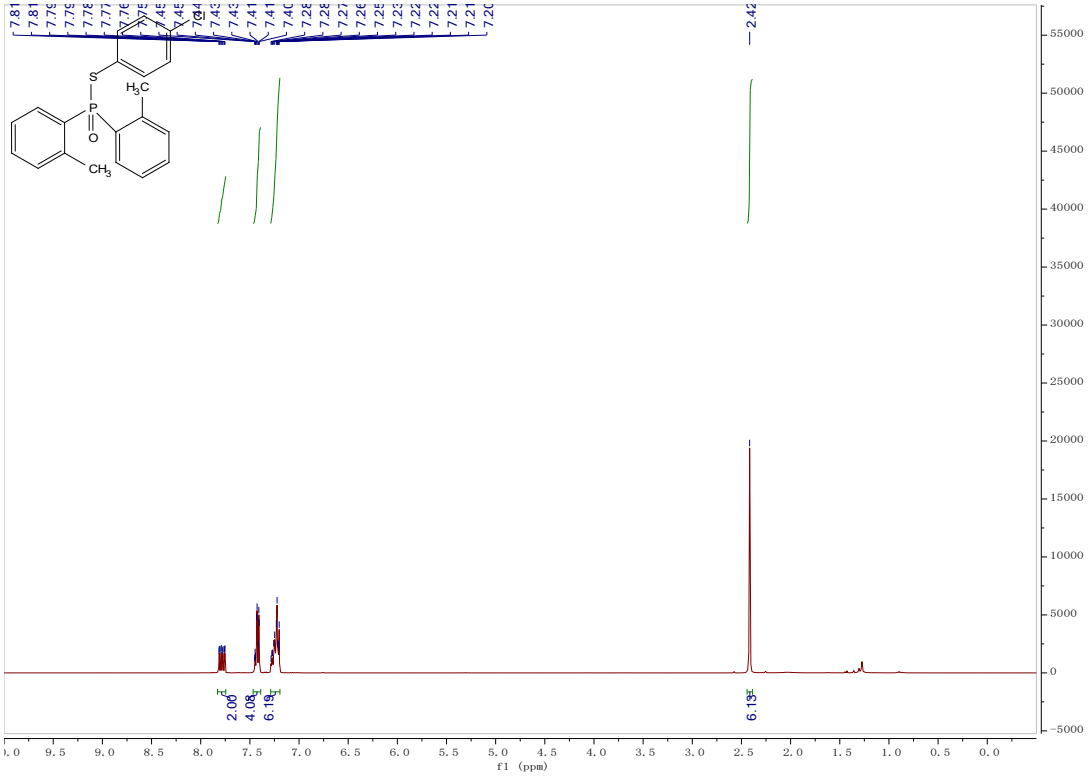
S-(4-chlorophenyl) bis(4-methoxyphenyl)phosphinothioate (3d)

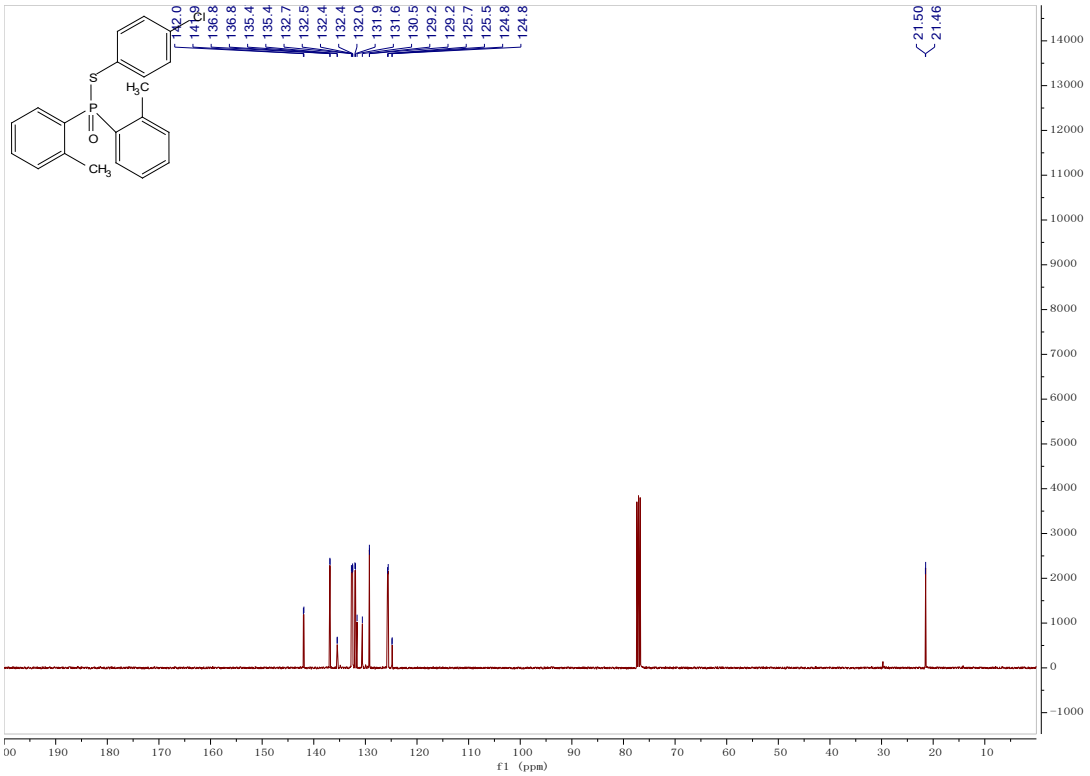


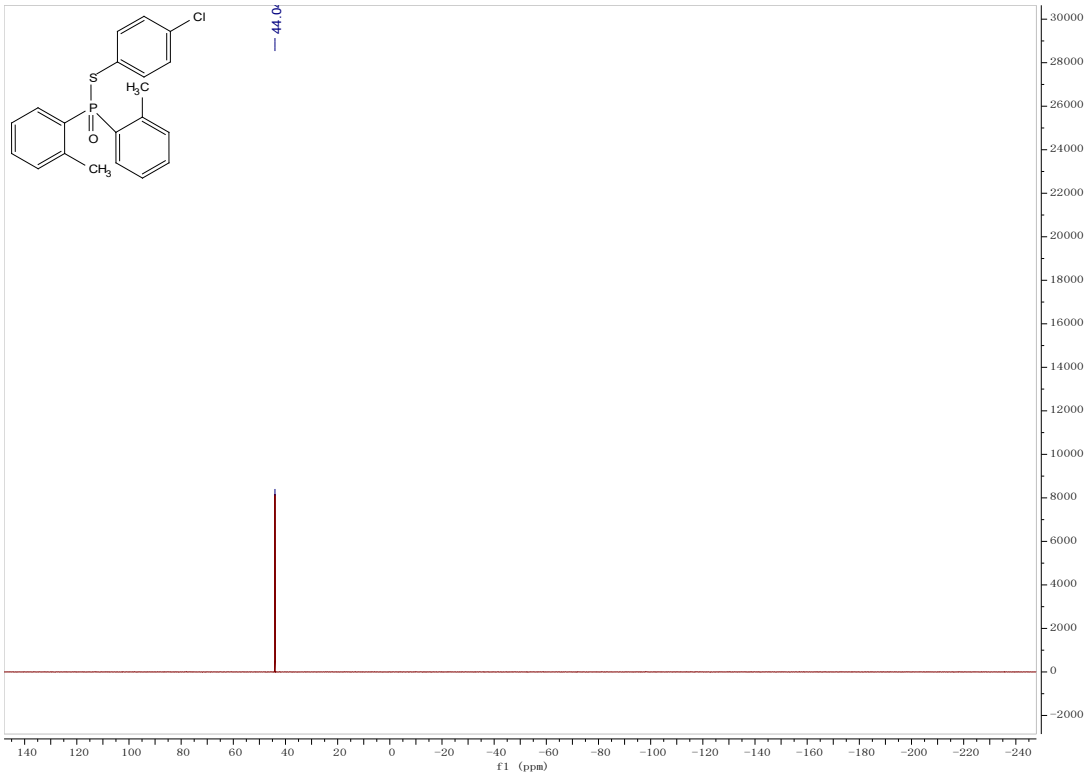

162.8
162.8
139.3
136.3
135.2
133.2
133.6
133.4
129.2
129.2
125.5
125.4
124.1
122.9
114.2
114.0
55.41
S
P
O
H3C
O
O
CH3
f1 (ppm)


Cl
41.8
S
P
O
H3C
O
O
CH3
f1 (ppm)

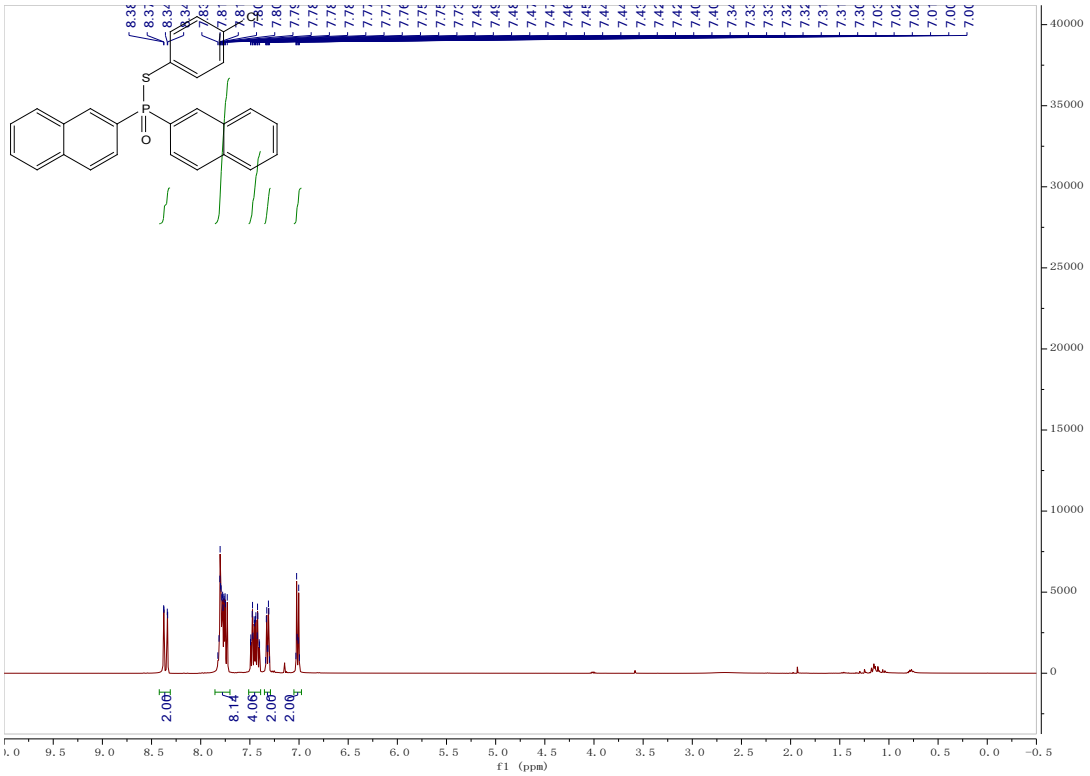
S-(4-chlorophenyl) di-o-tolylphosphinothioate (3e)

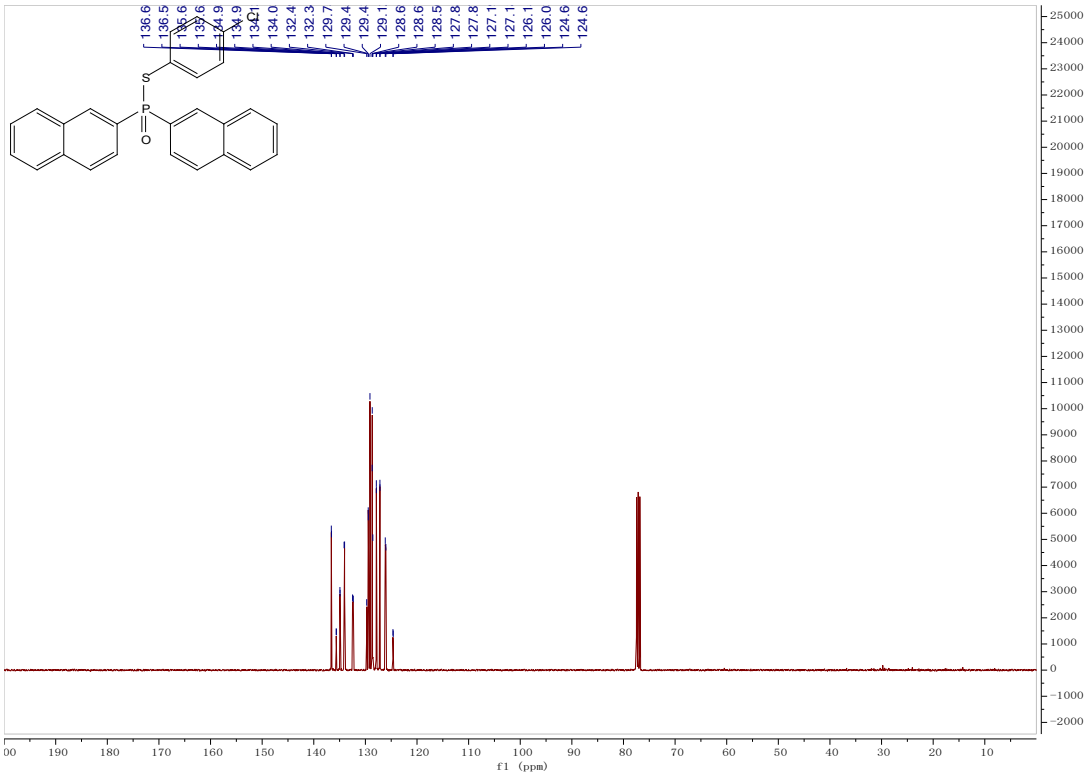


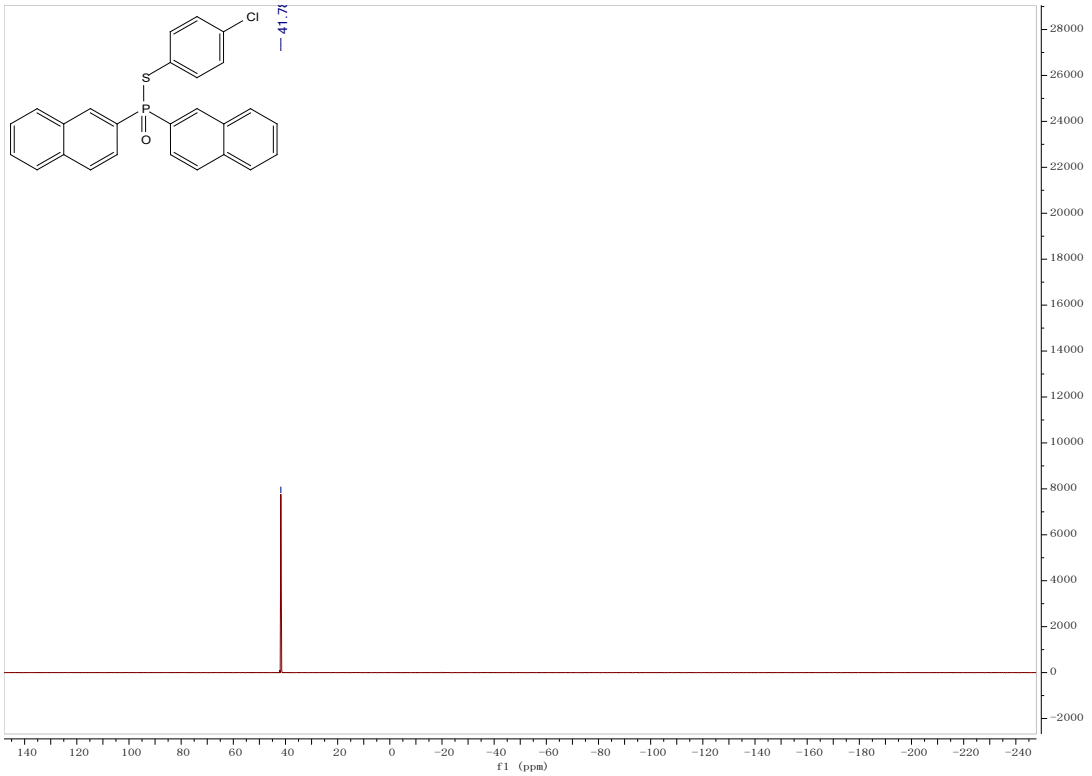




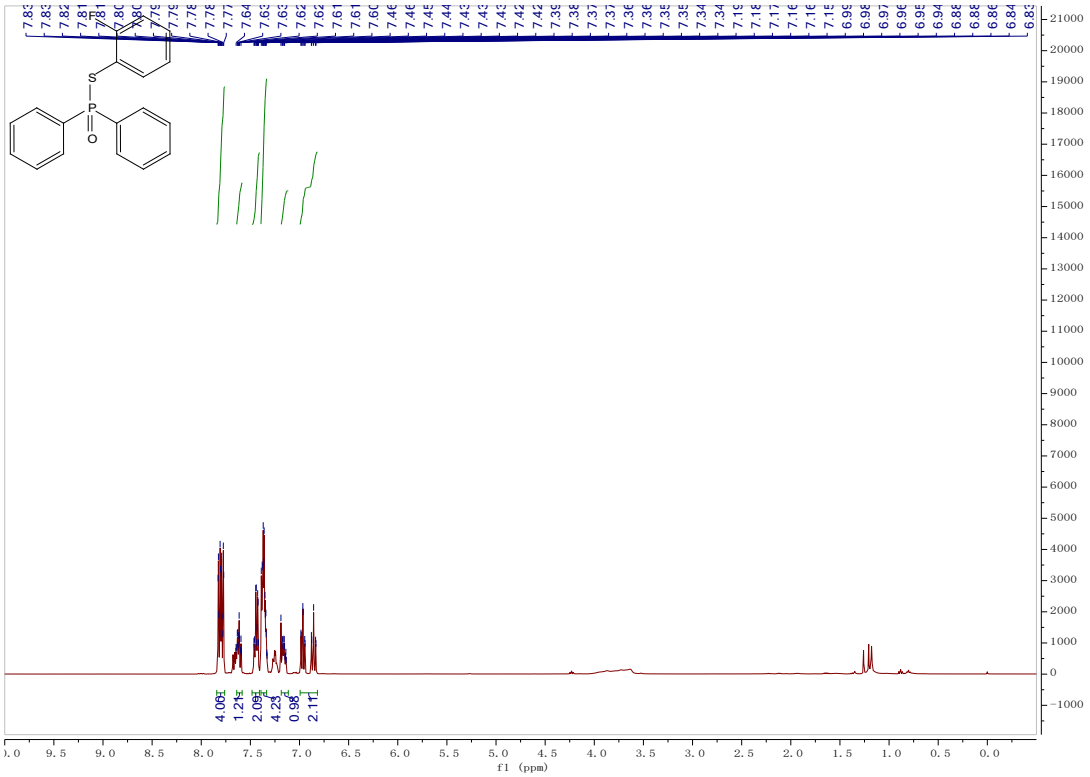
S-(4-chlorophenyl) di(naphthalen-2-yl)phosphinothioate (3f)

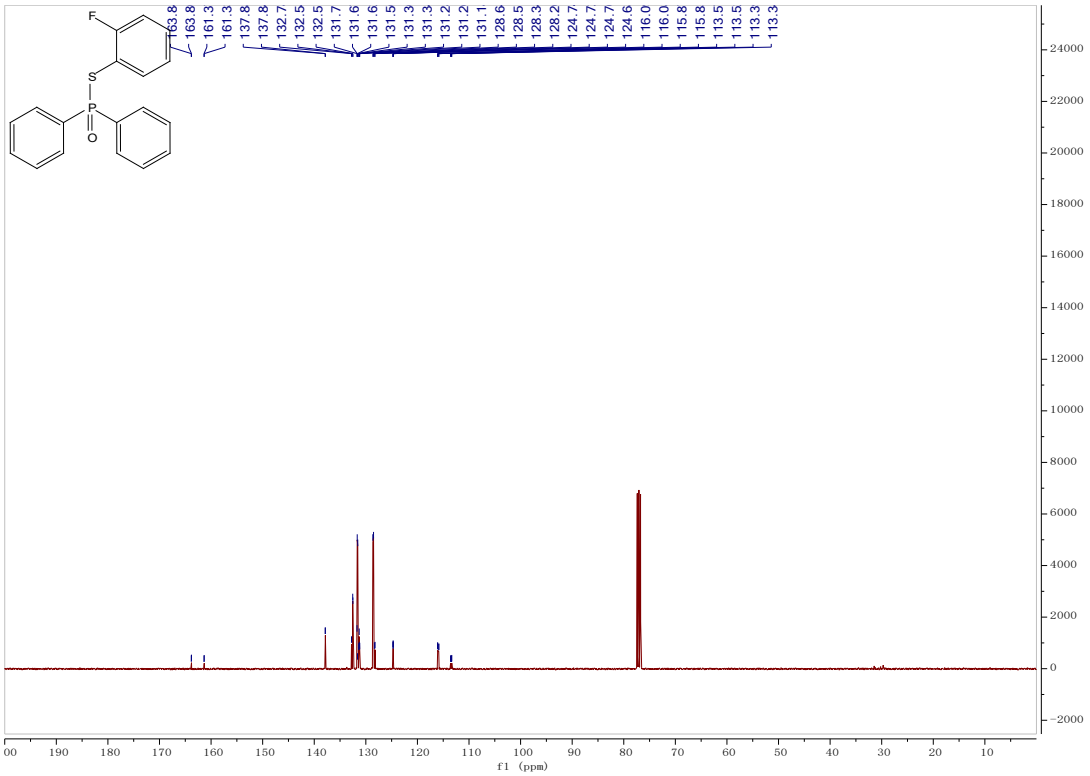


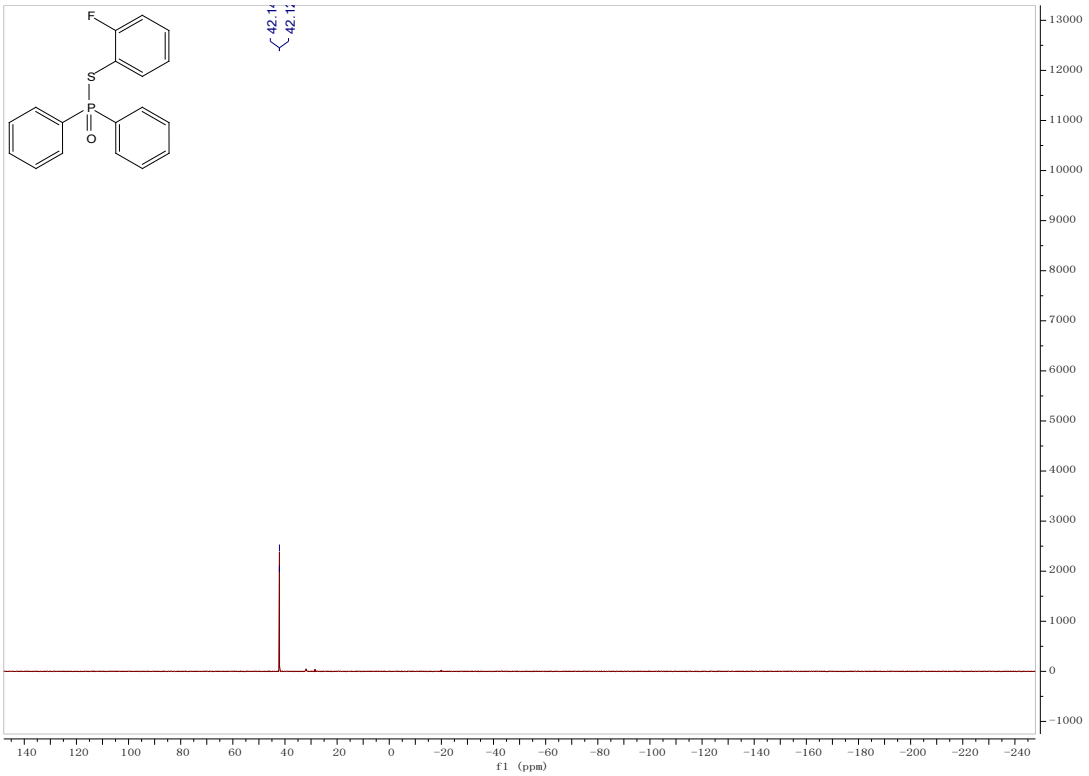

136.6
136.5
135.6
133.6
134.9
134.9
134.1
134.0
132.4
132.3
129.7
129.4
129.4
129.1
128.6
128.6
128.5
127.8
127.8
127.1
127.1
126.1
126.0
124.6
124.6
Cl
S
P
O
f1 (ppm)

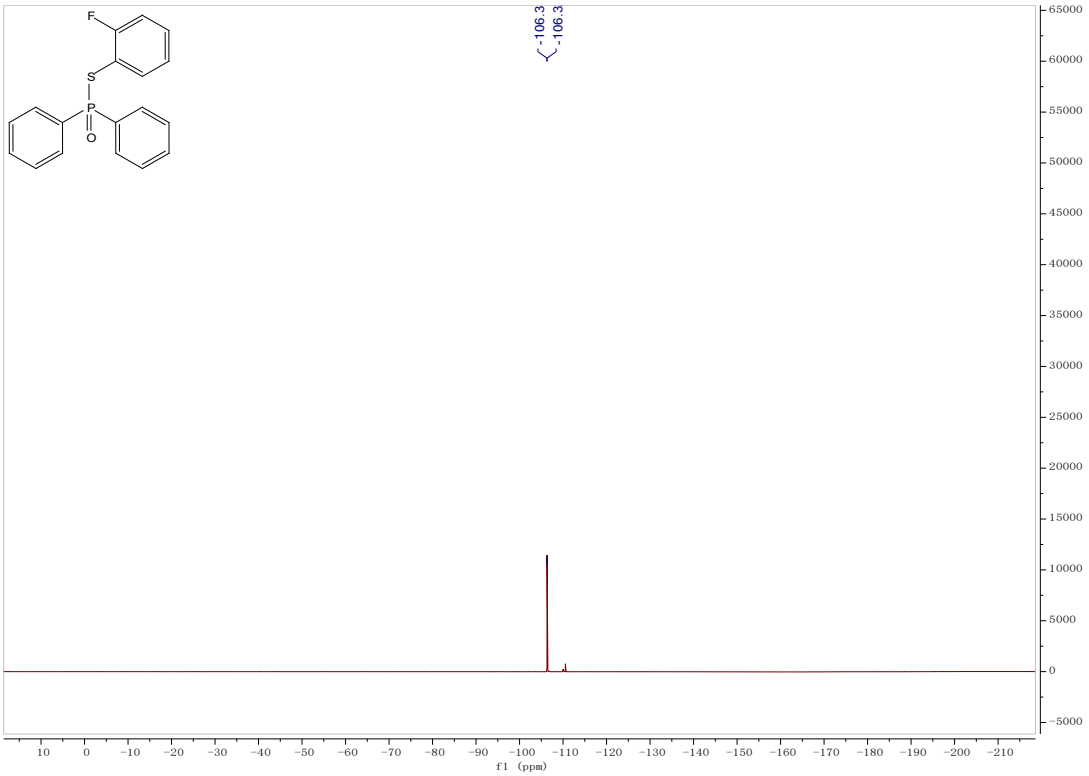

Cl
S
P
O
f1 (ppm)

S-(2-fluorophenyl) diphenylphosphinothioate (3g)

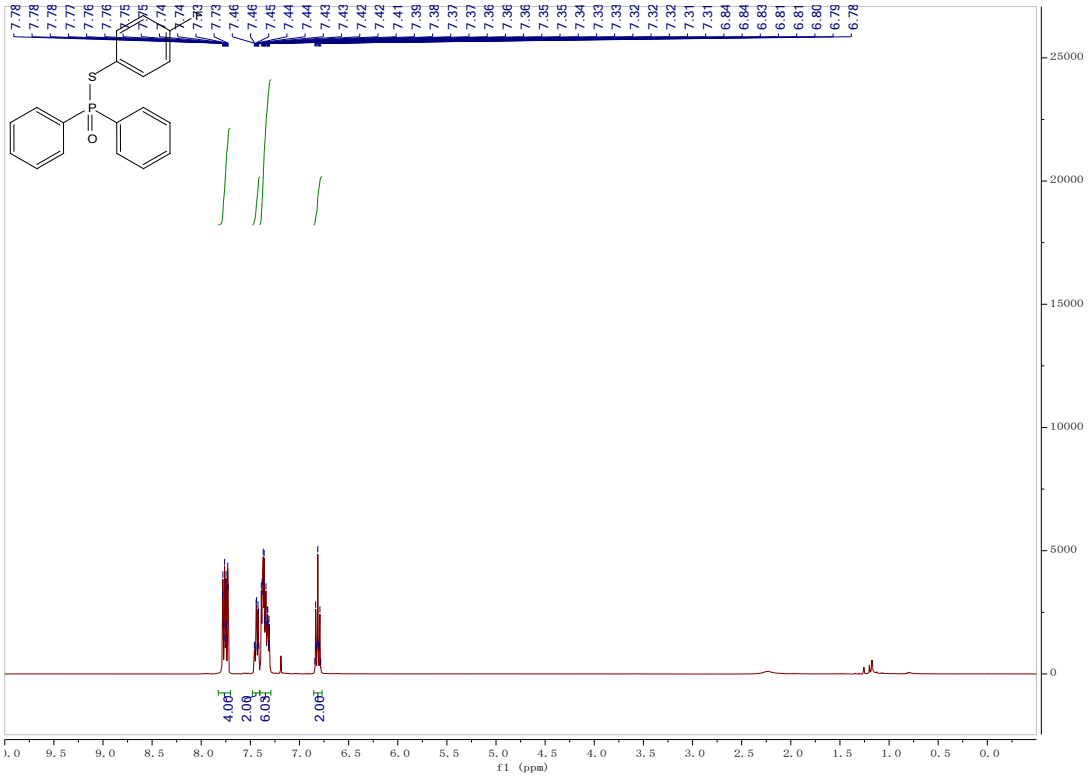


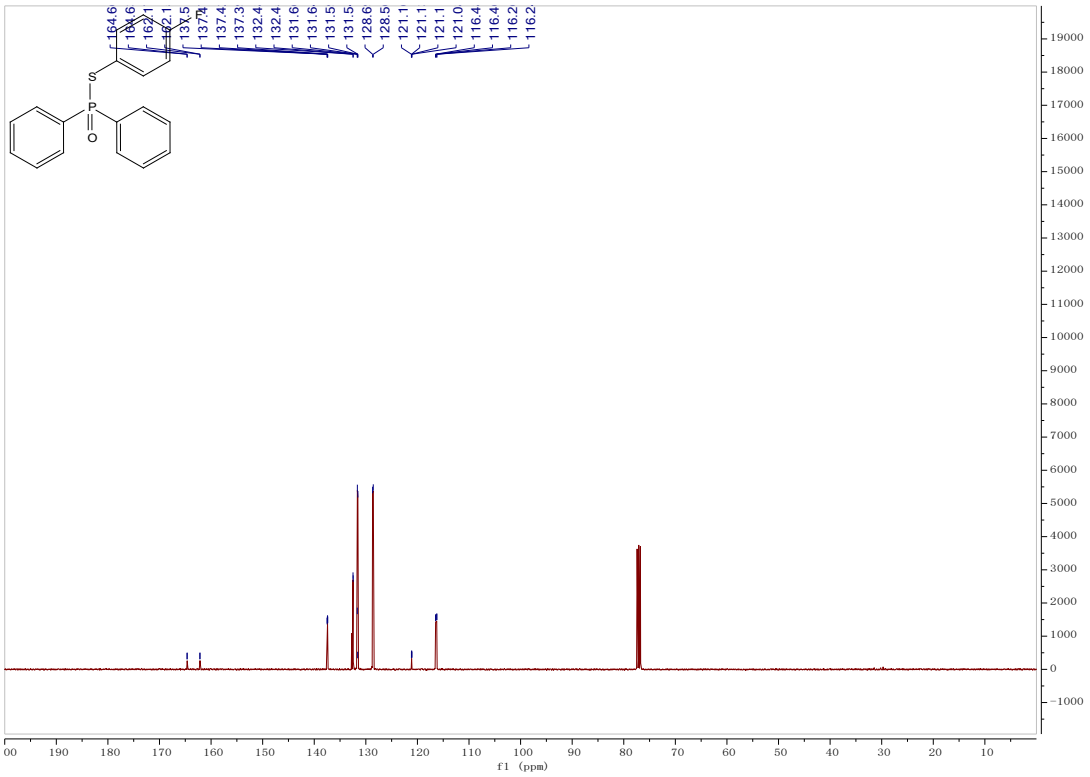


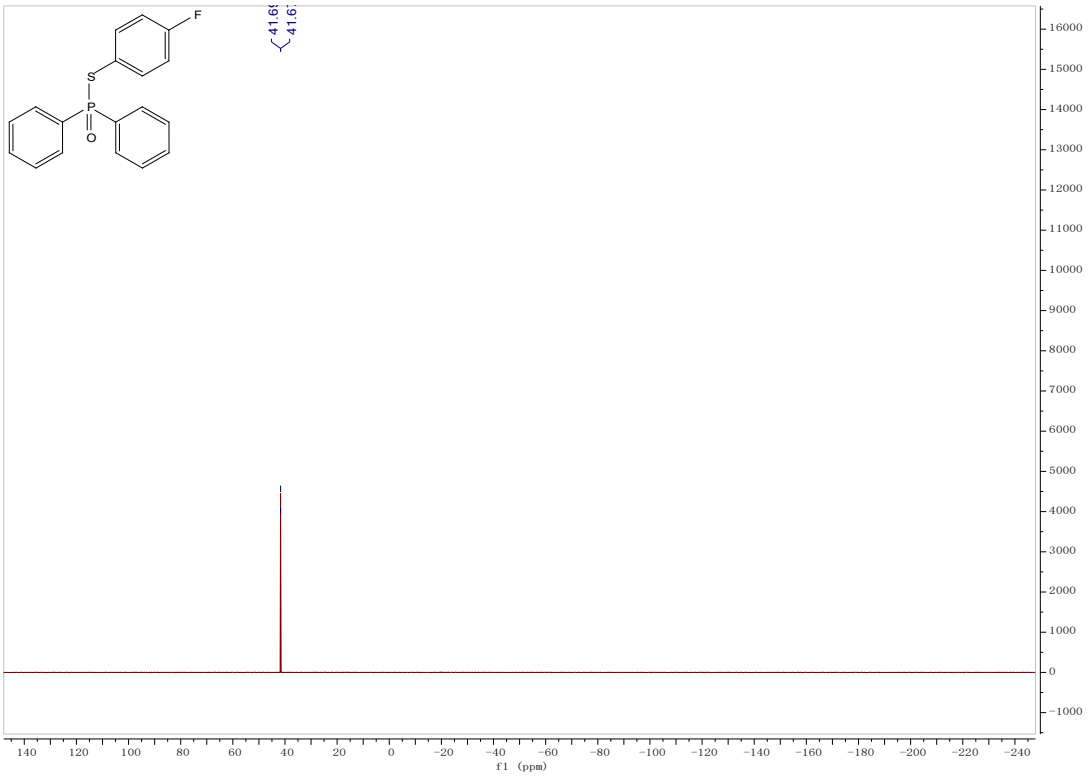

F
S
P
O
42.14
42.12
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
−1000
140 120 100 80 60 40 20 0 −20 −40 −60 −80 −100 −120 −140 −160 −180 −200 −220 −240
f1 (ppm)

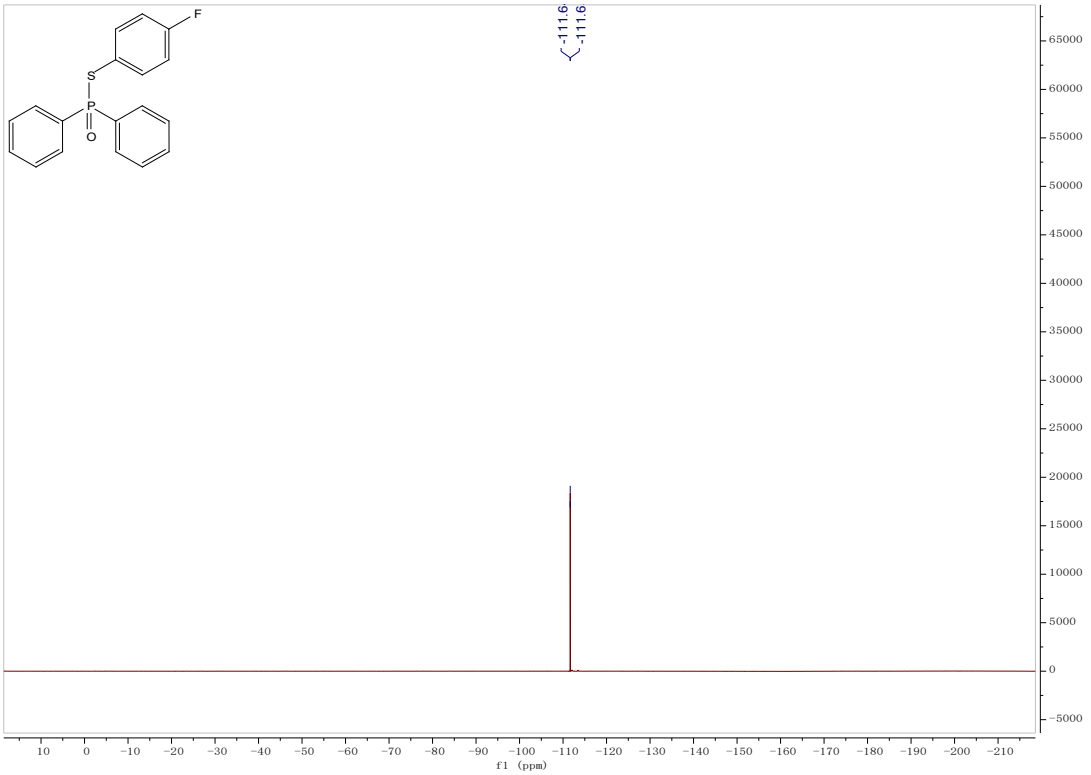

F
S
P
O
-106.3
-106.3
65000
60000
55000
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
−5000
10 0 −10 −20 −30 −40 −50 −60 −70 −80 −90 −100 −110 −120 −130 −140 −150 −160 −170 −180 −190 −200 −210
f1 (ppm)

S-(4-fluorophenyl) diphenylphosphinothioate (3h)

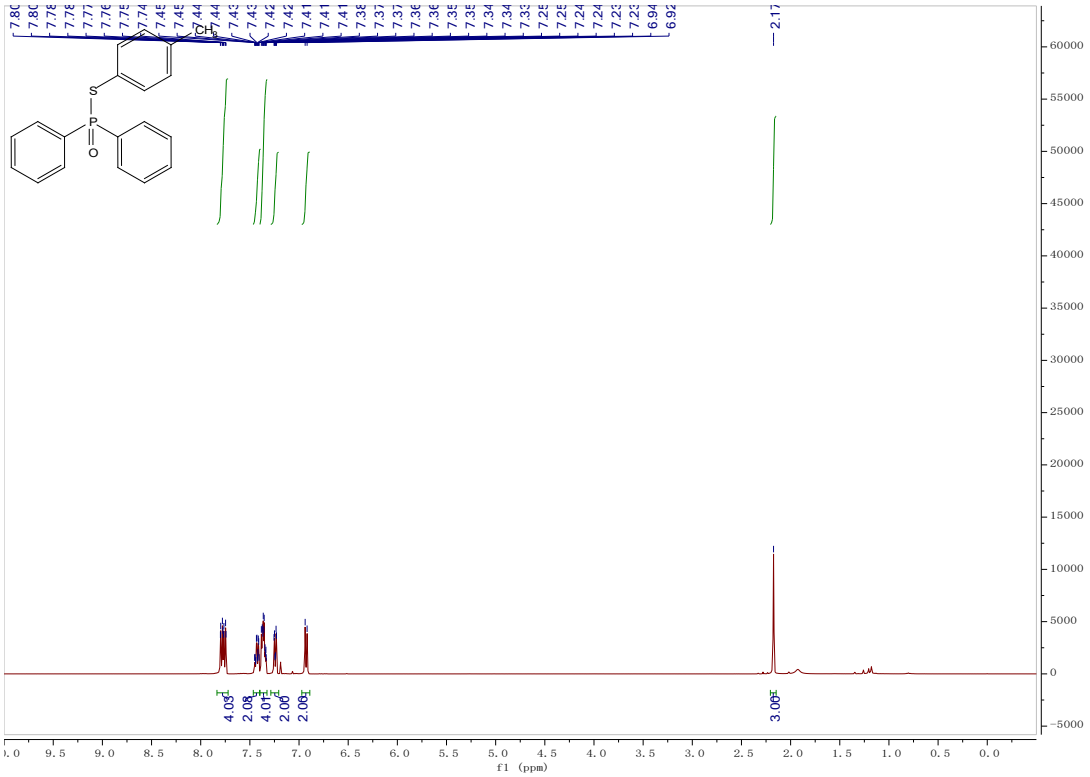


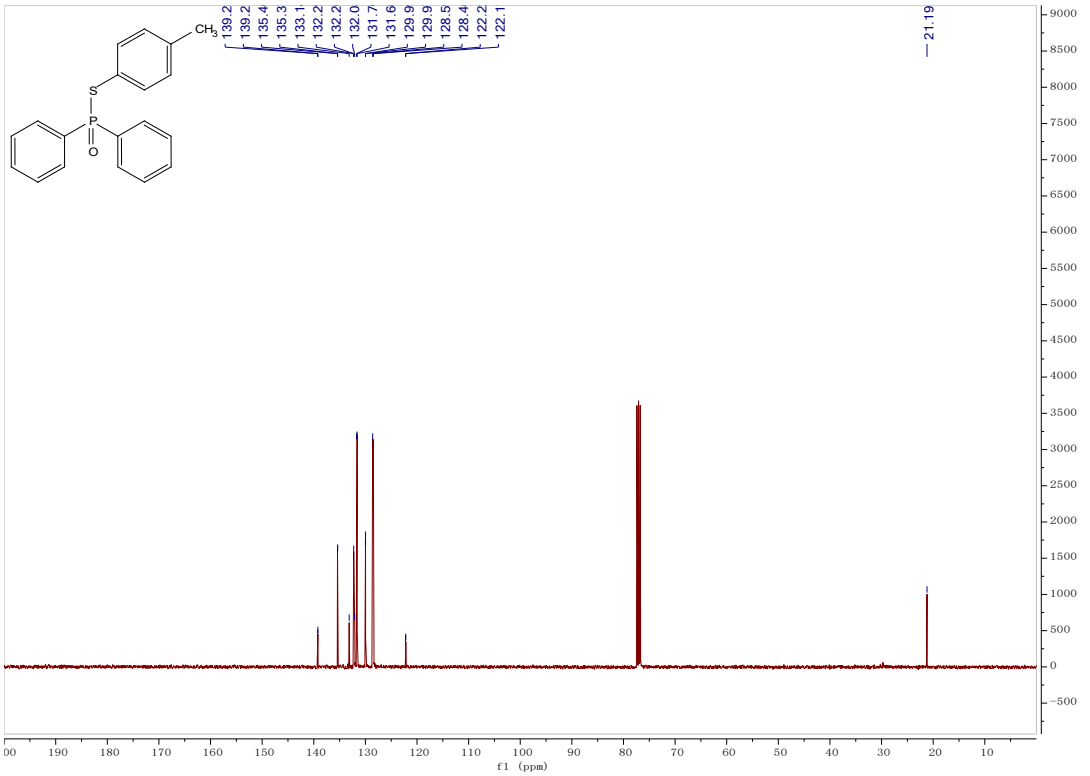


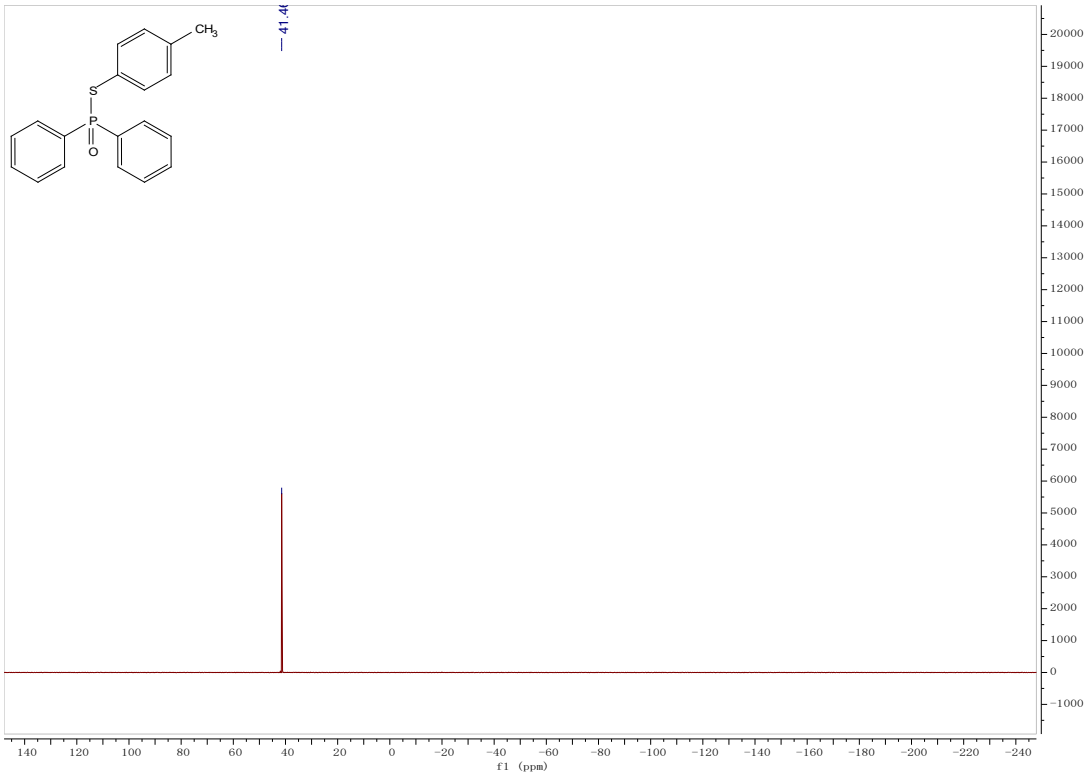

F
S
P
O
41.6
41.6
16000
15000
14000
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
140 120 100 80 60 40 20 0 -20 -40 -60 -80 -100 -120 -140 -160 -180 -200 -220 -240
f1 (ppm)


F
S
P
O
-111.6
-111.6
65000
60000
55000
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
-5000
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

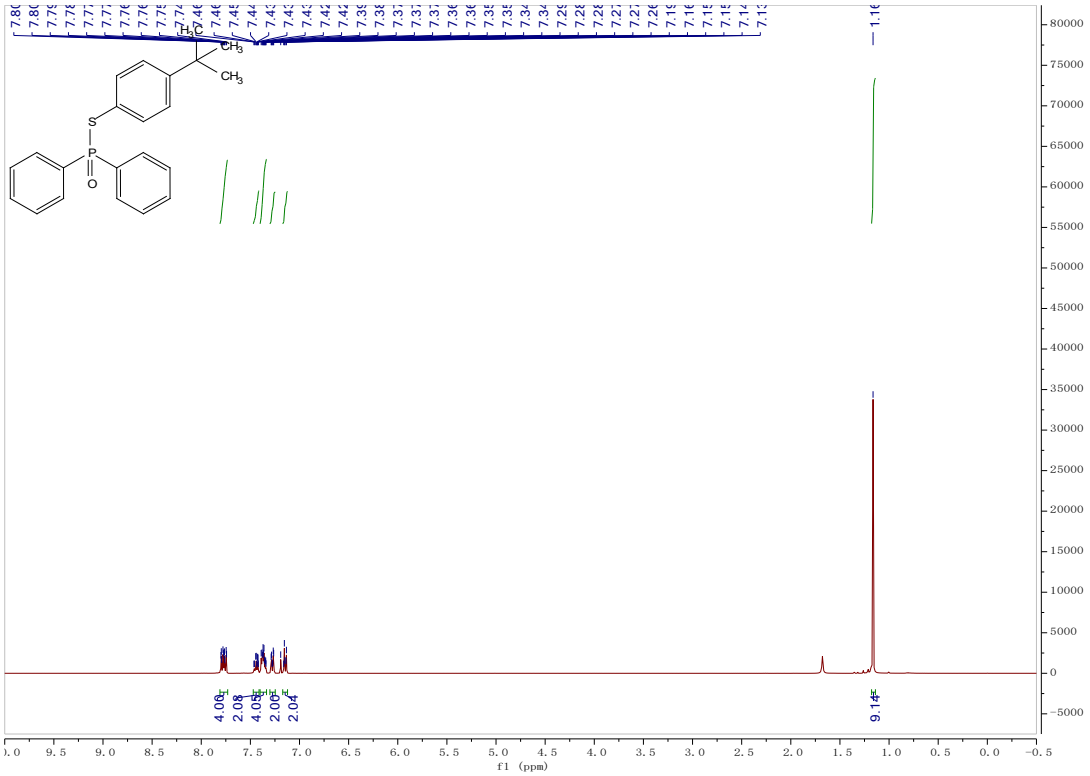
S-(p-tolyl) diphenylphosphinothioate (3i)

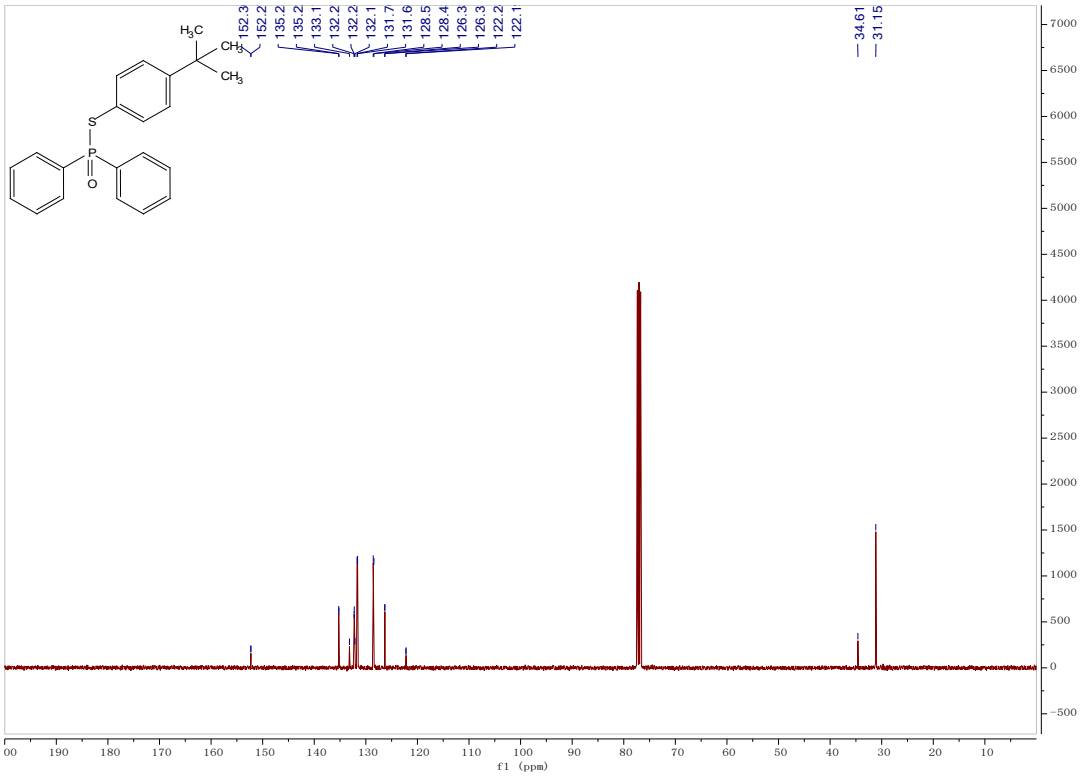


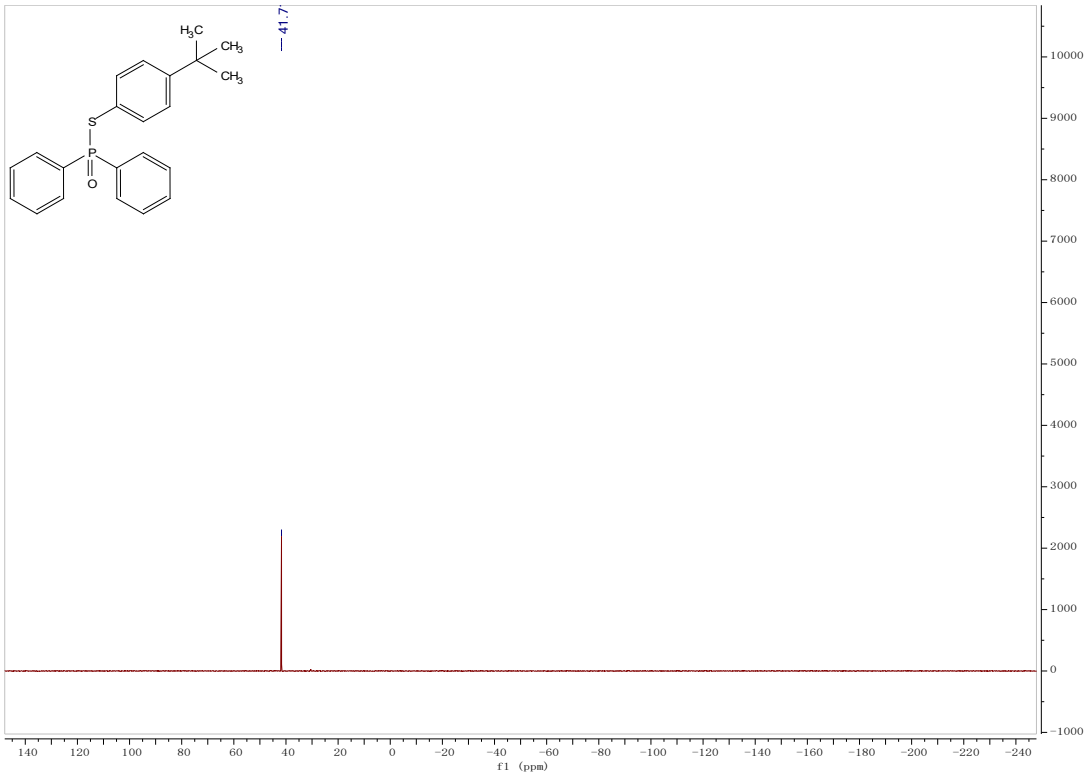




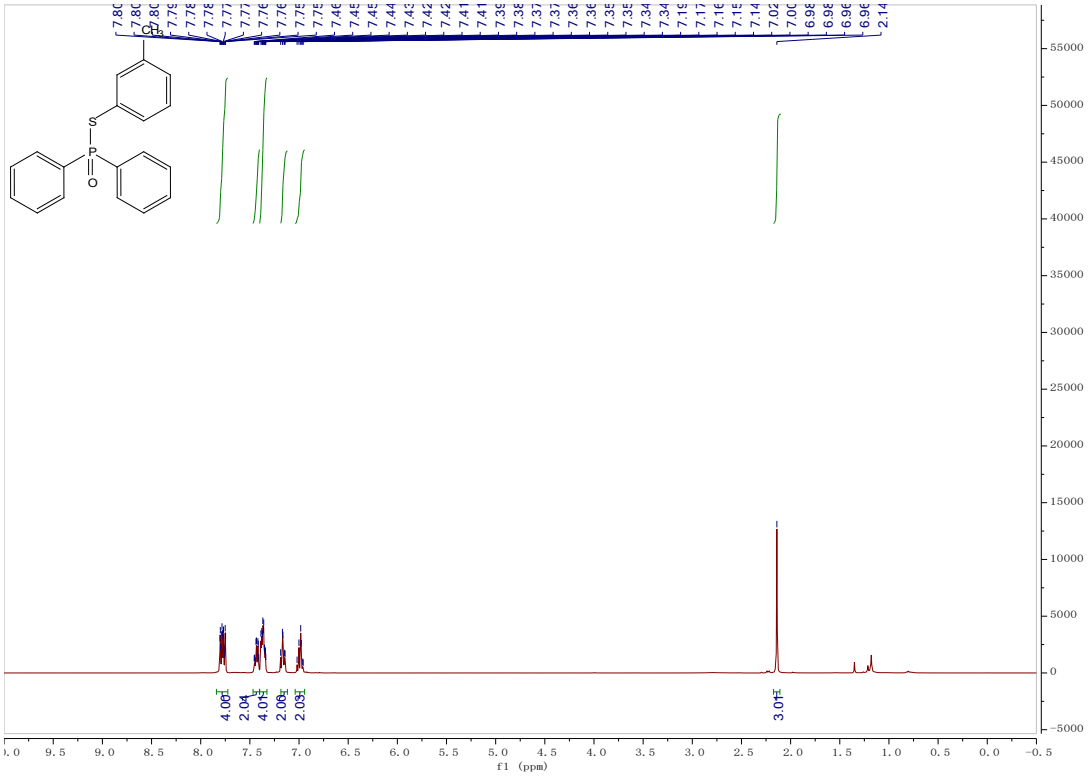
S-(4-(tert-butyl)phenyl) diphenylphosphinothioate (3j)

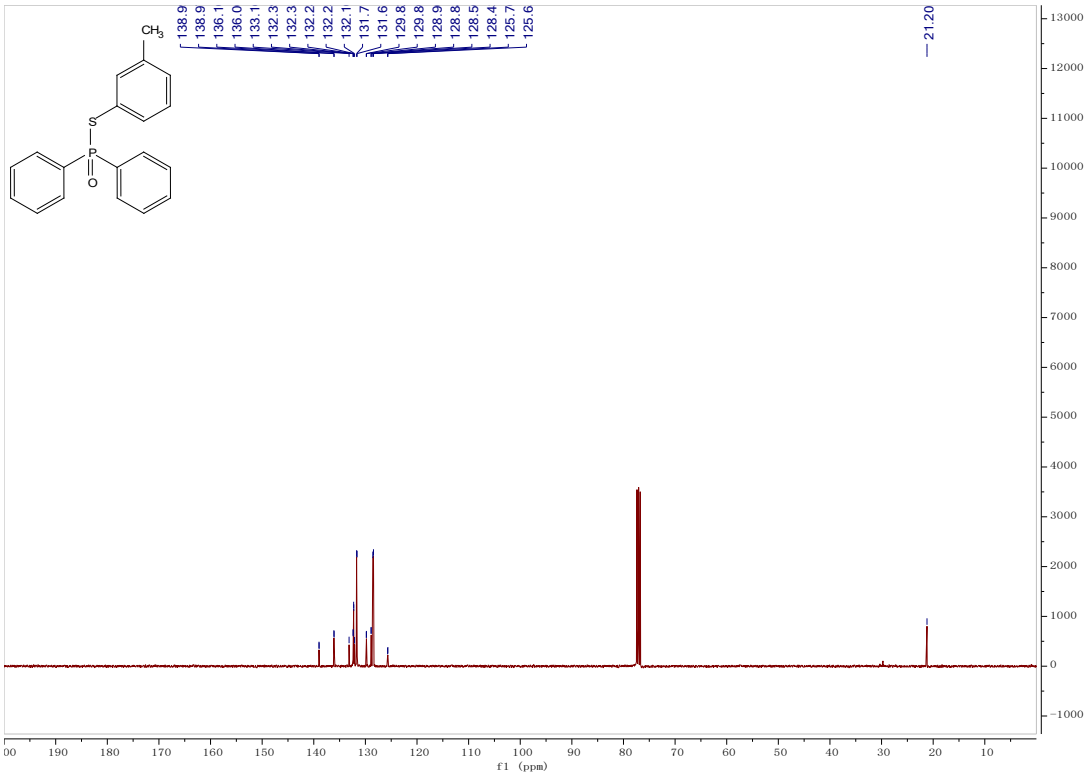


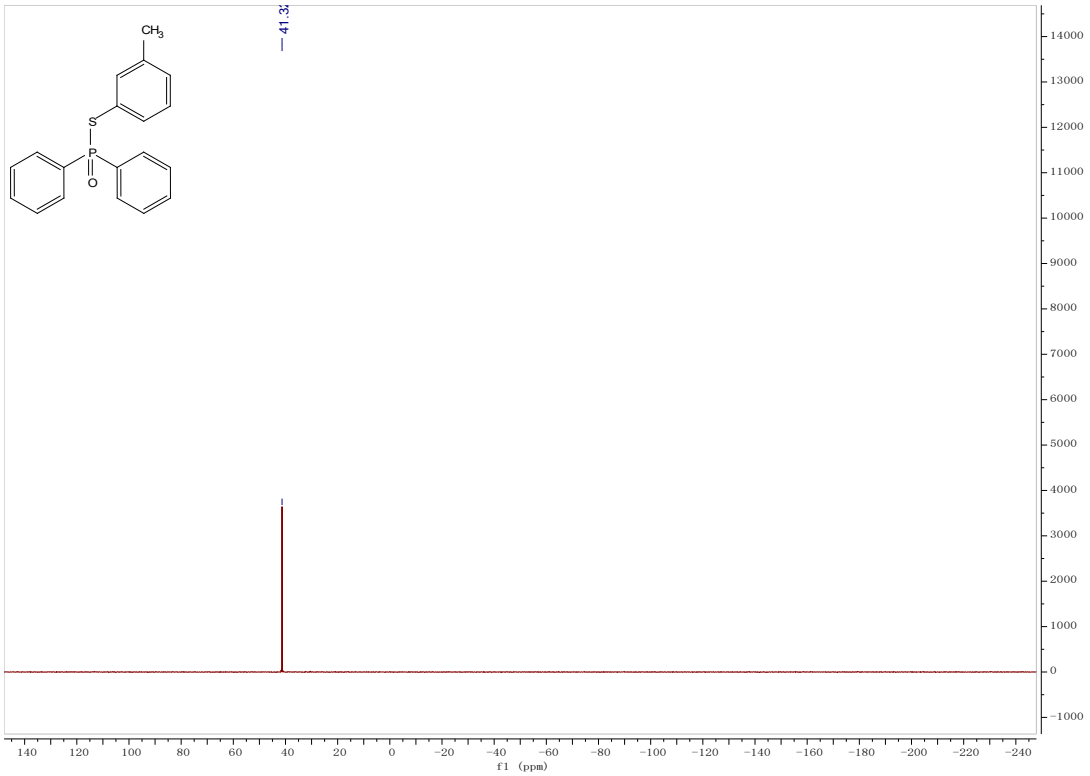

152.3
152.2
135.2
135.2
133.1
132.2
132.2
132.1
131.7
131.6
128.5
128.4
126.3
126.3
122.2
122.1
34.61
31.15
f1 (ppm)


41.7
f1 (ppm)

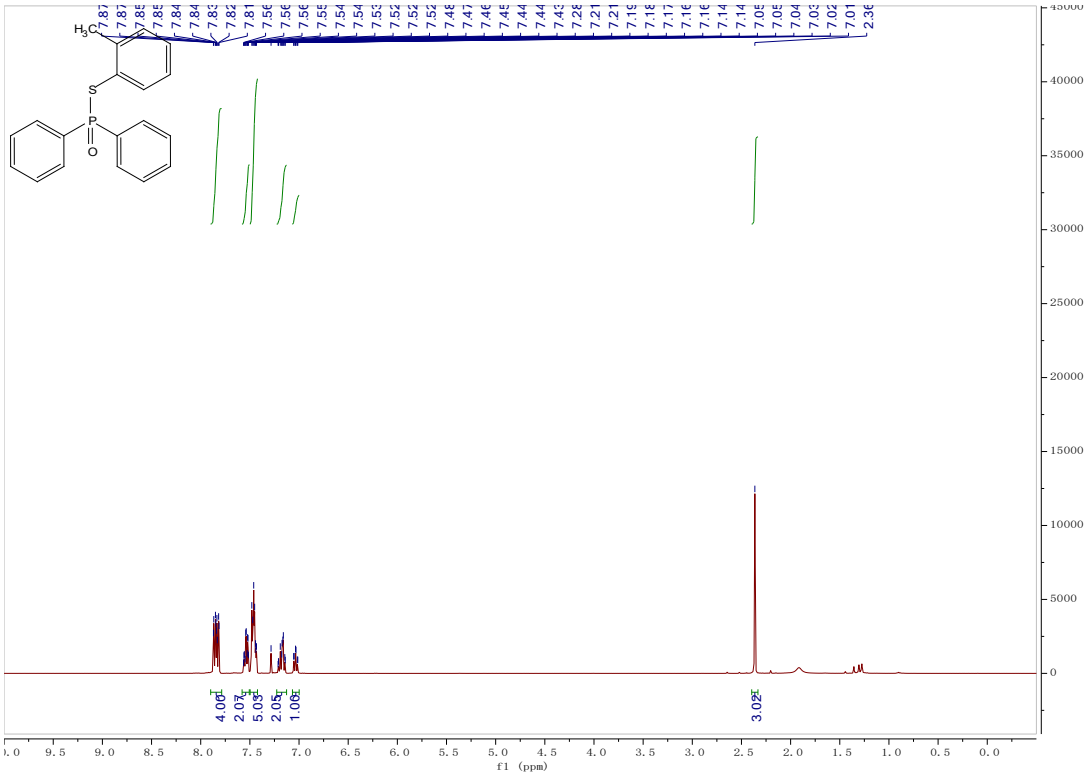
S-(m-tolyl) diphenylphosphinothioate (3k)

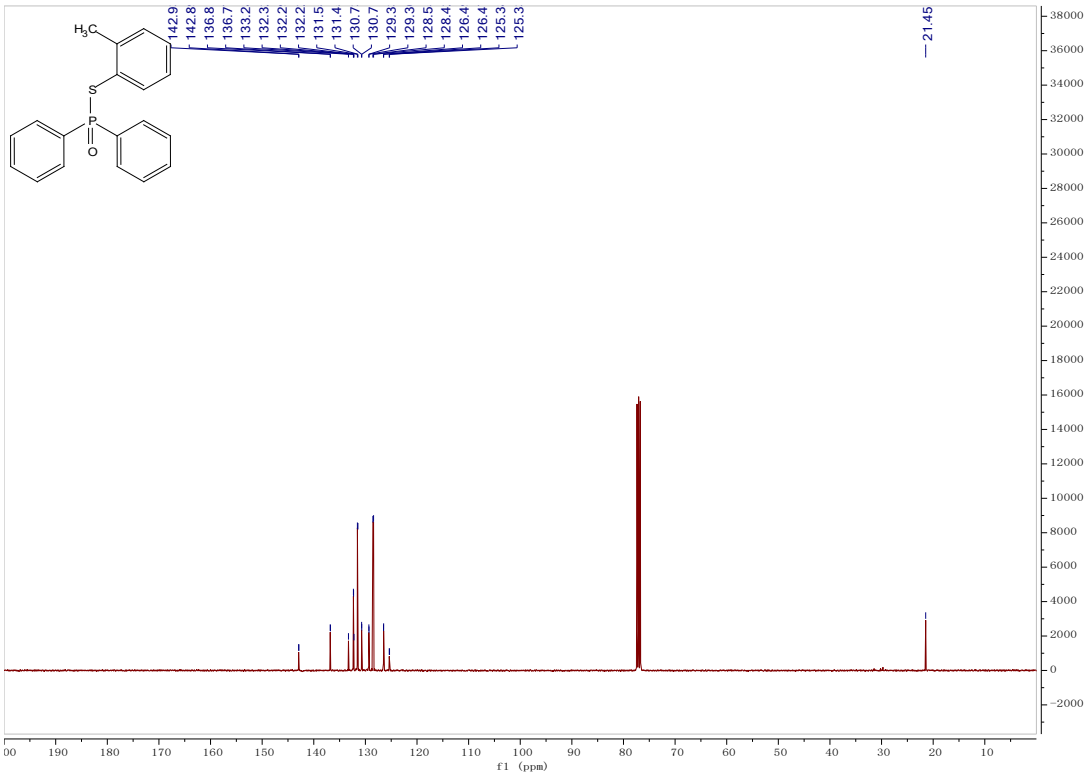


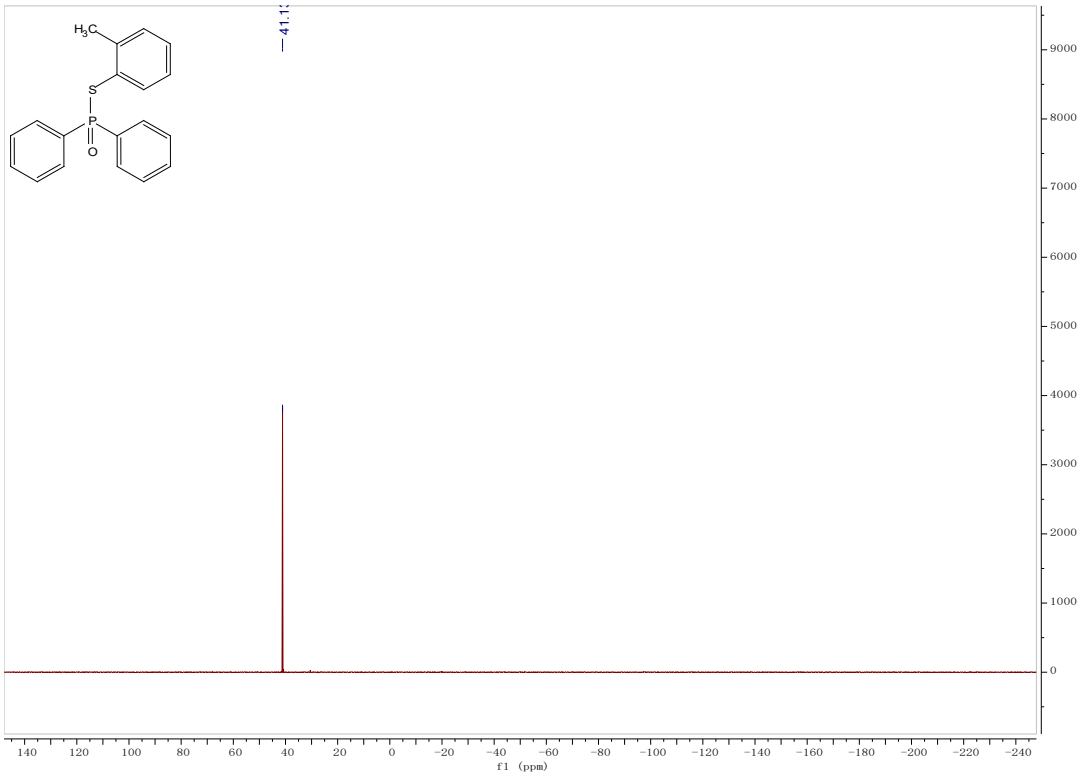




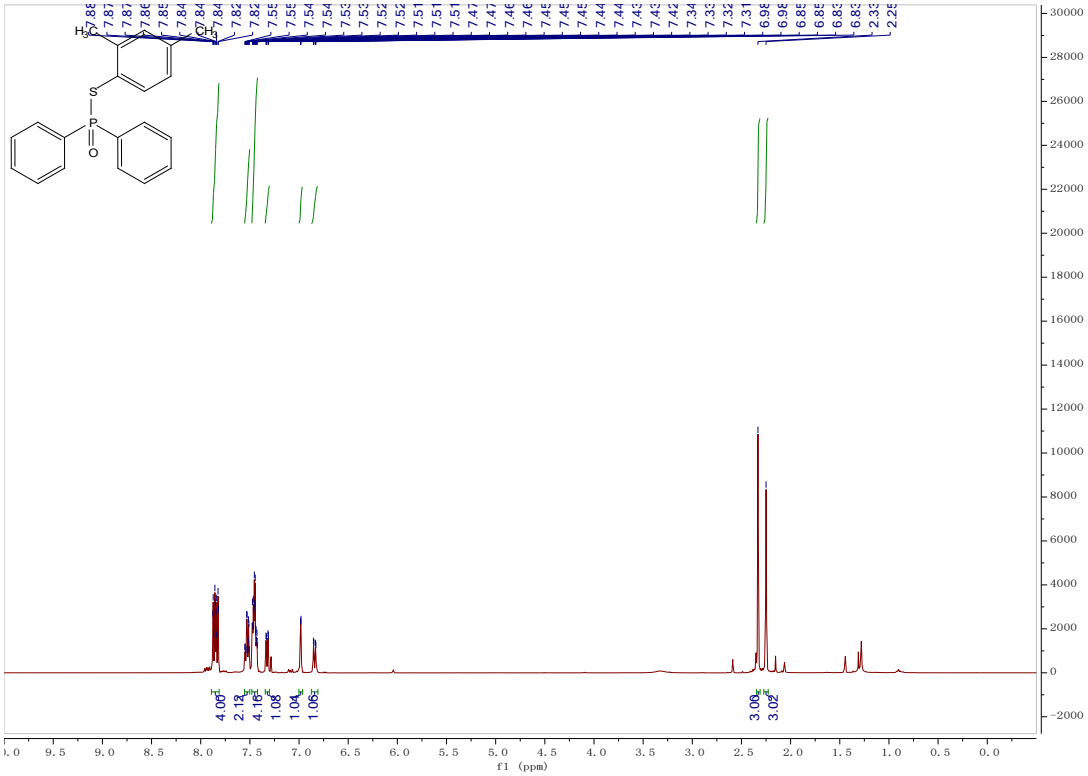
S-(o-tolyl) diphenylphosphinothioate (3l)

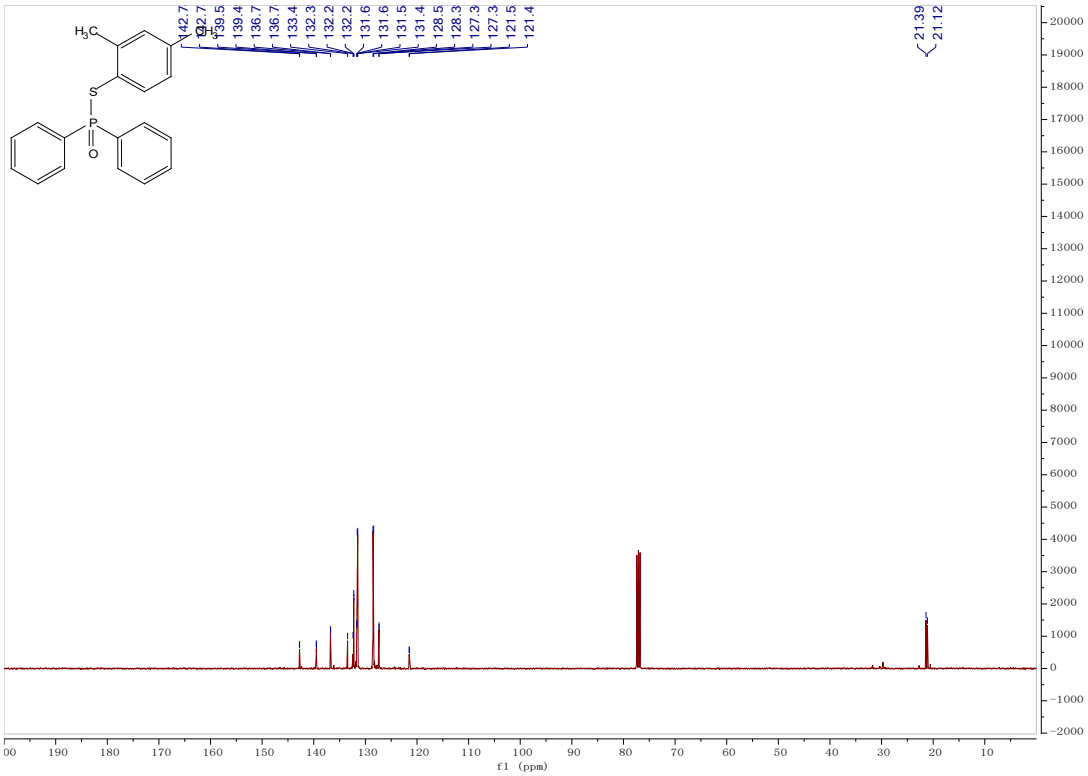


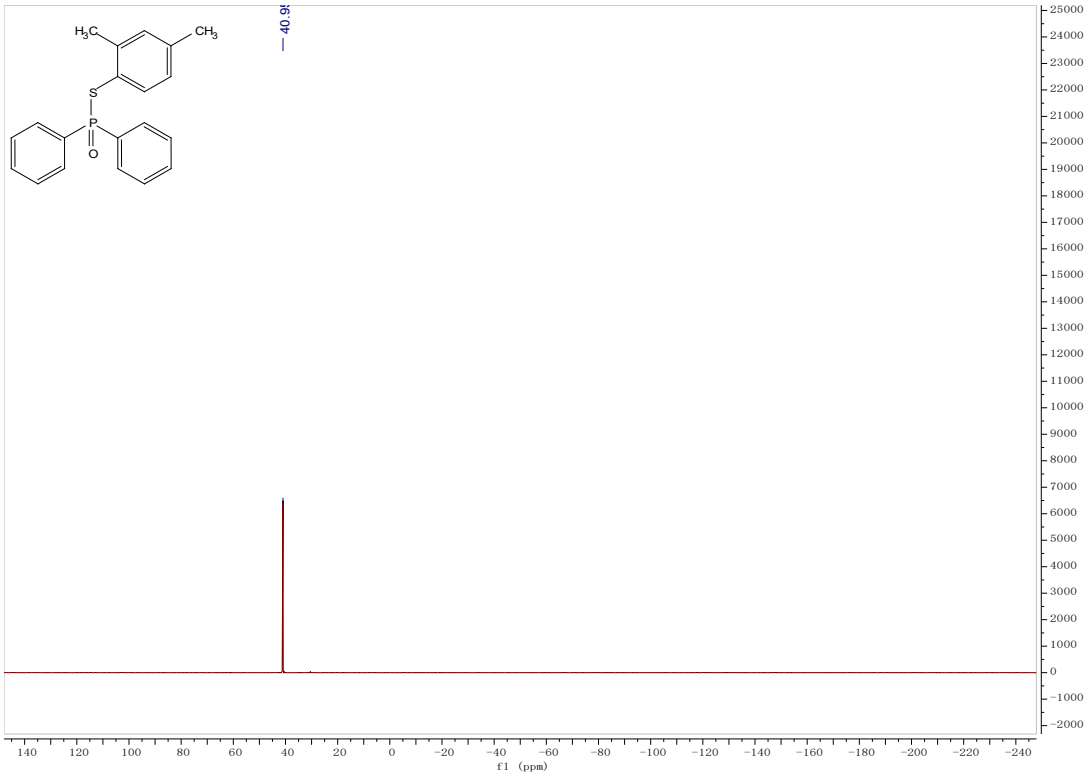

142.9
142.8
136.8
136.7
133.2
132.3
132.2
132.2
131.5
131.4
130.7
130.7
129.3
129.3
128.5
128.4
126.4
126.4
125.3
125.3
21.45
H3C
S
P
O
f1 (ppm)


H3C
S
P
O
f1 (ppm)

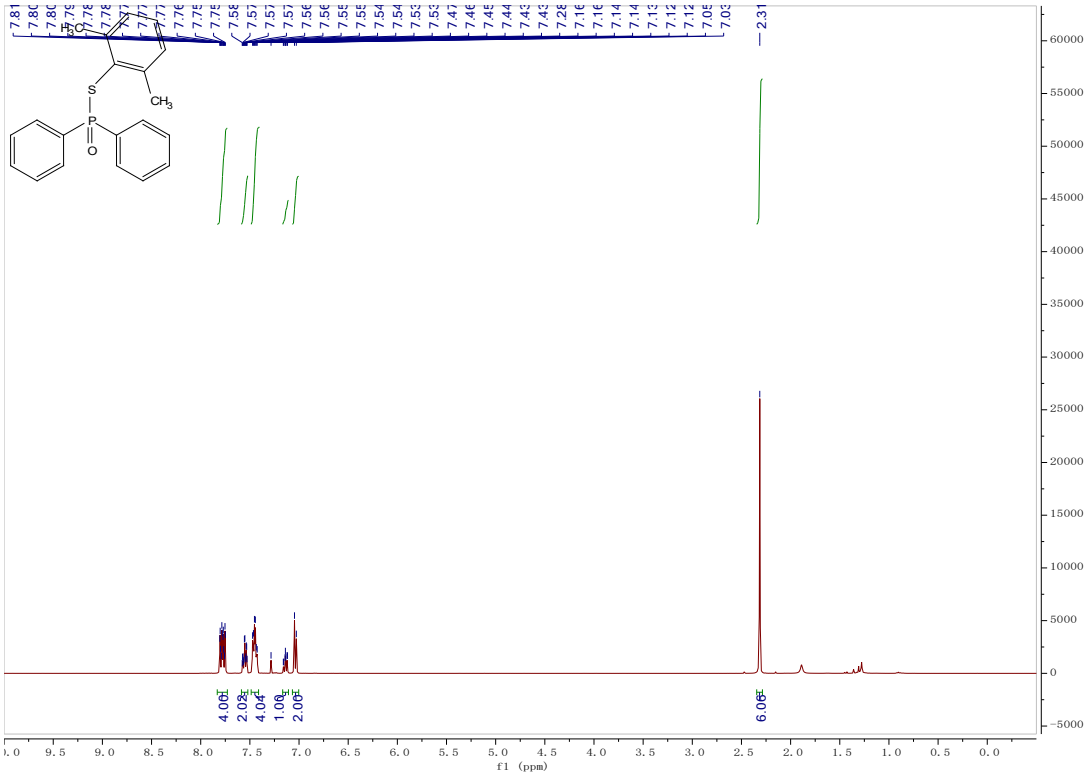
S-(2,4-dimethylphenyl) diphenylphosphinothioate (3m)

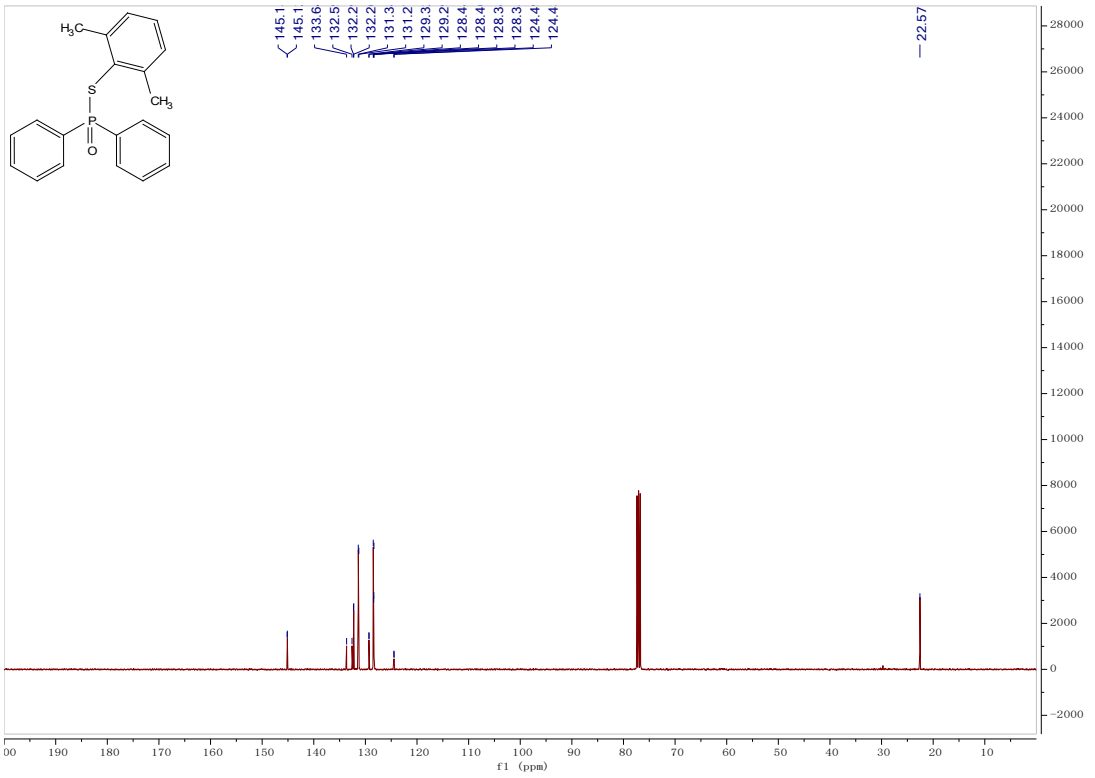


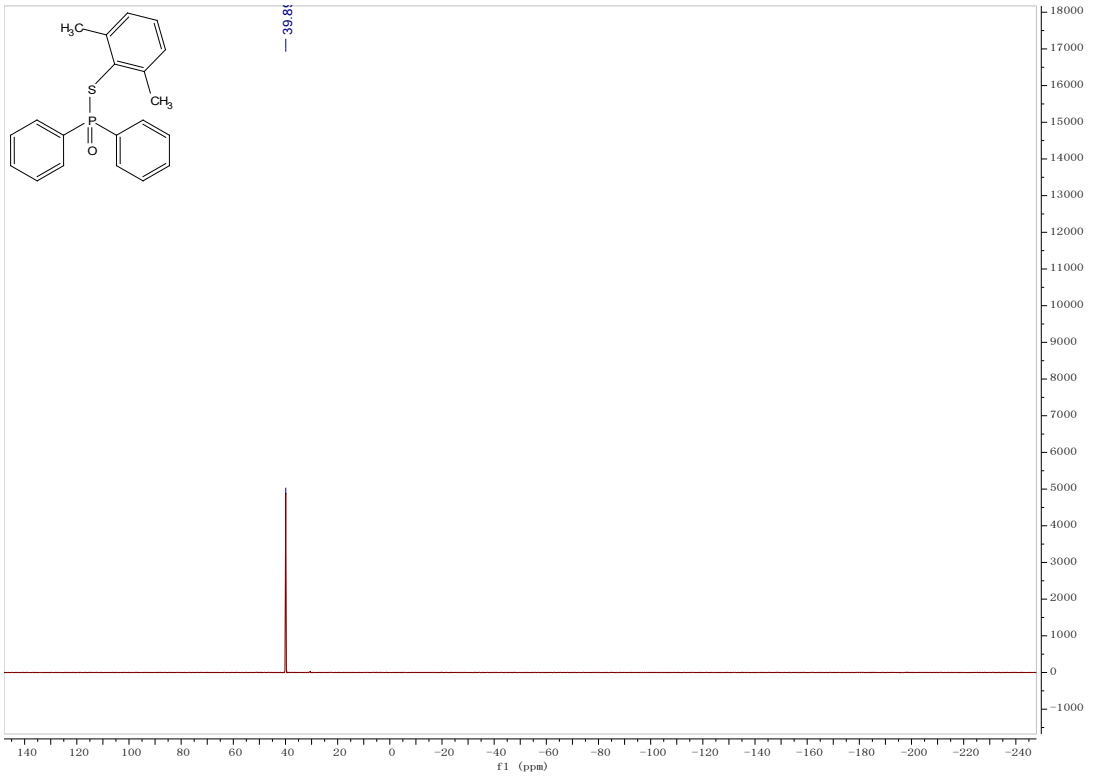




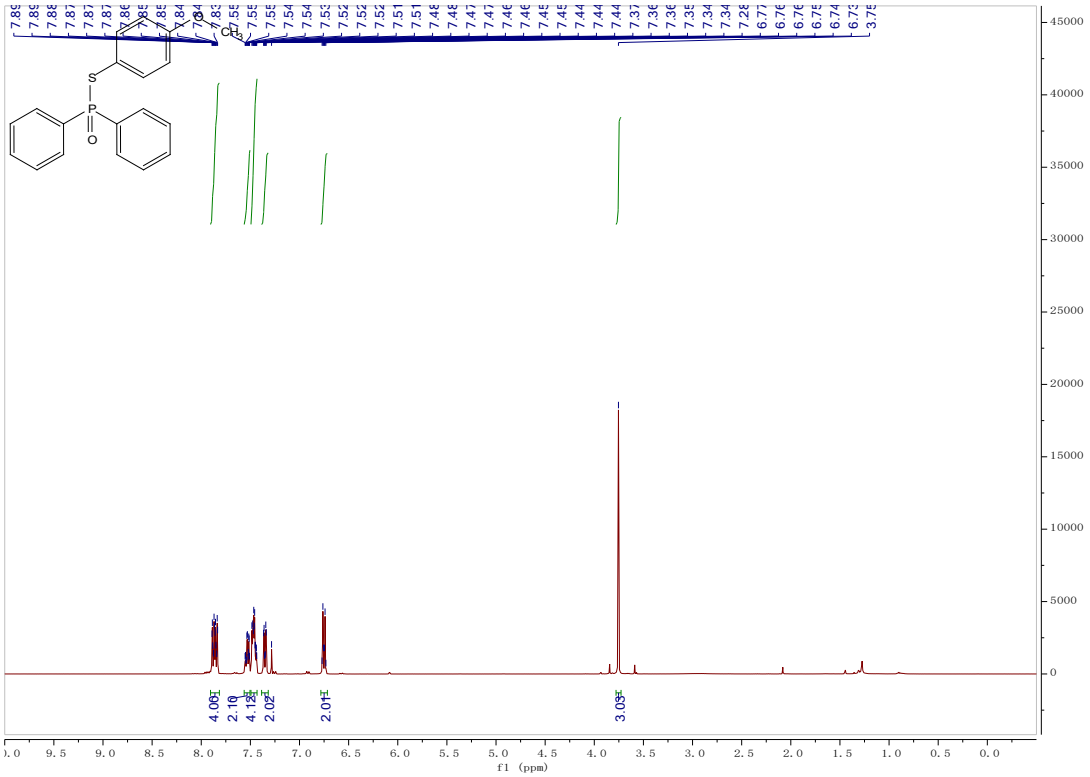
S-(2,6-dimethylphenyl) diphenylphosphinothioate (3n)

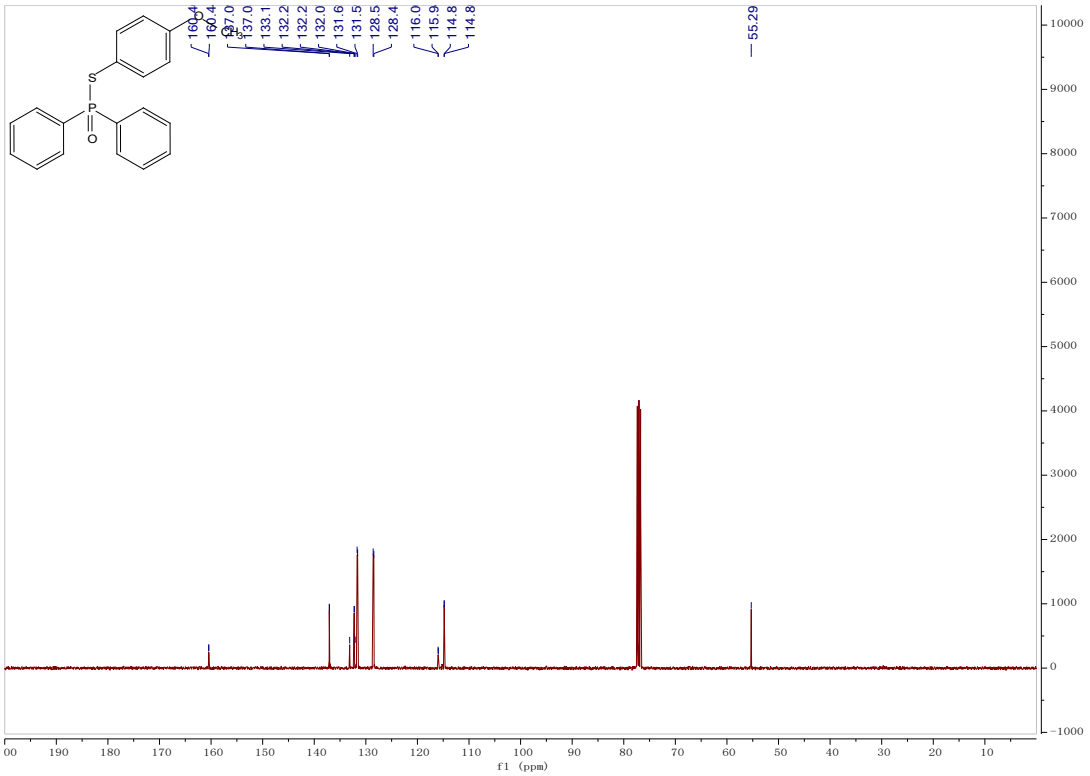


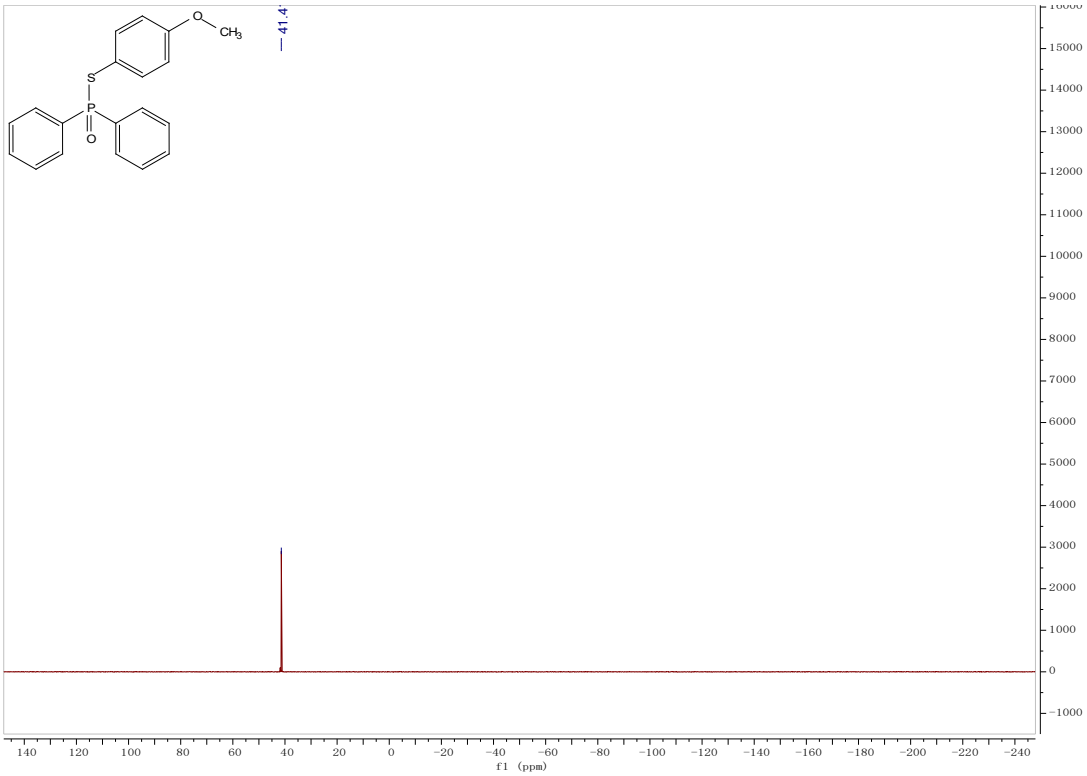

145.1
145.1
133.6
132.5
132.2
132.2
131.3
131.2
129.3
129.2
128.4
128.4
128.3
128.3
124.4
124.4
22.57
f1 (ppm)


39.8
f1 (ppm)

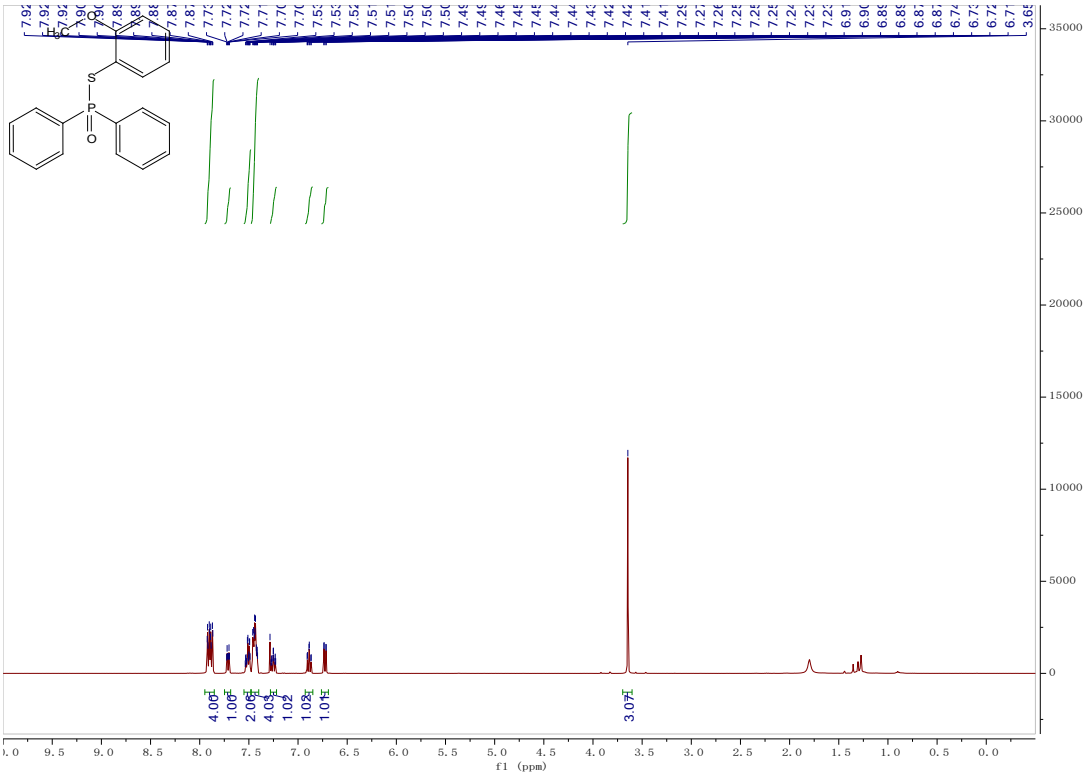
S-(4-methoxyphenyl) diphenylphosphinothioate (3o)

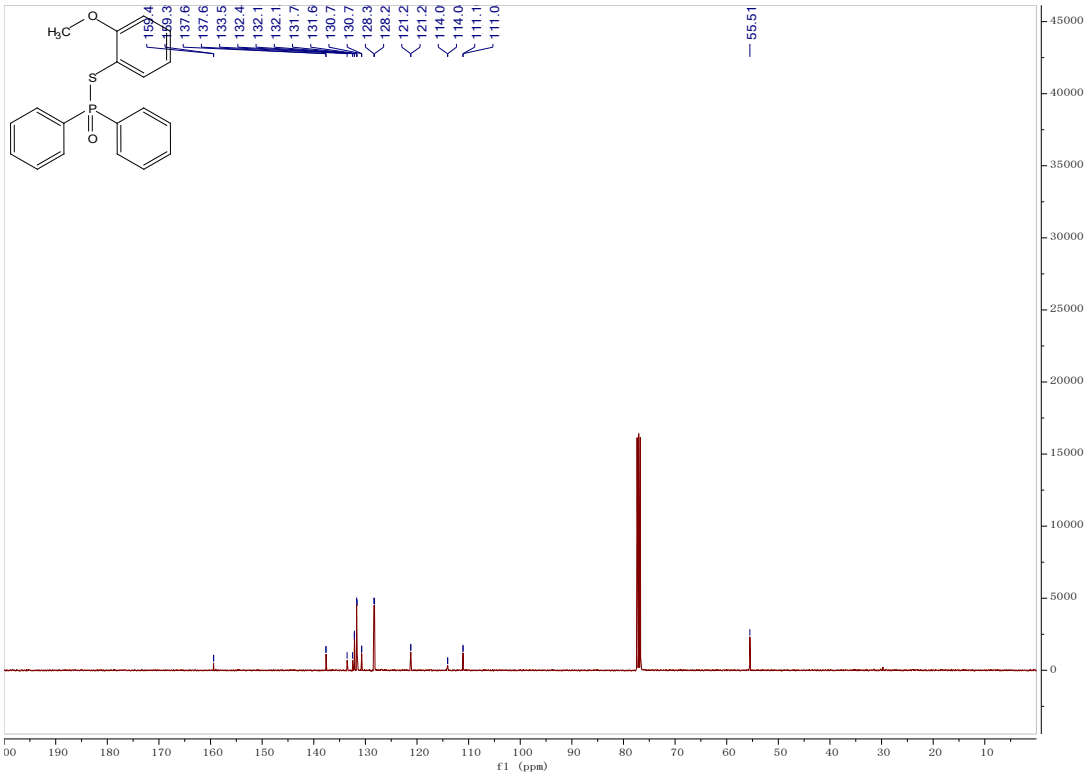


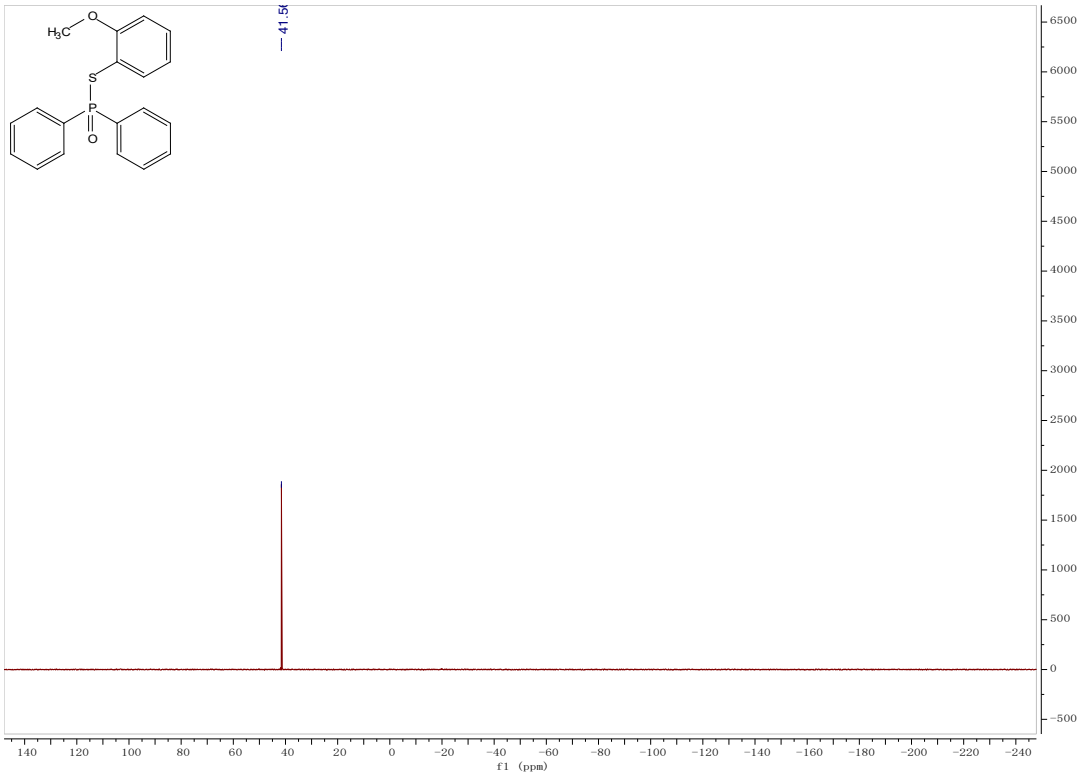




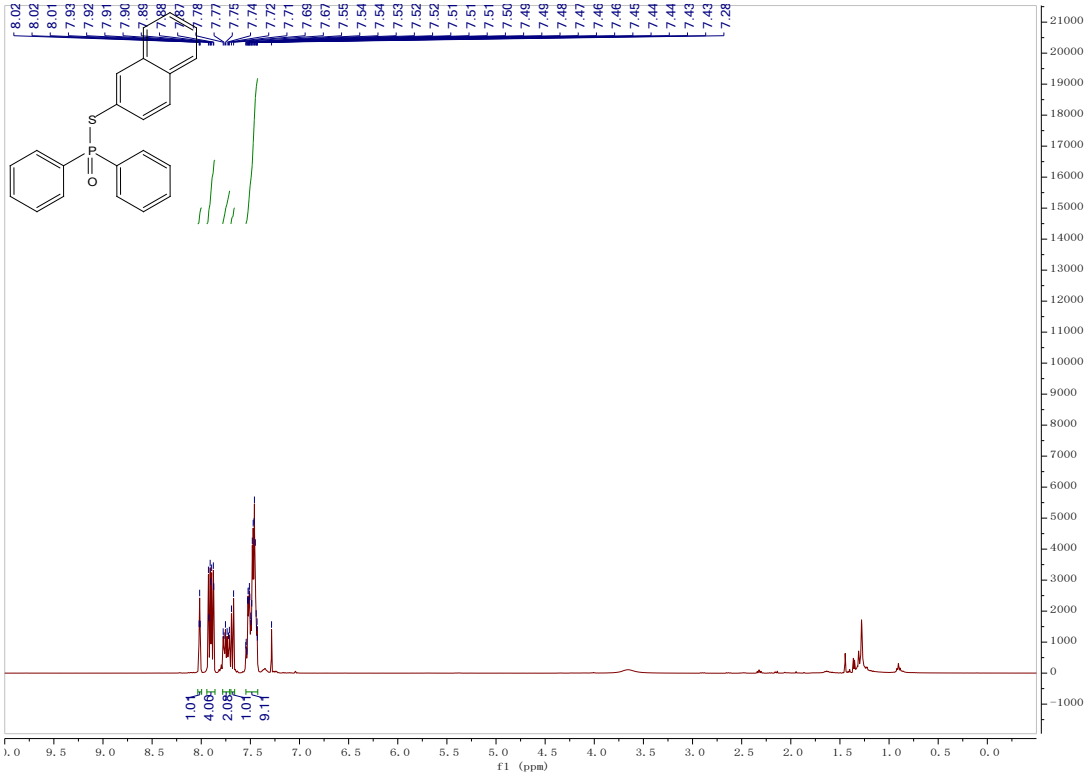
S-(2-methoxyphenyl) diphenylphosphinothioate (3p)

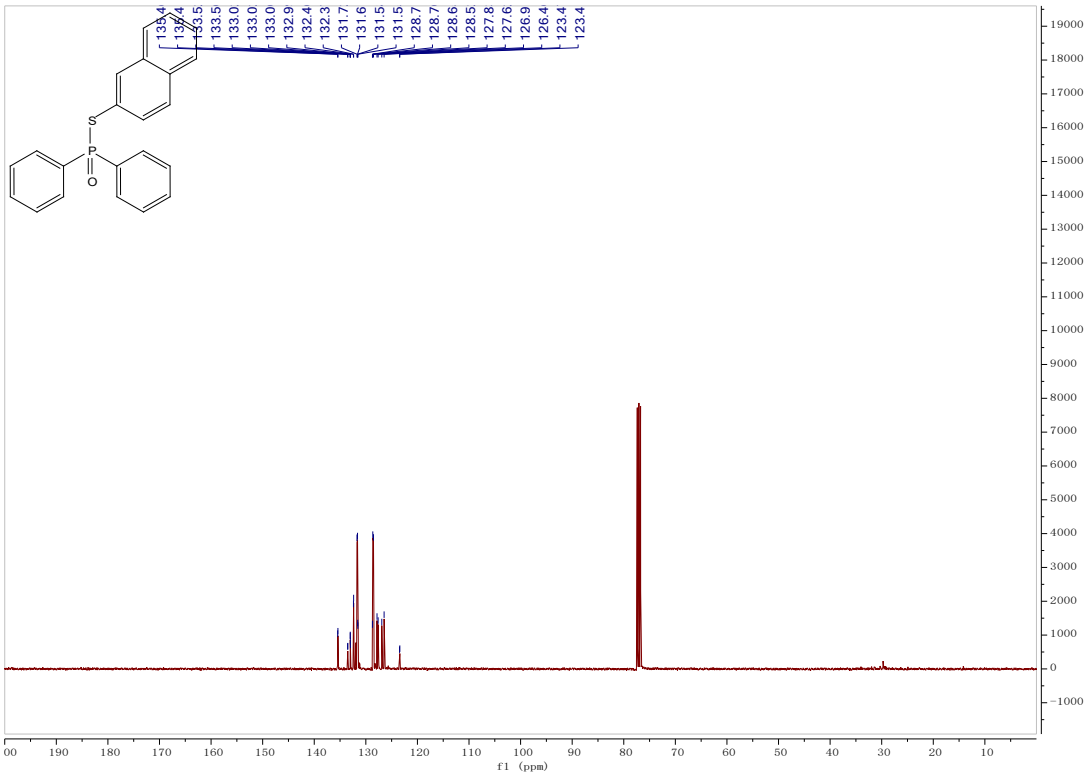


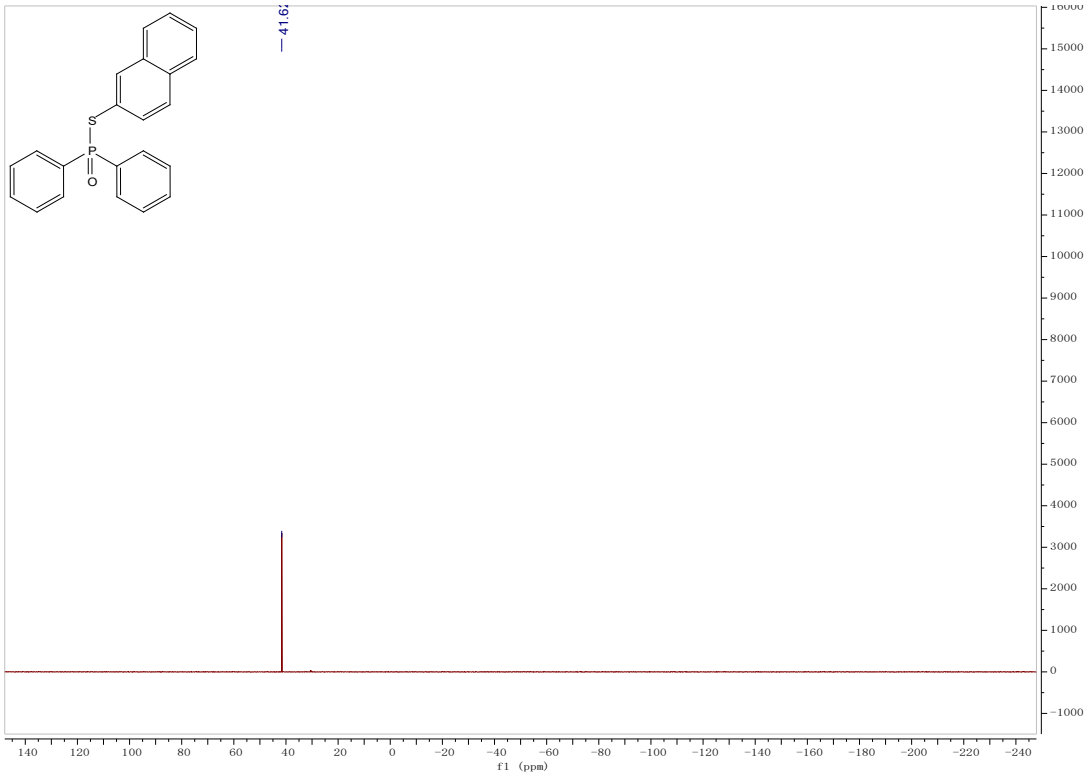

159.4
159.3
137.6
137.6
133.5
132.4
132.1
132.1
131.7
131.6
130.7
130.7
128.3
128.2
121.2
121.2
114.0
114.0
111.1
111.0
55.51
f1 (ppm)


41.5
f1 (ppm)

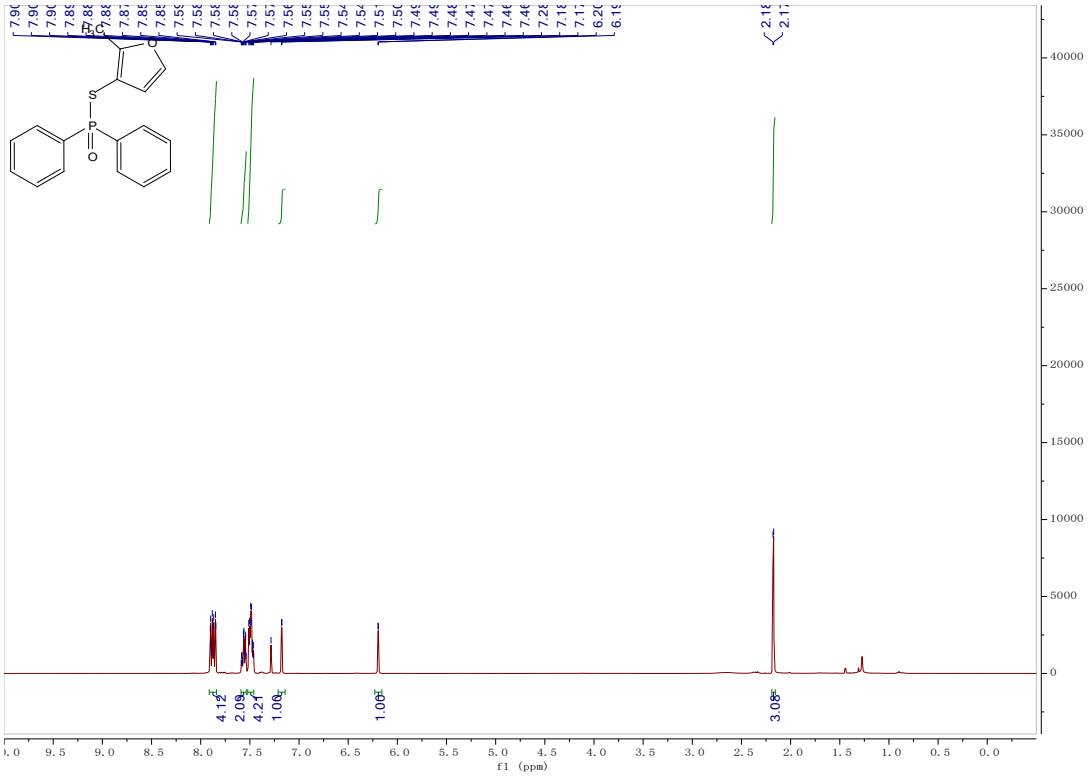
S-(naphthalen-2-yl) diphenylphosphinothioate (3q)

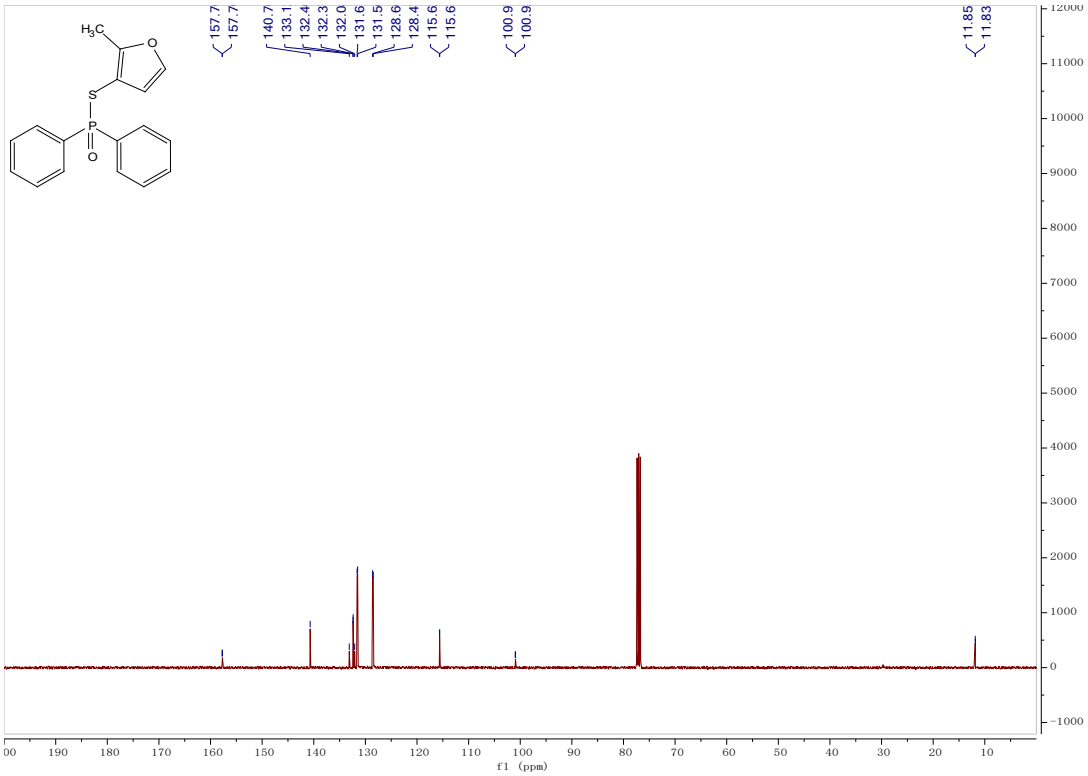


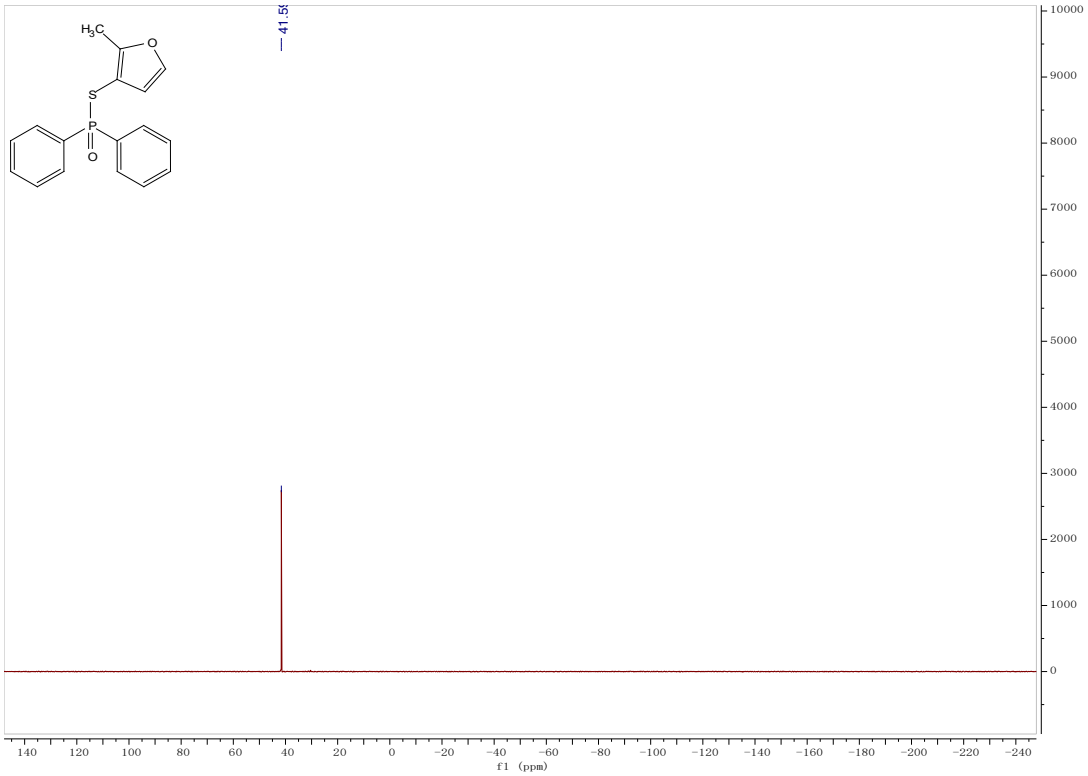




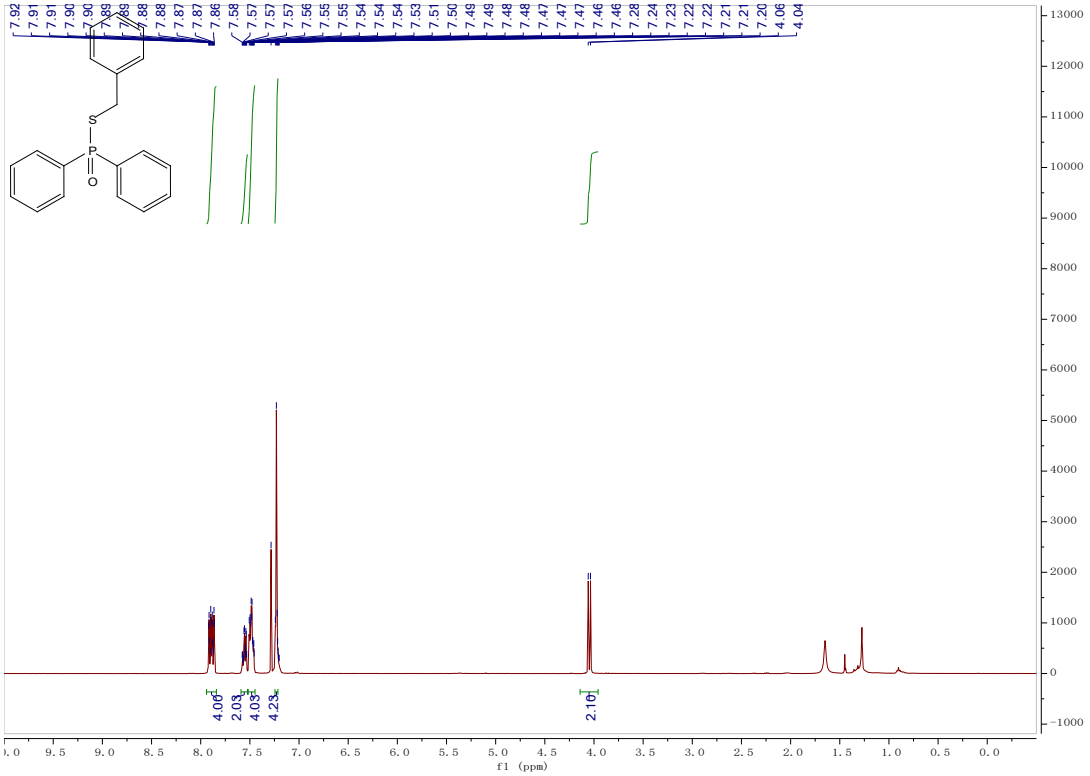
S-(2-methylfuran-3-yl) diphenylphosphinothioate (3r)

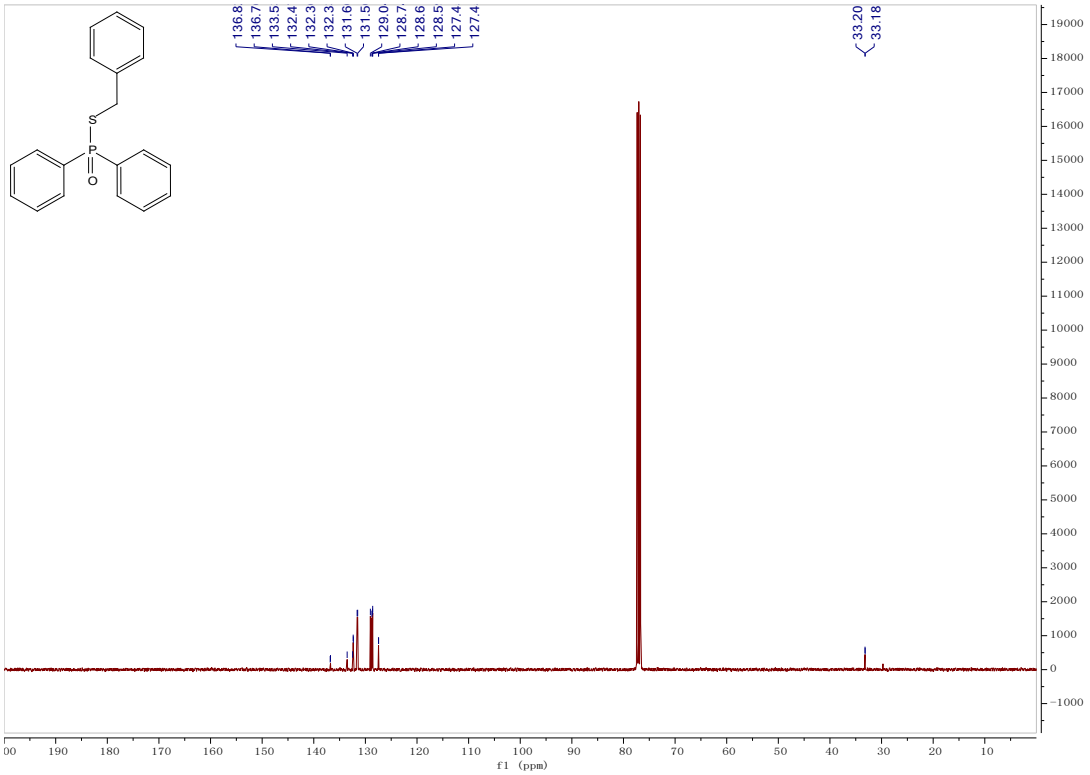


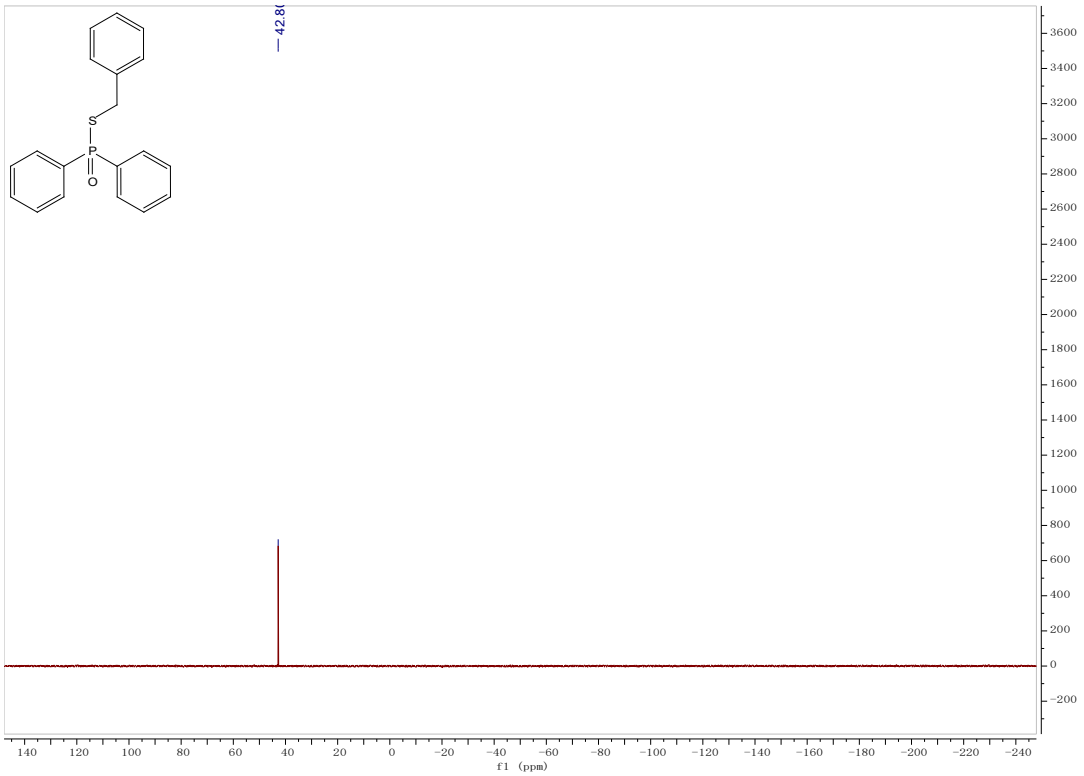

H3C
O
S
P
O
157.7
157.7
140.7
133.1
132.4
132.3
132.0
131.6
131.5
128.6
128.4
115.6
115.6
100.9
100.9
11.85
11.83
f1 (ppm)


H3C
O
S
P
O
41.5
f1 (ppm)

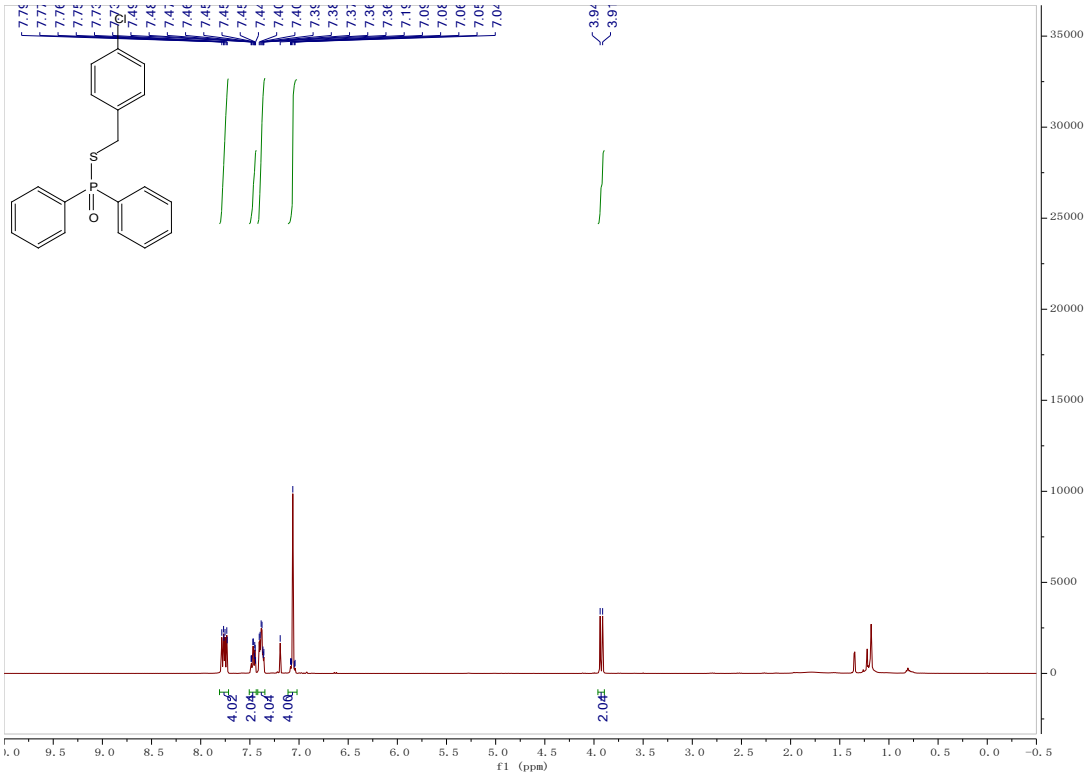
S-benzyl diphenylphosphinothioate (3s)

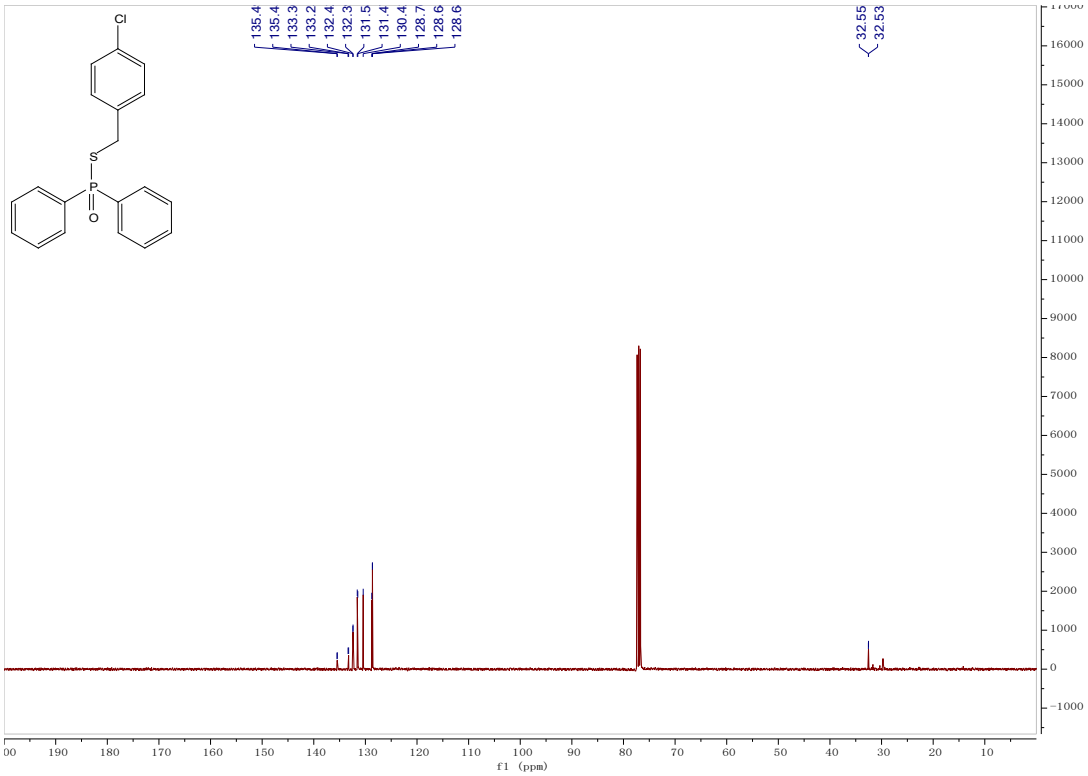


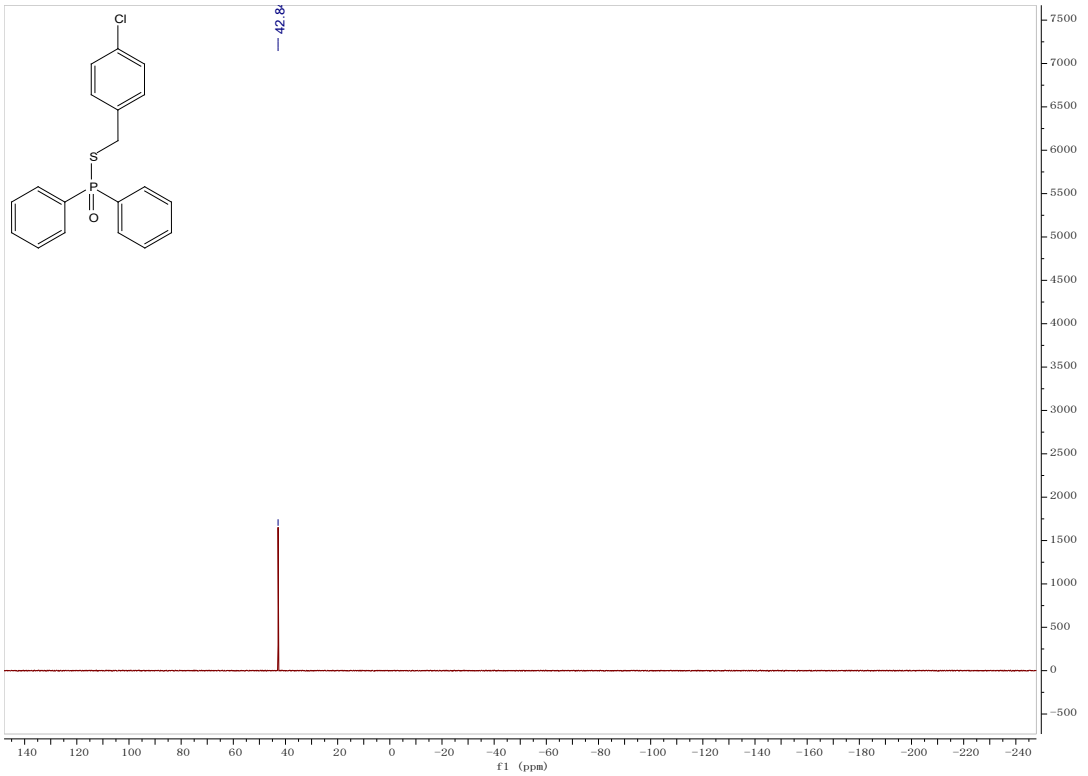




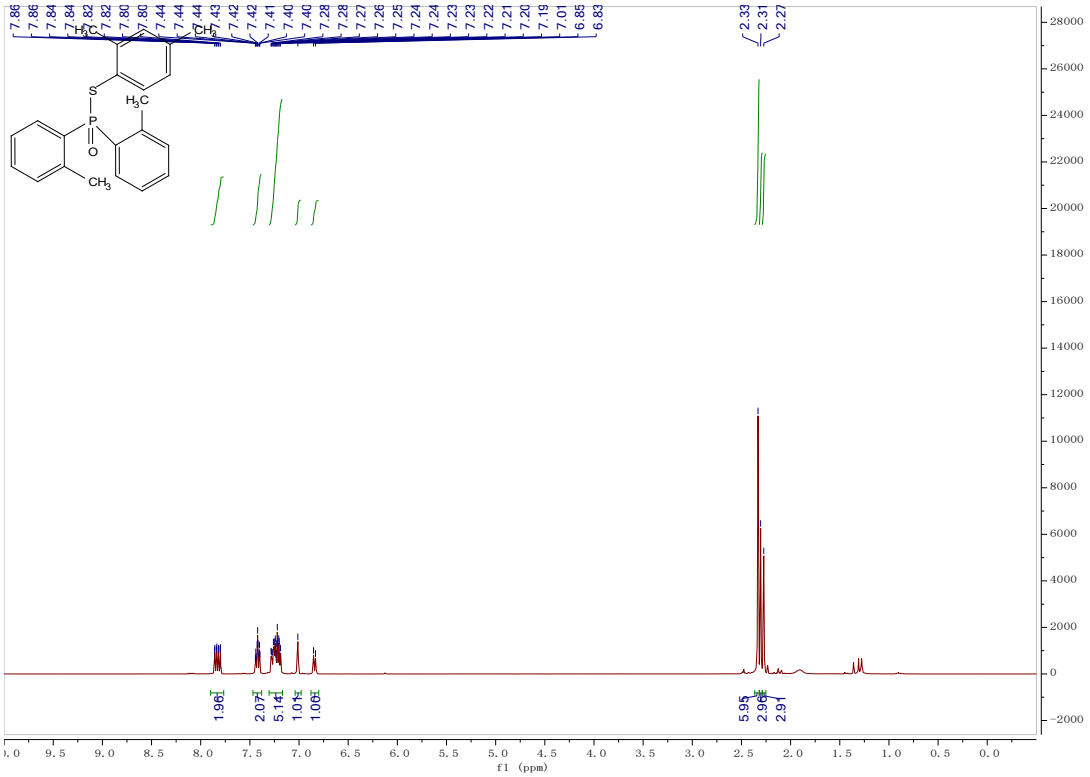
S-(4-chlorobenzyl) diphenylphosphinothioate (3t)

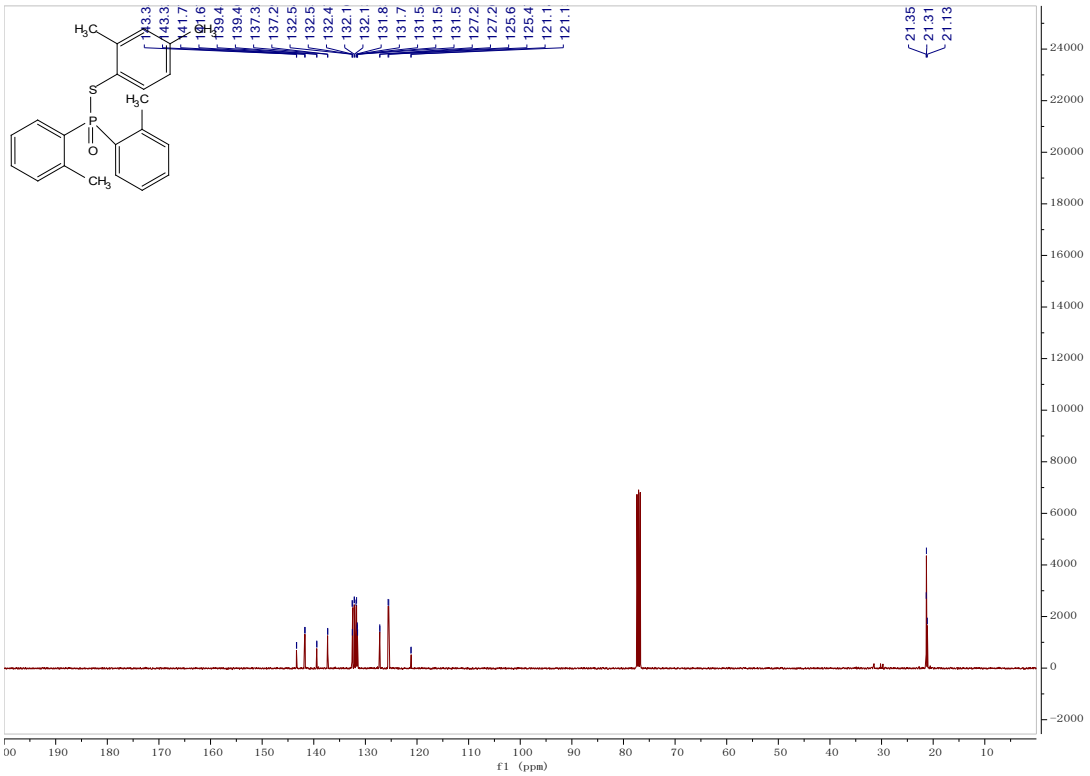


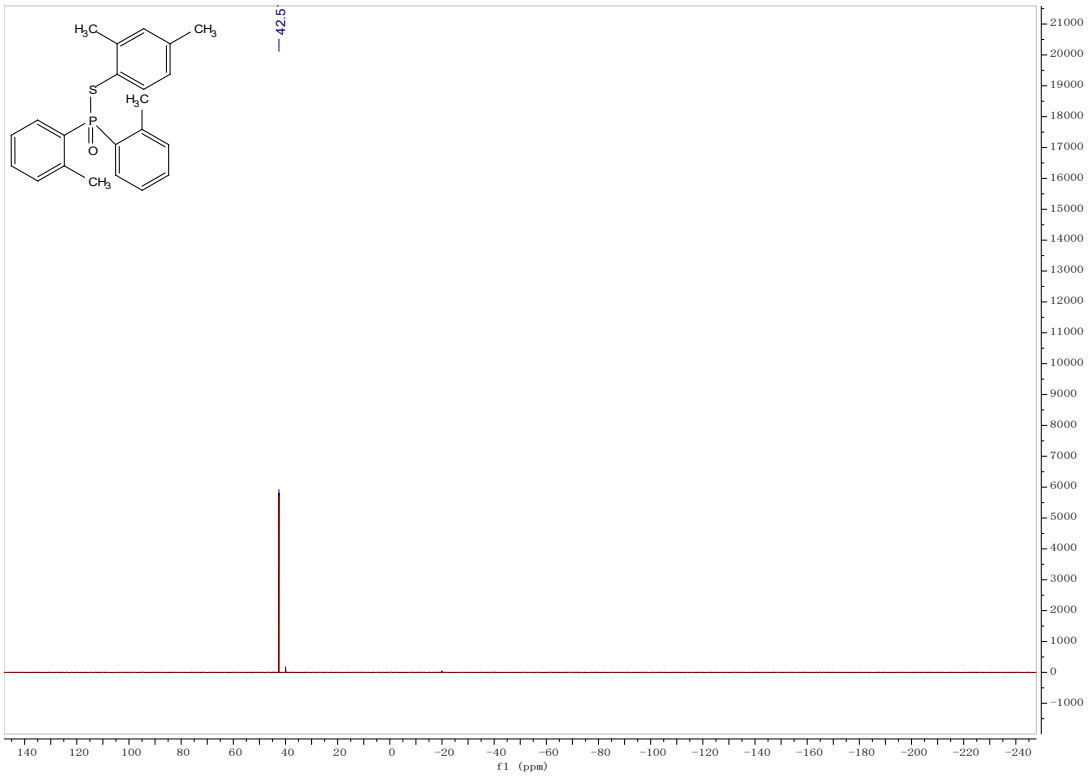

Cl
S
P
O
135.4
135.4
133.3
133.2
132.4
132.3
131.5
131.4
130.4
128.7
128.6
128.6
32.55
32.53
f1 (ppm)


Cl
S
P
O
42.8
f1 (ppm)

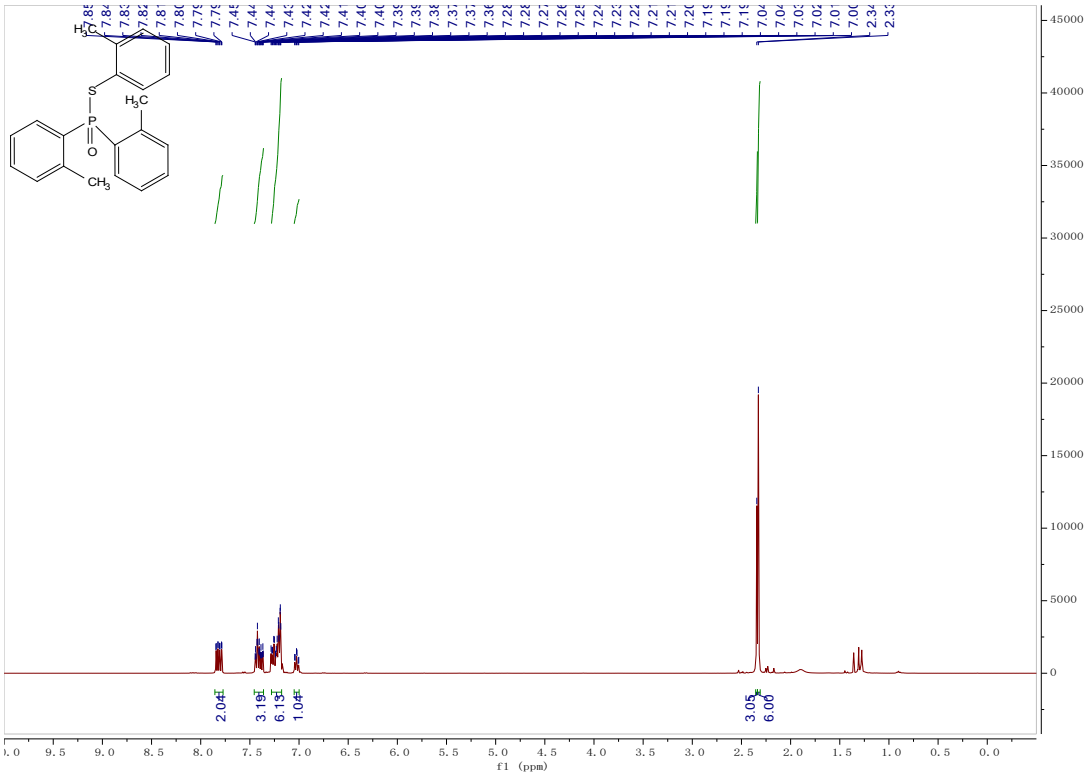
S-(2,4-dimethylphenyl) di-o-tolylphosphinothioate (3y)

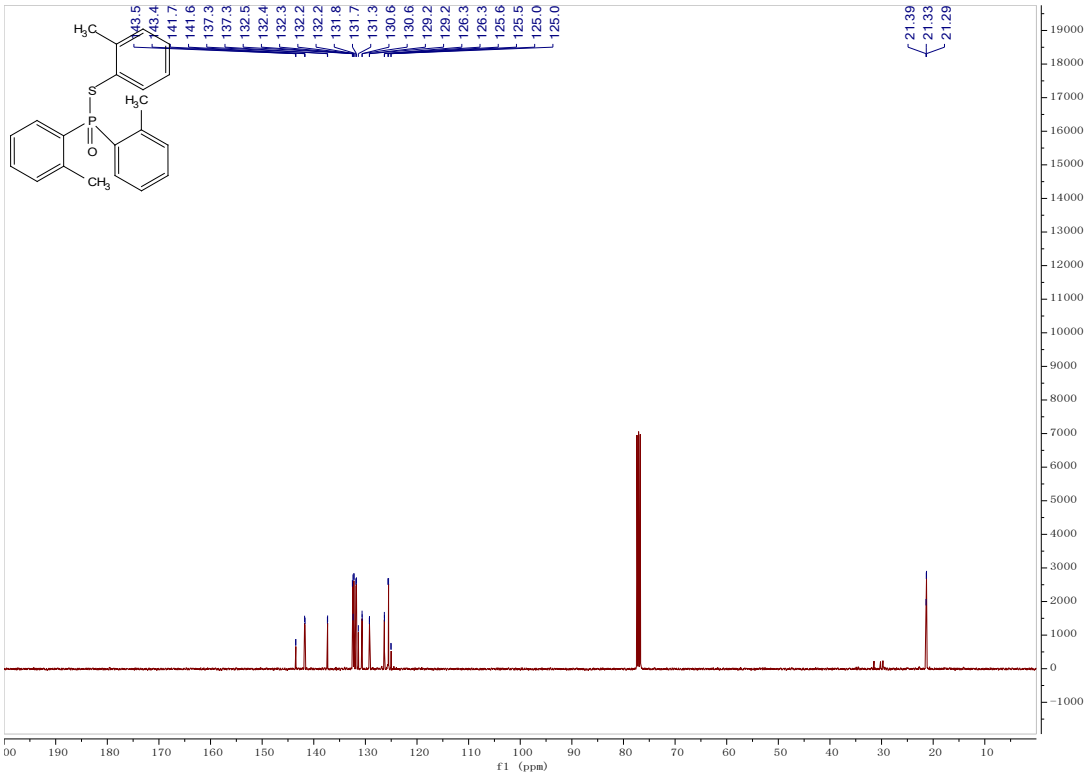


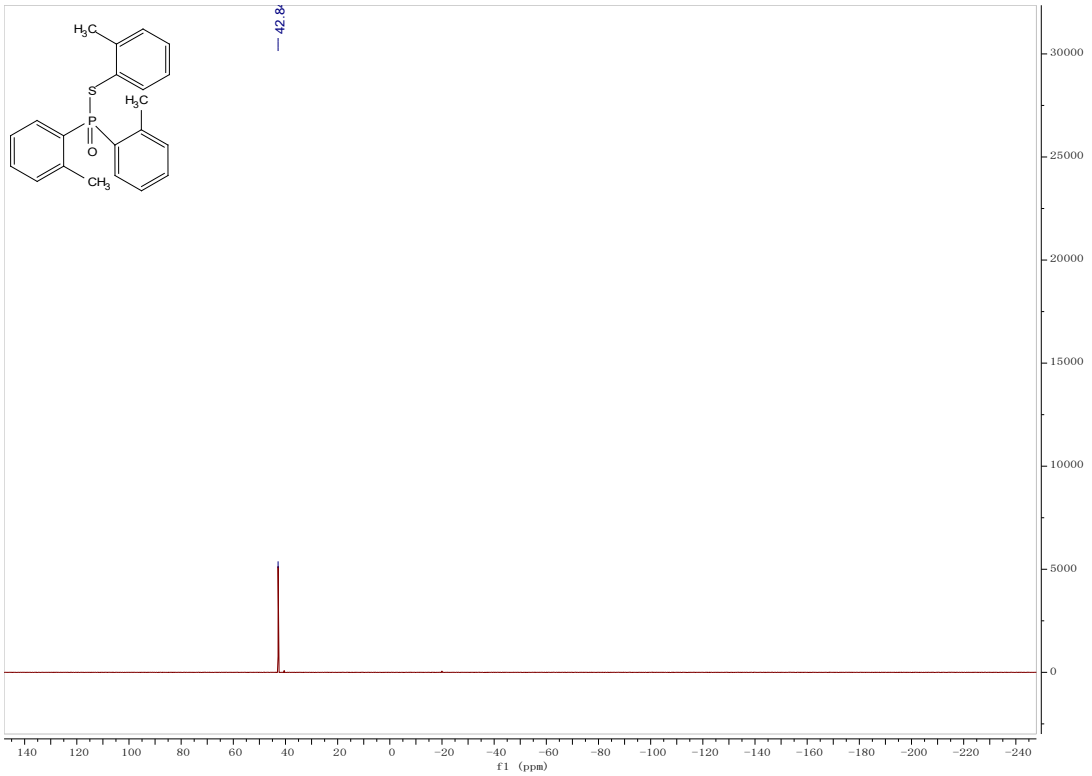




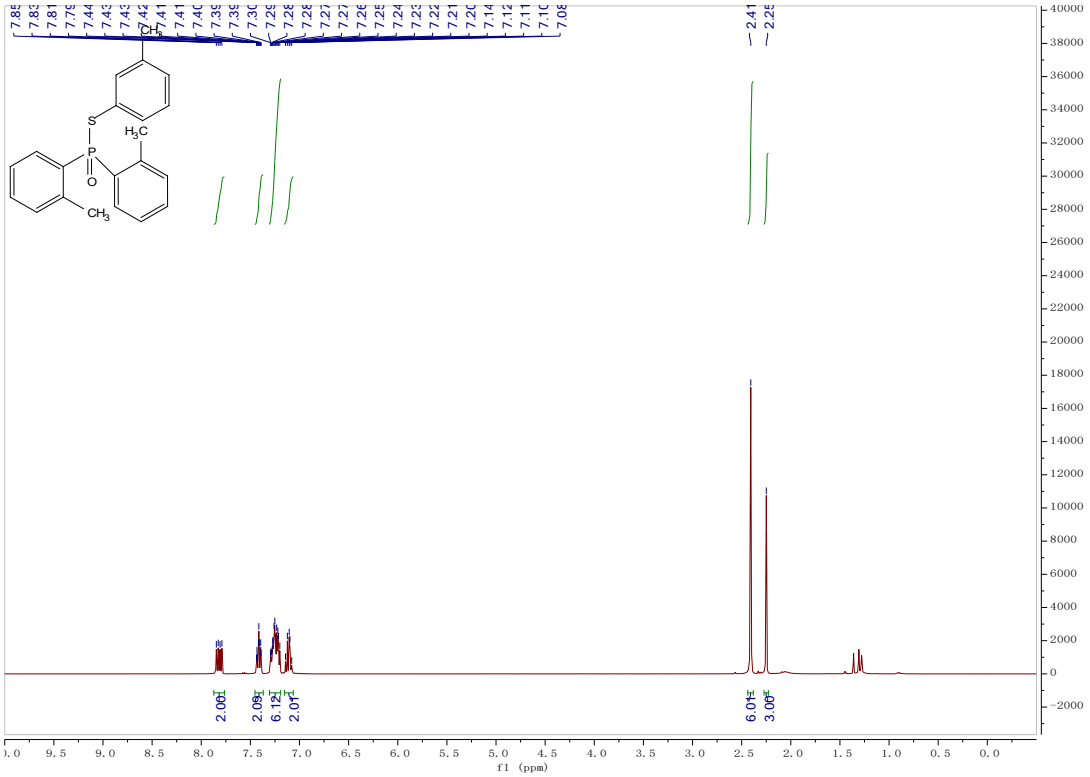
S-(o-tolyl) di-o-tolylphosphinothioate (3z)

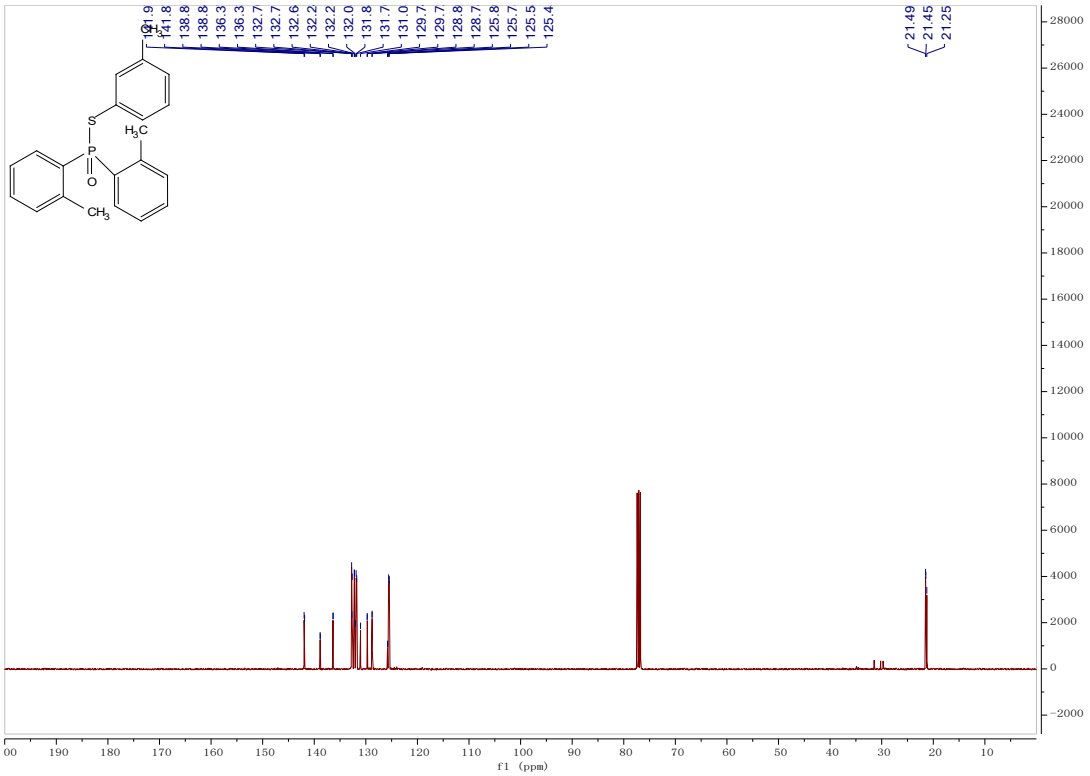


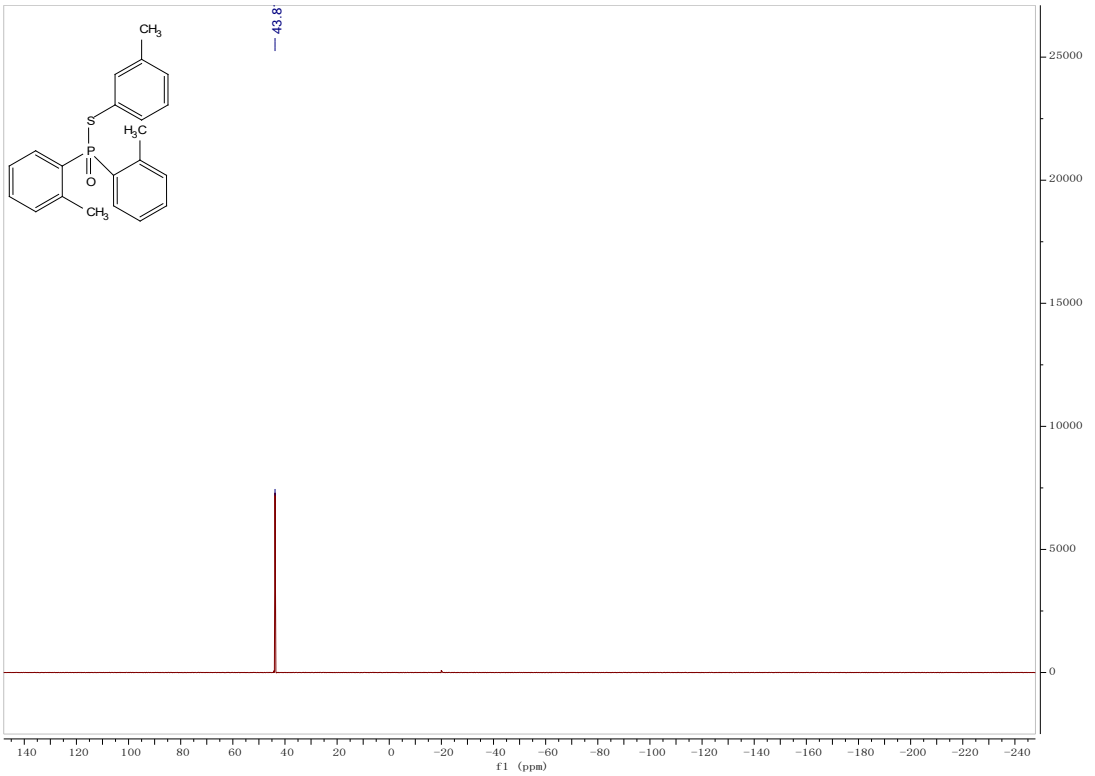

143.5
143.4
141.7
141.6
137.3
137.3
132.5
132.4
132.3
132.2
132.2
131.8
131.7
131.3
130.6
130.6
129.2
129.2
126.3
126.3
125.6
125.5
125.0
125.0
21.39
21.33
21.29
H3C
S
P
O
H3C
CH3
f1 (ppm)


42.8
H3C
S
P
O
H3C
CH3
f1 (ppm)

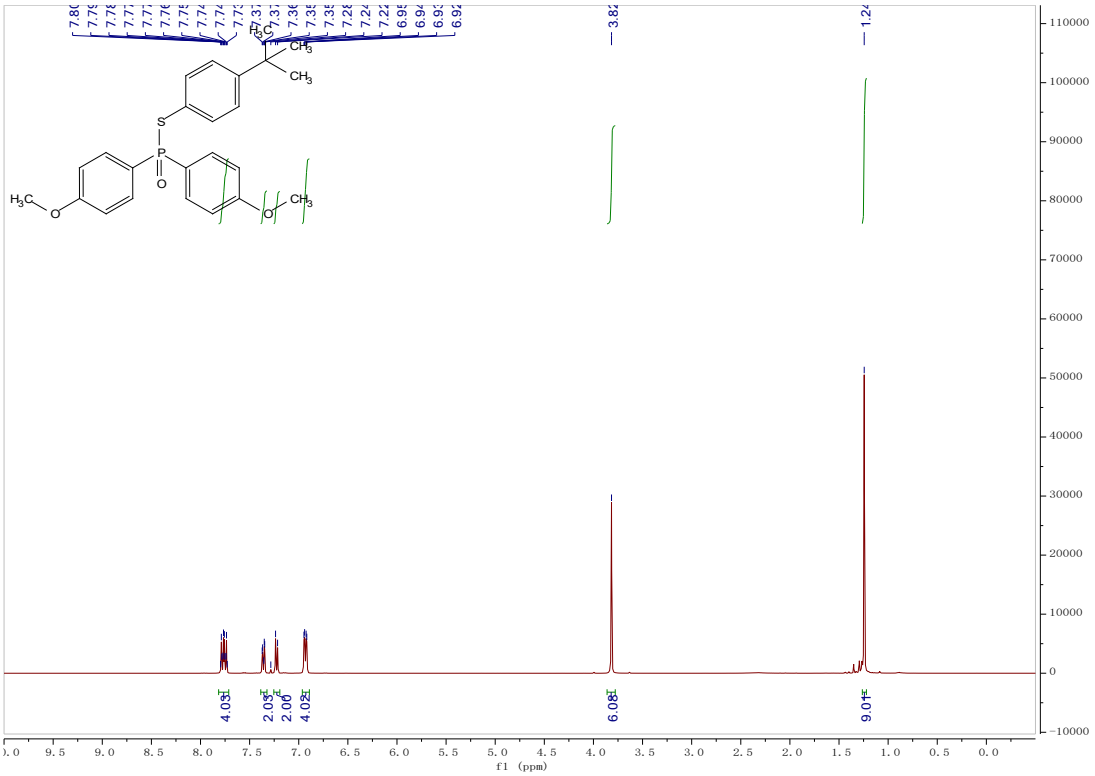
S-(m-tolyl) di-o-tolylphosphinothioate (3aa)

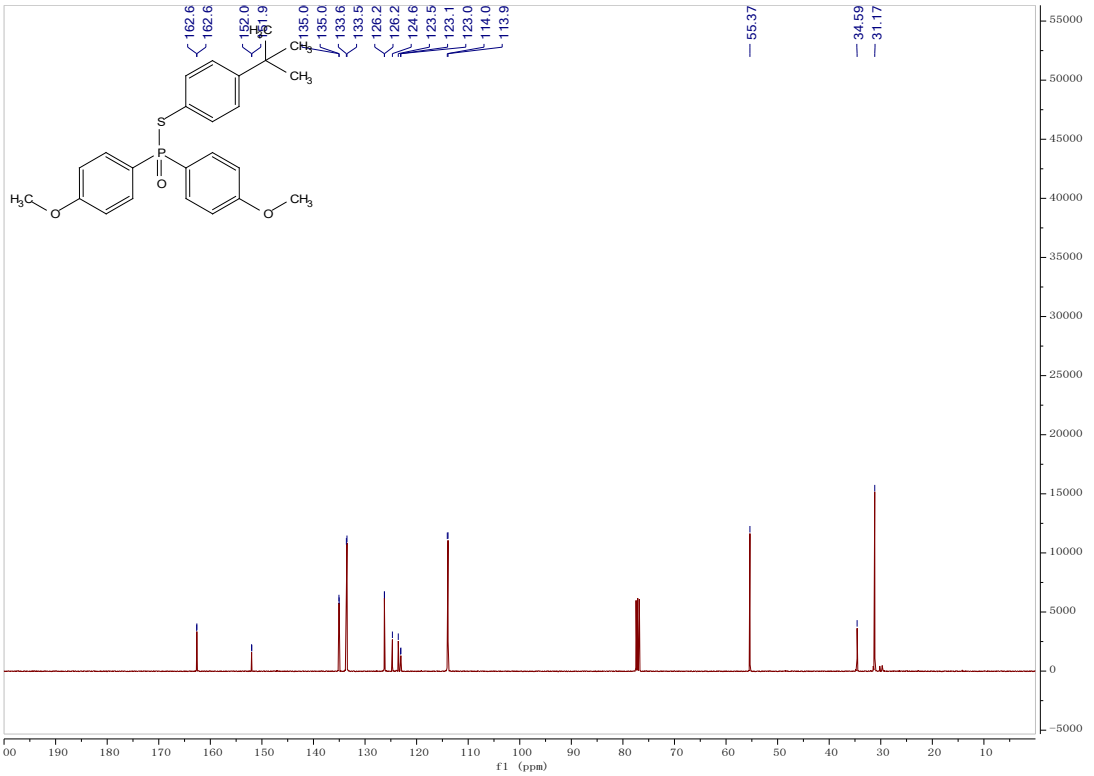


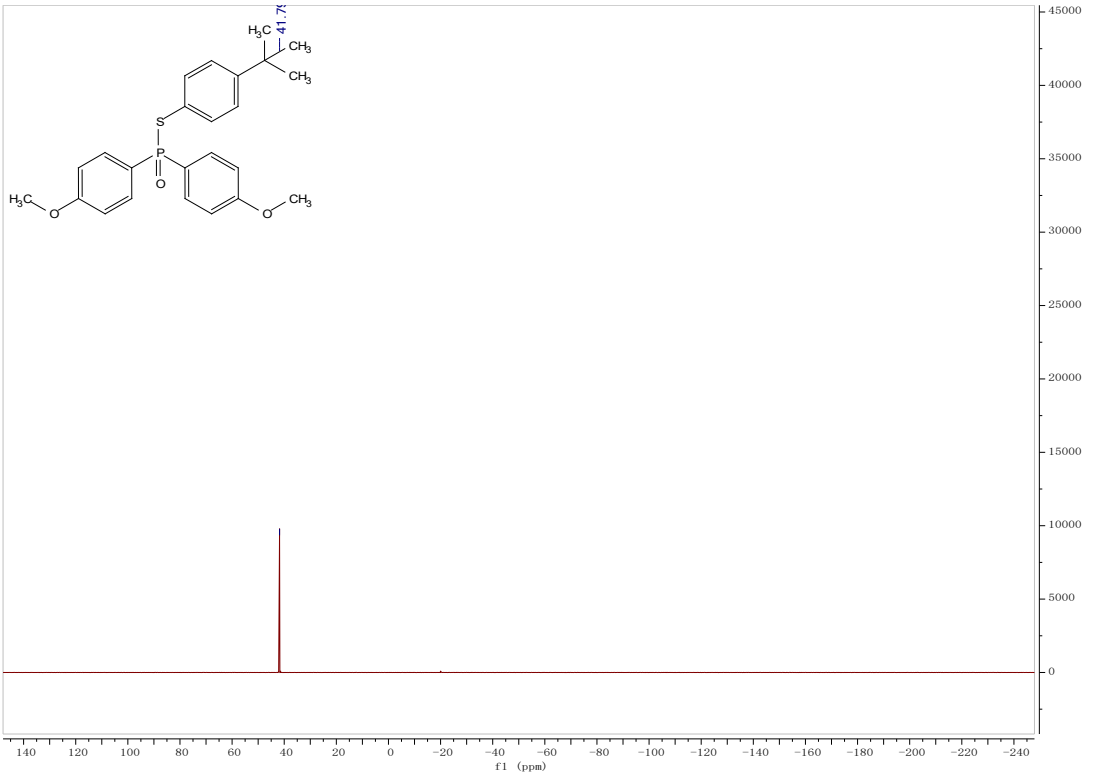




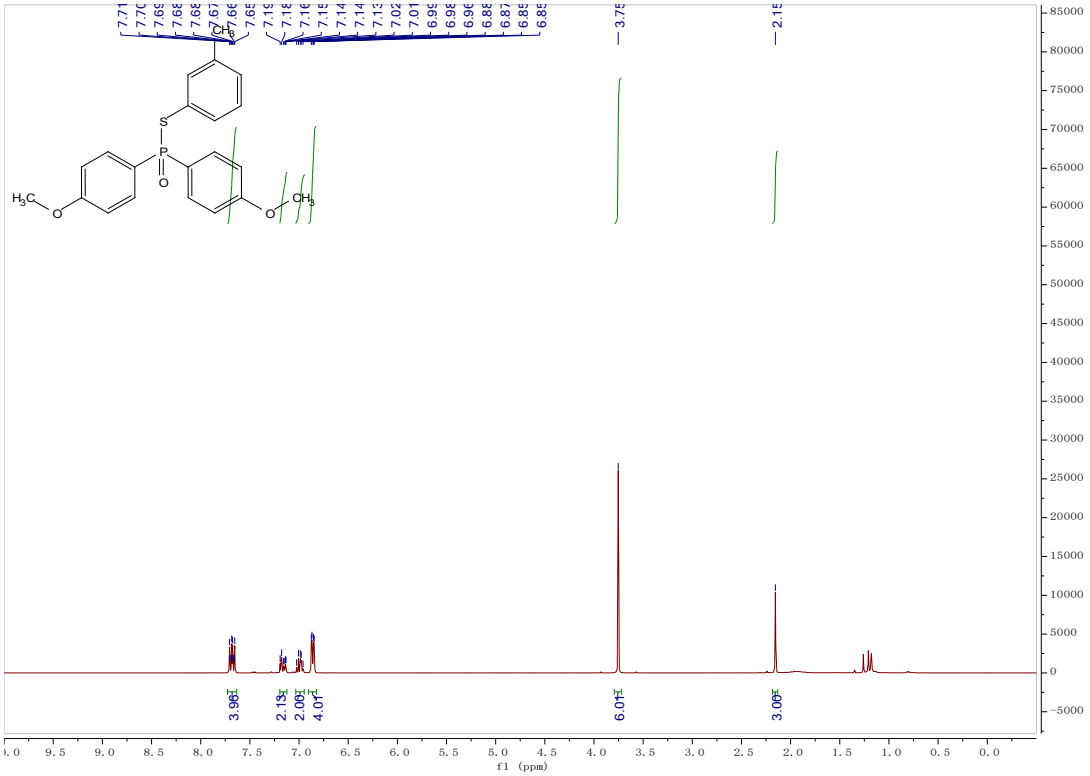
S-(4-(tert-butyl)phenyl) bis(4-methoxyphenyl)phosphinothioate (3ab)

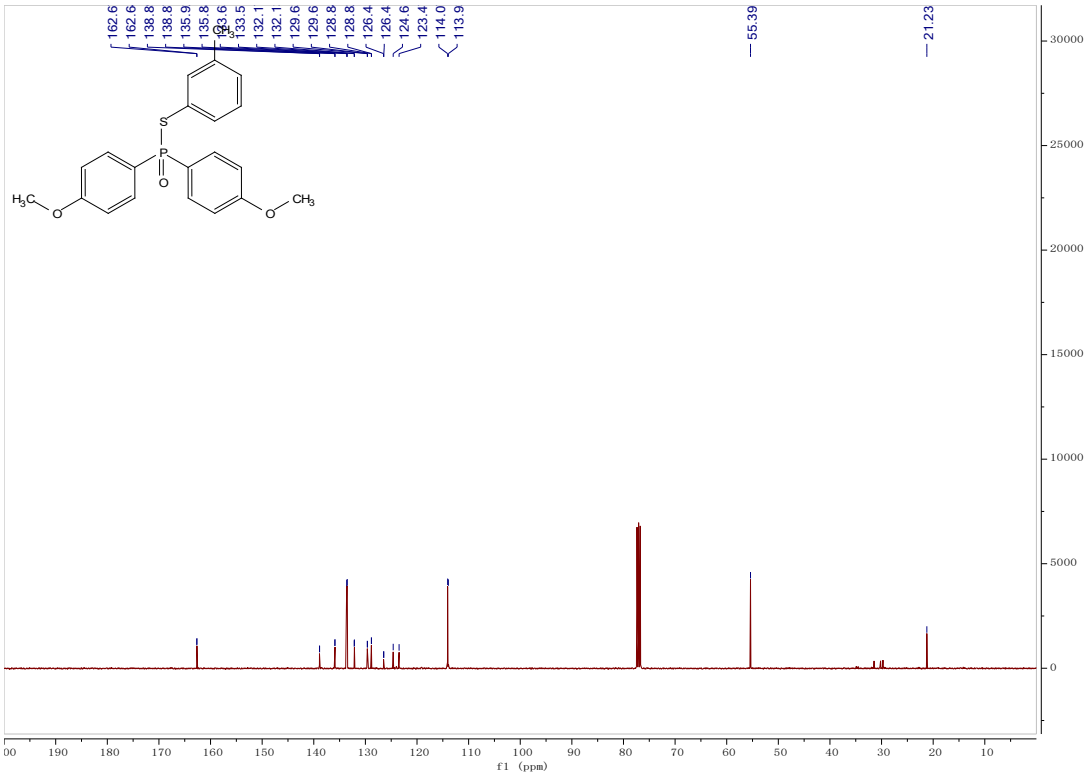


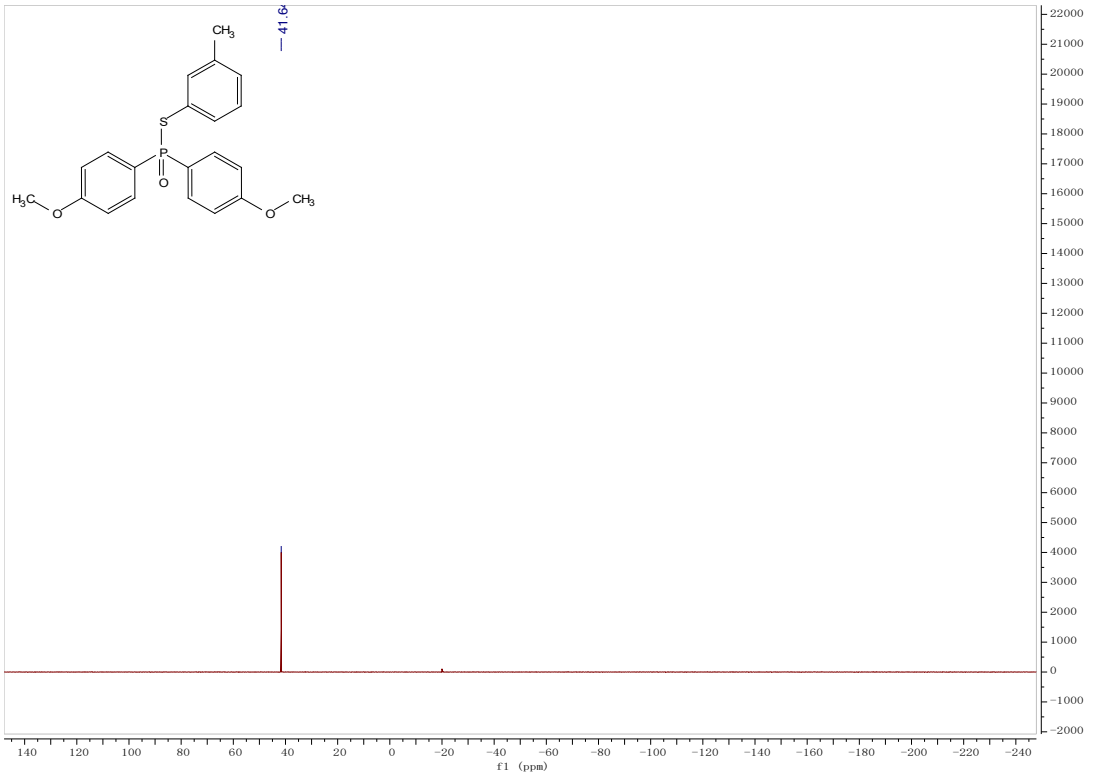

162.6
162.6
152.0
141.9
135.0
135.0
133.6
133.5
126.2
126.2
124.6
123.5
123.1
123.0
114.0
113.9
55.37
34.59
31.17
f1 (ppm)


41.7
f1 (ppm)

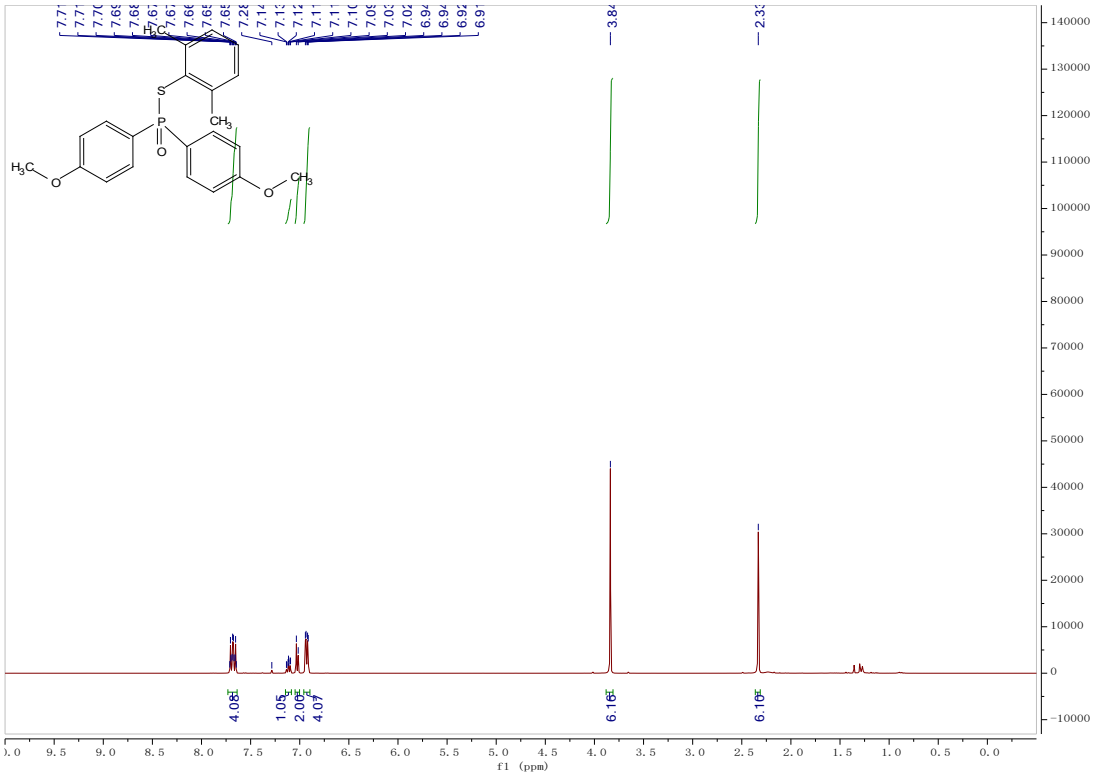
S-(m-tolyl) bis(4-methoxyphenyl)phosphinothioate (3ac)

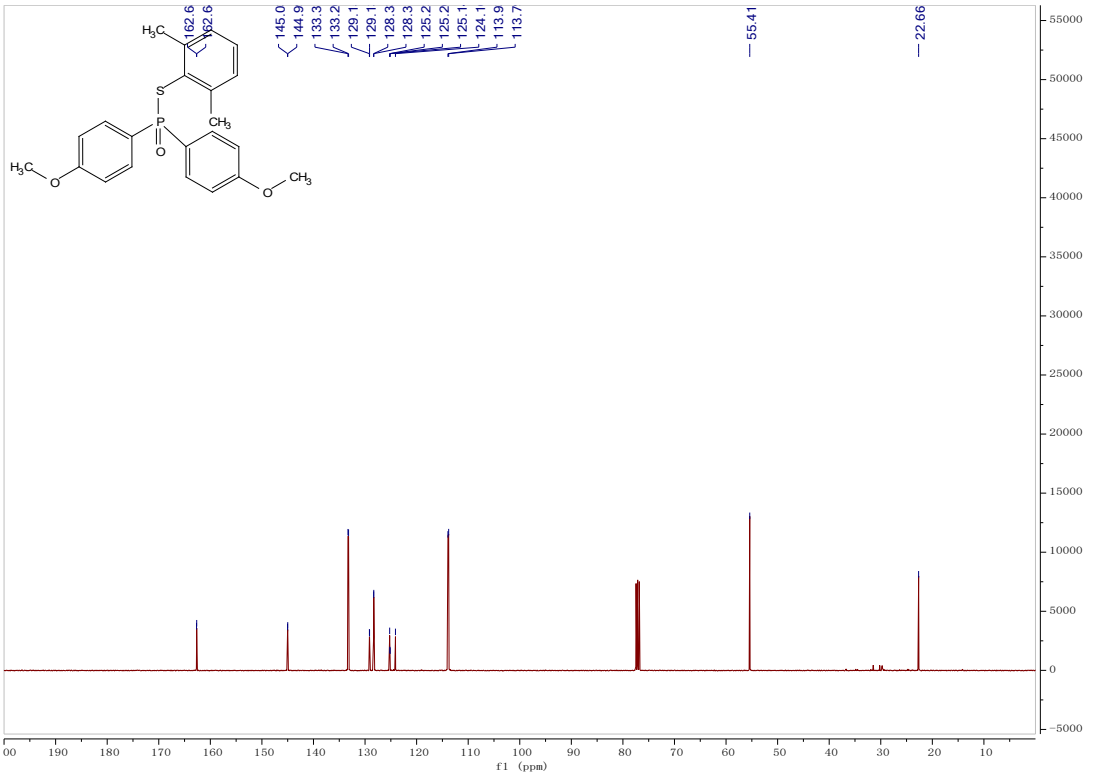


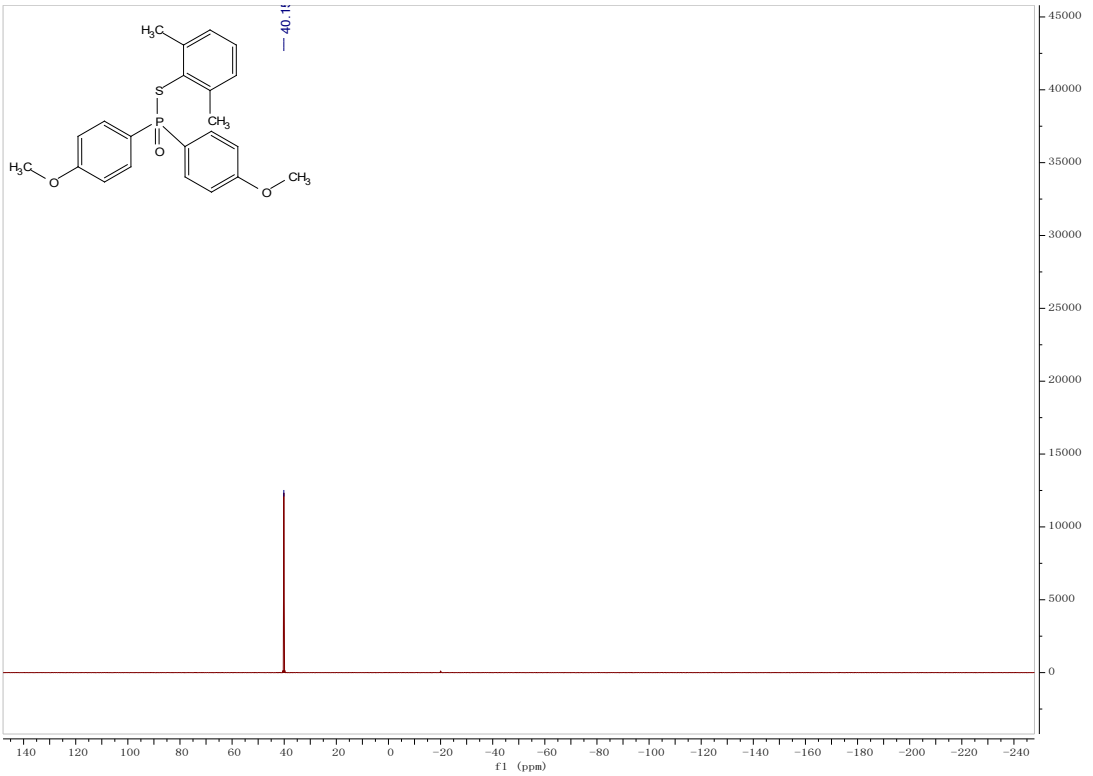




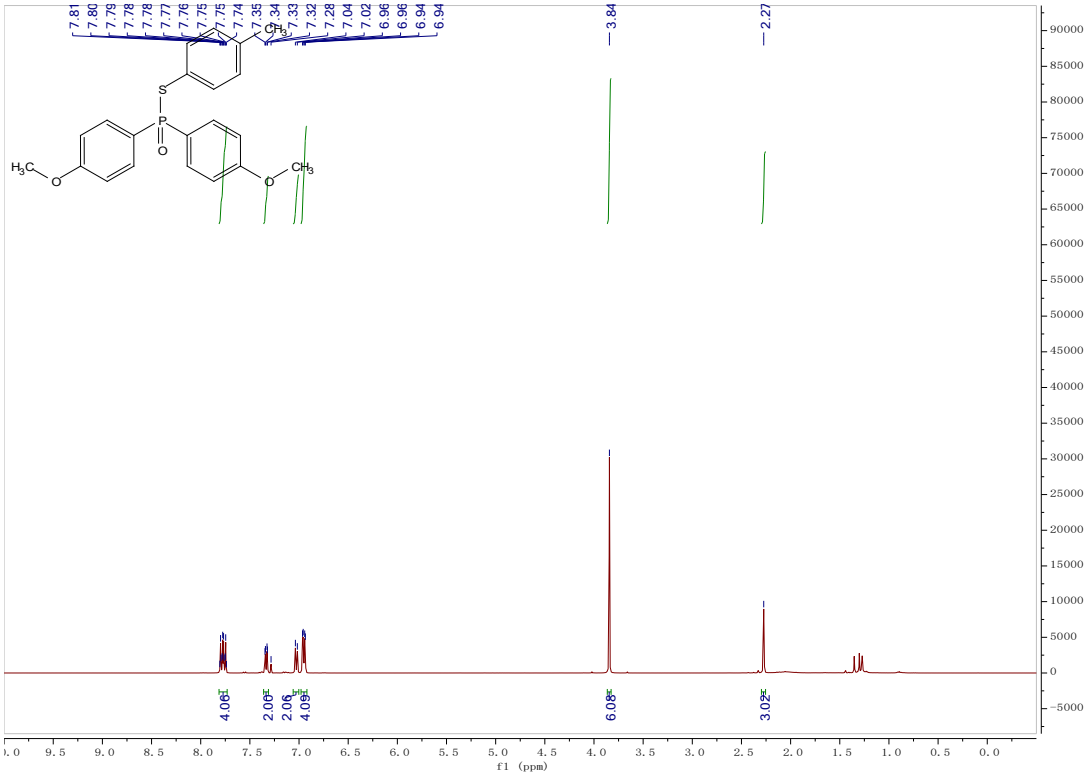
S-(2,6-dimethylphenyl) bis(4-methoxyphenyl)phosphinothioate (3ad)

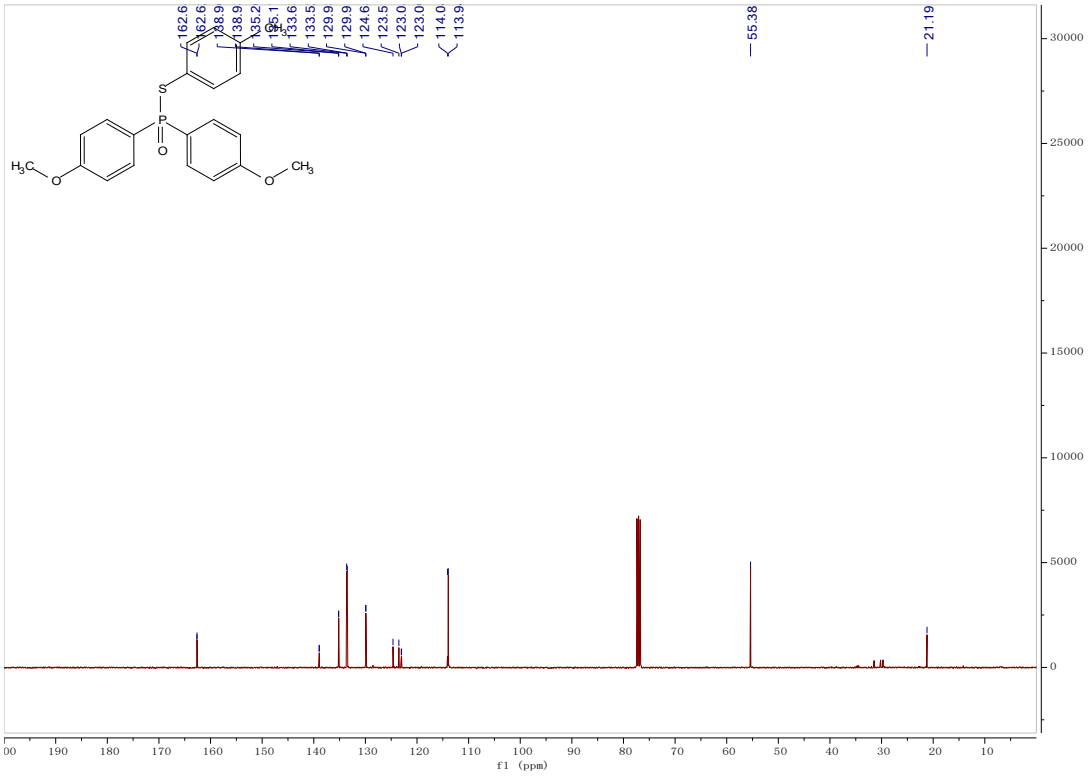


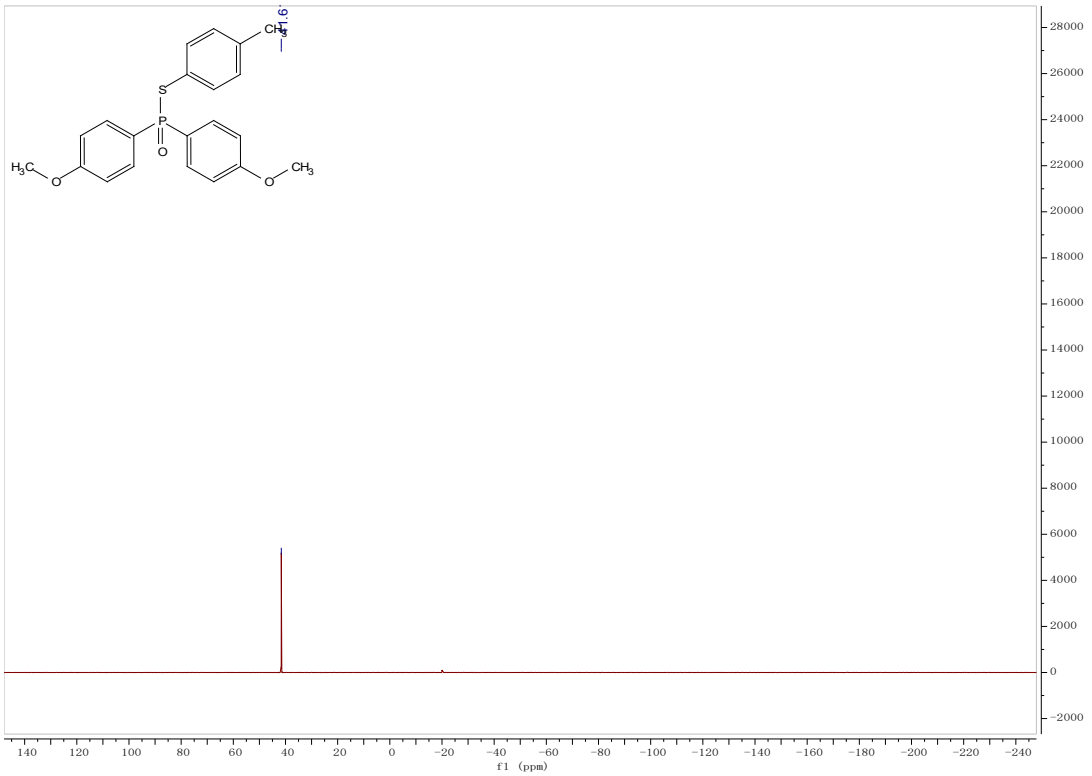

162.6
162.6
145.0
144.9
133.3
133.2
129.1
129.1
128.3
128.3
125.2
125.2
125.1
124.1
113.9
113.7
55.41
22.66
f1 (ppm)


40.1
f1 (ppm)

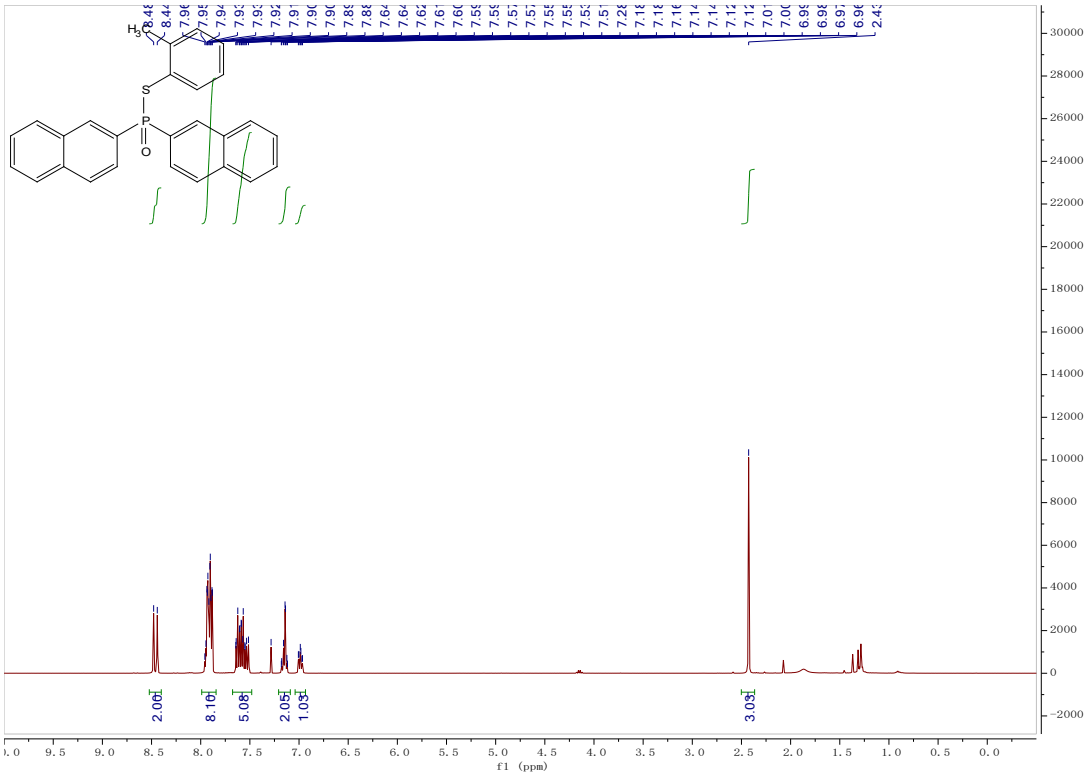
S-(p-tolyl) bis(4-methoxyphenyl)phosphinothioate (3ae)

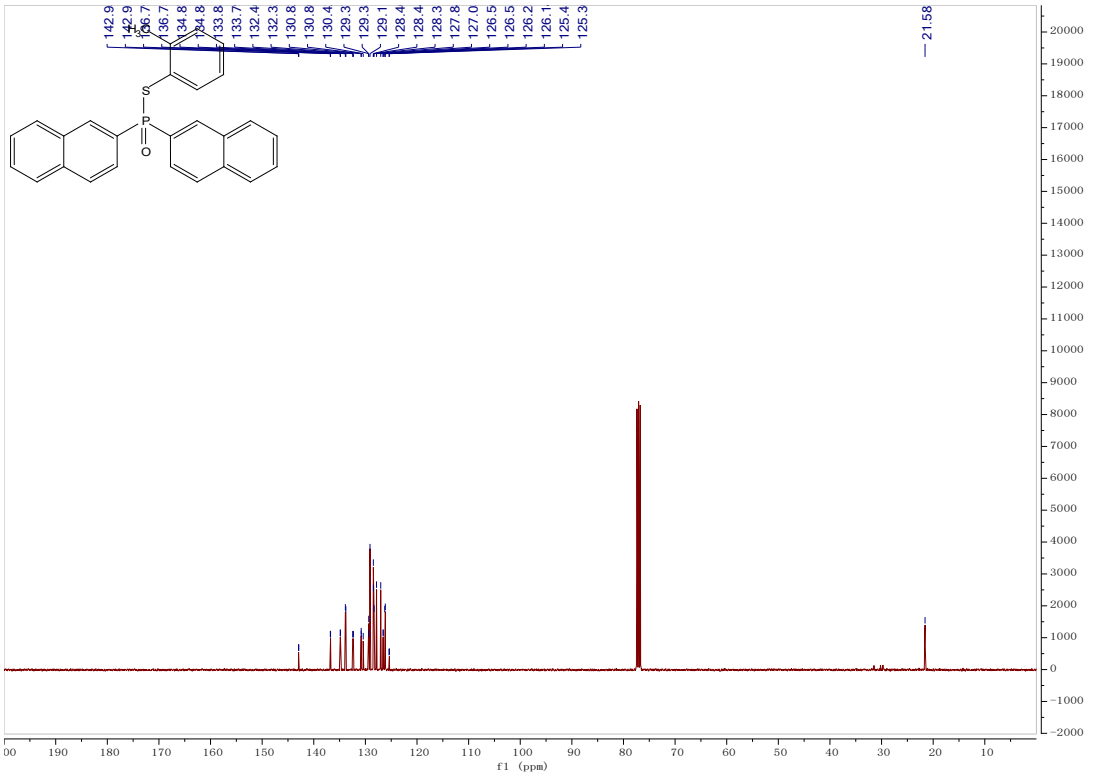


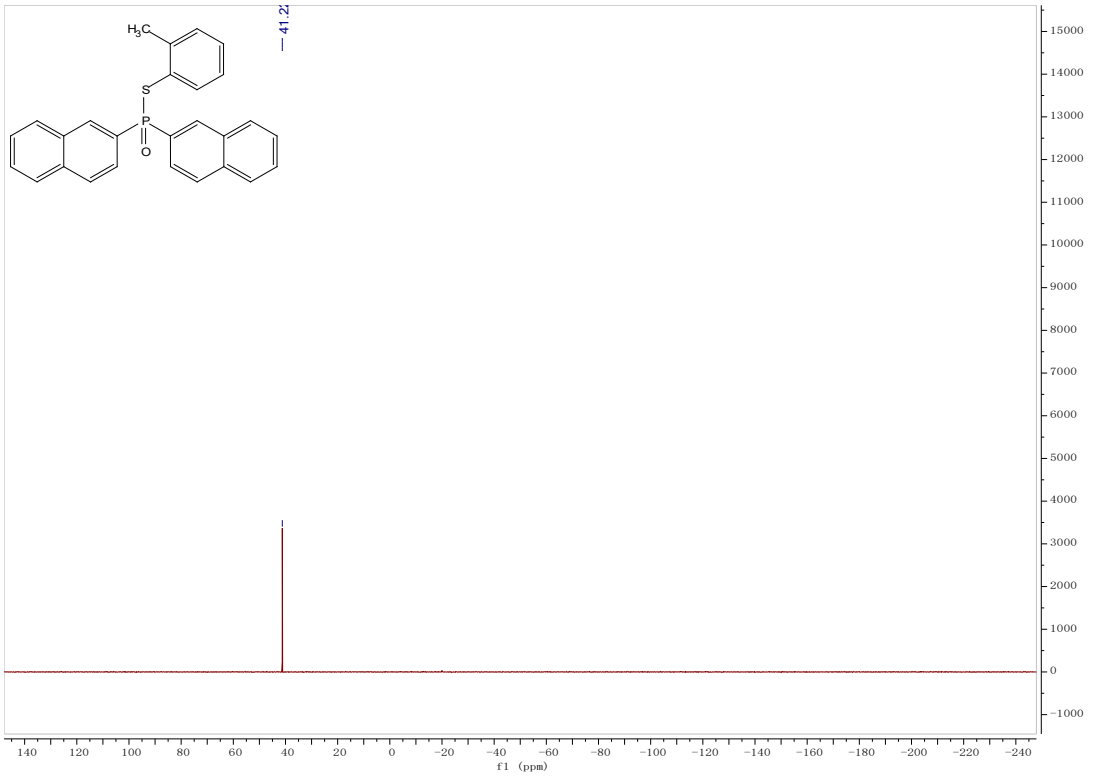




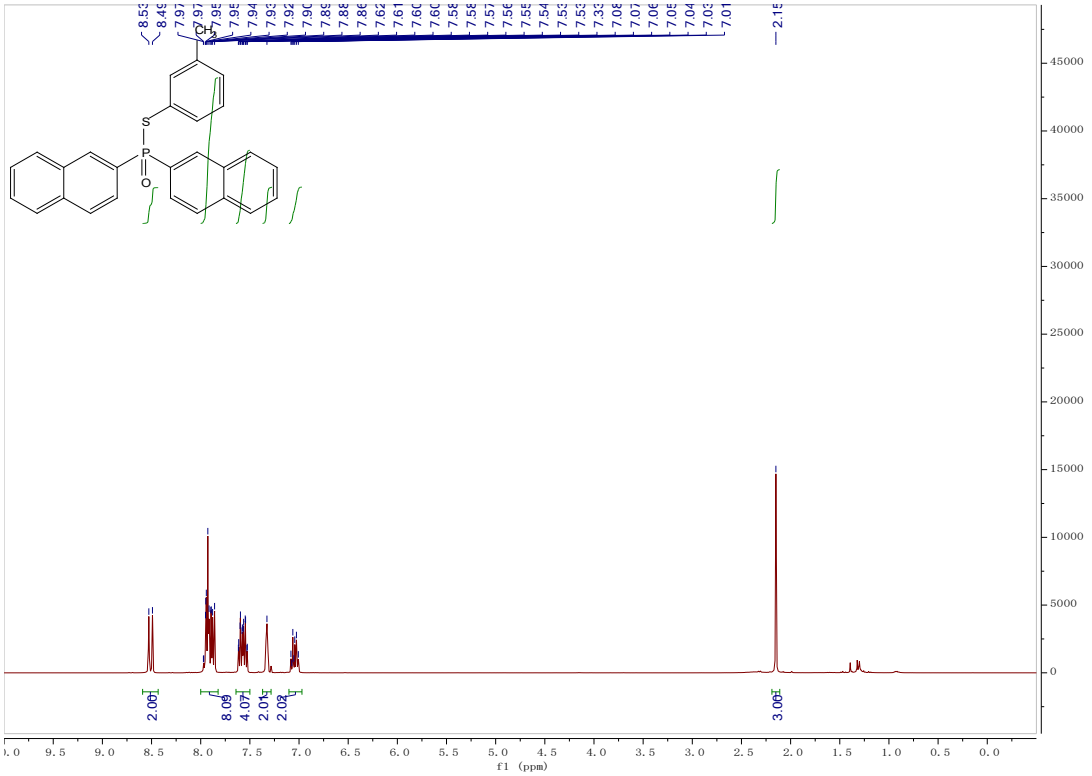
S-(o-tolyl) di(naphthalen-2-yl)phosphinothioate (3af)

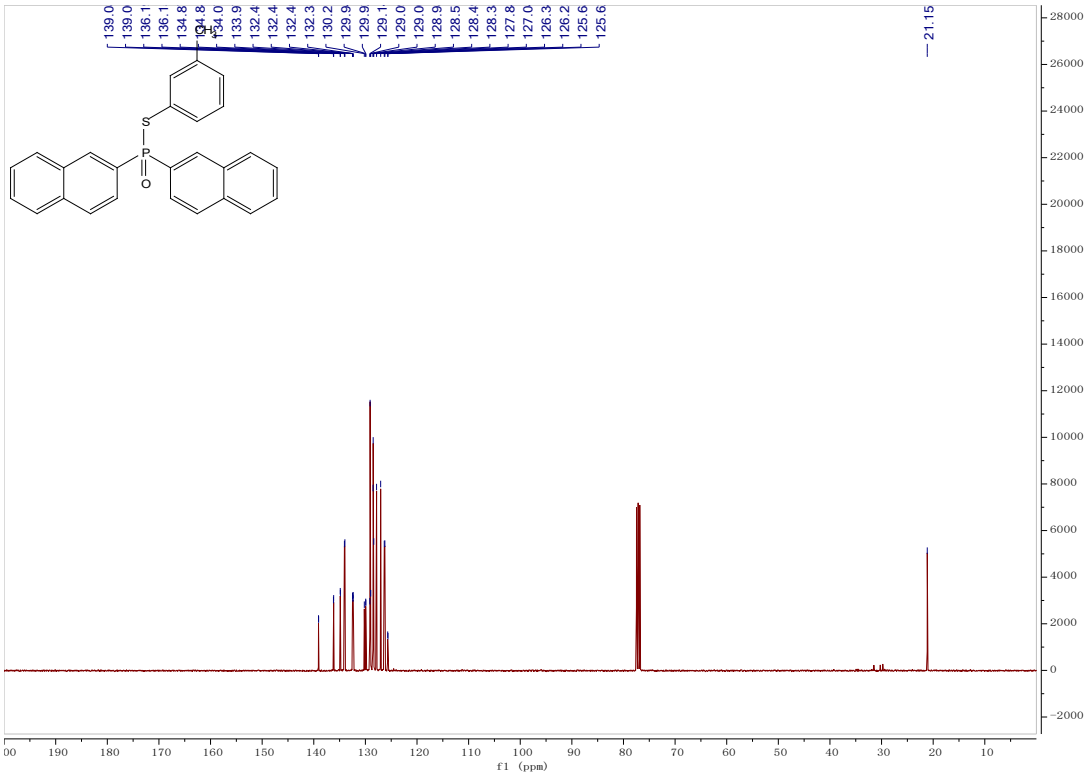


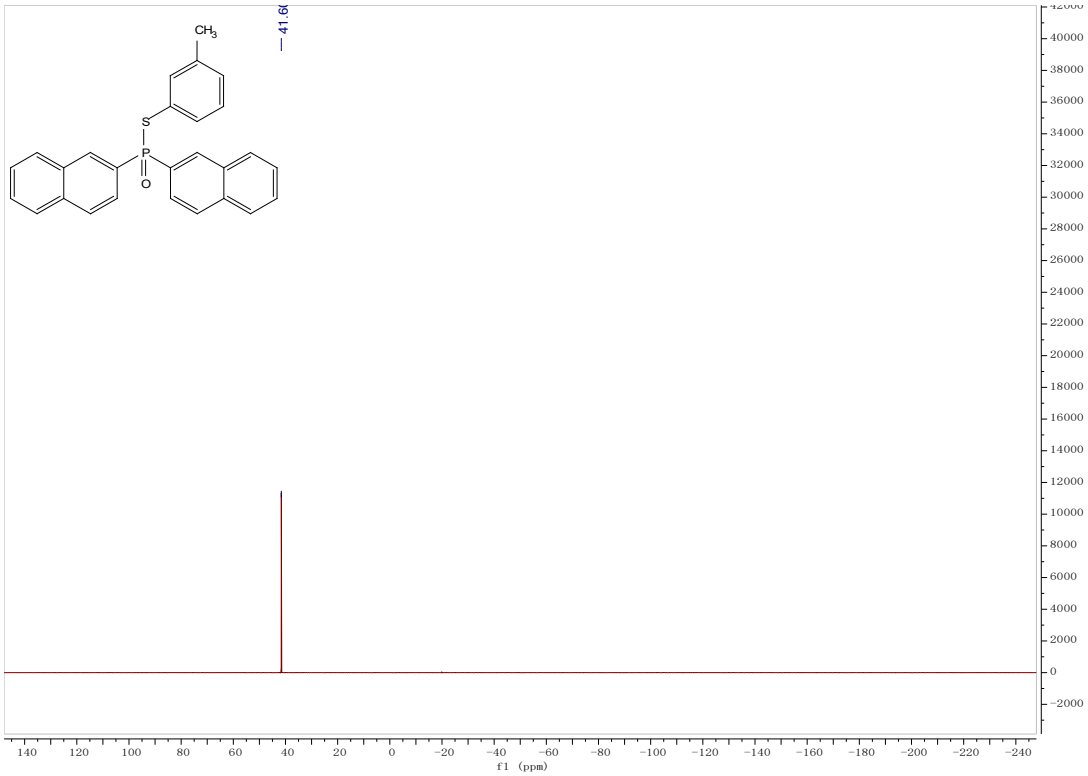

142.9
142.9
136.7
136.7
134.8
134.8
133.8
133.7
132.4
132.3
130.8
130.8
130.4
129.3
129.3
129.1
128.4
128.4
128.3
127.8
127.0
126.5
126.5
126.2
126.1
125.4
125.3
21.58
H3C
S
P
O
f1 (ppm)


41.2
H3C
S
P
O
f1 (ppm)

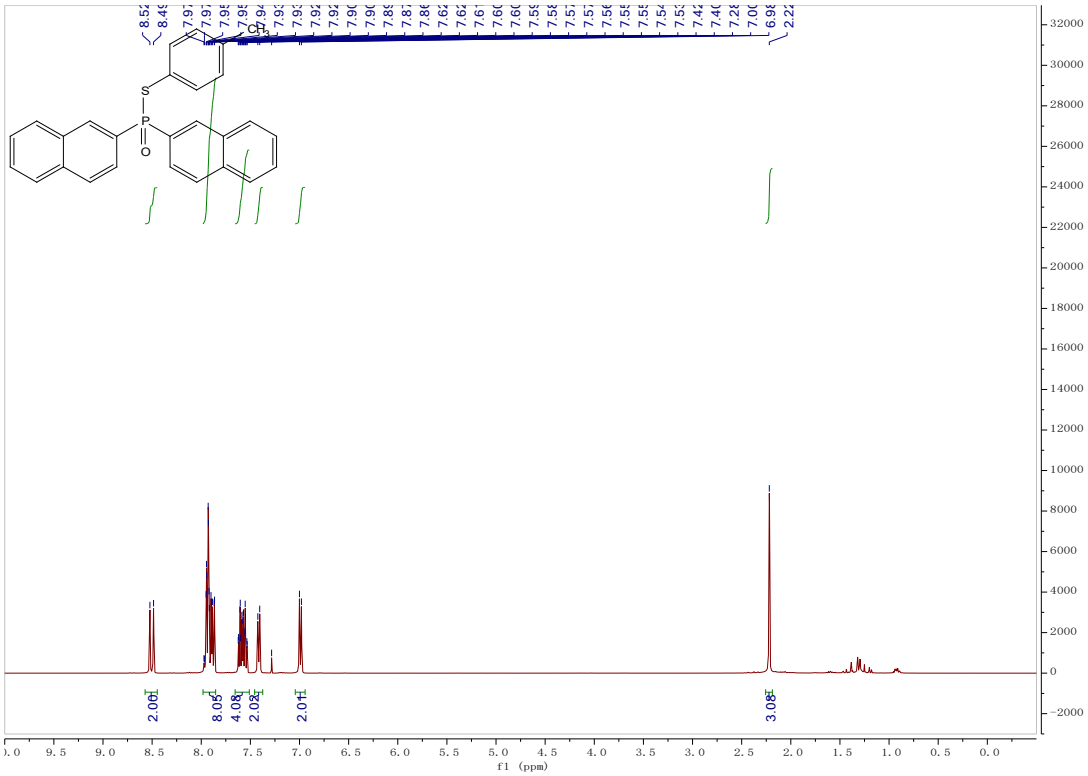
S-(m-tolyl) di(naphthalen-2-yl)phosphinothioate (3ag)

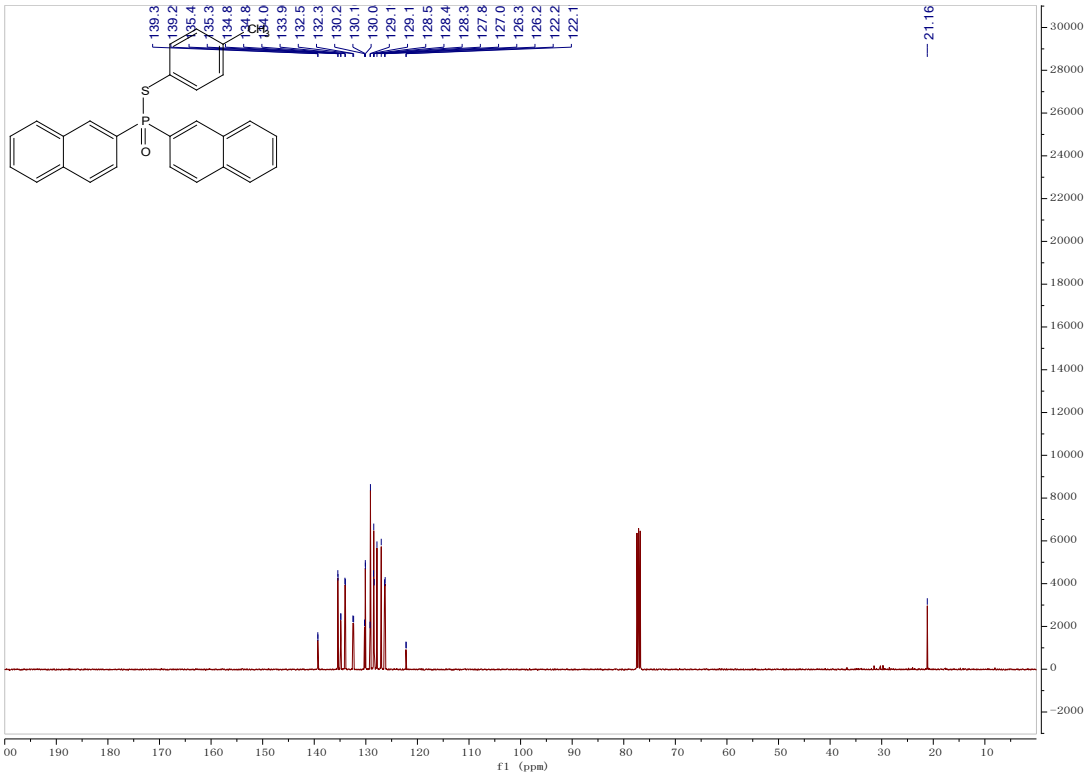


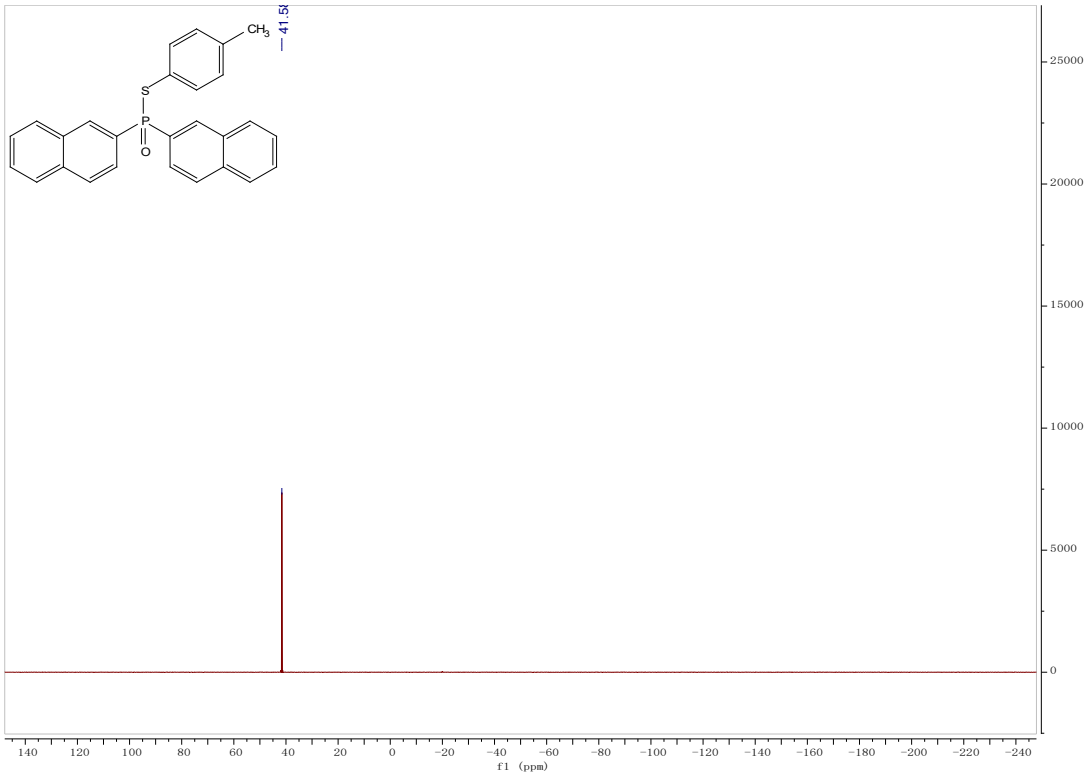




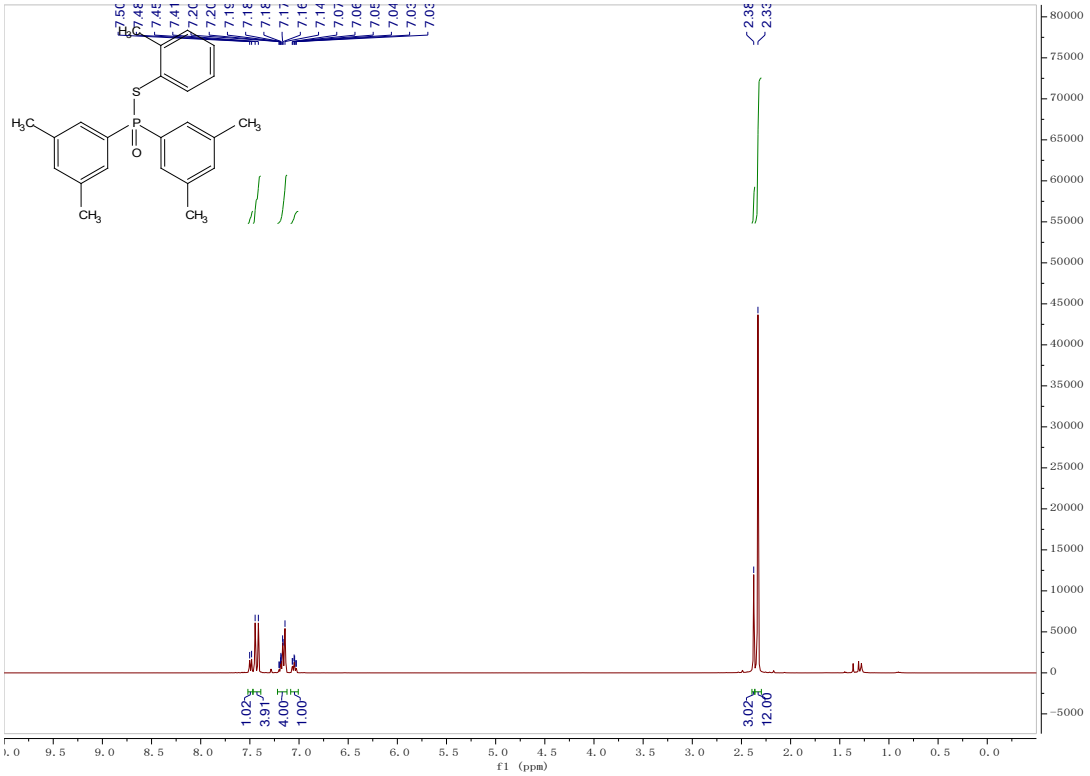
S-(p-tolyl) di(naphthalen-2-yl)phosphinothioate (3ah)

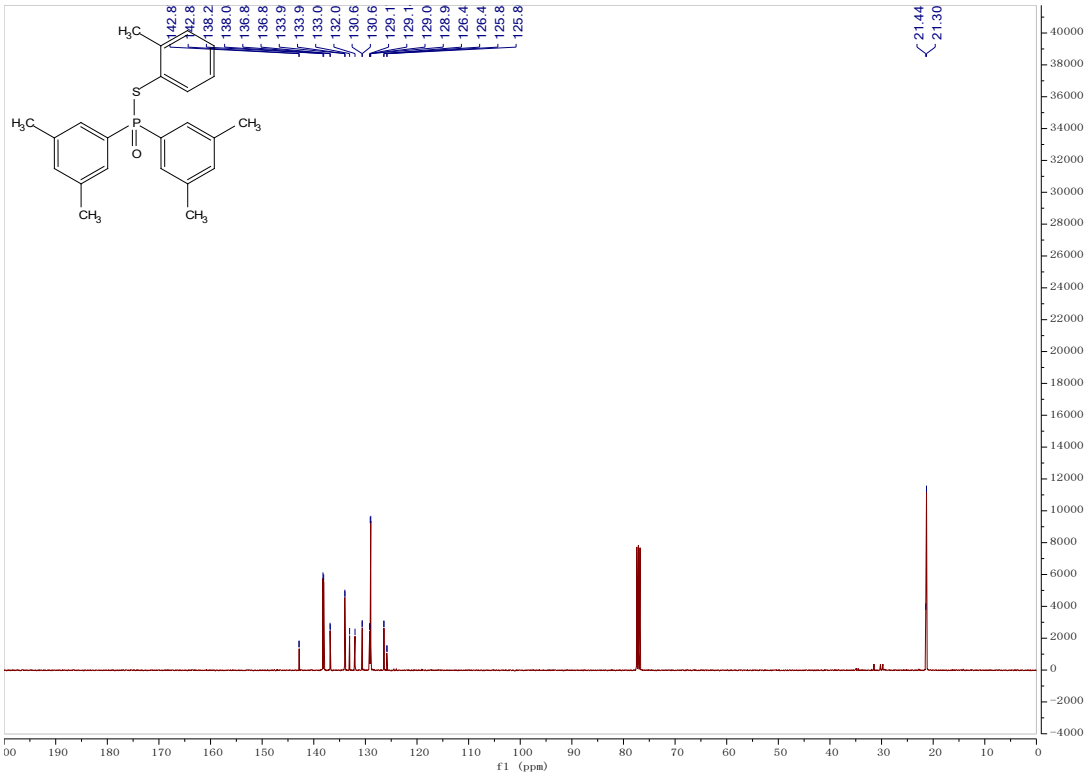


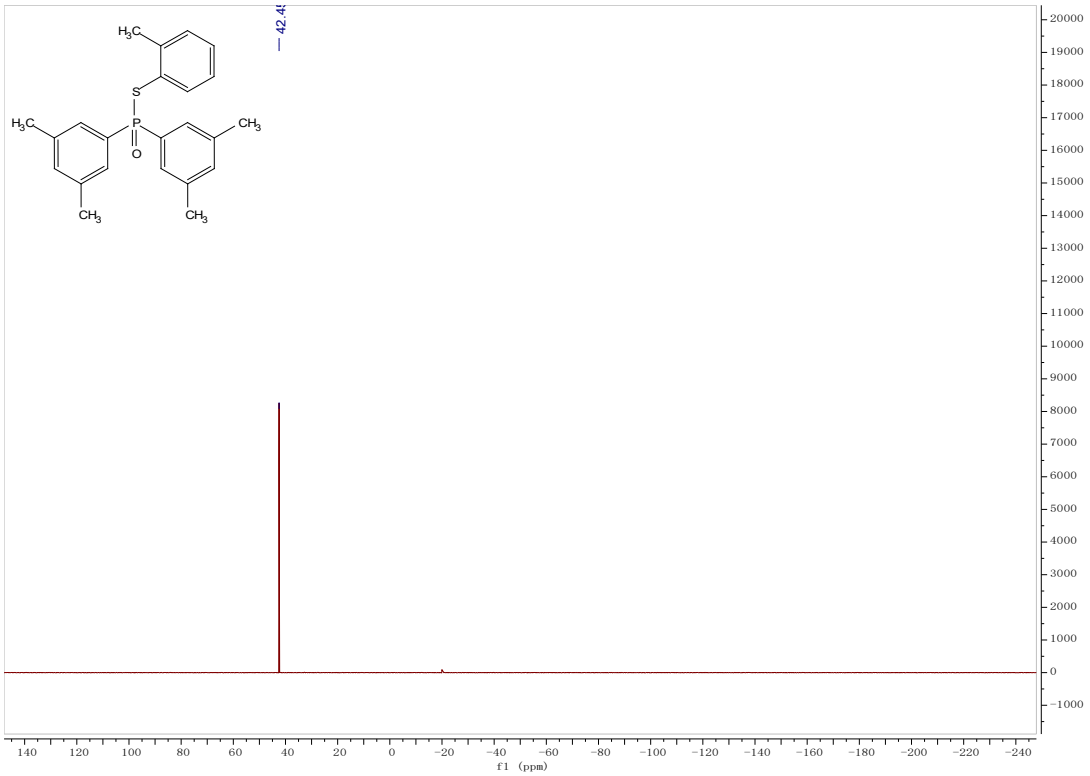

139.3
139.2
135.4
135.3
134.8
134.0
133.9
132.5
132.3
130.2
130.1
130.0
129.1
129.1
128.5
128.4
128.3
127.8
127.0
126.3
126.2
122.2
122.1
21.16
S
P
O
f1 (ppm)


CH3
41.5
S
P
O
f1 (ppm)

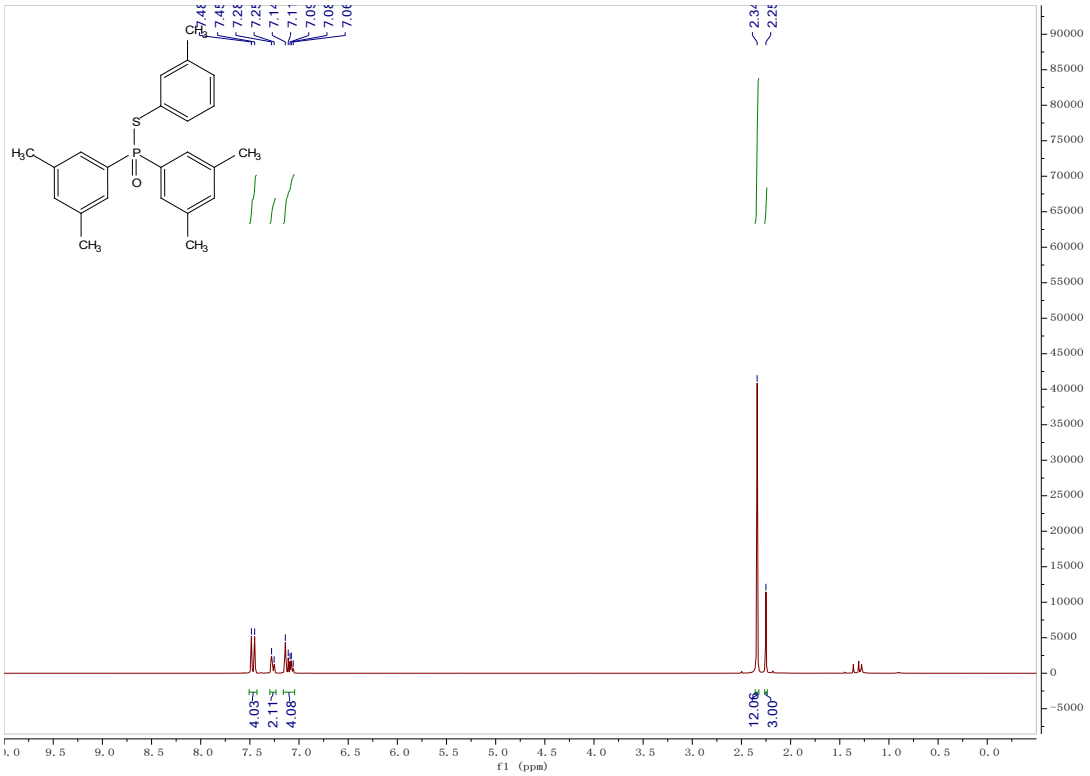
S-(o-tolyl) bis(3,5-dimethylphenyl)phosphinothioate (3ai)

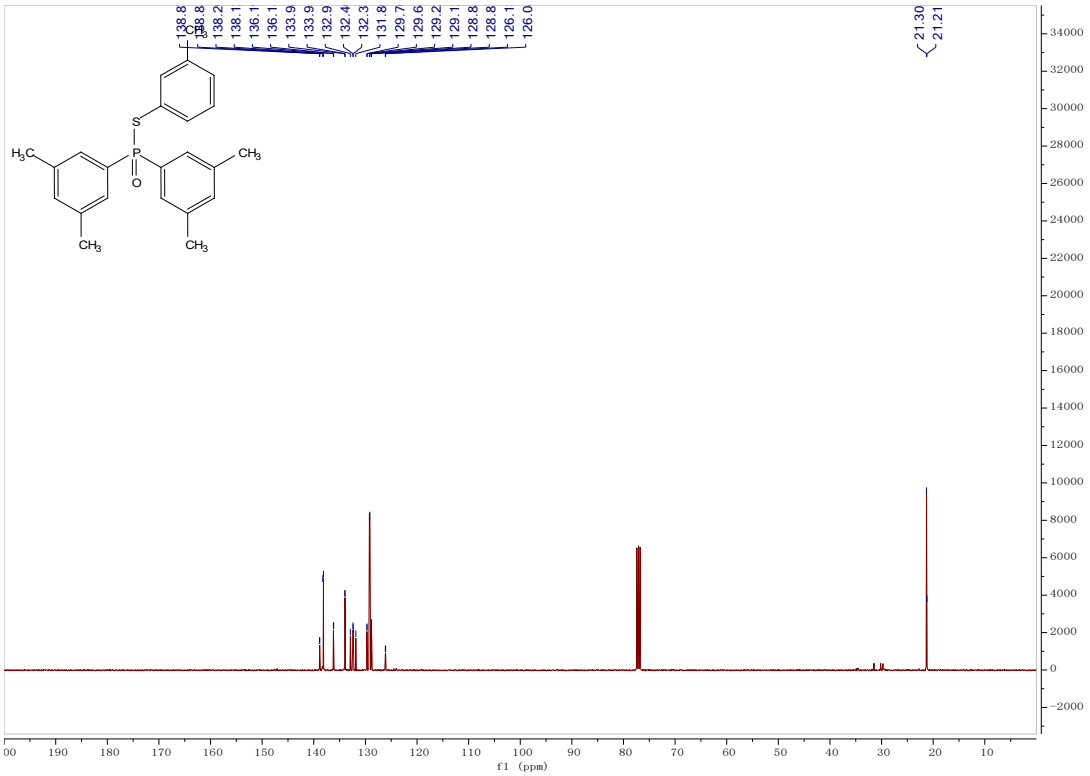


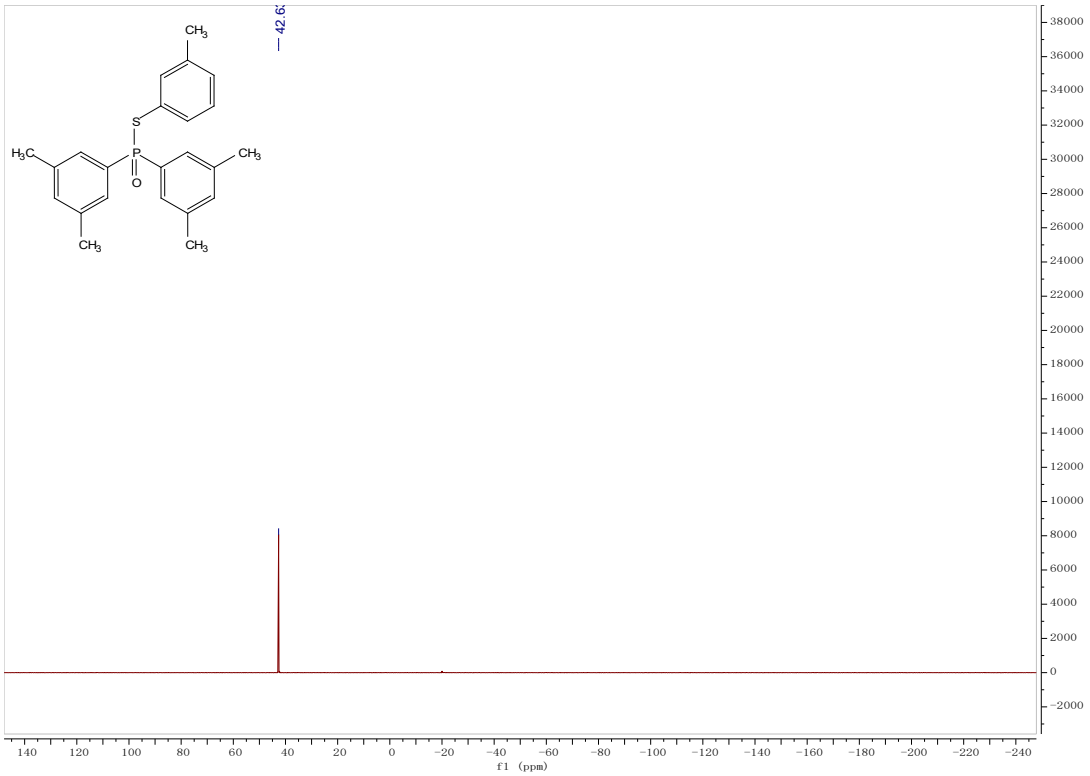




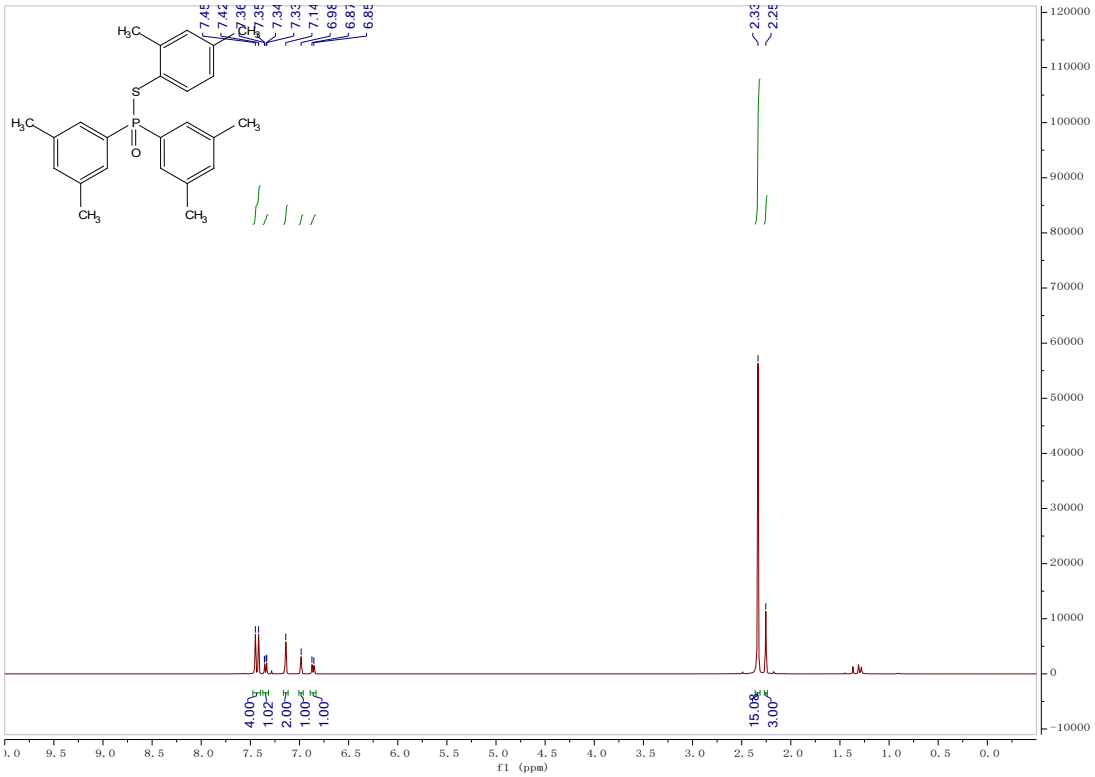
S-(m-tolyl) bis(3,5-dimethylphenyl)phosphinothioate (3aj)

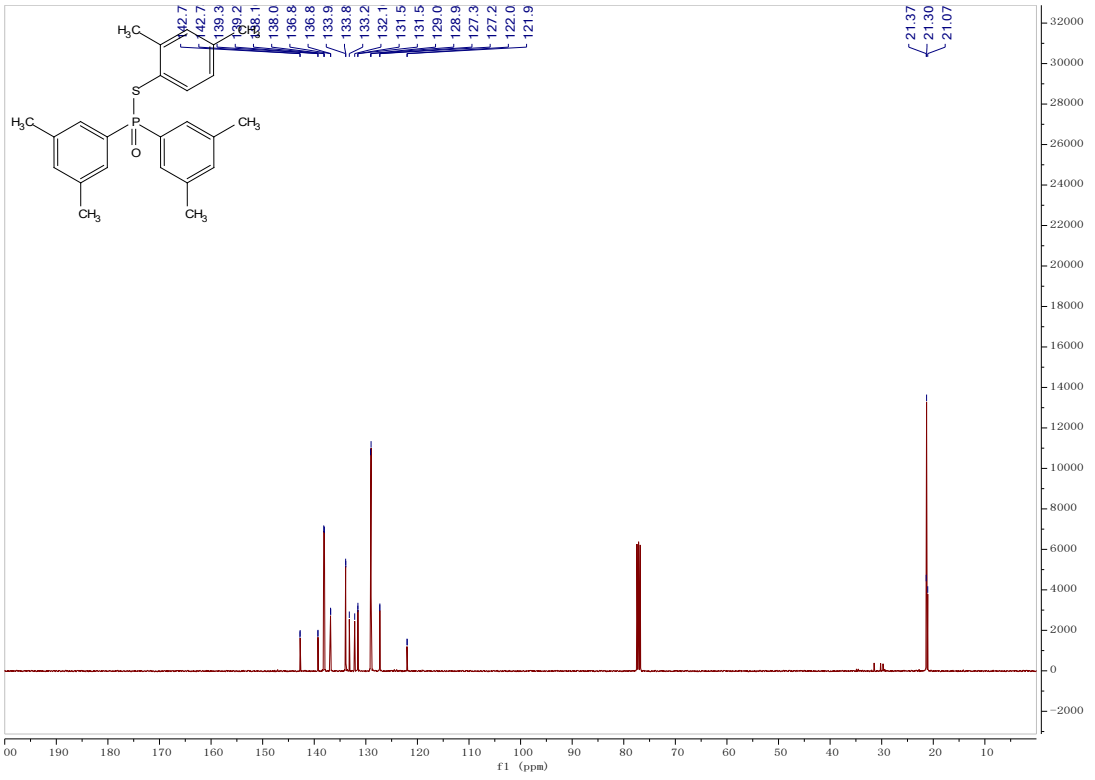


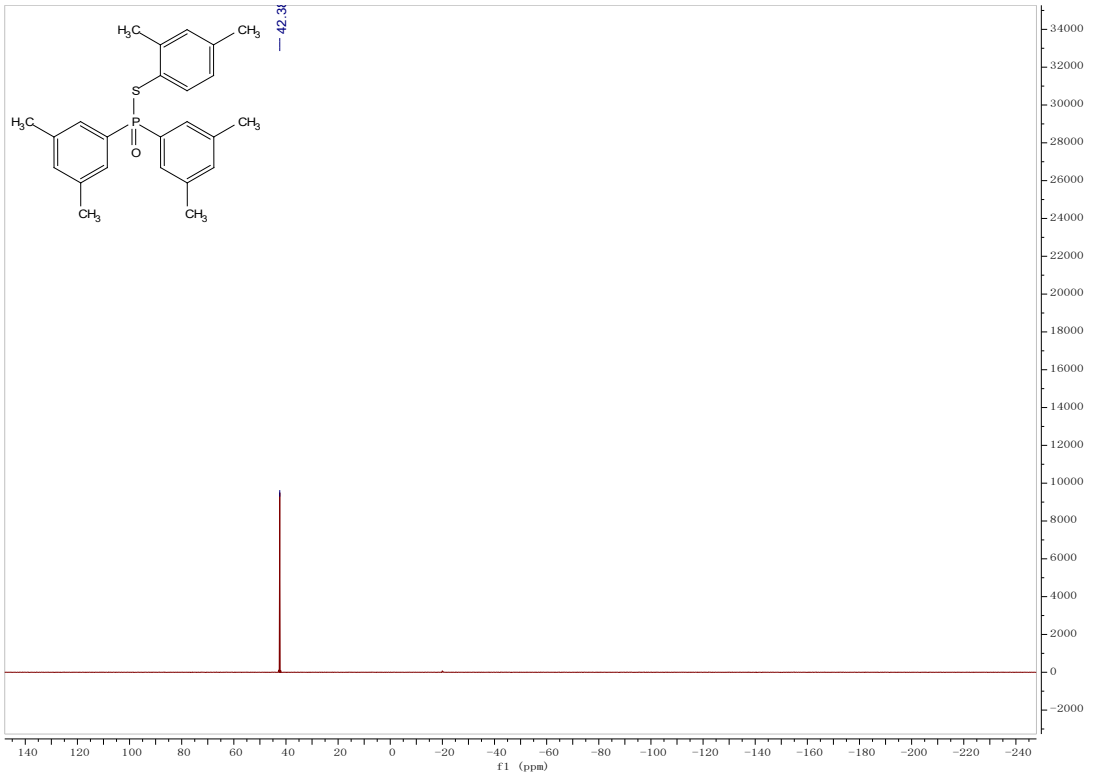

138.8
138.8
138.2
138.1
136.1
136.1
133.9
133.9
132.9
132.4
132.3
131.8
129.7
129.6
129.2
129.1
128.8
128.8
126.1
126.0
21.30
21.21
S
P
O
H3C
CH3
CH3
CH3
CH3
f1 (ppm)


42.6
S
P
O
H3C
CH3
CH3
CH3
CH3
CH3
f1 (ppm)

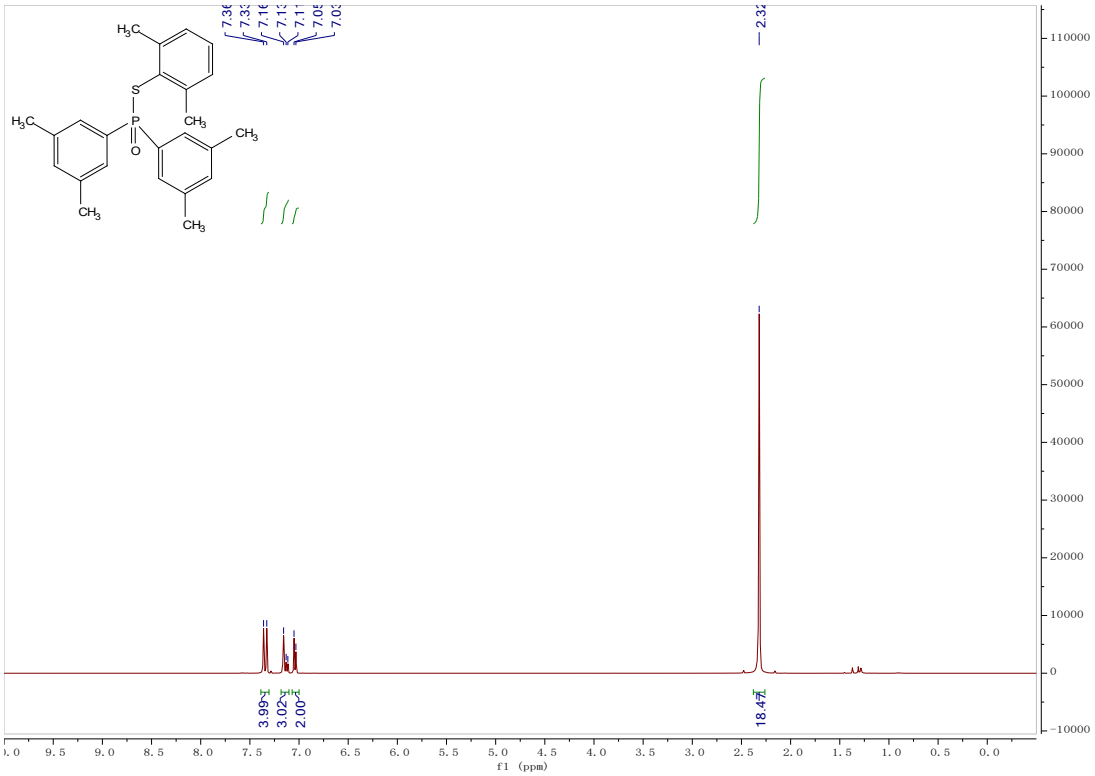
S-(2,4-dimethylphenyl) bis(3,5-dimethylphenyl)phosphinothioate (3ak)

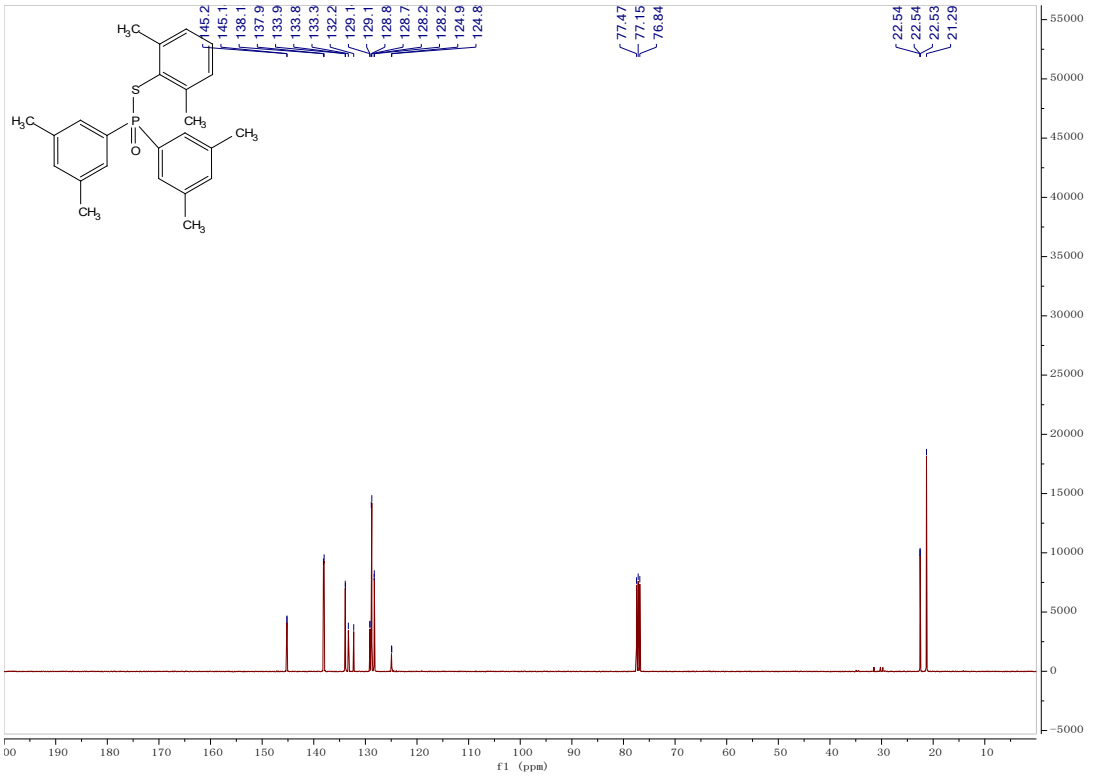


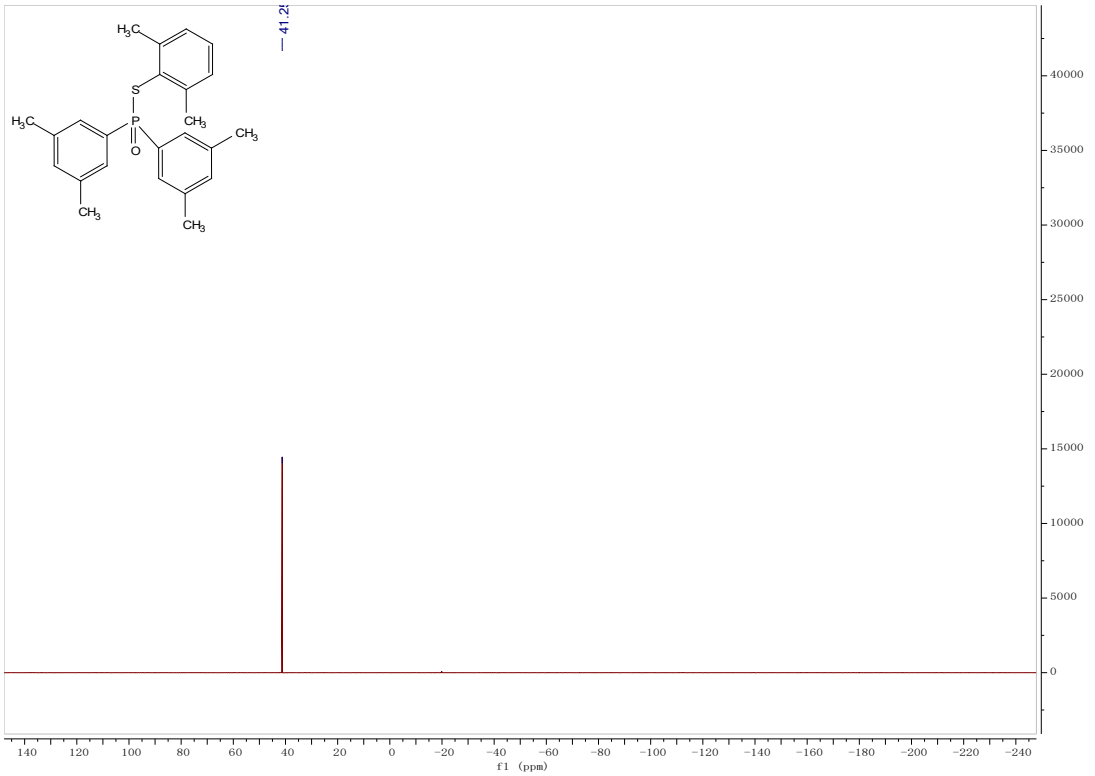




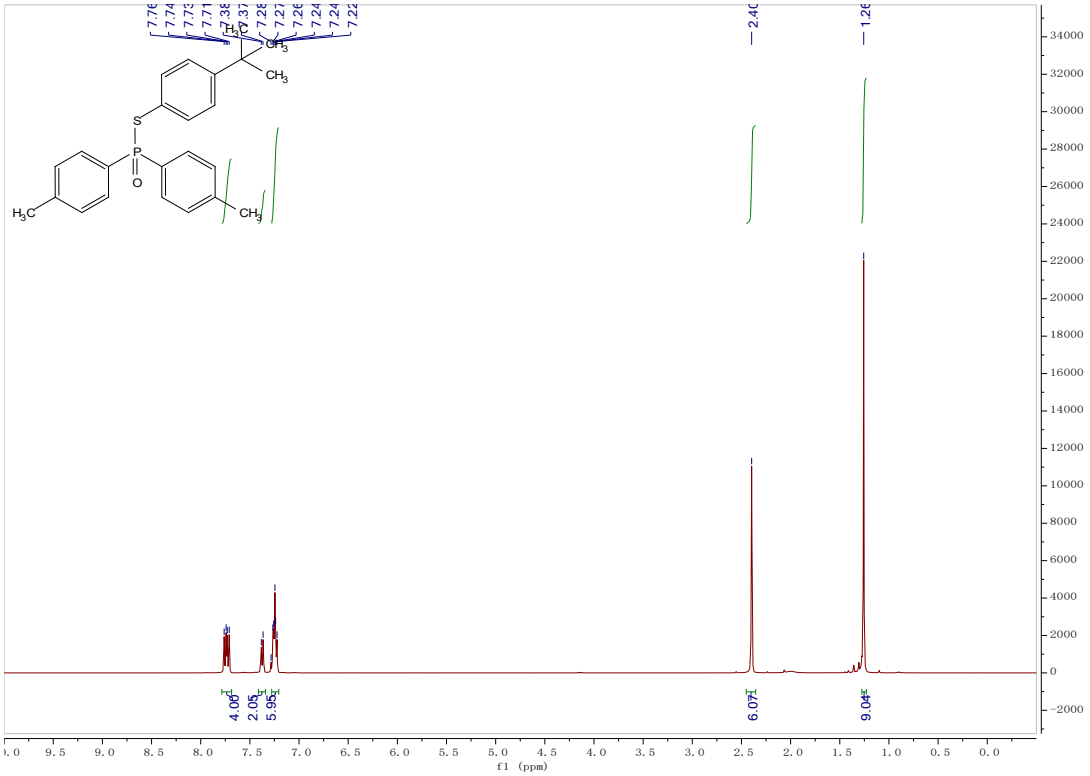
S-(2,6-dimethylphenyl) bis(3,5-dimethylphenyl)phosphinothioate (3al)

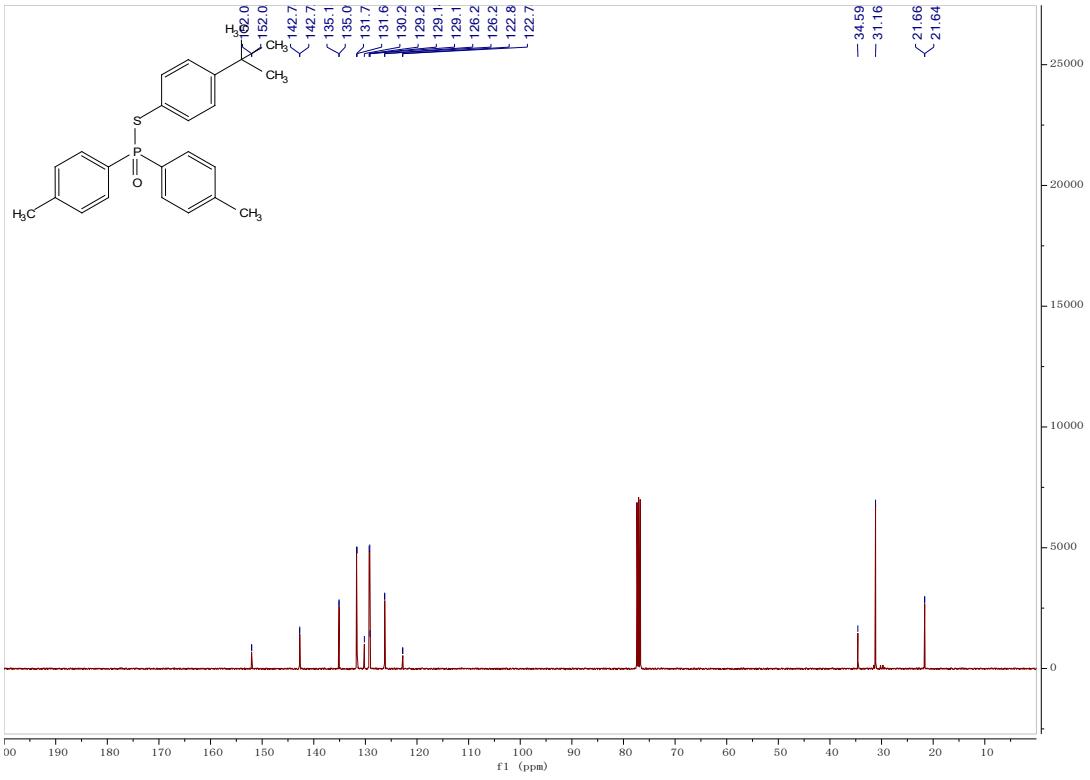


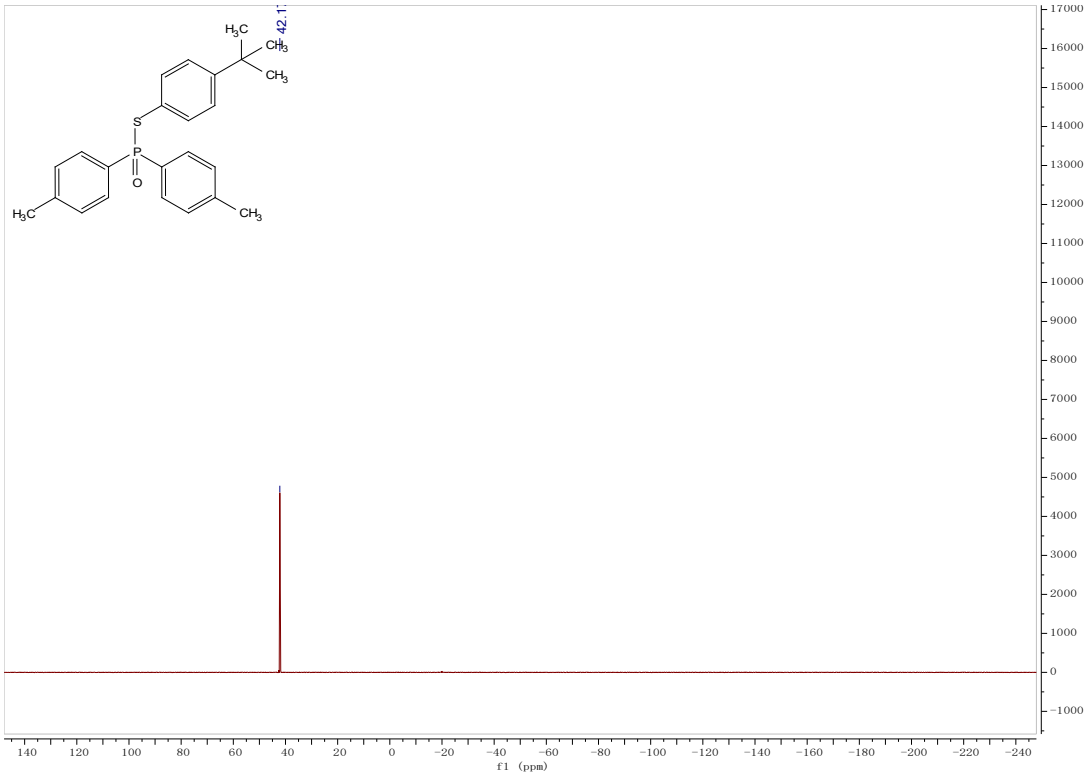

145.2
145.1
138.1
137.9
133.9
133.8
133.3
132.2
129.1
129.1
128.8
128.7
128.2
128.2
124.9
124.8
77.47
77.15
76.84
22.54
22.54
22.53
21.29
f1 (ppm)


41.2
f1 (ppm)

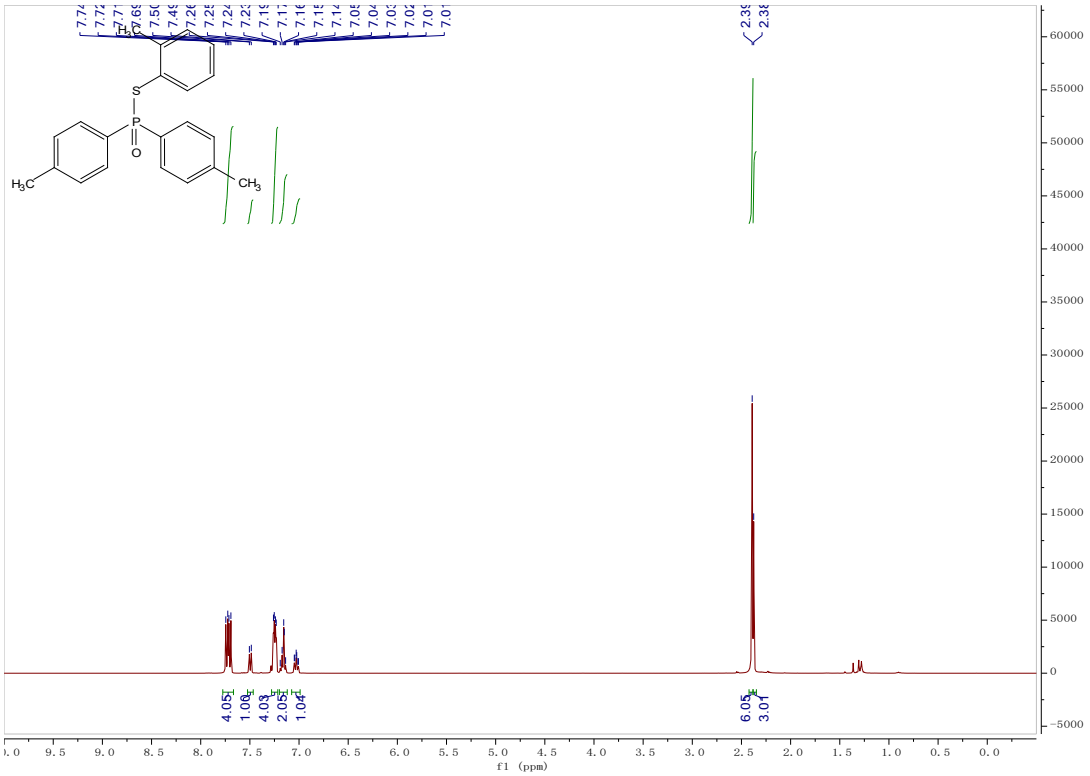
S-(4-(tert-butyl)phenyl) di-p-tolylphosphinothioate (3am)

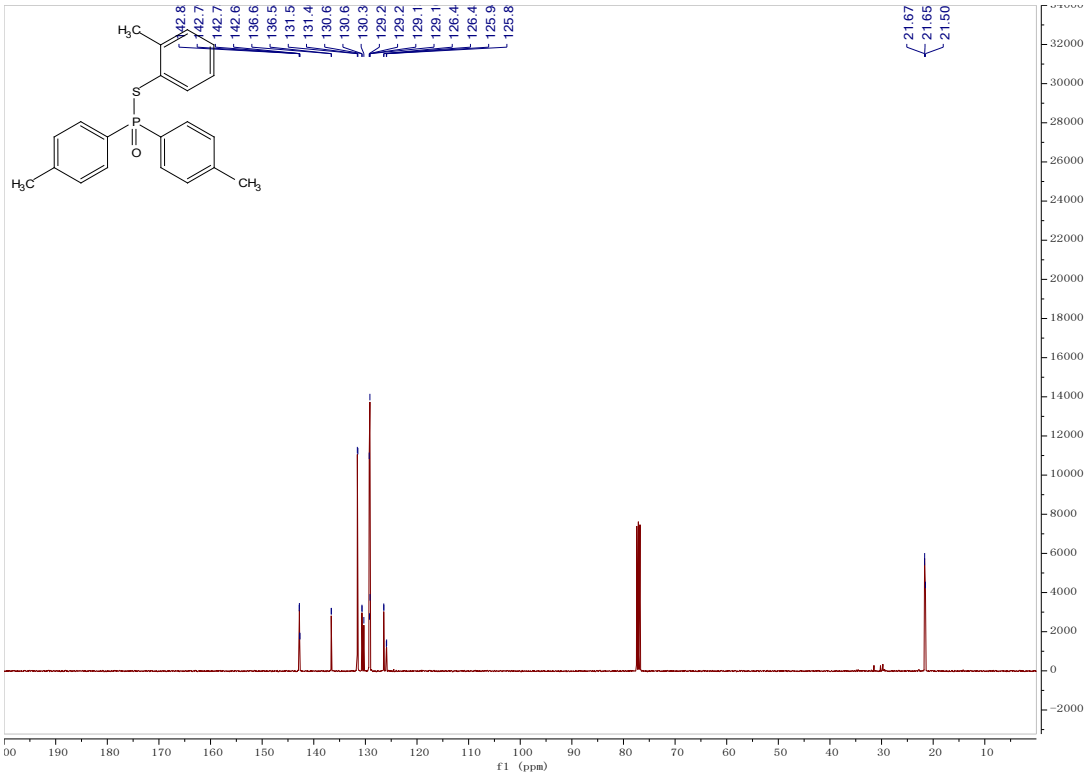


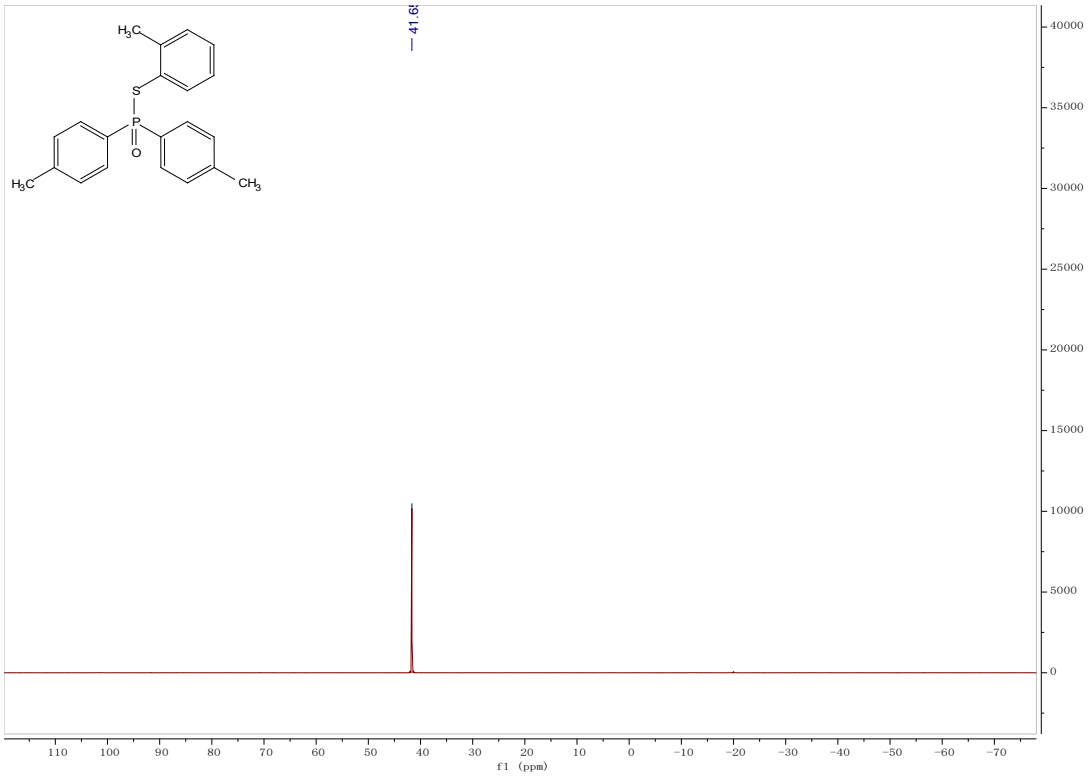




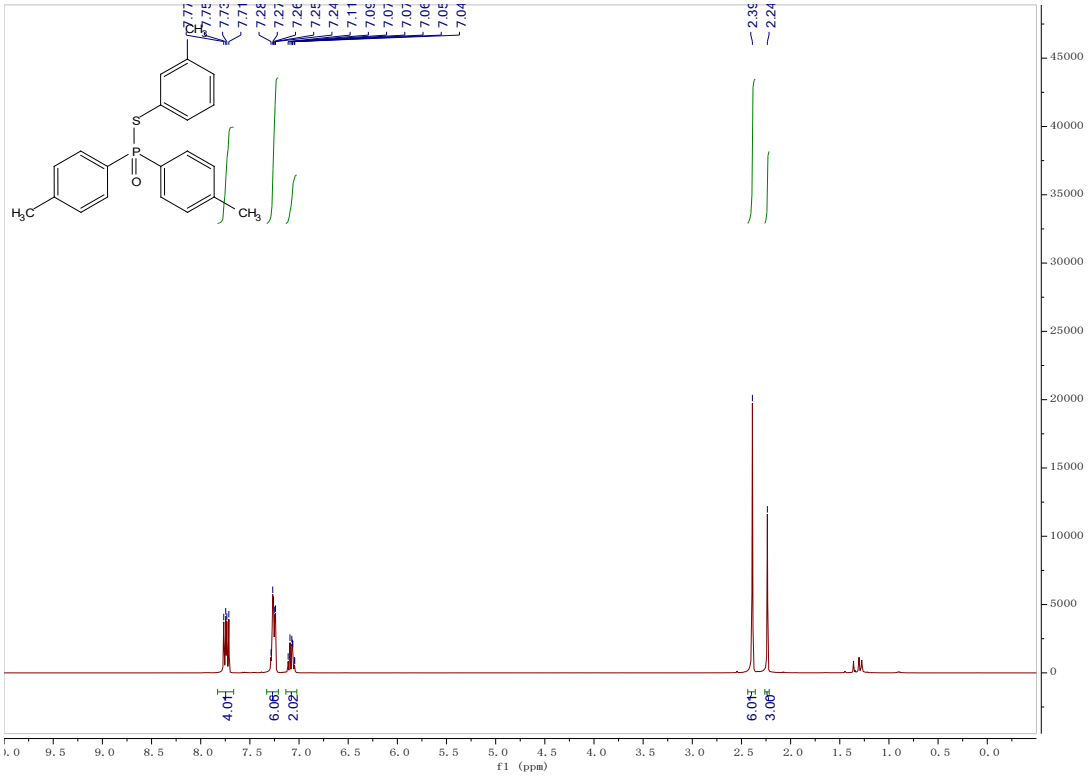
S-(o-tolyl) di-p-tolylphosphinothioate (3an)

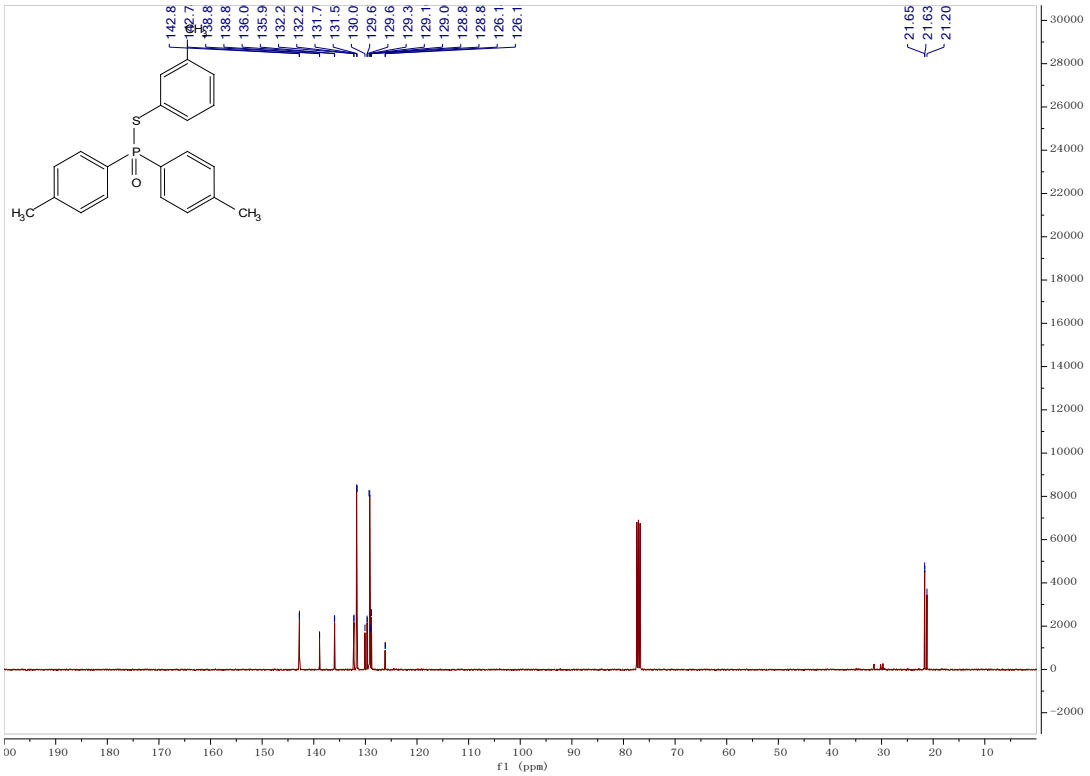


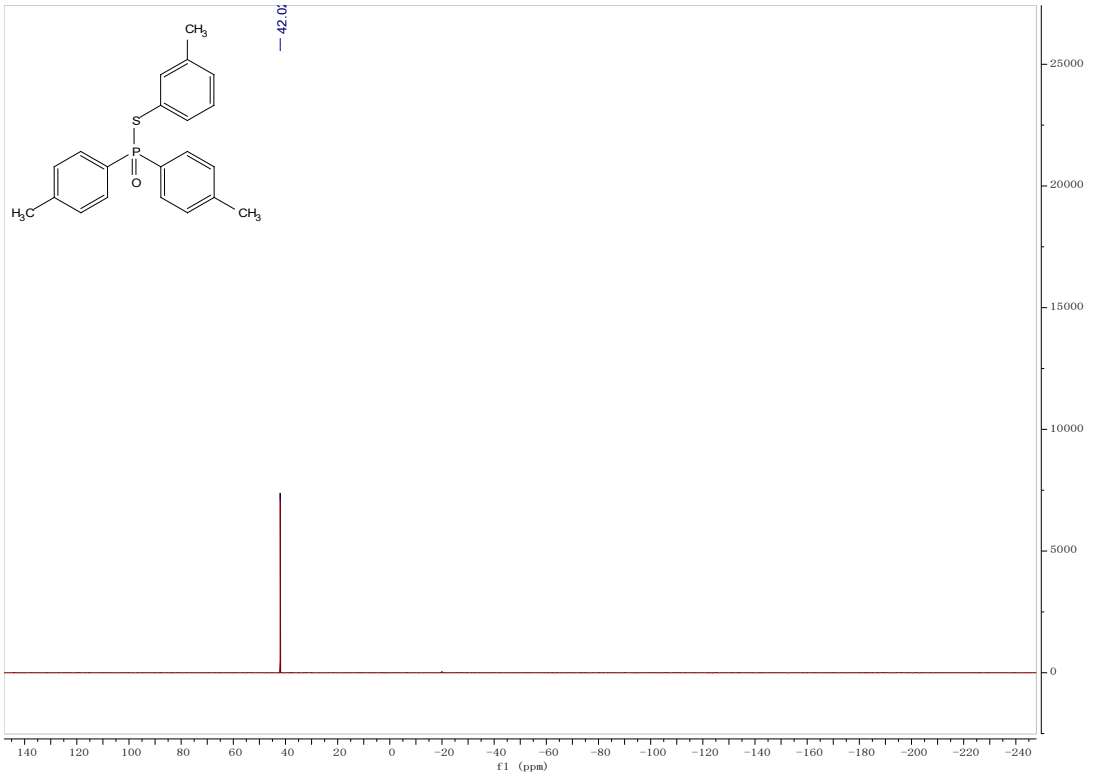

142.8
142.7
142.7
142.6
136.6
136.5
131.5
131.4
130.6
130.6
130.3
129.2
129.2
129.1
129.1
126.4
126.4
125.9
125.8
21.67
21.65
21.50
H3C
S
P
O
H3C
CH3
f1 (ppm)


41.6
H3C
S
P
O
H3C
CH3
f1 (ppm)

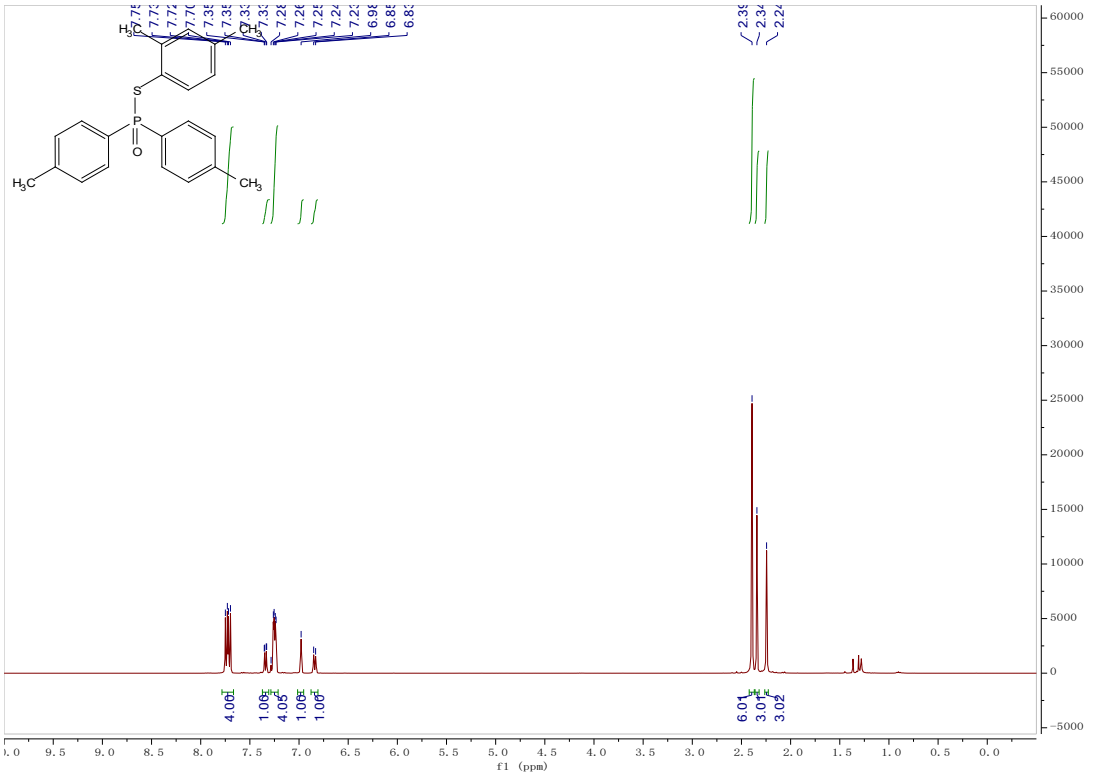
S-(m-tolyl) di-p-tolylphosphinothioate (3ao)

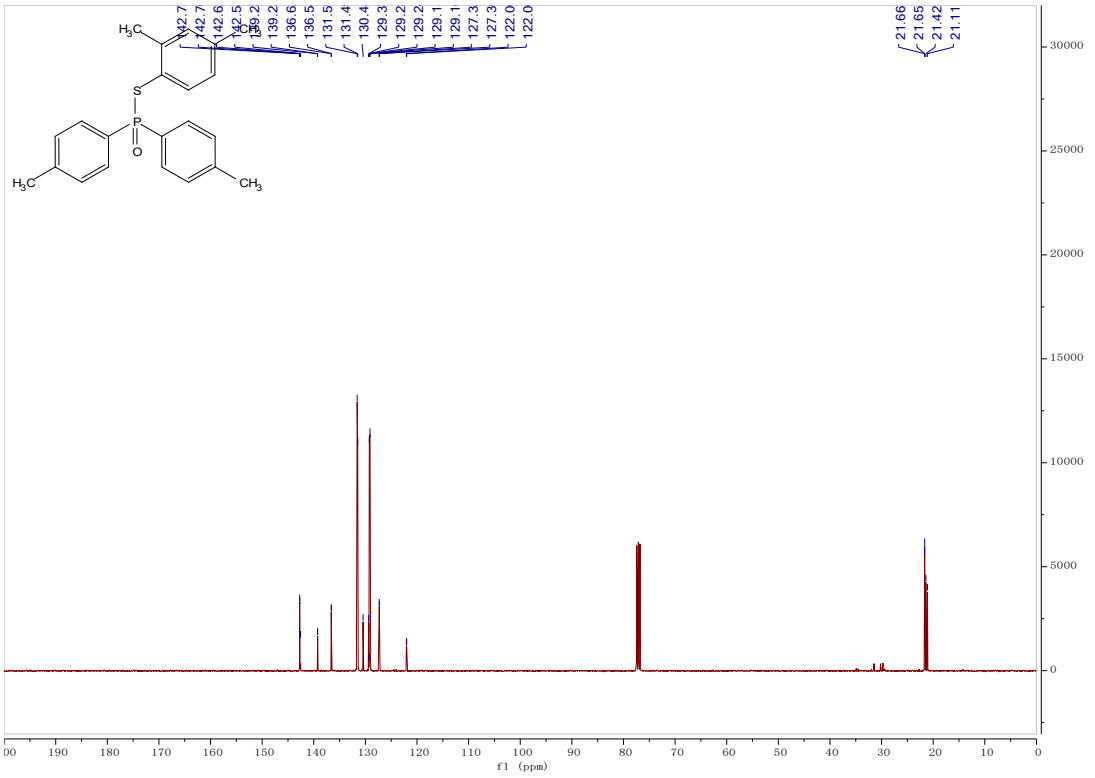


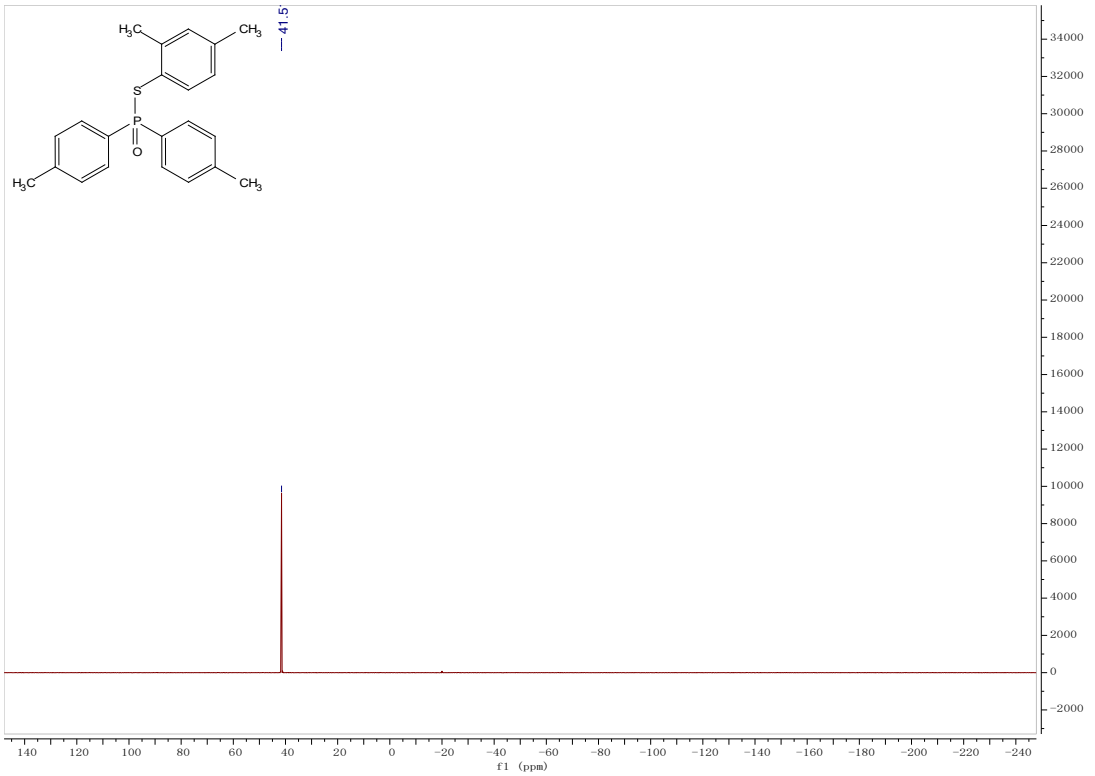




S-(2,4-dimethylphenyl) di-p-tolylphosphinothioate (3ap)




142.7
142.7
142.6
142.5
139.2
139.2
136.6
136.5
131.5
131.4
130.4
129.3
129.2
129.2
129.1
129.1
127.3
127.3
122.0
122.0
21.66
21.65
21.42
21.11
H3C
CH3
S
P
O
H3C
CH3
f1 (ppm)


41.5
H3C
CH3
S
P
O
H3C
CH3
f1 (ppm)