Electronic supplementary information (ESI)

Application of "hydrogen bonding interaction" in drug design Part Ⅱ: Design, synthesis, and SARs of thiophosphoramide derivatives as novel antiviral and antifungal agents

Aidang Lu[†,*], Yuanyuan Ma[†], Ziwen Wang[‡,*], Zhenghong Zhou[§], Qingmin Wang[§,*]

[†]School of Marine Science and Engineering, Hebei University of Technology, Tianjin 300130, China

[‡]Tianjin Key Laboratory of Structure and Performance for Functional Molecules, Key Laboratory of Inorganic-Organic Hybrid Functional Material Chemistry, Ministry of Education, College of Chemistry, Tianjin Normal University, Tianjin 300387, China

[§]State Key Laboratory of Elemento-Organic Chemistry, Research Institute of Elemento-Organic Chemistry, Nankai University, Tianjin 300071, China

Aidang Lu, Tel: 0086-22-60302241 Ext 205; Fax: 0086-22-60204274; e-mail: luaidang@hebut.edu.cn;

Ziwen Wang, Tel: 0086-22-23503792; Fax: 0086-22-23503792; e-mail: wangziwen2725@163.com;

Prof. Qingmin Wang, Tel.: 0086-22-23503952; Fax: 0086-22-23503952; e-mail: wangqm@nankai.edu.cn.

Contents

^{1}H NMR and ^{31}P NMR spectra of **1** ····S2

^{13}C NMR spectrum of **1** and ^{1}H NMR spectrum of **2** ····S3

^{31}P NMR and ^{13}C NMR spectra of **2** ····S4

^{1}H NMR and ^{31}P NMR spectra of **3** ····S5

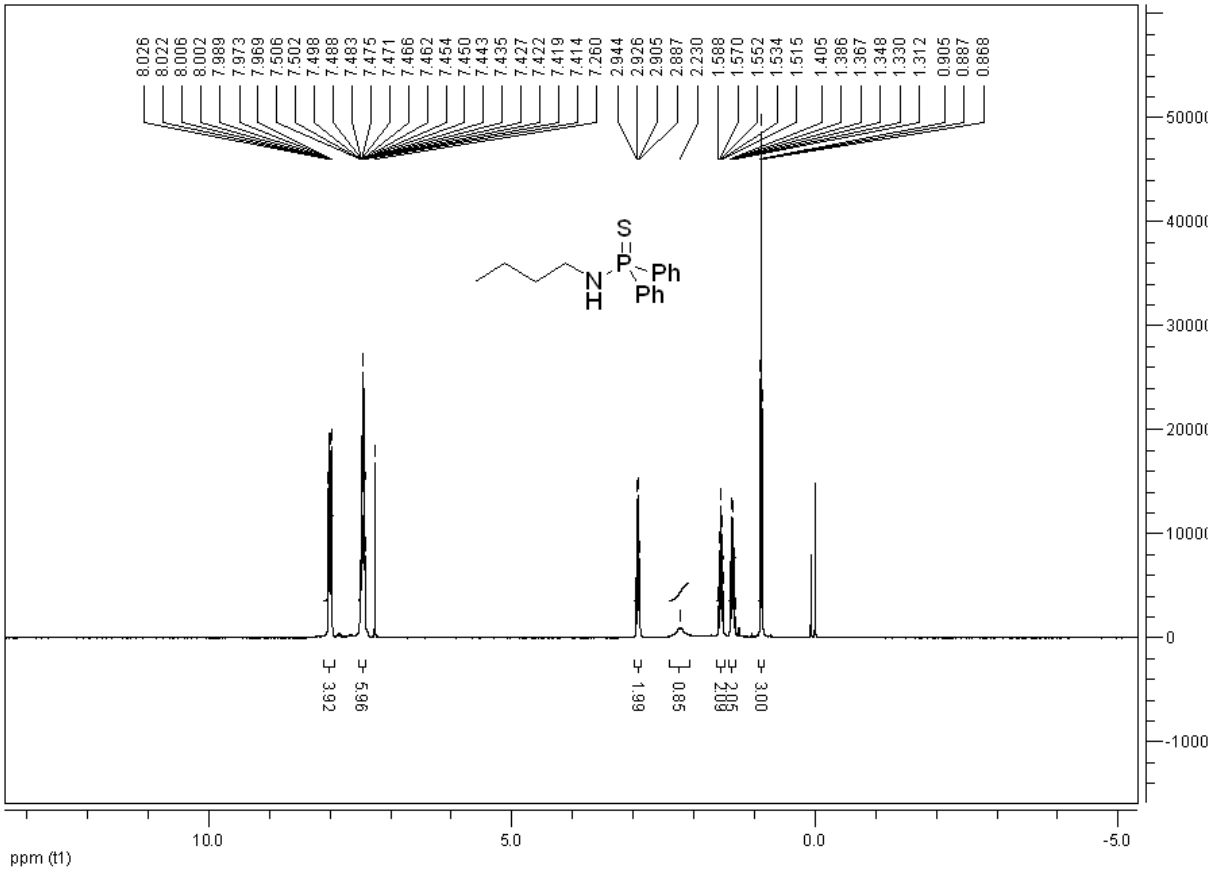
^{13}C NMR spectrum of **3** and ^{1}H NMR spectrum of **14** ····S6

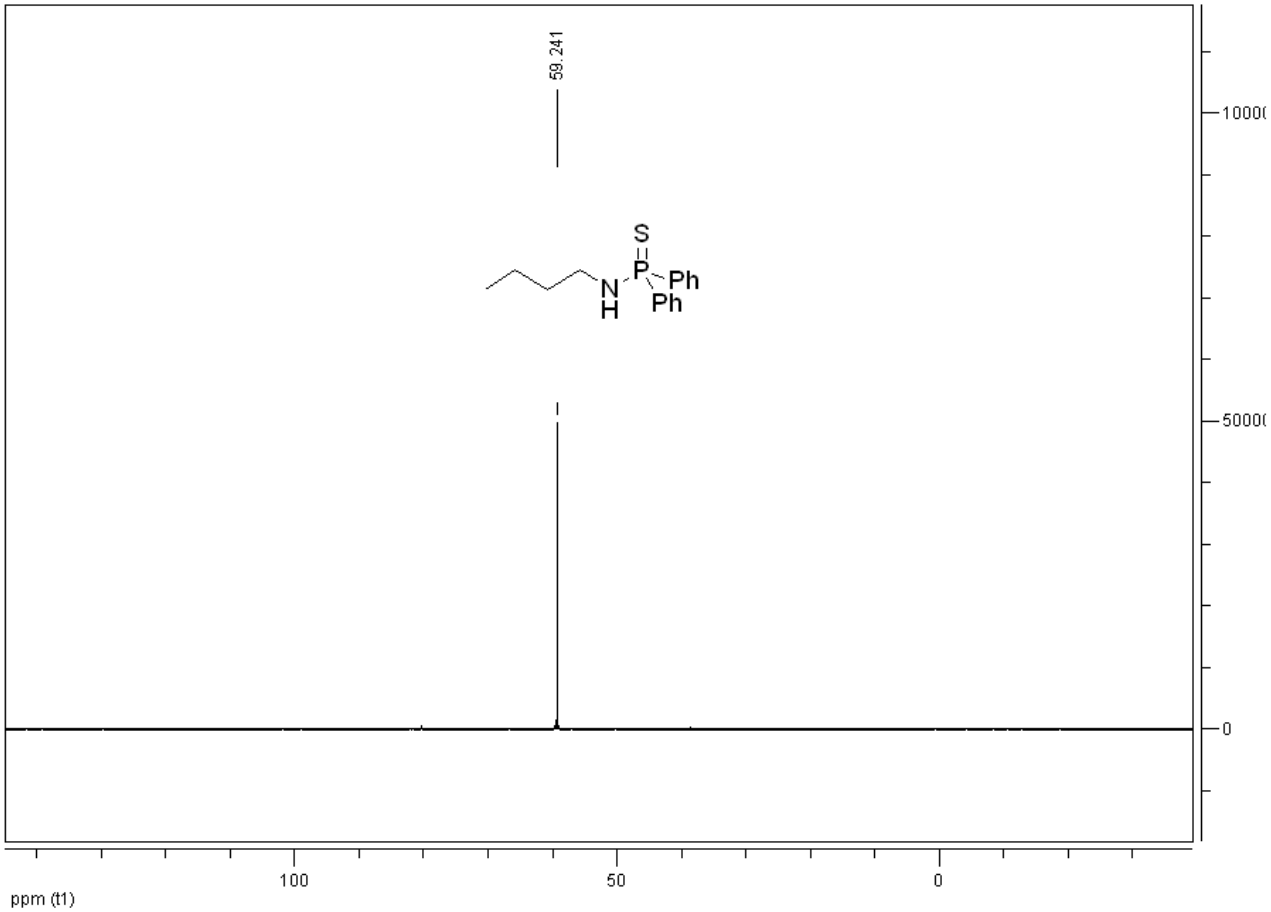
^{31}P NMR and ^{13}C NMR spectra of **14** ····S7

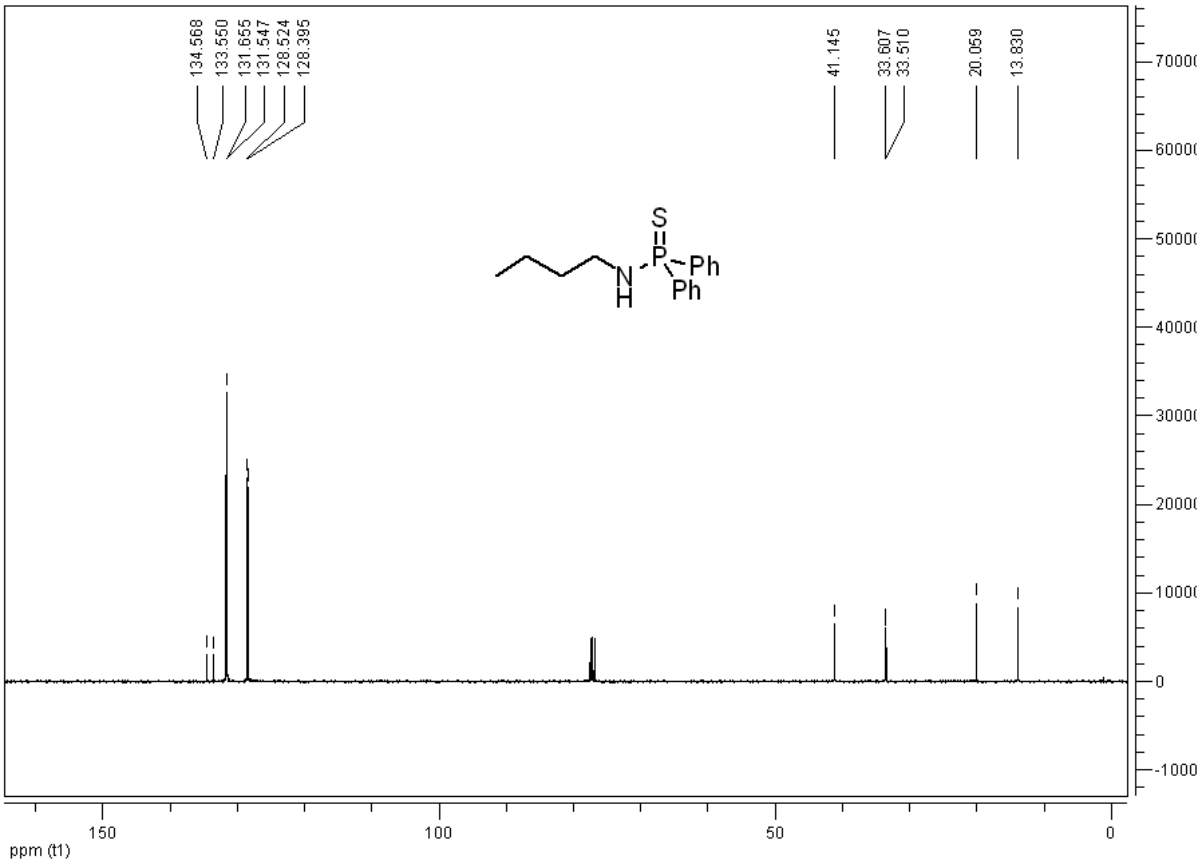
^{1}H NMR and ^{31}P NMR spectra of (*S*, *S*)-**17** ····S8

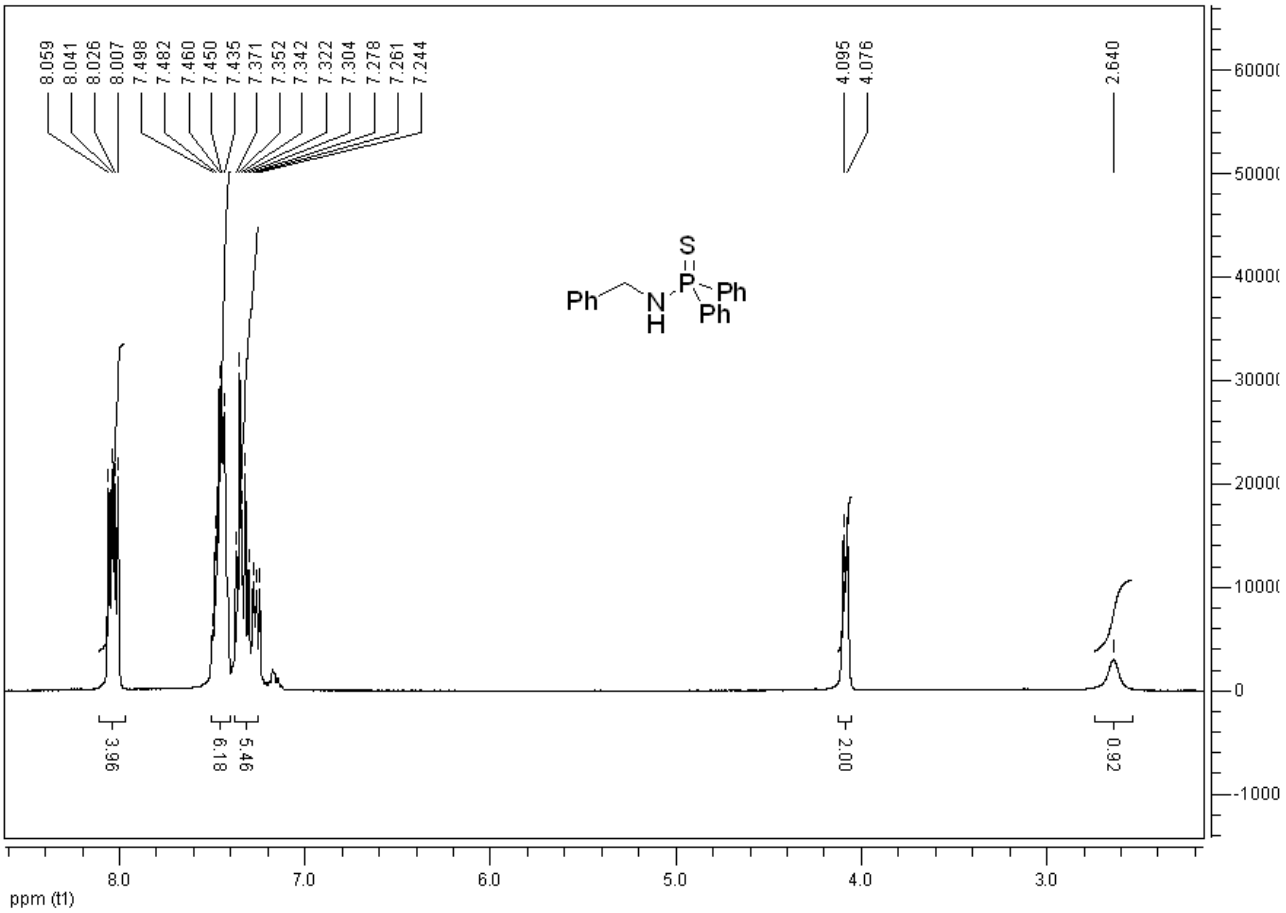
^{13}C NMR spectrum of (*S*,*S*)-**17** and ^{1}H NMR spectrum of (*R*,*R*)-**17**·HCl ····S9

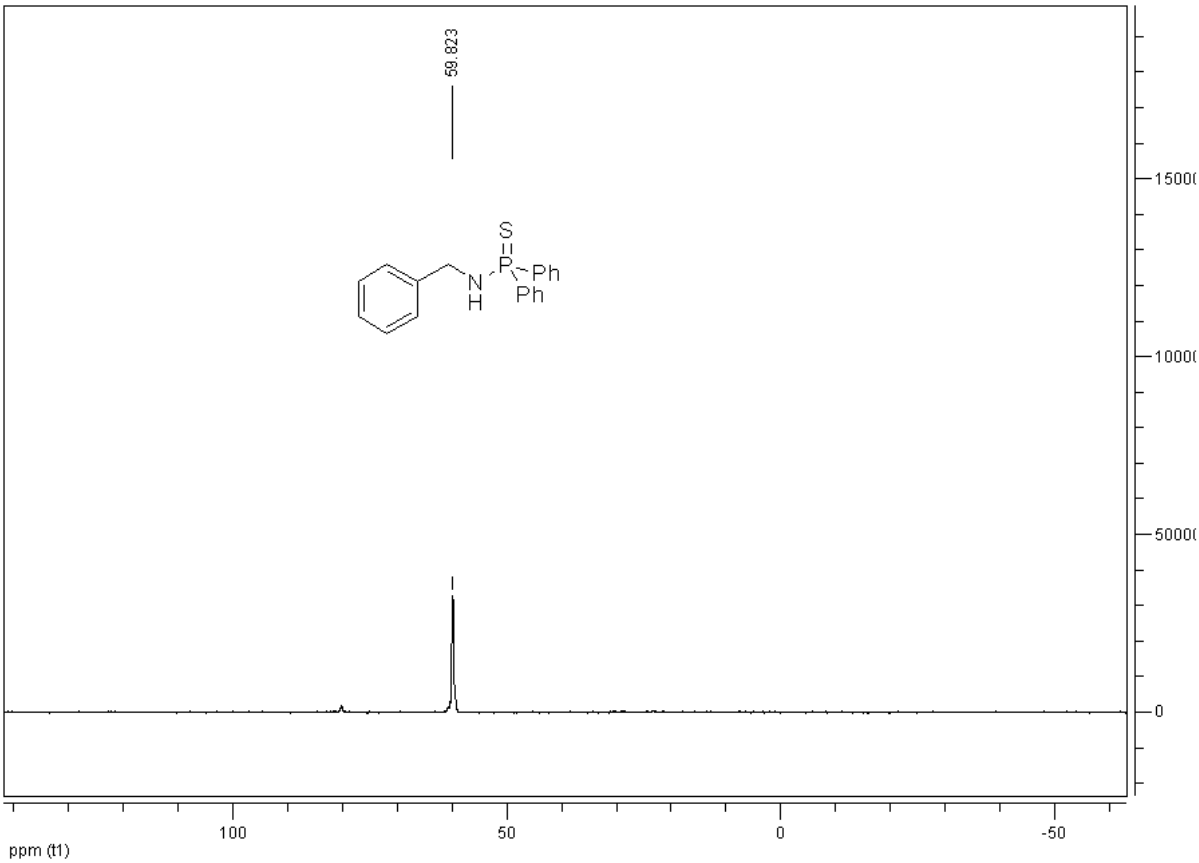
^{31}P NMR and ^{13}C NMR spectra of (*R*,*R*)-**17**·HCl ····S10

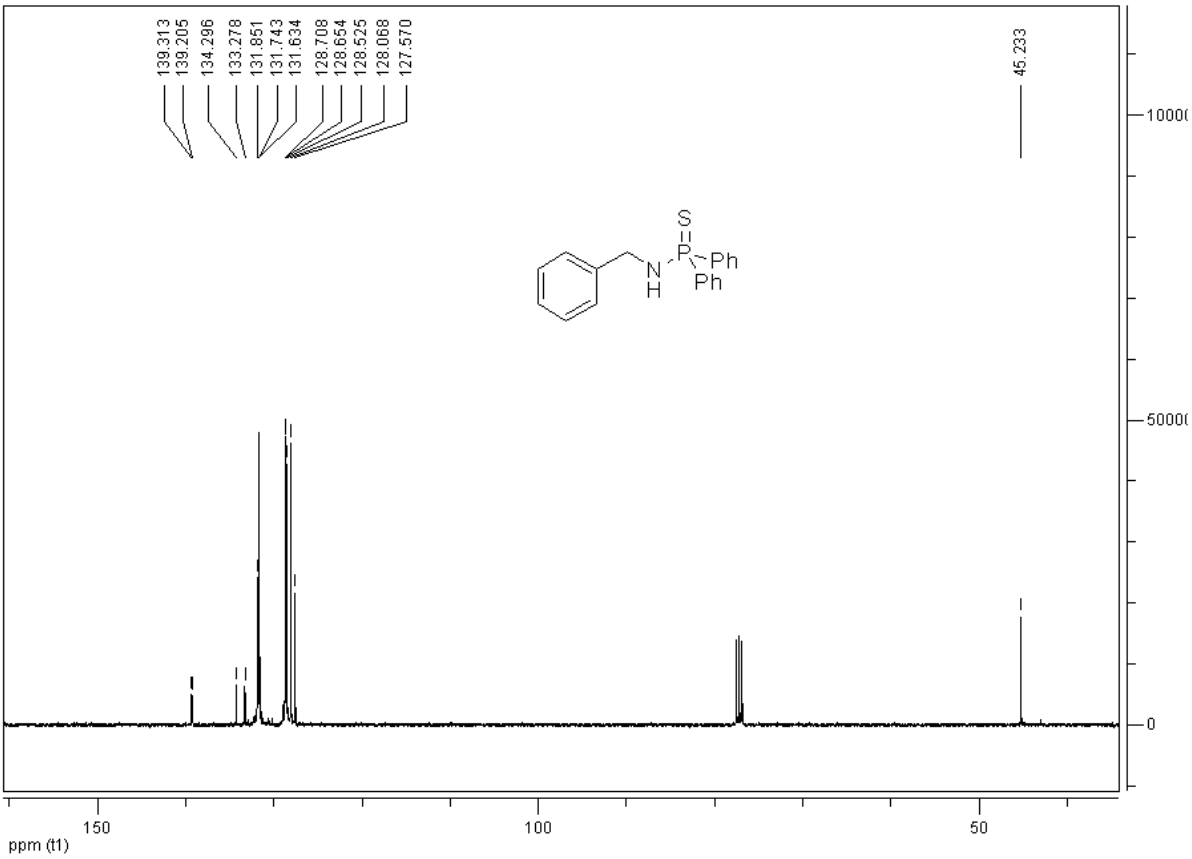

8.026
8.022
8.006
8.002
7.989
7.973
7.969
7.506
7.502
7.498
7.488
7.483
7.475
7.471
7.466
7.462
7.454
7.450
7.443
7.435
7.427
7.422
7.419
7.414
7.260
2.944
2.926
2.905
2.887
2.230
1.588
1.570
1.552
1.534
1.515
1.405
1.386
1.367
1.348
1.330
1.312
0.905
0.887
0.868
S
P
Ph
Ph
N
H
3.92
5.66
1.99
0.85
2.09
3.00
10.0
5.0
0.0
-5.0
ppm (t1)

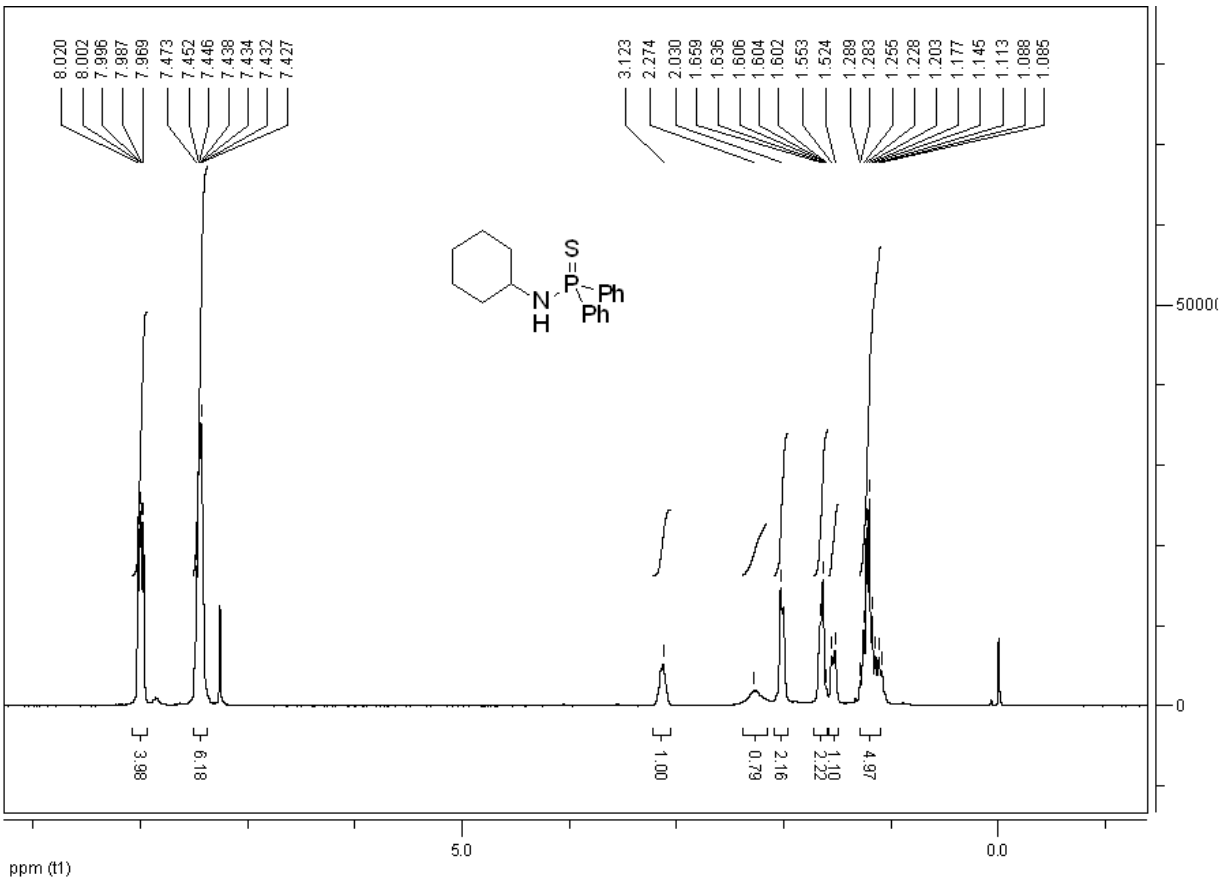

59.241
S
P
Ph
Ph
N
H
100
50
0
ppm (t1)

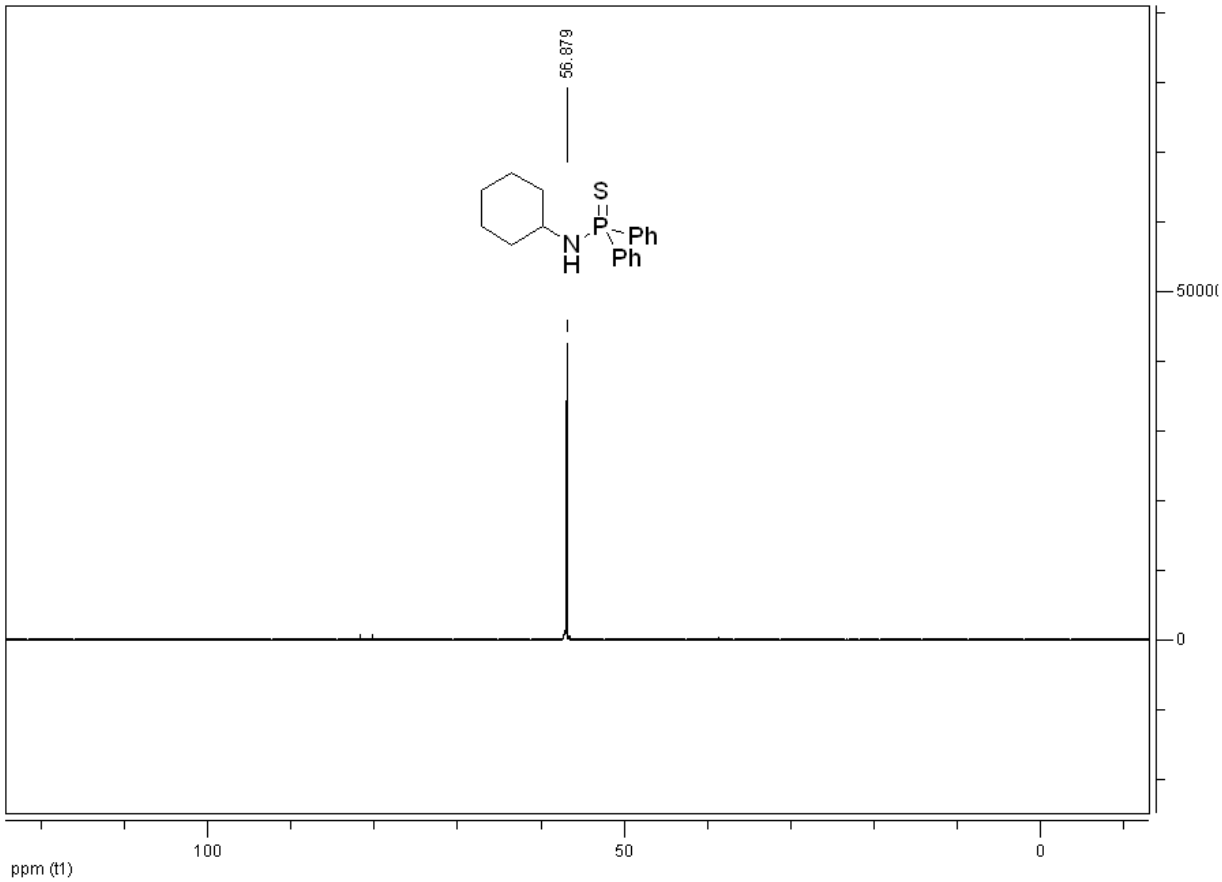

134.568
133.550
131.655
131.547
128.524
128.395
41.145
33.607
33.510
20.059
13.830
S
P
Ph
Ph
N
H
ppm (t1)

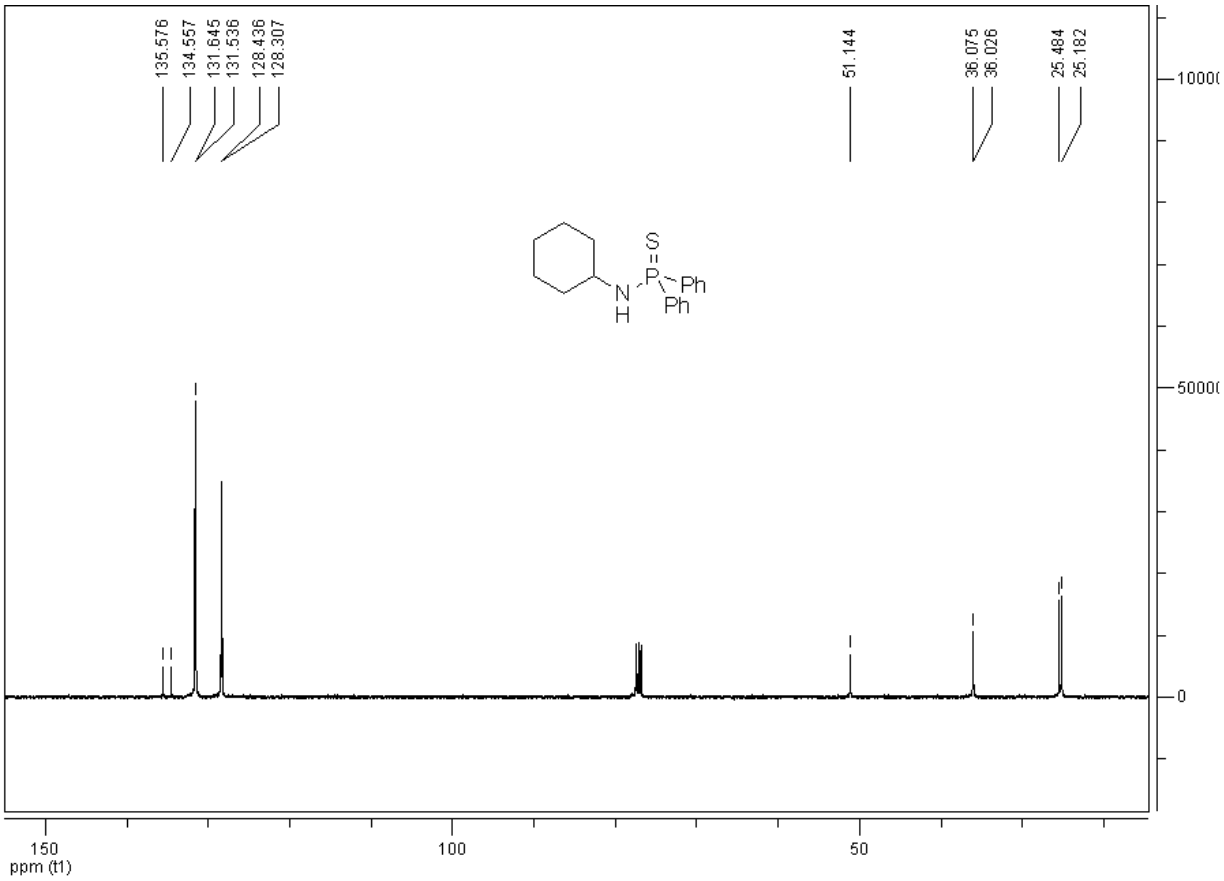

8.059
8.041
8.026
8.007
7.498
7.482
7.460
7.450
7.435
7.371
7.352
7.342
7.322
7.304
7.278
7.261
7.244
4.095
4.076
2.640
S
P
Ph
Ph
Ph
N
H
3.96
6.18
5.46
2.00
0.92
ppm (t1)

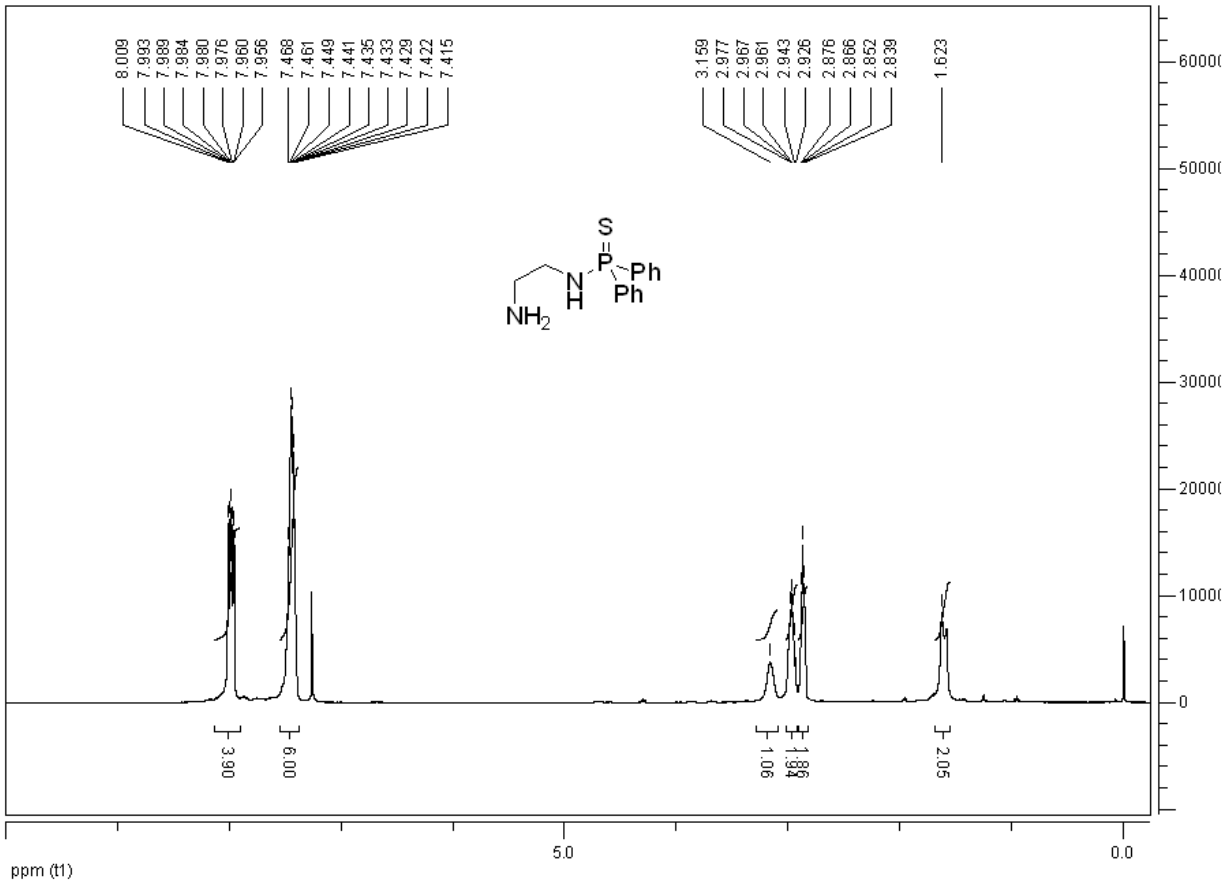

59.823
S
P
Ph
Ph
N
H
15000
10000
50000
0
100
50
0
-50
ppm (t1)

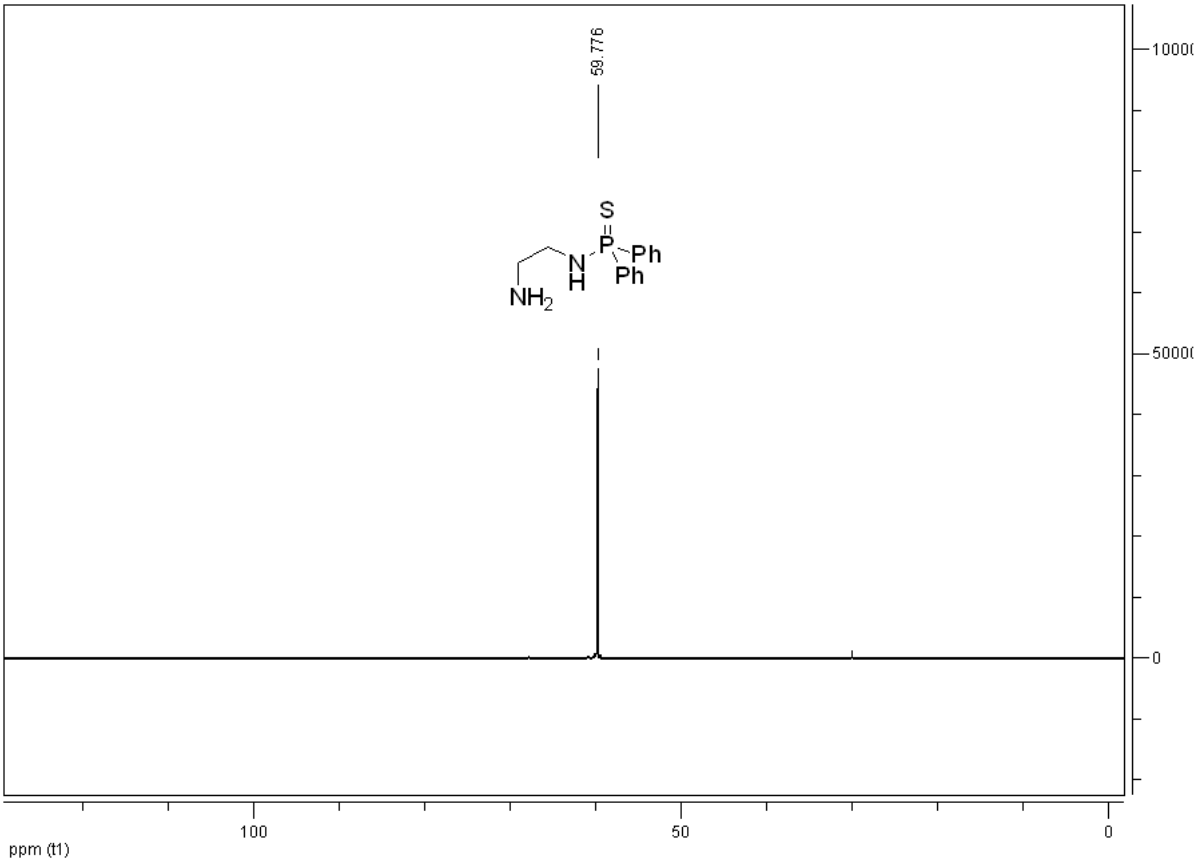

139.313
139.205
134.296
133.278
131.851
131.743
131.634
128.708
128.654
128.525
128.068
127.570
45.233
S
P
Ph
Ph
N
H
10000
50000
0
150
100
50
ppm (t1)

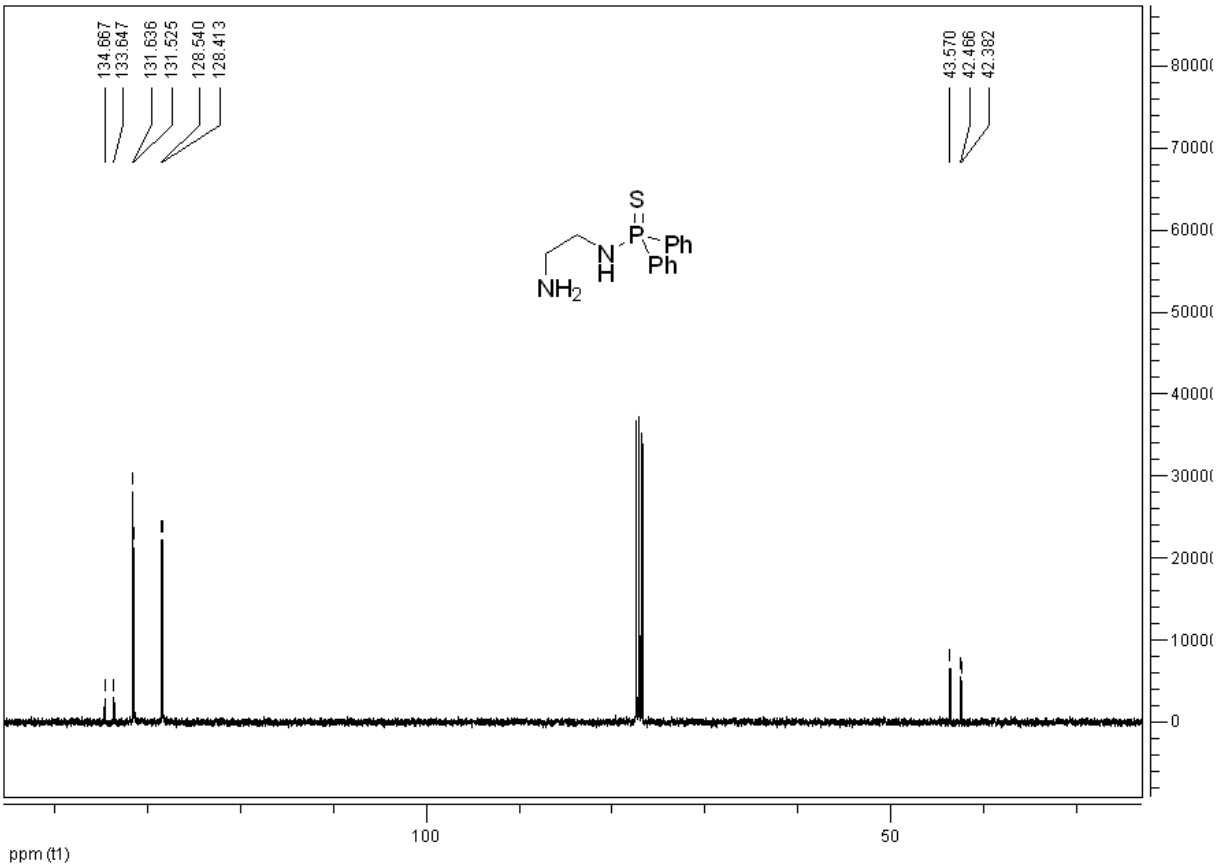

8.020
8.002
7.996
7.987
7.969
7.473
7.452
7.446
7.438
7.434
7.432
7.427
3.123
2.274
2.030
1.659
1.636
1.606
1.604
1.602
1.553
1.524
1.289
1.283
1.255
1.228
1.203
1.177
1.145
1.113
1.088
1.085
S
P
Ph
Ph
N
H
3.98
6.18
1.00
0.79
2.16
1.10
2.22
4.97
5000(
0
5.0
0.0
ppm (t1)

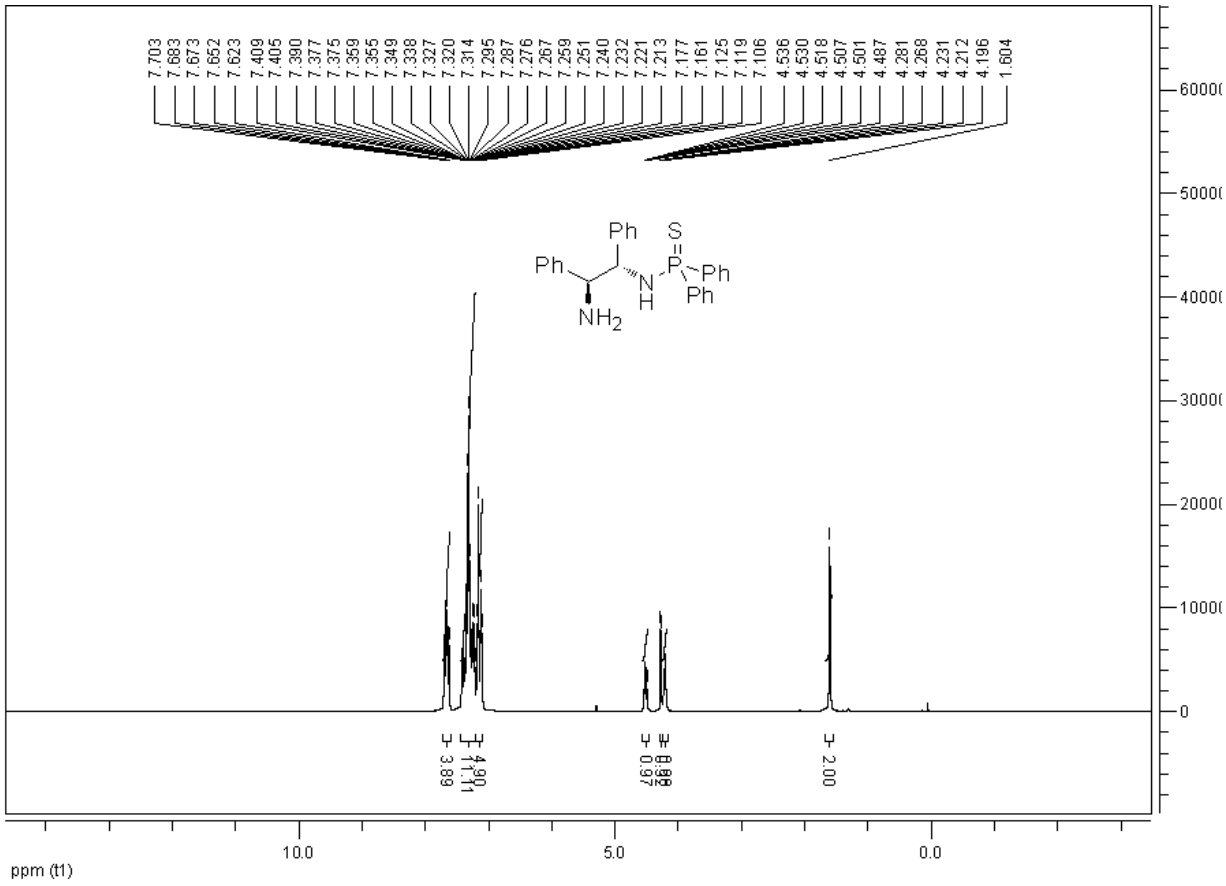

56.879
S
P
Ph
Ph
N
H
5000(
0
100
50
0
ppm (t1)

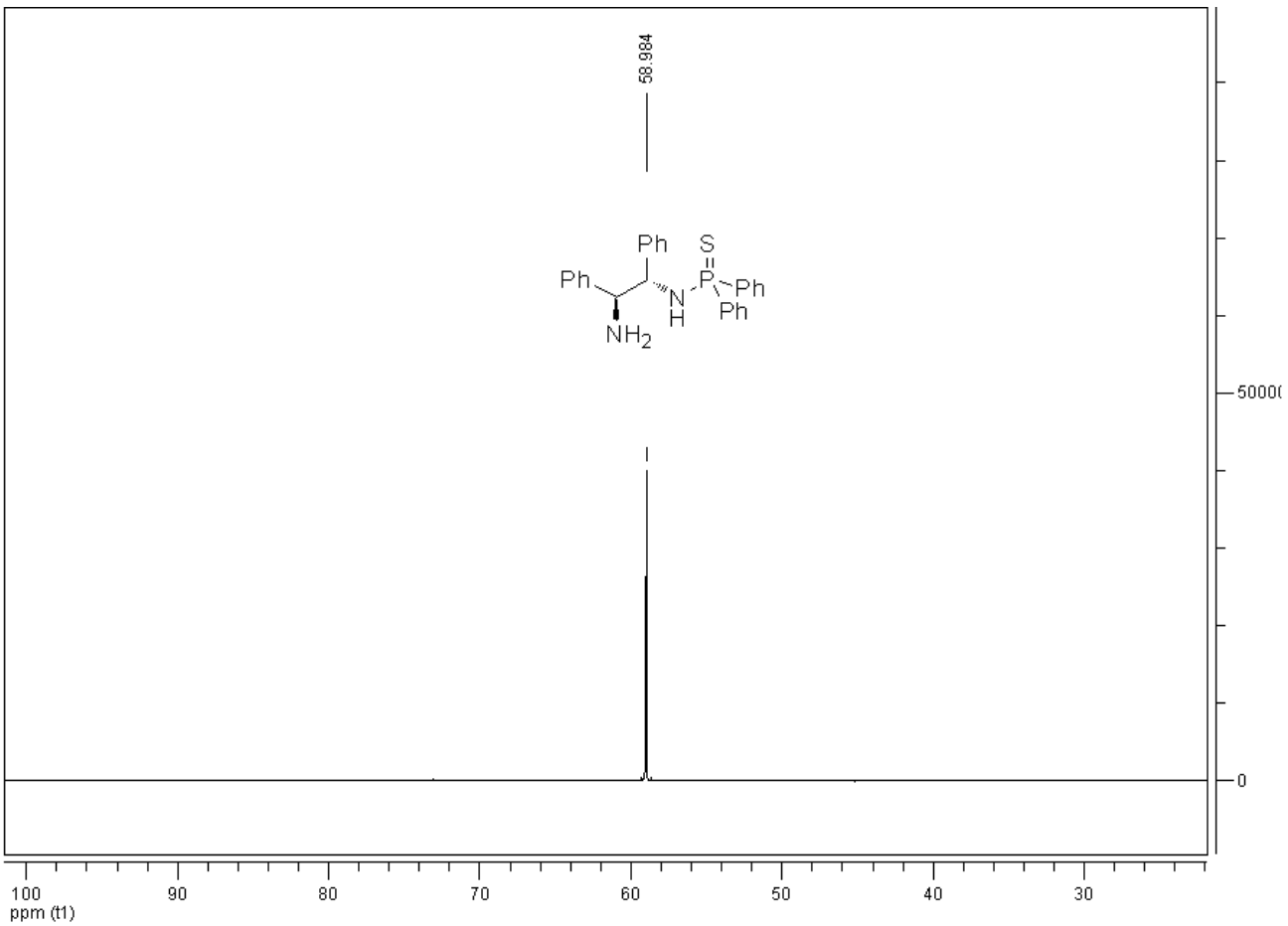

135.576
134.557
131.645
131.536
128.436
128.307
51.144
36.075
36.026
25.484
25.182
S
P
Ph
Ph
N
H
10000
50000
0
150
100
50
ppm (t1)

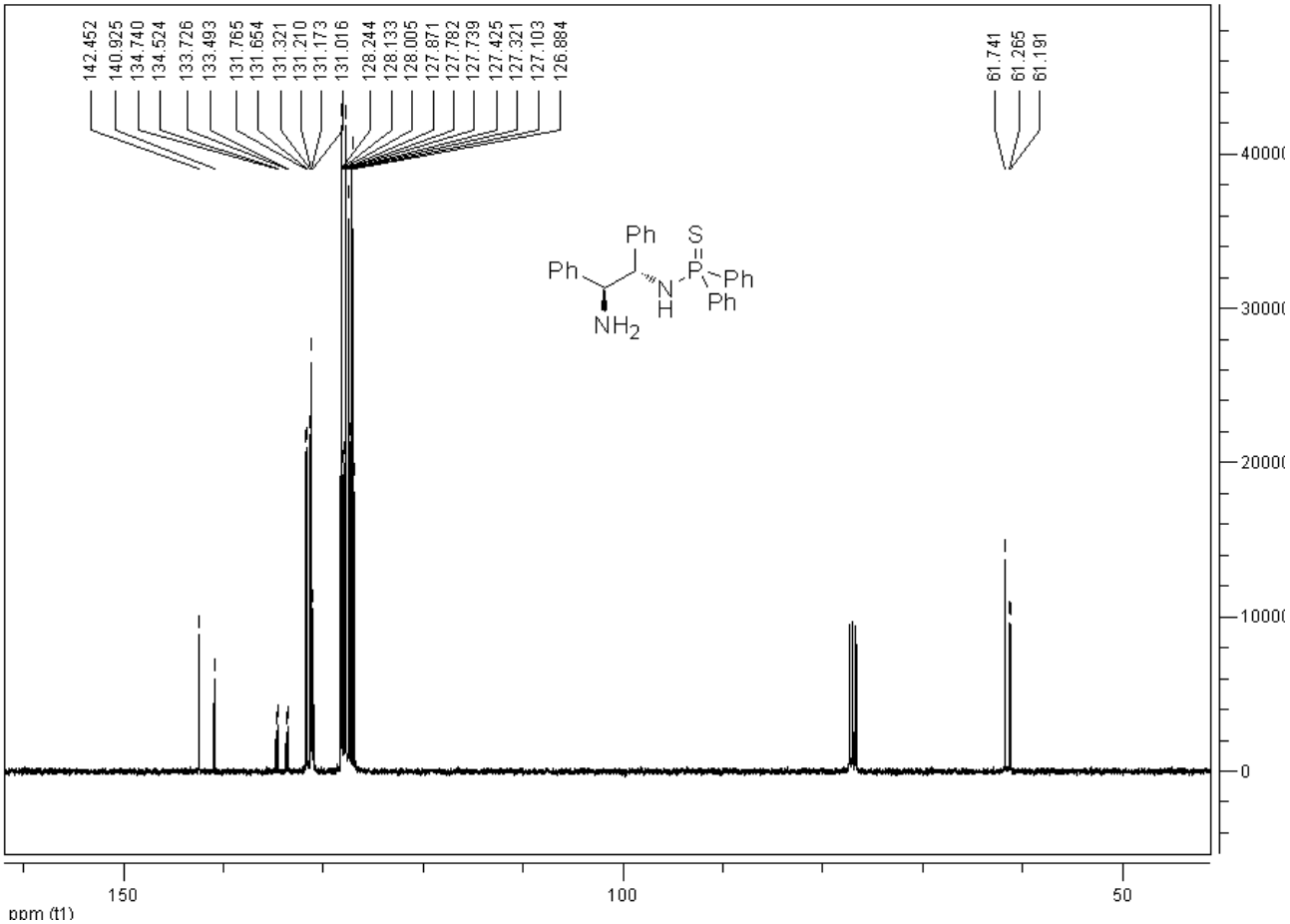

8.009
7.993
7.989
7.984
7.980
7.976
7.960
7.956
7.468
7.461
7.449
7.441
7.435
7.433
7.429
7.422
7.415
3.159
2.977
2.967
2.961
2.943
2.926
2.876
2.866
2.852
2.839
1.623
S
P
Ph
Ph
N
H
NH2
60000
50000
40000
30000
20000
10000
0
3.90
6.00
1.06
1.84
2.05
5.0
0.0
ppm (t1)

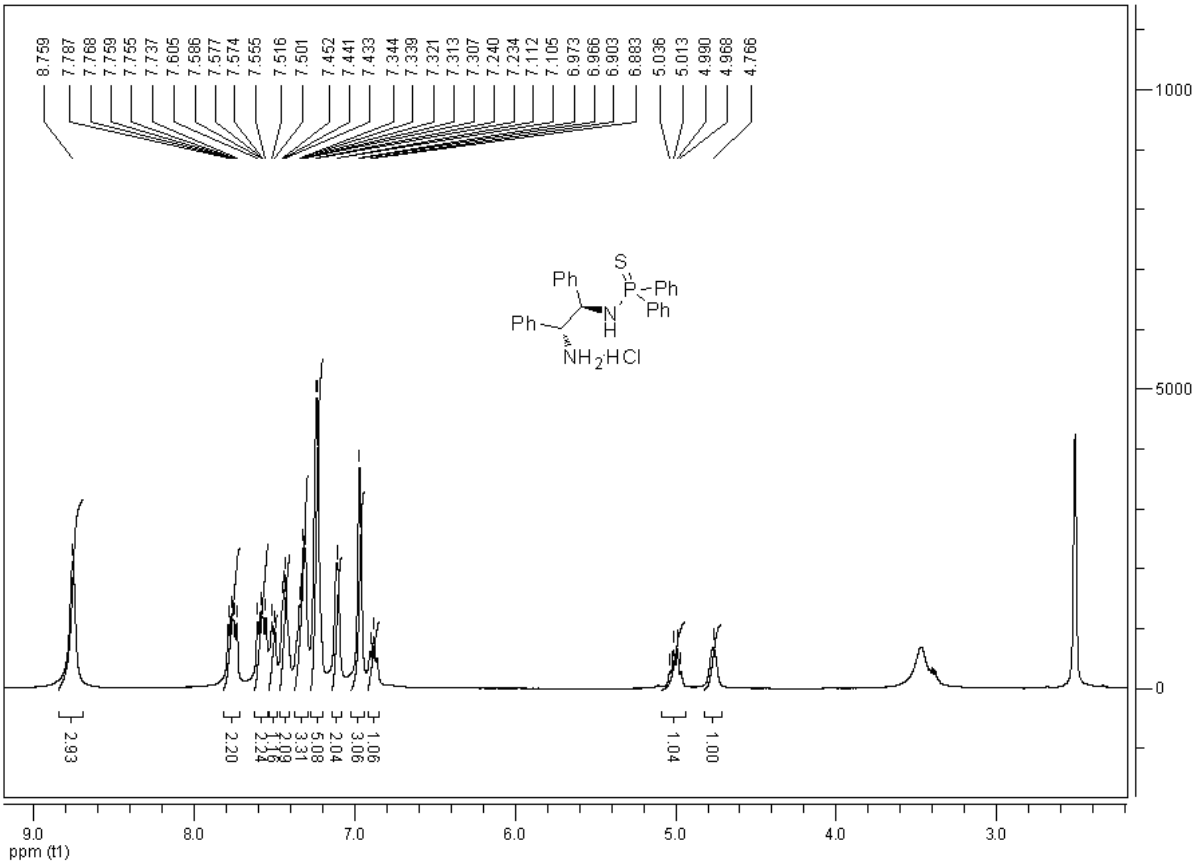

59.776
S
P
Ph
Ph
N
H
NH2
10000
50000
0
100
50
0
ppm (t1)

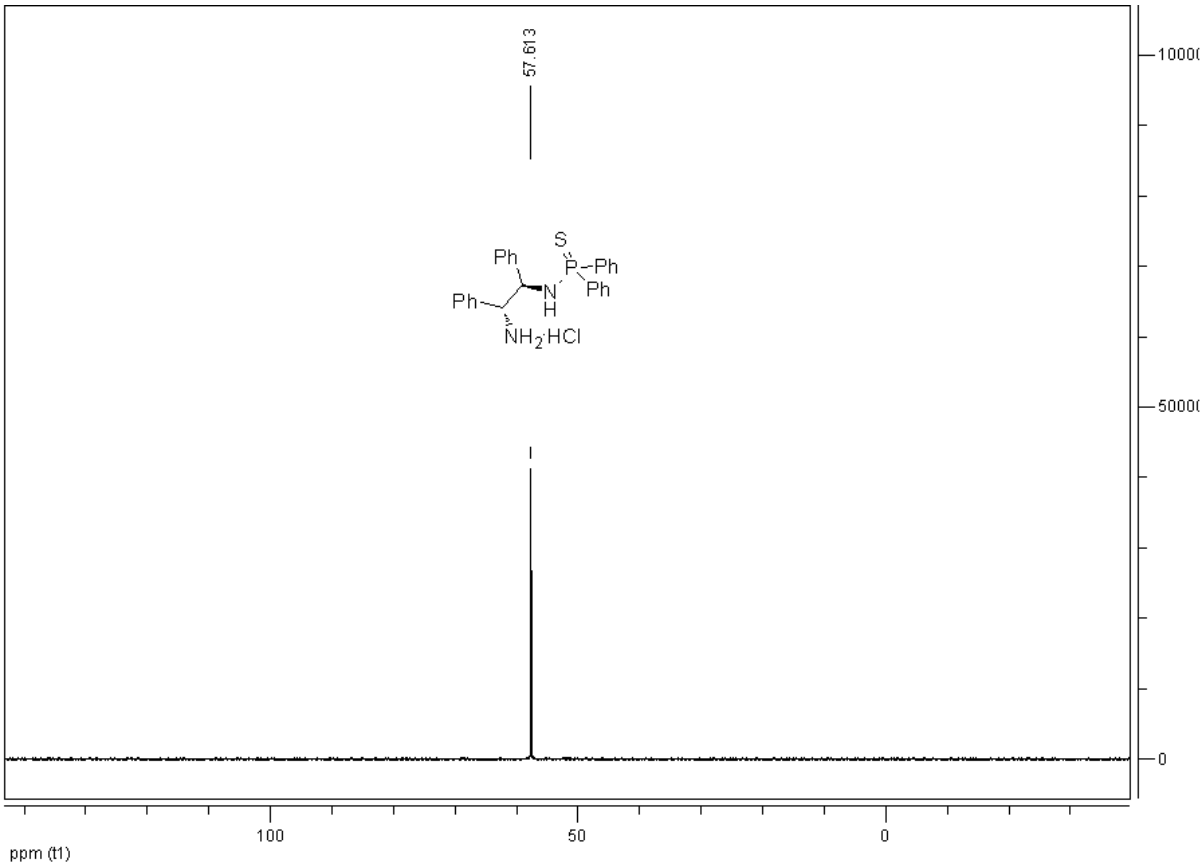

134.667
133.647
131.636
131.525
128.540
128.413
43.570
42.466
42.382
S
P
Ph
Ph
N
H
NH2
80000
70000
60000
50000
40000
30000
20000
10000
0
100
50
ppm (t1)

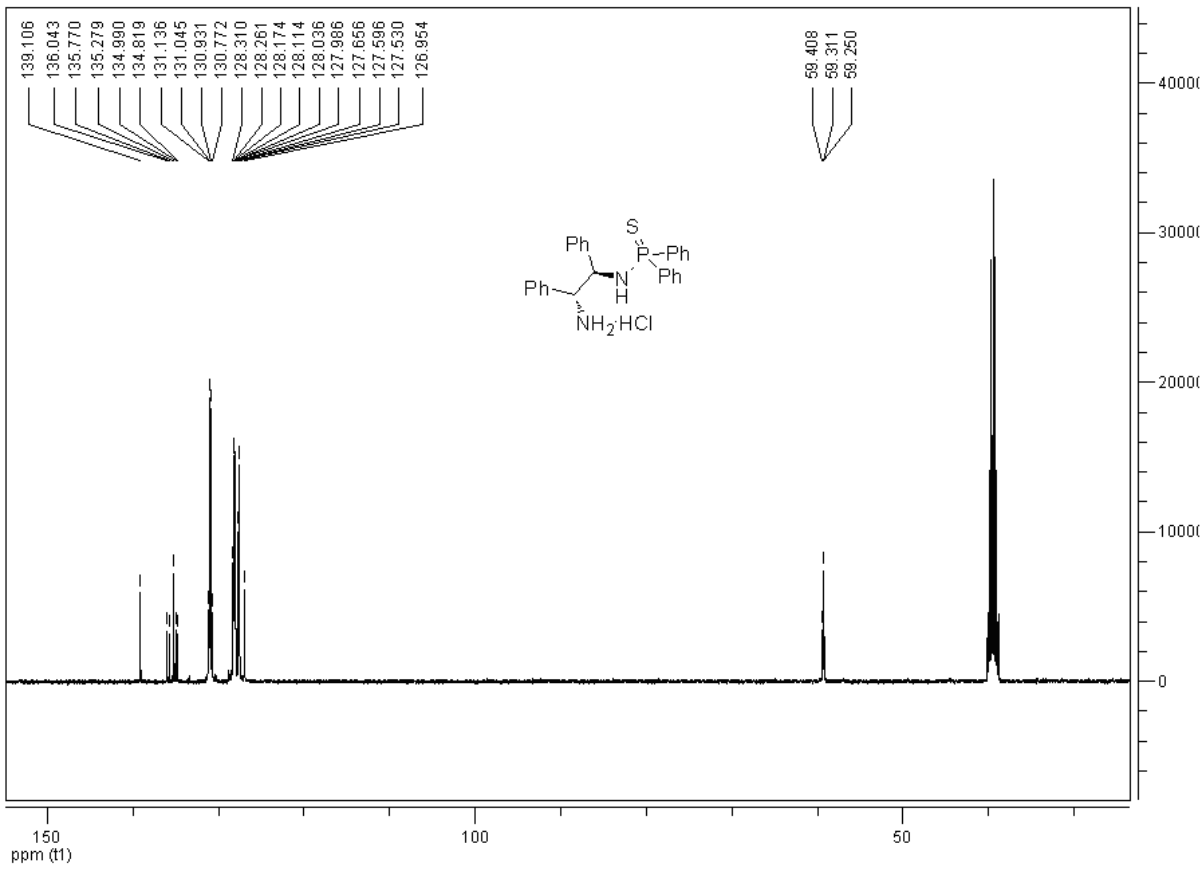

7.703
7.683
7.673
7.652
7.623
7.409
7.405
7.390
7.377
7.375
7.359
7.355
7.349
7.338
7.327
7.320
7.314
7.295
7.287
7.276
7.267
7.259
7.251
7.240
7.232
7.221
7.213
7.177
7.161
7.125
7.119
7.106
4.536
4.530
4.518
4.507
4.501
4.487
4.281
4.268
4.231
4.212
4.196
1.604
Ph
S
Ph
P
Ph
N
H
Ph
NH2
3.89
4.11
4.90
0.97
2.00
10.0
5.0
0.0
ppm (t1)


58.984
Ph
S
Ph
P
Ph
N
H
Ph
NH2
100
90
80
70
60
50
40
30
ppm (t1)


142.452
140.925
134.740
134.524
133.726
133.493
131.765
131.654
131.321
131.210
131.173
131.016
128.244
128.133
128.005
127.871
127.782
127.739
127.425
127.321
127.103
126.884
61.741
61.265
61.191
Ph
S
Ph
P
Ph
N
H
Ph
NH2
150
100
50
ppm (t1)


8.759
7.787
7.768
7.759
7.755
7.737
7.605
7.586
7.577
7.574
7.555
7.516
7.501
7.452
7.441
7.433
7.344
7.339
7.321
7.313
7.307
7.240
7.234
7.112
7.105
6.973
6.966
6.903
6.883
5.036
5.013
4.990
4.968
4.766
Ph
S
Ph
P
Ph
N
H
Ph
NH2HCl
2.93
2.20
2.14
1.31
5.08
2.04
3.06
1.04
1.00
9.0
8.0
7.0
6.0
5.0
4.0
3.0
ppm (t1)


57.613
Ph
S
P
Ph
Ph
Ph
N
H
NH2·HCl
10000
50000
0
100
50
0
ppm (t1)


139.106
136.043
135.770
135.279
134.990
134.819
131.136
131.045
130.931
130.772
128.310
128.261
128.174
128.114
128.036
127.986
127.656
127.596
127.530
126.954
59.408
59.311
59.250
Ph
S
P
Ph
Ph
Ph
N
H
NH2·HCl
40000
30000
20000
10000
0
150
100
50
ppm (t1)