

SUPPORTING INFORMATION

An approach to alicyclic ring-fused xantines

Kostiantyn Liubchak*, Andrey Tolmachev, Oleksandr O. Grygorenko, and
Kostiantyn Nazarenko

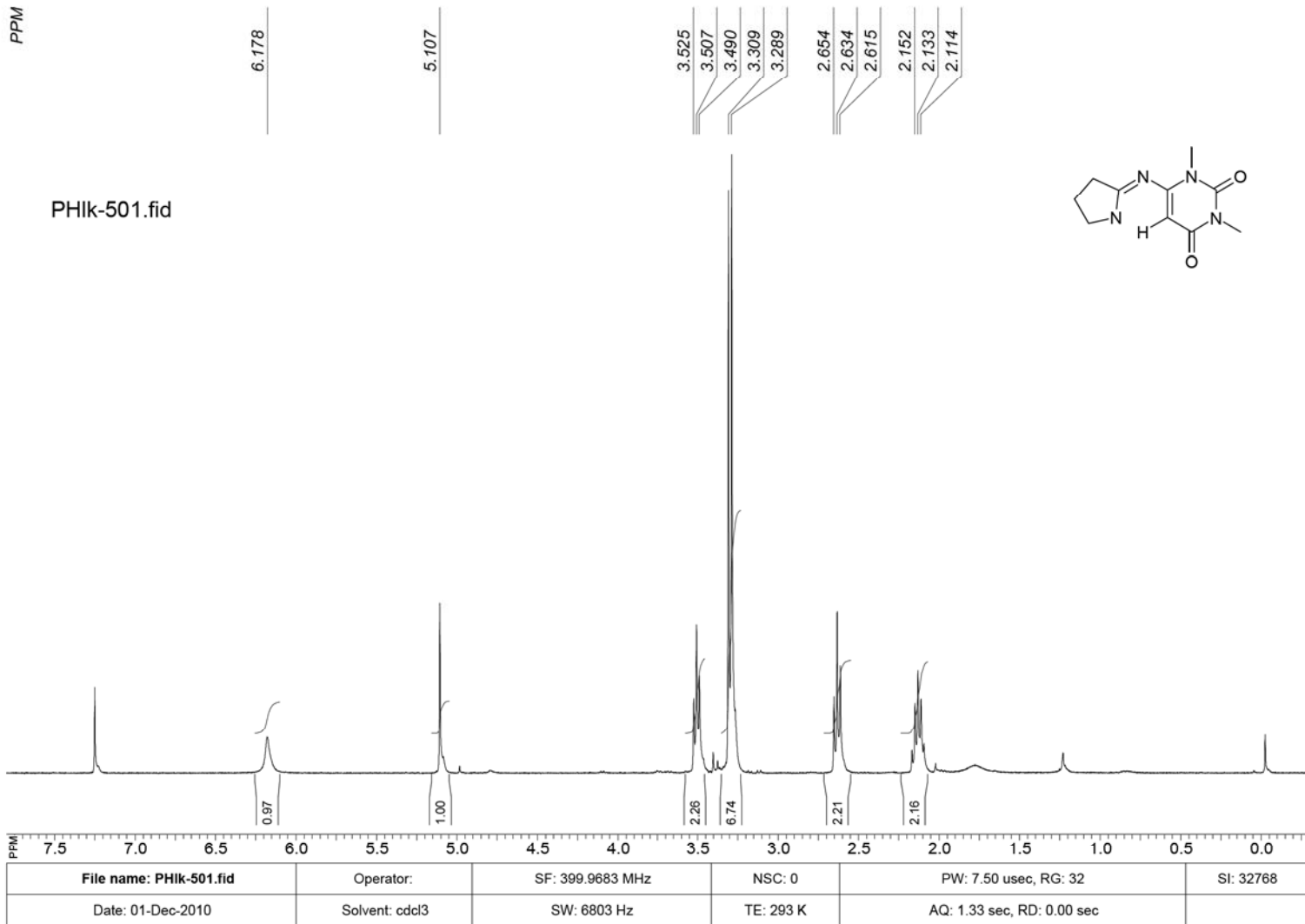
Corresponding author. Tel.: +380 50 707 12 10; e-mail: kliubchak@gmail.com

Content:

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3. Copies of ^1H and ^{13}C NMR spectra for compounds **3aa-3dc** – page S25 – S37

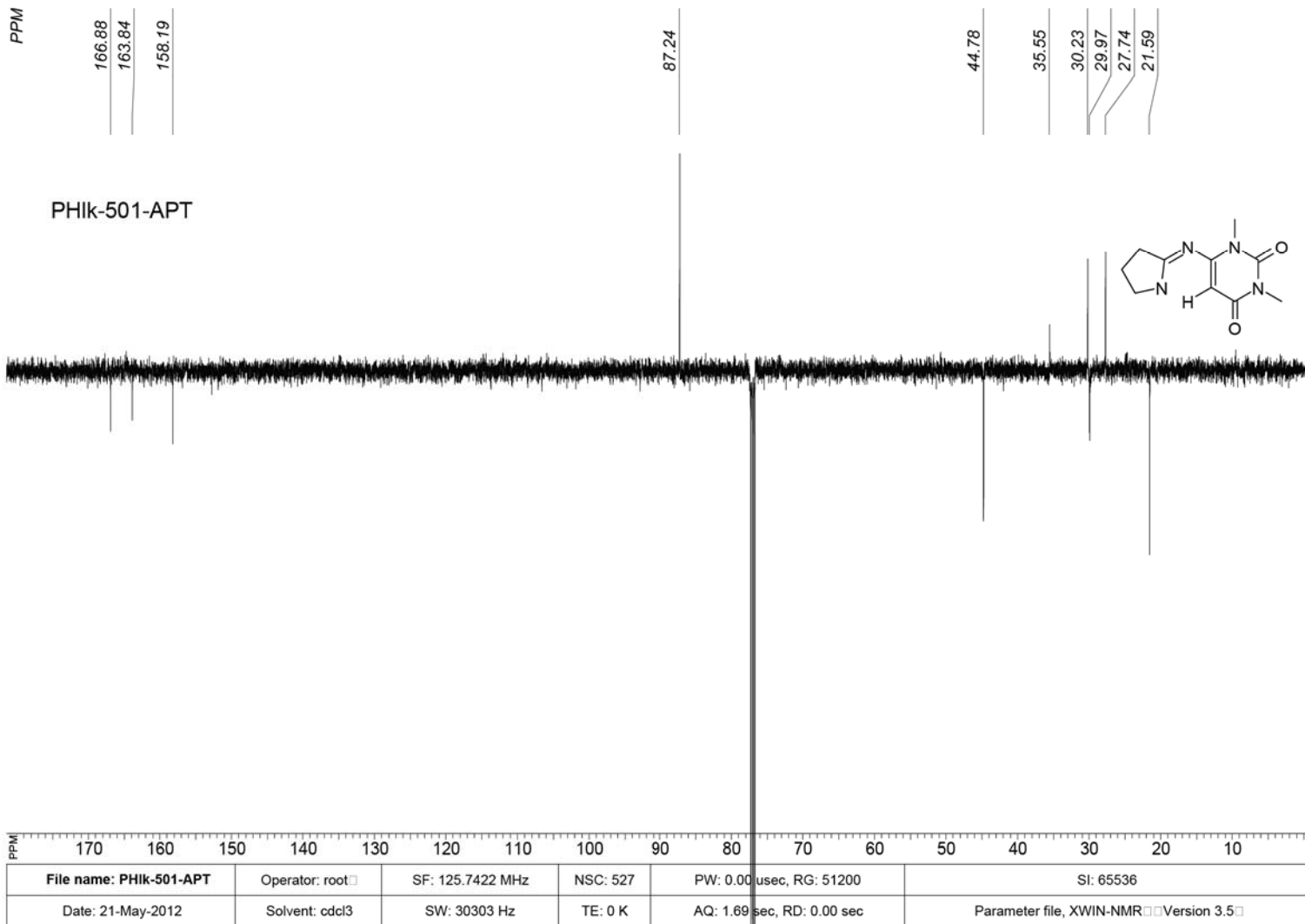
PPM

PHIk-501.fid



PPM

PHIk-501-APT



PPM

10.602

8.165

4.784

3.615

3.597

2.598

2.579

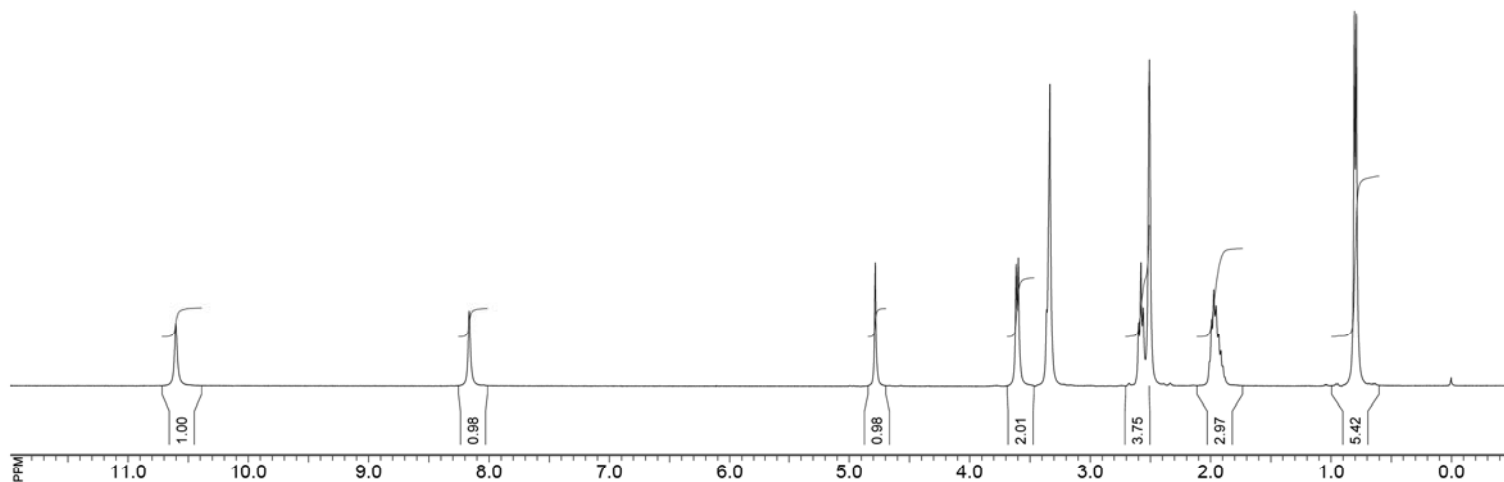
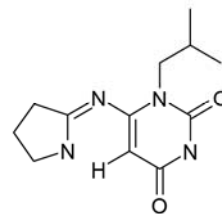
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1.974

0.807

0.790

PHIk-504.fid



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Date: 02-Feb-2011	Solvent: dms0-d6+ccl4	SW: 6803 Hz	TE: 293 K	AQ: 1.33 sec, RD: 0.00 sec	

PPM

167.72

163.75

160.35

152.35

86.76

48.36

44.67

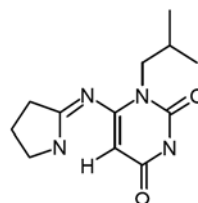
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27.73

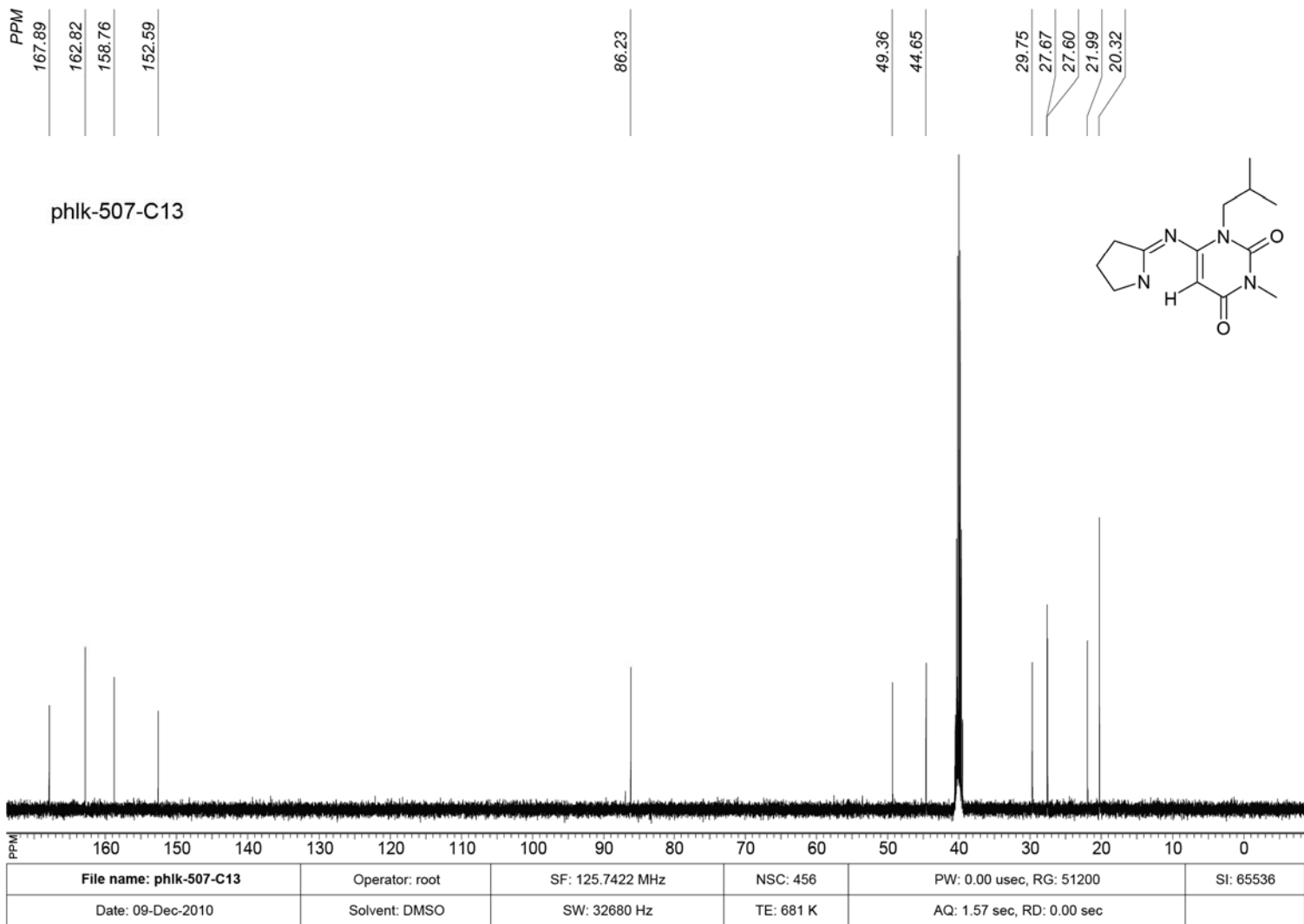
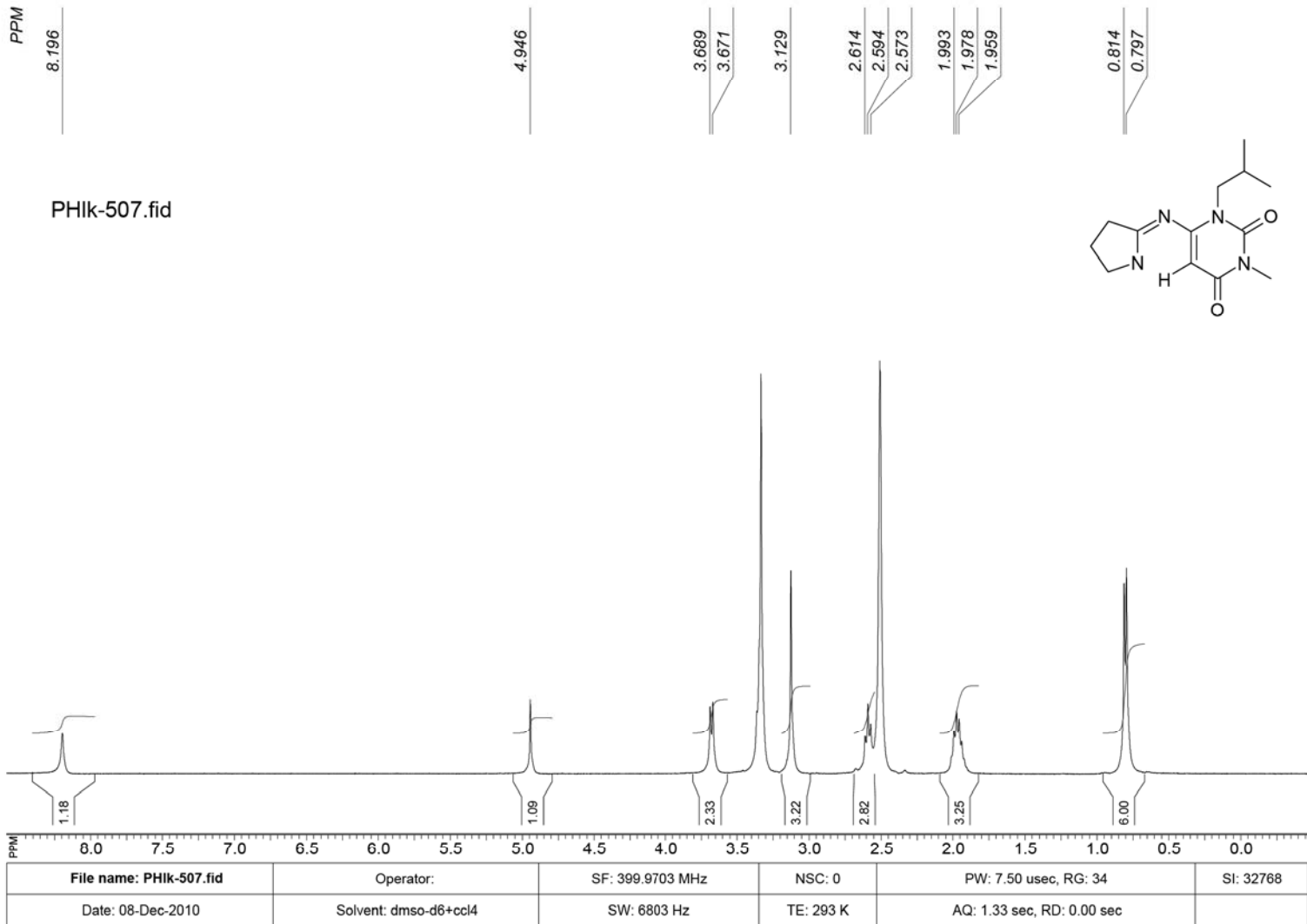
21.97

20.27

PHIk-504-APTC13



File name: PHIk-504-APTC13	Operator: root	SF: 125.7422 MHz	NSC: 116	PW: 0.00 usec, RG: 51200	SI: 65536
Date: 25-May-2012	Solvent: DMSO	SW: 30303 Hz	TE: 0 K	AQ: 1.69 sec, RD: 0.00 sec	Parameter file, XWIN-NMR Version 3.5



PPM

7.745

4.880

3.176

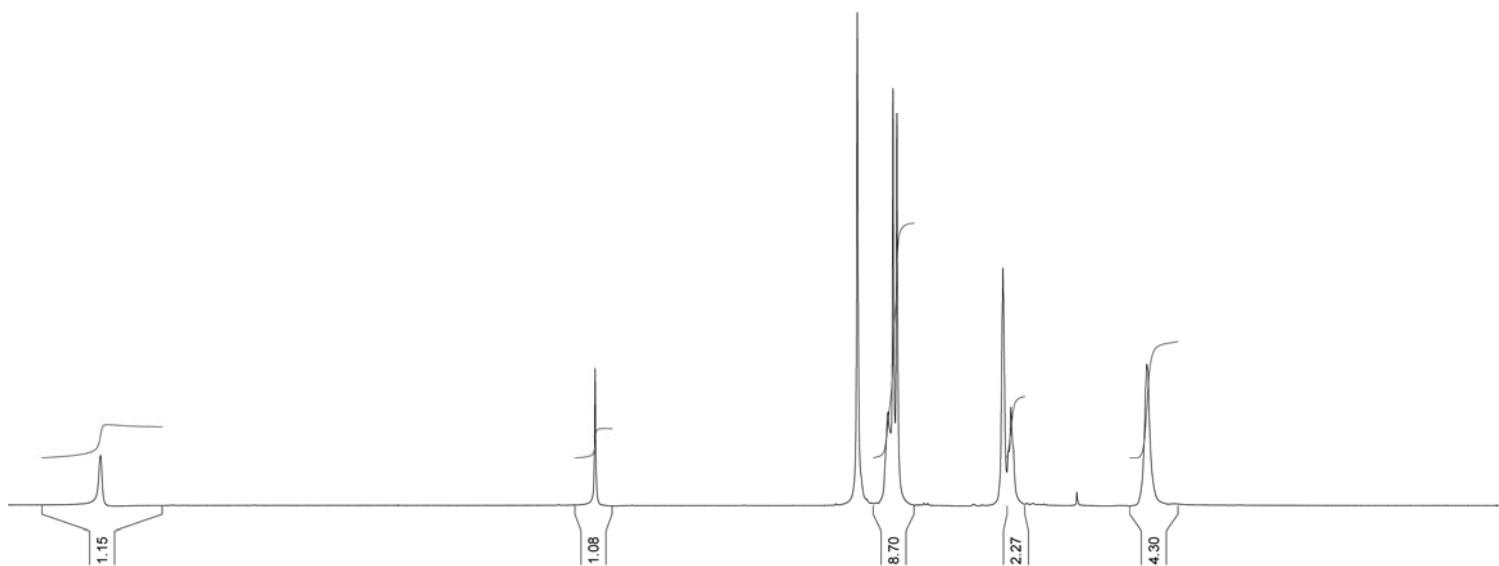
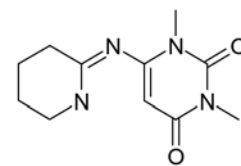
3.148

3.125

2.464

1.677

PHIk-510.fid



File name: PHIk-510.fid	Operator:	SF: 399.9703 MHz	NSC: 0	PW: 7.50 usec, RG: 22	SI: 32768
Date: 26-Jul-2011	Solvent: dms0-d6+ccl4	SW: 6803 Hz	TE: 293 K	AQ: 1.33 sec, RD: 0.00 sec	

PPM

162.78

161.40

157.55

152.78

107.36

86.67

41.60

30.12

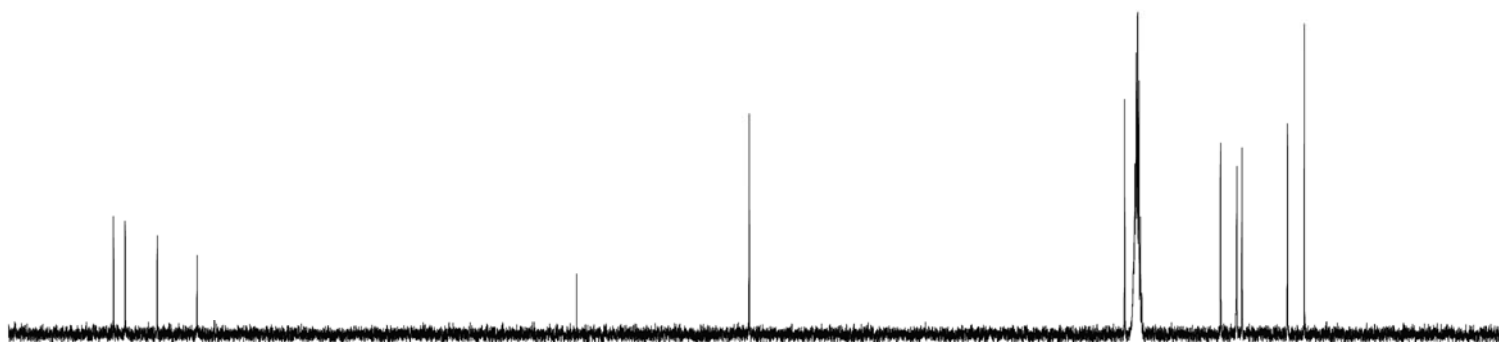
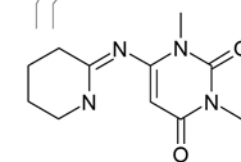
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27.56

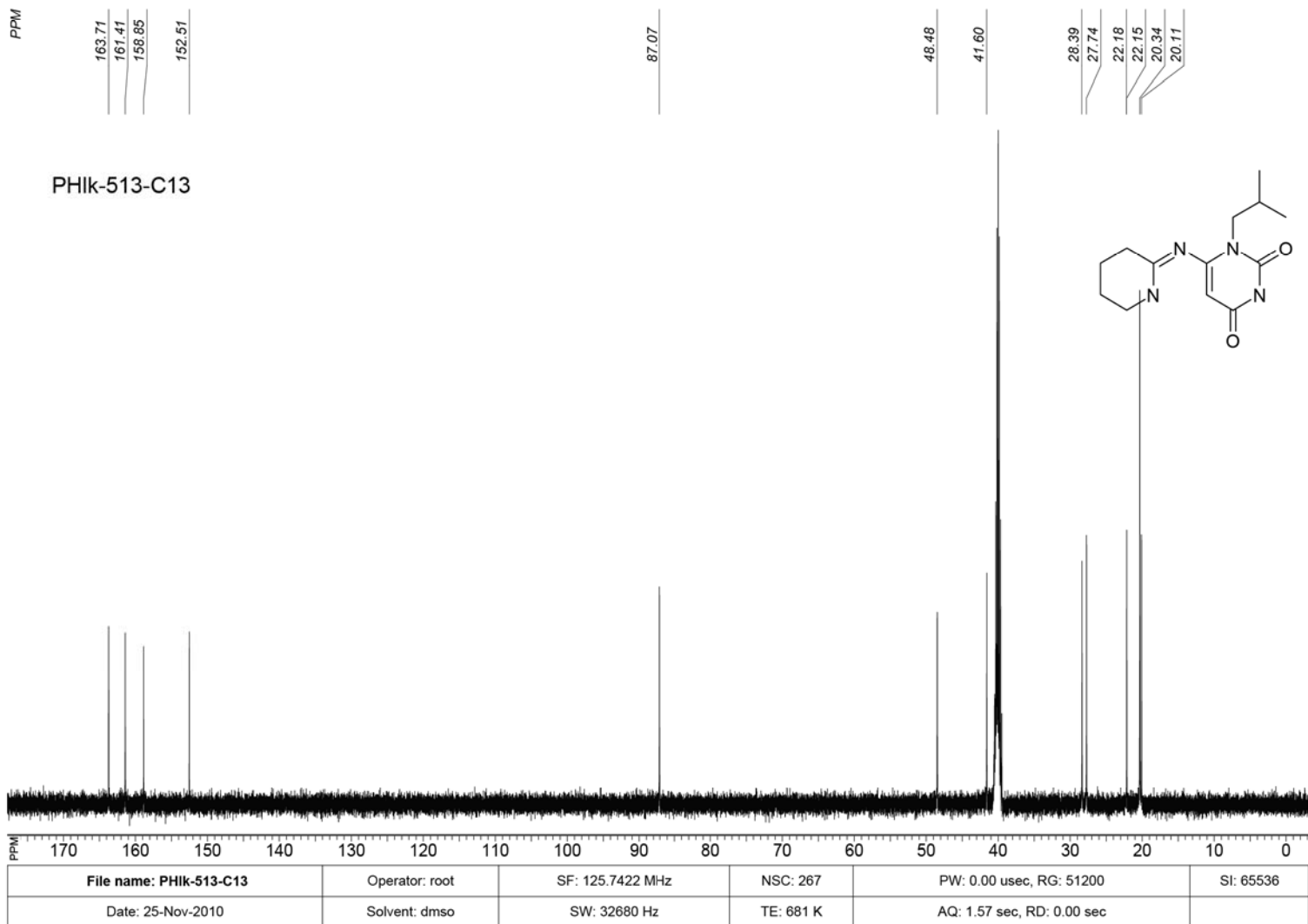
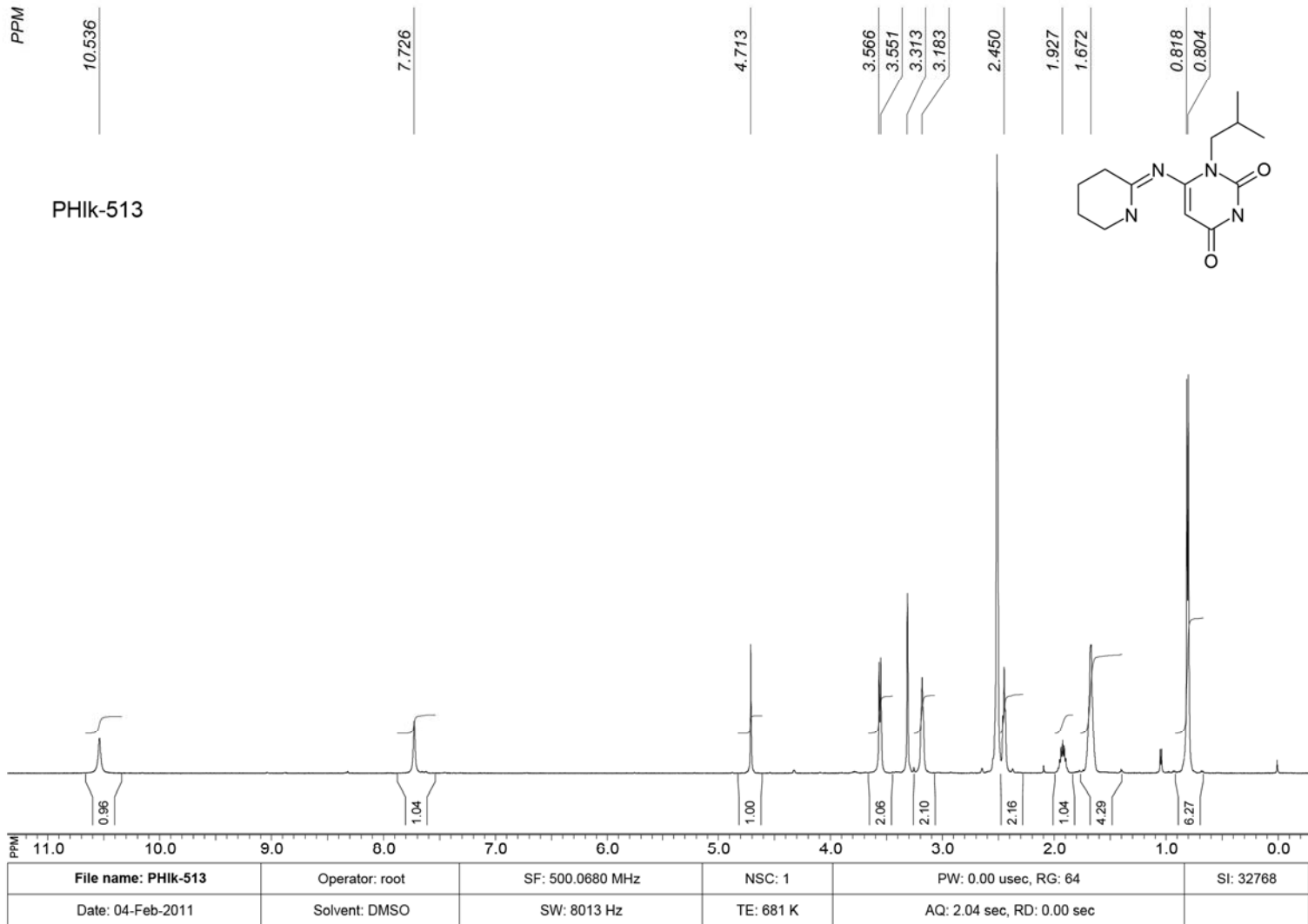
22.10

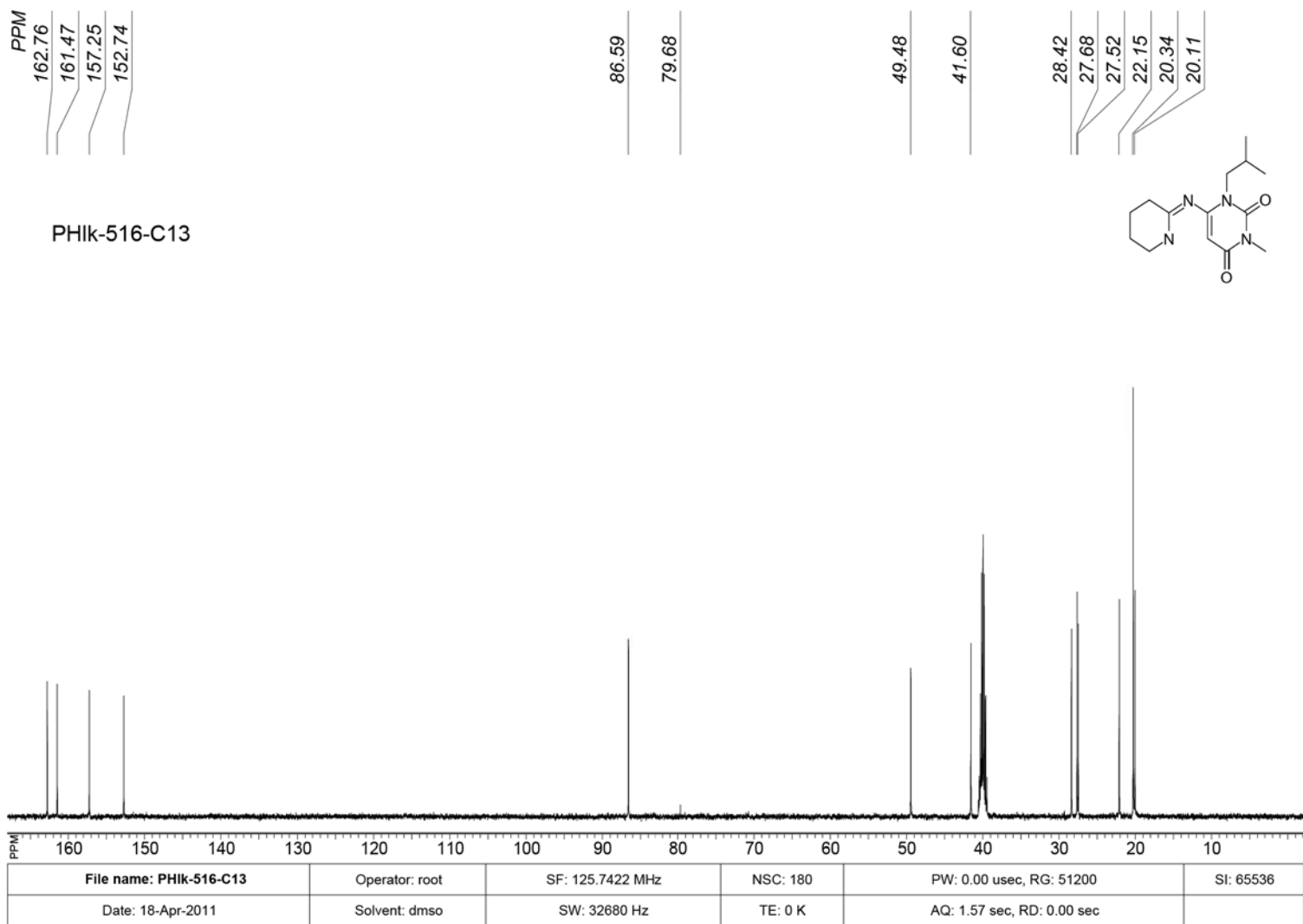
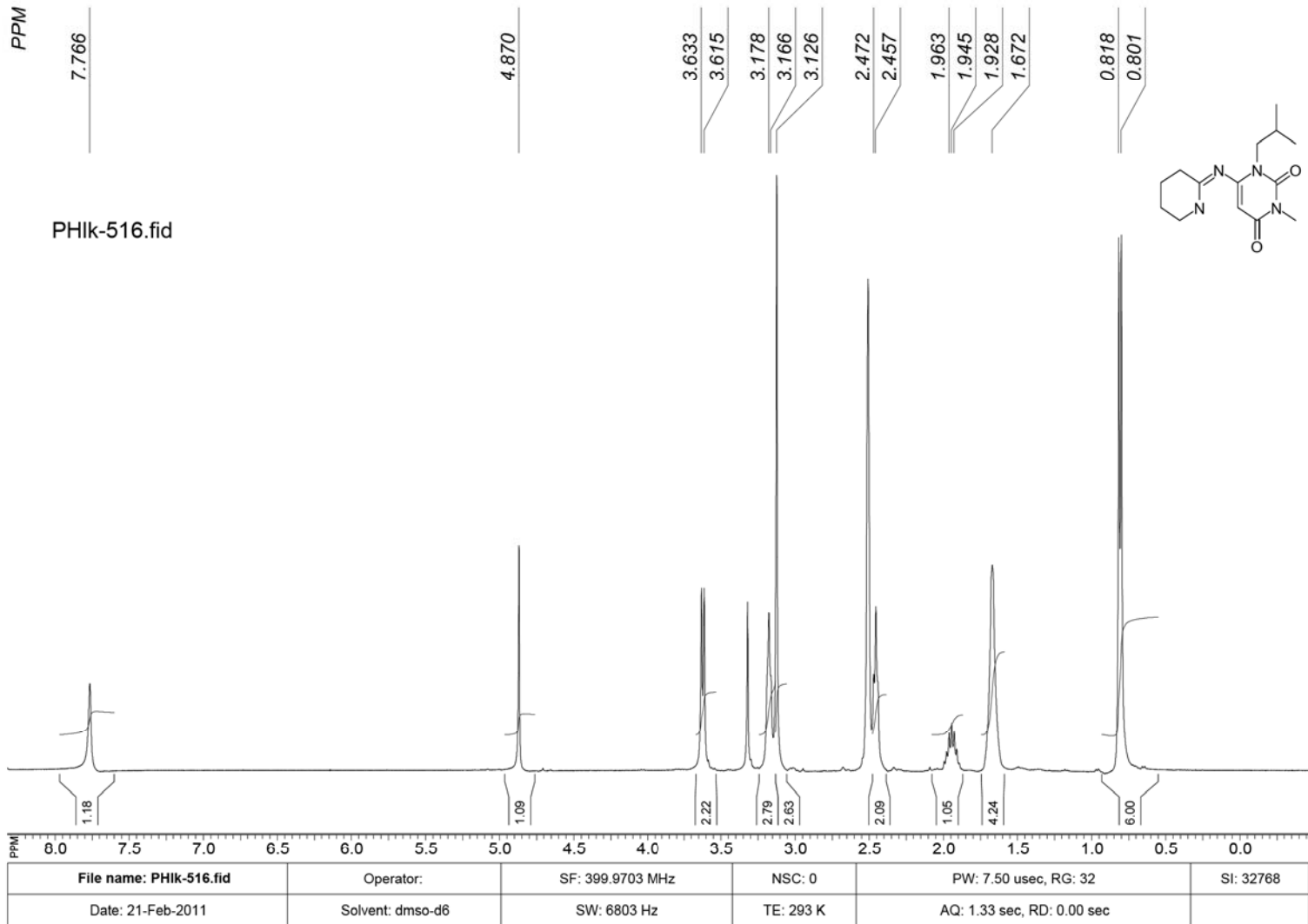
20.09

PHIk-510-C13



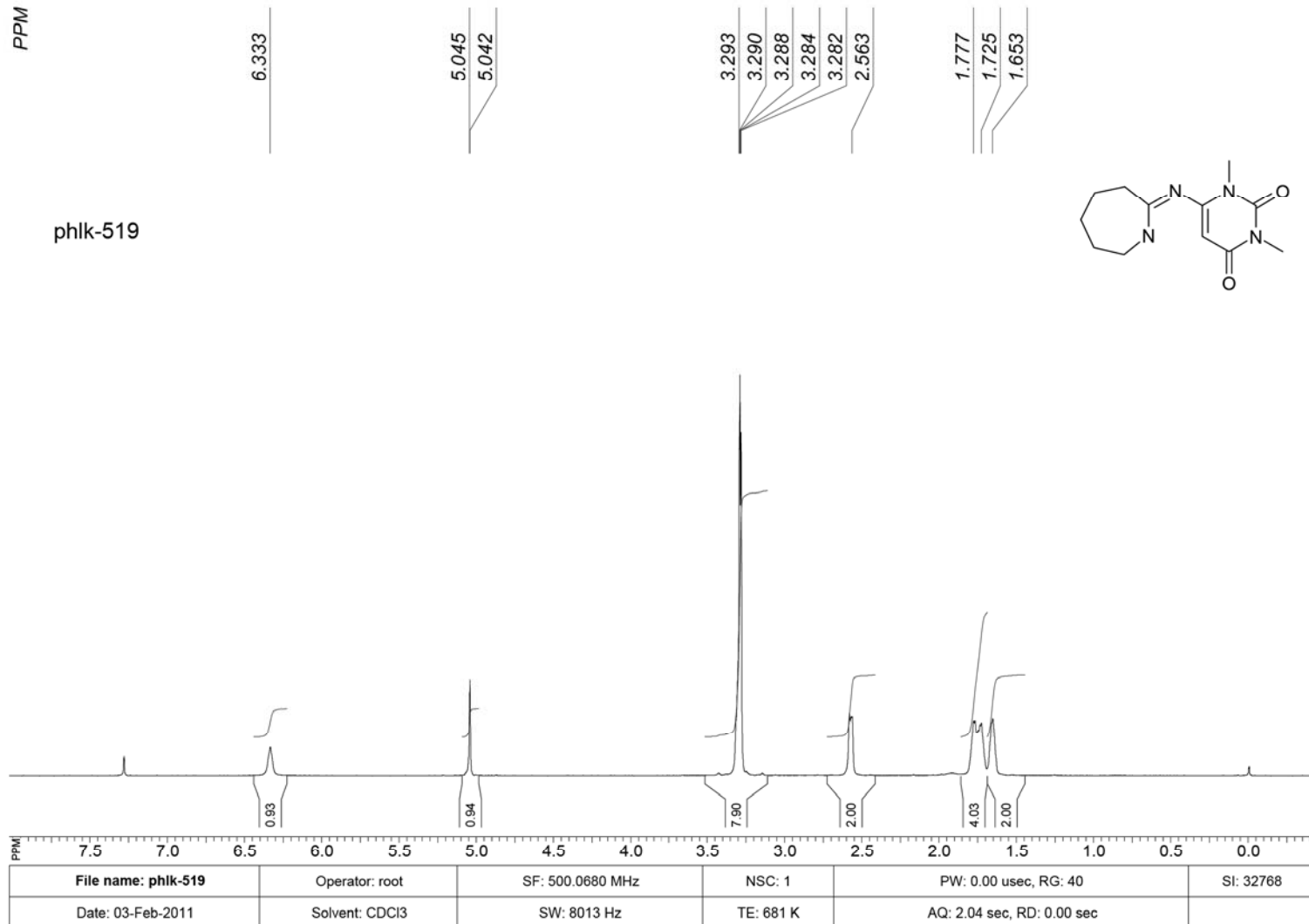
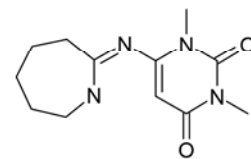
File name: PHIk-510-C13	Operator: root	SF: 125.7422 MHz	NSC: 140	PW: 0.00 usec, RG: 51200	SI: 65536
Date: 18-Apr-2011	Solvent: DMSO	SW: 32680 Hz	TE: 0 K	AQ: 1.57 sec, RD: 0.00 sec	





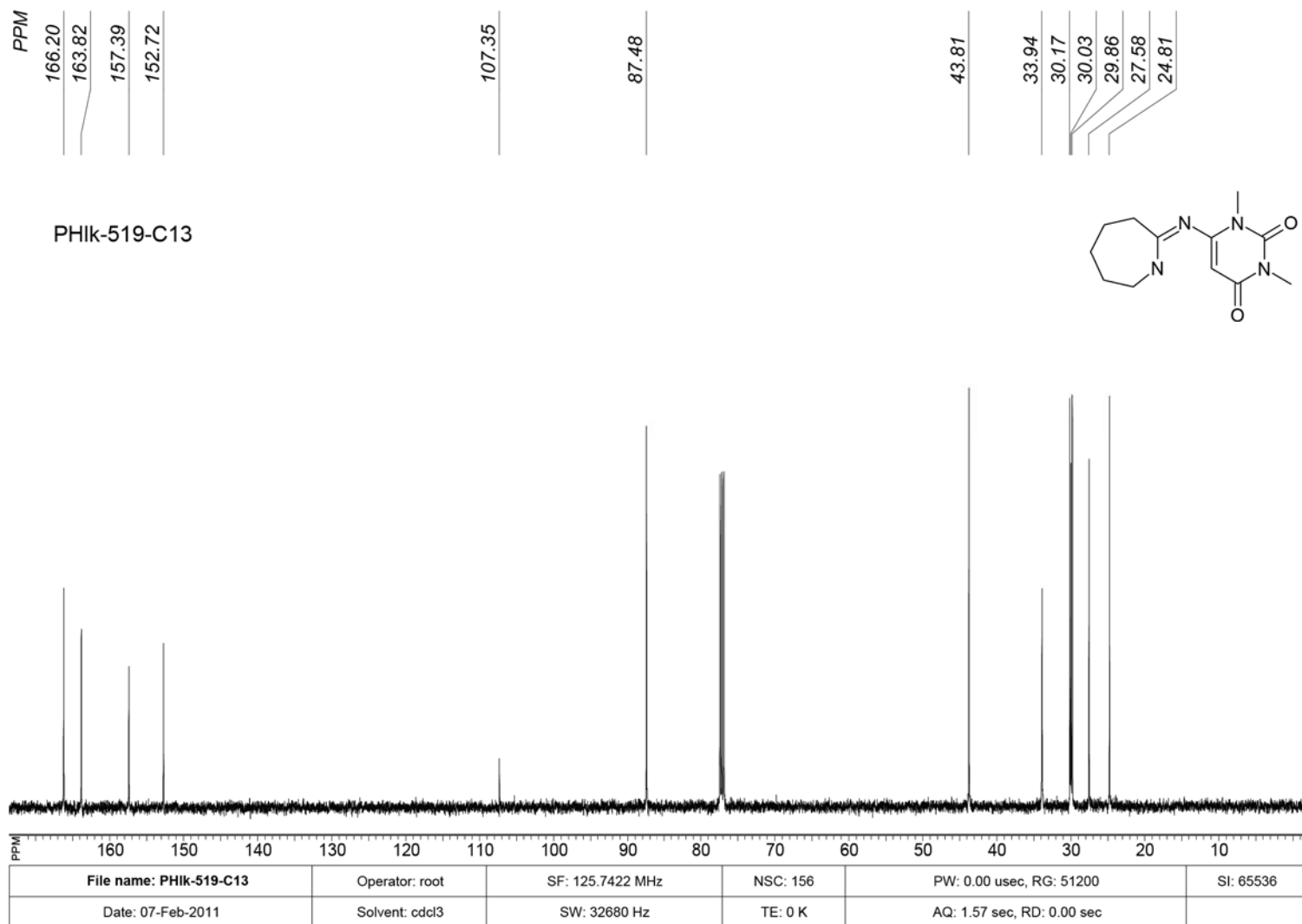
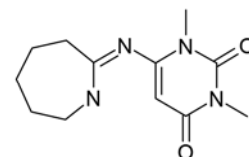
PPM

phlk-519



PPM

PHlk-519-C13



PPM

8.352

6.125

4.935

3.681

3.663

3.290

2.553

1.984

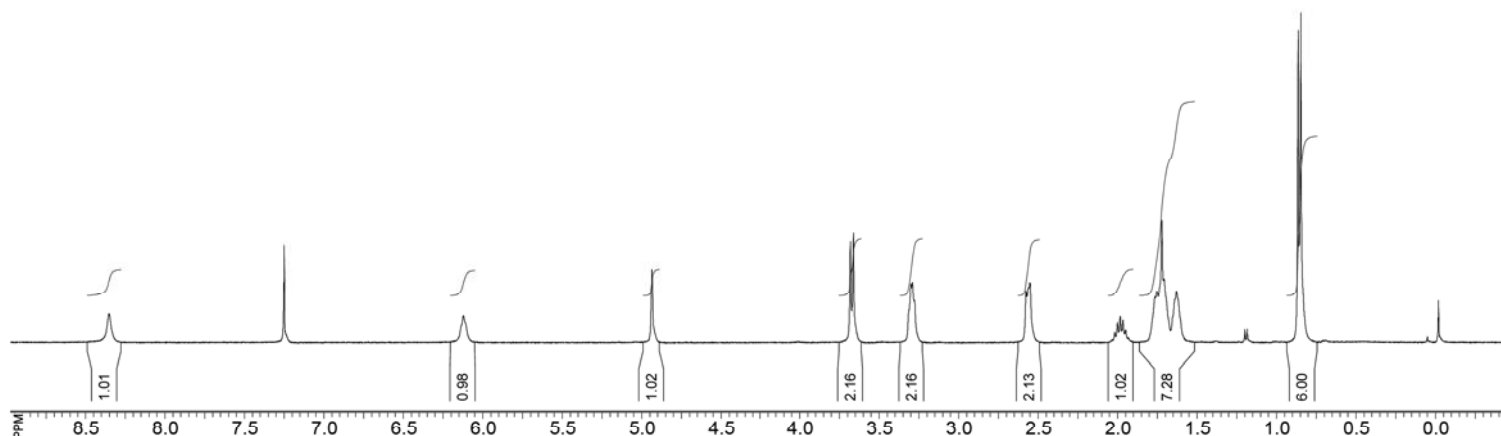
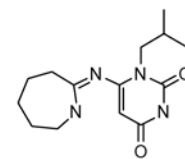
1.722

1.631

0.864

0.848

PHIk-522.fid



File name: PHIk-522.fid	Operator:	SF: 399.9683 MHz	NSC: 0	PW: 7.50 usec, RG: 32	SI: 32768
Date: 01-Feb-2011	Solvent: cdcl3	SW: 6803 Hz	TE: 293 K	AQ: 1.33 sec, RD: 0.00 sec	

PPM

156.65

155.22

151.61

147.38

107.19

45.91

30.80

29.62

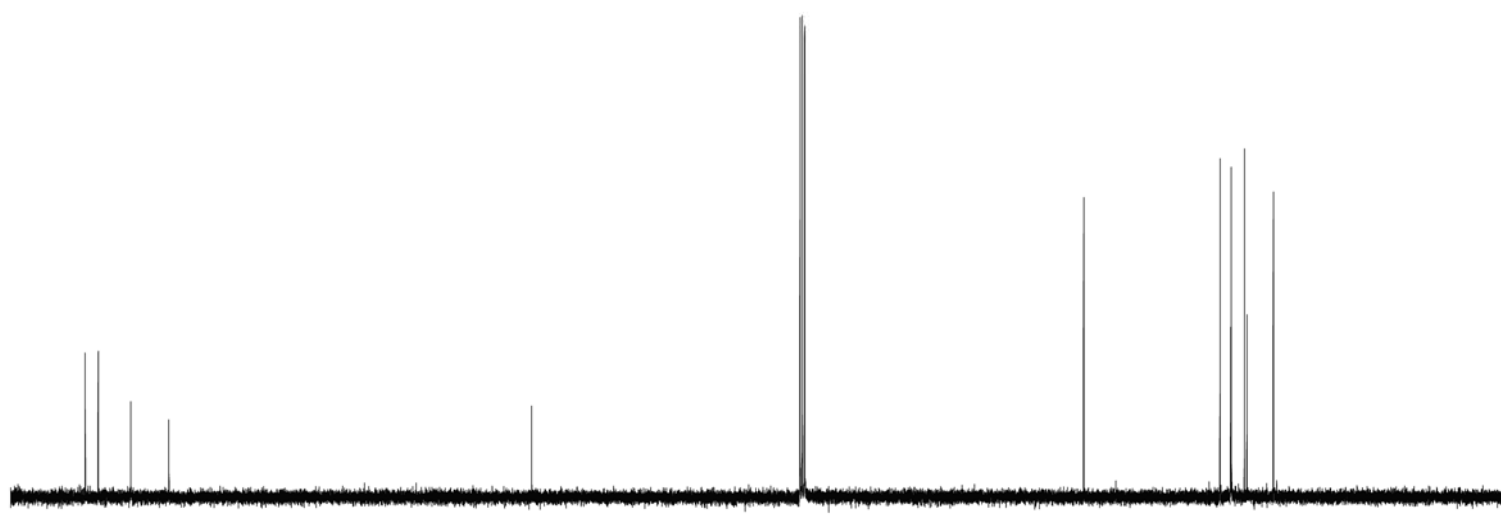
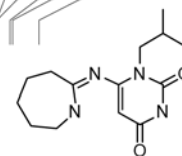
29.55

28.10

27.81

24.89

phIk-522-C13



File name: phIk-522-C13	Operator: root	SF: 125.7422 MHz	NSC: 337	PW: 0.00 usec, RG: 51200	SI: 65536
Date: 06-Oct-2011	Solvent: dmso	SW: 32680 Hz	TE: 0 K	AQ: 1.57 sec, RD: 0.00 sec	

PPM

7.712

4.773

3.619

3.603

3.205

3.133

2.514

1.950

1.670

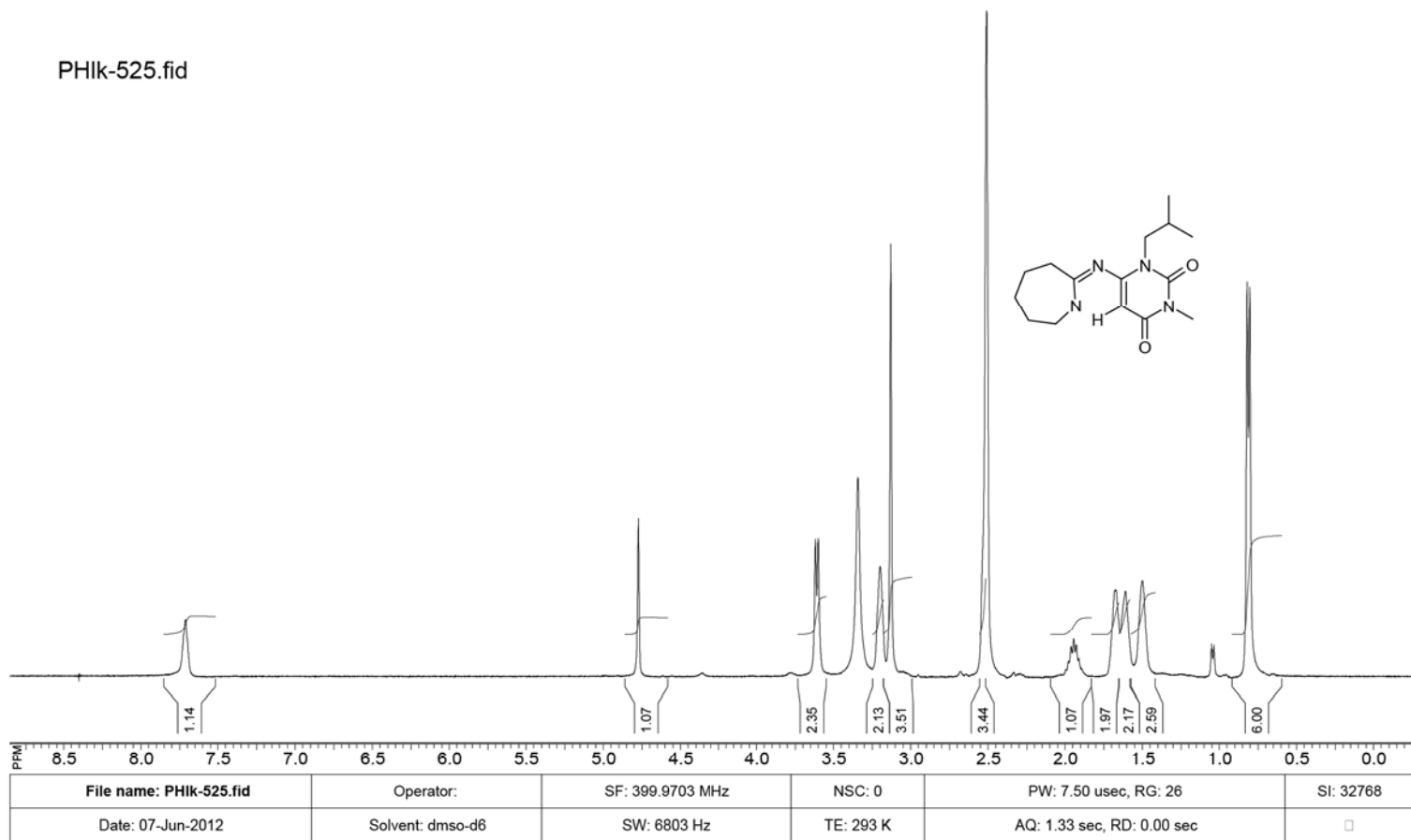
1.615

1.500

0.821

0.805

PHIk-525.fid



PPM

166.72

162.84

157.62

152.75

86.80

49.60

43.14

32.89

30.02

29.88

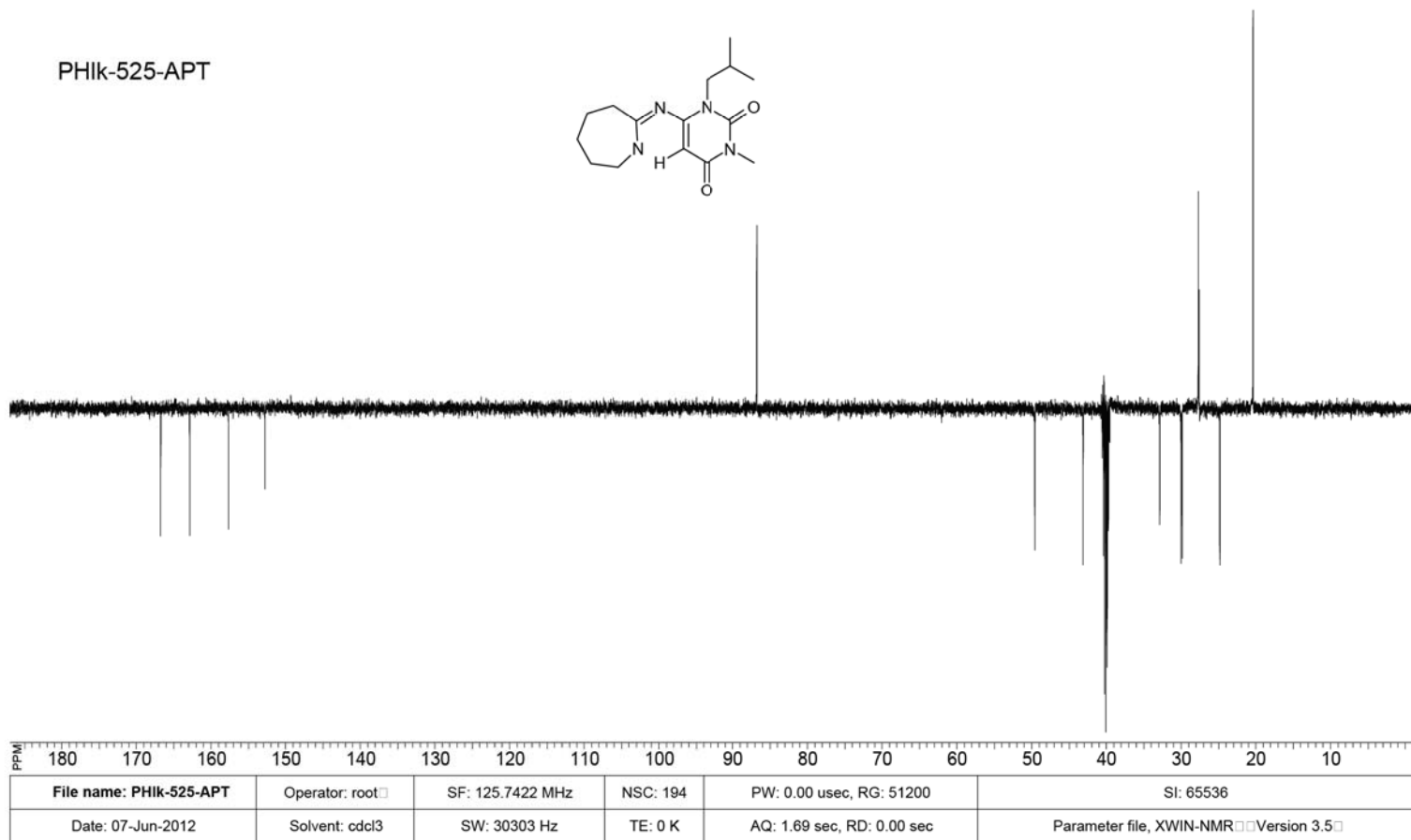
27.72

27.62

24.84

20.40

PHIk-525-APT



PPM

7,267

4,828

3,325

3,270

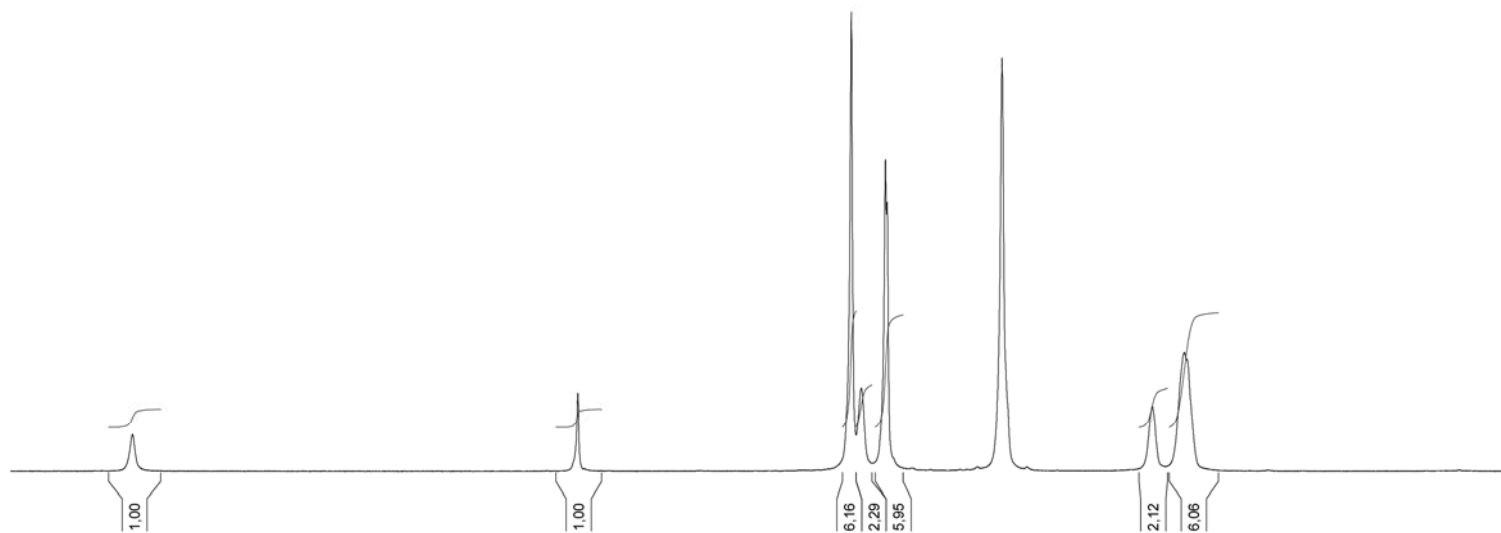
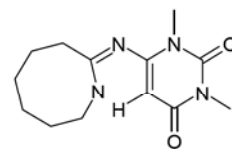
3,138

3,137

1,676

1,498

PHIk-528



File name: PHIk-528	Operator: root	SF: 500,0000 MHz	NSC: 1	PW: 0,00 usec, RG: 32	SI: 32768
Date: 20-январь-2011	Solvent: DMSO	SW: 8012 Hz	TE: 0 K	AQ: 2,04 sec, RD: 0,00 sec	

PPM

164,15

162,20

157,25

151,99

85,49

40,13

30,56

28,47

28,09

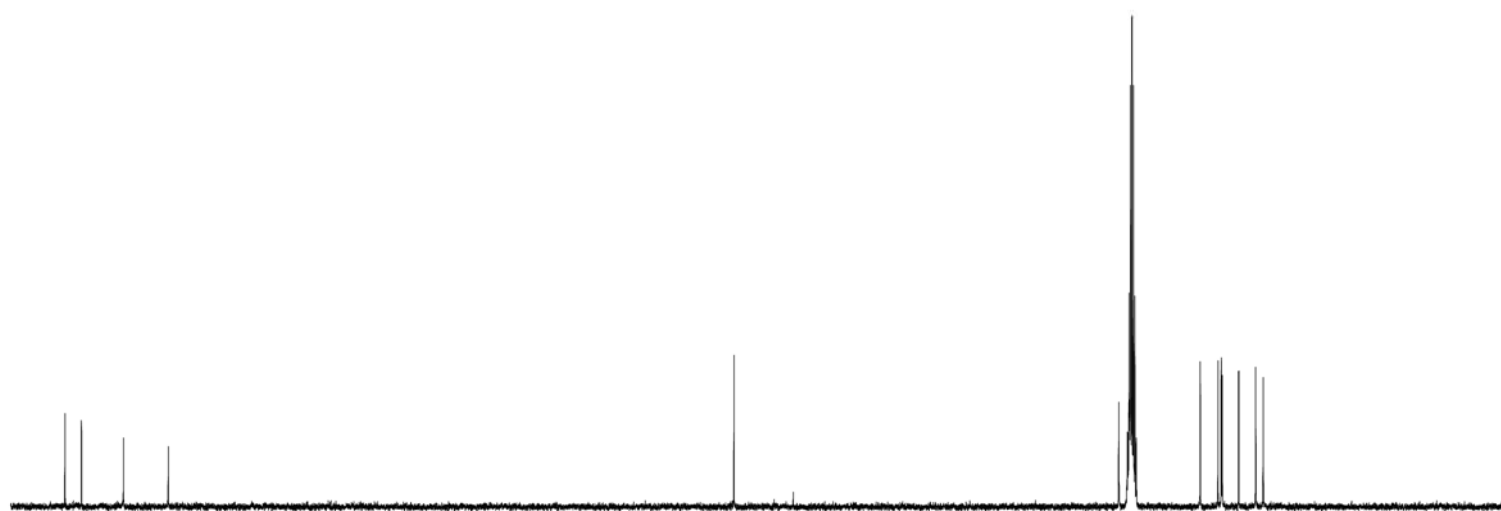
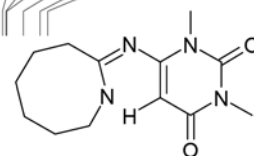
27,97

26,03

24,04

23,15

PHIk-528-C13



File name: PHIk-528-C13	Operator: root	SF: 125,0000 MHz	NSC: 243	PW: 0,00 usec, RG: 51200	SI: 65536
Date: 22-январь-2011	Solvent: DMSO	SW: 32679 Hz	TE: 0 K	AQ: 1,57 sec, RD: 0,00 sec	

PPM

10,057

6,794

4,129

2,967

2,951

2,714

1,935

1,374

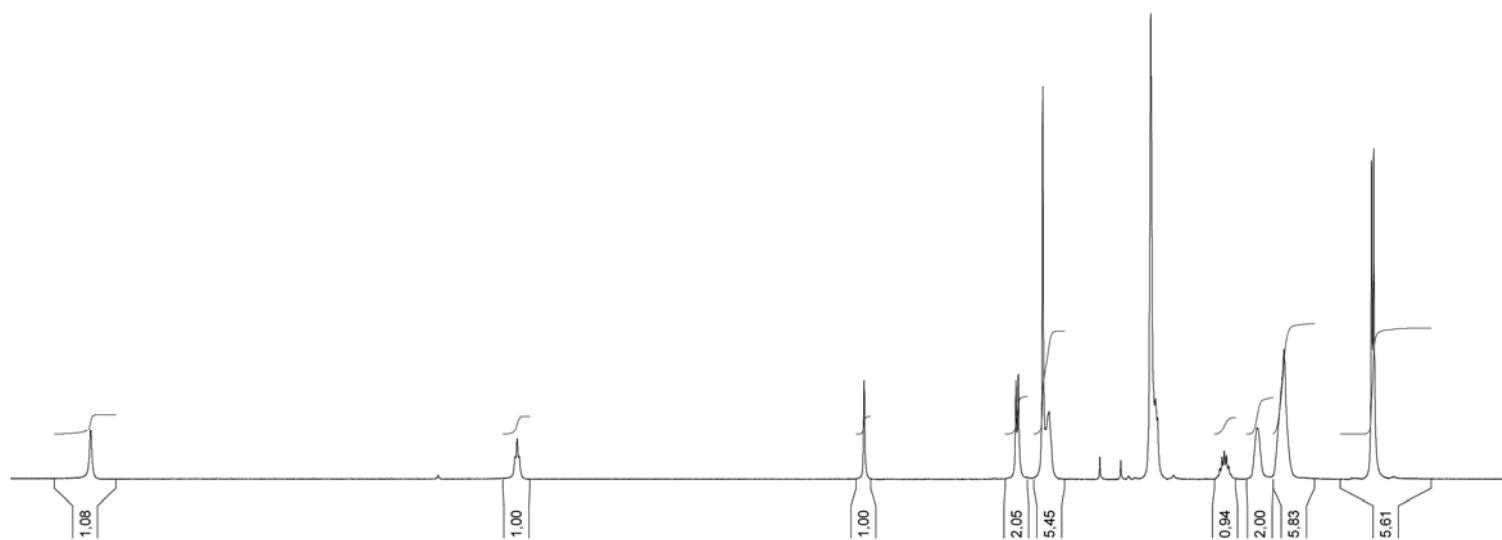
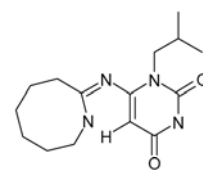
1,122

0,917

0,247

0,231

PHIk-531.fid



File name: PHIk-531.fid	Operator:	SF: 399,0000 MHz	NSC: 0	PW: 7,00 usec, RG: 28	SI: 32768
Date: 08-дек-2010	Solvent: dms0-d6+ccl4	SW: 6802 Hz	TE: 293 K	AQ: 1,33 sec, RD: 0,00 sec	

PPM

164,06

163,18

158,41

151,78

85,64

47,18

40,24

30,45

28,92

28,13

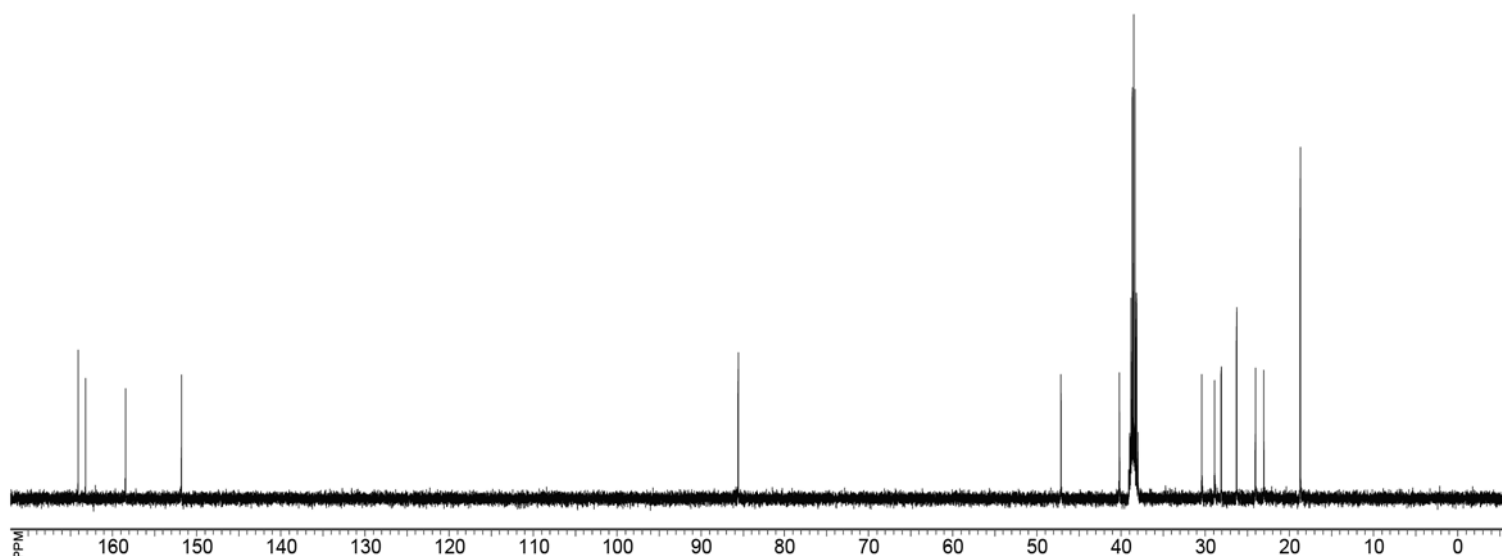
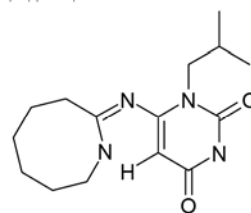
26,31

24,06

23,08

18,74

PHIk-531-C13



File name: PHIk-531-C13	Operator: root	SF: 125,0000 MHz	NSC: 384	PW: 0,00 usec, RG: 51200	SI: 65536
Date: 10-дек-2010	Solvent: DMSO	SW: 32679 Hz	TE: 0 K	AQ: 1,57 sec, RD: 0,00 sec	

PPM

5.971

5.111

3.734

3.719

3.389

3.306

2.521

2.038

1.886

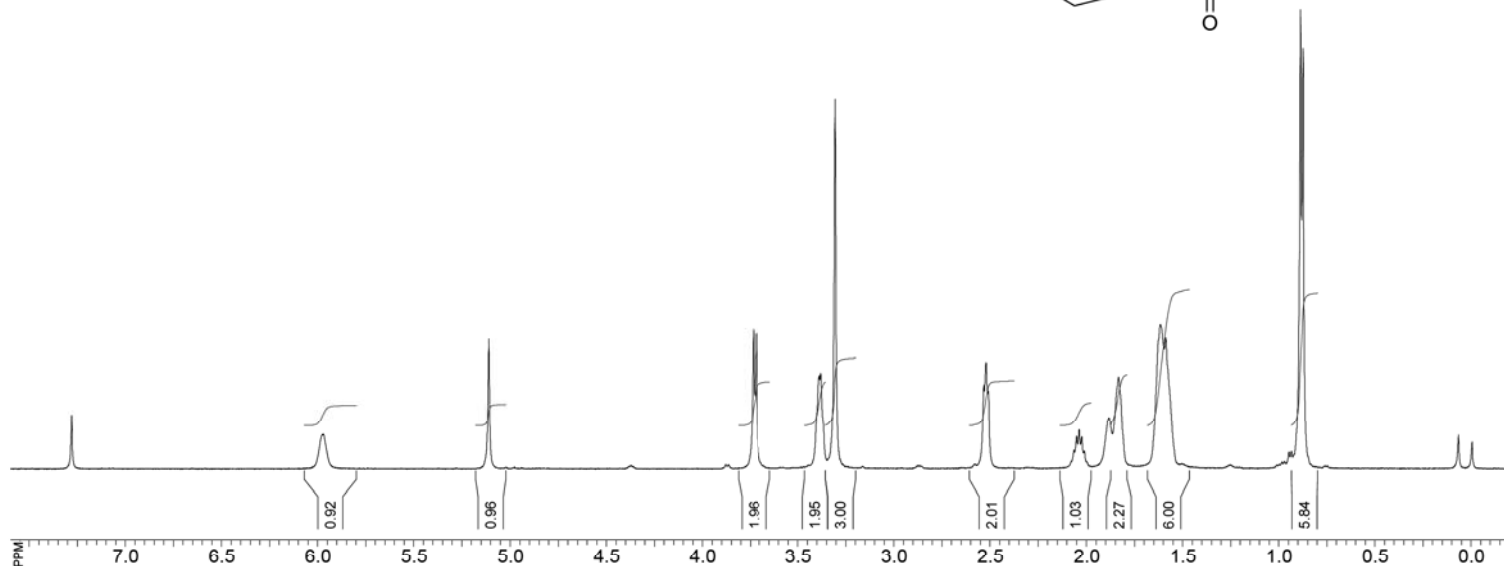
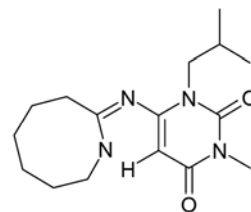
1.834

1.615

0.888

0.874

PHIk-534



File name: PHIk-534	Operator: root	SF: 500.0680 MHz	NSC: 1	PW: 0.00 usec, RG: 40	SI: 32768
Date: 28-Jan-2011	Solvent: CDCl3	SW: 8013 Hz	TE: 680 K	AQ: 2.04 sec, RD: 0.00 sec	

PPM

164.76

163.93

157.30

152.87

86.83

50.11

42.11

32.07

29.44

27.83

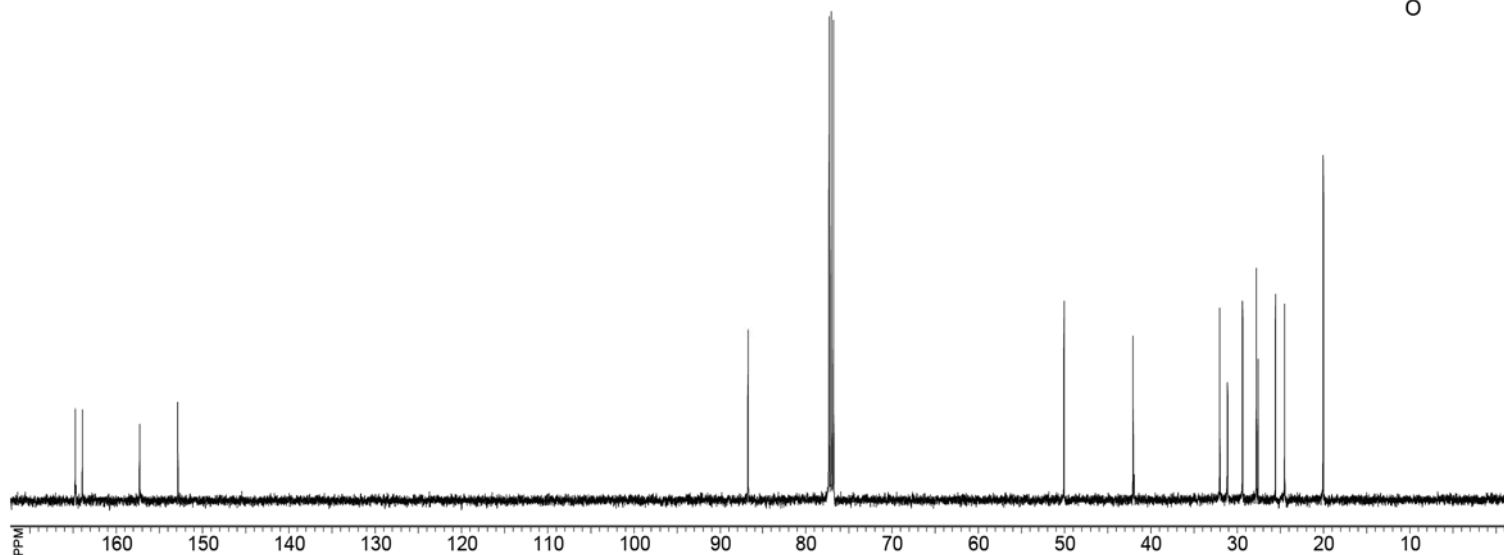
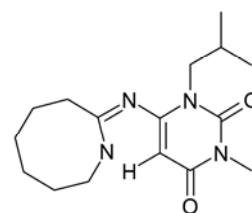
27.64

25.62

24.56

20.08

PHIk-534-C13

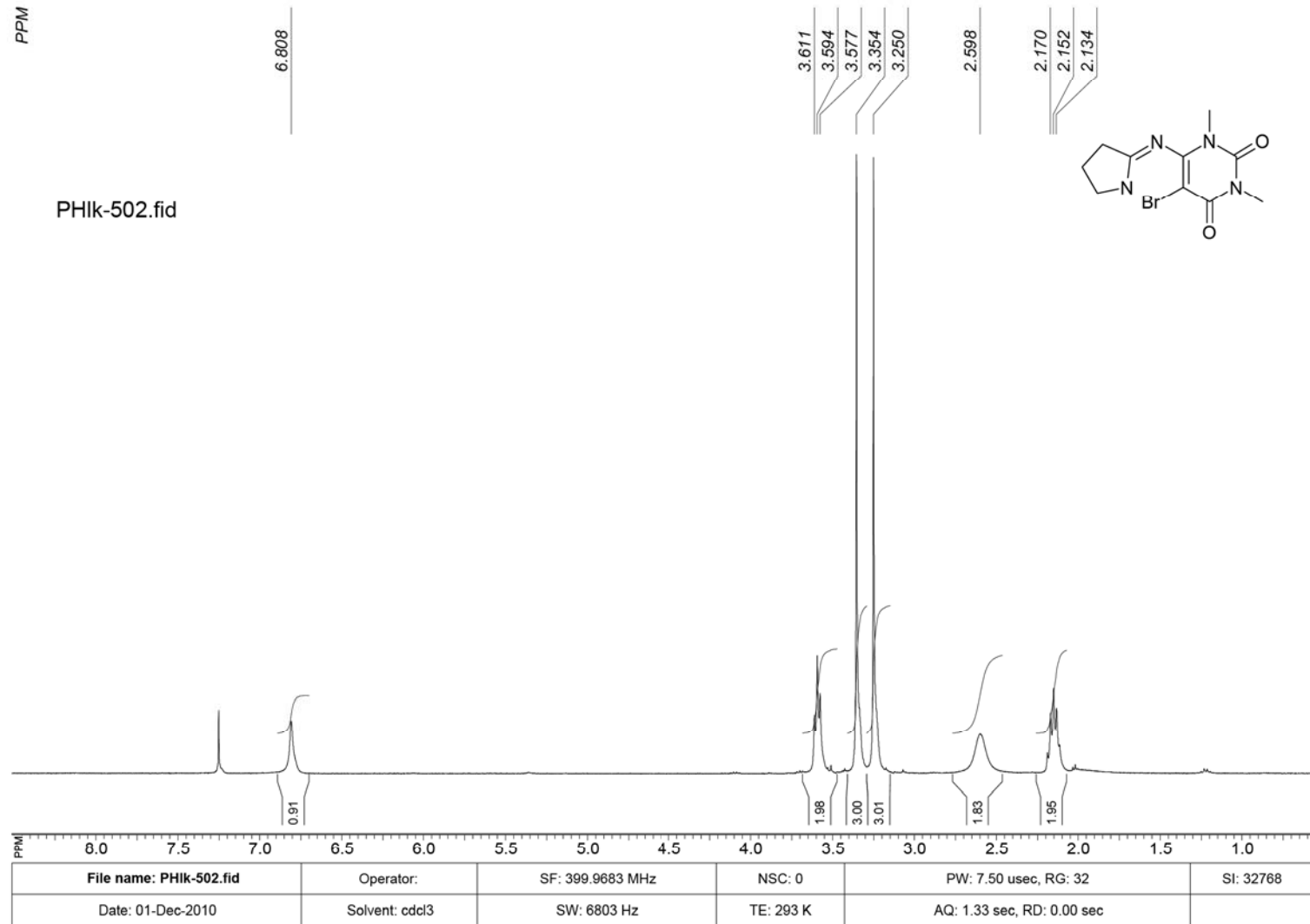


File name: PHIk-534-C13	Operator: root	SF: 125.7422 MHz	NSC: 185	PW: 0.00 usec, RG: 51200	SI: 65536
Date: 28-Jan-2011	Solvent: dmsO	SW: 32680 Hz	TE: 681 K	AQ: 1.57 sec, RD: 0.00 sec	

S13

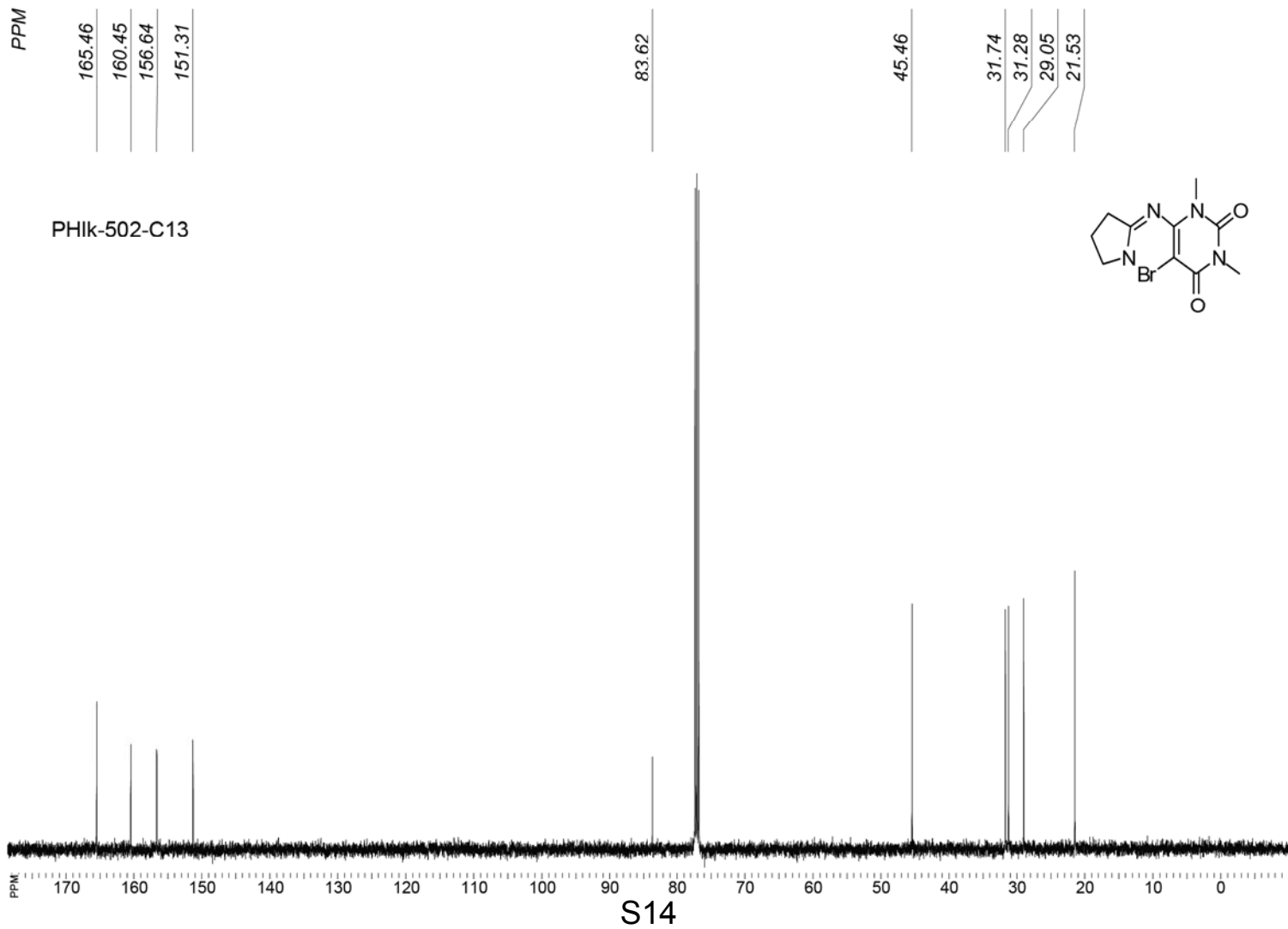
PPM

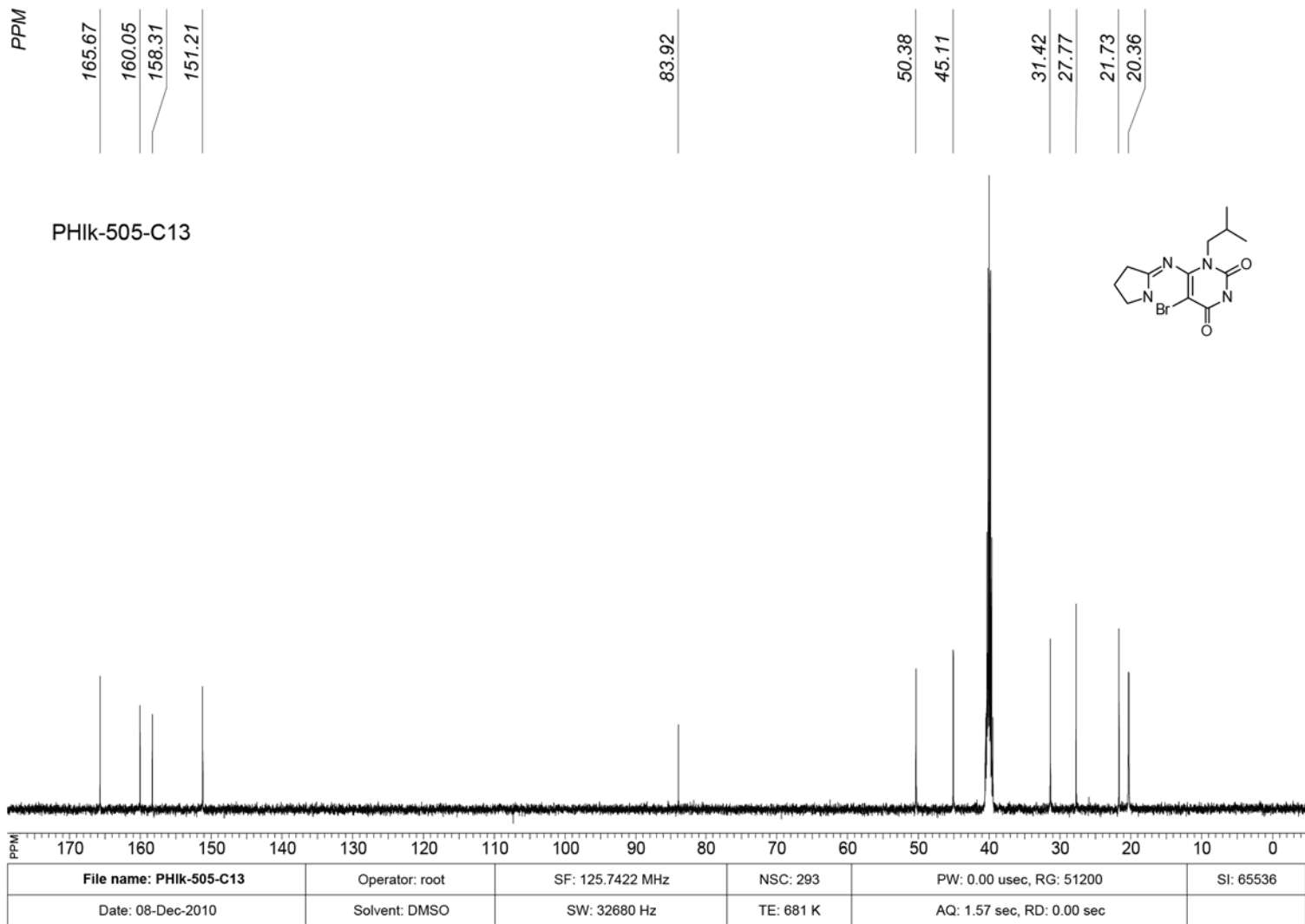
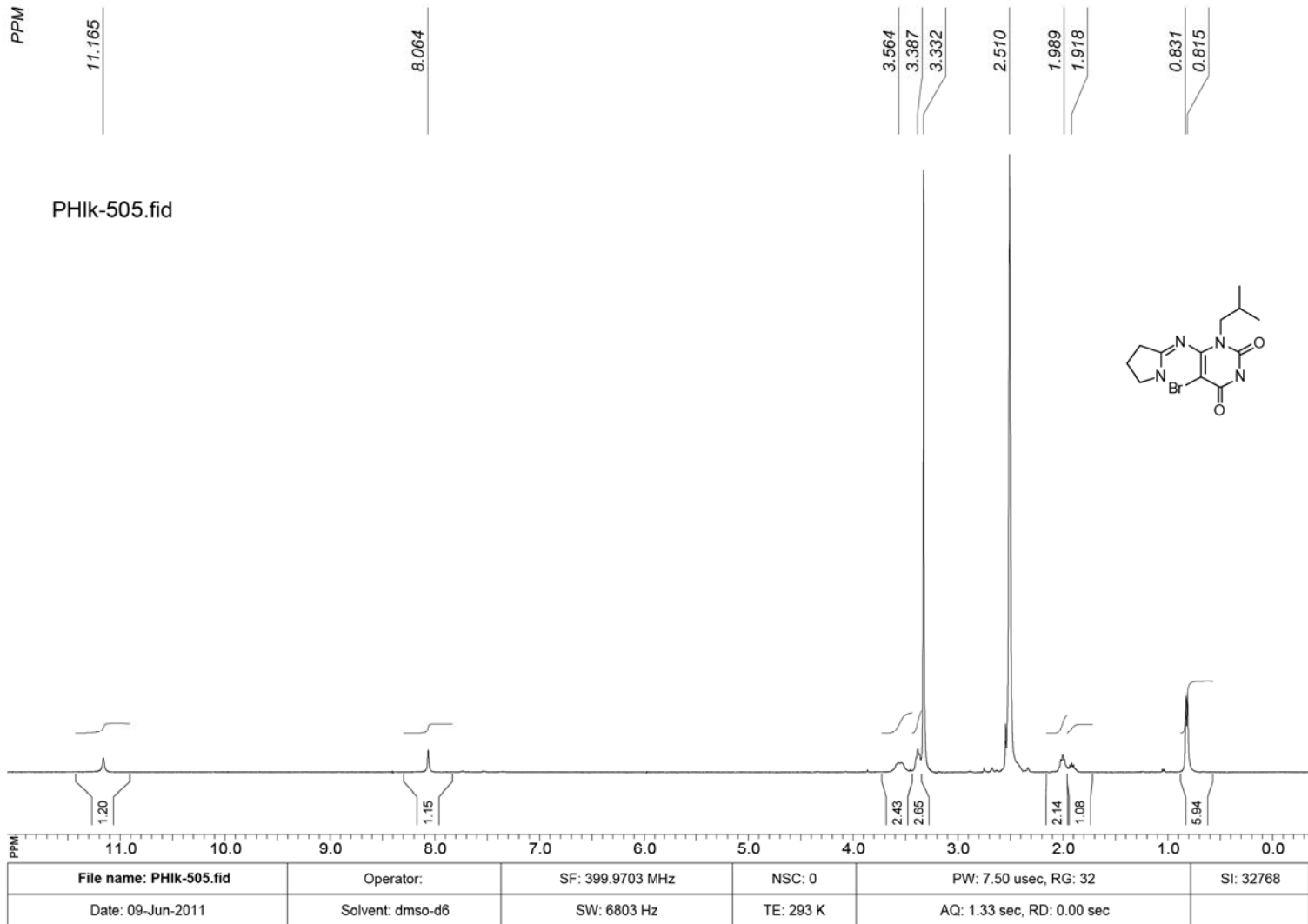
PHIk-502.fid



PPM

PHIk-502-C13





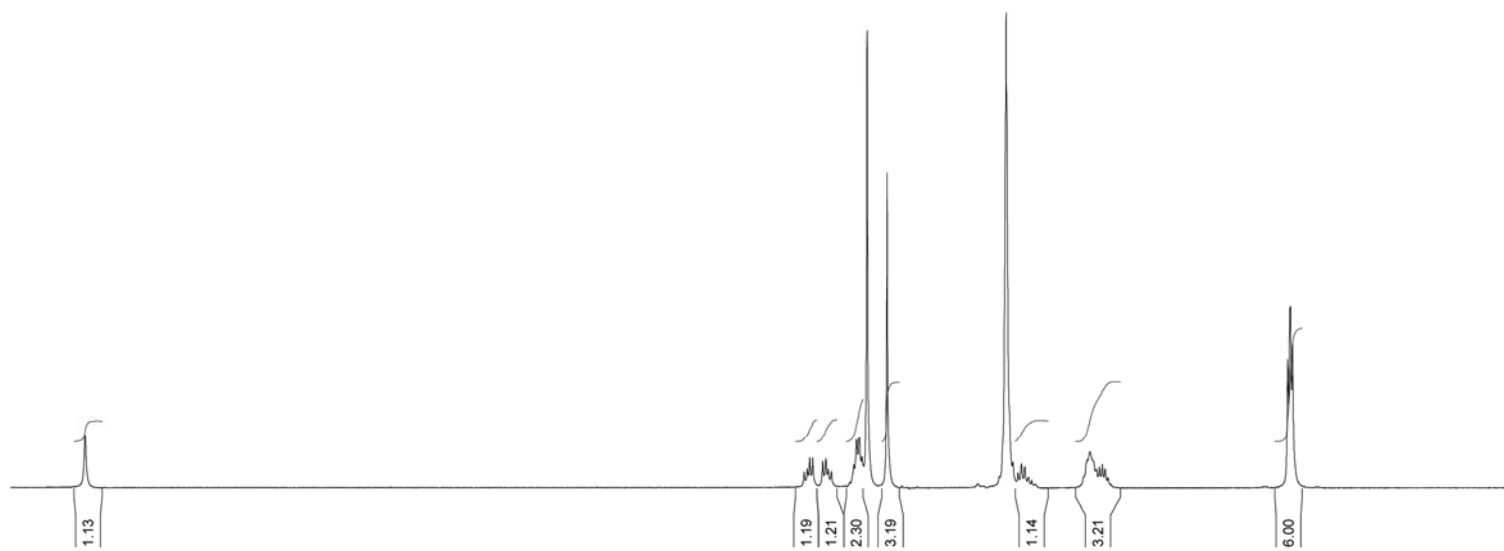
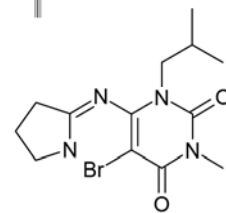
PPM

7.981

3.708
3.690
3.676
3.658
3.597
3.581
3.398
3.381
3.217
2.419
2.400
2.012
1.946
1.926

0.840
0.828
0.824
0.812

PHIk-508.fid



File name: PHIk-508.fid	Operator:	SF: 399.9703 MHz	NSC: 0	PW: 7.50 usec, RG: 34	SI: 32768
Date: 08-Dec-2010	Solvent: dms0-d6+ccl4	SW: 6803 Hz	TE: 293 K	AQ: 1.33 sec, RD: 0.00 sec	

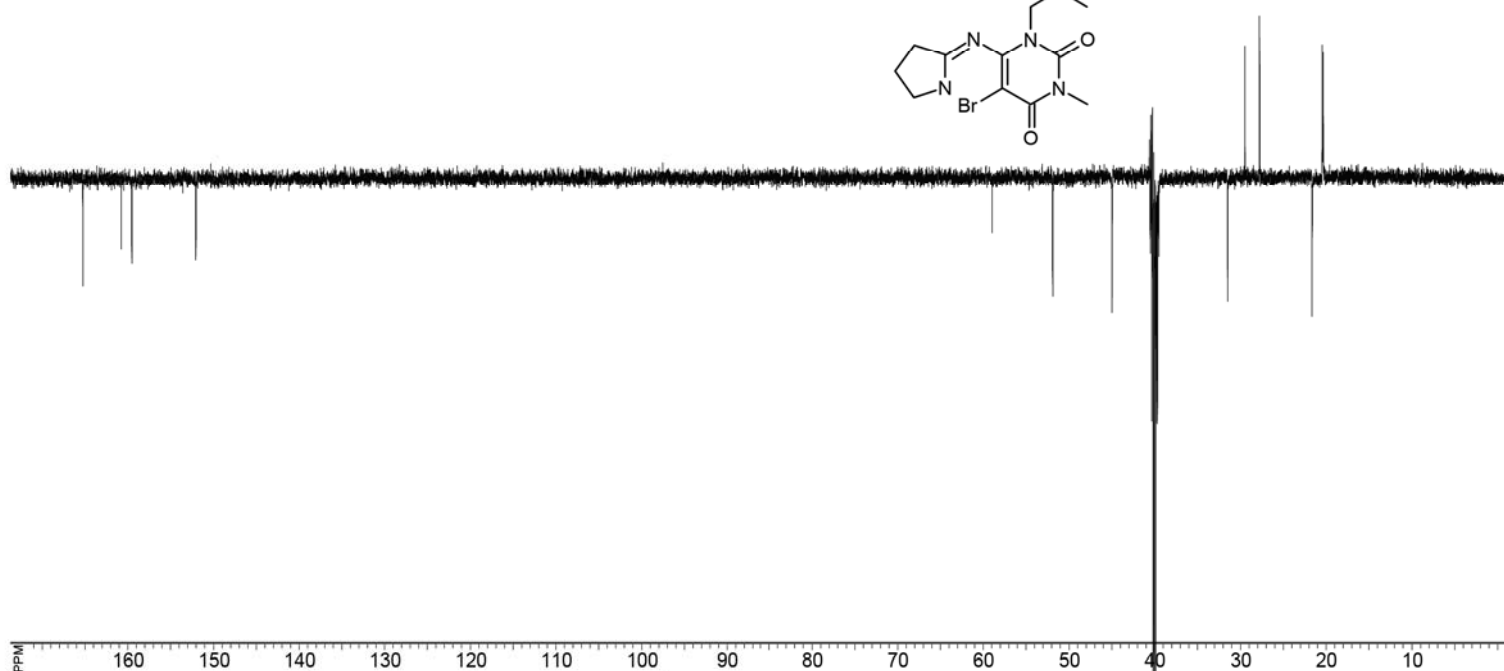
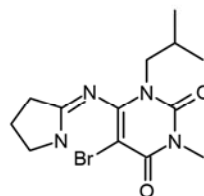
PPM

165.25
160.75
159.53
152.06

59.01
51.94
45.03

31.54
29.50
27.77
21.69
20.47
20.34

PHIk-508-APTC13



File name: PHIk-508-APTC13	Operator: root	SF: 125.7422 MHz	NSC: 264	PW: 0.00 usec, RG: 51200	SI: 65536
Date: 25-May-2012	Solvent: DMSO	SW: 30303 Hz	TE: 0 K	AQ: 1.69 sec, RD: 0.00 sec	Parameter file, XWIN-NMR Version 3.5

PPM

7.698

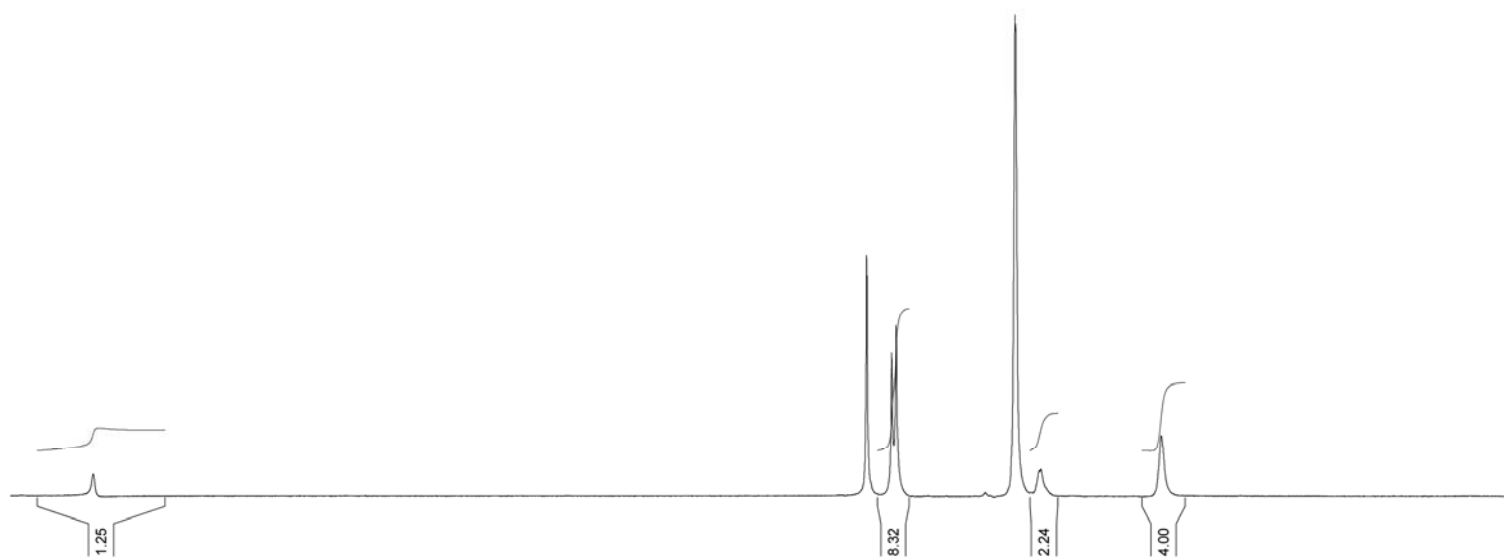
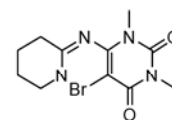
3.205

3.180

2.361

1.691

PHIk-511.fid



File name: PHIk-511.fid	Operator:	SF: 399.9703 MHz	NSC: 0	PW: 7.50 usec, RG: 24	SI: 32768
Date: 18-Apr-2011	Solvent: dms0-d6	SW: 6803 Hz	TE: 293 K	AQ: 1.33 sec, RD: 0.00 sec	

PPM

159.82

159.53

155.97

151.59

83.47

41.47

31.59

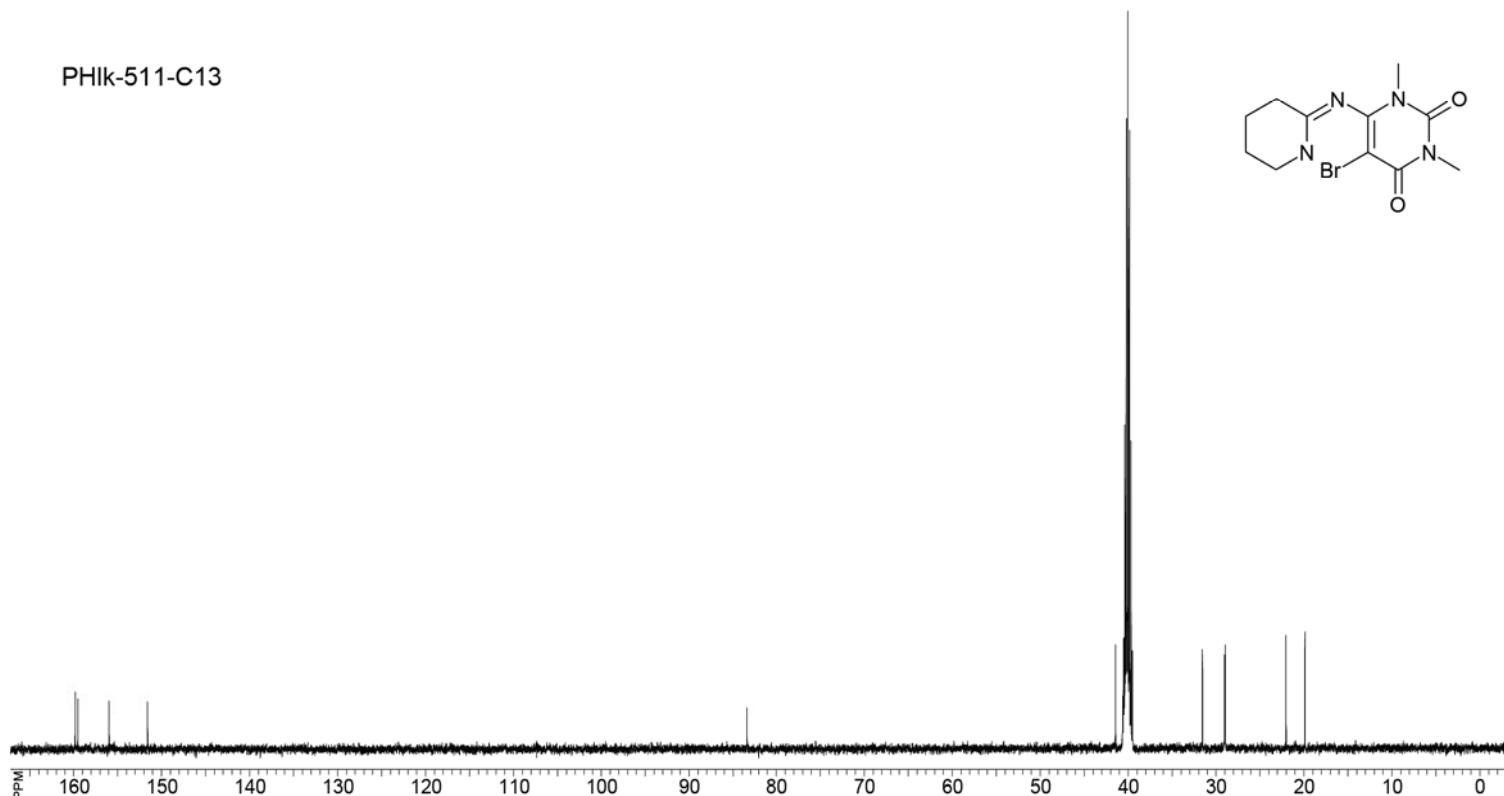
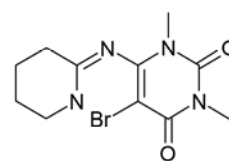
29.08

29.00

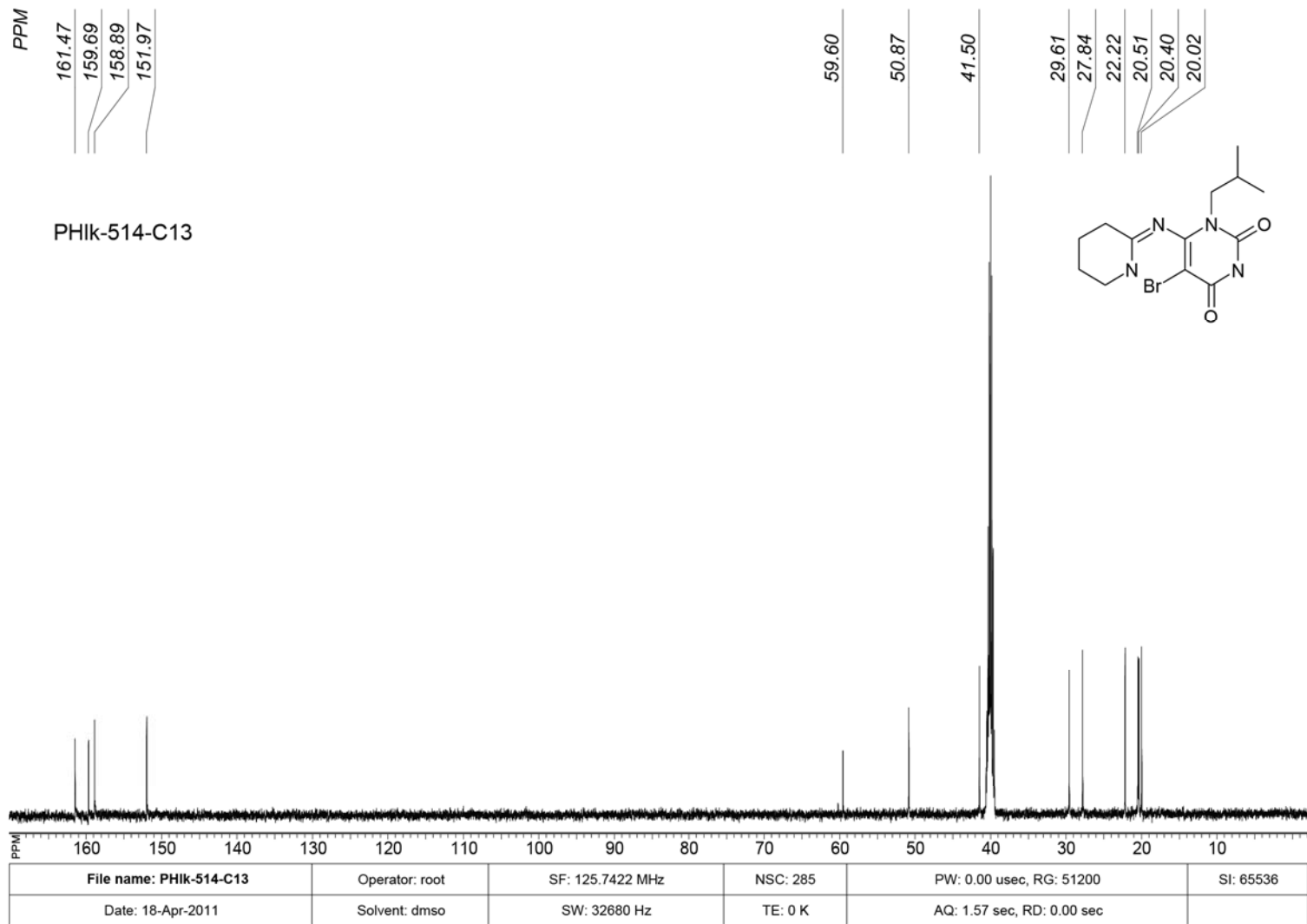
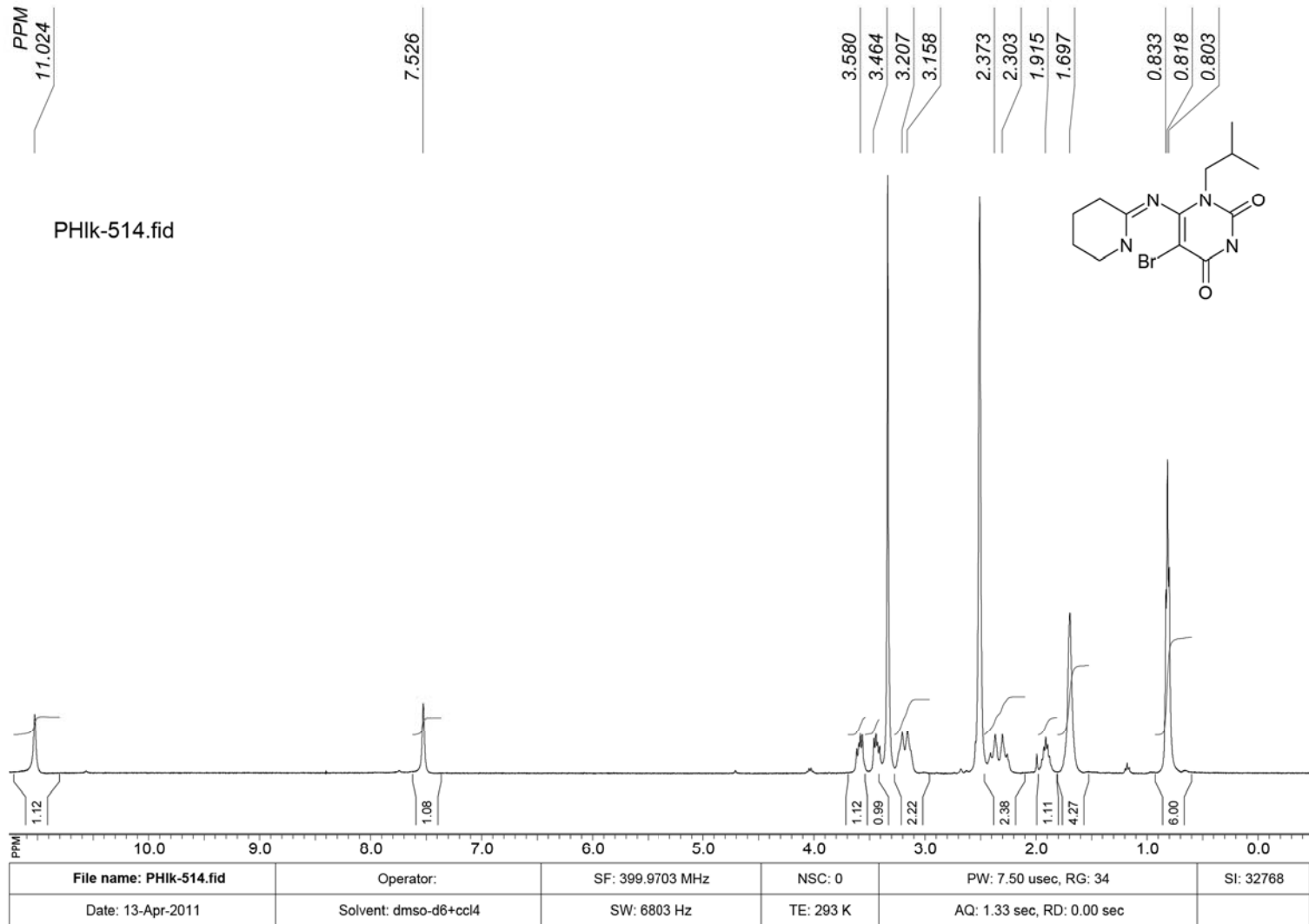
22.09

19.93

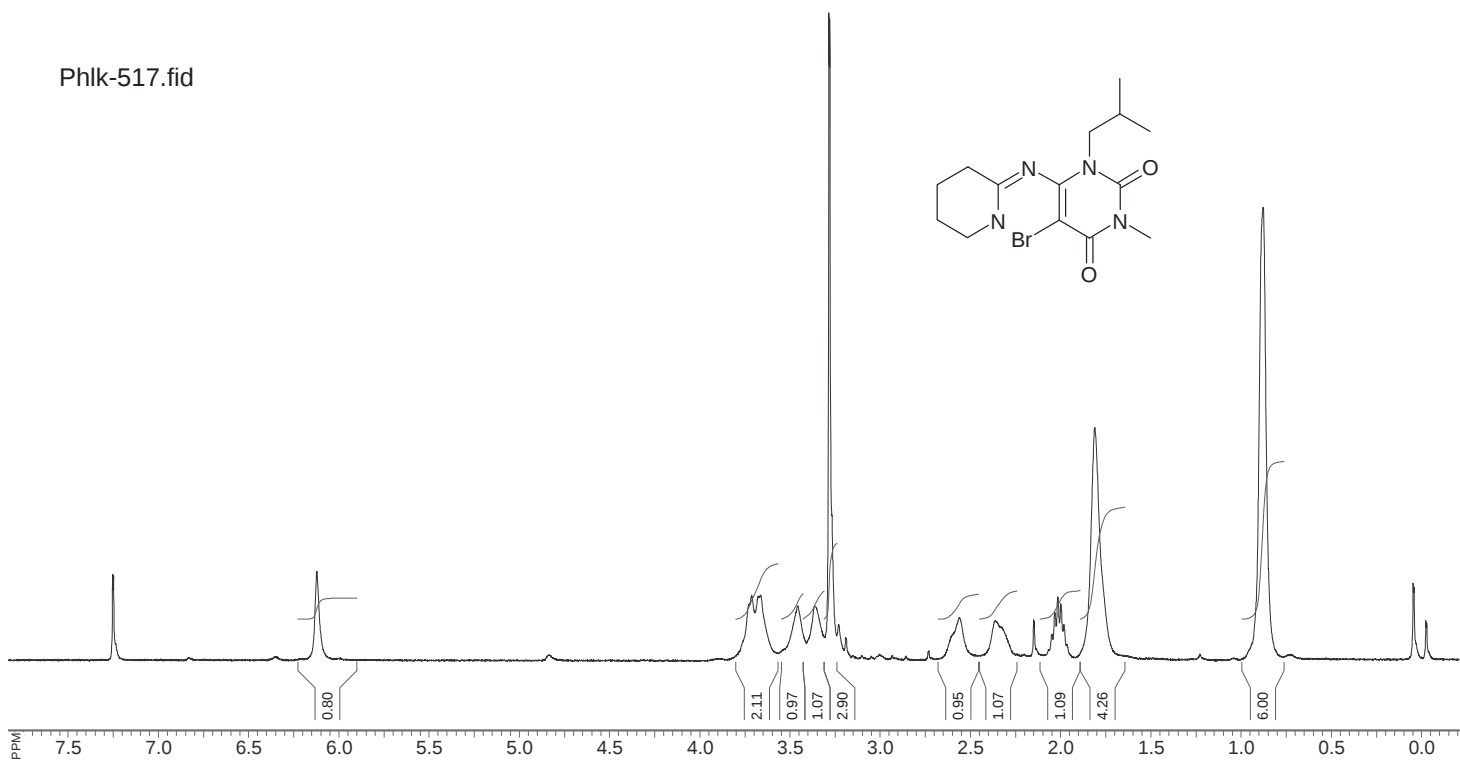
PHIk-511-C13



File name: PHIk-511-C13	Operator: root	SF: 125,7422 MHz	NSC: 478	PW: 0,00 usec, RG: 51200	SI: 65536
Date: 18-anp-2011	Solvent: DMSO	SW: 32680 Hz	TE: 0 K	AQ: 1,57 sec, RD: 0,00 sec	

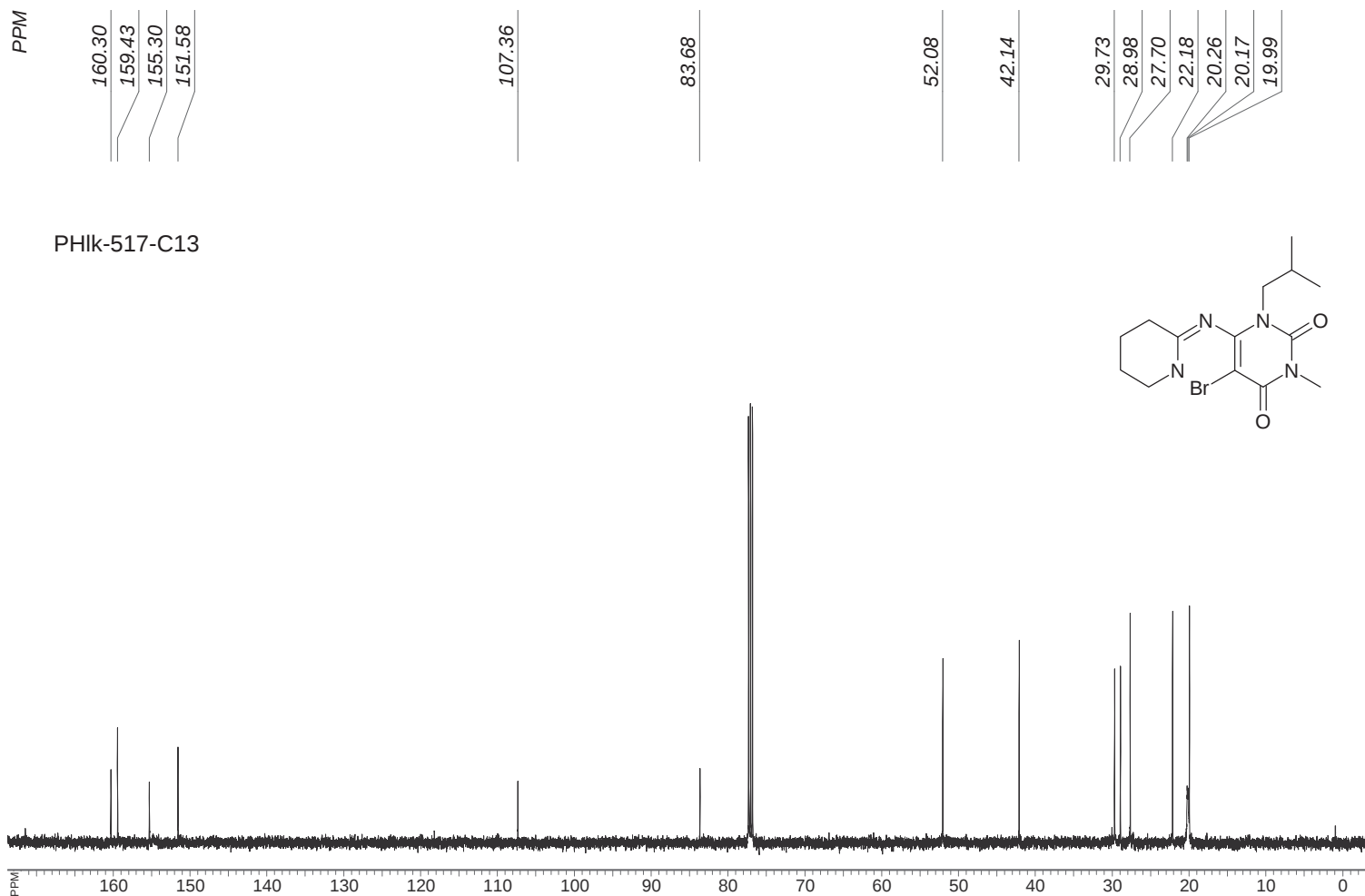


PPM



File name: Phlk-517.fid	Operator:	SF: 399.9683 MHz	NSC: 0	PW: 7.50 usec, RG: 22	SI: 32768
Date: 01-Mar-2011	Solvent: cdcl3	SW: 6803 Hz	TE: 293 K	AQ: 1.33 sec, RD: 0.00 sec	

PPM



File name: PHlk-517-C13	Operator: root	SF: 125.7422 MHz	NSC: 108	PW: 0.00 usec, RG: 51200	SI: 6553
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PPM

5.855

3.423

3.335

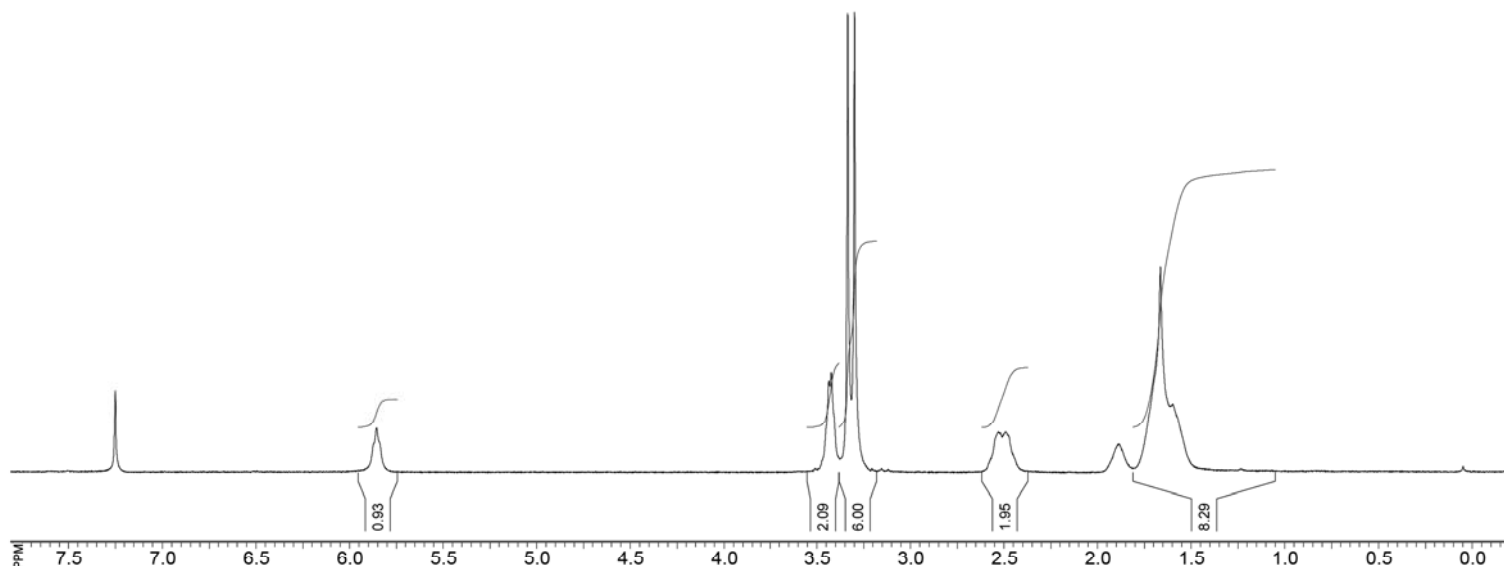
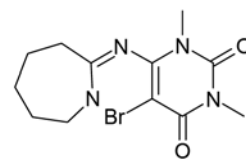
3.299

2.538

2.488

1.669

PHIk-520.fid



File name: PHIk-520.fid	Operator:	SF: 399.9683 MHz	NSC: 0	PW: 7.50 usec, RG: 26	SI: 32768
Date: 17-Apr-2011	Solvent: cdcl3	SW: 6803 Hz	TE: 293 K	AQ: 1.33 sec, RD: 0.00 sec	

PPM

163.40

160.08

154.66

151.57

83.96

42.49

32.00

31.46

30.43

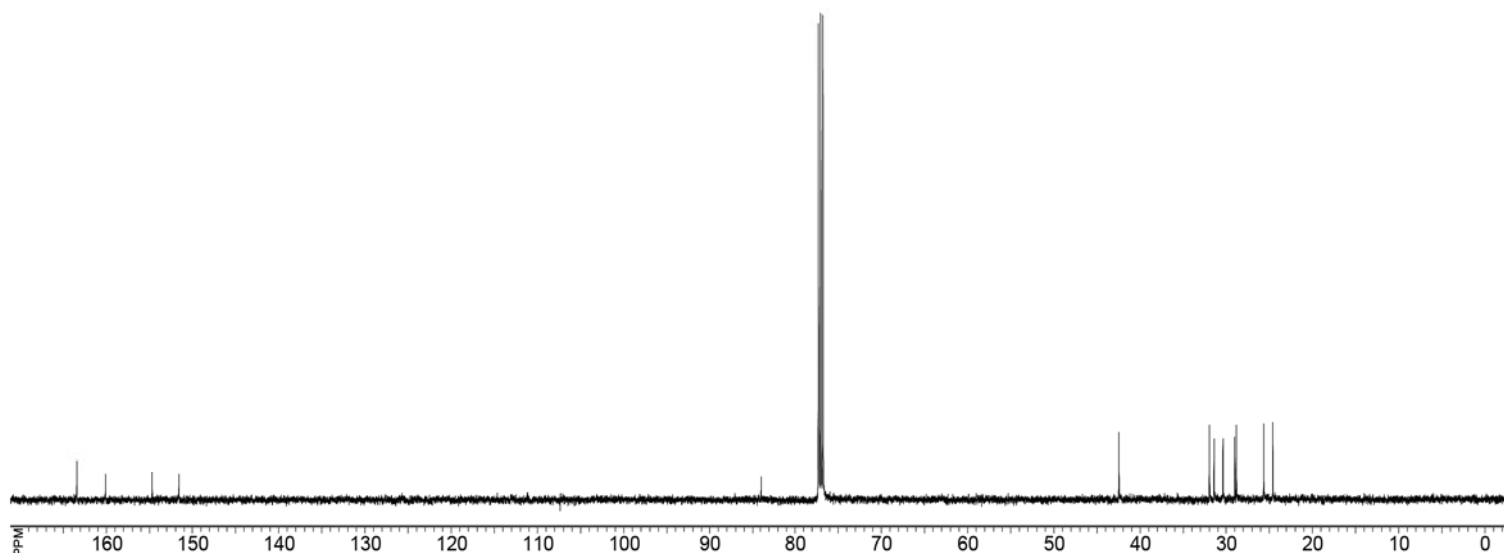
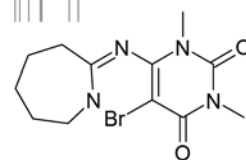
29.06

28.87

25.70

24.65

PHIk-520-C13



File name: PHIk-520-C13	Operator: root	SF: 125.7422 MHz	NSC: 590	PW: 0.00 usec, RG: 51200	SI: 65536
Date: 18-Apr-2011	Solvent: dms0	SW: 32680 Hz	TE: 680 K	AQ: 1.57 sec, RD: 0.00 sec	

S20

PPM

10.169

6.889

3.749

3.488

3.415

2.543

2.089

1.703

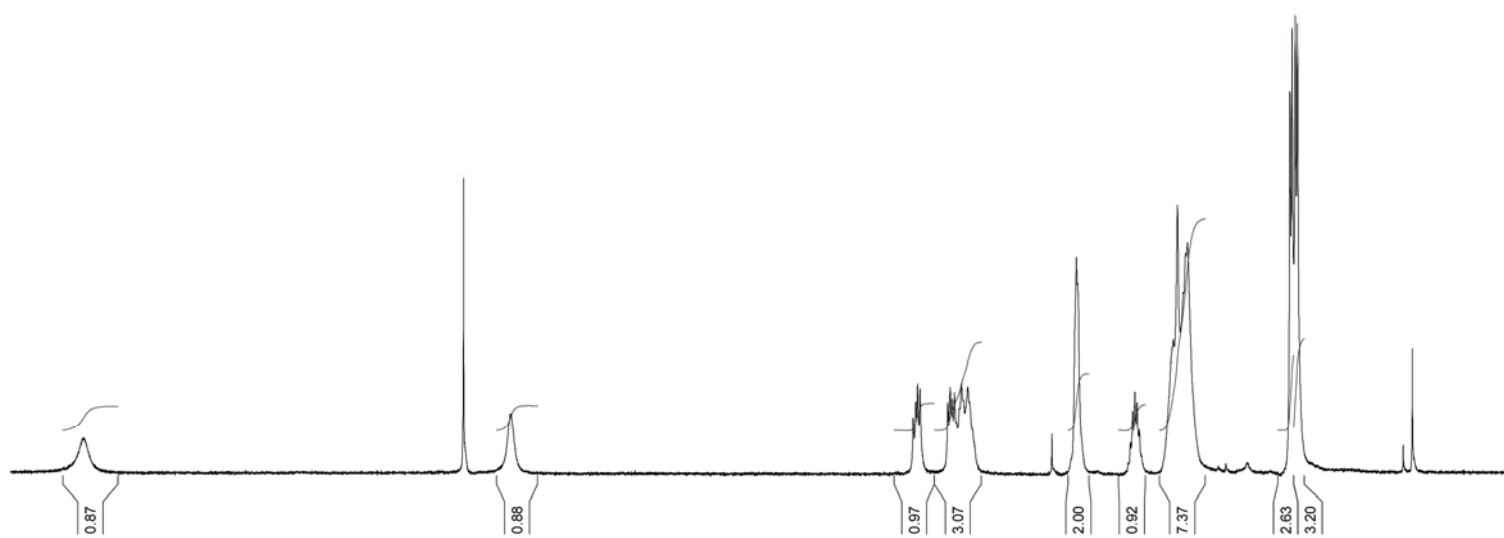
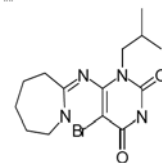
0.920

0.903

0.879

0.861

PHIk-523.fid



File name: PHIk-523.fid	Operator:	SF: 399.9683 MHz	NSC: 0	PW: 7.50 usec, RG: 32	SI: 32768
Date: 31-Jan-2011	Solvent: cdcl3	SW: 6803 Hz	TE: 293 K	AQ: 1.33 sec, RD: 0.00 sec	

PPM

164.15

160.80

157.50

151.84

84.23

51.40

44.10

35.39

30.49

29.73

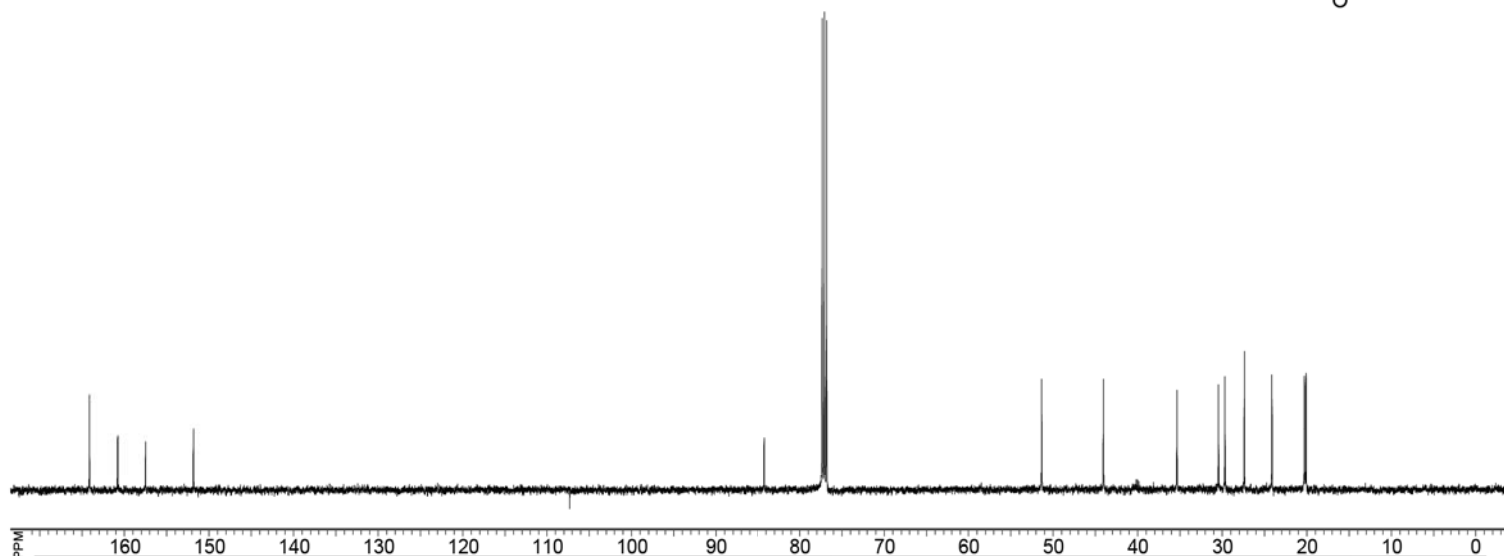
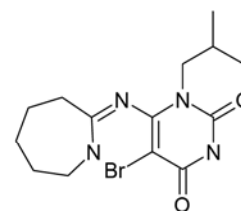
27.43

24.16

20.32

20.11

PHIk-523-C13



File name: PHIk-523-C13	Operator: root	SF: 125.7422 MHz	NSC: 283	PW: 0.00 usec, RG: 51200	SI: 65536
Date: 02-Feb-2011	Solvent: dmso	SW: 32680 Hz	TE: 681 K	AQ: 1.57 sec, RD: 0.00 sec	

PPM

6,293

3,806

3,628

3,416

3,276

2,571

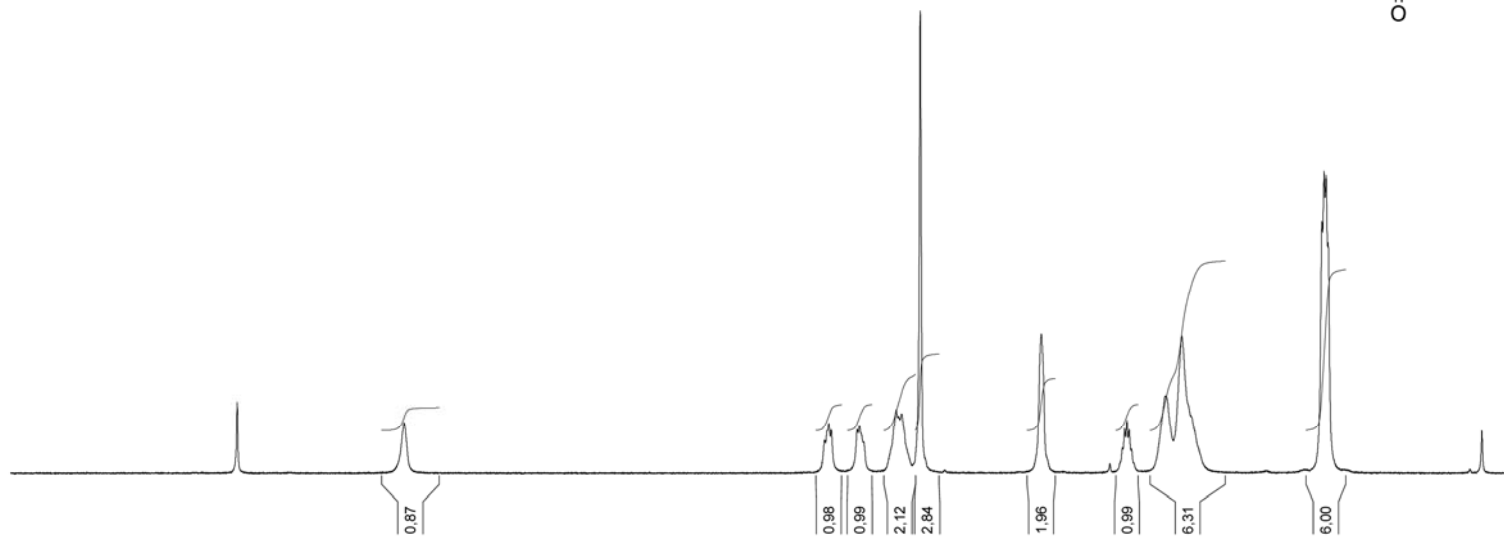
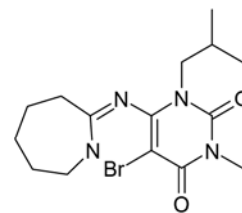
2,070

1,847

1,746

0,920

PHIk-526



File name: PHIk-526	Operator: root	SF: 500,000 MHz	NSC: 1	PW: 0,00 usec, RG: 40	SI: 32768
Date: 01-фев-2011	Solvent: DMSO	SW: 8012 Hz	TE: 681 K	AQ: 2,04 sec, RD: 0,00 sec	

PPM

163,58

159,58

154,40

150,74

82,47

50,66

42,69

33,67

28,86

28,18

27,40

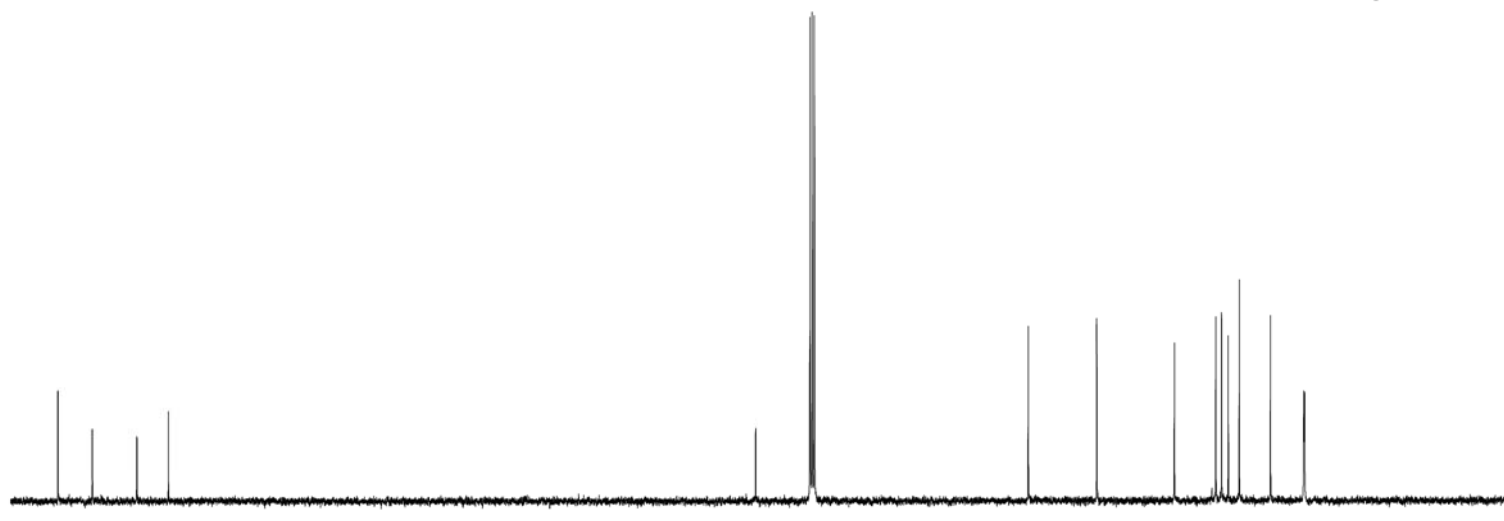
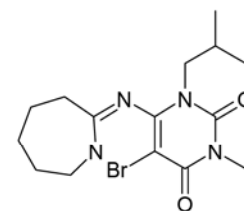
26,13

22,50

18,62

18,54

PHIk-526-C13



File name: PHIk-526-C13	Operator: root	SF: 125,000 MHz	NSC: 344	PW: 0,00 usec, RG: 51200	SI: 65536
Date: 02-фев-2011	Solvent: CDCl3	SW: 32679 Hz	TE: 681 K	AQ: 1,57 sec, RD: 0,00 sec	

PPM

6,064

3,455

3,352

3,280

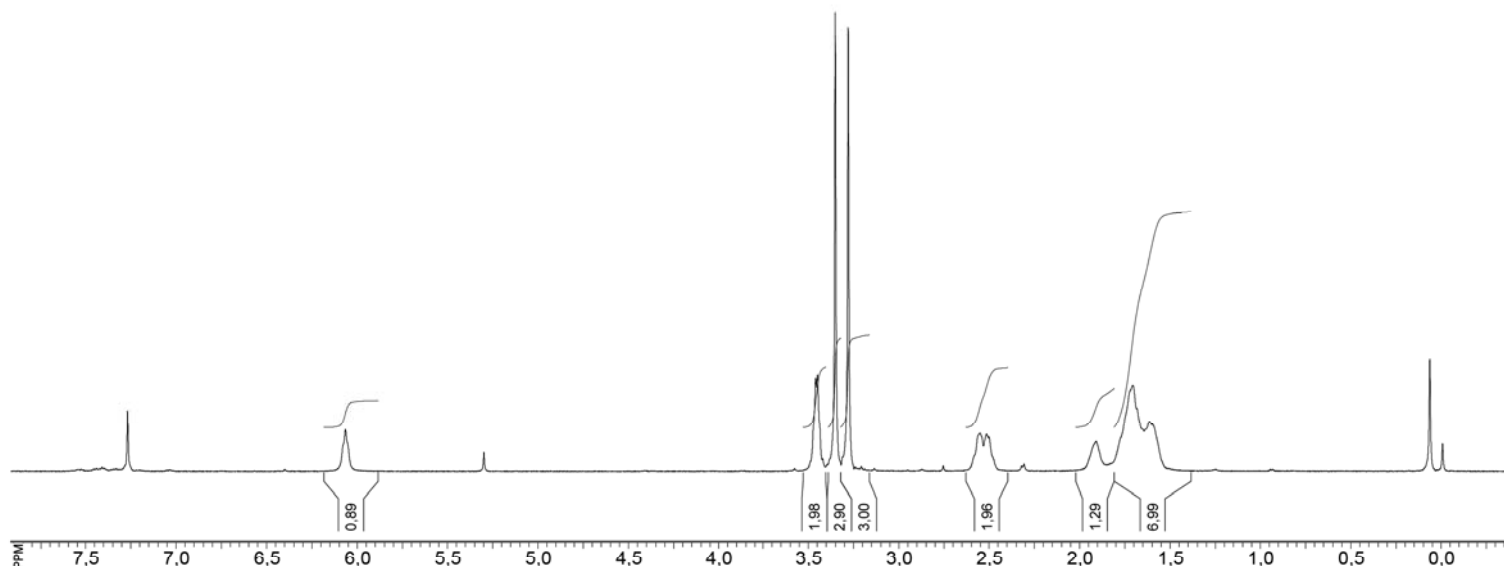
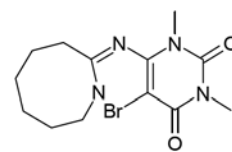
2,544

1,908

1,740

1,614

PHIk-529



File name: PHIk-529	Operator: root	SF: 500,000 MHz	NSC: 1	PW: 0,00 usec, RG: 40	SI: 32768
Date: 28-январь-2011	Solvent: CDCl3	SW: 8012 Hz	TE: 680 K	AQ: 2,04 sec, RD: 0,00 sec	

PPM

162,43

159,36

153,99

150,66

82,65

41,06

30,42

29,88

29,12

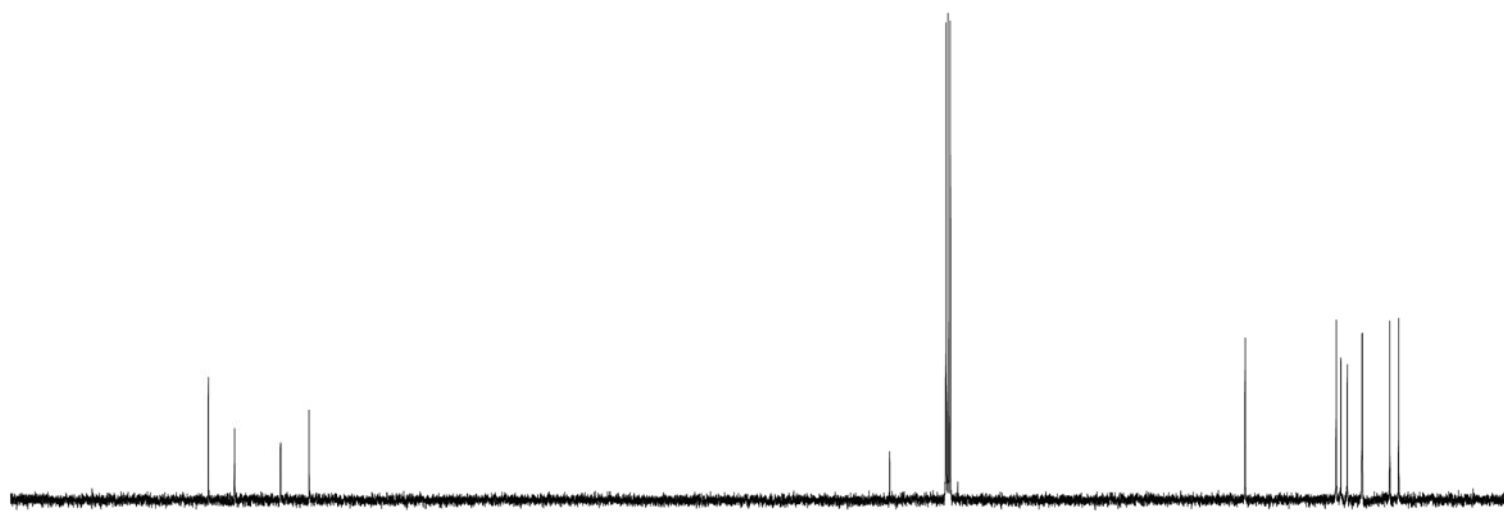
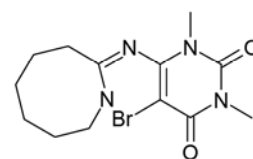
27,40

27,36

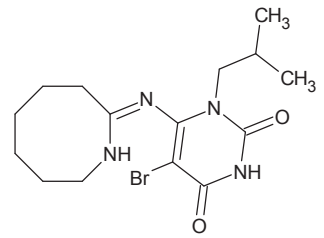
24,15

22,12

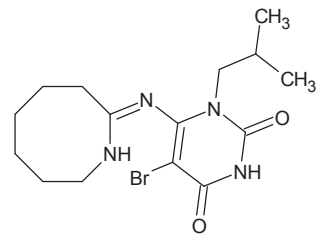
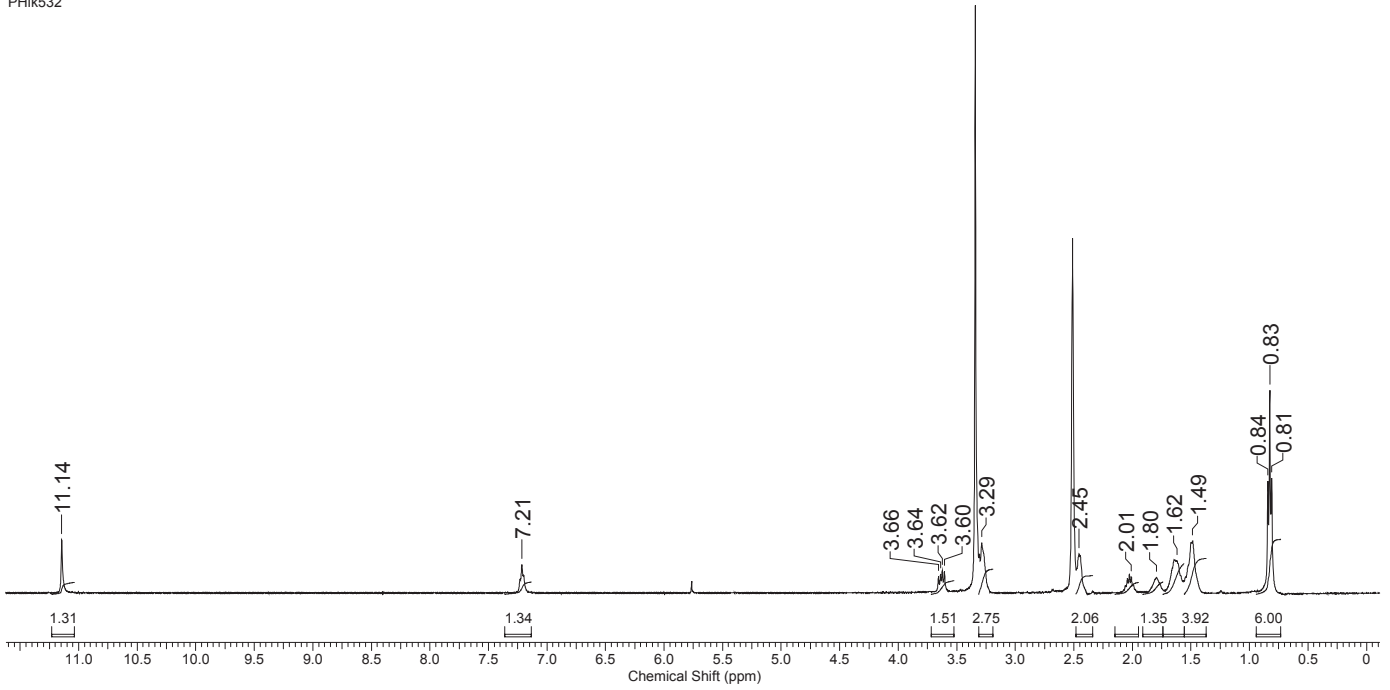
PHIk-529-C13



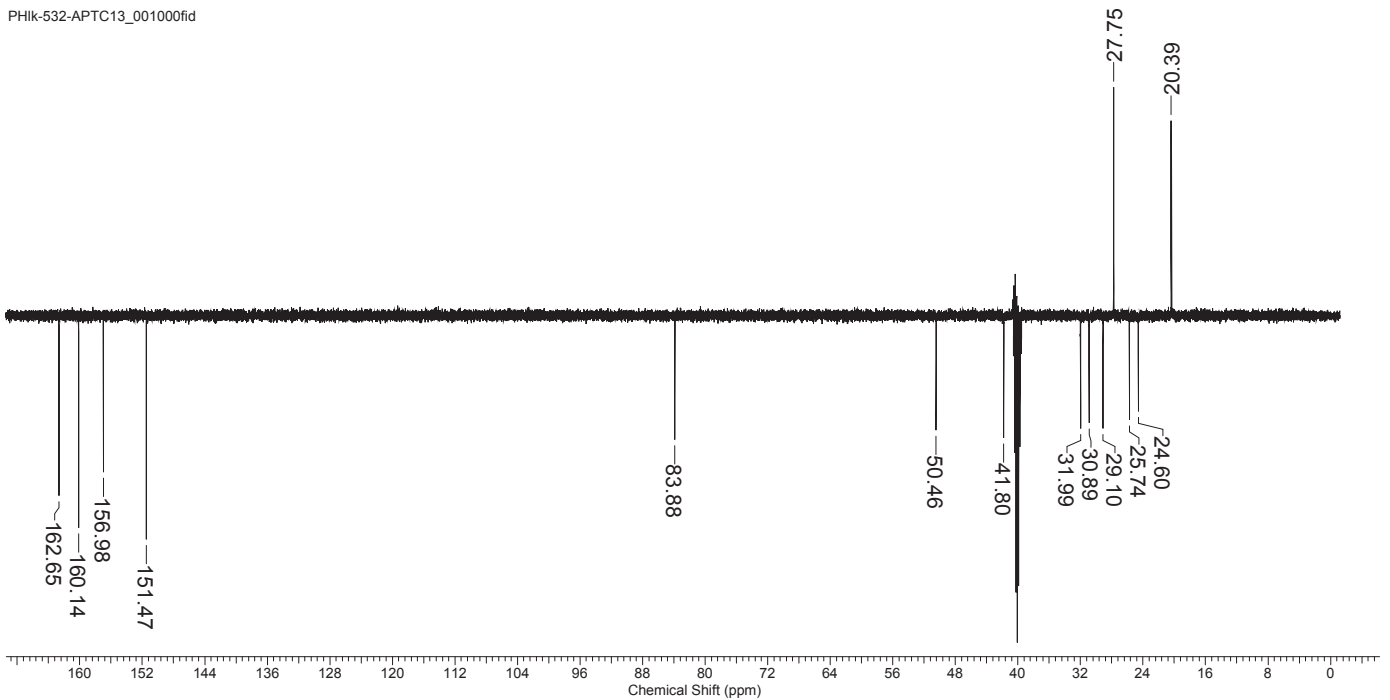
File name: PHIk-529-C13	Operator: root	SF: 125,000 MHz	NSC: 123	PW: 0,00 usec, RG: 51200	SI: 65536
Date: 28-январь-2011	Solvent: dmsO	SW: 32679 Hz	TE: 681 K	AQ: 1,57 sec, RD: 0,00 sec	



PHIk532

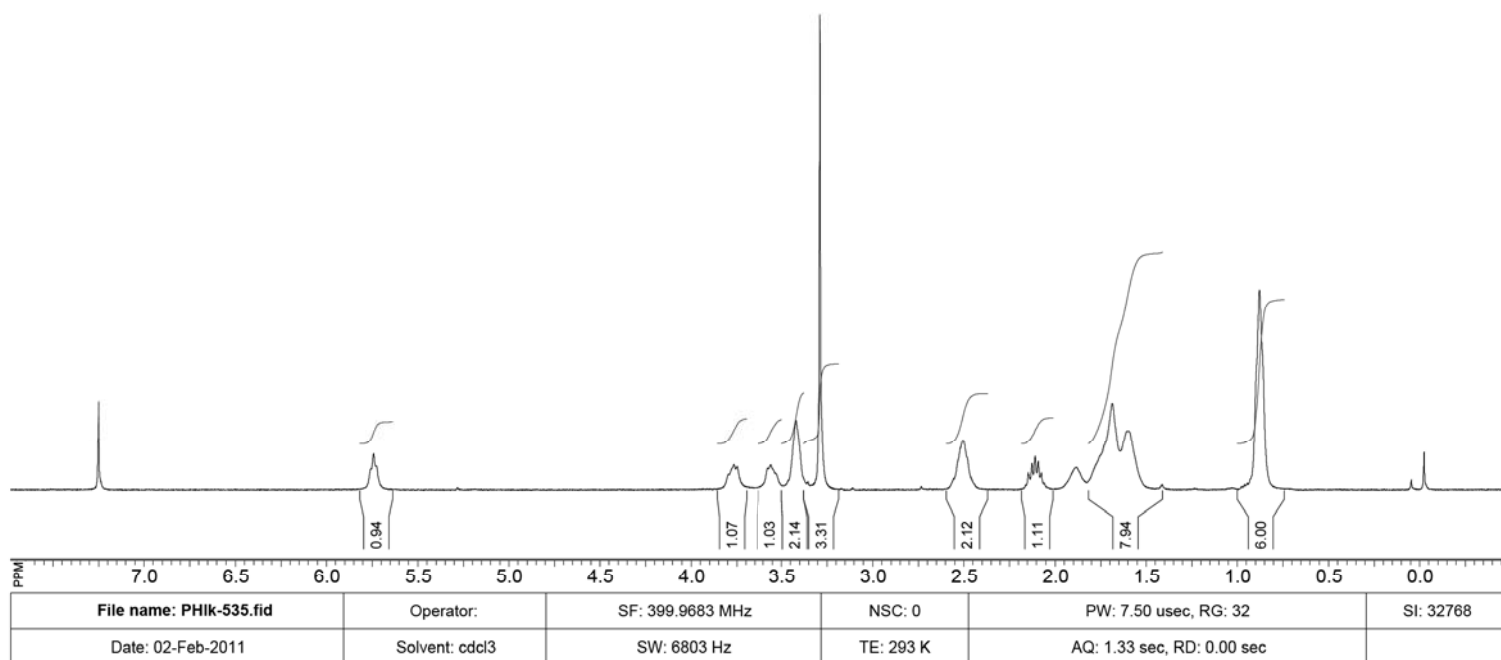
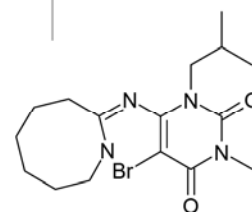


PHIk-532-APTC13_001000fid



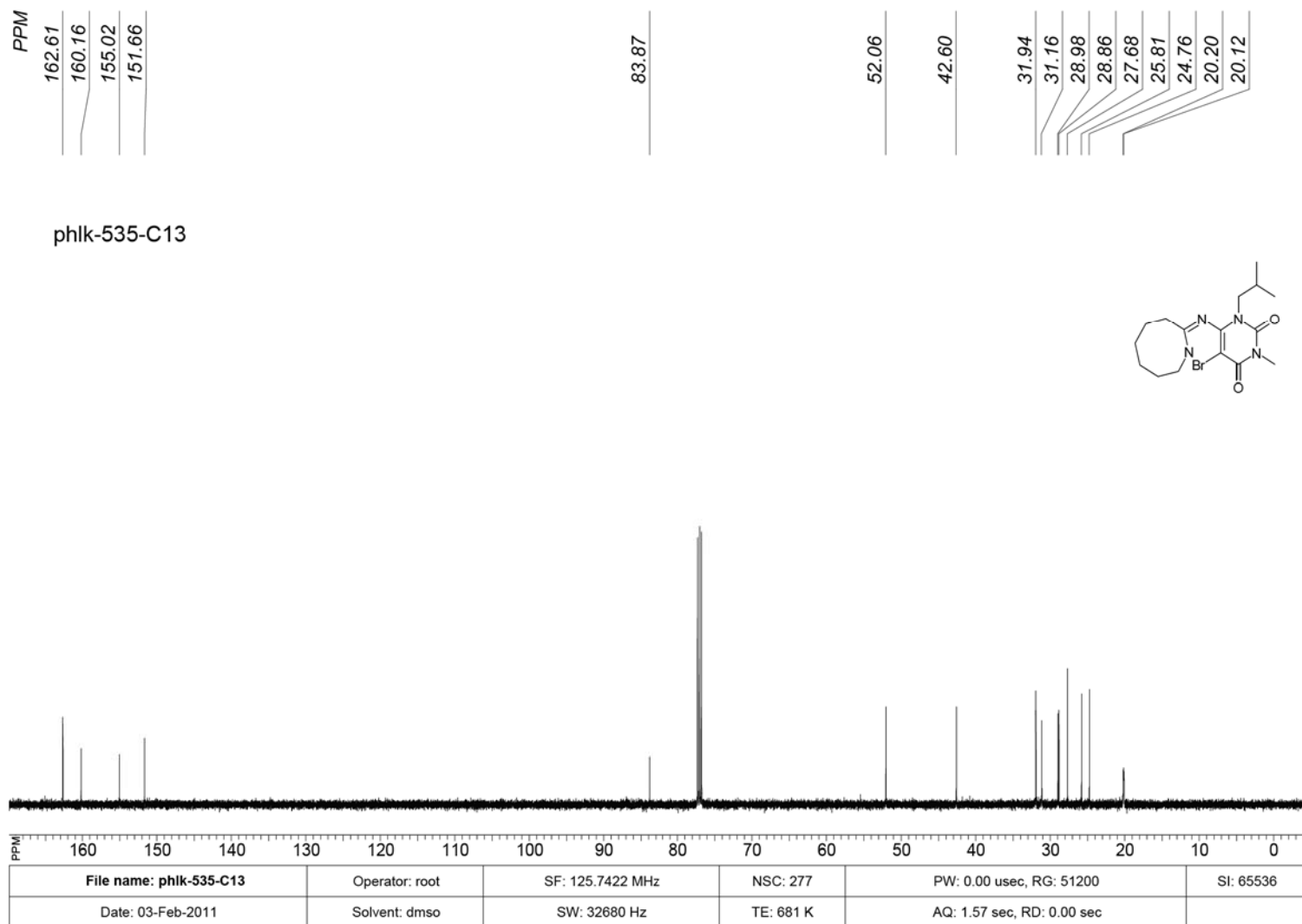
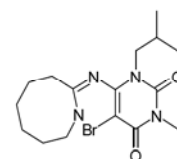
PPM

PHIk-535.fid



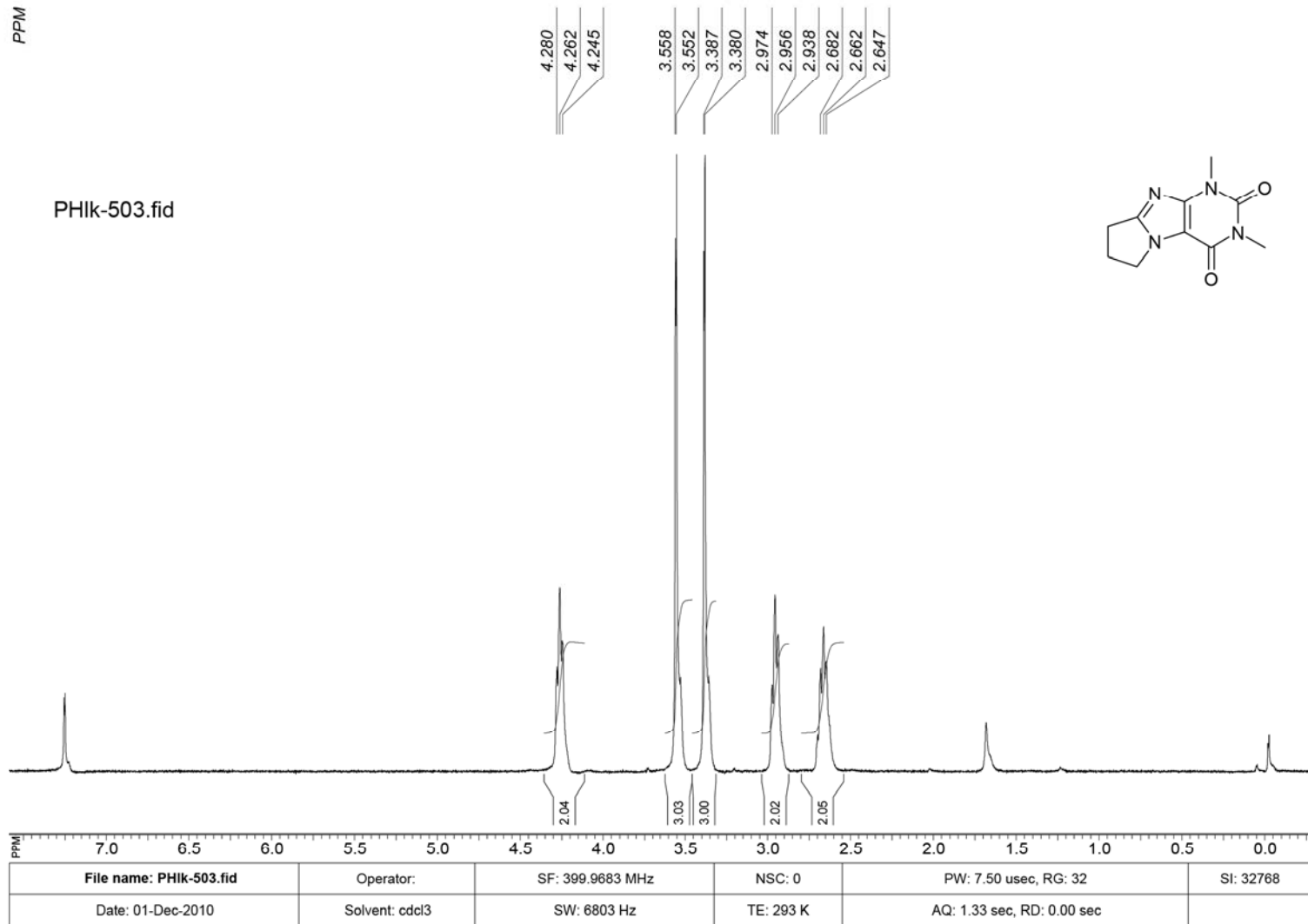
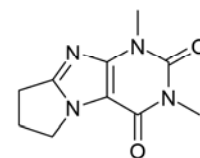
PPM

phlk-535-C13



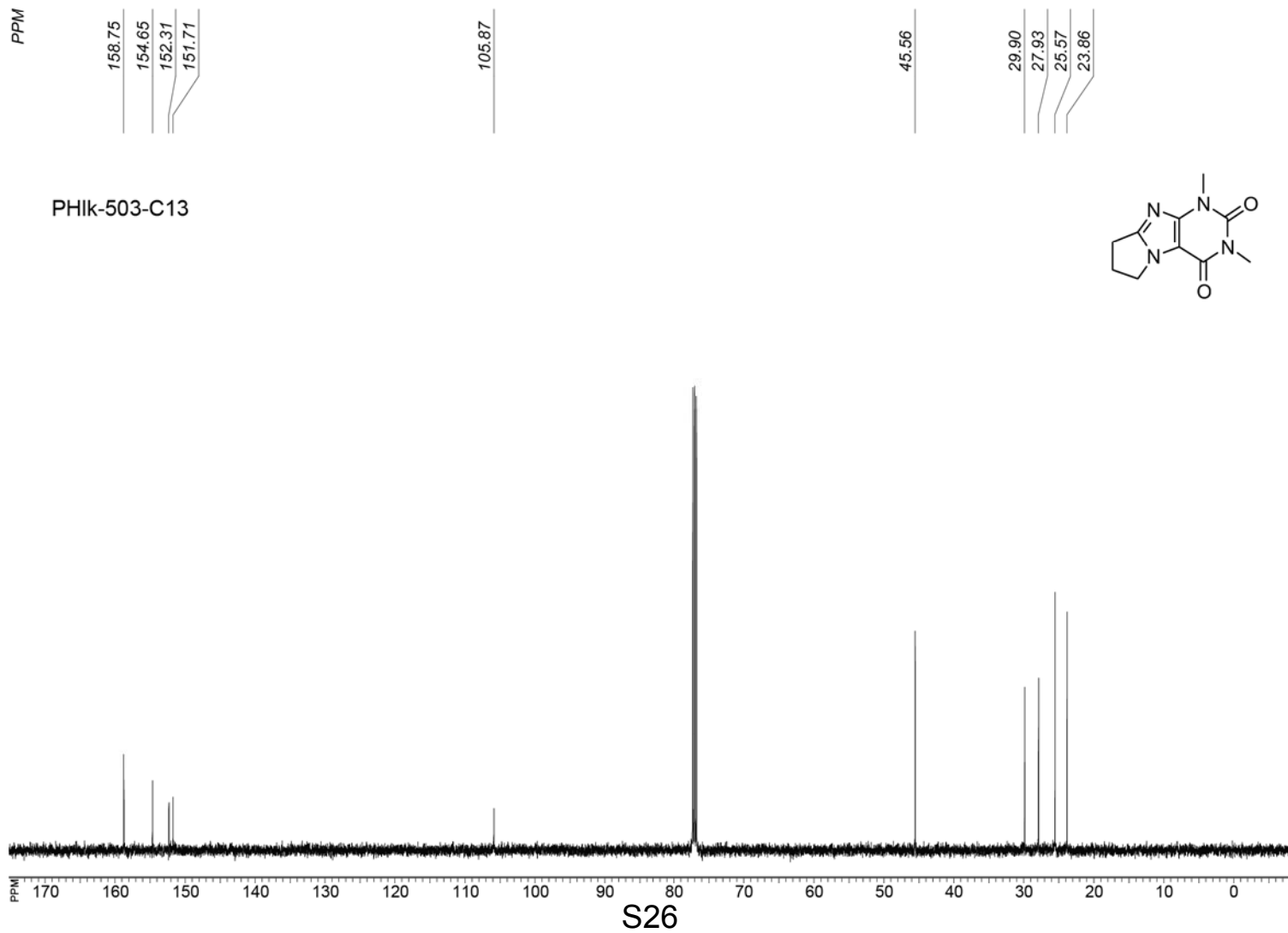
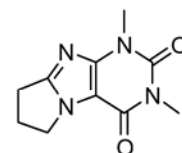
PPM

PHIk-503.fid



PPM

PHIk-503-C13



S26

PPM

8.495

4.273

4.255

4.238

3.872

3.853

2.984

2.965

2.946

2.700

2.680

2.662

2.643

2.626

2.335

2.317

2.300

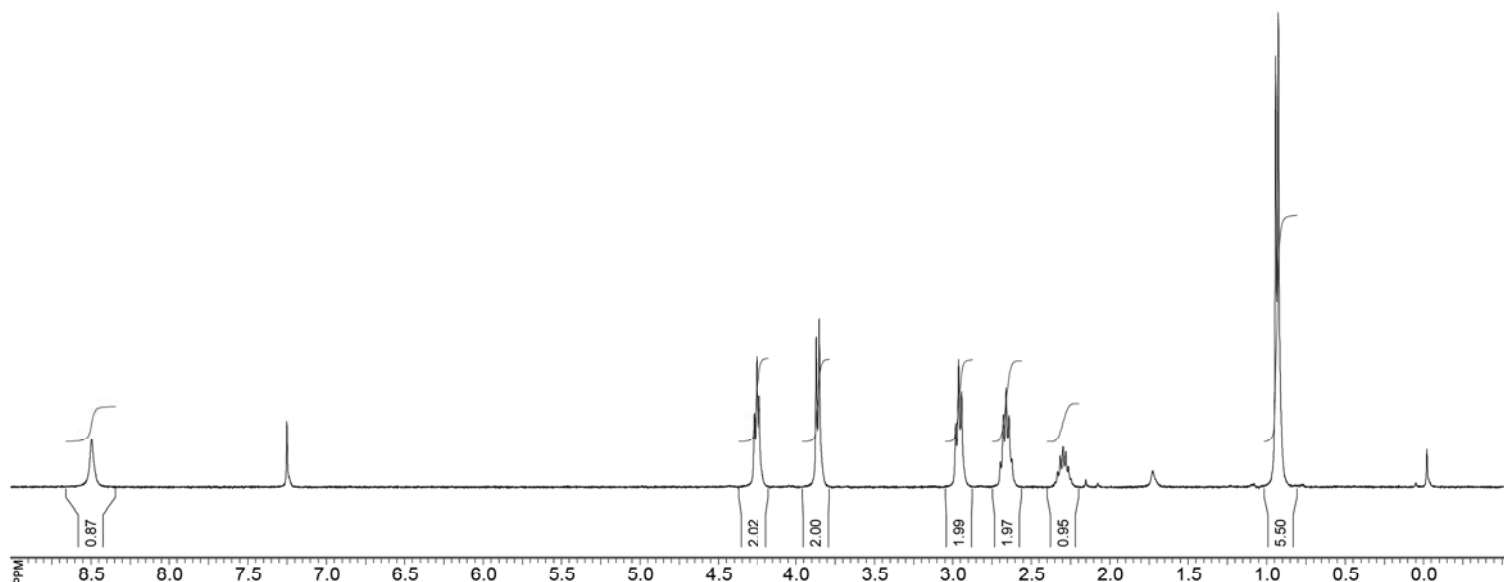
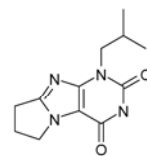
2.282

2.266

0.945

0.928

phlk-506.fid



File name: phlk-506.fid	Operator:	SF: 399.9683 MHz	NSC: 0	PW: 7.50 usec, RG: 28	SI: 32768
Date: 01-Dec-2010	Solvent: cdcl3	SW: 6803 Hz	TE: 293 K	AQ: 1.33 sec, RD: 0.00 sec	

PPM

159.21

151.04

107.35

106.01

49.90

45.61

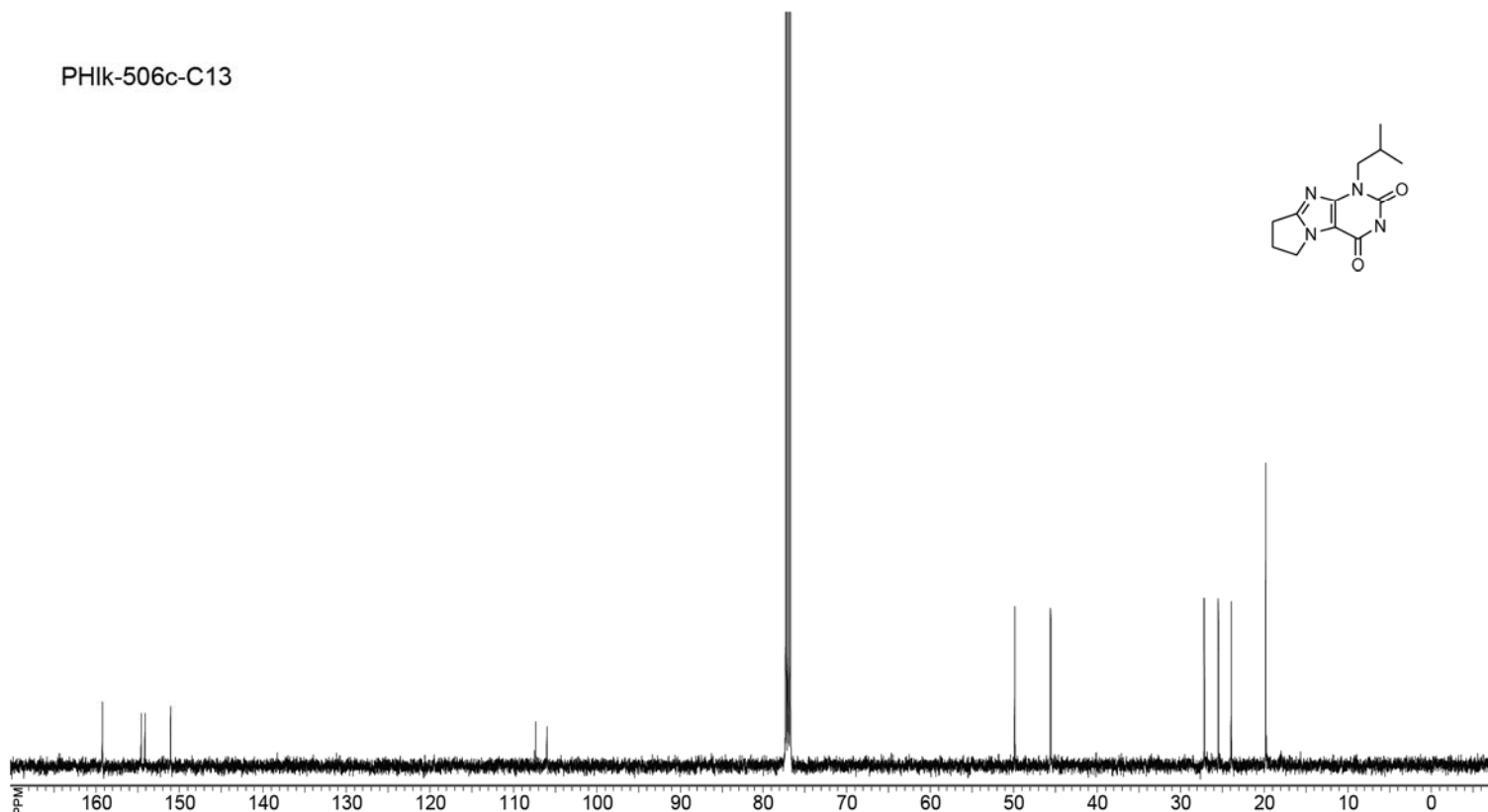
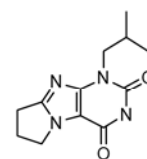
27.21

25.53

23.99

19.85

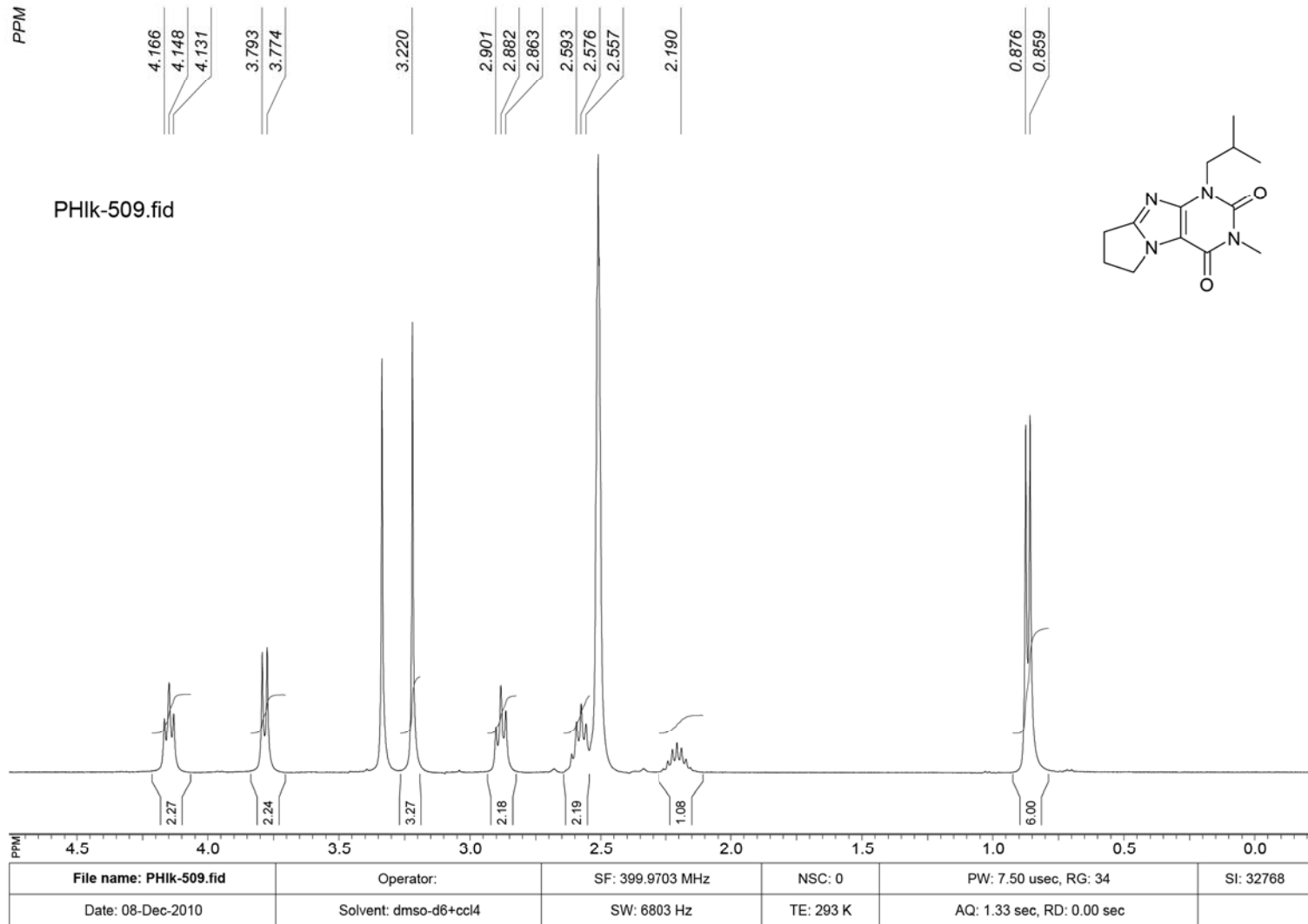
PHlk-506c-C13



File name: PHlk-506c-C13	Operator: root	SF: 125.7422 MHz	NSC: 447	PW: 0.00 usec, RG: 51200	SI: 65536
Date: 08-Jun-2011	Solvent: CDCl3	SW: 32680 Hz	TE: 682 K	AQ: 1.57 sec, RD: 0.00 sec	Parameter file, XWIN-NMR Version 3.5

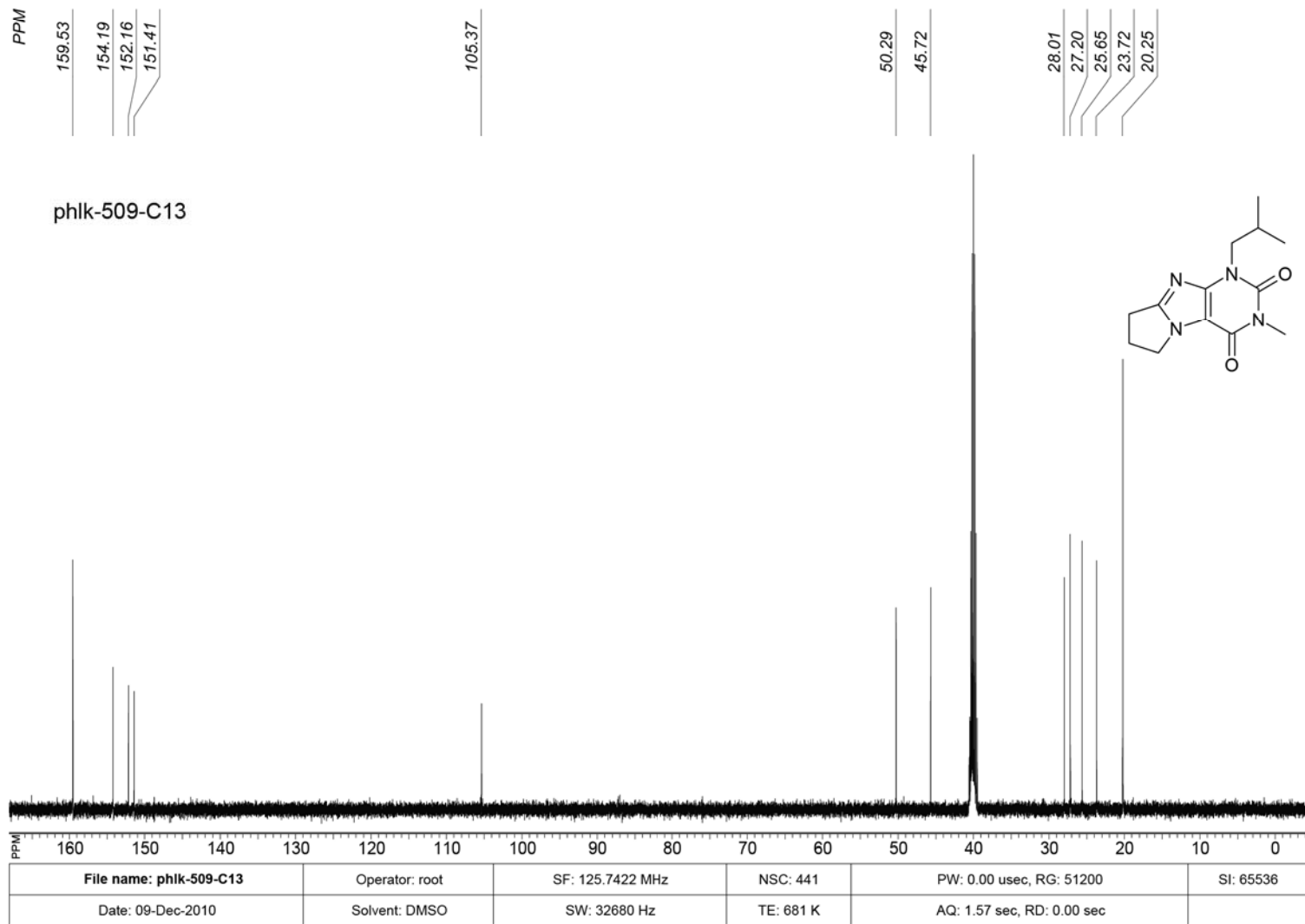
PPM

PHIk-509.fid



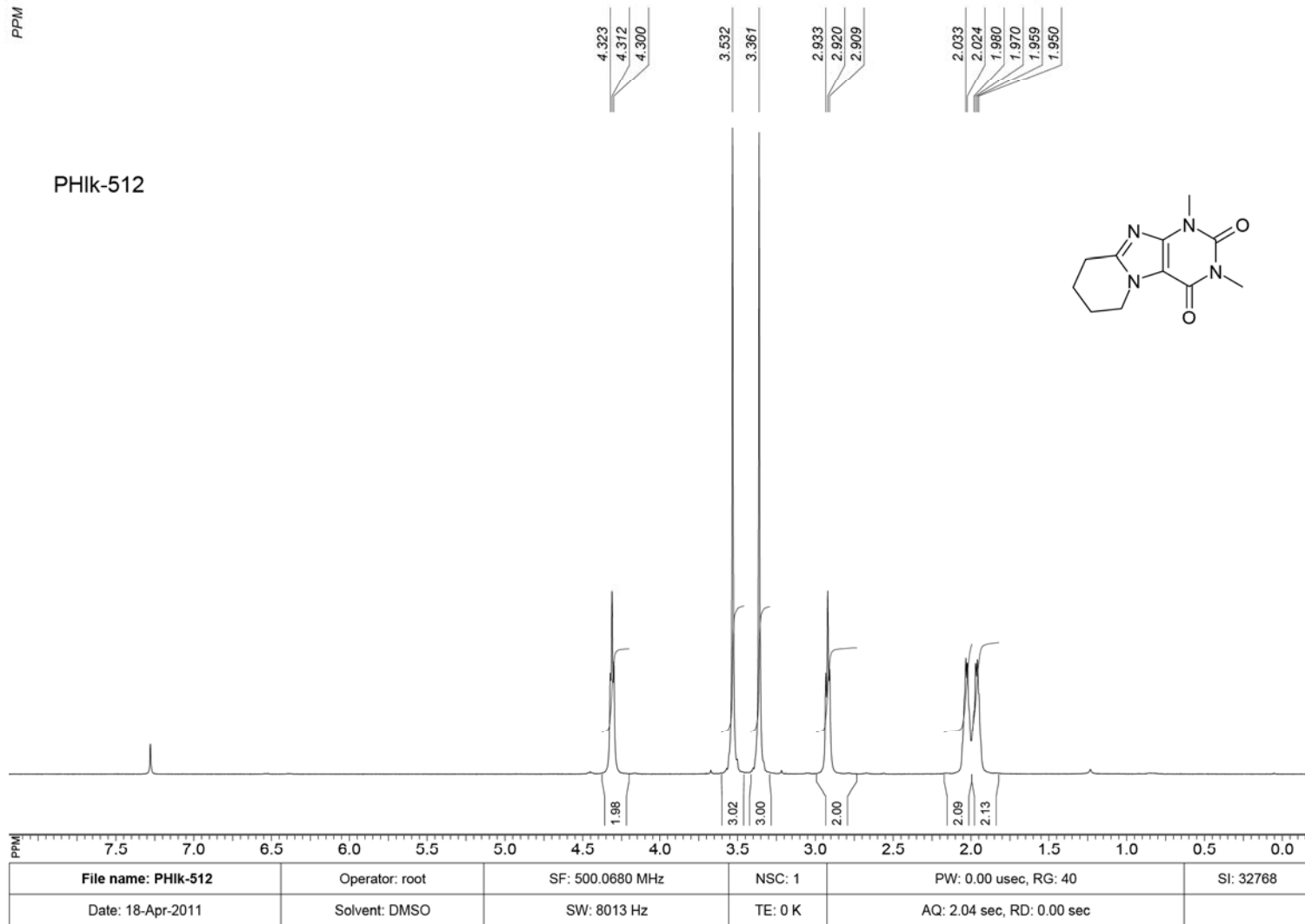
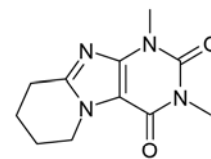
PPM

phlk-509-C13



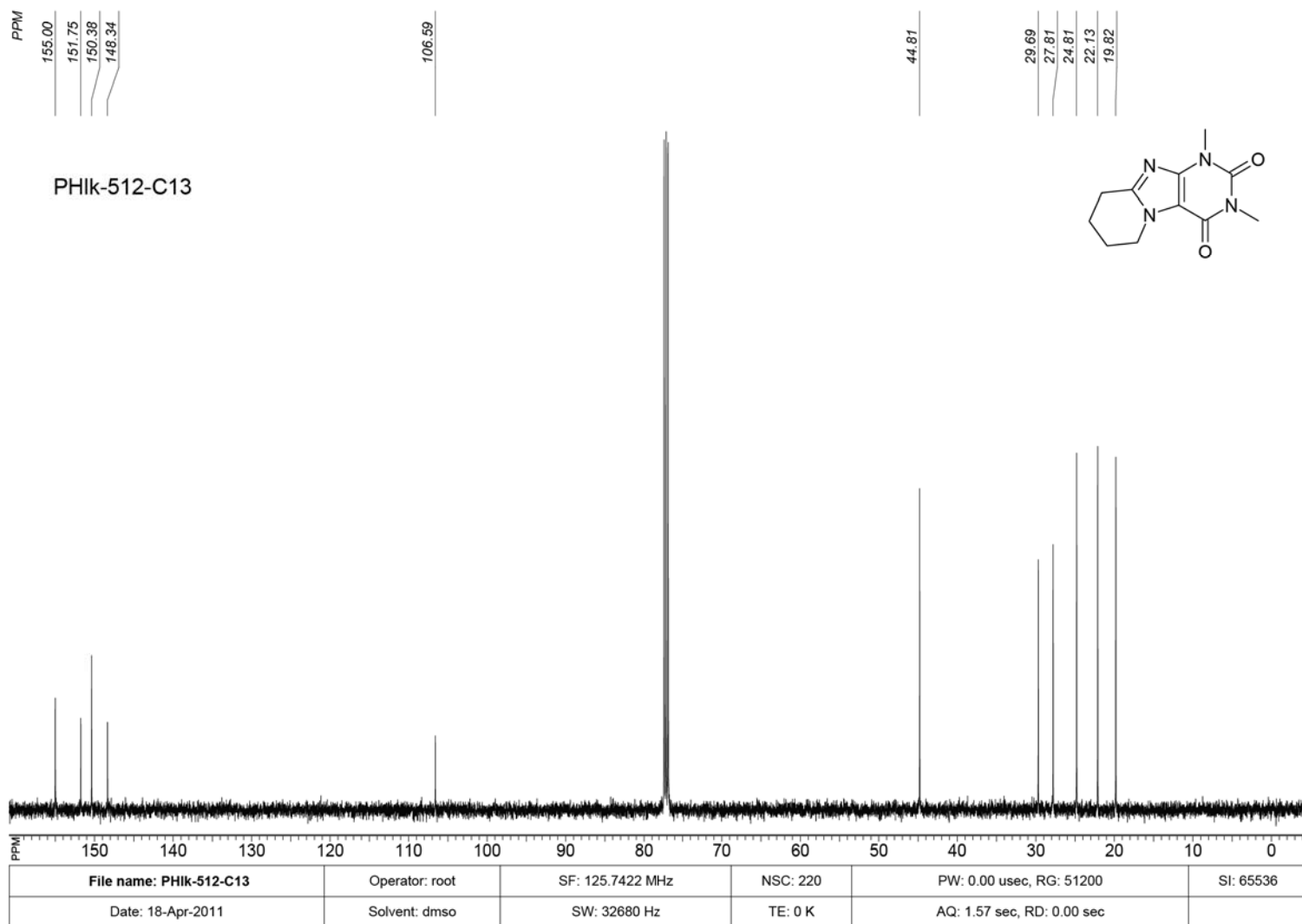
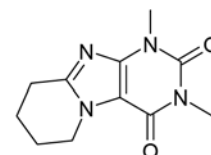
PPM

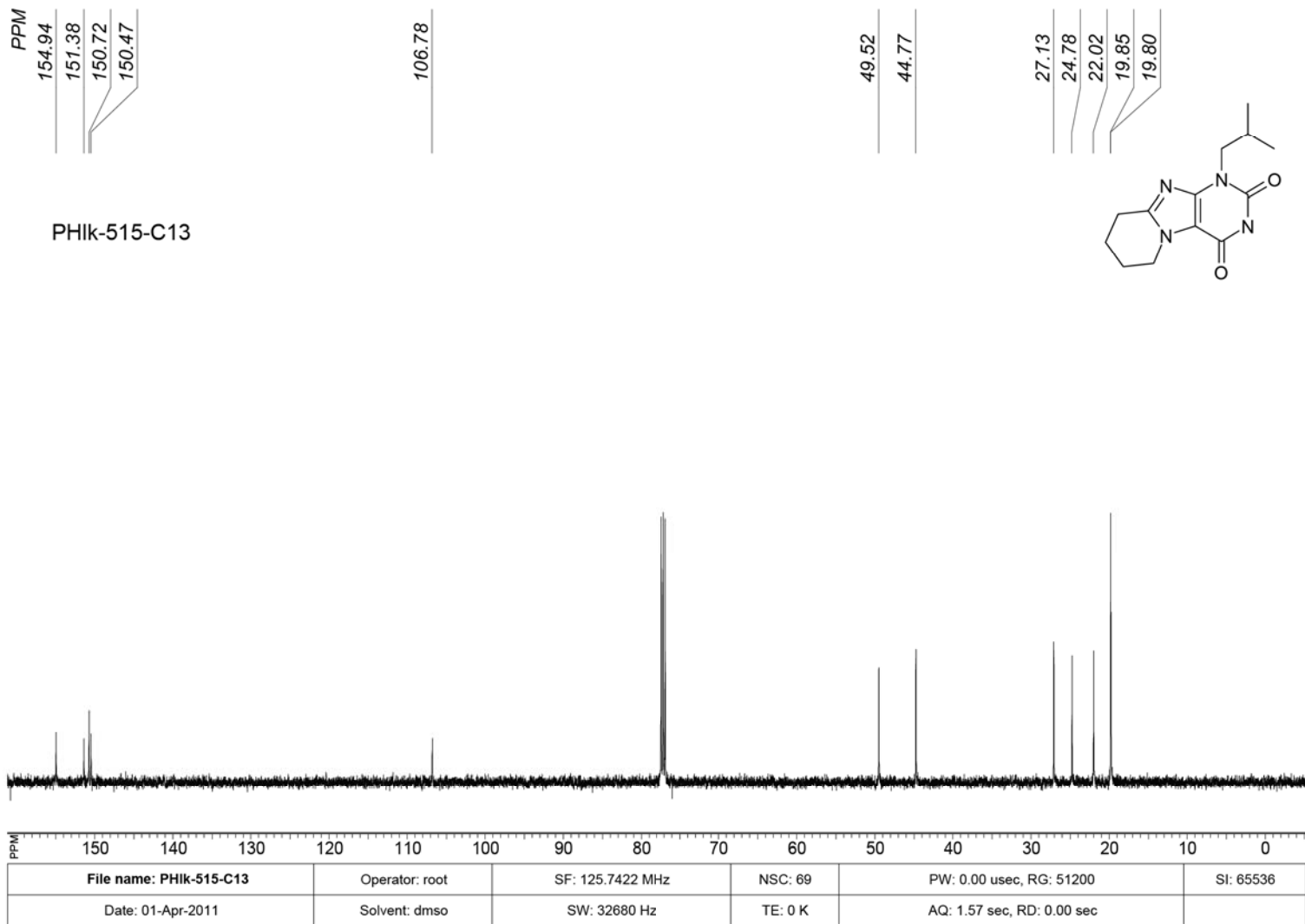
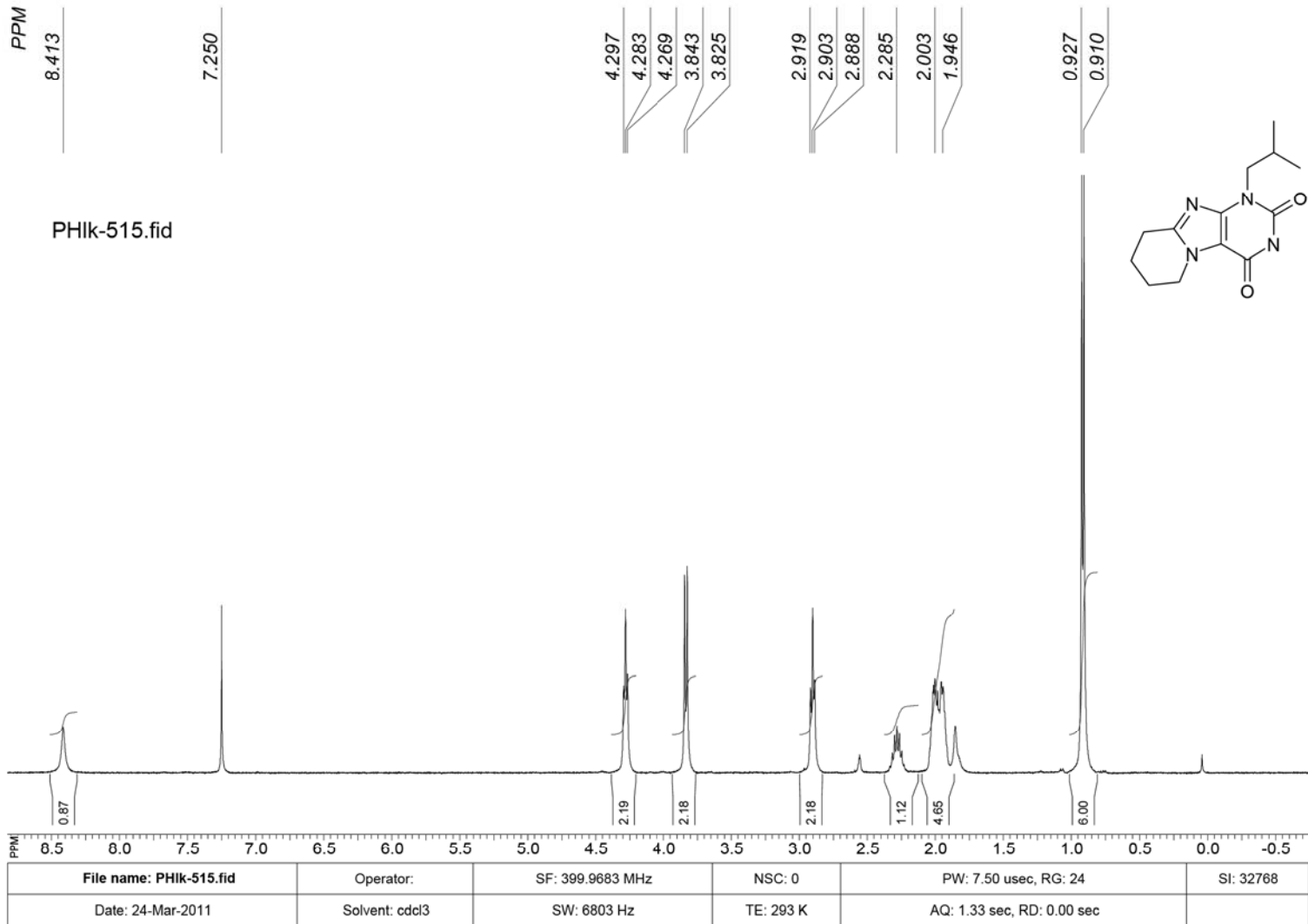
PHIk-512



PPM

PHIk-512-C13





PPM

4.203

3.778

3.214

2.843

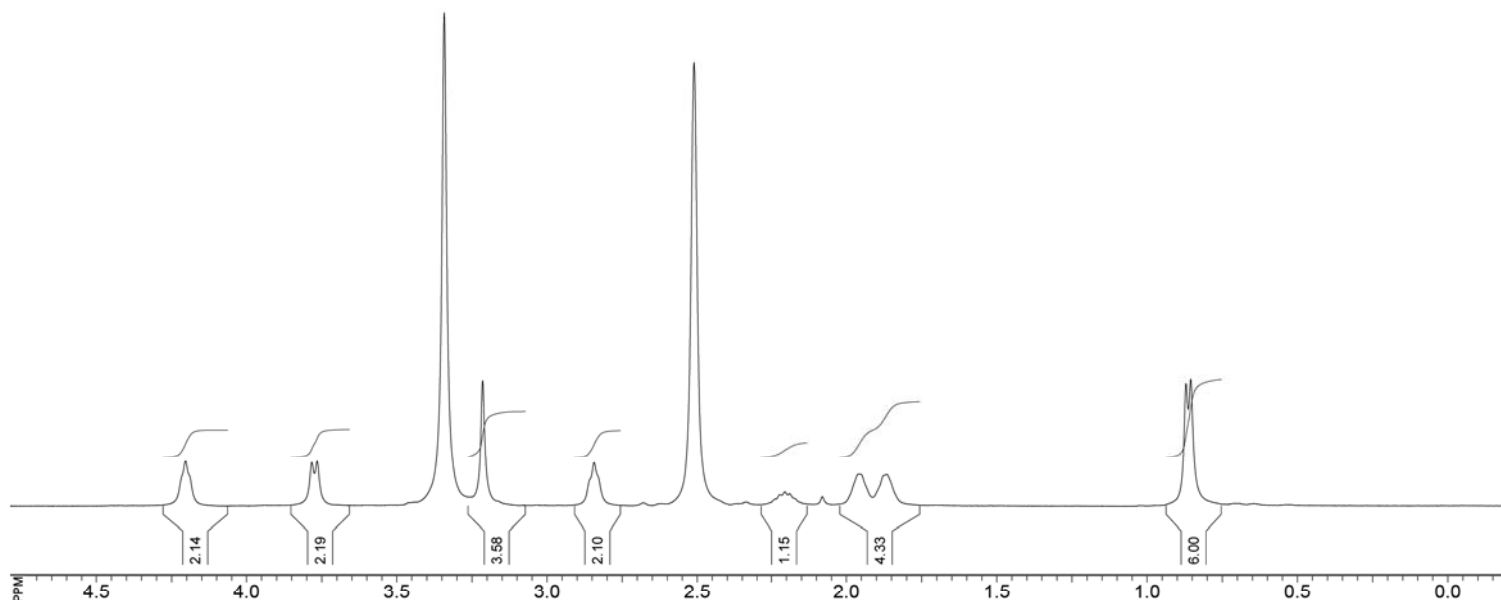
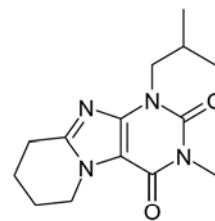
2.206

1.868

0.871

0.855

PHIk-518.fid



File name: PHIk-518.fid	Operator:	SF: 399.9703 MHz	NSC: 0	PW: 7.50 usec, RG: 32	SI: 32768
Date: 27-Jul-2011	Solvent: dms0-d6+ccl4	SW: 6803 Hz	TE: 293 K	AQ: 1.33 sec, RD: 0.00 sec	

PPM

154.58

151.49

150.87

148.29

106.16

50.08

44.87

27.93

27.18

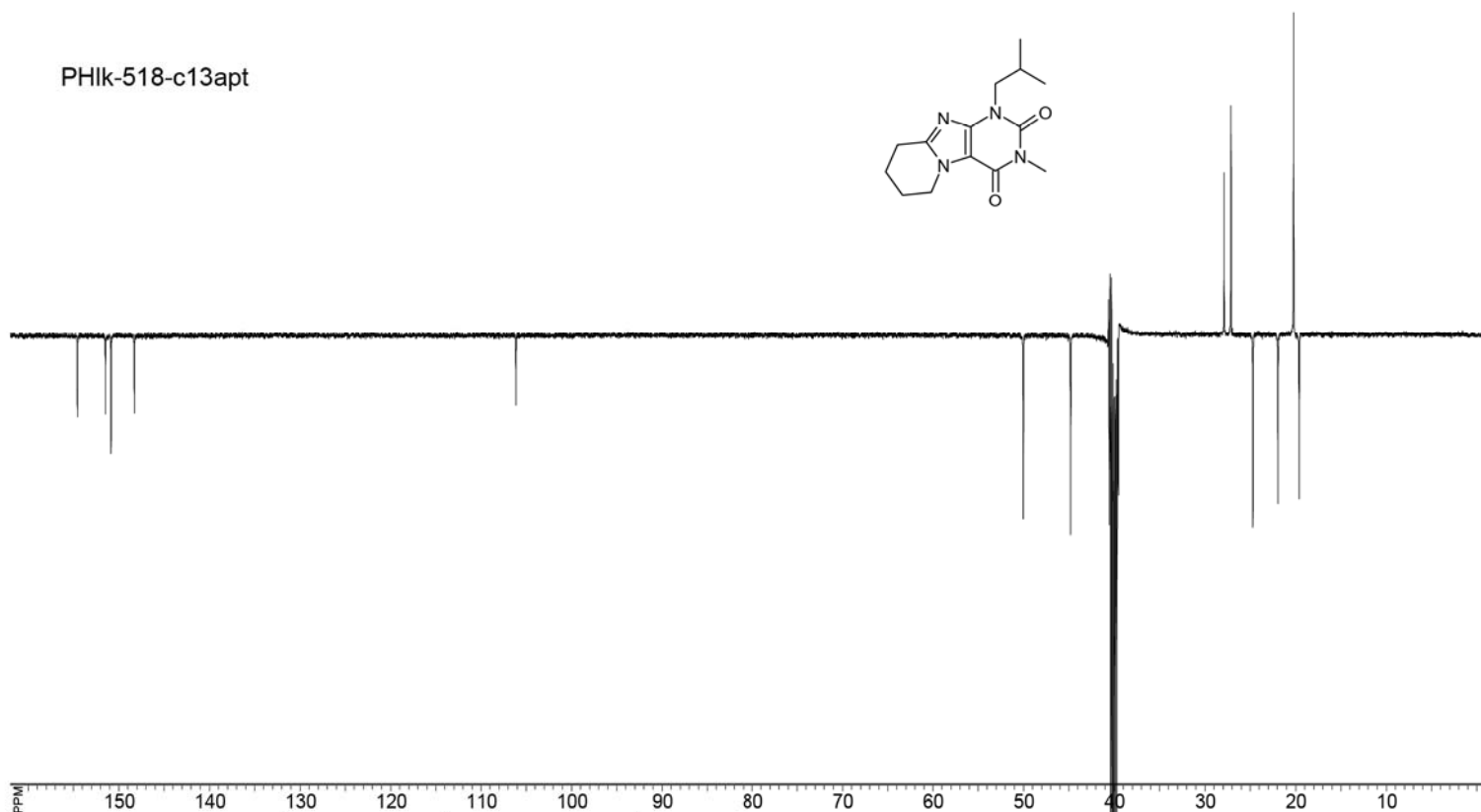
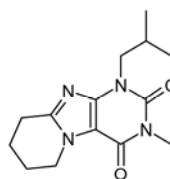
24.75

21.98

20.26

19.65

PHIk-518-c13apt



File name: PHIk-518-c13apt	Operator: root	SF: 125.7422 MHz	NSC: 15191	PW: 0.00 usec, RG: 51200	SI: 65536
Date: 27-May-2012	Solvent: dms0	SW: 30303 Hz	TE: 0 K	AQ: 1.69 sec, RD: 0.00 sec	Parameter file, XWIN-NMR Version 3.5

PPM

4.479

3.353

3.171

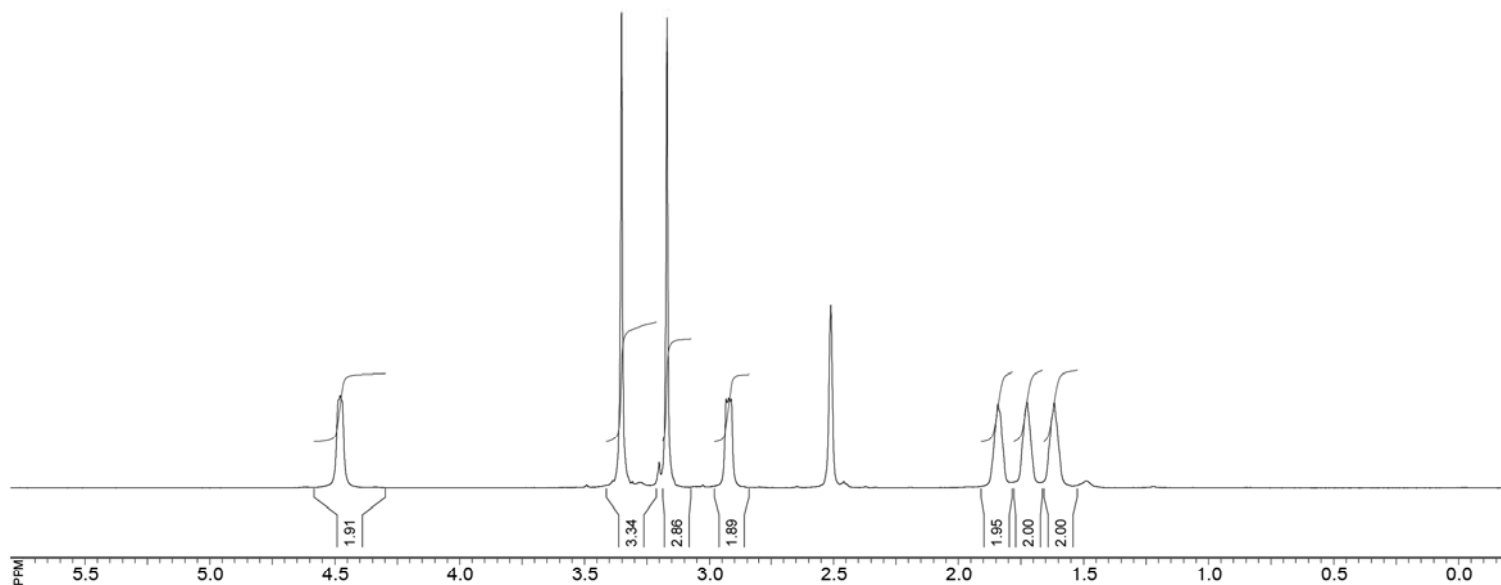
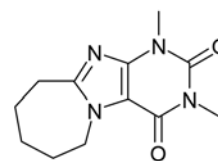
2.924

1.843

1.727

1.619

PHIk-521



File name: PHIk-521	Operator: root	SF: 500.0680 MHz	NSC: 1	PW: 0.00 usec, RG: 64	SI: 32768
Date: 22-May-2012	Solvent: dms0-d6+ccl4	SW: 8503 Hz	TE: 0 K	AQ: 1.93 sec, RD: 0.00 sec	Parameter file, XWIN-NMR Version 3.5

PPM

157.02

154.75

151.27

147.24

106.64

45.56

30.45

29.75

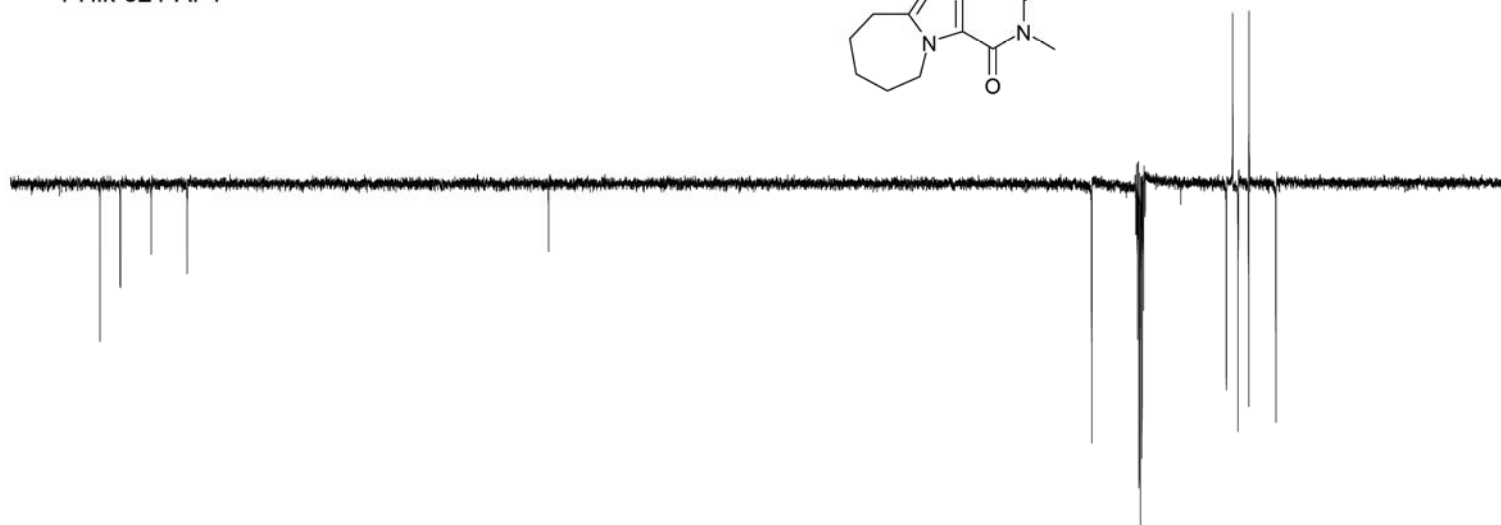
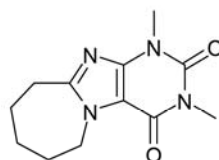
29.12

27.94

27.89

24.87

PHIk-521-APT



File name: PHIk-521-APT	Operator: root	SF: 125.7422 MHz	NSC: 202	PW: 0.00 usec, RG: 51200	SI: 65536
Date: 22-May-2012	Solvent: dms0	SW: 30303 Hz	TE: 0 K	AQ: 1.69 sec, RD: 0.00 sec	Parameter file, XWIN-NMR Version 3.5

PPM

8.300

4.485

3.853

3.834

2.921

2.275

1.901

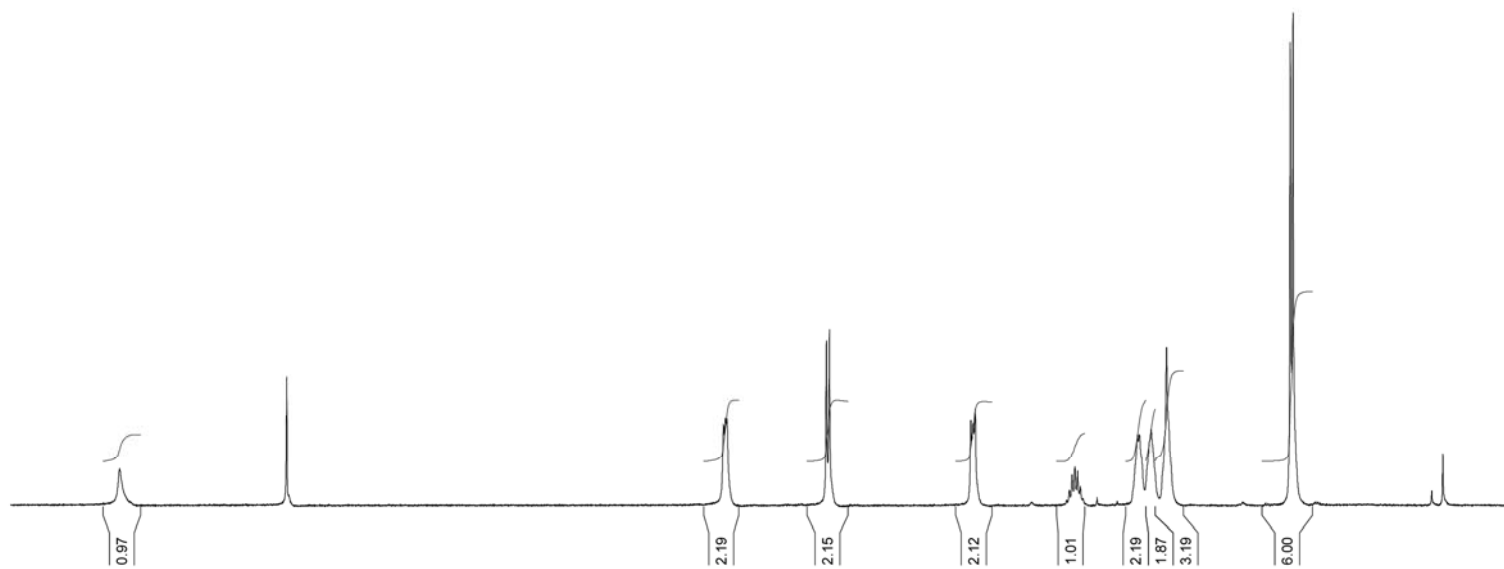
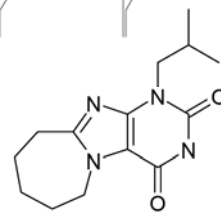
1.814

1.713

0.939

0.922

PHIk-524.fid



File name: PHIk-524.fid	Operator:	SF: 399.9683 MHz	NSC: 0	PW: 7.50 usec, RG: 32	SI: 32768
Date: 31-Jan-2011	Solvent: cddc3	SW: 6803 Hz	TE: 293 K	AQ: 1.33 sec, RD: 0.00 sec	

PPM

157.04

154.92

151.12

149.54

107.45

49.55

46.11

30.80

29.59

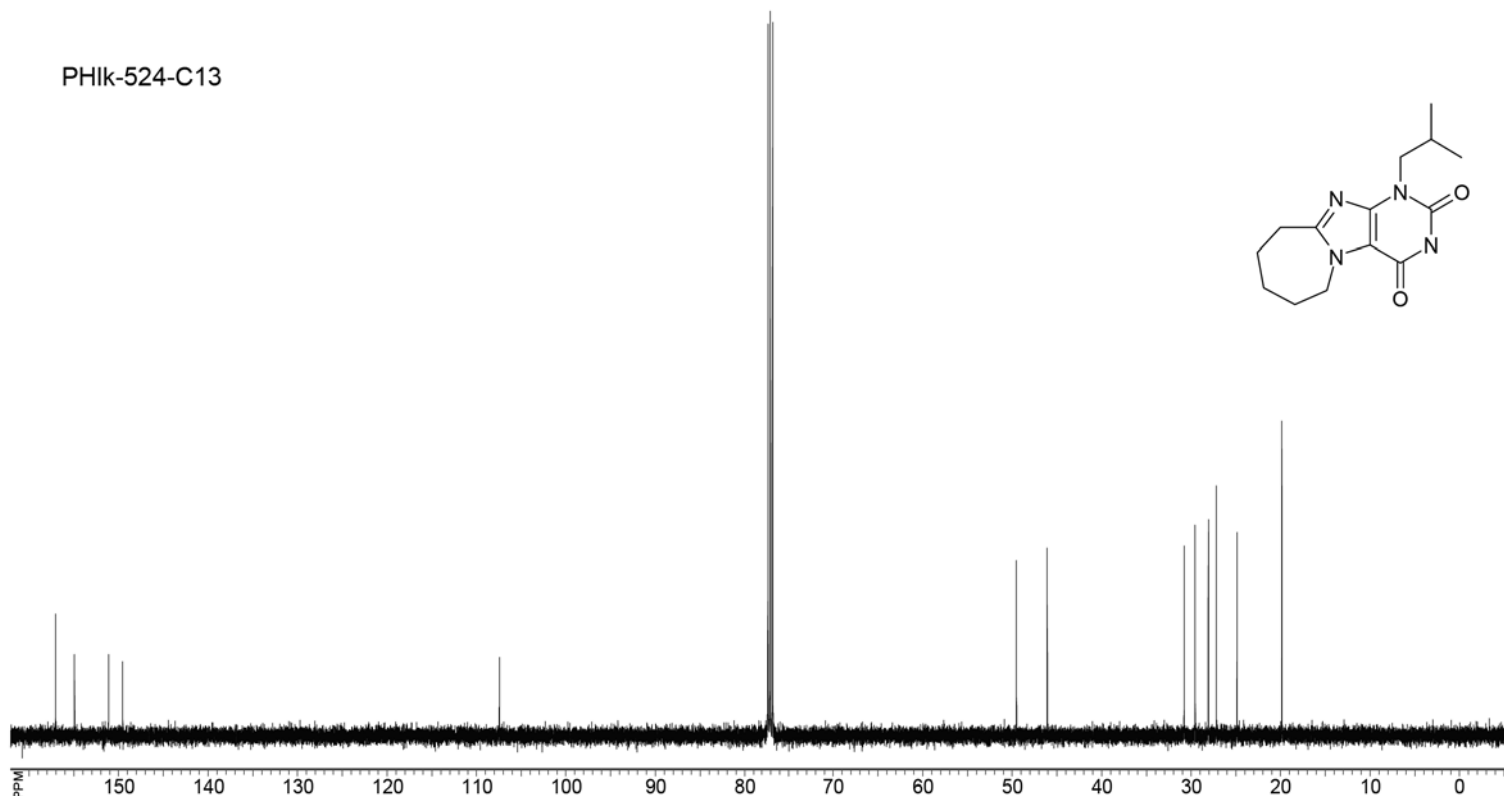
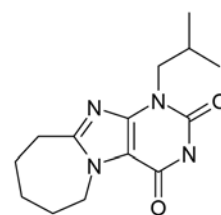
28.10

27.21

24.89

19.89

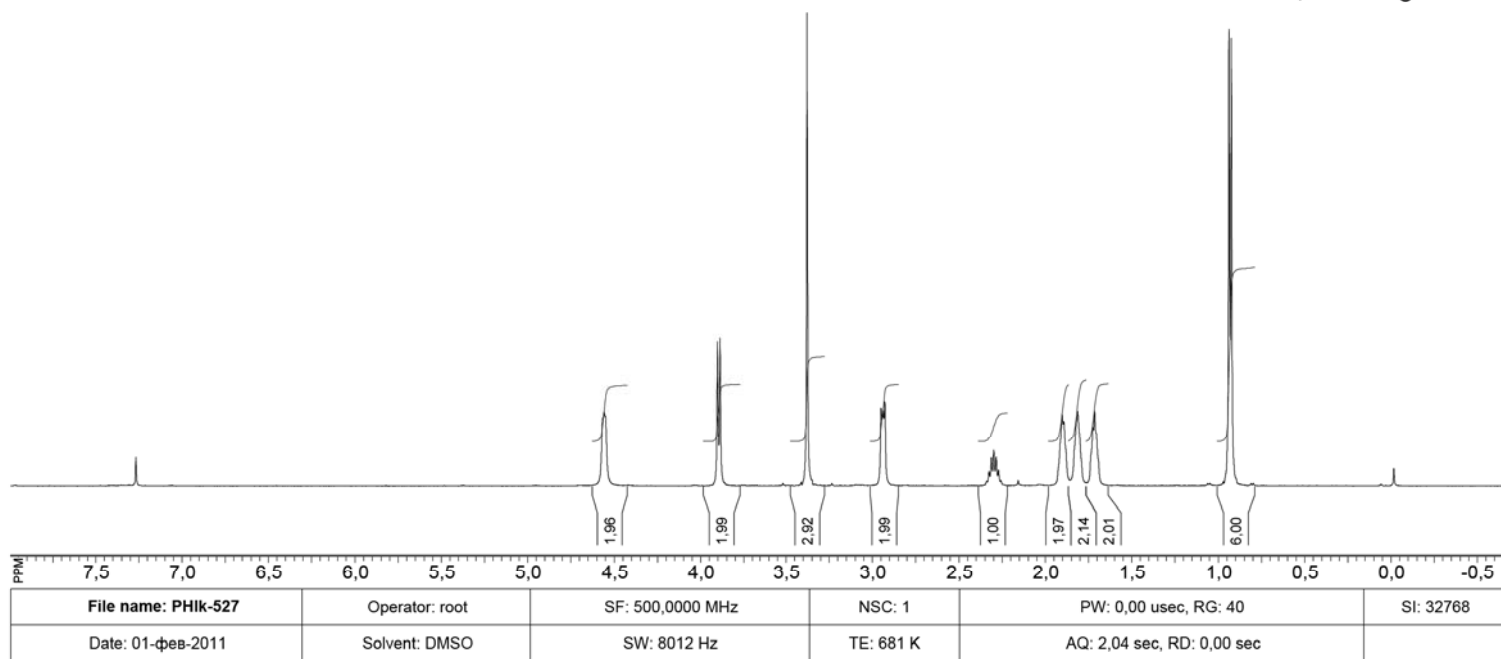
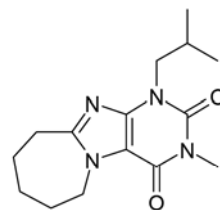
PHIk-524-C13



File name: PHIk-524-C13	Operator: root	SF: 125.7422 MHz	NSC: 443	PW: 0.00 usec, RG: 51200	SI: 65536
Date: 01-Feb-2011	Solvent: dms0	SW: 32680 Hz	TE: 681 K	AQ: 1.57 sec, RD: 0.00 sec	

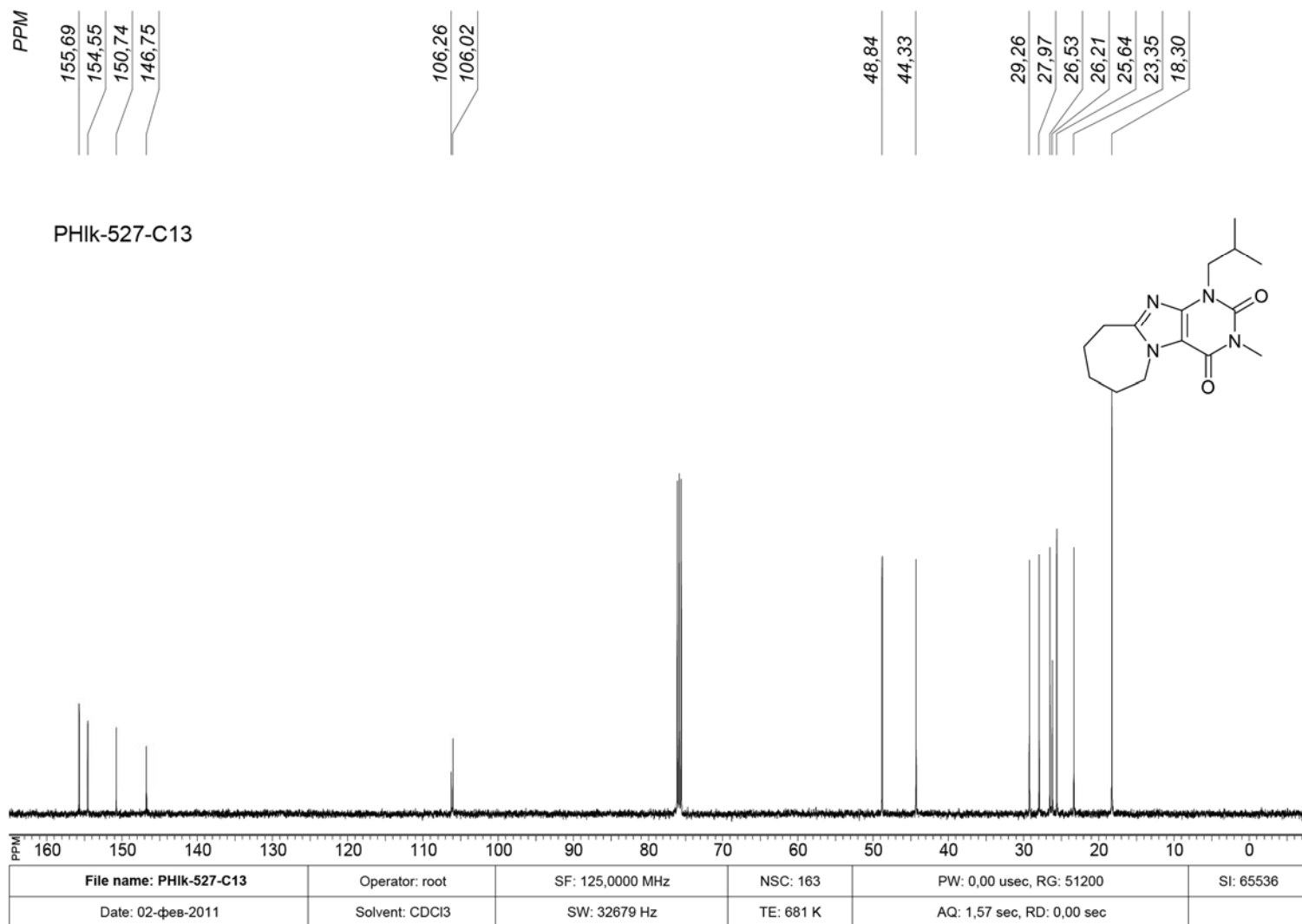
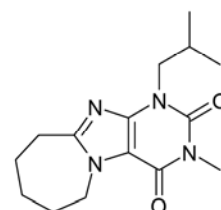
PPM

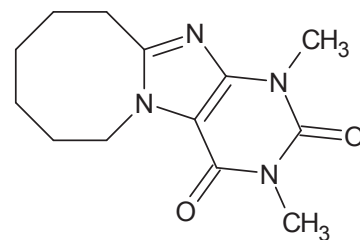
PHIk-527



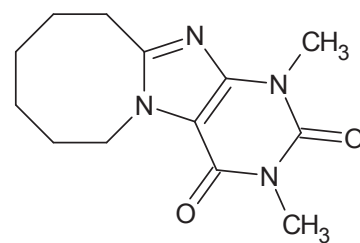
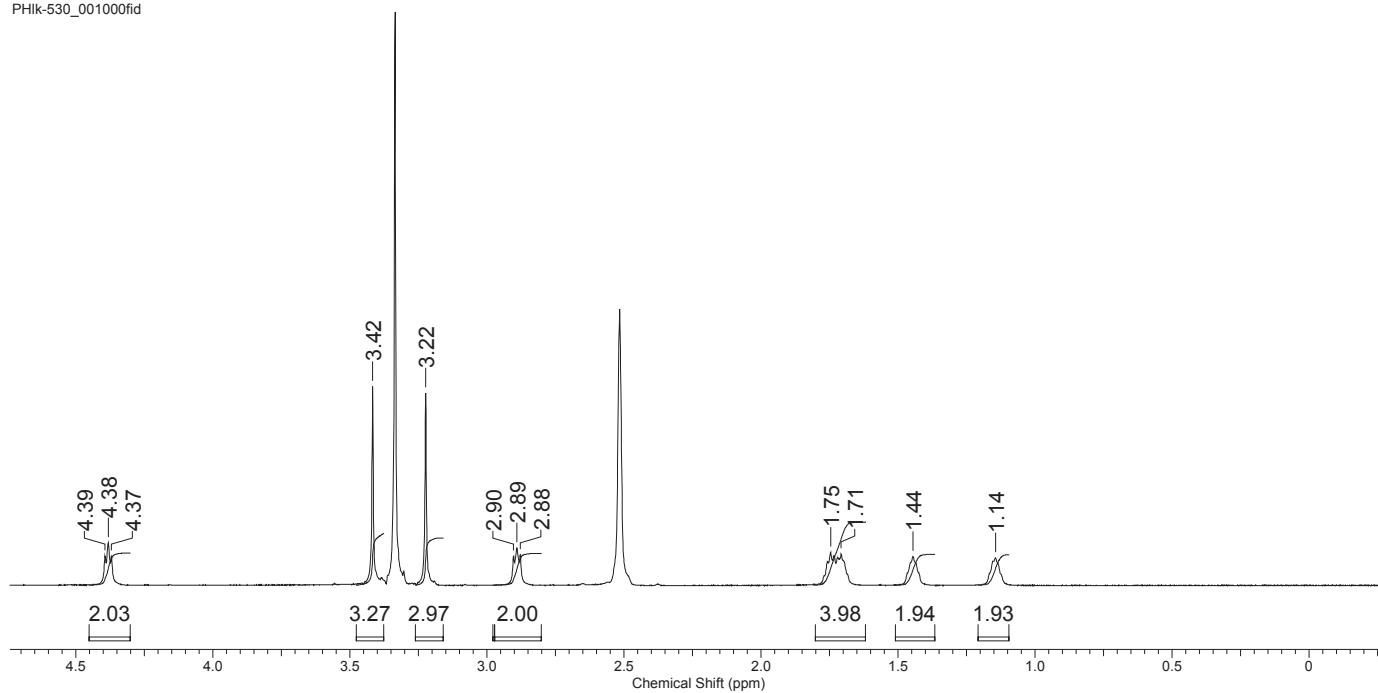
PPM

PHIk-527-C13

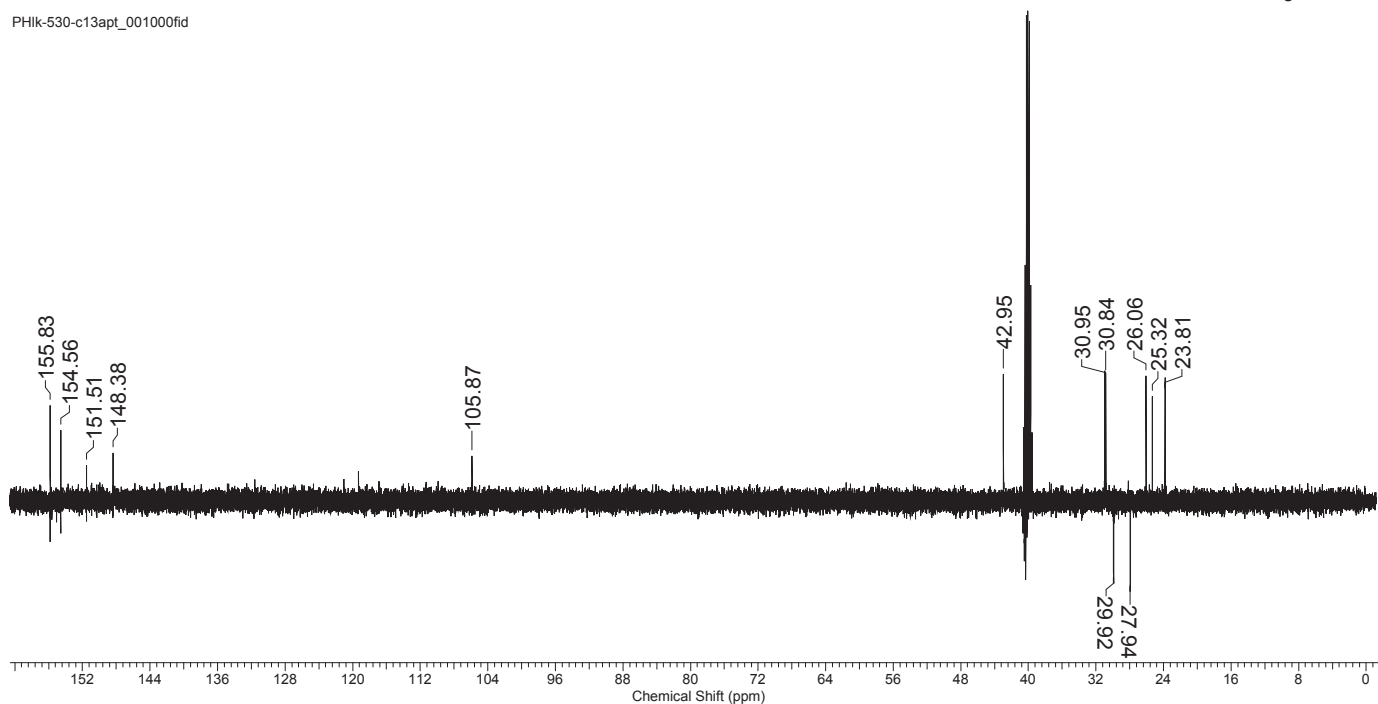




PHIk-530_001000fid



PHIk-530-c13apt_001000fid



PPM

10.987

4.340

3.737

3.723

2.861

2.182

1.733

1.679

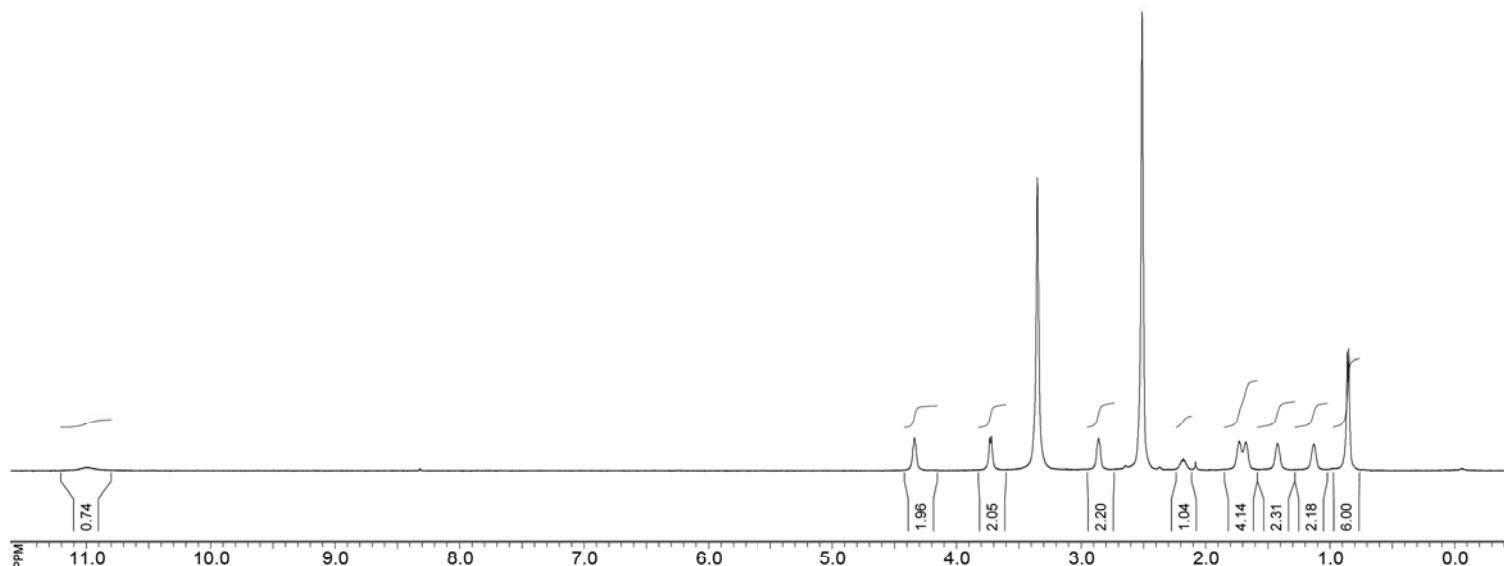
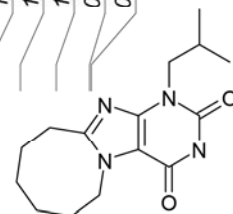
1.424

1.134

0.866

0.852

PHIk-533



File name: PHIk-533	Operator: root	SF: 500.0680 MHz	NSC: 1	PW: 0.00 usec, RG: 16	SI: 32768
Date: 14-Jan-2011	Solvent: DMSO	SW: 8013 Hz	TE: 0 K	AQ: 2.04 sec, RD: 0.00 sec	

PPM

154.92

154.21

150.58

149.26

105.10

47.60

41.45

29.50

29.36

25.67

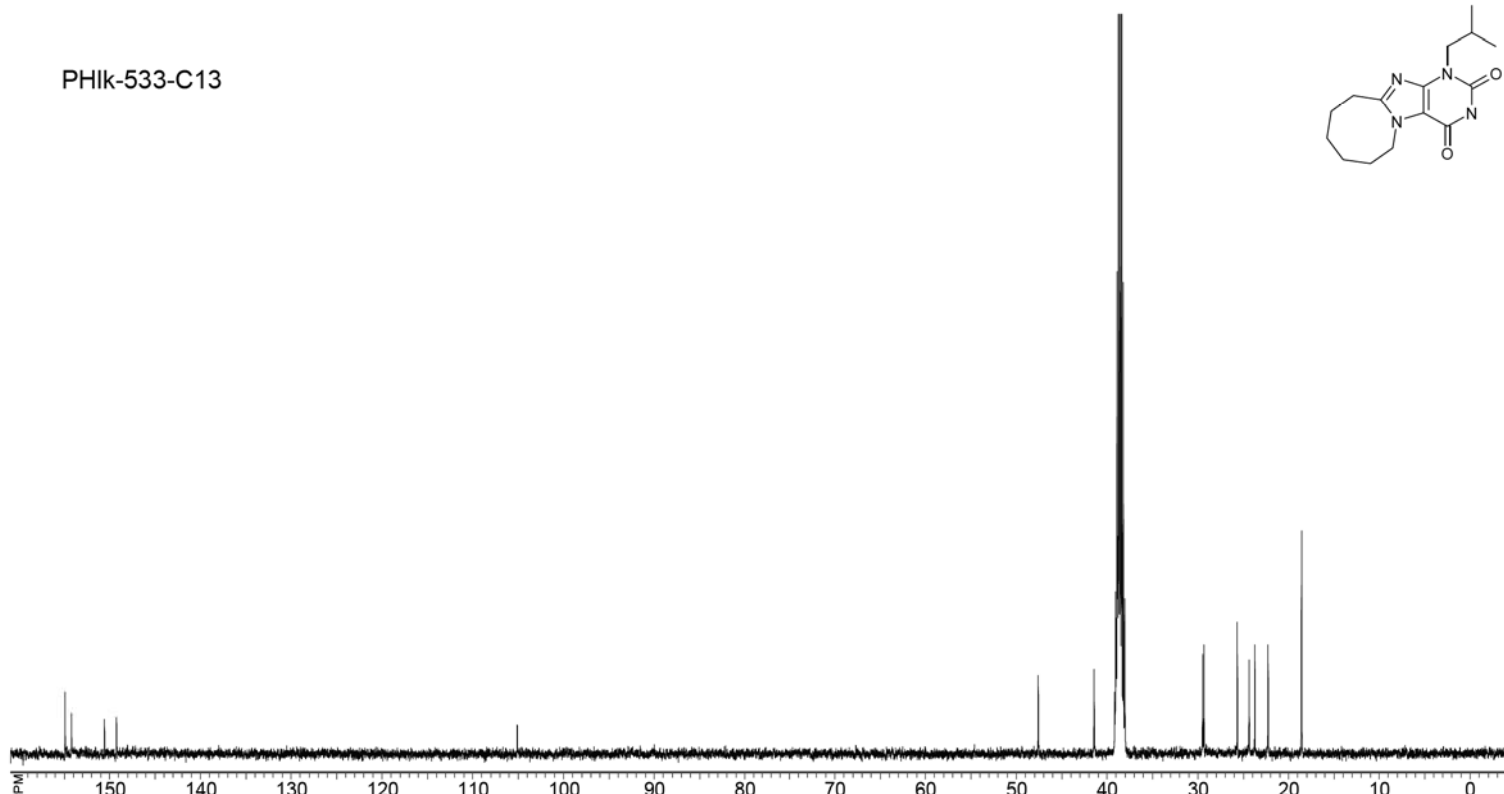
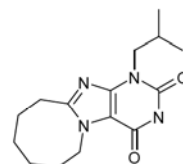
24.37

23.74

22.29

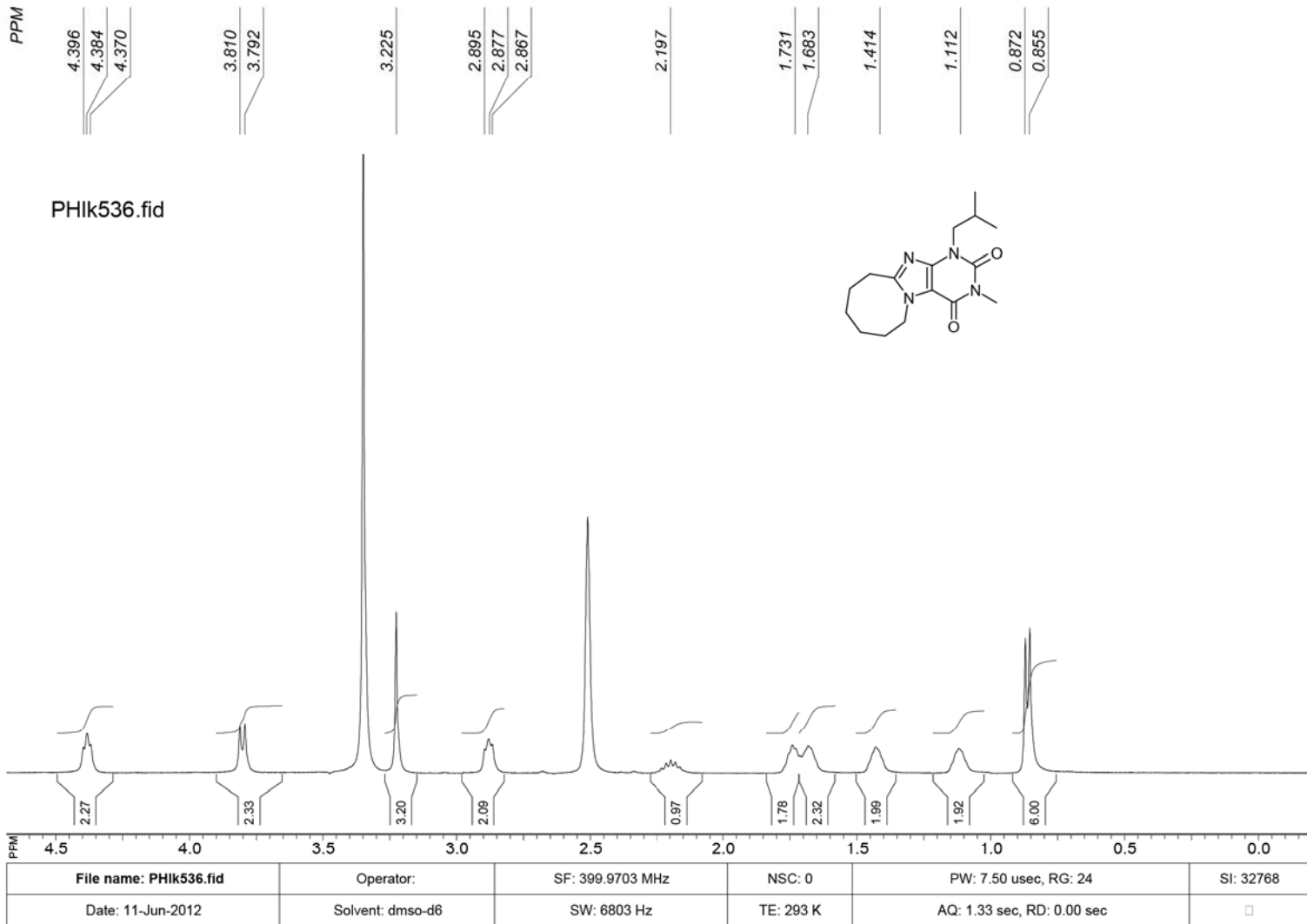
18.60

PHIk-533-C13



File name: PHIk-533-C13	Operator: root	SF: 125,0000 MHz	NSC: 343	PW: 0.00 usec, RG: 51200	SI: 65536
Date: 19-январь-2011	Solvent: DMSO	SW: 32679 Hz	TE: 0 K	AQ: 1.57 sec, RD: 0.00 sec	

PPM



PPM

