

Supplementary information

Catalyst-free Biginelli-type synthesis of new functionalized 4,7-dihydropyrazolo[1,5-*a*]pyrimidines

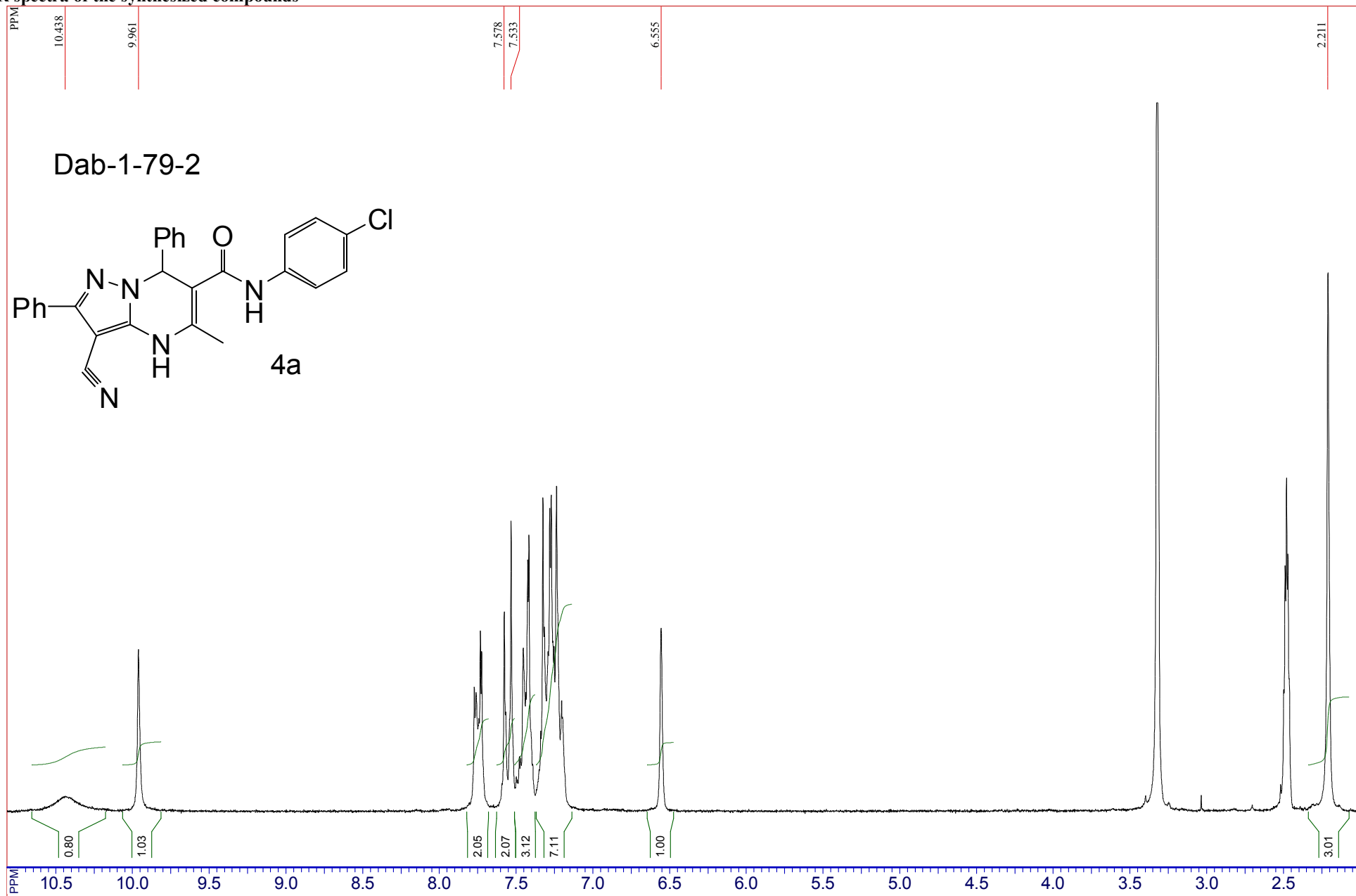
Maksim A. Kolosov,^a Dmitriy A. Beloborodov,^a Valeriy D. Orlov^a and Victor V. Dotsenko^{*b,c}

^aDepartment of Organic Chemistry, V.N. Karazin Kharkiv National University, Svobody sq., 4, 61022 Kharkiv, Ukraine

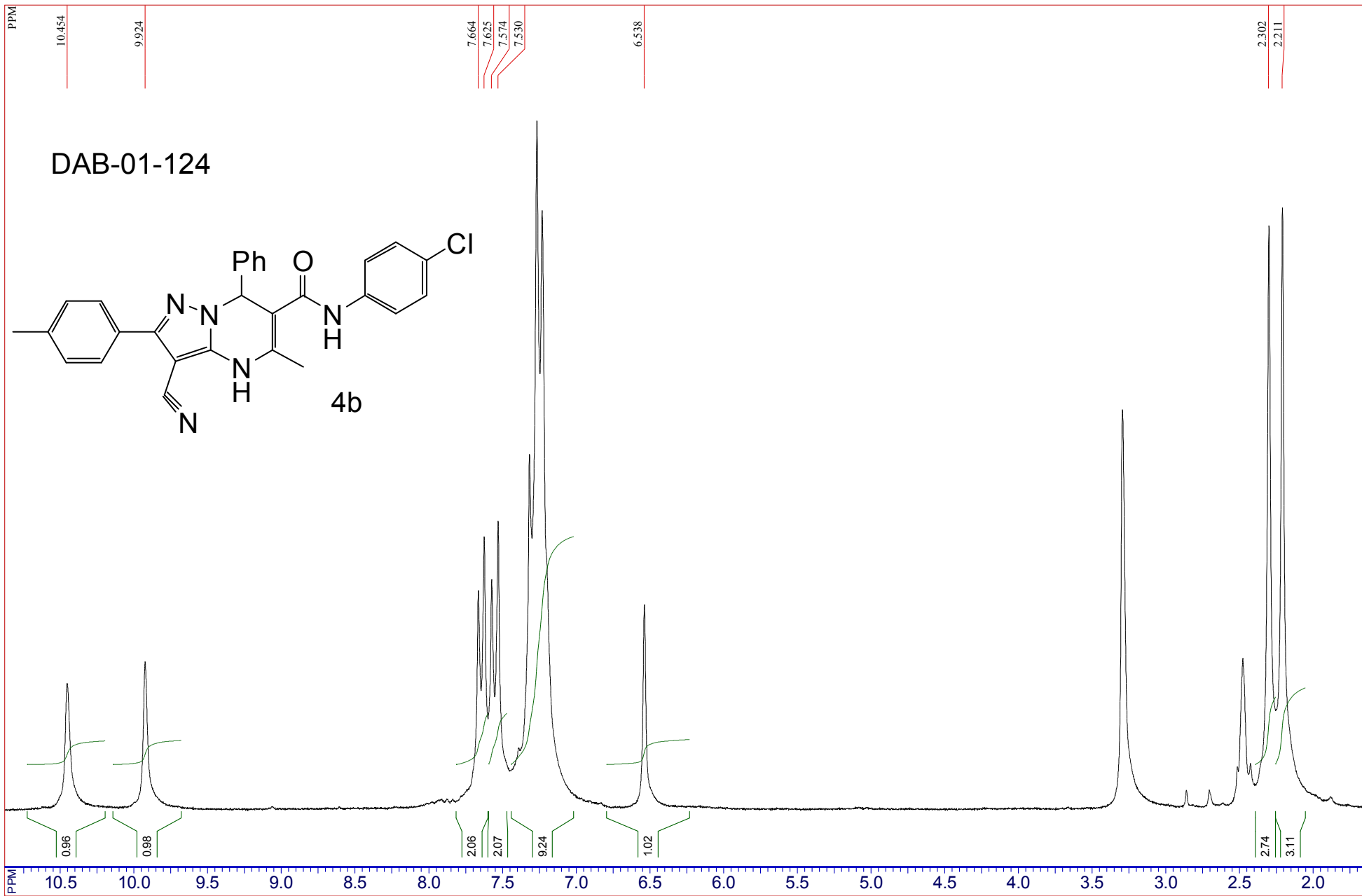
^bDepartment of Organic Chemistry & Technologies, Kuban State University, 149 Stavropolskaya str., 350040 Krasnodar, Russian Federation

^cDepartment of Chemistry, North Caucasus Federal University, 1a Pushkin St., 355009 Stavropol, Russian Federation

2. ¹H NMR spectra of the synthesized compounds

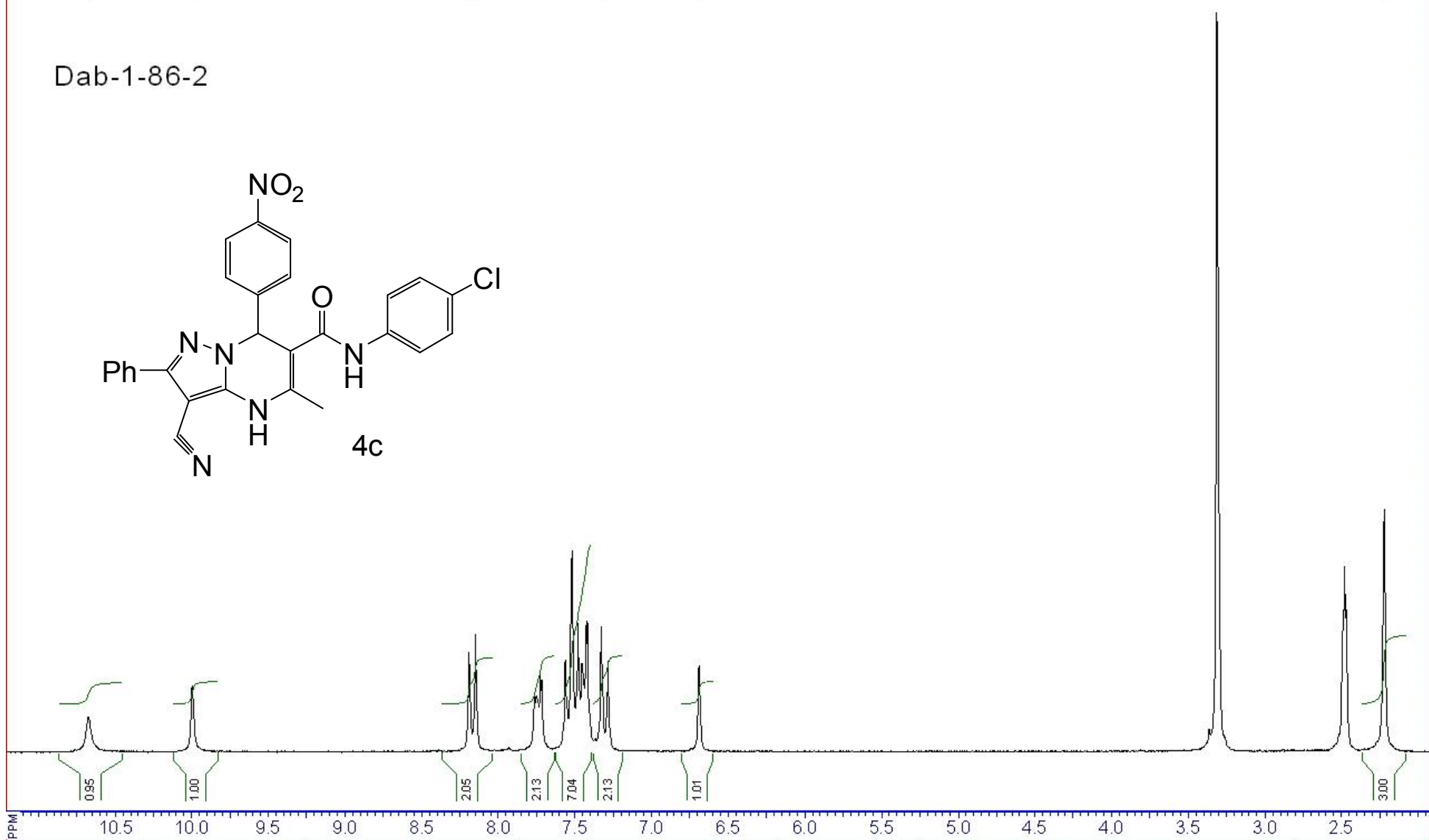
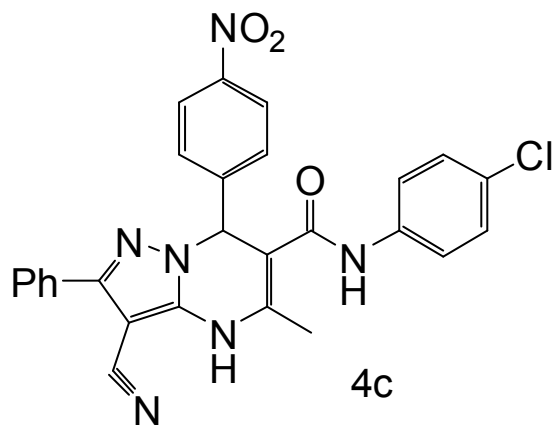


File name: Dab-1-79-2	Operator:	SF: 199.9704 MHz	NSC: 0	PW: 4.00 usec, RG: 28	SI: 32768
Date: 09-Jun-2008	Solvent: DMSO	SW: 5000 Hz	TE: 302 K	AQ: 1.99 sec, RD: 0.00 sec	

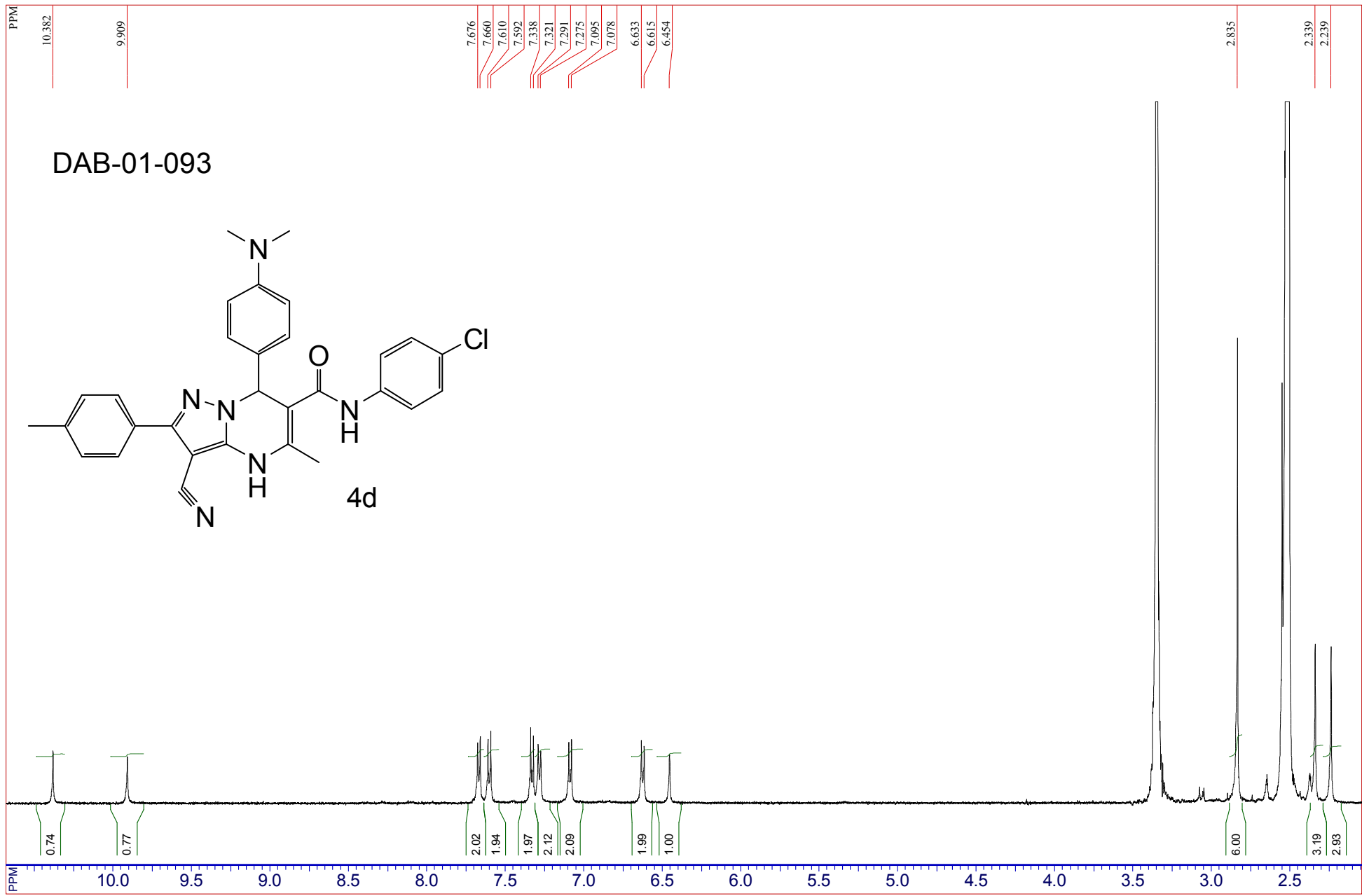


File name: DAB-01-124	Operator:	SF: 199.9704 MHz	NSC: 0	PW: 7.00 usec, RG: 34	SI: 32768
Date: 08-Dec-2008	Solvent: DMSO	SW: 5000 Hz	TE: 292 K	AQ: 2.00 sec, RD: 0.00 sec	

Dab-1-86-2



File name: Dab-1-86-2	Operator:	SF: 199.9704 MHz	NSC: 0	PW: 4.00 usec, RG: 30	SI: 32768
Date: 21-May-2008	Solvent: DMSO	SW: 5000 Hz	TE: 302 K	AQ: 1.99 sec, RD: 0.00 sec	



File name: DAB-01-093	Operator: root	SF: 500.0680 MHz	NSC: 1	PW: 0.00 usec, RG: 32	SI: 32768
Date: 12-Oct-2011	Solvent: DMSO	SW: 8013 Hz	TE: 0 K	AQ: 2.04 sec, RD: 0.00 sec	

PPM

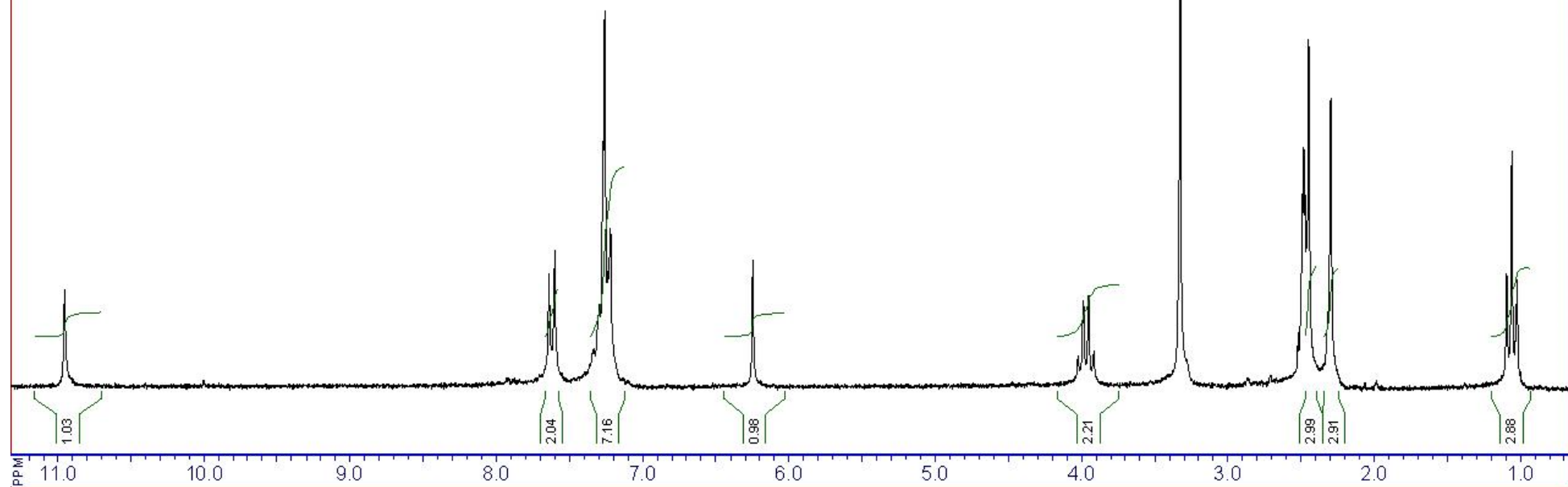
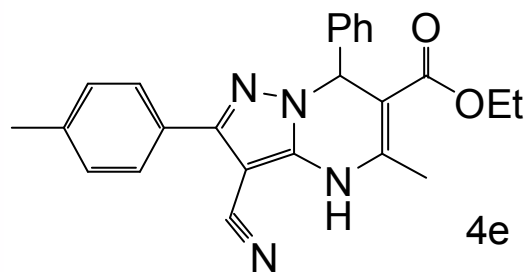
10.952

7.642
7.602

6.248

4.025
3.989
3.954
3.9182.450
2.2981.096
1.060
1.025

DAB-1-137



File name: DAB-1-137	Operator:	SF: 199.9704 MHz	NSC: 0	PW: 7.00 usec, RG: 32	SI: 32768
Date: 26-Jan-2009	Solvent: DMSO	SW: 5000 Hz	TE: 302 K	AQ: 1.92 sec, RD: 0.00 sec	

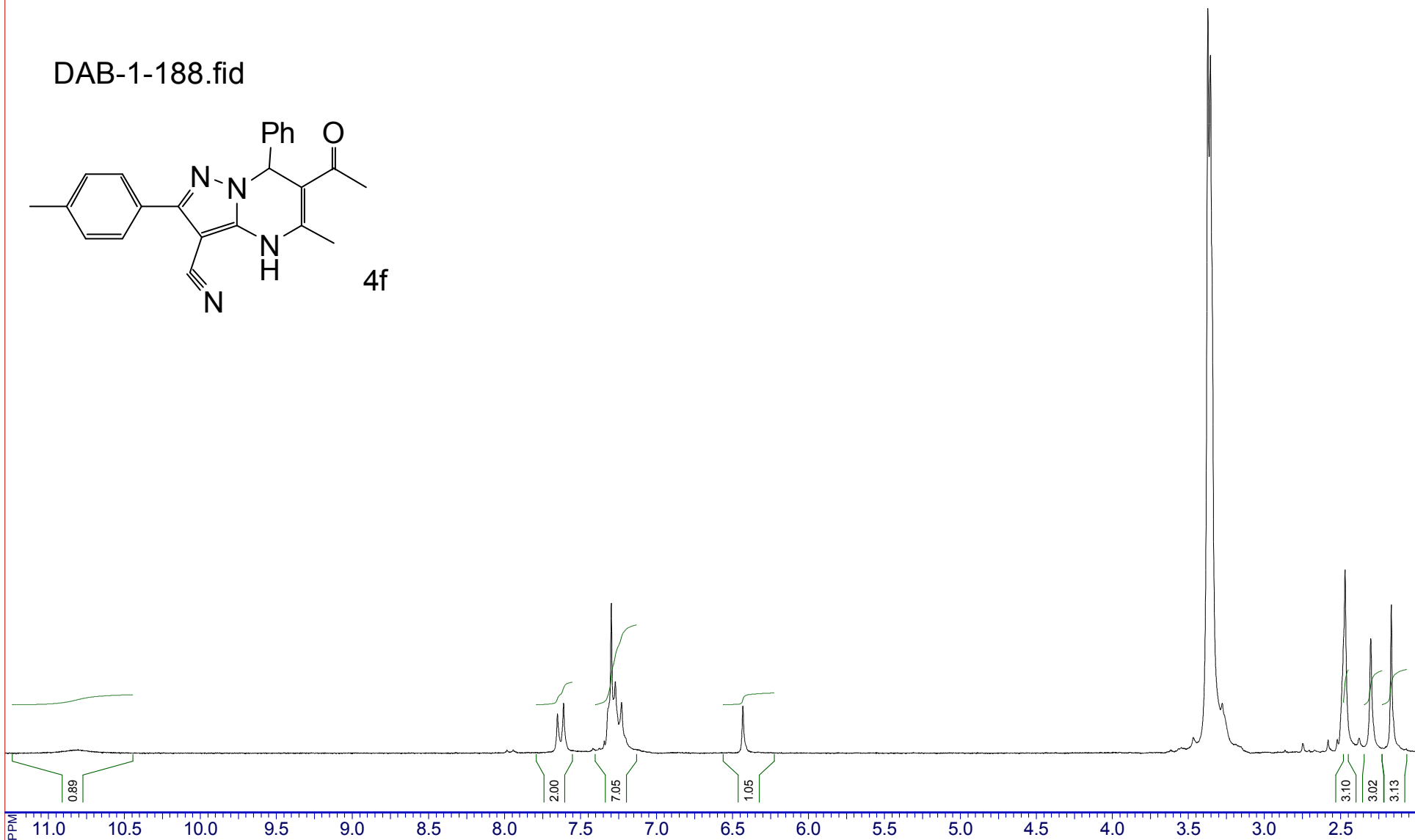
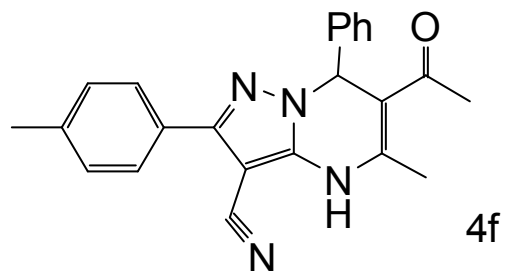
PPM

7.652
7.611

6.432

2.472
2.303
2.167

DAB-1-188.fid



File name: DAB-1-188.fid	Operator:	SF: 199.9704 MHz	NSC: 0	PW: 7.00 usec, RG: 39	SI: 32768
Date: 29-Jul-2009	Solvent: DMSO	SW: 5999 Hz	TE: 293 K	AQ: 1.99 sec, RD: 0.00 sec	

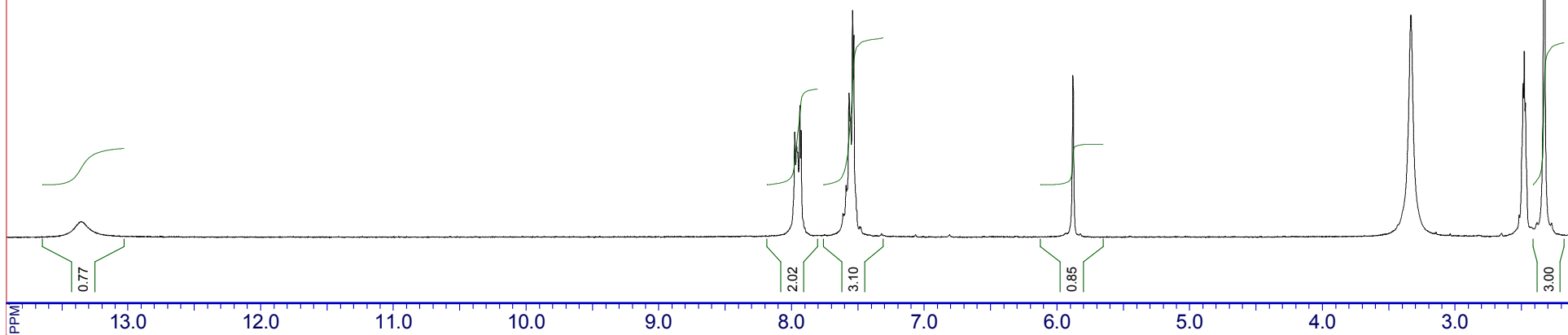
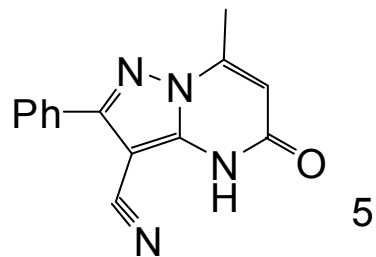
PPM

13.352

5.881

2.331

DAB-1-81



PPM

File name: DAB-1-81

Operator:

SF: 199.9704 MHz

NSC: 0

PW: 4.00 usec, RG: 36

SI: 32768

Date: 23-Apr-2008

Solvent: DMSO

SW: 5000 Hz

TE: 302 K

AQ: 1.99 sec, RD: 0.00 sec

PPM

7.930
7.8897.347
7.307

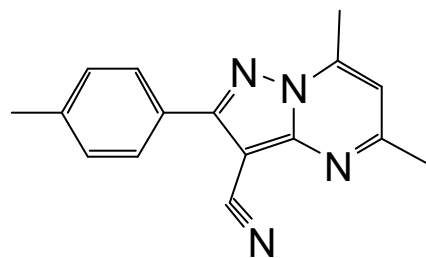
7.088

2.716

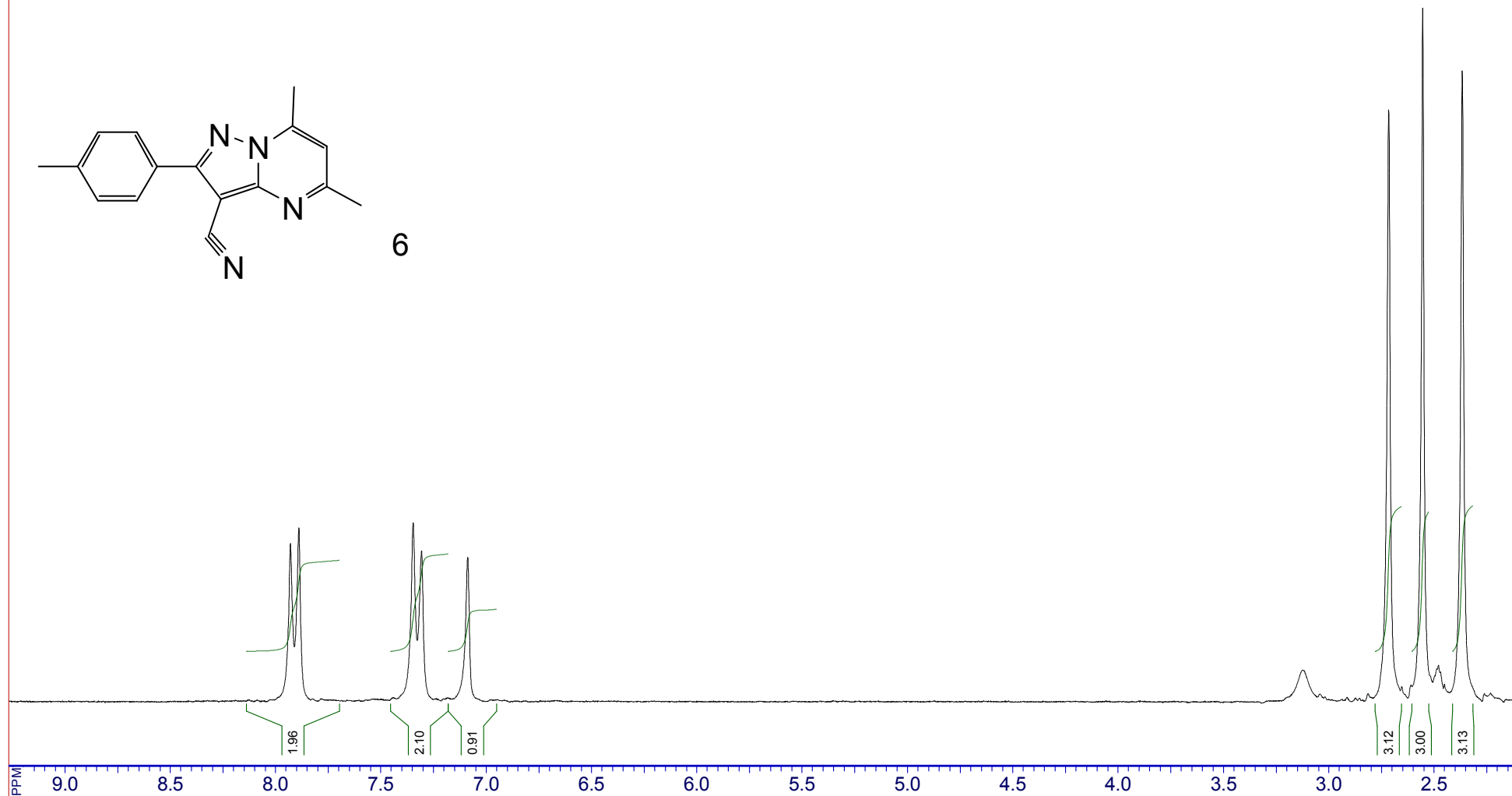
2.555

2.367

DAB-01-149



6



PPM

9.0

8.5

8.0

7.5

7.0

6.5

6.0

5.5

5.0

4.5

4.0

3.5

3.0

2.5

File name: DAB-01-149

Operator:

SF: 199.9706 MHz

NSC: 0

PW: 7.00 usec, RG: 32

SI: 32768

Date: 23-Feb-2009

Solvent: DMSO

SW: 5000 Hz

TE: 302 K

AQ: 2.56 sec, RD: 0.00 sec

PPM

11.322

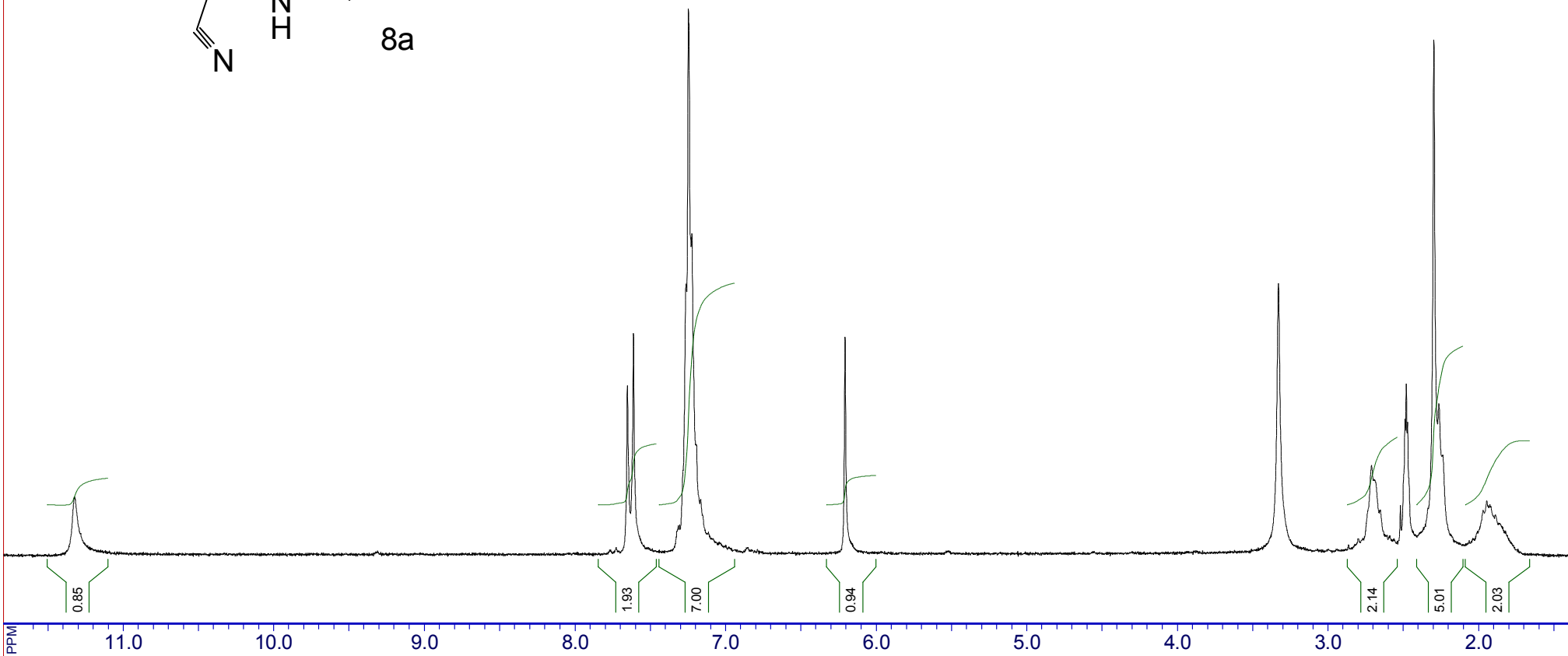
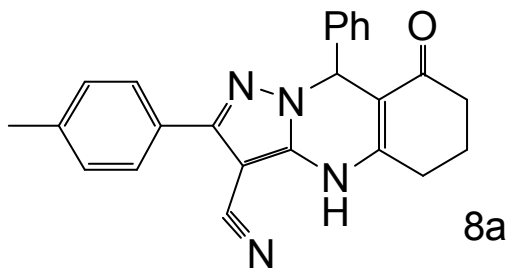
7.653

7.612

6.208

2.299

DAB-1-136



PPM

File name: DAB-1-136

Operator:

SF: 199.9704 MHz

NSC: 0

PW: 7.00 usec, RG: 32

SI: 32768

Date: 26-Jan-2009

Solvent: DMSO

SW: 5000 Hz

TE: 302 K

AQ: 1.92 sec, RD: 0.00 sec

PPM

11.183

7.662

7.628

7.260

7.227

7.050

7.015

6.593

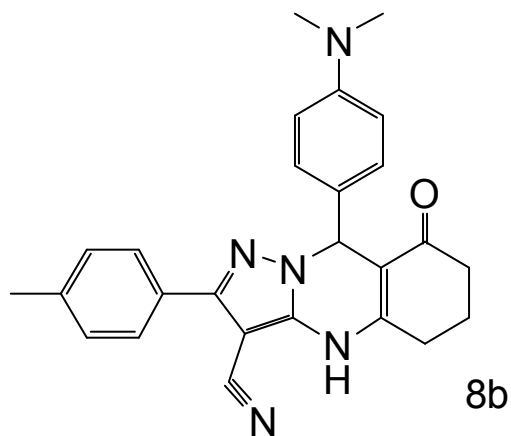
6.557

6.094

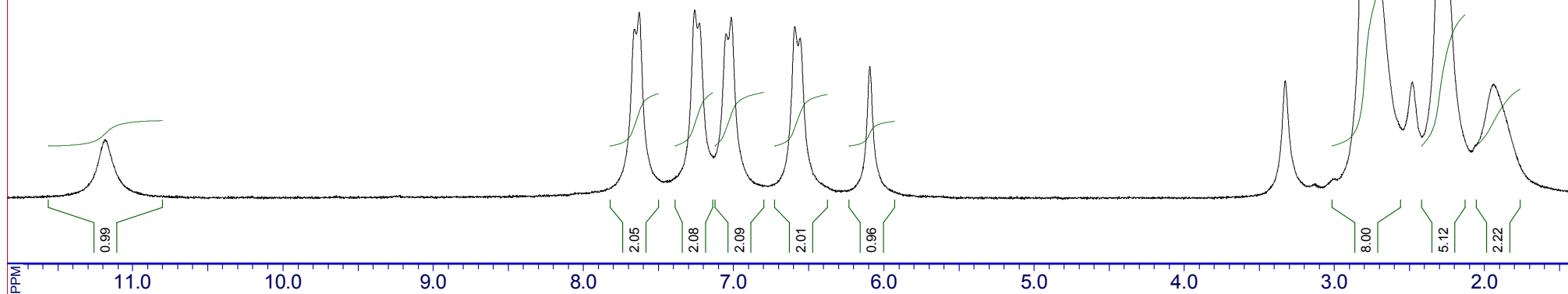
2.795

2.298

Dab-1-144



8b



File name: Dab-1-144

Operator:

SF: 199.9704 MHz

NSC: 0

PW: 7.00 usec, RG: 32

SI: 32768

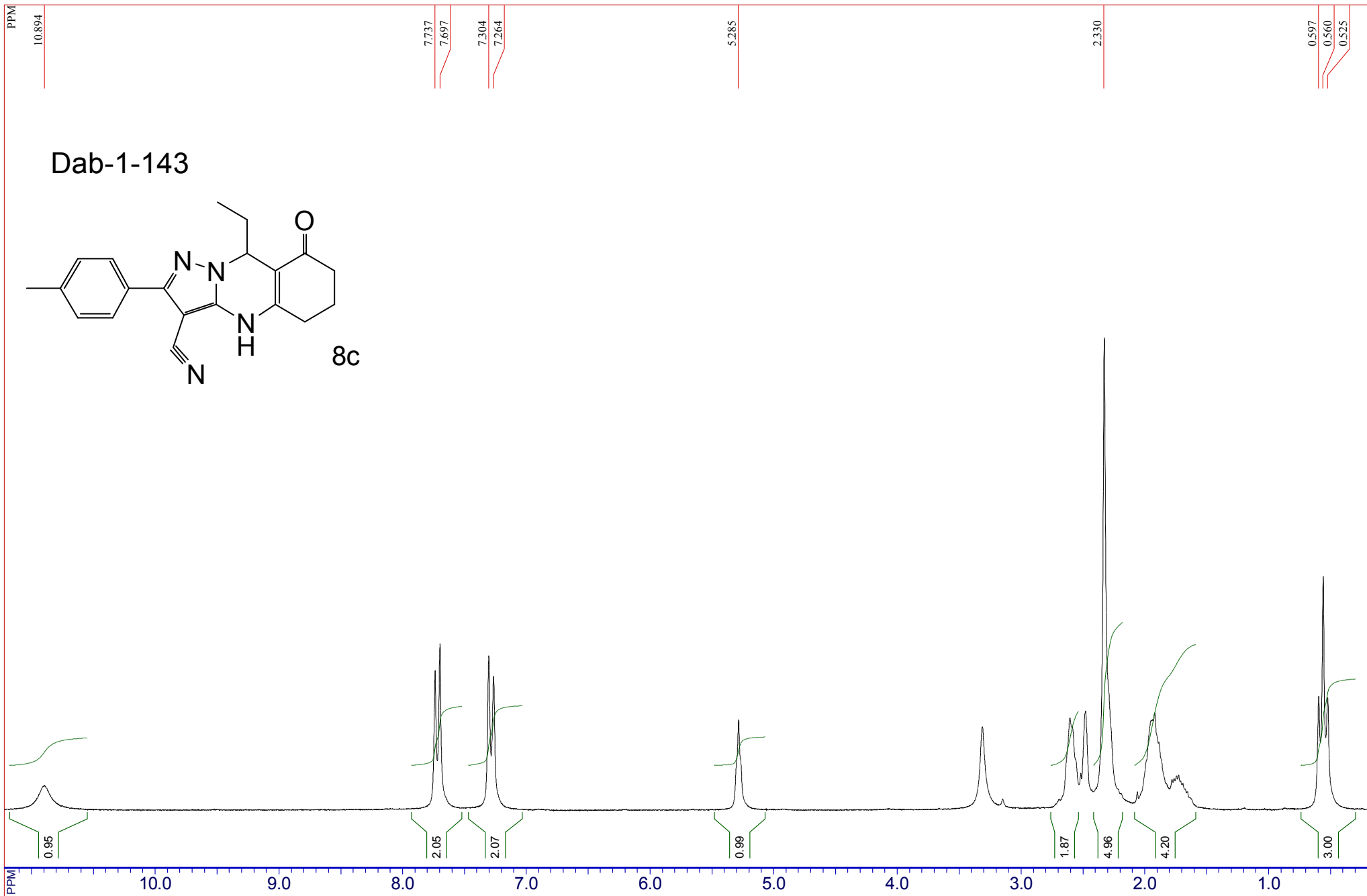
Date: 04-Feb-2009

Solvent: DMSO

SW: 5999 Hz

TE: 302 K

AQ: 1.92 sec, RD: 0.00 sec



File name: Dab-1-143	Operator:	SF: 199.9704 MHz	NSC: 0	PW: 7.00 usec, RG: 32	SI: 32768
Date: 04-Feb-2009	Solvent: DMSO	SW: 5999 Hz	TE: 302 K	AQ: 1.92 sec, RD: 0.00 sec	

PPM

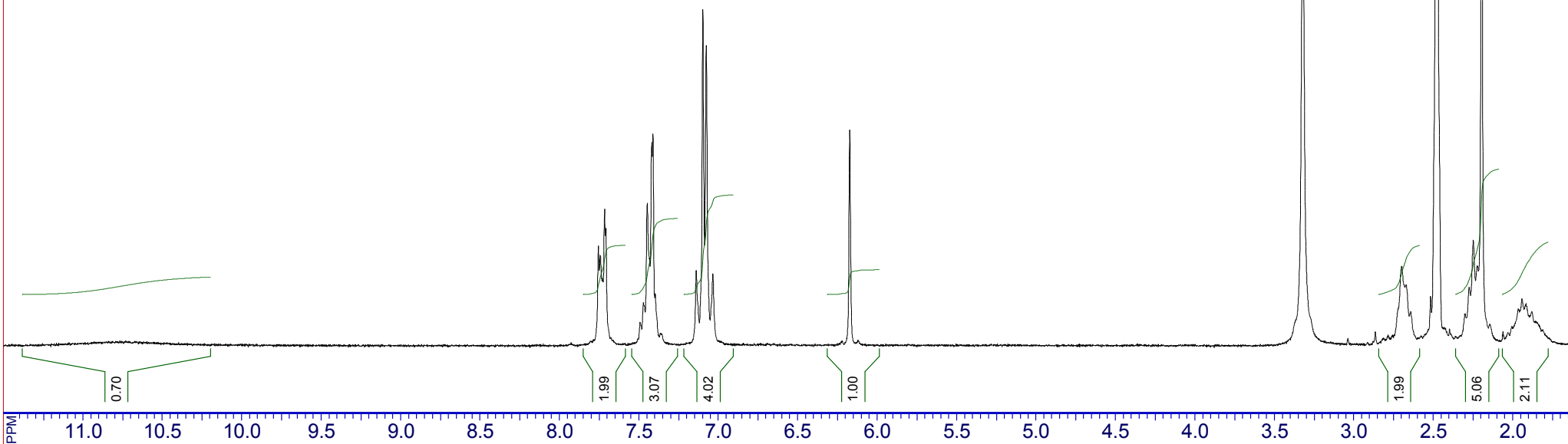
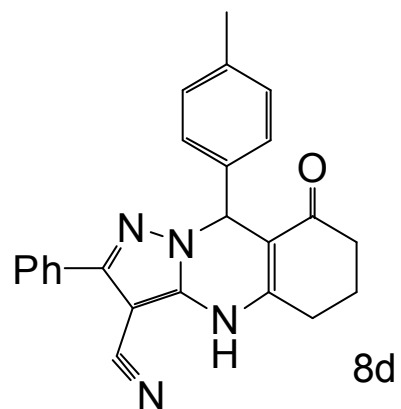
10.767

7.140
7.098
7.076
7.035

6.173

2.198

DAB-01-088



PPM

11.0 10.5 10.0 9.5 9.0 8.5 8.0

7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0

2.5 2.0

File name: DAB-01-088

Operator:

SF: 199.9704 MHz

NSC: 0

PW: 4.00 usec, RG: 39

SI: 32768

Date: 15-May-2008

Solvent: DMSO

SW: 5000 Hz

TE: 302 K

AQ: 1.99 sec, RD: 0.00 sec

PPM

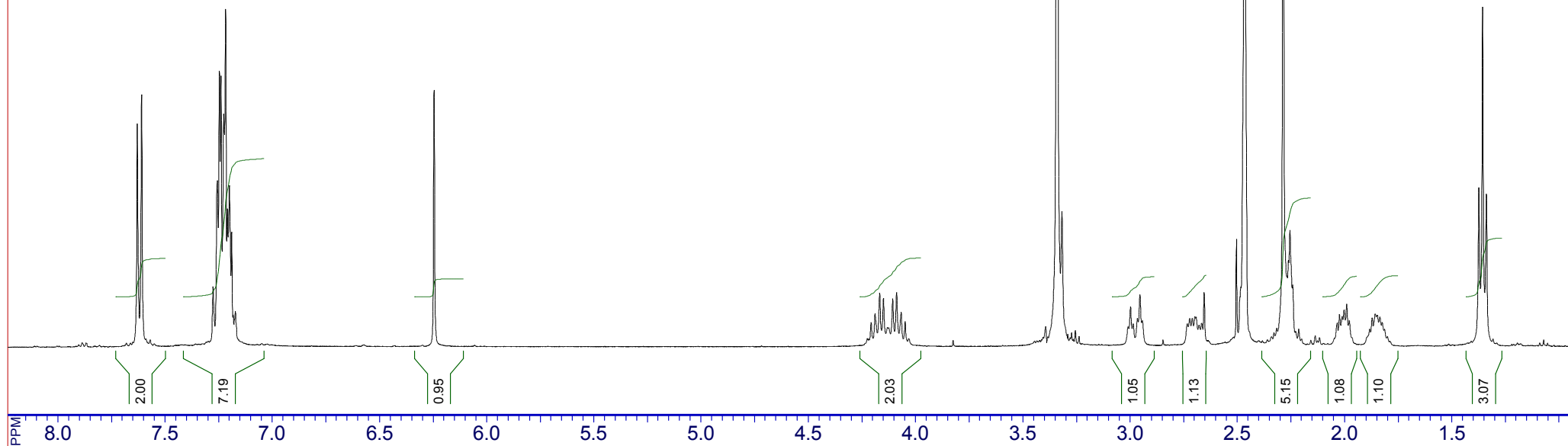
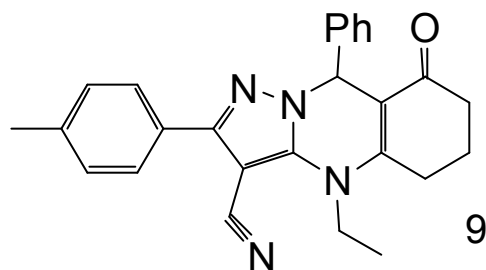
7.629
7.609

6.245

2.287

1.375
1.357
1.340

DAB-2-104-P1.fid



File name: DAB-2-104-P1.fid

Operator:

SF: 399.6338 MHz

NSC: 0

PW: 6.95 usec, RG: 30

SI: 32768

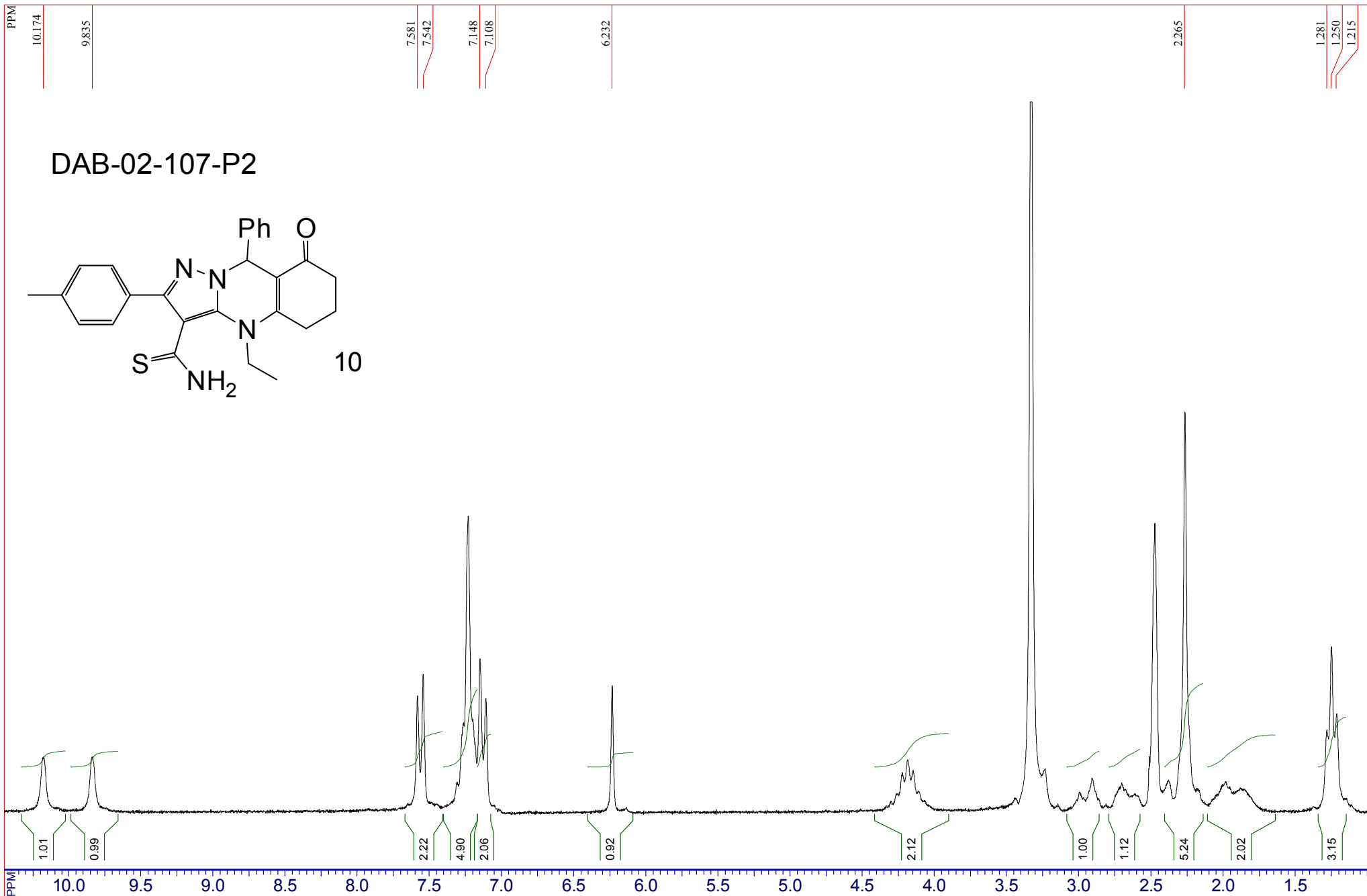
Date: 13-Sep-2015

Solvent: dms0

SW: 6410 Hz

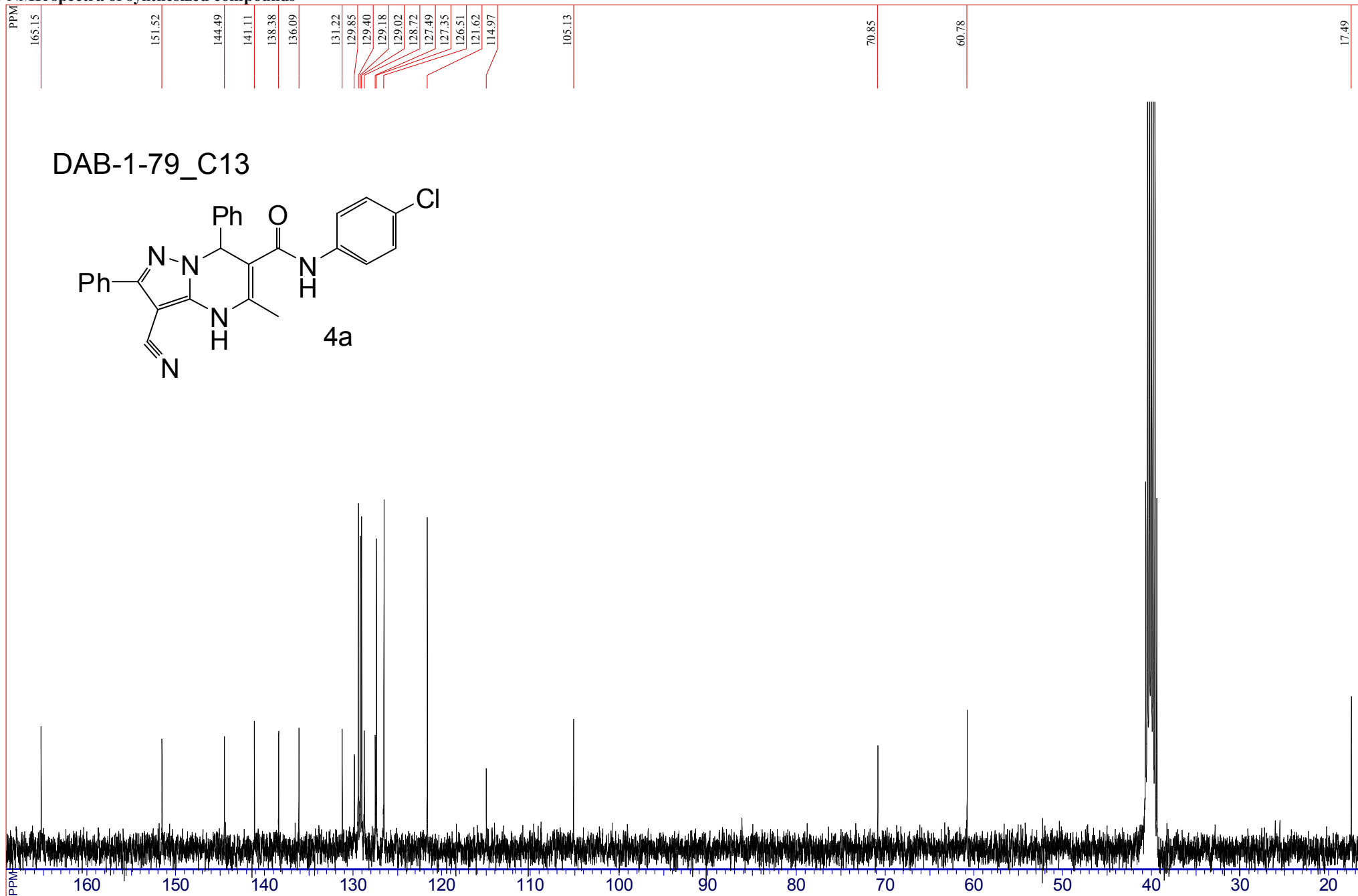
TE: 298 K

AQ: 2.56 sec, RD: 0.00 sec



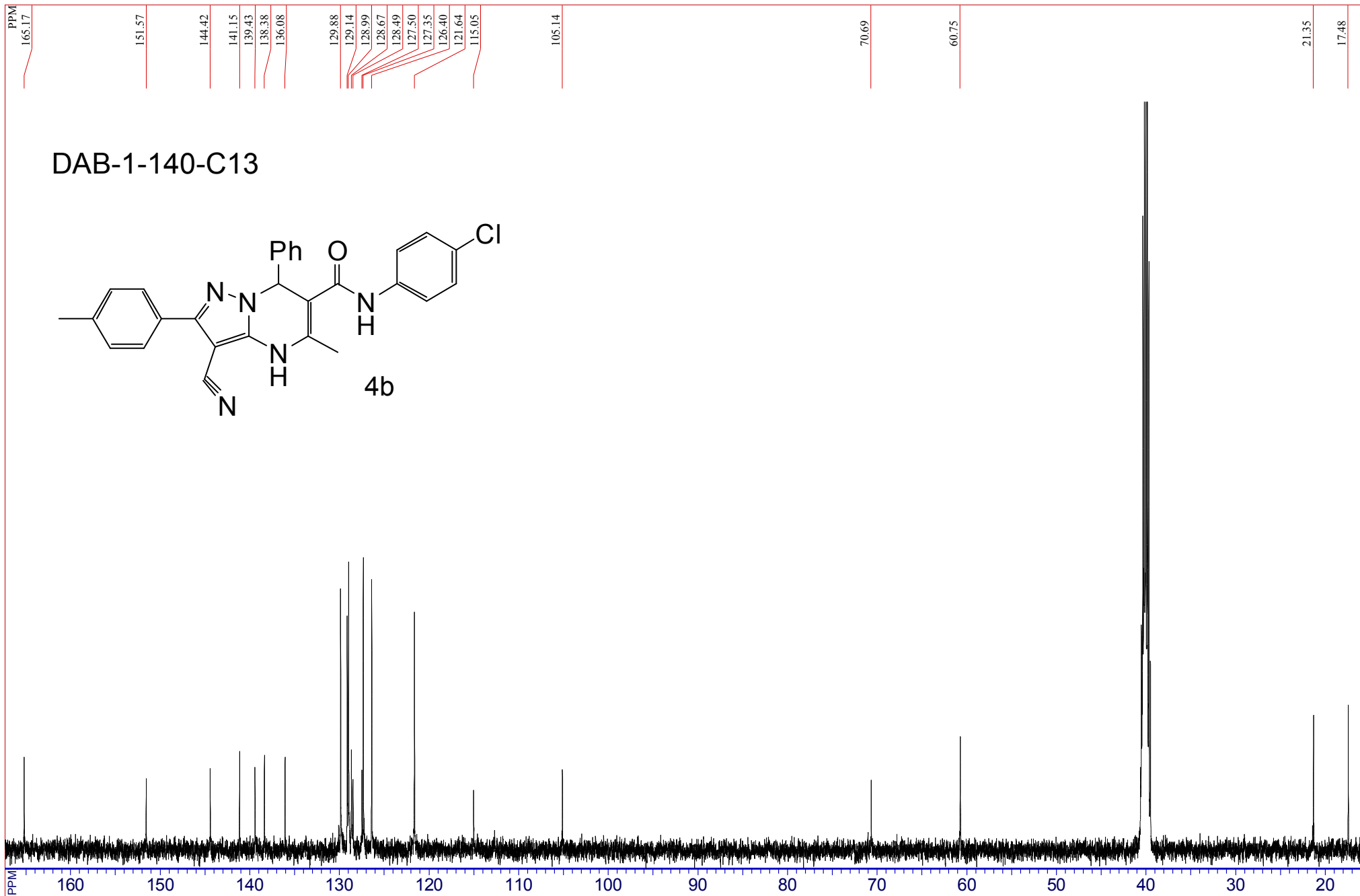
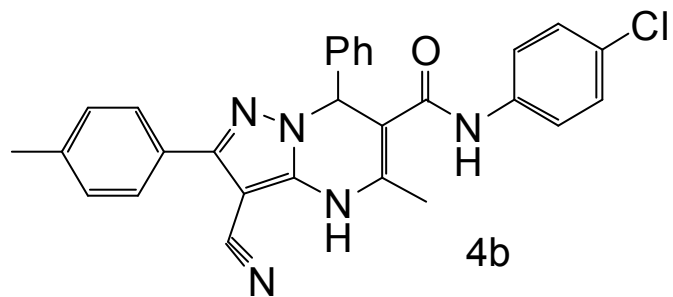
File name: DAB-02-107-P2	Operator:	SF: 199.9704 MHz	NSC: 0	PW: 7.00 usec, RG: 39	SI: 32768
Date: 19-Apr-2012	Solvent: DMSO	SW: 5501 Hz	TE: 302 K	AQ: 1.98 sec, RD: 0.00 sec	

3. ¹³C NMR spectra of synthesized compounds

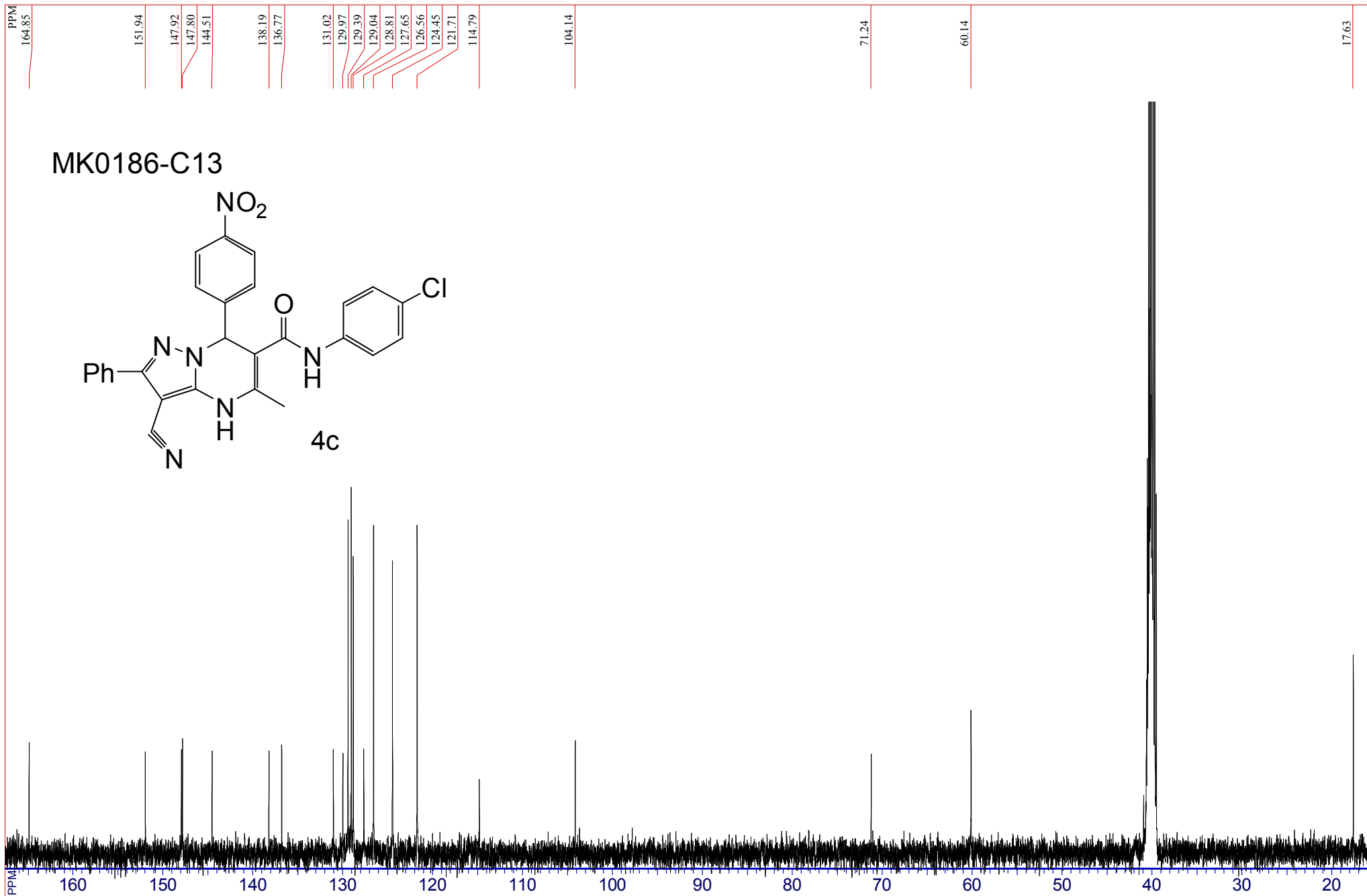


File name: DAB-1-79_C13	Operator: USER 1	SF: 100.6128 MHz	NSC: 298	PW: 0.00 usec, RG: 2050	SI: 32768
Date: 24-Sep-2015	Solvent: DMSO	SW: 24038 Hz	TE: 299 K	AQ: 1.36 sec, RD: 0.00 sec	Parameter file, TOPSPIN Version 2.1

DAB-1-140-C13

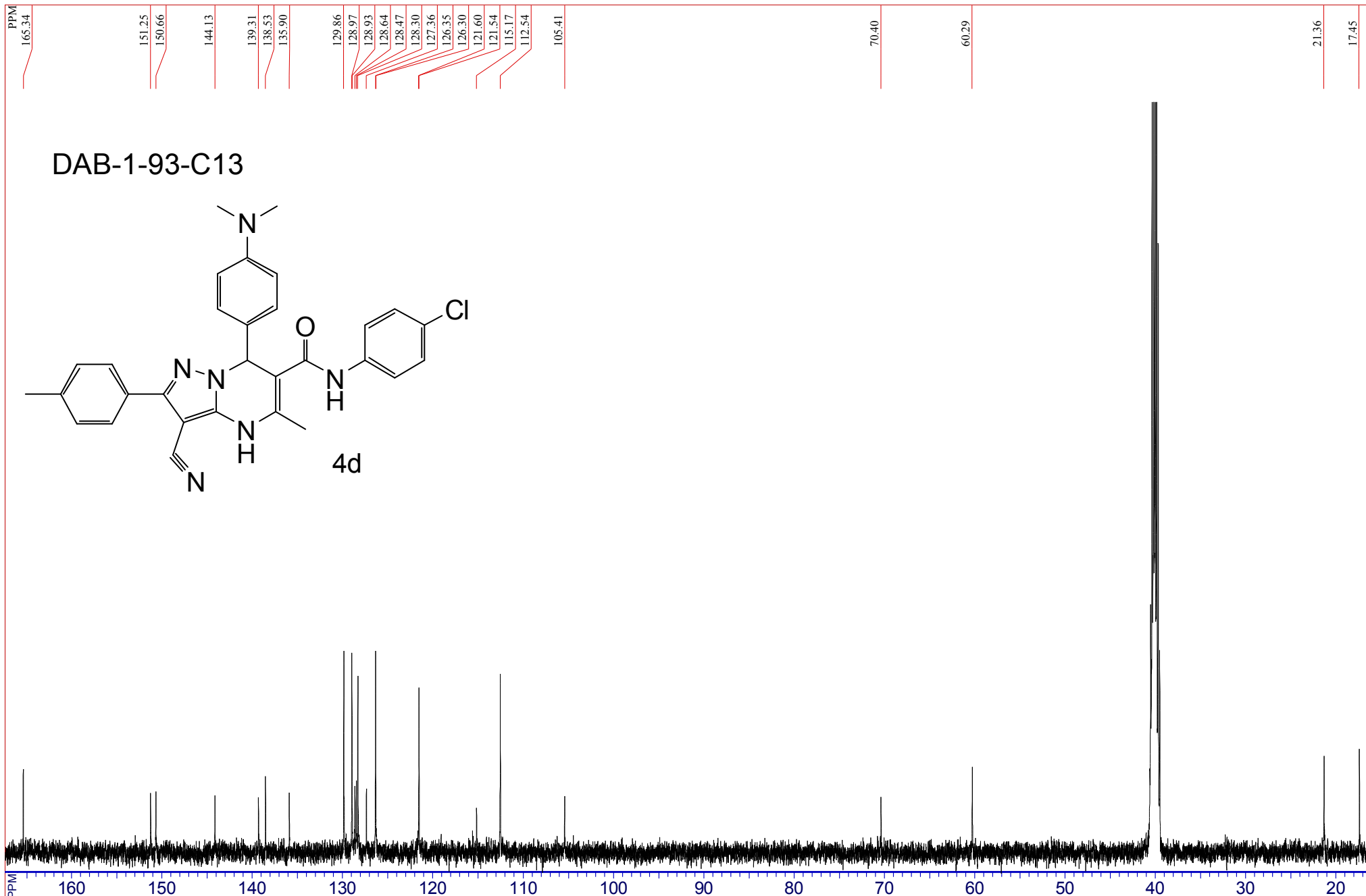
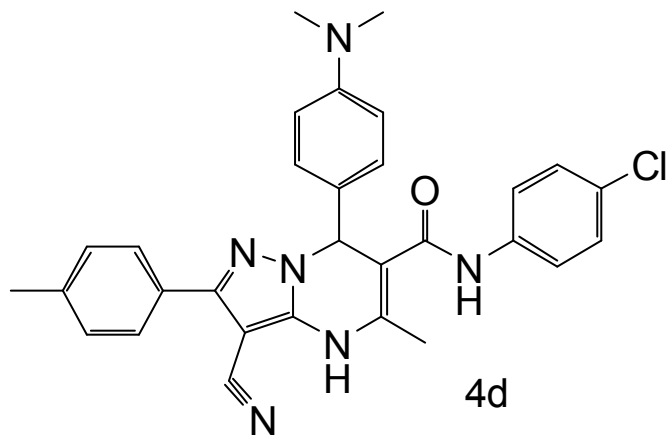


File name: DAB-1-140-C13	Operator: root	SF: 125.7422 MHz	NSC: 294	PW: 0.00 usec, RG: 51200	SI: 65536
Date: 29-May-2012	Solvent: dmsol	SW: 32680 Hz	TE: 0 K	AQ: 1.57 sec, RD: 0.00 sec	Parameter file, XWIN-NMR Version 3.5

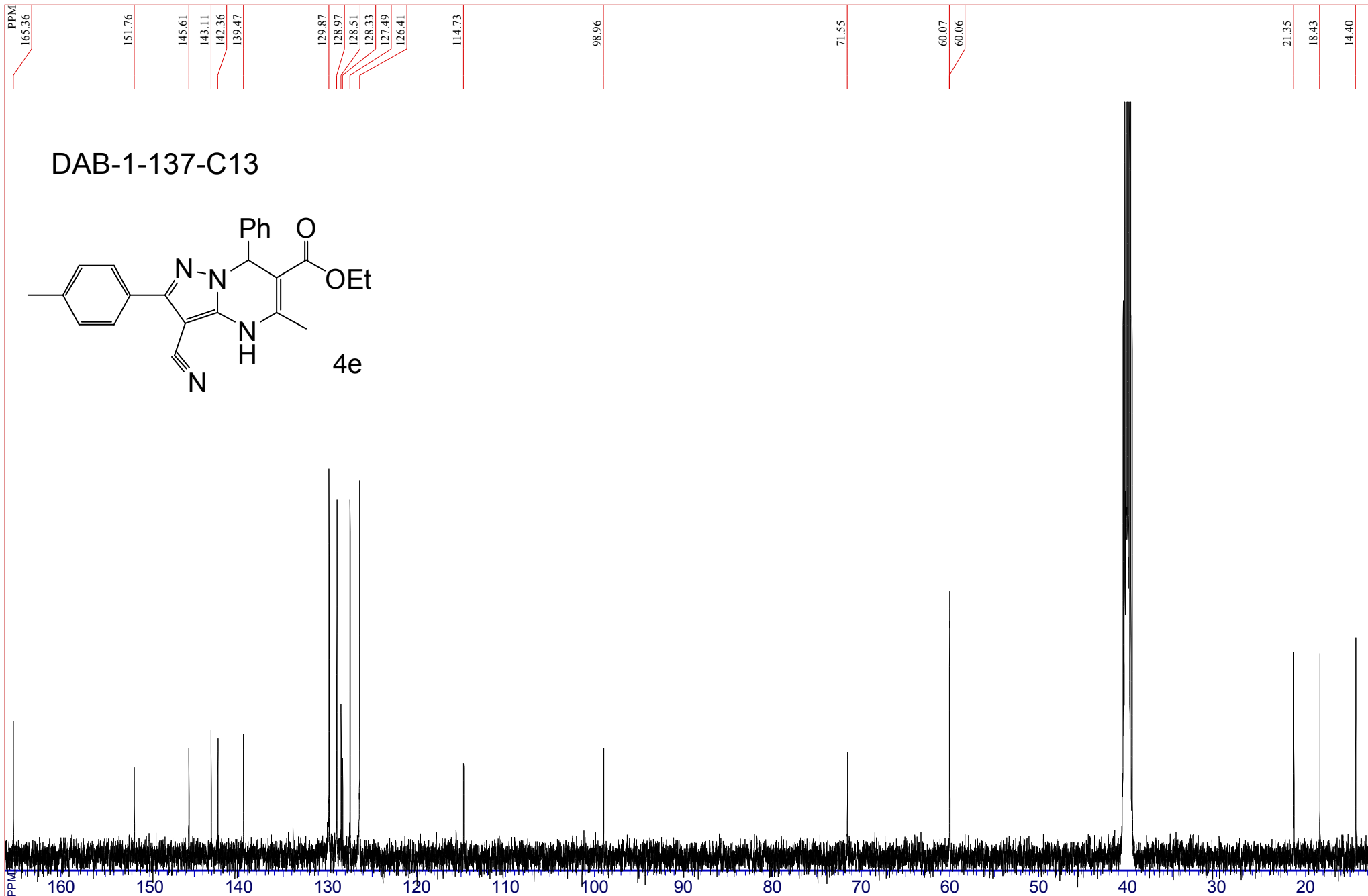


File name: MK0186-C13	Operator: root	SF: 125.7422 MHz	NSC: 276	PW: 0.00 usec, RG: 51200	SI: 65536
Date: 12-Apr-2012	Solvent: dms0	SW: 32680 Hz	TE: 0 K	AQ: 1.57 sec, RD: 0.00 sec	

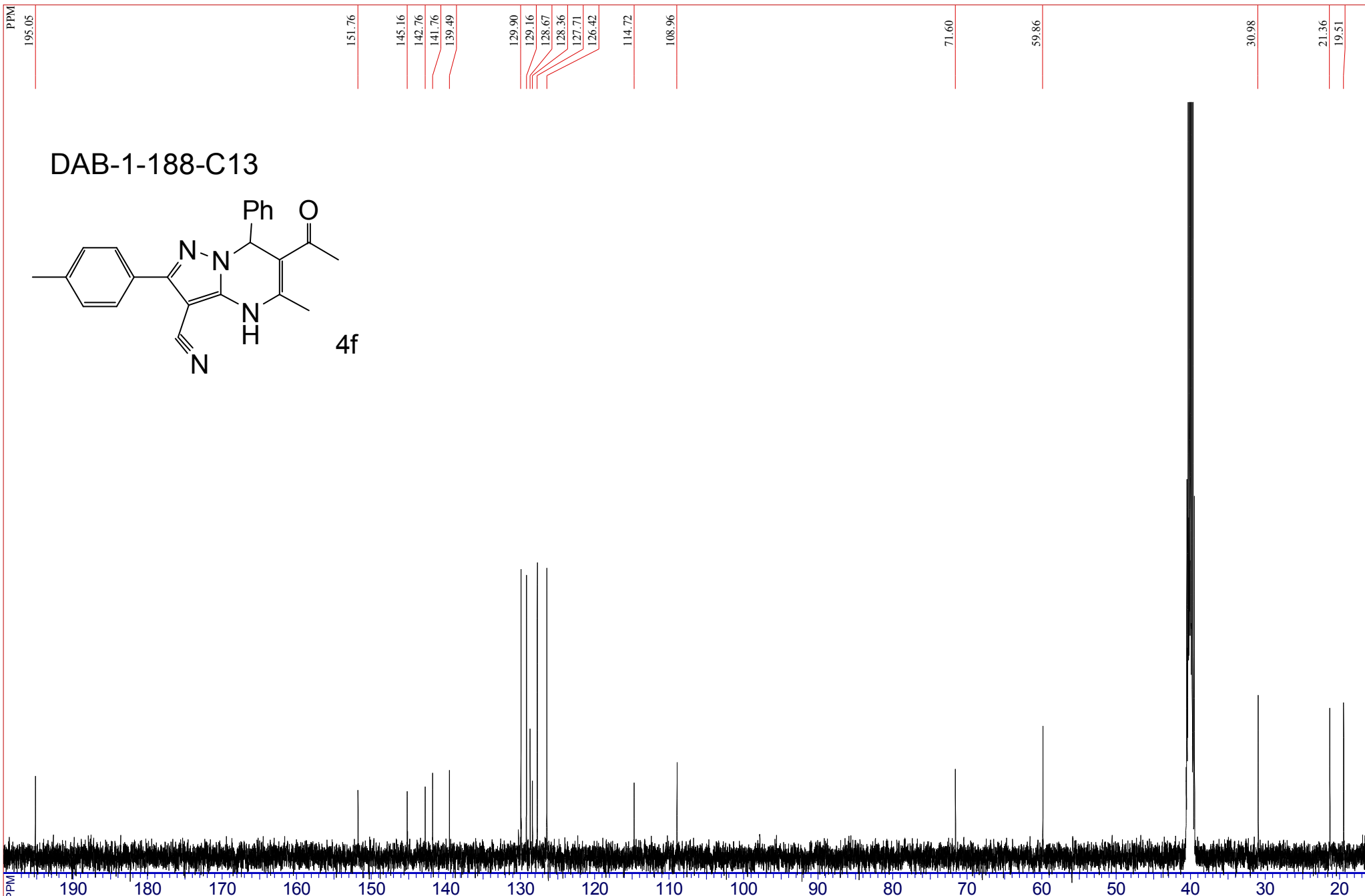
DAB-1-93-C13



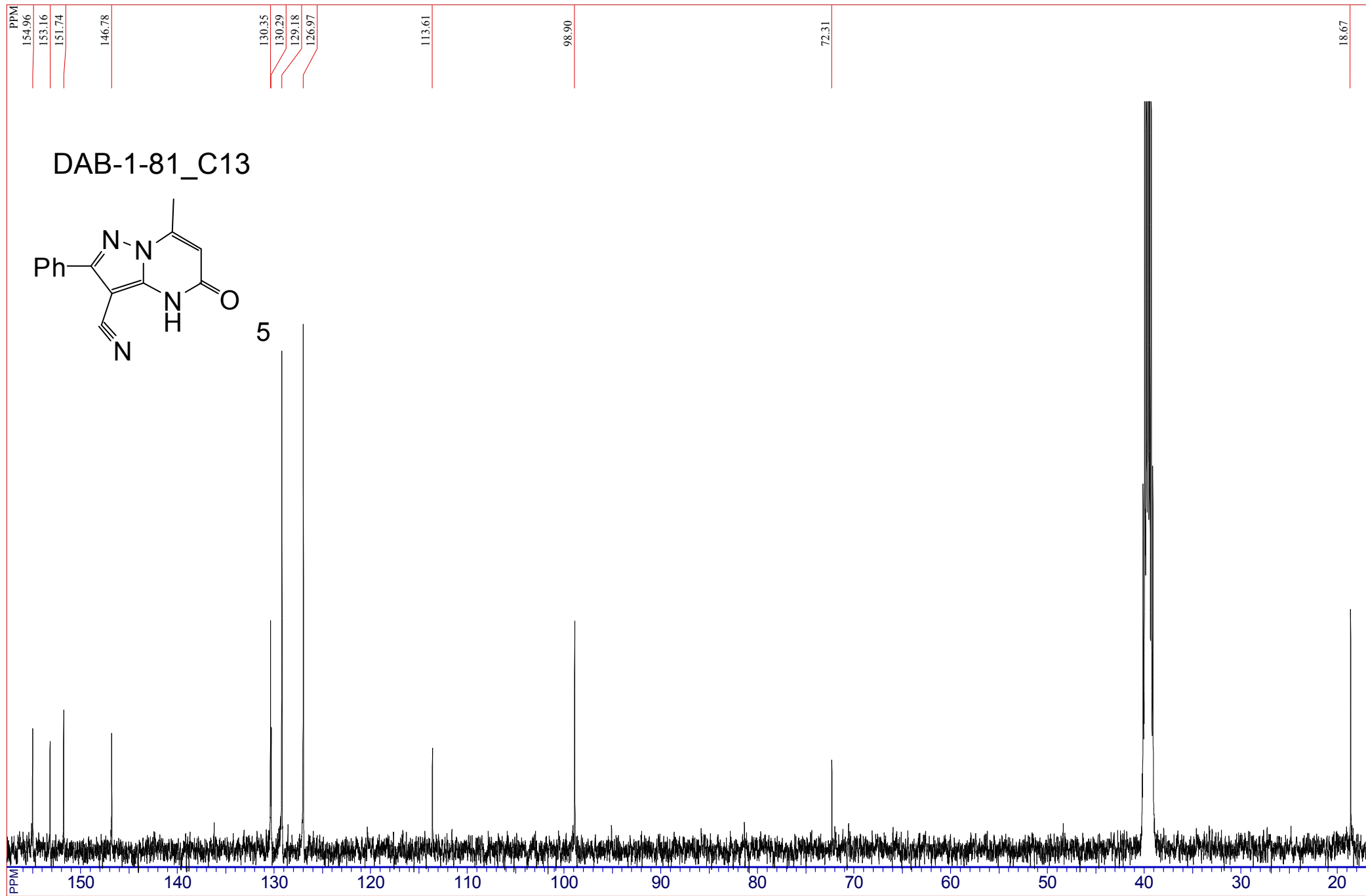
File name: DAB-1-93-C13	Operator: root	SF: 125.7422 MHz	NSC: 284	PW: 0.00 usec, RG: 51200	SI: 65536
Date: 29-May-2012	Solvent: dmso	SW: 32680 Hz	TE: 0 K	AQ: 1.57 sec, RD: 0.00 sec	Parameter file, XWIN-NMR Version 3.5



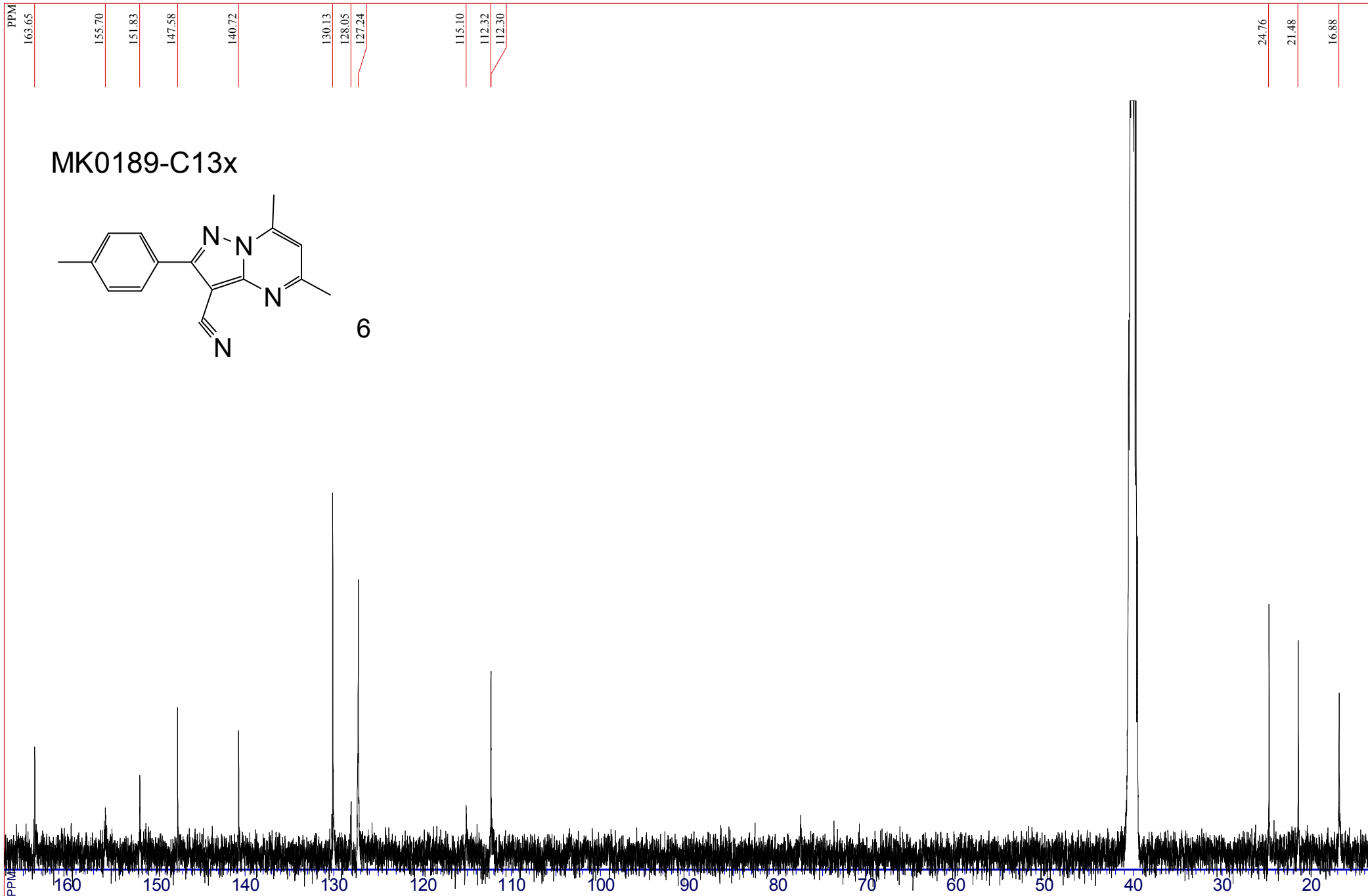
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Date: 29-May-2012	Solvent: dmso	SW: 32680 Hz	TE: 0 K	AQ: 1.57 sec, RD: 0.00 sec	Parameter file, XWIN-NMR Version 3.5



File name: DAB-1-188-C13	Operator: root	SF: 125.7422 MHz	NSC: 267	PW: 0.00 usec, RG: 51200	SI: 65536
Date: 29-May-2012	Solvent: dms0	SW: 32680 Hz	TE: 0 K	AQ: 1.57 sec, RD: 0.00 sec	Parameter file, XWIN-NMR Version 3.5



File name: DAB-1-81_C13	Operator: root	SF: 125.7126 MHz	NSC: 238	PW: 0.00 usec, RG: 51200	SI: 65536
Date: 24-Sep-2015	Solvent: dmso	SW: 32680 Hz	TE: 0 K	AQ: 1.57 sec, RD: 0.00 sec	Parameter file, XWIN-NMR Version 3.5



File name: MK0189-C13x

Operator: root

SF: 125.7422 MHz

NSC: 700

PW: 0.00 usec, RG: 51200

SI: 65536

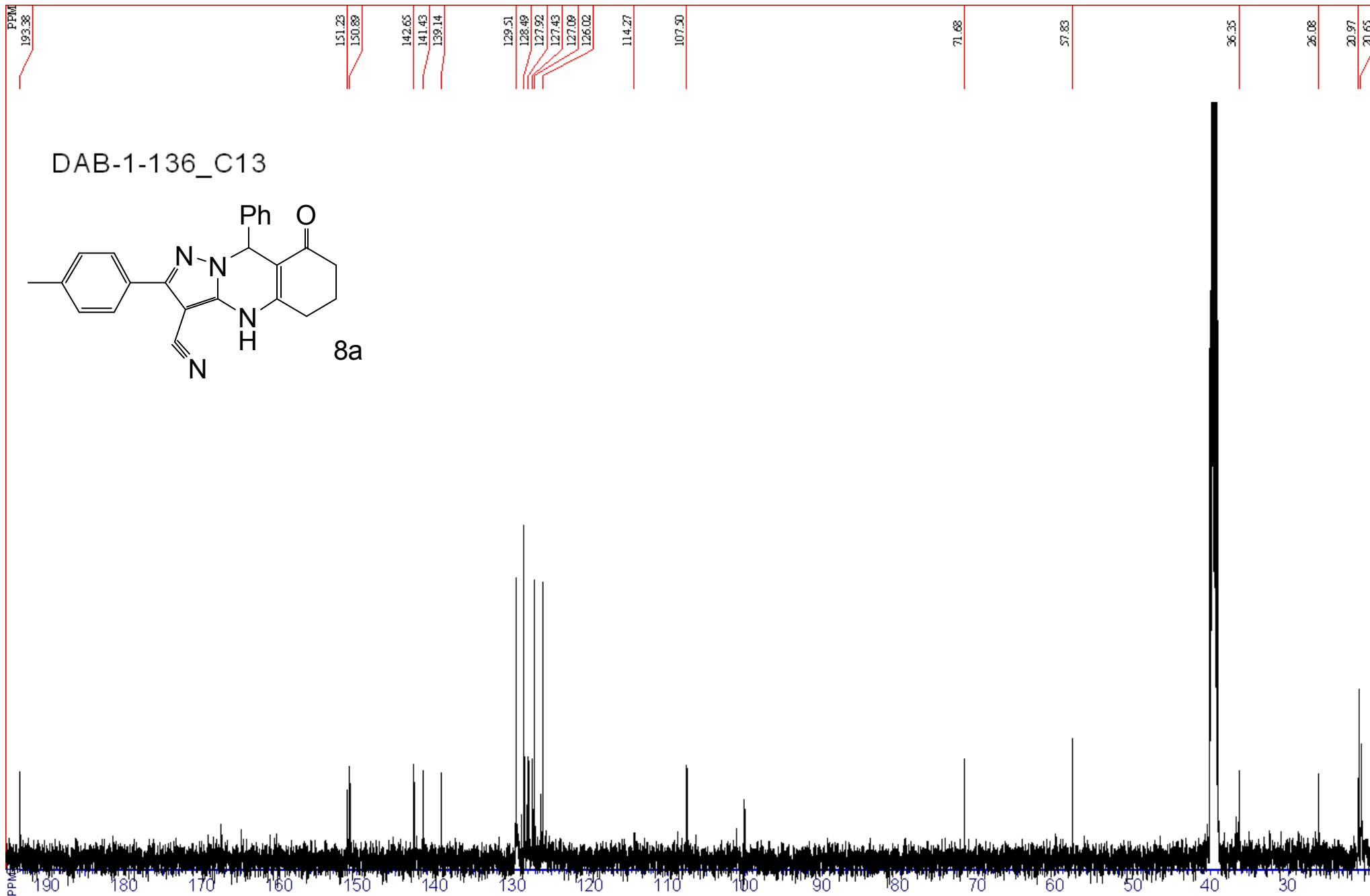
Date: 29-May-2012

Solvent: dms0

SW: 32680 Hz

TE: 0 K

AQ: 1.57 sec, RD: 0.00 sec



File name: DAB-1-136_C13	Operator: root	SF: 125.7126 MHz	NSC: 412	PW: 0.00 usec, RG: 51200	SI: 65536
Date: 24-Sep-2015	Solvent: dms0	SW: 32680 Hz	TE: 0 K	AQ: 1.57 sec, RD: 0.00 sec	

PPM

193.74

151.39

150.79

150.47

142.90

139.41

129.87

129.53

128.43

128.13

126.38

114.79

112.48

108.32

71.80

57.73

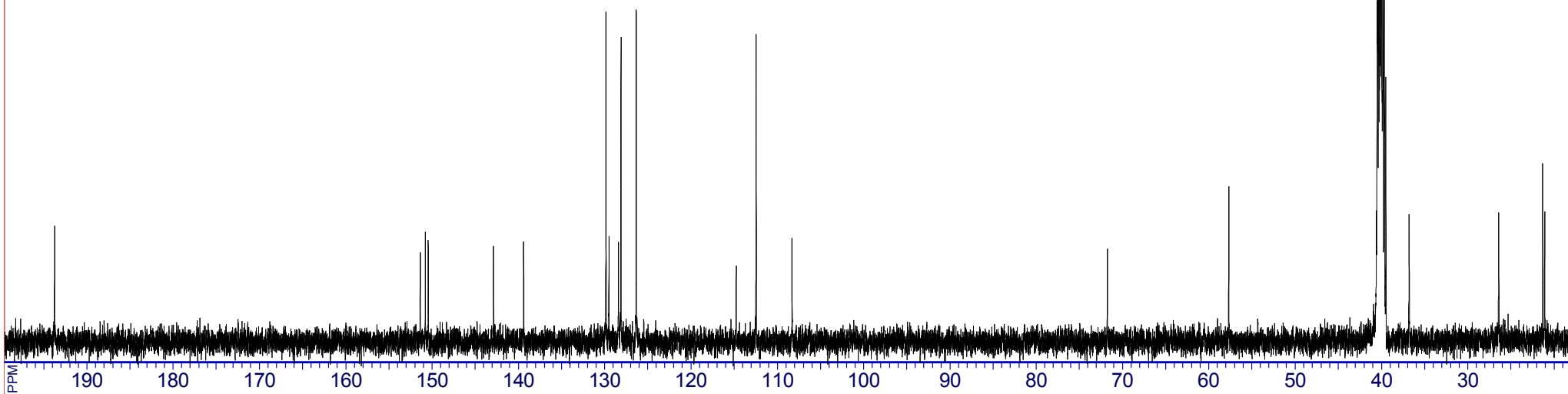
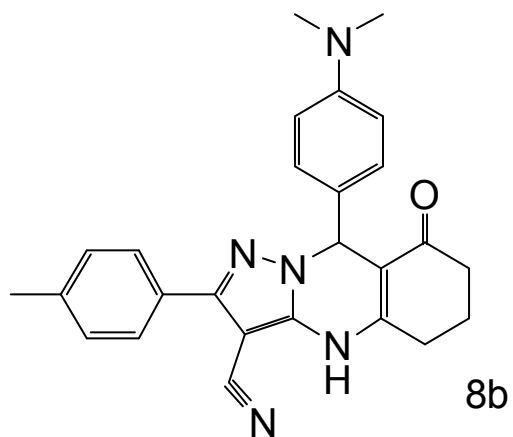
36.85

26.47

21.37

21.14

MK0187-C13



PPM

File name: MK0187-C13

Operator: root

SF: 125.7422 MHz

NSC: 186

PW: 0.00 usec, RG: 51200

SI: 65536

Date: 12-Apr-2012

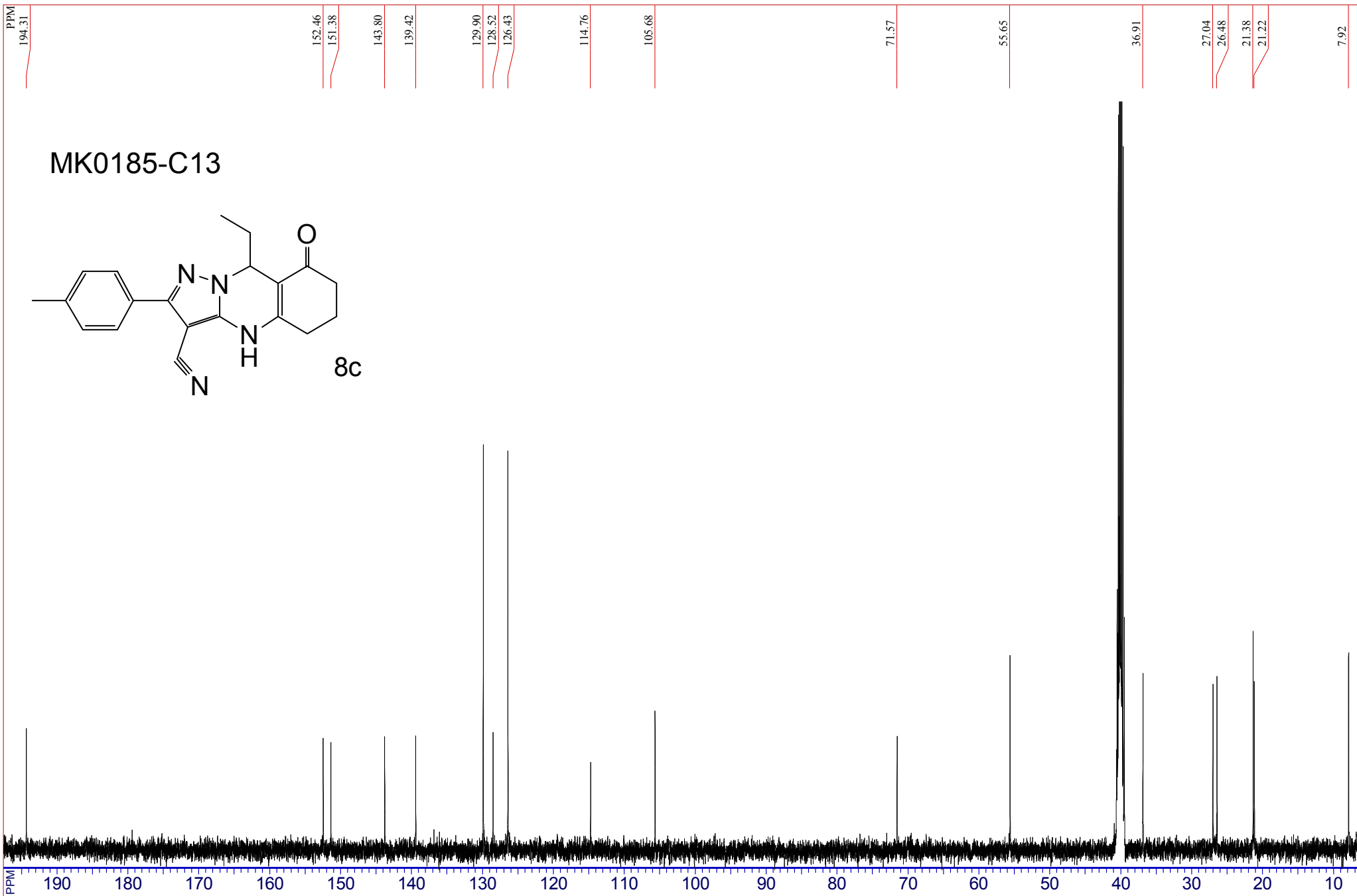
Solvent: dmsol

SW: 32680 Hz

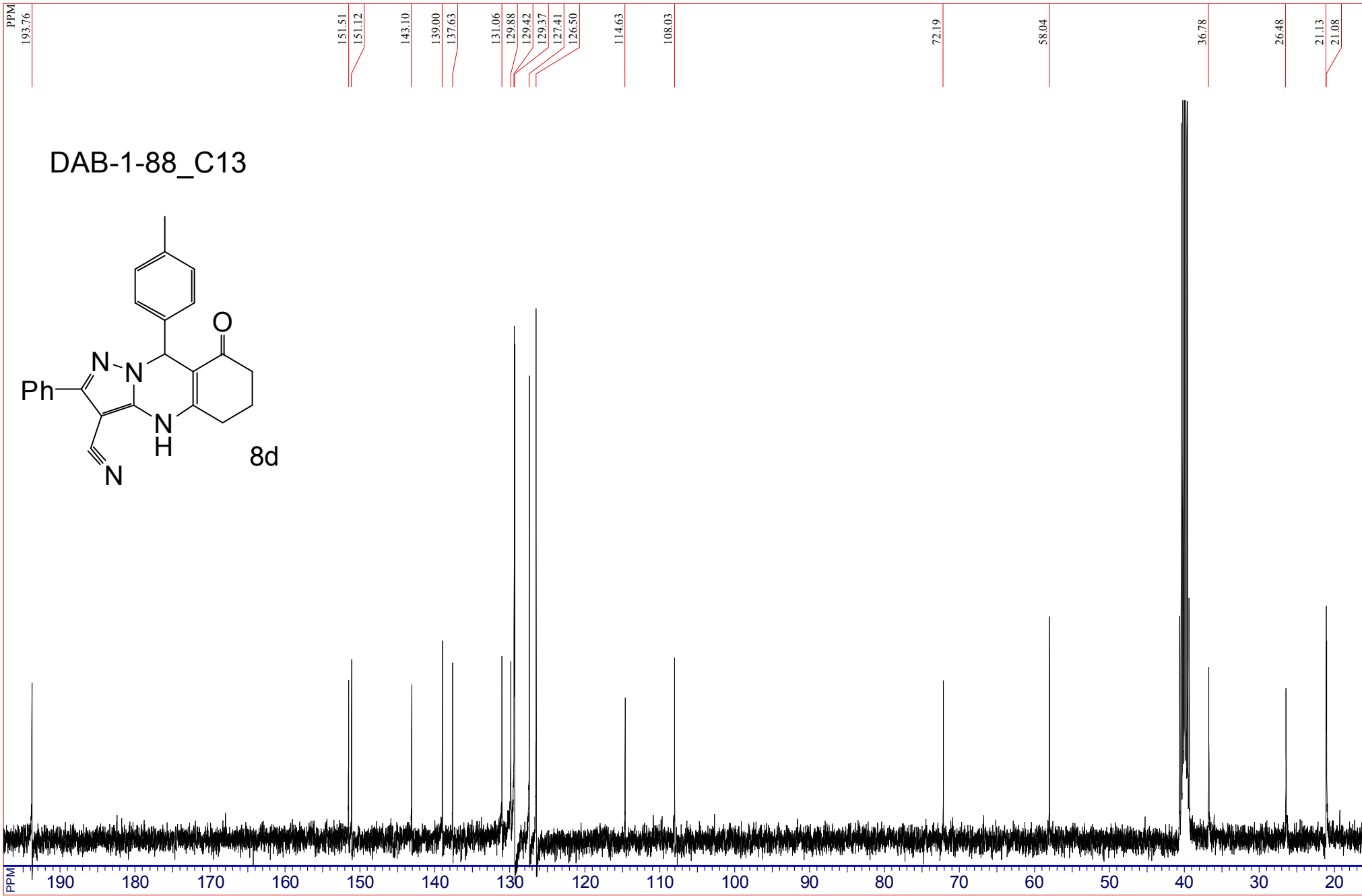
TE: 0 K

AQ: 1.57 sec, RD: 0.00 sec

Parameter file, XWIN-NMR Version 3.5



File name: MK0185-C13	Operator: root	SF: 125.7422 MHz	NSC: 201	PW: 0.00 usec, RG: 51200	SI: 65536
Date: 12-Apr-2012	Solvent: dms0	SW: 32680 Hz	TE: 0 K	AQ: 1.57 sec, RD: 0.00 sec	



File name: DAB-1-88_C13	Operator: USER 1	SF: 100.6128 MHz	NSC: 197	PW: 0.00 usec, RG: 2050	SI: 32768
Date: 24-Sep-2015	Solvent: DMSO	SW: 24038 Hz	TE: 299 K	AQ: 1.36 sec, RD: 0.00 sec	Parameter file, TOPSPIN Version 2.1

PPM
193.99

152.63
152.24

143.32
141.61
139.63

129.88
128.97
128.42
128.14
127.32
126.81

115.66

109.87

73.40

57.70

42.05

36.04

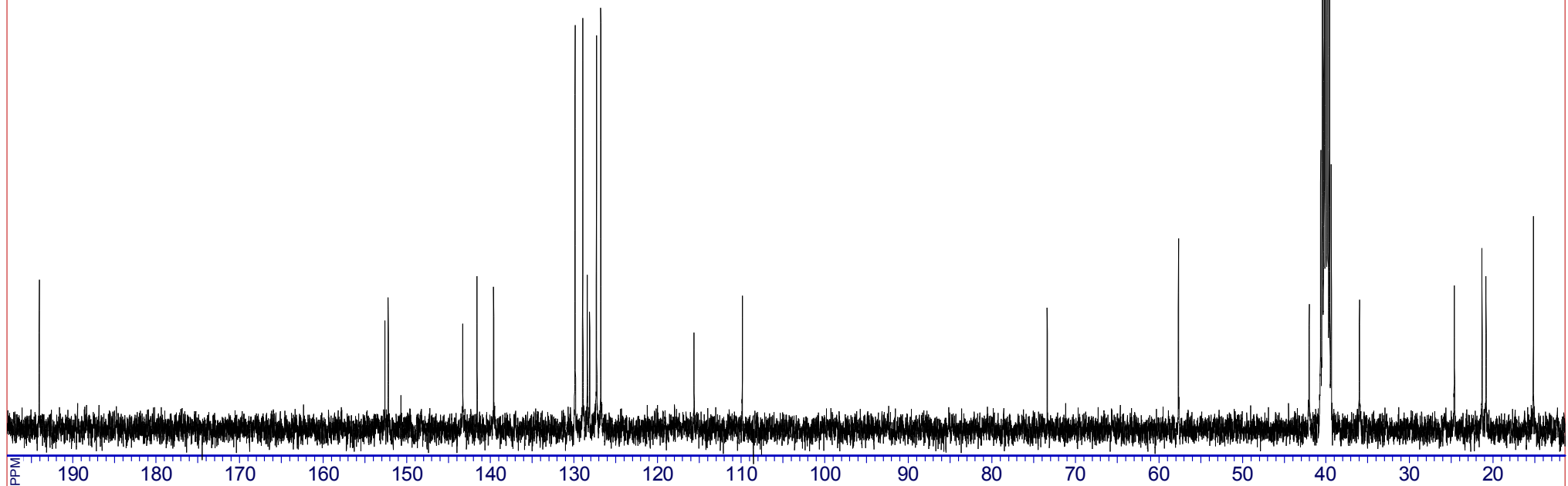
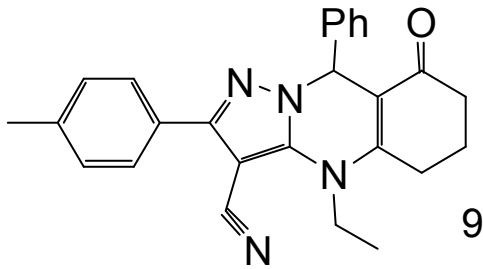
24.69

21.38

20.90

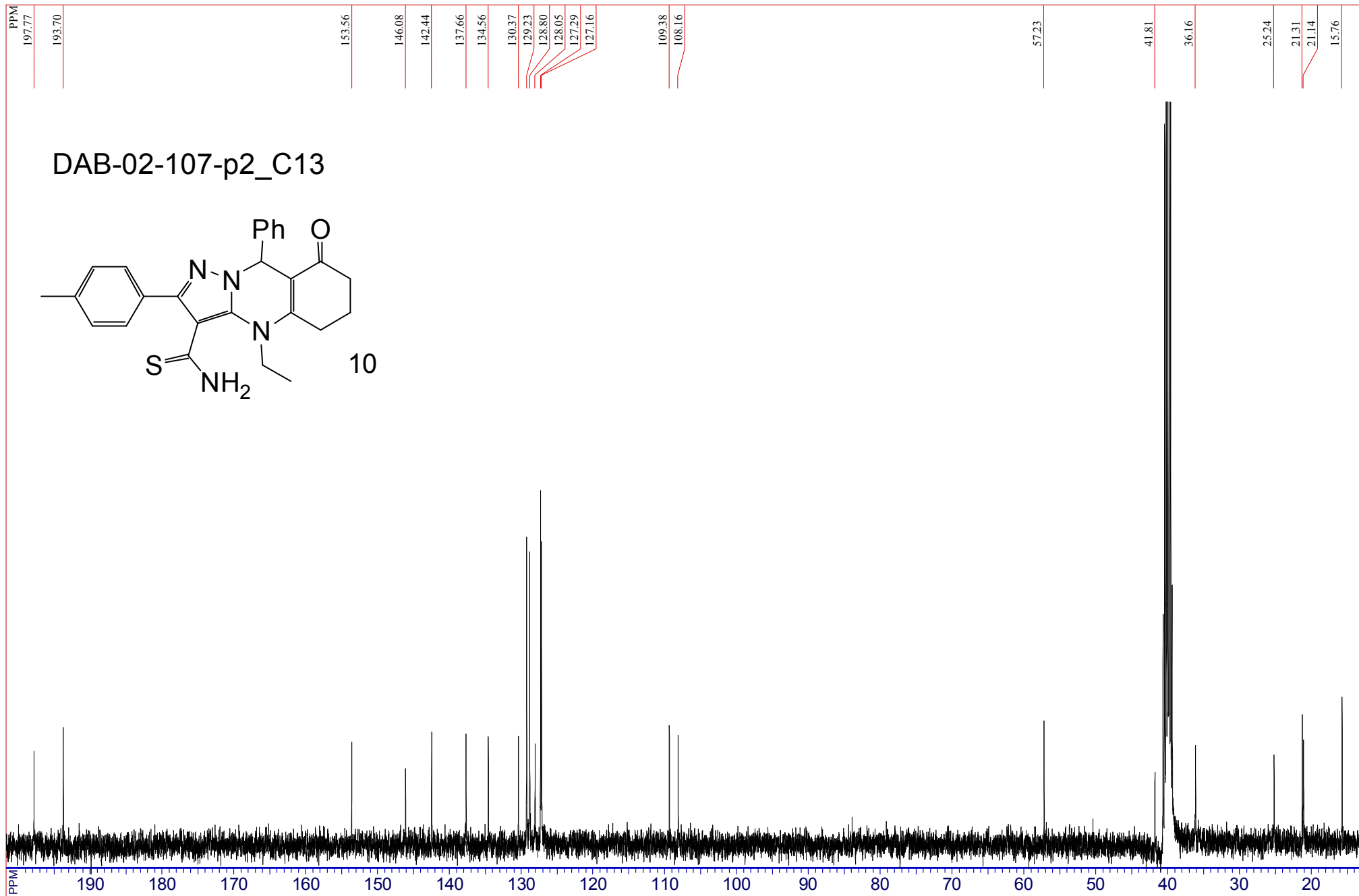
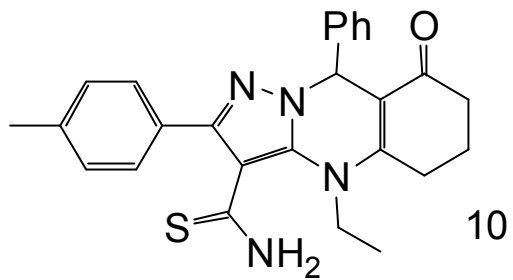
15.23

DAB-02-104-p1_C13



File name: DAB-02-104-p1_C13	Operator: USER 1	SF: 100.6128 MHz	NSC: 323	PW: 0.00 usec, RG: 2050	SI: 32768
Date: 24-Sep-2015	Solvent: DMSO	SW: 24038 Hz	TE: 299 K	AQ: 1.36 sec, RD: 0.00 sec	Parameter file, TOPSPIN Version 2.1

DAB-02-107-p2_C13

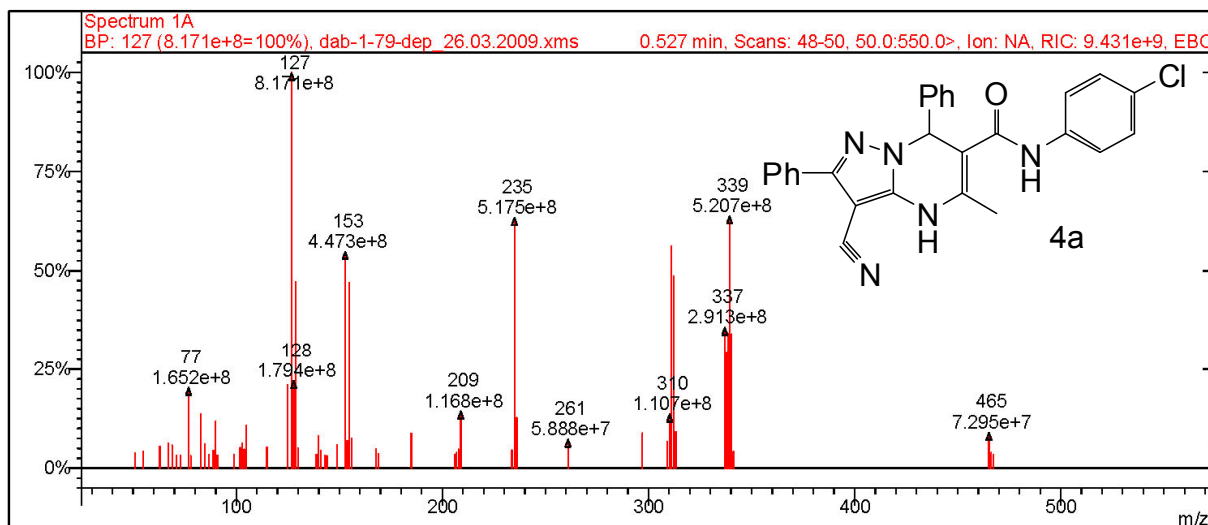


File name: DAB-02-107-p2_C13	Operator: USER 1	SF: 100.6128 MHz	NSC: 315	PW: 0.00 usec, RG: 2050	SI: 32768
Date: 24-Sep-2015	Solvent: DMSO	SW: 24038 Hz	TE: 299 K	AQ: 1.36 sec, RD: 0.00 sec	Parameter file, TOPSPIN Version 2.1

4. Mass-spectra of synthesized compounds

Print Date: 26 Mar 2009 18:48:48

Scan 49 from ..._data\my files\imk\mk-kolosov\dab-1-79-dep_26.03.2009.xms



Spectrum from ...iles\imk\mk-kolosov\dab-1-79-dep_26.03.2009.xms

Scan No: 49, Time: 0.527 minutes

3 points averaged. Background corrected (E).

Comment: 0.527 min. Scans: 48-50 50.0:550.0> Ion: NA RIC: 2.044e+10

Pair Count: 62 MW: 0 Formula: None

CAS No: None Acquired Range: 50 - 550 m/z

Method Description: EI

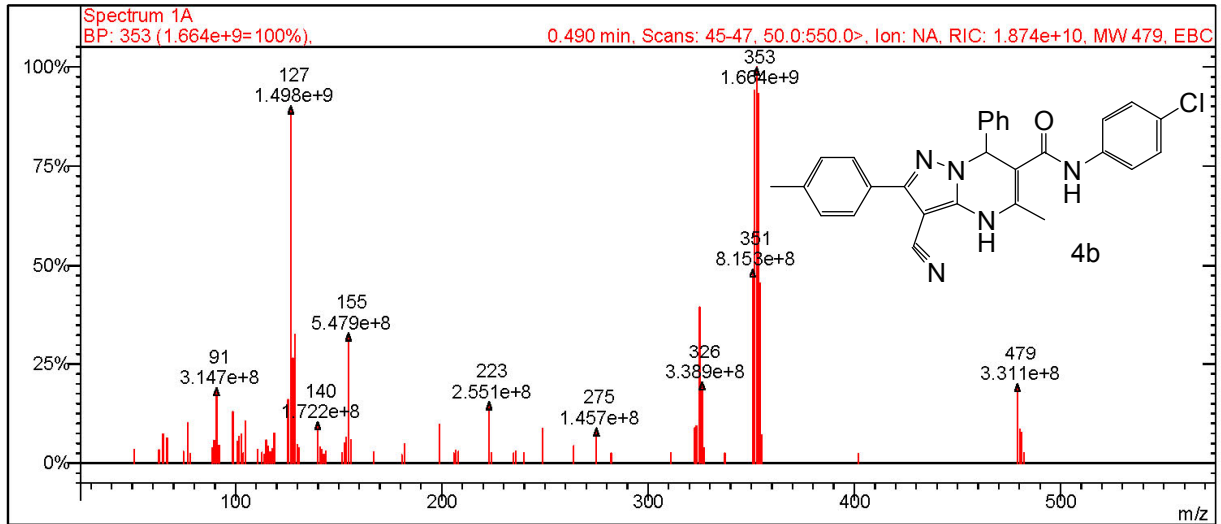
Scan 1 Channel Description: 50.0:550.0> EI;Det 0;WI Q1 Cal;ST 0.010

Scan Information: cp = 1.0 mTorr

Precursor Mass Range: 50 - 550 m/z

Ion	Int	Norm	Ion	Int	Norm	Ion	Int	Norm
51	3.079e+7	38	125	1.706e+8	209	209	1.168e+8	143
55	3.474e+7	42	127	8.171e+8	999	234	3.757e+7	46
63	4.440e+7	54	128	1.794e+8	219	235	5.175e+8	633
67	5.129e+7	63	129	3.851e+8	471	236	1.041e+8	127
69	4.658e+7	57	130	4.089e+7	50	261	5.888e+7	72
71	2.495e+7	31	139	2.778e+7	34	297	7.172e+7	88
73	2.486e+7	30	140	6.507e+7	80	309	5.467e+7	67
77	1.652e+8	202	141	3.624e+7	44	310	1.107e+8	135
78	2.493e+7	30	143	2.565e+7	31	311	4.586e+8	561
83	1.102e+8	135	144	2.518e+7	31	312	3.971e+8	485
85	4.901e+7	60	149	4.799e+7	59	313	7.483e+7	91
87	2.726e+7	33	153	4.473e+8	547	337	2.913e+8	356
89	3.608e+7	44	154	5.633e+7	69	338	2.400e+8	293
90	9.638e+7	118	155	3.841e+8	470	339	2.787e+8	341
91	2.614e+7	32	156	5.994e+7	73	339	5.207e+8	637
99	2.672e+7	33	168	3.967e+7	49	340	2.774e+8	339
102	4.166e+7	51	169	2.973e+7	36	341	3.411e+7	42
103	5.118e+7	63	185	7.127e+7	87	465	7.295e+7	89
104	3.830e+7	47	206	2.768e+7	34	466	3.163e+7	39
105	8.671e+7	106	207	3.186e+7	39	467	2.705e+7	33
115	4.266e+7	52	208	3.818e+7	47			

Scan 46 from ...data\my files\imk\mk-kolosov\dab-1-140-dep_31.03.2009.xms



Spectrum from ...les\imk\mk-kolosov\dab-1-140-dep_31.03.2009.xms

Scan No: 46, Time: 0.490 minutes

3 points averaged. Background corrected (E).

Name: DAB-1-140-DEP

Comment: Varian 1200 L; EI; electron energy 70 eV

Pair Count: 75 MW: 479 Formula: None

CAS No: None Acquired Range: 50 - 550 m/z

Method Description: EI

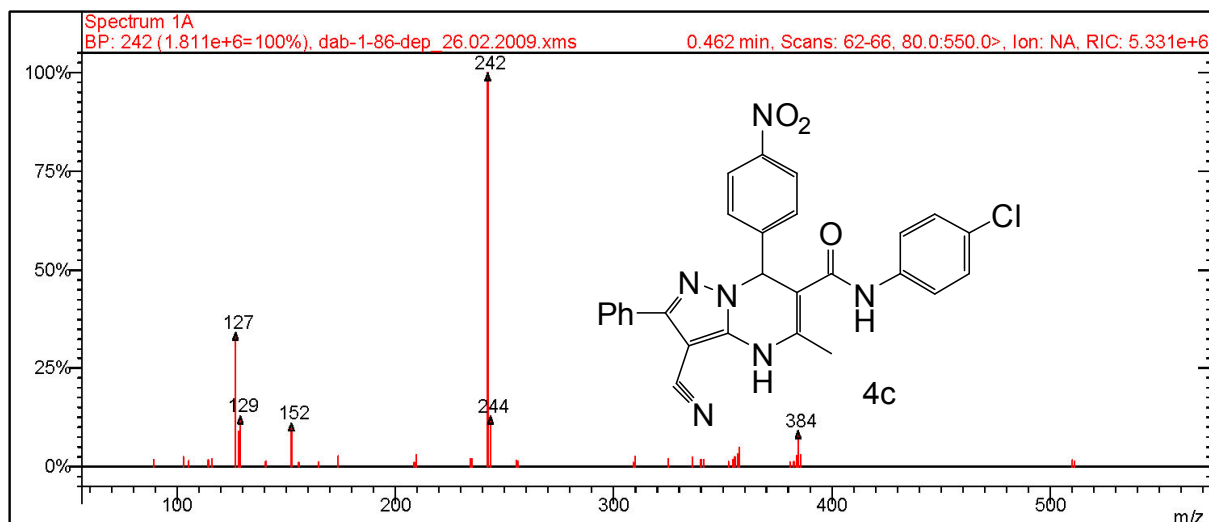
Scan 1 Channel Description: 50.0:550.0> EI;Det 0;WI Q1 Cal;ST 0.010

Scan Information: cp = 1.0 mTorr

Precursor Mass Range: 50 - 550 m/z

Ion	Int	Norm	Ion	Int	Norm	Ion	Int	Norm
51	5.659e+7	34	126	2.654e+8	159	235	4.029e+7	24
63	5.466e+7	33	127	1.498e+9	900	236	4.922e+7	30
65	1.209e+8	73	128	4.388e+8	263	240	4.158e+7	25
67	1.042e+8	63	129	5.420e+8	325	249	1.447e+8	87
75	4.724e+7	28	130	7.543e+7	45	264	7.140e+7	43
77	1.664e+8	100	131	6.191e+7	37	275	1.457e+8	87
78	3.857e+7	23	140	1.722e+8	103	282	4.094e+7	25
89	6.392e+7	38	141	6.660e+7	40	311	4.136e+7	25
90	9.401e+7	56	142	5.619e+7	34	323	1.480e+8	89
91	3.147e+8	189	143	3.609e+7	22	323	1.551e+8	93
92	7.324e+7	44	144	4.812e+7	29	325	6.569e+8	394
99	2.146e+8	129	152	4.119e+7	25	326	3.389e+8	204
101	9.000e+7	54	153	8.232e+7	49	327	6.280e+7	38
102	1.115e+8	67	154	1.082e+8	65	337	4.036e+7	24
103	1.198e+8	72	155	5.479e+8	329	351	8.153e+8	490
104	4.119e+7	25	156	9.641e+7	58	352	1.564e+9	939
105	1.759e+8	106	167	4.563e+7	27	353	1.664e+9	999
111	5.378e+7	32	181	3.335e+7	20	353	1.551e+9	932
113	4.405e+7	26	182	8.039e+7	48	354	7.584e+8	455
114	3.428e+7	21	199	1.616e+8	97	355	1.162e+8	70
115	9.513e+7	57	206	4.072e+7	24	402	3.974e+7	24
116	6.975e+7	42	207	5.237e+7	31	479	3.311e+8	199
117	4.659e+7	28	208	4.712e+7	28	480	1.421e+8	85
118	5.941e+7	36	223	2.551e+8	153	481	1.283e+8	77
119	1.248e+8	75	224	4.096e+7	25	482	4.223e+7	25

Scan 64 from ..._data\my files\mk\mk-kolosov\dab-1-86-dep_26.02.2009.xms



Spectrum from ...iles\mk\mk-kolosov\dab-1-86-dep_26.02.2009.xms

Scan No: 64, Time: 0.462 minutes

5 points averaged. Not background corrected.

Name: DAB-1-86

Comment: Varian1200L; EI; Electron Energy:70eV

Pair Count: 39 MW: 0 Formula: None

CAS No: None Acquired Range: 80 - 550 m/z

Method Description: EI

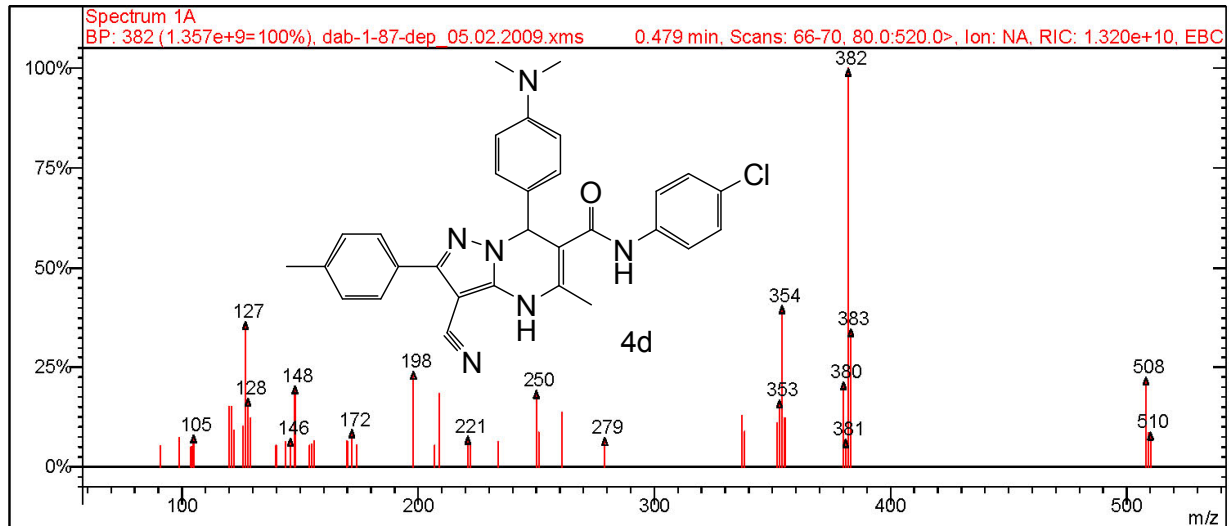
Scan 1 Channel Description: 80.0:550.0> EI;Det 0;WI Q1 Cal;ST 0.010

Scan Information: cp = 1.0 mTorr

Precursor Mass Range: 80 - 550 m/z

Ion	Int	Norm	Ion	Int	Norm	Ion	Int	Norm
89	29790	16	209	19450	11	341	29180	16
103	45475	25	210	52525	29	353	21790	12
105	25315	14	234	36095	20	354	31450	17
114	29450	16	235	36040	20	356	44870	25
116	36060	20	242	1.811e+6	999	357	57395	32
127	618525	341	244	229915	127	358	87380	48
128	160045	88	255	27410	15	381	19465	11
129	230265	127	256	23790	13	383	22055	12
141	23550	13	309	18860	10	384	49520	27
152	197930	109	310	46000	25	384	162580	90
156	18245	10	325	35715	20	386	54655	30
165	21170	12	336	41975	23	510	30710	17
174	47325	26	340	31610	17	511	23380	13

Scan 68 from ..._data\my files\imk\mk-kolosov\dab-1-87-dep_05.02.2009.xms



Spectrum from ...iles\imk\mk-kolosov\dab-1-87-dep_05.02.2009.xms

Scan No: 68, Time: 0.479 minutes

5 points averaged. Background corrected (E).

Comment: 0.479 min. Scans: 66-70 80.0:520.0> Ion: NA RIC: 1.611e+10

Pair Count: 44 MW: 0 Formula: None

CAS No: None Acquired Range: 80 - 520 m/z

Method Description: EI

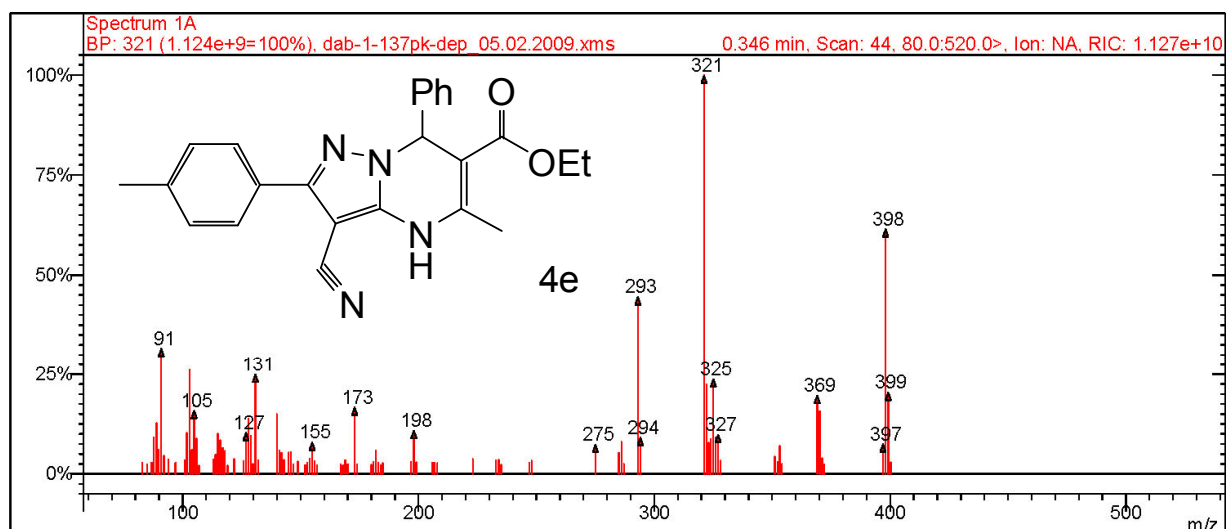
Scan 1 Channel Description: 80.0:520.0> EI;Det 0;WI Q1 Cal;ST 0.010

Scan Information: cp = 1.0 mTorr

Precursor Mass Range: 80 - 520 m/z

Ion	Int	Norm	Ion	Int	Norm	Ion	Int	Norm
91	7.100e+7	52	154	7.222e+7	53	279	9.818e+7	72
99	9.896e+7	73	155	7.692e+7	57	337	1.721e+8	127
104	6.814e+7	50	156	8.677e+7	64	338	1.188e+8	87
105	1.071e+8	79	170	8.761e+7	65	352	1.473e+8	108
120	2.045e+8	151	172	1.249e+8	92	353	2.256e+8	166
121	2.045e+8	151	174	7.350e+7	54	354	5.497e+8	405
122	1.218e+8	90	198	3.234e+8	238	355	1.655e+8	122
126	1.372e+8	101	207	7.217e+7	53	380	2.879e+8	212
127	4.955e+8	365	209	2.489e+8	183	381	9.228e+7	68
128	2.315e+8	170	221	1.022e+8	75	382	1.357e+9	999
129	1.659e+8	122	222	7.386e+7	54	383	4.713e+8	347
140	7.160e+7	53	234	8.457e+7	62	508	3.037e+8	224
144	8.504e+7	63	250	2.585e+8	190	509	1.138e+8	84
146	9.579e+7	71	251	1.161e+8	85	510	1.170e+8	86
148	2.742e+8	202	261	1.848e+8	136			

Scan 44 from ...ta\my files\imk\mk-kolosov\dab-1-137pk-dep_05.02.2009.xms



Spectrum from ...s\imk\mk-kolosov\dab-1-137pk-dep_05.02.2009.xms

Scan No: 44, Time: 0.346 minutes

No averaging. Not background corrected.

Name: DAB-1-137pK

Comment: 0.346 min. Scan: 44 80.0:520.0> Ion: NA RIC: 1.127e+10

Pair Count: 96 MW: 0 Formula: None

CAS No: None Acquired Range: 80 - 520 m/z

Method Description: EI

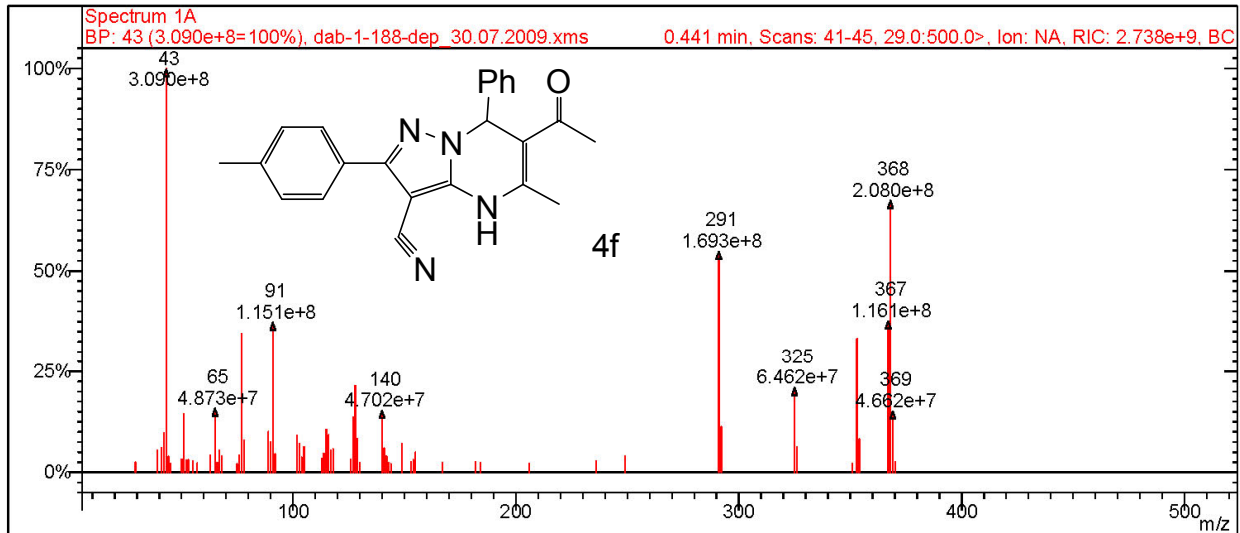
Scan 1 Channel Description: 80.0:520.0> EI;Det 0;WI Q1 Cal;ST 0.010

Scan Information: cp = 1.0 mTorr

Precursor Mass Range: 80 - 520 m/z

Ion	Int	Norm	Ion	Int	Norm	Ion	Int	Norm
83	3.113e+7	28	140	1.677e+8	149	223	4.097e+7	36
85	2.646e+7	24	141	6.595e+7	59	233	3.797e+7	34
87	3.142e+7	28	142	5.891e+7	52	234	3.982e+7	35
88	1.021e+8	91	143	3.891e+7	35	235	2.531e+7	22
89	1.425e+8	127	145	5.942e+7	53	247	3.090e+7	27
90	6.655e+7	59	146	6.165e+7	55	248	3.653e+7	32
91	3.537e+8	314	147	2.524e+7	22	275	8.140e+7	72
92	5.091e+7	45	149	3.454e+7	31	285	5.849e+7	52
94	3.885e+7	35	152	2.446e+7	22	286	8.955e+7	80
97	3.093e+7	27	153	3.136e+7	28	287	2.749e+7	24
101	3.772e+7	34	154	4.178e+7	37	293	4.994e+8	444
102	1.147e+8	102	155	8.795e+7	78	294	1.014e+8	90
103	2.933e+8	261	156	3.590e+7	32	321	1.124e+9	999
104	6.740e+7	60	157	2.479e+7	22	322	2.507e+8	223
105	1.771e+8	157	167	2.569e+7	23	323	8.712e+7	77
106	9.864e+7	88	168	2.383e+7	21	324	9.638e+7	86
107	2.295e+7	20	169	3.847e+7	34	325	2.660e+8	236
113	3.945e+7	35	170	2.654e+7	24	326	1.028e+8	91
114	5.383e+7	48	173	1.865e+8	166	327	1.096e+8	97
115	1.122e+8	100	174	2.640e+7	23	328	3.636e+7	32
116	9.492e+7	84	180	2.550e+7	23	351	4.821e+7	43
117	7.248e+7	64	181	3.354e+7	30	352	3.355e+7	30
118	6.425e+7	57	182	6.544e+7	58	353	7.833e+7	70
119	2.316e+7	21	183	2.998e+7	27	354	2.756e+7	24
122	4.098e+7	36	184	2.442e+7	22	369	2.195e+8	195
126	3.496e+7	31	185	3.014e+7	27	370	1.763e+8	157
127	1.148e+8	102	197	3.384e+7	30	371	4.396e+7	39
128	1.549e+8	138	198	1.209e+8	108	372	2.671e+7	24
129	1.070e+8	95	199	3.249e+7	29	397	8.255e+7	73
130	2.795e+7	25	206	3.138e+7	28	398	6.898e+8	613
131	2.792e+8	248	207	3.150e+7	28	399	2.283e+8	203
132	3.658e+7	33	208	2.938e+7	26	400	3.262e+7	29

Scan 43 from ...n_data\mk-kolosov\dab\07\dab-1-188-dep_30.07.2009.xms



Spectrum from ...mk-kolosov\dab\07\dab-1-188-dep_30.07.2009.xms

Scan No: 43, Time: 0.441 minutes

5 points averaged. Background corrected.

Name: DAB-1-188-DEP

Comment: Varian 1200 L; EI; electron energy 70 eV

Pair Count: 67 MW: 0 Formula: None

CAS No: None Acquired Range: 29 - 500 m/z

Method Description: EI

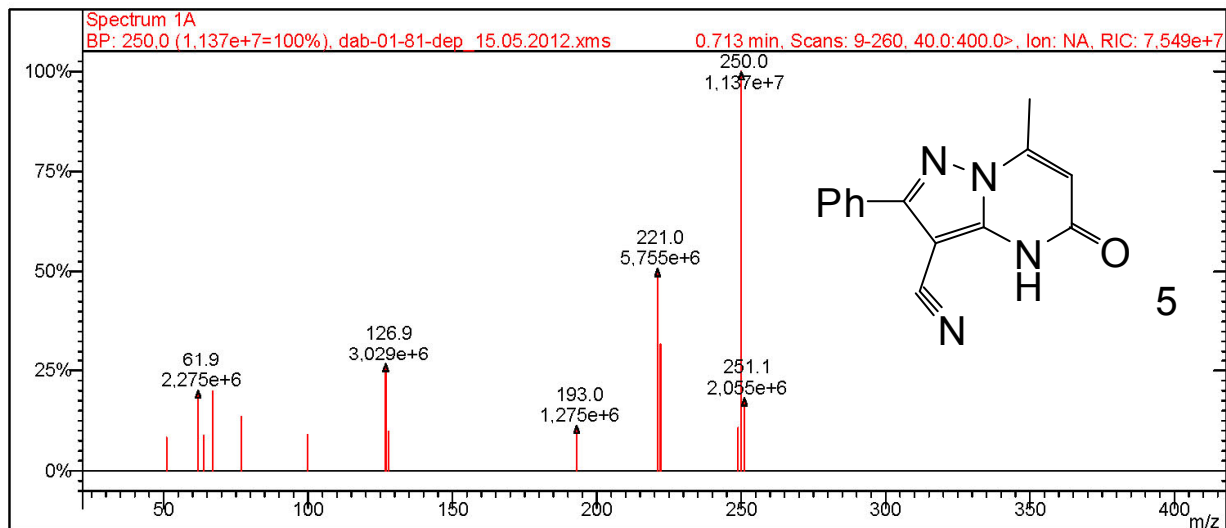
Scan 1 Channel Description: 29.0:500.0> EI;Det 0;WI Q1 Cal;ST 0.010

Scan Information: cp = 1.0 mTorr

Precursor Mass Range: 29 - 500 m/z

Ion	Int	Norm	Ion	Int	Norm	Ion	Int	Norm
29	7.651e+6	25	90	2.276e+7	74	144	6.370e+6	21
39	1.683e+7	54	91	1.151e+8	372	149	2.173e+7	70
41	1.869e+7	60	92	1.408e+7	46	153	7.516e+6	24
42	2.969e+7	96	102	2.828e+7	91	154	9.510e+6	31
43	3.090e+8	999	103	2.139e+7	69	155	1.532e+7	50
44	1.206e+7	39	104	1.145e+7	37	167	7.234e+6	23
45	6.450e+6	21	105	1.946e+7	63	182	8.038e+6	26
50	9.901e+6	32	113	1.050e+7	34	184	7.247e+6	23
51	4.429e+7	143	114	1.431e+7	46	206	6.189e+6	20
52	9.183e+6	30	115	3.273e+7	106	236	8.716e+6	28
53	9.430e+6	30	116	2.841e+7	92	249	1.203e+7	39
55	8.123e+6	26	117	1.661e+7	54	291	1.693e+8	547
57	6.883e+6	22	118	1.763e+7	57	292	3.491e+7	113
63	1.302e+7	42	126	9.753e+6	32	325	6.462e+7	209
65	4.873e+7	158	127	4.187e+7	135	326	1.918e+7	62
66	7.266e+6	23	128	6.624e+7	214	351	6.559e+6	21
67	1.644e+7	53	129	2.570e+7	83	353	1.027e+8	332
68	1.221e+7	39	130	7.354e+6	24	354	2.519e+7	81
75	6.230e+6	20	140	4.702e+7	152	367	1.161e+8	376
76	1.279e+7	41	141	1.831e+7	59	368	2.080e+8	672
77	1.065e+8	344	142	1.236e+7	40	369	4.662e+7	151
78	2.441e+7	79	143	7.148e+6	23	370	7.688e+6	25
89	3.095e+7	100						

Scan 135 from ...золе доценко\2015\вещества\5\dab-01-81-dep_15.05.2012.xms



Spectrum from ...ко\2015\вещества\5\dab-01-81-dep_15.05.2012.xms
 Scan No: 135, Time: 0.713 minutes
 252 points averaged. Not background corrected.
 Comment: 0.713 min. Scans: 9-260 40.0:400.0> Ion: NA RIC: 7,549e+7
 Pair Count: 14 MW: 0 Formula: None
 CAS No: None Acquired Range: 40.0 - 400.0 m/z

Method Description: EI

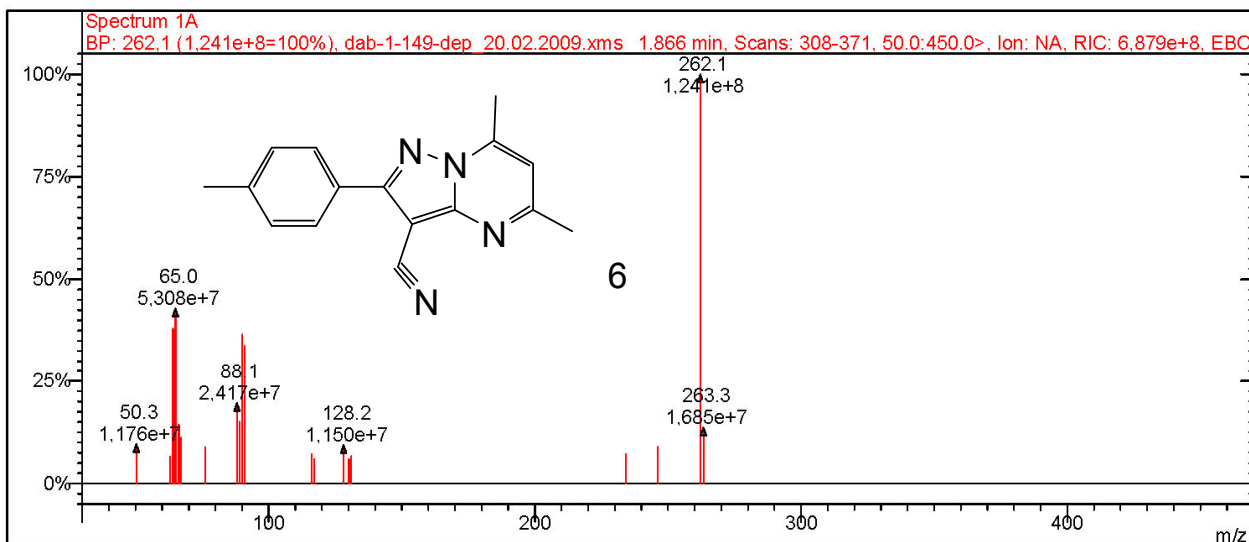
Scan 1 Channel Description: 40.0:400.0> EI;Det 1600;WI Q1 Cal;ST 0.010

Scan Information: cp = 1.0 mTorr

Precursor Mass Range: 40.0 - 400.0 m/z

Ion	Int	Norm	Ion	Int	Norm	Ion	Int	Norm
51.0	939670	83	99.9	1,022e+6	90	222.1	3,611e+6	317
61.9	2,275e+6	200	126.9	3,029e+6	266	248.9	1,217e+6	107
63.9	990337	87	127.9	1,107e+6	97	250.0	1,137e+7	999
66.9	2,240e+6	197	193.0	1,275e+6	112	251.1	2,055e+6	181
76.9	1,527e+6	134	221.0	5,755e+6	506			

Scan 339 from ...золе доценко\2015\вещества\6\dab-1-149-dep_20.02.2009.xms



Spectrum from ...ко\2015\вещества\6\dab-1-149-dep_20.02.2009.xms

Scan No: 339, Time: 1.866 minutes

64 points averaged. Background corrected (E).

Comment: 1.866 min. Scans: 308-371 50.0:450.0> Ion: NA RIC: 1,985e+9

Pair Count: 20 MW: 0 Formula: None

CAS No: None Acquired Range: 50.0 - 450.0 m/z

Method Description: EI

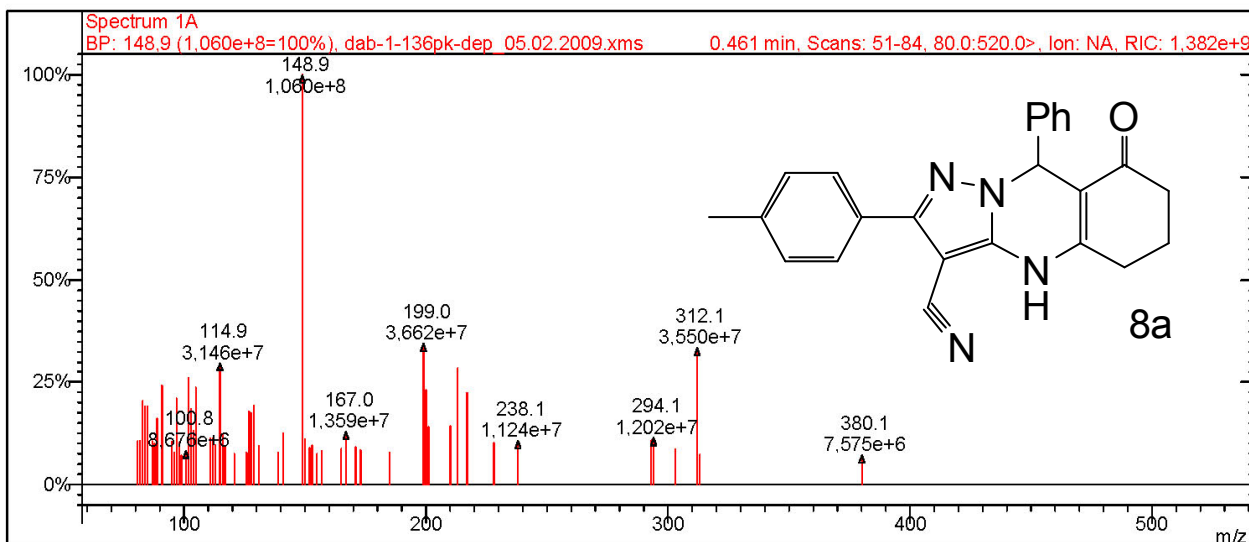
Scan 1 Channel Description: 50.0:450.0> EI;Det 0;WI Q1 Cal;ST 0.010

Scan Information: cp = 1.0 mTorr

Precursor Mass Range: 50.0 - 450.0 m/z

Ion	Int	Norm	Ion	Int	Norm	Ion	Int	Norm
50.3	1,176e+7	95	88.1	2,417e+7	195	130.1	7,298e+6	59
63.0	8,072e+6	65	89.0	1,863e+7	150	131.0	8,179e+6	66
64.1	4,710e+7	379	90.1	4,529e+7	365	234.3	8,855e+6	71
65.0	5,308e+7	427	91.0	4,188e+7	337	246.2	1,102e+7	89
66.2	1,774e+7	143	116.1	8,834e+6	71	262.1	1,241e+8	999
67.1	1,376e+7	111	117.2	7,306e+6	59	263.3	1,685e+7	136
76.1	1,088e+7	88	128.2	1,150e+7	93			

Scan 68 from ...е доценко\2015\вещества\8a\dab-1-136pk-dep_05.02.2009.xms



Spectrum from ...2015\вещества\8a\dab-1-136pk-dep_05.02.2009.xms

Scan No: 68, Time: 0.461 minutes

34 points averaged. Not background corrected.

Comment: 0.461 min. Scans: 51-84 80.0:520.0> Ion: NA RIC: 1,382e+9

Pair Count: 58 MW: 0 Formula: None

CAS No: None Acquired Range: 80.0 - 520.0 m/z

Method Description: EI

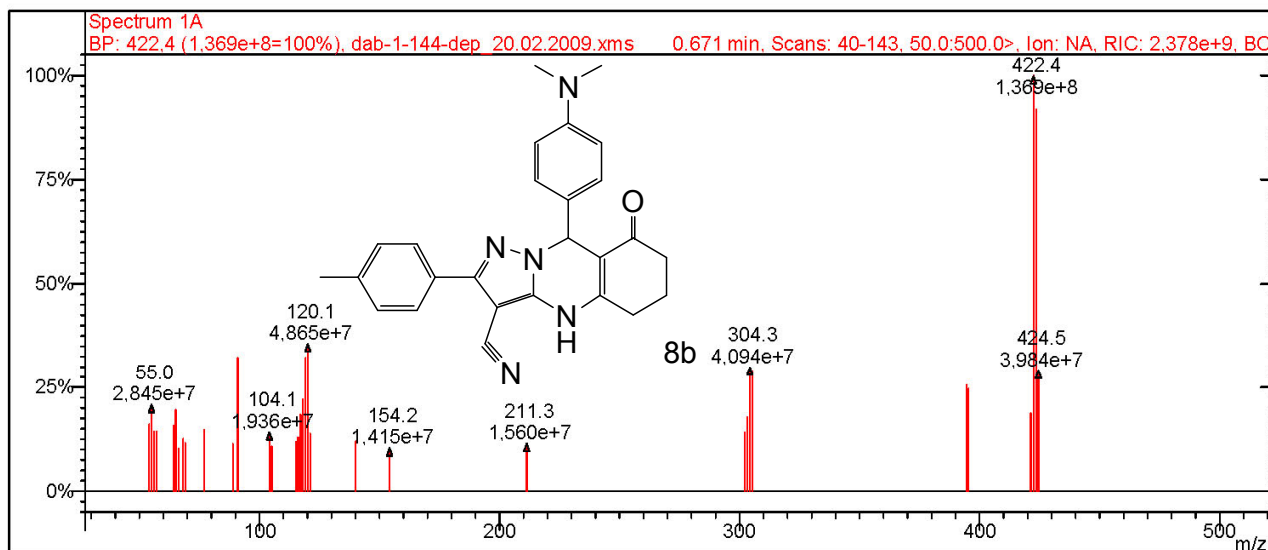
Scan 1 Channel Description: 80.0:520.0> EI;Det 0;WI Q1 Cal;ST 0.010

Scan Information: cp = 1.0 mTorr

Precursor Mass Range: 80.0 - 520.0 m/z

Ion	Int	Norm	Ion	Int	Norm	Ion	Int	Norm
80.9	1,116e+7	105	111.9	1,194e+7	113	165.0	9,175e+6	86
81.9	1,120e+7	106	113.0	1,017e+7	96	167.0	1,359e+7	128
82.9	2,156e+7	203	114.9	3,146e+7	297	171.0	9,653e+6	91
83.9	2,013e+7	190	116.0	1,275e+7	120	173.0	8,862e+6	84
85.0	2,010e+7	189	117.0	9,994e+6	94	185.0	8,113e+6	76
86.9	1,112e+7	105	120.9	7,842e+6	74	199.0	3,662e+7	345
87.9	1,051e+7	99	125.9	8,182e+6	77	200.0	2,433e+7	229
88.9	1,694e+7	160	126.9	1,879e+7	177	201.1	1,477e+7	139
90.9	2,556e+7	241	127.9	1,838e+7	173	210.0	1,507e+7	142
94.9	1,092e+7	103	128.9	2,021e+7	191	213.0	2,995e+7	282
95.9	8,131e+6	77	130.9	9,927e+6	94	217.0	2,365e+7	223
96.9	2,216e+7	209	139.0	8,079e+6	76	228.1	1,072e+7	101
98.0	1,075e+7	101	140.9	1,319e+7	124	238.1	1,124e+7	106
99.0	7,421e+6	70	148.9	1,060e+8	999	293.1	1,131e+7	107
100.8	8,676e+6	82	150.0	1,164e+7	110	294.1	1,202e+7	113
101.9	2,747e+7	259	151.9	9,395e+6	89	303.1	8,973e+6	85
102.9	1,953e+7	184	153.0	1,011e+7	95	312.1	3,550e+7	335
103.9	1,383e+7	130	155.0	7,856e+6	74	313.2	7,652e+6	72
104.9	2,500e+7	236	156.9	8,619e+6	81	380.1	7,575e+6	71
110.9	1,177e+7	111						

Scan 92 from ...оле доценко\2015\вещества\8b\dab-1-144-dep_20.02.2009.xms



Spectrum from ...o\2015\вещества\8b\dab-1-144-dep_20.02.2009.xms

Scan No: 92, Time: 0.671 minutes

104 points averaged. Background corrected.

Comment: 0.671 min. Scans: 40-143 50.0:500.0> Ion: NA RIC: 2,538e+9

Pair Count: 34 MW: 0 Formula: None

CAS No: None Acquired Range: 50.0 - 500.0 m/z

Method Description: EI

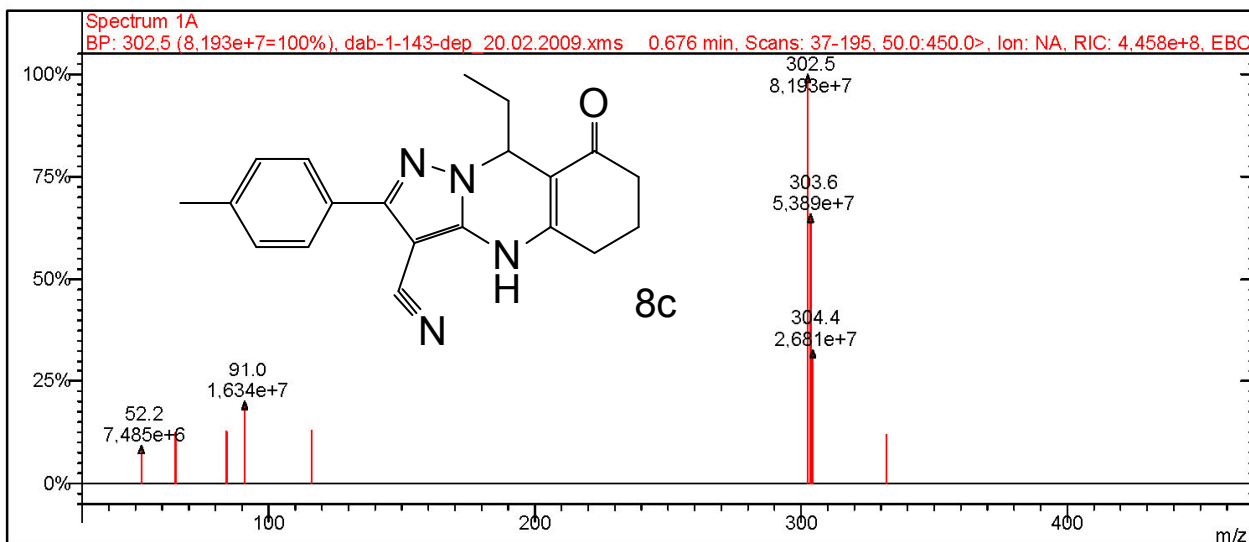
Scan 1 Channel Description: 50.0:500.0> EI;Det 0;WI Q1 Cal;ST 0.010

Scan Information: cp = 1.0 mTorr

Precursor Mass Range: 50.0 - 500.0 m/z

Ion	Int	Norm	Ion	Int	Norm	Ion	Int	Norm
54.1	2,189e+7	160	104.1	1,936e+7	141	211.3	1,560e+7	114
55.0	2,845e+7	208	105.2	1,467e+7	107	302.3	1,932e+7	141
56.2	1,963e+7	143	115.1	1,618e+7	118	303.2	2,433e+7	178
57.1	1,949e+7	142	116.1	1,765e+7	129	304.3	4,094e+7	299
64.2	2,148e+7	157	117.1	2,513e+7	183	305.2	3,975e+7	290
65.1	2,671e+7	195	118.1	3,008e+7	219	394.6	3,503e+7	256
66.2	1,390e+7	101	119.2	4,407e+7	322	395.4	3,378e+7	246
68.2	1,713e+7	125	120.1	4,865e+7	355	421.3	2,558e+7	187
69.1	1,581e+7	115	121.2	1,883e+7	137	422.4	1,369e+8	999
77.0	1,998e+7	146	140.0	1,633e+7	119	423.5	1,257e+8	917
88.9	1,545e+7	113	154.2	1,415e+7	103	424.5	3,984e+7	291
91.0	4,415e+7	322						

Scan 117 from ...оле доценко\2015\вещества\8c\dab-1-143-dep_20.02.2009.xms



Spectrum from ...o\2015\вещества\8c\dab-1-143-dep_20.02.2009.xms

Scan No: 117, Time: 0.676 minutes

159 points averaged. Background corrected (E).

Comment: 0.676 min. Scans: 37-195 50.0:450.0> Ion: NA RIC: 1,136e+9

Pair Count: 9 MW: 0 Formula: None

CAS No: None Acquired Range: 50.0 - 450.0 m/z

Method Description: EI

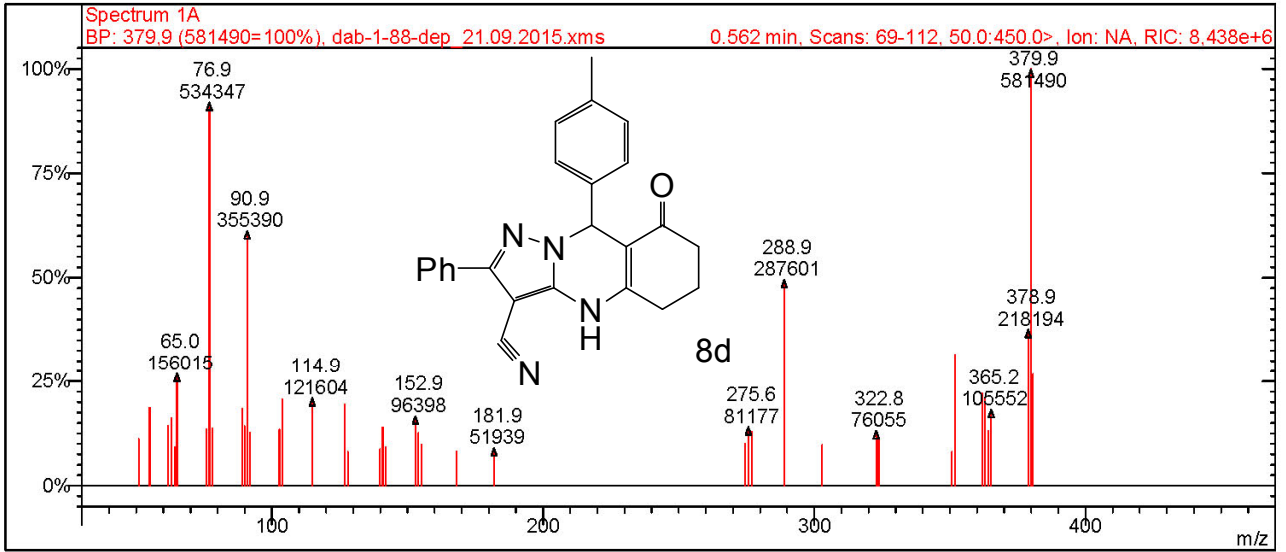
Scan 1 Channel Description: 50.0:450.0> EI;Det 1340;WI Q1 Cal;ST 0.010

Scan Information: cp = 1.1 mTorr

Precursor Mass Range: 50.0 - 450.0 m/z

Ion	Int	Norm	Ion	Int	Norm	Ion	Int	Norm
52.2	7,485e+6	91	91.0	1,634e+7	199	303.6	5,389e+7	657
65.0	1,015e+7	124	116.1	1,056e+7	129	304.4	2,681e+7	327
84.2	1,034e+7	126	302.5	8,193e+7	999	332.1	9,698e+6	118

Scan 91 from ...золе доценко\2015\вещества\8d\dab-1-88-dep_21.09.2015.xms



Spectrum from ...ко\2015\вещества\8d\dab-1-88-dep_21.09.2015.xms

Scan No: 91, Time: 0.562 minutes

44 points averaged. Not background corrected.

Comment: 0.562 min. Scans: 69-112 50.0:450.0> Ion: NA RIC: 8,438e+6

Pair Count: 42 MW: 0 Formula: None

CAS No: None Acquired Range: 50.0 - 450.0 m/z

Method Description: EI

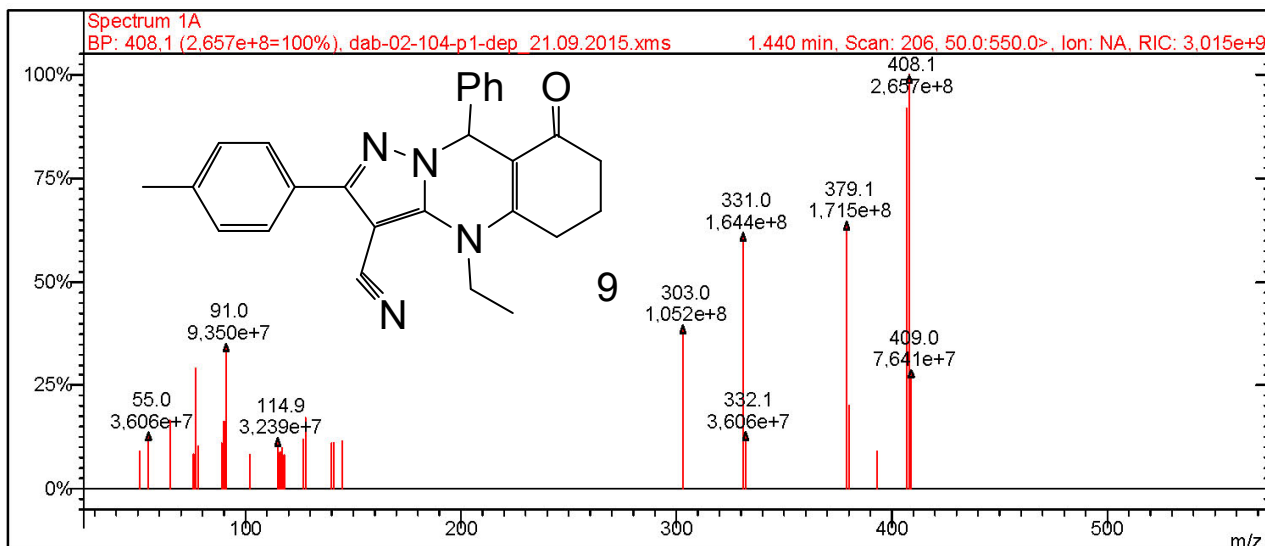
Scan 1 Channel Description: 50.0:450.0> EI;Det 1100;W1 Q1 Cal;ST 0.010

Scan Information: cp = 8.0 mTorr

Precursor Mass Range: 50.0 - 450.0 m/z

Ion	Int	Norm	Ion	Int	Norm	Ion	Int	Norm
51.0	64583	111	103.9	119614	205	277.0	74319	128
55.0	108156	186	114.9	121604	209	288.9	287601	494
61.8	83315	143	126.9	112262	193	302.9	56298	97
63.0	93527	161	128.1	46626	80	322.8	76055	131
64.1	53583	92	139.8	50259	86	323.7	65695	113
65.0	156015	268	140.9	80977	139	350.7	46628	80
75.9	78313	135	142.0	53388	92	351.9	183056	314
76.9	534347	918	152.9	96398	166	361.9	128155	220
78.0	79115	136	154.0	72758	125	363.0	120216	207
89.1	106308	183	155.1	57027	98	364.2	75975	131
90.0	82597	142	168.2	47137	81	365.2	105552	181
90.9	355390	611	181.9	51939	89	378.9	218194	375
92.0	72968	125	274.6	58325	100	379.9	581490	999
102.8	77575	133	275.6	81177	139	380.6	155262	267

Scan 206 from ... доценко\2015\вещества\9\dab-02-104-p1-dep_21.09.2015.xms



Spectrum from ...015\вещества\9\dab-02-104-p1-dep_21.09.2015.xms

Scan No: 206, Time: 1.440 minutes

No averaging. Not background corrected.

Comment: 1.440 min, Scan: 206 50.0:550.0> Ion: NA RIC: 3,015e+9

Pair Count: 28 MW: 0 Formula: None

CAS No: None Acquired Range: 50.0 - 550.0 m/z

Method Description: EI

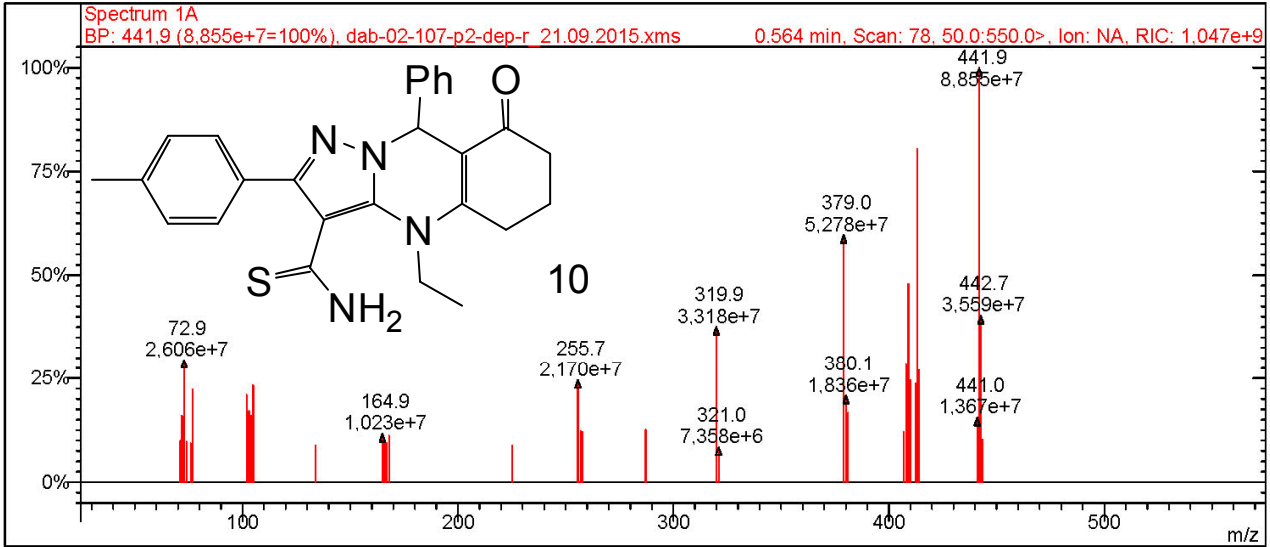
Scan 1 Channel Description: 50.0:550.0> EI;Det 0;WI Q1 Cal;ST 0.010

Scan Information: cp = 8.0 mTorr

Precursor Mass Range: 50.0 - 550.0 m/z

Ion	Int	Norm	Ion	Int	Norm	Ion	Int	Norm
51.0	2,393e+7	90	114.9	3,239e+7	122	303.0	1,052e+8	395
55.0	3,606e+7	136	116.0	2,328e+7	88	331.0	1,644e+8	618
64.9	4,359e+7	164	116.9	2,605e+7	98	332.1	3,606e+7	136
75.9	2,186e+7	82	117.9	2,133e+7	80	379.1	1,715e+8	645
76.9	7,757e+7	292	126.8	3,144e+7	118	380.0	5,312e+7	200
78.0	2,700e+7	101	127.9	4,536e+7	171	393.0	2,383e+7	90
89.0	2,893e+7	109	139.9	2,897e+7	109	407.0	2,439e+8	917
90.0	4,292e+7	161	140.9	2,909e+7	109	408.1	2,657e+8	999
91.0	9,350e+7	351	144.9	3,014e+7	113	409.0	7,641e+7	287
101.9	2,177e+7	82						

Scan 78 from ...ценко\2015\вещества\10\dab-02-107-p2-dep-r_21.09.2015.xms

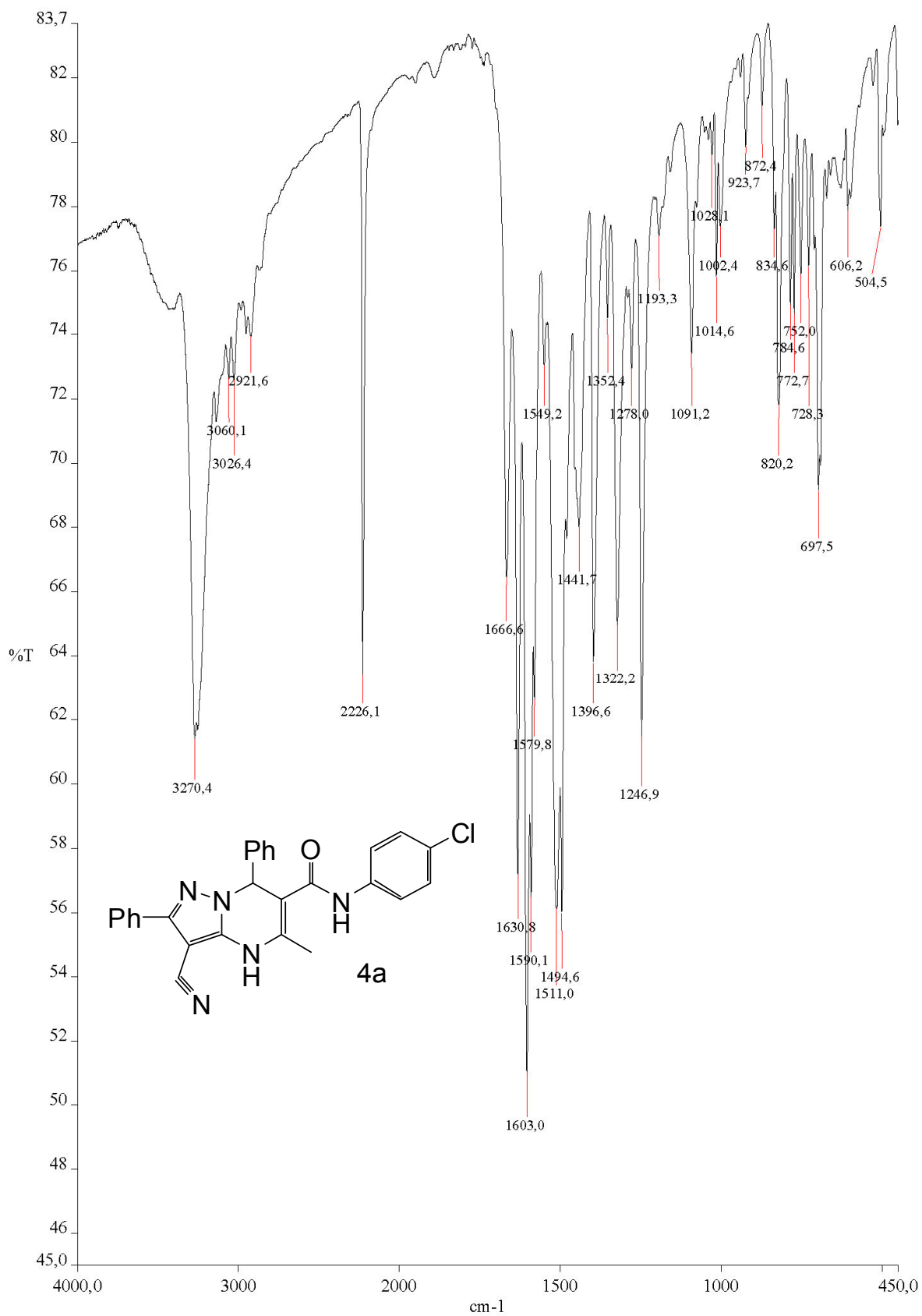


Spectrum from ...\вещества\10\dab-02-107-p2-dep-r_21.09.2015.xms
 Scan No: 78, Time: 0.564 minutes
 No averaging. Not background corrected.
 Comment: 0.564 min. Scan: 78 50.0:550.0> Ion: NA RIC: 1,047e+9
 Pair Count: 36 MW: 0 Formula: None
 CAS No: None Acquired Range: 50.0 - 550.0 m/z

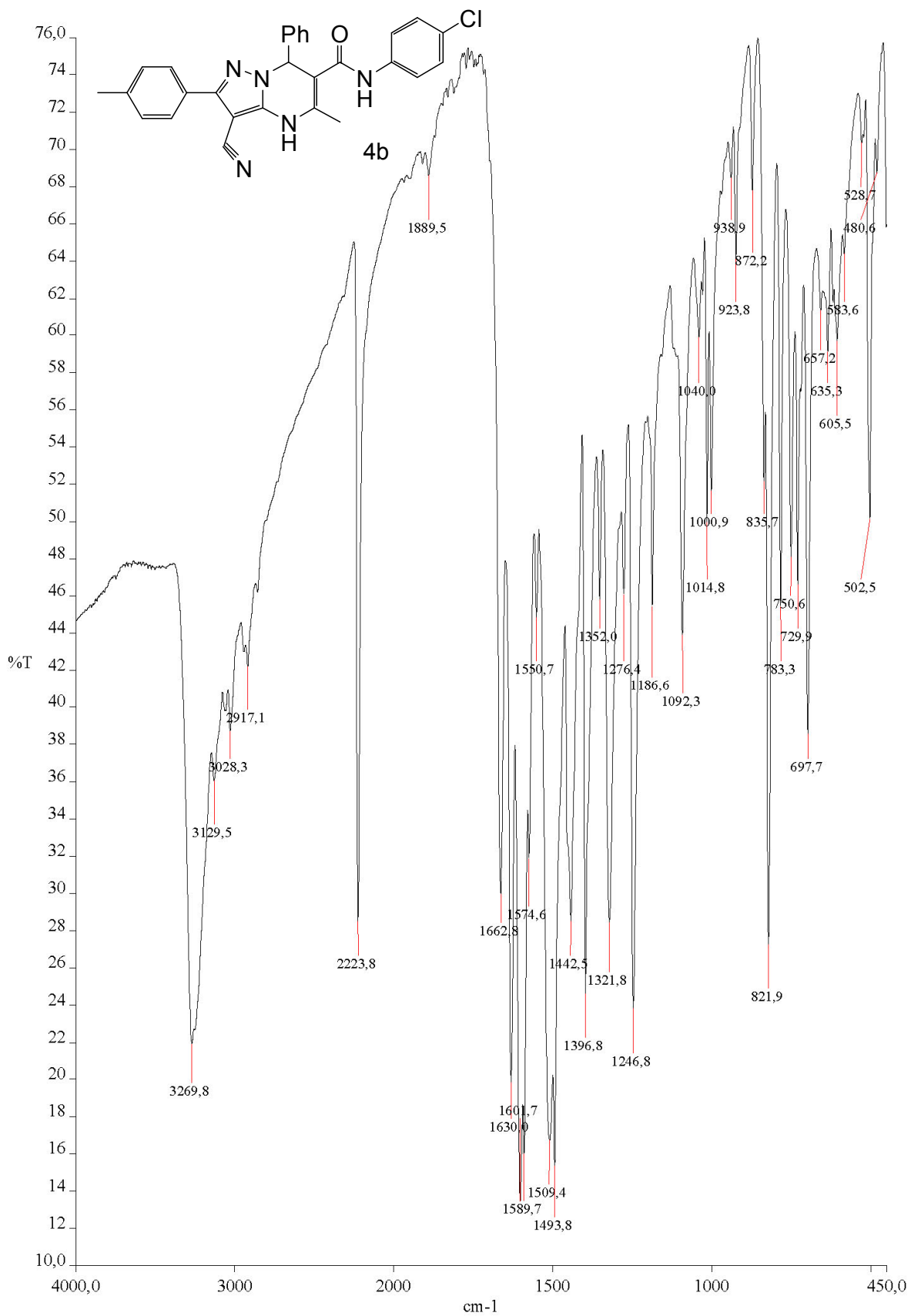
Method Description: EI
 Scan 1 Channel Description: 50.0:550.0> EI;Det 1100;WI Q1 Cal;ST 0.010
 Scan Information: cp = 8.0 mTorr
 Precursor Mass Range: 50.0 - 550.0 m/z

Ion	Int	Norm	Ion	Int	Norm	Ion	Int	Norm
71.1	8,773e+6	99	165.9	8,177e+6	92	381.0	1,471e+7	166
71.9	1,412e+7	159	166.9	8,217e+6	93	407.0	1,069e+7	121
72.9	2,606e+7	294	168.0	9,845e+6	111	408.0	2,505e+7	283
74.0	8,579e+6	97	225.1	7,788e+6	88	409.1	4,241e+7	478
75.9	8,227e+6	93	255.7	2,170e+7	245	410.1	2,173e+7	245
76.9	1,973e+7	223	256.9	1,083e+7	122	412.4	2,101e+7	237
101.9	1,854e+7	209	257.9	1,066e+7	120	413.1	7,117e+7	803
103.0	1,512e+7	171	287.1	1,110e+7	125	414.1	2,392e+7	270
104.0	1,409e+7	159	319.9	3,318e+7	374	441.0	1,367e+7	154
104.9	2,059e+7	232	321.0	7,358e+6	83	441.9	8,855e+7	999
133.9	7,658e+6	86	379.0	5,278e+7	595	442.7	3,559e+7	402
164.9	1,023e+7	115	380.1	1,836e+7	207	443.6	8,977e+6	101

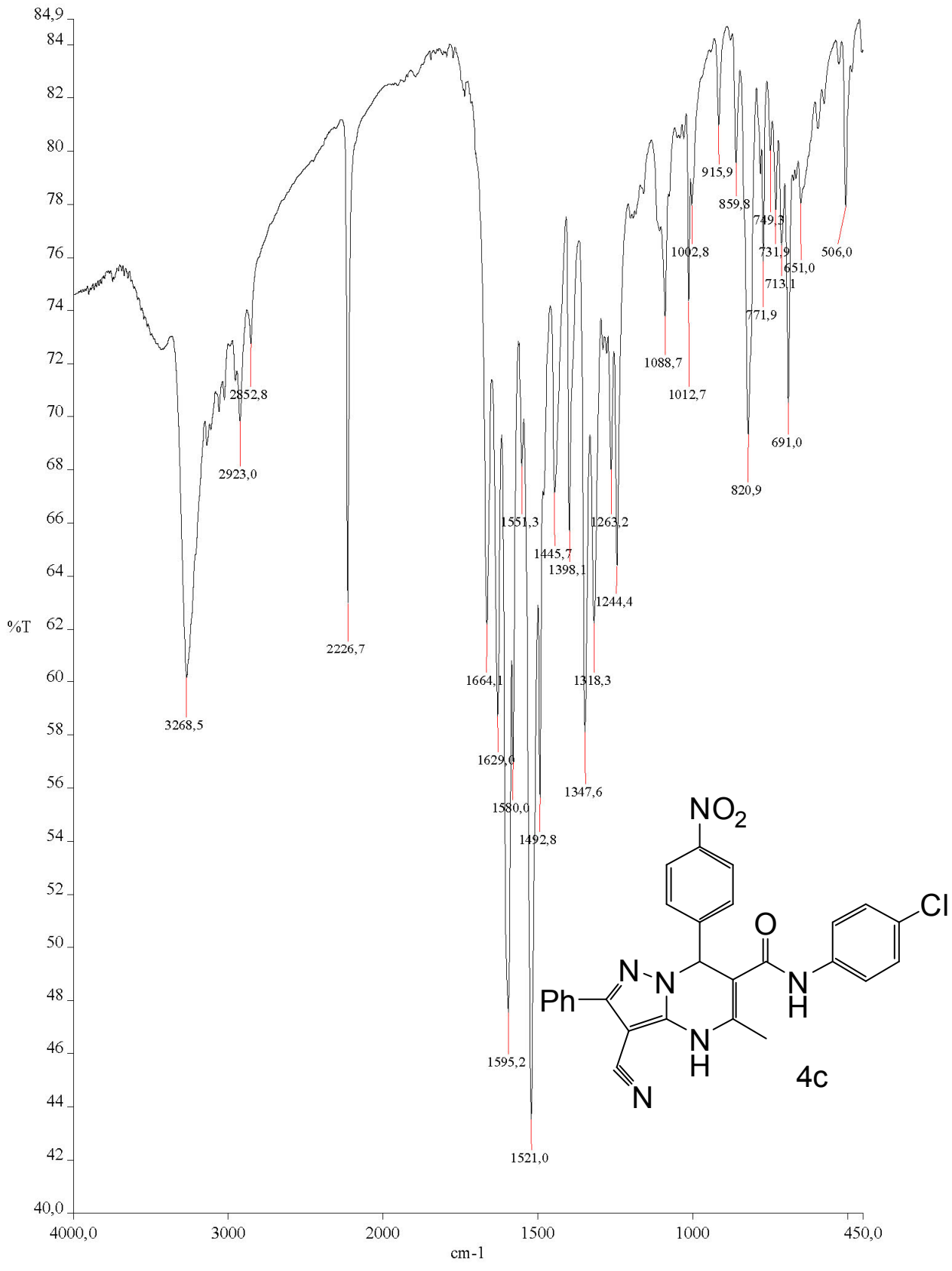
5. IR spectra of synthesized compounds



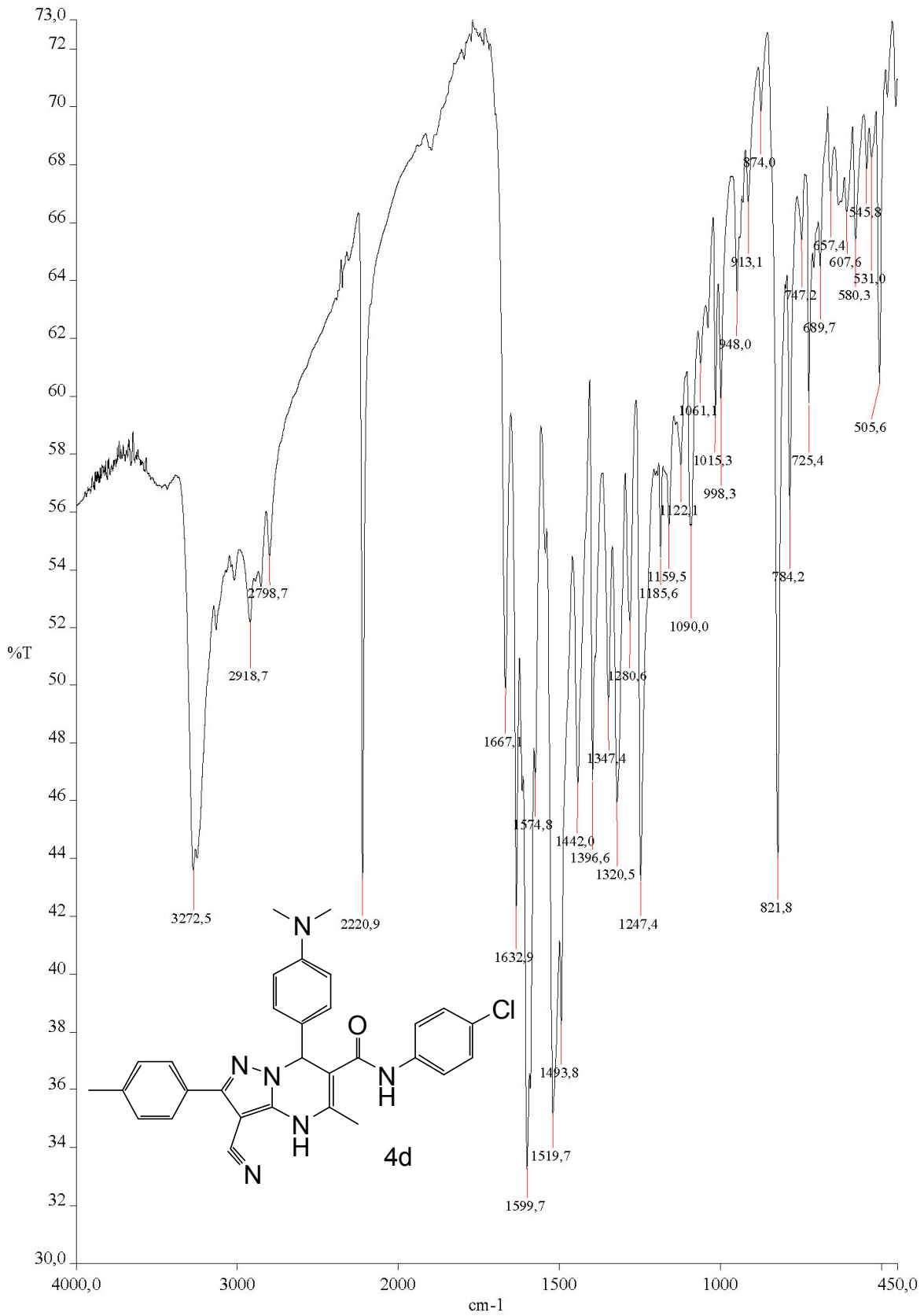
c:\pel_data\spectra\# 9438.sp - DAB-1-79



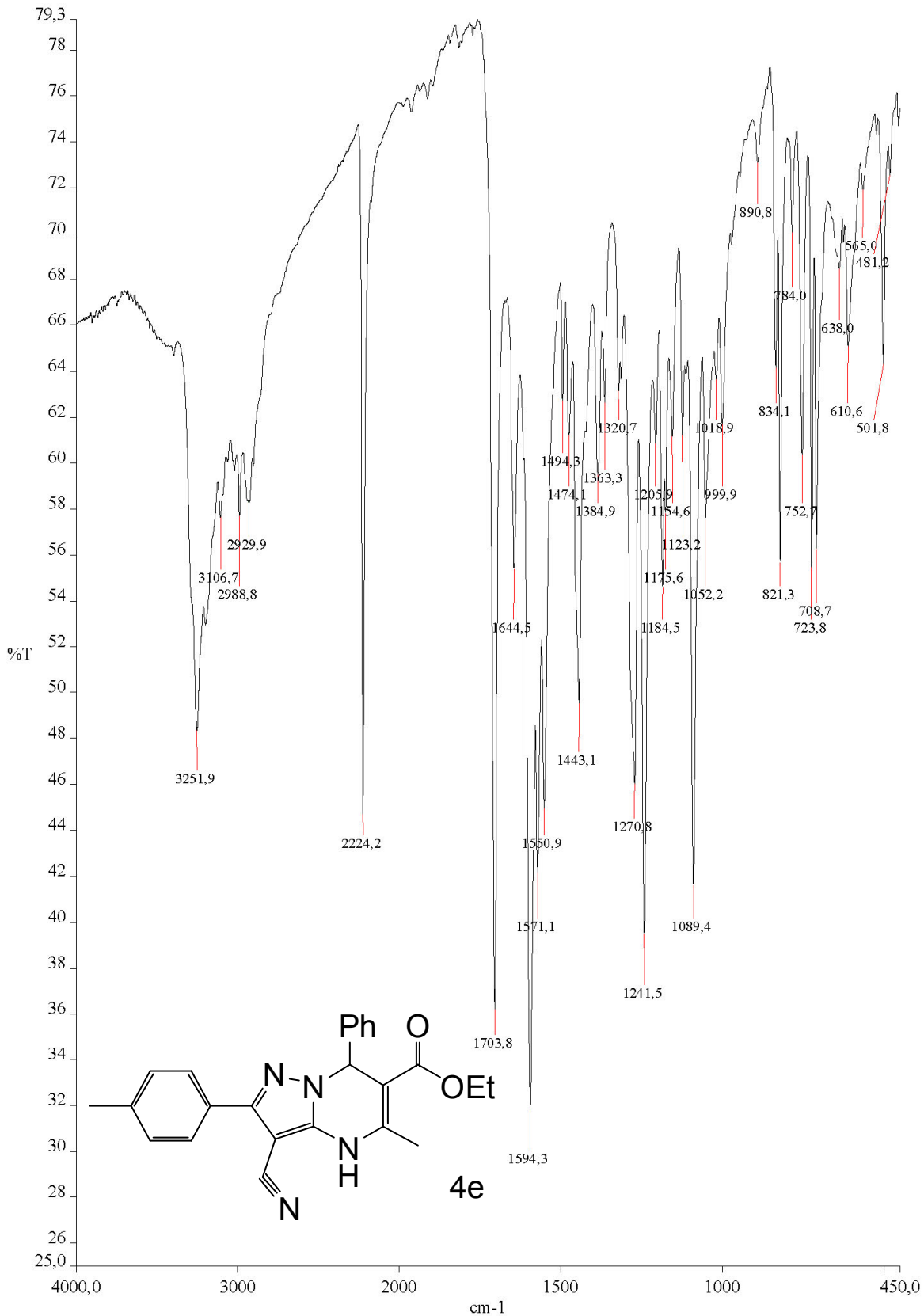
c:\pel_data\spectra\# 9443.sp - DAB-1-124



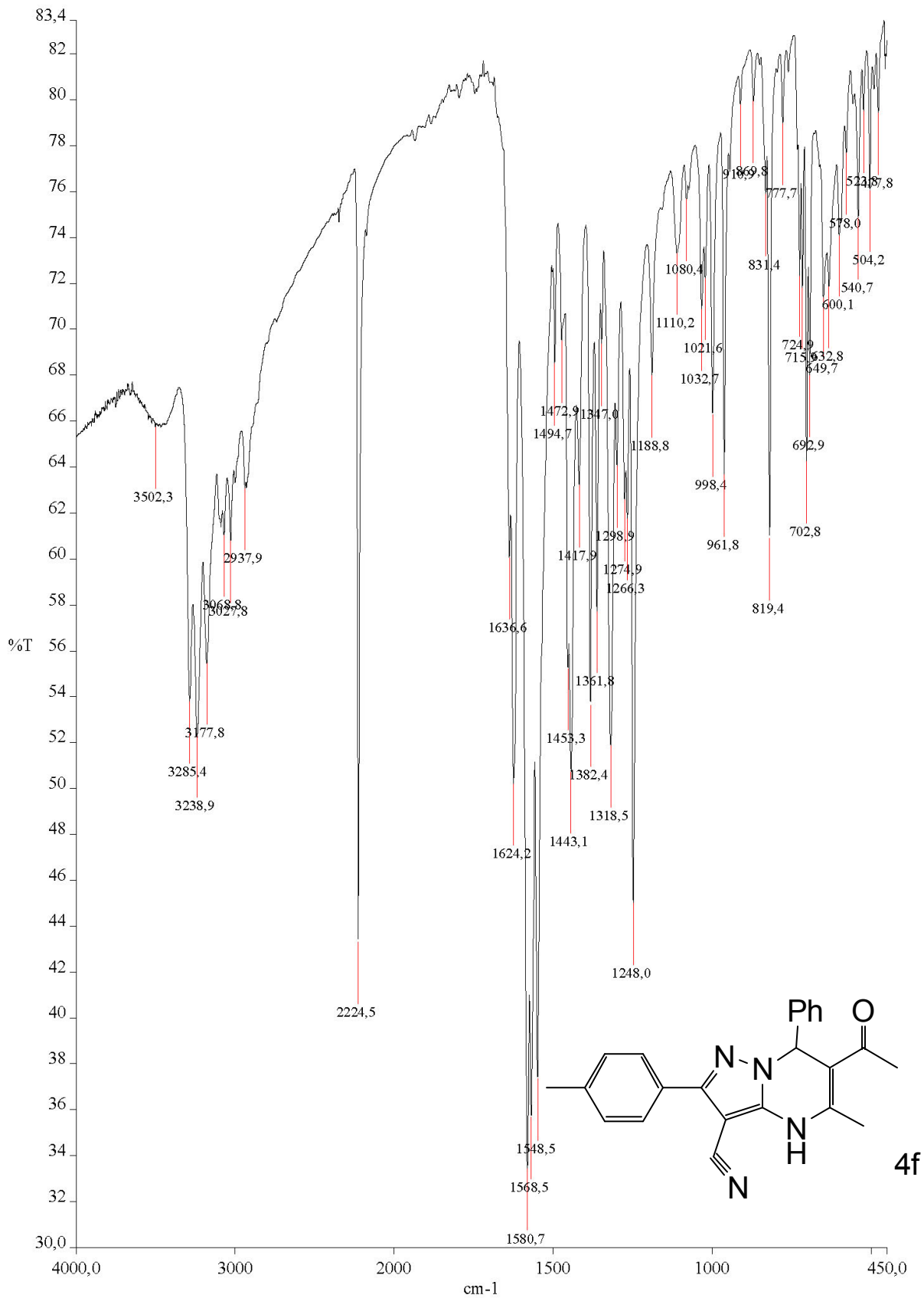
c:\pel_data\spectra# 9440.sp - DAB-1-86



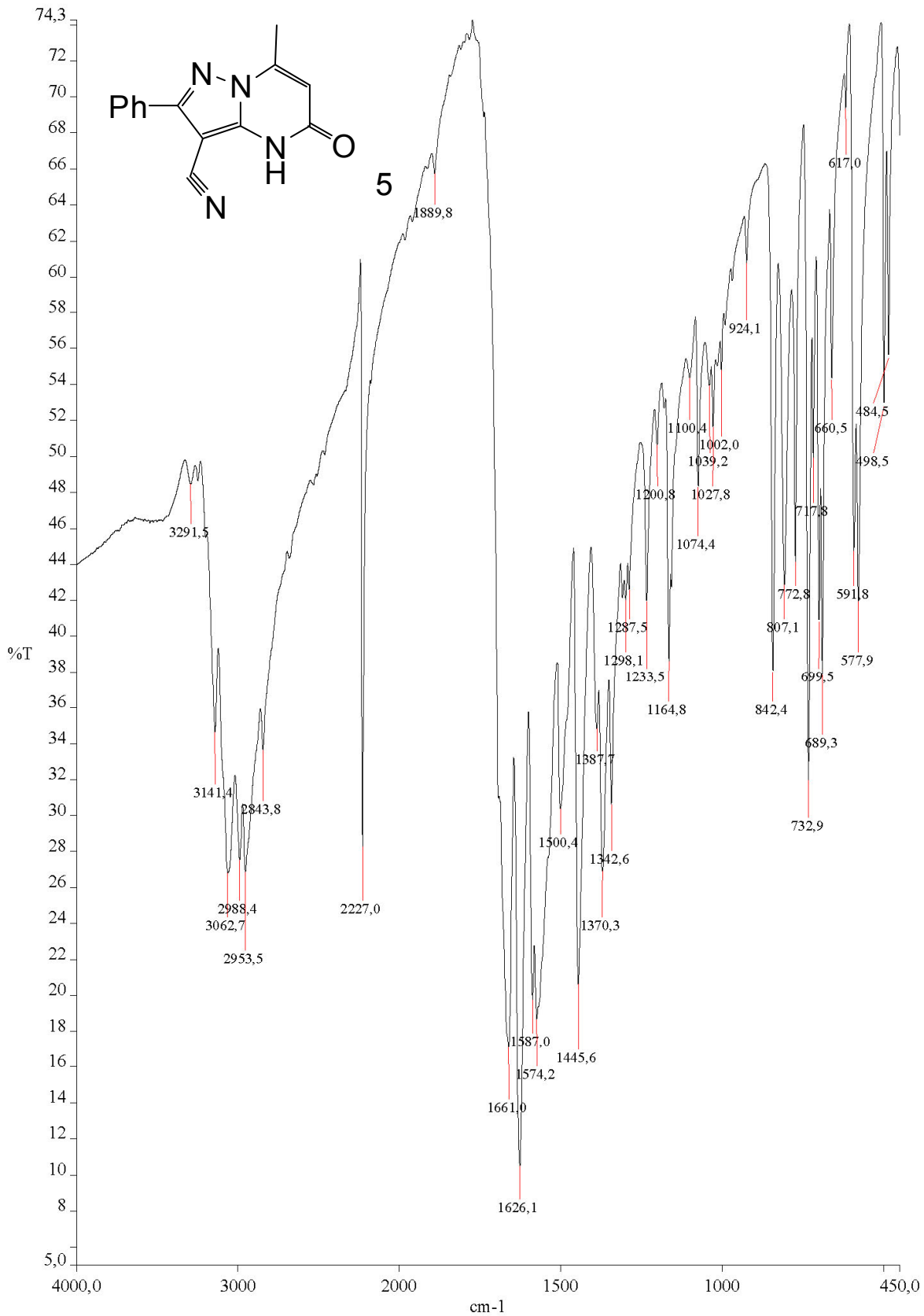
c:\pel_data\spectra# 9442.sp - DAB-1-93



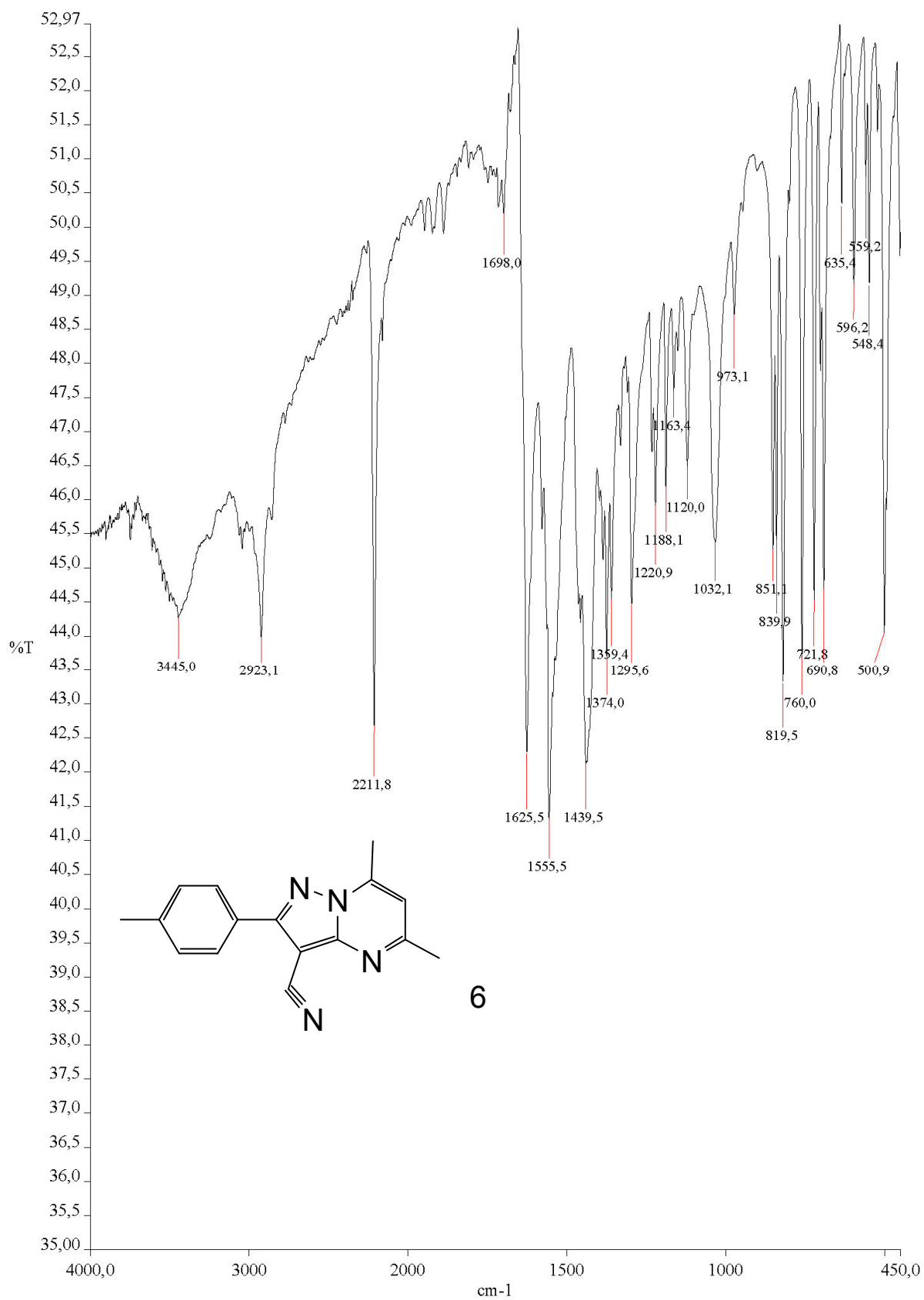
c:\pel_data\spectra# 9445.sp - DAB-1-137



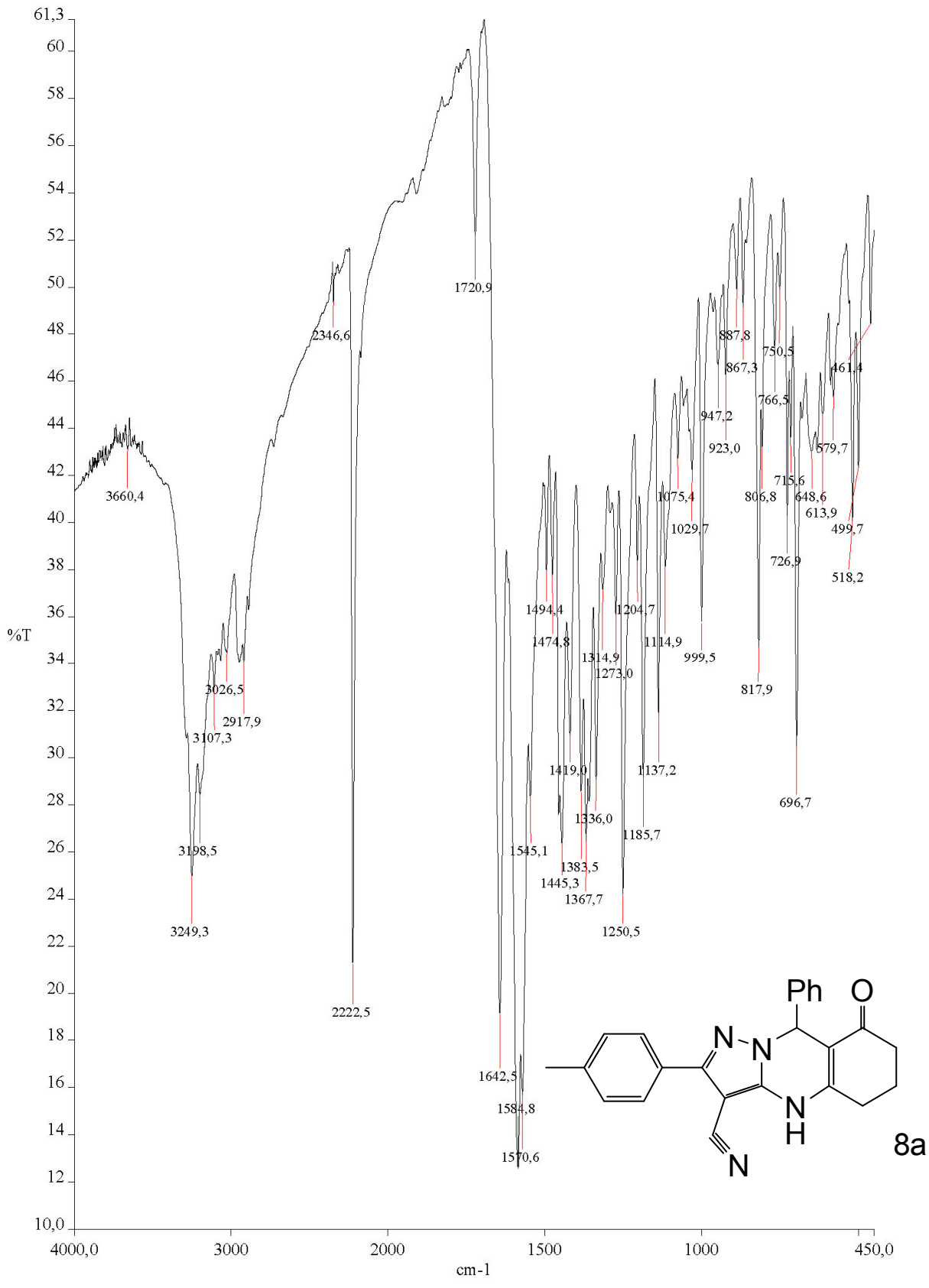
c:\pel_data\spectra# 9449.sp - DAB-1-188



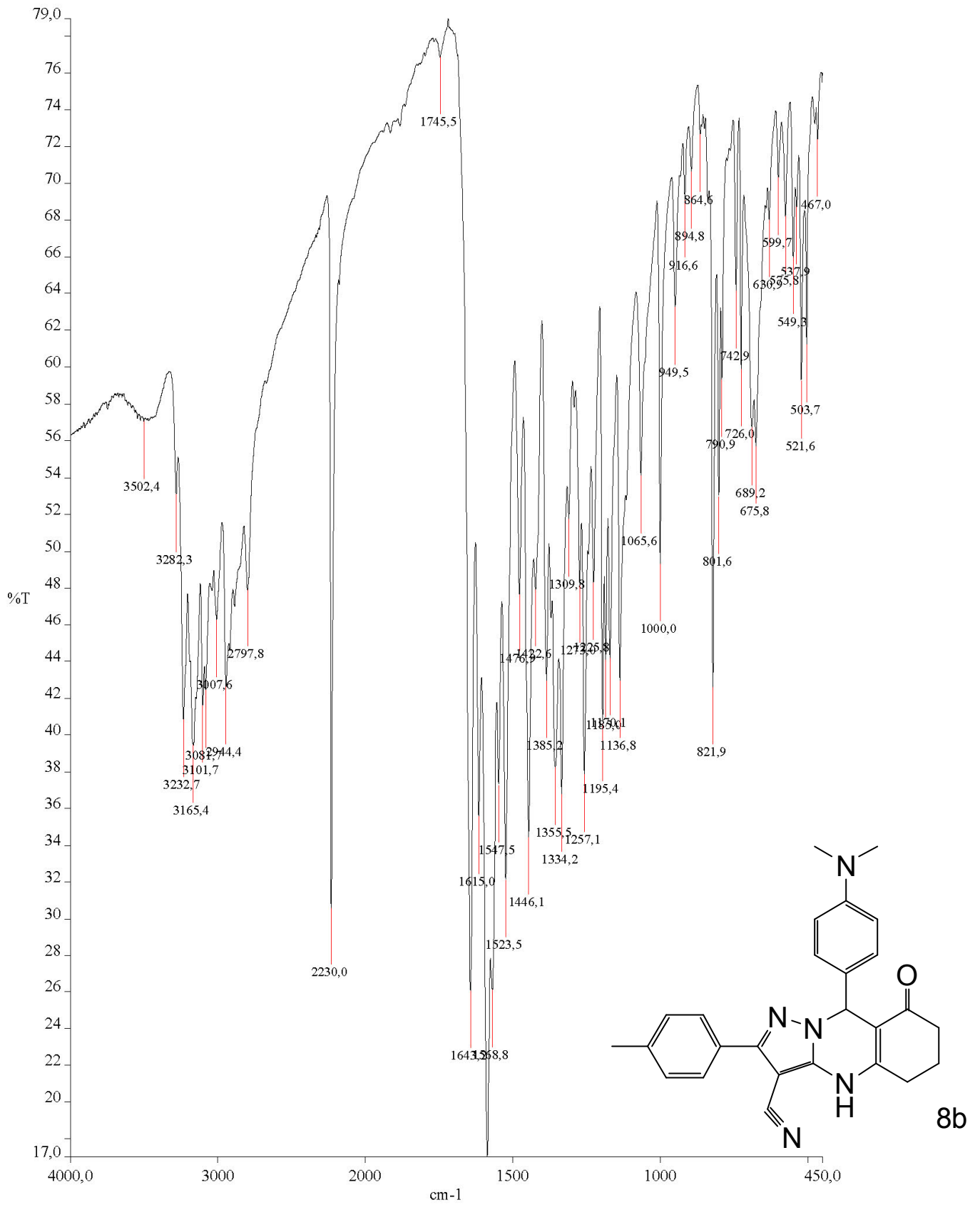
c:\pel_data\spectra# 9439.sp - DAB-1-81



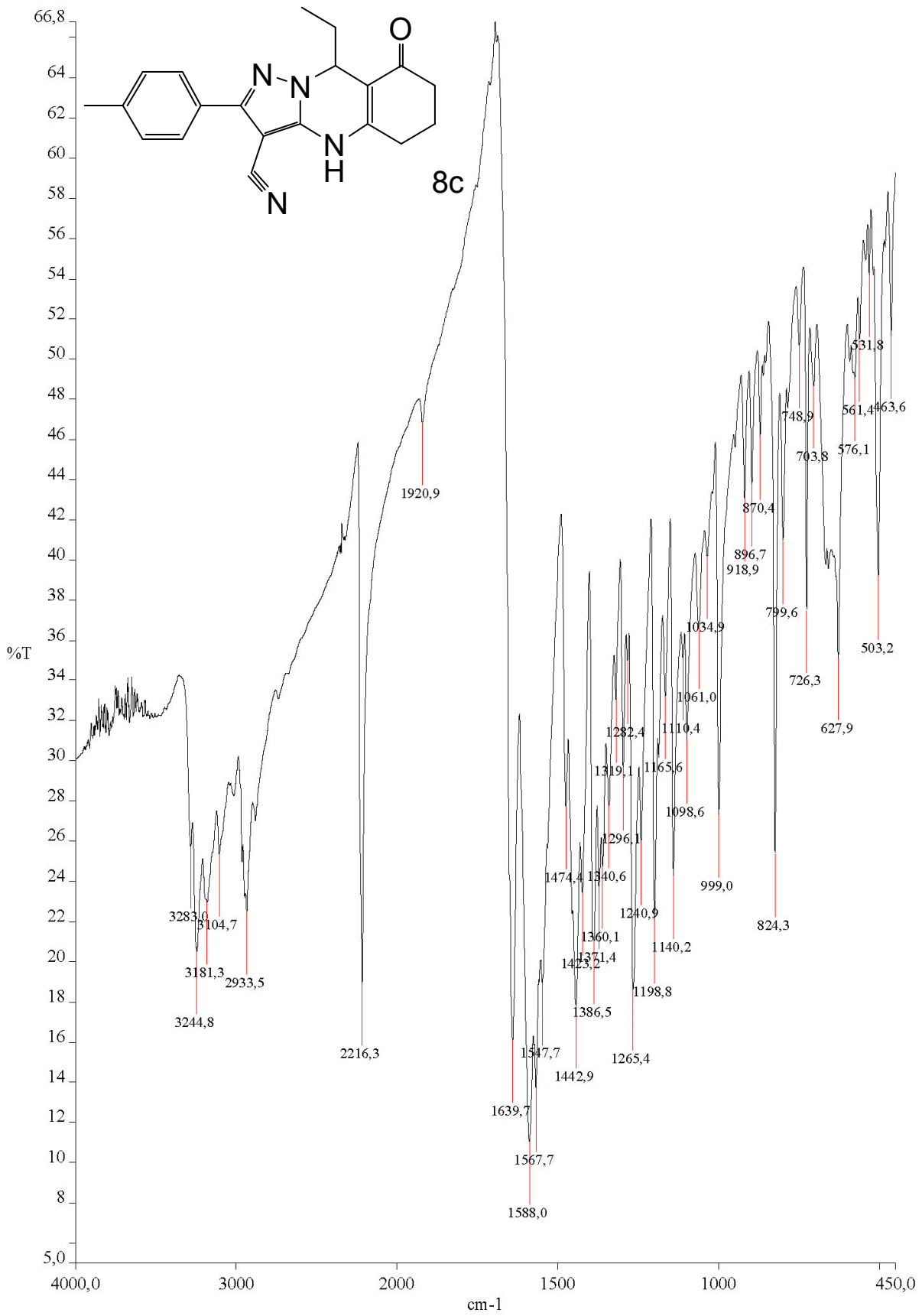
c:\pel_data\spectra\# 9448.sp - DAB-1-149



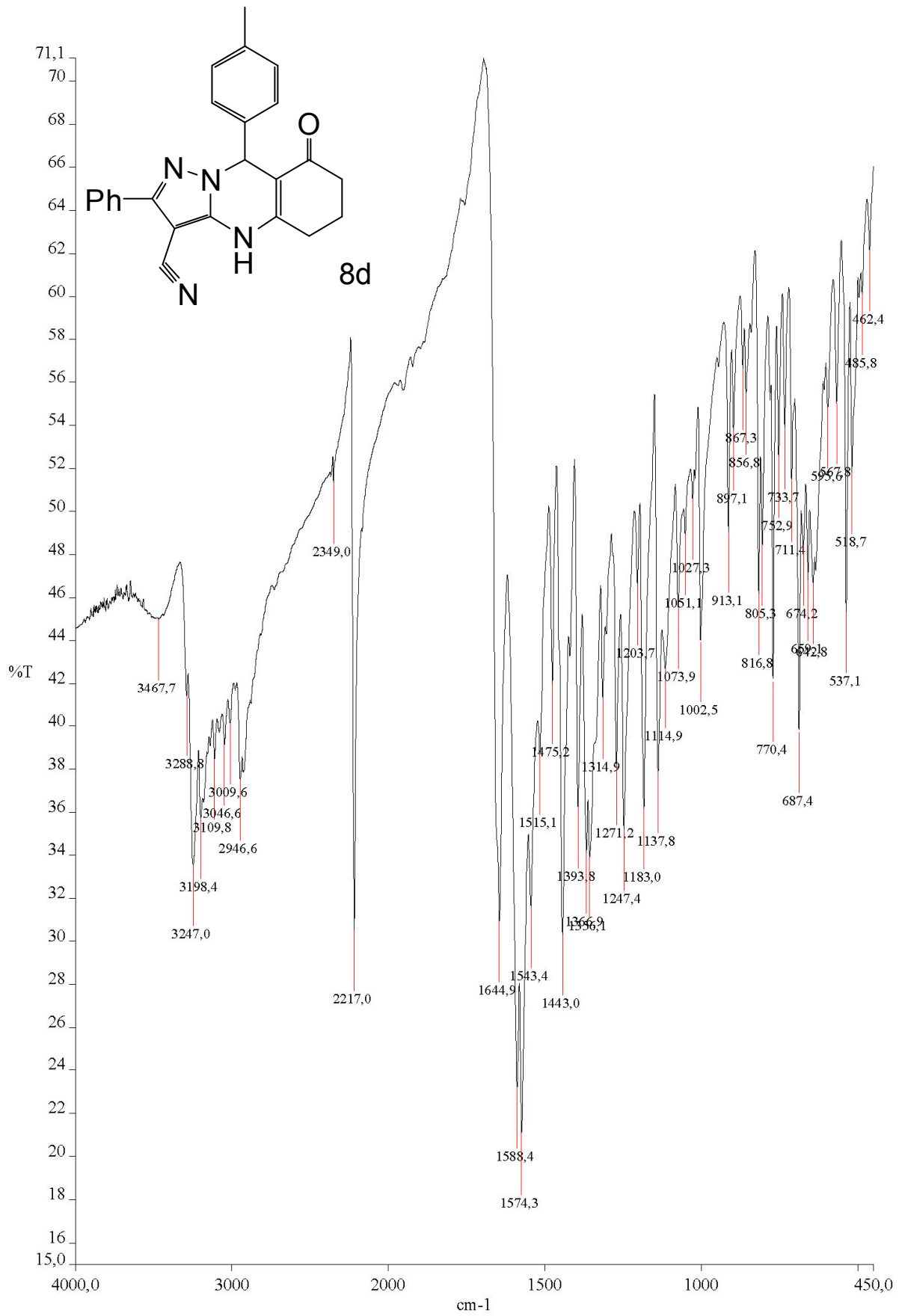
c:\pel_data\spectra# 9444.sp - DAB-1-136



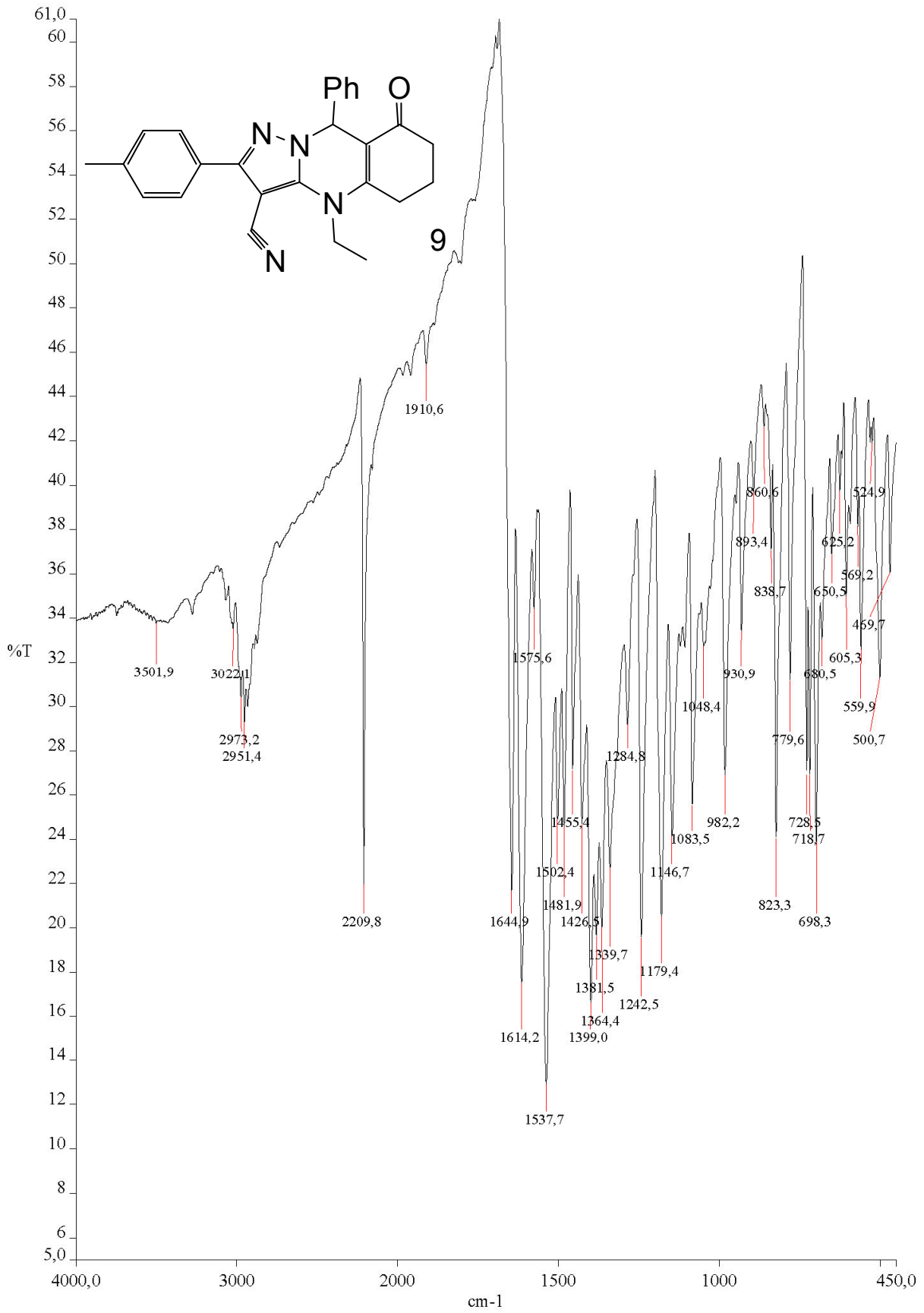
c:\pel_data\spectra\# 9447.sp - DAB-1-144



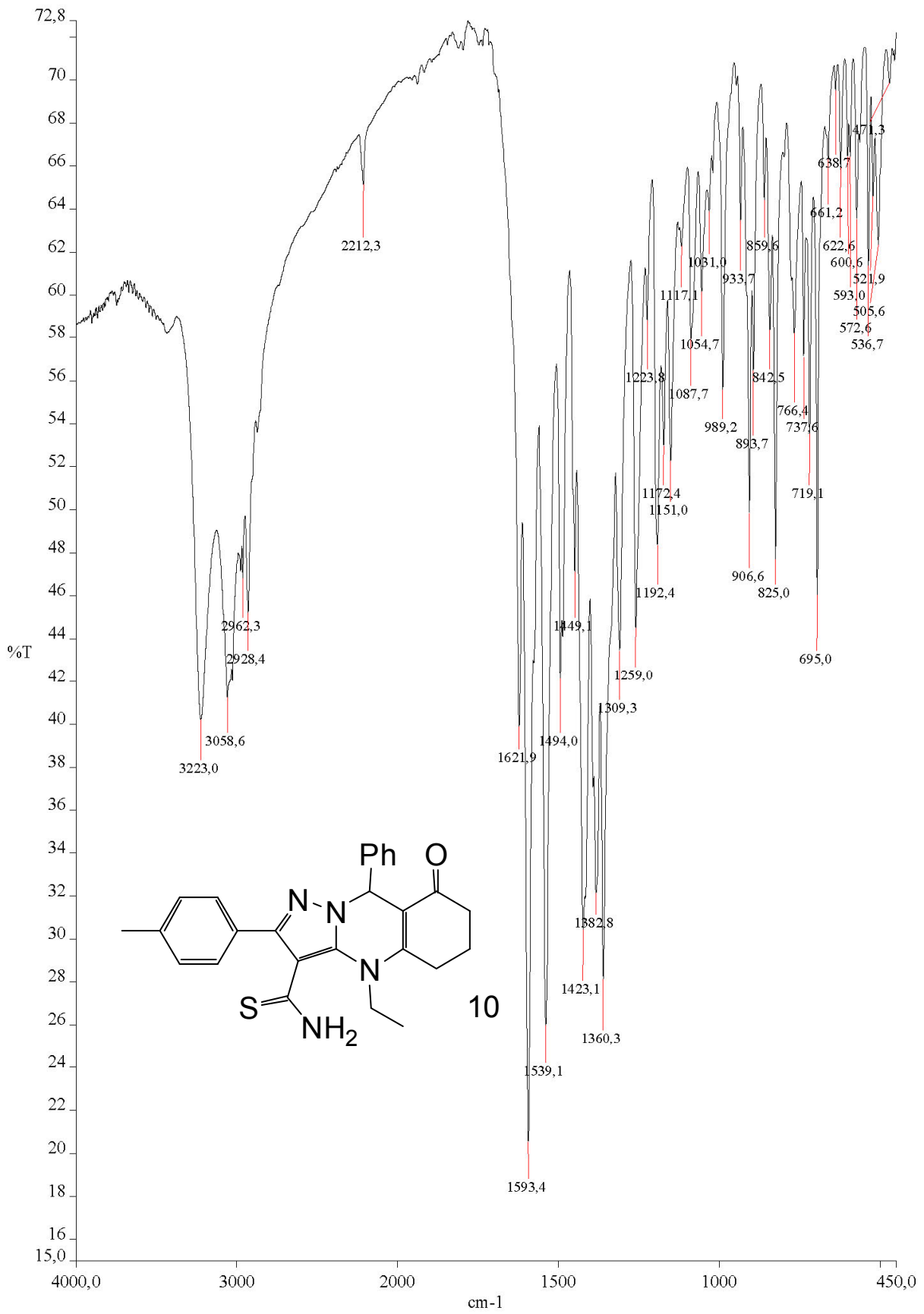
c:\pel_data\spectra# 9446.sp - DAB-1-143



c:\pel_data\spectra# 9441.sp - DAB-1-88



c:\pel_data\spectra# 9450.sp - DAB-2-104-P1



c:\pel_data\spectra# 9451.sp - DAB-2-107-P2