Supplementary Material

The synthesis of novel hexahydrodibenzo[*b,e*][1,4]diazepin-1-one derivatives

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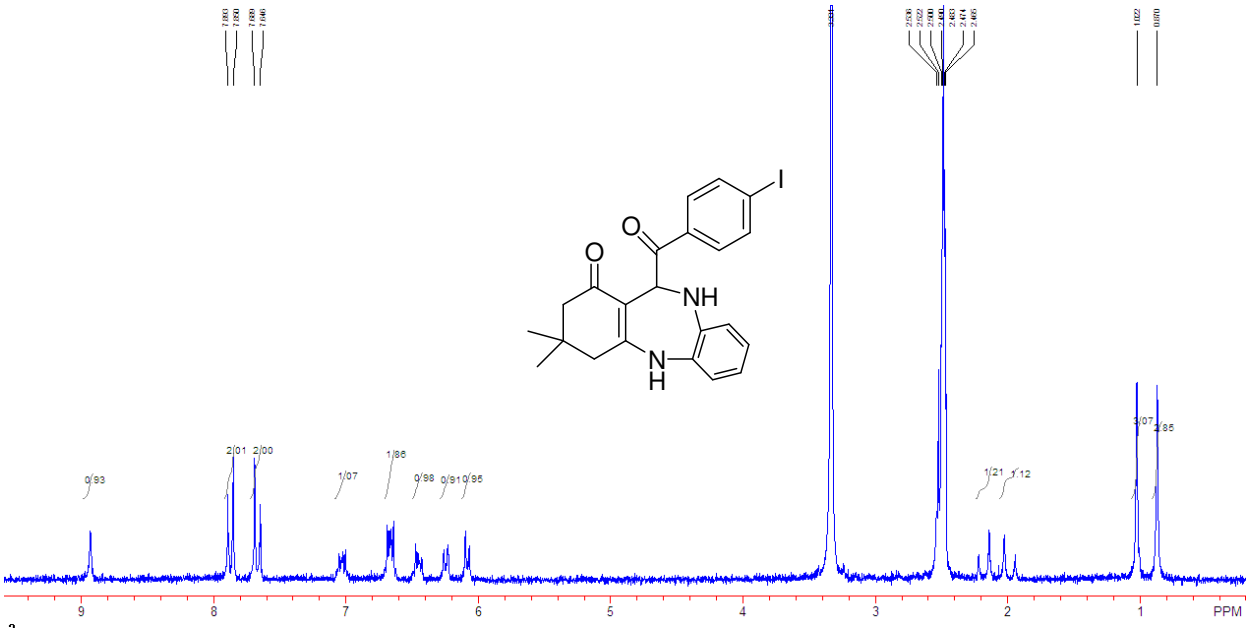
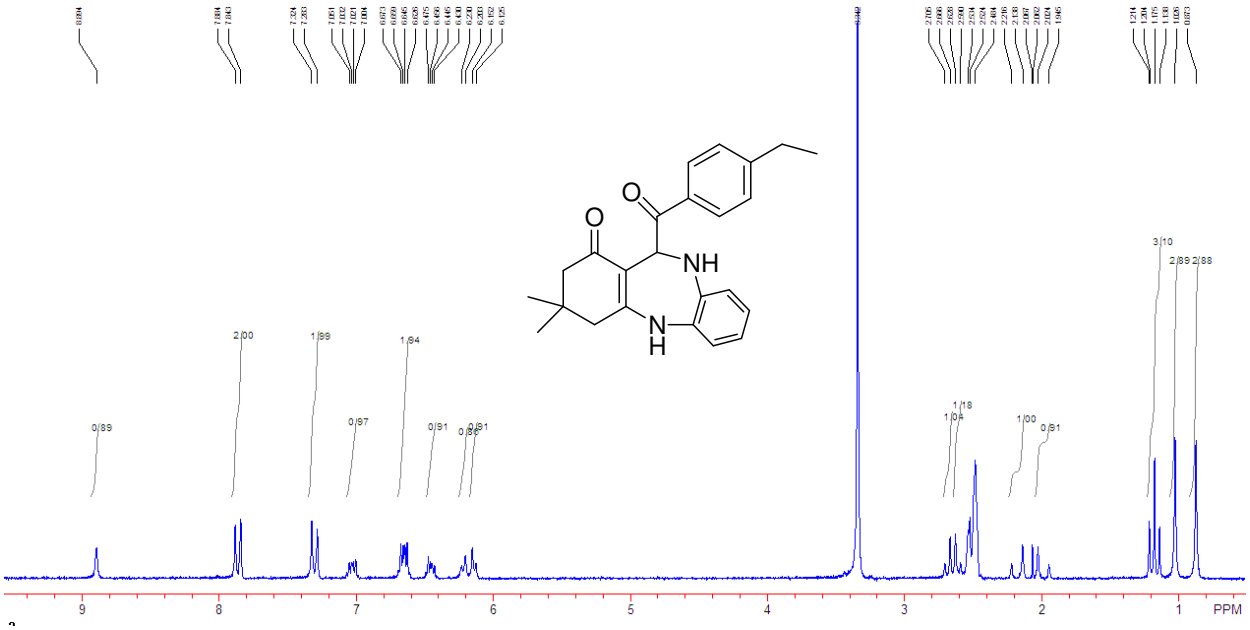
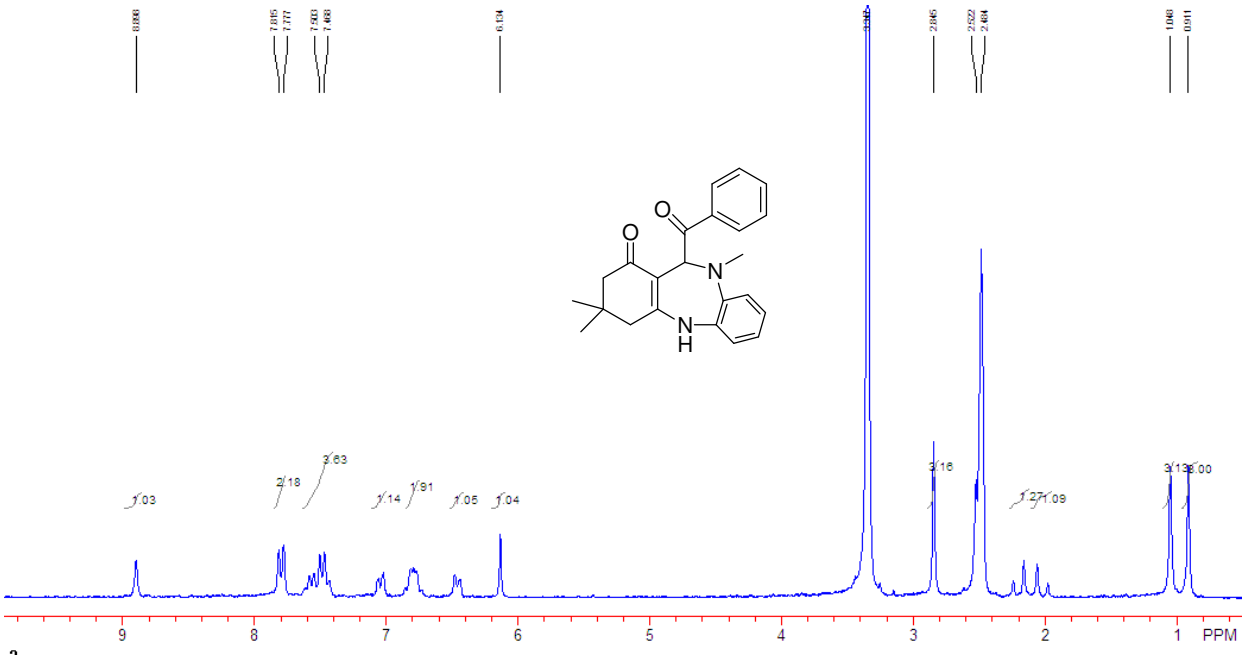


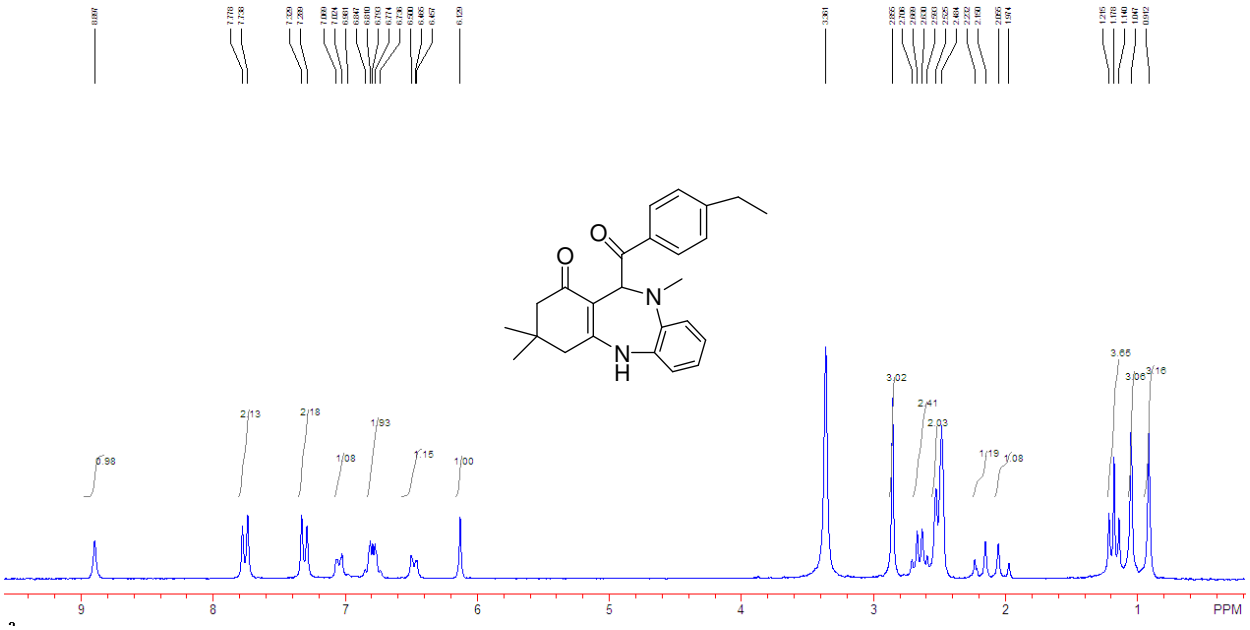
Compound **5k**



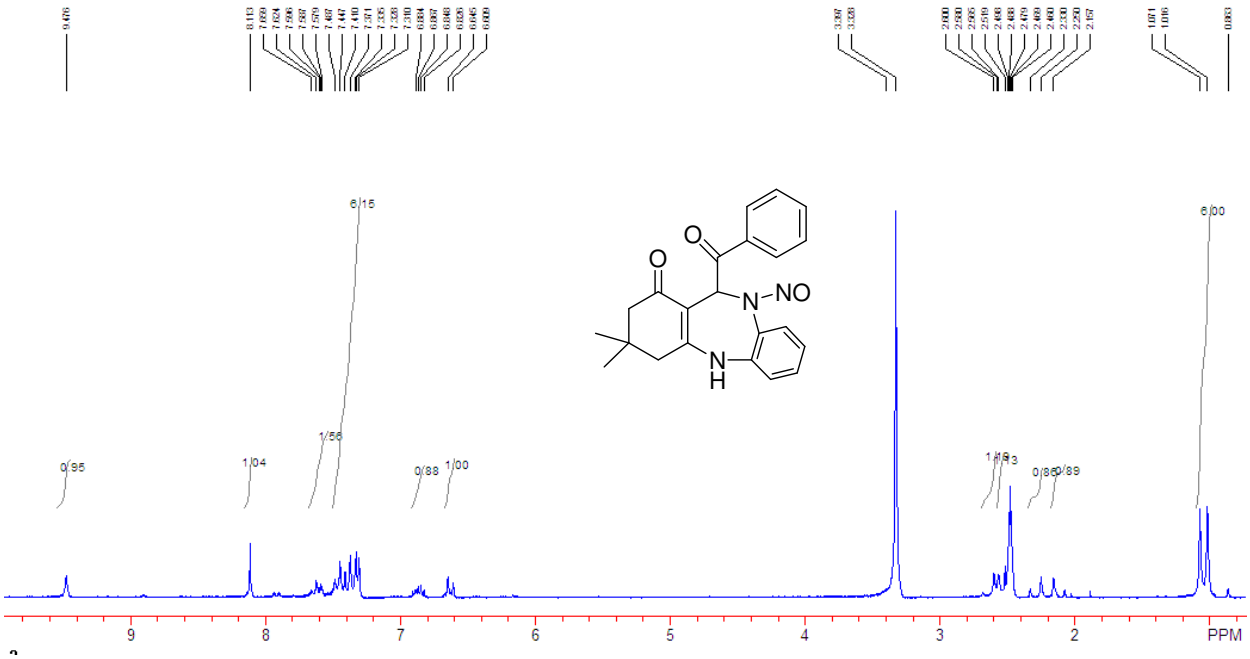
Compound **5g**



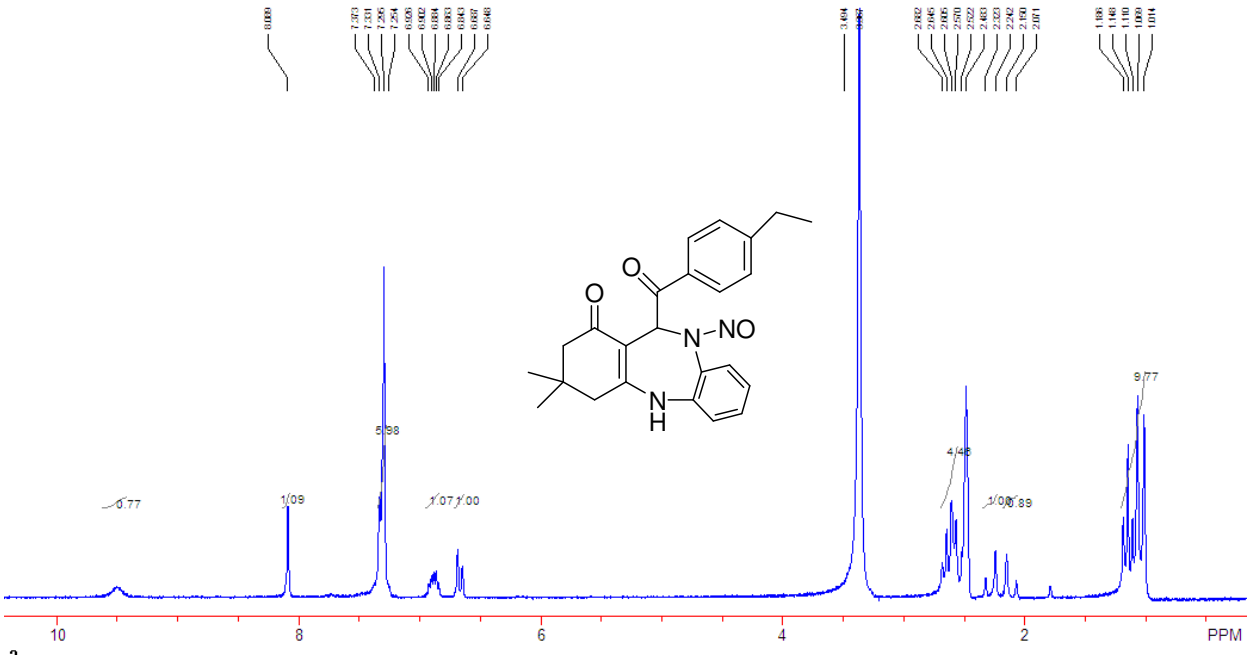
Compound **7a**



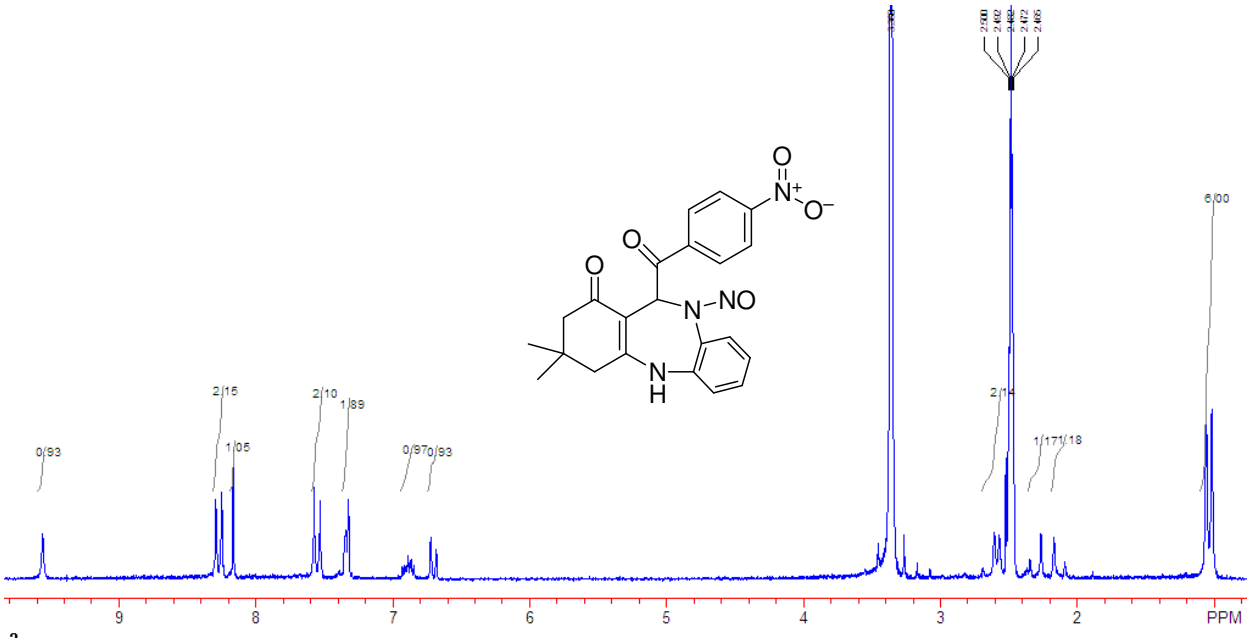
Compound **7b**



Compound **8a**



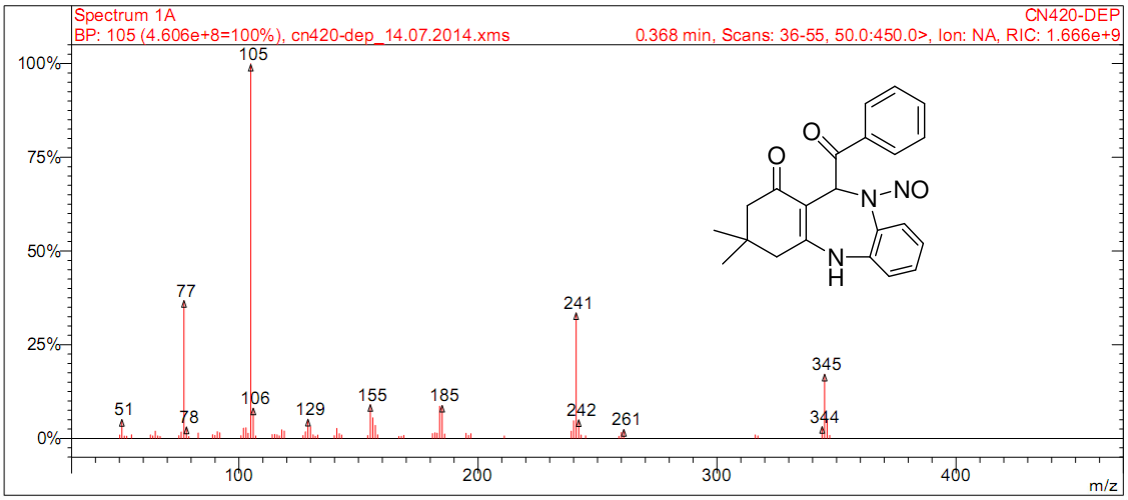
Compound **8b**



Compound **8d**

Print Date: 14 Jul 2014 19:56:23

Scan 45 from ...ata\otherfiles\univer\kolos\2014\cn420-dep_14.07.2014.xms



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Scan No: 45, Time: 0.368 minutes
20 points averaged. Not background corrected.
Name: CN420-DEP
Comment: Varian 1200L; EI; 70 eV
Pair Count: 77 MW: 0 Formula: None
CAS No: None Acquired Range: 50 - 450 m/z

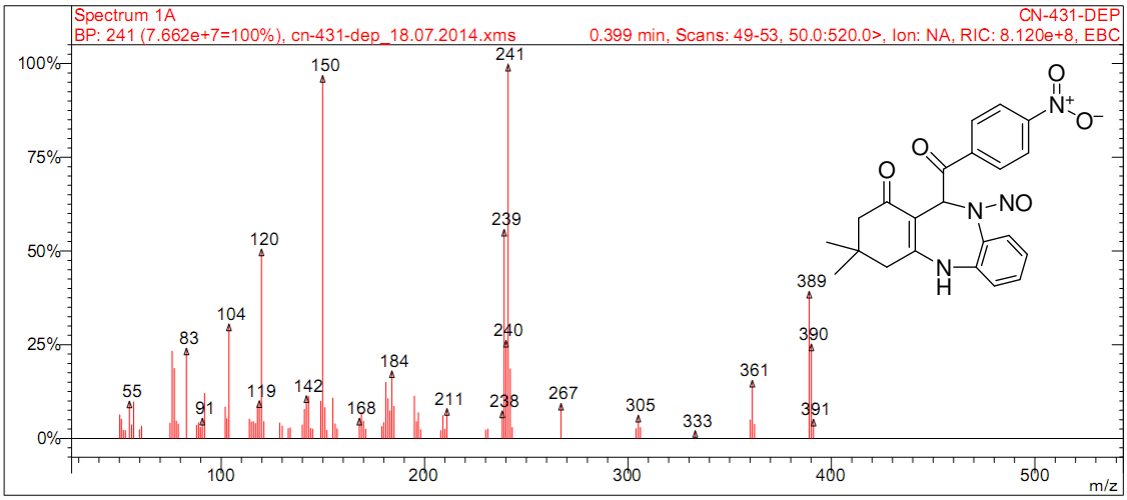
Method Description: EI
Scan 1 Channel Description: 50.0:450.0> EI;Det 1300;WI Q1 Cal;ST 0.010
Scan Information: cp = 7.4 mTorr
Precursor Mass Range: 50 - 450 m/z

Ion	Int	Norm	Ion	Int	Norm	Ion	Int	Norm
50	4.375e+6	9	107	3.174e+6	7	181	6.177e+6	13
51	2.350e+7	51	114	4.954e+6	11	182	7.043e+6	15
52	3.024e+6	7	115	5.070e+6	11	183	6.668e+6	14
53	2.966e+6	6	116	4.606e+6	10	184	3.965e+7	86
55	4.576e+6	10	117	3.216e+6	7	185	4.062e+7	88
63	4.467e+6	10	118	1.080e+7	23	186	5.446e+6	12
64	3.226e+6	7	119	9.235e+6	20	195	6.477e+6	14
65	9.032e+6	20	127	3.680e+6	8	196	3.843e+6	8
66	3.286e+6	7	128	8.319e+6	18	197	6.033e+6	13
67	2.664e+6	6	129	2.369e+7	51	211	3.140e+6	7
75	3.574e+6	8	130	1.455e+7	32	239	9.006e+6	20
76	8.007e+6	17	131	4.619e+6	10	240	2.189e+7	47
77	1.694e+8	367	132	2.783e+6	6	241	1.544e+8	335
78	1.420e+7	31	133	4.379e+6	9	242	2.300e+7	50
79	2.511e+6	5	140	3.587e+6	8	243	4.295e+6	9
83	6.701e+6	15	141	1.253e+7	27	245	3.362e+6	7
89	4.729e+6	10	142	5.974e+6	13	259	2.757e+6	6
90	3.917e+6	8	143	4.383e+6	10	260	7.498e+6	16
91	8.450e+6	18	154	3.775e+6	8	261	1.115e+7	24
92	7.044e+6	15	155	4.158e+7	90	316	4.418e+6	10
101	3.474e+6	8	156	2.554e+7	55	317	3.333e+6	7
102	1.275e+7	28	157	1.618e+7	35	344	1.472e+7	32
103	1.320e+7	29	158	4.527e+6	10	345	7.898e+7	171
104	6.430e+6	14	167	2.633e+6	6	346	2.308e+7	50
105	4.606e+8	999	168	2.860e+6	6	347	3.834e+6	8
106	3.724e+7	81	169	3.878e+6	8			

Compound **8a**

Print Date: 18 Jul 2014 17:51:24

Scan 51 from ...ta\otherfiles\univer\kolos\2014\cn-431-dep_18.07.2014.xms



Spectrum from ...les\univer\kolos\2014\cn-431-dep_18.07.2014.xms
Scan No: 51, Time: 0.399 minutes
5 points averaged. Background corrected (E).
Name: CN-431-DEP
Comment: Varian 1200 L; EI; 70 eV
Pair Count: 86 MW: 0 Formula: None
CAS No: None Acquired Range: 50 - 520 m/z

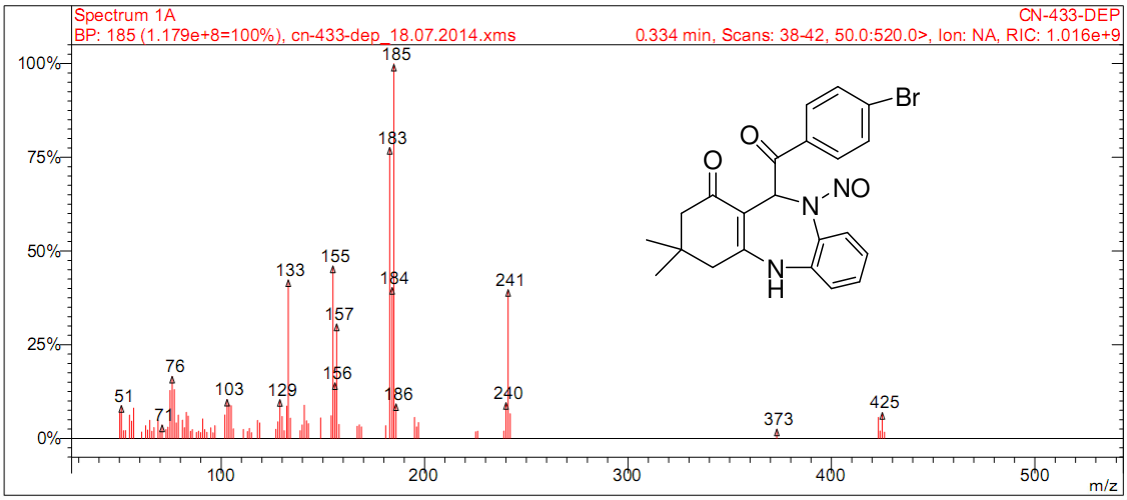
Method Description: EI
Scan 1 Channel Description: 50.0:520.0> EI;Det 1400;WI Q1 Cal;ST 0.010
Scan Information: cp = 7.4 mTorr
Precursor Mass Range: 50 - 520 m/z

Ion	Int	Norm	Ion	Int	Norm	Ion	Int	Norm
50	4.834e+6	63	120	3.873e+7	505	185	6.601e+6	86
51	3.979e+6	52	121	3.490e+6	46	195	8.689e+6	113
52	1.697e+6	22	129	3.181e+6	41	196	3.460e+6	45
53	1.597e+6	21	130	2.569e+6	34	197	5.274e+6	69
55	7.648e+6	100	133	2.038e+6	27	198	1.809e+6	24
56	2.807e+6	37	134	2.171e+6	28	208	1.626e+6	21
57	7.485e+6	98	140	2.781e+6	36	209	4.703e+6	61
60	1.818e+6	24	141	5.968e+6	78	210	1.931e+6	25
61	2.524e+6	33	142	8.723e+6	114	211	6.103e+6	80
75	3.147e+6	41	143	8.614e+6	112	230	1.722e+6	22
76	1.784e+7	233	144	2.057e+6	27	231	1.953e+6	25
77	1.433e+7	187	145	1.951e+6	25	238	5.637e+6	73
78	3.580e+6	47	149	7.612e+6	99	239	4.273e+7	557
79	2.972e+6	39	150	7.420e+7	967	240	2.006e+7	261
83	1.846e+7	241	151	6.311e+6	82	241	7.662e+7	999
88	2.705e+6	35	152	1.670e+6	22	242	1.424e+7	186
89	3.232e+6	42	155	8.259e+6	108	243	2.295e+6	30
90	2.279e+6	30	156	2.999e+6	39	267	7.176e+6	94
91	4.152e+6	54	157	2.006e+6	26	304	1.983e+6	26
92	9.233e+6	120	168	4.142e+6	54	305	4.773e+6	62
102	6.416e+6	84	169	5.379e+6	70	306	2.271e+6	30
103	4.031e+6	53	170	3.568e+6	47	333	1.599e+6	21
104	2.340e+7	305	171	1.936e+6	25	360	3.805e+6	50
114	4.002e+6	52	179	2.455e+6	32	361	1.187e+7	155
115	3.438e+6	45	180	3.280e+6	43	362	2.926e+6	38
116	3.470e+6	45	181	1.150e+7	150	389	3.007e+7	392
117	3.085e+6	40	182	8.159e+6	106	390	1.930e+7	252
118	6.781e+6	88	183	5.660e+6	74	391	3.949e+6	51
119	7.700e+6	100	184	1.382e+7	180			

Compound **8d**

Print Date: 18 Jul 2014 17:41:43

Scan 40 from ...ta\otherfiles\univer\kolos\2014\cn-433-dep_18.07.2014.xms



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Scan No: 40, Time: 0.334 minutes
5 points averaged. Not background corrected.
Name: CN-433-DEP
Comment: Varian 1200 L; EI; 70 eV
Pair Count: 90 MW: 0 Formula: None
CAS No: None Acquired Range: 50 - 520 m/z

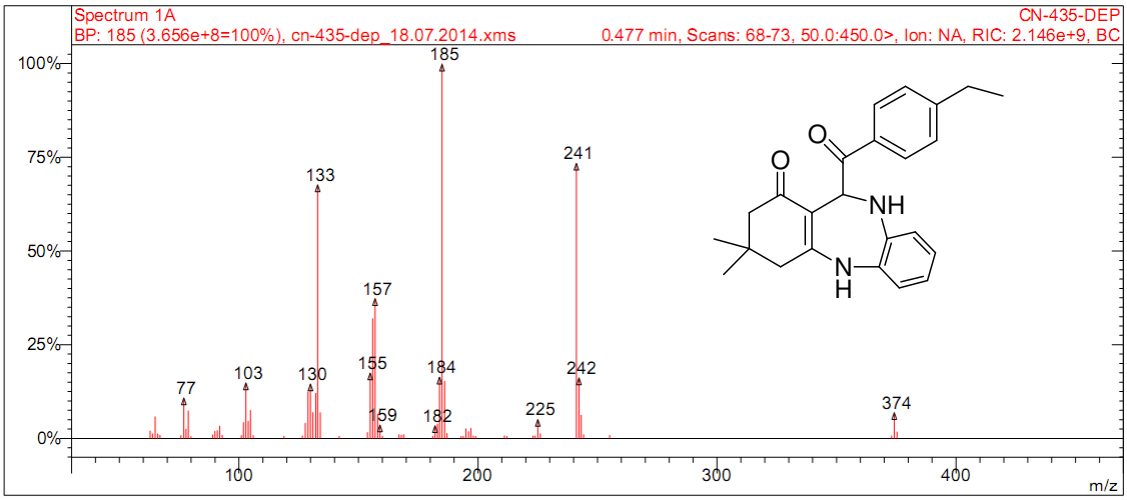
Method Description: EI
Scan 1 Channel Description: 50.0:520.0> EI;Det 0;WI Q1 Cal;ST 0.010
Scan Information: cp = 7.4 mTorr
Precursor Mass Range: 50 - 520 m/z

Ion	Int	Norm	Ion	Int	Norm	Ion	Int	Norm
50	8.265e+6	70	89	2.324e+6	20	142	5.583e+6	47
51	1.036e+7	88	90	1.875e+6	16	143	4.686e+6	40
52	2.476e+6	21	91	6.185e+6	52	149	6.512e+6	55
53	2.520e+6	21	92	2.860e+6	24	154	7.148e+6	61
55	7.379e+6	63	93	1.952e+6	17	155	5.425e+7	460
56	5.469e+6	46	95	3.416e+6	29	156	1.752e+7	148
57	9.568e+6	81	96	1.814e+6	15	157	3.602e+7	305
61	2.049e+6	17	97	4.055e+6	34	158	4.481e+6	38
63	4.060e+6	34	102	7.417e+6	63	167	3.868e+6	33
64	2.660e+6	23	103	1.230e+7	104	168	4.331e+6	37
65	5.778e+6	49	104	1.067e+7	90	169	3.667e+6	31
66	2.301e+6	19	105	1.034e+7	88	181	4.072e+6	34
67	3.482e+6	30	106	3.087e+6	26	183	9.151e+7	775
69	5.901e+6	50	111	2.893e+6	25	184	4.746e+7	402
70	2.344e+6	20	113	2.201e+6	19	185	1.179e+8	999
71	4.249e+6	36	114	3.168e+6	27	186	1.086e+7	92
73	2.837e+6	24	115	1.839e+6	16	195	6.669e+6	57
74	3.583e+6	30	118	5.711e+6	48	196	3.673e+6	31
75	1.514e+7	128	119	4.950e+6	42	197	5.053e+6	43
76	1.956e+7	166	127	2.907e+6	25	225	2.115e+6	18
77	1.539e+7	130	128	5.281e+6	45	226	2.327e+6	20
78	4.949e+6	42	129	1.220e+7	103	239	2.370e+6	20
79	7.352e+6	62	130	6.926e+6	59	240	1.125e+7	95
81	5.796e+6	49	131	2.478e+6	21	241	4.681e+7	397
82	3.447e+6	29	132	1.020e+7	86	242	7.805e+6	66
83	8.214e+6	70	133	4.990e+7	423	373	2.965e+6	25
84	7.065e+6	60	134	6.435e+6	55	423	6.672e+6	57
85	2.299e+6	19	139	2.496e+6	21	424	2.358e+6	20
86	2.830e+6	24	140	4.279e+6	36	425	8.175e+6	69
88	1.943e+6	16	141	1.050e+7	89	426	2.025e+6	17

Compound **8c**

Print Date: 18 Jul 2014 17:34:12

Scan 70 from ...ta\otherfiles\univer\kolos\2014\cn-435-dep_18.07.2014.xms



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Scan No: 70, Time: 0.477 minutes
6 points averaged. Background corrected.
Name: CN-435-DEP
Comment: Varian 1200 L; EI; 70 eV
Pair Count: 69 MW: 0 Formula: None
CAS No: None Acquired Range: 50 - 450 m/z

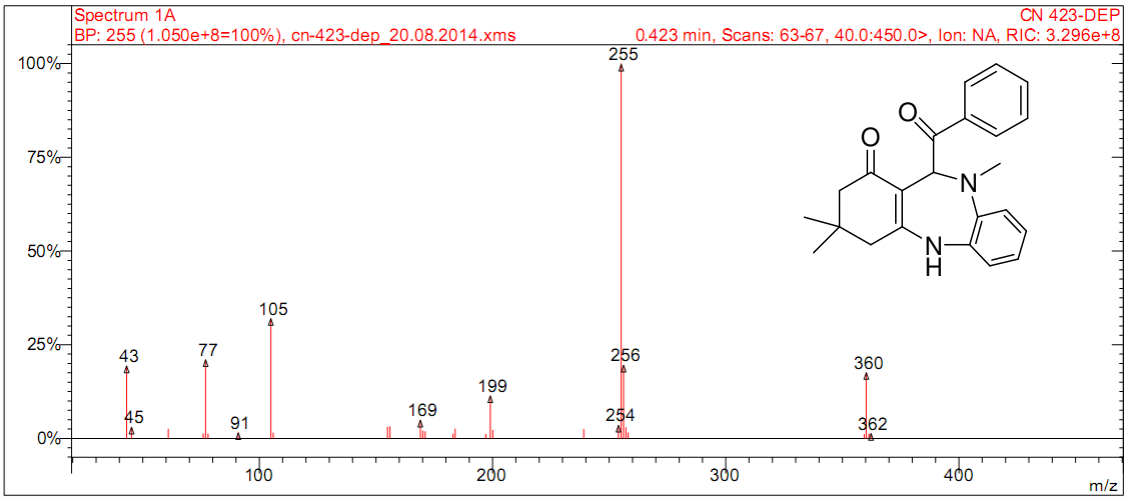
Method Description: EI
Scan 1 Channel Description: 50.0:450.0> EI;Det 1400;WI Q1 Cal;ST 0.010
Scan Information: cp = 7.4 mTorr
Precursor Mass Range: 50 - 450 m/z

Ion	Int	Norm	Ion	Int	Norm	Ion	Int	Norm
63	7.386e+6	20	128	1.497e+7	41	186	5.566e+7	152
64	4.545e+6	12	129	4.549e+7	124	187	4.940e+6	13
65	2.110e+7	58	130	5.306e+7	145	193	2.131e+6	6
66	4.501e+6	12	131	2.533e+7	69	194	2.097e+6	6
67	3.078e+6	8	132	4.417e+7	121	195	9.489e+6	26
76	2.853e+6	8	133	2.473e+8	676	196	6.764e+6	18
77	3.947e+7	108	134	2.515e+7	69	197	9.919e+6	27
78	9.017e+6	25	142	2.247e+6	6	198	2.456e+6	7
79	2.687e+7	73	154	5.880e+6	16	199	2.219e+6	6
80	1.829e+6	5	155	6.379e+7	174	211	2.685e+6	7
89	3.513e+6	10	156	1.170e+8	320	212	1.979e+6	5
90	6.990e+6	19	157	1.363e+8	373	223	2.645e+6	7
91	7.768e+6	21	158	2.381e+7	65	224	2.315e+6	6
92	1.210e+7	33	159	1.315e+7	36	225	1.847e+7	50
93	3.338e+6	9	160	2.206e+6	6	226	4.614e+6	13
101	2.952e+6	8	167	3.768e+6	10	241	2.683e+8	733
102	1.559e+7	43	168	3.328e+6	9	242	5.903e+7	161
103	5.414e+7	148	169	3.759e+6	10	243	2.275e+7	62
104	1.685e+7	46	181	2.336e+6	6	244	3.726e+6	10
105	2.749e+7	75	182	1.239e+7	34	255	3.115e+6	9
106	2.937e+6	8	183	1.420e+7	39	373	2.546e+6	7
119	2.129e+6	6	184	5.976e+7	163	374	2.509e+7	69
127	2.495e+6	7	185	3.656e+8	999	375	6.479e+6	18

Compound **5g**

Print Date: 20 Aug 2014 19:19:46

Scan 65 from ...ta\otherfiles\univer\kolos\2014\cn-423-dep_20.08.2014.xms

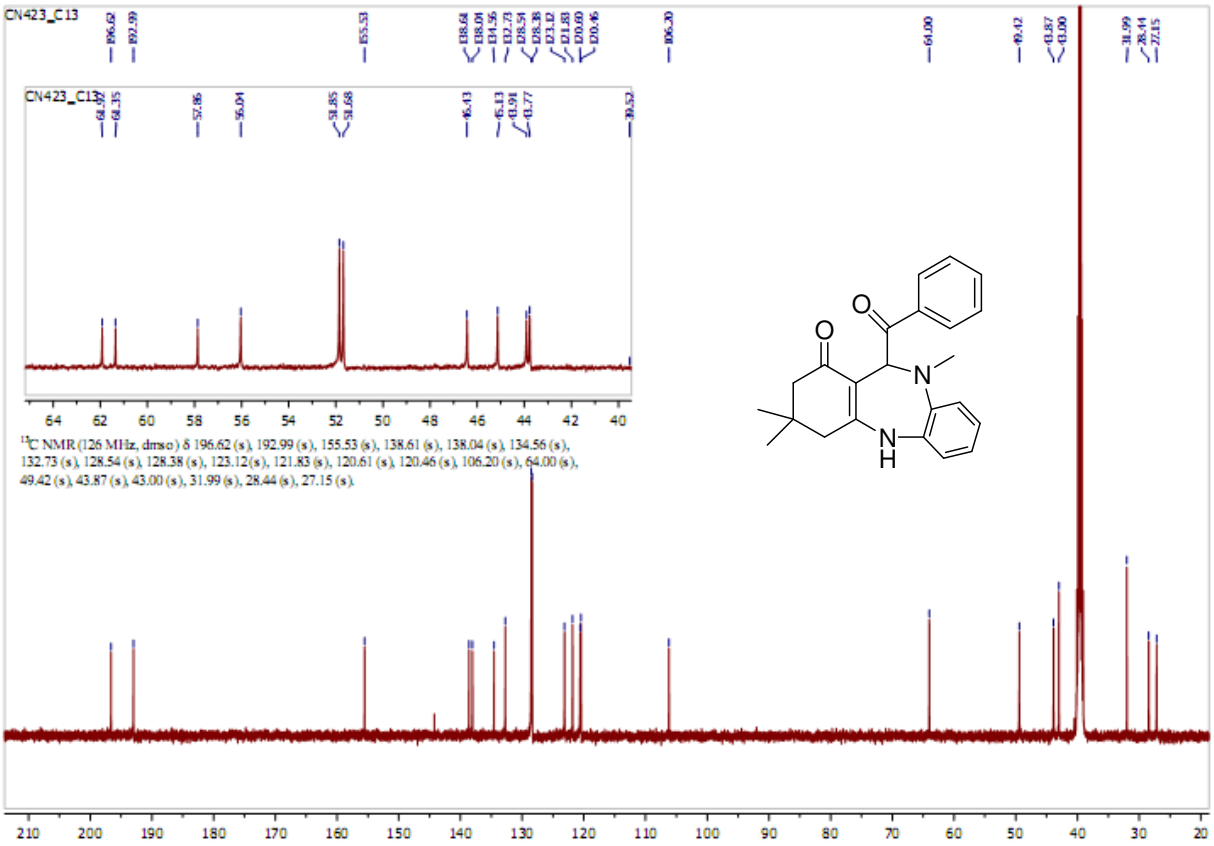


Spectrum from ...les\univer\kolos\2014\cn-423-dep_20.08.2014.xms
Scan No: 65, Time: 0.423 minutes
5 points averaged. Not background corrected.
Name: CN 423-DEP
Comment: Varian 1200L; EI; 70 eV
Pair Count: 29 MW: 0 Formula: None
CAS No: None Acquired Range: 40 - 450 m/z

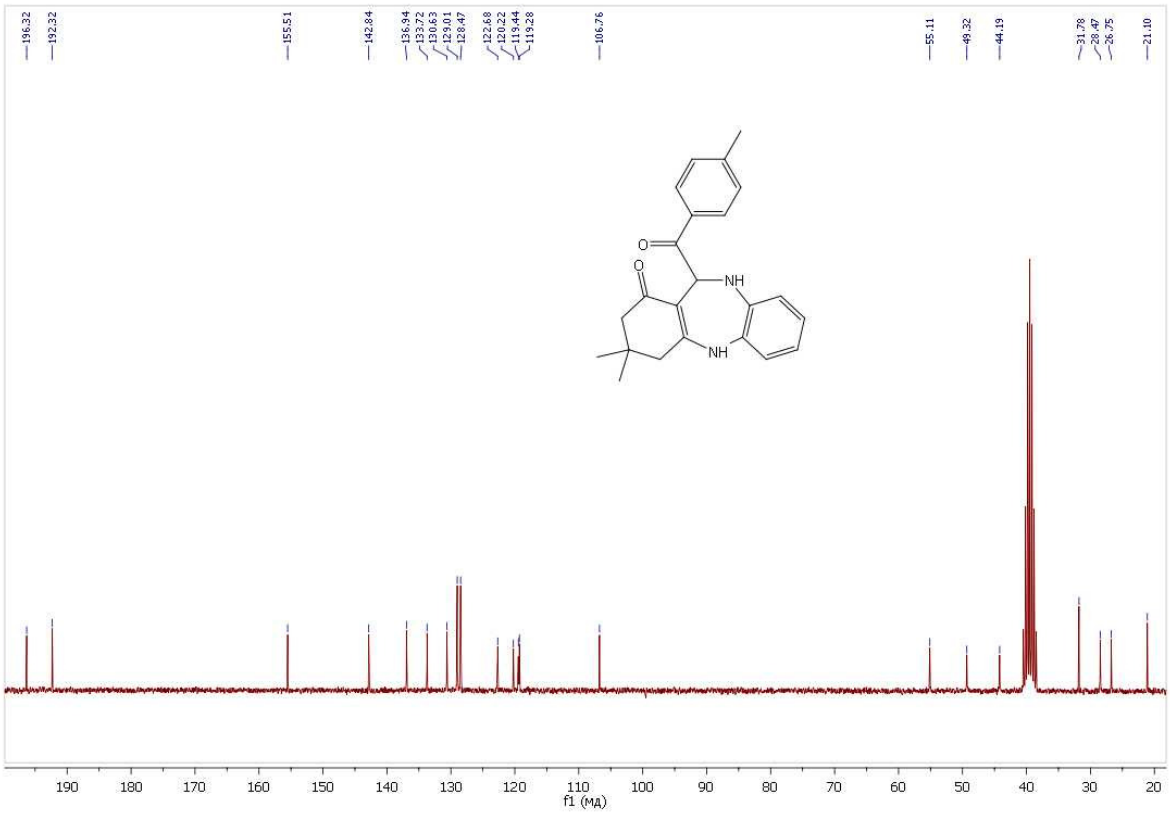
Method Description: EI
Scan 1 Channel Description: 40.0:450.0> EI;Det 1400;WI Q1 Cal;ST 0.010
Scan Information: cp = 7.4 mTorr
Precursor Mass Range: 40 - 450 m/z

Ion	Int	Norm	Ion	Int	Norm	Ion	Int	Norm
43	2.031e+7	193	156	3.341e+6	32	254	3.694e+6	35
45	3.160e+6	30	169	5.126e+6	49	255	1.050e+8	999
61	2.643e+6	25	170	2.088e+6	20	256	2.051e+7	195
76	1.355e+6	13	171	1.932e+6	18	257	3.055e+6	29
77	2.202e+7	210	183	1.276e+6	12	258	1.614e+6	15
78	1.306e+6	12	184	2.712e+6	26	359	1.142e+6	11
91	1.599e+6	15	197	1.181e+6	11	360	1.844e+7	176
105	3.356e+7	319	199	1.193e+7	114	361	1.286e+6	12
106	1.566e+6	15	200	2.294e+6	22	362	1.348e+6	13
155	3.185e+6	30	239	2.606e+6	25			

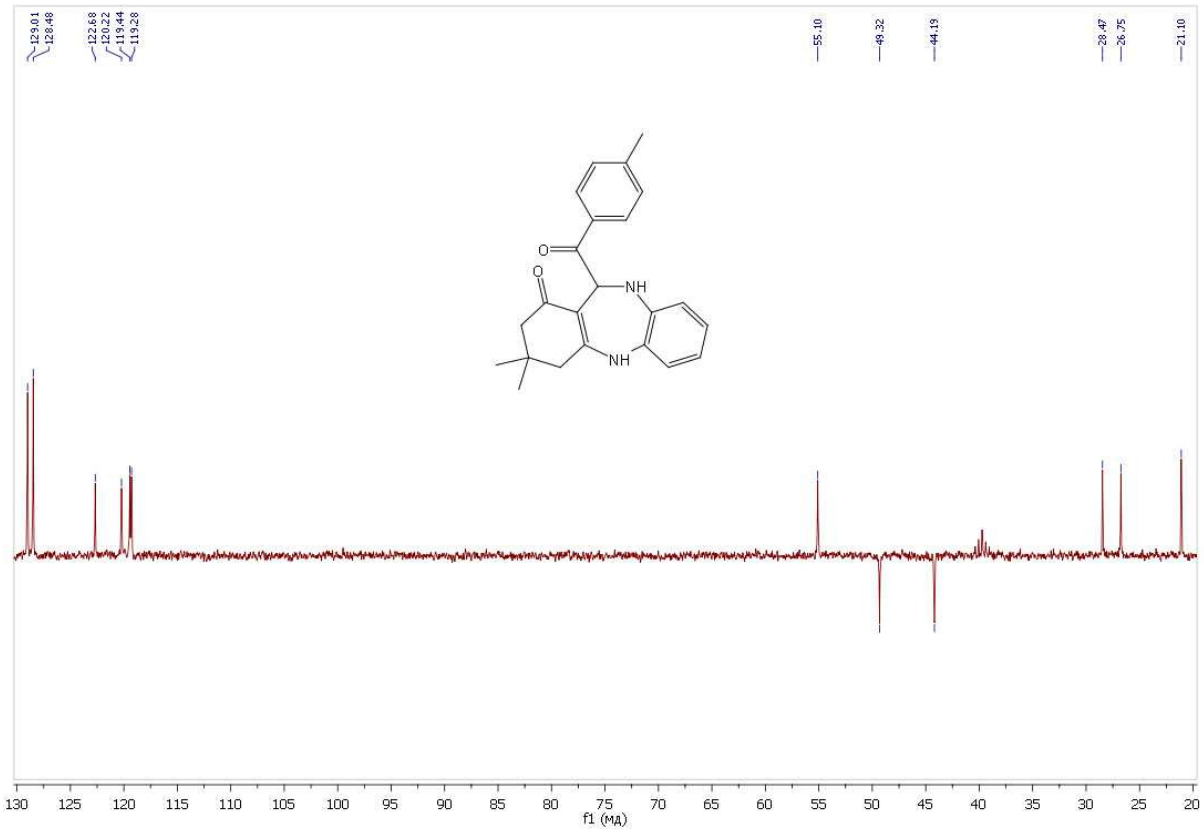
Compound **7a**



Compound **7a**



Compound **5f**



Compound **5f** (DEPT-135)

EuroEA Elemental Analyser

AutoRun name : Synth. Mix.-Chebanov-04.02.14-10.34
Date of print : 04-02-14
Time of print : 16:03

Sample source : kolos
Operator : fedoroff
Configuration : CHNS

Calibration Type : **K-Factor**

Results Summary for Element %

#	Type	Name	N %	C %	H %	S %	O %	Weight (mg)
1	sample	CN-436	6.703	70.952	5.553			1.048
2	sample	CN-438	7.401	76.353	6.692			0.933
3	sample	CN-440	7.242	77.312	7.233			1.055
4	sample	CN-443	7.403	76.430	5.791			0.812
5	sample	CN-444	7.451	69.311	5.750			1.383

EuroEA Elemental Analyser

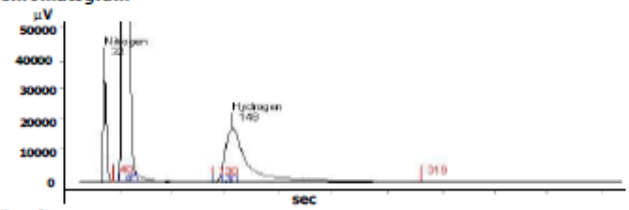
AutoRun name : Synth. Mix.-Chebanov-04.02.14-10.34
Date of print : 04-02-2014
Time of print : 16:07

Operator : fedoroff
Configuration : CHNS

Sample name : CN-443
Sample position # : 4
Type : sample
Sample weight : 0.812

Calibration : **k - factor**

Single Sample from AutoRun
Chromatogram



Results

Element	RT (s)	Start (s)	End (s)	Area (µV.s)	Area %
Nitrogen	32	28	40	108044	5.231
Carbon	49	45	130	1578905	76.448
Hydrogen	148	130	319	378271	18.315
Sulphur					
Oxygen					

Element	Element %	Intercep	Slope	Correlation	K-Factor
Nitrogen	7.403				7.657E-7
Carbon	76.430				2.908E-7
Hydrogen	5.791				1.133E-7
Sulphur					
Oxygen					

Compound **6f**

EuroEA Elemental Analyser

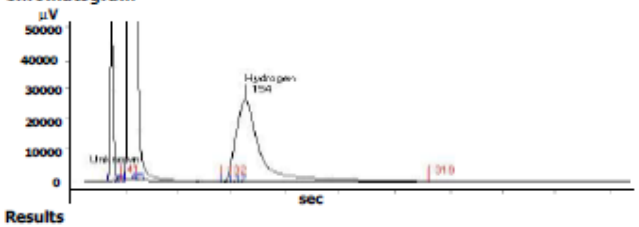
AutoRun name : Synth. Mix.-Chebanov-04.02.14-10.34
Date of print : 04-02-2014
Time of print : 16:05

Operator : fedoroff
Configuration : CHNS

Sample name : CN-438
Sample position # : 2
Type : sample
Sample weight : 0.933

Calibration : **k - factor**

Single Sample from AutoRun
Chromatogram



Results

Element	RT (s)	Start (s)	End (s)	Area (µV.s)	Area %
Nitrogen	33	29	41	136667	3.998
Carbon	49	45	132	2665249	77.958
Hydrogen	154	132	319	616889	18.044
Sulphur					
Oxygen					

Element	Element %	Intercep	Slope	Correlation	K-Factor
Nitrogen	7.401				7.657E-7
Carbon	76.353				2.908E-7
Hydrogen	6.692				1.133E-7
Sulphur					
Oxygen					

Compound **5f**

EuroEA Elemental Analyser

AutoRun name : Synth. Mix.-Chebanov-04.02.14-10.34
Date of print : 04-02-2014
Time of print : 16:08

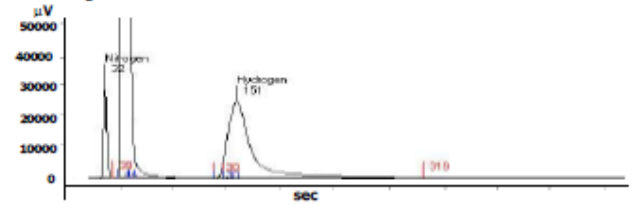
Operator : fedoroff
Configuration : CHNS

Sample name : CN-444
Sample position # : 5
Type : sample
Sample weight : 1.383

Calibration : **k - factor**

Single Sample from AutoRun

Chromatogram



Results

Element	RT (s)	Start (s)	End (s)	Area (µV.s)	Area %
Nitrogen	32	28	39	92781	3.235
Carbon	48	44	130	2209121	77.016
Hydrogen	151	130	319	566504	19.750
Sulphur					
Oxygen					

Element	Element %	Intercep	Slope	Correlation	K-Factor
Nitrogen	7.451				7.657E-7
Carbon	69.311				2.908E-7
Hydrogen	5.750				1.133E-7
Sulphur					
Oxygen					

Compound **5i**

EuroEA Elemental Analyser

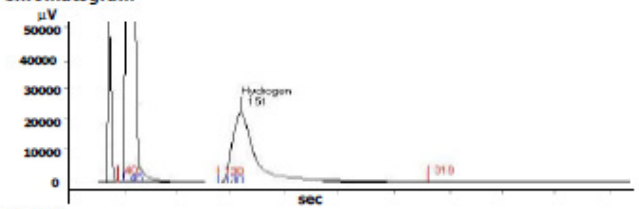
AutoRun name : Synth. Mix.-Chebanov-04.02.14-10.34
Date of print : 04-02-2014
Time of print : 16:06

Operator : fedoroff
Configuration : CHNS

Sample name : CN-440
Sample position # : 3
Type : sample
Sample weight : 1.055

Calibration : **k - factor**

Single Sample from AutoRun
Chromatogram



Results

Element	RT (s)	Start (s)	End (s)	Area (µV.s)	Area %
Nitrogen	32	16	40	153884	5.335
Carbon	49	45	130	2219693	76.955
Hydrogen	151	130	319	510828	17.710
Sulphur					
Oxygen					

Element	Element %	Intercep	Slope	Correlation	K-Factor
Nitrogen	7.242				7.657E-7
Carbon	77.312				2.908E-7
Hydrogen	7.233				1.133E-7
Sulphur					
Oxygen					

Compound **7b**

EuroEA Elemental Analyser

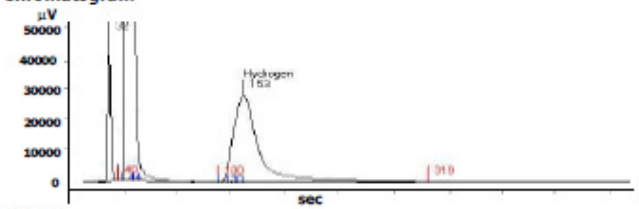
AutoRun name : Synth. Mix.-Chebanov-04.02.14-10.34
Date of print : 04-02-2014
Time of print : 16:04

Operator : fedoroff
Configuration : CHNS

Sample name : CN-436
Sample position # : 1
Type : sample
Sample weight : 1.048

Calibration : **k - factor**

Single Sample from AutoRun
Chromatogram



Results

Element	RT (s)	Start (s)	End (s)	Area (µV.s)	Area %
Nitrogen	32	16	40	131583	3.918
Carbon	48	44	130	2551064	75.967
Hydrogen	153	130	319	675492	20.115
Sulphur					
Oxygen					

Element	Element %	Intercep	Slope	Correlation	K-Factor
Nitrogen	6.703				7.657E-7
Carbon	70.952				2.908E-7
Hydrogen	5.553				1.133E-7
Sulphur					
Oxygen					

Compound **6b**