Electronic Supplementary Material (ESI) for RSC Advances.
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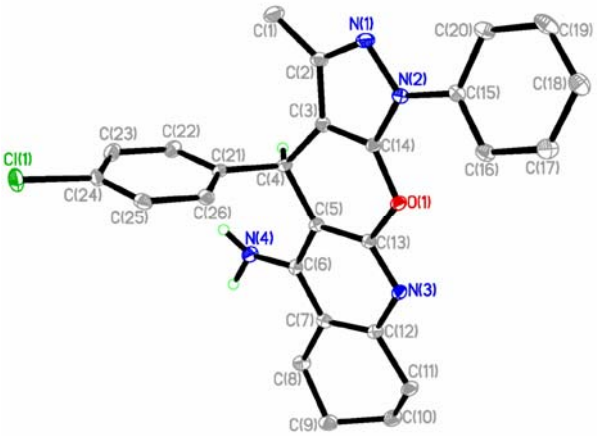
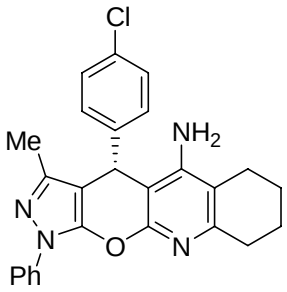
1. Crystallography data of Compound 10



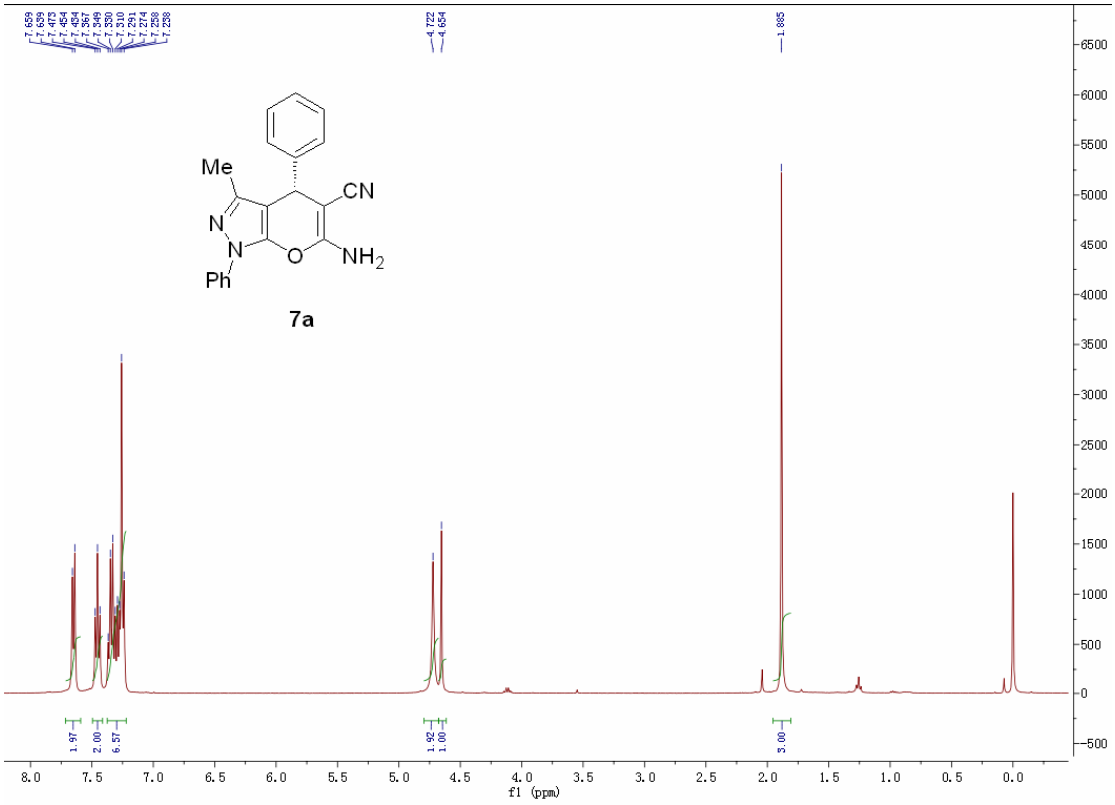


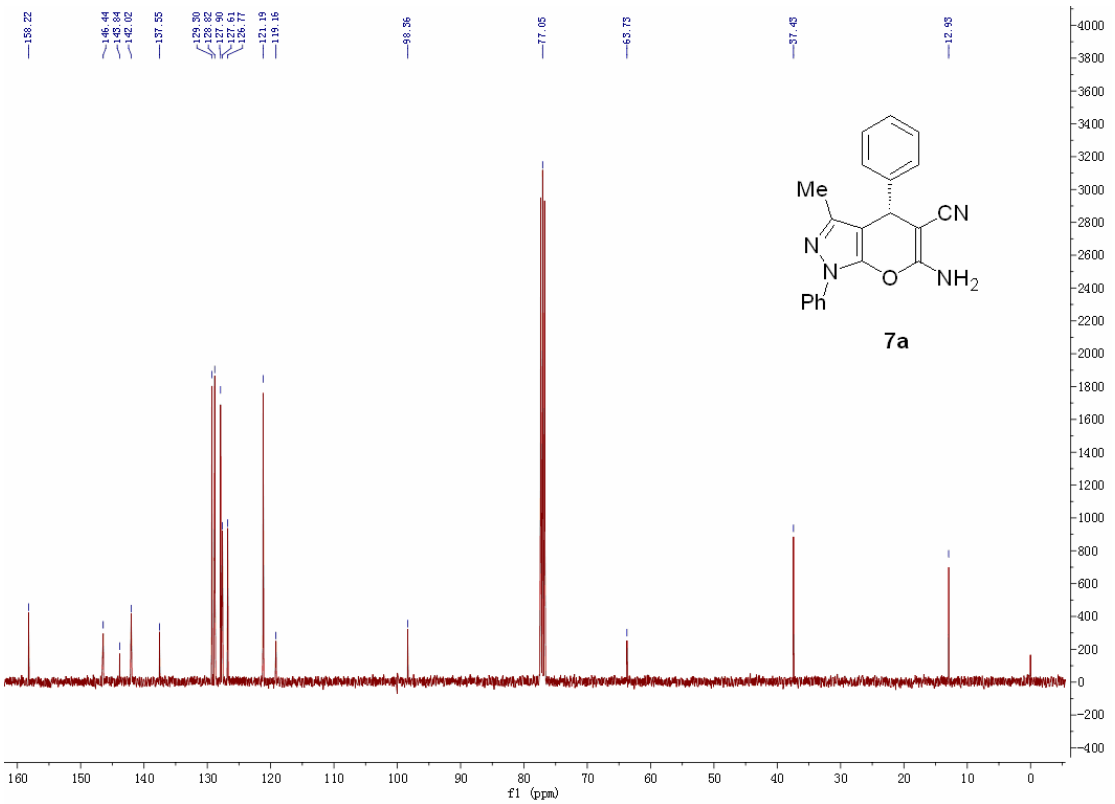
10

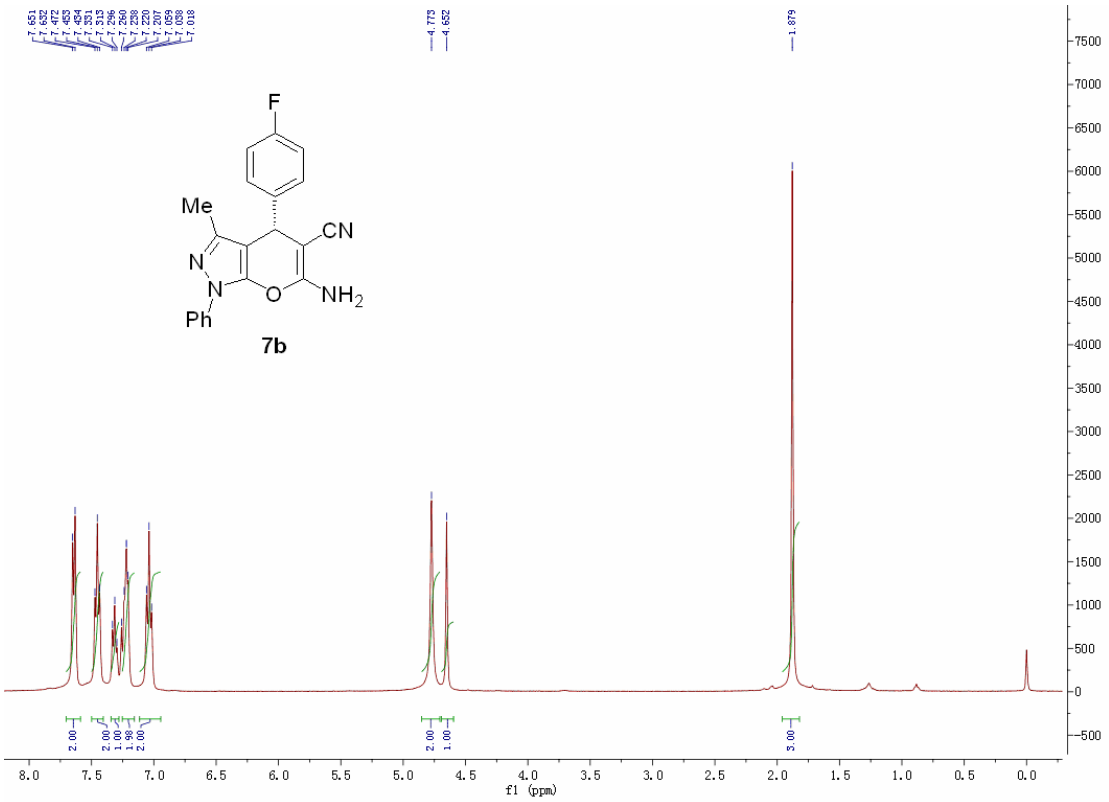
Identification code	shelxl
Empirical formula	C26 H23 Cl N4 O
Formula weight	442.93
Temperature	113(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)
Unit cell dimensions	a = 8.1418(16) A alpha = 90 deg.
	b = 12.894(3) A beta = 105.75(3) deg.
	c = 10.541(2) A gamma = 90 deg.
Volume	1065.1(4) A^3
Z, Calculated density	2, 1.381 Mg/m^3
Absorption coefficient	0.207 mm^-1
F(000)	464
Crystal size	0.20 x 0.18 x 0.12 mm
Theta range for data collection	2.01 to 28.10 deg.
Limiting indices	-9<=h<=10, -16<=k<=16, -13<=l<=13
Reflections collected / unique	10819 / 4910 [R(int) = 0.0301]
Completeness to theta = 28.10	99.1 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9756 and 0.9598
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4910 / 4 / 296
Goodness-of-fit on F^2	1.043
Final R indices [I>2sigma(I)]	R1 = 0.0312, wR2 = 0.0797

R indices (all data)	R1 = 0.0414, wR2 = 0.0828
Absolute structure parameter	-0.01(5)
Largest diff. peak and hole	0.209 and -0.296 e.A^-3

2. Copies of ^{1}H and ^{13}C NMR Spectra



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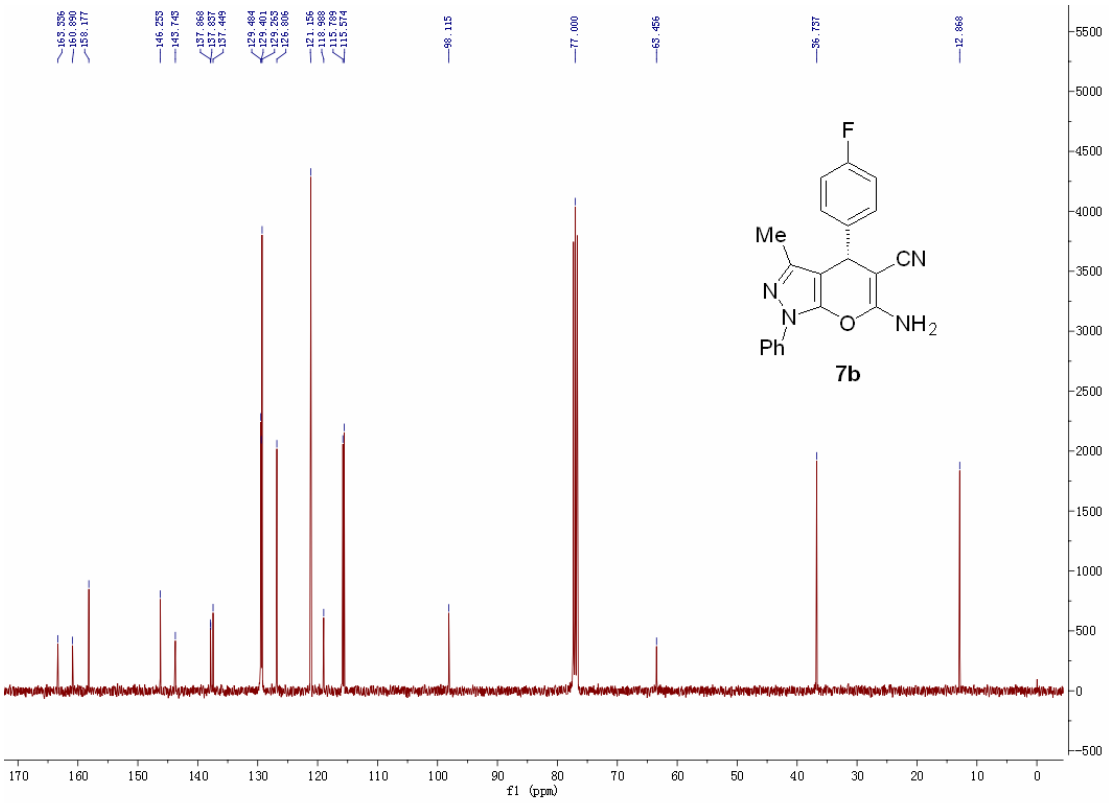
NH2
Ph
7b
f1 (ppm)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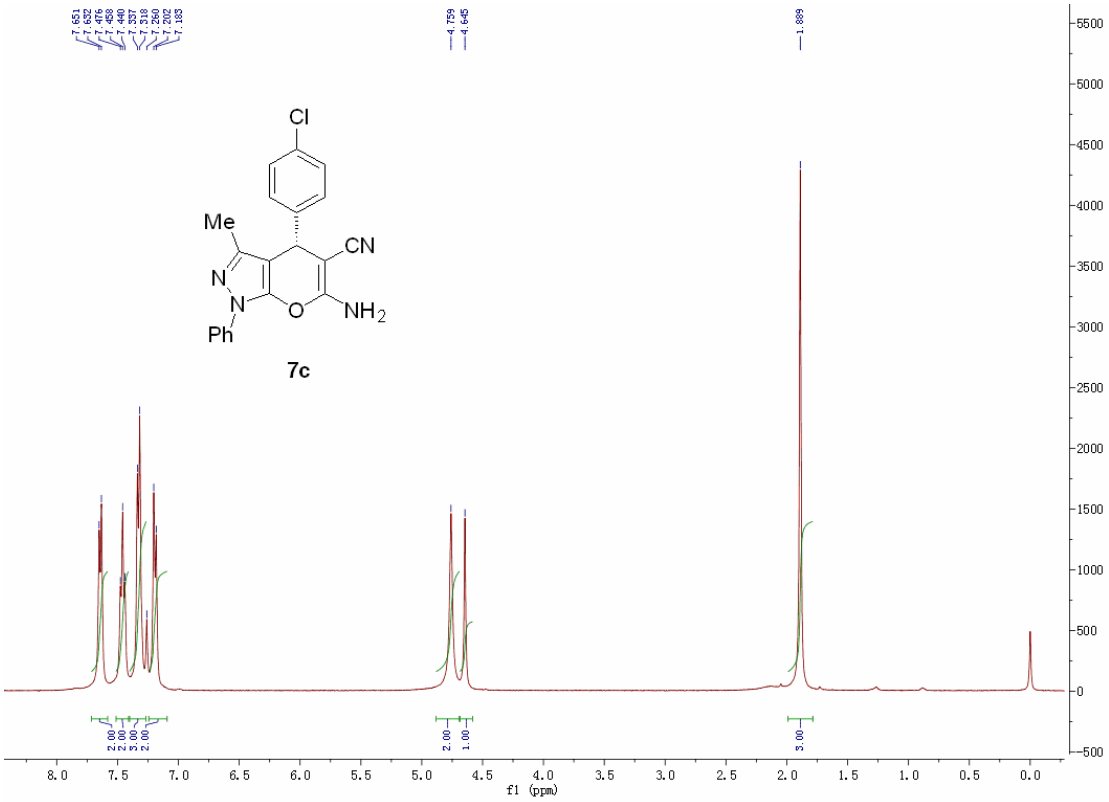
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NH2
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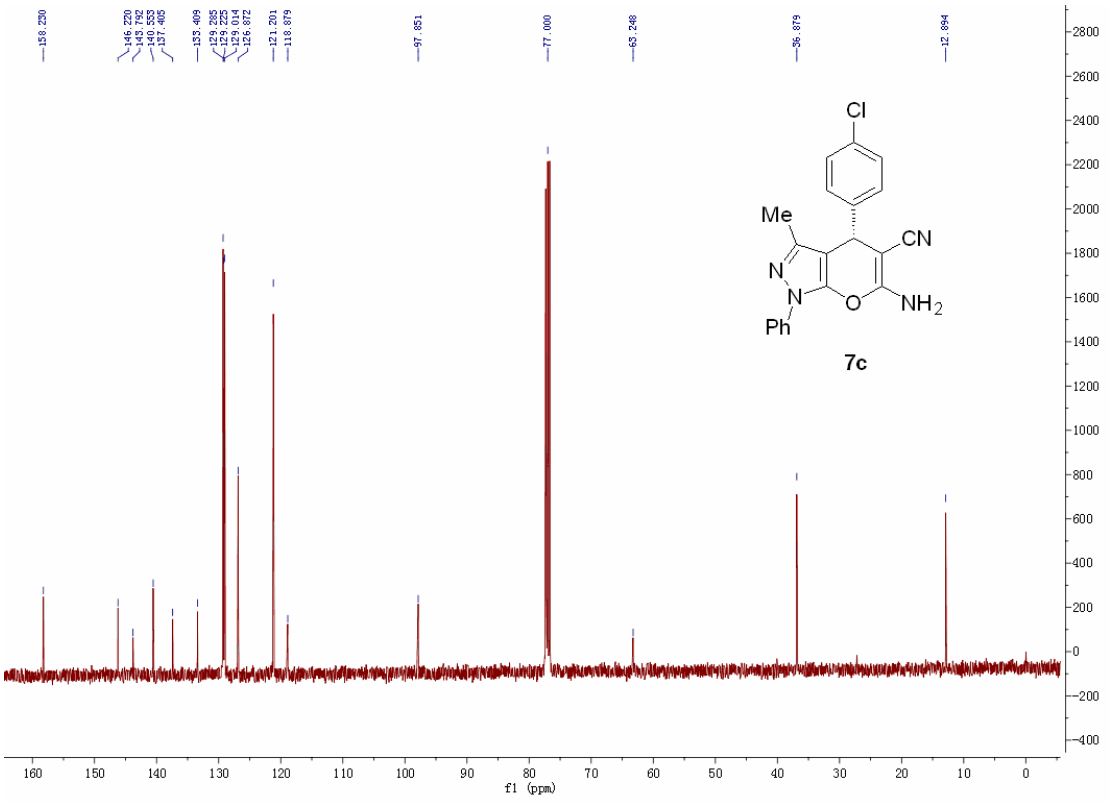
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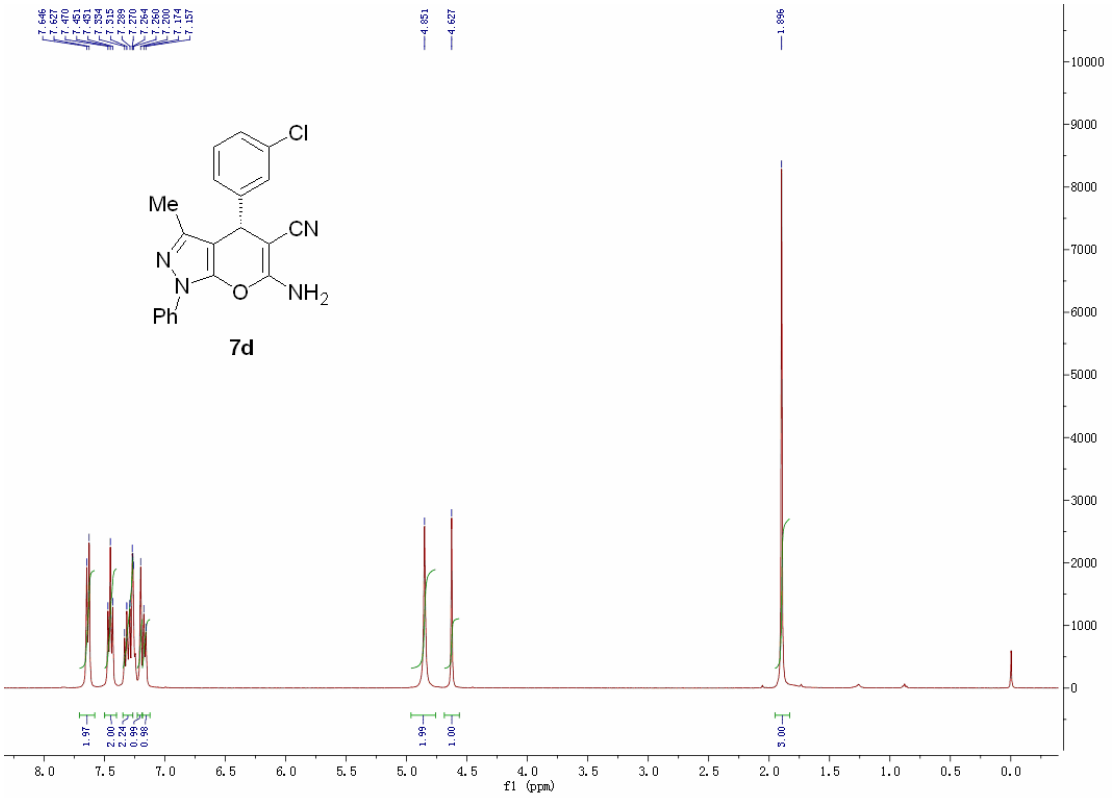
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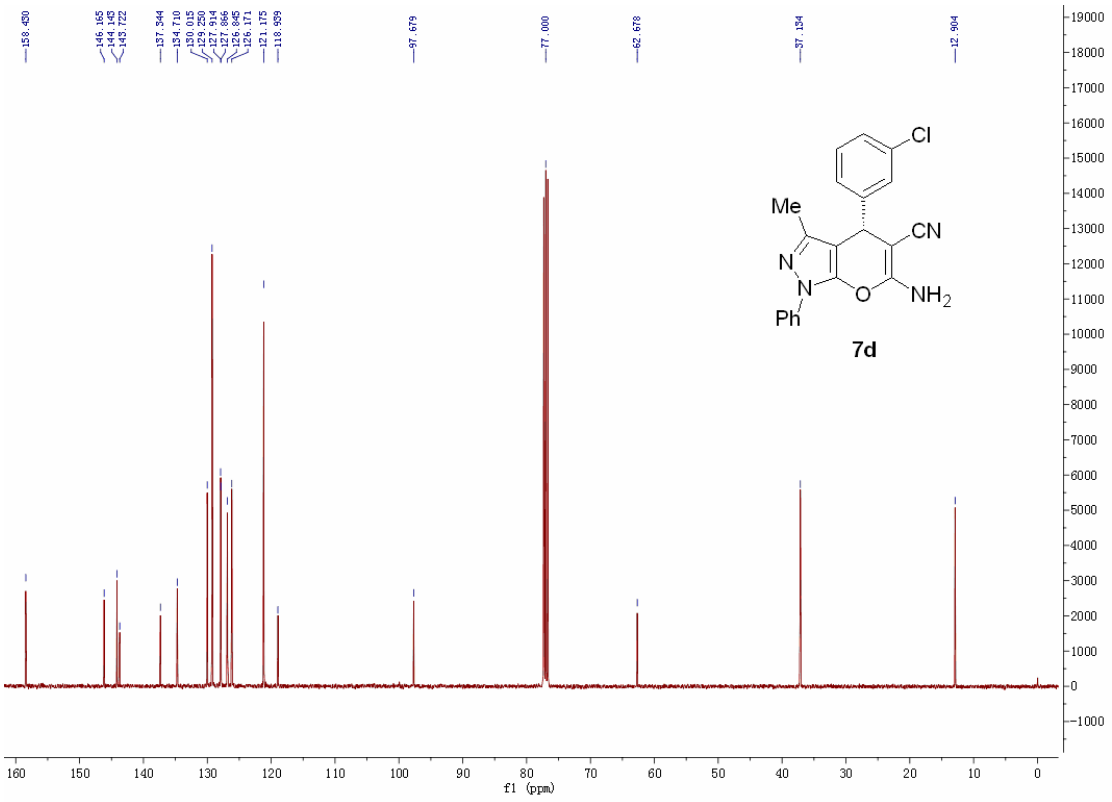
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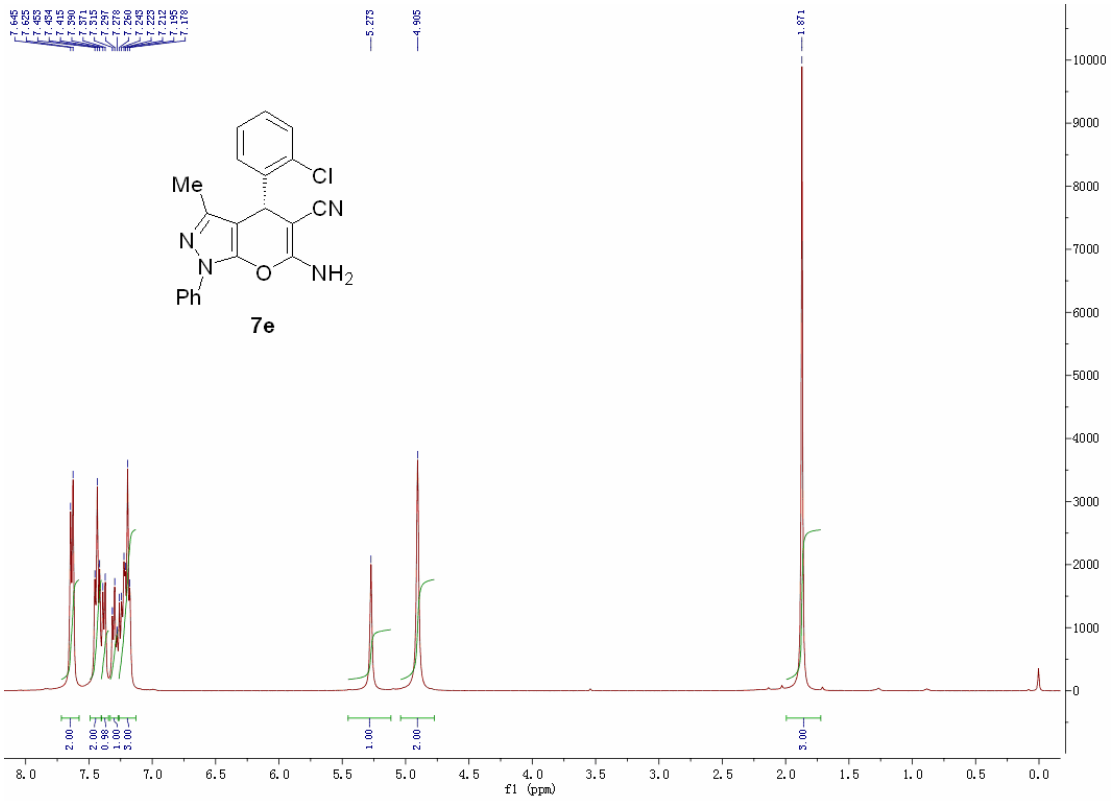
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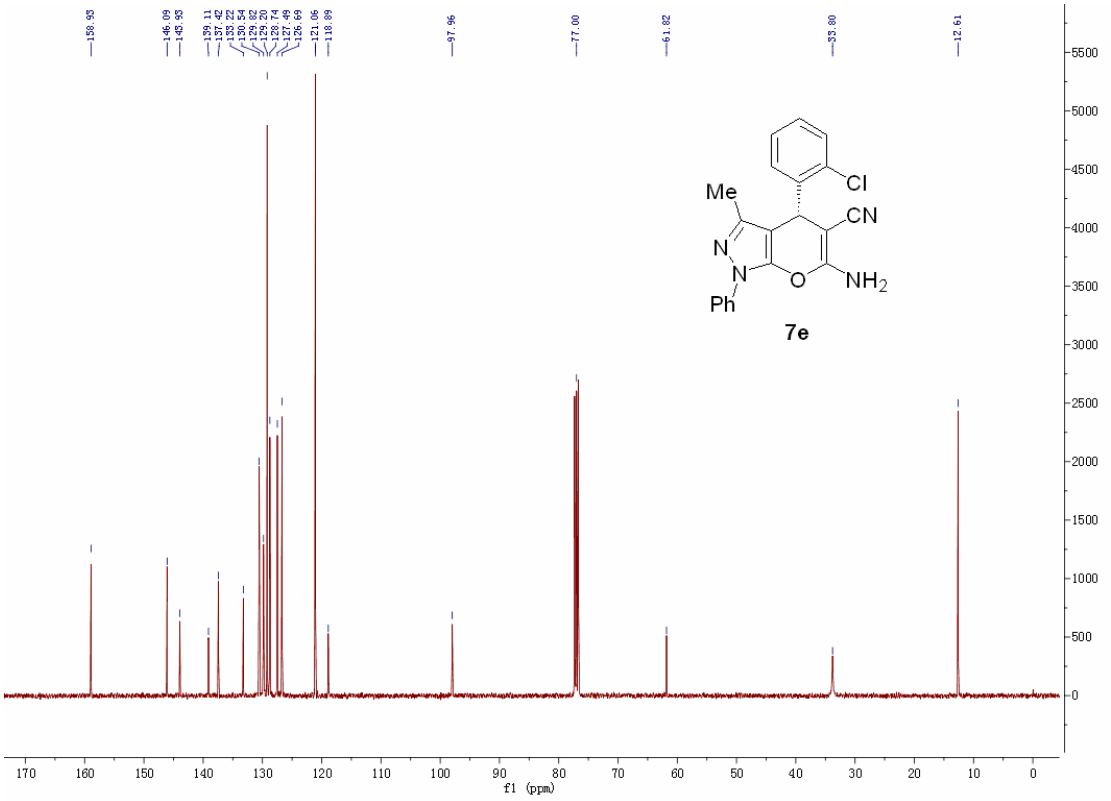
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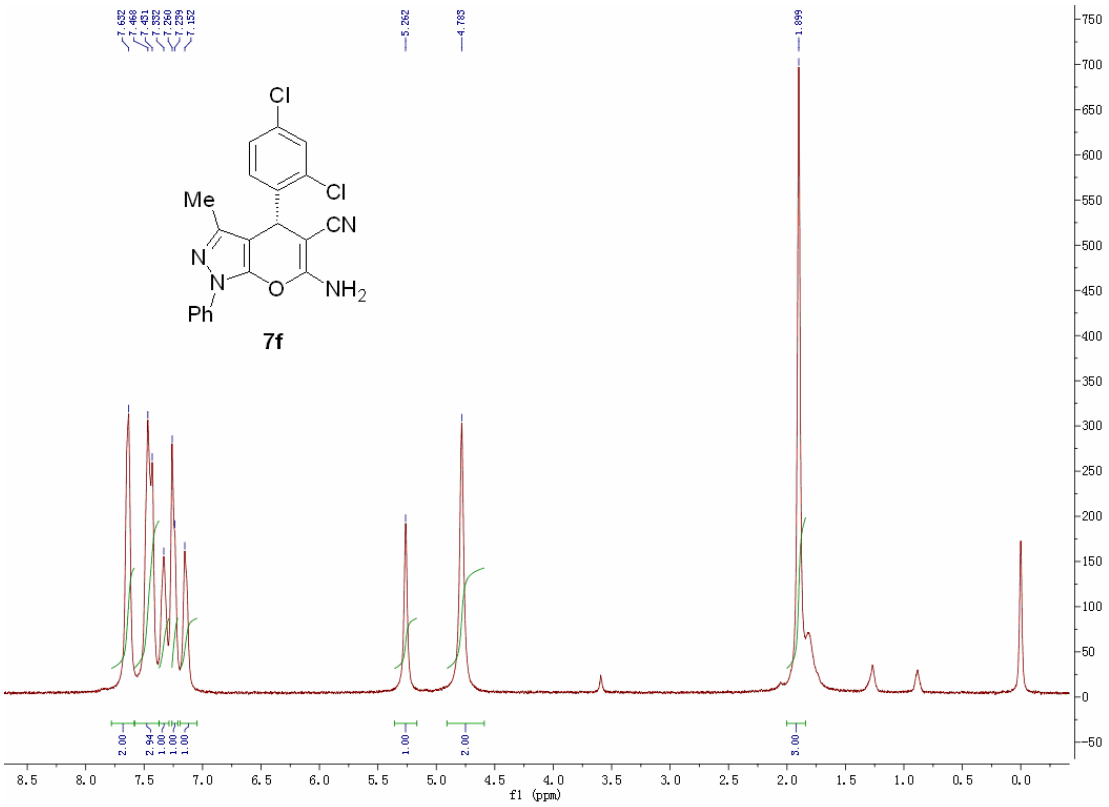
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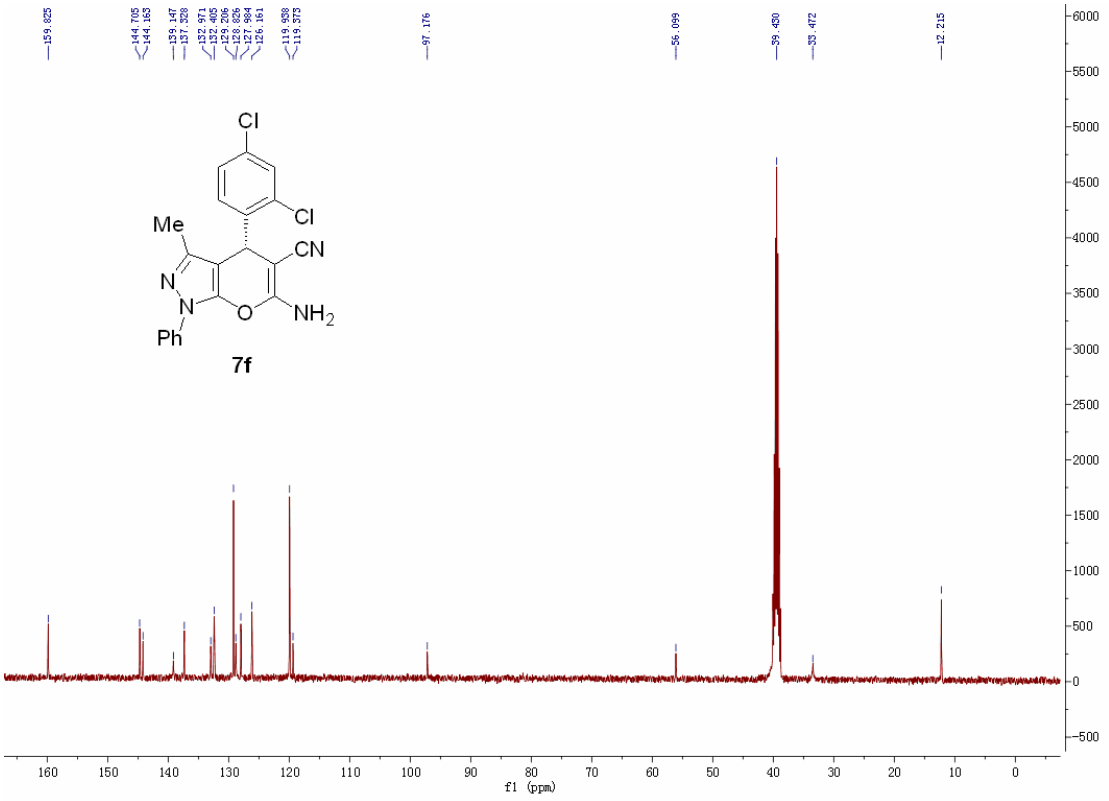
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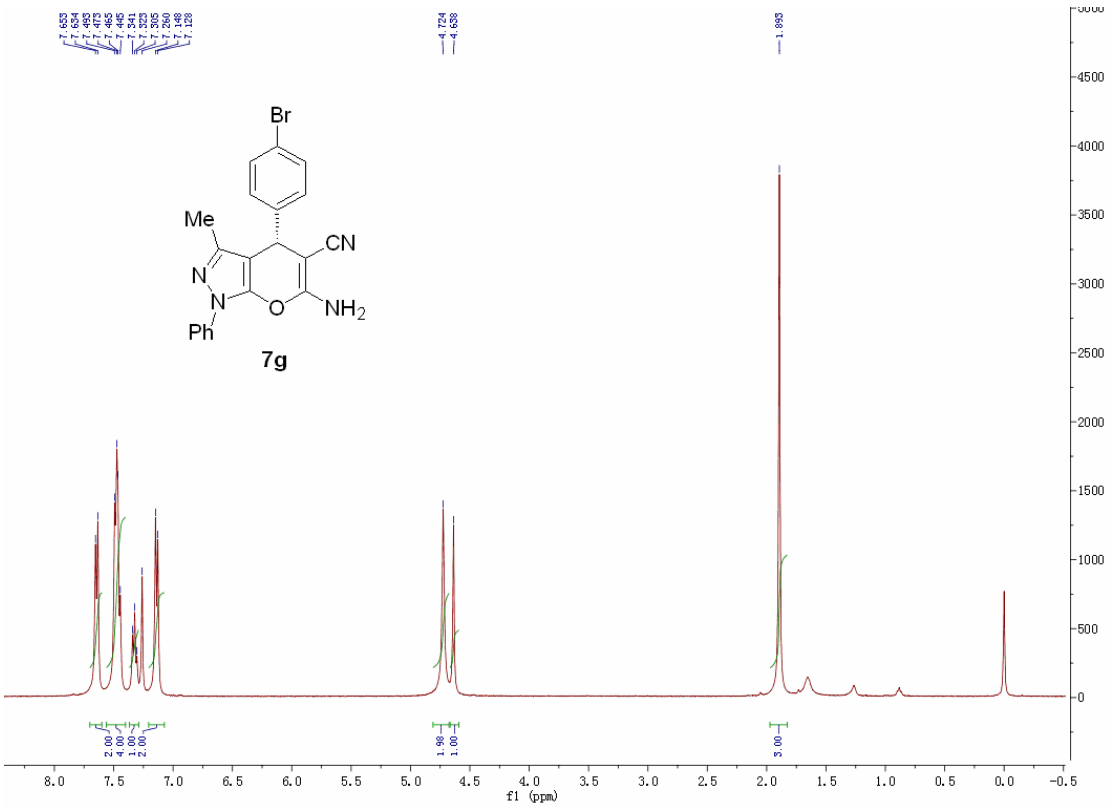
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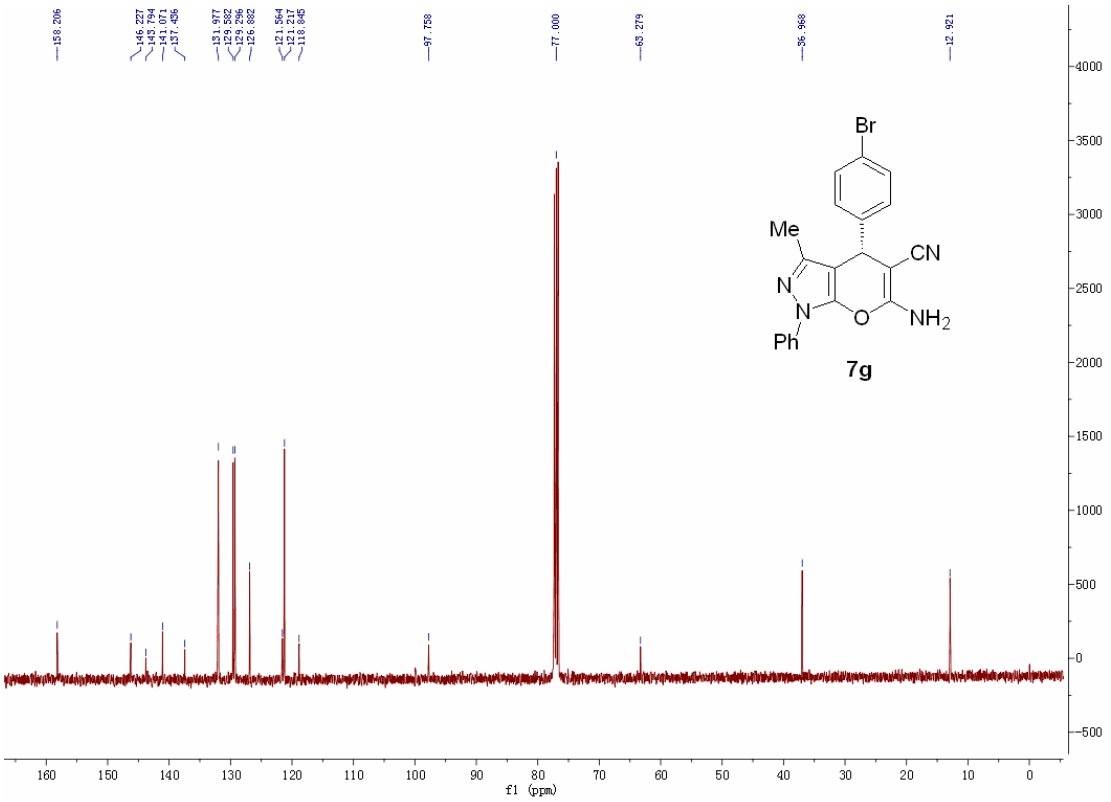
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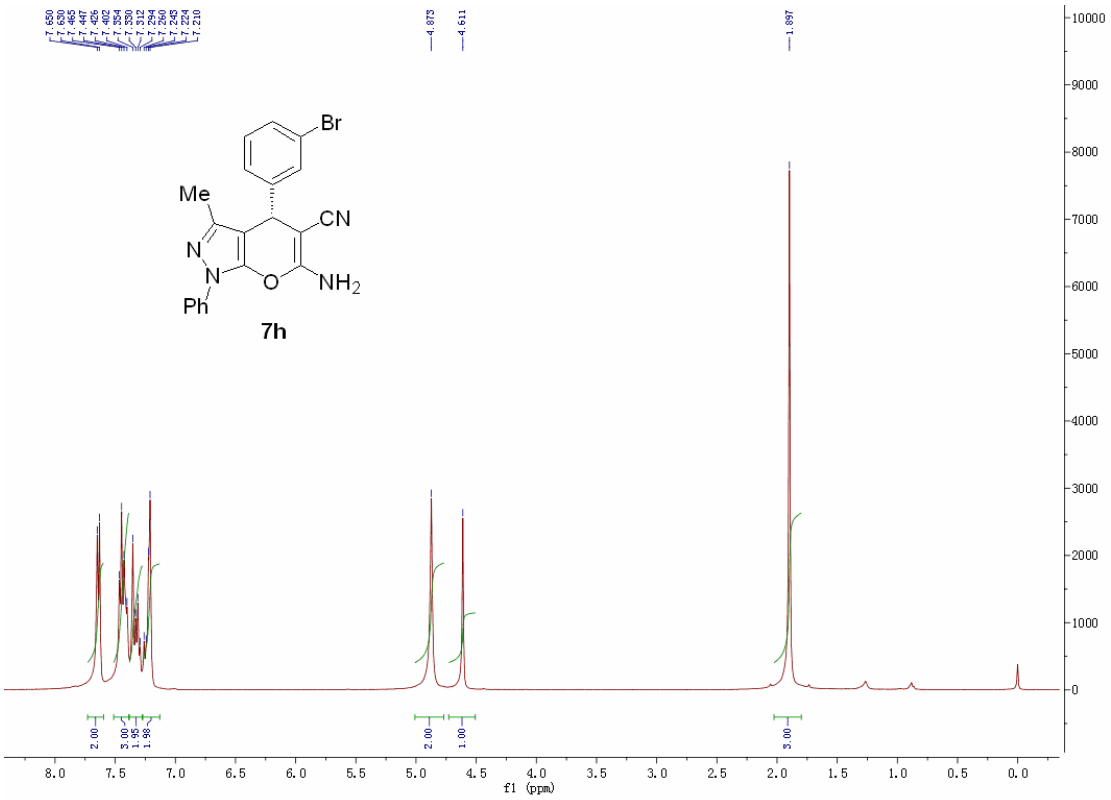
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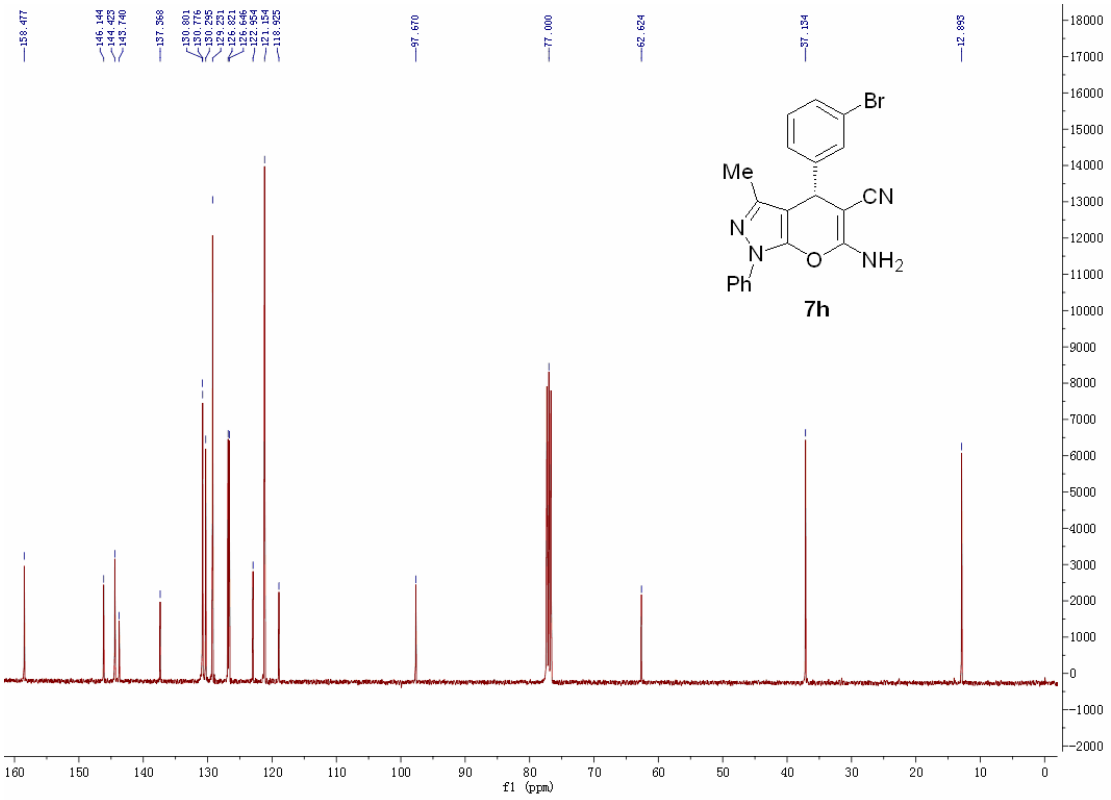
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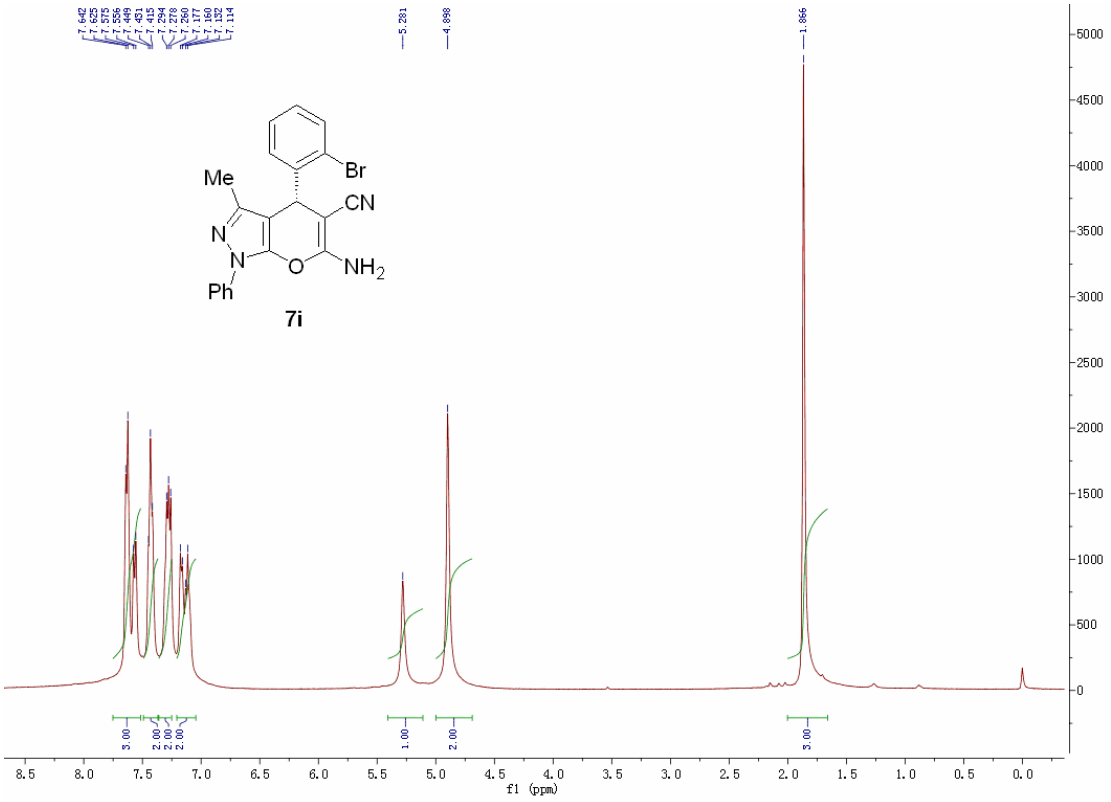
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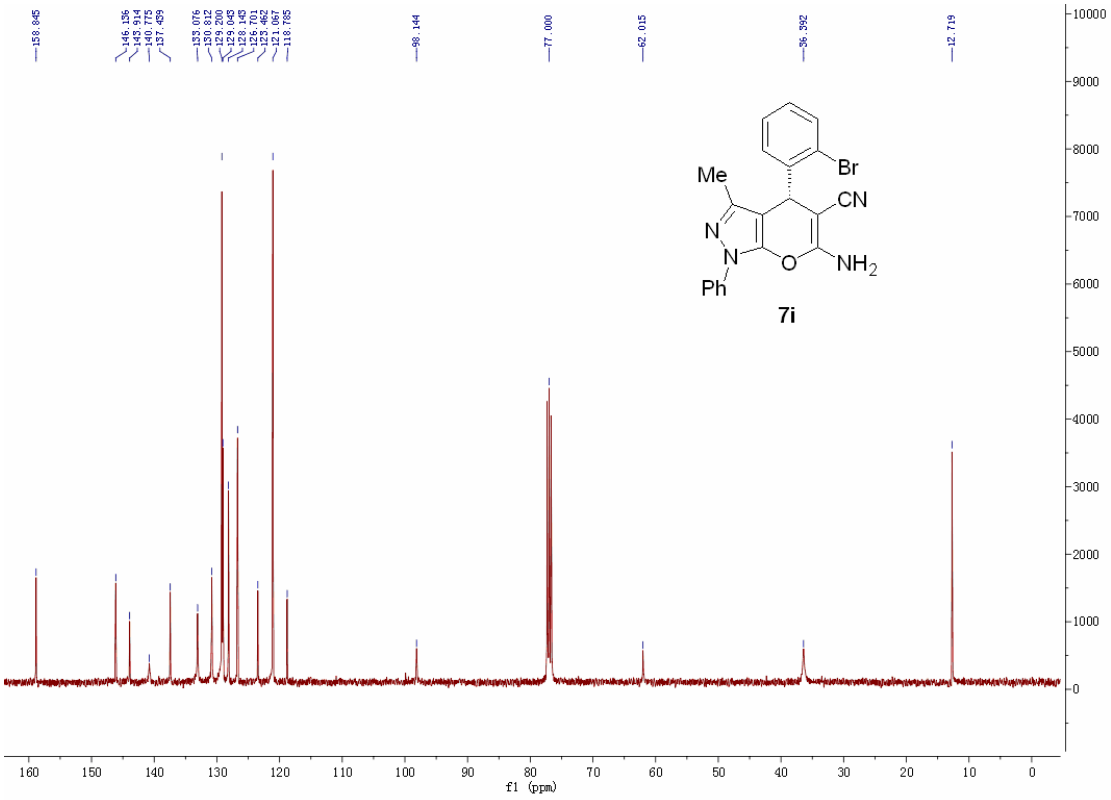
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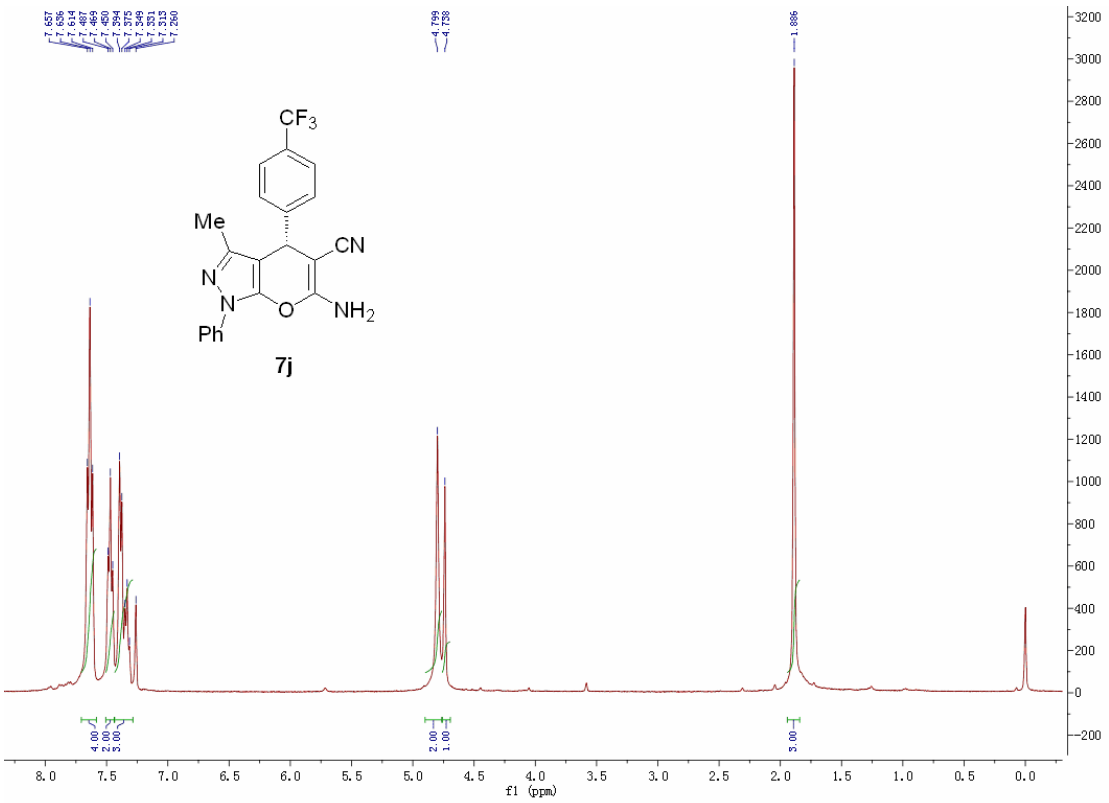
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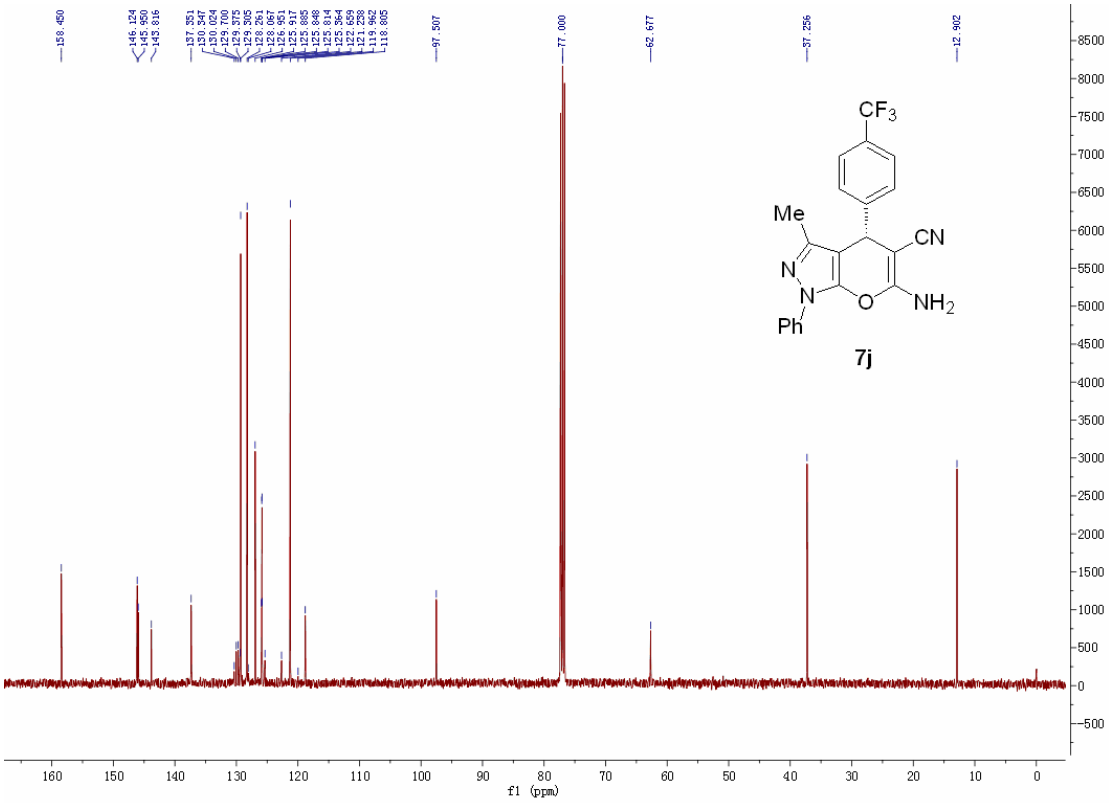
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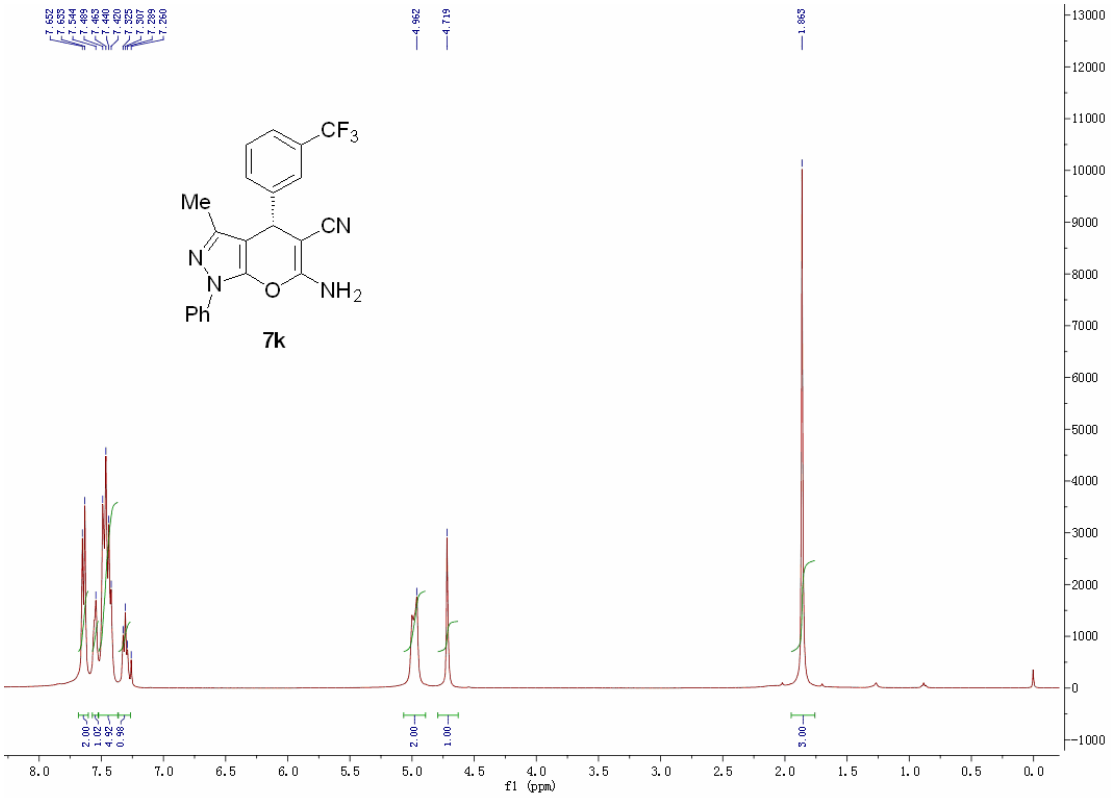
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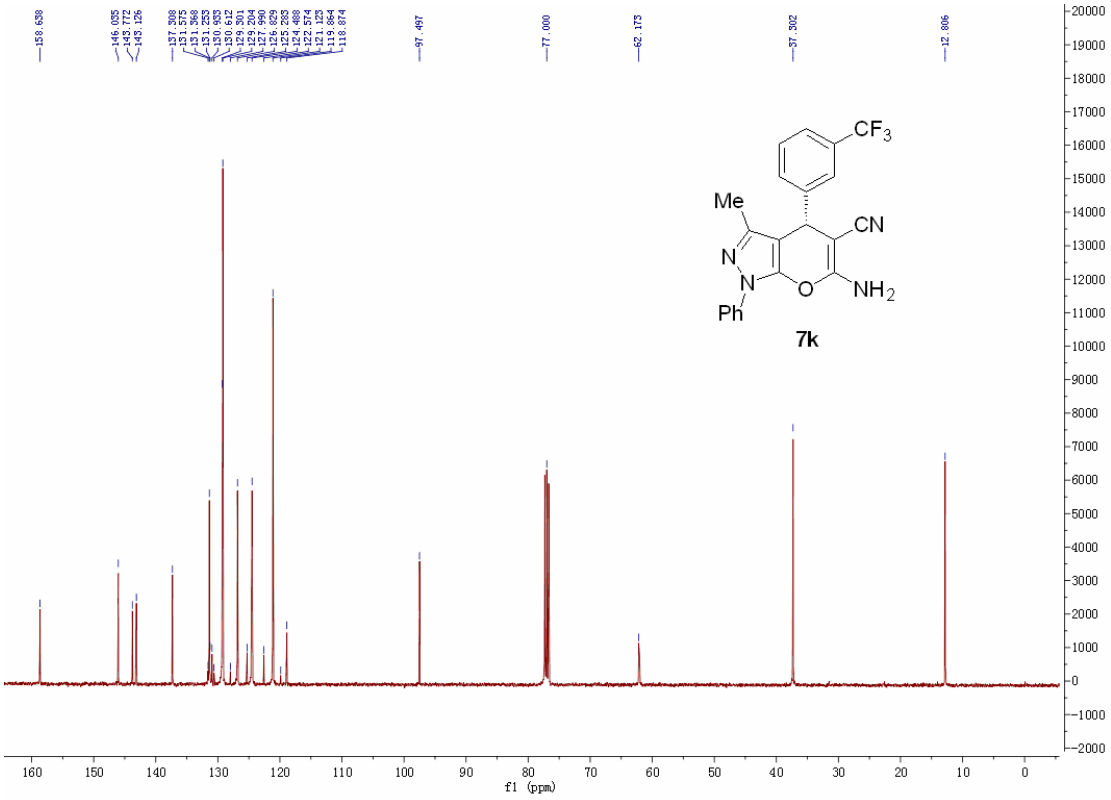
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N
O
NH2
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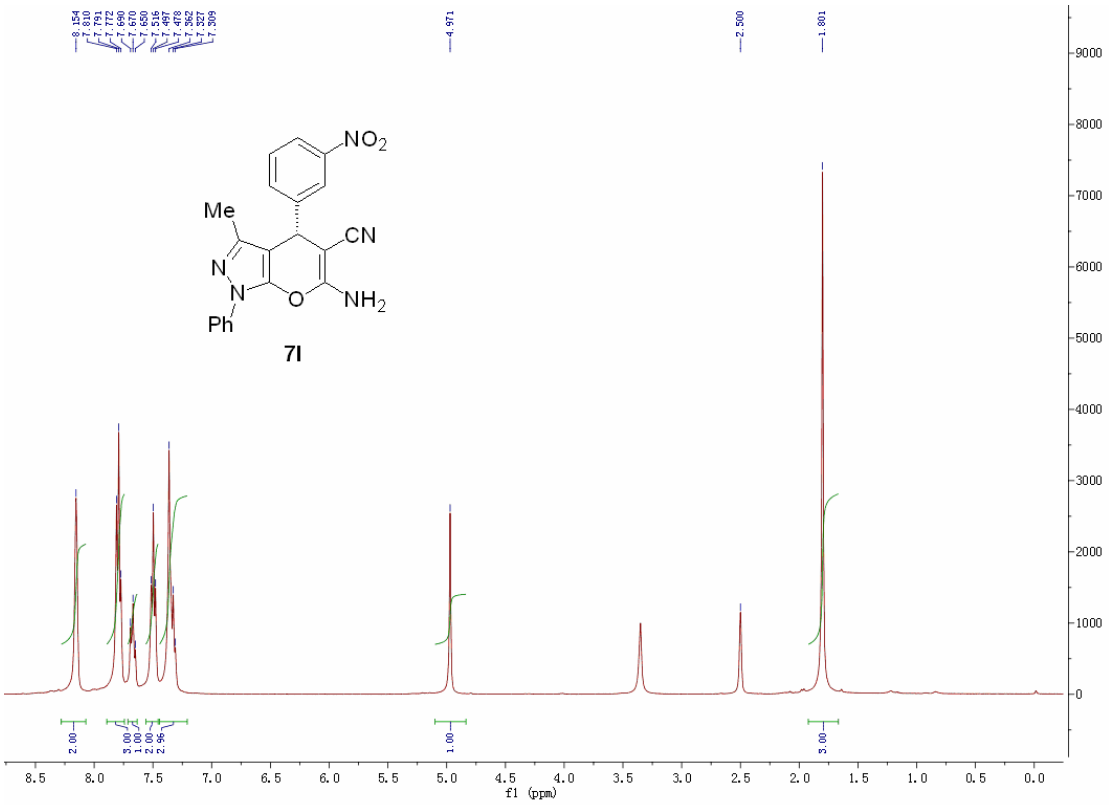
f1 (ppm)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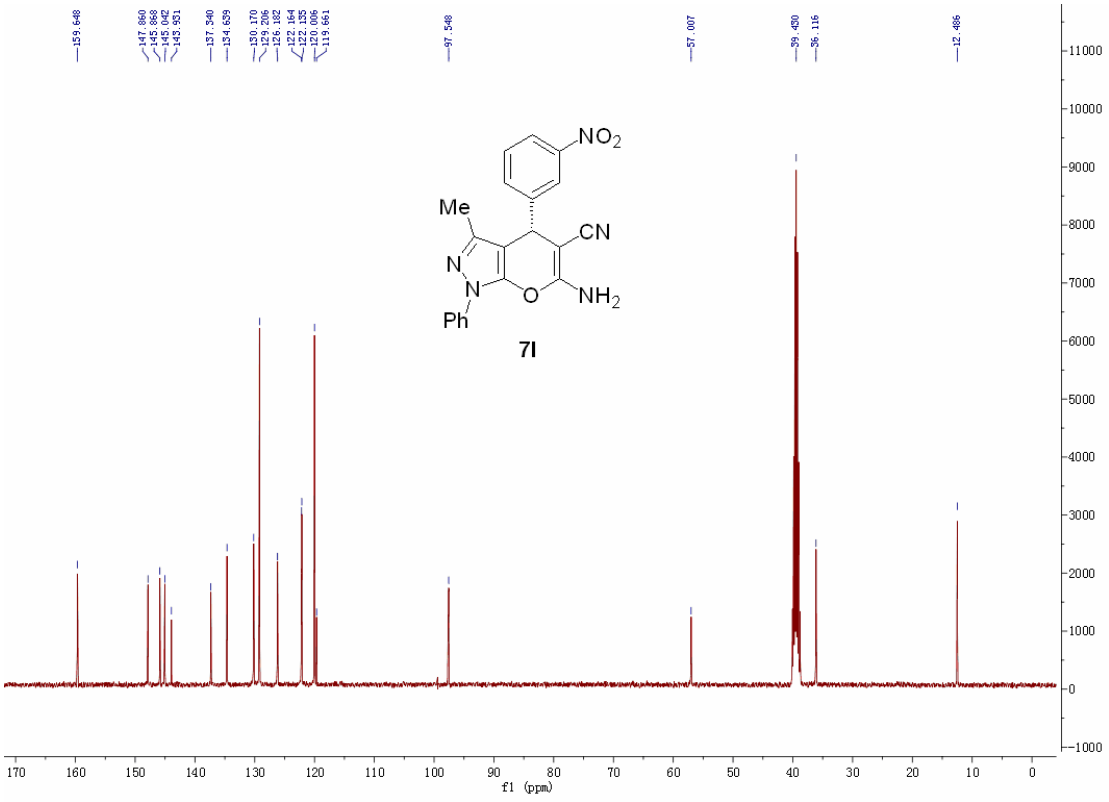
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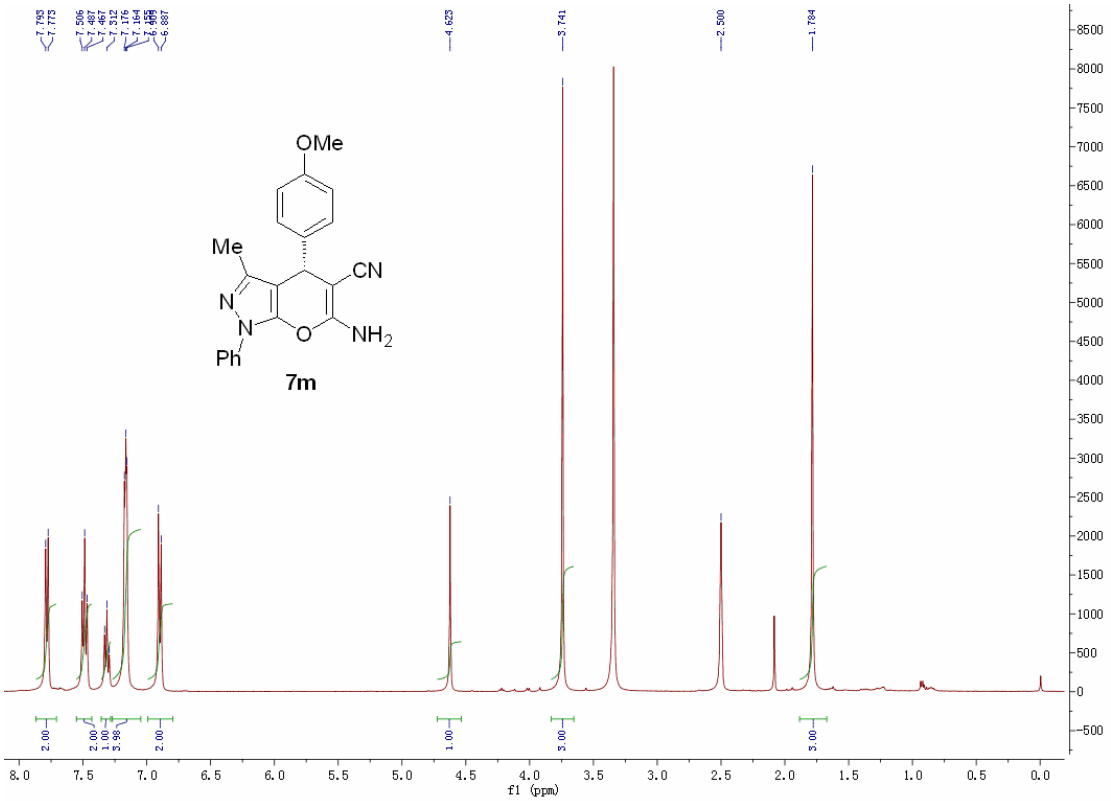
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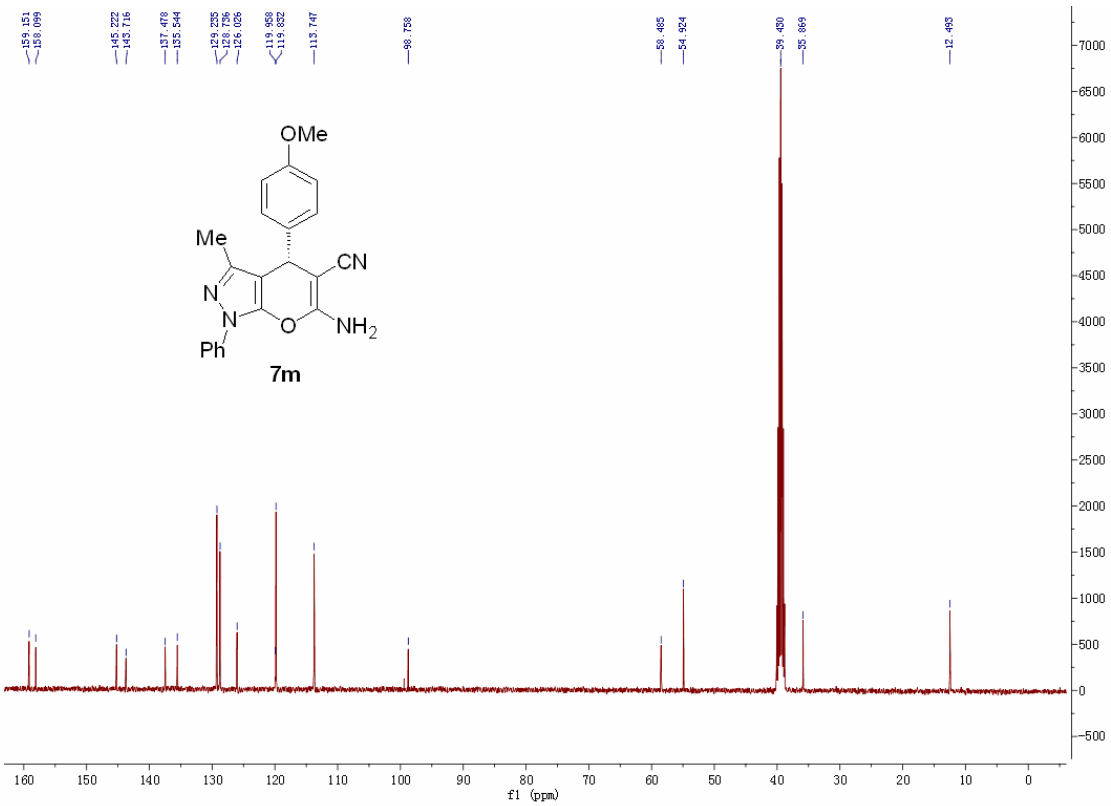
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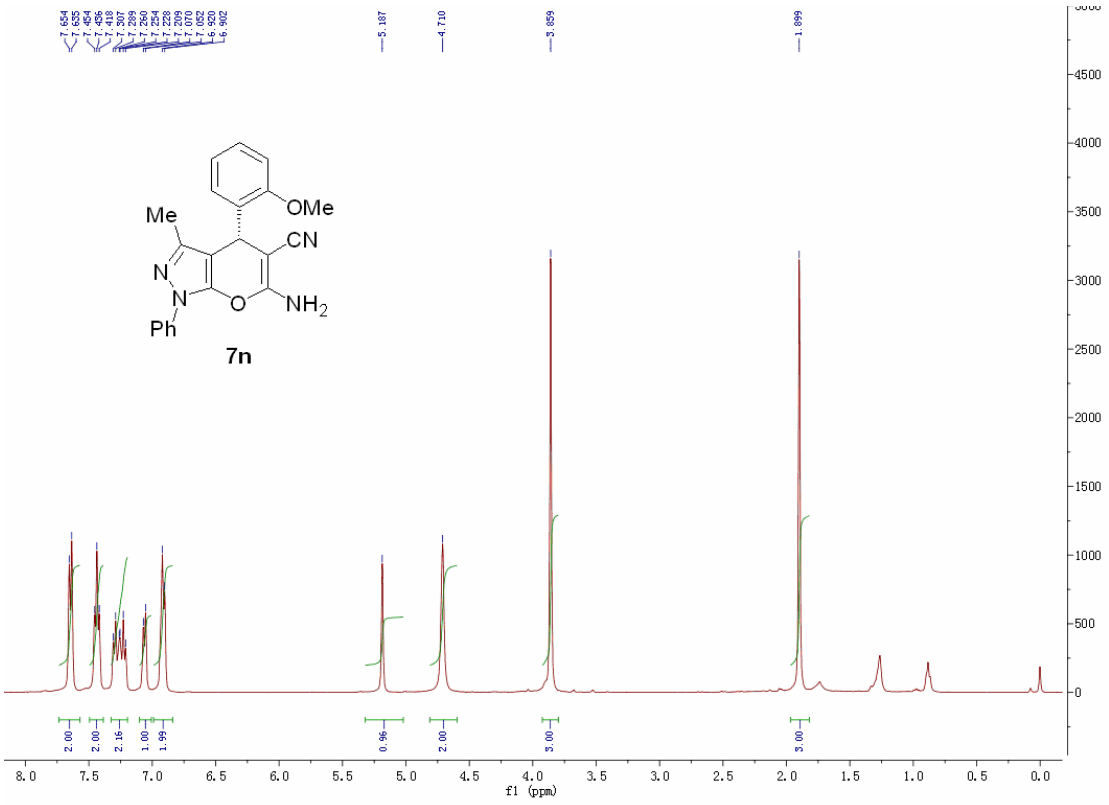
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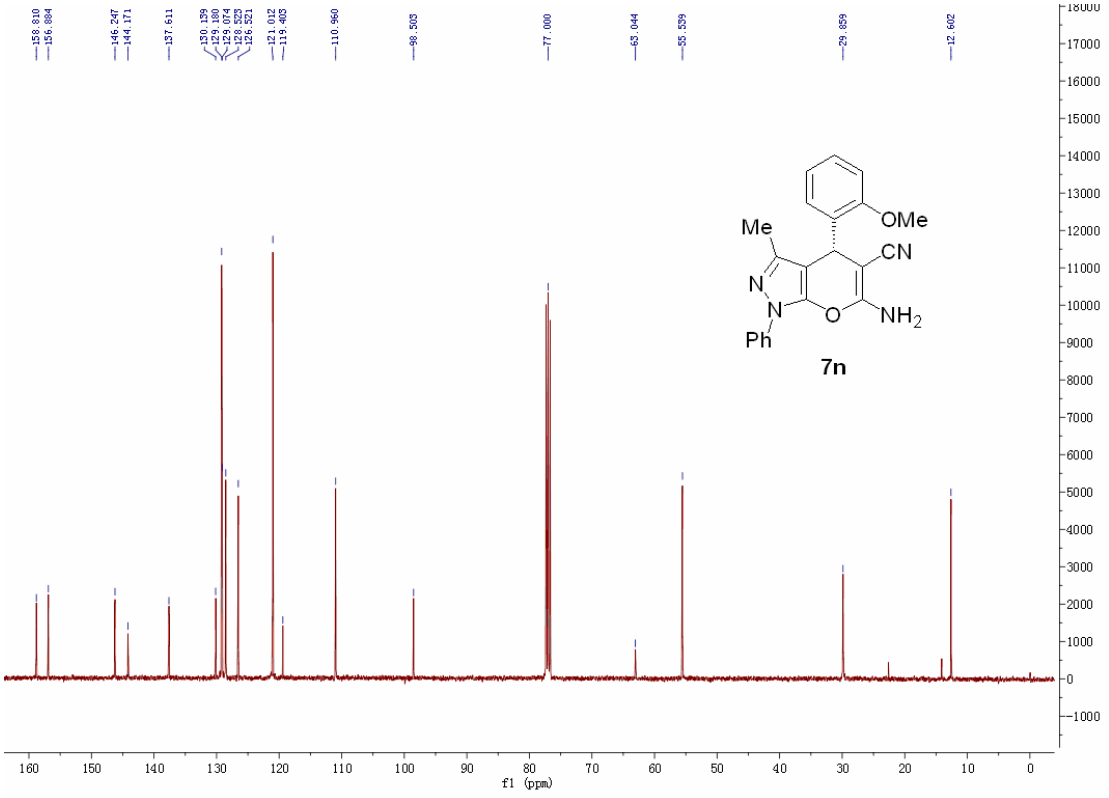
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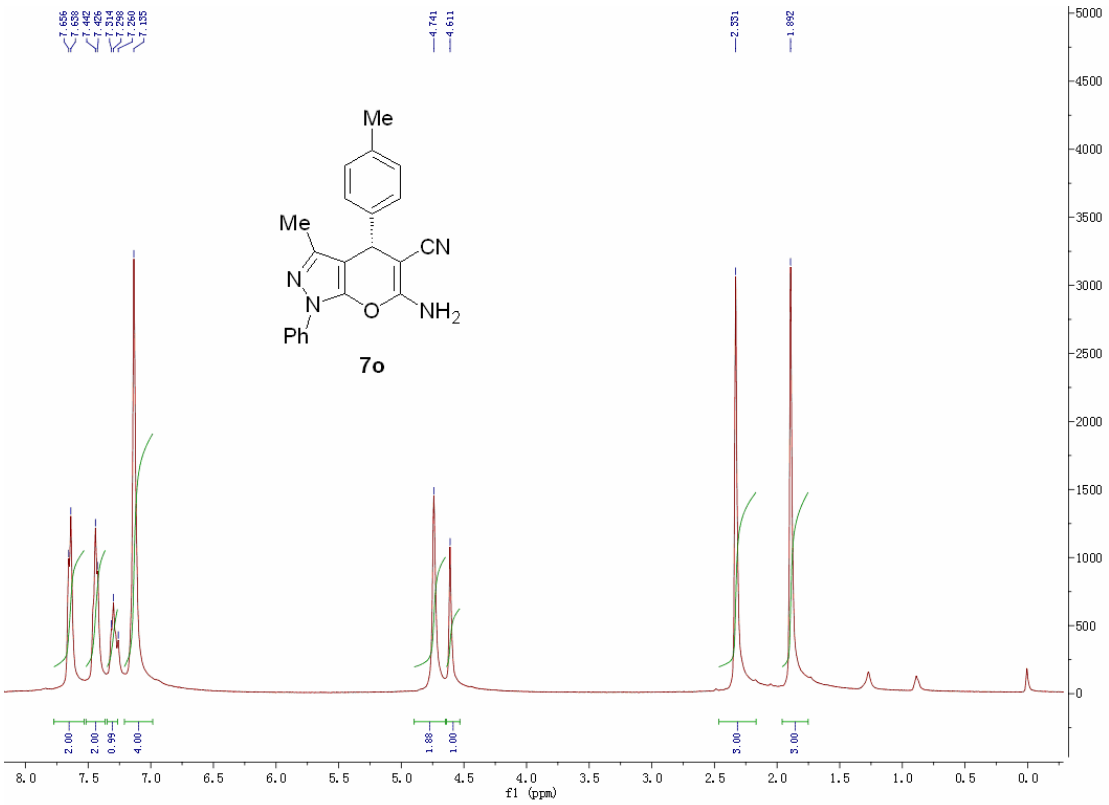
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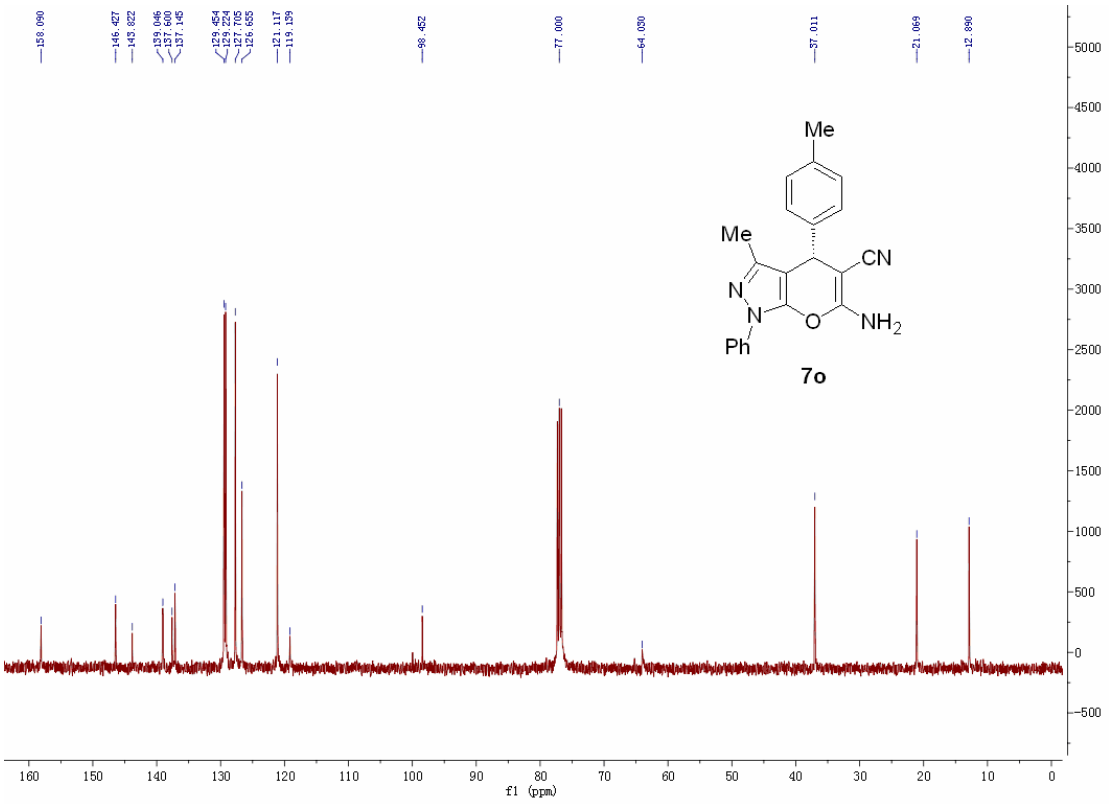
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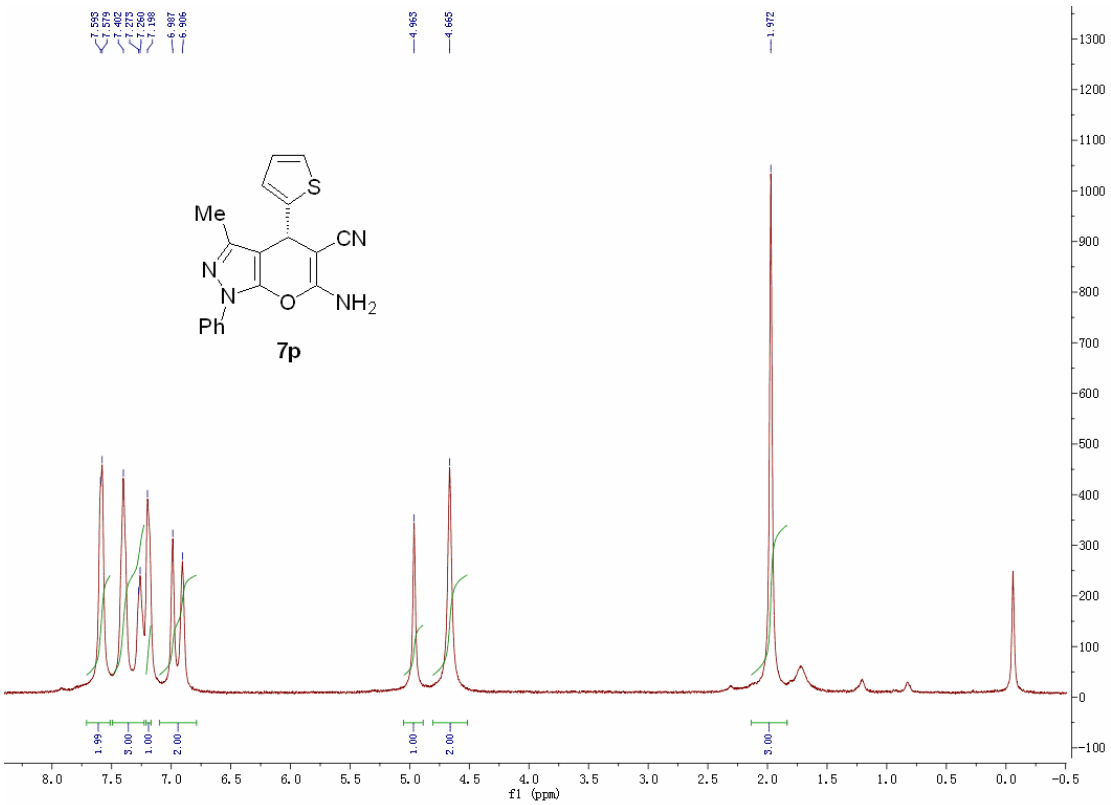
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N
N
O
NH2
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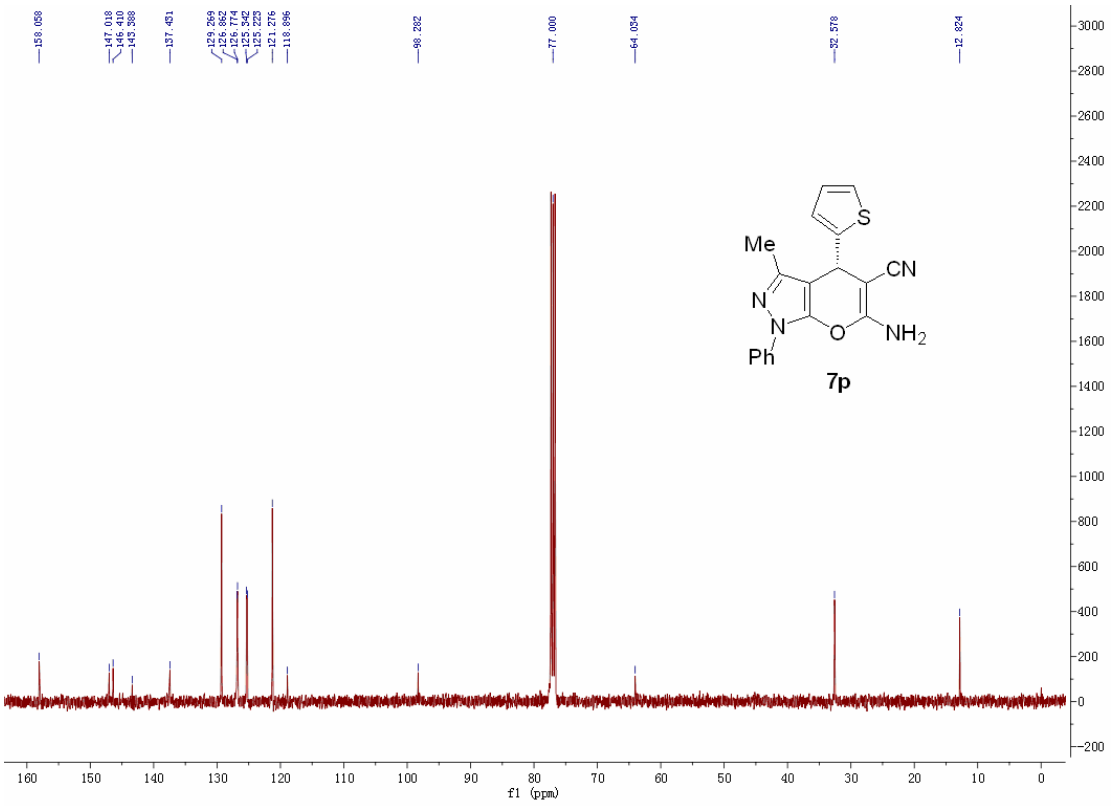
2.00
3.00
f1 (ppm)

7p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121.276
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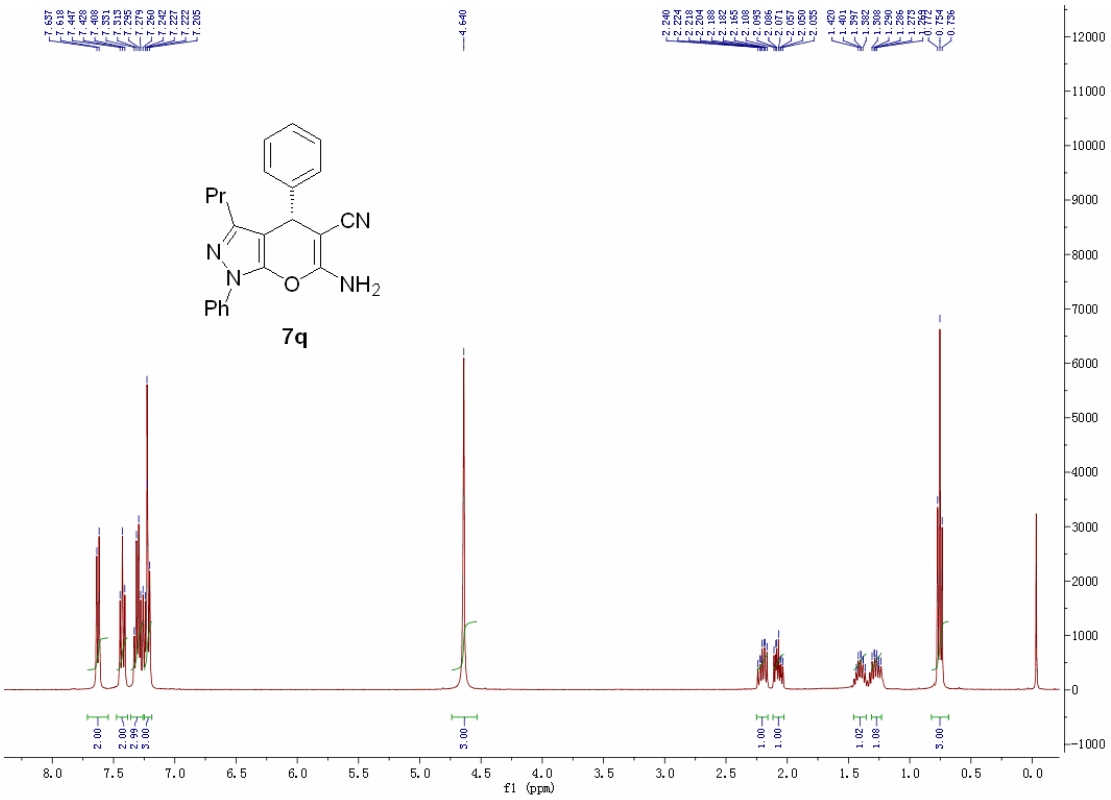
12.824
Me
CN
N
N
O
NH2
Ph
S
f1 (ppm)

7p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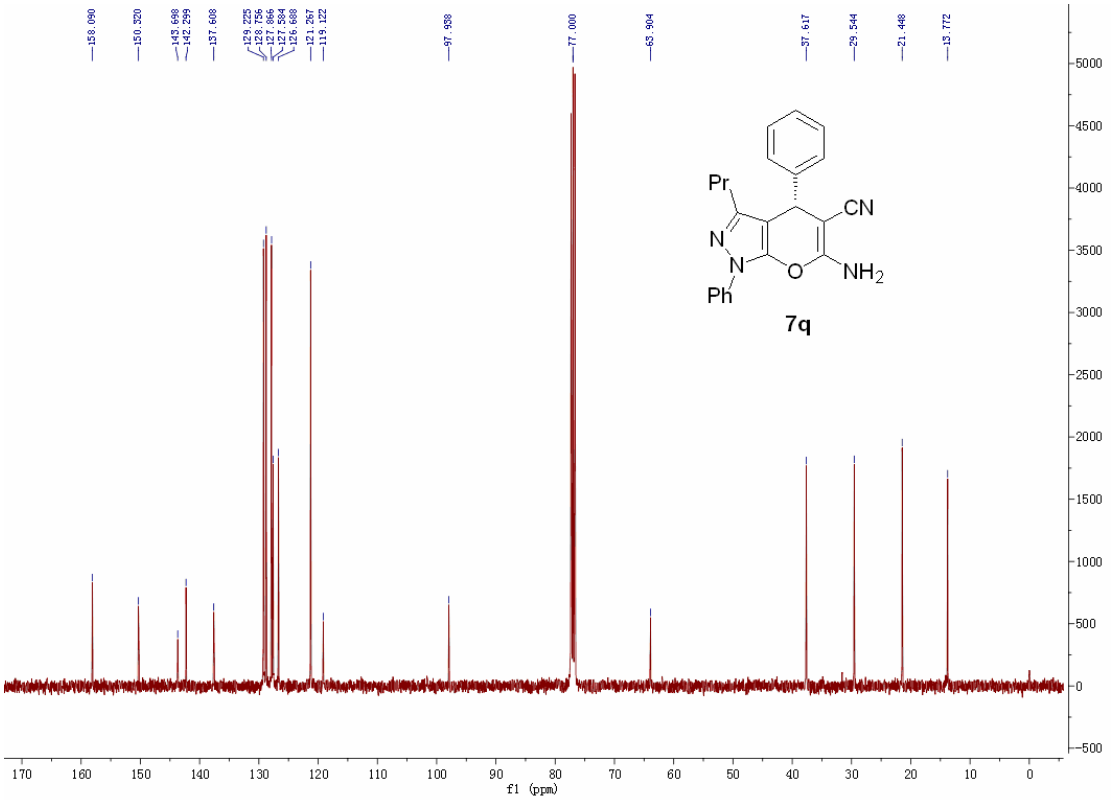
Ph
7q
f1 (ppm)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Ph
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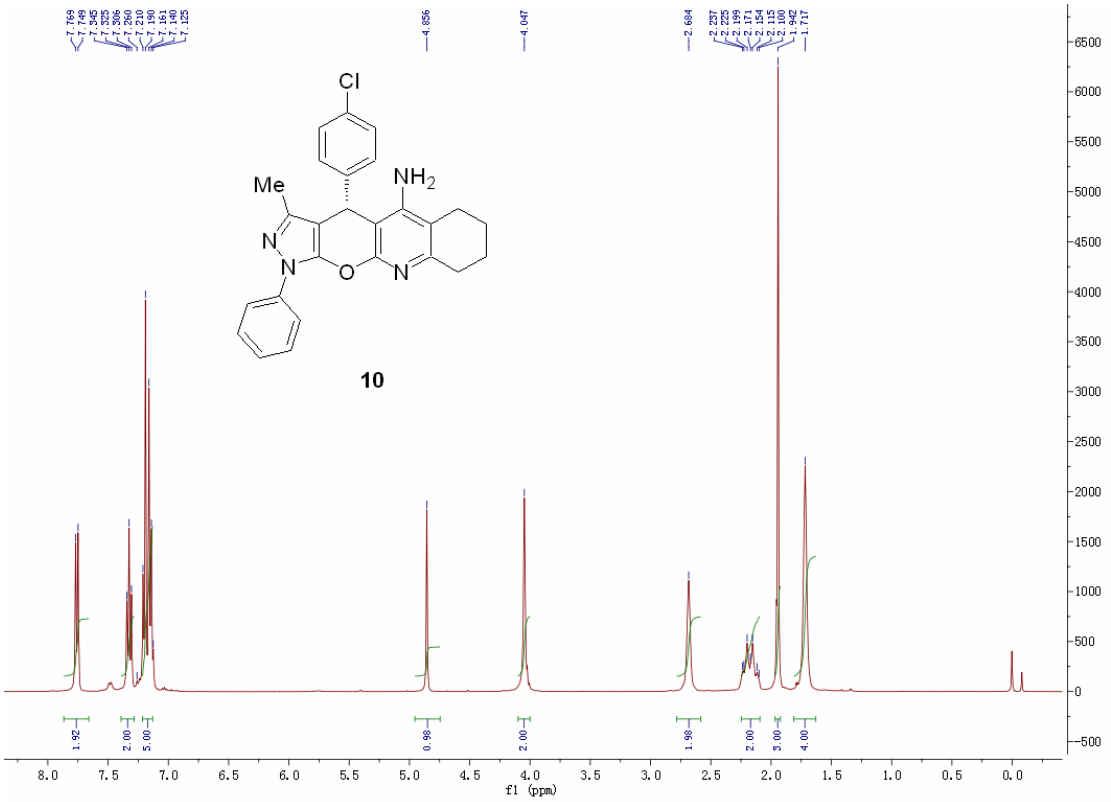
f1 (ppm)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NH2
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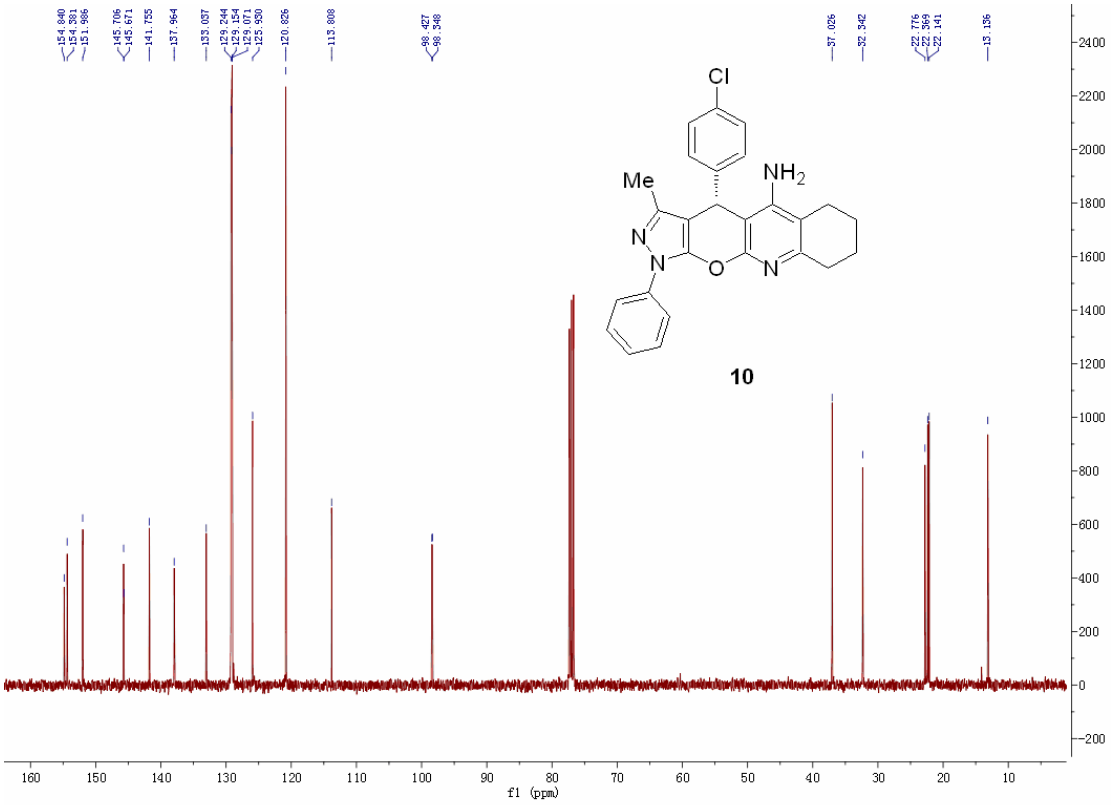
f1 (ppm)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Me
NH2
N
N
O
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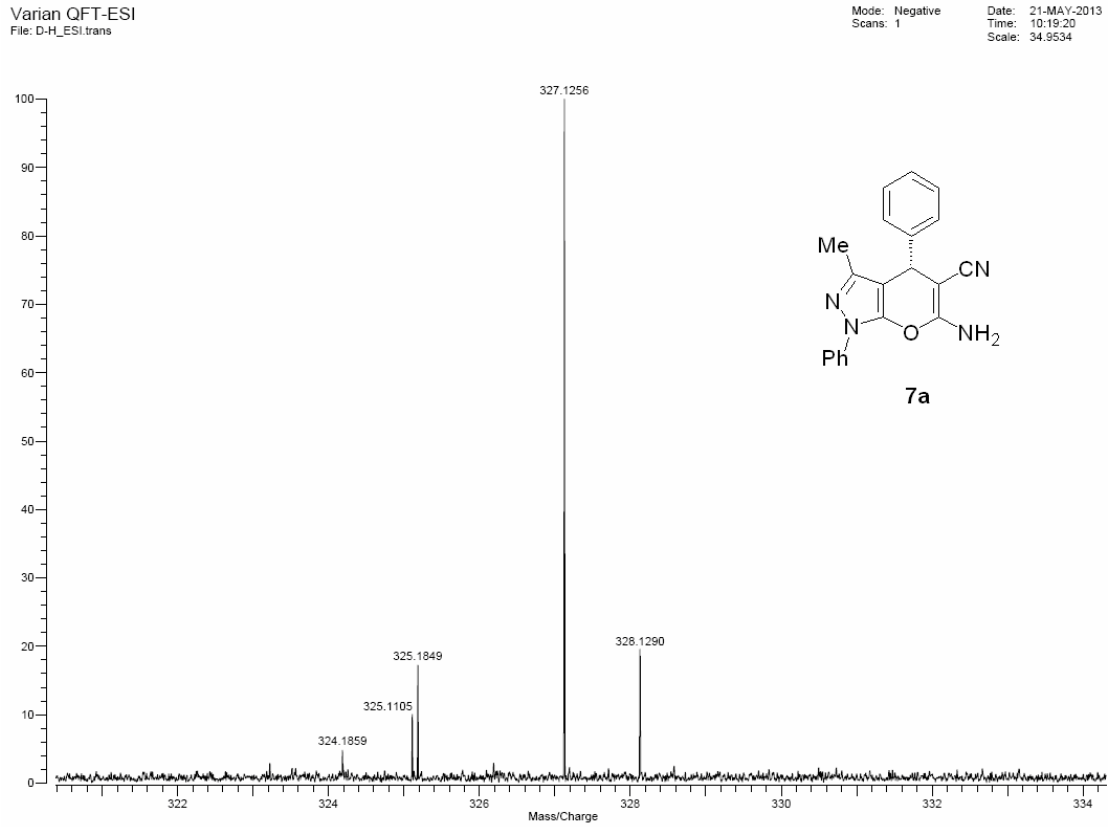
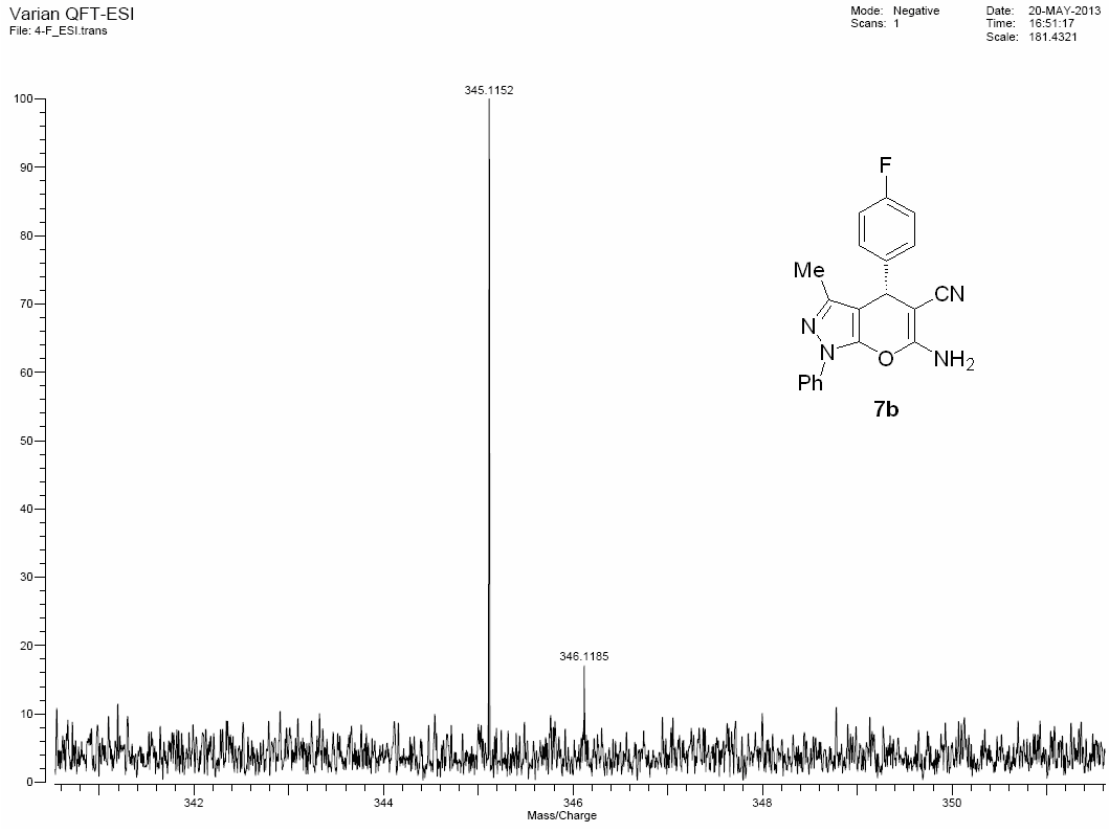
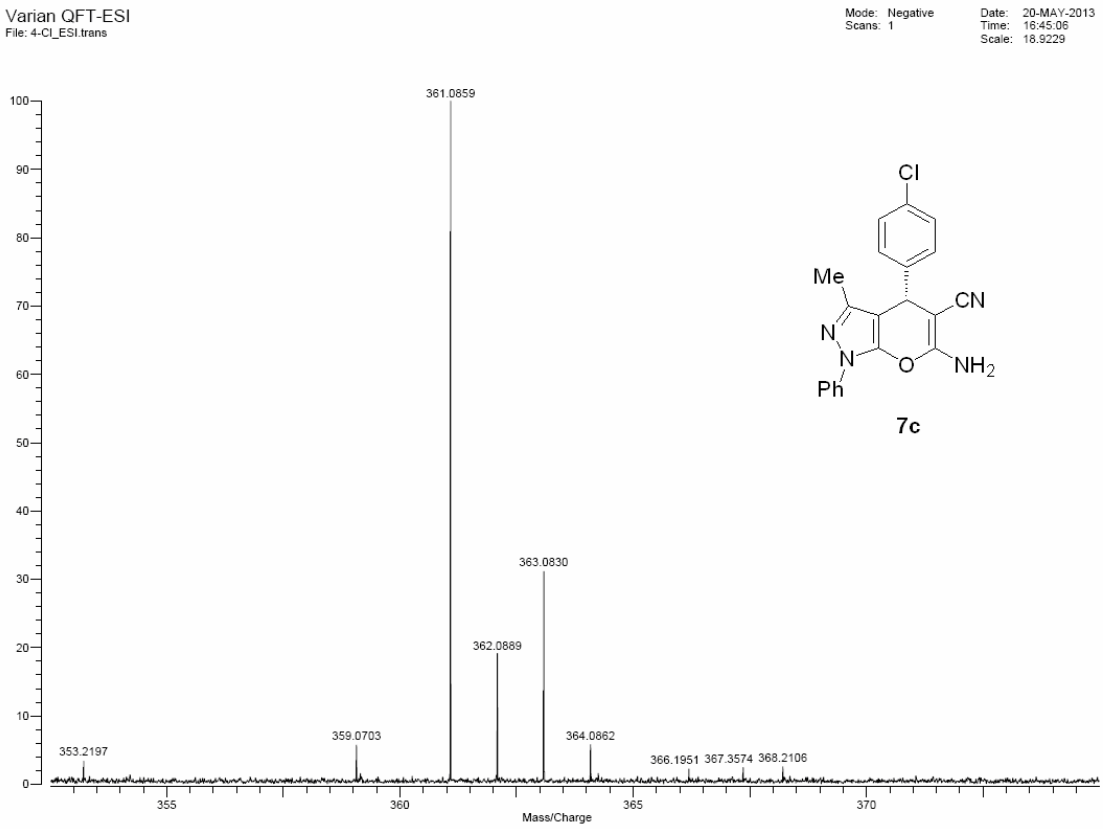
f1 (ppm)

2. Copies of HRMS spectra






Varian QFT-ESI
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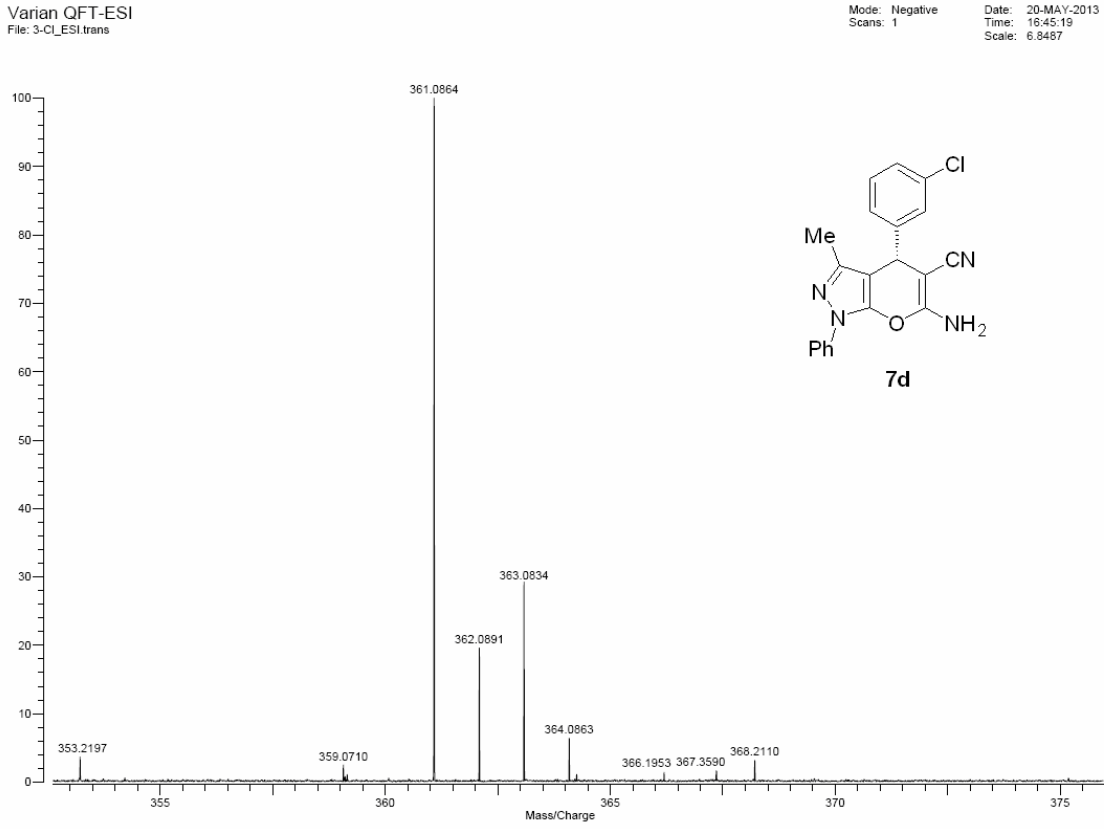
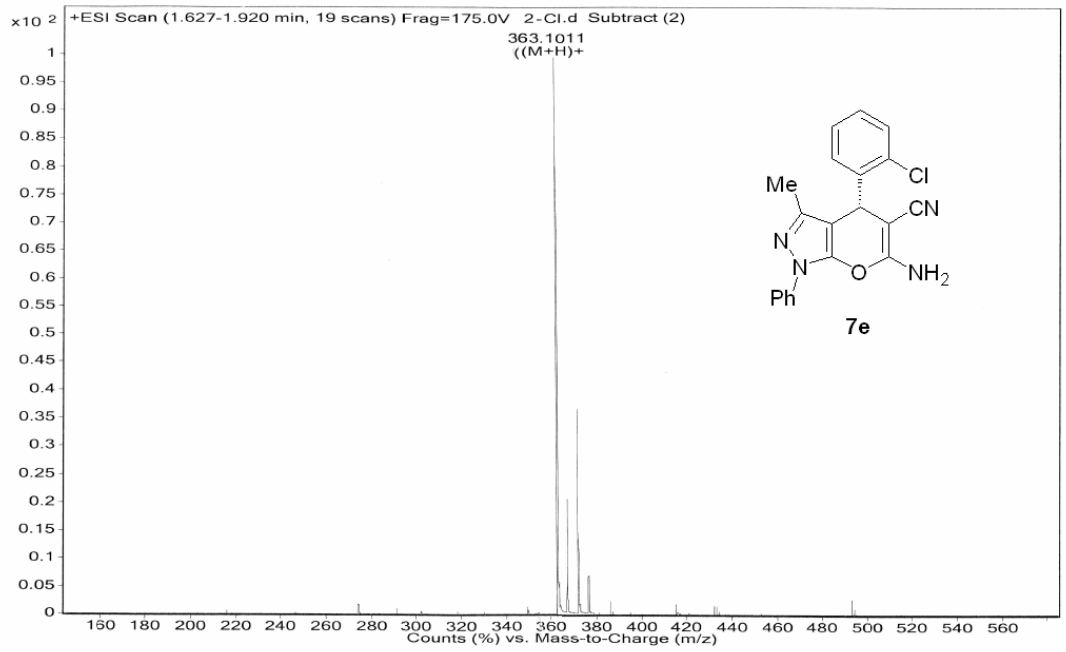
Mode: Negative
Scans: 1
Date: 20-MAY-2013
Time: 16:45:06
Scale: 18.9229
361.0859
363.0830
362.0889
359.0703
364.0862
353.2197
366.1951
367.3574
368.2106
Mass/Charge
Cl
Me
CN
N
N
O
NH2
Ph
7c


Varian QFT-ESI
File: 3-Cl_ESI.trans
Mode: Negative
Scans: 1
Date: 20-MAY-2013
Time: 16:45:19
Scale: 6.8487
361.0864
363.0834
362.0891
364.0863
353.2197
359.0710
366.1953
367.3590
368.2110
Mass/Charge
Cl
Me
CN
N
N
O
NH2
Ph
7d

Sample Name	lc/ms	**Position**	P1-A3	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	3	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Some Ions Missed
Data Filename	2-Cl.d	**ACQ Method**	chen-ms.m	**Comment**		**Acquired Time**	6/17/2013 11:54:15 AM



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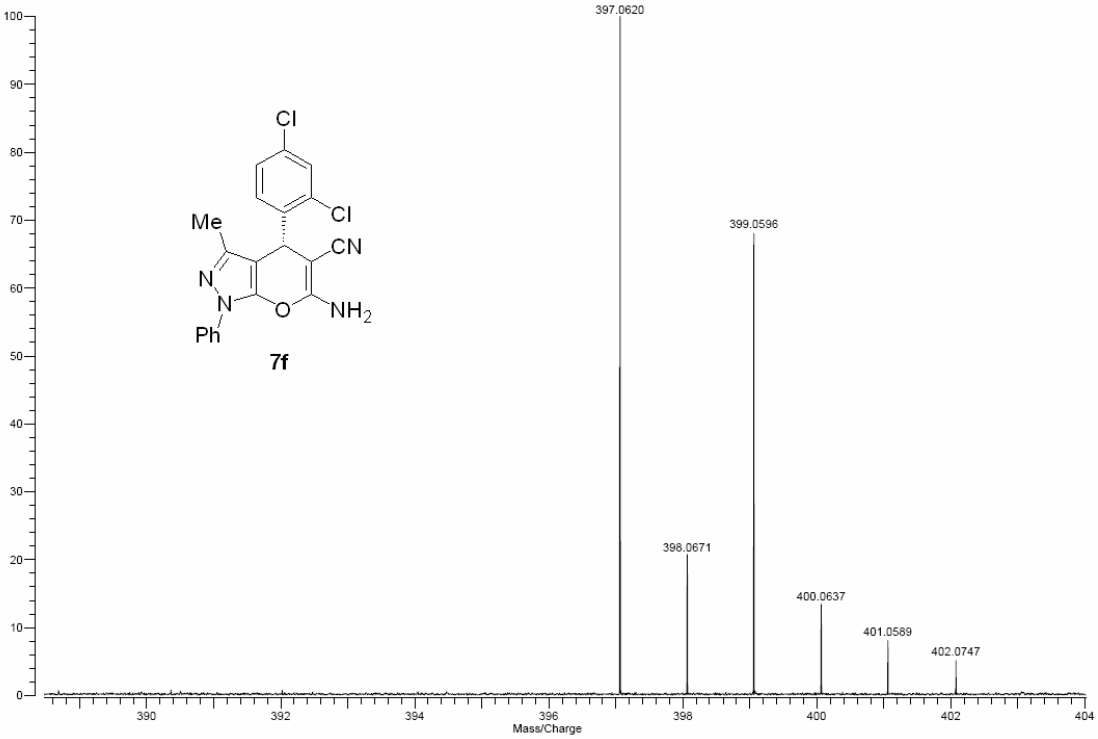
Varian ProMALDI
File: ZZH-WHX-2,4-CL -DHB-LASER60.trans

Mode: Positive
Scans: 1

Date: 24-MAY-2013
Time: 12:49:42
Scale: 9.8357



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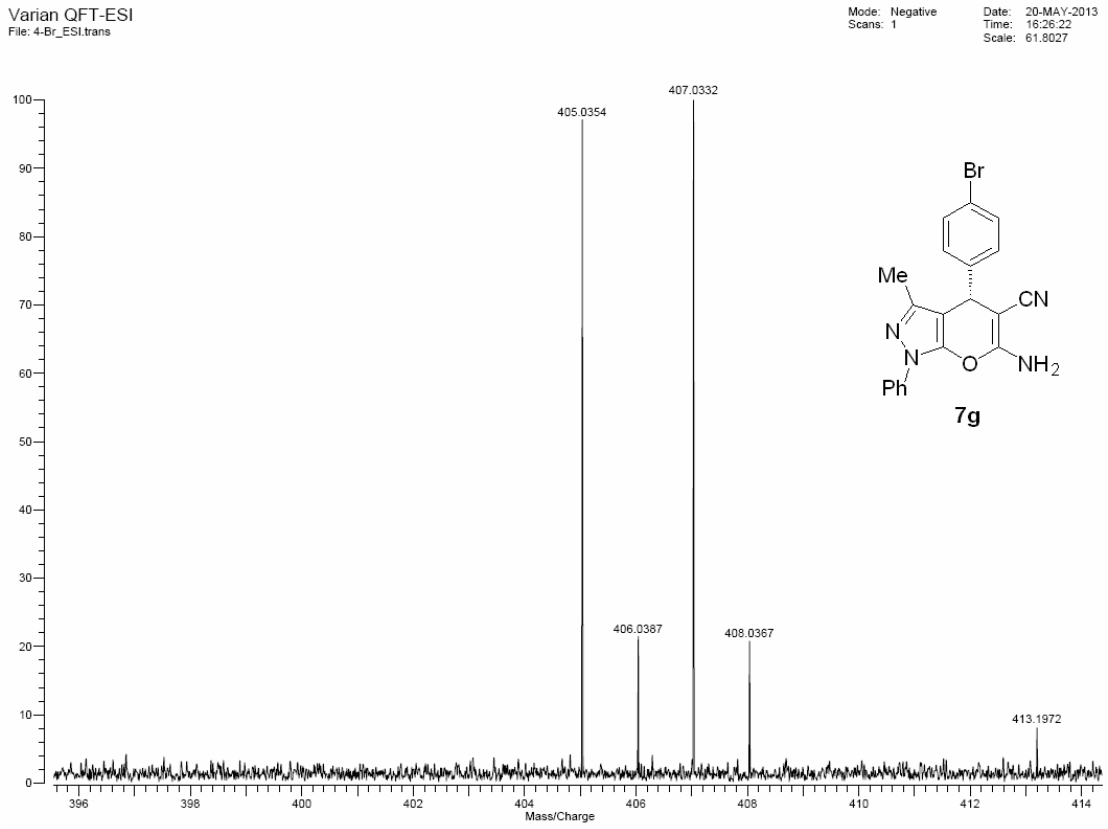
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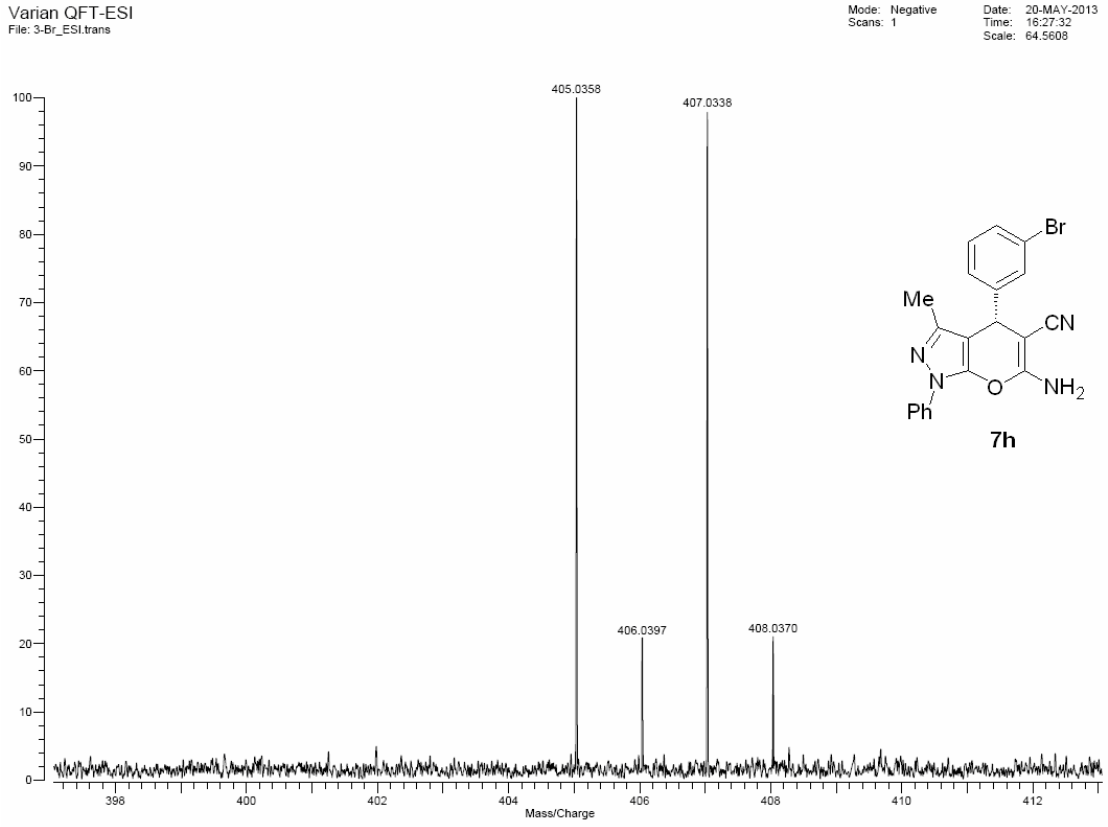
File: 4-Br_ESI.trans
Mode: Negative
Scans: 1
Date: 20-MAY-2013
Time: 16:26:22
Scale: 61.8027
405.0354
407.0332
406.0387
408.0367
413.1972
Mass/Charge
Br
Me
CN
N
N
O
NH2
Ph
7g


Varian QFT-ESI
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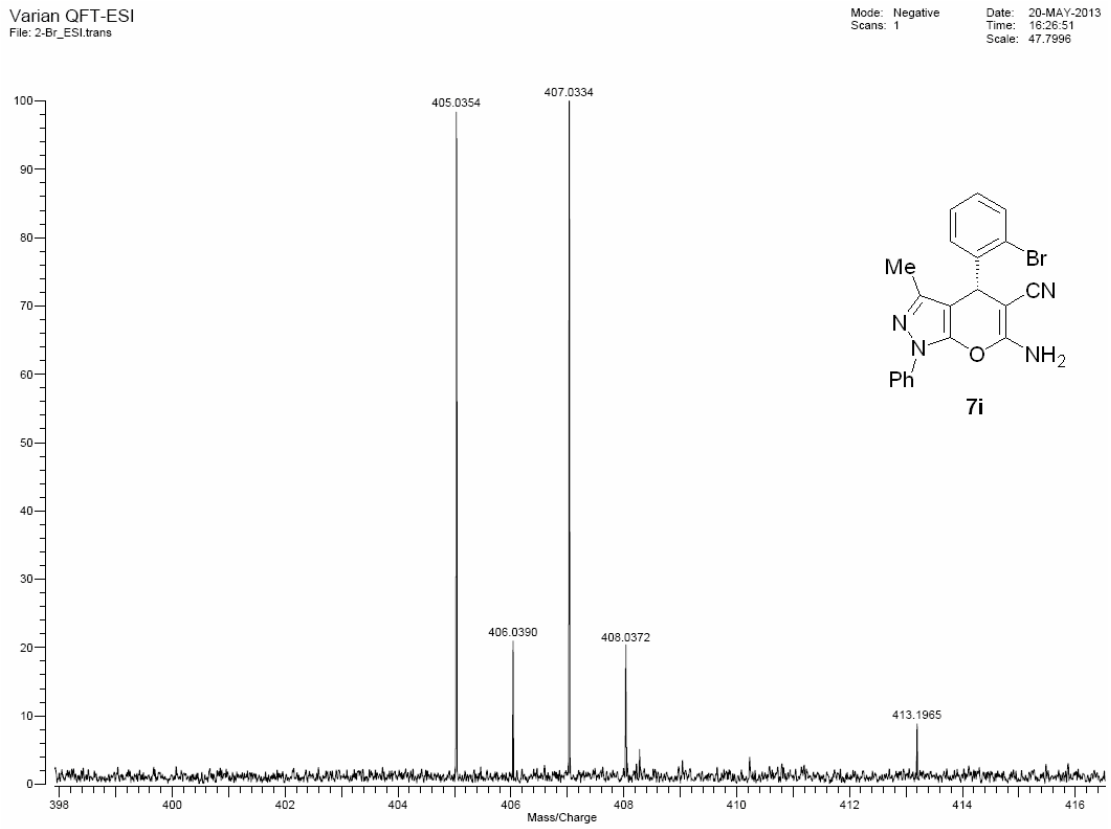
Mode: Negative
Scans: 1
Date: 20-MAY-2013
Time: 16:27:32
Scale: 64.5608
405.0358
407.0338
406.0397
408.0370
Mass/Charge
Br
Me
CN
N
N
O
NH2
Ph
7h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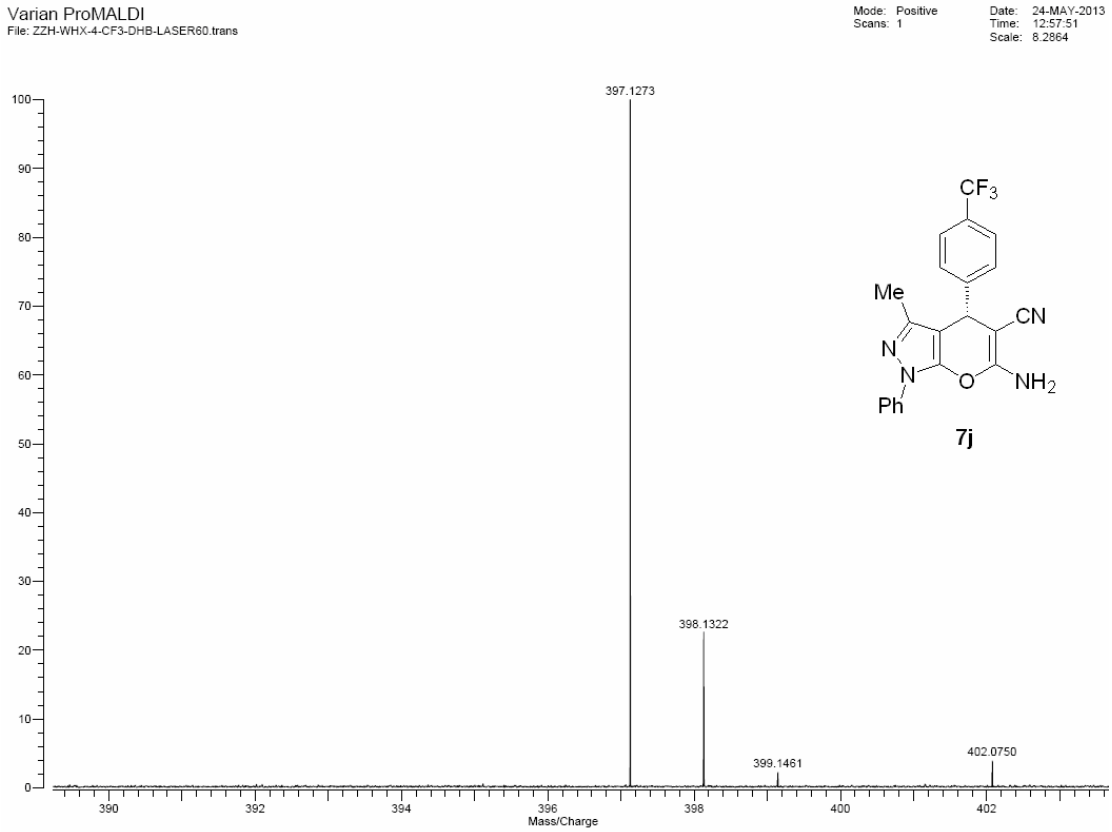
File: 2-Br_ESI.trans
Mode: Negative
Scans: 1
Date: 20-MAY-2013
Time: 16:26:51
Scale: 47.7996
405.0354
407.0334
406.0390
408.0372
413.1965
Mass/Charge
Me
Br
CN
N
N
O
NH2
Ph

7i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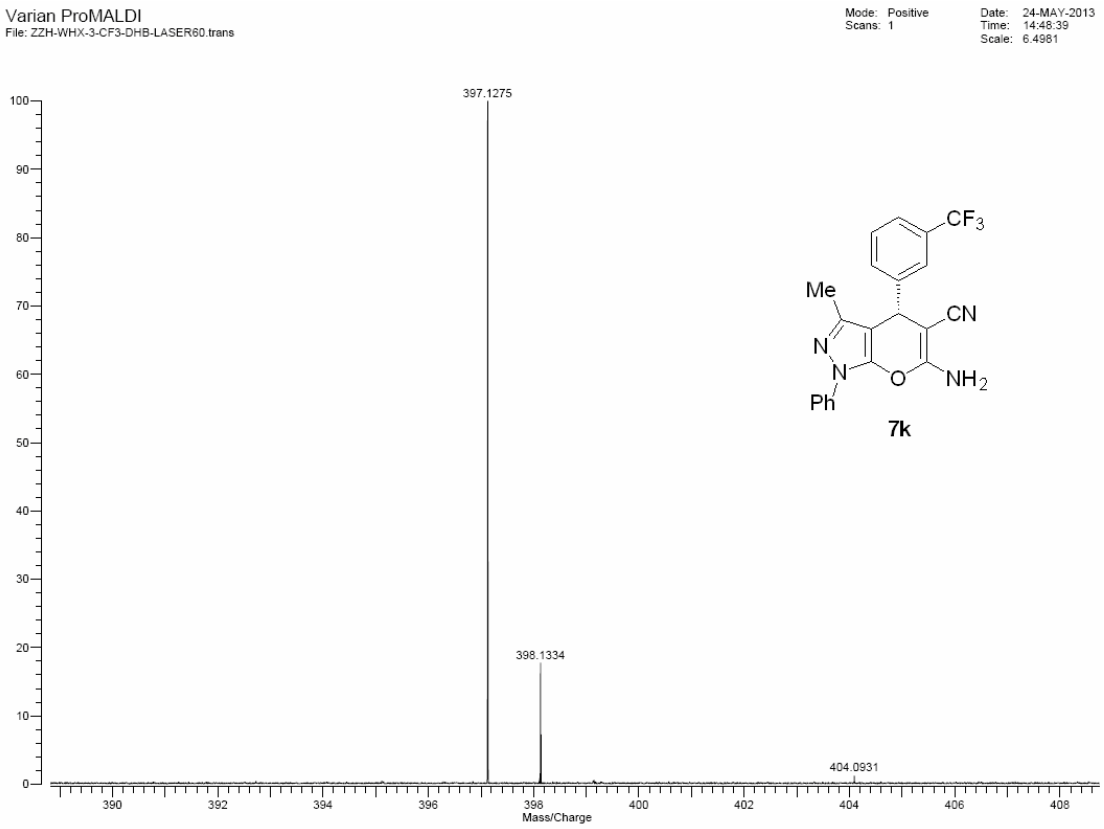
File: ZZH-WHX-4-CF3-DHB-LASER60.trans
Mode: Positive
Scans: 1
Date: 24-MAY-2013
Time: 12:57:51
Scale: 8.2864
397.1273
398.1322
399.1461
402.0750
Mass/Charge
CF3
Me
CN
N
N
O
NH2
Ph

7j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File: ZZH-WHX-3-CF3-DHB-LASER60.trans
Mode: Positive
Scans: 1
Date: 24-MAY-2013
Time: 14:48:39
Scale: 6.4981
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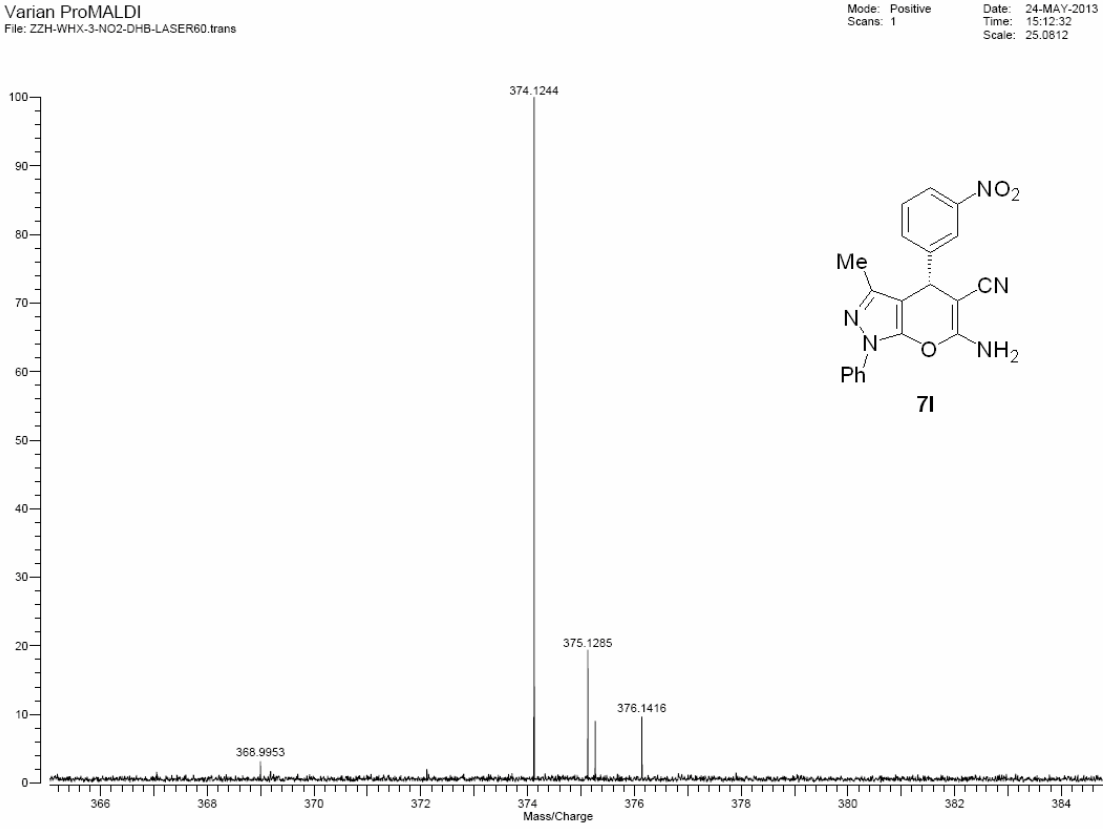
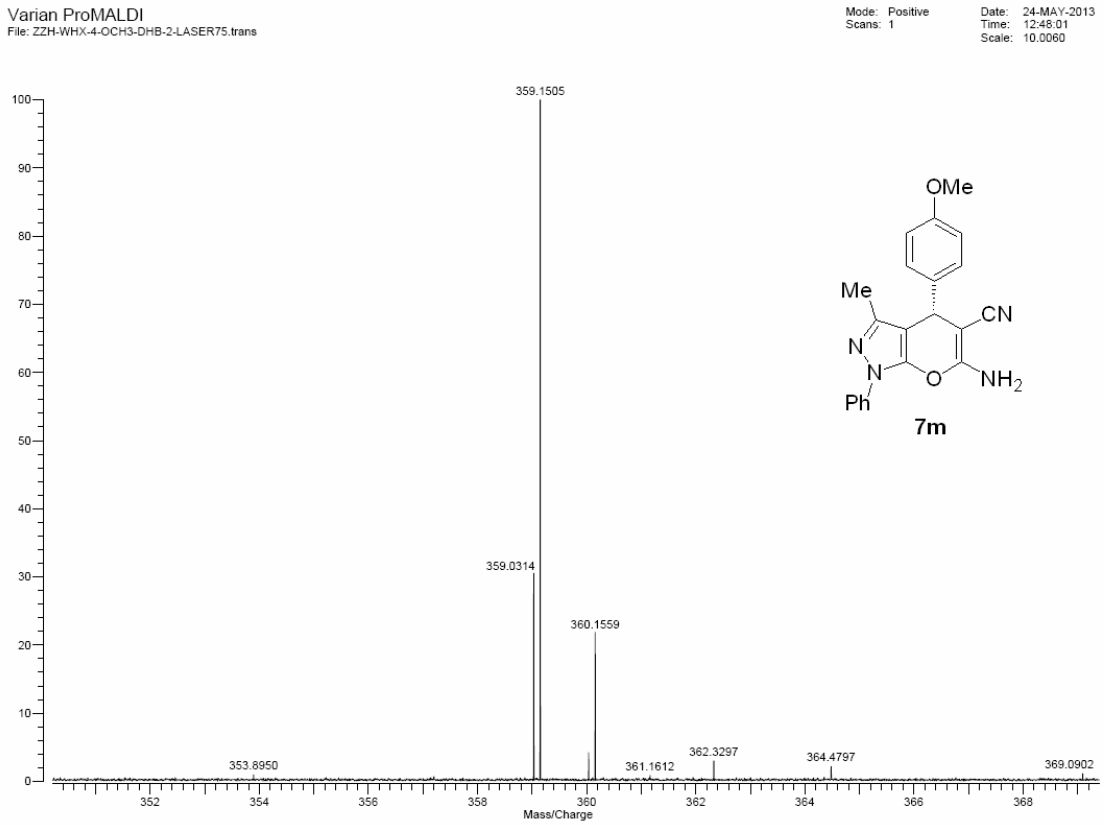
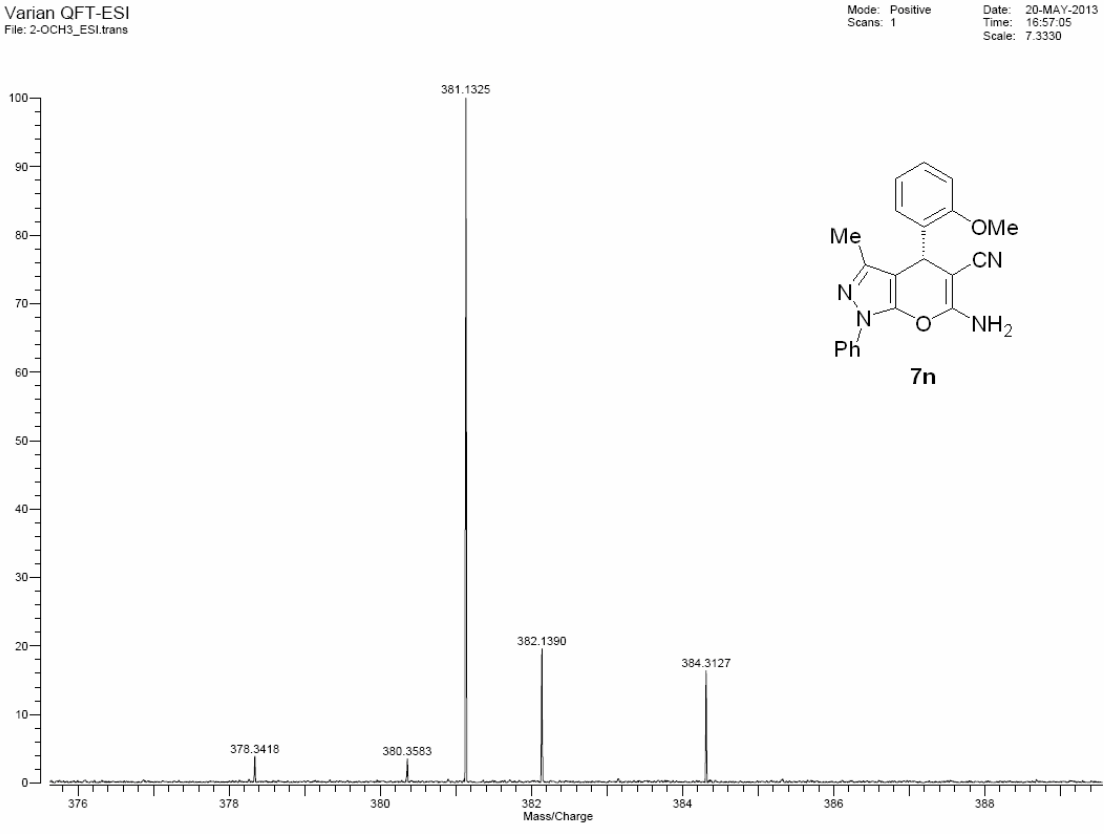
398.1334
404.0931
Mass/Charge
CF3
Me
CN
N
N
O
NH2
Ph

7k


Varian ProMALDI
File: ZZH-WHX-3-NO2-DHB-LASER60.trans
Mode: Positive
Scans: 1
Date: 24-MAY-2013
Time: 15:12:32
Scale: 25.0812
374.1244
375.1285
376.1416
368.9953
Mass/Charge
NO2
Me
CN
N
N
O
NH2
Ph

7l


Varian ProMALDI
File: ZZH-WHX-4-OCH3-DHB-2-LASER75.trans
Mode: Positive
Scans: 1
Date: 24-MAY-2013
Time: 12:48:01
Scale: 10.0060
359.1505
359.0314
360.1559
353.8950
361.1612
362.3297
364.4797
369.0902
Mass/Charge
OMe
Me
CN
N
N
O
NH2
Ph
7m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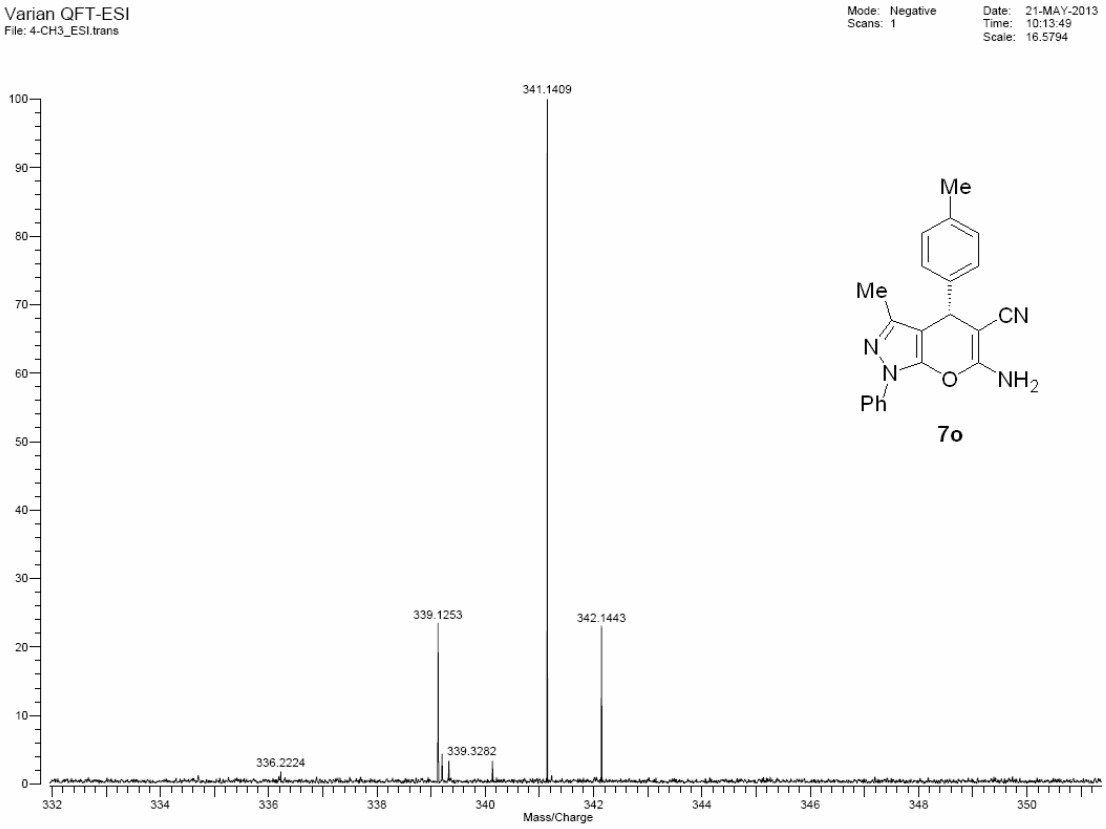
File: 2-OCH3_ESI.trans
Mode: Positive
Scans: 1
Date: 20-MAY-2013
Time: 16:57:05
Scale: 7.3330
381.1325
382.1390
384.3127
378.3418
380.3583
Mass/Charge
OMe
Me
CN
N
N
O
NH2
Ph
7n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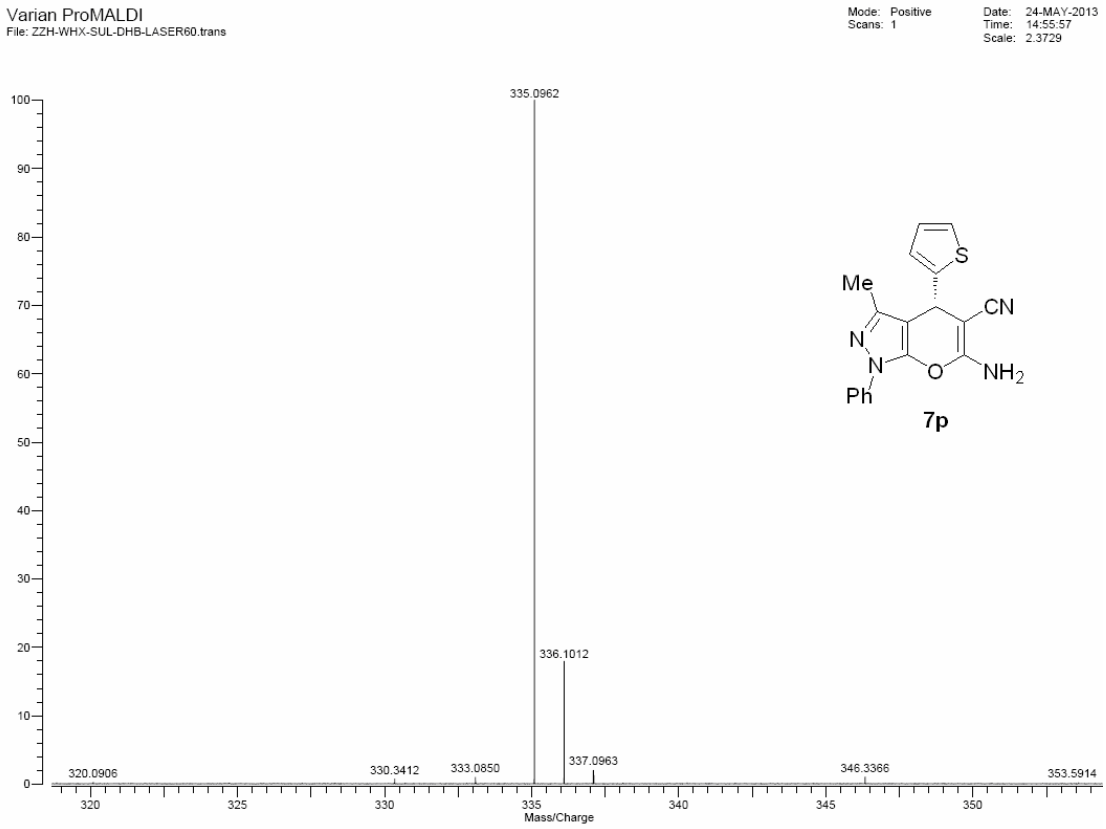
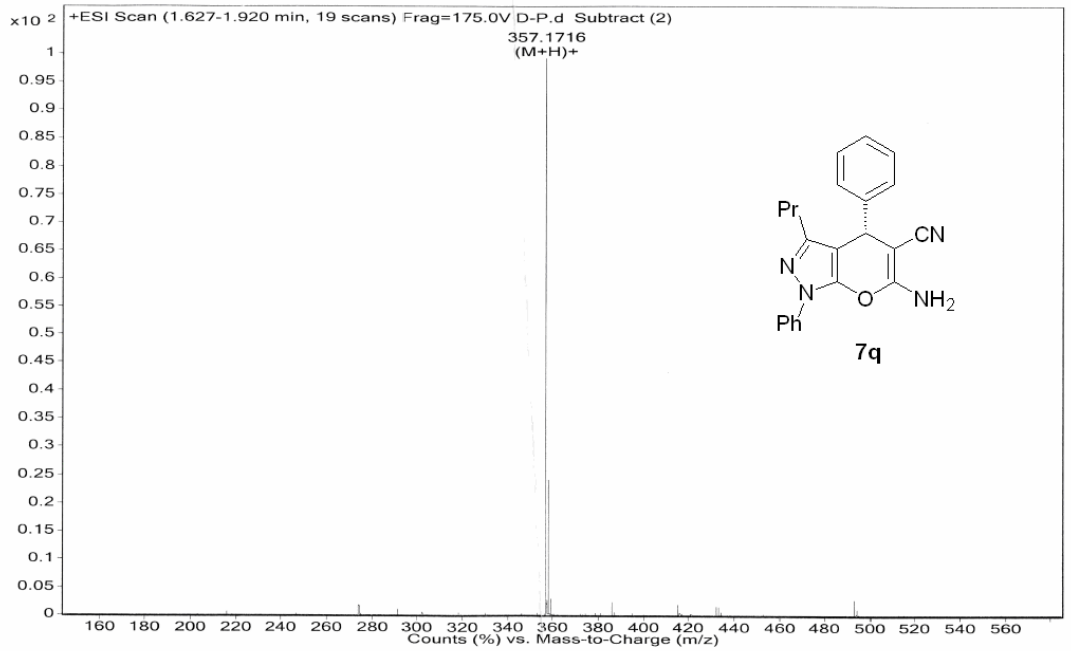
File: 4-CH3_ESI.trans
Mode: Negative
Scans: 1
Date: 21-MAY-2013
Time: 10:13:49
Scale: 16.5794
341.1409
339.1253
342.1443
336.2224
339.3282
Mass/Charge
Me
Me
CN
N
N
O
NH2
Ph
7o

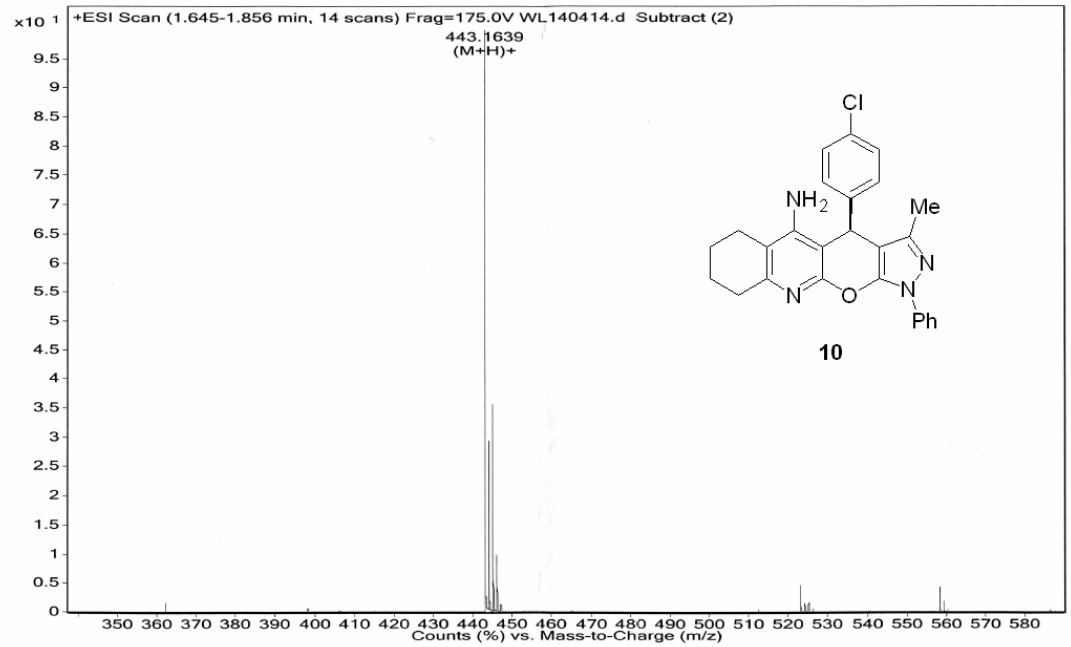

Varian ProMALDI
File: ZZH-WHX-SUL-DHB-LASER60.trans
Mode: Positive
Scans: 1
Date: 24-MAY-2013
Time: 14:55:57
Scale: 2.3729
335.0962
336.1012
320.0906
330.3412
333.0850
337.0963
346.3366
353.5914
Mass/Charge
S
Me
CN
N
N
O
NH2
Ph
7p

Sample Name	lc/ms	**Position**	P1-A3	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	3	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Some Ions Missed
Data Filename	D-P.d	**ACQ Method**	chen-ms.m	**Comment**		**Acquired Time**	6/17/2013 11:34:15 AM



7q

Sample Name	lc/ms	**Position**	P1-A4	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Some Ions Missed
Data Filename	WL140414.d	**ACQ Method**	chen-ms.m	**Comment**		**Acquired Time**	4/17/2015 9:46:56 AM



10

3. Copies of HPLC data

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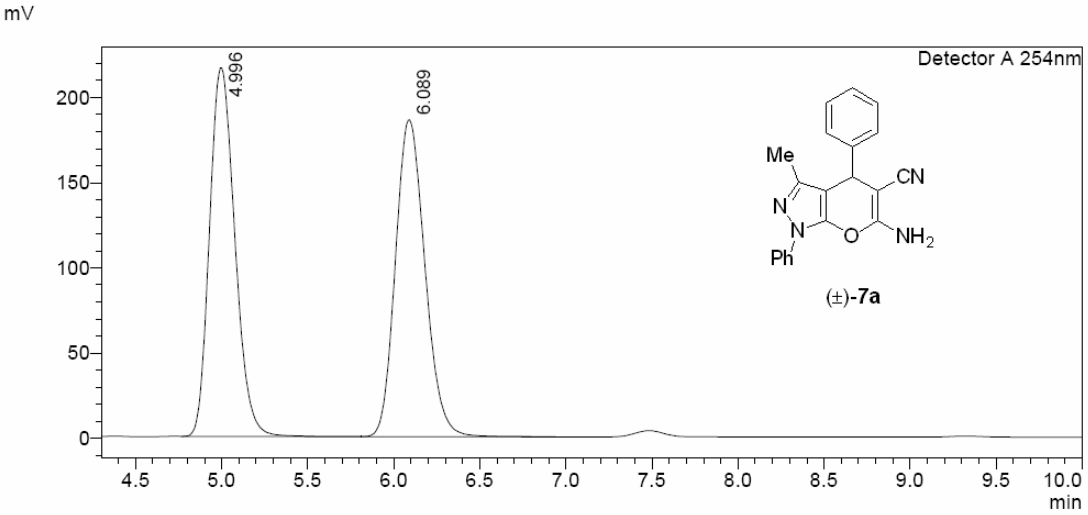

<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Height%	Area%
1	4.996	2218565	216367	53.760	49.977
2	6.089	2220565	186101	46.240	50.023
Total		4439129	402468	100.000	100.000

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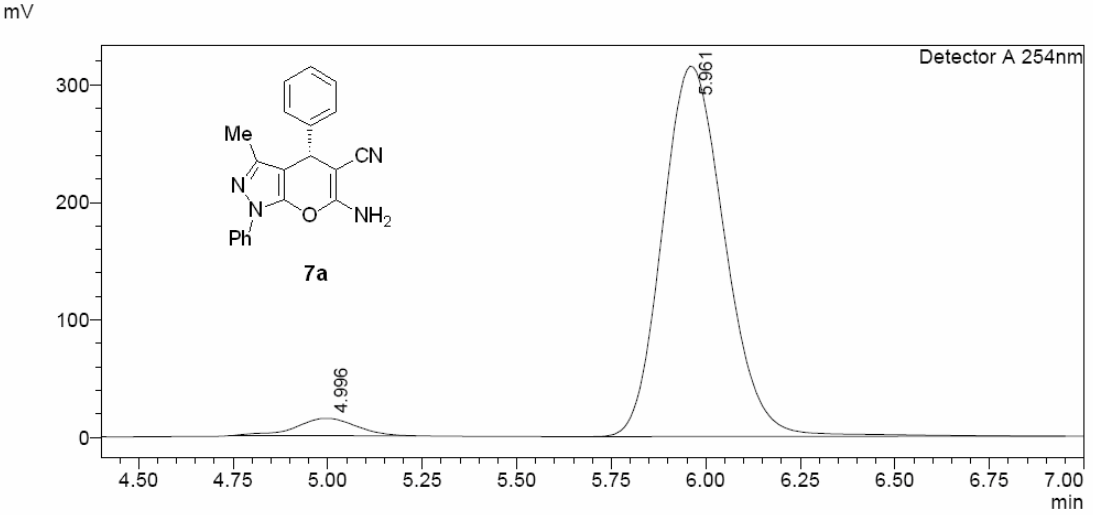

<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Height%	Area%
1	4.996	162201	14682	4.456	4.286
2	5.961	3622606	314788	95.544	95.714
Total		3784807	329470	100.000	100.000

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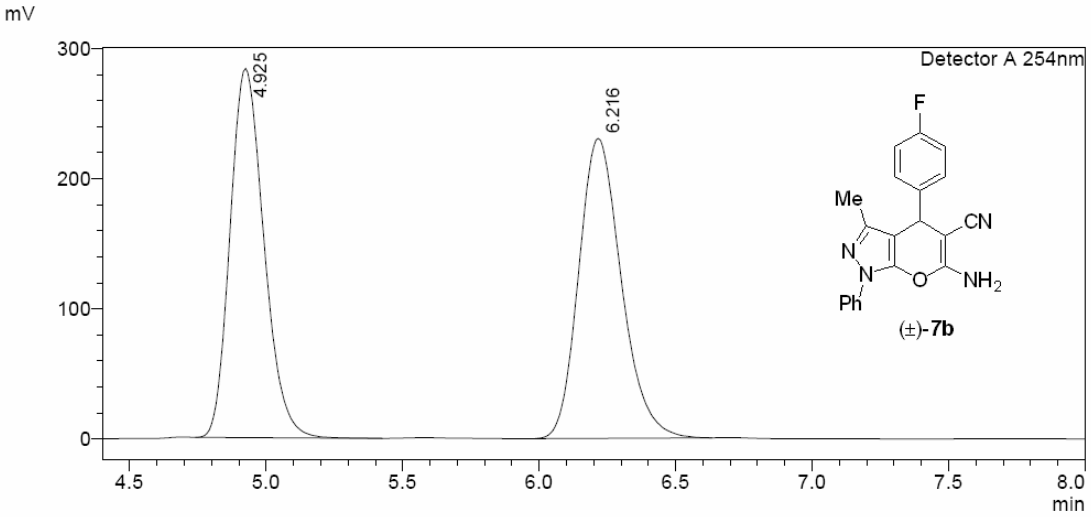

<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Height%	Area%
1	4.925	2446516	283771	55.165	49.406
2	6.216	2505358	230637	44.835	50.594
Total		4951874	514408	100.000	100.000

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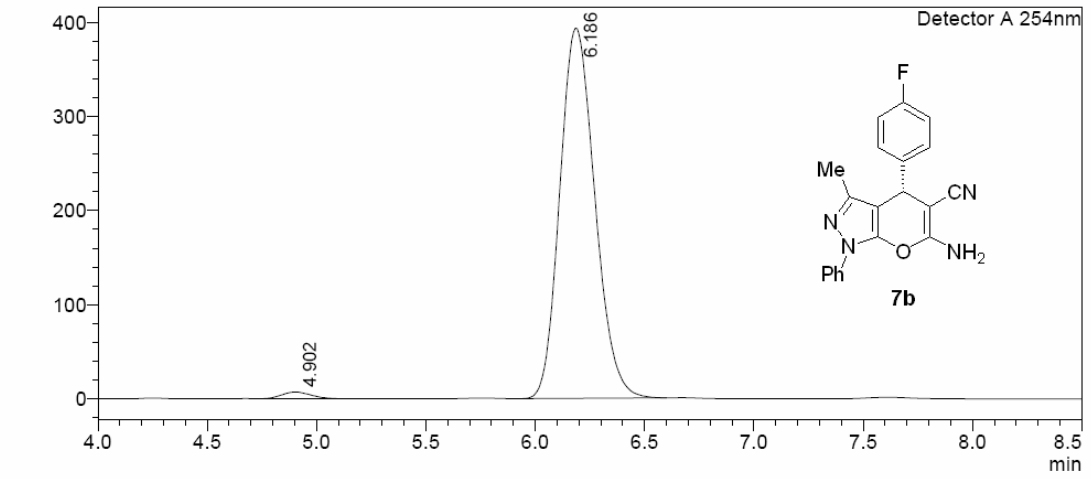

<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Height%	Area%
1	4.902	64568	7013	1.751	1.450
2	6.186	4388776	393515	98.249	98.550
Total		4453343	400529	100.000	100.000

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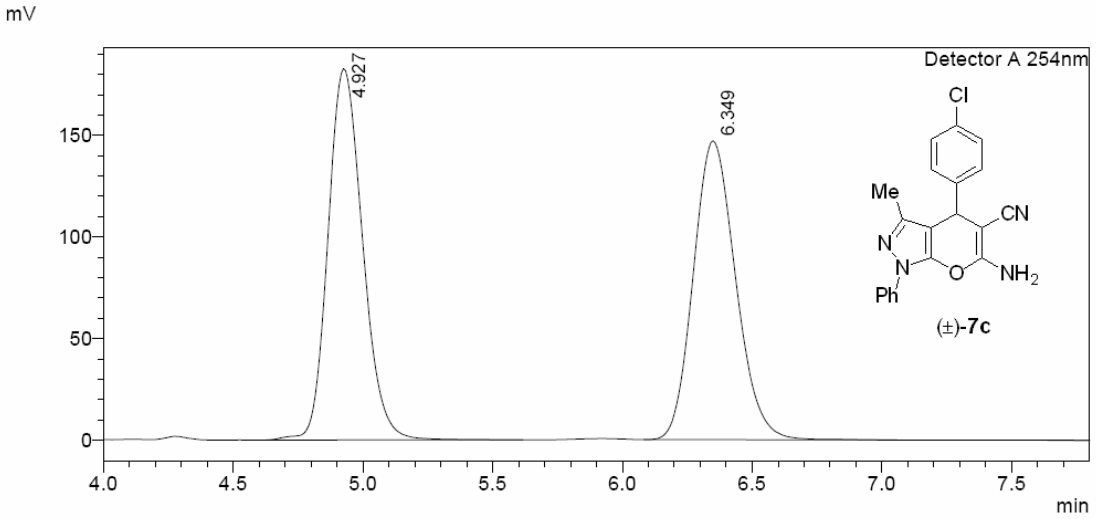

<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Conc.	Area/Height	Height%	Area%
1	4.927	50.419	9.289	55.405	50.419
2	6.349	49.581	11.349	44.595	49.581
Total				100.000	100.000

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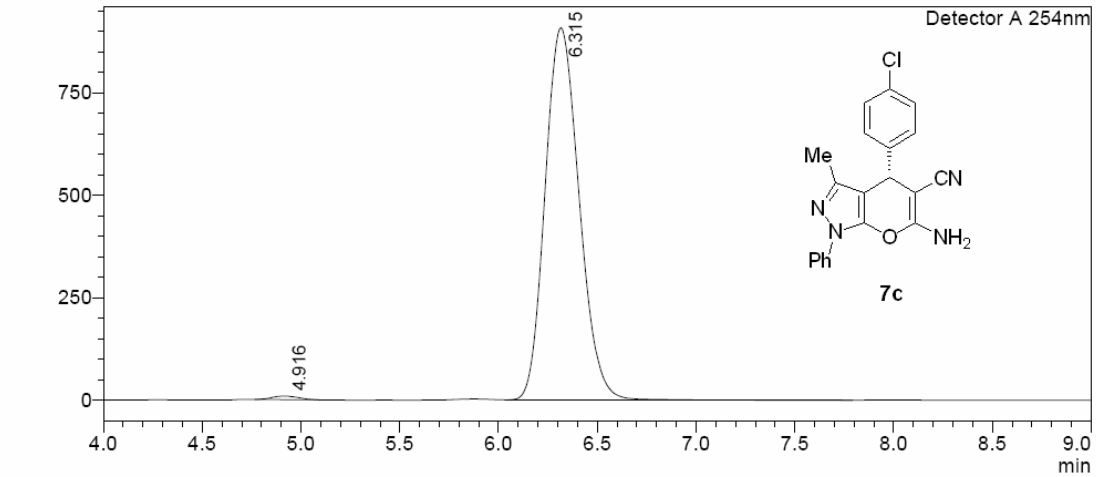


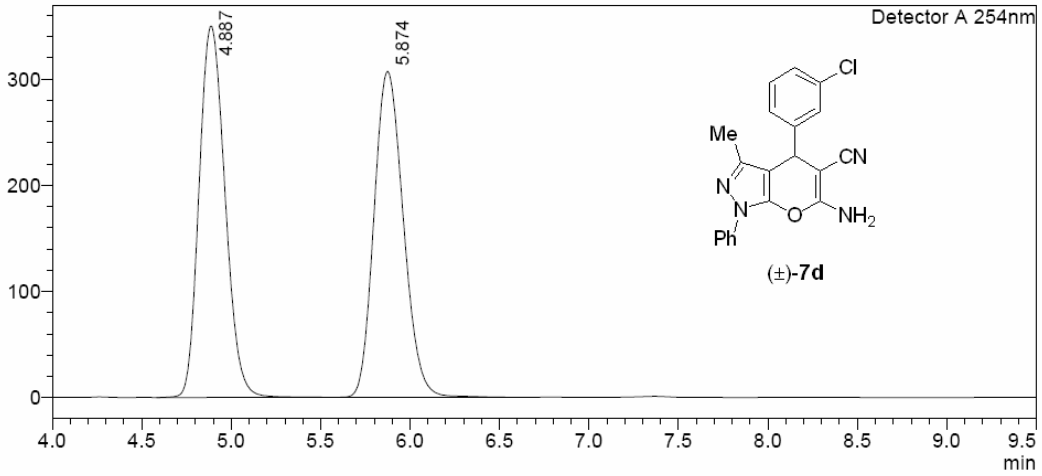
<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Height%	Area%
1	4.916	79824	8600	0.728	0.938	0.728
2	6.315	10880117	907991	99.272	99.062	99.272
Total		10959941	916591		100.000	100.000

<Chromatogram>

mV



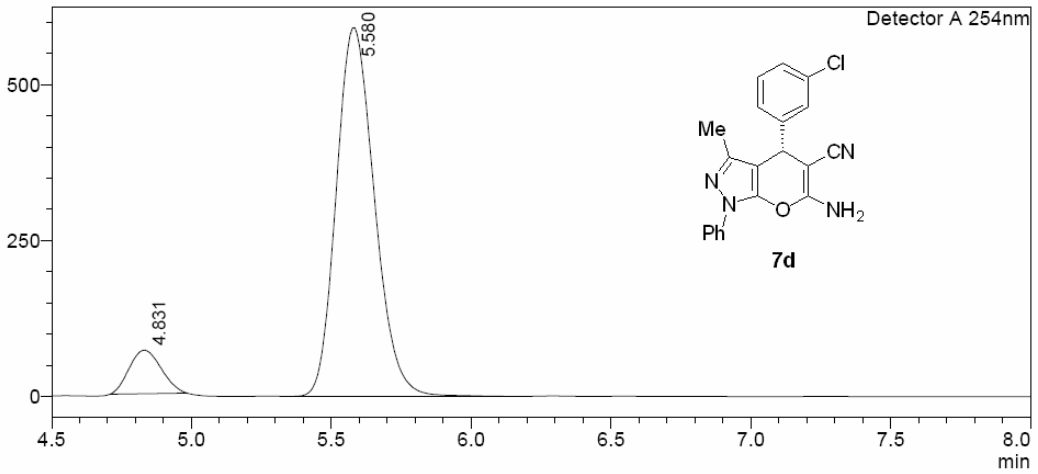
<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Height%	Area%
1	4.887	3523325	349196	53.220	50.186
2	5.874	3497198	306946	46.780	49.814
Total		7020523	656142	100.000	100.000

<Chromatogram>

mV



<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Height%	Area%
1	4.831	555600	69806	10.571	9.012
2	5.580	5609729	590520	89.429	90.988
Total		6165328	660325	100.000	100.000

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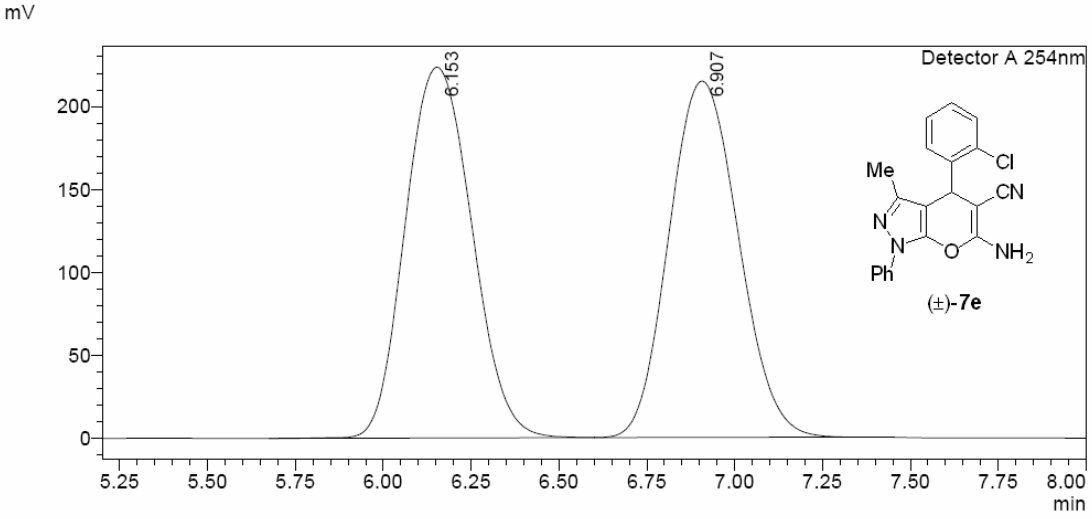
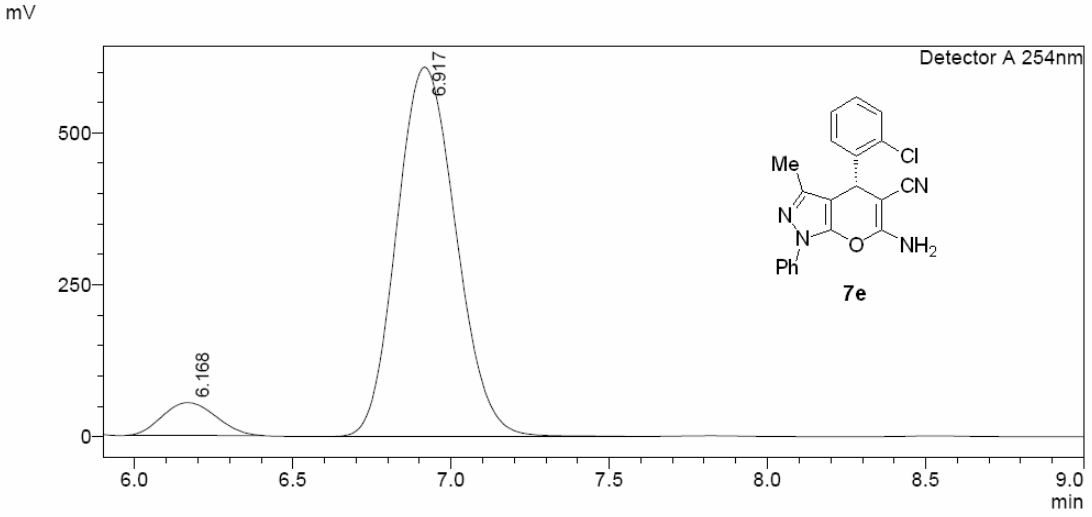


<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Height%	Area%
1	6.153	2945122	223426	50.988	49.921
2	6.907	2954392	214767	49.012	50.079
Total		5899514	438193	100.000	100.000

<Chromatogram>



<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Height%	Area%
1	6.168	638818	54120	8.177	7.460
2	6.917	7924180	607766	91.823	92.540
Total		8562998	661886	100.000	100.000

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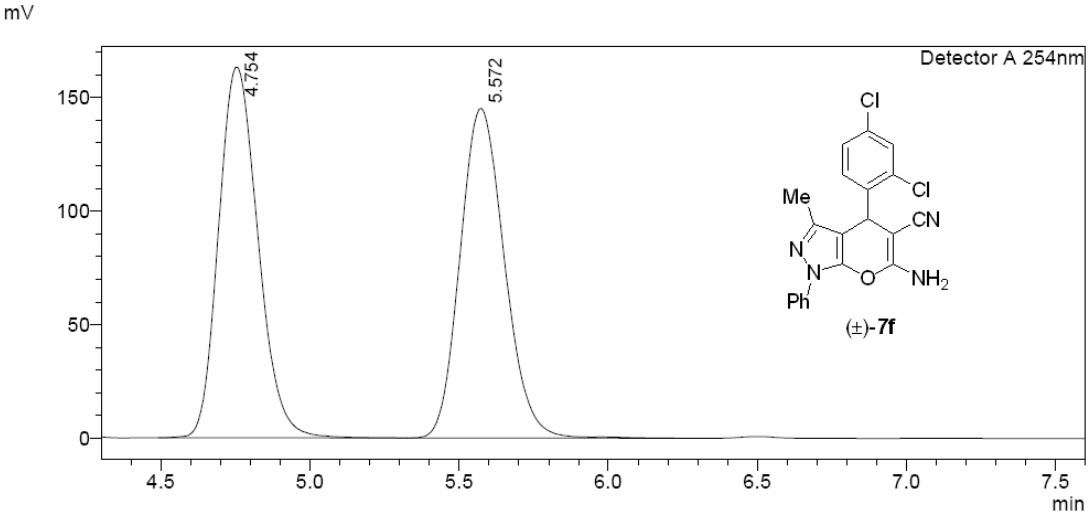

<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Height%	Area%
1	4.754	1503065	162993	52.905	50.044
2	5.572	1500431	145095	47.095	49.956
Total		3003497	308089	100.000	100.000

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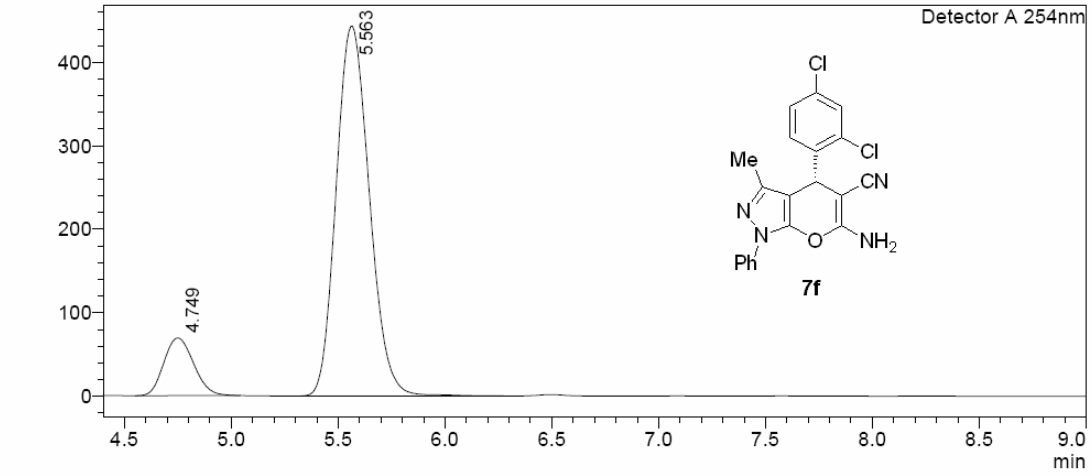

<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Height%	Area%
1	4.749	669937	69064	13.489	12.268
2	5.563	4790785	442925	86.511	87.732
Total		5460722	511990	100.000	100.000

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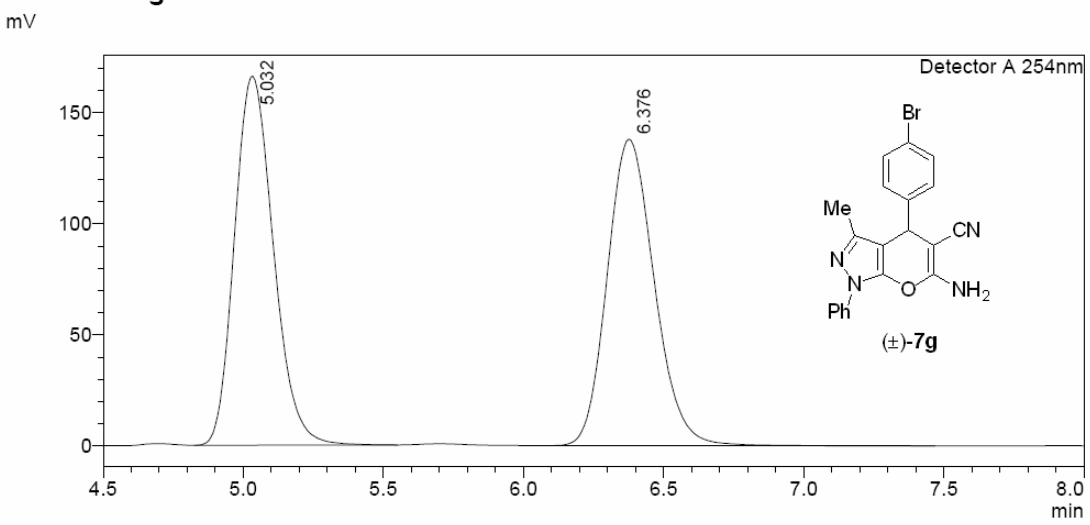
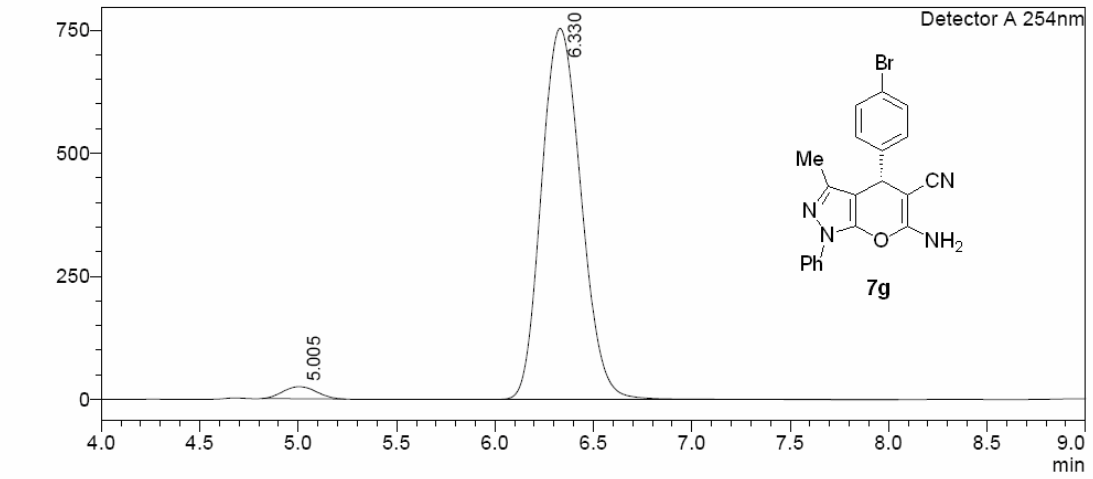


<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Height%	Area%
1	5.032	1606230	166140	54.632	49.893
2	6.376	1613117	137969	45.368	50.107
Total		3219346	304109	100.000	100.000

<Chromatogram>

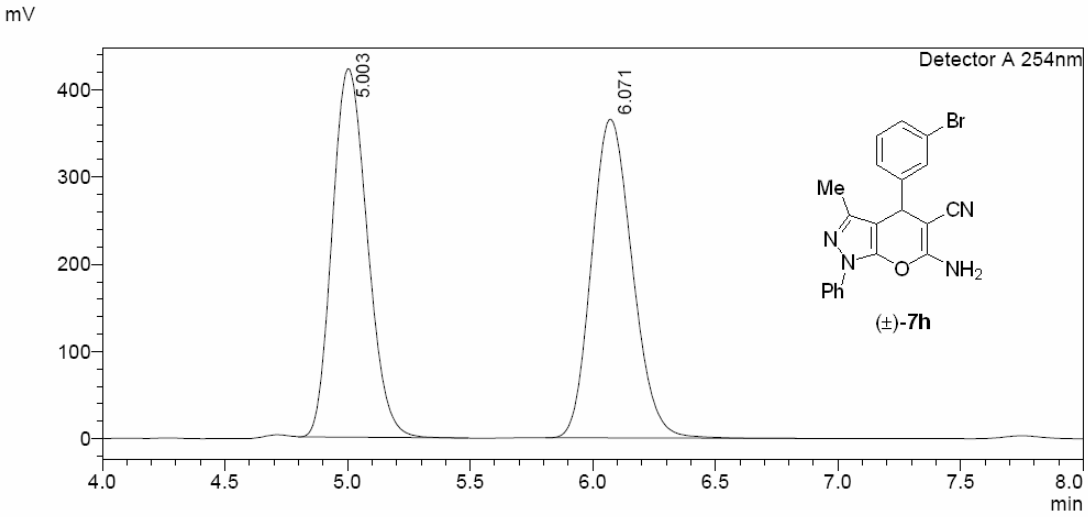


<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Height%	Area%
1	5.005	290322	24500	3.150	2.676
2	6.330	10559422	753205	96.850	97.324
Total		10849744	777705	100.000	100.000

<Chromatogram>

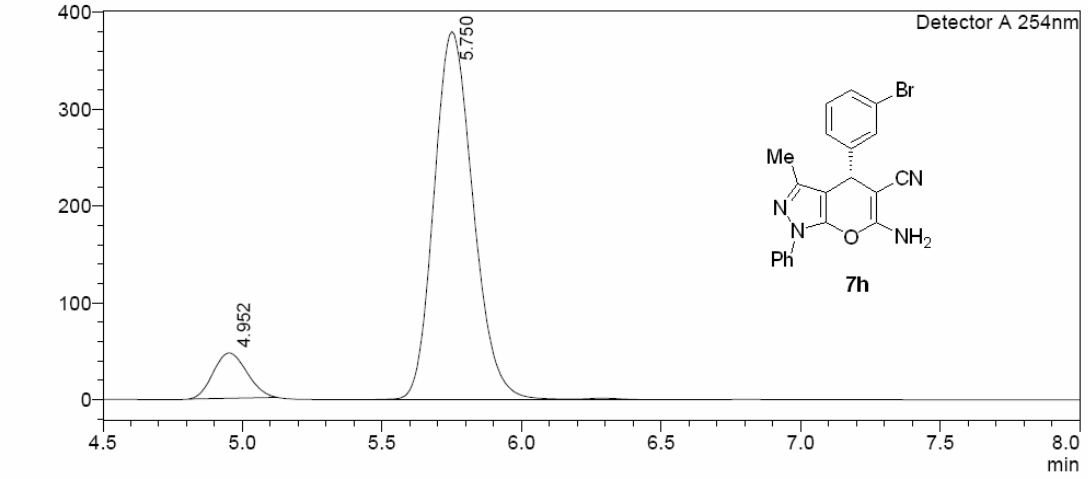


<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Conc.	Height	Area	Height%	Area%
1	5.003	49.840	421993	4199374	53.598	49.840
2	6.071	50.160	365342	4226311	46.402	50.160
Total			787335	8425685	100.000	100.000

<Chromatogram>

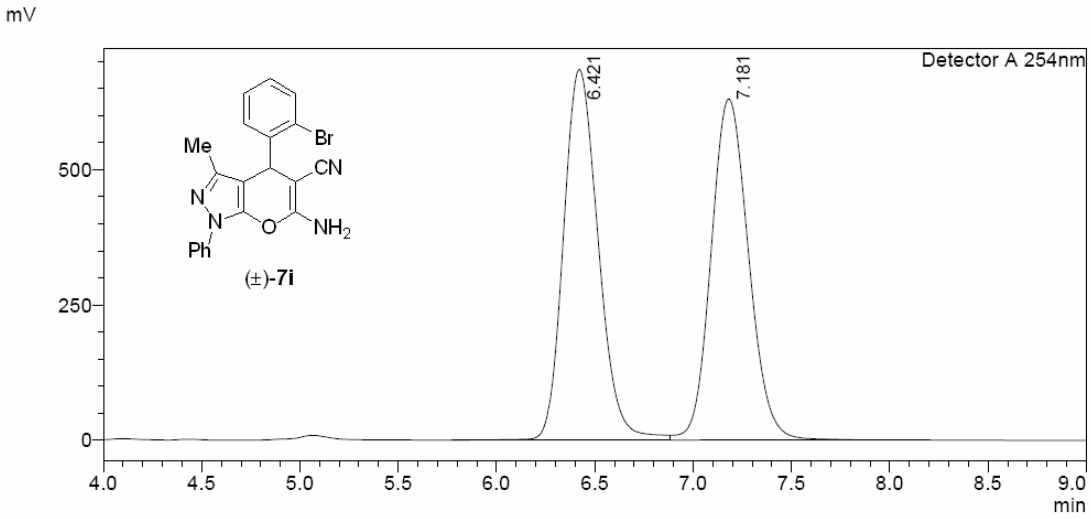


<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Height%	Area%
1	4.952	392318	46735	10.935	9.457
2	5.750	3755985	380648	89.065	90.543
Total		4148303	427383	100.000	100.000

<Chromatogram>

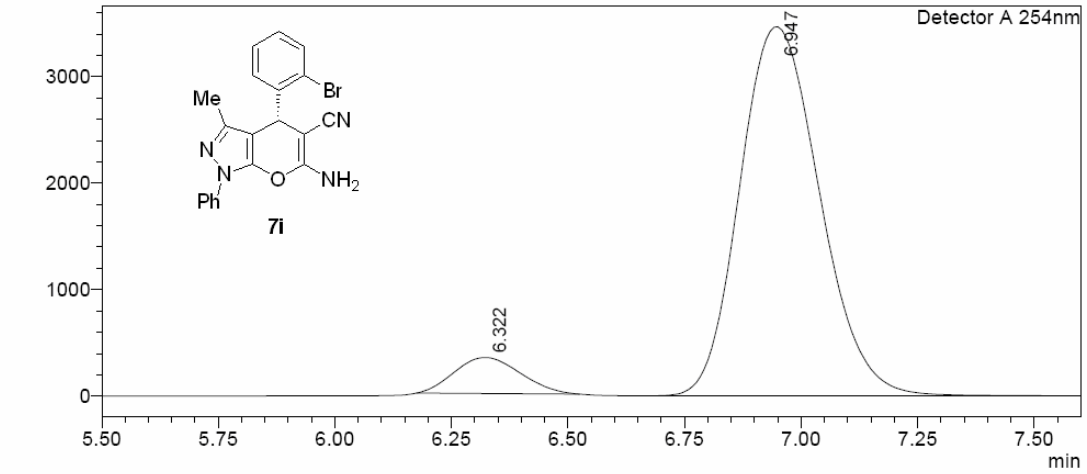


<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Conc.	Height	Area	Height%	Area%
1	6.421	50.217	683980	8421993	52.067	50.217
2	7.181	49.783	629682	8349290	47.933	49.783
Total			1313662	16771283	100.000	100.000

<Chromatogram>

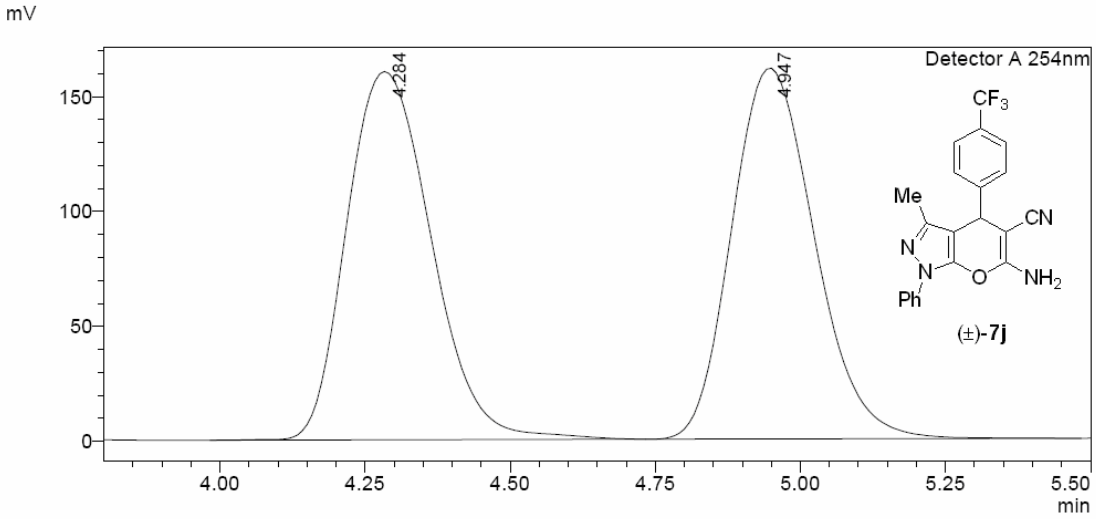


<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Height%	Area%
1	6.322	3352349	338840	8.904	7.519
2	6.947	41235262	3466734	91.096	92.481
Total		44587612	3805574	100.000	100.000

<Chromatogram>

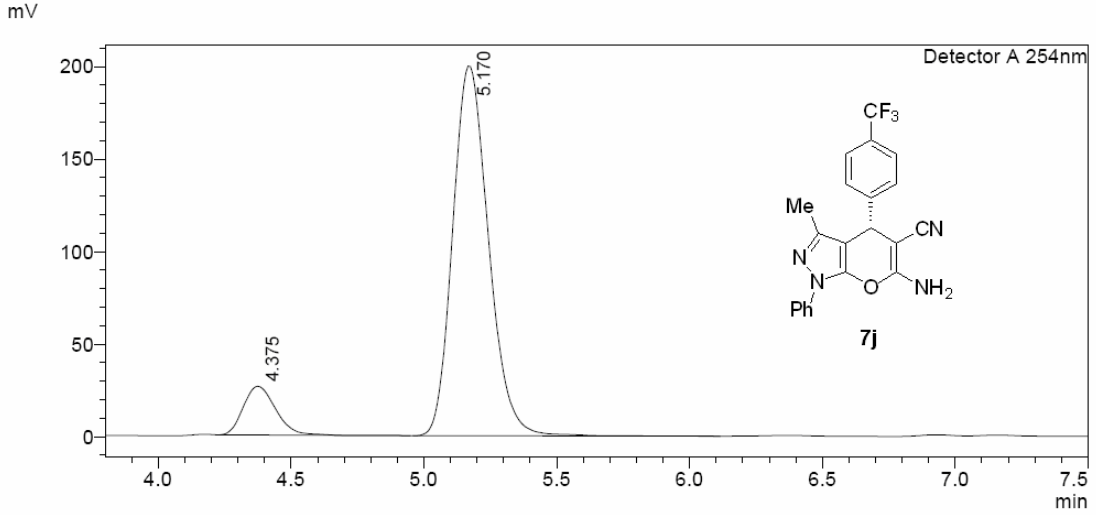


<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Height%	Area%
1	4.284	1625373	160332	49.842	50.316
2	4.947	1604985	161348	50.158	49.684
Total		3230358	321680	100.000	100.000

<Chromatogram>

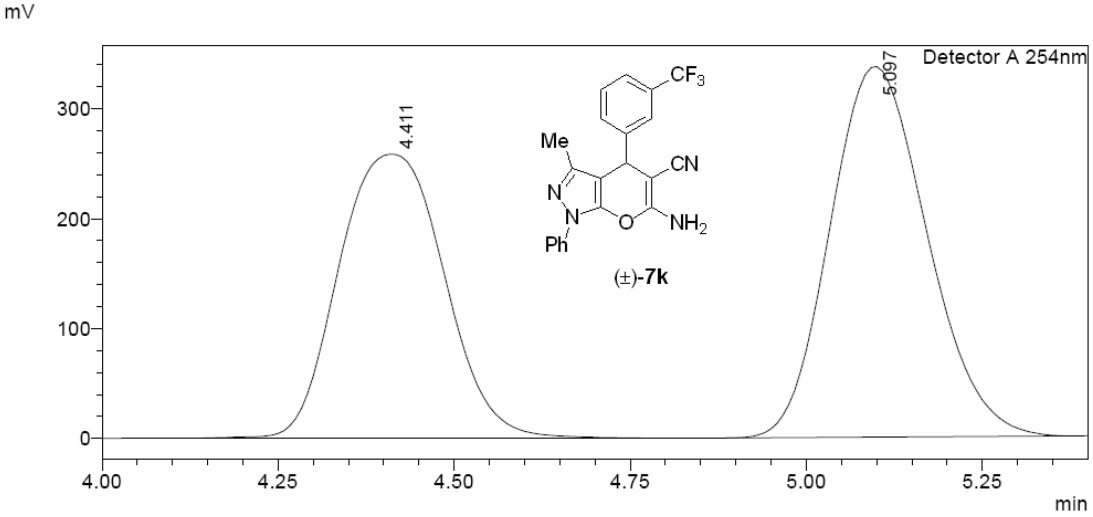


<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	4.375	224324	26274	10.687	11.624
2	5.170	1874779	199762	89.313	88.376
Total		2099103	226036	100.000	100.000

<Chromatogram>

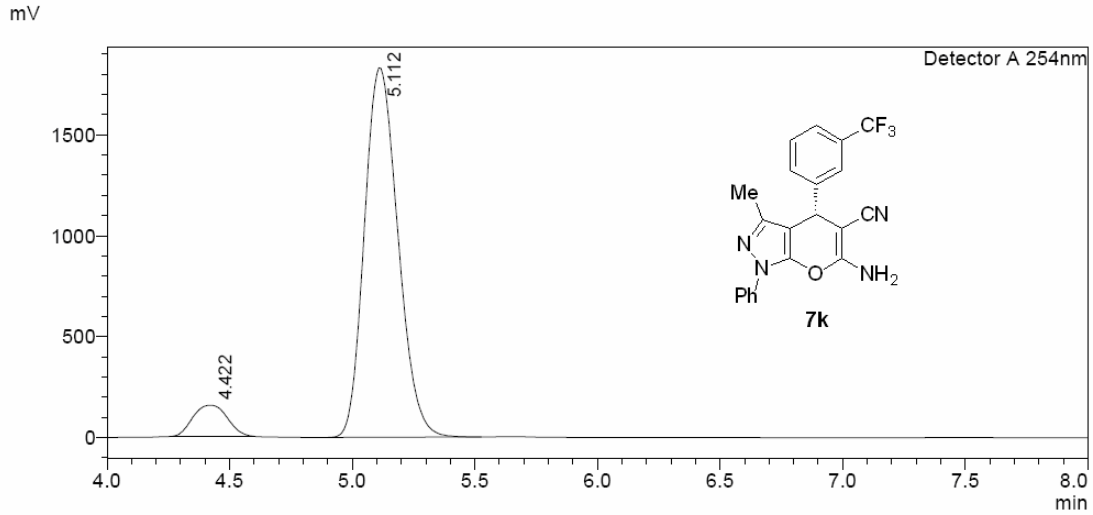


<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Height%	Area%
1	4.411	2687069	258525	43.379	45.410
2	5.097	3230289	337447	56.621	54.590
Total		5917357	595972	100.000	100.000

<Chromatogram>

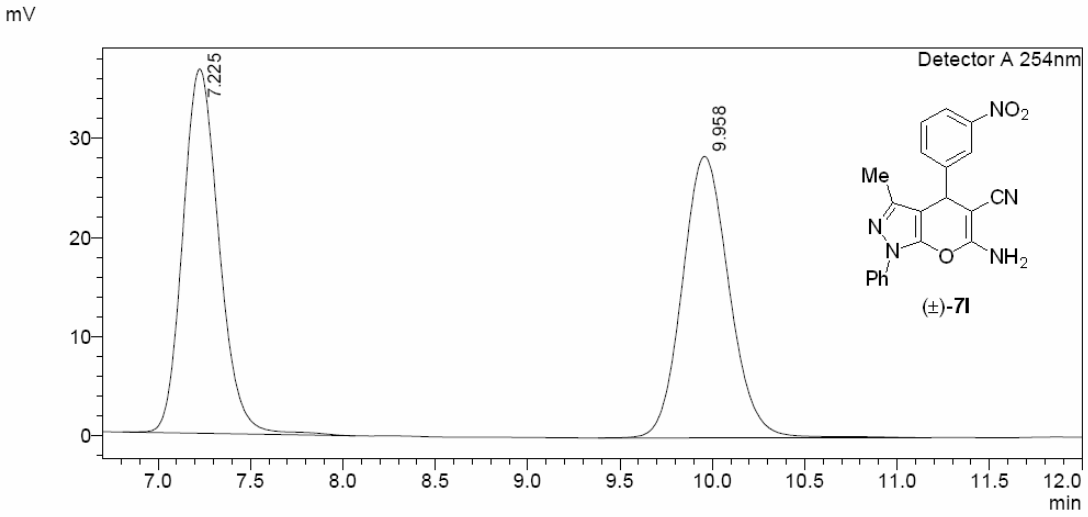


<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Height%	Area%
1	4.422	1495302	154036	7.764	7.887
2	5.112	17462984	1829863	92.236	92.113
Total		18958286	1983899	100.000	100.000

<Chromatogram>

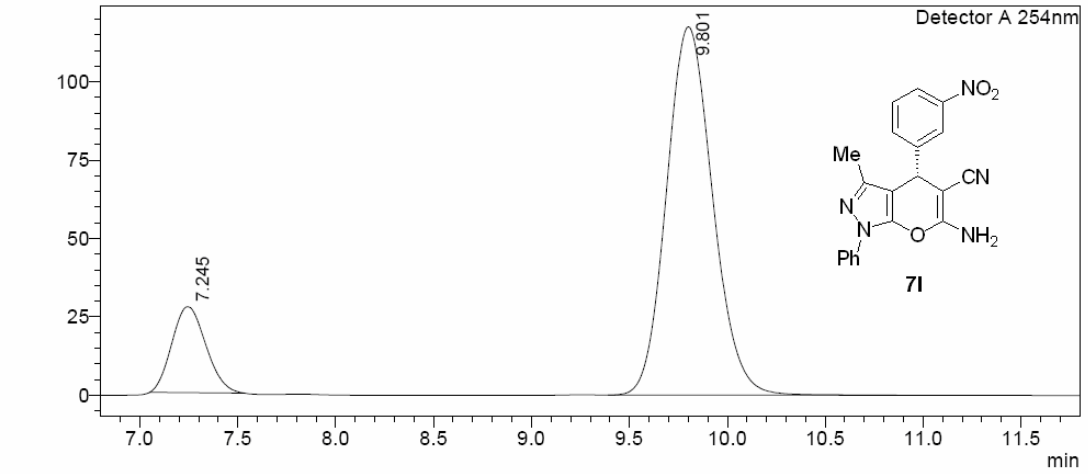


<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Height%	Area%
1	7.225	501370	36734	56.427	50.000
2	9.958	501364	28366	43.573	50.000
Total		1002734	65100	100.000	100.000

<Chromatogram>

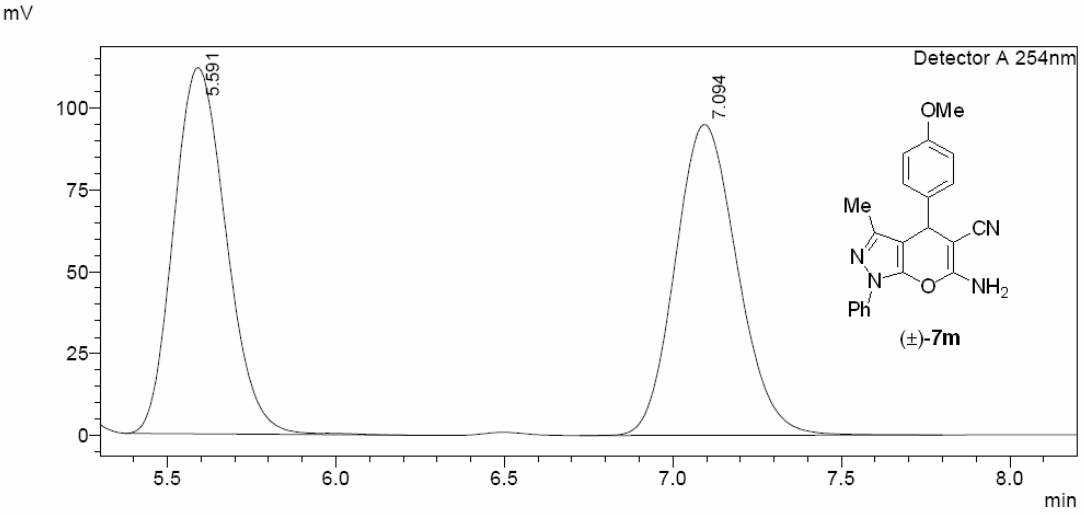


<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Height%	Area%
1	7.245	331265	27400	18.913	14.637
2	9.801	1931906	117473	81.087	85.363
Total		2263171	144873	100.000	100.000

<Chromatogram>

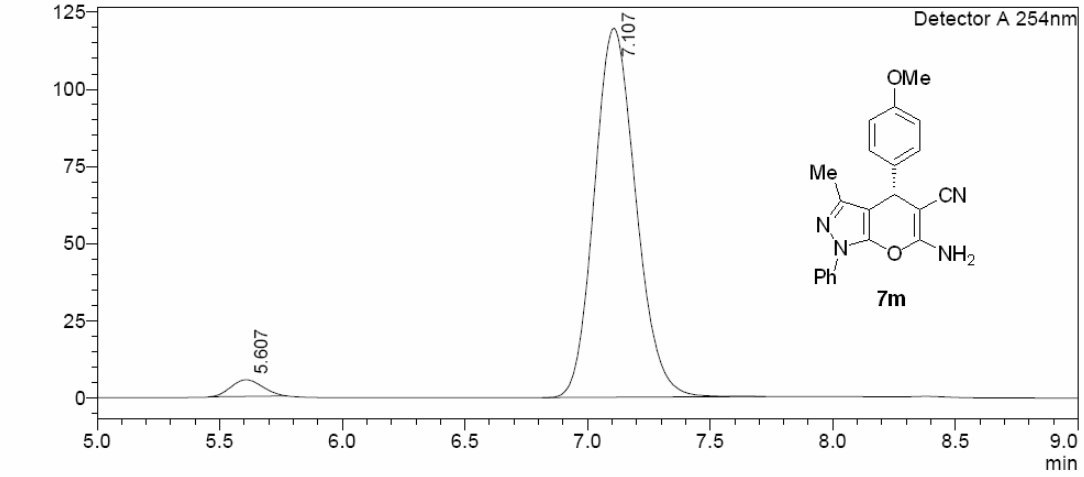


<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Height%	Area%
1	5.591	1214730	111866	54.100	49.945
2	7.094	1217400	94911	45.900	50.055
Total		2432130	206777	100.000	100.000

<Chromatogram>

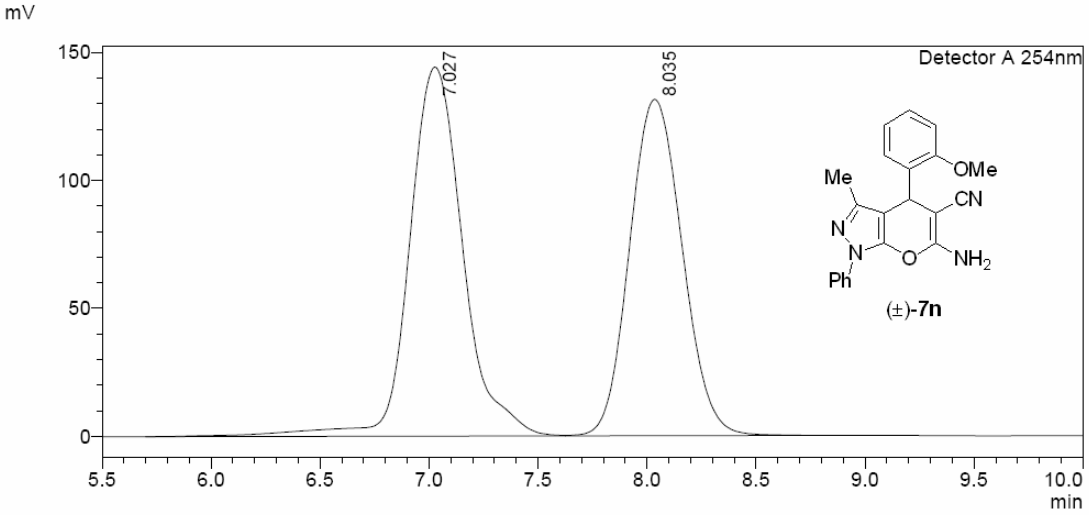


<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Height%	Area%
1	5.607	48480	5425	4.337	3.319
2	7.107	1412055	119664	95.663	96.681
Total		1460535	125088	100.000	100.000

<Chromatogram>

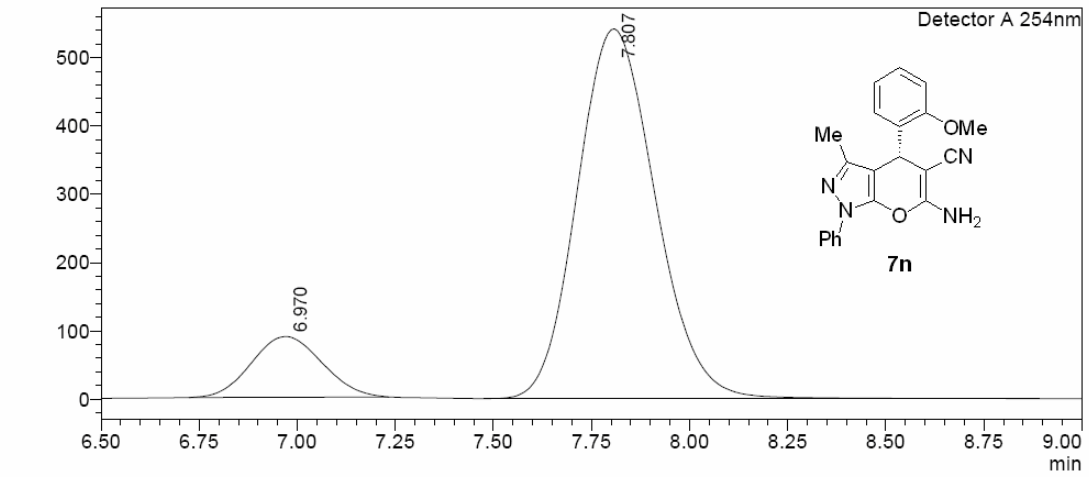


<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Height%	Area%
1	7.027	2455546	144130	52.312	52.601
2	8.035	2212680	131388	47.688	47.399
Total		4668226	275518	100.000	100.000

<Chromatogram>



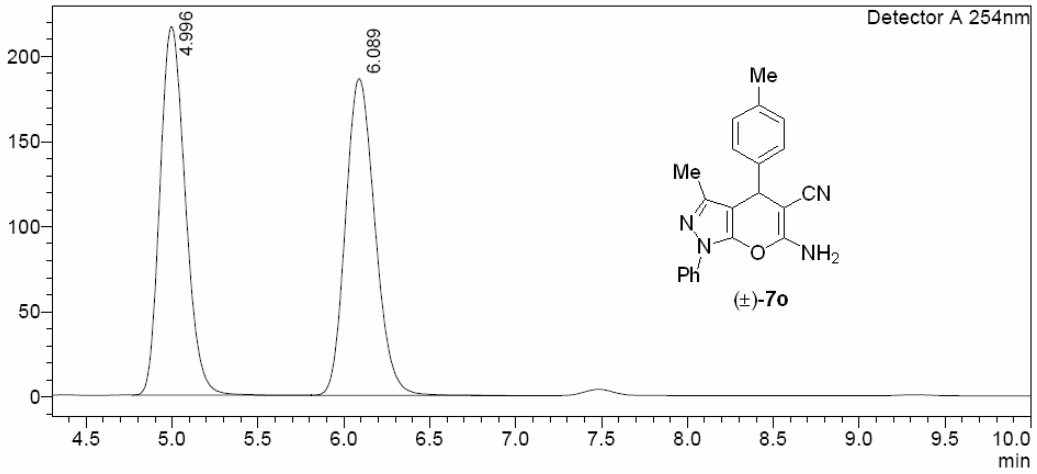
<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Height%	Area%
1	6.970	1108892	88691	14.077	12.882
2	7.807	7499003	541337	85.923	87.118
Total		8607895	630028	100.000	100.000

<Chromatogram>

mV



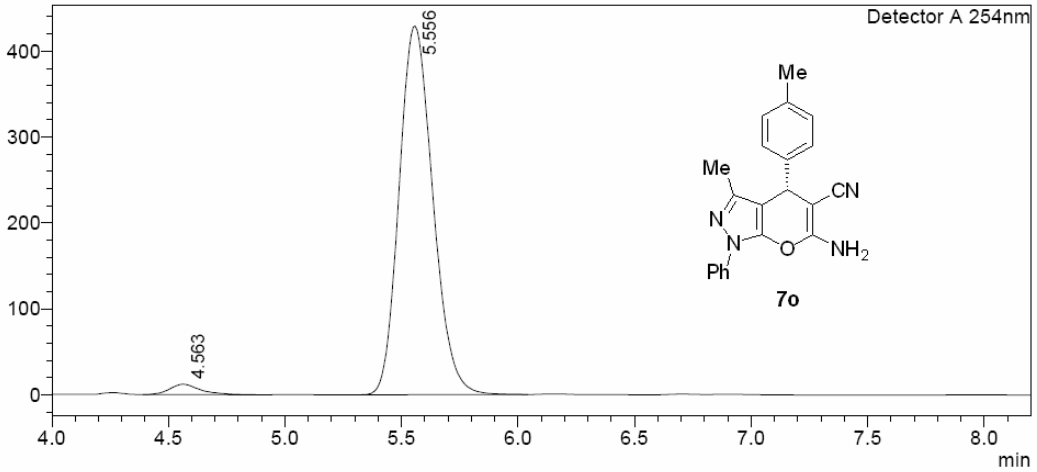
<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Height%	Area%
1	4.996	2218565	216367	53.760	49.977
2	6.089	2220565	186101	46.240	50.023
Total		4439129	402468	100.000	100.000

<Chromatogram>

mV

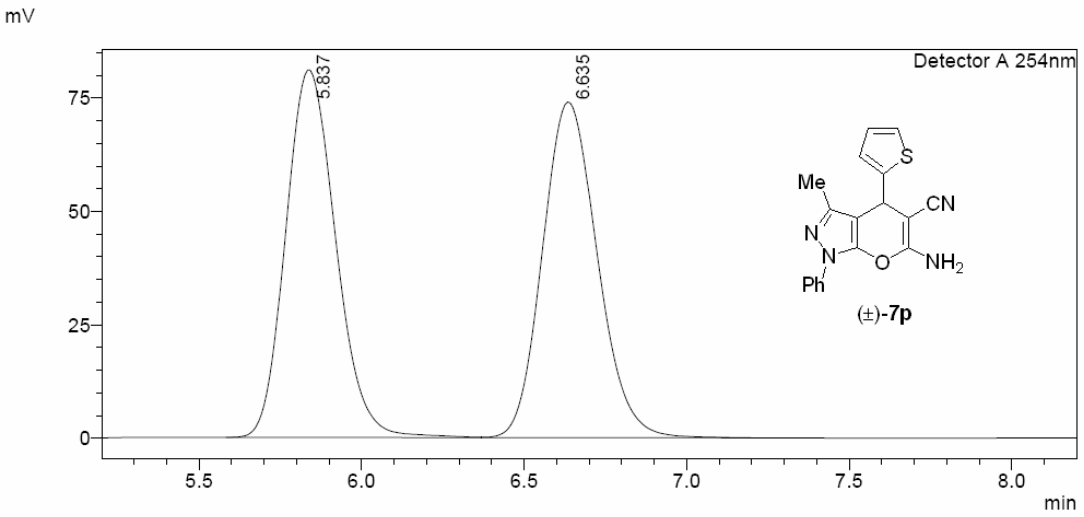


<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Height%	Area%
1	4.563	110469	11950	2.710	2.493
2	5.556	4321216	429080	97.290	97.507
Total		4431684	441030	100.000	100.000

<Chromatogram>



<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Height%	Area%
1	5.837	868317	80923	52.238	49.957
2	6.635	869795	73988	47.762	50.043
Total		1738112	154911	100.000	100.000

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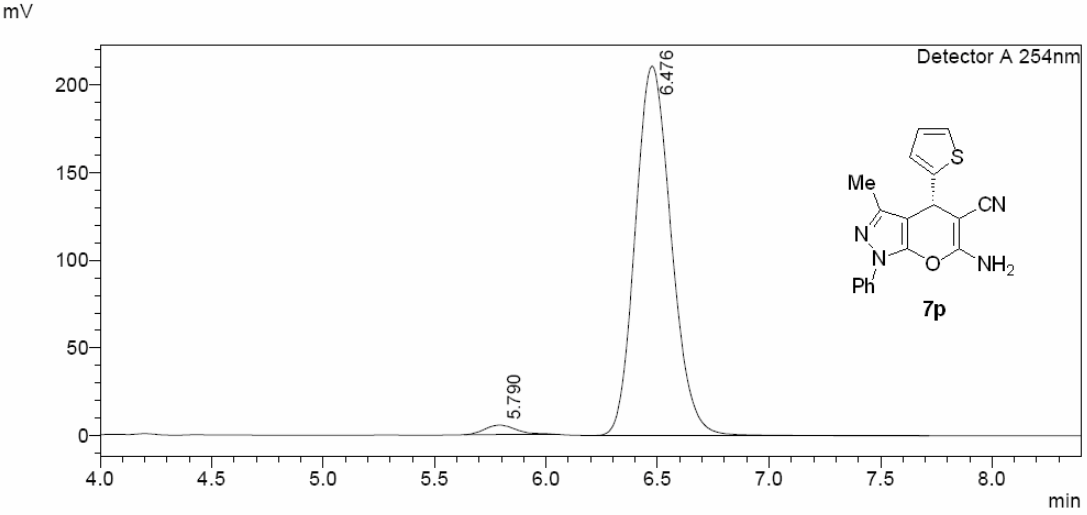
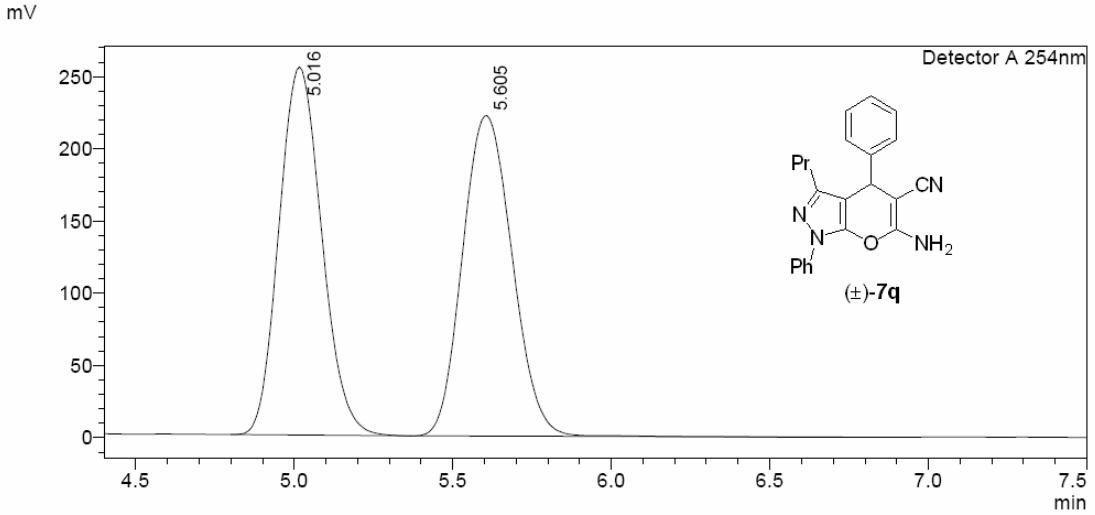


<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Height%	Area%
1	5.790	53587	5350	2.477	2.215
2	6.476	2366003	210605	97.523	97.785
Total		2419590	215954	100.000	100.000

<Chromatogram>



<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Height%	Area%
1	5.016	2389151	254873	53.460	49.709
2	5.605	2417125	221879	46.540	50.291
Total		4806276	476752	100.000	100.000

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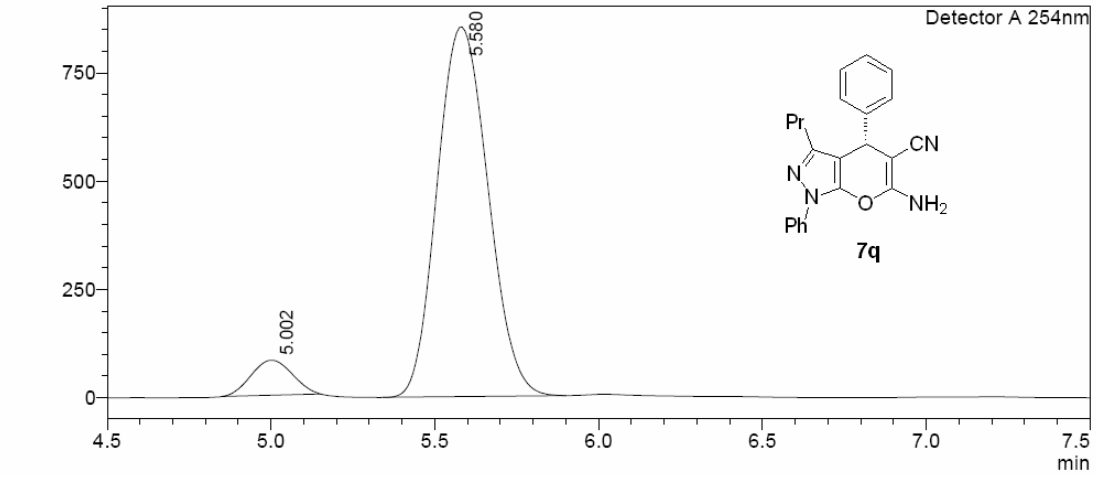

<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Height%	Area%
1	5.002	707003	80796	8.647	7.111
2	5.580	9235767	853560	91.353	92.889
Total		9942770	934355	100.000	100.000

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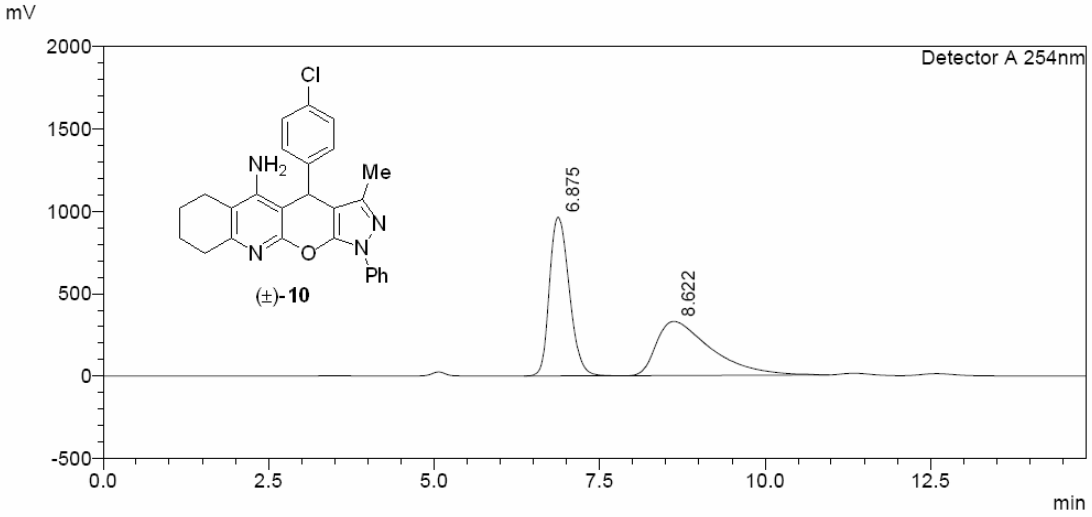

<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Height%	Area%
1	6.875	20086836	962995	51.547	74.530	51.547
2	8.622	18881130	329093	48.453	25.470	48.453
Total		38967966	1292088		100.000	100.000

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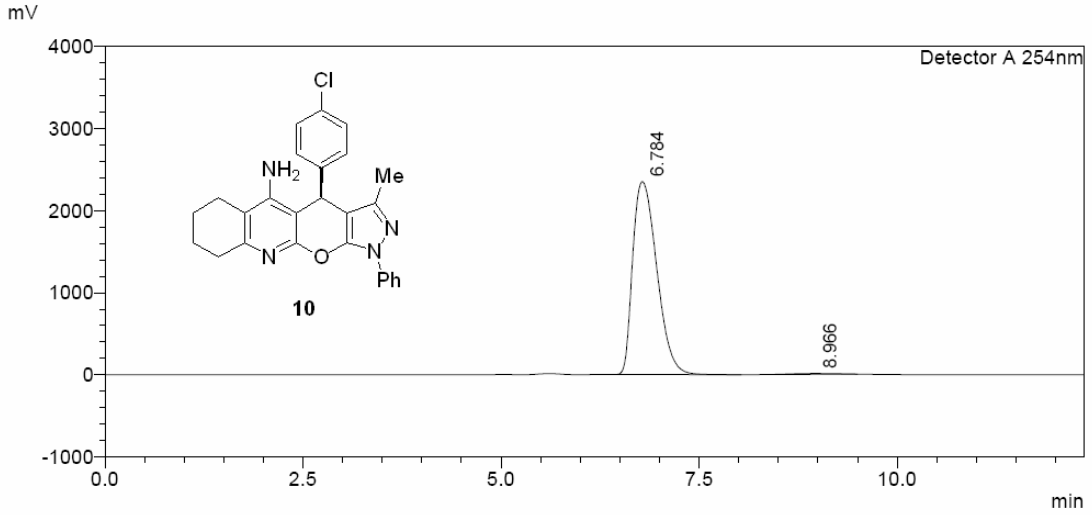

<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Height%	Area%
1	6.784	49790827	2352420	99.329	99.627	99.329
2	8.966	336562	8797	0.671	0.373	0.671
Total		50127389	2361217		100.000	100.000