Supplementary Information for:

Chiral Bifunctional Ferrocenylphosphines Catalyzed the highly Enantioselective [3+2] Cycloaddition Reaction

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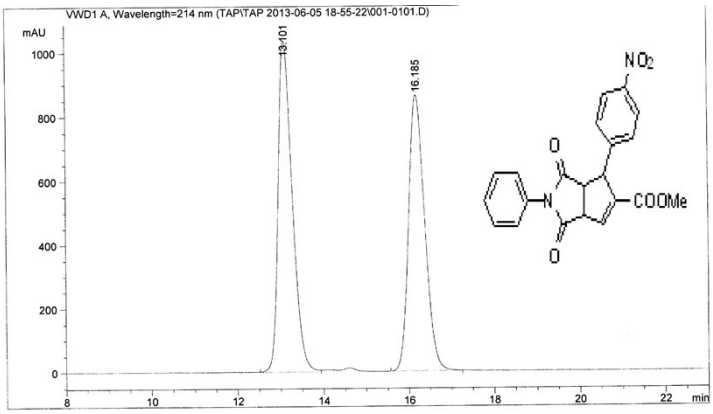
Content

I. HPLC chromatogram of the [3+2] cycloaddition products



Area Percent Report

Sorted By : Signal
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=214 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	13.101	BV	0.3506	2.36655e4	1037.29126	50.8613
2	16.185	BB	0.4110	2.28640e4	863.08838	49.1387
Totals :				4.65295e4	1900.37964	

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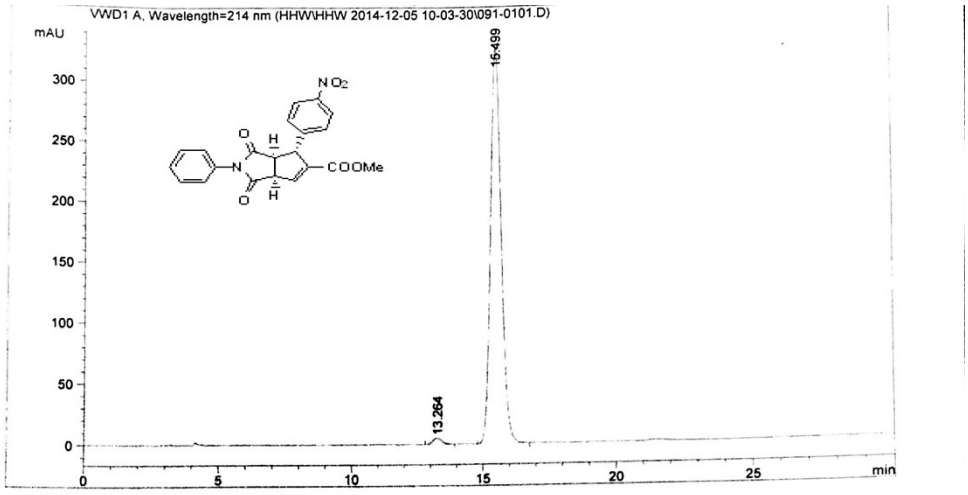

Area Percent Report

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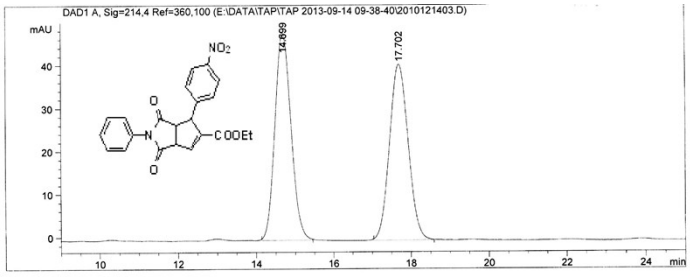
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=214 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	13.264	BB	0.3850	130.31323	5.23612	1.3971
2	15.499	BB	0.4353	9197.28418	327.57498	98.6029
Totals :				9327.59741	332.81110	



Area Percent Report

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Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=214,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.141	BB	0.1301	14.90601	1.60843	0.4914
2	4.716	BV	0.1769	14.26647	1.25253	0.4703
3	4.999	VB	0.1474	11.03178	1.09664	0.3637
4	6.565	BB	0.2076	47.74760	3.32418	1.5741
5	7.396	BB	0.2308	199.64729	13.17628	6.5817
6	14.699	BB	0.4454	1379.59326	48.28056	45.4805
7	17.702	BB	0.5222	1366.18384	40.84678	45.0384
Totals :				3033.37626	109.58540	

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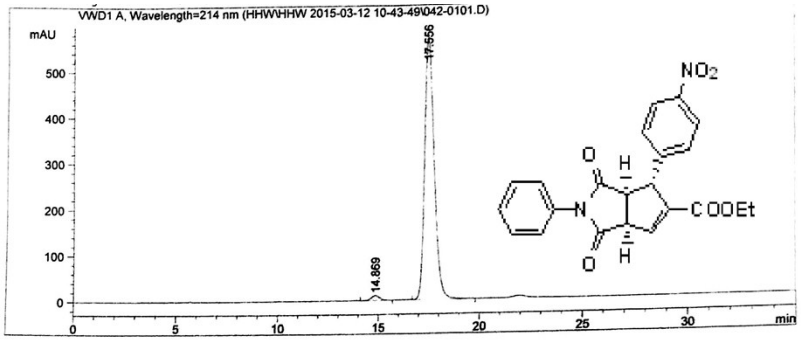

Area Percent Report

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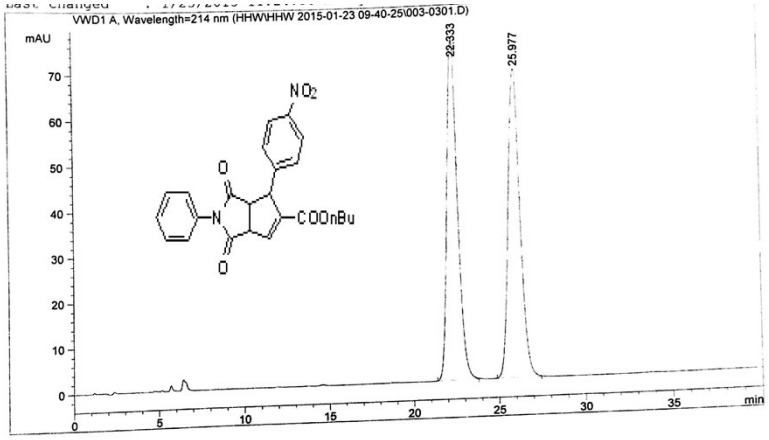
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=214 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	14.869	VB	0.4619	318.10962	10.48002	1.6798
2	17.556	BB	0.5044	1.86188e4	568.45850	98.3202
Totals :				1.89369e4	578.93851	



Area Percent Report

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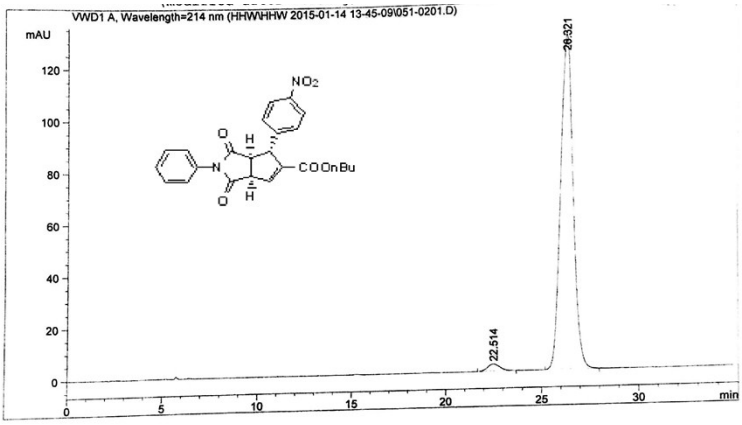
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=214 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	22.333	BB	0.6680	3277.39307	75.72830	50.0216
2	25.977	BB	0.7400	3274.55786	68.63902	49.9784
Totals :				6551.95093	144.36732	



Area Percent Report

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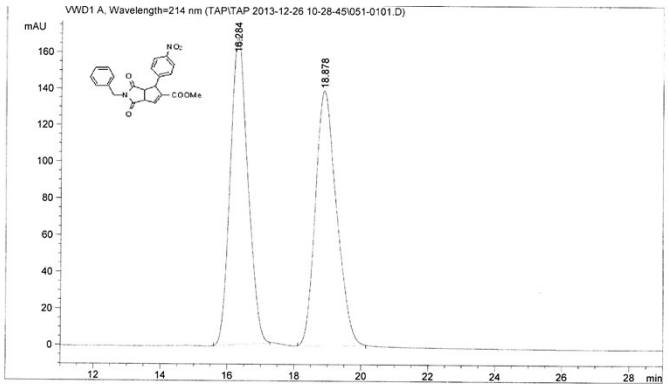
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=214 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	22.514	BB	0.6465	125.06725	2.74520	2.0992
2	26.321	BB	0.6980	5832.67480	129.67511	97.9008



Area Percent Report

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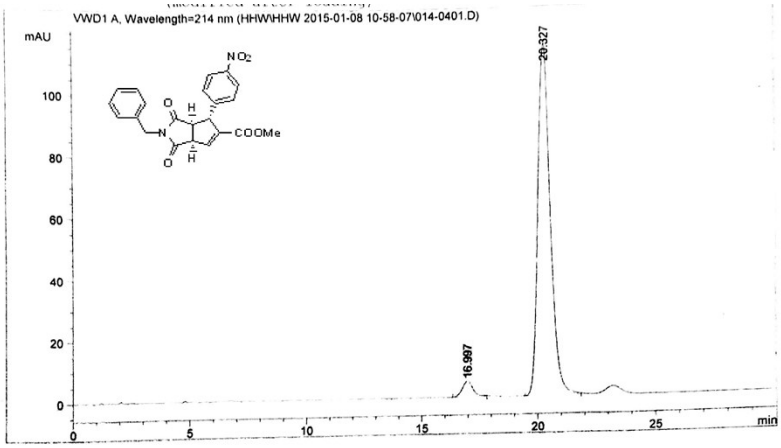
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=214 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	16.284	BB	0.5493	6142.51367	167.83238	50.0797
2	18.878	BB	0.6563	6122.96191	139.08620	49.9203
Totals :				1.22655e4	306.91858	

*** End of Report ***



Area Percent Report

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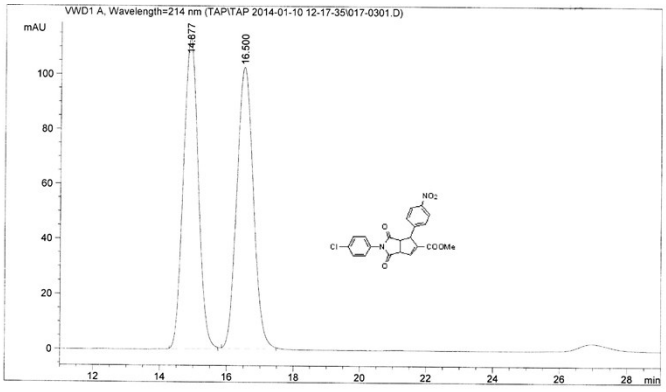
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=214 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	16.997	BB	0.4838	166.26436	5.21830	3.7825
2	20.327	BB	0.5653	4229.39844	115.16264	96.2175
Totals :				4395.66280	120.38094	



Area Percent Report

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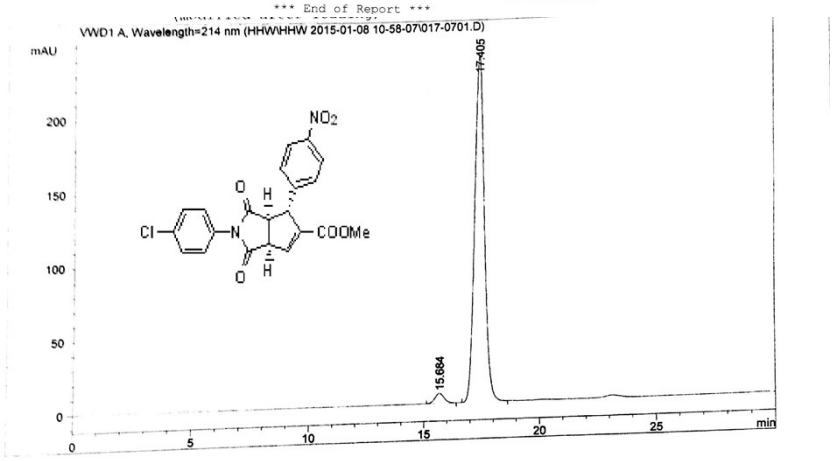
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=214 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	14.877	BB	0.4856	3489.09985	112.96248	49.8434
2	16.500	BB	0.5368	3511.01978	102.40843	50.1566
Totals :				7000.11963	215.37091	

*** End of Report ***

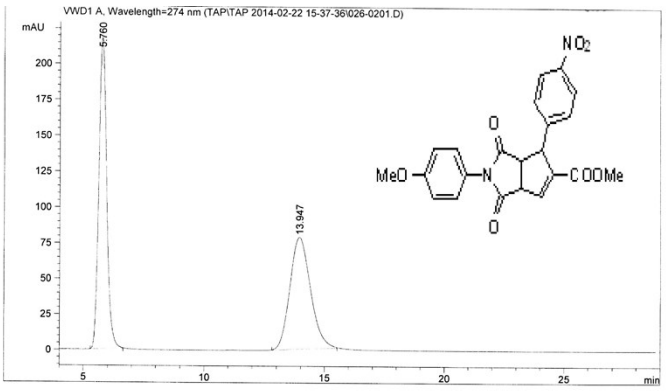


Area Percent Report

Sorted By : Signal
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=214 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	15.684	BB	0.4212	193.08649	7.02253	2.6621
2	17.405	BB	0.4551	7059.97705	240.16293	97.3379
Totals :				7253.06354	247.18546	



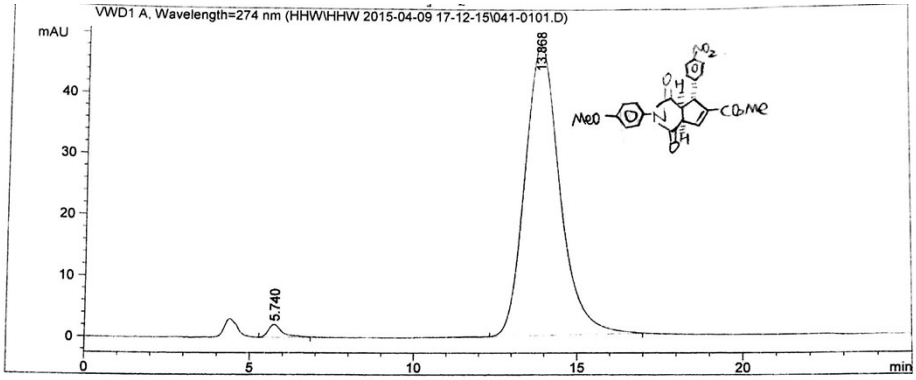
Area Percent Report

Sorted By : Signal
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=274 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	5.760	BB	0.3427	4872.44336	217.66606	50.8958
2	13.947	BB	0.9198	4700.91943	78.67982	49.1042
Totals :				9573.36279	296.34588	

*** End of Report ***



Area Percent Report

Sorted By : Signal
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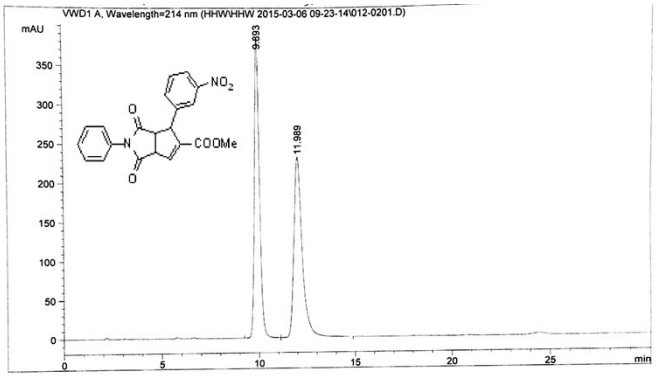
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=274 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	5.740	BB	0.4343	63.84350	2.12932	1.7397
2	13.868	BB	1.1449	3605.88232	48.12646	98.2603
Totals :				3669.72582	50.25578	



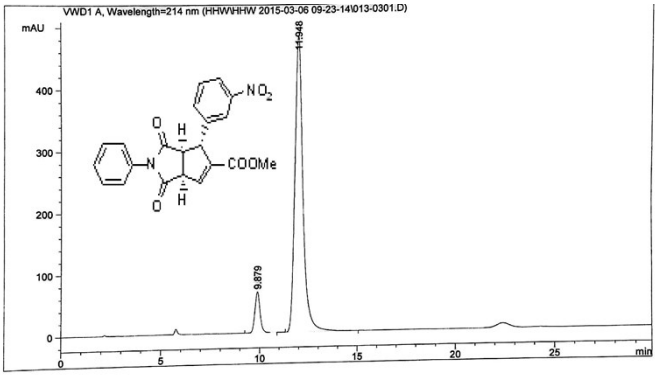
Area Percent Report

Sorted By : Signal
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=214 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	9.893	BV	0.2798	6983.59521	382.79703	49.7330
2	11.989	VB	0.4514	7058.58643	233.68265	50.2670
Totals :				1.40422e4	616.47968	

*** End of Report ***



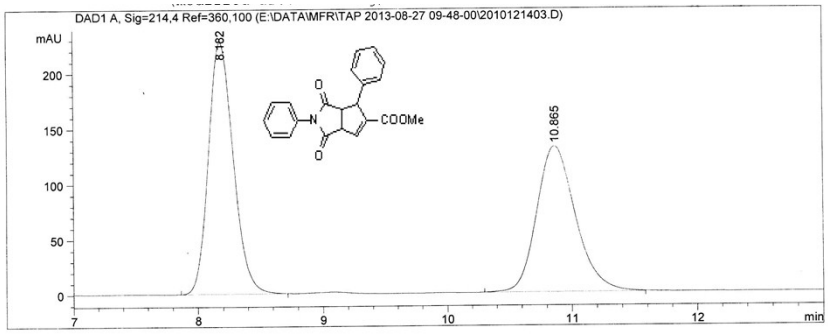
Area Percent Report

Sorted By : Signal
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=214 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	9.879	BB	0.2767	1216.43018	67.68273	8.0270
2	11.948	BB	0.4340	1.39378e4	485.45142	91.9730
Totals :				1.51542e4	553.13415	

*** End of Report ***

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                        Area Percent Report
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Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=214,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   8.182 BB    0.2135 3149.83032  227.56776  52.6031
   2  10.865 BB    0.3305 2838.09131  132.19363  47.3969

Totals :                  5987.92163  359.76140

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                        *** End of Report ***
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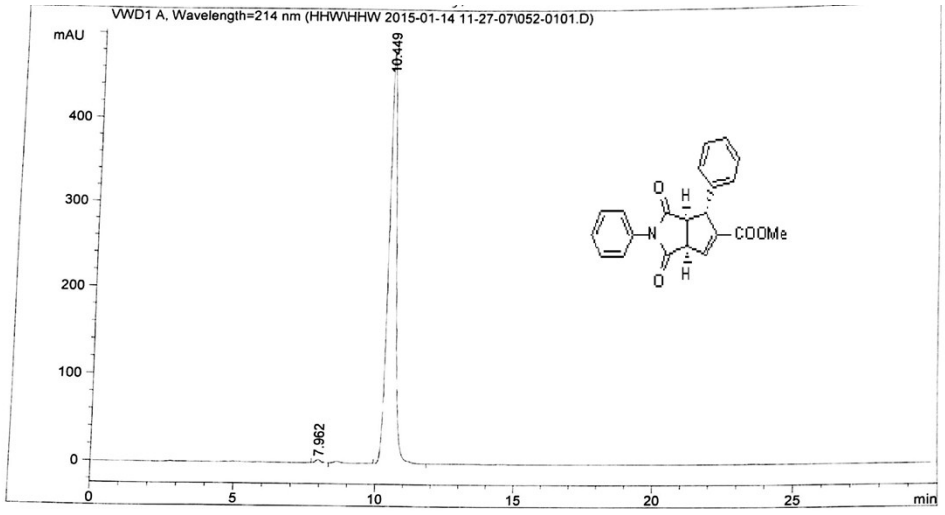


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                        Area Percent Report
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Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=214 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]  mAU   *s    [mAU   ]     %
----|-------|----|-------|----------|----------|--------|
   1   7.962 BB    0.1964   45.82819    3.60333   0.4875
   2  10.449 BB    0.2987 9354.30762  479.99799  99.5125

Totals :                  9400.13580  483.60132

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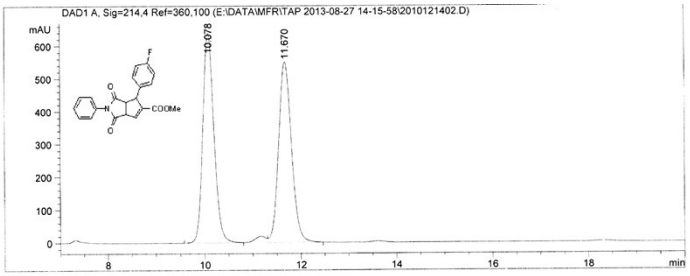

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Area Percent Report

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Sorted By : Signal
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=214,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.078	BB	0.2466	1.02153e4	638.70624	50.0120
2	11.670	VB	0.2869	1.02104e4	549.32574	49.9880

Totals : 2.04257e4 1188.03198

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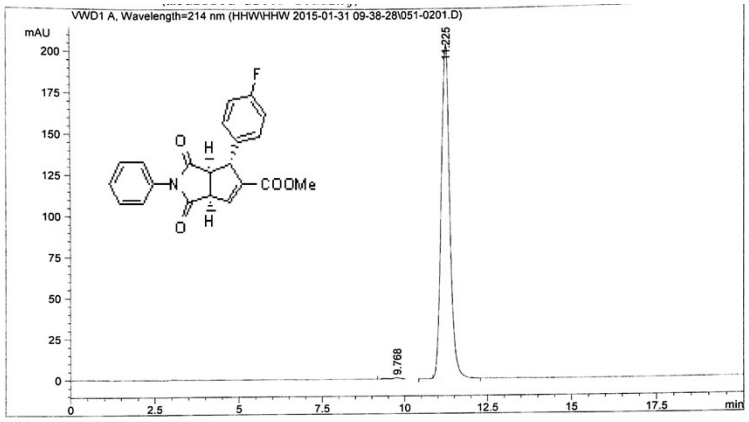
*** End of Report ***



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Area Percent Report

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Sorted By : Signal
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=214 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	9.768	BB	0.3192	18.14421	8.11136e-1	0.4876
2	11.225	BB	0.2827	3702.71094	202.99611	99.5124

Totals : 3720.85515 203.80725

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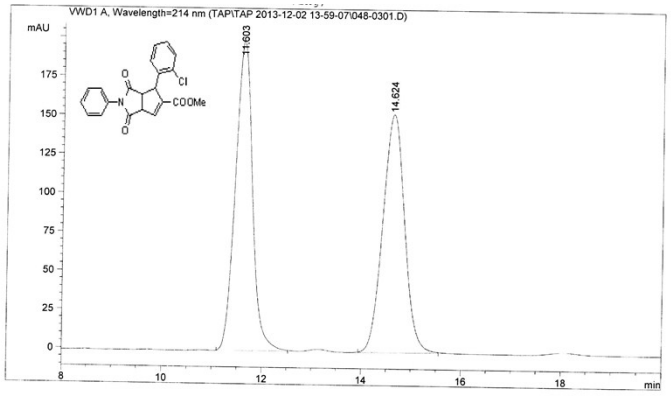
*** End of Report ***



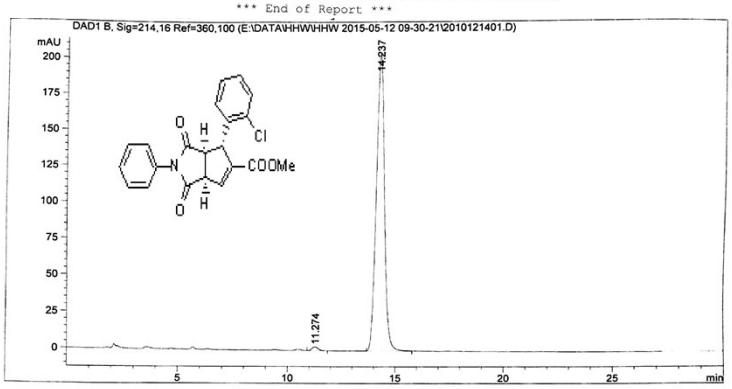
Area Percent Report

Sorted By : Signal
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=214 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	11.603	BB	0.3678	4714.86914	199.27615	50.1943
2	14.624	BB	0.4762	4678.37207	152.96103	49.8057
Totals :				9393.24121	352.23718	

*** End of Report ***



Area Percent Report

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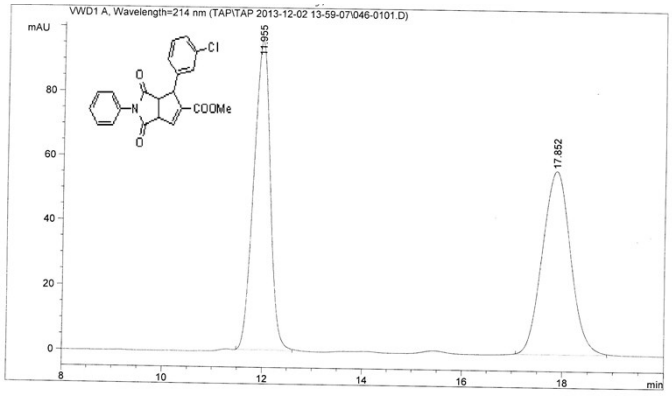
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 B, Sig=214,16 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.274	VB	0.3119	53.16908	2.67454	0.9766
2	14.237	BB	0.4031	5390.86084	204.77643	99.0234
Totals :				5444.02991	207.45096	

*** End of Report ***



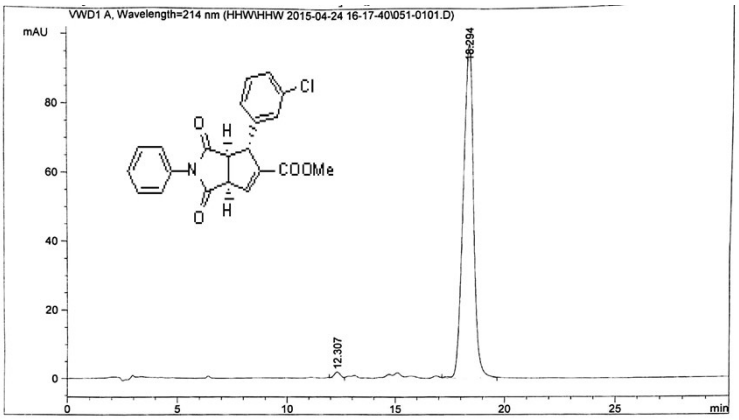
Area Percent Report

Sorted By : Signal
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=214 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	11.955	BB	0.3605	2192.09692	95.66399	49.9527
2	17.852	BB	0.6084	2196.24585	56.42459	50.0473
Totals :				4388.34277	152.08858	

*** End of Report ***



Area Percent Report

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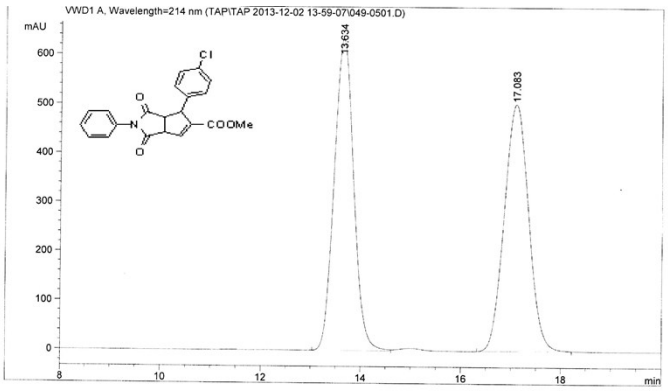
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=214 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	12.307	BV	0.3042	34.33590	1.77621	1.0596
2	18.294	VB	0.5112	3206.21851	96.91724	98.9404
Totals :				3240.55441	98.69344	

*** End of Report ***



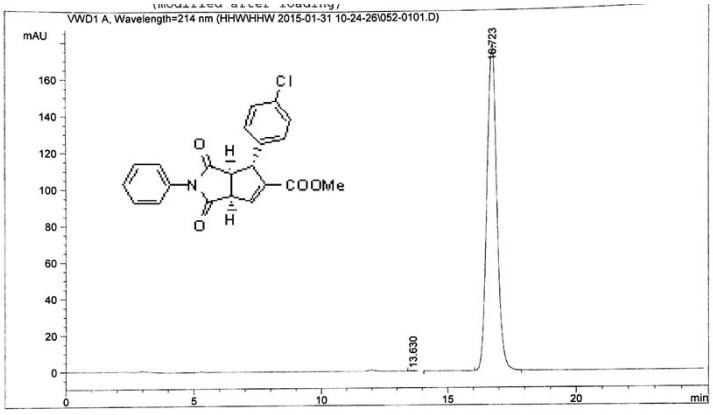
Area Percent Report

Sorted By : Signal
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=214 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	13.634	BB	0.4233	1.71187e4	632.81403	50.0954
2	17.083	BB	0.5328	1.70535e4	502.47000	49.9046
Totals :				3.41722e4	1135.28403	

*** End of Report ***



Area Percent Report

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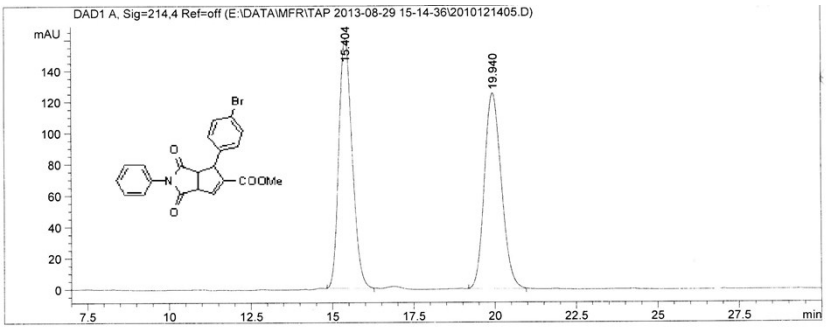
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=214 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	13.630	BB	0.2474	3.76061	2.09412e-1	0.0777
2	16.723	BB	0.4174	4834.52930	178.81114	99.9223
Totals :				4838.28991	179.02055	

*** End of Report ***



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Area Percent Report

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Sorted By : Signal
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=214,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.404	BB	0.4395	4529.70801	160.37756	49.8197
2	19.940	BB	0.5675	4562.49561	125.09035	50.1803

Totals : 9092.20361 285.46792

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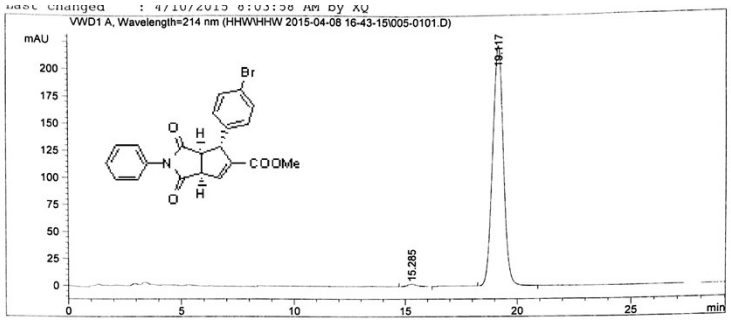
*** End of Report ***



==========

Area Percent Report

==========

Sorted By : Signal
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

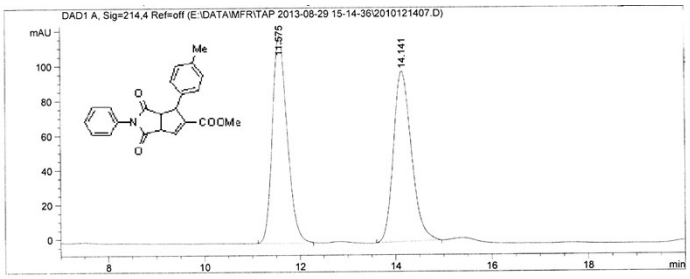
Signal 1: VWD1 A, Wavelength=214 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	15.285	BB	0.4828	66.75794	2.10963	0.8943
2	19.117	BB	0.5181	7397.72363	221.33163	99.1057

Totals : 7464.48158 223.44126

==========

*** End of Report ***



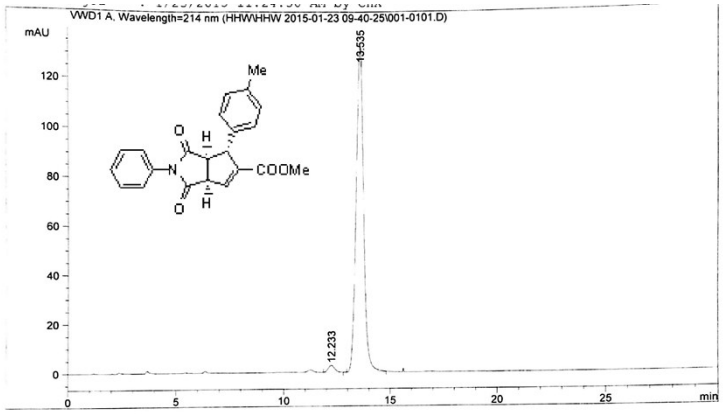
Area Percent Report

Sorted By : Signal
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=214,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.575	BB	0.3321	2585.47217	119.65311	50.1126
2	14.141	BB	0.4030	2573.84839	98.46755	49.8874
Totals :				5159.32056	218.12067	

*** End of Report ***



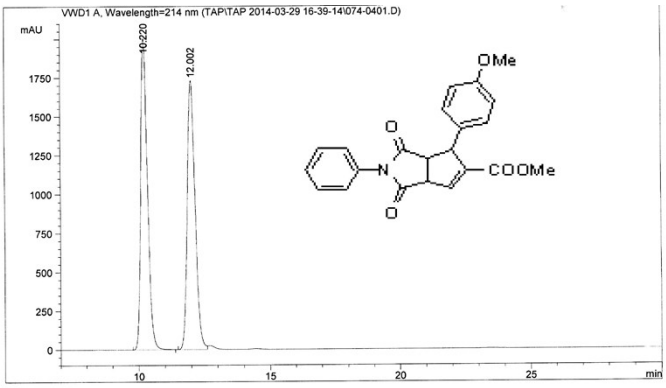
Area Percent Report

Sorted By : Signal
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

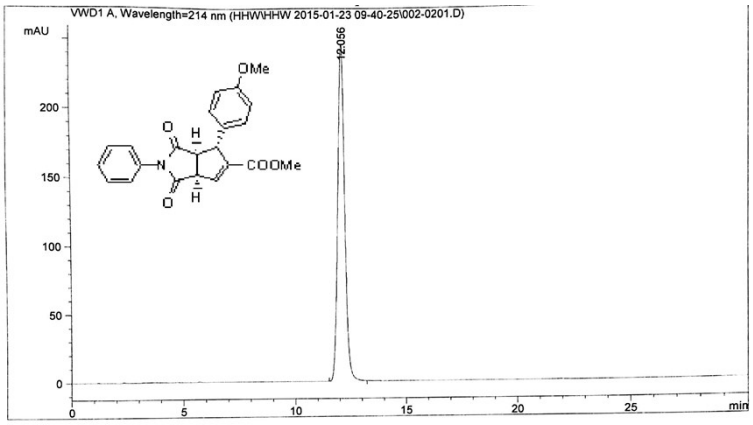
Signal 1: VWD1 A, Wavelength=214 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	12.233	BB	0.3230	59.61591	2.81290	1.8063
2	13.535	BB	0.3752	3240.87671	132.70505	98.1937
Totals :				3300.49261	135.51795	

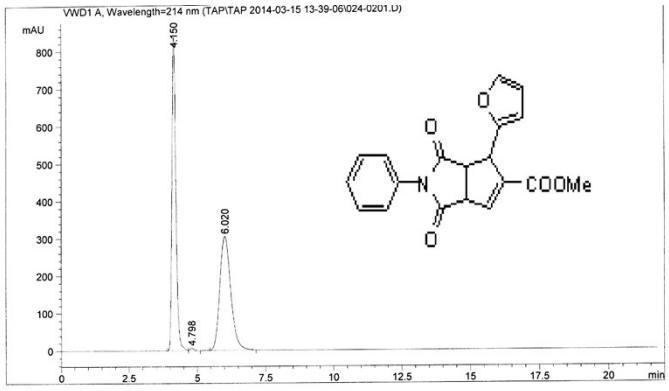
*** End of Report ***



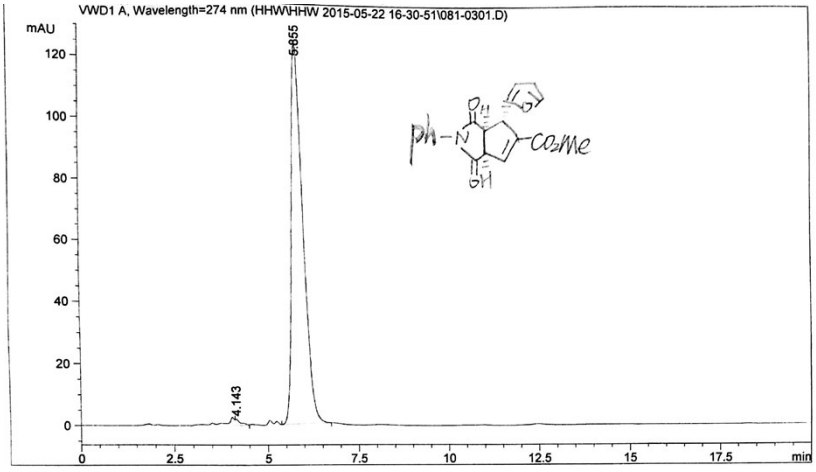

```
================================================================
                    Area Percent Report
================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=214 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]  mAU   *s   [mAU   ]      %
----|-------|----|-------|----------|----------|--------|
   1  10.220 BB    0.2764 3.57180e4  2003.82874  49.8687
   2  12.002 BV    0.3221 3.59204e4  1731.21252  50.1413

Totals :                  7.16384e4  3735.04126

================================================================
                    *** End of Report ***
```



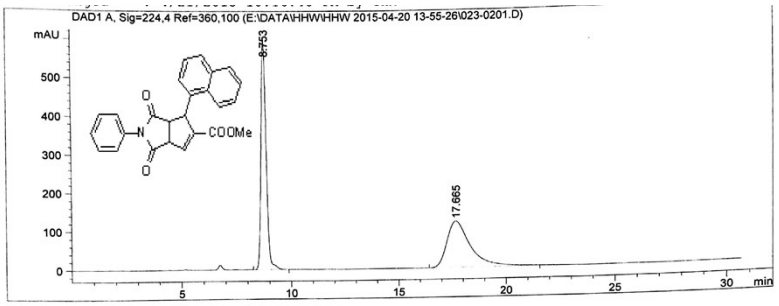

```
================================================================
                    Area Percent Report
================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=214 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]  mAU   *s   [mAU   ]      %
----|-------|----|-------|----------|----------|--------|
   1  12.056 BB    0.3355 5381.02441  247.21468 100.0000

Totals :                  5381.02441  247.21468

================================================================
                    *** End of Report ***
```



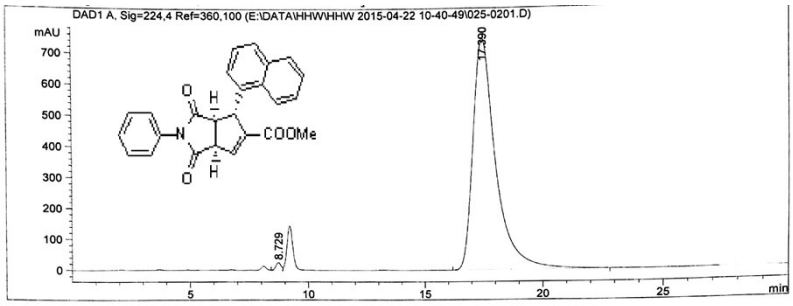

```
=====================================================================
                        Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=214 nm

Peak RetTime Type  Width     Area      Height      Area
  #   [min]        [min]  mAU   *s   [mAU   ]       %
----|-------|----|-------|----------|----------|--------|
   1   4.150 BV    0.1548 8462.98535  834.18024  49.9862
   2   4.798 VB    0.1419   58.83668    6.41843   0.3475
   3   6.020 BB    0.4284 8408.82617  303.14957  49.6663

Totals :                1.69306e4  1143.74824

=====================================================================
                        *** End of Report ***
```



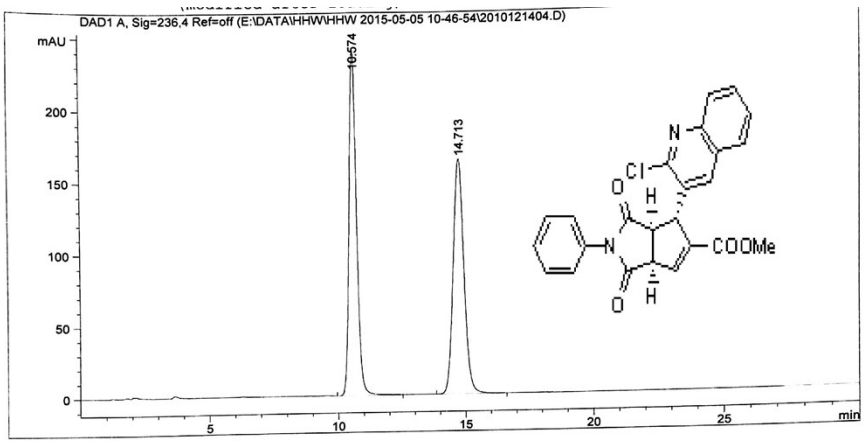

```
=====================================================================
                        Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=274 nm

Peak RetTime Type  Width     Area      Height      Area
  #   [min]        [min]  mAU   *s   [mAU   ]       %
----|-------|----|-------|----------|----------|--------|
   1   4.143 VB    0.1468   21.63298    2.01993   0.7960
   2   5.855 VB    0.3351 2696.01855  123.31822  99.2040

Totals :                   2717.65153  125.33815

=====================================================================
                        *** End of Report ***
```




```
================================================================================
                            Area Percent Report
================================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=224,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]    [mAU*s]    [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   8.753 VB    0.2529 9753.52832  596.07275  51.2286
   2  17.665 BB    1.1328 9285.68555  121.88516  48.7714

Totals :                  1.90392e4   717.95792

================================================================================
                            *** End of Report ***
```




```
================================================================================
                            Area Percent Report
================================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=224,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]    [mAU*s]    [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   8.729 VV    0.2308  377.05472   25.17243   0.7412
   2  17.390 BB    1.0048 5.04925e4   746.81250  99.2588

Totals :                  5.08696e4   771.98493

================================================================================
                            *** End of Report ***
```



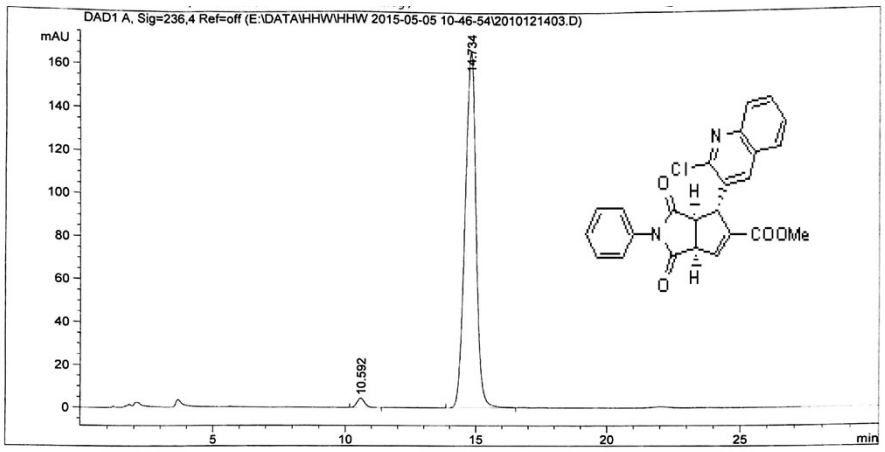
Area Percent Report

Sorted By : Signal
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=236,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.574	VV	0.3119	4887.16650	241.66545	49.9898
2	14.713	VV	0.4569	4889.16992	165.35890	50.0102

Totals : 9776.33643 407.02435



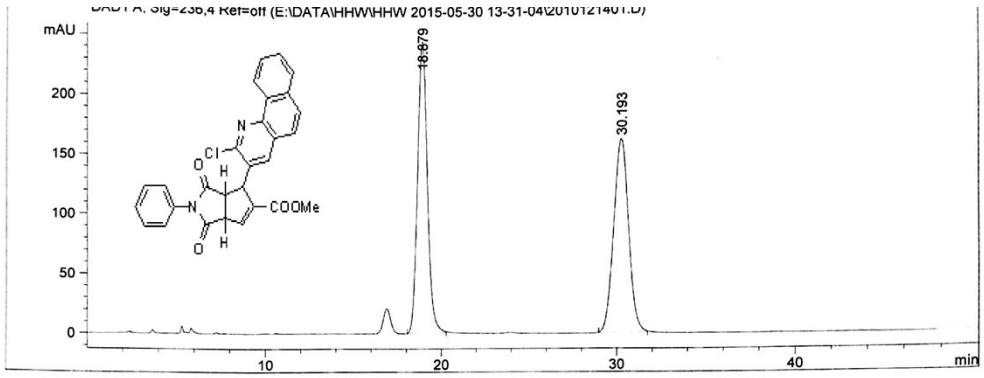
Area Percent Report

Sorted By : Signal
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

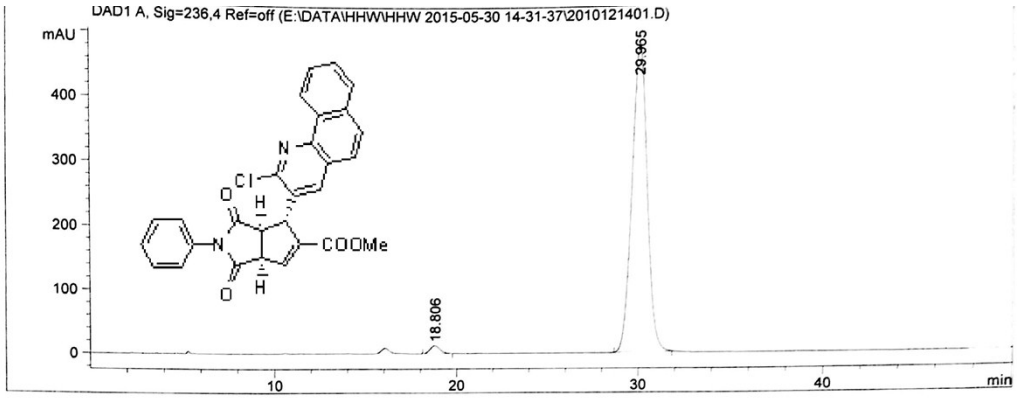
Signal 1: DAD1 A, Sig=236,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.592	VV	0.3251	91.70045	4.43735	1.8372
2	14.734	VV	0.4553	4899.69922	166.51833	98.1628

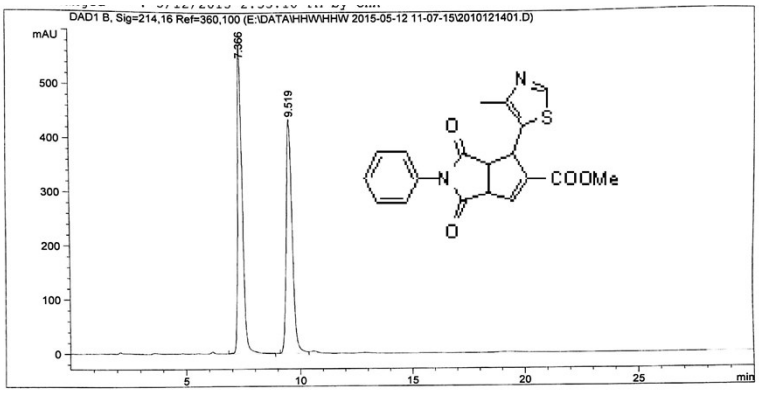
Totals : 4991.39967 170.95567



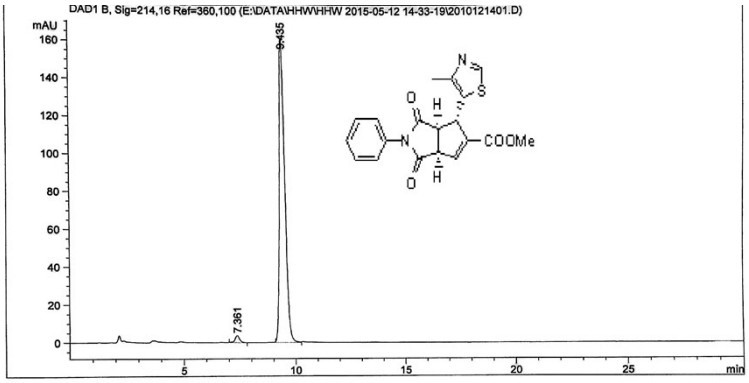

```
================================================================================
                          Area Percent Report
================================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=236,4 Ref=off

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  18.879 BB    0.5933 9482.30859  246.20564  50.0465
   2  30.193 BB    0.9074 9464.70020  162.53740  49.9535

Totals :                  1.89470e4   408.74304

================================================================================
                          *** End of Report ***
```




```
================================================================================
                          Area Percent Report
================================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=236,4 Ref=off

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  18.806 BB    0.5649  472.40665   12.55786   1.6739
   2  29.965 BB    0.8964 2.77489e4   480.02356  98.3261

Totals :                  2.82213e4   492.58142

================================================================================
                          *** End of Report ***
```

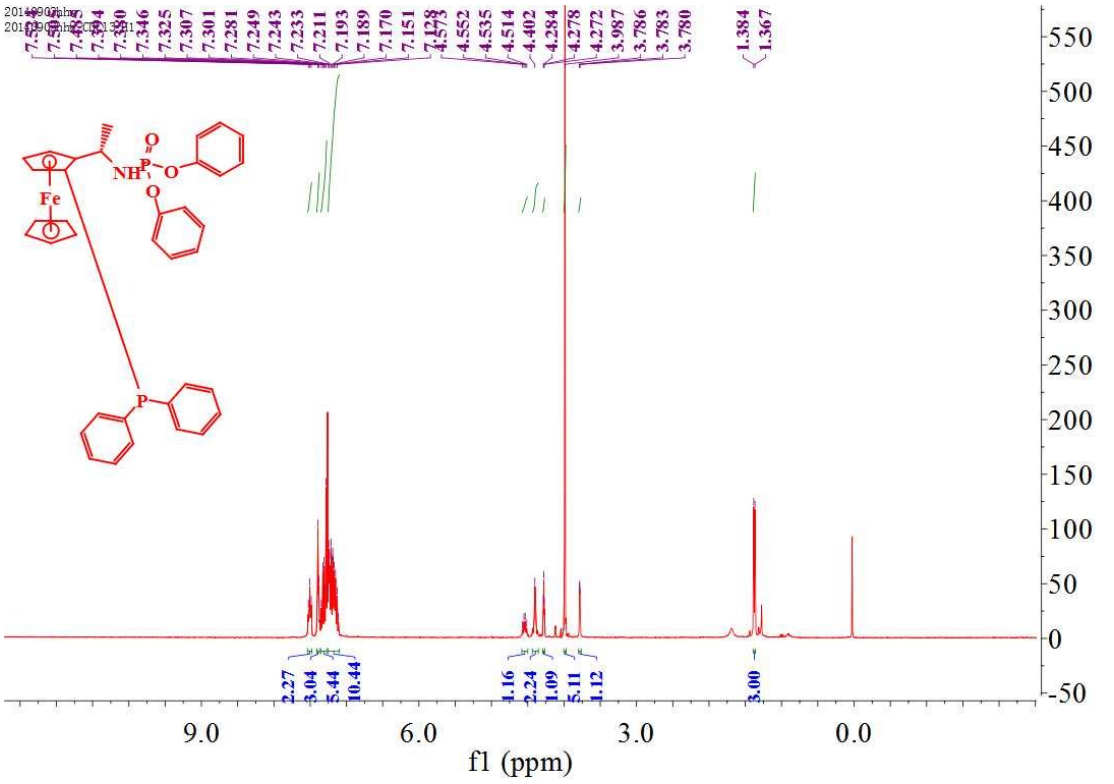


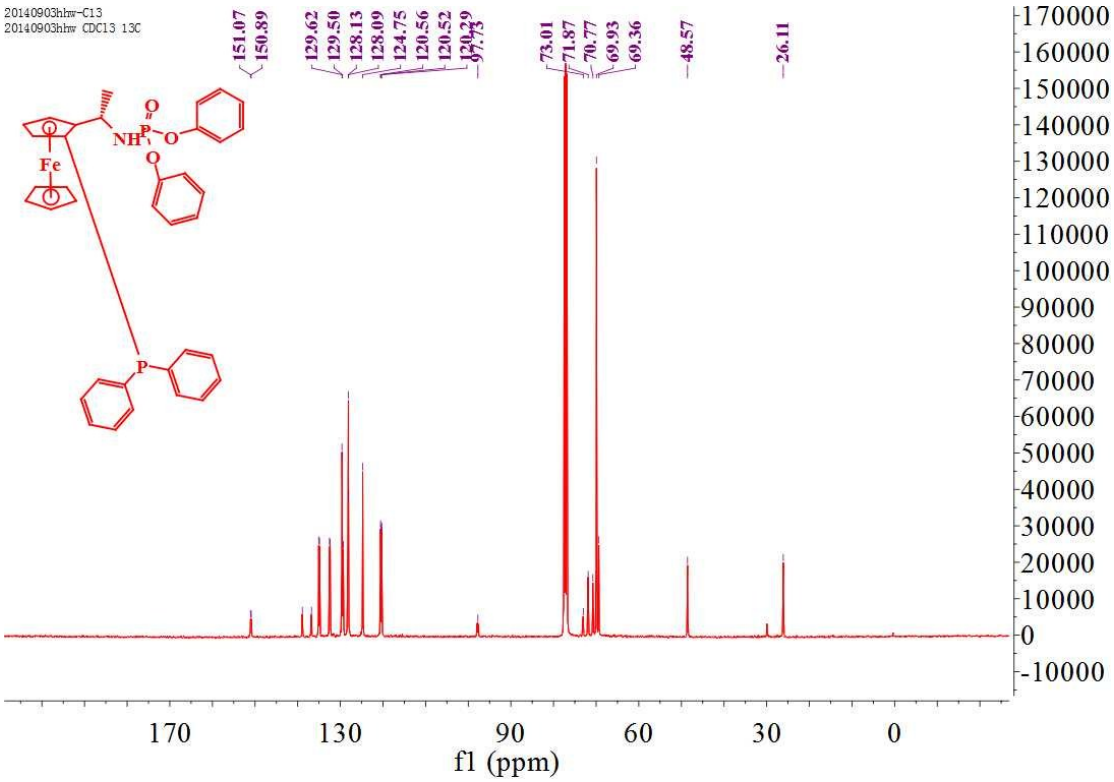

```
================================================================================
                          Area Percent Report
================================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 B, Sig=214,16 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   7.366 BB    0.2235 8193.29297  570.79108  50.4830
   2   9.519 BV    0.2779 8036.51709  438.24078  49.5170

Totals :                  1.62298e4  1009.03186

================================================================================
                          *** End of Report ***
```

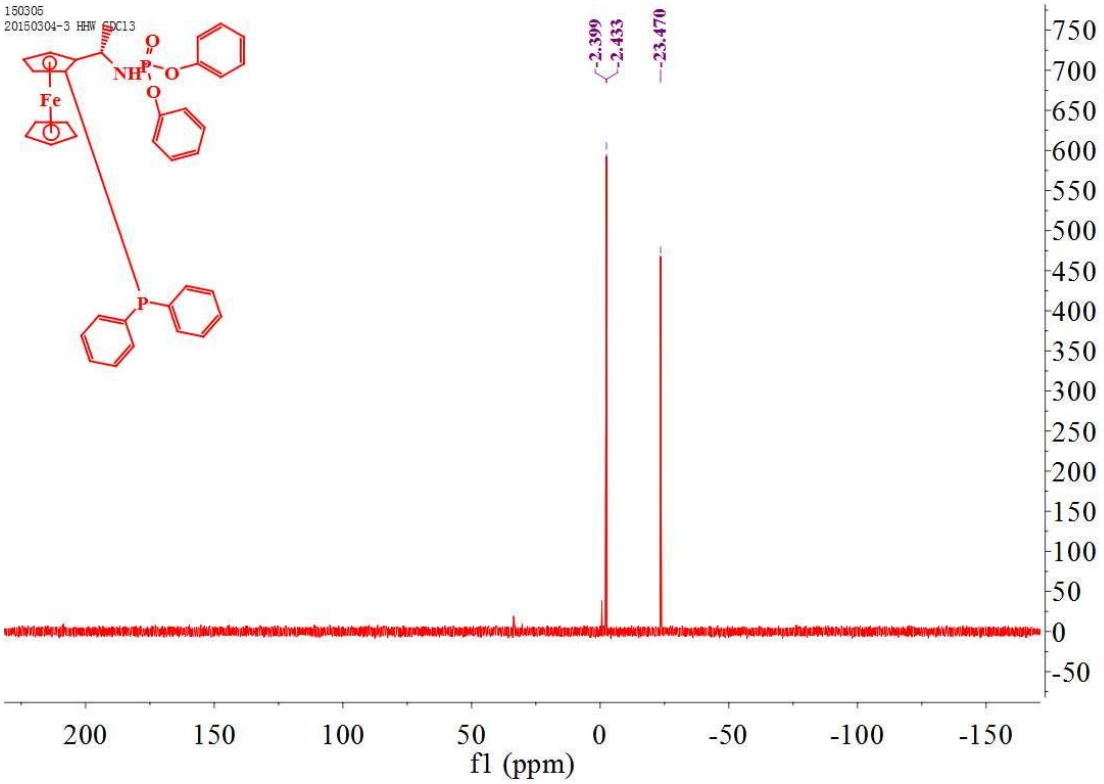


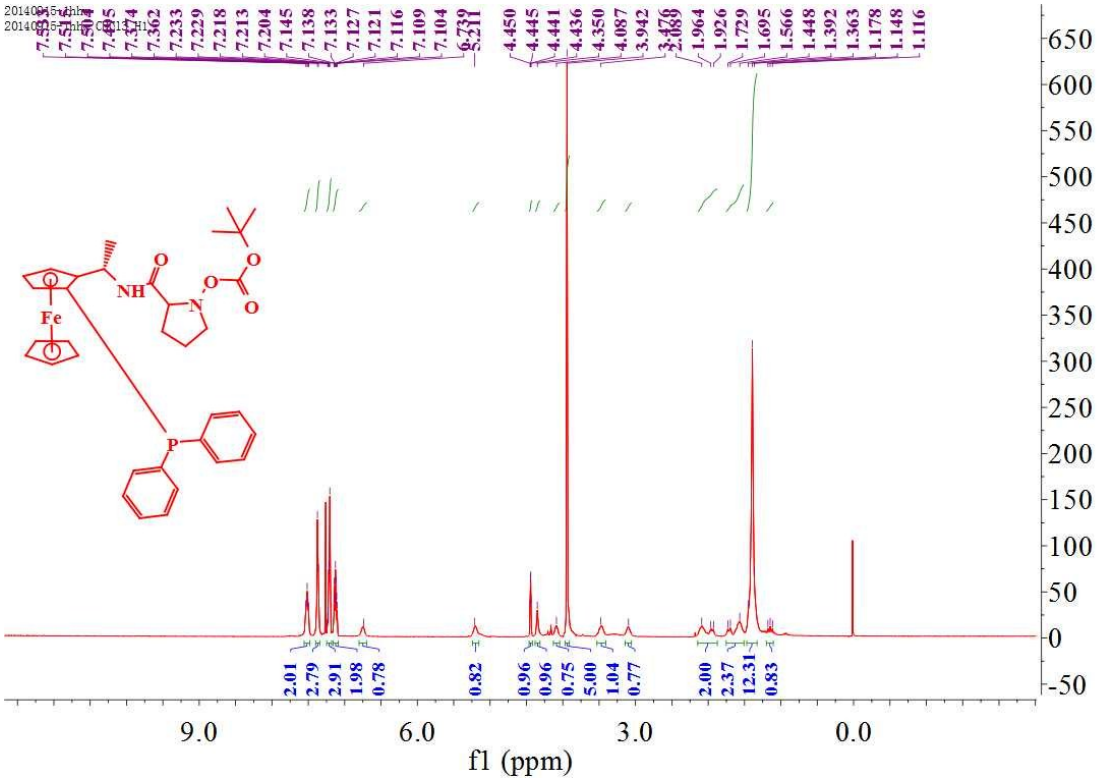

```
================================================================================
                          Area Percent Report
================================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 B, Sig=214,16 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   7.361 BB    0.2139   52.66909   3.70407   1.8520
   2   9.435 BB    0.2648 2791.22827  162.17851  98.1480

Totals :                  2843.89736  165.88258

================================================================================
                          *** End of Report ***
```

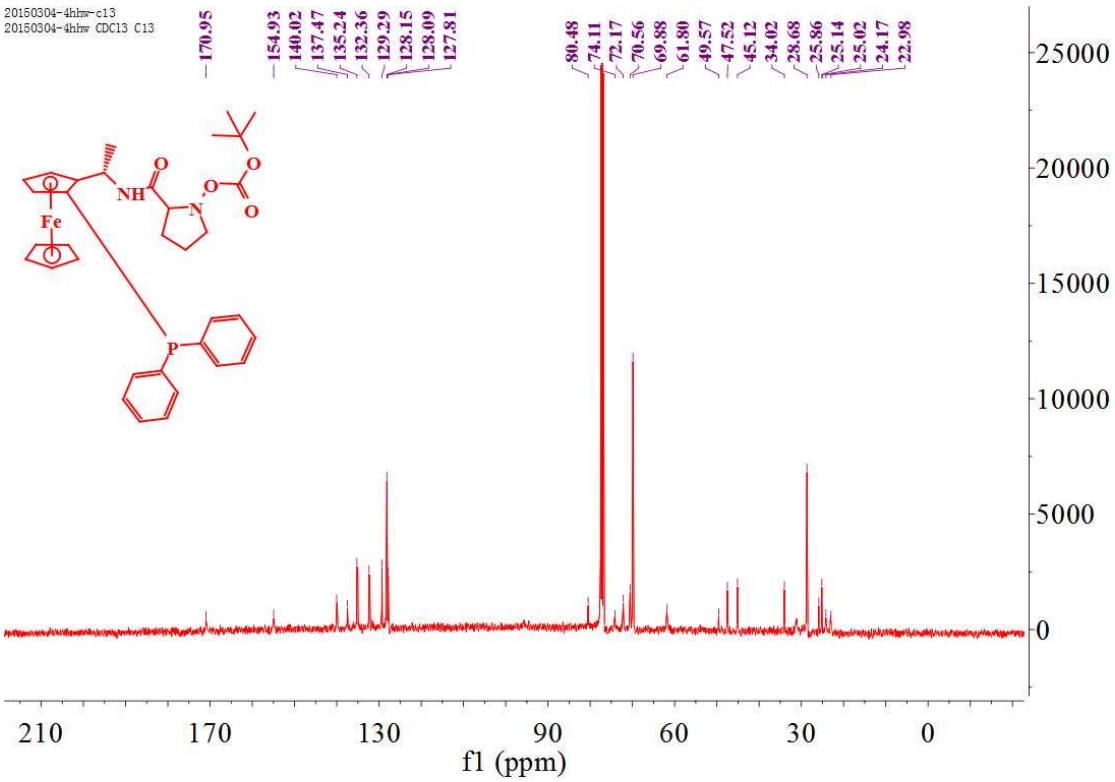
II. NMR/MS Spectra of the catalysts and the products

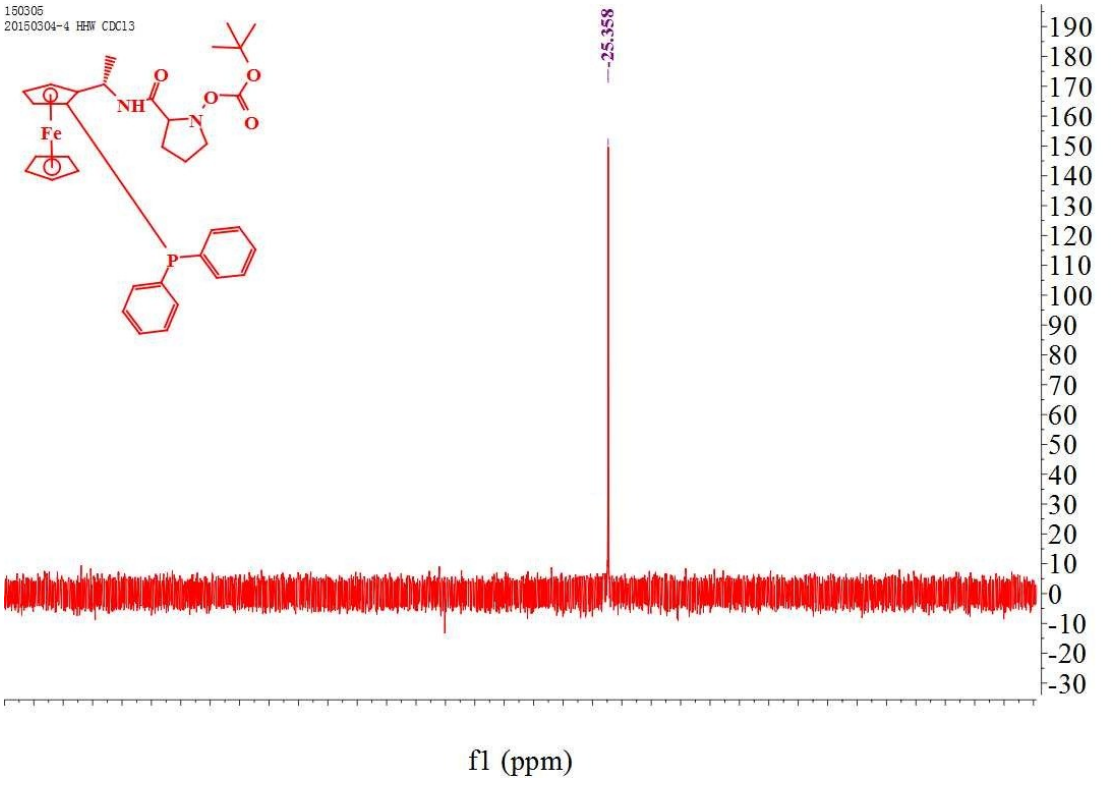


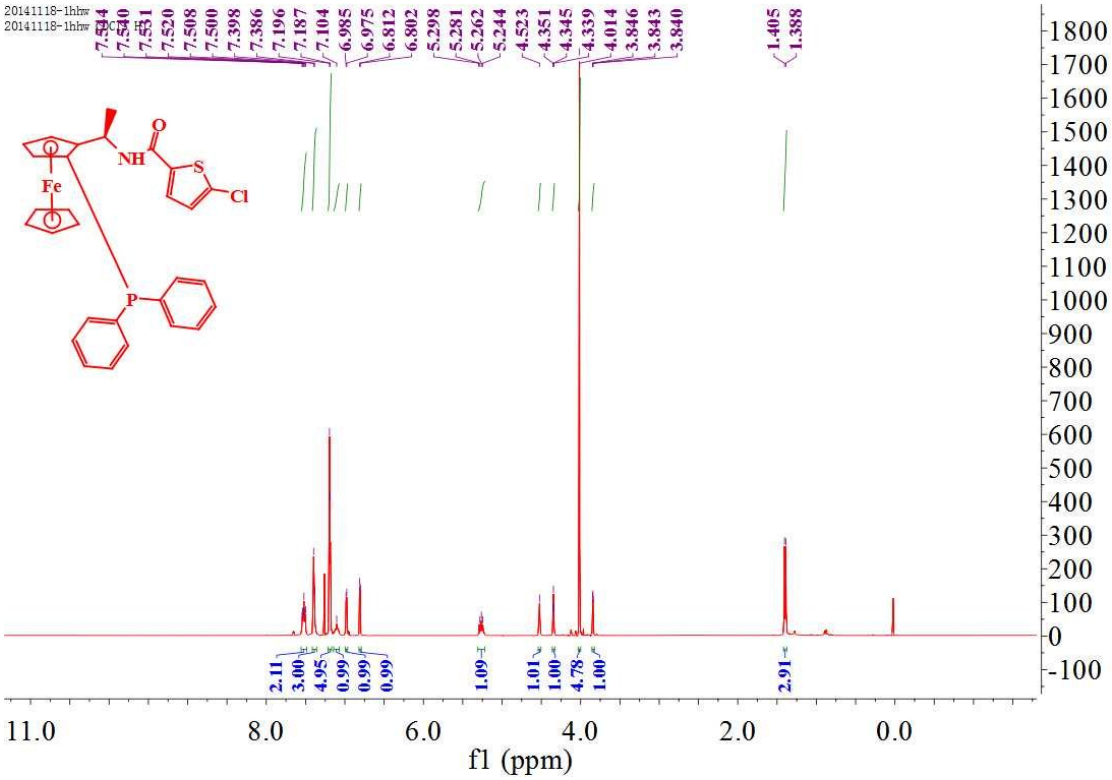


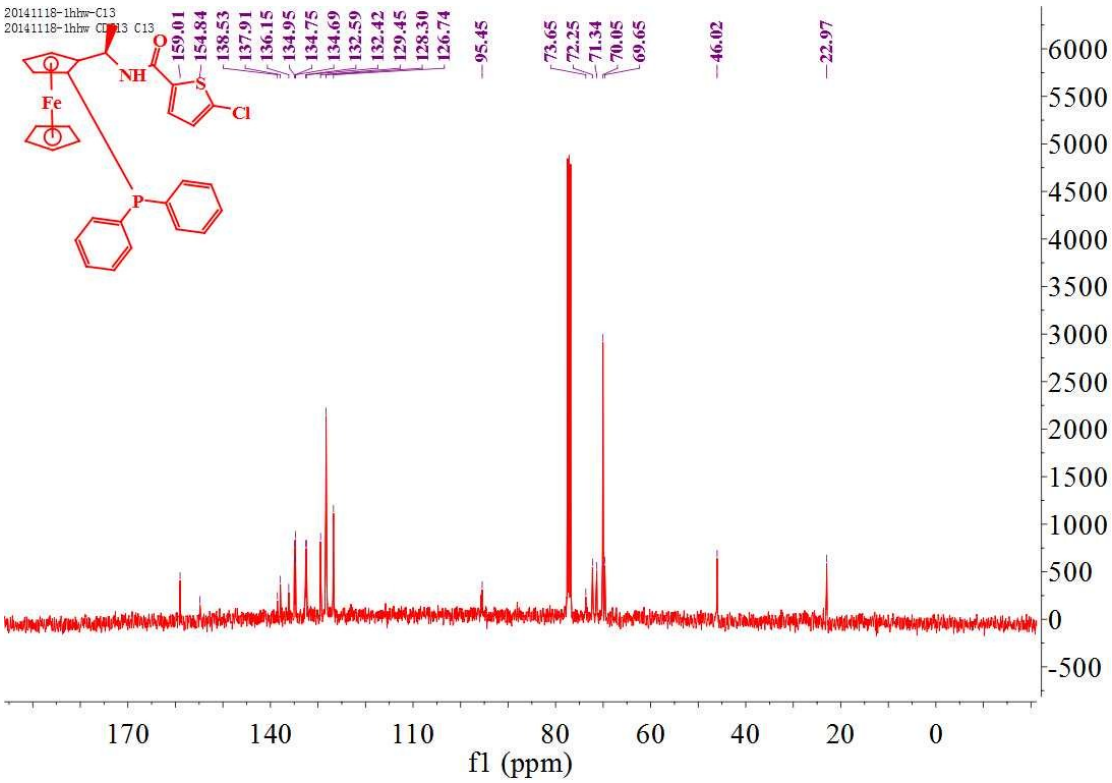

150305
20150304-3 HHW CDCl3
-2.399
-2.433
-23.470
f1 (ppm)

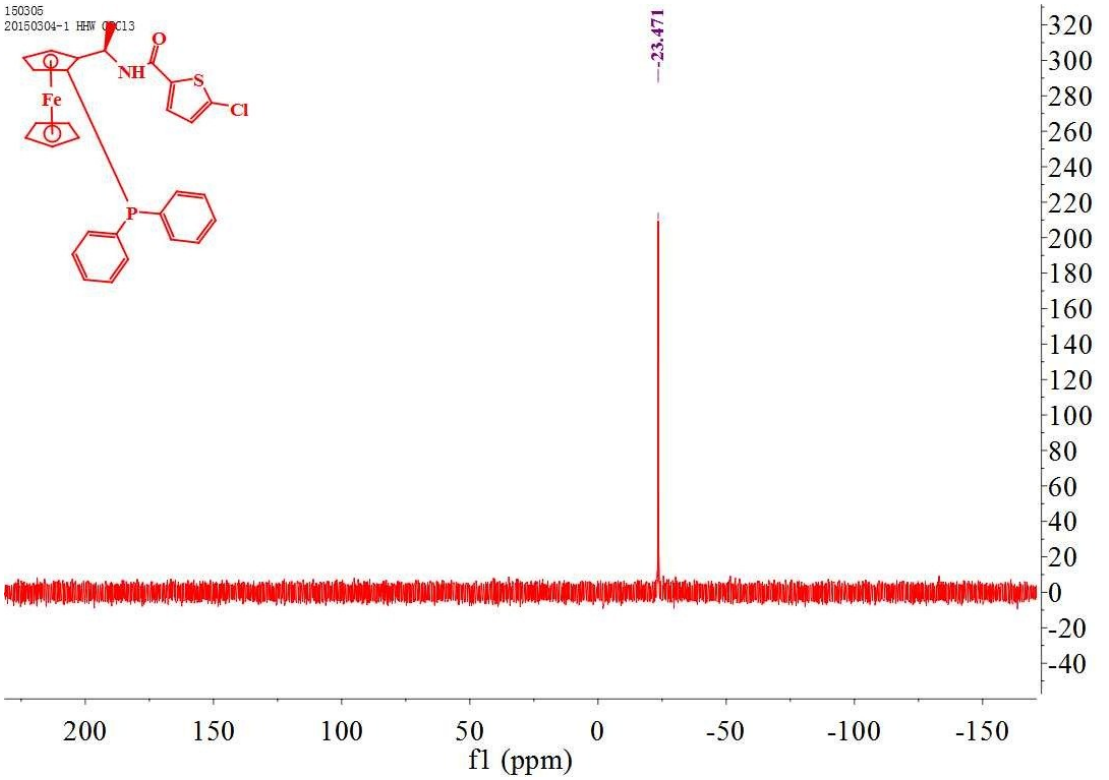

7.504
7.362
7.233
7.229
7.218
7.213
7.204
7.145
7.138
7.133
7.127
7.121
7.116
7.109
7.104
4.450
4.445
4.441
4.436
4.350
4.087
3.942
1.964
1.926
1.729
1.695
1.566
1.448
1.392
1.363
1.178
1.148
1.116
2.01
2.79
2.91
1.98
0.78
0.82
0.96
0.96
0.75
5.00
1.04
0.77
2.00
2.37
12.31
0.83
f1 (ppm)

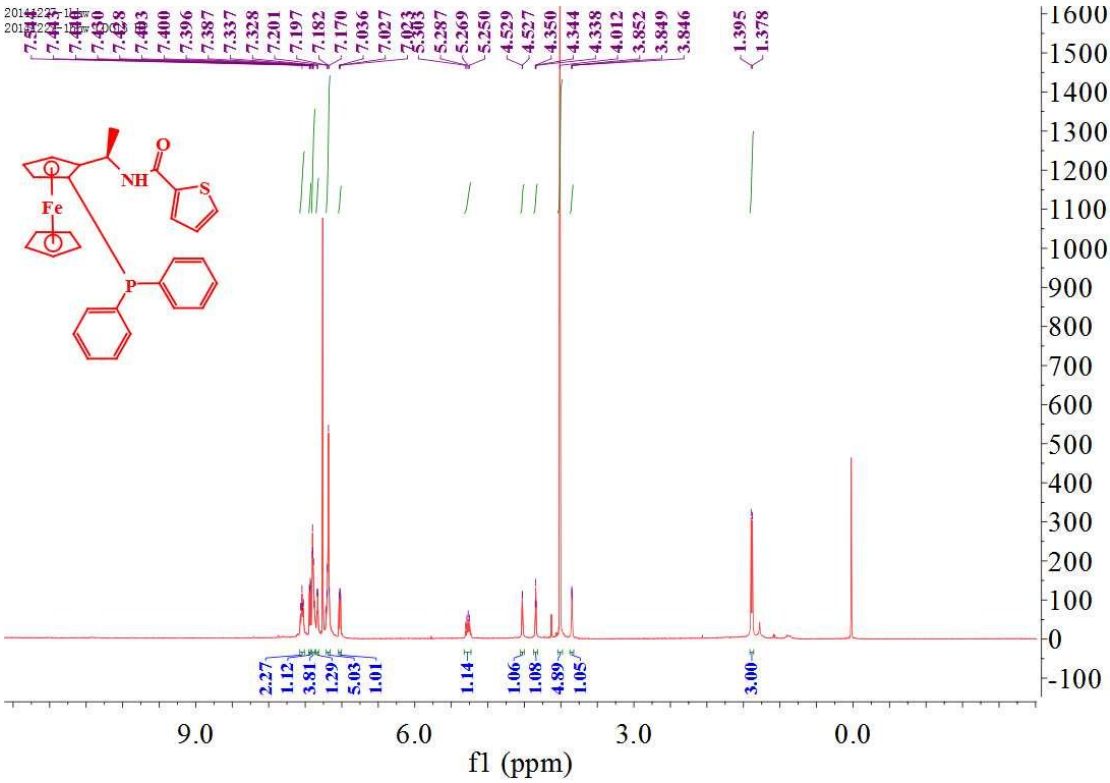

20150304-4hhw-c13
20150304-4hhw CDCl3 C13
170.95
154.93
140.02
137.47
135.24
132.36
129.29
128.15
128.09
127.81
80.48
74.11
72.17
70.56
69.88
61.80
49.57
47.52
45.12
34.02
28.68
25.86
25.14
25.02
24.17
22.98
25000
20000
15000
10000
5000
0
210
170
130
90
60
30
0
f1 (ppm)

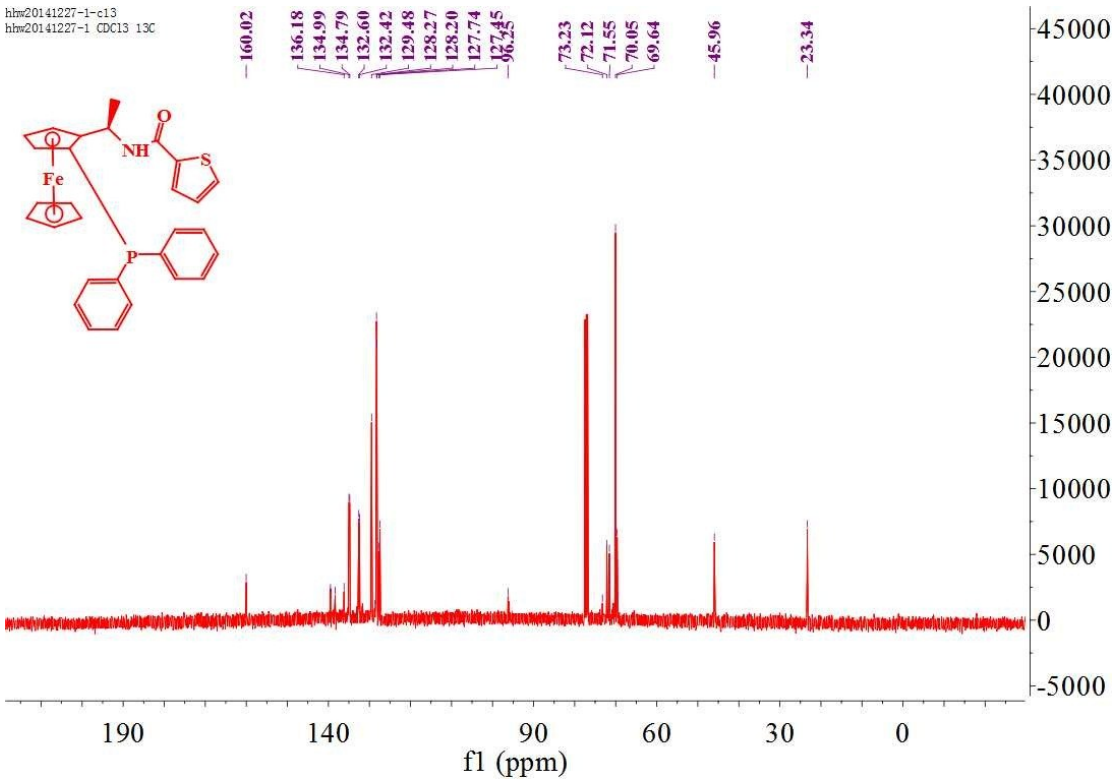

150305
20150304-4 HHW CDCl3
-25.358
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
-20
-30
f1 (ppm)

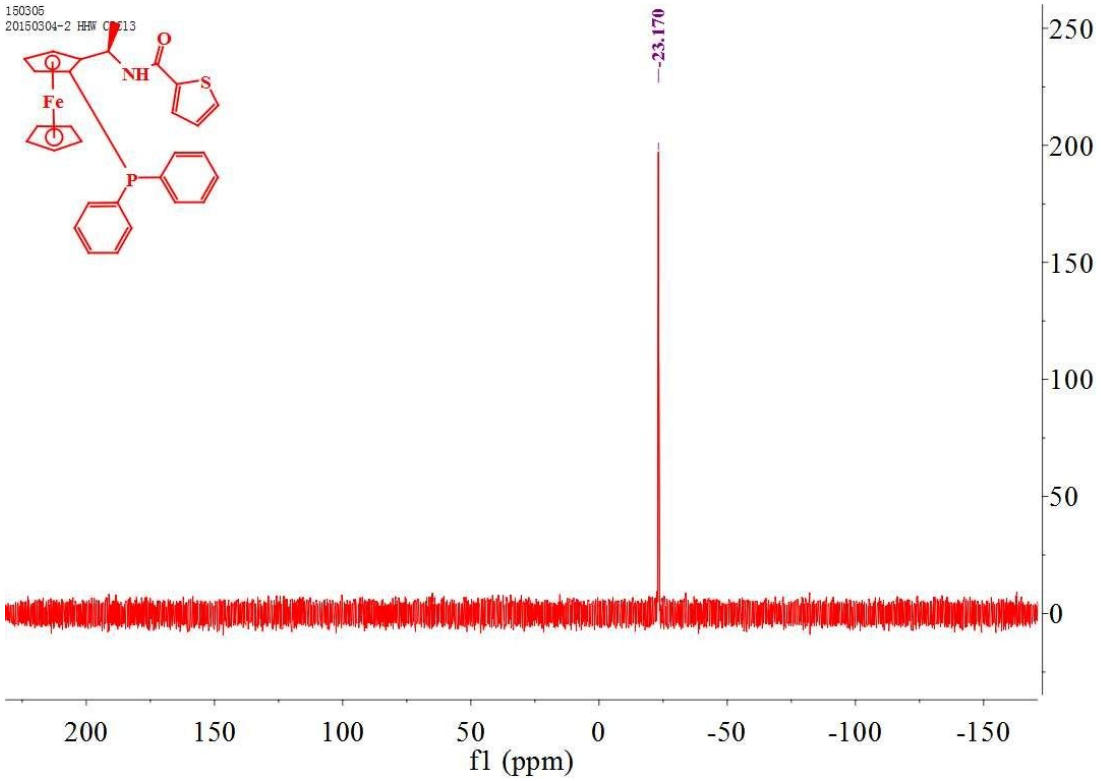

20141118-1hhw
20141118-1hhw
7.534
7.530
7.531
7.520
7.508
7.500
7.398
7.386
7.196
7.187
7.104
6.985
6.975
6.812
6.802
5.298
5.281
5.262
5.244
4.523
4.351
4.345
4.339
4.014
3.846
3.843
3.840
1.405
1.388
NH
O
S
Cl
Fe
P
2.11
3.00
4.95
0.99
0.99
0.99
1.09
1.01
1.00
4.78
1.00
2.91
11.0
8.0
6.0
4.0
2.0
0.0
f1 (ppm)

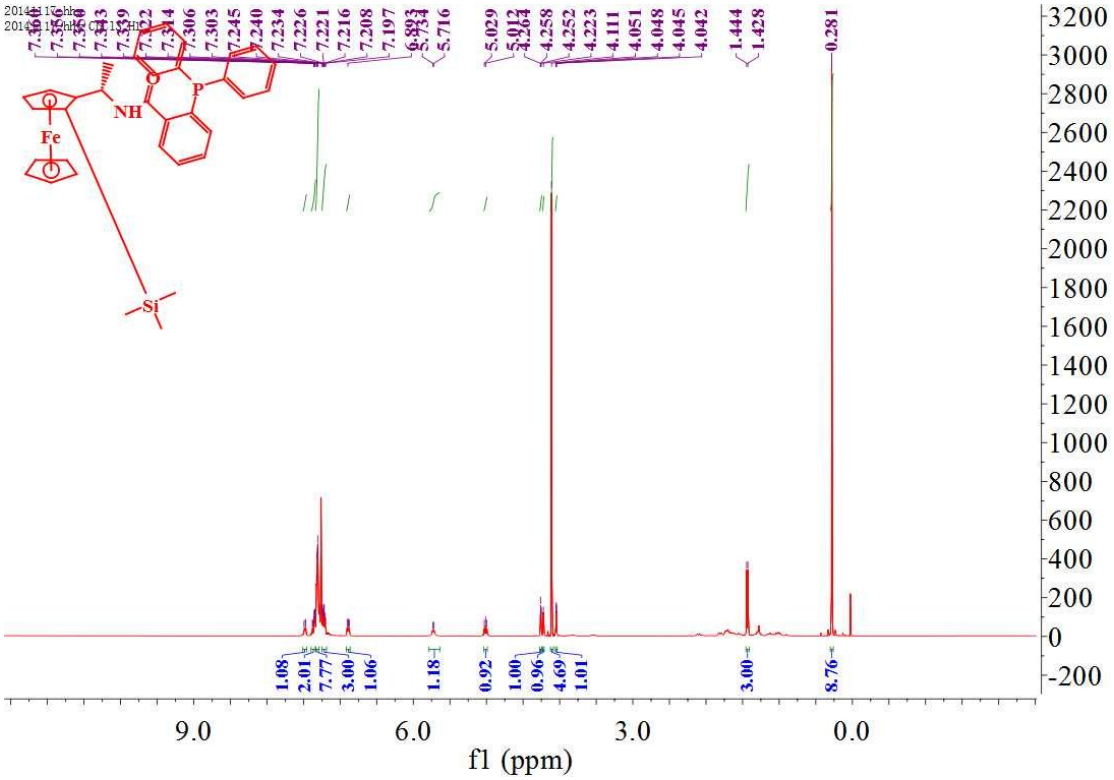

20141118-1hhw-C13
20141118-1hhw CDCl3 C13
159.01
154.84
138.53
137.91
136.15
134.95
134.75
134.69
132.59
132.42
129.45
128.30
126.74
95.45
73.65
72.25
71.34
70.05
69.65
46.02
22.97
NH
O
S
Cl
Fe
P
170
140
110
80
60
40
20
0
f1 (ppm)

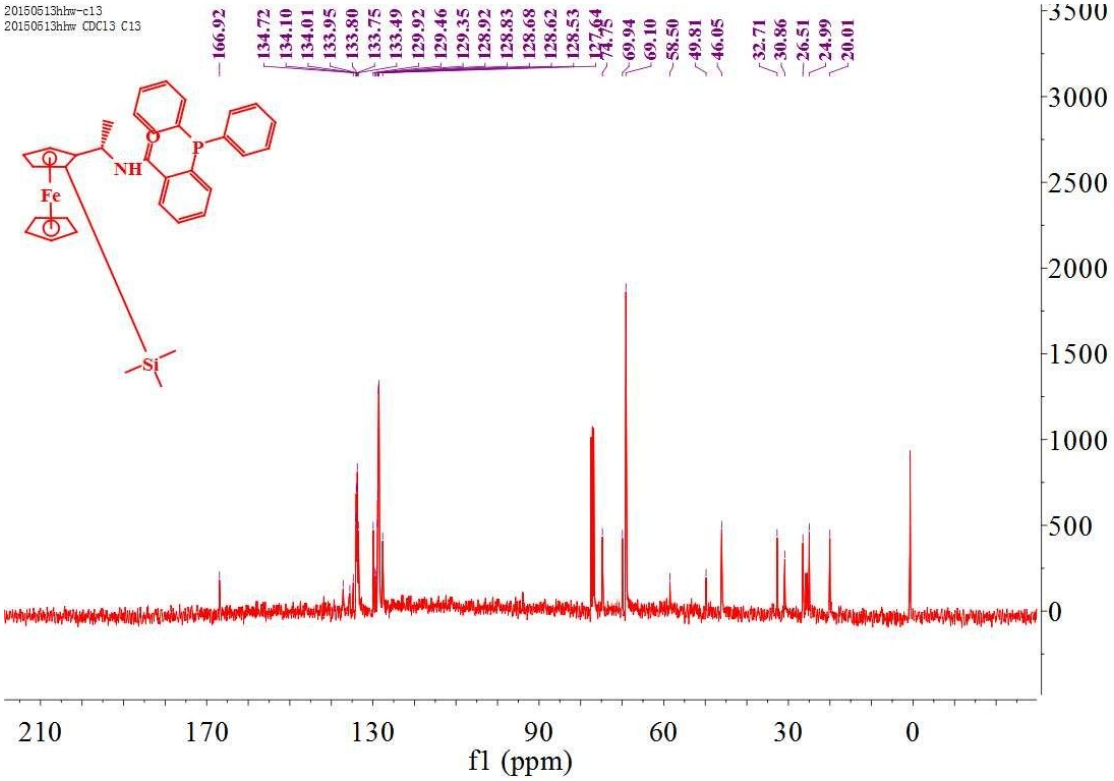

150305
20150304-1 HHW CDCl3
O
NH
S
Cl
Fe
P
-23.471
320
300
280
260
240
220
200
180
160
140
120
100
80
60
40
20
0
-20
-40
200
150
100
50
0
-50
-100
-150
f1 (ppm)

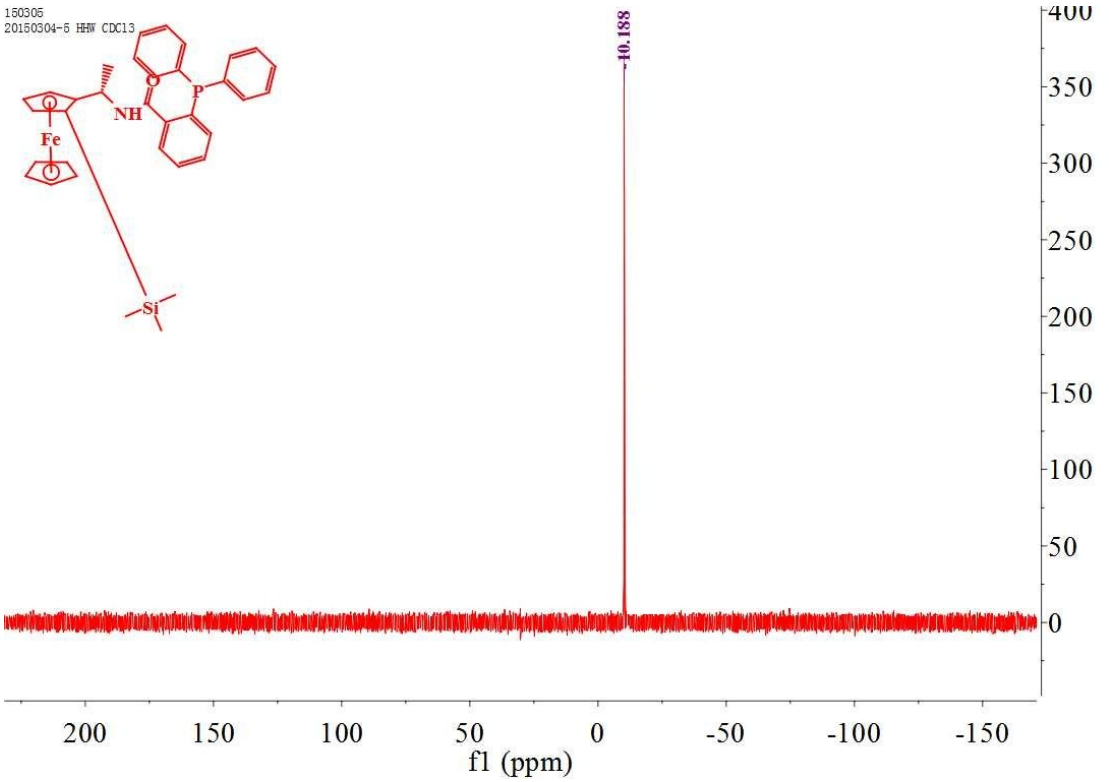

7.395
7.378
5.269
5.250
4.529
4.527
4.350
4.344
4.338
4.012
3.852
3.849
3.846
O
NH
S
Fe
P
2.27
1.12
3.81
1.29
5.03
1.01
1.14
1.06
1.08
4.89
1.05
3.00
1600
1500
1400
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
-100
9.0
6.0
3.0
0.0
f1 (ppm)

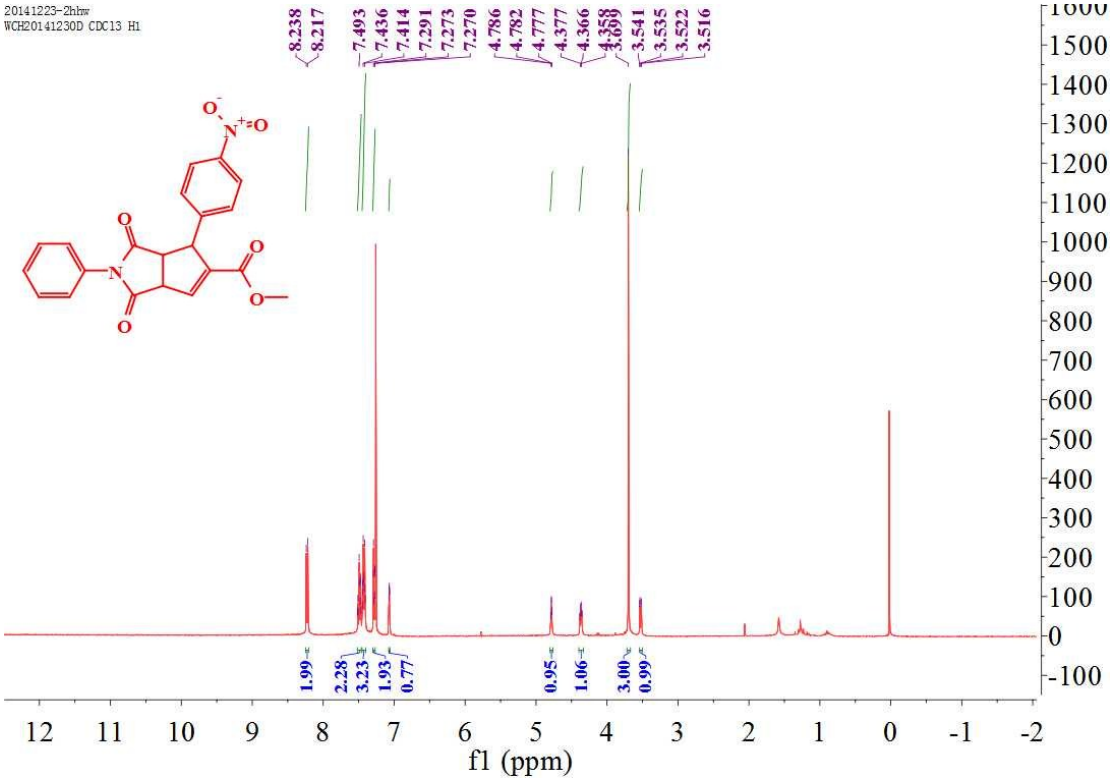

hhw20141227-1-c13
hhw20141227-1 CDCl3 13C
160.02
136.18
134.99
134.79
132.60
132.42
129.48
128.27
128.20
127.74
127.45
96.25
73.23
72.12
71.55
70.05
69.64
45.96
23.34
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
-5000
190
140
90
60
30
0
f1 (ppm)
O
NH
S
Fe
P

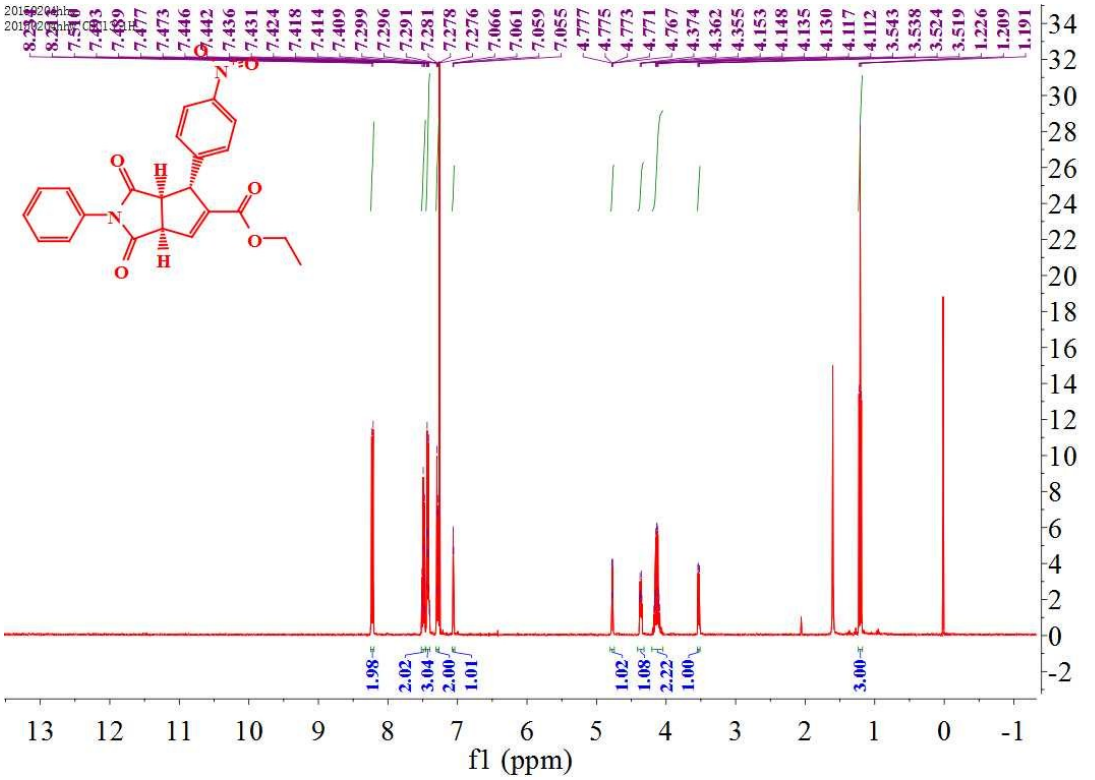

150305
20150304-2 HHW CDCl3
-23.170
250
200
150
100
50
0
200
150
100
50
0
-50
-100
-150
f1 (ppm)
O
NH
S
Fe
P

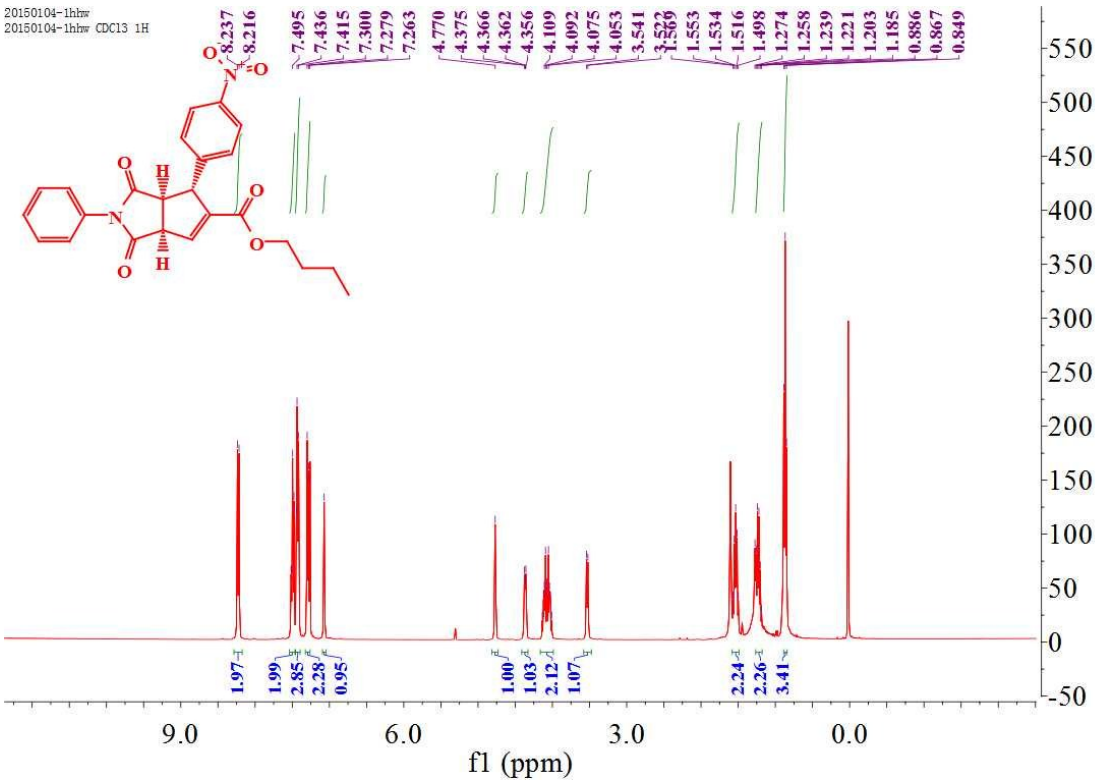

7.366
7.356
7.343
7.339
7.322
7.314
7.306
7.303
7.245
7.240
7.234
7.226
7.221
7.216
7.208
7.197
6.893
5.734
5.716
5.029
5.012
4.264
4.258
4.252
4.223
4.111
4.051
4.048
4.045
4.042
1.444
1.428
0.281
1.08
2.01
7.77
3.00
1.06
1.18
0.92
1.00
0.96
4.69
1.01
3.00
8.76
NH
O
P
Fe
Si
9.0
6.0
3.0
0.0
f1 (ppm)

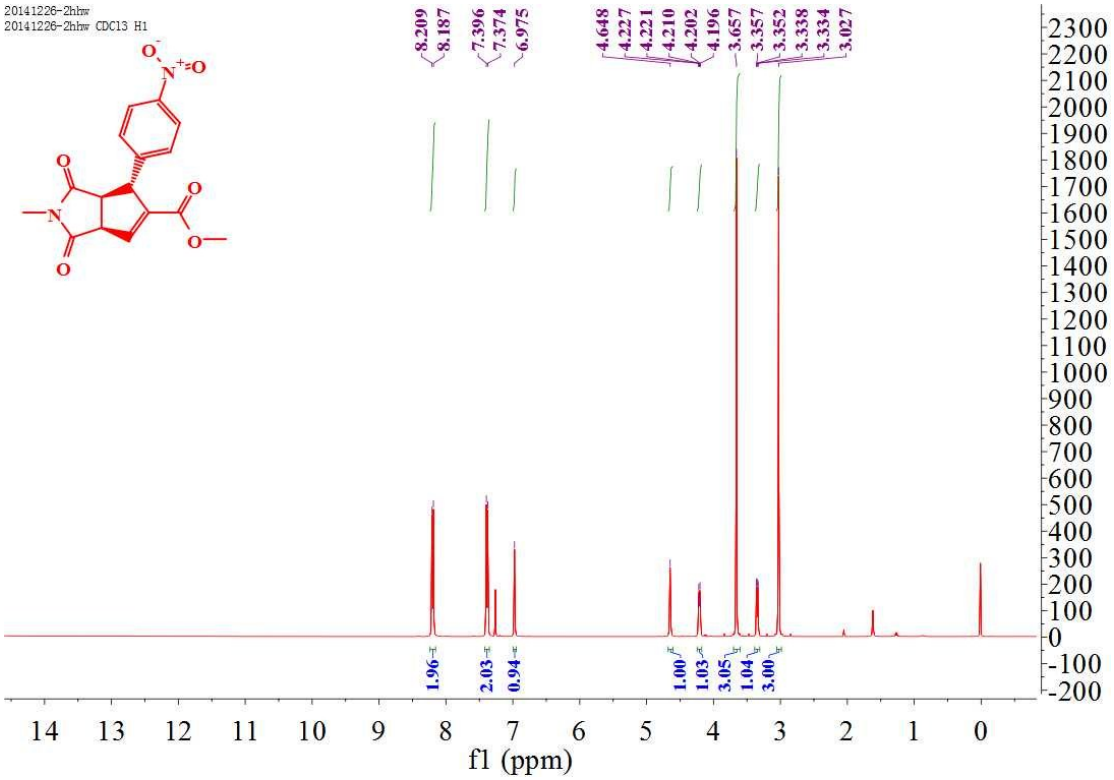

20150613hhw-c13
20150613hhw CDCl3 C13
166.92
134.72
134.10
134.01
133.95
133.80
133.75
133.49
129.92
129.46
129.35
128.92
128.83
128.68
128.62
128.53
69.94
69.10
58.50
49.81
46.05
32.71
30.86
26.51
24.99
20.01
NH
O
P
Fe
Si
210
170
130
90
60
30
0
f1 (ppm)

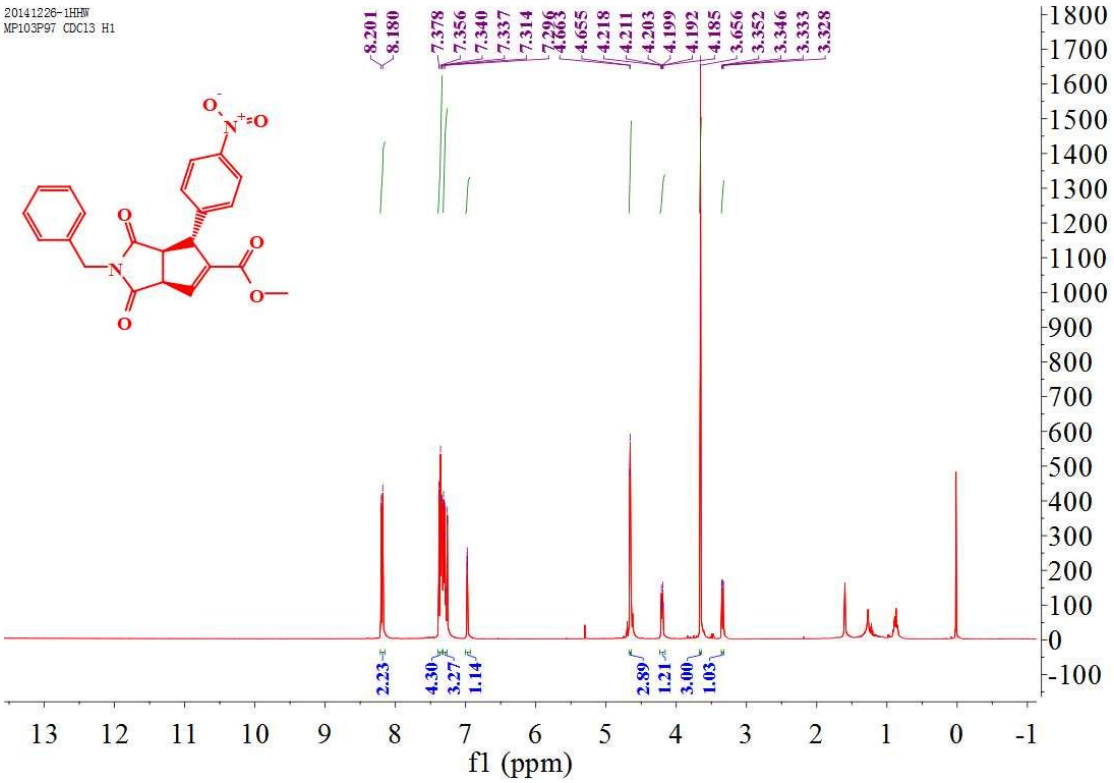

150305
20150304-6 HHW CDC13
O
P
NH
Fe
Si
10.188
400
350
300
250
200
150
100
50
0
200
150
100
50
0
-50
-100
-150
f1 (ppm)

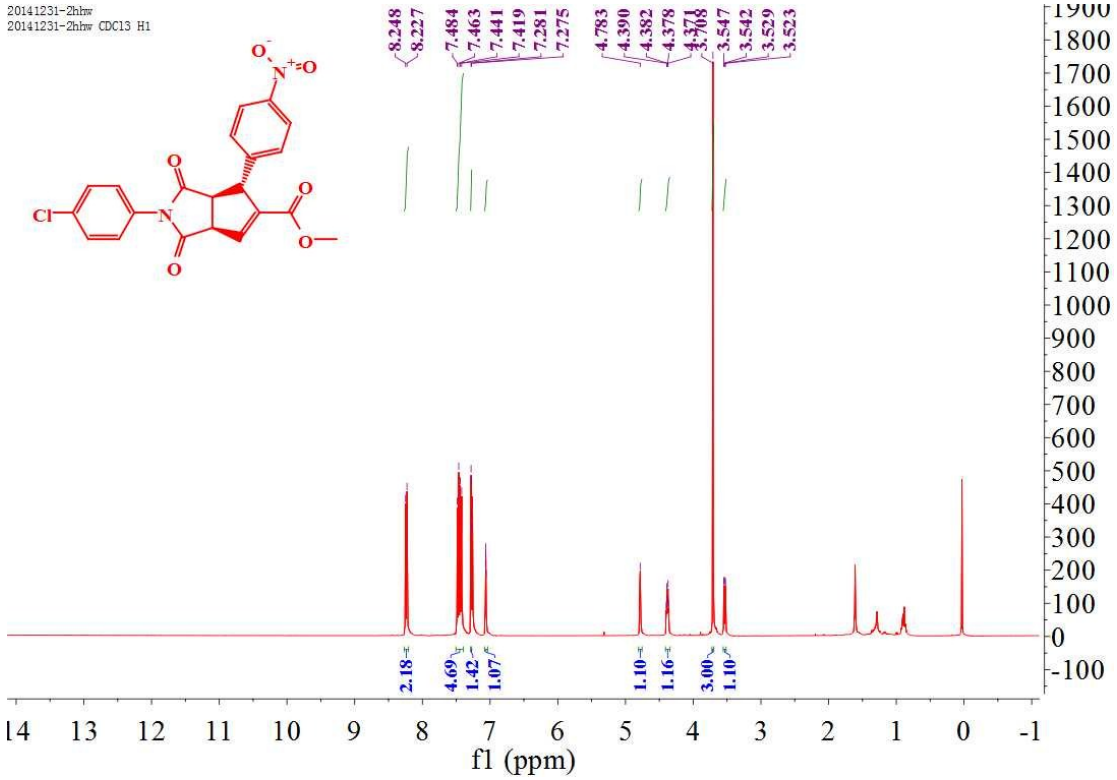

20141223-2hhw
WCH20141230D CDC13 H1
8.238
8.217
7.493
7.436
7.414
7.291
7.273
7.270
4.786
4.782
4.777
4.377
4.366
3.541
3.535
3.522
3.516
O
N
O
O
O
O
O
1.99
2.28
3.23
1.93
0.77
0.95
1.06
3.00
0.99
1600
1500
1400
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
-100
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
f1 (ppm)

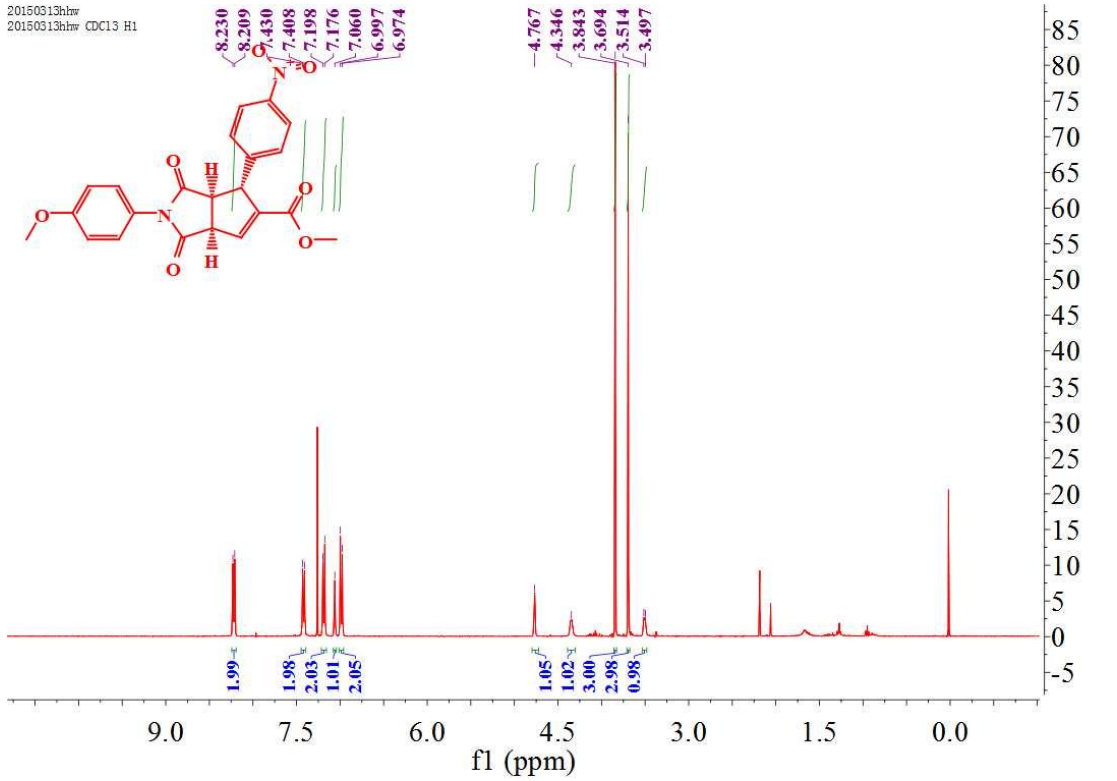

f1 (ppm)

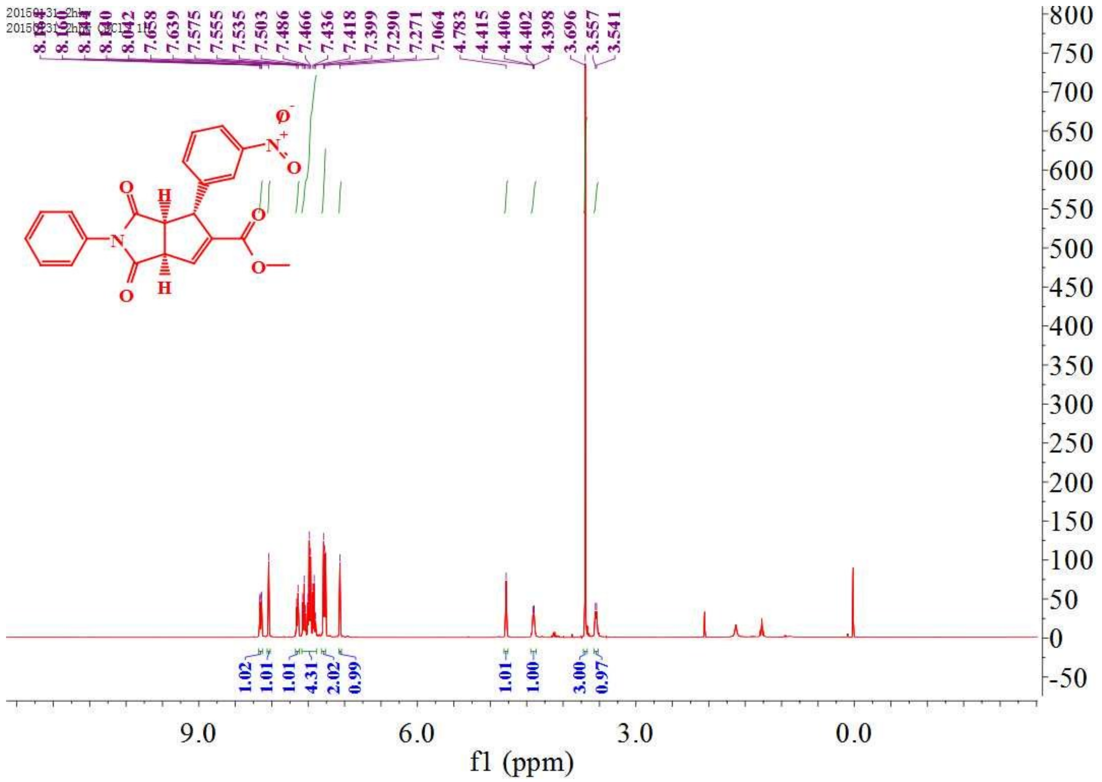

20150104-1hhw
20150104-1hhw CDCl3 1H
f1 (ppm)

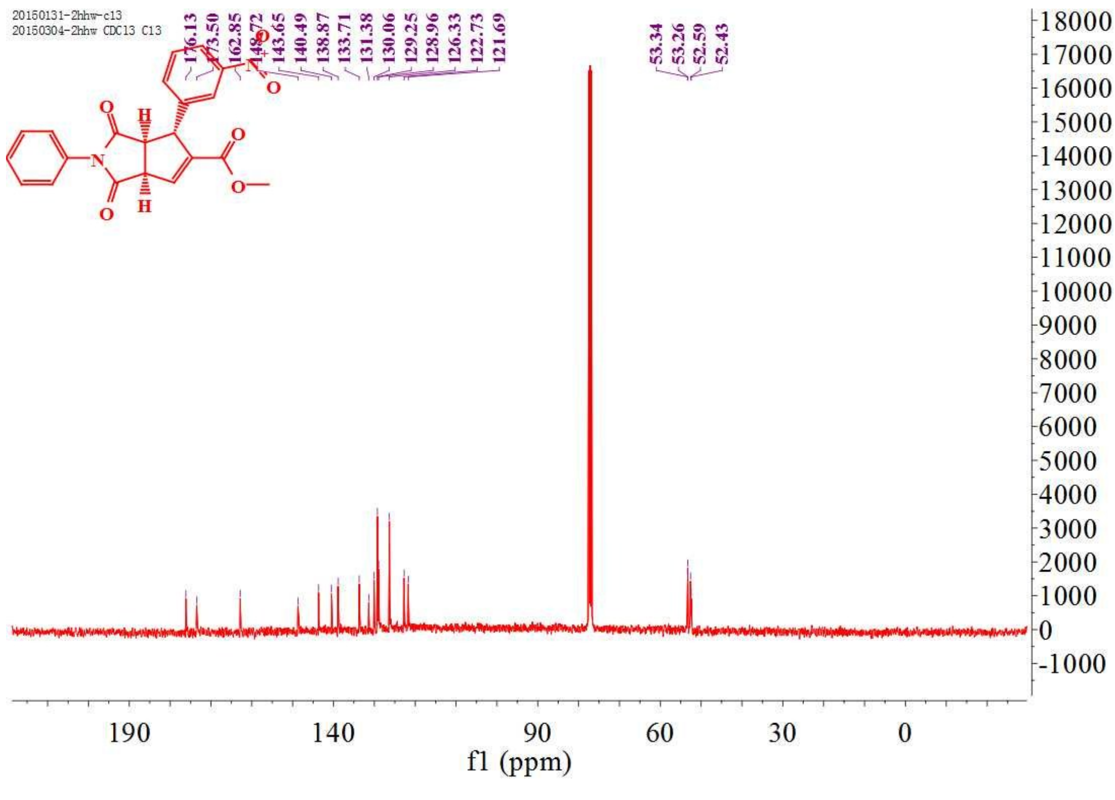

20141226-2hhw
20141226-2hhw CDCl3 H1
8.209
8.187
7.396
7.374
6.975
4.648
4.227
4.221
4.210
4.202
4.196
3.657
3.357
3.352
3.338
3.334
3.027
1.96
2.03
0.94
1.00
1.03
3.05
1.04
3.00
f1 (ppm)

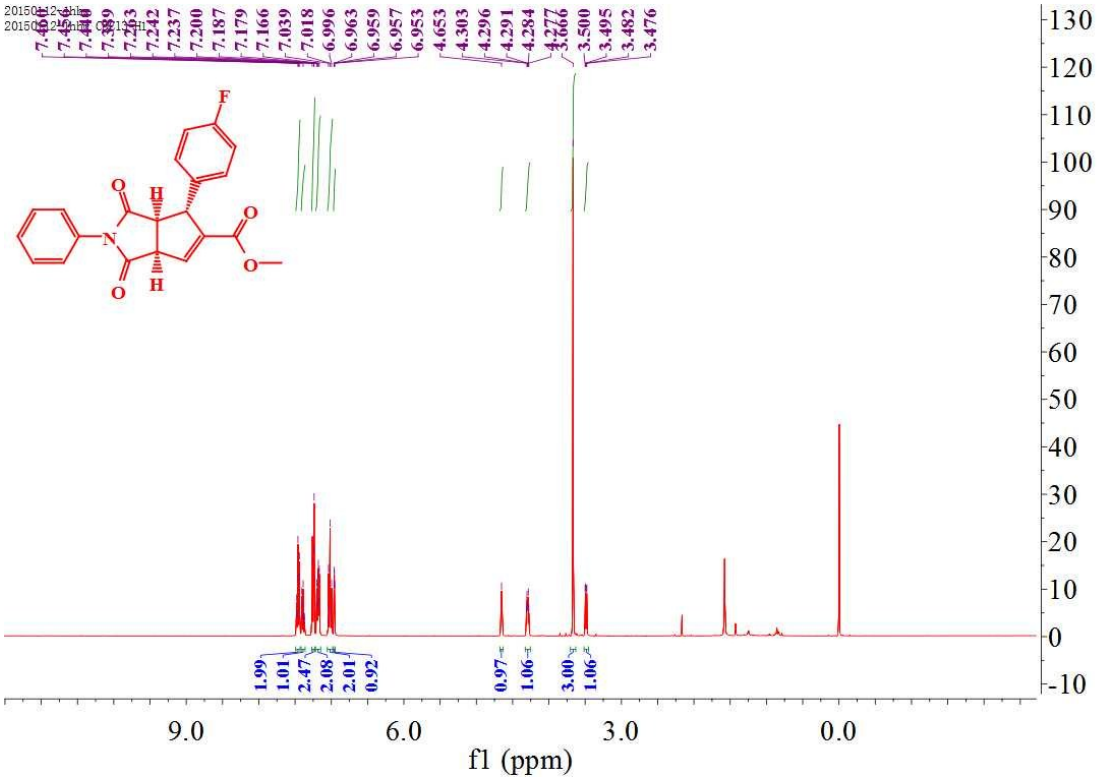

20141226-1HHW
MP103P97 CDCl3 H1
8.201
8.180
7.378
7.356
7.340
7.337
7.314
4.655
4.218
4.211
4.203
4.199
4.192
4.185
3.656
3.352
3.346
3.333
3.328
2.23
4.30
3.27
1.14
2.89
1.21
3.00
1.03
f1 (ppm)

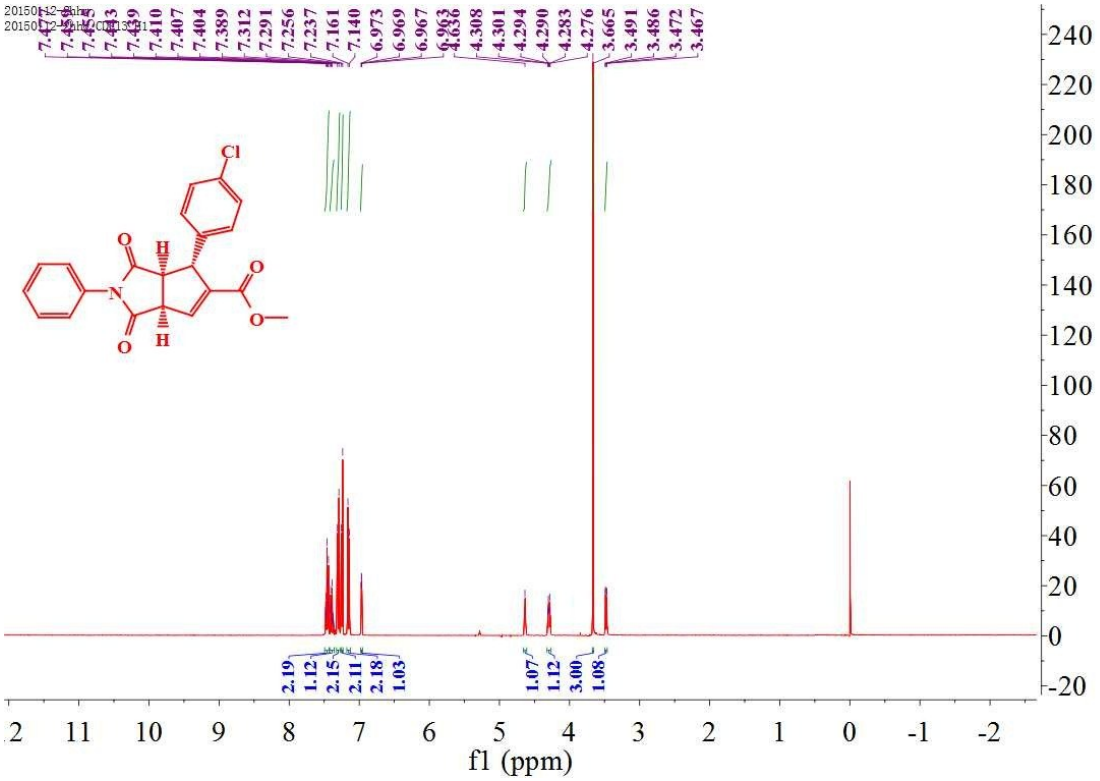

20141231-2hhw
20141231-2hhw CDCl3 H1
8.248
8.227
7.484
7.463
7.441
7.419
7.281
7.275
4.783
4.390
4.382
4.378
3.547
3.542
3.529
3.523
2.18
4.69
1.42
1.07
1.10
1.16
3.00
1.10
f1 (ppm)

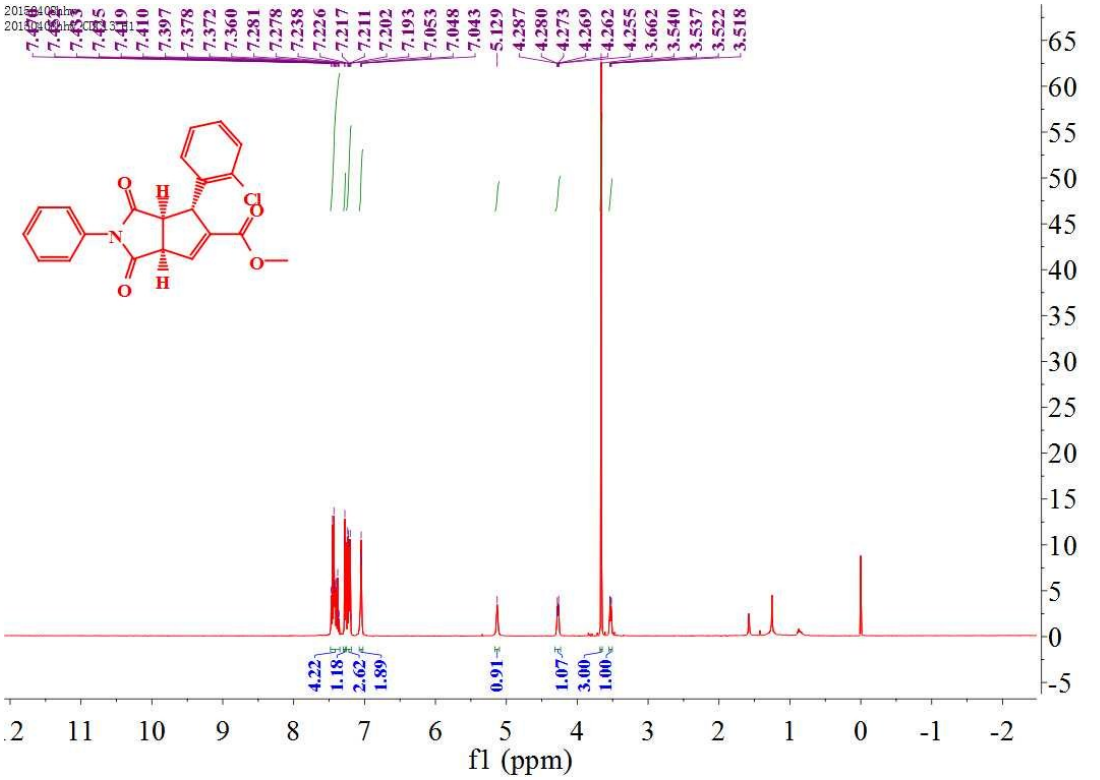

20150313hhw
20150313hhw CDCl3 H1
8.230
8.209
7.430
7.408
7.198
7.176
7.060
6.997
6.974
4.767
4.346
3.843
3.694
3.514
3.497
1.99
1.98
2.03
1.01
2.05
1.05
1.02
3.00
2.98
0.98
f1 (ppm)

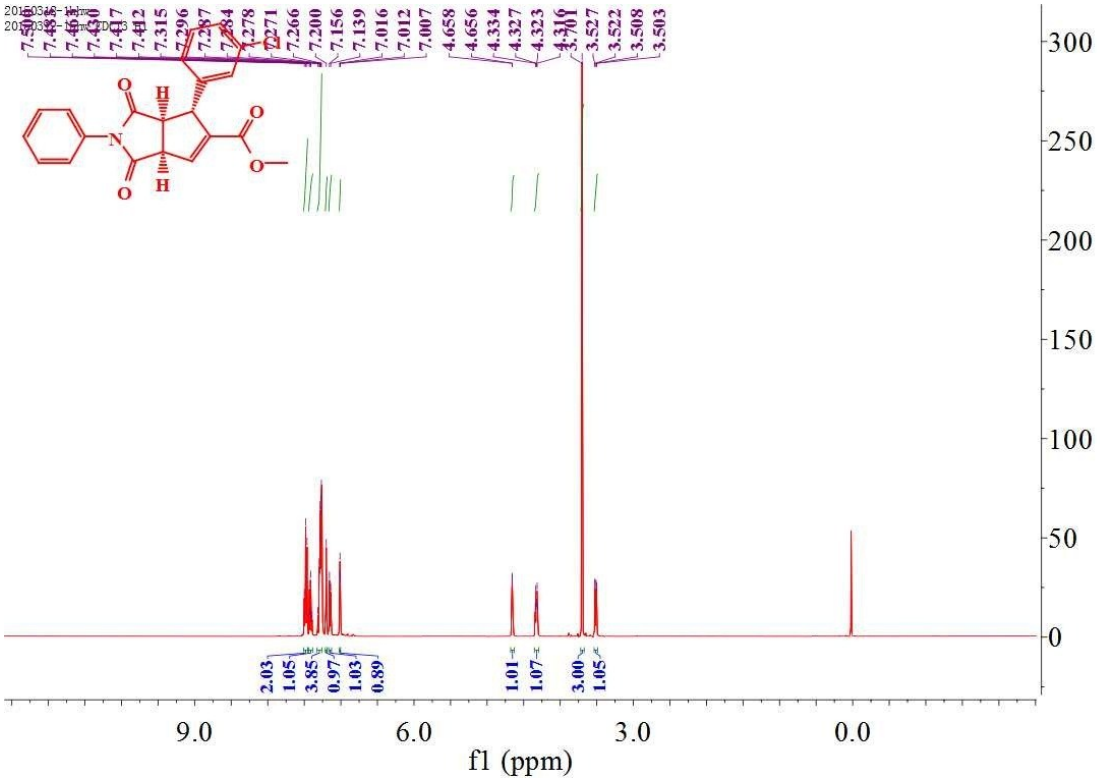

8.160
8.040
8.042
7.658
7.639
7.575
7.555
7.535
7.503
7.486
7.466
7.436
7.418
7.399
7.290
7.271
7.064
4.783
4.415
4.406
4.402
4.398
3.696
3.557
3.541
1.02
1.01
1.01
4.31
2.02
0.99
1.01
1.00
3.00
0.97
9.0
6.0
3.0
0.0
f1 (ppm)

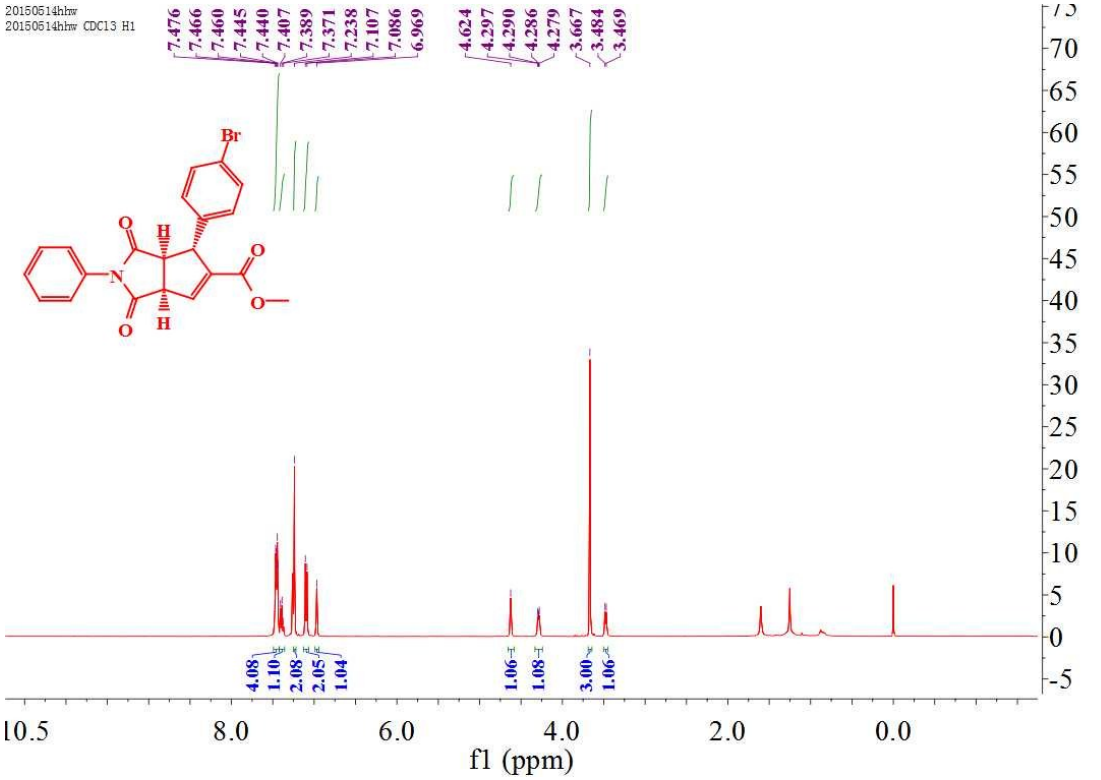

20150131-2hhw-c13
20150304-2hhw CDCl3 C13
176.13
173.50
162.85
148.72
143.65
140.49
138.87
133.71
131.38
130.06
129.25
128.96
126.33
122.73
121.69
53.34
53.26
52.59
52.43
190
140
90
60
30
0
f1 (ppm)

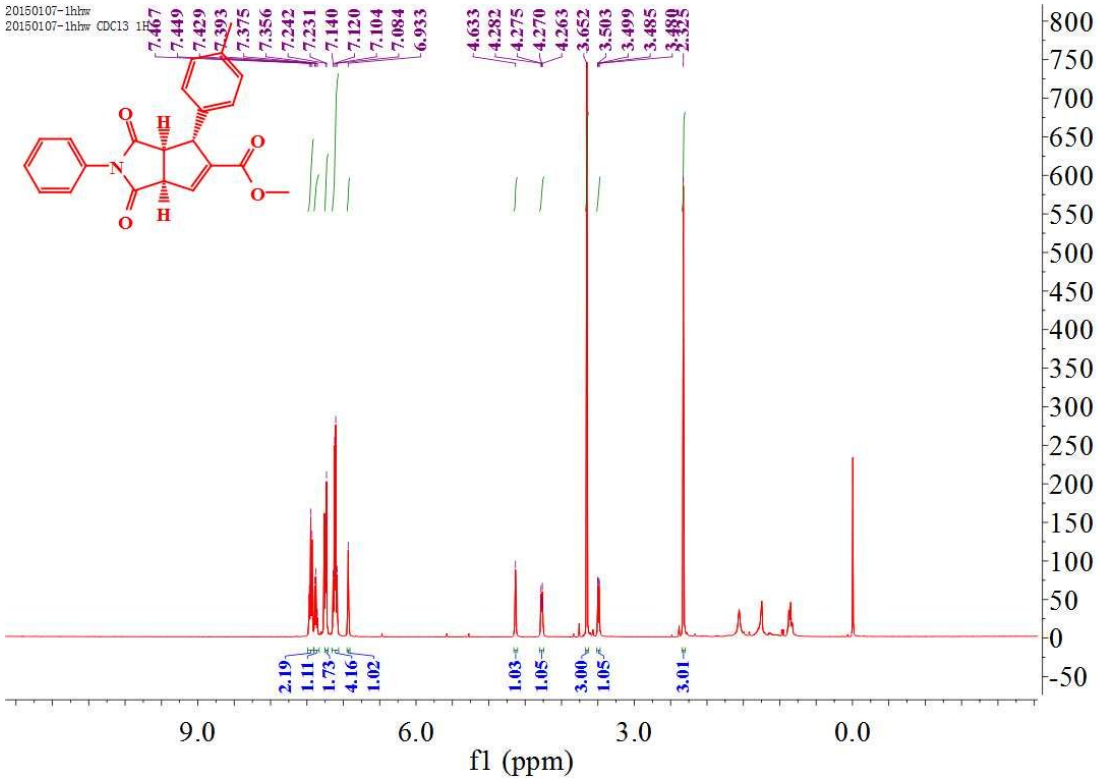

F
O
H
N
O
O
O
H
7.400
7.389
7.263
7.242
7.237
7.200
7.187
7.179
7.166
7.039
7.018
6.996
6.963
6.959
6.957
6.953
4.653
4.303
4.296
4.291
4.284
4.277
3.666
3.500
3.495
3.482
3.476
1.99
1.01
2.47
2.08
2.01
0.92
0.97
1.06
3.00
1.06
9.0
6.0
3.0
0.0
f1 (ppm)

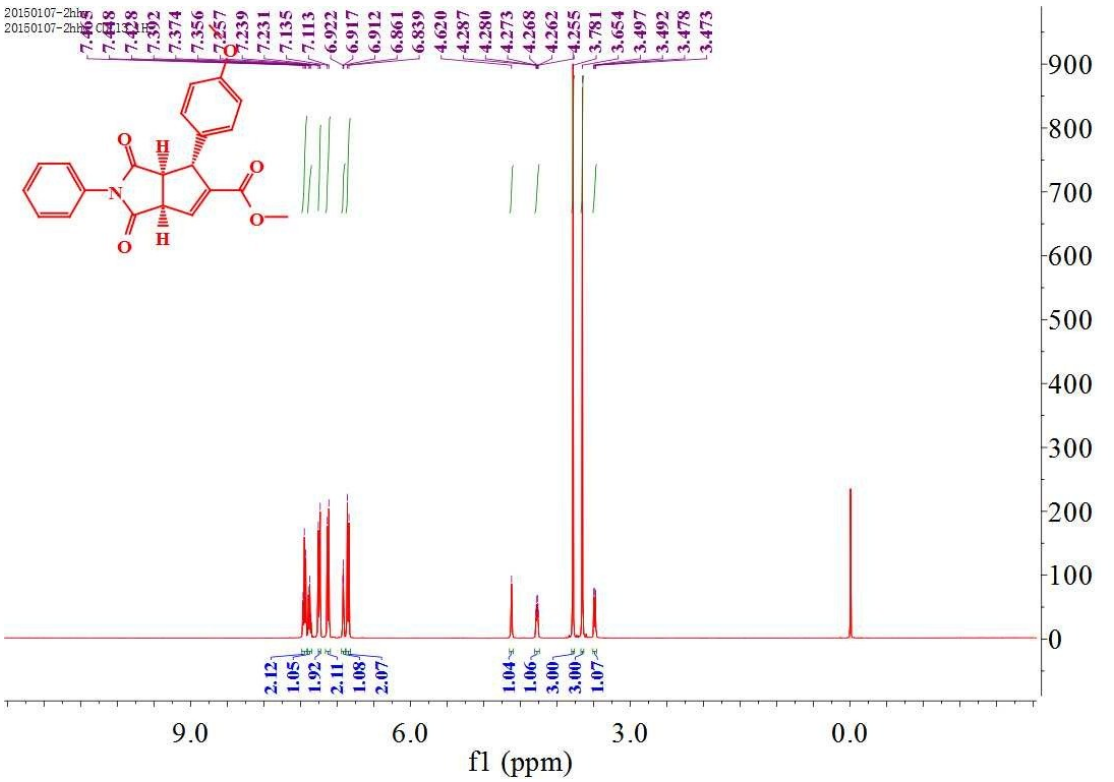

Cl
O
H
N
O
O
O
H
7.455
7.439
7.410
7.407
7.404
7.389
7.312
7.291
7.256
7.237
7.161
7.140
6.973
6.969
6.967
4.308
4.301
4.294
4.290
4.283
4.276
3.665
3.491
3.486
3.472
3.467
2.19
1.12
2.15
2.11
2.18
1.03
1.07
1.12
3.00
1.08
f1 (ppm)

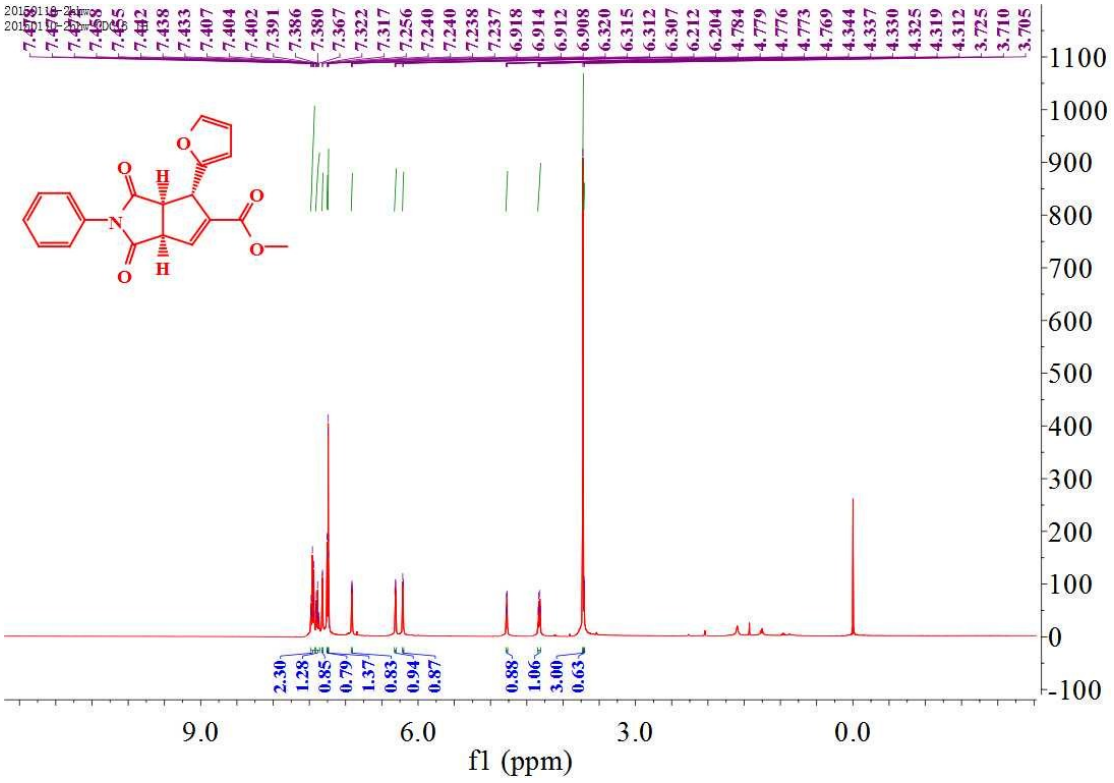

7.433
7.410
7.397
7.378
7.372
7.360
7.281
7.278
7.238
7.226
7.217
7.211
7.202
7.193
7.053
7.048
7.043
5.129
4.287
4.280
4.273
4.269
4.262
4.255
3.662
3.540
3.537
3.522
3.518
4.22
1.18
2.62
1.89
0.91
1.07
3.00
1.00
f1 (ppm)

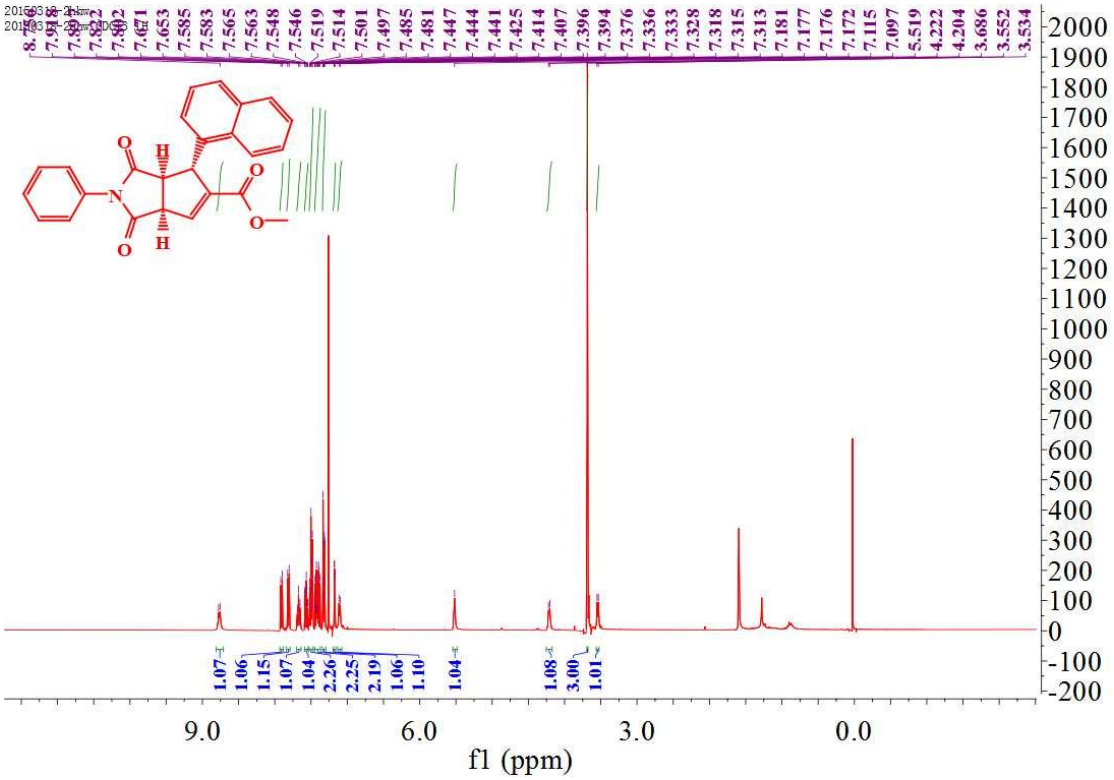

7.487
7.484
7.481
7.430
7.417
7.412
7.315
7.296
7.287
7.284
7.278
7.271
7.266
7.200
7.156
7.139
7.016
7.012
7.007
4.658
4.656
4.334
4.327
4.323
4.316
3.701
3.527
3.522
3.508
3.503
2.03
1.05
3.85
0.97
1.03
0.89
1.01
1.07
3.00
1.05
f1 (ppm)

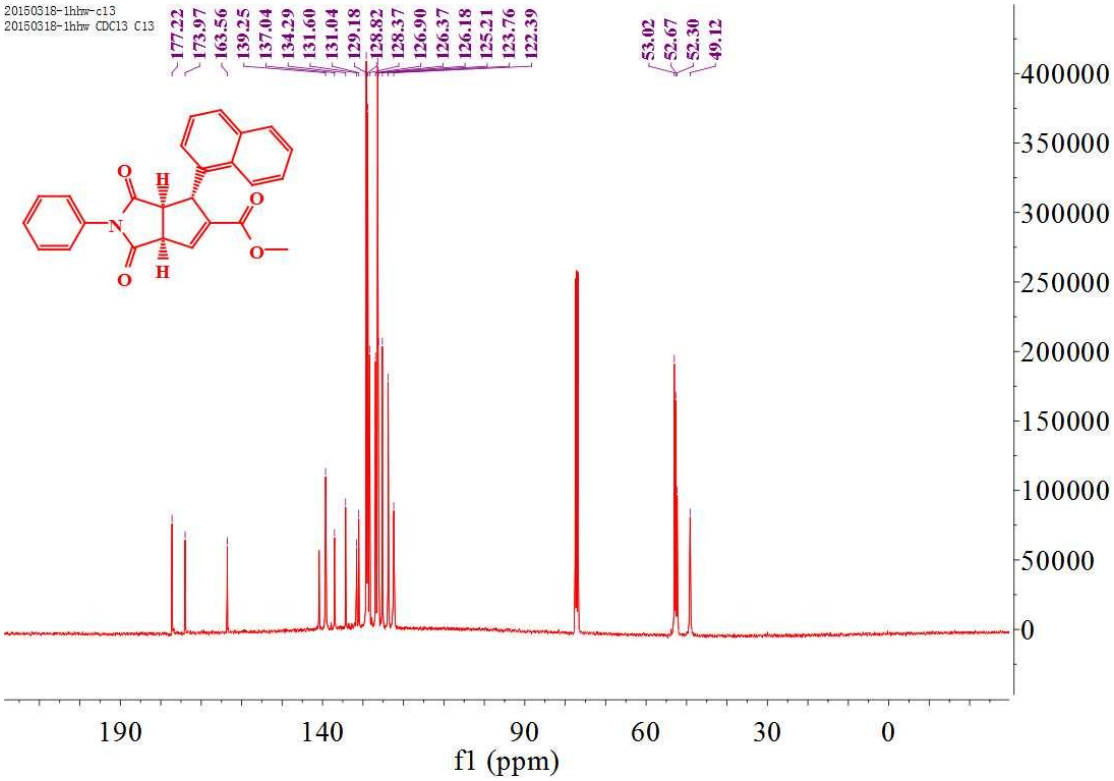

20150514hhw
20150514hhw CDCl3 H1
7.476
7.466
7.460
7.445
7.440
7.407
7.389
7.371
7.238
7.107
7.086
6.969
4.624
4.297
4.290
4.286
4.279
3.667
3.484
3.469
Br
O
H
N
O
O
O
H
4.08
1.10
2.08
2.05
1.04
1.06
1.08
3.00
1.06
10.5
8.0
6.0
4.0
2.0
0.0
f1 (ppm)

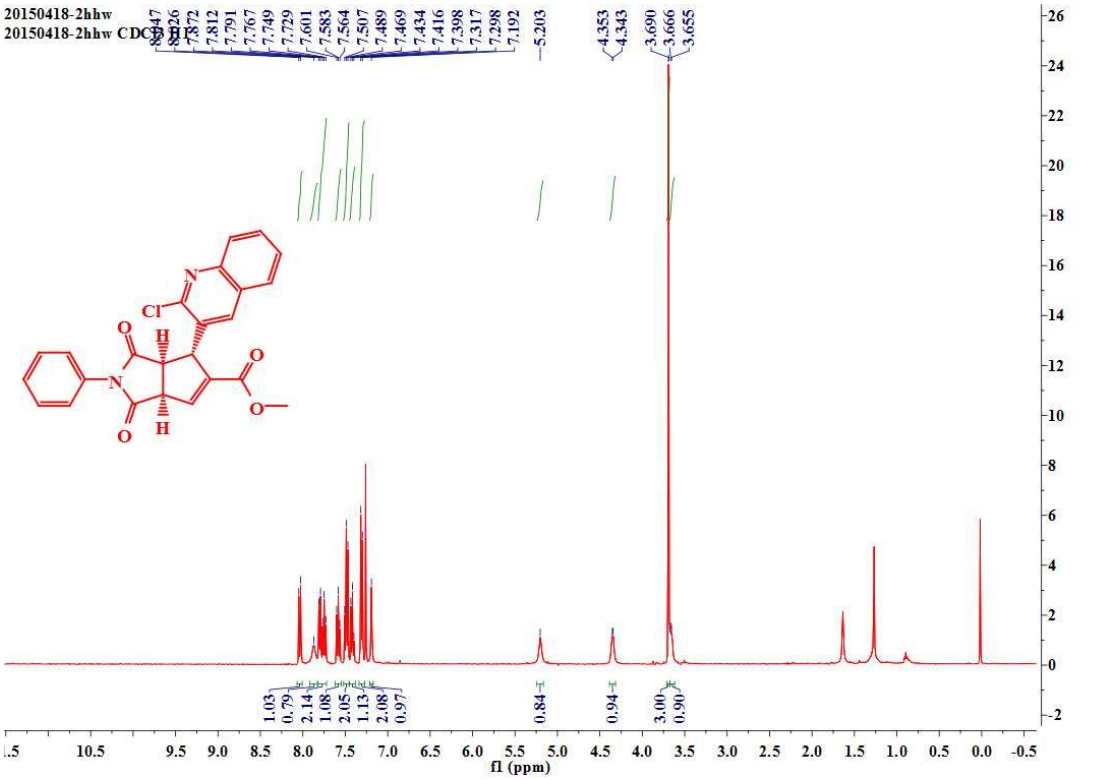

20150107-1hhw
20150107-1hhw CDCl3 1H
7.467
7.449
7.429
7.393
7.375
7.356
7.242
7.231
7.140
7.120
7.104
7.084
6.933
4.633
4.282
4.275
4.270
4.263
3.652
3.503
3.499
3.485
O
H
N
O
O
O
H
2.19
1.11
1.73
4.16
1.02
1.03
1.05
3.00
1.05
3.01
9.0
6.0
3.0
0.0
f1 (ppm)

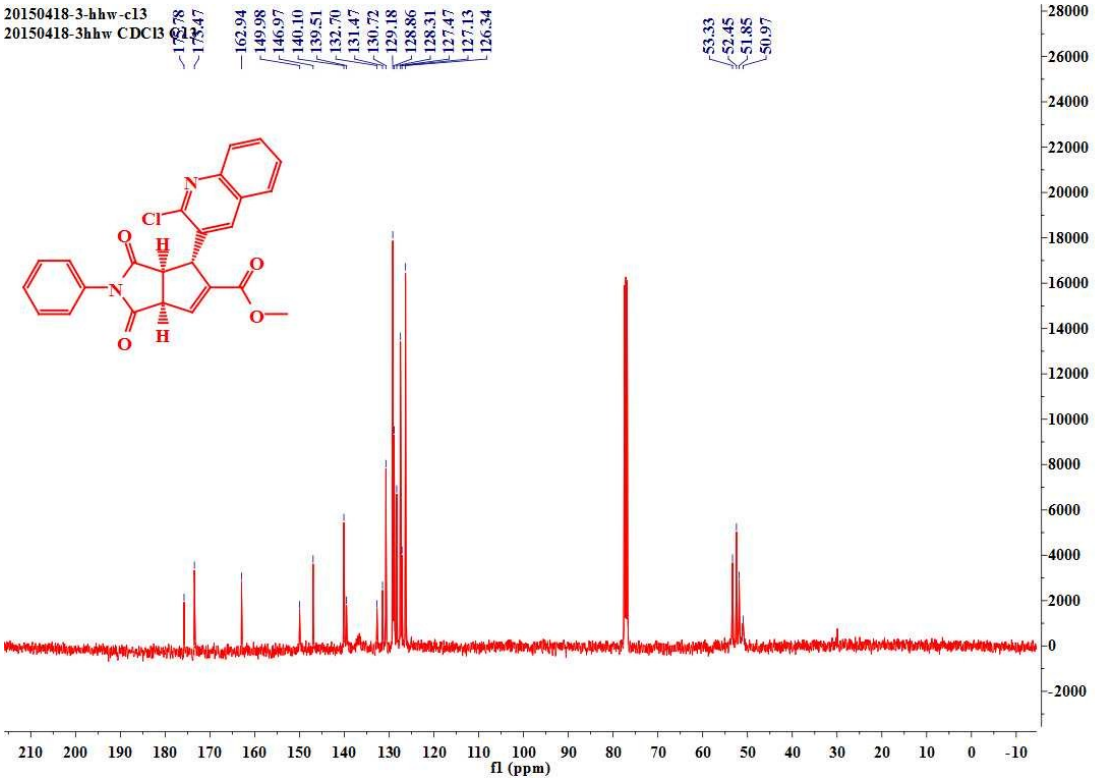

7.465
7.438
7.428
7.392
7.374
7.356
7.257
7.239
7.231
7.135
7.113
6.922
6.917
6.912
6.861
6.839
4.620
4.287
4.280
4.273
4.268
4.262
4.255
3.781
3.654
3.497
3.492
3.478
3.473
2.12
1.05
1.92
2.11
1.08
2.07
1.04
1.06
3.00
3.00
1.07
9.0
6.0
3.0
0.0
f1 (ppm)

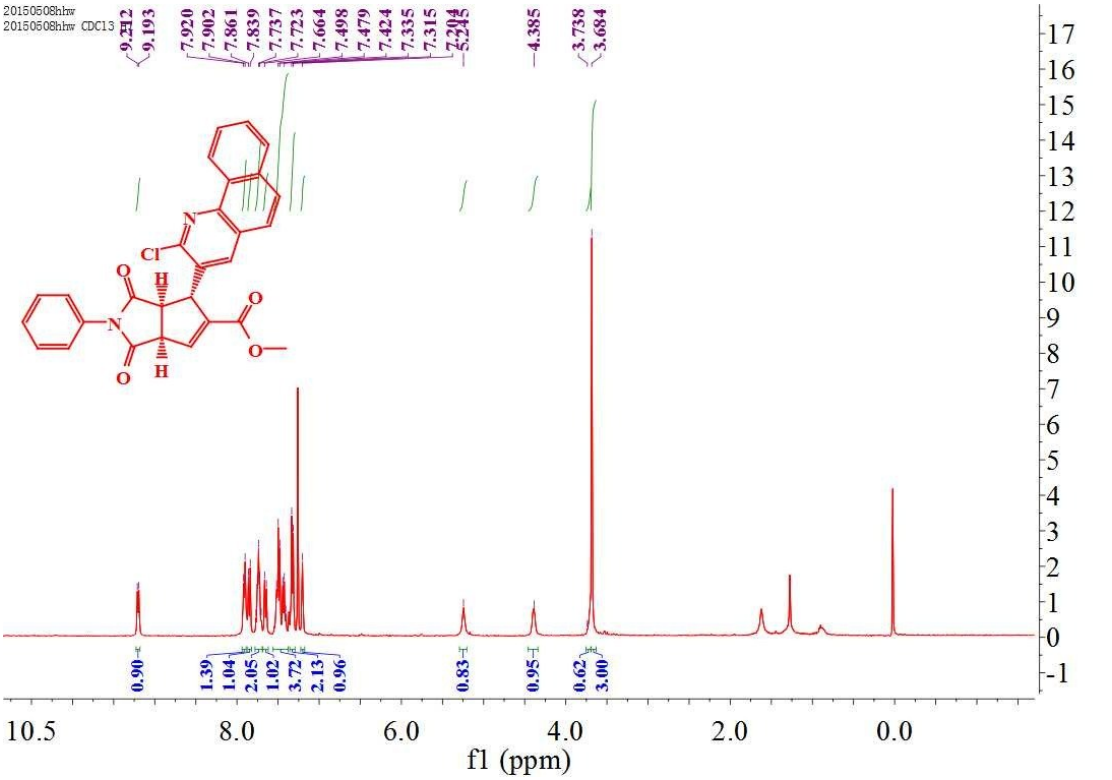

7.465
7.438
7.428
7.392
7.374
7.356
7.257
7.239
7.231
7.135
7.113
6.922
6.917
6.912
6.861
6.839
4.620
4.287
4.280
4.273
4.268
4.262
4.255
3.781
3.654
3.497
3.492
3.478
3.473
2.30
1.28
0.85
0.79
1.37
0.83
0.94
0.87
0.88
1.06
3.00
0.63
9.0
6.0
3.0
0.0
f1 (ppm)

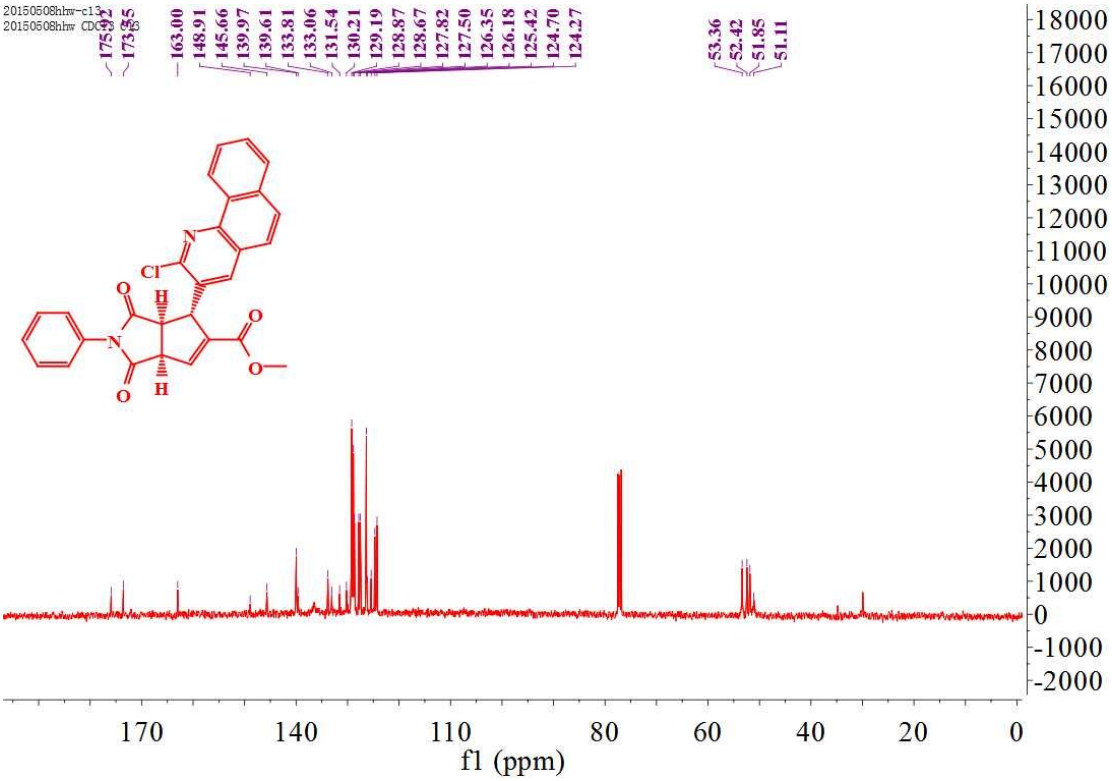

f1 (ppm)

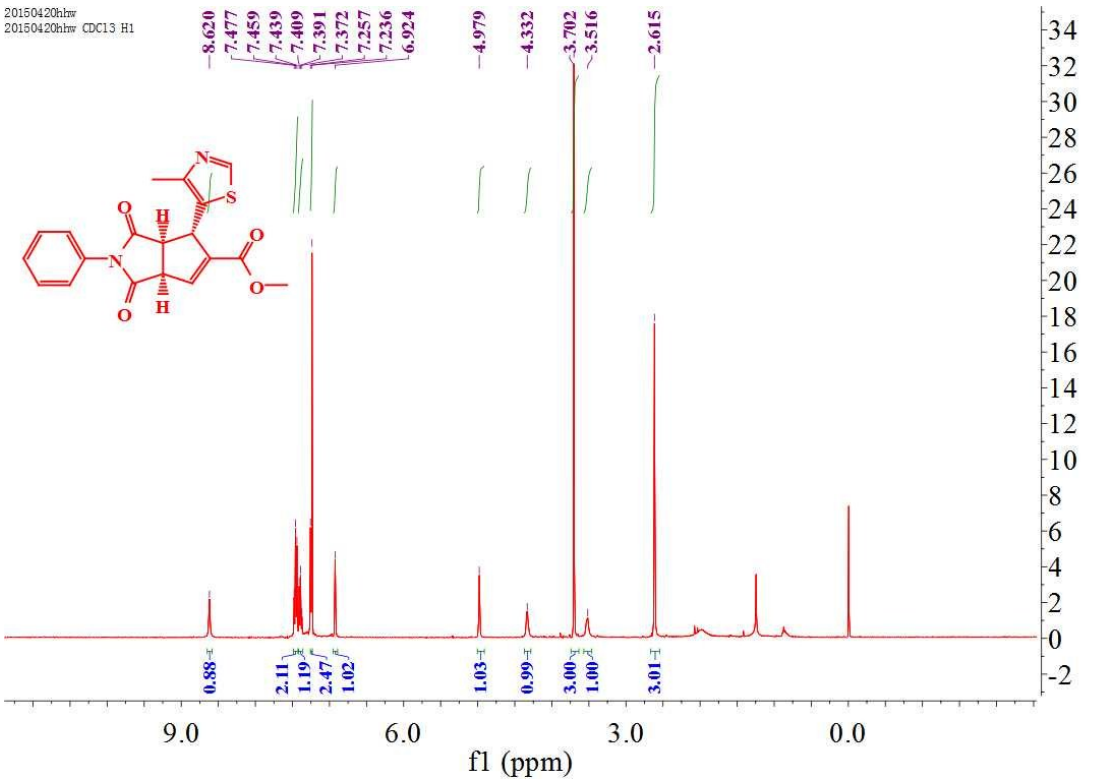

f1 (ppm)

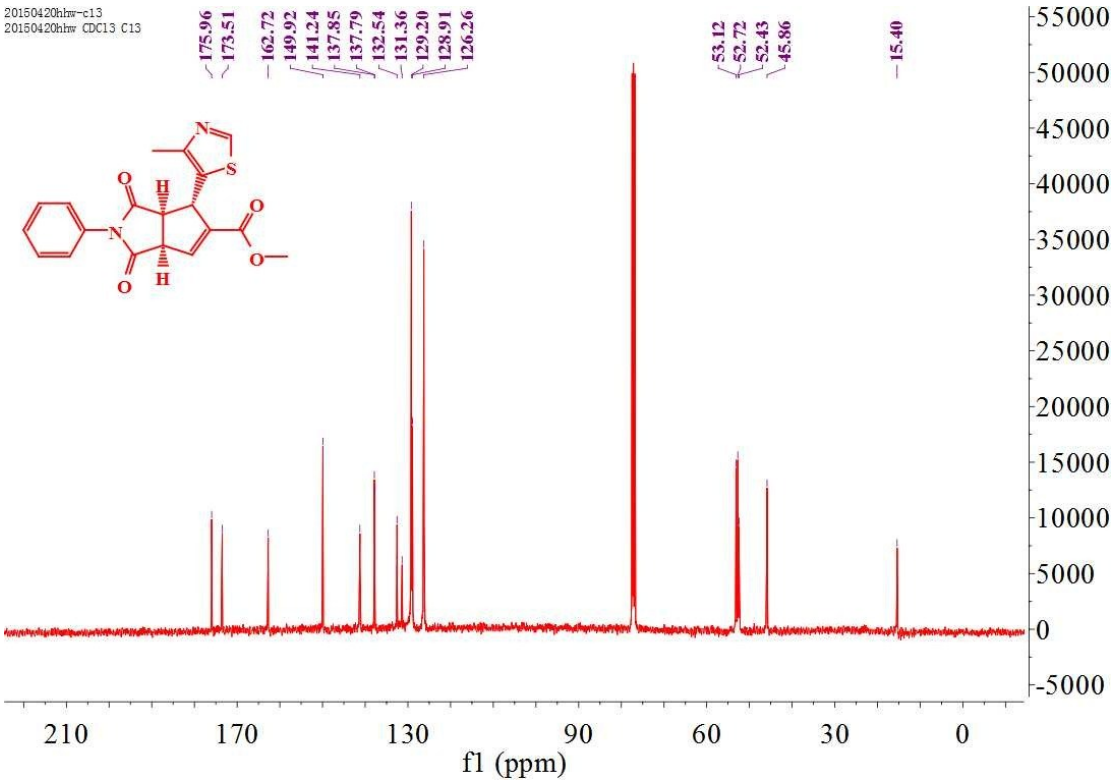

20150418-2hhw
20150418-2hhw CDCl3 H1
8.447
8.426
7.872
7.812
7.791
7.767
7.749
7.729
7.601
7.583
7.564
7.507
7.489
7.469
7.434
7.416
7.398
7.317
7.298
7.192
5.203
4.353
4.343
3.690
3.666
3.655
1.03
0.79
2.14
1.08
2.05
1.13
2.08
0.97
0.84
0.94
3.00
0.90
fl (ppm)

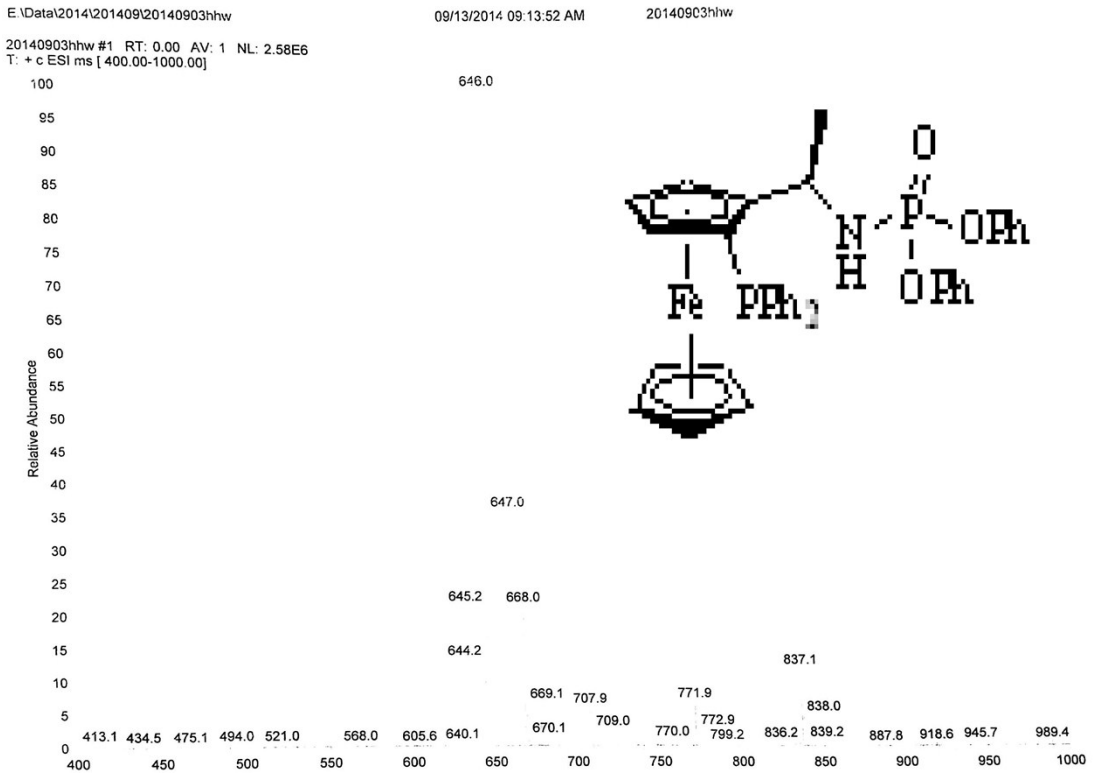

20150418-3-hhw-c13
20150418-3hhw CDCl3 C13
177.78
175.47
162.94
149.98
146.97
140.10
139.51
132.70
131.47
130.72
129.18
128.86
128.31
127.47
127.13
126.34
53.33
52.45
51.85
50.97
fl (ppm)


20150508hhw
20150508hhw CDCl3
9.212
9.193
7.920
7.902
7.861
7.839
7.737
7.723
7.664
7.498
7.479
7.424
7.335
7.315
4.385
3.738
3.684
0.90
1.39
1.04
2.05
1.02
3.72
2.13
0.96
0.83
0.95
0.62
3.00
f1 (ppm)


20150508hhw-c13
20150508hhw CDCl3
175.92
173.35
163.00
148.91
145.66
139.97
139.61
133.81
133.06
131.54
130.21
129.19
128.87
128.67
127.82
127.50
126.35
126.18
125.42
124.70
124.27
53.36
52.42
51.85
51.11
f1 (ppm)


20150420hhw
20150420hhw CDC13 H1
8.620
7.477
7.459
7.439
7.409
7.391
7.372
7.257
7.236
6.924
4.979
4.332
3.702
3.516
2.615
0.88
2.11
1.19
2.47
1.02
1.03
0.99
3.00
1.00
3.01
f1 (ppm)


20150420hhw-c13
20150420hhw CDC13 C13
175.96
173.51
162.72
149.92
141.24
137.85
137.79
132.54
131.36
129.20
128.91
126.26
53.12
52.72
52.43
45.86
15.40
f1 (ppm)



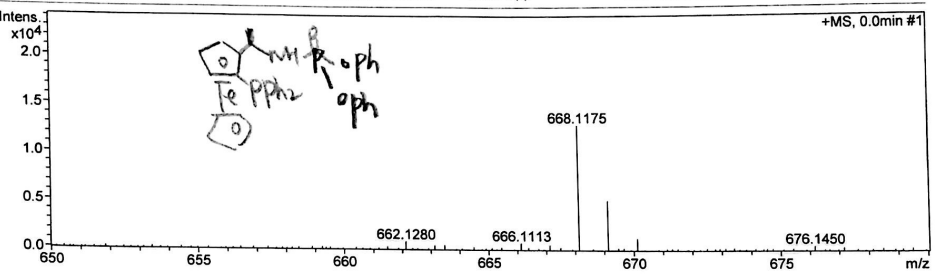
Mass Spectrum SmartFormula Report

Analysis Info

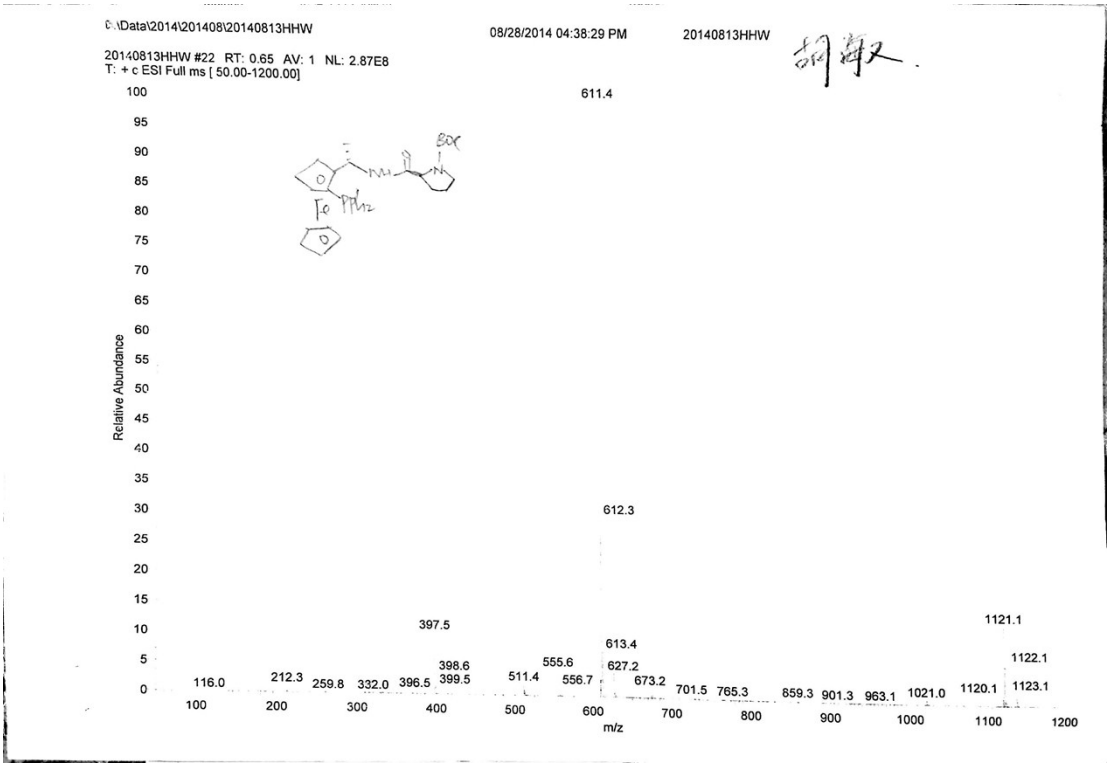
Analysis Name	D:\Data\2015\03.29\20140903HHW.d	Acquisition Date	3/29/2015 12:18:11 PM
Method	tune_POS_low.m		
Sample Name	20140903HHW	Operator	bruker
Comment		Instrument / Ser#	micrOTOF-Q II 10366

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Waste



Meas. m/z	Formula	m/z	err [ppm]	mSigma
668.1175	C 36 H 33 Fe N Na O 3 P 2	668.1178	0.5	11.7



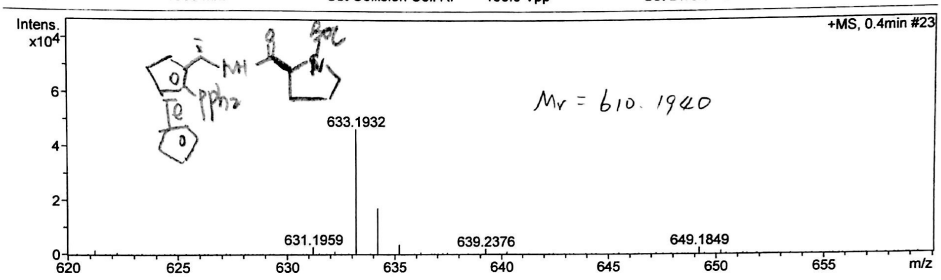
Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name	D:\Data\2014\11.13\20141111HHW.d	Acquisition Date	11/27/2014 3:32:10 PM
Method	tune_POS_low.m	Operator	bruker
Sample Name	ZJD20141031-2	Instrument / Ser#	micrOTOF-Q II 10366
Comment			

Acquisition Parameter

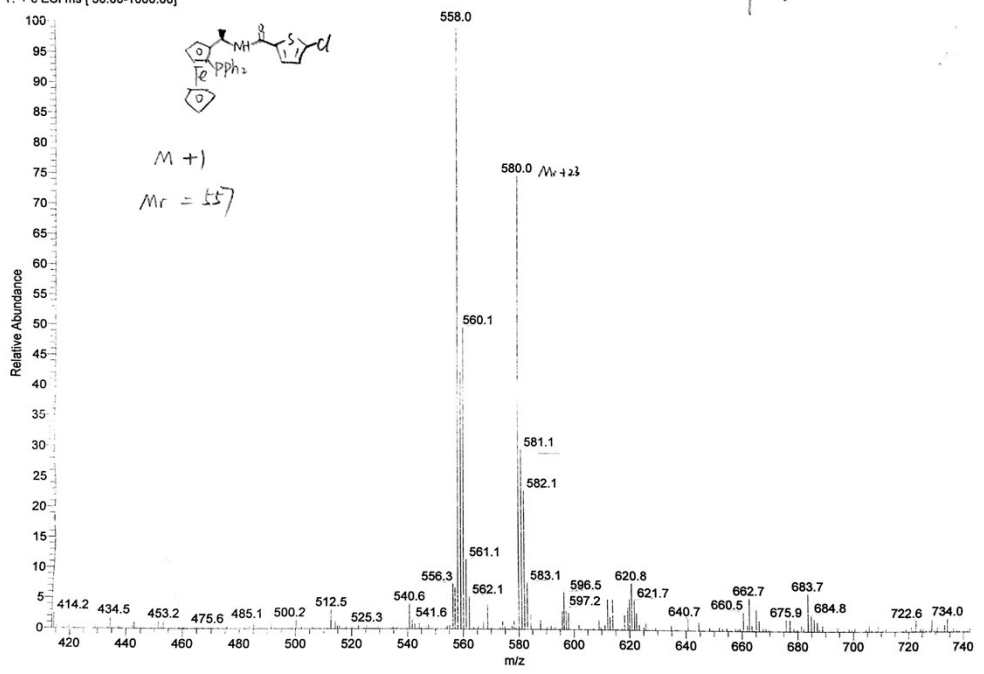
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Waste



Meas. m/z	Formula	m/z	err [ppm]	mSigma
633.1932	C 34 H 39 Fe N 2 Na O 3 P	633.1940	1.3	14.9

E:\Data\...\20141216-1HHW_141223101433 12/23/2014 10:14:33 AM 20141118-1HHW

20141216-1HHW_141223101433 #5 RT: 0.13 AV: 1 NL: 1.24E6
T: + c ESI ms [50.00-1000.00]



M+1

Mr = 557

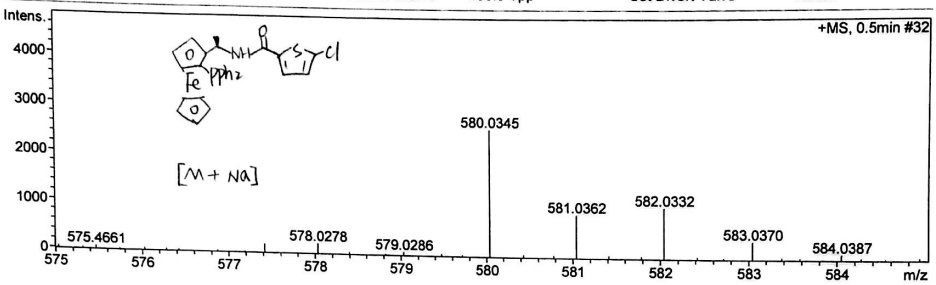
Mass Spectrum SmartFormula Report

Analysis Info

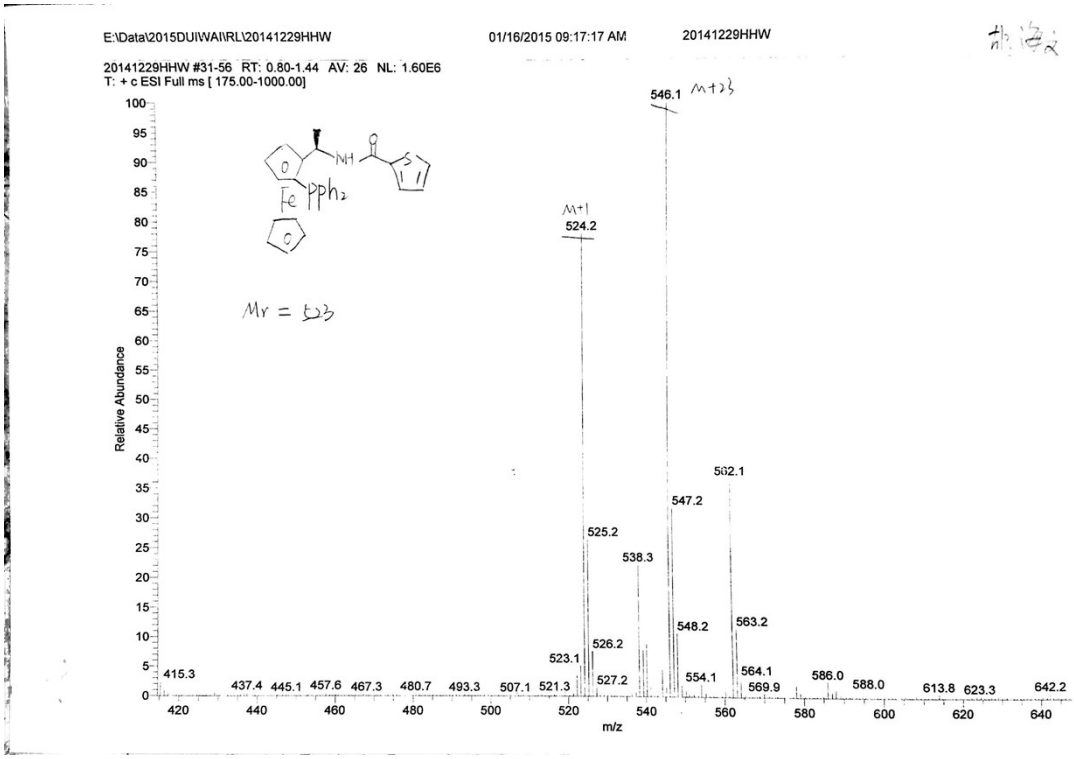
Analysis Name	D:\Data\2015\1.23\20141222-2HHW..d	Acquisition Date	1/22/2015 3:13:26 PM
Method	tune_POS_low.m		
Sample Name	20141222-2HHW.	Operator	bruker
Comment		Instrument / Ser#	micrOTOF-Q II 10366

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Waste



Meas. m/z	Formula	m/z	err [ppm]	mSigma
580.0345	C 29 H 25 Cl Fe N Na O P S	580.0325	-3.5	10.2



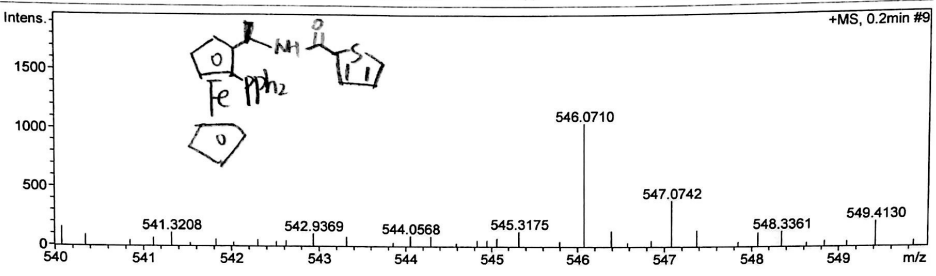
Mass Spectrum SmartFormula Report

Analysis Info

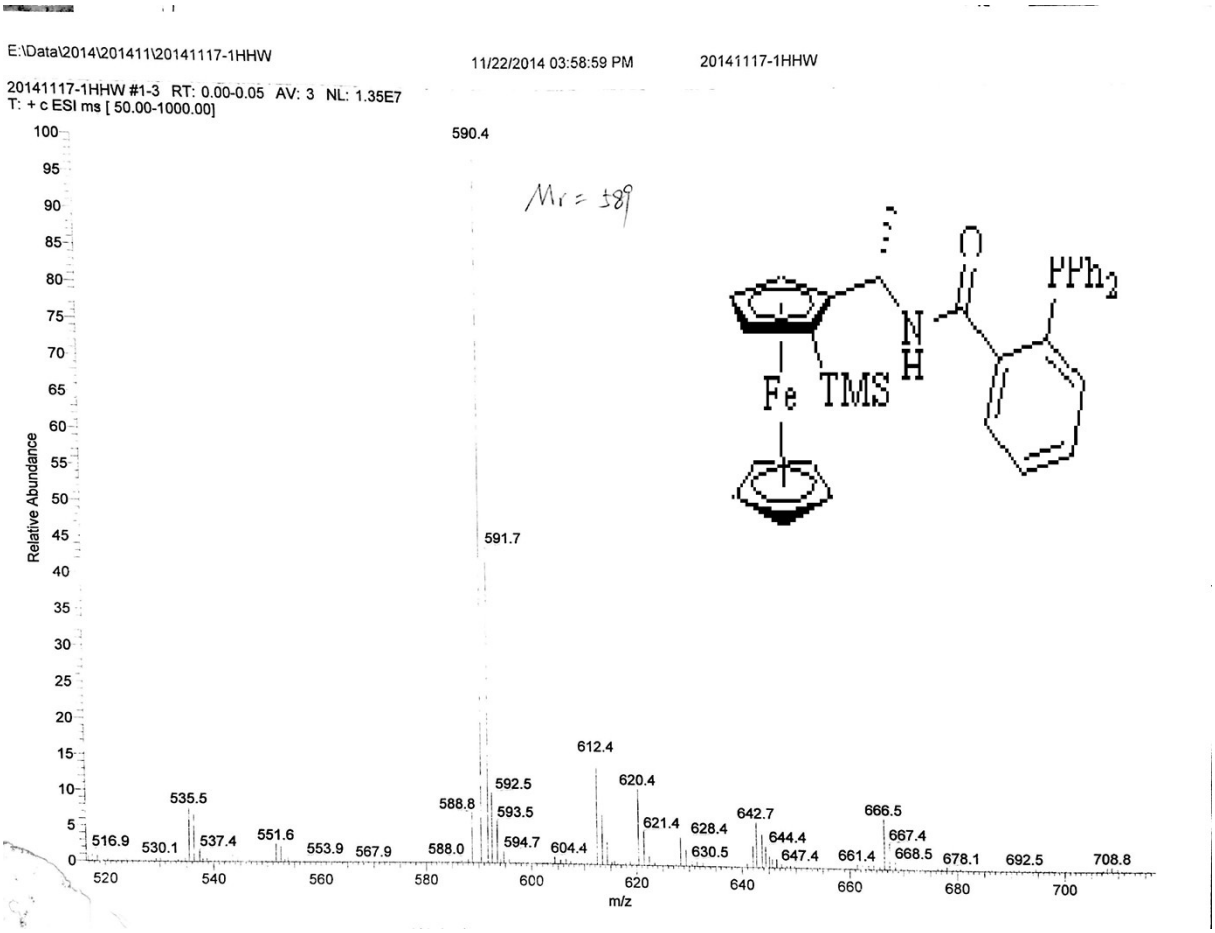
Analysis Name	D:\Data\2015\03.29\20141229HHW.d	Acquisition Date	3/29/2015 12:31:09 PM
Method	tune_POS_low.m	Operator	bruker
Sample Name	20141229HHW	Instrument / Ser#	micrOTOF-Q II 10366
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Waste



Meas. m/z	Formula	m/z	err [ppm]	mSigma
546.0710	C 29 H 26 Fe N Na O P S	546.0714	0.7	22.3



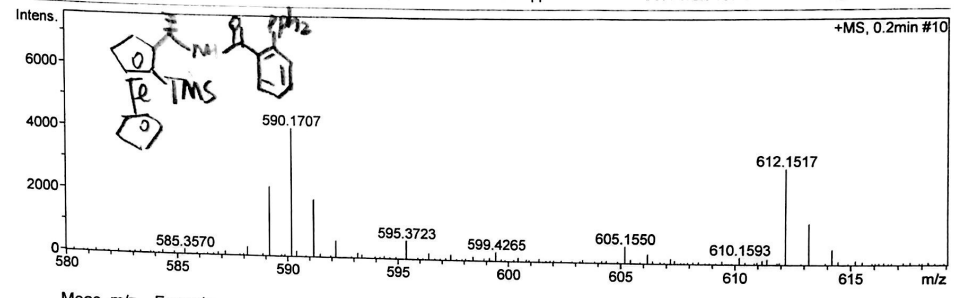
Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name	D:\Data\2015\03.29\20141117-1-HHW.d	Acquisition Date	3/29/2015 12:53:29 PM
Method	tune_POS_low.m	Operator	bruker
Sample Name	20141117-1-HHW	Instrument / Ser#	micrOTOF-Q II 10366
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Waste



Meas. m/z	Formula	m/z	err [ppm]	mSigma
612.1517	C 34 H 36 Fe N Na O P Si	612.1546	4.7	16.5

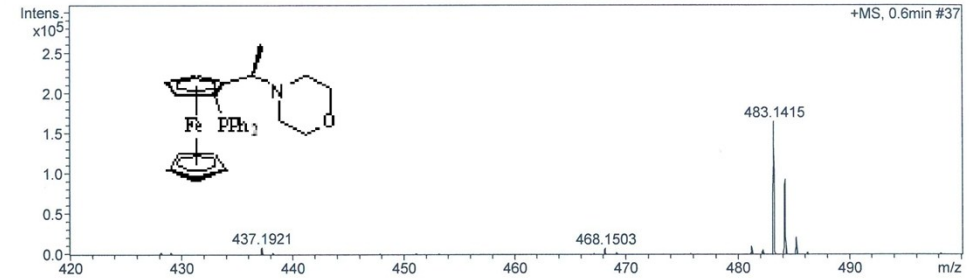
Mass Spectrum SmartFormula Report

Analysis Info

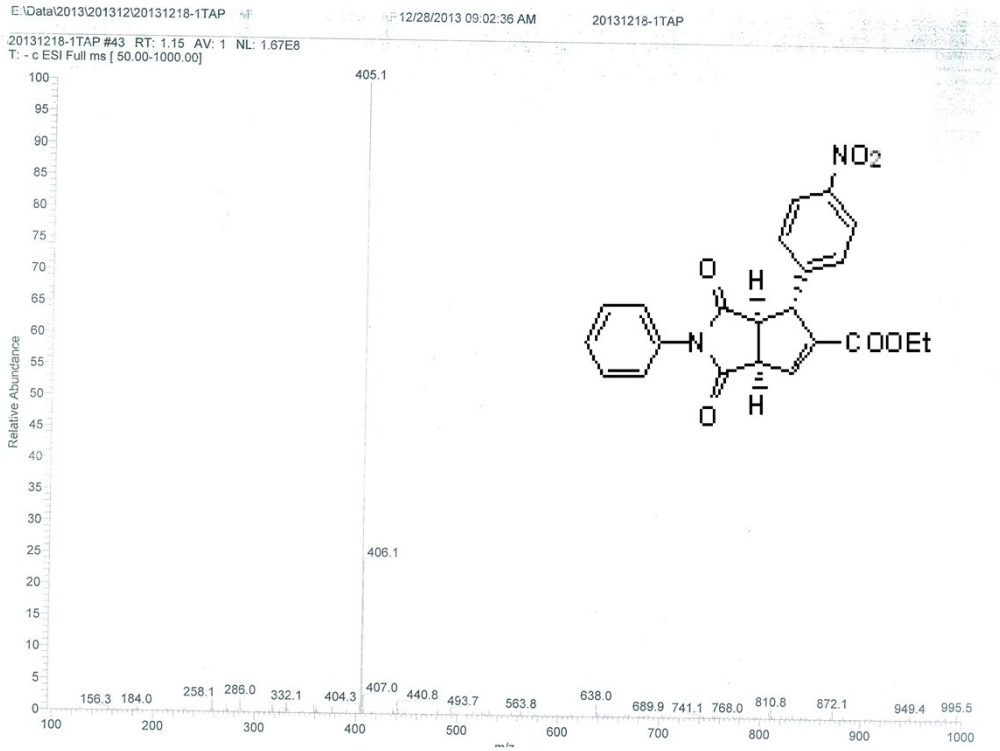
Analysis Name	D:\Data\2013\12.27\20131221-2TAP.d	Acquisition Date	12/27/2013 2:39:01 PM
Method	tune_POS_low.m	Operator	bruker
Sample Name	20131221-2TAP	Instrument / Ser#	micrOTOF-Q II 10366
Comment			

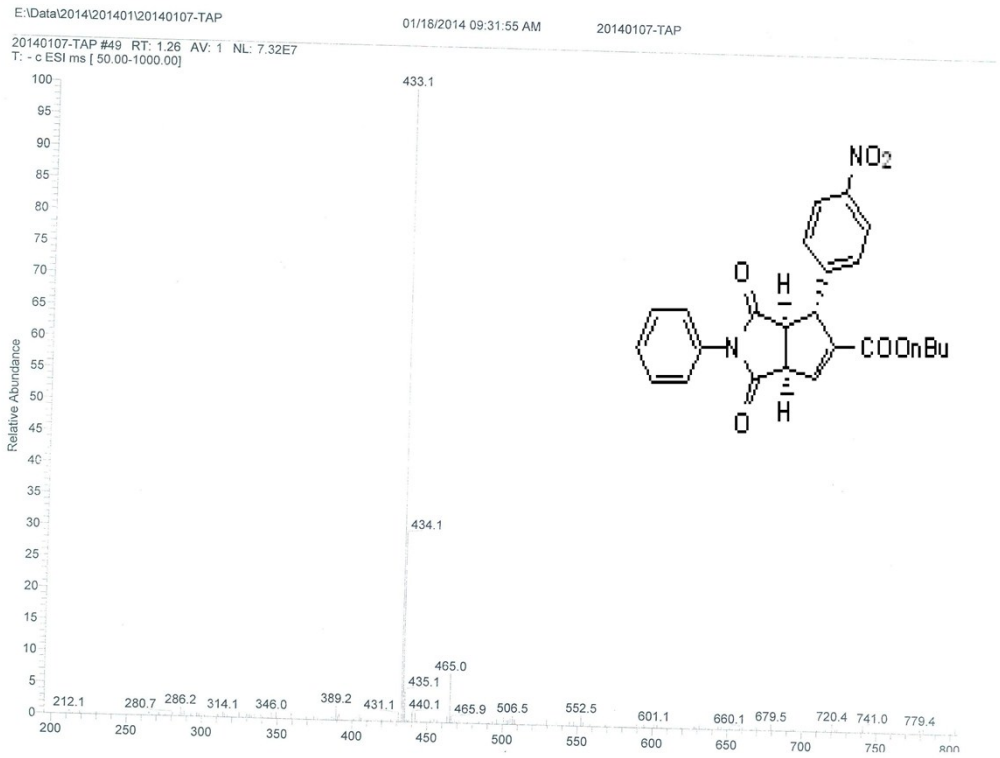
Acquisition Parameter

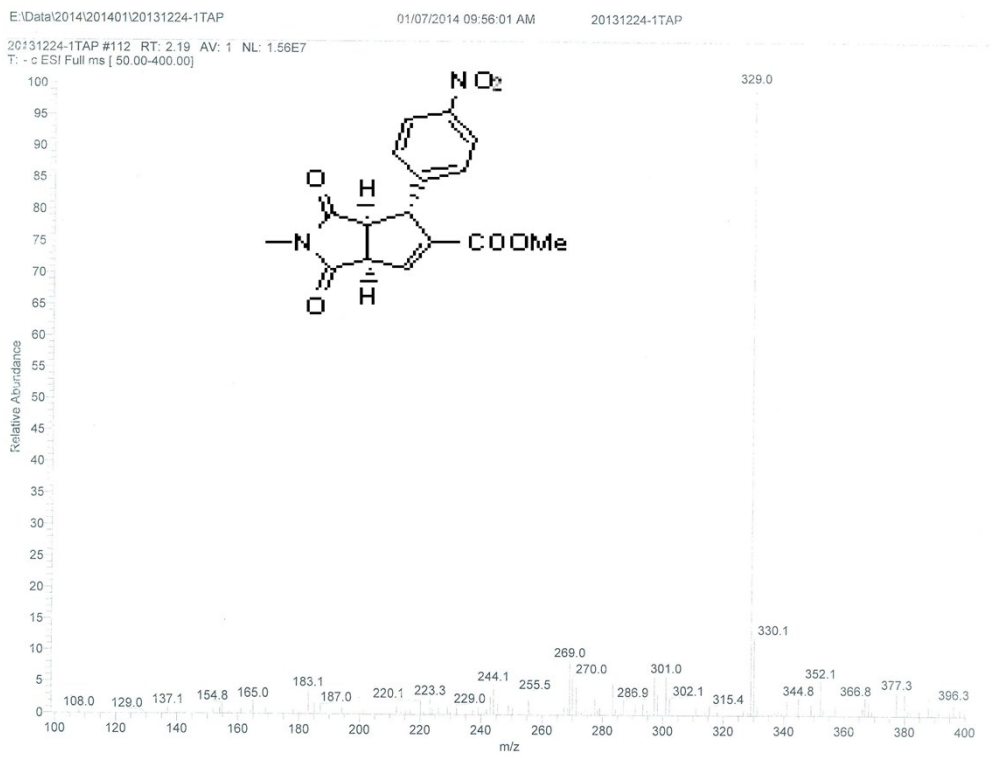
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Waste

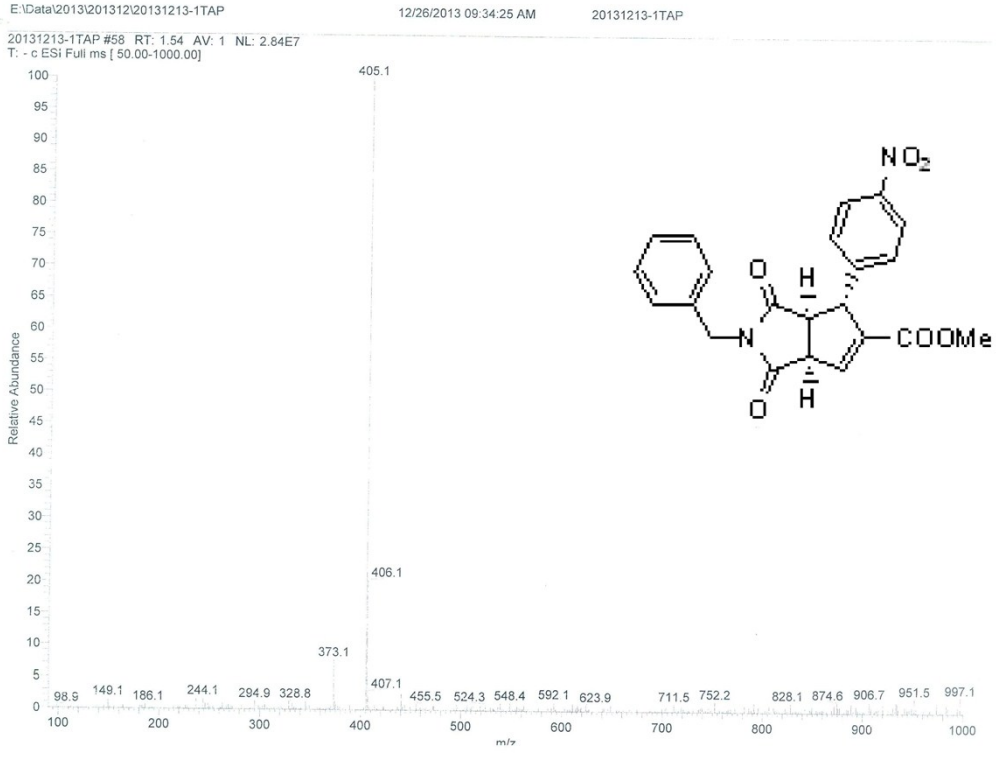


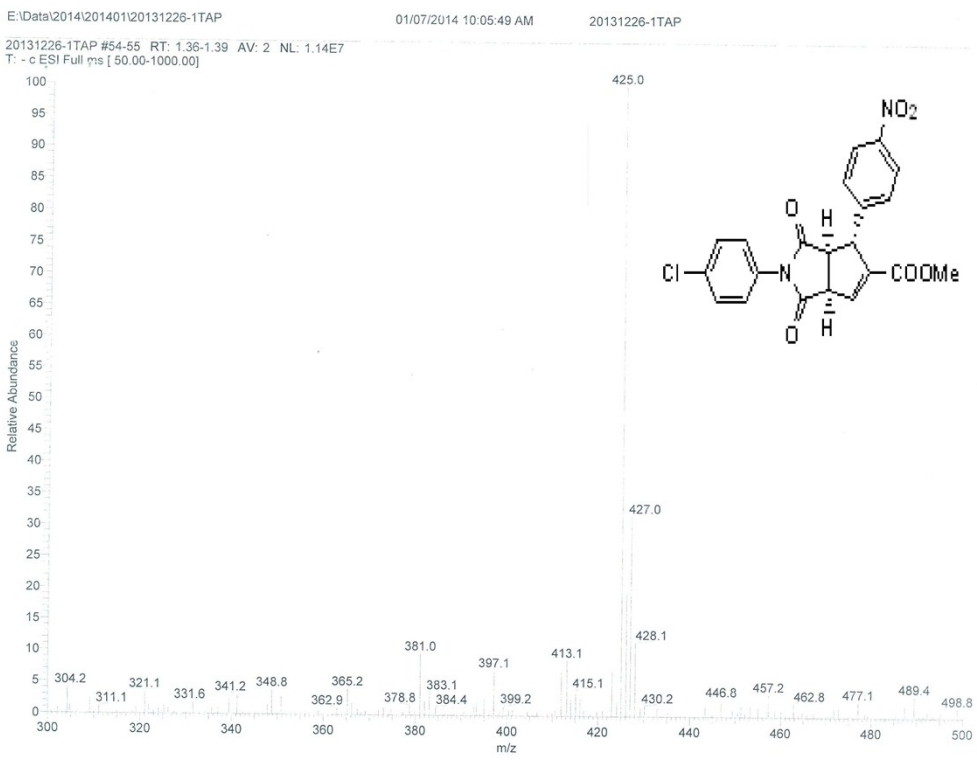
Meas. m/z	Formula	m/z	err [ppm]
483.1415	C 28 H 30 Fe N O P	483.1409	-1.3

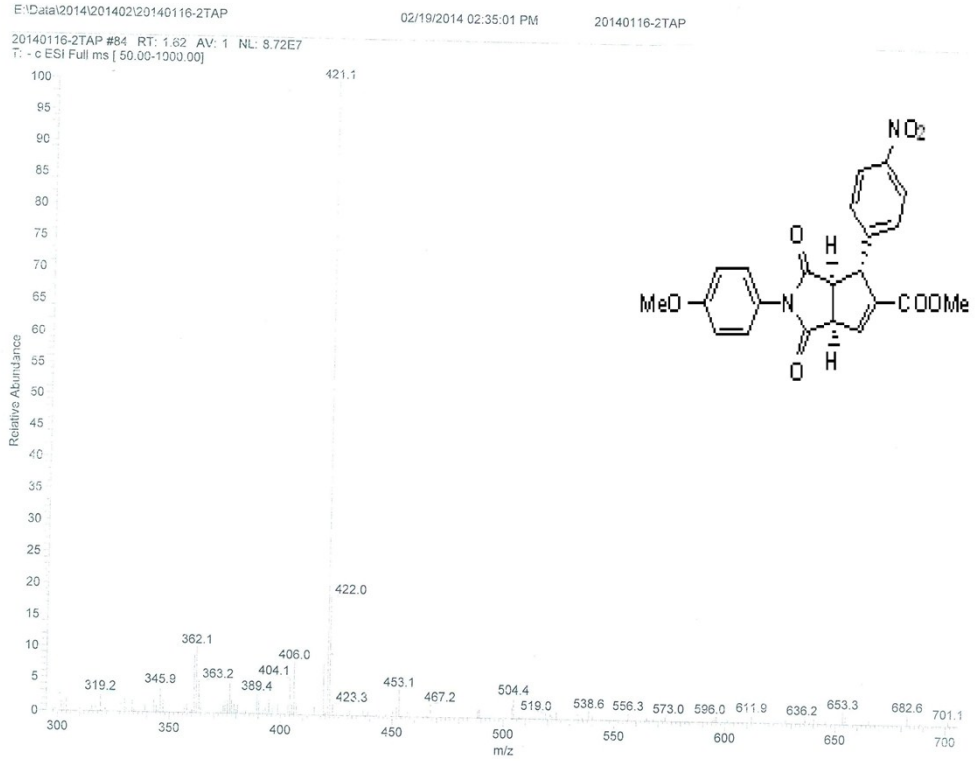

E:\Data\2013\201312\20131218-1TAP
12/28/2013 09:02:36 AM
20131218-1TAP
20131218-1TAP #43 RT: 1.15 AV: 1 NL: 1.67E8
T: - c ESI Full ms [50.00-1000.00]
Relative Abundance
405.1
406.1
156.3 184.0 258.1 286.0 332.1 404.3 407.0 440.8 493.7 563.8 638.0 689.9 741.1 768.0 810.8 872.1 949.4 995.5
m/z
NO2
O
H
N
COOEt
O
H

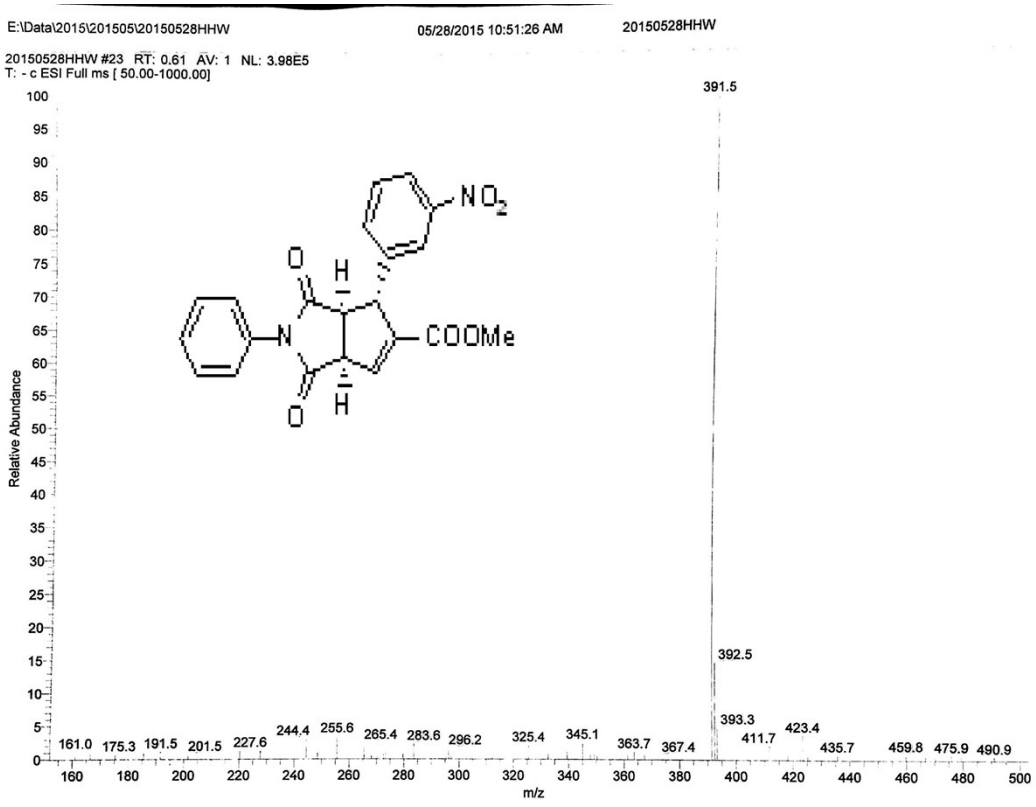

E:\Data\2014\201401\20140107-TAP
01/18/2014 09:31:55 AM
20140107-TAP
20140107-TAP #49 RT: 1.26 AV: 1 NL: 7.32E7
T: - c ESI ms [50.00-1000.00]
Relative Abundance
433.1
434.1
465.0
435.1
212.1 280.7 286.2 314.1 346.0 389.2 431.1 440.1 465.9 506.5 552.5 601.1 660.1 679.5 720.4 741.0 779.4
m/z
NO2
O
H
N
COOnBu
O
H


E:\Data\2014\201401\20131224-1TAP
01/07/2014 09:56:01 AM
20131224-1TAP
20131224-1TAP #112 RT: 2.19 AV: 1 NL: 1.56E7
T: - c ESI Full ms [50.00-400.00]
NO2
O
H
N
COOMe
O
H
Relative Abundance
m/z
329.0
330.1
269.0
270.0
301.0
352.1
244.1
255.5
183.1
108.0
129.0
137.1
154.8
165.0
187.0
220.1
223.3
229.0
286.9
302.1
315.4
344.8
366.8
377.3
396.3


E:\Data\2013\201312\20131213-1TAP
12/26/2013 09:34:25 AM
20131213-1TAP
20131213-1TAP #58 RT: 1.54 AV: 1 NL: 2.84E7
T: - c ESI Full ms [50.00-1000.00]
405.1
NO2
O
H
N
COOMe
O
H
Relative Abundance
m/z
406.1
373.1
407.1
98.9
149.1
186.1
244.1
294.9
328.8
455.5
524.3
548.4
592.1
623.9
711.5
752.2
828.1
874.6
906.7
951.5
997.1


E:\Data\2014\201401\20131226-1TAP
01/07/2014 10:05:49 AM
20131226-1TAP
20131226-1TAP #54-55 RT: 1.36-1.39 AV: 2 NL: 1.14E7
T: - c ESI Full ms [50.00-1000.00]
Relative Abundance
m/z
425.0
427.0
428.1
381.0
397.1
413.1
NO2
Cl
N
O
H
COOMe


E:\Data\2014\201402\20140116-2TAP
02/19/2014 02:35:01 PM
20140116-2TAP
20140116-2TAP #84 RT: 1.62 AV: 1 NL: 8.72E7
T: - c ESI Full ms [50.00-1000.00]
Relative Abundance
m/z
421.1
422.0
362.1
406.0
404.1
NO2
MeO
N
O
H
COOMe



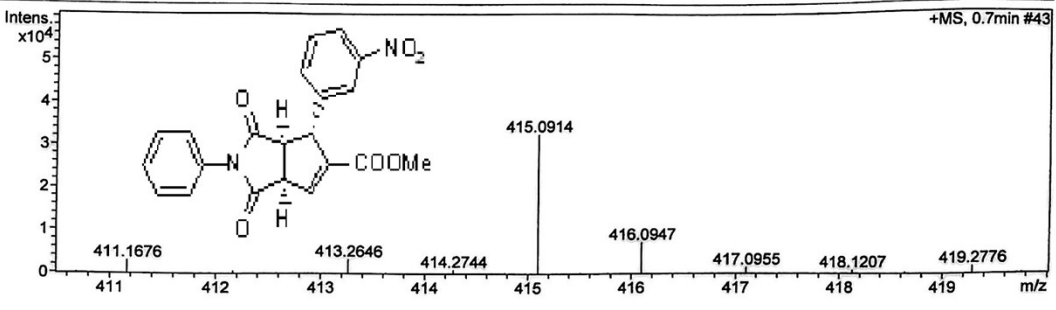
Mass Spectrum SmartFormula Report

Analysis Info

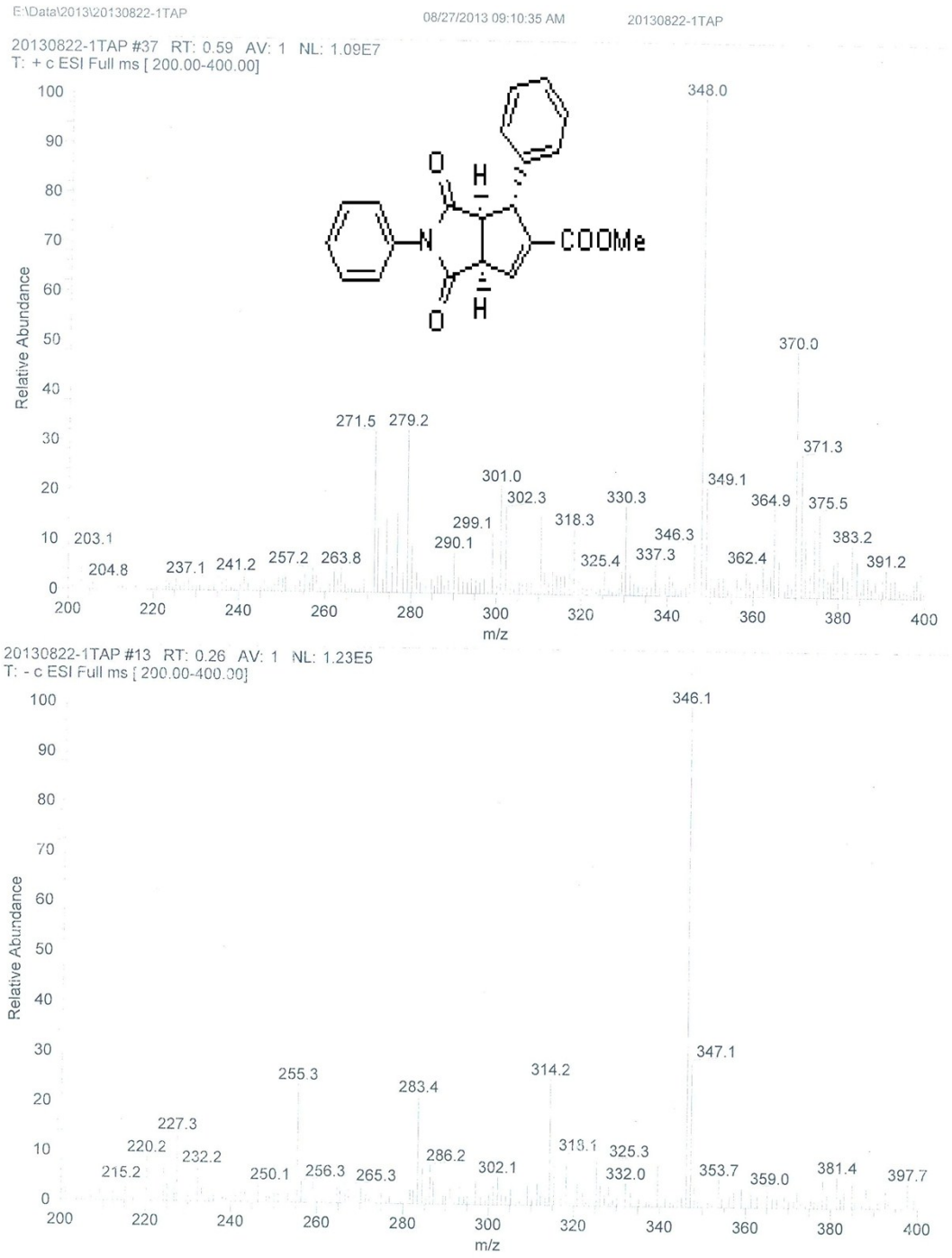
Analysis Name	D:\Data\2015\05.29\20150528HHW..d	Acquisition Date	5/29/2015 1:57:38 PM
Method	tune_POS_low.m		
Sample Name	20150528HHW.	Operator	bruker
Comment		Instrument / Ser#	micrOTOF-Q II 10366

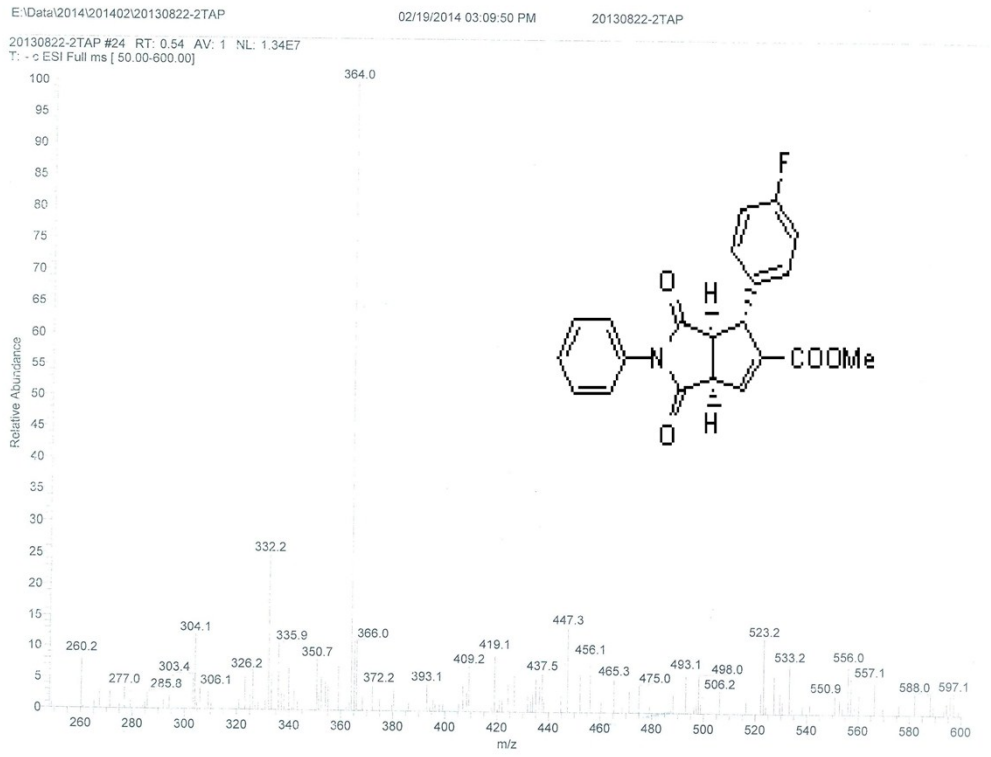
Acquisition Parameter

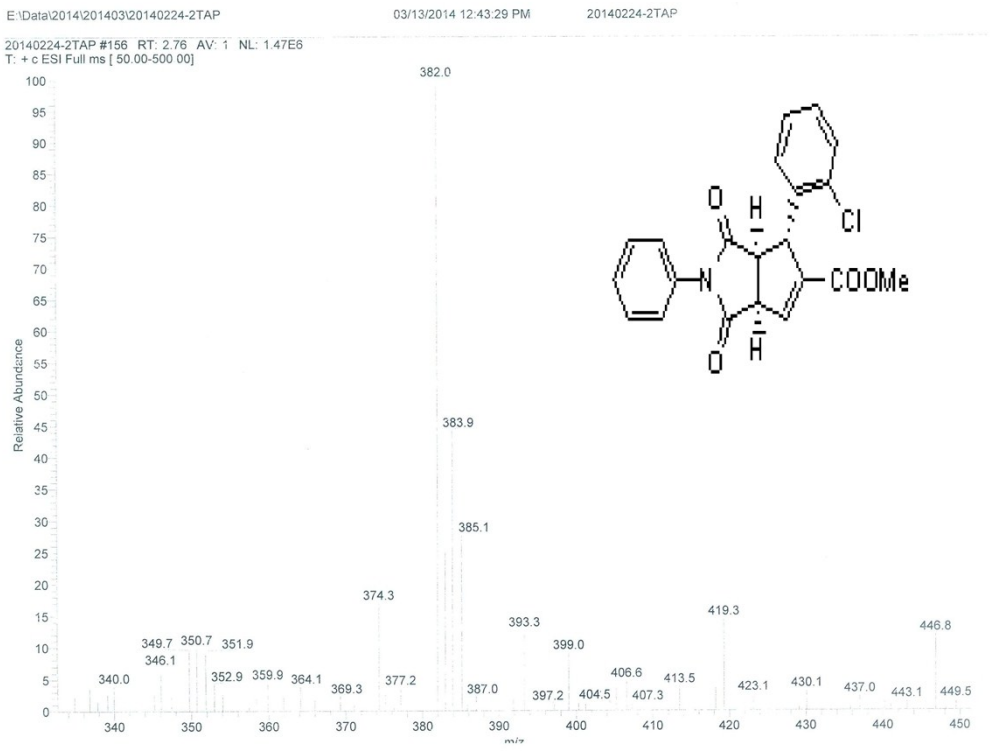
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Waste

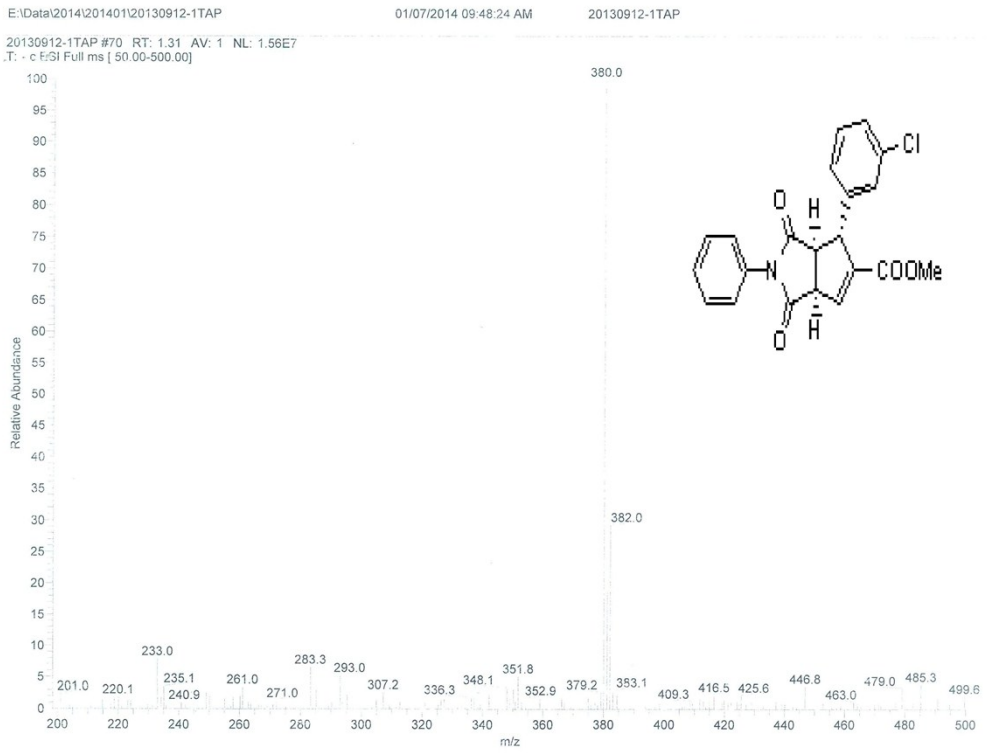


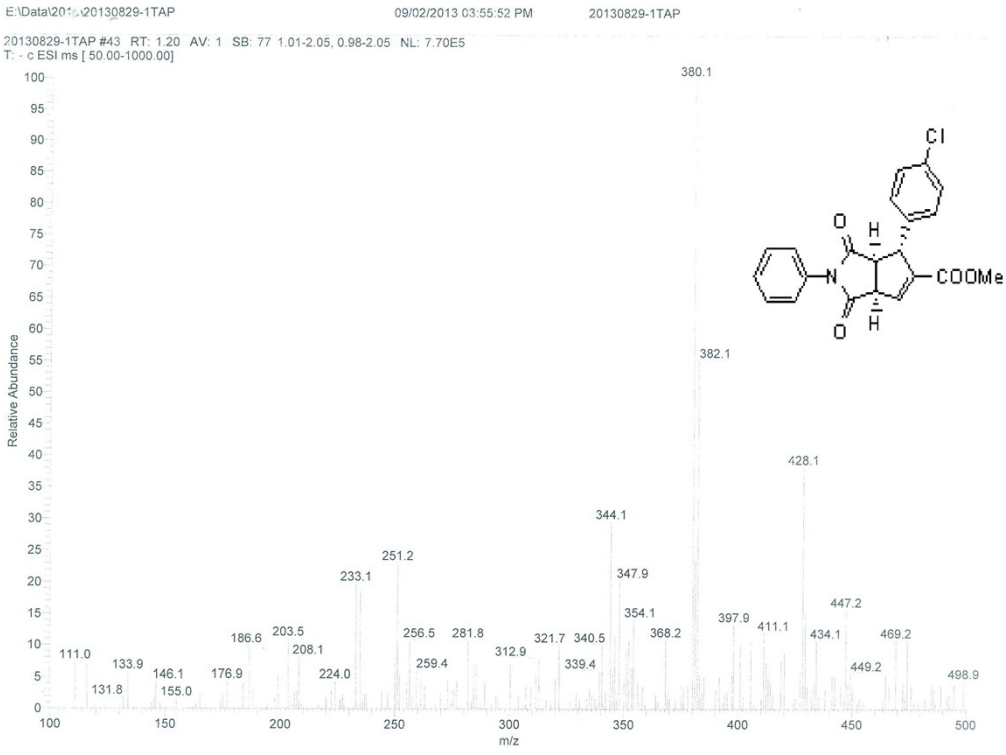
Meas. m/z	Formula	m/z	err [ppm]	mSigma
415.0914	C 21 H 16 N 2 Na O 6	415.0901	-3.2	8.0

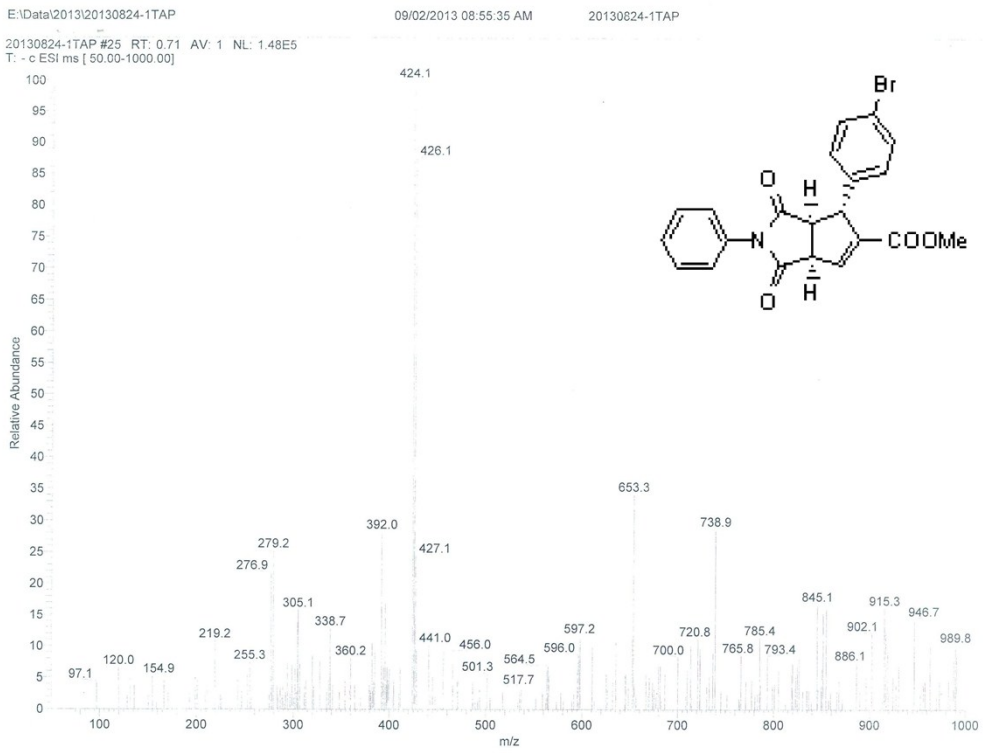

E:\Data\2013\20130822-1TAP
08/27/2013 09:10:35 AM
20130822-1TAP
20130822-1TAP #37 RT: 0.59 AV: 1 NL: 1.09E7
T: + c ESI Full ms [200.00-400.00]
Relative Abundance
m/z
348.0
370.0
271.5
279.2
371.3
301.0
349.1
302.3
330.3
364.9
375.5
318.3
299.1
346.3
383.2
290.1
203.1
325.4
337.3
362.4
391.2
204.8
237.1
241.2
257.2
263.8
20130822-1TAP #13 RT: 0.26 AV: 1 NL: 1.23E5
T: - c ESI Full ms [200.00-400.00]
Relative Abundance
m/z
346.1
347.1
255.3
314.2
283.4
227.3
220.2
232.2
286.2
313.1
325.3
215.2
250.1
256.3
265.3
302.1
332.0
353.7
359.0
381.4
397.7

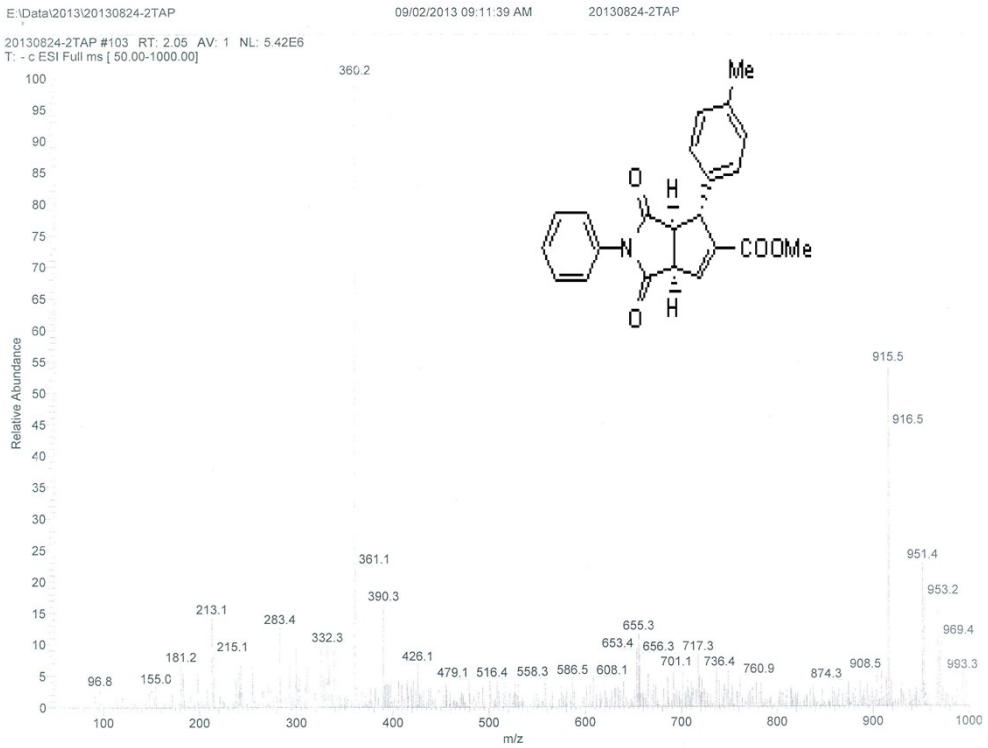

E:\Data\2014\201402\20130822-2TAP
02/19/2014 03:09:50 PM
20130822-2TAP
20130822-2TAP #24 RT: 0.54 AV: 1 NL: 1.34E7
T: - c ESI Full ms [50.00-600.00]
Relative Abundance
m/z
364.0
332.2
F
O
H
N
COOMe
O
H

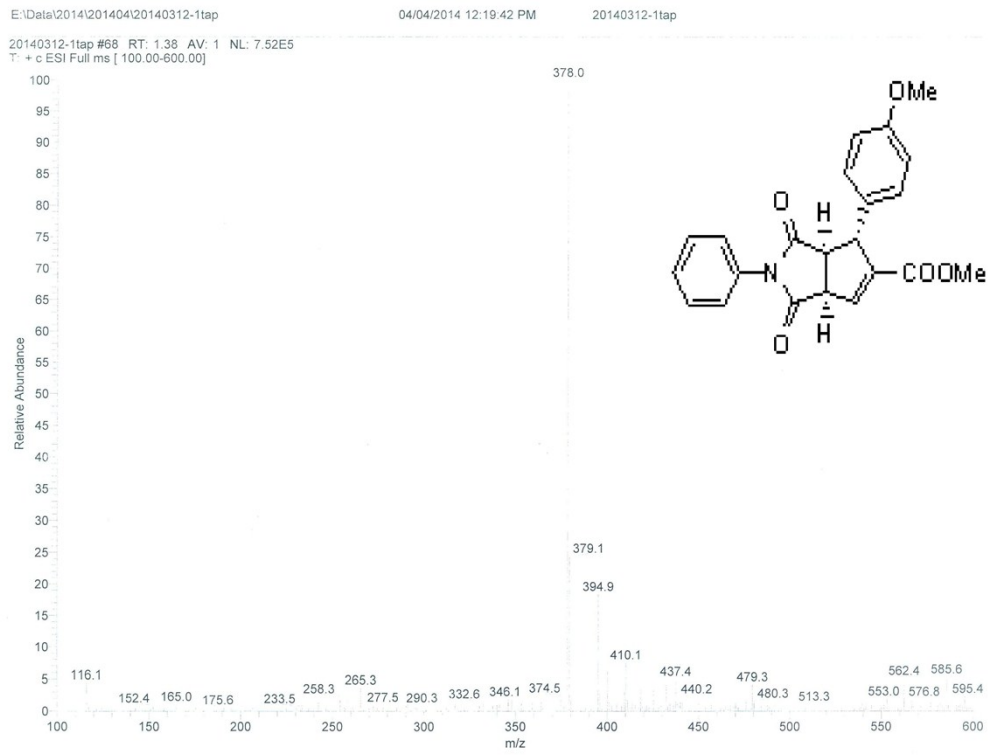

E:\Data\2014\201403\20140224-2TAP
03/13/2014 12:43:29 PM
20140224-2TAP
20140224-2TAP #156 RT: 2.76 AV: 1 NL: 1.47E6
T: + c ESI Full ms [50.00-500 00]
Relative Abundance
m/z
382.0
383.9
385.1
Cl
O
H
N
COOMe
O
H

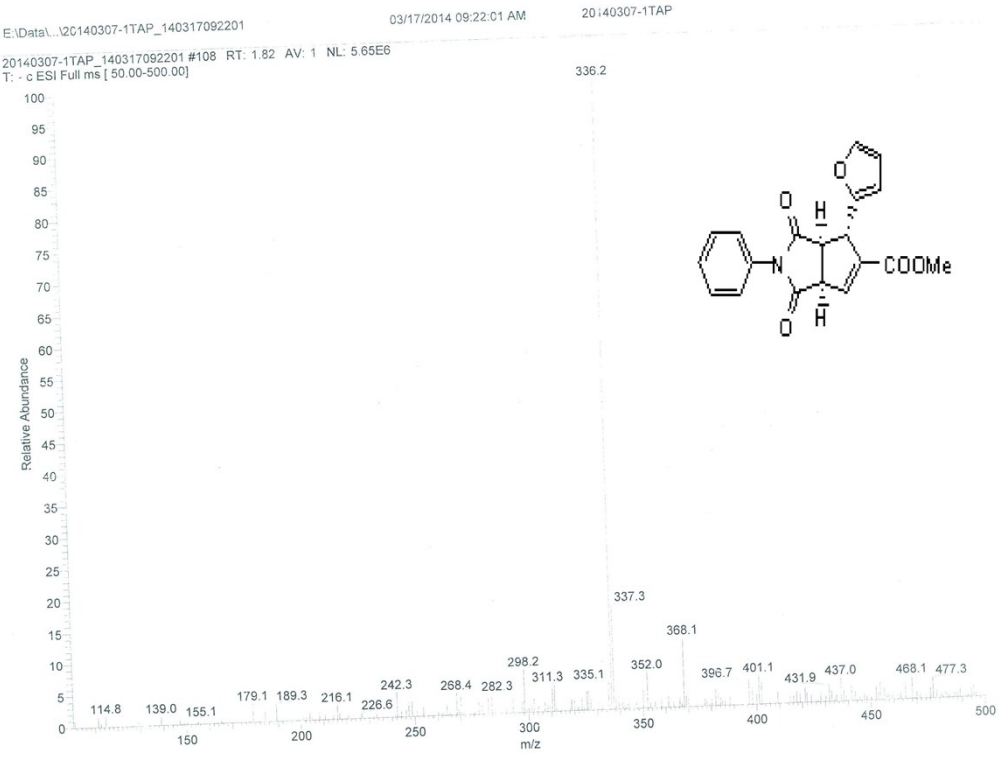

E:\Data\2014\201401\20130912-1TAP
01/07/2014 09:48:24 AM
20130912-1TAP
20130912-1TAP #70 RT: 1.31 AV: 1 NL: 1.56E7
T: - c ESI Full ms [50.00-500.00]
Relative Abundance
m/z
380.0
382.0
COOMe
Cl

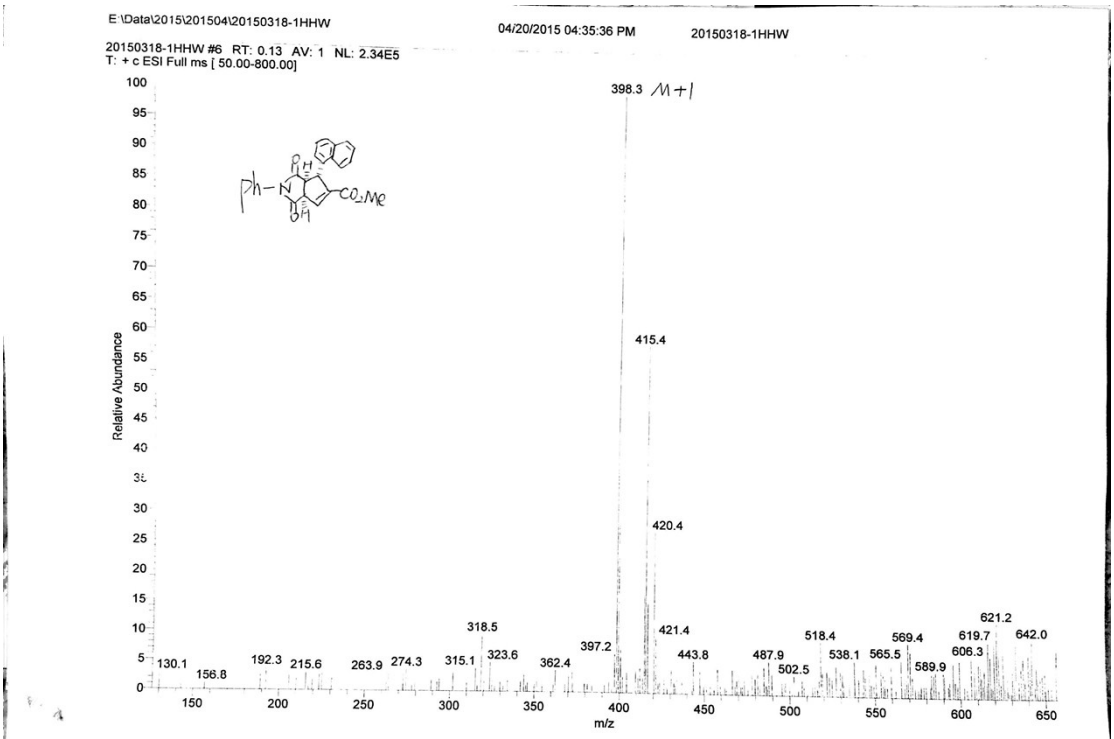

E:\Data\2013\20130829-1TAP
09/02/2013 03:55:52 PM
20130829-1TAP
20130829-1TAP #43 RT: 1.20 AV: 1 SB: 77 1.01-2.05, 0.98-2.05 NL: 7.70E5
T: - c ESI ms [50.00-1000.00]
Relative Abundance
m/z
380.1
382.1
428.1
344.1
251.2
233.1
COOMe
Cl


E:\Data\2013\20130824-1TAP
09/02/2013 08:55:35 AM
20130824-1TAP
20130824-1TAP #25 RT: 0.71 AV: 1 NL: 1.48E5
T: - c ESI ms [50.00-1000.00]
Br
O
H
N
COOMe
O
H
Relative Abundance
m/z
424.1
426.1
653.3
738.9
392.0
427.1
279.2
276.9
305.1
338.7
219.2
255.3
360.2
441.0
456.0
501.3
564.5
517.7
596.0
597.2
700.0
720.8
765.8
785.4
793.4
845.1
886.1
902.1
915.3
946.7
989.8
97.1
120.0
154.9


E:\Data\2013\20130824-2TAP
09/02/2013 09:11:39 AM
20130824-2TAP
20130824-2TAP #103 RT: 2.05 AV: 1 NL: 5.42E6
T: - c ESI Full ms [50.00-1000.00]
Me
O
H
N
COOMe
O
H
Relative Abundance
m/z
360.2
915.5
916.5
361.1
951.4
953.2
390.3
213.1
283.4
969.4
655.3
653.4
656.3
717.3
332.3
215.1
181.2
426.1
701.1
736.4
760.9
874.3
908.5
993.3
479.1
516.4
558.3
586.5
608.1
96.8
155.0


E:\Data\2014\201404\20140312-1tap
04/04/2014 12:19:42 PM
20140312-1tap
20140312-1tap #68 RT: 1.38 AV: 1 NL: 7.52E5
T: + c ESI Full ms [100.00-600.00]
Relative Abundance
m/z
OMe
COOMe
O
H
N
O
H
378.0
379.1
394.9
410.1
437.4
479.3
562.4
585.6
116.1
152.4
165.0
175.6
233.5
258.3
265.3
277.5
290.3
332.6
346.1
374.5
440.2
480.3
513.3
553.0
576.8
595.4


E:\Data\...\20140307-1TAP_140317092201
03/17/2014 09:22:01 AM
20140307-1TAP
20140307-1TAP_140317092201 #108 RT: 1.82 AV: 1 NL: 5.65E6
T: - c ESI Full ms [50.00-500.00]
Relative Abundance
m/z
O
O
H
N
O
H
COOMe
336.2
337.3
368.1
298.2
311.3
335.1
352.0
396.7
401.1
431.9
437.0
468.1
477.3
114.8
139.0
155.1
179.1
189.3
216.1
226.6
242.3
268.4
282.3



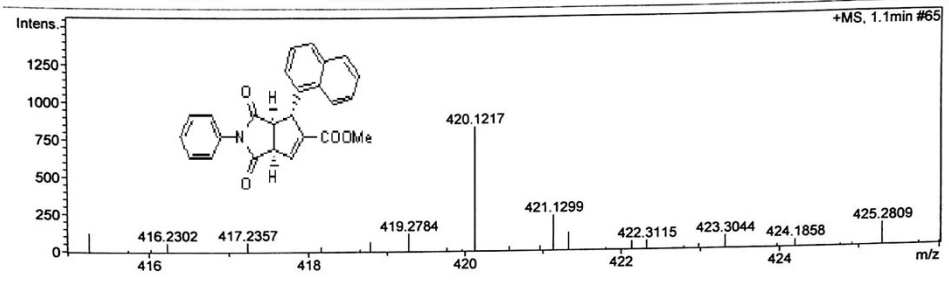
Mass Spectrum SmartFormula Report

Analysis Info

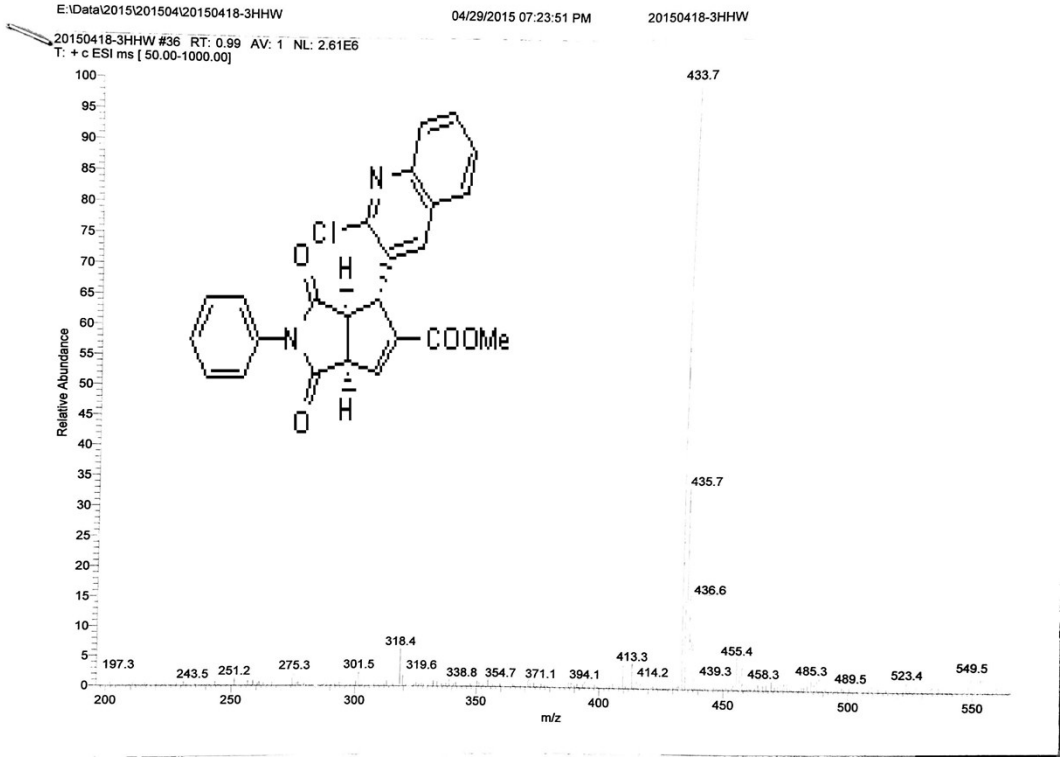
Analysis Name	D:\Data\2015\5.14\20150318-2HHW.d	Acquisition Date	5/15/2015 9:52:09 AM
Method	tune_POS_low.m	Operator	bruker
Sample Name	20150318-2HHW	Instrument / Ser#	micrOTOF-Q II 10366
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Waste



Meas. m/z	Formula	m/z	err [ppm]	mSigma
420.1217	C 25 H 19 N Na O 4	420.1206	-2.5	11.8



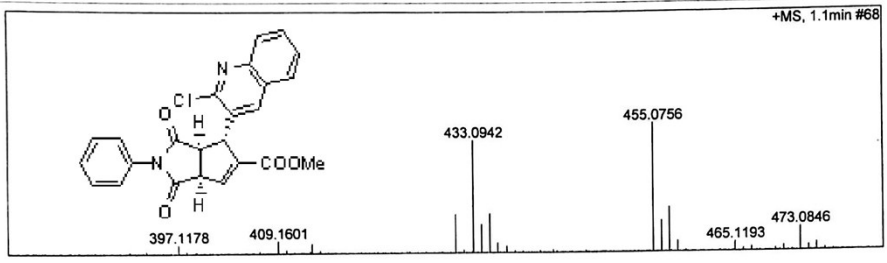
Mass Spectrum SmartFormula Report

Analysis Info

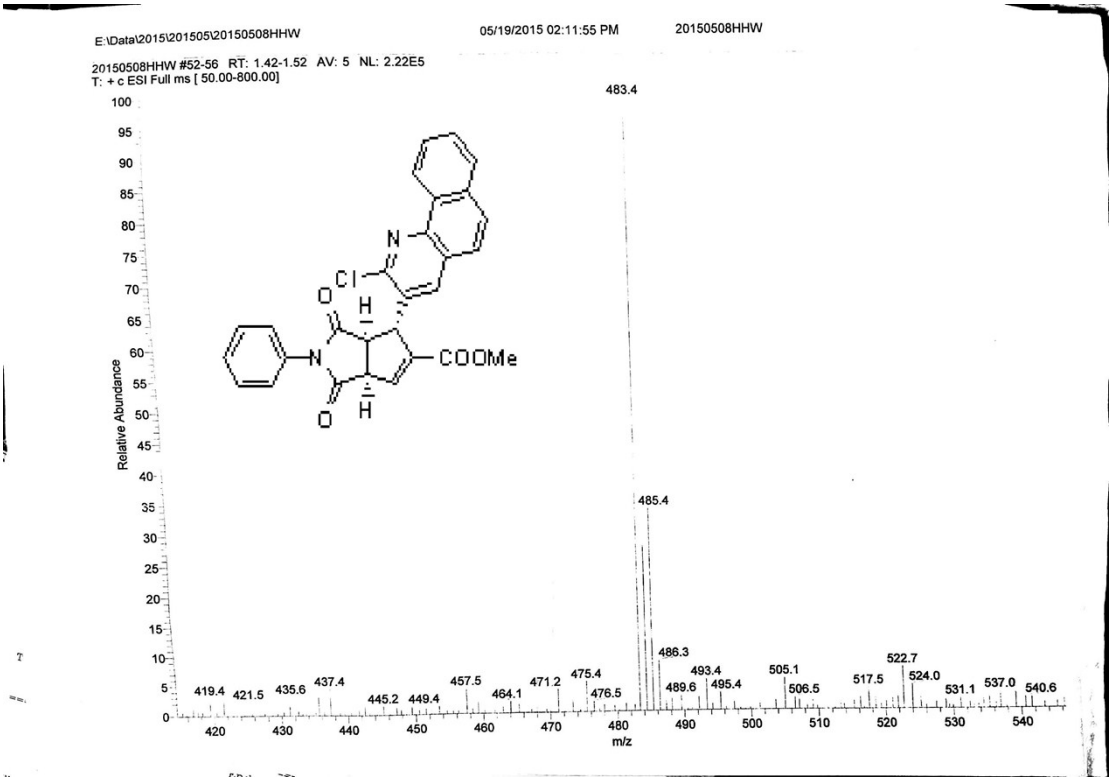
Analysis Name	D:\Data\2015\5.9\20150418-3HHW.d	Acquisition Date	5/9/2015 3:04:48 PM
Method	tune_POS_low.m		
Sample Name	20150418-3HHW	Operator	bruker
Comment		Instrument / Ser#	micrOTOF-Q II 10366

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Waste



Meas. m/z	Formula	m/z	err [ppm]	mSigma
433.0942	C 24 H 18 Cl N 2 O 4	433.0950	1.9	12.2



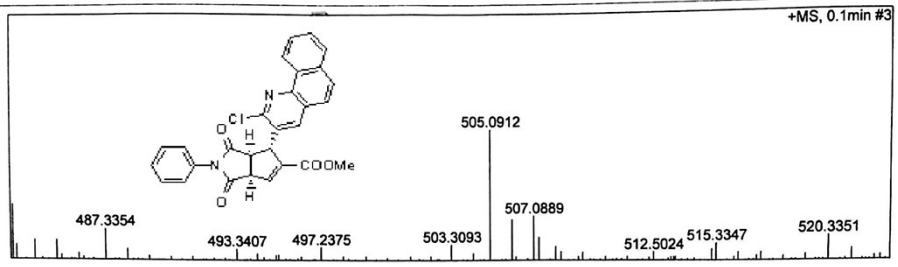
Mass Spectrum SmartFormula Report

Analysis Info

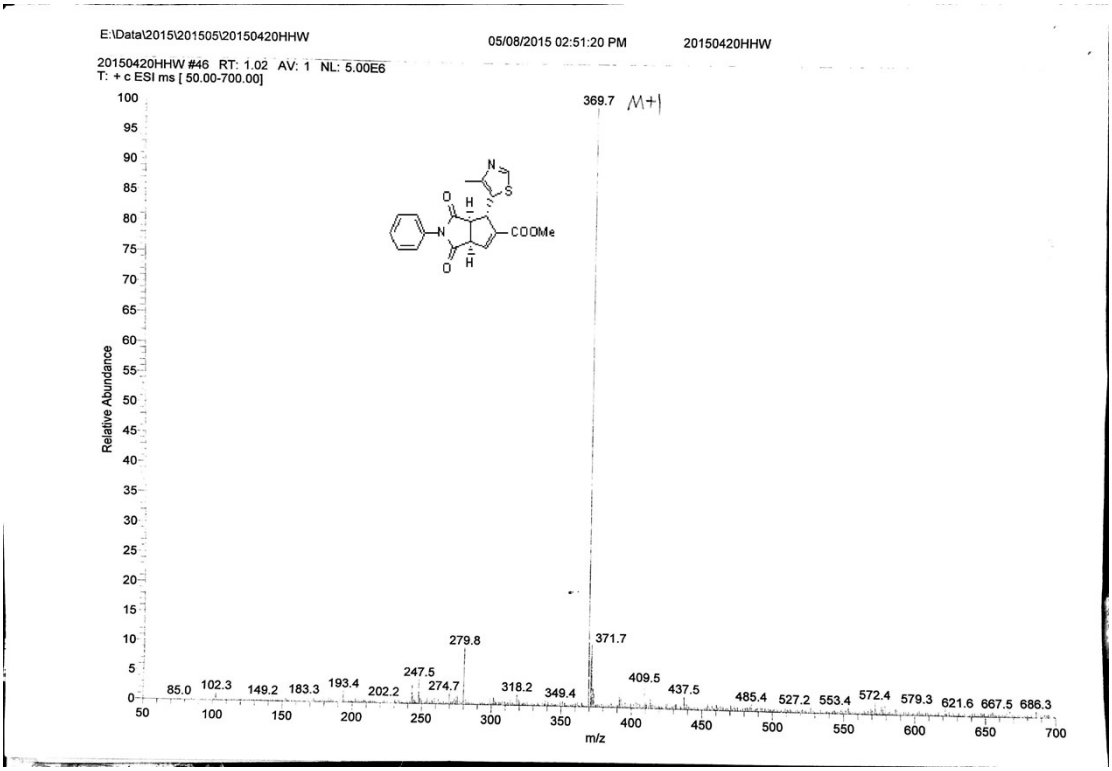
Analysis Name	D:\Data\2015\5.22\20150508HHW..d	Acquisition Date	5/22/2015 9:53:11 AM
Method	tune_POS_low.m	Operator	bruker
Sample Name	20150508HHW.	Instrument / Ser#	micrOTOF-Q II 10366
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Waste



Meas. m/z	Formula	m/z	err [ppm]	mSigma
505.0912	C 28 H 19 Cl N 2 Na O 4	505.0926	2.8	16.1



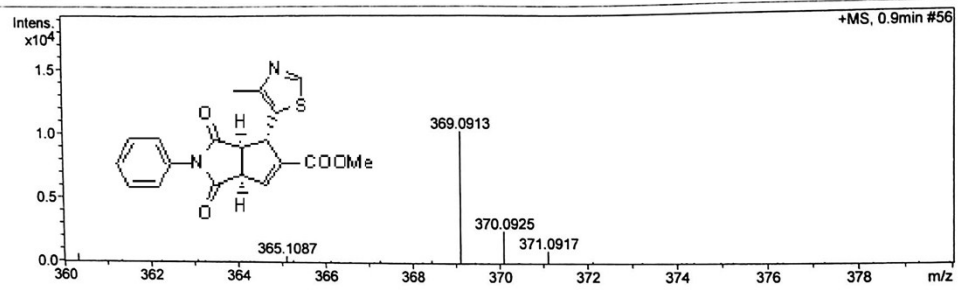
Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name	D:\Data\2015\5.14\20150420HHW.d	Acquisition Date	5/15/2015 10:04:32 AM
Method	tune_POS_low.m	Operator	bruker
Sample Name	20150420HHW	Instrument / Ser#	micrOTOF-Q II 10366
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Waste



Meas. m/z	Formula	m/z	err [ppm]	mSigma
369.0913	C 19 H 17 N 2 O 4 S	369.0904	-2.7	12.7