Supporting Information

Synthesis, Biological Evaluation and Mechanism Study of Chalcone Analogues as Novel Anti-cancer Agents

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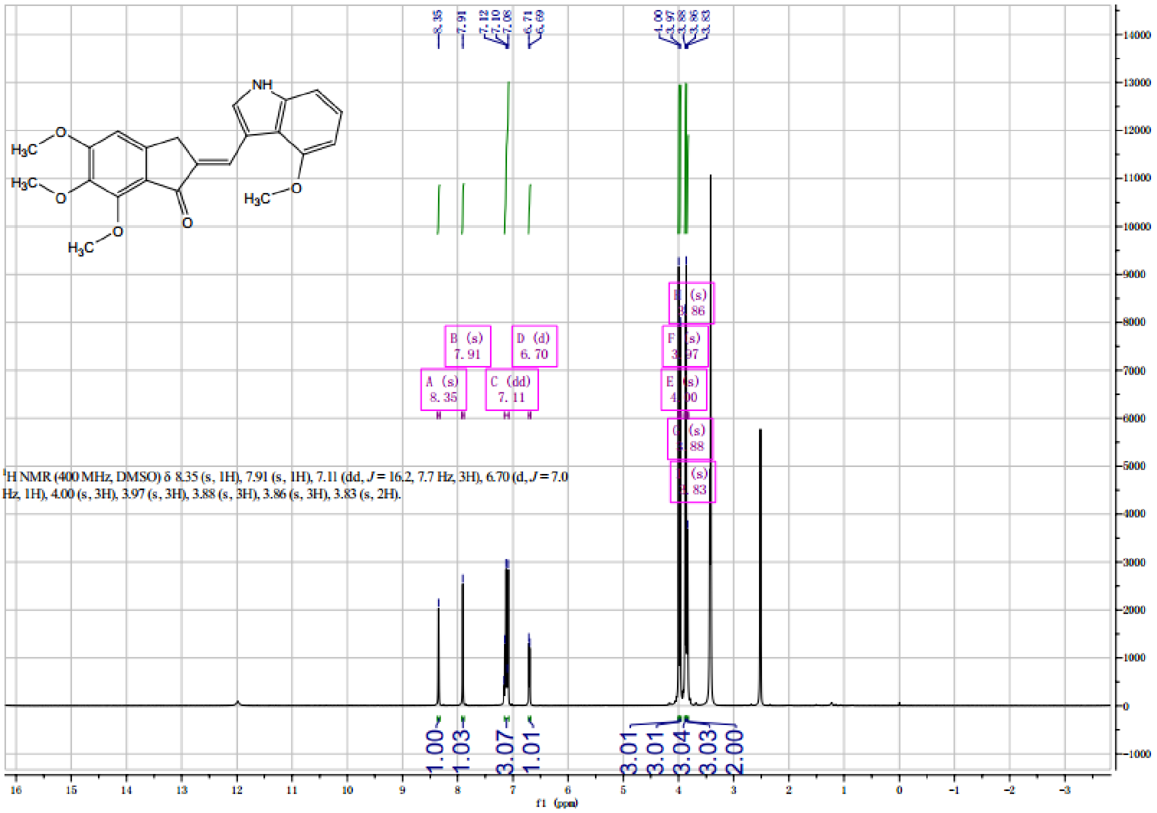
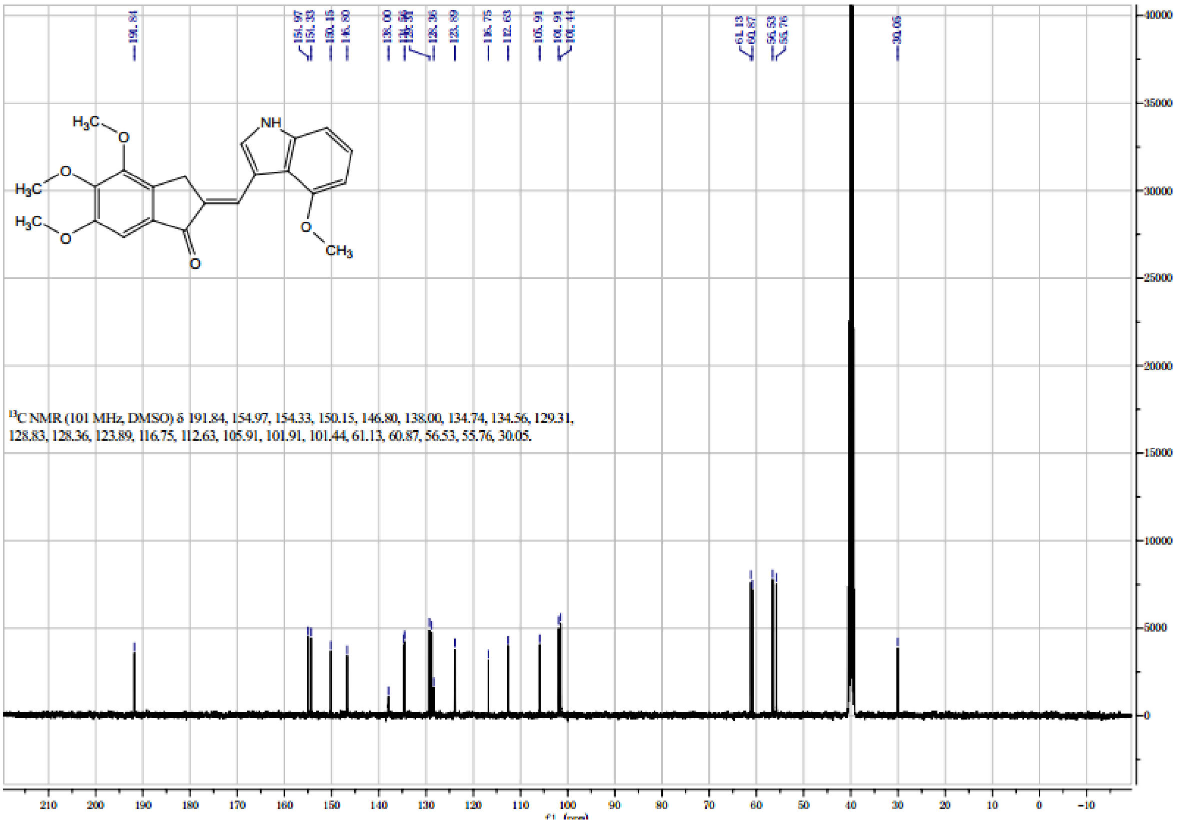
SI. NMR spectra of target compounds

8a

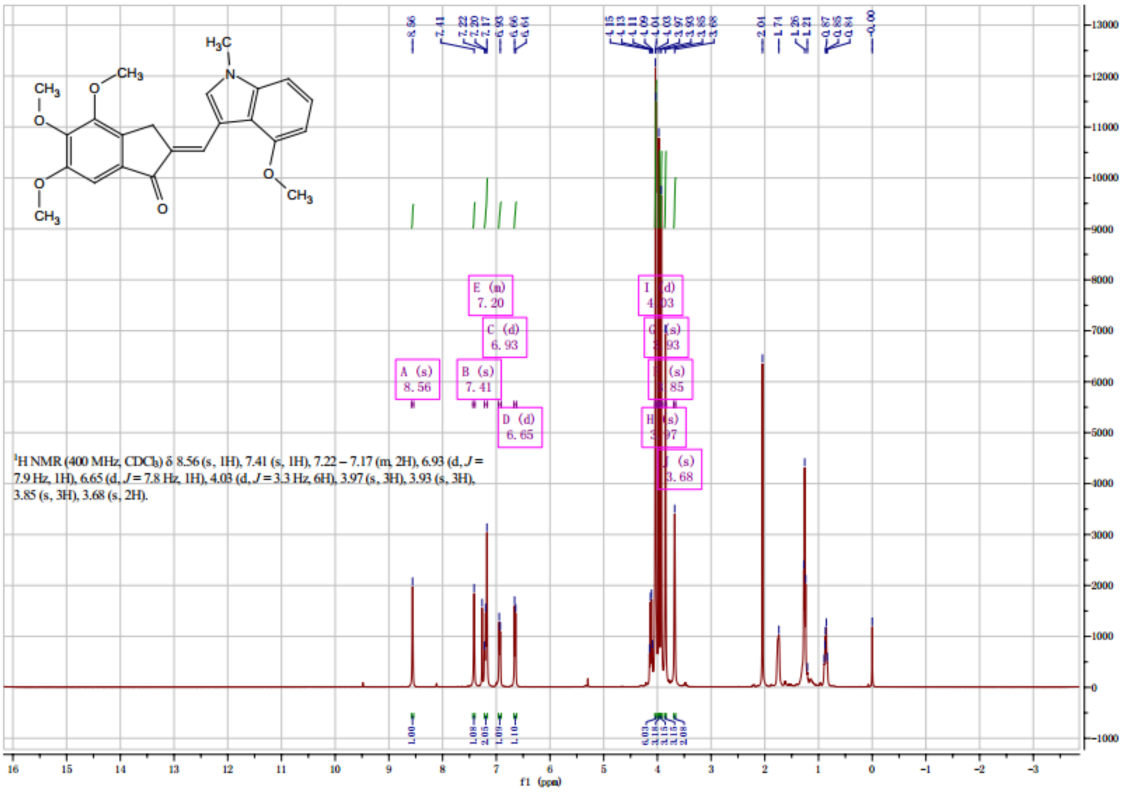


^{1}H NMR (400 MHz, DMSO) δ 8.35 (s, 1H), 7.91 (s, 1H), 7.11 (dd, *J* = 16.2, 7.7 Hz, 3H), 6.70 (d, *J* = 7.0 Hz, 1H), 4.00 (s, 3H), 3.97 (s, 3H), 3.88 (s, 3H), 3.86 (s, 3H), 3.83 (s, 2H).

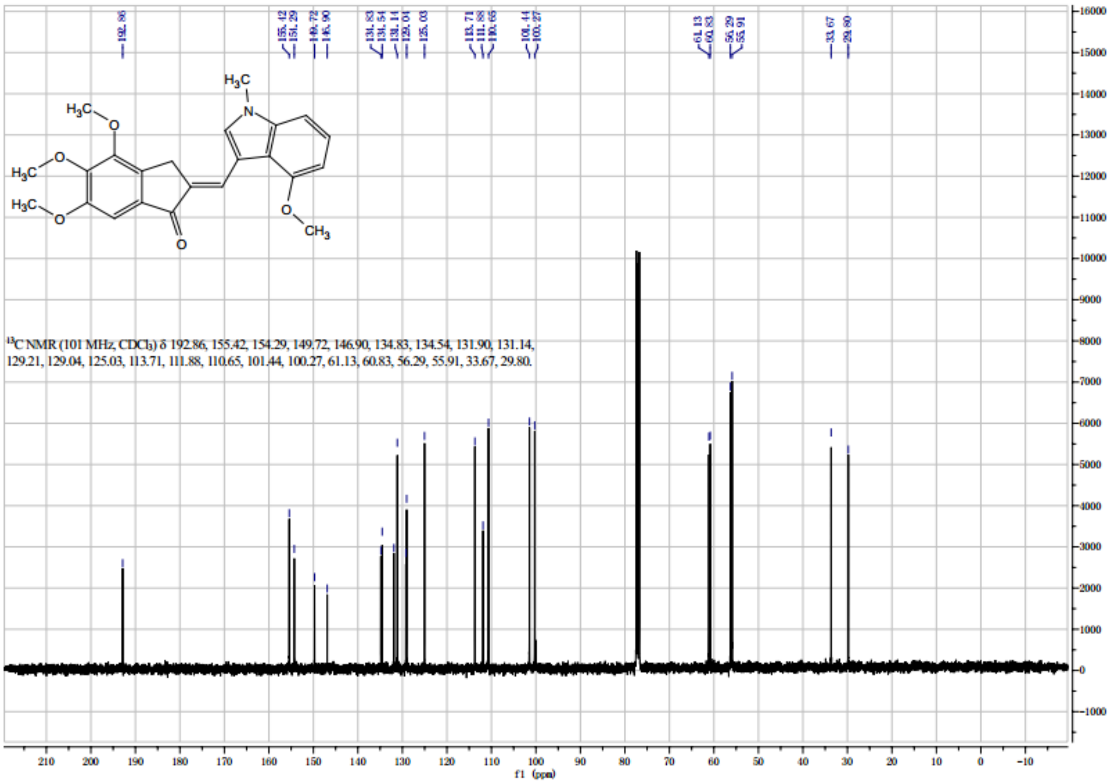


^{13}C NMR (101 MHz, DMSO) δ 191.84, 154.97, 154.33, 150.15, 146.80, 138.00, 134.74, 134.56, 129.31, 128.83, 128.36, 123.89, 116.75, 112.63, 105.91, 101.91, 101.44, 61.13, 60.87, 56.53, 55.76, 30.05.

8b

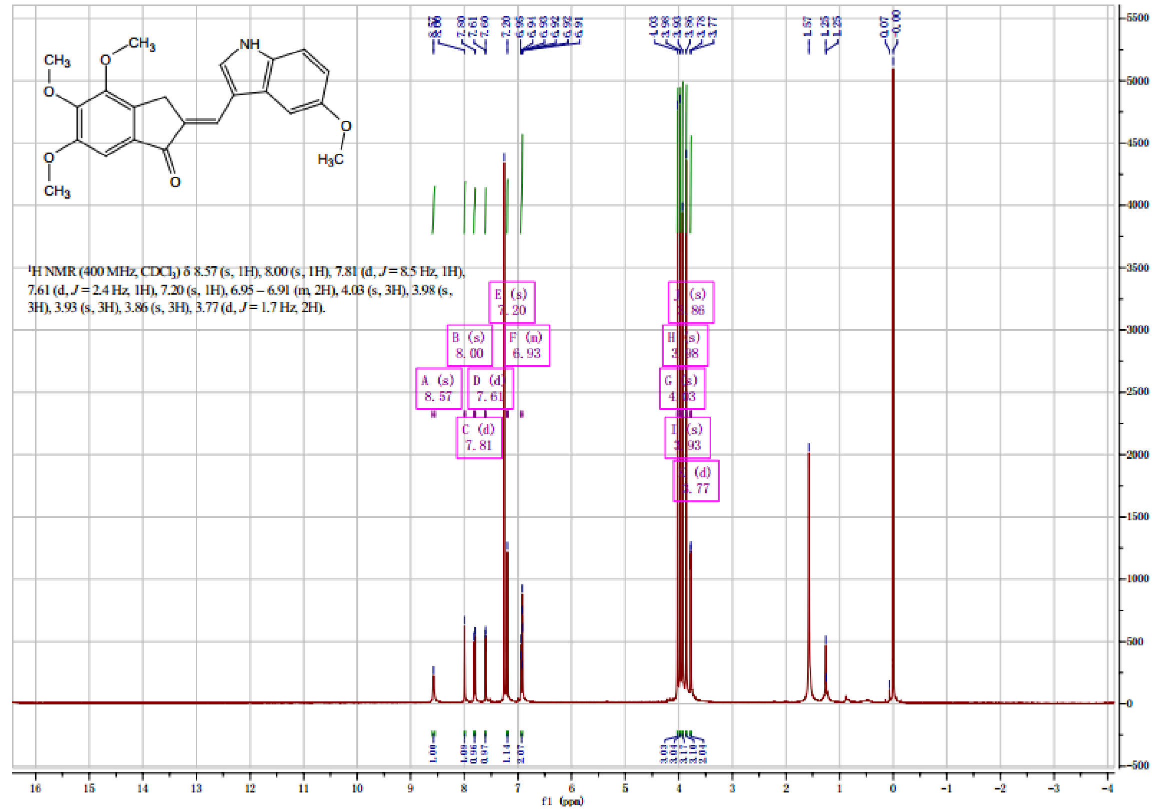


^{1}H NMR (400 MHz, CDCl$_3$) δ 8.56 (s, 1H), 7.41 (s, 1H), 7.22 – 7.17 (m, 2H), 6.93 (d, J = 7.9 Hz, 1H), 6.65 (d, J = 7.8 Hz, 1H), 4.03 (d, J = 3.3 Hz, 6H), 3.97 (s, 3H), 3.93 (s, 3H), 3.85 (s, 3H), 3.68 (s, 2H).

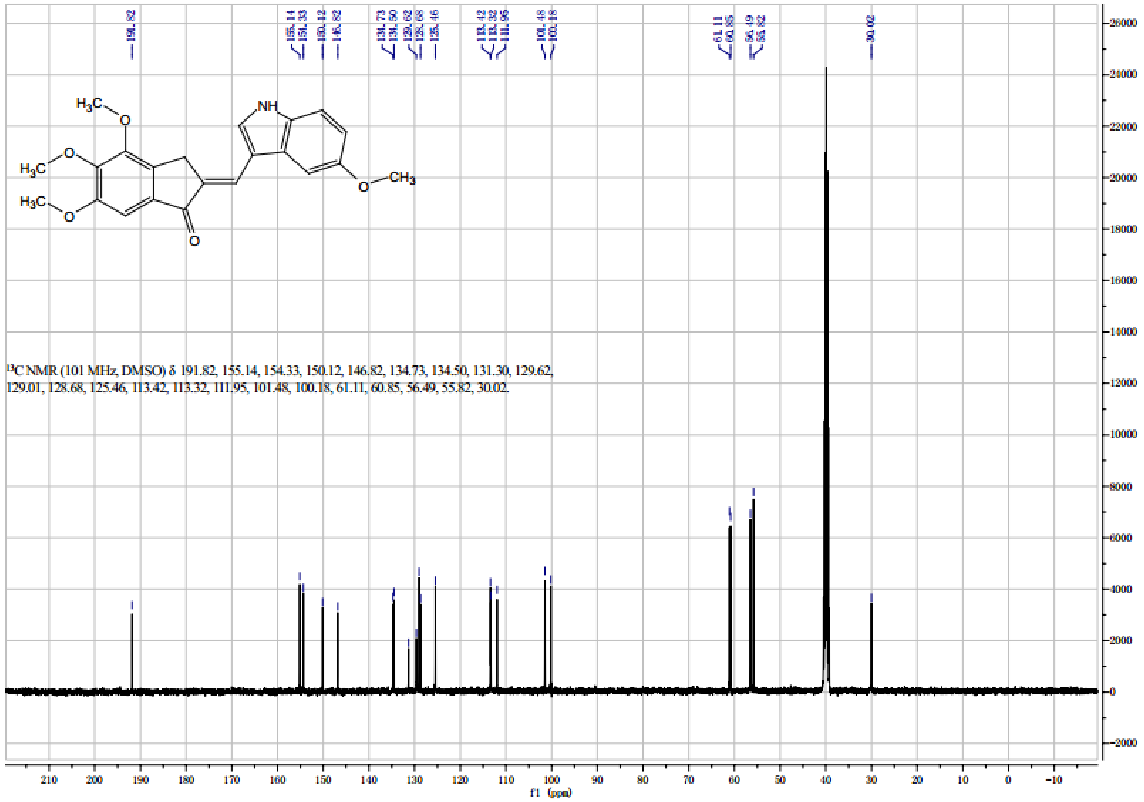


^{13}C NMR (101 MHz, CDCl$_3$) δ 192.86, 155.42, 154.29, 149.72, 146.90, 134.83, 134.54, 131.90, 131.14, 129.21, 129.04, 125.03, 113.71, 111.88, 110.65, 101.44, 100.27, 61.13, 60.83, 56.29, 55.91, 33.67, 29.80.

8c

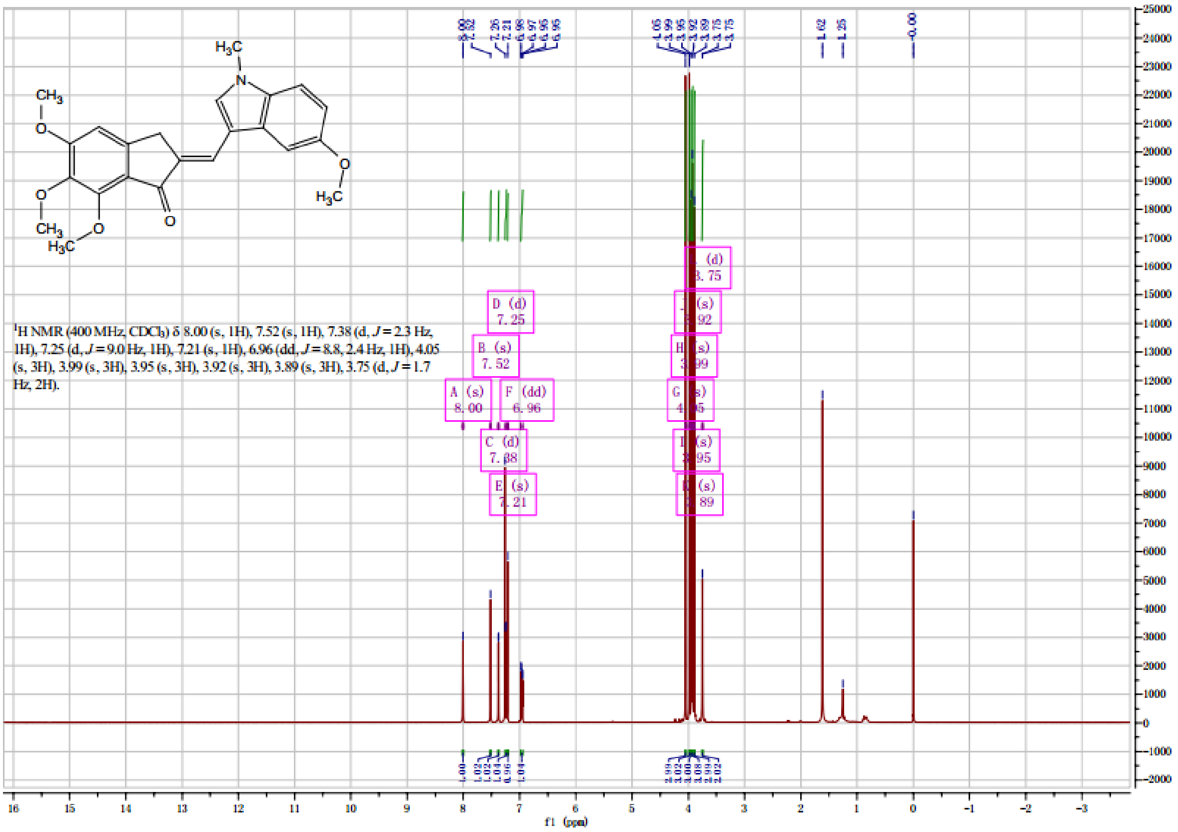


^{1}H NMR (400 MHz, CDCl$_3$) δ 8.57 (s, 1H), 8.00 (s, 1H), 7.81 (d, J = 8.5 Hz, 1H), 7.61 (d, J = 2.4 Hz, 1H), 7.20 (s, 1H), 6.95 – 6.91 (m, 2H), 4.03 (s, 3H), 3.98 (s, 3H), 3.93 (s, 3H), 3.86 (s, 3H), 3.77 (d, J = 1.7 Hz, 2H).

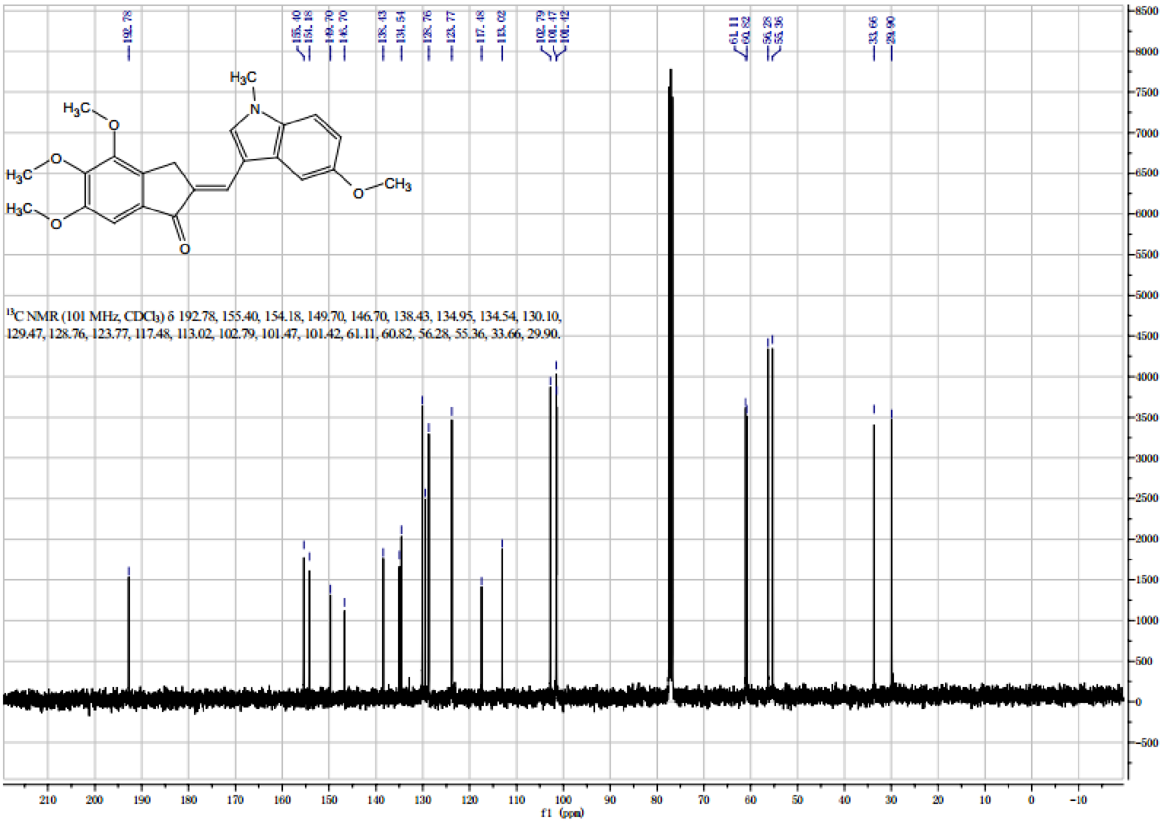


^{13}C NMR (101 MHz, DMSO) δ 191.82, 155.14, 154.33, 150.12, 146.82, 134.73, 134.50, 131.30, 129.62, 129.01, 128.68, 125.46, 113.42, 113.32, 111.95, 101.48, 100.18, 61.11, 60.85, 56.49, 55.82, 30.02.

8d

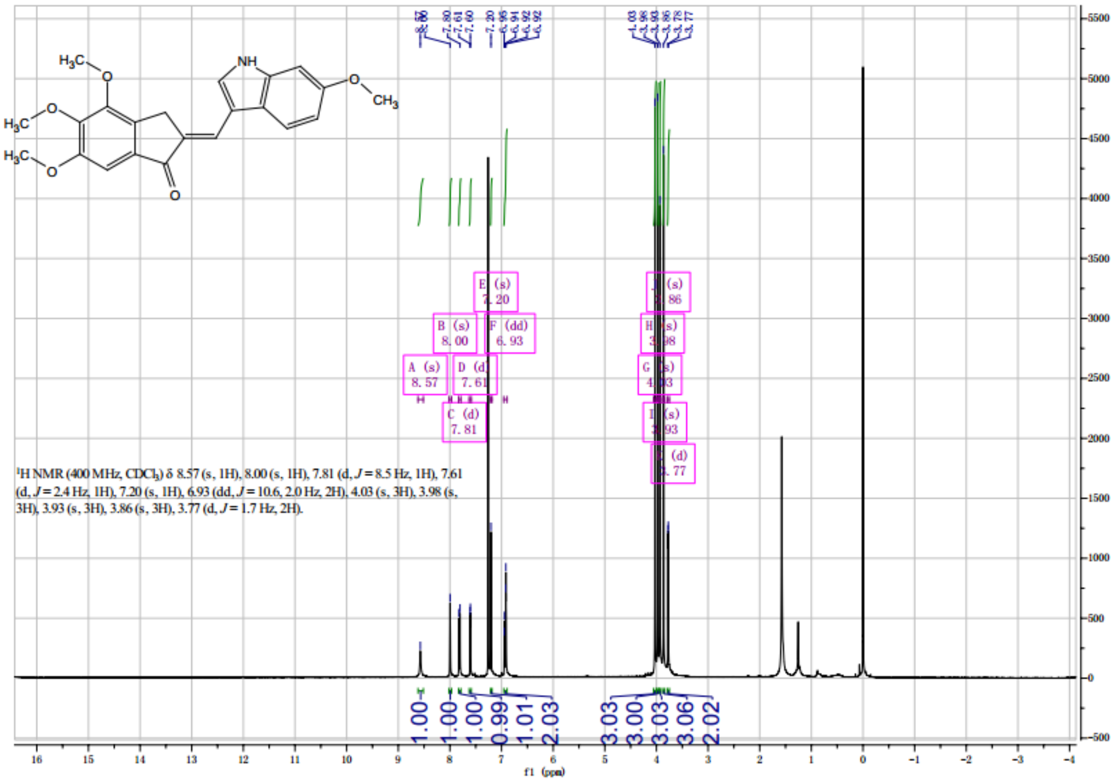


^{1}H NMR (400 MHz, CDCl$_3$) δ 8.00 (s, 1H), 7.52 (s, 1H), 7.38 (d, J = 2.3 Hz, 1H), 7.25 (d, J = 9.0 Hz, 1H), 7.21 (s, 1H), 6.96 (dd, J = 8.8, 2.4 Hz, 1H), 4.05 (s, 3H), 3.99 (s, 3H), 3.95 (s, 3H), 3.92 (s, 3H), 3.89 (s, 3H), 3.75 (d, J = 1.7 Hz, 2H).

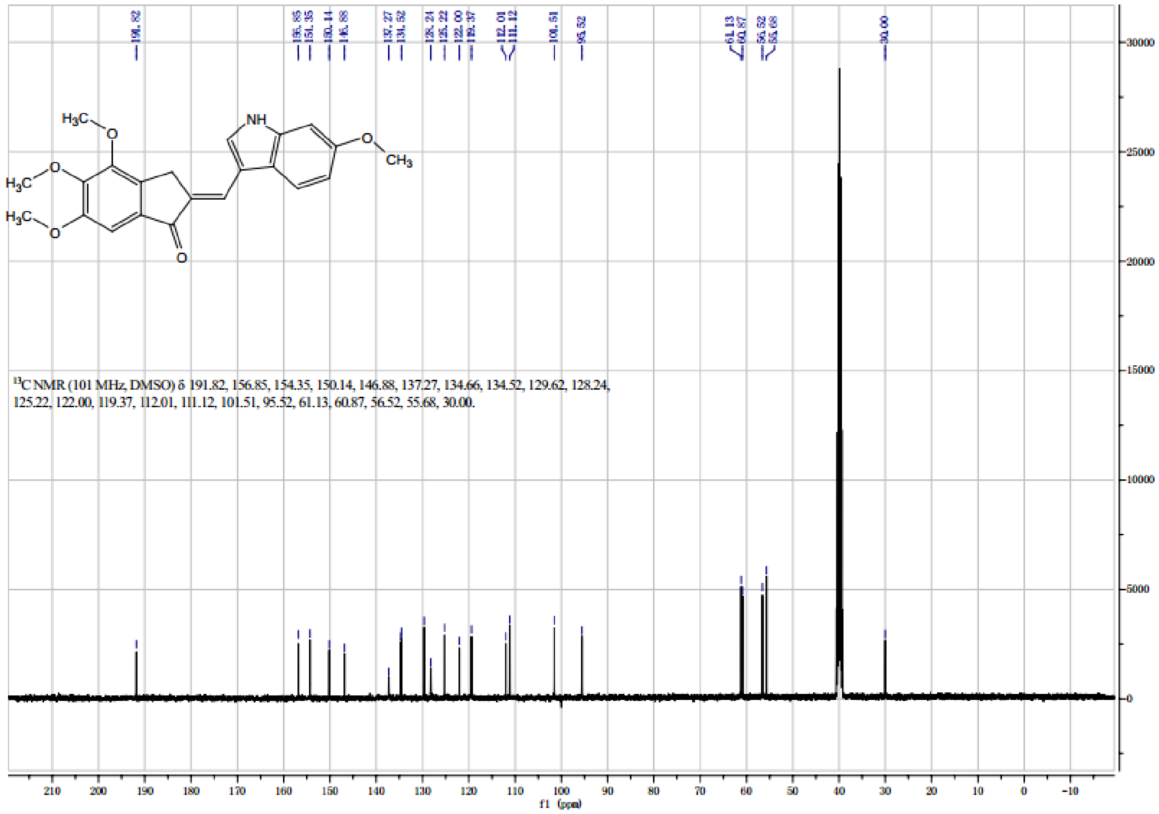


^{13}C NMR (101 MHz, CDCl$_3$) δ 192.78, 155.40, 154.18, 149.70, 146.70, 138.43, 134.95, 134.54, 130.10, 129.47, 128.76, 123.77, 117.48, 113.02, 102.79, 101.47, 101.42, 61.11, 60.82, 56.28, 55.36, 33.66, 29.90.

8e

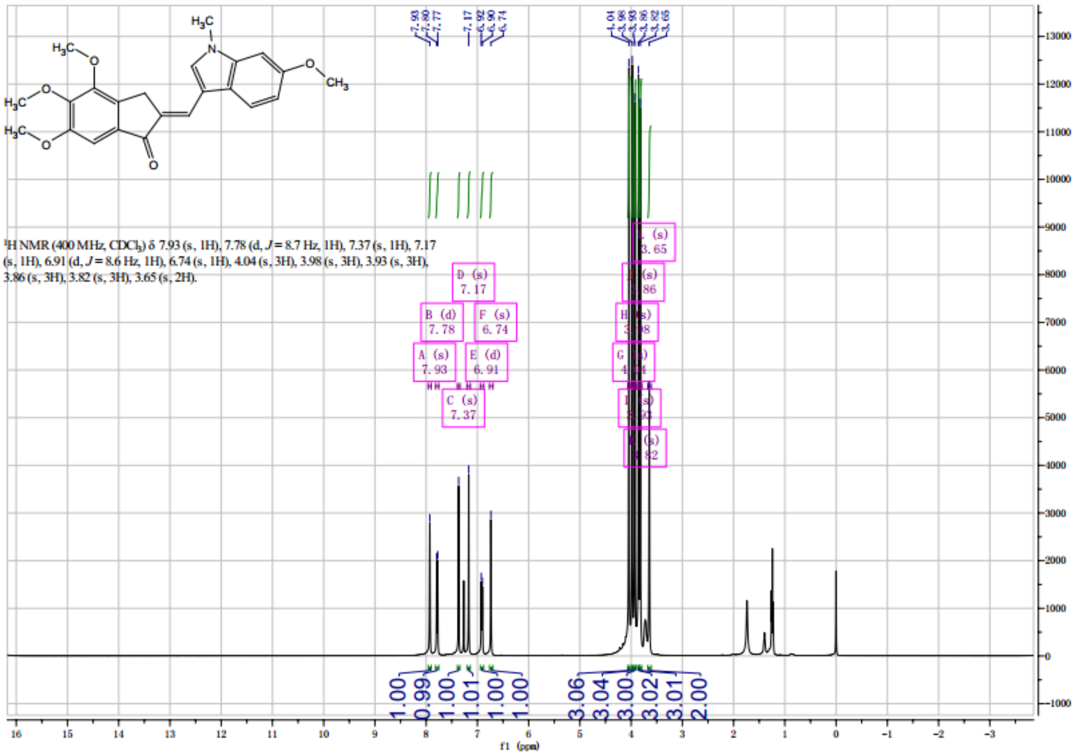


^{1}H NMR (400 MHz, CDCl$_3$) δ 8.57 (s, 1H), 8.00 (s, 1H), 7.81 (d, *J* = 8.5 Hz, 1H), 7.61 (d, *J* = 2.4 Hz, 1H), 7.20 (s, 1H), 6.93 (dd, *J* = 10.6, 2.0 Hz, 2H), 4.03 (s, 3H), 3.98 (s, 3H), 3.93 (s, 3H), 3.86 (s, 3H), 3.77 (d, *J* = 1.7 Hz, 2H).

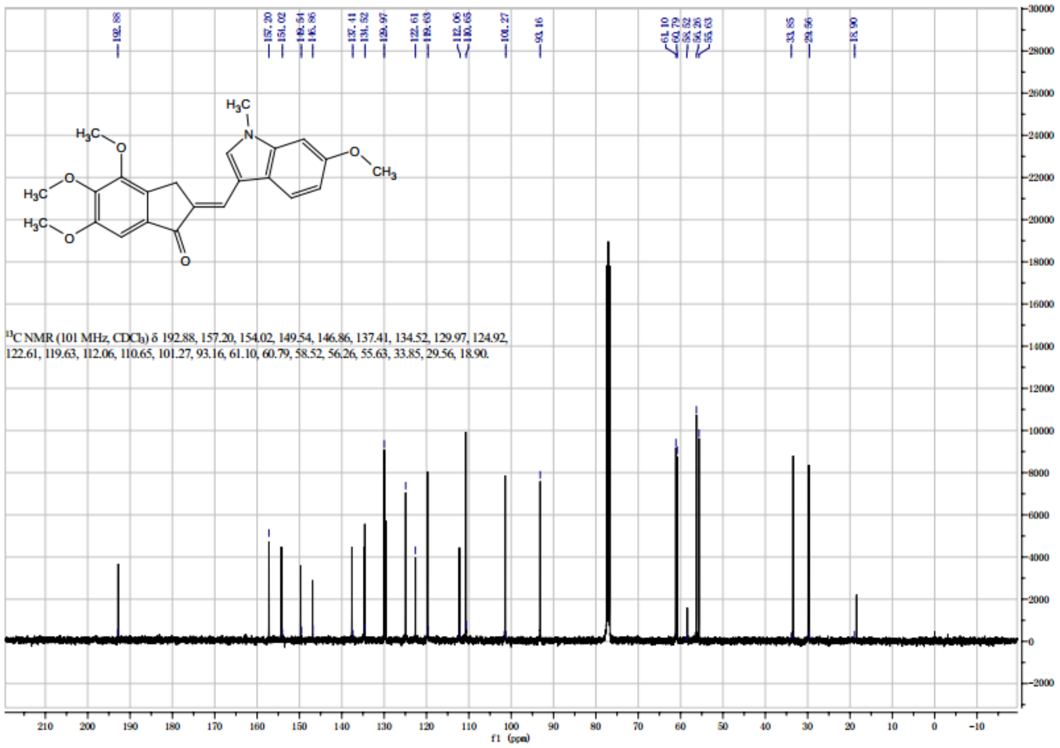


^{13}C NMR (101 MHz, DMSO) δ 191.82, 156.85, 154.35, 150.14, 146.88, 137.27, 134.66, 134.52, 129.62, 128.24, 125.22, 122.00, 119.37, 112.01, 111.12, 101.51, 95.52, 61.13, 60.87, 56.52, 55.68, 30.00.

8f

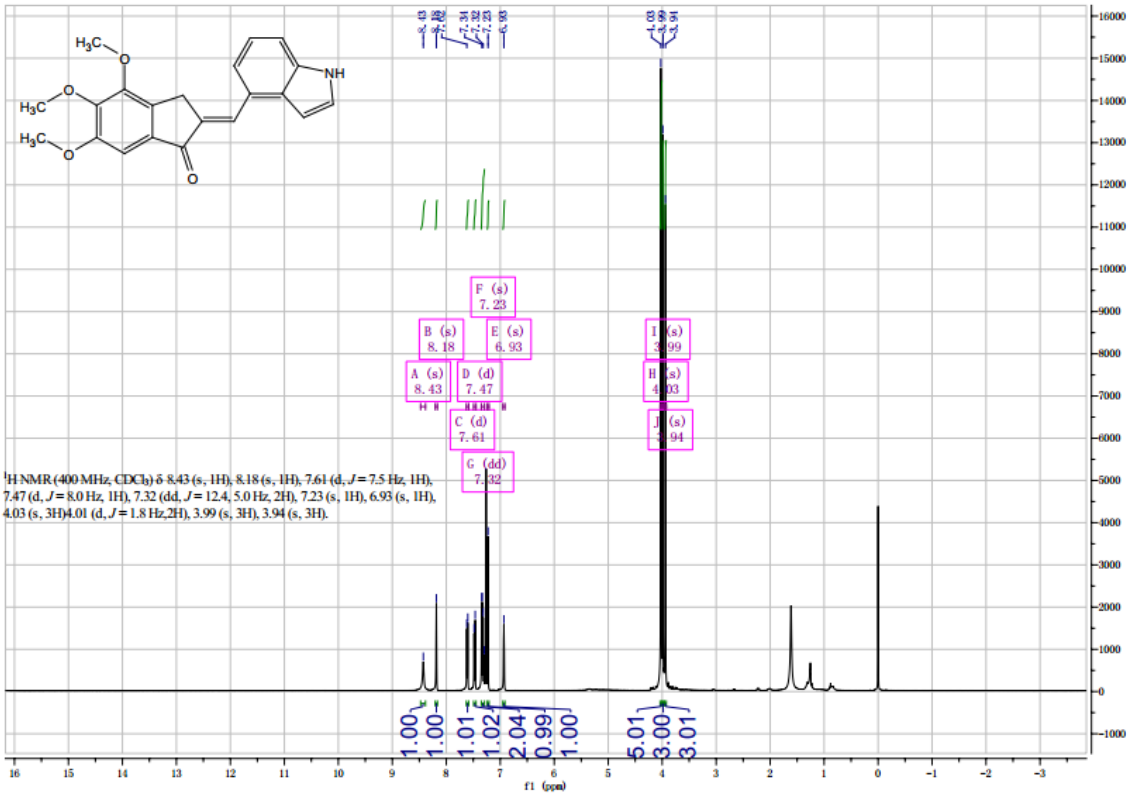


^{1}H NMR (400 MHz, CDCl$_3$) δ 7.93 (s, 1H), 7.78 (d, J = 8.7 Hz, 1H), 7.37 (s, 1H), 7.17 (s, 1H), 6.91 (d, J = 8.6 Hz, 1H), 6.74 (s, 1H), 4.04 (s, 3H), 3.98 (s, 3H), 3.93 (s, 3H), 3.86 (s, 3H), 3.82 (s, 3H), 3.65 (s, 2H).

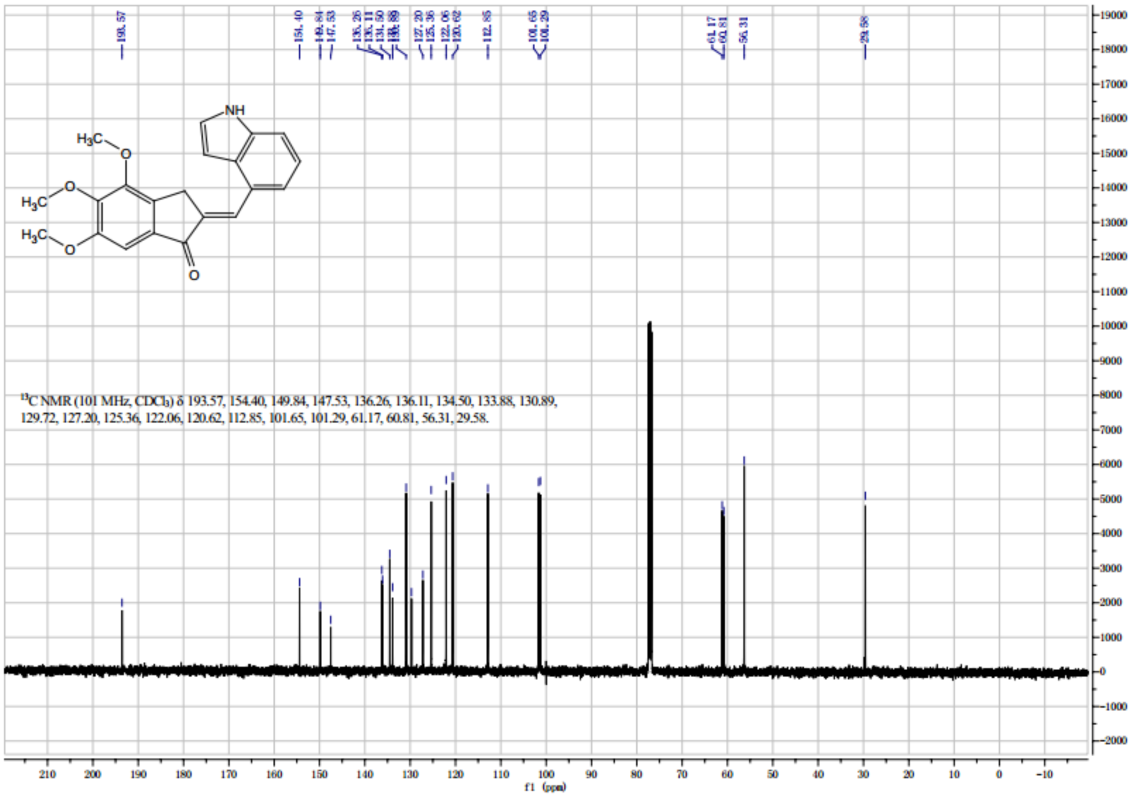


^{13}C NMR (101 MHz, CDCl$_3$) δ 192.88, 157.20, 154.02, 149.54, 146.86, 137.41, 134.52, 129.97, 124.92, 122.61, 119.63, 112.06, 110.65, 101.27, 93.16, 61.10, 60.79, 58.52, 56.26, 55.63, 33.85, 29.56, 18.90.

10a

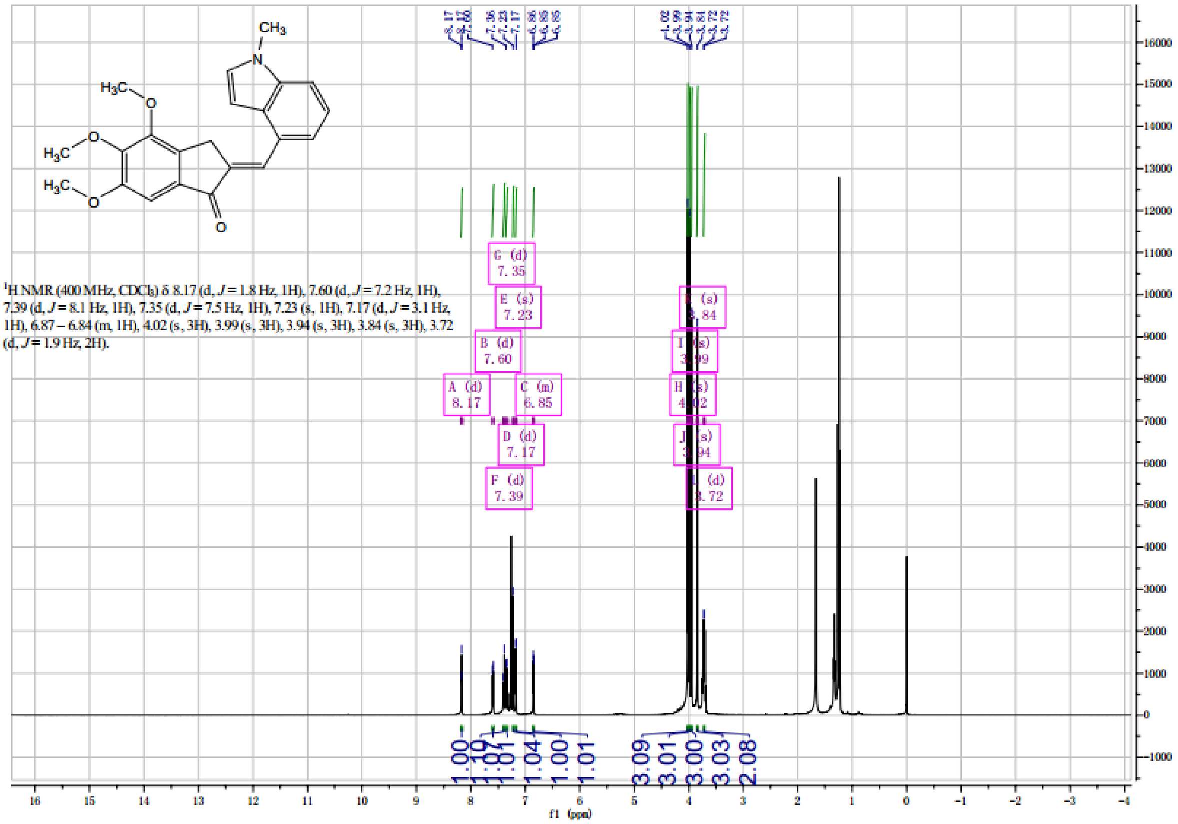


^1H NMR (400 MHz, $CDCl_3$) δ 8.43 (s, 1H), 8.18 (s, 1H), 7.61 (d, *J* = 7.5 Hz, 1H), 7.47 (d, *J* = 8.0 Hz, 1H), 7.32 (dd, *J* = 12.4, 5.0 Hz, 2H), 7.23 (s, 1H), 6.93 (s, 1H), 4.03 (s, 3H)4.01 (d, *J* = 1.8 Hz,2H), 3.99 (s, 3H), 3.94 (s, 3H).

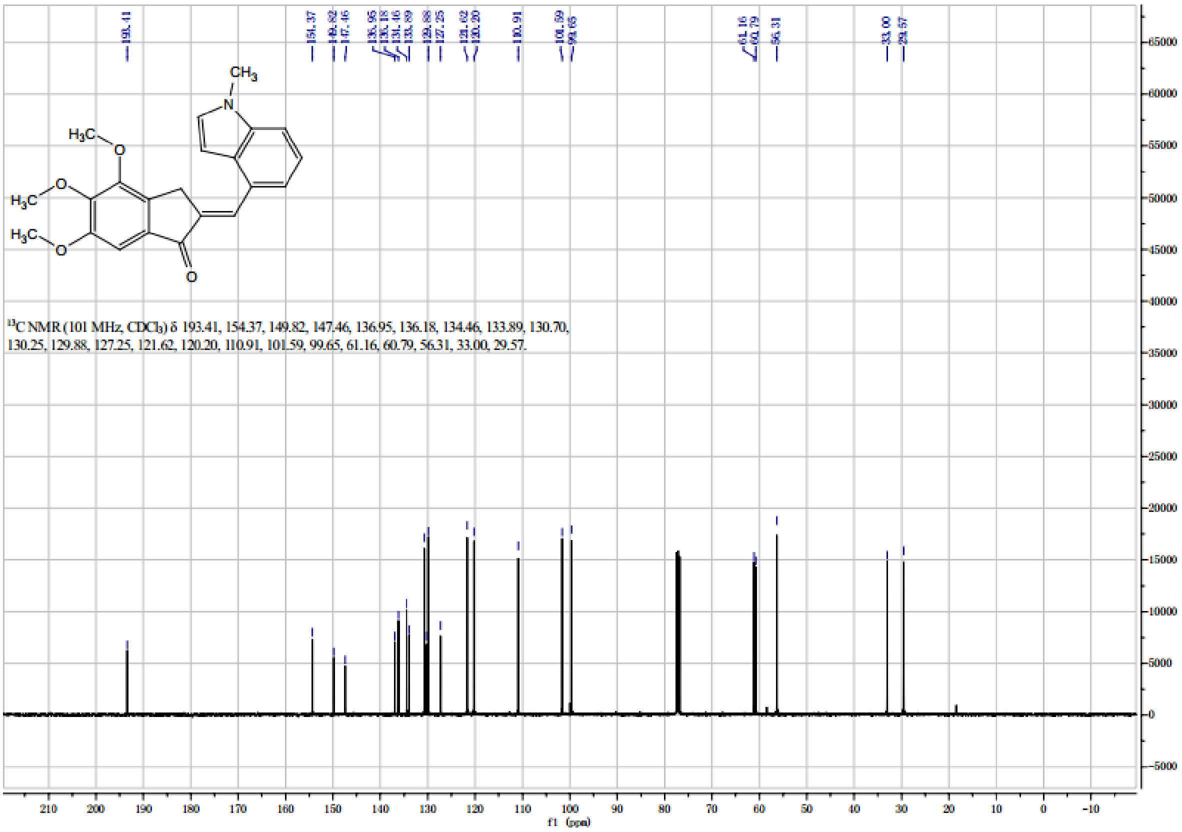


^{13}C NMR (101 MHz, $CDCl_3$) δ 193.57, 154.40, 149.84, 147.53, 136.26, 136.11, 134.50, 133.88, 130.89, 129.72, 127.20, 125.36, 122.06, 120.62, 112.85, 101.65, 101.29, 61.17, 60.81, 56.31, 29.58.

10b

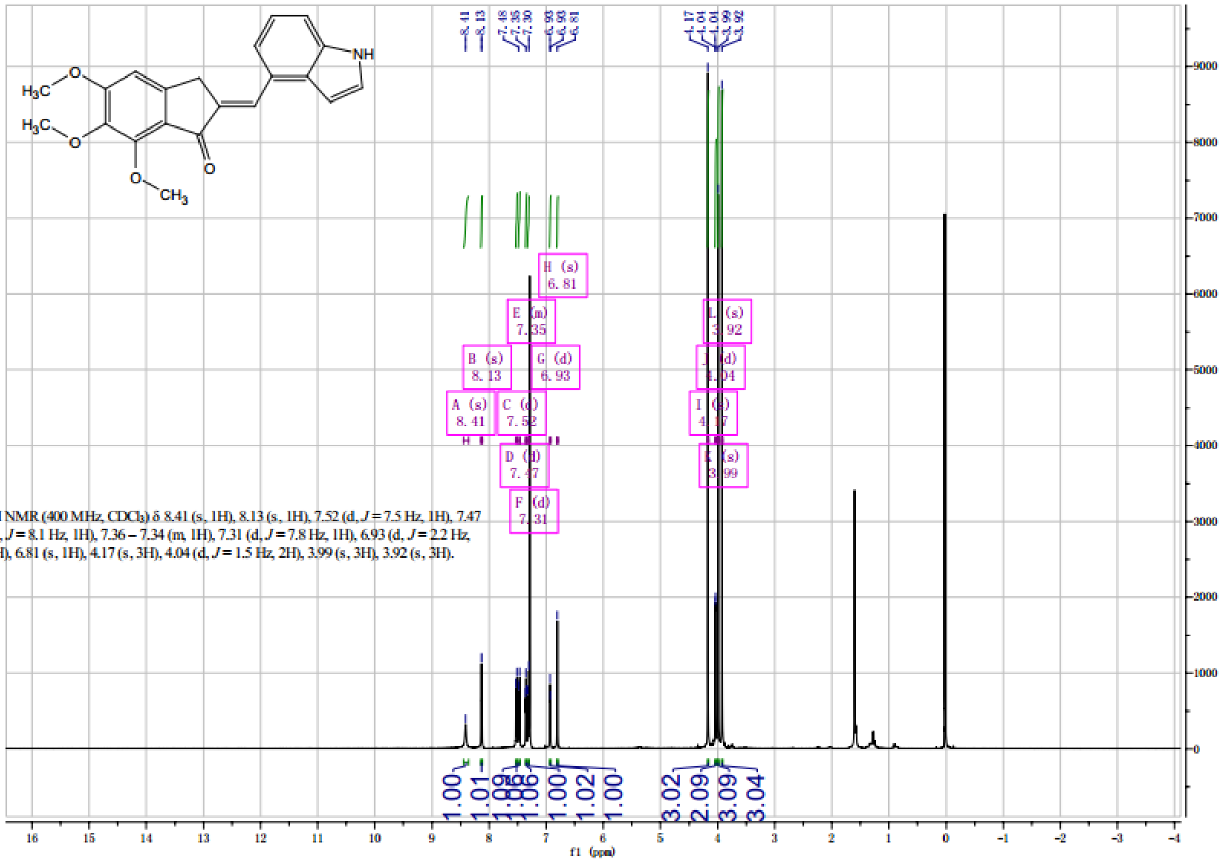


^{1}H NMR (400 MHz, CDCl$_3$) δ 8.17 (d, *J* = 1.8 Hz, 1H), 7.60 (d, *J* = 7.2 Hz, 1H), 7.39 (d, *J* = 8.1 Hz, 1H), 7.35 (d, *J* = 7.5 Hz, 1H), 7.23 (s, 1H), 7.17 (d, *J* = 3.1 Hz, 1H), 6.87 – 6.84 (m, 1H), 4.02 (s, 3H), 3.99 (s, 3H), 3.94 (s, 3H), 3.84 (s, 3H), 3.72 (d, *J* = 1.9 Hz, 2H).

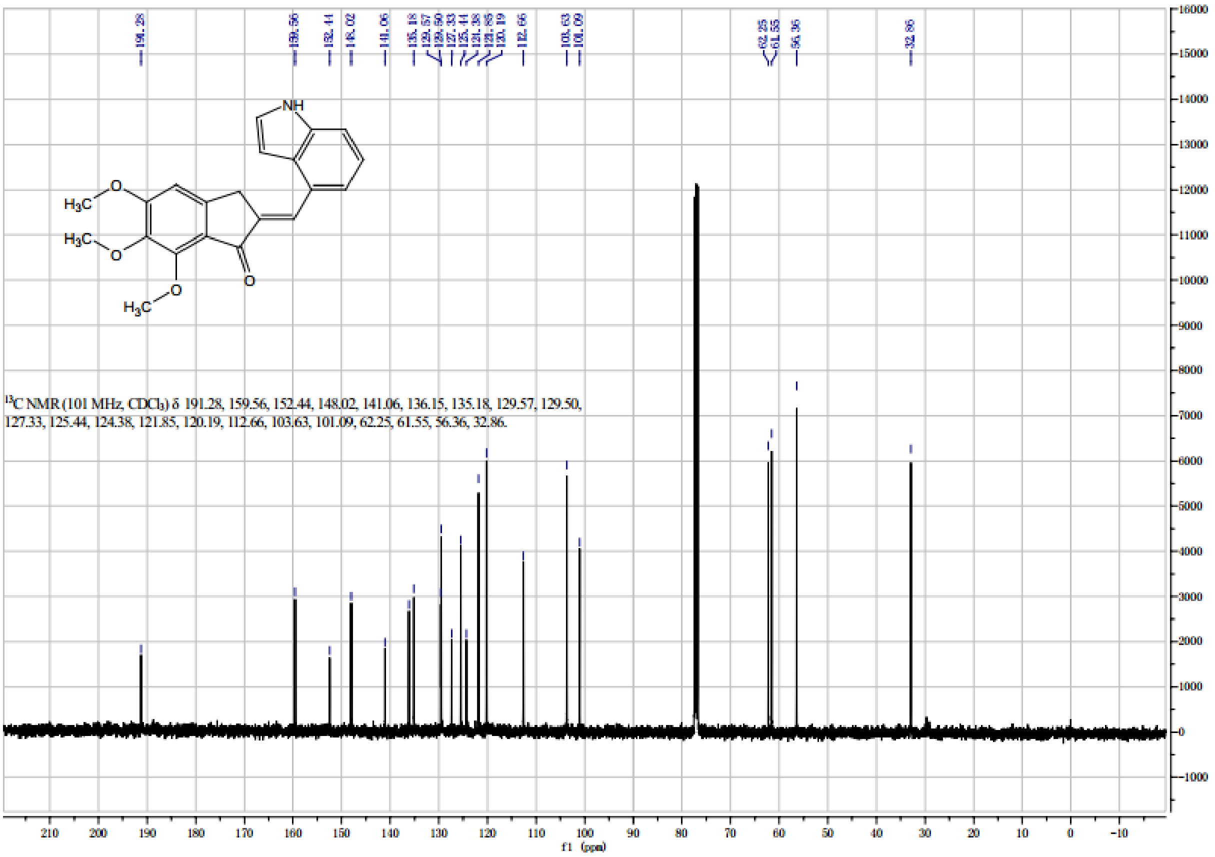


^{13}C NMR (101 MHz, CDCl$_3$) δ 193.41, 154.37, 149.82, 147.46, 136.95, 136.18, 134.46, 133.89, 130.70, 130.25, 129.88, 127.25, 121.62, 120.20, 110.91, 101.59, 99.65, 61.16, 60.79, 56.31, 33.00, 29.57.

10c

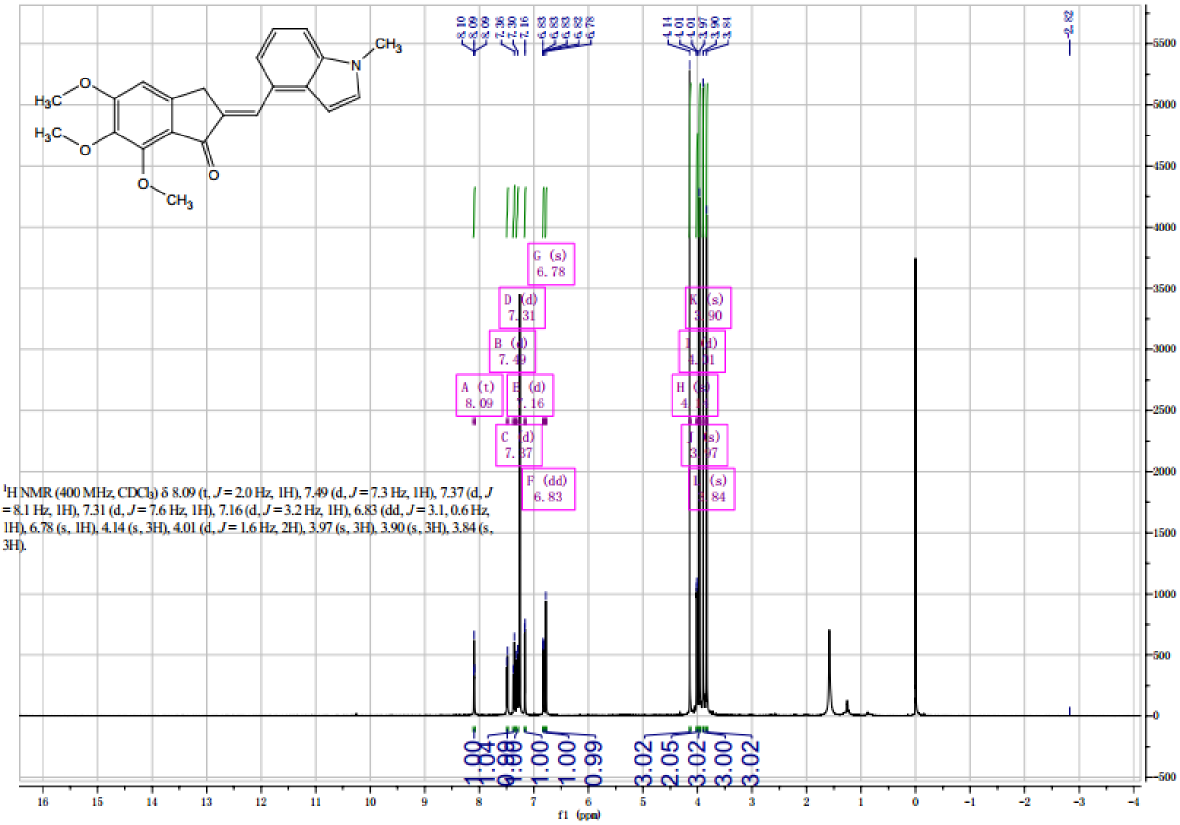


^{1}H NMR (400 MHz, CDCl$_3$) δ 8.41 (s, 1H), 8.13 (s, 1H), 7.52 (d, *J* = 7.5 Hz, 1H), 7.47 (d, *J* = 8.1 Hz, 1H), 7.36 – 7.34 (m, 1H), 7.31 (d, *J* = 7.8 Hz, 1H), 6.93 (d, *J* = 2.2 Hz, 1H), 6.81 (s, 1H), 4.17 (s, 3H), 4.04 (d, *J* = 1.5 Hz, 2H), 3.99 (s, 3H), 3.92 (s, 3H).

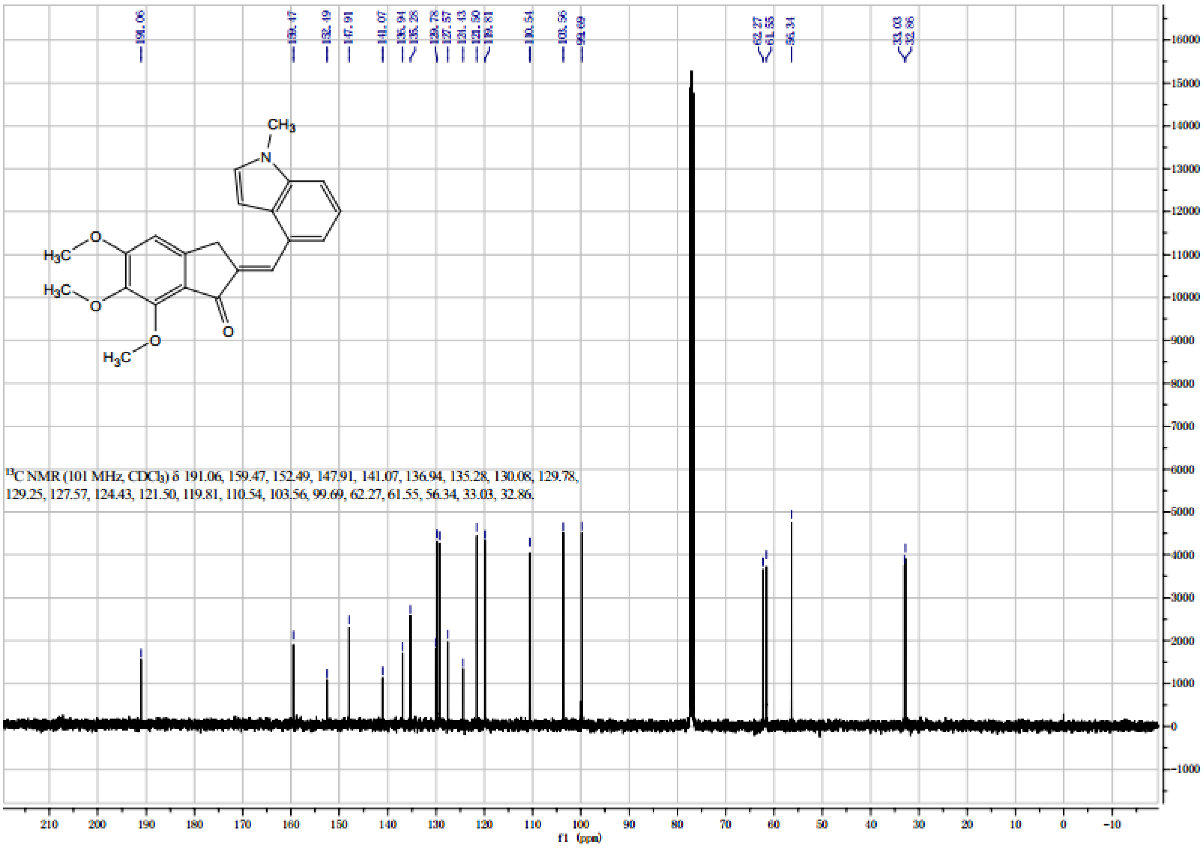


^{13}C NMR (101 MHz, CDCl$_3$) δ 191.28, 159.56, 152.44, 148.02, 141.06, 136.15, 135.18, 129.57, 129.50, 127.33, 125.44, 124.38, 121.85, 120.19, 112.66, 103.63, 101.09, 62.25, 61.55, 56.36, 32.86.

10d

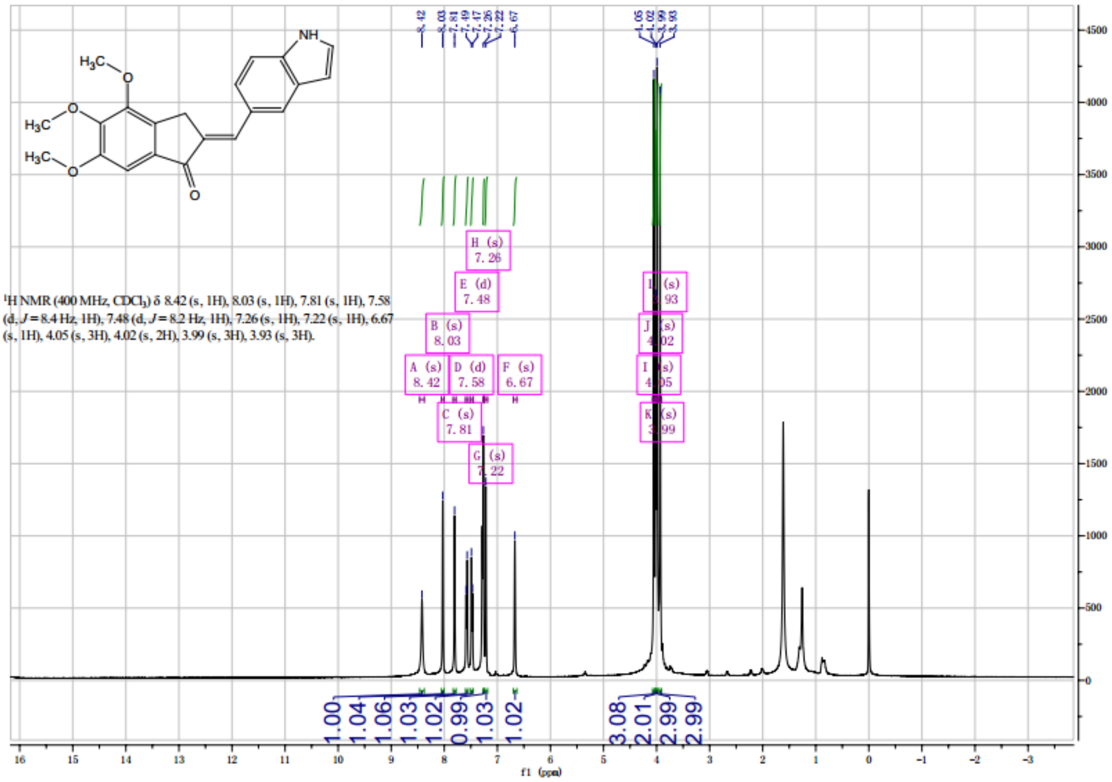


^{1}H NMR (400 MHz, CDCl$_3$) δ 8.09 (t, J = 2.0 Hz, 1H), 7.49 (d, J = 7.3 Hz, 1H), 7.37 (d, J = 8.1 Hz, 1H), 7.31 (d, J = 7.6 Hz, 1H), 7.16 (d, J = 3.2 Hz, 1H), 6.83 (dd, J = 3.1, 0.6 Hz, 1H), 6.78 (s, 1H), 4.14 (s, 3H), 4.01 (d, J = 1.6 Hz, 2H), 3.97 (s, 3H), 3.90 (s, 3H), 3.84 (s, 3H).

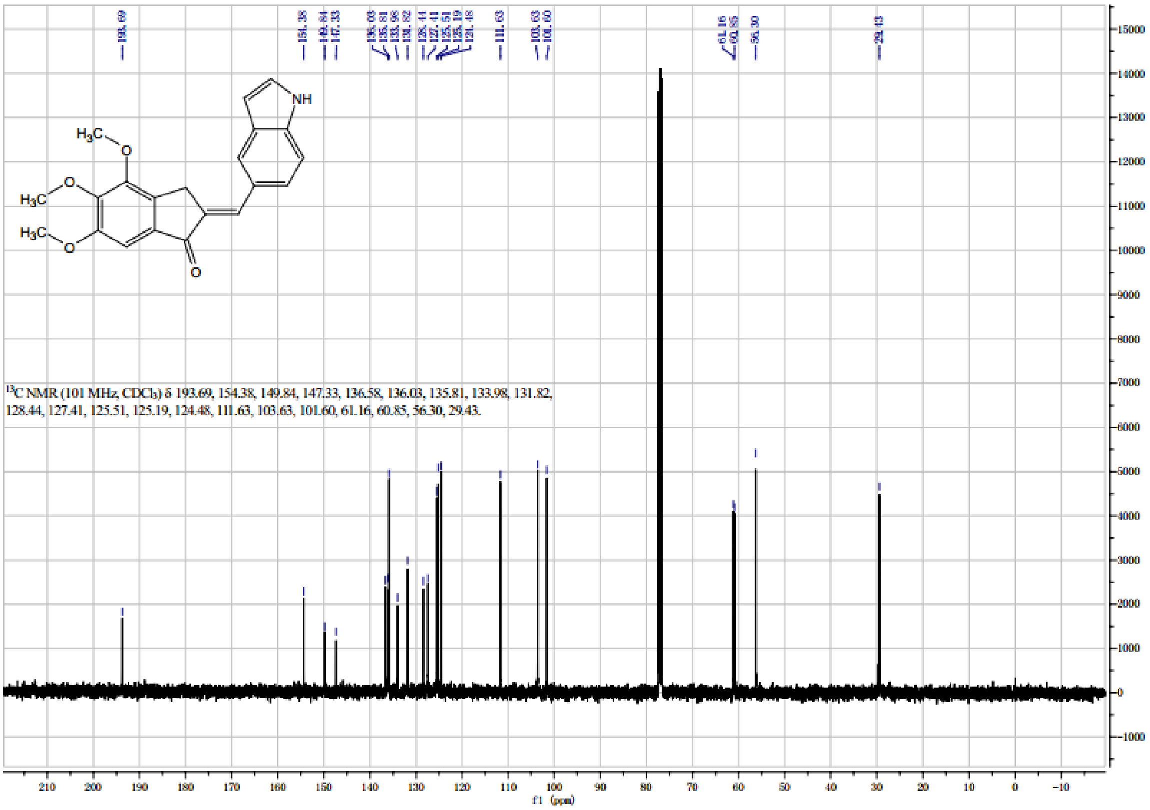


^{13}C NMR (101 MHz, CDCl$_3$) δ 191.06, 159.47, 152.49, 147.91, 141.07, 136.94, 135.28, 130.08, 129.78, 129.25, 127.57, 124.43, 121.50, 119.81, 110.54, 103.56, 99.69, 62.27, 61.55, 56.34, 33.03, 32.86.

11a

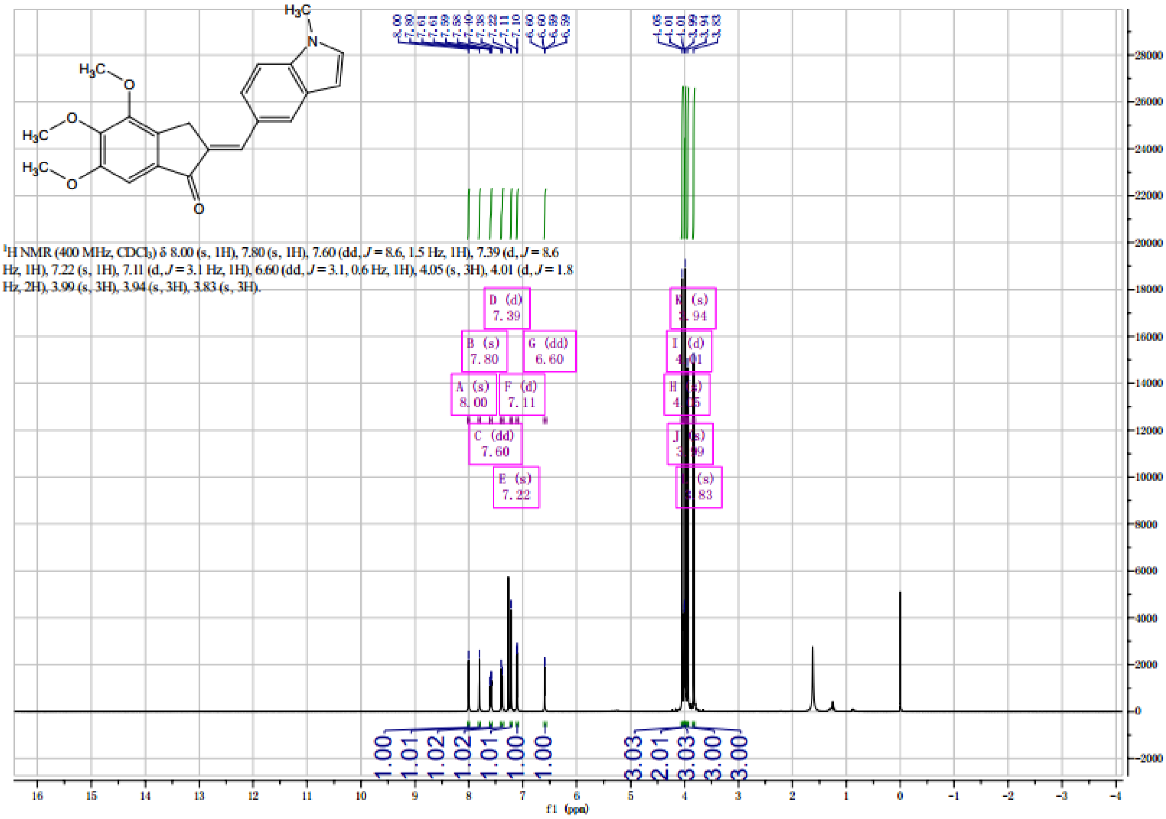


^{1}H NMR (400 MHz, CDCl$_3$) δ 8.42 (s, 1H), 8.03 (s, 1H), 7.81 (s, 1H), 7.58 (d, J = 8.4 Hz, 1H), 7.48 (d, J = 8.2 Hz, 1H), 7.26 (s, 1H), 7.22 (s, 1H), 6.67 (s, 1H), 4.05 (s, 3H), 4.02 (s, 2H), 3.99 (s, 3H), 3.93 (s, 3H).

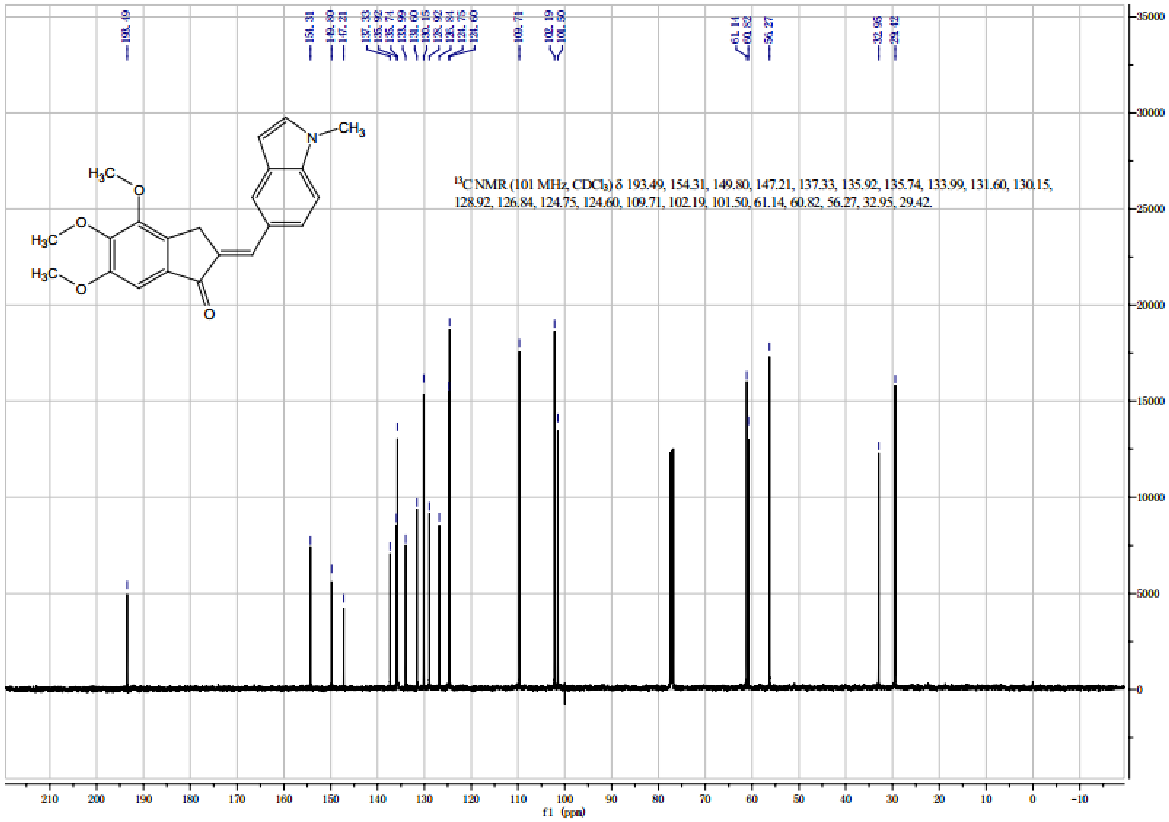


^{13}C NMR (101 MHz, CDCl$_3$) δ 193.69, 154.38, 149.84, 147.33, 136.58, 136.03, 135.81, 133.98, 131.82, 128.44, 127.41, 125.51, 125.19, 124.48, 111.63, 103.63, 101.60, 61.16, 60.85, 56.30, 29.43.

11b

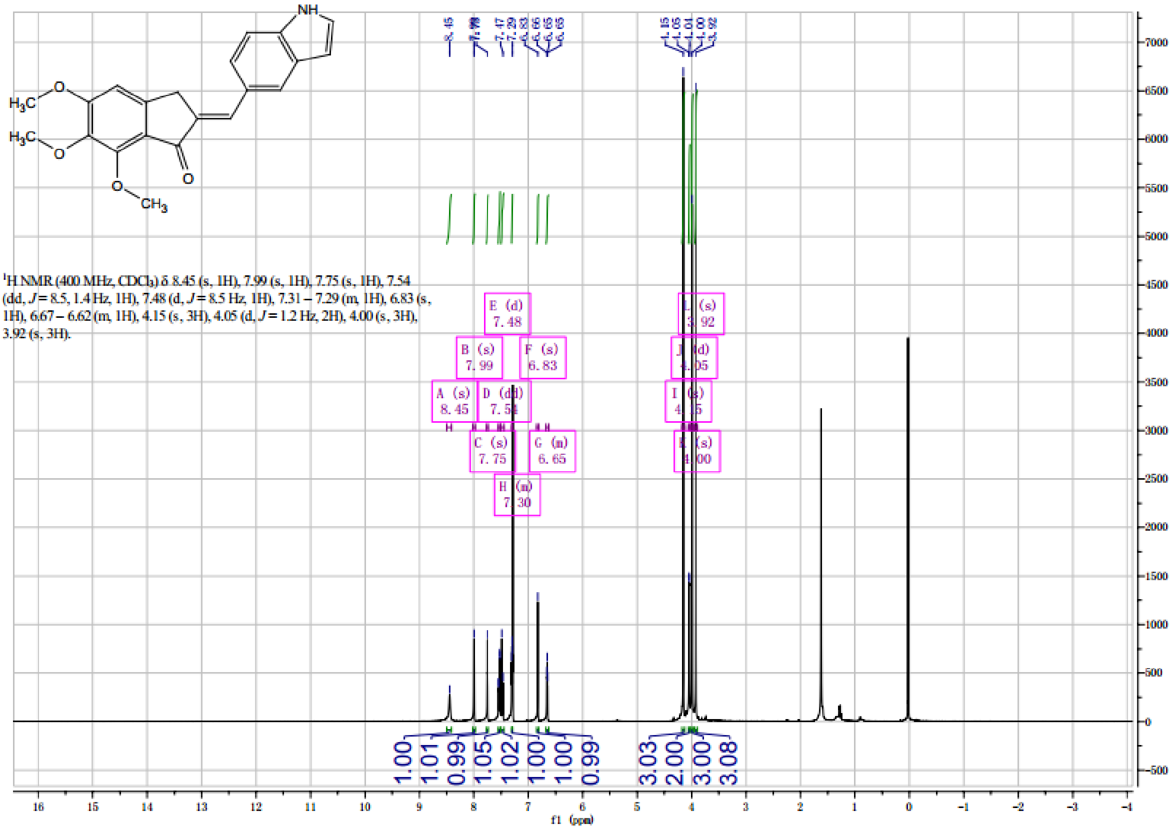


^{1}H NMR (400 MHz, CDCl$_3$) δ 8.00 (s, 1H), 7.80 (s, 1H), 7.60 (dd, J = 8.6, 1.5 Hz, 1H), 7.39 (d, J = 8.6 Hz, 1H), 7.22 (s, 1H), 7.11 (d, J = 3.1 Hz, 1H), 6.60 (dd, J = 3.1, 0.6 Hz, 1H), 4.05 (s, 3H), 4.01 (d, J = 1.8 Hz, 2H), 3.99 (s, 3H), 3.94 (s, 3H), 3.83 (s, 3H).

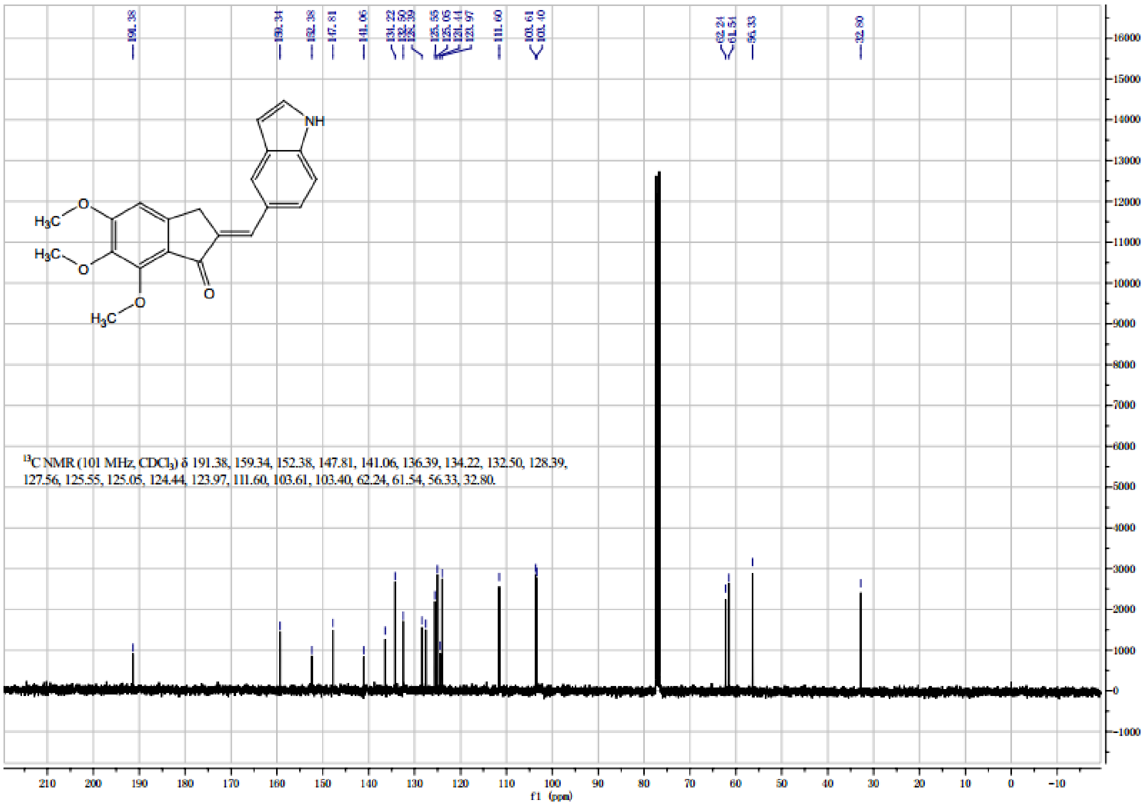


^{13}C NMR (101 MHz, CDCl$_3$) δ 193.49, 154.31, 149.80, 147.21, 137.33, 135.92, 135.74, 133.99, 131.60, 130.15, 128.92, 126.84, 124.75, 124.60, 109.71, 102.19, 101.50, 61.14, 60.82, 56.27, 32.95, 29.42.

11c

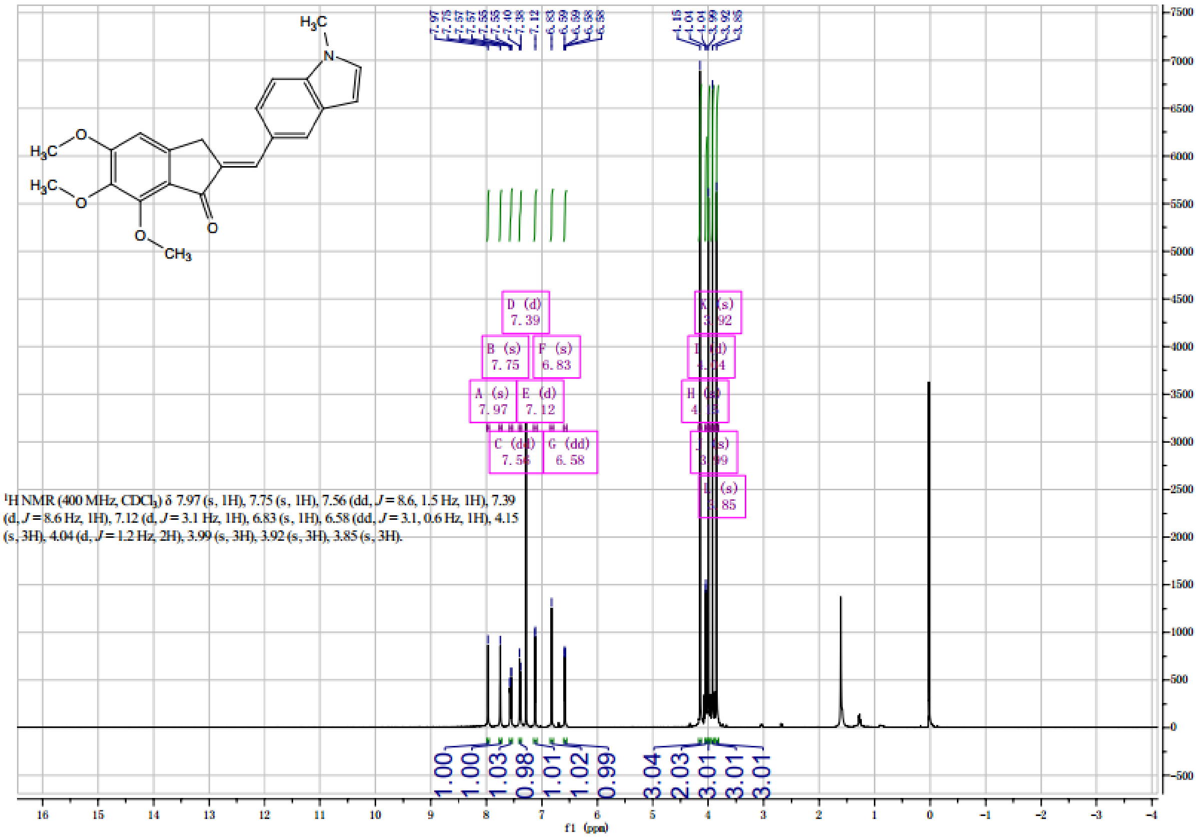


^{1}H NMR (400 MHz, $CDCl_3$) δ 8.45 (s, 1H), 7.99 (s, 1H), 7.75 (s, 1H), 7.54 (dd, *J* = 8.5, 1.4 Hz, 1H), 7.48 (d, *J* = 8.5 Hz, 1H), 7.31 – 7.29 (m, 1H), 6.83 (s, 1H), 6.67 – 6.62 (m, 1H), 4.15 (s, 3H), 4.05 (d, *J* = 1.2 Hz, 2H), 4.00 (s, 3H), 3.92 (s, 3H).

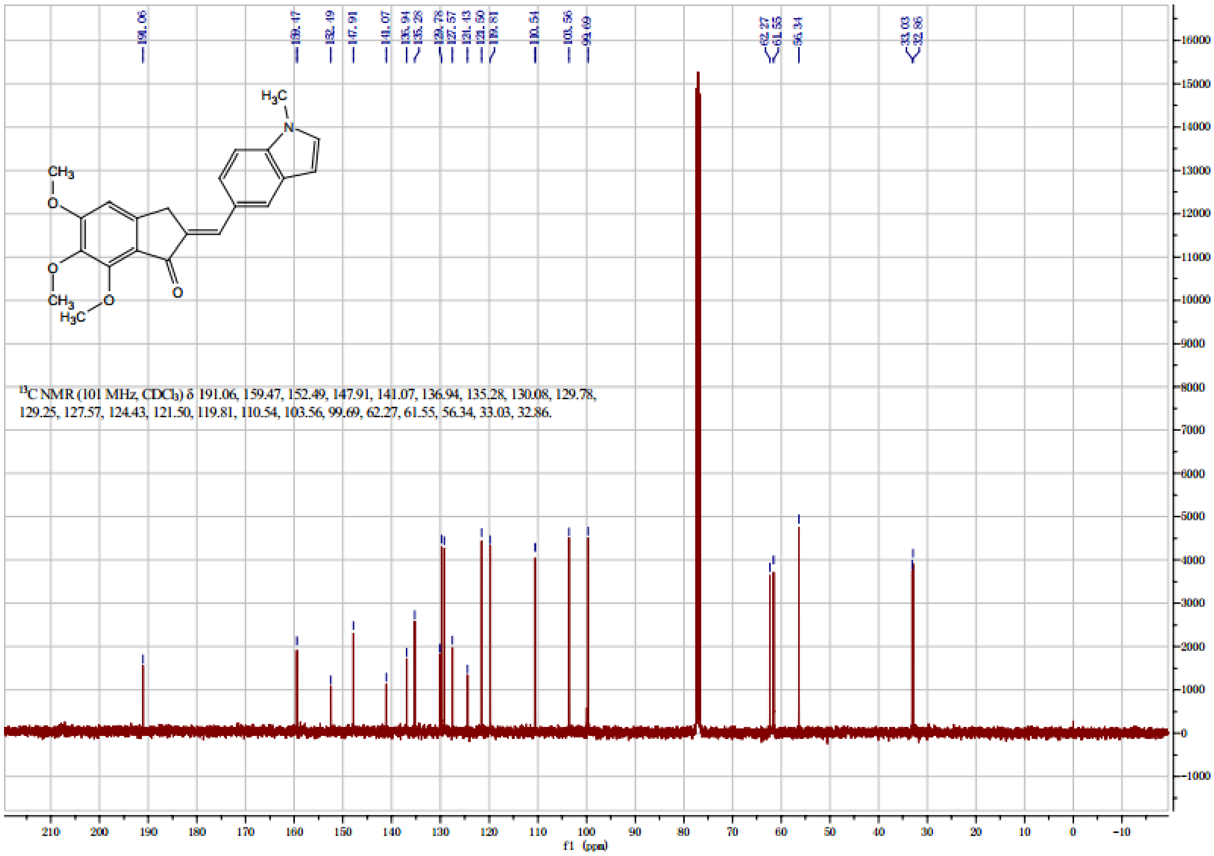


^{13}C NMR (101 MHz, $CDCl_3$) δ 191.38, 159.34, 152.38, 147.81, 141.06, 136.39, 134.22, 132.50, 128.39, 127.56, 125.55, 125.05, 124.44, 123.97, 111.60, 103.61, 103.40, 62.24, 61.54, 56.33, 32.80.

11d



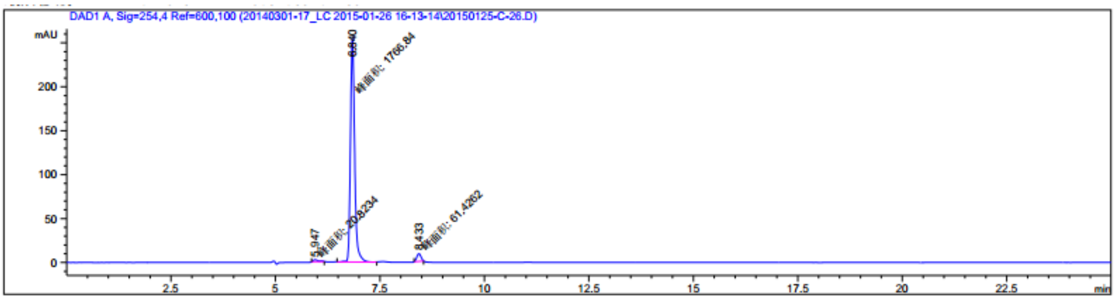
^{1}H NMR (400 MHz, CDCl$_3$) δ 7.97 (s, 1H), 7.75 (s, 1H), 7.56 (dd, *J* = 8.6, 1.5 Hz, 1H), 7.39 (d, *J* = 8.6 Hz, 1H), 7.12 (d, *J* = 3.1 Hz, 1H), 6.83 (s, 1H), 6.58 (dd, *J* = 3.1, 0.6 Hz, 1H), 4.15 (s, 3H), 4.04 (d, *J* = 1.2 Hz, 2H), 3.99 (s, 3H), 3.92 (s, 3H), 3.85 (s, 3H).



^{13}C NMR (101 MHz, CDCl$_3$) δ 191.06, 159.47, 152.49, 147.91, 141.07, 136.94, 135.28, 130.08, 129.78, 129.25, 127.57, 124.43, 121.50, 119.81, 110.54, 103.56, 99.69, 62.27, 61.55, 56.34, 33.03, 32.86.

SⅡ. HPLC chromatograms of target compounds

8a



Peak **Retention time** **Type** **Peak width** **Peak area** **Peak height** **Peak area**

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----|-------|----|-------|----------|----------|--------|
  1    5.947 MM    0.1528   20.82343    2.27158    1.1261
  2    6.840 MM    0.1164 1766.83618  252.99455   95.5519
  3    8.433 MM    0.1162   61.42618    8.81413    3.3220
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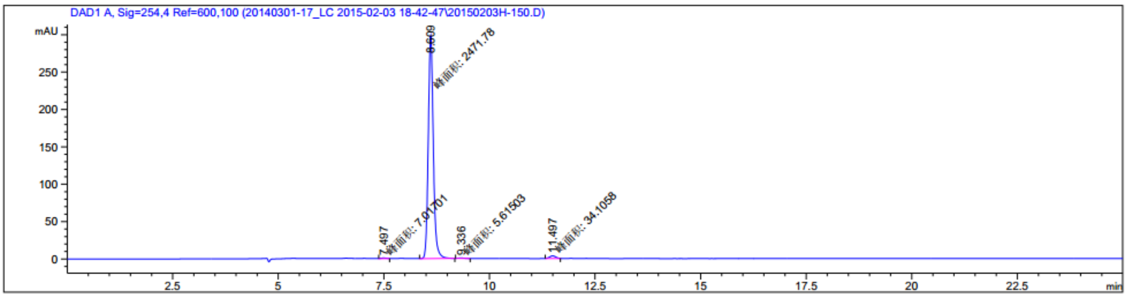
8b



Peak **Retention time** **Type** **Peak width** **Peak area** **Peak height** **Peak area**

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  #    [min]        [min]    [mAU*s]      [mAU]         %
----|-------|----|-------|----------|----------|--------|
  1    7.497 MM    0.1580    7.01701 7.40000e-1   0.2786
  2    8.609 MM    0.1382 2471.78442  298.17245  98.1442
  3    9.336 MM    0.1755    5.61503 5.33199e-1   0.2229
  4   11.497 MM    0.1659   34.10582    3.42686   1.3542
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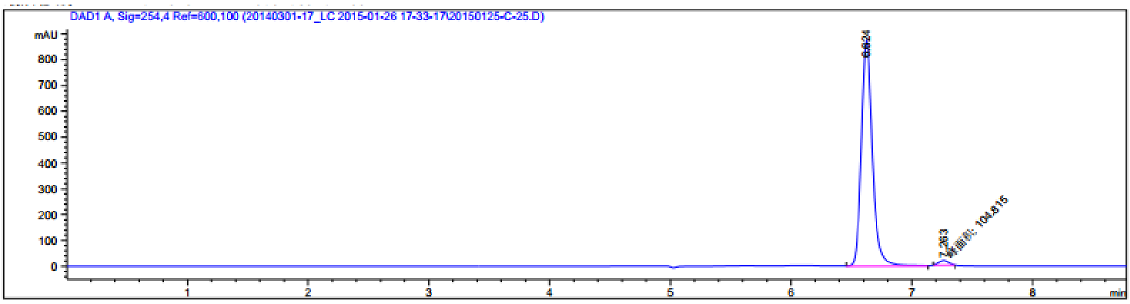
8c



Peak Retention time Type Peak width Peak area Peak height Peak area

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  1    6.624 VV    0.0966 5590.74316  874.41718  98.1597
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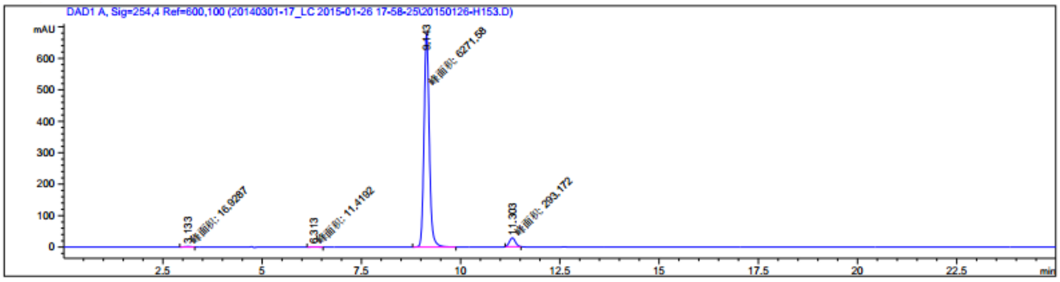
8d



Peak Retention time Type Peak width Peak area Peak height Peak area

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  1    3.133 MM    0.2036   16.92868    1.38594   0.2568
  2    6.313 MM    0.2386   11.41923 7.97671e-1   0.1732
  3    9.143 MM    0.1546 6271.58398  676.11389  95.1234
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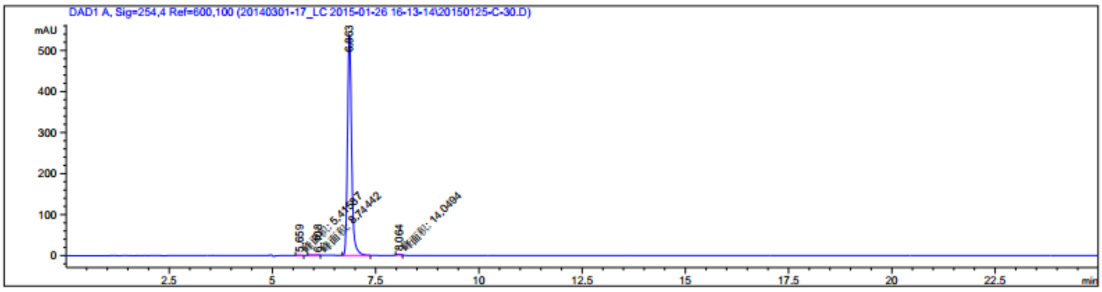
8e



Peak Retention time Type Peak width Peak area Peak height Peak area

```
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  3    6.863 BB    0.1076 3745.78003  535.80304  99.2525
  4    8.064 MM    0.1007   14.04943    2.32630   0.3723
```
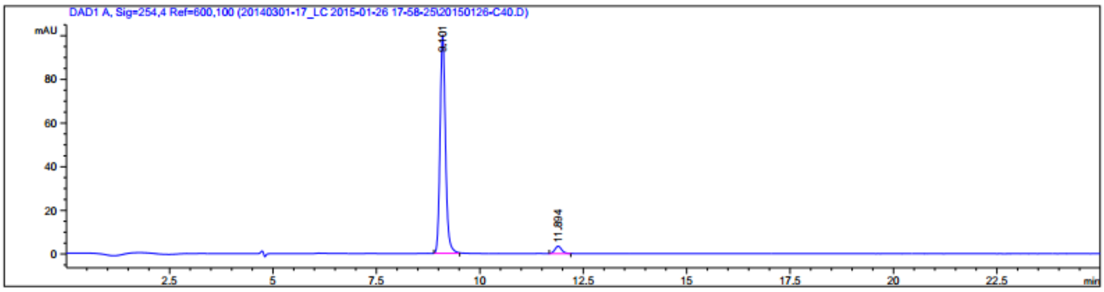
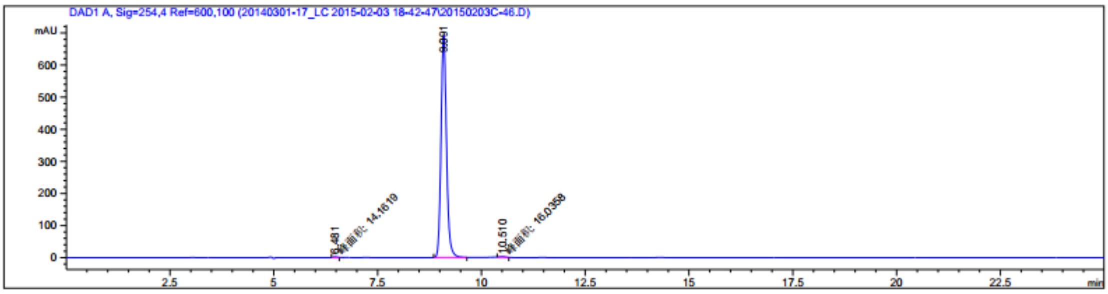

8f



Peak **Retention time** **Type** **Peak width** **Peak area** **Peak height** **Peak area**

```
  #     [min]          [min]    [mAU*s]      [mAU]        %
----|-------|----|-------|----------|----------|--------|
  1    9.101 BB     0.1383  908.48114   99.73994  95.9244
  2   11.894 BB     0.1785   38.59943    3.34932   4.0756
```

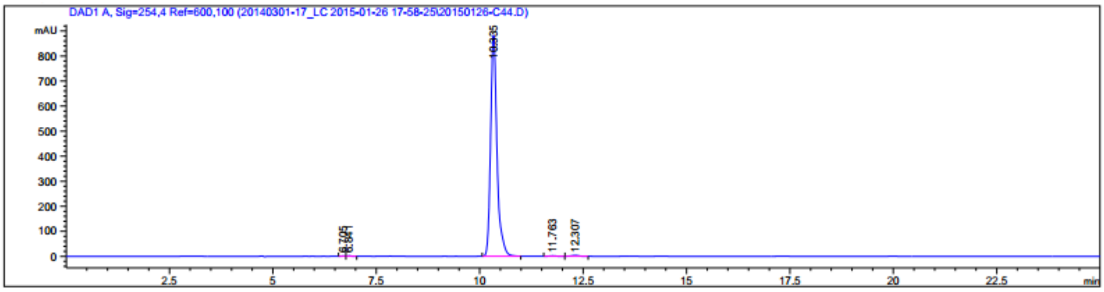
10a



Peak **Retention time** **Type** **Peak width** **Peak area** **Peak height** **Peak area**

```
  #     [min]          [min]    [mAU*s]      [mAU]        %
----|-------|----|-------|----------|----------|--------|
  1    6.481 MM     0.0983   14.16191    2.40131   0.2218
  2    9.091 BB     0.1414 6354.59326  690.33319  99.5270
  3   10.510 MM     0.1360   16.03581    1.96487   0.2512
```

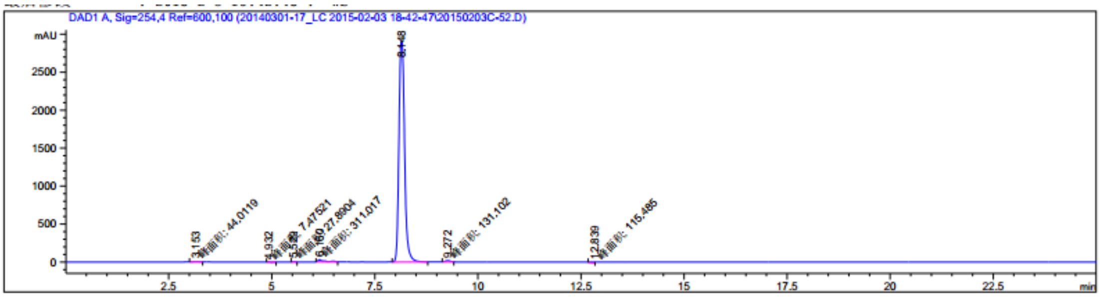
10b



Peak **Retention time** **Type** **Peak width** **Peak area** **Peak height** **Peak area**

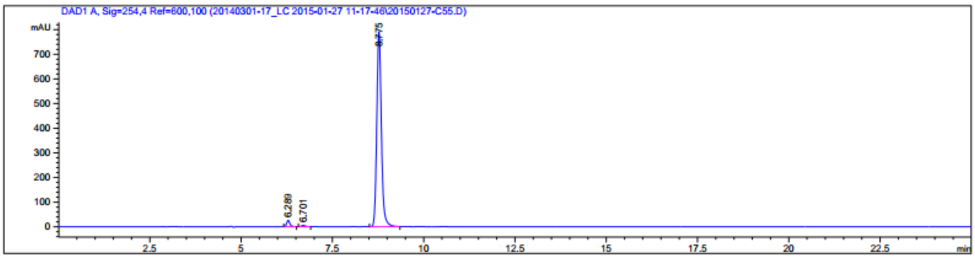
```
  #     [min]          [min]    [mAU*s]      [mAU]        %
----|-------|----|-------|----------|----------|--------|
  1    6.705 BV     0.0909   11.25573    1.90643   0.1171
  2    6.841 VB     0.1086   18.00187    2.42609   0.1873
  3   10.335 BB     0.1638 9511.89551  882.10077  98.9496
  4   11.763 BB     0.1880   23.20288    1.87931   0.2414
  5   12.307 BB     0.1955   48.50996    3.73635   0.5046
```

10c



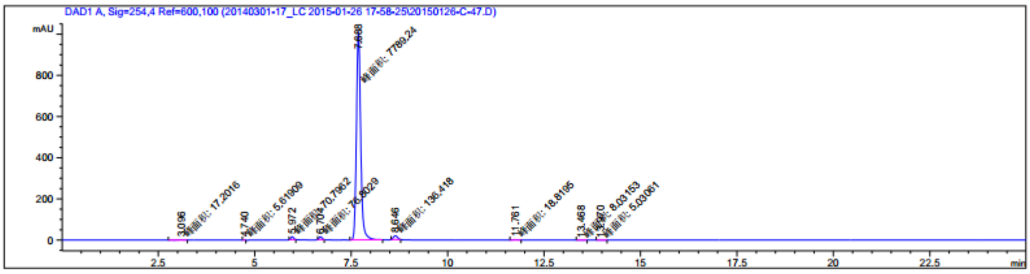
Peak #	Retention time [min]	Type	Peak width [min]	Peak area [mAU*s]	Peak height [mAU]	Peak area %
1	3.153	MM	0.1831	44.01191	4.00534	0.1558
2	4.932	MM	0.0996	7.47521	1.25040	0.0265
3	5.529	MM	0.0857	27.89041	5.42169	0.0987
4	6.160	MM	0.1805	311.01740	28.71350	1.1011
5	8.148	VB	0.1487	2.76086e4	2910.15405	97.7448
6	9.272	MM	0.1377	131.10223	15.86812	0.4642
7	12.839	MM	0.1186	115.48467	16.22391	0.4089

10d



Peak #	Retention time [min]	Type	Peak width [min]	Peak area [mAU*s]	Peak height [mAU]	Peak area %
1	6.289	BB	0.0961	158.81326	25.71469	2.2162
2	6.701	BB	0.1063	37.10743	5.25904	0.5178
3	8.775	VB	0.1348	6970.19092	791.03973	97.2660

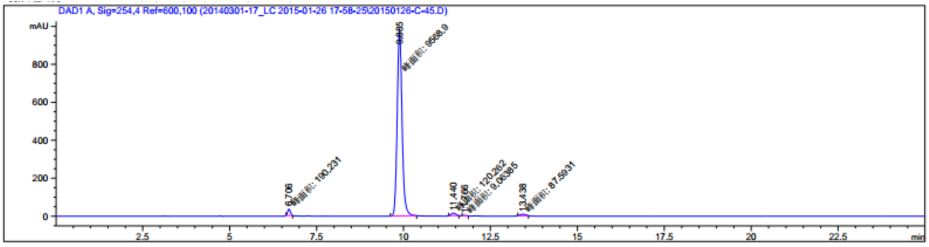
11a



Peak	Retention time	Type	Peak width	Peak area	Peak height	Peak area

```
   #    [min]          [min]    [mAU*s]      [mAU]          %
----|--------|----|--------|----------|----------|--------|
   1    3.096 MM    0.2171    17.20162     1.32028    0.2116
   2    4.740 MM    0.0632     5.61909     1.48231    0.0691
   3    5.972 MM    0.0837    70.79625    14.10119    0.8710
   4    6.704 MM    0.0915    76.80293    13.99040    0.9449
   5    7.688 MM    0.1294 7789.24072 1002.89917   95.8327
   6    8.646 MM    0.1229   136.41814    18.49550    1.6784
   7   11.761 MM    0.1897    18.81947     1.65361    0.2315
   8   13.468 MM    0.2662     8.03153 5.02806e-1    0.0988
   9   13.970 MM    0.1882     5.03061 3.37868e-1    0.0619
```

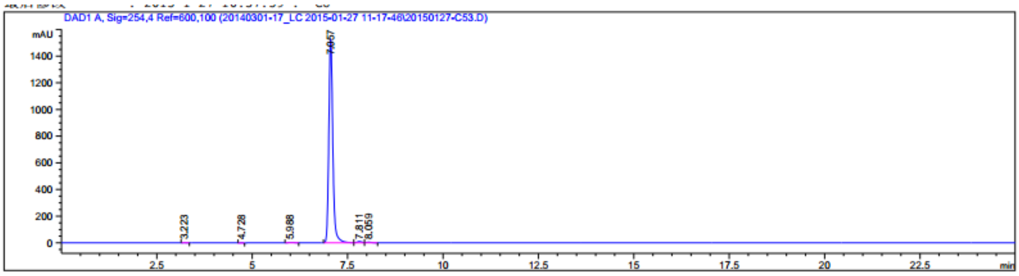
11b



Peak **Retention time** **Type** **Peak width** **Peak area** **Peak height** **Peak area**

```
   #    [min]          [min]    [mAU*s]      [mAU]          %
----|--------|----|--------|----------|----------|--------|
   1    6.706 MM    0.0937   190.23053    33.82433    1.9069
   2    9.885 MM    0.1632  9568.90137   977.41876   95.9187
   3   11.440 MM    0.1527   120.26173    13.13027    1.2055
   4   11.766 MM    0.1073     9.06385     1.40734    0.0909
   5   13.438 MM    0.1858    87.59314     7.85670    0.8780
```

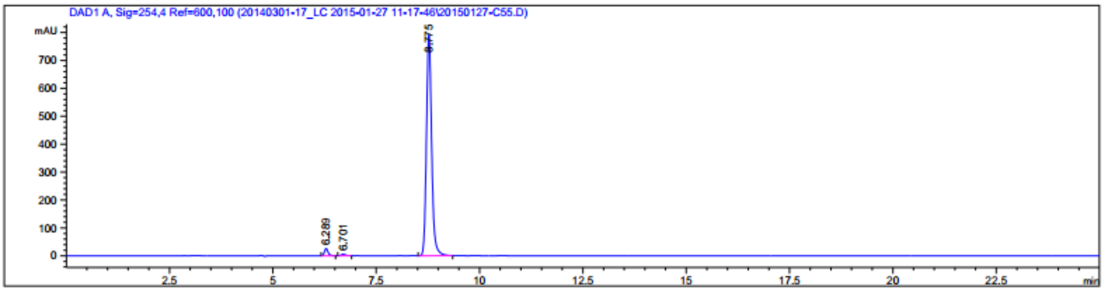
11c



Peak **Retention time** **Type** **Peak width** **Peak area** **Peak height** **Peak area**

```
   #    [min]          [min]    [mAU*s]      [mAU]          %
----|--------|----|--------|----------|----------|--------|
   1    3.223 BB    0.0818     7.40275     1.31160    0.0655
   2    4.728 BV    0.0906    16.64960     2.83334    0.1473
   3    5.988 BV    0.1468    29.86816     2.74786    0.2642
   4    7.057 BV    0.1130 1.11380e4   1529.22986   98.5142
   5    7.811 VV    0.1245    75.73344     9.15919    0.6699
   6    8.059 VB    0.1448    38.32880     4.03567    0.3390
```

11d

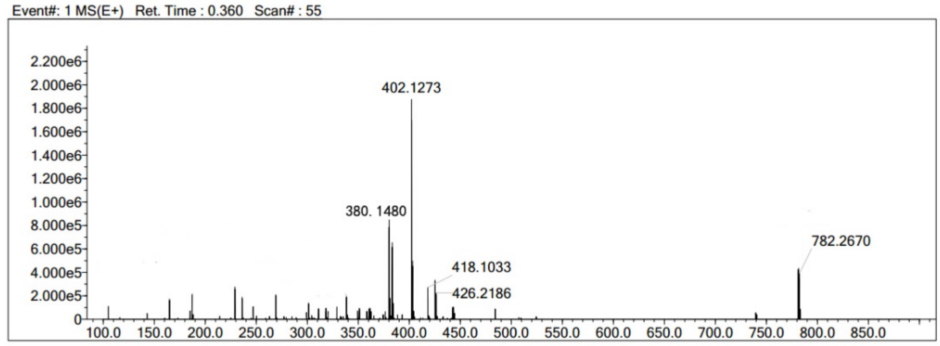


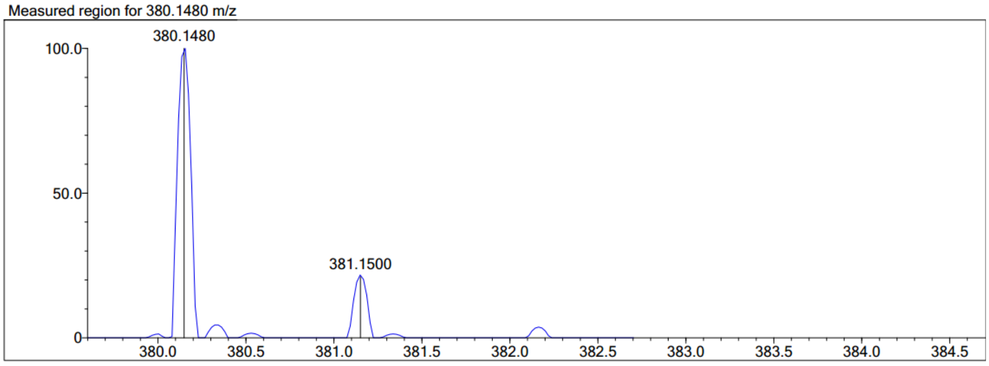
Peak Retention time Type Peak width Peak area Peak height Peak area

```
 #    [min]           [min]    [mAU*s]     [mAU]        %
----|-------|----|-------|----------|----------|--------|
  1   6.289 BB    0.0961  158.81326   25.71469   2.2162
  2   6.701 BB    0.1063   37.10743    5.25904   0.5178
  3   8.775 VB    0.1348 6970.19092  791.03973  97.2660
```

SⅢ.High resolution mass spectra of target compounds

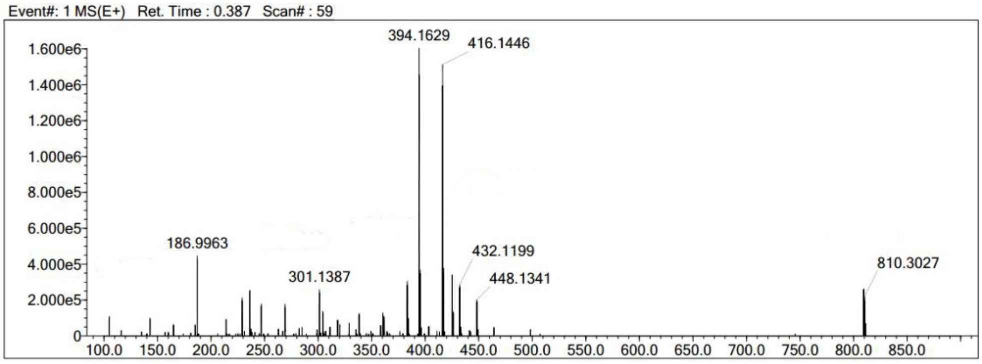
8a

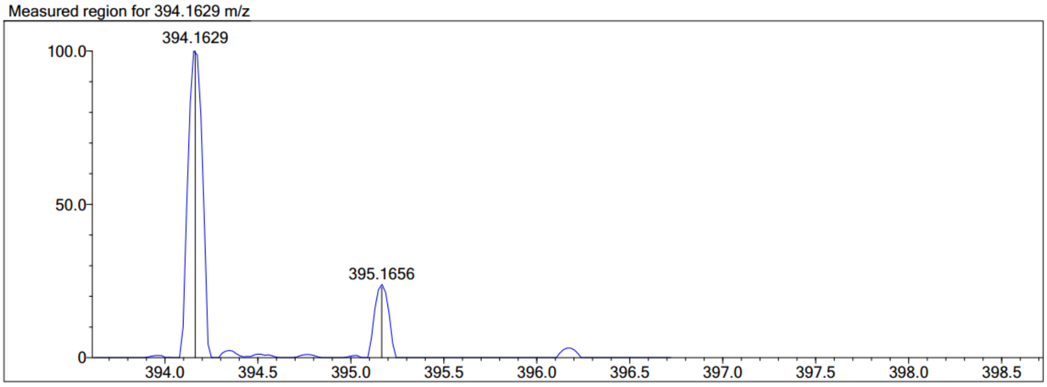




Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
2	85.07	C22 H21 N O5	[M+H]+	380.1480	380.1492	-1.2	-3.16	89.92	13.0

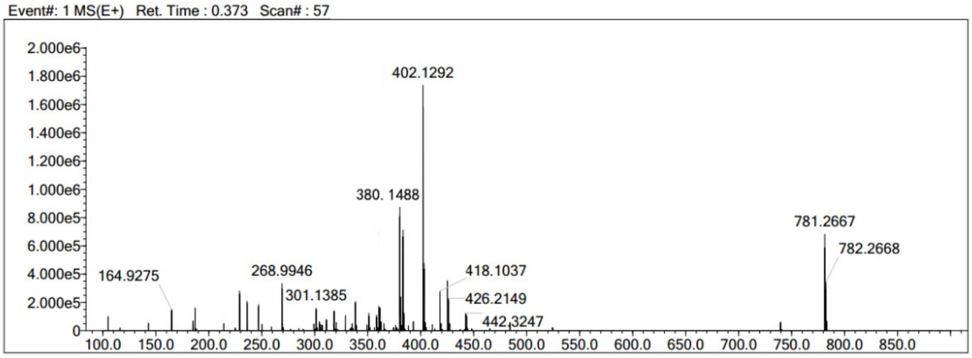
8b

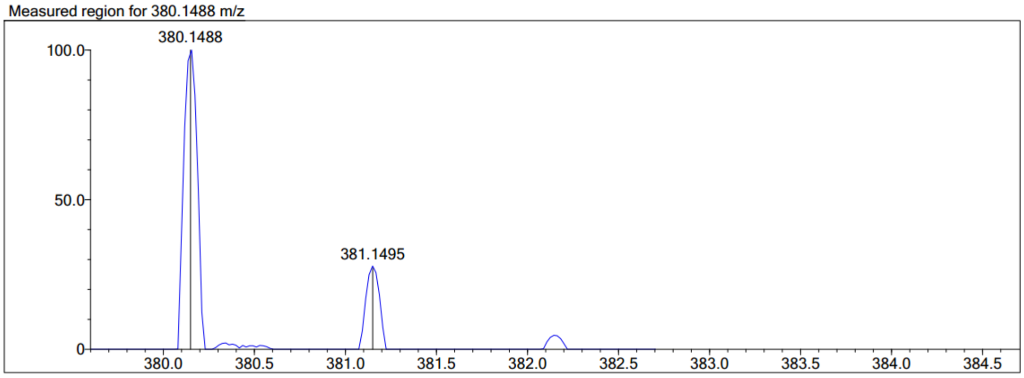




Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	84.53	C23 H23 N O5	[M+H]+	394.1629	394.1649	-2.0	-5.07	94.66	13.0

8c

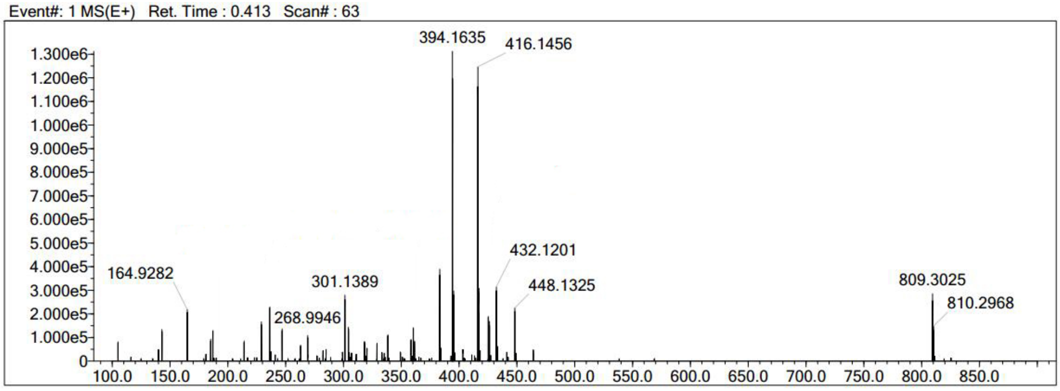




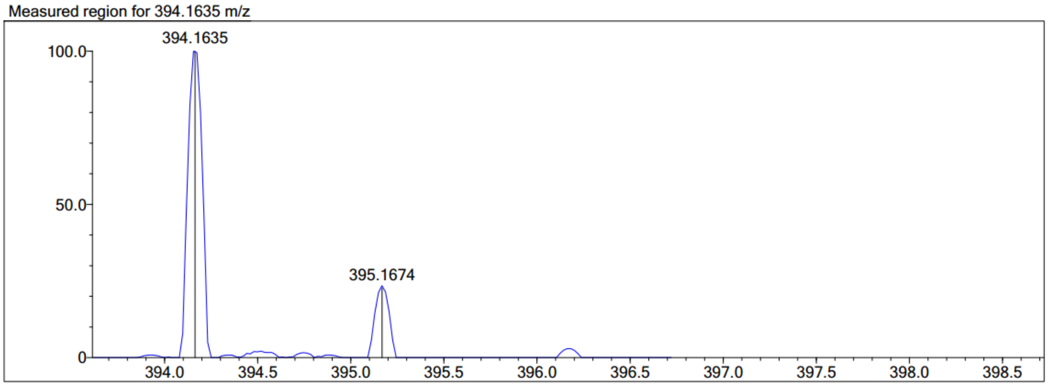
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	87.39	C22 H21 N O5	[M+H]+	380.1488	380.1492	-0.4	-1.05	87.50	13.0

8d

Event#: 1 MS(E+) Ret. Time : 0.413 Scan# : 63



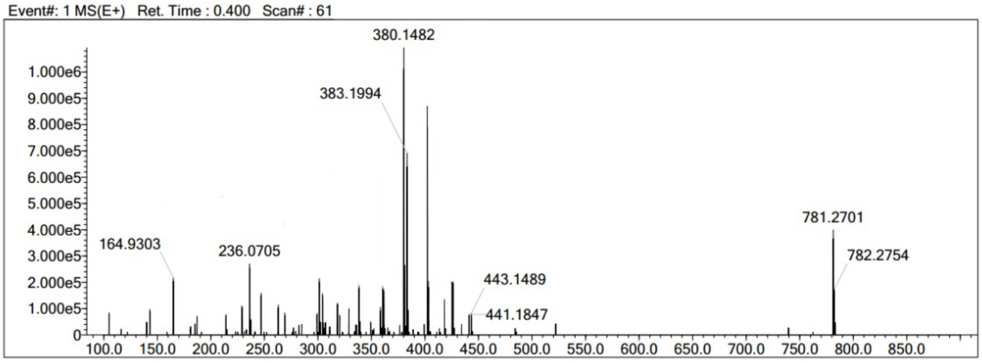
Measured region for 394.1635 m/z



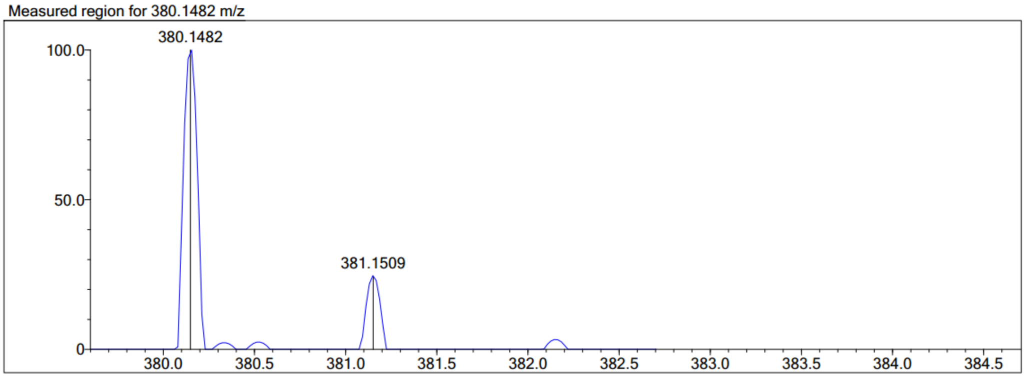
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	89.78	$C_{23}H_{23}NO_{5}$	[M+H]+	394.1635	394.1649	-1.4	-3.55	95.89	13.0

8e

Event#: 1 MS(E+) Ret. Time : 0.400 Scan# : 61



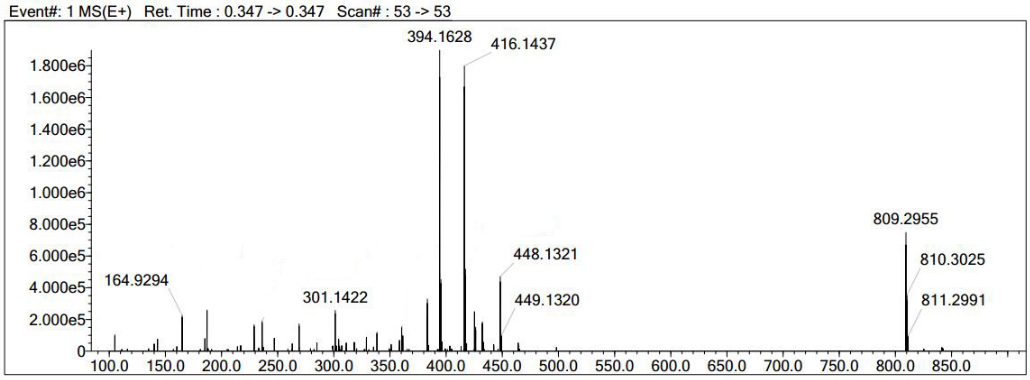
Measured region for 380.1482 m/z



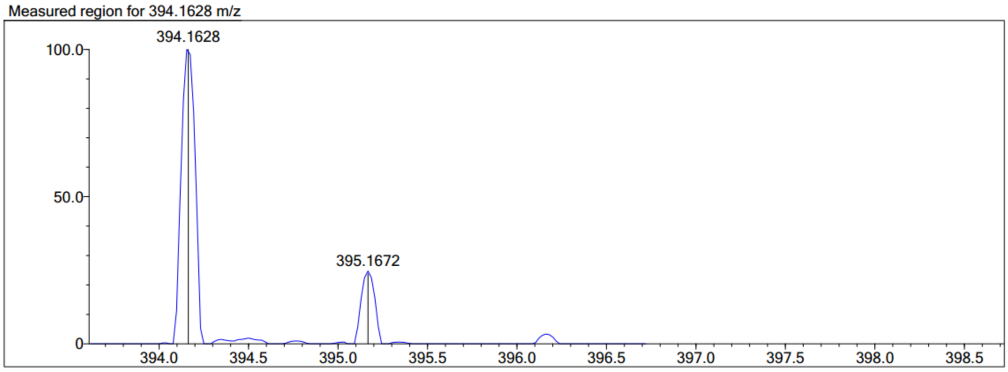
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
2	85.98	$C_{22}H_{21}NO_{5}$	[M+H]+	380.1482	380.1492	-1.0	-2.63	89.63	13.0

8f

Event#: 1 MS(E+) Ret. Time : 0.347 -> 0.347 Scan# : 53 -> 53



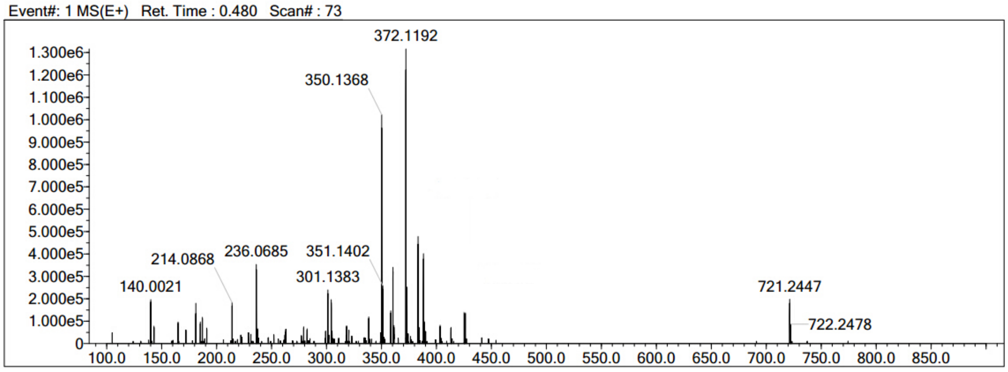
Measured region for 394.1628 m/z



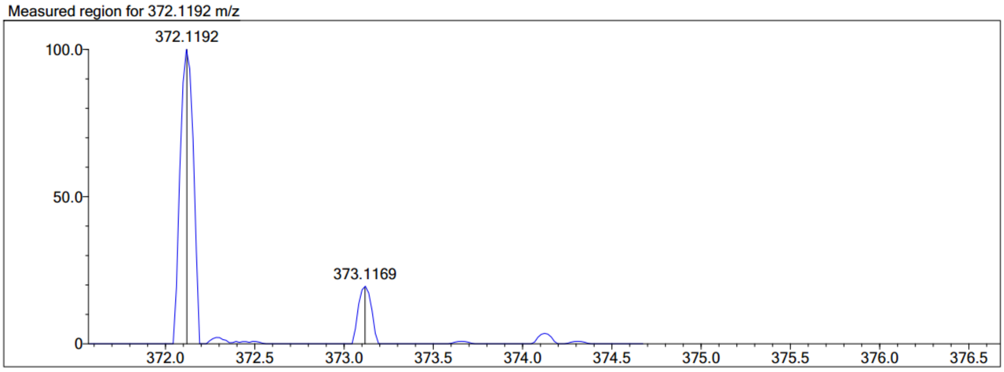
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
3	76.43	C23 H23 N O5	[M+H]+	394.1628	394.1649	-2.1	-5.33	88.16	13.0

10a

Event#: 1 MS(E+) Ret. Time : 0.480 Scan# : 73



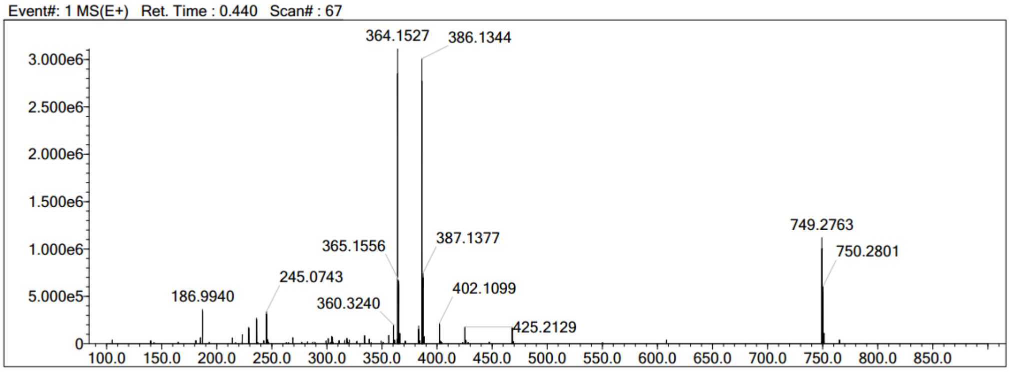
Measured region for 372.1192 m/z



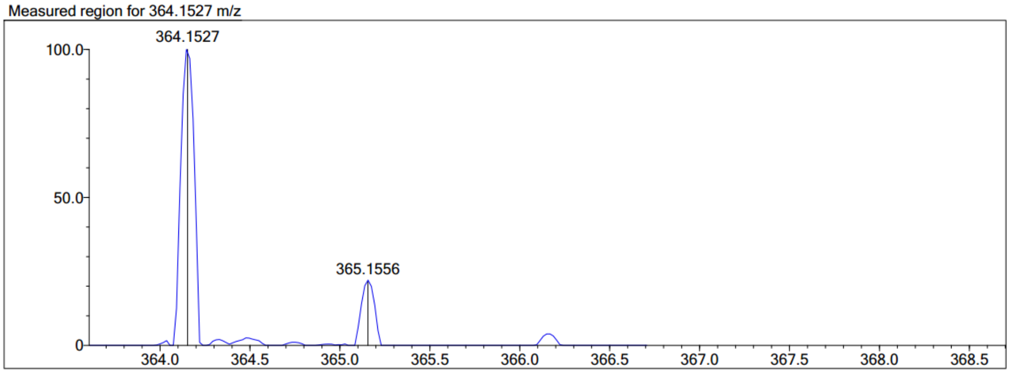
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
2	69.02	C21 H19 N O4	[M+Na]+	372.1192	372.1206	-1.4	-3.76	74.14	13.0

10b

Event#: 1 MS(E+) Ret. Time : 0.440 Scan# : 67



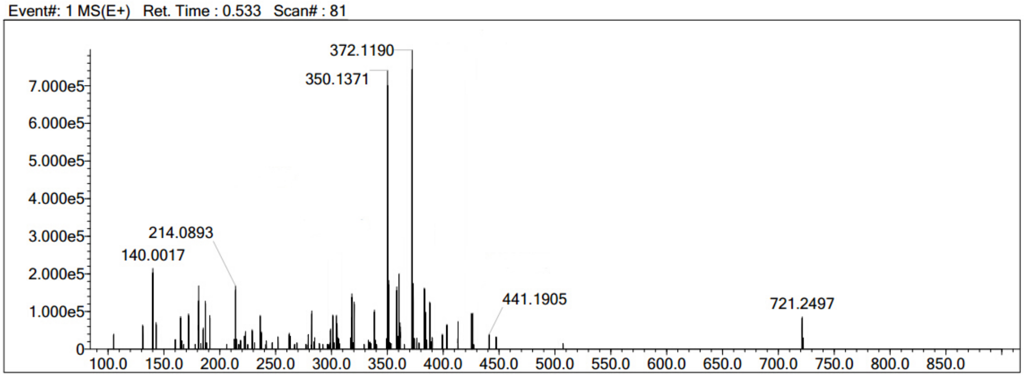
Measured region for 364.1527 m/z



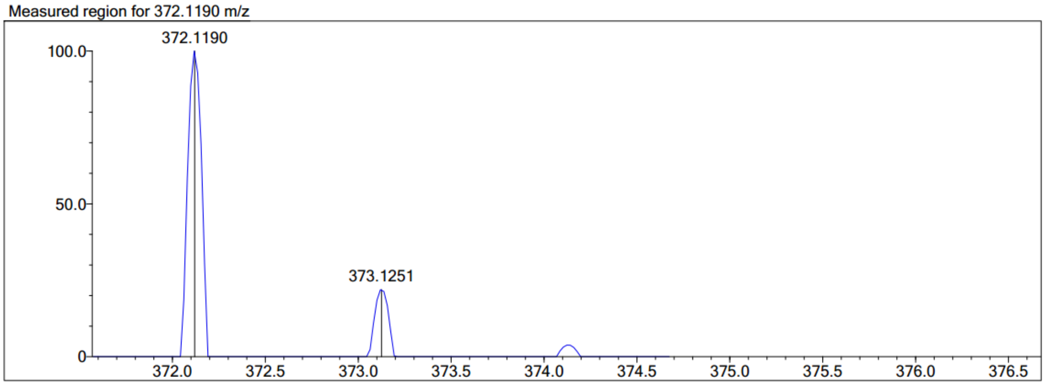
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	83.95	C22 H21 N O4	[M+H]+	364.1527	364.1543	-1.6	-4.39	91.73	13.0

10c

Event#: 1 MS(E+) Ret. Time : 0.533 Scan# : 81



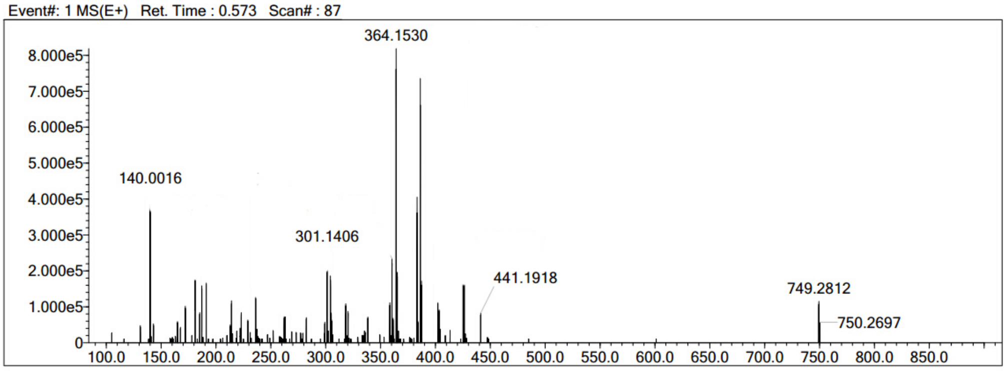
Measured region for 372.1190 m/z



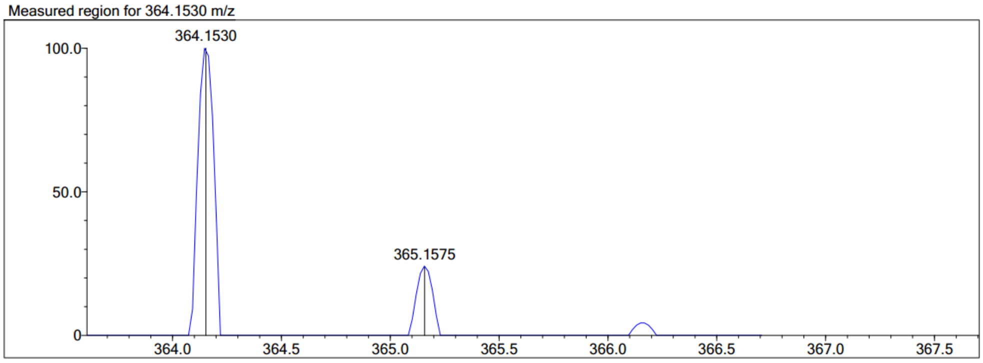
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
2	76.86	C21 H19 N O4	[M+Na]+	372.1190	372.1206	-1.6	-4.30	83.77	13.0

10d

Event#: 1 MS(E+) Ret. Time : 0.573 Scan# : 87



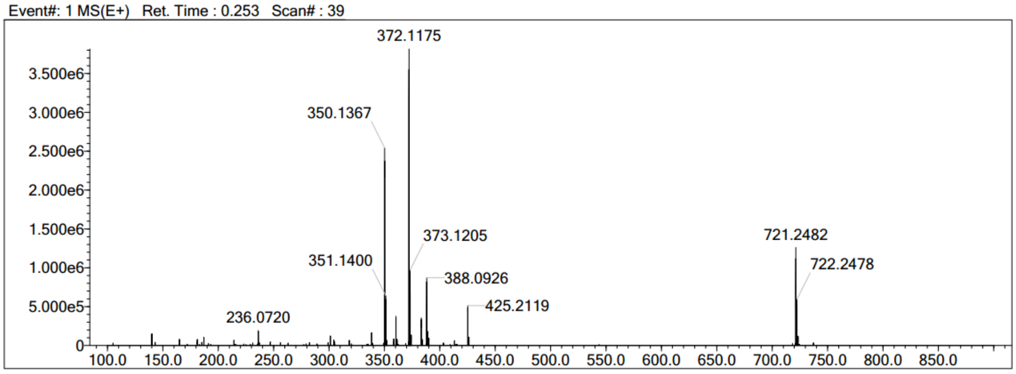
Measured region for 364.1530 m/z



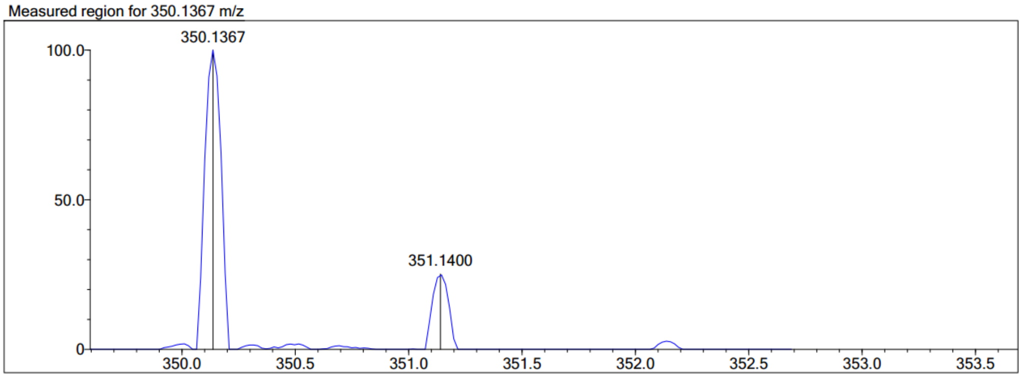
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	85.43	C22 H21 N O4	[M+H]+	364.1530	364.1543	-1.3	-3.57	91.30	13.0

11a

Event#: 1 MS(E+) Ret. Time : 0.253 Scan# : 39

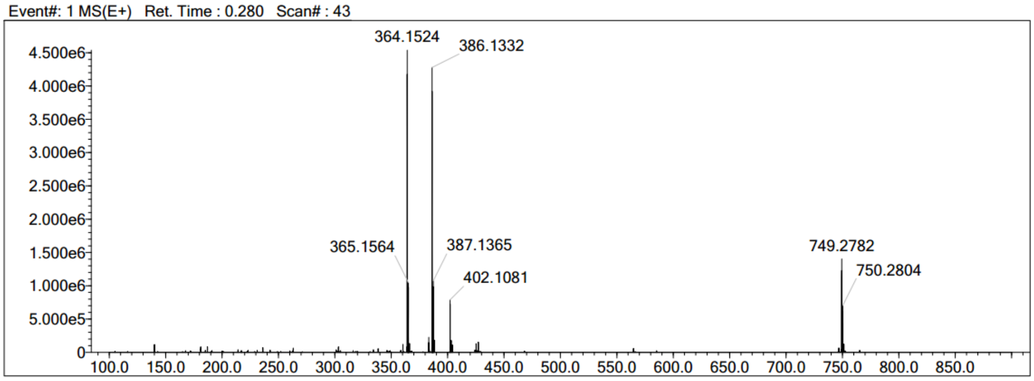


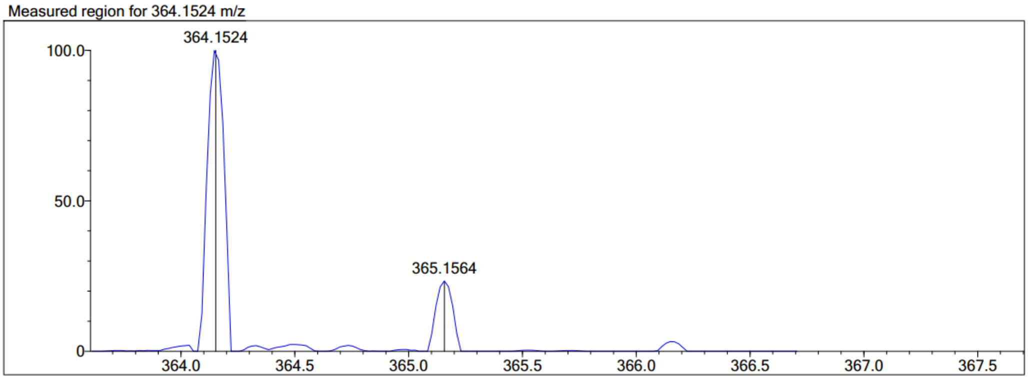
Measured region for 350.1367 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	62.51	C21 H19 N O4	[M+H]+	350.1367	350.1387	-2.0	-5.71	75.40	13.0

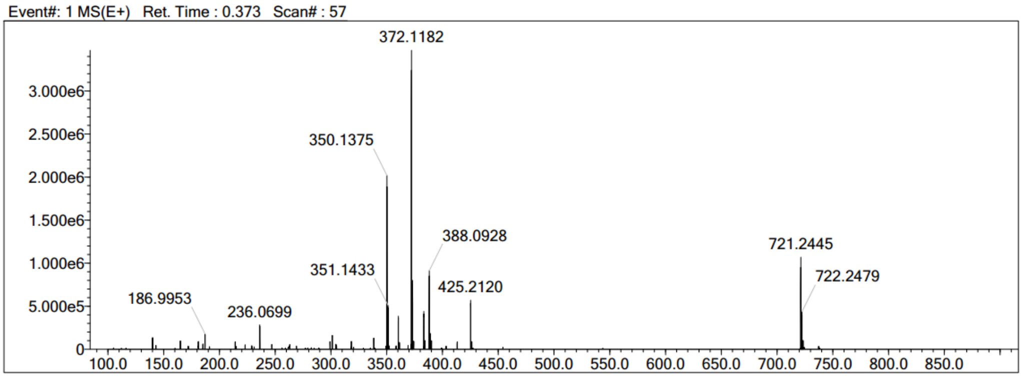
11b

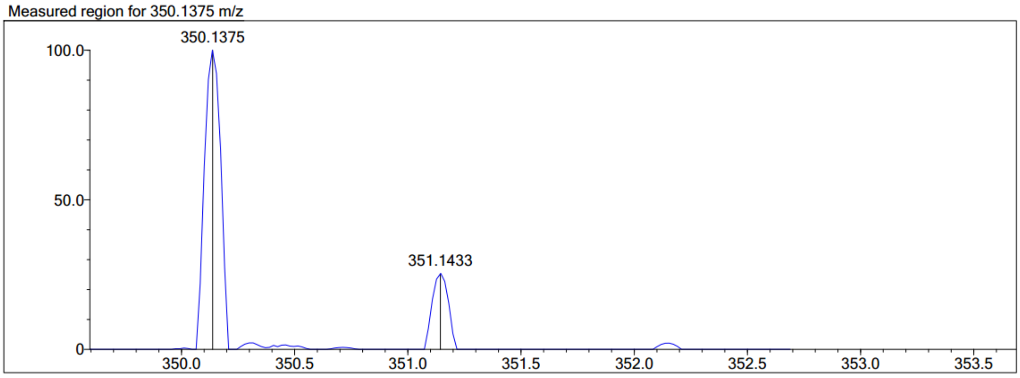




Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
2	78.66	C22 H21 N O4	[M+H]+	364.1524	364.1543	-1.9	-5.22	89.59	13.0

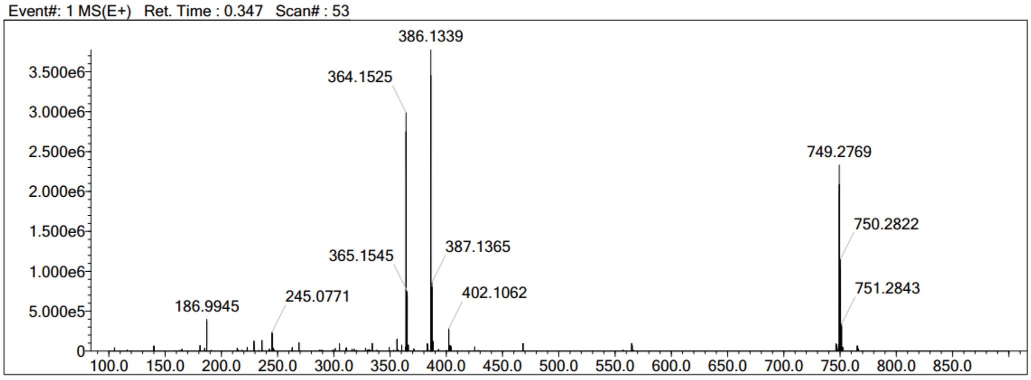
11c

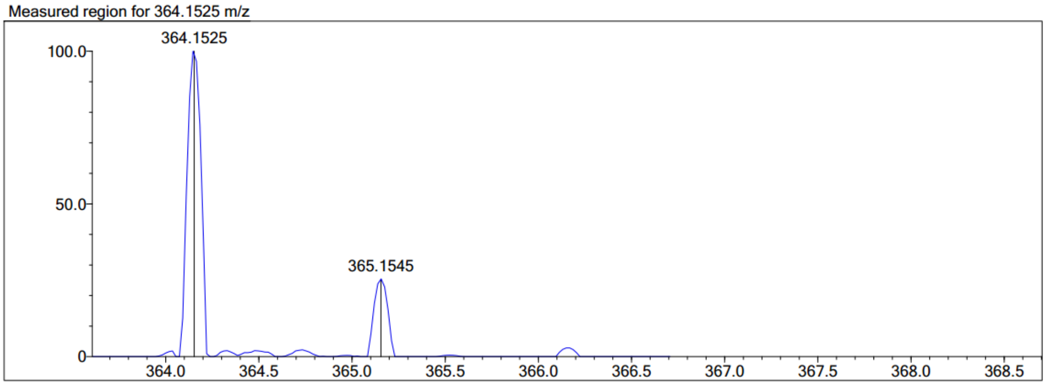




Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	73.38	C21 H19 N O4	[M+H]+	350.1375	350.1387	-1.2	-3.43	78.13	13.0

11d

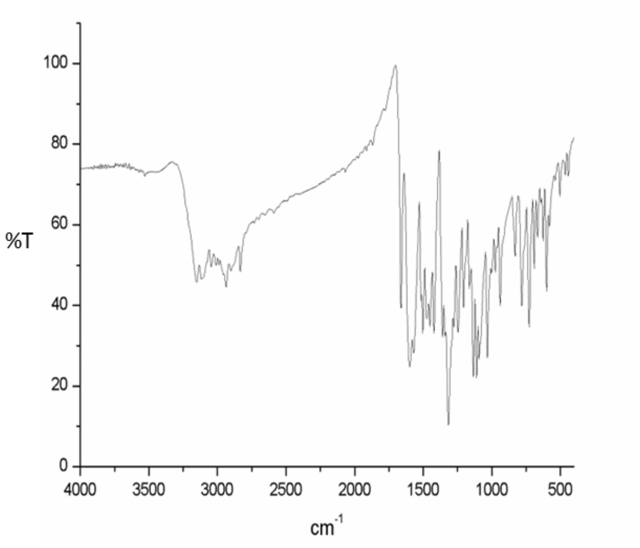




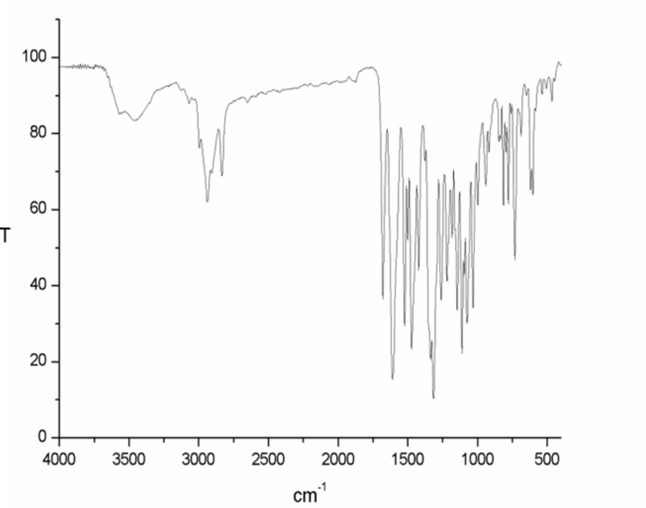
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	80.53	C22 H21 N O4	[M+H]+	364.1525	364.1543	-1.8	-4.94	89.33	13.0

SⅣ.IR spectra of target compounds

8a



8b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80
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3500
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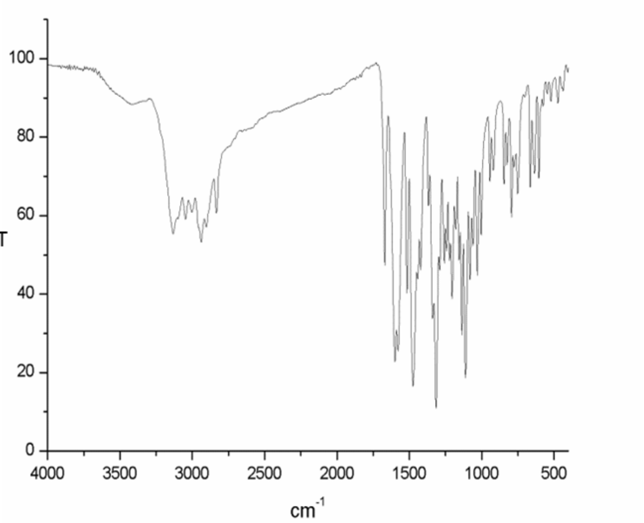
2000
1500
1000
500
cm^{-1}

8c


%T
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20
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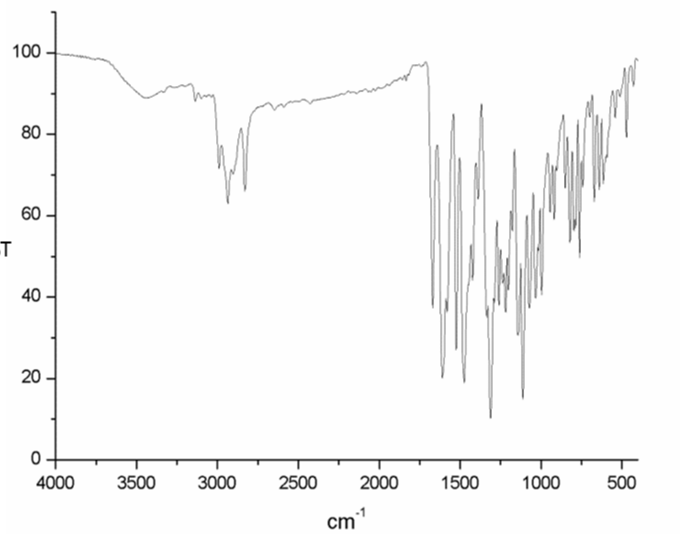
cm^{-1}

8d


%T
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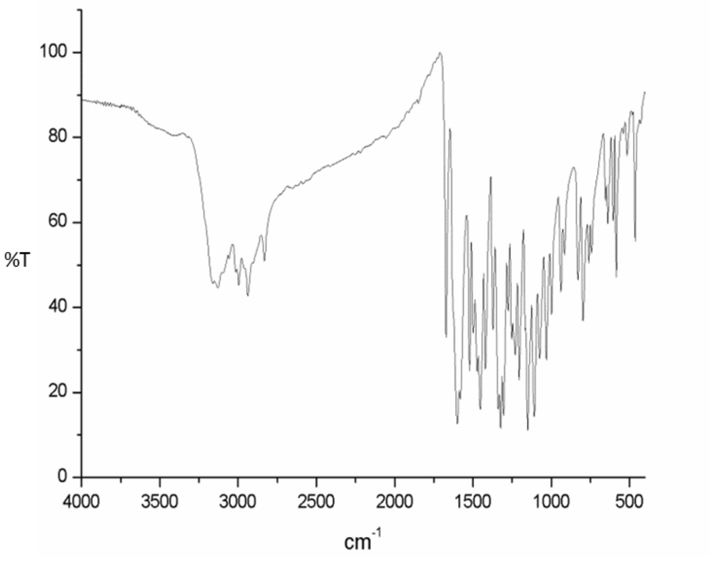
20
40
60
80
100
4000
3500
3000
2500
2000
1500
1000
500
cm^{-1}

8e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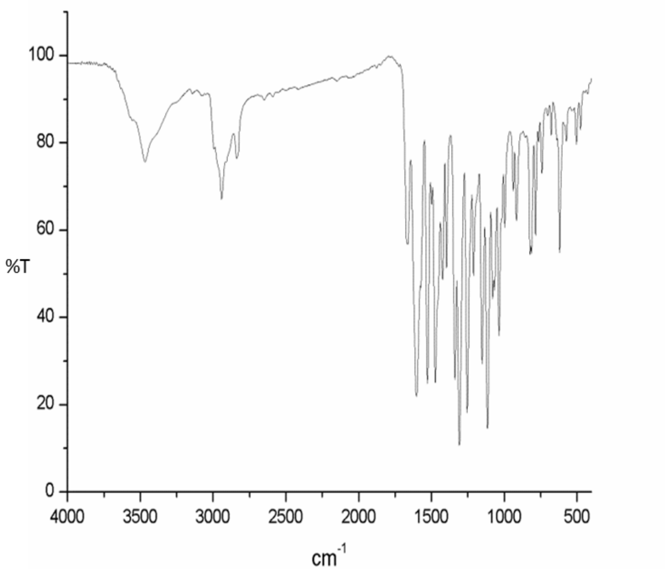
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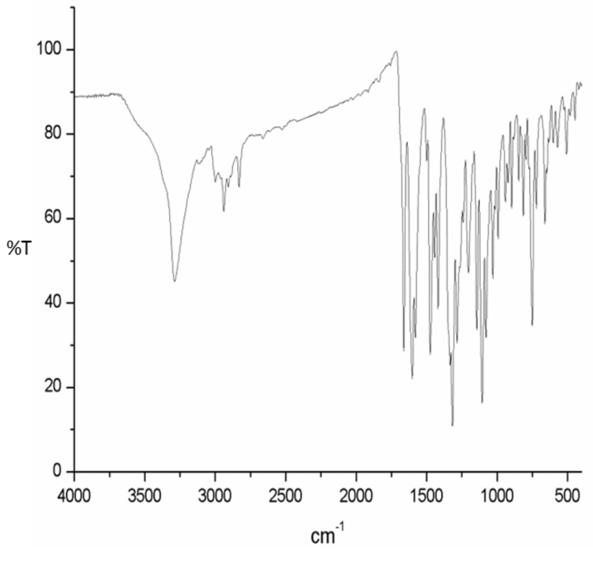
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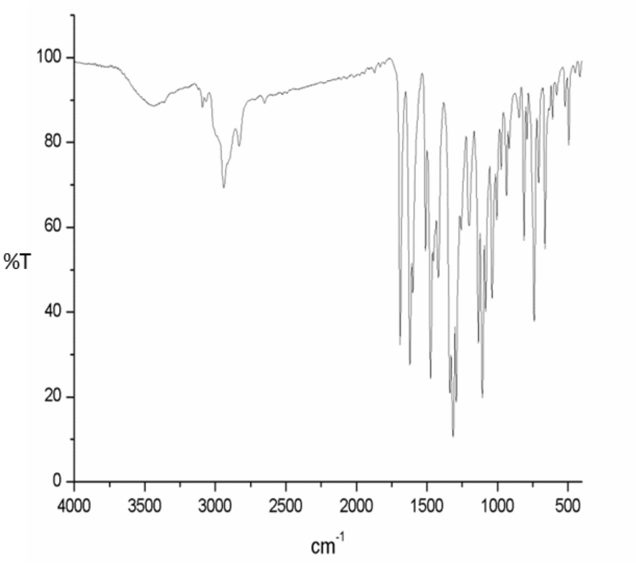
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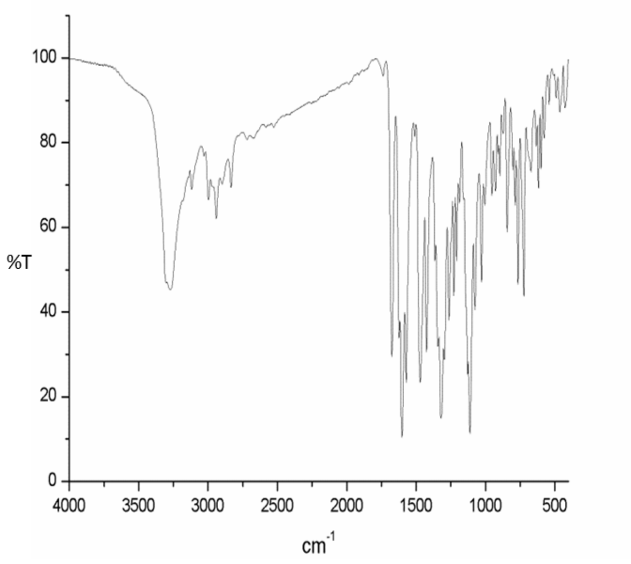
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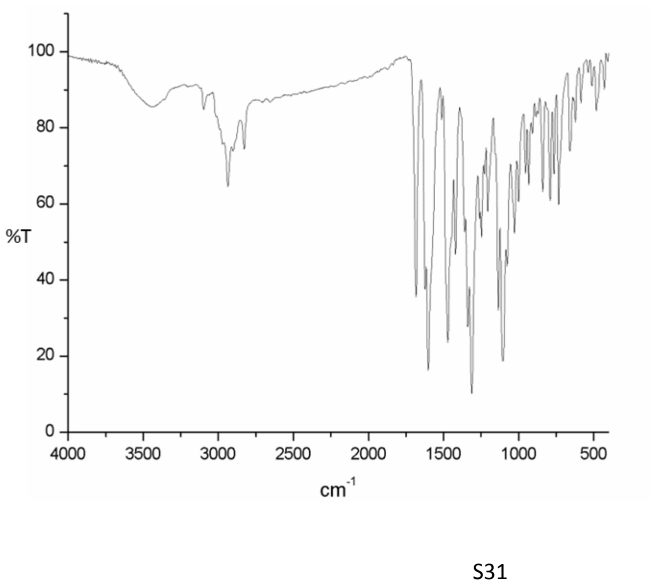
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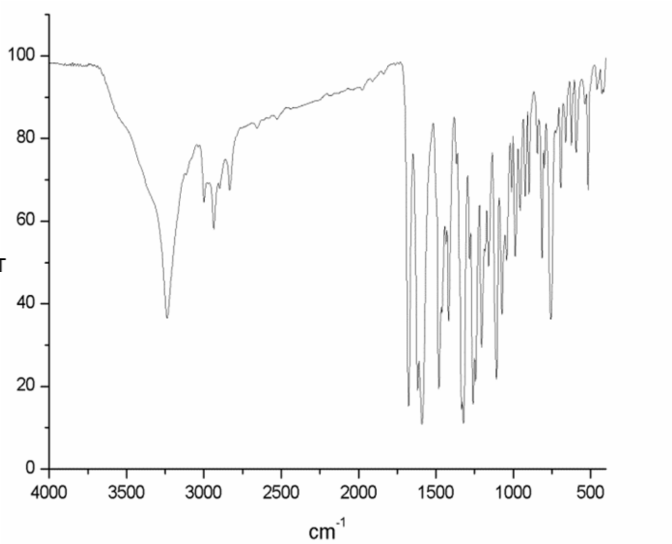
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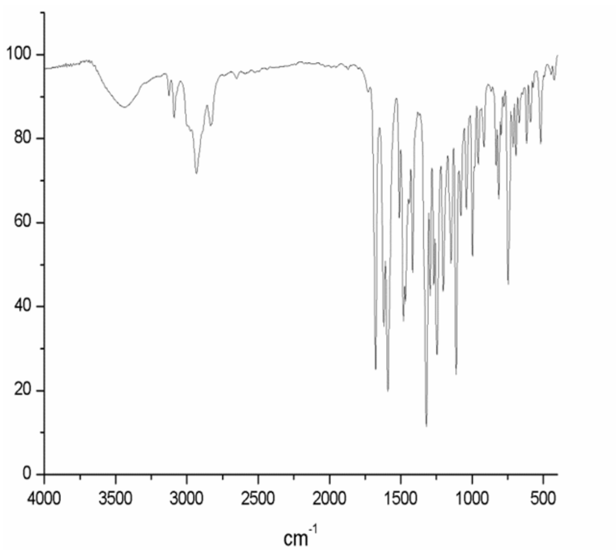
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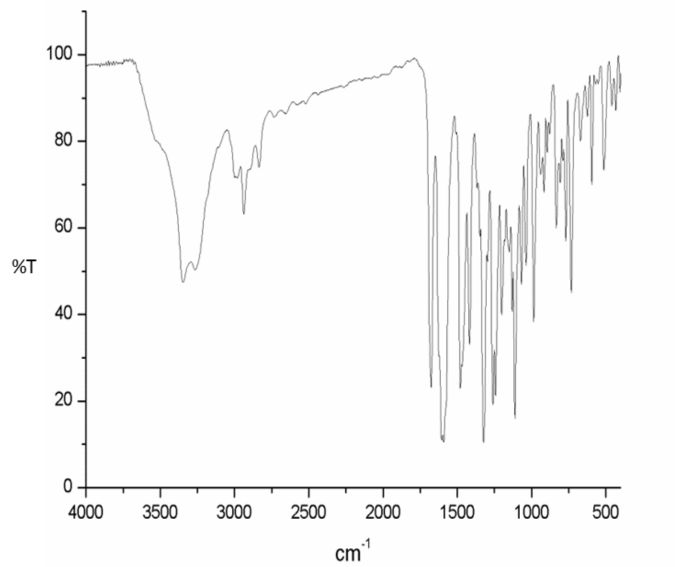
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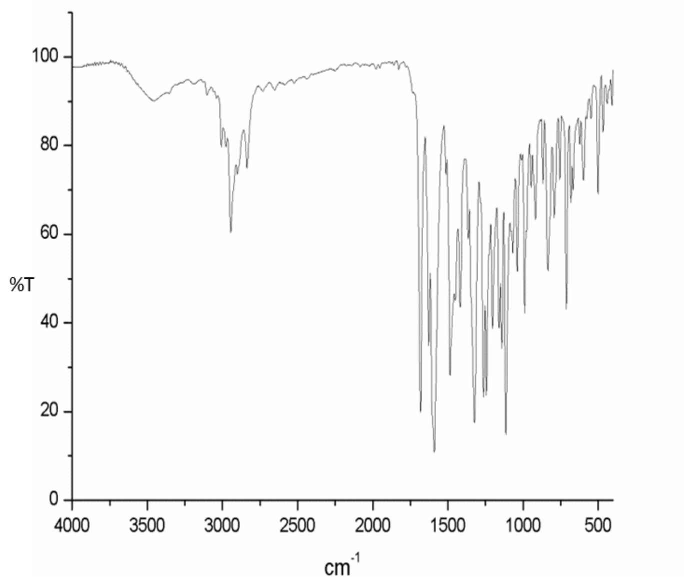
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