Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

1. Synthesize compounds

1.1 Materials and instruments

^{1}H and ^{13}C NMR spectra were recorded on Bruker DRX 500 MHz spectrometers with tetramethylsilane (TMS) as the internal standard (Bruker, Bremerhaven, Germany). MS and HRMS spectra were determined on a LCMS–IT–TOF mass spectrometer (Shimadzu, Kyoto, Japan). Column chromatography (CC): silica gel (200–300 mesh; Qingdao Makall Group CO., LTD; Qingdao; China). All reactions were monitored using thin-layer chromatography (TLC) on silica gel plates. Reaction reagents were purchased from J&K Scientific Ltd. Organic solvents were analytical reagent grade and purchased from Tianjin Chemical Reagent Co., Ltd. The synthesized compounds were named using ChemBioDraw Ultra software (v 12.0)

1.2 General procedure for the preparation of derivatives (6-14)

To a 100 ml flask charged with chlorosulfonic acid (25 mL) was added slowly 2-oxindole (50 mmol) at 0 ℃. After the addition, the reaction mixture was stirred at room temperature for 1.5 h. And then, the reaction mixture was heated to 68 ℃ for 1 h, cooled, and poured into ice water (200 mL). The precipitate was washed with water and dried in a vacuum oven to give 5-chlorosulfonyl-2-oxindole (**2**) which was used without further purification.

A mixture of 5-chloorosulfonyl-2-oxindole (5 mmol) and appropriate amine (10 mmol) in tetrahydrofuran (THF, 50 mL) was heated to refluxing and stirred for 3 h. And then, this mixture was concentrated under reduced pressure, and HCl (pH = 3, 25 mL) was added and stirred for 15 minutes. The crude product was filtered, washed with ice water (100 mL) and dried in a vacuum oven to give 5-sulfonylamido-2-oxindole (**3-5**) which was used without further purification.

To a mixture of compound **3(**or **4 or 5)** (0.5 mmol) and appropriate aldehyde (0.55 mmol) in ethanol (5 mL) was added piperidine (50 μL). The reaction mixture was heated to refluxing and stirred for 2 h, and TLC analysis indicated when the reaction was complete. The crude product was filtered, washed with ethanol and dried in a vacuum (if no solid precipitated, the crude product was chromatographed using a silica gel column) to afford the title compounds **6-14** as a yellow solid.

3 - (3, 5 - bis(trifluoromethyl)benzylidene) – N - (4 - bromophenyl) – 2 – oxoindoline – 5 – sulfonamide (6)

^{1}H NMR (Acetone-d_6, 500 MHz, ppm): δ10.17(s, 1H), 9.13(s, 1H), 8.38(s, 1H), 8.18(s, 1H), 8.12(s, 1H), 7.74(d, 1H, *J*= 8.0Hz),7.42(d, 2H, *J*= 8.5Hz), 7.20(d, 2H, *J*= 8.5Hz), 7.07(d, 1H, *J*= 8.0Hz); ^{13}C NMR (Acetone-d_6, 125 MHz, ppm): δ 166.7, 145.0, 137.7, 136.0, 135.0, 132.9, 132.1(2C), 131.9(2C), 131.1(2C), 129.4, 128.7, 124.8, 123.4(2C), 122.6(2C), 122.3, 119.6, 116.7, 110.0; ESIMS: *m/z* 588 $[M-H]^-$ HRESIMS: calc for $C_{23}H_{12}F_6BrN_2O_3S$ $[M-H]^-$ 588.9648, found 588.9662

N-(4-bromophenyl)-3-(3,4-difluorobenzylidene)-2-oxoindoline-5-sulfonamide (7)

^{1}H NMR (DMSO-d_6, 500 MHz, ppm): δ11.17(s, 1H), 10.34(s, 1H), 8.00(s, 1H), 7.71(s, 1H), 7.54-7.65(overlap, 2H), 7.37-7.44(overlap, 3H), 7.06(d, 2H, *J*= 8.5Hz), 7.00(d, 1H, *J*= 8.5Hz), 6.96(d, 2H, *J*= 8.5Hz); ^{13}C NMR (DMSO-d_6, 125MHz): ppm δ 167.5, 150.0, 149.2, 144.8, 137.7, 136.4, 132.0, 132.4(2C), 130.0, 126.8, 128.7, 125.2, 122.4(2C), 122.2, 121.1, 119.0, 117.9, 116.4, 111.0; ESIMS: *m/z* 488 $[M-H]^-$ HRESIMS: calc for $C_{21}H_{12}F_2BrN_2O_3S$ $[M-H]^-$ 488.9722, found 488.9726.

(E)-N-(4-bromophenyl)-3-(3-fluoro-4-hydroxybenzylidene)-2-oxoindoline-5-sulfonamide (8)

^{1}H NMR (DMSO-d_6, 500 MHz, ppm): δ 9.94(s, 1H), 9.16(s, 1H), 8.39(s, 1H), 8.12(s, 1H), 7.94(s, 1H), 7.72-7.76(overlap, 3H),7.42(d, 2H, *J*= 8.5Hz), 7.32(d, 1H, *J*= 8.5Hz), 7.26(d, 1H, *J*= 8.5Hz); ^{13}C NMR (DMSO-d_6, 125MHz, ppm): δ 167.9, 153.0, 151.1, 146.0, 143.0, 140.4, 138.5, 133.6, 132.1(2C), 132.0, 128.5, 126.8, 122.1(2C), 122.3, 120.4, 119.7, 117.4, 116.0, 110.4; ESIMS: *m/z* 488 $[M+H]^+$ HRESIMS: calc for $C_{21}H_{14}FBrN_2O_4S$ $[M+H]^+$ 488.99948, found 488.9914.

(E)-3-(3,5-bis(trifluoromethyl)benzylidene)-5-(morpholinosulfonyl)indolin-2-one (9)

^{1}H NMR (DMSO-d_6, 500 MHz, ppm): δ10.24(s, 1H), 8.43(s, 1H), 8.29(s, 1H), 8.16(s, 1H), 8.13(s, 1H), 7.74(d, 1H, *J*= 8.0Hz), 7.20(d, 1H, *J*= 8.0Hz), 3.68(t, 4H, *J*= 4.5Hz), 2.98(t, 4H, *J*= 4.5Hz); ^{13}C NMR (DMSO-d_6, 125 MHz, ppm): δ 166.8, 145.2, 137.5, 136.1, 135.3, 132.1, 130.3, 128.5(2C), 125.1, 123.4, 122.4(2C) 122.1, 120.2(2C), 110.0, 65.7(2C), 46.2(2C); ESIMS: *m/z* 507 $[M+H]^+$ HRESIMS: calc for $C_{21}H_{16}F_6BN_2O_4S$ $[M+H]^+$ 507.0808, found 507.0849.

(E)-3-(3,4-difluorobenzylidene)-5-(morpholinosulfonyl)indolin-2-one (10)

^{1}H NMR (DMSO-d_6, 500 MHz, ppm): δ10.08(s, 1H), 8.01(s, 1H), 7.72(s, 1H), 7.62-7.69(overlap, 2H), 7.13-7.18(overlap, 2H), 7.00(d, 1H, *J*= 8.5Hz), 3.69(t, 4H, *J*= 4.5Hz), 2.96(t, 4H, *J*= 4.5Hz); ^{13}C NMR (DMSO-d_6, 125MHz): ppm δ 167.3, 152.7, 146.4, 143.6, 138.9,

131.4, 129.8, 128.4, 126.4, 122.1, 121.8, 119.6, 118.9, 110.0, 109.3, 65.7(2C), 46.3(2C); ESIMS: *m/z* 405 $[M-H]^-$ HRESIMS: calc for $C_{19}H_{16}F_2N_2O_4S$ $[M-H]^-$ 405.0886, found 405.0726.

(E)-3-(3-fluoro-4-hydroxybenzylidene)-5-(morpholinosulfonyl)indolin-2-one (11)

^{1}H NMR (Pyridine-d_5, 500 MHz, ppm): δ11.34(s, 1H), 7.20(s, 1H), 6.94(s, 1H), 6.64(d, 1H, *J*= 8.5Hz), 6.48(d, 1H, *J*= 8.5Hz), 6.37(s, 1H), 6.07(d, 1H, *J*= 8.5Hz), 5.95(d, 1H, *J*= 8.5Hz), 2.37(t, 4H, *J*= 4.0Hz), 1.87(t, 4H, *J*= 4.0Hz); ^{13}C NMR (Pyridine-d_5, 125MHz): ppm δ 167.4, 151.5, 149.1, 143.7, 138.2, 130.8, 128.8, 127.5, 126.6, 122.4, 121.9, 119.2, 118.1, 116.6, 108.3, 64.8(2C), 45.2(2C); ESIMS: *m/z* 405 $[M+H]^+$ HRESIMS: calc for $C_{19}H_{17}FN_2O_5S$ $[M+H]^+$ 405.0992, found 405.0915.

(E)-3-(3,5-bis(trifluoromethyl)benzylidene)-5-((4-(pyrimidin-2-yl)piperazin-1-yl)sulfonyl)indolin-2-one (12)

^{1}H NMR (DMSO-d_6, 500 MHz, ppm): δ11.23 (s, 1H), 8.31 (s, 2H), 8.29(d, 2H, *J*= 4.5 Hz), 8.18 (s, 1H), 8.13 (s, 1H), 7.64(d, 1H, *J*= 8.0Hz), 7.04 (d, 1H, *J*= 8.0Hz), 6.60 (t, 1H, *J*=4.5Hz), 3.84 (t, 4H, *J*= 4.5Hz), 2.95 (t, 4H, *J*= 4.5Hz); ^{13}C NMR (DMSO-d_6, 125MHz, ppm): δ 167.4, 161.2, *158.4(2C)*, 145.6,136.2 *136.0*, 132.6*(2C)*,130.8*(2C)*, *130.5*, 128.9, 127.9, 125.3, 122.6*(2C)*, 121.8,120.5, *111.1*, *110.5*, 46.2(2C), 42.9(2C); ESIMS: *m/z* 584 $[M+H]^+$ HRESIMS: calc for $C_{25}H_{19}F_6N_5O_3S$ $[M+H]^+$ 584.1271, found 584.1186.

(E)-3-(3,4-difluorobenzylidene)-5-((4-(pyrimidin-2-yl)piperazin-1-yl)sulfonyl)indolin-2-one (13)

^{1}H NMR (DMSO-d_6, 500 MHz, ppm): δ11.20 (s, 1H), 8.29(d, 2H, *J*= 4.5 Hz), 8.09-8.11 (overlap, 3H), 7.59-7.70(overlap, 3H), 7.01 (d, 1H, *J*= 8.0Hz), 6.59 (t, 1H, *J*=4.5Hz), 3.82 (t, 4H, *J*= 4.5Hz), 2.94 (t, 4H, *J*= 4.5Hz); ^{13}C NMR (DMSO-d_6, 125MHz, ppm): δ 167.6, 161.2, *158.4(2C)*, 150.2, 147.3, 145.0,137.9, 130.8*(2C)*, 129.8, 127.7, 125.7, 121.8,120.0, *111.1*, *111.0*, *110.2*, 46.2(2C), 42.9(2C); ESIMS: *m/z* 484 $[M+H]^+$ HRESIMS: calc for $C_{23}H_{19}F_2N_5O_3S$ $[M+H]^+$ 484.1289, found 484.1249.

(E)-3-(3-fluoro-4-hydroxybenzylidene)-5-((4-(pyrimidin-2-yl)piperazin-1-yl)sulfonyl)indolin-2-one (14)

^{1}H NMR (Pyridine-d_5, 500 MHz, ppm): δ11.30 (s, 1H), 7.21(s, 1H), 7.11(d, 2H, *J*= 4.5 Hz), 7.01 (d, 1H, *J*= 8.0Hz), 6.95(s, 1H), 6.64 (d, 1H, *J*= 8.0Hz), 6.37(s, 1H), 6.11 (d, 1H, *J*= 8.0Hz), 5.92 (d, 1H, *J*= 8.0Hz), 5.22 (t, 1H, *J*=4.5Hz), 2.78 (t, 4H, *J*= 4.5Hz), 1.94 (t, 4H, *J*= 4.5Hz); ^{13}C

NMR (Pyridine-d_5, 125MHz, ppm): δ 167.4, 160.2, *156.7(2C)*, 148.8, 143.7, 138.2, 134.4, 130.8, 127.4, 126.3,125.8, 124.9,122.4,121.5, 121.0, *118.0*, *109.4*, *108.3*, 45.2(2C), 41.7(2C); ESIMS: *m/z* 482 $[M+H]^+$ HRESIMS: calc for $C_{23}H_{20}FN_5O_4S$ $[M+H]^+$ 482.1302, found 482.1293.

2. Anticancer activities assays

2.1. Materials

Dulbecco's modified Eagle's medium (DMEM), fetal bovine serum (FBS), and other cell culture reagents were purchased from Invitrogen (Carlsbad, CA, USA). The antibodies directed against caspase-3, 9, Bcl-2, Bax and p53 were purchased from Cell Signaling Technology (Danvers, MA, USA). The antibody directed against GAPDH was purchased from Abcam Trading Company Ltd (Shanghai, China). The high concentration Matrigel was purchased from BD Biosciences (Bedford, MA, USA). A NO detection kit was purchased from Applygen (Beijing, China). All the other reagents were purchased from Sigma, unless otherwise indicated.

2.2. Cell Culture and Proliferation Assay

The cells including Human lung cancer cell line, A549; Human hepatoma cell lines, Bel-7402 and HepG2; human cervical cancer cell line, HeLa; human colon cancer cell line, HCT116 and Humanumbilical vein endothelial cells, HUVECs were purchased from BOSTER, Ltd (Wuhan, China). The cells were maintained in DMEM supplemented with 10% FBS and 1% antibiotics at 37°C and in an atmosphere containing 5% CO_2. The cells were split 1:3 when they reached 80%–90% confluence. Cell proliferation was measured using the 3-(4, 5-dimethylthiazol-2-yl)-2, 5-diphenyltetrazolium bromide (MTT) colorimetric assay.

The cells (4×10^3 cells/well) with 10% FBS culture medium were seeded in a 96-well plate and incubated overnight. Next, the cells were treated with various amounts of compounds and incubated for 48 h. Subsequently, 20 μL of 5-mg/mL MTT was transferred into each well, and the cells were incubated for another 4 h. The medium in each well was carefully removed, and 150 μL DMSO was then added to each well. The samples were thoroughly agitated for 10 min on a shaker. Finally, the absorbance of the samples at 490 and 690 nm was measured against a background control (blank) using a microplate reader.

2.3. Wound Healing Assay

Briefly, the exponentially growing HUVECs (2.5×10^5 cells per well) were cultured in 6-well plates and starved overnight in 2% FBS medium until they reached 90% confluence. A single wound was then scratched in the center of the cell monolayers with a 200 μL sterile plastic pipette tip. The wounded monolayers were washed twice with 1 × PBS to remove the non-adherent cells and were incubated with various concentrations of compound 6 for 24 h in the presence of 1 μg/mL of mitomycin C (for mitotic inactivation). To measure the length of the endothelial cells that had migrated from the edge of the injured monolayer, images were obtained immediately after wounding and after a 24 h incubation period, using a phase-contrast microscope (Olympus, Tokyo, Japan. The length was measured by the Image Pro Plus v 6.0 software (Media Cybernetics, Inc., Bethesda, MD, USA).

2.4. Capillary-Like Tube Formation Assay

Briefly, high concentration Matrigel was added to a 96-well plate (50 μL per well) and allowed to polymerize for 1 h at 37 °C. The HUVECs (5.5×10^4 cells per well, 200 μL per well) with or without compound 6, were seeded onto the surface of the Matrigel. After a 7 h incubation period, cellular morphological changes and tubular structure formation were observed under a phase-contrast microscope (Olympus). The images were captured and the degree of tube formation was quantified by measuring the lengths of the tubes using the Image Pro Plus v 6.0 software.

2.5. Immunoblotting Analysis

Briefly, the HepG2 cells (2×10^5 cells per well) were cultured in 6-well plates. When they reached 80% confluence, the cells were treated with various concentrations of compound 6 for 12 h. Then the cells were washed with ice-cold PBS and lysed with lysis buffer (50 mMTris-HCl, 1% Triton X-100, 0.5% sodium deoxycholate, 150 mMNaCl, 1 mM EDTA, 1 mMphenylmethylsulfonyl fluoride (PMSF), 1-mM sodium orthovanadate, 1 mMNaF, and 0.2% protease inhibitor cocktail; pH 7.2). Proteins were separated by sodium dodecyl sulfate-polyacrylamide gel electrophoresis and were subsequently transferred to nitrocellulose membranes. The membranes were blocked with 5% skim milk in 1 × Tris-buffered saline containing 0.1% Tween 20 (TBST) for 1 h at room temperature and were then incubated overnight at 4 °C with a primary antibody. The following day, the membranes were washed with TBST and were probed with a secondary antibody. The bands were detected using enhanced chemiluminescence reagents (Thermo Fisher Scientific Inc., Shanghai, China).

2.6. NO Measurement

One means to investigate nitric oxide formation is to measure nitrite (NO^{2-}), which is one of two primary, stable and nonvolatile breakdown products of NO. The NO levels in the HUVECs were measured with the NO^{2-} detection kit. Briefly, the HUVECs were cultured in 24 wells plates (1×10^5 cells per well). After overnight incubation, the cells were starved for 16 h in 2% FBS containing medium. Then, the cells were exposed to 20% FBS containing medium with or without **compound6**. Twenty-four hours later, the supernatant was collected, and NO production was determined following the protocol supplied with the kit (Applygen, Beijing, China).

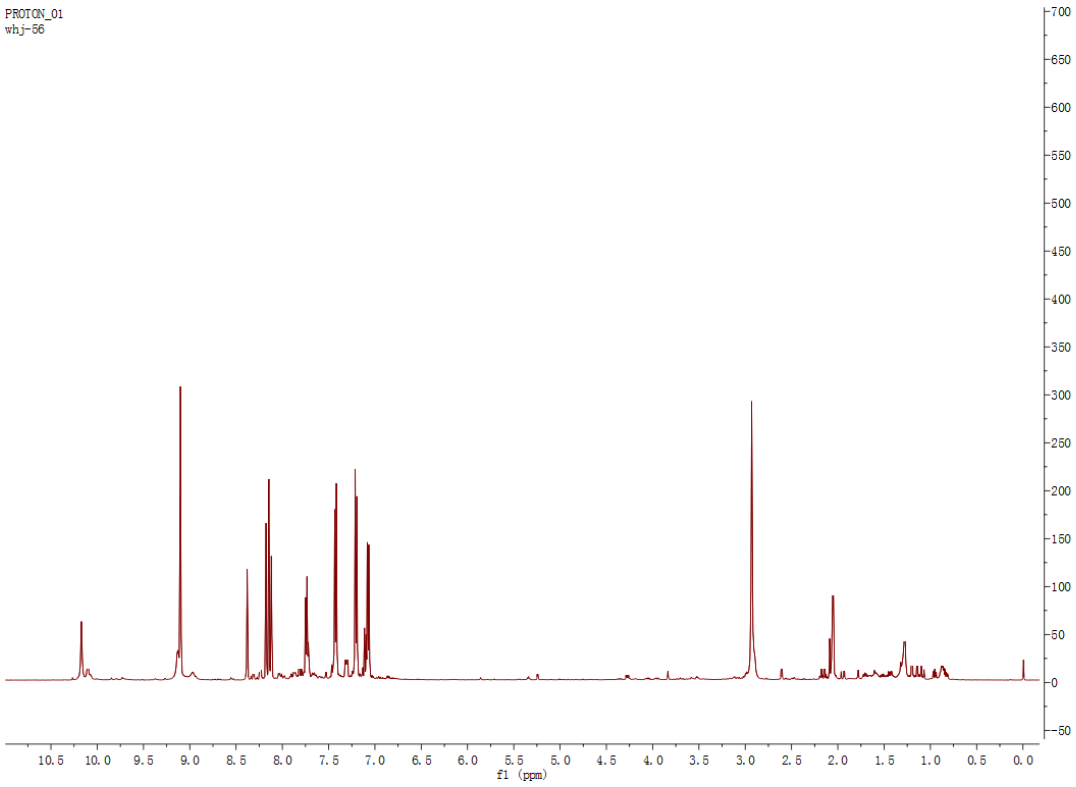
2.7. Statistical Analysis

All the experiments were performed at least three times, and the data are presented as mean ± SD values. Differences between the mean values were assessed using one-way analysis of variance. For all the analyses, $p < 0.05$ was considered significant. Statistical analyses were performed using SPSS 17.0 (SPSS, Inc., Chicago, IL, USA).

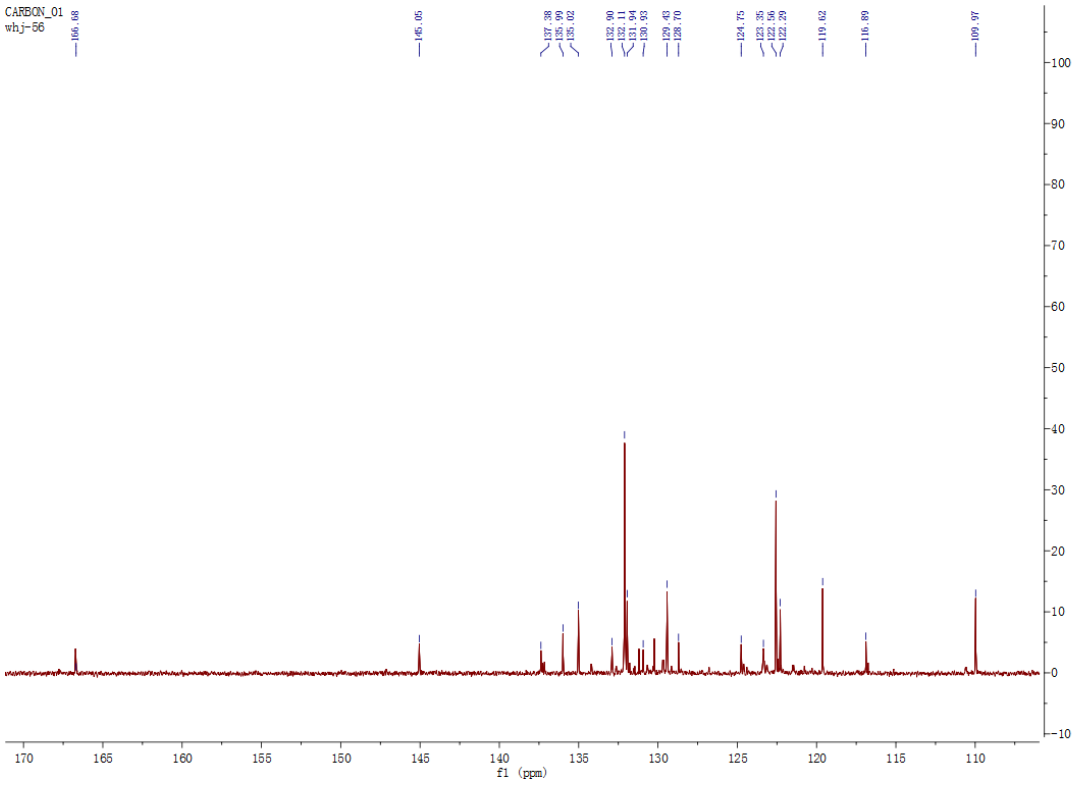
References

[1] Zheng, G.-h.; Shen, J.-j.; Zhan, Y.-c.; Yi, H.; Xue, S.-t.; Wang, Z.; Ji, X.-y.; Li, Z.-r. *Eur. J. Med. Chem.* **2014,** *81*, 277.

[2] Astin, J. W.; Batson, J.; Kadir, S.; Charlet, J.; Persad, R. A.; Gillatt, D.; Oxley, J. D.; Nobes, C. D. *Nat. Cell. Biol*. **2010**, *12*, 1194.



Compound 6 ^{1}H NMR



Compound 6 ^{13}C NMR

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N	3	2	5	S	2	0	1					

Error Margin (mDa): 20.0
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Max Isotopes: all
MSn Iso RI (%): 75.00

DBE Range: not fixed
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MSn Logic Mode: AND

Electron Ions: both
Use MSn Info: no
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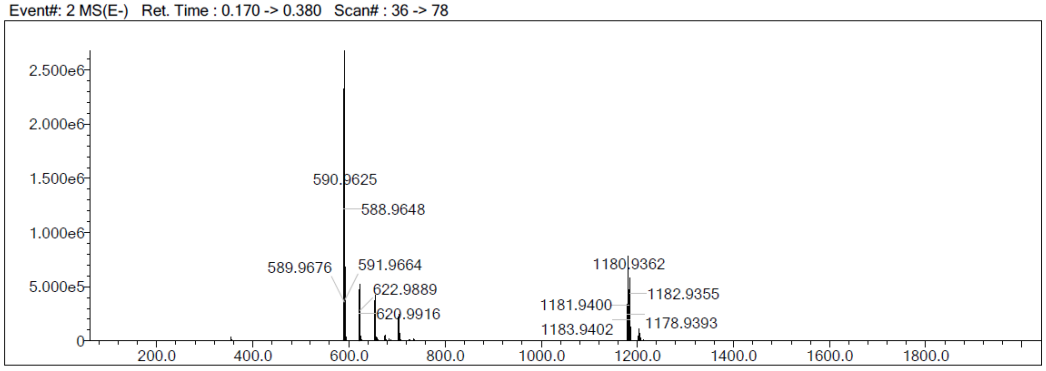
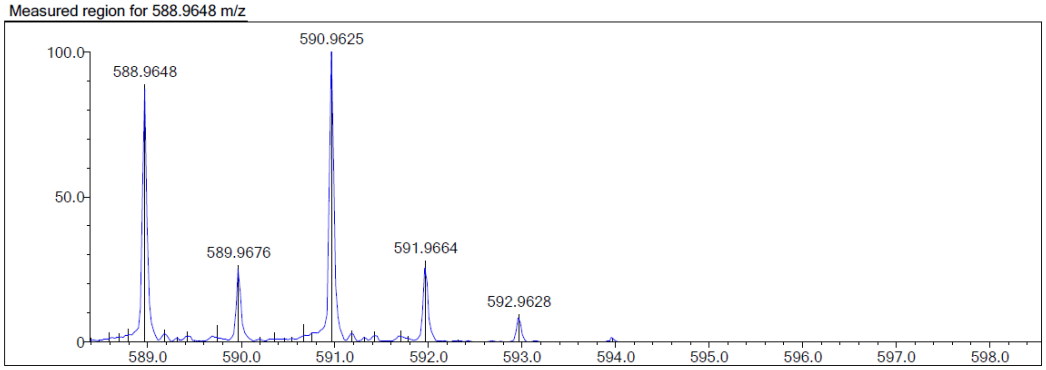
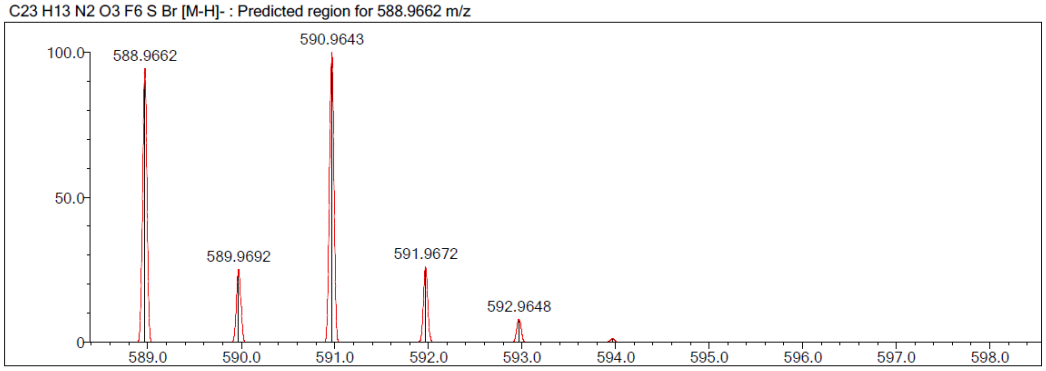


Measured region for 588.9648 m/z



C23 H13 N2 O3 F6 S Br [M-H]- : Predicted region for 588.9662 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
4	76.96	C23 H13 N2 O3 F6 S Br	[M-H]-	588.9648	588.9662	-1.4	-2.38	79.71	15.0

Compound 6 HR MS

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C	4	0	100	F	1	0	6	Br	1	0	4	
N	3	2	5	S	2	0	1					

Error Margin (mDa):	20.0	DBE Range:	not fixed	Electron Ions:	both
HC Ratio:	unlimited	Apply N Rule:	yes	Use MSn Info:	no
Max Isotopes:	all	Isotope RI (%):	1.00	Isotope Res:	10000
MSn Iso RI (%):	75.00	MSn Logic Mode:	AND	Max Results:	500

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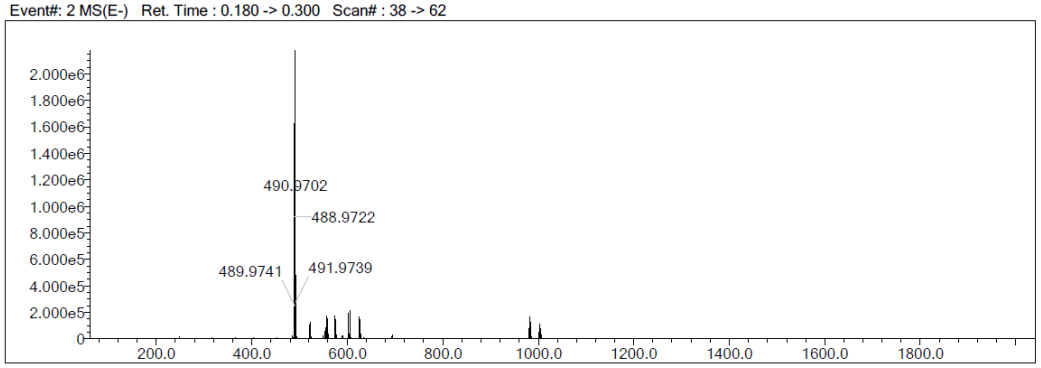
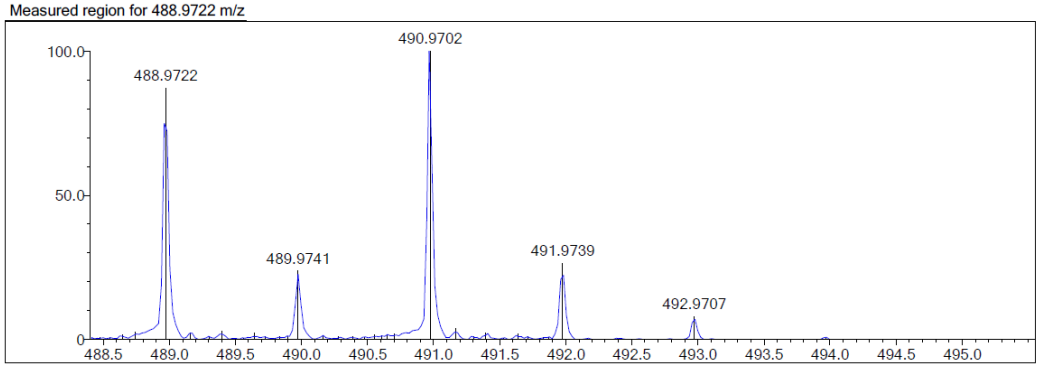
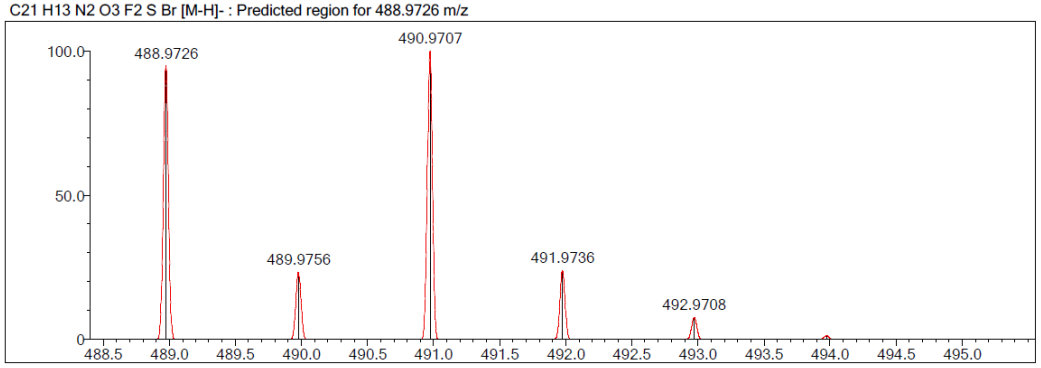


Measured region for 488.9722 m/z



C21 H13 N2 O3 F2 S Br [M-H]- : Predicted region for 488.9726 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
3	65.61	C21 H13 N2 O3 F2 S Br	[M-H]-	488.9722	488.9726	-0.4	-0.82	65.61	15.0

Compound 7 HR MS

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B	3	0	0	O	2	0	50	S	2	0	1	I	3	0	0	
C	4	19	50	F	1	0	6	Cl	1	0	0					

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Max Isotopes: all
MSn Iso RI (%): 75.00

DBE Range: 0.0 - 30.0
Apply N Rule: yes
Isotope RI (%): 1.00
MSn Logic Mode: OR

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Use MSn Info: yes
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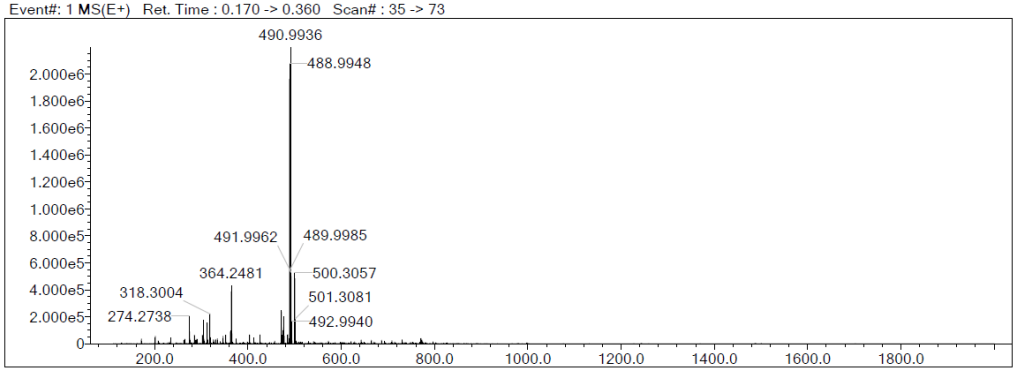
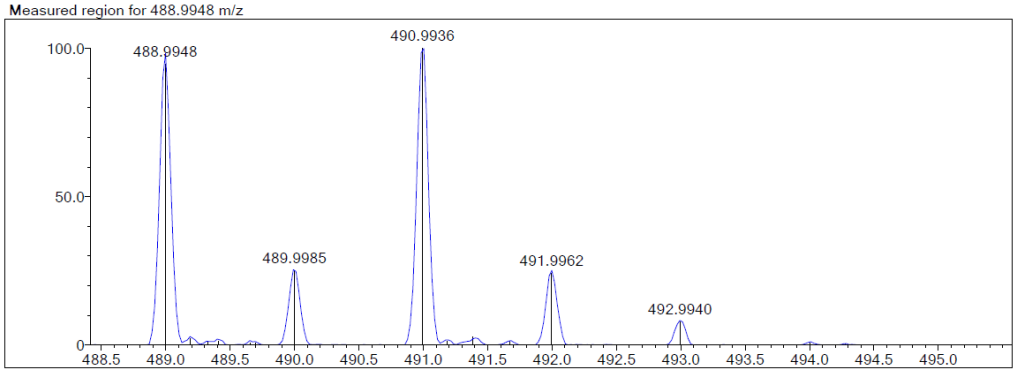
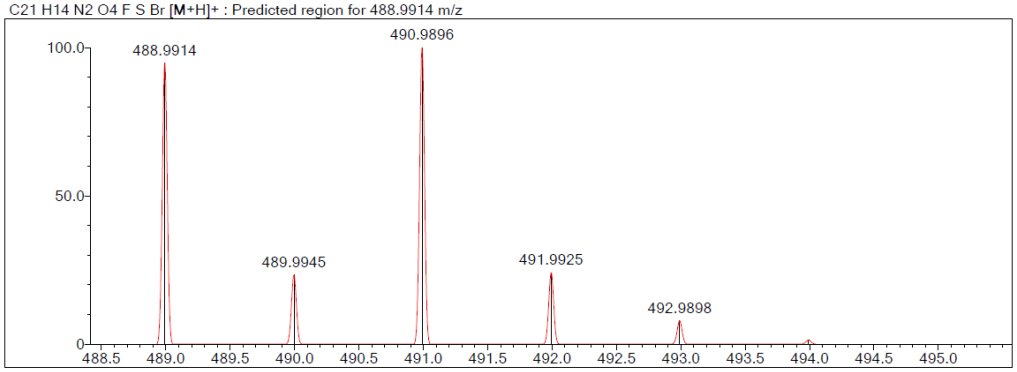


Measured region for 488.9948 m/z



C21 H14 N2 O4 F S Br [M+H]+ : Predicted region for 488.9914 m/z



Rank	Score	Ion	Formula (M)	Pred. m/z	Meas. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
16	70.23	[M+H]+	C21 H14 N2 O4 F S Br	488.9914	488.9948	3.4	6.95	99.61	15.0

Compound 8 HR MS

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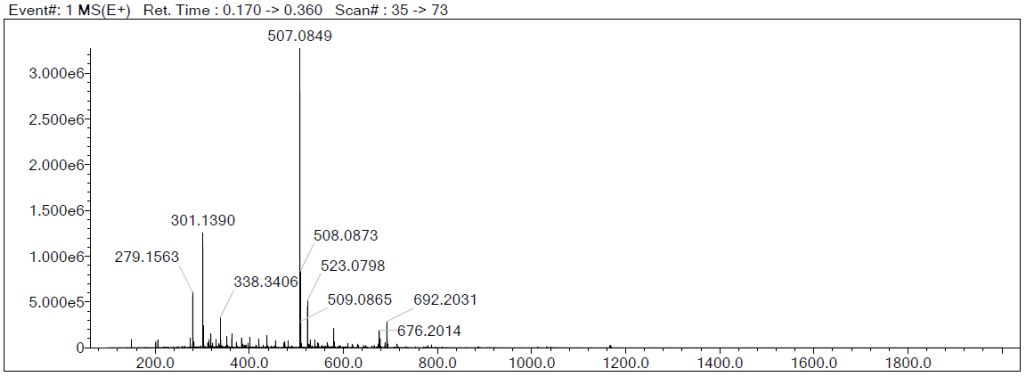
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	100	N	3	0	6	P	3	0	0	Br	1	0	2	H
B	3	0	0	O	2	0	50	S	2	0	1	I	3	0	0	
C	4	19	50	F	1	0	6	Cl	1	0	0					

Error Margin (mDa): 20.0
HC Ratio: 0.0 - 3.0
Max Isotopes: all
MSn Iso RI (%): 75.00

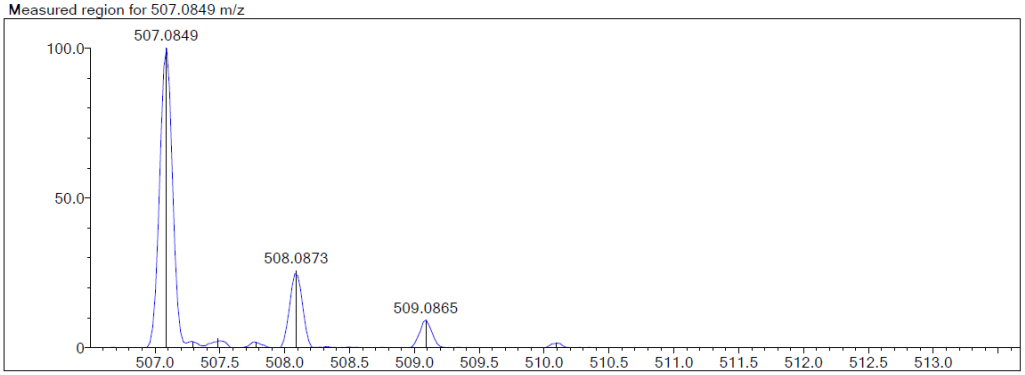
DBE Range: 0.0 - 30.0
Apply N Rule: yes
Isotope RI (%): 1.00
MSn Logic Mode: OR

Electron Ions: both
Use MSn Info: yes
Isotope Res: 10000
Max Results: 800

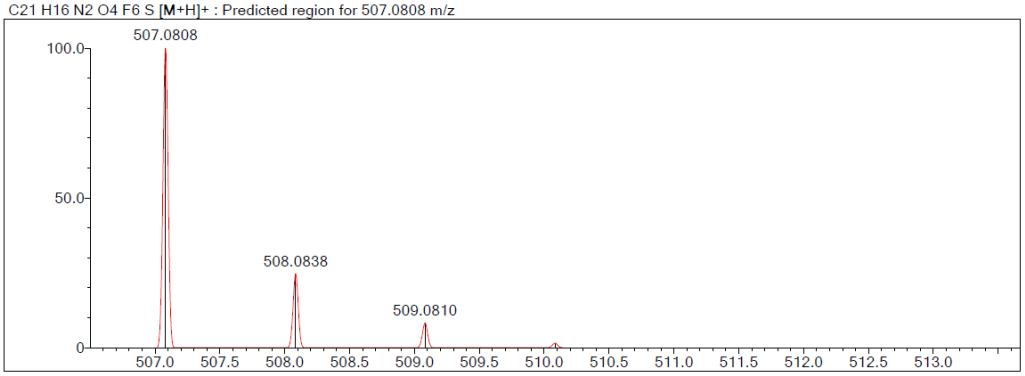
Event#: 1 MS(E+) Ret. Time : 0.170 -> 0.360 Scan# : 35 -> 73



Measured region for 507.0849 m/z



C21 H16 N2 O4 F6 S [M+H]+ : Predicted region for 507.0808 m/z



Rank	Score	Ion	Formula (M)	Pred. m/z	Meas. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
43	50.14	[M+H]+	C21 H16 N2 O4 F6 S	507.0808	507.0849	4.1	8.09	84.84	12.0

Compound 9 HR MS

Data File: D:\分子量测定\2015\2015-01-25\2015-01-25WLJ_62_29.lcd

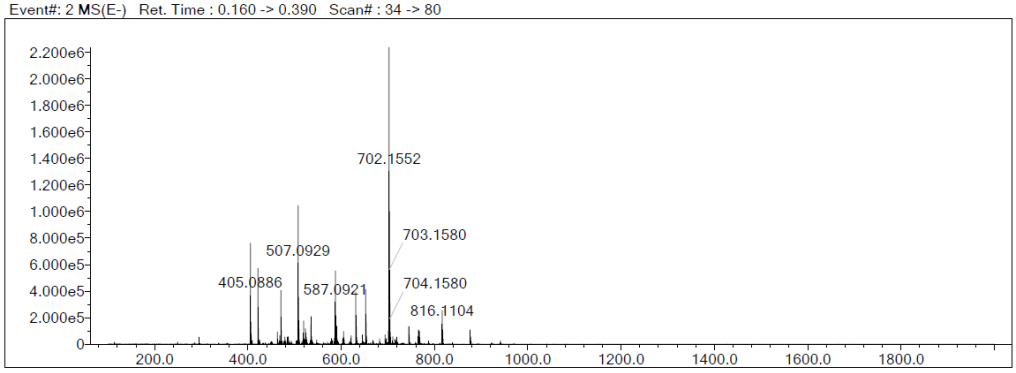
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	100	N	3	0	6	P	3	0	0	Br	1	0	2	H
B	3	0	0	O	2	0	50	S	2	0	1	I	3	0	0	
C	4	19	50	F	1	0	6	Cl	1	0	0					

Error Margin (mDa): 20.0
HC Ratio: 0.0 - 3.0
Max Isotopes: all
MSn Iso RI (%): 75.00

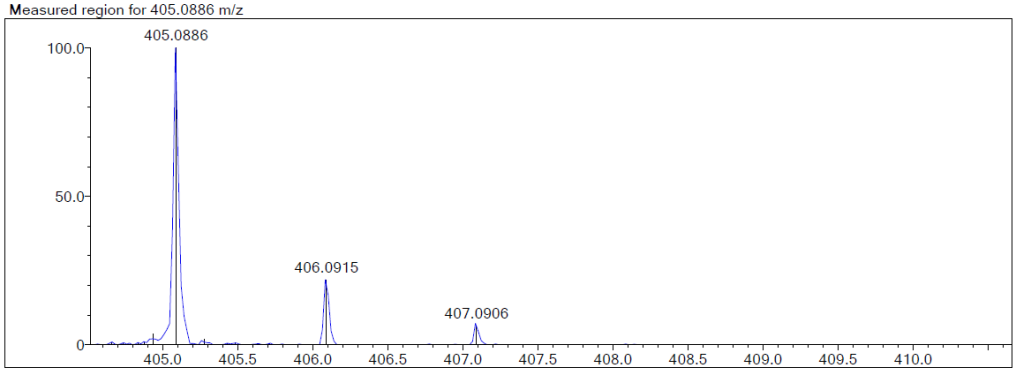
DBE Range: 0.0 - 30.0
Apply N Rule: yes
Isotope RI (%): 1.00
MSn Logic Mode: OR

Electron Ions: both
Use MSn Info: yes
Isotope Res: 10000
Max Results: 800

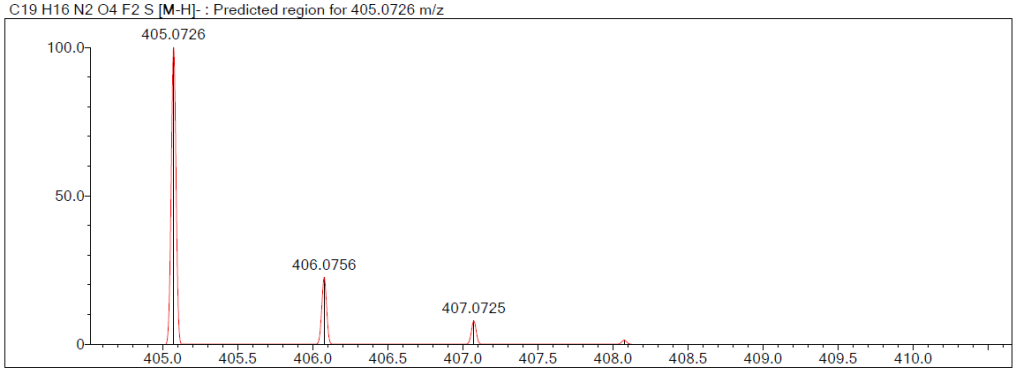
Event#: 2 MS(E-) Ret. Time : 0.160 -> 0.390 Scan# : 34 -> 80



Measured region for 405.0886 m/z



C19 H16 N2 O4 F2 S [M-H]- : Predicted region for 405.0726 m/z



Rank	Score	Ion	Formula (M)	Pred. m/z	Meas. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
84	0.00	[M-H]-	C19 H16 N2 O4 F2 S	405.0726	405.0886	16.0	39.50	14.27	12.0

Compound 10 HR MS

Data File: D:\分子量测定\2015\2015-01-25\2015-01-25WLJ_63_9.lcd

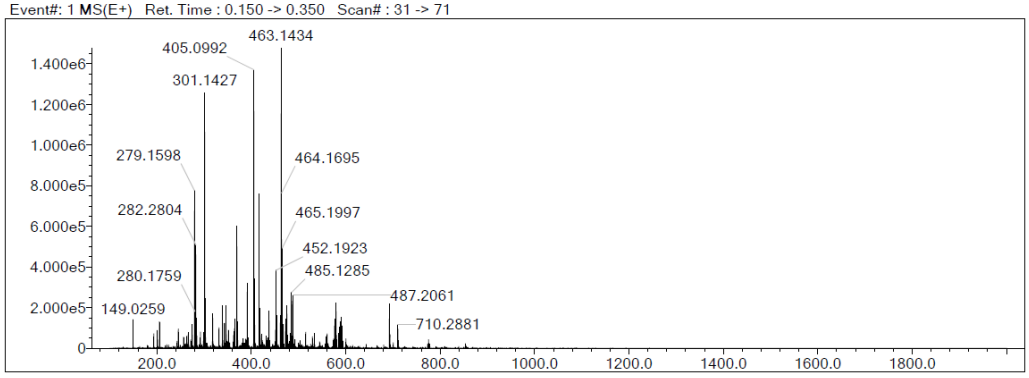
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	100	N	3	0	5	P	3	0	0	Br	1	0	2	H
B	3	0	0	O	2	0	50	S	2	0	1	I	3	0	0	
C	4	19	50	F	1	0	1	Cl	1	0	0					

Error Margin (mDa): 20.0
HC Ratio: 0.0 - 3.0
Max Isotopes: all
MSn Iso RI (%): 75.00

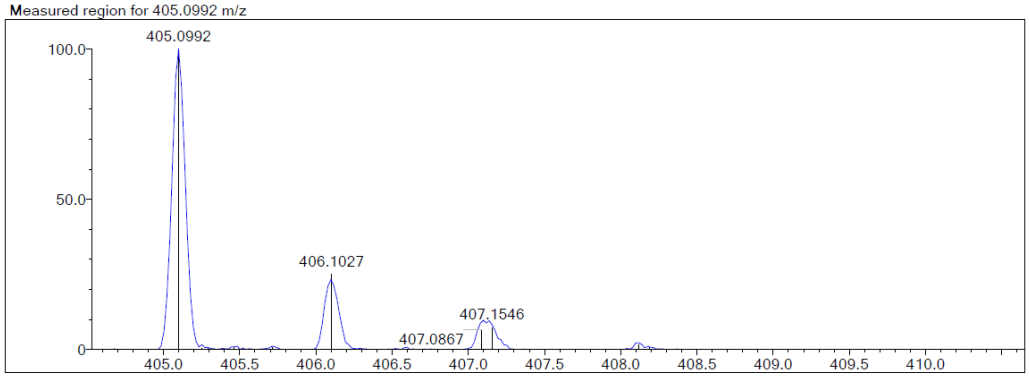
DBE Range: 0.0 - 30.0
Apply N Rule: yes
Isotope RI (%): 1.00
MSn Logic Mode: OR

Electron Ions: both
Use MSn Info: yes
Isotope Res: 10000
Max Results: 800

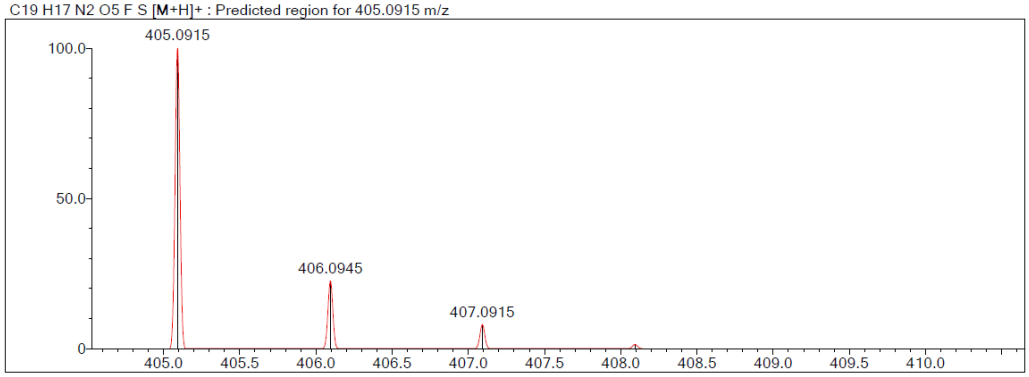
Event#: 1 MS(E+) Ret. Time : 0.150 -> 0.350 Scan# : 31 -> 71



Measured region for 405.0992 m/z



C19 H17 N2 O5 F S [M+H]+ : Predicted region for 405.0915 m/z



Rank	Score	Ion	Formula (M)	Pred. m/z	Meas. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
14	10.36	[M+H]+	C19 H17 N2 O5 F S	405.0915	405.0992	7.7	19.01	64.86	12.0

Compound 11 HR MS

Data File: D:\分子量测定\2015\2015-01-25\2015-01-25WLJ_WLJ-64_4.lcd

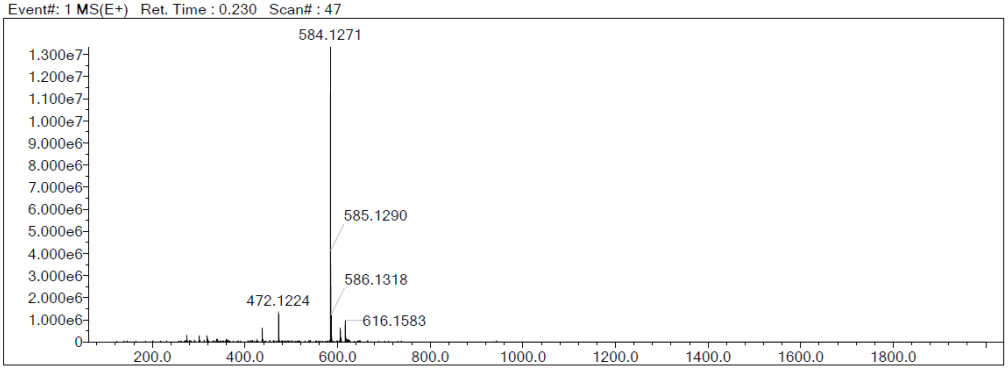
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	100	N	3	0	5	P	3	0	0	Br	1	0	0	H
B	3	0	0	O	2	0	50	S	2	0	1	I	3	0	0	
C	4	0	50	F	1	0	6	Cl	1	0	0					

Error Margin (mDa): 10.0
HC Ratio: 0.0 - 3.0
Max Isotopes: all
MSn Iso RI (%): 75.00

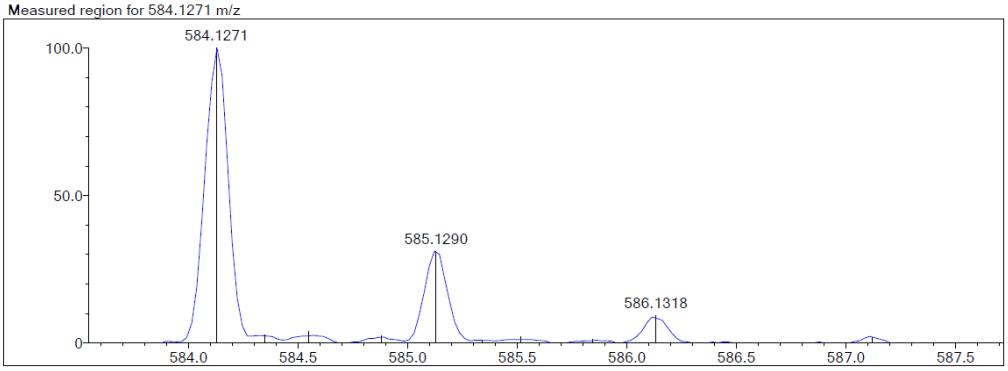
DBE Range: 0.0 - 30.0
Apply N Rule: yes
Isotope RI (%): 1.00
MSn Logic Mode: OR

Electron Ions: both
Use MSn Info: yes
Isotope Res: 10000
Max Results: 800

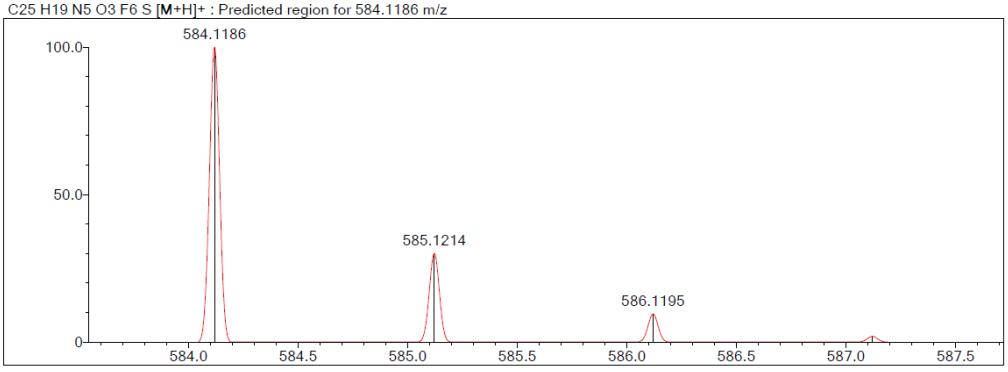
Event#: 1 MS(E+) Ret. Time : 0.230 Scan# : 47



Measured region for 584.1271 m/z



C25 H19 N5 O3 F6 S [M+H]+ : Predicted region for 584.1186 m/z



Rank	Score	Ion	Formula (M)	Pred. m/z	Meas. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
113	20.86	[M+H]+	C25 H19 N5 O3 F6 S	584.1186	584.1271	8.5	14.55	74.84	16.0

Compound 12 HR MS

Data File: D:\分子量测定\2015\2015-01-25\2015-01-25WLJ_65_35.lcd

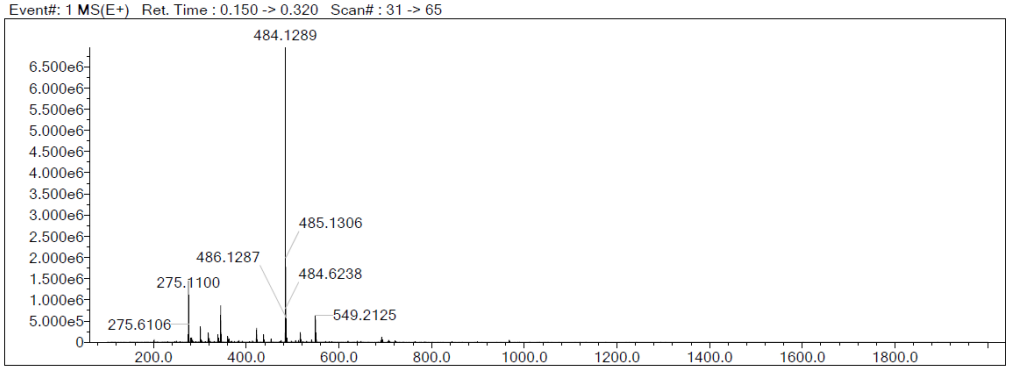
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	100	N	3	0	6	P	3	0	0	Br	1	0	2	H
B	3	0	0	O	2	0	50	S	2	0	1	I	3	0	0	
C	4	19	50	F	1	0	6	Cl	1	0	0					

Error Margin (mDa): 20.0
HC Ratio: 0.0 - 3.0
Max Isotopes: all
MSn Iso RI (%): 75.00

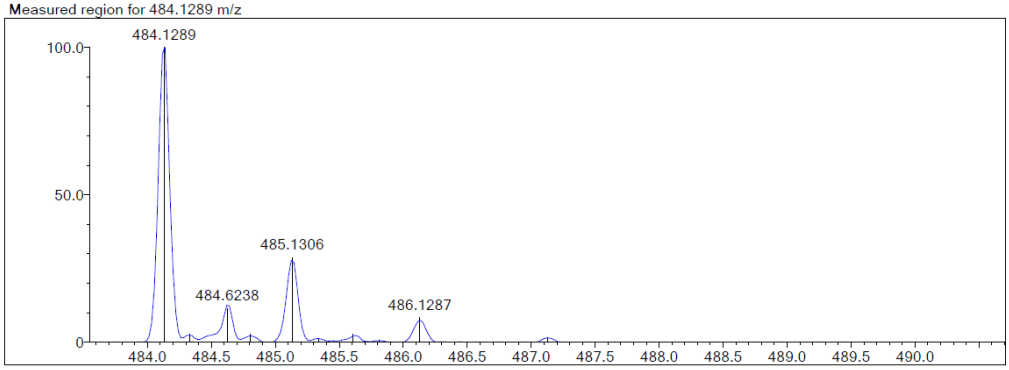
DBE Range: 0.0 - 30.0
Apply N Rule: yes
Isotope RI (%): 1.00
MSn Logic Mode: OR

Electron Ions: both
Use MSn Info: yes
Isotope Res: 10000
Max Results: 800

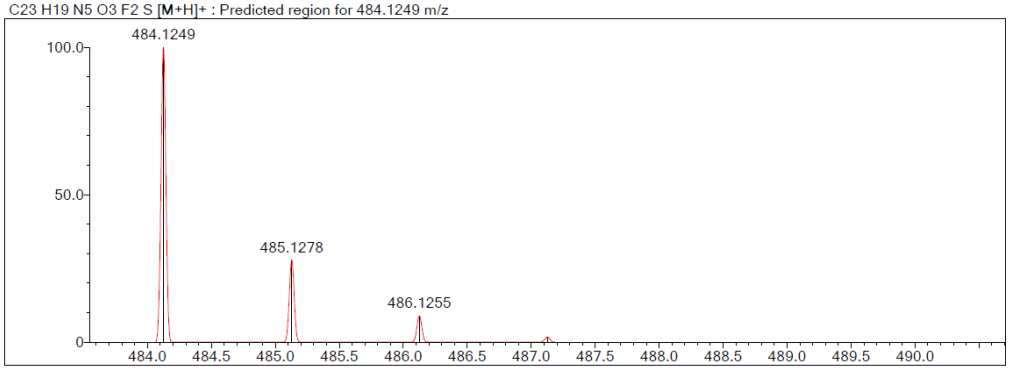
Event#: 1 MS(E+) Ret. Time : 0.150 -> 0.320 Scan# : 31 -> 65



Measured region for 484.1289 m/z



C23 H19 N5 O3 F2 S [M+H]+ : Predicted region for 484.1249 m/z



Rank	Score	Ion	Formula (M)	Pred. m/z	Meas. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
22	53.28	[M+H]+	C23 H19 N5 O3 F2 S	484.1249	484.1289	4.0	8.26	92.81	16.0

Compound 13 HR MS

Data File: D:\分子量测定\2015\2015-01-25\2015-01-25WLJ_66_7.lcd

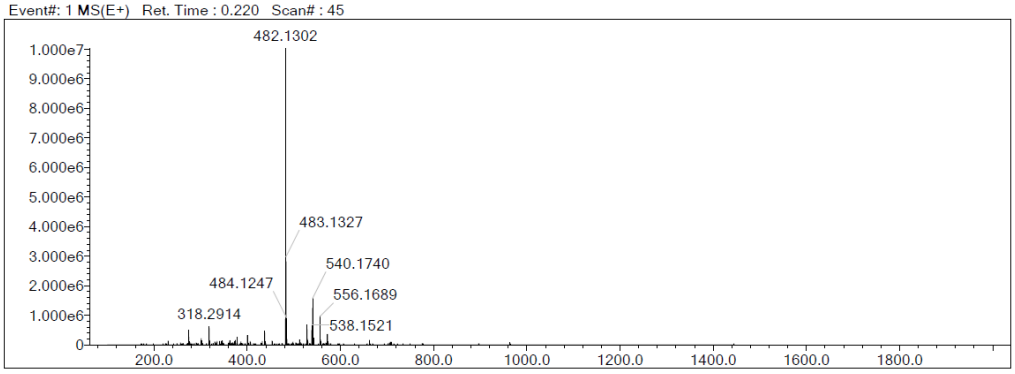
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	100	N	3	0	5	P	3	0	0	Br	1	0	2	H
B	3	0	0	O	2	0	50	S	2	0	1	I	3	0	0	
C	4	19	50	F	1	0	1	Cl	1	0	0					

Error Margin (mDa): 20.0
HC Ratio: 0.0 - 3.0
Max Isotopes: all
MSn Iso RI (%): 75.00

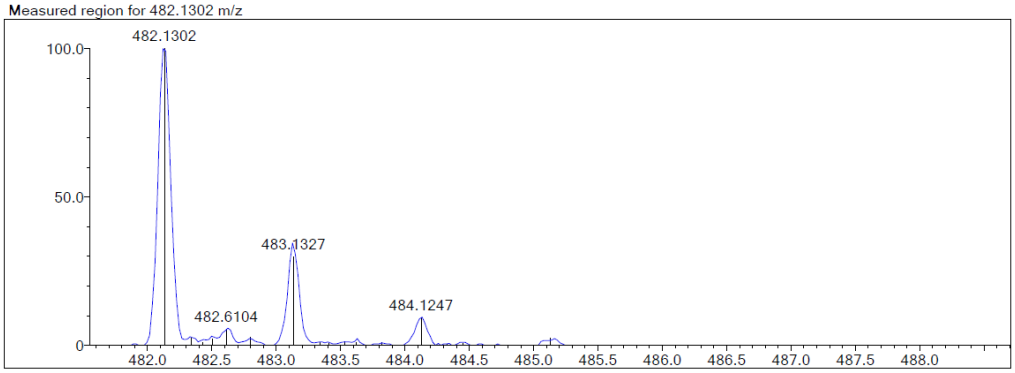
DBE Range: 0.0 - 30.0
Apply N Rule: yes
Isotope RI (%): 1.00
MSn Logic Mode: OR

Electron Ions: both
Use MSn Info: yes
Isotope Res: 10000
Max Results: 800

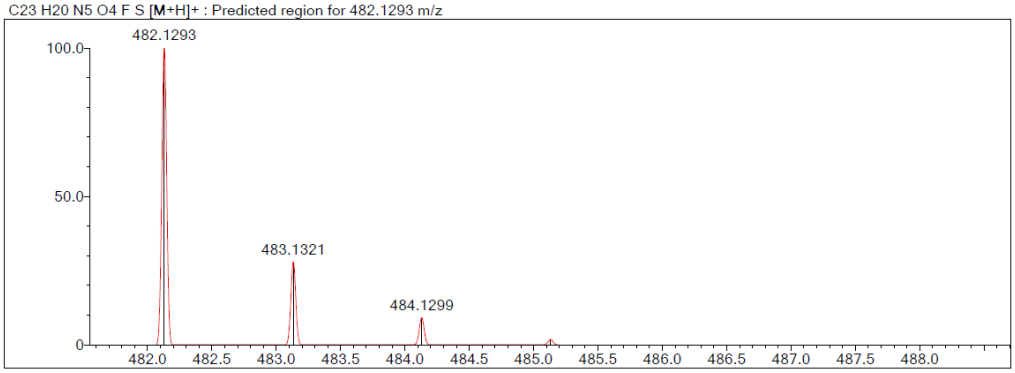
Event#: 1 MS(E+) Ret. Time : 0.220 Scan# : 45



Measured region for 482.1302 m/z



C23 H20 N5 O4 F S [M+H]+ : Predicted region for 482.1293 m/z



Rank	Score	Ion	Formula (M)	Pred. m/z	Meas. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
8	43.32	[M+H]+	C23 H20 N5 O4 F S	482.1293	482.1302	0.9	1.87	44.28	16.0

Compound 14 HR MS