Supporting information for

Discovery of Alkene-Conjugated Luciferins for Redshifted and Improved Bioluminescence Imaging *in vitro* and *in vivo*

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CONTENT

Cytotoxicity test

Cytotoxicity to ES-2-Fluc cells was determined using the CCK-8 method. ES-2-Fluc cells (8000 cells per well) were planted in a clear 96-well plate and grown for 24 hours at 37 °C. The wells were then filled with a variety of concentrations of the compounds (or DMSO control) dissolved in RPMI-1640. CCK-8 was added after an 8-hour incubation period at 37°C. A POLAR Star Omega microplate reader was used to determine cell viability.

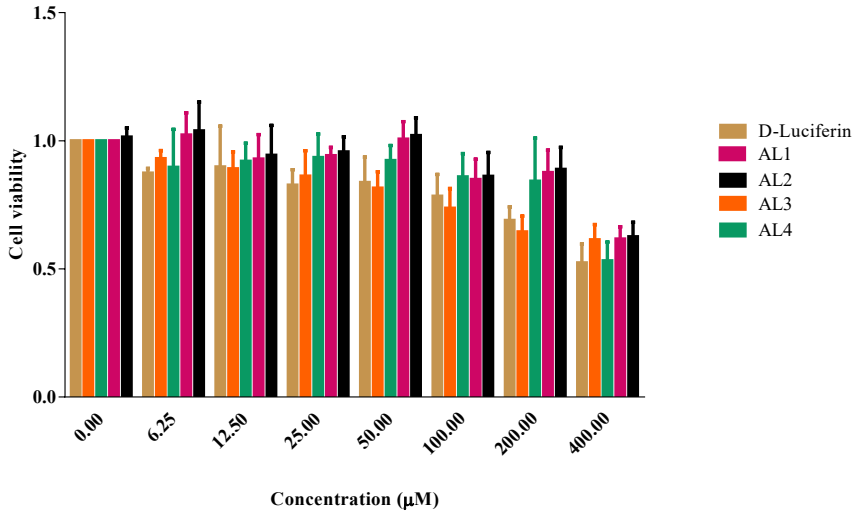
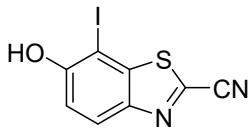


Figure S1. Cytotoxicity of novel D-Luciferin derivatives (CCK8 method)

Synthetic procedures

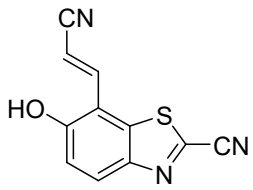
2-Cyano-6-hydroxy benzothiazole (A)



Hydroxybenzothiazole (16 mg, 91.3 μmol) was dissolved in toluene （7 mL）and the mixture was cooled to 0 °C. After stirred for 10 min, N-iodo succinimide (24.5 mg, 109 μmol) was added to the solution. The mixture was stirred for 10 h at room temperature. Upon completion, there was a large amount of insoluble matter, the mixture was filtered first, then collected solid. The filtrate was quenched with saturated $Na_2S_2O_3$ (2 x 20 mL), extracted with ethyl acetate (2 x 10 mL), washed the organic phase with saturated NaCl (2 x 20 mL), dried with anhydrous Na_2SO_4, filtered and concentrated under reduced pressure. The crude was purified by thin-layer chromatography (PE / EA = 2 / 1) affording product A as white solid (10mg, 36.45%). ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.43 (s, 1H), 8.10 (d, J = 8.9 Hz, 1H), 7.27 (d, J = 8.9 Hz, 1H).ESI-MS: found m/z 301.1 $[M-H]^-$

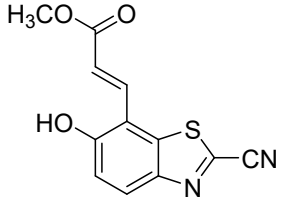
(E)-7-(2-cyanovinyl)-6-hydroxy-2-cyanobenzothiazole (B1)

Compound A (117 mg, 387 μmol) was dissolved in anhydrous acetonitrile (4 mL) of a



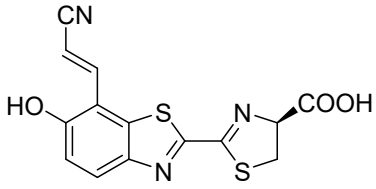
microwave reaction tube (10 mL). Acrylonitrile (61.7 mg, 1.16 mmol), palladium acetate (13.5 mg, 38.7 μmol) were added to the solution. The reaction temperature is 100 °C, and the microwave reaction time is 25 min. Upon completion, the mixture was diluted with ethyl acetate (10 mL), extracted with saturated NH_4Cl (2 x 20 mL), washed with saturated NaCl (2 x 20 mL), dried with anhydrous Na_2SO_4, then filtered and concentrated under reduced pressure. The mixture was purified by thin-layer chromatography (PE/EA=2/1) affording product B1 as light yellow solid (20 mg, 16%). ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.15 (d, J = 9.0 Hz, 1H), 7.79 (d, J = 16.8 Hz, 1H), 7.32 (d, J = 9.1 Hz, 1H), 6.49 (d, J = 16.7 Hz, 1H). ESI-MS: found m/z 226 $[M-H]^-$,452.57 $[2M-H]^-$

Methyl(E)-3-(2-cyano-6-hydroxybenzothiazol-7-yl)acrylate (B2)



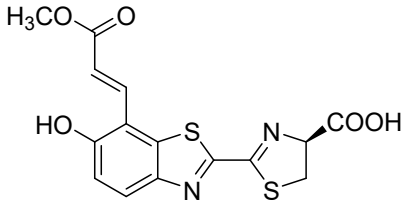
To a schlenk bottle of Compound A (200 mg, 662 μmol) in anhydrous acetonitrile (10 mL), were added tri-o-methyl phenyl phosphine (60.4 mg, 198 μmol), palladium acetate (34.67 mg, 99.31 μmol), Et_3N (276 μL, 1.99 μmol) under nitrogen pressure. The reaction mixture was heated to 70 °C for 8 h. Upon completion, the reaction solution was diluted with ethyl acetate (10 mL), washed with saturated NH_4Cl (2 x 20 mL), washed with saturated NaCl (2 x 20 mL), collected the upper organic phase, dried with anhydrous Na_2SO_4, filtered and concentrated under reduced pressure, separated and purified by thin-layer chromatography (PE/EA=1/1). The product was obtained 40 mg, with a yield of 23%. ^{1}H NMR (600 MHz, DMSO-d_6) δ 8.20 (d, J = 9.0 Hz, 1H), 8.04 (d, J = 16.4 Hz, 1H), 7.37 (d, J = 9.0 Hz, 1H), 6.55 (d, J = 16.4 Hz, 1H), 3.78 (s, 3H). ESI-MS found m/z 259.53 $[M-H]^-$

(S,E)-4,5-dihydro-2-(7-(2-cyano)-6-hydroxybenzothiazol-2-yl)thiazole-4-carboxylic acid (AL1)



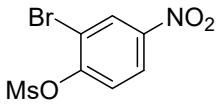
To a flask of compound B1 (26 mg, 114.42 μmol) in the solution of methanol (6 mL) and water (3 mL), were added K_2CO_3 (16.76 mg, 121.28 μmol) and D-cysteine (20.7 mg, 117.85 μmol), and react for about 20 min. Upon completion, the reaction solution was concentrated under reduced pressure until the organic solvent is completely evaporated, adjusted pH to 2-4 with HCl (1 M). Water (4 mL) was added to the crude, there are solid crystals. The mixture was store in the refrigerator until all the solids are deposited. The mixture were filtered and washed with petroleum ether, collected solid and dried as product AL1 (20 mg, 52%); mp: 166-168 °C. ^{1}H NMR (400 MHz, MeOD) δ 7.93 (d, J = 8.9 Hz, 1H), 7.82 (d, J = 16.9 Hz, 1H), 7.14 (d, J = 8.9 Hz, 1H), 6.39 (d, J = 16.9 Hz, 1H), 5.29 – 5.18 (m, 1H), 3.84 – 3.68 (m, 2H).^{13}C NMR (101 MHz, MeOD) δ 171.70, 165.84, 154.43, 148.88, 145.44, 144.02, 135.37, 127.38, 118.71, 118.03, 109.03, 95.90, 77.84, 34.94 ESI-MS found m/z 330 $[M-H]^-$, ESI-HRMS calcd: 331, found: 330.0005 $[M-H]^-$

(S,E)-4,5-dihydro-2-(7-(3-methoxy-3-oxoprop-1-en-1-yl)6-aminobenzothiazol-2-yl)thiazole -4 --Formic acid(AL2)



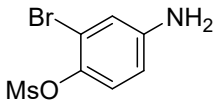
To a flask of compound B2 (40 mg, 153.7 μmol) in the mixture solution water (3 mL) and methanol (6 mL), was added K_2CO_3 (27.8 mg, 158 μmol). The mixture was stirred for 10 min. D-cysteine (22.7mg, 163 μmol) were added to the solution, the mixture was stirred for 20 min. The mixture was concentrated under reduced pressure until the methanol is completely evaporated in solution, then adjusted pH to 3, and placed it in the refrigerator to fully cool down. A large amount of solids precipitated out, then filtered, and rinsed the product with a small amount of petroleum ether and dried to obtain compound AL2 (40 mg, 72%); mp: 164-166°C. ^{1}H NMR (400 MHz, MeOD) δ 8.05 (d, *J* = 16.4 Hz, 1H), 7.83 (d, *J* = 8.9 Hz, 1H), 7.03 (d, *J* = 8.9 Hz, 1H), 6.54 (d, *J* = 16.4 Hz, 1H), 5.31 (t, *J* = 9.1 Hz, 1H), 3.73 (s, 3H), 3.69 (d, *J* = 3.2 Hz, 1H), 3.66 (d, *J* = 2.4 Hz, 1H). ^{13}C NMR (101 MHz, MeOD) δ 171.94, 168.05, 165.97, 157.67, 156.99, 147.35, 137.72, 136.11, 126.87, 119.56, 116.73, 114.05, 78.40, 50.81, 34.55. ESI-MS found m/z 363.5 $[M-H]^-$, ESI-HRMS calcd.: 364.39, found: 365.0259 $[M+H]^+$

2-bromo-4-nitrophenyl methanesulfonate (A')



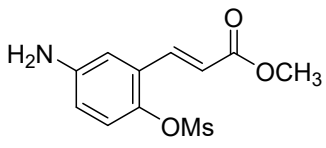
To a solution of 2-bromo-4-nitrophenol (100 mg, 458 μmol) and anhydrous Et_3N (6.7 mL, 48.4 mmol) in dry DCM (20 mL) under nitrogen, was added dropwise methanesulfonyl chloride (2.20 mL, 28.4 mmol). Then reaction mixture was stirred at 0 °C for 2 h. Upon completion, the reaction was quenched (1 M $NaHSO_4$) and washed with 1 M NaHSO4 (3 x 30 mL), saturated NH_4Cl (1 x 30 mL), and brine (3 x 30 mL). The organic phase was dried over anhydrous Na_2SO_4, filtered, and concentrated under reduced pressure. Purification by silica gel column chromatography (PE/EA=3/1) yield compound A' as light grey solid (101 mg, 75%); mp: 79-81°C.^{1}H NMR (400 MHz, DMSO-d_6) δ 8.61 (s, 1H), 8.34 (d, *J* = 9.0 Hz, 1H), 7.80 (d, *J* = 9.0 Hz, 1H), 3.64 (s, 3H). ESI-MS found m/z 298.99 $[M+H]^+$

3-amino-2-bromophenyl methanesulfonate (B')



A solution of Compound A' (300 mg, 1.01 mmol) in acetone (5 mL), a mixture of iron powder (362.13 mg, 6.48mmol) in acetic acid (3 mL), and water(10mL) were added to 40 mL schlenk bottle. The reaction mixture was heated to 70°C, stirred for 1.5 h, filtered hot through a pad of Celite. The filtrate was neutralized with saturated K_2CO_3 solution and washed with saturated EDTA solution (2 x 50 ml) to remove any additional iron species, extracted with ethyl acetate (50 mL), and dry with anhydrous Na_2SO_4, filtered and concentrated *in vacuo*. The residue was purified by Column chromatography on silica gel (PE/EA=2/5) affording compound B' as white solid (224 mg, 84%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.21 (d, *J* = 8.8 Hz, 2H), 6.90 (d, *J* = 2.8 Hz, 2H), 6.60 (dd, *J* = 8.8, 2.8 Hz, 2H), 3.80 (s, 3H), 3.20 (s, 5H). ESI-MS found m/z 287.93 $[M+Na]^+$

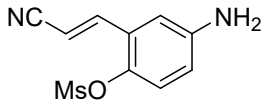
Methyl(E)-3-(5-amino-2-((methylsulfonyl)oxy)phenyl)acrylate (C'3)



Compound B' (224 mg, 841 μmol), tri-o-methylphenylphosphine (76.9 mg, 252 μmol), Et_3N (351 mL, 2.53 mmol), methyl acrylate (217.4 mg, 2.53 mmol)

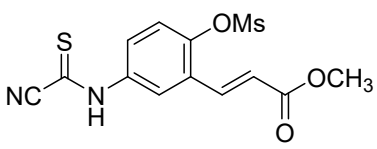
in ultra-dry acetonitrile (8 mL) were added to a 20 mL schlenk bottle vacuumed to replace nitrogen for three times. Then palladium acetate (44.1 mg, 126 μmol) was added under nitrogen pressure. The reaction was heated in a 70 ºC oil bath for 8 h, and the reaction was monitored by TLC. Upon completion, the reaction mixture was extracted with saturated NH_4Cl (2 x 20 ml), ethyl acetate (2 x 20 ml), dried with anhydrous Na_2SO_4, filtered and concentrated *in vacuo*. The residue was purified by Column chromatography on silica gel (PE/EA=3/1) affording compound C'3 as light yellow solid (133 mg, 58.1%); m.p: 102-104ºC. ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.71 (d, J = 16.1 Hz, 1H), 7.13 (d, J = 8.8 Hz, 1H), 6.98 (d, J = 2.7 Hz, 1H), 6.70 (dd, J = 8.8, 2.7 Hz, 1H), 6.43 (d, J = 16.0 Hz, 1H), 5.39 (s, 2H), 3.74 (s, 3H). ESI-MS found m/z 294.65 $[M+Na]^+$

(E) -4-amino-2-(2-cyano)phenylmethanesulfonate (C'4)



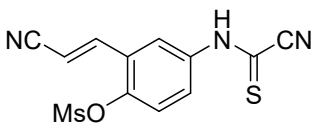
100 mg compound B', 43 mg N-methyldicyclohexylamine, 59.7μL acrylonitrile, 12.9 mg tris(dibenzylideneacetone) dipalladium, and tri-tert-butyl tetrafluoroborate were added into a 100 mL double-necked flask. Then 10.6 mg phosphine, 10mL ultra-dry 1.4-dioxane as solvent were added, vacuumed nitrogen replacement three times. The reaction was heated in a 120 ºC oil bath for 72 h, and the reaction was monitored by TLC. Upon completion, the reaction mixture was concentrated under reduced pressure. The residue was purified by Column chromatography on silica gel (PE/EA=4/1) affording compound C'4 as light grey solid (20 mg, 53%); mp: 102-104ºC. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.77 (d, J = 2.7 Hz, 1H), 8.41 (dd, J = 9.0, 2.8 Hz, 1H), 7.79 (dd, J = 19.0, 12.9 Hz, 2H), 6.90 (d, J = 16.7 Hz, 1H), 3.70 (s, 3H). ESI-MS found m/z 239.09 $[M+H]^+$

Methyl(E)-3-(5-((cyanocarbonyl)amino)-2-((methylsulfonyl)oxy)phenyl)acrylate (D'3)



To a flask of Compound C'3 (1.01 g, 3.72 mmol), was added Appel's salt (4, 5-dichloro-1, 2, 3-dithiazol-1-ium chloride, 931.49 mg, 4.47 mmol), followed by an nitrogen flush. Anhydrous THF (20 mL) and anhydrous ACN (20 mL) was immediately added and the reaction was stirred at room temperature for 5 min under nitrogen pressure. Upon consumption of starting material, anhydrous pyridine (618.44mg, 7.82 mmol) was slowly added. The reaction mixture was allowed to stir overnight, and the solution of $Na_2S_2O_3$ (1.51g， 7.82mmol) was added under nitrogen pressure. The mixture was stirred for 3h, and monitored by TLC. The mixture was extracted with ethyl acetate (2 x 50 ml), washed with 1 M $NaHSO_4$ (3 x 50 mL), dried with anhydrous Na_2SO_4, and purified by column chromatography on silica gel affording compound D'3 as white solid (1.06g, 80%); m.p: 185-187ºC. ^{1}H NMR (400 MHz, DMSO-d_6) δ 13.64 (s, 1H), 8.43 (d, J = 2.4 Hz, 1H), 7.91 (dd, J = 8.8, 2.5 Hz, 1H), 7.79 (d, J = 16.1 Hz, 1H), 7.63 (d, J= 8.8 Hz, 1H), 6.61 (d, J = 16.1 Hz, 1H), 3.76 (s, 3H), 3.57 (s, 3H). ESI-MS found m/z 339.05 $[M-H]^-$

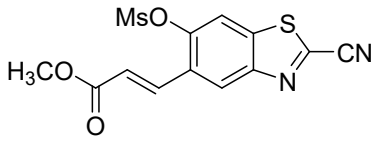
(E) -4-((cyanocarbonyl)amino)-2-(2-cyanovinyl)phenylmethanesulfonate (D'4)



To a flask of C'4 (500 mg, 2.1 mmol), was added Appel's salt (4, 5-dichloro-1, 2, 3-dithiazol-1-ium chloride, 525 mg,

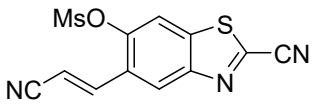
2.52 mmol), followed by an nitrogen flush. Anhydrous THF (10 mL) and anhydrous ACN (10 mL) was immediately added and the reaction was stirred at room temperature for 5 min under nitrogen pressure. Upon consumption of starting material, anhydrous pyridine (348.60mg, 4.41mmol) was slowly added. The reaction mixture was allowed to stir overnight, and the solution of $Na_2S_2O_3$ (995 mg，6.30mmol) was added under nitrogen pressure. The mixture was stirred for 3h, and monitored by TLC. The mixture was extracted with ethyl acetate (2 x 50 ml), washed with 1 M $NaHSO_4$ (3 x 50 mL), dried with anhydrous Na_2SO_4, and purified by column chromatography on silica gel affording compound D'4 as white solid (103 mg, 30%)；m.p:147-149 ^oC; ^1H NMR (400 MHz, DMSO-d_6) δ 8.30 (d, J = 2.3 Hz, 1H), 7.92 (dd, J = 8.8, 2.5 Hz, 1H), 7.76 (d, J = 16.7 Hz, 1H), 7.60 (d, J = 8.8 Hz, 1H), 6.48 (d, J = 16.7 Hz, 1H), 3.61 (d, J = 4.7 Hz, 3H).ESI-MS found m/z 306.10 $[M-H]^-$

Methyl(E)-3-(2-cyano-6-((methylsulfonyl)oxy)benzothiazol-5-yl)acrylate methyl (E'3)



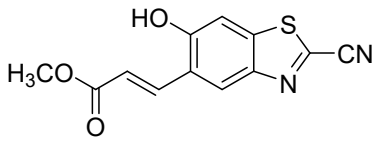
Compound D'3 (76 mg, 223 μmol), palladium chloride (8.09 mg, 26.8 μmol), copper (I) iodide (23.4 mg, 122 μmol), and TBAB (1512 mg, 46.9 μmol) were added in a 25 mL double-necked flask evacuated and replaced with nitrogen three times, and the mixed solution of DMSO (10 mL)and DMF (10 mL) as the reaction solvent was added. Then the mixture was heated in a 120 ºC oil bath for 4 h and the reaction was monitored by TLC. Upon completion, the mixture was diluted with ethyl acetate, extracted with saturated NH_4Cl, washed with water, dried with anhydrous Na_2SO_4, filtered and concentrated under reduced pressure, then purified by preparative thin layer chromatography (PE/EA=1/1) affording compound E'3 as light grey solid (25 mg, 36%); mp: 157-159^oC. ^1H NMR (400 MHz, DMSO-d_6) δ 8.93 (s, 1H), 8.54 (s, 1H), 7.88 (d, J = 16.1 Hz, 1H), 7.01 (d, J = 16.1 Hz, 1H), 3.78 (s, 3H), 3.62 (s, 3H). ESI-MS found m/z 361.87 $[M+Na]^+$

(F) -2-cyano-5-(2-cyanovinyl)benzothiazole-6-ylmethanesulfonate (E'4)



The reaction steps are the same as compound E'3, and the final product is 42.5 mg, and the yield is 40%; m.p: 249-251^oC. ^1H NMR (400 MHz, DMSO-d_6) δ 8.87 (s, 1H), 8.54 (s, 1H), 7.87 (d, J = 16.7 Hz, 1H), 6.84 (d, J = 16.6 Hz, 1H), 3.68 (s, 2H), 3.32 (s, 2H), 2.50 (s, 3H). ESI-MS found m/z 326.6 $[M+Na]^+$

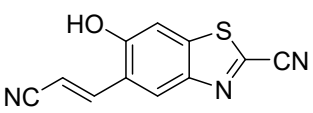
Methyl(E)-3-(2-cyano-6-hydroxybenzothiazol-5-yl)acrylate (F'3)



To a flask of compound E'3 (30 mg, 88.7 μmol), was added ultra-dry tetrahydrofuran (10 mL). 75% tetrabutylammonium fluoride solution was added dropwise into the reaction solution, followed by nitrogen flush. The reaction was stirred for 1h and monitored by TLC. Upon completion, the reaction solution was concentrated under reduced pressure, dissolved by ethyl acetate, washed with saturated NaCl, dried with anhydrous Na_2SO_4. The mixture was filtered, concentrated in vacuo and purified by thin-layer chromatography (PE/EA=2/3) affording product F'3 (13 mg, 56.3%). ^1H NMR (400 MHz, DMSO-d_6) δ 8.57 (s, 1H), 7.96 (d, J = 16.2 Hz, 1H), 7.68 (s, 1H), 6.89 (d, J =

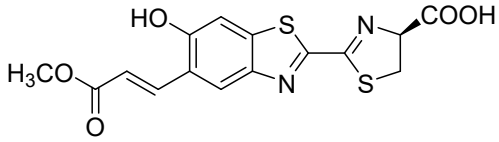
16.2 Hz, 1H), 3.74 (s, 3H). ESI-MS found m/z 259.53 [M-H]$^-$

(E) - 5 - (2-cyano vinyl) - 6-hydroxybenzothiazole-2-carbonitrile (F'4)



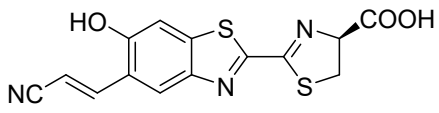
The experimental procedure was the same as that of F'3. The final product was 52 mg with a yield of 28%; m.p:339-341 ^{o}C.^{1}H NMR (400 MHz, DMSO-d_6) δ 11.51 (s, 1H), 8.49 (s, 1H), 7.79 (d, J = 16.8 Hz, 1H), 7.71 (s, 1H), 6.70 (d, J = 16.8 Hz, 1H). ESI-MS found m/z 226.16 [M-H]$^-$

(S,E)-4,5-dihydro-2-(5-(3-oxobut-1-en-1-yl)6-hydroxybenzothiazol-2-yl)thiazole-4-carboxylic acid (AL3)



Compound F'3 (41 mg, 157 μmol) was dissolved in the mixture solution methanol (8 mL) and water (4 mL). Then D-cysteine (20.2 mg, 167 μmol) and anhydrous K_2CO_3 (22.4 mg, 162 μmol) were added. After stirred at room temperature for 20 min, TLC was used to monitor the reaction. The crude was concentrated to remove methanol, adjusted pH to 2-3 with HCl (1M). A large amount of solid precipitated, filtrated, purified with HPLC to provide compound AL3 as a brown solid (30 mg, 53%); mp: 133-135^{o}C.^{1}H NMR (400 MHz, DMSO-d_6) δ 7.42 (s, 1H), 7.25 (d, J = 16.1 Hz, 1H), 6.60 (s, 1H), 5.95 (d, J = 16.1 Hz, 1H), 4.59 (s, 2H), 3.04 (s, 1H), 3.01 (s, 3H), 2.98 (d, J = 8.4 Hz, 1H). ^{13}C NMR (101 MHz, MeOD) δ 172.16, 167.92, 158.42, 156.45, 147.13, 140.11, 139.28, 129.72, 123.58, 122.99, 118.26, 106.46, 78.35, 51.11, 34.56.ESI-MS found m/z 365.19 [M+H]$^+$, ESI-HRMS calcd for:364.39, found: 363.0162 [M-H]$^-$

(S,E)-4,5-dihydro-2-(5-(2-cyanovinyl)-6-hydroxybenzothiazol-2-yl)thiazole-4-carboxylic acid (AL4）



To a flask of compound F'4 (46 mg, 202 μmol) in the solution of methanol (8 mL) and water (4 mL), were added D-cysteine (36.6 mg, 208 μmol) and anhydrous K_2CO_3 (29.7 mg, 215 μmol). After stirred at room temperature for 20 min, the reaction was basically completed. Methanol is removed by vacuum rotary evaporation, and water (5 mL) is added, and then the pH is adjusted to 2-3 with HCl (1M). A large amount of solid precipitated, filtrated, and washed the upper solid with petroleum ether (10 mL), and dried to provide product AL4 as solid (20mg , 33%); mp: 229-231^{o}C. ^{1}H NMR (400 MHz, MeOD) δ 8.18 (s, 1H), 7.78 (d, J = 16.8 Hz, 1H), 7.42 (s, 0H), 6.52 (d, J = 5.8 Hz, 0H), 5.41 (t, J = 9.1 Hz, 1H), 3.83 – 3.73 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 176.04, 169.73, 162.86, 160.26, 150.86, 150.38, 144.07, 127.35, 126.23, 122.42, 110.92, 100.75, 82.17, 38.45. ESI-HRMS calcd.: 331.36, found: 329.9995[M-H]$^-$

Bioluminescent spectra of novel substrates and D-luciferin under different pH conditions

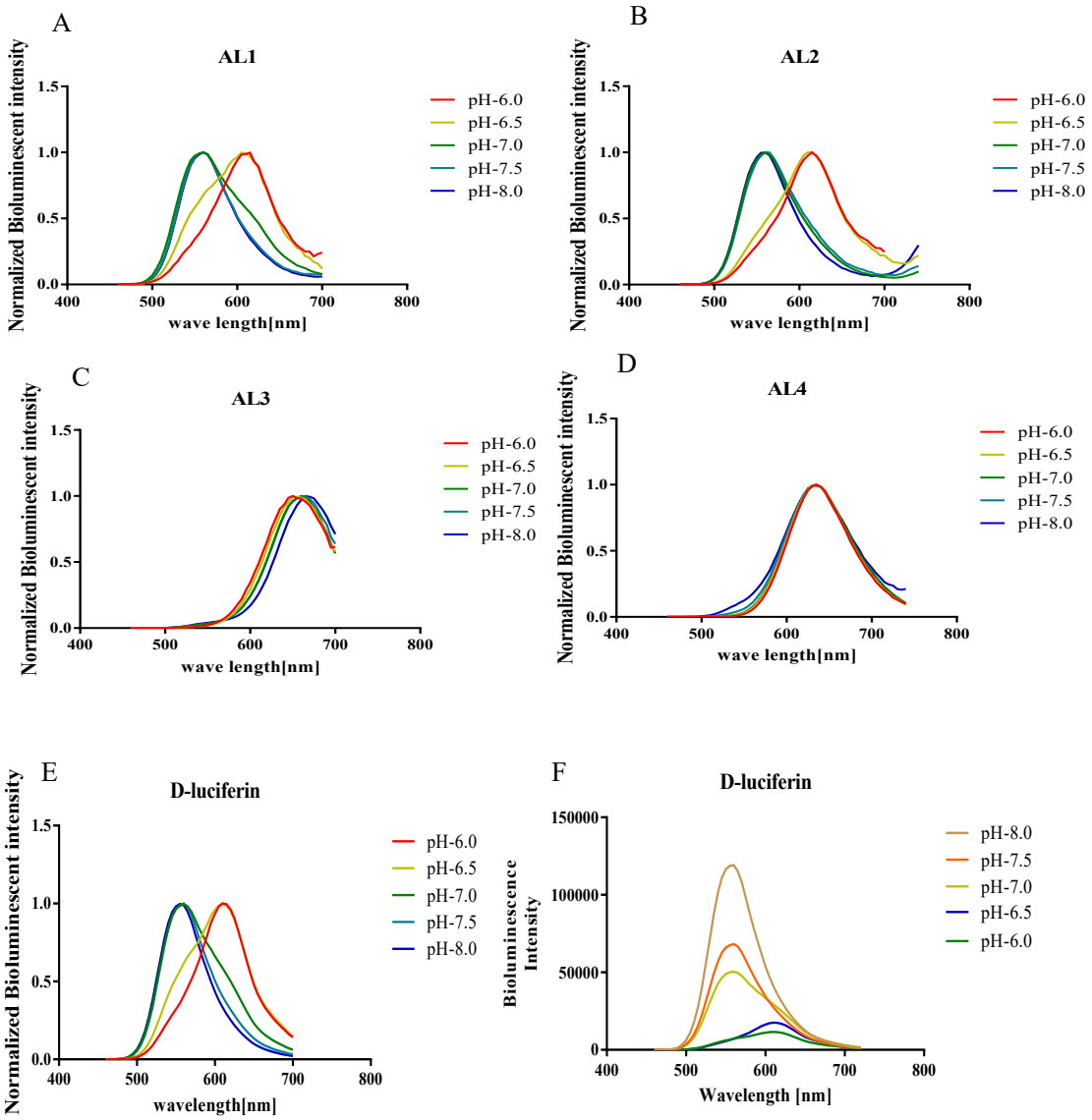


Figure S2: Normalized bioluminescent spectra of target products in various buffer solutions. The Normalized bioluminescent spectra of compound AL1(A)、AL2(B) 、AL3(C) 、AL4(D) 、D-luciferin(E) in various pH buffer solutions. The bioluminescent spectra of D-luciferin(F).

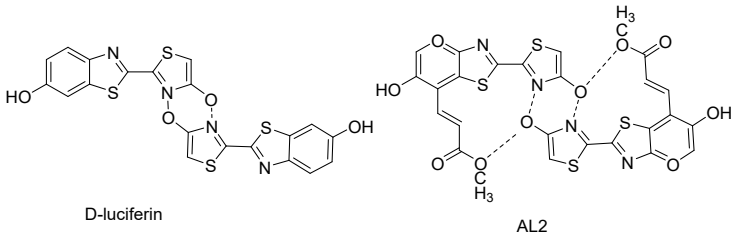


Figure S3: Possible excited state intermediates of D-luciferin and AL2. Dotted lines indicate hydrogen bonds

Tabularized values for graphs (Figures 4−6)

Table S1: Tabularized values for **Figure 4A**

Concentration (μM)	D-luciferin			AL-1			AL-2		
0.00	1.86E+07	1.52E+07	1.85E+07	1.10E+07	2.01E+06	2.66E+06	4.47E+07	6.11E+07	1.96E+07
2.50	3.08E+08	2.78E+08	2.74E+08	1.77E+07	9.23E+06	1.10E+07	3.97E+08	4.03E+08	4.21E+08
5.00	6.01E+08	5.32E+08	5.34E+08	1.78E+07	9.14E+06	1.09E+07	6.60E+08	6.44E+08	6.79E+08
10.00	9.77E+08	1.10E+09	1.04E+09	2.48E+07	1.40E+07	1.41E+07	8.70E+08	8.49E+08	8.90E+08
20.00	1.22E+08	2.02E+09	1.85E+09	3.17E+07	1.73E+07	2.15E+07	9.70E+08	1.05E+09	1.21E+09
40.00	3.19E+09	2.95E+09	2.91E+09	4.05E+07	4.09E+07	3.80E+07	1.91E+09	1.92E+09	1.98E+09
50.00	3.20E+09	3.11E+09	3.20E+09	4.40E+07	4.18E+07	3.89E+07	1.69E+09	1.69E+09	1.96E+09
75.00	3.79E+09	3.65E+09	3.70E+09	4.31E+07	4.33E+07	3.92E+07	2.13E+09	1.91E+09	2.12E+09
100.00	4.92E+09	4.93E+09	4.79E+09	4.63E+07	4.57E+07	4.72E+07	1.98E+09	1.87E+09	2.20E+09
Concentration (μM)	AL-3			AL-4					
0.00	1.18E+07	1.01E+07	1.03E+07	5.07E+06	3.47E+06	1.43E+06			
2.50	2.48E+08	2.71E+08	2.46E+08	1.93E+07	8.24E+06	7.83E+06			
5.00	3.25E+08	3.28E+08	3.25E+08	2.48E+07	9.14E+06	1.09E+07			
10.00	4.30E+08	4.31E+08	4.32E+08	1.78E+07	1.40E+07	1.41E+07			
20.00	5.72E+08	5.47E+08	5.27E+08	3.17E+07	1.73E+07	2.15E+07			
40.00	6.61E+08	6.27E+08	6.08E+08	3.62E+07	2.35E+07	2.79E+07			
50.00	6.94E+08	6.52E+08	6.53E+08	4.58E+07	2.50E+07	2.84E+07			
75.00	7.24E+08	6.84E+08	6.73E+08	5.17E+07	3.67E+07	3.45E+07			
100.00	7.02E+08	7.06E+08	7.24E+08	5.29E+07	3.69E+07	3.52E+07			

Table S2: Tabularized values for **Figure 4B**

Time (min)	D-luciferin			AL-1			AL-2		
0	3.80E+09	3.65E+09	3.75E+09	4.05E+07	4.09E+07	3.80E+07	1.91E+09	1.92E+09	1.98E+09
1	3.19E+09	2.95E+09	2.91E+09	3.58E+07	3.43E+07	3.13E+07	1.55E+09	1.54E+09	1.54E+09
2	2.84E+09	2.68E+09	2.59E+09	3.68E+07	2.94E+07	2.48E+07	1.10E+09	1.10E+09	1.08E+09
3	2.60E+09	2.46E+09	2.37E+09	2.89E+07	2.82E+07	3.10E+07	1.01E+09	1.01E+09	9.81E+08
4	2.40E+09	2.30E+09	2.20E+09	2.66E+07	2.63E+07	2.94E+07	9.30E+08	9.28E+08	8.96E+08
5	2.23E+09	2.15E+09	2.04E+09	2.86E+07	2.26E+07	2.14E+07	8.63E+08	8.55E+08	8.23E+08
6	1.94E+09	1.89E+09	1.76E+09	2.71E+07	2.67E+07	2.34E+07	8.03E+08	7.95E+08	7.62E+08
7	1.82E+09	1.78E+09	1.65E+09	2.54E+07	2.52E+07	2.28E+07	6.62E+08	6.54E+08	6.13E+08
9	1.71E+09	1.69E+09	1.55E+09	2.35E+07	2.48E+07	2.14E+07	5.97E+08	5.86E+08	5.42E+08
11	1.50E+09	1.49E+09	1.35E+09	2.27E+07	2.26E+07	1.98E+07	5.69E+08	5.55E+08	5.08E+08
13	1.40E+09	1.40E+09	1.27E+09	2.17E+07	2.03E+07	1.85E+07	5.38E+08	5.29E+08	4.79E+08
15	1.29E+09	1.29E+09	1.17E+09	2.10E+07	2.02E+07	1.76E+07	5.15E+08	5.07E+08	4.56E+08
17	1.20E+09	1.20E+09	1.08E+09	1.83E+07	1.70E+07	1.56E+07	4.95E+08	4.83E+08	4.35E+08
19	1.12E+09	1.12E+09	9.94E+08	1.75E+07	1.80E+07	1.56E+07	4.51E+08	4.41E+08	3.94E+08
21	1.05E+09	1.05E+09	9.22E+08	1.77E+07	1.72E+07	1.50E+07	4.31E+08	4.24E+08	3.75E+08
23	9.75E+08	9.80E+08	8.50E+08	1.62E+07	1.64E+07	1.42E+07	4.13E+08	4.05E+08	3.56E+08
25	9.13E+08	9.26E+08	7.92E+08	1.71E+07	1.56E+07	1.44E+07	3.93E+08	3.87E+08	3.42E+08
27	8.52E+08	8.68E+08	7.39E+08	1.57E+07	1.49E+07	1.25E+07	3.76E+08	3.71E+08	3.25E+08
29	7.98E+08	8.22E+08	6.94E+08	1.60E+07	1.44E+07	1.26E+07	3.60E+08	3.51E+08	3.10E+08

Time (min)	AL-3			AL-4		
0	7.37E+08	7.10E+08	7.25E+08	3.14E+07	2.36E+07	2.53E+07
1	6.20E+08	5.88E+08	5.73E+08	4.87E+07	2.59E+07	2.92E+07
2	5.41E+08	5.15E+08	5.58E+08	5.24E+07	3.04E+07	3.45E+07
3	4.80E+08	4.58E+08	4.89E+08	5.50E+07	3.78E+07	3.91E+07
4	4.53E+08	4.31E+08	4.57E+08	5.83E+07	4.06E+07	4.23E+07
5	4.03E+08	3.85E+08	4.03E+08	6.27E+07	4.38E+07	4.79E+07
6	3.80E+08	3.65E+08	3.80E+08	6.92E+07	4.91E+07	5.43E+07
7	3.60E+08	3.47E+08	3.59E+08	7.49E+07	5.08E+07	6.04E+07
9	3.20E+08	3.07E+08	3.18E+08	7.60E+07	5.58E+07	6.17E+07
11	2.76E+08	2.67E+08	2.76E+08	7.79E+07	5.81E+07	6.38E+07
13	2.51E+08	2.44E+08	2.49E+08	7.83E+07	5.93E+07	6.51E+07
15	2.28E+08	2.23E+08	2.29E+08	7.79E+07	5.95E+07	6.58E+07
17	2.11E+08	2.07E+08	2.12E+08	7.61E+07	5.87E+07	6.55E+07
19	1.96E+08	1.91E+08	1.95E+08	7.19E+07	5.57E+07	6.29E+07
21	1.79E+08	1.76E+08	1.78E+08	7.03E+07	5.43E+07	6.17E+07
23	1.66E+08	1.64E+08	1.65E+08	6.88E+07	5.32E+07	6.04E+07
25	1.54E+08	1.51E+08	1.54E+08	6.77E+07	5.26E+07	5.97E+07
27	1.44E+08	1.40E+08	1.43E+08	6.61E+07	5.19E+07	5.87E+07
29	1.30E+08	1.27E+08	1.26E+08	6.54E+07	5.16E+07	5.84E+07

Table S3: Tabularized values for **Figure 5A**

Concentration (μM)	D-luciferin			AL-1			AL-2		
0	7.02E+06	1.05E+07	5.87E+06	3.82E+05	3.88E+05	3.99E+05	1.61E+06	4.19E+06	3.13E+06
20	2.46E+08	2.57E+08	2.22E+08	5.59E+06	5.57E+06	5.77E+06	8.13E+07	8.82E+07	8.14E+07
50	3.19E+08	3.55E+08	3.57E+08	1.09E+07	1.11E+07	1.09E+07	2.08E+08	2.06E+08	1.95E+08
75	3.64E+08	3.52E+08	3.89E+08	1.34E+07	1.31E+07	1.40E+07	2.99E+08	2.86E+08	2.91E+08
100	4.91E+08	4.78E+08	5.20E+08	1.37E+07	1.42E+07	1.49E+07	2.87E+08	2.69E+08	2.80E+08
150	5.00E+08	4.44E+08	5.23E+08	1.36E+07	1.64E+07	1.65E+07	4.03E+08	3.71E+08	3.93E+08
200	4.46E+08	4.18E+08	5.20E+08	1.39E+07	1.54E+07	1.58E+07	4.07E+08	3.84E+08	3.82E+08
Concentration (μM)	AL-3			AL-4					
0	9.60E+05	7.69E+05	8.56E+05	7.17E+05	4.96E+05	9.44E+05			
20	1.85E+07	2.06E+07	1.90E+07	2.02E+07	1.95E+07	1.84E+07			
50	2.37E+07	2.62E+07	2.38E+07	3.90E+07	3.85E+07	3.46E+07			
75	2.83E+07	3.00E+07	3.13E+07	4.65E+07	4.13E+07	4.07E+07			
100	3.43E+07	3.63E+07	3.31E+07	4.77E+07	4.64E+07	4.28E+07			
150	3.66E+07	3.50E+07	3.81E+07	4.64E+07	4.68E+07	4.11E+07			
200	4.38E+07	4.21E+07	4.74E+07	4.78E+07	4.08E+07	4.38E+07			

Table S4: Tabularized values for **Figure 5B**

Time (min)	D-luciferin			AL-1			AL-2		
0	2.00E+08	1.90E+08	1.82E+08	7.46E+06	9.65E+06	1.11E+07	3.87E+07	1.26E+07	7.86E+06
5	5.00E+08	4.44E+08	5.23E+08	1.64E+07	1.65E+07	1.59E+07	3.79E+08	3.64E+08	3.84E+08
10	4.04E+08	3.57E+08	3.68E+08	1.57E+07	1.46E+07	1.36E+07	2.64E+08	2.64E+08	2.74E+08
15	3.23E+08	2.77E+08	2.58E+08	1.31E+07	1.25E+07	9.85E+06	1.58E+08	1.60E+08	1.66E+08
20	2.55E+08	2.16E+08	1.93E+08	1.05E+07	8.45E+06	8.40E+06	1.22E+08	1.19E+08	1.28E+08
25	2.07E+08	1.75E+08	1.56E+08	6.88E+06	5.94E+06	5.66E+06	1.02E+08	9.86E+07	1.08E+08
30	1.74E+08	1.49E+08	1.33E+08	5.60E+06	4.59E+06	4.65E+06	8.73E+07	8.54E+07	9.60E+07
40	1.42E+08	1.24E+08	1.03E+08	4.88E+06	3.85E+06	3.55E+06	8.60E+07	8.38E+07	9.48E+07
50	1.24E+08	1.07E+08	8.84E+07	3.96E+06	2.59E+06	2.47E+06	6.99E+07	6.81E+07	7.85E+07
Time (min)	AL-3			AL-4					
0	3.21E+06	5.01E+06	7.82E+06	1.47E+06	7.31E+05	1.60E+05			
5	3.66E+07	3.50E+07	3.81E+07	4.64E+07	4.68E+07	4.11E+07			
10	2.87E+07	2.96E+07	2.97E+07	3.67E+07	3.80E+07	3.27E+07			
15	2.39E+07	2.58E+07	2.17E+07	2.26E+07	2.50E+07	1.83E+07			
20	1.90E+07	2.25E+07	1.68E+07	1.89E+07	2.09E+07	1.53E+07			
25	1.61E+07	2.10E+07	1.48E+07	1.49E+07	1.79E+07	1.18E+07			
30	1.47E+07	1.82E+07	1.29E+07	1.43E+07	1.60E+07	1.11E+07			
40	1.32E+07	1.64E+07	1.12E+07	1.35E+07	1.53E+07	9.57E+06			
50	9.47E+06	1.27E+07	8.83E+06	1.33E+07	1.52E+07	1.02E+07			

Table S5: Tabularized values for **Figure 6B**

Time (min)	D-luciferin			AL2			AL-3		
0	9.37E+07	2.16E+08	6.74E+08	1.02E+09	8.98E+08	9.81E+08	8.82E+07	4.17E+07	9.70E+07
5	4.96E+08	7.26E+08	7.61E+08	1.16E+09	1.19E+09	1.13E+09	1.75E+08	2.62E+08	3.26E+08
10	6.27E+08	7.11E+08	8.43E+08	1.11E+09	9.98E+08	9.78E+08	1.40E+08	2.01E+08	3.03E+08
15	6.54E+08	6.10E+08	5.02E+08	7.37E+08	8.77E+08	8.35E+08	8.97E+07	9.86E+07	2.56E+08
20	2.91E+08	5.33E+08	2.11E+08	6.64E+08	7.70E+08	7.52E+08	5.03E+07	6.08E+07	2.11E+08
25	2.35E+08	3.69E+08	2.68E+08	6.27E+08	5.19E+08	6.13E+08	4.94E+07	4.17E+07	1.65E+08
30	3.24E+08	2.16E+08	1.72E+08	5.53E+08	5.08E+08	5.43E+08	3.32E+07	2.90E+07	1.36E+08
40	1.55E+08	1.93E+08	8.64E+07	4.15E+08	4.65E+08	4.45E+08	2.29E+07	2.06E+07	1.01E+08
50	1.87E+08	1.27E+08	6.42E+07	2.89E+08	3.16E+08	2.91E+08	2.77E+07	9.44E+06	6.78E+07
60	1.76E+08	7.53E+07	4.58E+07	2.40E+08	2.19E+08	2.23E+08	1.81E+07	6.35E+06	1.03E+07

Time (min)	AL-4		
0	3.99E+07	9.56E+06	7.93E+06
5	4.12E+07	1.44E+07	1.01E+07
10	4.44E+07	1.44E+07	6.46E+06
15	2.10E+07	1.11E+07	4.85E+06
20	1.72E+07	9.68E+06	4.44E+06
25	2.08E+07	6.26E+06	4.27E+06
30	2.10E+07	3.78E+06	4.11E+06
40	1.73E+07	1.23E+06	3.47E+06
50	1.29E+07	2.97E+06	3.21E+06
60	9.79E+06	3.19E+06	3.04E+06

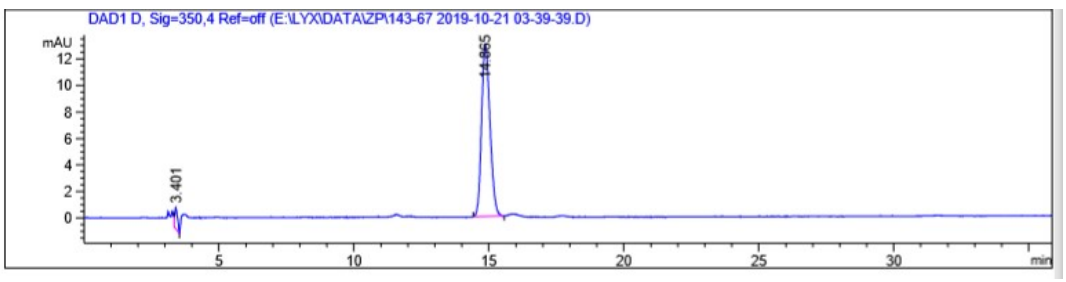
Table S6: Tabularized values for **Figure 6C**

Photon Flux (photons s-1)	AL2			D-luciferin		
1.5E+09	1.16E+09	1.19E+09	1.13E+09	4.96E+08	7.26E+08	7.61E+08

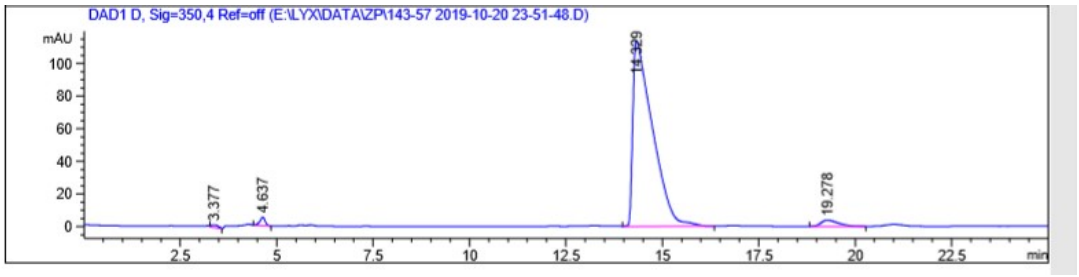
NMR, ESI-HRMS and HPLC spectra

HPLC spectra

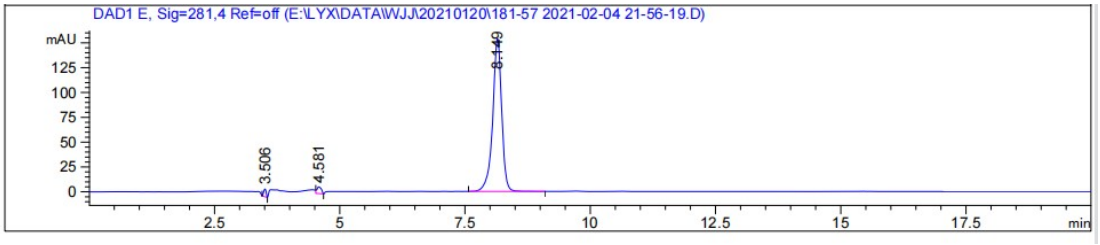
AL1



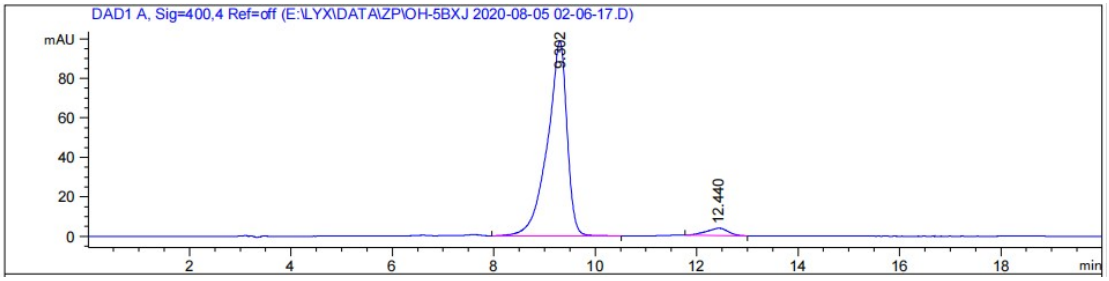
AL2



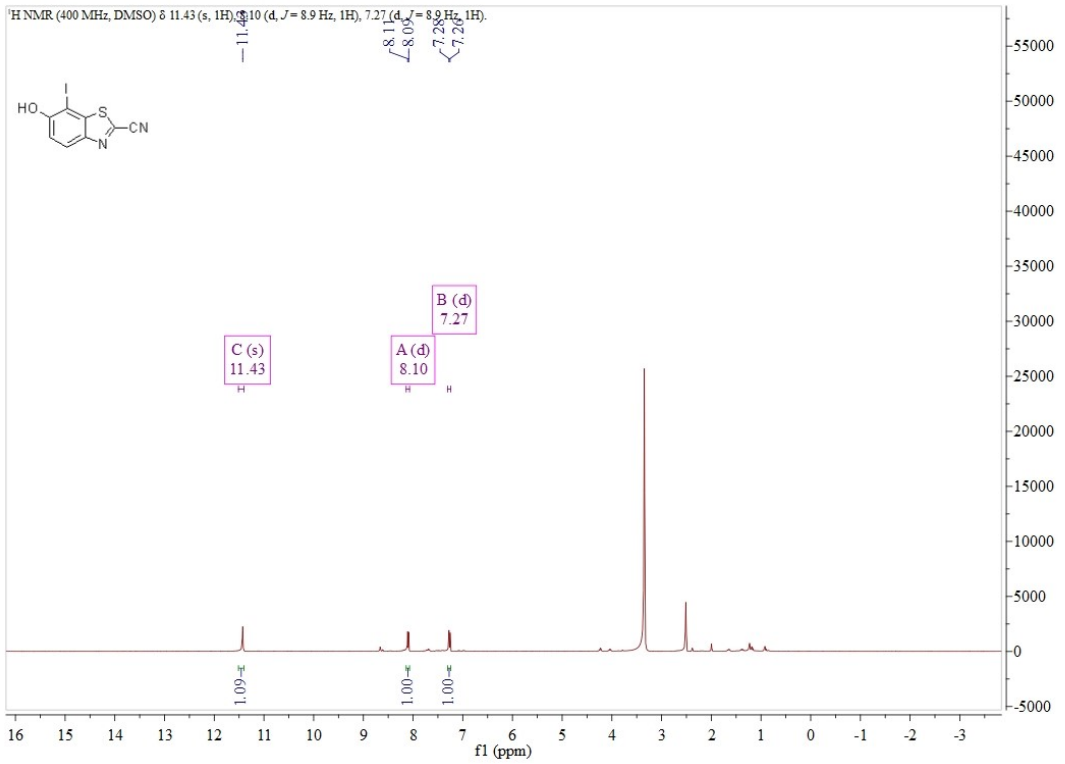
AL3

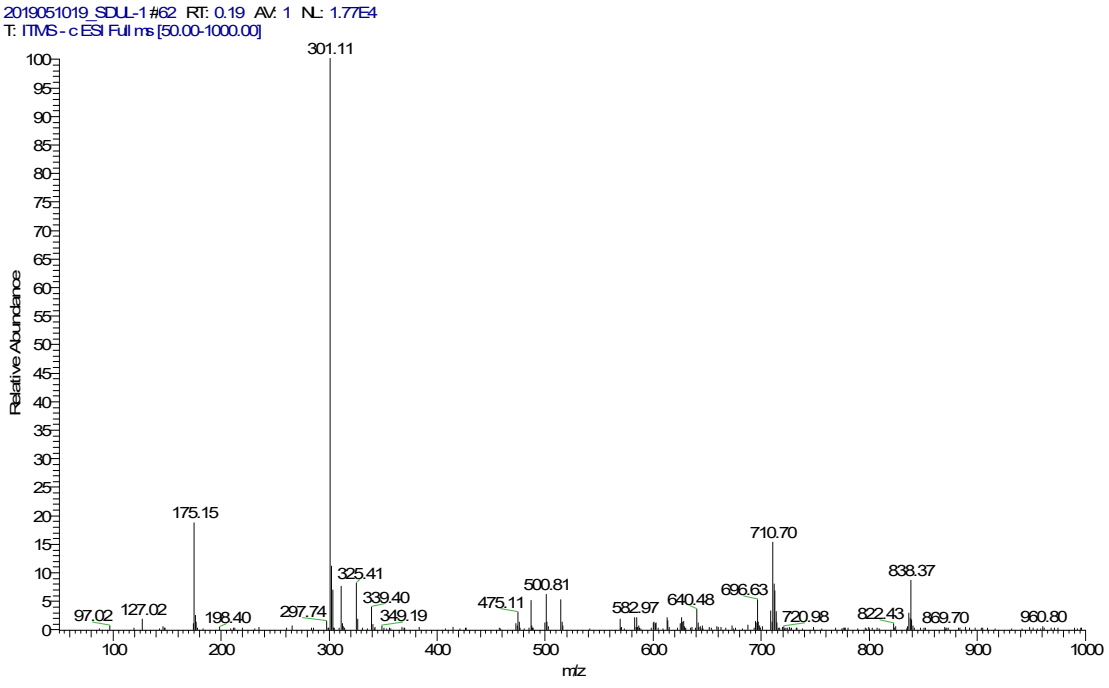


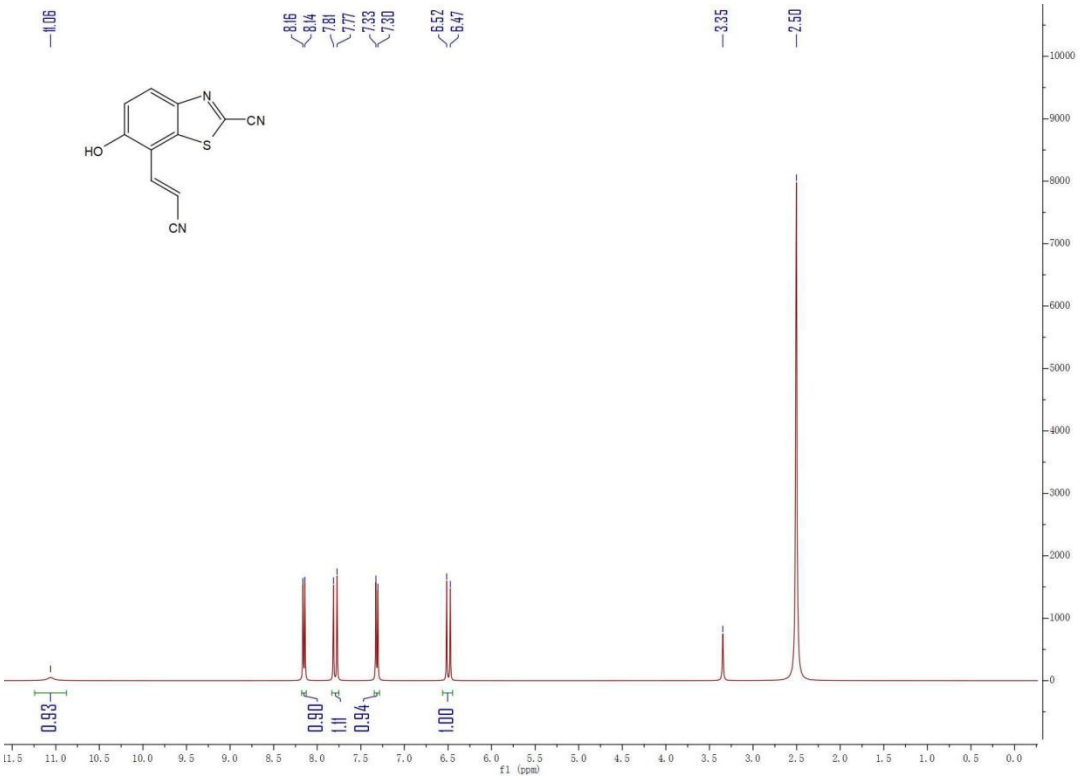
AL4



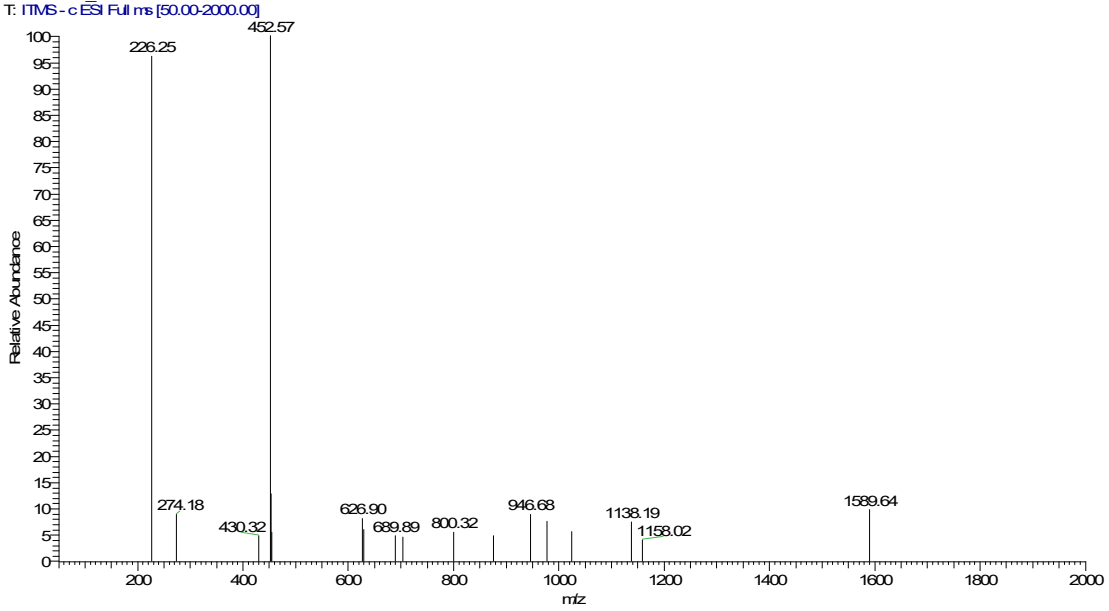
NMR and ESI-HRMS spectra

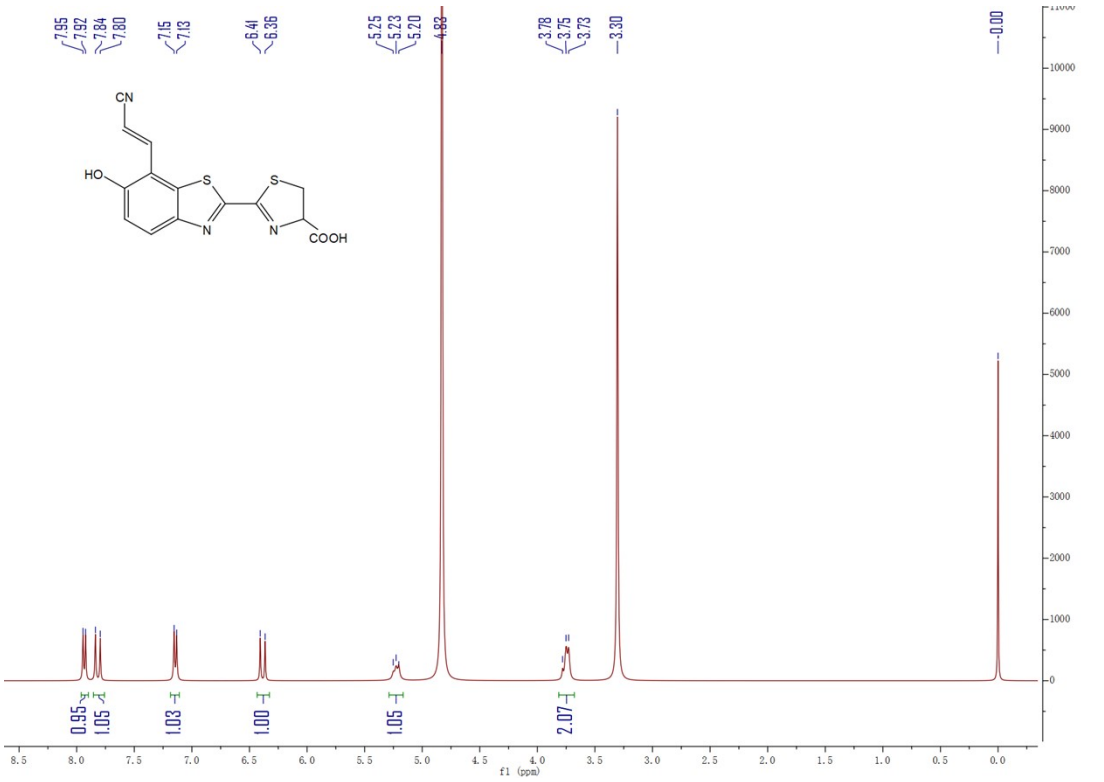

¹H NMR (400 MHz, DMSO) δ 11.43 (s, 1H), 8.10 (d, J = 8.9 Hz, 1H), 7.27 (d, J = 8.9 Hz, 1H).
11.43
8.11
8.09
7.28
7.26
HO
I
S
CN
N
B (d)
7.27
C (s)
11.43
A (d)
8.10
1.09
1.00
1.00
f1 (ppm)

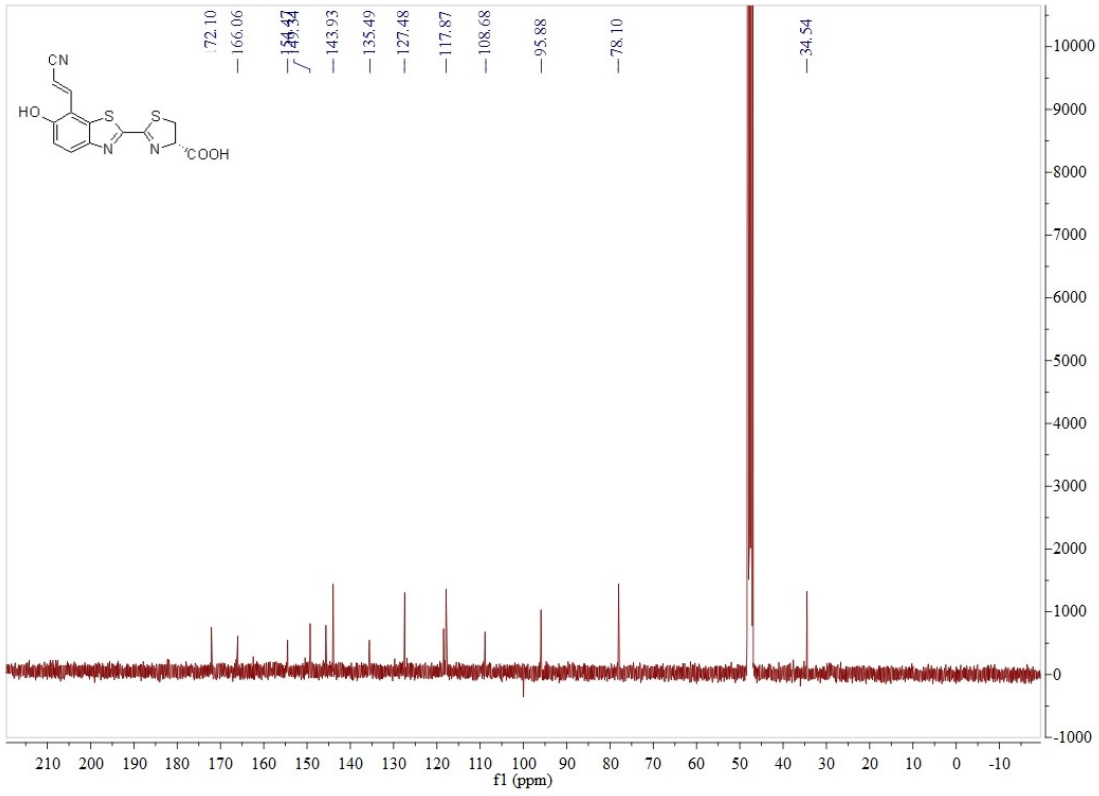

2019051019_SDUL-1 #62 RT: 0.19 AV: 1 NL: 1.77E4
T: ITMS - c ESI Full ms [50.00-1000.00]
301.11
175.15
325.41
339.40
500.81
710.70
838.37
97.02
127.02
198.40
297.74
349.19
475.11
582.97
640.48
696.63
720.98
822.43
869.70
960.80
Relative Abundance
m/z

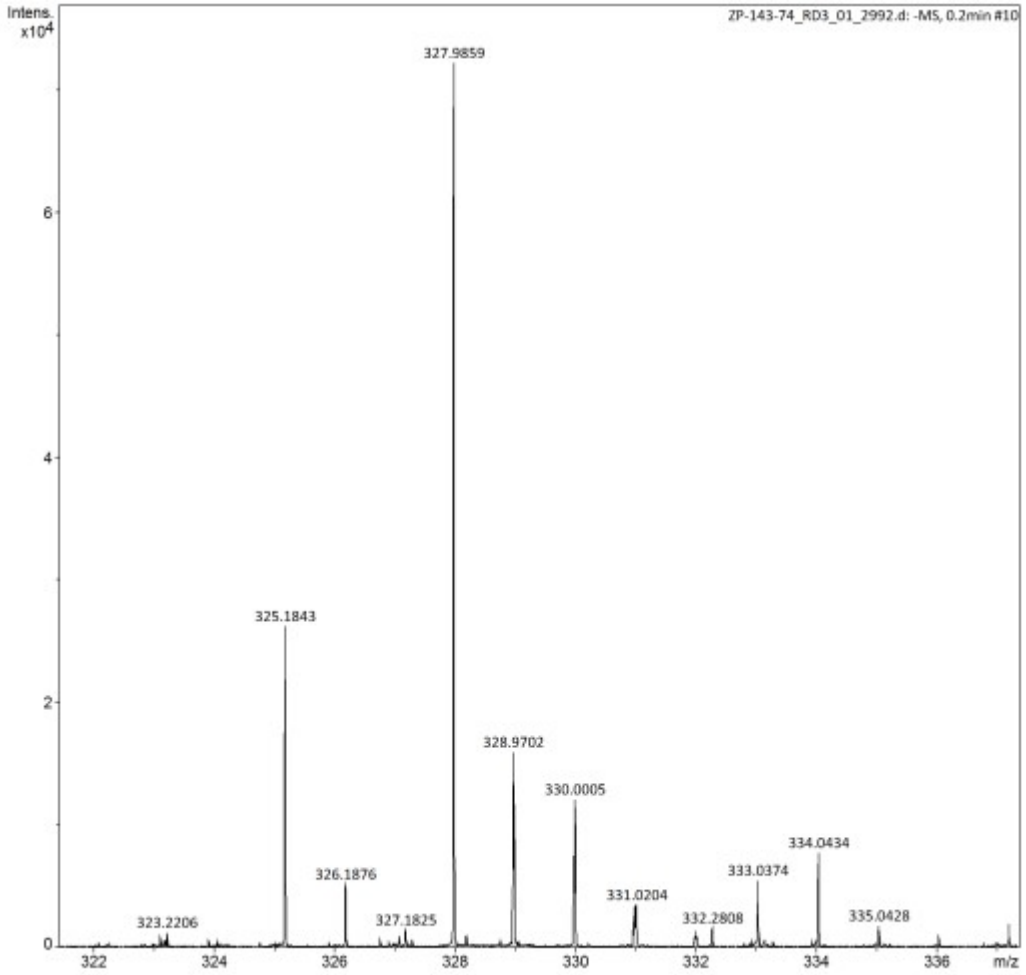


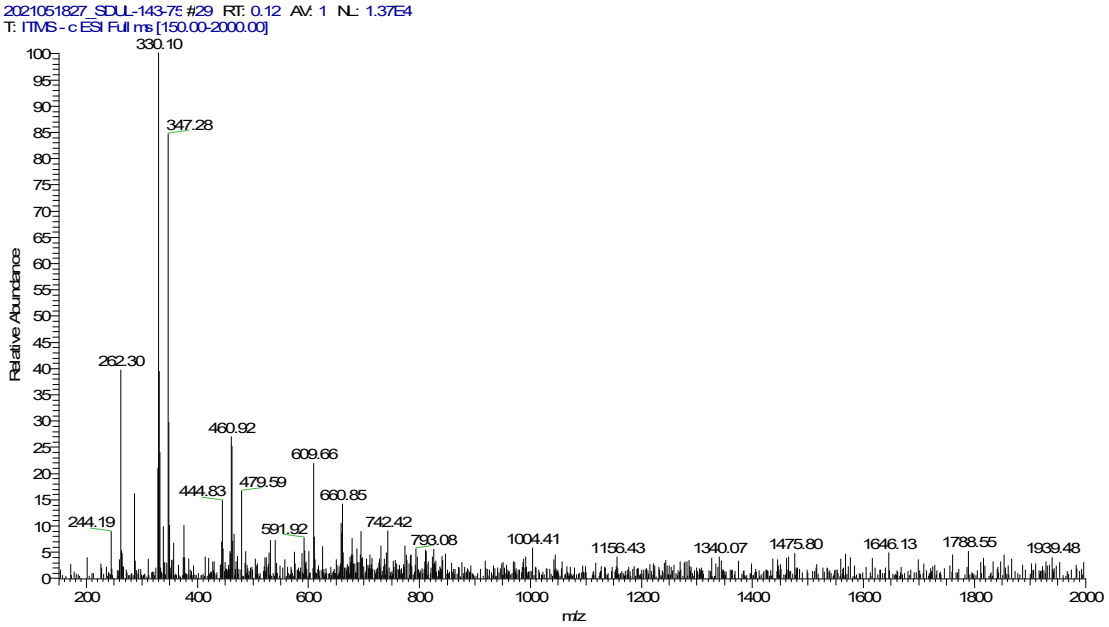
2021030921_SDLL-143-74 #99 RT: 0.43 AV: 1 NL: 3.22E2
T: ITMS - c ESI Full ms [50.00-2000.00]

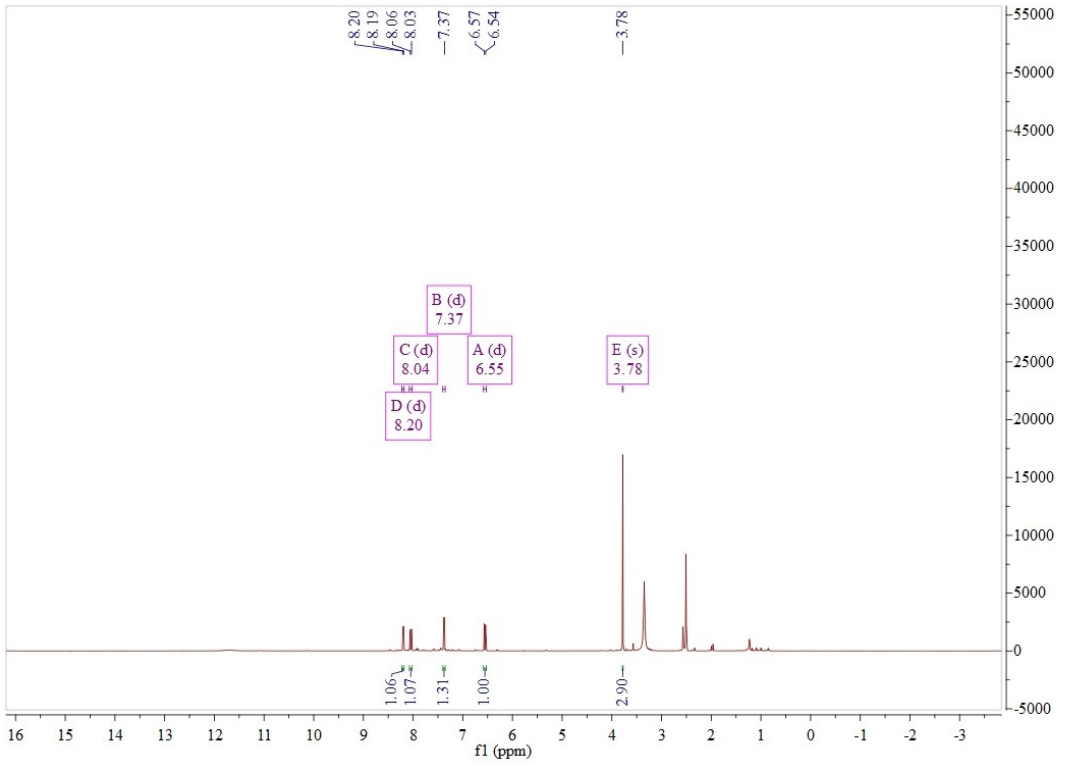


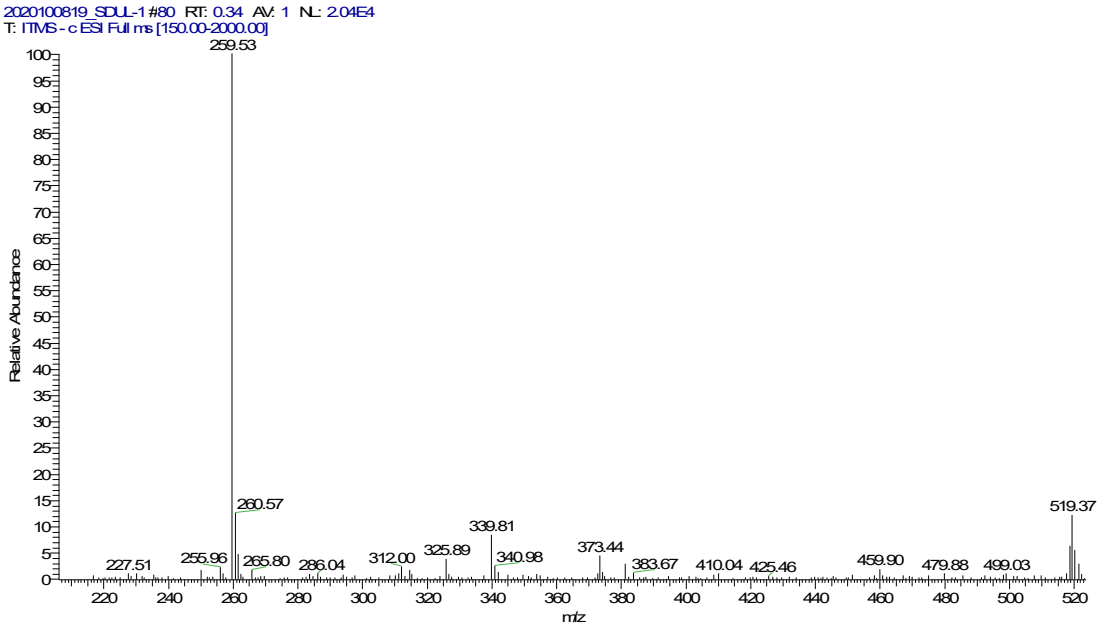

7.95
7.92
7.84
7.80
7.15
7.13
6.41
6.36
5.25
5.23
5.20
4.88
3.78
3.75
3.73
3.30
0.00
CN
HO
S
S
N
N
COOH
0.95
1.05
1.03
1.00
1.05
2.07
f1 (ppm)

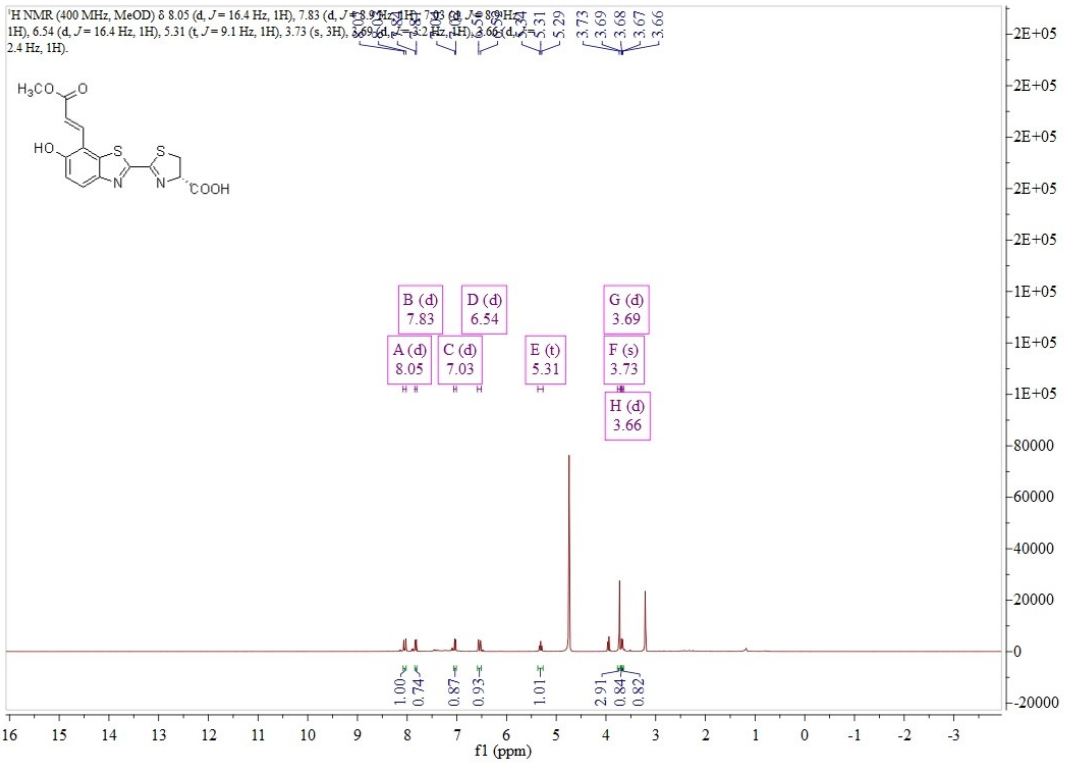

172.10
166.06
154.47
154.34
143.93
135.49
127.48
117.87
108.68
95.88
78.10
34.54
CN
HO
S
S
N
N
COOH
f1 (ppm)

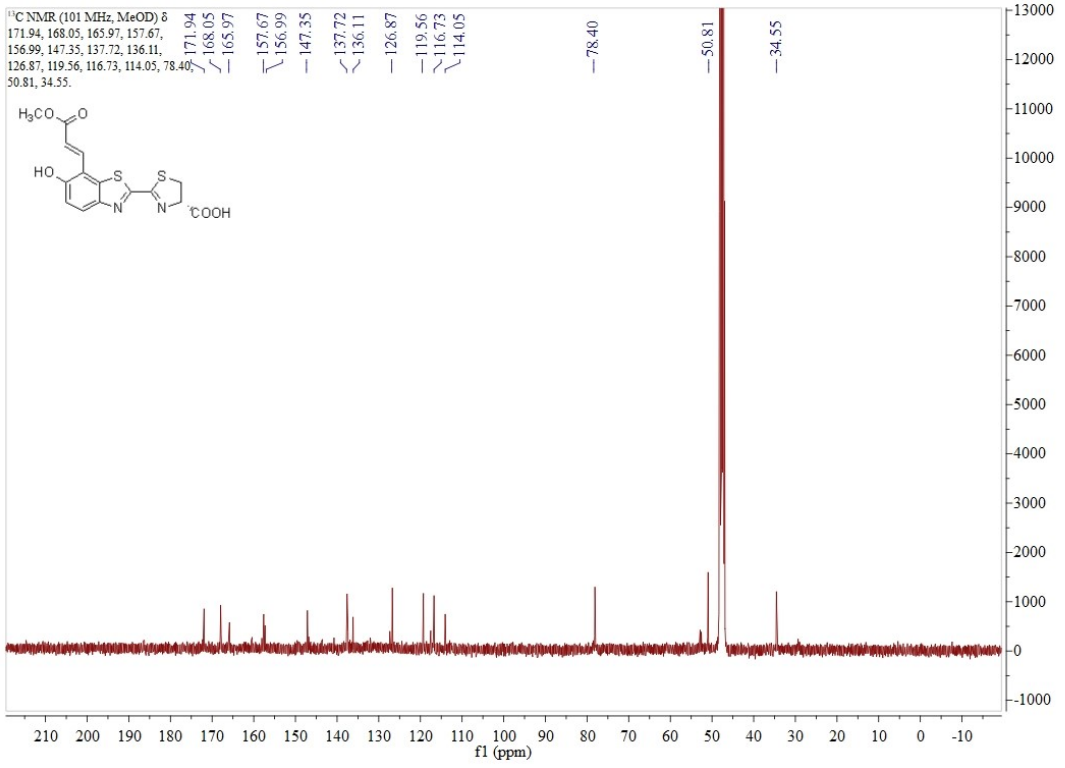

Intens.
x10^4
ZP-143-74_RD3_01_2992.d: -MS, 0.2min #10
327.9859
325.1843
328.9702
330.0005
326.1876
334.0434
333.0374
331.0204
323.2206
327.1825
332.2808
335.0428
m/z

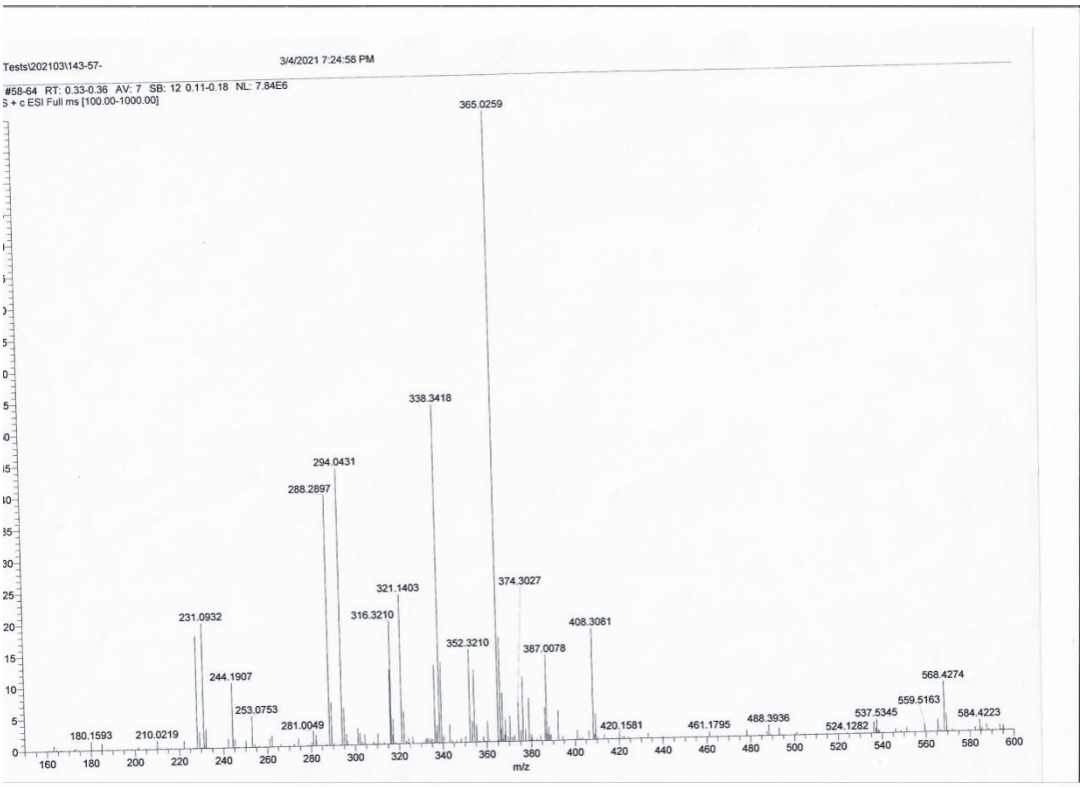

2021051827_SDUL-143-75 #29 RT: 0.12 AV: 1 NL: 1.37E4
T: ITMS - c ESI Full ms [150.00-2000.00]
330.10
347.28
262.30
460.92
609.66
444.83
479.59
660.85
244.19
591.92
742.42
793.08
1004.41
1156.43
1340.07
1475.80
1646.13
1788.55
1939.48
Relative Abundance
m/z

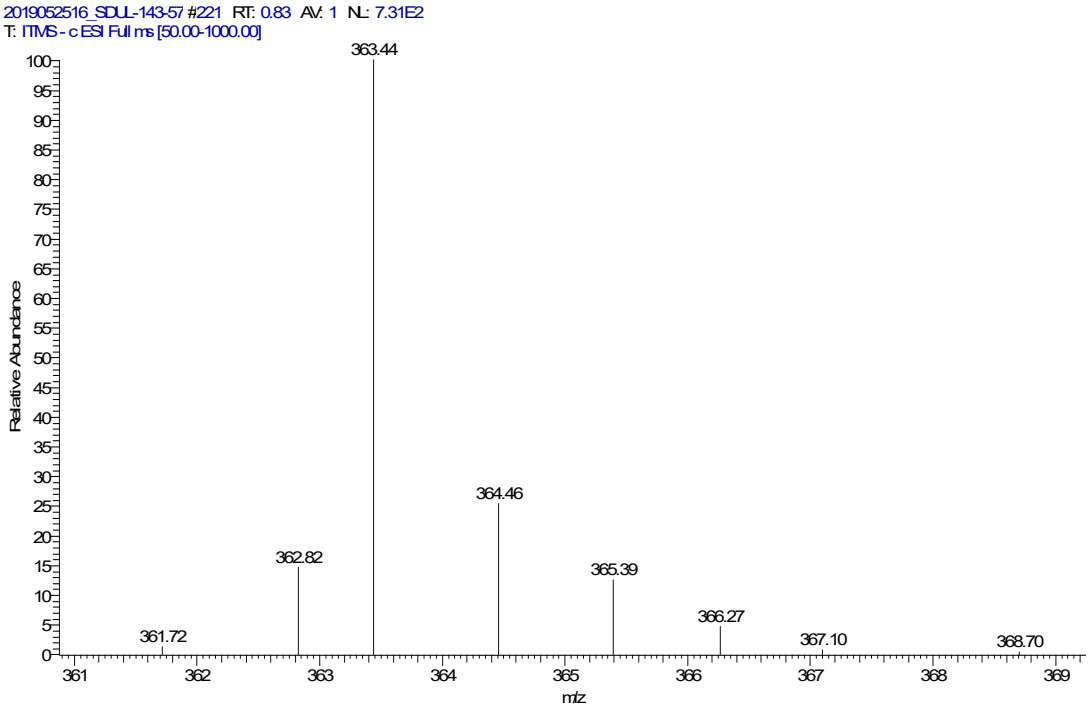

8.20
8.19
8.06
8.03
7.37
6.57
6.54
3.78
B (d)
7.37
C (d)
8.04
A (d)
6.55
E (s)
3.78
D (d)
8.20
1.06
1.07
1.31
1.00
2.90
f1 (ppm)

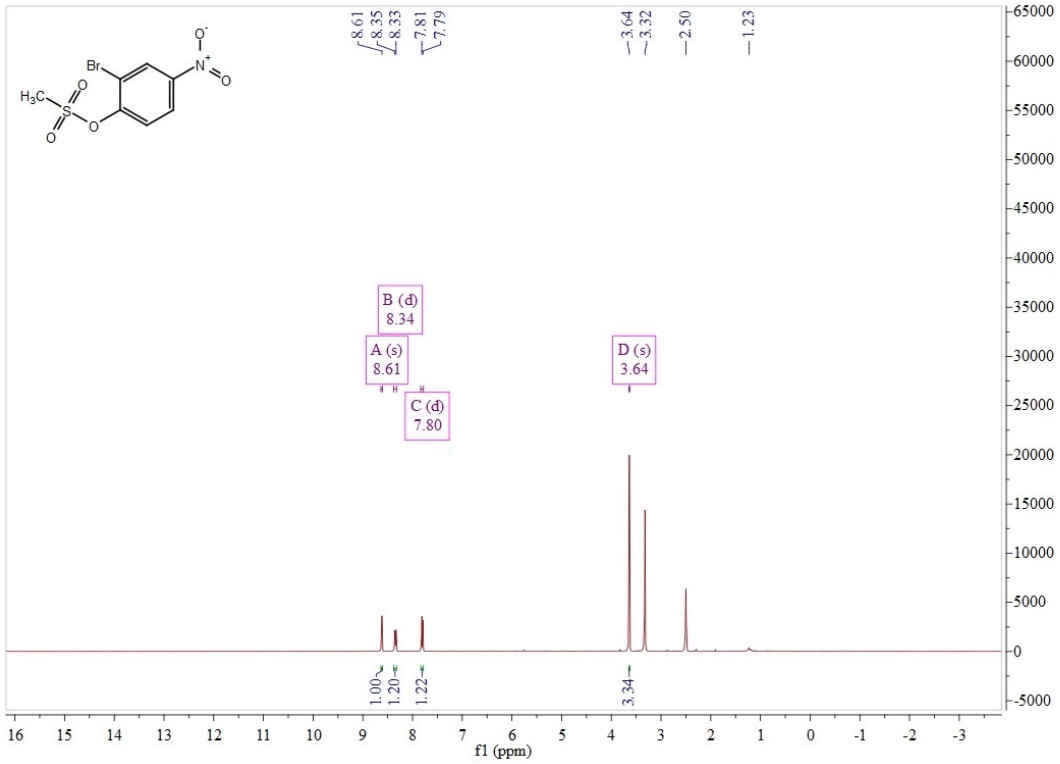

2020100819_SDLL-1 #80 RT: 0.34 AV: 1 NL: 2.04E4
T: ITMS - c ESI Full ms [150.00-2000.00]
Relative Abundance
m/z
259.53
260.57
339.81
519.37
227.51
255.96
265.80
286.04
312.00
325.89
340.98
373.44
383.67
410.04
425.46
459.90
479.88
499.03

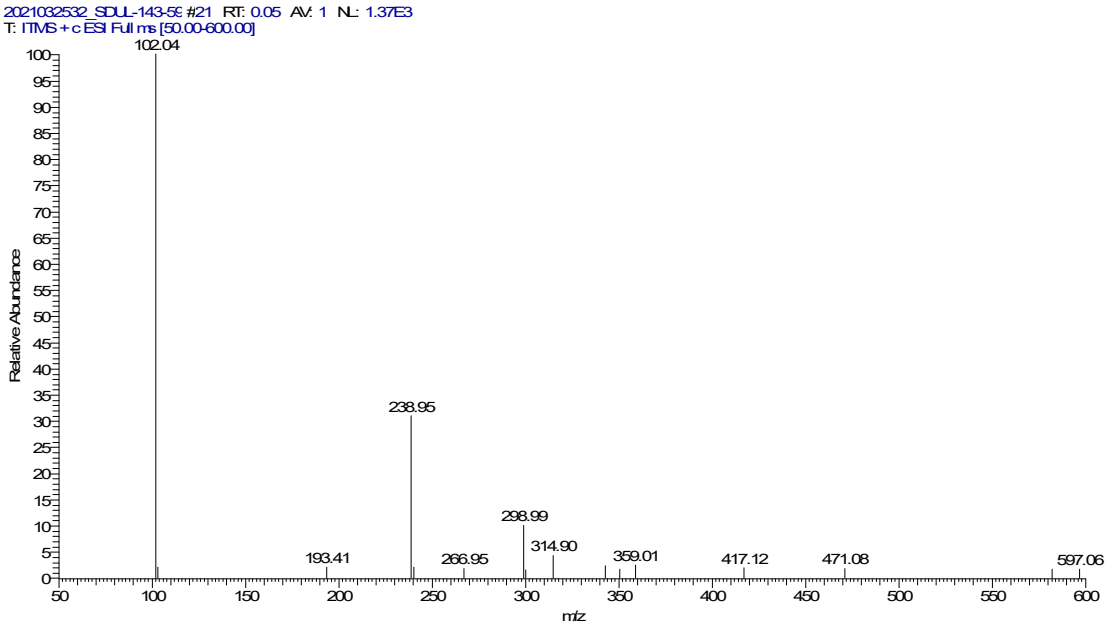

B (d) 7.83
D (d) 6.54
G (d) 3.69
A (d) 8.05
C (d) 7.03
E (t) 5.31
F (s) 3.73
H (d) 3.66
f1 (ppm)

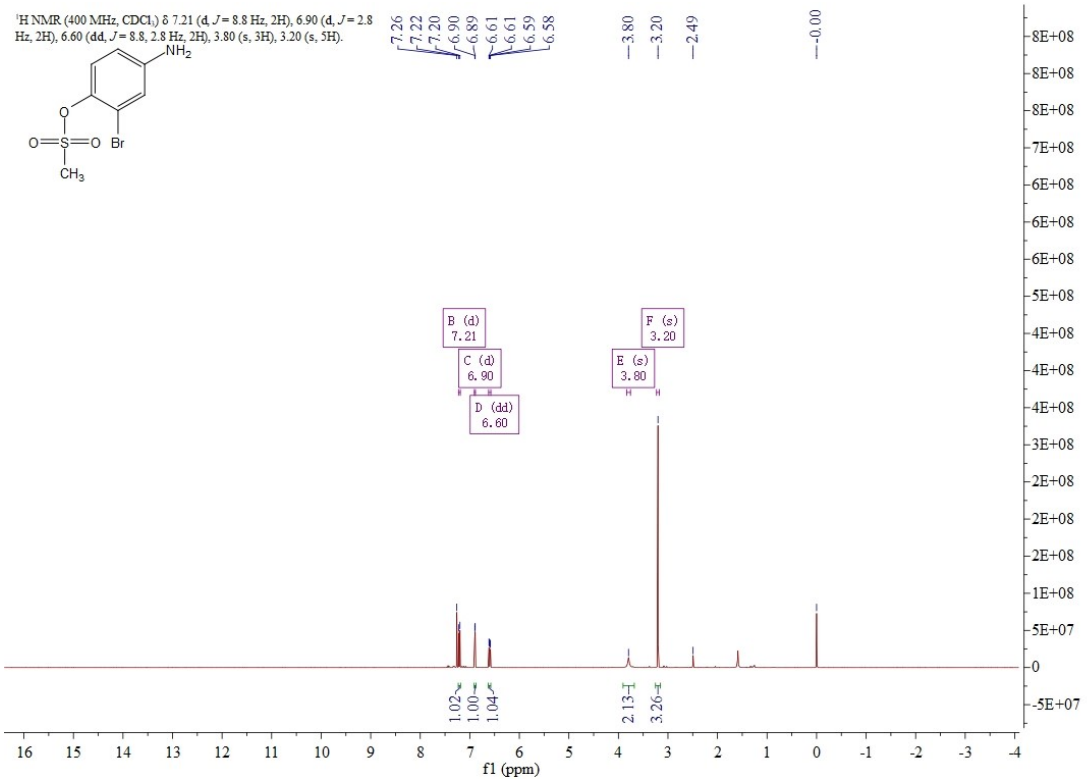

171.94
168.05
165.97
157.67
156.99
147.35
137.72
136.11
126.87
119.56
116.73
114.05
78.40
50.81
34.55
f1 (ppm)

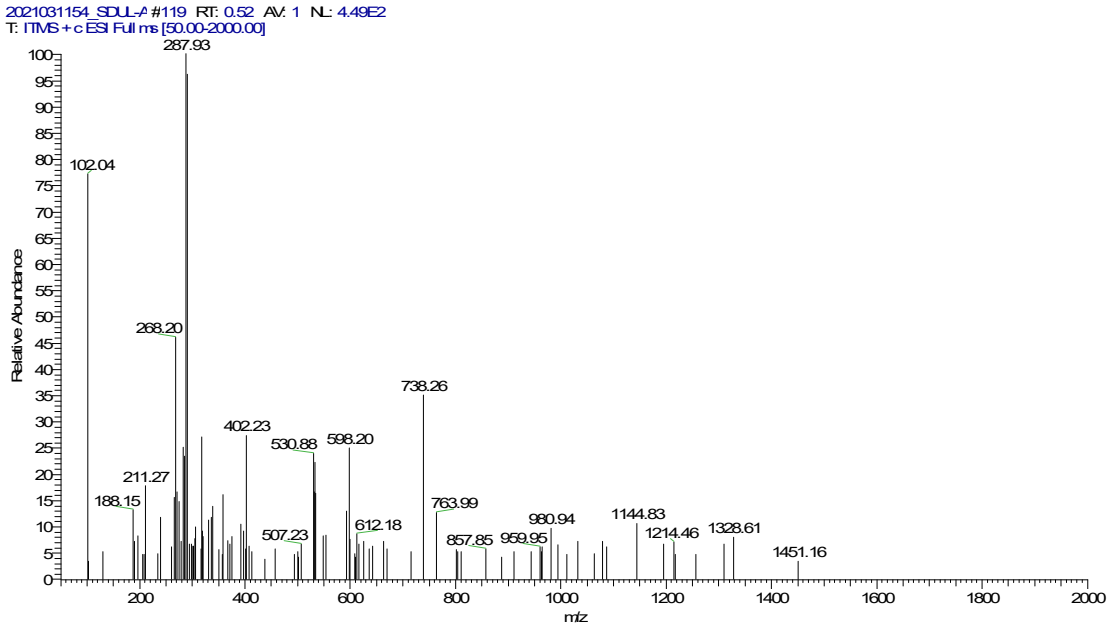

Tests\202103\143-57-
3/4/2021 7:24:58 PM
#58-64 RT: 0.33-0.36 AV: 7 SB: 12 0.11-0.18 NL: 7.84E6
S + c ESI Full ms [100.00-1000.00]
365.0259
338.3418
294.0431
288.2897
374.3027
321.1403
316.3210
231.0932
408.3081
352.3210
387.0078
244.1907
568.4274
559.5163
584.4223
537.5345
253.0753
281.0049
420.1581
461.1795
488.3936
524.1282
180.1593
210.0219
m/z

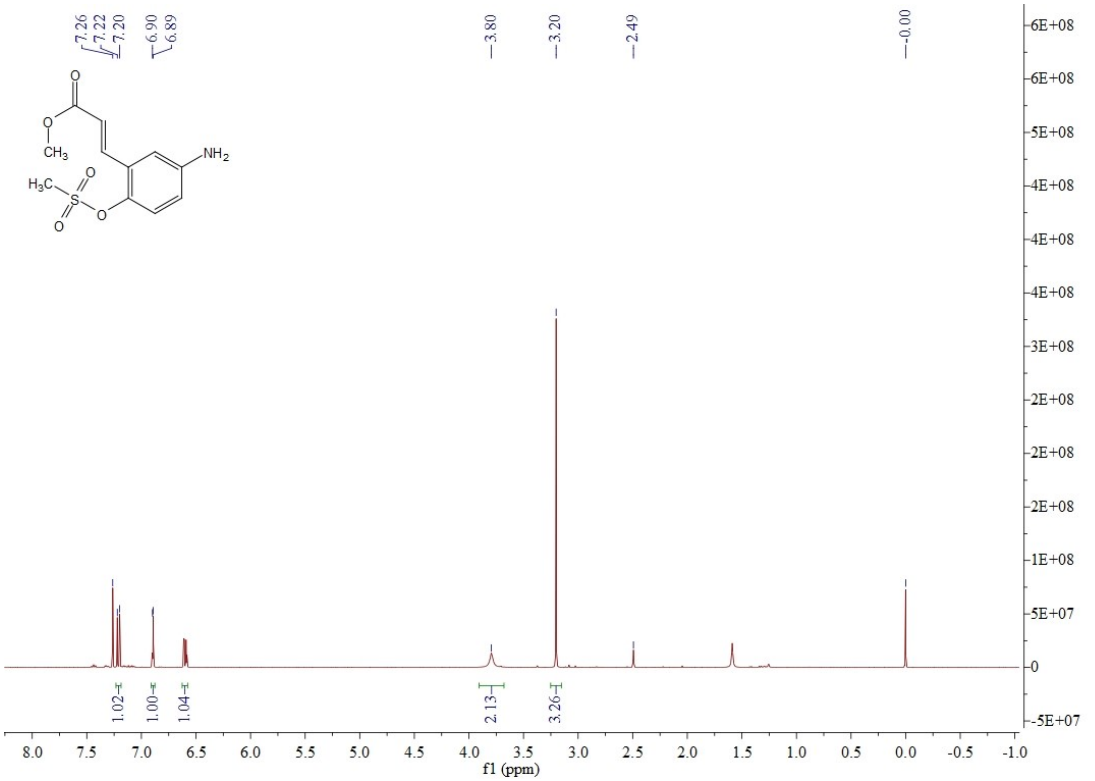

2019052516_SDUL-143-57 #221 RT: 0.83 AV: 1 NL: 7.31E2
T: ITMS - c ESI Full ms [50.00-1000.00]
363.44
364.46
362.82
365.39
366.27
361.72
367.10
368.70
Relative Abundance
m/z

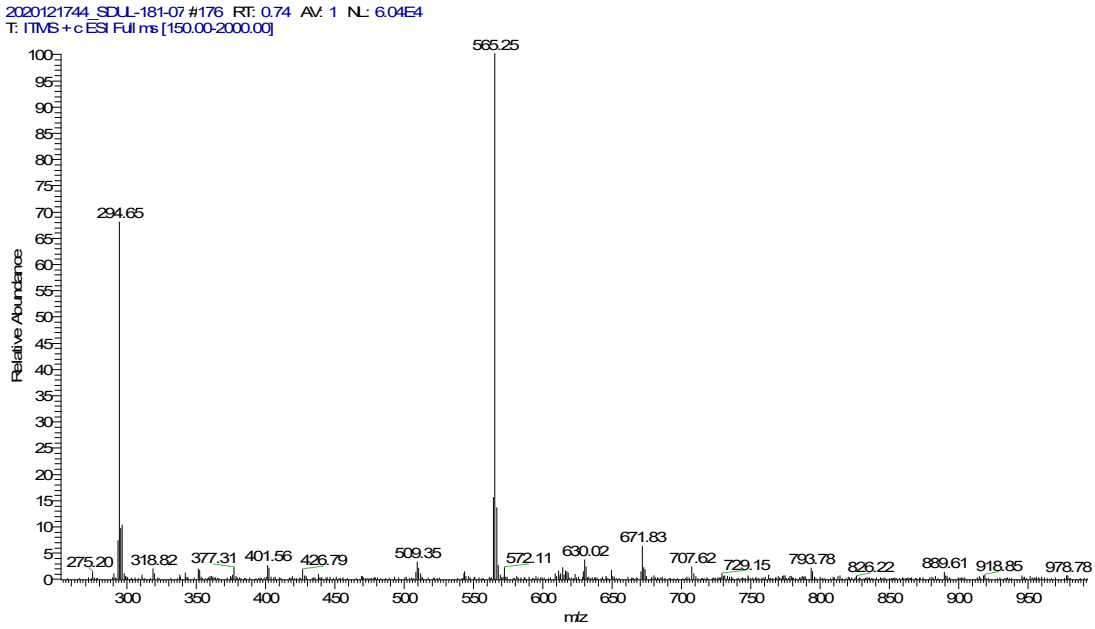

8.61
8.35
8.33
7.81
7.79
3.64
3.32
2.50
1.23
B (d)
8.34
A (s)
8.61
C (d)
7.80
D (s)
3.64
1.00
1.20
1.22
3.34
f1 (ppm)

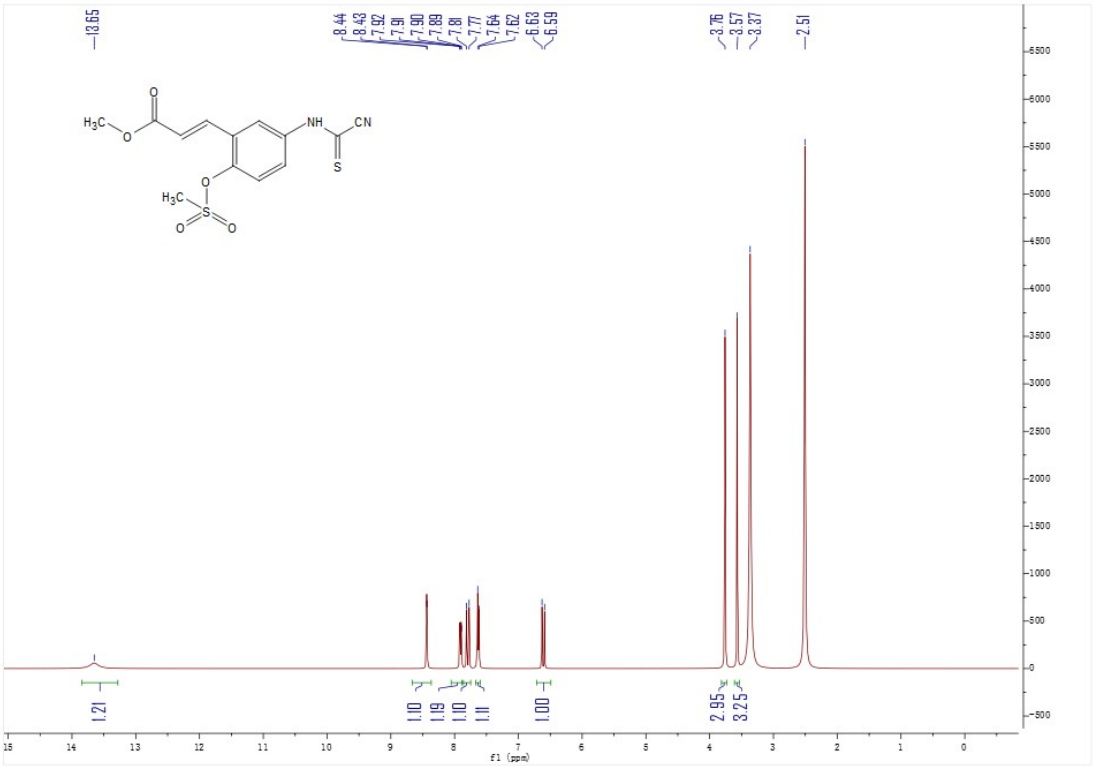

2021032532_SDUL-143-5 #21 RT: 0.05 AV: 1 NL: 1.37E3
T: ITMS + c ESI Full ms [50.00-600.00]
102.04
238.95
298.99
314.90
193.41
266.95
359.01
417.12
471.08
597.06
Relative Abundance
m/z

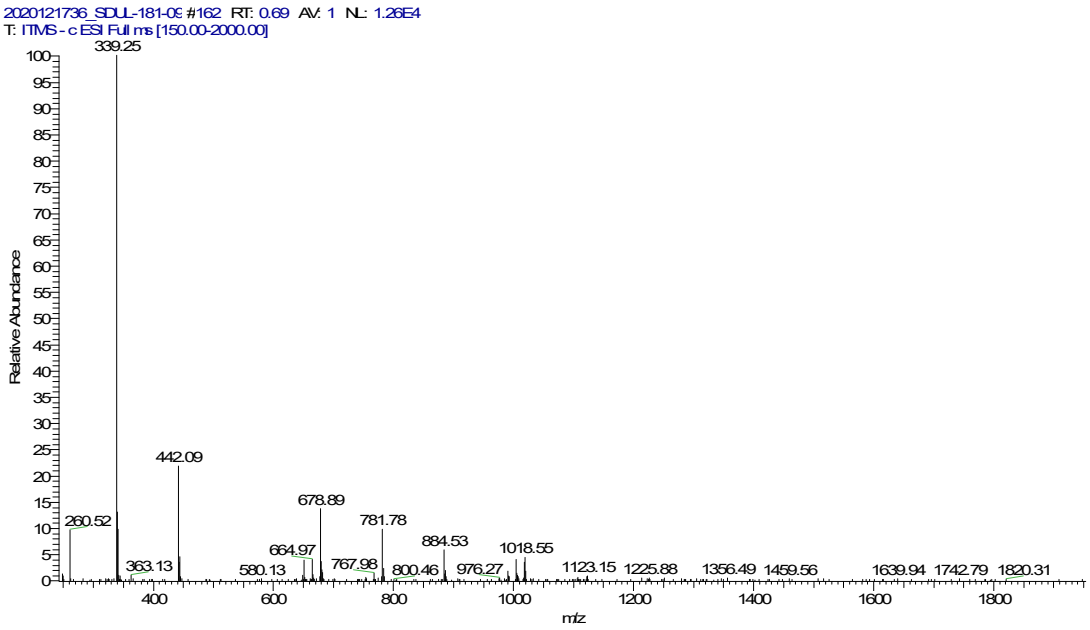

¹H NMR (400 MHz, CDCl₃) δ 7.21 (d, J = 8.8 Hz, 2H), 6.90 (d, J = 2.8 Hz, 2H), 6.60 (dd, J = 8.8, 2.8 Hz, 2H), 3.80 (s, 3H), 3.20 (s, 5H).
NH2
O
O=S=O
Br
CH3
7.26
7.22
7.20
6.90
6.89
6.61
6.61
6.59
6.58
3.80
3.20
2.49
0.00
B (d) 7.21
C (d) 6.90
D (dd) 6.60
F (s) 3.20
E (s) 3.80
1.02
1.00
1.04
2.13
3.26
f1 (ppm)

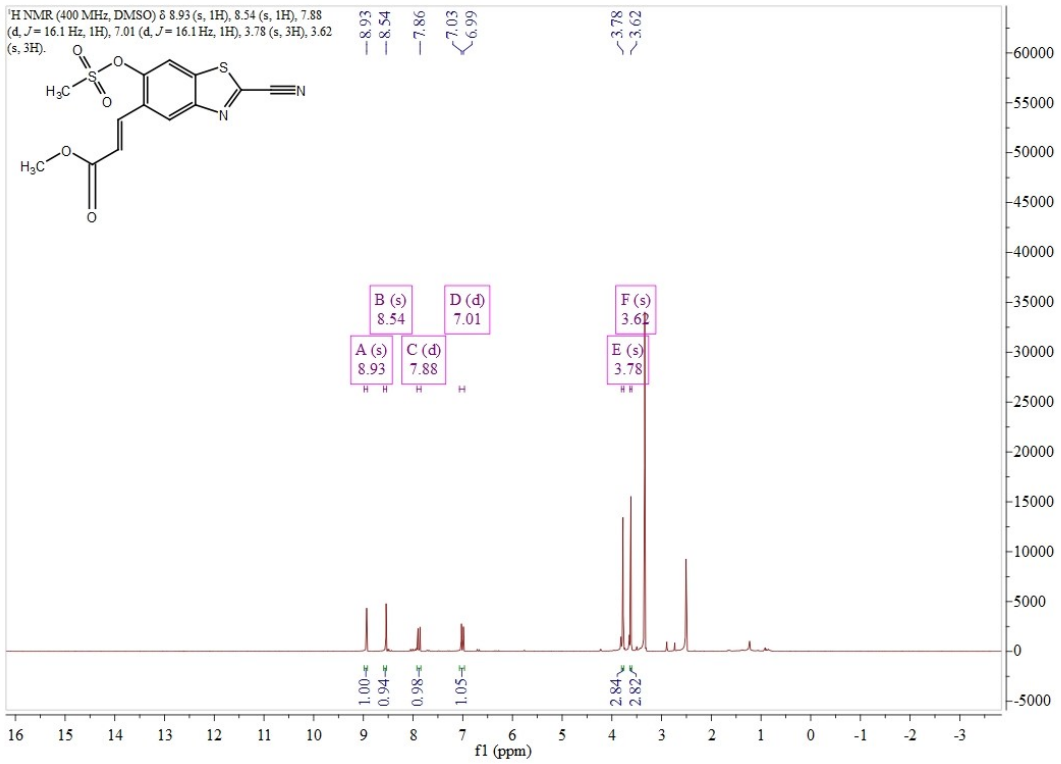

20210311154_SDUL-A #119 RT: 0.52 AV: 1 NL: 4.49E2
T: ITMS + c ESI Full ms [50.00-2000.00]
Relative Abundance
m/z
287.93
102.04
268.20
738.26
402.23
530.88
598.20
211.27
188.15
763.99
980.94
1144.83
1214.46
1328.61
507.23
612.18
857.85
959.95
1451.16

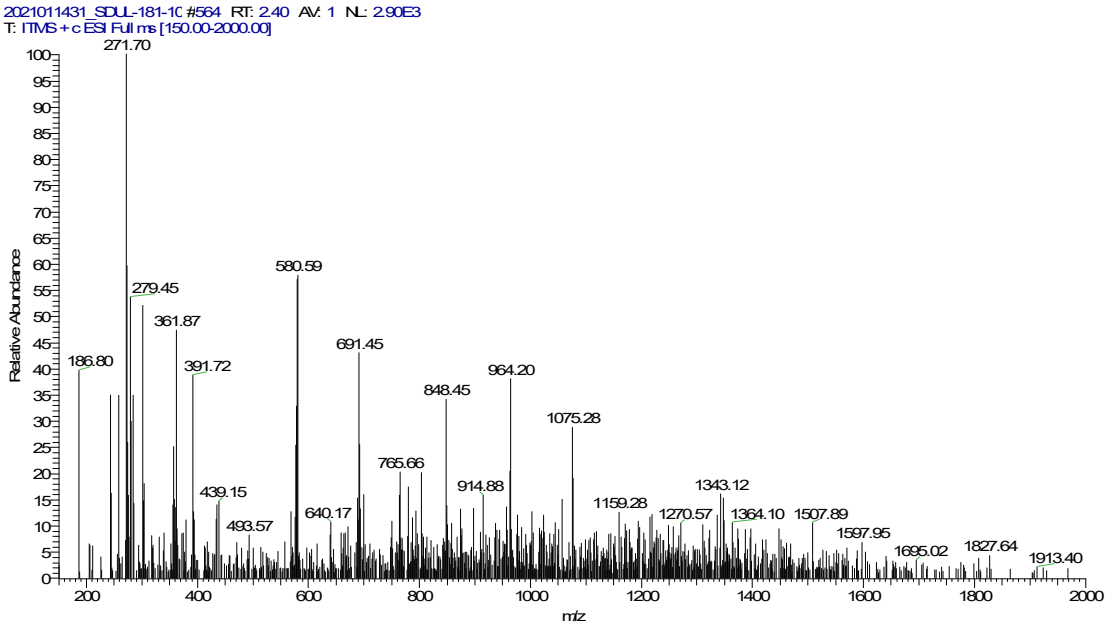

7.26
7.22
7.20
6.90
6.89
3.80
3.20
2.49
0.00
O
O
CH3
NH2
H3C
S
O
O
O
1.02
1.00
1.04
2.13
3.26
f1 (ppm)

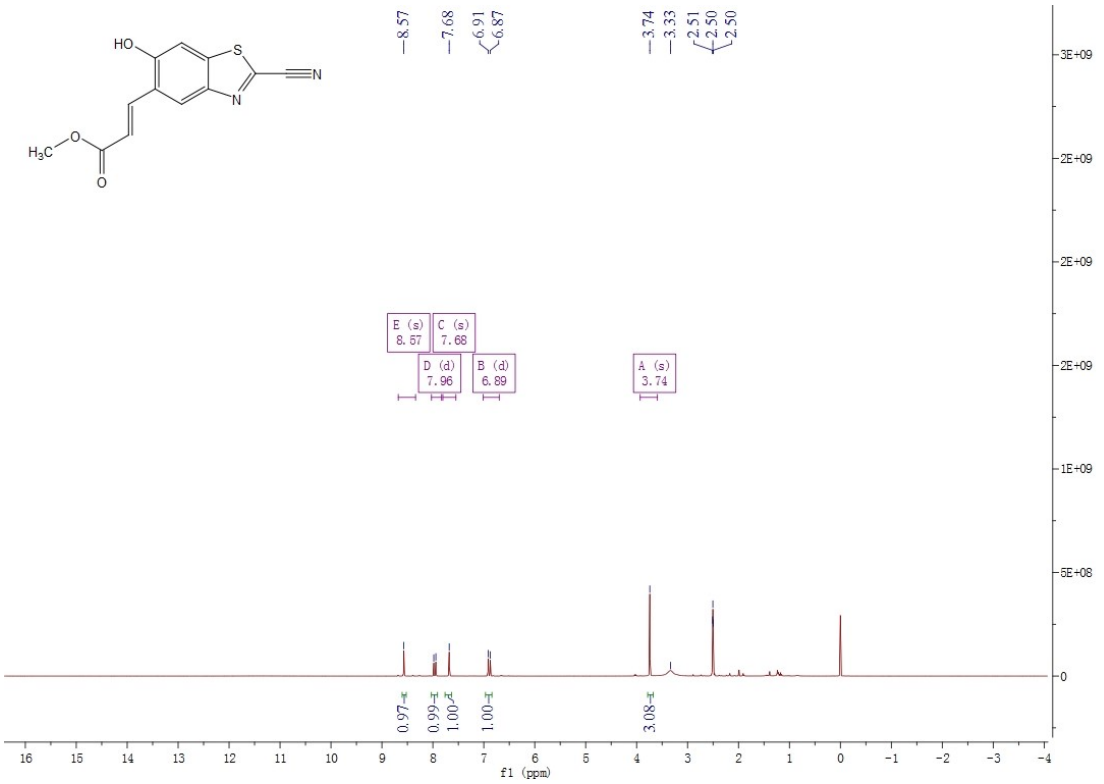

2020121744_SDUL-181-07 #176 RT: 0.74 AV: 1 NL: 6.04E4
T: ITMS + c ESI Full ms [150.00-2000.00]
565.25
294.65
Relative Abundance
275.20
318.82
377.31
401.56
426.79
509.35
572.11
630.02
671.83
707.62
729.15
793.78
826.22
889.61
918.85
978.78
m/z

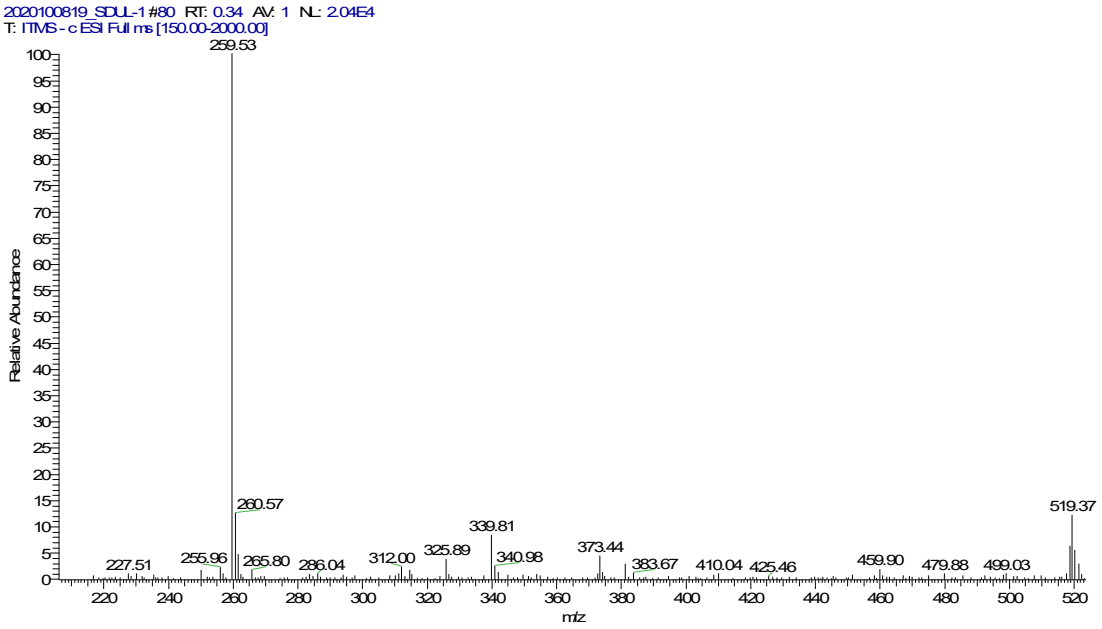

13.65
8.44
8.43
7.92
7.91
7.90
7.89
7.81
7.77
7.64
7.62
6.63
6.59
3.76
3.57
3.37
2.51
1.21
1.10
1.19
1.10
1.11
1.00
2.95
3.25
f1 (ppm)

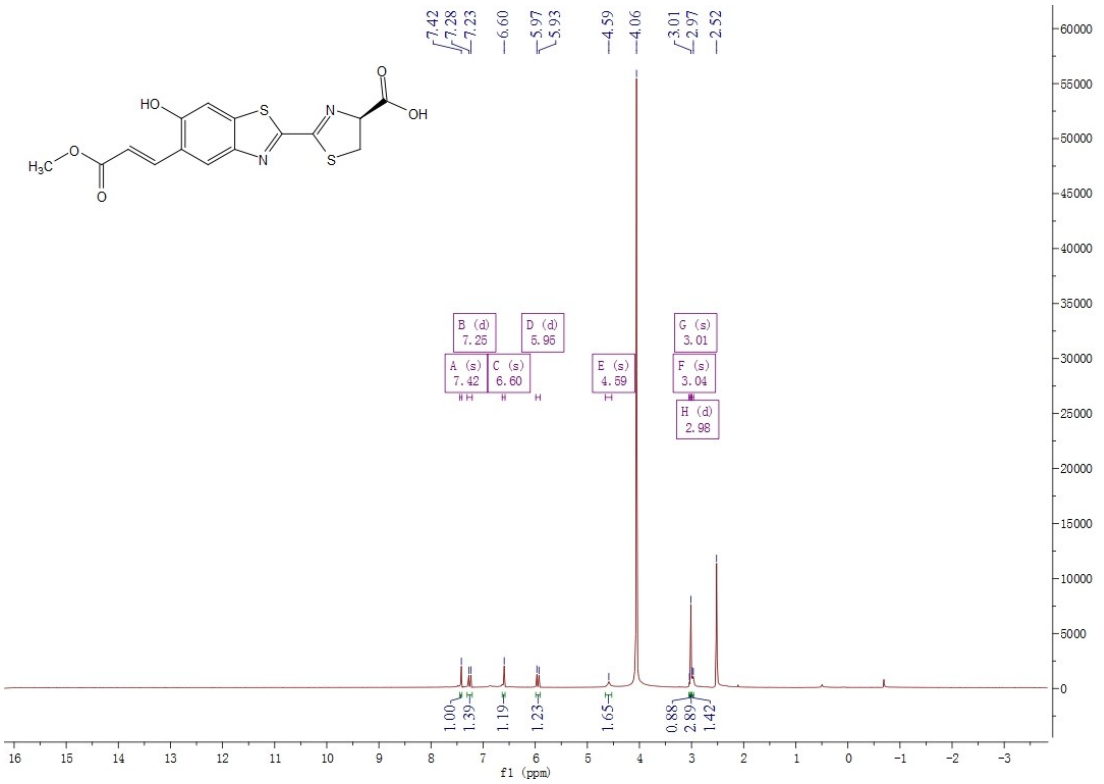

2020121736_SDUL-181-0 #162 RT: 0.69 AV: 1 NL: 1.26E4
T: ITMS - c ESI Full ms [150.00-2000.00]
Relative Abundance
m/z
339.25
442.09
678.89
781.78
884.53
1018.55
260.52
363.13
580.13
664.97
767.98
800.46
976.27
1123.15
1225.88
1356.49
1459.56
1639.94
1742.79
1820.31

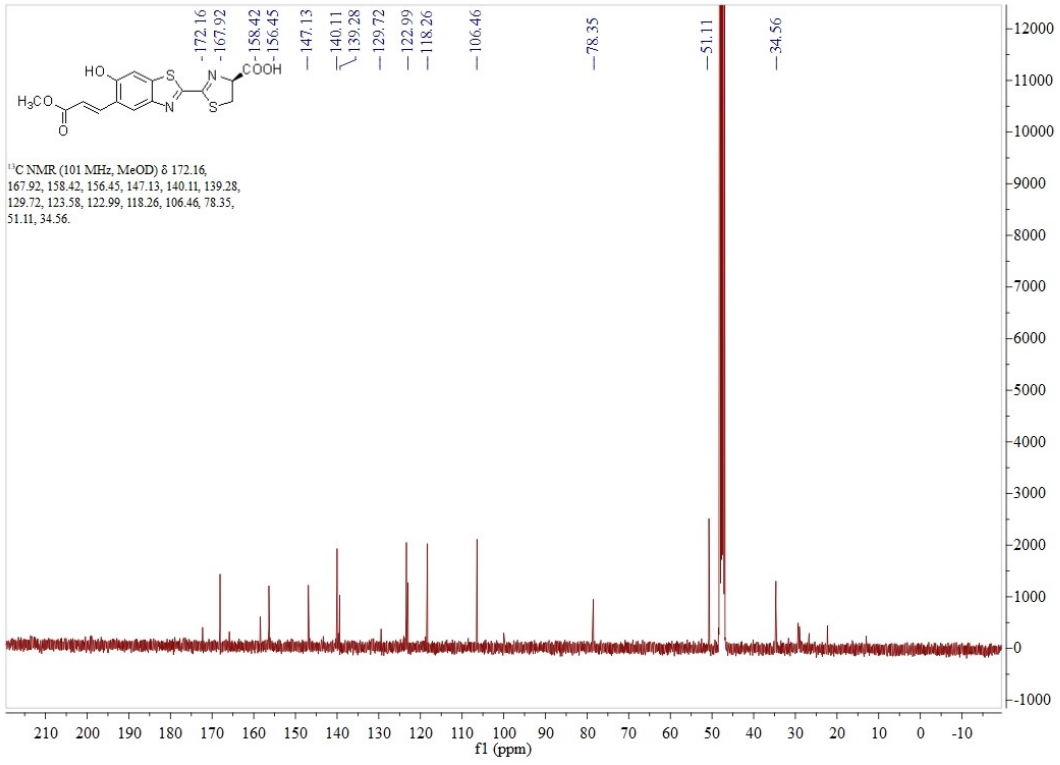

¹H NMR (400 MHz, DMSO) δ 8.93 (s, 1H), 8.54 (s, 1H), 7.88 (d, J = 16.1 Hz, 1H), 7.01 (d, J = 16.1 Hz, 1H), 3.78 (s, 3H), 3.62 (s, 3H).
8.93
8.54
7.86
7.03
6.99
3.78
3.62
B (s) 8.54
D (d) 7.01
F (s) 3.62
A (s) 8.93
C (d) 7.88
E (s) 3.78
1.00
0.94
0.98
1.05
2.84
2.82
f1 (ppm)

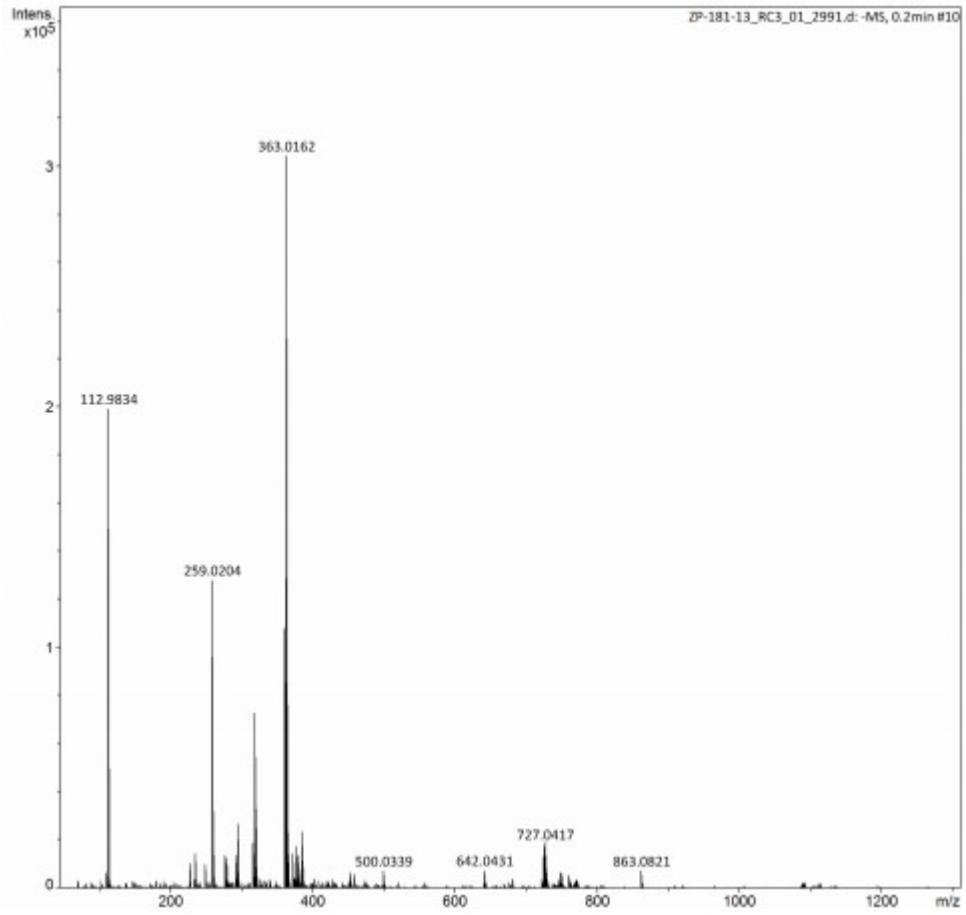

2021011431_SDUL-181-1C #564 RT: 2.40 AV: 1 NL: 2.90E3
T: ITMS + c ESI Full ms [150.00-2000.00]
Relative Abundance
m/z
271.70
279.45
361.87
391.72
186.80
439.15
493.57
580.59
640.17
691.45
765.66
848.45
914.88
964.20
1075.28
1159.28
1270.57
1343.12
1364.10
1507.89
1597.95
1695.02
1827.64
1913.40

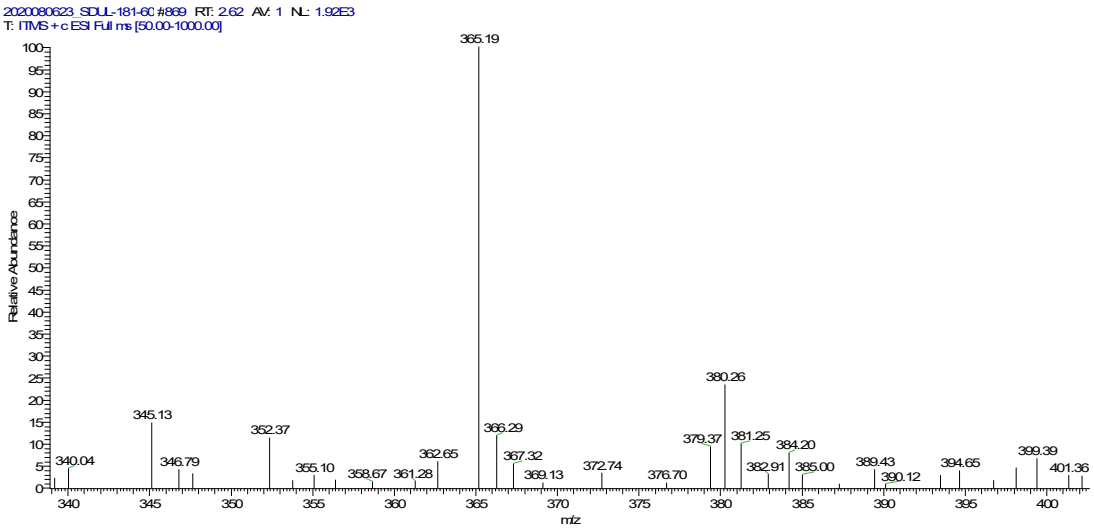

HO
S
N
N
O
H3C
O
8.57
7.68
6.91
6.87
3.74
3.33
2.51
2.50
2.50
E (s) 8.57
C (s) 7.68
D (d) 7.96
B (d) 6.89
A (s) 3.74
0.97
0.99
1.00
1.00
3.08
f1 (ppm)

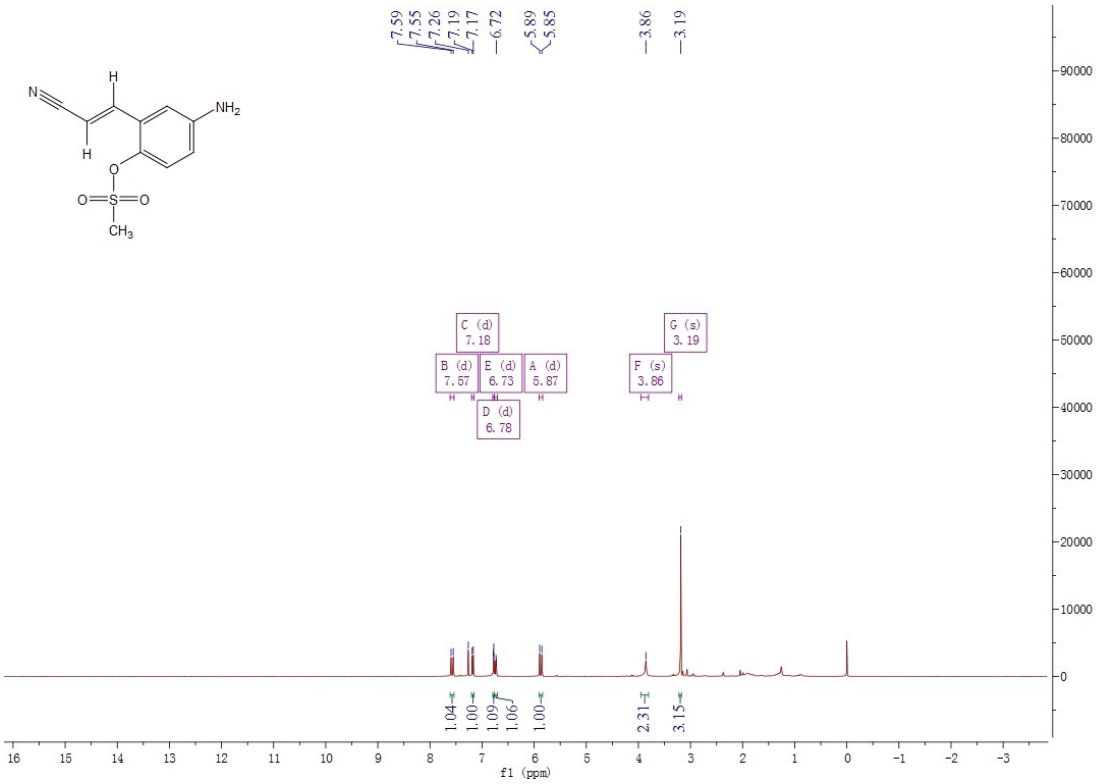

2020100819_SDUL-1 #80 RT: 0.34 AV: 1 NL: 2.04E4
T: ITMS - c ESI Full ms [150.00-2000.00]
Relative Abundance
m/z
259.53
260.57
339.81
519.37
227.51
255.96
265.80
286.04
312.00
325.89
340.98
373.44
383.67
410.04
425.46
459.90
479.88
499.03

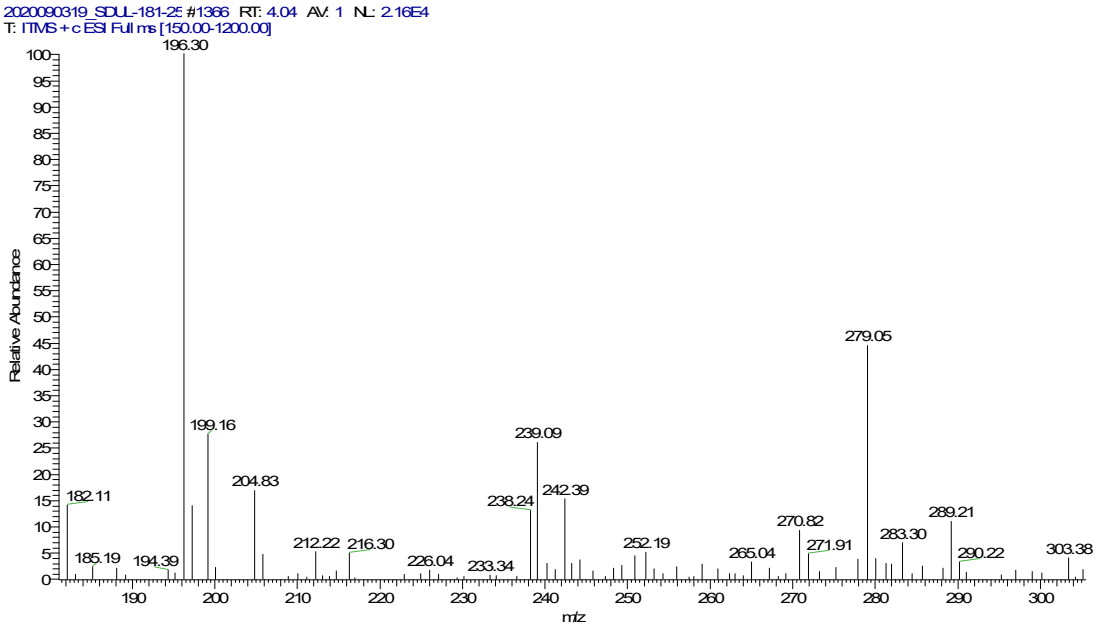

HO
S
N
OH
O
N
S
H3C
O
O
7.42
7.28
7.23
6.60
5.97
5.93
4.59
4.06
3.01
2.97
2.52
B (d) 7.25
D (d) 6.95
G (s) 3.01
A (s) 7.42
C (s) 6.60
E (s) 4.59
F (s) 3.04
H (d) 2.98
1.00
1.39
1.19
1.23
1.65
0.88
2.89
1.42
f1 (ppm)

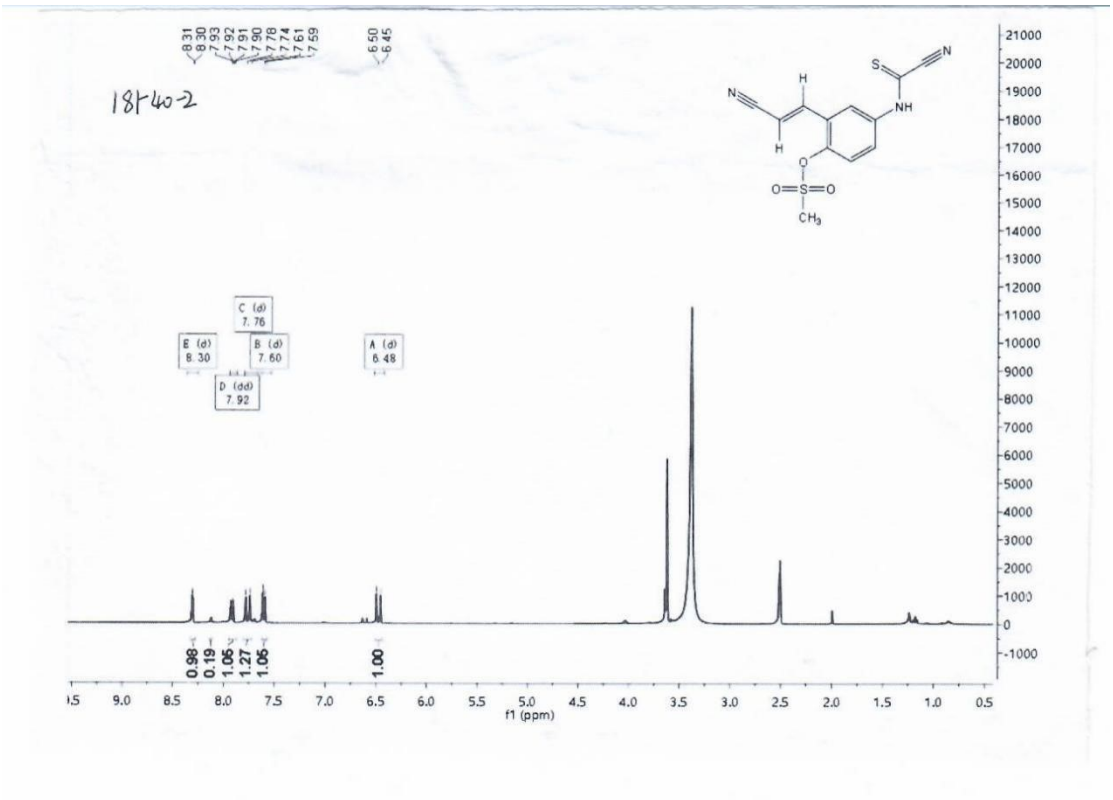

172.16
167.92
158.42
156.45
147.13
140.11
139.28
129.72
122.99
118.26
106.46
78.35
51.11
34.56
HO
S
N
COOH
H3CO
O
13C NMR (101 MHz, MeOD) δ 172.16, 167.92, 158.42, 156.45, 147.13, 140.11, 139.28, 129.72, 123.58, 122.99, 118.26, 106.46, 78.35, 51.11, 34.56.
f1 (ppm)

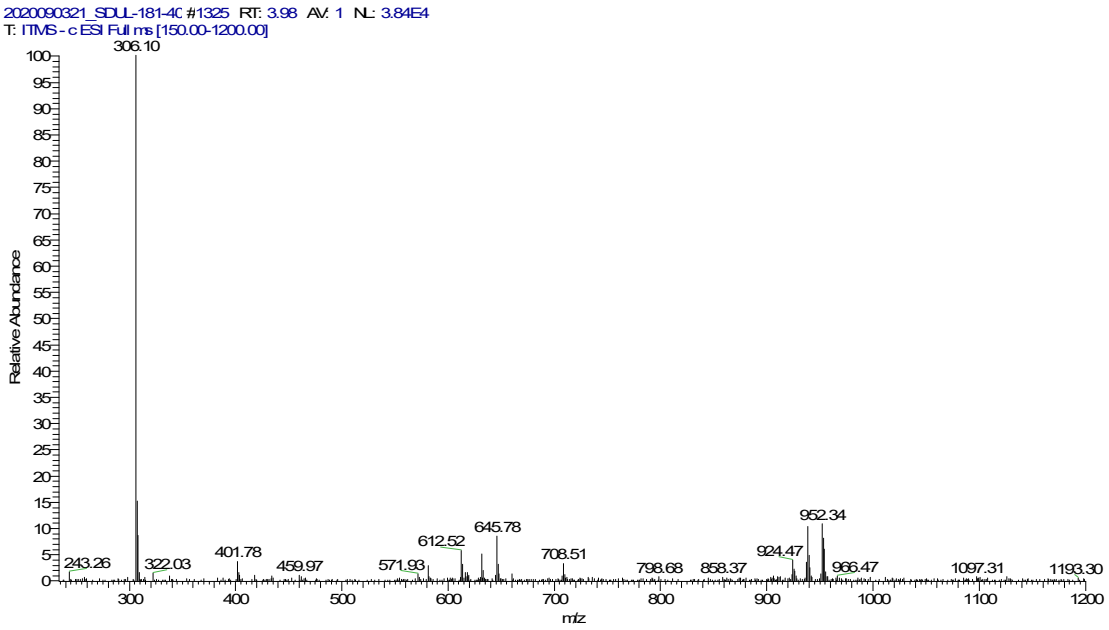

Intens.
x10^5
ZP-181-13_RC3_01_2991.d: -MS, 0.2min #10
363.0162
112.9834
259.0204
727.0417
500.0339
642.0431
863.0821
m/z

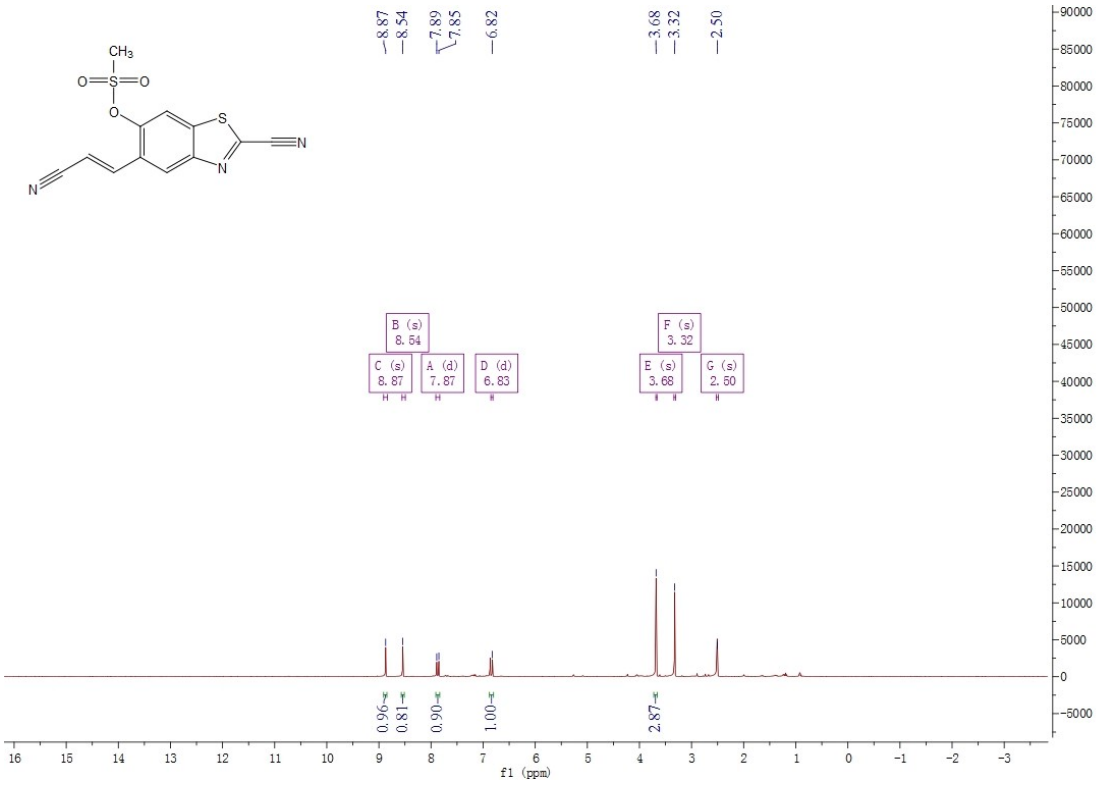

20200623_SDUL-181-6C #869 RT: 2.62 AV: 1 NL: 1.92E3
T: ITMS + c ESI Full ms [50.00-1000.00]
Relative Abundance
365.19
380.26
345.13
352.37
366.29
379.37
381.25
384.20
340.04
346.79
355.10
362.65
367.32
372.74
376.70
382.91
385.00
389.43
390.12
394.65
399.39
401.36
m/z

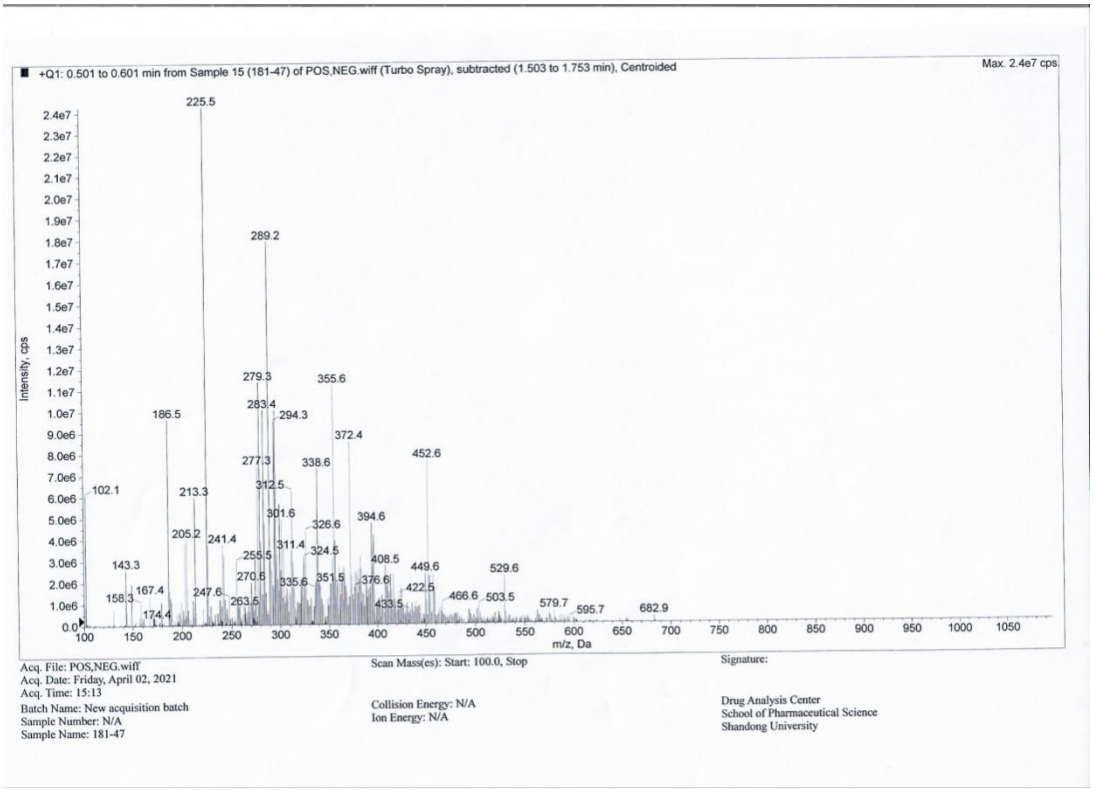

7.59
7.55
7.26
7.19
7.17
6.72
5.89
5.85
3.86
3.19
C (d) 7.18
B (d) 7.57
E (d) 6.73
A (d) 5.87
D (d) 6.78
G (s) 3.19
F (s) 3.86
1.04
1.00
1.09
1.06
1.00
2.31
3.15
f1 (ppm)

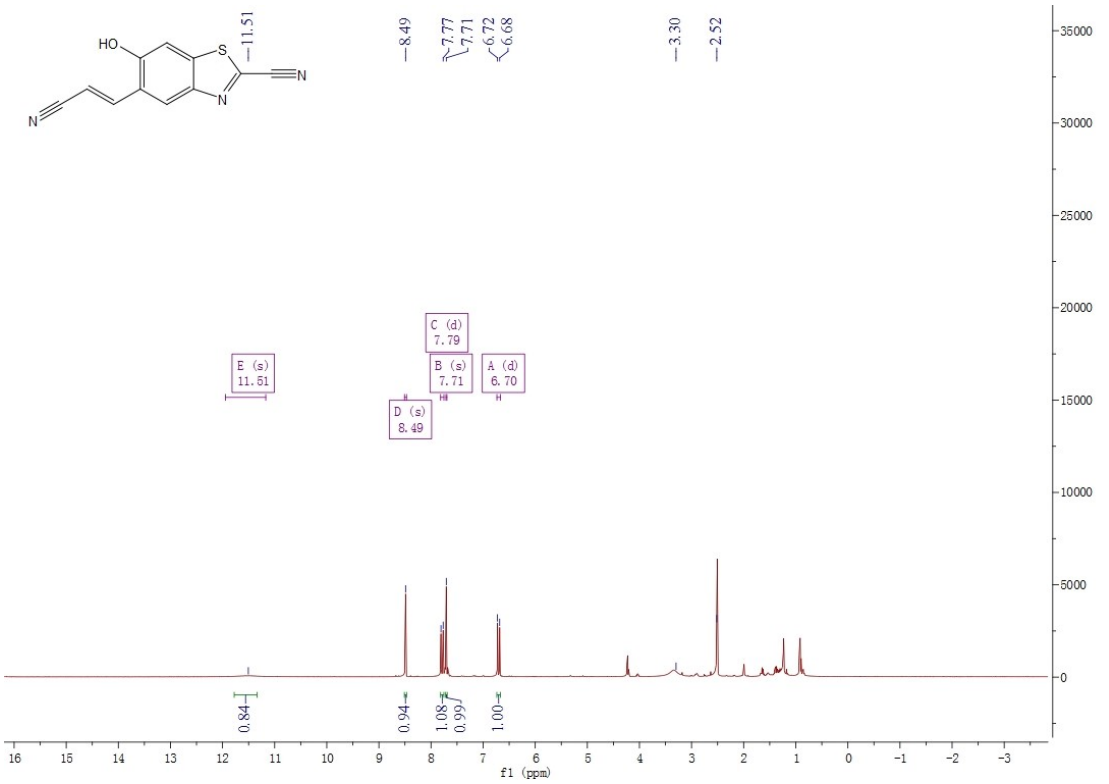

2020090319_SDUL-181-25 #1366 RT: 4.04 AV: 1 NL: 2.16E4
T: ITMS + c ESI Full ms [150.00-1200.00]
Relative Abundance
m/z
196.30
199.16
204.83
182.11
185.19
194.39
212.22
216.30
226.04
233.34
238.24
239.09
242.39
252.19
265.04
270.82
271.91
279.05
283.30
289.21
290.22
303.38

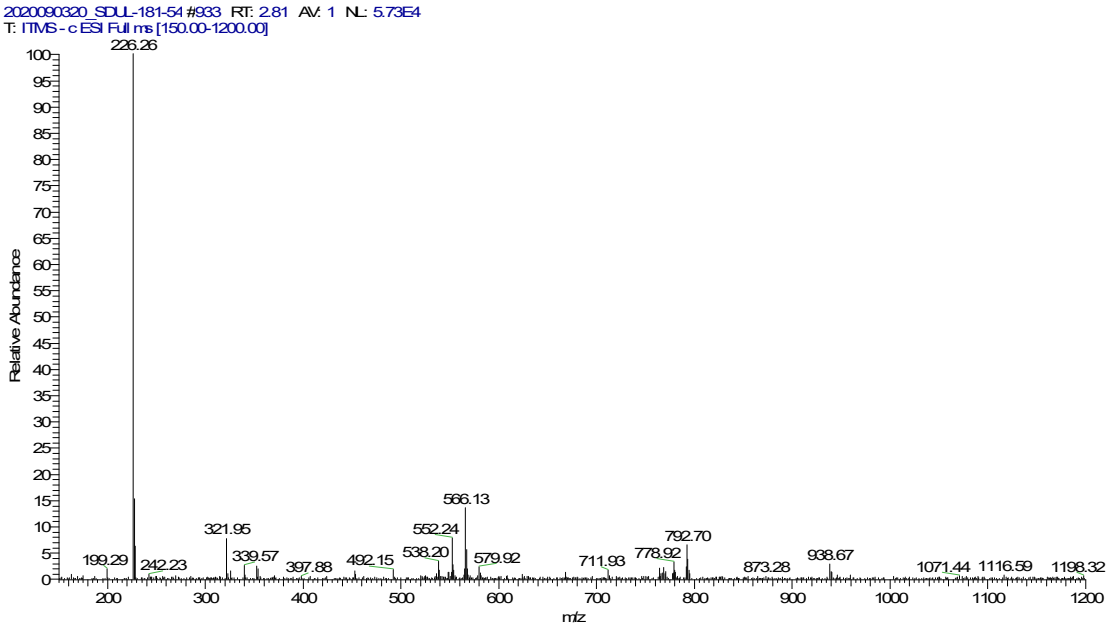

18f402
8.31
8.30
7.93
7.92
7.91
7.90
7.78
7.74
7.61
7.59
6.50
6.45
C (d) 7.76
E (d) 8.30
B (d) 7.60
A (d) 6.48
D (dd) 7.92
0.98
0.19
1.06
1.27
1.06
1.00
f1 (ppm)

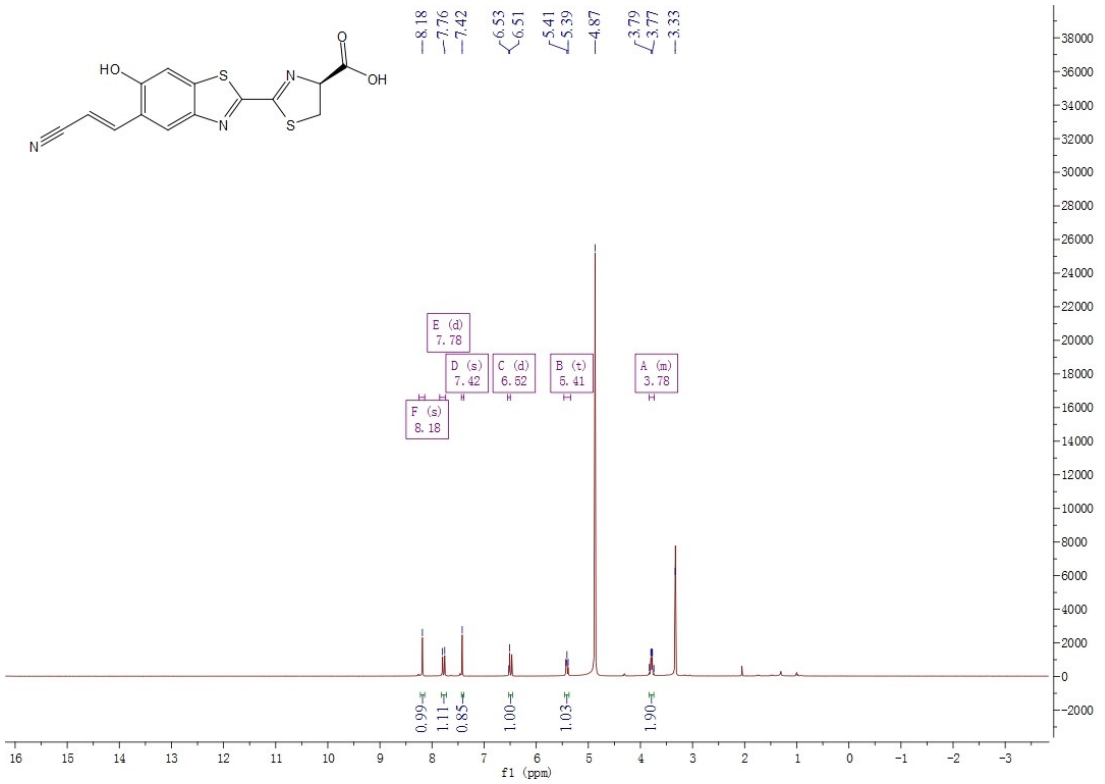

2020090321_SDUL-181-40 #1325 RT: 3.98 AV: 1 NL: 3.84E4
T: ITMS - c ESI Full ms [150.00-1200.00]
306.10
952.34
645.78
612.52
708.51
924.47
243.26
322.03
401.78
459.97
571.93
798.68
858.37
966.47
1097.31
1193.30
Relative Abundance
m/z

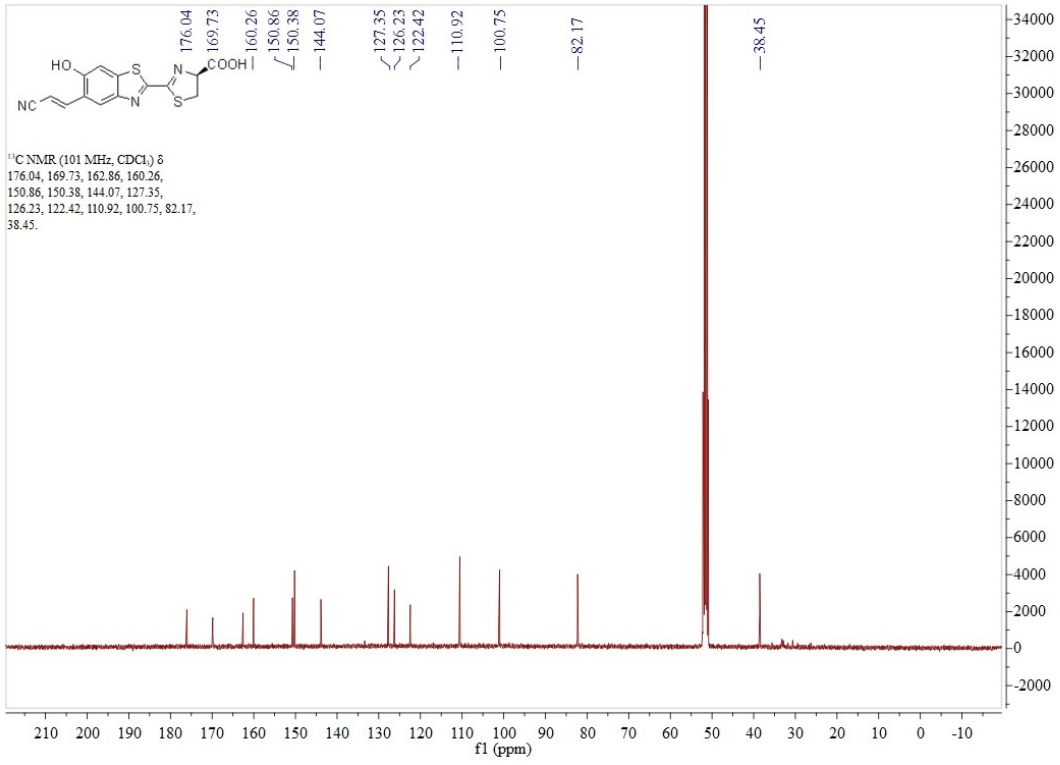

8.87
8.54
7.89
7.85
6.82
3.68
3.32
2.50
B (s) 8.54
C (s) 8.87
A (d) 7.87
D (d) 6.83
F (s) 3.32
E (s) 3.68
G (s) 2.50
0.96
0.81
0.90
1.00
2.87
f1 (ppm)

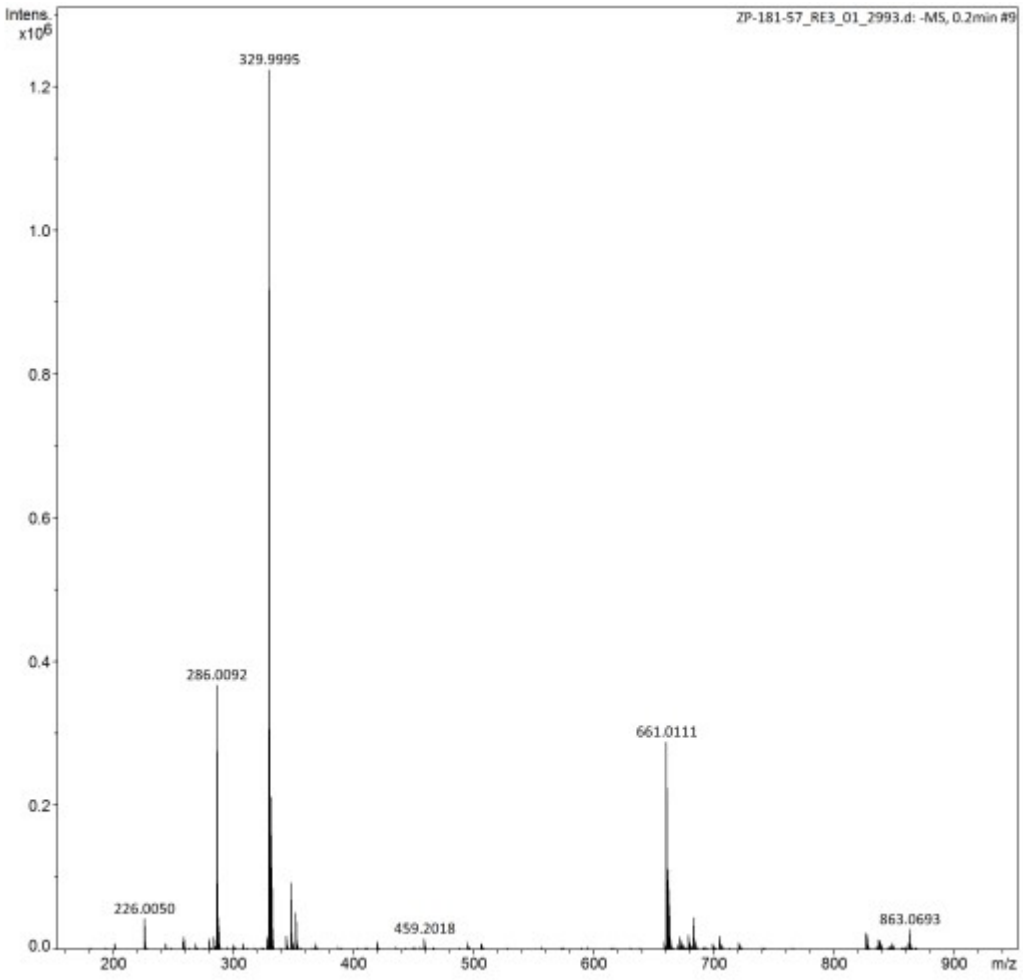

+Q1: 0.501 to 0.601 min from Sample 15 (181-47) of POS,NEG.wiff (Turbo Spray), subtracted (1.503 to 1.753 min), Centroided
Max. 2.4e7 cps
Intensity, cps
m/z, Da
225.5
289.2
279.3
355.6
283.4
294.3
186.5
372.4
452.6
277.3
338.6
102.1
312.5
213.3
301.6
394.6
326.6
205.2
241.4
311.4
324.5
255.5
408.5
449.6
529.6
143.3
270.6
335.6
351.5
376.6
422.5
158.3
167.4
247.6
263.5
433.5
466.6
503.5
579.7
595.7
682.9
174.4
Acq. File: POS,NEG.wiff
Acq. Date: Friday, April 02, 2021
Acq. Time: 15:13
Batch Name: New acquisition batch
Sample Number: N/A
Sample Name: 181-47
Scan Mass(es): Start: 100.0, Stop
Collision Energy: N/A
Ion Energy: N/A
Signature:
Drug Analysis Center
School of Pharmaceutical Science
Shandong University


HO
S
N
N
N
11.51
8.49
7.77
7.71
6.72
6.68
3.30
2.52
C (d)
7.79
E (s)
11.51
B (s)
7.71
A (d)
6.70
D (s)
8.49
0.84
0.94
1.08
0.99
1.00
f1 (ppm)


2020090320_SDUL-181-54 #933 RT: 2.81 AV: 1 NL: 5.73E4
T: ITMS - c ESI Full ms [150.00-1200.00]
Relative Abundance
m/z
226.26
566.13
321.95
552.24
792.70
199.29
242.23
339.57
397.88
492.15
538.20
579.92
711.93
778.92
873.28
938.67
1071.44
1116.59
1198.32


8.18
7.76
7.42
6.53
6.51
5.41
5.39
4.87
3.79
3.77
3.33
E (d) 7.78
D (s) 7.42
C (d) 6.52
B (t) 6.41
A (m) 3.78
F (s) 8.18
0.99
1.11
0.85
1.00
1.03
1.90
f1 (ppm)


176.04
169.73
160.26
150.86
150.38
144.07
127.35
126.23
122.42
110.92
100.75
82.17
38.45
^{13}C NMR (101 MHz, CDCl$_3$) δ
176.04, 169.73, 162.86, 160.26,
150.86, 150.38, 144.07, 127.35,
126.23, 122.42, 110.92, 100.75, 82.17,
38.45.
f1 (ppm)


ZP-181-57_RE3_01_2993.d: -MS, 0.2min #9
Intens.
x10^6
329.9995
286.0092
661.0111
226.0050
459.2018
863.0693
m/z