Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

Selective C3-H Nitration of 2-Sulfanilamidopyridines with *tert*-Butyl Nitrite

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1. General Information

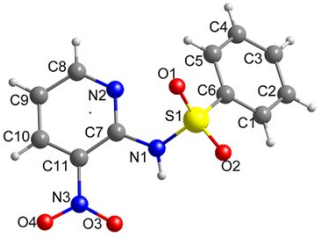
Unless otherwise noted, materials were purchased from commercial suppliers and used without further purification. The *N*-(pyridin-2-yl)arylsulfonamides were prepared according to reported methods.[1] All the reactions were carried out without any precautions to exclude air and moisture. All reactions were monitored by TLC (thin layer chromatography) and visualized using UV light. Products were purified by column chromatography by 100-200 mesh silica. Proton (^{1}H) and carbon (^{13}C) NMR spectra were taken on a Bruker AV-500 spectrometer operating at 500 MHz or 400 MHz for proton and 126 MHz or 101 MHz for carbon nuclei using $CDCl_3$ or DMSO-d_6 as solvent, respectively. Chemical shifts were referenced to the residual proton solvent peaks (^{1}H: $CDCl_3$, δ 7.26; DMSO-d_6, δ 2.50), solvent ^{13}C signals ($CDCl_3$, δ 77.00; DMSO-d_6, δ 39.60). Suitable crystals of compound **2a**, **2m** and **2n** were obtained by slowly evaporating a mixture of dichloromethane and petroleum ether solution at ambient temperature. Single crystal was chosen under an optical microscope and quickly coated with high vacuum grease to prevent decomposition. Intensity data and cell parameters were recorded at 295 K on a Rigaku R-Axis Rapid X-single crystal diffractometer, employing a Mo Kα radiation (λ = 0.71073 Å). The empirical absorption correction was applied by using the SADABS program. The structure was solved using direct method, and refined by full matrix least-squares on F^2. **CCDC 2157226 (2a)**, **CCDC 2158133 (2m)** and **CCDC 2158131 (2n)** contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from the Cambridge Crystallographic Data Centre.

2. General procedure for the C3-H nitration of 2-sulfanilamidopyridines

To a 10 mL vial, 2-sulfanilamidopyridines (**1a**-**1y**) (0.2 mmol) and $Cu(OAc)_2$ (5 mol %, 1.8 mg) were dissolved in PhCl (1.0 mL). ^{t}BuONO (4.0 mmol, 2.0 equiv, 24 μL) were then slowly added into the mixture. The reactions were then sealed and heated at 100 °C for 24 h. After that time, the reactions were monitored by TLC plate, and the solvent was removed under vacuum, the resulting solids were purified by flash column chromatography to afford the desired nitration products (**2a**-**2y**).

3. X-ray crystal structure data

Crystal data and structure refinement for **2a** (ball and stick at the 30% probability level)

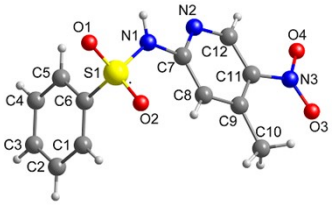


CCDC: 2157226

Table 1 Crystal data for **2a**	
Identification code	Shx97
Empirical formula	$C_{11}H_9N_3O_4S$
Formula weight	279.27
Temperature	295(2)

Crystal system	Triclinic
Space group	P-1
a/Å	7.3377(15)
b/Å	7.9190(16)
c/Å	11.426(2)
α/°	96.73(3)
β/°	99.02(3)
γ/°	109.40(3)
Volume/Å^3	608.2(2)
Z	2
ρ_{calc}mg/mm^3	1.525
μ/mm^{-1}	0.280
F(000)	288
Crystal size/mm^3	0.46 x 0.25 x 0.13
2Θ range for data collection	3.010 to 25.021°
Index ranges	-8<=h<=8, -9<=k<=9, -13<=l<=13
Reflections collected	4824
Independent reflections	2144 [R(int) = 0.0542]
Data/restraints/parameters	2144 / 0 / 172
Goodness-of-fit on F^2	1.145
Final R indexes [I>=2σ (I)]	R_1 = 0.0648, wR_2 = 0.1548
Final R indexes [all data]	R_1 = 0.1006, wR_2 = 0.2260
Largest diff. peak/hole / e Å^{-3}	0.481 / -0.728

Crystal data and structure refinement for **2m** (ball and stick at the 30% probability level)

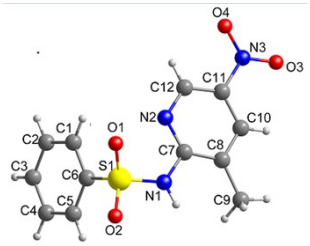


CCDC: 2158133

Table 2 Crystal data for **2m**	
Identification code	Shx97
Empirical formula	$C_{12}H_{11}N_3O_4S$
Formula weight	293.30
Temperature	293(2)
Crystal system	Monoclinic
Space group	$P2_1/c$
a/Å	6.9073(14)

b/Å	17.475(4)
c/Å	11.142(2)
α/°	90
β/°	96.86(3)
γ/°	90
Volume/Å^3	1335.2(5)
Z	4
ρ_{calc}mg/mm^3	1.459
μ/mm^{-1}	0.259
F(000)	608.0
Crystal size/mm^3	0.53 x 0.39 x 0.20
2Θ range for data collection	5.942 to 50.052°
Index ranges	-8<=h<=8, -20<=k<=20, -13<=l<=13
Reflections collected	10056
Independent reflections	2360 [R(int) = 0.0604, Rsigma = 0.0540]
Data/restraints/parameters	2360 / 18 / 181
Goodness-of-fit on F^2	1.210
Final R indexes [I>=2σ (I)]	R_1 = 0.0510, wR_2 = 0.1296
Final R indexes [all data]	R_1 = 0.0693, wR_2 = 0.1388
Largest diff. peak/hole / e Å^{-3}	0.31 / -0.30

Crystal data and structure refinement for **2n** (ball and stick at the 30% probability level)

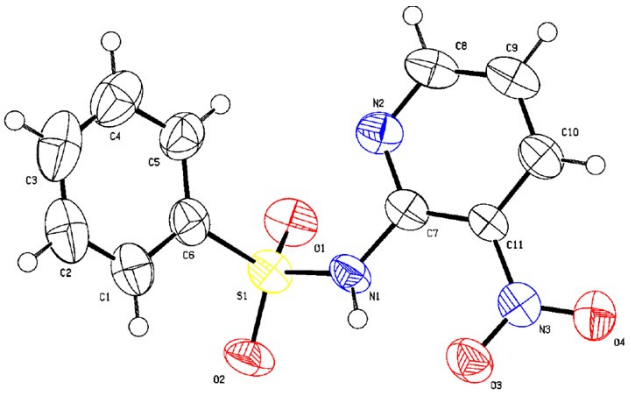


CCDC: 2158131

Table 3 Crystal data for **2n**	
Identification code	Shx97
Empirical formula	$C_{12}H_{11}N_3O_4S$
Formula weight	293.30
Temperature	293(2)
Crystal system	Monoclinic
Space group	$P2_1/n$
a/Å	8.0582(16)
b/Å	8.8182(18)
c/Å	18.340(4)
α/°	90

β/°	90.59(3)
γ/°	90
Volume/Å^3	1297.0(5)
Z	4
ρ_{calc}mg/mm^3	1.502
μ/mm^{-1}	0.267
F(000)	608.0
Crystal size/mm^3	0.37 x 0.32 x 0.28
2Θ range for data collection	6.424 to 50.044°
Index ranges	-9<=h<=9, -9<=k<=9, -21<=l<=21
Reflections collected	9935
Independent reflections	2288 [R(int) = 0.1049, Rsigma = 0.0688]
Data/restraints/parameters	2288 / 0 / 182
Goodness-of-fit on F^2	1.156
Final R indexes [I>=2σ (I)]	R_1 = 0.0434, wR_2 = 0.0937
Final R indexes [all data]	R_1 = 0.0777, wR_2 = 0.1404
Largest diff. peak/hole / e Å^{-3}	0.32 / -0.53

4. Hydrogen bonds data

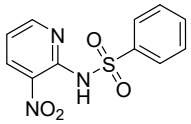


Hydrogen bonds with H..A < r(A) + 2.000 Angstroms and <DHA > 110 deg.
Appropriate HTAB instructions appended to .res file for future use.

D-H	d(D-H)	d(H..A)	<DHA	d(D..A)	A
N1-H1B	0.860	2.067	125.88	2.664	O3
N1-H1B	0.860	2.280	156.39	3.087	O3 [-x, -y+2, -z+1]
C5-H5A	0.930	2.684	114.91	3.189	N2
C8-H8A	0.930	2.657	125.51	3.286	O1 [-x+1, -y+1, -z+1]

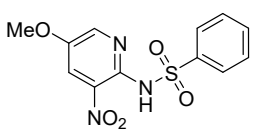
5. Characterization data

N-(3-nitropyridin-2-yl)benzenesulfonamide (**2a**)



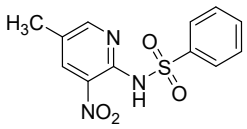
Followed General Procedure on 0.2 mmol scale. Purified *via* column chromatography (PE:EA = 10:1) on silica to obtain **2a**: 45.2 mg, 83% yield; Yellow solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.23 (s, 1H), 8.54 – 8.43 (m, 2H), 8.23 – 8.15 (m, 2H), 7.62 (t, *J* = 7.4 Hz, 1H), 7.53 (t, *J* = 7.6 Hz, 2H), 7.10 (dd, *J* = 8.3, 4.7 Hz, 1H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$) δ 154.1, 145.7, 139.2, 135.0, 133.7, 130.4, 128.8, 128.7, 118.1 ppm. HRMS (EI): m/z $[M+H]^+$ calcd for $C_{11}H_{10}N_3O_4S$: 280.0387, found: 280.0390.

N-(5-methoxy-3-nitropyridin-2-yl)benzenesulfonamide (**2b**)



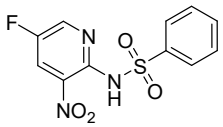
Followed General Procedure on 0.2 mmol scale. Purified *via* column chromatography (PE:EA = 10:1) on silica to obtain **2b**: 55.1 mg, 89% yield; Yellow solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.96 (s, 1H), 8.25 (d, *J* = 2.9 Hz, 1H), 8.18 – 8.12 (m, 2H), 7.93 (d, *J* = 2.9 Hz, 1H), 7.59 (t, *J* = 7.4 Hz, 1H), 7.51 (t, *J* = 7.6 Hz, 2H), 3.85 (s, 3H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$) δ 151.4, 143.4, 139.5, 133.4, 130.2, 128.7, 128.6, 117.4, 56.4 ppm. HRMS (EI): m/z $[M+H]^+$ calcd for $C_{12}H_{12}N_3O_5S$: 310.0492, found: 310.0490.

N-(5-methyl-3-nitropyridin-2-yl)benzenesulfonamide (**2c**)



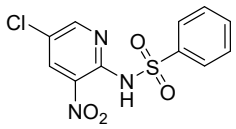
Followed General Procedure on 0.2 mmol scale. Purified *via* column chromatography (PE:EA = 8:1) on silica to obtain **2c**: 51.6 mg, 88% yield; Yellow solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.08 (s, 1H), 8.33 (m, 1H), 8.29 – 8.25 (m, 1H), 8.19 – 8.15 (m, 2H), 7.63 – 7.56 (m, 1H), 7.51 (m, 2H), 2.32 (s, 3H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$) δ 154.5, 143.5, 139.3, 134.7, 133.5, 130.0, 128.68, 128.61, 128.4, 17.2 ppm. HRMS (EI): m/z $[M+H]^+$ calcd for $C_{12}H_{12}N_3O_4S$: 294.0543, found: 294.0542.

N-(5-fluoro-3-nitropyridin-2-yl)benzenesulfonamide (**2d**)



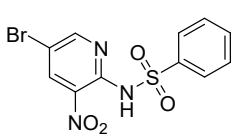
Followed General Procedure on 0.2 mmol scale. Purified *via* column chromatography (PE:EA = 5:1) on silica to obtain **2d**: 48.1 mg, 81% yield; Yellow solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.08 (s, 1H), 8.43 (d, *J* = 2.8 Hz, 1H), 8.25 (dd, *J* = 7.4, 2.8 Hz, 1H), 8.19 – 8.09 (m, 2H), 7.67 – 7.59 (m, 1H), 7.53 (dd, *J* = 8.5, 7.0 Hz, 2H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$) δ 153.8 (d, *J* = 257.0 Hz), 142.8 (d, *J* = 24.9 Hz), 142.0 (d, *J* = 1.9 Hz), 139.0, 133.8, 129.7 (d, *J* = 2.9 Hz), 128.8, 128.7, 121.8 (d, *J* = 23.5 Hz) ppm. HRMS (EI): m/z $[M+H]^+$ calcd for $C_{11}H_9FN_3O_4S$: 298.0292, found: 298.0288.

N-(5-chloro-3-nitropyridin-2-yl)benzenesulfonamide (**2e**)



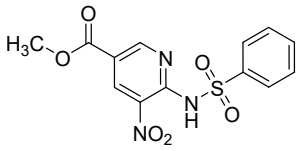
Followed General Procedure on 0.2 mmol scale. Purified *via* column chromatography (PE:EA = 8:1) on silica to obtain **2e**: 55.8 mg, 89% yield; Yellow solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.11 (s, 1H), 8.46 (q, *J* = 2.4 Hz, 2H), 8.17 (s, 1H), 8.15 (d, *J* = 1.4 Hz, 1H), 7.66 – 7.58 (m, 1H), 7.53 (t, *J* = 7.6 Hz, 2H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$) δ 152.8, 143.8, 138.8, 134.2, 133.8, 130.0, 128.76, 128.75, 125.2 ppm. HRMS (EI): m/z $[M+H]^+$ calcd for $C_{11}H_9ClN_3O_4S$: 313.9997, found: 313.9995.

N-(5-bromo-3-nitropyridin-2-yl)benzenesulfonamide (**2f**)



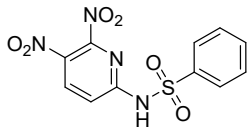
Followed General Procedure on 0.2 mmol scale. Purified *via* column chromatography (PE:EA = 10:1) on silica to obtain **2f**: 60.1 mg, 84% yield; Yellow solid; ^{1}H NMR (400 MHz, $CDCl_3$) 8.20 (d, J = 1.9 Hz, 1H), 8.15 (s, 1H), 8.13 (d, J = 1.3 Hz, 1H), 7.87 (d, J = 2.1 Hz, 1H), 7.75 (s, 1H), 7.60 (t, J = 7.4 Hz, 1H), 7.51 (t, J = 7.6 Hz, 2H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$) δ 147.5, 146.7, 142.6, 139.1, 133.5, 128.7, 128.5, 113.4, 107.0 ppm. HRMS (EI): m/z $[M+H]^+$ calcd for $C_{11}H_9BrN_3O_4S$: 357.9492, 359.9471, found: 357.9493, 359.9471.

methyl 5-nitro-6-(phenylsulfonamido)nicotinate (**2g**)



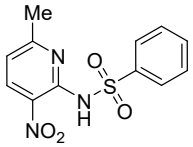
Followed General Procedure on 0.2 mmol scale. Purified *via* column chromatography (PE:EA = 8:1) on silica to obtain **2g**: 48.2 mg, 72% yield; Yellow solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.38 (s, 1H), 9.06 (d, J = 2.0 Hz, 1H), 9.03 (s, 1H), 8.21 (s, 1H), 8.19 (d, J = 1.4 Hz, 1H), 7.63 (t, J = 7.4 Hz, 1H), 7.54 (t, J = 7.7 Hz, 2H),, 3.95 (s, 3H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$) δ 163.3, 155.0, 147.8, 138.6, 136.3, 134.0, 129.6, 129.0, 128.8, 120.8, 52.9 ppm. HRMS (EI): m/z $[M+H]^+$ calcd for $C_{13}H_{12}N_3O_6S$: 338.0441, found: 338.0443.

N-(5,6-dinitropyridin-2-yl)benzenesulfonamide (**2h**)



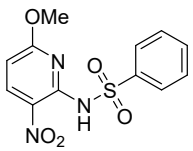
Followed General Procedure on 0.2 mmol scale. Purified *via* column chromatography (PE:EA = 5:1) on silica to obtain **2h**: 41.5 mg, 64% yield; Yellow solid; ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.48 (d, J = 8.9 Hz, 1H), 8.19 (d, J = 8.9 Hz, 1H), 7.92 – 7.86 (m, 2H), 7.67 (t, J = 7.4 Hz, 1H), 7.60 (t, J = 7.5 Hz, 2H) ppm; ^{13}C NMR (101 MHz, DMSO-d_6) δ 146.3, 145.7, 140.0, 135.0, 134.1, 133.5, 129.6, 126.9, 124.1 ppm. HRMS (EI): m/z $[M+H]^-$ calcd for $C_{11}H_7N_4O_6S$: 323.0092, found: 323.0088.

N-(6-methyl-3-nitropyridin-2-yl)benzenesulfonamide (**2i**)



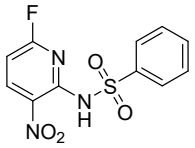
Followed General Procedure on 0.2 mmol scale. Purified *via* column chromatography (PE:EA = 10:1) on silica to obtain **2i**: 38.0 mg, 48% yield; Yellow solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.19 (s, 1H), 8.32 (d, J = 8.5 Hz, 1H), 8.20 (s, 1H), 8.18 (d, J = 1.3 Hz, 1H), 7.61 (t, J = 7.4 Hz, 1H), 7.53 (t, J = 7.6 Hz, 2H), 6.89 (d, J = 8.5 Hz, 1H), 2.48 (s, 3H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.3, 144.8, 139.2, 134.9, 133.6, 129.1, 128.4, 128.2, 118.0, 24.3. HRMS (EI): m/z $[M+H]^+$ calcd for $C_{12}H_{12}N_3O_4S$: 294.0543, found:294.0542.

N-(6-methoxy-3-nitropyridin-2-yl)benzenesulfonamide (**2j**)



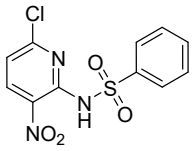
Followed General Procedure on 0.2 mmol scale. Purified *via* column chromatography (PE:EA = 10:1) on silica to obtain **2j**: 50.7 mg, 82% yield; Yellow solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.65 (s, 1H), 8.34 (d, J = 9.1 Hz, 1H), 8.09 (s, 1H), 8.07 (d, J = 1.4 Hz, 1H), 7.64 (t, J = 7.4 Hz, 1H), 7.54 (t, J = 7.7 Hz, 2H), 6.39 (d, J = 9.1 Hz, 1H), 3.77 (s, 3H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.9, 146.4, 139.8, 137.4, 133.6, 129.0, 127.8, 124.4, 106.1, 55.5 ppm. HRMS (EI): m/z $[M+H]^+$ calcd for $C_{12}H_{12}N_3O_5S$: 310.0492, found: 310.0490.

N-(6-fluoro-3-nitropyridin-2-yl)benzenesulfonamide (**2k**)



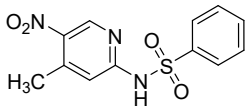
Followed General Procedure on 0.2 mmol scale. Purified *via* column chromatography (PE:EA = 8:1) on silica to obtain **2k**: 47.1 mg, 89% yield; Yellow solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 10.31 (s, 1H), 8.59 (dd, *J* = 8.9, 6.5 Hz, 1H), 8.31 – 8.15 (m, 2H), 7.65 (t, *J* = 7.4 Hz, 1H), 7.56 (t, *J* = 7.7 Hz, 2H), 6.64 (dd, *J* = 8.9, 3.5 Hz, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 163.6 (d, *J* = 253.7 Hz), 145.9 (d, *J* = 19.9 Hz), 140.8 (d, *J* = 11.0 Hz), 138.4, 134.1, 129.2, 128.8, 127.8, 103.7(d, *J* = 38.3 Hz) ppm. HRMS (EI): m/z $[M+H]^+$ calcd for $C_{11}H_9FN_3O_4S$: 298.0292, found: 298.0288.

N-(6-chloro-3-nitropyridin-2-yl)benzenesulfonamide (**2l**)



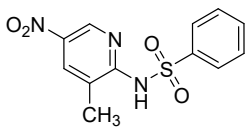
Followed General Procedure on 0.2 mmol scale. Purified *via* column chromatography (PE:EA = 10:1) on silica to obtain **2l**: 49.4 mg, 79% yield; Yellow solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.20 (s, 1H), 8.41 (d, *J* = 8.6 Hz, 1H), 8.28 – 8.15 (m, 2H), 7.65 (t, *J* = 7.4 Hz, 1H), 7.57 (t, *J* = 7.6 Hz, 2H), 7.03 (s, 1H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$) δ 155.6, 145.3, 138.3, 137.2, 134.1, 129.5, 128.8, 128.7, 118.4 ppm. HRMS (EI): m/z $[M+H]^+$ calcd for $C_{11}H_9ClN_3O_4S$: 313.9997, found: 313.9995.

N-(4-methyl-5-nitropyridin-2-yl)benzenesulfonamide (**2m**)



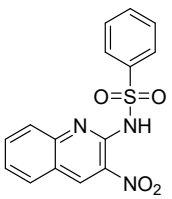
Followed General Procedure on 0.2 mmol scale. Purified *via* column chromatography (PE:EA = 2:1) on silica to obtain **2m**: 35.2 mg, 60% yield; Yellow solid; ^{1}H NMR (500 MHz, $CDCl_3$) 9.23 (s, 1H), 8.18 (d, *J* = 23.4 Hz, 3H), 7.65 – 7.46 (m, 3H), 6.90 (s, 1H), 2.51 (s, 3H) ppm. HRMS (EI): m/z $[M+H]^+$ calcd for $C_{12}H_{12}N_3O_4S$: 294.0543, found: 294.0542.

N-(3-methyl-5-nitropyridin-2-yl)benzenesulfonamide (**2n**)



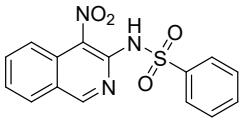
Followed General Procedure on 0.2 mmol scale. Purified *via* column chromatography (PE:EA = 2:1) on silica to obtain **2n**: 38.1 mg, 65% yield; Yellow solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.10 (s, 1H), 7.92 (d, *J* = 7.6 Hz, 1H)., 7.63 (t, *J* = 7.4 Hz, 1H), 7.53 (t, *J* = 7.6 Hz, 2H), 7.32 (s, 1H), 2.65 (s, 3H) ppm. HRMS (EI): m/z $[M+H]^+$ calcd for $C_{12}H_{12}N_3O_4S$: 294.0543, found: 294.0542.

N-(3-nitroquinolin-2-yl)benzenesulfonamide (**2o**)



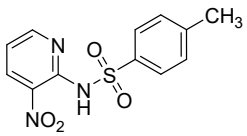
Followed General Procedure on 0.2 mmol scale. Purified *via* column chromatography (PE:EA = 2:1) on silica to obtain **2o**: 29.6 mg, 45% yield; Yellow solid; ^{1}H NMR (500 MHz, DMSO-d_6) δ 11.79 (s, 1H), 8.35 (d, *J* = 9.0 Hz, 1H), 8.11 (s, 2H), 8.00 (d, *J* = 7.5 Hz, 2H), 7.63 (t, *J* = 7.4 Hz, 1H), 7.56 (t, *J* = 7.7 Hz, 3H), 7.19 (s, 11H) ppm; ^{13}C NMR (126 MHz, DMSO-d_6) δ 162.0, 143.3, 141.5, 140.2, 133.1, 129.0, 127.8, 125.1, 124.3, 123.9, 123.7, 118.6, 116.0 ppm. HRMS (EI): m/z $[M+Na]^+$ calcd for $C_{15}H_{11}NaN_3O_4S$: 352.0362, found: 352.0362.

N-(4-nitroisoquinolin-3-yl)benzenesulfonamide (**2p**)



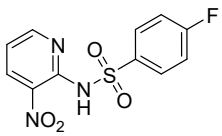
Followed General Procedure on 0.2 mmol scale. Purified *via* column chromatography (PE:EA = 3:1) on silica to obtain **2p**: 34.3 mg, 52% yield; Yellow solid; ^{1}H NMR (500 MHz, DMSO-d_6) δ 11.42 (s, 1H), 9.24 (s, 1H), 8.18 (d, J = 8.2 Hz, 1H), 8.00 (d, J = 7.5 Hz, 2H), 7.93 (t, J = 7.7 Hz, 1H), 7.82 (d, J = 8.6 Hz, 1H), 7.70 (t, J = 7.5 Hz, 1H), 7.65 (t, J = 7.3 Hz, 1H), 7.60 (t, J = 7.4 Hz, 2H);^{13}C NMR (126 MHz, DMSO-d_6) δ 154.8, 141.2, 138.6, 134.3, 133.0, 131.9, 129.0, 128.6, 128.3, 127.8, 127.3, 125.7, 120.1 ppm. HRMS (EI): m/z [M+Na]$^+$ calcd for $C_{15}H_{11}NaN_3O_4S$: 352.0362, found: 352.0362.

4-methyl-*N*-(3-nitropyridin-2-yl)benzenesulfonamide (**2q**)



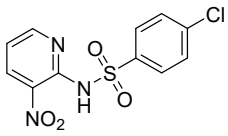
Followed General Procedure on 0.2 mmol scale. Purified *via* column chromatography (PE:EA = 10:1) on silica to obtain **2q**: 51.3 mg, 83% yield; Yellow solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.19 (s, 1H), 8.49 (dd, J = 9.9, 5.9 Hz, 2H), 8.07 (d, J = 8.1 Hz, 2H), 7.32 (d, J = 8.2 Hz, 2H), 7.08 (dd, J = 8.3, 4.7 Hz, 1H), 2.42 (s, 3H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$) δ 154.1, 145.8, 144.7, 136.3, 135.0, 130.4, 129.3, 128.9, 117.9, 21.6 ppm. HRMS (EI): m/z [M+H]$^+$ calcd for $C_{12}H_{12}N_3O_4S$: 294.0543, found: 294.0542.

4-fluoro-*N*-(3-nitropyridin-2-yl)benzenesulfonamide (**2r**)



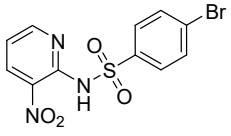
Followed General Procedure on 0.2 mmol scale. Purified *via* column chromatography (PE:EA = 8:1) on silica to obtain **2r**: 47.5 mg, 80% yield; Yellow solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.20 (s, 1H), 8.54 – 8.46 (m, 2H), 8.25 – 8.19 (m, 2H), 7.20 (t, J = 8.6 Hz, 2H), 7.12 (dd, J = 8.1, 4.9 Hz, 1H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$) 165.61 (d, J = 256.6 Hz), 154.00, 145.48, 135.11 (d, J = 3.5 Hz), 135.06, 131.83 (d, J = 9.7 Hz), 130.44, 118.23, 115.93 (d, J = 22.8 Hz) ppm. HRMS (EI): m/z [M+H]$^+$ calcd for $C_{11}H_9FN_3O_4S$: 298.0292, found: 298.0288.

4-chloro-*N*-(3-nitropyridin-2-yl)benzenesulfonamide (**2s**)



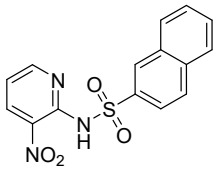
Followed General Procedure on 0.2 mmol scale. Purified *via* column chromatography (PE:EA = 10:1) on silica to obtain **2s**: 52.6 mg, 84% yield; Yellow solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.23 (s, 1H), 8.50 (d, J = 6.7 Hz, 2H), 8.14 (d, J = 8.7 Hz, 2H), 7.50 (d, J = 8.7 Hz, 2H), 7.17 – 7.10 (m, 1H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$) δ 154.0, 145.5, 140.3, 137.6, 135.1, 130.44, 130.40, 129.0, 118.3 ppm. HRMS (EI): m/z [M+H]$^+$ calcd for $C_{11}H_9ClN_3O_4S$: 313.9997, found: 313.9995.

4-bromo-*N*-(3-nitropyridin-2-yl)benzenesulfonamide (**2t**)



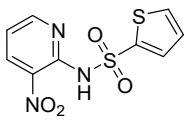
Followed General Procedure on 0.2 mmol scale. Purified *via* column chromatography (PE:EA = 10:1) on silica to obtain **2t**: 62.8 mg, 79% yield; Yellow solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.23 (s, 1H), 8.52 – 8.48 (m, 2H), 8.06 (d, J = 8.7 Hz, 2H), 7.67 (d, J = 8.7 Hz, 2H), 7.16 – 7.10 (m, 1H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$) δ 154.1, 145.4, 138.1, 137.9, 135.1, 132.0, 130.4, 128.9, 118.3 ppm. HRMS (EI): m/z [M+H]$^+$ calcd for $C_{11}H_9BrN_3O_4S$: 357.9492, 359.9471, found: 357.9493, 359.9471.

N-(3-nitropyridin-2-yl)naphthalene-2-sulfonamide (**2u**)



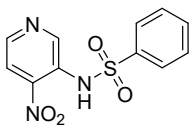
Followed General Procedure on 0.2 mmol scale. Purified *via* column chromatography (PE:EA = 6:1) on silica to obtain **2u**: 39.5 mg, 60% yield; Yellow solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.32 (s, 1H), 8.79 (s, 1H), 8.55 – 8.40 (m, 2H), 8.13 (dd, *J* = 8.7, 1.9 Hz, 1H), 8.02 (d, *J* = 7.8 Hz, 1H), 7.96 (d, *J* = 8.8 Hz, 1H), 7.90 (d, *J* = 7.9 Hz, 1H), 7.72 – 7.56 (m, 2H), 7.06 (dd, *J* = 8.2, 4.8 Hz, 1H) ppm; ^{13}C NMR (101 MHz, CDCl3 δ 154.1, 145.7, 136.0, 135.2, 135.0, 131.8, 130.9, 130.4, 129.5, 129.3, 128.9, 127.9, 127.6, 123.4, 118.0 ppm. HRMS (EI): m/z $[M+H]^+$ calcd for $C_{15}H_{12}N_3O_4S$: 330.0543, found: 330.0549.

N-(3-nitropyridin-2-yl)thiophene-2-sulfonamide (**2v**)



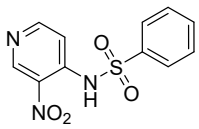
Followed General Procedure on 0.2 mmol scale. Purified *via* column chromatography (PE:EA = 8:1) on silica to obtain **2v**: 29.1 mg, 51% yield; Yellow solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.28 (s, 1H), 8.63 (dd, *J* = 4.6, 1.7 Hz, 1H), 8.53 (dd, *J* = 8.4, 1.7 Hz, 1H), 7.99 (dd, *J* = 3.8, 1.4 Hz, 1H), 7.67 (dd, *J* = 5.0, 1.4 Hz, 1H), 7.17 (dd, *J* = 8.3, 4.7 Hz, 1H), 7.10 (dd, *J* = 5.0, 3.9 Hz, 1H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$) δ 154.0, 145.5, 139.5, 135.2, 135.1, 134.0, 130.4, 127.0, 118.3 ppm. HRMS (EI): m/z $[M+H]^+$ calcd for $C_9H_8N_3O_4S_2$: 285.9951, found: 285.9956.

N-(4-nitropyridin-3-yl)benzenesulfonamide (**2w**)



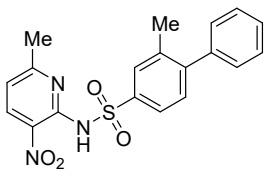
Followed General Procedure on 0.2 mmol scale. Purified *via* column chromatography (PE:EA = 8:1) on silica to obtain **2w**: 45.2 mg, 81% yield; Yellow solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.63 (s, 1H), 8.33 (dd, *J* = 8.4, 1.2 Hz, 1H), 8.28 (dd, *J* = 4.3, 1.3 Hz, 1H), 7.85 (d, *J* = 7.5 Hz, 2H), 7.65 – 7.57 (m, 2H), 7.50 (t, *J* = 7.8 Hz, 2H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.5, 143.0, 138.1, 134.1, 130.7, 130.3, 130.1, 129.6, 127.0 ppm. HRMS (EI): m/z $[M+H]^+$ calcd for $C_{11}H_{10}N_3O_4S$: 280.0387, found: 280.0390.

N-(3-nitropyridin-4-yl)benzenesulfonamide (**2x**)



Followed General Procedure on 0.2 mmol scale. Purified *via* column chromatography (PE:EA = 5:1) on silica to obtain **2x**: 43.5 mg, 78% yield; Yellow solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 10.27 (s, 1H), 9.30 (s, 1H), 8.58 (d, *J* = 5.9 Hz, 1H), 7.99 (d, *J* = 7.8 Hz, 2H), 7.68 (dd, *J* = 19.4, 6.7 Hz, 2H), 7.57 (t, *J* = 7.8 Hz, 2H) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ 155.0, 148.3, 140.8, 138.2, 134.5, 131.7, 129.8, 127.4, 111.7 ppm. HRMS (EI): m/z $[M+H]^+$ calcd for $C_{11}H_{10}N_3O_4S$: 280.0387, found: 280.0390.

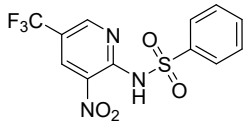
2-methyl-*N*-(6-methyl-3-nitropyridin-2-yl)-[1,1'-biphenyl]-4-sulfonamide (**2aa**)



Followed General Procedure on 0.2 mmol scale. Purified *via* column chromatography (PE:EA = 10:1) on silica to obtain **2aa**: 46.1 mg, 68% yield; Yellow solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.24 (s, 1H), 8.36 (d, *J* = 8.5 Hz, 1H), 8.13 (s, 1H), 8.10 – 8.05 (m, 1H), 7.42 (dt, *J* = 20.8, 7.4 Hz, 4H), 7.33 – 7.27 (m, 2H), 6.92 (d, *J* = 8.5 Hz, 1H), 2.54 (s, 3H), 2.35 (s, 3H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$.) δ 165.3, 147.3, 145.0, 134.0, 137.5, 136.1, 135.0, 130.9, 129.8, 128.7,

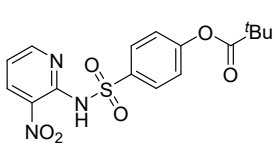
128.3, 128.2, 127.8, 126.7, 118.0, 24.5, 20.5 ppm. HRMS (EI): m/z $[M+H]^+$ calcd for $C_{19}H_{18}N_3O_4S$: 384.1013, found: 384.1017.

N-(3-nitro-5-(trifluoromethyl)pyridin-2-yl)benzenesulfonamide (**2ab**)



Followed General Procedure on 0.2 mmol scale. Purified *via* column chromatography (PE:EA = 8:1) on silica to obtain **2ab**: 54.2 mg, 78% yield; Yellow solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 10.34 (bs, 1H), 8.74 (s, 1H), 8.72 (s, 1H), 8.20 (d, *J* = 8.2 Hz, 2H), 7.65 (t, *J* = 7.5 Hz, 1H), 7.56 (t, *J* = 7.9 Hz, 2H) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ 150.9 (q, *J* = 3.6 Hz), 147.6, 138.6, 134.1, 132.9 (q, *J* = 3.5 Hz), 129.4, 129.0, 128.9, 122.1 (q, *J* = 272.6 Hz), 121.4 (q, *J* = 36.9 Hz) ppm. HRMS (EI): m/z $[M+H]^+$ calcd for $C_{12}H_9F_3N_3O_4S$: 348.0260, found: 348.0268.

4-(*N*-(3-nitropyridin-2-yl)sulfamoyl)phenyl pivalate (**2ac**)



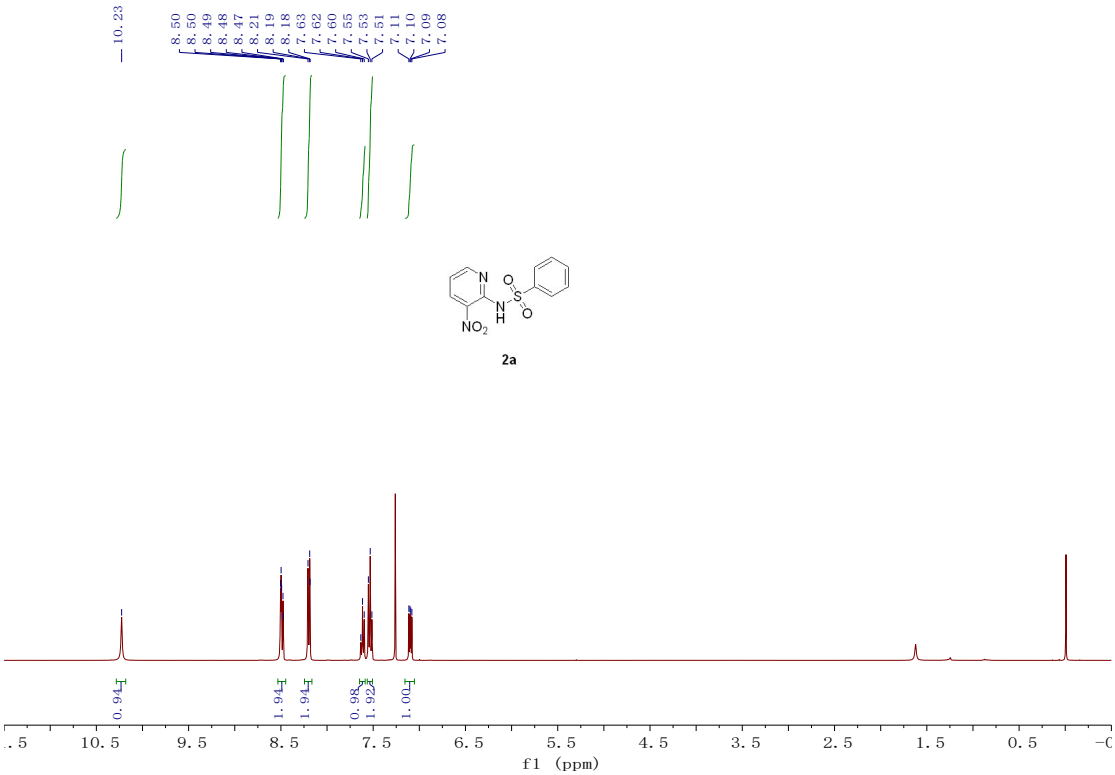
Followed General Procedure on 0.2 mmol scale. Purified *via* column chromatography (PE:EA = 8:1) on silica to obtain **2ac**: 43.0 mg, 64% yield; Yellow solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 10.21 (s, 1H), 8.49 – 8.48 (m, 2H), 8.22 (d, *J* = 8.7 Hz, 2H), 7.23 (d, *J* = 8.7 Hz, 2H), 7.11 – 7.08 (m, 1H), 1.35 (s, 9H) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ 176.3, 155.1, 154.1, 145.6, 136.1, 135.0, 130.7, 130.5, 121.9, 118.1, 39.2, 27.0 ppm. HRMS (EI): m/z $[M+H]^+$ calcd for $C_{16}H_{18}N_3O_6S$: 380.0911, found: 380.0916.

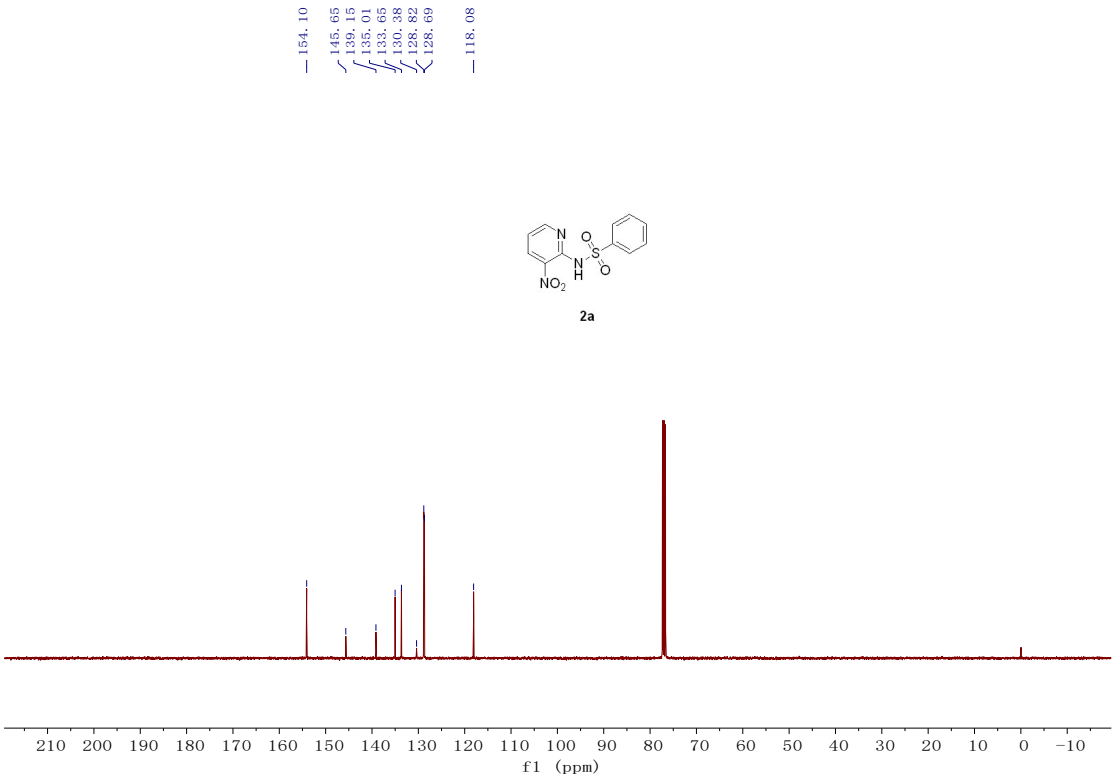
6. References

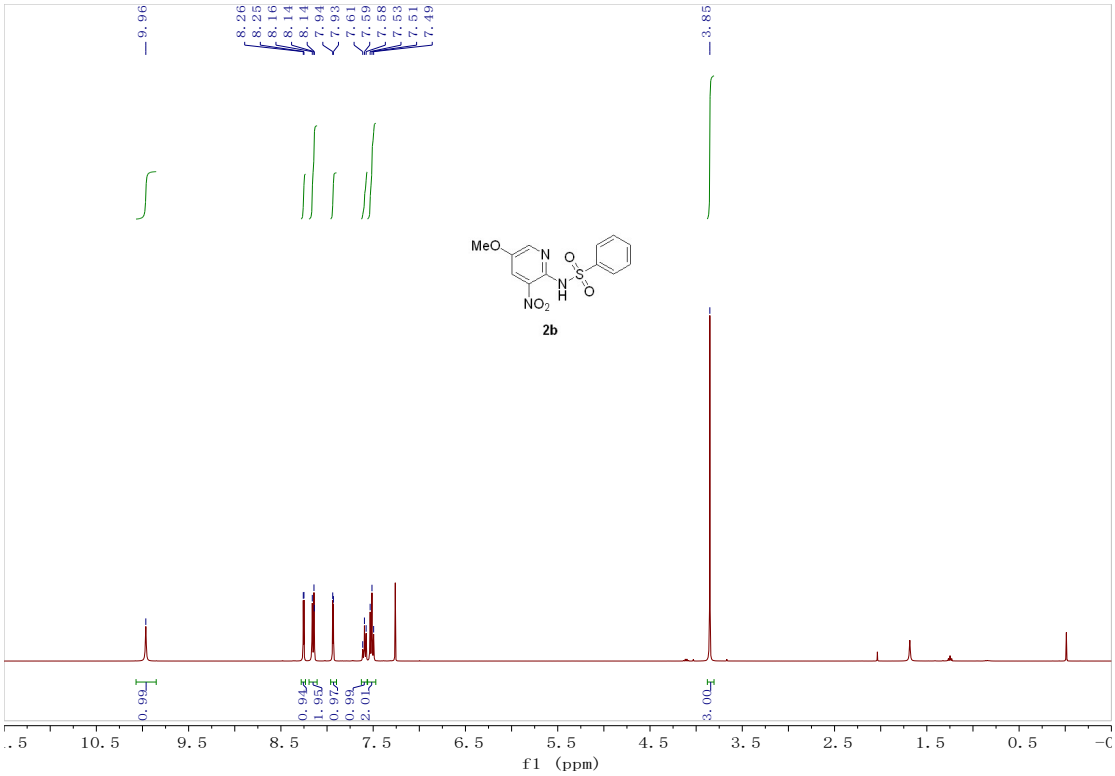
1. (a) X. Wang, A. Guram, M. Ronk, J. E. Milne, J. S. Tedrow and M. M. Faul, Copper-catalyzed *N*-arylation of sulfonamides with aryl bromides under mild conditions, *Tetrahedron Lett*, 2012, **53**, 7-10. (b) R. Adams and Leslie M. Werbel, Preparation of Quinol Imide Acetates. VI. Scope and Limitations, *J. Am. Chem. Soc*. 1958, **80**, 5799-5803. (c) J. P. English, J. H. Clark, R. G. Shepherd, H. W. Marson, J. Krapcho, and R. O. Roblin Jr, Studies in Chemotherapy. XIV. Antimalarials. The Synthesis of Substituted Metanilamides and Related Compounds[1], *J. Am. Chem. Soc*. 1946, **68**, 1039-1049. (d) S. Ayesa, C. Lindquist, T. Agback, K. Benkestock, B. Classon, I. Henderson, E. Hewitt, K. Jansson, A. Kallin, D. Sheppard and B. Samuelsson, Solid-phase parallel synthesis and SAR of 4-amidofuran-3-one inhibitors of cathepsin S: Effect of sulfonamides P3 substituents on potency and selectivity, *Bioorg. Med. Chem*., 2009, **17**,1307-1324. (e) S. Elbasil, K. M. Ghoneim, M. Khalifa and Y. M. Abouzeid, Synthesis of Certain N^1- andN^4-(5-Nitro-2-pyridyl) -Substituted Sulfonamides, *J. Pharm. Sci*., 1969, **58**, 907-909. (f) R. T. McGuire, C. M. Simon, A. A. Yadav, M. J. Ferguson and M Stradiotto, Nickel-Catalyzed Cross-Coupling of Sulfonamides With (Hetero)aryl Chlorides, *Angew. Chem. Int. Ed*., 2020, **59**, 8952-8956. (g) J. W. Chittum, C. G. Tindall, R. D. Howells, V. Coates and M. D. Shie, Benzenesulfonamides of primary aminopyridines and primary aminoquinolines, *J. Chem. Eng. Data*, 1974, **19**, 294-295. (h) A. Polley, G. Bairy, P. Das and R. Jana, Triple Mode of Alkylation with Ethyl Bromodifluoroacetate: *N*, or *O*-Difluoromethylation, *N*-Ethylation and *S*-(ethoxycarbonyl)difluoromethylation, *Adv. Synth. Catal*., 2018, **360**, 4161-4167. (h) H. Dorn and G Hilgetag, Strukturen und N → N′-Sulfonyl-Wanderung der Bis-arylsulfonyl-Derivate des 2-Amino-pyridins, 1964, **97**, 695-703. (i) T. A. Mastrukova, Y. N. SheinkerI, K. Kuznetsova, E. M. Peresleni, T. B. Sakharova and M. I. Kabachnik, The application of the Hammett equation to the theory of tautomeric equilibrium-II: Tautomerism of *α*-arylsulphaminopyridines, *Tetrahedron*, 1963, **19**, 357-372. (j) S. S. Chourasiya, D. Patel, C. M. Nagaraja, A. K. Chakraborti and P. V. Bharatam, *New J. Chem*., 2017, **41**, 8118-8129. (k) A. Arcoria, E. Maccarone, G. Musumarra

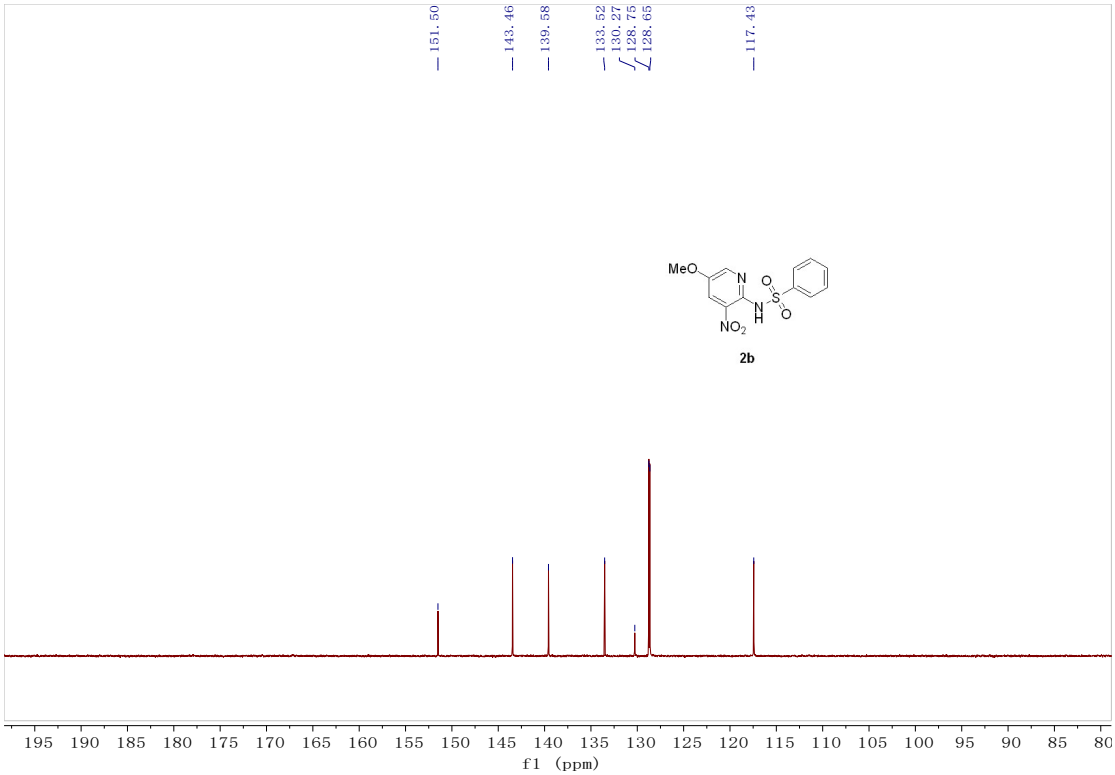
and G. A. Tomaselli, Ultraviolet and infrared absorption spectra of 2-thiophenesulfonamides, *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*, 1974, **30**, 611-618. (l) J. W. Chittum, C. G. Tindall, R. D. Howells, W. Coates and M. D. Shie, Benzenesulfonamides of primary aminopyridines and primary aminoquinolines. *J. Chem. Eng. Data*. 1974, **19**, 294-295. (m) K. Imaki, T. Okada, Y. Nakayama, Y. Nagao, K. Kobayashi, Y. Sakai, T. Mohri, T. Amino, K. Nakai and M. Kawamura, Non-peptidic inhibitors of human neutrophil elastase: the design and synthesis of sulfonanilide-containing inhibitors. *Bioorgan. Med. Chem.* 1996, **4**, 2115-2134.; (n) M. Kheirabadi, G. S. Creech, J. X. Qiao, D. S. Nirschl, D. K. Leahy, K. M. Boy, P. H. Carter and M. D. Eastgate, Leveraging a "Catch-Release" logic gate process for the synthesis and nonchromatographic purification of thioether- or amine-bridged macrocyclic peptides. *J. Org. Chem.* 2018, **83**, 4323-4335.

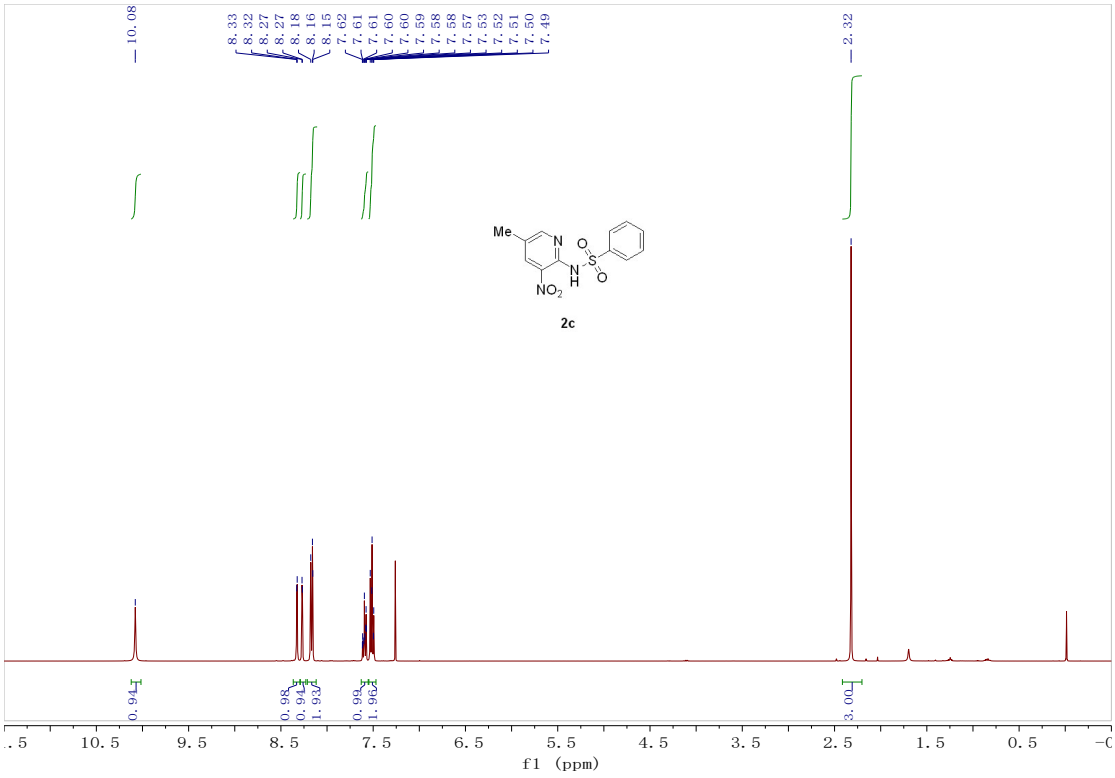
7. ^{1}H and ^{13}C NMR spectra

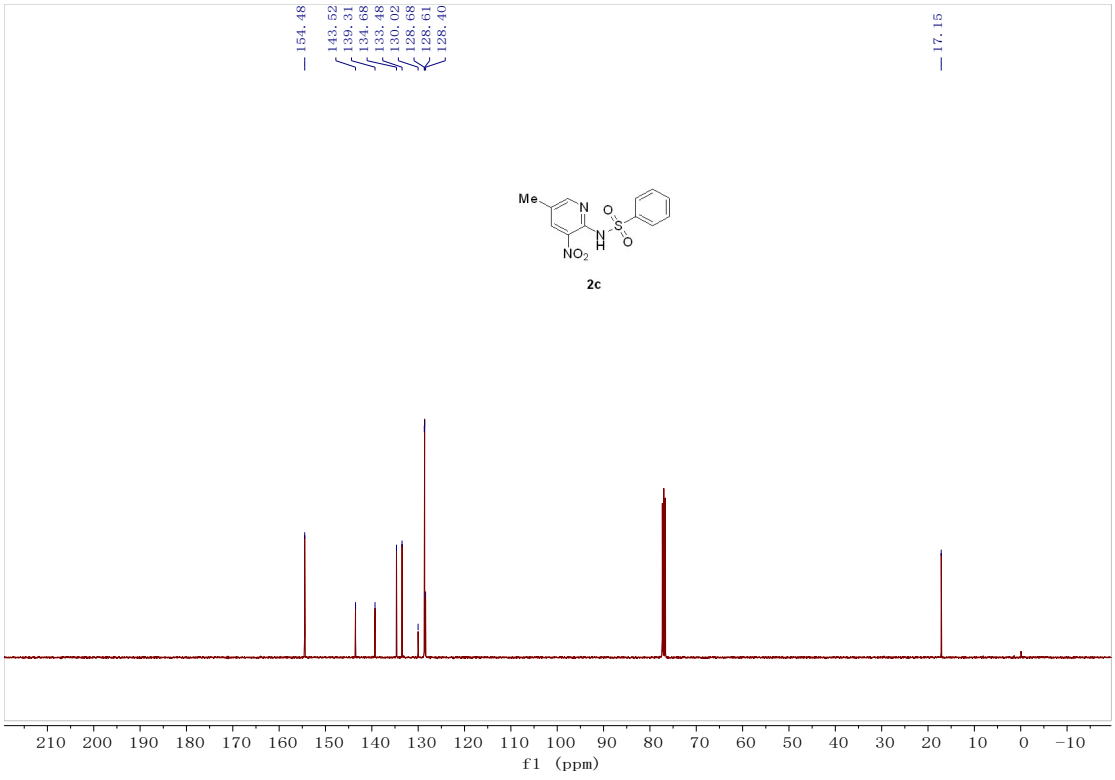


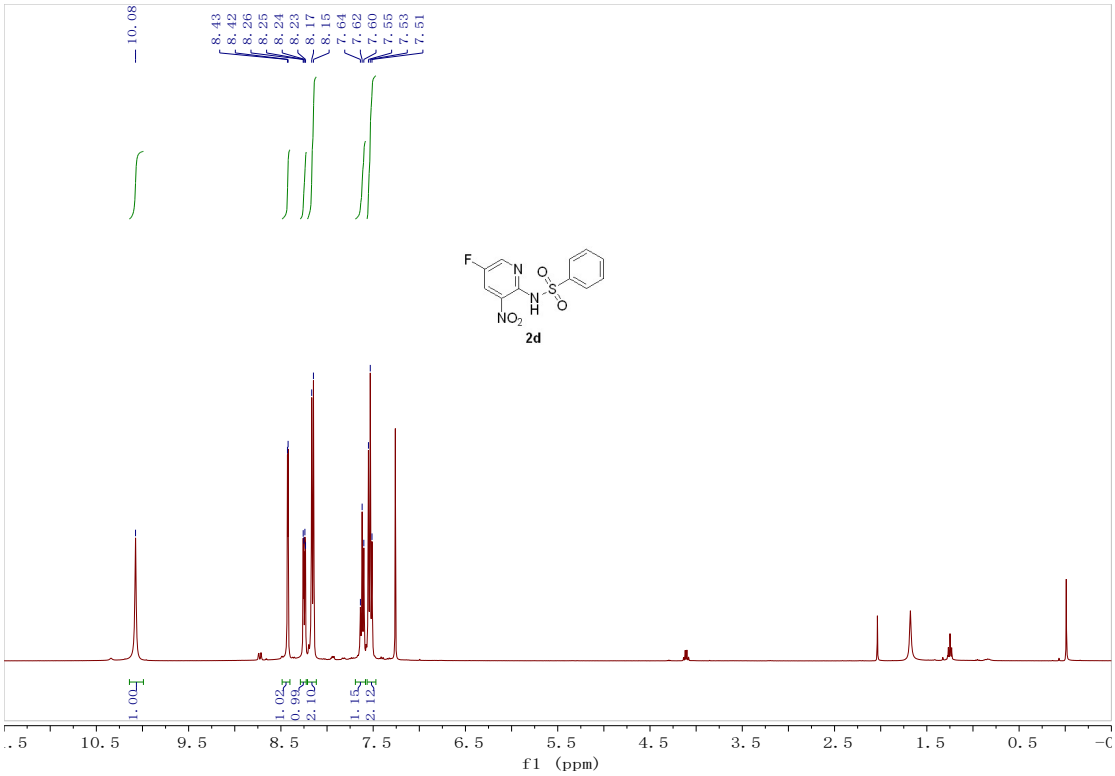


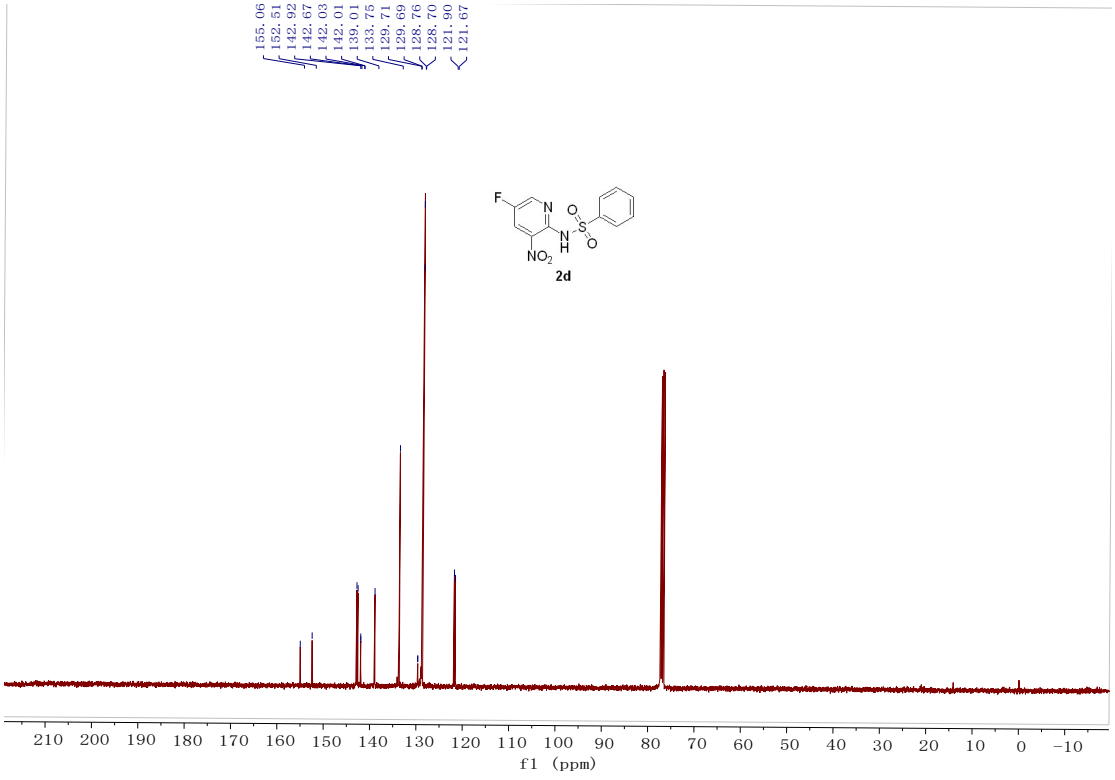

9.96
8.26
8.25
8.16
8.14
8.14
7.94
7.93
7.61
7.59
7.58
7.53
7.51
7.49
3.85
MeO
N
O
S
O
N
H
NO2
2b
0.99
0.94
1.95
0.97
0.99
2.01
3.00
f1 (ppm)

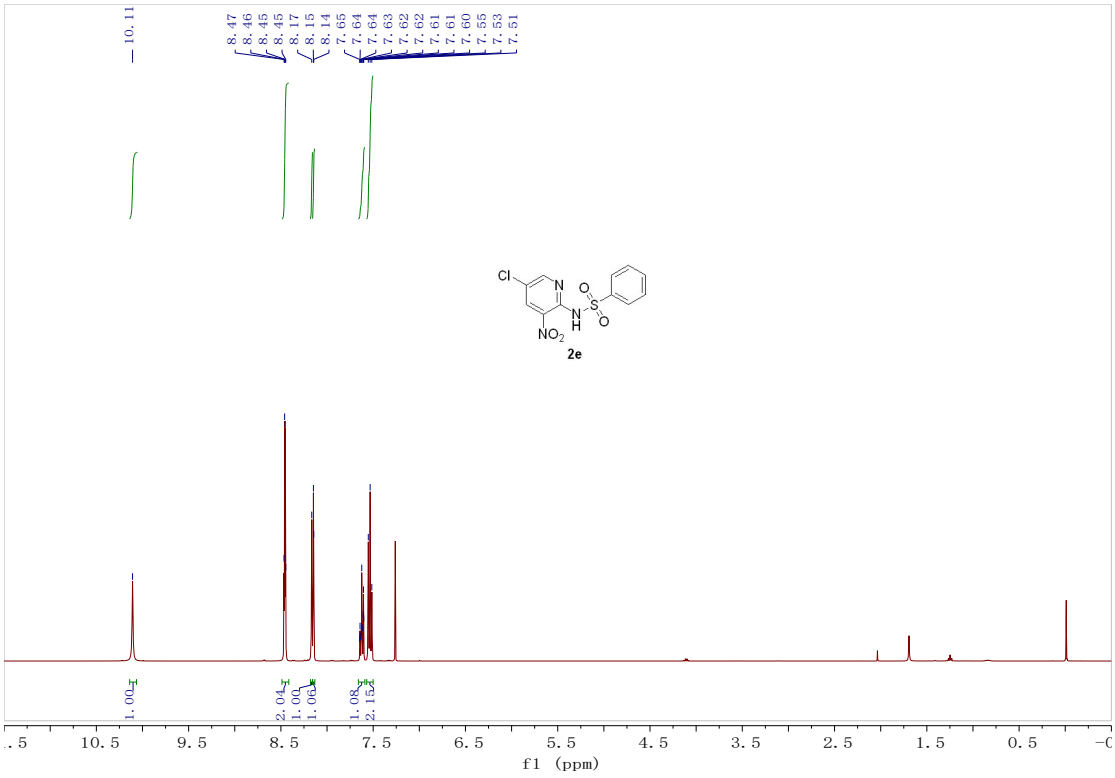

151.50
143.46
139.58
133.52
130.27
128.75
128.65
117.43
MeO
N
O
S
O
N
H
NO2
2b
f1 (ppm)

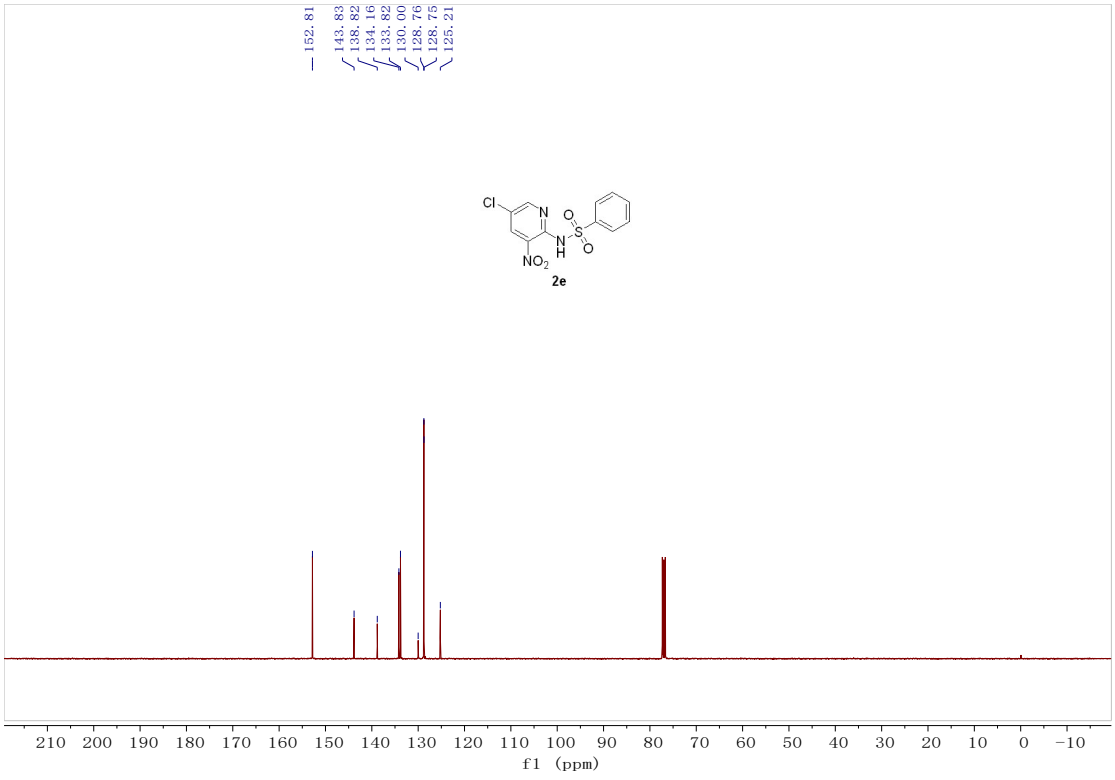

10.08
8.33
8.32
8.27
8.27
8.18
8.16
8.15
7.62
7.61
7.61
7.60
7.60
7.59
7.58
7.58
7.57
7.53
7.52
7.51
7.50
7.49
2.32
Me
N
O
S
N
H
O
NO2
2c
0.94
0.98
0.94
1.93
0.99
1.96
3.00
f1 (ppm)

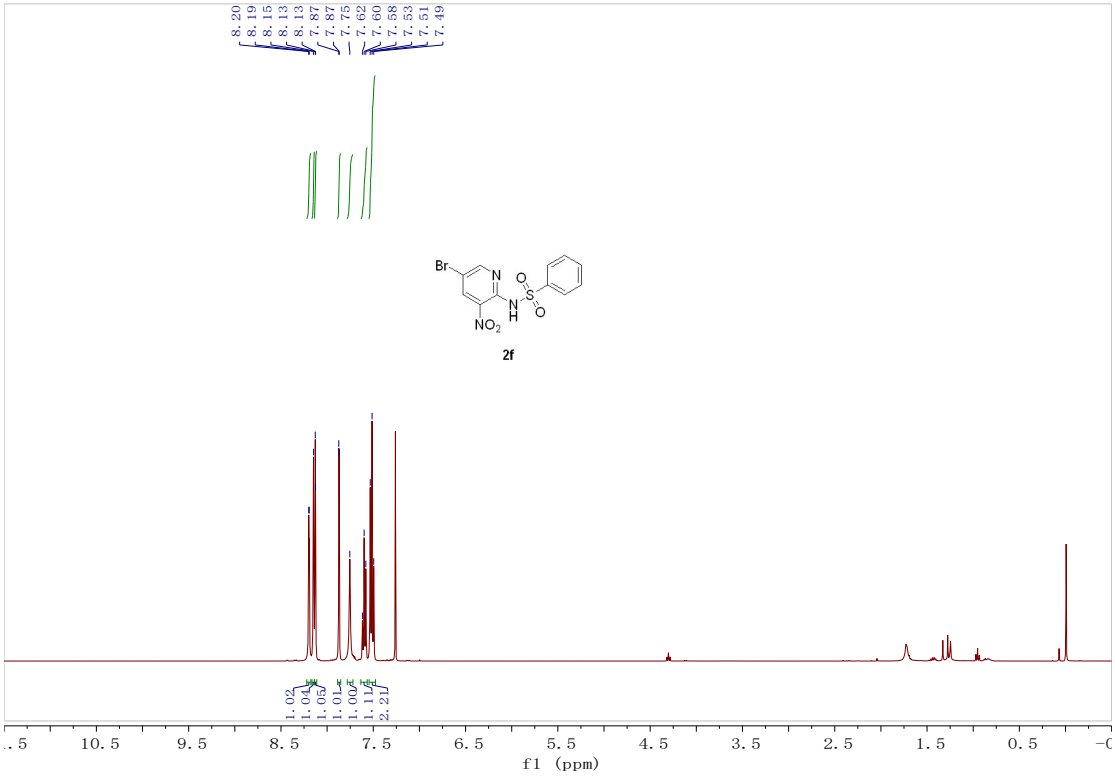

154.48
143.52
139.31
134.68
133.48
130.02
128.68
128.61
128.40
17.15
Me
N
O
S
N
H
O
NO2
2c
f1 (ppm)

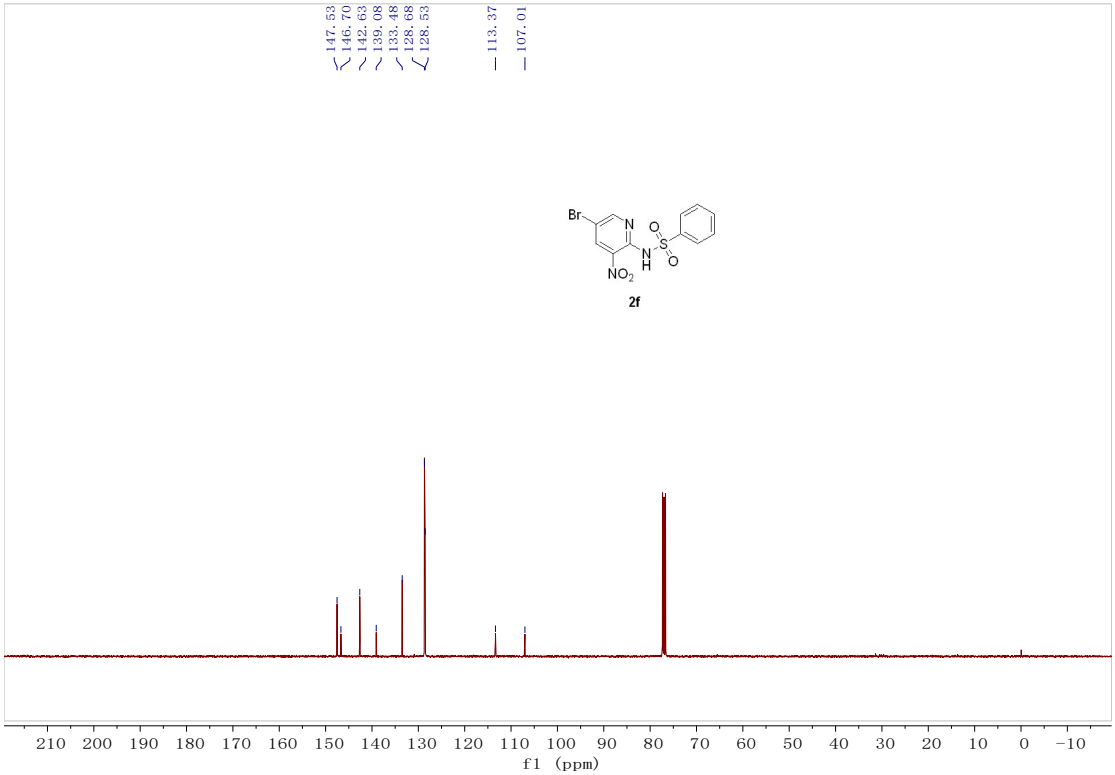

10.08
8.43
8.42
8.26
8.25
8.24
8.23
8.17
8.15
7.64
7.62
7.60
7.55
7.53
7.51
F
N
O
S
O
N
H
NO2
2d
1.00
1.02
0.99
2.10
1.15
2.12
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)

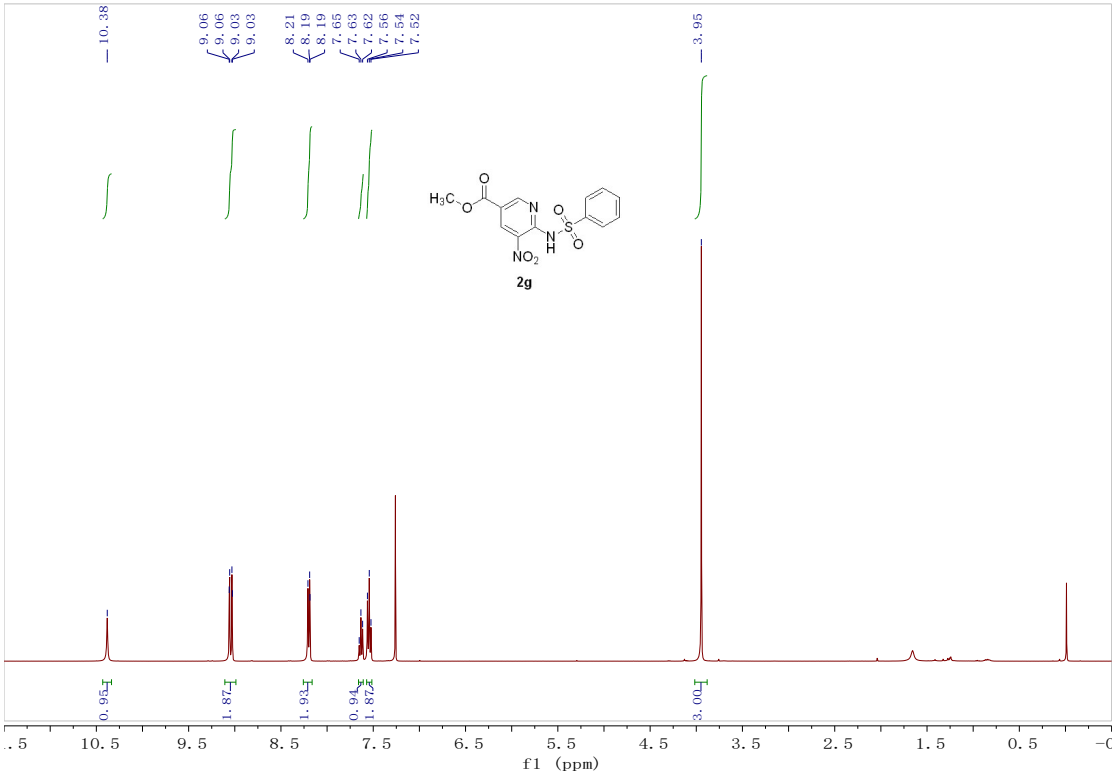

155.06
152.51
142.92
142.67
142.03
142.01
139.01
133.75
129.71
129.69
128.76
128.70
121.90
121.67
F
N
O
S
O
N
H
NO2
2d
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)


10.11
8.47
8.46
8.45
8.45
8.17
8.15
8.14
7.65
7.64
7.64
7.63
7.62
7.62
7.61
7.61
7.60
7.55
7.53
7.51
Cl
N
O
S
N
H
O
O
NO2
2e
1.00
2.04
1.00
1.08
2.15
f1 (ppm)

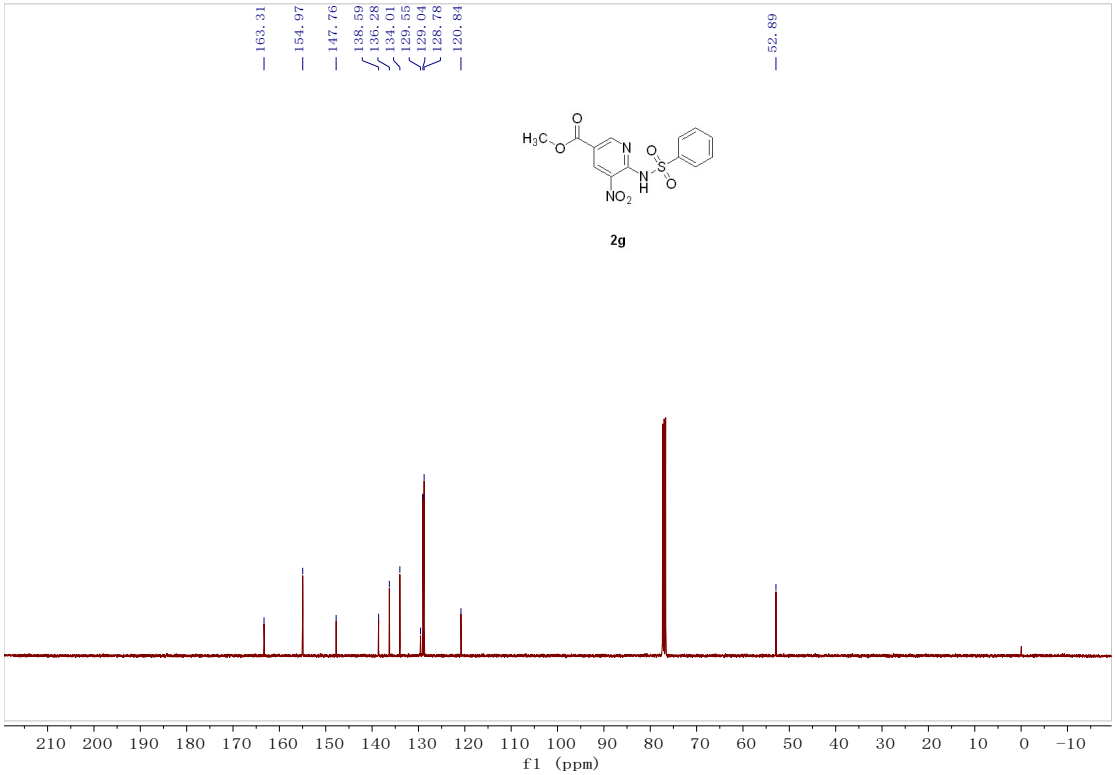

152.81
143.83
138.82
134.16
133.82
130.00
128.76
128.75
125.21
Cl
N
O
S
N
H
O
O
NO2
2e
f1 (ppm)


8.20
8.19
8.15
8.13
8.13
7.87
7.87
7.75
7.62
7.60
7.58
7.53
7.51
7.49
Br
N
O
S
O
N
H
NO2
2f
1.02
1.04
1.05
1.01
1.00
1.11
2.21
f1 (ppm)

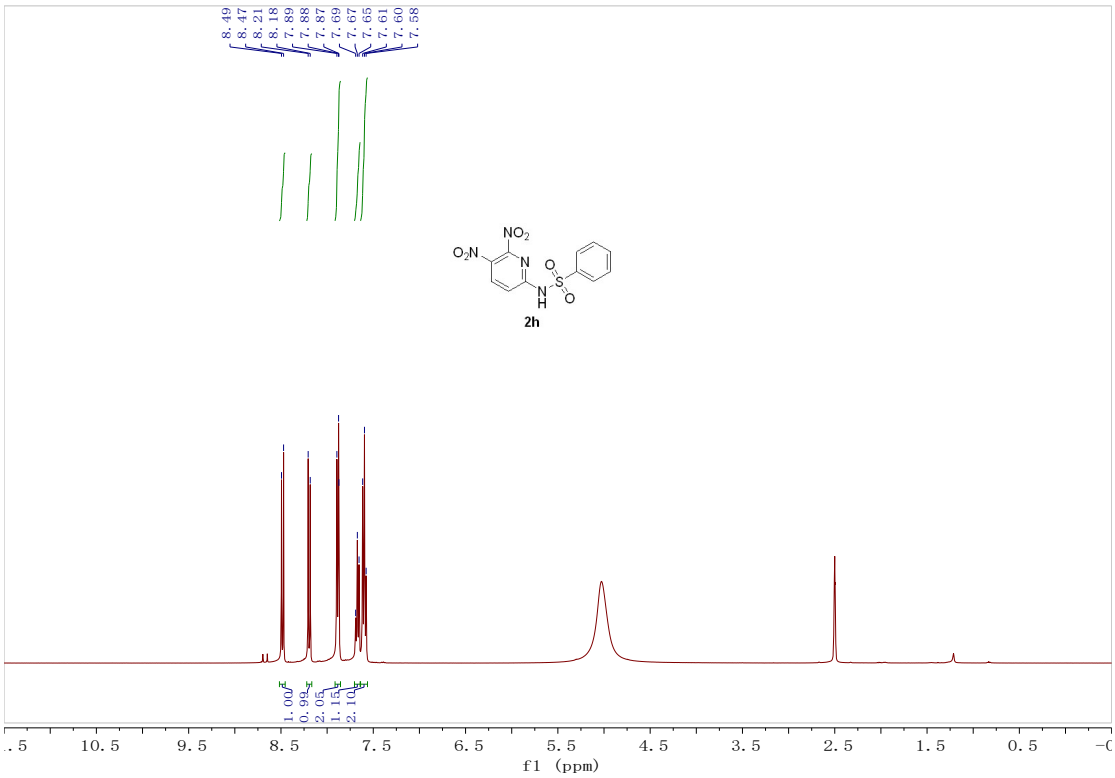

147.53
146.70
142.63
139.08
133.48
128.68
128.53
113.37
107.01
Br
N
O
S
O
N
H
NO2
2f
f1 (ppm)

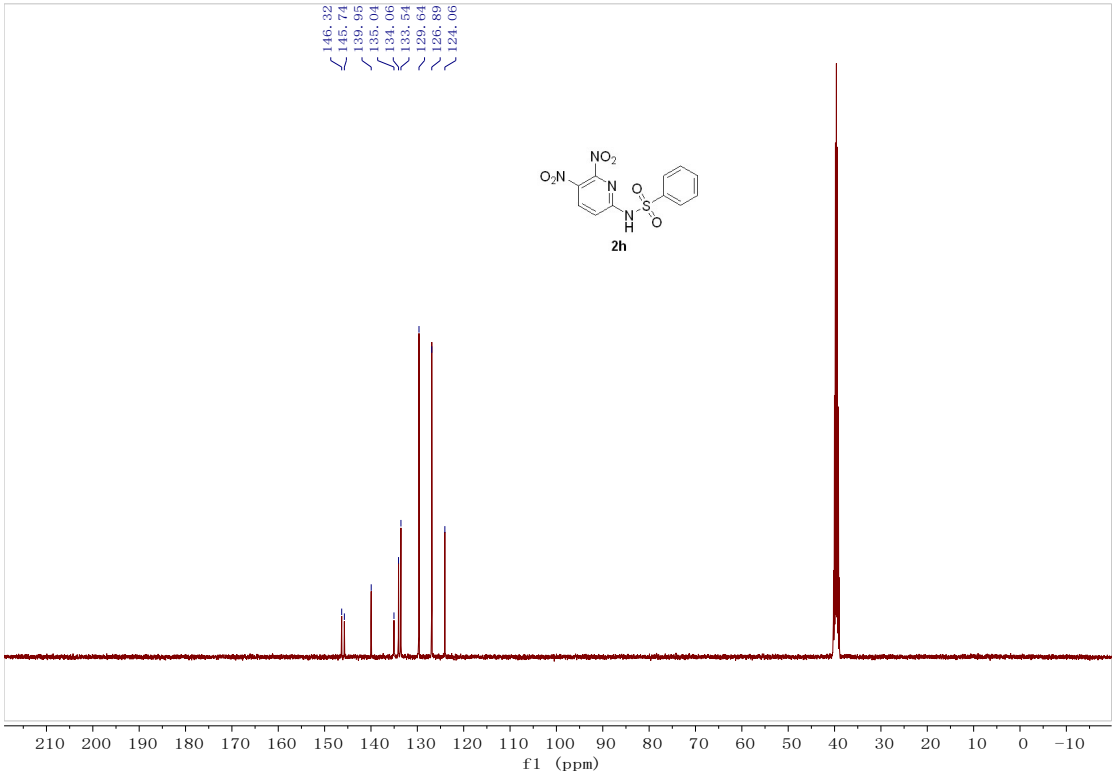

10.38
9.06
9.06
9.03
9.03
8.21
8.19
8.19
7.65
7.63
7.62
7.56
7.54
7.52
3.95
0.95
1.87
1.93
0.94
1.87
3.00
f1 (ppm)

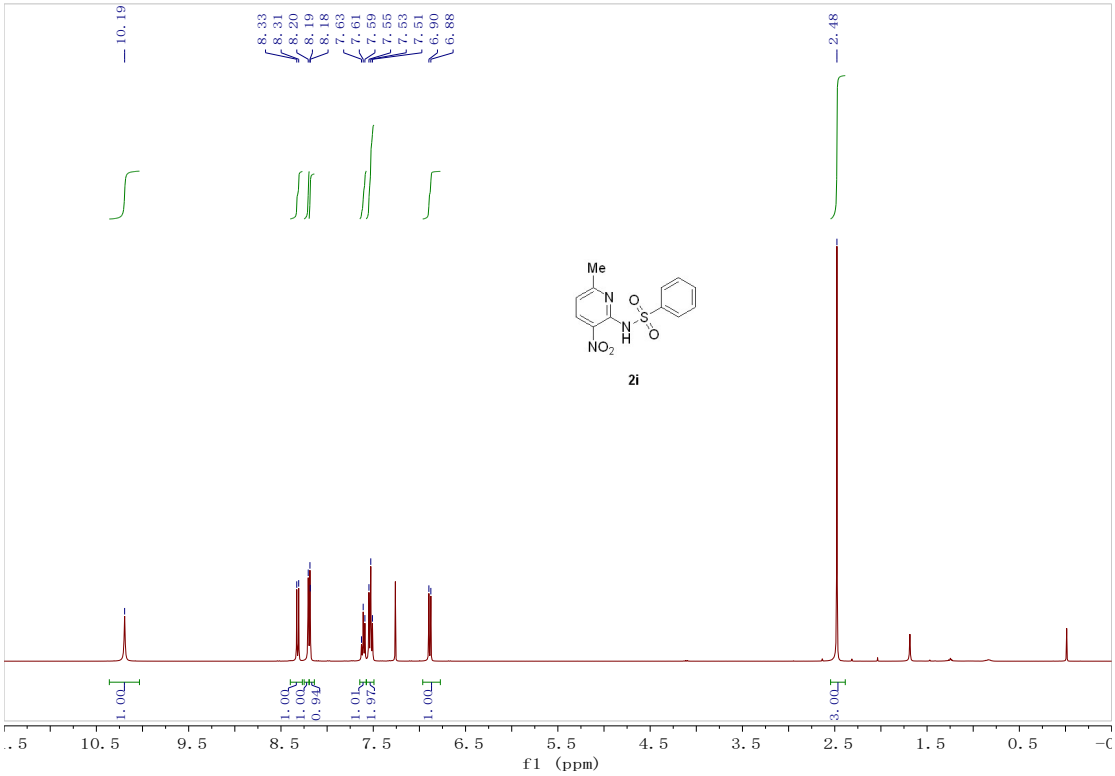
2g

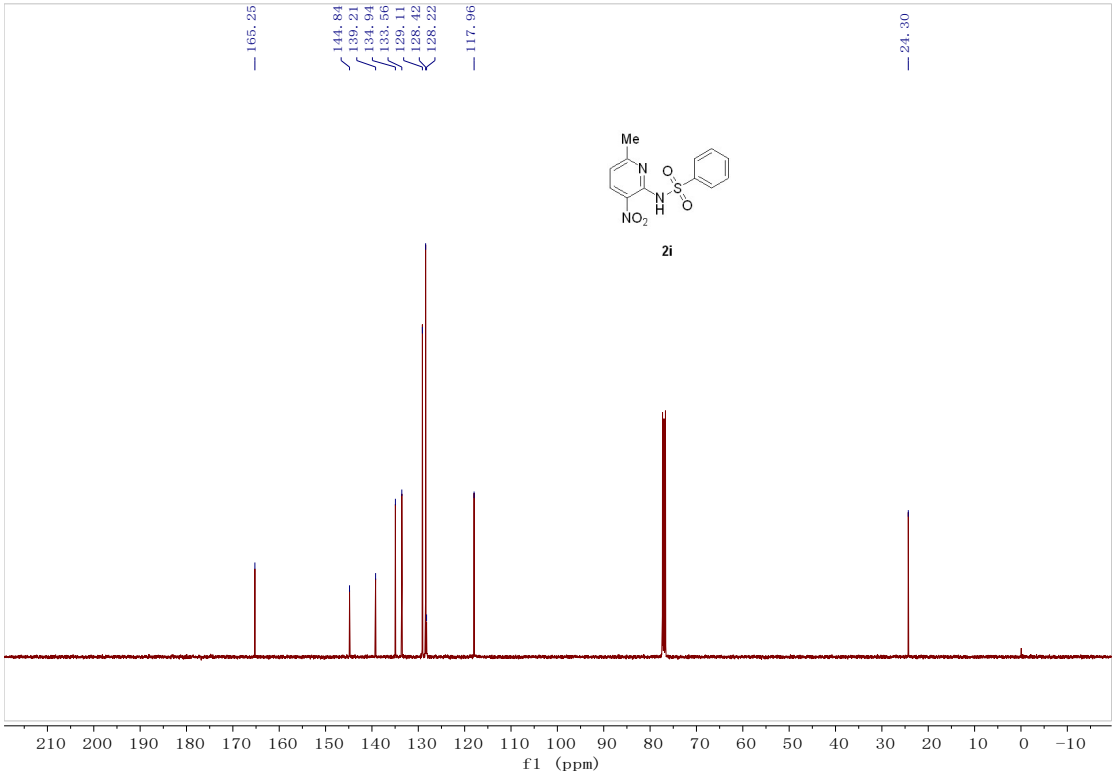

163.31
154.97
147.76
138.59
136.28
134.01
129.55
129.04
128.78
120.84
52.89
f1 (ppm)

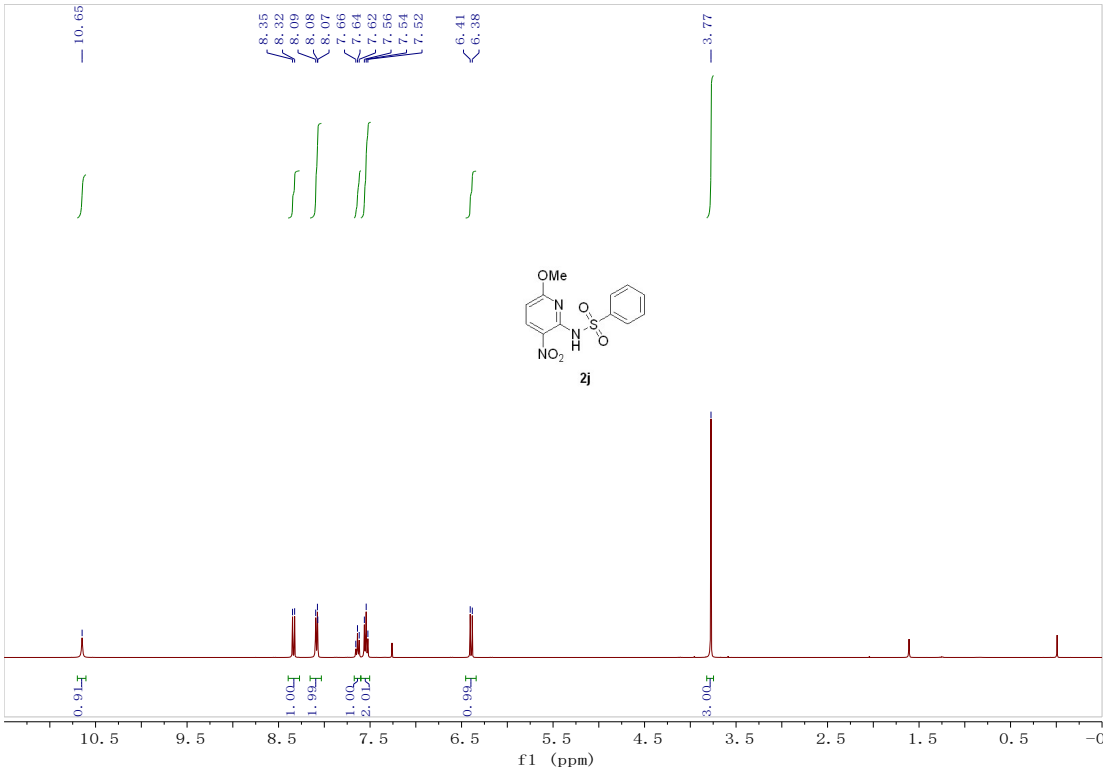
2g

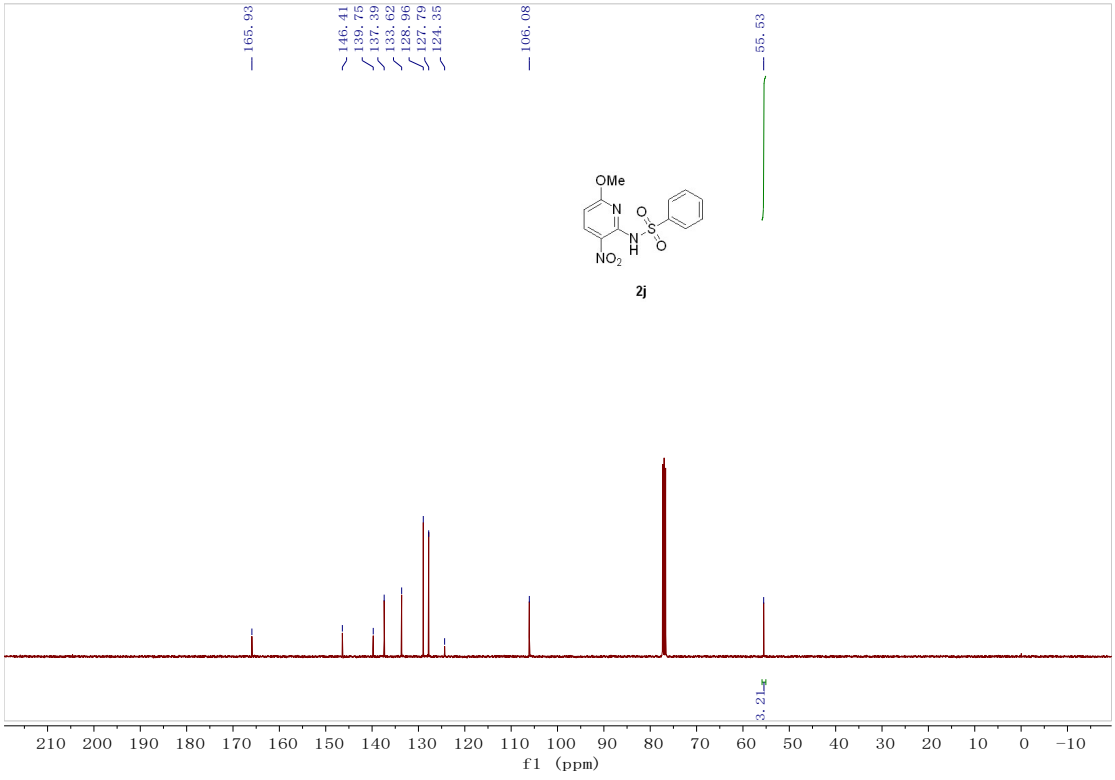

8.49
8.47
8.21
8.18
7.89
7.88
7.87
7.69
7.67
7.65
7.61
7.60
7.58
NO2
O2N
N
O
S
O
N
H
2h
1.00
0.99
2.05
1.15
2.10
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)

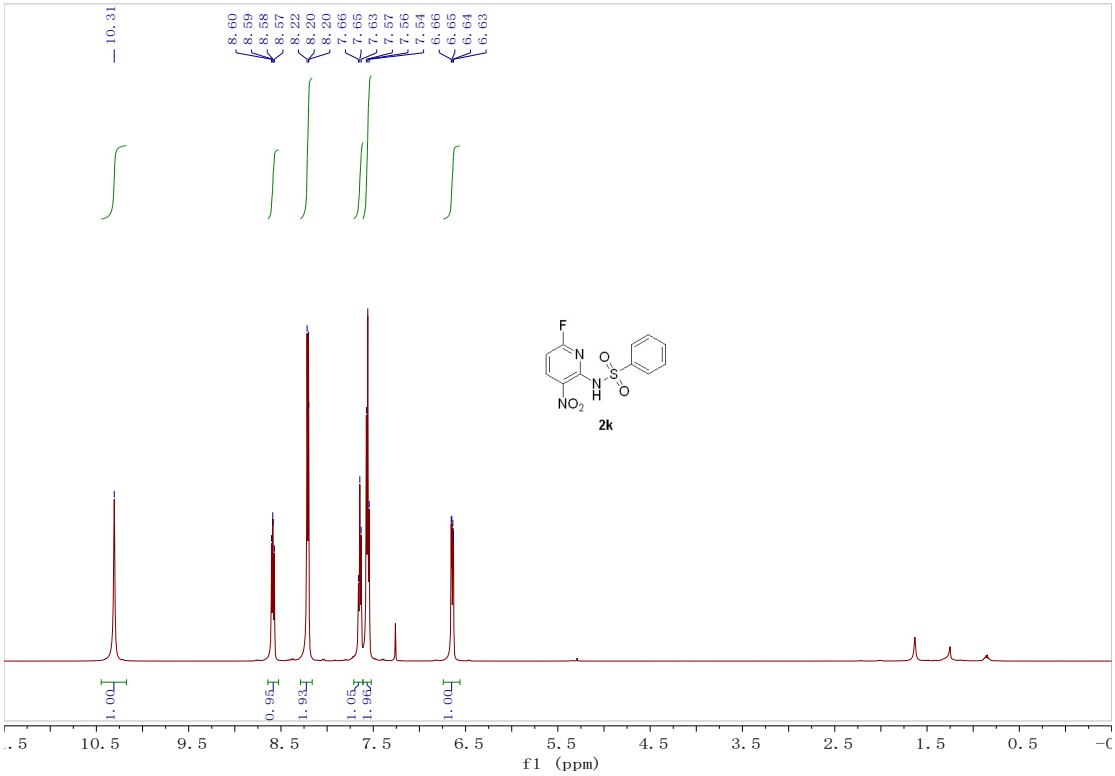

146.32
145.74
139.95
135.04
134.06
133.54
129.64
126.89
124.06
NO2
O2N
N
O
S
O
N
H
2h
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

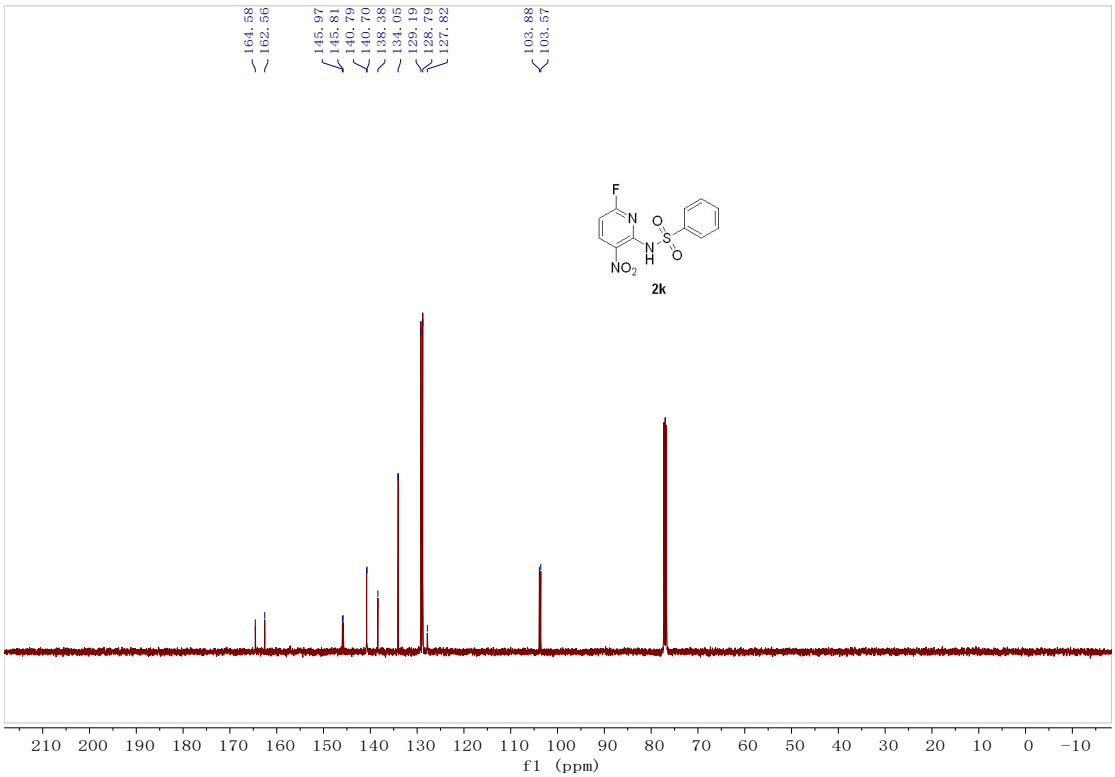

10.19
8.33
8.31
8.20
8.19
8.18
7.63
7.61
7.59
7.55
7.53
7.51
6.90
6.88
2.48
Me
N
O
S
N
H
O
NO2
2i
1.00
1.00
0.94
1.01
1.97
1.00
3.00
f1 (ppm)

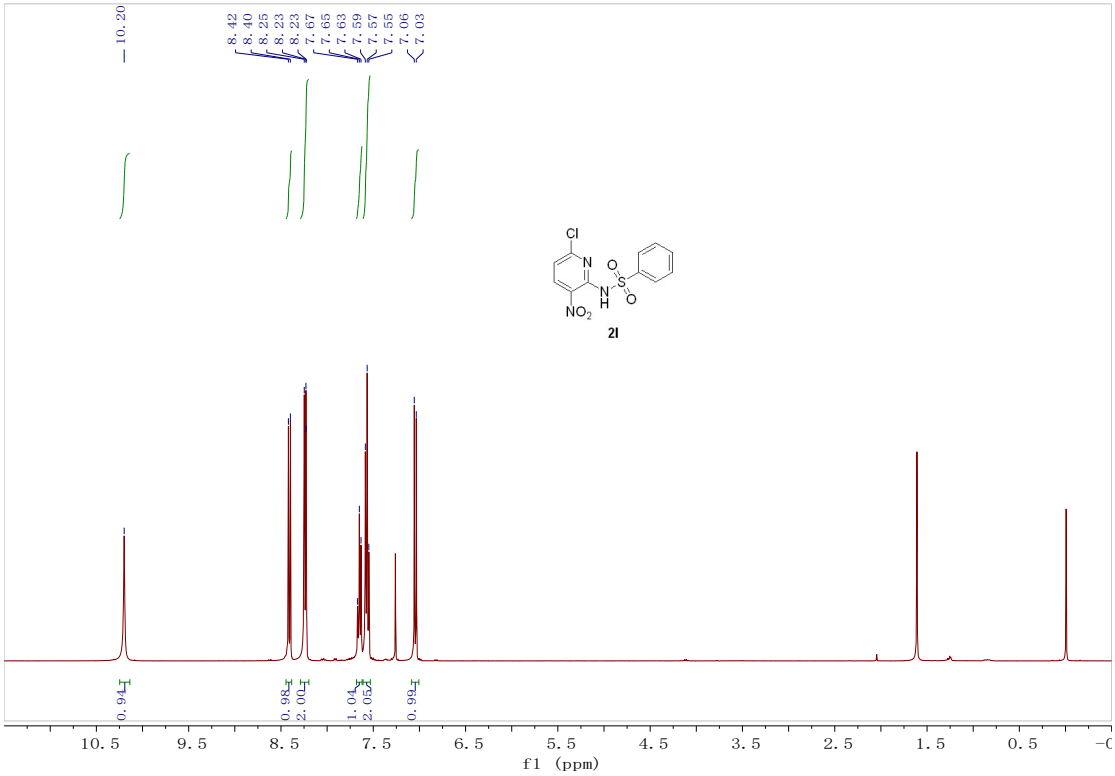

165.25
144.84
139.21
134.94
133.56
129.11
128.42
128.22
117.96
24.30
Me
N
O
S
N
H
O
NO2
2i
f1 (ppm)

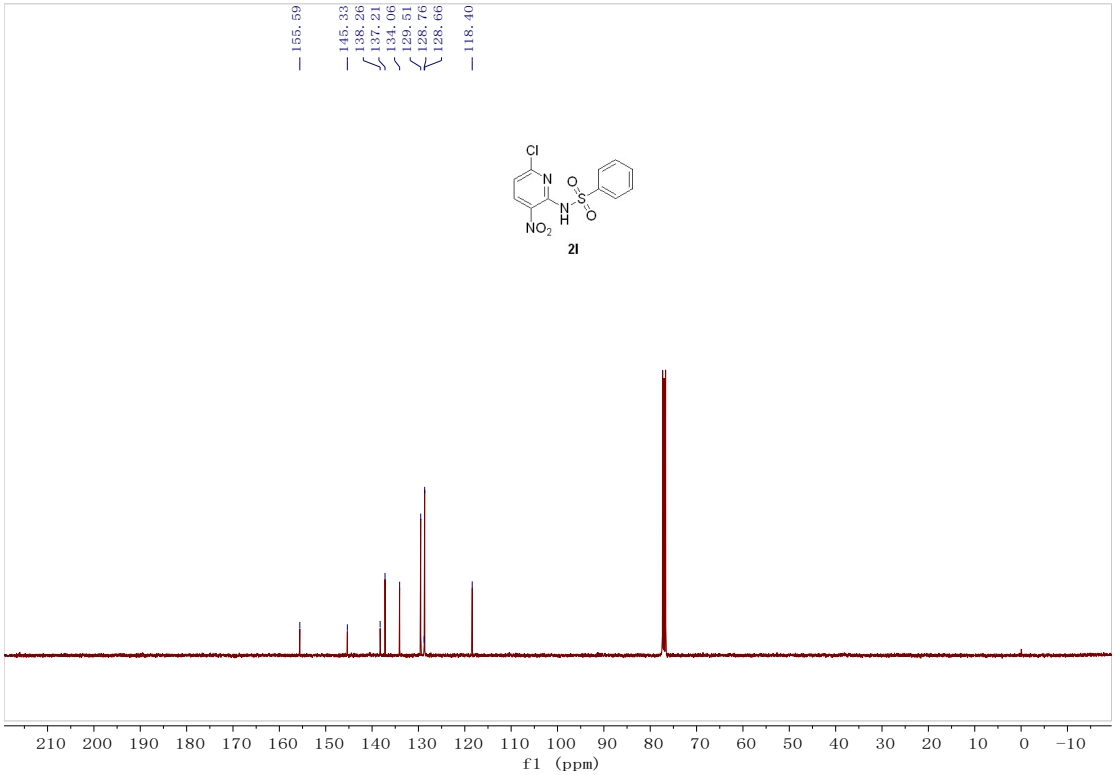

10.65
8.35
8.32
8.09
8.08
8.07
7.66
7.64
7.62
7.56
7.54
7.52
6.41
6.38
3.77
OMe
N
O
S
O
N
H
NO2
2j
0.91
1.00
1.99
1.00
2.01
0.99
3.00
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)

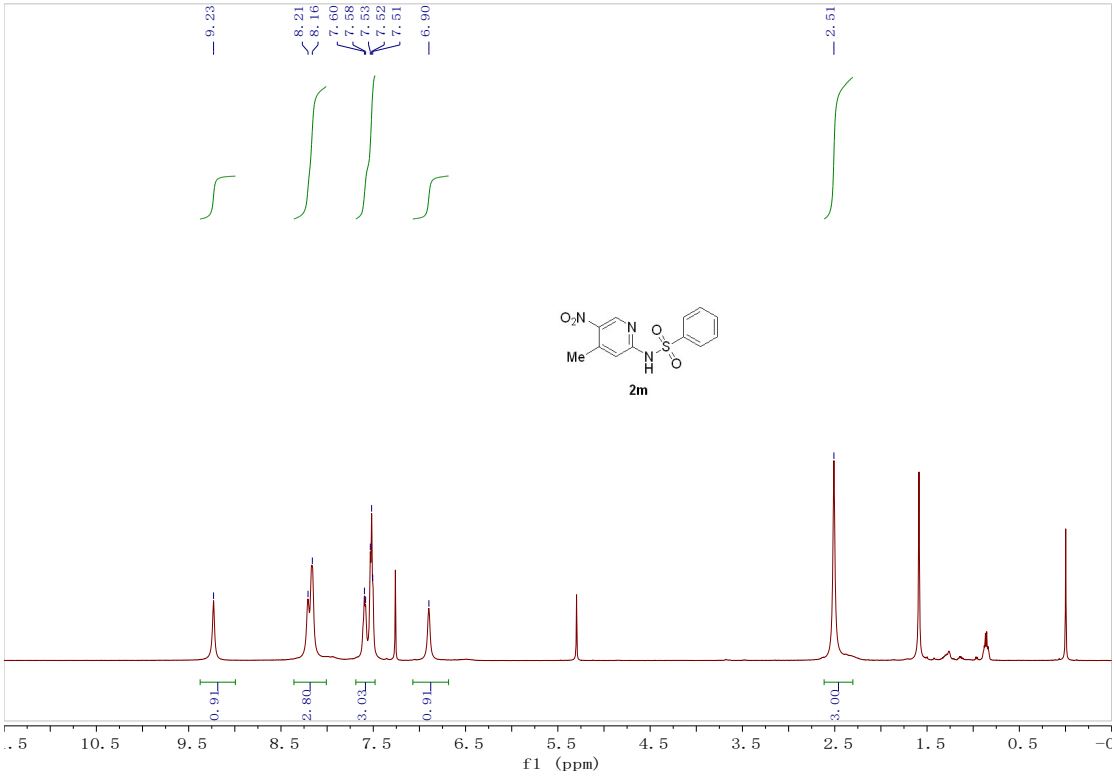

165.93
146.41
139.75
137.39
133.62
128.96
127.79
124.35
106.08
55.53
OMe
N
O
S
O
N
H
NO2
2j
3.21
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

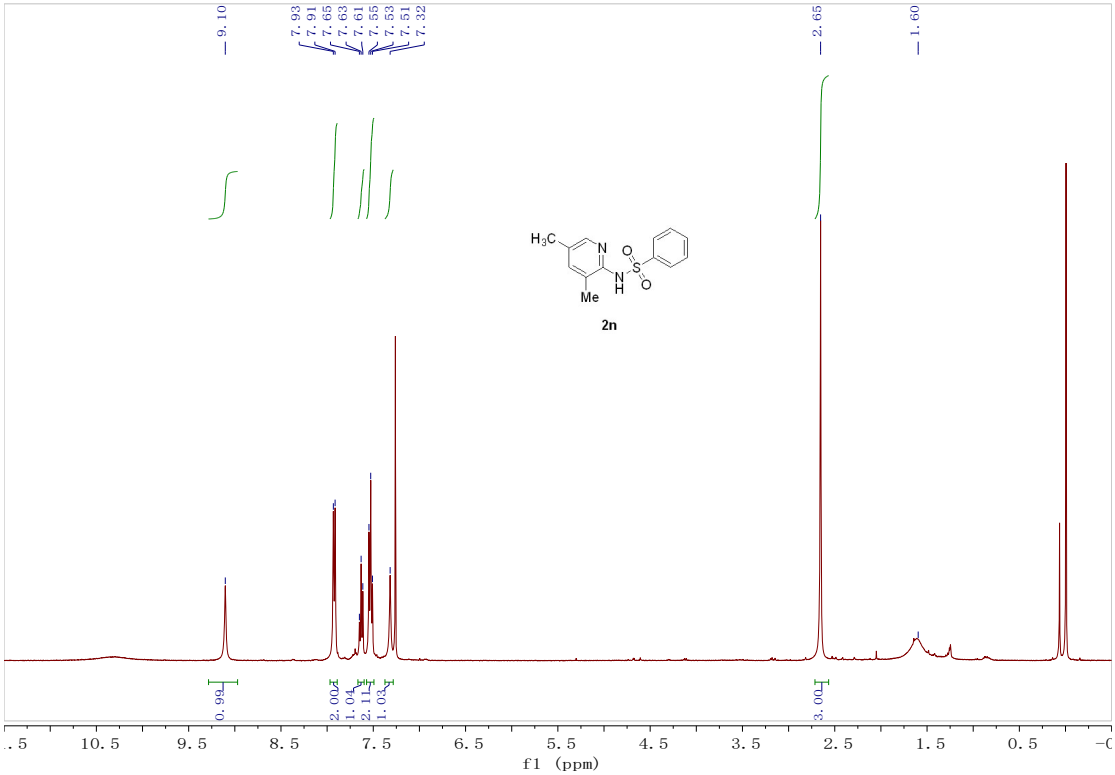

10.31
8.60
8.59
8.58
8.57
8.22
8.20
8.20
7.66
7.65
7.63
7.57
7.56
7.54
6.66
6.65
6.64
6.63
F
N
O
S
O
N
H
NO2
2k
1.00
0.95
1.93
1.05
1.96
1.00
f1 (ppm)

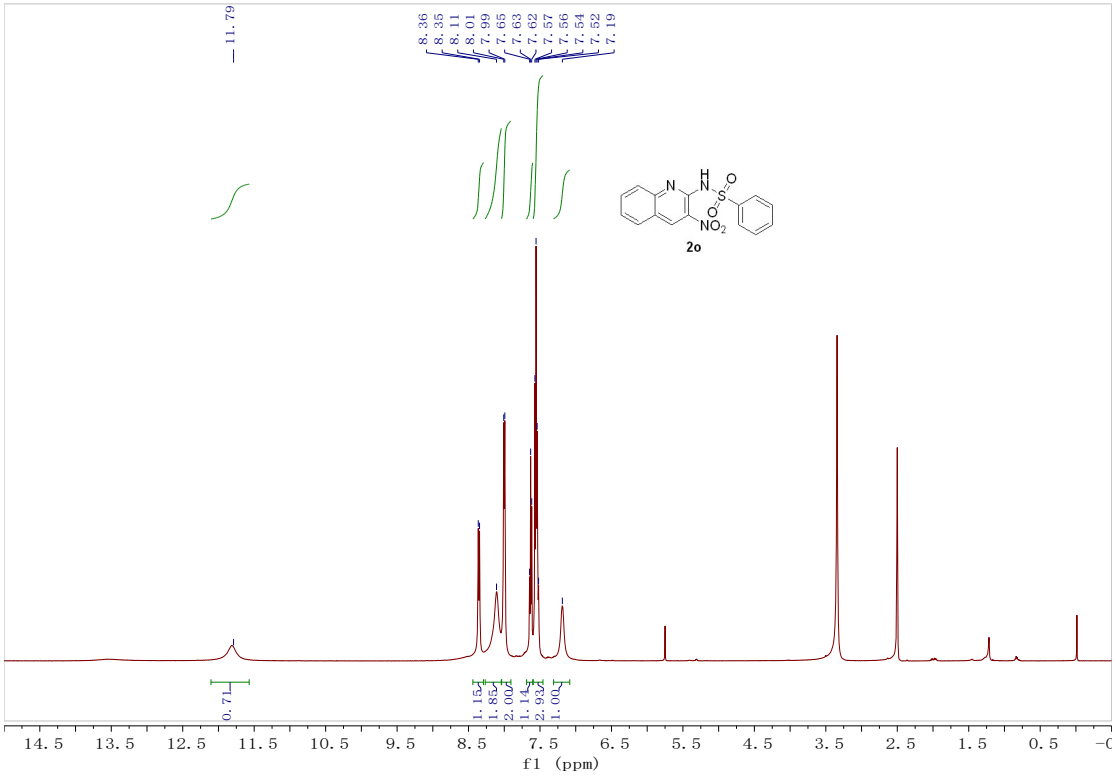

164.58
162.56
145.97
145.81
140.79
140.70
138.38
134.05
129.19
128.79
127.82
103.88
103.57
F
N
O
S
O
N
H
NO2
2k
f1 (ppm)

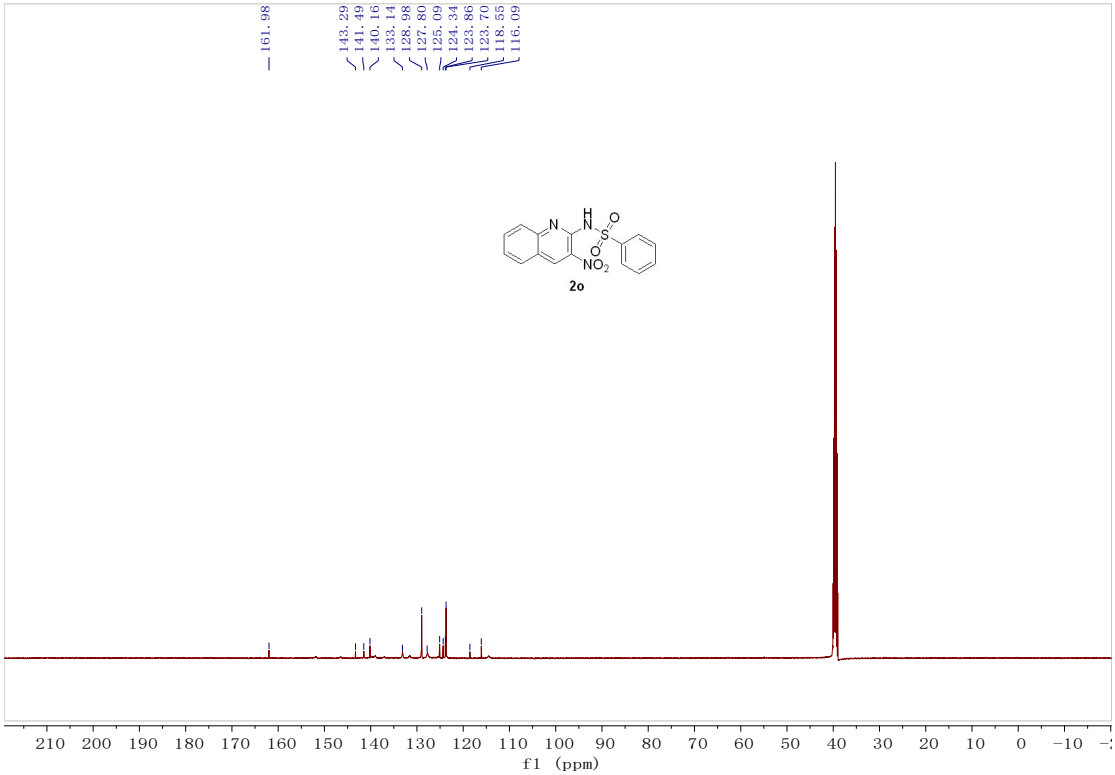

10.20
8.42
8.40
8.25
8.23
8.23
7.67
7.65
7.63
7.59
7.57
7.55
7.06
7.03
Cl
N
O
S
O
N
H
NO2
2l
0.94
0.98
2.00
1.04
2.05
0.99
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)

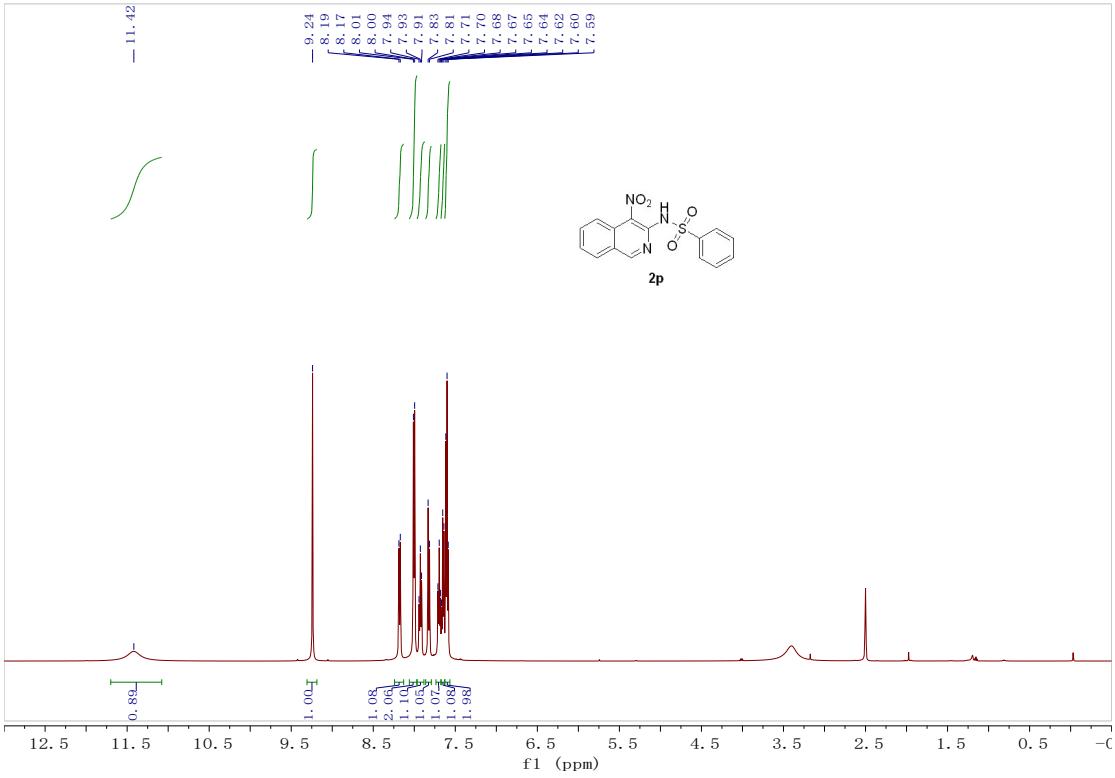

155.59
145.33
138.26
137.21
134.06
129.51
128.76
128.66
118.40
Cl
N
O
S
O
N
H
NO2
2l
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

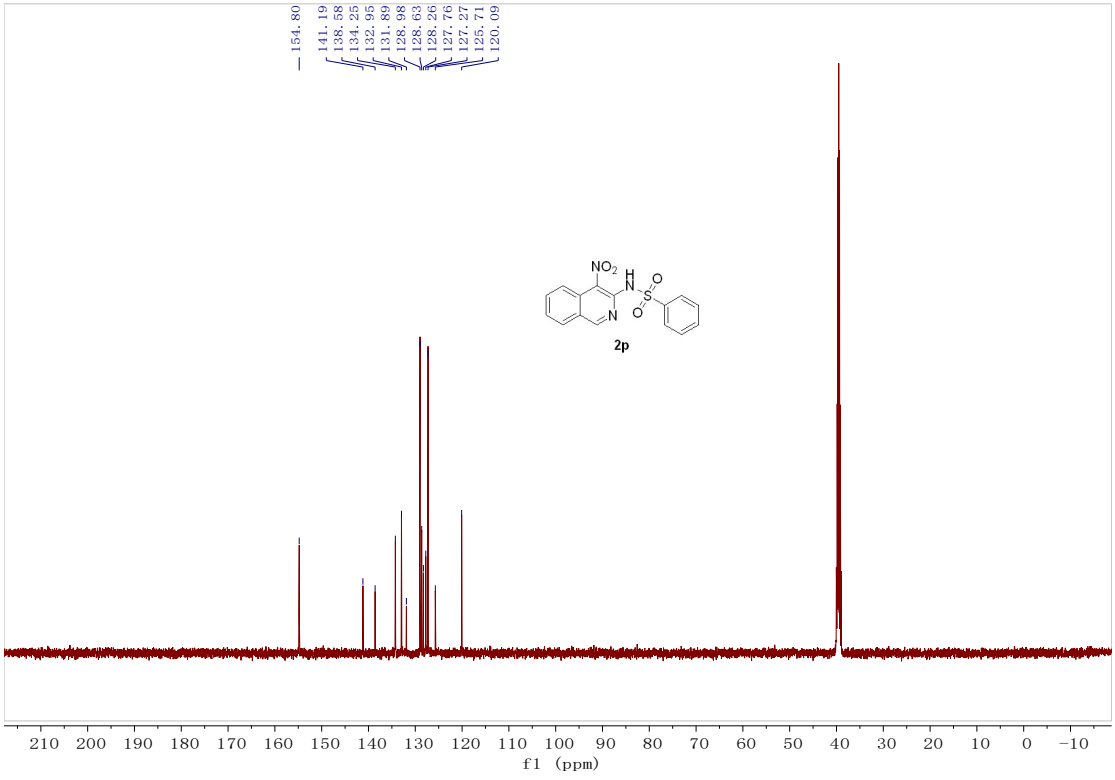

9.23
8.21
8.16
7.60
7.58
7.53
7.52
7.51
6.90
2.51
O2N
Me
N
O
S
O
N
H
2m
0.91
2.80
3.03
0.91
3.00
f1 (ppm)

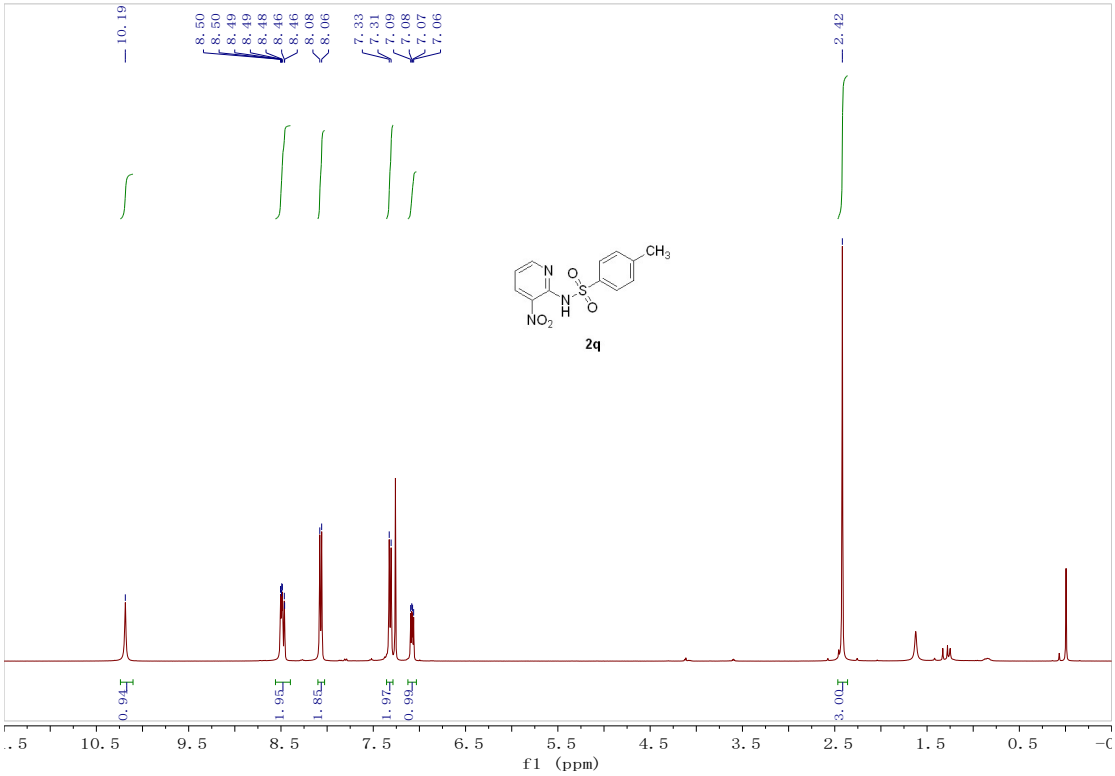

9.10
7.93
7.91
7.65
7.63
7.61
7.55
7.53
7.51
7.32
2.65
1.60
H3C
Me
N
O
S
O
N
H
2n
0.99
2.00
1.04
2.11
1.03
3.00
f1 (ppm)


11.79
8.36
8.35
8.11
8.01
7.99
7.65
7.63
7.62
7.57
7.56
7.54
7.52
7.19
2o
0.71
1.15
1.85
2.00
1.14
2.93
1.00
f1 (ppm)


161.98
143.29
141.49
140.16
133.14
128.98
127.80
125.09
124.34
123.86
123.70
118.55
116.09
2o
f1 (ppm)


11.42
9.24
8.19
8.17
8.01
8.00
7.94
7.93
7.91
7.83
7.81
7.71
7.70
7.68
7.67
7.65
7.64
7.62
7.60
7.59
NO2
H
N
O
S
O
N
2p
0.89
1.00
1.08
2.06
1.10
1.05
1.07
1.08
1.98
12.5
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)


154.80
141.19
138.58
134.25
132.95
131.89
128.98
128.63
128.26
127.76
127.27
125.71
120.09
NO2
H
N
O
S
O
N
2p
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)


10.19
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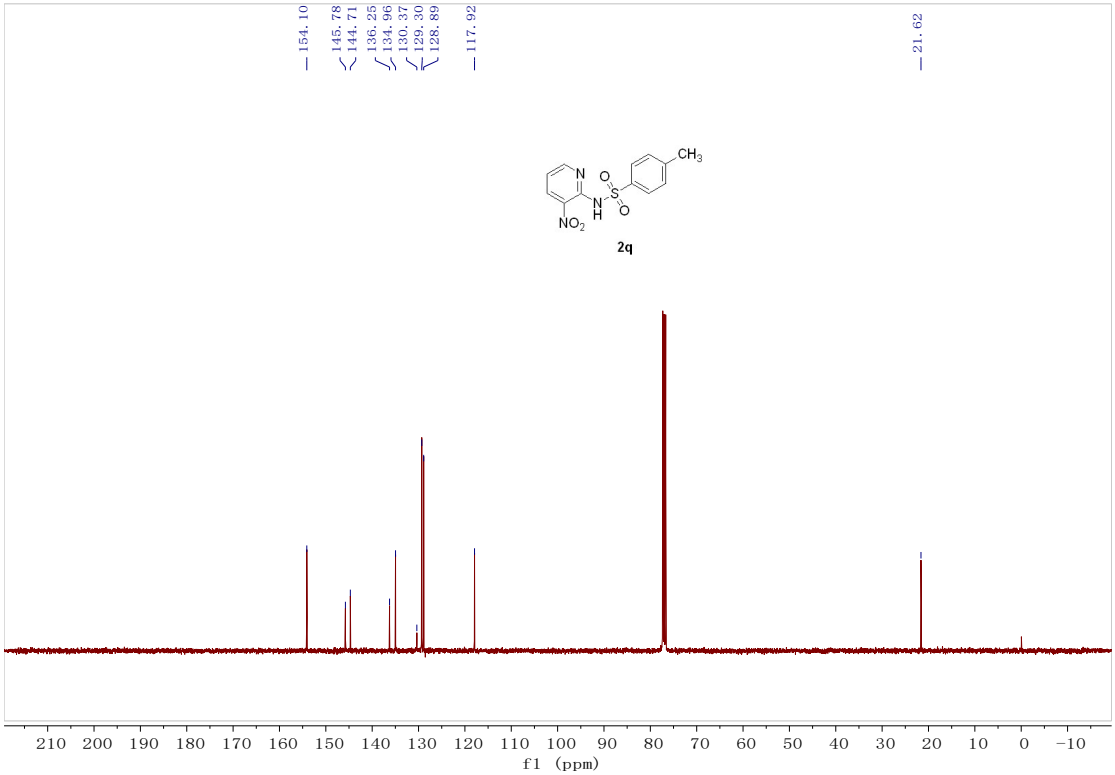
8.50
8.49
8.49
8.48
8.46
8.46
8.08
8.06
7.33
7.31
7.09
7.08
7.07
7.06
2.42
0.94
1.95
1.85
1.97
0.99
3.00
f1 (ppm)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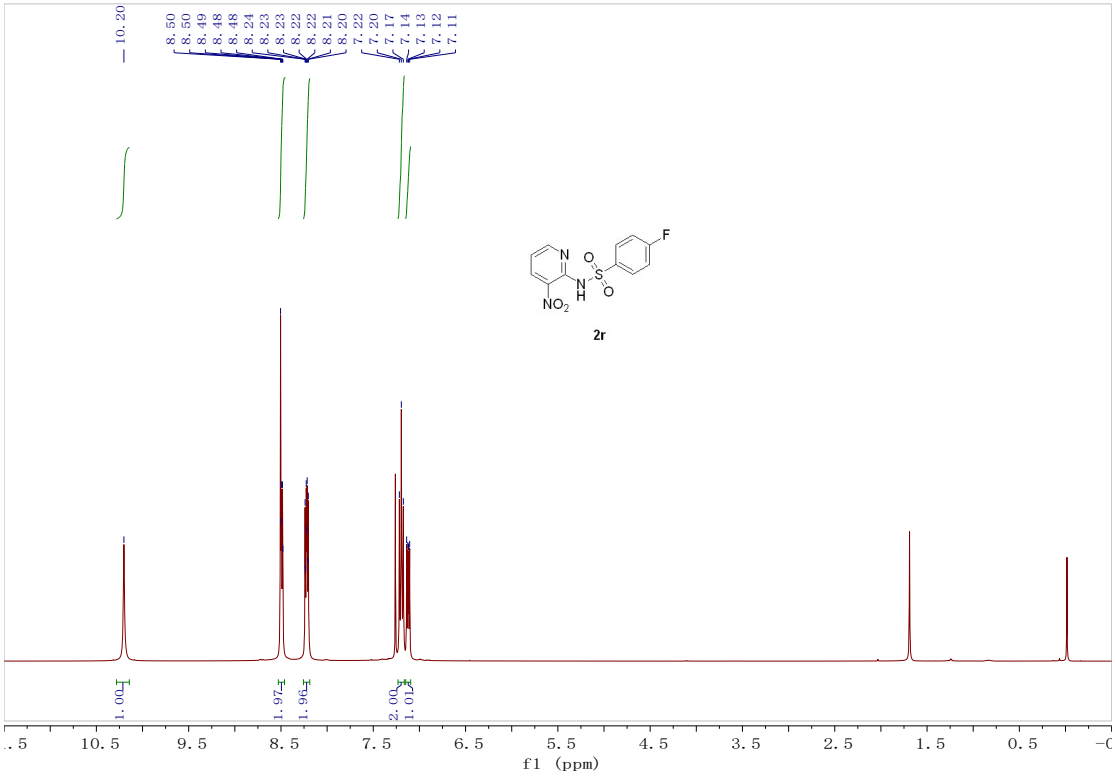
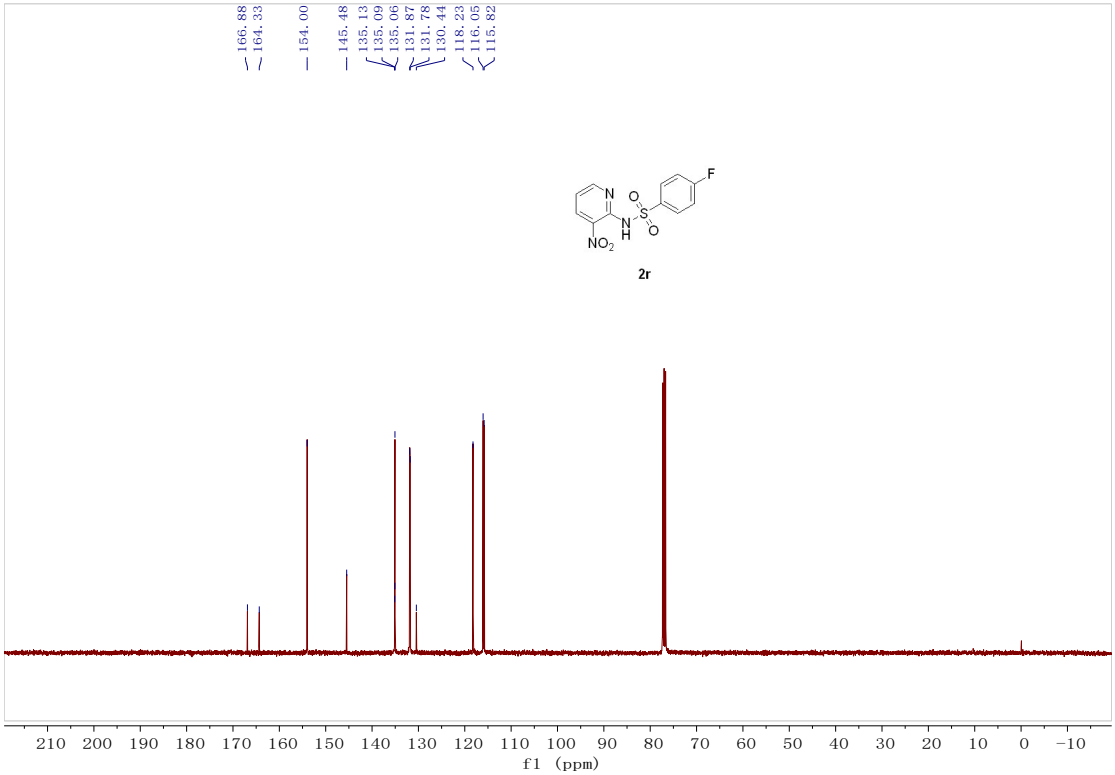
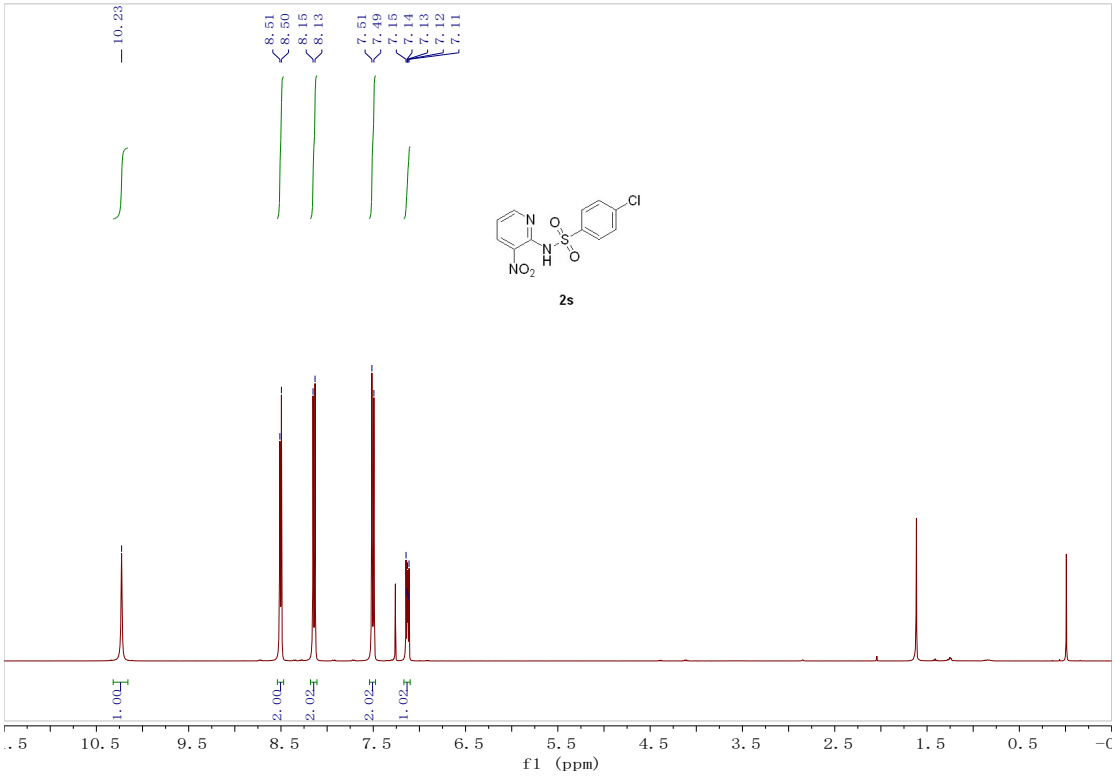
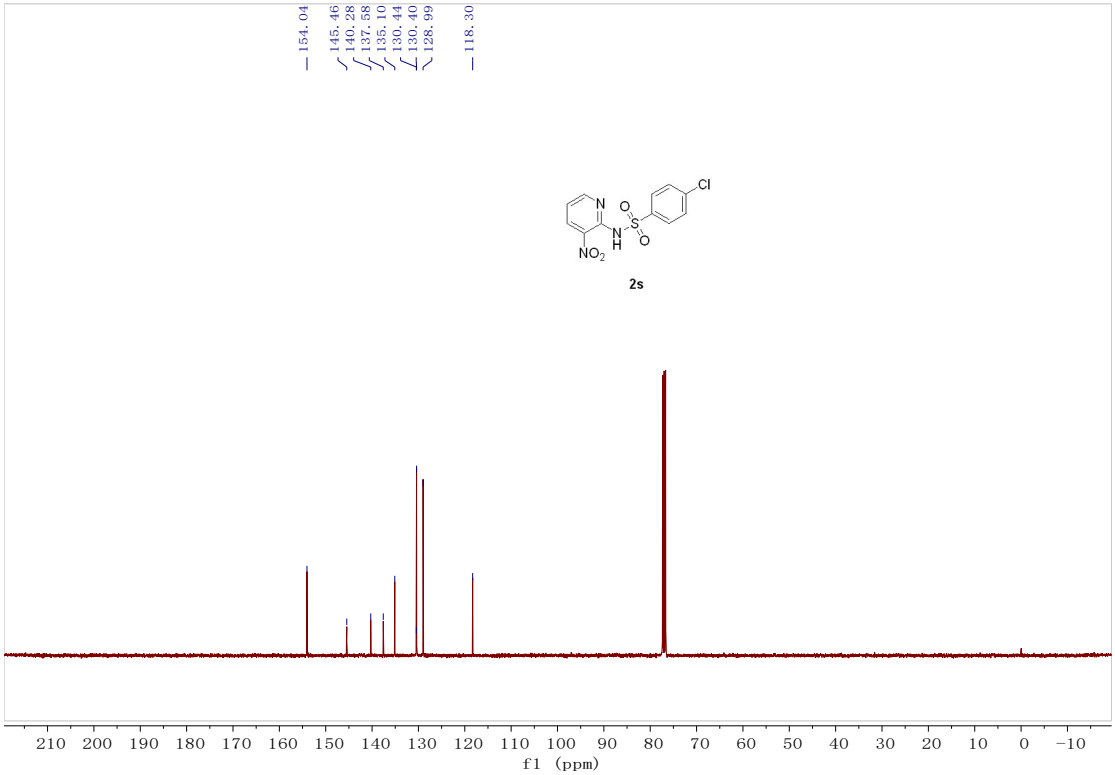
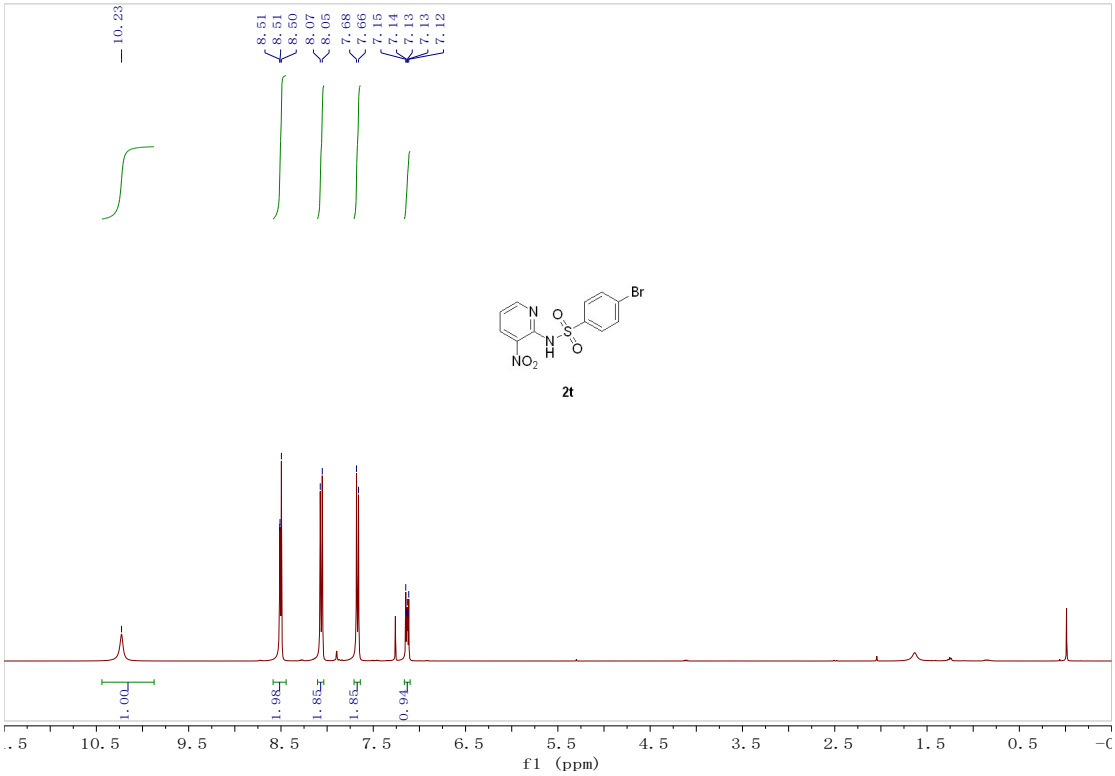
145.78
144.71
136.25
134.96
130.37
129.30
128.89
117.92
21.62
f1 (ppm)

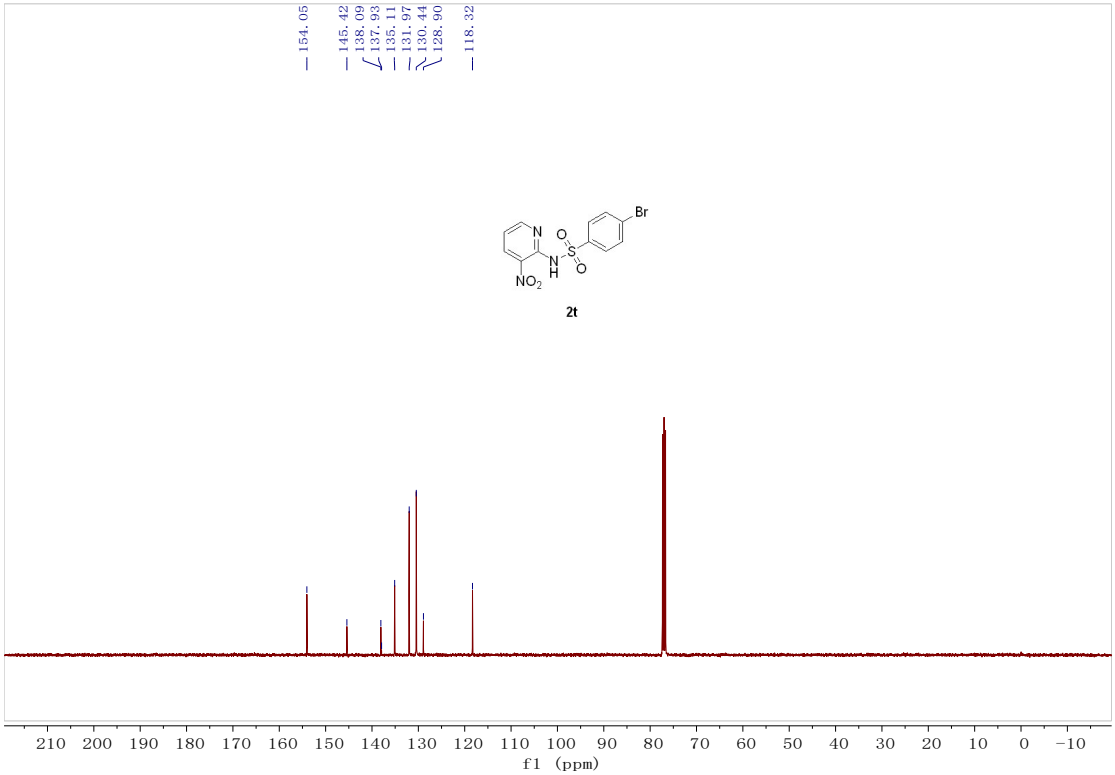

10.20
8.50
8.50
8.49
8.48
8.48
8.24
8.23
8.23
8.22
8.22
8.21
8.20
7.22
7.20
7.17
7.14
7.13
7.12
7.11
1.00
1.97
1.96
2.00
1.01
f1 (ppm)

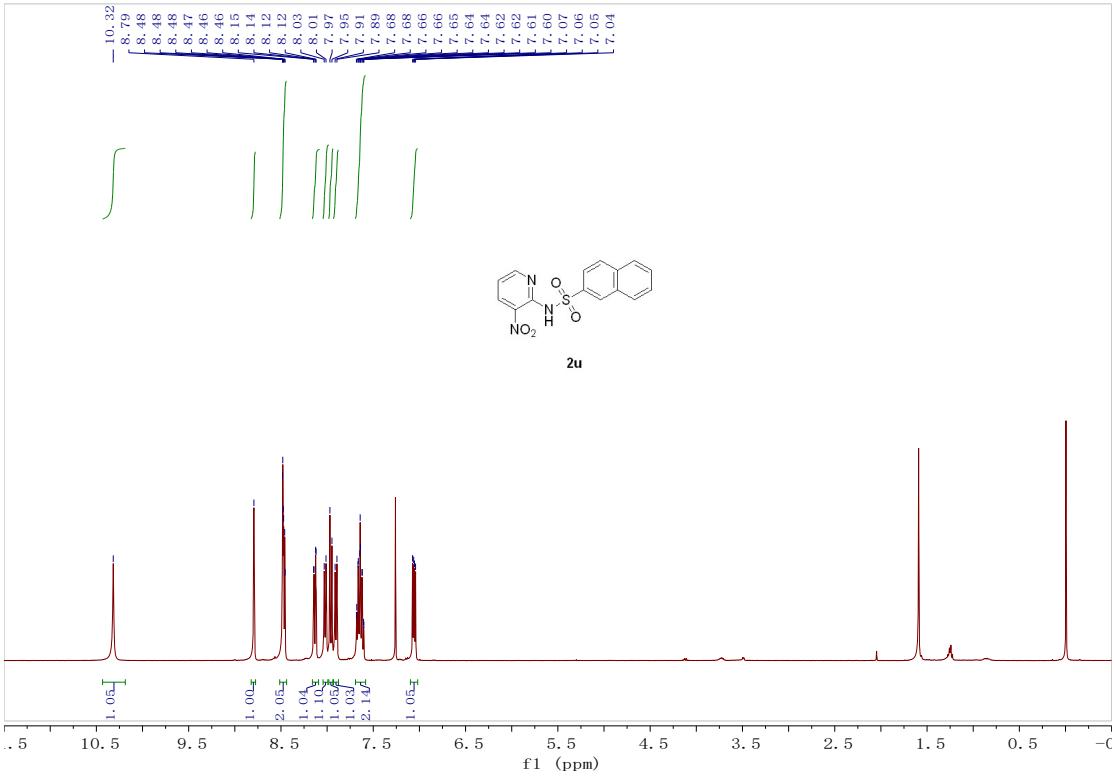

166.88
164.33
154.00
145.48
135.13
135.09
135.06
131.87
131.78
130.44
118.23
116.05
115.82
f1 (ppm)


10.23
8.51
8.50
8.15
8.13
7.51
7.49
7.15
7.14
7.13
7.12
7.11
Cl
N
O
S
N
H
O
NO2
2s
1.00
2.00
2.02
2.02
1.02
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)

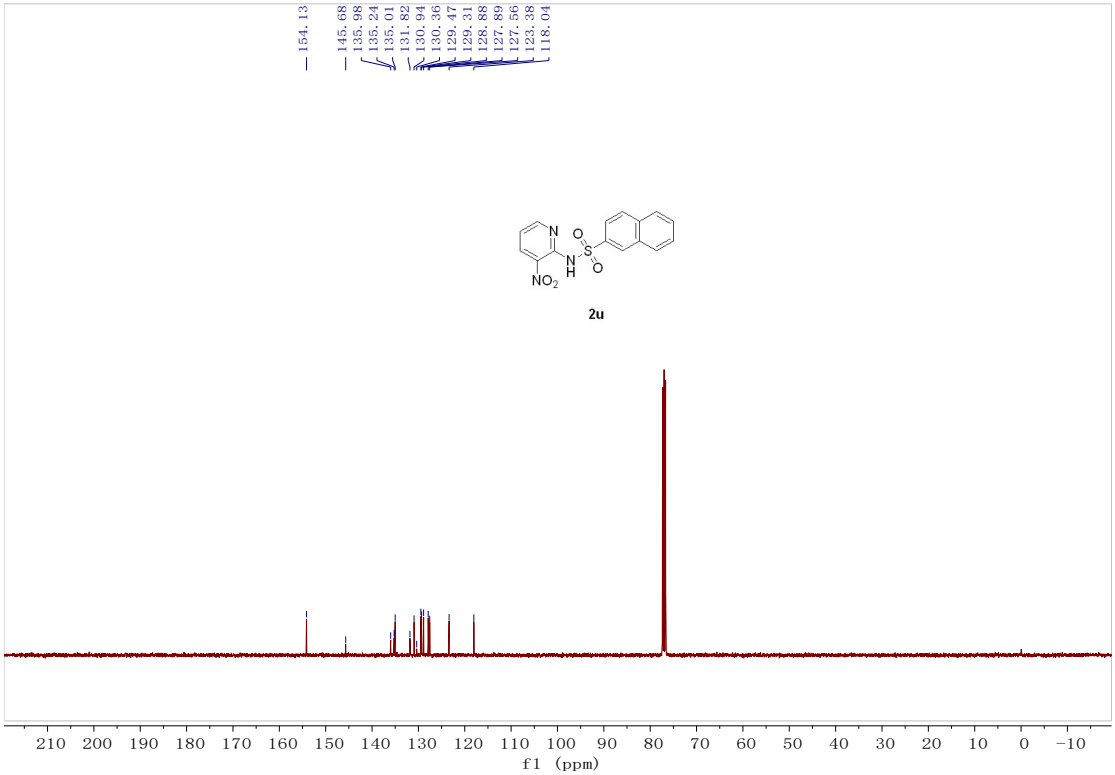

154.04
145.46
140.28
137.58
135.10
130.44
130.40
128.99
118.30
Cl
N
O
S
N
H
O
NO2
2s
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)


10.23
8.51
8.51
8.50
8.07
8.05
7.68
7.66
7.15
7.14
7.13
7.13
7.12
Br
N
O
S
O
N
H
NO2
2t
1.00
1.98
1.85
1.85
0.94
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)

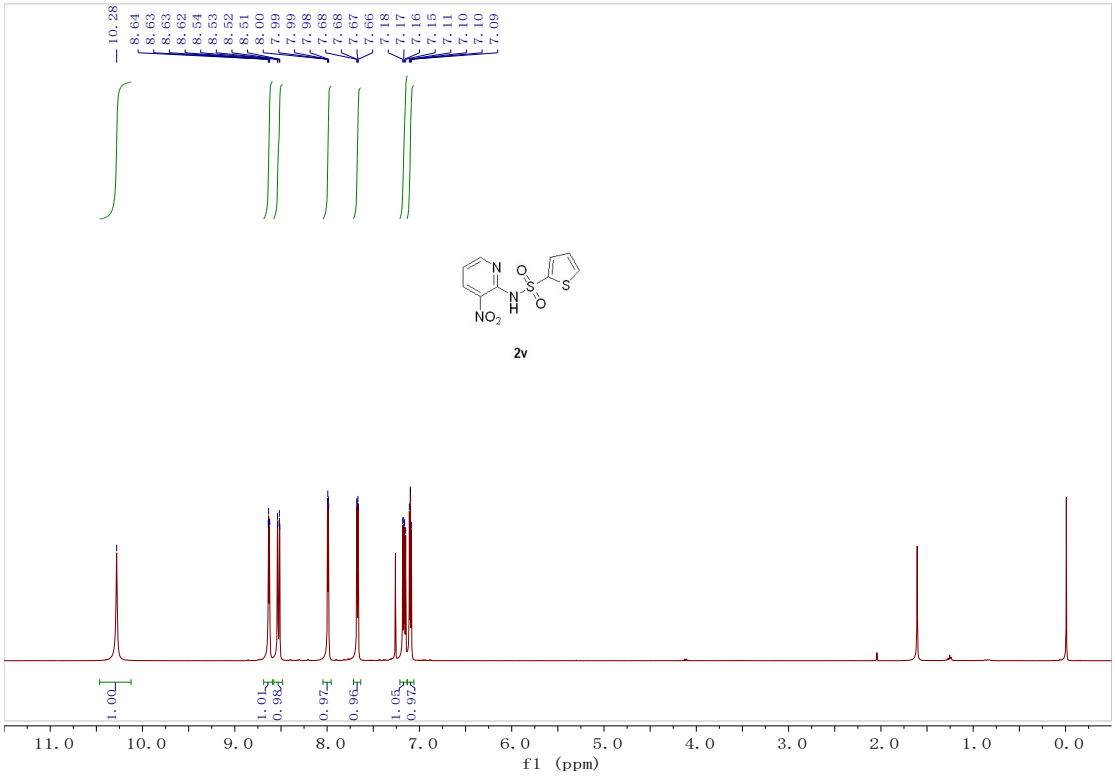

154.05
145.42
138.09
137.93
135.11
131.97
130.44
128.90
118.32
Br
N
O
S
O
N
H
NO2
2t
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

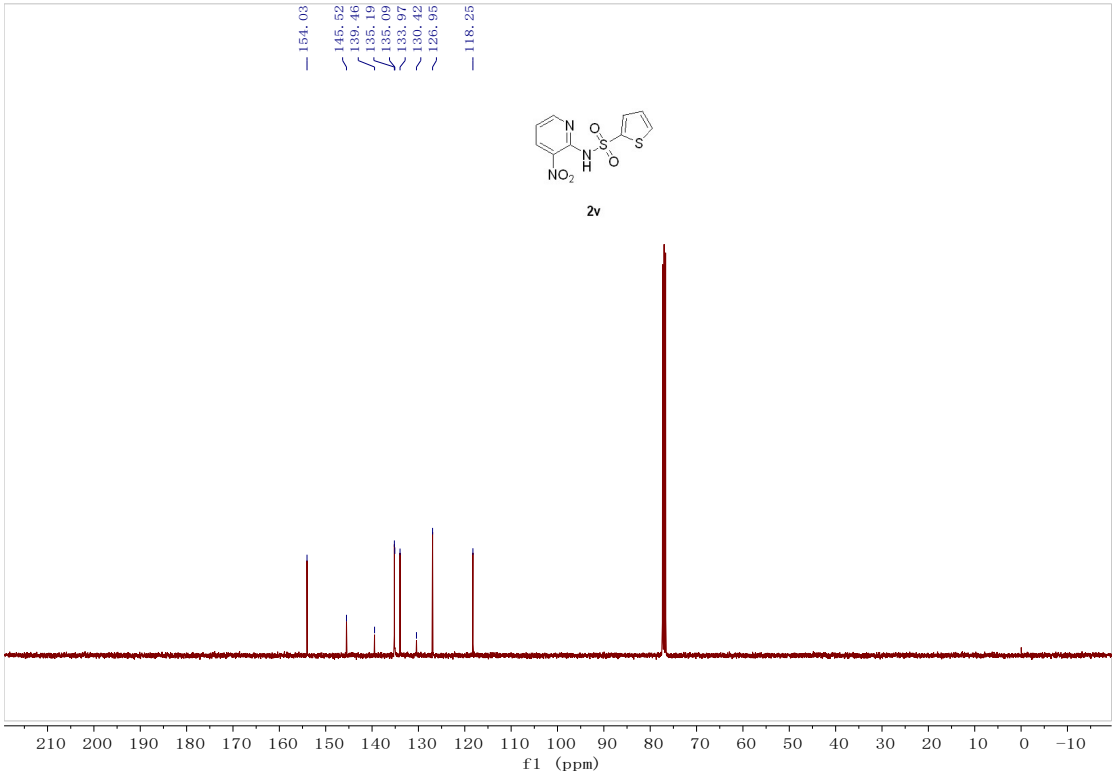

10.32
8.79
8.48
8.48
8.48
8.47
8.46
8.46
8.15
8.14
8.12
8.12
8.03
8.01
7.97
7.95
7.91
7.89
7.68
7.68
7.66
7.66
7.65
7.64
7.64
7.62
7.62
7.61
7.60
7.07
7.06
7.05
7.04
1.05
1.00
2.05
1.04
1.10
1.05
1.03
2.14
1.05
f1 (ppm)

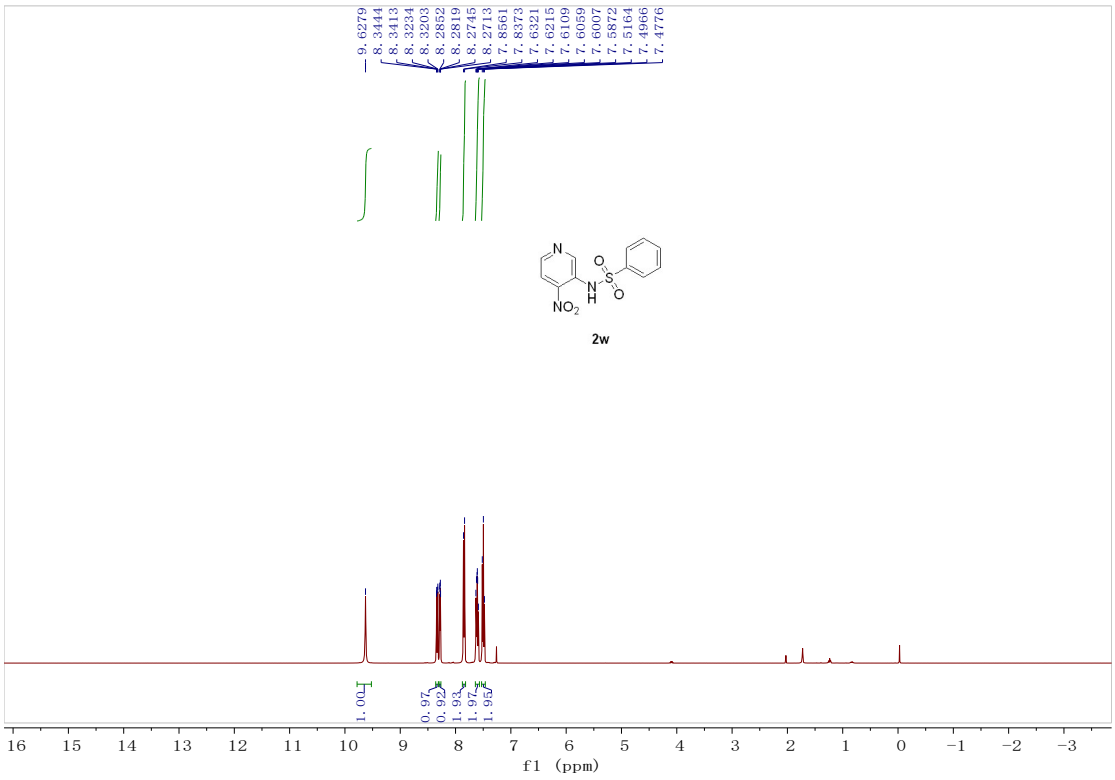
2u

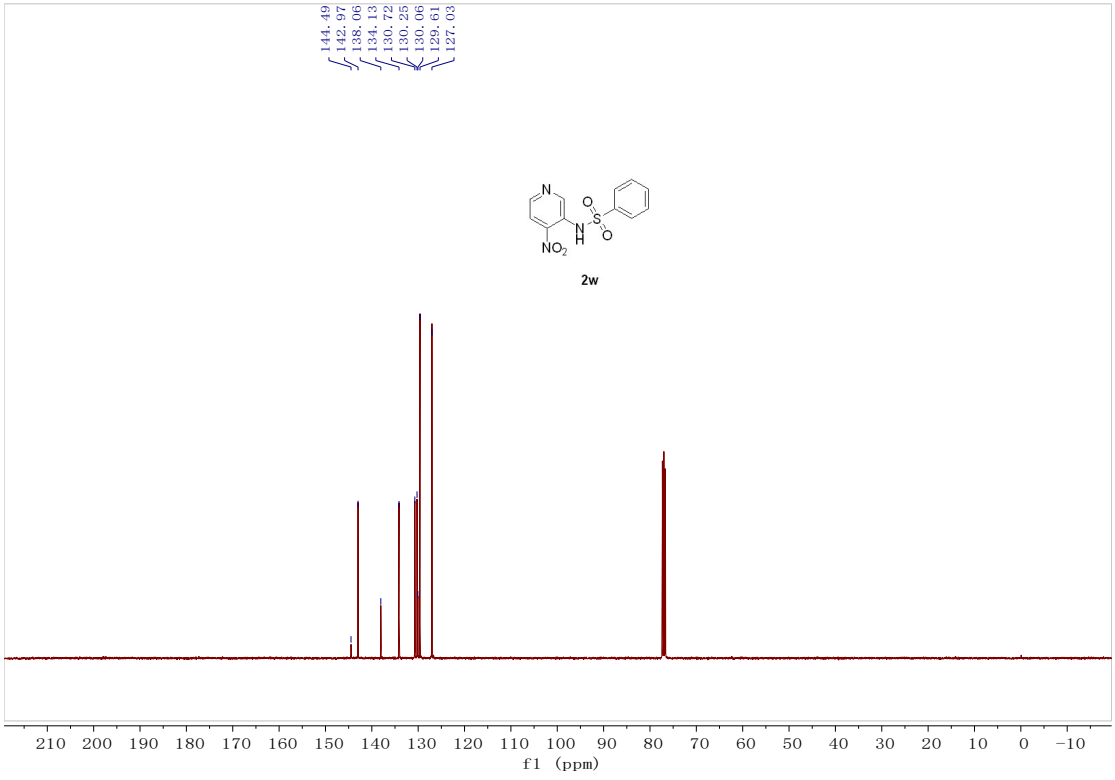

154.13
145.68
135.98
135.24
135.01
131.82
130.94
130.36
129.47
129.31
128.88
127.89
127.56
123.38
118.04
f1 (ppm)

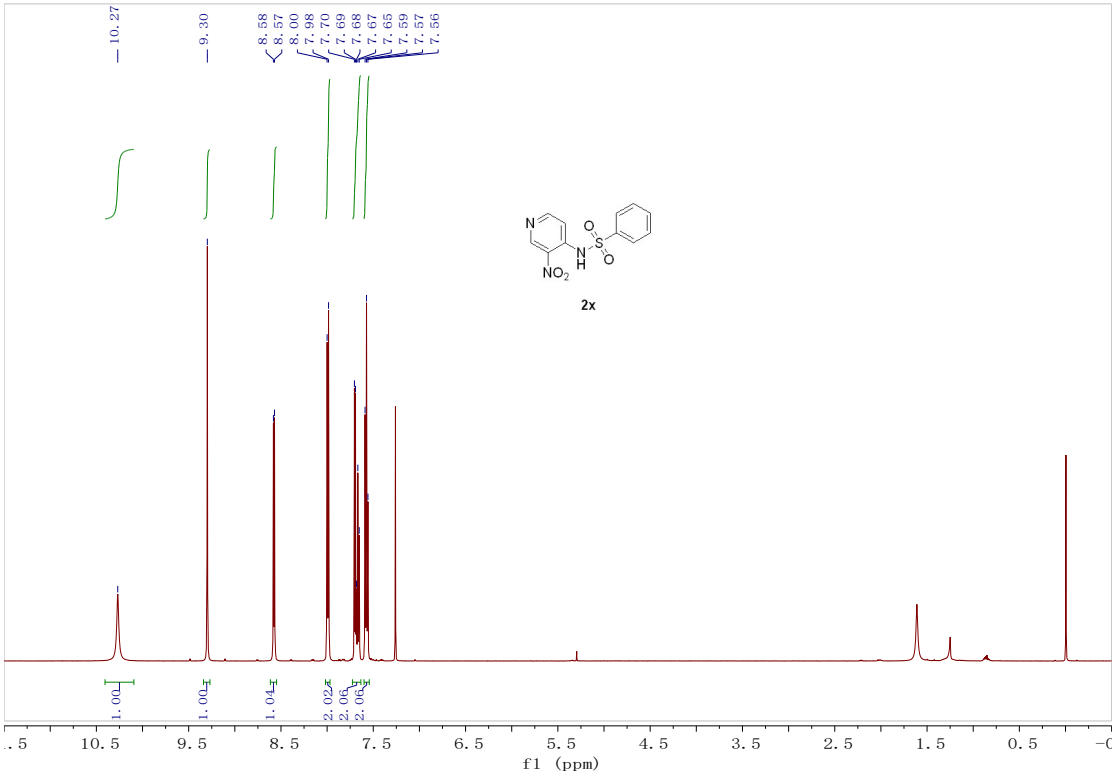
2u

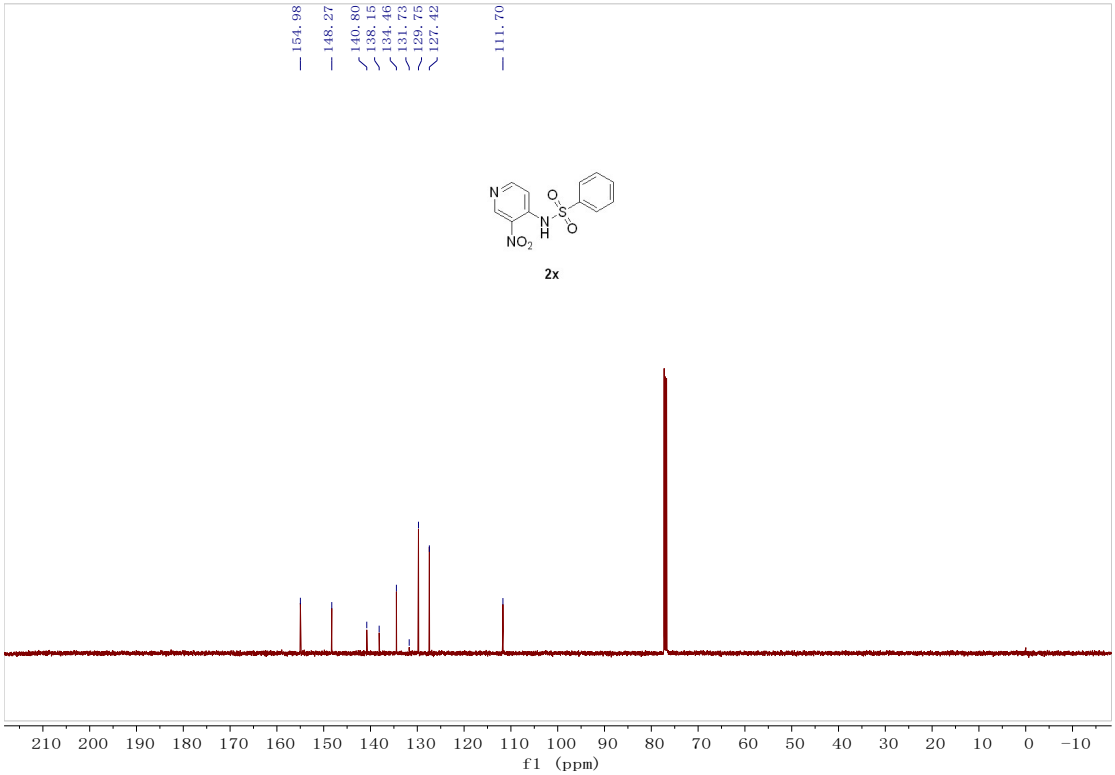

10.28
8.64
8.63
8.63
8.62
8.54
8.53
8.52
8.51
8.00
7.99
7.99
7.98
7.68
7.68
7.67
7.66
7.18
7.17
7.16
7.15
7.11
7.10
7.10
7.09
2v
1.00
1.01
0.98
0.97
0.96
1.05
0.97
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

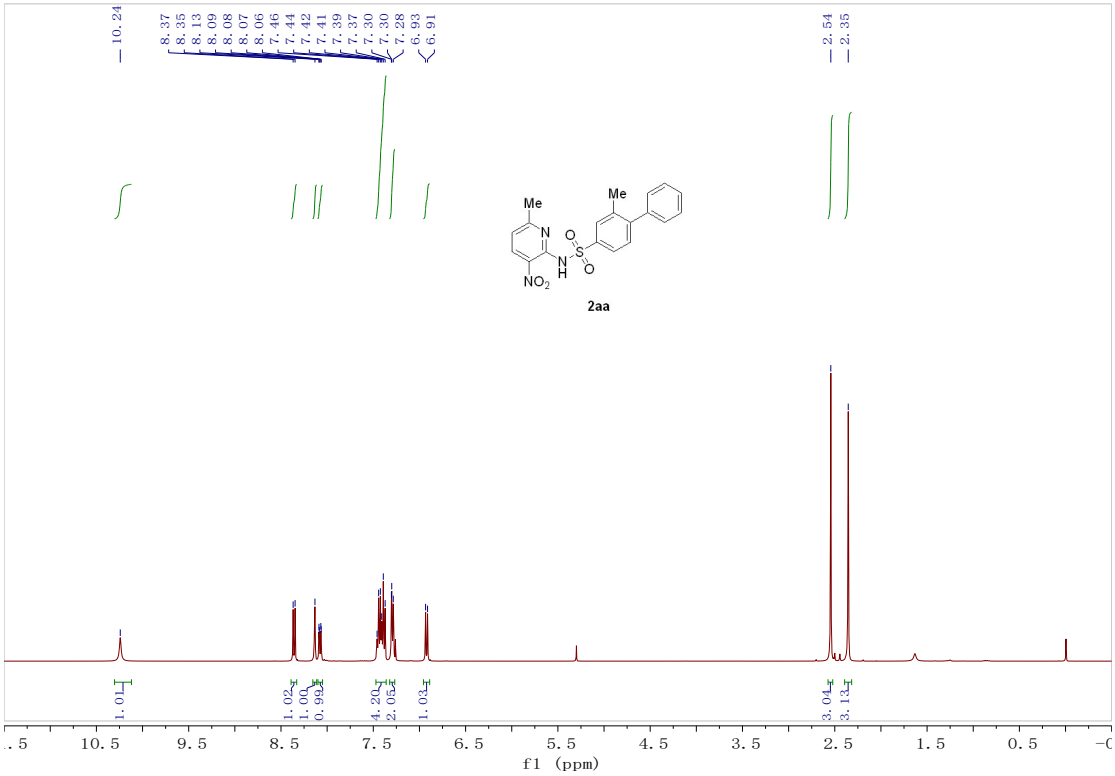

154.03
145.52
139.46
135.19
135.09
133.97
130.42
126.95
118.25
2v
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

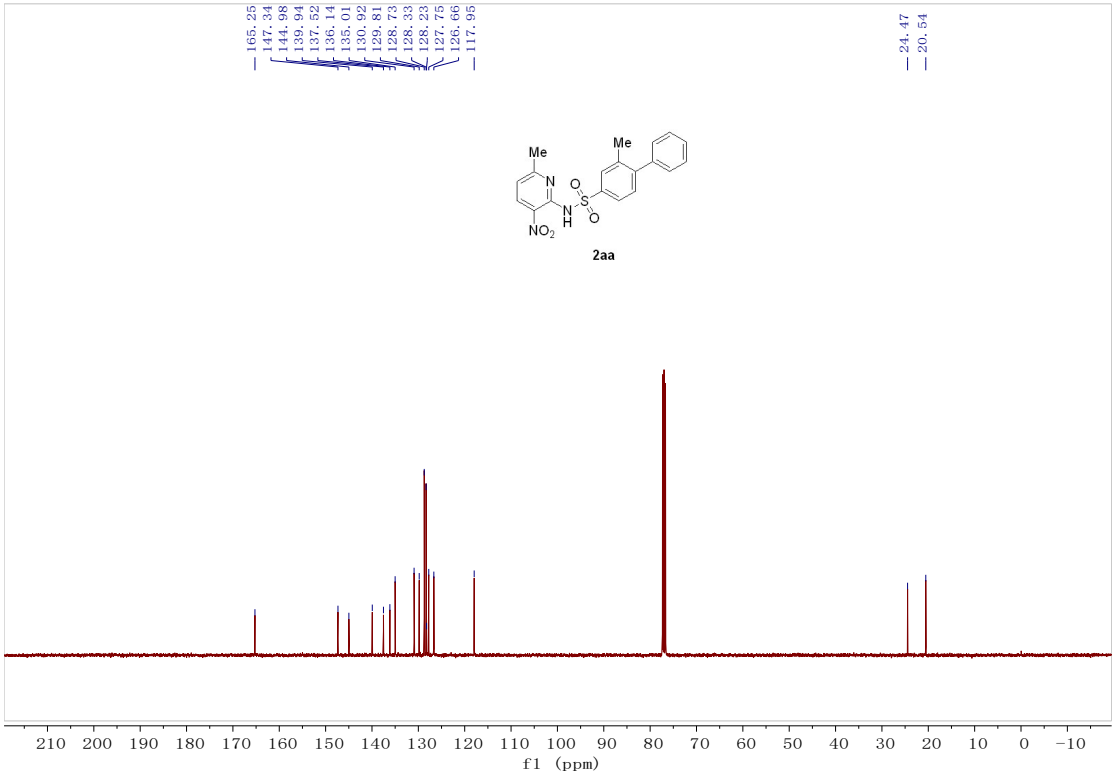

9.6279
8.3444
8.3413
8.3234
8.3203
8.2852
8.2819
8.2745
8.2713
7.8561
7.8373
7.6321
7.6215
7.6109
7.6059
7.6007
7.5872
7.5164
7.4966
7.4776
2w
1.00
0.97
0.92
1.93
1.97
1.95
f1 (ppm)

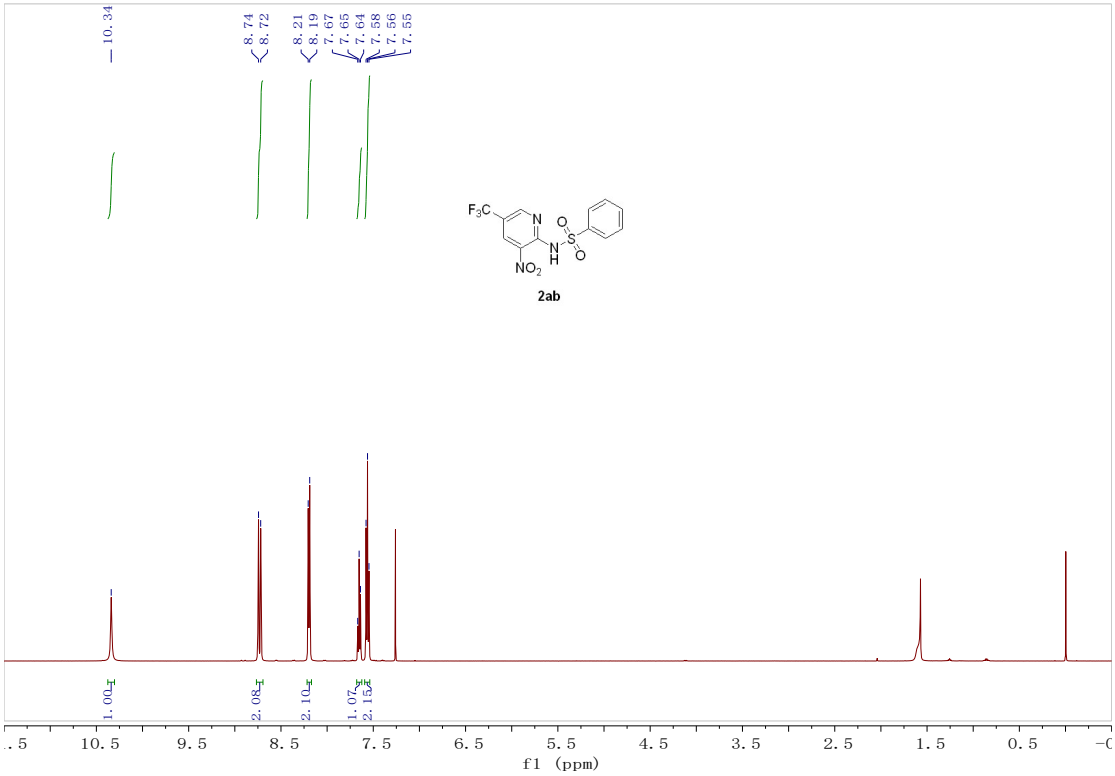

144.49
142.97
138.06
134.13
130.72
130.25
130.06
129.61
127.03
2w
f1 (ppm)

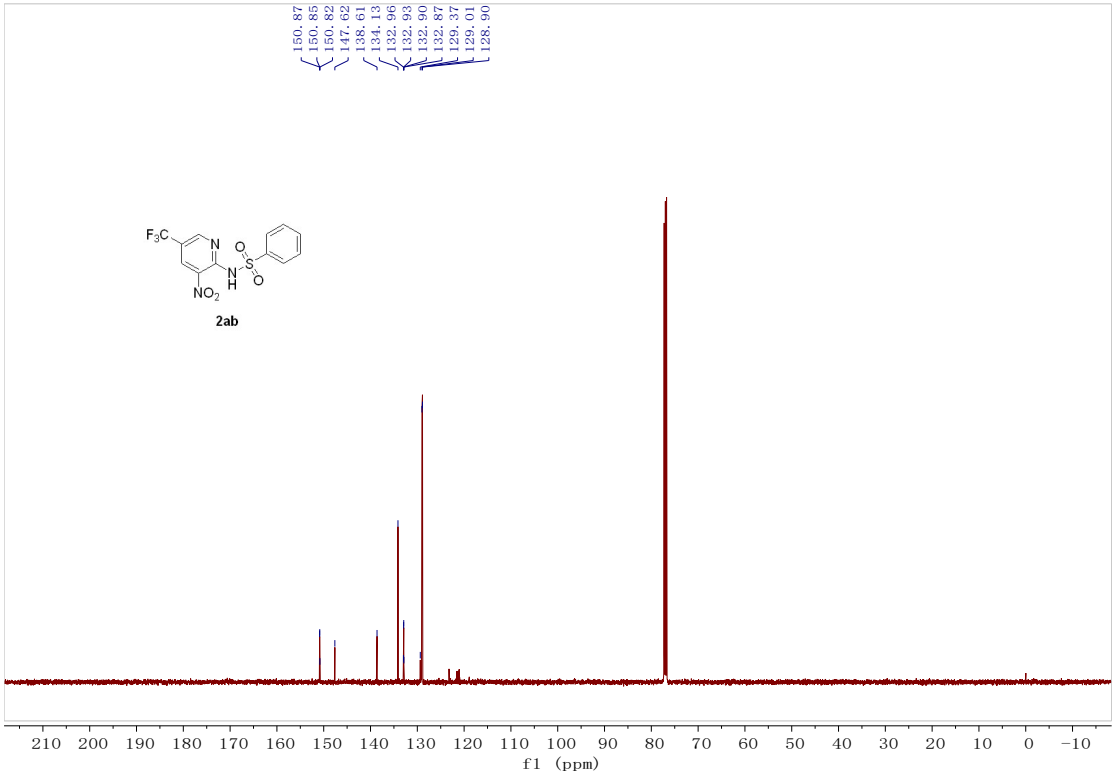

10.27
9.30
8.58
8.57
8.00
7.98
7.70
7.69
7.68
7.67
7.65
7.59
7.57
7.56
1.00
1.00
1.04
2.02
2.06
2.06
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)
2x

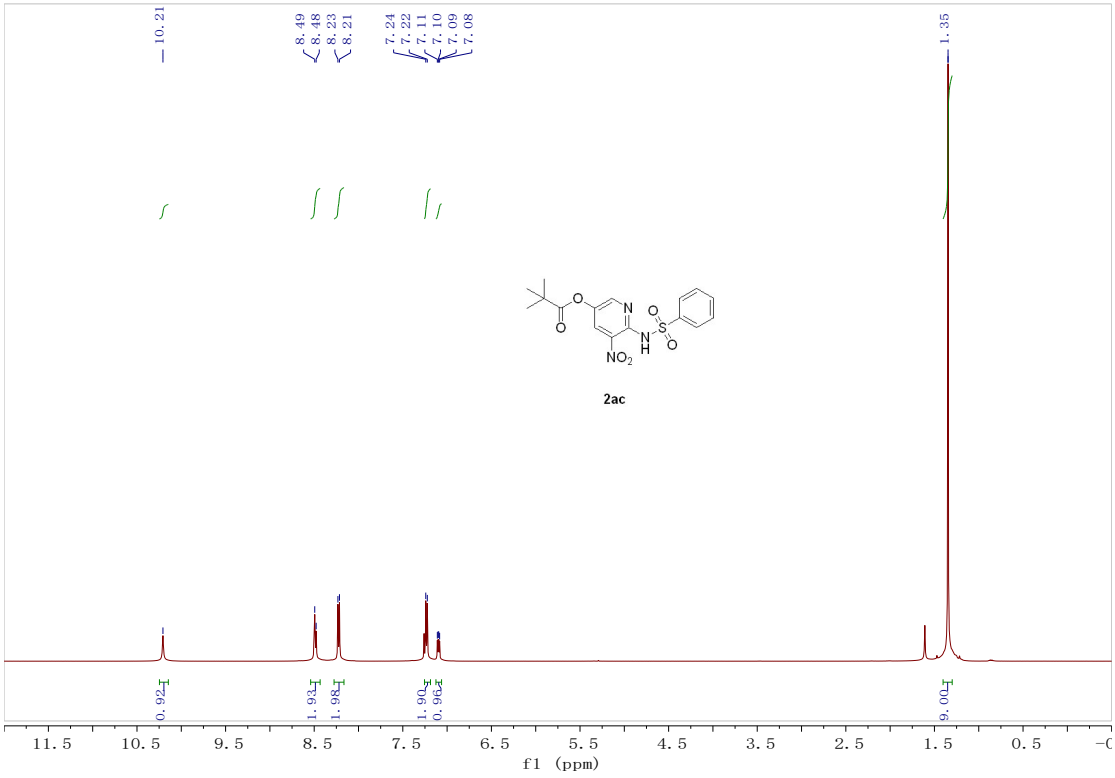

154.98
148.27
140.80
138.15
134.46
131.73
129.75
127.42
111.70
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)
2x

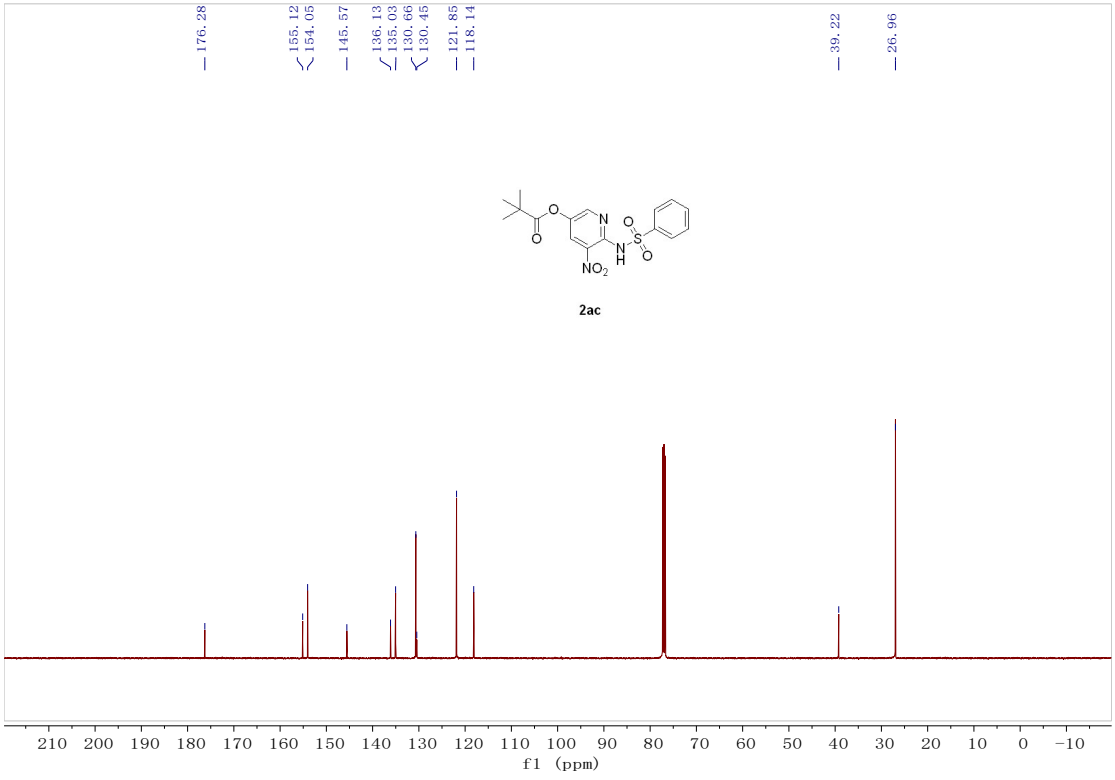

10.24
8.37
8.35
8.13
8.09
8.08
8.07
8.06
7.46
7.44
7.42
7.41
7.39
7.37
7.30
7.28
6.93
6.91
2.54
2.35
Me
Me
N
O
S
N
H
O
O
NO2
2aa
1.01
1.02
1.00
0.99
4.20
2.05
1.03
3.04
3.13
f1 (ppm)


165.25
147.34
144.98
139.94
137.52
136.14
135.01
130.92
129.81
128.73
128.33
128.23
127.75
126.66
117.95
24.47
20.54
Me
Me
N
O
S
N
H
O
O
NO2
2aa
f1 (ppm)


10.34
8.74
8.72
8.21
8.19
7.67
7.65
7.64
7.58
7.56
7.55
F3C
N
O
S
N
H
O
NO2
2ab
1.00
2.08
2.10
1.07
2.15
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)


150.87
150.85
150.82
147.62
138.61
134.13
132.96
132.93
132.90
132.87
129.37
129.01
128.90
F3C
N
O
S
N
H
O
NO2
2ab
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)


10.21
8.49
8.48
8.23
8.21
7.24
7.22
7.11
7.10
7.09
7.08
1.35
0.92
1.93
1.98
1.90
0.96
9.00
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)
2ac


176.28
155.12
154.05
145.57
136.13
135.03
130.66
130.45
121.85
118.14
39.22
26.96
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)
2ac