

Supporting Information

Construction of Nine-membered *N,N,O*-Heterocycles *via* Pd-catalyzed [6+3] Dipolar Cycloaddition

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NMR Specturm

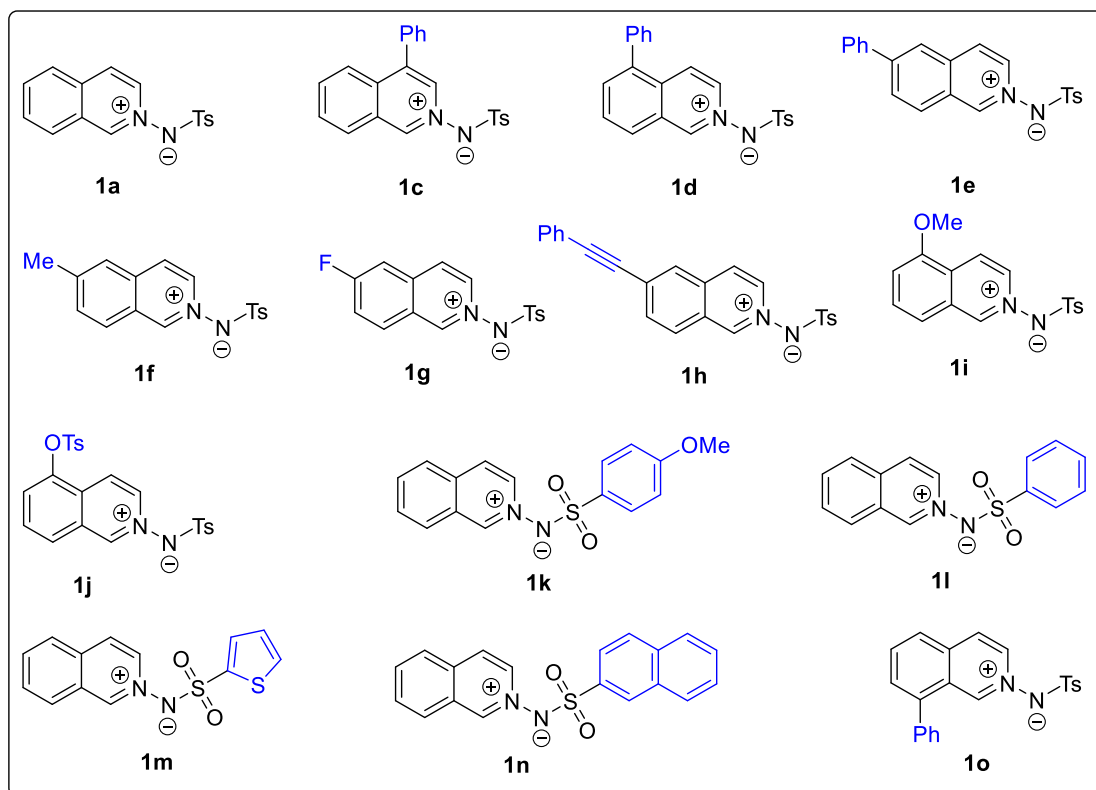
I. General Information

Flash column chromatography was performed over silica gel (200-300 mesh) purchased from Qindao Puke Co. Lit., China. All air or moisture sensitive reactions were conducted in oven-dried glassware under nitrogen atmosphere using anhydrous solvents. Anhydrous toluene, acetonitrile, dichloromethane, chloroform, methanol, and tetrahydrofuran were purified by the Innovative® solvent purification system. Other anhydrous solvents were purchased from J&K Scientific. ^1H , ^{13}C , and ^{19}F NMR spectra were collected on a Bruker AV 400 or AV 300 MHz NMR spectrometer using residue solvent peaks as an internal standard (^1H NMR: CDCl_3 at 7.26 ppm, $\text{DMSO-}d_6$ at 2.51 ppm; ^{13}C NMR: CDCl_3 at 77.15 ppm, $\text{DMSO-}d_6$ at 39.5 ppm). HRMS spectra were performed on a Waters mass spectrometer.

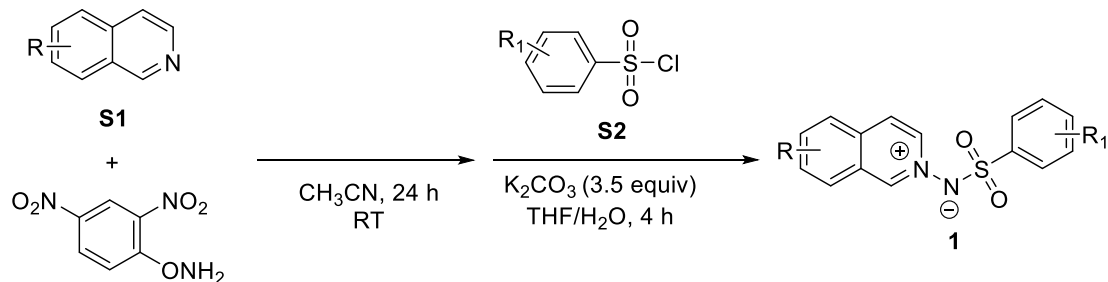
II. Preparation of Substrates 1 and 2

Substrates **1a**, **1c-1m** were synthesized according to the literature procedure.^[1]

Substrates **1a**, **1f-1g** and **1i-1l** are known compounds.



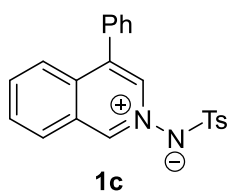
General Procedure A: Preparation of *N*-Iminoisoquinolinium Ylides **1**.



Under N₂ at room temperature, to a round-bottom flask charged with isoquinoline **S1** (1.30 g, 10 mmol, 1.0 equiv), O-(2,4-dinitrophenyl)hydroxylamine (2.19 g, 11 mmol, 1.1 equiv) and acetonitrile (40 mL). The mixture was allowed to stir for 24 h before it was filtered to give an orange precipitate. Then, dissolve the orange precipitate in

[1] P. Zhang, Y. Zhou, X. Han and J. Xu, H. Liu, *J. Org. Chem.* 2018, **83**, 3879-3888.

THF/H₂O (30 mL, 1:1) followed by adding K₂CO₃ (4.83 g, 35 mmol, 3.5 equiv) at room temperature. Next, arylsulfonyl chloride **S2** (20 mmol, 2 equiv) was added portion wise to the reaction mixture and stirred for another 4 h. The reaction mixture was diluted with water (20 mL) and extracted with dichloromethane (30 mL × 3). The combined organic layers were washed with water (30 mL × 2), dried over anhydrous Na₂SO₄, and concentrated under reduced pressure. The residue was purified by silica gel column chromatography (dichloromethane/EtOAc) to afford the desired *N*-iminoisoquinolinium ylides **1**.



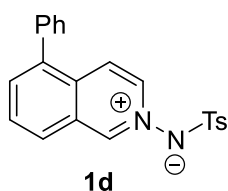
(4-Phenylisoquinolin-2-ium-2-yl)(tosyl)amide (1c) was prepared according to the General Procedure A as a yellow solid (chromatography eluent: dichloromethane/EtOAc = 5:1) in 35% yield (610 mg).

M.P. 196.2-197.4 °C.

¹H NMR (300MHz, CDCl₃) δ 9.30 (s, 1H), 8.12 (d, *J* = 7.5 Hz, 1H), 7.99-7.80 (m, 4H), 7.68 (d, *J* = 8.2 Hz, 2H), 7.54-7.51 (m, 3H), 7.32-7.28 (m, 2H), 7.18 (d, *J* = 8.0 Hz, 2H), 2.37 (s, 3H) ppm.

¹³C NMR (75MHz, CDCl₃) δ 145.9, 141.6, 139.2, 138.5, 136.9, 134.4, 133.7, 133.2, 130.4, 129.8, 129.7, 129.4, 129.22, 129.20, 128.5, 127.4, 125.5, 21.5 ppm.

HRMS (CI+) calculated for C₂₂H₁₉N₂O₂S [M + H]⁺: 375.1167, found: 375.1165.



(5-Phenylisoquinolin-2-ium-2-yl)(tosyl)amide (1d) was prepared according

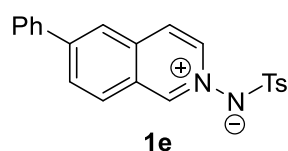
to the General Procedure A as a dark brown solid (chromatography eluent: dichloromethane/EtOAc = 5:1) in 33% yield (610 mg).

M.P. 214.6-216.6 °C.

¹H NMR (300MHz, CDCl₃) δ 9.33 (s, 1H), 8.08-8.04 (m, 2H), 7.91-7.86 (m, 3H), 7.68 (d, *J* = 8.2 Hz, 2H), 7.54-7.50 (m, 3H), 7.42-7.39 (m, 2H), 7.16 (d, *J* = 8.0 Hz, 2H), 2.35 (s, 3H) ppm.

¹³C NMR (75MHz, CDCl₃) δ 146.9, 141.6, 140.3, 139.3, 137.7, 137.1, 134.6 133.0, 130.3, 129.8, 129.4, 129.1, 128.9, 128.7, 128.1, 127.3, 123.3, 21.5 ppm.

HRMS (CI+) calculated for C₂₂H₁₉N₂O₂S [M + H]⁺: 375.1167, found: 375.1169.



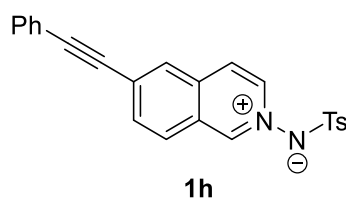
(6-Phenylisoquinolin-2-ium-2-yl)(tosyl)amide (1e) was prepared according to the General Procedure A as an orange red solid (chromatography eluent: dichloromethane/EtOAc = 5:1) in 65% yield (1.1 g).

M.P. 182.1-183 °C.

¹H NMR (300MHz, CDCl₃) δ 9.28 (s, 1H), 8.15-8.04 (m, 4H), 7.88 (d, *J* = 7.0 Hz, 1H), 7.73-7.64 (m, 4H), 7.57-7.48 (m, 3H), 7.16 (d, *J* = 8.0 Hz, 2H), 2.35 (s, 3H) ppm.

¹³C NMR (75MHz, CDCl₃) δ 147.3, 147.0, 141.6, 139.2, 138.6, 138.3, 135.2, 130.3, 129.6, 129.5, 129.4, 129.3, 127.8, 127.3, 127.1, 124.7, 124.3, 21.5 ppm.

HRMS (CI+) calculated for C₂₂H₁₉N₂O₂S [M + H]⁺: 375.1167, found: 375.1165.



(6-(Phenylethynyl)-isoquinolin-2-ium-2-yl)(tosyl)amide (1h) was prepared according to the General Procedure A as a brown solid (chromatography

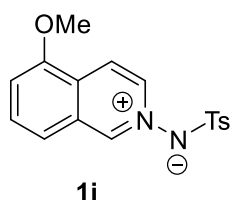
eluent: dichloromethane/EtOAc = 5:1) in 20% yield (310 mg).

M.P. 195.2-196.7 °C.

¹H NMR (300MHz, CDCl₃) δ 9.23 (s, 1H), 8.09 (t, *J* = 7.2 Hz, 2H), 8.00 (d, *J* = 8.6 Hz, 1H), 7.86 (dd, *J*₁ = 1.1, *J*₂ = 8.6 Hz, 1H), 7.78 (d, *J* = 7.0 Hz, 1H), 7.66 (d, *J* = 8.1 Hz, 2H), 7.60-7.58 (m, 2H), 7.44-7.41 (m, 3H), 7.17 (d, *J* = 8.0 Hz, 2H), 2.36 (s, 3H) ppm.

¹³C NMR (75MHz, CDCl₃) δ 146.4, 141.8, 139.1, 138.4, 134.3, 133.2, 132.1, 129.9, 129.8, 129.5, 129.4, 128.8, 128.6, 127.3, 127.1, 124.1, 121.9, 96.1, 88.0, 21.5 ppm.

HRMS (CI⁺) calculated for C₂₄H₁₉N₂O₂S [M + H]⁺: 399.1167, found: 399.1168.



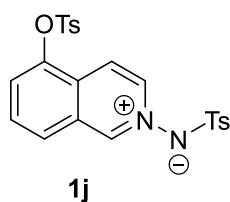
(5-Methoxyisoquinolin-2-ium-2-yl)(tosyl)amide (1i): was prepared according to the General Procedure A as a white solid (chromatography eluent: Dichloromethane/EtOAc = 5:1) in 49% yield (418 mg).

M.P. 228.8-230.1 °C.

¹H NMR (300MHz, DMSO-*d*₆) δ 9.49 (s, 1H), 8.23 (d, *J* = 7.1 Hz, 1H), 8.05 (dd, *J*₁ = 1.4 *J*₂ = 7.1 Hz 1H), 7.89-7.80 (m, 2H), 7.49 (d, *J* = 7.3 Hz 1H), 7.41 (d, *J* = 8.1 Hz 2H), 7.19 (d, *J* = 8.0 Hz, 2H), 4.01 (s, 3H), 2.29 (s, 3H) ppm.

¹³C NMR (101MHz, DMSO-*d*₆) δ 153.8, 147.4, 140.8, 139.4, 137.2, 131.5, 129.2, 128.8, 126.6, 126.1, 120.2, 119.7, 112.7, 56.4, 20.9 ppm.

HRMS (CI⁺) calculated for C₁₇H₁₇N₂O₃S [M + H]⁺:329.0960, found: 329.0960.



Tosyl(5-(tosyloxy)isoquinolin-2-ium-2-yl)amide (1j): was prepared according

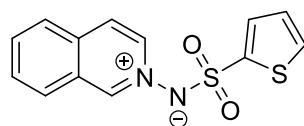
to the General Procedure A as a white solid (chromatography eluent: Dichloromethane/EtOAc = 1:1) in 15% yield (320 mg).

M.P. 215.9-216.7 °C.

¹H NMR (400MHz, CDCl₃) δ 9.34 (s, 1H), 8.03 (dd, *J*₁ = 1.2, *J*₂ = 7.2 Hz 1H), 7.96 (d, *J* = 8.3 Hz, 1H), 7.82 (d, *J* = 7.2 Hz 1H), 7.76-7.72 (m, 3H), 7.66-7.61 (m, 3H), 7.34 (d, *J* = 8.2 Hz 2H), 7.17 (d, *J* = 8.1 Hz, 2H), 2.46 (s, 3H), 2.36 (s, 3H) ppm.

¹³C NMR (101MHz, CDCl₃) δ 146.9, 145.5, 144.9, 142.0, 138.9, 138.0, 131.6, 130.8, 130.5, 129.5, 129.4, 128.7, 128.6, 127.4, 127.3, 126.5, 119.6, 22.0, 21.6 ppm.

HRMS (CI+) calculated for C₂₃H₂₁N₂O₅S₂ [M + H]⁺:469.0892, found: 469.0888.



1m

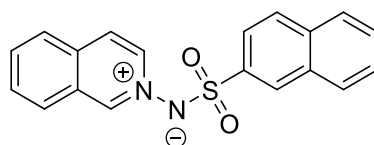
Isoquinolin-2-ium-2-yl(thiophen-2-ylsulfonyl)amide (1m) was prepared according to the General Procedure A as a yellow solid (chromatography eluent: dichloromethane/EtOAc = 5:1) in 39% yield (110 mg).

M.P. 223.8-225.7 °C.

¹H NMR (300MHz, DMSO-*d*₆) δ 9.60 (s, 1H), 8.40 (d, *J* = 8.1 Hz, 1H), 8.30 (d, *J* = 7.0 Hz, 1H), 8.22 (dd, *J*₁ = 1.6, *J*₂ = 7.2 Hz, 2H), 8.08 (dd, *J*₁ = 1.1, *J*₂ = 7.0 Hz, 1H), 7.96-7.91 (m, 1H), 7.72 (dd, *J*₁ = 1.3, *J*₂ = 5.0 Hz, 1H), 7.23 (dd, *J*₁ = 1.3, *J*₂ = 3.6 Hz, 1H), 7.01 (dd, *J*₁ = 3.6, *J*₂ = 5.0 Hz, 1H) ppm.

¹³C NMR (75MHz, DMSO-*d*₆) δ 148.2, 143.8, 137.7, 134.8, 134.7, 130.7, 130.5, 130.0, 129.1, 127.7, 127.2, 127.0, 125.3 ppm.

HRMS (CI+) calculated for C₁₃H₁₁N₂O₂S₂ [M + H]⁺: 292.0262, found: 292.0265.



1n

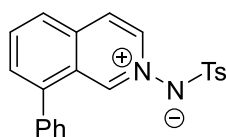
Isoquinolin-2-ium-2-yl(naphthalen-2-ylsulfonyl)amide (1n) was prepared according to the General Procedure A as a yellow solid (chromatography eluent: dichloromethane/EtOAc = 5:1) in 50% yield (170 mg).

M.P. 233.1-234.7 °C.

¹H NMR (300MHz, DMSO-*d*₆) δ 9.60 (s, 1H), 8.35 (d, *J* = 8.2 Hz, 1H), 8.18 (t, *J* = 7.0 Hz, 2H), 8.09-7.87 (m, 7H), 7.71 (dd, *J*₁ = 1.8, *J*₂ = 8.6 Hz, 1H), 7.64-7.52 (m, 2H) ppm.

¹³C NMR (75MHz, DMSO-*d*₆) δ 148.3, 139.5, 137.8, 134.7, 134.5, 133.6, 131.9, 130.5, 129.1, 128.9(2C), 127.8, 127.7, 127.6, 127.1, 127.0, 126.5, 125.3, 123.4 ppm.

HRMS (CI+) calculated for C₁₉H₁₅N₂O₂S [M + H]⁺: 335.0854, found: 335.0856.



1o

(8-Phenylisoquinolin-2-ium-2-yl)(tosyl)amide (1o) was prepared according to the General Procedure A as a yellow solid (chromatography eluent: dichloromethane/EtOAc = 5:1) in 48% yield (830 mg).

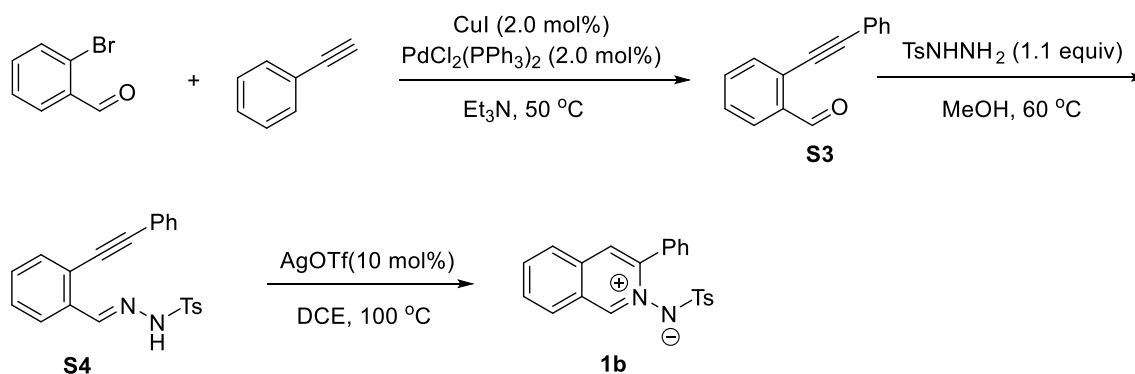
M.P. 217.2-219.2 °C.

¹H NMR (300MHz, CDCl₃) δ 8.97 (s, 1H), 8.28 (dd, *J*₁ = 1.5, *J*₂ = 7.0 Hz, 1H), 7.98-7.95 (m, 3H), 7.72 (dd, *J*₁ = 2.2, *J*₂ = 6.1 Hz, 1H), 7.57-7.47 (m, 5H), 7.22-7.19 (m, 2H), 7.12 (d, *J* = 8.0 Hz, 2H), 2.38 (s, 3H) ppm.

¹³C NMR (75MHz, CDCl₃) δ 146.3, 142.3, 141.4, 138.8, 138.3, 136.2, 135.2, 133.9, 131.0, 129.8, 129.3, 129.2, 129.1, 127.4, 126.5, 126.2, 124.9, 21.5 ppm.

HRMS (CI+) calculated for C₂₂H₁₉N₂O₂S [M + H]⁺: 375.1167, found: 375.1164.

Preparation of *N*-Iminoisoquinolinium Ylide **1b**^[2].



2-(Phenylethynyl)benzaldehyde (S3): Under N₂ at room temperature, to a round-bottom flask charged with 2-bromobenzaldehyde (1.85 g, 10 mmol, 1 equiv), CuI (38 mg, 0.2 mmol, 2.0 mol%), PdCl₂(PPh₃)₂ (140 mg, 0.2 mmol, 2.0 mol%) and Et₃N (30 mL) was added ethynylbenzene (1.03 g, 10.5 mmol, 1.05 equiv) dropwise. The mixture was allowed to stir at 50 °C for 12 h before it was filtered through a pad of Celite rinsing with Et₂O. The filtrate was concentrated under reduced pressure and purified by silica gel column chromatography (petroleum ether/EtOAc = 100:1) to afford **S3** in 70% yield (1.45 g).

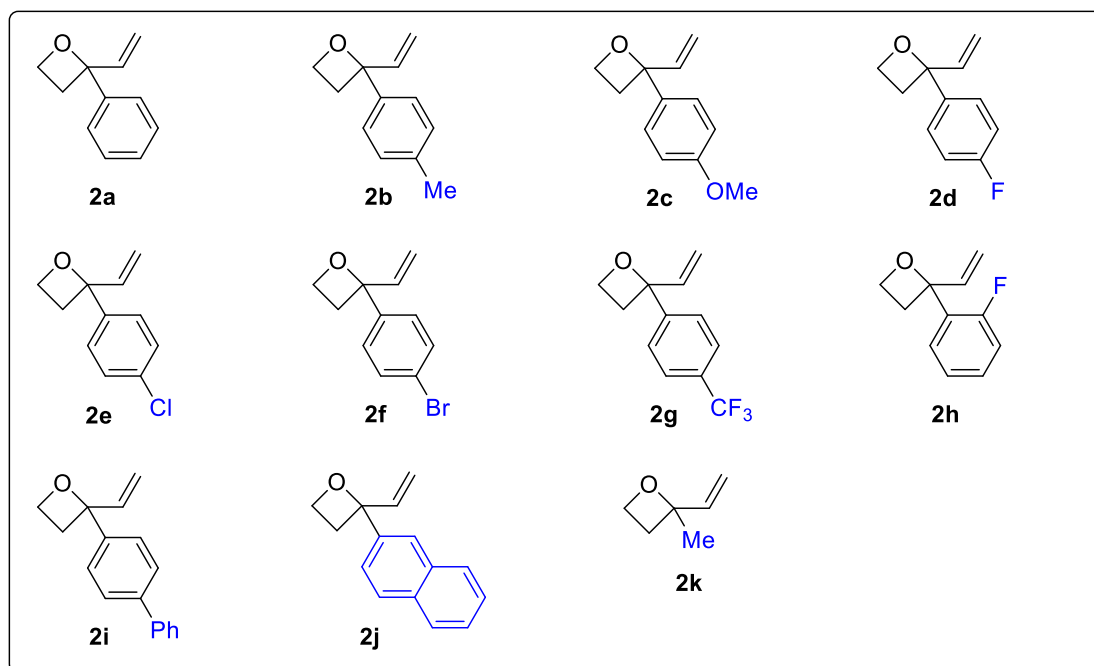
(*E*)-4-methyl-*N'*-(2-(phenylethynyl)benzylidene)benzenesulfonohydrazide (S4): To a solution of TsNHNH₂ (1.43 g, 7.7 mmol, 1.1 equiv) in the methanol (10 mL) was added the carbonyl compound **S3** (1.45 g, 7.0 mmol, 1.0 equiv) at 60 °C. The mixture was stirred approximately 30 min to give the crude product as precipitate. Wash the precipitate with petroleum ether and dry in vacuo to afford **S4** in 70% yield (1.82 g).

(3-Phenylisoquinolin-2-ium-2-yl)(tosyl)amide (1b): A Mixture of **S4** (0.90 g, 2.4 mmol, 1.0 equiv), AgOTf (61.7 mg, 0.24 mmol, 10 mol %) and 30

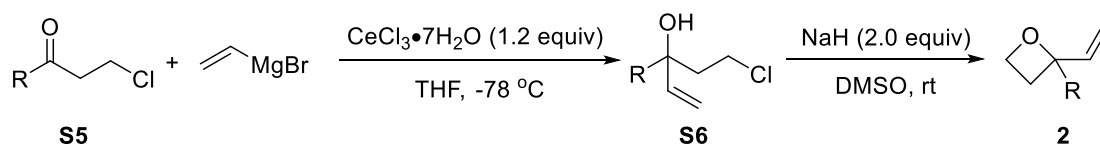
[2] (a) F. Liu, J.-Y. Wang, P. Zhou, G. Li, W.-J. Hao and S.-J. Tu, B. Jiang, *Angew. Chem. Int. Ed.*, 2017, **56**, 15570-15574; (b) F. Ye, X. Ma, Q. Xiao, H. Li, Y. Zhang and J. Wang, *J. Am. Chem. Soc.*, 2012, **134**, 5742-5745; (c) C. Wu, Q. Wang, J. Zhao, P. Li and F. Shi, *Synthesis*, 2012, **44**, 3033-3042.

dichloroethane (30 mL) was stirred at 100°C for 2 h. Then, the reaction mixture was diluted with water (20 mL) and extracted with EtOAc (30 mL × 3). The combined organic layers were washed with water (30 mL × 2), dried over anhydrous Na₂SO₄, and concentrated under reduced pressure. The residue was purified by silica gel column chromatography (petroleum ether/EtOAc = 1:1) to afford the desired *N*-iminoisoquinolinium ylide **1b** in 59% yield (527.5 mg).

Substrates **2a-2k** were synthesized according to the literature procedure,^[3] all of them are known compounds.



General Procedure B: Preparation of 2-Vinyl Oxetanes **2**.



[3] (a) H. Uno, T. Imai, K.e Harada and N. Shibata, *ACS Catal.* 2020, **10**, 1454-1459; (b) B. Guo, G.g Schwarzwald and J. T. Njardarson, *Angew. Chem. Int. Ed.* 2012, **51**, 5675-5678.

Allylic Alcohol (S6): To a flame dried 200 mL round bottom flask was charged with cerium chloride ($\text{CeCl}_3 \cdot 7\text{H}_2\text{O}$) (5.92 g, 24 mmol, 1.2 equiv) quickly. The flask was heated gradually to 140 °C in an oil bath under high vacuum and maintained at the same temperature for 2 h. Then the oil bath was removed and the flask was cooled to room temperature. THF (70 mL) was introduced with vigorous stirring. The suspension was well stirred under nitrogen at room temperature for 2 h. Then the mixture was cooled down to -78 °C followed by the addition of the vinyl magnesium bromide (1.0 M in THF, 30 mL, 1.2 equiv) via syringe. After being stirred for another 2 h at -78 °C, the corresponding β -chloro ketone **S5** (20 mmol, 1.0 equiv) in THF (50 mL) was added via syringe slowly. The reaction was maintained at -78 °C for 3 h, TLC indicated that all of the starting material was consumed. The reaction was quenched with 50 mL sat. NaHCO_3 . After separation, the aqueous layer was extracted with ether (3 x 15 mL). The combined organic layer was washed with water (30 mL), brine (30 mL), dried over anhydrous Na_2SO_4 , and concentrated under reduced pressure. The crude product was purified by flash column chromatography on silica gel to give the corresponding products **S6**.

2-Vinyl Oxetanes (2): To a 50 mL flame-dried round bottom flask charged with anhydrous DMSO (30 mL) and the corresponding allylic alcohol **S6** (4.2 mmol, 1.0 equiv). NaH (60% suspension in mineral oil, 336 mg, 8.4 mmol, 2.0 equiv) was added in one portion. Reaction was stirred at room temperature for 30 minutes. The reaction was then cooled down to 0 °C and quenched with sat. NaHCO_3 (15 mL) carefully. After separation, the aqueous layer was extracted with ethyl acetate (3 x 10 mL). The combined organic layer was washed with water (15 mL), brine (15 mL), dried over anhydrous Na_2SO_4 , and concentrated under reduced pressure. The crude product was purified by flash column chromatography to give the products **2**.

2-phenyl-2-vinyloxetane (2a) was prepared according to the General Procedure B as a colorless oil (chromatography eluent: petroleum ether/EtOAc = 20:1) in 71% yield (464.7 mg).

2-(*p*-Tolyl)-2-vinyloxetane (2b) was prepared according to the General Procedure B as a colorless oil (chromatography eluent: petroleum ether/EtOAc = 20:1) in 76% yield (953.4 mg).

2-(4-Methoxyphenyl)-2-vinyloxetane (2c) was prepared according to the General Procedure B as a colorless oil (chromatography eluent: petroleum ether/EtOAc = 20:1) in 61% yield (656.1 mg).

2-(4-Fluorophenyl)-2-vinyloxetane (2d) was prepared according to the General Procedure B as a colorless oil (chromatography eluent: petroleum ether/EtOAc = 20:1) in 90% yield (129 mg).

2-(4-Chlorophenyl)-2-vinyloxetane (2e) was prepared according to the General Procedure B as a colorless oil (chromatography eluent: petroleum ether/EtOAc = 20:1) in 76% yield (665 mg).

2-(4-Bromophenyl)-2-vinyloxetane (2f) was prepared according to the General Procedure B as a colorless oil (chromatography eluent: petroleum ether/EtOAc = 20:1) in 65% yield (837.5 mg).

2-(4-(Trifluoromethyl)phenyl)-2-vinyloxetane (2g) was prepared according to the General Procedure B as a colorless oil (chromatography eluent: petroleum ether/EtOAc = 20:1) in 94% yield (1.56 g).

2-(2-Fluorophenyl)-2-vinyloxetane (2h) was prepared according to the

General Procedure B as a colorless oil (chromatography eluent: petroleum ether/EtOAc = 20:1) in 99% yield (769.8 mg).

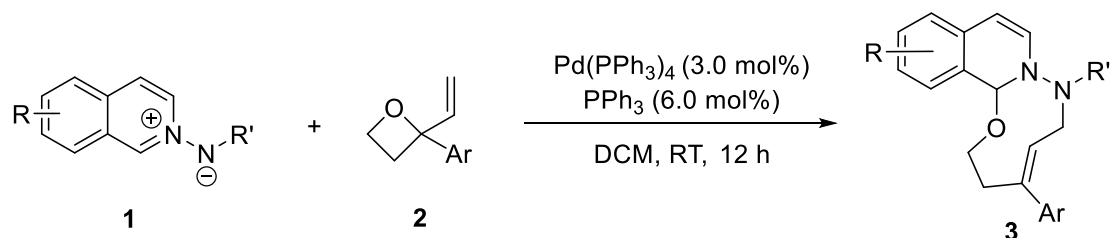
2-([1,1'-Biphenyl]-4-yl)-2-vinyloxetane (2i) was prepared according to the General Procedure B as a colorless oil (chromatography eluent: petroleum ether/EtOAc = 20:1) in 84% yield (498.1 mg).

2-(Naphthalen-2-yl)-2-vinyloxetane (2j) was prepared according to the General Procedure B as a colorless oil (chromatography eluent: petroleum ether/EtOAc = 20:1) in 50% yield (489.5 mg).

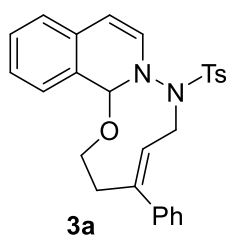
2-Methyl-2-vinyloxetane (2k) was prepared according to the General Procedure B as a colorless oil (chromatography eluent: petroleum ether/EtOAc = 20:1) in 46% yield (448.8 mg).

III. Synthesis of the Nine-membered Heterocycles

General Procedure C:



Under N₂ at room temperature, to a solution of *N*-iminoisoquinolinium ylides **1** (0.30 mmol, 1.0 equiv) and oxetane **2** (0.9 mmol, 3.0 equiv) in DCM (3.0 mL) was added Pd(PPh₃)₄ (10.4 mg, 0.009 mmol, 5.0 mol%) and PPh₃ (4.7 mg, 0.018 mmol, 10 mol%). The reaction mixture was stirred at room temperature for 12 h. The reaction mixture was directly concentrated and purified by silica gel column chromatography (petroleum ether/EtOAc) to afford the desired product **3**.



(E)-4-Phenyl-7-tosyl-2,3,6,7-tetrahydro-14bH-[1,3,4]xadiazonino[2,3-a]isoquinoline (3a) was prepared according to the General Procedure C as a light yellow solid (chromatography eluent: petroleum ether/EtOAc = 10:1) in 98% yield (134.8 mg).

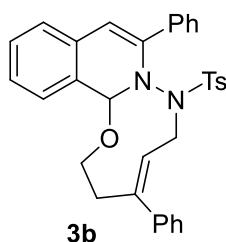
M.P. 136.2-137.0 °C.

¹H NMR (300MHz, CDCl₃) δ 7.68 (d, *J* = 8.2 Hz, 2H), 7.29-7.23 (m, 8H), 7.17-7.09 (m, 2H), 7.03 (d, *J* = 7.6 Hz, 1H), 6.05 (d, *J* = 7.7 Hz, 1H), 5.99 (s, 1H), 5.91 (t, *J* = 7.9 Hz, 1H), 5.4 (d, *J* = 7.7 Hz, 1H), 4.84 (q, *J* = 8.8 Hz, 1H), 4.5 (q, *J* =

7.1 Hz, 1H), 3.52-3.45 (m, 1H), 3.23 (t, $J = 9.1$ Hz, 1H), 3.00 (t, $J = 12.8$ Hz, 1H), 2.55 (dt, $J_1 = 4.1$, $J_2 = 10.5$ Hz, 1H), 2.42 (s, 3H) ppm.

^{13}C NMR (75MHz, CDCl_3) δ 146.8, 144.4, 143.2, 135.6, 134.8, 131.9, 129.9, 128.8, 128.5, 128.3, 127.9, 127.6, 127.6, 126.5, 125.8, 124.1, 121.8, 99.4, 88.8, 63.5, 49.2, 33.0, 21.7 ppm.

HRMS (CI+) calculated for $\text{C}_{27}\text{H}_{27}\text{N}_2\text{O}_3\text{S}$ $[\text{M} + \text{H}]^+$: 459.1742, found: 459.1741.



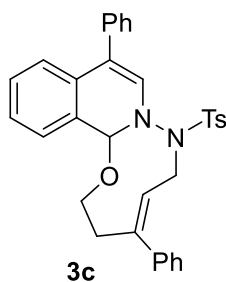
(*E*)-4,9-Diphenyl-7-tosyl-2,3,6,7-tetrahydro-14*b*H-[1,3,4]oxadiazonino[2,3-*a*]isquinoline (**3b**) was prepared according to the General Procedure C as a light yellow solid (chromatography eluent: petroleum ether/EtOAc = 10:1) in 96% yield (154.0 mg).

M.P. 142.0-143.1 °C.

^1H NMR (300MHz, CDCl_3) δ 7.42-7.08 (m, 14H), 7.01 (d, $J = 6.8$ Hz, 4H), 6.32 (q, $J = 6.6$ Hz, 1H), 6.19 (s, 1H), 5.70 (s, 1H), 4.79-4.64 (m, 2H), 3.81-3.75 (m, 1H), 3.61 (q, $J = 9.4$ Hz, 1H), 3.20-3.14 (m, 1H), 2.79(dd, $J_1 = 5.1$, $J_2 = 14.7$ Hz, 1H), 2.42 (s, 3H) ppm.

^{13}C NMR (75MHz, CDCl_3) δ 144.1, 144.0, 143.2, 142.7, 136.1, 135.1, 130.5, 129.4, 128.9, 128.8, 128.7, 128.68, 128.60, 128.1, 128.0, 127.5, 127.1, 125.9, 125.5, 124.9, 124.2, 104.8, 90.3, 63.9, 52.5, 33.7, 21.7 ppm.

HRMS (CI+) calculated for $\text{C}_{33}\text{H}_{31}\text{N}_2\text{O}_3\text{S}$ $[\text{M} + \text{H}]^+$: 535.2055, found: 535.2057.



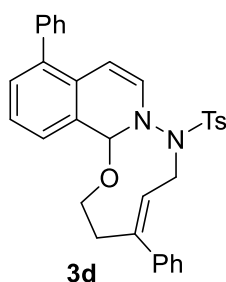
(*E*)-4,10-Diphenyl-7-tosyl-2,3,6,7-tetrahydro-14*b*H-[1,3,4]oxadiazonino[2,3-*a*]isoquinoline (**3c**) was prepared according to the General Procedure C as a light yellow solid (chromatography eluent: petroleum ether/EtOAc = 10:1) in 49% yield (78.4 mg).

M.P. 132.9-134.0 °C.

¹H NMR (300MHz, CDCl₃) δ 7.70 (d, *J* = 8.3 Hz, 2H), 7.30-7.17 (m, 13H), 7.13-7.10 (m, 1H), 6.98 (td, *J*₁ = 2.5, *J*₂ = 4.4 Hz, 2H), 6.12 (d, *J* = 0.7 Hz, 1H), 5.89 (d, *J* = 1.2 Hz, 1H), 5.82 (t, *J* = 7.6 Hz, 1H), 4.88 (q, *J* = 8.0 Hz, 1H), 4.42 (q, *J* = 7.2 Hz, 1H), 3.63-3.57 (m, 1H), 3.39 (td, *J*₁ = 2.3, *J*₂ = 9.1 Hz, 1H), 3.15(td, *J*₁ = 2.6, *J*₂ = 9.1 Hz, 1H), 2.63-2.56 (m, 1H), 2.42 (s, 3H) ppm.

¹³C NMR (75MHz, CDCl₃) δ 146.6, 144.5, 142.7, 137.2, 135.1, 132.6, 131.6, 129.9, 129.5, 128.6, 128.5, 128.4, 128.3, 128.26, 128.21, 127.6, 126.8, 126.6, 126.3, 122.9, 121.4, 113.5, 89.6, 64.1, 48.9, 33.1, 21.7 ppm.

HRMS (CI⁺) calculated for C₃₃H₃₁N₂O₃S [M + H]⁺: 535.2055, found: 535.2064.



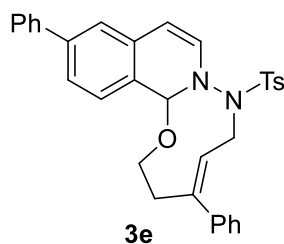
(*E*)-4,11-Diphenyl-7-tosyl-2,3,6,7-tetrahydro-14*b*H-[1,3,4]oxadiazonino[2,3-*a*]isoquinoline (**3d**) was prepared according to the General Procedure C as a light yellow solid (chromatography eluent: petroleum ether/EtOAc = 10:1) in 44% yield (71.0 mg).

M.P. 145.9-146.4 °C.

¹H NMR (300MHz, CDCl₃) δ 7.68 (d, *J* = 8.3 Hz, 2H), 7.43-7.18 (m, 14H), 7.10 (dd, *J*₁ = 2.0, *J*₂ = 7.0 Hz, 1H), 6.00(s, 1H), 5.97 (dd, *J*₁ = 1.3, *J*₂ = 7.9 Hz, 1H), 5.90 (t, *J* = 7.7 Hz, 1H), 5.46 (d, *J* = 7.9 Hz, 1H), 4.84 (q, *J* = 8.1 Hz, 1H), 4.42 (q, *J* = 13.6 Hz, 1H), 3.60-3.53 (m, 1H), 3.35 (td, *J*₁ = 2.4, *J*₂ = 8.8 Hz, 1H), 3.07 (td, *J*₁ = 2.6, *J*₂ = 14.3 Hz, 1H), 2.64-2.57 (m, 1H), 2.42 (s, 3H) ppm.

¹³C NMR (75MHz, CDCl₃) δ 146.4, 144.5, 143.0, 140.6, 137.0, 135.3, 134.0, 130.2, 129.9(3C), 129.2, 128.5, 128.4, 128.2, 127.6, 127.2, 127.1, 126.6, 125.7, 121.7, 97.8, 89.5, 64.0, 49.1, 33.1, 21.8 ppm.

HRMS (CI+) calculated for C₃₃H₃₁N₂O₃S [M + H]⁺: 535.2055, found: 535.2062.



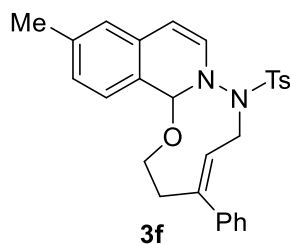
(E)-4,12-Diphenyl-7-tosyl-2,3,6,7-tetrahydro-14bH-[1,3,4]oxadiazonino[2,3-a]isoquinoline (3e) was prepared according to the General Procedure C as a light yellow solid (chromatography eluent: petroleum ether/EtOAc = 10:1) in 46% yield (74.1 mg).

M.P. 156.7-158.0 °C.

¹H NMR (300MHz, CDCl₃) δ 7.70 (d, *J* = 8.2 Hz, 2H), 7.58(d, *J* = 7.2 Hz, 2H), 7.45-7.25 (m, 12H), 7.18 (d, *J* = 8.0 Hz, 1H), 6.06 (t, *J* = 7.8 Hz, 2H), 5.90 (t, *J* = 7.8 Hz, 1H), 5.44 (d, *J* = 7.7 Hz, 1H), 4.86 (q, *J* = 8.7 Hz, 1H), 4.50 (q, *J* = 7.1 Hz, 1H), 3.57-3.50 (m, 1H), 3.29 (t, *J* = 7.0 Hz, 1H), 3.04 (t, *J* = 12.7 Hz, 1H), 2.57 (dt, *J*₁ = 3.8, *J*₂ = 10.8 Hz, 1H), 2.42 (s, 3H) ppm.

¹³C NMR (75MHz, CDCl₃) δ 146.9, 144.5, 143.1, 141.7, 140.9, 135.6, 135.1, 132.3, 130.0, 128.9, 128.5(2C), 128.3, 127.6, 127.5, 127.3, 126.6, 126.5, 124.8, 122.8, 121.7, 99.4, 88.8, 63.7, 49.2, 33.1, 21.8 ppm.

HRMS (CI+) calculated for C₃₃H₃₁N₂O₃S [M + H]⁺: 535.2055, found: 535.2062.



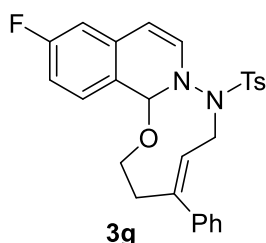
(*E*)-12-Methyl-4-phenyl-7-tosyl-2,3,6,7-tetrahydro-14*bH*-[1,3,4]oxadiazonino[2,3-*a*]isoquinoline (**3f**) was prepared according to the General Procedure C as a light yellow solid (chromatography eluent: petroleum ether/EtOAc = 10:1) in 94% yield (133.3 mg).

M.P. 122.2-123.8 °C.

¹H NMR (300MHz, CDCl₃) δ 7.68 (d, *J* = 8.2 Hz, 2H), 7.28-7.23 (m, 7H), 6.98 (q, *J* = 7.8 Hz, 2H), 6.84 (s, 1H), 6.03 (d, *J* = 7.7 Hz, 1H), 5.97 (s, 1H), 5.90 (t, *J* = 8.0 Hz, 1H), 5.32 (d, *J* = 7.7 Hz, 1H), 4.83 (q, *J* = 9.0 Hz, 1H), 4.51 (q, *J* = 7.1 Hz, 1H), 3.49-3.43 (m, 1H), 3.21 (t, *J* = 6.9 Hz, 1H), 2.97 (t, *J* = 16.9 Hz, 1H), 2.53 (dd, *J*₁ = 4.2, *J*₂ = 14.5 Hz, 1H), 2.42 (s, 3H), 2.32 (s, 3H) ppm.

¹³C NMR (75MHz, CDCl₃) δ 146.9, 144.4, 143.3, 138.6, 135.8, 135.1, 131.9, 129.9, 128.5, 128.3, 127.8, 127.6, 126.8, 126.5, 124.9, 124.5, 121.9, 99.2, 88.6, 63.3, 49.3, 33.1, 21.7, 21.4 ppm.

HRMS (CI+) calculated for C₂₈H₂₉N₂O₃S [M + H]⁺: 473.1899, found: 473.1902.



(*E*)-12-Fluoro-4-phenyl-7-tosyl-2,3,6,7-tetrahydro-14*bH*-[1,3,4]oxadiazonino[2,3-*a*]isoquinoline (**3g**) was prepared according to the General Procedure C as a light yellow solid (chromatography eluent: petroleum ether/EtOAc = 10:1) in

95% yield (135.5 mg).

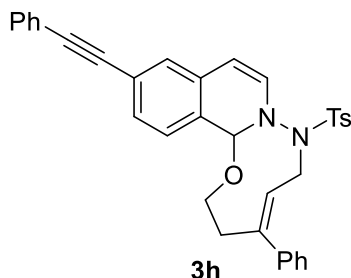
M.P. 159.4-160.2 °C.

¹H NMR (300MHz, CDCl₃) δ 7.67 (d, *J* = 8.3 Hz, 2H), 7.29-7.24 (m, 7H), 7.08 (q, *J* = 5.6 Hz, 1H), 6.83 (td, *J*₁ = 2.6, *J*₂ = 8.5 Hz, 1H), 6.70 (dd, *J*₁ = 2.5, *J*₂ = 9.6 Hz, 1H), 6.06 (d, *J* = 7.7 Hz, 1H), 6.00 (s, 1H), 5.89 (t, *J* = 7.8 Hz, 1H), 5.32 (d, *J* = 7.7 Hz, 1H), 4.83 (q, *J* = 8.8 Hz, 1H), 4.47 (q, *J* = 7.1 Hz, 1H), 3.52-3.46 (m, 1H), 3.22 (td, *J*₁ = 2.2, *J*₂ = 8.9 Hz, 1H), 3.02 (td, *J*₁ = 2.2, *J*₂ = 8.9 Hz, 1H), 2.59-2.51 (m, 1H), 2.43 (s, 3H) ppm.

¹³C NMR (75MHz, CDCl₃) δ 163.0 (d, *J* = 244.5 Hz), 147.0, 144.6, 143.0, 135.6 (d, *J* = 27.8 Hz), 134.0 (d, *J* = 9.0 Hz), 129.9 (d, *J* = 6.8 Hz), 129.7, 128.5, 128.3, 127.7, 126.4, 123.6, 123.5, 121.6, 113.0 (d, *J* = 22.5 Hz), 110.0 (d, *J* = 21.8 Hz), 98.6, 88.4, 63.5, 49.1, 33.0, 21.7 ppm.

¹⁹F NMR (282MHz, CDCl₃) δ -113.4 ppm.

HRMS (CI⁺) calculated for C₂₇H₂₆FN₂O₃S [M + H]⁺: 477.1648, found: 477.1651.



(E)-4-Phenyl-12-(phenylethynyl)-7-tosyl-2,3,6,7-tetrahydro-14bH-[1,3,4]oxadiazonino[2,3-a]isoquinoline (3h) was prepared according to the General Procedure C as a light yellow solid (chromatography eluent: petroleum ether/EtOAc = 10:1) in 66% yield (110.3 mg).

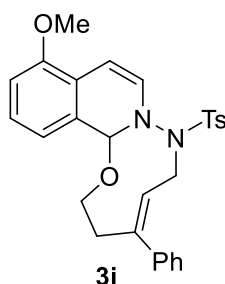
M.P. 152.9-154.1 °C.

¹H NMR (300MHz, CDCl₃) δ 7.67 (d, *J* = 8.2 Hz, 2H), 7.52 (dd, *J*₁ = 4.0, *J*₂ = 7.5 Hz, 2H), 7.35-7.23 (m, 12H), 7.09 (q, *J* = 8.0 Hz, 1H), 6.06 (d, *J* = 7.7 Hz, 1H), 5.98 (s, 1H), 5.91 (t, *J* = 7.9 Hz, 1H), 5.37 (d, *J* = 7.7 Hz, 1H), 4.84 (q, *J* = 8.8 Hz, 1H), 4.48 (q, *J* = 7.2 Hz, 1H), 3.54-3.47 (m, 1H), 3.25 (t, *J* = 6.7 Hz, 1H), 3.01 (t, *J* =

12.9 Hz, 1H), 2.60-2.53 (m, 1H), 2.43 (s, 3H) ppm.

¹³C NMR (75MHz, CDCl₃) δ 146.9, 144.6, 143.0, 135.4, 132.0(2C), 131.8, 130.0, 128.8, 128.5, 128.4(2C), 128.3, 128.0, 127.7, 127.4, 127.2, 126.5, 123.8, 123.3, 121.8, 98.8, 89.7, 89.2, 88.5, 63.6, 49.1, 33.0, 21.8 ppm.

HRMS (CI⁺) calculated for C₃₅H₃₁N₂O₃S [M + H]⁺: 559.2055, found: 559.2065.



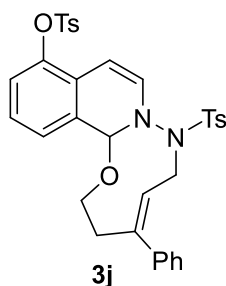
(E)-11-Methoxy-4-phenyl-7-tosyl-2,3,6,7-tetrahydro-14bH-[1,3,4]oxadiazonin o[2,3-a]isoquinoline (3i): was prepared according to the General Procedure C as a light yellow solid (chromatography eluent: petroleum ether/EtOAc = 10:1) in 75% yield (100.8 mg).

M.P. 140.2-141.7 °C.

¹H NMR (400MHz, CDCl₃) δ 7.69 (d, *J* = 8.2 Hz 2H), 7.31-7.24 (m, 7H), 7.11 (d, *J* = 7.9 Hz, 1H), 6.76 (q, *J* = 8.0 Hz, 2H), 6.05 (dd, *J*₁ = 1.0, *J*₂ = 6.8 Hz 1H), 5.99 (s, 1H) 5.91 (t, *J* = 7.9 Hz, 1H), 5.74 (d, *J* = 7.9 Hz, 1H), 4.84 (q, *J* = 8.8 Hz, 1H), 4.48 (q, *J* = 7.2 Hz, 1H), 3.83 (s, 3H), 3.51-3.45 (m, 1H), 3.27-3.21 (m, 1H), 3.02-2.97 (m, 1H), 2.59-2.53 (m, 1H), 2.42 (s, 3H) ppm.

¹³C NMR (101MHz, CDCl₃) δ 153.0, 146.8, 144.4, 143.1, 135.6, 133.9, 129.9, 128.6, 128.5, 128.3, 127.6, 126.5, 126.4, 121.8, 120.1, 109.6, 93.6, 88.6, 63.4, 55.6, 49.1, 33.0, 29.8, 21.7 ppm.

HRMS (CI⁺) calculated for C₂₈H₂₉N₂O₄S [M + H]⁺:489.1848, found: 489.1848.



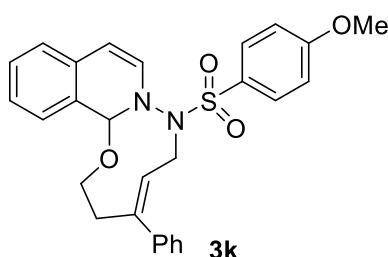
(E)-4-Phenyl-7-tosyl-2,3,6,7-tetrahydro-14bH-[1,3,4]oxadiazonino[2,3-a]isoquinolin-11-yl 4-methylbenzenesulfonate (3j): was prepared according to the General Procedure A as a white solid (chromatography eluent: petroleum ether/EtOAc = 10:1) in 90% yield (169.5 mg).

M.P. 157.7-160.7 °C.

¹H NMR (400MHz, CDCl₃) δ 7.66 (d, *J* = 8.3 Hz 2H), 7.60 (d, *J* = 8.2 Hz 2H), 7.35-7.28 (m, 4H), 7.25-7.23 (m, 3H), 7.15-7.05 (m, 4H), 6.98 (d, *J* = 7.2 Hz, 1H), 5.98 (dd, *J*₁ = 0.9, *J*₂ = 7.9 Hz 1H), 5.89 (s, 1H) 5.84 (t, *J* = 7.8 Hz, 1H), 5.42 (d, *J* = 7.9 Hz, 1H), 4.76 (q, *J* = 8.7 Hz, 1H), 4.39 (q, *J* = 7.2 Hz, 1H), 3.36-3.32 (m, 1H), 2.96-2.93 (m, 2H), 2.49 (q, *J* = 6.5 Hz, 1H), 2.43 (s, 3H), 2.32 (s, 3H) ppm.

¹³C NMR (101MHz, CDCl₃) δ 146.9, 145.5, 144.7, 143.2, 143.0, 135.5, 135.0, 132.6, 130.0, 129.8, 129.4, 128.6, 128.5, 128.3, 127.8, 126.7, 126.6, 126.1, 125.9, 122.2, 121.6, 93.0, 87.8, 63.2, 48.7, 33.0, 21.8, 21.7 ppm.

HRMS (CI⁺) calculated for C₃₄H₃₃N₂O₆S₂ [M + H⁺]:629.1780, found: 629.1780.



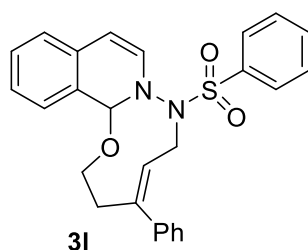
(E)-7-((4-Methoxyphenyl)sulfonyl)-4-phenyl-2,3,6,7-tetrahydro-14bH-[1,3,4]oxadiazonino[2,3-a]isoquinoline (3k) was prepared according to the General Procedure C as a light yellow solid (chromatography eluent: petroleum ether/EtOAc = 10:1) in 85% yield (120.8 mg).

M.P. 141.1-143.8 °C.

¹H NMR (300MHz, CDCl₃) δ 7.73-7.69 (m, 2H), 7.30-7.23 (m, 6H), 7.17-7.09 (m, 2H), 7.03 (d, *J* = 7.7 Hz, 1H), 6.92-6.87 (m, 2H), 6.06 (dd, *J*₁ = 1.1, *J*₂ = 7.7 Hz, 1H), 5.98 (s, 1H), 5.91 (t, *J* = 7.9 Hz, 1H), 5.40 (d, *J* = 7.7 Hz, 1H), 4.83 (q, *J* = 8.6 Hz, 1H), 4.46 (q, *J* = 7.2 Hz, 1H), 3.80 (s, 3H), 3.52-3.45 (m, 1H), 3.28-3.20 (m, 1H), 3.05-2.97 (m, 1H), 2.60-2.53 (m, 1H) ppm.

¹³C NMR (75MHz, CDCl₃) δ 163.6, 146.7, 143.1, 134.5, 131.9, 130.5, 129.8, 128.8, 128.5, 127.9(2C), 127.6, 126.5, 125.8, 124.1, 121.8, 114.4, 99.4, 88.9, 63.5, 55.8, 49.0, 33.0 ppm.

HRMS (CI⁺) calculated for C₂₇H₂₇N₂O₄S [M + H]⁺: 475.1692, found: 475.1693.



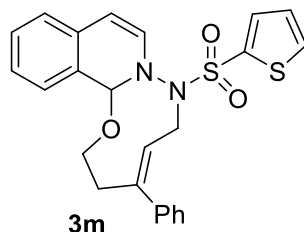
(E)-4-Phenyl-7-(phenylsulfonyl)-2,3,6,7-tetrahydro-14bH-[1,3,4]oxadiazonino[2,3-a]isoquinoline (31) was prepared according to the General Procedure C as a light yellow solid (chromatography eluent: petroleum ether/EtOAc = 10:1) in 65% yield (86.1 mg).

M.P. 107.1-108.8 °C.

¹H NMR (300MHz, CDCl₃) δ 7.79 (d, *J* = 7.3 Hz, 2H), 7.57 (t, *J* = 7.4 Hz, 1H), 7.43 (t, *J* = 7.9 Hz, 2H), 7.30-7.21 (m, 6H), 7.16-7.10 (m, 2H), 7.02 (d, *J* = 7.7 Hz, 1H), 6.04 (dd, *J*₁ = 0.9, *J*₂ = 7.7 Hz, 1H), 5.97 (s, 1H), 5.91 (t, *J* = 8.0 Hz, 1H), 5.37 (d, *J* = 7.7 Hz, 1H), 4.86 (q, *J* = 8.9 Hz, 1H), 4.53 (q, *J* = 7.2 Hz, 1H), 3.50-3.43 (m, 1H), 3.25-3.18 (m, 1H), 3.01-2.94 (m, 1H), 2.57-2.50 (m, 1H) ppm.

¹³C NMR (75MHz, CDCl₃) δ 146.9, 143.1, 138.5, 134.8, 133.4, 131.8, 129.2, 128.8, 128.4, 128.2, 127.9, 127.6, 127.5, 126.4, 125.8, 124.1, 121.7, 99.4, 88.7, 63.4, 49.3, 33.0 ppm.

HRMS (CI+) calculated for C₂₆H₂₅N₂O₃S [M + H]⁺: 445.1586, found: 445.1588.



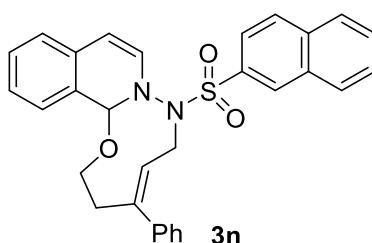
(E)-4-Phenyl-7-(thiophen-2-ylsulfonyl)-2,3,6,7-tetrahydro-14bH-[1,3,4]oxadiazonino[2,3-a]isoquinoline (3m) was prepared according to the General Procedure C as a light yellow solid (chromatography eluent: petroleum ether/EtOAc = 10:1) in 91% yield (122.6 mg).

M.P. 113.8-114.6 °C.

¹H NMR (300MHz, CDCl₃) δ 7.64 (dd, J₁ = 1.3, J₂ = 5.0 Hz, 1H), 7.56 (dd, J₁ = 1.3, J₂ = 3.8 Hz, 1H), 7.31-7.24 (m, 6H), 7.16 (d, J = 3.9 Hz, 2H), 7.09-7.03 (m, 2H), 6.10 (t, J = 1.3 Hz, 2H), 5.93 (t, J = 7.9 Hz, 1H), 5.42 (d, J = 7.5 Hz, 1H), 4.87 (q, J = 8.8 Hz, 1H), 4.52 (q, J = 7.2 Hz, 1H), 3.55-3.48 (m, 1H), 3.30-3.22 (m, 1H), 3.06-2.97 (m, 1H), 2.61-2.53 (m, 1H) ppm.

¹³C NMR (75MHz, CDCl₃) δ 147.1, 143.1, 138.9, 134.3, 134.2, 133.6, 131.8, 128.9, 128.5(2C), 128.0, 127.9, 127.7, 126.5, 125.9, 124.2, 121.5, 99.7, 88.8, 63.6, 49.6, 33.0 ppm.

HRMS (CI+) calculated for C₂₄H₂₃N₂O₃S₂ [M + H]⁺: 451.1150, found: 451.1147.



(E)-7-(Naphthalen-2-ylsulfonyl)-4-phenyl-2,3,6,7-tetrahydro-14bH-[1,3,4]oxadiazonino[2,3-a]isoquinoline (3n) was prepared according to the General Procedure C as a light yellow solid (chromatography eluent: petroleum

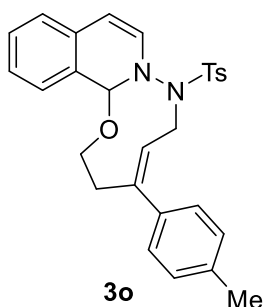
ether/EtOAc = 10:1) in 53% yield (78.7 mg).

M.P. 146.8-148.0 °C.

¹H NMR (300MHz, CDCl₃) δ 8.35 (s, 1H), 7.92 (d, *J* = 8.6 Hz, 2H), 7.84-7.76 (m, 2H), 7.65-7.60 (m, 3H), 7.31-7.00 (m, 8H), 6.05 (d, *J* = 7.7 Hz, 1H), 5.99 (s, 1H), 5.94 (t, *J* = 8.0 Hz, 1H), 5.35 (d, *J* = 9.5 Hz, 1H), 4.92 (q, *J* = 8.8 Hz, 1H), 4.58 (q, *J* = 7.4 Hz, 1H), 3.49-3.43 (m, 1H), 3.24 (t, *J* = 9.0 Hz, 1H), 3.98 (q, *J* = 13.6 Hz, 1H), 2.57 (dd, *J*₁ = 4.5, *J*₂ = 14.6 Hz, 1H) ppm.

¹³C NMR (75MHz, CDCl₃) δ 146.9, 143.1, 135.4, 135.2, 134.8, 133.2, 132.3, 132.1, 131.9, 131.8, 130.0, 129.5, 129.2, 128.7, 128.5, 128.4, 128.0, 127.7, 126.5, 125.8, 124.2, 123.1, 121.8, 99.6, 89.0, 63.5, 49.5, 33.1 ppm.

HRMS (CI⁺) calculated for C₃₀H₂₇N₂O₃S [M + H]⁺: 495.1742, found: 495.1750.



(E)-4-(*p*-tolyl)-7-tosyl-2,3,6,7-tetrahydro-14*b*H-[1,3,4]oxadiazonino[2,3-*a*]isoquinoline (3o) was prepared according to the General Procedure C as a light yellow solid (chromatography eluent: petroleum ether/EtOAc = 10:1) in 90% yield (127.4 mg).

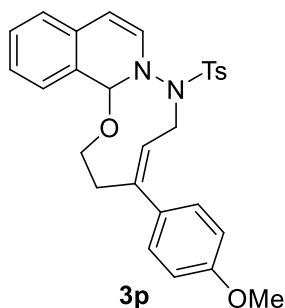
M.P. 134.2-135.0 °C.

¹H NMR (300MHz, CDCl₃) δ 7.68 (d, *J* = 8.3 Hz, 2H), 7.28-7.09 (m, 9H), 7.02 (d, *J* = 7.7 Hz, 1H), 6.05 (dd, *J*₁ = 1.1, *J*₂ = 7.7 Hz, 1H), 6.00 (s, 1H), 5.89 (t, *J* = 7.9 Hz, 1H), 5.36 (d, *J* = 7.7 Hz, 1H), 4.83 (q, *J* = 8.9 Hz, 1H), 4.51 (q, *J* = 7.2 Hz, 1H), 3.50-3.43 (m, 1H), 3.21 (td, *J*₁ = 2.0, *J*₂ = 8.7 Hz, 1H), 3.01-2.93 (m, 1H), 2.57-2.49 (m, 1H), 2.42 (s, 3H), 2.32 (s, 3H) ppm.

¹³C NMR (75MHz, CDCl₃) δ 146.7, 144.4, 140.3, 137.4, 135.8, 135.1, 132.0, 129.9, 129.2, 128.8, 128.3, 127.9, 127.6, 126.4, 125.7, 124.1, 121.1, 99.2, 88.7, 63.5, 49.4,

33.0, 21.7, 21.2 ppm.

HRMS (CI+) calculated for C₂₈H₂₉N₂O₃S [M + H]⁺: 473.1899, found: 473.1900.



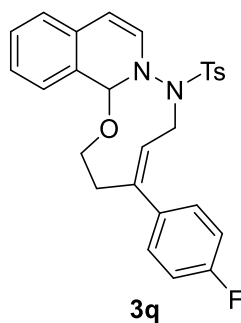
(E)-4-(4-Methoxyphenyl)-7-tosyl-2,3,6,7-tetrahydro-14bH-[1,3,4]oxadiazonin o[2,3-a]isoquinoline (3p) was prepared according to the General Procedure C as a light yellow solid (chromatography eluent: petroleum ether/EtOAc = 10:1) in 91% yield (133.2 mg).

M.P. 133.4-135.7 °C.

¹H NMR (300MHz, CDCl₃) δ 7.68 (d, *J* = 8.3 Hz, 2H), 7.29-7.02 (m, 8H), 6.83 (dt, *J*₁ = 3.0, *J*₂ = 8.8 Hz 2H), 6.05 (dd, *J*₁ = 1.2, *J*₂ = 7.7 Hz 1H), 5.97 (s, 1H), 5.86 (t, *J* = 7.9 Hz, 1H), 5.37 (d, *J* = 7.7 Hz, 1H), 4.82 (q, *J* = 8.8 Hz, 1H), 4.47 (q, *J* = 7.2 Hz, 1H), 3.79 (s, 3H), 3.50-3.43 (m, 1H), 3.24-3.17 (m, 1H), 3.00-2.93 (m, 1H), 2.57-2.49 (m, 1H), 2.42 (s, 3H) ppm.

¹³C NMR (75MHz, CDCl₃) δ 159.3, 146.2, 144.4, 135.7, 135.4, 134.8, 131.9, 129.9, 128.8, 128.3, 127.9, 127.7, 127.6, 125.8, 124.1, 120.4, 113.9, 99.3, 88.8, 63.5, 55.4, 49.2, 32.9, 21.8 ppm.

HRMS (CI+) calculated for C₂₈H₂₉N₂O₄S [M + H]⁺: 489.1848, found: 489.1852.



(*E*)-4-(4-Fluorophenyl)-7-tosyl-2,3,6,7-tetrahydro-14*b*H-[1,3,4]oxadiazonino[2,3-*a*]isoquinoline (**3q**) was prepared according to the General Procedure C as a light yellow solid (chromatography eluent: petroleum ether/EtOAc = 10:1) in 80% yield (114.1 mg).

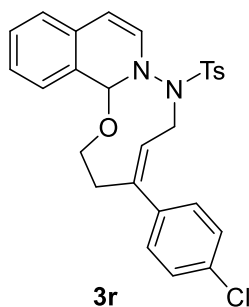
M.P. 142.9-144.1 °C.

¹H NMR (300MHz, CDCl₃) δ 7.67 (d, *J* = 8.3 Hz, 2H), 7.29-7.09 (m, 7H), 7.05-6.94 (m, 3H), 6.02 (dd, *J*₁ = 1.2, *J*₂ = 7.7 Hz, 1H), 5.98 (s, 1H), 5.86 (t, *J* = 7.8 Hz, 1H), 5.39 (d, *J* = 7.7 Hz, 1H), 4.81 (q, *J* = 8.5 Hz, 1H), 4.43 (q, *J* = 7.2 Hz, 1H), 3.52-3.45 (m, 1H), 3.26-3.18 (m, 1H), 3.05-2.96 (m, 1H), 2.56-2.50 (m, 1H), 2.42 (s, 3H) ppm.

¹³C NMR (75MHz, CDCl₃) δ 162.4 (d, *J* = 245.3 Hz), 145.7, 144.5, 139.0 (d, *J* = 3.0 Hz), 135.4, 134.2, 131.8, 129.9, 128.8, 128.4, 128.2 (d, *J* = 8.3 Hz), 127.9, 127.6, 125.9, 124.2, 121.8, 115.3 (d, *J* = 21.0 Hz), 99.5, 89.0, 63.4, 48.9, 33.1, 21.7 ppm.

¹⁹F NMR (282MHz, CDCl₃) δ -114.9 ppm.

HRMS (CI⁺) calculated for C₂₇H₂₆FN₂O₃S [M + H]⁺: 477.1648, found: 477.1647.



(*E*)-4-(4-Chlorophenyl)-7-tosyl-2,3,6,7-tetrahydro-14*b*H-[1,3,4]oxadiazonino[2,3-*a*]isoquinoline (**3r**) was prepared according to the General Procedure C as a light yellow solid (chromatography eluent: petroleum ether/EtOAc = 10:1) in 86% yield (126.9 mg).

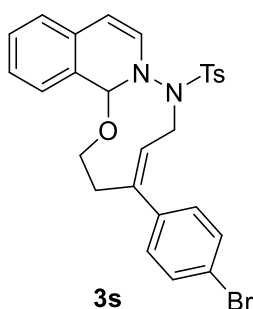
M.P. 139.2-141.3 °C.

¹H NMR (300MHz, CDCl₃) δ 7.67 (d, *J* = 8.3 Hz, 2H), 7.30-7.09 (m, 9H), 7.04 (d, *J* = 7.7 Hz, 1H), 6.01 (dd, *J*₁ = 1.2, *J*₂ = 7.7 Hz 1H), 5.98 (s, 1H), 5.89 (t, *J* = 7.8 Hz,

1H), 5.40 (d, $J = 7.7$ Hz, 1H), 4.82 (q, $J = 8.6$ Hz, 1H), 4.43 (q, $J = 7.2$ Hz, 1H), 3.51-3.44 (m, 1H), 3.25-3.17 (m, 1H), 3.04-2.96 (m, 1H), 2.55-2.47 (m, 1H), 2.42 (s, 3H) ppm.

^{13}C NMR (75MHz, CDCl_3) δ 145.6, 144.6, 141.4, 135.3, 134.2, 133.5, 131.8, 129.9, 128.9, 128.6, 128.3, 127.9, 127.8, 127.6, 125.9, 124.2, 122.3, 99.6, 89.0, 63.4, 48.9, 32.9, 21.7 ppm.

HRMS (CI+) calculated for $\text{C}_{27}\text{H}_{26}\text{ClN}_2\text{O}_3\text{S}$ $[\text{M} + \text{H}]^+$: 493.1353, found: 493.1360.



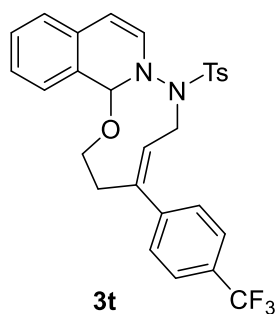
(*E*)-4-(4-Bromophenyl)-7-tosyl-2,3,6,7-tetrahydro-14*b*H-[1,3,4]oxadiazonino[2,3-*a*]isoquinoline (**3s**) was prepared according to the General Procedure C as a light yellow solid (chromatography eluent: petroleum ether/EtOAc = 10:1) in 86% yield (138.2 mg).

M.P. 134.7-136.0 °C.

^1H NMR (300MHz, CDCl_3) δ 7.67 (d, $J = 8.3$ Hz, 2H), 7.41 (dd, $J_1 = 1.7$, $J_2 = 5.0$ Hz, 2H), 7.30-7.09 (m, 7H), 7.04 (d, $J = 7.7$ Hz, 1H), 6.01 (d, $J = 8.8$ Hz, 1H), 5.98 (s, 1H), 5.89 (t, $J = 7.8$ Hz, 1H), 5.38 (d, $J = 5.9$ Hz, 1H), 4.81 (q, $J = 8.6$ Hz, 1H), 4.43 (q, $J = 8.6$ Hz, 1H), 3.51-3.44 (m, 1H), 3.25-3.17 (m, 1H), 3.04-2.96 (m, 1H), 2.54-2.47 (m, 1H), 2.42 (s, 3H) ppm.

^{13}C NMR (75MHz, CDCl_3) δ 145.6, 144.5, 141.9, 135.3, 134.2, 131.8, 131.6, 129.9, 128.9, 128.3, 128.2, 127.9, 127.6, 125.9, 124.2, 122.4, 121.7, 99.6, 89.0, 63.4, 48.9, 32.9, 21.7 ppm.

HRMS (CI+) calculated for $\text{C}_{27}\text{H}_{26}\text{BrN}_2\text{O}_3\text{S}$ $[\text{M} + \text{H}]^+$: 537.0848, found: 537.0844.



(E)-7-Tosyl-4-(4-(trifluoromethyl)phenyl)-2,3,6,7-tetrahydro-14bH-[1,3,4]oxadiazonino[2,3-a]isoquinoline (3t) was prepared according to the General Procedure C as a light yellow solid (chromatography eluent: petroleum ether/EtOAc = 10:1) in 92% yield (144.9 mg).

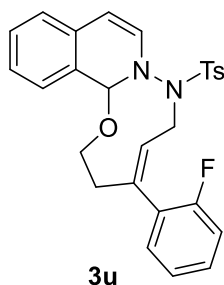
M.P. 144.8-147.7 °C.

¹H NMR (300MHz, CDCl₃) δ 7.68 (d, *J* = 8.3 Hz, 2H), 7.55(d, *J* = 8.2 Hz, 2H), 7.37 (d, *J* = 8.1 Hz, 2H), 7.30-7.10 (m, 5H), 7.05 (d, *J* = 7.7 Hz, 1H), 6.00 (d, *J* = 4.7 Hz, 2H), 5.95 (t, *J* = 8.0 Hz, 1H), 5.40 (d, *J* = 7.9 Hz, 1H), 4.84 (q, *J* = 8.5 Hz, 1H), 4.44 (q, *J* = 7.1 Hz, 1H), 3.54-3.47 (m, 1H), 3.27-3.20 (m, 1H), 3.10-3.03 (m, 1H), 2.58-2.53 (m, 1H), 2.42 (s, 3H) ppm.

¹³C NMR (75MHz, CDCl₃) δ 146.2, 145.6, 144.6, 135.2, 134.0, 131.8, 130.0, 129.6 (q, *J* = 32.3 Hz), 128.9, 128.4, 127.9, 127.6, 126.8, 126.1, 126.0, 125.5 (q, *J* = 3.8 Hz), 124.2, 123.6, 99.7, 89.1, 63.4, 48.8, 32.9, 21.8 ppm.

¹⁹F NMR (282MHz, CDCl₃) δ -62.5 ppm.

HRMS (CI⁺) calculated for C₂₈H₂₆F₃N₂O₃S [M + H]⁺: 527.1616, found: 527.1620.



(E)-4-(2-Fluorophenyl)-7-tosyl-2,3,6,7-tetrahydro-14bH-[1,3,4]oxadiazonino[2,3-a]isoquinoline (3u) was prepared according to the General Procedure C as a light yellow solid (chromatography eluent: petroleum ether/EtOAc = 10:1) in

85% yield (121.4 mg).

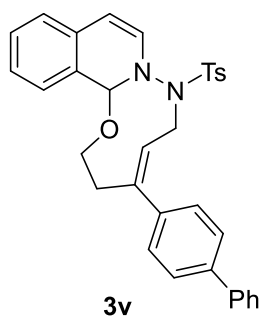
M.P. 145.3-146.1 °C.

¹H NMR (300MHz, CDCl₃) δ 7.68 (d, *J* = 8.3 Hz, 2H), 7.23-6.96 (m, 10H), 6.10 (d, *J* = 6.7 Hz, 1H), 5.99 (s, 1H), 5.84 (t, *J* = 8.0 Hz, 1H), 5.43 (d, *J* = 7.7 Hz, 1H), 4.85 (q, *J* = 8.9 Hz, 1H), 4.52 (q, *J* = 7.2 Hz, 1H), 3.48-3.41 (m, 1H), 3.28 (t, *J* = 9.3 Hz, 1H), 2.96 (q, *J* = 9.7 Hz, 1H), 2.46 (s, 1H), 2.42 (s, 3H) ppm.

¹³C NMR (75MHz, CDCl₃) δ 159.7 (d, *J* = 245.3 Hz), 144.5, 143.4, 135.7, 135.2, 131.9, 131.7 (d, *J* = 14.3 Hz), 130.4 (d, *J* = 3.8 Hz), 129.9, 129.2 (d, *J* = 8.3 Hz), 128.8, 128.3, 127.9, 127.6, 125.8, 124.9, 124.3, 124.2, 115.8 (d, *J* = 22.5 Hz), 99.4, 88.7, 63.4, 49.2, 33.7, 21.8 ppm.

¹⁹F NMR (282MHz, CDCl₃) δ -114.4 ppm.

HRMS (CI⁺) calculated for C₂₇H₂₆FN₂O₃S [M + H]⁺: 477.1648, found: 477.1647.



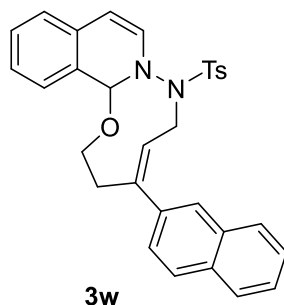
(E)-4-([1,1'-Biphenyl]-4-yl)-7-tosyl-2,3,6,7-tetrahydro-14bH-[1,3,4]oxadiazono[2,3-a]isoquinoline (3v) was prepared according to the General Procedure C as a light yellow solid (chromatography eluent: petroleum ether/EtOAc = 10:1) in 92% yield (147.4 mg).

M.P. 139.4-142.5 °C.

¹H NMR (300MHz, CDCl₃) δ 7.69 (d, *J* = 8.3 Hz, 2H), 7.58-7.23 (m, 12H), 7.18-7.09 (m, 2H), 7.04 (d, *J* = 7.6 Hz, 1H), 6.06 (dd, *J*₁ = 1.2, *J*₂ = 7.7 Hz, 1H), 5.98 (t, *J* = 5.5 Hz, 2H), 5.40 (d, *J* = 7.7 Hz, 1H), 4.86 (q, *J* = 8.8 Hz, 1H), 4.51 (q, *J* = 7.2 Hz, 1H), 3.55-3.48 (m, 1H), 3.30-3.22 (m, 1H), 3.07-2.99 (m, 1H), 2.63-2.56 (m, 1H), 2.42 (s, 3H) ppm.

^{13}C NMR (75MHz, CDCl_3) δ 146.3, 144.5, 141.9, 140.7, 140.5, 135.6, 134.7, 131.9, 129.9, 128.9, 128.8, 128.3, 127.9, 127.6, 127.5, 127.2, 127.1, 126.9, 125.8, 124.2, 121.8, 99.4, 88.9, 63.5, 49.2, 32.9, 21.7 ppm.

HRMS (CI+) calculated for $\text{C}_{33}\text{H}_{31}\text{N}_2\text{O}_3\text{S}$ $[\text{M} + \text{H}]^+$: 535.2055, found: 535.2068.



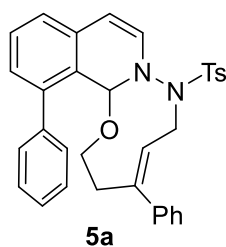
(*E*)-4-(Naphthalen-2-yl)-7-tosyl-2,3,6,7-tetrahydro-14*b*H-[1,3,4]oxadiazoninolo[2,3-*a*]isoquinoline (**3w**) was prepared according to the General Procedure C as a light yellow solid (chromatography eluent: petroleum ether/EtOAc = 10:1) in 89% yield (135.6 mg).

M.P. 145.7-147.3 °C.

^1H NMR (300MHz, CDCl_3) δ 7.81-7.69 (m, 6H), 7.47-7.42 (m, 3H), 7.30-7.24 (m, 3H), 7.18-7.09 (m, 2H), 7.04 (d, $J = 6.6$ Hz, 1H), 6.07(t, $J = 7.7$ Hz, 2H), 6.02 (s, 1H), 5.39 (d, $J = 7.7$ Hz, 1H), 4.89 (q, $J = 8.8$ Hz, 1H), 4.54 (q, $J = 7.1$ Hz, 1H), 3.58-3.51 (m, 1H), 3.33-3.25 (m, 1H), 3.13-3.06 (m, 1H), 2.72-2.64 (m, 1H), 2.42 (s, 3H) ppm.

^{13}C NMR (75MHz, CDCl_3) δ 146.6, 144.5, 140.3, 135.6, 134.7, 133.4, 132.8, 131.9, 130.0, 128.8, 128.3, 128.2, 128.1, 128.0, 127.7, 127.6, 126.4, 126.1, 125.8, 125.2, 124.8, 124.2, 122.4, 99.5, 88.9, 63.6, 49.3, 33.0, 21.8 ppm.

HRMS (CI+) calculated for $\text{C}_{31}\text{H}_{29}\text{N}_2\text{O}_3\text{S}$ $[\text{M} + \text{H}]^+$: 509.1899, found: 509.1903.



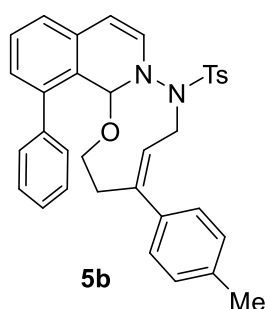
4,12-Diphenyl-5-tosyl-4-vinyl-2,3,4,5-tetrahydro-12*b*H-[1,3,4]oxadiazepino[2,3-*a*]isoquinoline (5a) was prepared according to the General Procedure C as a light yellow solid (chromatography eluent: petroleum ether/EtOAc = 10:1) in 90% yield (144.1 mg).

M.P. 150.5-152.7 °C.

¹H NMR (300MHz, CDCl₃) δ 7.63 (d, *J* = 8.3 Hz, 2H), 7.39-7.21 (m, 11H), 7.19-7.16 (m, 2H), 7.10-7.04 (m, 2H), 5.93-5.89 (m, 2H), 5.75 (dd, *J* = 6.2, *J* = 7.5 Hz, 1H), 5.58 (d, *J* = 7.4 Hz, 1H), 4.81 (q, *J* = 6.1 Hz, 1H), 4.15 (q, *J* = 7.7 Hz, 1H), 3.26-3.09 (m, 2H), 2.84-2.79 (m, 1H), 2.44 (s, 3H), 2.39 (d, *J* = 3.6 Hz, 1H) ppm.

¹³C NMR (75MHz, CDCl₃) δ 146.2, 144.5, 142.3, 141.0, 140.5, 134.1, 131.4, 129.8, 129.4, 128.7, 128.4, 128.2, 128.0, 127.7, 127.5, 127.3, 126.6(2C), 126.3, 123.8, 120.3, 101.4, 88.2, 65.1, 48.2, 33.1, 21.8 ppm.

HRMS (CI⁺) calculated for C₃₃H₃₁N₂O₃S [M + H]⁺: 535.2055, found: 535.2065.



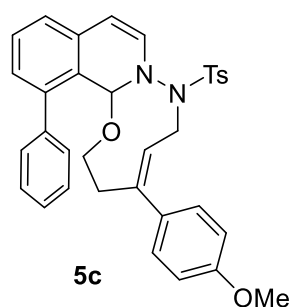
12-Phenyl-4-(*p*-tolyl)-5-tosyl-4-vinyl-2,3,4,5-tetrahydro-12*b*H-[1,3,4]oxadiazepino[2,3-*a*]isoquinoline (5b) was prepared according to the General Procedure C as a light yellow solid (chromatography eluent: petroleum ether/EtOAc = 10:1) in 95% yield (156.4 mg).

M.P. 128.5-130.6 °C.

$^1\text{H NMR}$ (400MHz, CDCl_3) δ 7.64 (d, $J = 6.2$ Hz, 2H), 7.40-7.23 (m, 5H), 7.25-7.22 (m, 3H), 7.11-7.04 (m, 6H), 5.94 (dd, $J_1 = 1.2$, $J_2 = 7.6$ Hz, 1H), 5.88 (d, $J = 1.3$ Hz, 1H), 5.75 (t, $J = 7.0$ Hz, 1H), 5.58 (d, $J = 7.6$ Hz, 1H), 4.81 (q, $J = 6.3$ Hz, 1H), 4.18 (q, $J = 7.7$ Hz, 1H), 3.23 (dt, $J_1 = 10.8$, $J_2 = 2.6$ Hz, 1H), 3.12 (td, $J_1 = 13.9$, $J_2 = 3.2$ Hz, 1H), 2.84 (dt, $J_1 = 3.8$, $J_2 = 11.8$ Hz, 1H), 2.45 (s, 3H), 2.41 (d, $J = 14.6$ Hz, 1H), 2.31 (s, 3H) ppm.

$^{13}\text{C NMR}$ (101MHz, CDCl_3) δ 146.1, 144.4, 141.0, 140.5, 139.5, 137.3, 134.3, 131.7, 131.5, 129.8, 129.4, 129.1, 128.7, 128.2, 128.0, 127.7, 127.3, 126.4, 126.2, 123.8, 119.6, 101.2, 88.1, 65.1, 48.4, 33.0, 21.8, 21.2 ppm.

HRMS (CI $^+$) calculated for $\text{C}_{34}\text{H}_{33}\text{N}_2\text{O}_3\text{S}$ [$\text{M} + \text{H}$] $^+$: 549.2212, found: 549.2221.



4-(4-Methoxyphenyl)-12-phenyl-5-tosyl-4-vinyl-2,3,4,5-tetrahydro-12bH-[1,3,4]oxadiazepino[2,3-a]isoquinoline (5c) was prepared according to the General Procedure C as a light yellow solid (chromatography eluent: petroleum ether/EtOAc = 10:1) in 89% yield (150.7 mg).

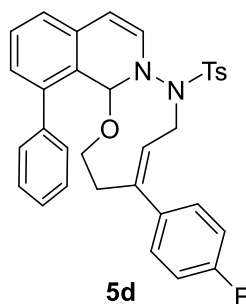
M.P. 123.8-125.0 °C.

$^1\text{H NMR}$ (400MHz, CDCl_3) δ 7.63 (d, $J = 8.2$ Hz, 2H), 7.38-7.23 (m, 8H), 7.14-7.05 (m, 4H), 6.78(d, $J = 8.7$ Hz, 2H), 5.91 (t, $J = 7.6$ Hz, 2H), 5.71 (t, $J = 6.8$ Hz, 1H), 5.58 (d, $J = 7.6$ Hz, 1H), 4.80 (dd, $J_1 = 6.1$, $J_2 = 13.9$ Hz, 1H), 4.14 (q, $J = 7.8$ Hz, 1H), 3.77 (s, 3H), 3.22 (td, $J_1 = 11.1$, $J_2 = 2.6$ Hz, 1H), 3.11 (td, $J_1 = 13.8$, $J_2 = 3.0$ Hz, 1H), 2.82 (dt, $J_1 = 11.7$, $J_2 = 3.6$ Hz, 1H), 2.45 (s, 3H), 2.40 (t, $J = 3.1$ Hz, 1H) ppm.

$^{13}\text{C NMR}$ (101MHz, CDCl_3) δ 159.2, 145.6, 144.4, 141.0, 140.5, 134.7, 134.1, 131.5, 131.4, 129.8, 129.4, 128.7, 128.2, 128.0, 127.7(2C), 127.3, 126.3, 123.8, 118.7, 113.8,

101.3, 88.2, 65.1, 55.4, 48.3, 33.0, 21.8 ppm.

HRMS (CI⁺) calculated for C₃₄H₃₃N₂O₄S [M + H]⁺: 565.2161, found: 565.2169.



4-(4-Fluorophenyl)-12-phenyl-5-tosyl-4-vinyl-2,3,4,5-tetrahydro-12*b*H-[1,3,4]oxadiazepino[2,3-*a*]isoquinoline (5d) was prepared according to the General Procedure C as a light yellow solid (chromatography eluent: petroleum ether/EtOAc = 10:1) in 85% yield (140.8 mg).

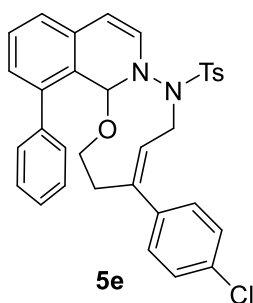
M.P. 131.2-134.9 °C.

¹H NMR (400MHz, CDCl₃) δ 7.69-7.61 (m, 4H), 7.56-7.53 (m, 1H), 7.48-7.44 (m, 2H), 7.38-7.28 (m, 3H), 7.15-7.05 (m, 4H), 6.92(t, *J* = 8.6 Hz, 2H), 5.88 (t, *J* = 8.8 Hz, 2H), 5.70 (t, *J* = 7.2 Hz, 1H), 5.59 (d, *J* = 7.6 Hz, 1H), 4.79 (dd, *J*₁ = 5.7, *J*₂ = 14.1 Hz, 1H), 4.09 (q, *J* = 7.8 Hz, 1H), 3.23-3.11(m, 2H), 2.80-2.76 (m, 1H), 2.45 (s, 3H), 2.35 (t, *J* = 11.0 Hz, 1H) ppm.

¹³C NMR (101MHz, CDCl₃) δ 162.2 (d, *J* = 247.5 Hz), 145.1, 144.6, 140.9, 140.5, 138.2 (d, *J* = 3.0 Hz), 132.2 (d, *J* = 10.1 Hz), 131.9 (d, *J* = 2.0 Hz), 130.9 (d, *J* = 41.4 Hz), 129.8, 129.4, 128.8, 128.6 (d, *J* = 12.1 Hz), 128.1 (d, *J* = 8.0 Hz), 128.2, 128.0, 127.4 (d, *J* = 43.4 Hz), 126.3, 123.9, 120.3, 115.2 (d, *J* = 21.2 Hz), 101.6, 88.4, 64.9, 48.0, 33.2, 21.8 ppm.

¹⁹F NMR (282MHz, CDCl₃) δ -115.1 ppm.

HRMS (CI⁺) calculated for C₃₃H₃₀FN₂O₃S [M + H]⁺: 553.1961, found: 553.1968.



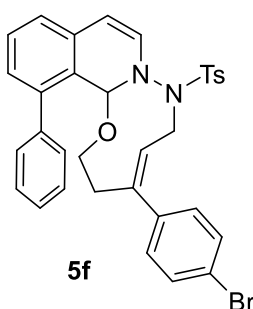
4-(4-Chlorophenyl)-12-phenyl-5-tosyl-4-vinyl-2,3,4,5-tetrahydro-12*b*H-[1,3,4]oxadiazepino[2,3-*a*]isoquinoline (5e) was prepared according to the General Procedure C as a light yellow solid (chromatography eluent: petroleum ether/EtOAc = 10:1) in 97% yield (165.8 mg).

M.P. 150.3-152.4 °C.

¹H NMR (400MHz, CDCl₃) δ 7.57-7.45 (m, 4H), 7.39-7.29 (m, 4H), 7.23(t, *J* = 6.3 Hz, 4H), 7.14-7.06 (m, 4H), 5.88 (t, *J* = 7.8 Hz, 2H), 5.74 (dd, *J*₁ = 6.0, *J*₂ = 10.3 Hz, 1H), 5.59 (d, *J* = 7.6 Hz, 1H), 4.80 (dd, *J*₁ = 5.7, *J*₂ = 14.1 Hz, 1H), 4.12 (q, *J* = 7.4 Hz, 1H), 3.23-3.11(m, 2H), 2.80-2.76 (m, 1H), 2.45 (s, 3H), 2.36 (t, *J* = 11.2 Hz, 1H) ppm.

¹³C NMR (101MHz, CDCl₃) δ 144.9, 144.6, 140.9, 140.7, 140.4, 133.9, 133.4, 132.3, 131.2, 129.8, 129.2, 128.8, 128.5, 128.2, 128.1, 127.9, 127.7, 127.3, 126.3, 123.9, 120.8, 101.6, 88.4, 64.9, 48.0, 33.0, 21.8 ppm.

HRMS (CI⁺) calculated for C₃₃H₃₀ClN₂O₃S [M + H]⁺: 569.1666, found: 569.1672.



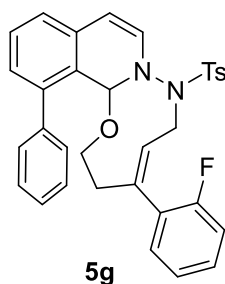
4-(4-Bromophenyl)-12-phenyl-5-tosyl-4-vinyl-2,3,4,5-tetrahydro-12*b*H-[1,3,4]oxadiazepino[2,3-*a*]isoquinoline (5f) was prepared according to the General Procedure C as a light yellow solid (chromatography eluent: petroleum ether/EtOAc = 10:1) in 93% yield (171.2 mg).

M.P. 151.3-153.5 °C.

¹H NMR (400MHz, CDCl₃) δ 7.63 (d, *J* = 7.5 Hz, 2H), 7.38-7.24 (m, 10H), 7.11-7.04 (m, 4H), 5.88(t, *J* = 8.5 Hz, 2H), 5.75 (t, *J* = 6.6 Hz, 1H), 6.59 (d, *J* = 7.6 Hz, 1H), 4.80 (dd, *J*₁ = 5.7, *J*₂ = 14.1 Hz, 1H), 4.12 (q, *J* = 7.8 Hz, 1H), 3.22-3.10 (m, 2H), 2.77 (dd, *J*₁ = 6.0, *J*₂ = 11.7 Hz 1H), 2.45 (s, 3H), 2.36 (t, *J* = 11.4 Hz, 1H) ppm.

¹³C NMR (101MHz, CDCl₃) δ 144.9, 144.6, 141.1, 140.9, 140.4, 133.9, 131.5, 131.2, 130.8, 129.8, 129.4, 128.8, 128.3, 128.2, 128.0, 127.7, 127.3, 126.3, 123.9, 121.6, 120.8, 101.6, 88.4, 64.9, 48.0, 32.9, 21.8 ppm.

HRMS (CI⁺) calculated for C₃₃H₃₀BrN₂O₃S [M + H]⁺: 613.1161, found: 613.1171.



4-(2-Fluorophenyl)-12-phenyl-5-tosyl-4-vinyl-2,3,4,5-tetrahydro-12*b*H-[1,3,4]oxadiazepino[2,3-*a*]isoquinoline (5g) was prepared according to the General Procedure C as a light yellow solid (chromatography eluent: petroleum ether/EtOAc = 10:1) in 82% yield (136.6 mg).

M.P. 114.5-115.2 °C.

¹H NMR (400MHz, CDCl₃) δ 7.64 (d, *J* = 8.3 Hz, 2H), 7.40-7.30 (m, 5H), 7.24-7.17 (m, 3H), 7.13-7.02 (m, 6H), 5.98 (dd, *J*₁ = 1.2, *J*₂ = 7.6 Hz, 1H), 5.89 (d, *J* = 1.2 Hz, 1H), 5.72 (t, *J* = 6.9 Hz, 1H), 5.63 (d, *J* = 7.6 Hz, 1H), 4.82 (q, *J* = 6.3 Hz, 1H), 4.18 (q, *J* = 7.7 Hz, 1H), 3.26-3.20(m, 1H), 3.11-3.05(m, 1H), 2.82 (dt, *J*₁ = 3.7, *J*₂ = 12.0 Hz 1H), 2.45 (s, 3H), 2.39 (t, *J* = 7.8 Hz, 1H) ppm.

¹³C NMR (101MHz, CDCl₃) δ 159.6 (d, *J* = 247.5 Hz), 144.4, 142.7, 140.9, 140.4, 134.3, 132.2 (d, *J* = 10.1 Hz), 131.7, 131.3, 130.8, 130.7, 129.8, 129.4, 129.1 (d, *J* = 8.1 Hz), 128.6, 128.2, 128.1, 127.4 (d, *J* = 47.5 Hz), 126.2, 124.2 (d, *J* = 3.0 Hz),

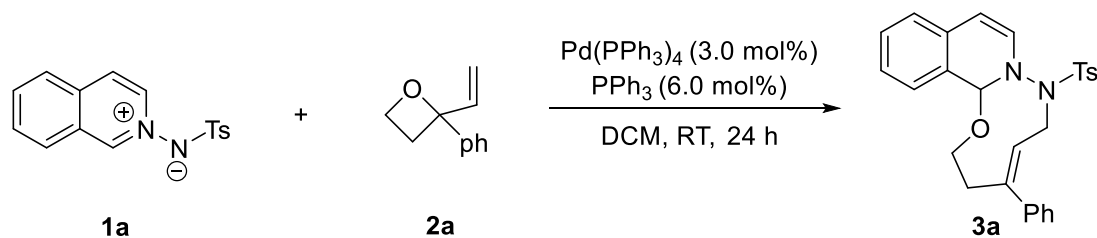
123.8, 123.5, 115.5 (d, $J = 22.2$ Hz), 101.5, 88.1, 65.0, 48.2, 33.7, 21.8 ppm.

^{19}F NMR (282MHz, CDCl_3) δ -114.9 ppm.

HRMS (CI+) calculated for $\text{C}_{33}\text{H}_{30}\text{FN}_2\text{O}_3\text{S}$ $[\text{M} + \text{H}]^+$: 535.1961, found: 553.1965.

IV. Gram-scale Synthesis

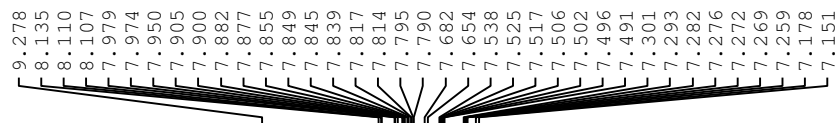
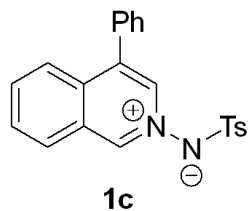
Gram-scale synthesis:



Under N₂ at room temperature, to a solution of *N*-iminoisoquinolinium ylide **1a** (0.89 g, 3.0 mmol) and 2-vinyl oxetane **2a** (0.96 g, 9.0 mmol) in DCM (30 mL) was added Pd(PPh₃)₄ (104 mg, 0.09 mmol, 3.0 mol%) and PPh₃ (47.2 mg, 0.18 mmol, 6.0 mol%). The reaction mixture was stirred at room temperature for 24 h. The reaction mixture was directly concentrated and purified by silica gel column chromatography (petroleum ether/EtOAc = 10:1) to afford the desired product **3a** in 87% yield (1.20 g).

NMR Spectrum

3sjwei 4423 xhl-1-81-h-fr 1h cdcl3



2.350

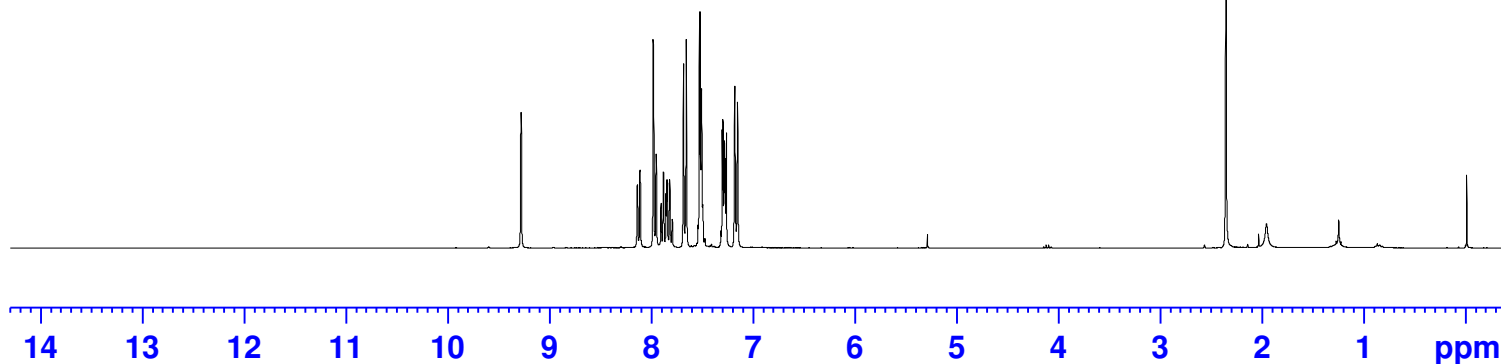


Current Data Parameters
NAME 2021-4--11Project 1 data
EXPNO 4423
PROCNO 1

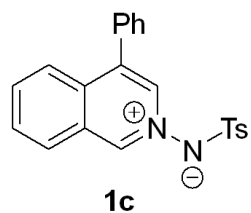
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Time 21.22
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PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 161
DW 83.200 usec
DE 6.50 usec
TE 296.2 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 300.1318534 MHz
NUC1 1H
P1 10.00 usec
PLW1 14.00000000 W

F2 - Processing parameters
SI 65536
SF 300.1300073 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



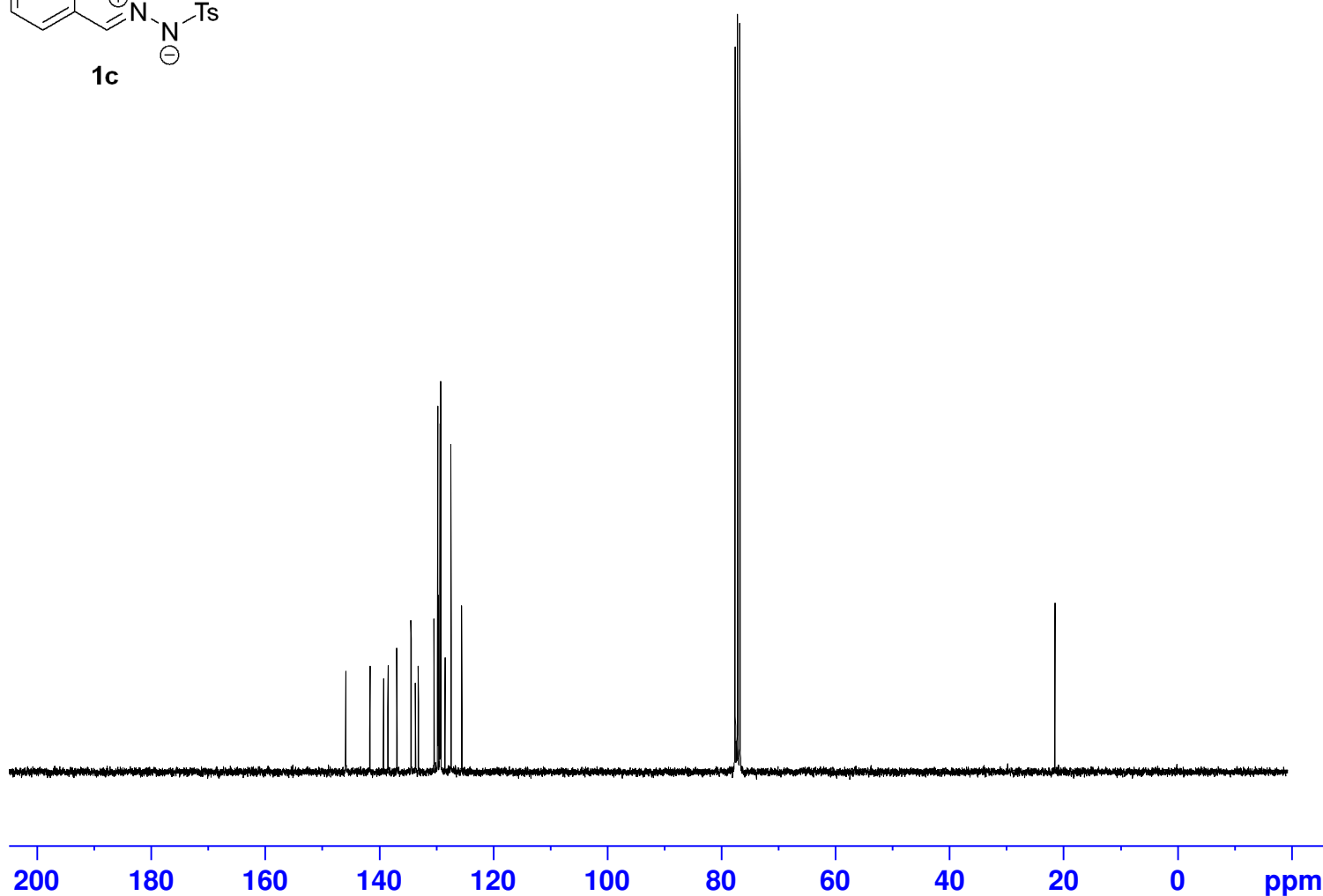
3sjwei 4424 xhl-1-81-c-fr 13c cdcl3



145.87
141.64
139.24
138.48
136.92
134.43
133.68
133.15
130.41
129.76
129.68
129.36
129.22
129.20
128.47
127.41
125.53

77.57
77.15
76.73

21.47



Current Data Parameters
NAME 2021-4--11Project 1 data
EXPNO 4424
PROCNO 1

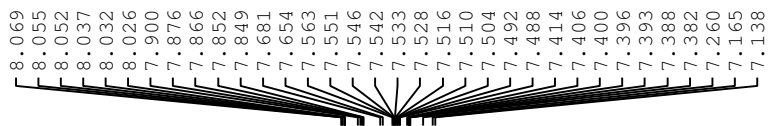
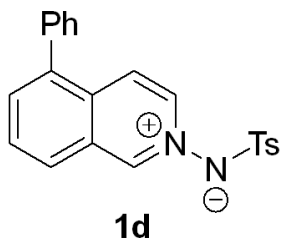
F2 - Acquisition Parameters
Date_ 20210704
Time 22.30
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PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 1024
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175317 sec
RG 203
DW 27.733 usec
DE 6.50 usec
TE 296.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 75.4752949 MHz
NUC1 13C
P1 9.50 usec
PLW1 34.20000076 W

===== CHANNEL f2 =====
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.17284000 W
PLW13 0.14000000 W

F2 - Processing parameters
SI 32768
SF 75.4677432 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

3sjwei 4421 xh1-1-78-h-fr 1h cdcl3



2.337

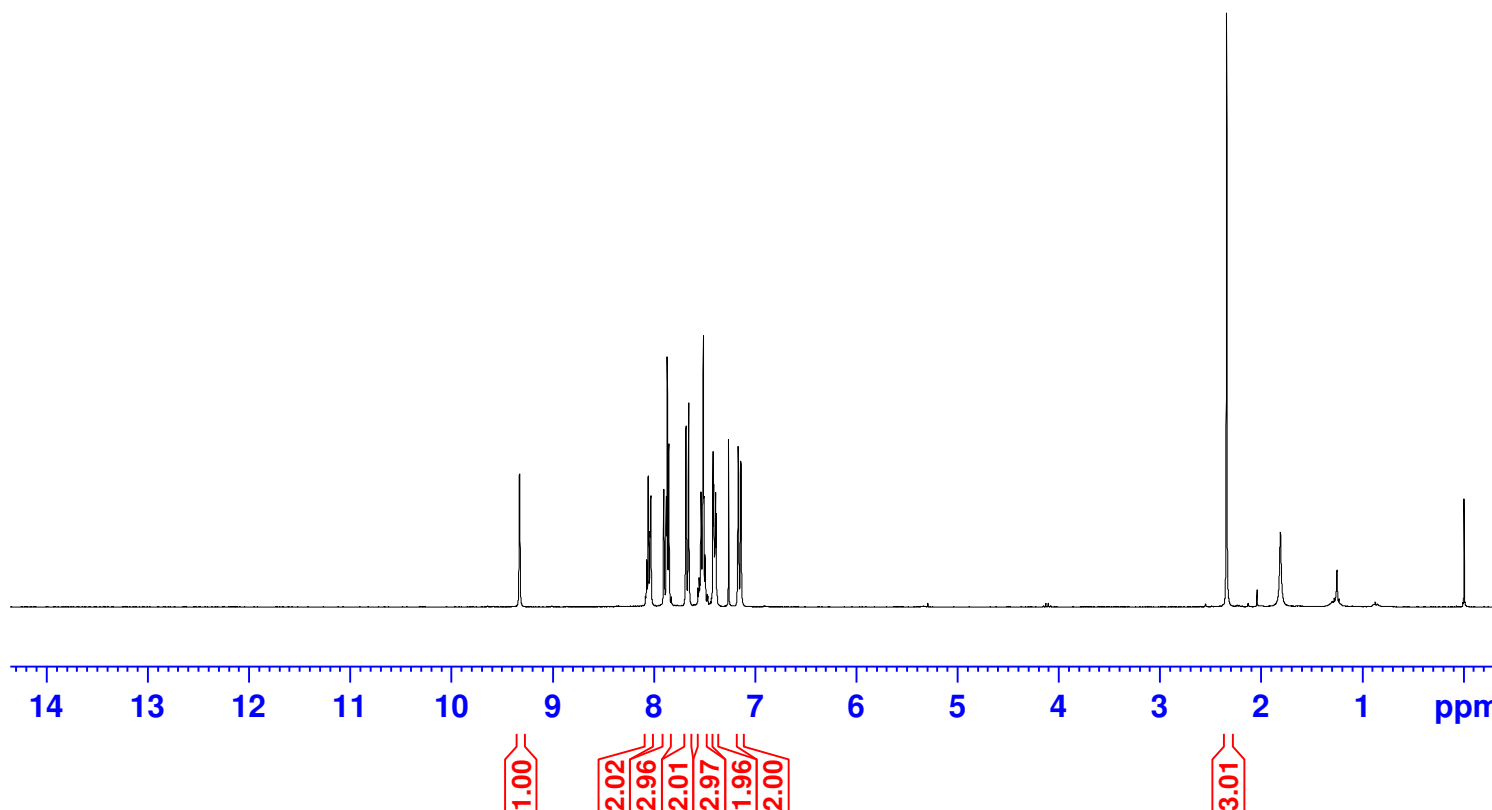


Current Data Parameters
NAME 2021-4--11Project 1 data
EXPNO 4421
PROCNO 1

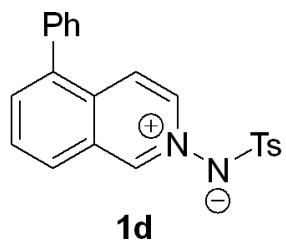
F2 - Acquisition Parameters
Date_ 20210704
Time 20.09
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 203
DW 83.200 usec
DE 6.50 usec
TE 296.1 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 300.1318534 MHz
NUC1 1H
P1 10.00 usec
PLW1 14.00000000 W

F2 - Processing parameters
SI 65536
SF 300.1300072 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



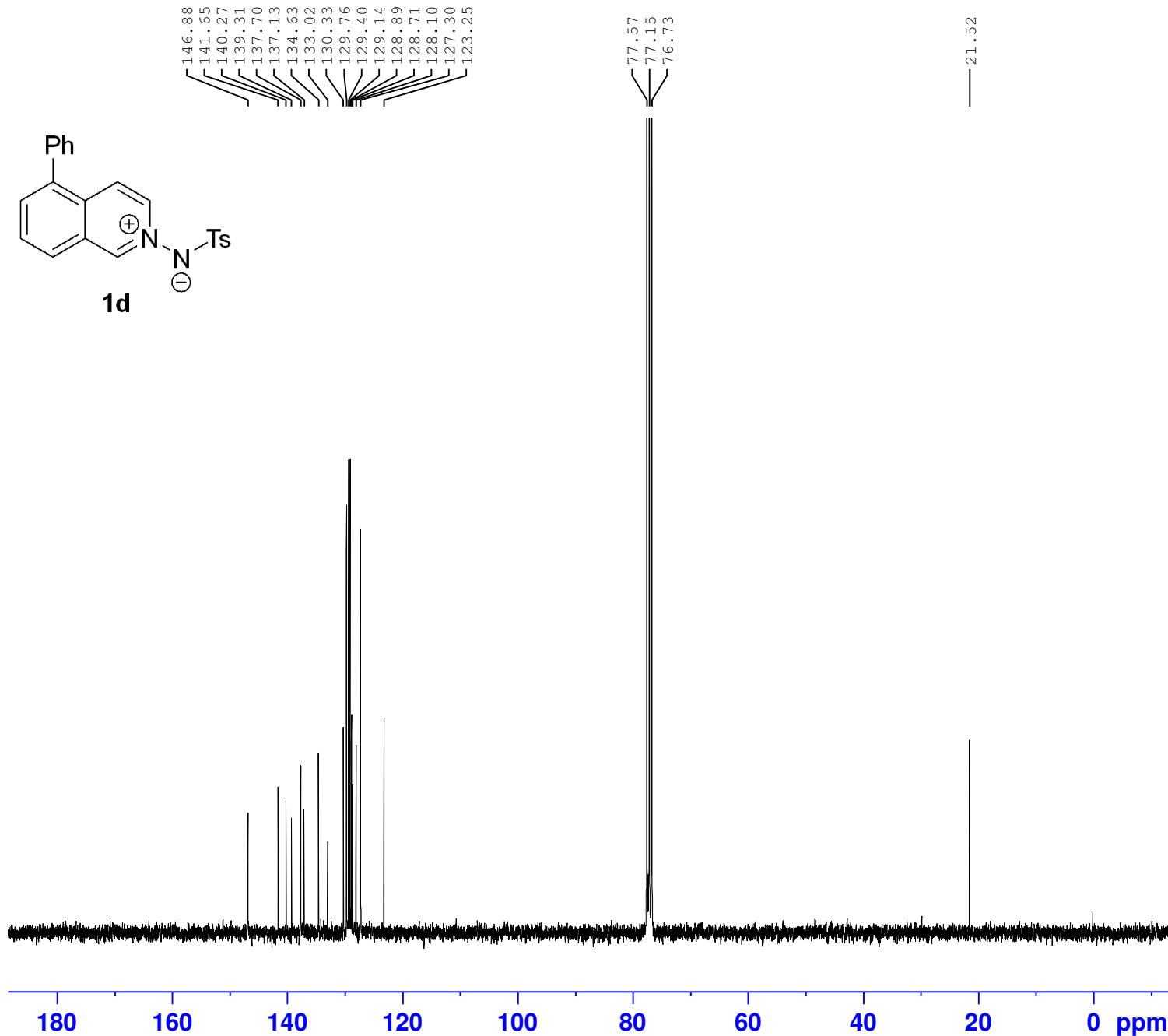
3sjwei 4422 xh1-1-78-c-fr 13c cdcl3



146.88
141.65
140.27
139.31
137.70
137.13
134.63
133.02
130.33
129.76
129.40
129.14
128.89
128.71
128.10
127.30
123.25

77.57
77.15
76.73

— 21.52



Current Data Parameters
NAME 2021-4--11Project 1 data
EXPNO 4422
PROCNO 1

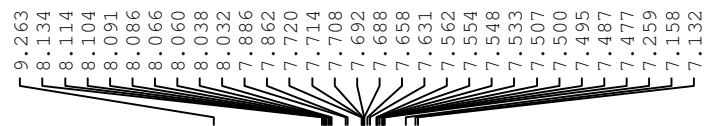
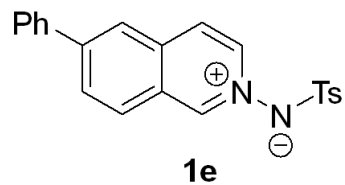
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Time 21.17
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PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 1024
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175317 sec
RG 203
DW 27.733 usec
DE 6.50 usec
TE 296.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 75.4752949 MHz
NUC1 13C
P1 9.50 usec
PLW1 34.20000076 W

===== CHANNEL f2 =====
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.17284000 W
PLW13 0.14000000 W

F2 - Processing parameters
SI 32768
SF 75.4677415 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

3sjwei 4436 xh1-1-66-h-fr 1h cdcl3



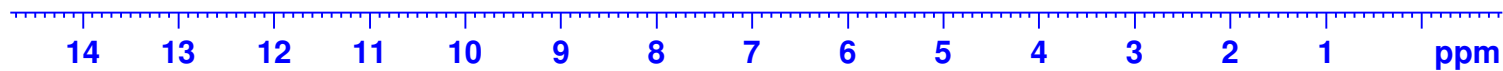
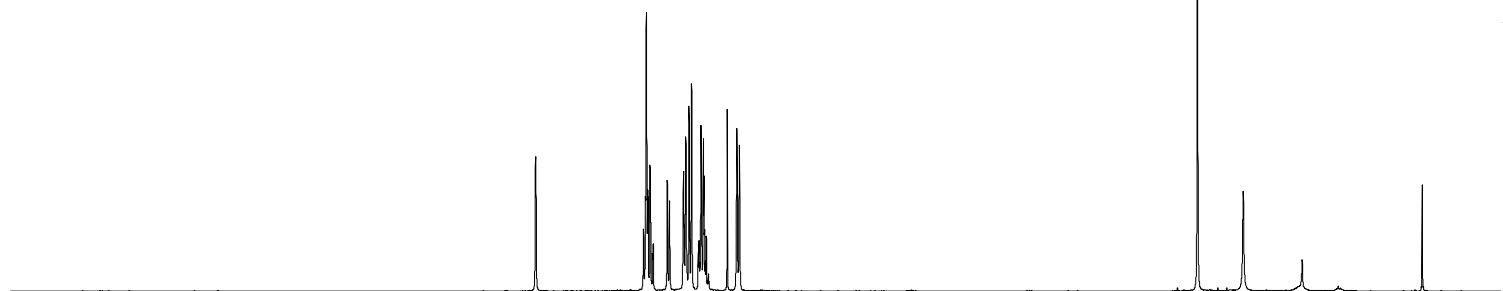
2.339

Current Data Parameters
NAME 2021-4--11Project 1 data
EXPNO 4436
PROCNO 1

F2 - Acquisition Parameters
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Time 9.14
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 181
DW 83.200 usec
DE 6.50 usec
TE 296.2 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 300.1318534 MHz
NUC1 1H
P1 10.00 usec
PLW1 14.00000000 W

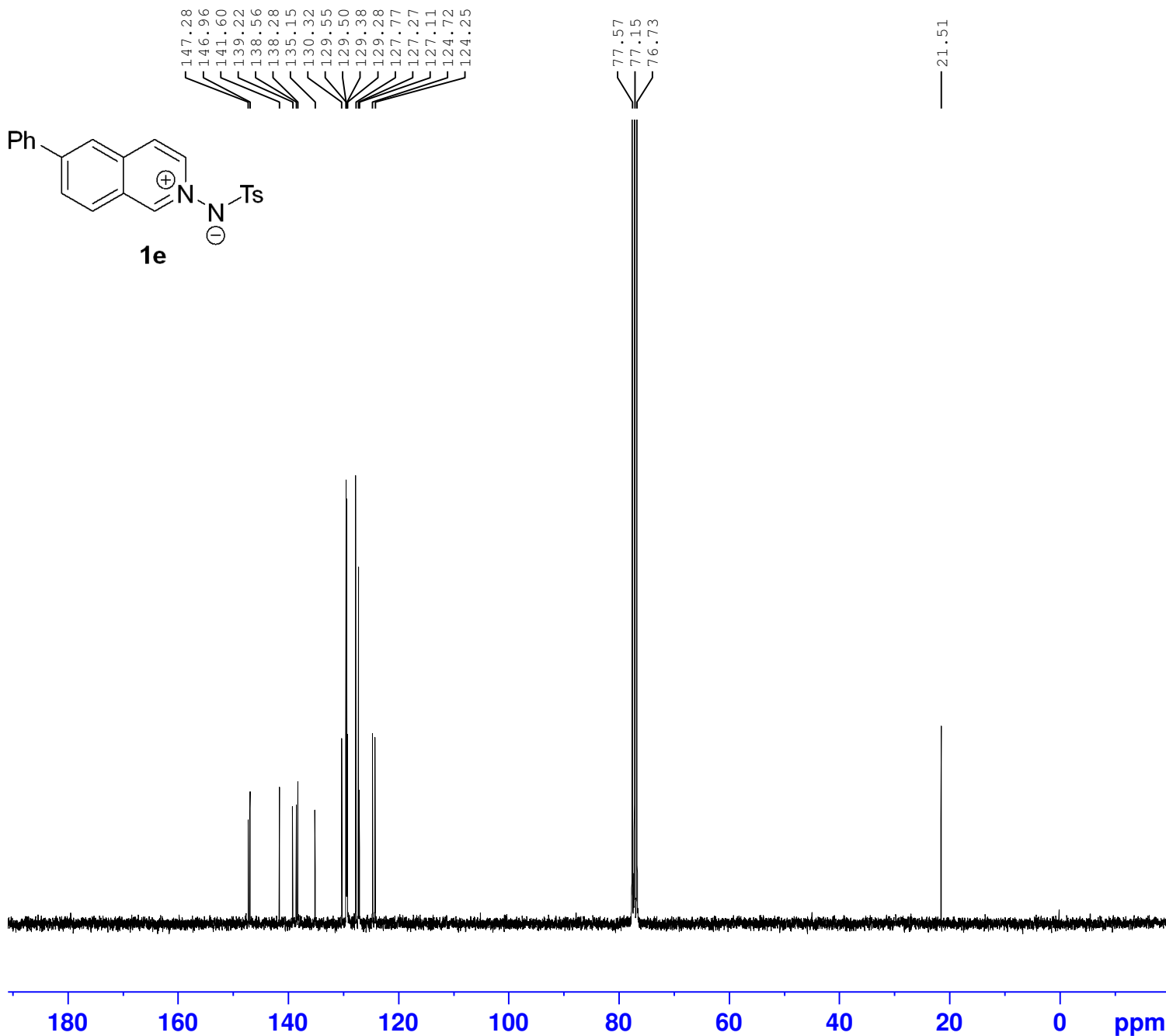
F2 - Processing parameters
SI 65536
SF 300.1300075 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



1.00
4.21
1.01
4.16
3.11
2.09

3.14

3sjwei 4459 xh1-1-66-1c-fr 13c cdcl3



Current Data Parameters
NAME 2021-4--11Project 1 data
EXPNO 4459
PROCNO 1

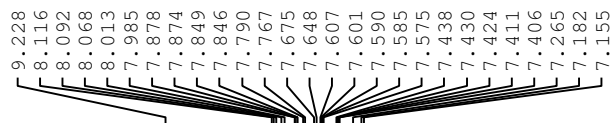
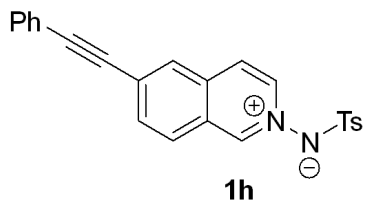
F2 - Acquisition Parameters
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INSTRUM spect
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PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175317 sec
RG 203
DW 27.733 usec
DE 6.50 usec
TE 296.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 75.4752949 MHz
NUC1 13C
P1 9.50 usec
PLW1 34.20000076 W

==== CHANNEL f2 =====
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.17284000 W
PLW13 0.14000000 W

F2 - Processing parameters
SI 32768
SF 75.4677426 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

3sjwei 4437 xh1-2-13-h-fr 1h cdcl3



— 2.358

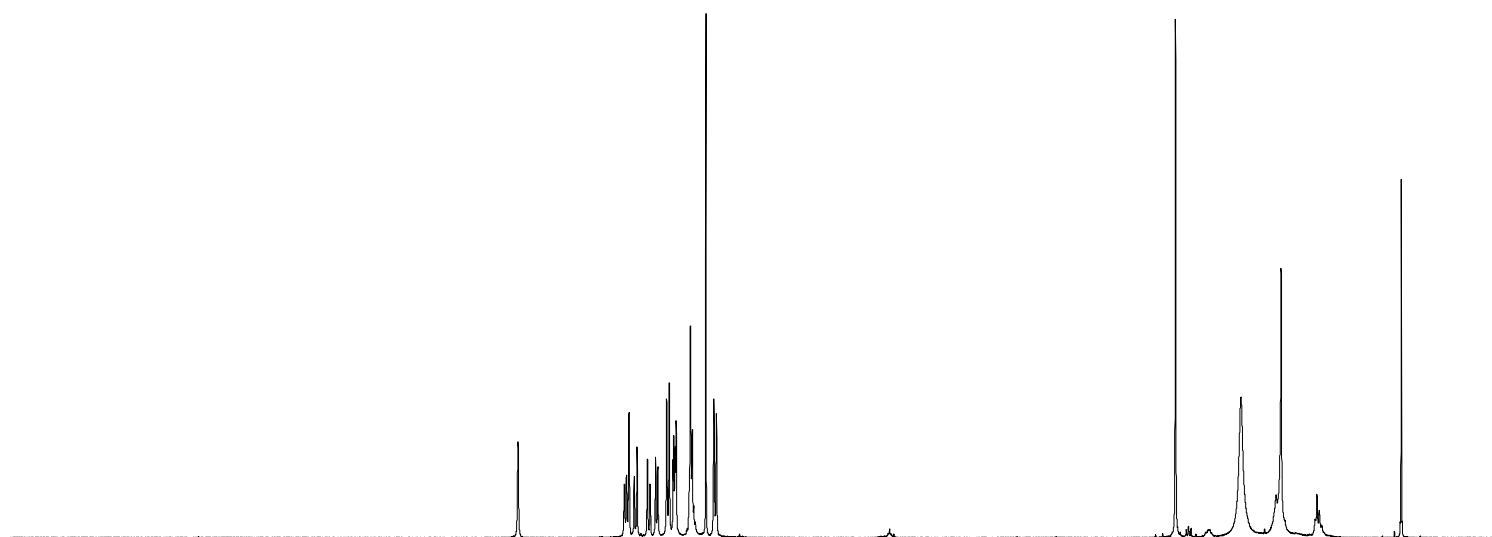


Current Data Parameters
NAME 2021-4--11Project 1 data
EXPNO 4437
PROCNO 1

F2 - Acquisition Parameters
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INSTRUM spect
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PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 203
DW 83.200 usec
DE 6.50 usec
TE 296.1 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 300.1318534 MHz
NUC1 1H
P1 10.00 usec
PLW1 14.00000000 W

F2 - Processing parameters
SI 65536
SF 300.1300057 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

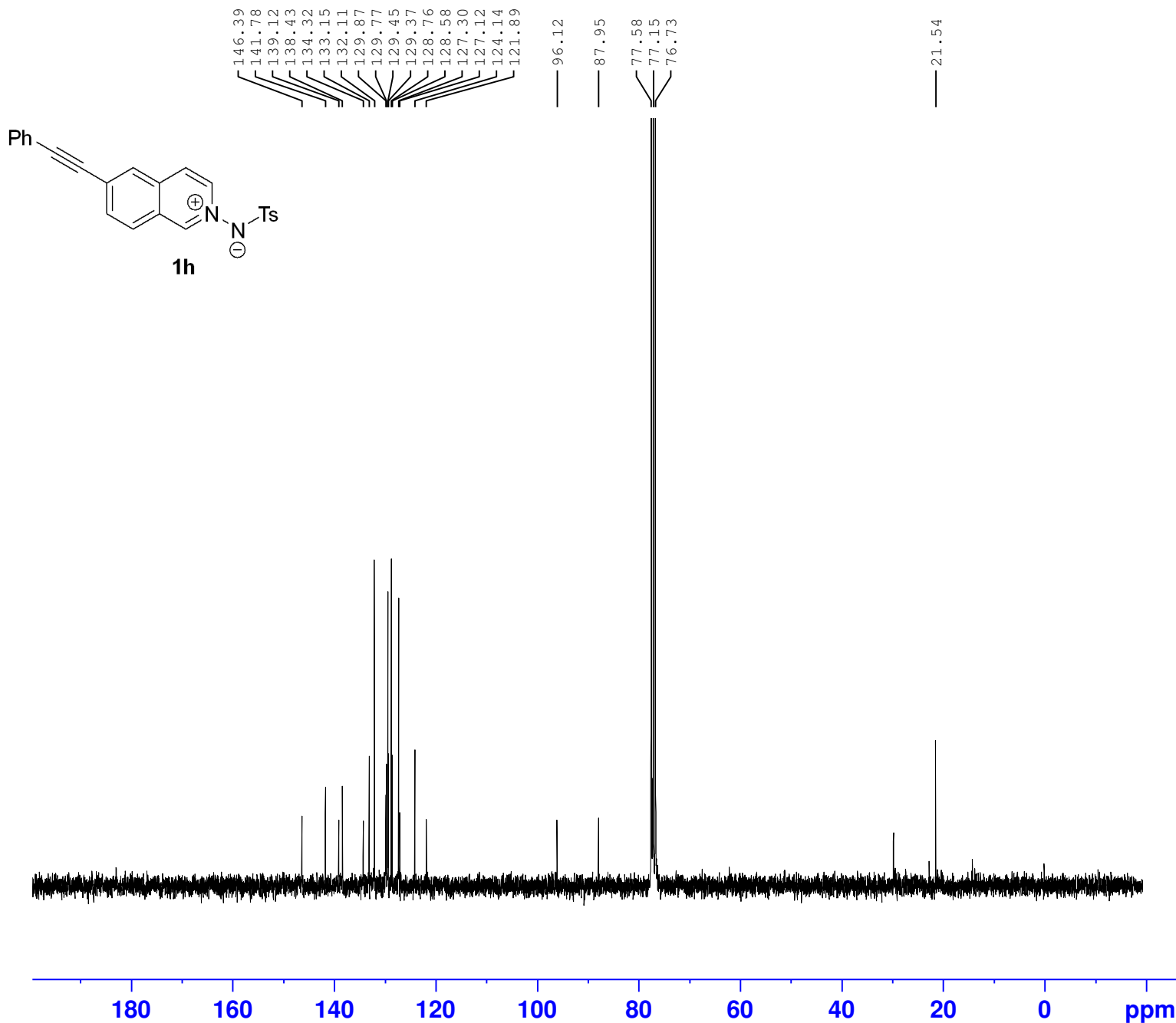


14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm

0.90
1.98
1.03
1.03
1.05
2.06
2.08
3.09
2.02

3.00

3sjwei 4512 xh1-2-13-c-fr 13c cdcl3



Current Data Parameters
NAME 2021-4--11Project 1 data
EXPNO 4512
PROCNO 1

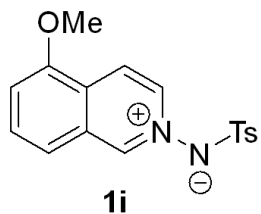
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Time 12.51
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PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175317 sec
RG 203
DW 27.733 usec
DE 6.50 usec
TE 296.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 75.4752949 MHz
NUC1 13C
P1 9.50 usec
PLW1 34.20000076 W

===== CHANNEL f2 =====
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.17284000 W
PLW13 0.14000000 W

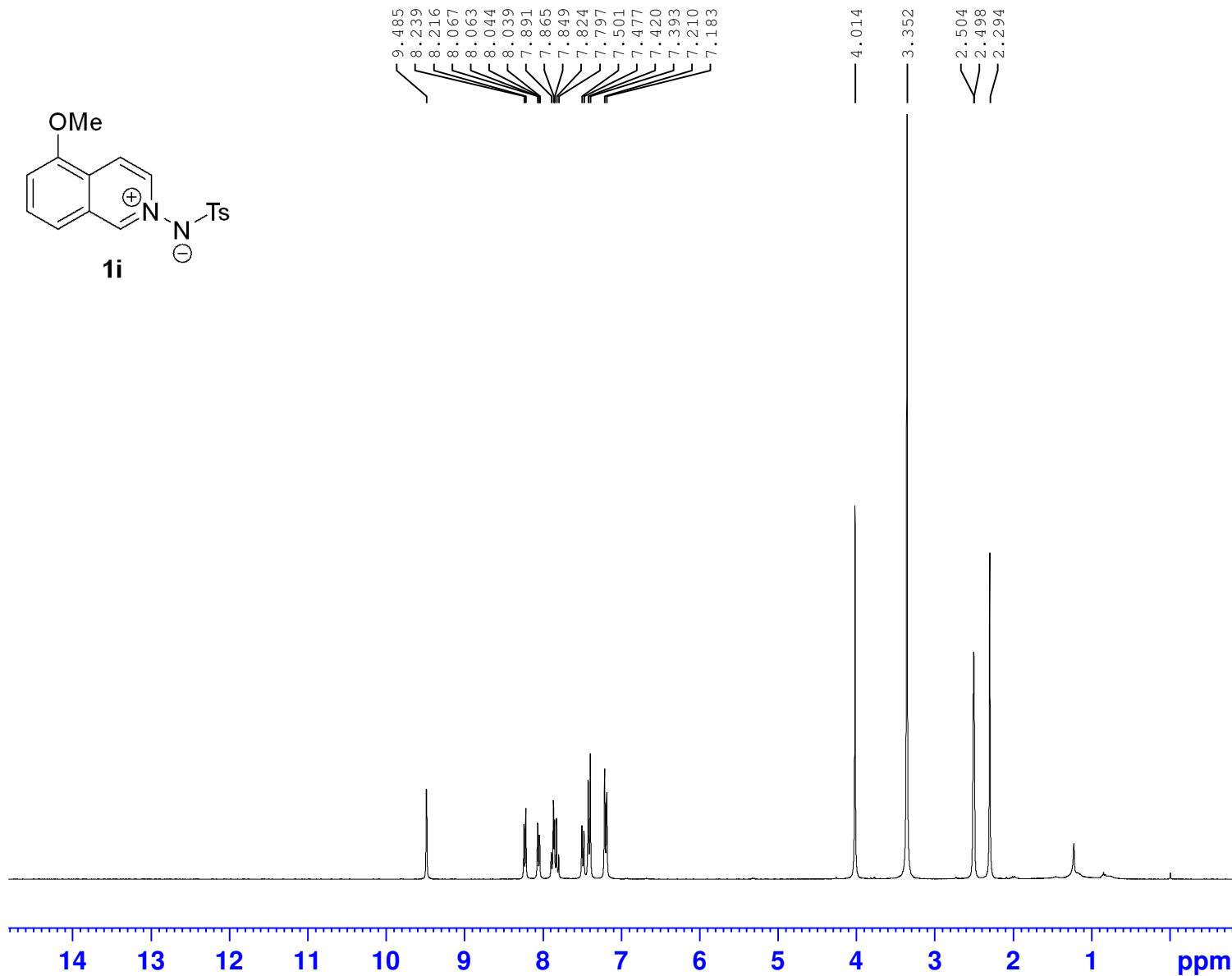
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WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

3sjwei 6002 xh1 1h dms0



9.485
8.239
8.216
8.067
8.063
8.044
8.039
7.891
7.865
7.849
7.824
7.797
7.501
7.477
7.420
7.393
7.210
7.183

4.014
3.352
2.504
2.498
2.294



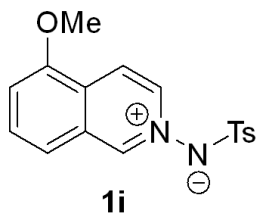
Current Data Parameters
NAME 220721-300M
EXPNO 6002
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220721
Time 14.08
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 203
DW 83.200 usec
DE 6.50 usec
TE -59.1 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 300.1318534 MHz
NUC1 1H
P1 10.00 usec
PLW1 14.00000000 W

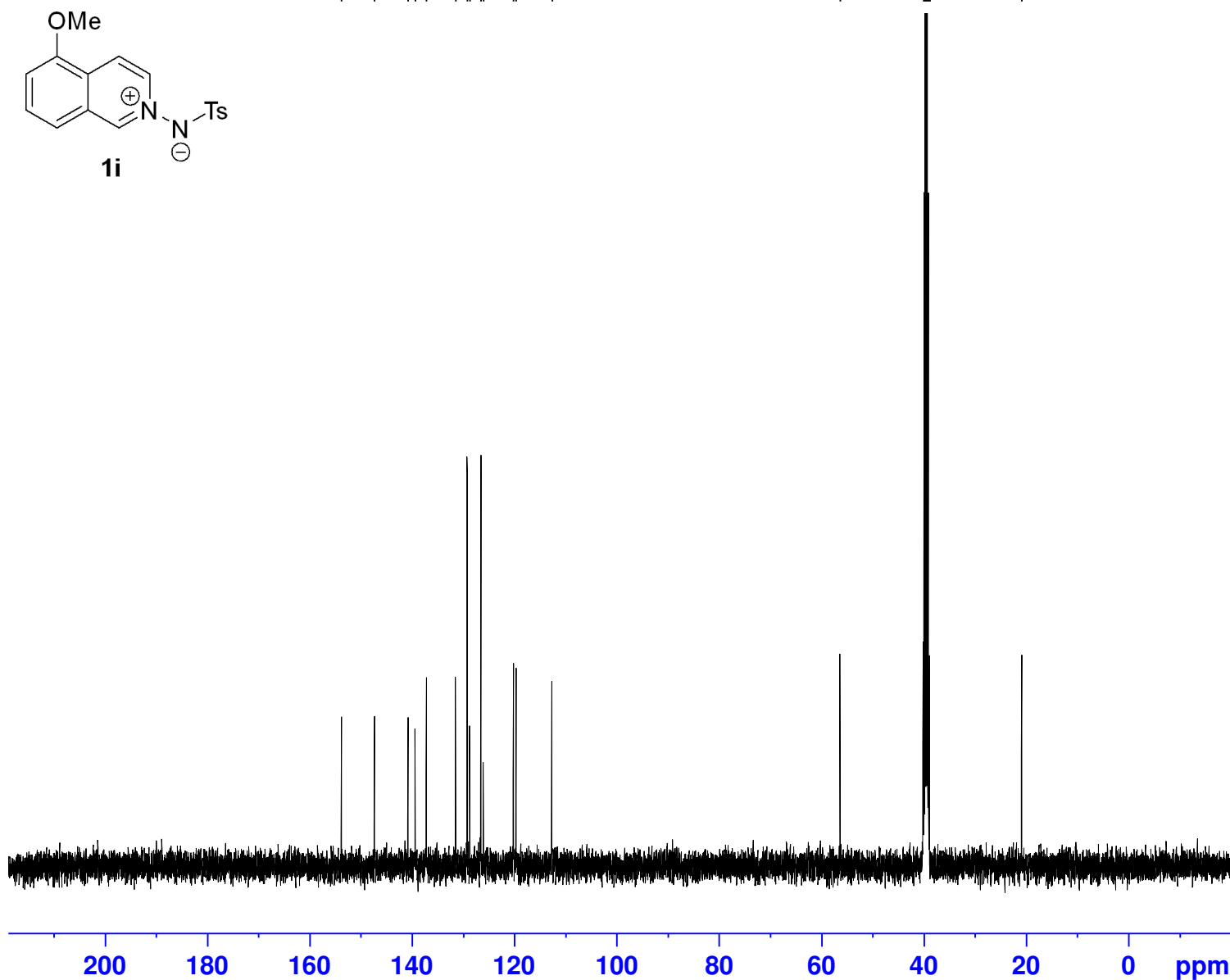
F2 - Processing parameters
SI 65536
SF 300.1300024 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

XHL-1-41



153.83
147.36
140.82
139.42
137.22
131.51
129.24
128.76
126.55
126.07
120.21
119.66
112.68

56.37
40.12
39.91
39.71
39.50
39.29
39.08
38.87
20.86



Current Data Parameters
NAME 220721-400
EXPNO 41
PROCNO 1

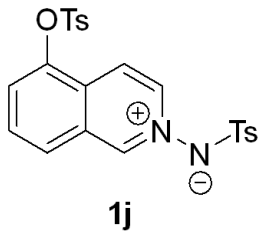
F2 - Acquisition Parameters
Date_ 20220721
Time 19.26
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 50
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 193.13
DW 20.800 usec
DE 6.50 usec
TE 295.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 13C
P1 12.00 usec
PLW1 53.00000000 W
SFO1 100.6379178 MHz

==== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.37246999 W
PLW13 0.30170000 W
SFO2 400.1916008 MHz

F2 - Processing parameters
SI 32768
SF 100.6279047 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

xh1-5-38



9.341
8.041
8.038
8.023
8.020
7.966
7.945
7.828
7.810
7.764
7.758
7.744
7.738
7.724
7.660
7.639
7.633
7.613
7.352
7.331
7.260
7.185
7.164

2.465
2.360

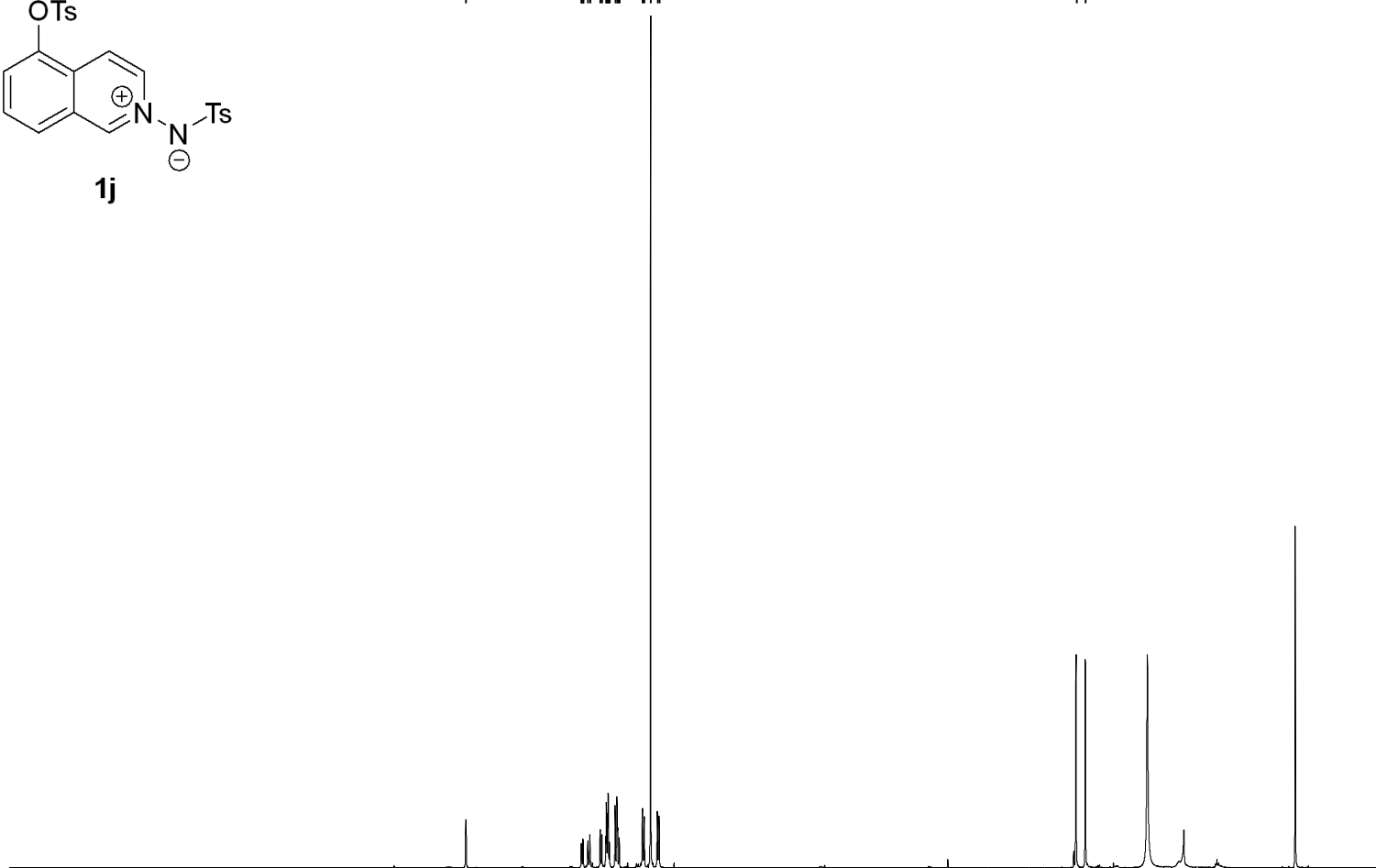


Current Data Parameters
NAME 220728-400
EXPNO 93
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220728
Time 21.58
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 193.13
DW 60.800 usec
DE 6.50 usec
TE 294.7 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 14.68 usec
PLW1 14.00000000 W
SFO1 400.1924713 MHz

F2 - Processing parameters
SI 65536
SF 400.1900162 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

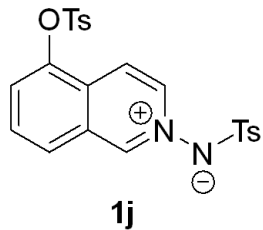


14 13 12 11 10 9 8 7 6 5 4 3 2 1 ppm

0.98
1.02
0.96
1.08
3.03
2.96
2.09
2.07

3.36
3.05

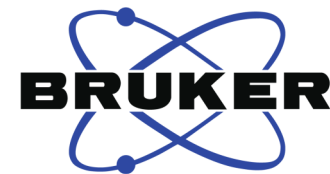
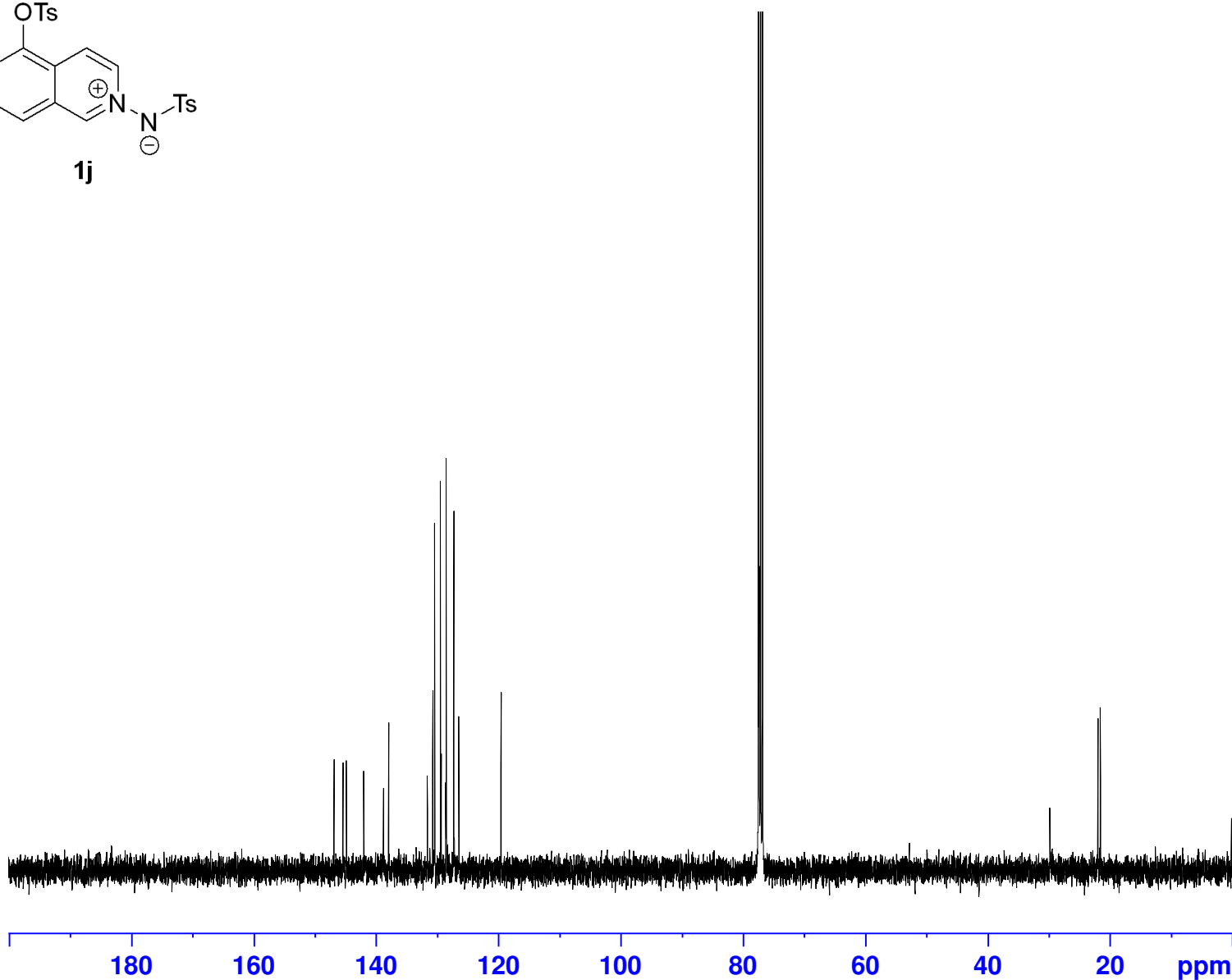
XHL-5-38



146.91
145.44
144.89
142.05
138.83
137.97
131.63
130.76
130.45
129.53
129.36
128.67
128.58
127.33
127.28
126.50
119.59

77.46
77.15
76.83

29.82
21.96
21.56



Current Data Parameters
NAME 220730-400
EXPNO 119
PROCNO 1

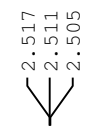
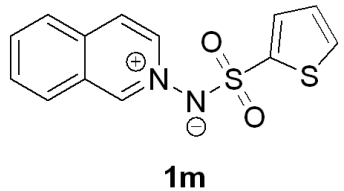
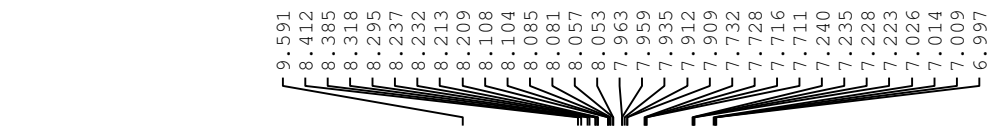
F2 - Acquisition Parameters
Date_ 20220729
Time 23.37
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 193.13
DW 20.800 usec
DE 6.50 usec
TE 295.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 13C
P1 12.00 usec
PLW1 53.00000000 W
SFO1 100.6379178 MHz

==== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.37246999 W
PLW13 0.30170000 W
SFO2 400.1916008 MHz

F2 - Processing parameters
SI 32768
SF 100.6278459 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

3sjwei 5597 xh1-3-2 1h dms0

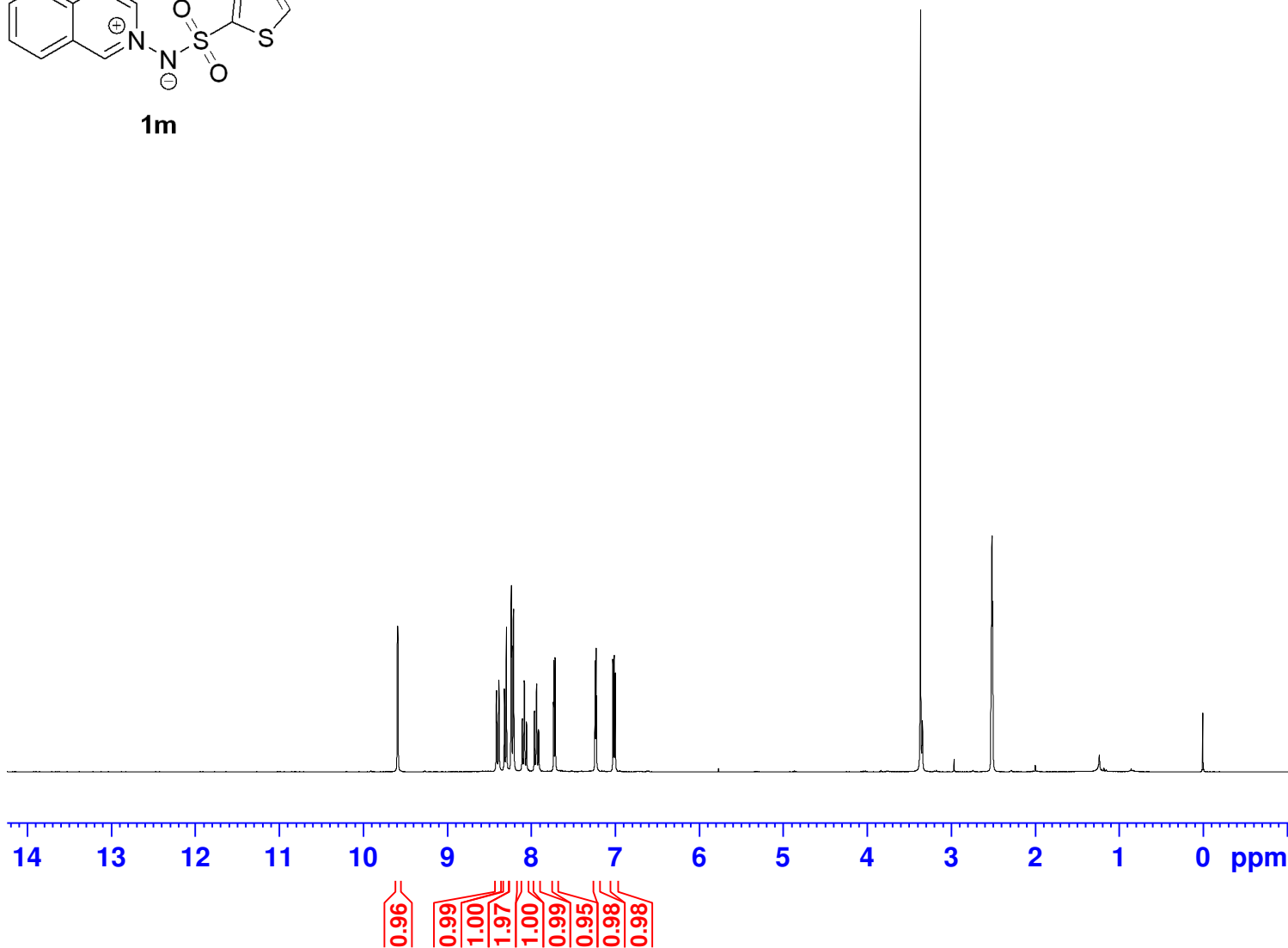


Current Data Parameters
NAME 2021-4--11Project 1 data
EXPNO 5597
PROCNO 1

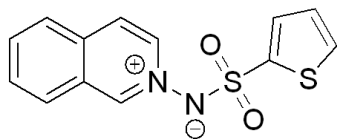
F2 - Acquisition Parameters
Date_ 20211030
Time 3.34
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 203
DW 83.200 usec
DE 6.50 usec
TE -59.1 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 300.1318534 MHz
NUC1 1H
P1 10.00 usec
PLW1 14.00000000 W

F2 - Processing parameters
SI 65536
SF 300.1299989 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



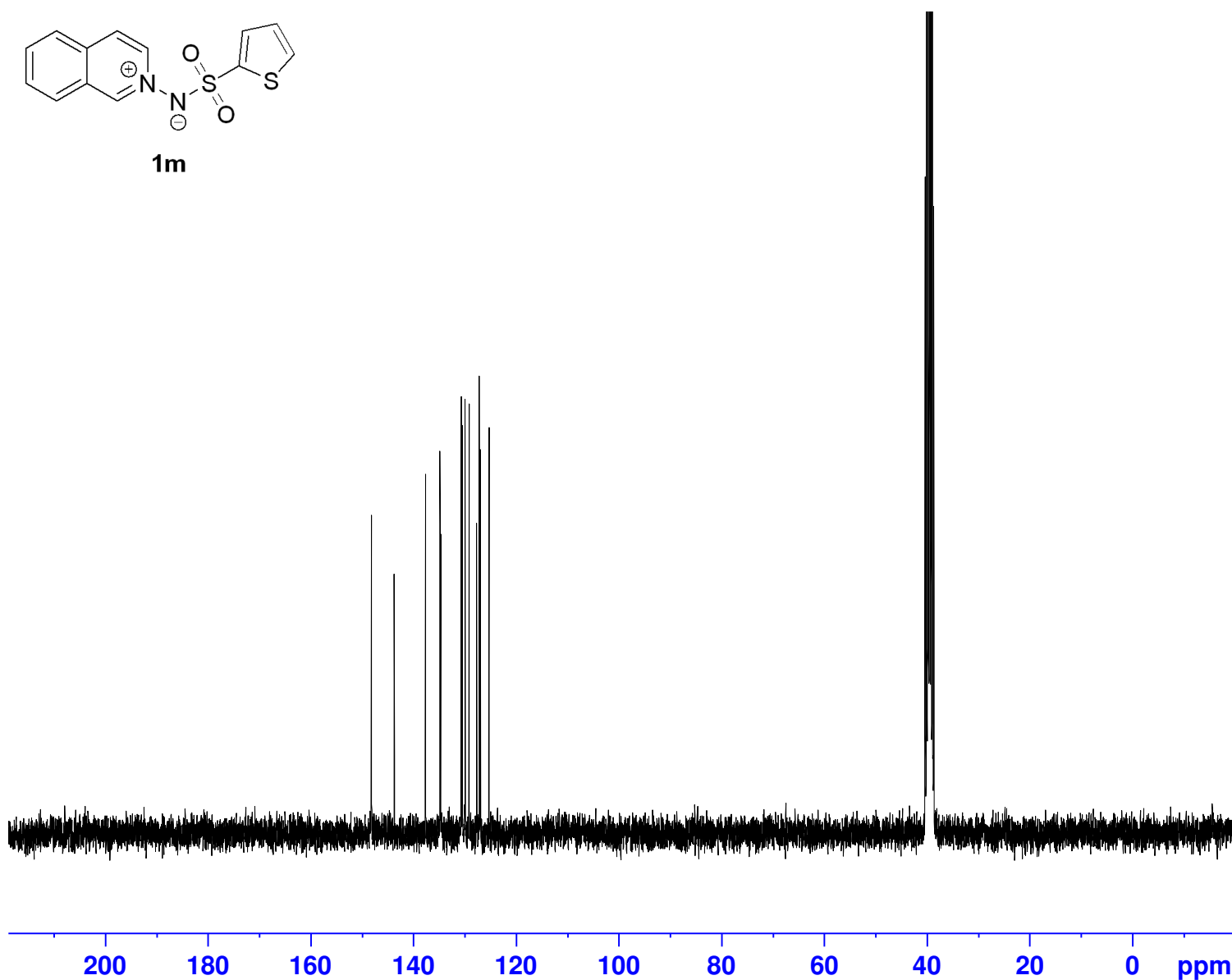
3sjwei 5598 xhl-3-2 13c dms0



1m

148.19
143.75
137.67
134.84
134.69
130.71
130.49
129.97
129.14
127.71
127.19
126.99
125.29

40.32
40.04
39.77
39.49
39.21
38.93
38.65



Current Data Parameters
NAME 2021-4--11Project 1 data
EXPNO 5598
PROCNO 1

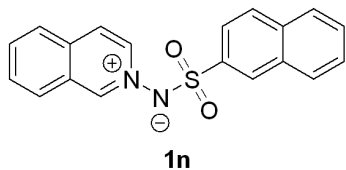
F2 - Acquisition Parameters
Date_ 20211030
Time 4.42
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175317 sec
RG 203
DW 27.733 usec
DE 6.50 usec
TE -59.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 75.4752949 MHz
NUC1 13C
P1 9.50 usec
PLW1 34.20000076 W

===== CHANNEL f2 =====
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.17284000 W
PLW13 0.14000000 W

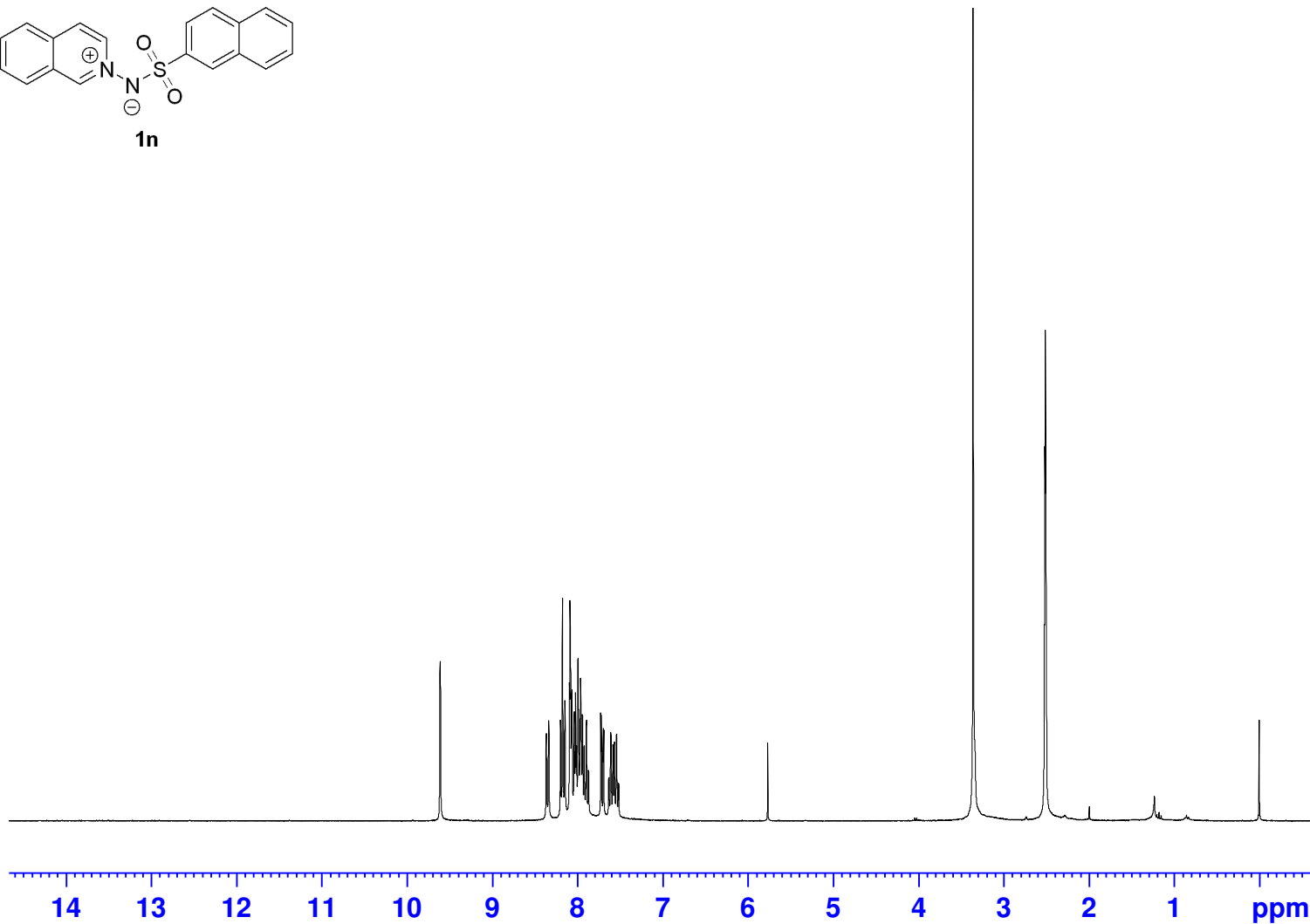
F2 - Processing parameters
SI 32768
SF 75.4677850 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

3sjwei 5595 xh1-2-100 1h dms0



9.611
8.365
8.338
8.199
8.176
8.149
8.095
8.089
8.072
8.066
8.041
8.037
8.023
8.014
8.010
7.994
7.964
7.943
7.922
7.919
7.895
7.871
7.868
7.727
7.721
7.698
7.692
7.635
7.631
7.612
7.608
7.586
7.581
7.569
7.564
7.542
7.538
7.519
7.515

2.515
2.509
2.503



Current Data Parameters
NAME 2021-4--11Project 1 data
EXPNO 5595
PROCNO 1

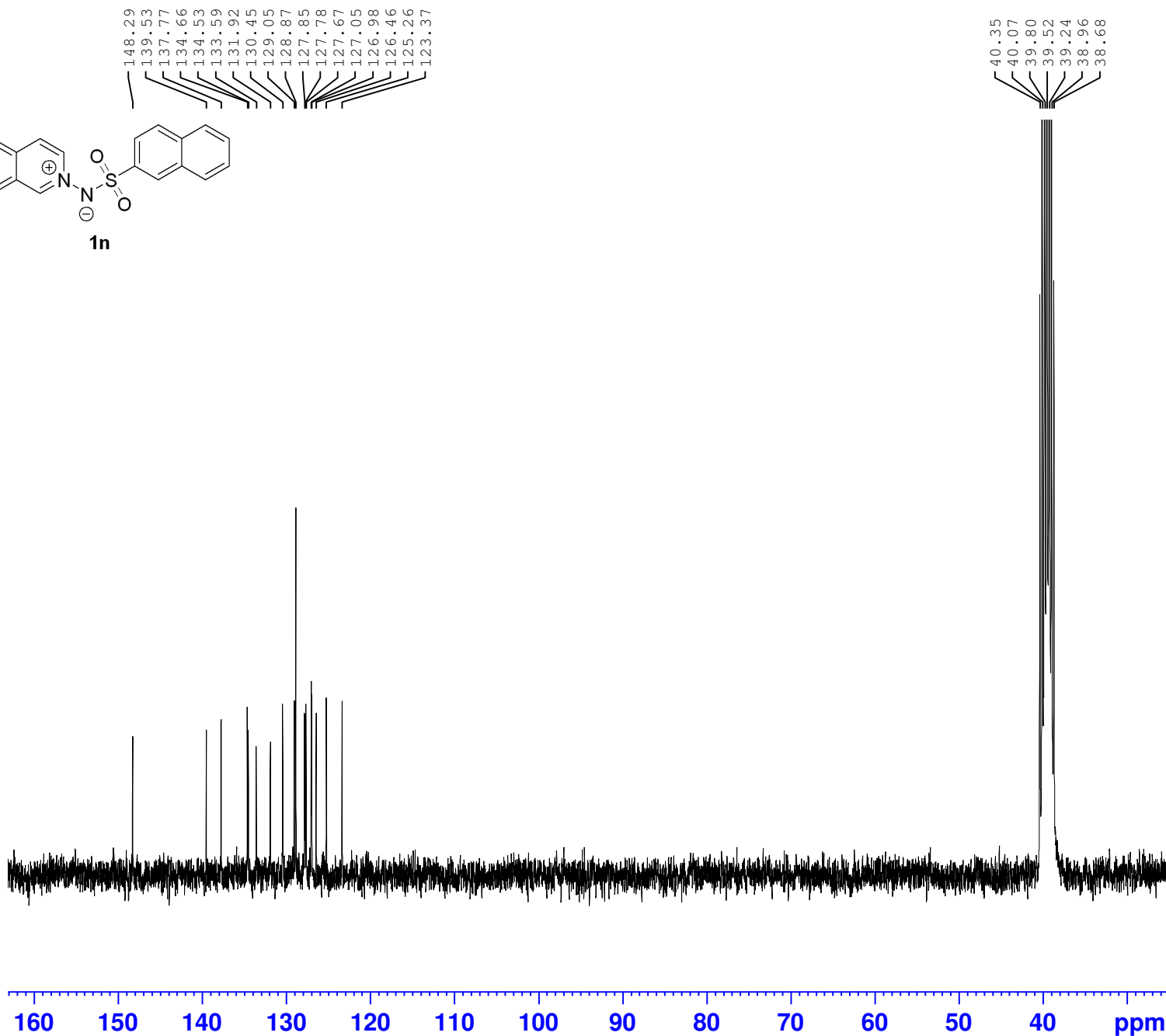
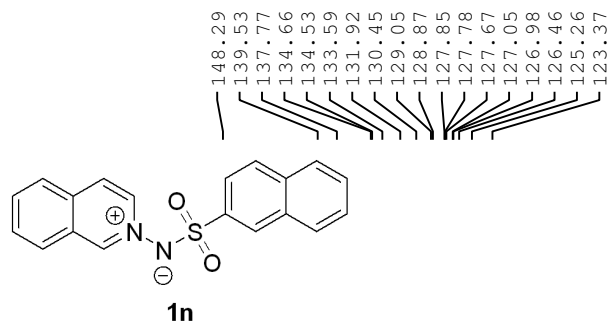
F2 - Acquisition Parameters
Date_ 20211030
Time 2.22
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 203
DW 83.200 usec
DE 6.50 usec
TE -59.1 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 300.1318534 MHz
NUC1 1H
P1 10.00 usec
PLW1 14.00000000 W

F2 - Processing parameters
SI 65536
SF 300.1299995 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1.00
1.07
2.05
7.67
1.08
2.18

3sjwei 5596 xhl-2-100 13c dms0



Current Data Parameters
NAME 2021-4--11Project 1 data
EXPNO 5596
PROCNO 1

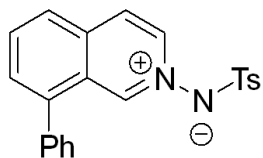
F2 - Acquisition Parameters
Date_ 20211030
Time 3.29
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175317 sec
RG 203
DW 27.733 usec
DE 6.50 usec
TE -59.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 75.4752949 MHz
NUC1 13C
P1 9.50 usec
PLW1 34.20000076 W

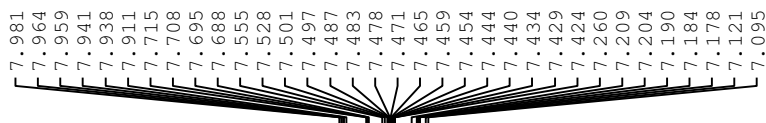
===== CHANNEL f2 =====
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.17284000 W
PLW13 0.14000000 W

F2 - Processing parameters
SI 32768
SF 75.4677828 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

3sjwei 4425 xh1-1-82-h-fr 1h cdcl3



1o



2.362

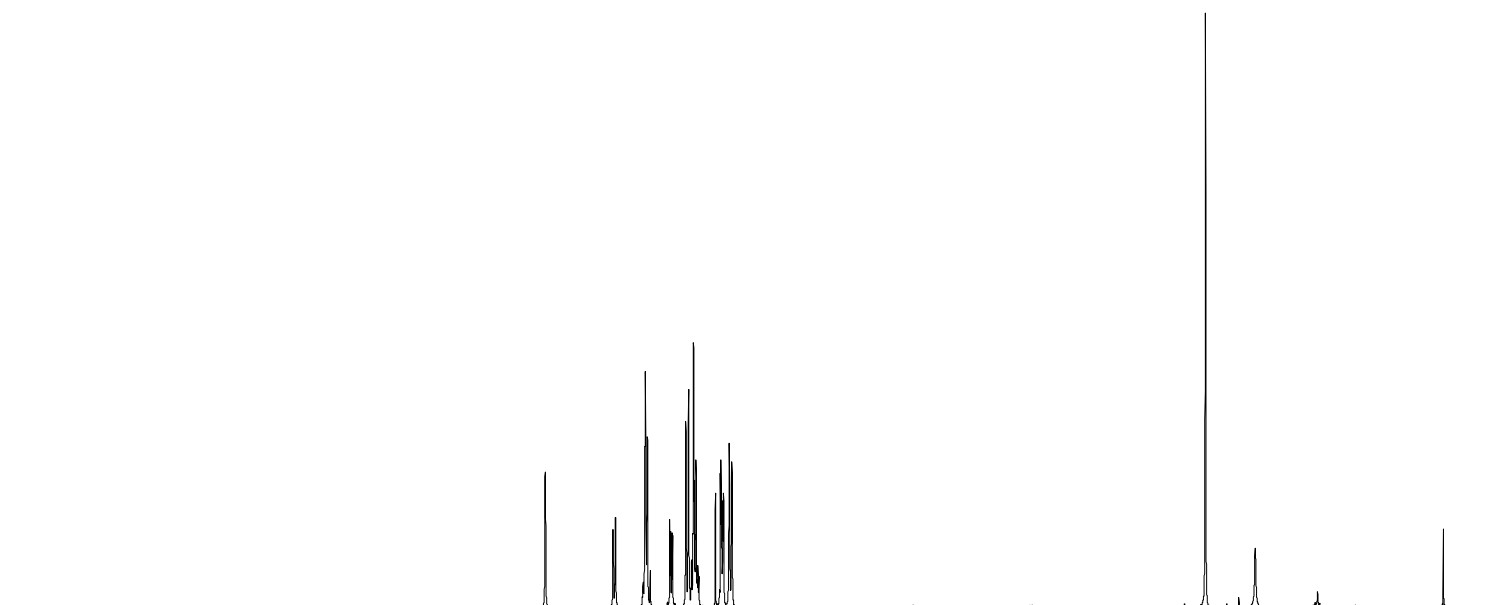


Current Data Parameters
NAME 2021-4--11Project 1 data
EXPNO 4425
PROCNO 1

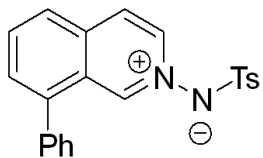
F2 - Acquisition Parameters
Date_ 20210704
Time 22.35
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 161
DW 83.200 usec
DE 6.50 usec
TE 296.2 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 300.1318534 MHz
NUC1 1H
P1 10.00 usec
PLW1 14.00000000 W

F2 - Processing parameters
SI 65536
SF 300.1300072 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



3sjwei 4426 xhl-1-82-c-fr 13c cdcl3

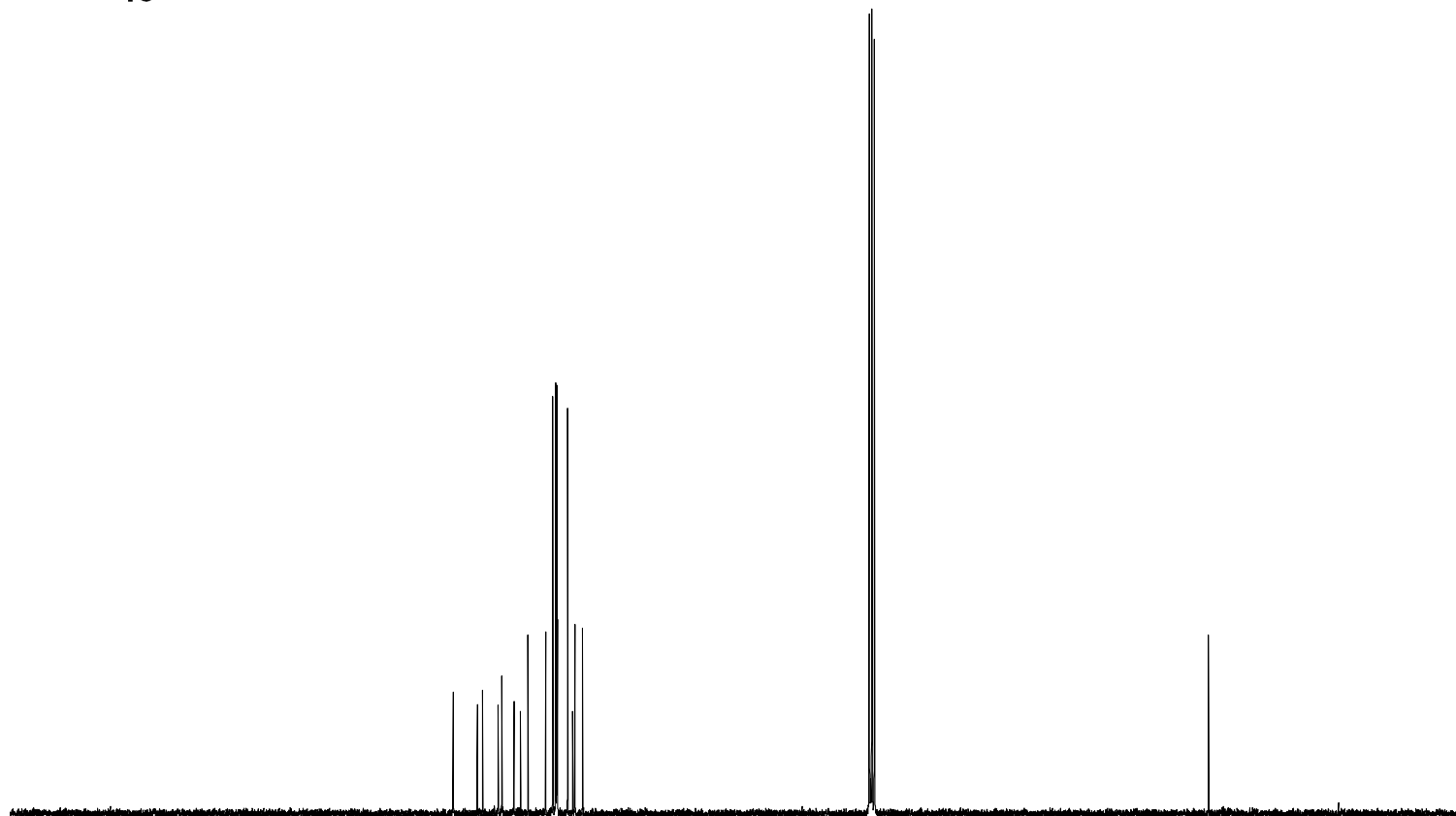


1o

146.28
142.30
141.42
138.83
138.25
136.23
135.15
133.92
130.99
129.81
129.34
129.16
129.06
127.38
126.54
126.18
124.91

77.57
77.15
76.73

21.54



Current Data Parameters
NAME 2021-4--11Project 1 data
EXPNO 4426
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210704
Time 23.43
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 1024
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175317 sec
RG 203
DW 27.733 usec
DE 6.50 usec
TE 296.1 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

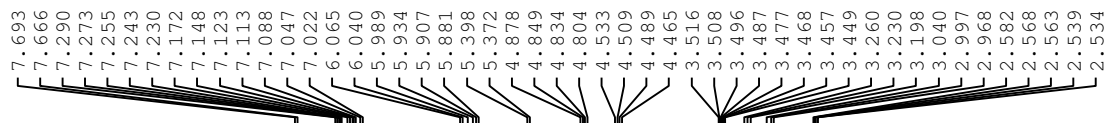
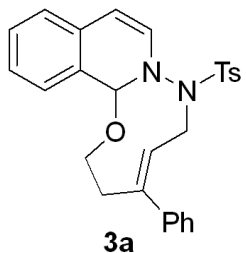
===== CHANNEL f1 =====
SFO1 75.4752949 MHz
NUC1 13C
P1 9.50 usec
PLW1 34.2000076 W

===== CHANNEL f2 =====
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 14.0000000 W
PLW12 0.1728400 W
PLW13 0.1400000 W

F2 - Processing parameters
SI 32768
SF 75.4677433 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

200 180 160 140 120 100 80 60 40 20 0 ppm

3sjwei 5512 xh1-3-29-2 1h cdcl3

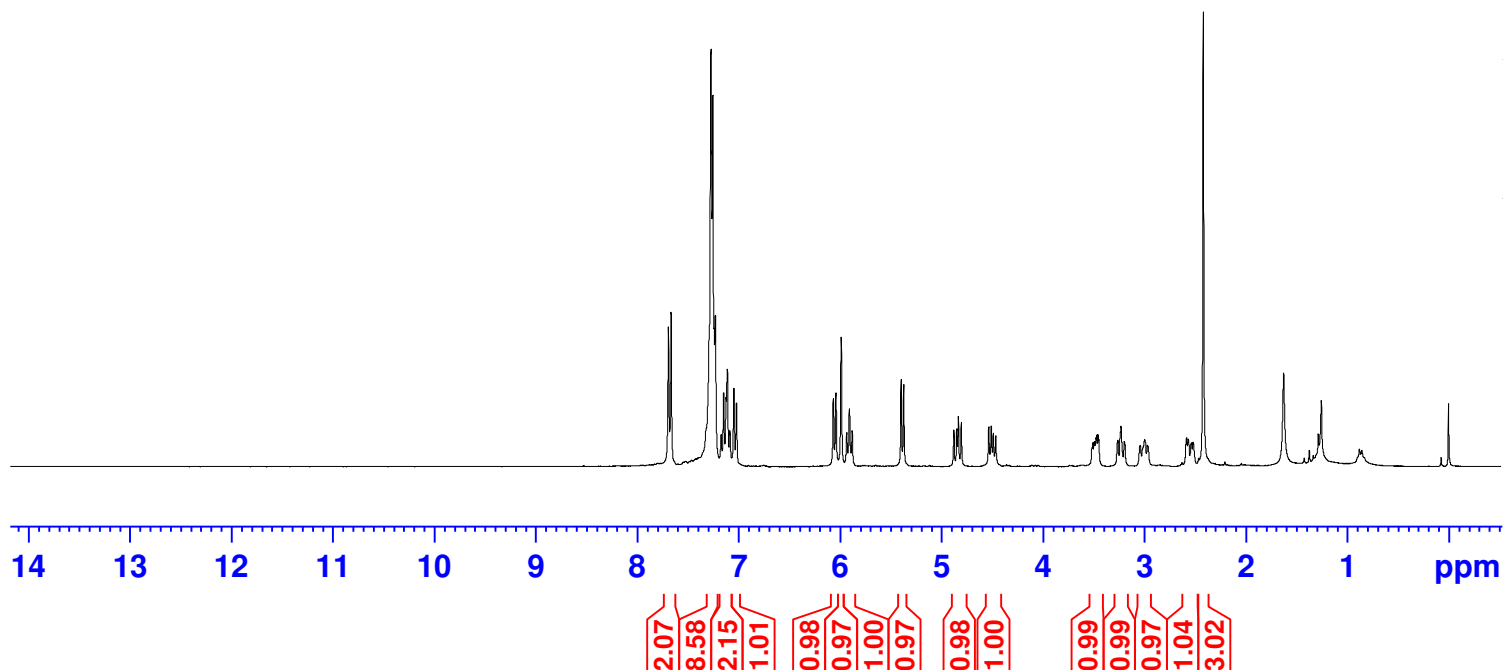


Current Data Parameters
NAME 2021-4--11Project 1 data
EXPNO 5512
PROCNO 1

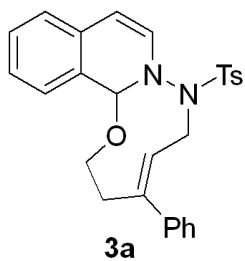
F2 - Acquisition Parameters
Date_ 20211013
Time 9.16
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 128
DW 83.200 usec
DE 6.50 usec
TE -59.1 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 300.1318534 MHz
NUC1 1H
P1 10.00 usec
PLW1 14.00000000 W

F2 - Processing parameters
SI 65536
SF 300.1300088 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



3sjwei 5523 xh1-3-29-2 13c cdcl3



146.82
144.43
143.15
135.59
134.78
131.89
129.91
128.80
128.49
128.29
127.91
127.61
127.58
126.49
125.78
124.14
121.82

99.35

88.81

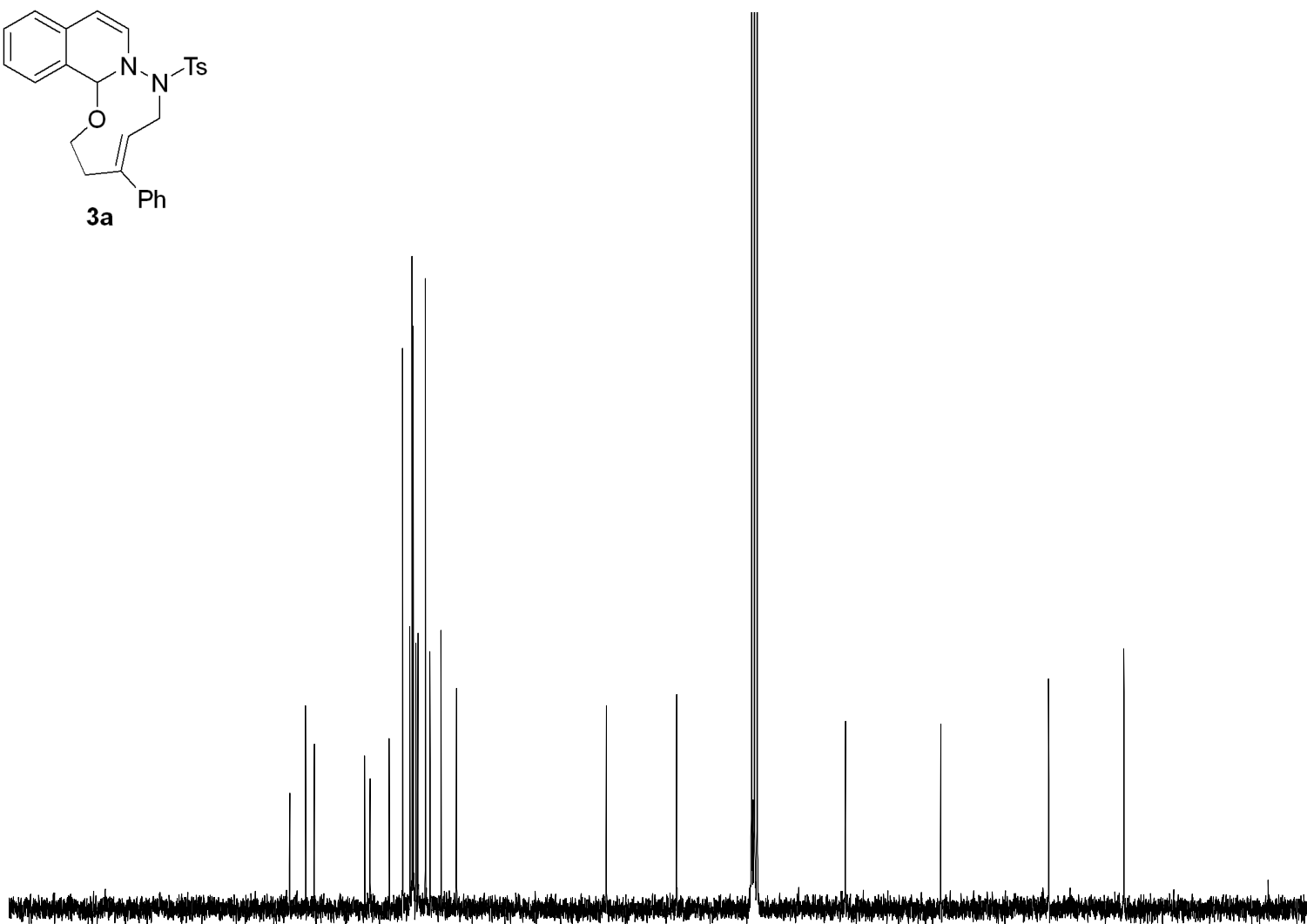
77.57
77.15
76.73

63.50

49.21

33.03

21.74



180 160 140 120 100 80 60 40 20 ppm



Current Data Parameters
NAME 2021-4--11Project 1 data
EXPNO 5523
PROCNO 1

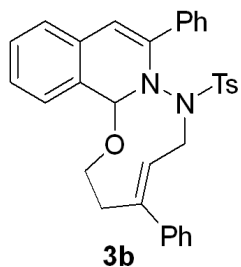
F2 - Acquisition Parameters
Date_ 20211013
Time 12.42
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 800
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175317 sec
RG 203
DW 27.733 usec
DE 6.50 usec
TE -59.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 75.4752949 MHz
NUC1 13C
P1 9.50 usec
PLW1 34.20000076 W

===== CHANNEL f2 =====
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.17284000 W
PLW13 0.14000000 W

F2 - Processing parameters
SI 32768
SF 75.4677420 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

3sjwei 5274 xh1-2-83 1h cdcl3



7.417
7.408
7.401
7.376
7.366
7.361
7.341
7.336
7.316
7.311
7.280
7.239
7.232
7.210
7.207
7.196
7.190
7.184
7.178
7.167
7.159
7.132
7.108
7.084
7.024
7.002
6.996
6.350
6.328
6.315
6.293
6.186
5.698
4.791
4.770
4.745
4.721
4.685
4.673
4.638
3.812
3.806
3.795
3.787
3.771
3.764
3.753
3.746
3.645
3.614
3.607
3.573
3.215
3.188
3.171
3.166

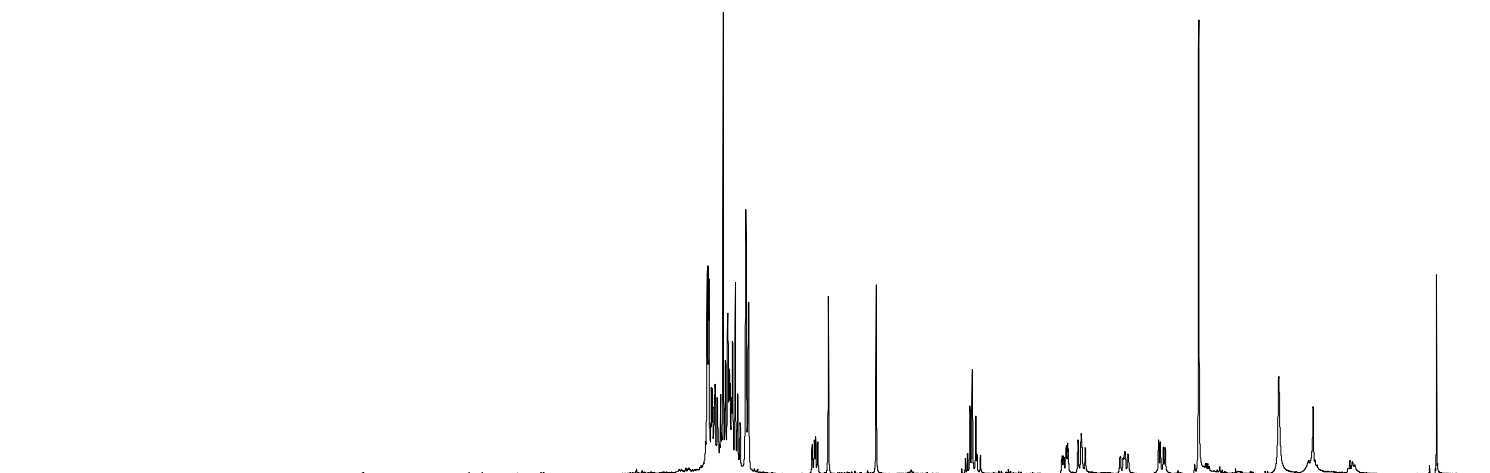


Current Data Parameters
NAME 2021-4--11Project 1 data
EXPNO 5274
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210909
Time 9.13
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 181
DW 83.200 usec
DE 6.50 usec
TE -59.1 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 300.1318534 MHz
NUC1 1H
P1 10.00 usec
PLW1 14.00000000 W

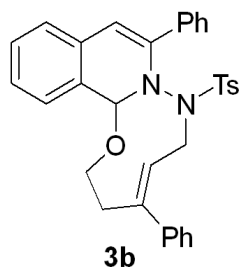
F2 - Processing parameters
SI 65536
SF 300.1300087 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



14 13 12 11 10 9 8 7 6 5 4 3 2 1 ppm

8.00
8.47
4.27
1.00
0.99
1.02
2.09
1.01
1.19
1.02
1.12
3.30

3sjwei 5287 xh1-2-83 13c cdcl3



144.06
143.98
143.23
142.73
136.07
135.05
130.48
129.39
128.94
128.81
128.73
128.68
128.60
128.07
127.95
127.53
127.10
125.91
125.50
124.88
124.18
104.79

90.35

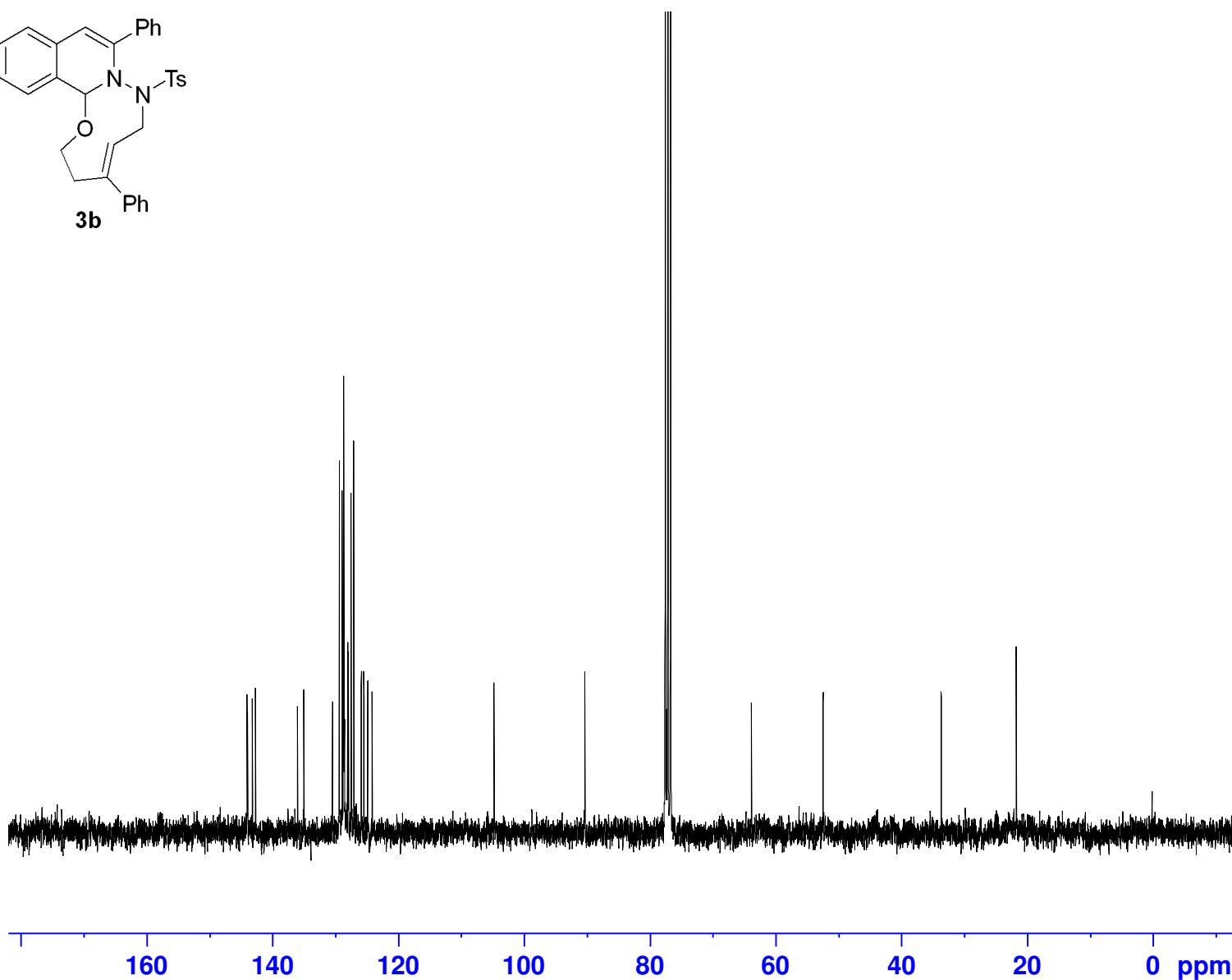
77.57
77.15
76.72

63.85

52.46

33.66

21.74



Current Data Parameters
NAME 2021-4--11Project 1 data
EXPNO 5287
PROCNO 1

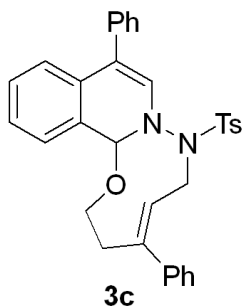
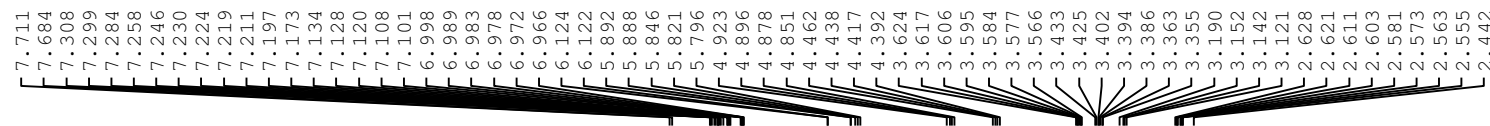
F2 - Acquisition Parameters
Date_ 20210909
Time 11.41
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 1024
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175317 sec
RG 203
DW 27.733 usec
DE 6.50 usec
TE -59.1 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 75.4752949 MHz
NUC1 13C
P1 9.50 usec
PLW1 34.20000076 W

===== CHANNEL f2 =====
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.17284000 W
PLW13 0.14000000 W

F2 - Processing parameters
SI 32768
SF 75.4677406 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

3sjwei 5358 xhl-1-84 1h cdcl3

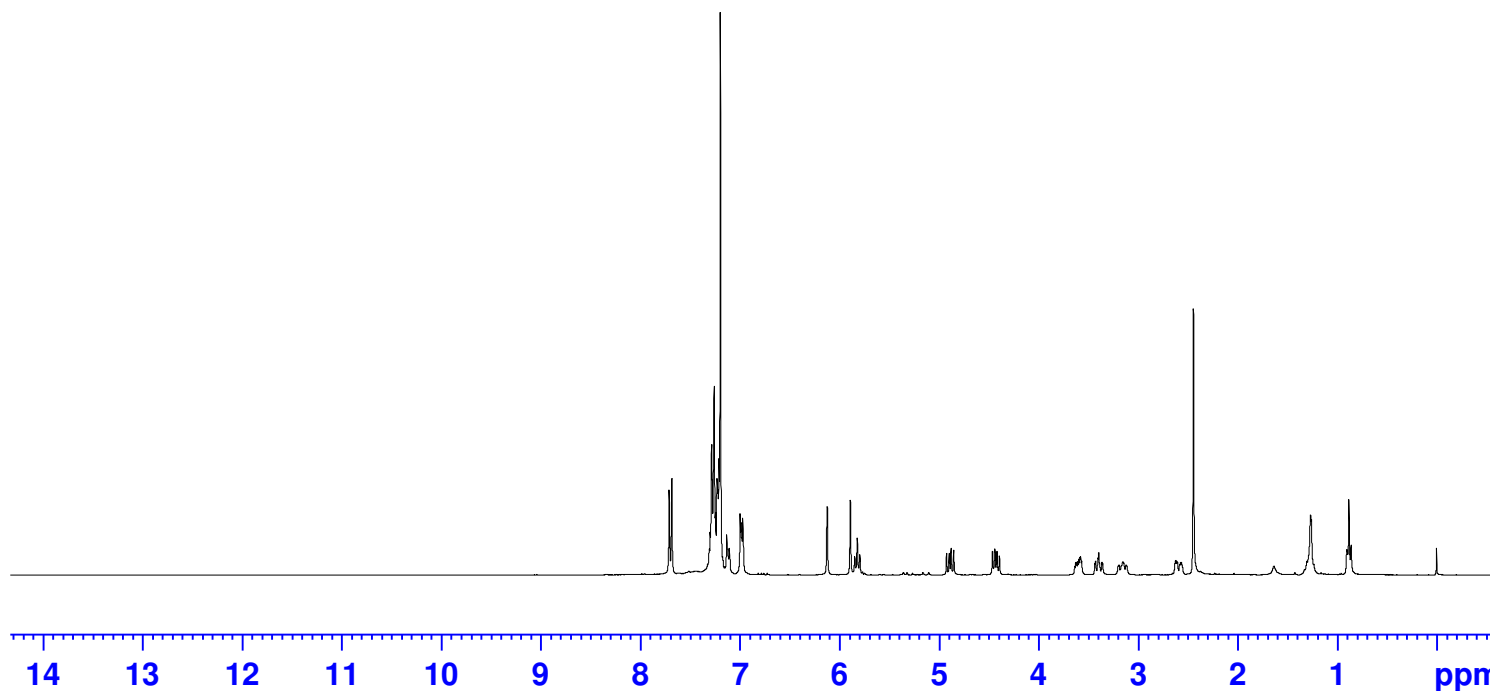


Current Data Parameters
NAME 2021-4--11Project 1 data
EXPNO 5358
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210917
Time 9.16
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 71.8
DW 83.200 usec
DE 6.50 usec
TE -59.1 K
D1 1.00000000 sec
TD0 1

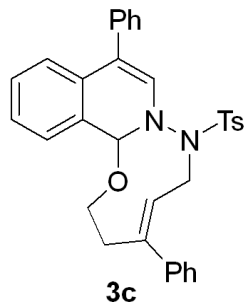
==== CHANNEL f1 =====
SFO1 300.1318534 MHz
NUC1 1H
P1 10.00 usec
PLW1 14.00000000 W

F2 - Processing parameters
SI 65536
SF 300.1300152 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



2.07
13.69
1.18
2.03
0.98
0.97
1.00
0.97
1.11
1.06
1.00
0.99
0.99
3.03

3sjwei 5379 xh1-1-84 13c cdcl3



146.64
144.54
142.74
137.24
135.12
132.61
131.63
129.93
129.53
128.64
128.58
128.41
128.39
128.26
128.21
127.57
126.78
126.63
126.28
122.87
121.39
113.46

89.56

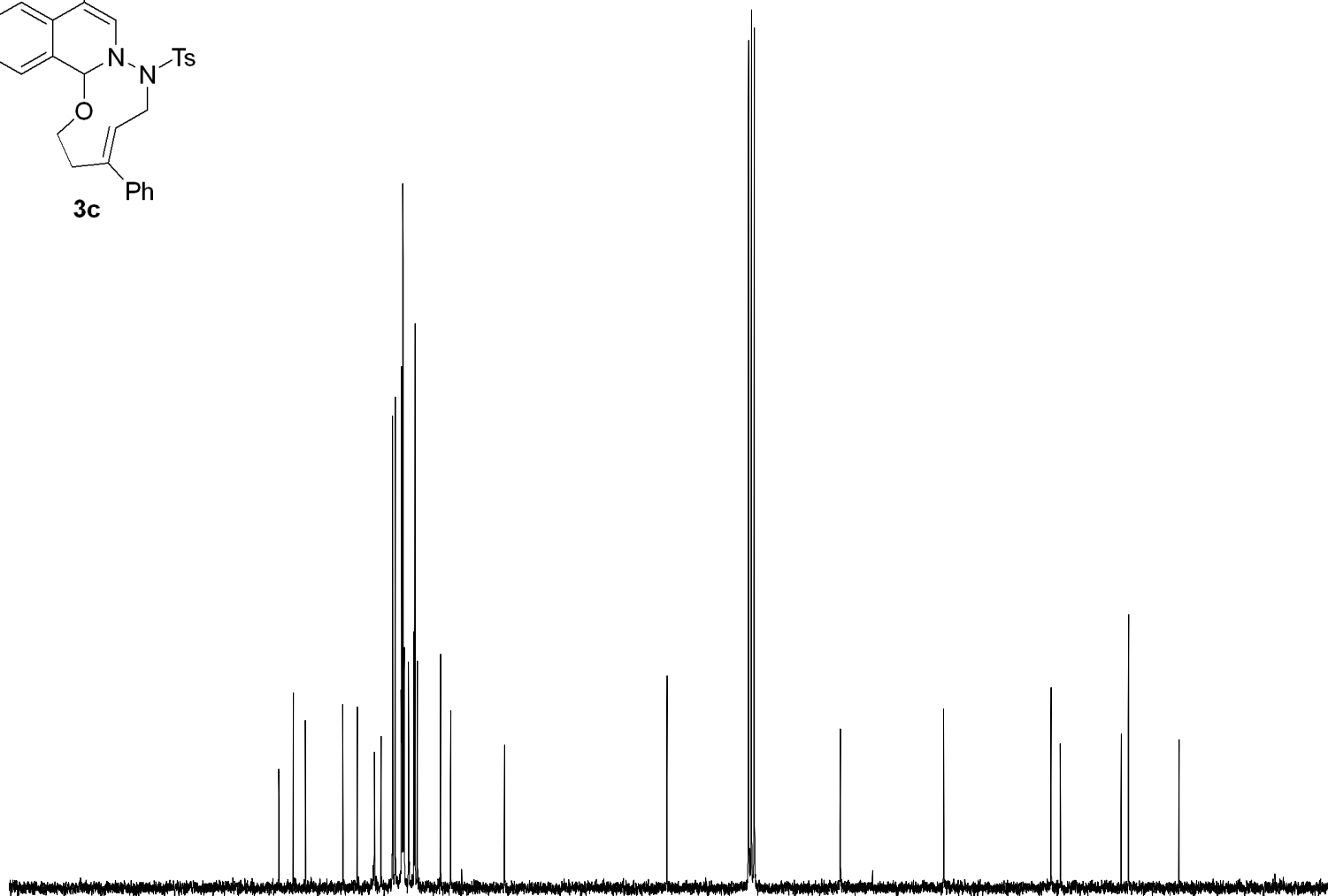
77.57
77.15
76.73

64.06

48.86

33.08

21.68



Current Data Parameters
NAME 2021-4--11Project 1 data
EXPNO 5379
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210917
Time 12.35
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 700
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175317 sec
RG 203
DW 27.733 usec
DE 6.50 usec
TE -59.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 75.4752949 MHz
NUC1 13C
P1 9.50 usec
PLW1 34.20000076 W

===== CHANNEL f2 =====
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.17284000 W
PLW13 0.14000000 W

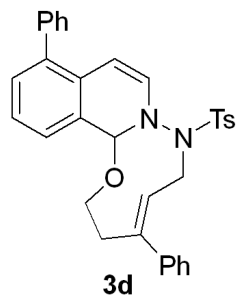
F2 - Processing parameters
SI 32768
SF 75.4677448 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

180 160 140 120 100 80 60 40 20 ppm

3sjwei 5345 xh1-1-83 1h cdcl3



7.696
7.669
7.433
7.427
7.422
7.402
7.399
7.381
7.354
7.348
7.335
7.332
7.328
7.323
7.289
7.276
7.267
7.255
7.234
7.228
7.204
7.179
7.120
7.114
7.097
7.090
5.998
5.988
5.984
5.962
5.957
5.918
5.892
5.866
5.478
5.452
4.885
4.858
4.840
4.813
4.463
4.438
4.418
4.393
3.594
3.585
3.575
3.564
3.554
3.545
3.535
3.396
3.388
3.367
3.358
3.348
3.327
3.080
3.071
2.644
2.636
2.625
2.616
2.587
2.576
2.421

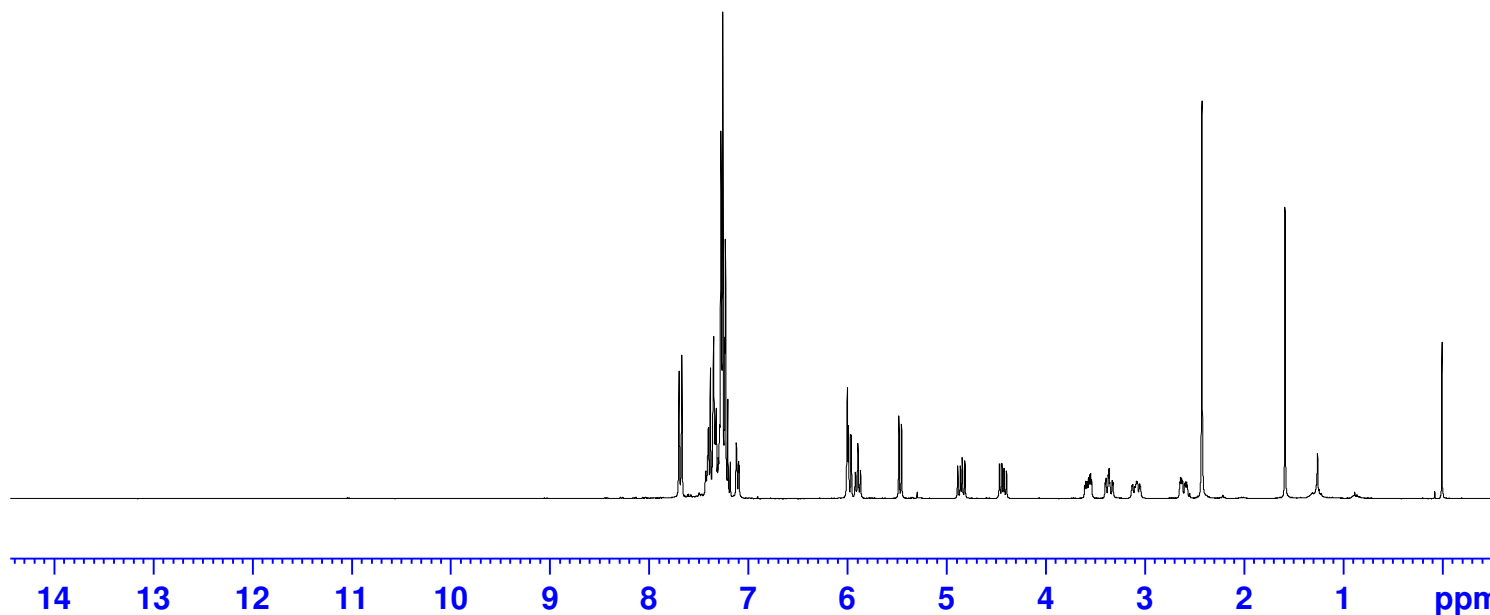


Current Data Parameters
NAME 2021-4--11Project 1 data
EXPNO 5345
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210916
Time 9.13
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 181
DW 83.200 usec
DE 6.50 usec
TE -59.1 K
D1 1.00000000 sec
TD0 1

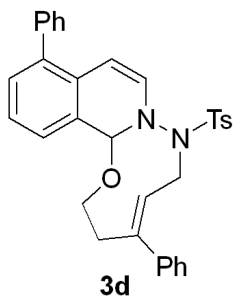
==== CHANNEL f1 =====
SFO1 300.1318534 MHz
NUC1 1H
P1 10.00 usec
PLW1 14.00000000 W

F2 - Processing parameters
SI 65536
SF 300.1300087 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



2.06
5.65
10.59
1.03
0.94
1.05
1.00
1.00
1.01
1.01
1.02
1.04
1.00
1.02
3.11

3sjwei 5365 xh1-1-83 13c cdcl3



146.44
144.50
143.01
140.57
136.97
135.32
134.01
130.19
129.90
129.17
128.51
128.42
128.24
127.64
127.15
127.09
126.57
125.66
121.69

97.77

89.47

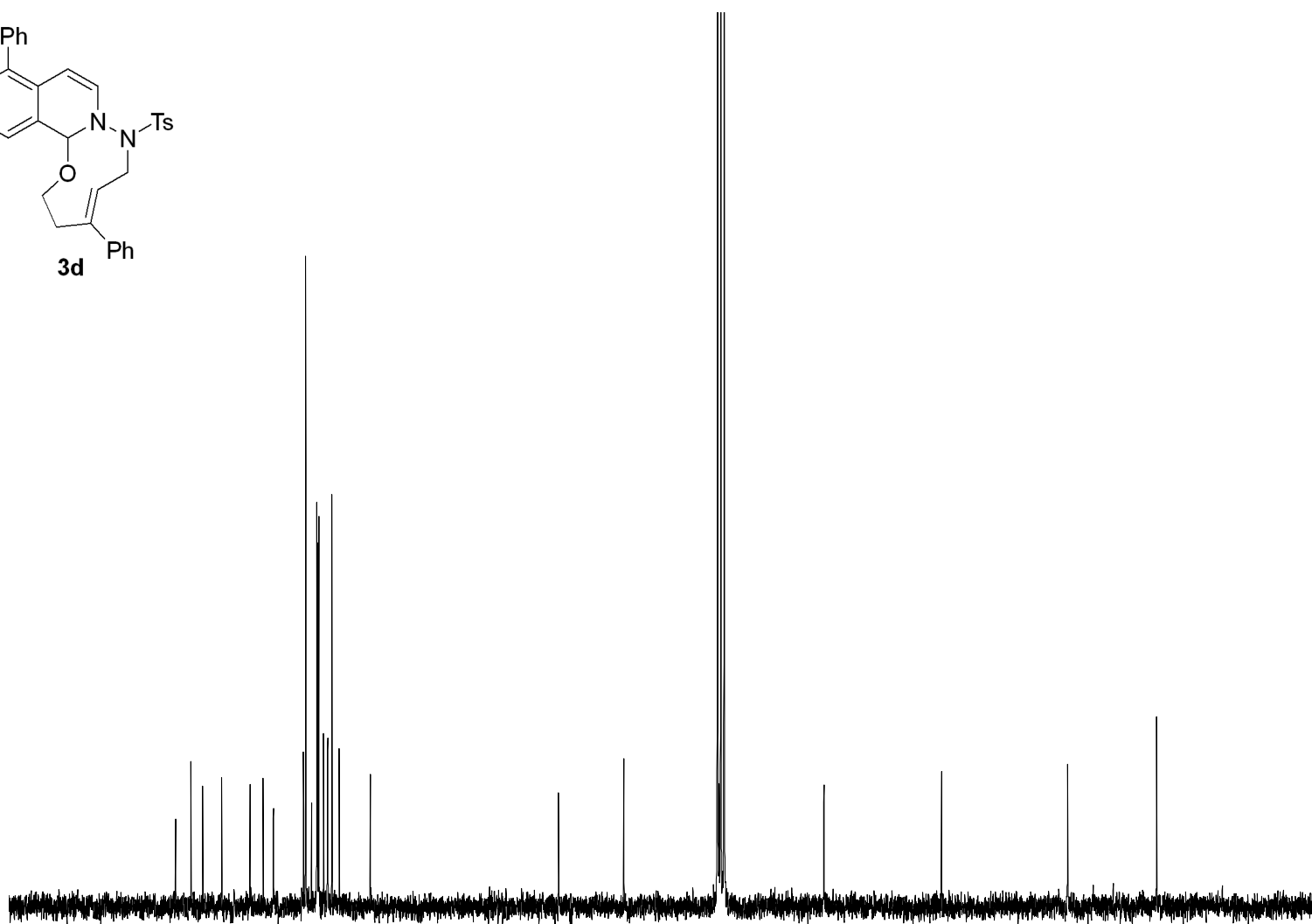
77.57
77.15
76.73

64.04

49.08

33.07

21.76



Current Data Parameters
NAME 2021-4--11Project 1 data
EXPNO 5365
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210916
Time 11.58
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175317 sec
RG 203
DW 27.733 usec
DE 6.50 usec
TE -59.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

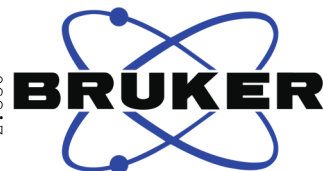
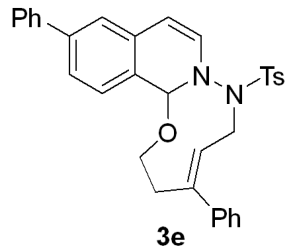
===== CHANNEL f1 =====
SFO1 75.4752949 MHz
NUC1 13C
P1 9.50 usec
PLW1 34.20000076 W

===== CHANNEL f2 =====
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.17284000 W
PLW13 0.14000000 W

F2 - Processing parameters
SI 32768
SF 75.4677405 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

3sjwei 5326 xh1-1-74 1h cdcl3



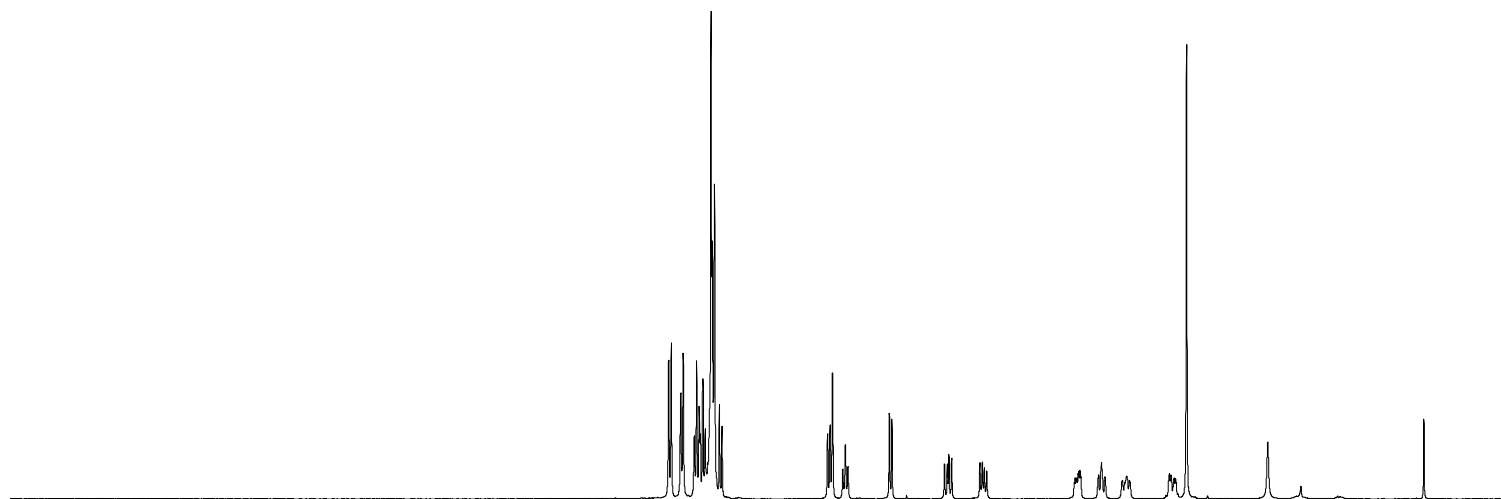
7.715
7.688
7.591
7.566
7.453
7.429
7.403
7.395
7.389
7.364
7.341
7.282
7.271
7.247
7.196
7.169
6.090
6.064
6.041
5.936
5.909
5.883
5.460
5.434
4.897
4.868
4.852
4.823
4.534
4.510
4.490
4.466
3.572
3.563
3.552
3.543
3.532
3.523
3.512
3.504
3.322
3.299
3.292
3.259
3.079
3.036
3.008
2.599
2.586
2.580
2.556
2.550

Current Data Parameters
NAME 2021-4--11Project 1 data
EXPNO 5326
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210915
Time 9.05
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 144
DW 83.200 usec
DE 6.50 usec
TE -59.1 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 300.1318534 MHz
NUC1 1H
P1 10.00 usec
PLW1 14.00000000 W

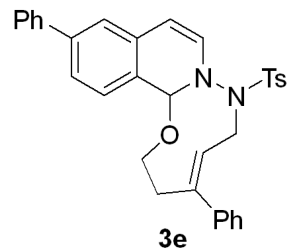
F2 - Processing parameters
SI 65536
SF 300.1300108 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



14 13 12 11 10 9 8 7 6 5 4 3 2 1 ppm

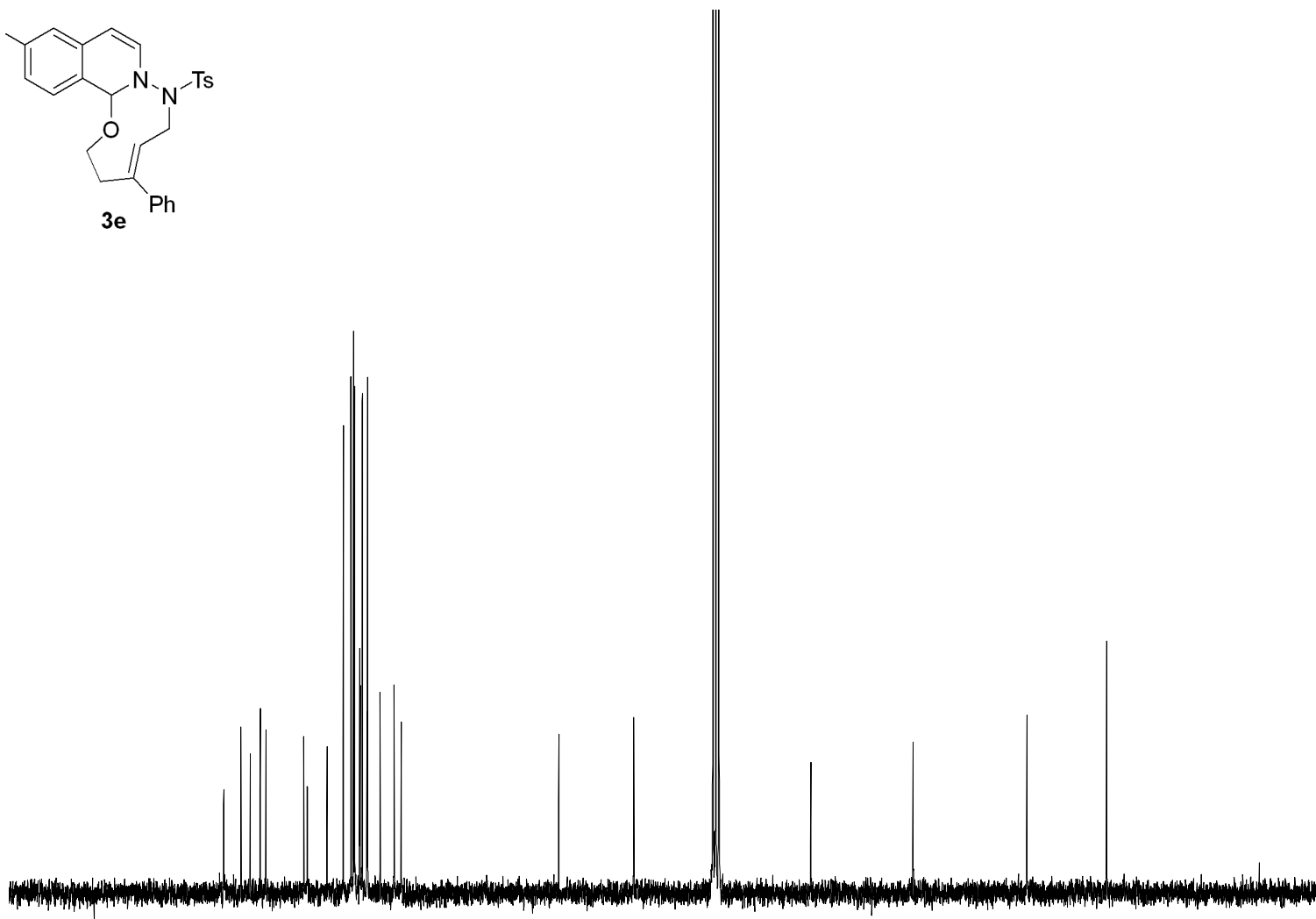
2.04
2.06
4.25
8.44
1.02
2.03
1.00
0.99
1.00
0.99
1.01
1.02
1.00
1.03
3.03

3sjwei 5344 xh1-1-74 13c cdcl3



146.90
144.46
143.12
141.73
140.89
135.55
135.05
132.25
129.95
128.86
128.50
128.34
127.63
127.56
127.25
126.61
126.51
124.74
122.75
121.73

99.41
88.79
77.57
77.15
76.72
63.68
49.20
33.06
21.76



Current Data Parameters
NAME 2021-4--11Project 1 data
EXPNO 5344
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210915
Time 14.21
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 600
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175317 sec
RG 203
DW 27.733 usec
DE 6.50 usec
TE -59.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

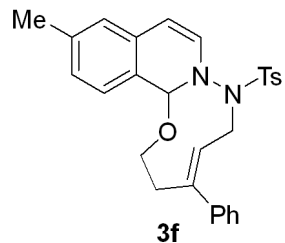
===== CHANNEL f1 =====
SFO1 75.4752949 MHz
NUC1 13C
P1 9.50 usec
PLW1 34.20000076 W

===== CHANNEL f2 =====
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.17284000 W
PLW13 0.14000000 W

F2 - Processing parameters
SI 32768
SF 75.4677421 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

3sjwei 5316 xh1-2-20 1h cdcl3



7.695
7.668
7.287
7.272
7.267
7.255
7.238
7.230
7.017
6.991
6.976
6.947
6.843
6.046
6.020
5.968
5.927
5.901
5.874
5.335
5.309
4.872
4.842
4.828
4.798
4.551
4.527
4.507
4.483
3.494
3.486
3.474
3.465
3.455
3.446
3.434
3.426
3.240
3.217
3.210
3.177
3.172
3.013
2.969
2.940
2.562
2.548

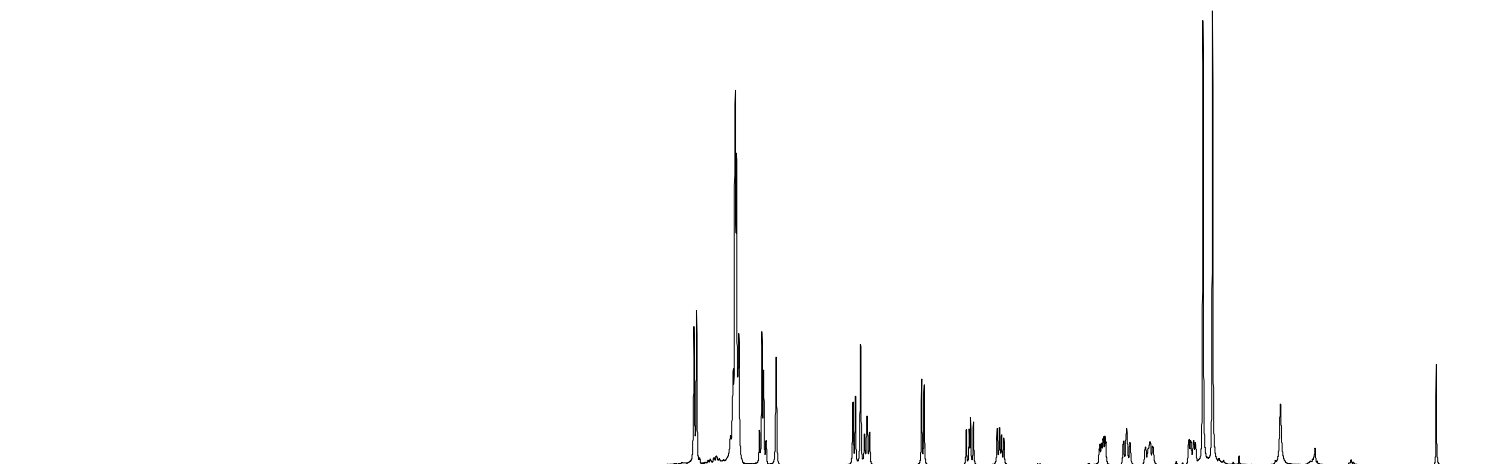


Current Data Parameters
NAME 2021-4--11Project 1 data
EXPNO 5316
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210914
Time 8.56
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 161
DW 83.200 usec
DE 6.50 usec
TE -59.1 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 300.1318534 MHz
NUC1 1H
P1 10.00 usec
PLW1 14.00000000 W

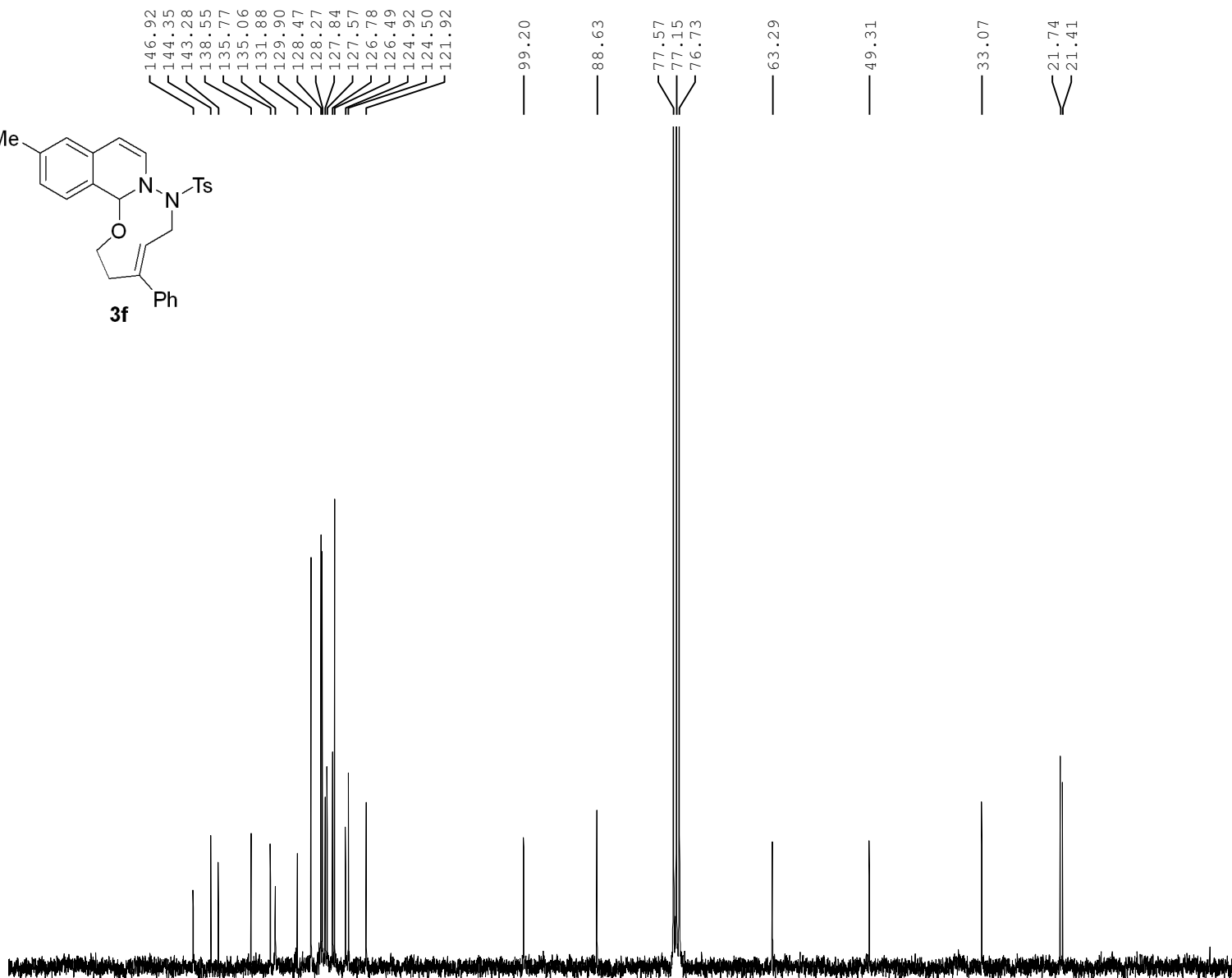
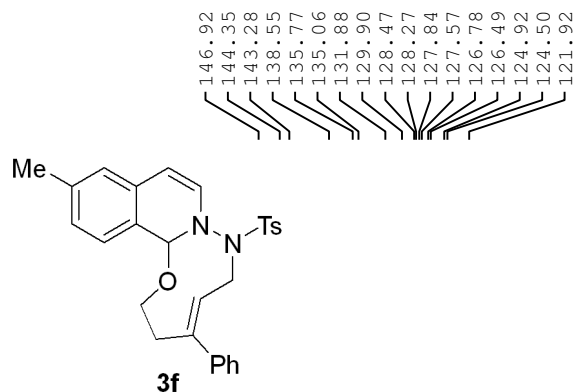
F2 - Processing parameters
SI 65536
SF 300.1300088 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



14 13 12 11 10 9 8 7 6 5 4 3 2 1 ppm

2.23
7.92
2.03
0.99
0.98
0.95
1.00
0.98
0.98
1.00
1.01
1.00
0.99
1.04
3.12
3.17

3sjwei 5328 xh1-2-20 13c cdcl3



Current Data Parameters
NAME 2021-4--11Project 1 data
EXPNO 5328
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210914
Time 10.59
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 1024
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175317 sec
RG 203
DW 27.733 usec
DE 6.50 usec
TE -59.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 75.4752949 MHz
NUC1 13C
P1 9.50 usec
PLW1 34.20000076 W

===== CHANNEL f2 =====
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.17284000 W
PLW13 0.14000000 W

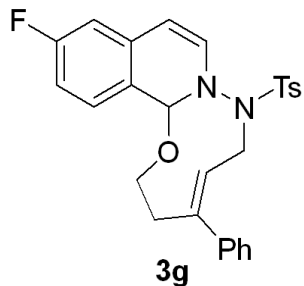
F2 - Processing parameters
SI 32768
SF 75.4677414 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

3sjwei 5222 xh1-2-76 1h cdcl3



7.686
7.659
7.298
7.280
7.269
7.257
7.243
7.103
7.084
7.074
7.056
6.872
6.863
6.843
6.835
6.815
6.806
6.728
6.720
6.696
6.688
6.083
6.058
5.984
5.913
5.887
5.860
5.338
5.312
4.870
4.841
4.826
4.797
4.511
4.487
4.466
4.443
3.529
3.520
3.509
3.500
3.489
3.480
3.469
3.460
3.260
3.252
3.230
3.222
3.213
3.190
3.183
3.066
3.058
3.018
3.010
2.988
2.588
2.581
2.568
2.561
2.540
2.532
2.520
2.512
2.425

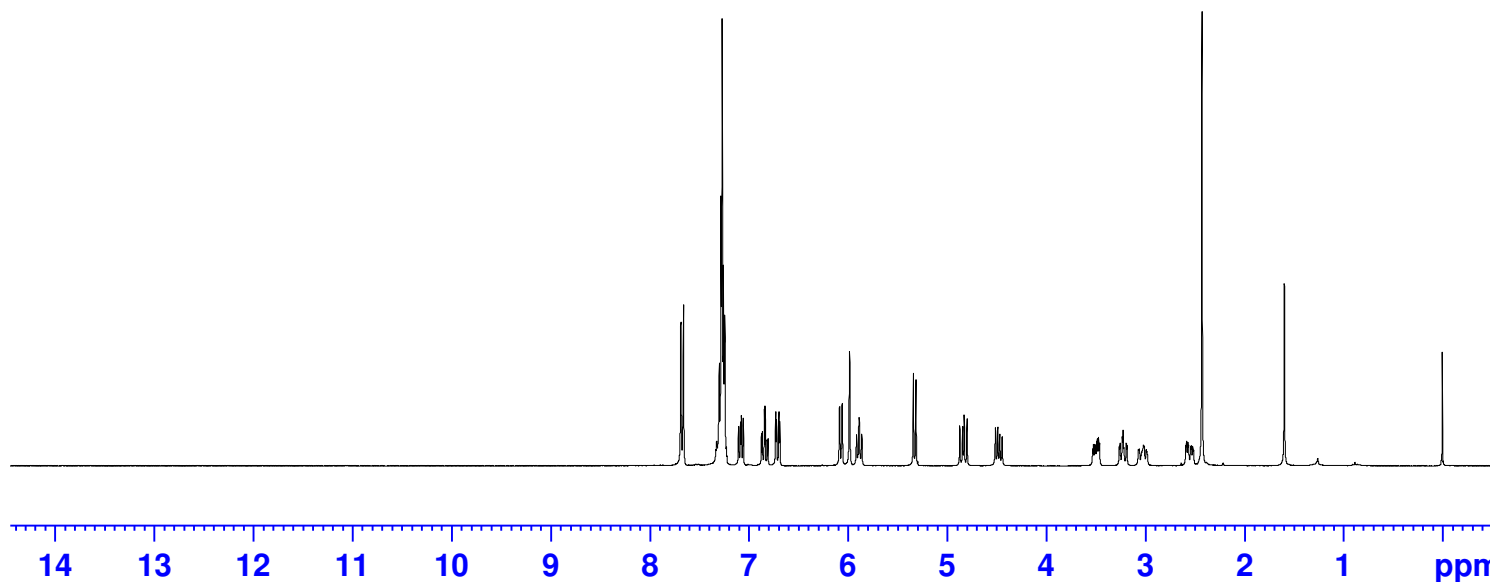


Current Data Parameters
NAME 2021-4--11Project 1 data
EXPNO 5222
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210906
Time 9.07
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 161
DW 83.200 usec
DE 6.50 usec
TE -59.1 K
D1 1.00000000 sec
TD0 1

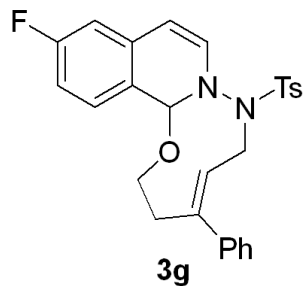
==== CHANNEL f1 =====
SFO1 300.1318534 MHz
NUC1 1H
P1 10.00 usec
PLW1 14.00000000 W

F2 - Processing parameters
SI 65536
SF 300.1300082 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

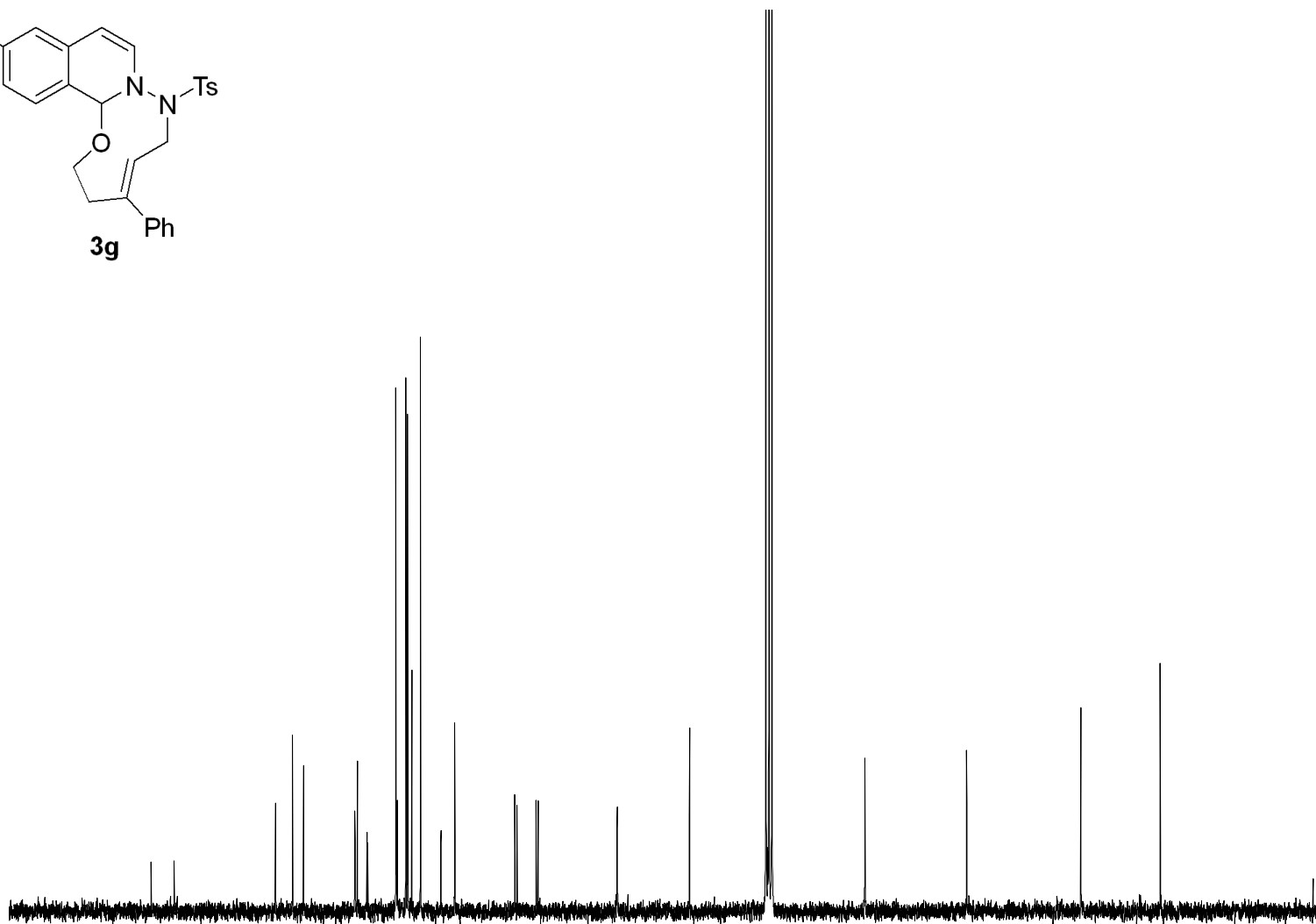


2.02
7.65
1.02
1.01
0.98
0.97
0.96
0.96
0.96
0.98
0.96
1.00
1.01
1.00
1.01
3.02

3sjwei 5227 xh1-2-76 13c cdcl3



164.59
161.33
146.98
144.58
143.02
135.75
135.39
134.05
133.93
129.96
129.88
129.76
128.53
128.31
127.69
126.46
123.58
123.55
121.62
113.11
112.81
110.11
109.82
98.64
98.61
88.38
77.57
77.15
76.73
63.56
49.16
32.99
21.75



Current Data Parameters
NAME 2021-4--11Project 1 data
EXPNO 5227
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210906
Time 11.43
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175317 sec
RG 203
DW 27.733 usec
DE 6.50 usec
TE -59.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

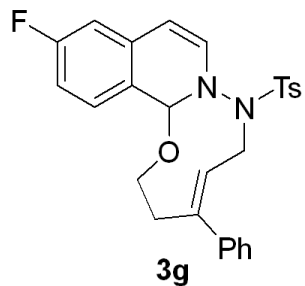
===== CHANNEL f1 =====
SFO1 75.4752949 MHz
NUC1 13C
P1 9.50 usec
PLW1 34.20000076 W

===== CHANNEL f2 =====
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.17284000 W
PLW13 0.14000000 W

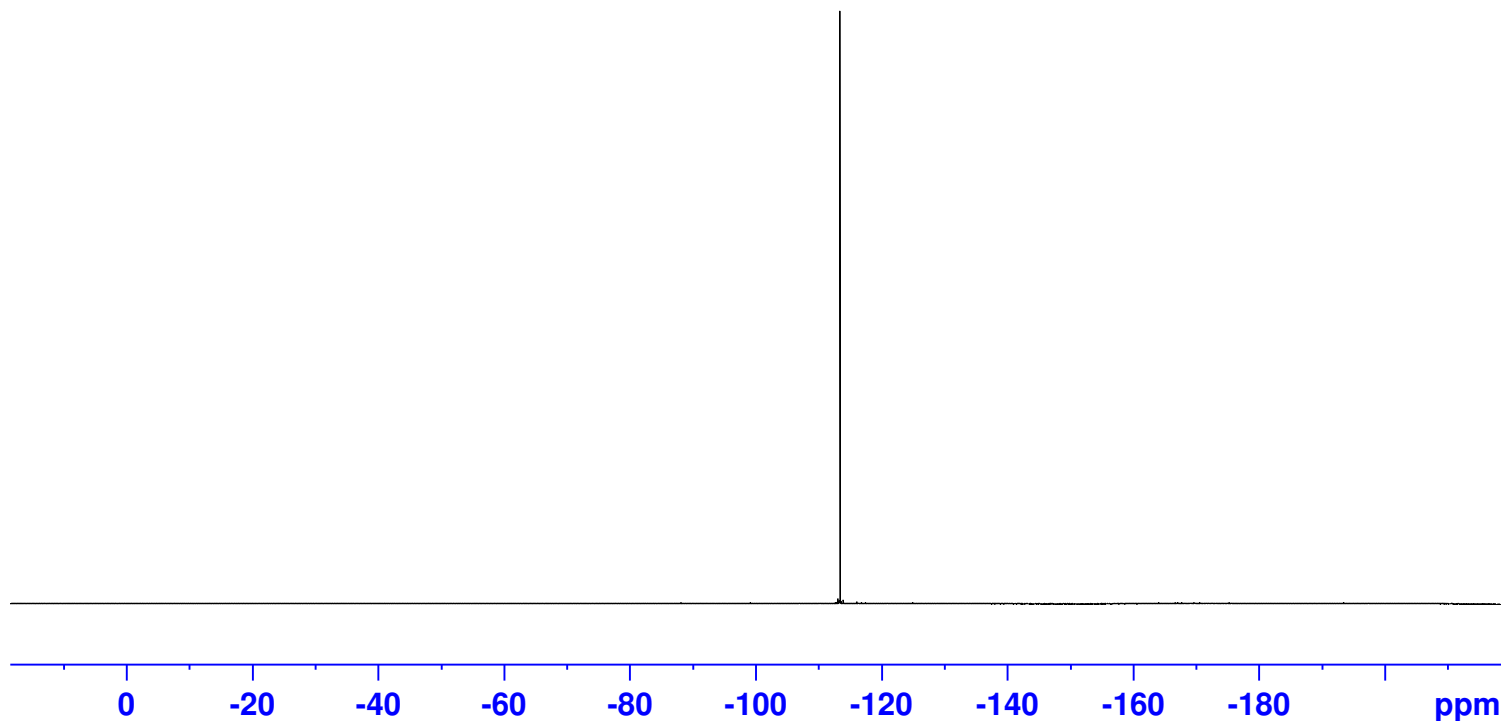
F2 - Processing parameters
SI 32768
SF 75.4677410 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

3sjwei 5228 xh1-2-76 19f cdcl3



-113.398



Current Data Parameters
NAME 0906sjw
EXPNO 5228
PROCNO 1

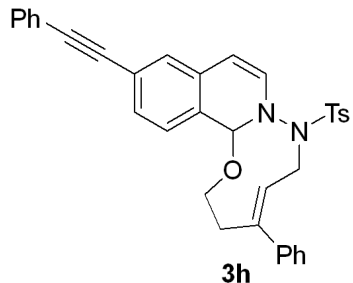
F2 - Acquisition Parameters
Date_ 20210906
Time 11.45
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgfhigqn.2
TD 131072
SOLVENT CDC13
NS 16
DS 4
SWH 66964.289 Hz
FIDRES 0.510897 Hz
AQ 0.9786710 sec
RG 203
DW 7.467 usec
DE 6.50 usec
TE -59.1 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 282.3761148 MHz
NUC1 19F
P1 14.50 usec
PLW1 10.39999962 W

==== CHANNEL f2 =====
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.17284000 W

F2 - Processing parameters
SI 65536
SF 282.4043552 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

3sjwei 5066 xh1-2-35 1h cdcl3



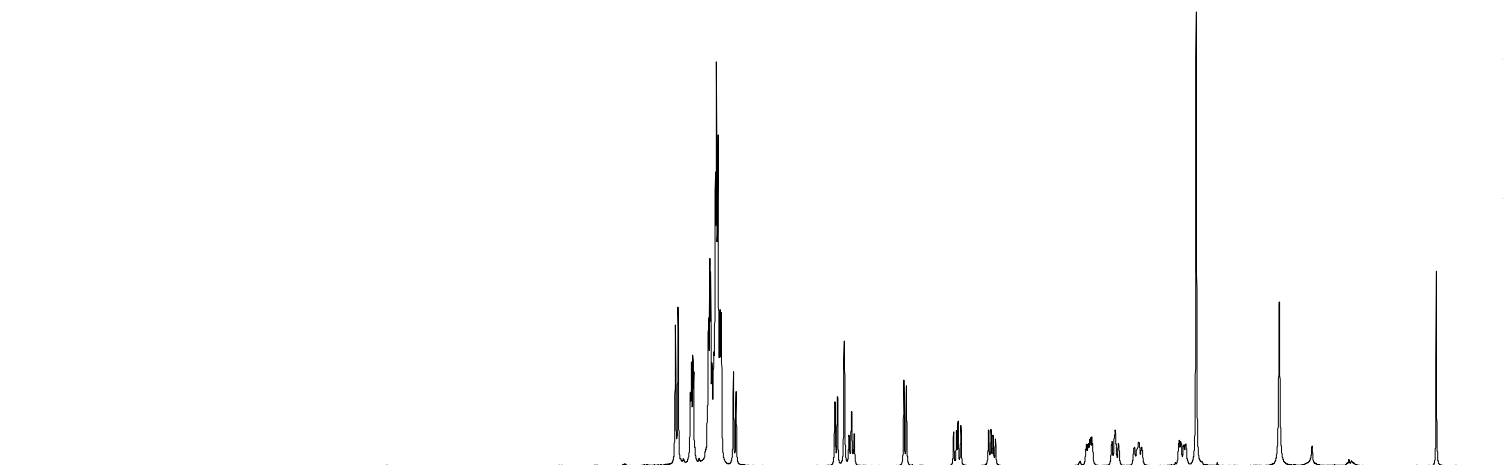
7.690
7.662
7.538
7.525
7.513
7.506
7.355
7.352
7.341
7.333
7.321
7.317
7.302
7.295
7.284
7.275
7.265
7.258
7.239
7.228
7.102
7.076
6.076
6.051
5.983
5.935
5.908
5.882
5.380
5.355
4.878
4.848
4.833
4.804
4.524
4.500
4.479
4.455
3.541
3.533
3.522
3.513
3.502
3.493
3.482
3.474
3.276
3.253
3.246
3.214
3.051
3.008
2.979
2.597
2.584

Current Data Parameters
NAME 2021-4--11Project 1 data
EXPNO 5066
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210825
Time 9.10
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 203
DW 83.200 usec
DE 6.50 usec
TE -59.1 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 300.1318534 MHz
NUC1 1H
P1 10.00 usec
PLW1 14.00000000 W

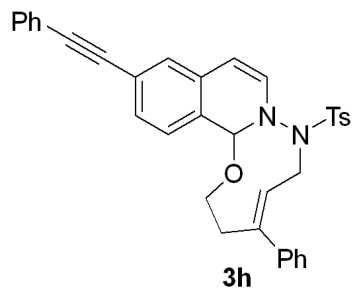
F2 - Processing parameters
SI 65536
SF 300.1300078 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



14 13 12 11 10 9 8 7 6 5 4 3 2 1 ppm

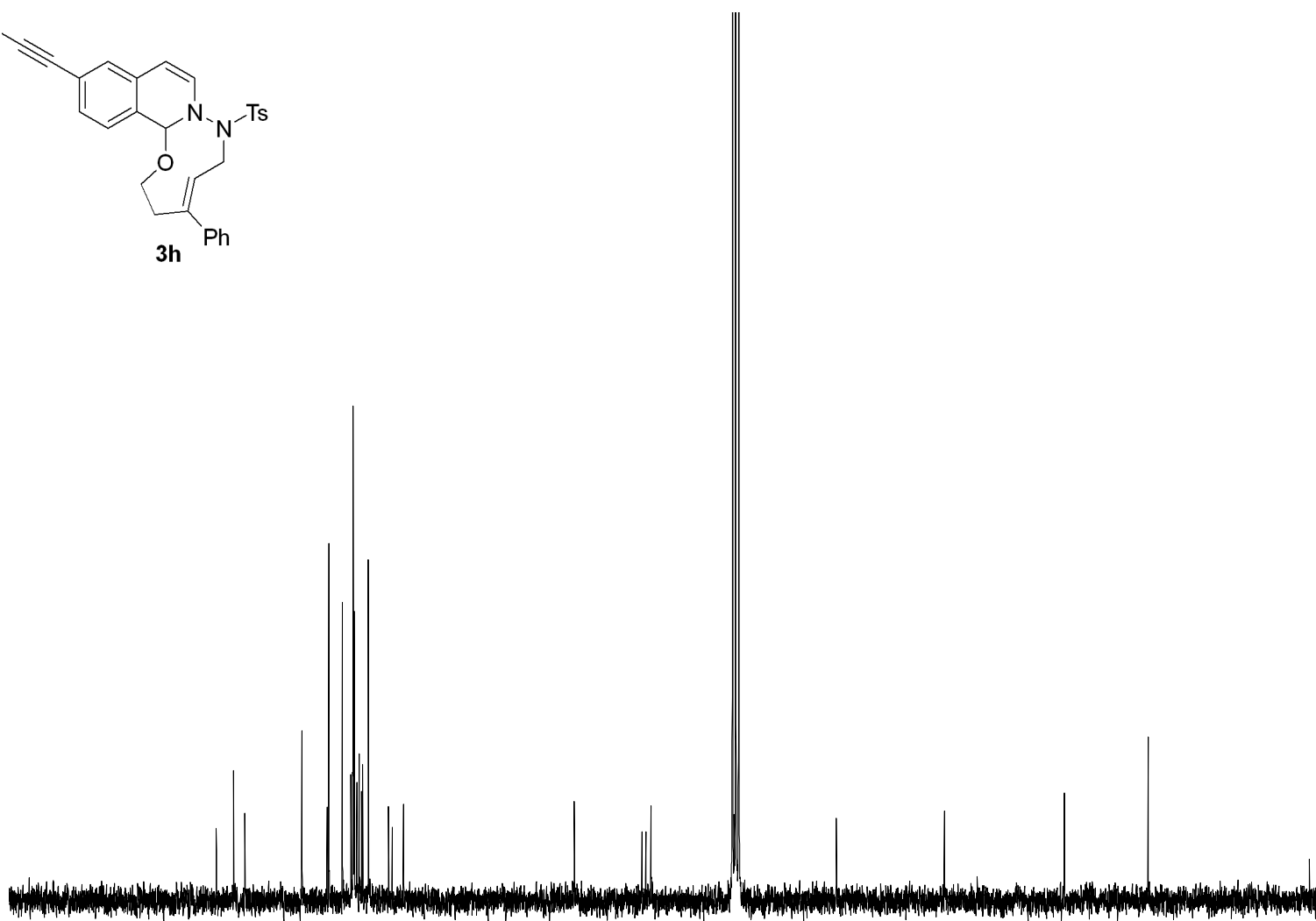
2.02
2.17
3.86
9.35
1.06
0.99
0.98
1.00
0.96
0.97
0.98
0.99
1.03
0.99
1.06
3.07

3sjwei 5081 xh1-2-35 13c cdcl3



146.87
144.56
143.04
135.38
132.00
131.76
129.96
128.80
128.54
128.49
128.35
128.01
127.69
127.36
127.22
126.47
123.75
123.25
121.75

98.81
89.72
89.21
88.53
77.57
77.15
76.73
63.64
49.13
33.03
21.77



Current Data Parameters
NAME 2021-4--11Project 1 data
EXPNO 5081
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210825
Time 11.34
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 1024
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175317 sec
RG 203
DW 27.733 usec
DE 6.50 usec
TE -59.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

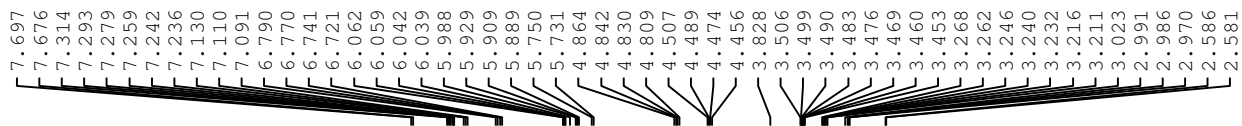
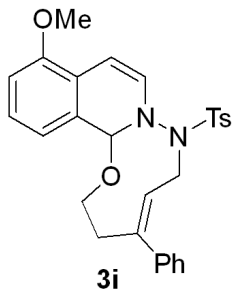
===== CHANNEL f1 =====
SFO1 75.4752949 MHz
NUC1 13C
P1 9.50 usec
PLW1 34.20000076 W

===== CHANNEL f2 =====
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.17284000 W
PLW13 0.14000000 W

F2 - Processing parameters
SI 32768
SF 75.4677404 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

xh1-5-31

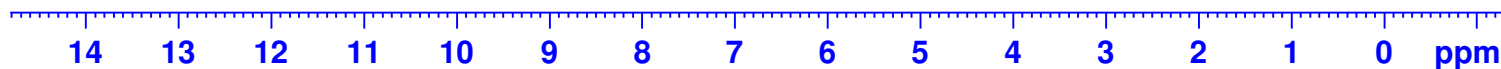
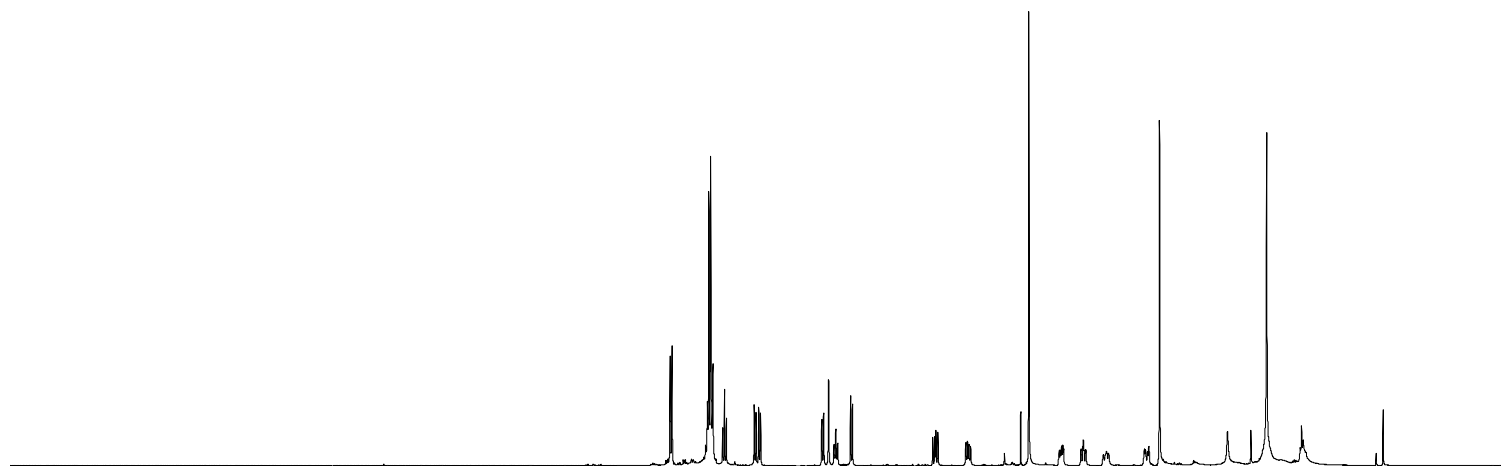


Current Data Parameters
NAME 220726-400
EXPNO 64
PROCNO 1

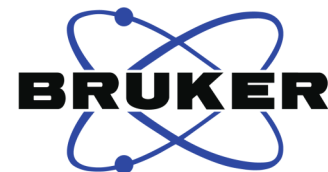
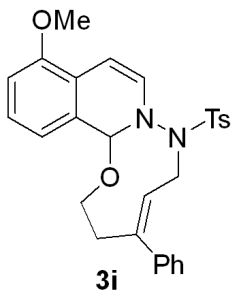
F2 - Acquisition Parameters
Date_ 20220726
Time 16.28
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 6
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 75.43
DW 60.800 usec
DE 6.50 usec
TE 294.7 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 14.68 usec
PLW1 14.00000000 W
SFO1 400.1924713 MHz

F2 - Processing parameters
SI 65536
SF 400.1900188 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



XHL-5-31



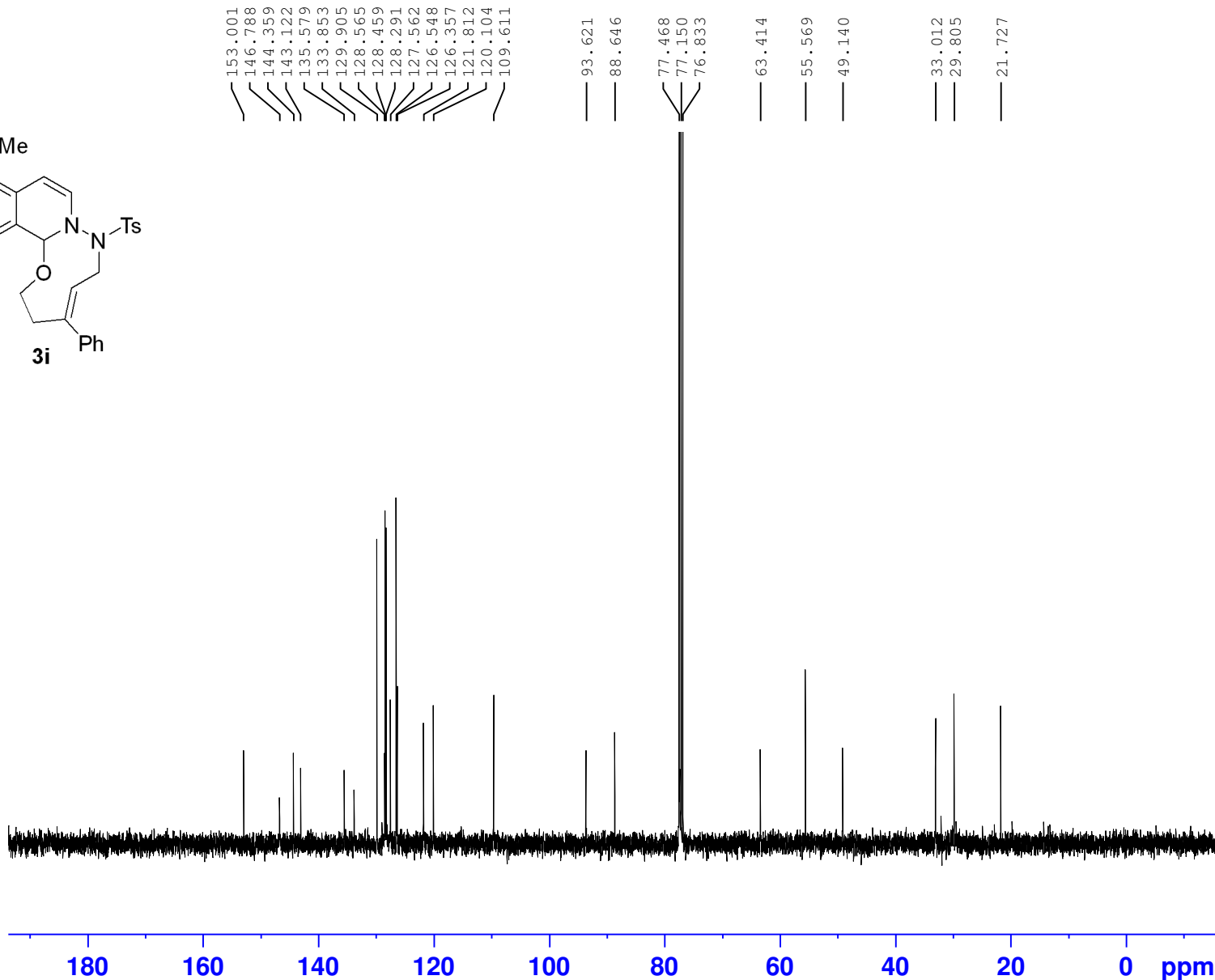
Current Data Parameters
 NAME 220725-400
 EXPNO 60
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20220725
 Time 16.44
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 65
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 193.13
 DW 20.800 usec
 DE 6.50 usec
 TE 295.3 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

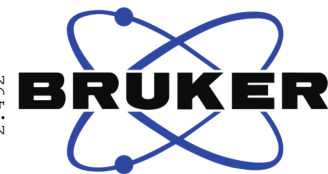
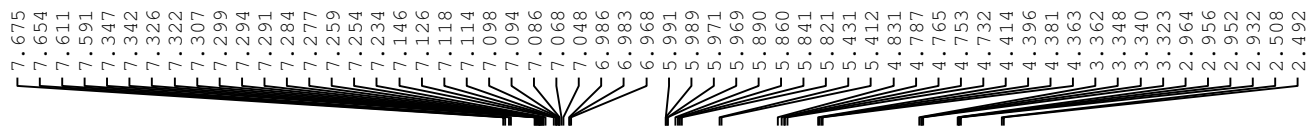
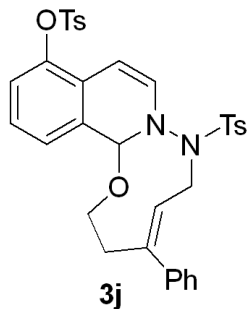
===== CHANNEL f1 =====
 NUC1 13C
 P1 12.00 usec
 PLW1 53.00000000 W
 SFO1 100.6379178 MHz

===== CHANNEL f2 =====
 CPDPRG[2] waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PLW2 14.00000000 W
 PLW12 0.37246999 W
 PLW13 0.30170000 W
 SFO2 400.1916008 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6278493 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



XHL-5-40

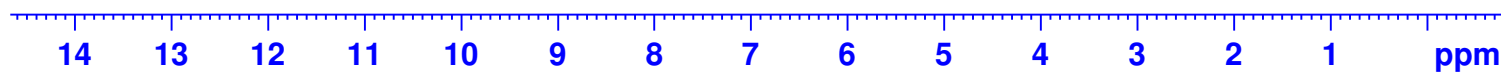
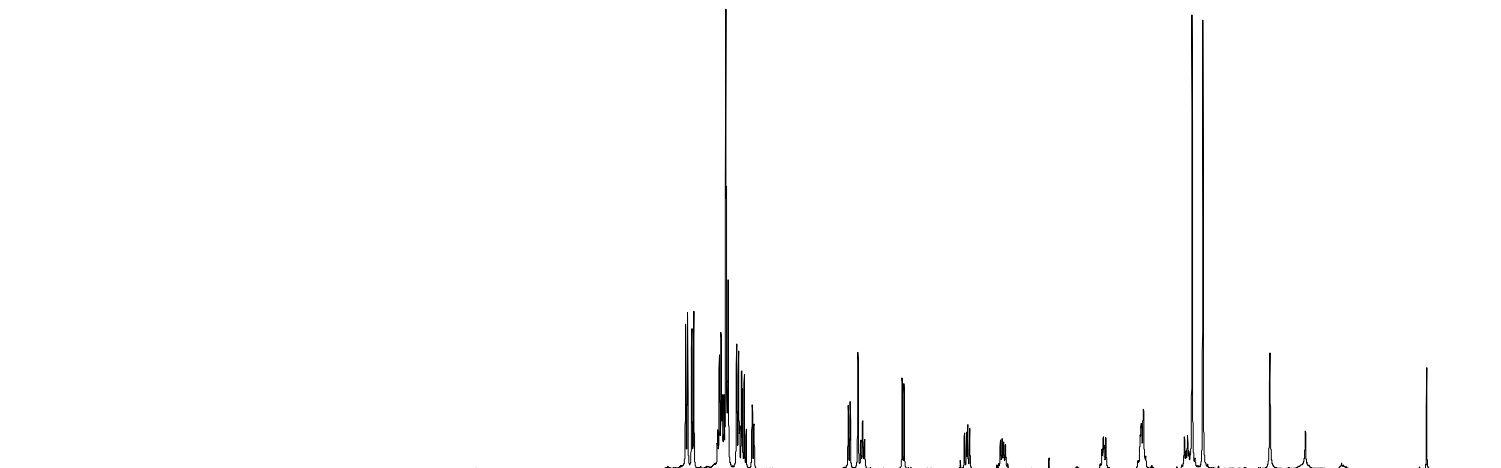


Current Data Parameters
 NAME 220729-400
 EXPNO 101
 PROCNO 1

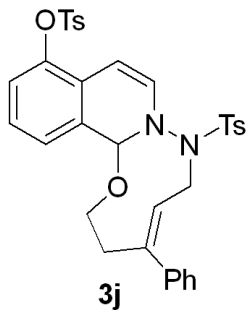
F2 - Acquisition Parameters
 Date_ 20220729
 Time 21.00
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 8
 DS 2
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9845889 sec
 RG 113.67
 DW 60.800 usec
 DE 6.50 usec
 TE 294.8 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 1H
 P1 14.68 usec
 PLW1 14.00000000 W
 SFO1 400.1924713 MHz

F2 - Processing parameters
 SI 65536
 SF 400.1900171 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

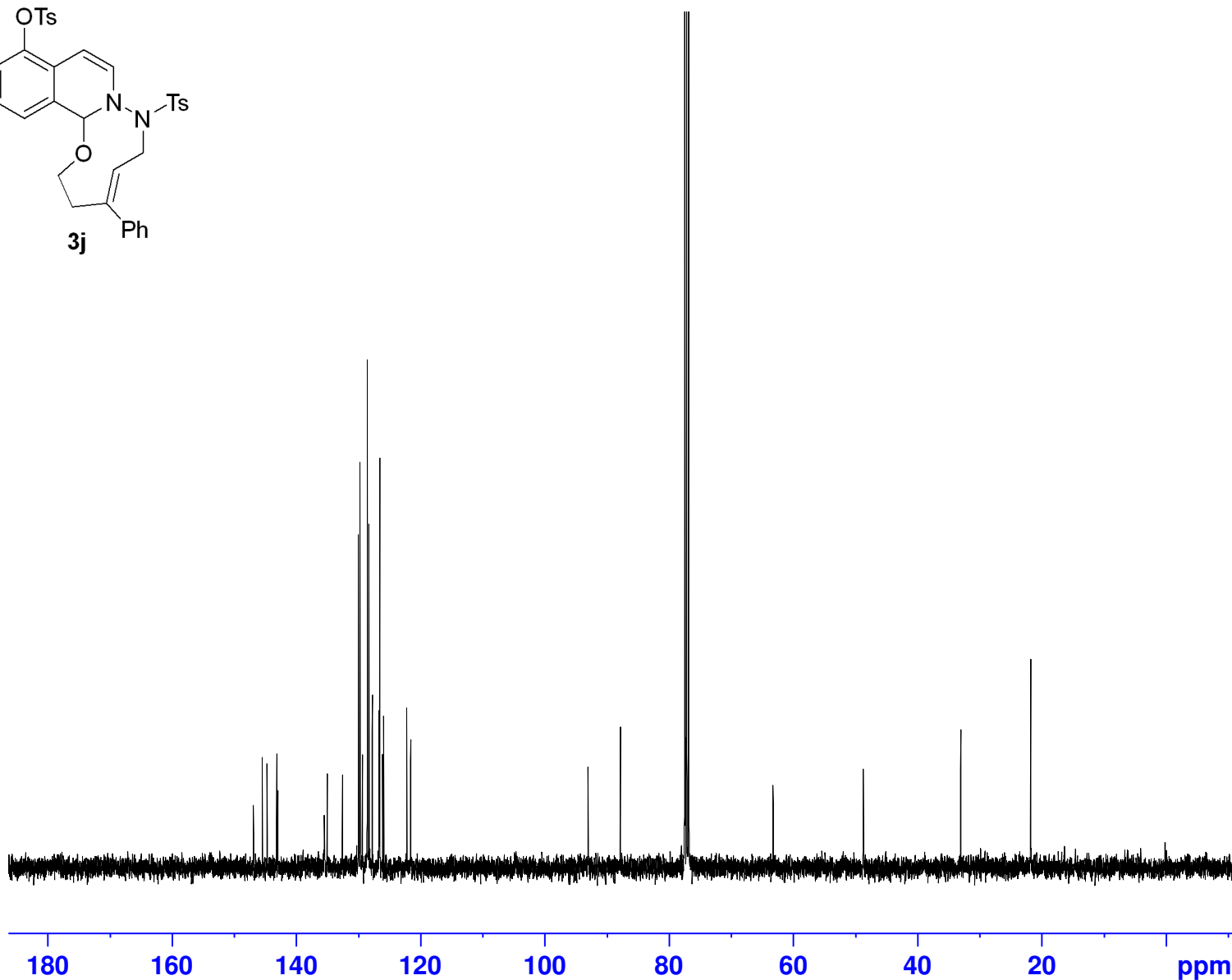


XHL-5-40



146.91
145.50
144.71
143.18
142.98
135.50
135.02
132.60
130.00
129.75
129.38
128.58
128.57
128.31
127.78
126.70
126.57
126.11
125.93
122.22
121.60

93.04
87.82
77.47
77.15
76.83
63.23
48.71
33.02
21.76
21.73



Current Data Parameters
NAME 220729-400
EXPNO 102
PROCNO 1

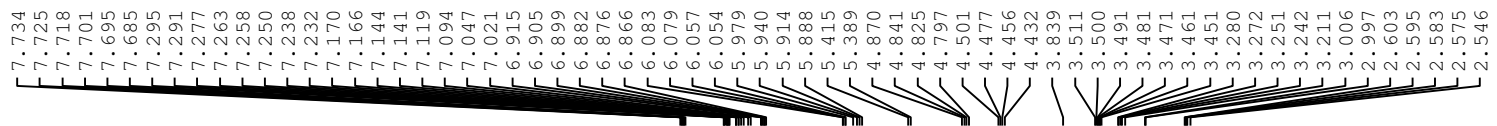
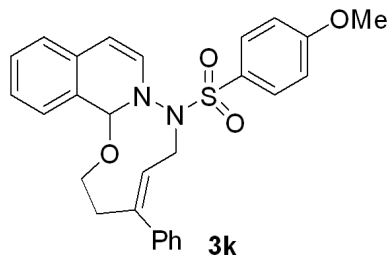
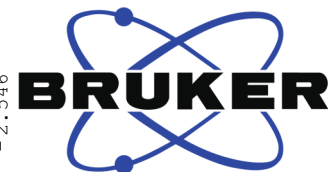
F2 - Acquisition Parameters
Date_ 20220729
Time 21.04
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 166
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 193.13
DW 20.800 usec
DE 6.50 usec
TE 295.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 13C
P1 12.00 usec
PLW1 53.00000000 W
SFO1 100.6379178 MHz

==== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.37246999 W
PLW13 0.30170000 W
SFO2 400.1916008 MHz

F2 - Processing parameters
SI 32768
SF 100.6278481 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

3sjwei 5458 xh1-3-15 1h cdcl3

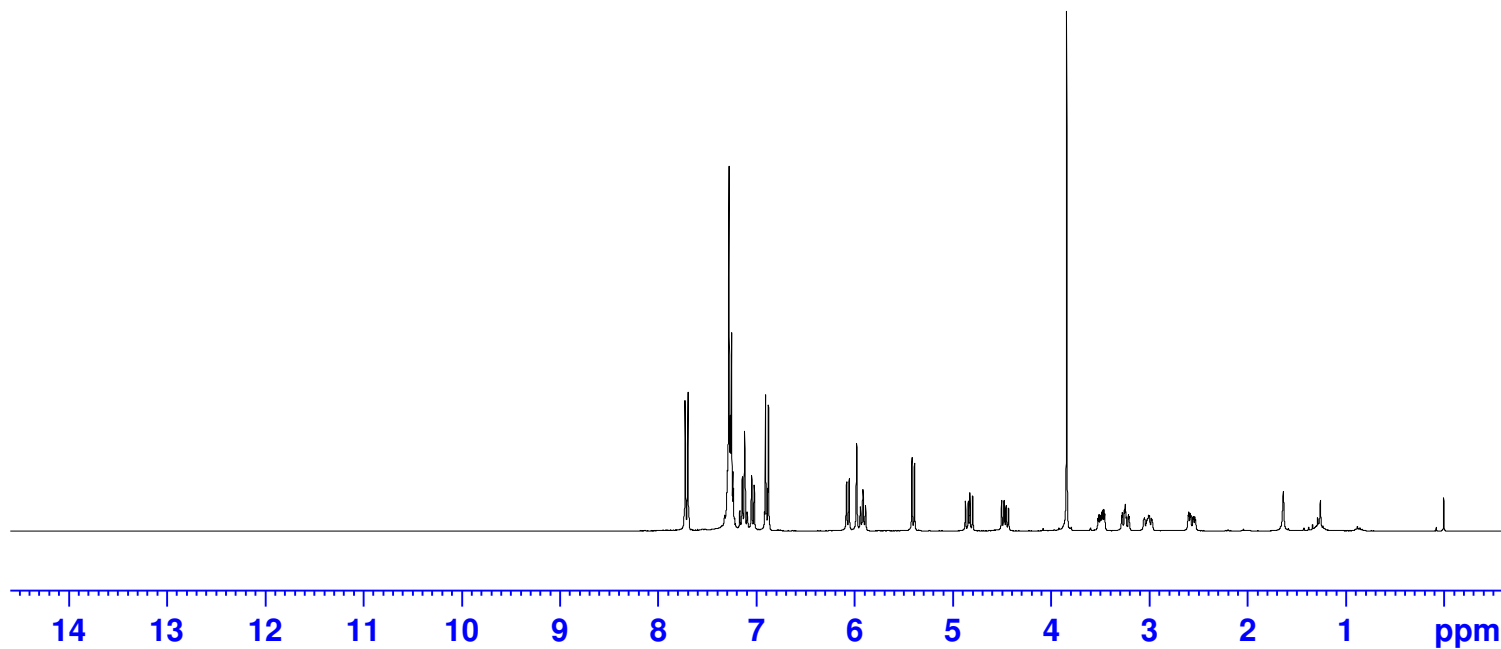


Current Data Parameters
NAME 2021-4--11Project 1 data
EXPNO 5458
PROCNO 1

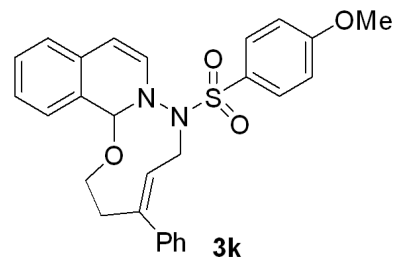
F2 - Acquisition Parameters
Date_ 20210929
Time 9.32
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 101
DW 83.200 usec
DE 6.50 usec
TE -59.1 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 300.1318534 MHz
NUC1 1H
P1 10.00 usec
PLW1 14.00000000 W

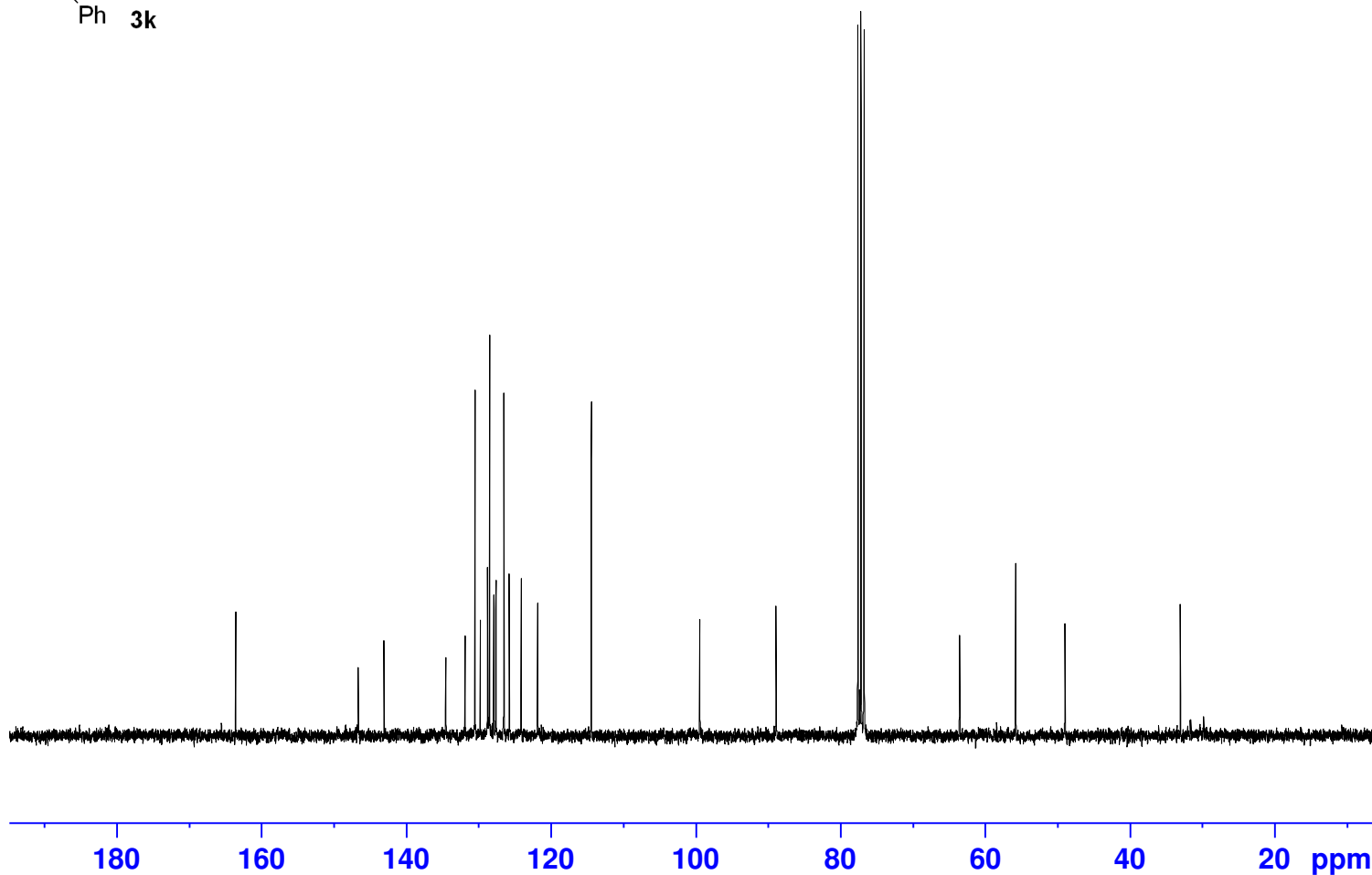
F2 - Processing parameters
SI 65536
SF 300.1300103 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



3sjwei 5456 xh1-3-15 13c cdcl3



163.59
146.66
143.08
134.54
131.85
130.50
129.77
128.78
128.49
127.90
127.60
126.50
125.77
124.13
121.84
114.43
99.43
88.89
77.57
77.15
76.72
63.52
55.76
48.95
33.01



Current Data Parameters
NAME 2021-4--11Project 1 data
EXPNO 5456
PROCNO 1

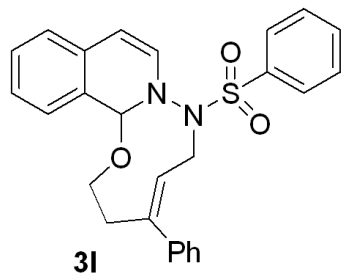
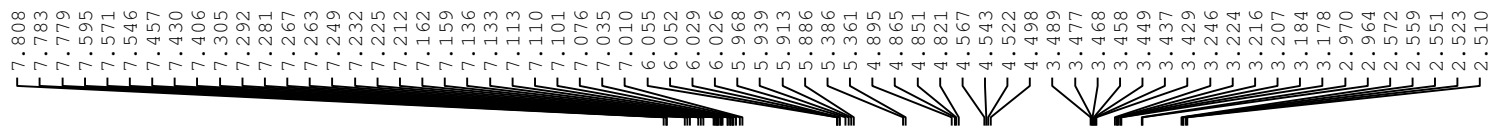
F2 - Acquisition Parameters
Date_ 20210928
Time 13.36
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 648
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175317 sec
RG 203
DW 27.733 usec
DE 6.50 usec
TE -59.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 75.4752949 MHz
NUC1 13C
P1 9.50 usec
PLW1 34.20000076 W

===== CHANNEL f2 =====
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.17284000 W
PLW13 0.14000000 W

F2 - Processing parameters
SI 32768
SF 75.4677421 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

3sjwei 5427 xh1-3-9 1h cdcl3

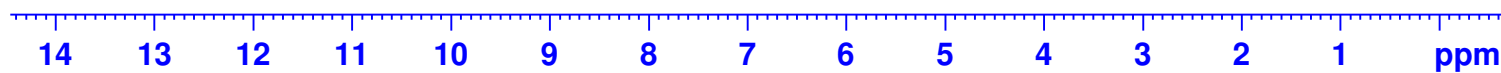
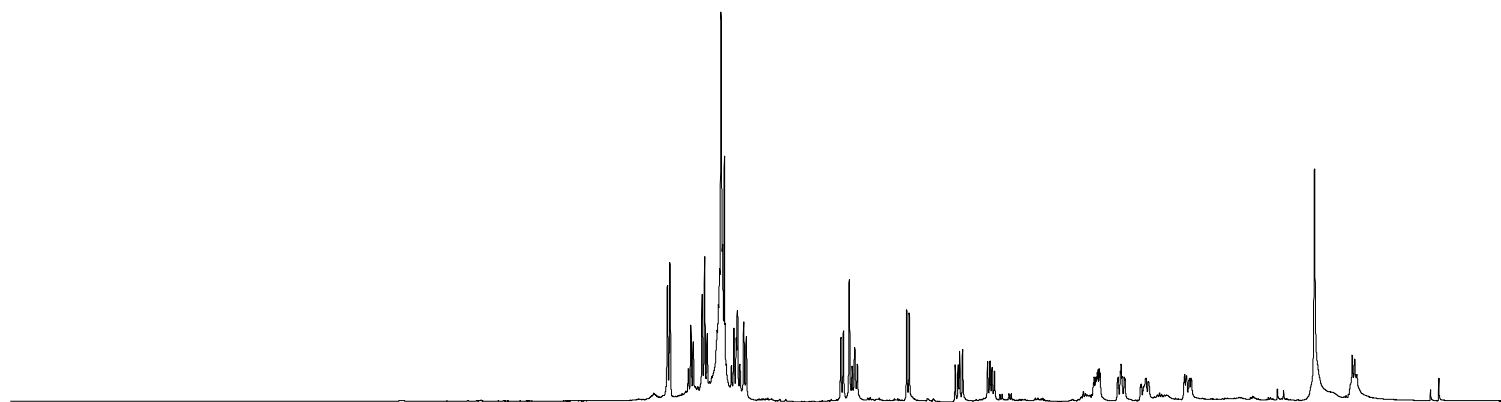


Current Data Parameters
NAME 2021-4--11Project 1 data
EXPNO 5427
PROCNO 1

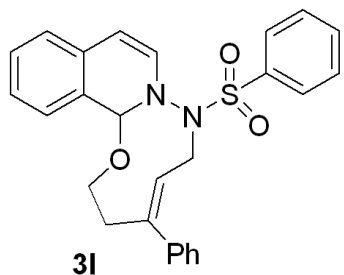
F2 - Acquisition Parameters
Date_ 20210927
Time 9.14
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 32
DW 83.200 usec
DE 6.50 usec
TE -59.1 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 300.1318534 MHz
NUC1 1H
P1 10.00 usec
PLW1 14.00000000 W

F2 - Processing parameters
SI 65536
SF 300.1300154 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



3sjwei 5459 xh1-3-9 13c cdcl3



146.88
143.07
138.51
134.79
133.42
131.79
129.24
128.79
128.44
128.18
127.85
127.58
127.47
126.41
125.80
124.11
121.71

99.40

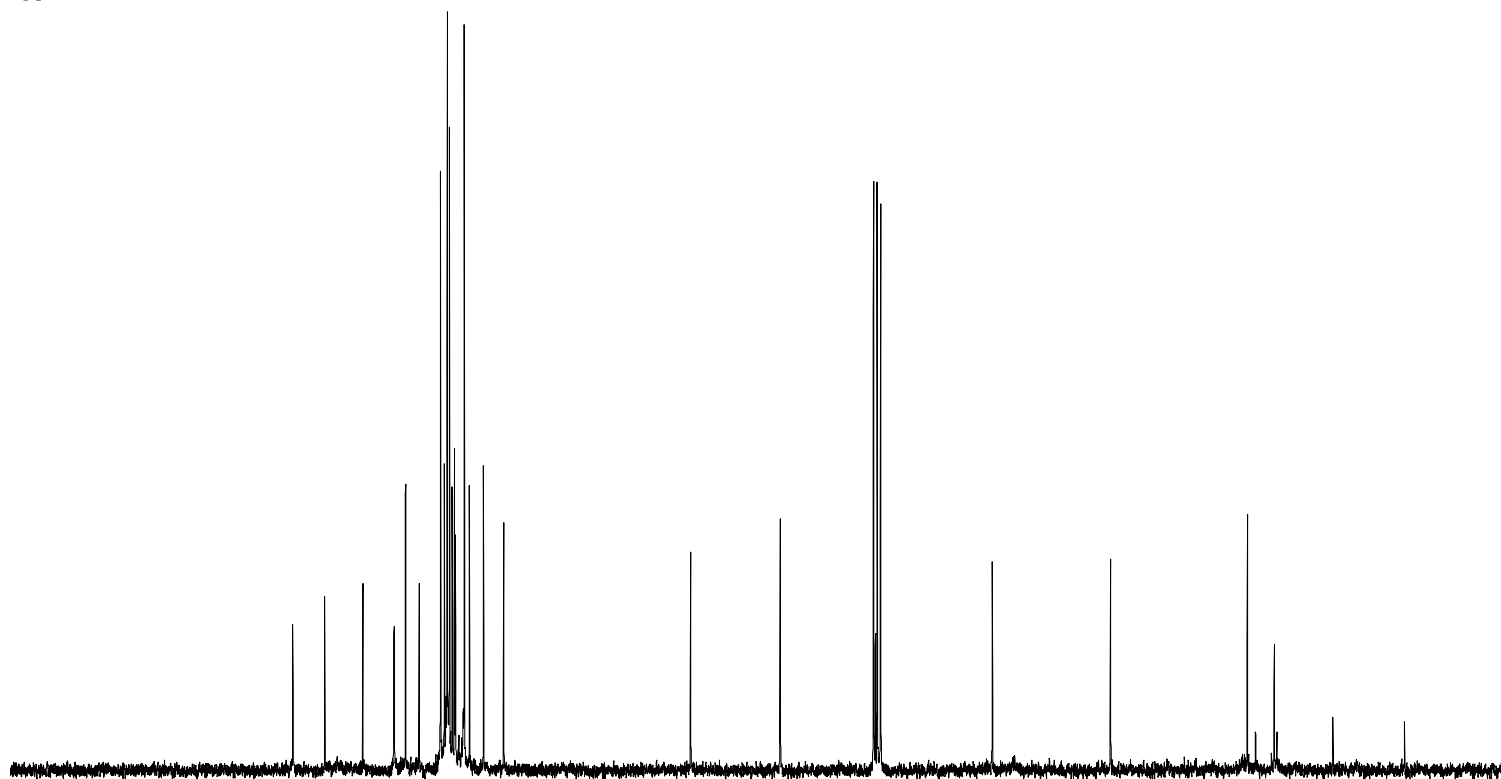
88.70

77.57
77.15
76.73

63.39

49.28

32.96



Current Data Parameters
NAME 2021-4--11Project 1 data
EXPNO 5459
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210927
Time 12.20
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 500
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175317 sec
RG 203
DW 27.733 usec
DE 6.50 usec
TE -59.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

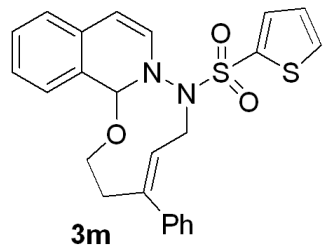
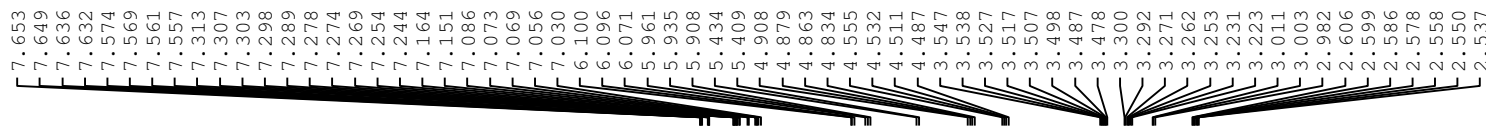
===== CHANNEL f1 =====
SFO1 75.4752949 MHz
NUC1 13C
P1 9.50 usec
PLW1 34.20000076 W

===== CHANNEL f2 =====
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.17284000 W
PLW13 0.14000000 W

F2 - Processing parameters
SI 32768
SF 75.4677484 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

3sjwei 5428 xh1-3-11 1h cdcl3

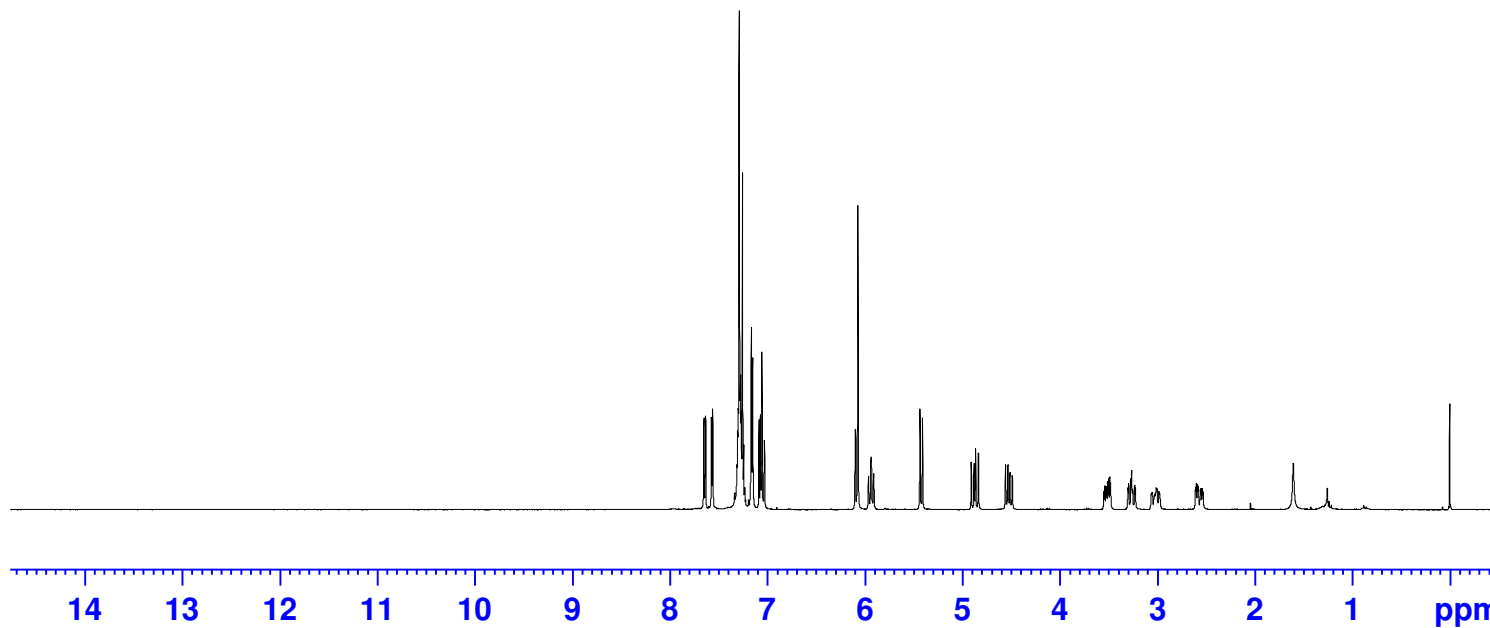


Current Data Parameters
NAME 2021-4--11Project 1 data
EXPNO 5428
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210927
Time 9.19
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 161
DW 83.200 usec
DE 6.50 usec
TE -59.1 K
D1 1.00000000 sec
TD0 1

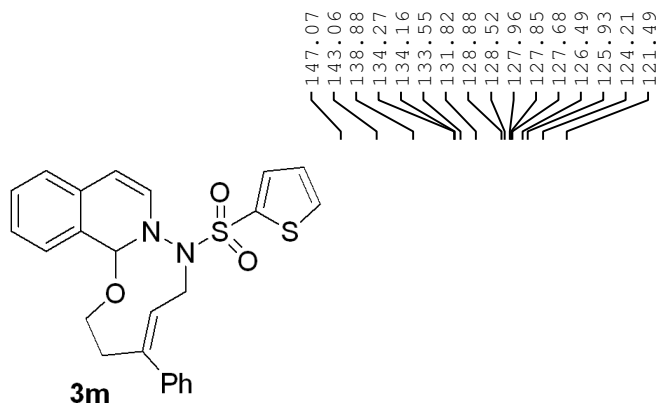
==== CHANNEL f1 =====
SFO1 300.1318534 MHz
NUC1 1H
P1 10.00 usec
PLW1 14.00000000 W

F2 - Processing parameters
SI 65536
SF 300.1300091 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



0.96
0.98
6.55
1.92
2.00
1.89
0.98
0.98
0.98
1.00
1.00
1.01
0.98
0.99

3sjwei 5425 xh1-3-11 13c cdcl3



147.07
143.06
138.88
134.27
134.16
133.55
131.82
128.88
128.52
127.96
127.85
127.68
126.49
125.93
124.21
121.49

99.70

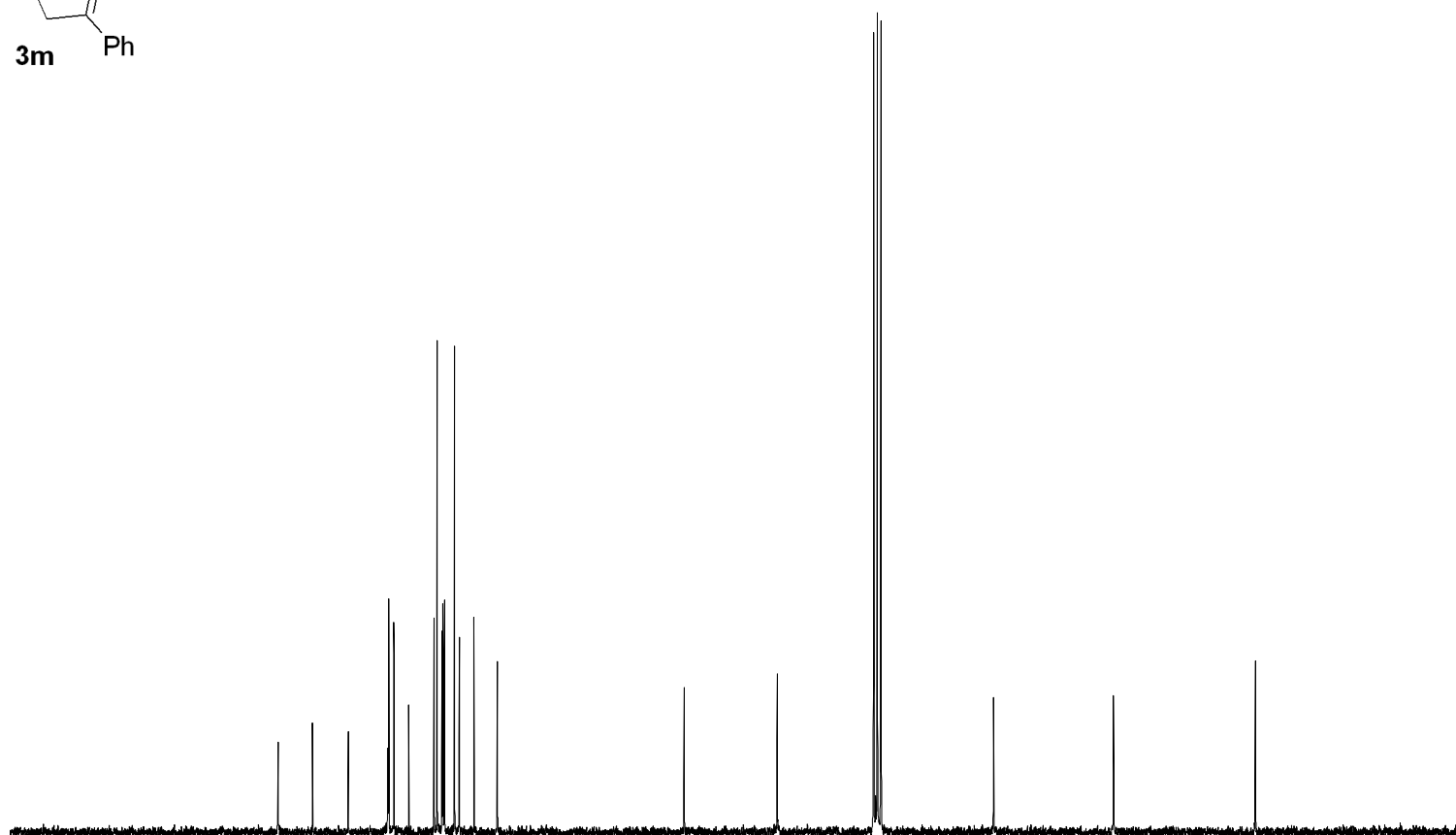
88.84

77.57
77.15
76.73

63.59

49.58

33.03



Current Data Parameters
NAME 2021-4--11Project 1 data
EXPNO 5425
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210926
Time 11.49
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175317 sec
RG 203
DW 27.733 usec
DE 6.50 usec
TE -59.1 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

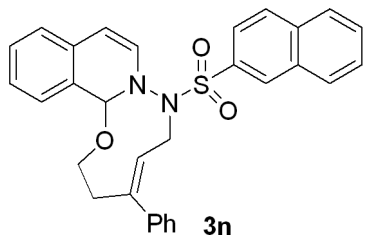
===== CHANNEL f1 =====
SFO1 75.4752949 MHz
NUC1 13C
P1 9.50 usec
PLW1 34.2000076 W

===== CHANNEL f2 =====
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 14.0000000 W
PLW12 0.17284000 W
PLW13 0.14000000 W

F2 - Processing parameters
SI 32768
SF 75.4677422 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 ppm

3sjwei 5504 xh1-3-10 1h cdcl3



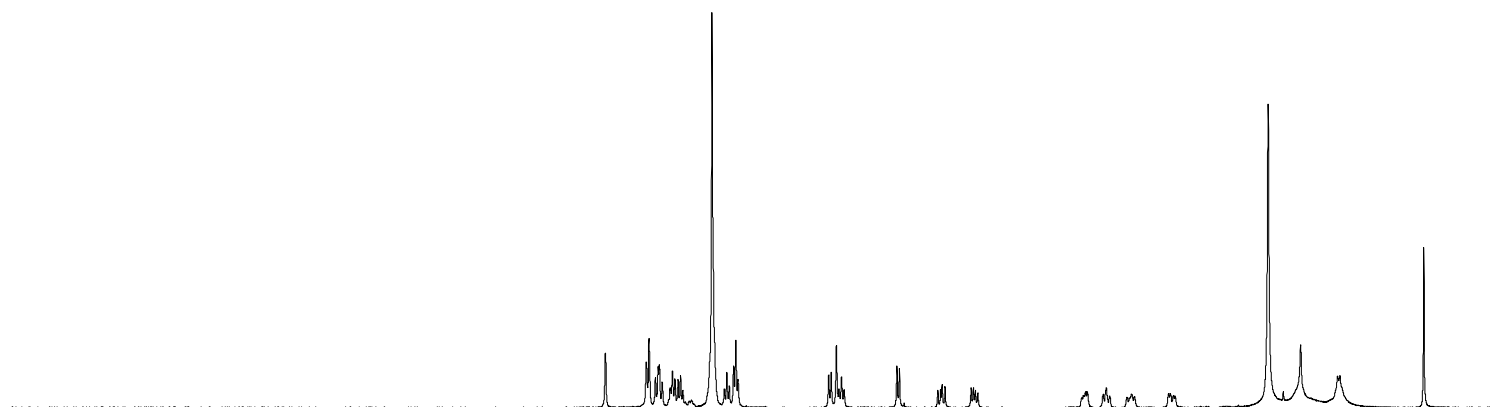
8.347
7.931
7.902
7.837
7.809
7.798
7.769
7.764
7.684
7.663
7.639
7.607
7.581
7.557
7.261
7.132
7.108
7.083
7.039
7.016
6.994
6.069
6.043
5.991
5.965
5.939
5.911
5.374
5.348
4.956
4.927
4.912
4.883
4.617
4.592
4.572
4.548
3.485
3.472
3.465
3.453
3.445
3.433
3.268
3.238
3.206
3.200
3.024
2.978
2.953
2.601
2.586
2.553
2.537

Current Data Parameters
NAME 2021-4--11Project 1 data
EXPNO 5504
PROCNO 1

F2 - Acquisition Parameters
Date_ 20211010
Time 9.20
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 203
DW 83.200 usec
DE 6.50 usec
TE -59.1 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 300.1318534 MHz
NUC1 1H
P1 10.00 usec
PLW1 14.00000000 W

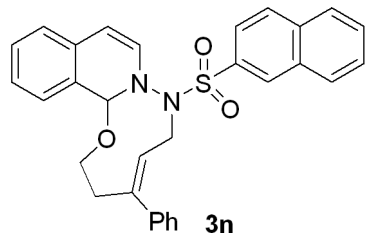
F2 - Processing parameters
SI 65536
SF 300.1300067 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



14 13 12 11 10 9 8 7 6 5 4 3 2 1 ppm

1.02
2.20
2.23
3.19
9.06
1.21
2.18
1.00
0.98
1.10
1.04
1.01
1.00
1.01
1.03
0.99
1.02

3sjwei 5513 xh1-3-10 13c cdcl3



146.85
143.10
135.41
135.17
134.79
133.24
132.27
132.14
131.86
131.78
130.02
129.54
129.24
128.71
128.54
128.49
127.99
127.71
126.49
125.84
124.18
123.09
121.80

99.60

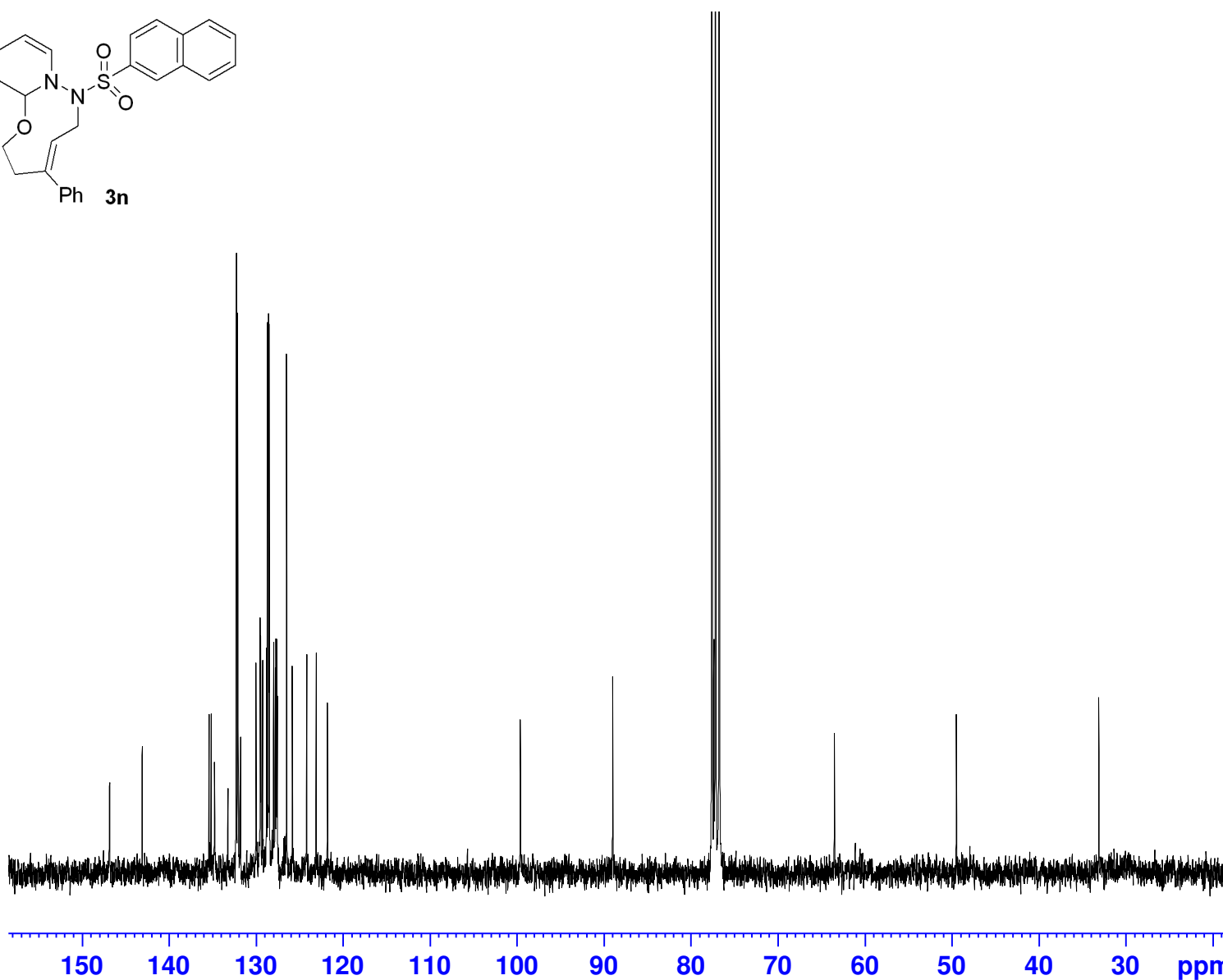
88.99

77.57
77.15
76.73

63.48

49.46

33.07



Current Data Parameters
NAME 2021-4--11Project 1 data
EXPNO 5513
PROCNO 1

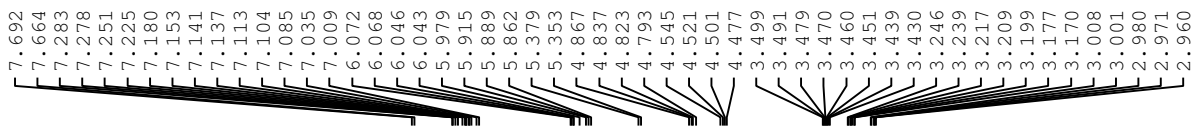
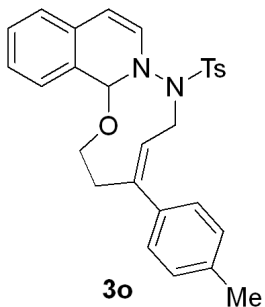
F2 - Acquisition Parameters
Date_ 20211011
Time 12.27
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 1024
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175317 sec
RG 203
DW 27.733 usec
DE 6.50 usec
TE -59.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 75.4752949 MHz
NUC1 13C
P1 9.50 usec
PLW1 34.20000076 W

===== CHANNEL f2 =====
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.17284000 W
PLW13 0.14000000 W

F2 - Processing parameters
SI 32768
SF 75.4677421 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

3sjwei 5033 xh1-2-53 1h cdcl3

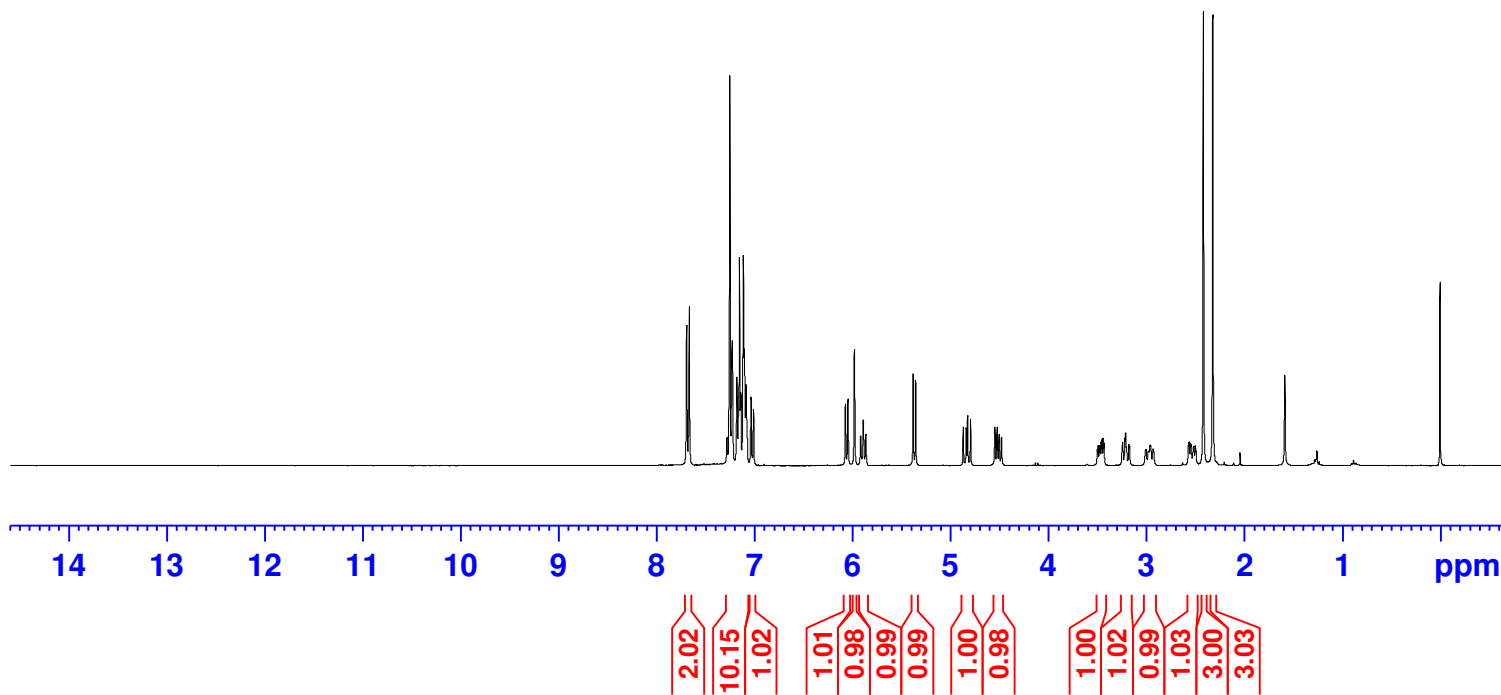


Current Data Parameters
NAME 2021-4--11Project 1 data
EXPNO 5033
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210807
Time 9.09
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 144
DW 83.200 usec
DE 6.50 usec
TE 296.2 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 300.1318534 MHz
NUC1 1H
P1 10.00 usec
PLW1 14.00000000 W

F2 - Processing parameters
SI 65536
SF 300.1300099 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



3sjwei 5045 xh1-2-53 13c cdcl3

146.69
144.37
140.25
137.44
135.75
135.05
131.95
129.90
129.18
128.78
128.27
127.92
127.57
126.38
125.74
124.11
121.13

99.23

88.71

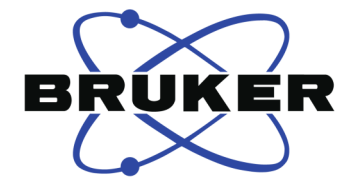
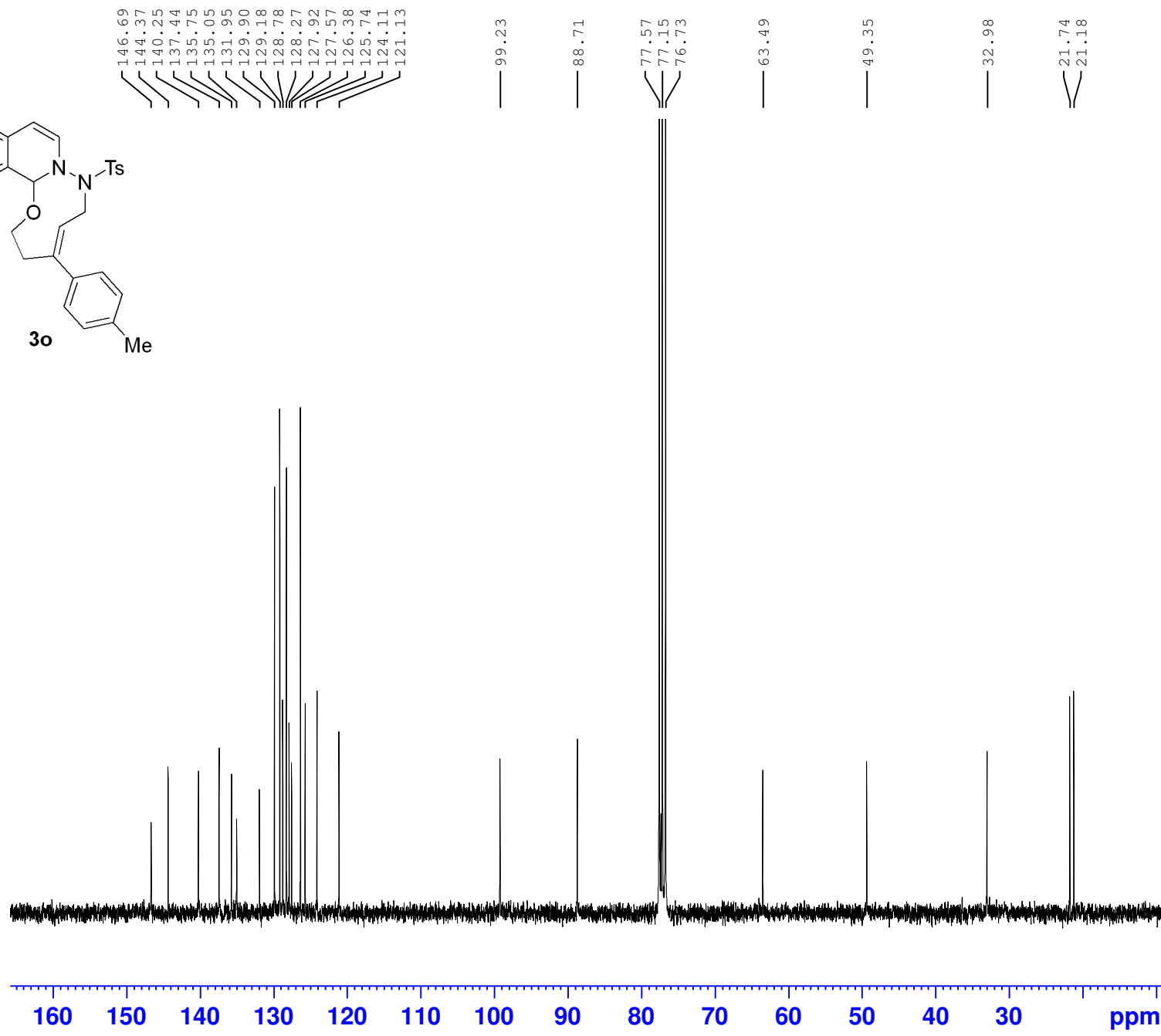
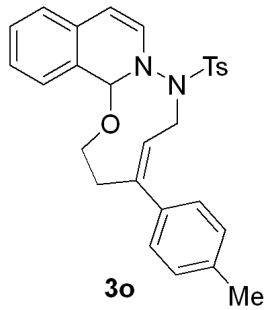
77.57
77.15
76.73

63.49

49.35

32.98

21.74
21.18



Current Data Parameters
NAME 2021-4--11Project 1 data
EXPNO 5045
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210807
Time 11.01
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 800
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175317 sec
RG 203
DW 27.733 usec
DE 6.50 usec
TE 296.2 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 75.4752949 MHz
NUC1 13C
P1 9.50 usec
PLW1 34.2000076 W

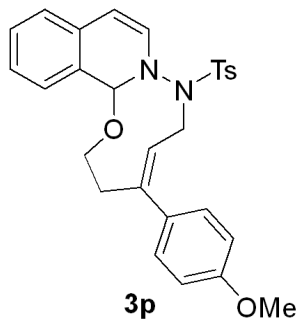
===== CHANNEL f2 =====
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 14.0000000 W
PLW12 0.1728400 W
PLW13 0.1400000 W

F2 - Processing parameters
SI 32768
SF 75.4677415 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

3sjwei 5213 xh1-2-74 1h cdcl3



7.691
7.664
7.287
7.281
7.258
7.238
7.228
7.206
7.199
7.189
7.170
7.166
7.144
7.140
7.121
7.117
7.105
7.101
7.080
7.041
7.015
6.853
6.843
6.836
6.820
6.813
6.068
6.064
6.042
6.038
5.969
5.887
5.861
5.834
5.390
5.364
4.857
4.828
4.813
4.783
4.513
4.489
4.468
4.444
3.789
3.495
3.483
3.474
3.464
3.455
3.444
3.435
3.244
3.237
3.216
3.207
3.176
3.168
2.956
2.948
2.574
2.566
2.553
2.546
2.505
2.419

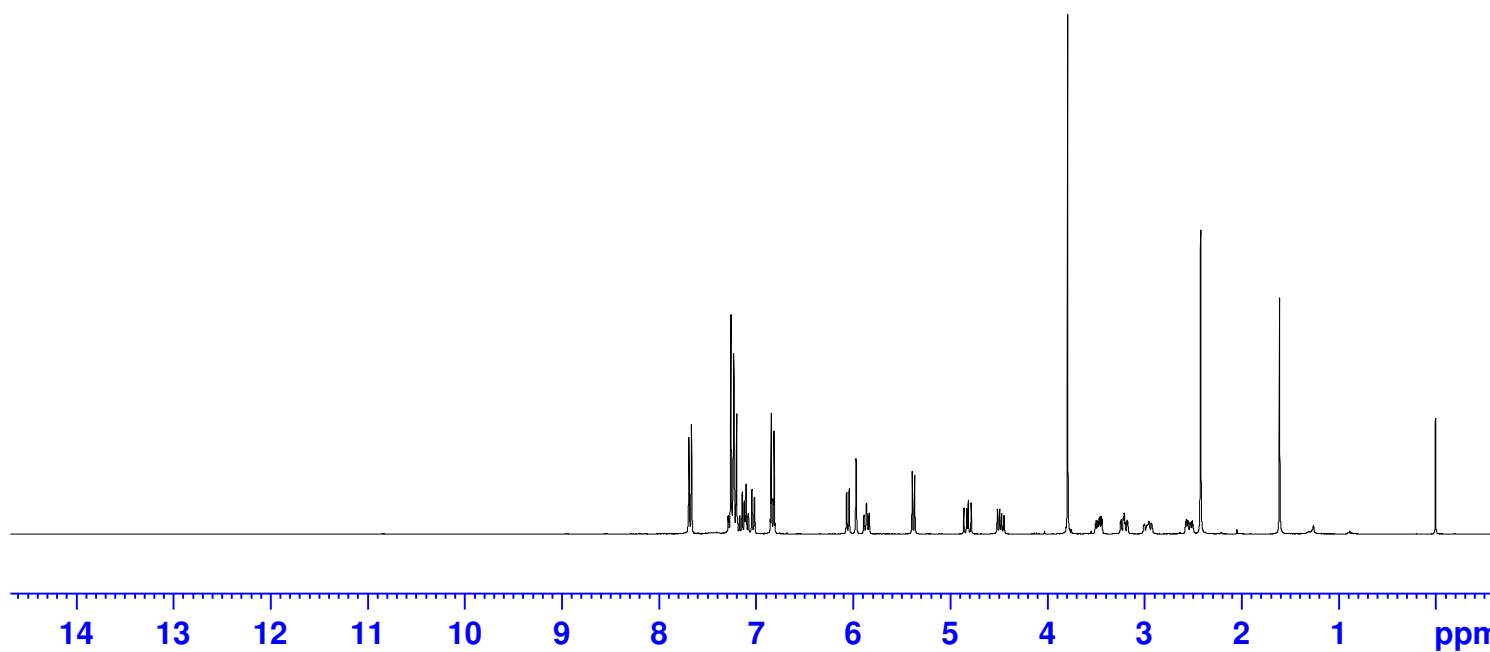


Current Data Parameters
NAME 2021-4--11Project 1 data
EXPNO 5213
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210904
Time 10.00
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 181
DW 83.200 usec
DE 6.50 usec
TE -59.1 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 300.1318534 MHz
NUC1 1H
P1 10.00 usec
PLW1 14.00000000 W

F2 - Processing parameters
SI 65536
SF 300.130078 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



2.04
5.80
2.11
1.03
2.05
1.00
1.00
1.00
1.00
1.01
1.01
3.09
1.03
1.02
1.02
1.03
3.06

3sjwei 5214 xh1-2-74 13c cdcl3



Current Data Parameters
NAME 2021-4--11Project 1 data
EXPNO 5214
PROCNO 1

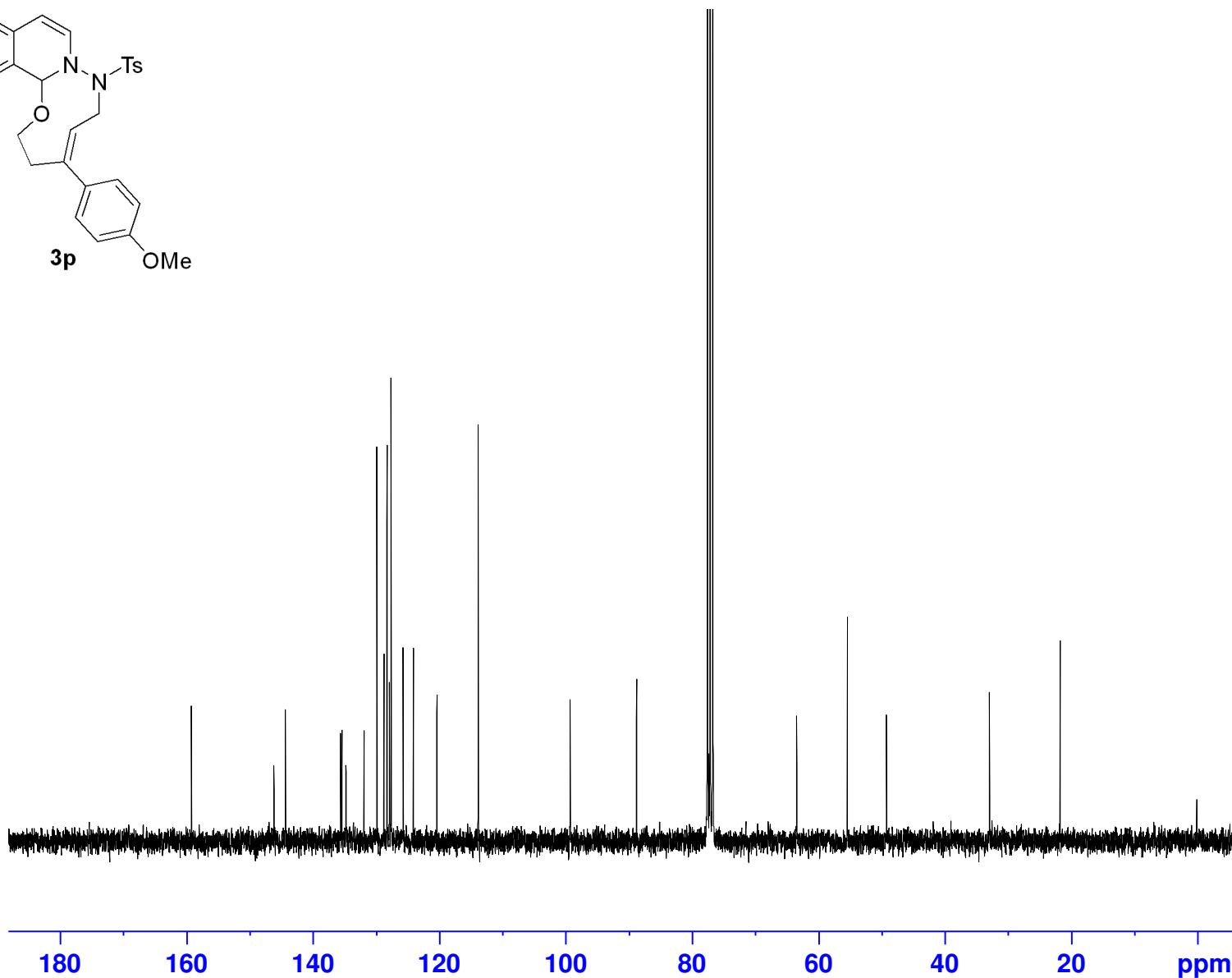
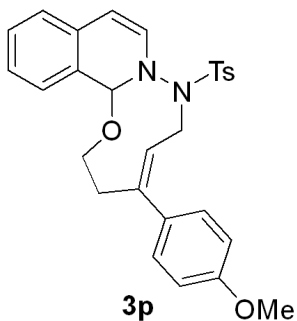
F2 - Acquisition Parameters
Date_ 20210904
Time 10.53
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 800
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175317 sec
RG 203
DW 27.733 usec
DE 6.50 usec
TE -59.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 75.4752949 MHz
NUC1 13C
P1 9.50 usec
PLW1 34.20000076 W

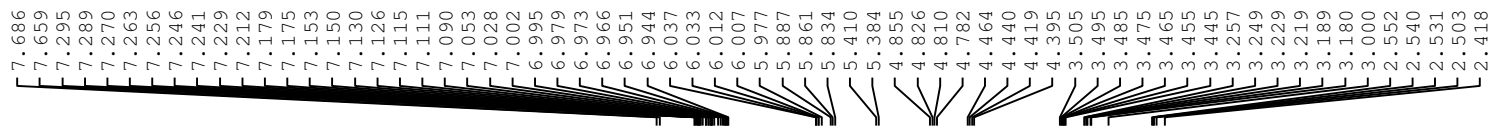
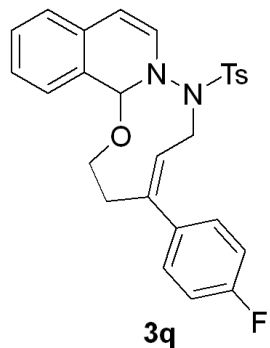
===== CHANNEL f2 =====
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.17284000 W
PLW13 0.14000000 W

F2 - Processing parameters
SI 32768
SF 75.4677406 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

159.27
146.20
144.40
135.65
135.43
134.80
131.93
129.90
128.79
128.31
127.92
127.66
127.61
125.76
124.12
120.40
113.86
99.32
88.80
77.57
77.15
76.73
63.45
55.42
49.24
32.93
21.75



3sjwei 5018 xh1-2-52 1h cdcl3

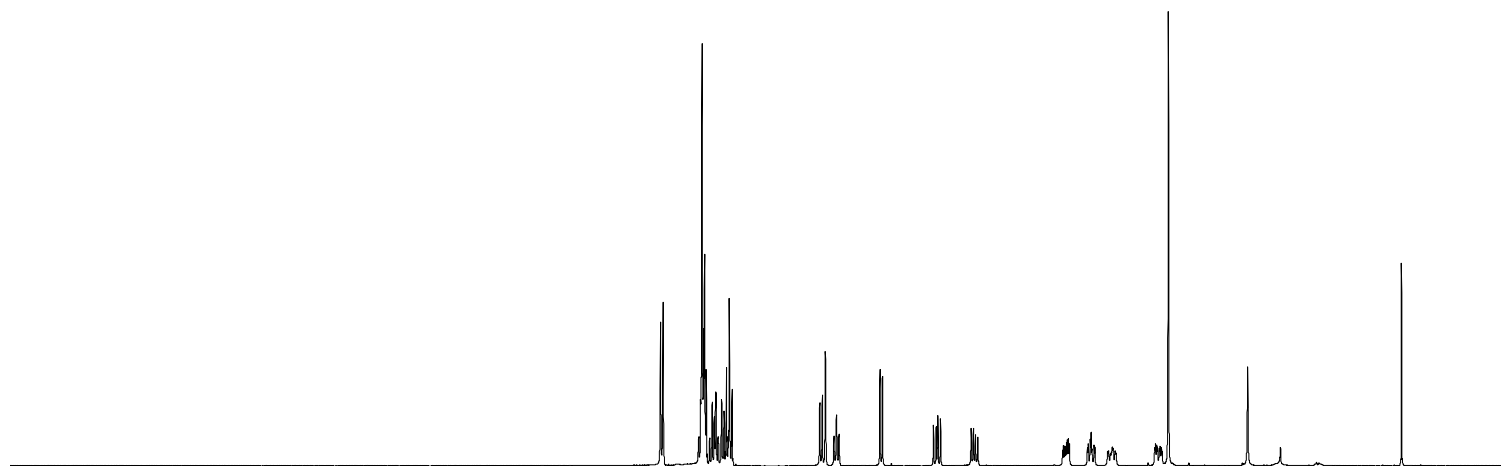


Current Data Parameters
NAME 2021-4--11Project 1 data
EXPNO 5018
PROCNO 1

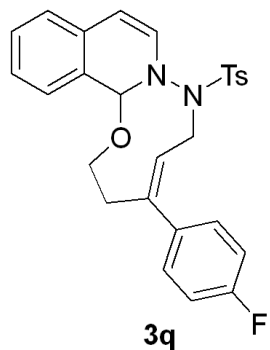
F2 - Acquisition Parameters
Date_ 20210806
Time 9.13
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 144
DW 83.200 usec
DE 6.50 usec
TE 296.1 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 300.1318534 MHz
NUC1 1H
P1 10.00 usec
PLW1 14.00000000 W

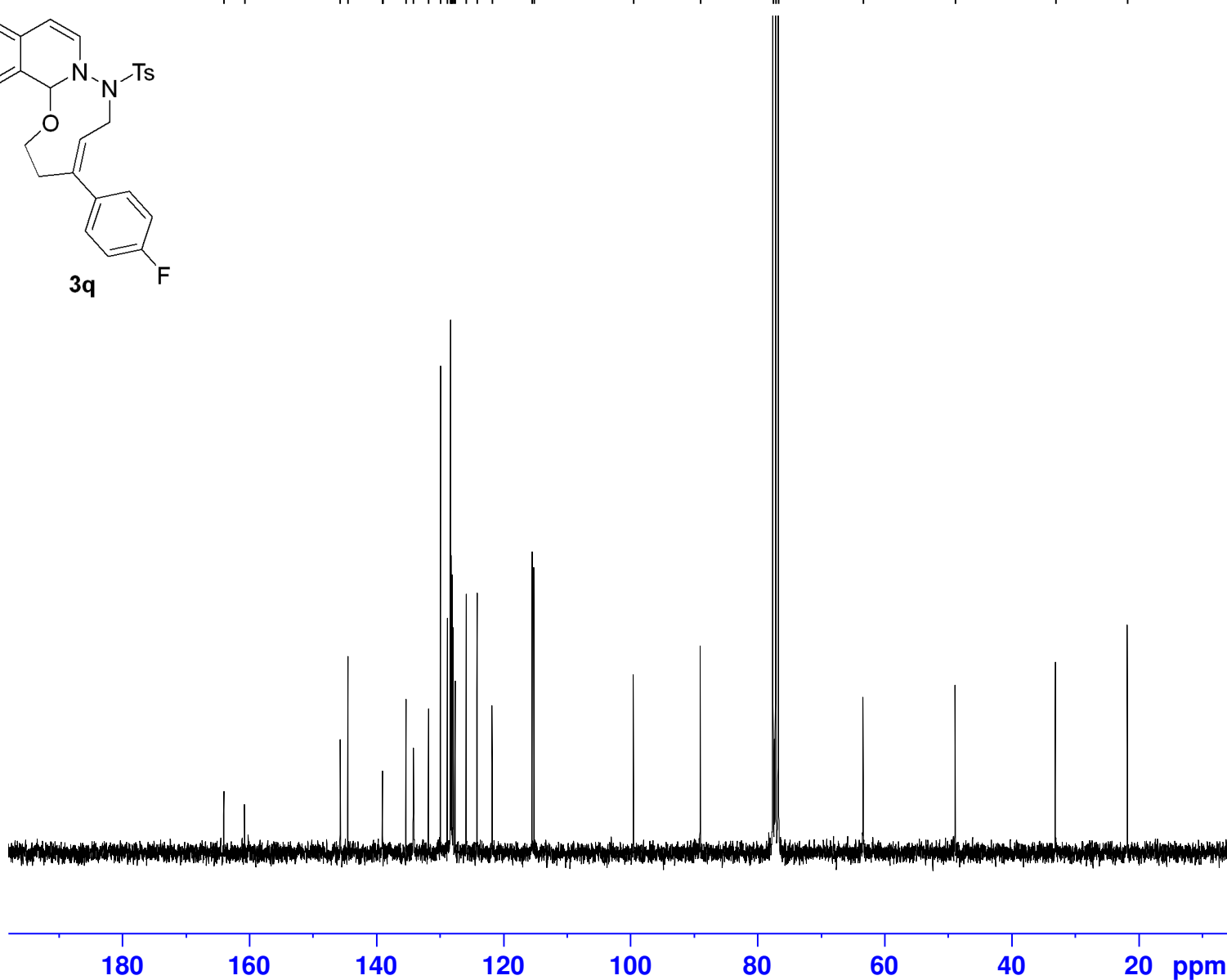
F2 - Processing parameters
SI 65536
SF 300.1300080 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



3sjwei 5029 xh1-2-52 13c cdcl3



164.05
160.78
145.72
144.51
139.06
139.02
135.36
134.18
131.82
129.92
128.84
128.36
128.22
128.11
127.91
127.62
125.86
124.16
121.79
115.48
115.20
99.54
89.02
77.57
77.15
76.72
63.37
48.88
33.09
21.74



Current Data Parameters
NAME 2021-4--11Project 1 data
EXPNO 5029
PROCNO 1

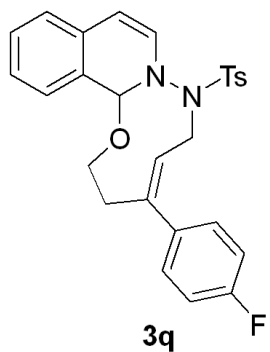
F2 - Acquisition Parameters
Date_ 20210806
Time 12.37
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 800
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175317 sec
RG 203
DW 27.733 usec
DE 6.50 usec
TE 296.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 75.4752949 MHz
NUC1 13C
P1 9.50 usec
PLW1 34.20000076 W

===== CHANNEL f2 =====
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.17284000 W
PLW13 0.14000000 W

F2 - Processing parameters
SI 32768
SF 75.4677411 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

3sjwei 5030 xh1-2-52 19f cdcl3



-114.941



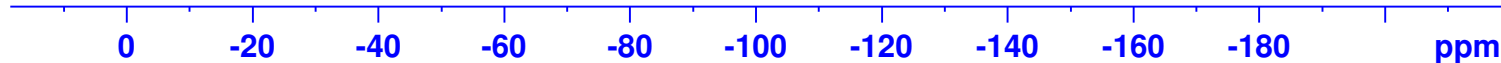
Current Data Parameters
NAME 0806sjw
EXPNO 5030
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210806
Time 12.39
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgfhigqn.2
TD 131072
SOLVENT CDC13
NS 16
DS 4
SWH 66964.289 Hz
FIDRES 0.510897 Hz
AQ 0.9786710 sec
RG 203
DW 7.467 usec
DE 6.50 usec
TE 296.1 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 282.3761148 MHz
NUC1 19F
P1 14.50 usec
PLW1 10.39999962 W

==== CHANNEL f2 =====
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.17284000 W

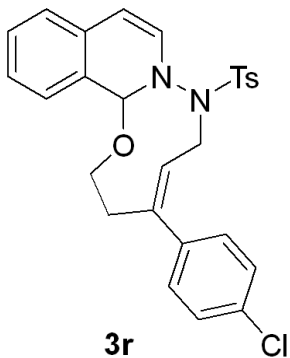
F2 - Processing parameters
SI 65536
SF 282.4043552 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



3sjwei 4975 xh1-2-44 1h cdcl3



7.685
7.657
7.295
7.290
7.272
7.266
7.257
7.245
7.229
7.217
7.210
7.203
7.188
7.181
7.176
7.154
7.151
7.131
7.127
7.113
7.110
7.088
7.051
7.025
6.025
6.021
5.999
5.995
5.977
5.918
5.892
5.866
5.402
5.376
4.856
4.827
4.811
4.782
4.470
4.446
4.425
4.401
3.504
3.493
3.483
3.474
3.464
3.453
3.444
3.249
3.241
3.221
3.212
3.202
3.181
3.173
2.995
2.986
2.550
2.542
2.530
2.522
2.502
2.493
2.481
2.418

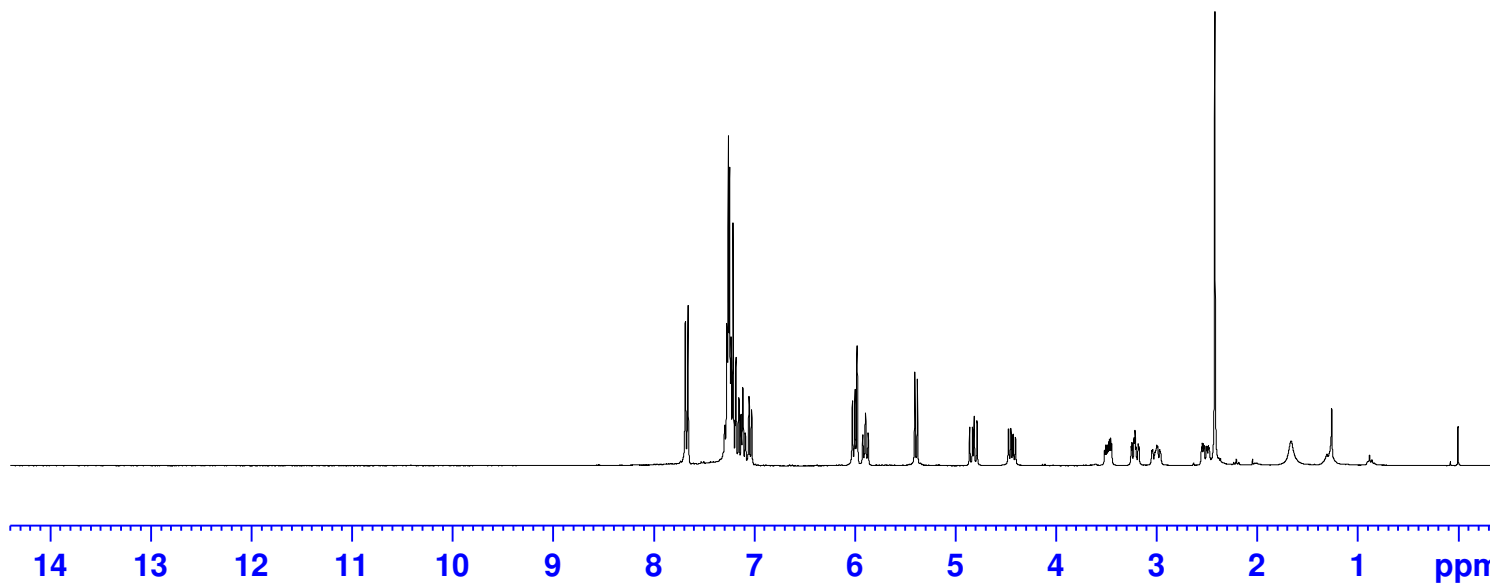


Current Data Parameters
NAME 2021-4--11Project 1 data
EXPNO 4975
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210804
Time 9.09
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 144
DW 83.200 usec
DE 6.50 usec
TE 296.1 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 300.1318534 MHz
NUC1 1H
P1 10.00 usec
PLW1 14.00000000 W

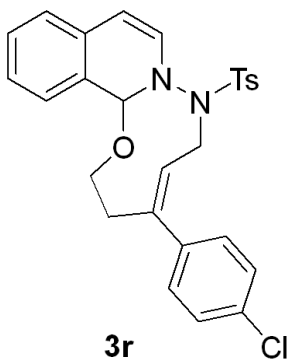
F2 - Processing parameters
SI 65536
SF 300.1300082 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



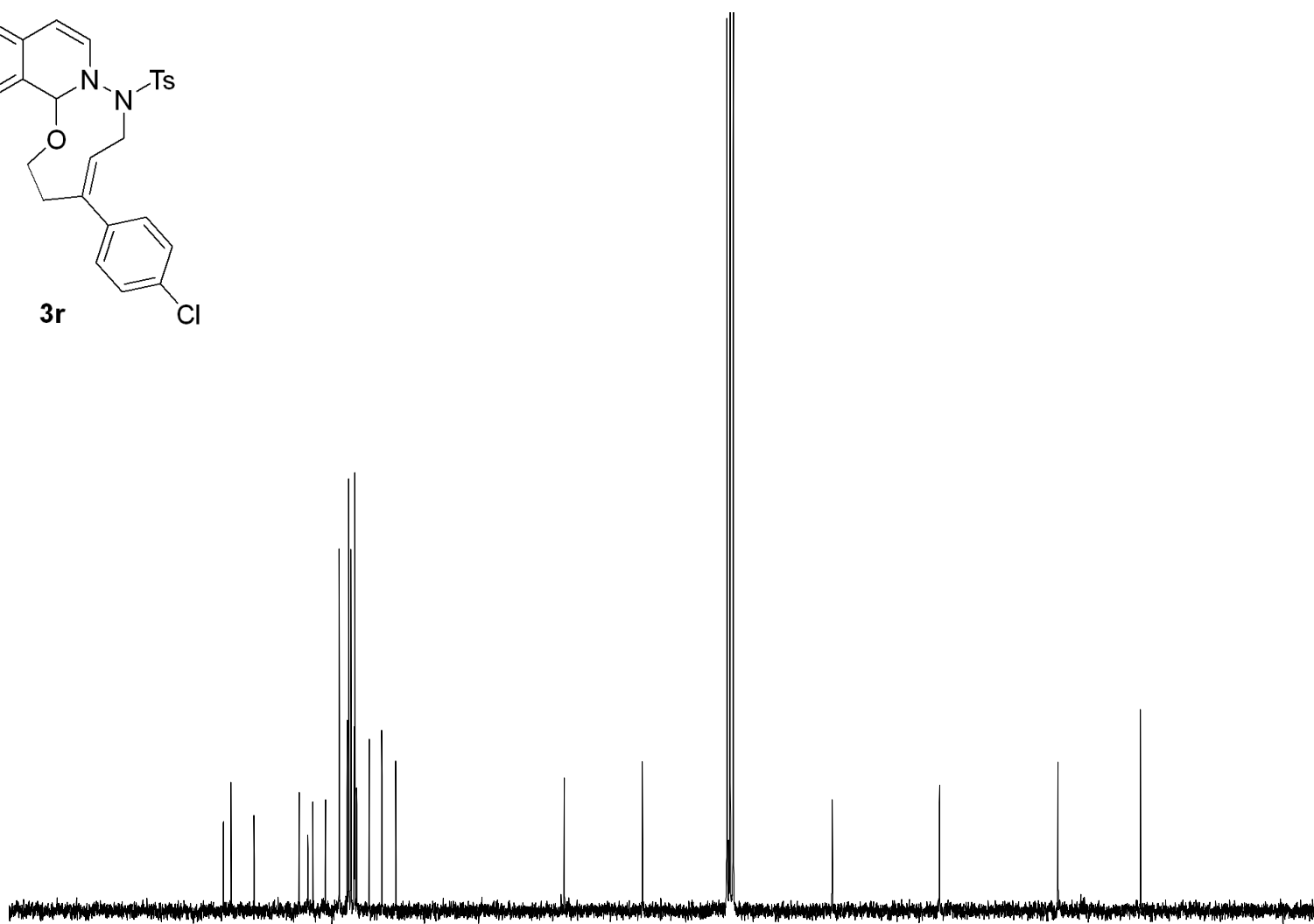
2.08
7.49
2.83
1.03
2.00
1.00
0.99
0.99
0.98
1.00
1.04
1.00
1.04
3.17

3sjwei 4991 xh1-2-44 13c cdcl3

145.58
144.54
141.42
135.33
134.16
133.50
131.80
129.93
128.86
128.64
128.34
127.92
127.83
127.57
125.88
124.17
122.30
99.55
89.00
77.57
77.15
76.72
63.35
48.88
32.89
21.74



3r



170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm



Current Data Parameters
NAME 2021-4--11Project 1 data
EXPNO 4991
PROCNO 1

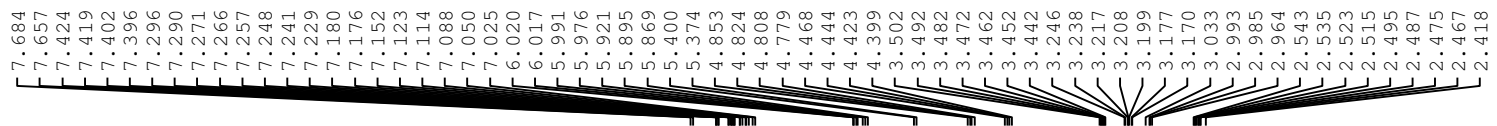
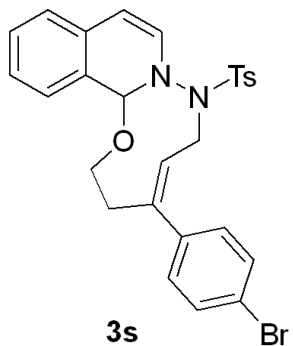
F2 - Acquisition Parameters
Date_ 20210804
Time 12.44
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 700
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175317 sec
RG 203
DW 27.733 usec
DE 6.50 usec
TE 296.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 75.4752949 MHz
NUC1 13C
P1 9.50 usec
PLW1 34.20000076 W

===== CHANNEL f2 =====
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.17284000 W
PLW13 0.14000000 W

F2 - Processing parameters
SI 32768
SF 75.4677416 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

3sjwei 4954 xh1-2-48 1h cdcl3

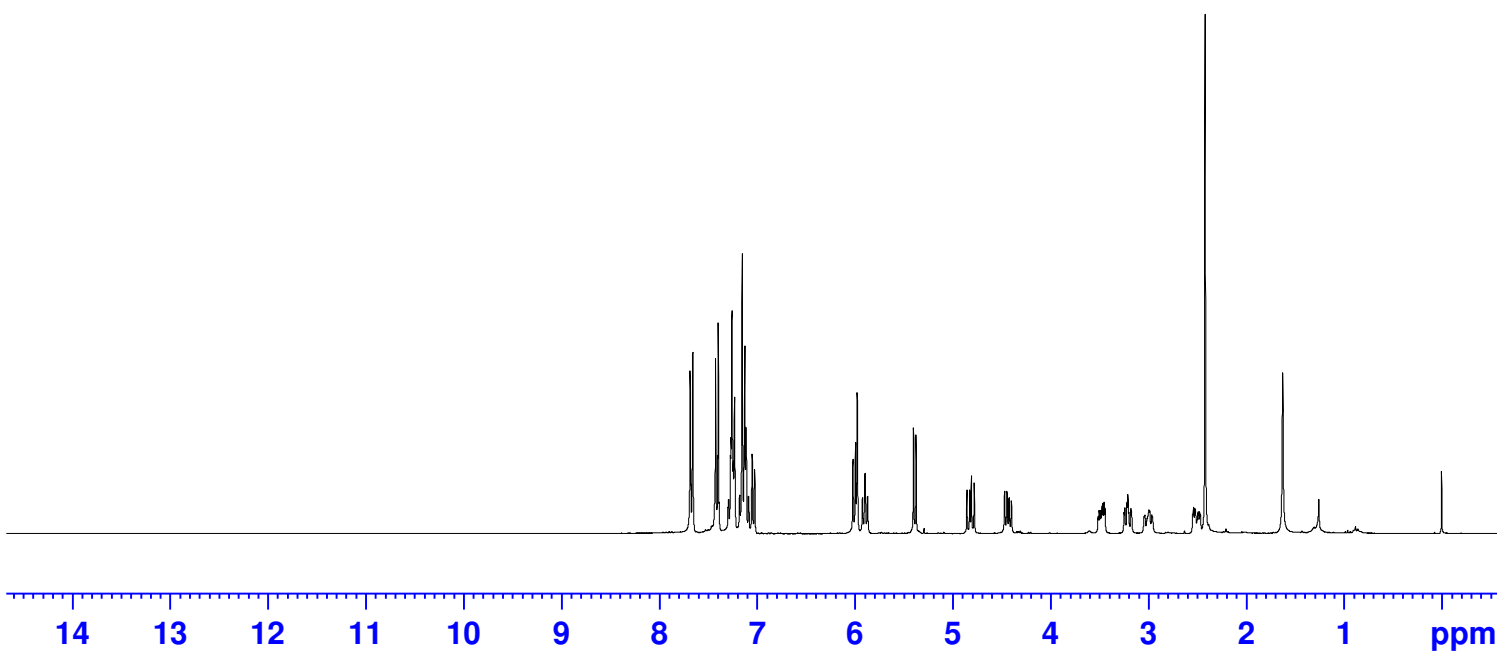


Current Data Parameters
NAME 2021-4--11Project 1 data
EXPNO 4954
PROCNO 1

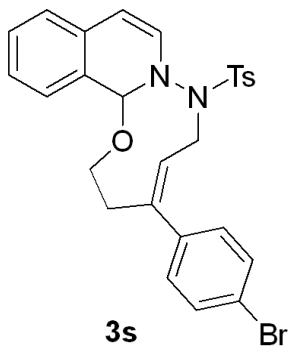
F2 - Acquisition Parameters
Date_ 20210803
Time 9.27
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 144
DW 83.200 usec
DE 6.50 usec
TE 296.2 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 300.1318534 MHz
NUC1 1H
P1 10.00 usec
PLW1 14.00000000 W

F2 - Processing parameters
SI 65536
SF 300.1300079 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



3sjwei 4970 xh1-2-48 13c cdcl3



145.63
144.54
141.92
135.33
134.18
131.80
131.60
129.93
128.86
128.34
128.17
127.92
127.56
125.89
124.17
122.36
121.65

99.55

88.99

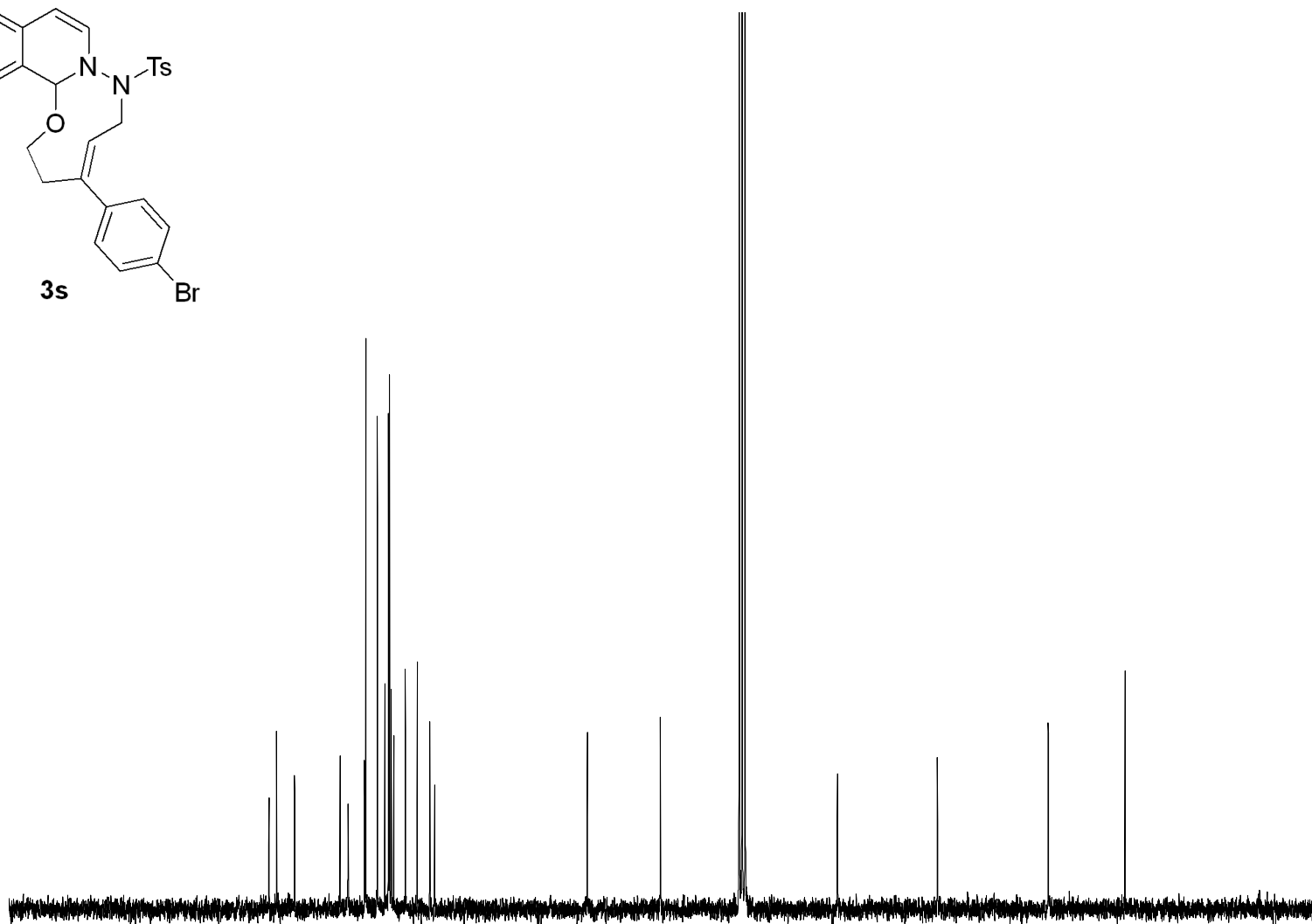
77.57
77.15
76.73

63.36

48.89

32.85

21.74



Current Data Parameters
NAME 2021-4--11Project 1 data
EXPNO 4970
PROCNO 1

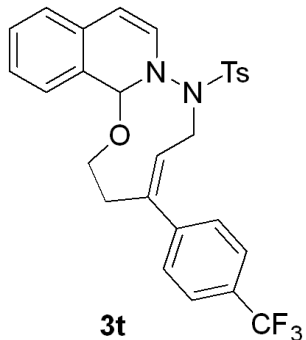
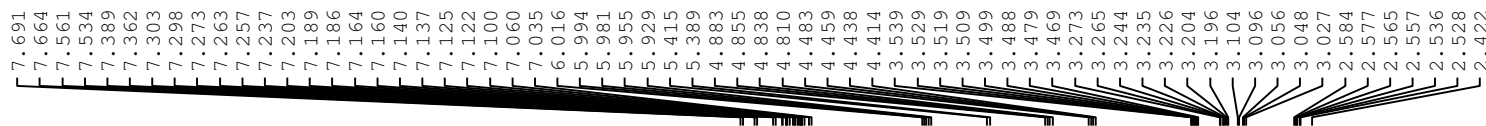
F2 - Acquisition Parameters
Date_ 20210803
Time 11.35
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 700
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175317 sec
RG 203
DW 27.733 usec
DE 6.50 usec
TE 296.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 75.4752949 MHz
NUC1 13C
P1 9.50 usec
PLW1 34.20000076 W

===== CHANNEL f2 =====
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.17284000 W
PLW13 0.14000000 W

F2 - Processing parameters
SI 32768
SF 75.4677415 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

3sjwei 5481 xh1-3-20 1h cdcl3

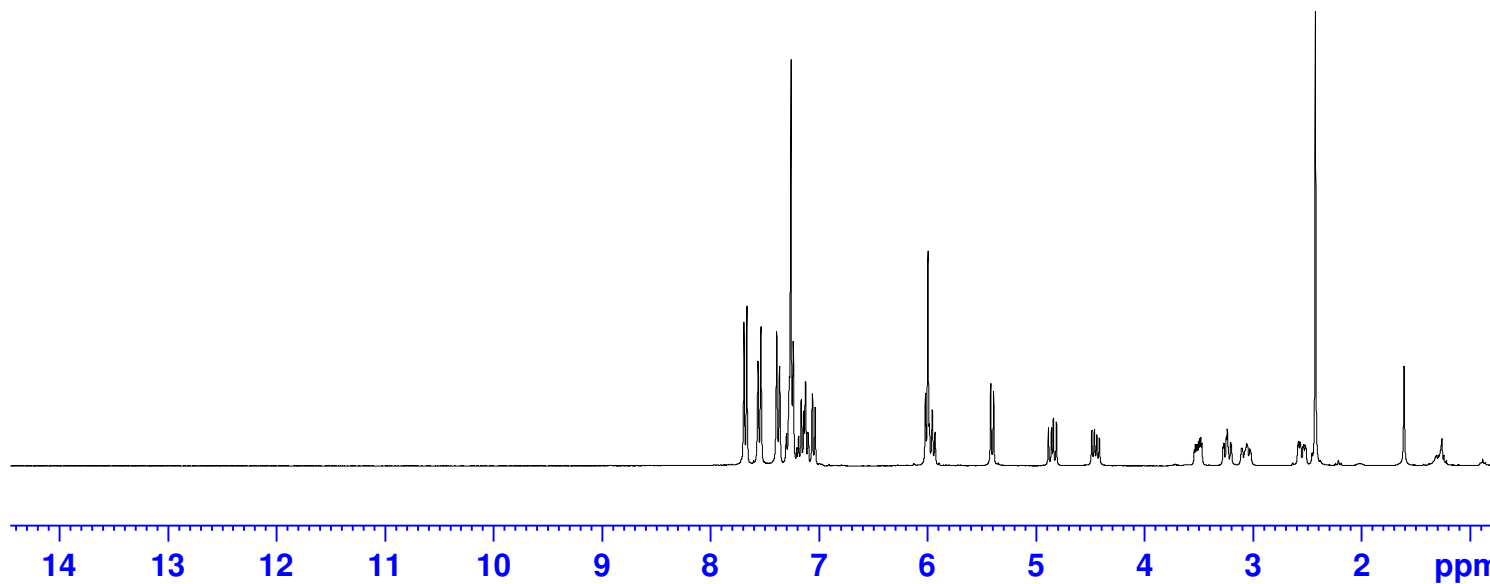


Current Data Parameters
NAME 2021-4--11Project 1 data
EXPNO 5481
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210930
Time 9.16
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 144
DW 83.200 usec
DE 6.50 usec
TE -59.1 K
D1 1.00000000 sec
TD0 1

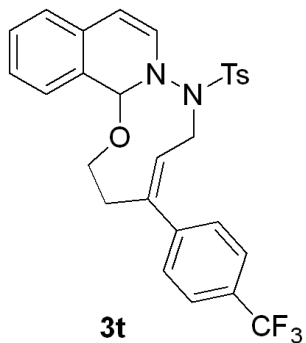
==== CHANNEL f1 =====
SFO1 300.1318534 MHz
NUC1 1H
P1 10.00 usec
PLW1 14.00000000 W

F2 - Processing parameters
SI 65536
SF 300.1300082 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



2.02
2.04
2.04
4.35
2.22
1.00
1.92
1.02
1.00
1.00
0.99
0.99
1.01
0.99
1.01
3.02

3sjwei 5497 xh1-3-20 13c cdcl3



146.62
145.56
144.62
135.22
133.97
131.76
130.29
129.96
129.86
129.43
128.99
128.91
128.37
127.94
127.57
126.84
125.95
125.57
125.52
125.47
125.42
124.21
123.60
99.67

89.09

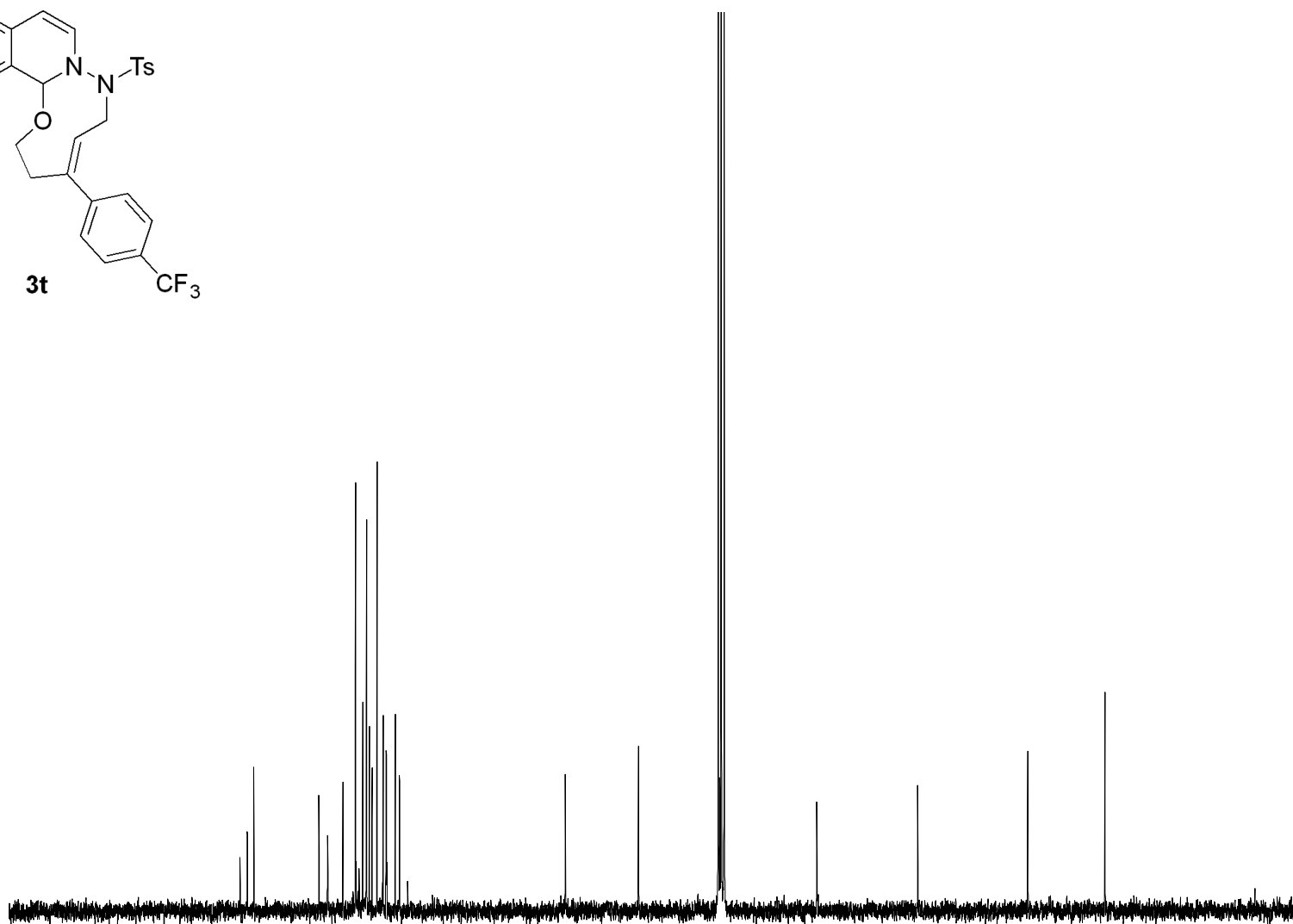
77.57
77.15
76.72

63.35

48.79

32.90

21.75



Current Data Parameters
NAME 2021-4--11Project 1 data
EXPNO 5497
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210930
Time 12.46
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 600
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175317 sec
RG 203
DW 27.733 usec
DE 6.50 usec
TE -59.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 75.4752949 MHz
NUC1 13C
P1 9.50 usec
PLW1 34.20000076 W

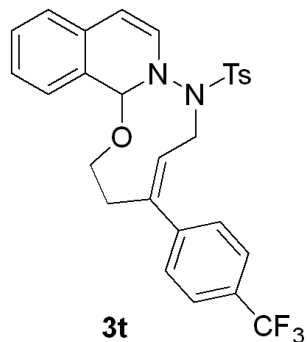
===== CHANNEL f2 =====
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.17284000 W
PLW13 0.14000000 W

F2 - Processing parameters
SI 32768
SF 75.4677412 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

3sjwei 5498 xh1-3-20 19fcdcl3

— -62.514



3t



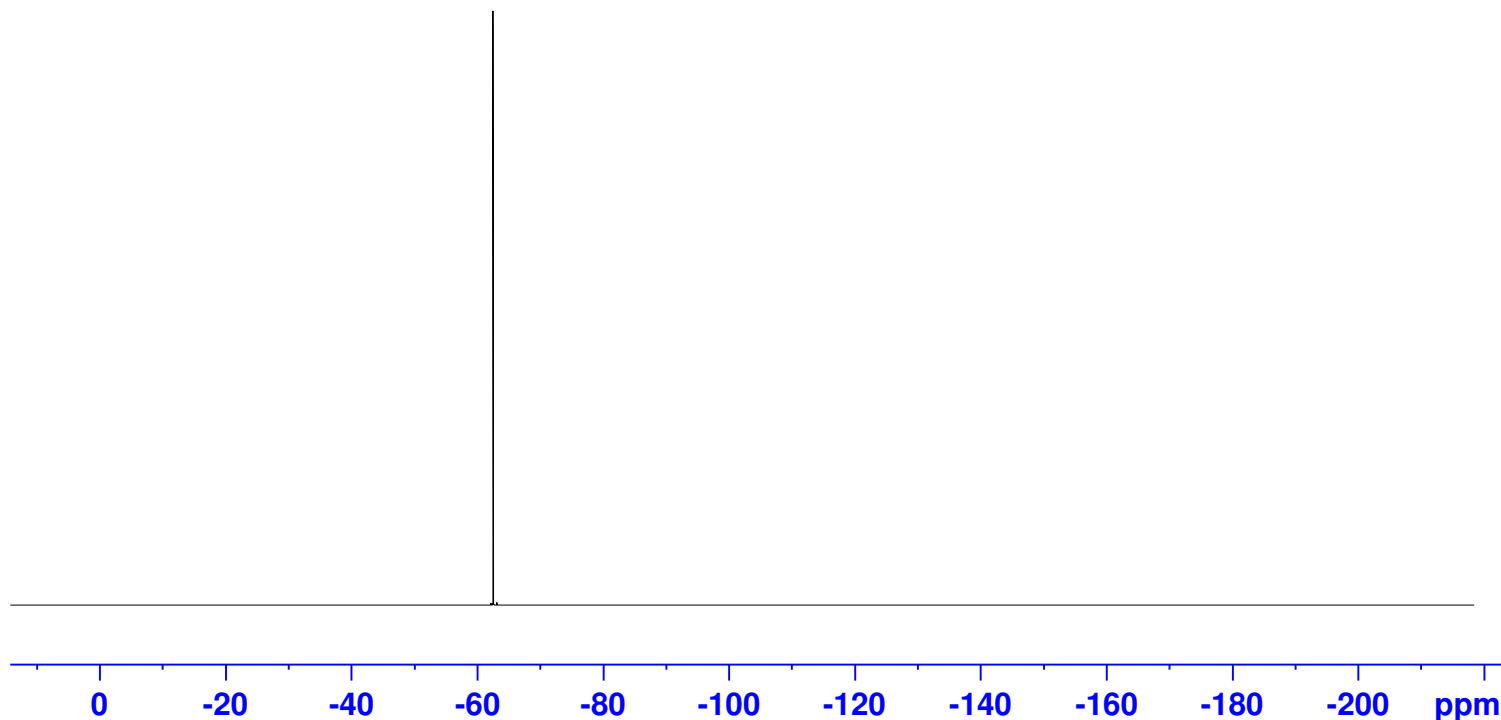
Current Data Parameters
NAME 0930sjw
EXPNO 5498
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210930
Time 12.48
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgfhigqn.2
TD 131072
SOLVENT CDCl3
NS 16
DS 4
SWH 66964.289 Hz
FIDRES 0.510897 Hz
AQ 0.9786710 sec
RG 203
DW 7.467 usec
DE 6.50 usec
TE -59.1 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 282.3761148 MHz
NUC1 19F
P1 14.50 usec
PLW1 10.39999962 W

==== CHANNEL f2 =====
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.17284000 W

F2 - Processing parameters
SI 65536
SF 282.4043552 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



3sjwei 5502 xh1-3-4 1h cdcl3

7.691
7.663
7.233
7.213
7.204
7.180
7.156
7.132
7.114
7.094
7.072
7.046
7.021
6.993
6.986
6.957
6.116
6.091
5.999
5.872
5.845
5.818
5.443
5.417
4.889
4.860
4.845
4.815
4.564
4.540
4.519
4.495
3.476
3.468
3.457
3.448
3.436
3.428
3.417
3.408
3.310
3.279
3.246
3.004
2.972
2.959
2.931
2.463
2.425

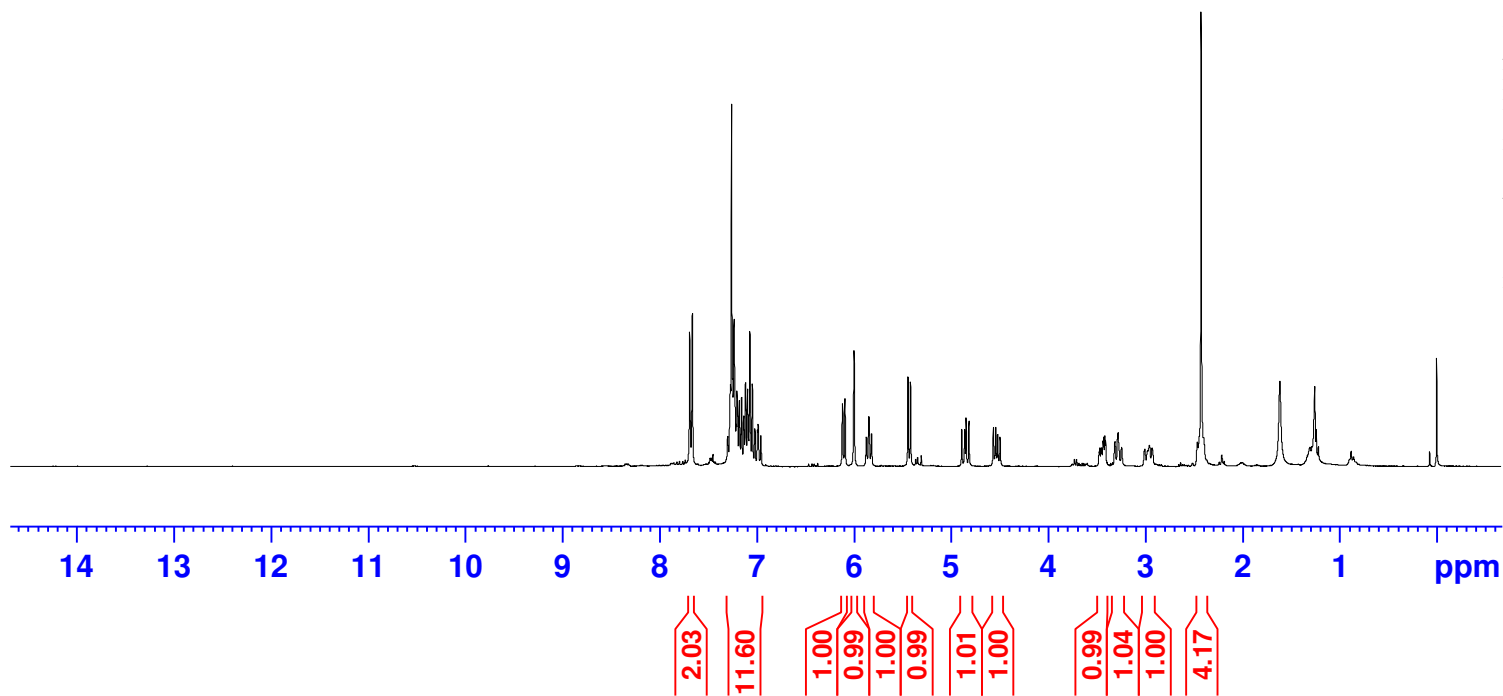
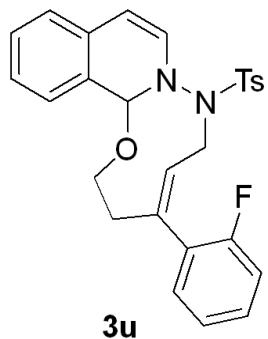


Current Data Parameters
NAME 2021-4--11Project 1 data
EXPNO 5502
PROCNO 1

F2 - Acquisition Parameters
Date_ 20211010
Time 9.09
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 181
DW 83.200 usec
DE 6.50 usec
TE -59.1 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 300.1318534 MHz
NUC1 1H
P1 10.00 usec
PLW1 14.00000000 W

F2 - Processing parameters
SI 65536
SF 300.1300073 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



3sjwei 5511 xh1-3-4 13c cdcl3



Current Data Parameters
NAME 2021-4--11Project 1 data
EXPNO 5511
PROCNO 1

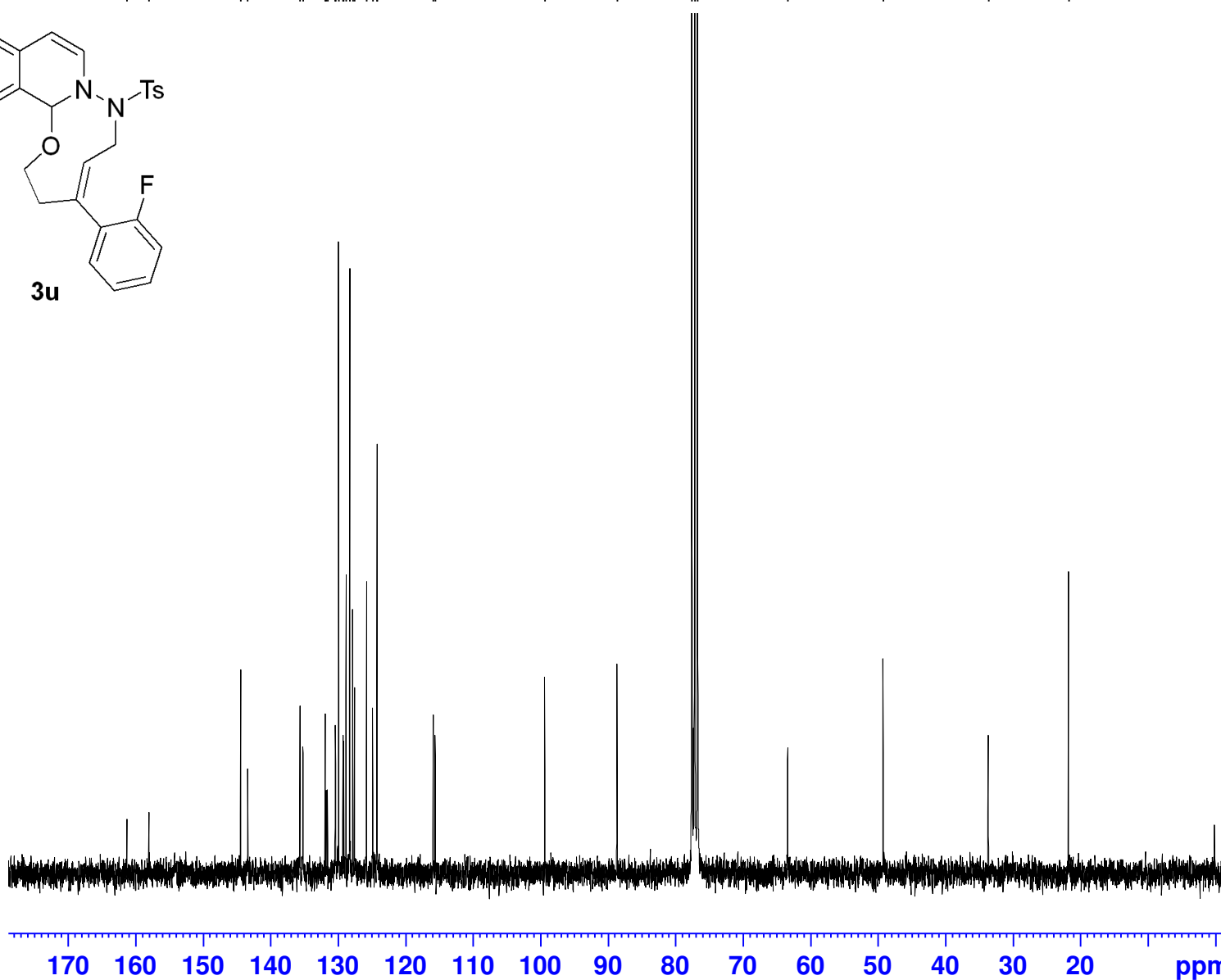
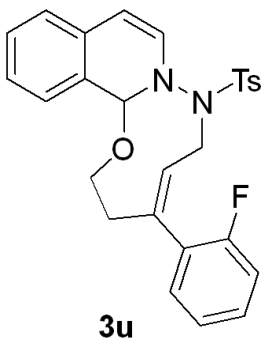
F2 - Acquisition Parameters
Date_ 20211009
Time 13.26
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1500
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175317 sec
RG 203
DW 27.733 usec
DE 6.50 usec
TE -59.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO 1

===== CHANNEL f1 =====
SFO1 75.4752949 MHz
NUC1 13C
P1 9.50 usec
PLW1 34.20000076 W

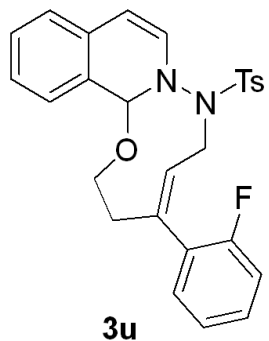
===== CHANNEL f2 =====
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.17284000 W
PLW13 0.14000000 W

F2 - Processing parameters
SI 32768
SF 75.4677402 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

161.33
158.06
144.46
143.41
135.66
135.22
131.92
131.76
131.57
130.45
130.40
129.94
129.30
129.19
128.84
128.29
127.85
127.57
125.80
124.89
124.27
124.22
115.92
115.62
99.38
88.67
77.57
77.15
76.73
63.37
49.23
33.65
21.76



3sjwei 5509 xhl-3-4 19f cdcl3



-114.359



Current Data Parameters
NAME 211009sjw
EXPNO 5509
PROCNO 1

F2 - Acquisition Parameters
Date_ 20211009
Time 9.22
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgfhigqn.2
TD 131072
SOLVENT CDCl3
NS 16
DS 4
SWH 66964.289 Hz
FIDRES 0.510897 Hz
AQ 0.9786710 sec
RG 203
DW 7.467 usec
DE 6.50 usec
TE -59.1 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
TD0 1

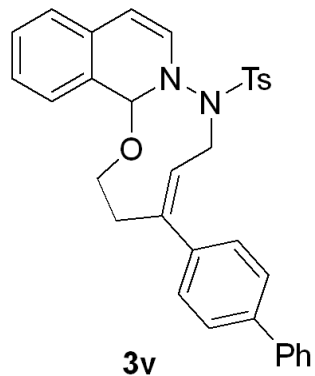
==== CHANNEL f1 =====
SFO1 282.3761148 MHz
NUC1 19F
P1 14.50 usec
PLW1 10.39999962 W

==== CHANNEL f2 =====
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.17284000 W

F2 - Processing parameters
SI 65536
SF 282.4043552 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



3sjwei 4976 xh1-2-46 1h cdcl3



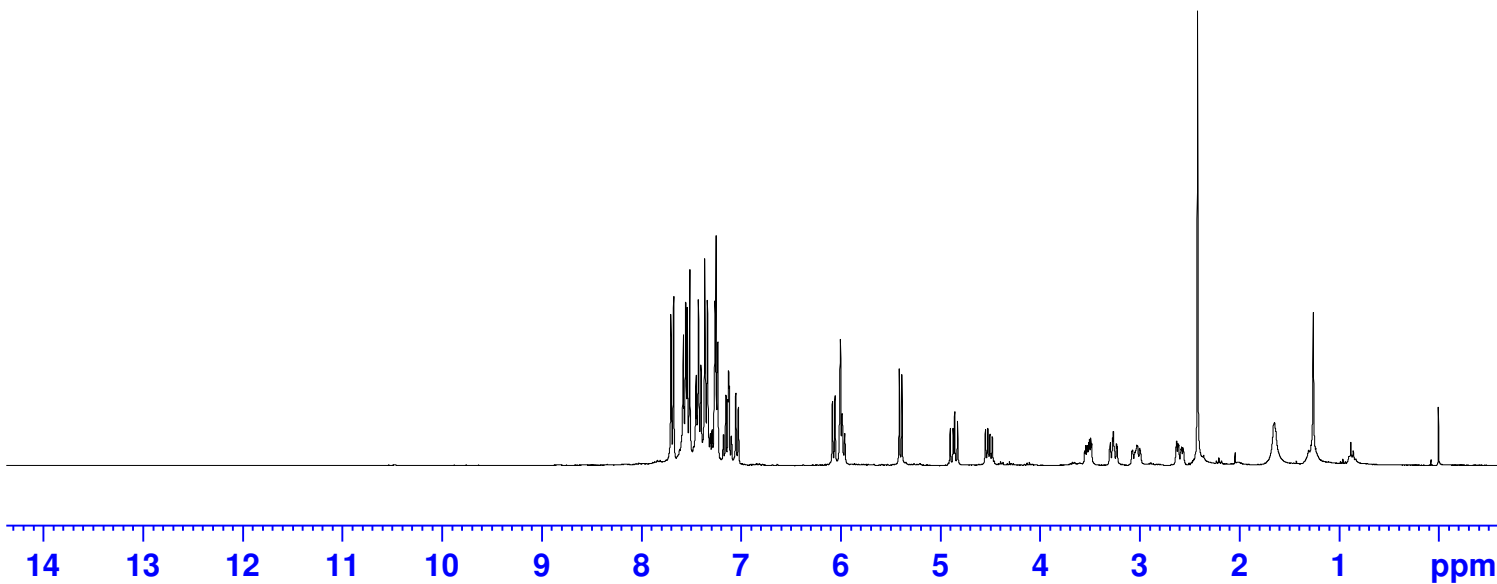
7.703
7.675
7.583
7.578
7.554
7.541
7.519
7.513
7.450
7.444
7.426
7.421
7.401
7.364
7.357
7.336
7.260
7.250
7.245
7.238
7.232
7.179
7.175
7.153
7.149
7.130
7.125
7.118
7.097
7.051
7.026
6.083
6.080
6.058
6.054
6.003
5.985
5.957
5.410
5.385
4.899
4.870
4.855
4.826
4.546
4.522
4.501
4.477
3.541
3.529
3.520
3.510
3.501
3.489
3.481
3.292
3.271
3.262
3.253
3.231
3.026
3.020
2.626
2.613
2.606
2.417

Current Data Parameters
NAME 2021-4--11Project 1 data
EXPNO 4976
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210804
Time 9.13
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 144
DW 83.200 usec
DE 6.50 usec
TE 296.1 K
D1 1.00000000 sec
TD0 1

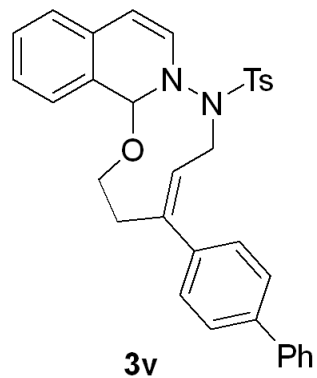
==== CHANNEL f1 =====
SFO1 300.1318534 MHz
NUC1 1H
P1 10.00 usec
PLW1 14.00000000 W

F2 - Processing parameters
SI 65536
SF 300.1300104 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

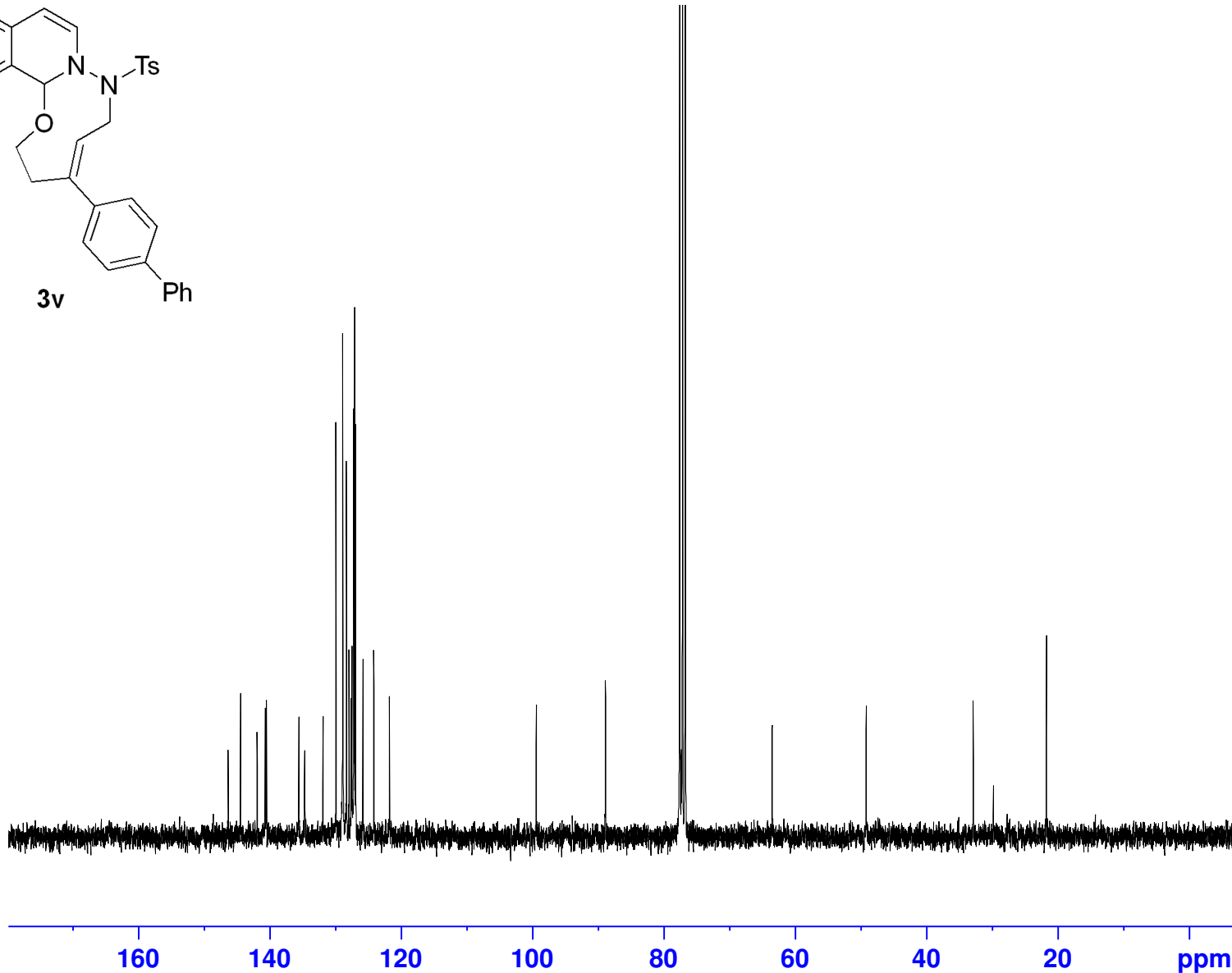


2.05
4.95
3.07
3.29
1.48
1.11
2.15
0.99
0.98
1.95
1.02
1.01
1.02
1.00
1.03
0.96
0.96
3.18

3sjwei 5003 xh1-2-46 13c cdcl3



146.34
144.46
141.92
140.68
140.50
135.57
134.69
131.91
129.92
128.91
128.82
128.32
127.94
127.60
127.48
127.22
127.10
126.91
125.81
124.16
121.78
99.42
88.88
77.57
77.15
76.73
63.51
49.19
32.88
21.74



Current Data Parameters
NAME 2021-4--11Project 1 data
EXPNO 5003
PROCNO 1

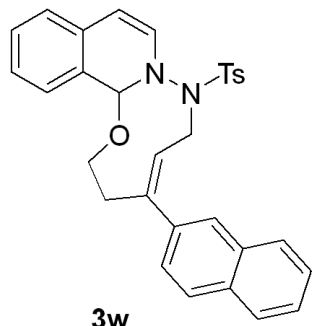
F2 - Acquisition Parameters
Date_ 20210805
Time 10.51
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 800
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175317 sec
RG 203
DW 27.733 usec
DE 6.50 usec
TE 296.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 75.4752949 MHz
NUC1 13C
P1 9.50 usec
PLW1 34.20000076 W

===== CHANNEL f2 =====
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.17284000 W
PLW13 0.14000000 W

F2 - Processing parameters
SI 32768
SF 75.4677415 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

3sjwei 5510 xhl-3-3 13c cdcl3



146.62
144.47
140.33
135.61
134.72
133.37
132.84
131.94
129.95
128.84
128.34
128.23
128.16
127.96
127.66
127.61
126.40
126.13
125.83
125.23
124.79
124.18
122.42
99.46

88.85

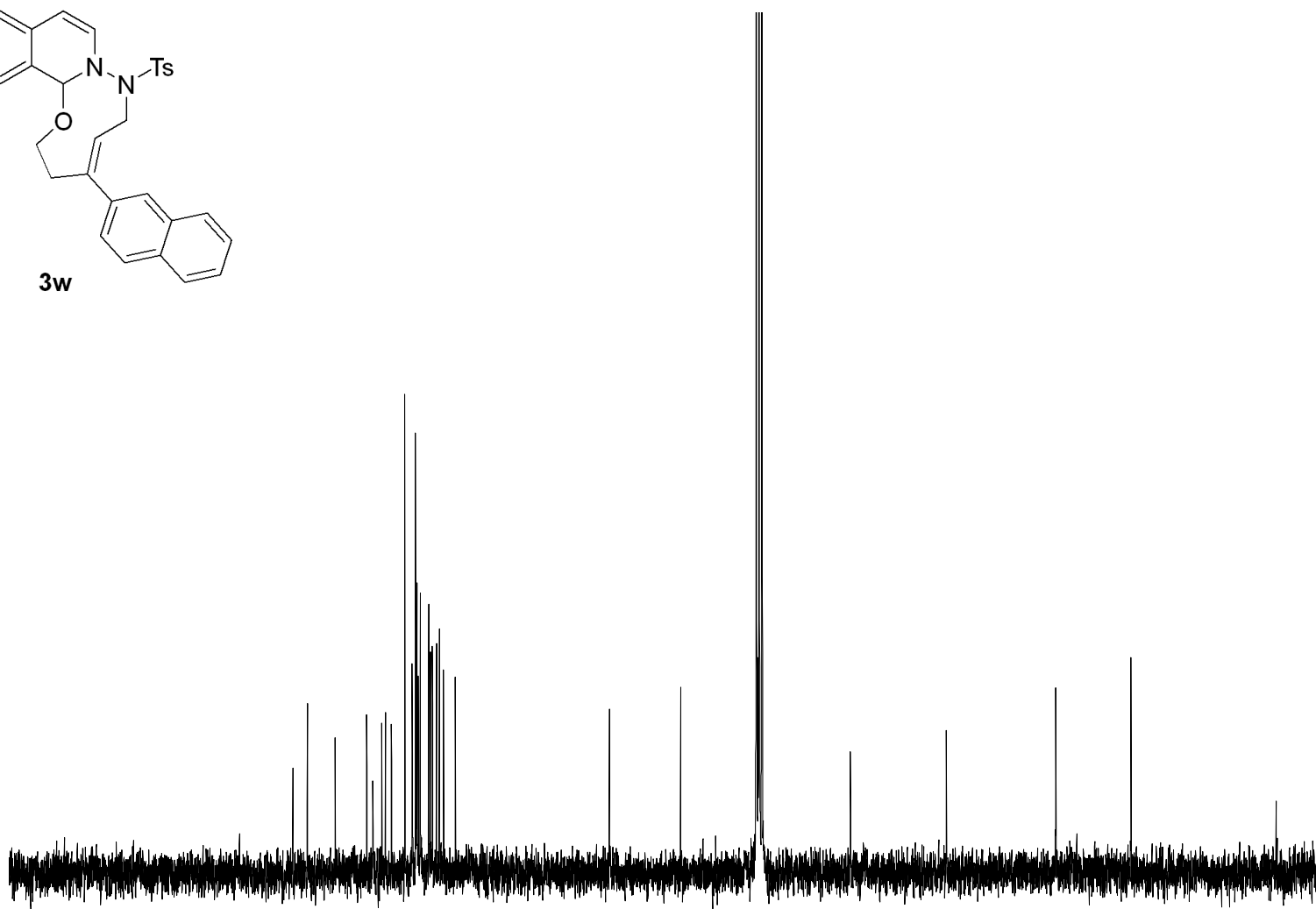
77.58
77.15
76.73

63.57

49.28

32.97

21.77



Current Data Parameters
NAME 2021-4--11Project 1 data
EXPNO 5510
PROCNO 1

F2 - Acquisition Parameters
Date_ 20211009
Time 11.45
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1500
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175317 sec
RG 203
DW 27.733 usec
DE 6.50 usec
TE -59.1 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 75.4752949 MHz
NUC1 13C
P1 9.50 usec
PLW1 34.20000076 W

===== CHANNEL f2 =====
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.17284000 W
PLW13 0.14000000 W

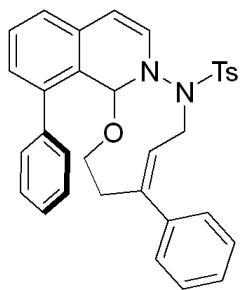
F2 - Processing parameters
SI 32768
SF 75.4677399 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

180 160 140 120 100 80 60 40 20 ppm

3sjwei 5624 xh1-3-76 1h cdcl3



7.641
7.614
7.391
7.381
7.376
7.361
7.352
7.336
7.328
7.323
7.319
7.314
7.293
7.279
7.268
7.251
7.244
7.237
7.226
7.208
7.188
7.181
7.173
7.171
7.168
7.162
7.156
7.103
7.099
7.077
7.073
7.068
7.064
7.043
7.039
5.927
5.923
5.897
5.893
5.889
5.777
5.756
5.752
5.731
5.593
5.568
4.846
4.825
4.799
4.779
4.184
4.158
4.137
4.111
3.226
3.219
3.186
3.140
3.130
2.831
2.819
2.805
2.792
2.440
2.395
2.383



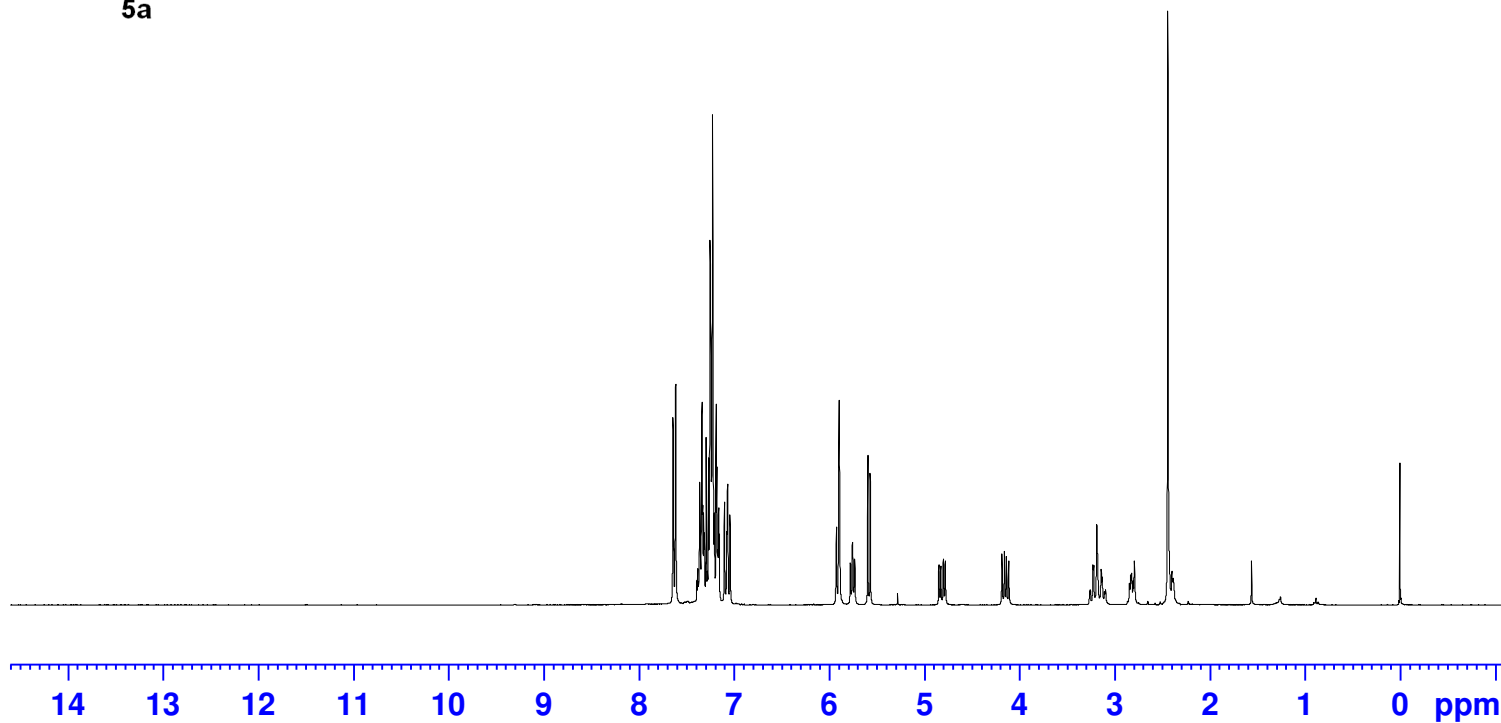
5a

Current Data Parameters
NAME 2021-4--11Project 1 data
EXPNO 5624
PROCNO 1

F2 - Acquisition Parameters
Date_ 20211123
Time 9.06
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 114
DW 83.200 usec
DE 6.50 usec
TE -59.1 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 300.1318534 MHz
NUC1 1H
P1 10.00 usec
PLW1 14.00000000 W

F2 - Processing parameters
SI 65536
SF 300.1300120 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



2.08
11.70
2.10
2.08
2.02
1.00
0.99
0.99
1.00
2.01
0.96
4.07

3sjwei 5631 xh1-3-76 13c cdcl3



Current Data Parameters
NAME 2021-4--11Project 1 data
EXPNO 5631
PROCNO 1

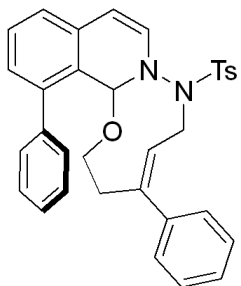
F2 - Acquisition Parameters
Date_ 20211123
Time 11.15
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175317 sec
RG 203
DW 27.733 usec
DE 6.50 usec
TE -59.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 75.4752949 MHz
NUC1 13C
P1 9.50 usec
PLW1 34.20000076 W

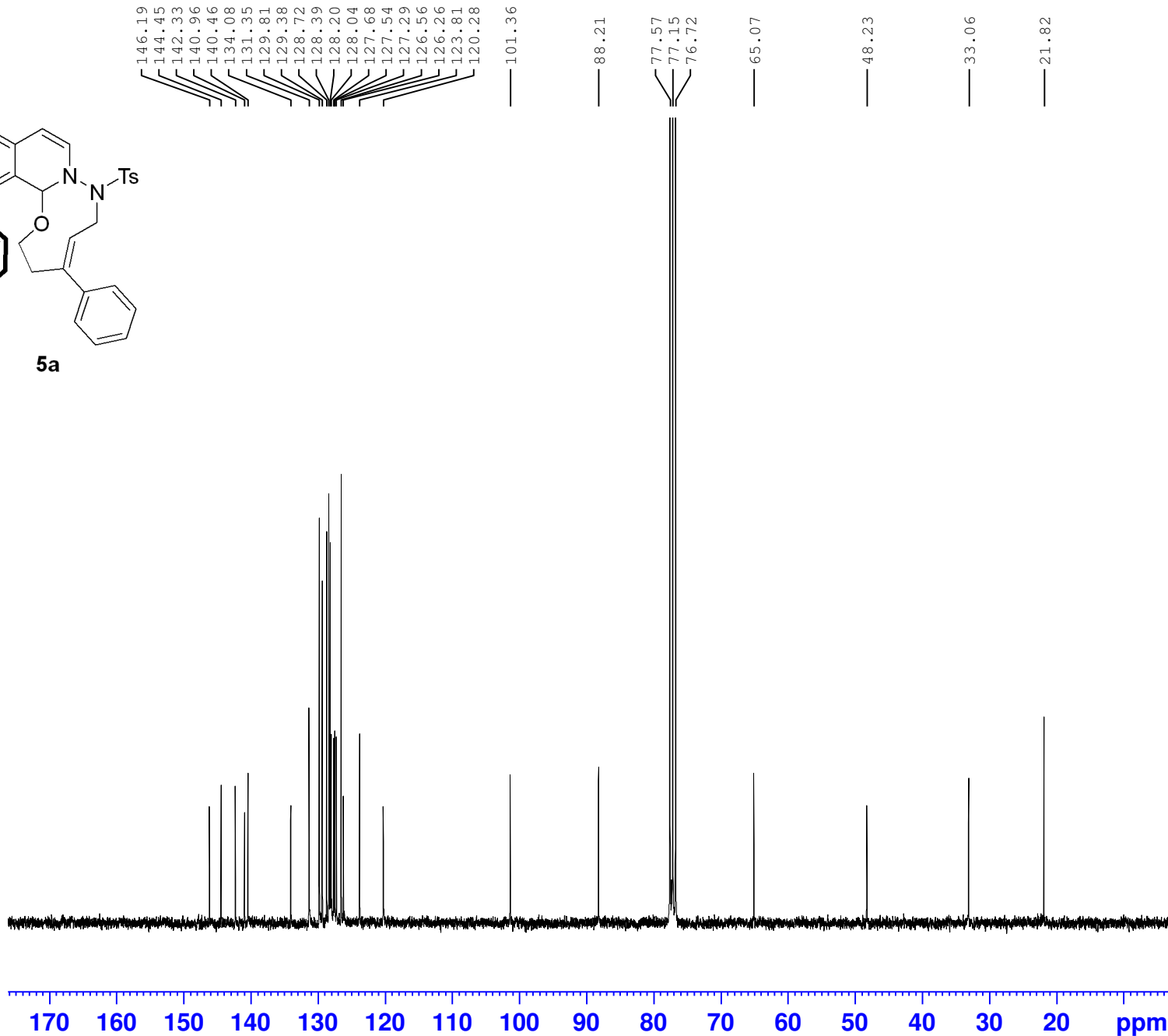
===== CHANNEL f2 =====
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.17284000 W
PLW13 0.14000000 W

F2 - Processing parameters
SI 32768
SF 75.4677433 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

146.19
144.45
142.33
140.96
140.46
134.08
131.35
129.81
129.38
128.72
128.39
128.20
128.04
127.68
127.54
127.29
126.56
126.26
123.81
120.28
101.36
88.21
77.57
77.15
76.72
65.07
48.23
33.06
21.82

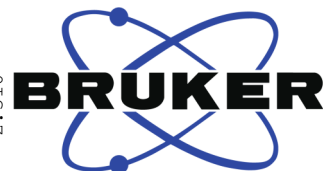


5a



170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

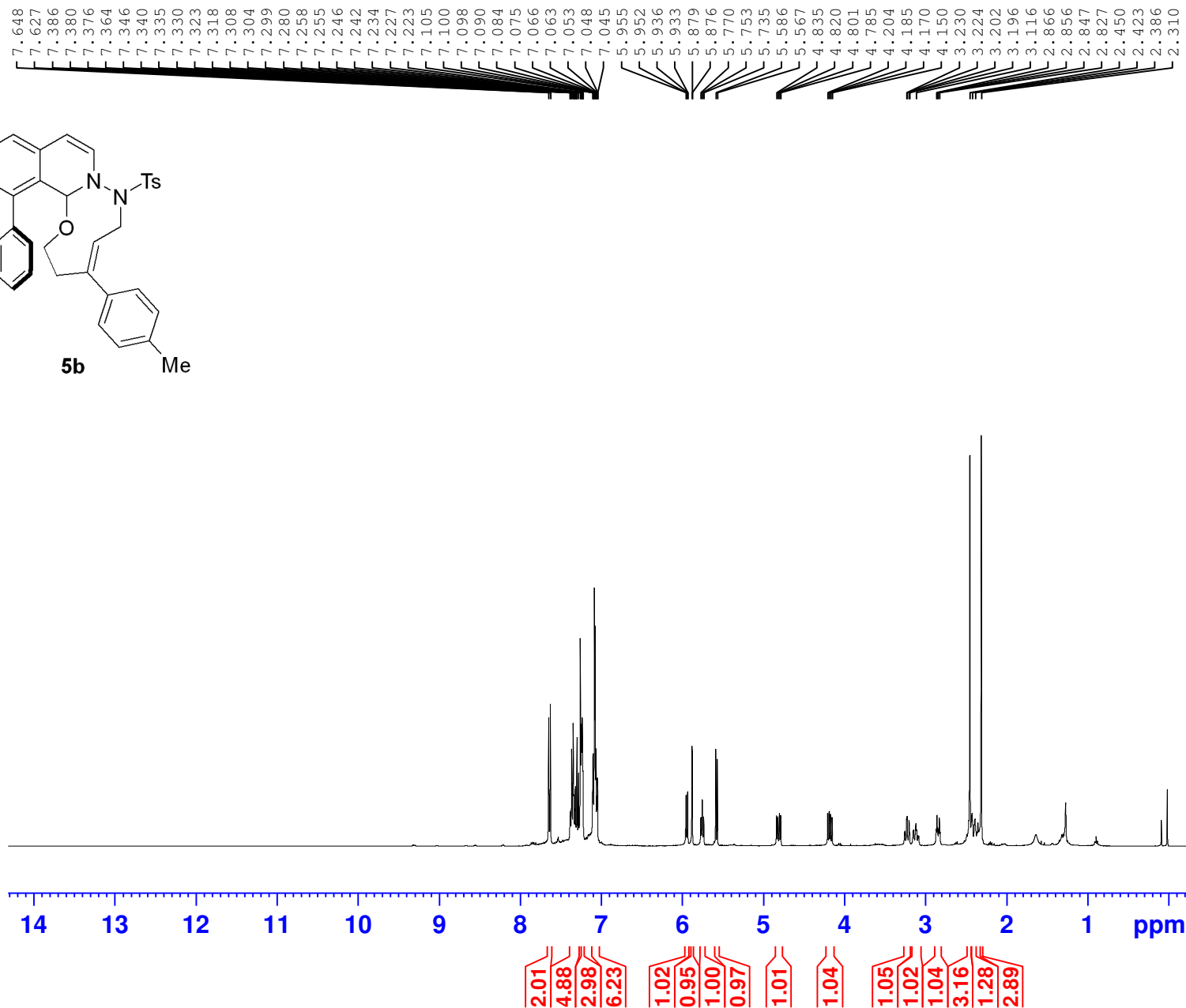
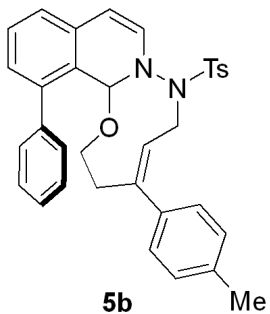
XHL-4-57



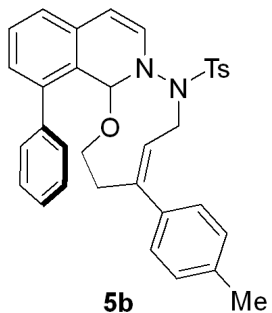
Current Data Parameters
NAME 2021-4--11Project 1 data
EXPNO 7
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220531
Time 20.26 h
INSTRUM Avance
PROBHD Z116098_0833 (
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8196.722 Hz
FIDRES 0.250144 Hz
AQ 3.9976959 sec
RG 81.3802
DW 61.000 usec
DE 13.54 usec
TE 294.7 K
D1 1.00000000 sec
TD0 1
SFO1 400.1324708 MHz
NUC1 1H
P0 3.33 usec
P1 10.00 usec
PLW1 20.73200035 W

F2 - Processing parameters
SI 65536
SF 400.1300105 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



XHL-4-57-c



146.11
144.40
141.02
140.47
139.47
137.32
134.26
131.72
131.45
129.81
129.37
129.09
128.67
128.17
128.03
127.65
127.26
126.41
126.18
123.78
119.61
101.21

88.08

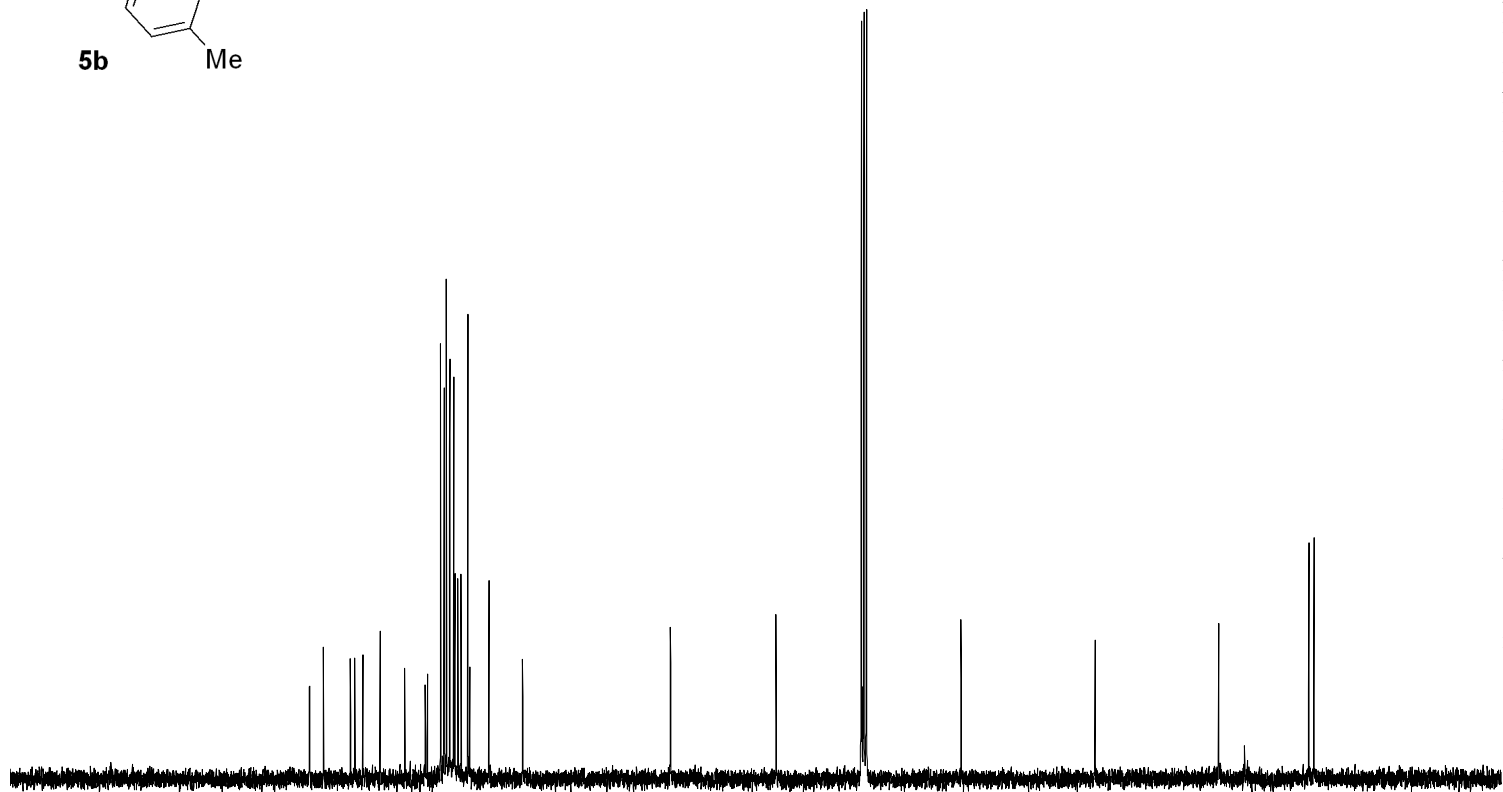
77.46
77.15
76.83

65.06

48.38

33.00

21.81
21.17



180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

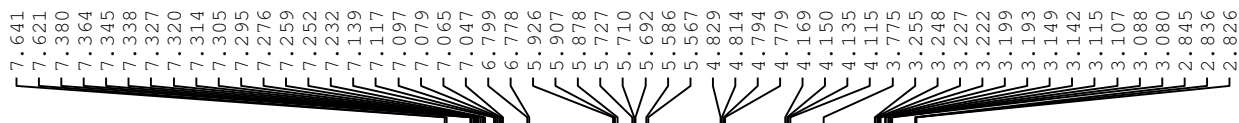
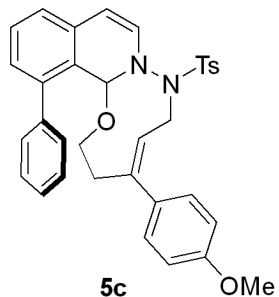


Current Data Parameters
NAME 2021-4--11Project 1 data
EXPNO 8
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220531
Time 20.41 h
INSTRUM Avance
PROBHD Z116098_0833 (
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 254
DS 4
SWH 23809.523 Hz
FIDRES 0.726609 Hz
AQ 1.3762560 sec
RG 51.55
DW 21.000 usec
DE 6.50 usec
TE 294.8 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1
SFO1 100.6228298 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 87.89900208 W
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz65
PCPD2 90.00 usec
PLW2 20.73200035 W
PLW12 0.25595000 W
PLW13 0.12874000 W

F2 - Processing parameters
SI 32768
SF 100.6127606 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

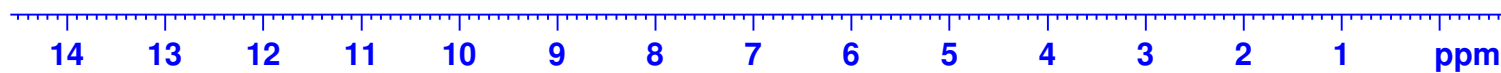
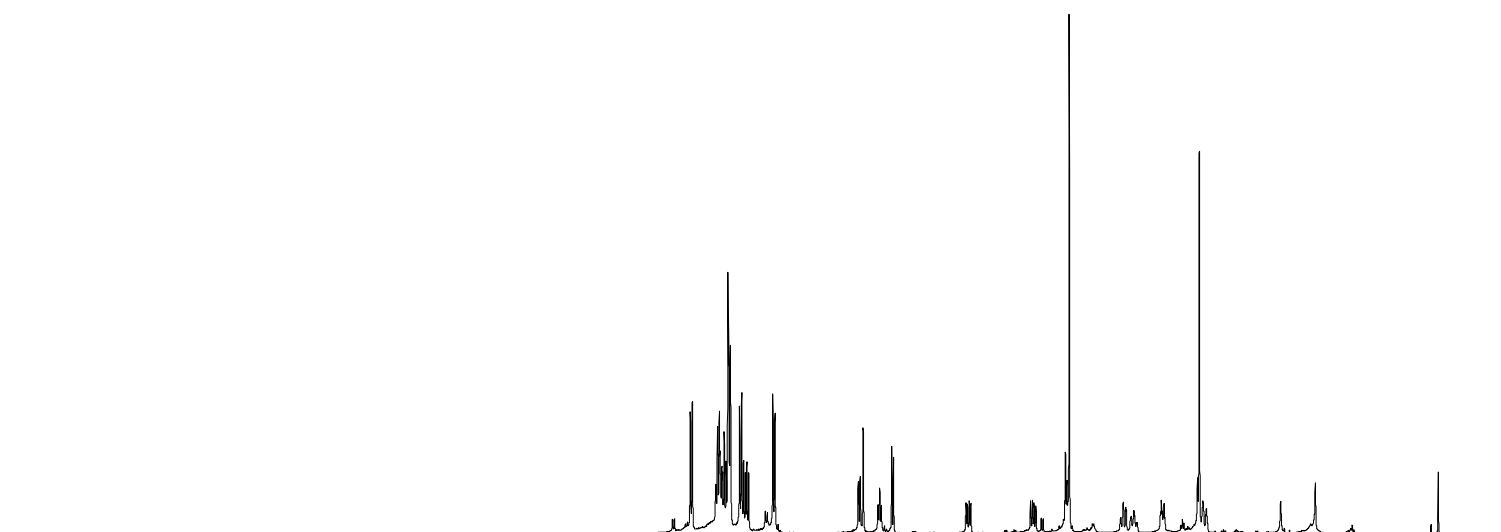
XHL-4-70



Current Data Parameters
NAME 2021-4--11Project 1 data
EXPNO 11
PROCNO 1

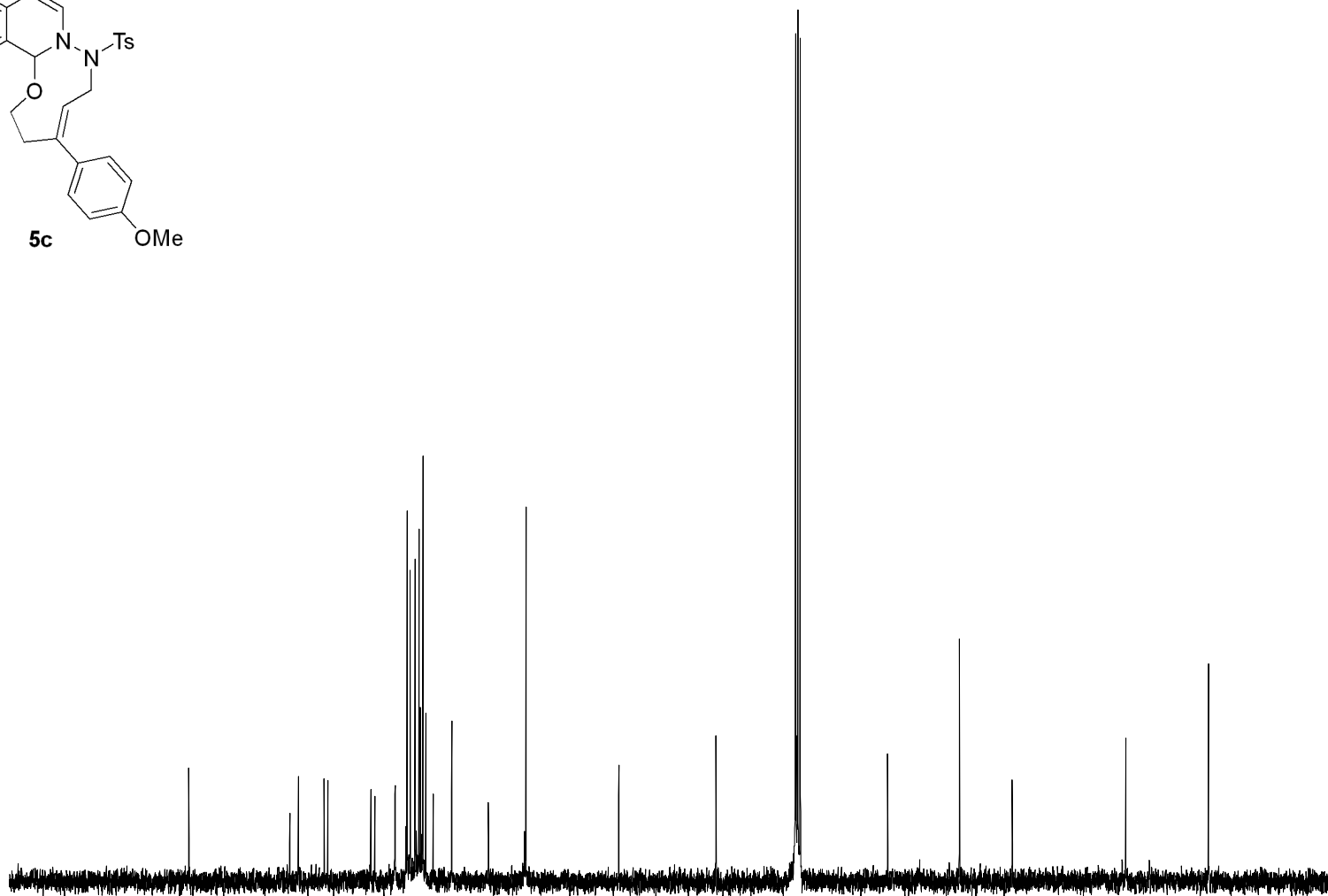
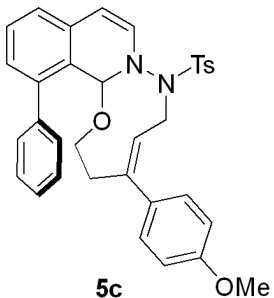
F2 - Acquisition Parameters
Date_ 20220531
Time 21.07 h
INSTRUM Avance
PROBHD Z116098_0833 (
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8196.722 Hz
FIDRES 0.250144 Hz
AQ 3.9976959 sec
RG 92.3873
DW 61.000 usec
DE 13.54 usec
TE 294.2 K
D1 1.00000000 sec
TD0 1
SFO1 400.1324708 MHz
NUC1 1H
P0 3.33 usec
P1 10.00 usec
PLW1 20.73200035 W

F2 - Processing parameters
SI 65536
SF 400.1300104 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



XHL-4-70-C

159.20
145.60
144.42
140.98
140.47
134.69
134.13
131.45
131.39
129.80
129.38
128.72
128.18
128.01
127.66
127.27
126.26
123.78
118.84
113.77
101.27
88.20
77.46
77.15
76.83
65.06
55.38
48.27
32.96
21.81



180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

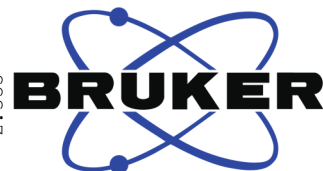


Current Data Parameters
NAME 2021-4--11Project 1 data
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220531
Time 21.23 h
INSTRUM Avance
PROBHD Z116098_0833 (
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 254
DS 4
SWH 23809.523 Hz
FIDRES 0.726609 Hz
AQ 1.3762560 sec
RG 51.55
DW 21.000 usec
DE 6.50 usec
TE 294.5 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1
SFO1 100.6228298 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 87.89900208 W
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz65
PCPD2 90.00 usec
PLW2 20.73200035 W
PLW12 0.25595000 W
PLW13 0.12874000 W

F2 - Processing parameters
SI 32768
SF 100.6127605 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

XHL-4-58-H

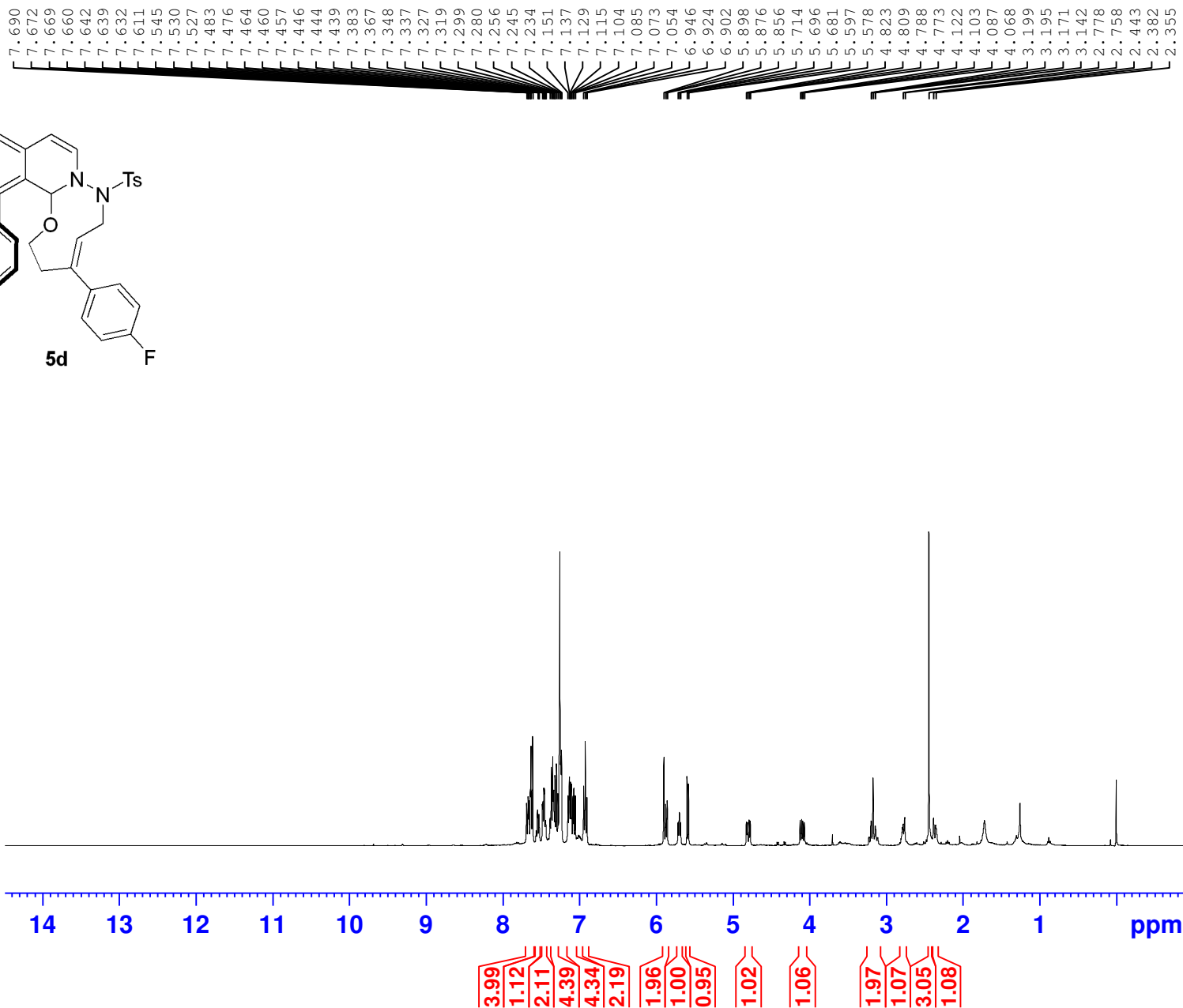
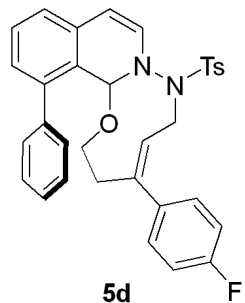


Current Data Parameters
NAME 2021-4--11Project 1 data
EXPNO 30
PROCNO 1

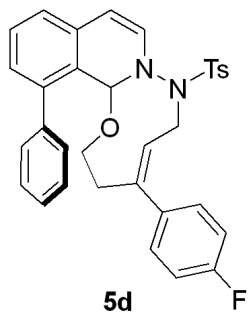
F2 - Acquisition Parameters
Date_ 20220601
Time 16.12
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 113.67
DW 60.800 usec
DE 6.50 usec
TE 294.8 K
D1 1.0000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 14.40 usec
PLW1 14.0000000 W
SFO1 400.1924713 MHz

F2 - Processing parameters
SI 65536
SF 400.1900184 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



XHL-4-58-C



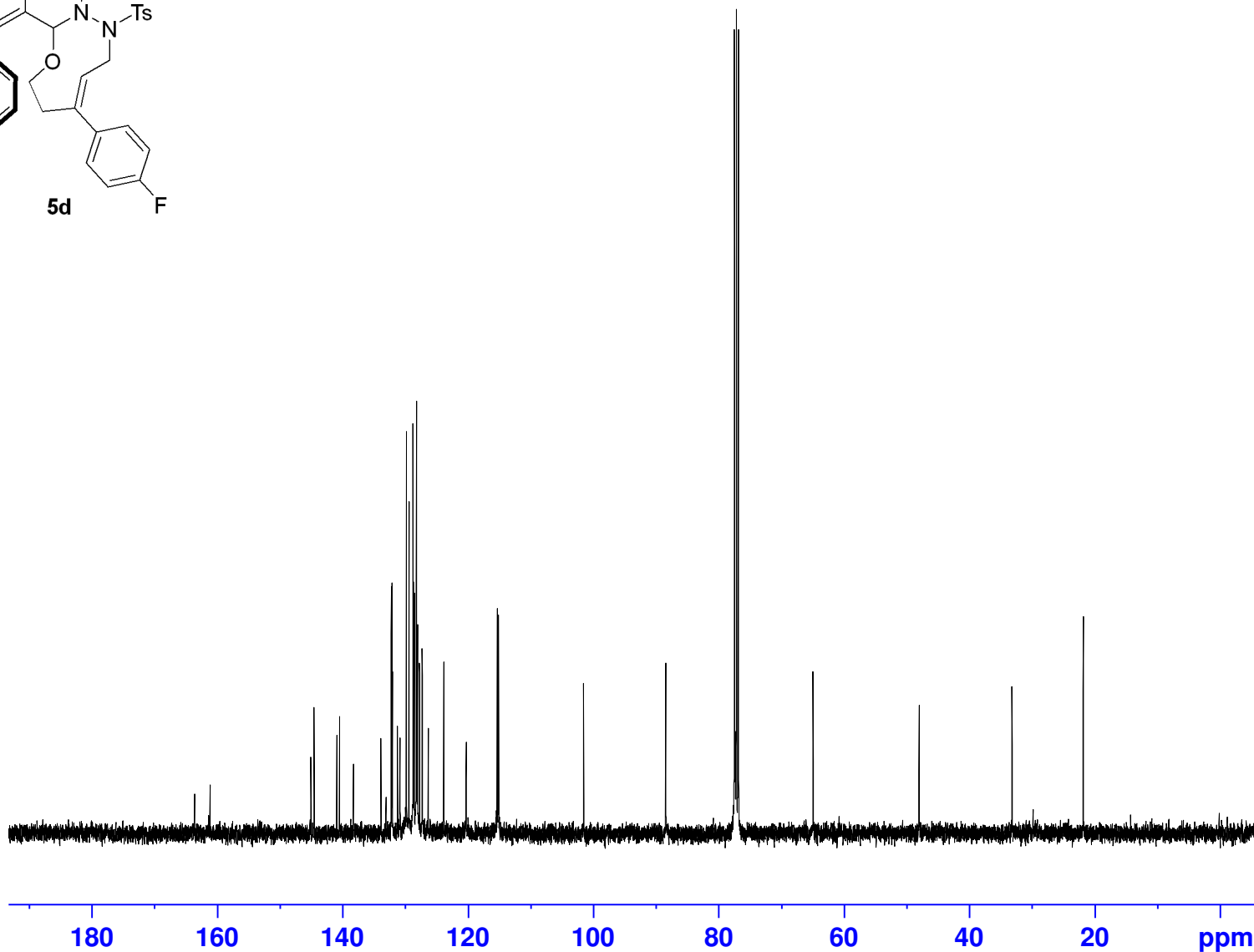
163.62
161.18
145.08
144.56
140.93
140.47
138.30
138.27
133.91
133.10
132.25
132.16
132.09
132.06
131.26
130.85
129.83
129.42
128.79
128.69
128.57
128.28
128.22
128.20
128.06
127.73
127.30
126.34
123.85
120.29
115.33
115.11
101.55
88.44
77.46
77.15
76.83

64.92

47.99

33.17

21.80

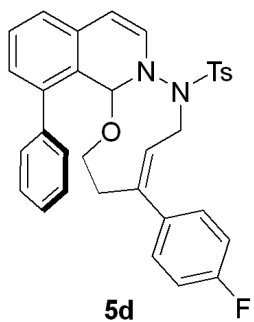


Current Data Parameters
NAME 2021-4--11Project 1 data
EXPNO 1
PROCNO 1

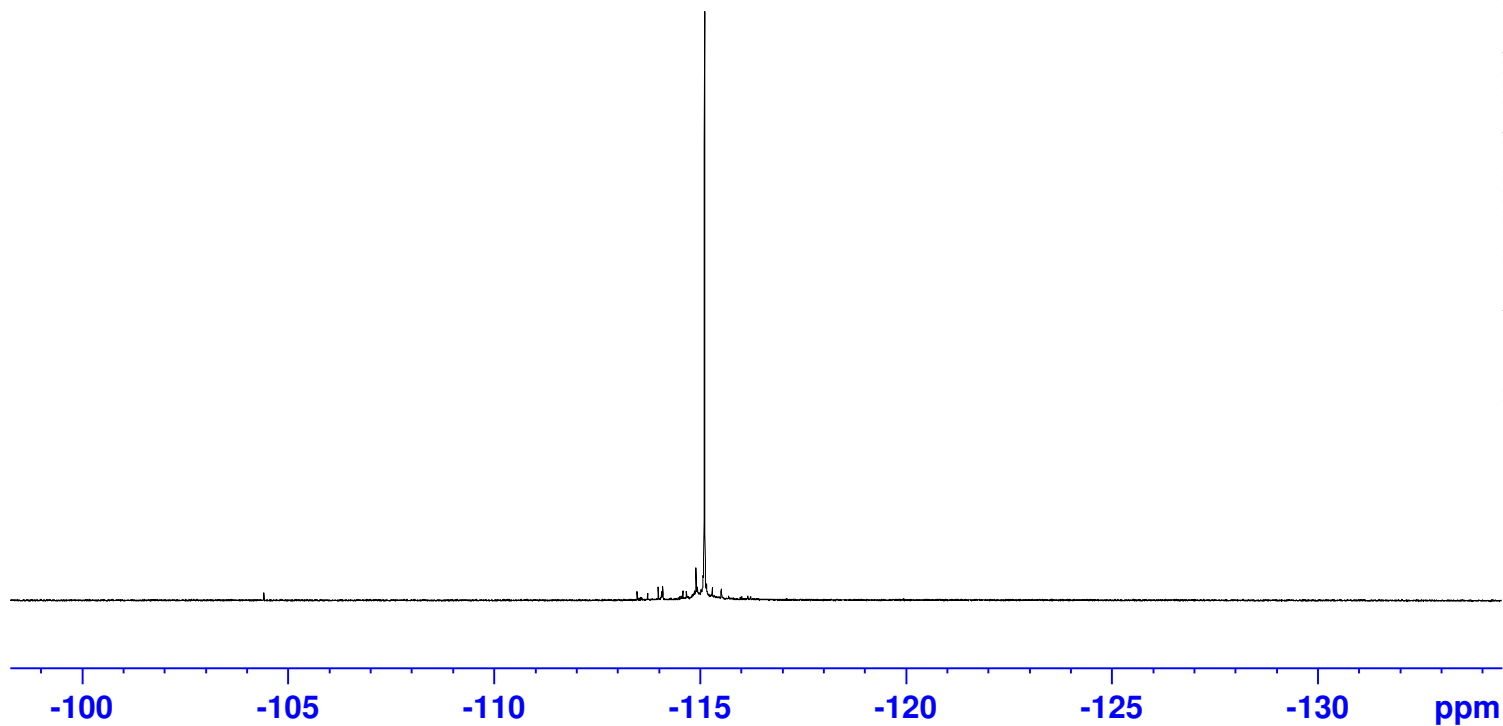
F2 - Acquisition Parameters
Date_ 20220603
Time 11.54 h
INSTRUM Avance
PROBHD Z116098_0833 (
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 512
DS 4
SWH 23809.523 Hz
FIDRES 0.726609 Hz
AQ 1.3762560 sec
RG 47.095
DW 21.000 usec
DE 6.50 usec
TE 298.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6228298 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 87.89900208 W
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz65
PCPD2 90.00 usec
PLW2 20.73200035 W
PLW12 0.25595000 W
PLW13 0.12874000 W

F2 - Processing parameters
SI 32768
SF 100.6127587 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

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— -115.12



Current Data Parameters
NAME 2021-4--11Project 1 data
EXPNO 2
PROCNO 1

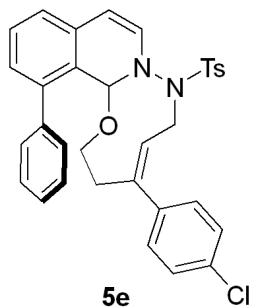
F2 - Acquisition Parameters
Date_ 20220603
Time 11.23 h
INSTRUM Avance
PROBHD Z116098_0833 (
PULPROG zgig
TD 131072
SOLVENT CDC13
NS 16
DS 4
SWH 90909.094 Hz
FIDRES 1.387163 Hz
AQ 0.7208960 sec
RG 101
DW 5.500 usec
DE 6.50 usec
TE 298.4 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 376.4607164 MHz
NUC1 19F
P1 18.00 usec
PLW1 16.73100090 W
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 20.73200035 W
PLW12 0.25595000 W

F2 - Processing parameters
SI 65536
SF 376.4983662 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

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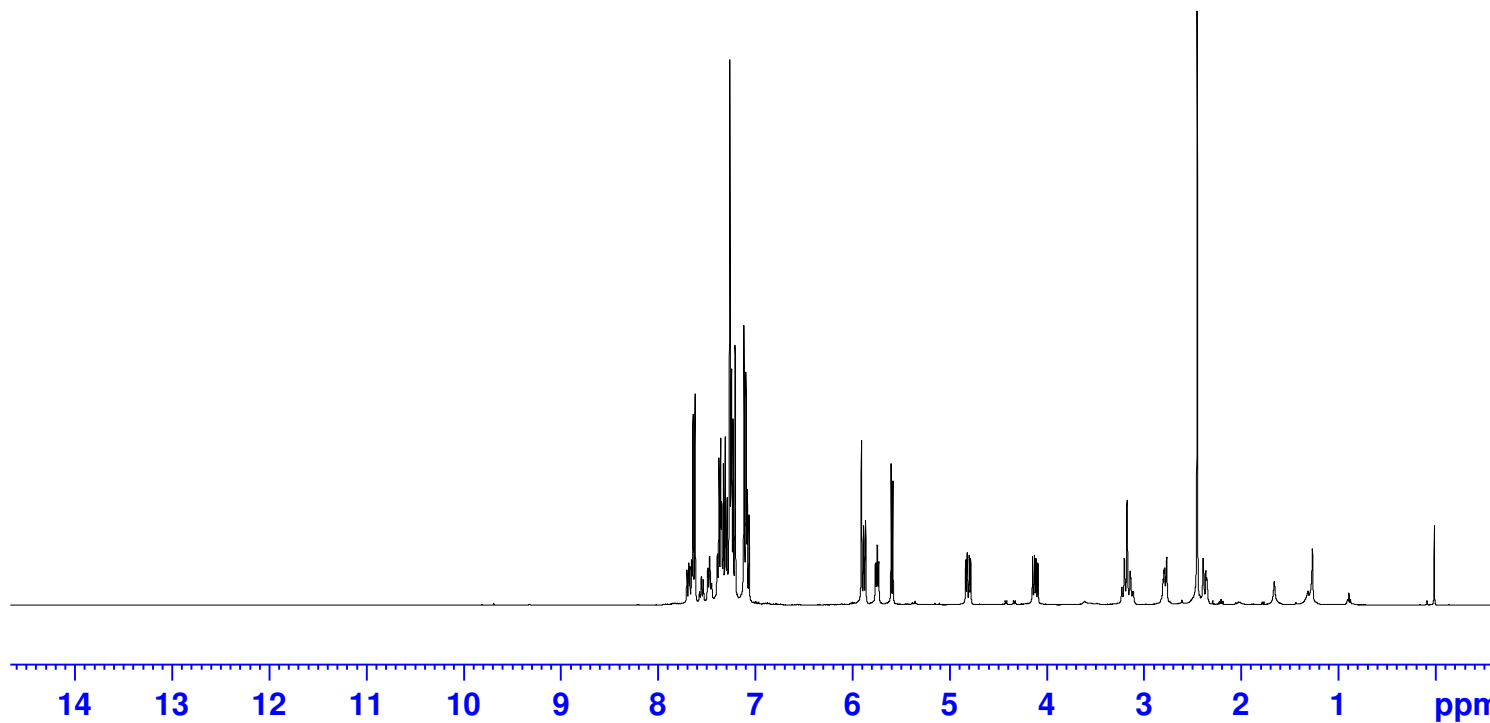
7.701
7.684
7.680
7.671
7.654
7.650
7.639
7.618
7.554
7.550
7.490
7.483
7.470
7.463
7.393
7.388
7.372
7.354
7.348
7.343
7.340
7.333
7.326
7.317
7.307
7.297
7.288
7.260
7.242
7.226
7.205
7.115
7.110
7.094
7.082
7.063
5.903
5.883
5.864
5.761
5.746
5.742
5.727
5.600
5.581
4.831
4.817
4.796
4.781
4.143
4.124
4.108
4.089
3.200
3.196
3.171
3.139
3.132
2.792
2.783
2.772
2.763
2.449
2.388
2.360
2.351



Current Data Parameters
NAME 2021-4--11Project 1 data
EXPNO 3
PROCNO 1

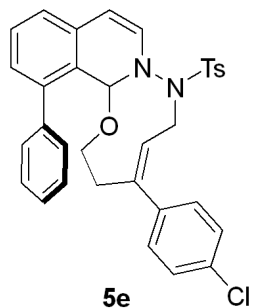
F2 - Acquisition Parameters
Date_ 20220531
Time 19.44 h
INSTRUM Avance
PROBHD Z116098_0833 (
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8196.722 Hz
FIDRES 0.250144 Hz
AQ 3.9976959 sec
RG 91.6422
DW 61.000 usec
DE 13.54 usec
TE 294.5 K
D1 1.0000000 sec
TD0 1
SFO1 400.1324708 MHz
NUC1 1H
P0 3.33 usec
P1 10.00 usec
PLW1 20.73200035 W

F2 - Processing parameters
SI 65536
SF 400.1300103 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



4.54
4.76
3.91
4.13
2.03
1.00
0.96
1.03
1.03
2.06
1.05
2.88
1.00

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144.91
144.58
140.92
140.66
140.44
133.86
133.40
132.25
131.22
129.84
129.40
128.77
128.54
128.23
128.08
127.92
127.73
127.31
126.28
123.86
120.78
101.56

88.39

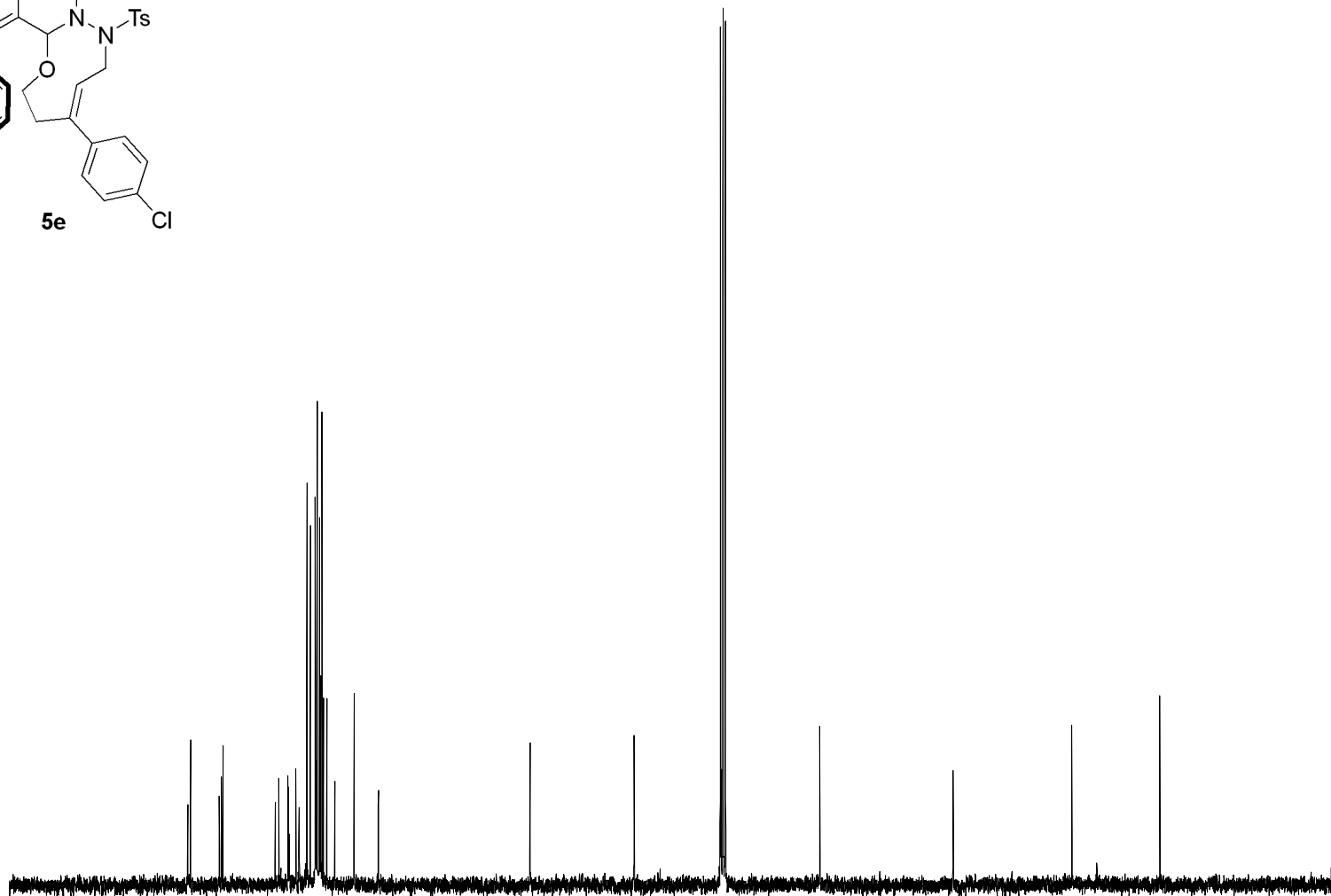
77.46
77.15
76.83

64.88

47.99

32.95

21.82



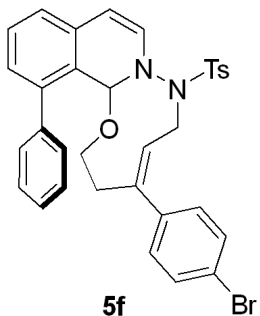
Current Data Parameters
NAME 2021-4--11Project 1 data
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220531
Time 19.59 h
INSTRUM Avance
PROBHD Z116098_0833 (
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 254
DS 4
SWH 23809.523 Hz
FIDRES 0.726609 Hz
AQ 1.3762560 sec
RG 51.55
DW 21.000 usec
DE 6.50 usec
TE 295.2 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1
SFO1 100.6228298 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 87.89900208 W
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz65
PCPD2 90.00 usec
PLW2 20.73200035 W
PLW12 0.25595000 W
PLW13 0.12874000 W

F2 - Processing parameters
SI 32768
SF 100.6127605 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

XHL-4-67-H



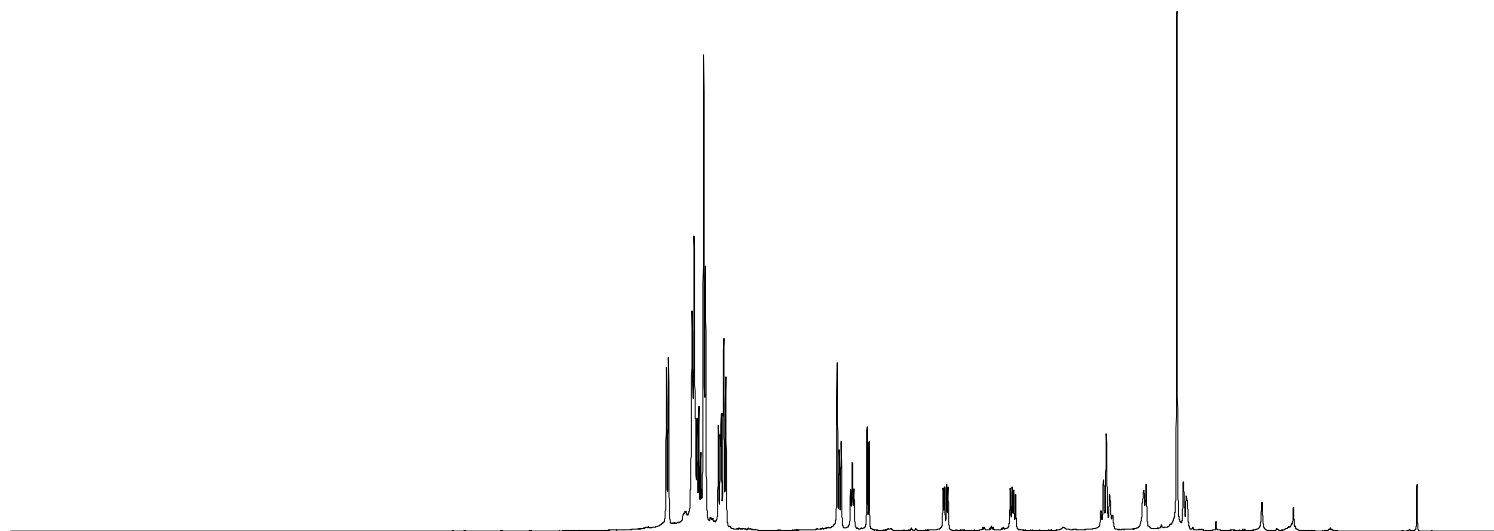
7.638
7.619
7.378
7.374
7.357
7.343
7.328
7.307
7.290
7.288
7.260
7.243
7.110
7.091
7.082
7.063
7.054
7.035
5.903
5.882
5.863
5.766
5.749
5.733
5.598
5.579
4.826
4.812
4.791
4.776
4.144
4.124
4.108
4.089
3.221
3.195
3.168
3.134
3.102
2.800
2.784
2.770
2.762
2.450
2.384
2.356
2.348



Current Data Parameters
NAME 2021-4--11Project 1 data
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220531
Time 20.05 h
INSTRUM Avance
PROBHD Z116098_0833 (
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8196.722 Hz
FIDRES 0.250144 Hz
AQ 3.9976959 sec
RG 101
DW 61.000 usec
DE 13.54 usec
TE 294.4 K
D1 1.00000000 sec
TD0 1
SFO1 400.1324708 MHz
NUC1 1H
P0 3.33 usec
P1 10.00 usec
PLW1 20.73200035 W

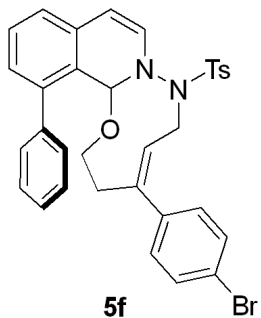
F2 - Processing parameters
SI 65536
SF 400.1300111 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



14 13 12 11 10 9 8 7 6 5 4 3 2 1 ppm

2.10
11.49
4.10
1.98
1.02
0.98
1.02
1.01
2.02
1.07
3.00
1.02

XHL-4-67-C



144.94
144.58
141.14
140.92
140.43
133.85
131.49
131.22
130.83
129.84
129.39
128.76
128.26
128.23
128.09
127.74
127.31
126.27
123.86
121.56
120.84
101.55

88.38

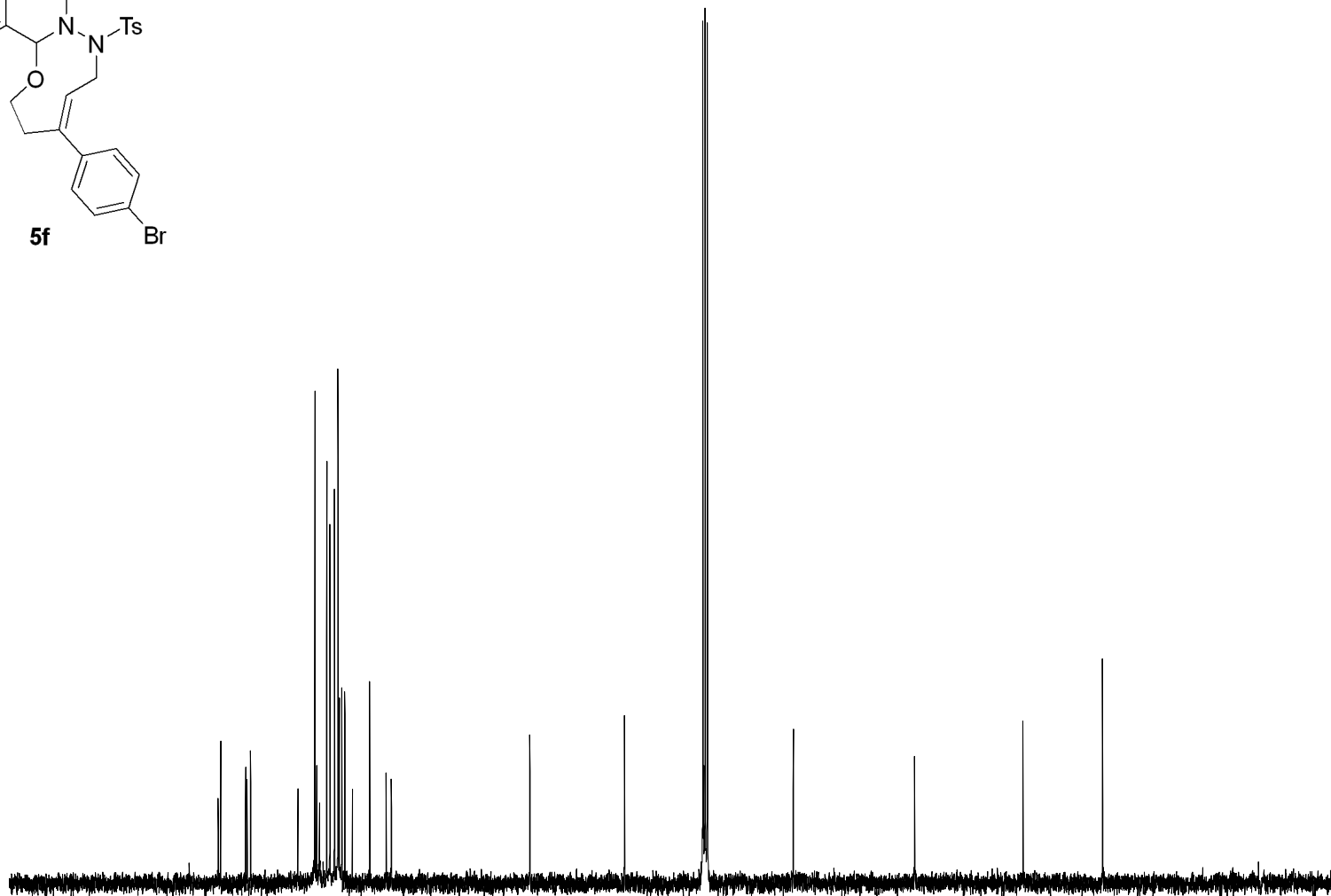
77.46
77.15
76.83

64.87

47.99

32.91

21.82



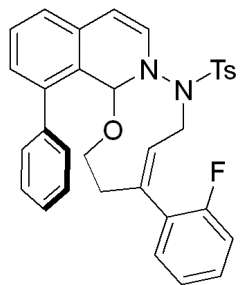
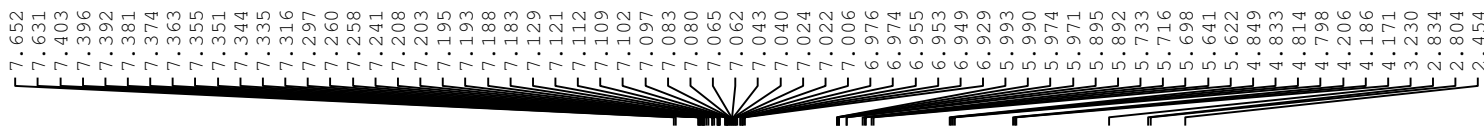
Current Data Parameters
NAME 2021-4--11Project 1 data
EXPNO 6
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220531
Time 20.20 h
INSTRUM Avance
PROBHD Z116098_0833 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 254
DS 4
SWH 23809.523 Hz
FIDRES 0.726609 Hz
AQ 1.3762560 sec
RG 53.2129
DW 21.000 usec
DE 6.50 usec
TE 295.2 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1
SFO1 100.6228298 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 87.89900208 W
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz65
PCPD2 90.00 usec
PLW2 20.73200035 W
PLW12 0.25595000 W
PLW13 0.12874000 W

F2 - Processing parameters
SI 32768
SF 100.6127613 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

160 140 120 100 80 60 40 20 ppm

XHL-4-71-H

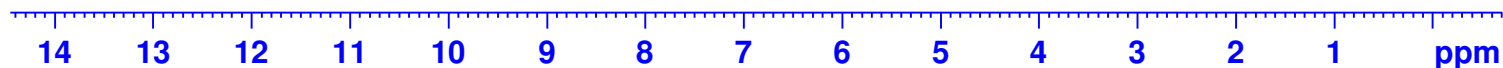
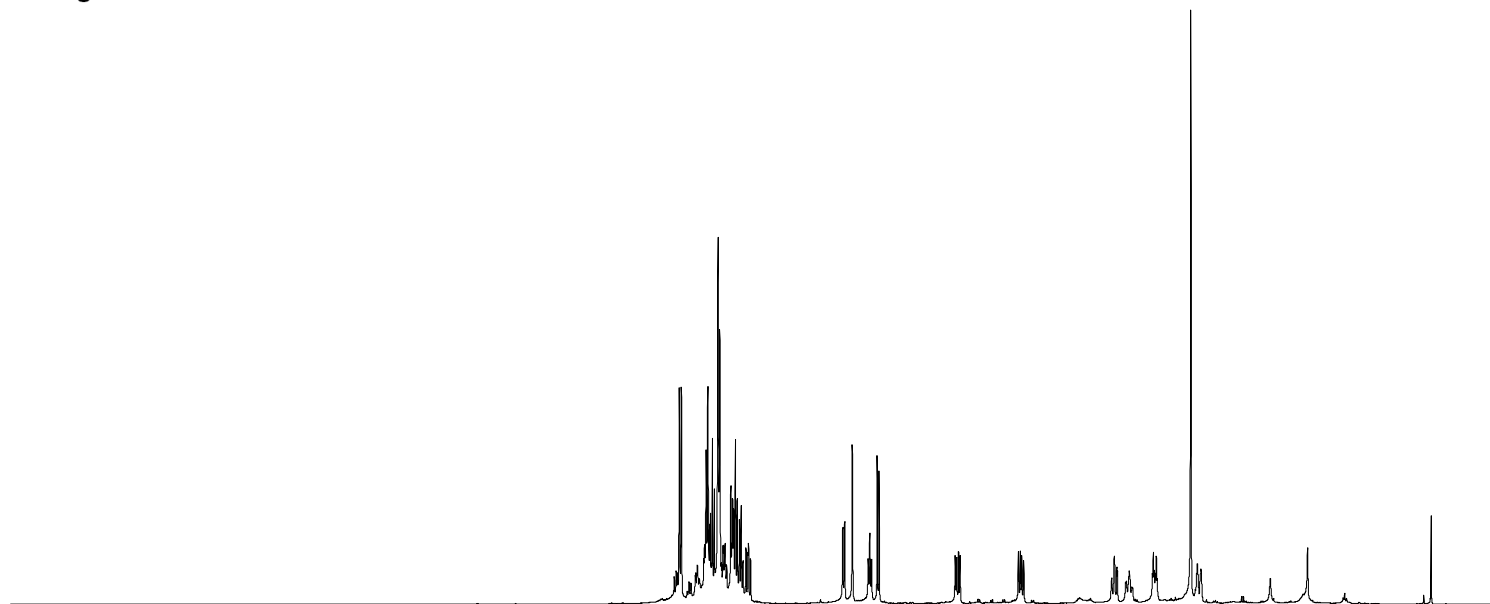


5g

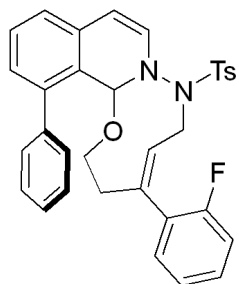
Current Data Parameters
 NAME 2021-4--11Project 1 data
 EXPNO 9
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20220531
 Time 20.47 h
 INSTRUM Avance
 PROBHD Z116098_0833 (
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 16
 DS 2
 SWH 8196.722 Hz
 FIDRES 0.250144 Hz
 AQ 3.9976959 sec
 RG 60.6061
 DW 61.000 usec
 DE 13.54 usec
 TE 294.5 K
 D1 1.0000000 sec
 TD0 1
 SFO1 400.1324708 MHz
 NUC1 1H
 P0 3.33 usec
 P1 10.00 usec
 PLW1 20.73200035 W

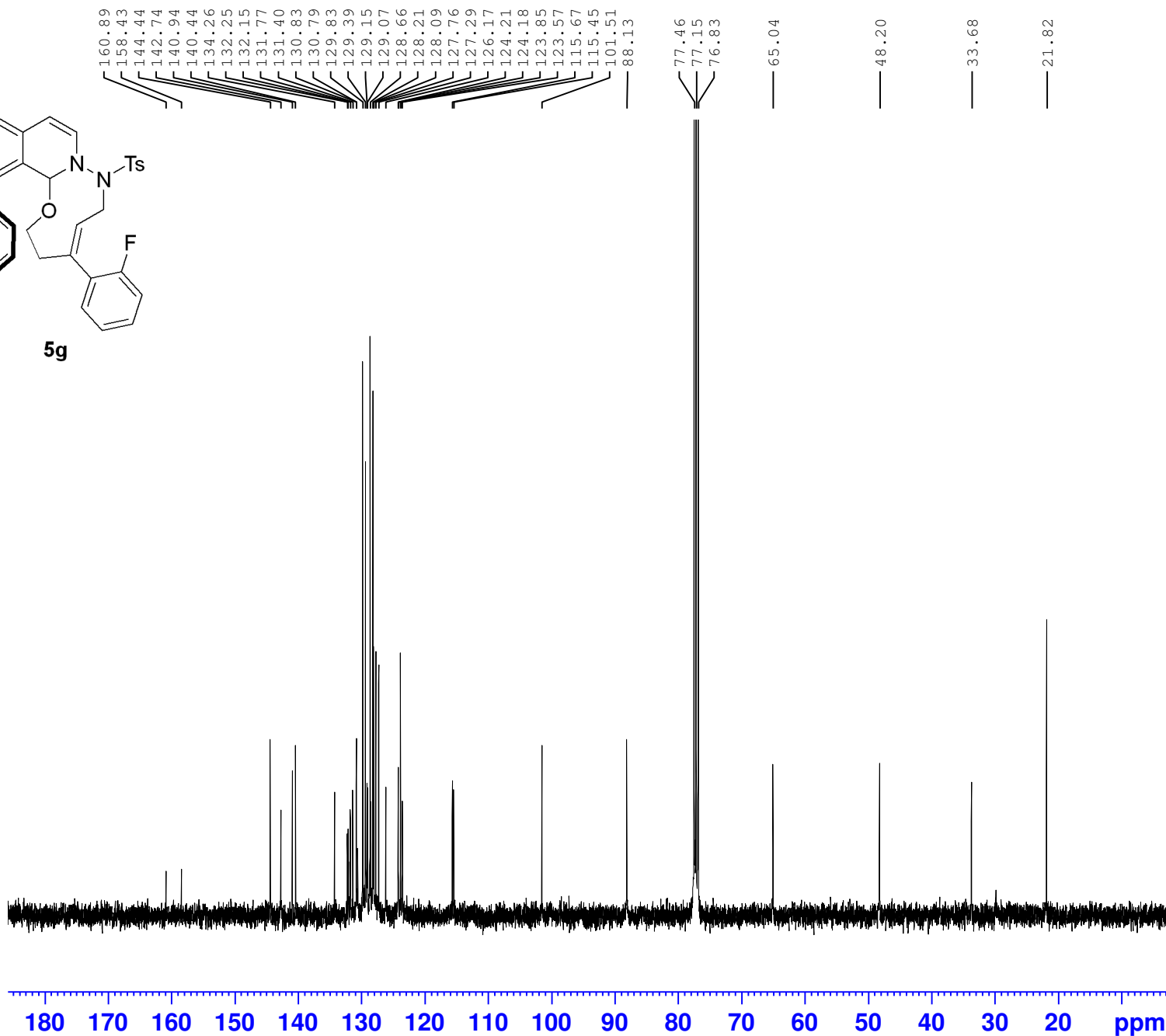
F2 - Processing parameters
 SI 65536
 SF 400.1300109 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



XHL-4-71-C



5g

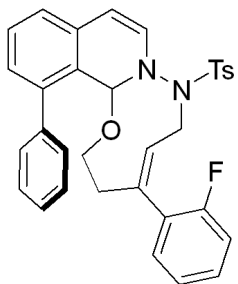


Current Data Parameters
NAME 2021-4--11Project 1 data
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220531
Time 21.03 h
INSTRUM Avance
PROBHD Z116098_0833 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 254
DS 4
SWH 23809.523 Hz
FIDRES 0.726609 Hz
AQ 1.3762560 sec
RG 49.9878
DW 21.000 usec
DE 6.50 usec
TE 294.8 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1
SFO1 100.6228298 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 87.89900208 W
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz65
PCPD2 90.00 usec
PLW2 20.73200035 W
PLW12 0.25595000 W
PLW13 0.12874000 W

F2 - Processing parameters
SI 32768
SF 100.6127612 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

XHL-4-71



5g

-114.90



Current Data Parameters
NAME 220605
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220605
Time 16.30 h
INSTRUM Avance
PROBHD z116098_0833 (
PULPROG zgig
TD 131072
SOLVENT CDCl3
NS 16
DS 4
SWH 90909.094 Hz
FIDRES 1.387163 Hz
AQ 0.7208960 sec
RG 101
DW 5.500 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 376.4607164 MHz
NUC1 19F
P1 18.00 usec
PLW1 16.73100090 W
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 20.73200035 W
PLW12 0.25595000 W

F2 - Processing parameters
SI 65536
SF 376.4983662 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

