Supporting Information

Gold-catalyzed [5+2]-Annulations of 1,3-Diyn-1-amides with Anthranils Bearing no C(6)-substituents

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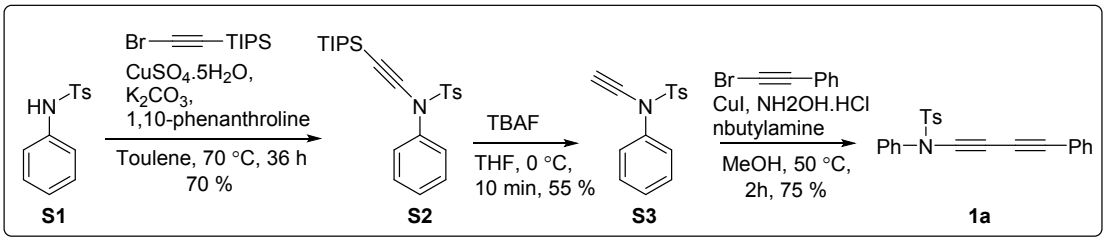
Contents:

(1) Representative Synthetic procedures

1.1. General procedure:

Unless otherwise noted, all reactions were carried out under a N_2 atmosphere in reaction tube. Tetrahydrofuran was dried with sodium benzophenone and distilled before use. Dichloroethane were dried over CaH_2 and distilled before use. The triethylamine (Et_3N) were stored over 4 Å molecular sieves prior to use. Reagents were purchased from commercial sources and used without purification, unless otherwise stated. Reactions were magnetically stirred and monitored by thin layer chromatography carried out on 0.25 mm E. Merck silica gel plate (60f- 254) using UV light as visualizing agents and/or potassium permanganate ($KMnO_4$). ^1H NMR and ^{13}C NMR spectra were recorded on a Bruker 400, Varian 400, 500, and 600 MHz spectrometers using chloroform-*d* ($CDCl_3$) as the internal standard. Chemical shifts are reported in parts per million (ppm). Multiplicities are indicated by s (singlet), d (doublet), t (triplet), q (quartet), and m (multiplet). Coupling constants *J* are reported in Hertz (Hz). Benzisoxazoles (**2a-2i**) were synthesized following similar synthetic procedure [S5]. 1,3-diynamides **1a, 1d, 1i, 1j, 1w** were synthesized using similar procedures. [s4b] The other ynamides **12a**, **12b** were synthesized using similar procedure. [s4c]

1.2. Synthetic procedure for preparation of starting materials:



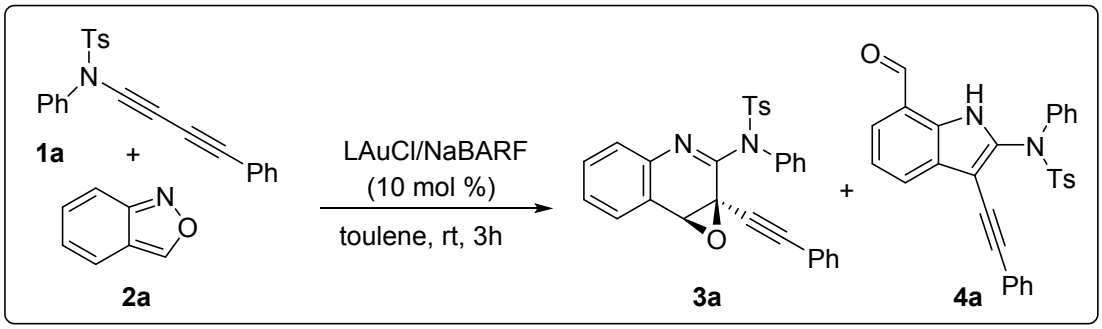
Tosyl amide **S1** was synthesized as per literature procedure. [s1]

In dry sealed tube, a mixture of **S1** (1.0 g, 4.05 mmol), K_2CO_3 (1.1 g, 8.1 mmol), $CuSO_{4.5}H_2O$ (101 mg, 0.4 mmol), and 1,10-phenanthroline (146 mg, 0.8 mmol) was added a solution of (bromoethynyl)triisopropylsilane (1.15 g, 4.5 mmol) in dry toluene. The reaction mixture was capped and heated in an oil bath at 70°C for 36 h while being monitored with TLC analysis. After completion, the reaction mixture was cooled to room temperature and diluted with ether and filtered through celite, and the filtrate was concentrated under vacuum. The crude products were purified by flash column chromatography using silica gel (eluent: EA/Hexane) to afford the desired product **S2**

(70%) as a yellow solid. [s2] To a solution of N-((triisopropylsilyl) ethynyl) benzenesulfonamide **S2** (1.0 g, 2.3 mmol) in THF (10 mL) was added n-tetrabutyl ammonium fluoride (1.0M in THF, 3.5 mL, 3.5 mmol) at 0 °C, and the resulting mixture was stirred at 0 °C for 10 mins. The crude products were purified by flash column chromatography using silica gel (eluent: EA/Hexane) to afford the desired ynamide substrate **S3** (55%) as a white solid. [s2] In a two-neck flask equipped with a reflux condenser were introduced under nitrogen atmosphere CuI (11 mg, 0.06 mmol) and NH_2OH•HCl (23 mg, 0.3 mmol) in MeOH (2 mL). To the mixture was added *n*-butylamine (162 mg, 0.2 mL, 2.2 mmol, 2 equiv.) followed by MeOH (1.5 mL) and ynamide **S3** (300 mg, 1.1 mmol). The resulting solution was heated to 50 °C and solution of (bromoethynyl)benzene (240mg, 1.3 mmol) [s3b] in MeOH (1.5 mL) was added slowly within 10 minutes. The reaction mixture was further heated at 50 °C for 2 h. Then ether and brine were added, the layers separated, and the aqueous layer was extracted 3 times with ether. The combined organic layers were washed with brine, dried over $MgSO_4$ and concentrated under reduced pressure. The residue was purified by flash column chromatography using silica gel (eluent: EA and Hexane) to afford the desired 4-methyl-N-phenyl-N-(phenylbuta-1,3-diyn-1-yl)benzenesulfonamide **1a** (246 mg, 0.66 mmol, 75%) as a yellow solid.[s4] Similarly, other diynamide (**1b-1w**) were synthesized.

(2) Standard procedures for catalytic operations]

Standard procedure for the synthesis of 4-methyl-N-phenyl-N-((1a*R*,7b*S*)-1a-(phenylethynyl)-1a,7b-dihydrooxireno[2,3-*c*]quinolin-2-yl)benzenesulfonamide (3a) and N-(7-formyl-3-(phenylethynyl)-1*H*-indol-2-yl)-4-methyl-N-phenylbenzenesulfonamide (4a).

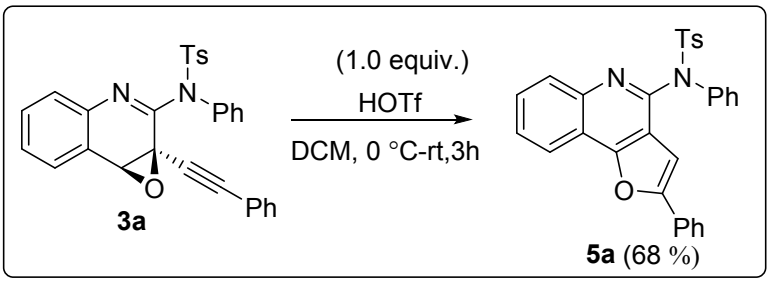


A catalytic tube was charged with LAuCl (11.4 mg, 0.021) and NaBARF (19.1 mg, 0.021 mmol), and to this mixture was added dry toulene (0.5 mL). The resulting mixture was stirred at room temperature for 10 min. To this mixture was added a 2.5 ml dry toulene solution of 4-methyl-N-phenyl-N-(phenylbuta-1,3-diyn-1-

yl)benzenesulfonamide (**1a**) (80 mg, 0.215 mmol) and benzo[*c*]isoxazole (**2a**) (35 mg, 0.237 mmol). After stirring at room temprature for 3 h, the reaction mixture was filtered over a short celite bed, concentrated, and eluted through a silica column (5-8% EA/hexane) to give the desired 4-methyl-N-phenyl-N-((1a*R*,7b*S*)-1a-(phenylethynyl)-1a,7b-dihydrooxireno[2,3-*c*]quinolin-2-yl)benzenesulfonamide (**3a**) in (71.9 mg, 0.14 mmol, 68%) as a white solid and N-(7-formyl-3-(phenylethynyl)-1*H*-indol-2-yl)-4-methyl-N-phenylbenzenesulfonamide (**4a**) in (18 mg, 0.03 mmol, 17 %) as a yellow solid.

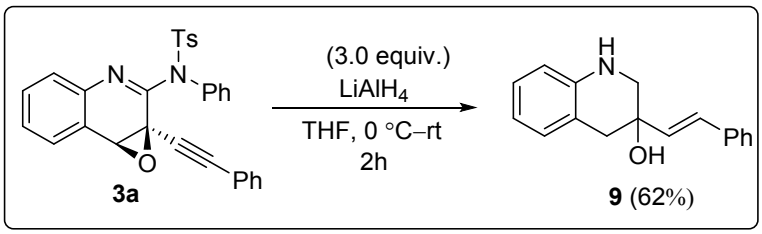
(3) Synthetic procedures for chemical functionalizations:

(3.1) Standard procedure for the synthesis of 4-methyl-N-phenyl-N-(2-phenylfuro[3,2-c]quinolin-4-yl)benzenesulfonamide (5a)



To a solution of 4-methyl-N-phenyl-N-((1a*R*,7b*S*)-1a-(phenylethynyl)-1a,7b-dihydrooxireno[2,3-c]quinolin-2-yl)benzenesulfonamide **3a** (50 mg, 0.102 mmol) in 1 ml DCM was added triflic acid (16.5 mg, 0.011 mmol) slowly at 0℃, after 10 min allowed the reaction solution at room temperature around 3 hours. Monitered the reaction by TLC, once reaction completed add 2 ml water and extract with ether (2 ml×3) times. The solution was concentrated under reduced pressure. The crude mass was purified by silica gel chromatography (EA:Hexane) gave the desired product 4-methyl-N-phenyl-N-(2-phenylfuro[3,2-c]quinolin-4-yl)benzenesulfonamide **5a** (34 mg, 0.069, 68 %) as white solid.

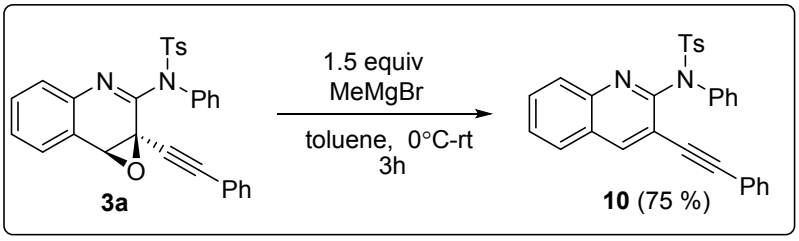
(3.2) Standard procedure for the synthesis of (*E*)-3-styryl-1,2,3,4-tetrahydroquinolin-3-ol (9)



To a solution of **3a** (50 mg, 0.10 mmol) in 3 ml dry THF, was added Lithium aluminium hydride (11 mg, 0.30 mmol) at 0 ℃, monitered the reaction by TLC. Add 3 ml water

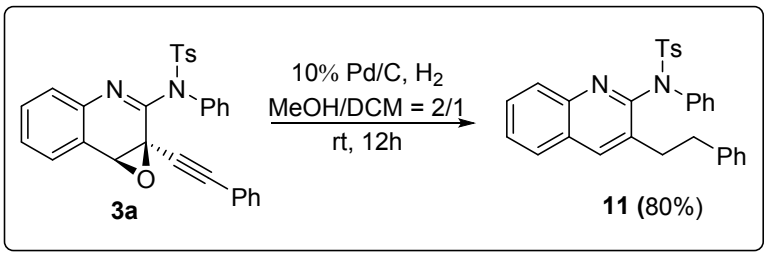
after completion of the reaction and extract with ether (2 ml×3) times. After concentrated under reduced pressure, crude residue was purified by silica gel column chromatography obtained **9** (16 mg, 0.06 mmol, 62 %) as white solid.

(3.3) **Standard procedure for the synthesis of 4-methyl-N-phenyl-N-(3-(phenylethynyl)quinolin-2-yl)benzenesulfonamide (10)**



To a solution of **3a** (80 mg, 0.16 mmol) in 2 ml dry toluene wad added methyl magnesium bromide (3.0 M, 82µL, 0.245mmol) at ℃. Allowed the reaction at room temperature for 3 hours. Once reaction completed, add 2 ml NH_4Cl and extract with ether (2 ml×3) times. The solution was concentrated under reduced pressure. Crude mass was purified by silica gel chromatography (EA:Hexane) delievered **10** (58 mg, 0.12 mmol, 75 %) as white solid.

(3.4) Standard procedure for the synthesis of 4-methyl-N-(3-phenethylquinolin-2-yl)-*N*-phenylbenzenesulfonamide (11)



To a solution of 10% Pd/C (50.0 mg) in methanol (2 mL) was added methanol (3 mL) solution of **3a** (80.0 mg, 0.163 mmol), and reaction mixture was stirred for 12 hours at room temperature. The reaction mixture was passed through a short bed of silica after completion of reaction, washed with ethyl acetate, and concentrated. The crude product was purified by flash chromatography on silica gel column (EA/Hexane) to afford **11** (62.4 mg, 0.13 mmol, 80%) as a yellow liquid.

(4) References:

[s1] X. Nie, G. Wang; *J. Org. Chem.*, **2006**, *71*, 4734-4741.

[s2] a) A. Hentz, P. Retailleau, V. Gandon, K. Cariou, R. H. Dodd; *Angew. Chem. Int.*

Ed., **2014**, *53*, 8333-8337. b) Y. C. Hsu, S. A. Hsieh, R. S. Liu; *Chem. Eur. J.* **2019**, *25*, 5288-5297.

[s3] a) Y. Tang, L. Shen, B. T. Dellaria, R. P. Hsung; *Tetrahedron Lett.*, **2008**, *49*, 6404-6409. b) Y. Gao, G. Wu. Q. Zhou, J. Wang; *Angew. Chem. Int. Ed.*, **2018**, *57*, 2716-2720.

[s4] a) I. Talbi, C. Alayrac, J. Lohier, S. Touil, B. Witulski; *Org. Lett.*, **2016**, *18*, 2656-2659. b) M. Skaria, Y. C. Hsu, Y. T. Jiang, M. Y. Lu, T. C. Kuo, M. J. Cheng, R. S. Liu; *Org. Lett.* **2020**, *22*, 4478–4482. c) L. Q. Yang, K. B. Wang, C. Y. Li; *Eur. J. Org. Chem*. **2013**, 2775–2779

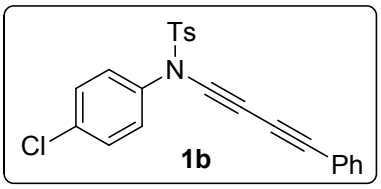
[s5] (a) Compound (**2a-2h**): a) R. L. Sahani, R-S. Liu; *Angew. Chem. Int. Ed*., **2017**, *56*, 12736-12740; b) J. Chauhan, S. Fletcher, *Tetrahedron Lett*. **2012**, *53*, 4951- 4954; c) H. Jin, L. Huang, J. Xie, M. Rudolph, F. Rominger and A. S. K. Hashmi, *Angew. Chem. Int. Ed*, **2016**, *55*, 794-797; d) H. Jin, B. Tian, X. Song, J. Xie, M. Rudolph, F. Rominger, A. S. K. Hashmi, *Angew. Chem. Int. Ed*. **2016**, *55*, 12688- 12692; e) F. Wang, P. Xu, S. Y. Wang, S. J. Ji, *Org. Lett*. **2018**, *20*, 2204−2207.

(b) Compound **2i**: M. Chiarini, L. D. Vecchio, F. Marinelli, L. Rossi, A. Arcadi, *Synthesis*, **2016**, *48*, 3017-3030.

Note: 1) The spectroscopic data of the 1,3-diynamides **1b, 1c, 1e, 1f, 1g, 1h, 1k, 1l, 1m, 1n, 1o, 1p, 1q, 1r, 1s, 1t** and **1u** are provided below.
2) As **4o** yield mention in manuscript was less than 5 % that's why **s**pectral data of compound **4o** was not provided because **4o** was difficult to isolate, its yield calculated from crude nmr.

(4) Spectral data for compounds:

Spectral data for *N*-(4-chlorophenyl)-4-methyl-*N*-(phenylbuta-1,3-diyn-1-yl)benzenesulfonamide (1b)

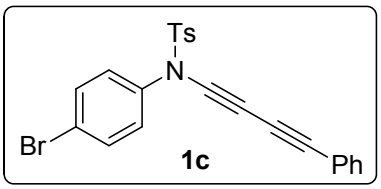


1b

Yellow solid; (523 mg, 1.29 mmol, 79%); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.58 (d, J = 8.4 Hz, 2H), 7.45 (td, J = 8.4, 1.2 Hz, 2H), 7.35-7.26 (m, 7H), 7.18-7.16 (m, 2H), 2.43 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 145.6, 136.5, 134.6, 132.6, 132.4, 129.9, 129.4, 129.1, 128.4, 128.1, 127.5, 121.7, 81.7, 73.7, 73.1, 58.1, 21.7; ESI-MS (M+Na) calcd.

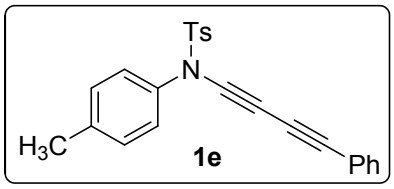
for $C_{23}H_{16}ClNNaO_2S$: 428.0488; Found: 428.0531.

Spectral data for *N*-(4-bromophenyl)-4-methyl-*N*-(phenylbuta-1,3-diyn-1-yl)benzenesulfonamide (1c)



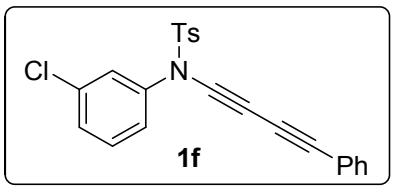
Yellow solid; (520 mg, 1.15 mmol, 81 %); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.59 (d, *J* = 8.4 Hz, 2H), 7.45 (t, *J* = 7.8 Hz, 4H), 7.33-7.28 (m, 5H), 7.11 (d, *J* = 8.4, 2H), 2.43 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 145.7, 137.1, 132.4, 132.3, 129.9, 129.6, 129.1, 128.4, 128.1, 127.7, 122.6, 121.7, 81.7, 73.6, 73.1, 58.2, 21.7; ESI-MS (M+Na) calcd. for $C_{23}H_{16}BrNNaO_2S$: 471.9983; Found: 473.9956.

Spectral data for 4-methyl-*N*-(phenylbuta-1,3-diyn-1-yl)-*N*-(*p*-tolyl)benzenesulfonamide (1e)



Yellow liquid; (560 mg, 1.45 mmol, 83%); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.60 (d, *J* = 8.4 Hz, 2H), 7.44 (d, *J* = 7.8 Hz, 2H), 7.33-7.27 (m, 5H), 7.13-7.07 (m, 4H), 2.43 (s, 3H), 2.33 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 145.3, 138.9, 135.4, 133.0, 132.3, 129.9, 129.7, 128.9, 128.4, 128.2, 126.3, 121.9, 81.3, 74.6, 73.5, 57.4, 21.7, 21.1; ESI-MS (M+Na) calcd. for $C_{24}H_{19}NNaO_2S$: 408.1034; Found: 408.1031.

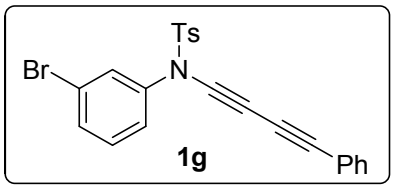
Spectral data for *N*-(3-chlorophenyl)-4-methyl-*N*-(phenylbuta-1,3-diyn-1-yl)benzenesulfonamide (1f)



Yellow liquid; (274 mg, 0.67 mmol, 69 %); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.61 (d, *J* = 8.4 Hz, 2H), 7.47-7.45 (m, 2H), 7.34-7.24 (m, 8H), 7.19-7.16 (m, 1H), 2.44 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 145.7, 139.1, 134.7, 132.7, 132.4, 130.2, 129.9, 129.2, 128.8, 128.4, 128.2, 126.2, 124.3, 121.8, 81.8, 73.5, 73.1, 58.5, 21.8; EI-MS calcd. for $C_{23}H_{16}ClNO_2S$: 405.0590; Found: 405.0585.

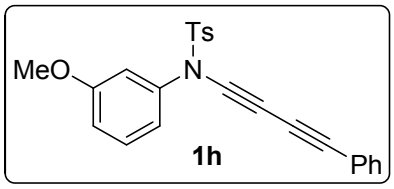
Spectral data for *N*-(3-bromophenyl)-4-methyl-*N*-(phenylbuta-1,3-diyn-1-

yl)benzenesulfonamide (1g)



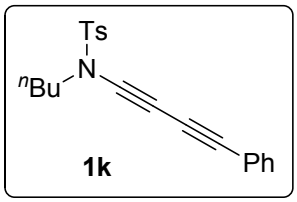
Brown Liquid; (387 mg, 0.85 mmol, 86 %); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.60 (d, *J* = 8.0 Hz, 2H), 7.45 (t, *J* = 7.5 Hz, 3H), 7.38 (s,1 H), 7.35-7.28 (m, 5H), 7.23-7.18 (m, 2H), 2.44 (s, 3H) ; ^{13}C NMR (150 MHz, $CDCl_3$): δ 146.0, 139.5, 132.9, 132.7, 131.9, 130.7, 130.1, 129.4, 129.3, 128.7, 128.4, 125.1, 122.7, 121.9, 82.1, 73.7, 73.4, 58.7, 22.0; EI-MS calcd. for $C_{23}H_{16}BrNO_2S$: 449.0085; Found: 449.0080.

Spectral data for *N*-(3-methoxyphenyl)-4-methyl-*N*-(phenylbuta-1,3-diyn-1-yl)benzenesulfonamide (1h)



Brown Liquid; (186 mg, 0.46 mmol, 70%); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.62 (d, *J* = 8.4 Hz, 2H), 7.46-7.44 (m, 2H), 7.32-7.27 (m, 5H), 7.20 (t, *J* = 8.4 Hz, 1H), 6.80-6.77 (m, 2H), 3.74 (s, 3H), 2.43 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 160.0, 145.4, 138.9, 133.0, 132.3, 129.8, 129.7, 128.9, 128.4, 128.2, 121.9, 118.3, 114.7, 111.9, 81.5, 74.2, 73.4, 57.8, 55.5, 21.7; EI-MS calcd. for $C_{24}H_{19}NO_3S$: 401.1086; Found: 401.1083

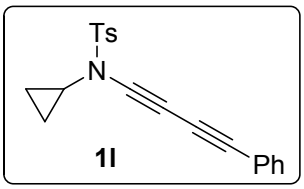
Spectral data for *N*-butyl-4-methyl-*N*-(phenylbuta-1,3-diyn-1-yl)benzenesulfonamide (1k)



White solid; (1.50 g, 4.27 mmol, 74%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.80 (d, *J* = 8.0 Hz, 2H), 7.45 (d, *J* = 78.0 Hz, 2H), 7.36-7.26 (m, 5H), 3.34 (t, *J* = 7.2 Hz, 2H), 2.44 (s, 3H), 1.66-1.57 (m, 2H), 1.37-1.27 (m, 2H), 0.89 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 145.0, 134.4, 132.3, 130.0, 128.9, 128.3, 127.5, 122.0, 80.9, 74.1, 73.5, 58.1, 51.3, 29.8, 21.6, 19.4, 13.5; EI-MS (M) calcd. for $C_{21}H_{21}NO_2S$: 351.1293; Found: 351.1296.

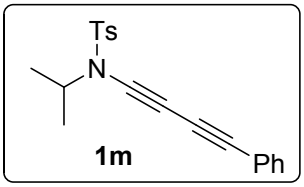
Spectral data for *N*-cyclopropyl-4-methyl-*N*-(phenylbuta-1,3-diyn-1-

yl)benzenesulfonamide (1l)



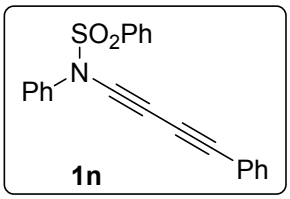
Yellow liquid; (484 mg, 1.44 mmol, 68 %); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.84 (d, *J* = 8.4 Hz, 2H), 7.46-7.44 (m, 2H), 7.36 (d, *J* = 8.4 Hz, 2H), 7.37-7.27 (m, 3H), 2.80-2.77 (m, 1H), 2.45 (s, 3H), 0.87-0.84 (m, 2H), 0.80-0.76 (m, 2H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 145.2, 133.9, 132.3, 129.9, 128.9, 128.4, 127.9, 122.0, 81.1, 73.5, 73.4, 57.9, 32.9, 21.7, 6.7; ESI-MS (M+Na) calcd. for $C_{20}H_{17}NNaO_2S$: 358.08788; Found: 358.0873

Spectral data for *N*-isopropyl-4-methyl-*N*-(phenylbuta-1,3-diyn-1-yl)benzenesulfonamide (1m)



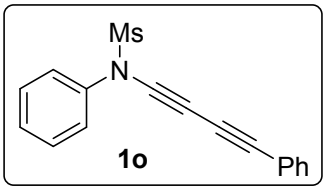
Yellow liquid; (259 mg, 0.70 mmol, 73%); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.80 (d, *J* = 8.4 Hz, 2H), 7.47-7.45 (m, 2H), 7.34-7.28 (m, 5H), 4.16-4.10 (m, 1H), 2.43 (s, 3H), 1.12 (q, *J* = 7.2 Hz, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 144.9, 135.6, 132.3, 129.9, 128.9, 128.4, 127.4, 122.1, 80.8, 73.8, 71.4, 60.1, 53.2, 21.7, 20.9; ESI-MS (M+Na) calcd. for $C_{20}H_{19}NNaO_2S$: 360.1034; Found: 360.1034.

Spectral data for *N*-phenyl-*N*-(phenylbuta-1,3-diyn-1-yl)benzenesulfonamide (1n)



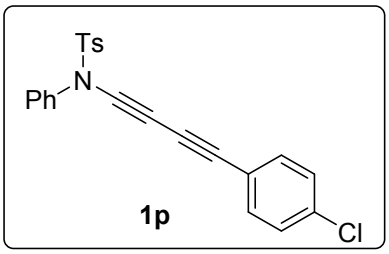
White solid; (533 mg, 1.49 mmol, 45%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.73 (d, *J* = 7.2 Hz, 2H), 7.66 (t, *J* = 7.2 Hz, 1H), 7.51 (d, *J* = 7.2 Hz, 2H), 7.47 (dd, *J* = 8.0, 1.2 Hz, 2H), 7.32~7.28 (m, 6H), 7.23-7.22 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 137.8, 135.7, 134.2, 132.3, 129.3, 129.1, 128.8, 128.3, 128.0, 126.2, 121.7, 81.5, 74.1, 73.2, 57.7, one 'C' merge with others; ESI-MS (M+Na) calcd. for $C_{22}H_{15}NNaO_2S$: 380.0721; Found: 380.07139.

Spectral data for *N*-phenyl-*N*-(phenylbuta-1,3-diyn-1-yl)methanesulfonamide (1o)



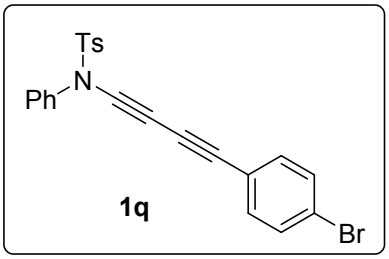
Brown solid; (324 mg, 0.87 mmol, 75%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.51-7.28(m, 10H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 137.7, 132.3, 129.6, 129.1, 128.8, 128.4, 125.6, 121.7, 81.9, 73.3, 72.9, 58.4, 37.6; ESI-MS (M+H) calcd. for $C_{17}H_{14}NO_2S$: 296.0745; Found: 296.0743.

Spectral data for *N*-((4-chlorophenyl)buta-1,3-diyn-1-yl)-4-methyl-*N*-phenylbenzenesulfonamide (1p)



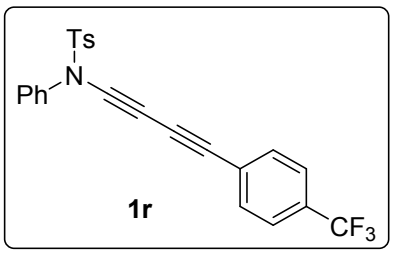
White solid; (940 mg, 2.32 mmol, 63%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.58 (d, *J* = 8.4 Hz, 2H), 7.38-7.20 (m, 11H), 2.42 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 145.4, 137.9, 135.1, 133.5, 132.9, 129.7, 129.3, 128.8, 128.1, 126.3, 120.4, 80.2, 74.9, 74.4, 57.5, 21.7, one 'C' merge with others; ESI-MS (M+Na) calcd. for $C_{23}H_{16}ClNNaO_2S$: 428.0488; Found: 428.05002.

Spectral data for *N*-((4-bromophenyl)buta-1,3-diyn-1-yl)-4-methyl-*N*-phenylbenzenesulfonamide (1q)



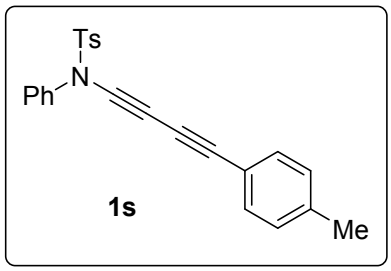
White solid; (860 mg, 1.91 mmol, 52%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.59 (d, *J* = 8.4 Hz, 2H), 7.42 (d, *J* = 8.4 Hz, 2H), 7.32-7.27 (m, 7H), 7.24-7.20 (m, 2H), 2.42 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 145.4, 137.9, 133.6, 132.9, 131.7, 129.7, 129.3, 128.7, 128.1, 126.3, 123.4, 120.9, 80.3, 74.9, 74.6, 57.6, 21.7; ESI-MS (M+Na) calcd. for $C_{23}H_{16}BrNNaO_2S$: 471.9983; Found: 471.99804.

Spectral data for 4-methyl-*N*-phenyl-*N*-((4-(trifluoromethyl)phenyl)buta-1,3-diyn-1-yl)benzenesulfonamide (1r)



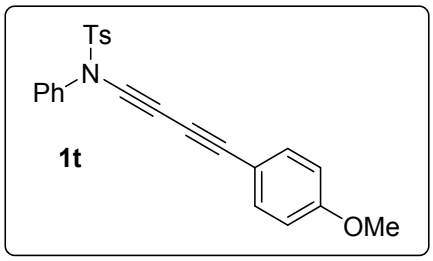
White solid; (350 mg, 0.80 mmol, 70%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.59 (d, *J* = 5.6 Hz, 2H), 7.54 (s, 4H), 7.35-7.32 (m, 3H), 7.29 (d, *J* = 5.6 Hz, 2H), 7.25-7.21 (m, 2H), 2.43 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 145.6, 137.7, 132.9, 132.4, 130.7, 130.5, 130.3, 130.1, 129.8, 129.3, 128.8, 128.1, 126.4, 126.3, 125.8, 125.3, 124.6, 122.8, 121.9, 79.9, 75.8, 75.6, 57.4, 21.7; ESI-MS (M+Na) calcd. for $C_{24}H_{16}F_3NNaO_2S$: 462.0752; Found: 462.07779.

Spectral data for 4-methyl-*N*-phenyl-*N*-(*p*-tolylbuta-1,3-diyn-1-yl)benzene sulfonamide (1s)



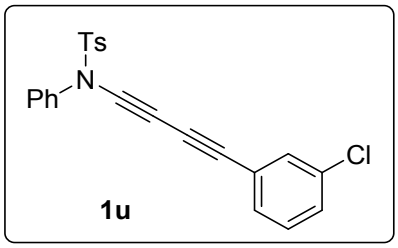
Yellow solid; (247 mg, 0.64 mmol, 68%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.59 (d, *J* = 8.4 Hz, 2H), 7.36-7.21 (m, 9H), 7.09 (d, *J* = 8.0 Hz, 2H), 2.42 (s, 3H), 2.32 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 145.3, 139.4, 138.0, 132.8, 132.2, 129.7, 129.2, 129.1, 128.6, 128.1, 126.2, 118.7, 81.7, 74.0, 72.7, 57.8, 21.6, 21.5; ESI-MS (M+H) calcd. for $C_{24}H_{20}NO_2S$: 386.1215; Found: 386.12195.

Spectral data for *N*-((4-methoxyphenyl)buta-1,3-diyn-1-yl)-4-methyl-*N*-phenylbenzenesulfonamide (1t)



Yellow solid; (720 mg, 1.79 mmol, 49%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.59 (d, *J* = 8.4 Hz, 2H), 7.40 (d, *J* = 8.4 Hz, 2H), 7.32-7.21 (m, 7H), 6.81 (d, *J* = 8.8 Hz, 2H), 3.78 (s, 3H), 2.42 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 160.2, 145.3, 138.1, 134.1, 133.0, 129.7, 129.2, 128.6, 128.1, 126.3, 114.2, 113.8, 81.6, 73.8, 72.1, 57.9, 55.3, 21.7; ESI-MS (M+Na) calcd. for $C_{24}H_{19}NNaO_3S$: 424.0983; Found: 424.09817.

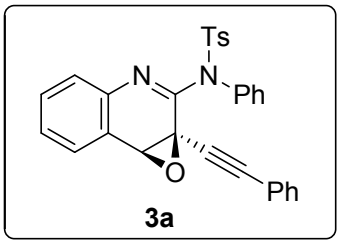
Spectral data for *N*-((3-chlorophenyl)buta-1,3-diyn-1-yl)-4-methyl-*N*-phenylbenzenesulfonamide (1u)



1u

Yellow solid; (263 mg, 0.64 mmol, 44%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.58 (d, *J* = 5.6 Hz, 2H), 7.42 (s, 1H), 7.33-7.28 (m, 7H), 7.23-7.20 (m, 3H), 2.43 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 145.5, 137.8, 134.2, 132.9, 132.0, 130.4, 129.8, 129.6, 129.3, 129.3, 128.8, 128.1, 126.3, 123.7, 79.9, 75.0, 74.6, 57.4, 21.7; ESI-MS (M+Na) calcd. for $C_{23}H_{16}ClNNaO_2S$: 428.0488; Found: 428.04764.

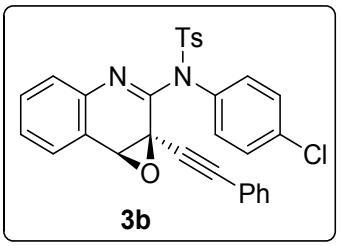
Spectral data for 4-methyl-*N*-phenyl-*N*-((1a*R*,7b*S*)-1a-(phenylethynyl)-1a,7b-dihydrooxireno[2,3-*c*]quinolin-2-yl)benzenesulfonamide (3a)



3a

White solid; (71.9 mg, 0.14 mmol, 68%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.76 (d, *J* = 8.0 Hz, 2H), 7.58-7.48 (m, 3H), 7.40-7.35 (m, 5H), 7.34-7.29 (m, 5H), 7.25 (d, *J* = 8.0 Hz, 2H), 4.65 (s, 1H), 2.40 (s, 3H), two 'C' merge with others; ^{13}C NMR (100 MHz, $CDCl_3$): δ 151.6, 143.9, 141.0, 136.9, 136.1, 131.9, 130.4, 130.4, 129.6, 129.2, 129.1, 128.7, 128.6, 128.3, 127.4, 123.3, 121.3, 86.5, 83.2, 65.5, 53.3, 21.5; ESI-MS (M+H) calcd. for $C_{30}H_{23}N_2O_3S$: 491.1423; Found: 491.14231

Spectral data for *N*-(4-chlorophenyl)-4-methyl-*N*-((1aR,7bS)-1a-(phenylethynyl)-1a,7b-dihydrooxireno[2,3-*c*]quinolin-2-yl)benzenesulfonamide (3b)

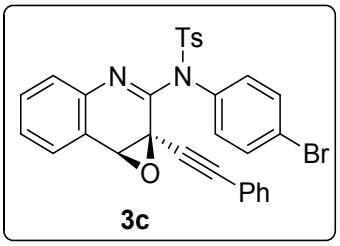


3b

White solid; (61 mg, 0.11 mmol, 80%); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.74 (d, *J* = 8.4 Hz, 2H), 7.59 (d, *J* = 6.6Hz, 1H), 7.53-7.49 (m, 2H), 7.35-7.25(m, 10H), 7.25 (d, *J* =

8.4Hz, 2H), 4.65 (s, 1H), 2.41 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 151.3, 144.3, 140.9, 135.7, 135.3, 134.9, 131.9, 131.6, 130.6, 129.7, 129.3, 128.9, 128.8, 128.7, 128.4, 127.6, 123.3, 121.1, 86.9, 83.0, 65.5, 53.2, 21.6, one 'C' merge with others; ESI-MS (M+Na) calcd. for $C_{30}H_{21}ClN_2NaO_3S$: 547.0859; Found: 547.0856.

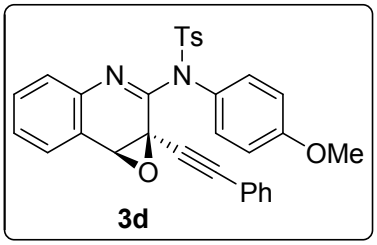
Spectral data for *N*-(4-bromophenyl)-4-methyl-*N*-((1aR,7bS)-1a-(phenylethynyl)-1a,7b-dihydrooxireno[2,3-*c*]quinolin-2-yl)benzenesulfonamide (3c)



3c

White solid; (96 mg, 0.16 mmol, 76 %); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.74 (d, *J* = 8.4 Hz, 2H), 7.58 (d, *J* = 7.2 Hz, 1H), 7.53-7.48 (m, 4H), 7.37-7.30(m, 6H), 7.27-7.23(m, 4H), 4.65 (s, 1H), 2.41 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 151.2, 144.3, 140.8, 135.8, 135.7, 131.9, 131.9, 131.8, 130.6, 129.7, 128.8, 128.7, 128.4, 127.6, 123.3, 123.1, 121.0, 86.9, 82.9, 65.5, 53.2, 21.6, one 'C' merge with others; ESI-MS (M+Na) calcd. for $C_{30}H_{21}BrN_2NaO_3S$: 591.0354; Found: 591.0361

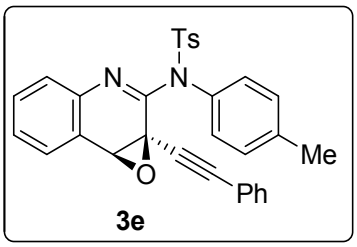
Spectral data for *N*-(4-methoxyphenyl)-4-methyl-*N*-((1a*R*,7b*S*)-1a-(phenylethynyl)-1a,7b-dihydrooxireno[2,3-*c*]quinolin-2-yl)benzenesulfonamide (3d)



3d

Yellow solid; (65 mg, 0.12 mmol, 84 %); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.76 (d, *J* = 8.4 Hz, 2H), 7.56 (d, *J* = 7.2 Hz, 1H), 7.52-7.47 (m, 2H), 7.35-7.25 (m, 10H), 6.86 (d, *J* = 9.6 Hz, 2H), 4.62 (s, 1H), 3.80 (s, 3H), 2.40 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 151.9, 151.5, 143.9, 141.1, 135.9, 131.9, 131.8, 130.5, 129.8, 129.3, 129.2, 129.0, 128.6, 128.5, 128.3, 127.3, 123.2, 121.3, 113.8, 86.4, 83.4, 65.5, 55.4, 53.2, 21.6; ESI-MS (M+Na) calcd. for $C_{31}H_{24}N_2NaO_4S$: 543.1354; Found: 543.1368

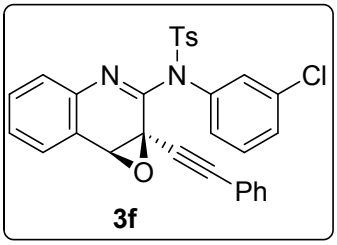
Spectral data for 4-methyl-*N*-((1a*R*,7b*S*)-1a-(phenylethynyl)-1a,7b-dihydrooxireno[2,3-*c*]quinolin-2-yl)-*N*-(*p*-tolyl)benzenesulfonamide (3e)



3e

White solid; (59 mg, 0.11 mmol, 76 %); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.75 (d, *J* = 8.4 Hz, 2H), 7.57 (d, *J* = 7.2 Hz, 1H), 7.52-7.47 (m, 2H), 7.36-7.29 (m, 6H), 7.25 (t, *J* = 9.0, 4H), 7.16 (d, *J* = 7.6 Hz, 2H), 4.63 (s, 1H), 2.40 (s, 3H), 2.38 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 151.6, 143.9, 141.0, 138.9, 136.0, 133.9, 131.9, 130.5, 130.3, 129.7, 129.3, 129.2, 1291.1, 128.6, 128.3, 127.3, 123.2, 121.3, 86.4, 83.2, 65.5, 53.2, 21.6, 21.3, one 'C' merge with others; ESI-MS (M+Na) calcd. for $C_{31}H_{24}N_2NaO_3S$: 527.1508; Found: 527.1351

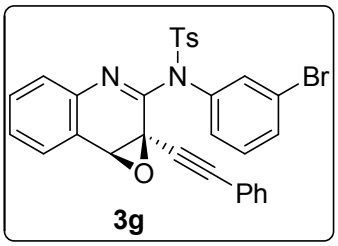
Spectral data for *N*-(3-chlorophenyl)-4-methyl-*N*-((1aR,7b*S*)-1a-(phenylethynyl)-1a,7b-dihydrooxireno[2,3-*c*]quinolin-2-yl)benzenesulfonamide (3f)



3f

Yellow solid; (62 mg, 0.11 mmol, 80 %); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.75 (d, *J* = 8.4 Hz, 2H), 7.59 (d, *J* = 7.2 Hz, 1H), 7.54-7.49 (m, 3H), 7.36-7.25 (m, 10H), 7.16 (td, *J* = 7.8, 1.2 Hz, 1H), 4.66 (s, 1H), 2.41 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 151.3, 144.3, 140.8, 137.9, 135.8, 134.3, 132.0, 130.8, 130.6, 129.6, 129.5, 129.3, 129.0, 128.8, 128.7, 128.4, 128.0, 127.7, 123.4, 120.9, 86.9, 82.8, 65.6, 53.3, 21.6, one 'C' merge with others; ESI-MS (M+Na) calcd. for $C_{30}H_{21}ClN_2NaO_3S$: 547.0859; Found: 547.0858

Spectral data for *N*-(3-bromophenyl)-4-methyl-*N*-((1aR,7b*S*)-1a-(phenylethynyl)-1a,7b-dihydrooxireno[2,3-*c*]quinolin-2-yl)benzenesulfonamide (3g)

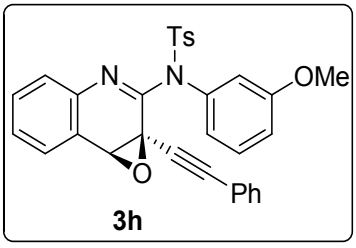


3g

Yellow solid; (59 mg, 0.10 mmol, 78 %); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.72 (d, *J* = 8.4 Hz, 2H), 7.67 (s, 1H), 7.56 (d, *J* = 7.8 Hz, 1H), 7.51-7.46 (m, 3H), 7.35-7.28 (m,

6H), 7.24-7.16(m, 4H), 4.63 (s, 1H), 2.38 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 151.3, 144.3, 140.8, 138.0, 135.8, 133.7, 132.1, 131.9, 130.6, 129.8, 129.6, 129.3, 128.8, 128.7, 128.4, 128.3, 127.7, 123.4, 122.1, 120.9, 87.0, 82.6, 65.5, 53.3, 21.6, one 'C' merge with others; ESI-MS (M+Na) calcd. for $C_{30}H_{21}BrN_2NaO_3S$: 591.0354; Found: 591.036.

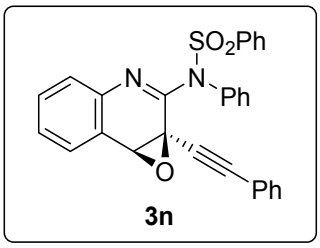
Spectral data for *N*-(3-methoxyphenyl)-4-methyl-*N*-((1aR,7b*S*)-1a-(phenylethynyl)-1a,7b-dihydrooxireno[2,3-*c*]quinolin-2-yl)benzenesulfonamide (3h)



3h

White solid; (55 mg, 0.10 mmol, 71 %); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.73 (d, *J* = 8.4 Hz, 2H), 7.55 (d, *J* = 7.8 Hz, 1H), 7.49-7.45 (m, 2H), 7.33-7.25 (m, 6H), 7.21 (d, *J* = 8.4 Hz, 3H), 6.97 (t, *J* = 8.4 Hz, 1H), 6.92 (dd, *J* = 8.4, 1.8 Hz, 1H), 6.81 (td, *J* = 7.8, 1.2 Hz, 1H), 4.61 (s, 1H), 3.54 (s, 3H), 2.37 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 159.7, 151.6, 144.0, 140.9, 137.8, 136.1, 132.0, 130.5, 129.7, 129.3, 129.2, 129.0, 128.6, 128.3, 127.4, 123.3, 122.2, 121.3, 115.7, 115.6, 86.5, 83.1, 65.7, 55.2, 53.4, 21.6, one 'C' merge with others; ESI-MS (M+Na) calcd. for $C_{31}H_{24}N_2NaO_4S$: 543.1354; Found: 543.1356.

Spectral data for *N*-phenyl-*N*-((1a*R*,7b*S*)-1a-(phenylethynyl)-1a,7b-dihydrooxireno[2,3-*c*]quinolin-2-yl)benzenesulfonamide (3n)

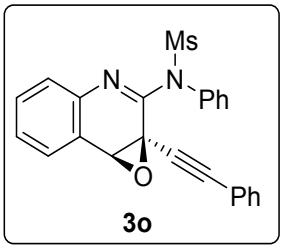


3n

White solid; (100.7 mg, 0.21 mmol, 75%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.86 (d, *J* = 7.6 Hz, 2H), 7.59-7.54 (m, 2H), 7.52-7.49 (m, 2H), 7.45 (t, *J* = 8.0 Hz, 3H), 7.47-7.39 (m, 5H), 7.34-7.31 (m, 5H), 4.65 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 151.5, 140.9, 139.1, 136.6, 133.1, 132.0, 130.5, 130.3, 129.5, 129.3, 129.2, 128.9, 128.7, 128.6, 128.3, 128.0, 127.5, 123.3, 121.2, 86.6, 83.1, 65.5, 53.3; ESI-MS (M+Na) calcd. for $C_{29}H_{21}N_2NaO_3S$: 499.1092; Found: 499.1092.

Spectral data for *N*-phenyl-*N*-((1a*R*,7b*S*)-1a-(phenylethynyl)-1a,7b-

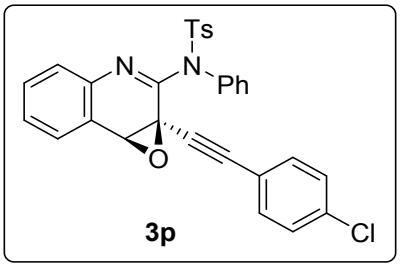
dihydrooxireno[2,3-*c*]quinolin-2-yl)methanesulfonamide (3o)



3o

White solid; (73 mg, 0.17 mmol, 62%); ^{1}H NMR (700 MHz, $CDCl_3$): δ 7.63 (d, *J* = 7.7 Hz, 2H), 7.60 (d, *J* = 7.7 Hz, 1H), 7.53-7.49 (m, 3H), 7.44-7.40 (m, 3H), 7.37-7.31 (m, 2H), 7.30-7.27 (m, 4H), 4.70 (s, 3H), 3.45 (s,3H); ^{13}C NMR (175 MHz, $CDCl_3$): δ 152.4, 140.7, 136.4, 131.9, 130.6, 129.7, 129.3, 129.2, 128.9, 128.9, 128.2, 127.8, 123.5, 121.1, 86.6, 82.8, 65.6, 53.5, 40.4, one 'C' merge with others; ESI-MS (M+Na) calcd. for $C_{24}H_{18}N_2NaO_3S$: 437.0936; Found: 437.0927.

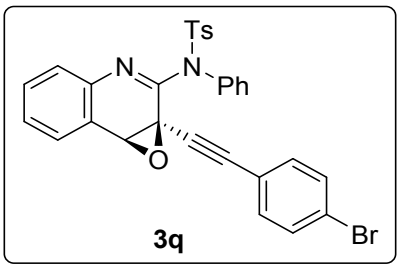
Spectral data for *N*-((1a*R*,7bS)-1a-((4-chlorophenyl)ethynyl)-1a,7b-dihydrooxireno[2,3-*c*]quinolin-2-yl)-4-methyl-*N*-phenylbenzenesulfonamide (3p)



3p

White solid; (70.8 mg, 0.13 mmol, 64%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.73 (d, *J* = 8.4 Hz, 2H), 7.58 (d, *J* = 7.6 Hz, 1H), 7.53-7.48 (m, 2H), 7.40-7.36 (m, 5H), 7.34-7.27 (m, 3H), 7.25-7.21 (m, 4H), 4.64 (s, 1H), 2.40 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 151.4, 144.1, 141.0, 136.7, 136.0, 135.4, 133.2, 130.6, 130.3, 129.7, 129.3, 128.8, 128.7, 128.7, 127.5, 123.2, 119.7, 85.4, 84.2, 65.5, 53.3, 21.6, two 'C' merge with others; ESI-MS (M+H) calcd. for $C_{30}H_{22}ClN_2O_3S$: 525.1040; Found: 525.10558

Spectral data for *N*-((1a*R*,7bS)-1a-((4-bromophenyl)ethynyl)-1a,7b-dihydrooxireno[2,3-*c*]quinolin-2-yl)-4-methyl-*N*-phenylbenzenesulfonamide (3q)

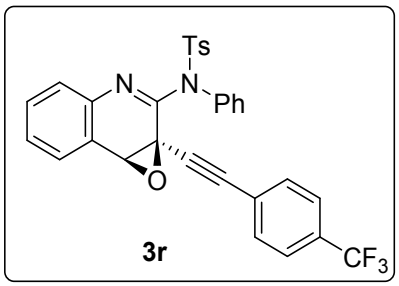


3q

White solid; (75.4 mg, 0.13 mmol, 70%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.72 (d, *J* = 8.4 Hz, 2H), 7.58 (d, *J* = 8.0 Hz, 1H), 7.53-7.49 (m, 2H), 7.48-7.43 (3, 2H), 7.40-7.29

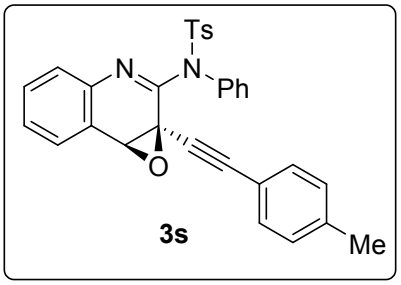
(m, 5H), 7.25-7.23 (m, 3H), 7.17-7.14 (m, 2H), 4.63 (s, 1H), 2.40 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 151.4, 144.1, 141.0, 136.8, 136.1, 133.4, 131.7, 130.6, 130.4, 129.7, 129.3, 128.8, 128.7, 128.7, 127.5, 123.7, 123.2, 120.2, 85.5, 84.4, 65.6, 53.3, 21.6, two 'C' merge with others; ESI-MS (M+Na) calcd. for $C_{30}H_{21}BrN_2NaO_3S$: 591.0354; Found: 591.03652

Spectral data for 4-methyl-*N*-phenyl-*N*-((1a*R*,7b*S*)-1a-((4-(trifluoromethyl)phenyl)ethynyl)-1a,7b-dihydrooxireno[2,3-*c*]quinolin-2-yl)benzenesulfonamide (3r)



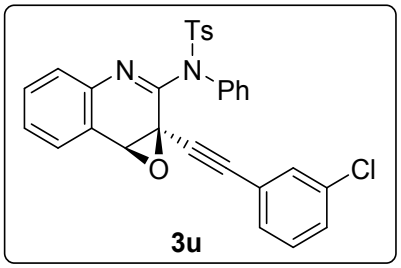
White solid; (73.4 mg, 0.13 mmol, 57%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.72 (d, *J* = 8.4 Hz, 2H), 7.60-7.56 (m, 3H), 7.52-7.50 (m, 2H), 7.42-7.30 (m, 8H), 7.25 (d, *J* = 8.0 Hz, 2H), 4.67 (s, 1H), 2.40 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 151.1, 144.1, 140.9, 136.7, 135.9, 132.2, 131.0, 130.6, 130.3, 129.6, 129.4, 129.3, 129.2, 128.8, 128.7, 128.7, 128.2, 127.9, 127.6, 125.3, 125.2, 125.0, 123.6, 123.0, 122.3, 85.5, 84.9, 65.5, 53.1, 21.6; ESI-MS (M+Na) calcd. for $C_{31}H_{21}F_3N_2NaO_3S$: 581.1123; Found: 581.11064

Spectral data for 4-methyl-*N*-phenyl-*N*-((1a*R*,7b*S*)-1a-(*p*-tolylethynyl)-1a,7b-dihydrooxireno[2,3-*c*]quinolin-2-yl)benzenesulfonamide (3s)



White solid; (34.9 mg, 0.07 mmol, 27%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.74 (d, *J* = 8.4 Hz, 2H), 7.57 (d, *J* = 7.2 Hz, 1H), 7.53-7.47 (m, 2H), 7.39-7.38 (m, 5H), 7.31 (td, *J* = 7.2, 2.0 Hz, 1H), 7.25-7.19 (m, 4H), 7.11 (d, *J* = 8.0 Hz, 2H), 4.62 (s, 1H), 2.40 (s, 3H), 2.35 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 151.7, 144.0, 141.0, 139.4, 136.7, 136.1, 131.9, 130.5, 129.7, 129.3, 129.0, 128.7, 128.6, 127.4, 123.4, 118.2, 86.8, 82.5, 65.5, 53.3, 21.6, 21.5, two 'C' merge with others; ESI-MS (M+Na) calcd. for $C_{31}H_{24}N_2NaO_3S$: 527.1405; Found: 527.13978.

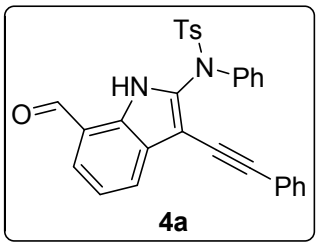
Spectral data for *N*-((1a*R*,7b*S*)-1a-((3-chlorophenyl)ethynyl)-1a,7b-dihydrooxireno[2,3-*c*]quinolin-2-yl)-4-methyl-*N*-phenylbenzenesulfonamide (3u)



3u

White solid; (70.5 mg, 0.13 mmol, 65%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.74 (d, *J* = 5.6 Hz, 2H), 7.57 (d, *J* = 5.2 Hz, 1H), 7.53-7.49 (m, 2H), 7.43-7.37 (m, 5H), 7.36-7.31 (m, 2H), 7.28-7.19 (m, 5H), 4.64 (s, 1H), 2.39 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 151.2, 144.1, 140.9, 136.7, 135.9, 134.1, 131.8, 130.6, 130.3, 130.1, 129.7, 129.6, 129.5, 129.3, 128.8, 128.7, 128.7, 127.5, 123.1, 122.9, 84.9, 84.3, 65.5, 53.2, 21.6, one 'C' merge with others; ESI-MS (M+Na) calcd. for $C_{30}H_{21}ClN_2O_3S$: 547.0859; Found: 547.08523

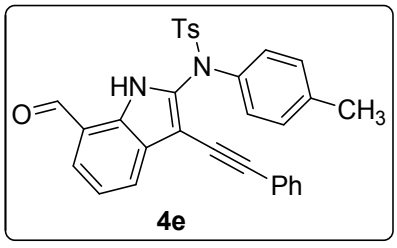
Spectral data for *N*-(7-formyl-3-(phenylethynyl)-1H-indol-2-yl)-4-methyl-*N*-phenylbenzenesulfonamide (4a)



4a

Yellow solid; (18 mg, 0.03 mmol, 17 %); ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.47 (s, 1H), 10.12 (s, 1H), 7.95 (d, *J* = 8.0 Hz, 1H), 7.72 (d, *J* = 8.0 Hz, 3H), 7.54 (dt, *J* = 8.4, 1.2 Hz, 2H), 7.36-7.29 (m, 7H), 7.24-7.19 (m, 2H), 7.17 (d, *J* = 8.0 Hz, 2H), 2.21 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 192.9, 144.4, 139.9, 137.2, 136.7, 131.7, 130.5, 130.3, 129.7, 129.3, 129.0, 128.4, 128.3, 128.2, 128.1, 128.0, 127.2, 123.4, 120.7, 96.2, 94.7, 80.6, 21.2, one 'C' merge with others; ESI-MS (M+Na) calcd. for $C_{30}H_{22}N_2NaO_3S$: 513.1249; Found: 513.12725.

Spectral data for *N*-(7-formyl-3-(phenylethynyl)-1*H*-indol-2-yl)-4-methyl-*N*-(*p*-tolyl)benzenesulfonamide (4e)

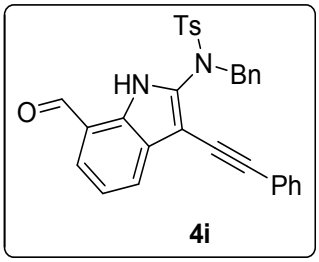


4e

Yellow solid; (8 mg, 0.015 mmol, 10 %); ^{1}H NMR (600 MHz, $CDCl_3$): δ 10.44 (s, 1H),

10.11 (s, 1H), 7.93 (d, *J* = 7.8 Hz, 1H), 7.71 (d, *J* = 8.4 Hz, 3H), 7.41 (d, *J* = 8.4 Hz, 2H), 7.32-7.29 (m, 4H), 7.21-7.20 (m, 2H), 7.17 (d, *J* = 7.8 Hz, 2H), 7.12 (d, *J* = 7.8 Hz, 2H), 2.29 (s, 3H), 2.22 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 192.9, 144.3, 138.6, 137.4, 137.1, 136.6, 131.1, 130.4, 130.2, 129.9, 129.7, 129.5, 129.0, 128.5, 128.2, 128.1, 127.9, 127.1, 123.4, 120.6, 95.7, 94.5, 80.7, 21.4, 21.1; ESI-MS (M+Na) calcd. for $C_{31}H_{24}N_2NaO_3S$: 527.1405; Found: 527.1410.

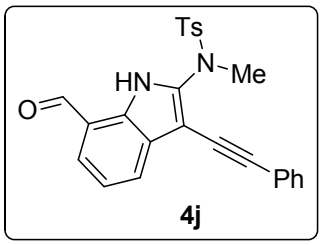
Spectral data for *N*-benzyl-*N*-(7-formyl-3-(phenylethynyl)-1H-indol-2-yl)-4-methylbenzenesulfonamide (4i)



4i

White solid; (50.3 mg, 0.10 mmol, 56%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.14 (s, 1H), 10.01 (s, 1H), 7.90 (d, *J* = 8.0 Hz, 1H), 7.68 (d, *J* = 8.0 Hz, 2H), 7.61 (d, *J* = 7.2 Hz, 1H), 7.38-7.32 (m, 5H), 7.28-7.15 (m, 8H), 5.07 (s, 2H), 2.16 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 192.5, 144.4, 136.6, 135.2, 134.7, 130.9, 130.2, 129.9, 129.8, 128.7, 128.6, 128.5, 128.2, 128.0, 128.0, 127.8, 126.6, 123.1, 120.4, 120.3, 95.8, 94.4, 80.0, 53.3, 21.2; ESI-MS (M+Na) calcd. for $C_{31}H_{24}N_2NaO_3S$: 527.1405; Found: 527.14095

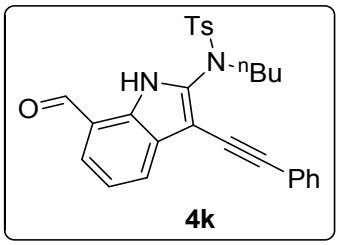
Spectral data for *N*-(7-formyl-3-(phenylethynyl)-1H-indol-2-yl)-*N*,4-dimethylbenzenesulfonamide (4j)



4j

White solid; (60.6 mg, 0.14 mmol, 65%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.34 (s, 1H), 10.12 (s, 1H), 7.92 (d, *J* = 8.0 Hz, 1H), 7.71 (d, *J* = 7.2 Hz, 1H), 7.61 (d, *J* = 8.4 Hz, 2H), 7.34-7.26 (m, 4H), 7.18-7.12 (m, 4H), 3.49 (s, 3H), 2.15 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 192.7, 144.5, 138.8, 133.3, 130.8, 130.0, 129.9, 129.7, 128.8, 128.1, 127.9, 127.9, 126.6, 123.1, 120.5, 95.0, 93.0, 79.8, 37.9, 21.3, one 'C' merge with others; ESI-MS (M+Na) calcd. for $C_{25}H_{20}N_2NaO_3S$: 451.1092; Found: 451.10852

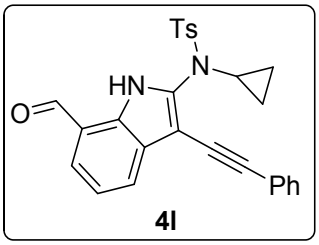
Spectral data for *N*-butyl-*N*-(7-formyl-3-(phenylethynyl)-1H-indol-2-yl)-4-methylbenzenesulfonamide (4k)



4k

White solid; (70.6 mg, 0.15 mmol, 67%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.27 (s, 1H), 10.13 (s, 1H), 7.95 (d, *J* = 8.0 Hz, 1H), 7.72 (d, *J* = 7.2 Hz, 1H), 7.62 (d, *J* = 8.0 Hz, 2H), 7.35-7.27 (m, 4H), 7.24-7.13 (m, 4H), 3.87 (t, *J* = 6.8 Hz, 2H), 2.12 (s, 3H), 1.56-1.49 (m, 2H), 1.39-1.33 (m, 2H), 0.85 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 192.8, 144.2, 136.9, 134.7, 130.8, 130.3, 130.0, 129.7, 128.8, 128.1, 127.9, 127.7, 126.7, 123.1, 120.5, 120.4, 95.2, 94.2, 79.7, 49.7, 30.6, 21.2, 19.6, 13.6; ESI-MS (M+Na) calcd. for $C_{28}H_{26}N_2NaO_3S$: 493.1562; Found: 493.15637.

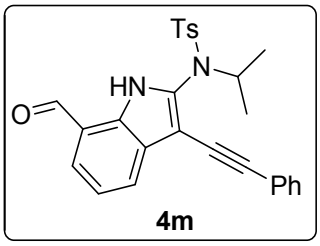
Spectral data for *N*-cyclopropyl-*N*-(7-formyl-3-(phenylethynyl)-1*H*-indol-2-yl)-4-methylbenzenesulfonamide (4l)



4l

Yellow solid; (49 mg, 0.11 mmol, 61 %); ^{1}H NMR (600 MHz, $CDCl_3$): δ 10.14 (s, 1H), 10.11 (s, 1H), 7.95 (d, *J* = 7.8 Hz, 1H), 7.71 (d, *J* = 7.2 Hz, 3H), 7.35 (t, *J* = 7.8 Hz, 1H), 7.26 (t, *J* = 8.4 Hz, 3H), 7.19 (d, *J* = 7.8 Hz, 2H), 7.11-7.10 (m, 2H), 3.17-3.14 (m, 1H), 2.17 (s, 3H), 0.95 (d, *J* = 7.2 Hz, 2H), 0.84 (d, *J* = 6.6 Hz, 2H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 192.8, 144.5, 139.1, 133.9, 130.9, 130.2, 129.9, 129.7, 128.9, 128.3, 128.1, 127.9, 126.8, 123.3, 120.5, 120.4, 94.1, 93.9, 80.3, 32.0, 21.4, 8.4 ; ESI-MS (M+Na) calcd. for $C_27H_{22}N_2NaO_3S$: 477.1249; Found: 477.1237.

Spectral data for *N*-(7-formyl-3-(phenylethynyl)-1*H*-indol-2-yl)-*N*-isopropyl-4-methylbenzenesulfonamide (4m)

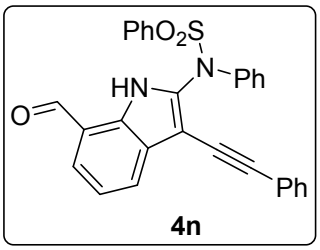


4m

Yellow solid; (46mg, 0.10 mmol, 57 %); ^{1}H NMR (600 MHz, $CDCl_3$): δ 10.12 (s, 1H), 10.03 (s, 1H), 8.01 (d, *J* = 7.8 Hz, 1H), 7.78 (d, *J* = 8.4 Hz, 2H), 7.74 (dd, *J* = 7.8, 1.8

Hz, 1H), 7.35 (t, *J* = 7.8 Hz, 1H), 7.30-7.28 (m, 3H), 7.22-7.20 (m, 2H), 7.12 (d, *J* = 7.8 Hz, 2H), 4.66-4.59 (m, 1H), 2.16 (s, 3H), 1.26 (d, *J* = 7.2 Hz, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 192.9, 143.7, 137.7, 133.0, 131.1, 130.8, 130.5, 129.6, 128.8, 128.2, 127.9, 127.7, 127.4, 123.4, 120.6, 120.5, 99.8, 93.9, 81.3, 54.2, 22.4, 21.3.; ESI-MS (M+Na) calcd. for $C_{27}H_{24}N_2NaO_3S$: 479.1405; Found: 479.1413

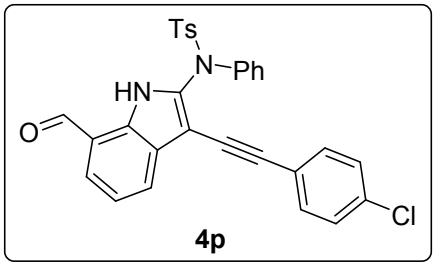
Spectral data for *N*-(7-formyl-3-(phenylethynyl)-1*H*-indol-2-yl)-*N*-phenylbenzenesulfonamide (4n)



4n

White solid; (20.2 mg, 0.04 mmol, 15%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.61 (s, 1H), 10.14 (s, 1H), 7.96 (d, *J* = 8.0 Hz, 1H), 7.88 (d, *J* = 7.2 Hz, 2H), 7.72 (dd, *J* = 7.2, 0.8 Hz, 1H), 7.55-7.53 (m, 2H), 7.48-7.45 (m, 2H), 7.427.38 (m, 2H), 7.357.27 (m, 7H), 7.24-7.21 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 193.0, 139.7, 139.6, 137.0, 133.3, 131.2, 130.4, 130.4, 129.3, 129.0, 128.9, 128.3, 128.2, 128.0, 127.2, 123.0, 120.7, 96.3, 94.8, 80.5, three 'C' merge with others; ESI-MS (M+Na) calcd. for $C_{29}H_{20}N_2NaO_3S$: 499.1092; Found: 499.10884

Spectral data for *N*-(3-((4-chlorophenyl)ethynyl)-7-formyl-1H-indol-2-yl)-4-methyl-*N*-phenylbenzenesulfonamide (4p)

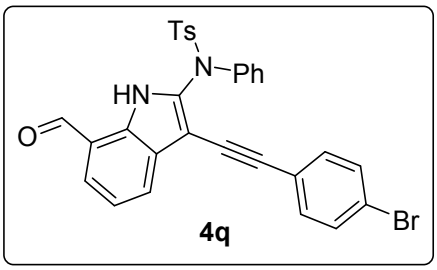


4p

White solid; (17.2 mg, 0.03 mmol, 14%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.46 (s, 1H), 10.12 (s, 1H), 7.92 (d, *J* = 7.6 Hz, 1H), 7.71 (d, *J* = 8.0 Hz, 3H), 7.48 (d, *J* = 8.4 Hz, 2H), 7.34-7.23 (m, 6H), 7.19 (d, *J* = 8.4, 2H), 7.11 (d, *J* = 8.4 Hz, 2H), 2.26 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 192.9, 144.4, 139.7, 137.5, 136.6, 133.9, 132.3, 130.4, 130.3, 129.8, 129.3, 128.8, 128.5, 128.3, 128.3, 128.1, 127.1, 121.8, 120.8, 120.7, 95.6, 93.5, 81.7, 21.5; ESI-MS (M+H) calcd. for $C_{30}H_{22}ClN_2O_3S$: 525.1040; Found: 525.10559

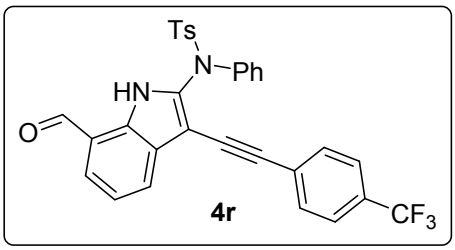
Spectral data for *N*-(3-((4-bromophenyl)ethynyl)-7-formyl-1H-indol-2-yl)-4-

methyl-*N*-phenylbenzenesulfonamide (4q)



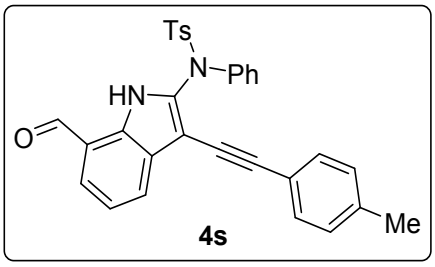
White solid; (14.8 mg, 0.03 mmol, 17%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.48 (s, 1H), 10.11 (s, 1H), 7.92 (d, *J* = 8.0 Hz, 1H), 7.71 (t, *J* = 7.2 Hz, 3H), 7.49-7.47 (m, 2H), 7.42 (dt, *J* = 6.8, 1.6 Hz, 2H), 7.34-7.28 (m, 4H), 7.19 (d, *J* = 8.0 Hz, 2H), 7.05 (d, *J* = 6.8 Hz, 2H), 2.26 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 192.9, 144.4, 139.7, 137.5, 136.6, 132.5, 131.4, 130.4, 130.3, 129.7, 129.3, 128.8, 128.3, 128.2, 128.1, 127.0, 122.3, 122.1, 120.7, 120.7, 95.6, 93.6, 82.0, 21.5; ESI-MS (M+Na) calcd. for $C_{30}H_{21}BrN_2NaO_3S$: 591.0354; Found: 591.03569

Spectral data for *N*-(7-formyl-3-((4-(trifluoromethyl)phenyl)ethynyl)-1H-indol-2-yl)-4-methyl-*N*-phenylbenzenesulfonamide (4r)



Yellow solid; (27.6 mg, 0.05 mmol, 21%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.53 (s, 1H), 10.13 (s, 1H), 7.93 (d, *J* = 8.0 Hz, 1H), 7.75-7.70 (m, 3H), 7.54 (d, *J* = 8.0 Hz, 2H), 7.48 (dd, *J* = 8.0, 1.6 Hz, 2H), 7.36-7.27 (m, 6H), 7.19 (d, *J* = 8.0 Hz, 2H), 2.24 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 193.0, 144.0, 139.7, 138.0, 136.7, 131.2, 130.3, 129.7, 129.3, 128.8, 128.4, 128.2, 128.1, 127.2, 126.9, 125.1, 120.9, 120.7, 95.1, 93.3, 83.5, 21.4; ESI-MS (M+Na) calcd. for $C_{31}H_{21}F_3N_2NaO_3S$: 581.1123; Found: 581.11242

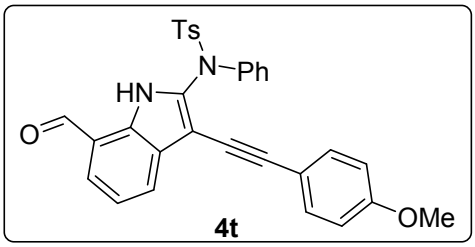
Spectral data for *N*-(7-formyl-3-(p-tolylethynyl)-1H-indol-2-yl)-4-methyl-*N*-phenylbenzenesulfonamide (4s)



Yellow oil; (23.3 mg, 0.05 mmol, 18%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.41 (s, 1H),

10.11 (s, 1H), 7.95 (d, *J* = 8.0 Hz, 1H), 7.71 (d, *J* = 8.4 Hz, 3H), 7.54-7.52 (m, 2H), 7.34-7.27 (m, 4H), 7.17 (d, *J* = 8.0 Hz, 2H), 7.10 (s, 4H), 2.36 (s, 3H), 2.24 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 192.9, 144.3, 139.8, 138.1, 137.0, 136.6, 131.1, 130.4, 130.3, 129.7, 129.2, 128.9, 128.4, 128.2, 128.1, 127.2, 120.6, 120.5, 120.2, 96.5, 94.8, 79.9, 21.5, 21.4; ESI-MS (M+Na) calcd. for $C_{31}H_{24}N_2NaO_3S$: 527.1405; Found: 527.13929

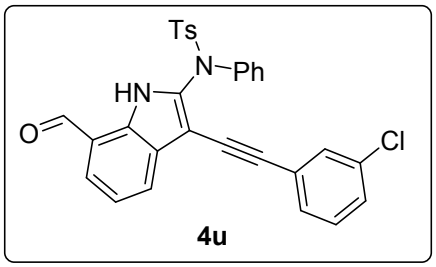
Spectral data for *N*-(7-formyl-3-(p-tolylethynyl)-1H-indol-2-yl)-4-methyl-*N*-phenylbenzenesulfonamide (4t)



4t

Yellow oil; (18.1 mg, 0.03 mmol, 18%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.45 (s, 1H), 10.11 (s, 1H), 7.94 (d, *J* = 8.0 Hz, 1H), 7.72 (t, *J* = 8.0 Hz, 3H), 7.53 (dd, *J* = 8.4, 1.2 Hz, 2H), 7.34-7.27 (m, 4H), 7.18-7.13 (m, 4H), 6.83 (d, *J* = 8.8 Hz, 2H), 3.82 (s, 3H), 2.25 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 192.9, 159.4, 144.3, 139.9, 136.8, 136.7, 132.6, 130.4, 130.3, 129.7, 129.2, 128.9, 128.3, 128.2, 128.1, 127.3, 120.6, 120.5, 115.5, 113.8, 96.6, 94.5, 79.1, 55.3, 21.5; ESI-MS (M+Na) calcd. for $C_{31}H_{24}N_2NaO_4S$: 543.1355; Found: 543.13432

Spectral data for *N*-(3-((3-chlorophenyl)ethynyl)-7-formyl-1H-indol-2-yl)-4-methyl-*N*-phenylbenzenesulfonamide (4u)

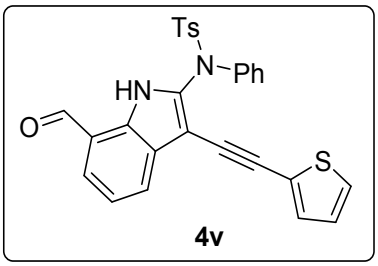


4u

Yellow oil; (15.1 mg, 0.03 mmol, 14%); ^{1}H NMR (600 MHz, $CDCl_3$): δ 10.59 (s, 1H), 10.13 (s, 1H), 7.92 (d, *J* = 7.8 Hz, 1H), 7.72 (d, *J* = 8.4 Hz, 3H), 7.51 (d, *J* = 7.8 Hz, 2H), 7.35-7.28 (m, 4H), 7.26 (d, *J* = 7.8 Hz, 1H), 7.22-7.12 (m, 3H), 7.09 (d, *J* = 7.2 Hz, 2H), 2.27 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 192.9, 144.5, 139.7, 137.7, 136.7, 134.0, 130.9, 130.4, 130.3, 129.8, 129.4, 129.3, 129.2, 128.9, 128.4, 128.3, 128.1, 128.1, 127.0, 125.0, 120.8, 120.7, 95.4, 93.2, 82.1, 21.4; ESI-MS (M+Na) calcd. for $C_{30}H_{21}ClN_2NaO_3S$: 547.0859; Found: 547.08432

Spectral data for *N*-(7-formyl-3-(thiophen-2-ylethynyl)-1H-indol-2-yl)-4-methyl-

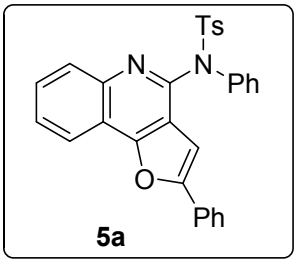
***N*-phenylbenzenesulfonamide (4v)**



4v

Yellow oil; (13.1 mg, 0.026 mmol, 18%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.45 (s, 1H), 10.11 (s, 1H), 7.91 (d, *J* = 7.6 Hz, 1H), 7.71 (t, *J* = 8.0 Hz, 3H), 7.46 (d, *J* = 7.6 Hz, 2H), 7.34-7.29 (m, 4H), 7.25-7.20 (m, 3H), 7.00-6.95 (m, 2H), 2.29 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 192.9, 144.5, 139.6, 137.5, 136.5, 131.4, 130.3, 130.2, 129.7, 129.3, 128.7, 128.5, 128.4, 128.0, 127.1, 126.9, 123.4, 120.7, 120.6, 95.5, 87.6, 84.3, 21.5; ESI-MS (M+Na) calcd. for $C_{28}H_{20}N_2NaO_3S_2$: 519.0813; Found: 519.08035.

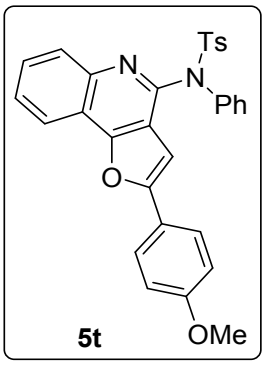
Spectral data for 4-methyl-*N*-phenyl-*N*-(2-phenylfuro[3,2-*c*]quinolin-4-yl)benzenesulfonamide (5a)



5a

White solid; (28.0 mg, 0.06 mmol, 40%); ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.22 (dd, *J* = 9.0, 0.6 Hz, 1H), 8.00 (d, *J* = 8.4 Hz, 1H), 7.96 (d, *J* = 8.4 Hz, 2H), 7.70 (d, *J* = 7.8 Hz, 2H), 7.64 (dt, *J* = 7.2, 1.2 Hz, 1H), 7.56-7.54 (m, 1H), 7.48-7.46 (m, 2H), 7.41.7.38 (m, 5H), 7.33-7.30 (m, 3H), 6.29 (s, 1H), 2.43 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 155.9, 155.7, 147.5, 143.9, 143.7, 139.6, 137.2, 129.9, 129.7, 129.5, 129.2, 128.9, 128.8, 128.8, 128.7, 128.5, 128.5, 126.3, 124.8, 119.8, 117.6, 116.1, 100.2, 21.6; ESI-MS (M+H) calcd. for $C_{30}H_{23}N_2O_3S$: 491.1429; Found: 491.14416

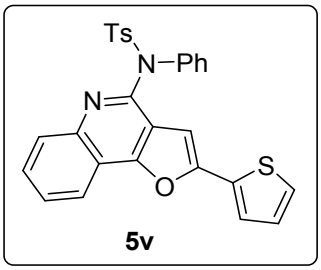
Spectral data for *N*-(2-(4-methoxyphenyl)furo[3,2-*c*]quinolin-4-yl)-4-methyl-*N*-phenylbenzenesulfonamide (5t)



5t

Brown oil; (36.2 mg, 0.07 mmol, 36%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.20 (d, *J* = 8.0 Hz, 1H), 7.99 (d, *J* = 8.4 Hz, 1H), 7.95 (d, *J* = 8.4 Hz, 2H), 7.63 (t, *J* = 8.4 Hz, 3H), 7.54 (t, *J* = 7.6 Hz, 1H), 7.45 (dd, *J* = 6.4, 3.2 Hz, 2H), 7.38-7.37 (m, 3H), 7.30 (d, *J* = 8.0 Hz, 2H), 6.92 (d, *J* = 8.0 Hz, 2H), 6.15 (s, 1H), 3.82 (s, 3H), 2.43 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 160.2, 156.6, 155.9, 147.4, 143.7, 143.6, 139.6, 137.1, 129.9, 129.7, 129.2, 128.8, 128.7, 128.5, 128.2, 126.4, 126.2, 122.3, 119.7, 117.9, 116.1, 114.3, 98.5, 55.4, 21.6; ESI-MS (M+Na) calcd. for $C_{31}H_{24}N_2NaO_4S$: 543.1355; Found: 543.13574

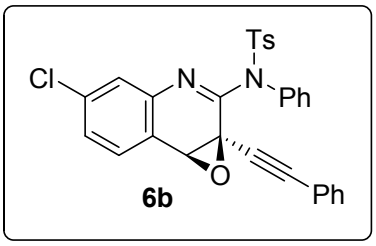
Spectral data for 4-methyl-*N*-phenyl-*N*-(2-(thiophen-2-yl)furo[3,2-*c*]quinolin-4-yl)benzenesulfonamide (5v)



5v

Green sticky solid; (20.7 mg, 0.04 mmol, 48%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.19 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.99 (d, *J* = 8.4 Hz, 1H), 7.94 (d, *J* = 8.4 Hz, 2H), 7.66-7.62 (m, 1H), 7.54 (dt, *J* = 7.2, 1.2 Hz, 1H), 7.46-7.43 (m, 2H), 7.39-7.37 (m, 4H), 7.32-7.29 (m, 3H), 7.07-7.05 (m, 1H), 6.12 (s, 1H), 2.43 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 156.6, 151.1, 147.3, 143.9, 143.7, 139.5, 137.1, 132.1, 129.9, 129.7, 129.2, 128.8, 128.7, 128.6, 127.9, 126.4, 125.2, 119.9, 117.6, 116.1, 100.0, 21.7, one 'C' merge with others; ESI-MS (M+Na) calcd. for $C_{28}H_{20}N_2NaO_3S$: 519.0813; Found: 519.08052

Spectral data for *N*-((1a*R*,7b*S*)-5-chloro-1a-(phenylethynyl)-1a,7b-dihydrooxireno[2,3-*c*]quinolin-2-yl)-4-methyl-*N*-phenylbenzenesulfonamide (6b)

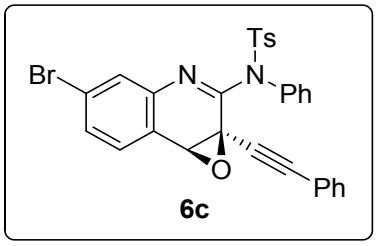


6b

White solid; (74.5 mg, 0.14 mmol, 66%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.71 (d, *J* = 8.0Hz, 2H), 7.52-7.50 (m, 2H), 7.43-7.33 (m, 6H), 7.32-7.25 (m, 7H), 4.60 (s, 1H), 2.41 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 152.9, 144.2, 142.0, 136.4, 136.0, 135.7, 131.9, 130.4, 130.2, 129.5, 129.2, 128.9, 128.7, 128.7, 128.3, 127.2, 121.7, 121.0, 86.7, 82.8, 64.9, 53.2, 21.6, one 'C' merge with others; ESI-MS (M+Na) calcd. for $C_{30}H_{21}ClN_2NaO_3S$: 547.0859; Found: 547.08564

Spectral data for *N*-((1a*R*,7b*S*)-5-bromo-1a-(phenylethynyl)-1a,7b-

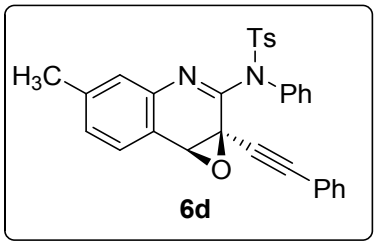
dihydrooxireno[2,3-*c*]quinolin-2-yl)-4-methyl-*N*-phenylbenzenesulfonamide (6c)



6c

Yellow solid; (112.1 mg, 0.20 mmol, 78%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.71 (d, *J* = 8.0 Hz, 2H), 7.66 (s, 1H), 7.43-7.25 (m, 14H), 4.60 (s, 1H), 2.41 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 152.9, 144.2, 142.1, 136.4, 135.6, 131.9, 131.2, 130.4, 130.1, 129.5, 129.2, 128.9, 128.7, 128.6, 128.2, 124.0, 122.1, 121.0, 86.7, 82.8, 65.0, 53.2, 21.6, one 'C' merge with others; ESI-MS (M+Na) calcd. for $C_{30}H_{21}BrN_2NaO_3S$: 591.0354; Found: 591.03233

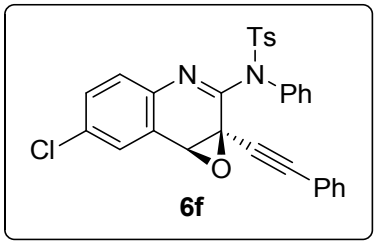
Spectral data for 4-methyl-*N*-((1a*R*,7b*S*)-5-methyl-1a-(phenylethynyl)-1a,7b-dihydrooxireno[2,3-*c*] quinolin-2-yl)-*N*-phenylbenzenesulfonamide (6d)



6d

White solid; (80.3 mg, 0.16 mmol, 63%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.74 (dd, *J* = 8.4, 1.6 Hz, 2H), 7.46 (d, *J* = 7.6 Hz,1H), 7.40-7.34 (m, 6H), 7.33-7.29 (m, 6H), 7.26 (s, 1H), 7.14-7.12 (m, 1H), 4.62 (s, 1H), 2.43 (s, 3H), 2.40 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 151.6, 143.9, 140.8, 140.6, 136.6, 135.8, 131.8, 130.3, 129.5, 129.0, 129.0, 128.6, 128.5, 128.2, 128.2, 121.2, 120.3, 86.3, 83.3, 65.3, 53.1, 21.5, 21.3, two 'C' merge with others; ESI-MS (M+Na) calcd. for $C_{31}H_{24}N_2NaO_3S$: 527.1405; Found: 527.14085

Spectral data for *N*-((1a*R*,7b*S*)-6-chloro-1a-(phenylethynyl)-1a,7b-dihydrooxireno[2,3-*c*] quinolin-2-yl)-4-methyl-*N*-phenylbenzenesulfonamide (6f)

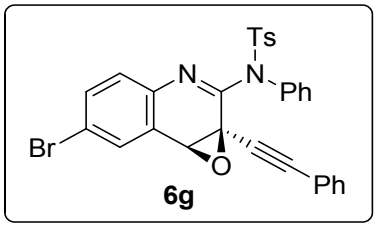


6f

White solid; (90.0 mg, 0.17 mmol, 64%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.71 (d, *J* =

8.4 Hz, 2H), 7.56 (s, 1H), 7.45-7.29 (m, 12H), 7.24 (d, *J* = 8.4 Hz, 2H), 4.57 (s, 1H), 2.40 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 151.8, 144.1, 139.5, 136.5, 135.8, 132.6, 131.9, 130.5, 130.4, 129.8, 129.6, 129.3, 129.0, 128.9, 128.7, 128.3, 124.7, 121.0, 86.7, 82.7, 64.8, 53.1, 21.6, one 'C' merge with others; ESI-MS (M+Na) calcd. for $C_{30}H_{21}ClN_2NaO_3S$: 547.0859; Found: 547.08566

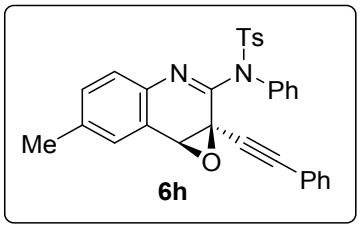
Spectral data for *N*-((1a*R*,7b*S*)-6-bromo-1a-(phenylethynyl)-1a,7b-dihydrooxireno[2,3-*c*] quinolin-2-yl)-4-methyl-*N*-phenylbenzenesulfonamid*e* (6g)



6g

White solid; (70.5 mg, 0.12 mmol, 52%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.74-7.69 (m, 3H), 7.59 (dd, *J* = 8.4, 2.4 Hz, 1H), 7.41-7.38 (m, 6H), 7.35-7.30 (m, 5H), 7.24 (d, J = 8.0 Hz, 2H), 4.56 (s, 1H), 2.39 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 152.0, 144.1, 139.9, 136.5, 135.8, 133.5, 131.9, 130.4, 130.0, 129.6, 129.3, 128.9, 128.7, 128.3, 125.0, 121.0, 120.5, 86.7, 82.7, 64.7, 53.2, 21.6, two 'C' merge with others; ESI-MS (M+Na) calcd. for $C_{30}H_{21}BrN_2NaO_3S$: 591.0354; Found: 591.03440

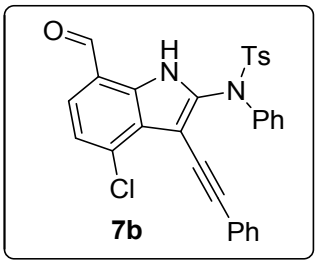
Spectral data for 4-methyl-*N*-((1a*R*,7b*S*)-6-methyl-1a-(phenylethynyl)-1a,7b-dihydrooxireno[2,3-*c*] quinolin-2-yl)-*N*-phenylbenzenesulfonamide (6h)



6h

Yellow solid; (66 mg, 0.13 mmol, 63%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.74 (d, *J* = 8.0 Hz, 2H), 7.43-7.38 (m, 7H), 7.35-7.28 (m, 6H), 7.23 (d, *J* = 8.0 Hz, 2H), 4.59 (s, 1H), 2.40 (s, 3H), 2.39 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 150.7, 143.9, 138.7, 137.7, 136.7, 136.0, 131.9, 131.2, 130.3, 129.7, 129.6, 129.1, 128.6, 128.5, 128.2, 123.1, 121.3, 86.4, 83.3, 65.5, 53.2, 21.6, 21.2, two 'C' merge with others; ESI-MS (M+H) calcd. for $C_{31}H_{25}N_2O_3S$: 505.1586; Found: 505.15971

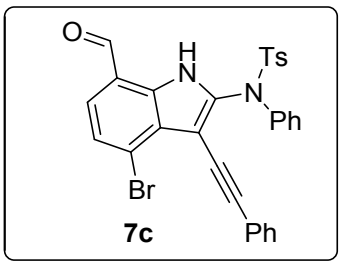
Spectral data for *N*-(4-chloro-7-formyl-3-(phenylethynyl)-1*H*-indol-2-yl)-4-methyl-*N*-phenylbenzenesulfonamide (7b)



7b

White solid; (34.3 mg, 0.06 mmol, 18%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.49 (s, 1H), 10.06 (s, 1H), 7.89 (s, 1H), 7.69 (t, *J* = 8.4 Hz, 3H), 7.51 (d, *J* = 7.6 Hz, 2H), 7.35-7.30 (m, 6H), 7.20-7.17 (m, 4H), 2.22 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 191.8, 144.6, 139.5, 138.3, 136.4, 131.2, 130.2, 129.8, 129.6, 129.3, 128.7, 128.5, 128.5, 128.2, 128.1, 128.1, 126.5, 123.0, 121.1, 95.5, 95.1, 79.8, 21.4, one 'C' merge with others; ESI-MS (M+Na) calcd. for $C_{30}H_{21}ClN_2NaO_3S$: 547.0859; Found: 547.08325

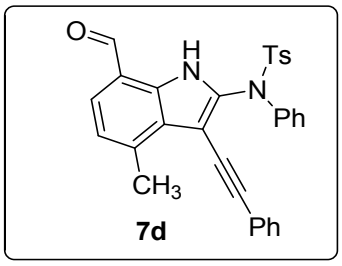
Spectral data for *N*-(4-bromo-7-formyl-3-(phenylethynyl)-*1H*-indol-2-yl)-4-methyl-*N*-phenylbenzenesulfonamide (7c)



7c

White solid; (19.5 mg, 0.03 mmol, 14%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.52 (s, 1H), 10.06 (s, 1H), 8.05 (s, 1H), 7.80 (s, 1H), 7.70 (d, *J* = 8.0 Hz, 2H), 7.51 (d, *J* = 7.2 Hz, 2H), 7.33-7.30 (m, 6H), 7.24-7.17 (m, 4H), 2.22 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 191.8, 144.6, 139.5, 138.2, 136.4, 132.3, 131.2, 130.7, 129.8, 129.4, 129.3, 129.0, 128.5, 128.4, 128.2, 128.1, 123.0, 121.5, 113.4, 95.4, 95.0, 79.8, 21.4, one 'C' merge with others; ESI-MS (M+Na) calcd. for $C_{30}H_{21}BrN_2NaO_3S$: 519.0354; Found: 591.03578

Spectral data for *N*-(7-formyl-4-methyl-3-(phenylethynyl)-1H-indol-2-yl)-4-methyl-*N*-phenylbenzenesulfonamide (7d)

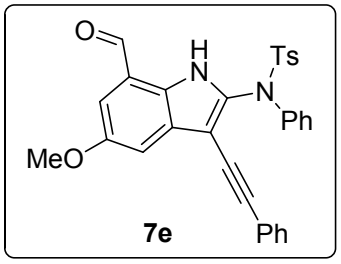


7d

Yellow solid; (35.3 mg, 0.07 mmol, 31%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.26 (s, 1H), 10.06 (s, 1H), 7.73 (s, 1H), 7.70 (d, *J* = 8.4 Hz, 2H), 7.54-7.51 (m, 3H), 7.34-7.28 (m, 6H), 7.22-7.19 (m, 2H), 7.16 (d, *J* = 8.4 Hz, 2H), 2.51 (s, 3H), 2.22 (s, 3H); ^{13}C

NMR (100 MHz, $CDCl_3$): δ 192.9, 144.3, 139.9, 137.1, 136.6, 131.6, 131.1, 130.3, 129.7, 129.2, 129.1, 128.8, 128.3, 128.1, 128.1, 127.9, 127.1, 123.4, 120.5, 95.7, 94.4, 80.9, 21.4, 21.1, one 'C' merge with others; ESI-MS (M+Na) calcd. for $C_{31}H_{24}N_2NaO_3S$: 527.1405; Found: 527.13984

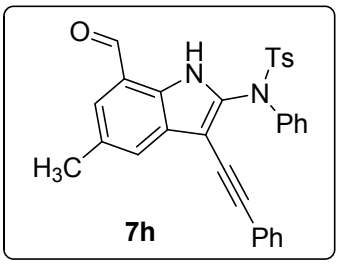
Spectral data for *N*-(7-formyl-5-methoxy-3-(phenylethynyl)-1H-indol-2-yl)-4-methyl-*N*-phenylbenzenesulfonamide (7e)



7e

White solid; mp: (50.3 mg, 0.10 mmol, 34%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.36 (s, 1H), 10.06 (s, 1H), 7.73 (d, *J* = 8.0 Hz, 2H), 7.55 (d, *J* = 7.2 Hz, 2H), 7.42 (s, 1H), 7.34-7.30 (m, 7H), 7.23-7.22 (m, 2H), 7.16 (d, *J* = 7.6 Hz, 2H), 3.90 (s, 3H), 2.20 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 192.5, 154.6, 144.3, 139.9, 137.5, 136.7, 131.1, 129.7, 129.2, 128.3, 128.2, 128.2, 128.1, 127.9, 125.5, 123.4, 121.0, 119.0, 109.9, 95.7, 94.6, 80.8, 56.2, 21.4, one 'C' merge with others; ESI-MS (M+Na) calcd. for $C_{31}H_{24}N_2NaO_4S$: 543.1355; Found: 543.13478

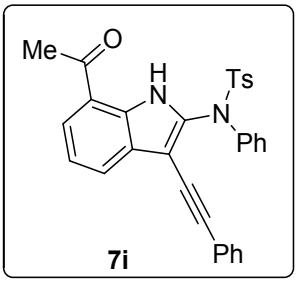
Spectral data for *N*-(7-formyl-5-methyl-3-(phenylethynyl)-1H-indol-2-yl)-4-methyl-*N*-phenylbenzenesulfonamide (7h)



7h

White solid; (7.5 mg, 0.01 mmol, 6%); ^{1}H NMR (400 MHz, CD_2Cl_2): δ 10.63 (s, 1H), 10.07 (s, 1H), 7.76 (d, *J* = 8.0 Hz, 2H), 7.64 (d, *J* = 7.6 Hz, 1H), 7.54 (d, *J* = 7.2 Hz, 2H), 7.38-7.32 (m, 6H), 7.24-7.19 (m, 4H), 7.09 (d, *J* = 7.2 Hz, 1H), 2.87 (s, 3H), 2.25 (s, 3H); ^{13}C NMR (100 MHz, CD_2Cl_2): δ 192.9, 145.1, 141.5, 140.5, 137.7, 137.3, 131.0, 130.9, 130.2, 129.6, 128.6, 128.4, 128.3, 126.9, 123.8, 122.7, 119.4, 96.9, 94.9, 83.3, 21.6, 19.7, three 'C' merge with others; ESI-MS (M+Na) calcd. for $C_{31}H_{24}N_2NaO_3S$: 527.1405; Found: 527.13885

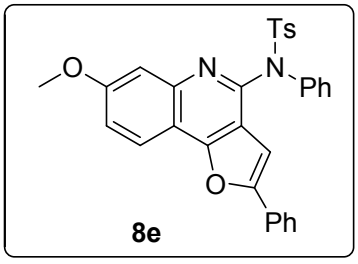
Spectral data for *N*-(7-acetyl-3-(phenylethynyl)-1H-indol-2-yl)-4-methyl-*N*-phenylbenzenesulfonamide (7i)



7i

Yellow solid; (65.7 mg, 0.13 mmol, 52%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.72 (s, 1H), 7.90 (d, *J* = 7.6 Hz, 1H), 7.82 (d, *J* = 7.6Hz, 1H), 7.71 (d, *J* = 8.4 Hz, 2H), 7.53 (dt, *J* = 7.0, 2.0 Hz, 2H), 7.34-7.28 (m, 6H), 7.24-7.16 (m, 5H), 2.69 (s, 3H), 2.22 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 199.8, 144.3, 139.8, 136.9, 136.5, 131.4, 131.0, 129.6, 129.1, 128.2, 128.0, 127.9, 127.8, 126.6, 126.2, 126.2, 123.3, 120.3, 120.1, 95.6, 94.4, 80.9, 26.4, 21.3, one 'C' merge with others; ESI-MS (M+Na) calcd. for $C_{31}H_{24}N_2NaO_3S$: 527.1405; Found: 527.14237

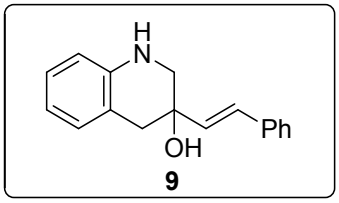
Spectral data for *N*-(7-methoxy-2-phenylfuro[3,2-*c*]quinolin-4-yl)-4-methyl-N-phenylbenzenesulfonamid*e* (8e)



8e

White solid; (64.3 mg, 0.12 mmol, 52%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.89 (d, *J* = 8.0 Hz, 3H), 7.76 (d, *J* = 7.6Hz, 2H), 7.49-7.46 (m, 3H), 7.42 (t, *J* = 7.6 Hz, 2H), 7.35-7.34 (m, 4H), 7.30-7.26 (m, 3H), 6.50 (s, 1H), 3.99 (s, 3H), 2.43 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 158.1, 156.4, 155.9, 145.4, 143.6, 139.7, 139.6, 137.0, 130.5, 129.5, 129.1, 129.0, 128.8, 128.8, 128.2, 124.9, 120.5, 118.7, 117.0, 100.3, 98.3, 55.8, 21.6, two 'C' merge with others; ESI-MS (M+H) calcd. for $C_{31}H_{25}N_2O_4S$: 521.1535; Found: 521.15523

Spectral data for (*E*)-3-styryl-1,2,3,4-tetrahydroquinolin-3-ol (9)

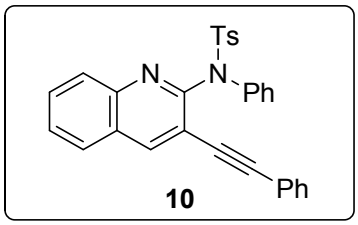


9

White solid; (25.6 mg, 0.10 mmol, 62%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.41 (d, *J* = 7.2 Hz, 2H), 7.33 (d, *J* = 7.2 Hz, 2H), 7.25-7.22 (m, 1H), 7.06-7.00(m, 2H), 6.82 (d, *J* = 16.0 Hz, 1H), 6.72 (d, *J* = 7.2 Hz, 1H), 6.61 (d, *J* = 7.8 Hz, 1H), 6.34 (d, *J* = 16.0 Hz,

1H), 4.01 (s, 1H), 3.27 (d, *J* = 11.2 Hz, 1H), 3.14-3.09 (m, 2H), 2.84-2.80 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 142.7, 136.7, 132.6, 130.6, 129.1, 128.6, 127.6, 127.1, 126.5, 119.1, 118.5, 114.3, 68.0, 51.6, 40.1; ESI-MS (M+H) calcd. for $C_{17}H_{18}NO$: 252.1388; Found: 252.13913

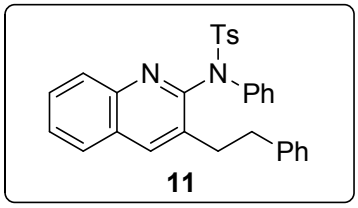
Spectral data for 4-methyl-*N*-phenyl-*N*-(3-(phenylethynyl)quinolin-2-yl)benzenesulfonamide (10)



10

White solid; (47.5 mg, 0.10 mmol, 75%); ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.29 (s, 1H), 7.95 (d, *J* = 8.4 Hz, 1H), 7.81 (d, *J* = 10.2 Hz, 2H), 7.74 (d, *J* = 7.8 Hz, 1H), 7.69 (t, *J* = 7.8 Hz, 1H), 7.55-7.51 (m, 3H), 7.48-7.47 (m, 2H), 7.38-7.36 (m, 3H), 7.26-7.23 (m, 5H), 7.24~7.23 (m, 3H), 2.42 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 152.8, 145.6, 143.4, 142.1, 139.4, 136.9, 131.7, 130.3, 129.3, 129.2, 128.8, 128.7, 128.7, 128.6, 128.3, 127.7, 127.4, 127.1, 126.6, 122.7, 117.1, 95.9, 84.9, 21.6; ESI-MS (M+H) calcd. for $C_{30}H_{23}N_2O_2S$: 475.1480; Found: 475.14919

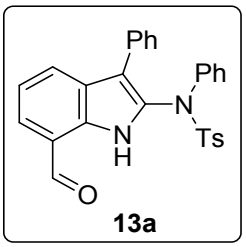
Spectral data for 4-methyl-*N*-(3-phenethylquinolin-2-yl)-*N*-phenylbenzenesulfonamide (11)



11

Colorless oil; (67.7 mg, 0.14 mmol, 80%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.88 (t, *J* = 8.4 Hz, 1H), 7.73-7.64 (m, 4H), 7.52-7.45 (m, 3H), 7.29-7.17 (m, 10H), 3.08 (t, *J* = 6.8 Hz, 2H), 2.94 (t, *J* = 9.2 Hz, 2H), 2.45 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 152.8, 145.6, 143.4, 141.2, 139.6, 138.5, 136.4, 133.4, 129.4, 129.0, 128.9, 128.5, 128.3, 128.0, 127.4, 127.0, 126.9, 126.0, 35.8, 33.2, 21.6, three 'C' merge with others; ESI-MS (M+Na) calcd. for $C_{30}H_{26}N_2NaO_2S$: 501.1613; Found: 501.16335

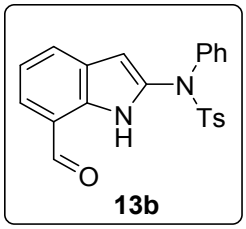
Spectra data for N-(7-formyl-3-phenyl-1*H*-indol-2-yl)-4-methyl-N-phenylbenzenesulfonamide (13a)



13a

Yellow Solid; (62.8 mg, 0.13 mmol, 78%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.17 (s, 1H), 10.11 (s, 1H), 7.86 (d, *J* = 7.7 Hz, 1H), 7.70 (d, *J* = 7.0 Hz, 1H), 7.58 (d, *J* = 8.4 Hz, 2H), 7.31-7.23 (m, 8H), 7.16-7.12 (m, 3H), 7.06 (d, *J* = 6.3 Hz, 2H), 2.43 (s, 3H); ^{13}C NMR (175 MHz, $CDCl_3$): δ193.3, 144.5, 140.5, 136.3, 131.9, 131.2, 130.9, 129.9, 129.6, 129.0, 128.3, 127.8, 127.5, 127.3, 127.1, 126.8, 120.3, 120.2, 120.2, 115.5, 21.7; ESI-MS (M+Na) calcd. for $C_{28}H_{22}N_2NaO_3S$: 489.1249; Found: 489.1248

Spectra data for N-(7-formyl-3-phenyl-1*H*-indol-2-yl)-4-methyl-N-phenylbenzenesulfonamide (13b)

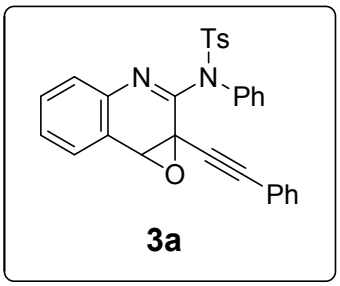


13b

White Solid; (70.8 mg, 0.18 mmol, 82%); ^{1}H NMR (700 MHz, $CDCl_3$): δ 10.50 (s, 1H), 10.08 (s, 1H), 7.69 (d, *J* = 7.7 Hz, 1H), 7.59 (dd, *J* = 9.1, 7.7 Hz, 3H), 7.37-7.36 (m, 3H), 7.26-7.22 (m, 3H), 7.19 (d, *J* = 7.0 Hz, 1H), 5.95 (d, *J* = 2.8 Hz, 1H), 2.42 (s, 3H); ^{13}C NMR (175 MHz, $CDCl_3$): δ 193.0, 144.5, 139.3, 137.1, 135.4, 131.2, 129.7, 129.5, 128.8, 128.7, 128.4, 128.2, 127.9, 127.2, 120.1, 119.9, 95.5, 21.6 ESI-MS (M+Na) calcd. for $C_{22}H_{18}N_2NaO_3S$: 413.0936; Found: 413.0972.

(3) X-ray crystallographic structure and data for compound 3a, 4a, and 5a.

3.1. X-ray crystallographic structure and data for compound 3a



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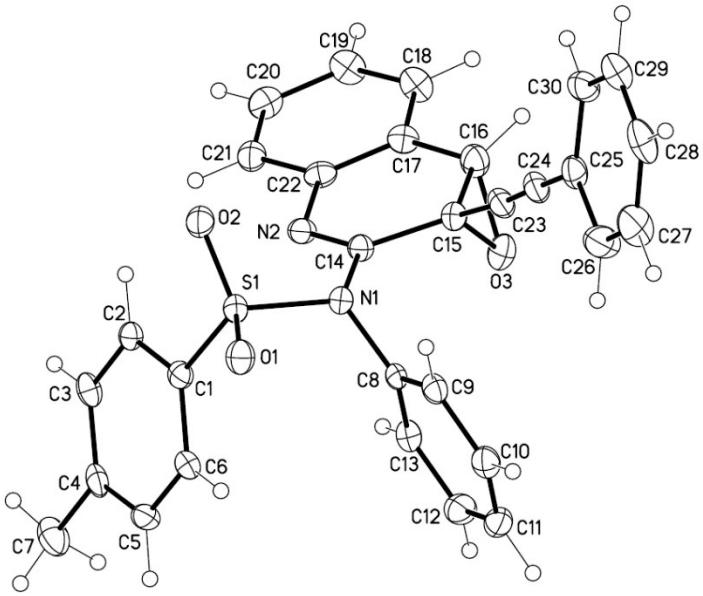


Figure S1 - Molecular structure of compound 3a

Table 1. Crystal data and structure refinement for 191051lt_0m_a.

Identification code	191051lt_0m_a	
Empirical formula	C30 H22 N2 O3 S	
Formula weight	490.55	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 42.369(2) Å	α= 90°.
	b = 8.2398(4) Å	β= 105.722(3)°.
	c = 14.1141(7) Å	γ = 90°.
Volume	4743.1(4) $Å^3$	
Z	8	
Density (calculated)	1.374 Mg/m^3	
Absorption coefficient	0.173 mm^{-1}	

F(000)	2048
Crystal size	0.15 x 0.03 x 0.03 mm^3
Theta range for data collection	0.999 to 26.395°.
Index ranges	-52<=h<=51, -10<=k<=10, -12<=l<=17
Reflections collected	20380
Independent reflections	4837 [R(int) = 0.0435]
Completeness to theta = 25.242°	99.6 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7454 and 0.6706
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4837 / 0 / 326
Goodness-of-fit on F^2	1.210
Final R indices [I>2sigma(I)]	R1 = 0.0833, wR2 = 0.2087
R indices (all data)	R1 = 0.0943, wR2 = 0.2145
Extinction coefficient	n/a
Largest diff. peak and hole	1.166 and -0.525 e.$Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 191051lt_0m_a. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
S(1)	4162(1)	4895(1)	7758(1)	17(1)
N(1)	3892(1)	3402(5)	7290(3)	18(1)
N(2)	3761(1)	3033(5)	8778(3)	18(1)
O(1)	4302(1)	5293(4)	6970(2)	23(1)
O(2)	3985(1)	6103(4)	8138(2)	24(1)
O(3)	3363(1)	306(4)	7503(2)	26(1)
C(1)	4475(1)	4052(5)	8714(3)	18(1)
C(2)	4467(1)	4248(5)	9683(3)	18(1)
C(3)	4714(1)	3544(5)	10425(3)	20(1)
C(4)	4964(1)	2644(5)	10214(3)	21(1)
C(5)	4969(1)	2513(6)	9234(4)	22(1)
C(6)	4725(1)	3203(6)	8481(3)	20(1)
C(7)	5223(1)	1862(6)	11030(4)	31(1)
C(8)	3992(1)	2223(5)	6661(3)	17(1)
C(9)	3948(1)	2584(6)	5672(3)	20(1)
C(10)	4050(1)	1468(6)	5083(3)	22(1)
C(11)	4192(1)	25(6)	5475(3)	23(1)

C(12)	4231(1)	-330(6)	6460(4)	25(1)
C(13)	4131(1)	771(6)	7063(3)	21(1)
C(14)	3683(1)	2832(5)	7854(3)	18(1)
C(15)	3375(1)	2011(6)	7262(3)	20(1)
C(16)	3155(1)	1422(6)	7852(3)	24(1)
C(17)	3249(1)	1763(6)	8915(3)	20(1)
C(18)	3050(1)	1323(6)	9505(4)	26(1)
C(19)	3149(1)	1626(6)	10510(4)	26(1)
C(20)	3445(1)	2403(6)	10925(3)	24(1)
C(21)	3641(1)	2866(5)	10339(3)	21(1)
C(22)	3545(1)	2554(5)	9329(3)	20(1)
C(23)	3237(1)	2503(6)	6248(3)	22(1)
C(24)	3117(1)	3008(6)	5439(3)	23(1)
C(25)	2994(1)	3656(6)	4470(3)	22(1)
C(26)	3143(1)	3291(7)	3722(4)	33(1)
C(27)	3028(1)	3983(8)	2800(4)	36(1)
C(28)	2765(1)	5033(7)	2601(4)	32(1)
C(29)	2612(1)	5393(7)	3326(4)	31(1)
C(30)	2723(1)	4706(6)	4251(4)	27(1)

Table 3. Bond lengths [Å] and angles [°] for 191051lt_0m_a.

S(1)-O(2)	1.434(3)
S(1)-O(1)	1.434(3)
S(1)-N(1)	1.688(4)
S(1)-C(1)	1.759(5)
N(1)-C(14)	1.420(6)
N(1)-C(8)	1.454(5)
N(2)-C(14)	1.266(6)
N(2)-C(22)	1.412(6)
O(3)-C(16)	1.449(6)
O(3)-C(15)	1.450(6)
C(1)-C(6)	1.383(6)
C(1)-C(2)	1.387(6)
C(2)-C(3)	1.392(6)
C(2)-H(2)	0.9500
C(3)-C(4)	1.390(7)
C(3)-H(3)	0.9500

C(4)-C(5)	1.392(7)
C(4)-C(7)	1.504(6)
C(5)-C(6)	1.387(6)
C(5)-H(5)	0.9500
C(6)-H(6)	0.9500
C(7)-H(7A)	0.9800
C(7)-H(7B)	0.9800
C(7)-H(7C)	0.9800
C(8)-C(13)	1.386(6)
C(8)-C(9)	1.390(6)
C(9)-C(10)	1.384(6)
C(9)-H(9)	0.9500
C(10)-C(11)	1.379(7)
C(10)-H(10)	0.9500
C(11)-C(12)	1.386(7)
C(11)-H(11)	0.9500
C(12)-C(13)	1.387(7)
C(12)-H(12)	0.9500
C(13)-H(13)	0.9500
C(14)-C(15)	1.505(6)
C(15)-C(23)	1.450(6)
C(15)-C(16)	1.489(6)
C(16)-C(17)	1.472(6)
C(16)-H(16)	1.0000
C(17)-C(18)	1.384(6)
C(17)-C(22)	1.394(6)
C(18)-C(19)	1.389(7)
C(18)-H(18)	0.9500
C(19)-C(20)	1.387(7)
C(19)-H(19)	0.9500
C(20)-C(21)	1.377(7)
C(20)-H(20)	0.9500
C(21)-C(22)	1.395(6)
C(21)-H(21)	0.9500
C(23)-C(24)	1.192(7)
C(24)-C(25)	1.429(6)
C(25)-C(30)	1.401(7)
C(25)-C(26)	1.403(7)

C(26)-C(27)	1.384(7)
C(26)-H(26)	0.9500
C(27)-C(28)	1.379(8)
C(27)-H(27)	0.9500
C(28)-C(29)	1.381(7)
C(28)-H(28)	0.9500
C(29)-C(30)	1.383(7)
C(29)-H(29)	0.9500
C(30)-H(30)	0.9500

O(2)-S(1)-O(1)	120.0(2)
O(2)-S(1)-N(1)	106.59(19)
O(1)-S(1)-N(1)	104.05(19)
O(2)-S(1)-C(1)	110.4(2)
O(1)-S(1)-C(1)	107.5(2)
N(1)-S(1)-C(1)	107.7(2)
C(14)-N(1)-C(8)	116.7(4)
C(14)-N(1)-S(1)	118.7(3)
C(8)-N(1)-S(1)	116.6(3)
C(14)-N(2)-C(22)	120.2(4)
C(16)-O(3)-C(15)	61.8(3)
C(6)-C(1)-C(2)	121.3(4)
C(6)-C(1)-S(1)	119.0(3)
C(2)-C(1)-S(1)	119.7(3)
C(1)-C(2)-C(3)	118.5(4)
C(1)-C(2)-H(2)	120.7
C(3)-C(2)-H(2)	120.7
C(4)-C(3)-C(2)	121.6(4)
C(4)-C(3)-H(3)	119.2
C(2)-C(3)-H(3)	119.2
C(3)-C(4)-C(5)	118.1(4)
C(3)-C(4)-C(7)	120.3(4)
C(5)-C(4)-C(7)	121.6(4)
C(6)-C(5)-C(4)	121.4(4)
C(6)-C(5)-H(5)	119.3
C(4)-C(5)-H(5)	119.3
C(1)-C(6)-C(5)	119.0(4)
C(1)-C(6)-H(6)	120.5

C(5)-C(6)-H(6)	120.5
C(4)-C(7)-H(7A)	109.5
C(4)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	109.5
C(4)-C(7)-H(7C)	109.5
H(7A)-C(7)-H(7C)	109.5
H(7B)-C(7)-H(7C)	109.5
C(13)-C(8)-C(9)	121.4(4)
C(13)-C(8)-N(1)	119.3(4)
C(9)-C(8)-N(1)	119.3(4)
C(10)-C(9)-C(8)	118.9(4)
C(10)-C(9)-H(9)	120.5
C(8)-C(9)-H(9)	120.5
C(11)-C(10)-C(9)	120.3(4)
C(11)-C(10)-H(10)	119.9
C(9)-C(10)-H(10)	119.9
C(10)-C(11)-C(12)	120.4(4)
C(10)-C(11)-H(11)	119.8
C(12)-C(11)-H(11)	119.8
C(11)-C(12)-C(13)	120.2(4)
C(11)-C(12)-H(12)	119.9
C(13)-C(12)-H(12)	119.9
C(8)-C(13)-C(12)	118.8(4)
C(8)-C(13)-H(13)	120.6
C(12)-C(13)-H(13)	120.6
N(2)-C(14)-N(1)	120.4(4)
N(2)-C(14)-C(15)	125.2(4)
N(1)-C(14)-C(15)	114.5(4)
C(23)-C(15)-O(3)	118.2(4)
C(23)-C(15)-C(16)	119.7(4)
O(3)-C(15)-C(16)	59.1(3)
C(23)-C(15)-C(14)	118.7(4)
O(3)-C(15)-C(14)	112.7(4)
C(16)-C(15)-C(14)	114.6(4)
O(3)-C(16)-C(17)	116.6(4)
O(3)-C(16)-C(15)	59.1(3)
C(17)-C(16)-C(15)	118.2(4)
O(3)-C(16)-H(16)	116.8

C(17)-C(16)-H(16)	116.8
C(15)-C(16)-H(16)	116.8
C(18)-C(17)-C(22)	119.7(4)
C(18)-C(17)-C(16)	121.7(4)
C(22)-C(17)-C(16)	118.6(4)
C(17)-C(18)-C(19)	120.1(5)
C(17)-C(18)-H(18)	119.9
C(19)-C(18)-H(18)	119.9
C(20)-C(19)-C(18)	120.2(4)
C(20)-C(19)-H(19)	119.9
C(18)-C(19)-H(19)	119.9
C(21)-C(20)-C(19)	119.9(4)
C(21)-C(20)-H(20)	120.1
C(19)-C(20)-H(20)	120.1
C(20)-C(21)-C(22)	120.3(4)
C(20)-C(21)-H(21)	119.8
C(22)-C(21)-H(21)	119.8
C(17)-C(22)-C(21)	119.7(4)
C(17)-C(22)-N(2)	123.1(4)
C(21)-C(22)-N(2)	117.2(4)
C(24)-C(23)-C(15)	175.4(5)
C(23)-C(24)-C(25)	176.3(5)
C(30)-C(25)-C(26)	118.4(4)
C(30)-C(25)-C(24)	120.4(4)
C(26)-C(25)-C(24)	121.2(5)
C(27)-C(26)-C(25)	120.2(5)
C(27)-C(26)-H(26)	119.9
C(25)-C(26)-H(26)	119.9
C(28)-C(27)-C(26)	120.6(5)
C(28)-C(27)-H(27)	119.7
C(26)-C(27)-H(27)	119.7
C(27)-C(28)-C(29)	119.9(5)
C(27)-C(28)-H(28)	120.0
C(29)-C(28)-H(28)	120.0
C(28)-C(29)-C(30)	120.3(5)
C(28)-C(29)-H(29)	119.9
C(30)-C(29)-H(29)	119.9
C(29)-C(30)-C(25)	120.6(5)

C(29)-C(30)-H(30)	119.7
C(25)-C(30)-H(30)	119.7

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 191051lt_0m_a. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

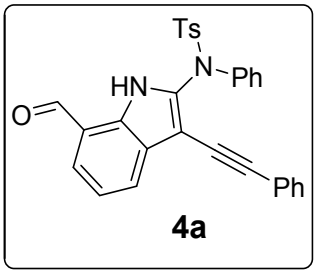
	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
S(1)	18(1)	15(1)	16(1)	0(1)	2(1)	-2(1)
N(1)	17(2)	18(2)	19(2)	-4(2)	3(2)	-1(2)
N(2)	17(2)	20(2)	19(2)	0(2)	5(2)	2(2)
O(1)	26(2)	21(2)	23(2)	1(1)	6(1)	-5(1)
O(2)	23(2)	19(2)	24(2)	-2(1)	0(1)	2(1)
O(3)	31(2)	21(2)	27(2)	-4(1)	7(2)	-6(1)
C(1)	17(2)	13(2)	22(2)	1(2)	4(2)	-2(2)
C(2)	17(2)	15(2)	22(2)	-2(2)	4(2)	-3(2)
C(3)	19(2)	22(2)	17(2)	3(2)	2(2)	-7(2)
C(4)	18(2)	17(2)	24(2)	0(2)	-3(2)	-5(2)
C(5)	15(2)	20(2)	31(2)	-3(2)	7(2)	-1(2)
C(6)	15(2)	22(2)	22(2)	-3(2)	3(2)	-3(2)
C(7)	25(3)	26(3)	36(3)	5(2)	-4(2)	-1(2)
C(8)	13(2)	18(2)	20(2)	-5(2)	5(2)	-5(2)
C(9)	17(2)	18(2)	22(2)	0(2)	3(2)	-3(2)
C(10)	21(2)	28(2)	20(2)	-2(2)	8(2)	-6(2)
C(11)	23(2)	22(2)	26(2)	-5(2)	10(2)	-4(2)
C(12)	24(2)	20(2)	32(3)	1(2)	7(2)	1(2)
C(13)	20(2)	23(2)	19(2)	-2(2)	2(2)	-4(2)
C(14)	17(2)	16(2)	21(2)	-1(2)	5(2)	-1(2)
C(15)	19(2)	21(2)	18(2)	-3(2)	3(2)	-1(2)
C(16)	23(2)	27(2)	24(2)	-3(2)	8(2)	-6(2)
C(17)	21(2)	21(2)	20(2)	3(2)	6(2)	2(2)
C(18)	23(2)	30(3)	23(2)	5(2)	5(2)	-2(2)
C(19)	26(3)	29(3)	23(2)	8(2)	8(2)	0(2)
C(20)	30(3)	25(2)	18(2)	3(2)	6(2)	5(2)
C(21)	22(2)	18(2)	21(2)	0(2)	2(2)	1(2)
C(22)	22(2)	17(2)	22(2)	3(2)	9(2)	4(2)
C(23)	16(2)	28(2)	22(2)	-3(2)	3(2)	-3(2)

C(24)	17(2)	29(3)	22(2)	-5(2)	2(2)	-4(2)
C(25)	21(2)	28(2)	17(2)	-3(2)	2(2)	-4(2)
C(26)	25(3)	50(3)	23(2)	-4(2)	6(2)	5(2)
C(27)	32(3)	63(4)	13(2)	-3(2)	6(2)	-6(3)
C(28)	26(3)	44(3)	20(2)	4(2)	-1(2)	-13(2)
C(29)	21(2)	37(3)	32(3)	-2(2)	1(2)	-5(2)
C(30)	20(2)	36(3)	25(2)	-4(2)	8(2)	-1(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^{-3}) for 191051lt_0m_a.

	x	y	z	U(eq)
H(2)	4296	4848	9838	22
H(3)	4713	3682	11092	24
H(5)	5143	1938	9078	26
H(6)	4731	3095	7816	24
H(7A)	5205	2268	11666	47
H(7B)	5441	2125	10954	47
H(7C)	5193	682	11002	47
H(9)	3851	3580	5405	24
H(10)	4021	1697	4405	27
H(11)	4263	-729	5068	27
H(12)	4327	-1332	6723	30
H(13)	4157	535	7739	25
H(16)	2915	1385	7512	29
H(18)	2845	813	9222	31
H(19)	3014	1300	10915	31
H(20)	3511	2615	11612	29
H(21)	3843	3401	10623	26
H(26)	3324	2566	3850	39
H(27)	3131	3733	2298	43
H(28)	2688	5508	1967	38
H(29)	2431	6115	3189	37
H(30)	2615	4949	4743	32

3.2. X-ray crystallographic structure and data for compound 4a



CCDC : 1996554

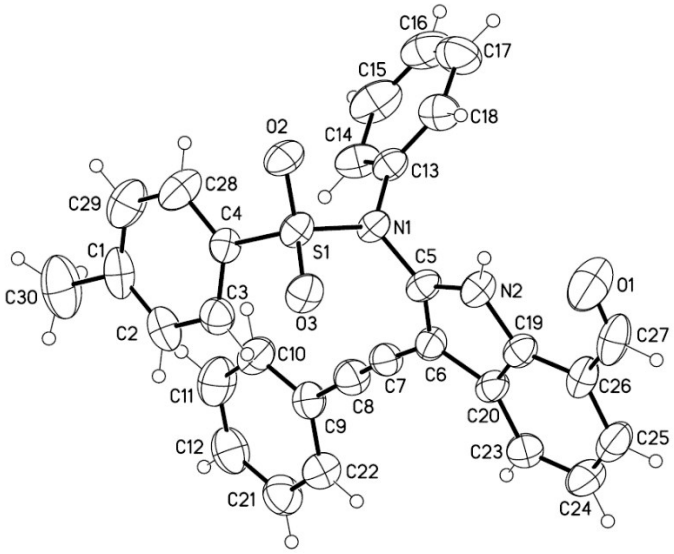


Figure S2 - Molecular structure of compound 4a

Table 1. Crystal data and structure refinement for mo_191107_0m.

Identification code	mo_191107_0m	
Empirical formula	C30 H22 N2 O3 S	
Formula weight	490.55	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 8.7173(19) Å	α= 91.258(7)°.
	b = 9.0625(18) Å	β= 97.362(7)°.
	c = 15.386(4) Å	γ = 92.766(6)°.
Volume	1203.6(4) $Å^3$	
Z	2	
Density (calculated)	1.354 Mg/m^3	
Absorption coefficient	0.171 mm^{-1}	
F(000)	512	

Crystal size	0.05 x 0.03 x 0.03 mm^3
Theta range for data collection	2.251 to 26.503°.
Index ranges	-10<=h<=10, -11<=k<=11, -19<=l<=19
Reflections collected	21928
Independent reflections	4977 [R(int) = 0.1699]
Completeness to theta = 25.242°	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7454 and 0.6578
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4977 / 0 / 326
Goodness-of-fit on F^2	1.024
Final R indices [I>2sigma(I)]	R1 = 0.0811, wR2 = 0.1152
R indices (all data)	R1 = 0.2446, wR2 = 0.1696
Extinction coefficient	n/a
Largest diff. peak and hole	0.264 and -0.444 e.$Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for mo_191107_0m. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	533(6)	2311(6)	2746(4)	55(2)
C(2)	1547(6)	3464(6)	3086(3)	52(1)
C(3)	2545(6)	4162(5)	2590(3)	44(1)
C(4)	2532(5)	3713(5)	1724(3)	36(1)
C(5)	6719(5)	4653(4)	2014(3)	37(1)
C(6)	7059(5)	4661(5)	2907(3)	39(1)
C(7)	6245(6)	3847(5)	3512(3)	42(1)
C(8)	5646(6)	3213(5)	4062(3)	46(1)
C(9)	4890(6)	2505(5)	4728(3)	40(1)
C(10)	3744(6)	1385(5)	4540(3)	51(1)
C(11)	3070(6)	745(6)	5214(4)	65(2)
C(12)	3524(7)	1195(6)	6072(4)	60(2)
C(13)	5858(5)	2321(5)	1233(3)	37(1)
C(14)	5277(6)	1165(5)	1701(3)	52(1)
C(15)	5605(7)	-284(5)	1486(4)	65(2)
C(16)	6533(7)	-535(6)	841(4)	68(2)
C(17)	7107(7)	610(6)	399(4)	66(2)
C(18)	6753(6)	2029(5)	594(3)	50(1)

C(19)	8804(6)	6200(5)	2343(3)	38(1)
C(20)	8381(5)	5656(5)	3131(3)	39(1)
C(21)	4654(6)	2307(6)	6265(3)	54(1)
C(22)	5330(6)	2961(5)	5603(3)	46(1)
C(23)	9226(6)	6121(5)	3922(3)	50(1)
C(24)	10489(6)	7094(6)	3917(4)	60(2)
C(25)	10924(6)	7602(5)	3137(4)	54(1)
C(26)	10098(6)	7172(5)	2327(3)	46(1)
C(27)	10587(6)	7692(5)	1522(4)	61(2)
C(28)	1515(6)	2603(5)	1362(4)	62(2)
C(29)	516(7)	1903(6)	1876(4)	66(2)
C(30)	-558(7)	1520(6)	3300(4)	86(2)
N(1)	5566(4)	3829(3)	1459(2)	35(1)
N(2)	7783(4)	5573(4)	1665(2)	39(1)
O(1)	9941(5)	7409(4)	790(3)	83(1)
O(2)	3450(4)	4103(3)	224(2)	48(1)
O(3)	4121(4)	6095(3)	1380(2)	47(1)
S(1)	3901(2)	4558(1)	1123(1)	39(1)

Table 3. Bond lengths [Å] and angles [°] for mo_191107_0m.

C(1)-C(29)	1.379(7)
C(1)-C(2)	1.384(7)
C(1)-C(30)	1.521(7)
C(2)-C(3)	1.369(6)
C(2)-H(19)	0.9300
C(3)-C(4)	1.384(6)
C(3)-H(2)	0.9300
C(4)-C(28)	1.368(6)
C(4)-S(1)	1.758(5)
C(5)-C(6)	1.368(6)
C(5)-N(2)	1.384(5)
C(5)-N(1)	1.406(5)
C(6)-C(20)	1.430(6)
C(6)-C(7)	1.436(7)
C(7)-C(8)	1.194(6)
C(8)-C(9)	1.435(7)
C(9)-C(10)	1.388(6)

C(9)-C(22)	1.399(6)
C(10)-C(11)	1.381(7)
C(10)-H(11)	0.9300
C(11)-C(12)	1.376(7)
C(11)-H(10)	0.9300
C(12)-C(21)	1.374(7)
C(12)-H(1)	0.9300
C(13)-C(18)	1.360(6)
C(13)-C(14)	1.396(6)
C(13)-N(1)	1.445(5)
C(14)-C(15)	1.399(6)
C(14)-H(3)	0.9300
C(15)-C(16)	1.380(7)
C(15)-H(4)	0.9300
C(16)-C(17)	1.362(7)
C(16)-H(5)	0.9300
C(17)-C(18)	1.372(6)
C(17)-H(6)	0.9300
C(18)-H(7)	0.9300
C(19)-N(2)	1.375(5)
C(19)-C(26)	1.400(6)
C(19)-C(20)	1.405(6)
C(20)-C(23)	1.384(6)
C(21)-C(22)	1.373(6)
C(21)-H(9)	0.9300
C(22)-H(8)	0.9300
C(23)-C(24)	1.378(7)
C(23)-H(15)	0.9300
C(24)-C(25)	1.386(7)
C(24)-H(14)	0.9300
C(25)-C(26)	1.395(6)
C(25)-H(13)	0.9300
C(26)-C(27)	1.441(7)
C(27)-O(1)	1.209(6)
C(27)-H(12)	0.9300
C(28)-C(29)	1.390(7)
C(28)-H(18)	0.9300
C(29)-H(17)	0.9300

C(30)-H(30A)	0.9600
C(30)-H(30B)	0.9600
C(30)-H(30C)	0.9600
N(1)-S(1)	1.651(3)
N(2)-H(16)	0.8600
O(2)-S(1)	1.435(3)
O(3)-S(1)	1.437(3)

C(29)-C(1)-C(2)	118.0(5)
C(29)-C(1)-C(30)	120.2(6)
C(2)-C(1)-C(30)	121.8(6)
C(3)-C(2)-C(1)	121.8(5)
C(3)-C(2)-H(19)	119.1
C(1)-C(2)-H(19)	119.1
C(2)-C(3)-C(4)	119.2(5)
C(2)-C(3)-H(2)	120.4
C(4)-C(3)-H(2)	120.4
C(28)-C(4)-C(3)	120.4(5)
C(28)-C(4)-S(1)	121.4(4)
C(3)-C(4)-S(1)	118.1(4)
C(6)-C(5)-N(2)	109.7(4)
C(6)-C(5)-N(1)	129.9(4)
N(2)-C(5)-N(1)	120.4(4)
C(5)-C(6)-C(20)	106.8(4)
C(5)-C(6)-C(7)	127.1(4)
C(20)-C(6)-C(7)	126.1(4)
C(8)-C(7)-C(6)	175.2(5)
C(7)-C(8)-C(9)	177.6(5)
C(10)-C(9)-C(22)	118.8(5)
C(10)-C(9)-C(8)	122.6(5)
C(22)-C(9)-C(8)	118.5(5)
C(11)-C(10)-C(9)	119.6(5)
C(11)-C(10)-H(11)	120.2
C(9)-C(10)-H(11)	120.2
C(12)-C(11)-C(10)	121.0(5)
C(12)-C(11)-H(10)	119.5
C(10)-C(11)-H(10)	119.5
C(21)-C(12)-C(11)	119.8(5)

C(21)-C(12)-H(1)	120.1
C(11)-C(12)-H(1)	120.1
C(18)-C(13)-C(14)	119.9(4)
C(18)-C(13)-N(1)	120.3(4)
C(14)-C(13)-N(1)	119.7(4)
C(13)-C(14)-C(15)	118.8(5)
C(13)-C(14)-H(3)	120.6
C(15)-C(14)-H(3)	120.6
C(16)-C(15)-C(14)	119.6(5)
C(16)-C(15)-H(4)	120.2
C(14)-C(15)-H(4)	120.2
C(17)-C(16)-C(15)	120.8(5)
C(17)-C(16)-H(5)	119.6
C(15)-C(16)-H(5)	119.6
C(16)-C(17)-C(18)	119.7(6)
C(16)-C(17)-H(6)	120.1
C(18)-C(17)-H(6)	120.1
C(13)-C(18)-C(17)	121.2(5)
C(13)-C(18)-H(7)	119.4
C(17)-C(18)-H(7)	119.4
N(2)-C(19)-C(26)	130.2(4)
N(2)-C(19)-C(20)	108.0(4)
C(26)-C(19)-C(20)	121.8(4)
C(23)-C(20)-C(19)	119.8(5)
C(23)-C(20)-C(6)	133.1(5)
C(19)-C(20)-C(6)	107.1(4)
C(22)-C(21)-C(12)	120.0(5)
C(22)-C(21)-H(9)	120.0
C(12)-C(21)-H(9)	120.0
C(21)-C(22)-C(9)	120.8(5)
C(21)-C(22)-H(8)	119.6
C(9)-C(22)-H(8)	119.6
C(24)-C(23)-C(20)	119.0(5)
C(24)-C(23)-H(15)	120.5
C(20)-C(23)-H(15)	120.5
C(23)-C(24)-C(25)	121.1(5)
C(23)-C(24)-H(14)	119.4
C(25)-C(24)-H(14)	119.4

C(24)-C(25)-C(26)	121.8(5)
C(24)-C(25)-H(13)	119.1
C(26)-C(25)-H(13)	119.1
C(25)-C(26)-C(19)	116.5(5)
C(25)-C(26)-C(27)	120.9(5)
C(19)-C(26)-C(27)	122.6(4)
O(1)-C(27)-C(26)	126.2(5)
O(1)-C(27)-H(12)	116.9
C(26)-C(27)-H(12)	116.9
C(4)-C(28)-C(29)	119.5(5)
C(4)-C(28)-H(18)	120.2
C(29)-C(28)-H(18)	120.2
C(1)-C(29)-C(28)	121.0(5)
C(1)-C(29)-H(17)	119.5
C(28)-C(29)-H(17)	119.5
C(1)-C(30)-H(30A)	109.5
C(1)-C(30)-H(30B)	109.5
H(30A)-C(30)-H(30B)	109.5
C(1)-C(30)-H(30C)	109.5
H(30A)-C(30)-H(30C)	109.5
H(30B)-C(30)-H(30C)	109.5
C(5)-N(1)-C(13)	118.1(3)
C(5)-N(1)-S(1)	120.1(3)
C(13)-N(1)-S(1)	121.7(3)
C(19)-N(2)-C(5)	108.5(4)
C(19)-N(2)-H(16)	125.8
C(5)-N(2)-H(16)	125.8
O(2)-S(1)-O(3)	121.14(18)
O(2)-S(1)-N(1)	107.93(18)
O(3)-S(1)-N(1)	105.32(18)
O(2)-S(1)-C(4)	106.4(2)
O(3)-S(1)-C(4)	109.1(2)
N(1)-S(1)-C(4)	106.10(18)

Symmetry transformations used to generate equivalent atoms:

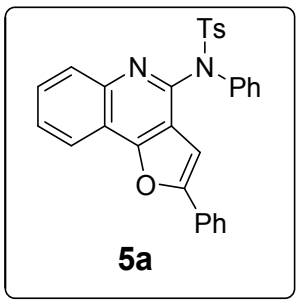
Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for mo_191107_0m. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	34(4)	57(4)	78(4)	25(3)	15(3)	9(3)
C(2)	43(4)	59(3)	57(3)	13(3)	18(3)	10(3)
C(3)	42(3)	40(3)	52(3)	2(2)	7(3)	4(2)
C(4)	34(3)	40(3)	35(3)	7(2)	4(2)	0(2)
C(5)	39(3)	30(3)	38(3)	1(2)	-6(2)	2(2)
C(6)	33(3)	38(3)	45(3)	-3(2)	3(2)	-1(2)
C(7)	37(3)	45(3)	43(3)	-7(3)	-1(3)	10(3)
C(8)	46(4)	48(3)	44(3)	0(3)	5(3)	4(3)
C(9)	38(3)	40(3)	42(3)	8(2)	3(2)	7(3)
C(10)	46(4)	48(3)	54(3)	-2(3)	-5(3)	-1(3)
C(11)	53(4)	56(4)	84(5)	13(3)	12(3)	-13(3)
C(12)	54(4)	68(4)	61(4)	14(3)	25(3)	0(3)
C(13)	41(3)	30(3)	38(3)	2(2)	-2(2)	-2(2)
C(14)	70(4)	44(3)	39(3)	0(2)	-2(3)	-1(3)
C(15)	88(5)	34(3)	68(4)	11(3)	-11(4)	-10(3)
C(16)	87(5)	42(4)	69(4)	-10(3)	-20(4)	16(3)
C(17)	72(5)	58(4)	67(4)	-12(3)	4(3)	23(4)
C(18)	58(4)	43(3)	47(3)	2(2)	1(3)	10(3)
C(19)	38(3)	35(3)	39(3)	2(2)	-3(2)	2(2)
C(20)	35(3)	37(3)	41(3)	-4(2)	-8(2)	8(2)
C(21)	55(4)	59(4)	50(3)	4(3)	15(3)	1(3)
C(22)	50(4)	42(3)	44(3)	3(2)	4(3)	-1(3)
C(23)	46(4)	64(4)	40(3)	-7(3)	2(3)	3(3)
C(24)	51(4)	69(4)	54(4)	-13(3)	-10(3)	1(3)
C(25)	41(4)	46(3)	71(4)	-6(3)	-9(3)	-5(3)
C(26)	33(3)	42(3)	62(4)	7(3)	-3(3)	-4(3)
C(27)	38(4)	56(3)	86(5)	19(3)	0(3)	-16(3)
C(28)	60(4)	61(4)	59(4)	-1(3)	-7(3)	-18(3)
C(29)	54(4)	57(4)	83(5)	10(3)	0(3)	-18(3)
C(30)	62(5)	80(4)	126(6)	38(4)	41(4)	2(4)
N(1)	35(2)	29(2)	38(2)	1(2)	-4(2)	0(2)
N(2)	42(3)	36(2)	37(2)	9(2)	1(2)	-7(2)
O(1)	68(3)	113(3)	62(3)	19(2)	-4(2)	-28(3)
O(2)	53(2)	56(2)	32(2)	2(2)	-7(2)	-4(2)
O(3)	48(2)	24(2)	66(2)	4(2)	1(2)	-1(2)
S(1)	39(1)	36(1)	41(1)	6(1)	-1(1)	-2(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^{-3}) for mo_191107_0m.

	x	y	z	U(eq)
H(19)	1551	3774	3666	62
H(2)	3223	4930	2834	53
H(11)	3433	1067	3962	61
H(10)	2298	-1	5086	78
H(1)	3067	749	6520	72
H(3)	4683	1354	2148	62
H(4)	5201	-1074	1776	78
H(5)	6769	-1496	705	82
H(6)	7735	431	-32	79
H(7)	7132	2805	284	60
H(9)	4960	2615	6845	65
H(8)	6090	3716	5737	55
H(15)	8946	5780	4448	60
H(14)	11058	7415	4445	72
H(13)	11791	8247	3154	65
H(12)	11483	8303	1571	73
H(18)	1492	2320	775	74
H(17)	-174	1148	1629	79
H(30A)	-1534	1282	2949	130
H(30B)	-715	2152	3787	130
H(30C)	-114	628	3515	130
H(16)	7803	5726	1117	47

3.3. X-ray crystallographic structure and data for compound 5a



5a

CCDC : 1996563

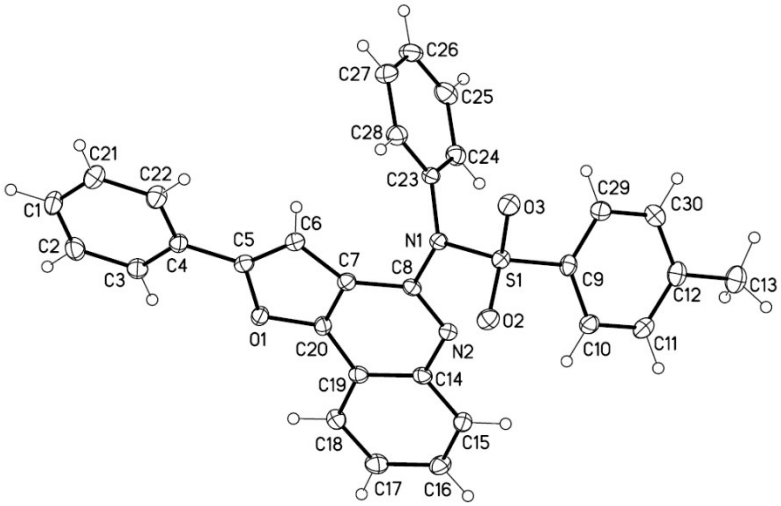


Figure S2 - Molecular structure of compound 5a

Table 1. Crystal data and structure refinement for mo_191113lt_0m.

Identification code	mo_191113LT_0m	
Empirical formula	C30 H22 N2 O3 S	
Formula weight	490.55	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 11.8170(2) Å	α= 90°.
	b = 9.2806(2) Å	β= 94.1040(10)°.
	c = 21.6826(4) Å	γ = 90°.
Volume	2371.81(8) $Å^3$	
Z	4	
Density (calculated)	1.374 Mg/m^3	
Absorption coefficient	0.173 mm^{-1}	
F(000)	1024	
Crystal size	0.15 x 0.12 x 0.11 mm^3	
Theta range for data collection	1.728 to 26.414°.	
Index ranges	-14<=h<=14, -11<=k<=11, -27<=l<=26	
Reflections collected	27010	
Independent reflections	4860 [R(int) = 0.0320]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7454 and 0.6992	
Refinement method	Full-matrix least-squares on F^2	

Data / restraints / parameters	4860 / 0 / 326
Goodness-of-fit on F^2	1.026
Final R indices [I>2sigma(I)]	R1 = 0.0324, wR2 = 0.0775
R indices (all data)	R1 = 0.0431, wR2 = 0.0833
Extinction coefficient	n/a
Largest diff. peak and hole	0.331 and -0.449 e.Å^{-3}

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for mo_191113lt_0m. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
S(1)	9558(1)	1453(1)	1218(1)	16(1)
O(1)	5477(1)	989(1)	-700(1)	17(1)
O(2)	9638(1)	2879(1)	975(1)	21(1)
O(3)	10527(1)	520(1)	1237(1)	21(1)
N(1)	8583(1)	590(1)	764(1)	15(1)
N(2)	7128(1)	2244(1)	942(1)	15(1)
C(1)	5384(2)	-2050(2)	-2620(1)	28(1)
C(2)	4594(1)	-1207(2)	-2347(1)	24(1)
C(3)	4874(1)	-538(2)	-1785(1)	20(1)
C(4)	5957(1)	-698(2)	-1494(1)	16(1)
C(5)	6258(1)	0(2)	-902(1)	16(1)
C(6)	7161(1)	-123(2)	-487(1)	16(1)
C(7)	6953(1)	833(2)	12(1)	15(1)
C(8)	7524(1)	1269(2)	582(1)	14(1)
C(9)	9101(1)	1553(2)	1974(1)	17(1)
C(10)	8588(1)	2801(2)	2174(1)	18(1)
C(11)	8270(1)	2872(2)	2776(1)	20(1)
C(12)	8447(1)	1712(2)	3180(1)	20(1)
C(13)	8087(1)	1815(2)	3832(1)	26(1)
C(14)	6095(1)	2883(2)	772(1)	15(1)
C(15)	5663(1)	3899(2)	1177(1)	18(1)
C(16)	4622(1)	4517(2)	1042(1)	21(1)
C(17)	3968(1)	4158(2)	493(1)	21(1)
C(18)	4361(1)	3175(2)	90(1)	18(1)
C(19)	5428(1)	2522(2)	223(1)	15(1)
C(20)	5924(1)	1481(2)	-143(1)	15(1)
C(21)	6456(2)	-2230(2)	-2329(1)	28(1)

C(22)	6747(1)	-1553(2)	-1769(1)	22(1)
C(23)	8571(1)	-974(2)	795(1)	15(1)
C(24)	7881(1)	-1653(2)	1195(1)	19(1)
C(25)	7834(1)	-3146(2)	1205(1)	24(1)
C(26)	8463(1)	-3949(2)	812(1)	25(1)
C(27)	9156(1)	-3259(2)	417(1)	24(1)
C(28)	9219(1)	-1765(2)	409(1)	20(1)
C(29)	9292(1)	385(2)	2367(1)	21(1)
C(30)	8957(1)	473(2)	2969(1)	23(1)

Table 3. Bond lengths [Å] and angles [°] for mo_191113lt_0m.

S(1)-O(2)	1.4298(11)
S(1)-O(3)	1.4338(10)
S(1)-N(1)	1.6655(12)
S(1)-C(9)	1.7640(14)
O(1)-C(20)	1.3633(16)
O(1)-C(5)	1.3940(17)
N(1)-C(8)	1.4307(17)
N(1)-C(23)	1.4538(18)
N(2)-C(8)	1.3034(18)
N(2)-C(14)	1.3825(18)
C(1)-C(2)	1.383(2)
C(1)-C(21)	1.385(2)
C(1)-H(1)	0.9500
C(2)-C(3)	1.386(2)
C(2)-H(10)	0.9500
C(3)-C(4)	1.393(2)
C(3)-H(7)	0.9500
C(4)-C(22)	1.393(2)
C(4)-C(5)	1.4596(19)
C(5)-C(6)	1.3507(19)
C(6)-C(7)	1.4329(19)
C(6)-H(6)	0.9500
C(7)-C(20)	1.3768(19)
C(7)-C(8)	1.4239(19)
C(9)-C(29)	1.388(2)
C(9)-C(10)	1.391(2)

C(10)-C(11)	1.385(2)
C(10)-H(5)	0.9500
C(11)-C(12)	1.395(2)
C(11)-H(4)	0.9500
C(12)-C(30)	1.390(2)
C(12)-C(13)	1.508(2)
C(13)-H(22)	0.9800
C(13)-H(3)	0.9800
C(13)-H(2)	0.9800
C(14)-C(15)	1.410(2)
C(14)-C(19)	1.4198(19)
C(15)-C(16)	1.370(2)
C(15)-H(14)	0.9500
C(16)-C(17)	1.411(2)
C(16)-H(13)	0.9500
C(17)-C(18)	1.367(2)
C(17)-H(12)	0.9500
C(18)-C(19)	1.410(2)
C(18)-H(11)	0.9500
C(19)-C(20)	1.405(2)
C(21)-C(22)	1.388(2)
C(21)-H(9)	0.9500
C(22)-H(8)	0.9500
C(23)-C(24)	1.384(2)
C(23)-C(28)	1.384(2)
C(24)-C(25)	1.387(2)
C(24)-H(15)	0.9500
C(25)-C(26)	1.386(2)
C(25)-H(19)	0.9500
C(26)-C(27)	1.385(2)
C(26)-H(18)	0.9500
C(27)-C(28)	1.388(2)
C(27)-H(16)	0.9500
C(28)-H(17)	0.9500
C(29)-C(30)	1.393(2)
C(29)-H(21)	0.9500
C(30)-H(20)	0.9500

O(2)-S(1)-O(3)	119.69(6)
O(2)-S(1)-N(1)	106.76(6)
O(3)-S(1)-N(1)	104.13(6)
O(2)-S(1)-C(9)	109.02(7)
O(3)-S(1)-C(9)	107.57(6)
N(1)-S(1)-C(9)	109.28(6)
C(20)-O(1)-C(5)	105.96(10)
C(8)-N(1)-C(23)	116.17(11)
C(8)-N(1)-S(1)	120.38(9)
C(23)-N(1)-S(1)	117.48(9)
C(8)-N(2)-C(14)	119.13(12)
C(2)-C(1)-C(21)	119.79(14)
C(2)-C(1)-H(1)	120.1
C(21)-C(1)-H(1)	120.1
C(1)-C(2)-C(3)	120.20(14)
C(1)-C(2)-H(10)	119.9
C(3)-C(2)-H(10)	119.9
C(2)-C(3)-C(4)	120.33(14)
C(2)-C(3)-H(7)	119.8
C(4)-C(3)-H(7)	119.8
C(22)-C(4)-C(3)	119.26(13)
C(22)-C(4)-C(5)	120.07(13)
C(3)-C(4)-C(5)	120.66(13)
C(6)-C(5)-O(1)	110.89(12)
C(6)-C(5)-C(4)	132.87(13)
O(1)-C(5)-C(4)	116.24(12)
C(5)-C(6)-C(7)	106.27(12)
C(5)-C(6)-H(6)	126.9
C(7)-C(6)-H(6)	126.9
C(20)-C(7)-C(8)	116.25(12)
C(20)-C(7)-C(6)	106.45(12)
C(8)-C(7)-C(6)	137.27(13)
N(2)-C(8)-C(7)	123.25(13)
N(2)-C(8)-N(1)	119.04(12)
C(7)-C(8)-N(1)	117.71(12)
C(29)-C(9)-C(10)	120.94(13)
C(29)-C(9)-S(1)	118.87(11)
C(10)-C(9)-S(1)	120.17(11)

C(11)-C(10)-C(9)	119.15(14)
C(11)-C(10)-H(5)	120.4
C(9)-C(10)-H(5)	120.4
C(10)-C(11)-C(12)	121.10(14)
C(10)-C(11)-H(4)	119.5
C(12)-C(11)-H(4)	119.5
C(30)-C(12)-C(11)	118.75(13)
C(30)-C(12)-C(13)	121.23(14)
C(11)-C(12)-C(13)	120.03(14)
C(12)-C(13)-H(22)	109.5
C(12)-C(13)-H(3)	109.5
H(22)-C(13)-H(3)	109.5
C(12)-C(13)-H(2)	109.5
H(22)-C(13)-H(2)	109.5
H(3)-C(13)-H(2)	109.5
N(2)-C(14)-C(15)	118.25(12)
N(2)-C(14)-C(19)	123.29(13)
C(15)-C(14)-C(19)	118.40(13)
C(16)-C(15)-C(14)	120.41(13)
C(16)-C(15)-H(14)	119.8
C(14)-C(15)-H(14)	119.8
C(15)-C(16)-C(17)	120.75(14)
C(15)-C(16)-H(13)	119.6
C(17)-C(16)-H(13)	119.6
C(18)-C(17)-C(16)	120.39(13)
C(18)-C(17)-H(12)	119.8
C(16)-C(17)-H(12)	119.8
C(17)-C(18)-C(19)	119.71(13)
C(17)-C(18)-H(11)	120.1
C(19)-C(18)-H(11)	120.1
C(20)-C(19)-C(18)	125.73(13)
C(20)-C(19)-C(14)	113.92(12)
C(18)-C(19)-C(14)	120.34(13)
O(1)-C(20)-C(7)	110.43(12)
O(1)-C(20)-C(19)	125.44(12)
C(7)-C(20)-C(19)	124.12(12)
C(1)-C(21)-C(22)	120.36(15)
C(1)-C(21)-H(9)	119.8

C(22)-C(21)-H(9)	119.8
C(21)-C(22)-C(4)	120.05(14)
C(21)-C(22)-H(8)	120.0
C(4)-C(22)-H(8)	120.0
C(24)-C(23)-C(28)	120.88(13)
C(24)-C(23)-N(1)	119.44(13)
C(28)-C(23)-N(1)	119.64(13)
C(23)-C(24)-C(25)	119.43(14)
C(23)-C(24)-H(15)	120.3
C(25)-C(24)-H(15)	120.3
C(26)-C(25)-C(24)	120.19(15)
C(26)-C(25)-H(19)	119.9
C(24)-C(25)-H(19)	119.9
C(27)-C(26)-C(25)	119.90(14)
C(27)-C(26)-H(18)	120.1
C(25)-C(26)-H(18)	120.1
C(26)-C(27)-C(28)	120.28(15)
C(26)-C(27)-H(16)	119.9
C(28)-C(27)-H(16)	119.9
C(23)-C(28)-C(27)	119.30(15)
C(23)-C(28)-H(17)	120.3
C(27)-C(28)-H(17)	120.3
C(9)-C(29)-C(30)	119.05(14)
C(9)-C(29)-H(21)	120.5
C(30)-C(29)-H(21)	120.5
C(12)-C(30)-C(29)	121.01(14)
C(12)-C(30)-H(20)	119.5
C(29)-C(30)-H(20)	119.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for mo_191113lt_0m. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
S(1)	14(1)	16(1)	17(1)	-2(1)	1(1)	0(1)
O(1)	17(1)	18(1)	15(1)	-3(1)	0(1)	1(1)

O(2)	21(1)	18(1)	23(1)	-1(1)	4(1)	-3(1)
O(3)	15(1)	24(1)	24(1)	-3(1)	1(1)	3(1)
N(1)	15(1)	14(1)	16(1)	-1(1)	-1(1)	1(1)
N(2)	17(1)	14(1)	15(1)	1(1)	1(1)	1(1)
C(1)	42(1)	23(1)	17(1)	-4(1)	-3(1)	-3(1)
C(2)	28(1)	23(1)	21(1)	2(1)	-6(1)	-4(1)
C(3)	22(1)	18(1)	20(1)	1(1)	1(1)	-2(1)
C(4)	20(1)	14(1)	15(1)	0(1)	1(1)	-3(1)
C(5)	18(1)	14(1)	18(1)	0(1)	4(1)	-1(1)
C(6)	16(1)	15(1)	17(1)	0(1)	2(1)	0(1)
C(7)	17(1)	14(1)	15(1)	1(1)	3(1)	-1(1)
C(8)	16(1)	13(1)	15(1)	3(1)	2(1)	-1(1)
C(9)	14(1)	20(1)	15(1)	-2(1)	-1(1)	-1(1)
C(10)	19(1)	16(1)	20(1)	-2(1)	-1(1)	-1(1)
C(11)	18(1)	19(1)	22(1)	-6(1)	2(1)	0(1)
C(12)	15(1)	26(1)	19(1)	-3(1)	0(1)	-5(1)
C(13)	26(1)	33(1)	21(1)	-4(1)	5(1)	-4(1)
C(14)	17(1)	13(1)	16(1)	2(1)	3(1)	0(1)
C(15)	21(1)	17(1)	16(1)	-1(1)	1(1)	-1(1)
C(16)	23(1)	18(1)	21(1)	-3(1)	5(1)	4(1)
C(17)	17(1)	21(1)	25(1)	0(1)	2(1)	5(1)
C(18)	18(1)	19(1)	18(1)	1(1)	0(1)	1(1)
C(19)	17(1)	13(1)	16(1)	2(1)	3(1)	-1(1)
C(20)	17(1)	15(1)	14(1)	0(1)	0(1)	-3(1)
C(21)	36(1)	27(1)	21(1)	-6(1)	4(1)	5(1)
C(22)	22(1)	24(1)	20(1)	-3(1)	2(1)	0(1)
C(23)	16(1)	13(1)	16(1)	0(1)	-2(1)	1(1)
C(24)	18(1)	21(1)	19(1)	0(1)	0(1)	2(1)
C(25)	24(1)	22(1)	25(1)	6(1)	-1(1)	-2(1)
C(26)	28(1)	14(1)	31(1)	2(1)	-7(1)	1(1)
C(27)	27(1)	20(1)	26(1)	-4(1)	-1(1)	7(1)
C(28)	21(1)	20(1)	21(1)	0(1)	2(1)	2(1)
C(29)	23(1)	20(1)	21(1)	-2(1)	-2(1)	6(1)
C(30)	26(1)	23(1)	21(1)	3(1)	-2(1)	2(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^{3}) for mo_191113lt_0m.

	x	y	z	U(eq)
H(1)	5191	-2503	-3006	33
H(10)	3856	-1086	-2545	29
H(7)	4326	31	-1597	24
H(6)	7806	-722	-519	19
H(5)	8457	3594	1901	22
H(4)	7925	3725	2915	24
H(22)	8307	932	4058	40
H(3)	7262	1934	3822	40
H(2)	8458	2645	4040	40
H(14)	6096	4158	1546	21
H(13)	4337	5194	1320	25
H(12)	3251	4601	403	26
H(11)	3917	2933	-278	22
H(9)	6995	-2821	-2513	33
H(8)	7487	-1673	-1574	27
H(15)	7444	-1101	1460	23
H(19)	7369	-3620	1482	28
H(18)	8418	-4971	815	30
H(16)	9590	-3810	150	29
H(17)	9703	-1291	142	24
H(21)	9647	-462	2228	26
H(20)	9079	-325	3240	28

(7) Computational details

Geometries were optimized using the B3LYP functional, the 6-31G** basis for light atoms, and a double-*z* contraction of the Los Alamos valence functions and pseudopotentials for gold. Hessians at these geometries provided the zero-point energy and vibrational enthalpy and entropy. Solvation free energies G_{solv} were computed in toluene with the CPCM continuum model. The electronic energy E_{elec} was evaluated with the same functional and the 6-311++G** basis and a triple- *z* contraction of the Los Alamos valence functions augmented with diffuse *s* and *p* functions for gold. Gibbs

free energies of organometallic species were computed according to the following equation:

$$G = E_{elec} + G_{solv} + ZPE + H_{vib} + 4kT - TS_{vib}$$

Species	E_{elec}	G_{solv}	$ZPE + H_{vib} + 4kT - TS_{vib}$	G_{total}(hartree)
Benzo[c]isoxazole	-399.7682573	-0.0037519	0.075015	-399.6969942
A	-2745.511509	-0.029182	0.660579	-2744.880112
B	-3145.293387	-0.032221	0.764975	-3144.560633
C	-3145.332874	-0.029353	0.761860	-3144.600367
D	-3145.314195	-0.029420	0.765701	-3144.577915
E	-1890.039061	-0.009762	0.378476	-1889.670347
F	-3145.322372	-0.033609	0.763922	-3144.592059
TS_{AB}	-3145.273587	-0.0293272	0.760904	-3144.542011
TS_{BC}	-3145.288236	-0.0308428	0.762569	-3144.55651
TS_{CD}	-3145.31417	-0.02917868	0.766278	-3144.577071
TS_{CF}	-3145.302886	-0.0324847	0.762336	-3144.573035
1a	-1490.19882	-0.0071132	0.276072	-1489.929862

Coordinates of optimized structures

Benzo[c]isoxazole

C	0.00000000	-0.75787300	0.00000000
C	-0.53956500	0.57933900	0.00000000
C	0.32802300	1.71036900	0.00000000
C	1.67700400	1.47978000	0.00000000
C	2.21382200	0.14594700	0.00000000
C	1.41371300	-0.96388300	0.00000000
C	-1.89701400	0.36104000	0.00000000
H	-0.07308100	2.71885400	0.00000000
H	2.36862400	2.31650600	0.00000000
H	3.29330200	0.02617600	0.00000000
H	1.81836700	-1.96978900	0.00000000
H	-2.76326500	1.00606700	0.00000000
O	-2.14352000	-0.95463800	0.00000000
N	-0.95309600	-1.68414700	0.00000000

A

C	-1.74271100	-0.00490200	-0.42952000
C	-0.82602500	0.89093900	-0.51958300

C	-0.84299400	2.26860800	-0.71759600
C	-0.78870700	3.47391000	-0.89842500
N	-2.56854600	-0.97067000	-0.30294200
C	-3.13535700	-1.69412500	-1.42528800
C	-2.88647000	-3.06186300	-1.56577900
C	-3.92096000	-0.99676500	-2.34702200
C	-3.43775200	-3.73533300	-2.65672500
H	-2.28125700	-3.58230600	-0.83333900
C	-4.45540900	-1.68173000	-3.43720100
H	-4.10435600	0.06397500	-2.20877900
C	-4.21718800	-3.04964200	-3.59099200
H	-3.25057600	-4.79757000	-2.77778200
H	-5.06116200	-1.14718600	-4.16189400
H	-4.63837300	-3.58045800	-4.43894800
S	-3.11109800	-1.43648300	1.44650100
O	-2.91677000	-2.88141200	1.51225700
O	-2.36052800	-0.49261300	2.26484000
C	-4.83690800	-1.04327700	1.44536500
C	-5.76315000	-2.03937300	1.12010300
C	-5.23564000	0.25679600	1.77614700
C	-7.11659700	-1.71544000	1.13134900
H	-5.42951000	-3.04241400	0.88037700
C	-6.59437700	0.55270200	1.77985800
H	-4.49920900	1.00702900	2.04241200
C	-7.55433900	-0.42275800	1.46053600
H	-7.84654300	-2.48111600	0.88580400
H	-6.91832900	1.55549700	2.04265600
C	-9.02496400	-0.09567900	1.50398900
H	-9.59689500	-0.72551300	0.81775300
H	-9.42436300	-0.26285400	2.51178900
H	-9.21090400	0.95128200	1.24995500
Au	1.07047800	-0.10801900	-0.36742700
P	3.18720800	-1.19201000	-0.47743200
C	4.05502600	-0.50191100	-2.04334300
C	2.83922300	-3.08584100	-0.51794300
C	4.34689100	-0.87624900	0.93188000
C	4.07926700	0.02729100	1.99124600
C	5.58297000	-1.55639800	0.92925600

C	5.06528000	0.22010500	2.97622100
C	2.81801600	0.81020400	2.19255200
C	6.53764600	-1.36072100	1.92250900
H	5.81593900	-2.24805800	0.13162000
C	6.27913900	-0.45885300	2.95267100
H	4.85309800	0.91546900	3.78227600
C	2.78607600	2.18266800	1.90110700
C	1.70657600	0.22591500	2.82178500
H	7.47524600	-1.90645700	1.88478900
H	7.01281500	-0.28783200	3.73444900
C	1.66390500	2.94984300	2.22010500
H	3.65057800	2.65059700	1.43867800
C	0.58566100	0.99475200	3.14326400
H	1.73210300	-0.82833000	3.08178700
C	0.56382800	2.35826600	2.84356400
H	1.65401300	4.01135500	1.99092300
H	-0.26747600	0.52647700	3.62240800
H	-0.30384900	2.95818300	3.10034900
C	-0.74992300	4.88023700	-1.10307700
C	0.48701200	5.55196000	-1.20095800
C	-1.94549900	5.62151800	-1.20962100
C	0.52172900	6.92866200	-1.39914100
H	1.40688100	4.98164300	-1.12199500
C	-1.89994200	6.99780100	-1.40764100
H	-2.89721900	5.10550600	-1.13572300
C	-0.66903700	7.65353100	-1.50255800
H	1.47699000	7.43897000	-1.47448800
H	-2.82393000	7.56188900	-1.48898300
H	-0.63785100	8.72768700	-1.65762900
C	3.21100400	-0.86046200	-3.28330800
H	2.15924300	-0.58258000	-3.16230100
H	3.60282600	-0.31091400	-4.14655100
H	3.26518300	-1.92507400	-3.52667900
C	4.07159300	1.03344900	-1.86688700
H	3.06226600	1.45082600	-1.80250000
H	4.62794900	1.33571100	-0.97465200
H	4.56690200	1.48224900	-2.73535800
C	5.50552700	-0.97638500	-2.25845800

H	5.59372500	-2.06078200	-2.35251800
H	5.87170200	-0.53988000	-3.19462500
H	6.17072700	-0.63791300	-1.46188900
C	1.58328400	-3.34339100	-1.38053300
H	0.70688400	-2.81977900	-0.98903000
H	1.71647500	-3.04891600	-2.42338300
H	1.36739400	-4.41788400	-1.36529500
C	3.98434700	-3.95901400	-1.06704300
H	4.89964900	-3.88696600	-0.47747700
H	3.66604700	-5.00707300	-1.02868900
H	4.21735900	-3.73252400	-2.11032800
C	2.52285100	-3.49710500	0.93620100
H	3.39167900	-3.40514200	1.59196800
H	1.70665200	-2.90072400	1.35760500
H	2.20397600	-4.54541500	0.94485000

B

C	-1.76093600	0.65428800	-0.56129700
C	-0.43940400	0.99913700	-0.53471000
C	-0.07933400	2.35507300	-0.64423200
C	0.29665700	3.51346400	-0.75346200
N	-2.34735100	-0.62954300	-0.49924100
C	-2.63911700	-1.34710200	-1.72052000
C	-1.60582900	-1.75047100	-2.57455200
C	-3.97160200	-1.60621400	-2.06144000
C	-1.90962000	-2.41181200	-3.76374900
H	-0.57843700	-1.53347600	-2.30286900
C	-4.26781200	-2.27873800	-3.24812500
H	-4.76554600	-1.28209200	-1.39710400
C	-3.23869900	-2.68123600	-4.10072600
H	-1.10737600	-2.72169300	-4.42677400
H	-5.30245200	-2.48085300	-3.50825300
H	-3.47061600	-3.19994900	-5.02596700
S	-2.23587300	-1.50170700	0.98475900
O	-1.28055200	-2.60472300	0.83345500
O	-2.03721200	-0.46942300	2.01158600
C	-3.85366600	-2.22864000	1.20752700
C	-4.03969800	-3.58353100	0.92975100

C	-4.90129600	-1.43968000	1.69126700
C	-5.29865100	-4.14686200	1.13025000
H	-3.20915200	-4.18007100	0.57041800
C	-6.15132500	-2.02071600	1.88270700
H	-4.73567000	-0.39402600	1.92749700
C	-6.37135000	-3.38065100	1.60762900
H	-5.44858200	-5.20106600	0.91502700
H	-6.96917100	-1.41411100	2.26203500
C	-7.72079600	-4.00798800	1.85463200
H	-7.89301500	-4.86200600	1.19415700
H	-7.79436900	-4.37300900	2.88633600
H	-8.53141200	-3.28913800	1.70582700
Au	1.17863000	-0.29427000	-0.32958700
P	3.12837300	-1.71461400	-0.36901000
C	3.89204200	-1.44443100	-2.12612700
C	2.63508300	-3.53527900	-0.00750600
C	4.47920800	-1.30219800	0.84062200
C	4.38891900	-0.29210000	1.83424500
C	5.70106100	-1.99533000	0.71075200
C	5.52594600	-0.01855500	2.61974900
C	3.18740600	0.53481000	2.16669300
C	6.80839400	-1.71489900	1.50539000
H	5.79845900	-2.77369400	-0.03230600
C	6.72188200	-0.71066300	2.46664500
H	5.44599500	0.75110000	3.38094400
C	3.25265500	1.93090100	2.02382700
C	2.04959000	-0.02481800	2.76918000
H	7.72743900	-2.27636400	1.36862600
H	7.57293700	-0.47232900	3.09738200
C	2.20751500	2.74325100	2.46368300
H	4.13550100	2.37757000	1.57491600
C	1.00408800	0.78818900	3.21269600
H	1.99358400	-1.09703700	2.91932500
C	1.08276900	2.17335500	3.06321900
H	2.27594200	3.82043300	2.34338600
H	0.13116700	0.33265100	3.66845500
H	0.27573800	2.80790500	3.41812400
C	0.77470200	4.84795000	-0.87263300

C	2.16215300	5.10745300	-0.87392000
C	-0.12166700	5.93064900	-0.99115900
C	2.63241500	6.41182900	-0.99198000
H	2.85295700	4.27576300	-0.78291700
C	0.35709000	7.23196800	-1.10699600
H	-1.18948400	5.73537700	-0.98900100
C	1.73340500	7.47585000	-1.10846800
H	3.70146800	6.60140100	-0.99420500
H	-0.34083800	8.05886200	-1.19728500
H	2.10416800	8.49217200	-1.20047200
C	2.74138400	-1.35059100	-3.15472200
H	2.05507100	-0.53141200	-2.92476000
H	3.17386700	-1.15993300	-4.14393200
H	2.16145600	-2.27399100	-3.22249600
C	4.60707100	-0.07654700	-2.07813900
H	3.93987400	0.71631300	-1.72332100
H	5.49151200	-0.09421500	-1.43730700
H	4.92959100	0.18941500	-3.09137300
C	4.87568900	-2.52190800	-2.62192300
H	4.39925300	-3.49881000	-2.73479600
H	5.23899000	-2.22580500	-3.61300900
H	5.75480000	-2.63055800	-1.98516500
C	1.60015400	-3.98610100	-1.05774200
H	0.74980500	-3.30193500	-1.11540200
H	2.04062100	-4.09784100	-2.05262800
H	1.20966700	-4.96733200	-0.76469800
C	3.79691300	-4.54722800	0.03026700
H	4.49246700	-4.34320000	0.84667500
H	3.37378800	-5.54245400	0.20927000
H	4.35800400	-4.59917200	-0.90476600
C	1.96572200	-3.52593400	1.38417600
H	2.66407900	-3.20671900	2.16406900
H	1.07441000	-2.89548300	1.41015000
H	1.65209400	-4.54813400	1.62629200
C	-3.32491800	2.52466800	0.22075300
C	-4.12637300	3.47392200	-0.49246300
C	-3.24251400	2.52603800	1.63318100
C	-3.93919700	3.15289400	-1.82300100

C	-4.87147700	4.46062000	0.21467800
C	-3.97618000	3.49569700	2.27699000
H	-2.64264700	1.78482500	2.14857500
H	-4.31923200	3.56604200	-2.74758400
C	-4.78292200	4.45580800	1.58204200
H	-5.48232500	5.18154300	-0.31738600
H	-3.94705300	3.53957700	3.36145100
H	-5.33257100	5.18938100	2.16199000
N	-2.73133100	1.70758700	-0.66297900
O	-3.11981200	2.11784400	-1.95641600

C

C	-1.92920000	0.41505800	-0.79789000
C	-0.71794600	0.95980200	-0.13743300
C	-0.74331300	2.24845100	0.28443100
C	-0.72482700	3.42276500	0.67459400
N	-2.55769700	-0.73883600	-0.31309700
C	-3.43846300	-1.49029400	-1.17871500
C	-2.90399100	-2.44108900	-2.05243400
C	-4.81433000	-1.24907500	-1.13722000
C	-3.76131400	-3.16475600	-2.88025800
H	-1.83189500	-2.59198600	-2.08857900
C	-5.66409900	-1.97541500	-1.97051100
H	-5.20746100	-0.50101200	-0.45717100
C	-5.13863300	-2.93467900	-2.83900100
H	-3.35266800	-3.90431400	-3.56175400
H	-6.73347200	-1.79092200	-1.94293100
H	-5.80184800	-3.49945600	-3.48721400
S	-2.12417600	-1.40642600	1.21834100
O	-1.33119000	-2.61803200	1.00066800
O	-1.56297600	-0.26663500	1.96255300
C	-3.67749300	-1.87039800	1.95028300
C	-4.09012700	-3.20336700	1.89321900
C	-4.43625300	-0.89817600	2.60905600
C	-5.29349300	-3.55767800	2.49761600
H	-3.47677900	-3.94201700	1.39012700
C	-5.63540200	-1.27567400	3.20540500
H	-4.08531700	0.12656900	2.66403700

C	-6.08326500	-2.60629000	3.16068700
H	-5.62364100	-4.59162500	2.45603500
H	-6.23149900	-0.52852200	3.72168100
C	-7.36774600	-3.00934600	3.84020000
H	-7.83611600	-3.86075200	3.33924100
H	-7.17746600	-3.30588700	4.87893700
H	-8.08569300	-2.18506600	3.86311300
Au	1.06504100	-0.08852600	-0.21519900
P	3.07488600	-1.38031700	-0.58009300
C	4.05205300	-0.49020000	-1.97182500
C	2.49235900	-3.15824200	-1.05677900
C	4.29392700	-1.54889700	0.81178200
C	4.29630000	-0.75976700	1.98952700
C	5.33378600	-2.48633800	0.64089000
C	5.34229100	-0.93695900	2.91664900
C	3.28254700	0.26530600	2.38855600
C	6.34765100	-2.65738100	1.57791100
H	5.36497600	-3.09356700	-0.25253400
C	6.35545200	-1.86952100	2.72659400
H	5.33354200	-0.33048300	3.81676300
C	3.67379100	1.60860600	2.50720700
C	1.99999600	-0.10364600	2.82537700
H	7.12434200	-3.39561300	1.40425000
H	7.13813100	-1.98189100	3.47059200
C	2.80711600	2.55766400	3.05030800
H	4.67167500	1.90227000	2.19394100
C	1.13536700	0.84571000	3.37546000
H	1.69095600	-1.14315200	2.77133200
C	1.53751800	2.17682900	3.49146200
H	3.13689900	3.58795900	3.15416900
H	0.15037400	0.53736200	3.70682700
H	0.87104900	2.91022900	3.93600800
C	-0.69504600	4.75592800	1.11131600
C	0.53782700	5.36186500	1.46283700
C	-1.89269100	5.50959900	1.19976200
C	0.56426000	6.68314800	1.88718700
H	1.44709400	4.77430200	1.39821900
C	-1.85248400	6.82902800	1.62740500

H	-2.83289300	5.03984000	0.93120000
C	-0.62696600	7.41488800	1.96937700
H	1.50674900	7.14942800	2.15530100
H	-2.76851300	7.40653000	1.69722100
H	-0.60065800	8.44800200	2.30280100
C	3.19813600	-0.47370100	-3.25459600
H	2.18682500	-0.10010900	-3.07677300
H	3.67934800	0.18395600	-3.98808200
H	3.11676400	-1.46321400	-3.71175900
C	4.25549400	0.95994900	-1.47916600
H	3.30352700	1.47448100	-1.31685800
H	4.83002900	0.99889100	-0.54898200
H	4.81604200	1.51620900	-2.23937600
C	5.43523800	-1.09486200	-2.27890300
H	5.38169500	-2.12994200	-2.62196600
H	5.89355700	-0.50996700	-3.08476800
H	6.10641100	-1.04686300	-1.41894200
C	1.14450600	-3.02859200	-1.80442000
H	0.36206400	-2.65627000	-1.13928300
H	1.18677700	-2.37787400	-2.67973900
H	0.84276400	-4.02752000	-2.14174800
C	3.45479400	-3.96491100	-1.95244700
H	4.42763100	-4.15624500	-1.49676100
H	3.00002800	-4.94389600	-2.14185000
H	3.61368900	-3.49257400	-2.92459700
C	2.23422100	-3.92093900	0.26056200
H	3.15069300	-4.11747500	0.82095600
H	1.53429600	-3.38285800	0.90780300
H	1.77359000	-4.88558200	0.01893300
C	-1.99150600	2.00094200	-2.65198900
C	-1.16731500	1.90554800	-3.80764000
C	-2.61691800	3.23067500	-2.37426400
C	-0.46273300	0.67223100	-4.18786700
C	-0.99761200	3.03260900	-4.62786300
C	-2.42448700	4.33391700	-3.20213400
H	-3.27888100	3.29171600	-1.51703700
H	0.02915400	0.72988100	-5.18346900
C	-1.61107500	4.24521000	-4.33593300

H	-0.36610900	2.94032400	-5.50845100
H	-2.92176100	5.26978300	-2.96380700
H	-1.46840300	5.10534900	-4.98129500
N	-2.32940200	0.88164100	-1.91644100
O	-0.37459000	-0.34634800	-3.51903500

D

C	-2.16684500	0.22424800	-0.70260200
C	-0.79274600	0.92172600	-0.76853900
C	-0.81492000	2.21352300	-0.17213900
C	-0.81981800	3.31906800	0.34359800
N	-2.26416200	-1.14408800	-0.44502100
C	-3.22481000	-1.95945700	-1.15833800
C	-2.73218800	-2.84974400	-2.11743800
C	-4.59764900	-1.87576900	-0.90237100
C	-3.62052300	-3.65916200	-2.82701400
H	-1.66352900	-2.90283900	-2.29397300
C	-5.47809200	-2.68105500	-1.62372900
H	-4.96415300	-1.18492100	-0.15334800
C	-4.99235600	-3.57286700	-2.58334600
H	-3.24016200	-4.35246100	-3.57075900
H	-6.54472200	-2.61503800	-1.43251300
H	-5.68274500	-4.20000800	-3.13918800
S	-1.55344600	-1.82301900	1.00284000
O	-0.68240800	-2.92400100	0.59020200
O	-1.04106900	-0.66822900	1.74519600
C	-2.93134400	-2.51280800	1.89721500
C	-3.21832900	-3.87494200	1.77998000
C	-3.67642100	-1.68000600	2.73786200
C	-4.27622300	-4.40229200	2.51538300
H	-2.61798700	-4.50363900	1.13255600
C	-4.73018800	-2.22920700	3.46236400
H	-3.42165800	-0.63023800	2.83421200
C	-5.04689200	-3.59398200	3.36519400
H	-4.50537400	-5.46074200	2.43128500
H	-5.31144500	-1.59154700	4.12243700
C	-6.16779600	-4.18463600	4.18298200
H	-6.62115300	-5.04344500	3.68074900

H	-5.79393200	-4.53395900	5.15319800
H	-6.95108900	-3.44824700	4.38204700
Au	1.11205500	-0.04058400	-0.52998500
P	3.25382700	-1.08974100	-0.80622400
C	4.17183200	-0.05279800	-2.13783700
C	2.89758000	-2.90331300	-1.38097500
C	4.45917300	-1.17473400	0.60771400
C	4.41002600	-0.35106200	1.76142900
C	5.54476000	-2.06520100	0.47655700
C	5.44564800	-0.46218800	2.71055800
C	3.36233200	0.66014100	2.10460800
C	6.54938700	-2.16793800	1.43328200
H	5.62021600	-2.69071900	-0.40095600
C	6.50055800	-1.35517600	2.56322500
H	5.39584000	0.16851500	3.59243500
C	3.72360200	2.01491100	2.18911100
C	2.07707700	0.27897000	2.51796000
H	7.36206900	-2.87310300	1.28907700
H	7.27321600	-1.41530600	3.32365100
C	2.82311800	2.96471800	2.67122600
H	4.72380800	2.31883900	1.89292900
C	1.18007700	1.22949300	3.01034600
H	1.78623800	-0.76609800	2.48815900
C	1.55050200	2.57201500	3.09060000
H	3.12261300	4.00689600	2.73682100
H	0.19425800	0.90992800	3.32823300
H	0.85458800	3.30803300	3.48100500
C	-0.82776300	4.61435200	0.93411300
C	0.34480000	5.39827300	0.95566000
C	-2.01293500	5.13431900	1.49470900
C	0.32468200	6.67053300	1.51957600
H	1.25841000	4.99440600	0.53270300
C	-2.01935300	6.40282700	2.06716600
H	-2.91606300	4.53294500	1.47509400
C	-0.85370300	7.17403500	2.07827000
H	1.22963800	7.27036000	1.52883800
H	-2.93385400	6.79376900	2.50269200
H	-0.86324300	8.16484800	2.52222300

C	3.34799500	-0.04887300	-3.44132500
H	2.31231800	0.26028300	-3.26803000
H	3.79919300	0.66351500	-4.14191000
H	3.34004100	-1.02488800	-3.93361600
C	4.23786300	1.38766600	-1.58417200
H	3.24282900	1.79900400	-1.39004000
H	4.81542800	1.44188700	-0.65761600
H	4.73412300	2.02771700	-2.32310500
C	5.60938100	-0.52209700	-2.43218700
H	5.65287200	-1.53038200	-2.84748400
H	6.04901500	0.15412300	-3.17462600
H	6.24204700	-0.48585000	-1.54274700
C	1.57075600	-2.89491000	-2.17782600
H	0.72959600	-2.60285500	-1.54662900
H	1.60432200	-2.23534400	-3.04831200
H	1.38130300	-3.91297600	-2.53888400
C	3.96287900	-3.56196400	-2.28294400
H	4.94736900	-3.65390500	-1.82260500
H	3.62816900	-4.58033100	-2.51163300
H	4.07795500	-3.04151700	-3.23670000
C	2.68106900	-3.75137600	-0.10884800
H	3.59679400	-3.88072100	0.47122400
H	1.91212800	-3.31928400	0.53782000
H	2.33050500	-4.74564700	-0.40902000
C	-3.41809900	2.07870700	-1.57402600
C	-2.60670400	2.59439100	-2.63988200
C	-4.57653900	2.80673300	-1.21990100
C	-1.41655000	1.96407800	-3.05003400
C	-3.02723000	3.75071400	-3.35887800
C	-4.91184600	3.97389100	-1.88141400
H	-5.20547100	2.40733900	-0.43189800
H	-1.00888600	2.19539600	-4.03827200
C	-4.14603100	4.44920600	-2.97077800
H	-2.42654500	4.08982300	-4.19849100
H	-5.80387500	4.51613800	-1.58197200
H	-4.44801900	5.34683400	-3.49874800
N	-3.25477800	0.84838800	-1.00047200
O	-0.71305100	1.11472400	-2.39990200

E

C	-1.77935400	-0.00362600	-0.33147800
C	-1.39389900	1.43852500	-0.54251100
C	-0.07282000	1.89619100	-0.18502800
C	0.98517200	2.37687400	0.16503800
N	-0.73055000	-0.96647900	-0.23926500
C	-0.89426800	-2.06372400	0.68884900
C	-1.69638400	-3.17445700	0.40621500
C	-0.21632300	-1.97409800	1.90773400
C	-1.80997400	-4.19399800	1.35036700
H	-2.21396000	-3.22888500	-0.54228800
C	-0.34194600	-2.99408100	2.85119600
H	0.39911600	-1.10184700	2.10217100
C	-1.13722400	-4.10610300	2.57156500
H	-2.43158200	-5.05752500	1.13326000
H	0.18268400	-2.92062400	3.79912900
H	-1.23412200	-4.90281100	3.30342000
S	0.13440500	-1.32591200	-1.71110800
O	-0.32685400	-2.61754000	-2.22808100
O	0.03480200	-0.11252000	-2.52097200
C	1.82002300	-1.54632300	-1.15603100
C	2.25808900	-2.81778600	-0.78095800
C	2.68275900	-0.44965600	-1.14378400
C	3.57903100	-2.98045700	-0.37043000
H	1.57708600	-3.65989600	-0.82084800
C	4.00036000	-0.63461300	-0.73194400
H	2.32421500	0.52340600	-1.45627100
C	4.46853700	-1.89705700	-0.33982100
H	3.92582500	-3.96667500	-0.07415900
H	4.67486900	0.21674900	-0.71588200
C	5.90754500	-2.09172800	0.07205400
H	6.01299000	-2.91519900	0.78408400
H	6.53350700	-2.32975300	-0.79679400
H	6.31847900	-1.18753700	0.53009600
C	2.23709200	2.94347900	0.55336400
C	2.72770700	4.09339400	-0.09604700
C	2.99896200	2.36632600	1.58795800

C	3.94683800	4.64794900	0.28393100
H	2.14433400	4.53870100	-0.89514400
C	4.21697300	2.92891200	1.96071300
H	2.62567800	1.47966600	2.08935500
C	4.69503900	4.06981200	1.31202900
H	4.31417600	5.53449700	-0.22432800
H	4.79403700	2.47641200	2.76182100
H	5.64473600	4.50626000	1.60645100
C	-4.03764000	0.50566400	0.01197700
C	-3.86641700	1.90563300	-0.05617700
C	-5.30574800	-0.01735700	0.30804600
C	-2.53713200	2.42223700	-0.41752000
C	-4.94271400	2.75204500	0.22139900
C	-6.37781500	0.83462900	0.55194600
H	-5.41522000	-1.09566200	0.35297500
H	-2.28883600	3.43921300	-0.11554100
C	-6.19664800	2.22185400	0.52007200
H	-4.79892600	3.82870600	0.18187100
H	-7.35558700	0.42073500	0.77937400
H	-7.03231400	2.88587300	0.71860200
N	-2.98428200	-0.39820600	-0.13668300
O	-2.00229400	2.04666500	-1.69198800

F

C	1.30521500	-1.27551900	0.86929900
C	0.77328100	-0.03557500	1.43449900
C	1.52431600	1.18704000	1.38574900
C	2.18623900	2.18990400	1.58130200
N	2.07049200	-1.48180700	-0.24023400
C	2.81658800	-2.72408400	-0.36044300
C	2.30192100	-3.81854600	-1.05855000
C	4.07840600	-2.78005200	0.23743800
C	3.06596100	-4.98061400	-1.15442600
H	1.32183300	-3.75698500	-1.51447100
C	4.83137200	-3.94969100	0.14108200
H	4.45901600	-1.91432100	0.77012000
C	4.32649100	-5.04874900	-0.55596900
H	2.67031400	-5.83833500	-1.68900000

H	5.80946500	-4.00029700	0.60889400
H	4.91248800	-5.95959900	-0.62987500
S	1.97523000	-0.51420800	-1.74510000
O	1.48402300	-1.45456100	-2.74964000
O	1.22057700	0.69214000	-1.41480300
C	3.66266100	-0.09997800	-2.10170200
C	4.42788700	-0.95936300	-2.89604200
C	4.17314600	1.11101500	-1.62573400
C	5.73582000	-0.59458400	-3.20127700
H	4.00383300	-1.88387100	-3.27023700
C	5.48260000	1.45423700	-1.94948800
H	3.55235600	1.77019200	-1.03001700
C	6.28335500	0.61239300	-2.73818400
H	6.34018000	-1.25534400	-3.81590100
H	5.88631500	2.39761000	-1.59304800
C	7.68849900	1.01193000	-3.11106500
H	8.33736500	0.13886300	-3.22119100
H	7.69463400	1.54548700	-4.06935900
H	8.12886400	1.67742200	-2.36396200
Au	-1.19692800	0.01922600	0.31392800
P	-3.31317000	-0.47929900	-0.67436300
C	-4.52557800	-0.87911400	0.75802100
C	-2.98484400	-1.98533300	-1.84498900
C	-4.17813300	0.83092500	-1.66409200
C	-3.88150700	2.21592700	-1.60175500
C	-5.26118900	0.41864000	-2.46812000
C	-4.68874900	3.10887000	-2.33352000
C	-2.77375900	2.86335000	-0.83419800
C	-6.03477600	1.31720400	-3.19549000
H	-5.52188000	-0.62844700	-2.52134200
C	-5.74816600	2.67852200	-3.12395500
H	-4.45168400	4.16676500	-2.28295100
C	-3.08636600	3.74895500	0.20929000
C	-1.43629000	2.74852000	-1.24602800
H	-6.85548100	0.95244200	-3.80513700
H	-6.33974000	3.39915800	-3.68018300
C	-2.08829100	4.50630100	0.82404100
H	-4.12089300	3.86142900	0.52157400

C	-0.43986900	3.51238300	-0.63484500
H	-1.17787900	2.09380400	-2.07214600
C	-0.76436600	4.39690800	0.39503400
H	-2.35058600	5.19699100	1.62042000
H	0.58598600	3.41567300	-0.97178900
H	0.01059400	5.00558600	0.84923500
C	2.97676400	3.35640400	1.81811800
C	2.41589800	4.48661800	2.44730900
C	4.34037000	3.38644200	1.46083700
C	3.19329400	5.61543800	2.69373400
H	1.37270100	4.46313500	2.74424600
C	5.10902600	4.52138900	1.70688400
H	4.78864200	2.51020100	1.00357200
C	4.53930400	5.63966200	2.32041900
H	2.74870100	6.47827200	3.18046900
H	6.15849500	4.53134600	1.42778300
H	5.14215100	6.52167900	2.51302700
C	-4.00355500	-2.09546300	1.54735100
H	-2.96513700	-1.96122100	1.86478300
H	-4.61584000	-2.22012000	2.44803200
H	-4.07414200	-3.02553300	0.97767100
C	-4.51912500	0.36082500	1.67850200
H	-3.52448500	0.55943300	2.08842300
H	-4.86028500	1.25910000	1.15676300
H	-5.20406300	0.18306900	2.51571200
C	-5.97577700	-1.13897500	0.30562200
H	-6.06823800	-2.00233400	-0.35566300
H	-6.58214800	-1.34471300	1.19516000
H	-6.41153900	-0.27085800	-0.19285400
C	-1.87093500	-2.85569700	-1.21725000
H	-0.92185700	-2.31905100	-1.16464300
H	-2.11876400	-3.21505800	-0.21632400
H	-1.71885700	-3.73325200	-1.85604200
C	-4.19149100	-2.91066900	-2.11071300
H	-5.03311900	-2.41675800	-2.59753200
H	-3.86253200	-3.70684000	-2.78801000
H	-4.55351200	-3.39459800	-1.20065000
C	-2.45257400	-1.41392300	-3.17682100

H	-3.21151400	-0.85333900	-3.72620600
H	-1.58415800	-0.76583700	-3.02246600
H	-2.12514700	-2.24712100	-3.80856300
C	0.46167600	-2.00048300	2.73230600
C	-0.18059000	-2.83064000	3.72424000
C	0.43493900	-0.51146200	2.88360800
C	-0.02557500	-4.30785500	3.79789000
C	-1.03882800	-2.20574400	4.59658900
C	-0.66013600	0.03576600	3.73175200
H	1.35104100	-0.26687400	3.45989400
H	-0.61399300	-4.76707300	4.62379800
C	-1.31998000	-0.78850400	4.57845000
H	-1.56447900	-2.81989300	5.32575300
H	-0.83012300	1.10830900	3.72777000
H	-2.06249600	-0.39820900	5.26669800
N	1.03083300	-2.40229000	1.62164100
O	0.66590700	-4.97922800	3.06549900

TS_{AB}

C	1.55802800	0.07938200	0.41783200
C	0.47289700	0.82092800	0.53165100
C	0.38397500	2.20247300	0.73596800
C	0.18688800	3.39506600	0.90729800
N	2.01517900	-1.15393900	0.32461800
C	2.24227000	-2.00312600	1.47560800
C	1.59597400	-3.24095700	1.55924600
C	3.10224600	-1.57628400	2.49192800
C	1.81981800	-4.05326200	2.67211200
H	0.93363900	-3.55796600	0.76329600
C	3.30139300	-2.39026800	3.60673900
H	3.59995200	-0.61772700	2.41348300
C	2.66682100	-3.63068400	3.69787300
H	1.32075400	-5.01520200	2.73902800
H	3.96244900	-2.05652700	4.40063000
H	2.83097300	-4.26370200	4.56431300
S	2.38259600	-1.79586200	-1.31560600
O	1.47236000	-2.91873000	-1.54426200
O	2.34836400	-0.60758900	-2.16864400

C	4.04597000	-2.40842300	-1.17581600
C	4.25694600	-3.78207300	-1.03477800
C	5.11360900	-1.50712300	-1.23363600
C	5.56468700	-4.25255900	-0.94725100
H	3.41383000	-4.46224400	-1.00616500
C	6.41075600	-2.00094600	-1.14257500
H	4.93208800	-0.44586000	-1.35996000
C	6.65877200	-3.37626800	-0.99995000
H	5.73824600	-5.31935800	-0.83995900
H	7.24746000	-1.30974400	-1.18998100
C	8.07105700	-3.90097600	-0.93841900
H	8.74868000	-3.17647900	-0.47855400
H	8.12777400	-4.83410400	-0.37182200
H	8.44935100	-4.10725000	-1.94710400
Au	-1.37475300	-0.19629100	0.37710200
P	-3.49097500	-1.30830600	0.41146600
C	-4.37591000	-0.71578100	2.01997800
C	-3.16107600	-3.19725900	0.34743700
C	-4.65010500	-0.93179400	-0.98788500
C	-4.33667300	-0.06854100	-2.06868500
C	-5.94491200	-1.49000000	-0.93588300
C	-5.33280500	0.20102700	-3.02590800
C	-3.02419700	0.60871400	-2.31621700
C	-6.91179900	-1.21554200	-1.89820800
H	-6.21204000	-2.15395300	-0.12590100
C	-6.60414800	-0.35786900	-2.95211400
H	-5.08303300	0.86195100	-3.84998600
C	-2.91760800	1.99769600	-2.14216300
C	-1.93875200	-0.08784300	-2.87070600
H	-7.89559100	-1.66768100	-1.81914300
H	-7.34430400	-0.12800500	-3.71249800
C	-1.74934300	2.67161500	-2.50105800
H	-3.75948600	2.54977200	-1.73406400
C	-0.77177200	0.58743200	-3.23446300
H	-2.01622000	-1.15731800	-3.03856500
C	-0.67657900	1.96809000	-3.05100200
H	-1.68272800	3.74604600	-2.35816900
H	0.06060900	0.03373200	-3.65615500

H	0.22838200	2.49471300	-3.33911600
C	-0.04690100	4.78466900	1.11267400
C	-1.21077400	5.21529100	1.78373800
C	0.87080000	5.74976800	0.64802200
C	-1.44242100	6.57238200	1.98750500
H	-1.91854200	4.47534000	2.14320300
C	0.62452300	7.10509400	0.84792800
H	1.76440700	5.42492600	0.12518700
C	-0.52843400	7.52036900	1.51958600
H	-2.33899900	6.89283000	2.50933800
H	1.33339600	7.84125600	0.48071000
H	-0.71457700	8.57843700	1.67663300
C	-3.32843100	-0.60506200	3.15141200
H	-2.51993700	0.08427200	2.89368200
H	-3.82674700	-0.21938400	4.04839600
H	-2.88221300	-1.56694300	3.41185400
C	-4.91112700	0.70057100	1.71617900
H	-4.12003000	1.36170200	1.34630300
H	-5.72044200	0.68914300	0.98262300
H	-5.30181100	1.13578300	2.64301400
C	-5.52909100	-1.60693100	2.51990000
H	-5.19204700	-2.61032100	2.79208900
H	-5.94843100	-1.15273000	3.42512100
H	-6.34699800	-1.69236200	1.80263300
C	-2.35174700	-3.59980100	1.59676000
H	-1.47352400	-2.96459700	1.74552700
H	-2.95717700	-3.57358500	2.50687900
H	-2.00260000	-4.63143800	1.47142100
C	-4.41252300	-4.09119600	0.24643800
H	-4.95391100	-3.93497600	-0.68853200
H	-4.08664600	-5.13770400	0.26034200
H	-5.10503300	-3.95815300	1.08021500
C	-2.30253200	-3.43444100	-0.91515700
H	-2.83832200	-3.15082400	-1.82615600
H	-1.35341400	-2.89184100	-0.88916100
H	-2.07494800	-4.50415300	-0.99045900
C	3.51644100	2.31469000	-0.33344600
C	4.14696600	3.36141200	0.42518600

C	3.39516000	2.41060400	-1.74789300
C	4.06021900	2.91858300	1.72600400
C	4.67096500	4.51617600	-0.22517400
C	3.90897600	3.53924100	-2.33601700
H	2.92230900	1.61547900	-2.31058300
H	4.37380900	3.32040100	2.67890000
C	4.54312300	4.58716000	-1.58715400
H	5.15502200	5.30237500	0.34424100
H	3.83836700	3.65032400	-3.41388500
H	4.93014900	5.44765200	-2.12293600
N	3.12972700	1.32073400	0.47641200
O	3.45610900	1.73048000	1.76773200

TS_{BC}

C	1.83046900	0.60426100	0.47853800
C	0.49103100	0.99135000	0.53475400
C	0.16507100	2.33891500	0.65986500
C	-0.20334500	3.50303100	0.78304400
N	2.27638400	-0.74590300	0.48493400
C	2.62133500	-1.39917900	1.72459600
C	1.62520900	-1.74671800	2.64442600
C	3.96671700	-1.64244700	2.02704900
C	1.97576400	-2.33985200	3.85685700
H	0.58814600	-1.54236200	2.40428800
C	4.30964500	-2.25018200	3.23549800
H	4.73434000	-1.35346900	1.31782300
C	3.31631700	-2.59886700	4.15196500
H	1.20080600	-2.60560100	4.56968100
H	5.35383900	-2.44143600	3.46375900
H	3.58536600	-3.06618400	5.09441300
S	2.20670400	-1.61098300	-0.99046700
O	1.26345300	-2.72642100	-0.84883700
O	1.99521200	-0.57512400	-2.01225200
C	3.83074800	-2.31869100	-1.22633200
C	4.04295500	-3.66672400	-0.93457500
C	4.86029500	-1.51576700	-1.72579500
C	5.31049300	-4.20940800	-1.13813600
H	3.22574100	-4.27458900	-0.56374200

C	6.11904200	-2.07658700	-1.92055200
H	4.67203500	-0.47628100	-1.97169000
C	6.36560500	-3.42908100	-1.63169500
H	5.48124100	-5.25829900	-0.91260300
H	6.92289500	-1.45948700	-2.31264300
C	7.72479100	-4.03421500	-1.88114100
H	7.91126700	-4.88684600	-1.22277100
H	7.80395000	-4.39519500	-2.91386200
H	8.52373700	-3.30261500	-1.73092600
Au	-1.14828100	-0.27360800	0.37410100
P	-3.12863200	-1.65968700	0.44057500
C	-4.07353800	-1.10187800	2.02224200
C	-2.59757200	-3.51263900	0.45094400
C	-4.35797000	-1.45943900	-0.93969800
C	-4.24774900	-0.50121900	-1.97955900
C	-5.50668000	-2.27772700	-0.91356600
C	-5.30198600	-0.38672200	-2.90635800
C	-3.08883300	0.40844700	-2.23637400
C	-6.52691000	-2.16275300	-1.85292000
H	-5.62015100	-3.01749700	-0.13434300
C	-6.42902800	-1.19916600	-2.85394900
H	-5.20724200	0.34941700	-3.69844100
C	-3.26039400	1.79900100	-2.14515400
C	-1.87518200	-0.08926700	-2.73725300
H	-7.39054100	-2.81793500	-1.79453600
H	-7.21588800	-1.08658900	-3.59356200
C	-2.24450200	2.66930300	-2.54168000
H	-4.20271500	2.19549000	-1.77735000
C	-0.86126200	0.78172000	-3.14320900
H	-1.73699300	-1.16065900	-2.84344400
C	-1.04647700	2.16184100	-3.04876000
H	-2.39542700	3.74250600	-2.46847900
H	0.06747700	0.37181900	-3.52502200
H	-0.26540800	2.84202700	-3.37626700
C	-0.66358300	4.83587100	0.92148600
C	-2.05028300	5.10861100	0.93377400
C	0.24859800	5.90676000	1.04890900
C	-2.50466900	6.41540500	1.07200100

H	-2.74955000	4.28511500	0.83437300
C	-0.21602700	7.21002600	1.18563800
H	1.31336300	5.69805600	1.03612400
C	-1.59079000	7.46653500	1.19830700
H	-3.57094500	6.61861900	1.08269100
H	0.48960000	8.02917200	1.28362200
H	-1.94979000	8.48548300	1.30670000
C	-3.18233000	-1.36514800	3.25324200
H	-2.17734600	-0.94972200	3.12974200
H	-3.63608000	-0.88419800	4.12746800
H	-3.09463500	-2.43138200	3.47904900
C	-4.28197900	0.42185500	1.86710800
H	-3.33181000	0.95999700	1.80099700
H	-4.87758200	0.66260700	0.98129500
H	-4.82335900	0.79560900	2.74403900
C	-5.45284300	-1.74957200	2.25135100
H	-5.40931400	-2.83774300	2.32776200
H	-5.85332900	-1.37428400	3.20029000
H	-6.16762200	-1.48187600	1.47105600
C	-1.30857100	-3.64493800	1.29079900
H	-0.48807400	-3.06535600	0.86515000
H	-1.45213900	-3.35295900	2.33372200
H	-1.00066200	-4.69716400	1.28613600
C	-3.63501700	-4.50861800	1.00468000
H	-4.56090500	-4.53717700	0.42798600
H	-3.20204100	-5.51423300	0.95347000
H	-3.87810300	-4.31865900	2.05320500
C	-2.25482200	-3.87505100	-1.01048500
H	-3.12774700	-3.83295100	-1.66655600
H	-1.47134100	-3.22569400	-1.41244200
H	-1.86622300	-4.89952900	-1.03348000
C	3.12448100	2.58879900	-0.34812000
C	3.91228100	3.57199000	0.32012500
C	2.81278800	2.72697600	-1.72170400
C	4.05937900	3.12598500	1.63551100
C	4.39804800	4.71170100	-0.37163600
C	3.29600000	3.84901900	-2.36168200
H	2.23853100	1.95836200	-2.22479700

H	4.63824800	3.57802400	2.43969100
C	4.07959400	4.84148300	-1.70170700
H	5.00192700	5.45131700	0.14406600
H	3.07561700	3.98165300	-3.41684700
H	4.42788400	5.69993400	-2.26541800
N	2.83000100	1.53419600	0.43266600
O	3.45543400	2.02011900	1.89586700

TS_{CD}

C	-2.15968900	0.20388900	-0.70069000
C	-0.79586100	0.91383000	-0.71607300
C	-0.84311100	2.20361500	-0.13629400
C	-0.86664600	3.31613400	0.36713700
N	-2.23957800	-1.16715200	-0.43816500
C	-3.17764100	-2.00017200	-1.16069100
C	-2.66050900	-2.88334300	-2.11333300
C	-4.55433300	-1.93974900	-0.91904300
C	-3.52759700	-3.70904500	-2.83040700
H	-1.58956100	-2.91795100	-2.27970700
C	-5.41361100	-2.76137400	-1.64734900
H	-4.94021100	-1.25365500	-0.17538600
C	-4.90303900	-3.64626700	-2.60046900
H	-3.12791700	-4.39676700	-3.56919600
H	-6.48309400	-2.71325400	-1.46702000
H	-5.57691500	-4.28617700	-3.16201300
S	-1.54159400	-1.82465600	1.02272300
O	-0.64713600	-2.91492400	0.63170200
O	-1.05645600	-0.65622100	1.76314200
C	-2.91909000	-2.52938200	1.90616300
C	-3.18376800	-3.89654600	1.79561300
C	-3.68707600	-1.70217200	2.73155000
C	-4.24240100	-4.43483700	2.52201400
H	-2.56596400	-4.52056900	1.16019700
C	-4.74110300	-2.26226800	3.44730700
H	-3.44956000	-0.64794400	2.82318200
C	-5.03568200	-3.63240200	3.35641800
H	-4.45432700	-5.49725800	2.44293000
H	-5.34010100	-1.62886900	4.09552700

C	-6.15736000	-4.23431300	4.16492500
H	-6.59089100	-5.10400800	3.66392100
H	-5.79032300	-4.57017300	5.14247500
H	-6.95453900	-3.50883700	4.34836200
Au	1.11494000	-0.02514400	-0.51554800
P	3.26326300	-1.05687600	-0.81166900
C	4.16240100	-0.00646800	-2.14517900
C	2.91663800	-2.87090900	-1.39011800
C	4.47866800	-1.13888100	0.59365300
C	4.42807200	-0.32588600	1.75483800
C	5.57294600	-2.01636400	0.44784800
C	5.47080700	-0.43423700	2.69651200
C	3.37221400	0.67131000	2.11345300
C	6.58472100	-2.11660400	1.39727300
H	5.64946400	-2.63339900	-0.43559000
C	6.53427000	-1.31446200	2.53469700
H	5.41982400	0.18789900	3.58438300
C	3.72215700	2.02802800	2.21305800
C	2.09145700	0.27435900	2.52616200
H	7.40400300	-2.81164900	1.24176400
H	7.31224900	-1.37300900	3.28979300
C	2.81545100	2.96408500	2.71020300
H	4.71872100	2.34403000	1.91732000
C	1.18773400	1.21113600	3.03255700
H	1.80971200	-0.77287000	2.48541200
C	1.54725600	2.55564500	3.12833200
H	3.10784800	4.00739800	2.78977900
H	0.20566500	0.87924500	3.34921400
H	0.84668100	3.28065700	3.53103600
C	-0.90193800	4.61620200	0.94208200
C	0.28059500	5.37583200	1.06815500
C	-2.12451700	5.16631100	1.38212100
C	0.23418200	6.65372400	1.61691700
H	1.22082700	4.94756800	0.73802000
C	-2.15821500	6.44081300	1.93910800
H	-3.03393800	4.58309100	1.28039500
C	-0.98169600	7.18692300	2.05519400
H	1.14638300	7.23534500	1.70797100

H	-3.10111400	6.85629600	2.28116300
H	-1.01217100	8.18250900	2.48743500
C	3.32772500	-0.00319000	-3.44182600
H	2.29103700	0.29695300	-3.25906700
H	3.76765600	0.71582800	-4.14280400
H	3.32376100	-0.97708200	-3.93841000
C	4.22090200	1.43172500	-1.58459100
H	3.22391700	1.83470400	-1.38305900
H	4.80335200	1.48570400	-0.66100100
H	4.70809000	2.07915600	-2.32310700
C	5.60137200	-0.46219500	-2.45355500
H	5.65008900	-1.46832600	-2.87356100
H	6.02886500	0.22090300	-3.19676900
H	6.24120500	-0.42419500	-1.56933100
C	1.58325000	-2.86955100	-2.17574500
H	0.74570600	-2.58613900	-1.53578200
H	1.60399600	-2.20628700	-3.04382200
H	1.39822500	-3.88763000	-2.53904400
C	3.97991700	-3.51752300	-2.30298700
H	4.96816800	-3.60469200	-1.84979800
H	3.65087400	-4.53715800	-2.53422400
H	4.08452600	-2.99162600	-3.25497400
C	2.71676500	-3.72523200	-0.11947800
H	3.63782100	-3.84886100	0.45336800
H	1.94886100	-3.30196900	0.53429500
H	2.37249300	-4.72138700	-0.42067900
C	-3.43206700	2.03492500	-1.60093600
C	-2.61958100	2.57588100	-2.65059800
C	-4.61148200	2.73334600	-1.25856900
C	-1.40947500	1.97067500	-3.05946200
C	-3.05183300	3.73082400	-3.36057000
C	-4.96259700	3.90160400	-1.91208000
H	-5.24399000	2.31166300	-0.48511000
H	-1.00412400	2.23041000	-4.04356200
C	-4.19066500	4.40474900	-2.98216300
H	-2.44659400	4.09040800	-4.18845700
H	-5.87102300	4.42041300	-1.62039000
H	-4.50172700	5.30200700	-3.50549500

N	-3.25124000	0.80437700	-1.02760300
O	-0.70158700	1.13113000	-2.41696600

TS_{CF}

C	1.35940900	-1.43707400	0.71195300
C	0.68794000	-0.18622300	1.18544900
C	1.46292100	0.95764200	1.39983000
C	2.13099000	1.91870200	1.76335300
N	2.35481800	-1.44975400	-0.25129800
C	3.23582100	-2.60415200	-0.31947500
C	2.83890600	-3.79448100	-0.93491400
C	4.50381800	-2.47943600	0.25370900
C	3.72923700	-4.86643200	-0.97354500
H	1.84853800	-3.87693500	-1.36429700
C	5.38586000	-3.55950000	0.21333800
H	4.78845700	-1.54250800	0.72179700
C	4.99897600	-4.75157200	-0.40172100
H	3.42593600	-5.79614500	-1.44433300
H	6.37145400	-3.46817200	0.65909100
H	5.68514600	-5.59244600	-0.43337400
S	2.15643600	-0.58008300	-1.78505600
O	1.80314000	-1.57441100	-2.79617000
O	1.25492100	0.53631100	-1.49289400
C	3.79484100	0.02825200	-2.11113400
C	4.60566400	-0.65470800	-3.02002500
C	4.22320800	1.20217100	-1.48514800
C	5.87410900	-0.14898300	-3.29424500
H	4.24467200	-1.55635400	-3.50127300
C	5.49501300	1.68736600	-1.77463500
H	3.57042200	1.72653800	-0.79629000
C	6.33841900	1.02464000	-2.68177200
H	6.51271400	-0.67363600	-3.99898200
H	5.83608800	2.60157800	-1.29692500
C	7.69963700	1.58092100	-3.01625600
H	7.63976800	2.24962300	-3.88359900
H	8.11254800	2.16014600	-2.18597200
H	8.40681300	0.78577800	-3.26723700
Au	-1.30012900	-0.00452200	0.41923100

P	-3.45896200	-0.29537700	-0.59550300
C	-4.72927500	-0.59621400	0.81221300
C	-3.22285100	-1.81117700	-1.77561600
C	-4.20460200	1.07958300	-1.59732300
C	-3.76194100	2.42593200	-1.58222300
C	-5.34796300	0.76670900	-2.36234100
C	-4.49356600	3.38234100	-2.31424800
C	-2.56181900	2.97542200	-0.87983400
C	-6.04392000	1.72402600	-3.09303200
H	-5.72146700	-0.24644500	-2.37712000
C	-5.61538400	3.04899600	-3.06394100
H	-4.14440400	4.40982500	-2.29932800
C	-2.73571000	3.93261400	0.13274300
C	-1.26413500	2.71119800	-1.34476400
H	-6.91561700	1.43323100	-3.67090500
H	-6.14437300	3.81534100	-3.62216100
C	-1.64167300	4.62142400	0.65738700
H	-3.73765600	4.15709400	0.48781300
C	-0.17159500	3.40840900	-0.82617900
H	-1.10926800	1.99135800	-2.14178800
C	-0.35869900	4.37148700	0.16630200
H	-1.79751700	5.37077800	1.42836300
H	0.81992000	3.19854900	-1.21140700
H	0.49004800	4.93204100	0.54522000
C	2.93097200	3.00836000	2.19440600
C	2.33482600	4.17699500	2.71873600
C	4.34055800	2.92568000	2.12964700
C	3.12952100	5.22974100	3.16028300
H	1.25355600	4.23630100	2.77679100
C	5.12495100	3.98946800	2.56216800
H	4.80028600	2.02411400	1.73755600
C	4.52271700	5.14112200	3.07888000
H	2.66518800	6.12242500	3.56756900
H	6.20694800	3.92068200	2.50666100
H	5.13865300	5.96701900	3.42124900
C	-4.33238900	-1.86604200	1.58850600
H	-3.28507900	-1.84158200	1.90171600
H	-4.95224100	-1.93670500	2.49016000

H	-4.50043600	-2.77655400	1.00720100
C	-4.61117800	0.62759100	1.74765100
H	-3.60767900	0.72114200	2.17380600
H	-4.85107000	1.56099900	1.23038700
H	-5.32328400	0.51368200	2.57329400
C	-6.19466600	-0.71696100	0.35246300
H	-6.35897300	-1.55128000	-0.33272800
H	-6.81814000	-0.89534500	1.23626100
H	-6.55453500	0.19830500	-0.12095200
C	-2.25386600	-2.81575400	-1.10976700
H	-1.26833500	-2.38284100	-0.92731400
H	-2.63132500	-3.21175100	-0.16526600
H	-2.11682500	-3.66529700	-1.78780000
C	-4.50120400	-2.59069200	-2.14912800
H	-5.22449000	-2.00407600	-2.71634900
H	-4.20965400	-3.42976600	-2.79080100
H	-5.00222700	-3.01627100	-1.27616400
C	-2.54889600	-1.26445100	-3.05284000
H	-3.20400200	-0.59680300	-3.61711900
H	-1.61995000	-0.73116700	-2.82546000
H	-2.28805500	-2.10837900	-3.70114800
C	0.30575100	-2.39135400	2.38783200
C	-0.66765600	-3.31130300	2.88598300
C	0.47229800	-1.11500400	3.04318600
C	-0.91804700	-4.65430300	2.29472900
C	-1.48158600	-2.89632500	3.93017000
C	-0.43901800	-0.72041400	4.07391200
H	1.49316000	-0.77423200	3.17256700
H	-1.59273500	-5.28344400	2.91799800
C	-1.40390400	-1.59910000	4.50188200
H	-2.23334400	-3.58849500	4.30384600
H	-0.31210700	0.24569000	4.55271000
H	-2.07855300	-1.33039900	5.30800000
N	1.01655600	-2.59020500	1.26244700
O	-0.47554600	-5.06278600	1.24363900

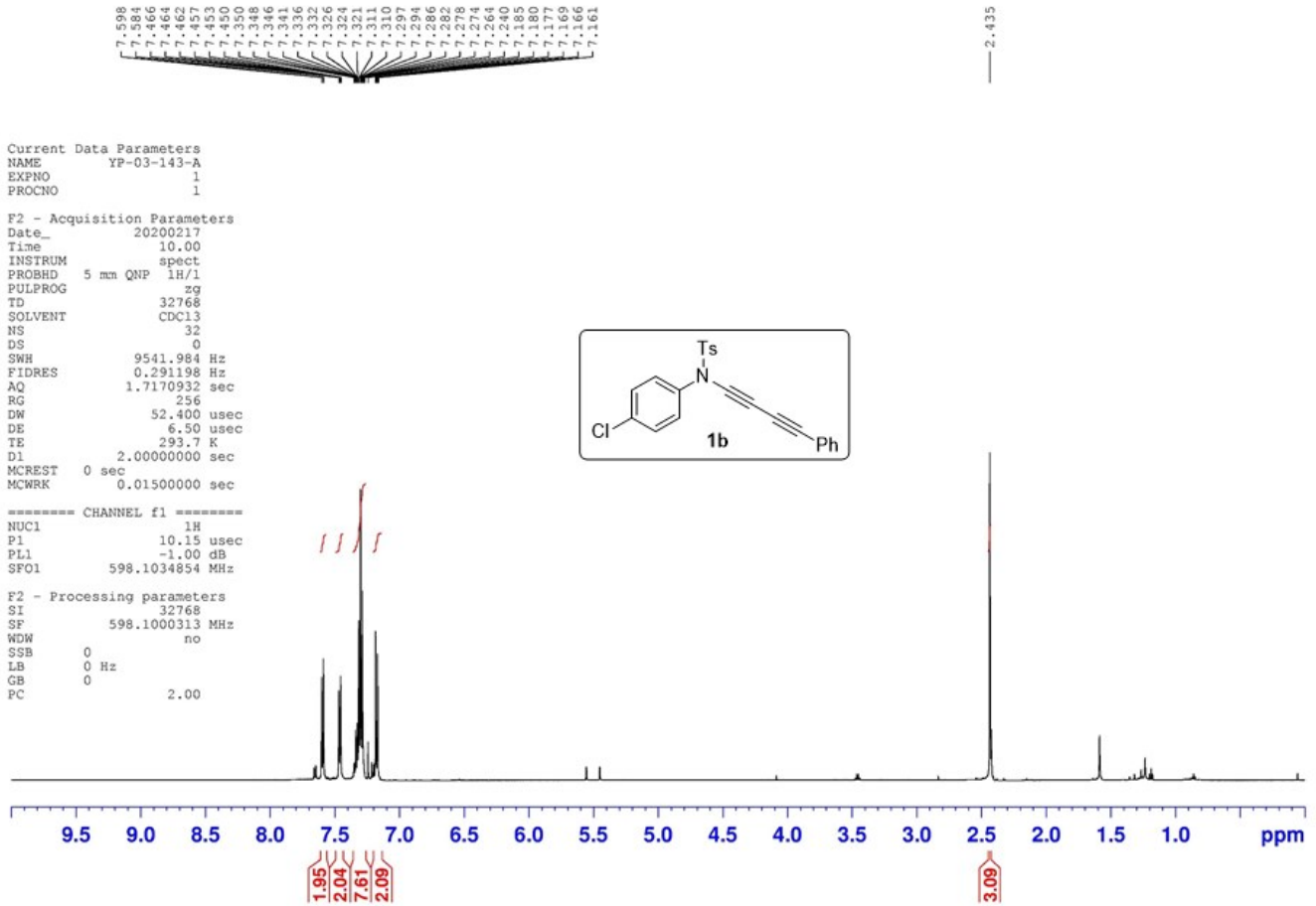
1a

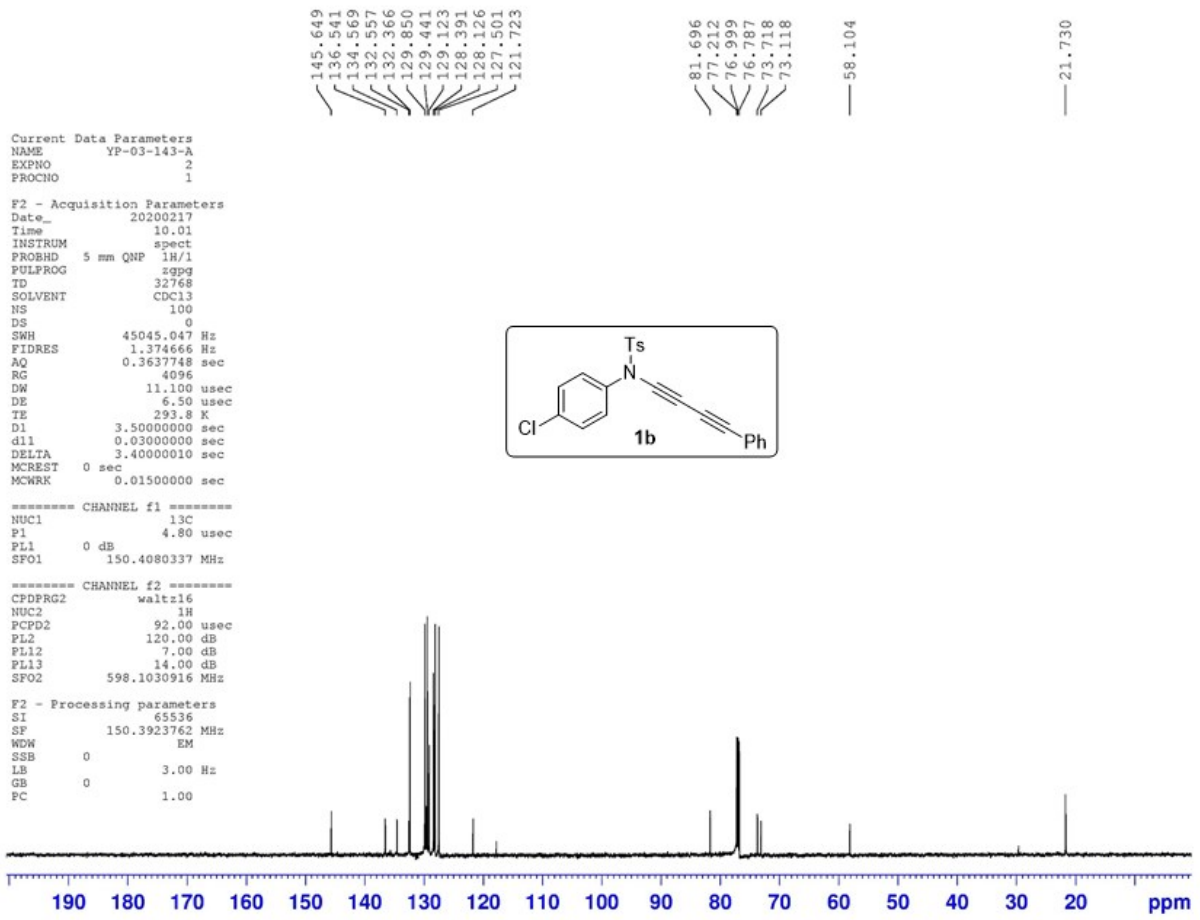
C	-0.03684400	-1.01855900	-0.61135500

C	-1.23184500	-0.83210900	-0.44756500
C	-2.56243400	-0.62533300	-0.26949300
C	-3.75904900	-0.43854700	-0.10805200
N	1.27156900	-1.23718300	-0.80523200
C	2.02606200	-1.98192000	0.17502800
C	2.99768000	-2.89159800	-0.25332600
C	1.76432200	-1.80952100	1.53845400
C	3.71637000	-3.61877500	0.69457400
H	3.18216000	-3.01620800	-1.31276200
C	2.47661800	-2.55582700	2.47542700
H	0.99801400	-1.10787200	1.85119200
C	3.45743700	-3.45707300	2.05696500
H	4.47190100	-4.32467400	0.36351600
H	2.26735700	-2.42786800	3.53318300
H	4.01291100	-4.03538800	2.78903000
S	2.11189600	-0.02267700	-1.79872500
O	3.42730300	-0.59346400	-2.07787500
O	1.16159900	0.32059400	-2.84970500
C	2.31108400	1.37665400	-0.70919900
C	3.47194000	1.48622000	0.05951800
C	1.28585800	2.32183800	-0.61815500
C	3.60152800	2.56618900	0.92909300
H	4.25788400	0.74596000	-0.03693900
C	1.43677600	3.39159600	0.25990500
H	0.39852000	2.22184000	-1.23242200
C	2.59172200	3.53256300	1.04356000
H	4.50357900	2.66154000	1.52708800
H	0.64534800	4.13209700	0.33520400
C	2.75654000	4.71578900	1.96549900
H	3.41723100	4.48105800	2.80456200
H	3.19568600	5.56749000	1.43160800
H	1.79486800	5.04599200	2.36837100
C	-5.15288300	-0.21972100	0.06975500
C	-5.98052200	0.05875700	-1.03781100
C	-5.73100500	-0.27708400	1.35477100
C	-7.34317800	0.27687000	-0.85893500
H	-5.54007800	0.10086600	-2.02840800
C	-7.09632900	-0.06552500	1.52105700

H	-5.09784800	-0.49034500	2.20967400
C	-7.90651800	0.21400800	0.41790500
H	-7.96920400	0.49276900	-1.71966000
H	-7.52989600	-0.11586100	2.51551200
H	-8.97095500	0.38131200	0.55240000

Spectra of key Compounds

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134.569
132.557
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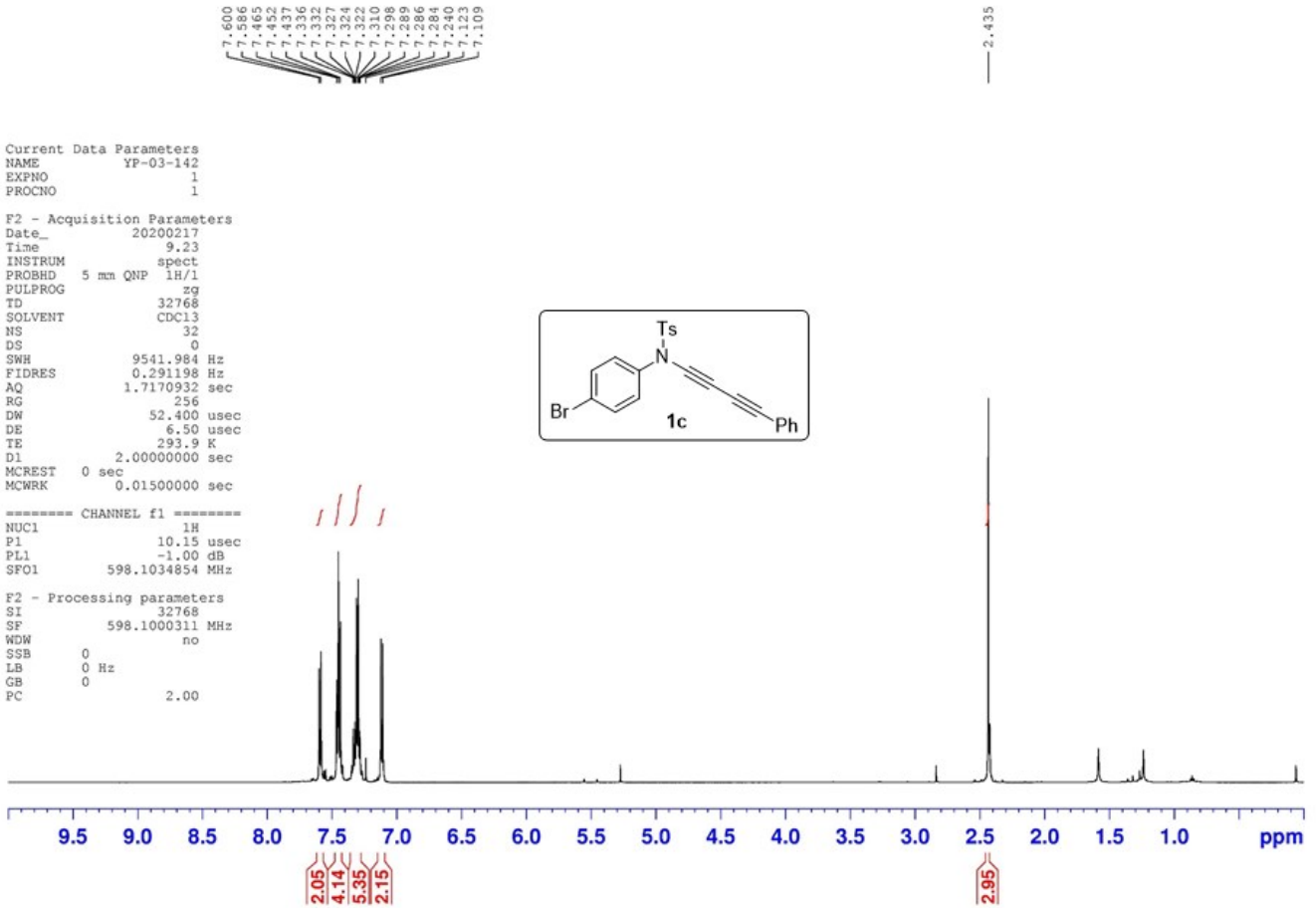
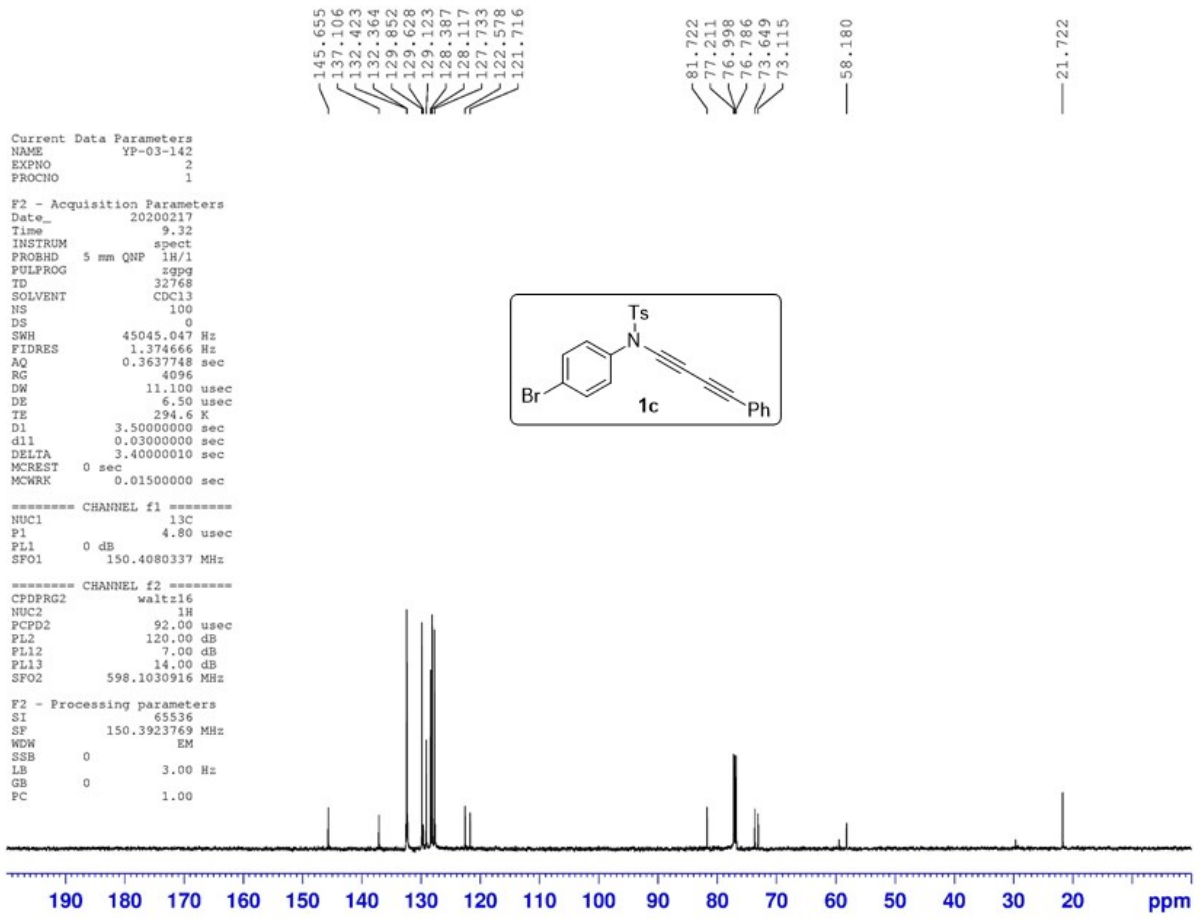
129.123
128.391
128.126
127.501
121.723
81.696
77.212
76.999
76.787
73.718
73.118
58.104
21.730
Current Data Parameters
NAME YP-03-143-A
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200217
Time 10.01
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 100
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 293.8 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0 dB
SFO1 150.4080337 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 7.00 dB
PL13 14.00 dB
SFO2 598.1030916 MHz
F2 - Processing parameters
SI 65536
SF 150.3923762 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
Ts
N
Cl
Ph
1b
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


7.600
7.586
7.465
7.452
7.437
7.336
7.332
7.327
7.324
7.322
7.310
7.298
7.289
7.286
7.284
7.240
7.123
7.109
2.435
Current Data Parameters
NAME YP-03-142
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200217
Time 9.23
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 9541.984 Hz
FIDRES 0.291198 Hz
AQ 1.7170932 sec
RG 256
DW 52.400 usec
DE 6.50 usec
TE 293.9 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.15 usec
PL1 -1.00 dB
SFO1 598.1034854 MHz
F2 - Processing parameters
SI 32768
SF 598.1000311 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 2.00
Ts
N
Br
Ph
1c
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
2.05
4.14
5.35
2.15
2.95


145.655
137.106
132.423
132.364
129.852
129.628
129.123
128.387
128.117
127.733
122.578
121.716
81.722
77.211
76.998
76.786
73.649
73.115
58.180
21.722
Current Data Parameters
NAME YP-03-142
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200217
Time 9.32
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 100
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 294.6 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0 dB
SFO1 150.4080337 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 7.00 dB
PL13 14.00 dB
SFO2 598.1030916 MHz
F2 - Processing parameters
SI 65536
SF 150.3923769 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
Ts
N
Br
Ph
1c
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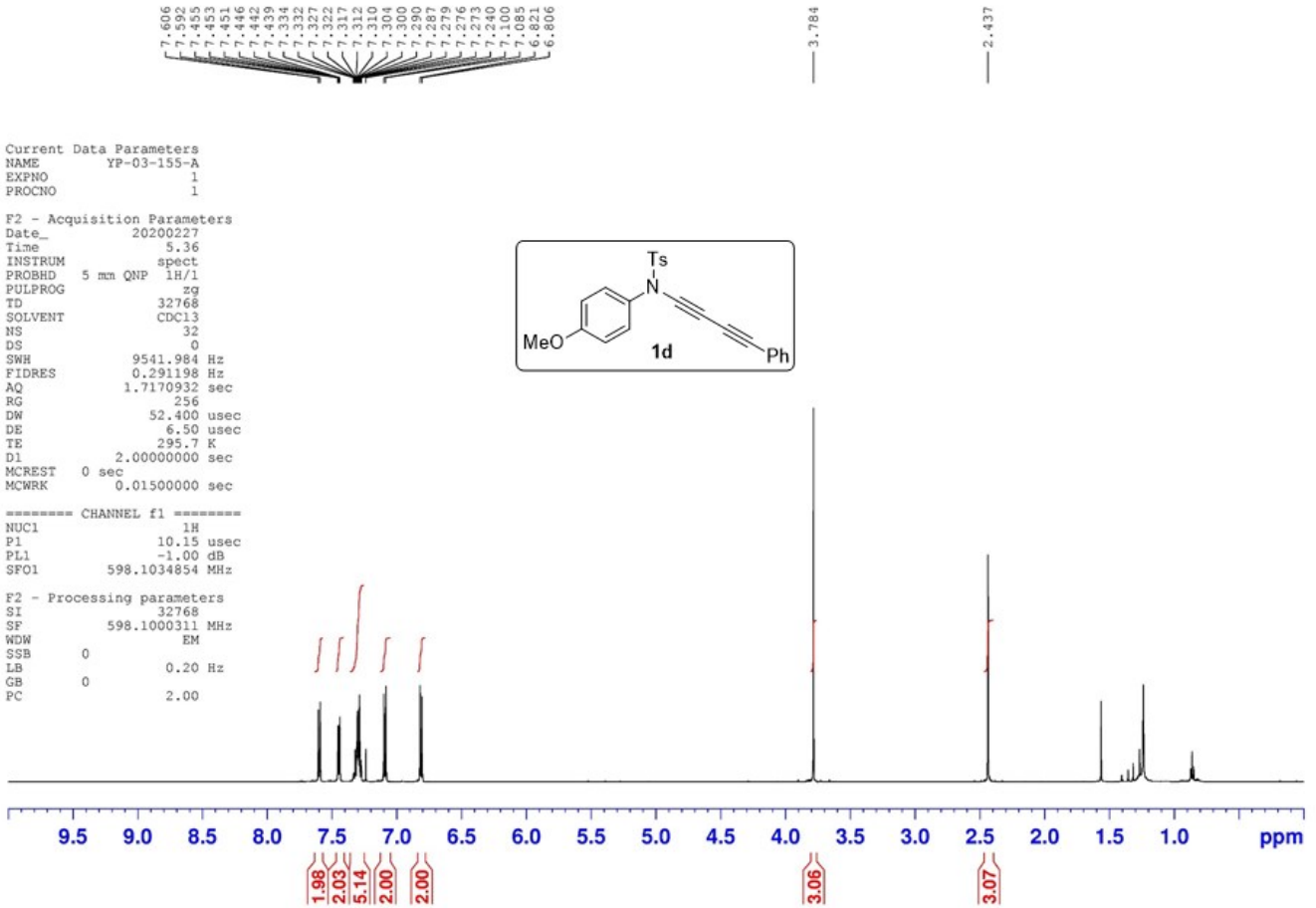
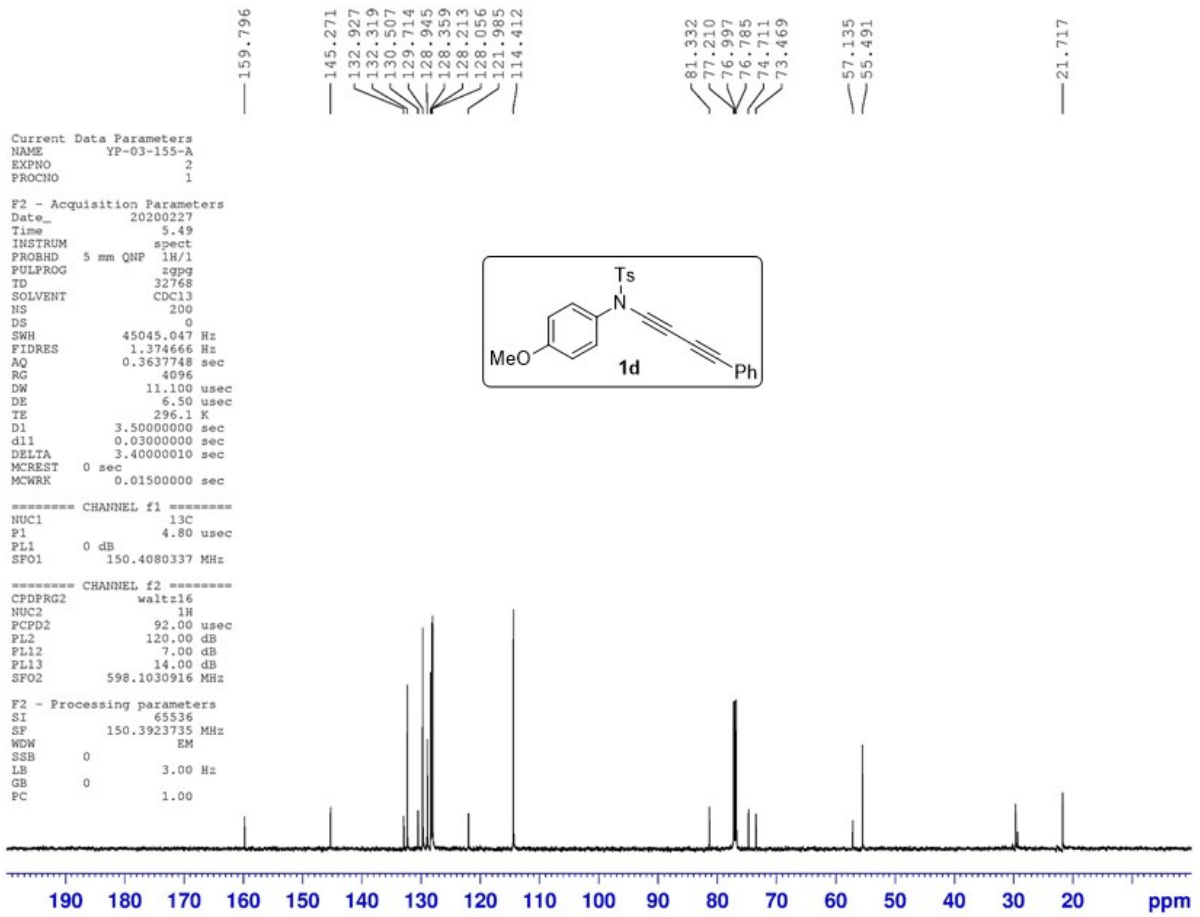

7.606
7.592
7.455
7.453
7.451
7.446
7.442
7.439
7.334
7.332
7.327
7.322
7.317
7.312
7.310
7.304
7.300
7.290
7.287
7.279
7.276
7.273
7.240
7.100
7.085
6.821
6.806
3.784
2.437
Current Data Parameters
NAME YP-03-155-A
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200227
Time 5.36
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDC13
NS 32
DS 0
SWH 9541.984 Hz
FIDRES 0.291198 Hz
AQ 1.7170932 sec
RG 256
DW 52.400 usec
DE 6.50 usec
TE 295.7 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.15 usec
PL1 -1.00 dB
SFO1 598.1034854 MHz
F2 - Processing parameters
SI 32768
SF 598.1000311 MHz
WDW EM
SSB 0
LB 0.20 Hz
GB 0
PC 2.00
Ts
N
MeO
1d
Ph
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.98
2.03
5.14
2.00
2.00
3.06
3.07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130.507
129.714
128.945
128.359
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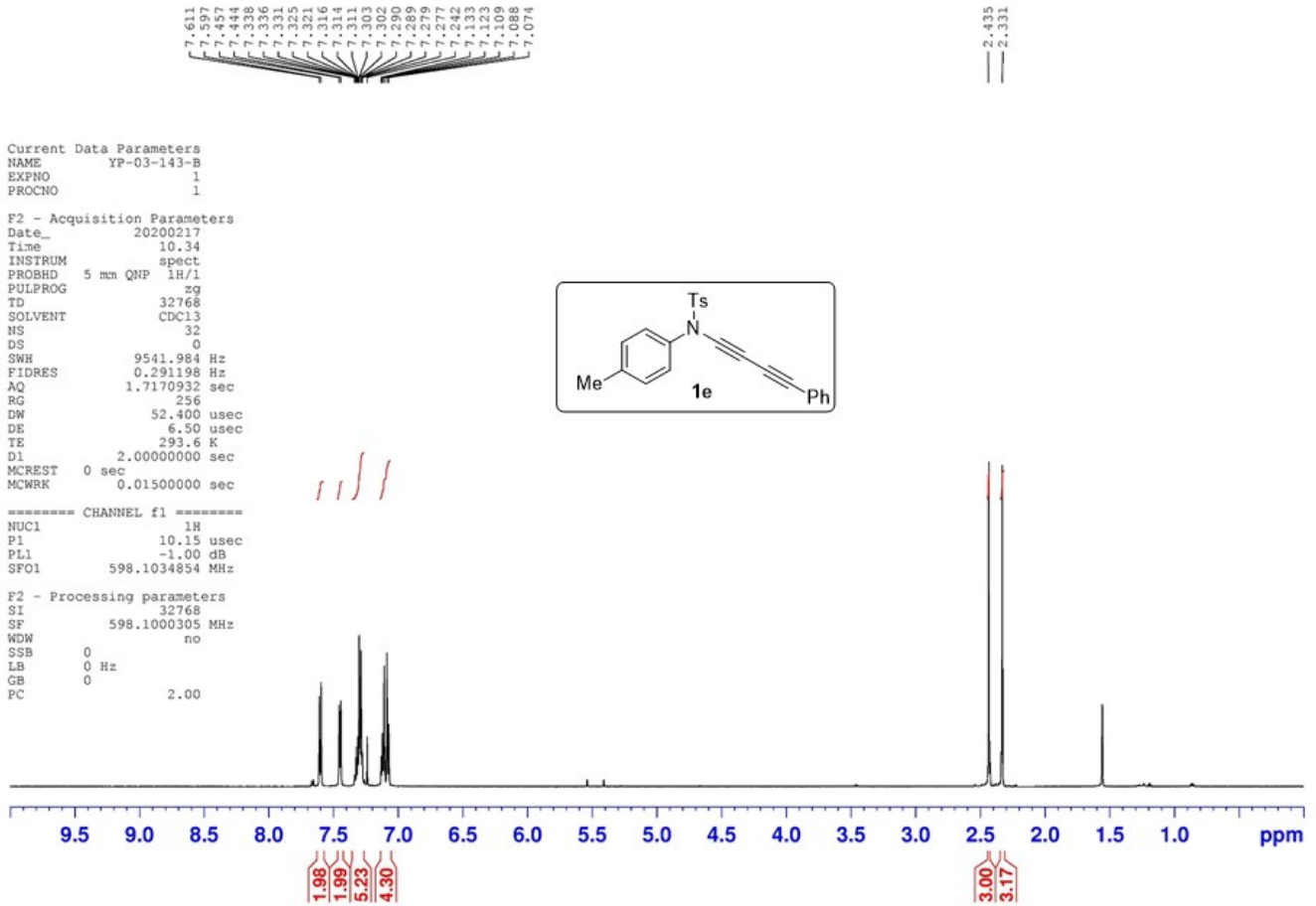
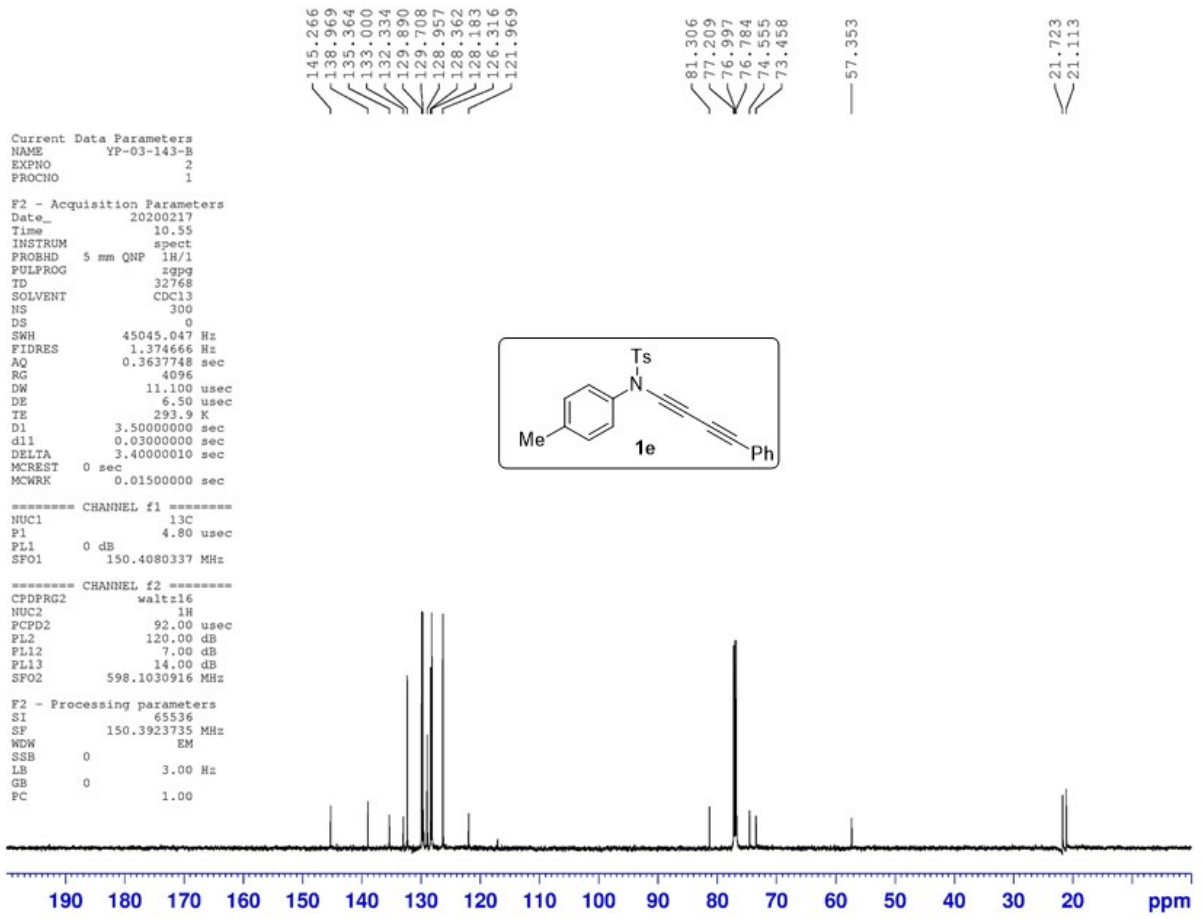
128.056
121.985
114.412
81.332
77.210
76.997
76.785
74.711
73.469
57.135
55.491
21.717
Current Data Parameters
NAME YP-03-155-A
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200227
Time 5.49
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 200
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 296.1 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0 dB
SFO1 150.4080337 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 7.00 dB
PL13 14.00 dB
SFO2 598.1030916 MHz
F2 - Processing parameters
SI 65536
SF 150.3923735 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
Ts
N
MeO
Ph
1d
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


7.611
7.597
7.457
7.444
7.338
7.336
7.331
7.325
7.321
7.316
7.314
7.311
7.303
7.302
7.290
7.289
7.279
7.277
7.242
7.133
7.123
7.109
7.088
7.074
2.435
2.331
Current Data Parameters
NAME YP-03-143-B
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200217
Time 10.34
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 9541.984 Hz
FIDRES 0.291198 Hz
AQ 1.7170932 sec
RG 256
DW 52.400 usec
DE 6.50 usec
TE 293.6 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.15 usec
PL1 -1.00 dB
SFO1 598.1034854 MHz
F2 - Processing parameters
SI 32768
SF 598.1000305 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 2.00
Ts
N
Me
Ph
1e
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
1.98
1.99
5.23
4.30
3.00
3.17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133.000
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129.708
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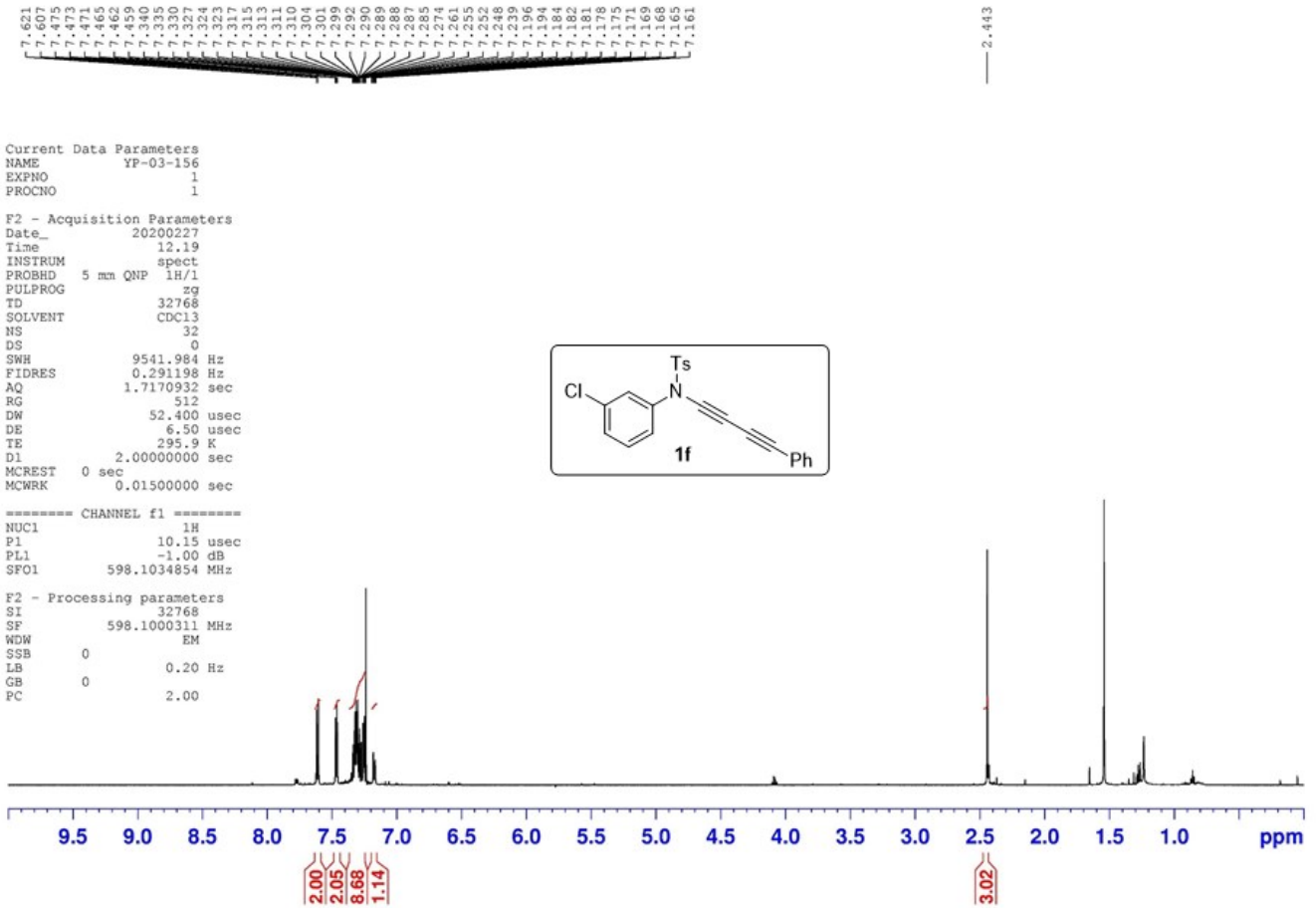
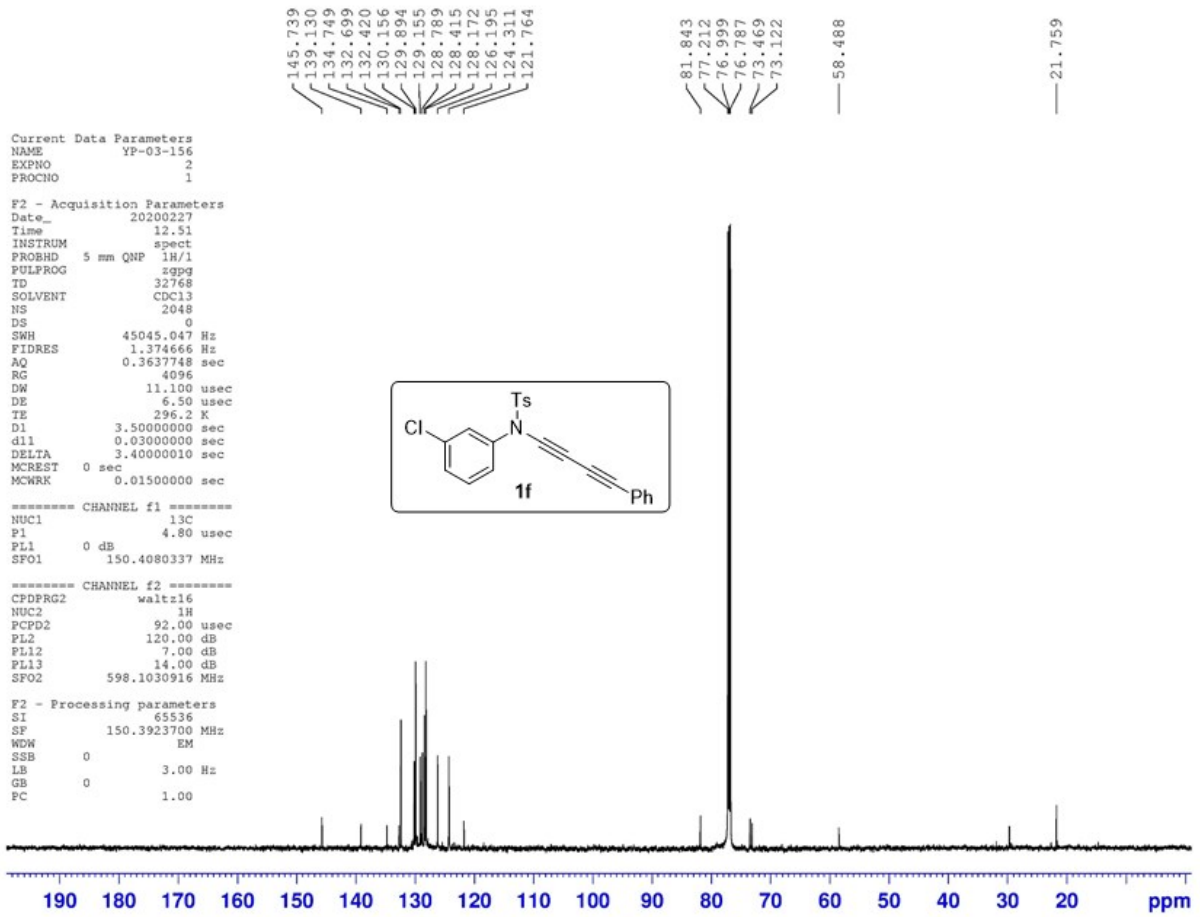
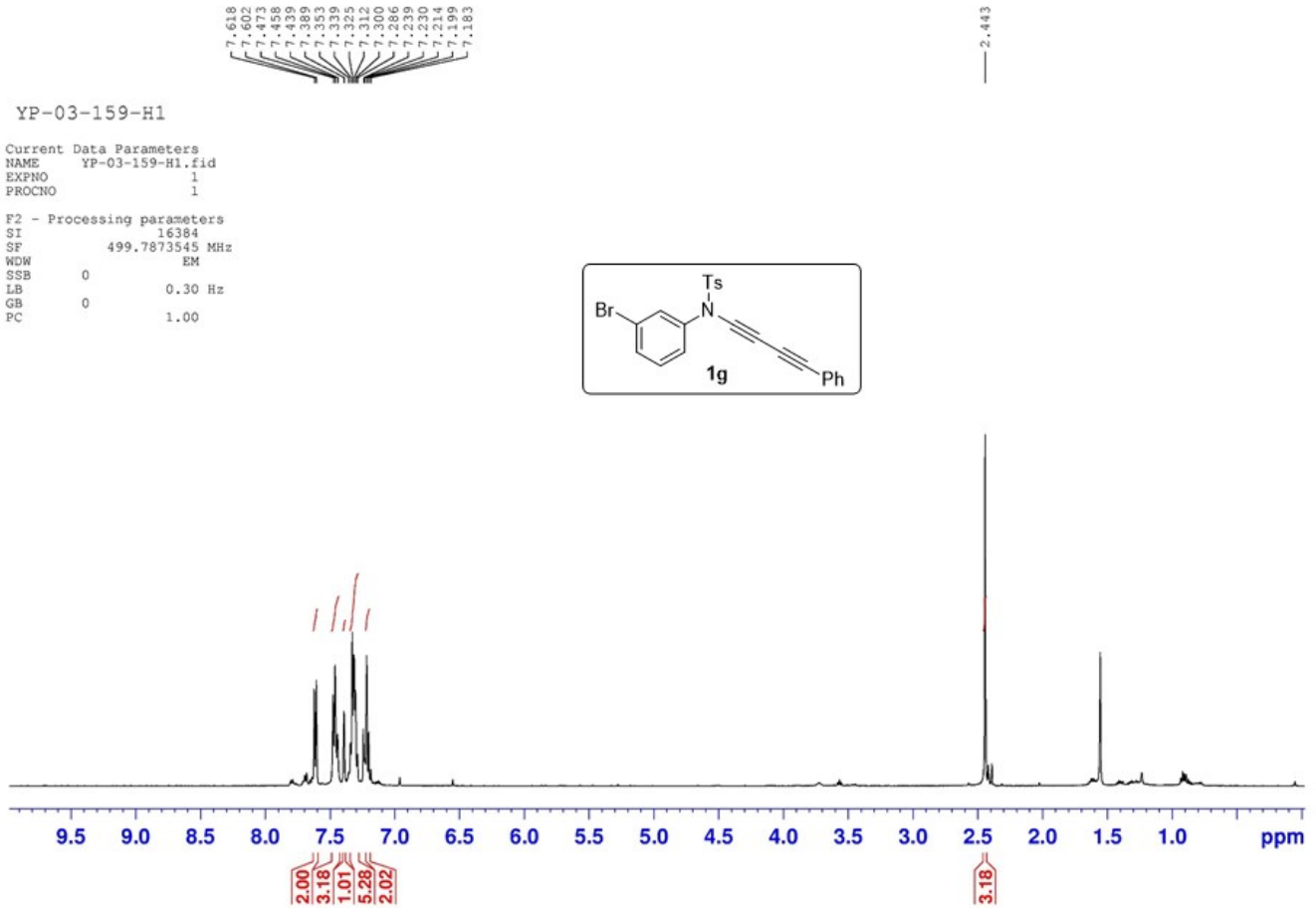
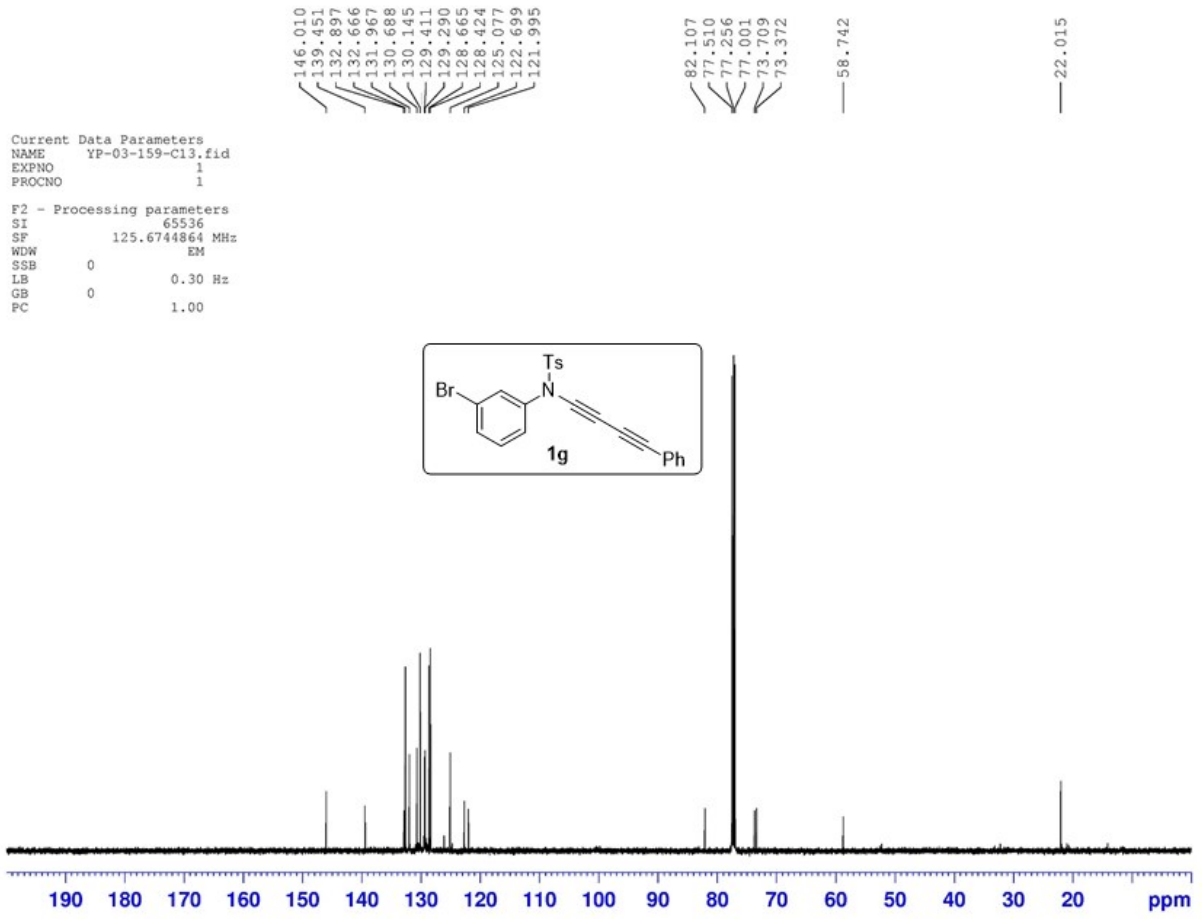
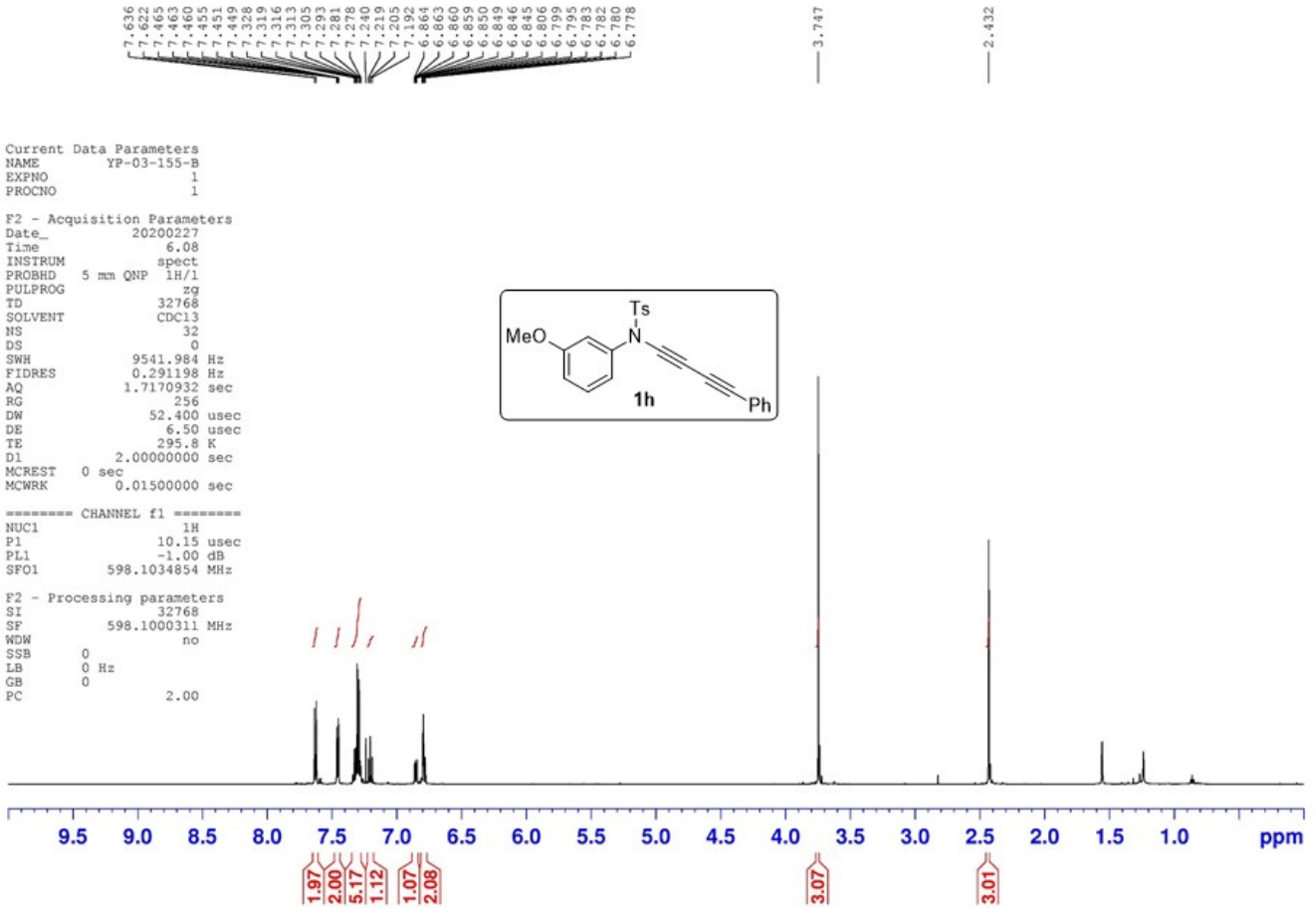
128.183
126.316
121.969
81.306
77.209
76.997
76.784
74.555
73.458
57.353
21.723
21.113
Current Data Parameters
NAME YP-03-143-B
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200217
Time 10.55
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDC13
NS 300
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 293.9 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0 dB
SFO1 150.4080337 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 7.00 dB
PL13 14.00 dB
SFO2 598.1030916 MHz
F2 - Processing parameters
SI 65536
SF 150.3923735 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
Ts
N
Me
Ph
1e
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

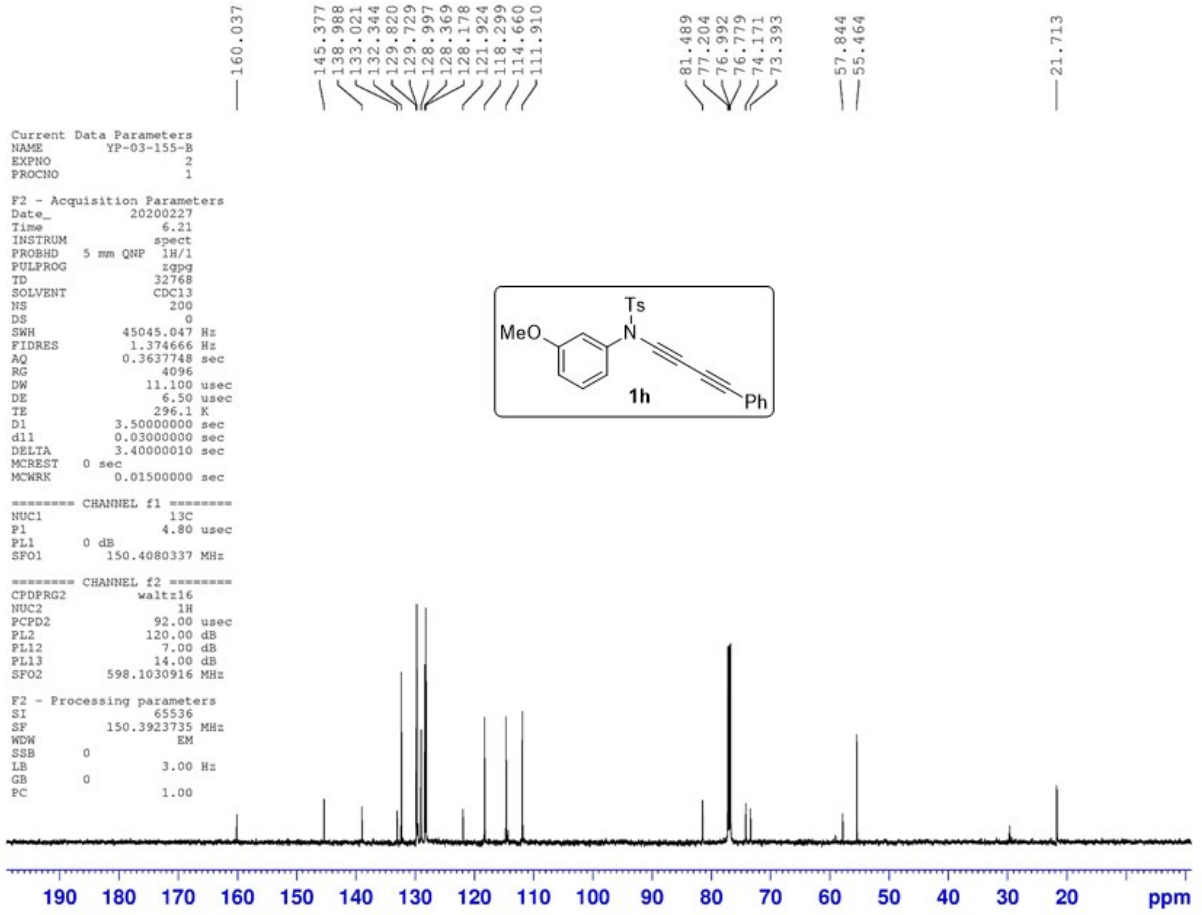

7.621
7.607
7.475
7.473
7.471
7.465
7.462
7.459
7.340
7.335
7.330
7.327
7.324
7.323
7.317
7.315
7.313
7.311
7.310
7.304
7.301
7.299
7.292
7.290
7.289
7.288
7.287
7.285
7.274
7.261
7.255
7.252
7.248
7.239
7.196
7.194
7.184
7.182
7.181
7.178
7.175
7.171
7.169
7.168
7.165
7.161
2.443
Current Data Parameters
NAME YP-03-156
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200227
Time 12.19
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 9541.984 Hz
FIDRES 0.291198 Hz
AQ 1.7170932 sec
RG 512
DW 52.400 usec
DE 6.50 usec
TE 295.9 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.15 usec
PL1 -1.00 dB
SFO1 598.1034854 MHz
F2 - Processing parameters
SI 32768
SF 598.1000311 MHz
WDW EM
SSB 0
LB 0.20 Hz
GB 0
PC 2.00
Cl
N
Ts
Ph
1f
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
2.00
2.05
8.68
1.14
3.02

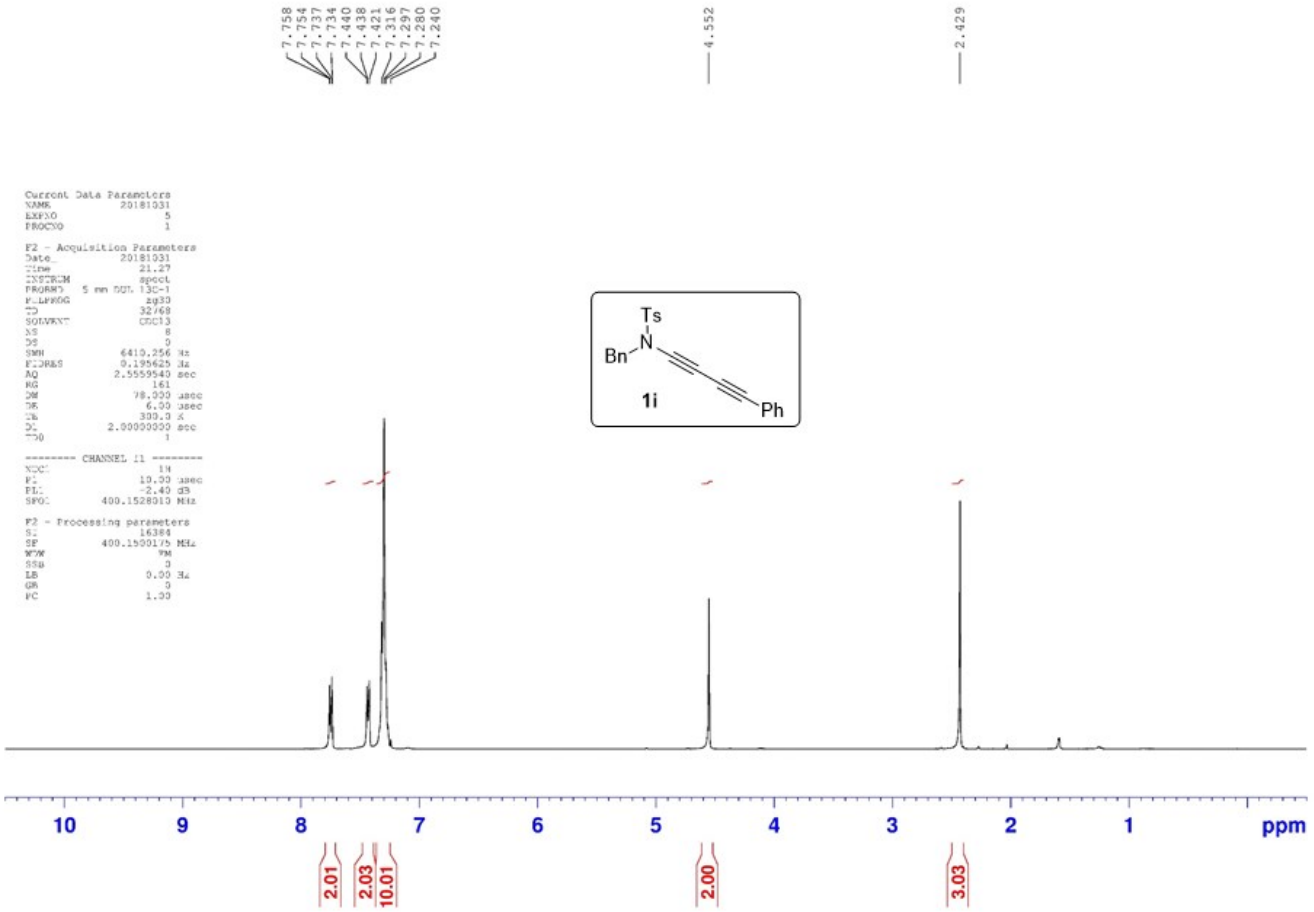

145.739
139.130
134.749
132.699
132.420
130.156
129.894
129.155
128.789
128.415
128.172
126.195
124.311
121.764
81.843
77.212
76.999
76.787
73.469
73.122
58.488
21.759
Current Data Parameters
NAME YP-03-156
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200227
Time 12.51
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 2048
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 296.2 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0 dB
SFO1 150.4080337 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 7.00 dB
PL13 14.00 dB
SFO2 598.1030916 MHz
F2 - Processing parameters
SI 65536
SF 150.3923700 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
Ts
N
Cl
Ph
1f
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

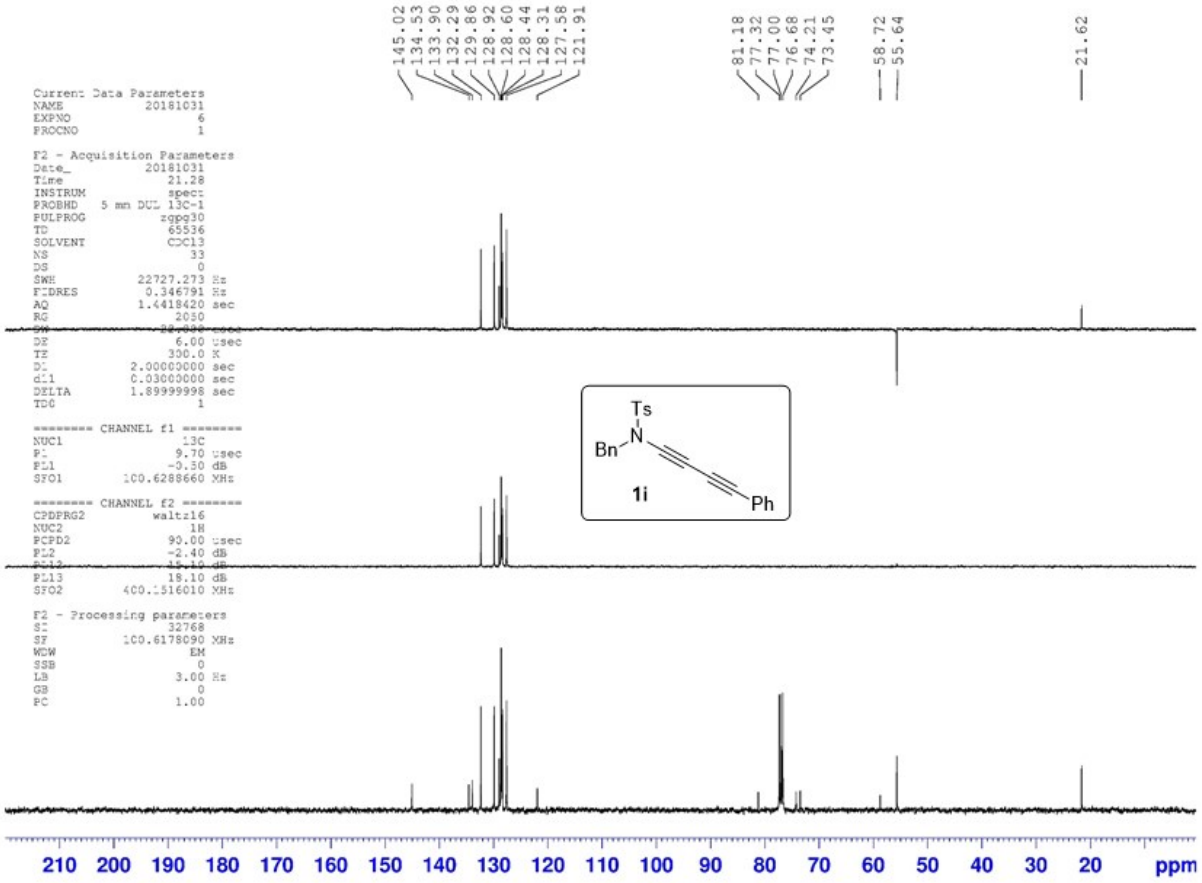

7.618
7.602
7.473
7.458
7.439
7.389
7.353
7.339
7.325
7.312
7.300
7.286
7.239
7.230
7.214
7.199
7.183
2.443
YP-03-159-H1
Current Data Parameters
NAME YP-03-159-H1.fid
EXPNO 1
PROCNO 1
F2 - Processing parameters
SI 16384
SF 499.7873545 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
Ts
N
Br
Ph
1g
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
2.00
3.18
1.01
5.28
2.02
3.18

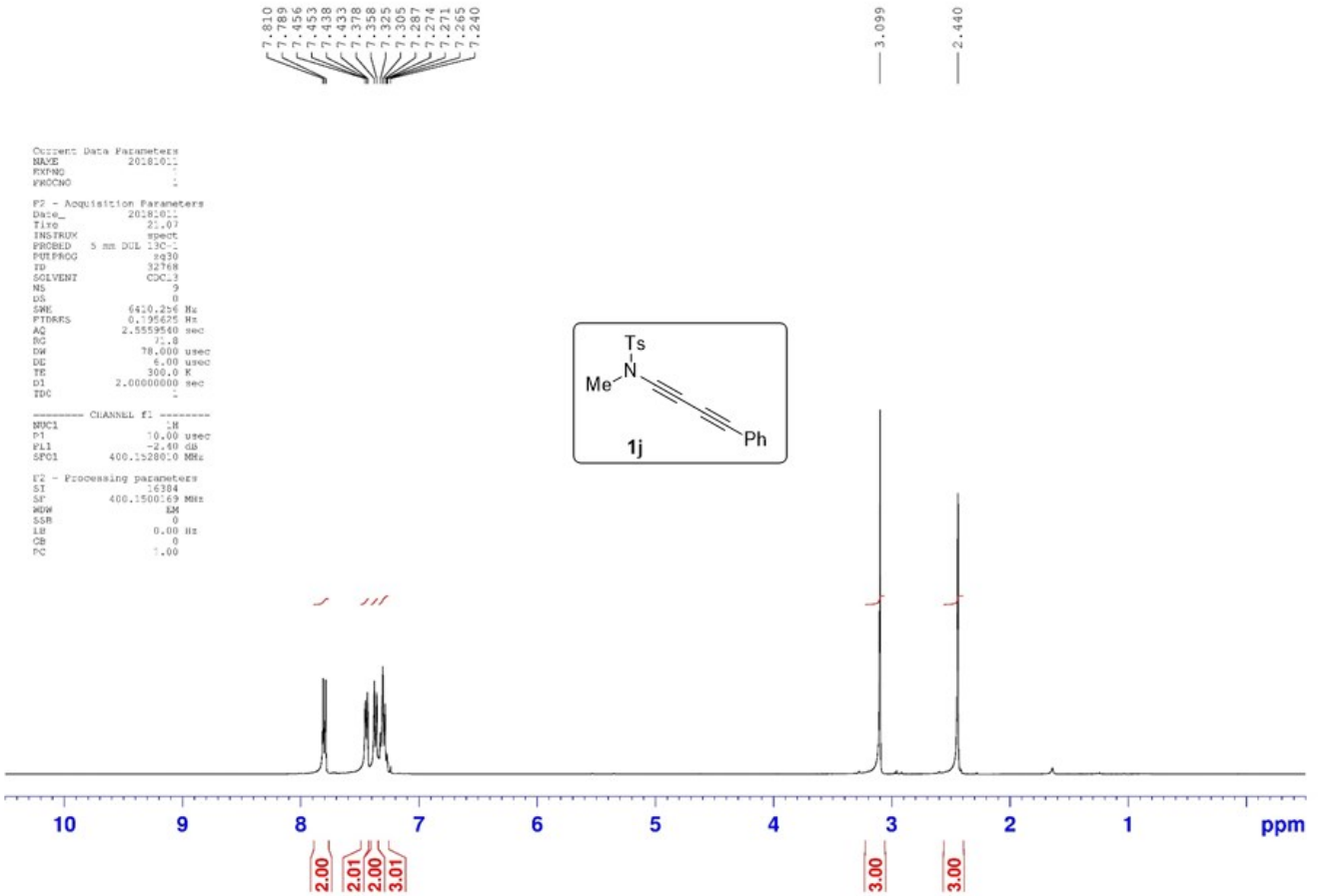

146.010
139.451
132.897
132.666
131.967
130.688
130.145
129.411
129.290
128.665
128.424
125.077
122.699
121.995
82.107
77.510
77.256
77.001
73.709
73.372
58.742
22.015
Current Data Parameters
NAME YP-03-159-C13.fid
EXPNO 1
PROCNO 1
F2 - Processing parameters
SI 65536
SF 125.6744864 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
Ts
N
Br
Ph
1g
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

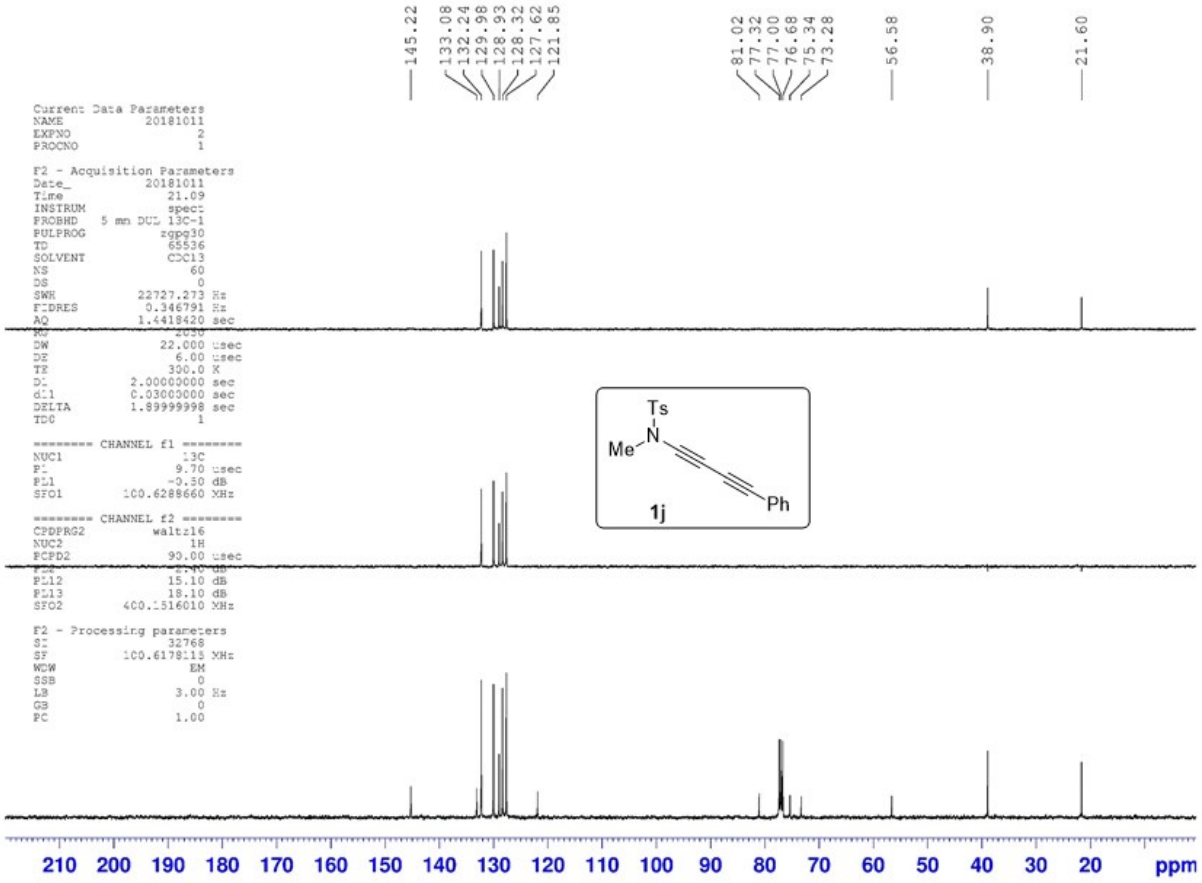

7.636
7.622
7.465
7.463
7.460
7.455
7.451
7.449
7.328
7.319
7.316
7.313
7.305
7.293
7.281
7.278
7.240
7.219
7.205
7.192
6.864
6.863
6.860
6.859
6.850
6.849
6.846
6.845
6.806
6.799
6.795
6.783
6.782
6.780
6.778
3.747
2.432
Current Data Parameters
NAME YP-03-155-B
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200227
Time 6.08
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 9541.984 Hz
FIDRES 0.291198 Hz
AQ 1.7170932 sec
RG 256
DW 52.400 usec
DE 6.50 usec
TE 295.8 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.15 usec
PL1 -1.00 dB
SFO1 598.1034854 MHz
F2 - Processing parameters
SI 32768
SF 598.1000311 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 2.00
Ts
N
MeO
Ph
1h
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
1.97
2.00
5.17
1.12
1.07
2.08
3.07
3.01

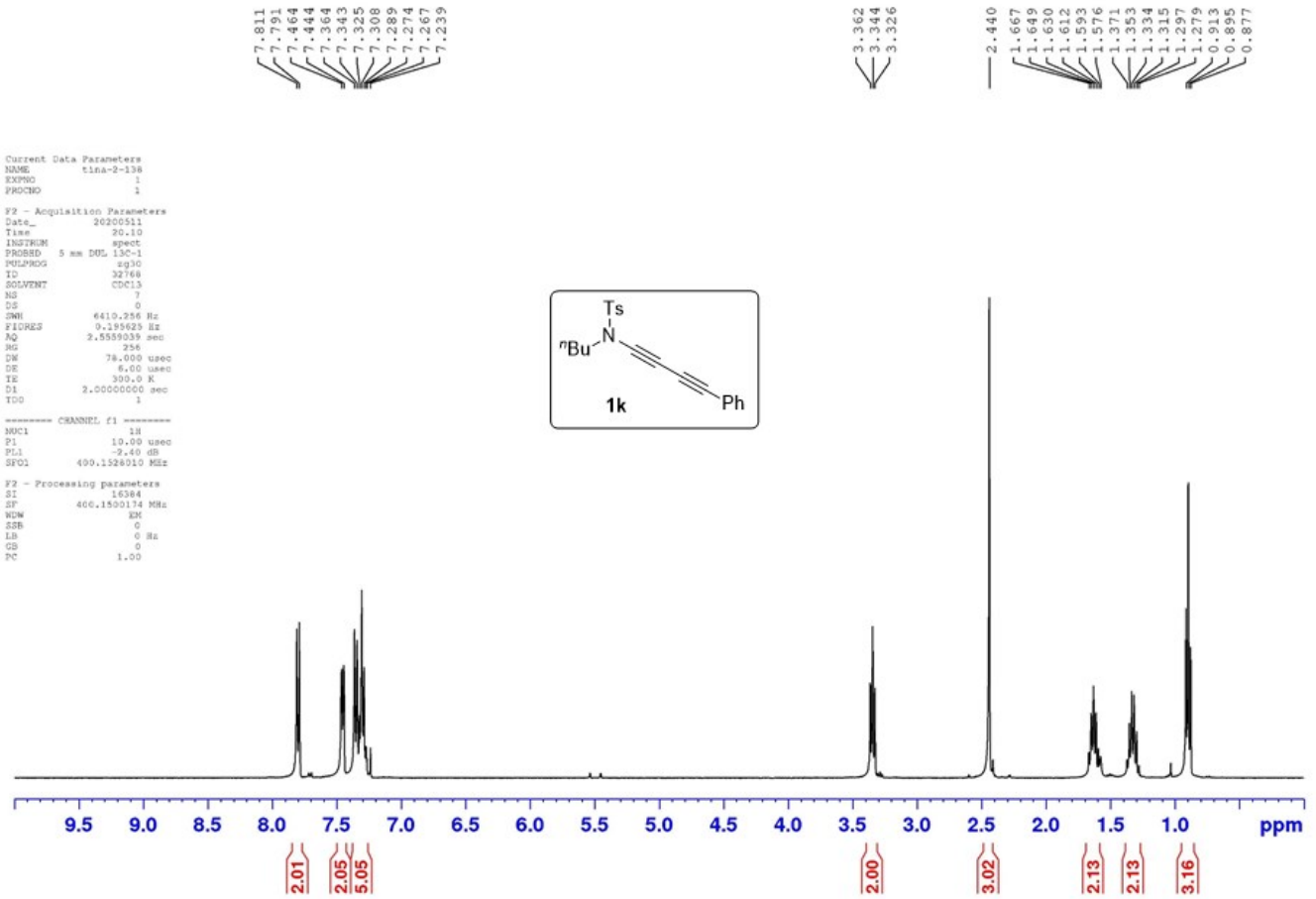

160.037
145.377
138.988
133.021
132.344
129.820
129.729
128.997
128.369
128.178
121.924
118.299
114.660
111.910
81.489
77.204
76.992
76.779
74.171
73.393
57.844
55.464
21.713
Current Data Parameters
NAME YP-03-155-B
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200227
Time 6.21
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDC13
NS 200
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 296.1 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0 dB
SFO1 150.4080337 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 7.00 dB
PL13 14.00 dB
SFO2 598.1030916 MHz
F2 - Processing parameters
SI 65536
SF 150.3923735 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
Ts
N
MeO
Ph
1h
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

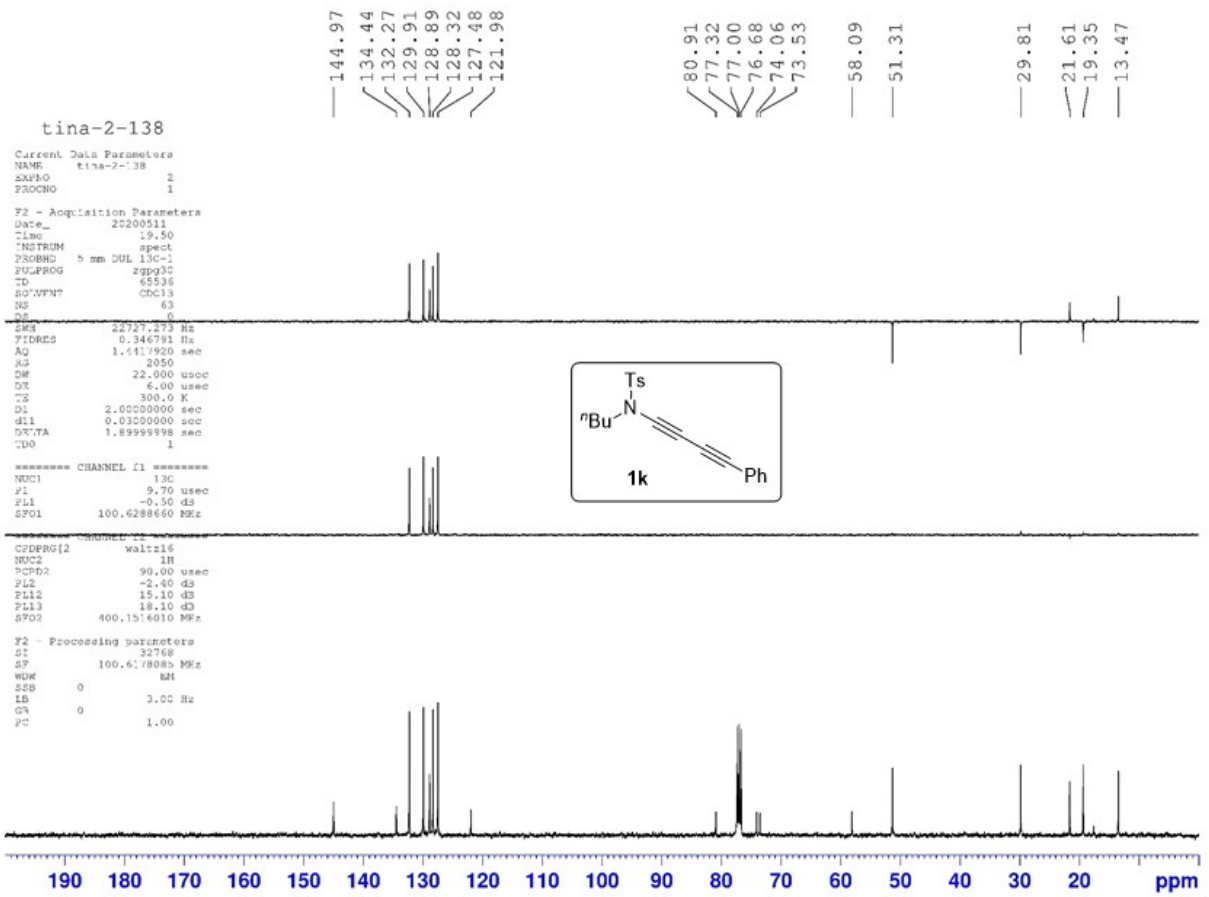

7.758
7.754
7.737
7.734
7.440
7.438
7.421
7.316
7.297
7.280
7.240
4.552
2.429
Ts
N
Bn
1i
Ph
10
9
8
7
6
5
4
3
2
1
ppm
2.01
2.03
10.01
2.00
3.03

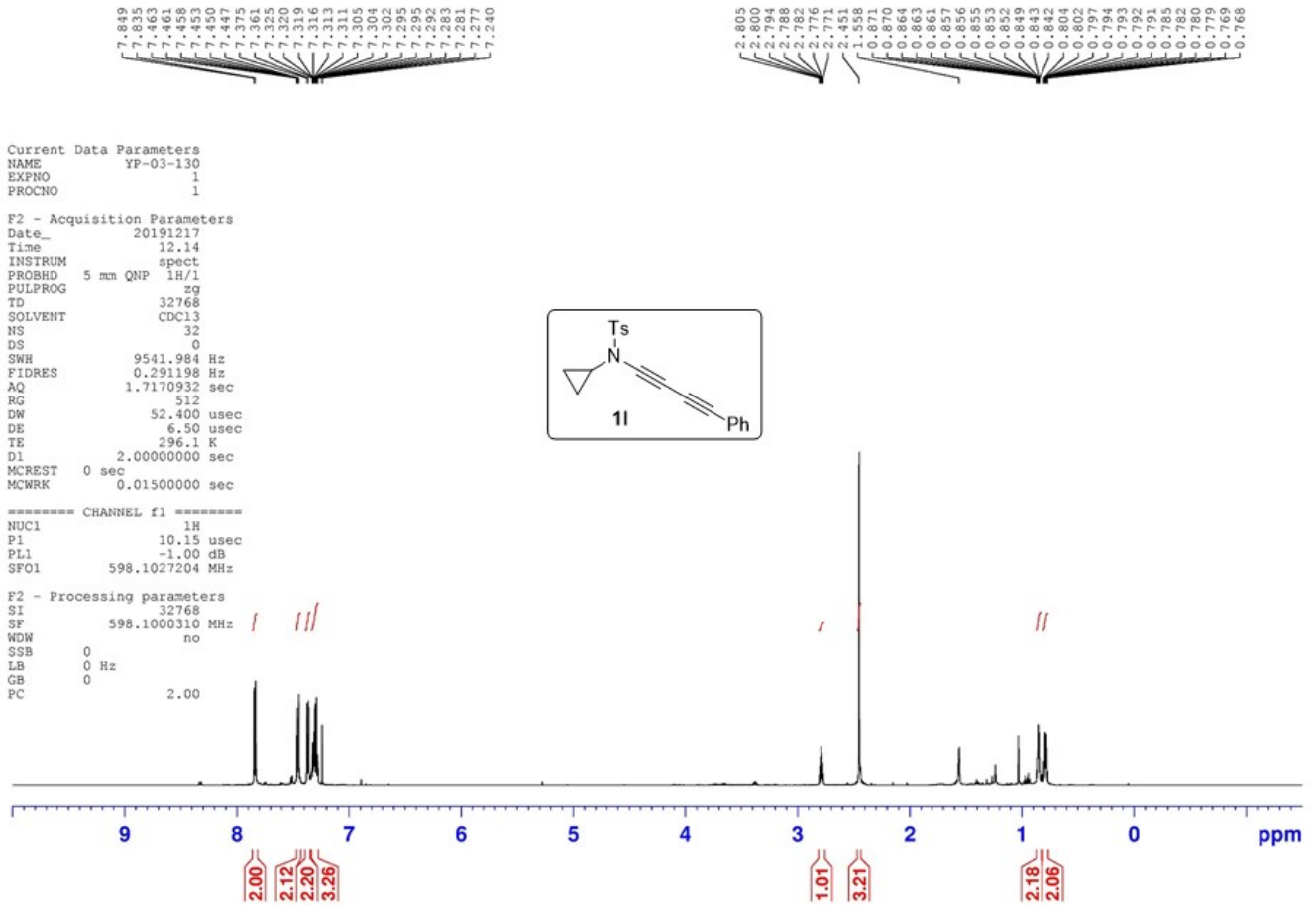

145.02
134.53
133.90
132.29
129.86
128.92
128.60
128.44
128.31
127.58
121.91
81.18
77.32
77.00
76.68
74.21
73.45
58.72
55.64
21.62
Current Data Parameters
NAME 20181031
EXPNO 6
PROCNO 1
F2 - Acquisition Parameters
Date_ 20181031
Time 21.28
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 33
DS 0
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4418420 sec
RG 2050
DW 22.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.70 usec
PL1 -0.50 dB
SFO1 100.6288660 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.40 dB
PL12 15.10 dB
PL13 18.10 dB
SFO2 400.1516010 MHz
F2 - Processing parameters
SI 32768
SF 100.6178090 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
Ts
N
Bn
1i
Ph
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


7.810
7.789
7.456
7.453
7.438
7.433
7.378
7.358
7.325
7.305
7.287
7.274
7.271
7.265
7.240
3.099
2.440
Ts
N
Me
Ph
1j
10
9
8
7
6
5
4
3
2
1
ppm
2.00
2.01
2.00
3.01
3.00
3.00


145.22
133.08
132.24
129.98
128.93
128.32
127.62
121.85
81.02
77.32
77.00
76.68
75.34
73.28
56.58
38.90
21.60
Current Data Parameters
NAME 20181011
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20181011
Time 21.09
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 60
DS 0
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4418420 sec
DW 22.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.70 usec
PL1 -0.30 dB
SFO1 100.6288660 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL12 15.10 dB
PL13 18.10 dB
SFO2 400.1516010 MHz
F2 - Processing parameters
SI 32768
SF 100.6178115 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
Ts
N
Me
Ph
1j
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


7.811
7.791
7.464
7.444
7.364
7.343
7.325
7.308
7.289
7.274
7.267
7.239
3.362
3.344
3.326
2.440
1.667
1.649
1.630
1.612
1.593
1.576
1.371
1.353
1.334
1.315
1.297
1.279
0.913
0.895
0.877
Current Data Parameters
NAME tina-2-138
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200511
Time 20.10
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 7
DS 0
SWH 6410.256 Hz
FIDRES 9.195625 Hz
AQ 2.5559039 sec
RG 256
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1326010 MHz
F2 - Processing parameters
SI 16384
SF 400.1300174 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00
Ts
N
nBu
1k
Ph
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
2.01
2.05
5.05
2.00
3.02
2.13
2.13
3.16


144.97
134.44
132.27
129.91
128.89
128.32
127.48
121.98
80.91
77.32
77.00
76.68
74.06
73.53
58.09
51.31
29.81
21.61
19.35
13.47
tina-2-138
Ts
N
nBu
Ph
1k
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


7.849
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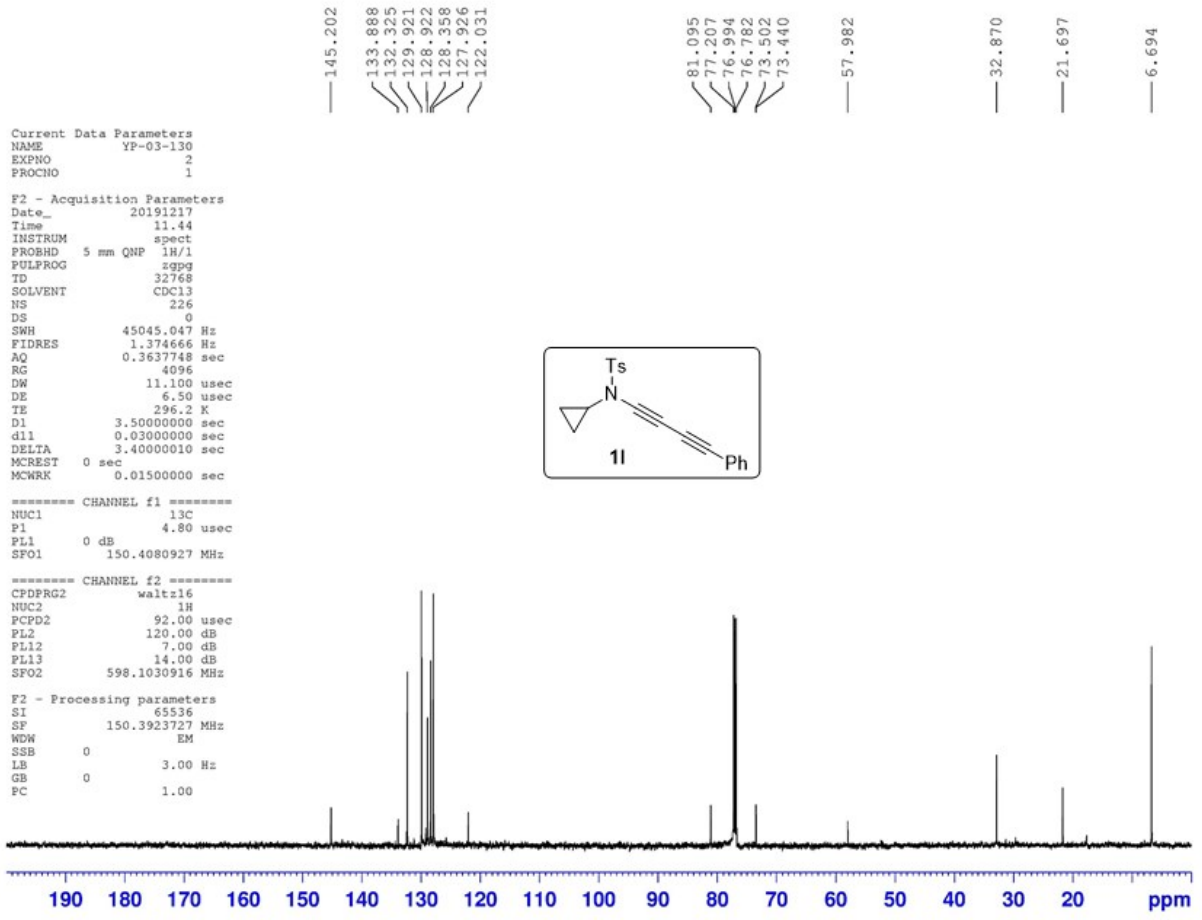
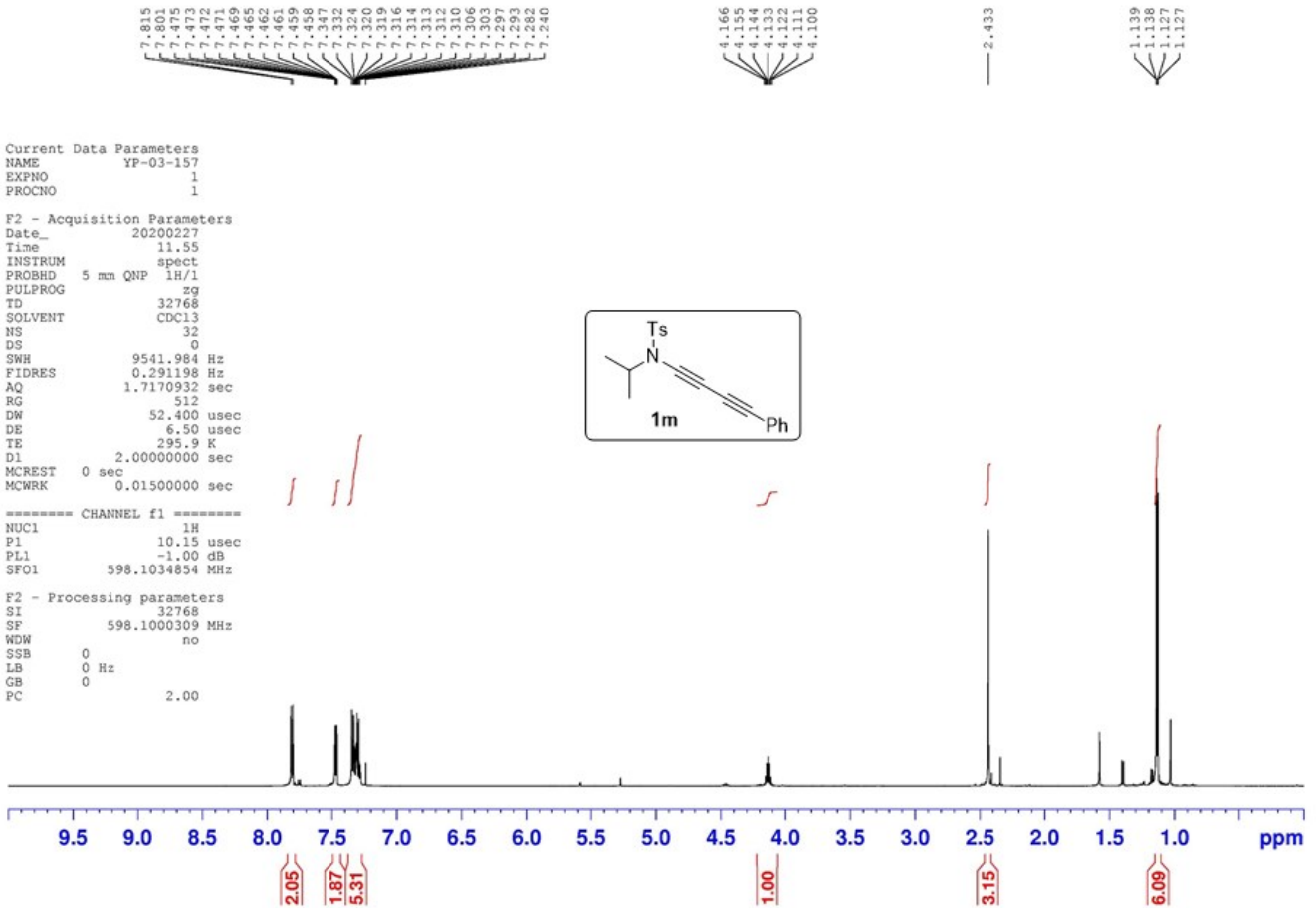
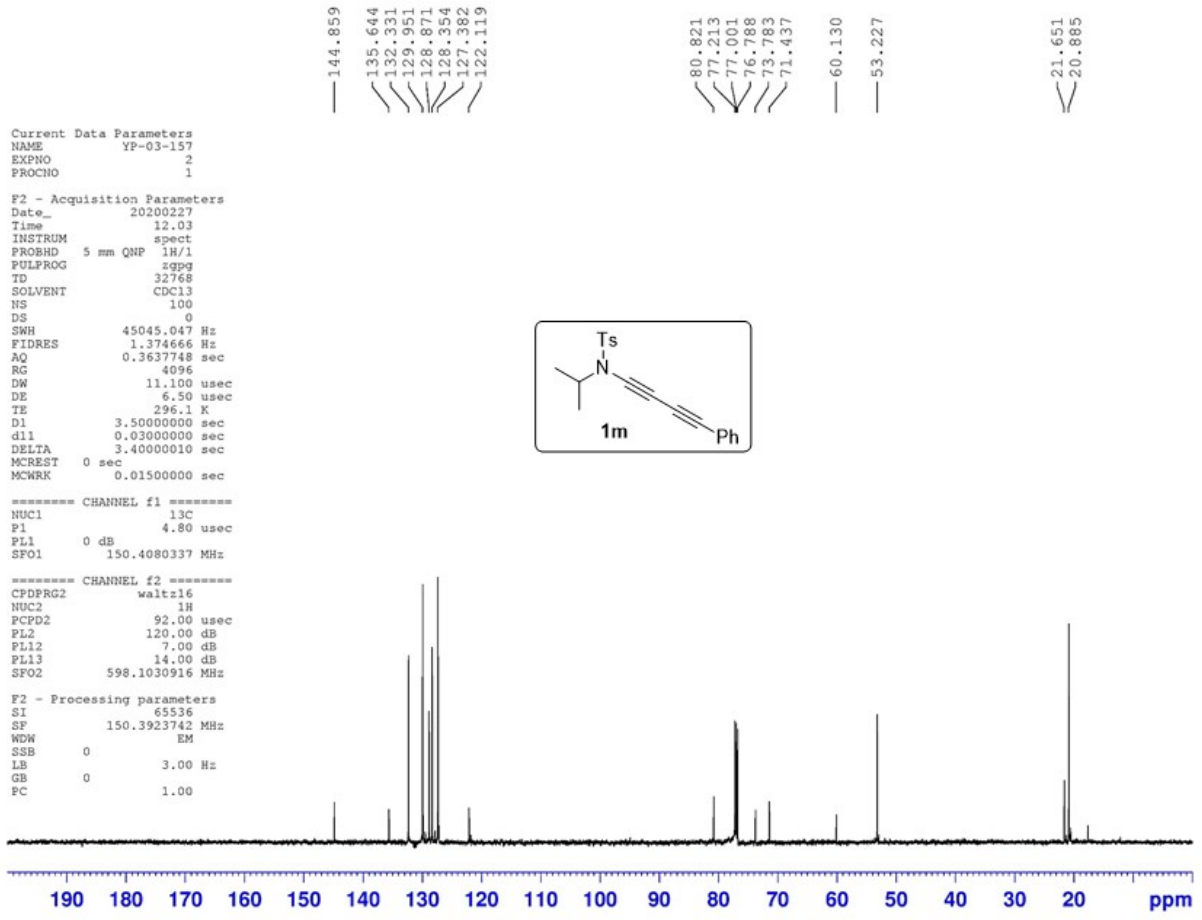
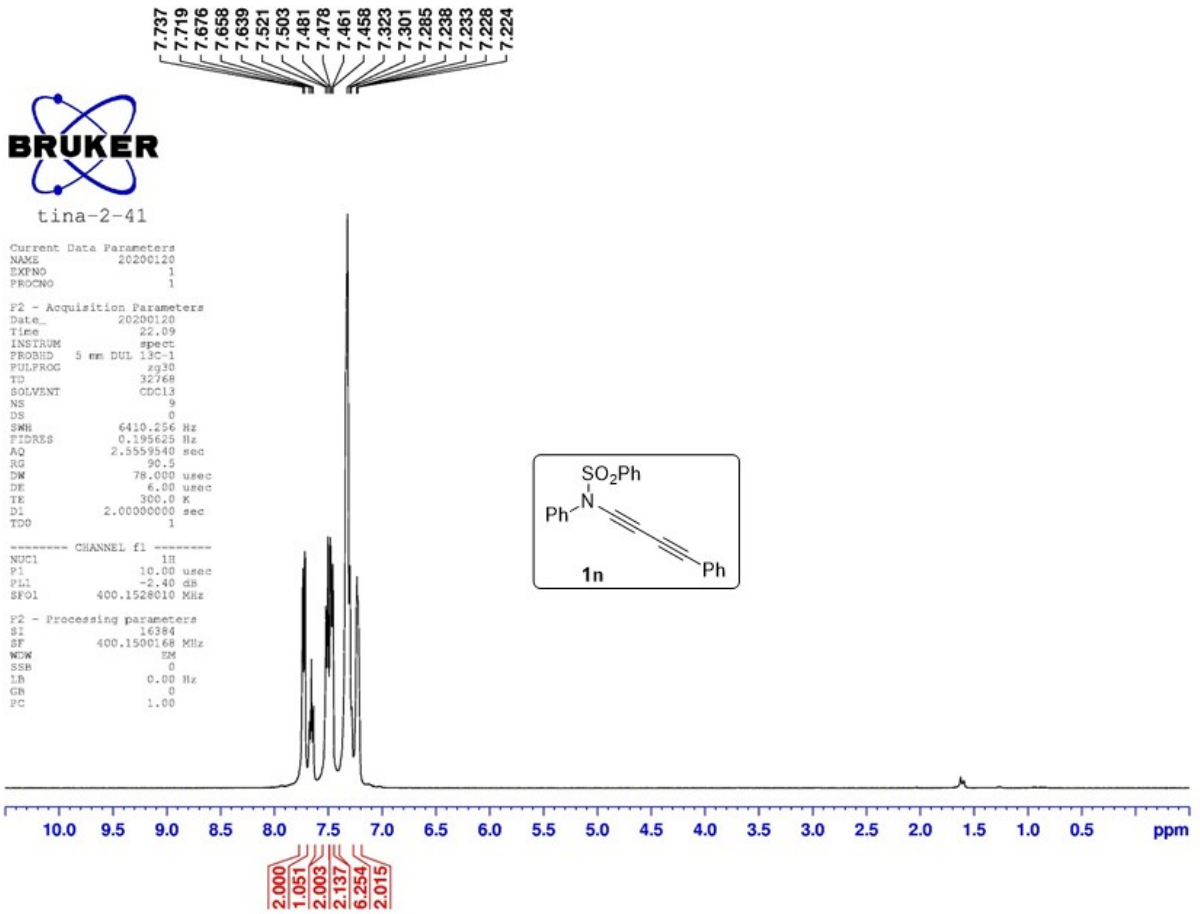
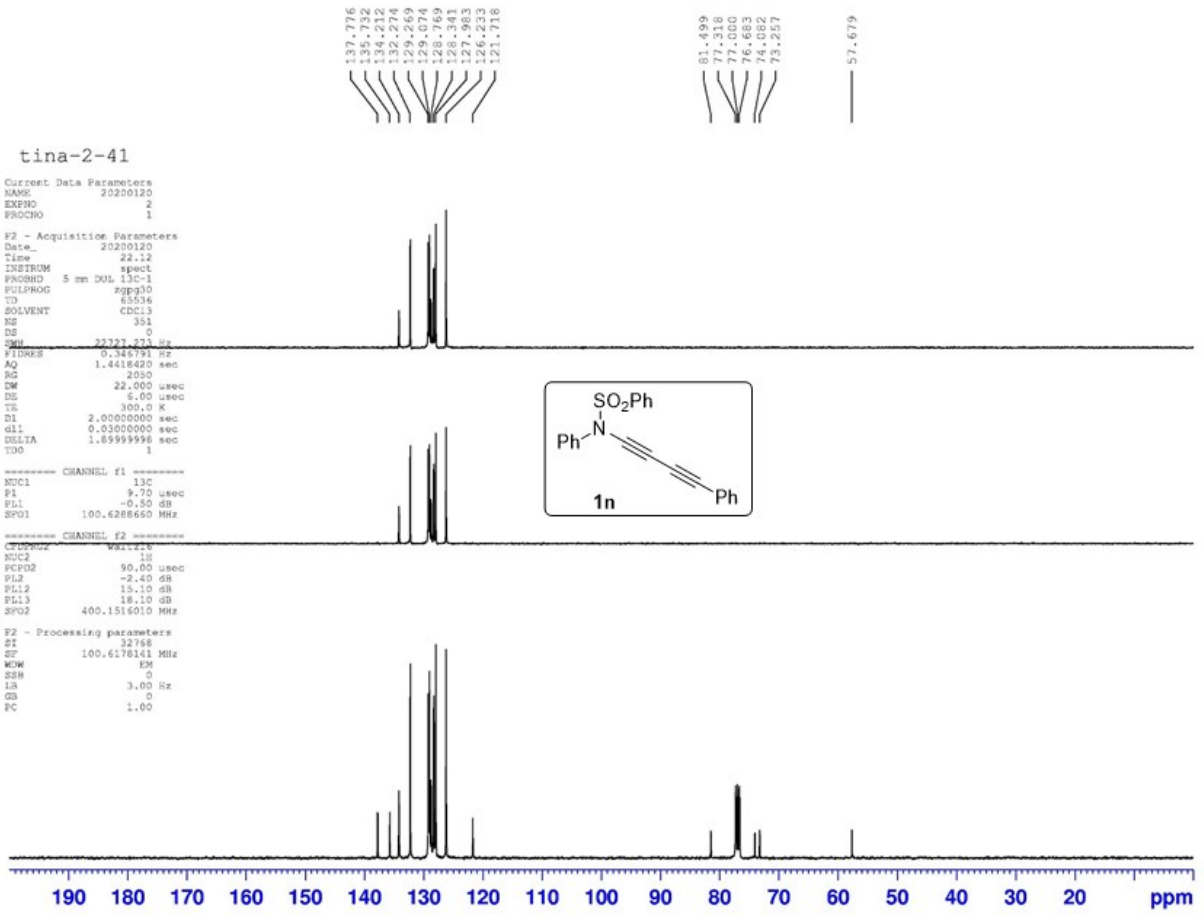
7.463
7.461
7.458
7.453
7.450
7.447
7.375
7.361
7.325
7.320
7.319
7.316
7.313
7.311
7.305
7.304
7.302
7.295
7.295
7.292
7.283
7.281
7.277
7.240
2.805
2.800
2.794
2.788
2.782
2.776
2.771
2.451
1.558
0.871
0.870
0.864
0.863
0.861
0.857
0.856
0.855
0.853
0.852
0.849
0.843
0.842
0.804
0.802
0.797
0.794
0.793
0.792
0.791
0.785
0.782
0.780
0.779
0.769
0.768
Current Data Parameters
NAME YP-03-130
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20191217
Time 12.14
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 9541.984 Hz
FIDRES 0.291198 Hz
AQ 1.7170932 sec
RG 512
DW 52.400 usec
DE 6.50 usec
TE 296.1 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.15 usec
PL1 -1.00 dB
SFO1 598.1027204 MHz
F2 - Processing parameters
SI 32768
SF 598.1000310 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 2.00
Ts
N
1l
Ph
9
8
7
6
5
4
3
2
1
0
ppm
2.00
2.12
2.20
3.26
1.01
3.21
2.18
2.06

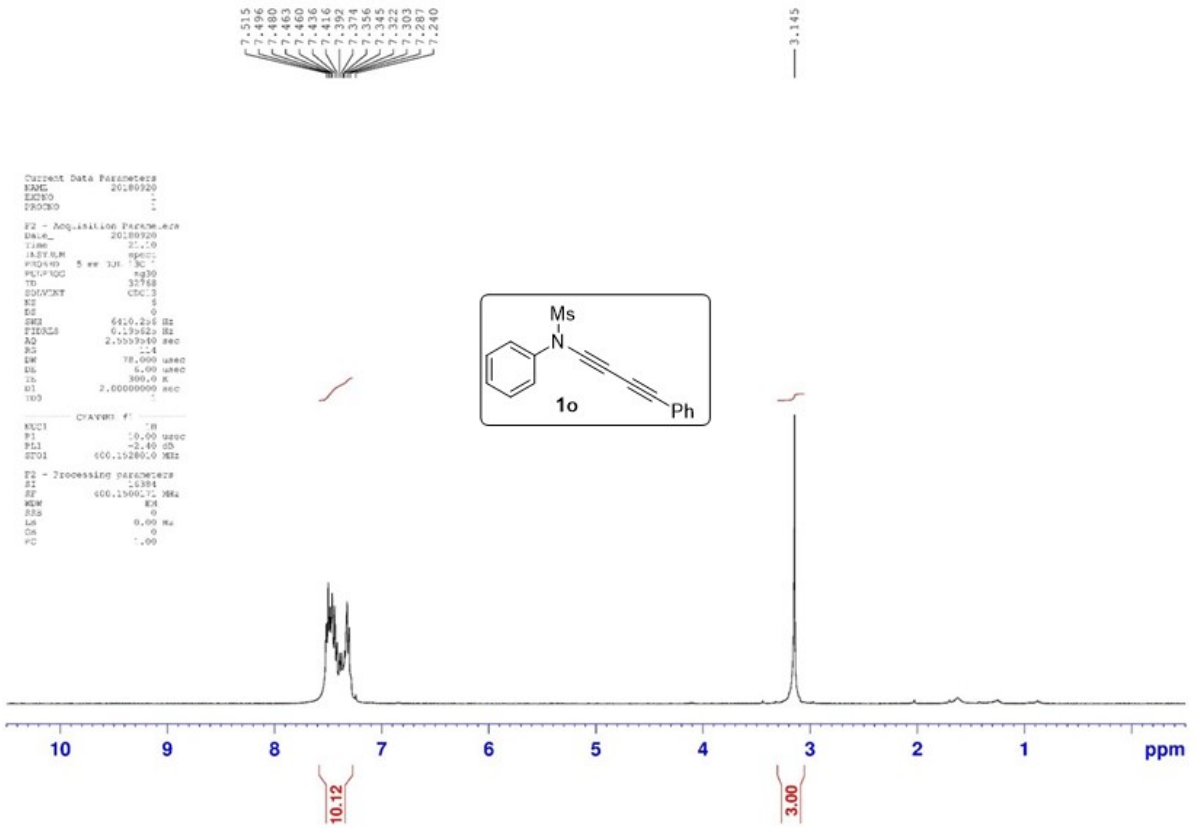

145.202
133.888
132.325
129.921
128.922
128.358
127.926
122.031
81.095
77.207
76.994
76.782
73.502
73.440
57.982
32.870
21.697
6.694
Current Data Parameters
NAME YP-03-130
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20191217
Time 11.44
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 226
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 296.2 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0 dB
SFO1 150.4080927 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 7.00 dB
PL13 14.00 dB
SFO2 598.1030916 MHz
F2 - Processing parameters
SI 65536
SF 150.3923727 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
Ts
N
Ph
1l
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

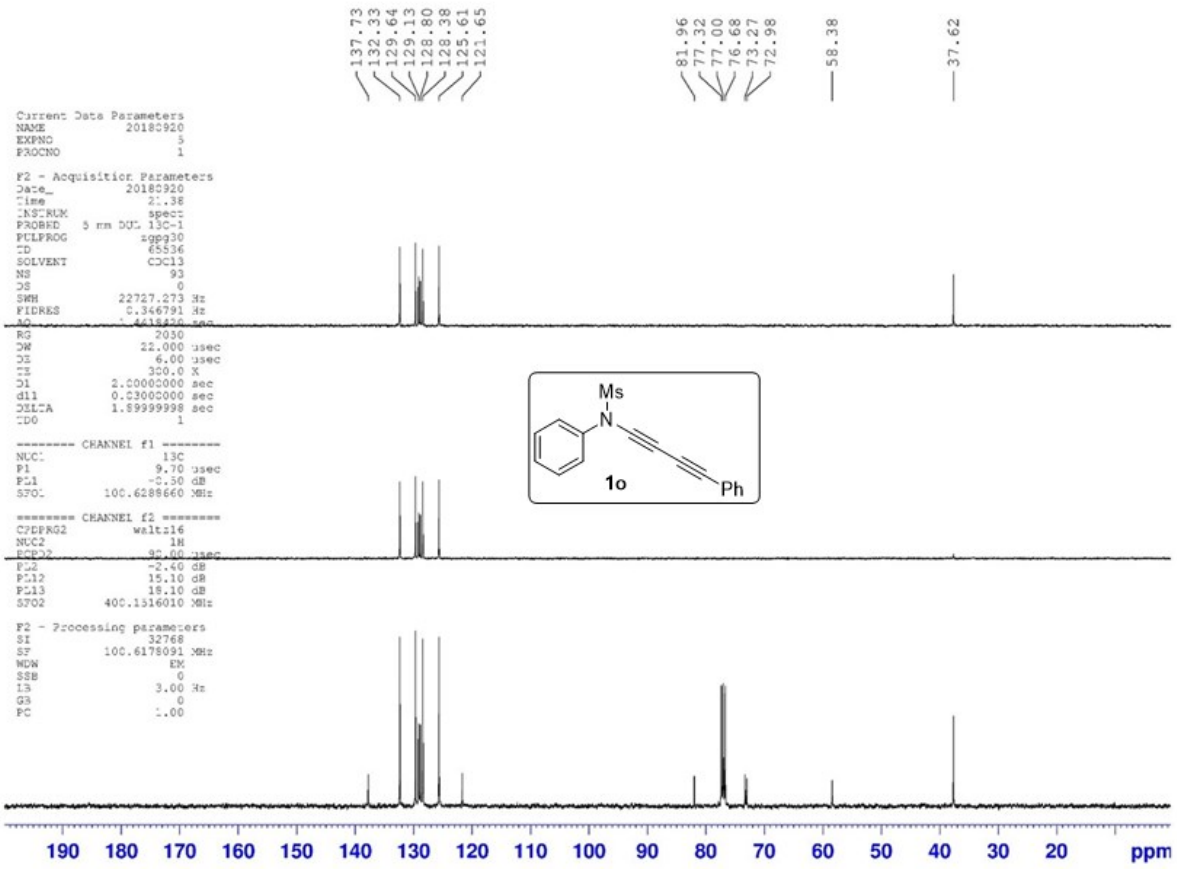

7.815
7.801
7.475
7.473
7.472
7.471
7.469
7.465
7.462
7.461
7.459
7.458
7.347
7.332
7.324
7.320
7.319
7.316
7.314
7.313
7.312
7.310
7.306
7.303
7.297
7.293
7.282
7.240
4.166
4.155
4.144
4.133
4.122
4.111
4.100
2.433
1.139
1.138
1.127
1.127
Current Data Parameters
NAME YP-03-157
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200227
Time 11.55
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 9541.984 Hz
FIDRES 0.291198 Hz
AQ 1.7170932 sec
RG 512
DW 52.400 usec
DE 6.50 usec
TE 295.9 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.15 usec
PL1 -1.00 dB
SFO1 598.1034854 MHz
F2 - Processing parameters
SI 32768
SF 598.1000309 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 2.00
Ts
N
1m
Ph
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
2.05
1.87
5.31
1.00
3.15
6.09

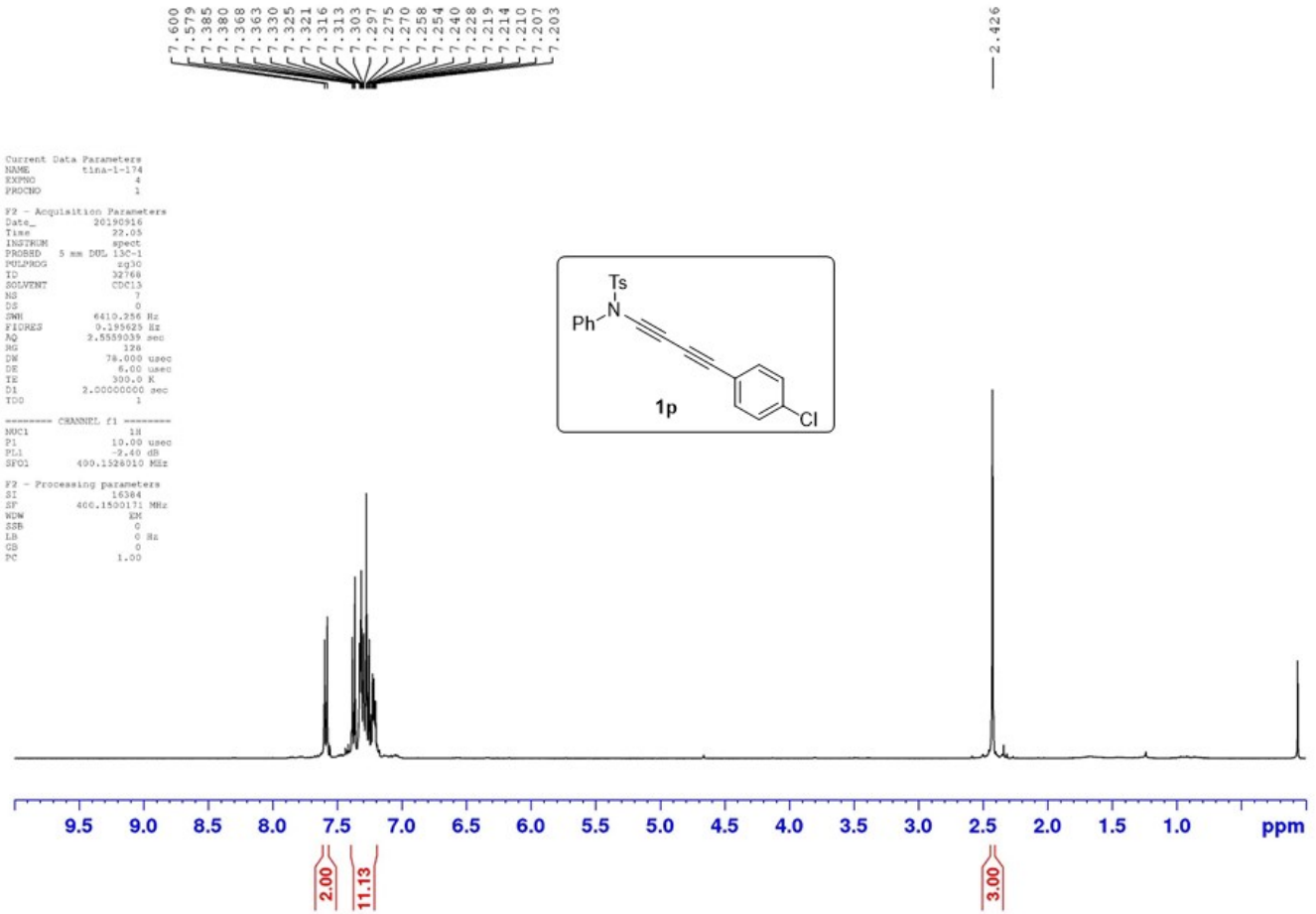

144.859
135.644
132.331
129.951
128.871
128.354
127.382
122.119
80.821
77.213
77.001
76.788
73.783
71.437
60.130
53.227
21.651
20.885
Current Data Parameters
NAME YP-03-157
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200227
Time 12.03
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 100
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 296.1 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0 dB
SFO1 150.4080337 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 7.00 dB
PL13 14.00 dB
SFO2 598.1030916 MHz
F2 - Processing parameters
SI 65536
SF 150.3923742 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
Ts
N
1m
Ph
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

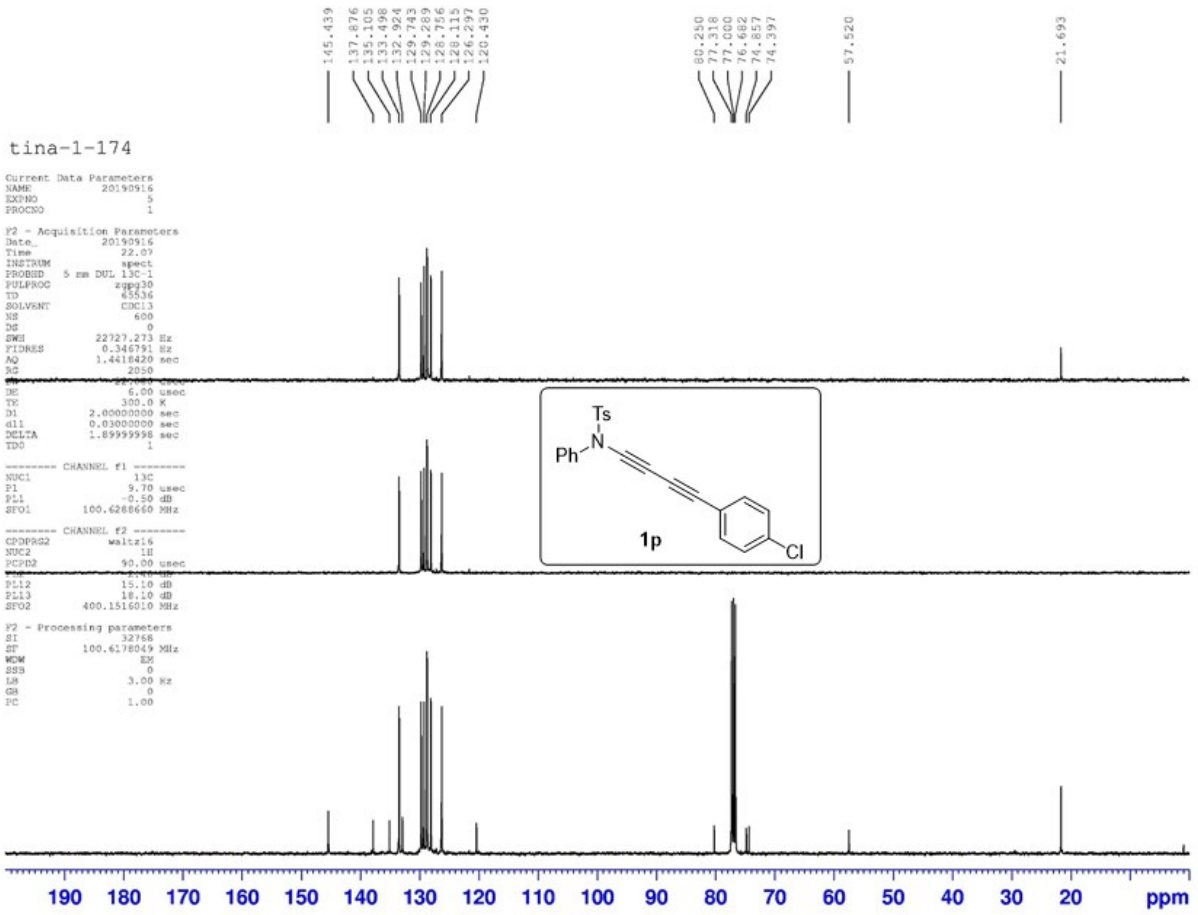

7.737
7.719
7.676
7.658
7.639
7.521
7.503
7.481
7.478
7.461
7.458
7.323
7.301
7.285
7.238
7.233
7.228
7.224
BRUKER
tina-2-41
Current Data Parameters
NAME 20200120
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200120
Time 22.09
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 9
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 90.5
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz
F2 - Processing parameters
SI 16384
SF 400.1500168 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
SO2Ph
Ph
N
Ph
1n
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
2.000
1.051
2.003
2.137
6.254
2.015

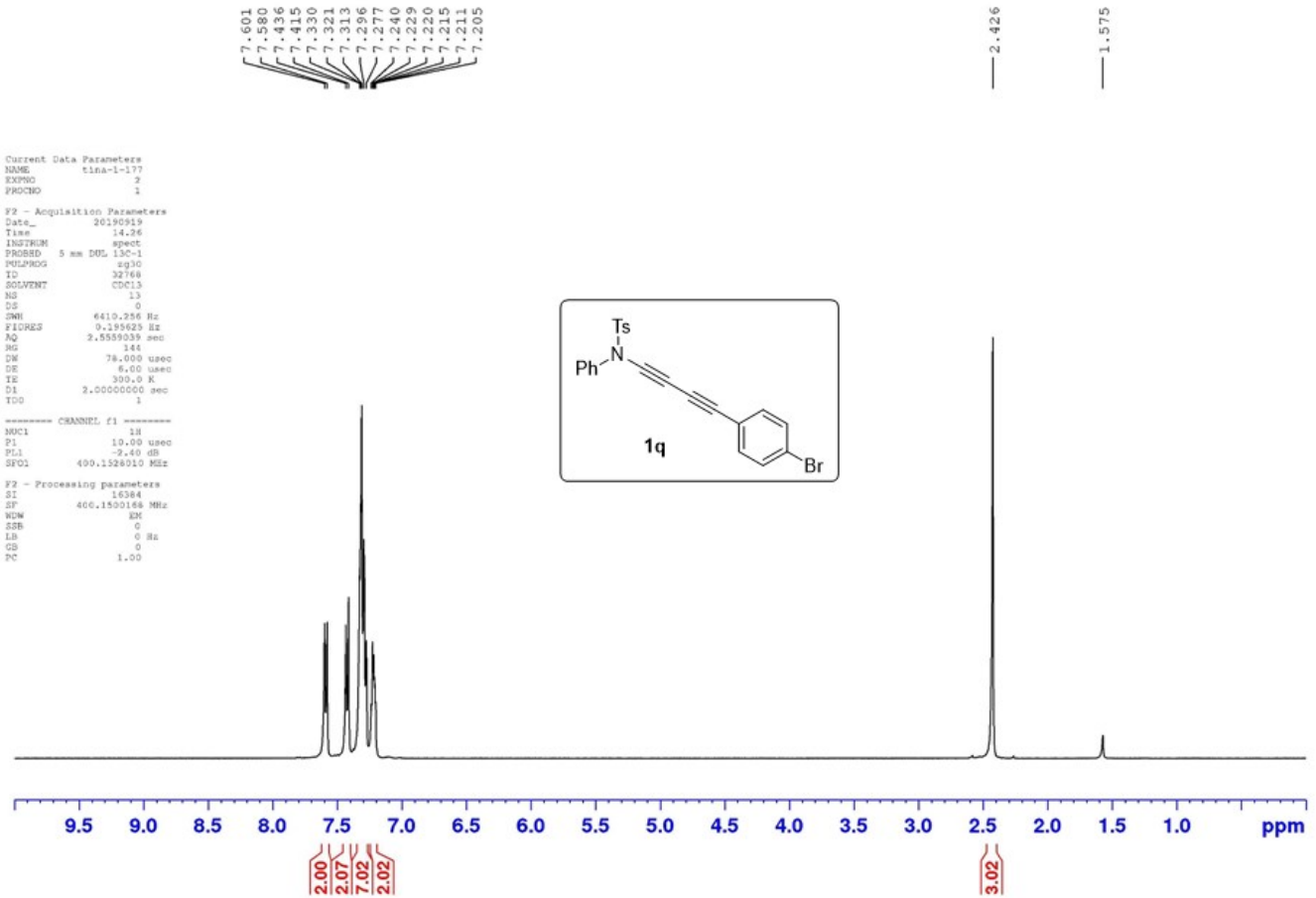

137.776
135.732
134.212
132.274
129.269
129.074
128.769
128.341
127.983
126.233
121.718
81.499
77.318
77.000
76.683
74.082
73.257
57.679
tina-2-41
Current Data Parameters
NAME 20200120
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200120
Time 22.12
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 351
DS 0
SWH 22321.273 Hz
FIDRES 0.346791 Hz
AQ 1.4418420 sec
RG 2050
DW 22.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.70 usec
PL1 -0.50 dB
SFO1 100.6288660 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.40 dB
PL12 15.10 dB
PL13 18.10 dB
SFO2 400.1516010 MHz
F2 - Processing parameters
SI 32768
SF 100.6178141 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
SO2Ph
N
Ph
Ph
1n
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

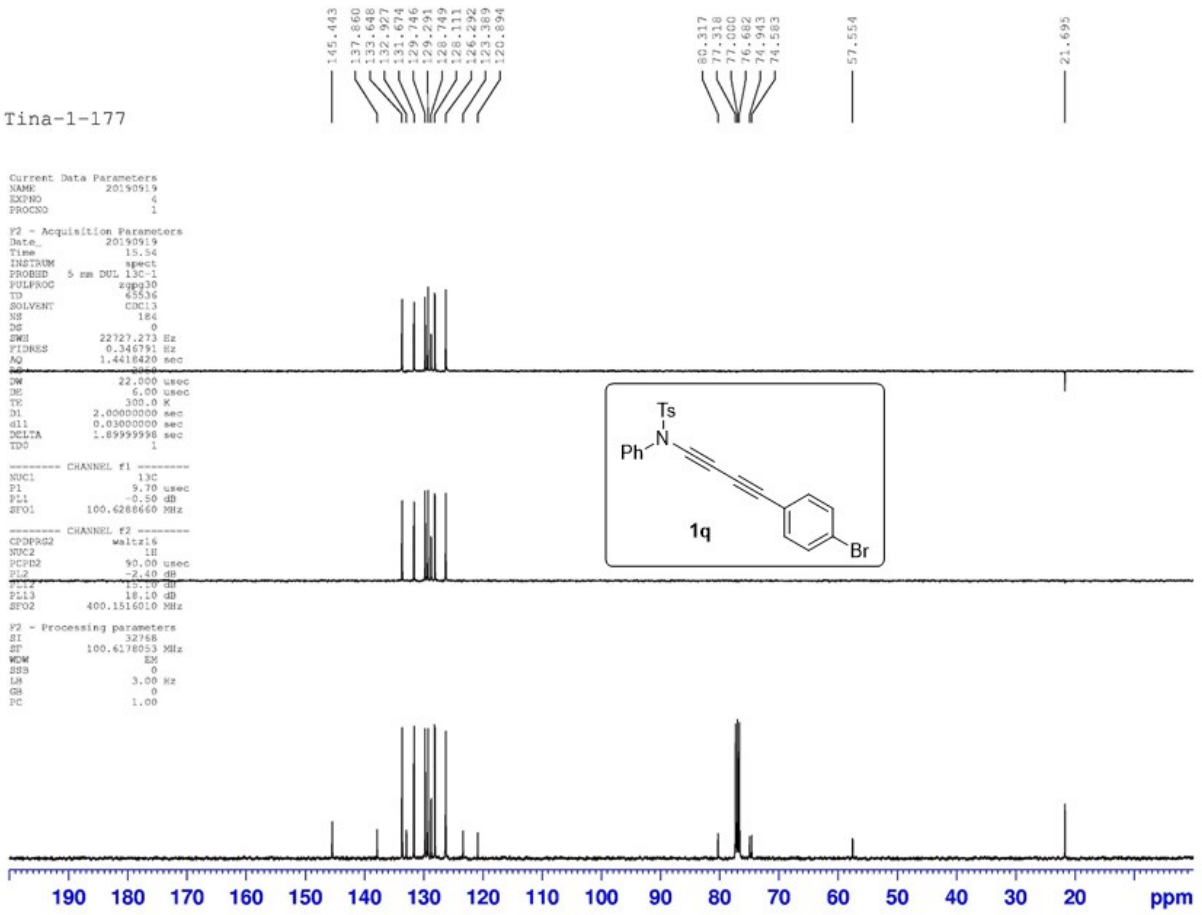

7.515
7.496
7.480
7.463
7.460
7.436
7.392
7.374
7.356
7.345
7.322
7.303
7.287
7.240
3.145
Ms
N
Ph
1o
10
9
8
7
6
5
4
3
2
1
ppm
10.12
3.00

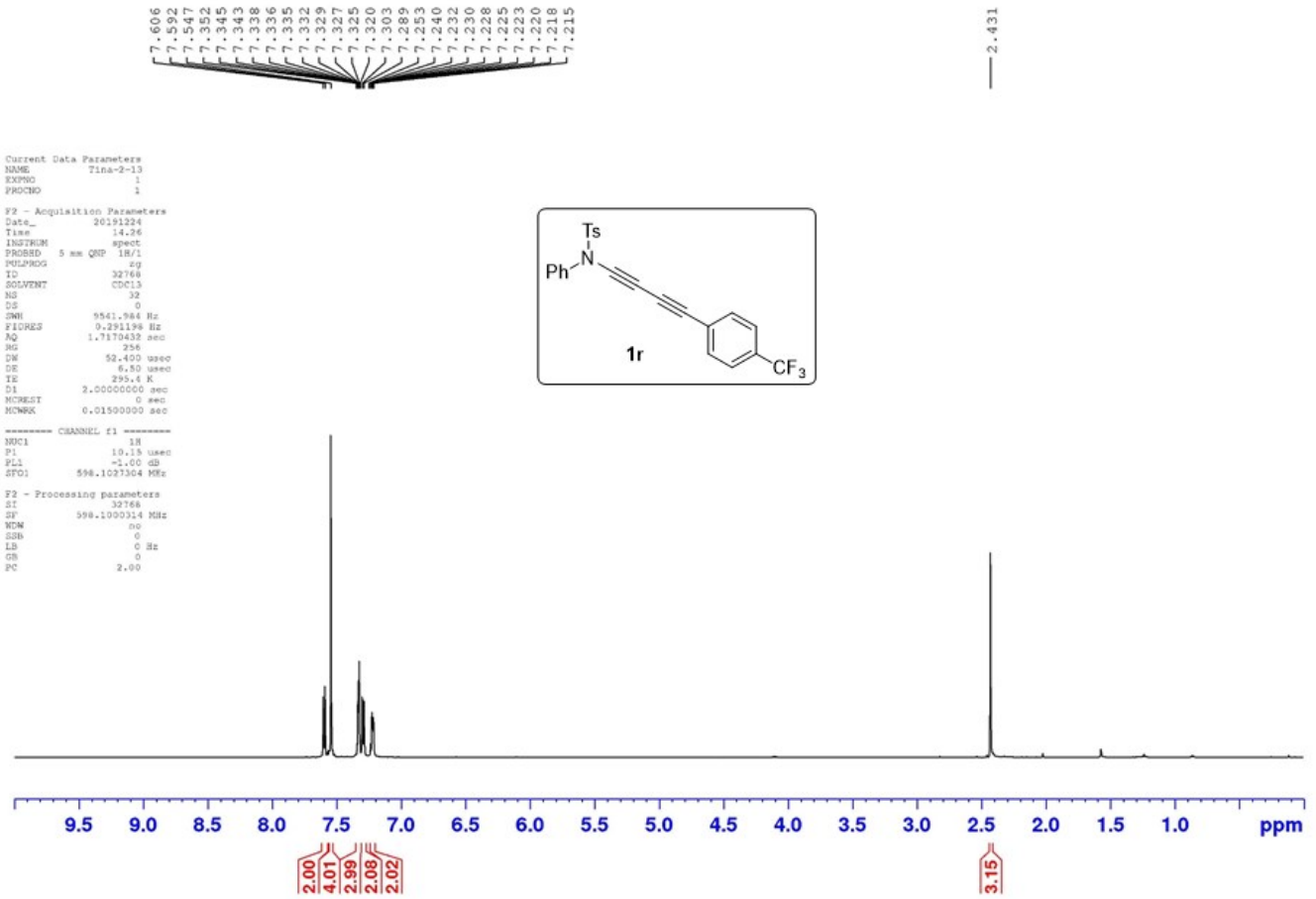

137.73
132.33
129.64
129.13
128.80
128.38
125.61
121.65
81.96
77.32
77.00
76.68
73.27
72.98
58.38
37.62
Ms
N
Ph
1o
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

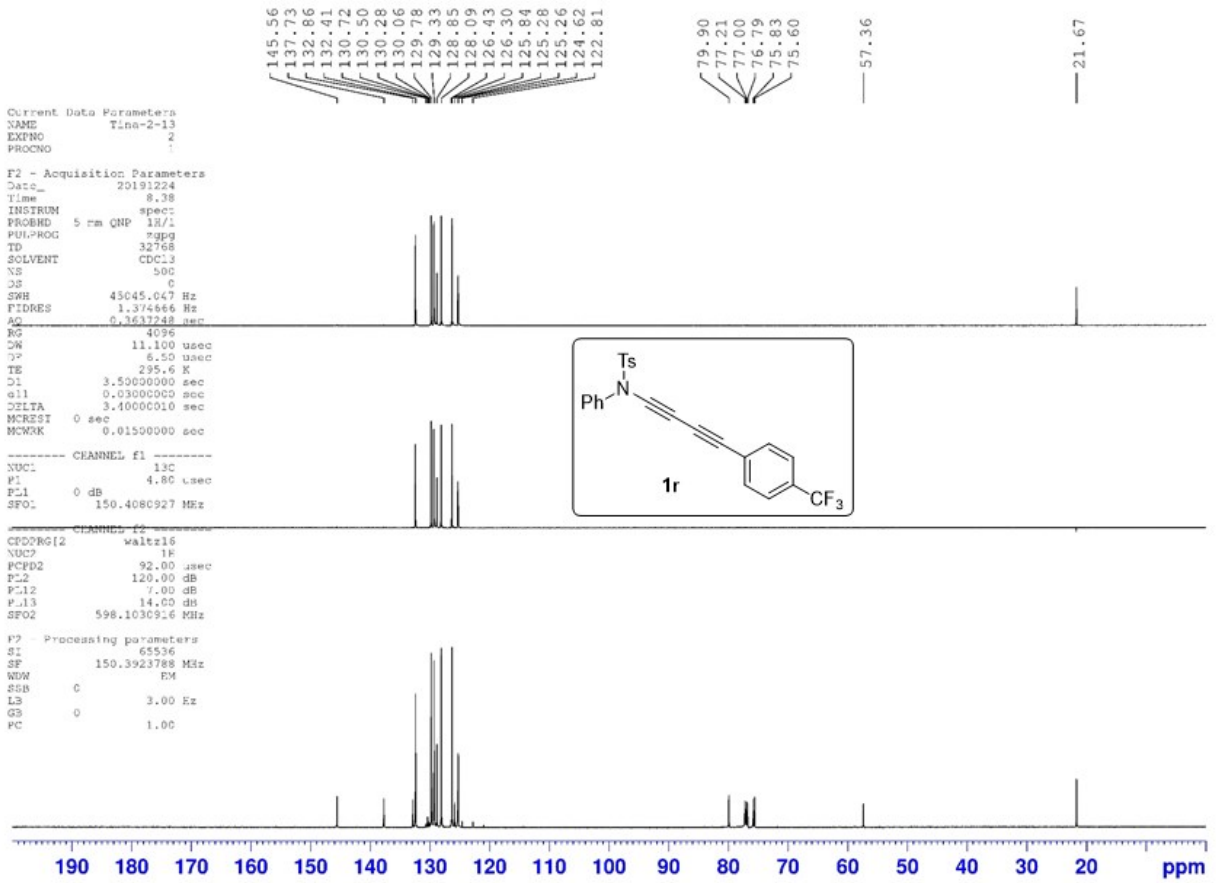

7.600
7.579
7.385
7.380
7.368
7.363
7.330
7.325
7.321
7.316
7.313
7.303
7.297
7.275
7.270
7.258
7.254
7.240
7.228
7.219
7.214
7.210
7.207
7.203
2.426
Current Data Parameters
NAME tina-1-174
EXPNO 4
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190916
Time 22.05
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 7
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559039 sec
RG 128
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1326010 MHz
F2 - Processing parameters
SI 16384
SF 400.1300171 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00
Ts
N
Ph
1p
Cl
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
2.00
11.13
3.00

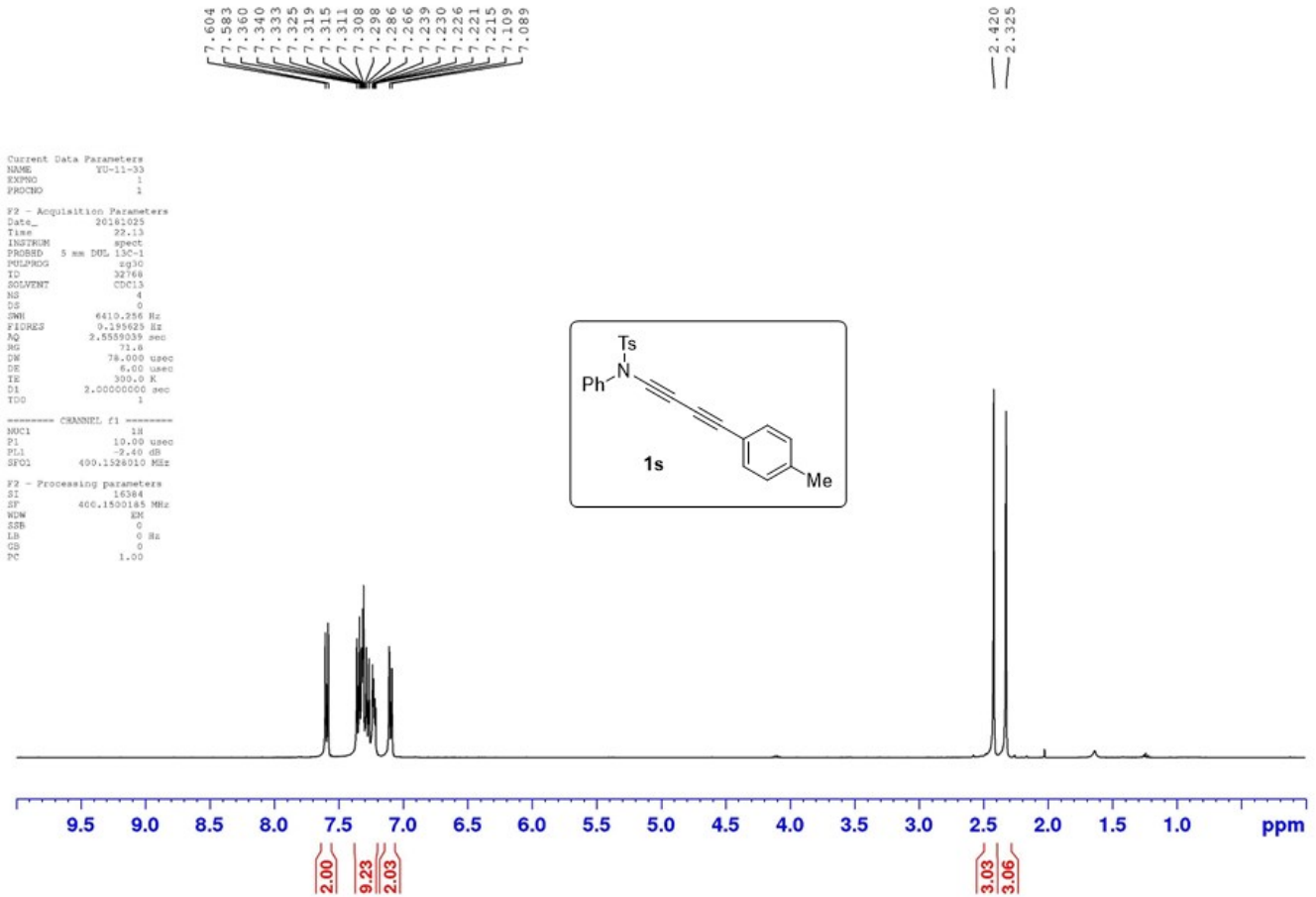

145.439
137.876
135.105
133.498
132.924
129.743
129.289
128.756
128.115
126.297
126.430
80.250
77.318
77.000
76.682
74.857
74.397
57.520
21.693
tina-1-174
Current Data Parameters
NAME 20190916
EXPNO 5
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190916
Time 22.07
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 600
DS 0
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4418420 sec
RG 2050
DW 22.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.70 usec
PL1 -0.50 dB
SFO1 100.6288660 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL12 15.10 dB
PL13 18.10 dB
SFO2 400.1516010 MHz
F2 - Processing parameters
SI 32768
SF 100.6178049 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
Ts
N
Ph
1p
Cl
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

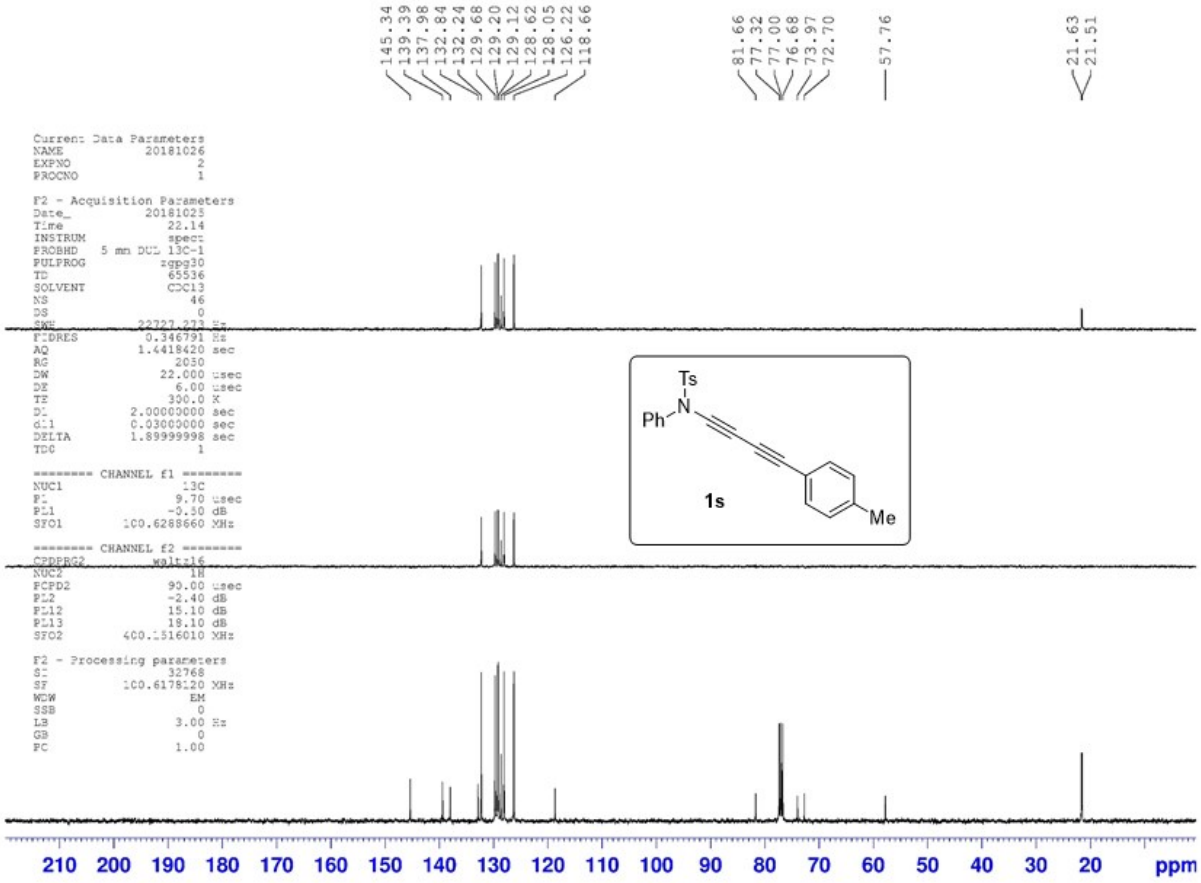

7.601
7.580
7.436
7.415
7.330
7.321
7.313
7.296
7.277
7.240
7.229
7.220
7.215
7.211
7.205
2.426
1.575
Current Data Parameters
NAME tina-1-177
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190919
Time 14.26
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 13
DS 0
SWH 6410.256 Hz
FIDRES 9.195625 Hz
AQ 2.5559039 sec
RG 144
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1326010 MHz
F2 - Processing parameters
SI 16384
SF 400.1300164 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00
Ts
N
Ph
1q
Br
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
2.00
2.07
7.02
2.02
3.02

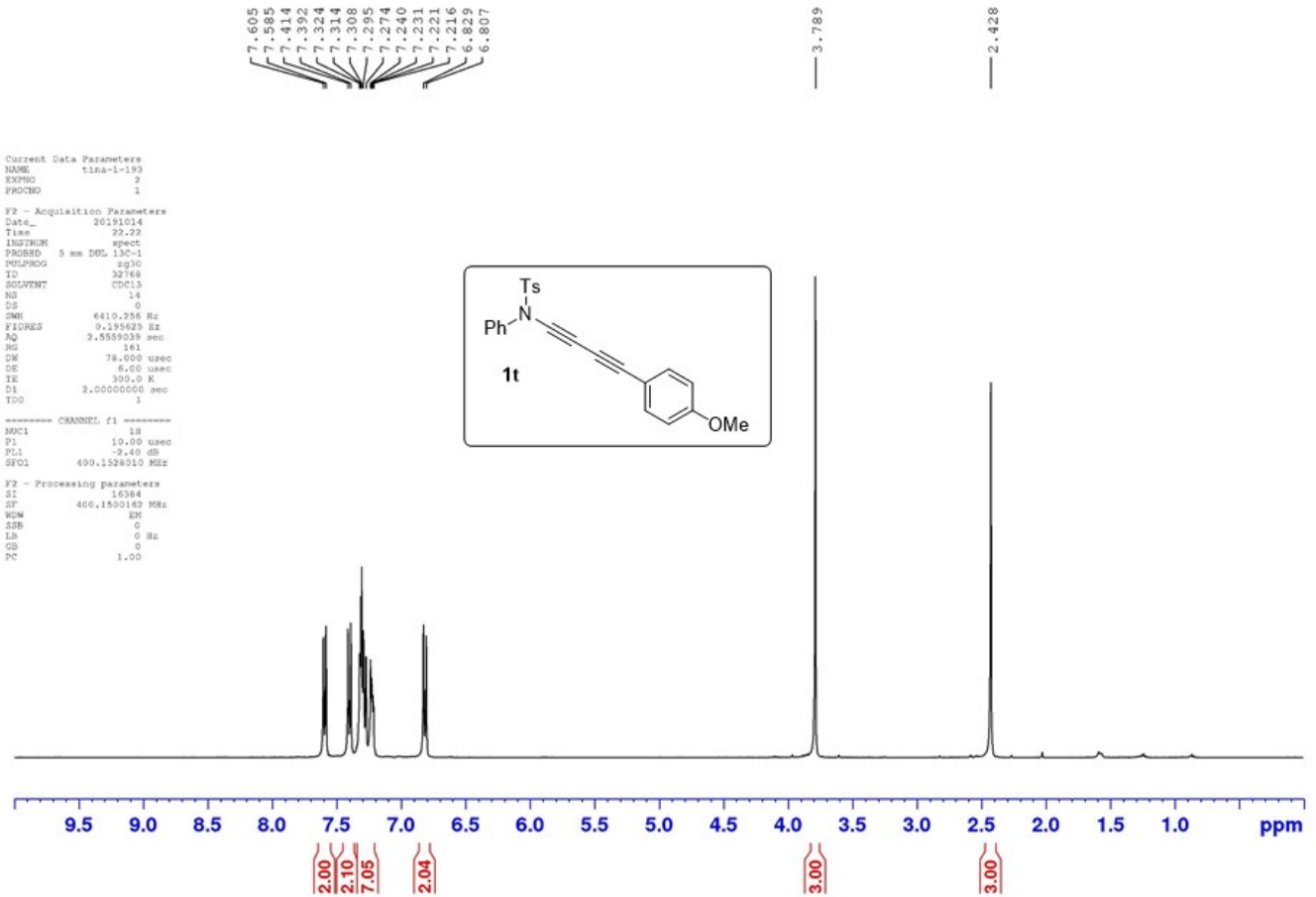

Tina-1-177
145.443
137.860
133.648
132.927
131.674
129.746
129.291
128.749
128.111
126.292
123.389
120.894
80.317
77.318
77.000
76.682
74.943
74.563
57.554
21.695
Current Data Parameters
NAME 20190919
EXPNO 6
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190919
Time 15.54
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 184
DS 0
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4418420 sec
RG 8268
DW 22.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.70 usec
PL1 -0.50 dB
SFO1 100.6288660 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.40 dB
PL12 15.10 dB
PL13 18.10 dB
SFO2 400.1516010 MHz
F2 - Processing parameters
SI 32768
SF 100.6178053 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
Ts
N
Ph
1q
Br
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

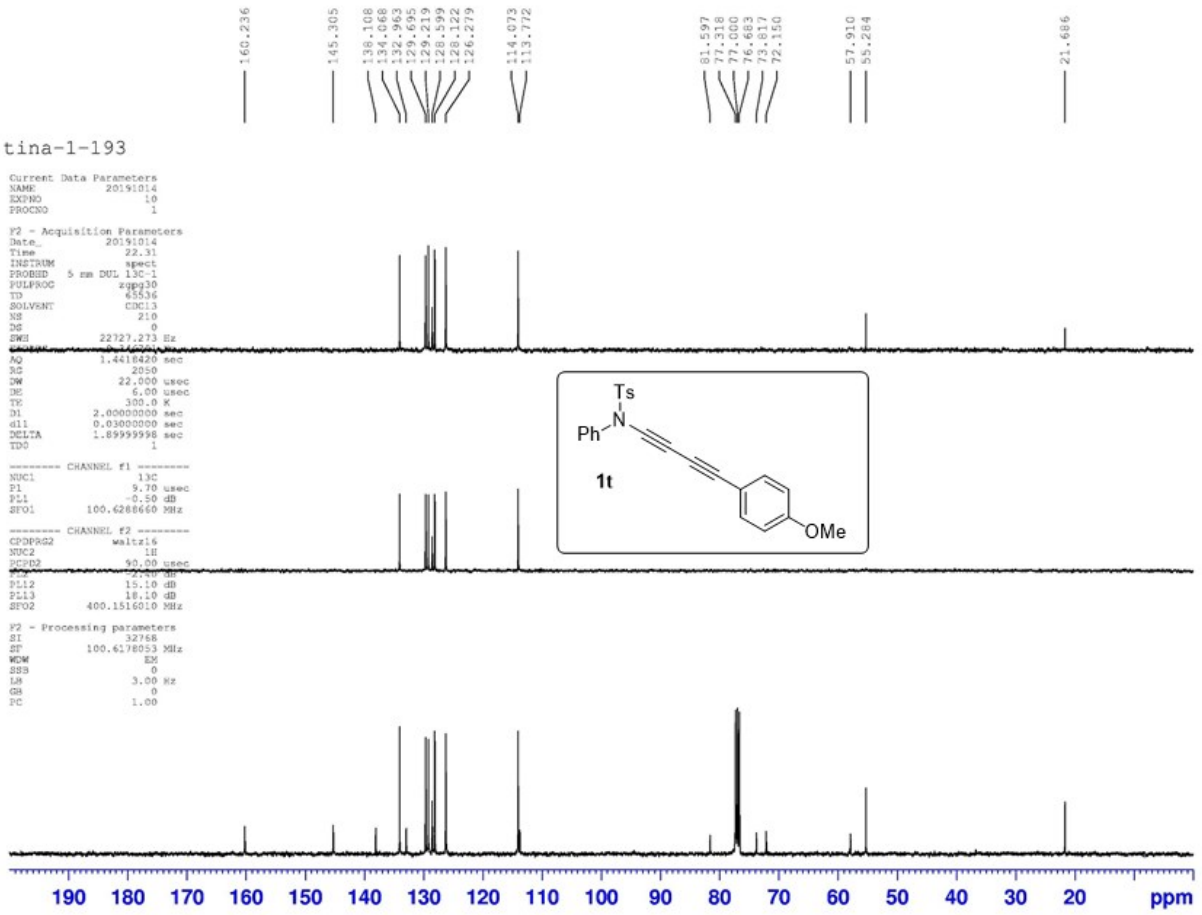

7.606
7.592
7.547
7.352
7.345
7.343
7.338
7.336
7.335
7.332
7.329
7.327
7.325
7.320
7.303
7.289
7.253
7.240
7.232
7.230
7.228
7.225
7.223
7.220
7.218
7.215
2.431
Current Data Parameters
NAME Tina-2-13
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20191224
Time 14.26
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 9541.984 Hz
FIDRES 0.291199 Hz
AQ 1.7170432 sec
RG 256
DW 52.400 usec
DE 6.50 usec
TE 295.4 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.15 usec
PL1 -1.00 dB
SFO1 598.1027304 MHz
F2 - Processing parameters
SI 32768
SF 598.1000314 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 2.00
Ts
N
Ph
1r
CF3
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
2.00
4.01
2.99
2.08
2.02
3.15

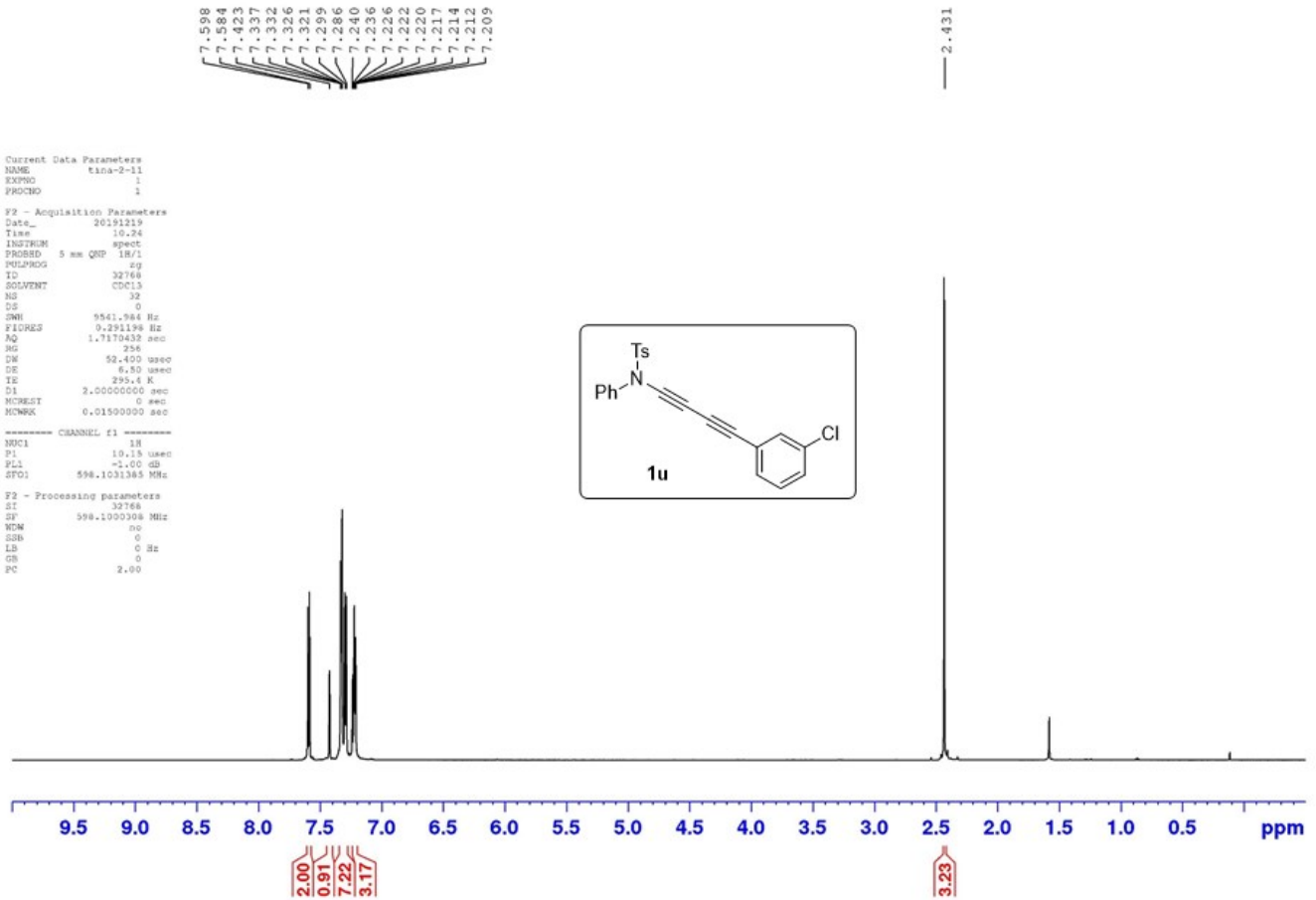

145.56
137.73
132.86
132.41
130.72
130.50
130.28
130.06
129.78
129.33
128.85
128.09
126.43
126.30
125.84
125.28
125.26
124.62
122.81
79.90
77.21
77.00
76.79
75.83
75.60
57.36
21.67
Current Data Parameters
NAME Tina-2-13
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20191224
Time 8.38
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 500
DS 0
SWH 43045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3611248 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 295.6 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
-------- CHANNEL f1 --------
NUC1 13C
P1 4.80 usec
PL1 0 dB
SFO1 150.4080927 MHz
-------- CHANNEL f2 --------
CPDPRG[2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 7.00 dB
PL13 14.00 dB
SFO2 598.1030916 MHz
F2 - Processing parameters
SI 65536
SF 150.3923788 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
Ts
N
Ph
1r
CF3
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

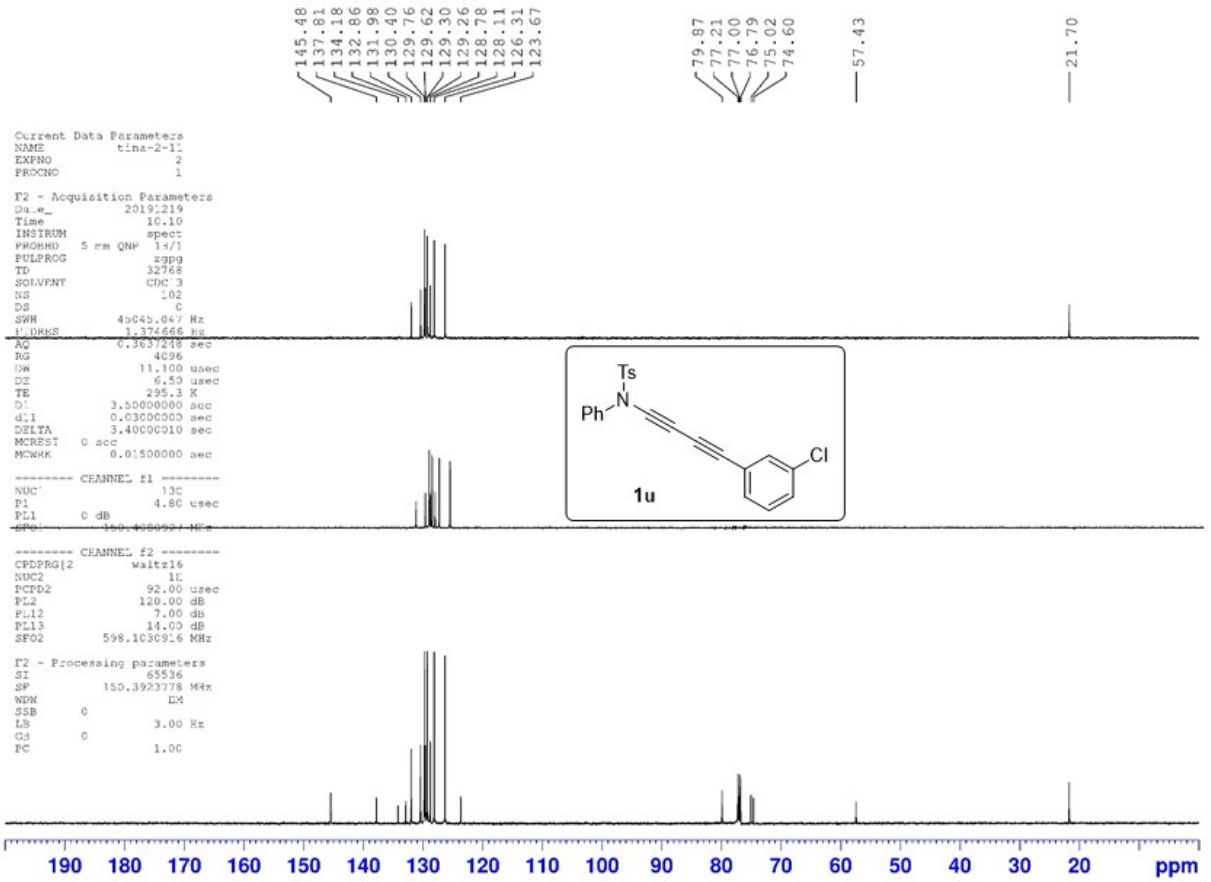

7.604
7.583
7.360
7.340
7.333
7.325
7.319
7.315
7.311
7.308
7.298
7.286
7.266
7.239
7.230
7.226
7.221
7.215
7.109
7.089
2.420
2.325
Current Data Parameters
NAME YU-11-33
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161025
Time 22.13
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 4
DS 0
SWH 6410.256 Hz
FIDRES 9.195625 Hz
AQ 2.5559039 sec
RG 71.8
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1326010 MHz
F2 - Processing parameters
SI 16384
SF 400.1300185 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00
Ts
N
Ph
1s
Me
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
2.00
9.23
2.03
3.03
3.06

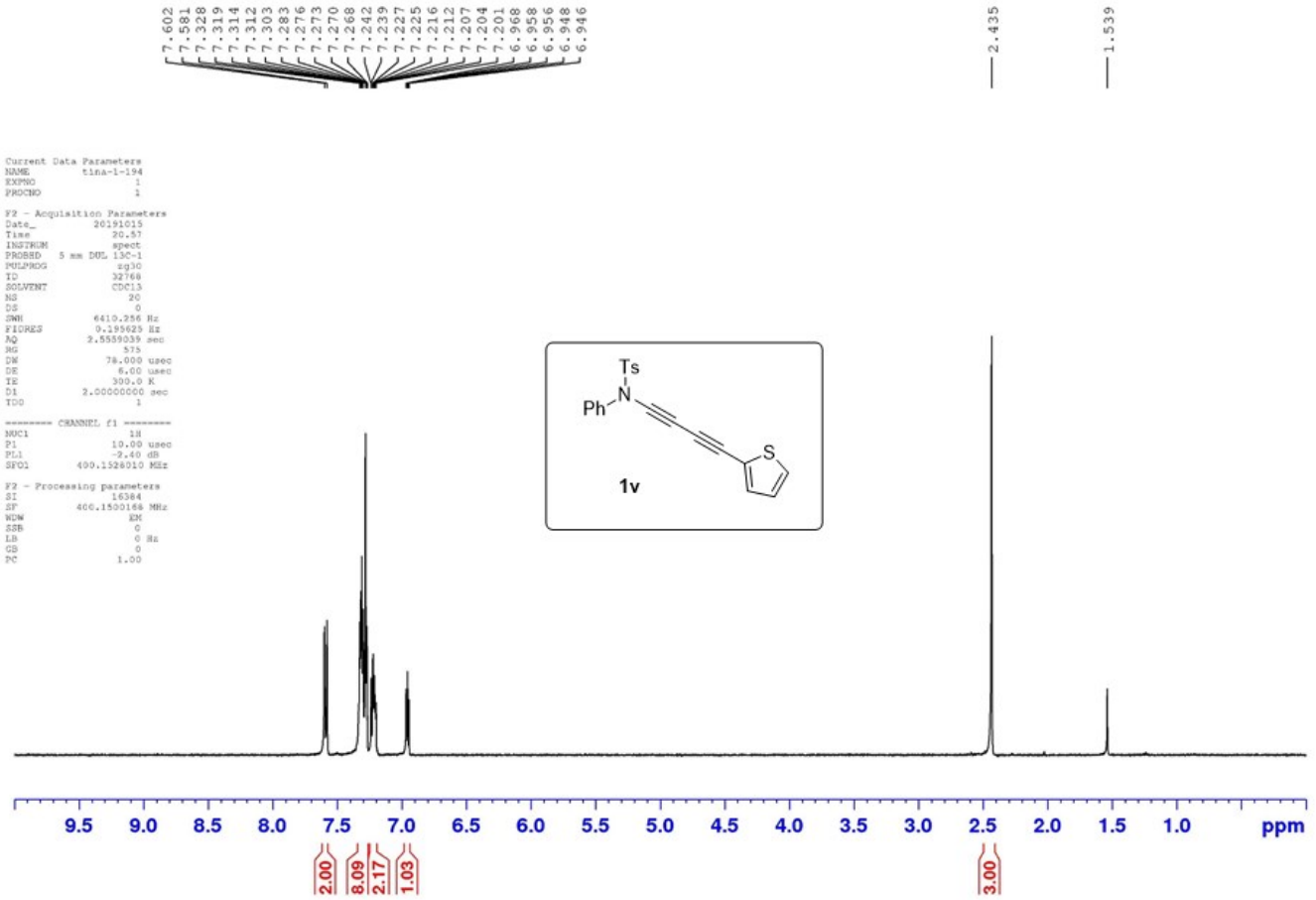

145.34
139.39
137.98
132.84
132.24
129.68
129.20
129.12
128.62
128.05
126.22
118.66
81.66
77.32
77.00
76.68
73.97
72.70
57.76
21.63
21.51
Current Data Parameters
NAME 20181026
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20181025
Time 22.14
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 46
DS 0
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4418420 sec
RG 2030
DW 22.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.70 usec
PL1 -0.50 dB
SFO1 100.6288660 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.40 dB
PL12 15.10 dB
PL13 18.10 dB
SFO2 400.1516010 MHz
F2 - Processing parameters
SI 32768
SF 100.6178120 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
Ts
N
Ph
1s
Me
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

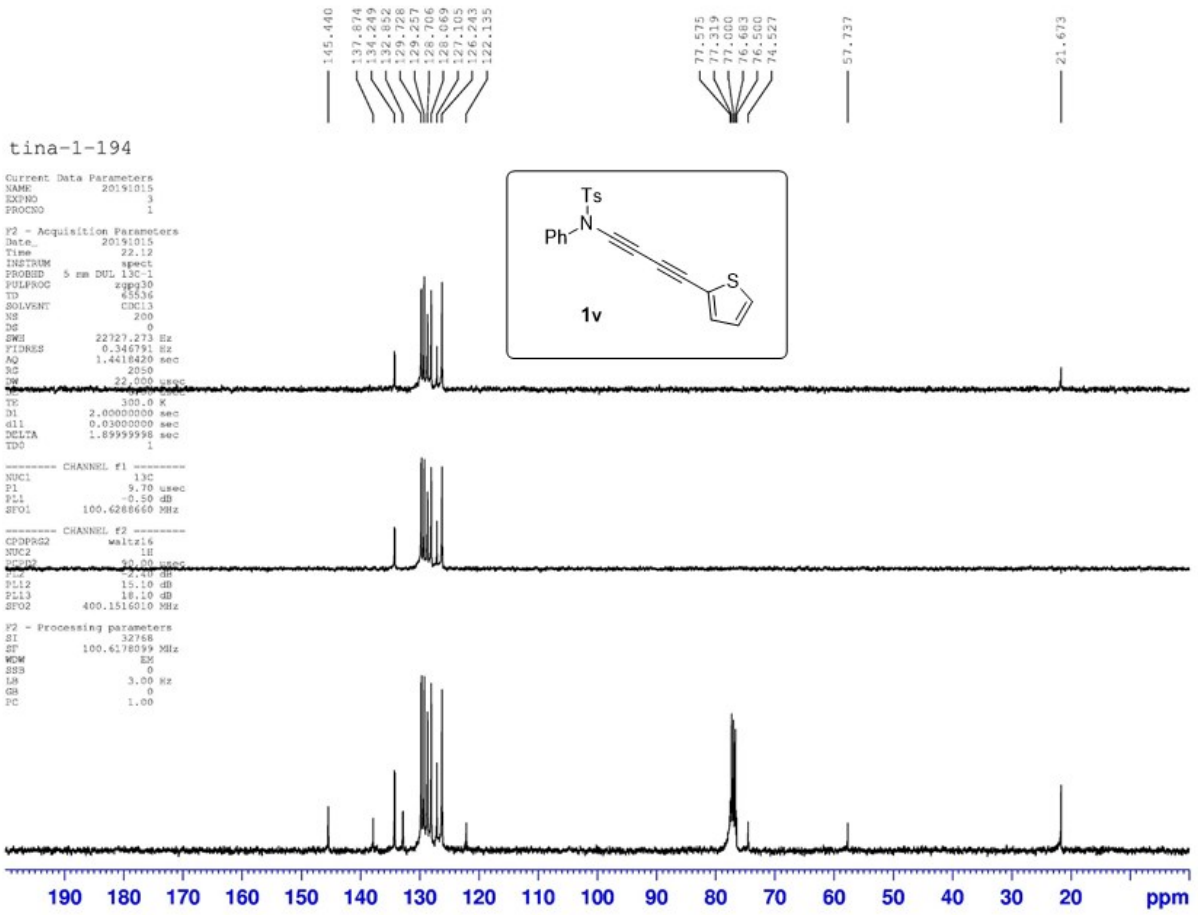

7.605
7.585
7.414
7.392
7.324
7.314
7.308
7.295
7.274
7.240
7.231
7.221
7.216
6.829
6.807
3.789
2.428
Current Data Parameters
NAME tina-1-193
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20191014
Time 22.22
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 6410.256 Hz
FIDRES 9.195625 Hz
AQ 2.5559039 sec
RG 161
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1326010 MHz
F2 - Processing parameters
SI 16384
SF 400.1300163 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00
Ts
N
Ph
1t
OMe
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
2.00
2.10
7.05
2.04
3.00
3.00

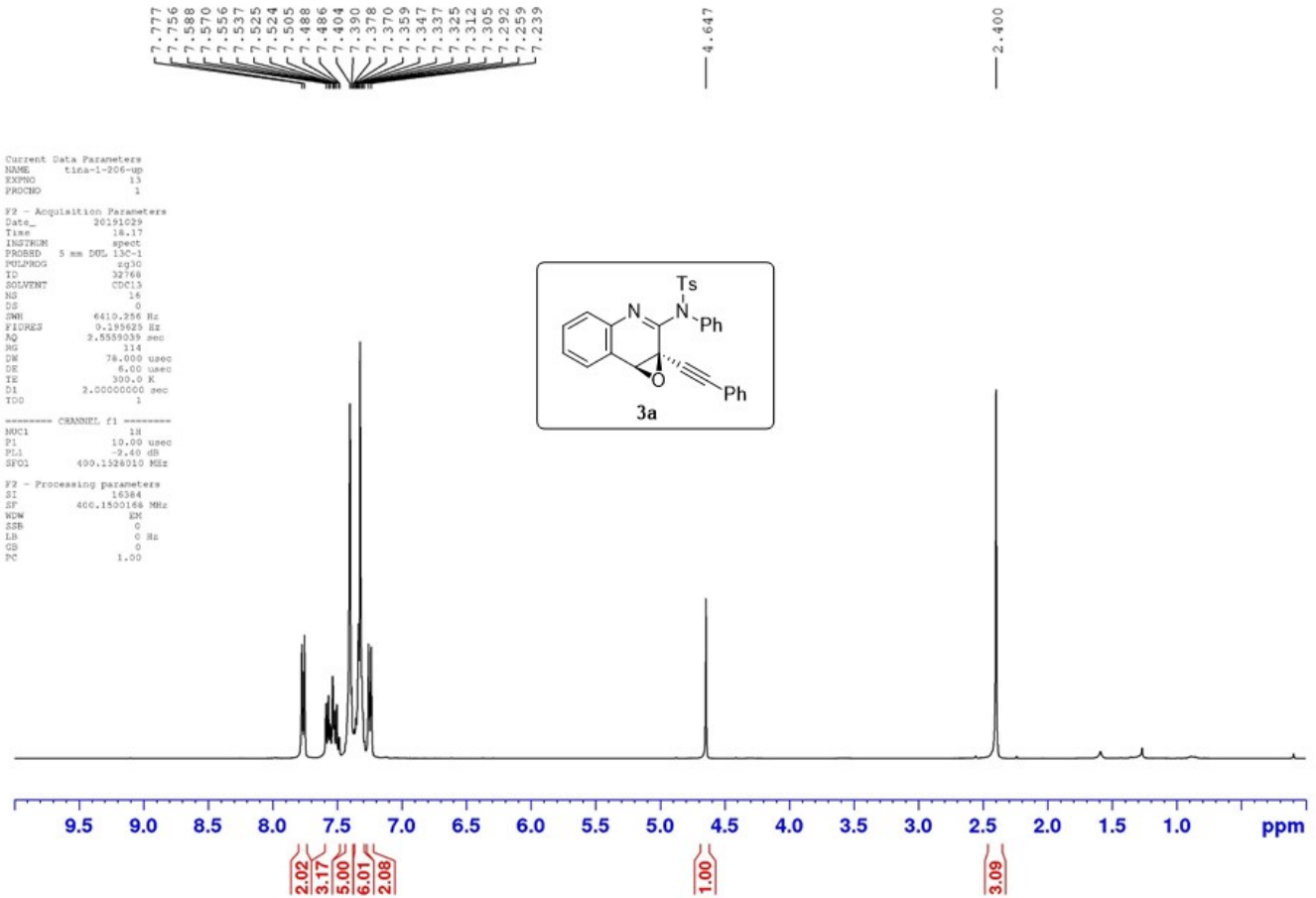

160.236
145.305
138.108
134.668
132.963
129.695
129.219
128.599
128.122
126.279
114.073
113.772
81.597
77.318
77.000
76.683
73.817
72.150
57.910
55.264
21.686
tina-1-193
Current Data Parameters
NAME 20191014
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20191014
Time 22.31
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 210
DS 0
SWH 22727.273 Hz
AQ 1.4418420 sec
RG 2050
DW 22.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.70 usec
PL1 -0.50 dB
SFO1 100.6288660 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL12 15.10 dB
PL13 18.10 dB
SFO2 400.1516010 MHz
F2 - Processing parameters
SI 32768
SF 100.6178053 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
Ts
N
Ph
1t
OMe
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

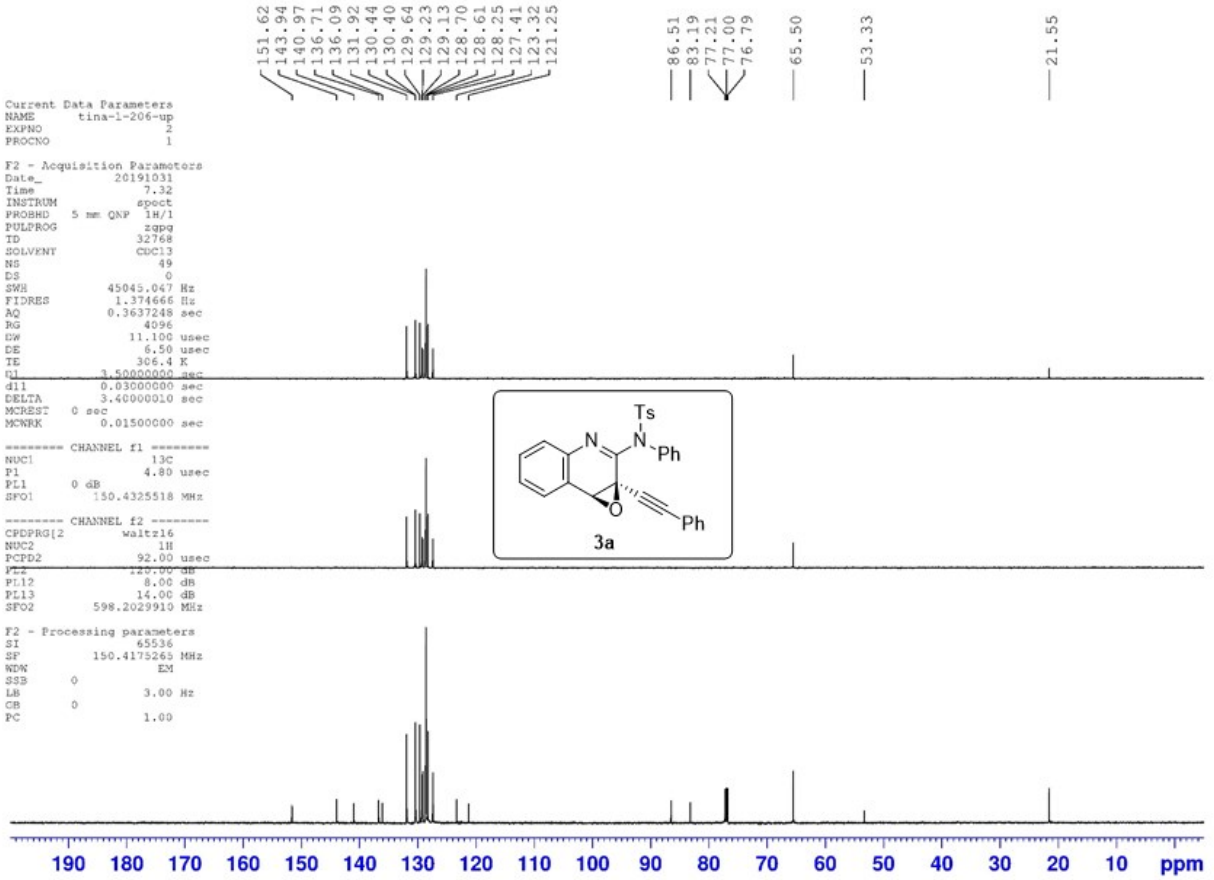

7.598
7.584
7.423
7.337
7.332
7.326
7.321
7.299
7.286
7.240
7.236
7.226
7.222
7.220
7.217
7.214
7.212
7.209
2.431
Current Data Parameters
NAME tina-2-11
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20191219
Time 10.24
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 9541.984 Hz
FIDRES 0.291199 Hz
AQ 1.7170432 sec
RG 256
DW 52.400 usec
DE 6.50 usec
TE 295.4 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.15 usec
PL1 -1.00 dB
SFO1 598.1031385 MHz
F2 - Processing parameters
SI 32768
SF 598.1000308 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 2.00
Ts
N
Ph
Cl
1u
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
2.00
0.91
7.22
3.17
3.23

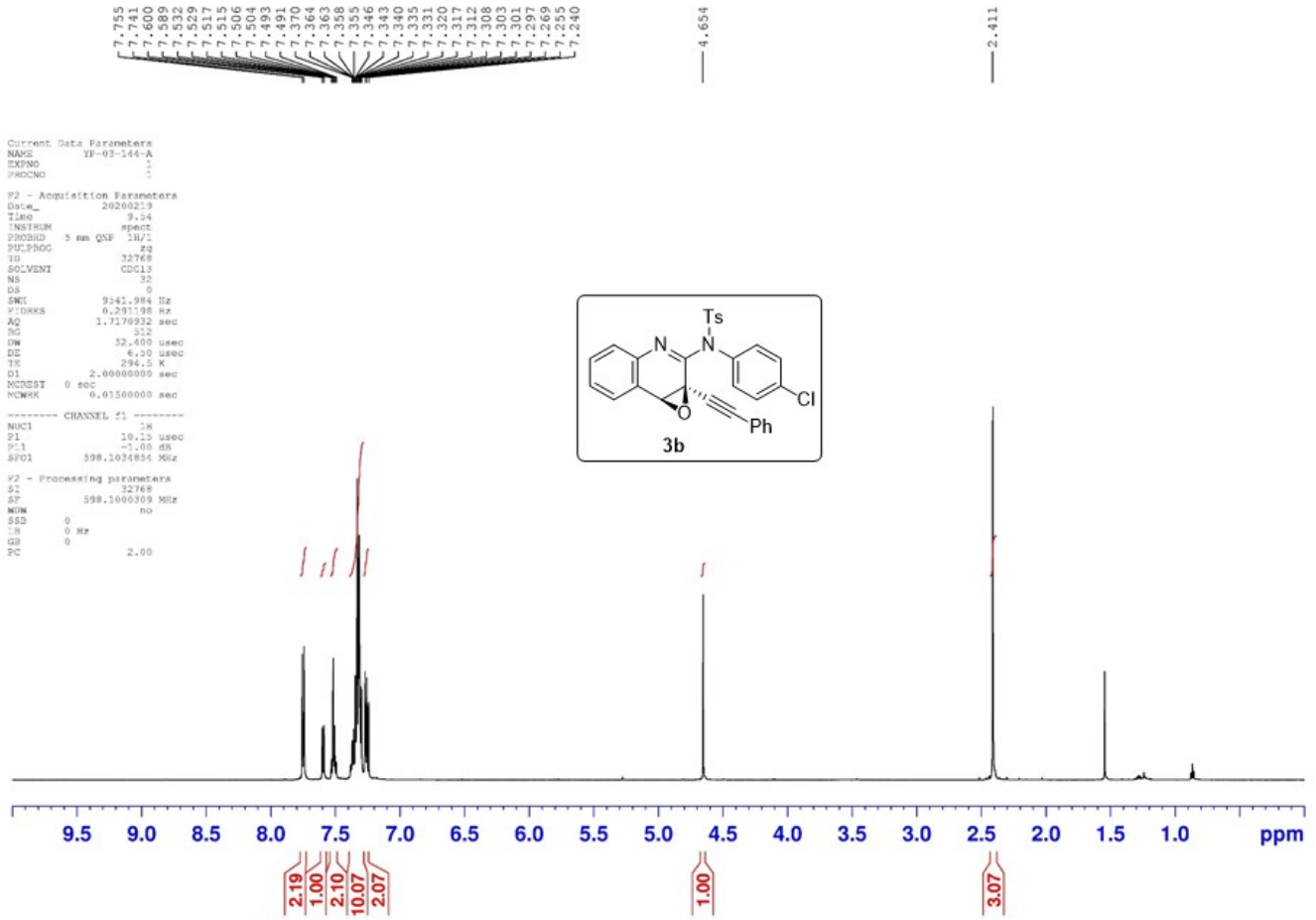

145.48
137.81
134.18
132.86
131.98
130.40
129.76
129.62
129.30
129.26
128.78
128.11
126.31
123.67
79.87
77.21
77.00
76.79
75.02
74.60
57.43
21.70
Current Data Parameters
NAME tina-2-11
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20191219
Time 10.10
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 102
DS 0
SWH 49645.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637248 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 295.3 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
-------- CHANNEL f1 --------
NUC1 13C
P1 4.80 usec
PL1 0 dB
SFO1 150.4060924 MHz
-------- CHANNEL f2 --------
CPDPRG[2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 7.00 dB
PL13 14.00 dB
SFO2 598.1030916 MHz
F2 - Processing parameters
SI 65536
SF 150.3923778 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
Ts
N
Ph
Cl
1u
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

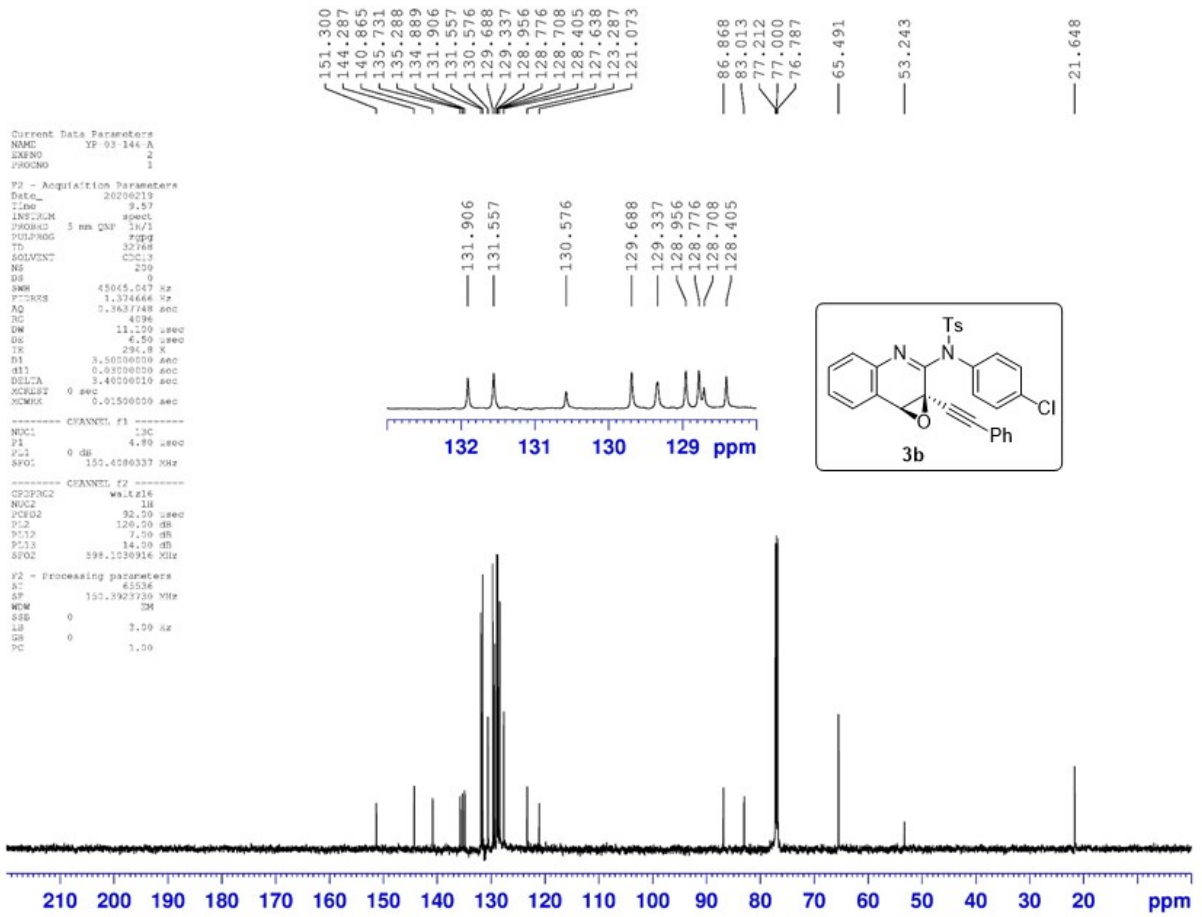

7.602
7.581
7.328
7.319
7.314
7.312
7.303
7.283
7.276
7.273
7.270
7.268
7.242
7.239
7.227
7.225
7.216
7.212
7.207
7.204
7.201
6.968
6.958
6.956
6.948
6.946
2.435
1.539
Current Data Parameters
NAME tina-1-194
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20191015
Time 20.57
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 20
DS 0
SWH 6410.256 Hz
FIDRES 9.195625 Hz
AQ 2.5559039 sec
RG 575
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1324010 MHz
F2 - Processing parameters
SI 16384
SF 400.1300164 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00
Ts
N
Ph
S
1v
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
2.00
8.09
2.17
1.03
3.00

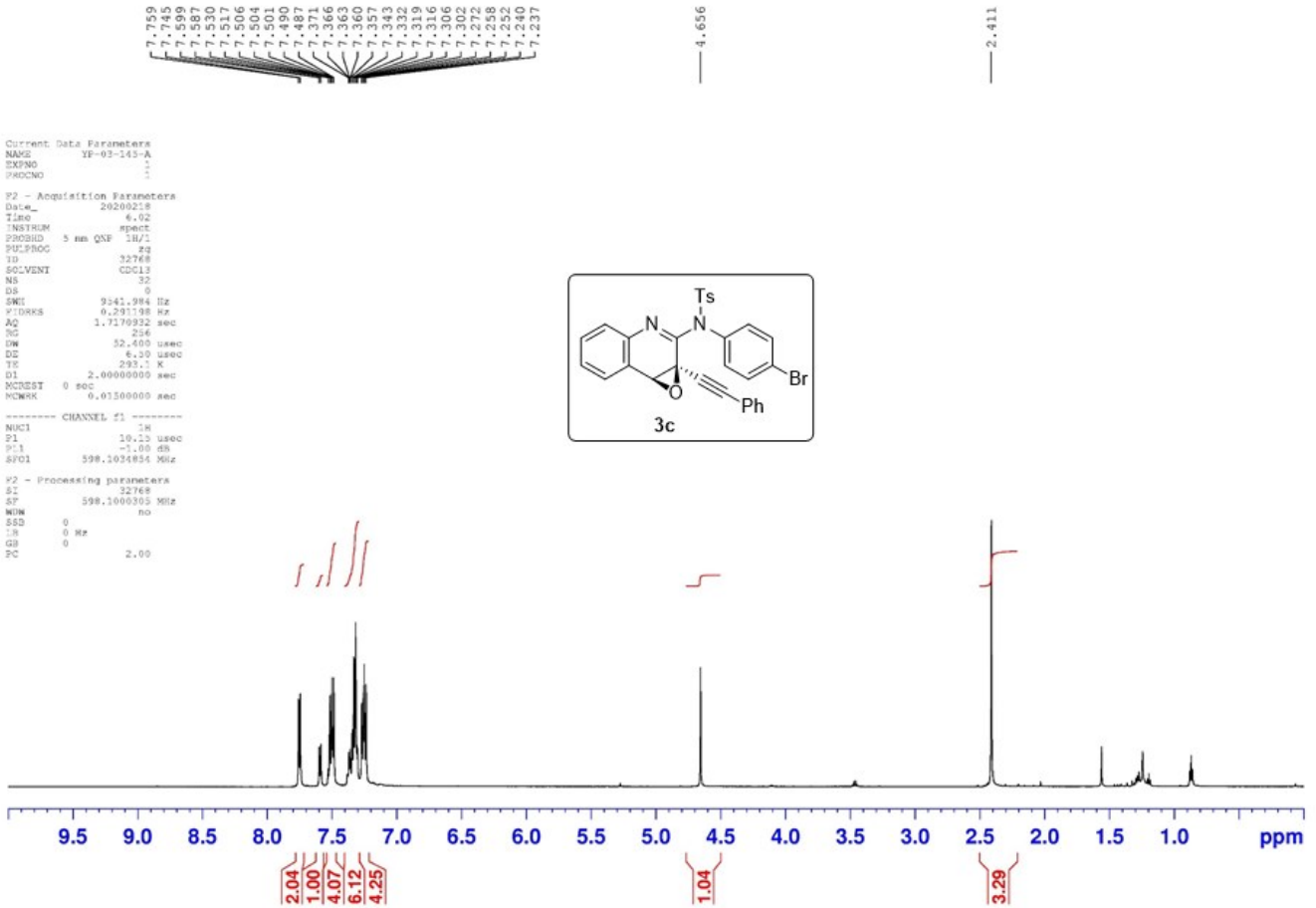

145.440
137.874
134.249
132.852
129.728
129.257
128.706
128.069
127.105
126.243
122.135
77.575
77.319
77.000
76.683
76.500
74.527
57.737
21.673
tina-1-194
Current Data Parameters
NAME 20191015
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20191015
Time 22.12
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 200
DS 0
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4418420 sec
RG 2050
DW 22.000 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.70 usec
PL1 -0.50 dB
SFO1 100.6288660 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD 80.00 usec
PL2 -1.00 dB
PL12 15.10 dB
PL13 18.10 dB
SFO2 400.1516010 MHz
F2 - Processing parameters
SI 32768
SF 100.6178099 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
Ts
N
Ph
S
1v
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

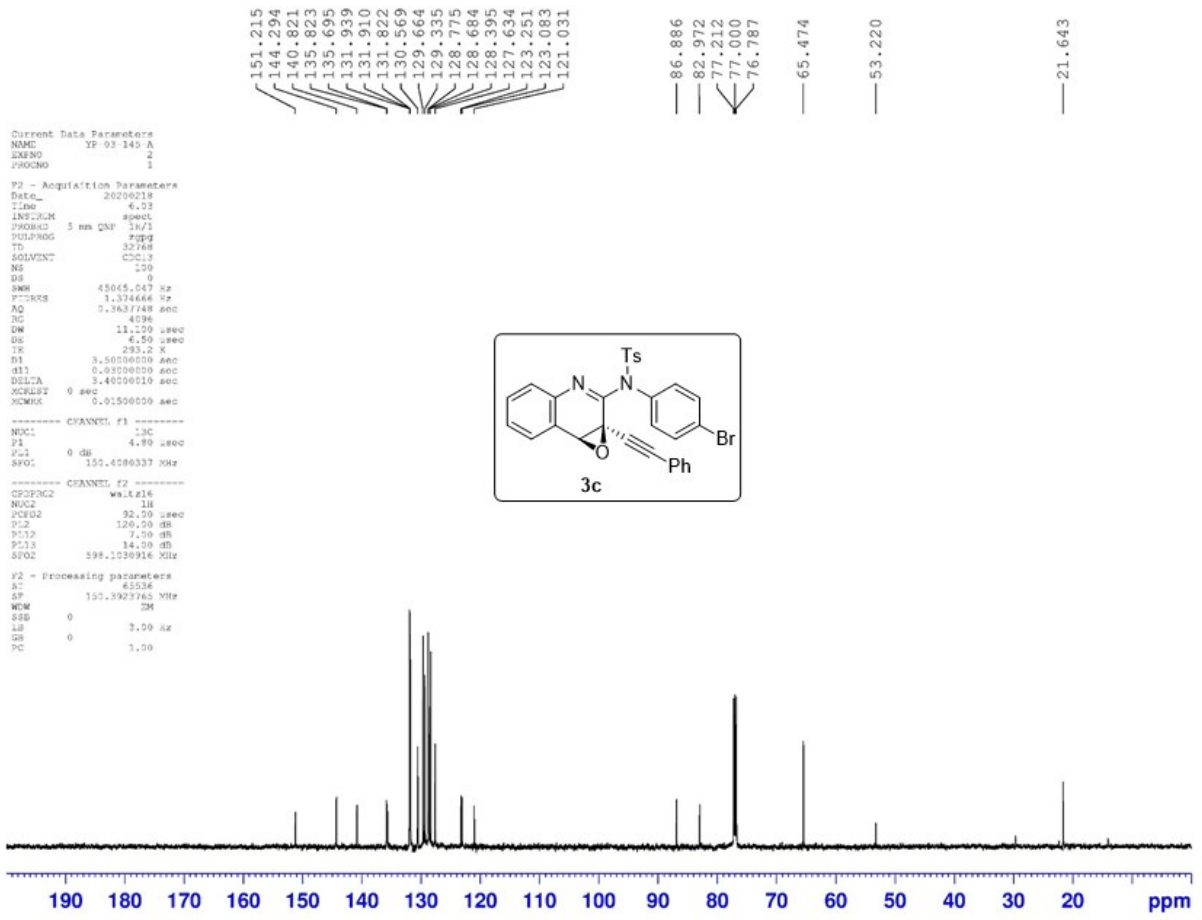

7.777
7.756
7.688
7.570
7.556
7.537
7.525
7.524
7.505
7.488
7.486
7.404
7.390
7.378
7.370
7.359
7.347
7.337
7.325
7.312
7.305
7.292
7.259
7.239
4.647
2.400
Current Data Parameters
NAME tina-1-206-up
EXPNO 13
PROCNO 1
F2 - Acquisition Parameters
Date_ 20191029
Time 18.17
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 6410.256 Hz
FIDRES 9.195625 Hz
AQ 2.5559039 sec
RG 114
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1326010 MHz
F2 - Processing parameters
SI 16384
SF 400.1300164 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00
Ts
N
N
Ph
O
Ph
3a
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
2.02
3.17
5.00
6.01
2.08
1.00
3.09


151.62
143.94
140.97
136.71
136.09
131.92
130.44
130.40
129.64
129.23
129.13
128.70
128.61
128.25
127.41
123.32
121.25
86.51
83.19
77.21
77.00
76.79
65.50
53.33
21.55
Current Data Parameters
NAME tina-1-206-up
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20191031
Time 7.32
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 49
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637248 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 306.4 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0 dB
SFO1 150.4325518 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 8.00 dB
PL13 14.00 dB
SFO2 598.2029910 MHz
F2 - Processing parameters
SI 65536
SF 150.4175265 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
Ts
N
N
Ph
O
Ph
3a
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


7.755
7.741
7.600
7.589
7.532
7.529
7.517
7.515
7.506
7.504
7.493
7.491
7.370
7.364
7.363
7.358
7.355
7.346
7.343
7.340
7.335
7.331
7.320
7.317
7.312
7.308
7.303
7.301
7.297
7.269
7.255
7.240
4.654
2.411
Current Data Parameters
NAME YF-03-144-A
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200219
Time 9.04
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 9541.984 Hz
FIDRES 0.291198 Hz
AQ 1.7170932 sec
RG 512
DW 52.400 usec
DE 6.50 usec
TE 294.5 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
-------- CHANNEL f1 --------
NUC1 1H
P1 10.15 usec
PL1 -1.00 dB
SFO1 598.1034834 MHz
F2 - Processing parameters
SI 32768
SF 598.1000309 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 2.00
Ts
N
N
Cl
O
Ph
3b
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
2.19
1.00
2.10
10.07
2.07
1.00
3.07


151.300
144.287
140.865
135.731
135.288
134.889
131.906
131.557
130.576
129.688
129.337
128.956
128.776
128.708
128.405
127.638
123.287
121.073
86.868
83.013
77.212
77.000
76.787
65.491
53.243
21.648
131.906
131.557
130.576
129.688
129.337
128.956
128.776
128.708
128.405
132
131
130
129
ppm
Ts
N
N
Cl
O
Ph
3b
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


7.759
7.745
7.599
7.587
7.530
7.517
7.506
7.504
7.501
7.490
7.487
7.371
7.366
7.363
7.360
7.357
7.343
7.332
7.319
7.316
7.306
7.302
7.272
7.258
7.252
7.240
7.237
4.656
2.411
Current Data Parameters
NAME YF-03-145-A
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200218
Time 6.02
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 9541.984 Hz
FIDRES 0.291198 Hz
AQ 1.7170932 sec
RG 256
DW 52.400 usec
DE 6.50 usec
TE 293.1 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
-------- CHANNEL f1 --------
NUC1 1H
P1 10.15 usec
PL1 -1.00 dB
SFO1 598.1034834 MHz
F2 - Processing parameters
SI 32768
SF 598.1000305 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 2.00
Ts
N
N
Br
O
Ph
3c
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
2.04
1.00
4.07
6.12
4.25
1.04
3.29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144.294
140.821
135.823
135.695
131.939
131.910
131.822
130.569
129.664
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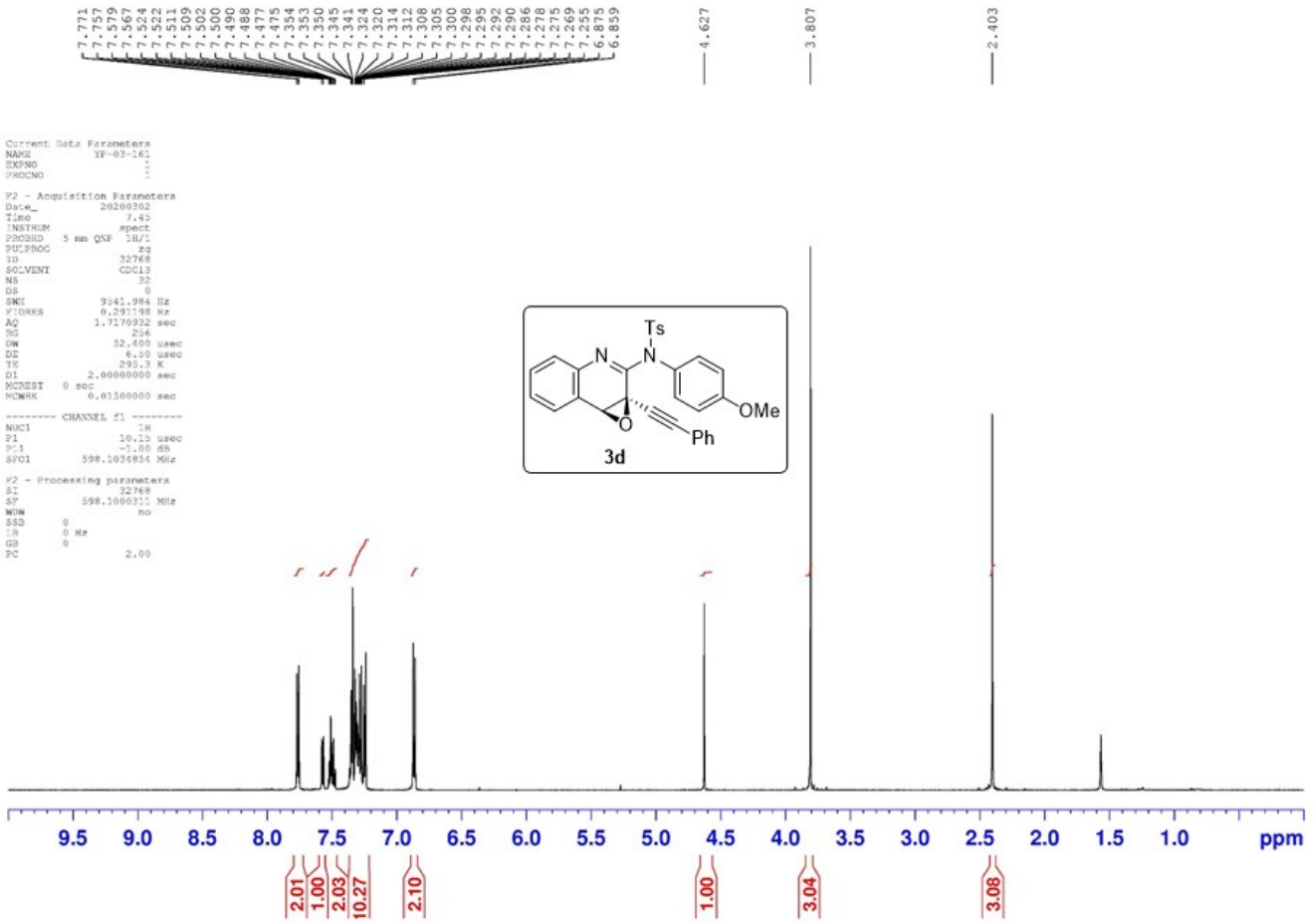
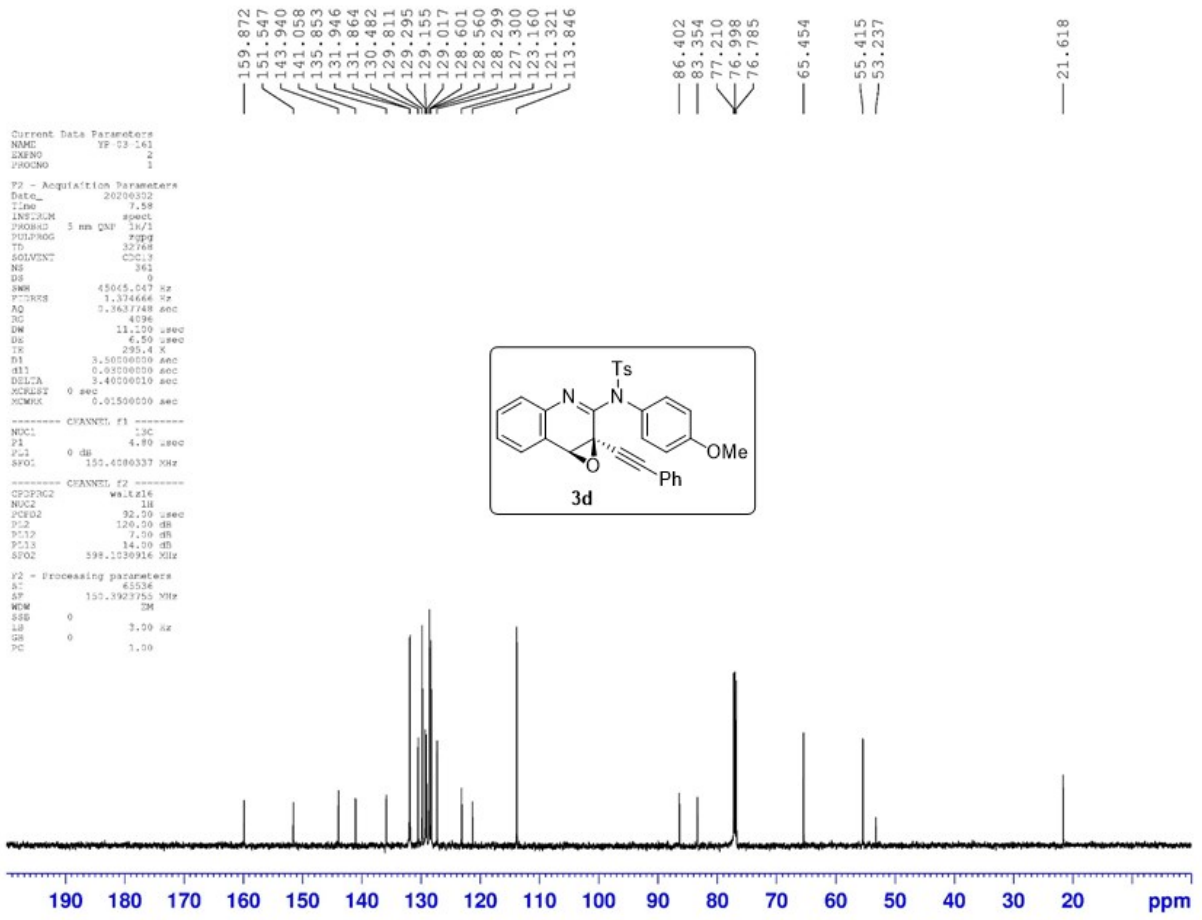
128.775
128.684
128.395
127.634
123.251
123.083
121.031
86.886
82.972
77.212
77.000
76.787
65.474
53.220
21.643
Ts
N
N
O
Br
Ph
3c
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


7.771
7.757
7.579
7.567
7.524
7.522
7.511
7.509
7.502
7.500
7.490
7.488
7.477
7.475
7.354
7.353
7.350
7.345
7.341
7.324
7.320
7.314
7.312
7.308
7.305
7.300
7.298
7.295
7.292
7.290
7.286
7.278
7.275
7.269
7.255
6.875
6.859
4.627
3.807
2.403
Current Data Parameters
NAME YF-03-161
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200302
Time 7.45
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 9541.984 Hz
FIDRES 0.291198 Hz
AQ 1.7170932 sec
RG 256
DW 52.400 usec
DE 6.50 usec
TE 293.3 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
-------- CHANNEL f1 --------
NUC1 1H
P1 10.15 usec
PL1 -1.00 dB
SFO1 598.1034854 MHz
F2 - Processing parameters
SI 32768
SF 598.1000311 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 2.00
Ts
N
N
O
OMe
Ph
3d
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
2.01
1.00
2.03
10.27
2.10
1.00
3.04
3.08


159.872
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143.940
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135.853
131.946
131.864
130.482
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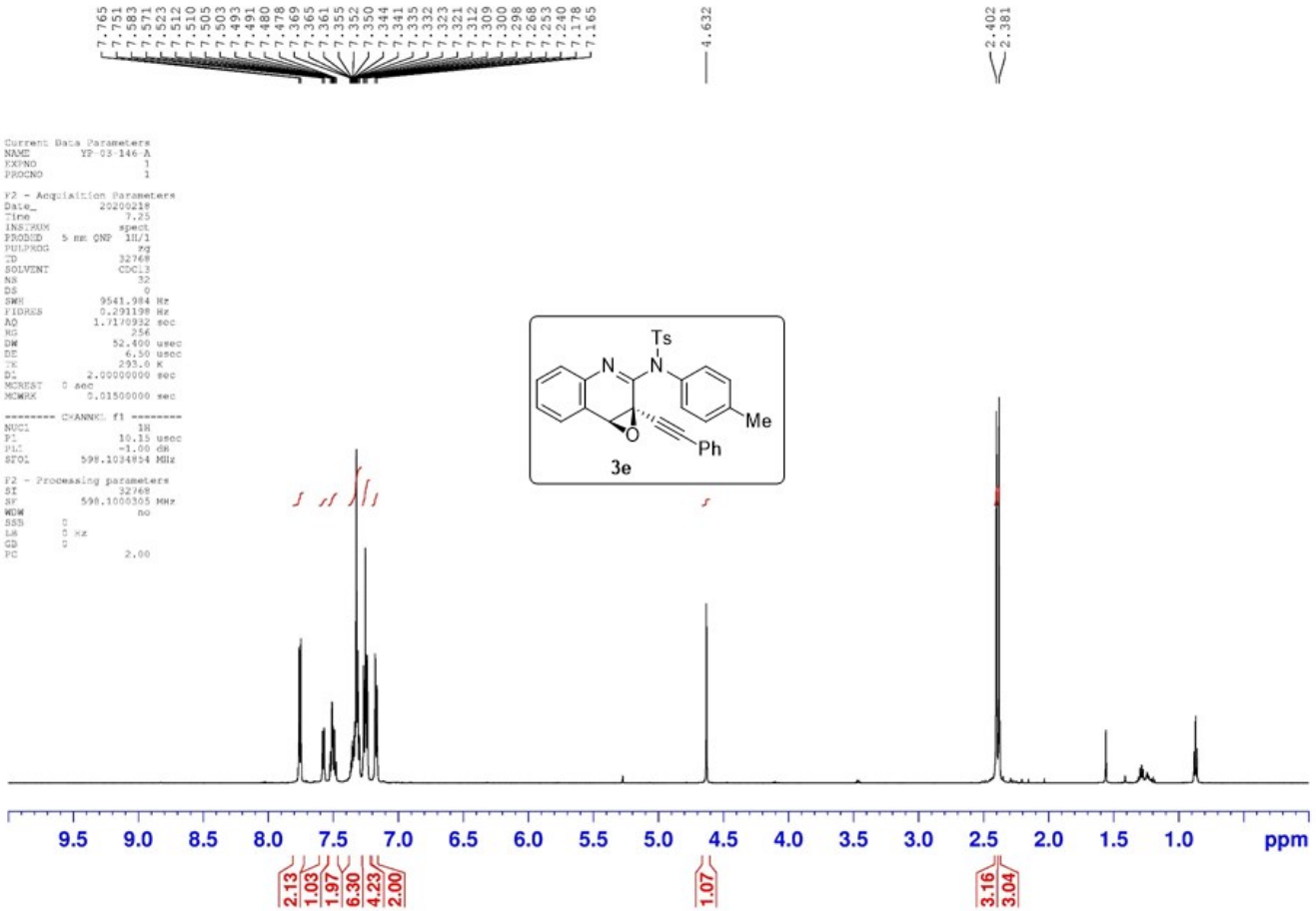
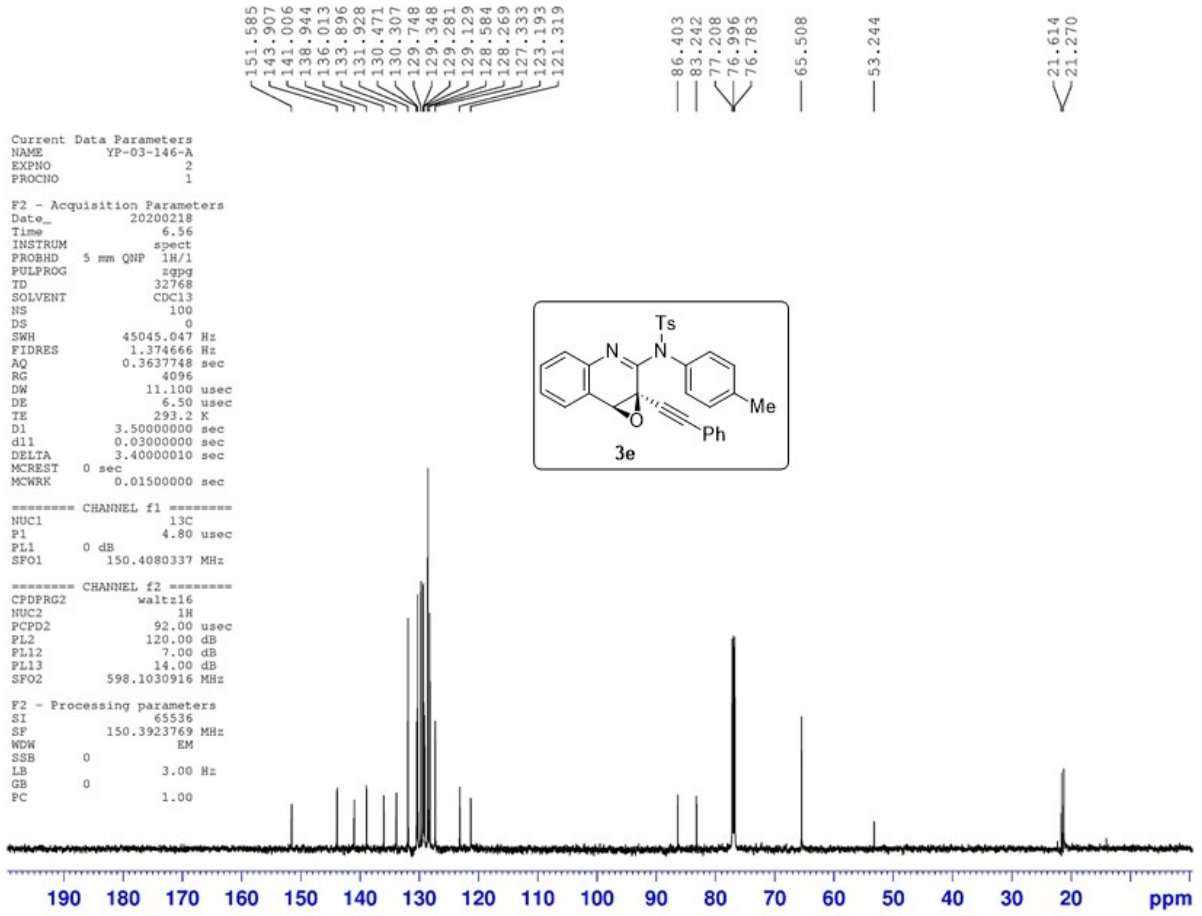
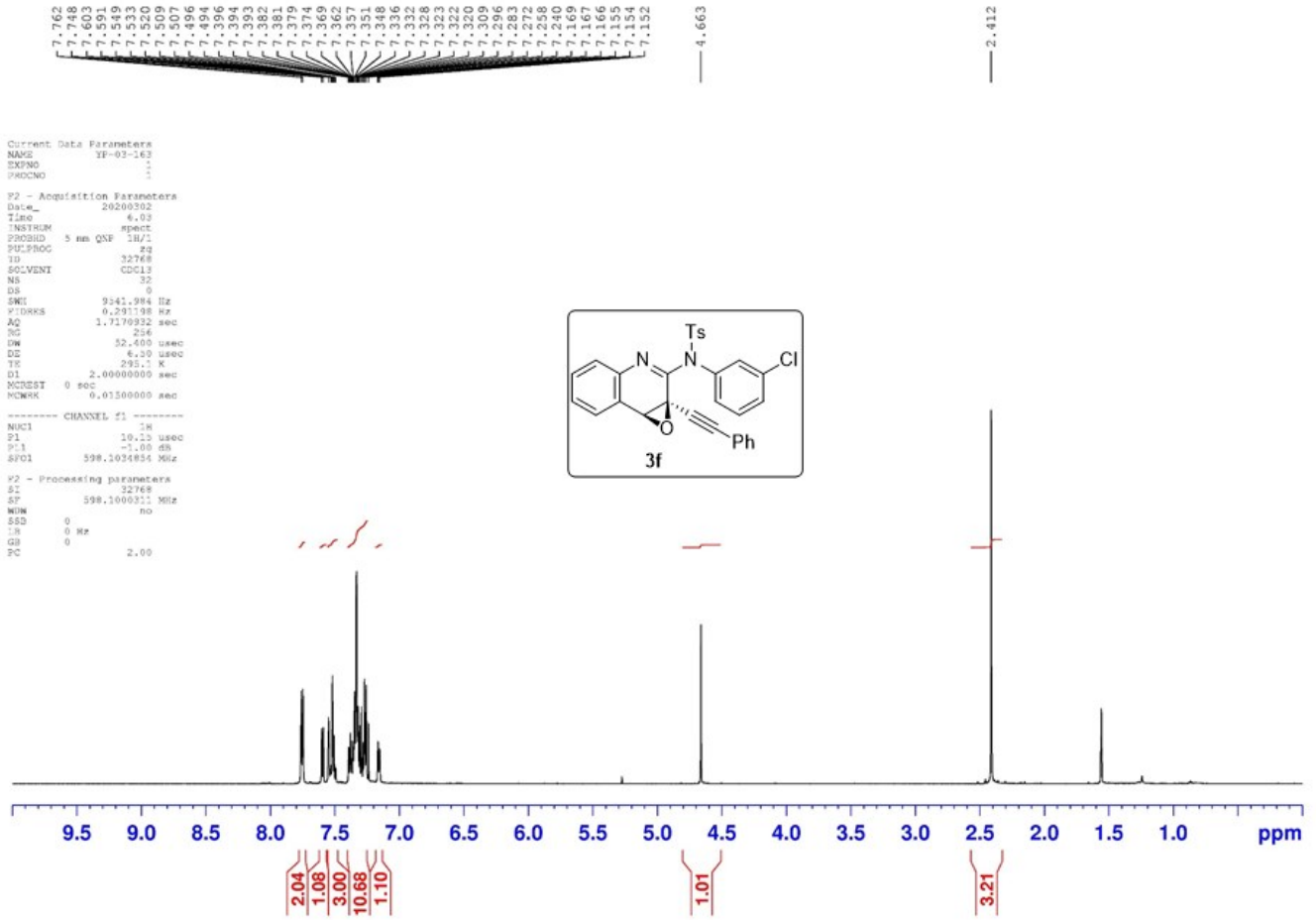
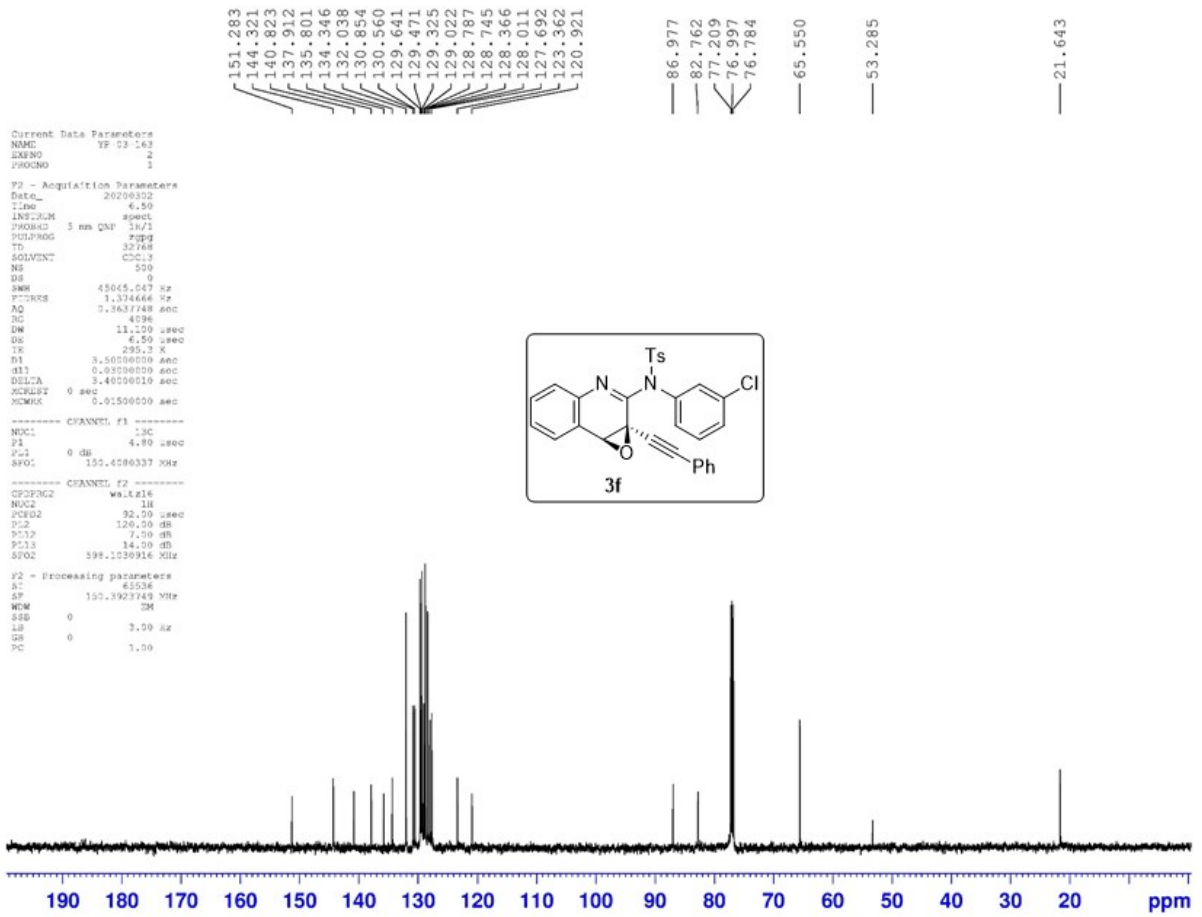
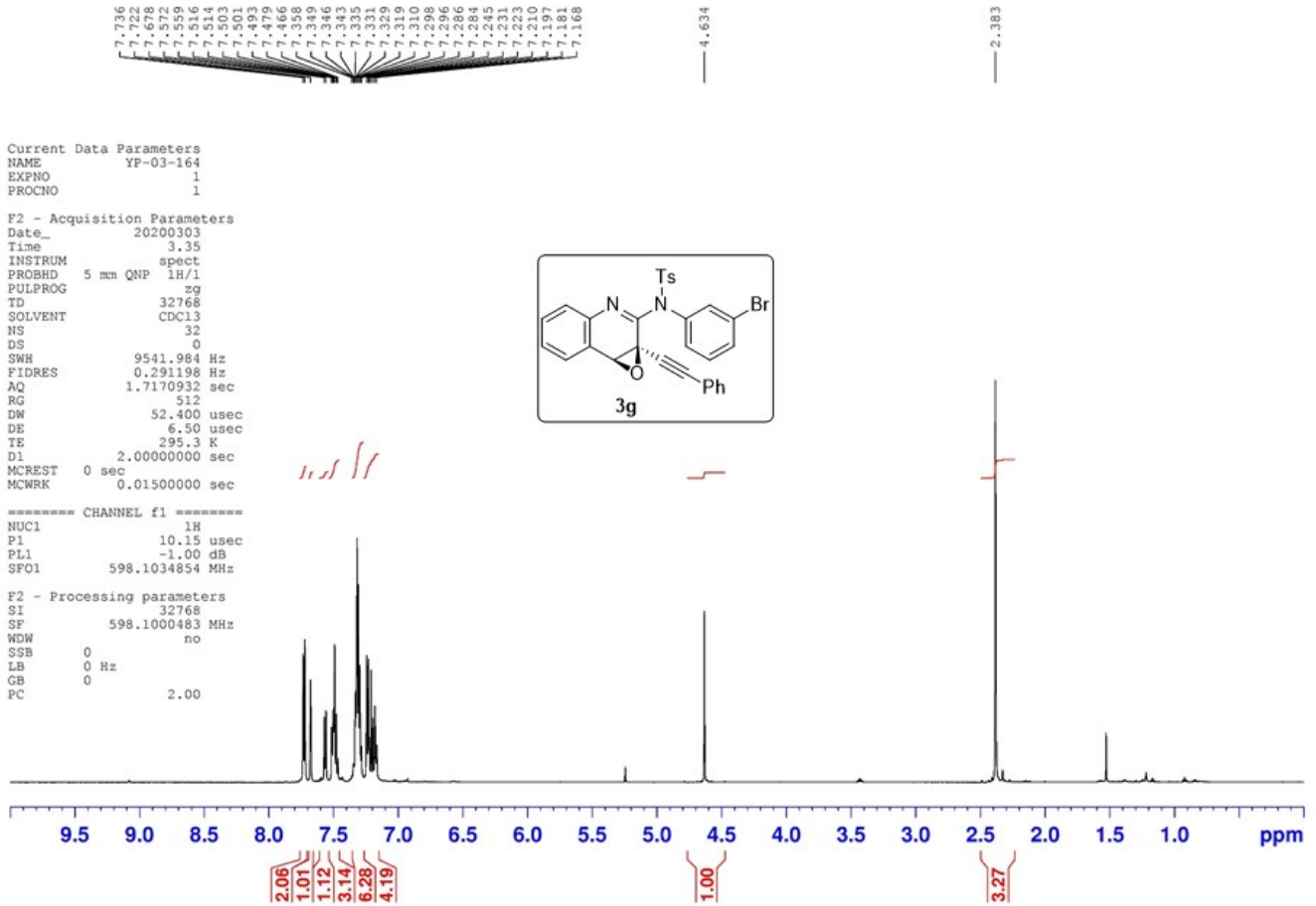
129.295
129.155
129.017
128.601
128.560
128.299
127.300
123.160
121.321
113.846
86.402
83.354
77.210
76.998
76.785
65.454
55.415
53.237
21.618
Current Data Parameters
NAME YF-03-161
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200302
Time 7.58
INSTRUM spect
PROBHD 5 mm CNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 361
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 295.4 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
-------- CHANNEL f1 --------
NUC1 13C
P1 4.80 usec
PL1 0 dB
SFO1 150.4080337 MHz
-------- CHANNEL f2 --------
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.20 usec
PL2 120.00 dB
PL12 7.00 dB
PL13 14.00 dB
SFO2 599.1030916 MHz
F2 - Processing parameters
SI 65536
SF 150.3923755 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
Ts
N
N
OMe
O
Ph
3d
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

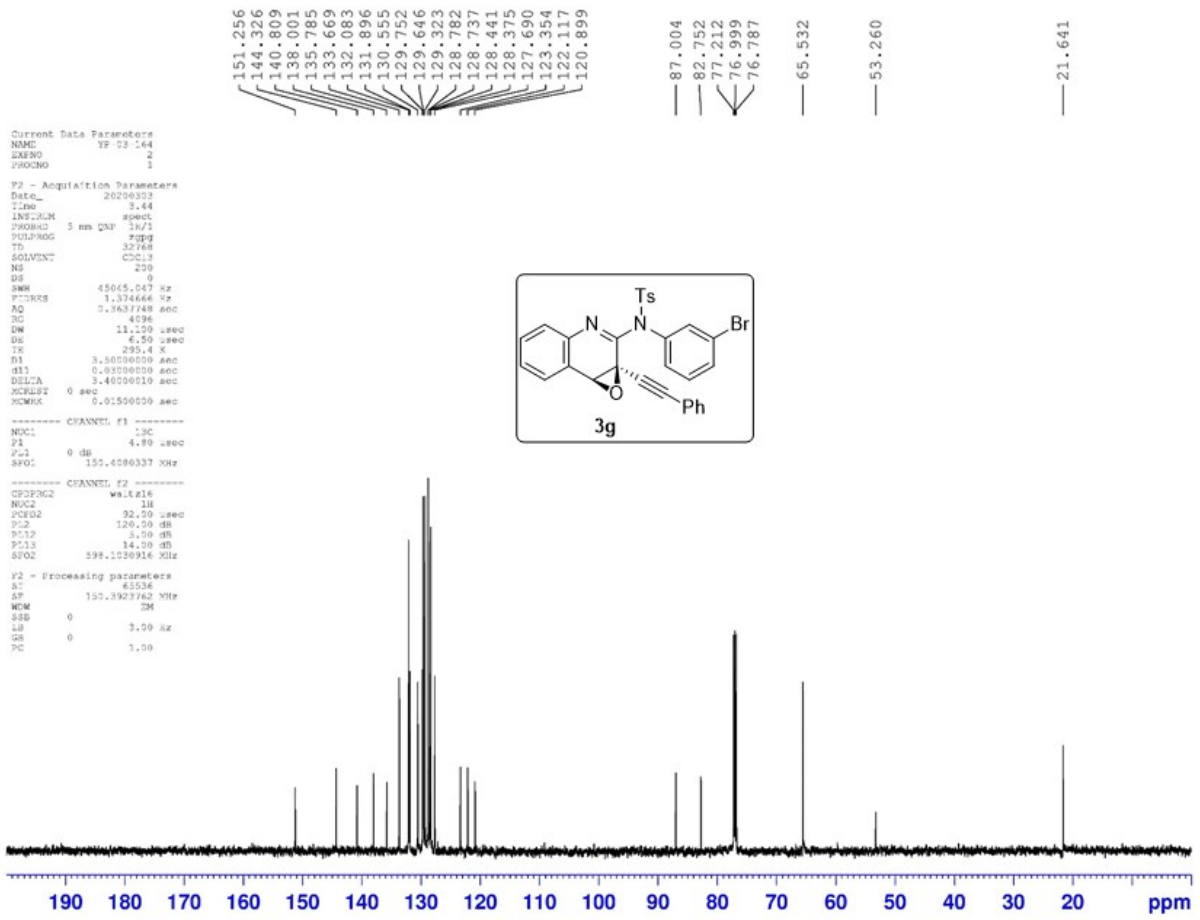

7.765
7.751
7.583
7.571
7.523
7.512
7.510
7.505
7.503
7.493
7.491
7.480
7.478
7.369
7.365
7.361
7.355
7.352
7.350
7.344
7.341
7.335
7.332
7.323
7.321
7.312
7.309
7.300
7.298
7.268
7.253
7.240
7.178
7.165
4.632
2.402
2.381
Current Data Parameters
NAME YP-03-146-A
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200218
Time 7.25
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 9541.984 Hz
FIDRES 0.291198 Hz
AQ 1.7170932 sec
RG 256
DW 52.400 usec
DE 6.50 usec
TE 293.0 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
-------- CHANNEL f1 --------
NUC1 1H
P1 10.15 usec
PL1 -1.00 dB
SFO1 598.1034854 MHz
F2 - Processing parameters
SI 32768
SF 598.1000305 MHz
WDW no
SSB 0
LB 0.30 Hz
GB 0
PC 2.00
Ts
N
N
O
Me
Ph
3e
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
2.13
1.03
1.97
6.30
4.23
2.00
1.07
3.16
3.04

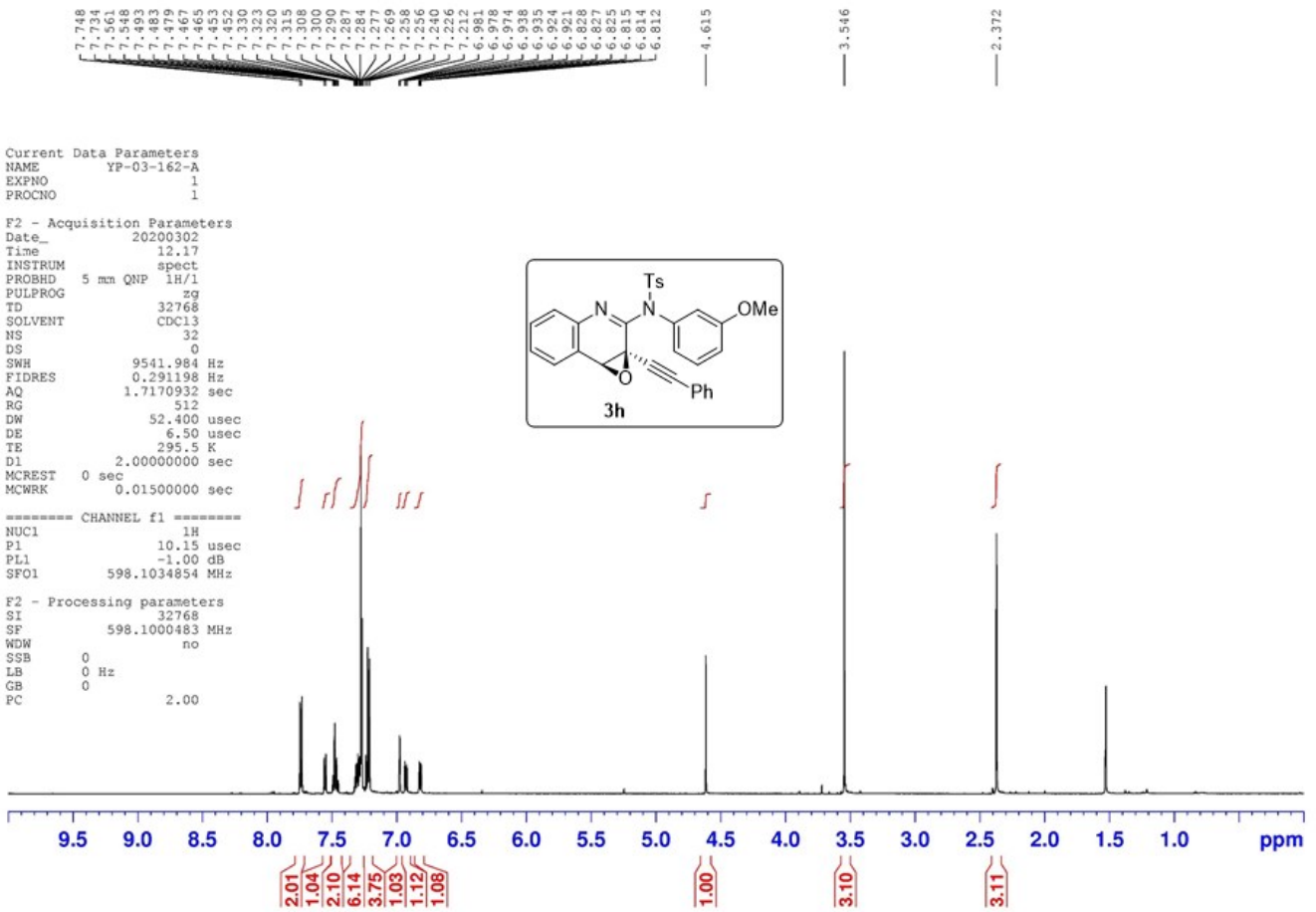

151.585
143.907
141.006
138.944
136.013
133.896
131.928
130.471
130.307
129.748
129.348
129.281
129.129
128.584
128.269
127.333
123.193
121.319
86.403
83.242
77.208
76.996
76.783
65.508
53.244
21.614
21.270
Current Data Parameters
NAME YP-03-146-A
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200218
Time 6.56
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 100
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 293.2 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0 dB
SFO1 150.4080337 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 7.00 dB
PL13 14.00 dB
SFO2 598.1030916 MHz
F2 - Processing parameters
SI 65536
SF 150.3923769 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
Ts
N
N
O
Me
Ph
3e
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

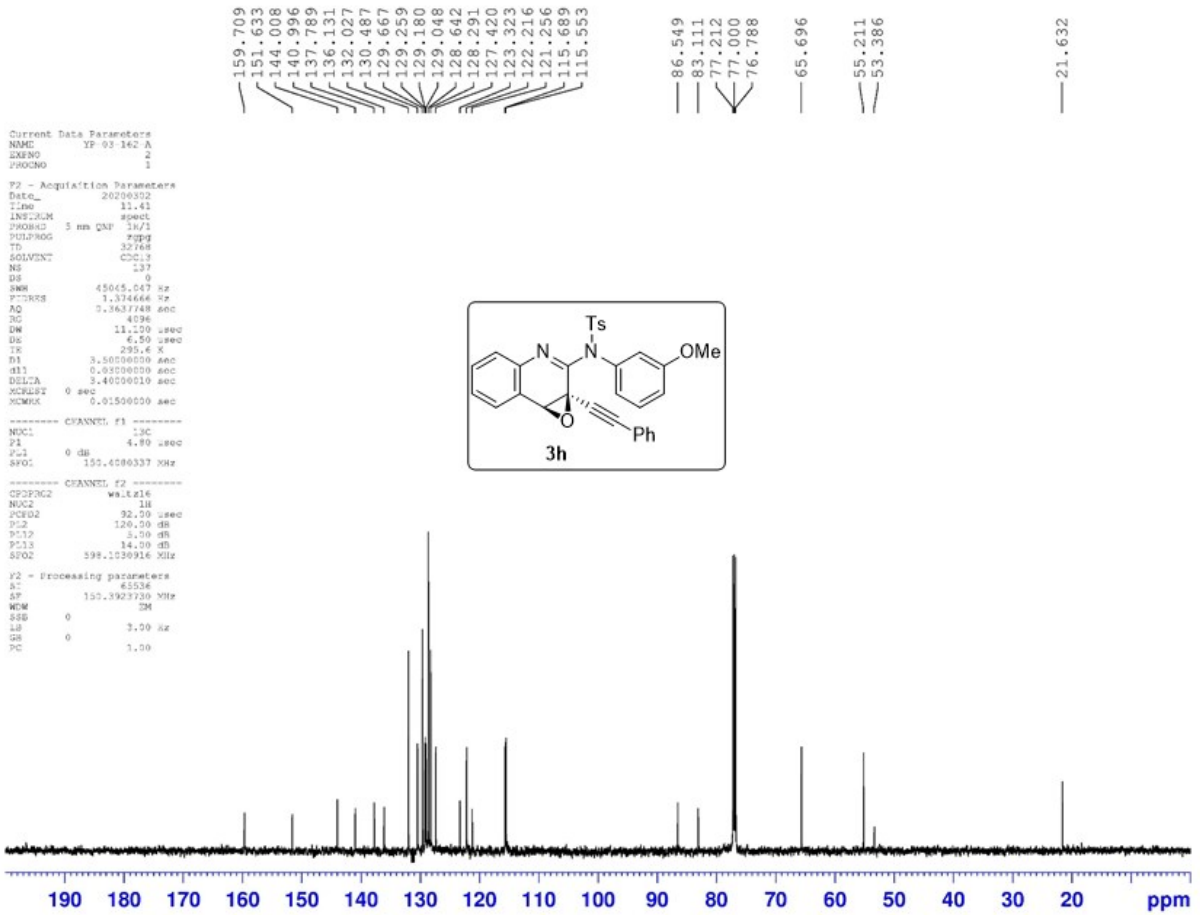

7.762
7.748
7.603
7.591
7.549
7.533
7.520
7.509
7.507
7.496
7.494
7.396
7.394
7.393
7.382
7.381
7.379
7.374
7.369
7.362
7.357
7.351
7.348
7.336
7.332
7.328
7.323
7.322
7.320
7.309
7.296
7.283
7.272
7.258
7.240
7.169
7.167
7.166
7.155
7.154
7.152
4.663
2.412
Current Data Parameters
NAME YF-03-163
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200302
Time 6.03
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 9541.984 Hz
FIDRES 0.291198 Hz
AQ 1.7170932 sec
RG 256
DW 52.400 usec
DE 6.50 usec
TE 295.1 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
-------- CHANNEL f1 --------
NUC1 1H
P1 10.15 usec
PL1 -1.00 dB
SFO1 598.1034834 MHz
F2 - Processing parameters
SI 32768
SF 598.1000311 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 2.00
Ts
N
N
Cl
O
Ph
3f
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
2.04
1.08
3.00
10.68
1.10
1.01
3.21

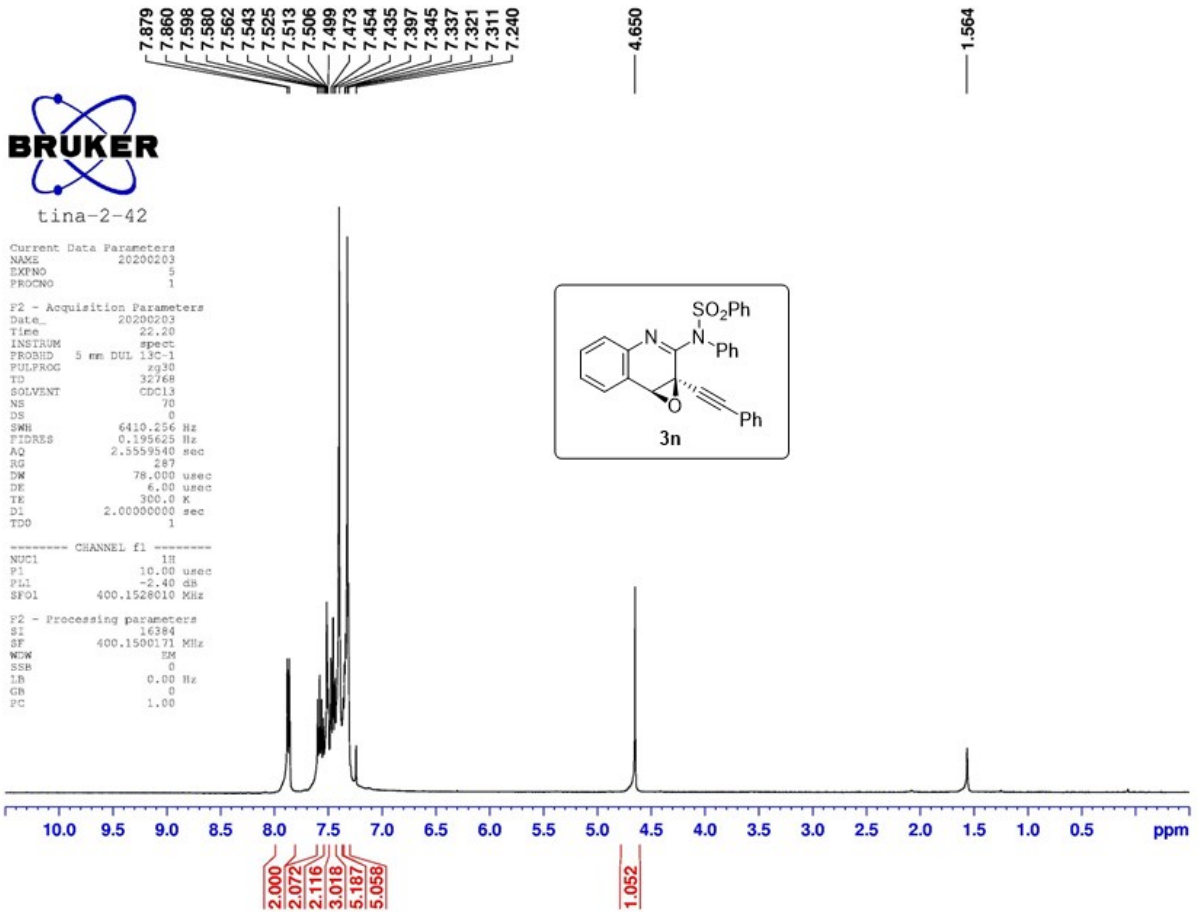

151.283
144.321
140.823
137.912
135.801
134.346
132.038
130.854
130.560
129.641
129.471
129.325
129.022
128.787
128.745
128.366
128.011
127.692
123.362
120.921
86.977
82.762
77.209
76.997
76.784
65.550
53.285
21.643
Ts
N
N
Cl
O
Ph
3f
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

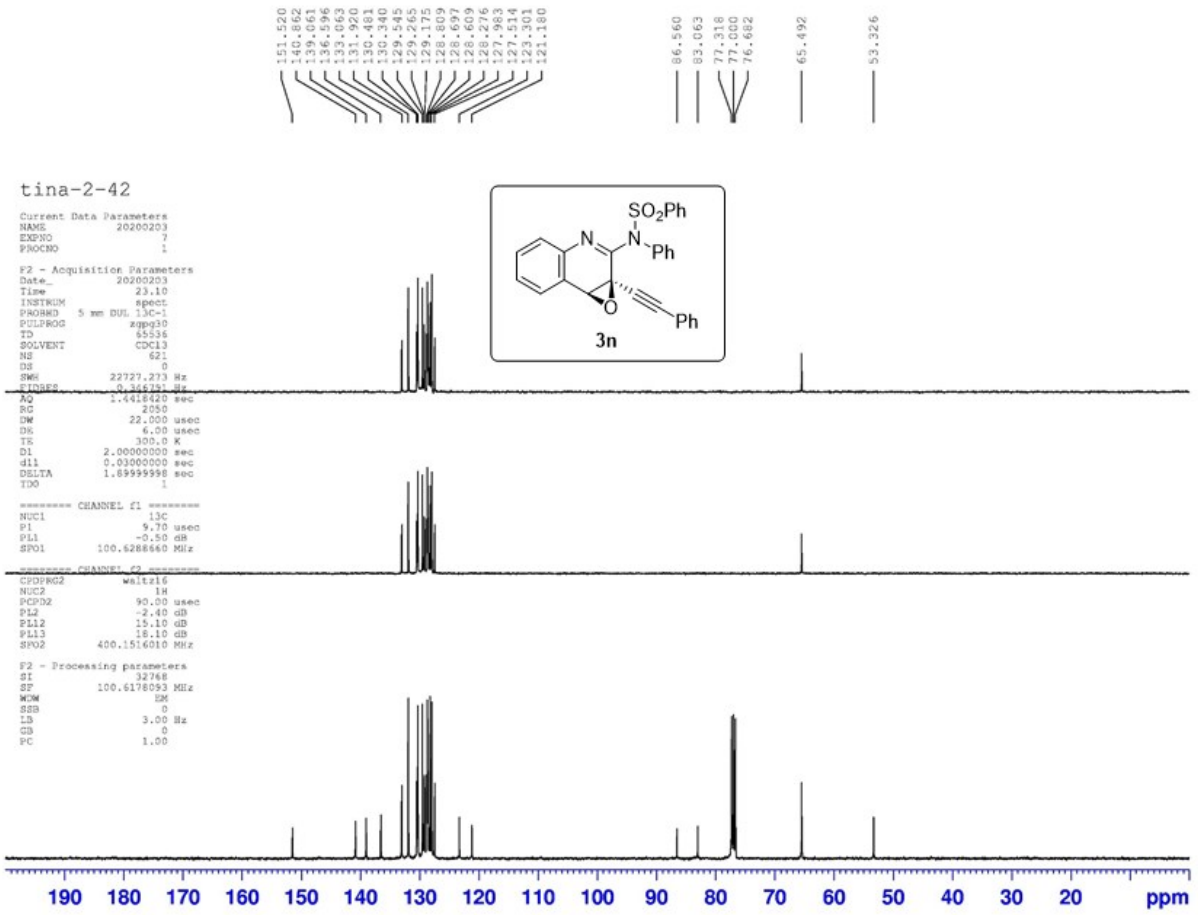

7.736
7.722
7.678
7.572
7.559
7.516
7.514
7.503
7.501
7.493
7.479
7.466
7.358
7.349
7.346
7.343
7.335
7.331
7.329
7.319
7.310
7.298
7.296
7.286
7.284
7.245
7.231
7.223
7.210
7.197
7.181
7.168
4.634
2.383
Current Data Parameters
NAME YP-03-164
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200303
Time 3.35
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 9541.984 Hz
FIDRES 0.291198 Hz
AQ 1.7170932 sec
RG 512
DW 52.400 usec
DE 6.50 usec
TE 295.3 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.15 usec
PL1 -1.00 dB
SFO1 598.1034854 MHz
F2 - Processing parameters
SI 32768
SF 598.1000483 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 2.00
Ts
N
N
Br
O
Ph
3g
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
2.06
1.01
1.12
3.14
6.28
4.19
1.00
3.27

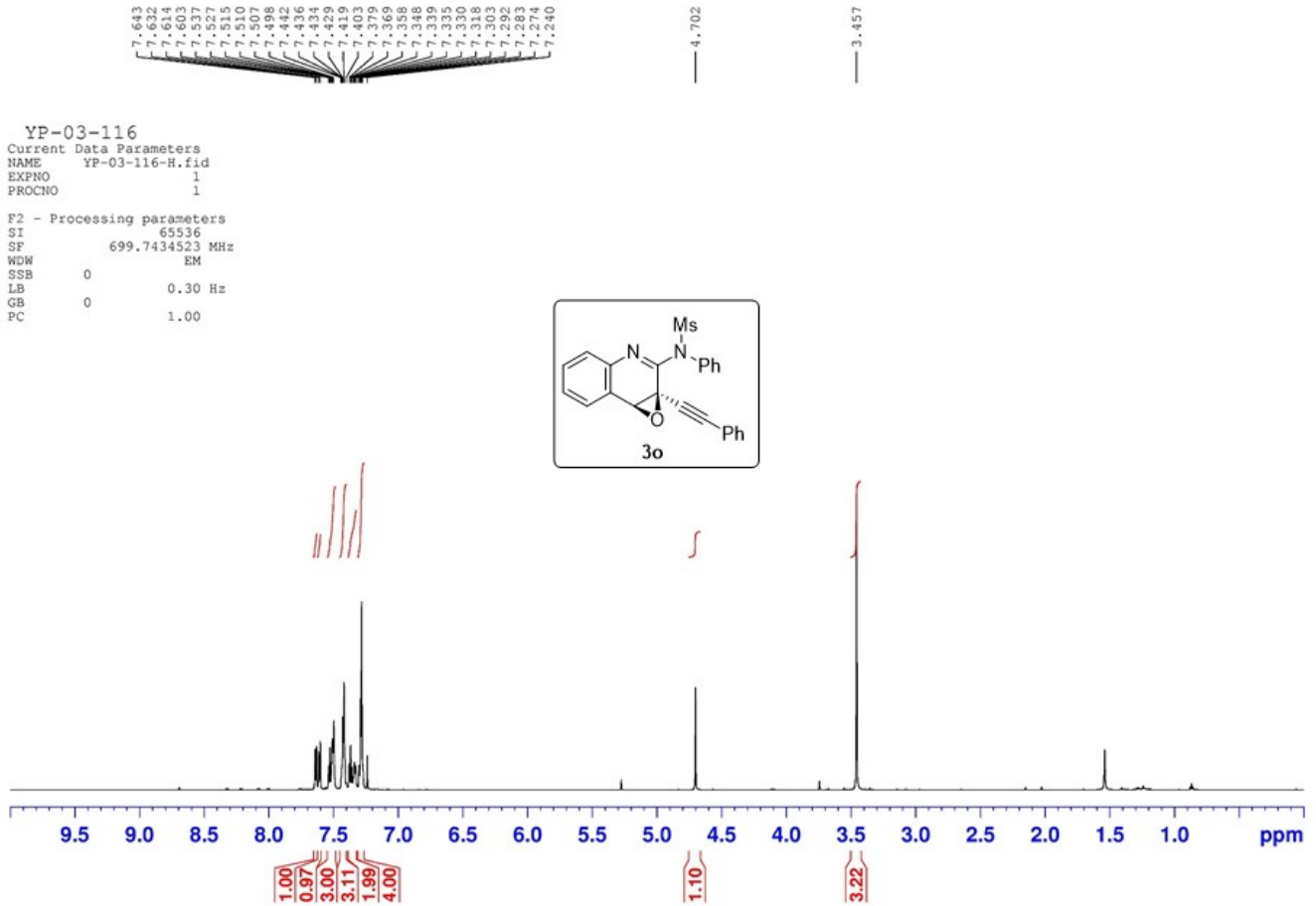

151.256
144.326
140.809
138.001
135.785
133.669
132.083
131.896
130.555
129.752
129.646
129.323
128.782
128.737
128.441
128.375
127.690
123.354
122.117
120.899
87.004
82.752
77.212
76.999
76.787
65.532
53.260
21.641
Ts
N
N
Br
O
Ph
3g
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

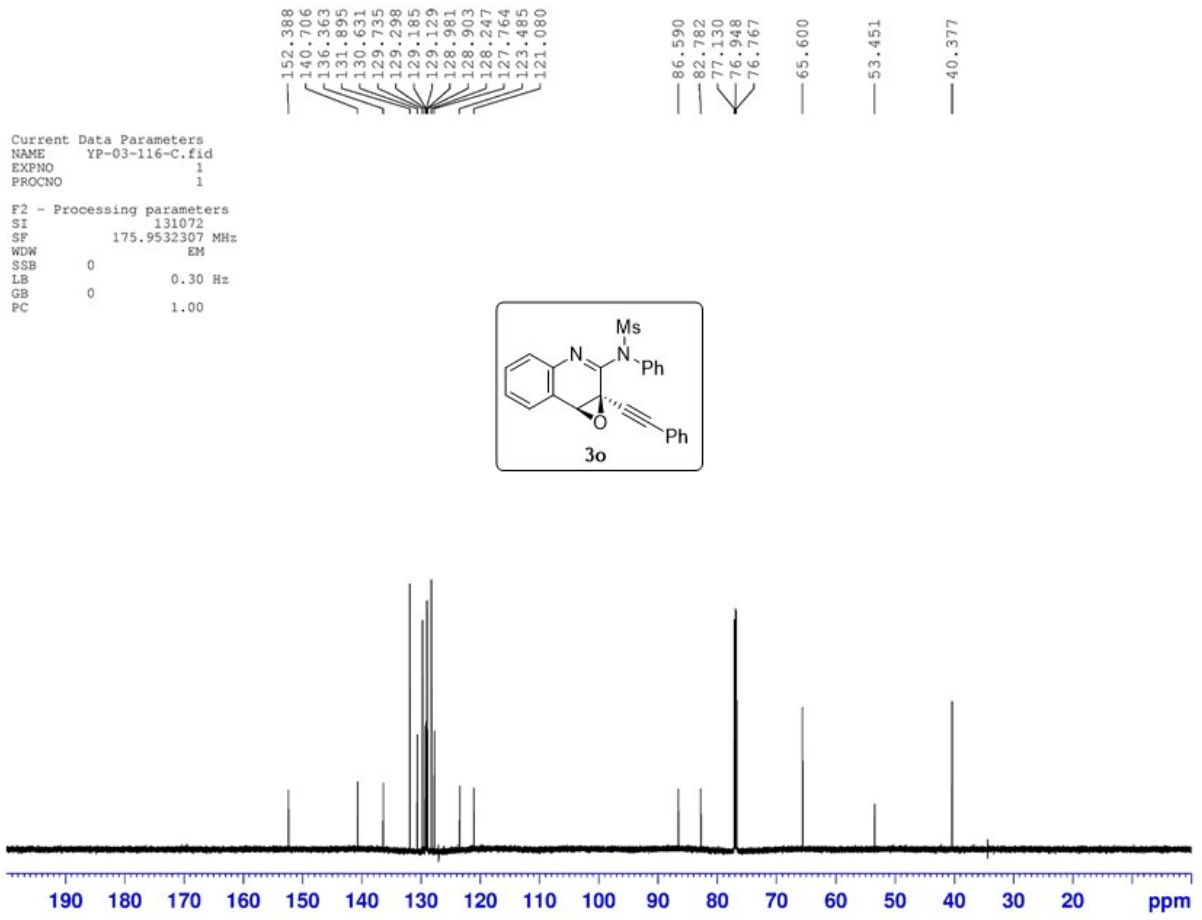

7.748
7.734
7.561
7.548
7.493
7.483
7.479
7.467
7.465
7.453
7.452
7.330
7.323
7.320
7.315
7.308
7.300
7.290
7.287
7.284
7.277
7.269
7.258
7.256
7.240
7.226
7.212
6.981
6.978
6.974
6.938
6.935
6.924
6.921
6.828
6.827
6.825
6.815
6.814
6.812
4.615
3.546
2.372
Current Data Parameters
NAME YP-03-162-A
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200302
Time 12.17
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 9541.984 Hz
FIDRES 0.291198 Hz
AQ 1.7170932 sec
RG 512
DW 52.400 usec
DE 6.50 usec
TE 295.5 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.15 usec
PL1 -1.00 dB
SFO1 598.1034854 MHz
F2 - Processing parameters
SI 32768
SF 598.1000483 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 2.00
Ts
N
N
OMe
O
Ph
3h
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
2.01
1.04
2.10
6.14
3.75
1.03
1.12
1.08
1.00
3.10
3.11

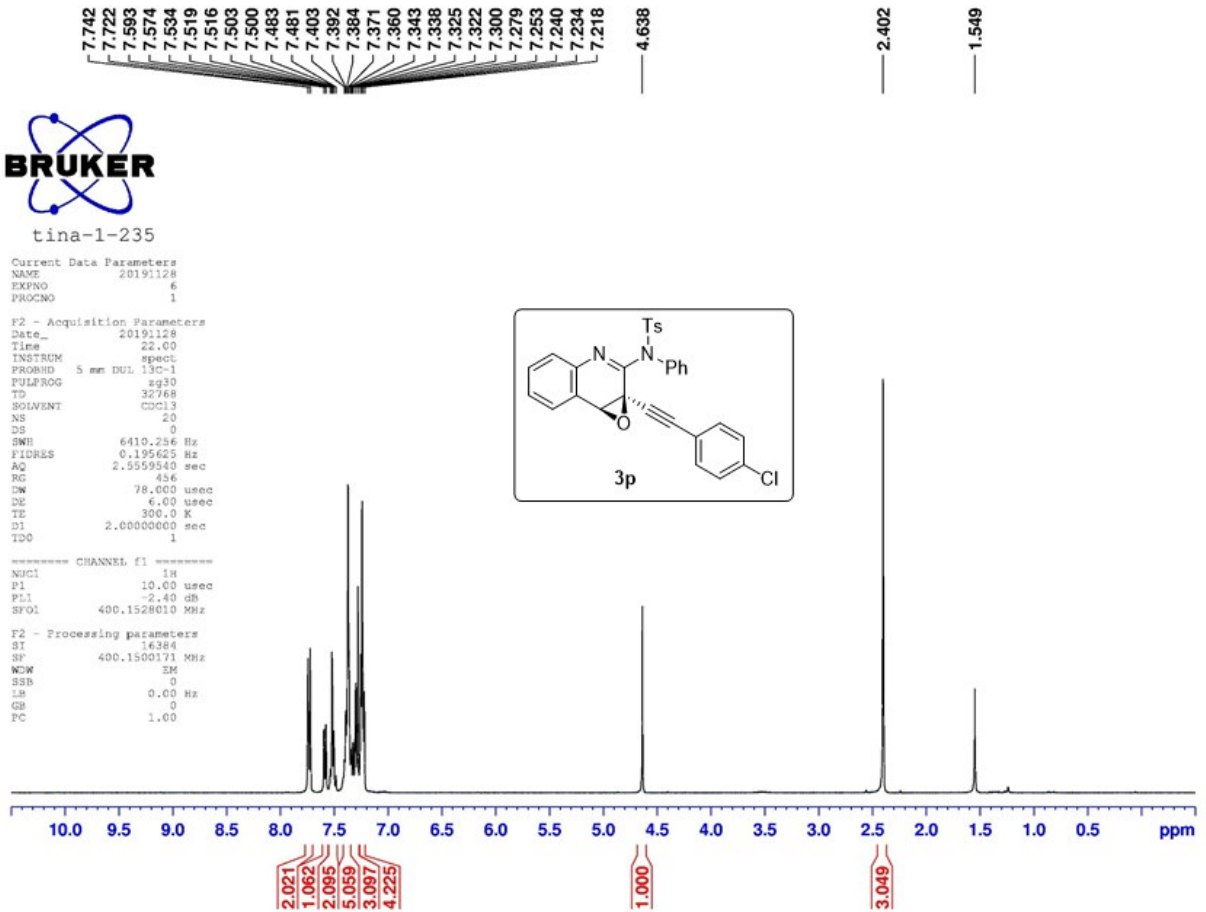

159.709
151.633
144.008
140.996
137.789
136.131
132.027
130.487
129.667
129.259
129.180
129.048
128.642
128.291
127.420
123.323
122.216
121.256
115.689
115.553
86.549
83.111
77.212
77.000
76.788
65.696
55.211
53.386
21.632
Ts
N
N
OMe
O
Ph
3h
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

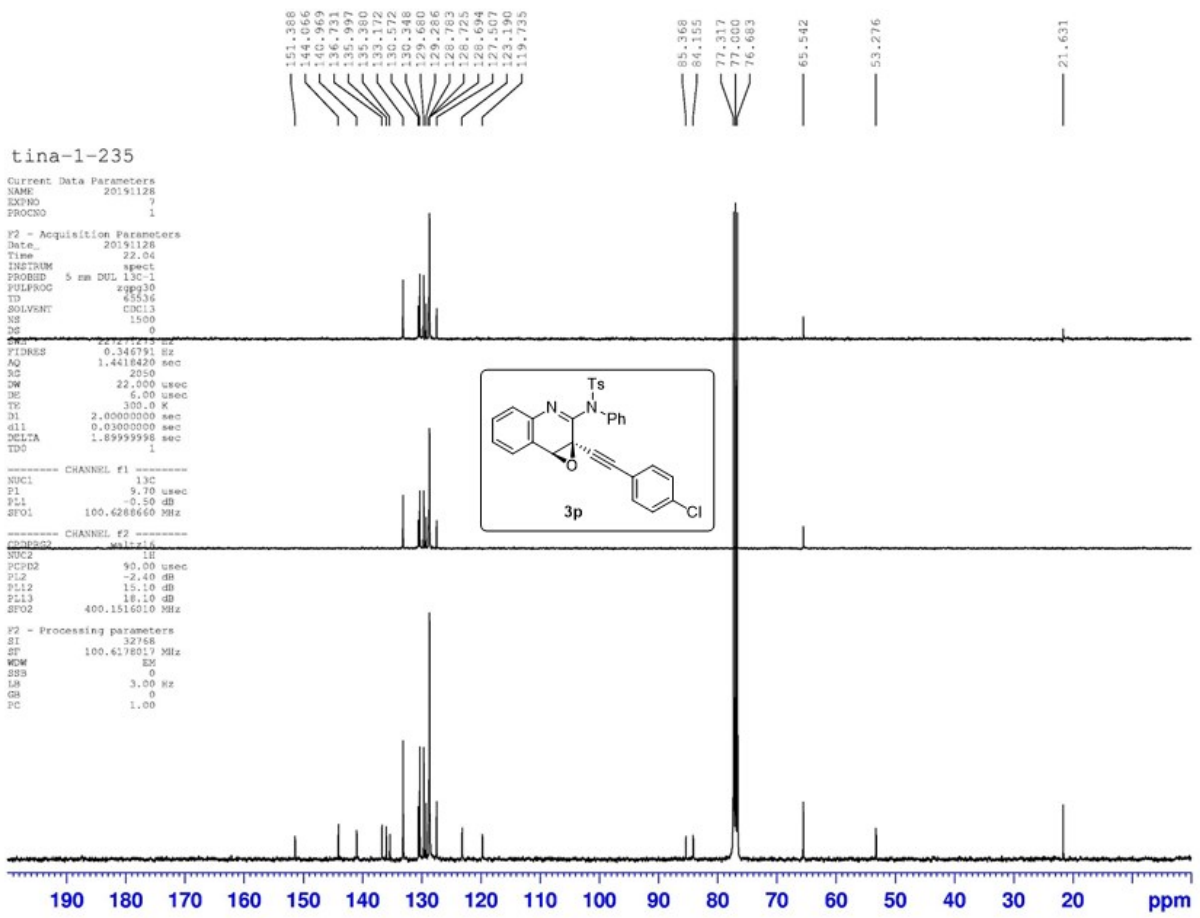

7.879
7.860
7.598
7.580
7.562
7.543
7.525
7.513
7.506
7.499
7.473
7.454
7.435
7.397
7.345
7.337
7.321
7.311
7.240
4.650
1.564
BRUKER
tina-2-42
Current Data Parameters
NAME 20200203
EXPNO 5
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200203
Time 22.20
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 70
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 287
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz
F2 - Processing parameters
SI 16384
SF 400.1500171 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
SO2Ph
N
N
Ph
O
Ph
3n
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
2.000
2.072
2.116
3.018
5.187
5.058
1.052

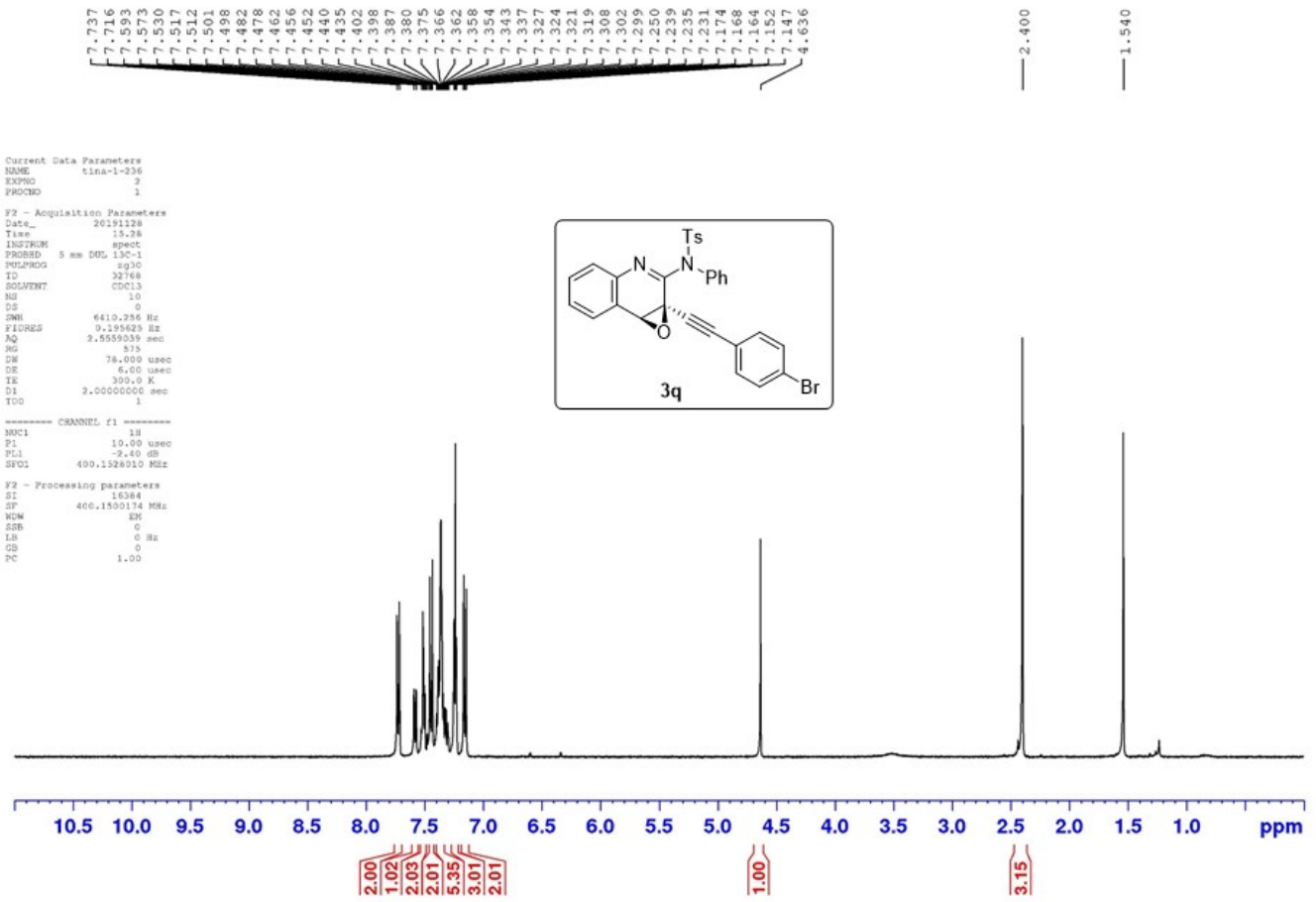

151.520
140.662
139.061
136.596
133.063
131.920
131.481
130.340
129.545
129.265
129.175
128.809
128.697
128.609
128.276
127.983
127.514
123.301
121.180
86.560
83.063
77.318
77.000
76.682
65.492
53.326
tina-2-42
Current Data Parameters
NAME 20200203
EXPNO 7
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200203
Time 23.10
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 621
DS 0
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4418420 sec
RG 2050
DW 22.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.70 usec
PL1 -0.50 dB
SFO1 100.6288660 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.40 dB
PL12 15.10 dB
PL13 18.10 dB
SFO2 400.1516010 MHz
F2 - Processing parameters
SI 32768
SF 100.6178093 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
SO2Ph
N
N
Ph
O
Ph
3n
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

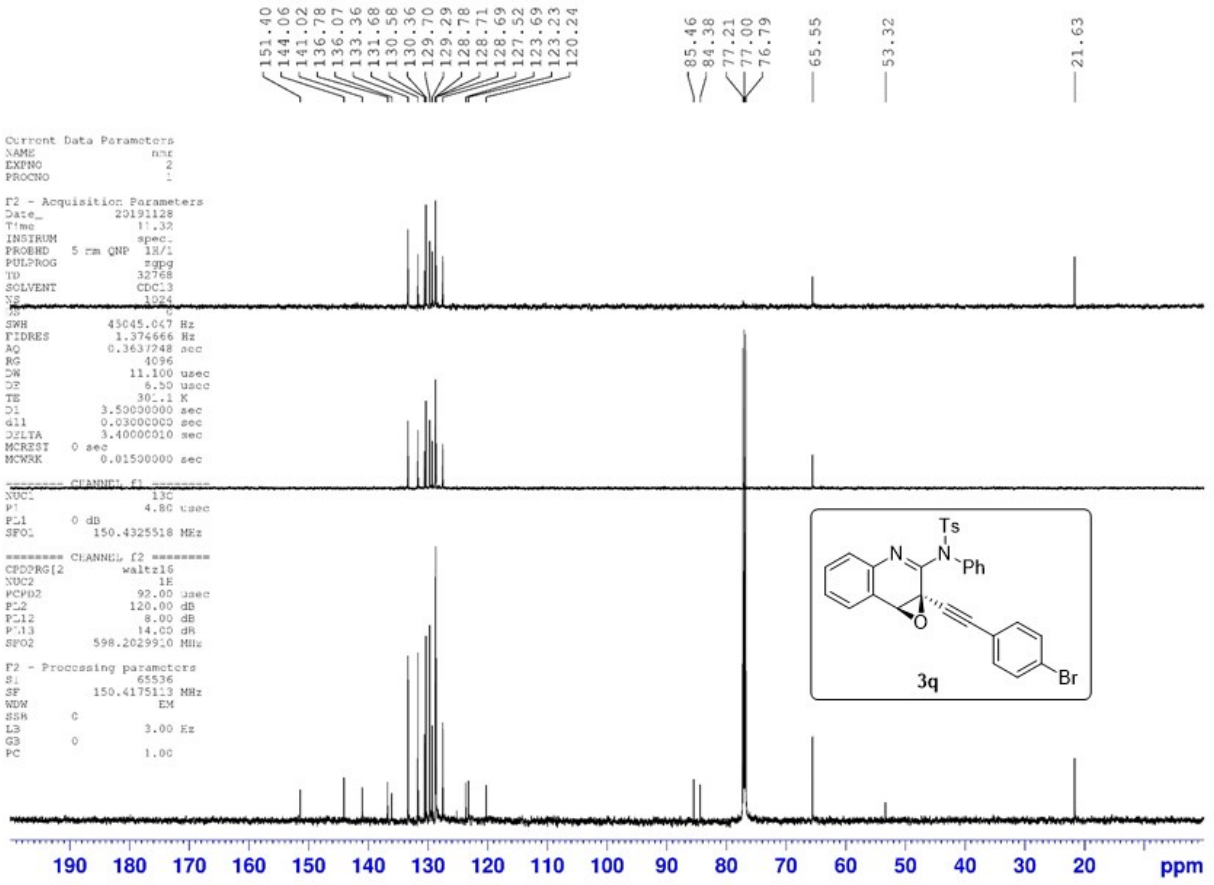

7.643
7.632
7.614
7.603
7.537
7.527
7.515
7.510
7.507
7.498
7.442
7.436
7.434
7.429
7.419
7.403
7.379
7.369
7.358
7.348
7.339
7.335
7.330
7.318
7.303
7.292
7.283
7.274
7.240
4.702
3.457
YP-03-116
Current Data Parameters
NAME YP-03-116-H.fid
EXPNO 1
PROCNO 1
F2 - Processing parameters
SI 65536
SF 699.7434523 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
Ms
N
N
Ph
O
Ph
3o
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.00
0.97
3.00
3.11
1.99
4.00
1.10
3.22

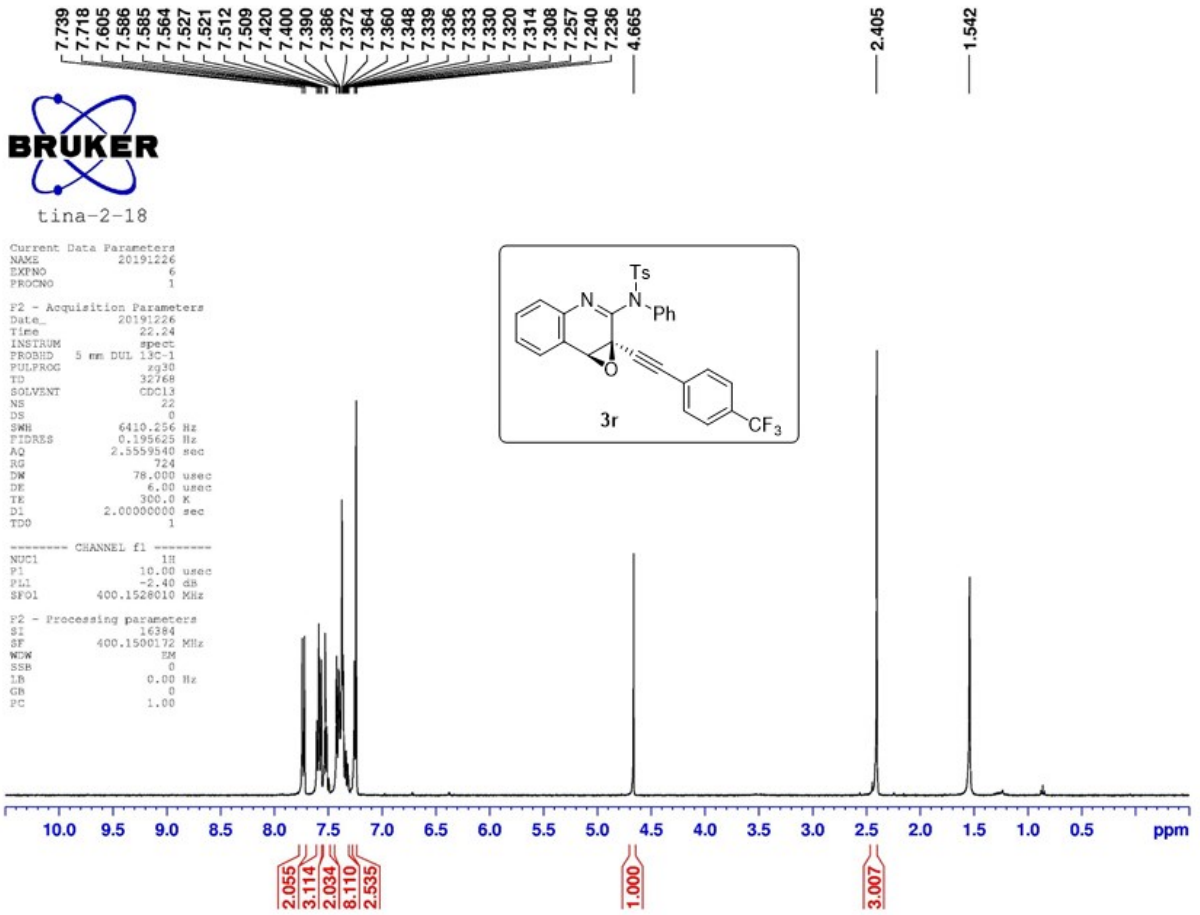

152.388
140.706
136.363
131.895
130.631
129.735
129.298
129.185
129.129
128.981
128.903
128.247
127.764
123.485
121.080
86.590
82.782
77.130
76.948
76.767
65.600
53.451
40.377
Current Data Parameters
NAME YP-03-116-C.fid
EXPNO 1
PROCNO 1
F2 - Processing parameters
SI 131072
SF 175.9532307 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
Ms
N
N
Ph
O
Ph
3o
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

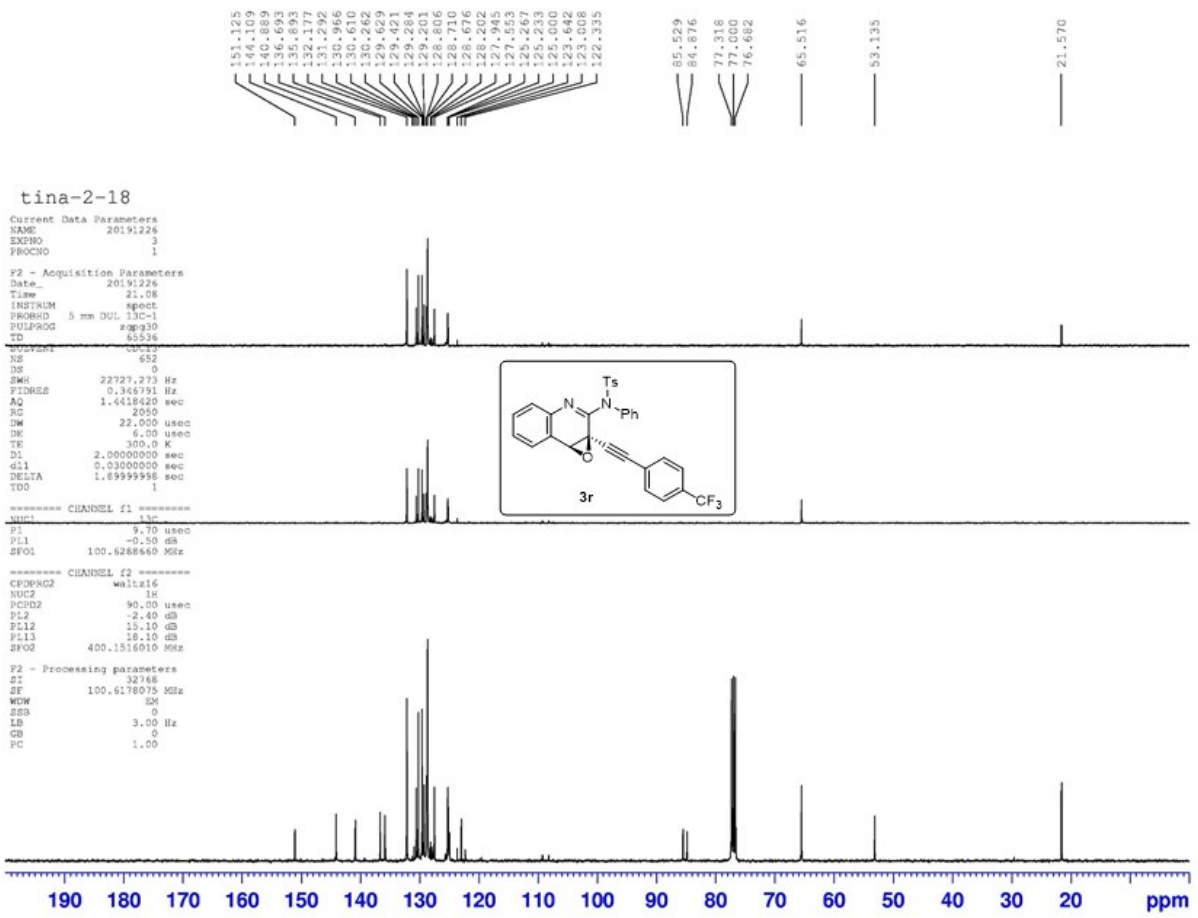

7.742
7.722
7.593
7.574
7.534
7.519
7.516
7.503
7.500
7.483
7.481
7.403
7.392
7.384
7.371
7.360
7.343
7.338
7.325
7.322
7.300
7.279
7.253
7.240
7.234
7.218
4.638
2.402
1.549
BRUKER
tina-1-235
Current Data Parameters
NAME 20191128
EXPNO 6
PROCNO 1
F2 - Acquisition Parameters
Date_ 20191128
Time 22.00
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 20
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 456
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz
F2 - Processing parameters
SI 16384
SF 400.1500171 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
Ts
N
N
Ph
O
3p
Cl
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
2.021
1.062
2.095
5.059
3.097
4.225
1.000
3.049

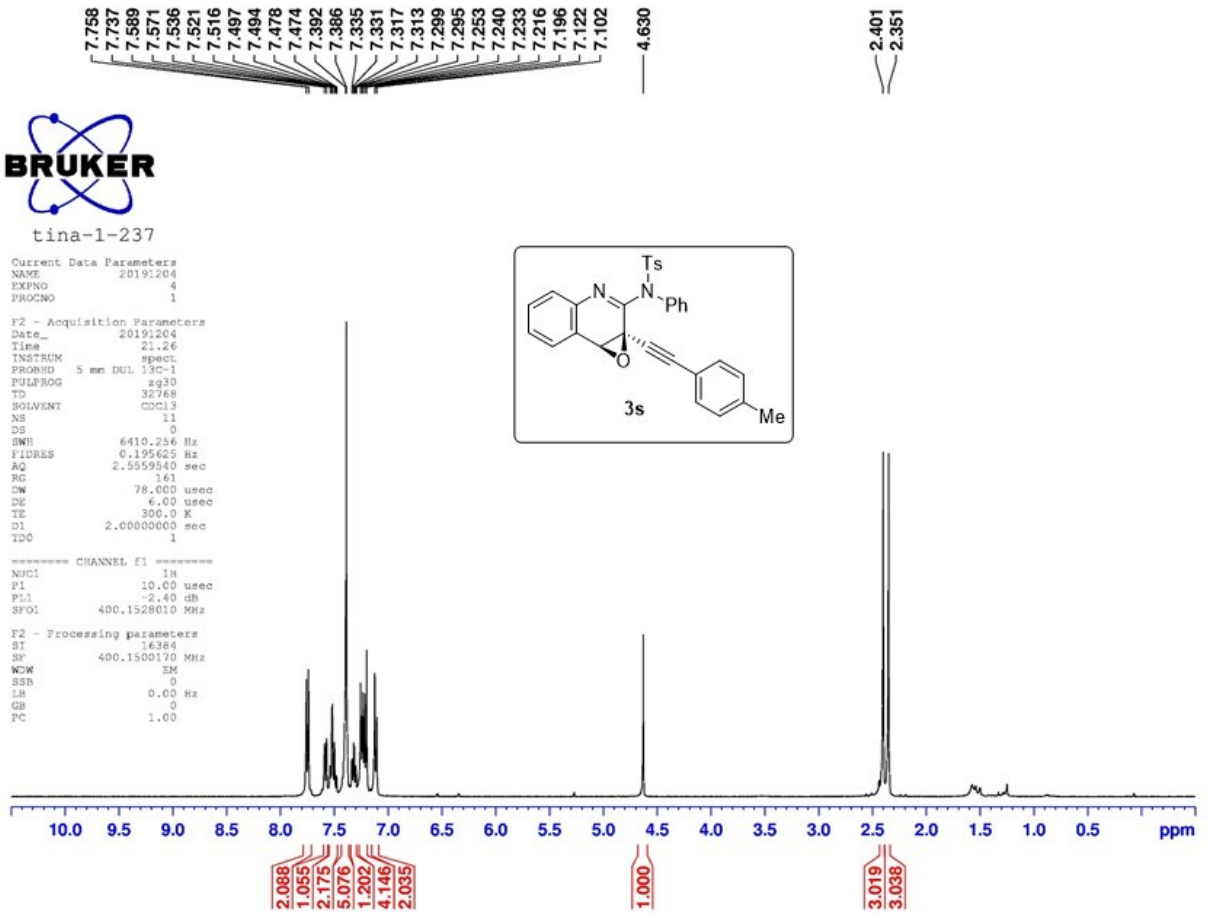

151.388
144.066
140.969
136.731
135.997
135.380
133.172
130.572
130.348
129.680
129.286
128.763
128.725
128.694
127.507
123.190
119.735
85.368
84.155
77.317
77.000
76.683
65.542
53.276
21.631
tina-1-235
Current Data Parameters
NAME 20191128
EXPNO 7
PROCNO 1
F2 - Acquisition Parameters
Date_ 20191128
Time 22.04
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1500
DS 0
SWH 27247.275 Hz
FIDRES 0.346791 Hz
AQ 1.4418420 sec
RG 2050
DW 22.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.70 usec
PL1 -0.50 dB
SFO1 100.6288660 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.40 dB
PL12 15.10 dB
PL13 18.10 dB
SFO2 400.1516010 MHz
F2 - Processing parameters
SI 32768
SF 100.6178017 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
Ts
N
N
Ph
O
Cl
3p
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


7.737
7.716
7.593
7.573
7.530
7.517
7.512
7.501
7.498
7.482
7.478
7.462
7.456
7.452
7.440
7.435
7.402
7.398
7.387
7.380
7.375
7.366
7.362
7.358
7.354
7.343
7.337
7.327
7.324
7.321
7.319
7.308
7.302
7.299
7.250
7.239
7.235
7.231
7.174
7.168
7.164
7.152
7.147
4.636
2.400
1.540
Current Data Parameters
NAME tina-1-236
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20191128
Time 15.28
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 10
DS 0
SWH 6410.256 Hz
FIDRES 9.195625 Hz
AQ 2.5559039 sec
RG 575
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1526010 MHz
F2 - Processing parameters
SI 16384
SF 400.1500174 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00
Ts
N
N
Ph
O
Br
3q
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
2.00
1.02
2.03
2.01
5.35
3.01
2.01
1.00
3.15


151.40
144.06
141.02
136.78
136.07
133.36
131.68
130.58
130.36
129.70
129.29
128.78
128.71
128.69
127.52
123.69
123.23
120.24
85.46
84.38
77.21
77.00
76.79
65.55
53.32
21.63
Current Data Parameters
NAME nmr
EXPNO 2
PROCNO 1
f2 - Acquisition Parameters
Date_ 20191128
Time 17.32
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 1024
DS 4
SWH 43045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637248 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 301.1 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0 dB
SFO1 150.4325518 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 8.00 dB
PL13 14.00 dB
SFO2 598.2029910 MHz
f2 - Processing parameters
SI 65536
SF 150.4175113 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
Ts
N
N
Ph
O
Br
3q
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


7.739
7.718
7.605
7.586
7.585
7.564
7.527
7.521
7.512
7.509
7.420
7.400
7.390
7.386
7.372
7.364
7.360
7.348
7.339
7.336
7.333
7.330
7.320
7.314
7.308
7.257
7.240
7.236
4.665
2.405
1.542
BRUKER
tina-2-18
Current Data Parameters
NAME 20191226
EXPNO 6
PROCNO 1
F2 - Acquisition Parameters
Date_ 20191226
Time 22.24
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 22
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 724
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz
F2 - Processing parameters
SI 16384
SF 400.1500172 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
Ts
N
N
Ph
O
3r
CF3
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
2.055
3.114
2.034
8.110
2.535
1.000
3.007


151.125
144.109
140.889
136.693
135.893
132.177
131.292
130.966
130.610
130.262
129.629
129.421
129.284
129.201
128.806
128.710
128.676
128.202
127.945
127.553
125.267
125.233
125.000
123.642
123.008
122.335
85.529
84.876
77.318
77.000
76.682
65.516
53.135
21.570
tina-2-18
Current Data Parameters
NAME 20191226
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20191226
Time 21.08
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 652
DS 0
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4418420 sec
RG 2050
DW 22.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.70 usec
PL1 -0.50 dB
SFO1 100.6268660 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.40 dB
PL12 15.10 dB
PL13 18.10 dB
SFO2 400.1516010 MHz
F2 - Processing parameters
SI 32768
SF 100.6178075 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
Ts
N
N
Ph
O
CF3
3r
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm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7.589
7.571
7.536
7.521
7.516
7.497
7.494
7.478
7.474
7.392
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7.335
7.331
7.317
7.313
7.299
7.295
7.253
7.240
7.233
7.216
7.196
7.122
7.102
4.630
2.401
2.351
BRUKER
tina-1-237
Current Data Parameters
NAME 20191204
EXPNO 4
PROCNO 1
F2 - Acquisition Parameters
Date_ 20191204
Time 21.26
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 11
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 161
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz
F2 - Processing parameters
SI 16384
SF 400.1500170 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
Ts
N
N
Ph
O
3s
Me
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
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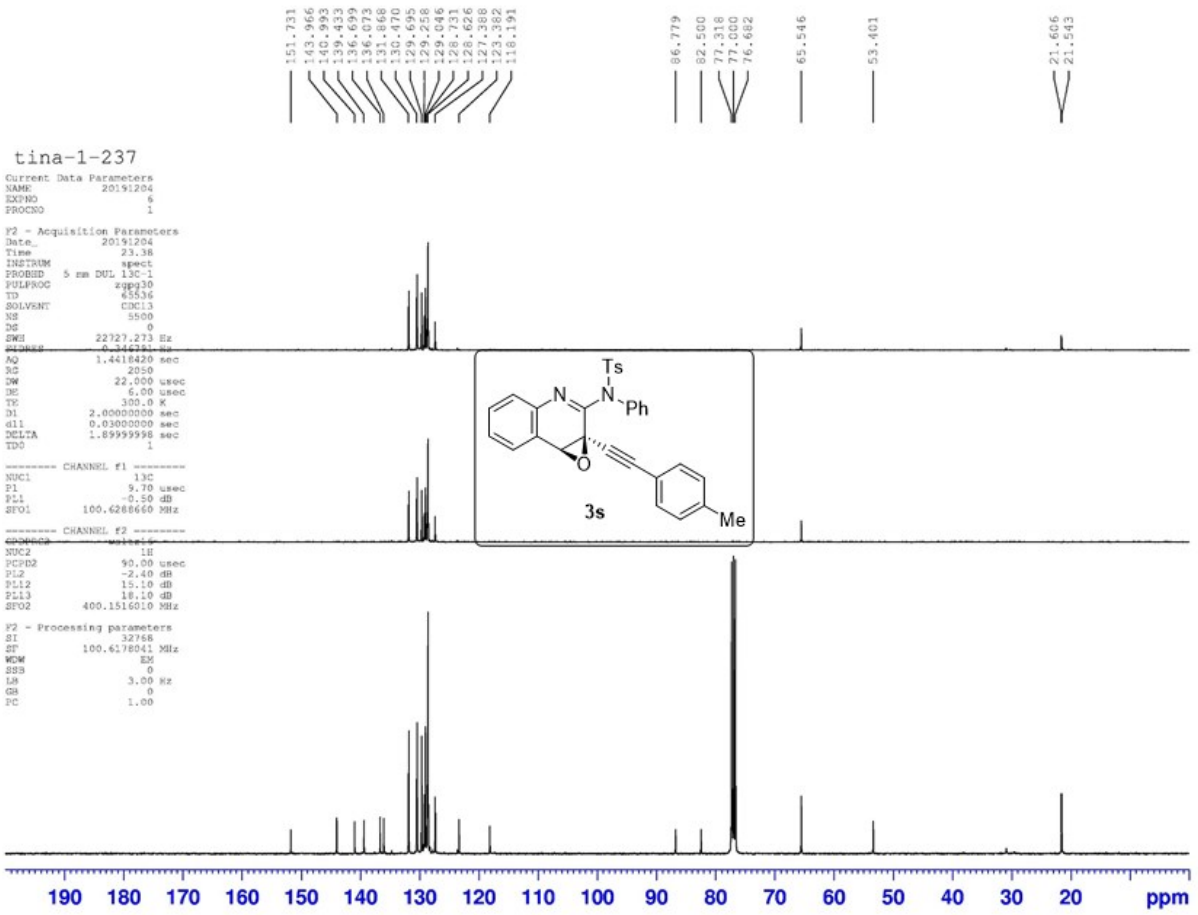
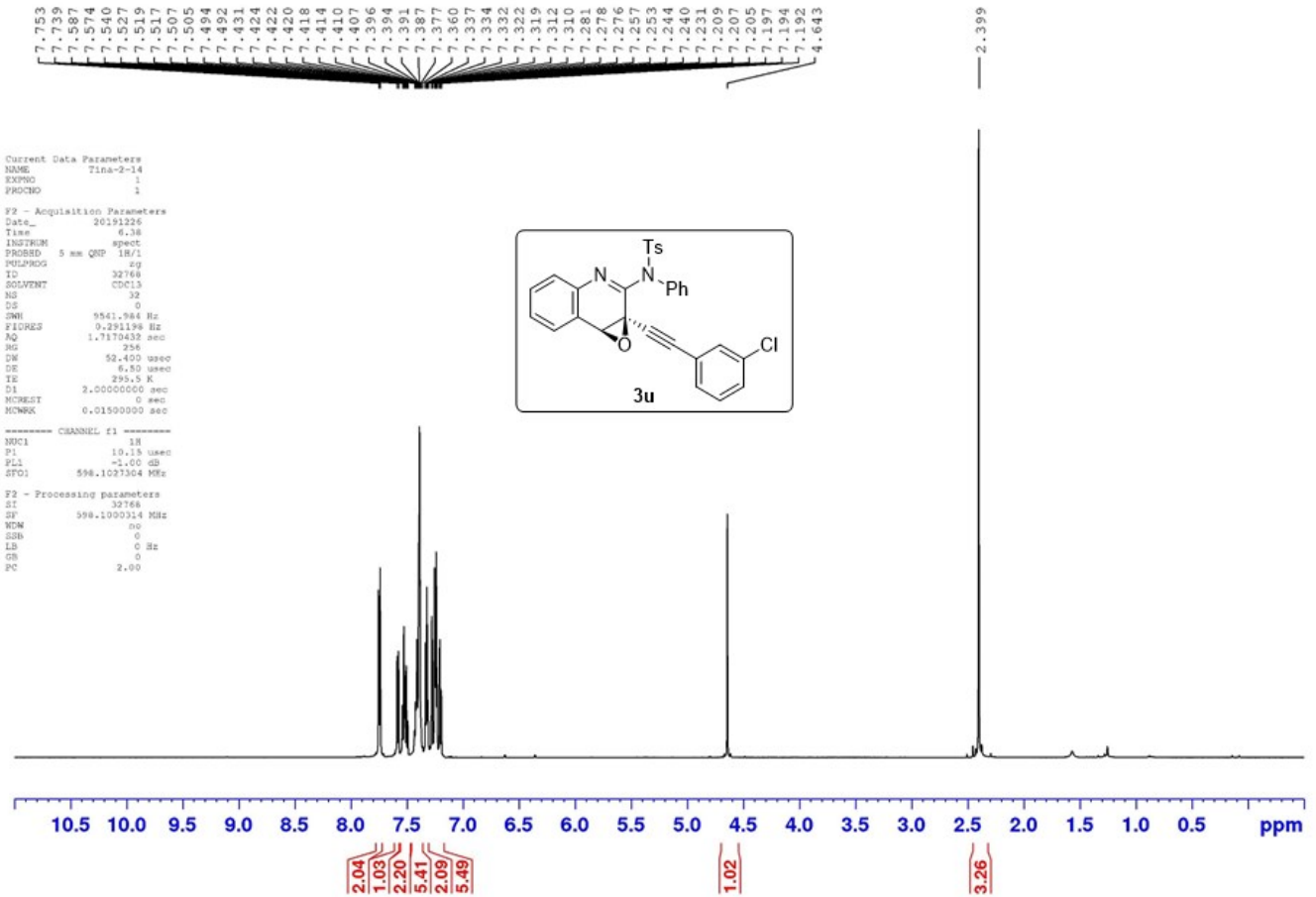
1.055
2.175
5.076
1.202
4.146
2.035
1.000
3.019
3.038


151.731
143.966
140.993
139.433
136.699
136.073
131.868
130.470
129.695
129.258
128.646
128.131
128.626
127.368
123.382
118.191
86.779
82.500
77.318
77.000
76.682
65.546
53.401
21.606
21.543
tina-1-237
Current Data Parameters
NAME 20191204
EXPNO 6
PROCNO 1
F2 - Acquisition Parameters
Date_ 20191204
Time 23.38
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 5500
DS 0
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4418420 sec
RG 2050
DW 22.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.70 usec
PL1 -0.50 dB
SFO1 100.6288660 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.40 dB
PL12 15.10 dB
PL13 18.10 dB
SFO2 400.1516010 MHz
F2 - Processing parameters
SI 32768
SF 100.6178041 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
Ts
N
N
Ph
O
3s
Me
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


7.753
7.739
7.587
7.574
7.540
7.527
7.519
7.517
7.507
7.505
7.494
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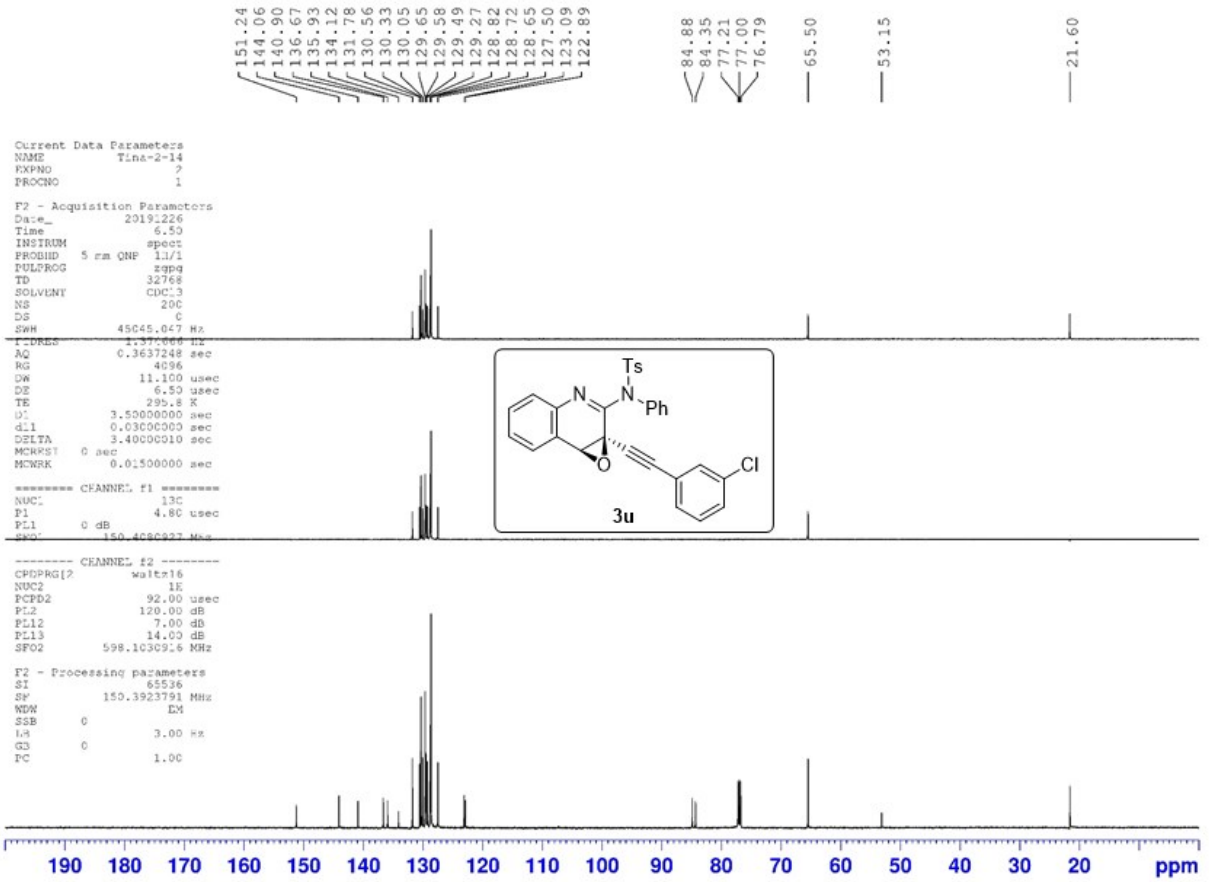
7.431
7.424
7.422
7.420
7.418
7.414
7.410
7.407
7.396
7.394
7.391
7.387
7.377
7.360
7.337
7.334
7.332
7.322
7.319
7.312
7.310
7.281
7.278
7.276
7.257
7.253
7.244
7.240
7.231
7.209
7.207
7.205
7.197
7.194
7.192
4.643
2.399
Current Data Parameters
NAME Tina-2-14
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20191226
Time 6.38
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 9541.984 Hz
FIDRES 0.291199 Hz
AQ 1.7170432 sec
RG 256
DW 52.400 usec
DE 6.50 usec
TE 295.5 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.15 usec
PL1 -1.00 dB
SFO1 598.1027304 MHz
F2 - Processing parameters
SI 32768
SF 598.1000314 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 2.00
Ts
N
N
Ph
O
Cl
3u
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
2.04
1.03
2.20
5.41
2.09
5.49
1.02
3.26


151.24
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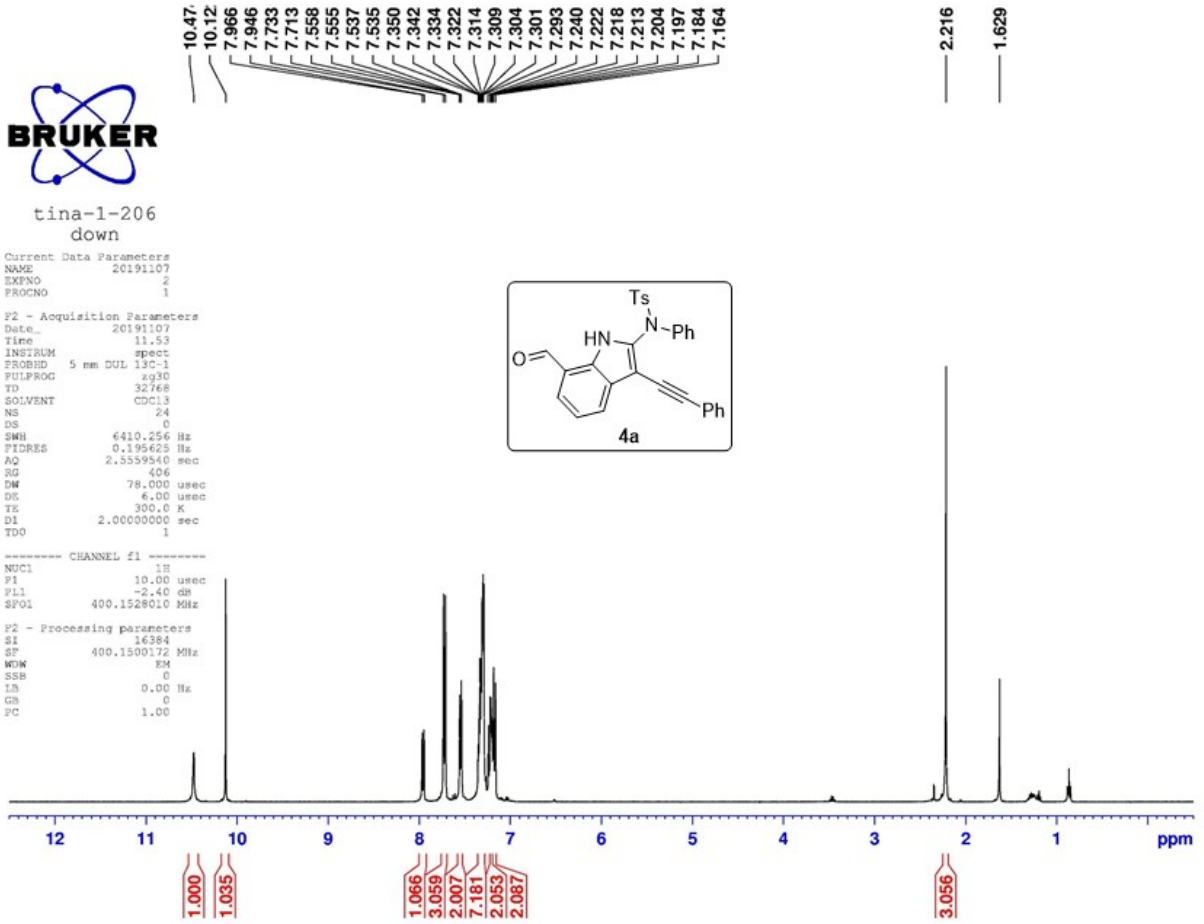
140.90
136.67
135.93
134.12
131.78
130.56
130.33
130.05
129.65
129.58
129.49
129.27
128.82
128.72
128.65
127.50
123.09
122.89
84.88
84.35
77.21
77.00
76.79
65.50
53.15
21.60
Current Data Parameters
NAME Tina-2-14
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20191226
Time 6.50
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 200
DS 0
SWH 45045.047 Hz
FIDRES 1.375066 Hz
AQ 0.3637248 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 295.8 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0 dB
SFO1 150.4080927 MHz
-------- CHANNEL f2 --------
CPDPRG[2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 7.00 dB
PL13 14.00 dB
SFO2 598.1030916 MHz
F2 - Processing parameters
SI 65536
SF 150.3923791 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
Ts
N
N
Ph
O
Cl
3u
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm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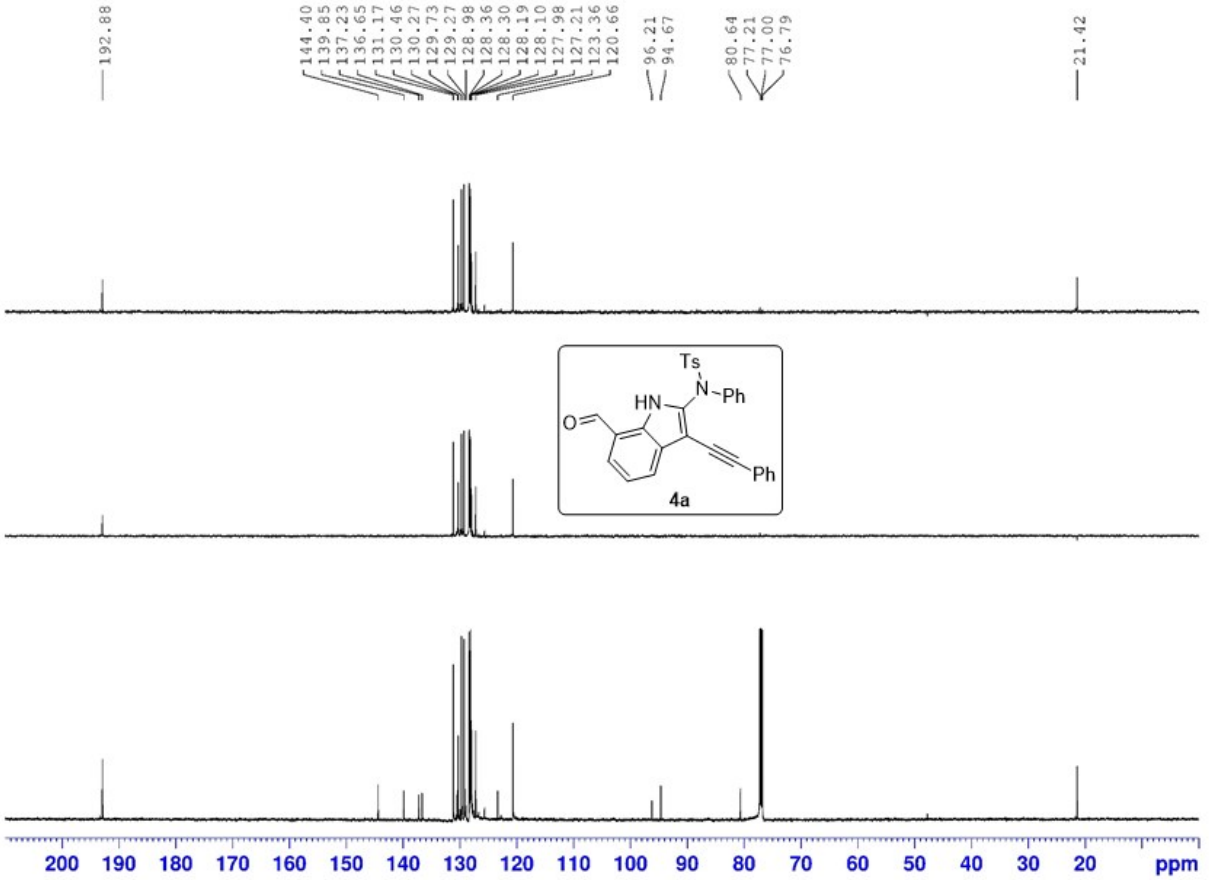
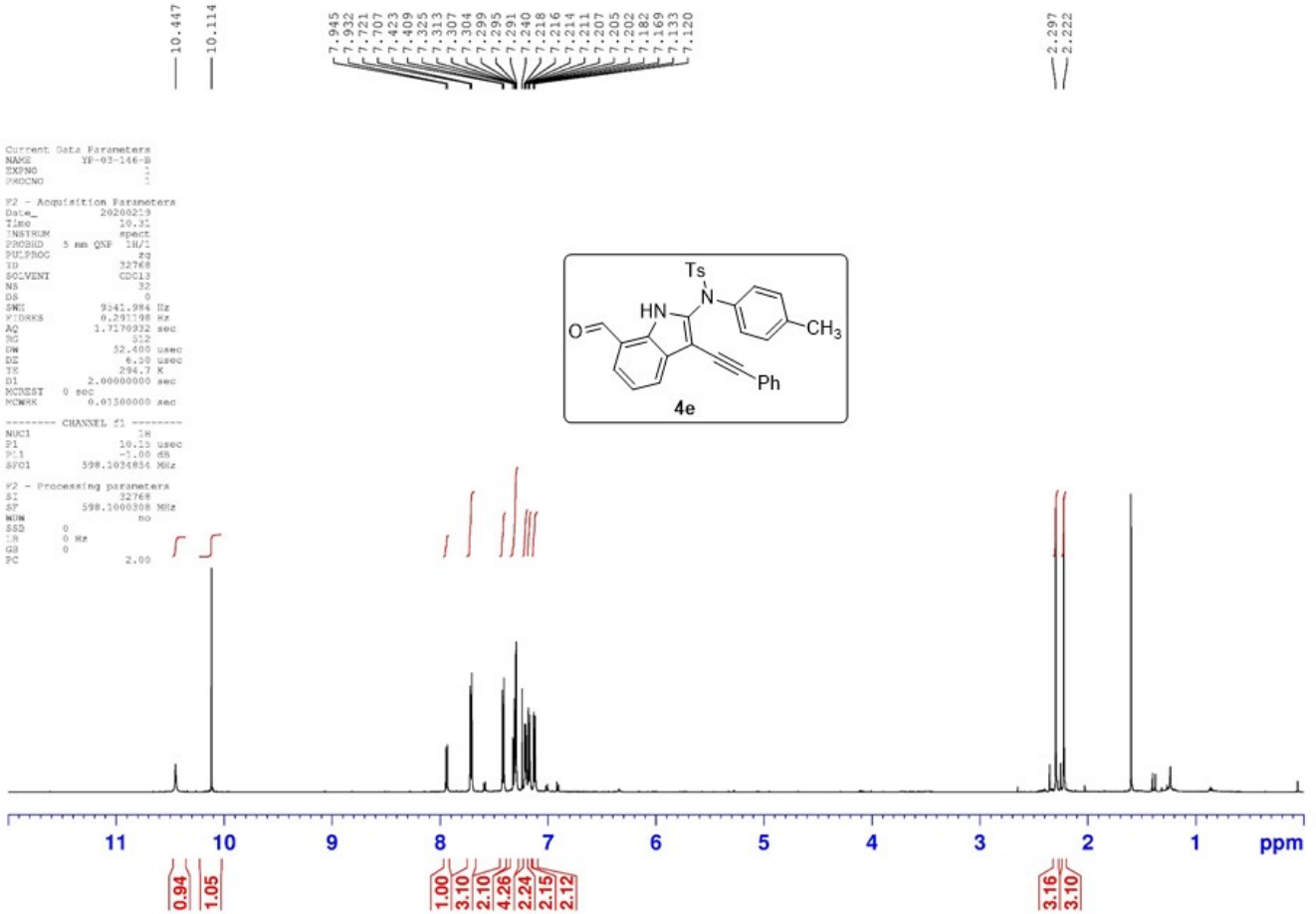
7.946
7.733
7.713
7.558
7.555
7.537
7.535
7.350
7.342
7.334
7.322
7.314
7.309
7.304
7.301
7.293
7.240
7.222
7.218
7.213
7.204
7.197
7.184
7.164
2.216
1.629
BRUKER
tina-1-206
down
Current Data Parameters
NAME 20191107
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20191107
Time 11.53
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 24
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 406
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz
F2 - Processing parameters
SI 16384
SF 400.1500172 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
Ts
N
Ph
HN
O
Ph
4a
12
11
10
9
8
7
6
5
4
3
2
1
ppm
1.000
1.035
1.066
3.059
2.007
7.181
2.053
2.087
3.056


192.88
144.40
139.85
137.23
136.65
131.17
130.46
130.27
129.73
129.27
128.98
128.36
128.30
128.19
128.10
127.98
127.21
123.36
120.66
96.21
94.67
80.64
77.21
77.00
76.79
21.42
Ts
N
Ph
HN
O
Ph
4a
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


10.447
10.114
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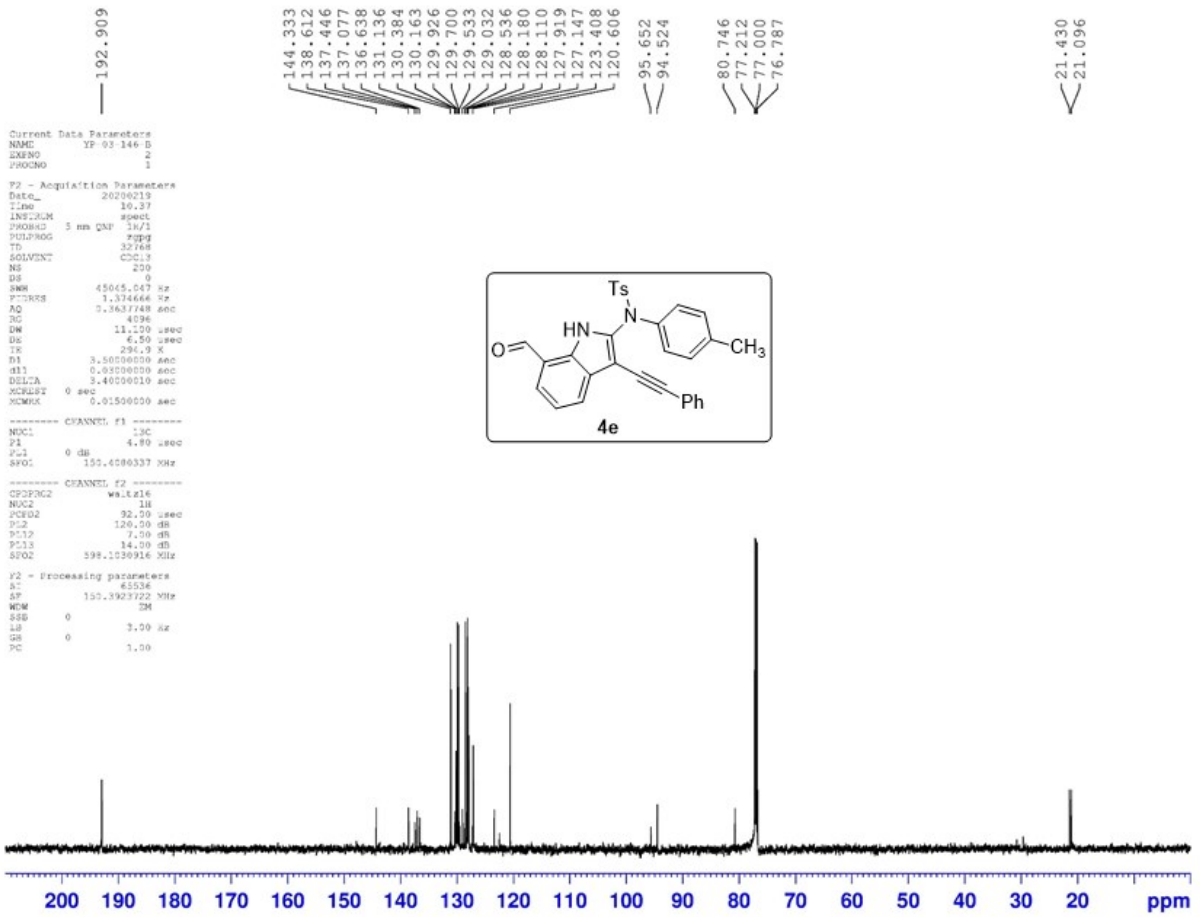
7.932
7.721
7.707
7.423
7.409
7.325
7.313
7.307
7.304
7.299
7.295
7.291
7.240
7.218
7.216
7.214
7.211
7.207
7.205
7.202
7.182
7.169
7.133
7.120
2.297
2.222
Current Data Parameters
NAME YF-03-146-B
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200219
Time 10.31
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 9541.984 Hz
FIDRES 0.291198 Hz
AQ 1.7170932 sec
RG 512
DW 52.400 usec
DE 6.50 usec
TE 294.7 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
-------- CHANNEL f1 --------
NUC1 1H
P1 10.15 usec
PL1 -1.00 dB
SFO1 598.1034834 MHz
F2 - Processing parameters
SI 32768
SF 598.1000308 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 2.00
Ts
N
HN
O
CH3
Ph
4e
11
10
9
8
7
6
5
4
3
2
1
ppm
0.94
1.05
1.00
3.10
2.10
4.26
2.24
2.15
2.12
3.16
3.10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138.612
137.446
137.077
136.638
131.136
130.384
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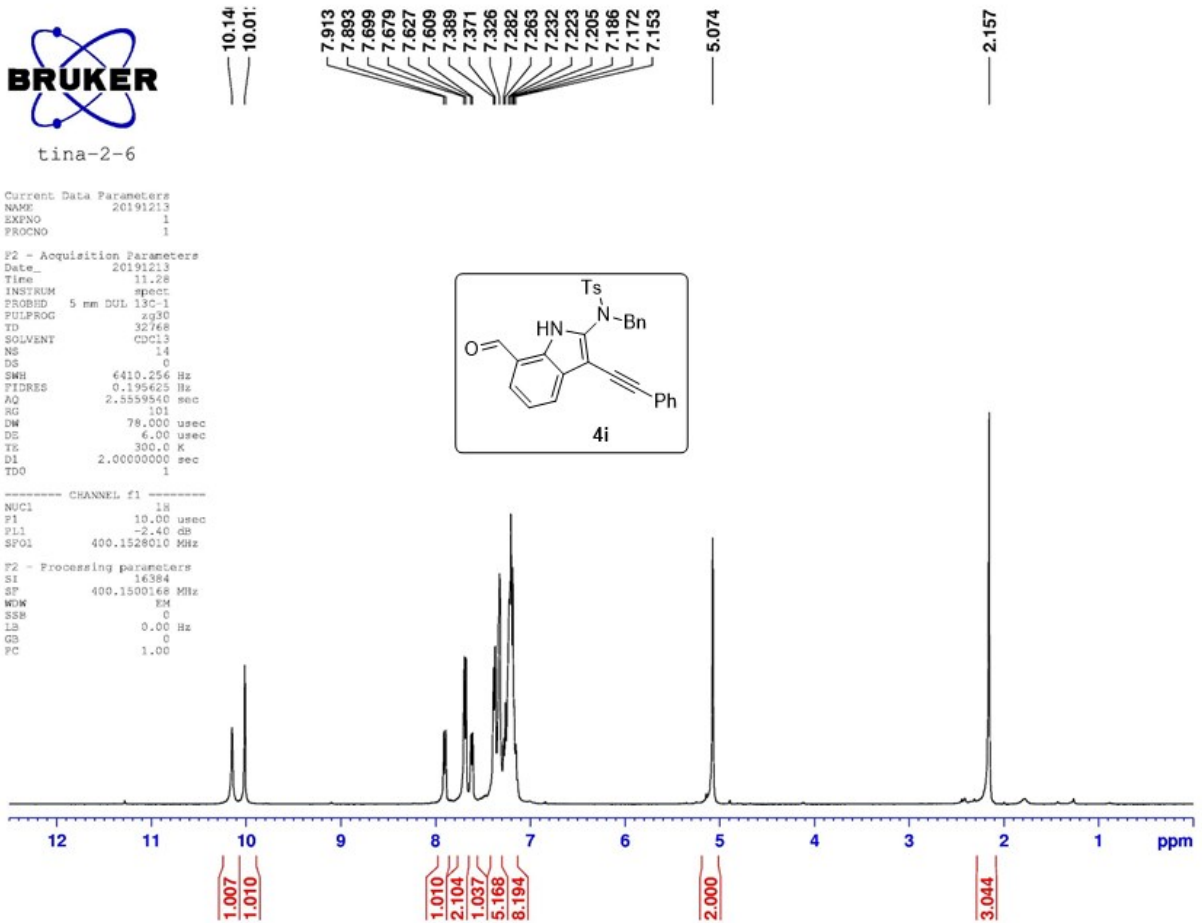
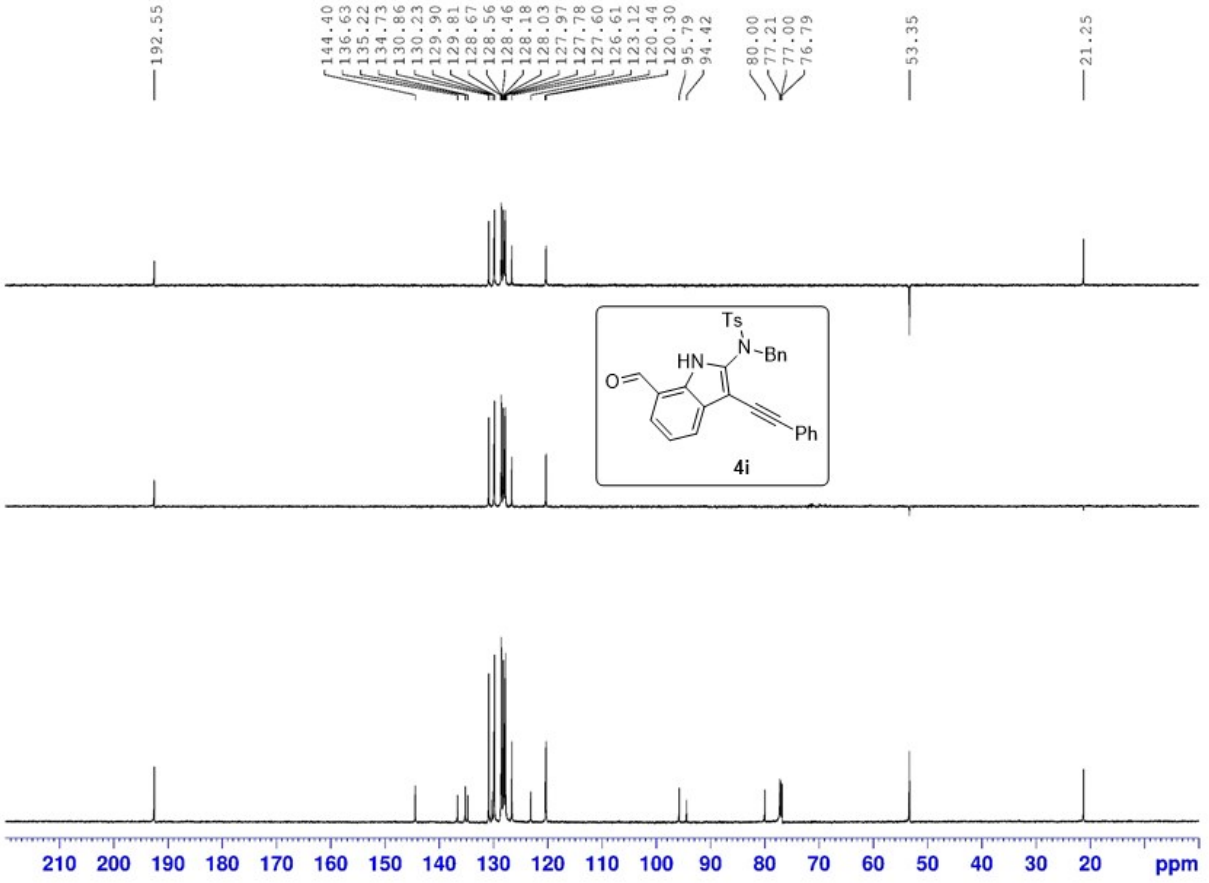
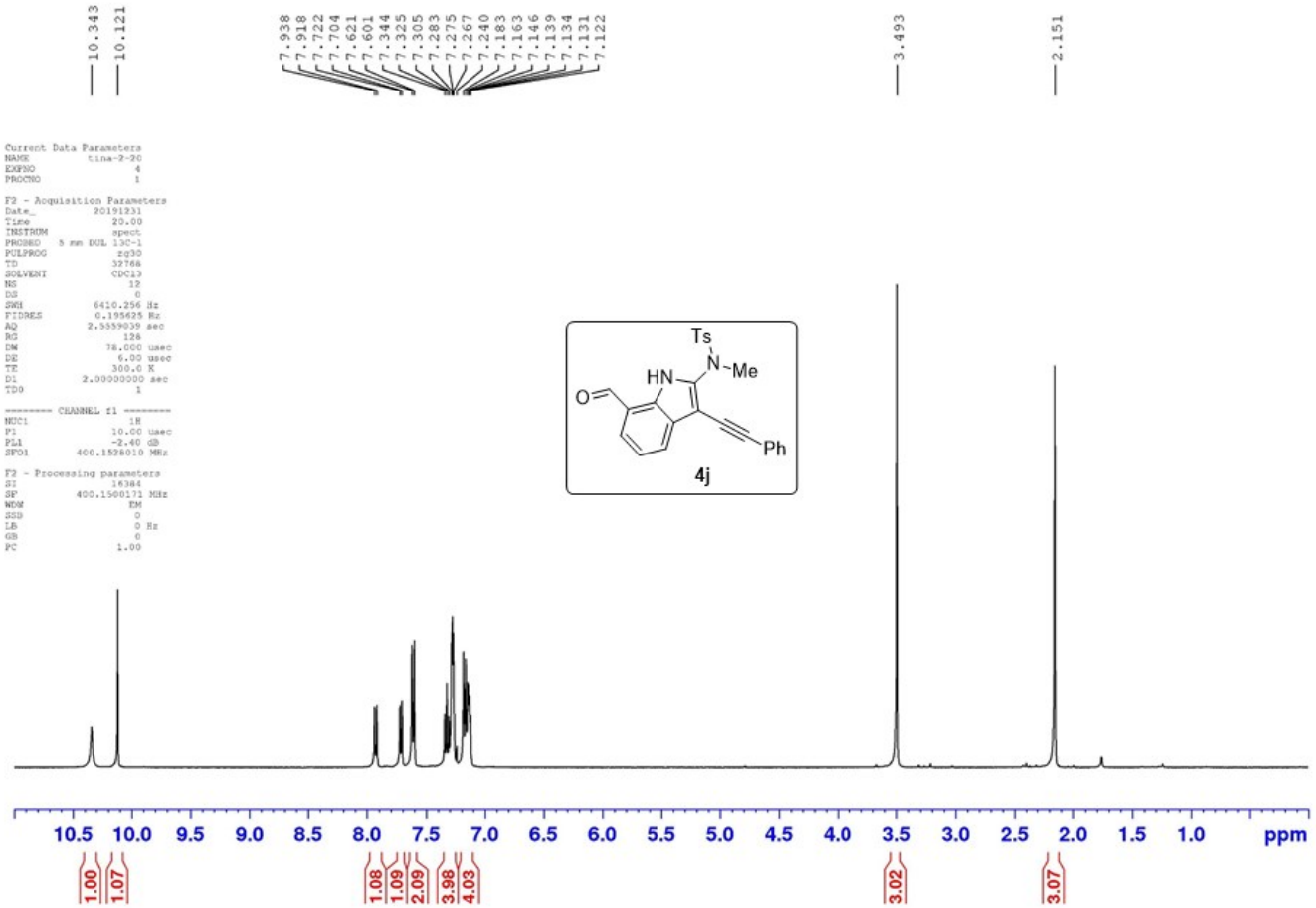
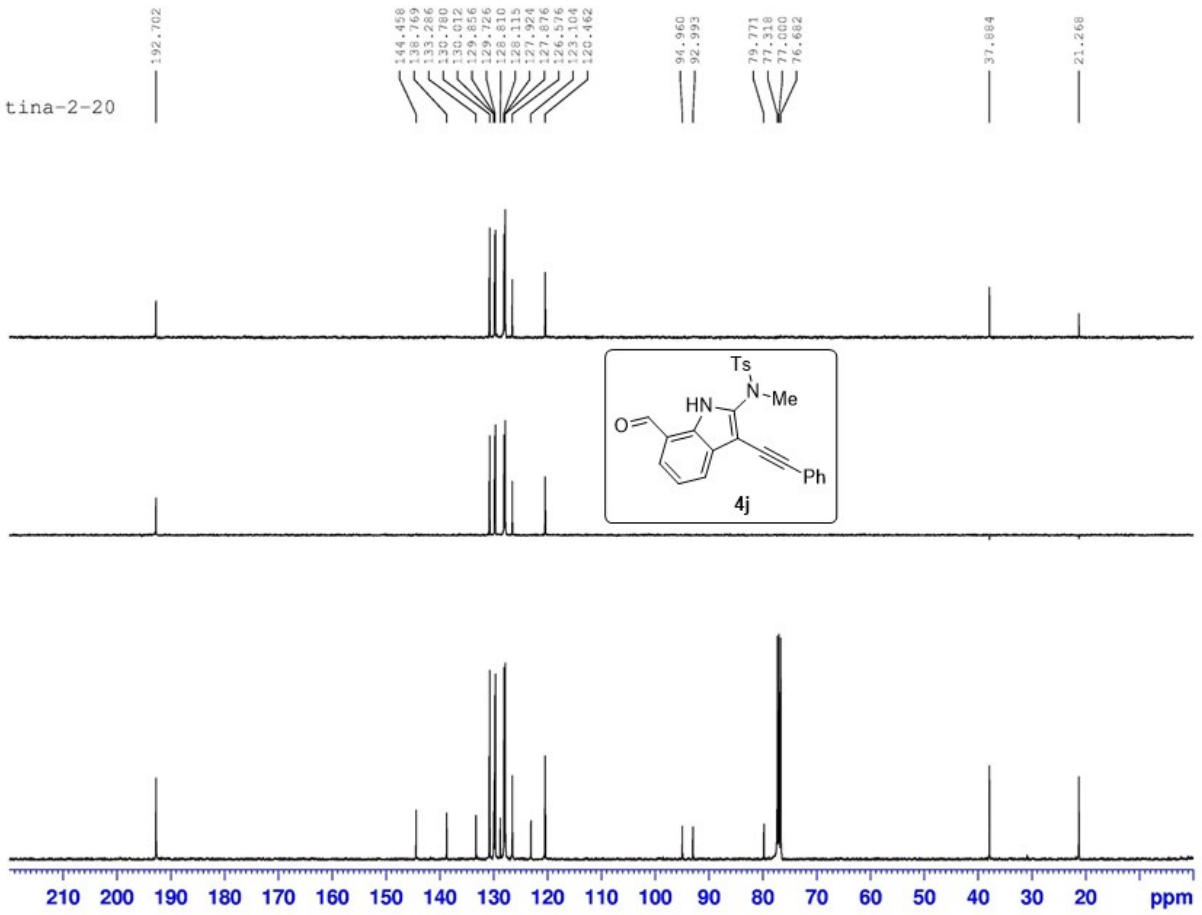
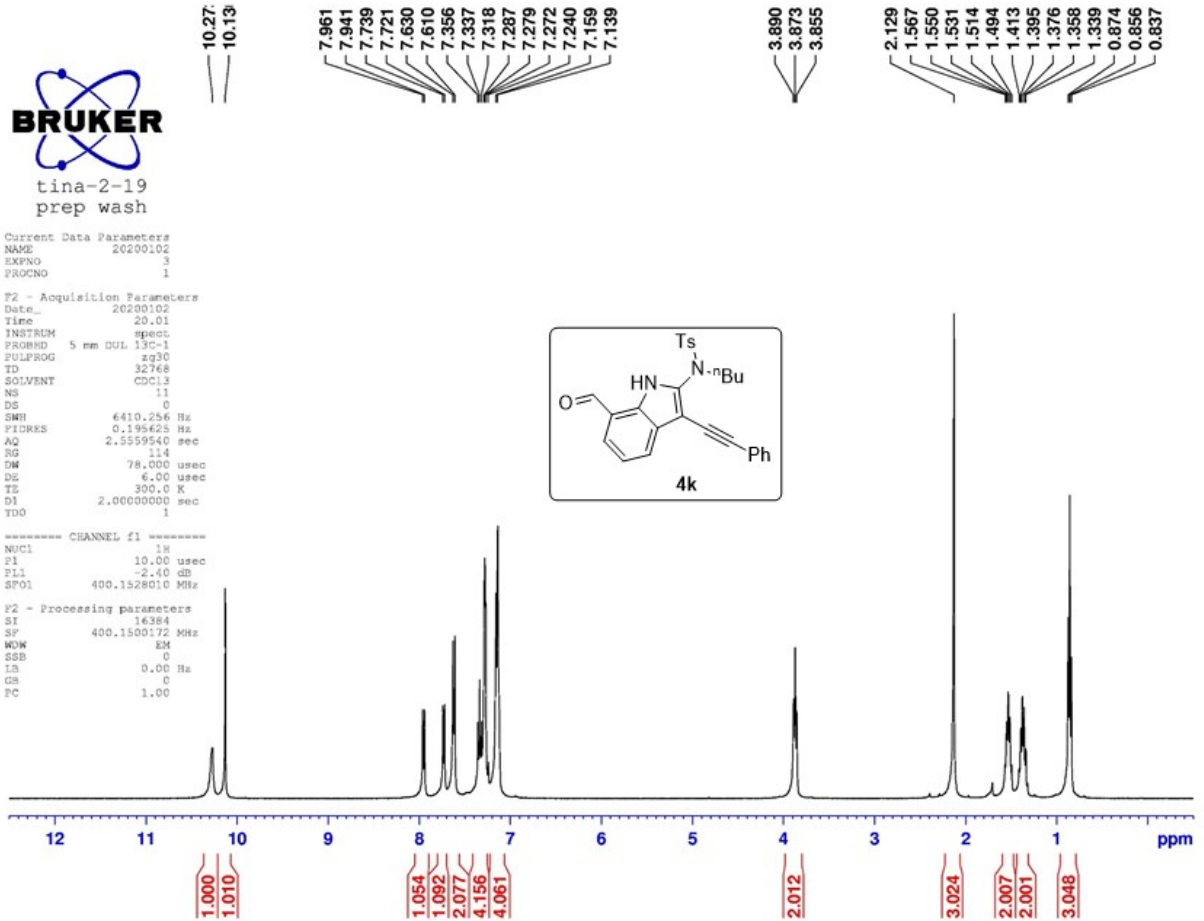
129.926
129.700
129.533
129.032
128.536
128.180
128.110
127.919
127.147
123.408
120.606
95.652
94.524
80.746
77.212
77.000
76.787
21.430
21.096
Ts
N
HN
O
CH3
Ph
4e
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

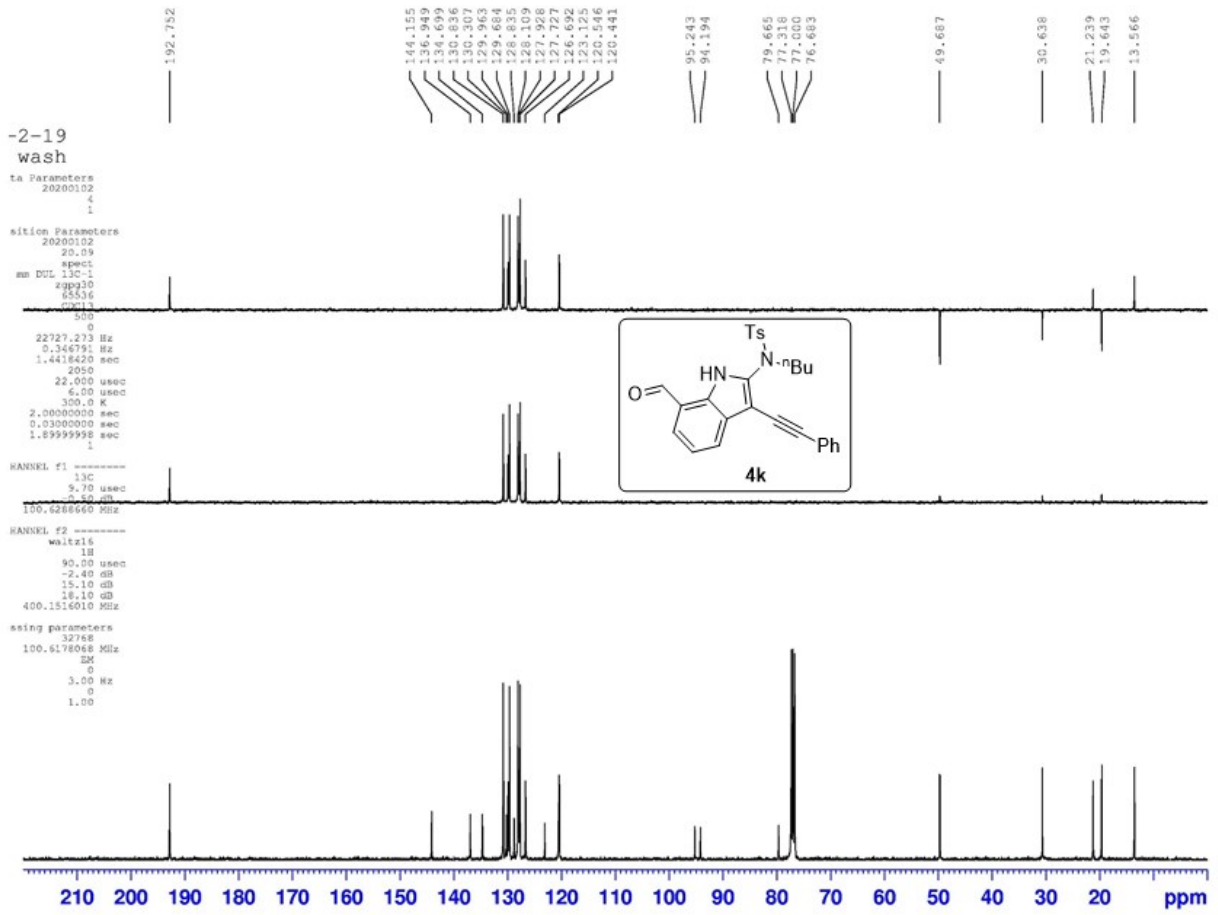

BRUKER
tina-2-6
10.14
10.01
7.913
7.893
7.699
7.679
7.627
7.609
7.389
7.371
7.326
7.282
7.263
7.232
7.223
7.205
7.186
7.172
7.153
5.074
2.157
Current Data Parameters
NAME 20191213
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20191213
Time 11.28
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 14
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 101
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
-------- CHANNEL f1 --------
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz
F2 - Processing parameters
SI 16384
SF 400.1500168 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
Ts
N
Bn
HN
O
Ph
4i
12
11
10
9
8
7
6
5
4
3
2
1
ppm
1.007
1.010
1.010
2.104
1.037
5.168
8.194
2.000
3.044

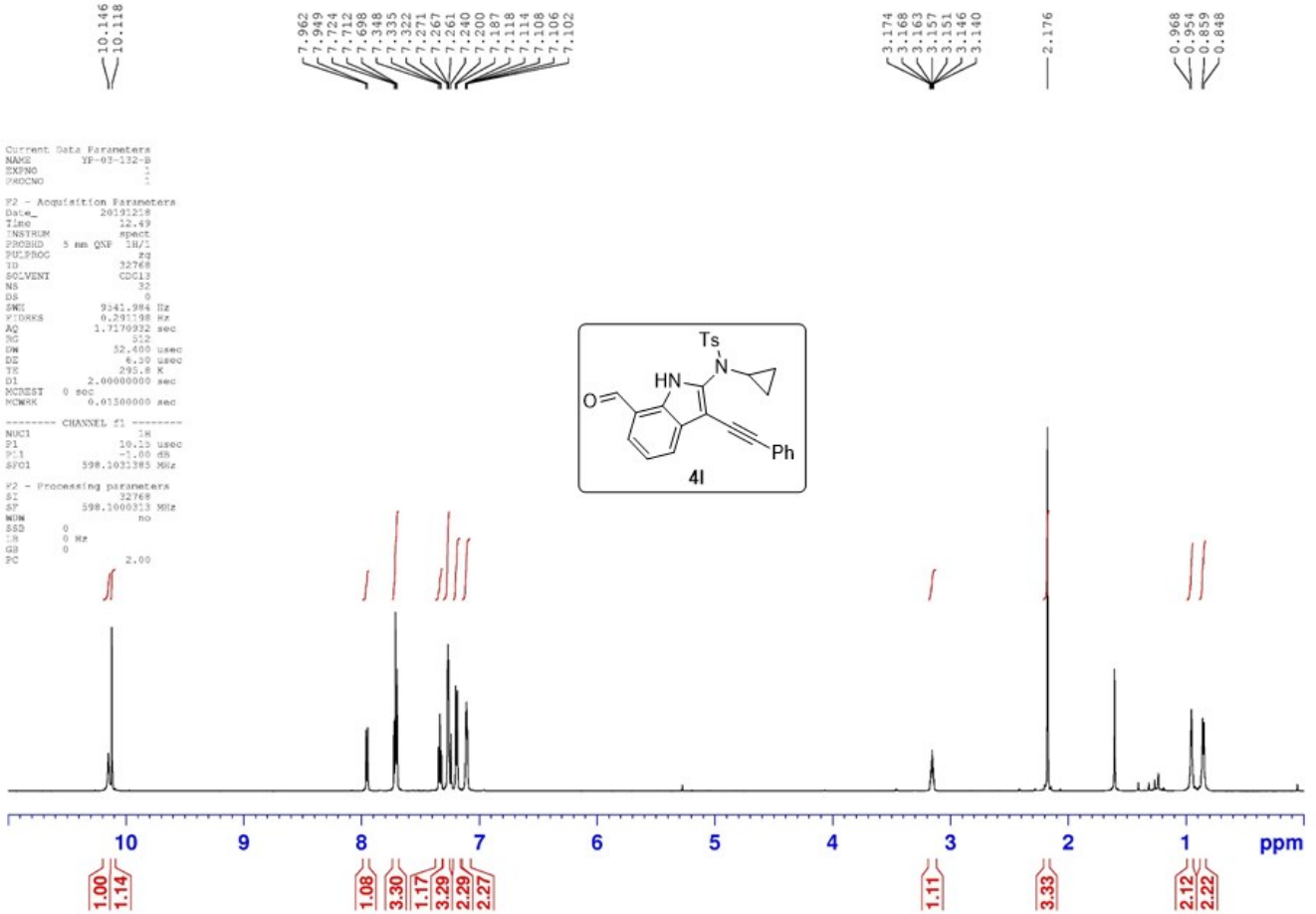

192.55
144.40
136.63
135.22
134.73
130.86
130.23
129.90
129.81
128.67
128.56
128.46
128.18
128.03
127.97
127.78
127.60
126.61
123.12
120.44
120.30
95.79
94.42
80.00
77.21
77.00
76.79
53.35
21.25
Ts
N
Bn
HN
O
Ph
4i
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

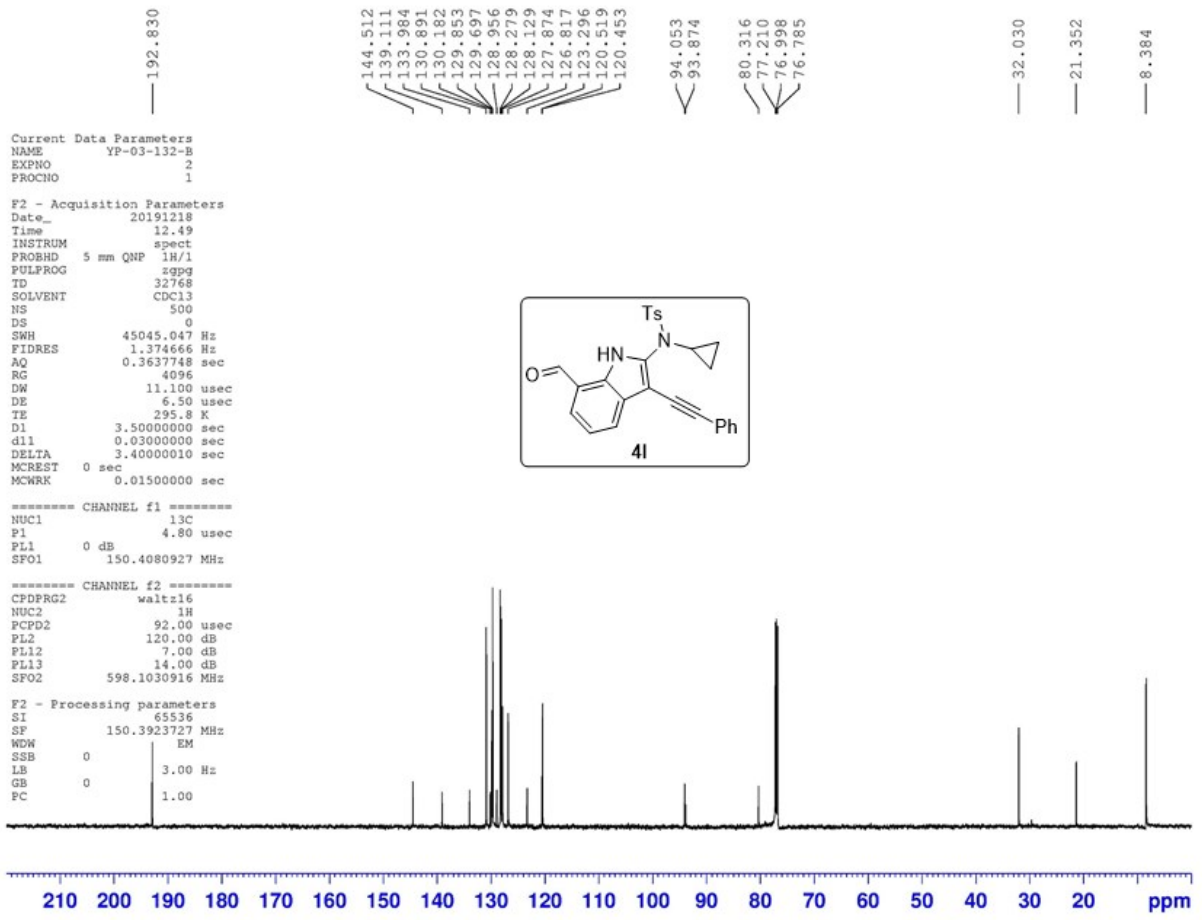

10.343
10.121
7.938
7.918
7.722
7.704
7.621
7.601
7.344
7.325
7.305
7.283
7.275
7.267
7.240
7.183
7.163
7.146
7.139
7.134
7.131
7.122
3.493
2.151
Current Data Parameters
NAME tina-2-20
EXPNO 4
PROCNO 1
F2 - Acquisition Parameters
Date_ 20191231
Time 20.00
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 12
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559039 sec
RG 126
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz
F2 - Processing parameters
SI 16384
SF 400.1500171 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00
Ts
N
Me
HN
O
Ph
4j
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
1.00
1.07
1.08
1.09
2.09
3.98
4.03
3.02
3.07

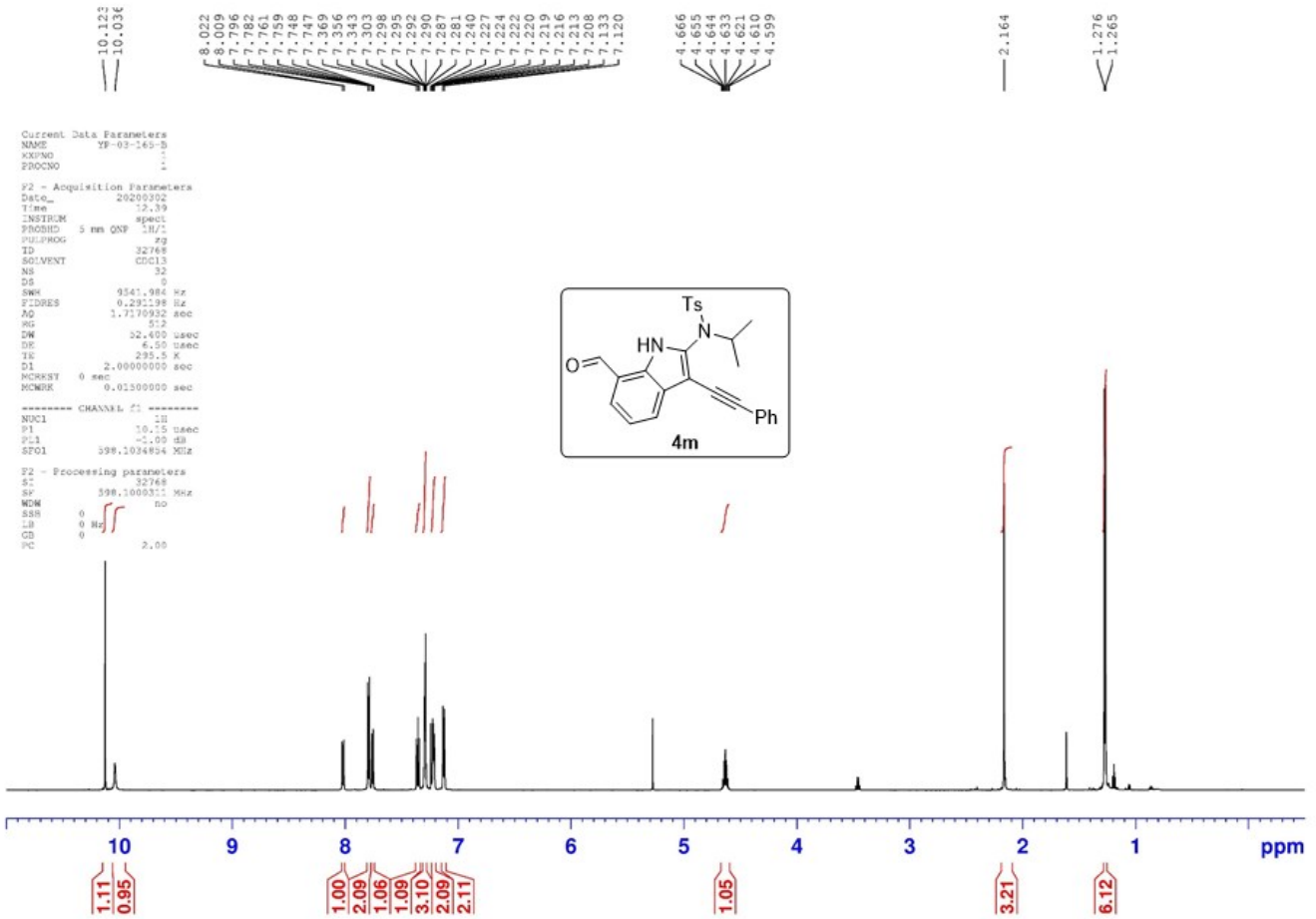

tina-2-20
192.702
144.458
138.769
133.286
131.760
130.012
129.656
129.726
128.810
128.115
127.924
127.876
126.576
123.104
120.462
94.960
92.993
79.771
77.318
77.000
76.682
37.884
21.268
Ts
N
Me
HN
O
Ph
4j
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

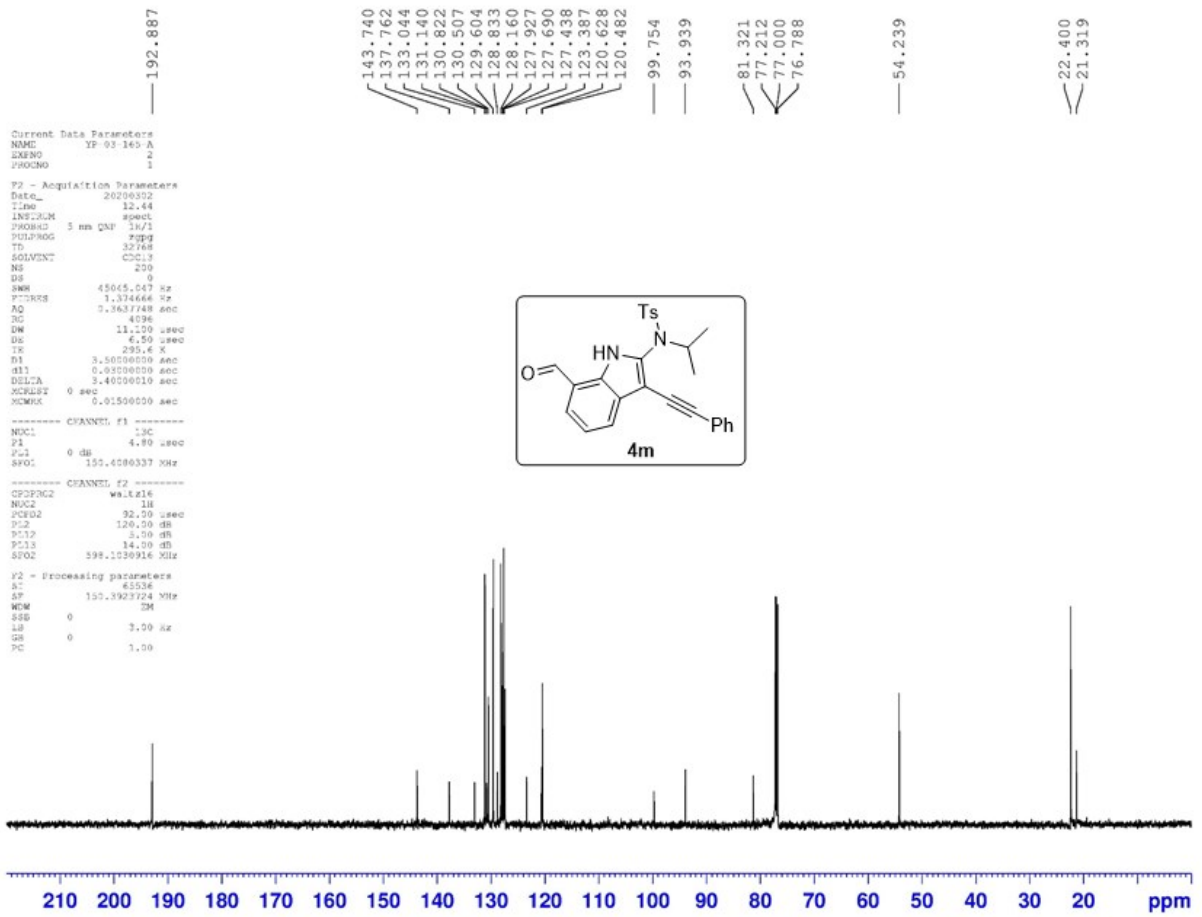

10.27
10.13
7.961
7.941
7.739
7.721
7.630
7.610
7.356
7.337
7.318
7.287
7.279
7.272
7.240
7.159
7.139
3.890
3.873
3.855
2.129
1.567
1.550
1.531
1.514
1.494
1.413
1.395
1.376
1.358
1.339
0.874
0.856
0.837
BRUKER
tina-2-19
prep wash
Current Data Parameters
NAME 20200102
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200102
Time 20.01
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 11
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 114
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz
F2 - Processing parameters
SI 16384
SF 400.1500172 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
Ts
N-nBu
HN
O
Ph
4k
12
11
10
9
8
7
6
5
4
3
2
1
ppm
1.000
1.010
1.054
1.092
2.077
4.156
4.061
2.012
3.024
2.007
2.001
3.048

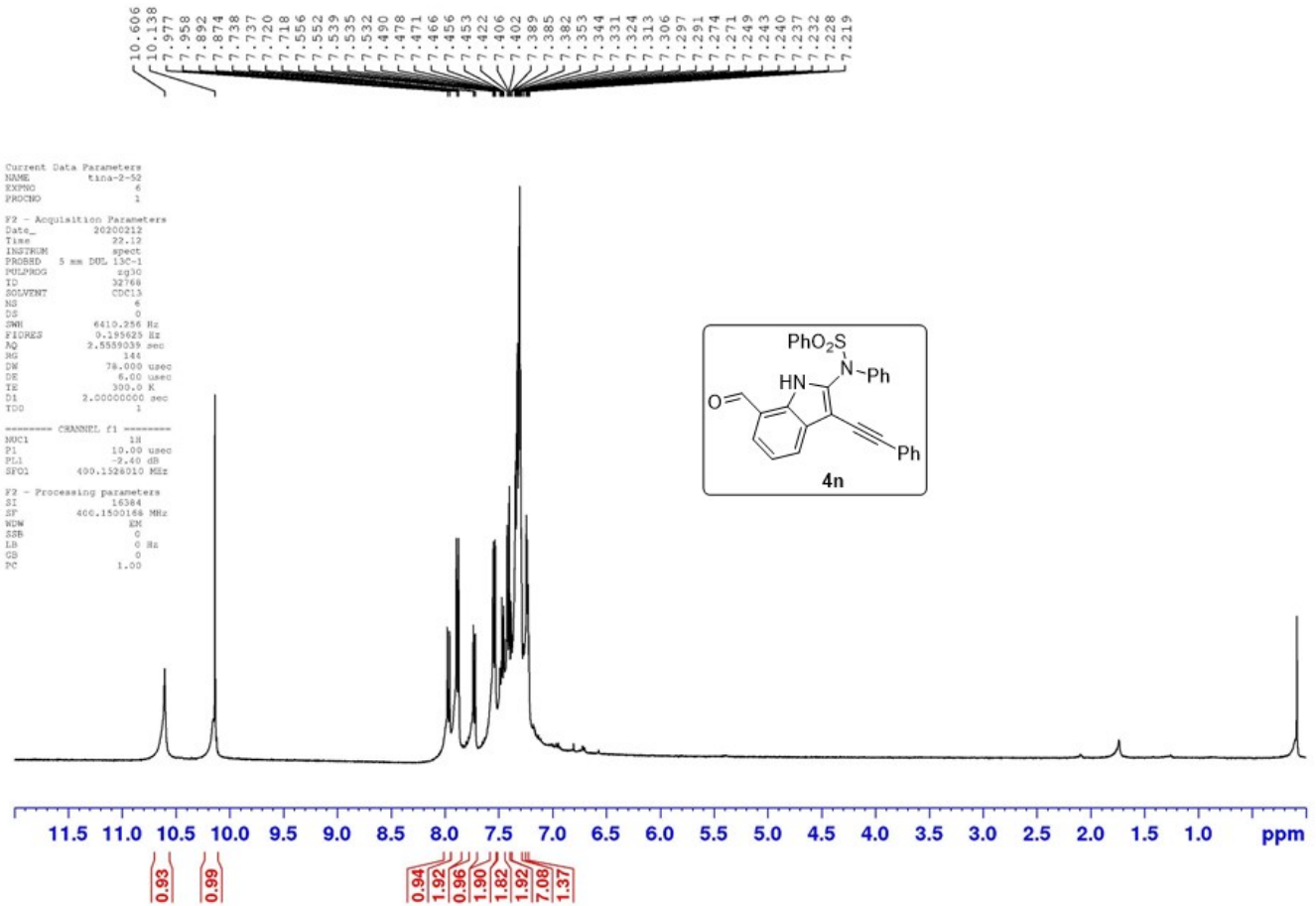

192.752
144.155
136.949
134.699
130.836
130.307
129.963
129.684
128.835
128.109
127.928
127.727
126.692
123.125
120.546
120.441
95.243
94.194
79.665
77.318
77.000
76.683
49.687
30.638
21.239
19.643
13.566
-2-19
wash
Ts
N-nBu
HN
O
Ph
4k
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

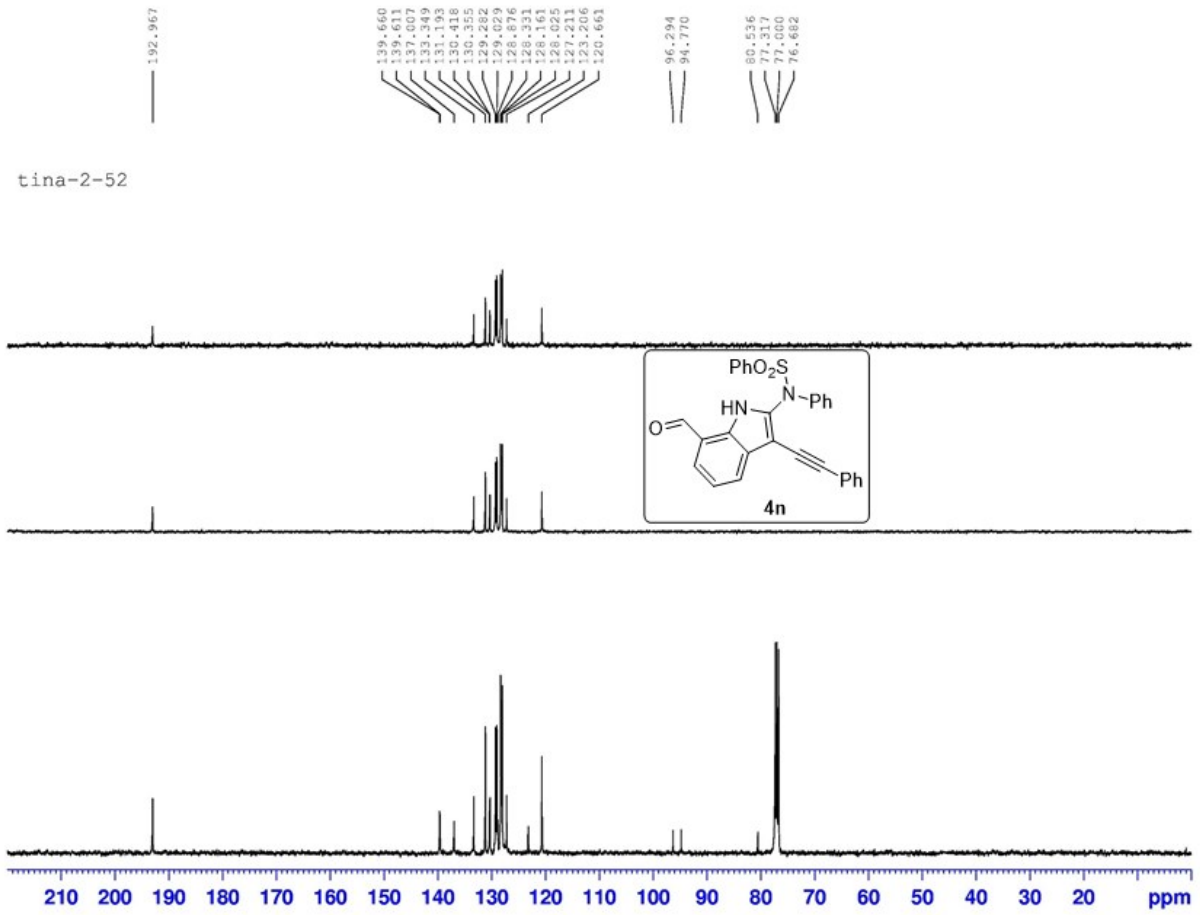

10.146
10.118
7.962
7.949
7.724
7.712
7.698
7.348
7.335
7.322
7.271
7.267
7.261
7.240
7.200
7.187
7.118
7.114
7.108
7.106
7.102
3.174
3.168
3.163
3.157
3.151
3.146
3.140
2.176
0.968
0.954
0.859
0.848
Ts
N
HN
O
Ph
4l
10
9
8
7
6
5
4
3
2
1
ppm
1.00
1.14
1.08
3.30
1.17
3.29
2.29
2.27
1.11
3.33
2.12
2.22

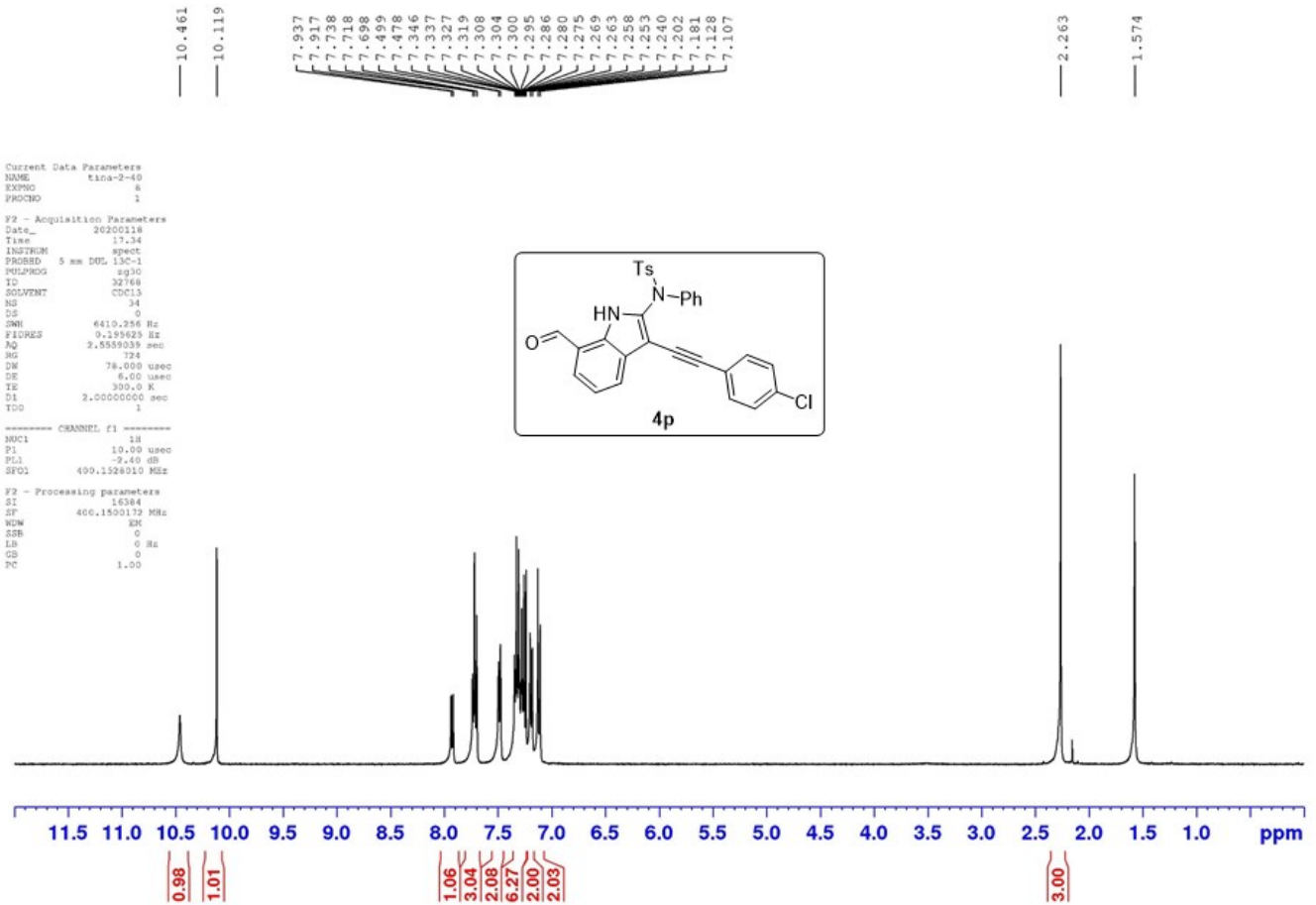

192.830
144.512
139.111
133.984
130.891
130.182
129.853
129.697
128.956
128.279
128.129
127.874
126.817
123.296
120.519
120.453
94.053
93.874
80.316
77.210
76.998
76.785
32.030
21.352
8.384
Current Data Parameters
NAME YP-03-132-B
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20191218
Time 12.49
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 500
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 295.8 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0 dB
SFO1 150.4080927 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 7.00 dB
PL13 14.00 dB
SFO2 598.1030916 MHz
F2 - Processing parameters
SI 65536
SF 150.3923727 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
Ts
N
HN
O
Ph
4l
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

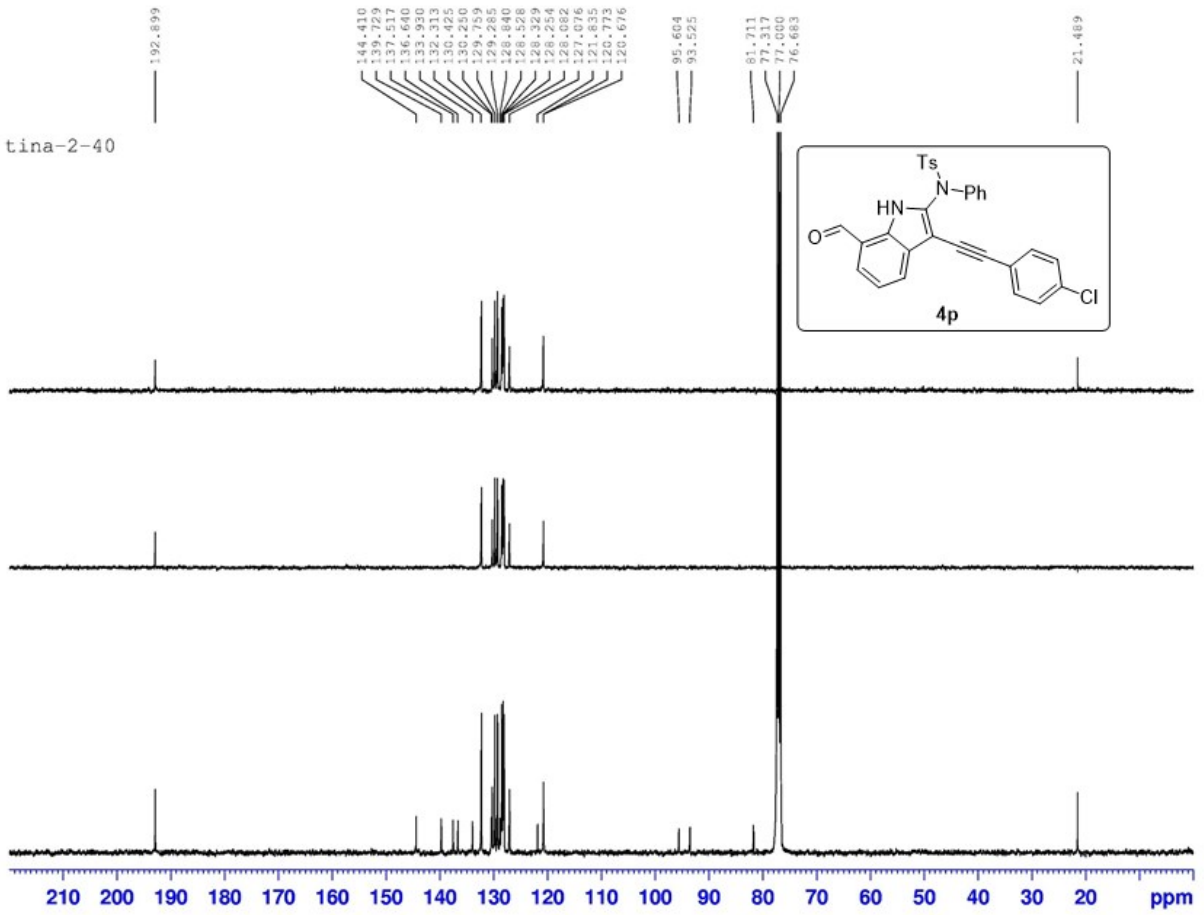

10.123
10.036
8.022
8.009
7.796
7.782
7.761
7.759
7.748
7.747
7.369
7.356
7.343
7.303
7.298
7.295
7.292
7.290
7.287
7.281
7.240
7.227
7.224
7.222
7.220
7.219
7.216
7.213
7.208
7.133
7.120
4.666
4.655
4.644
4.633
4.621
4.610
4.599
2.164
1.276
1.265
Current Data Parameters
NAME YP-03-165-5
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200302
Time 12.39
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 9541.984 Hz
FIDRES 0.291198 Hz
AQ 1.7170932 sec
RG 512
DW 52.400 usec
DE 6.50 usec
TE 295.5 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
-------- CHANNEL f1 --------
NUC1 1H
P1 10.75 usec
PL1 -1.00 dB
SFO1 598.1034894 MHz
F2 - Processing parameters
SI 32768
SF 598.1000311 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 2.00
Ts
N
HN
O
Ph
4m
10
9
8
7
6
5
4
3
2
1
ppm
1.11
0.95
1.00
2.09
1.06
1.09
3.10
2.09
2.11
1.05
3.21
6.12

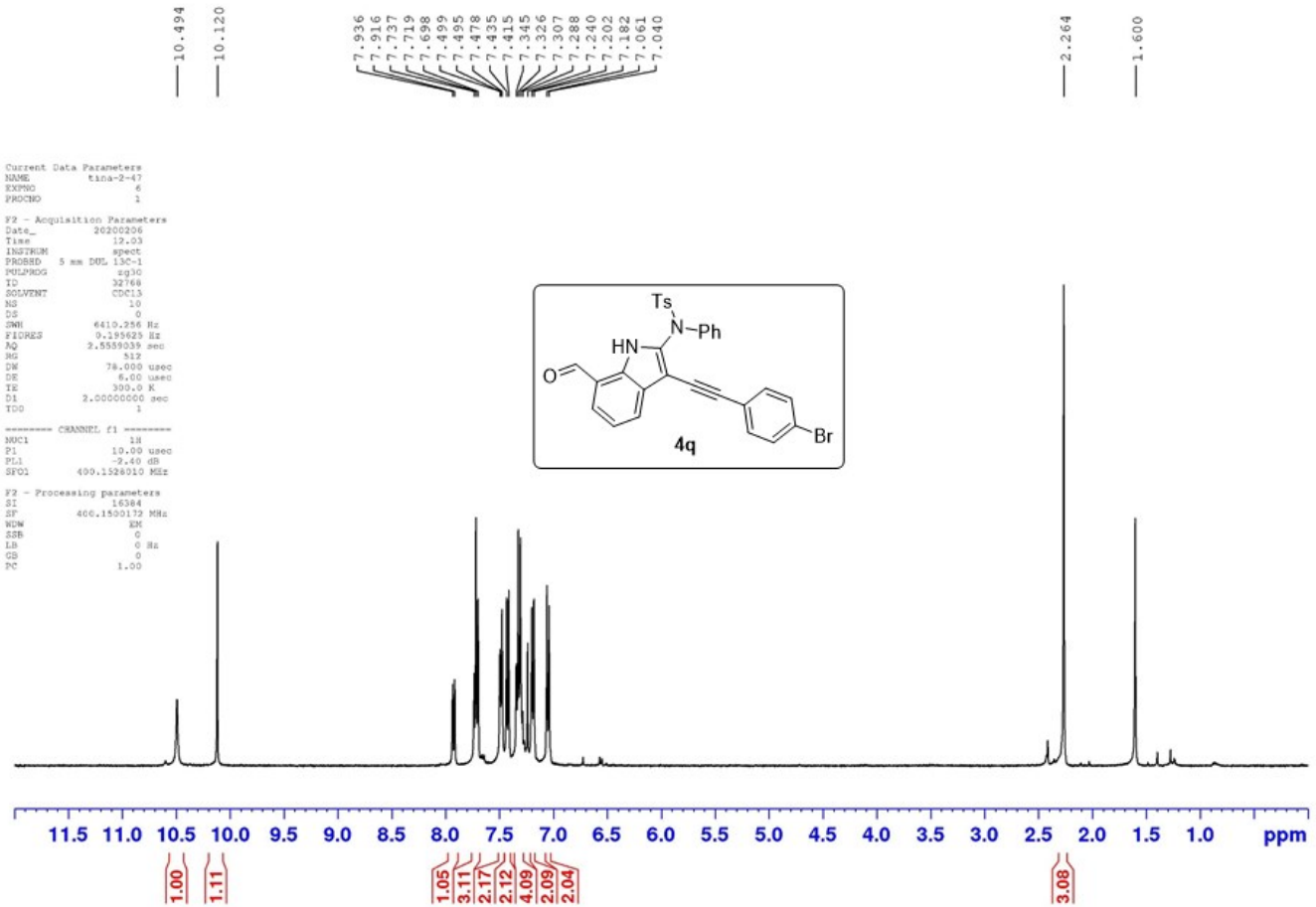

192.887
143.740
137.762
133.044
131.140
130.822
130.507
129.604
128.833
128.160
127.927
127.690
127.438
123.387
120.628
120.482
99.754
93.939
81.321
77.212
77.000
76.788
54.239
22.400
21.319
Ts
N
HN
O
Ph
4m
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

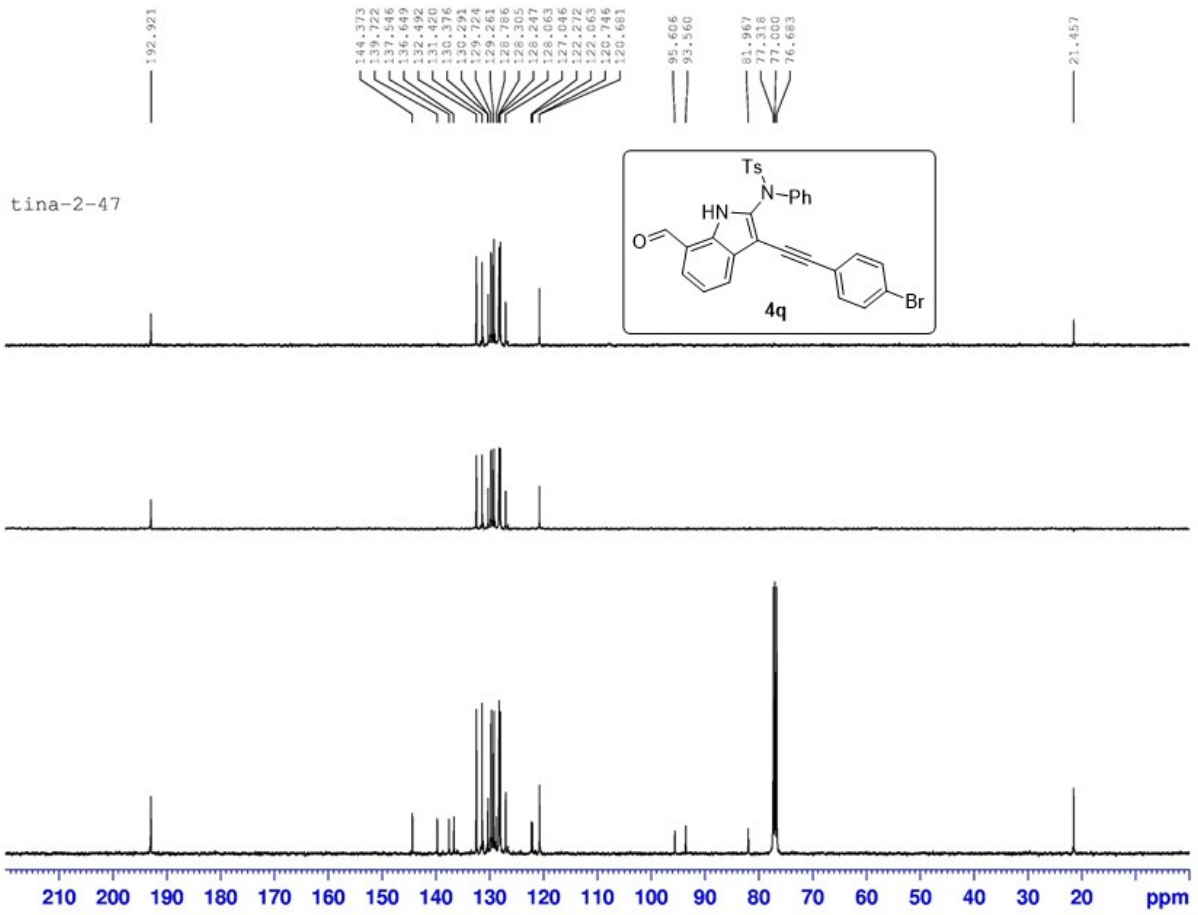

10.606
10.138
7.977
7.958
7.892
7.874
7.738
7.737
7.720
7.718
7.556
7.552
7.539
7.535
7.532
7.490
7.478
7.471
7.466
7.456
7.453
7.422
7.406
7.402
7.389
7.385
7.382
7.353
7.344
7.331
7.324
7.313
7.306
7.297
7.291
7.274
7.271
7.249
7.243
7.240
7.237
7.232
7.228
7.219
Current Data Parameters
NAME tina-2-52
EXPNO 6
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200212
Time 22.12
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 4
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559039 sec
RG 144
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1326010 MHz
F2 - Processing parameters
SI 16384
SF 400.1300164 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00
PhO2S
N
Ph
HN
O
Ph
4n
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
0.93
0.99
0.94
1.92
0.96
1.90
1.82
1.92
7.08
1.37

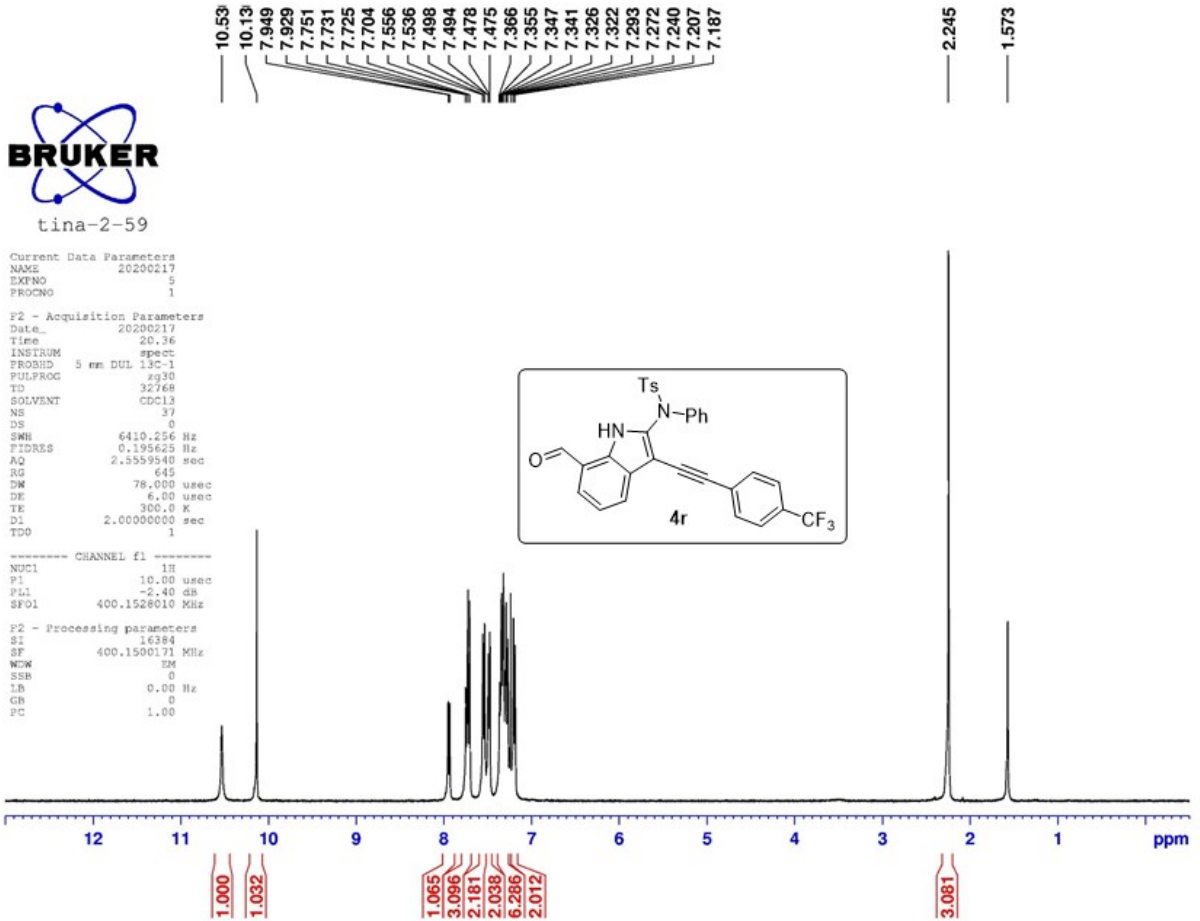

192.967
139.660
139.611
137.007
133.349
131.193
130.418
130.355
129.282
129.029
128.876
128.331
128.161
128.025
127.211
123.206
120.661
96.294
94.770
80.536
77.317
77.000
76.682
tina-2-52
PhO2S
N
Ph
HN
O
Ph
4n
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

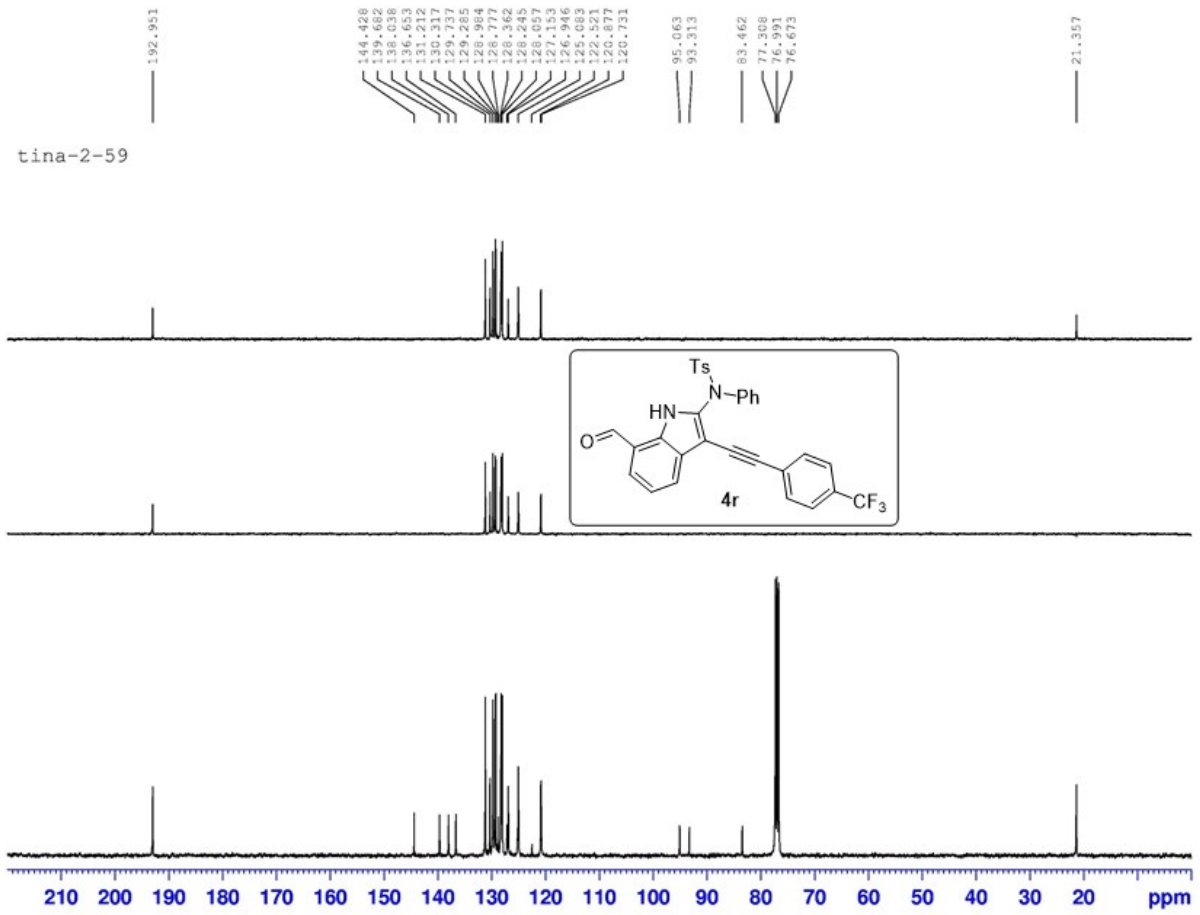

10.461
10.119
7.937
7.917
7.738
7.718
7.698
7.499
7.478
7.346
7.337
7.327
7.319
7.308
7.304
7.300
7.295
7.286
7.280
7.275
7.269
7.263
7.258
7.253
7.240
7.202
7.181
7.128
7.107
2.263
1.574
Current Data Parameters
NAME tina-2-40
EXPNO 6
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200118
Time 17.34
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 34
DS 0
SWH 6410.256 Hz
FIDRES 9.195625 Hz
AQ 2.5559039 sec
RG 724
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1326010 MHz
F2 - Processing parameters
SI 16384
SF 400.1300173 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00
Ts
N
Ph
HN
O
Cl
4p
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
0.98
1.01
1.06
3.04
2.08
6.27
2.00
2.03
3.00

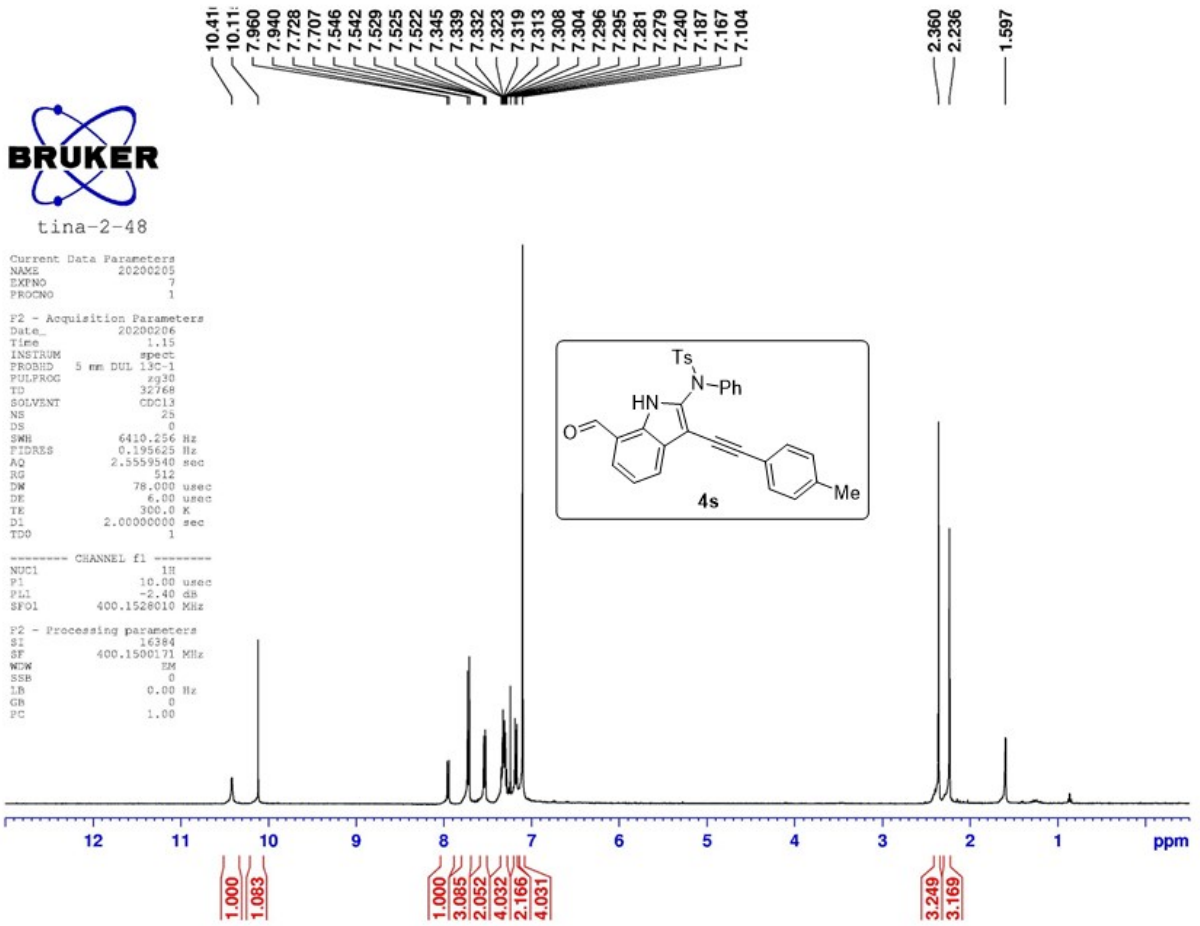

192.899
144.410
139.729
137.517
136.640
133.930
132.313
130.425
130.250
129.759
129.285
128.840
128.528
128.329
128.254
128.082
127.076
121.635
120.773
120.676
95.604
93.525
81.711
77.317
77.000
76.683
21.489
tina-2-40
Ts
N–Ph
HN
O
Cl
4p
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

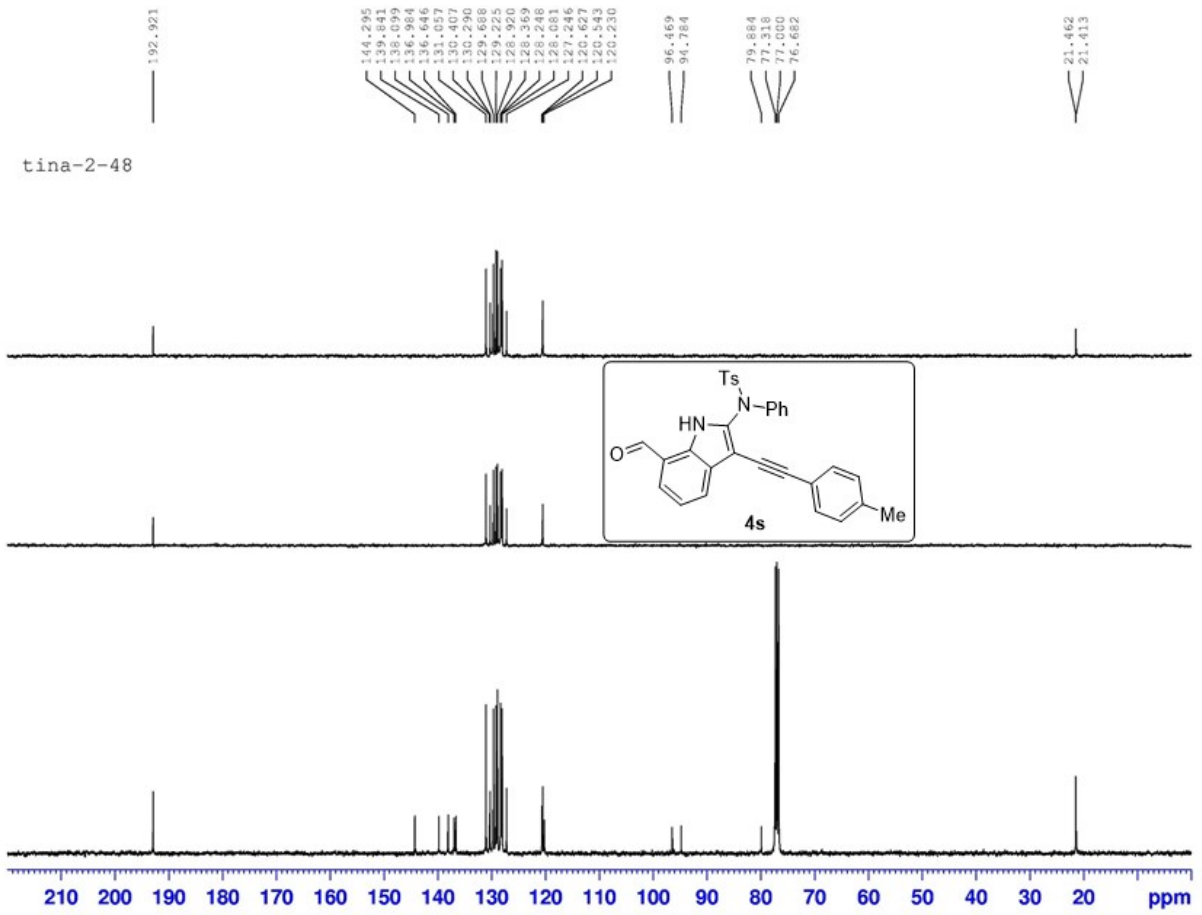

10.494
10.120
7.936
7.916
7.737
7.719
7.698
7.499
7.495
7.478
7.435
7.415
7.345
7.326
7.307
7.288
7.240
7.202
7.182
7.061
7.040
2.264
1.600
Current Data Parameters
NAME tina-2-47
EXPNO 6
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200206
Time 12.03
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 10
DS 0
SWH 6410.256 Hz
FIDRES 9.195625 Hz
AQ 2.5559039 sec
RG 512
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1326010 MHz
F2 - Processing parameters
SI 16384
SF 400.1300173 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00
Ts
N–Ph
HN
O
Br
4q
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.00
1.11
1.05
3.11
2.17
2.12
4.09
2.09
2.04
3.08

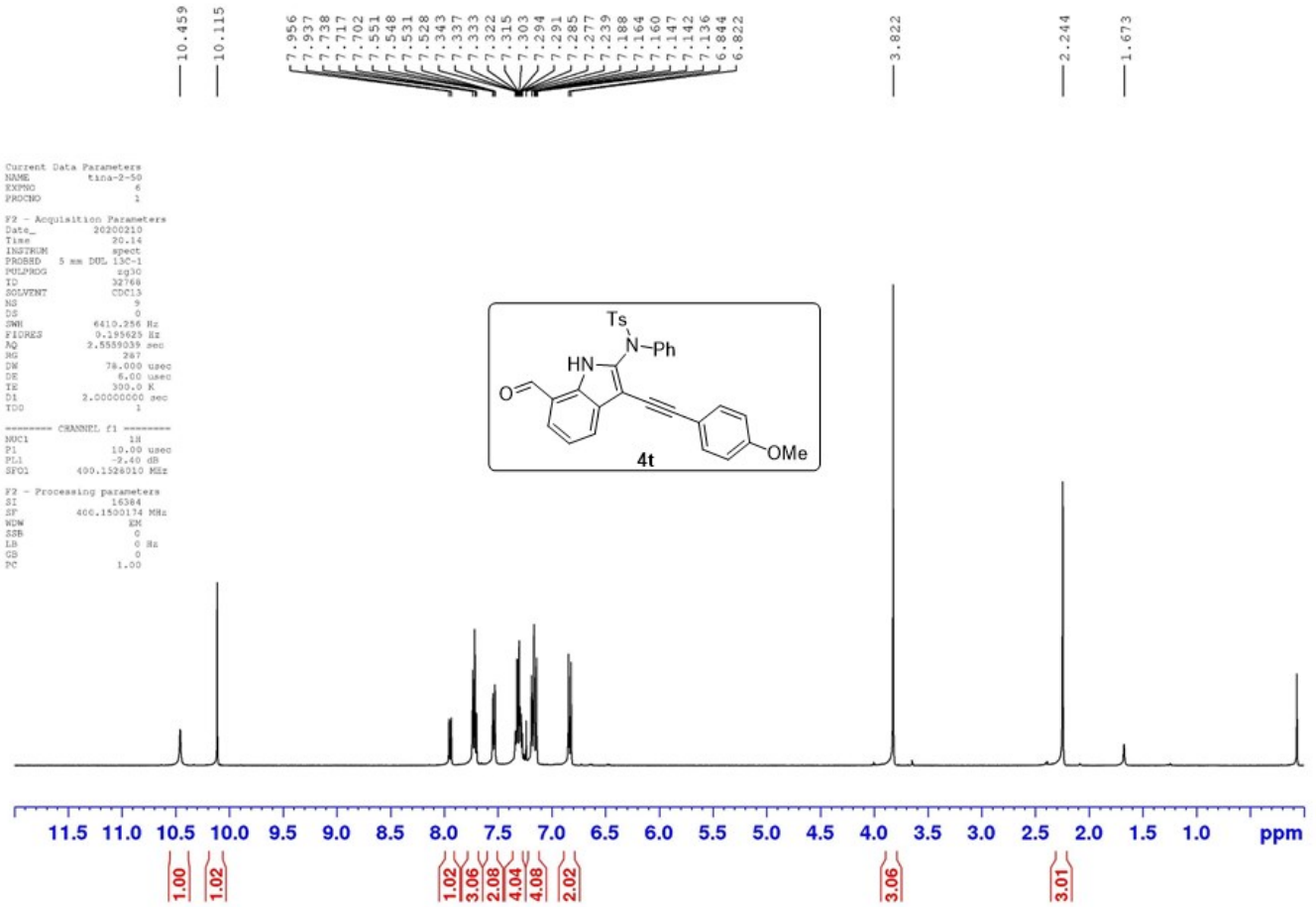

192.921
144.373
139.722
137.546
136.649
132.492
131.420
130.376
130.291
129.724
129.261
128.786
128.305
128.247
128.063
127.046
122.272
122.663
120.746
120.661
95.666
93.560
81.967
77.318
77.000
76.683
21.457
tina-2-47
Ts
N–Ph
HN
O
Br
4q
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

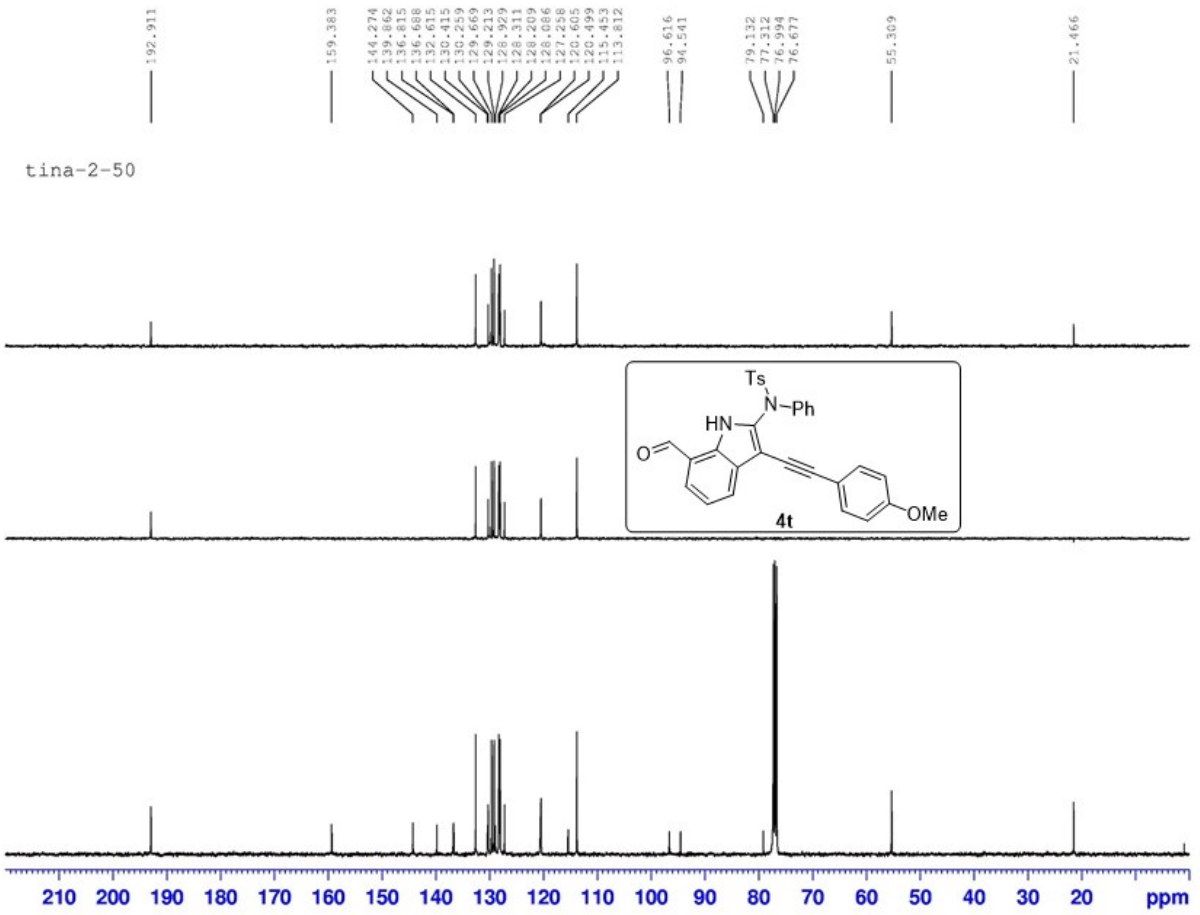

10.53
10.13
7.949
7.929
7.751
7.731
7.725
7.704
7.556
7.536
7.498
7.494
7.478
7.475
7.366
7.355
7.347
7.341
7.326
7.322
7.293
7.272
7.240
7.207
7.187
2.245
1.573
BRUKER
tina-2-59
Current Data Parameters
NAME 20200217
EXPNO 5
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200217
Time 20.36
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 37
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 645
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz
F2 - Processing parameters
SI 16384
SF 400.1500171 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
Ts
N–Ph
HN
O
4r
CF3
12
11
10
9
8
7
6
5
4
3
2
1
ppm
1.000
1.032
1.065
3.096
2.181
2.038
6.286
2.012
3.081

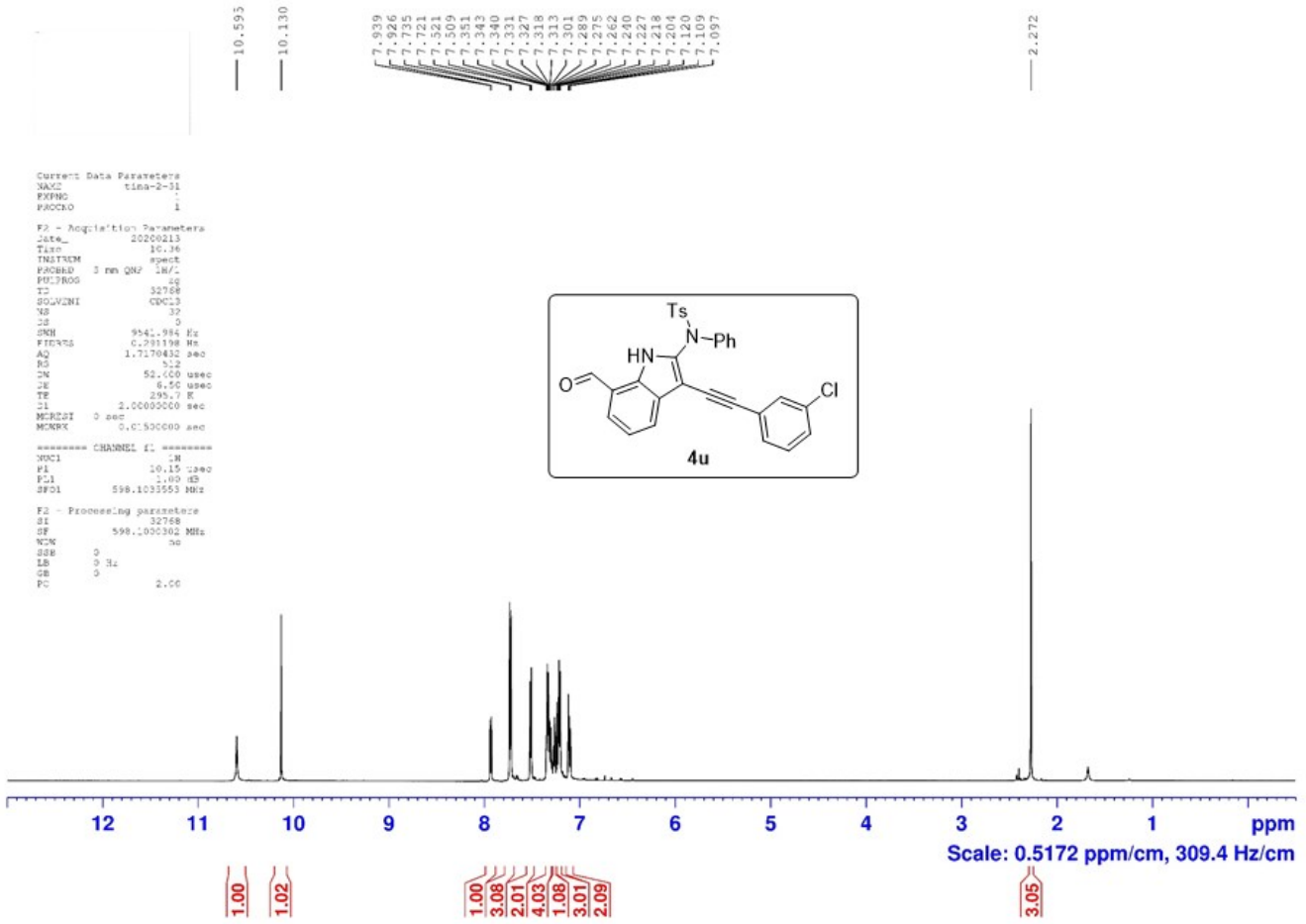

192.951
144.428
139.682
138.038
136.653
131.212
130.317
129.737
129.285
128.984
128.777
128.362
128.245
128.057
127.153
126.946
125.683
122.521
120.977
120.731
95.063
93.313
83.462
77.308
76.991
76.673
21.357
tina-2-59
Ts
N–Ph
HN
O
4r
CF3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

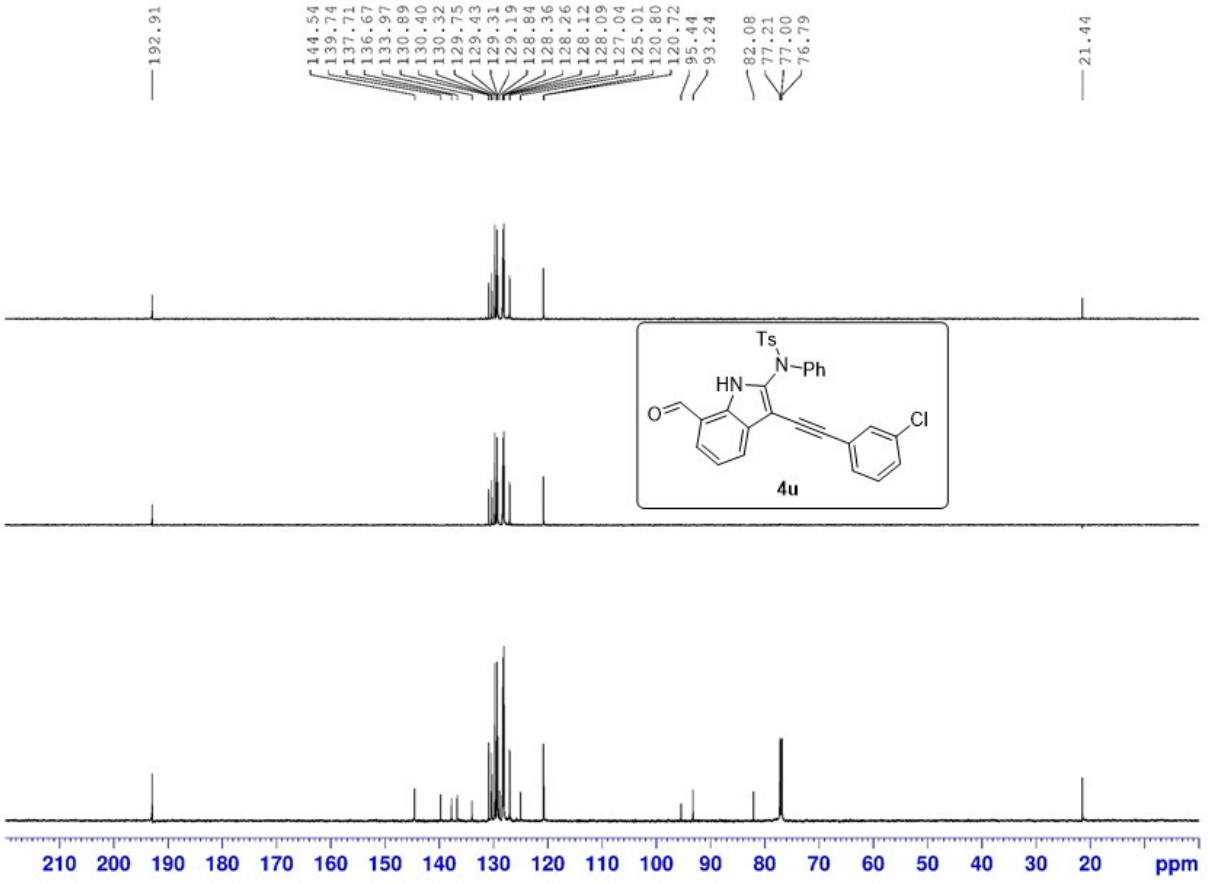

10.41
10.11
7.960
7.940
7.728
7.707
7.546
7.542
7.529
7.525
7.522
7.345
7.339
7.332
7.323
7.319
7.313
7.308
7.304
7.296
7.295
7.281
7.279
7.240
7.187
7.167
7.104
2.360
2.236
1.597
BRUKER
tina-2-48
Current Data Parameters
NAME 20200205
EXPNO 7
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200206
Time 1.15
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 25
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 512
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz
F2 - Processing parameters
SI 16384
SF 400.1500171 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
Ts
N–Ph
HN
O
Me
4s
12
11
10
9
8
7
6
5
4
3
2
1
ppm
1.000
1.083
1.000
3.085
2.052
4.032
2.166
4.031
3.249
3.169

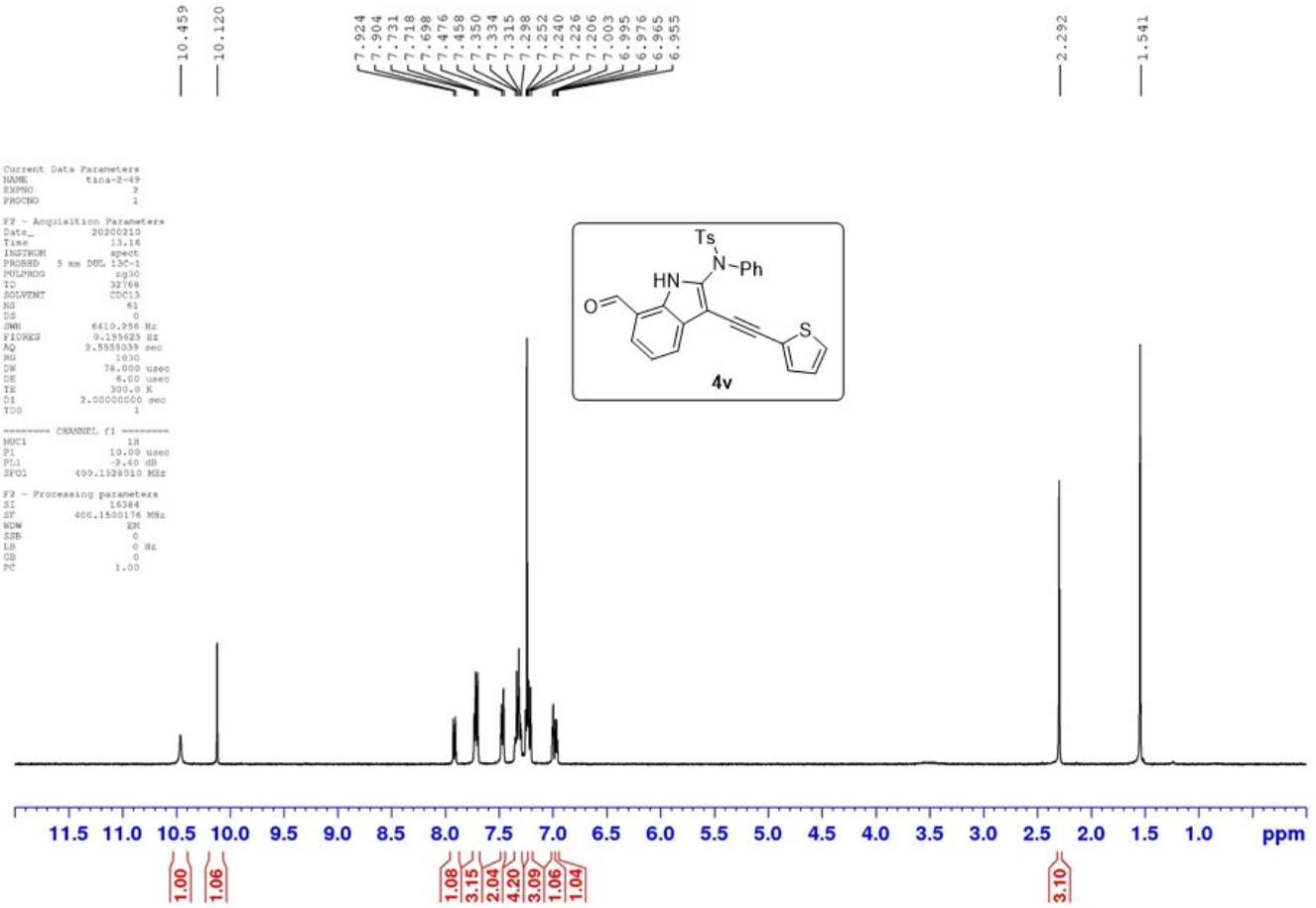

192.921
144.295
139.641
138.099
136.984
136.646
131.057
130.407
130.290
129.668
129.225
128.920
128.569
128.248
128.061
127.246
126.627
126.543
126.230
96.469
94.784
79.684
77.318
77.000
76.682
21.462
21.413
tina-2-48
Ts
N
Ph
HN
O
Me
4s
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

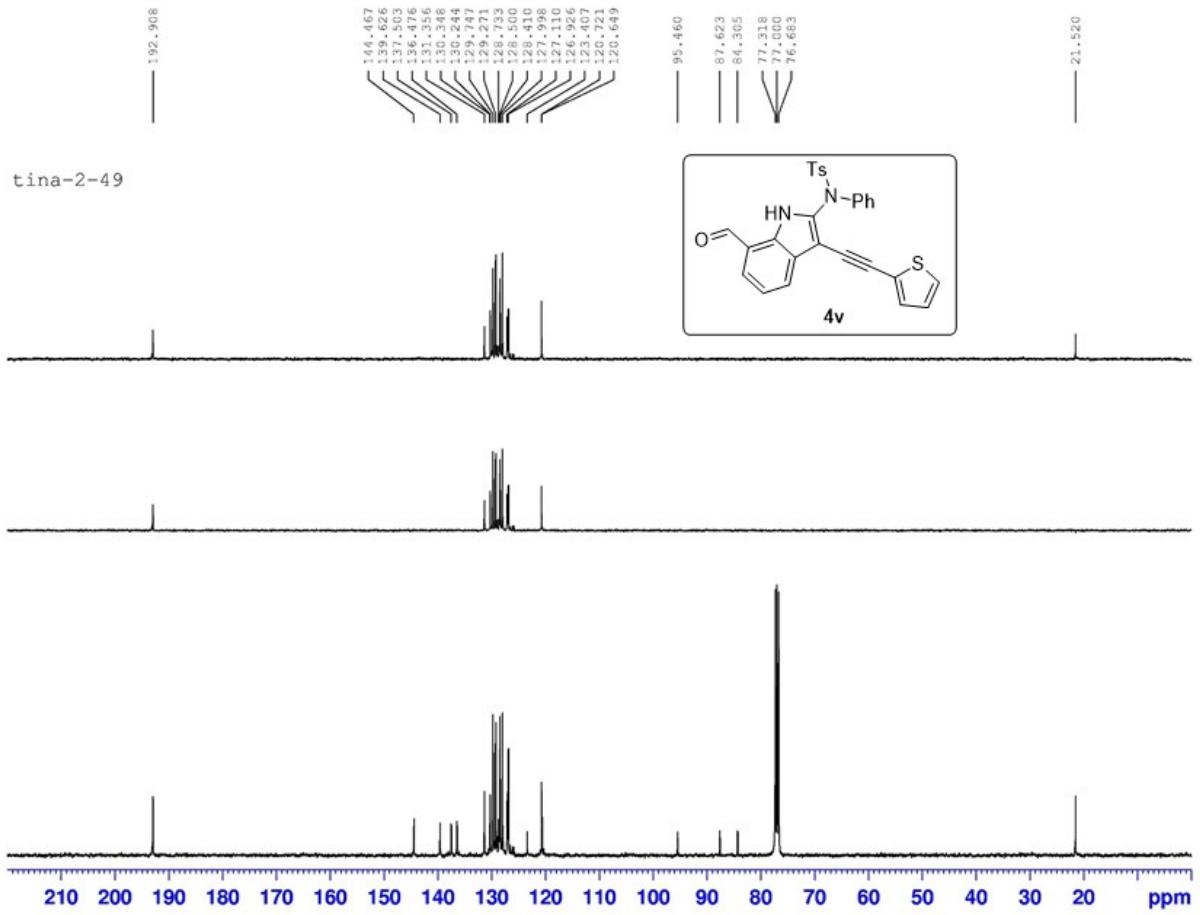

10.459
10.115
7.956
7.937
7.738
7.717
7.702
7.551
7.548
7.531
7.528
7.343
7.337
7.333
7.322
7.315
7.303
7.294
7.291
7.285
7.277
7.239
7.188
7.164
7.160
7.147
7.142
7.136
6.844
6.822
3.822
2.244
1.673
Current Data Parameters
NAME tina-2-50
EXPNO 6
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200210
Time 20.14
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 9
DS 0
SWH 6410.256 Hz
FIDRES 9.195625 Hz
AQ 2.5559039 sec
RG 287
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1326010 MHz
F2 - Processing parameters
SI 16384
SF 400.1300174 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00
Ts
N–Ph
HN
O
OMe
4t
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.00
1.02
1.02
3.06
2.08
4.04
4.08
2.02
3.06
3.01

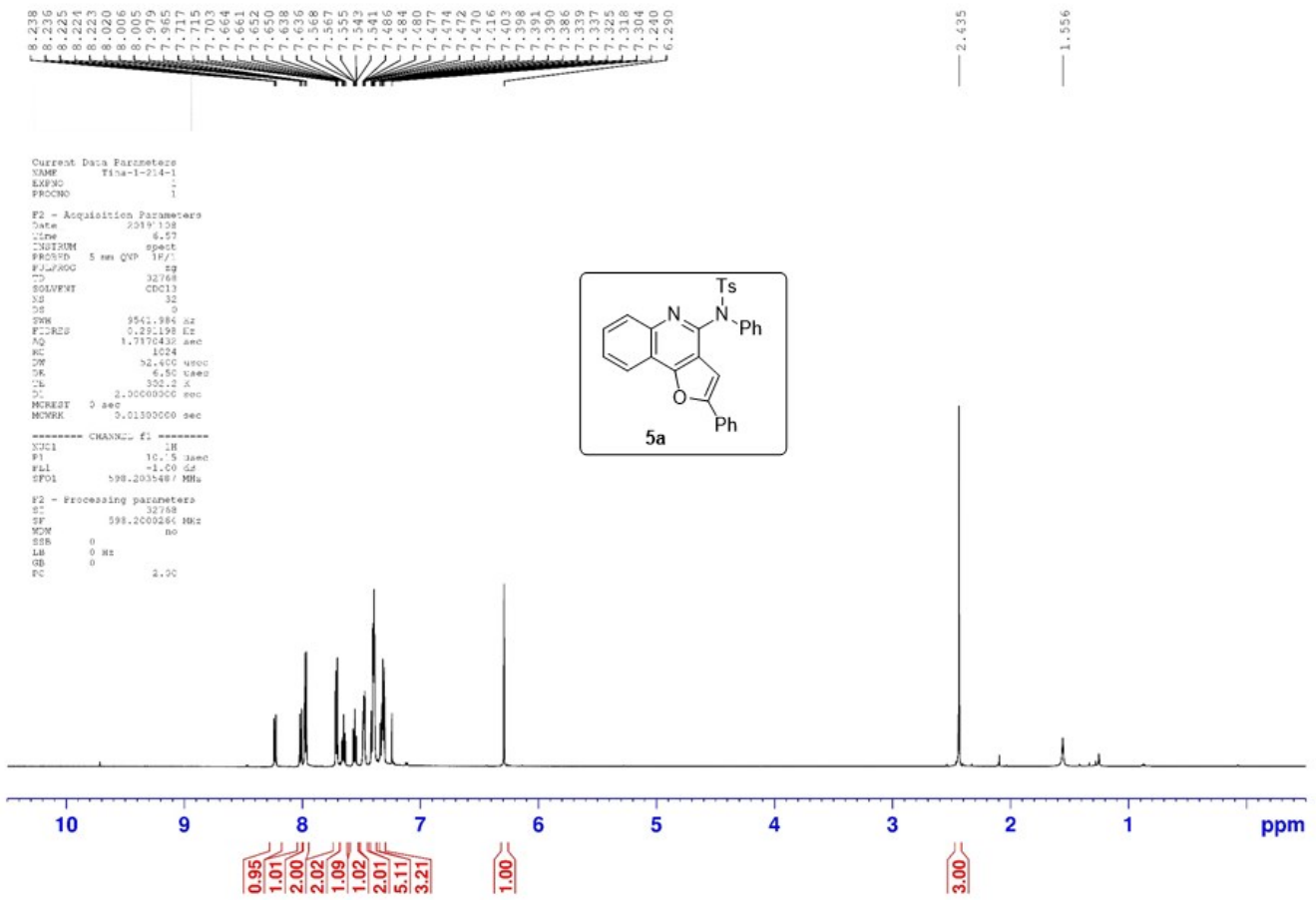

192.911
159.383
144.274
139.862
136.815
136.688
132.615
130.415
130.259
129.669
129.213
128.929
128.311
128.209
128.086
127.258
120.605
120.499
115.453
113.812
96.616
94.541
79.132
77.312
76.994
76.677
55.309
21.466
tina-2-50
Ts
N–Ph
HN
O
OMe
4t
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

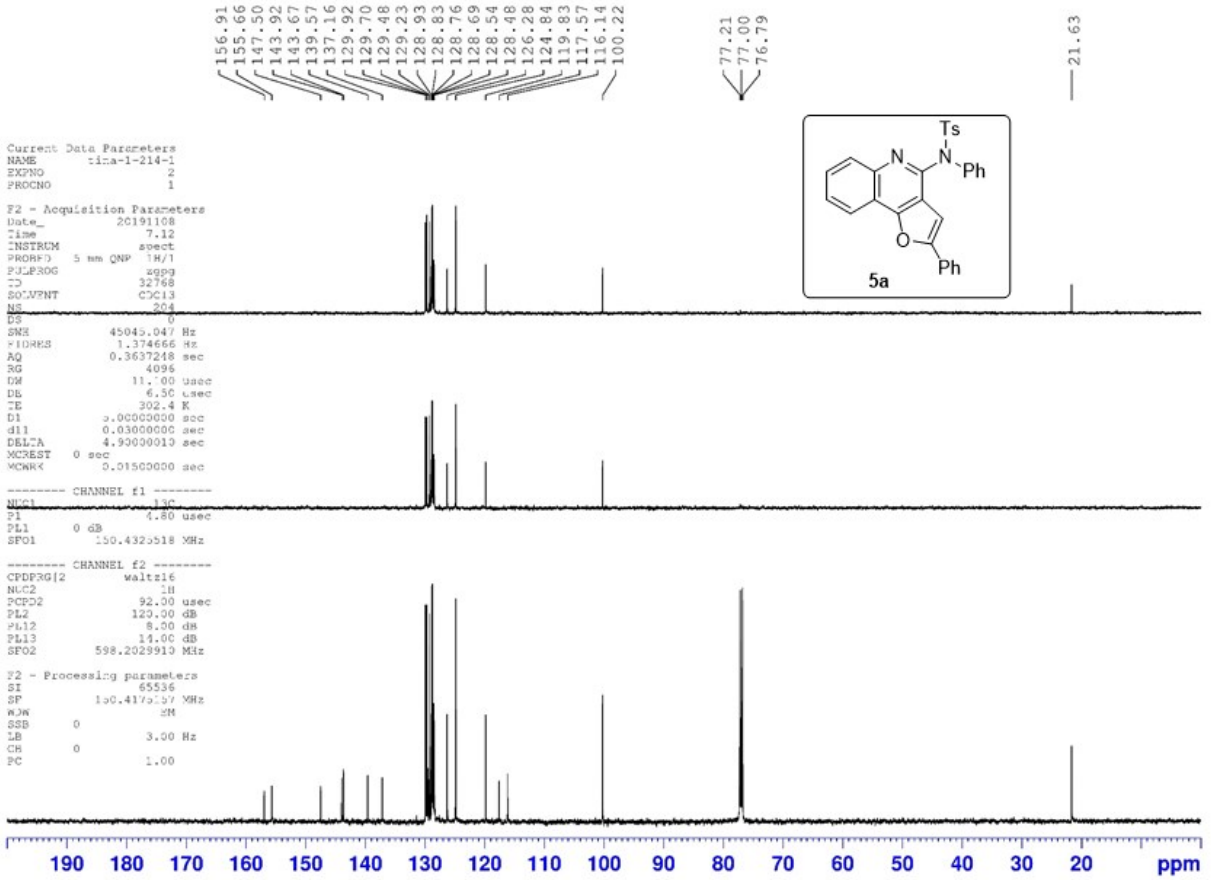

10.595
10.130
7.939
7.926
7.735
7.721
7.521
7.509
7.351
7.343
7.340
7.331
7.327
7.318
7.313
7.301
7.289
7.275
7.262
7.240
7.227
7.218
7.204
7.120
7.109
7.097
2.272
Ts
N–Ph
HN
O
Cl
4u
12
11
10
9
8
7
6
5
4
3
2
1
ppm
Scale: 0.5172 ppm/cm, 309.4 Hz/cm
1.00
1.02
1.00
3.08
2.01
4.03
1.08
3.01
2.09
3.05

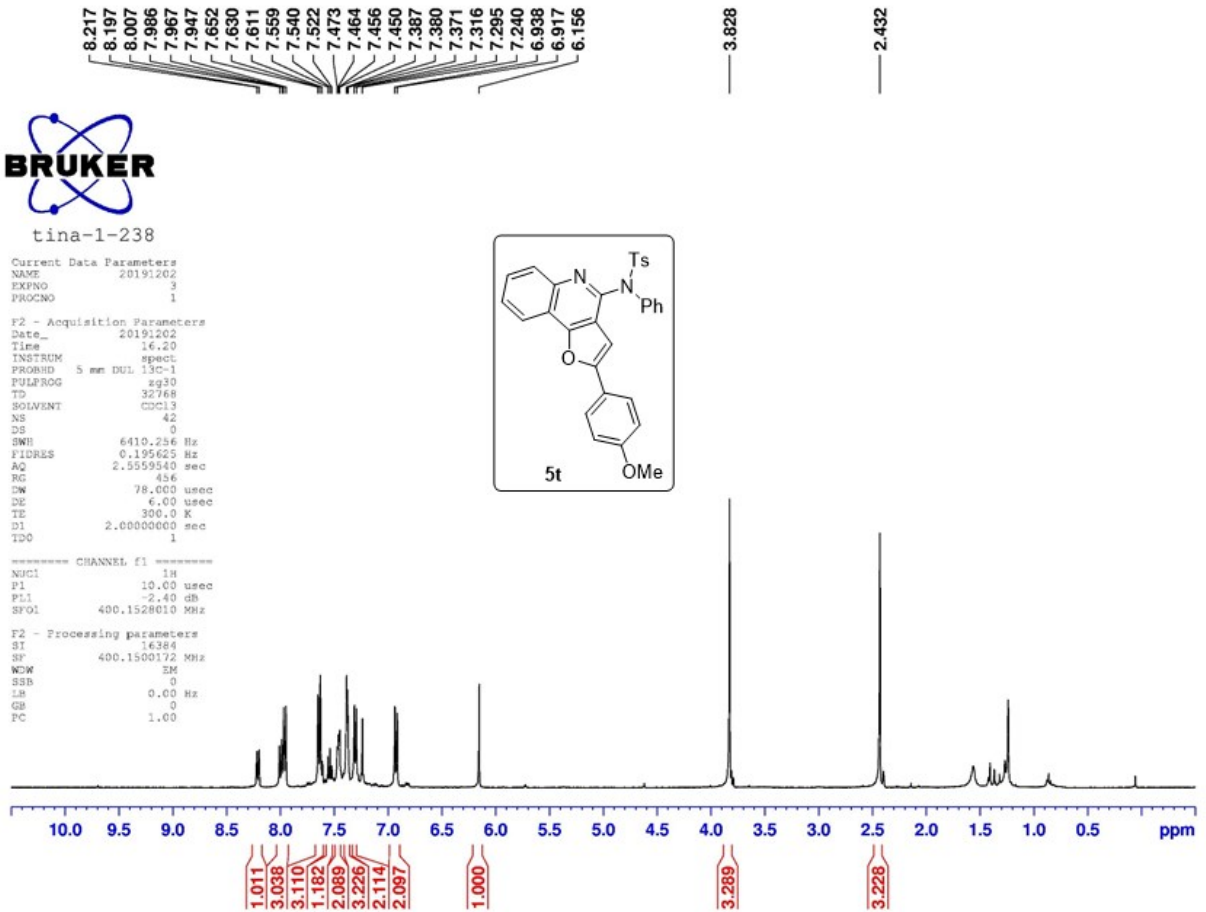

192.91
144.54
139.74
137.71
136.67
133.97
130.89
130.40
130.32
129.75
129.43
129.31
129.19
128.84
128.36
128.26
128.12
128.09
127.04
125.01
120.80
120.72
95.44
93.24
82.08
77.21
77.00
76.79
21.44
Ts
N
Ph
HN
O
Cl
4u
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

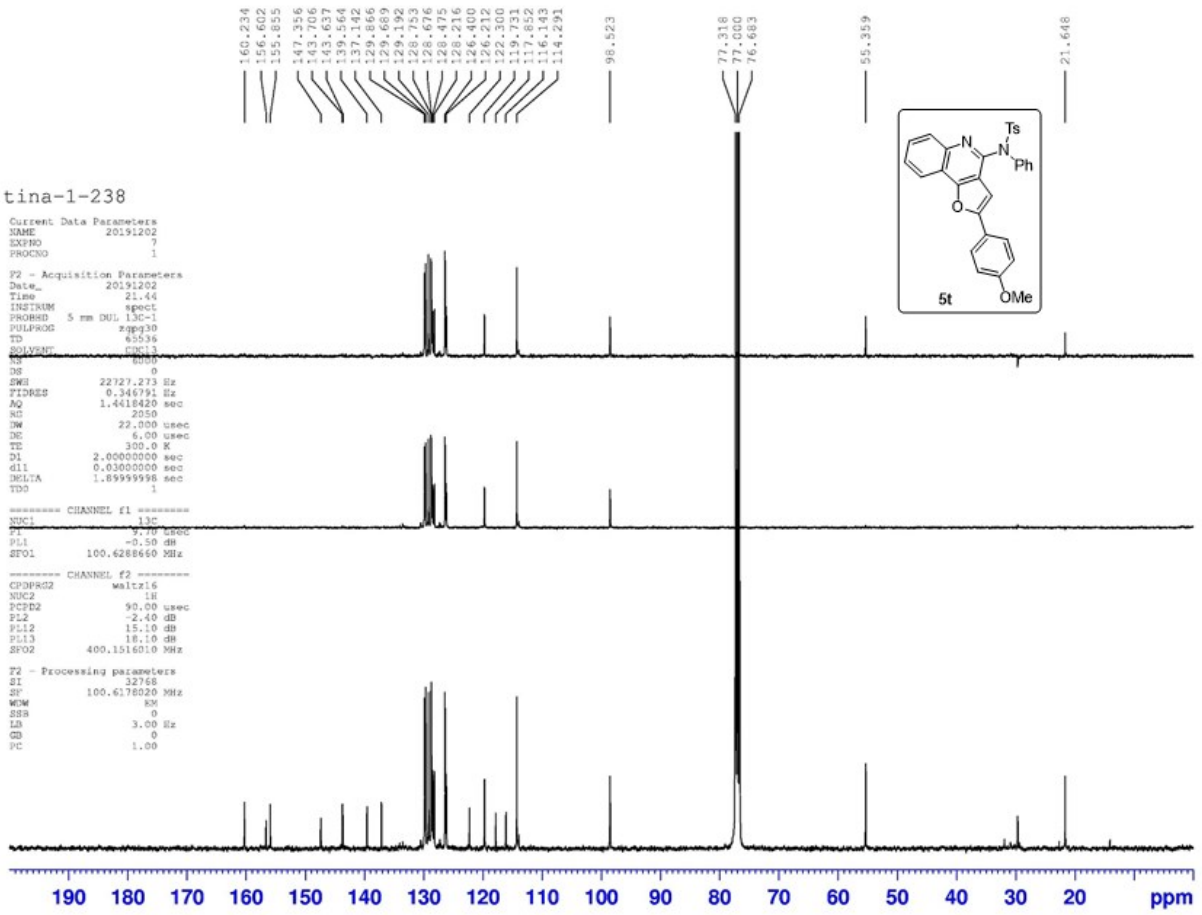

10.459
10.120
7.924
7.904
7.731
7.718
7.698
7.476
7.458
7.350
7.334
7.315
7.298
7.252
7.240
7.226
7.206
7.003
6.995
6.976
6.965
6.955
2.292
1.541
Current Data Parameters
NAME tina-2-49
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200210
Time 13.16
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 61
DS 0
SWH 6410.256 Hz
FIDRES 9.195625 Hz
AQ 2.5559039 sec
RG 1030
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1326010 MHz
F2 - Processing parameters
SI 16384
SF 400.1300176 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00
Ts
N
Ph
HN
O
S
4v
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.00
1.06
1.08
3.15
2.04
4.20
3.09
1.06
1.04
3.10

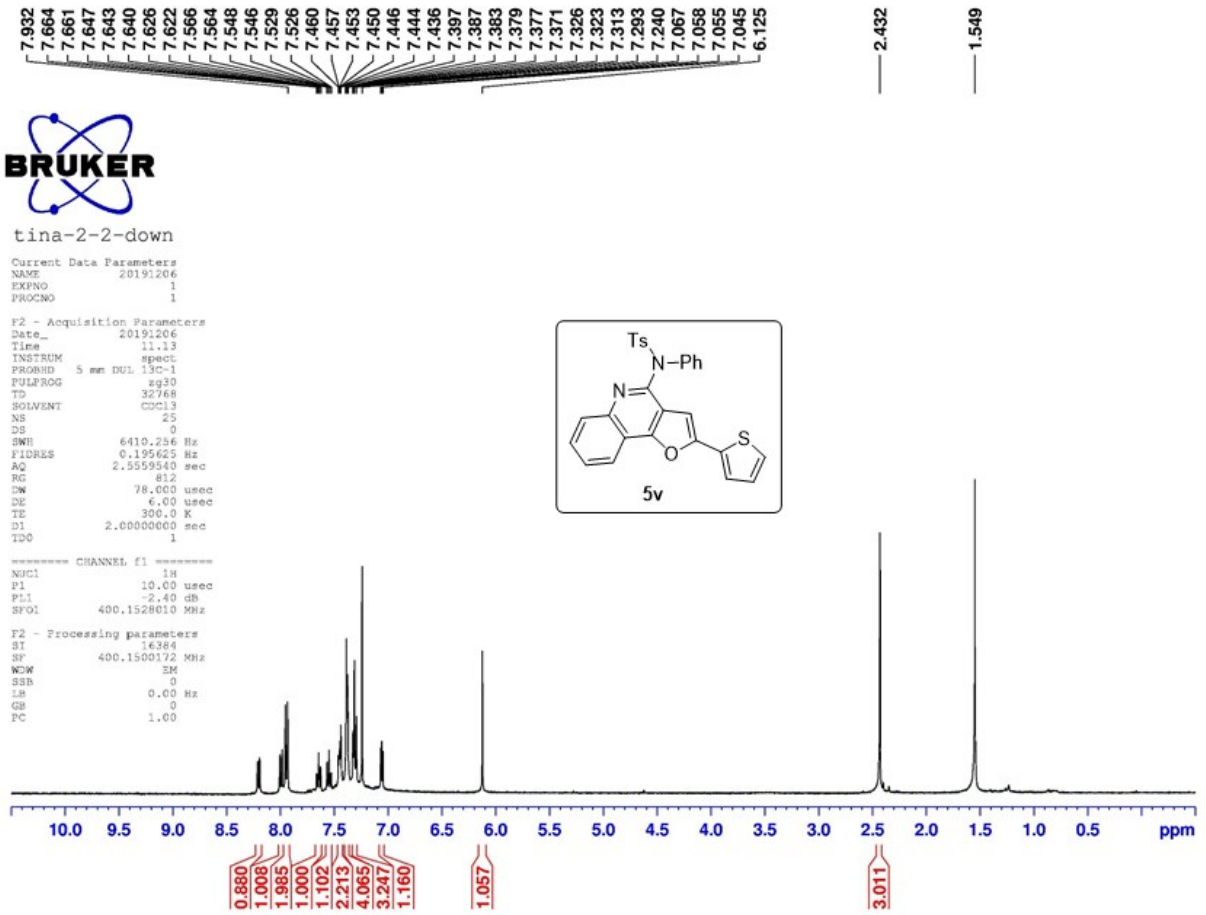

192.908
144.467
139.626
137.503
136.476
131.356
131.248
130.244
129.747
129.271
128.733
128.500
128.410
127.998
127.110
126.926
123.407
120.721
120.649
95.460
87.623
84.305
77.318
77.000
76.683
21.520
tina-2-49
Ts
N
Ph
HN
O
S
4v
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

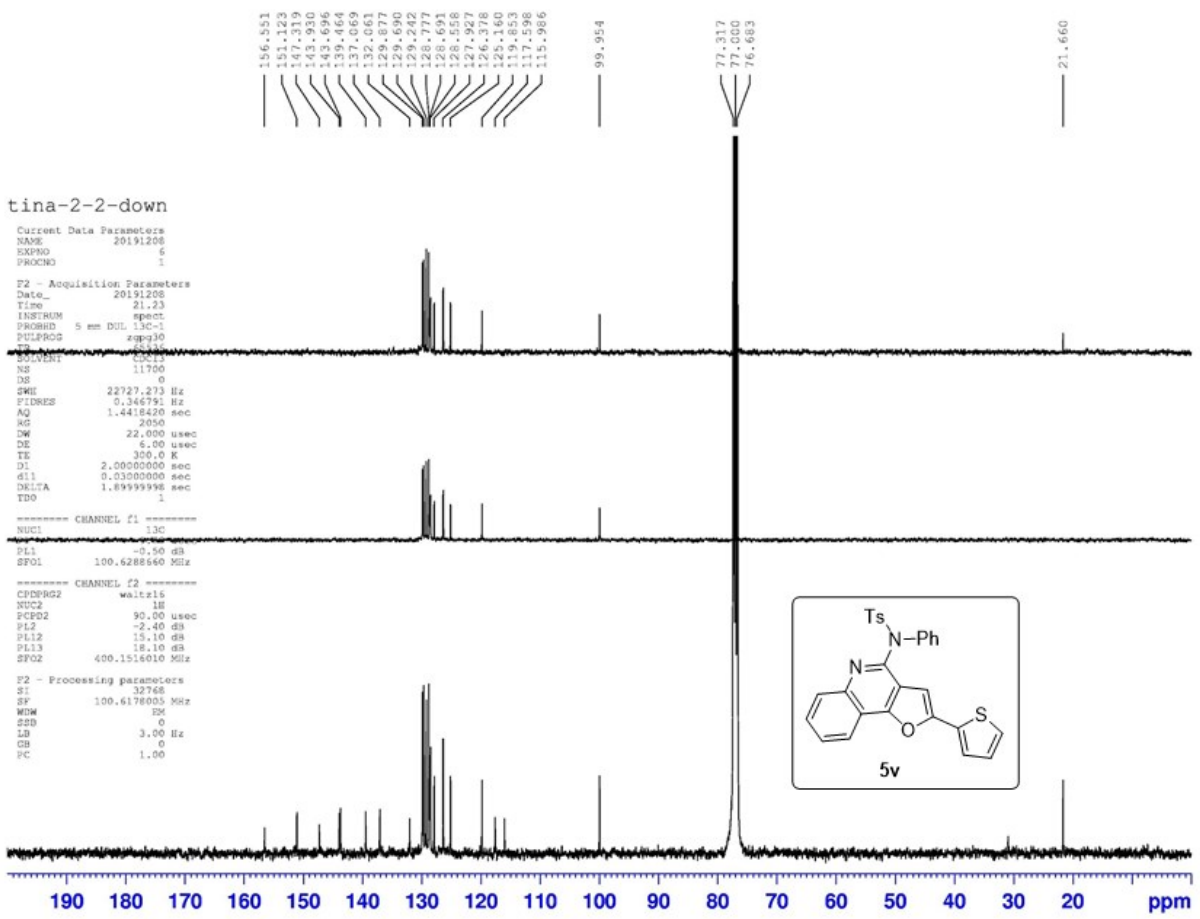

8.238
8.236
8.225
8.224
8.223
8.020
8.006
8.005
7.979
7.965
7.717
7.715
7.703
7.664
7.661
7.652
7.650
7.638
7.636
7.568
7.567
7.555
7.543
7.541
7.486
7.484
7.480
7.477
7.474
7.472
7.470
7.416
7.403
7.398
7.391
7.390
7.386
7.339
7.337
7.325
7.318
7.304
7.240
6.290
2.435
1.556
Current Data Parameters
NAME Tina-1-214-1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date 20191108
Time 6.57
INSTRUM spect
PROBHD 5 mm QNP 1H/
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 9541.984 Hz
FIDRES 0.291198 Hz
AQ 1.7170432 sec
RG 1024
DW 52.400 usec
DE 6.50 usec
TE 300.2 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01300000 sec
-------- CHANNEL f1 --------
NUC1 1H
P1 10.75 usec
PL1 -1.00 dB
SFO1 599.2035487 MHz
F2 - Processing parameters
SI 32768
SF 599.2000286 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 2.00
Ts
N
N
Ph
O
Ph
5a
10
9
8
7
6
5
4
3
2
1
ppm
0.95
1.01
2.00
2.02
1.09
1.02
2.01
5.11
3.21
1.00
3.00

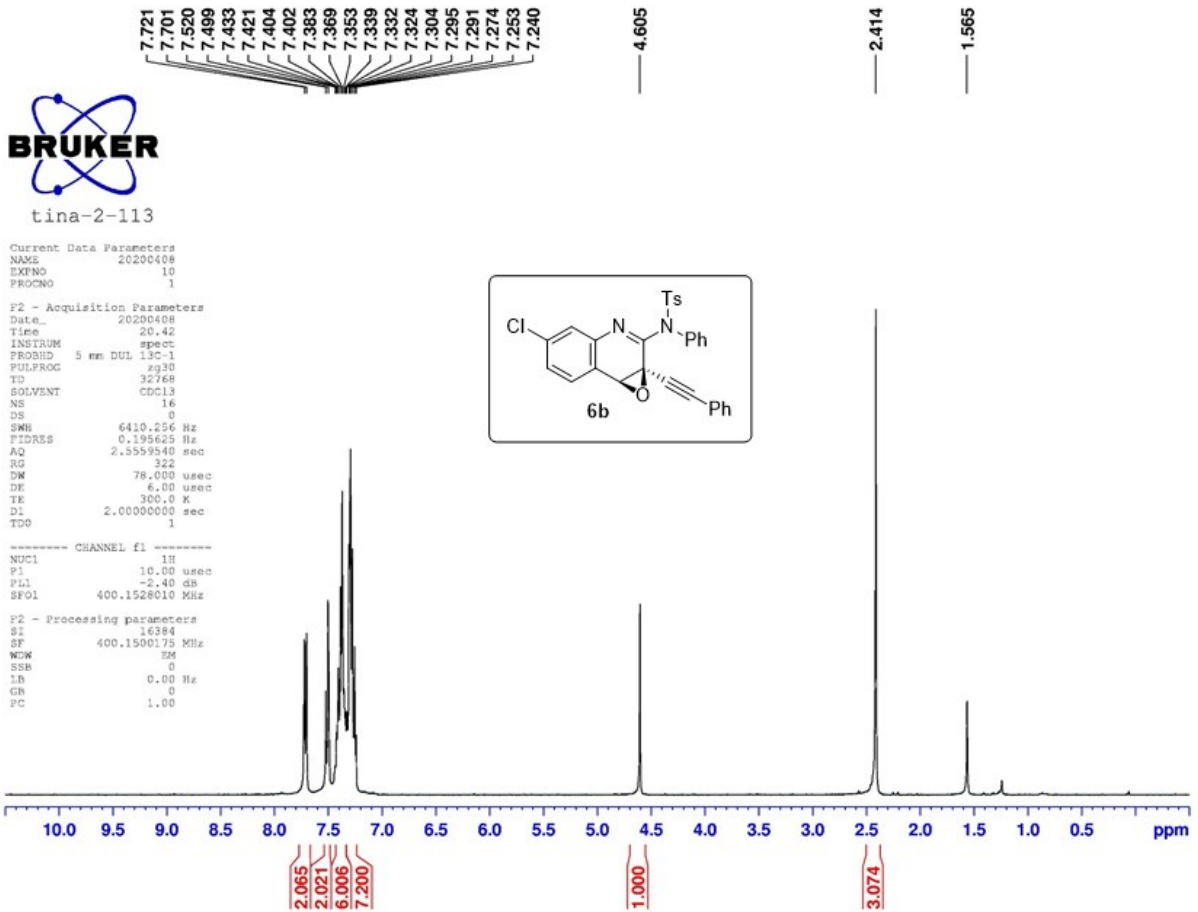

156.91
155.66
147.50
143.92
143.67
139.57
137.16
129.92
129.70
129.48
129.23
128.93
128.83
128.76
128.69
128.54
128.48
126.28
124.84
119.83
117.57
116.14
100.22
77.21
77.00
76.79
21.63
Ts
N
N
Ph
O
Ph
5a
Current Data Parameters
NAME tina-1-214-1
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20191108
Time 7.12
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 204
DS 4
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637248 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 302.4 K
D1 3.00000000 sec
d11 0.03000000 sec
DELTA 4.99000013 sec
MCREST 0 sec
MCWRK 0.01500000 sec
-------- CHANNEL f1 --------
NUC1 13C
P1 4.80 usec
PL1 0 dB
SFO1 150.4320518 MHz
-------- CHANNEL f2 --------
CPDPRG[2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 8.00 dB
PL13 14.00 dB
SFO2 598.2029910 MHz
F2 - Processing parameters
SI 65536
SF 150.4179197 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

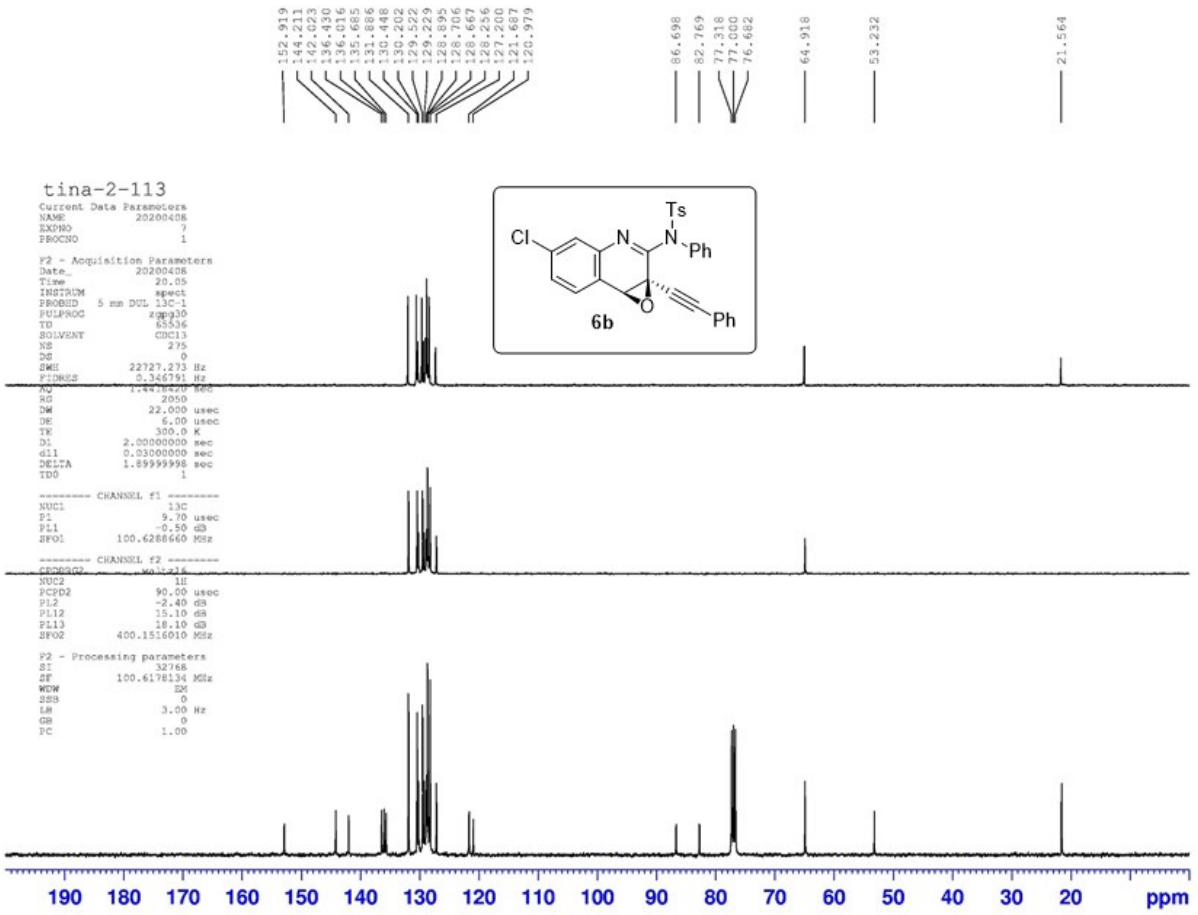

8.217
8.197
8.007
7.986
7.967
7.947
7.652
7.630
7.611
7.559
7.540
7.522
7.473
7.464
7.456
7.450
7.387
7.380
7.371
7.316
7.295
7.240
6.938
6.917
6.156
3.828
2.432
BRUKER
tina-1-238
Current Data Parameters
NAME 20191202
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20191202
Time 16.20
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 42
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 456
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz
F2 - Processing parameters
SI 16384
SF 400.1500172 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
N
Ts
N
Ph
O
5t
OMe
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
1.011
3.038
3.110
1.182
2.089
3.226
2.114
2.097
1.000
3.289
3.228

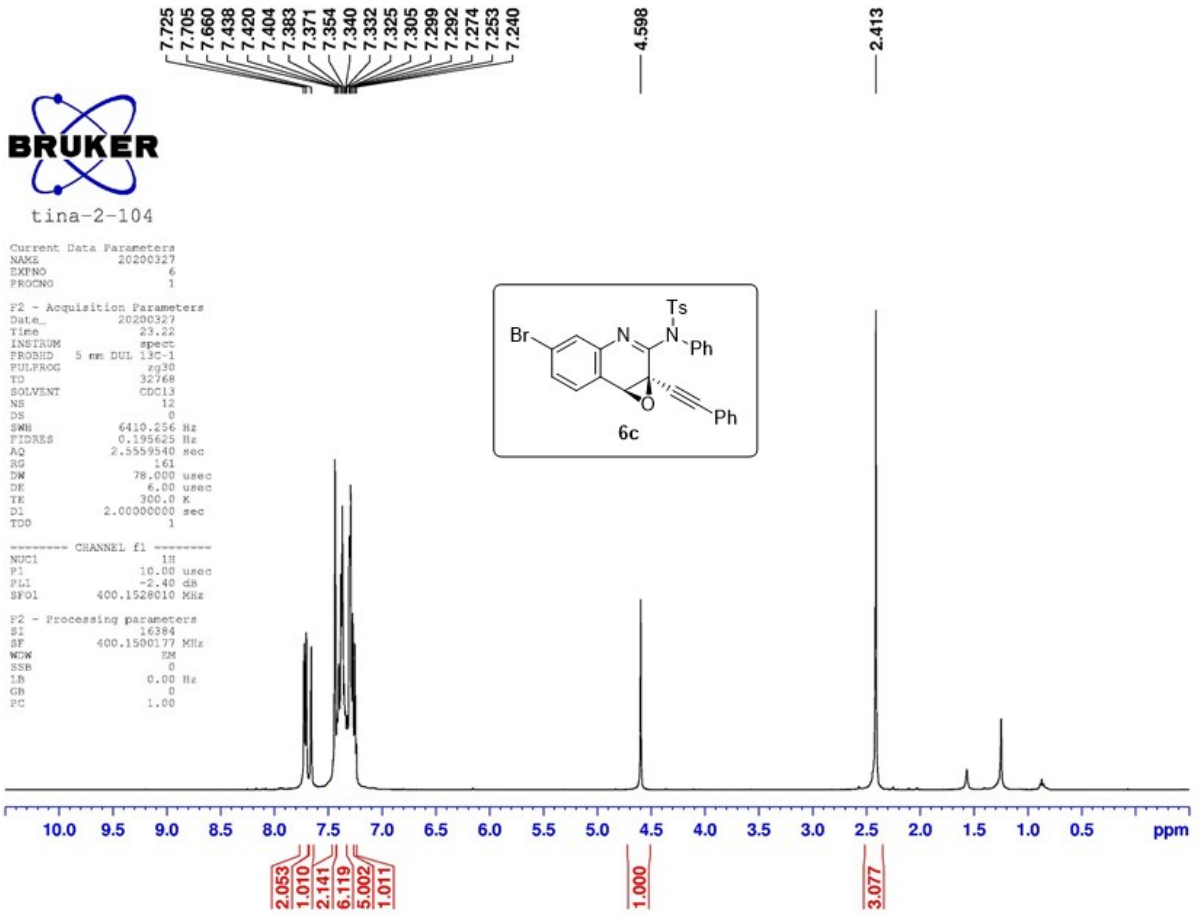

160.234
156.602
155.855
147.356
143.706
143.637
139.564
137.142
129.866
129.689
129.192
128.753
128.676
128.475
126.216
126.400
126.212
122.300
119.731
117.852
116.143
114.291
98.523
77.318
77.000
76.683
55.359
21.648
tina-1-238
Current Data Parameters
NAME 20191202
EXPNO 7
PROCNO 1
F2 - Acquisition Parameters
Date_ 20191202
Time 21.44
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 8000
DS 0
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4418420 sec
RG 2050
DW 22.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.70 usec
PL1 -0.50 dB
SFO1 100.6288660 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.40 dB
PL12 15.10 dB
PL13 18.10 dB
SFO2 400.1516010 MHz
F2 - Processing parameters
SI 32768
SF 100.6178020 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
Ts
N
N
Ph
O
5t
OMe
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

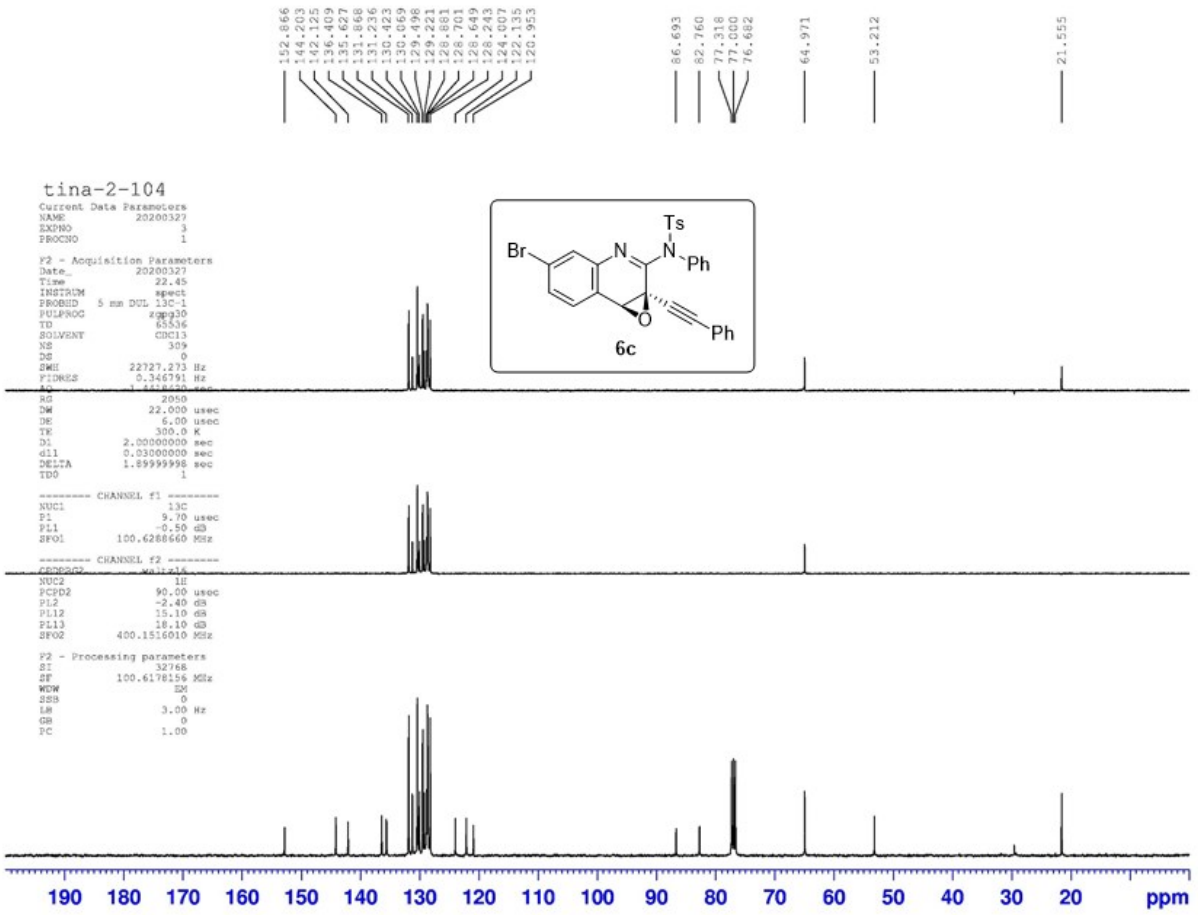

7.932
7.664
7.661
7.647
7.643
7.640
7.626
7.622
7.566
7.564
7.548
7.546
7.529
7.526
7.460
7.457
7.453
7.450
7.446
7.444
7.436
7.397
7.387
7.383
7.379
7.377
7.371
7.326
7.323
7.313
7.293
7.240
7.067
7.058
7.055
7.045
6.125
2.432
1.549
BRUKER
tina-2-2-down
Current Data Parameters
NAME 20191206
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20191206
Time 11.13
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 25
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 812
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz
F2 - Processing parameters
SI 16384
SF 400.1500172 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
Ts
N–Ph
N
O
S
5v
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
0.880
1.008
1.985
1.000
1.102
2.213
4.065
3.247
1.160
1.057
3.011

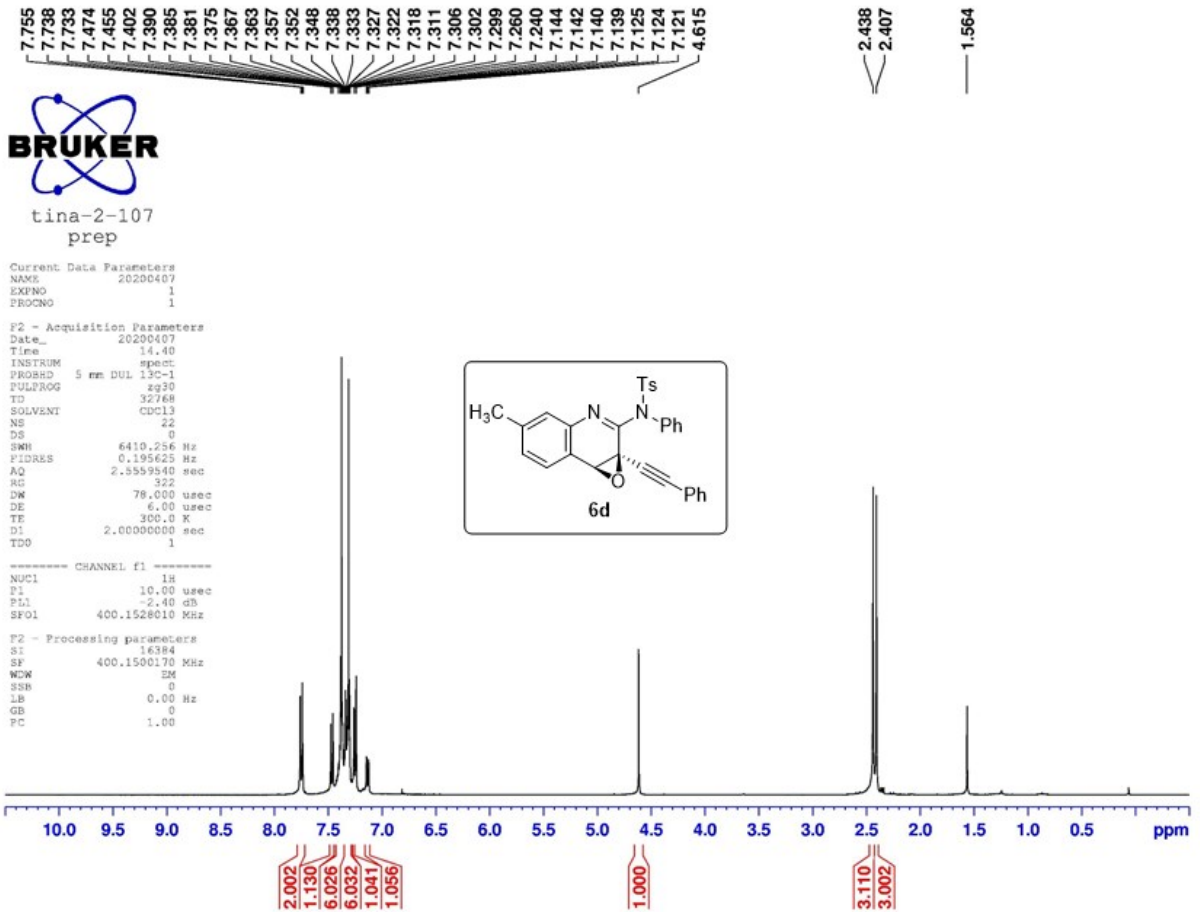

156.551
151.123
147.319
143.930
143.696
139.464
137.069
132.061
129.877
129.690
129.242
128.777
128.691
128.558
127.927
126.378
125.160
119.853
117.598
115.986
99.954
77.317
77.000
76.683
21.660
tina-2-2-down
Current Data Parameters
NAME 20191208
EXPNO 6
PROCNO 1
F2 - Acquisition Parameters
Date_ 20191208
Time 21.23
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
SOLVENT CDCl3
NS 11700
DS 0
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4418420 sec
RG 2050
DW 22.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
PL1 -0.50 dB
SFO1 100.6288660 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.40 dB
PL12 15.10 dB
PL13 18.10 dB
SFO2 400.1516010 MHz
F2 - Processing parameters
SI 32768
SF 100.6178005 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
Ts
N–Ph
N
O
S
5v
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

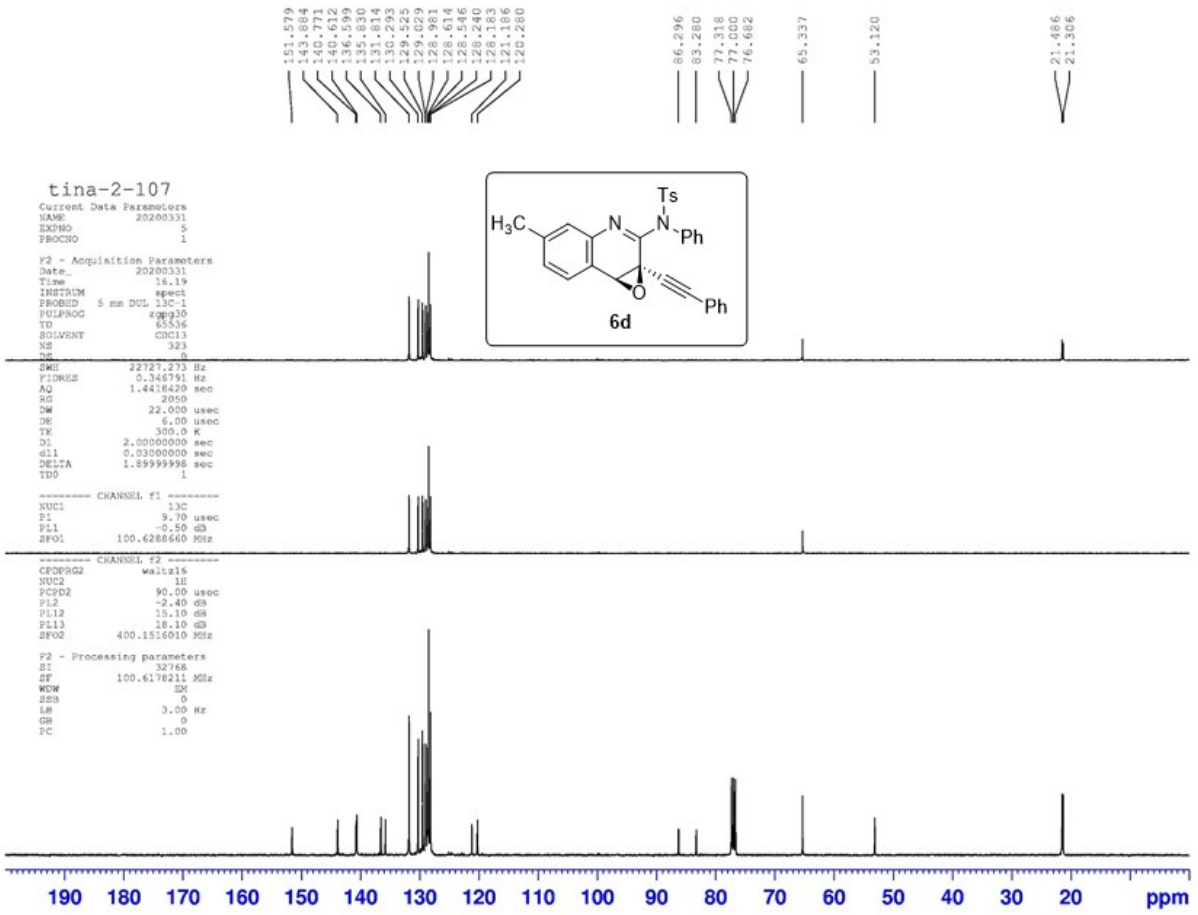

7.721
7.701
7.520
7.499
7.433
7.421
7.404
7.402
7.383
7.369
7.353
7.339
7.332
7.324
7.304
7.295
7.291
7.274
7.253
7.240
4.605
2.414
1.565
BRUKER
tina-2-113
Current Data Parameters
NAME 20200408
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200408
Time 20.42
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 322
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz
F2 - Processing parameters
SI 16384
SF 400.1500175 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
Cl
N
Ts
N
Ph
O
Ph
6b
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
2.065
2.021
6.006
7.200
1.000
3.074


152.919
144.211
142.623
136.430
136.016
131.685
131.886
130.448
130.202
129.522
129.229
128.895
128.706
128.667
128.256
127.200
121.687
120.979
86.698
82.769
77.318
77.000
76.682
64.918
53.232
21.564
tina-2-113
Current Data Parameters
NAME 20200408
EXPNO 7
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200408
Time 20.05
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 275
DS 0
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4418420 sec
RG 2050
DW 22.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.70 usec
PL1 -0.50 dB
SFO1 100.6288660 MHz
======== CHANNEL f2 ========
NUC2 1H
PCPD2 90.00 usec
PL2 -2.40 dB
PL12 15.10 dB
PL13 18.10 dB
SFO2 400.1516010 MHz
F2 - Processing parameters
SI 32768
SF 100.6178134 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
Cl
N
Ts
N
Ph
O
Ph
6b
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


7.725
7.705
7.660
7.438
7.420
7.404
7.383
7.371
7.354
7.340
7.332
7.325
7.305
7.299
7.292
7.274
7.253
7.240
4.598
2.413
BRUKER
tina-2-104
Current Data Parameters
NAME 20200327
EXPNO 6
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200327
Time 23.22
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 12
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 161
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz
F2 - Processing parameters
SI 16384
SF 400.1500177 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
Br
N
Ts
N
Ph
O
Ph
6c
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
2.053
1.010
2.141
6.119
5.002
1.011
1.000
3.077


152.866
144.203
142.125
136.409
135.627
131.868
131.236
130.423
130.069
129.498
129.221
128.881
128.701
128.649
128.243
124.007
122.135
120.953
86.693
82.760
77.318
77.000
76.682
64.971
53.212
21.555
tina-2-104
Current Data Parameters
NAME 20200327
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200327
Time 22.45
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 309
DS 0
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4418629 sec
RG 2050
DW 22.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.70 usec
PL1 -0.50 dB
SFO1 100.6288660 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.40 dB
PL12 15.10 dB
PL13 18.10 dB
SFO2 400.1516010 MHz
F2 - Processing parameters
SI 32768
SF 100.6178156 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
Br
N
Ts
N
Ph
O
Ph
6c
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


7.755
7.738
7.733
7.474
7.455
7.402
7.390
7.385
7.381
7.375
7.367
7.363
7.357
7.352
7.348
7.338
7.333
7.327
7.322
7.318
7.311
7.306
7.302
7.299
7.260
7.240
7.144
7.142
7.140
7.139
7.125
7.124
7.121
4.615
2.438
2.407
1.564
BRUKER
tina-2-107
prep
Current Data Parameters
NAME 20200407
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200407
Time 14.40
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 22
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 322
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz
F2 - Processing parameters
SI 16384
SF 400.1500170 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
Ts
N
N
Ph
H3C
O
Ph
6d
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
2.002
1.130
6.026
6.032
1.041
1.056
1.000
3.110
3.002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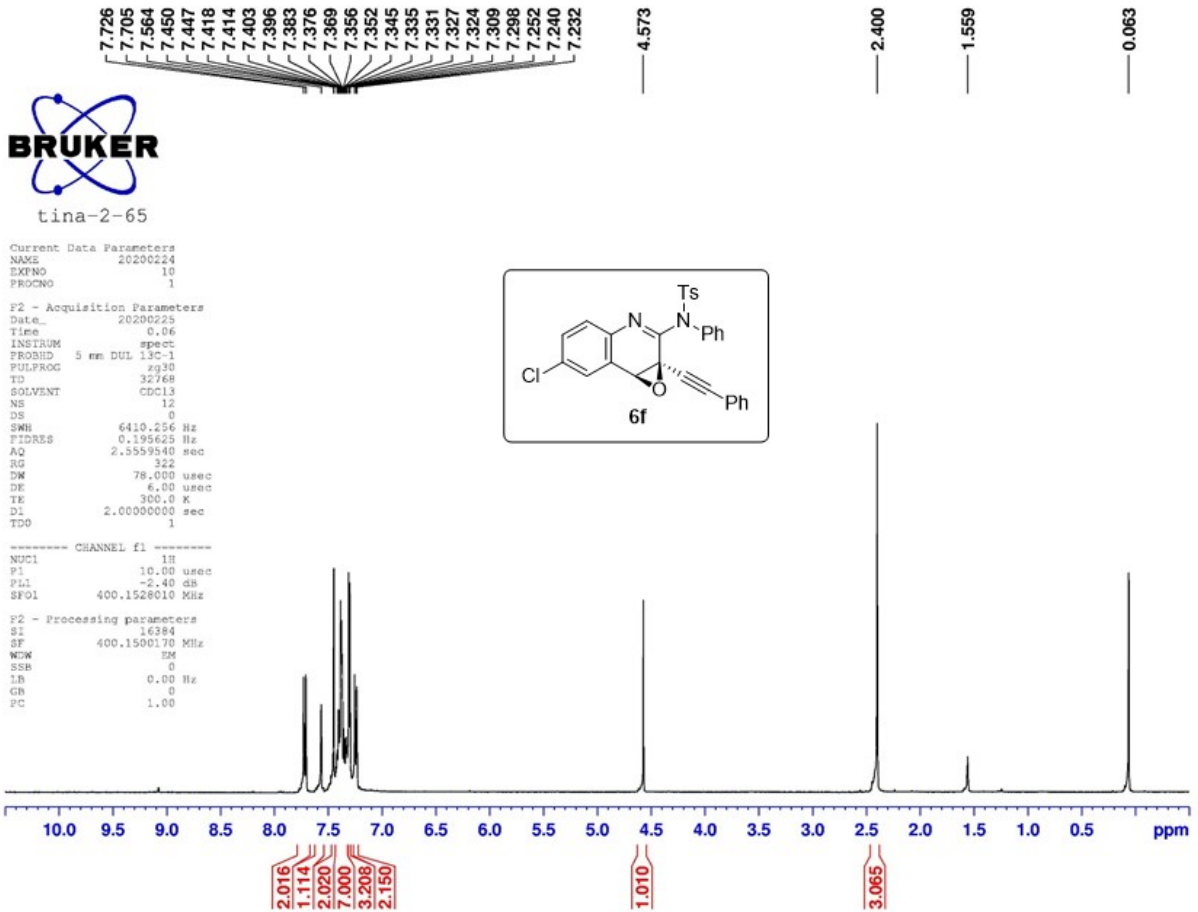
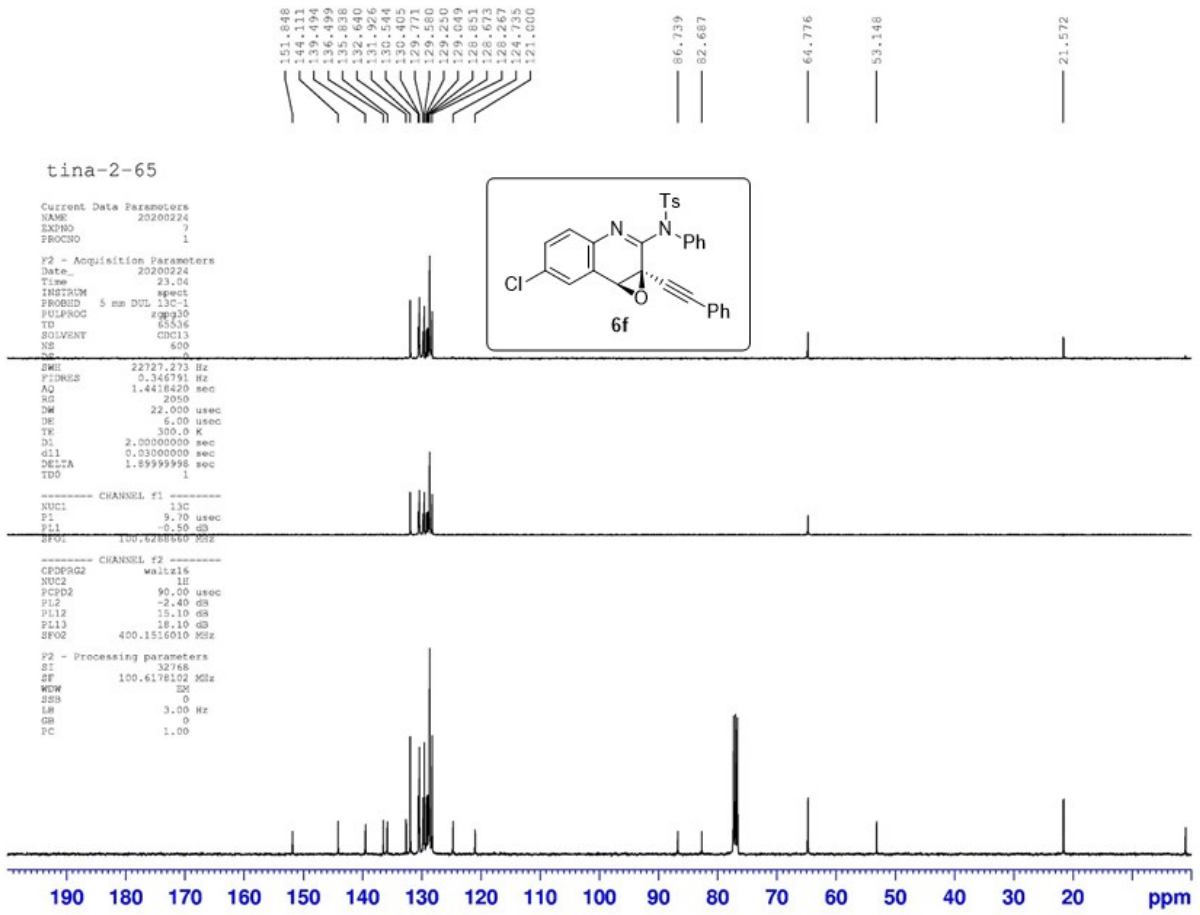
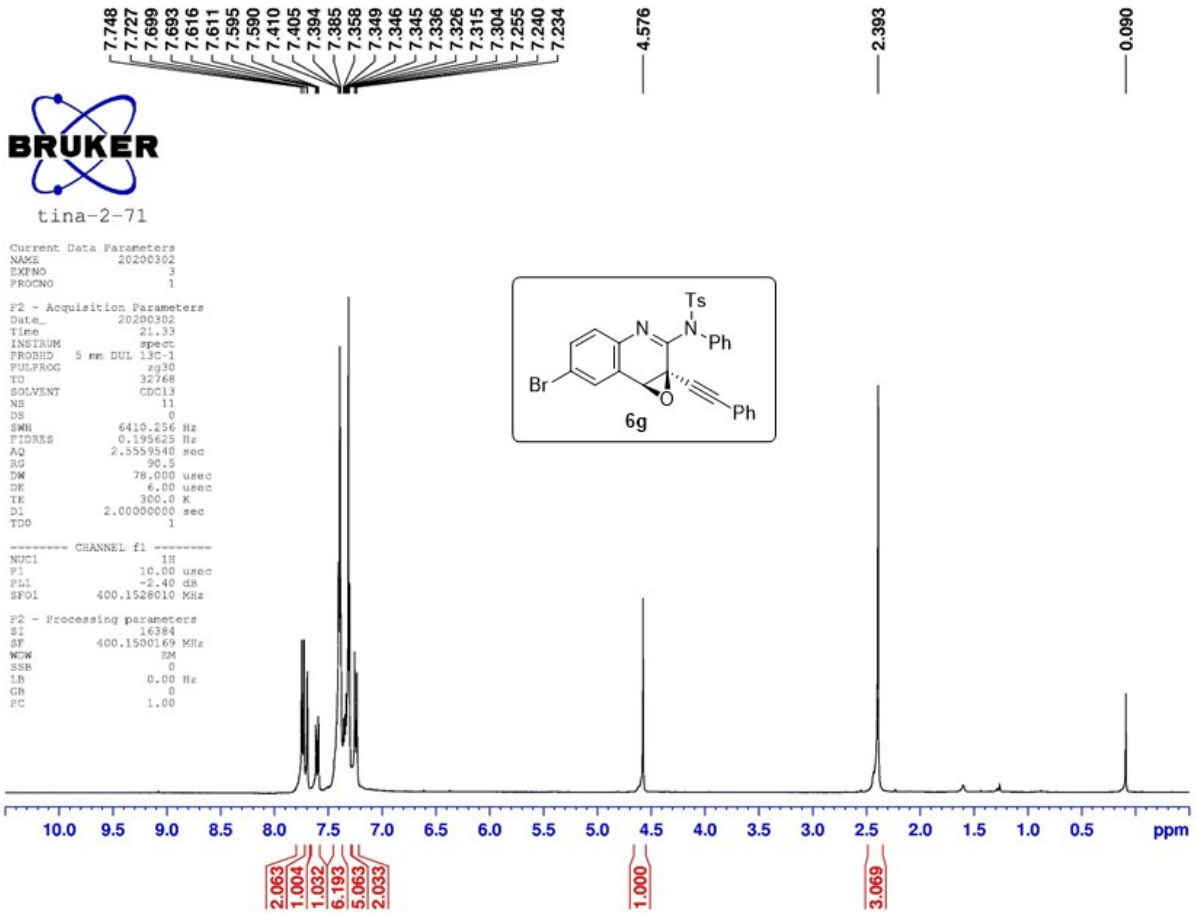
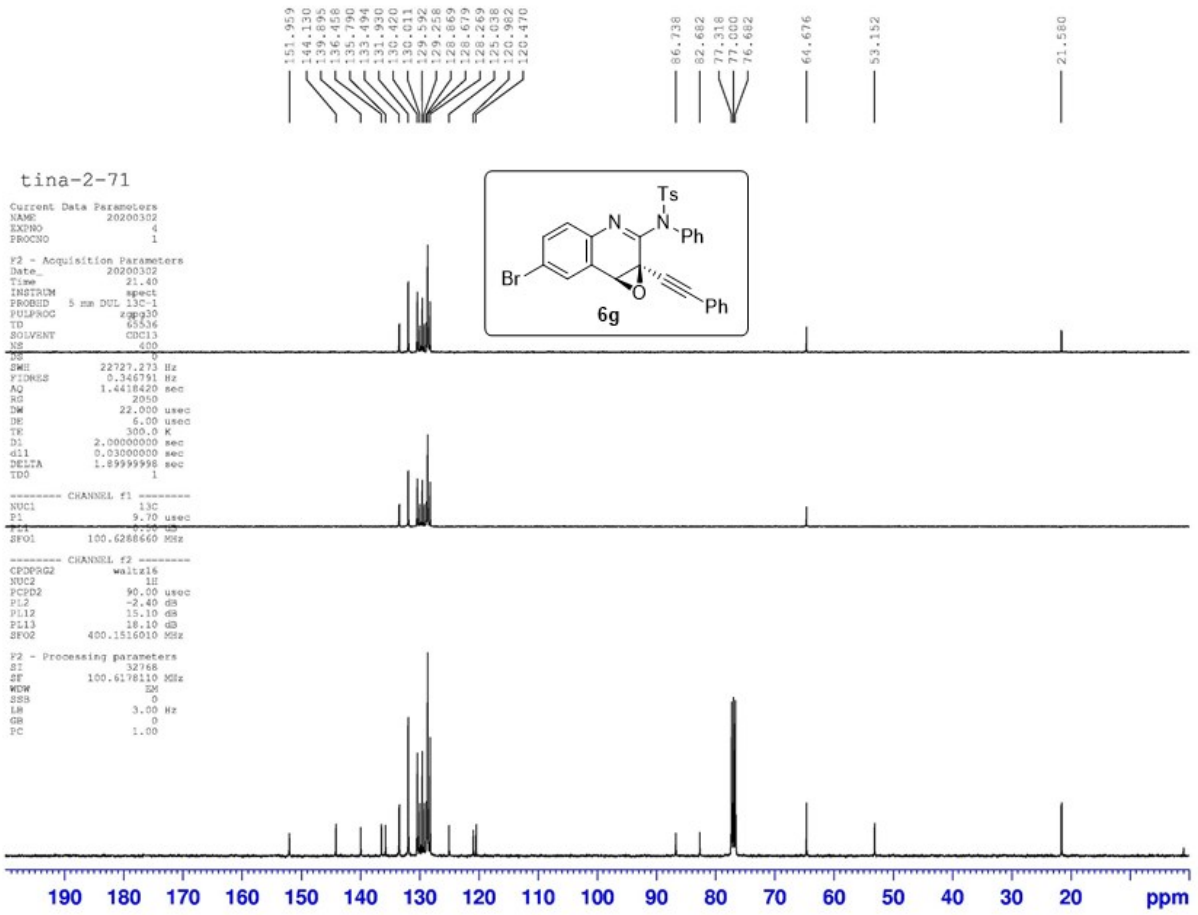
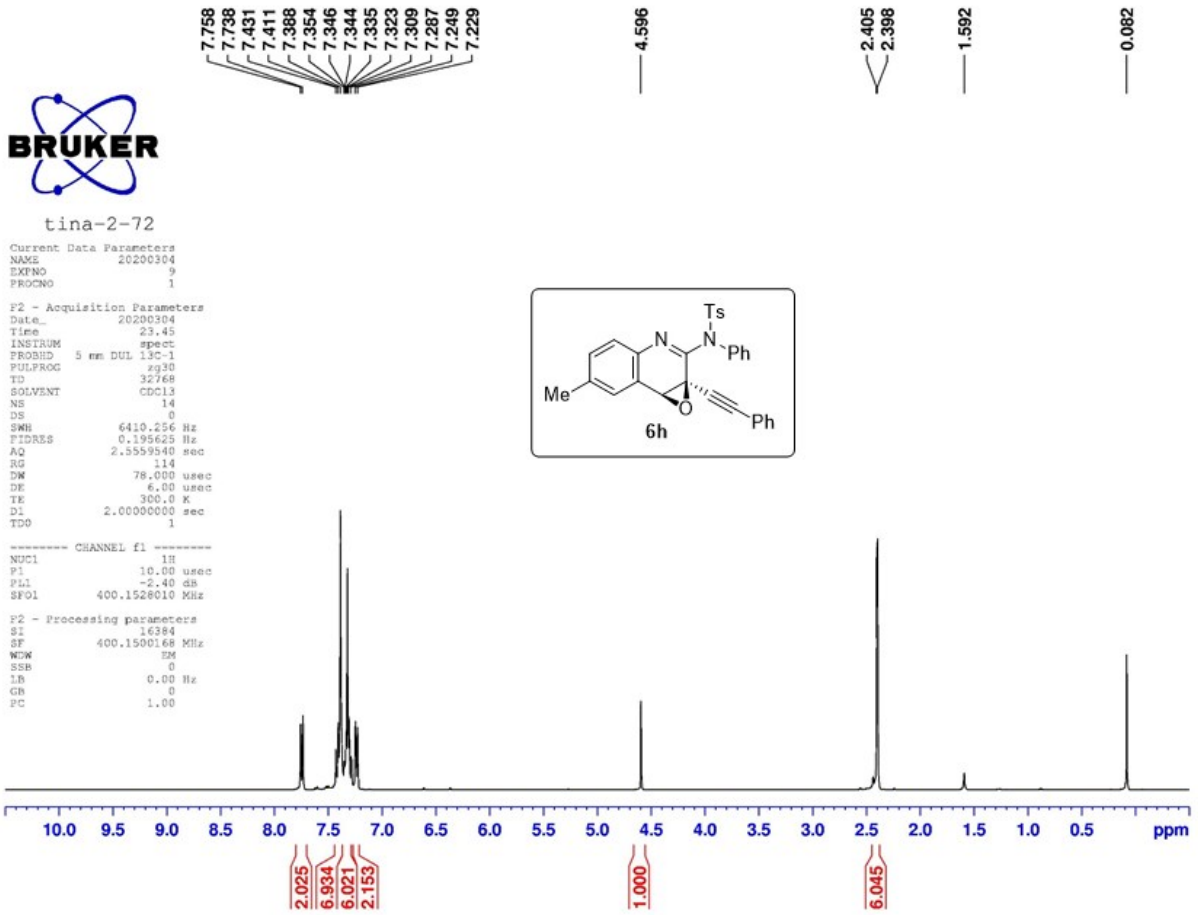
143.884
140.771
140.612
136.599
135.830
131.814
130.293
129.525
129.029
128.981
128.614
128.546
128.240
128.183
121.186
120.280
86.296
83.280
77.318
77.000
76.682
65.337
53.120
21.486
21.306
tina-2-107
Current Data Parameters
NAME 20200331
EXPNO 5
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200331
Time 16.19
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 323
DS 0
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4418420 sec
RG 2050
DW 22.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.70 usec
PL1 -0.50 dB
SFO1 100.6288660 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.40 dB
PL12 15.10 dB
PL13 18.10 dB
SFO2 400.1516010 MHz
F2 - Processing parameters
SI 32768
SF 100.6178211 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
Ts
N
N
Ph
H3C
O
Ph
6d
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

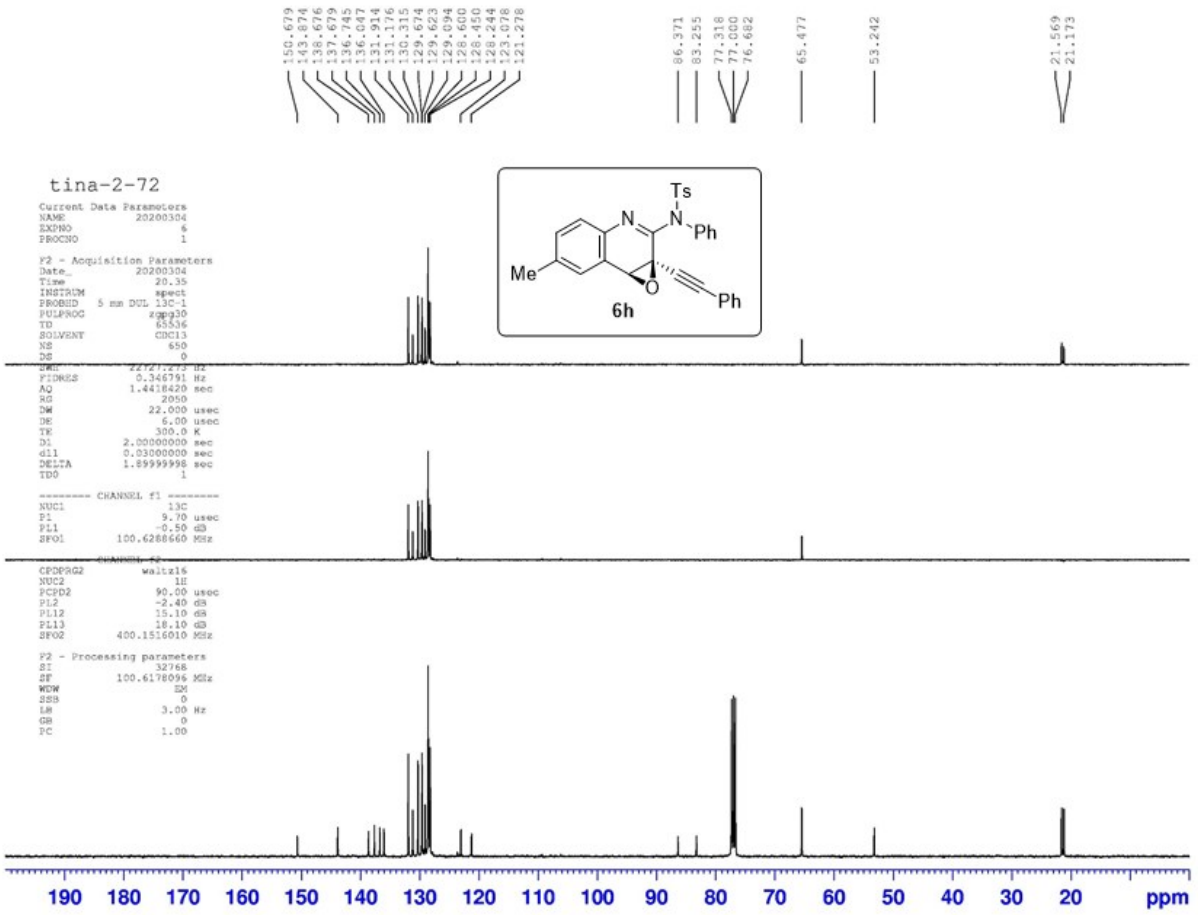

7.726
7.705
7.564
7.450
7.447
7.418
7.414
7.403
7.396
7.383
7.376
7.369
7.356
7.352
7.345
7.335
7.331
7.327
7.324
7.309
7.298
7.252
7.240
7.232
4.573
2.400
1.559
0.063
BRUKER
tina-2-65
Current Data Parameters
NAME 20200224
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200225
Time 0.06
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 12
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 322
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz
F2 - Processing parameters
SI 16384
SF 400.1500170 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
Ts
N
N
Ph
Cl
O
Ph
6f
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
2.016
1.114
2.020
7.000
3.208
2.150
1.010
3.065


151.848
144.111
139.494
136.499
135.838
132.640
131.926
130.544
130.405
129.771
129.580
129.250
129.049
128.851
128.673
128.267
124.735
121.000
86.739
82.687
64.776
53.148
21.572
tina-2-65
Current Data Parameters
NAME 20200224
EXPNO 7
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200224
Time 23.04
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 600
DS 0
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4418420 sec
RG 2050
DW 22.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.70 usec
PL1 -0.50 dB
SFO1 100.6288660 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.40 dB
PL12 15.10 dB
PL13 18.10 dB
SFO2 400.1516010 MHz
F2 - Processing parameters
SI 32768
SF 100.6178102 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
Ts
N
N
Ph
Cl
O
Ph
6f
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


7.748
7.727
7.699
7.693
7.616
7.611
7.595
7.590
7.410
7.405
7.394
7.385
7.358
7.349
7.346
7.345
7.336
7.326
7.315
7.304
7.255
7.240
7.234
4.576
2.393
0.090
BRUKER
tina-2-71
Current Data Parameters
NAME 20200302
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200302
Time 21.33
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 11
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 90.5
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz
F2 - Processing parameters
SI 16384
SF 400.1500169 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
Ts
N
N
Ph
Br
O
Ph
6g
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
2.063
1.004
1.032
6.193
5.063
2.033
1.000
3.069


151.959
144.130
139.695
136.458
135.790
133.494
131.930
130.420
130.011
129.592
129.258
128.669
128.679
128.269
125.638
120.982
120.470
86.738
82.682
77.318
77.000
76.682
64.676
53.152
21.580
tina-2-71
Current Data Parameters
NAME 20200302
EXPNO 4
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200302
Time 21.40
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 400
DS 0
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4418420 sec
RG 2050
DW 22.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.70 usec
PL1 0.00 dB
SFO1 100.6268660 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.40 dB
PL12 15.10 dB
PL13 18.10 dB
SFO2 400.1516010 MHz
F2 - Processing parameters
SI 32768
SF 100.6178110 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
Ts
N
N
Ph
Br
O
Ph
6g
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


7.758
7.738
7.431
7.411
7.388
7.354
7.346
7.344
7.335
7.323
7.309
7.287
7.249
7.229
4.596
2.405
2.398
1.592
0.082
BRUKER
tina-2-72
Current Data Parameters
NAME 20200304
EXPNO 9
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200304
Time 23.45
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 14
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 114
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz
F2 - Processing parameters
SI 16384
SF 400.1500168 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
Ts
N
N
Ph
Me
O
Ph
6h
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
2.025
6.934
6.021
2.153
1.000
6.045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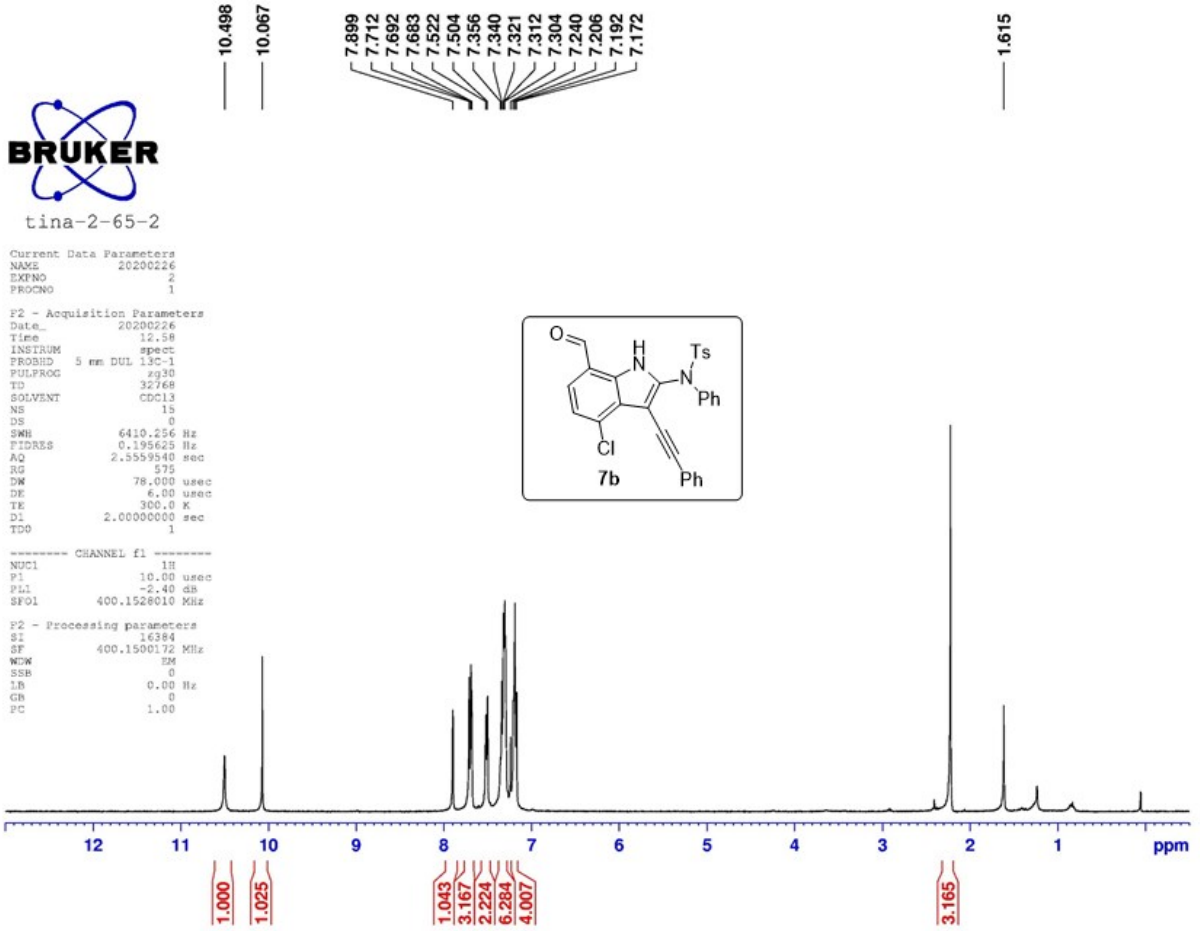
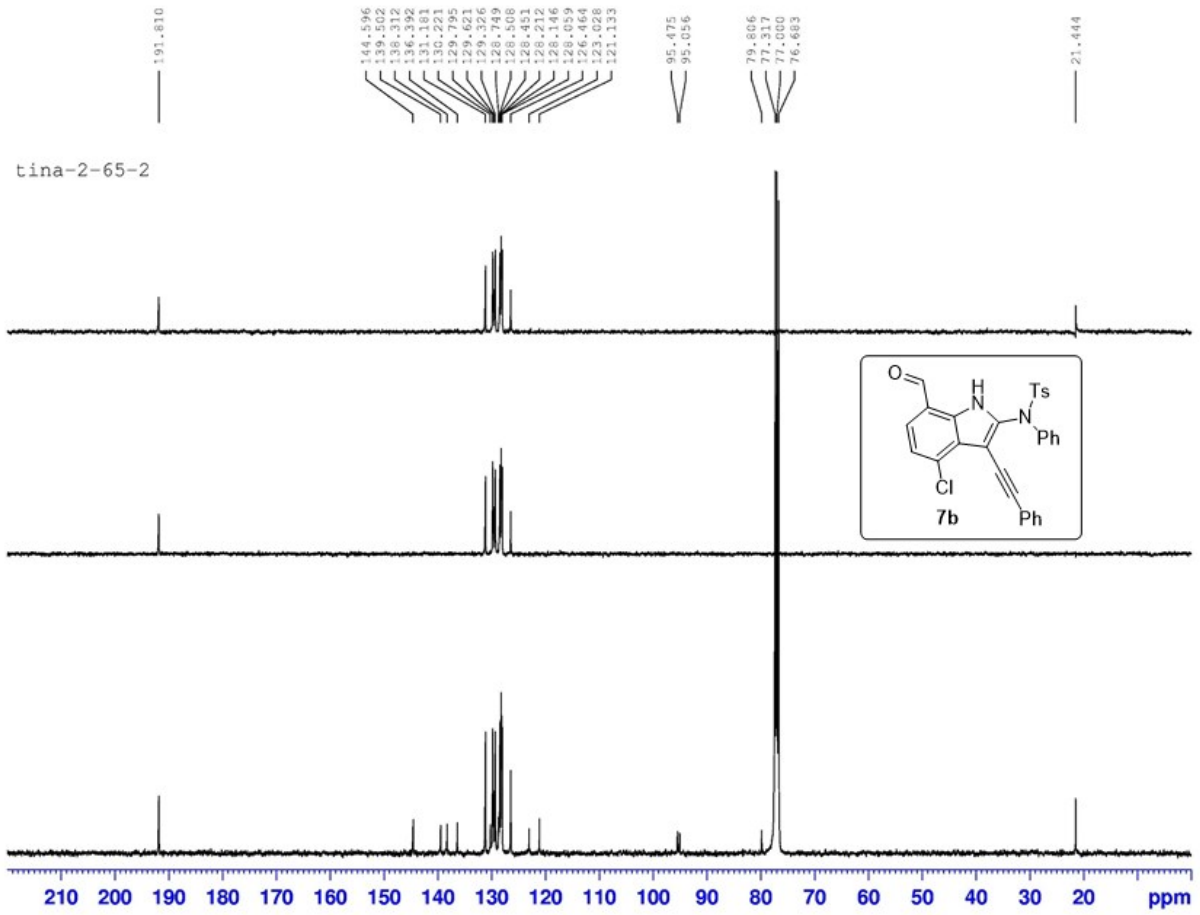
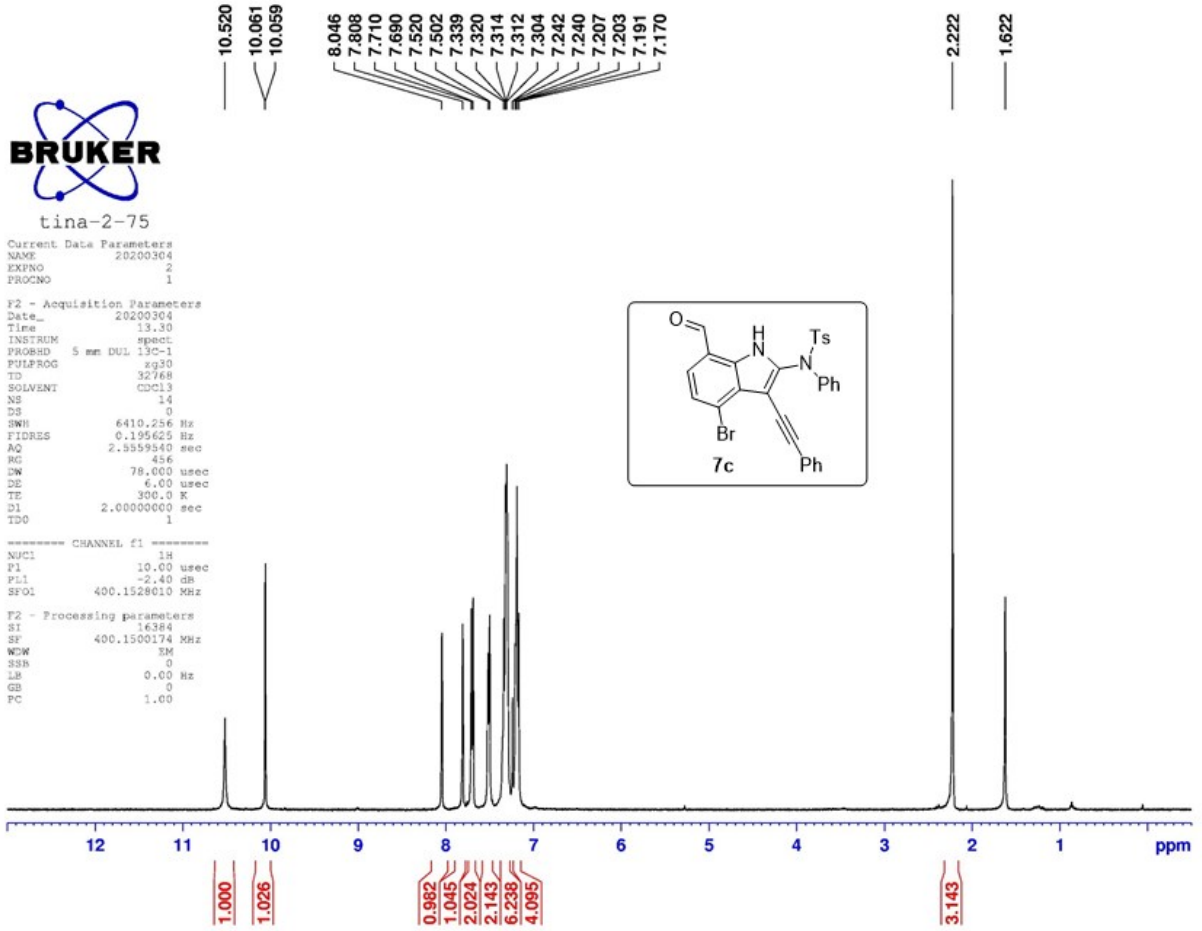
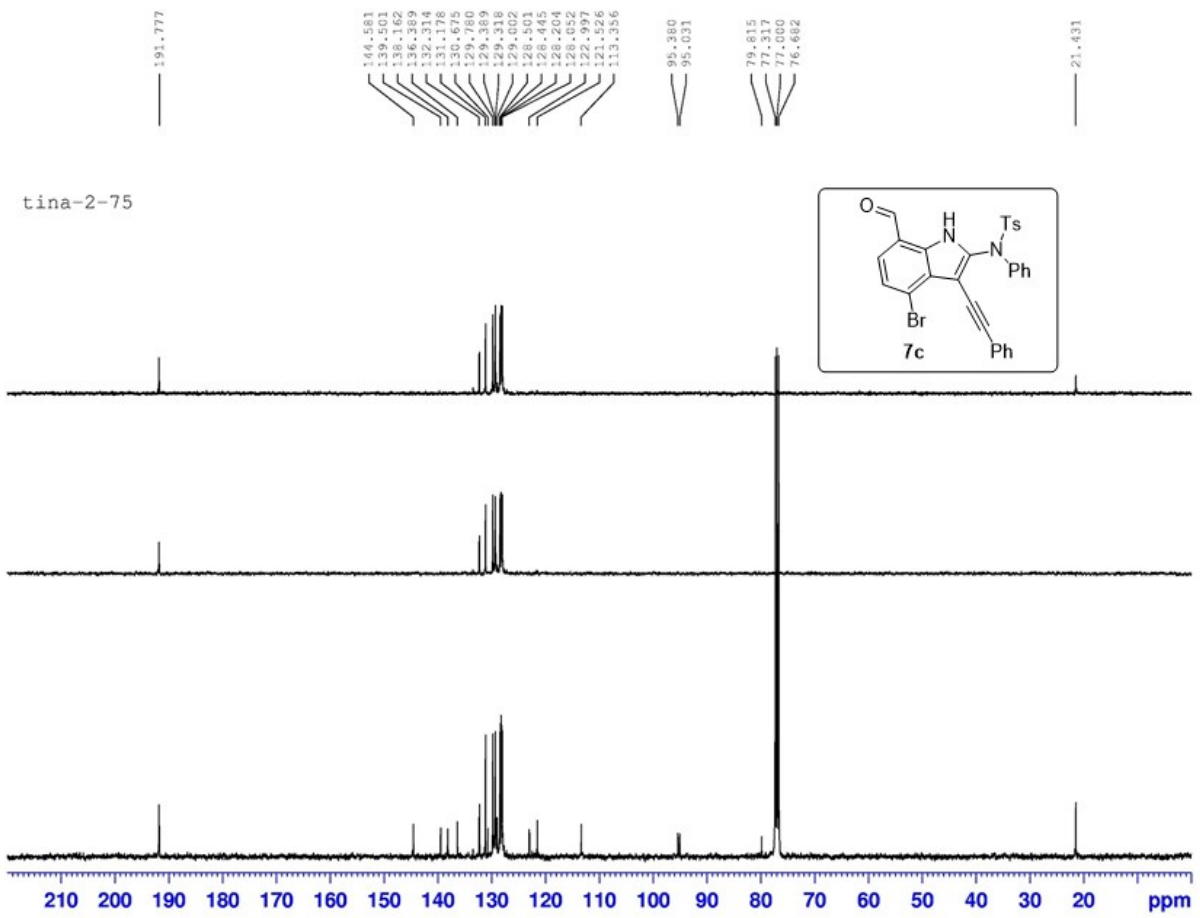
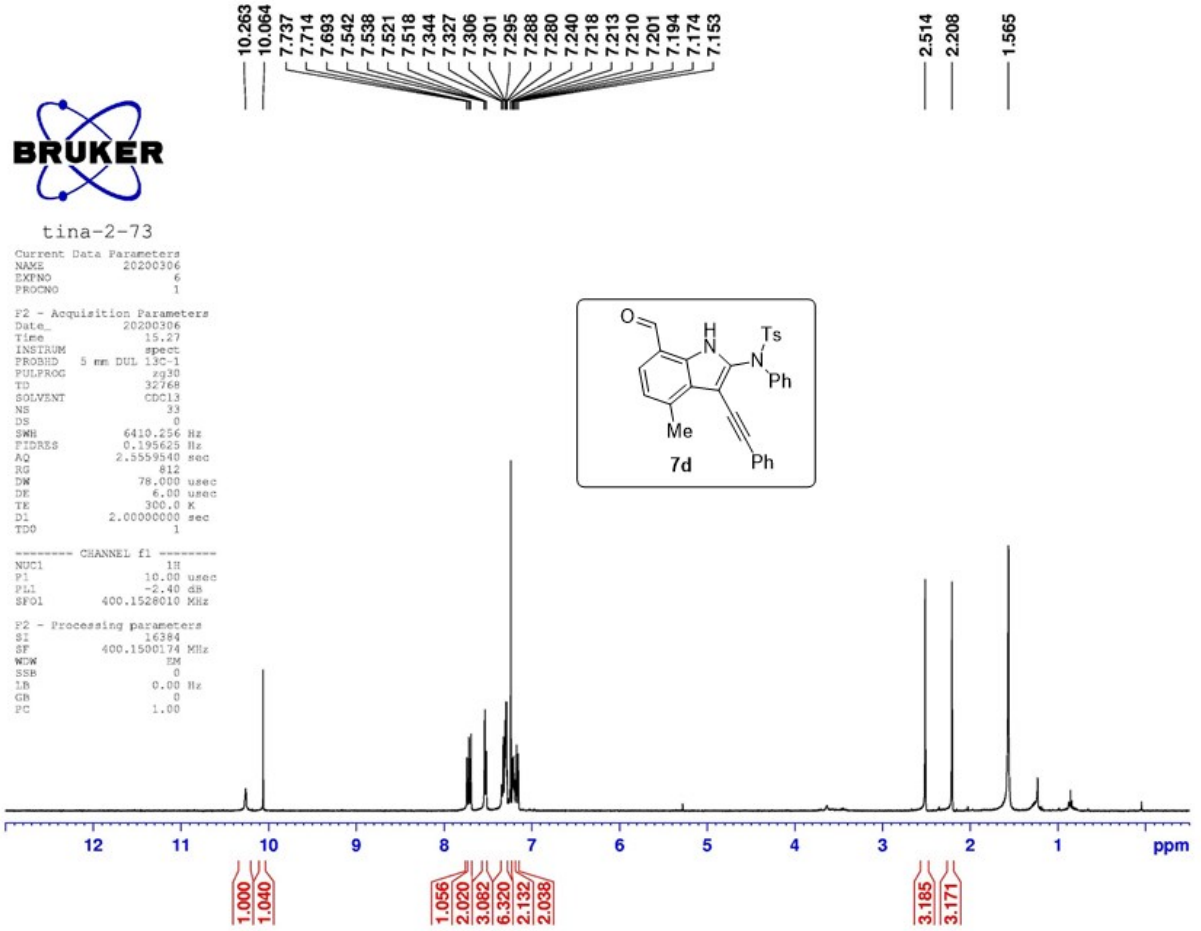
143.874
138.676
137.679
136.745
136.047
131.914
131.176
130.315
129.674
129.623
129.094
128.600
128.450
128.244
123.078
121.278
86.371
83.255
77.318
77.000
76.682
65.477
53.242
21.569
21.173
tina-2-72
Current Data Parameters
NAME 20200304
EXPNO 6
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200304
Time 20.35
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 650
DS 0
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4418420 sec
RG 2050
DW 22.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.70 usec
PL1 -0.50 dB
SFO1 100.6288660 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.40 dB
PL12 15.10 dB
PL13 18.10 dB
SFO2 400.1516010 MHz
F2 - Processing parameters
SI 32768
SF 100.6178096 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
Ts
N
N
Ph
Me
O
Ph
6h
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

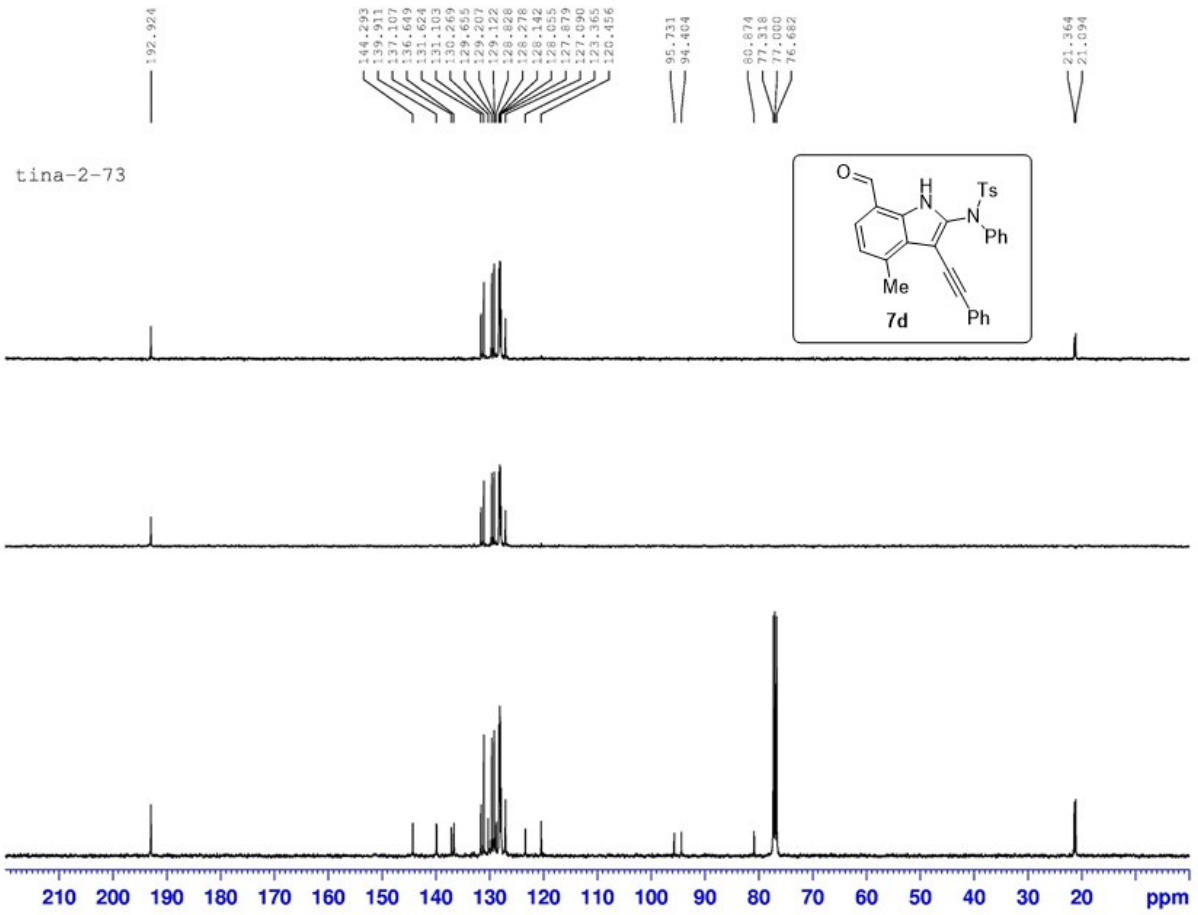

10.498
10.067
7.899
7.712
7.692
7.683
7.522
7.504
7.356
7.340
7.321
7.312
7.304
7.240
7.206
7.192
7.172
1.615
BRUKER
tina-2-65-2
Current Data Parameters
NAME 20200226
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200226
Time 12.58
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 15
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 575
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz
F2 - Processing parameters
SI 16384
SF 400.1500172 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
O
H
N
Ts
N
Ph
Cl
7b
Ph
12
11
10
9
8
7
6
5
4
3
2
1
ppm
1.000
1.025
1.043
3.167
2.224
6.284
4.007
3.165

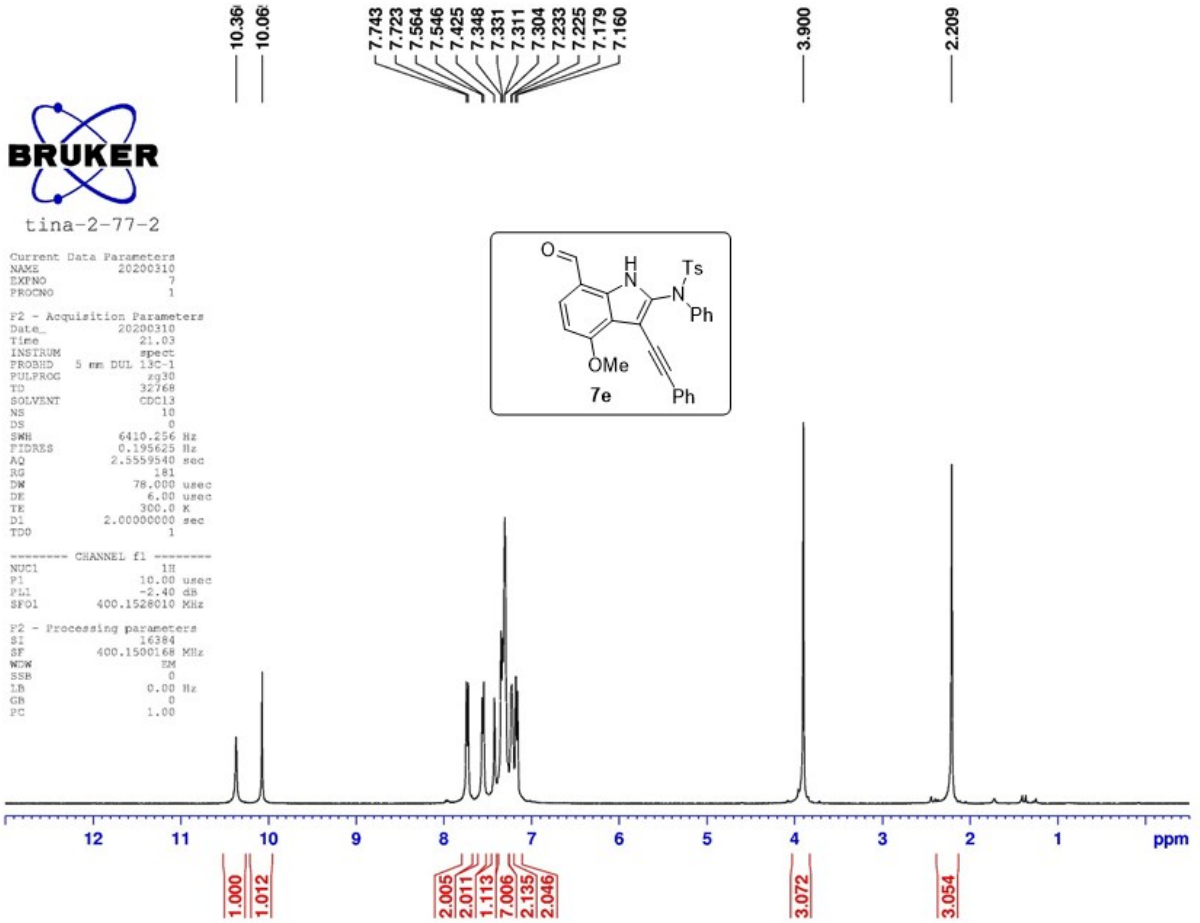

191.810
144.596
139.502
138.312
136.392
131.181
130.221
129.795
129.621
129.326
128.749
128.508
128.451
128.212
128.146
128.059
126.464
123.028
121.133
95.475
95.056
79.806
77.317
77.000
76.683
21.444
tina-2-65-2
O
H
N
Ts
N
Ph
Cl
7b
Ph
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

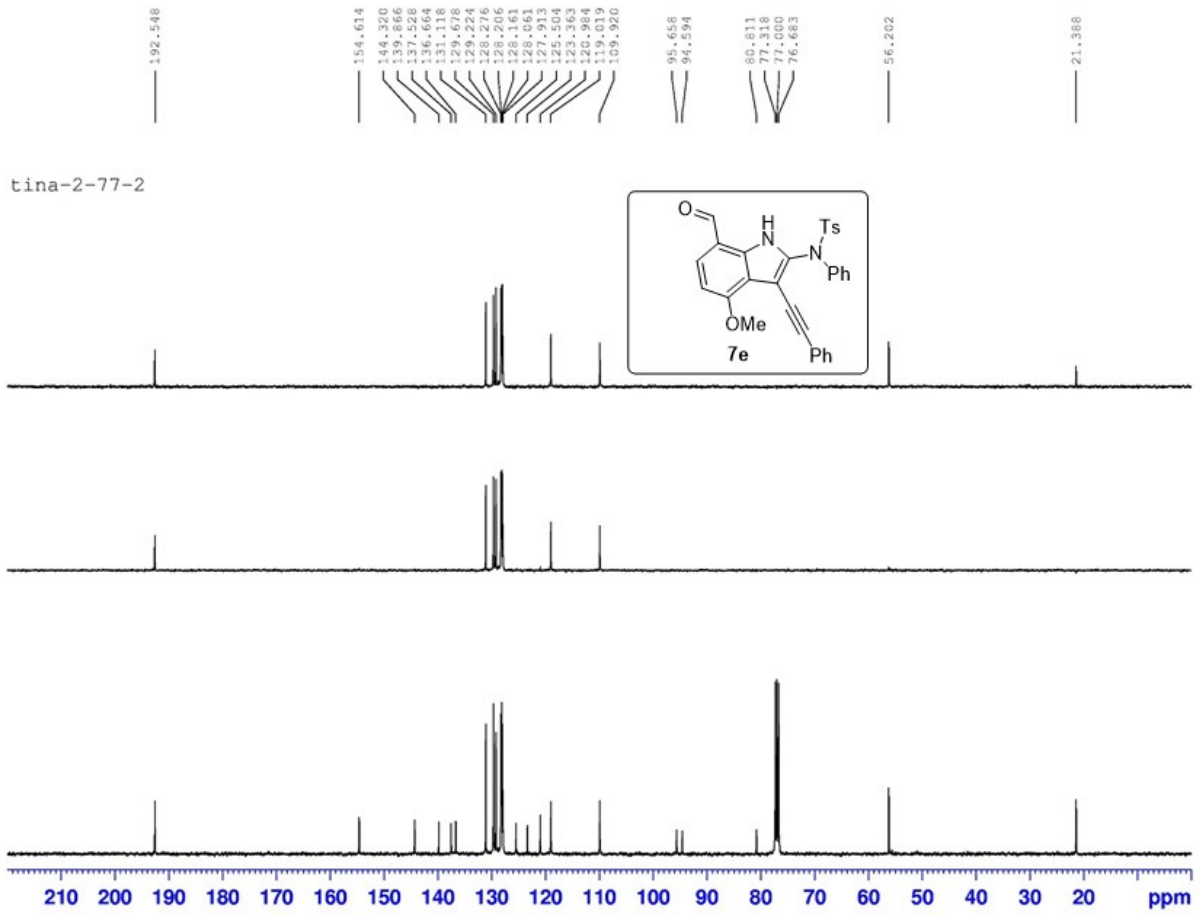

10.520
10.061
10.059
8.046
7.808
7.710
7.690
7.520
7.502
7.339
7.320
7.314
7.312
7.304
7.242
7.240
7.207
7.203
7.191
7.170
2.222
1.622
BRUKER
tina-2-75
Current Data Parameters
NAME 20200304
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200304
Time 13.30
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 14
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 456
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz
F2 - Processing parameters
SI 16384
SF 400.1500174 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
O
H
N
Ts
N
Ph
Br
7c
Ph
12
11
10
9
8
7
6
5
4
3
2
1
ppm
1.000
1.026
0.982
1.045
2.024
2.143
6.238
4.095
3.143

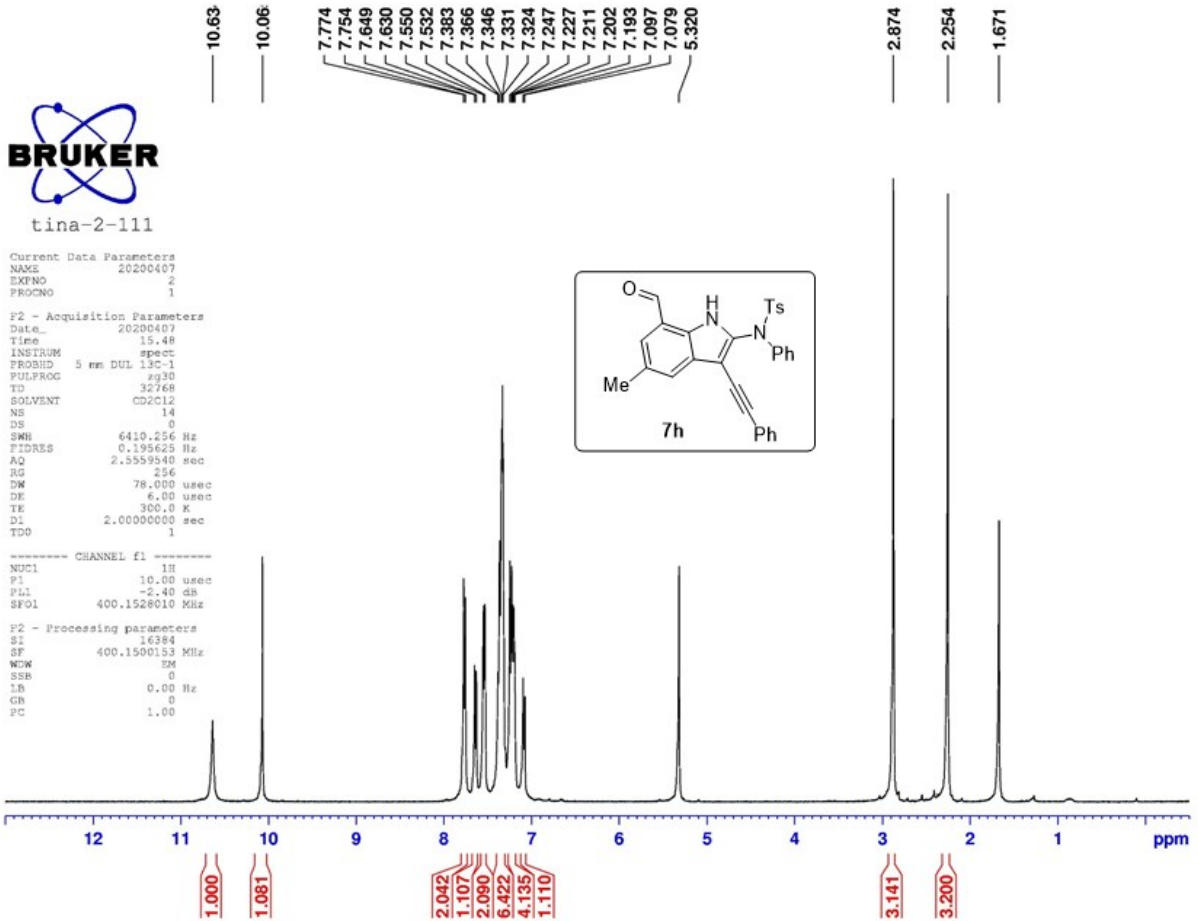

191.777
144.581
139.501
138.162
136.389
132.314
131.178
130.675
129.760
129.389
129.318
129.002
128.501
128.445
128.204
128.052
122.997
121.526
113.356
95.380
95.031
79.815
77.317
77.000
76.682
21.431
tina-2-75
O
H
N
Ts
N
Ph
Br
7c
Ph
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

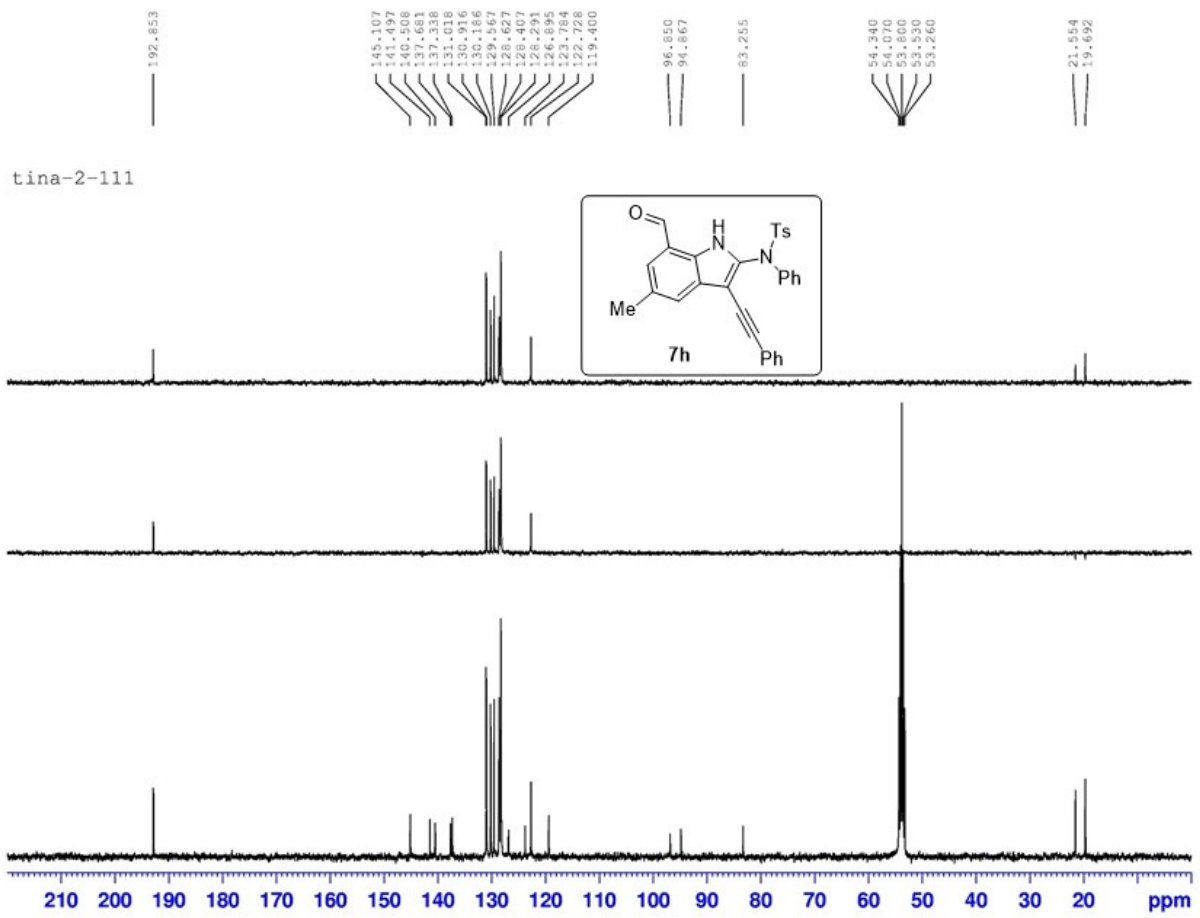

10.263
10.064
7.737
7.714
7.693
7.542
7.538
7.521
7.518
7.344
7.327
7.306
7.301
7.295
7.288
7.280
7.240
7.218
7.213
7.210
7.201
7.194
7.174
7.153
2.514
2.208
1.565
BRUKER
tina-2-73
Current Data Parameters
NAME 20200306
EXPNO 6
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200306
Time 15.27
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 33
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 812
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz
F2 - Processing parameters
SI 16384
SF 400.1500174 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
O
H
N
Ts
N
Ph
Me
Ph
7d
12
11
10
9
8
7
6
5
4
3
2
1
ppm
1.000
1.040
1.056
2.020
3.082
6.320
2.132
2.038
3.185
3.171

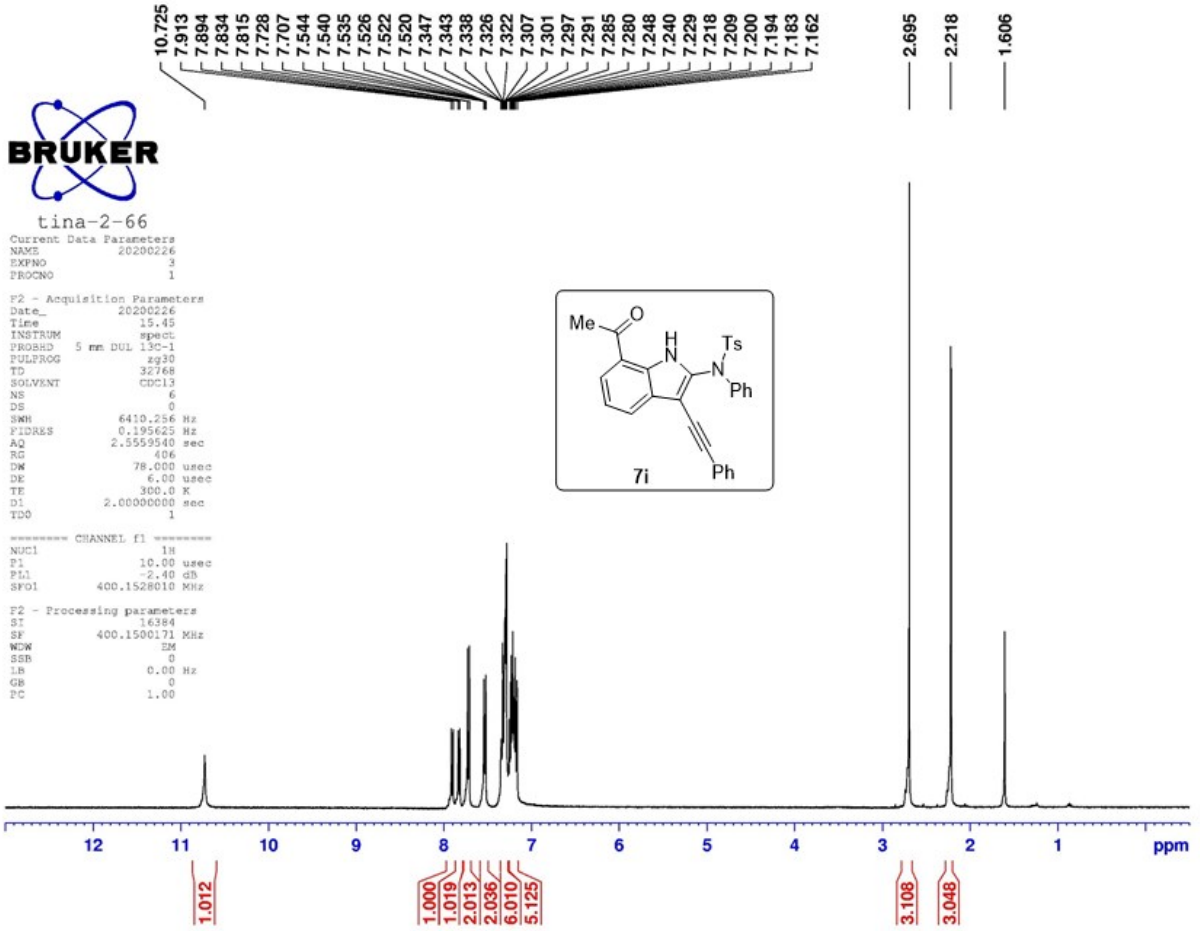

192.924
144.293
139.911
137.107
136.649
131.624
131.103
130.269
129.655
129.207
129.122
128.828
128.278
128.142
128.055
127.879
127.090
123.365
120.456
95.731
94.404
80.874
77.318
77.000
76.682
21.364
21.094
tina-2-73
O
H
N
Ts
N
Ph
Me
Ph
7d
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

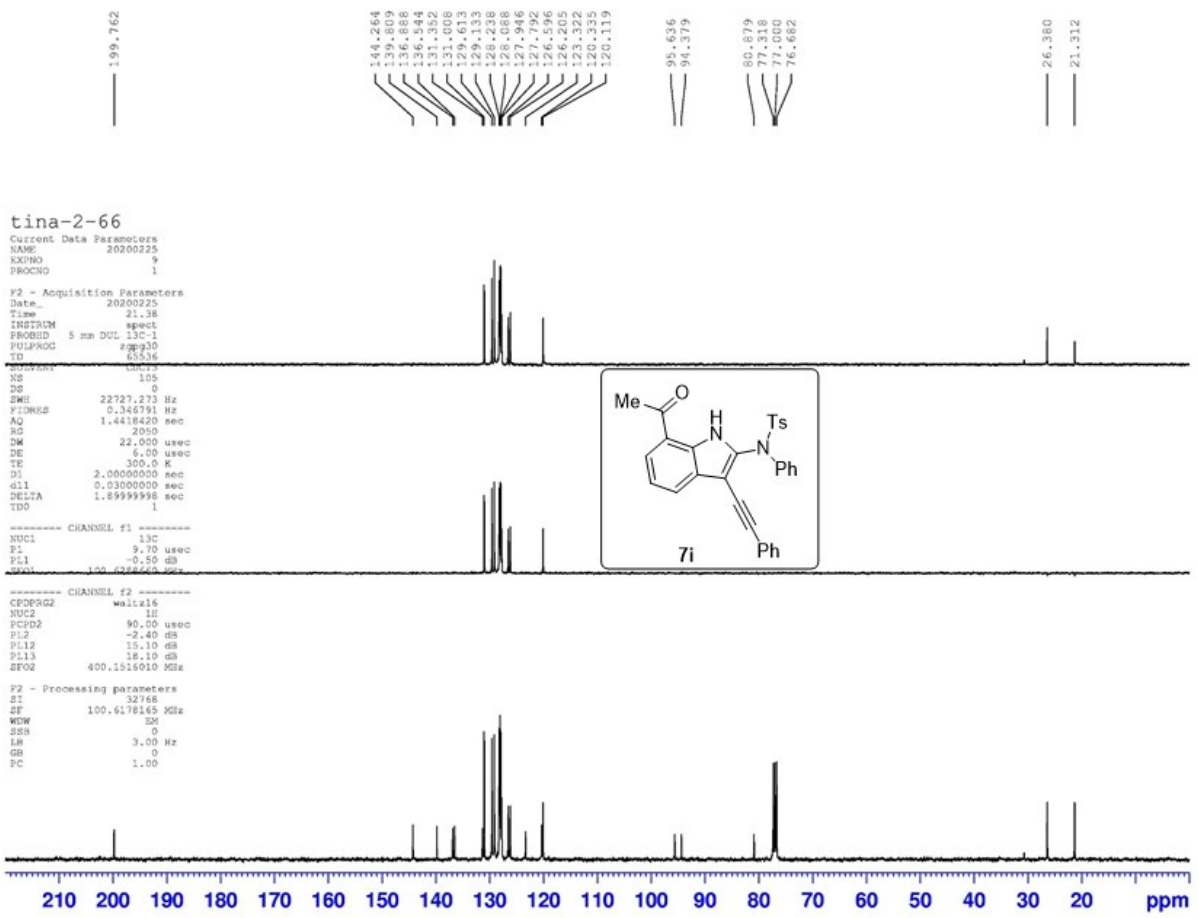

10.36
10.06
7.743
7.723
7.564
7.546
7.425
7.348
7.331
7.311
7.304
7.233
7.225
7.179
7.160
3.900
2.209
BRUKER
tina-2-77-2
Current Data Parameters
NAME 20200310
EXPNO 7
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200310
Time 21.03
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 10
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 181
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz
F2 - Processing parameters
SI 16384
SF 400.1500168 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
O
H
N
Ts
N
Ph
OMe
7e
Ph
12
11
10
9
8
7
6
5
4
3
2
1
ppm
1.000
1.012
2.005
2.011
1.113
7.006
2.135
2.046
3.072
3.054

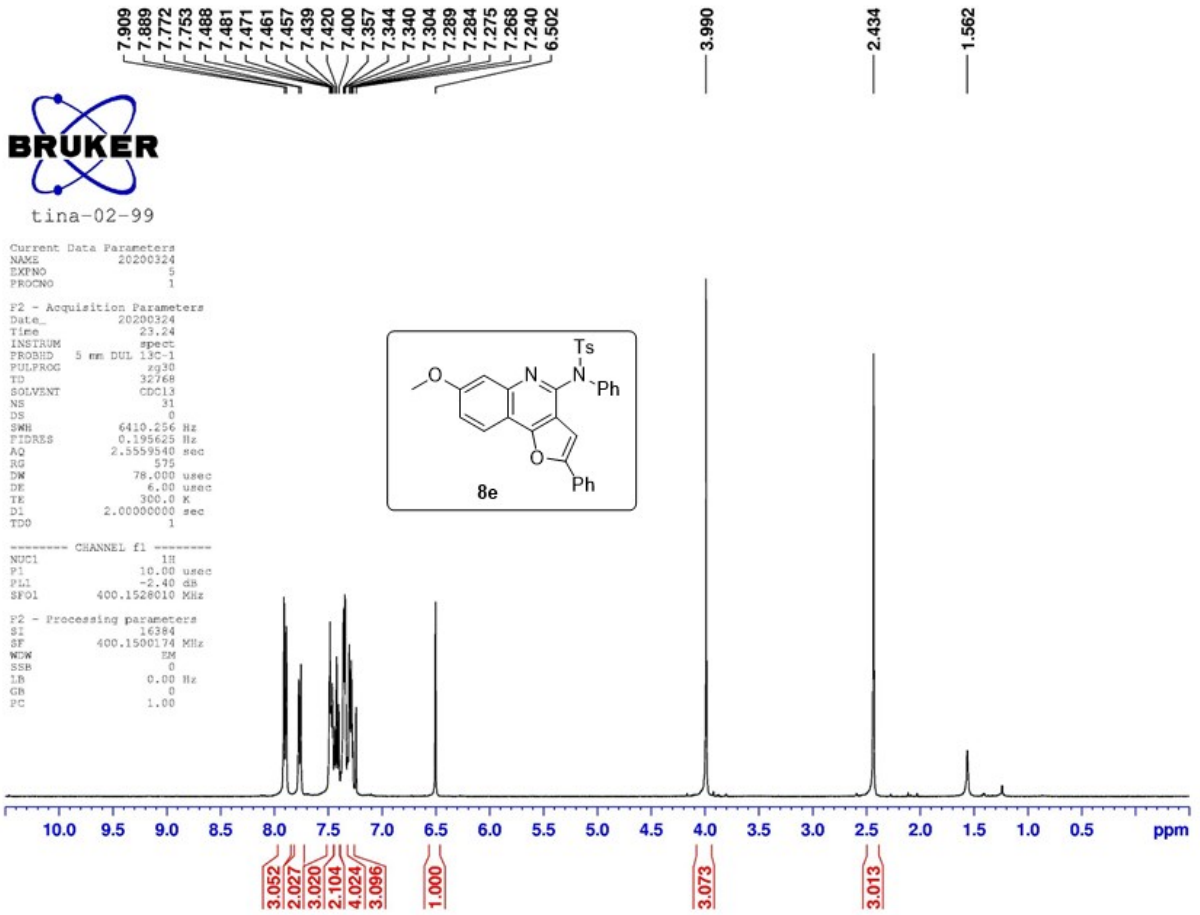

192.548
154.614
144.320
139.866
137.528
136.664
131.118
129.678
129.224
128.276
128.206
128.161
128.061
127.913
125.504
123.363
120.984
119.019
109.920
95.658
94.594
80.611
77.318
77.000
76.683
56.202
21.388
tina-2-77-2
O
H
N
Ts
N
Ph
OMe
7e
Ph
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

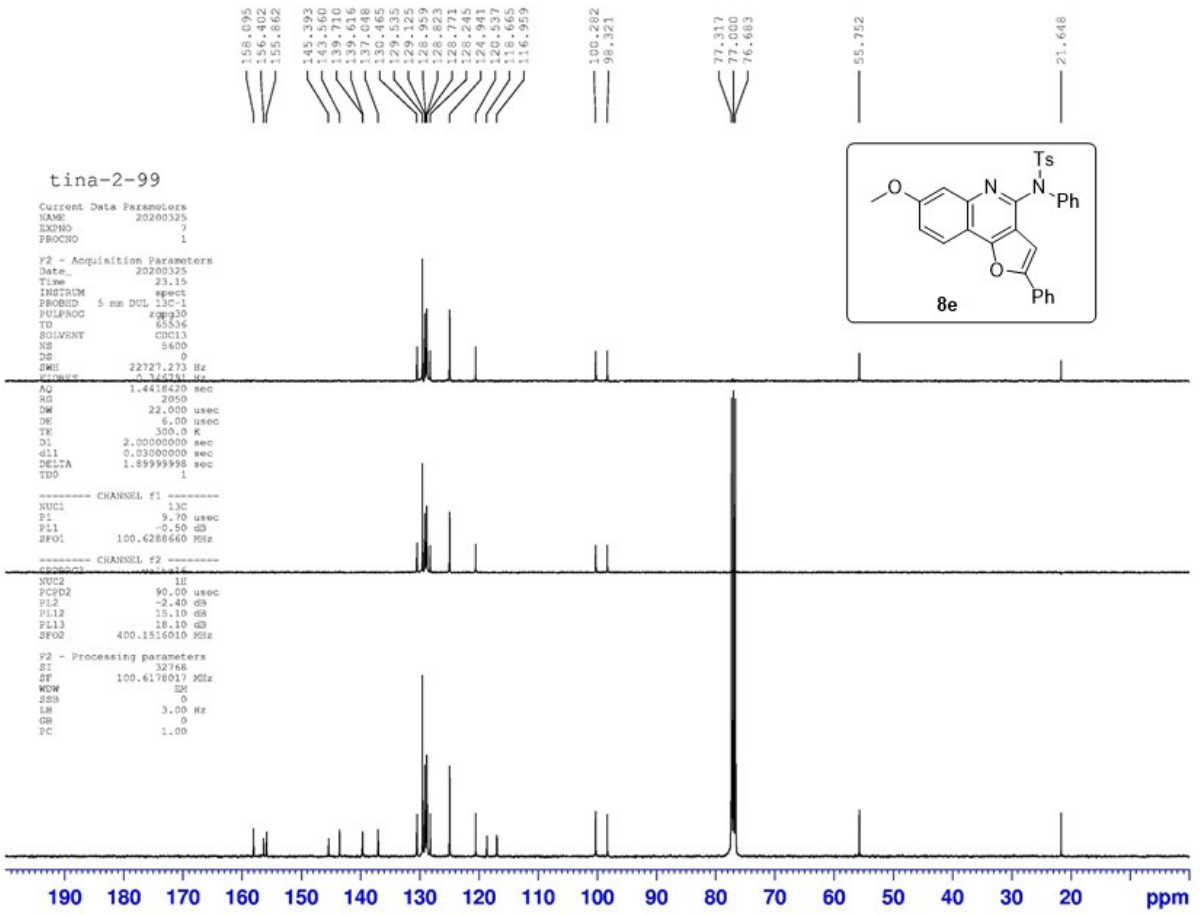

10.63
10.06
7.774
7.754
7.649
7.630
7.550
7.532
7.383
7.366
7.346
7.331
7.324
7.247
7.227
7.211
7.202
7.193
7.097
7.079
5.320
2.874
2.254
1.671
BRUKER
tina-2-111
Current Data Parameters
NAME 20200407
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200407
Time 15.48
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CD2Cl2
NS 14
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 256
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz
F2 - Processing parameters
SI 16384
SF 400.1500153 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
O
H
N
Ts
N
Ph
Me
7h
Ph
12
11
10
9
8
7
6
5
4
3
2
1
ppm
1.000
1.081
2.042
1.107
2.090
6.422
4.135
1.110
3.141
3.200

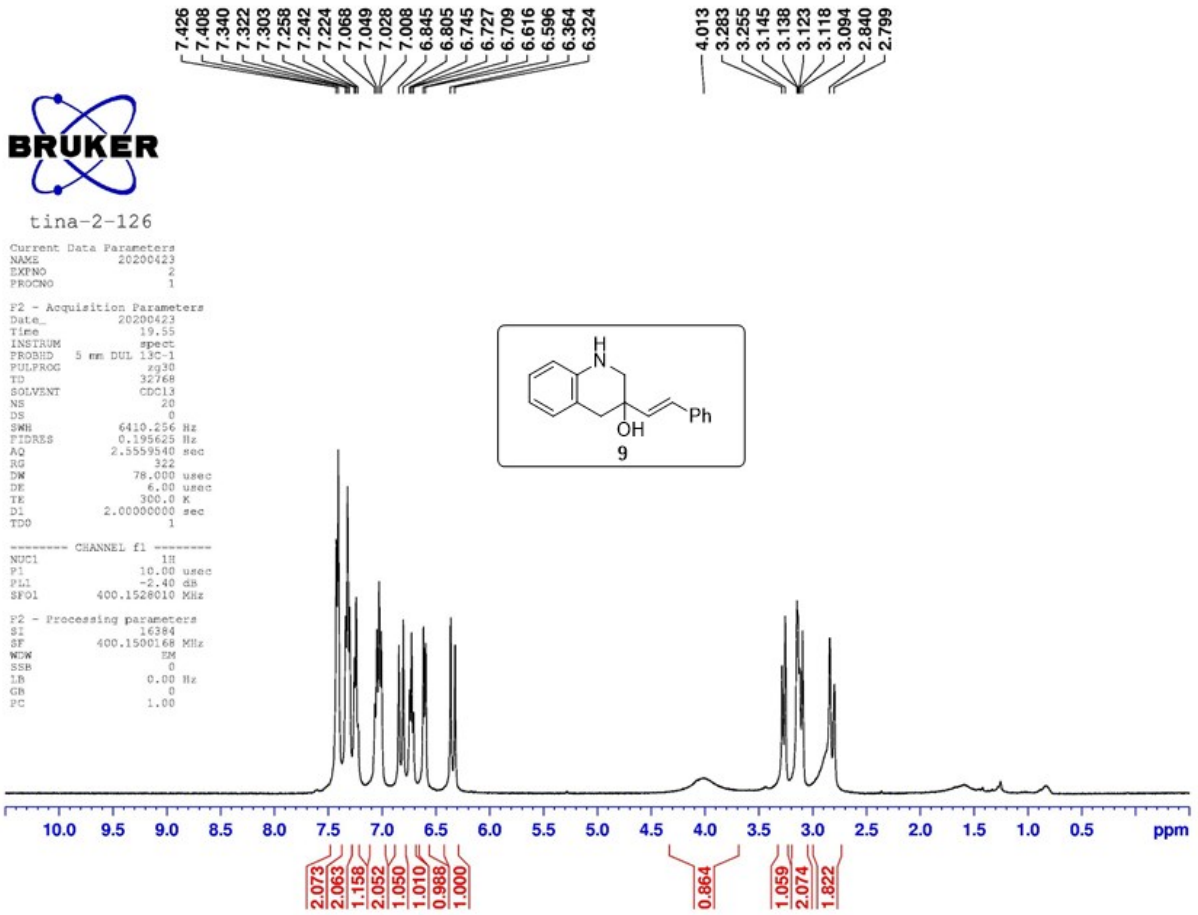

192.853
145.107
141.497
140.508
137.681
137.338
131.018
130.916
130.186
129.567
128.627
128.407
128.291
126.895
123.784
122.728
119.400
96.850
94.867
83.255
54.340
54.070
53.800
53.530
53.260
21.554
19.692
tina-2-111
O
H
N
Ts
N
Ph
Me
7h
Ph
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

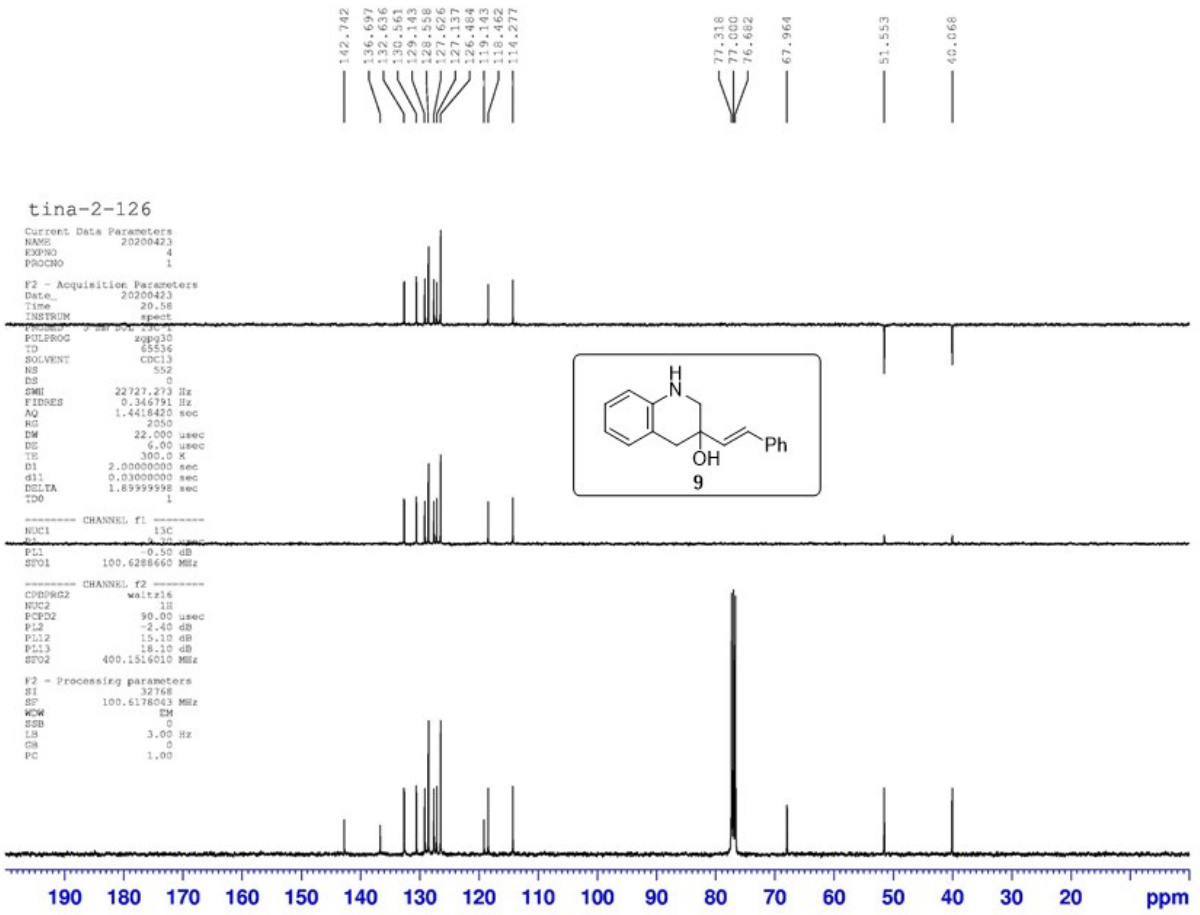

10.725
7.913
7.894
7.834
7.815
7.728
7.707
7.544
7.540
7.535
7.526
7.522
7.520
7.347
7.343
7.338
7.326
7.322
7.307
7.301
7.297
7.291
7.285
7.280
7.248
7.240
7.229
7.218
7.209
7.200
7.194
7.183
7.162
2.695
2.218
1.606
BRUKER
tina-2-66
Current Data Parameters
NAME 20200226
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200226
Time 15.45
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 6
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 406
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz
F2 - Processing parameters
SI 16384
SF 400.1500171 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
Me
O
H
N
Ts
N
Ph
Ph
7i
12
11
10
9
8
7
6
5
4
3
2
1
ppm
1.012
1.000
1.019
2.013
2.036
6.010
5.125
3.108
3.048

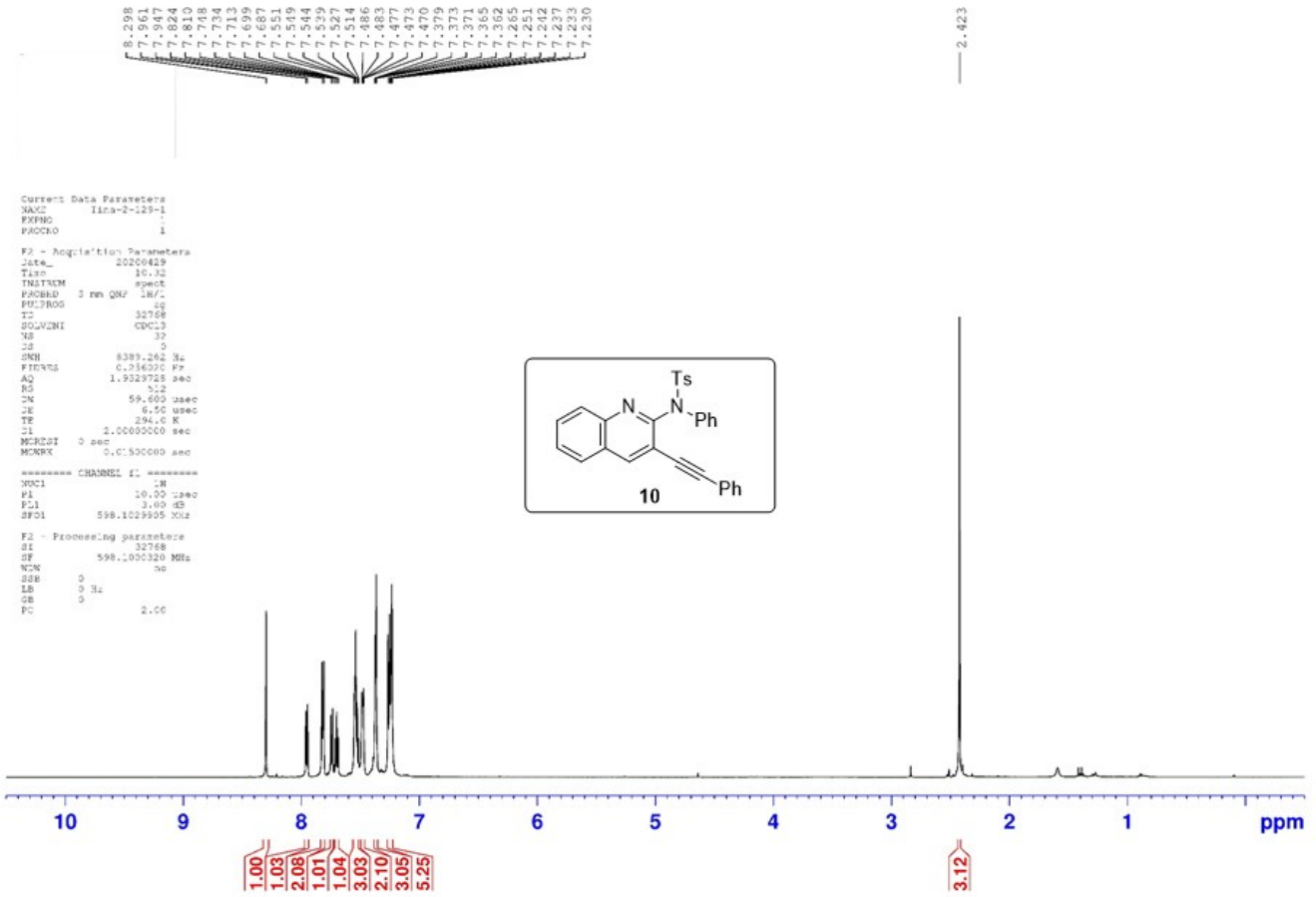

199.762
144.264
139.809
136.888
136.544
131.352
131.008
129.613
129.133
128.238
128.088
127.946
127.792
126.596
126.205
123.322
120.335
120.119
95.636
94.379
80.879
77.318
77.000
76.682
26.380
21.312
tina-2-66
Current Data Parameters
NAME 20200225
EXPNO 9
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200225
Time 21.38
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
NS 105
DS 0
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4418420 sec
RG 2050
DW 22.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
CHANNEL f1
NUC1 13C
P1 9.70 usec
PL1 -0.50 dB
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.40 dB
PL12 15.10 dB
PL13 18.10 dB
SFO2 400.1516010 MHz
F2 - Processing parameters
SI 32768
SF 100.6178165 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
Me
O
H
N
Ts
N
Ph
Ph
7i
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

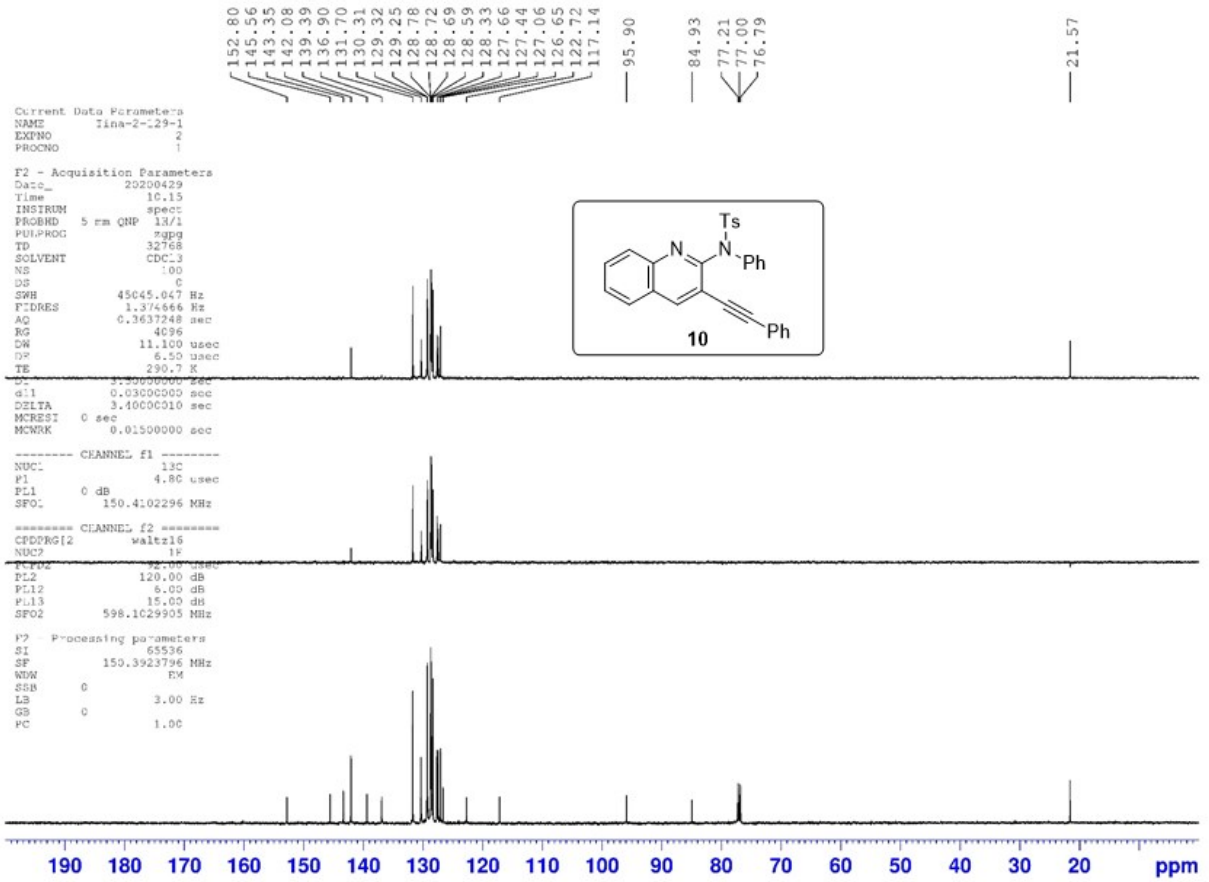

7.909
7.889
7.772
7.753
7.488
7.481
7.471
7.461
7.457
7.439
7.420
7.400
7.357
7.344
7.340
7.304
7.289
7.284
7.275
7.268
7.240
6.502
3.990
2.434
1.562
BRUKER
tina-02-99
Current Data Parameters
NAME 20200324
EXPNO 5
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200324
Time 23.24
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 31
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 575
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz
F2 - Processing parameters
SI 16384
SF 400.1500174 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
Ts
N
N
Ph
O
O
Ph
8e
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
3.052
2.027
3.020
2.104
4.024
3.096
1.000
3.073
3.013

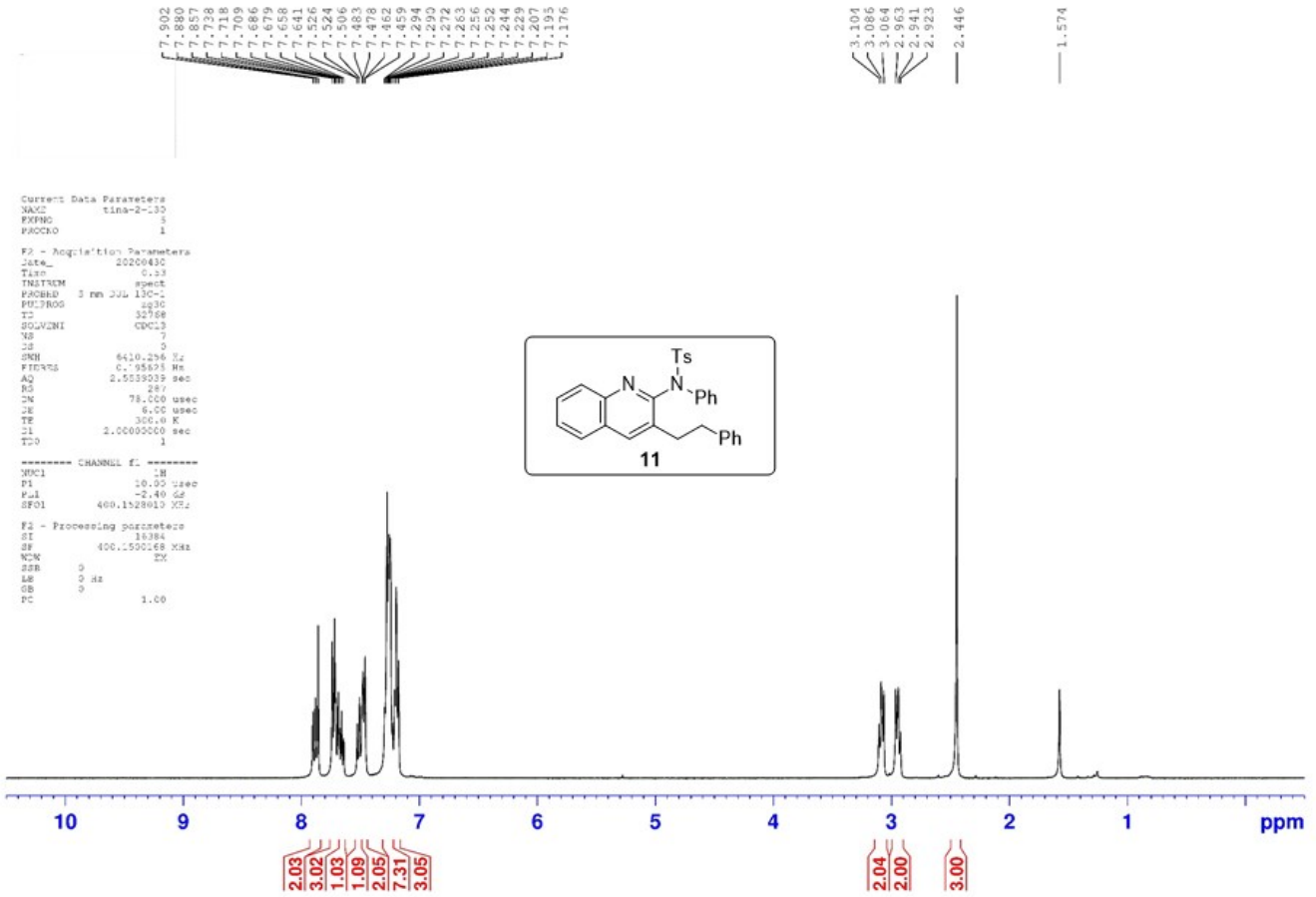

158.095
156.402
155.862
145.393
143.560
139.710
139.616
137.048
130.465
129.535
129.125
128.959
128.823
128.771
126.245
124.941
120.537
118.665
116.959
100.262
98.321
77.317
77.000
76.683
55.752
21.648
tina-2-99
Current Data Parameters
NAME 20200325
EXPNO 7
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200325
Time 23.15
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 5600
DS 0
SWH 22727.273 Hz
AQ 1.4418420 sec
RG 2050
DW 22.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.70 usec
PL1 -0.50 dB
SFO1 100.6288660 MHz
======== CHANNEL f2 ========
NUC2 1H
PCPD2 90.00 usec
PL2 -2.40 dB
PL12 15.10 dB
PL13 18.10 dB
SFO2 400.1516010 MHz
F2 - Processing parameters
SI 32768
SF 100.6178017 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
Ts
N
N
Ph
O
O
Ph
8e
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

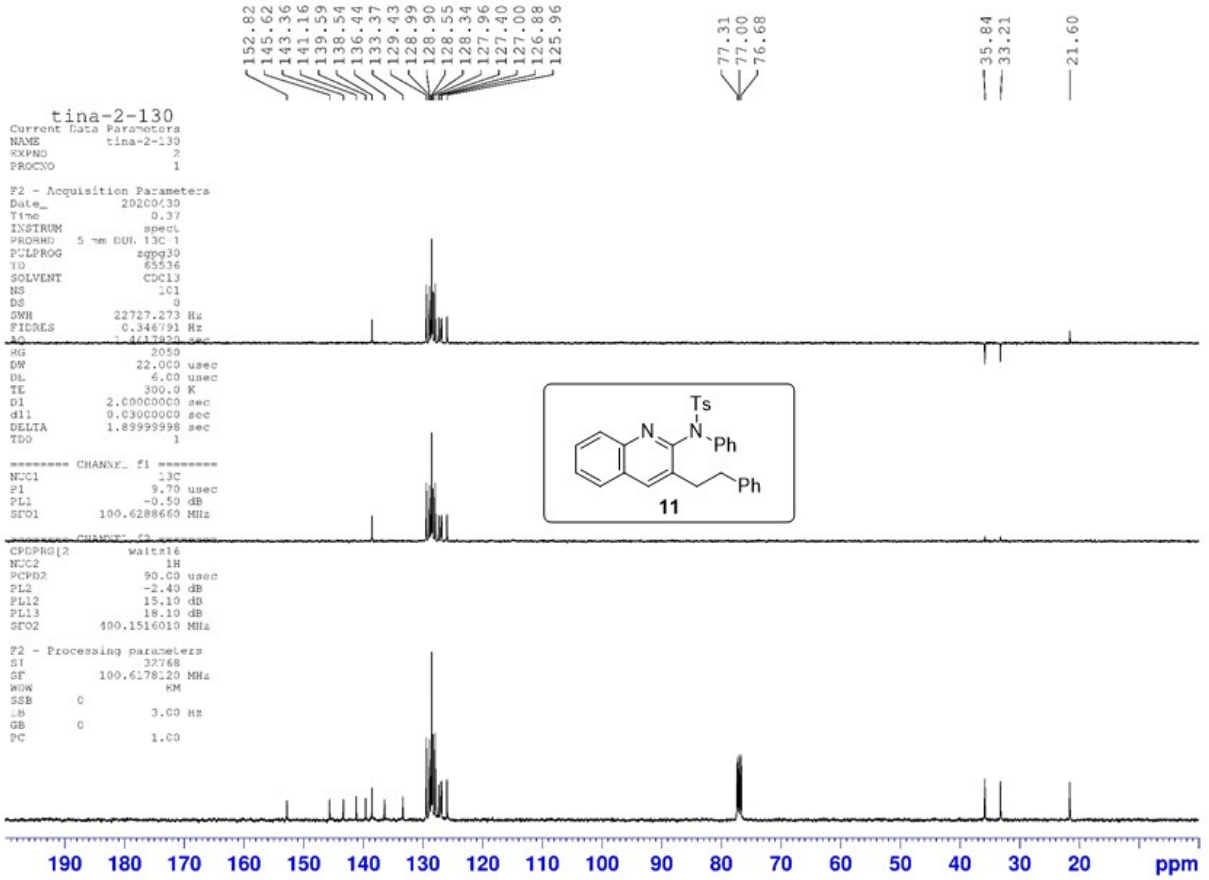

7.426
7.408
7.340
7.322
7.303
7.258
7.242
7.224
7.068
7.049
7.028
7.008
6.845
6.805
6.745
6.727
6.709
6.616
6.596
6.364
6.324
4.013
3.283
3.255
3.145
3.138
3.123
3.118
3.094
2.840
2.799
BRUKER
tina-2-126
Current Data Parameters
NAME 20200423
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200423
Time 19.55
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 20
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 322
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz
F2 - Processing parameters
SI 16384
SF 400.1500168 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
H
N
OH
Ph
9
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
2.073
2.063
1.158
2.052
1.050
1.010
0.988
1.000
0.864
1.059
2.074
1.822

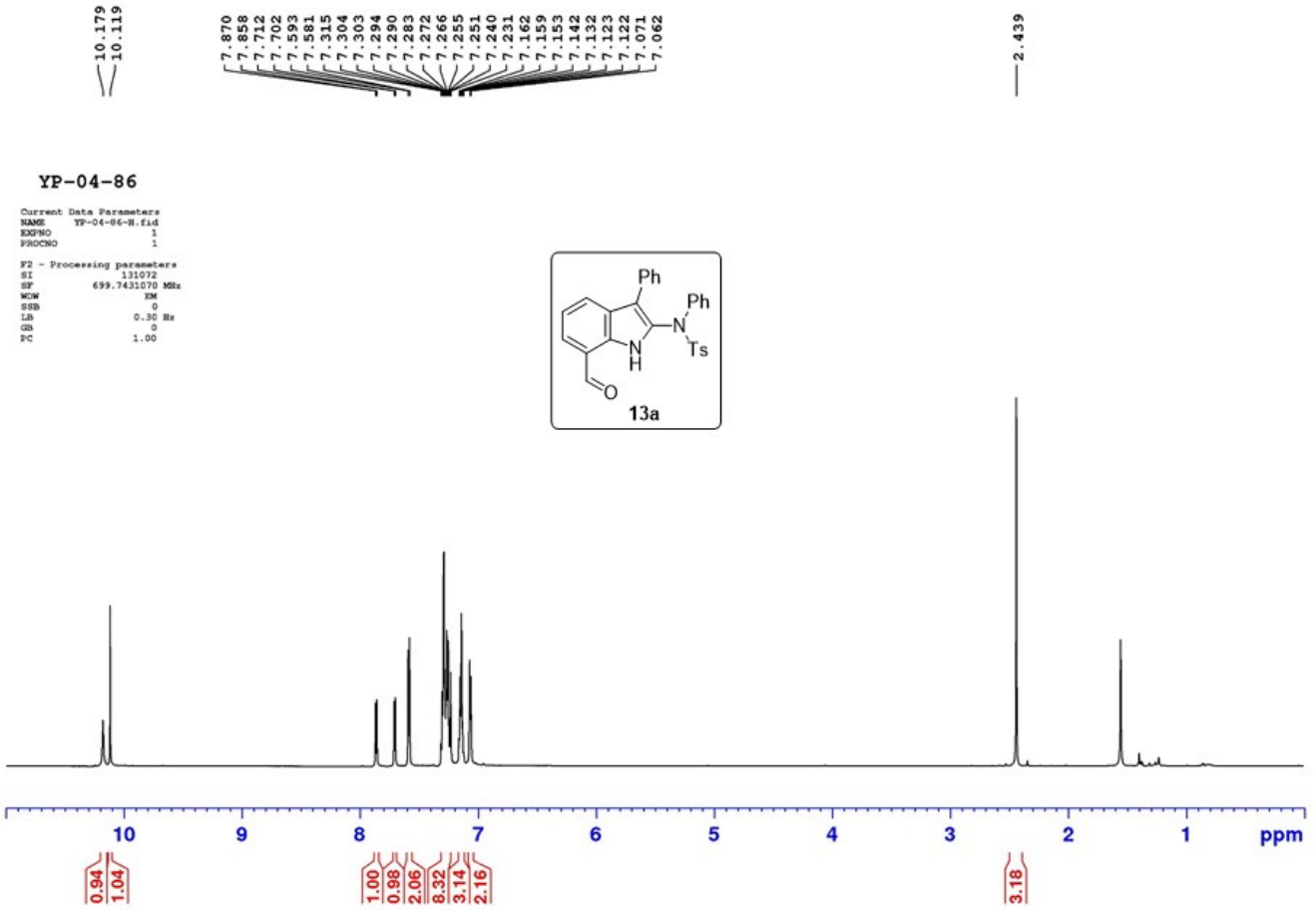

142.742
136.697
132.636
130.361
129.143
128.558
127.626
127.137
126.484
119.143
118.462
114.277
77.318
77.000
76.682
67.964
51.553
40.068
tina-2-126
Current Data Parameters
NAME 20200423
EXPNO 4
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200423
Time 20.58
INSTRUM spect
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 552
DS 0
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4418420 sec
RG 2050
DW 22.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
CHANNEL f1
NUC1 13C
PL1 -0.50 dB
SFO1 100.6288660 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.40 dB
PL12 15.10 dB
PL13 18.10 dB
SFO2 400.1516010 MHz
F2 - Processing parameters
SI 32768
SF 100.6178043 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
H
N
OH
Ph
9
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

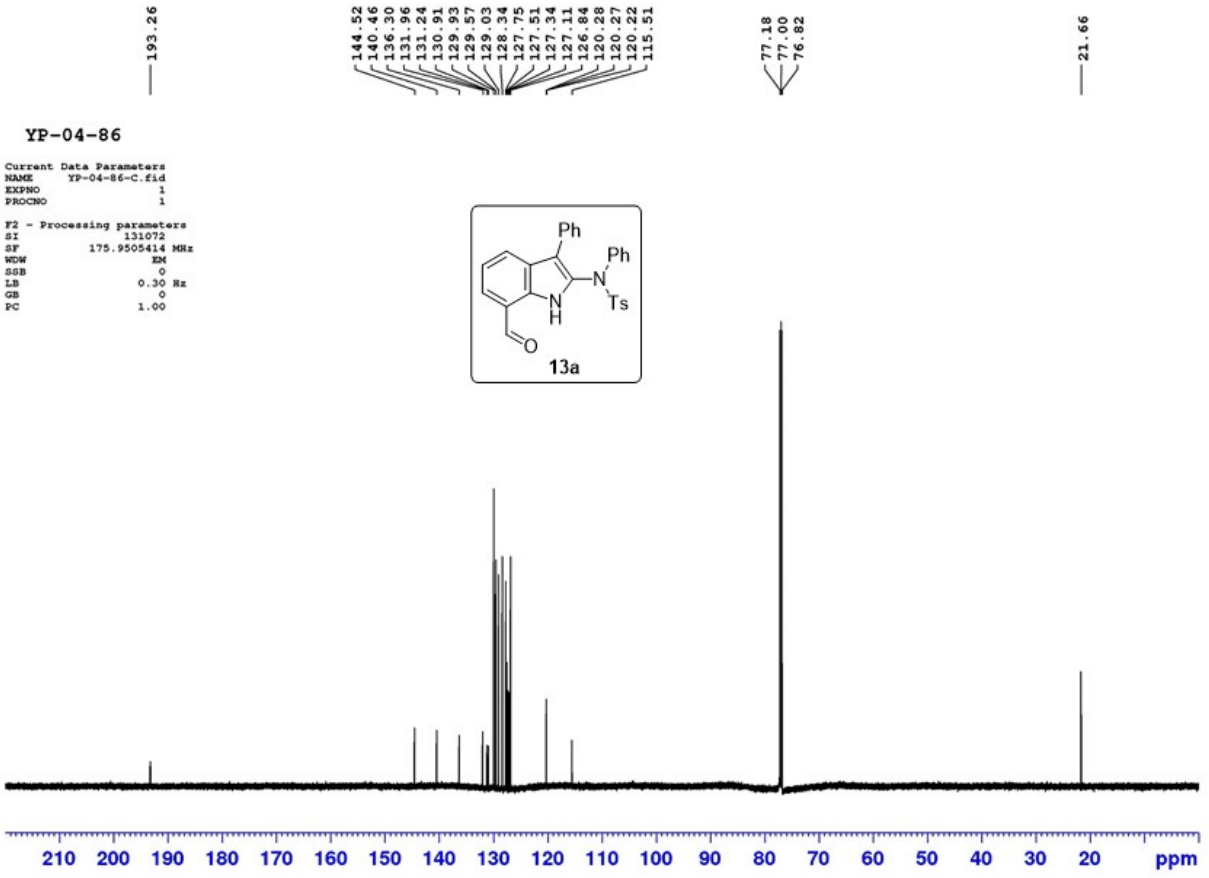

8.298
7.961
7.947
7.824
7.810
7.748
7.734
7.713
7.699
7.687
7.551
7.549
7.544
7.539
7.527
7.514
7.486
7.483
7.477
7.473
7.470
7.379
7.373
7.371
7.365
7.362
7.265
7.251
7.242
7.237
7.233
7.230
2.423
Ts
N
N
Ph
Ph
10
10
9
8
7
6
5
4
3
2
1
ppm
1.00
1.03
2.08
1.01
1.04
3.03
2.10
3.05
5.25
3.12

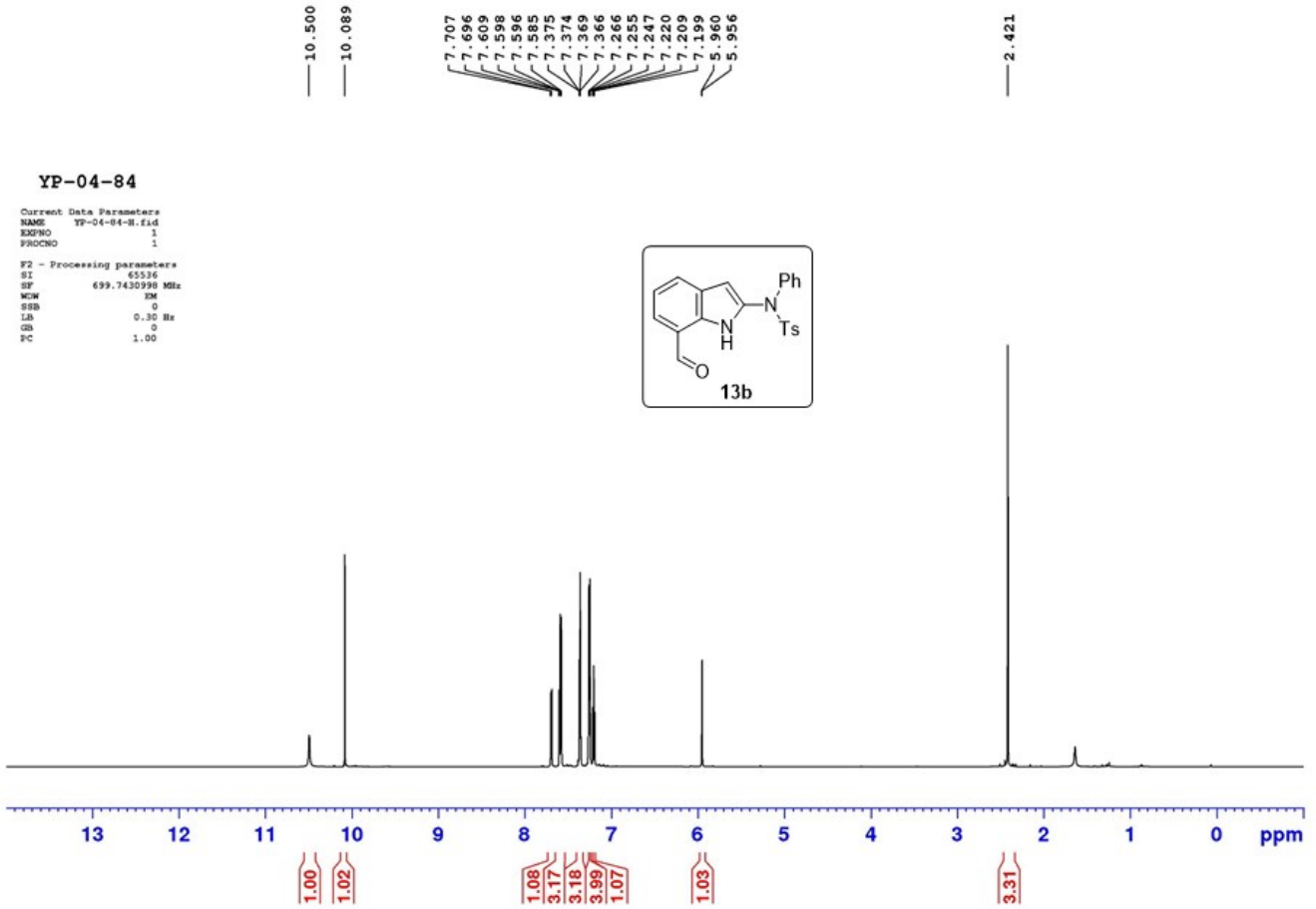

152.80
145.56
143.35
142.08
139.39
136.90
131.70
130.31
129.32
129.25
128.78
128.72
128.69
128.59
128.33
127.66
127.44
127.06
126.65
122.72
117.14
95.90
84.93
77.21
77.00
76.79
21.57
Current Data Parameters
NAME Tina-2-129-1
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200429
Time 16.15
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 100
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637248 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 290.7 K
D1 3.00000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
-------- CHANNEL f1 --------
NUC1 13C
P1 4.80 usec
PL1 0 dB
SFO1 150.4102296 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 6.00 dB
PL13 15.00 dB
SFO2 598.1029905 MHz
F2 - Processing parameters
SI 65536
SF 150.3923796 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
Ts
N
N
Ph
Ph
10
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

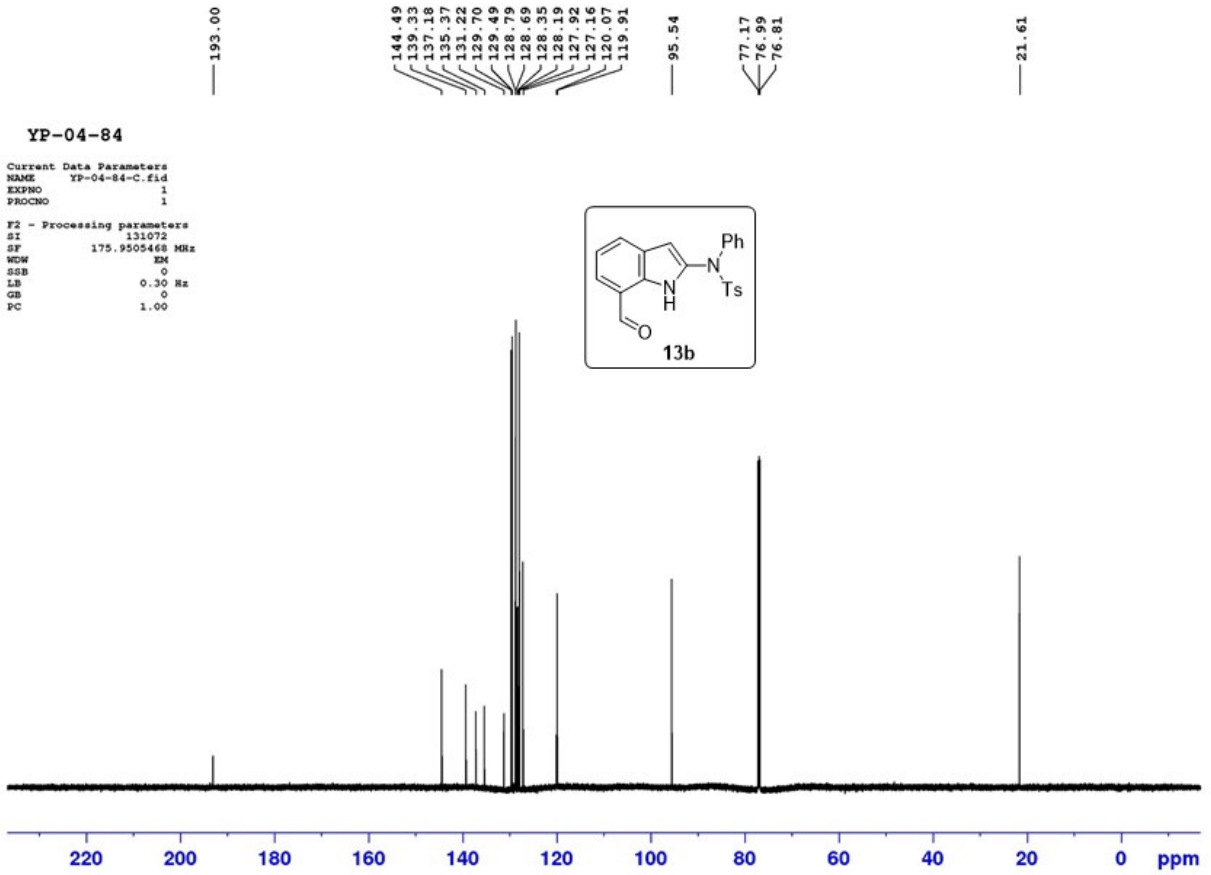

7.902
7.880
7.857
7.738
7.718
7.709
7.686
7.679
7.658
7.641
7.526
7.524
7.506
7.483
7.478
7.462
7.459
7.294
7.290
7.272
7.263
7.256
7.252
7.244
7.229
7.207
7.195
7.176
3.104
3.086
3.064
2.963
2.941
2.923
2.446
1.574
Ts
N
N
Ph
Ph
11
10
9
8
7
6
5
4
3
2
1
ppm
2.03
3.02
1.03
1.09
2.05
7.31
3.05
2.04
2.00
3.00


152.82
145.62
143.36
141.16
139.59
138.54
136.44
133.37
129.43
128.99
128.90
128.55
128.34
127.96
127.40
127.00
126.88
125.96
77.31
77.00
76.68
35.84
33.21
21.60
tina-2-130
Current Data Parameters
NAME tina-2-130
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200430
Time 0.37
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 101
DS 0
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4417920 sec
RG 2050
DW 22.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.70 usec
PL1 -0.50 dB
SFO1 100.6288660 MHz
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.40 dB
PL12 15.10 dB
PL13 18.10 dB
SFO2 400.1516010 MHz
F2 - Processing parameters
SI 32768
SF 100.6178120 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
Ts
N
N
Ph
Ph
11
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


10.179
10.119
7.870
7.858
7.712
7.702
7.593
7.581
7.315
7.304
7.303
7.294
7.290
7.283
7.272
7.266
7.255
7.251
7.240
7.231
7.162
7.159
7.153
7.142
7.132
7.123
7.122
7.071
7.062
2.439
YP-04-86
Current Data Parameters
NAME YP-04-86-H.fid
EXPNO 1
PROCNO 1
F2 - Processing parameters
SI 131072
SF 699.7431070 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
Ph
Ph
N
Ts
N
H
O
13a
10
9
8
7
6
5
4
3
2
1
ppm
0.94
1.04
1.00
0.98
2.06
8.32
3.14
2.16
3.18


193.26
144.52
140.46
136.30
131.96
131.24
130.91
129.93
129.57
129.03
128.34
127.75
127.51
127.34
127.11
126.84
120.28
120.27
120.22
115.51
77.18
77.00
76.82
21.66
YP-04-86
Current Data Parameters
NAME YP-04-86-C.fid
EXPNO 1
PROCNO 1
F2 - Processing parameters
SI 131072
SF 175.9505414 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
Ph
Ph
N
Ts
N
H
O
13a
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


10.500
10.089
7.707
7.696
7.609
7.598
7.596
7.585
7.375
7.374
7.369
7.366
7.266
7.255
7.247
7.220
7.209
7.199
5.960
5.956
2.421
YP-04-84
Current Data Parameters
NAME YP-04-84-H.fid
EXPNO 1
PROCNO 1
F2 - Processing parameters
SI 65536
SF 699.7430998 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
Ph
N
Ts
N
H
O
13b
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.02
1.08
3.17
3.18
3.99
1.07
1.03
3.31


193.00
144.49
139.33
137.18
135.37
131.22
129.70
129.49
128.79
128.69
128.35
128.19
127.92
127.16
120.07
119.91
95.54
77.17
76.99
76.81
21.61
YP-04-84
Current Data Parameters
NAME YP-04-84-C.fid
EXPNO 1
PROCNO 1
F2 - Processing parameters
SI 131072
SF 175.9505468 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
Ph
N
Ts
N
H
O
13b
220
200
180
160
140
120
100
80
60
40
20
0
ppm