Supporting Information for:

Chemoselective Double Annulation of Two Different Isocyanides: Rapid Access to Trifluoromethylated Indole-Fused Heterocycles

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I. General Information

All reagents were purchased from commercial sources and used without further purification, unless otherwise indicated. All reactions were monitored by TLC, which was performed on precoated aluminum sheets of silica gel 60 (F254). The products were purified by flash column chromatography on silica gel (300−400 mesh). Melting points were uncorrected. ^{1}H-NMR and ^{13}C-NMR spectra were recorded at 25 ºC on a Varian 400 MHz and 500 MHz, respectively, and TMS as the internal standard. All chemical shifts are given in ppm. High-resolution mass spectra (HRMS) were obtained using a Bruker microTOF II focus spectrometer (ESI).

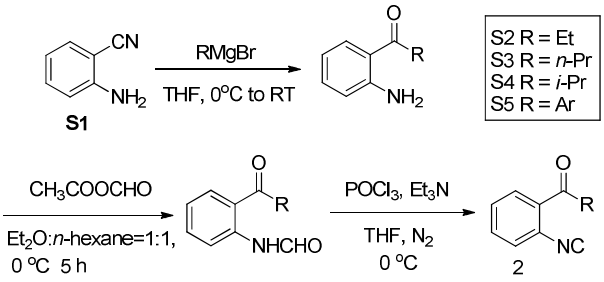
II. Synthesis and analytical data of substrates

1. Synthesis and analytical data of substrates **1**.

2. The starting materials **2** were prepared according to the literature procedures[1].

3. Synthesis and analytical data of ^{18}O-(2-isocyanophenyl)(phenyl)methanone.

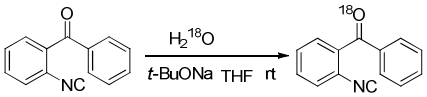
General experimental procedure for the preparation of substrates 1:



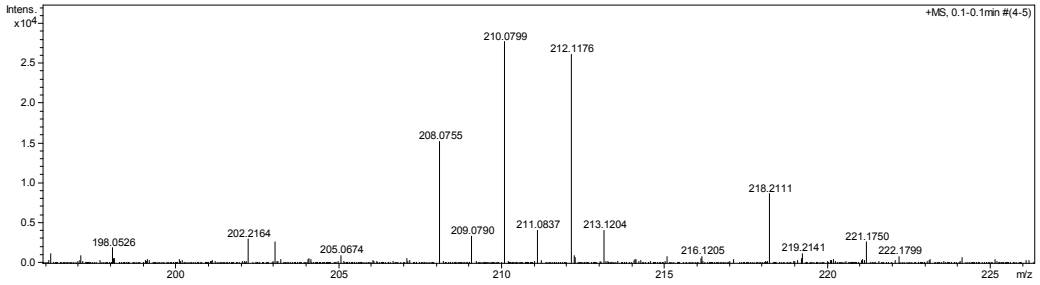
Ketones **S2, S3, S4,** and **S5** were prepared from **S1** according to literature procedures.[2] (2-Aminophenyl)(phenyl)methanone and 2-aminophenyl ethanone are commercially available. Isocyanides **1** were prepared according to the literature procedures[3c] by the typical formylation and dehydration procedure.[3]

Preparation of ^{18}O-(2-isocyanophenyl)(phenyl)methanone:

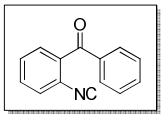
1. Zhang, X.; Gao, Y. L.; Xu, X. X. *Chem. Commun*. **2017**, *53*, 2427-2430
2. Mondal, S.; Mohamed, R. K.; Manoharan, M.; Phan, H.; Alabugin, L. V. *Org. Lett*. **2013**, *15*, 5650-5653.
3. (a) Neochoritis, C. G.; Stotani, S.; Mishra, B.; Dömling, A. *Org. Lett.* **2015**, *17*, 2002−2005. (b) Sisko, J.; Mellinger, M.; Sheldrake, P. W.; Baine, N. H. *Tetrahedron Lett*. **1996**, *37*, 8113−8116. (c) Kobayashi, K.; Yoneda, K.; Miyamoto, K.; Morikawa, O.; Konishi, H. *Tetrahedron Lett*. **2004**, *60*, 11639−11645. (d) Kobayashi, K.; Okamura, Y.; Fukamachi, S.; Konishi, H. *Tetrahedron* **2010**, *66*, 7961−7964.



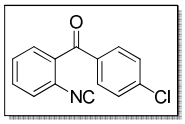
To a solution of (2-isocyanophenyl)(phenyl)methanone (**1**) (0.063 g, 0.3 mmol) and *t*-BuONa (0.029g, 0.3 mmol) in THF (2 ml) $H_2{}^{18}O$ (0.054 mL, 3 mmol) was added. The reaction mixture was stirred at room temperature. After the reaction was finished as indicated by TLC (reaction time, 30 min), the resulting mixture was poured into water (10 mL) and extracted with DCM (CH_2Cl_2, 10 mL). The combined organic layer was dried over anhydrous Na_2SO_4 and concentrated *in vacuo*. Purification of the crude product with flash column chromatography (petroleum ether /EtOAc = 15:1) to give 1a-^{18}O.



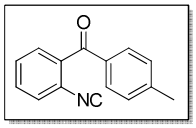
Analytical data of compounds 1



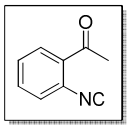
1a, (2-Isocyanophenyl)(phenyl)methanone.[3c] Yield: 0.94 g, 91 %. Pale yellow solid. m.p. 83-85 ºC. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.48-7.52 (m, 5H), 7.55-7.56 (m, 1H), 7.64 (t, *J* = 7.2 Hz, 1H), 7.81 (d, *J* = 7.2 Hz, 2H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 127.8, 128.7, 129.1, 129.4, 130.0, 131.4, 133.9, 136.1, 136.2, 169.0, 193.6. Mass Spectrometry: HRMS (ESI-TOF) (m/z): Calcd for $C_{14}H_9NNaO^+$ ($[M + Na]^+$) 230.0576, found 230.0581.



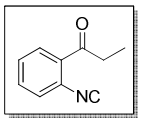
1b, (4-Chlorophenyl)(2-isocyanophenyl)methanone.[3d] Yield: 1.07 g, 89 %. Yellow solid. m.p. 90-93 ºC. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.46-7.59 (m, 6H), 7.76 (d, *J* = 7.2 Hz, 2H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 127.9, 129.1, 129.2, 129.3, 131.3, 131.6, 133.9, 134.4, 135.6, 140.6, 169.2, 192.4. Mass Spectrometry: HRMS (ESI-TOF) (m/z): Calcd for $C_{14}H_8NClNaO^+$ ($[M + Na]^+$) 264.0187, found 264.0187.



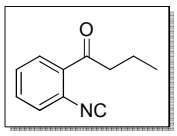
1c, (2-Isocyanophenyl)(*p*-tolyl)methanone. Yield: 0.95 g, 86 %. Yellow solid. m.p. 106-108 ºC. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 2.43 (s, 3H), 7.28 (d, J = 8.0 Hz, 2H), 7.48-7.54 (m, 4H), 7.70-7.72 (m, 2H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 21.7, 124.2, 127.7, 129.0, 129.2, 129.4, 130.2, 131.1, 133.5, 145.0, 168.7, 193.2. Mass Spectrometry: HRMS (ESI-TOF) (m/z): Calcd for $C_{15}H_{11}NNaO^+$ ($[M + Na]^+$) 244.0733, found 244.0741.



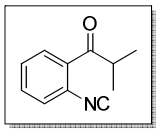
1d, 1-(2-Isocyanophenyl)ethanone.[3c] Yield: 0.52 g, 71 %. Yellow oil. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 2.71 (s, 3H), 7.47-7.53 (m, 2H), 7.55-7.59 (m, 1H), 7.79 (d, J = 7.6 Hz, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 29.5, 123.7, 128.7, 129.4, 132.5, 134.9, 169.8, 196.8.



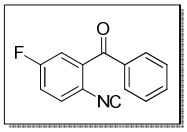
1e, 1-(2-Isocyanophenyl)propan-1-one. Yield: 0.54 g, 68 %. Yellow oil. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 1.24 (t, J = 8.0 Hz, 3H), 3.04 (q, J = 7.2 Hz, 2H), 7.46-7.56 (m, 3H), 7.72 (q, J = 6.0 Hz, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 7.99, 35.0, 128.7, 128.9, 129.4, 132.1, 135.5, 169.4, 200.4. Mass Spectrometry: HRMS (ESI-TOF) (m/z): Calcd for $C_{10}H_9NNaO^+$ ($[M + Na]^+$) 182.0576, found 182.0583.



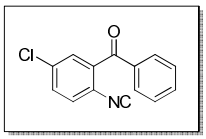
1f, 1-(2-Isocyanophenyl)butan-1-one. Yield: 0.57 g, 66 %. Yellow oil. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 1.00 (t, J = 7.2 Hz, 3H), 1.73-1.80 (m, 2H), 2.98 (t, J = 7.6 Hz, 2H), 7.45-7.55 (m, 3H), 7.69 (q, J = 6.0 Hz, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 13.5, 17.5, 43.6, 128.6, 128.8, 129.4, 132.0, 135.8, 169.5, 200.1. Mass Spectrometry: HRMS (ESI-TOF) (m/z): Calcd for $C_{11}H_{11}NNaO^+$ ($[M + Na]^+$) 196.0733, found 196.0721.



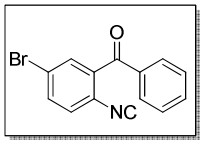
1g, 1-(2-Isocyanophenyl)-2-methylpropan-1-one. Yield: 0.55 g, 64 %. Yellow oil. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 1.21 (s, 3H), 1.22 (s, 3H), 3.38-3.49 (m, 1H), 7.45-7.50 (m, 3H), 7.57-7.59 (m, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 18.2, 39.0, 128.3, 128.4, 129.3, 131.6, 136.2, 169.0, 204.8. Mass Spectrometry: HRMS (ESI-TOF) (m/z): Calcd for $C_{11}H_{11}NNaO^+$ ($[M + Na]^+$) 196.0733, found 196.0741.



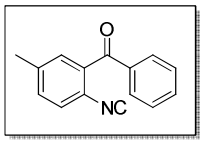
1h, (5-Fluoro-2-isocyanophenyl)(phenyl)methanone. Yield: 0.91 g, 81 %. Yellow solid. m.p. 73-75 ºC. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.20-7.28 (m, 2H), 7.51 (t, *J* = 6.8 Hz, 3H), 7.65 (t, *J* = 7.2 Hz, 1H), 7.81 (d, *J* = 7.6 Hz, 2H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 116.5 (d, *J* = 25.5 Hz), 118.5 (d, *J* = 23.1 Hz), 128.8, 129.8 (d, *J* = 8.7 Hz), 129.9, 134.3, 135.3, 138.2 (d, *J* = 6.9 Hz), 161.5 (d, *J* = 283.2 Hz), 169.0, 192.0. Mass Spectrometry: HRMS (ESI-TOF) (m/z): Calcd for $C_{14}H_8NFNaO^+$ ([M + Na]$^+$) 248.0482, found 248.0484.



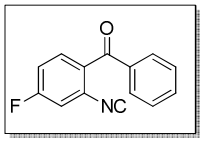
1i, (5-Chloro-2-isocyanophenyl)(phenyl)methanone.[3c] Yield: 1.05 g, 87 %. Yellow solid. m.p. 82-84 ºC. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.43-7.51 (m, 5H), 7.64-7.67 (m, 1H), 7.80 (d, *J* = 7.6 Hz, 2H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 128.8, 128.9, 129.2, 129.9, 131.4, 134.3, 135.3, 135.4, 137.5, 170.2, 192.0. Mass Spectrometry: HRMS (ESI-TOF) (m/z): Calcd for $C_{14}H_8NClNaO^+$ ([M + Na]$^+$) 264.0187, found 264.0191.



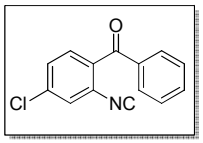
1j, (5-Bromo-2-isocyanophenyl)(phenyl)methanone. Yield: 1.25 g, 88 %. Yellow solid. m.p. 105-107 ºC. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.37 (d, *J* = 8.4 Hz, 1H), 7.51 (t, *J* = 8.0 Hz, 2H), 7.63-7.70 (m, 3H), 7.79-7.81 (m, 2H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 123.2, 128.8, 129.0, 129.9, 132.1, 134.3, 137.6, 170.5, 191.9. Mass Spectrometry: HRMS (ESI-TOF) (m/z): Calcd for $C_{14}H_8NBrNaO^+$ ([M + Na]$^+$) 307.9681, found 307.9680.



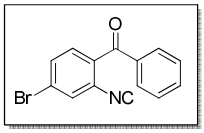
1k, (2-Isocyano-5-methylphenyl)(phenyl)methanone. Yield: 0.87 g, 79 %. Yellow solid. m.p. 102-104 ºC. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 2.42 (s, 3H), 7.30 (s, 1H), 7.33-7.39 (m, 2H), 7.49 (t, *J* = 8.0 Hz, 2H), 7.60-7.64 (m, 1H), 7.79-7.82 (m, 2H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 21.3, 127.6, 128.7, 129.8, 130.0, 132.0, 133.9, 136.0, 136.2, 139.8, 168.1, 194.0. Mass Spectrometry: HRMS (ESI-TOF) (m/z): Calcd for $C_{15}H_{11}NNaO^+$ ([M + Na]$^+$) 244.0733, found 244.0742.



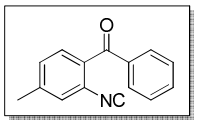
1l, (4-Fluoro-2-isocyanophenyl)(phenyl)methanone. Yield: 0.92 g, 82 %. Yellow solid. m.p. 64-66 ºC. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.24 (t, *J* = 8.0 Hz, 2H), 7.48-7.56 (m, 3H), 7.64 (t, *J* = 7.2 Hz, 1H), 7.79 (d, *J* = 7.2 Hz, 2H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 115.4 (d, *J* = 25.5 Hz), 116.7 (d, *J* = 21.3 Hz), 120.7, 129.9, 131.7 (d, *J* = 9.4 Hz), 132.2 (d, *J* = 3.8 Hz), 134.0, 136.0, 164.3 (d, *J* = 253.3 Hz), 170.4, 192.4. Mass Spectrometry: HRMS (ESI-TOF) (m/z): Calcd for $C_{14}H_8NFNaO^+$ ($[M + Na]^+$) 248.0482, found 248.0485.



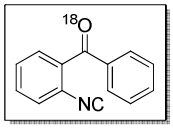
1m, (4-Chloro-2-isocyanophenyl)(phenyl)methanone. Yield: 1.05 g, 87 %. Yellow solid. m.p. 71-73 ºC. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.48-7.52 (m, 5H), 7.63-7.67 (m, 1H), 7.78-7.80 (m, 2H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 127.9, 128.8, 129.6, 130.0, 130.7, 134.2, 134.4, 135.9, 137.4, 170.8, 192. 6. Mass Spectrometry: HRMS (ESI-TOF) (m/z): Calcd for $C_{14}H_8NClNaO^+$ ($[M + Na]^+$) 264.0187, found 264.0187.



1n, (4-Bromo-2-isocyanophenyl)(phenyl)methanone. Yield: 1.24 g, 87 %. Yellow solid. m.p. 90-92 ºC. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.39-7.41 (m, 1H), 7.48-7.52 (m, 2H), 7.63-7.67 (m, 3H), 7.78-7.80 (m, 2H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 125.0, 128.8, 129.9, 130.6, 130.7, 132.4, 134.1, 134.8, 135.8, 170.8, 192.6. Mass Spectrometry: HRMS (ESI-TOF) (m/z): Calcd for $C_{14}H_8NBrlNaO^+$ ($[M + Na]^+$) 307.9681, found 307.9680.

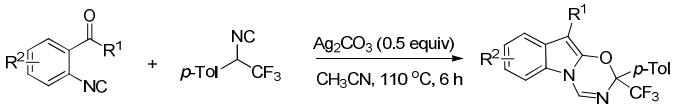


1o, (2-Isocyano-4-methylphenyl)(phenyl)methanone. Yield: 0.85 g, 77 %. Yellow solid. m.p. 93-95 ºC. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 2.44 (s, 3H), 7.29-7.31 (m, 2H), 7.41 (d, *J* = 8.4 Hz, 1H), 7.46-7.50 (m, 2H), 7.59-7.63 (m, 1H), 7.78-7.81 (m, 2H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 21.1, 128.3, 128.6, 129.6, 129.7, 129.9, 133.1, 133.7, 136.4, 142.5, 168.4, 193.6. Mass Spectrometry: HRMS (ESI-TOF) (m/z): Calcd for $C_{15}H_{11}NNaO^+$ ($[M + Na]^+$) 244.0733, found 244.0740.



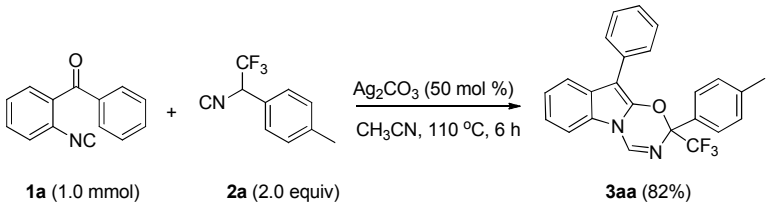
1a-^{18}O, ^{18}O-(2-Isocyanophenyl)(phenyl)methanone. Pale yellow solid. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.48-7.51 (m, 6H), 7.61-7.66 (m, 1H), 7.80-7.82 (m, 2H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 127.8, 128.7, 129.1, 129.4, 130.0, 131.4, 133.9, 136.1, 136.2, 168.9, 193.7. Mass Spectrometry: HRMS (ESI-TOF) (m/z): Calcd for $C_{14}H_9N^{18}O$ ([M + H]$^+$) 210.0799, found 210.0799.

III. Synthetic procedures and analytical data of compounds 3



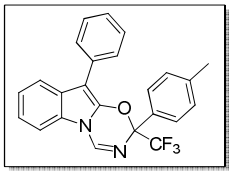
General procedure for the synthesis of 3 (taking 3aa as an example): To a solution of (2-isocyanophenyl)(phenyl)methanone (**1**) (42 mg, 0.2 mmol) and 1-methyl-4-(2,2,2-trifluoro-1-isocyanoethyl)benzene (**2a**) (79 mg, 0.4 mmol) in CH_3CN (2 ml) Ag_2CO_3 (0.028 g, 0.1 mmol) was added. The reaction mixture was heated at 110 ºC under stirring in sealed tube. After the reaction was finished as indicated by TLC (reaction time, 6 h), the resulting mixture was poured into water (10 mL) and extracted with DCM (CH_2Cl_2, 10 mL×3). The combined organic layer was dried over anhydrous Na_2SO_4 and concentrated *in vacuo*. Purification of the crude product with flash column chromatography (petroleum ether /EtOAc = 30:1) to give **3aa** (0.074 g, 91%).

1mmol Scale Synthesis of 3aa



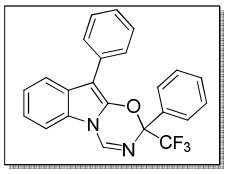
To a solution of (2-isocyanophenyl)(phenyl)methanone (**1**) (207 mg, 1.0 mmol) and 1-methyl-4-(2,2,2-trifluoro-1-isocyanoethyl)benzene (**2a**) (398 mg, 2.0 mmol) in CH_3CN (2.0 ml) Ag_2CO_3 (140 mg, 0.5 mmol) was added. The reaction mixture was heated at 110 ºC under stirring in sealed tube. After the reaction was finished as indicated by TLC (reaction time, 6 h), the resulting mixture was poured into water (10.0 mL) and extracted with DCM (CH_2Cl_2, 10.0 mL×3). The combined organic layer was dried over anhydrous Na_2SO_4 and concentrated *in vacuo*. Purification of the crude product with flash column chromatography (petroleum ether /EtOAc = 30:1) to give **3aa** (333 mg, 82%).

Analytical data of compounds 3



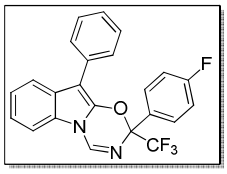
3aa, 10-Phenyl-2-(*p*-tolyl)-2-(trifluoromethyl)-2*H*-[1,3,5]oxadiazino[3,2-*a*]indole.

For **3aa**, yield: 73.9 mg, 91 %, pale yellow solid. m.p. 110-112 ºC. NMR Spectroscopy: ^{1}H NMR ($CDCl_3$, 500 MHz) δ 2.30 (s, 3H), 7.14 (d, *J* = 8.0 Hz, 2H), 7.19-7.24 (m, 2H), 7.35-7.39 (m, 2H), 7.53 (t, *J* = 8.0 Hz, 2H), 7.58 (d, *J* = 8.5 Hz, 2H), 7.73-7.78 (m, 3H), 8.38 (s, 1H). ^{13}C NMR ($CDCl_3$, 125 MHz) δ 21.1, 91.9 (q, *J* = 32.0 Hz), 99.4, 108.2, 119.6, 122.1 (q, *J* = 282.7 Hz), 122.7, 124.1, 126.6, 127.2, 127.5, 128.0, 128.7, 129.1, 129.7, 131.2 138.8, 139.0, 140.4. Mass Spectrometry: HRMS (ESI-TOF) (m/z): Calcd for $C_{24}H_{17}F_3N_2O$ ($[M + H]^+$) 407.1366, found 407.1353.



3ab, 2,10-Diphenyl-2-(trifluoromethyl)-2*H*-[1,3,5]oxadiazino[3,2-*a*]indole.

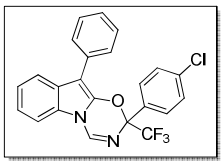
For **3ab**, yield: 62.0 mg, 79 %, pale yellow solid. m.p. 116-118ºC. NMR Spectroscopy: ^{1}H NMR ($CDCl_3$, 500 MHz) δ 7.19-7.25 (m, 2H), 7.33-7.40 (m, 5H), 7.53 (t, *J* = 7.6 Hz, 2H), 7.69-7.78 (m, 5H), 8.39 (s, 1H). ^{13}C NMR ($CDCl_3$, 151 MHz) δ 91.8 (q, *J* = 32.4 Hz), 99.4, 108.2, 119.7, 122.0 (q, *J* = 284.4 Hz), 122.8, 124.1, 126.7, 127.1, 127.6, 128.0, 128.4, 128.7, 128.8, 130.2, 131.1, 134.1, 138.7, 139.0. Mass Spectrometry: HRMS (ESI-TOF) (m/z): Calcd for $C_{23}H_{15}F_3N_2O$ ($[M + H]^+$) 393.1209, found 393.1198.



3ac, 2-(4-Fluorophenyl)-10-phenyl-2-(trifluoromethyl)-2*H*-[1,3,5]oxadiazino[3,2-*a*]indole.

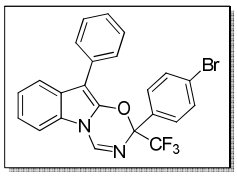
For **3ac**, yield: 73.8 mg, 90 %, white solid. m.p. 105-107ºC. NMR Spectroscopy: ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.00-7.03 (m, 1H), 7.25-7.32 (m, 3H), 7.37-7.42 (m, 2H), 7.53 (t, *J* = 7.2 Hz, 2H), 7.62-7.75 (m, 5H), 8.39 (s, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 91.7 (q, *J* = 34.0 Hz), 99.7 (d, *J* = 9.8 Hz), 108.3, 115.5 (d, *J* = 21.7 Hz), 119.8, 121.9 (q, *J* = 282.7 Hz), 123.0, 124.3, 126.8 (d, *J* =

3.6 Hz), 127.1, 128.0, 128.7, 128.8, 129.1, 129.8 (d, J = 8.2 Hz), 130.9 (d, J = 5.6 Hz), 132.7, 136.6, 138.3 (d, J = 9.3 Hz), 139.3 (d, J = 10.1 Hz), 163.8 (d, J = 248.9 Hz). Mass Spectrometry: HRMS (ESI-TOF) (m/z): Calcd for $C_{23}H_{14}F_4N_2O$ ($[M + H]^+$) 411.1115, found 411.1097.



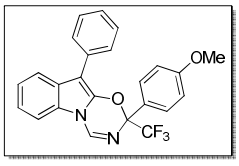
3ad, 2-(4-Chlorophenyl)-10-phenyl-2-(trifluoromethyl)-2*H*-[1,3,5]oxadiazino[3,2-*a*]indole.

For **3ad**, yield: 71.6 mg, 84 %, white solid. m.p. 111-113ºC. NMR Spectroscopy: ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.21-7.31 (m, 4H), 7.35-7.41 (m, 2H), 7.53 (t, J = 6.8 Hz, 2H), 7.63 (d, J = 8.0 Hz, 2H), 7.74 (d, J = 7.2 Hz, 3H), 8.38 (s, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 91.4 (q, J = 31.7 Hz), 99.8, 108.3, 119.8, 121.9 (q, J = 283.0 Hz), 123.0, 124.3, 126.8, 127.1, 128.0, 128.7, 128.8, 129.1, 130.9, 132.8, 136.6, 138.3, 139.2. Mass Spectrometry: HRMS (ESI-TOF) (m/z): Calcd for $C_{23}H_{14}ClF_3N_2O$ ($[M + H]^+$) 427.0820, found 427.0802.



3ae, 2-(4-Bromophenyl)-10-phenyl-2-(trifluoromethyl)-2*H*-[1,3,5]oxadiazino[3,2-*a*]indole.

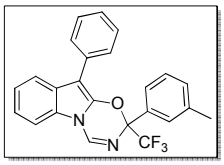
For **3ae**, yield: 79.9 mg, 85 %, white solid. m.p. 141-143ºC. NMR Spectroscopy: ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.21-7.28 (m, 2H), 7.37-7.41 (m, 2H), 7.46 (d, J = 7.4 Hz, 2H), 7.51-7.57 (m, 4H), 7.74 (d, J = 7.2 Hz, 3H), 8.38 (s, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 91.5 (q, J = 31.8 Hz), 99.8, 108.3, 119.8, 121.8 (q, J = 283.0 Hz), 123.0, 124.3, 124.9, 126.8, 127.0, 128.0, 128.6, 128.8, 129.4, 130.9, 131.7, 133.3, 138.3, 139.3. Mass Spectrometry: HRMS (ESI-TOF) (m/z): Calcd for $C_{23}H_{14}BrF_3N_2O$ ($[M + H]^+$) 471.0314, found 471.0285.



3af, 2-(4-Methoxyphenyl)-10-phenyl-2-(trifluoromethyl)-2*H*-[1,3,5]oxadiazino[3,2-*a*]indole.

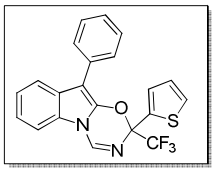
For **3af**, yield: 64.2 mg, 76 %, white solid. m.p. 136-138ºC. NMR Spectroscopy: ^{1}H NMR ($CDCl_3$, 400 MHz) δ 3.74 (s, 3H), 6.83 (d, J = 7.6 Hz, 2H), 7.22-7.24 (m, 2H), 7.36-7.38 (m, 2H), 7.25 (t, J

= 7.6 Hz, 2H), 7.61 (d, *J* = 7.6 Hz, 2H), 7.75-7.77 (m, 3H), 8.37 (s, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 55.2, 91.8 (q, *J* = 31.7 Hz), 99.4, 108.2, 113.8, 119.6, 122.1 (q, *J* = 282.6 Hz), 124.1, 125.9, 126.6, 127.1, 128.0, 128.7, 128.8, 129.1, 131.2, 138.8, 139.0, 161.0. Mass Spectrometry: HRMS (ESI-TOF) (m/z): Calcd for $C_{24}H_{17}F_3N_2O_2$ ($[M + Na]^+$) 445.1134, found 445.1136.



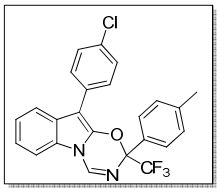
3ag, 10-Phenyl-2-(*m*-tolyl)-2-(trifluoromethyl)-2*H*-[1,3,5]oxadiazino[3,2-*a*]indole.

For **3ag**, yield: 65.0 mg, 80 %, white solid. m.p. 113-115ºC. NMR Spectroscopy: ^{1}H NMR ($CDCl_3$, 400 MHz) δ 2.26 (s, 3H), 7.15-7.21 (m, 2H), 7.22-7.24 (m, 2H), 7.35-7.42 (m, 2H), 7.47-7.54 (m, 4H), 7.72-7.77 (m, 3H), 8.38 (s, 1H). ^{13}C NMR ($CDCl_3$, 151 MHz) δ 21.3, 91.9 (q, *J* = 32.1 Hz), 99.6, 108.3, 119.6, 122.0 (q, *J* = 284.4 Hz), 122.7, 124.1, 124.7, 126.7, 127.1, 128.0, 128.2, 128.3, 128.7, 128.8, 131.0, 131.1, 134.0, 138.1, 138.8, 139.0. Mass Spectrometry: HRMS (ESI-TOF) (m/z): Calcd for $C_{24}H_{17}F_3N_2O$ ($[M + Na]^+$) 429.1185, found 429.1185.



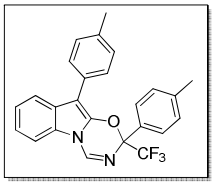
3ah, 10-Phenyl-2-(thiophen-2-yl)-2-(trifluoromethyl)-2*H*-[1,3,5]oxadiazino[3,2-*a*]indole.

For **3ah**, yield: 35.8 mg, 45 %, white solid. m.p. 146-148ºC. NMR Spectroscopy: ^{1}H NMR ($CDCl_3$, 400 MHz) δ 6.98 (d, *J* = 6.8 Hz, 1H), 7.25 (t, *J* = 7.2 Hz, 2H), 7.37 (t, *J* = 7.2 Hz, 3H), 7.42 (d, *J* = 6.8 Hz, 1H), 7.51 (t, *J* = 7.2 Hz, 2H), 7.75 (d, *J* = 7.2 Hz, 3H), 8.39 (s, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 90.7 (q, *J* = 32.6 Hz), 100.1, 108.3, 119.8, 121.6 (q, *J* = 282.6 Hz), 123.0, 124.3, 126.8, 127.1, 127.2, 128.0, 128.5, 128.7, 129.0, 130.9, 136.1, 138.3, 139.9. Mass Spectrometry: HRMS (ESI-TOF) (m/z): Calcd for $C_{21}H_{13}F_3N_2OS$ ($[M + Na]^+$) 421.0593, found 421.0585.



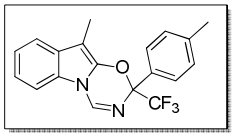
3ba, 10-(4-Chlorophenyl)-2-(*p*-tolyl)-2-(trifluoromethyl)-2*H*-[1,3,5]oxadiazino[3,2-*a*]indole.

For **3ba**, yield: 64.3 mg, 73 %, white solid. m.p. 145-147ºC. NMR Spectroscopy: ^{1}H NMR ($CDCl_3$, 400 MHz) δ 2.29 (s, 3H), 7.13 (d, *J* = 8.0 Hz, 2H), 7.18-7.25 (m, 2H), 7.36 (d, *J* = 7.2 Hz, 1H), 7.48 (d, *J* = 8.0 Hz, 2H), 7.54 (d, *J* = 7.6 Hz, 2H), 7.66-7.69 (m, 3H), 8.35 (s, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 21.1, 92.0 (q, *J* = 31.9 Hz), 98.3, 108.3, 119.4, 122.0 (q, *J* = 282.7 Hz), 122.9, 124.2, 126.7, 127.5, 128.6, 129.0, 129.1, 129.2, 129.7, 131.0, 132.3, 138.9, 139.0, 140.5. Mass Spectrometry: HRMS (ESI-TOF) (m/z): Calcd for $C_{24}H_{16}ClF_3N_2O$ ($[M + Na]^+$) 463.0795, found 463.0803.



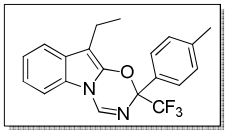
3ca, 2,10-Di-*p*-tolyl-2-(trifluoromethyl)-2*H*-[1,3,5]oxadiazino[3,2-*a*]indole.

For **3ca**, yield: 55.5 mg, 66 %, white solid. m.p. 114-116ºC. NMR Spectroscopy: ^{1}H NMR ($CDCl_3$, 400 MHz) δ 2.29 (s, 3H), 2.44 (s, 3H), 7.13 (d, *J* = 8.0 Hz, 2H), 7.19-7.24 (m, 2H), 7.32-7.39 (m, 3H), 7.57 (d, *J* = 7.6 Hz, 2H), 7.65 (d, *J* = 7.6 Hz, 2H), 7.71 (d, *J* = 7.2 Hz, 1H), 8.37 (s, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 21.1, 21.3, 91.9 (q, *J* = 31.5 Hz), 99.4, 108.2, 119.7, 122.1 (q, *J* = 282.8 Hz), 122.6, 124.0, 127.3, 127.6, 127.9, 128.2, 128.7, 129.1, 129.5, 131.2, 136.4, 138.6, 139.0, 140.3. Mass Spectrometry: HRMS (ESI-TOF) (m/z): Calcd for $C_{25}H_{19}F_3N_2O$ ($[M + Na]^+$) 443.1342, found 443.1329.



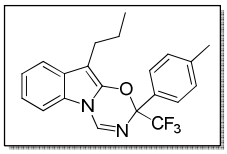
3da, 10-Methyl-2-(*p*-tolyl)-2-(trifluoromethyl)-2*H*-[1,3,5]oxadiazino[3,2-*a*]indole.

For **3da**, yield: 27.5 mg, 40 %, white solid. m.p. 88-90 ºC. NMR Spectroscopy: ^{1}H NMR ($CDCl_3$, 400 MHz) δ 2.20 (s, 3H), 2.31 (s, 3H), 7.10-7.20 (m, 4H), 7.27 (d, *J* = 7.6 Hz, 1H), 7.33 (d, *J* = 7.2 Hz, 1H), 7.63 (d, *J* = 8.4 Hz, 2H), 8.25 (s, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 6.1, 21.1, 91.5 (q, *J* = 31.6 Hz), 93.7, 107.9, 118.4, 122.2 (q, *J* = 282.2 Hz), 122.2, 123.4, 127.6, 128.4, 129.1, 129.3, 131.6, 138.6, 139.1, 140.2. Mass Spectrometry: HRMS (ESI-TOF) (m/z): Calcd for $C_{19}H_{15}F_3N_2O$ ($[M + H]^+$) 345.1209, found 345.1207.



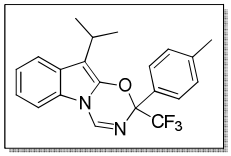
3ea, 10-Ethyl-2-(*p*-tolyl)-2-(trifluoromethyl)-2*H*-[1,3,5]oxadiazino[3,2-*a*]indole.

For **3ea**, yield: 34.4 mg, 48 %, white solid. m.p. 82-84ºC. NMR Spectroscopy: ^{1}H NMR ($CDCl_3$, 400 MHz) δ 1.31 (t, *J* = 7.6 Hz, 3H), 2.30 (s, 3H), 2.67-2.75 (m, 2H), 7.09-7.18 (m, 4H), 7.27 (d, *J* = 7.2 Hz, 1H), 7.37 (d, *J* = 6.8 Hz, 1H), 7.64 (d, *J* = 8.0 Hz, 2H), 8.26 (s, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 13.7, 15.3, 21.1, 91.4 (q, *J* = 31.6 Hz), 99.8, 99.9, 108.0, 118.7, 122.1, 122.2 (q, *J* = 282.2 Hz), 123.4, 127.6, 128.5, 128.6, 129.0, 131.6, 138.2, 139.2, 140.3. Mass Spectrometry: HRMS (ESI-TOF) (m/z): Calcd for $C_{20}H_{17}F_3N_2O$ ($[M+Na]^+$) 381.1185, found 381.1196.



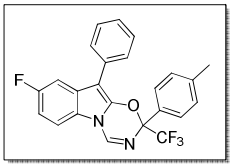
3fa, 10-Propyl-2-(*p*-tolyl)-2-(trifluoromethyl)-2*H*-[1,3,5]oxadiazino[3,2-*a*]indole.

For **3fa**, yield: 37.2 mg, 50 %, white solid. m.p. 80-82 ºC. NMR Spectroscopy: ^{1}H NMR ($CDCl_3$, 400 MHz) δ 1.01 (t, *J* = 7.2Hz, 3H), 1.71-1.72 (m, 2H), 2.32 (s, 3H), 2.64-2.68 (m, 2H), 7.13-7.17 (m, 4H), 7.29-7.31 (m, 1H), 7.36-7.38 (m, 1H), 7.64 (d, *J* = 8.4 Hz, 2H), 8.29 (s, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 14.1, 21.1, 22.2, 23.9, 91.4 (q, *J* = 31.5 Hz), 98.2, 108.0, 118.8, 122.1, 122.2 (q, *J* = 282.4 Hz), 123.4, 127.6, 128.5, 129.0, 131.6, 138.7, 139.1, 140.2. Mass Spectrometry: HRMS (ESI-TOF) (m/z): Calcd for $C_{21}H_{19}F_3N_2O$ ($[M + Na]^+$) 395.1342, found 395.1351.



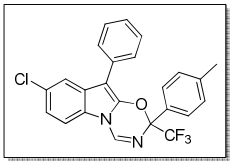
3ga, 10-Isopropyl-2-(*p*-tolyl)-2-(trifluoromethyl)-2*H*-[1,3,5]oxadiazino[3,2-*a*]indole

For **3ga**, yield: 38.0 mg, 51 %, white solid. m.p. 81-83ºC. NMR Spectroscopy: ^{1}H NMR ($CDCl_3$, 400 MHz) δ 1.43 (q, *J* = 6.8 Hz, 6H), 2.32 (s, 3H), 3.18-3.25 (m, 1H), 7.12-7.17 (m, 4H), 7.31 (d, *J* = 7.2 Hz, 1H), 7.43 (d, *J* = 7.2 Hz, 1H), 7.65 (d, *J* = 8.0 Hz, 2H), 8.29 (s, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 21.1, 21.9, 22.0, 23.9, 91.3 (q, *J* = 31.5 Hz), 103.9, 108.1, 119.3, 122.0, 122.2 (q, *J* = 282.5 Hz), 123.3, 127.7, 128.0, 128.6, 129.0, 131.6, 137.6, 139.3, 140.3. Mass Spectrometry: HRMS (ESI-TOF) (m/z): Calcd for $C_{21}H_{19}F_3N_2O$ ($[M + Na]^+$) 395.1342, found 395.1351.



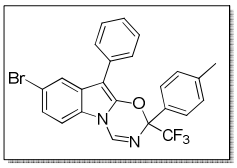
3ha, 8-Fluoro-10-phenyl-2-(*p*-tolyl)-2-(trifluoromethyl)-2*H*-[1,3,5]oxadiazino[3,2-*a*]indole.

For **3ha**, yield: 52.6 mg, 62 %, white solid. m.p. 163-165ºC. NMR Spectroscopy: ^{1}H NMR ($CDCl_3$, 400 MHz) δ 2.29 (s, 3H), 6.91 (t, *J* = 8.8 Hz, 1H), 7.14 (d, *J* = 7.6 Hz, 2H), 7.28-7.30 (m, 1H), 7.35-7.41 (m, 2H), 7.51-7.58 (m, 4H), 7.71 (d, *J* = 7.2 Hz, 2H), 8.32 (s, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 21.1, 91.9 (q, *J* = 32.1 Hz), 99.5 (d, *J* = 3.3 Hz), 106.1 (d, *J* = 25.6 Hz), 109.1 (d, *J* = 9.6 Hz), 110.2 (d, *J* = 25.7 Hz), 122.0 (q, *J* = 282.6 Hz), 124.9, 126.9, 127.5, 127.8, 128.4 (d, *J* = 10.1 Hz), 128.9, 129.1, 130.8 (d, *J* = 30.7 Hz), 138.8, 139.9, 140.5, 160.3 (d, *J* = 238.6 Hz). Mass Spectrometry: HRMS (ESI-TOF) (m/z): Calcd for $C_{24}H_{16}F_4N_2O$ ($[M+Na]^+$) 447.1091, found 447.1082.



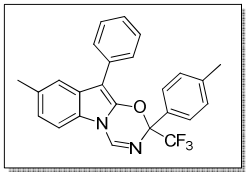
3ia, 8-Chloro-10-phenyl-2-(*p*-tolyl)-2-(trifluoromethyl)-2*H*-[1,3,5]oxadiazino[3,2-*a*]indole.

For **3ia**, yield: 66.1 mg, 75 %, white solid. m.p. 160-162ºC. NMR Spectroscopy: ^{1}H NMR ($CDCl_3$, 400 MHz) δ 2.29 (s, 3H), 7.13-7.15 (m, 3H), 7.27 (d, *J* = 8.4 Hz, 1H), 7.35-7.39 (m, 1H), 7.51-7.57 (m, 4H), 7.67-7.71 (m, 3H), 8.31 (s, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 21.1, 92.0 (q, *J* = 31.9 Hz), 99.2, 109.2, 119.5, 121.9 (q, *J* = 282.6 Hz), 122.8, 127.0, 127.5, 127.9, 128.5, 128.9, 129.2, 129.9, 130.4, 130.9, 138.6, 139.6, 140.6. Mass Spectrometry: HRMS (ESI-TOF) (m/z): Calcd for $C_{24}H_{16}ClF_3N_2O$ ($[M + Na]^+$) 463.0795, found 463.0783.



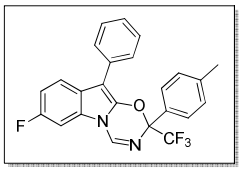
3ja, 8-Bromo-10-phenyl-2-(*p*-tolyl)-2-(trifluoromethyl)-2*H*-[1,3,5]oxadiazino[3,2-*a*]indole.

For **3ja**, yield: 82.3 mg, 85 %, white solid. m.p. 164-166 ºC. NMR Spectroscopy: ^{1}H NMR ($CDCl_3$, 400 MHz) δ 2.29 (s, 3H), 7.14 (d, *J* = 7.6 Hz, 2H), 7.23 (d, *J* = 7.6 Hz, 1H), 7.29 (d, *J* = 8.4 Hz, 1H), 7.37 (t, *J* = 7.2 Hz, 1H), 7.51-7.57 (m, 4H), 7.69 (d, *J* = 7.2 Hz, 2H), 7.82 (s, 1H), 8.32 (s, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 21.1, 92.0 (q, *J* = 32.0 Hz), 99.1, 109.6, 117.5, 121.9 (q, *J* = 282.8 Hz), 122.4, 125.5, 127.0, 127.3, 127.5, 127.9, 128.9, 129.2, 130.4, 130.8, 138.6, 139.4, 140.6. Mass Spectrometry: HRMS (ESI-TOF) (m/z): Calcd for $C_{24}H_{16}BrF_3N_2O$ ($[M + Na]^+$) 507.0290, found 507.0274.



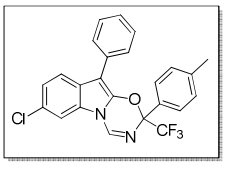
3ka, 8-Methyl-10-phenyl-2-(*p*-tolyl)-2-(trifluoromethyl)-2*H*-[1,3,5]oxadiazino[3,2-*a*]indole.

For **3ka**, yield: 52.9 mg, 63 %, white solid. m.p. 202-204 ºC. NMR Spectroscopy: ^{1}H NMR ($CDCl_3$, 400 MHz) δ 2.29 (s, 3H), 2.40 (s, 3H), 7.02 (d, *J* = 8.0 Hz, 1H), 7.12 (d, *J* = 7.6 Hz, 2H), 7.26 (d, *J* = 9.6 Hz, 1H), 7.34-7.38 (m, 1H), 7.52-7.58 (m, 5H), 7.75 (d, *J* = 7.2 Hz, 2H), 8.34 (s, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 21.1, 21.6, 91.8 (q, *J* = 31.9 Hz), 99.2, 107.9, 119.8, 122.1 (q, *J* = 282.7 Hz), 123.7, 126.6, 126.8, 127.3, 127.6, 128.1, 128.7, 129.1, 131.2, 131.3, 133.8, 138.9, 139.1, 140.3. Mass Spectrometry: HRMS (ESI-TOF) (m/z): Calcd for $C_{25}H_{19}F_3N_2O$ ($[M + Na]^+$) 443.1342, found 443.1333.



3la, 7-Fluoro-10-phenyl-2-(*p*-tolyl)-2-(trifluoromethyl)-2*H*-[1,3,5]oxadiazino[3,2-*a*]indole.

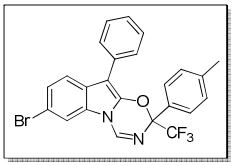
For **3la**, yield: 59.3 mg, 70 %, white solid. m.p. 165-167 ºC. NMR Spectroscopy: ^{1}H NMR ($CDCl_3$, 400 MHz) δ 2.28 (s, 3H), 6.93-6.98 (m, 1H), 7.08 (d, *J* = 8.4 Hz, 1H), 7.13 (d, *J* = 8.0 Hz, 2H), 7.34-7.38 (m, 1H), 7.49-7.54 (m, 4H), 7.61-7.63 (m, 1H), 7.72 (d, *J* = 7.2 Hz, 2H), 8.28 (s, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 21.1, 91.9 (q, *J* = 32.0 Hz), 96.3 (d, *J* = 27.4 Hz), 99.2, 111.7 (d, *J* = 23.0 Hz), 120.5 (d, *J* = 9.2 Hz), 122.0 (q, *J* = 282.7Hz), 123.2, 126.8, 127.5, 127.9, 128.7 (d, *J* = 11.7 Hz), 128.8, 129.1, 130.9 (d, *J* = 14.4 Hz), 138.7, 138.8, 140.5, 159.7 (d, *J* = 239.9 Hz). Mass Spectrometry: HRMS (ESI-TOF) (m/z): Calcd for $C_{24}H_{16}F_4N_2O$ ($[M + Na]^+$) 447.1091, found 447.1089.



3ma, 7-Chloro-10-phenyl-2-(*p*-tolyl)-2-(trifluoromethyl)-2*H*-[1,3,5]oxadiazino[3,2-*a*]indole.

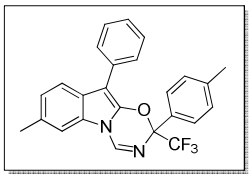
For **3ma**, yield: 57.2 mg, 65 %, white solid. m.p. 190-192 ºC. NMR Spectroscopy: ^{1}H NMR ($CDCl_3$, 400 MHz) δ 2.29 (s, 3H), 7.14 (d, *J* = 7.6 Hz, 2H), 7.19 (d, *J* = 8.4 Hz, 1H), 7.35-7.37 (m, 2H), 7.50-7.56 (m, 4H), 7.61 (d, *J* = 8.4 Hz, 2H), 7.71 (d, *J* = 7.2 Hz, 2H), 8.31 (s, 1H). ^{13}C NMR

($CDCl_3$, 100 MHz) δ 21.1, 92.0 (q, *J* = 31.9 Hz), 99.3, 108.8, 120.5, 122.0 (q, *J* = 282.7 Hz), 123.4, 124.4, 125.6, 126.9, 127.5, 127.9, 128.5, 128.8, 129.2, 130.6, 130.9, 138.6, 139.0, 140.5. Mass Spectrometry: HRMS (ESI-TOF) (m/z): Calcd for $C_{24}H_{16}ClF_3N_2O$ ($[M + H]^+$) 441.0976, found 441.0954.



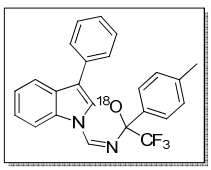
3na, 7-Bromo-10-phenyl-2-(*p*-tolyl)-2-(trifluoromethyl)-2*H*-[1,3,5]oxadiazino[3,2-*a*]indole.

For **3na**, yield: 92.0 mg, 95 %, white solid. m.p. 199-201 ºC. NMR Spectroscopy: ^1H NMR ($CDCl_3$, 400 MHz) δ 2.29 (s, 3H), 7.14 (d, *J* = 7.6 Hz, 2H), 7.32 (d, *J* = 8.0 Hz, 1H), 7.37 (t, *J* = 7.2 Hz, 1H), 7.50-7.56 (m, 6H), 7.70 (d, *J* = 7.2 Hz, 2H), 8.31 (s, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 21.1, 92.0 (q, *J* = 32.0 Hz), 99.4, 111.6, 115.7, 120.8, 121.9 (q, *J* = 282.6 Hz), 126.0, 126.9, 127.1, 127.5, 127.9, 128.8, 128.2, 129.3, 130.6, 130.8, 138.6, 138.9, 140.5. Mass Spectrometry: HRMS (ESI-TOF) (m/z): Calcd for $C_{24}H_{16}BrF_3N_2O$ ($[M + Na]^+$) 507.0290, found 507.0300.



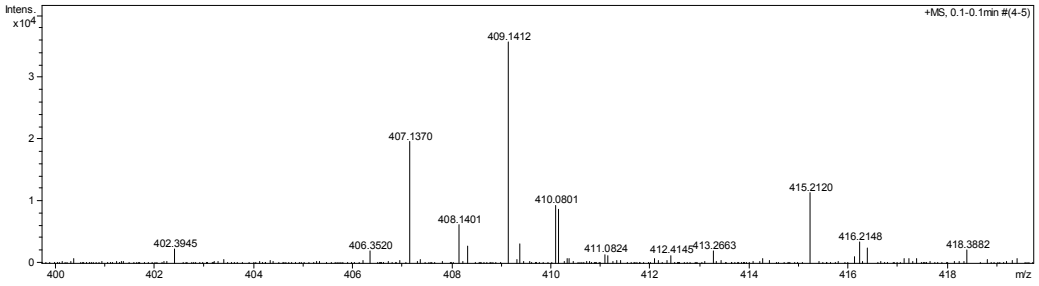
3oa, 7-Methyl-10-phenyl-2-(*p*-tolyl)-2-(trifluoromethyl)-2*H*-[1,3,5]oxadiazino[3,2-*a*]indole.

For **3oa**, yield: 74.8 mg, 89 %, white solid. m.p. 212-214 ºC. NMR Spectroscopy: ^1H NMR ($CDCl_3$, 400 MHz) δ 2.28 (s, 3H), 2.42 (s, 3H), 7.05 (d, *J* = 8.0 Hz, 1H), 7.11 (d, *J* = 7.6 Hz, 2H), 7.19 (s, 1H), 7.34 (t, *J* = 7.2 Hz, 1H), 7.51 (t, *J* = 7.2 Hz, 2H), 7.56 (d, *J* = 7.6 Hz, 2H), 7.61 (d, *J* = 8.0 Hz, 1H), 7.76 (d, *J* = 7.2 Hz, 2H), 8.34 (s, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 21.1, 21.5, 91.8 (q, *J* = 31.7 Hz), 99.3, 108.6, 119.4, 122.1 (q, *J* = 282.6 Hz), 124.6, 125.2, 126.5, 127.6, 127.9, 128.7, 129.0, 129.1, 131.2, 131.4, 132.8, 138.3, 139.1, 140.3. Mass Spectrometry: HRMS (ESI-TOF) (m/z): Calcd for $C_{25}H_{19}F_3N_2O$ ($[M + Na]^+$) 443.1342, found 443.1339.



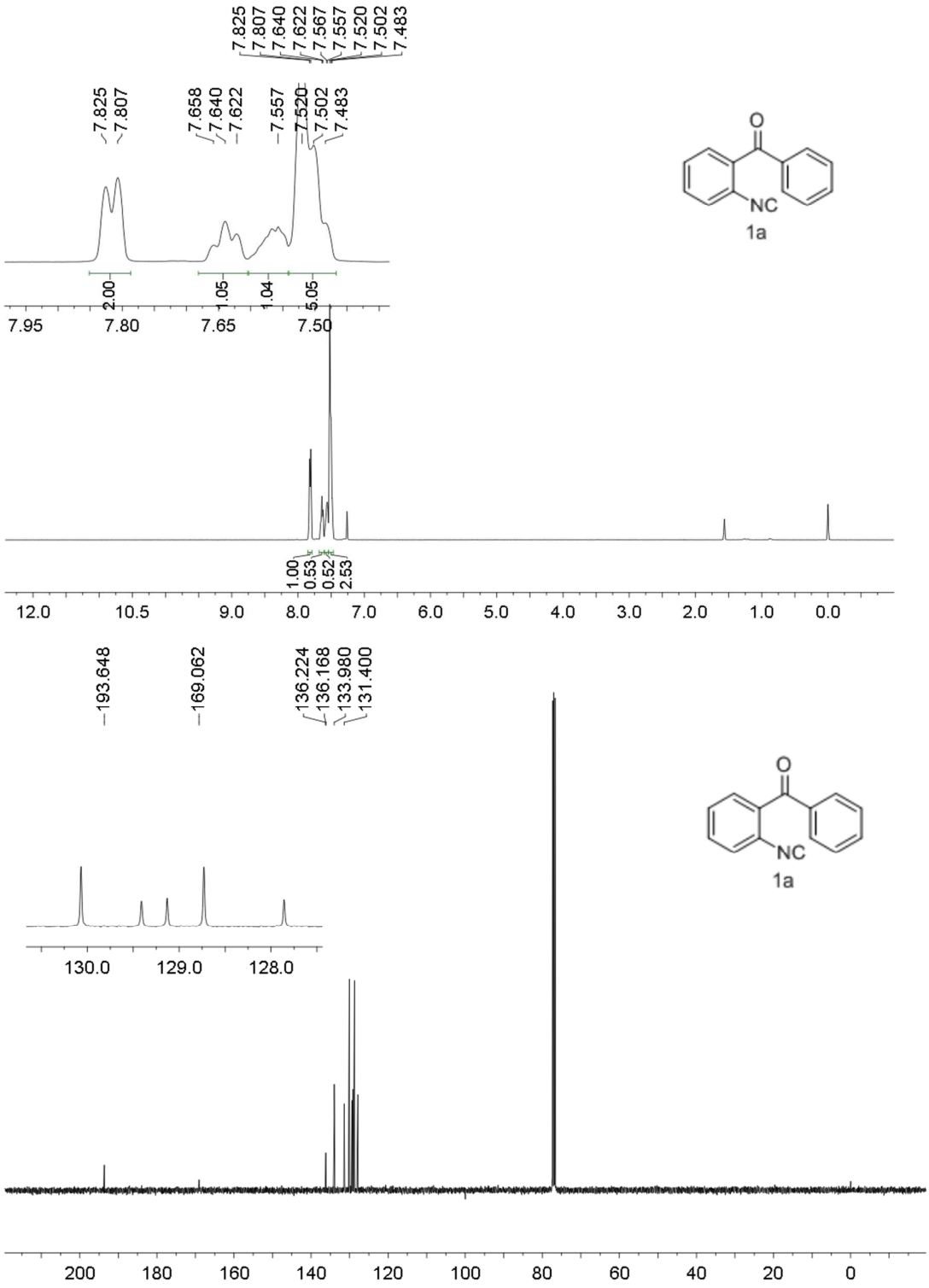
3aa-^{18}O, ^{18}O-10-Phenyl-2-(*p*-tolyl)-2-(trifluoromethyl)-2*H*-[1,3,5]oxadiazino[3,2-*a*]indole.

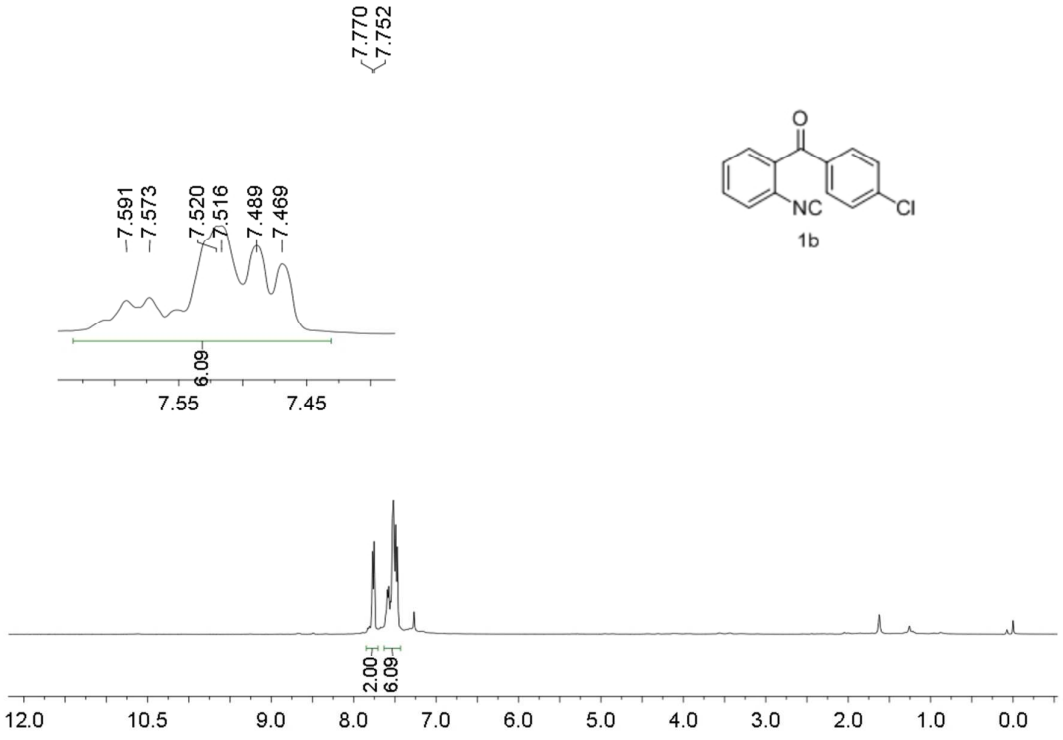
For **3aa-^{18}O**, yield: 66.1 mg, 81 %, white solid. NMR Spectroscopy: ^{1}H NMR ($CDCl_3$, 400 MHz) δ 2.26 (s, 3H), 7.15-7.34 (m, 4H), 7.36-7.38 (m, 2H), 7.47-7.54 (m, 4H), 7.71-7.75 (m, 3H), 8.37 (s, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 21.3, 91.9 (q, J = 31.8 Hz), 99.6, 108.3, 119.7, 122.0 (q, J = 282.7 Hz), 122.7, 124.1, 124.7, 126.7, 128.0, 128.2, 128.3, 128.7, 128.8, 131.0, 131.1, 134.0, 138.1, 138.8, 139.0. Mass Spectrometry: HRMS (ESI-TOF) (m/z): Calcd for $C_{24}H_{18}F_3N_2{}^{18}O$ ([M + H]$^+$) 409.1408, found 409.1412.



IV. Copies of ^{1}H NMR and ^{13}C NMR spectra of compounds

Copies of ^{1}H NMR and ^{13}C NMR spectra of compounds 1

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7.573
7.520
7.516
7.489
7.469
6.09
7.55
7.45
O
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Cl
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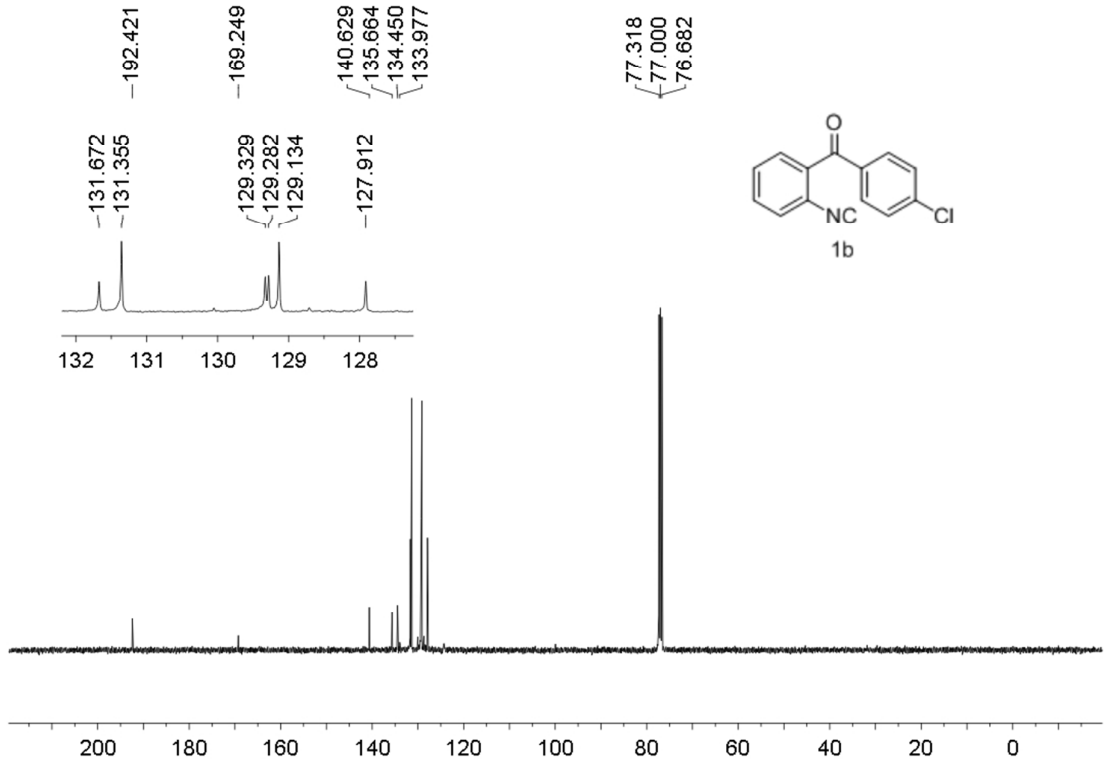
6.09
12.0
10.5
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0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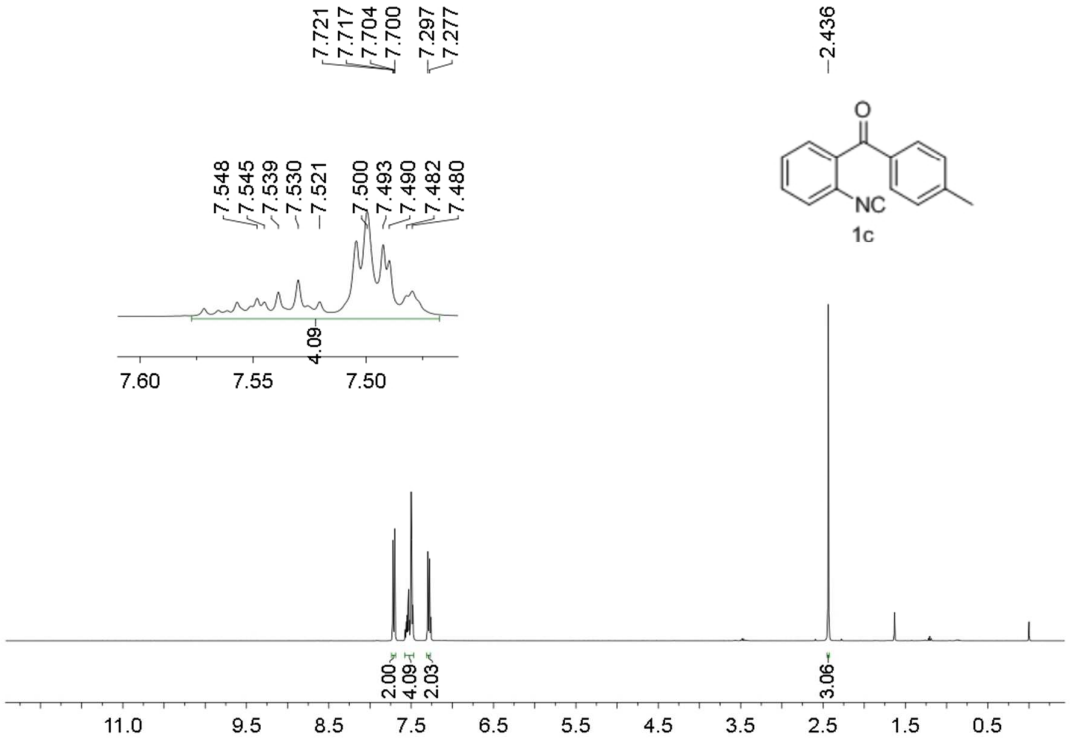
140.629
135.664
134.450
133.977
77.318
77.000
76.682
131.672
131.355
129.329
129.282
129.134
127.912
O
NC
Cl
1b
132
131
130
129
128
200
180
160
140
120
100
80
60
40
20
0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7.704
7.700
7.297
7.277
2.436
7.548
7.545
7.539
7.530
7.521
7.500
7.493
7.490
7.482
7.480
4.09
7.60
7.55
7.50
O
NC
1c
2.00
4.09
2.03
3.06
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9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
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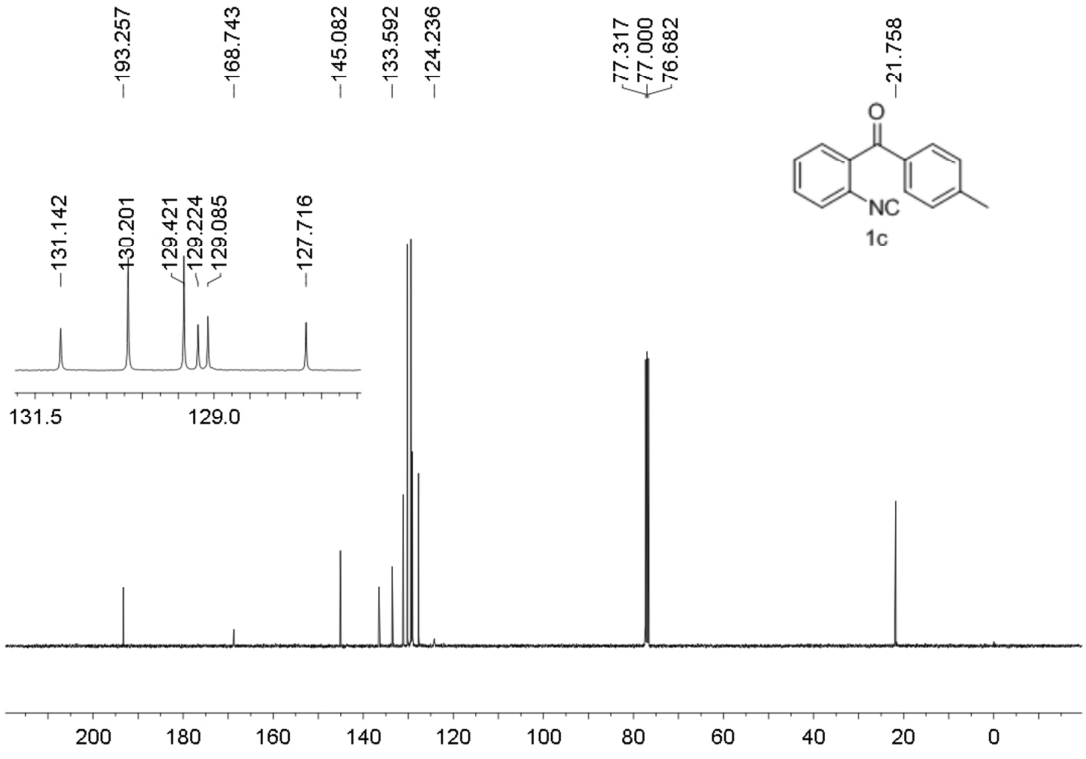
0.5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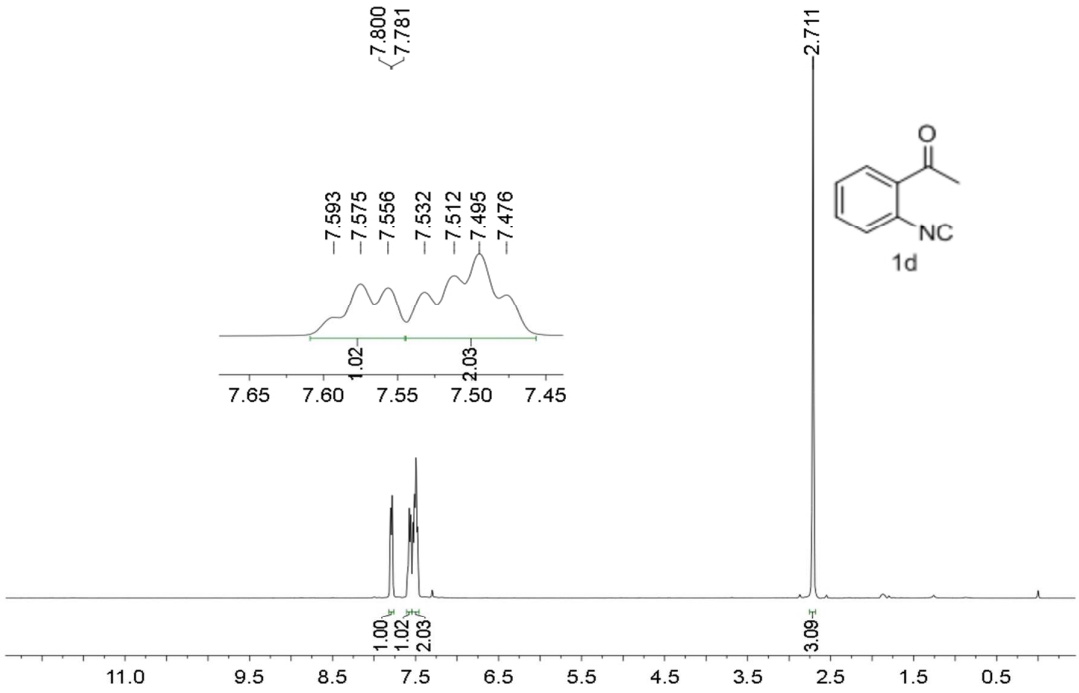
145.082
133.592
124.236
77.317
77.000
76.682
21.758
131.142
130.201
129.421
129.224
129.085
127.716
131.5
129.0
O
NC
1c
200
180
160
140
120
100
80
60
40
20
0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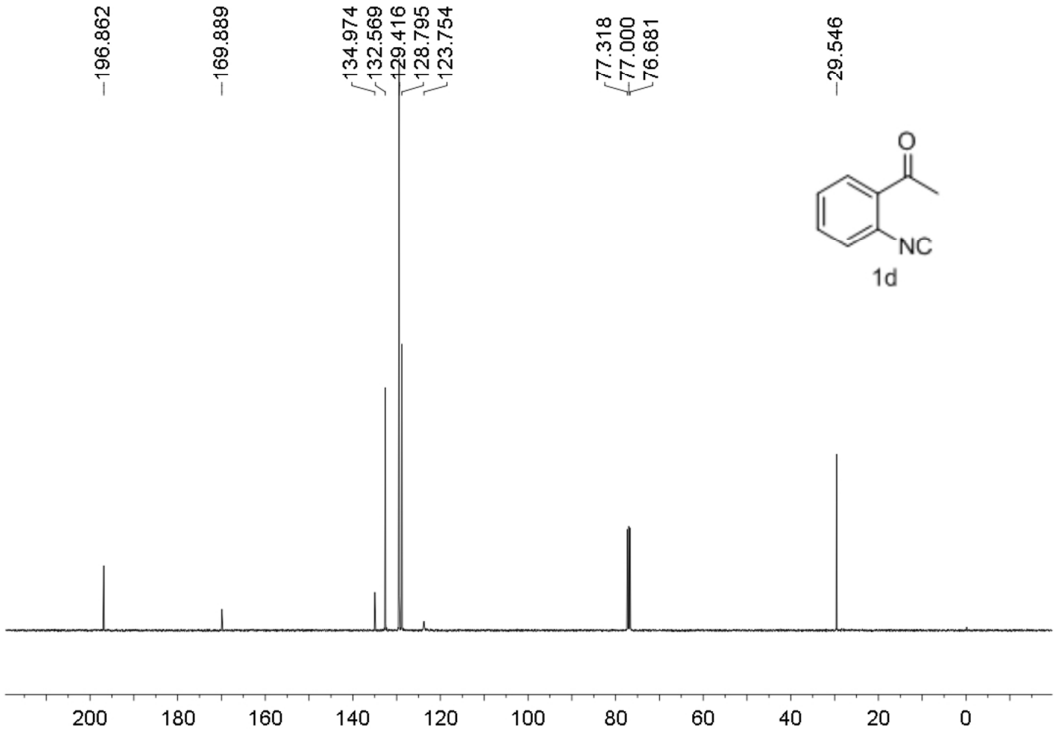
2.711
7.593
7.575
7.556
7.532
7.512
7.495
7.476
1.02
2.03
7.65
7.60
7.55
7.50
7.45
O
NC
1d
1.00
1.02
2.03
3.09
11.0
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5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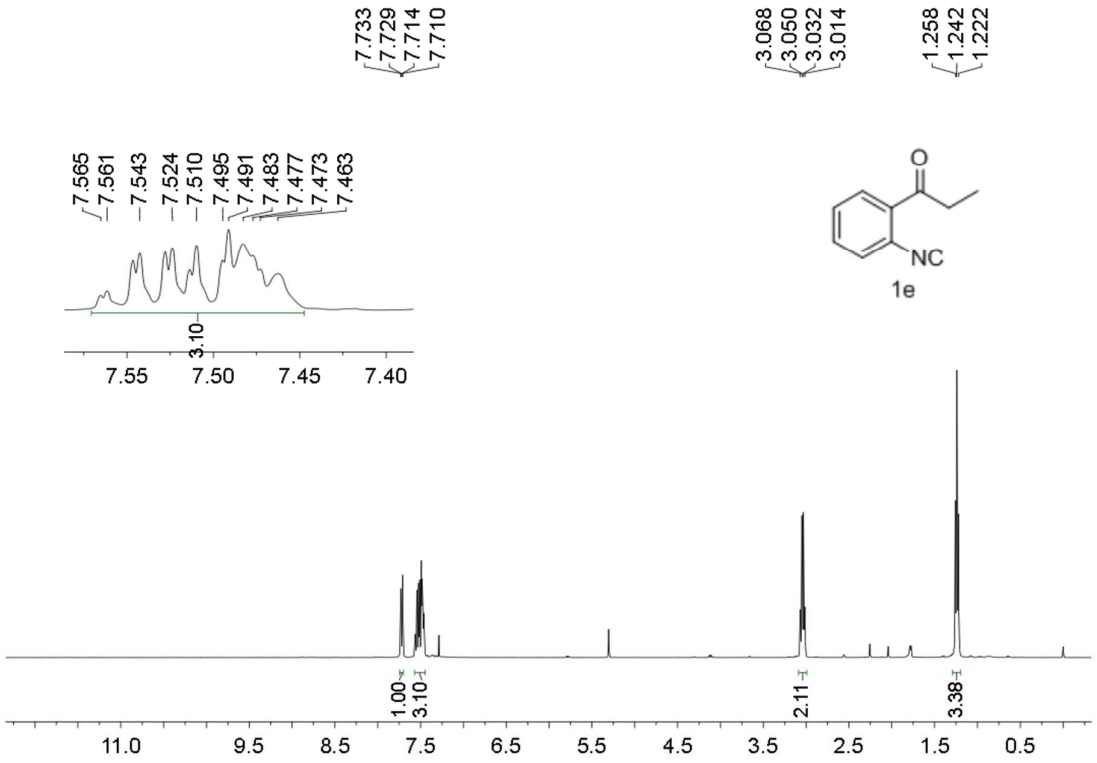
80
60
40
20
0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3.050
3.032
3.014
1.258
1.242
1.222
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7.561
7.543
7.524
7.510
7.495
7.491
7.483
7.477
7.473
7.463
3.10
7.55
7.50
7.45
7.40
O
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1e
1.00
3.10
2.11
3.38
11.0
9.5
8.5
7.5
6.5
5.5
4.5
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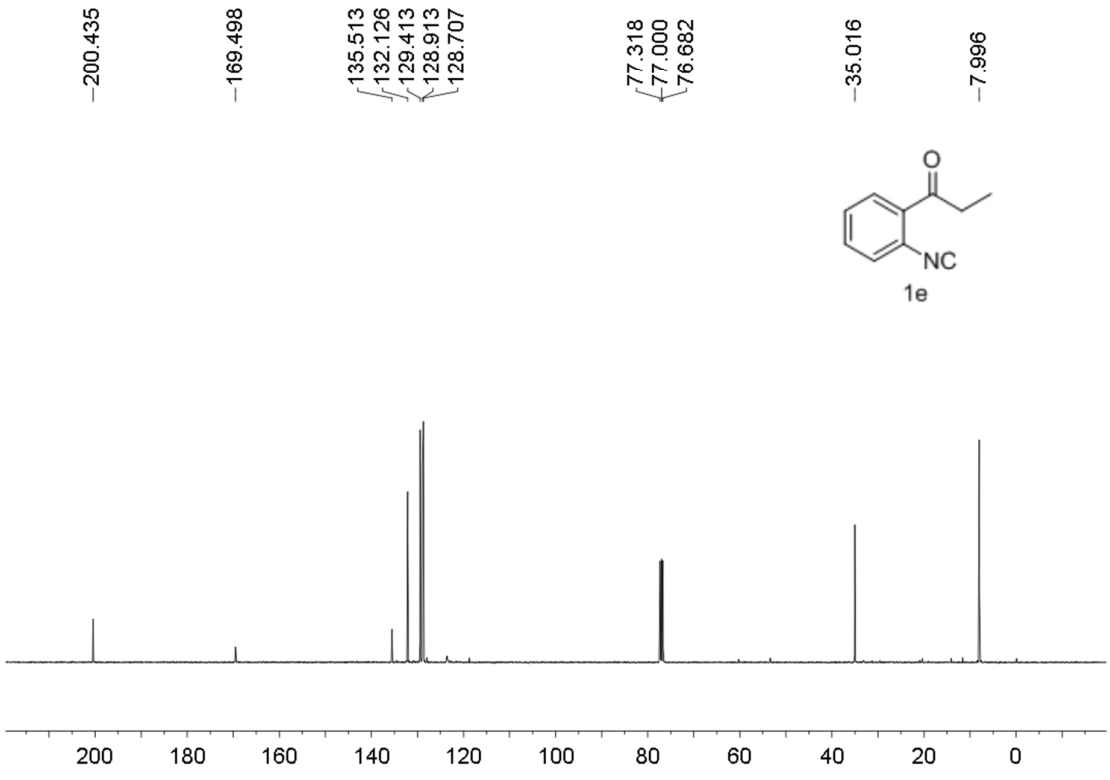
1.5
0.5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7.996
O
NC
1e
200
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140
120
100
80
60
40
20
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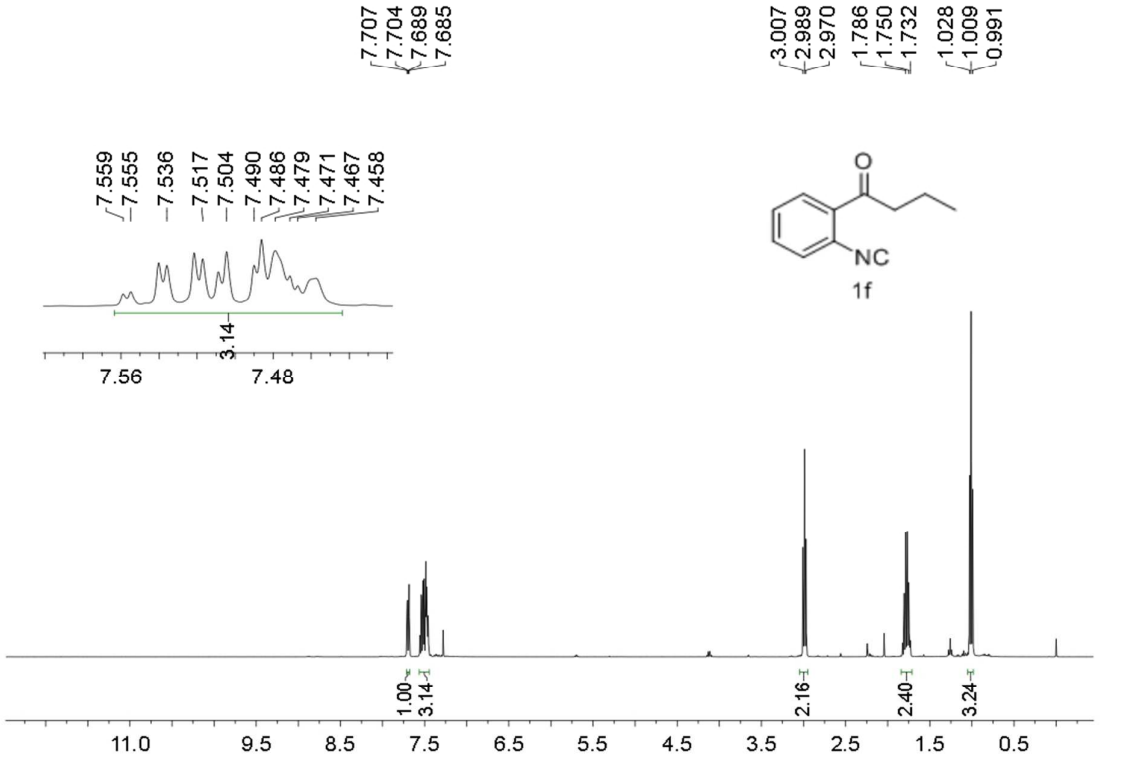
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7.685
3.007
2.989
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1.732
1.028
1.009
0.991
7.559
7.555
7.536
7.517
7.504
7.490
7.486
7.479
7.471
7.467
7.458
3.14
7.56
7.48
O
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1f
1.00
3.14
2.16
2.40
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9.5
8.5
7.5
6.5
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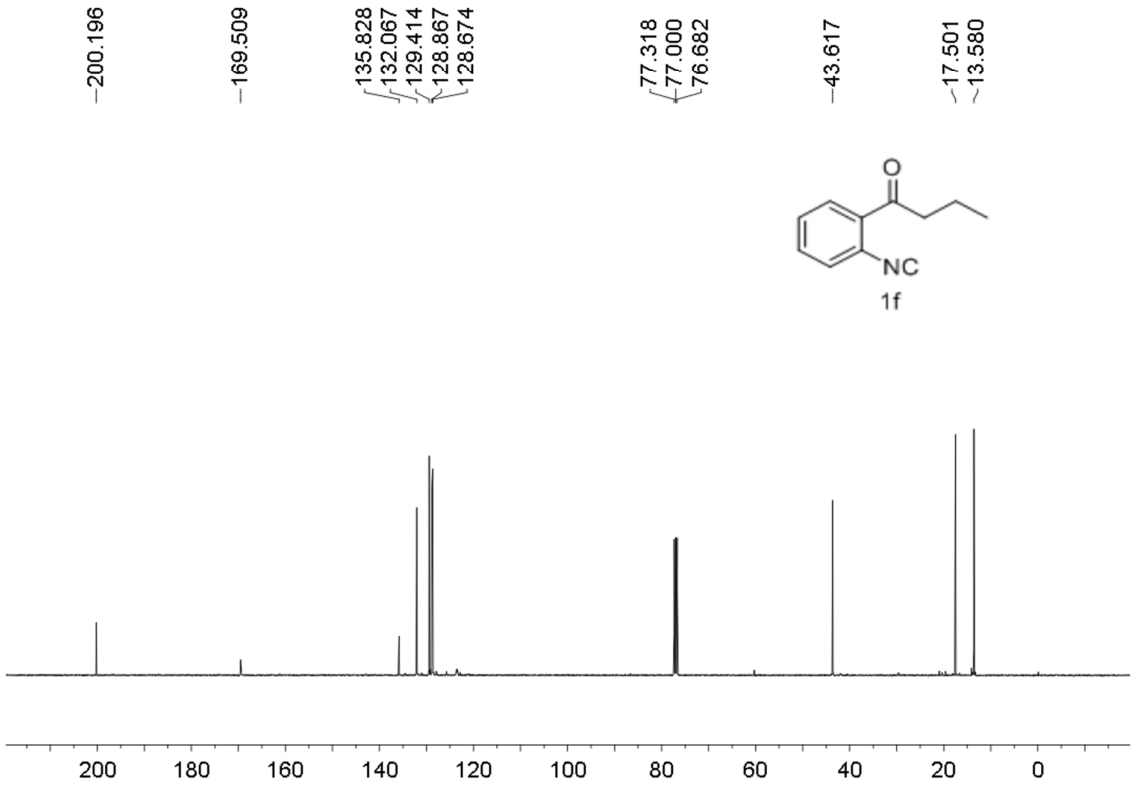
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128.867
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77.000
76.682
43.617
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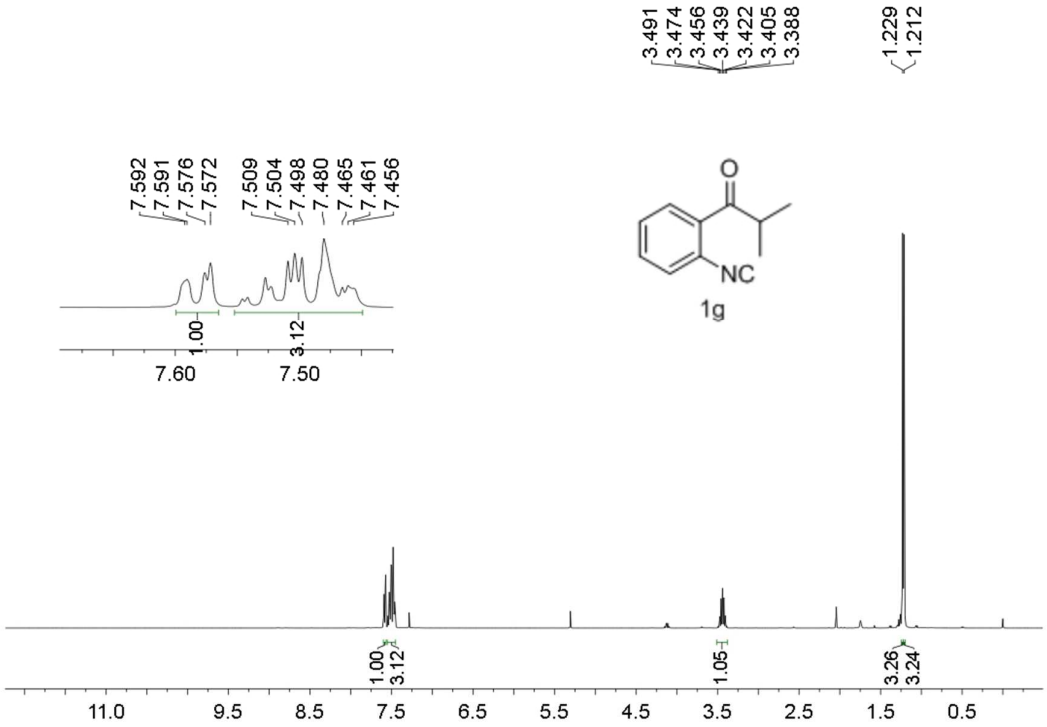
13.580
O
NC
1f
200
180
160
140
120
100
80
60
40
20
0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7.572
7.509
7.504
7.498
7.480
7.465
7.461
7.456
O
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1g
1.00
3.12
7.60
7.50
1.00
3.12
1.05
3.26
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4.5
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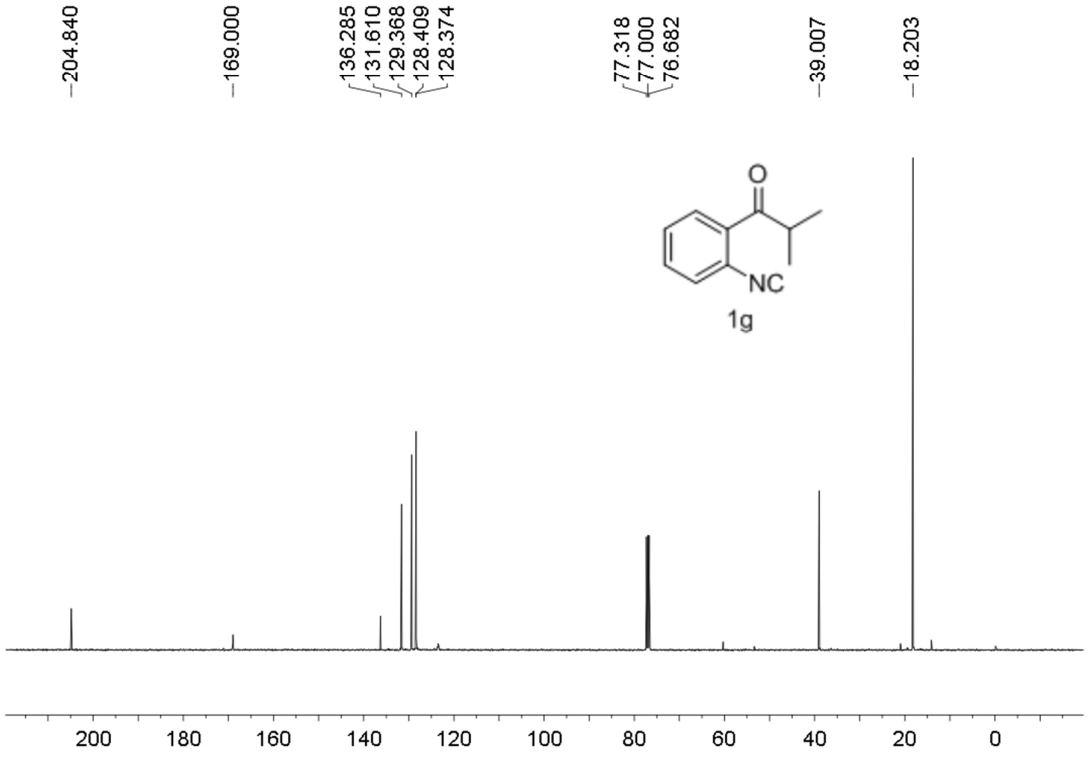
0.5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128.409
128.374
77.318
77.000
76.682
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O
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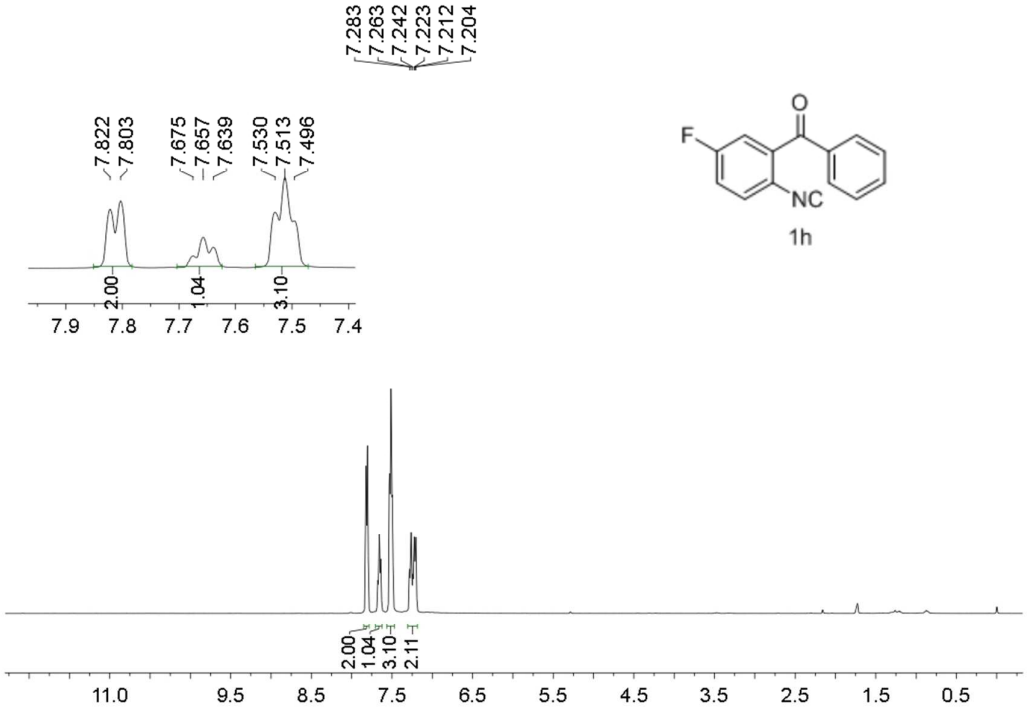
1g
200
180
160
140
120
100
80
60
40
20
0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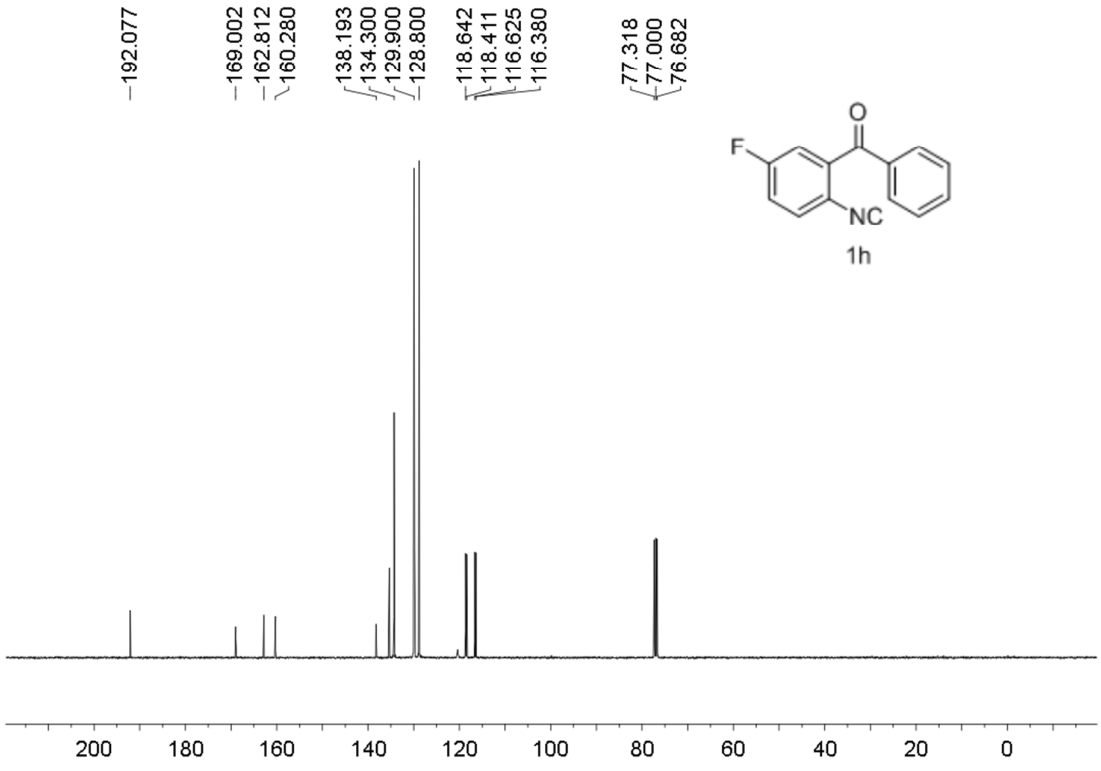
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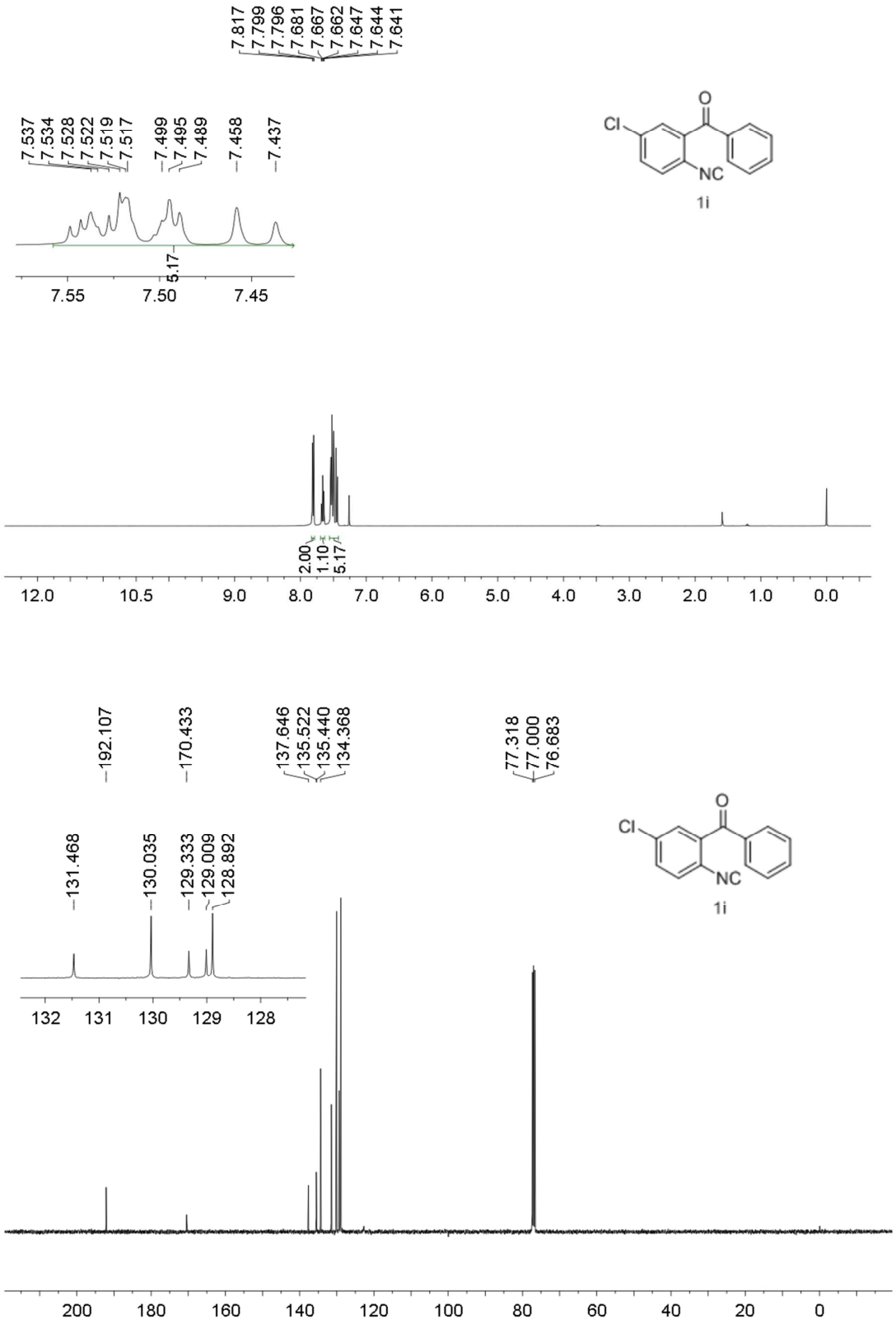
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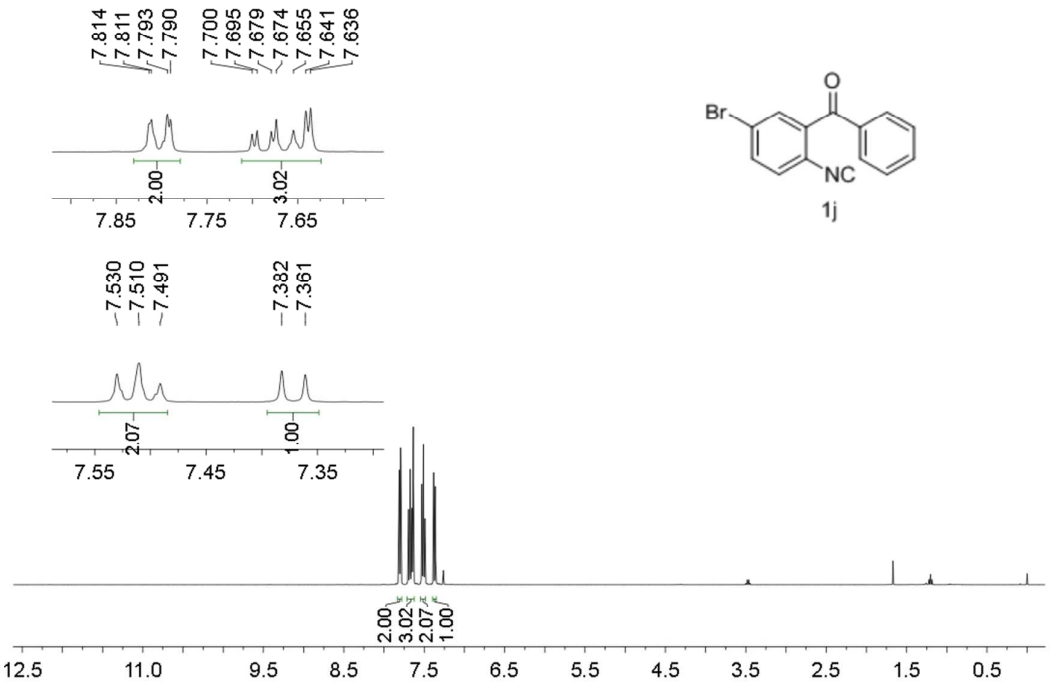
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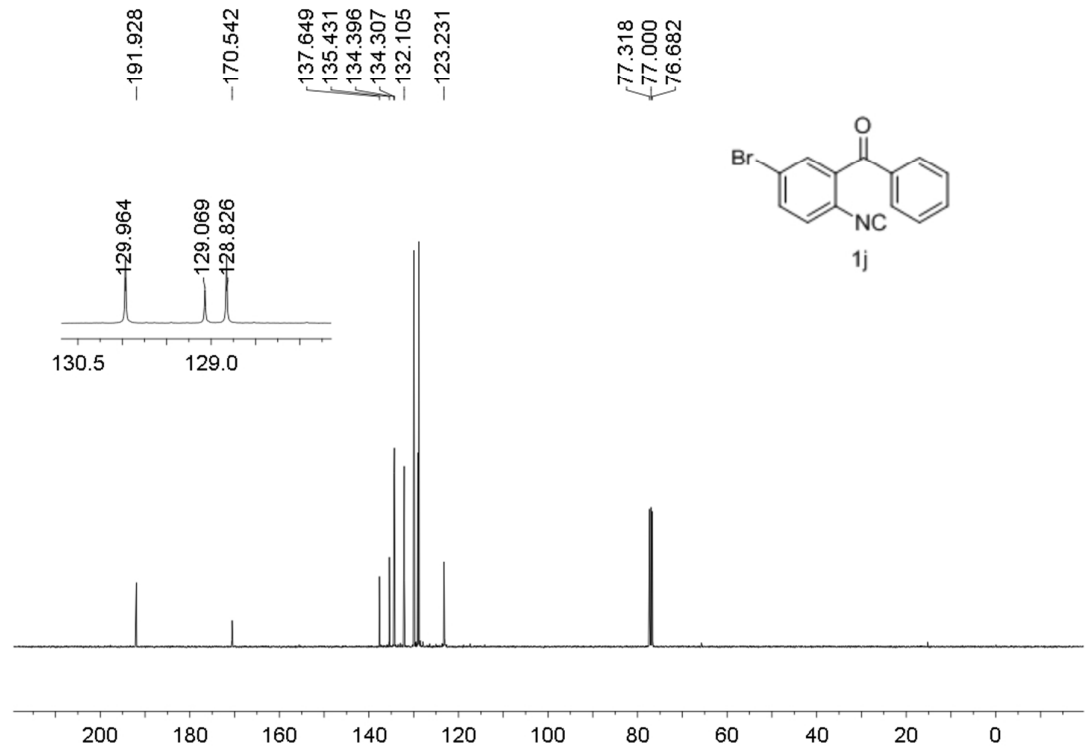
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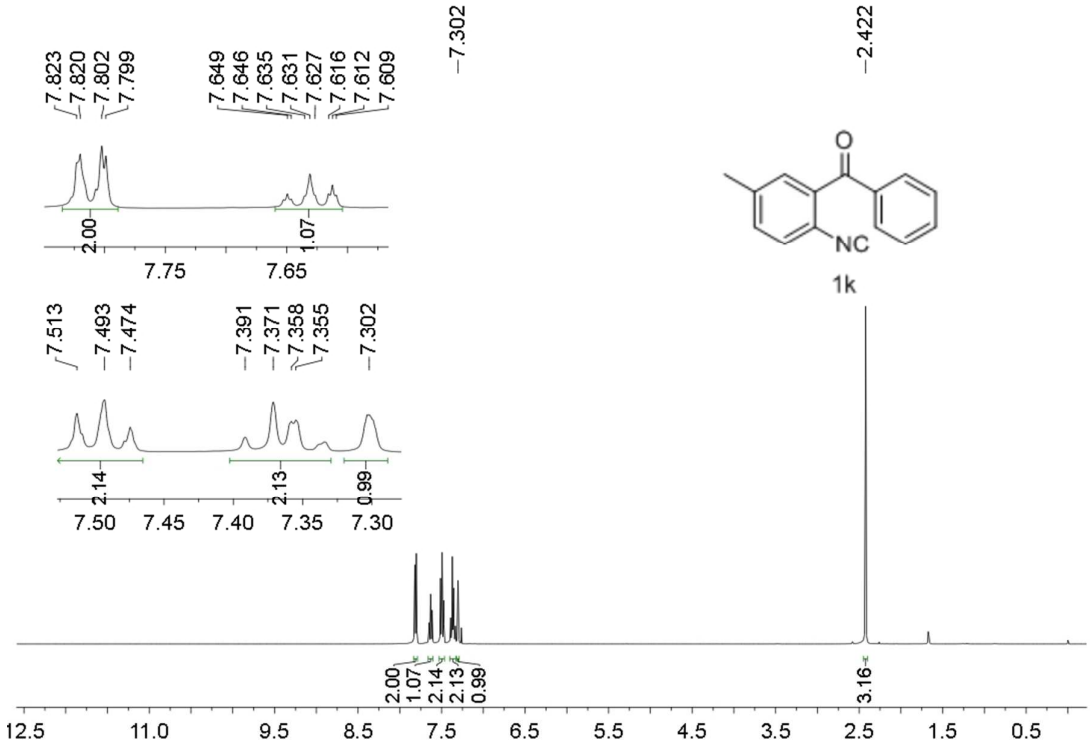
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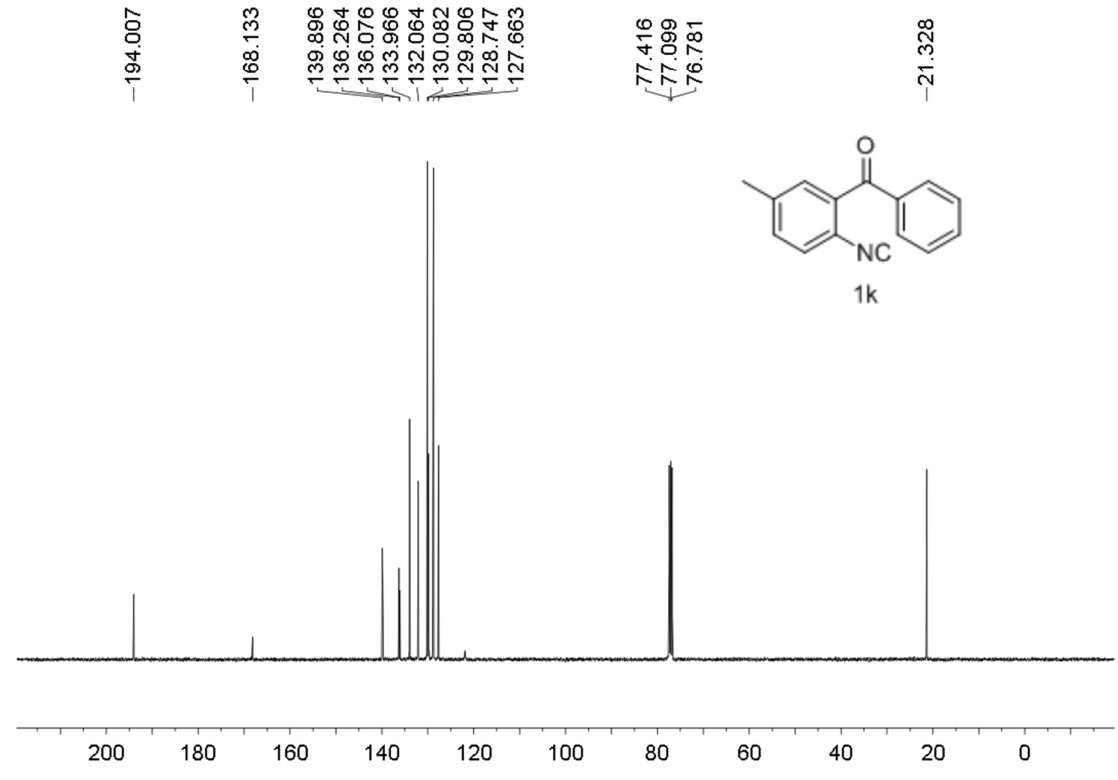
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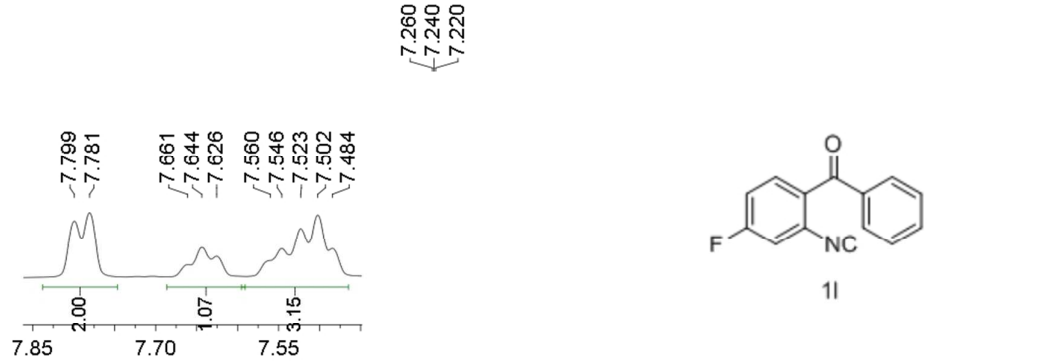
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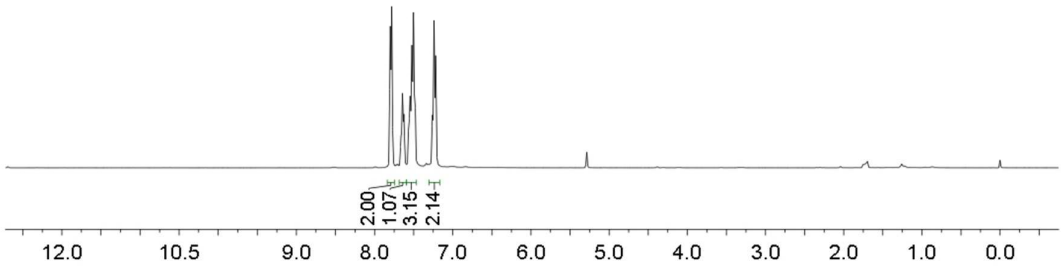
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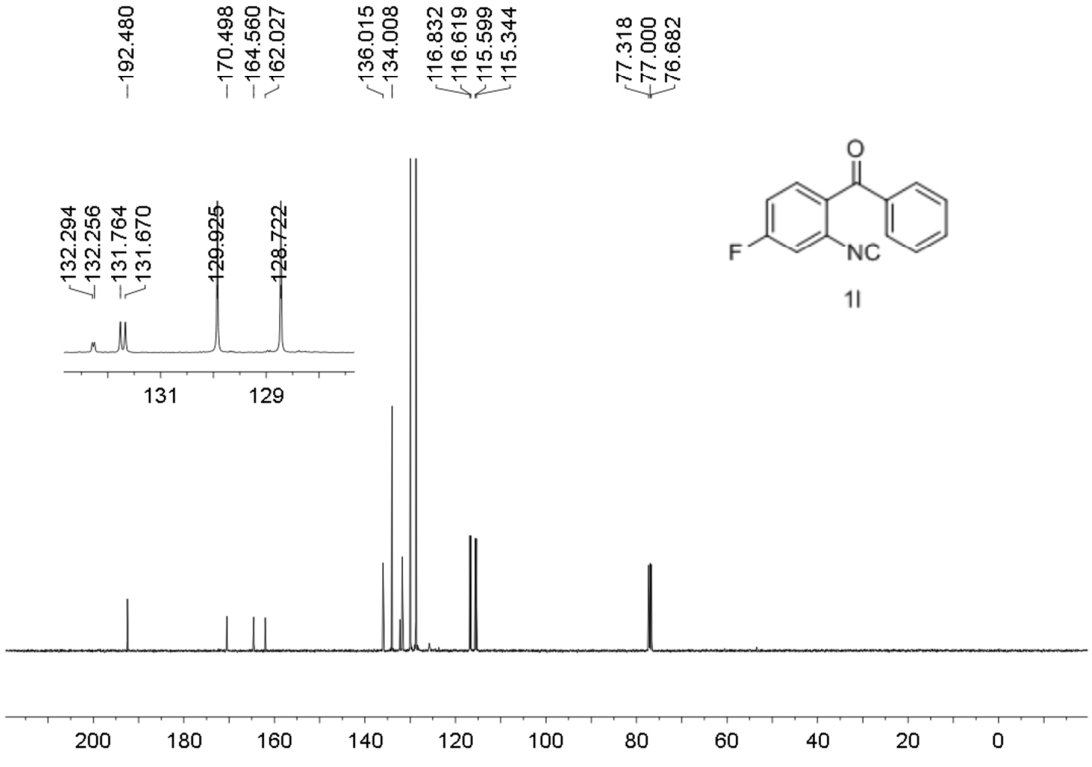
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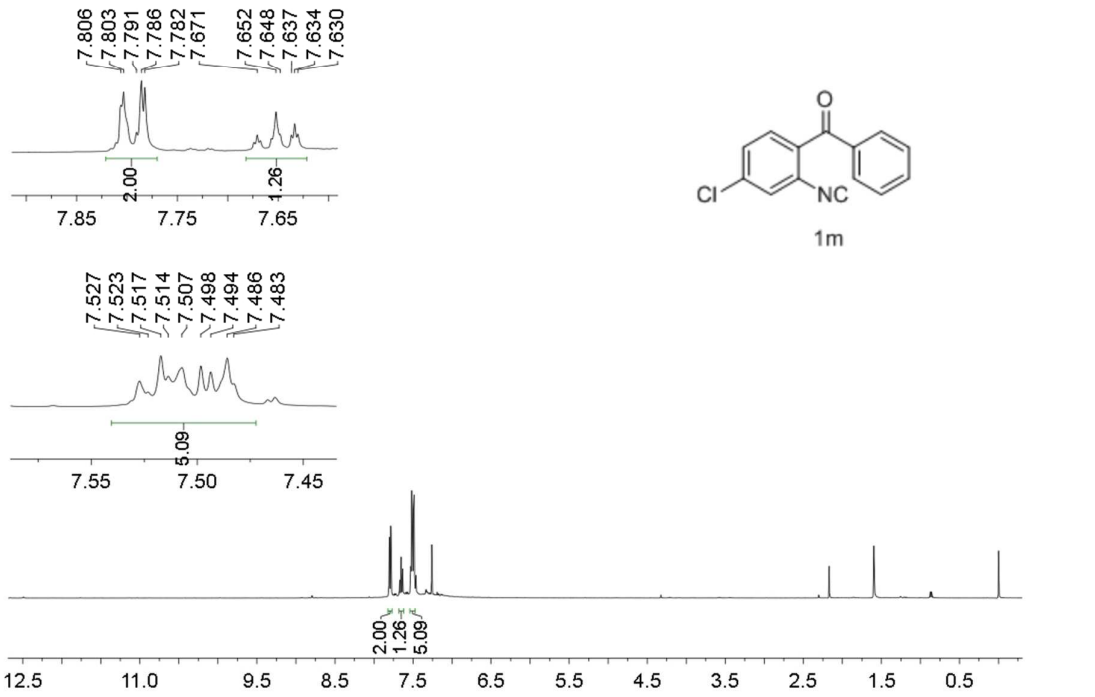
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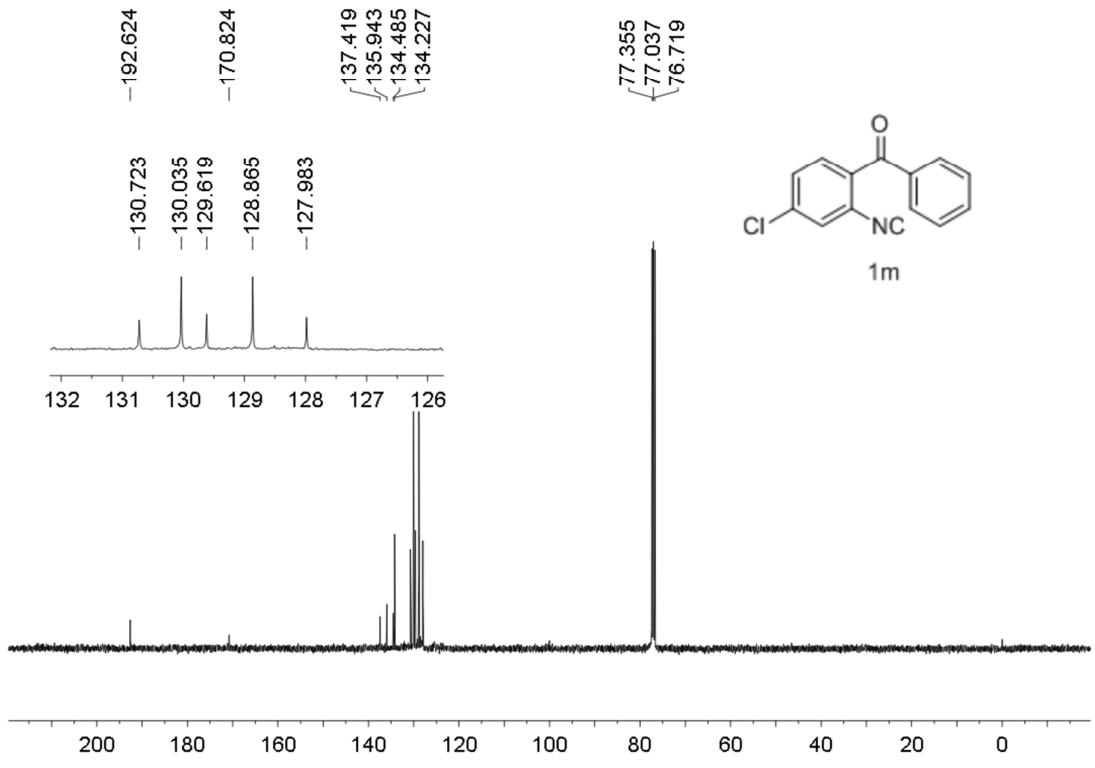
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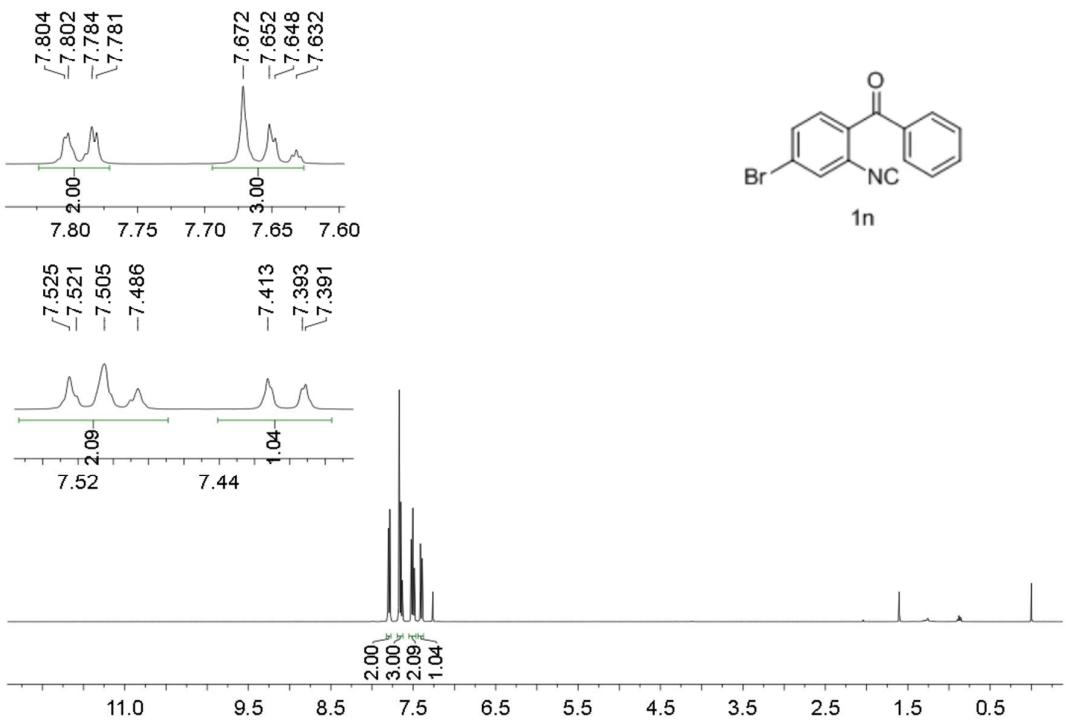
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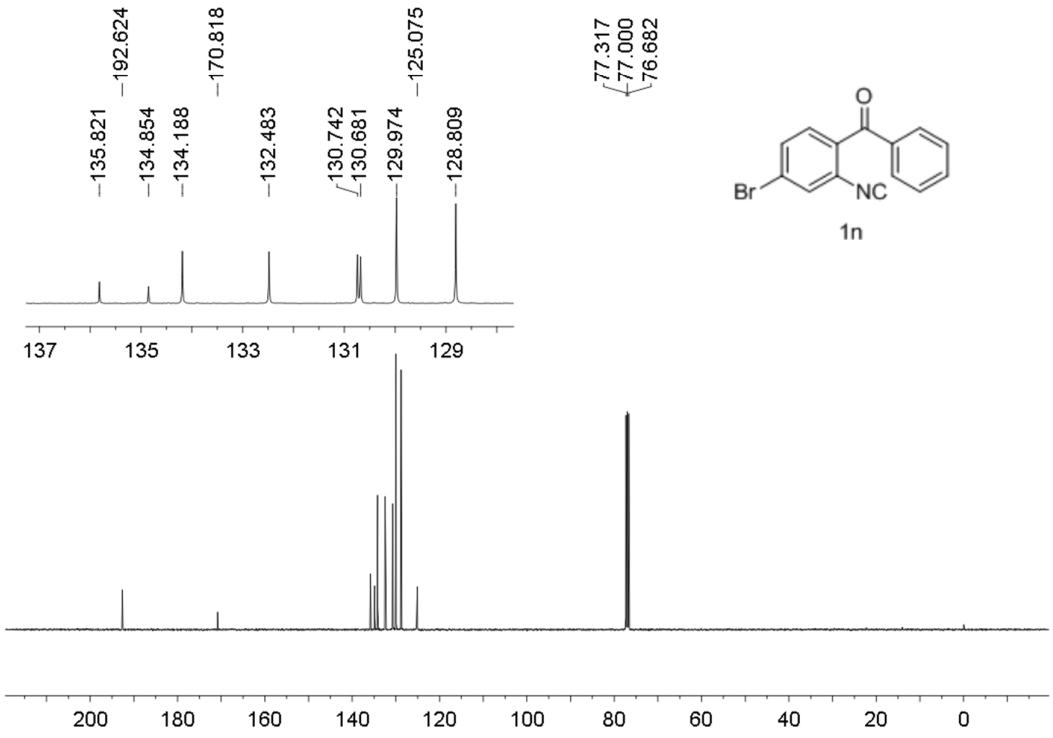
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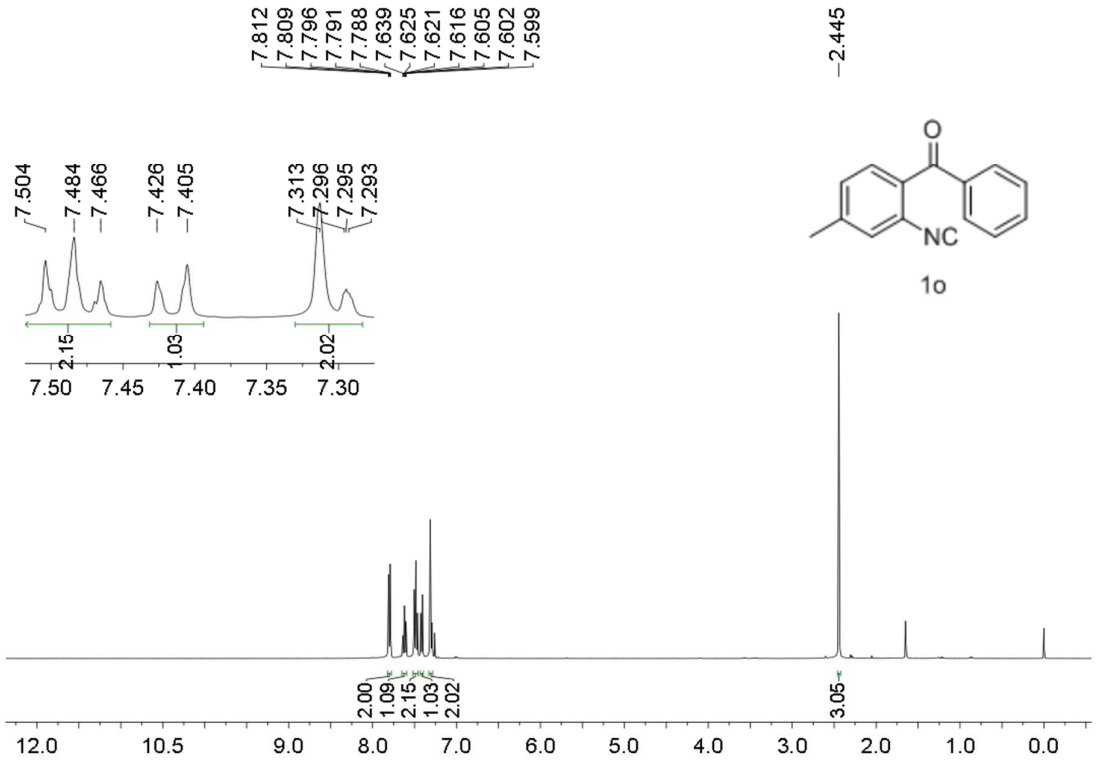
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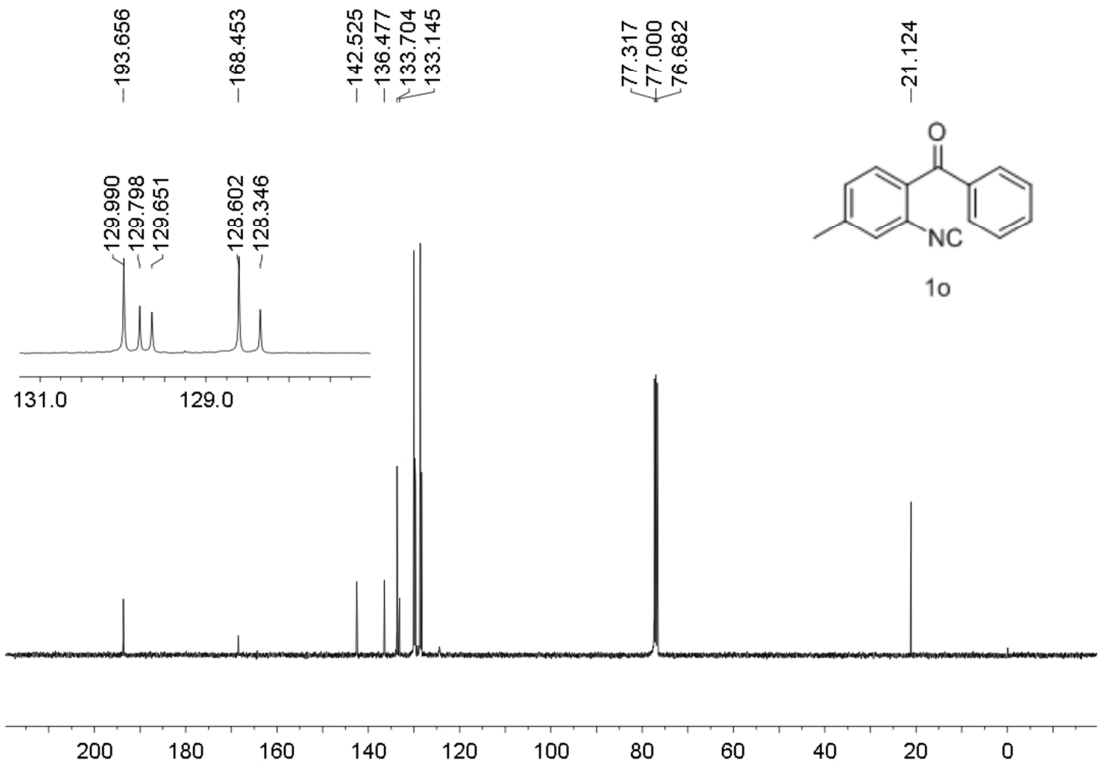
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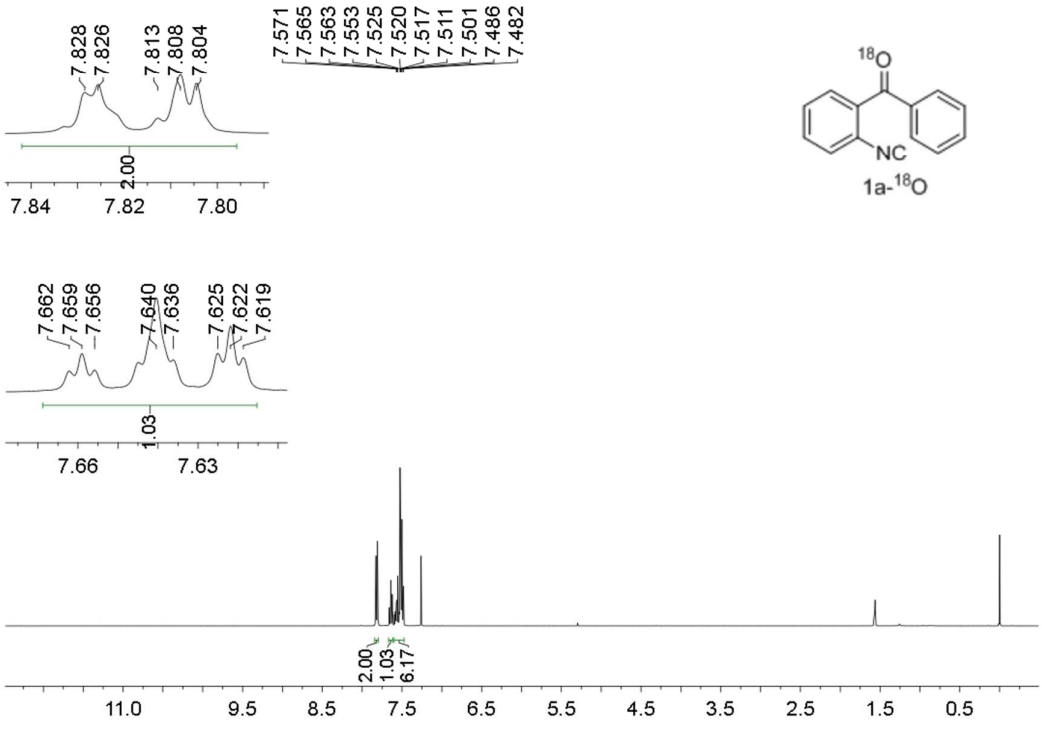
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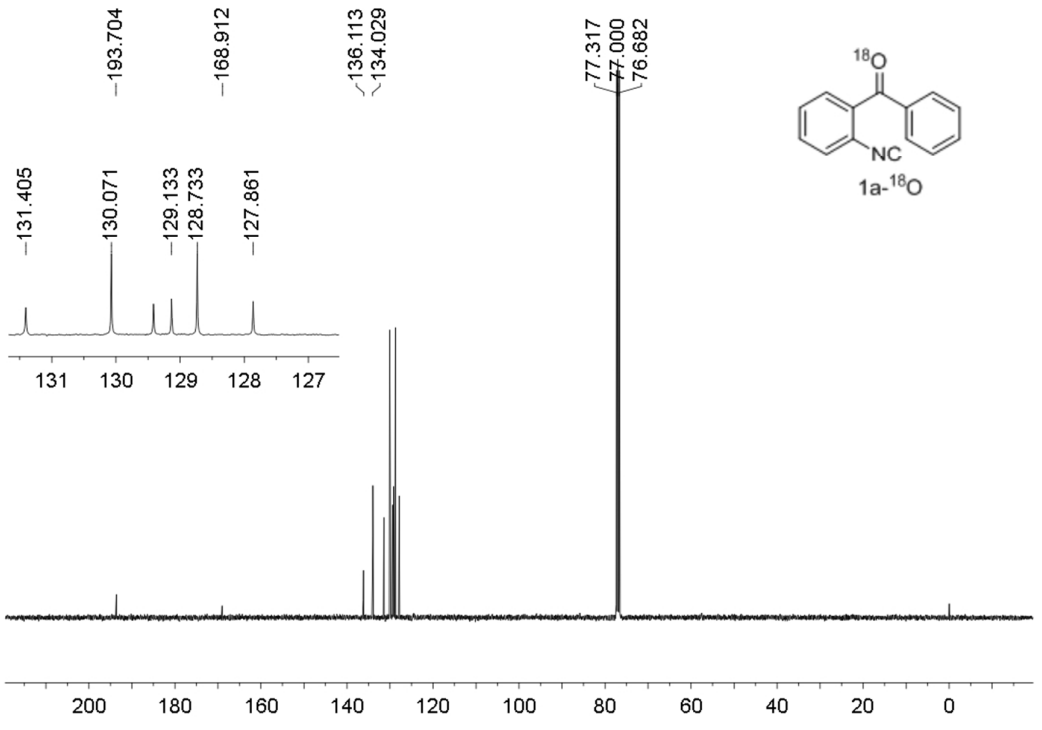
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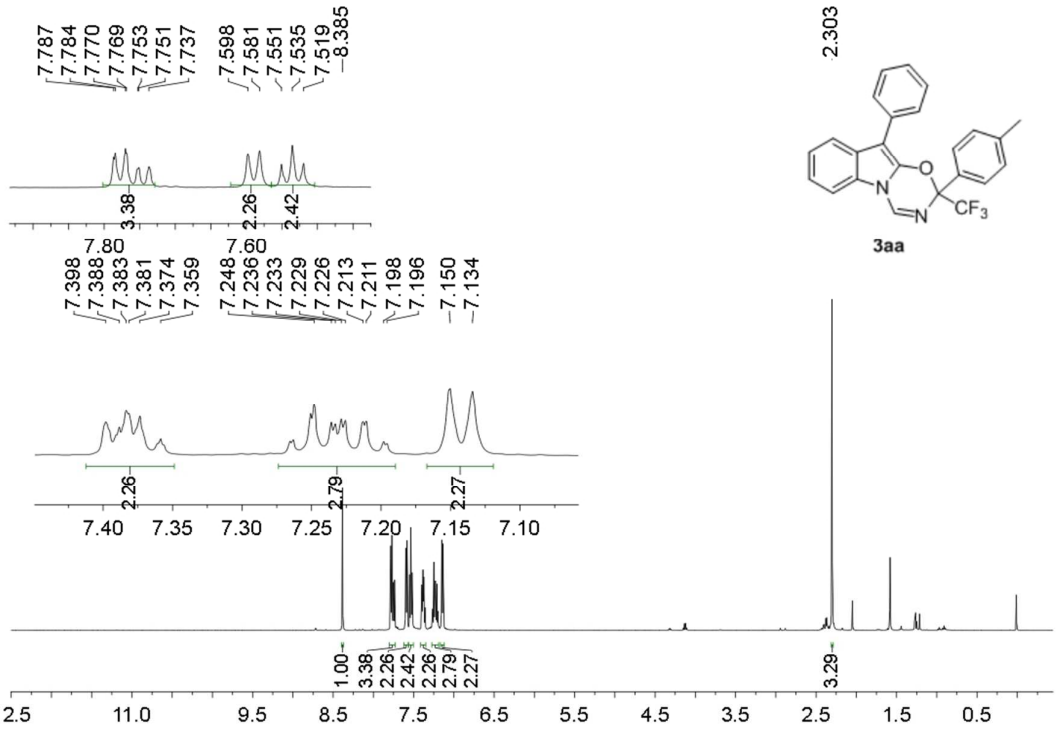
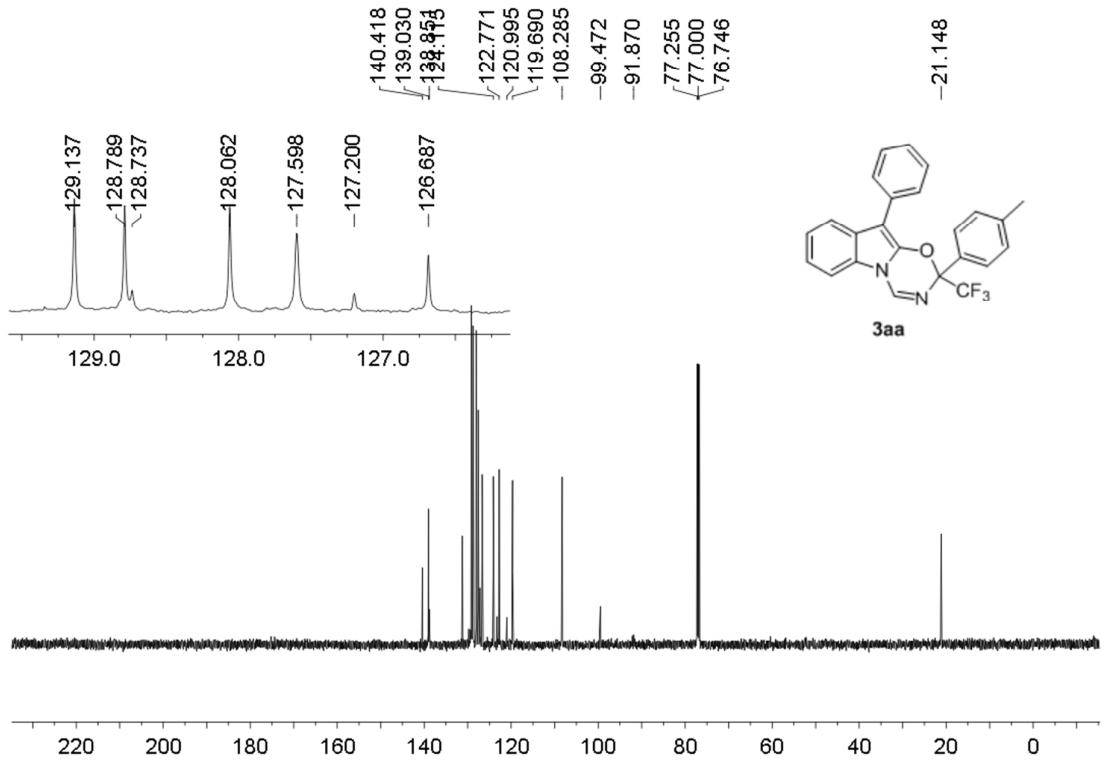
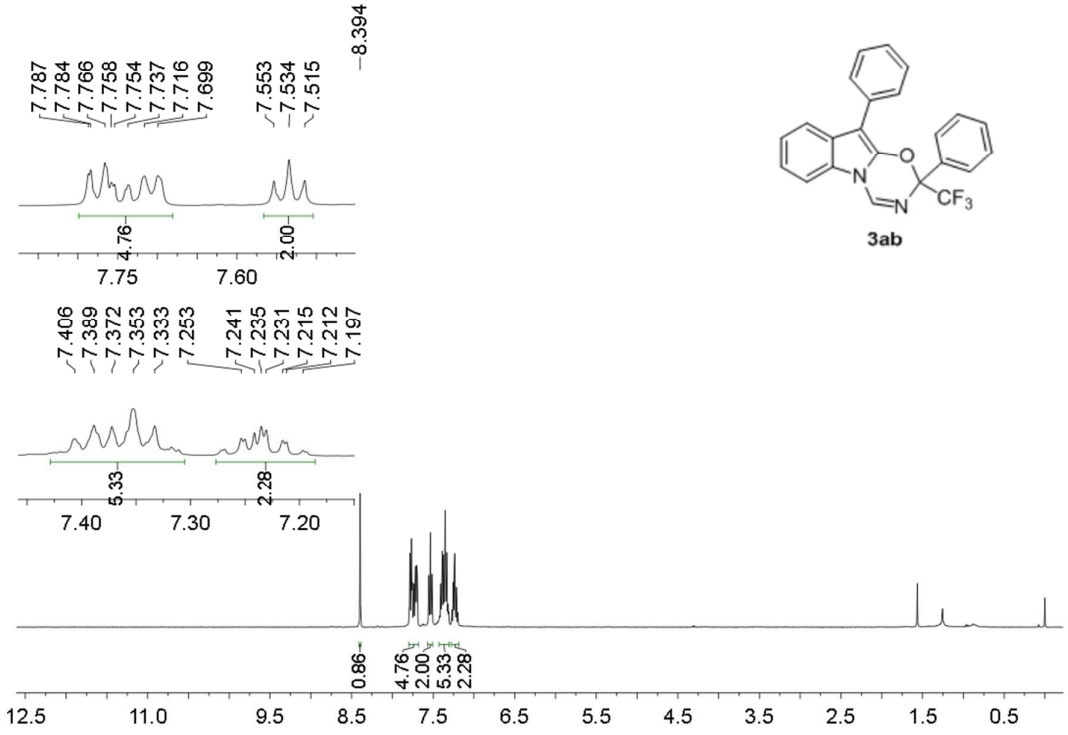
Copies of ^{1}H NMR and ^{13}C NMR spectra of compounds 3



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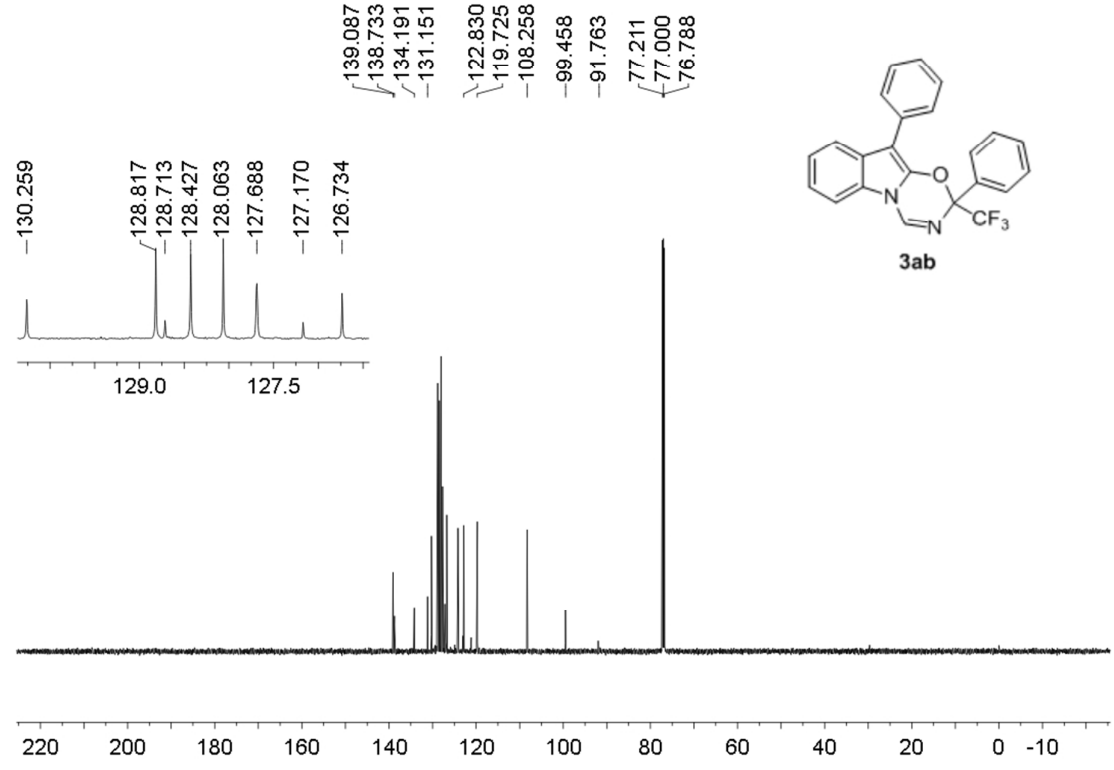
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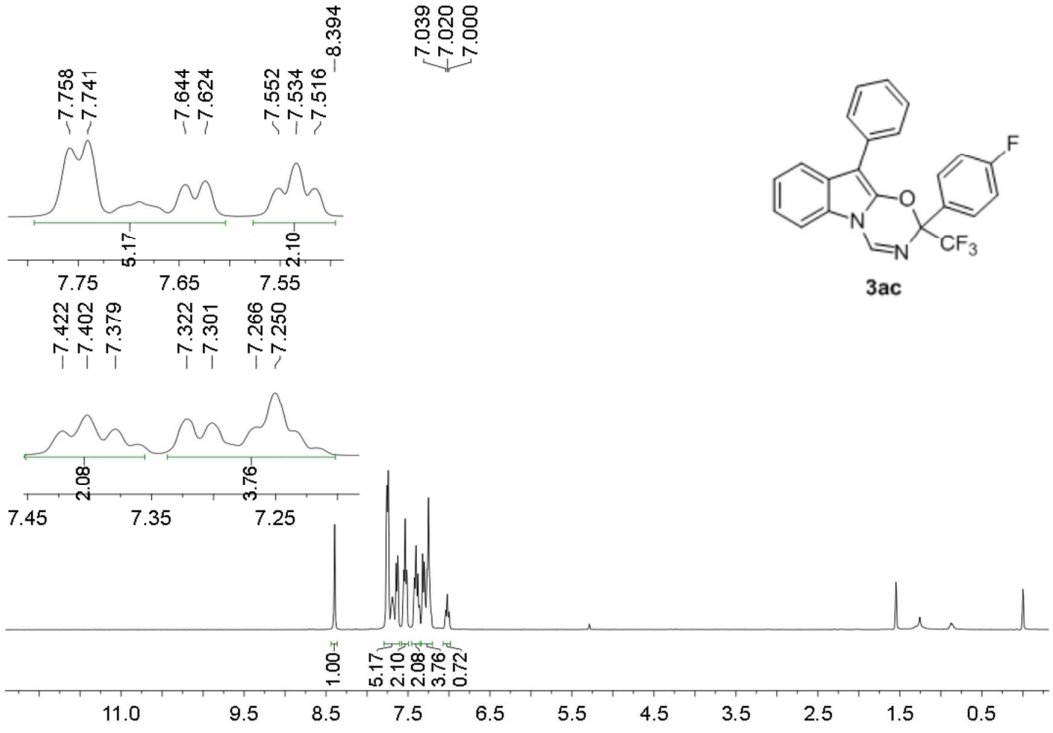
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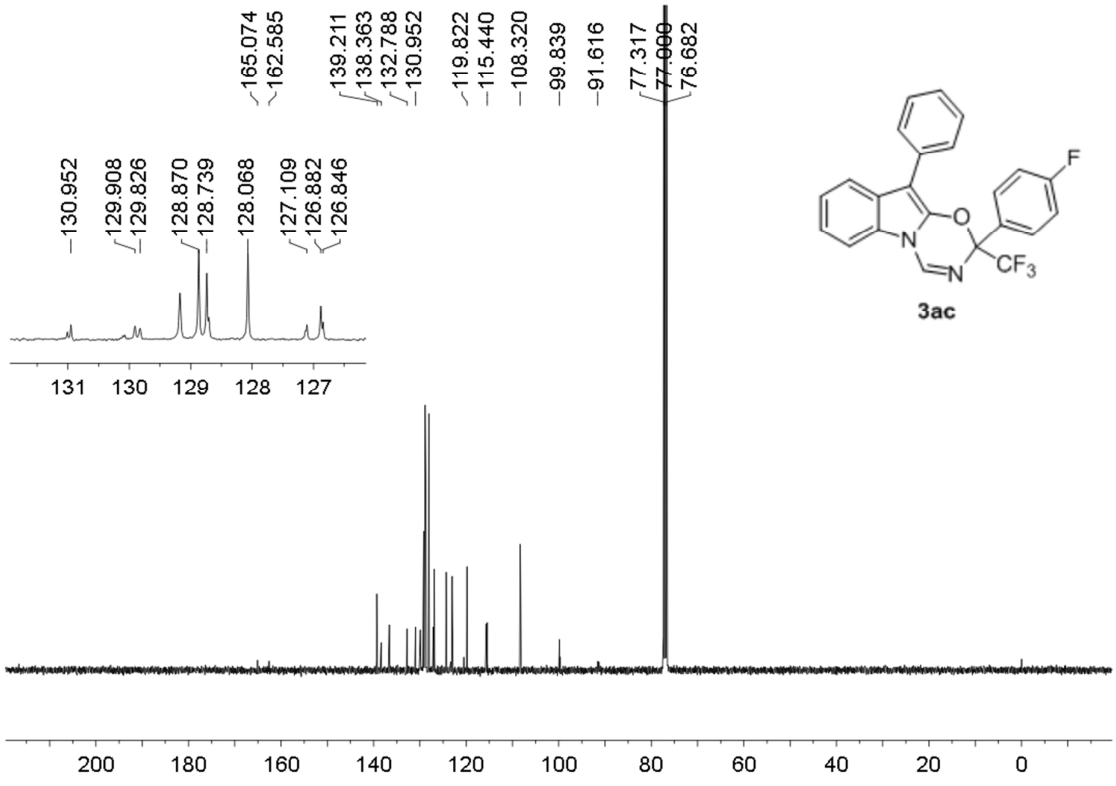
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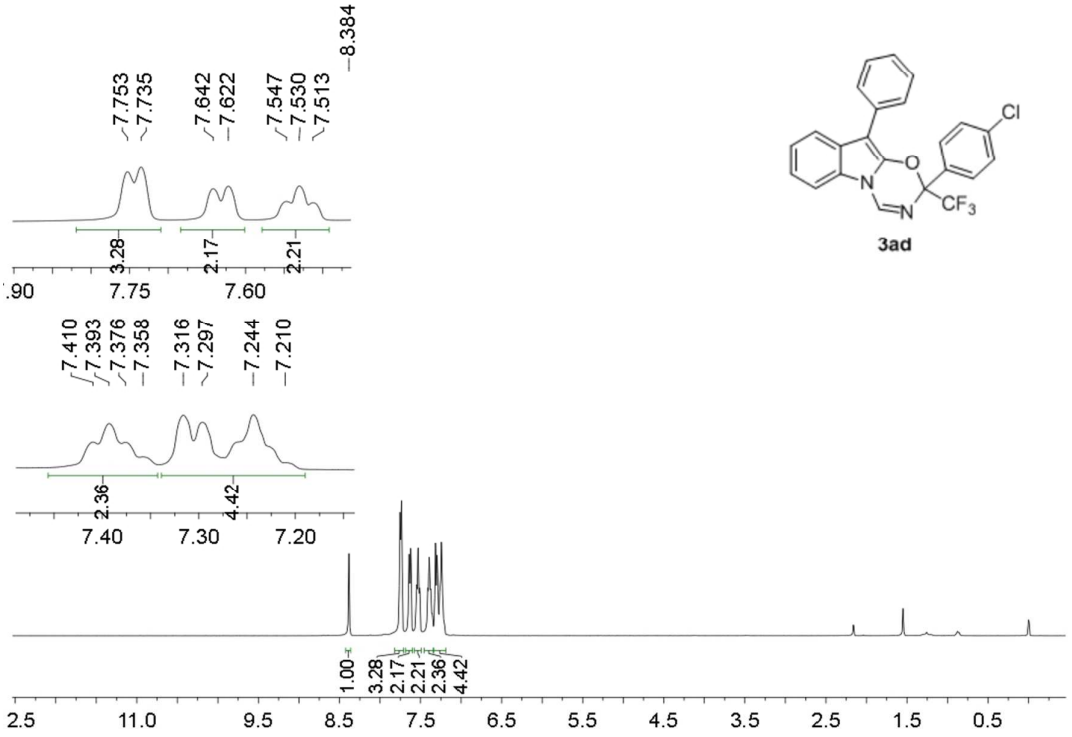
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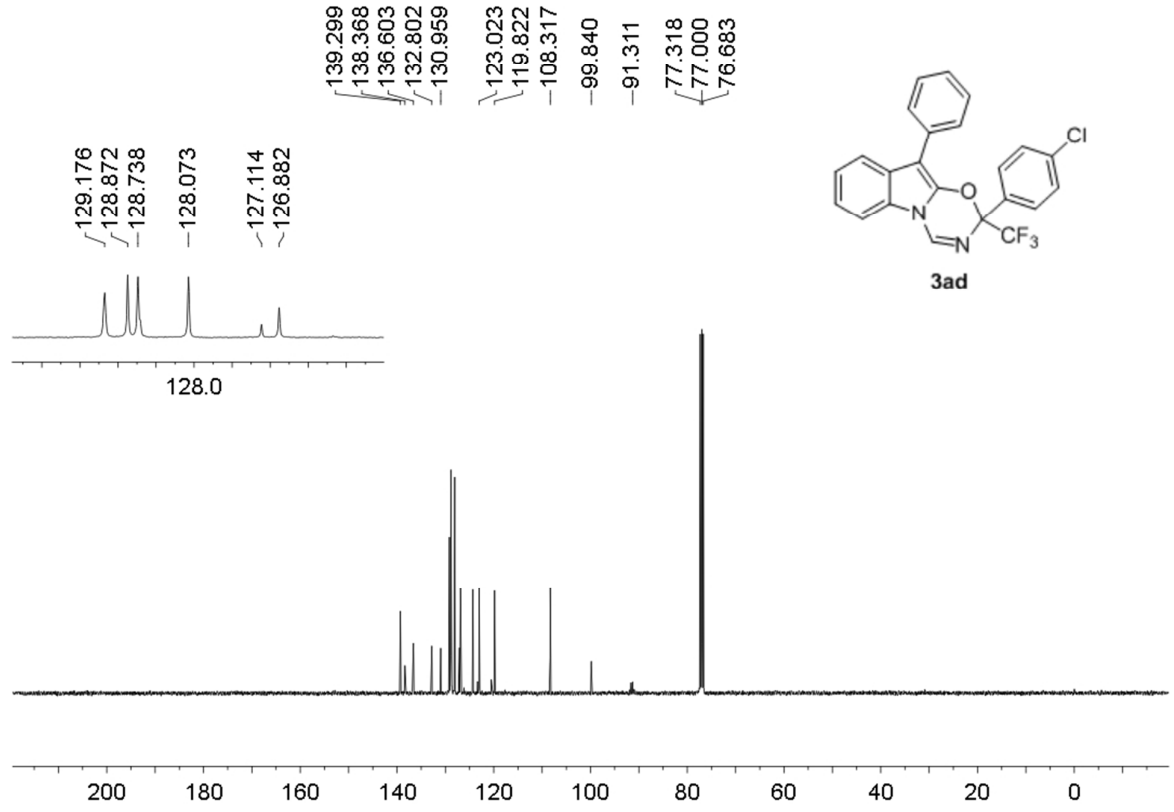
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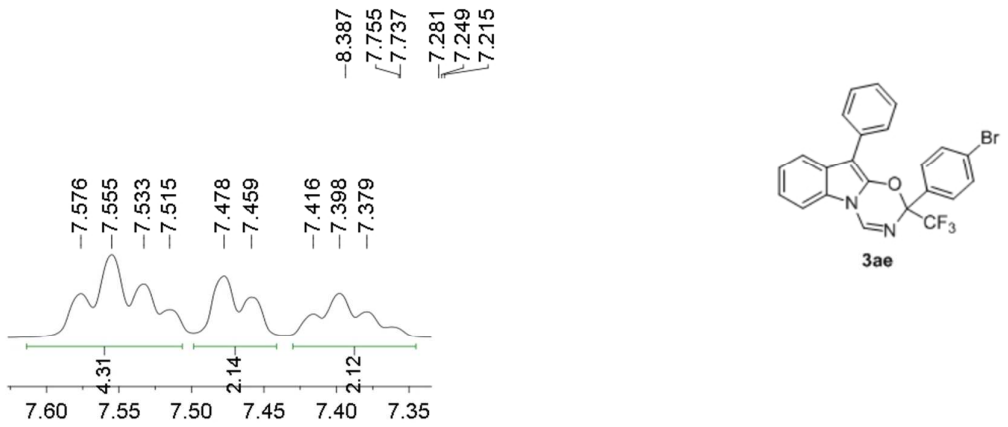
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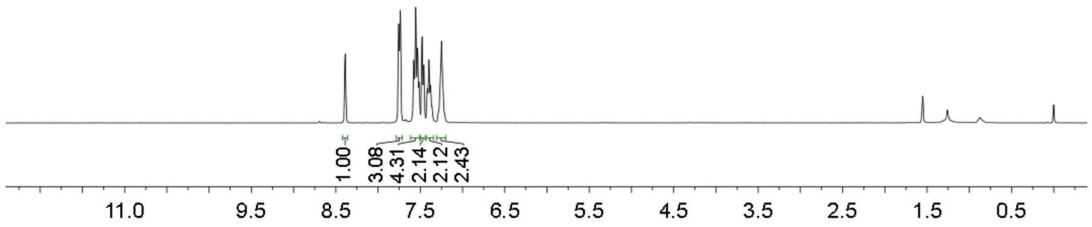
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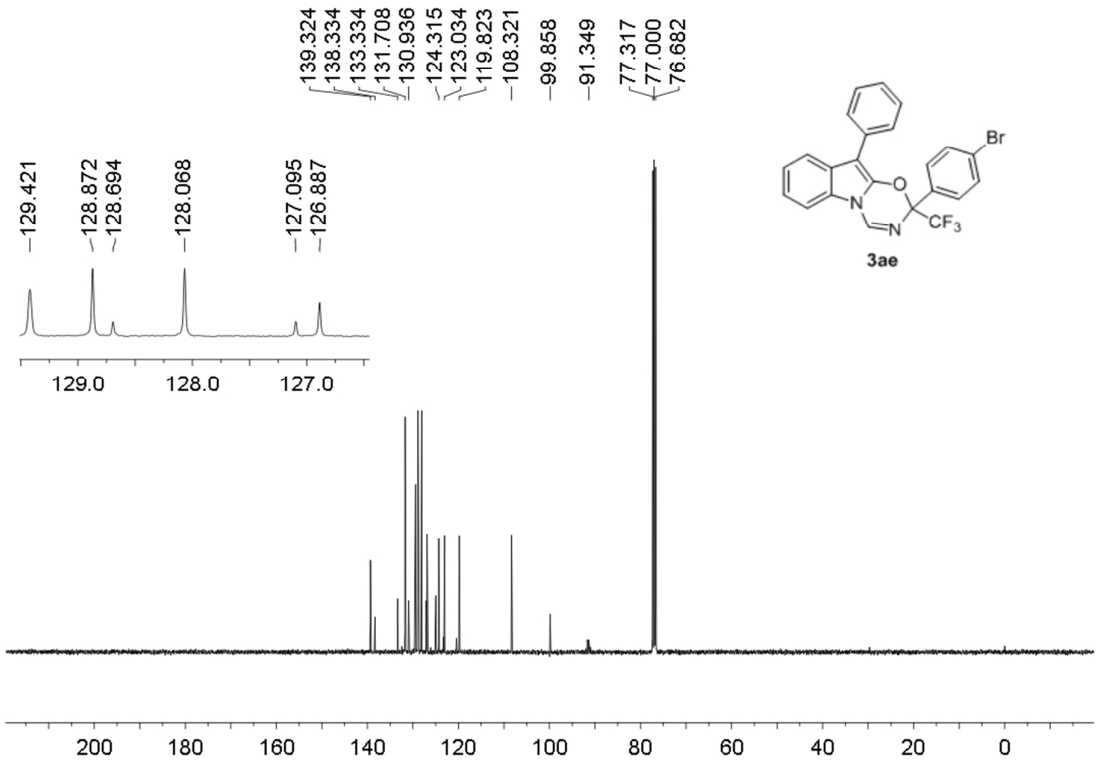
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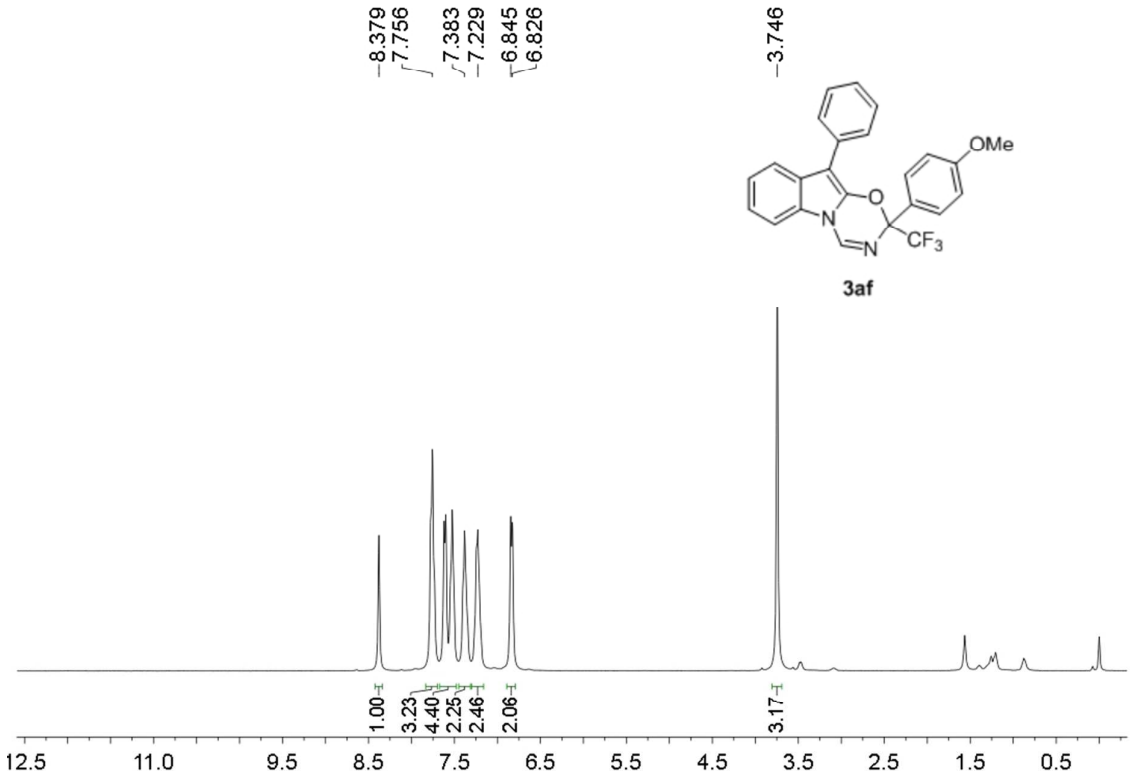
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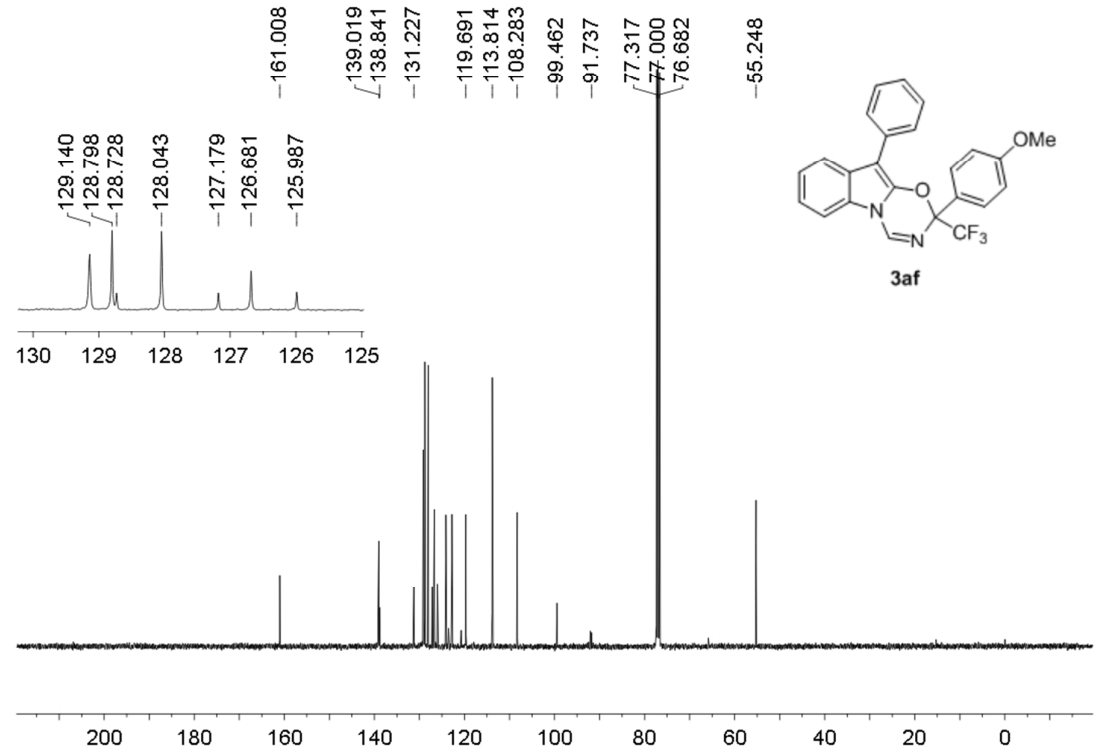
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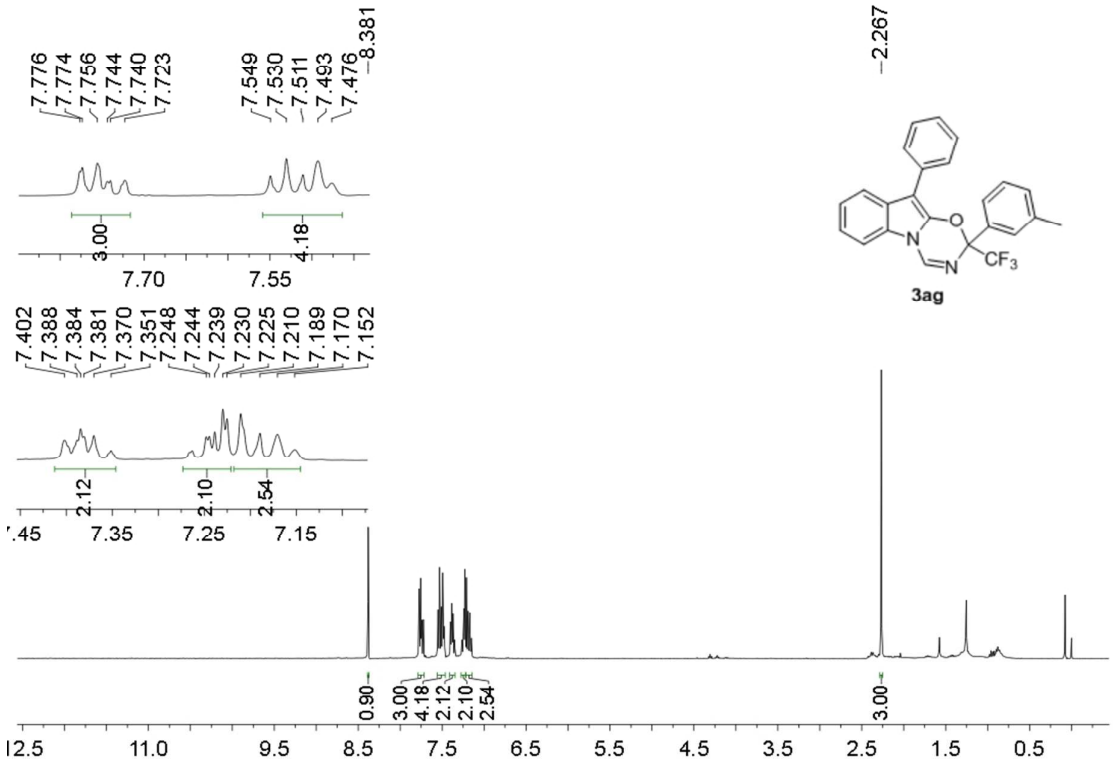
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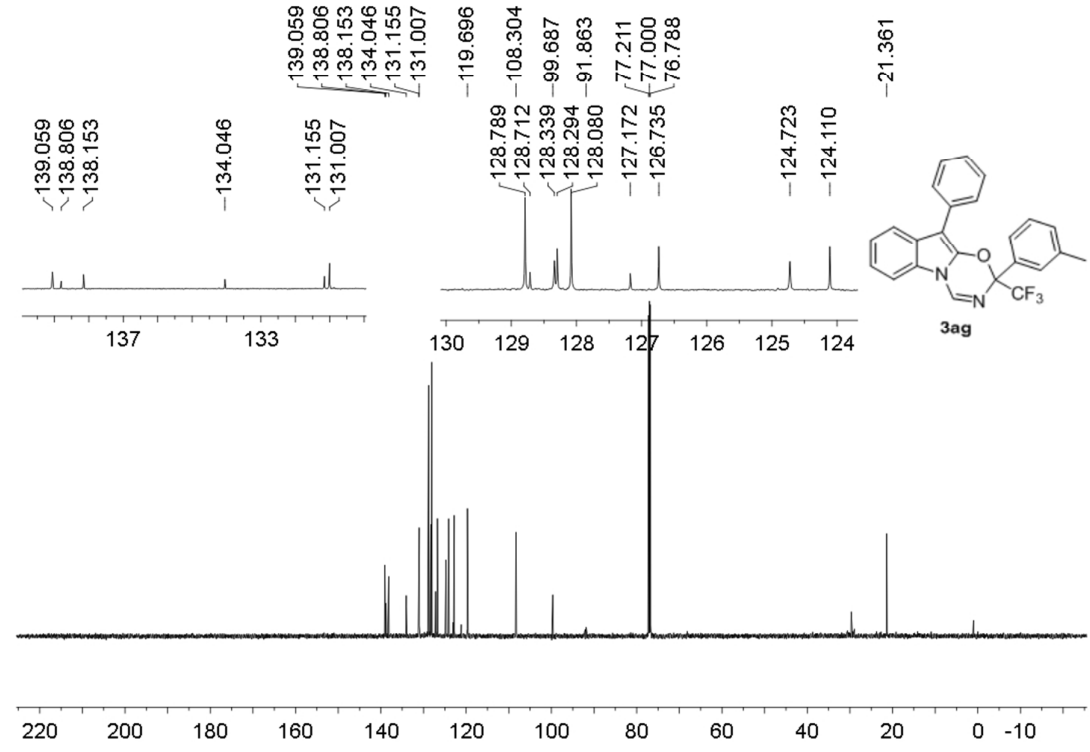
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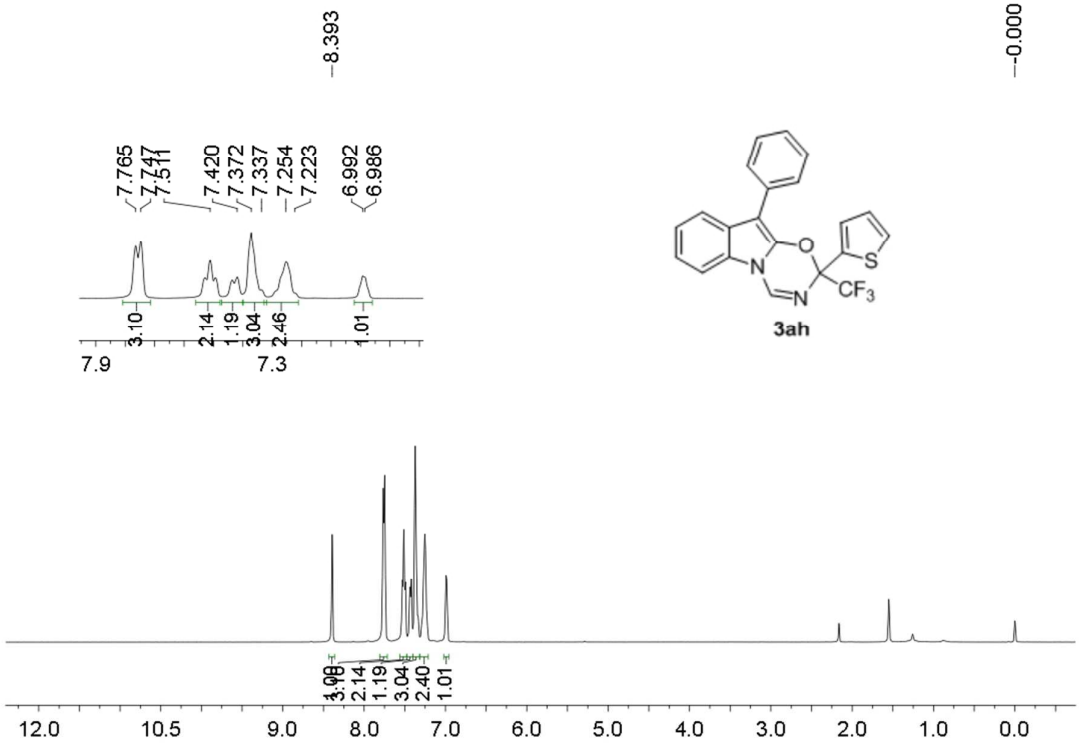
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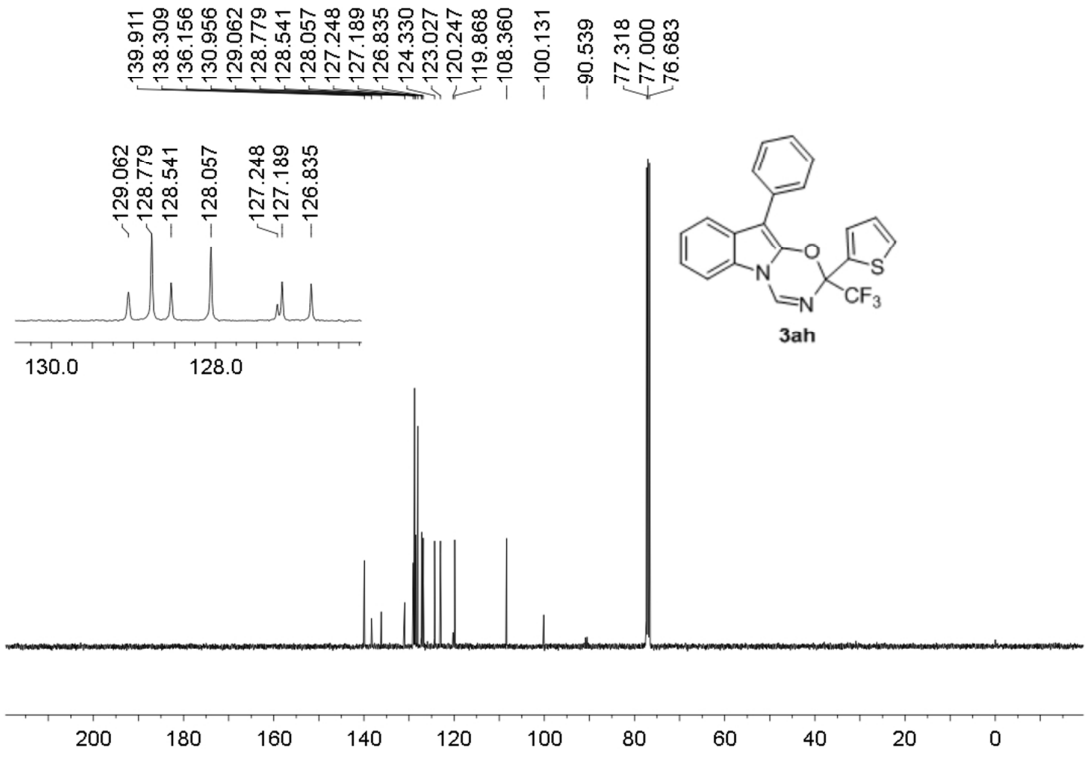
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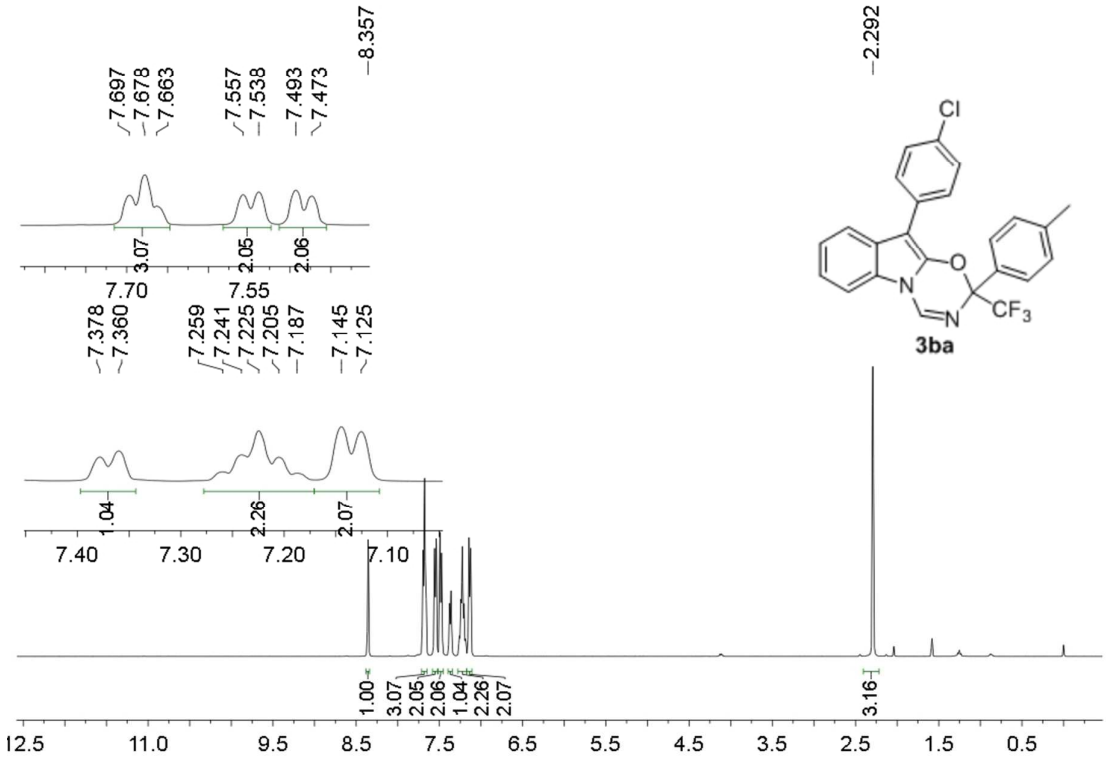
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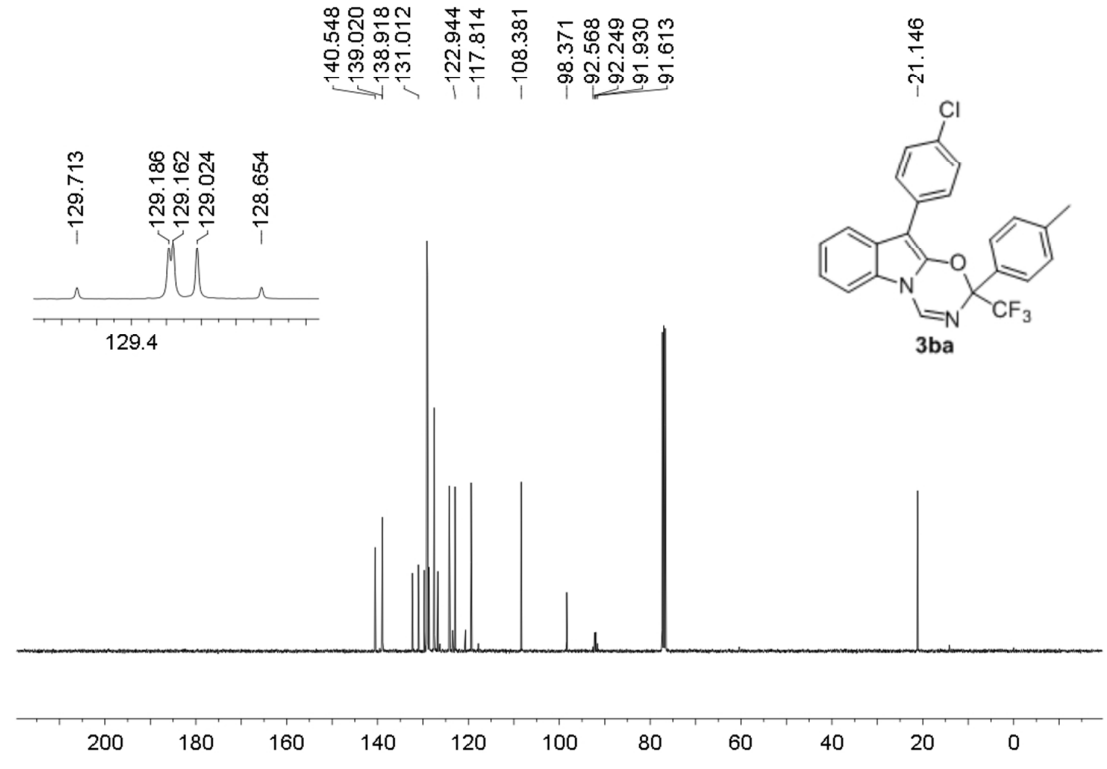
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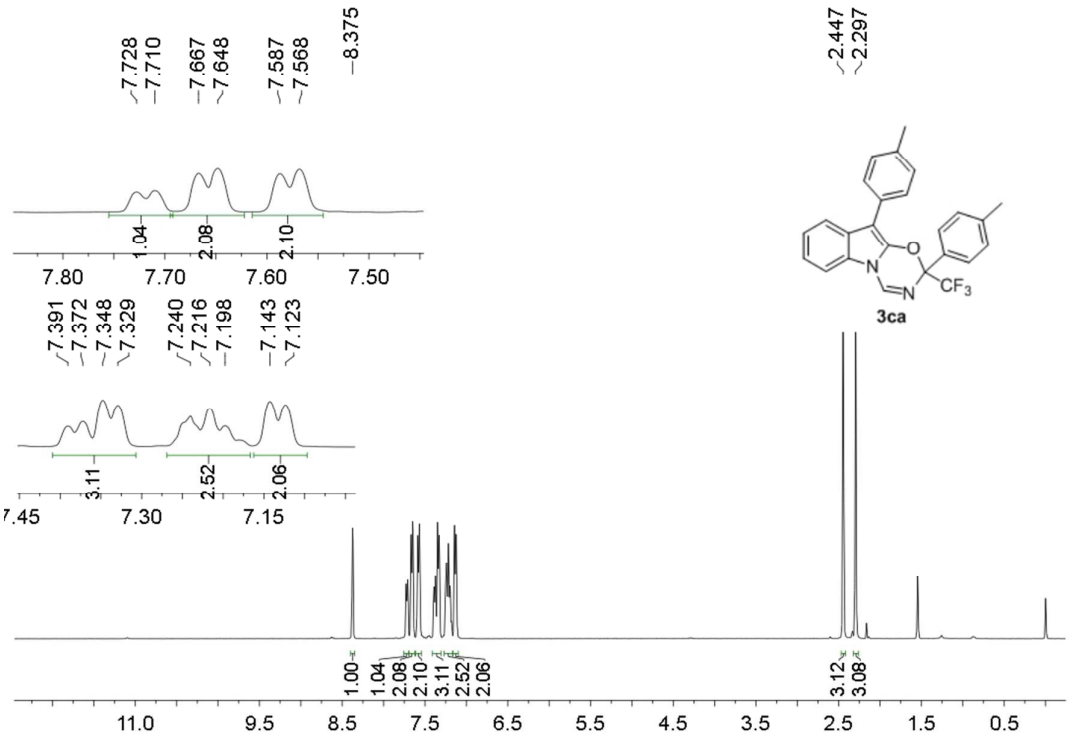
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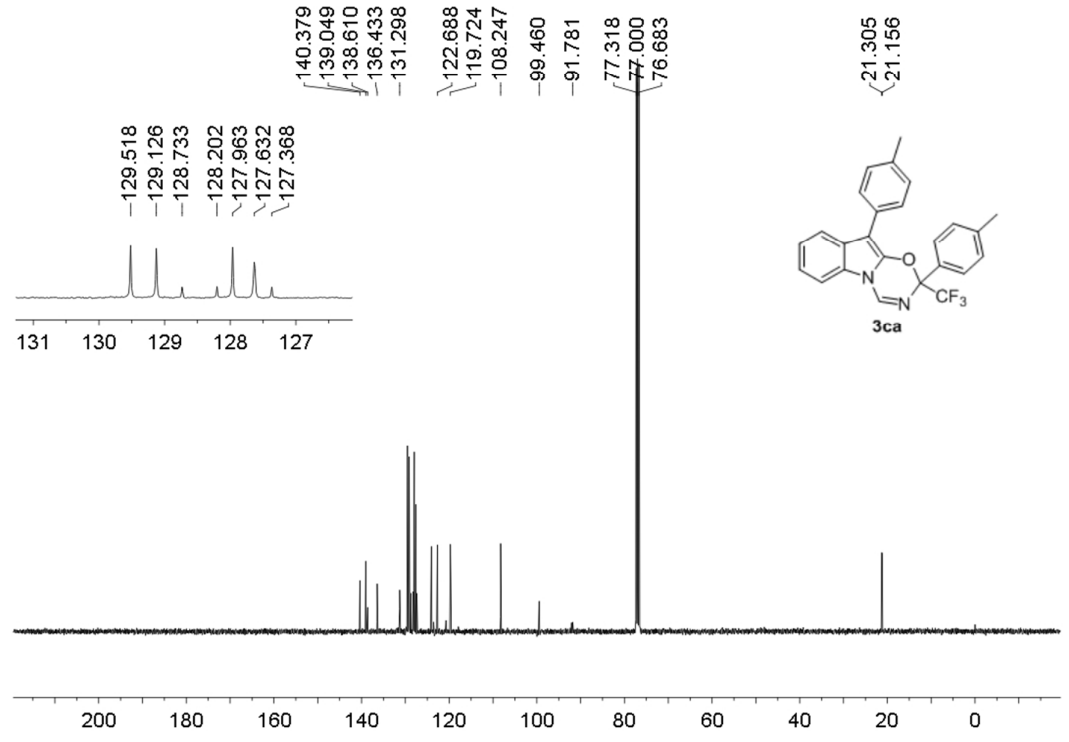
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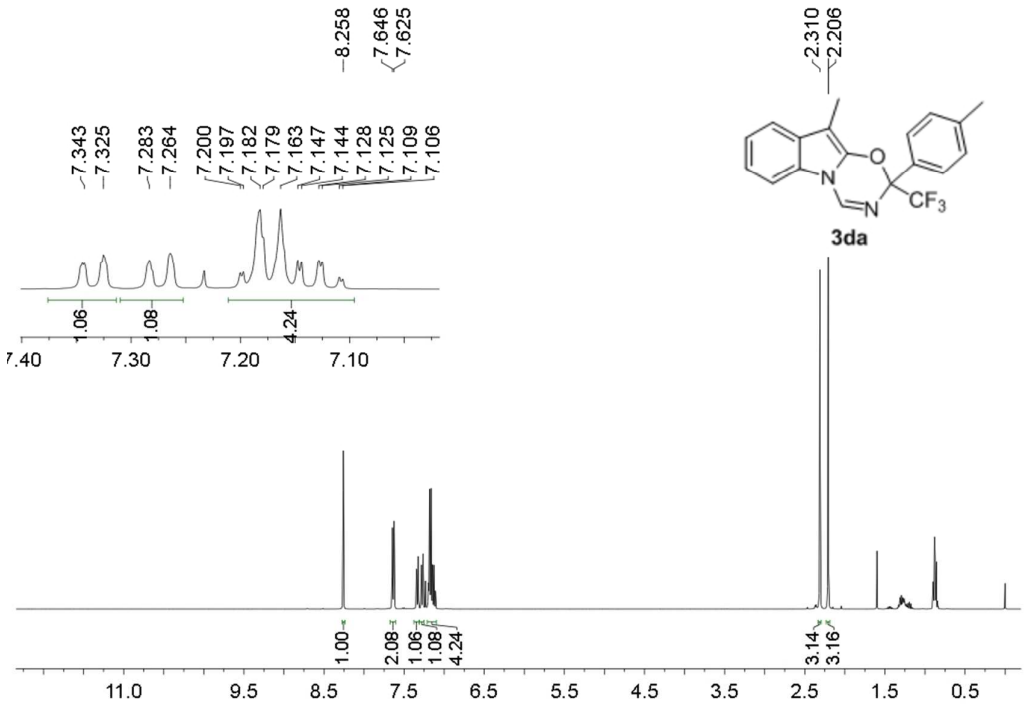
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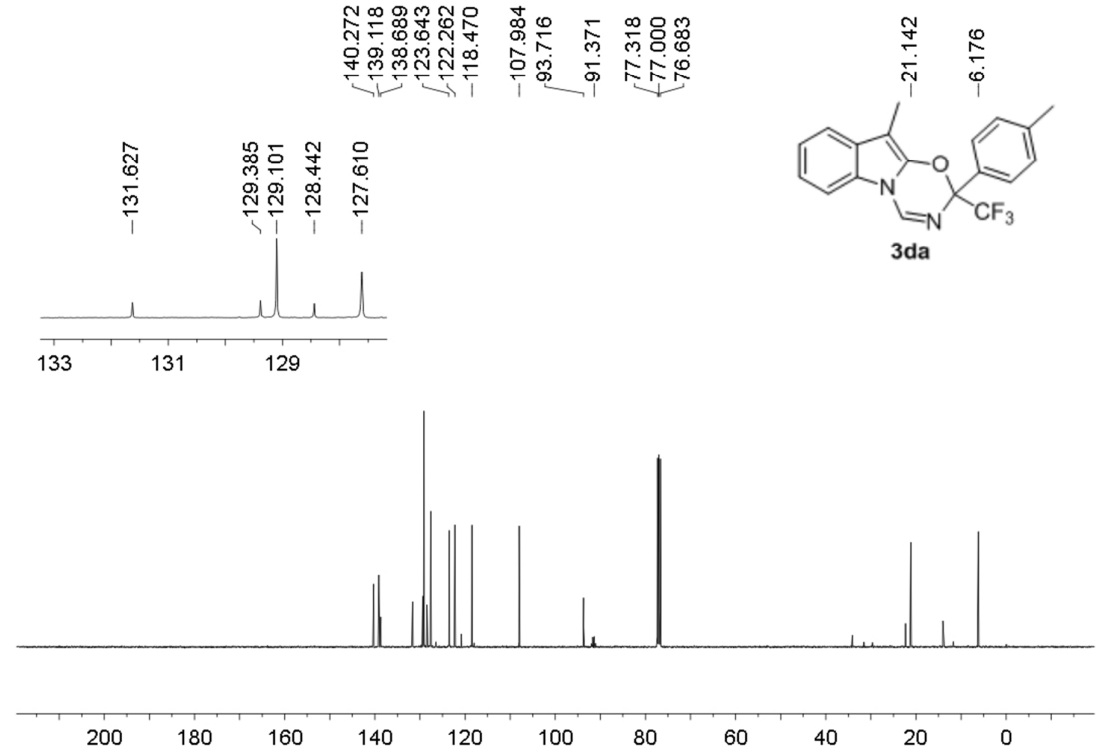
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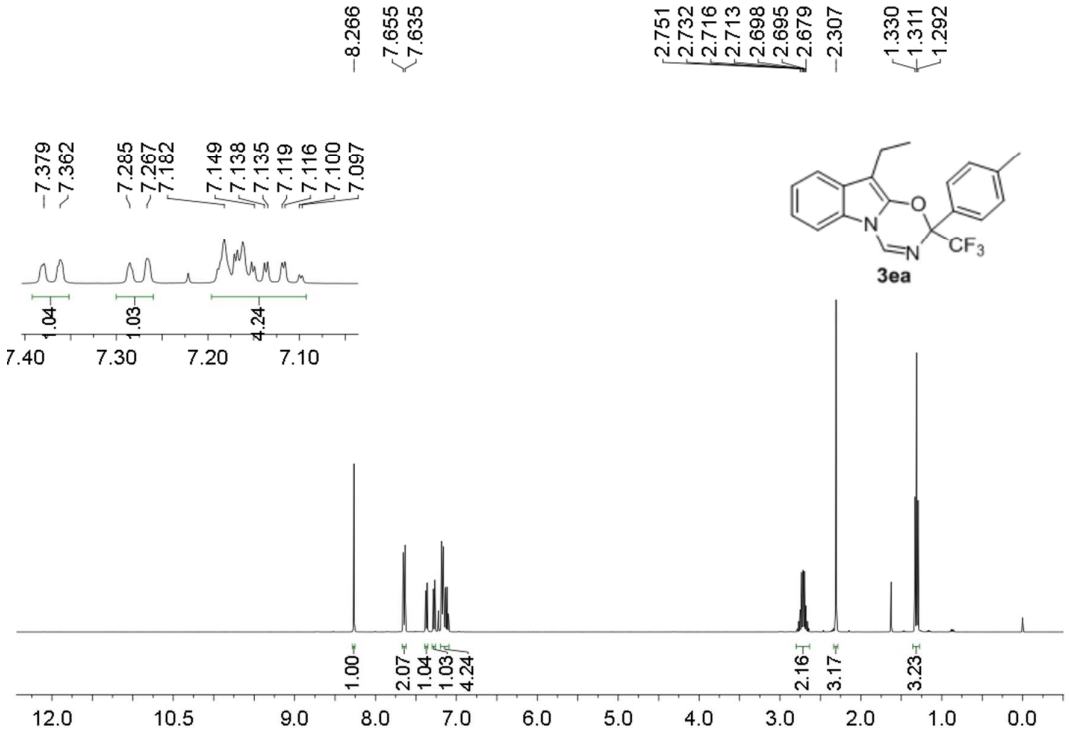
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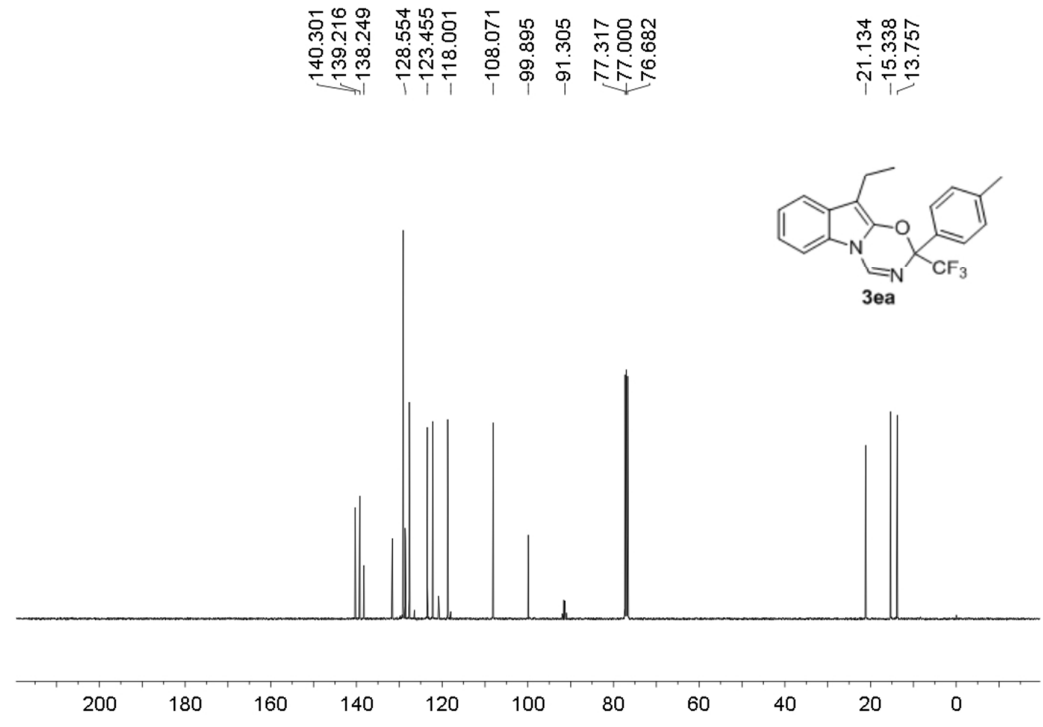
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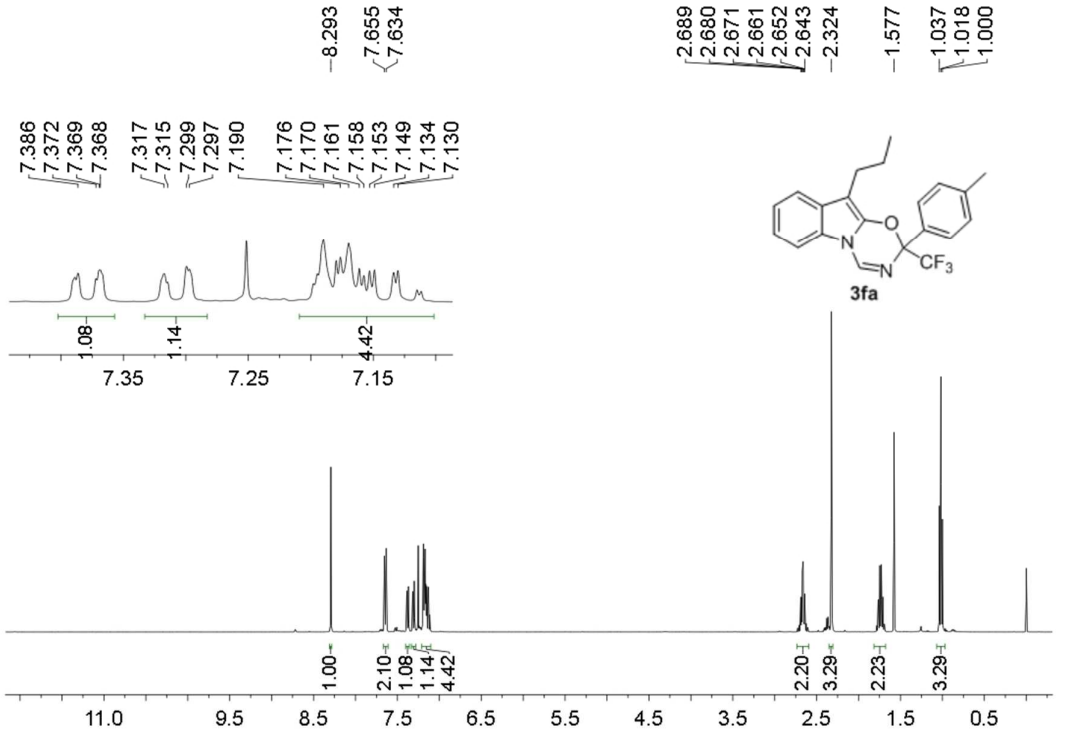
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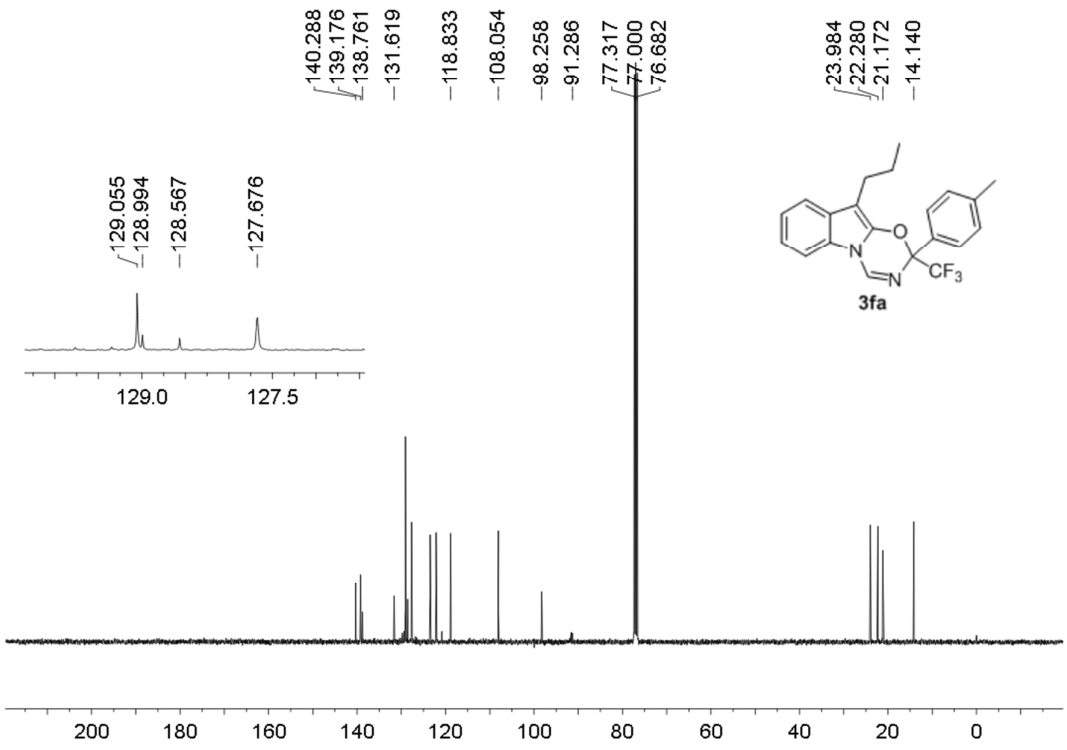
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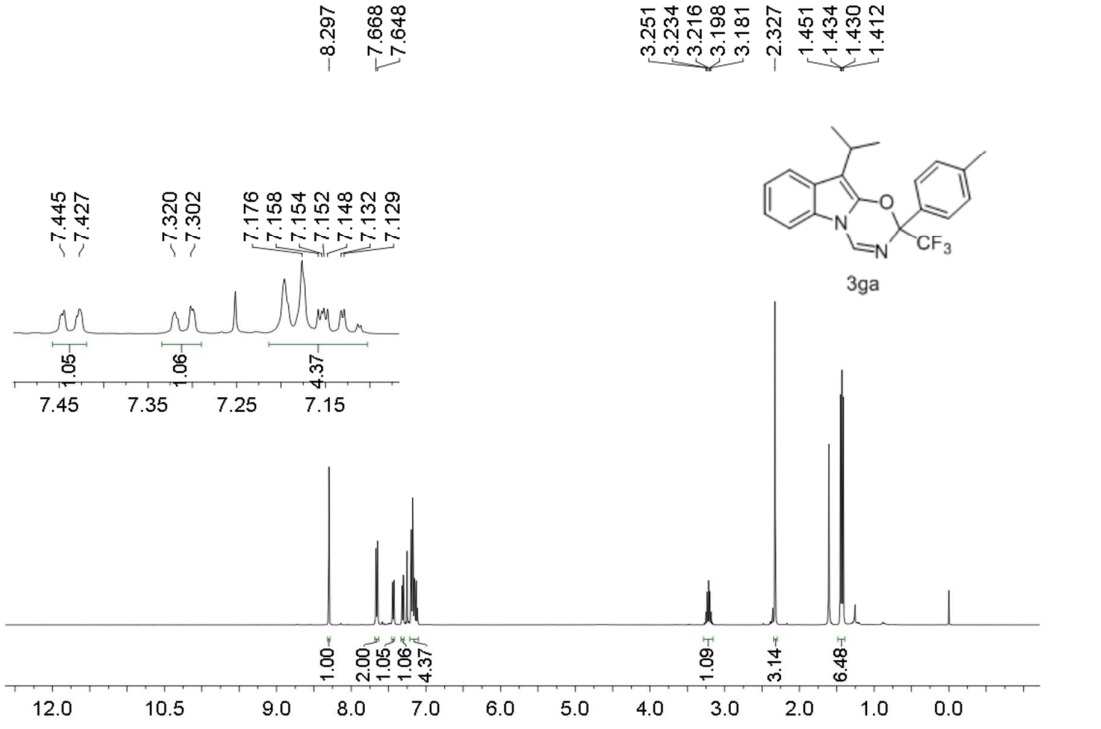
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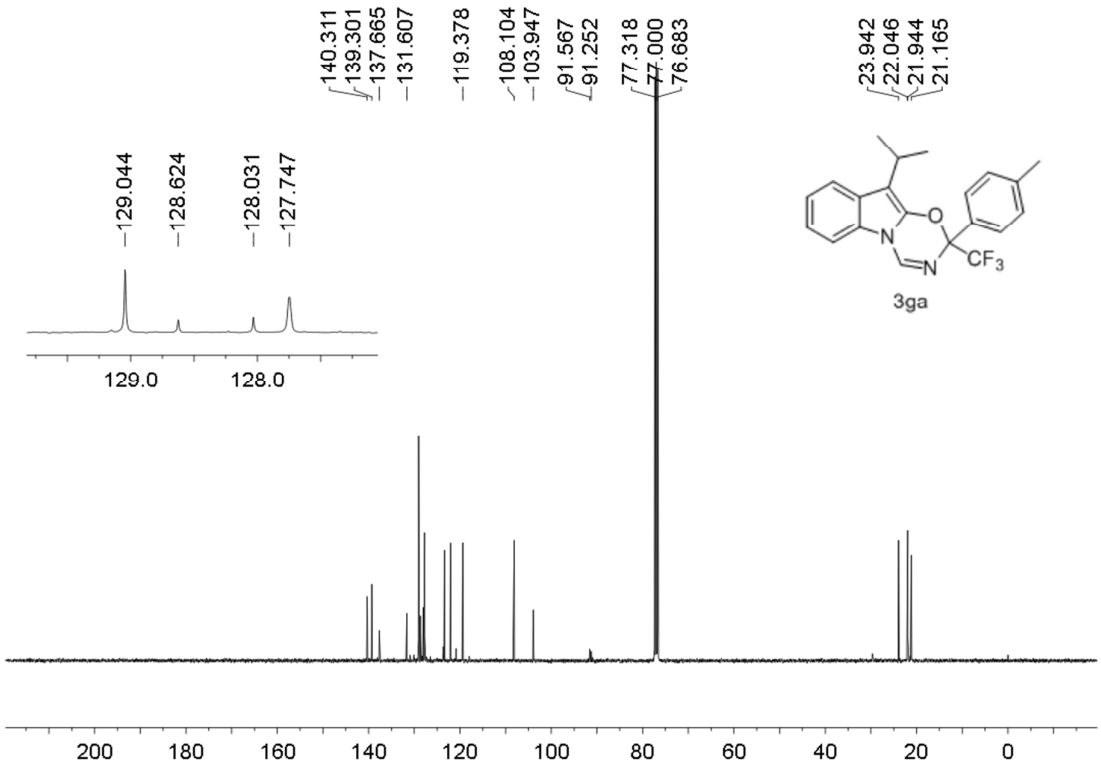
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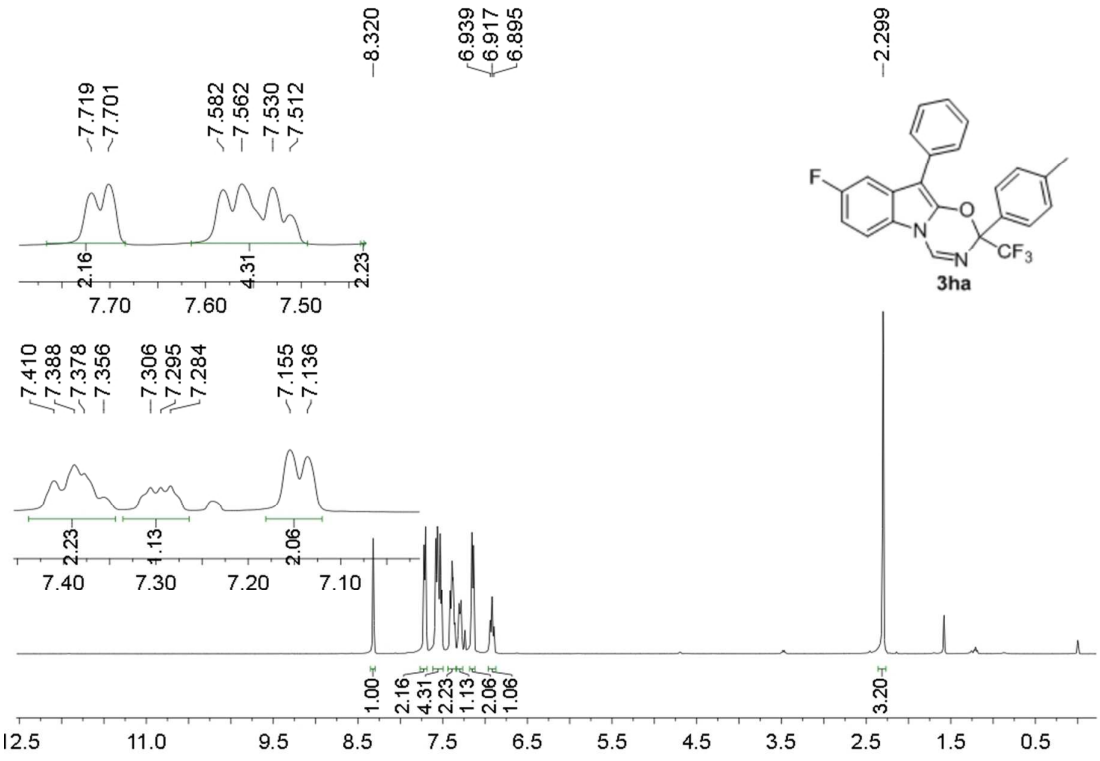
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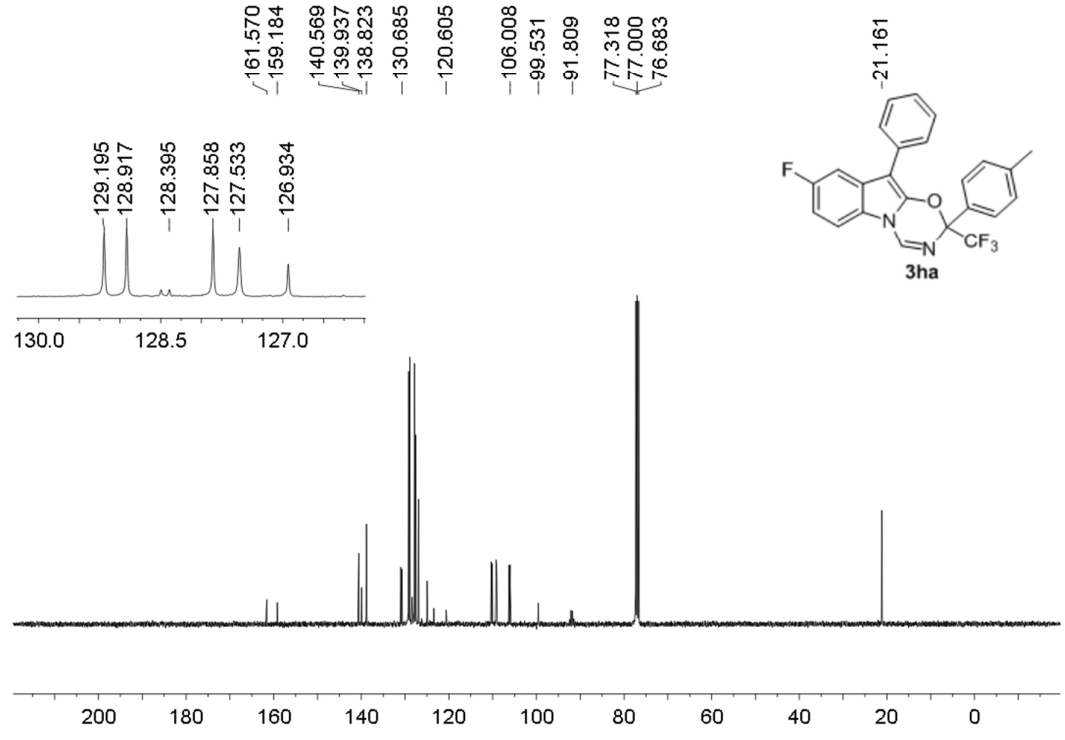
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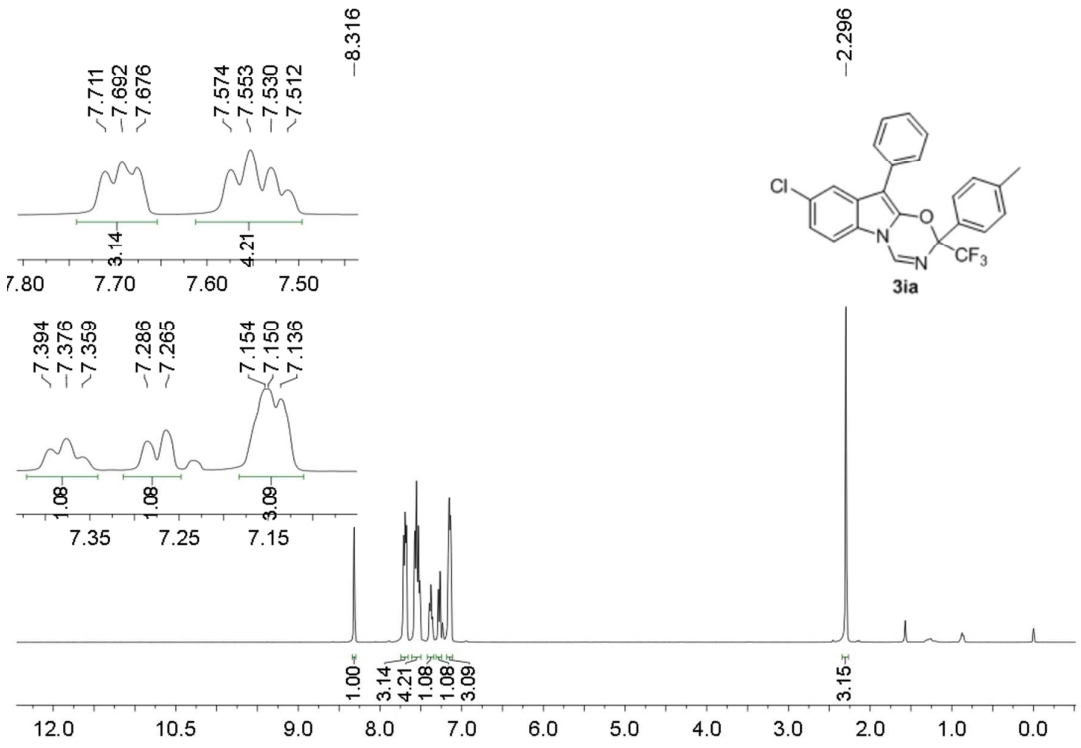
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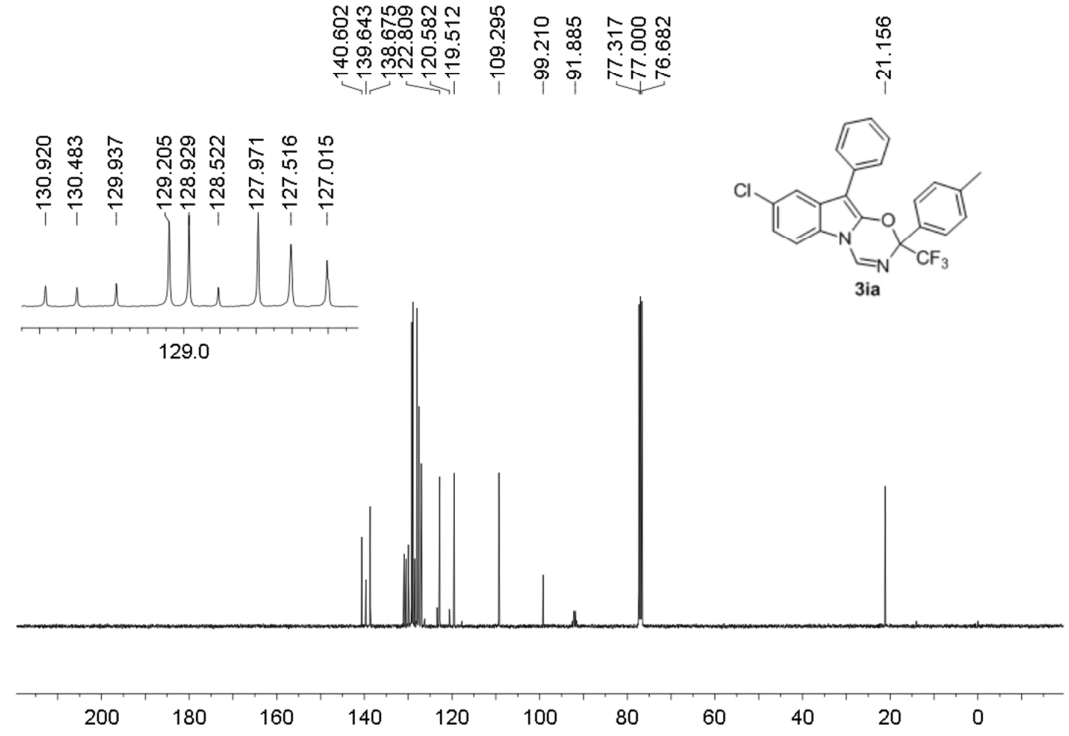
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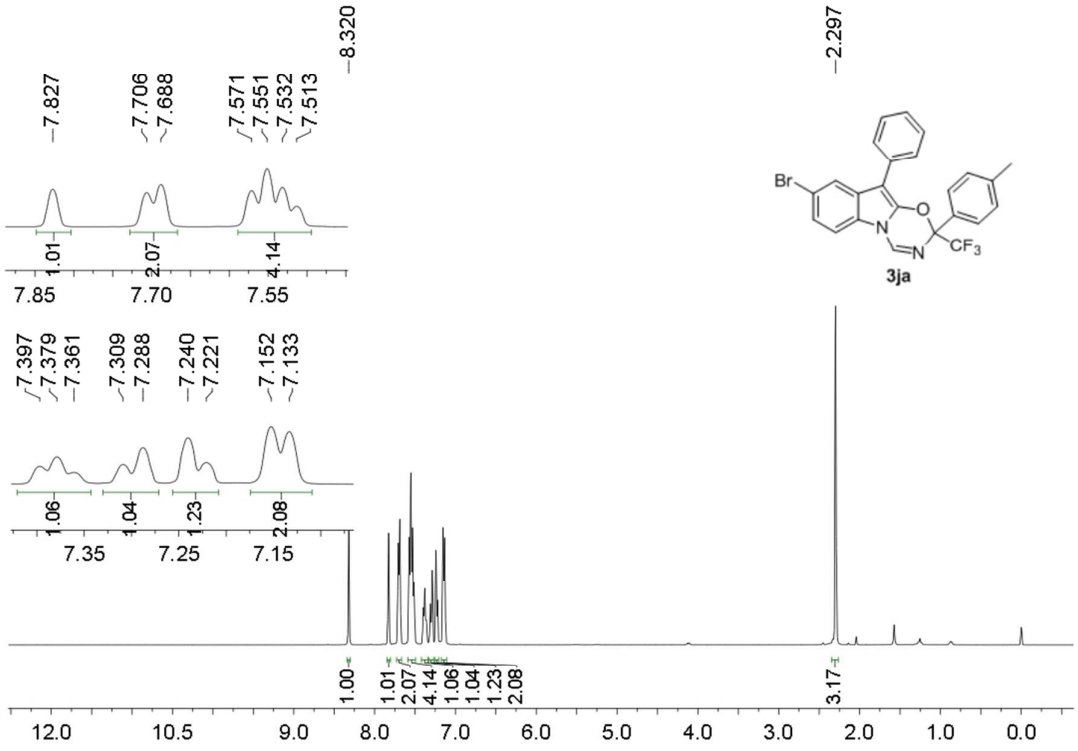
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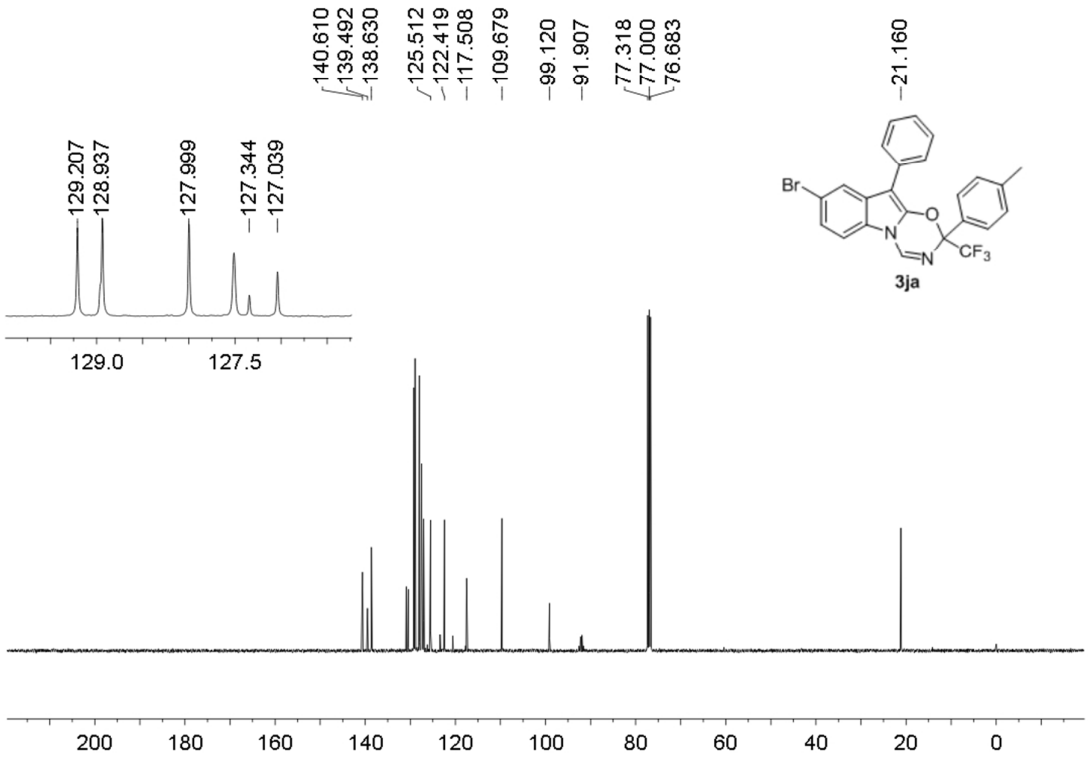
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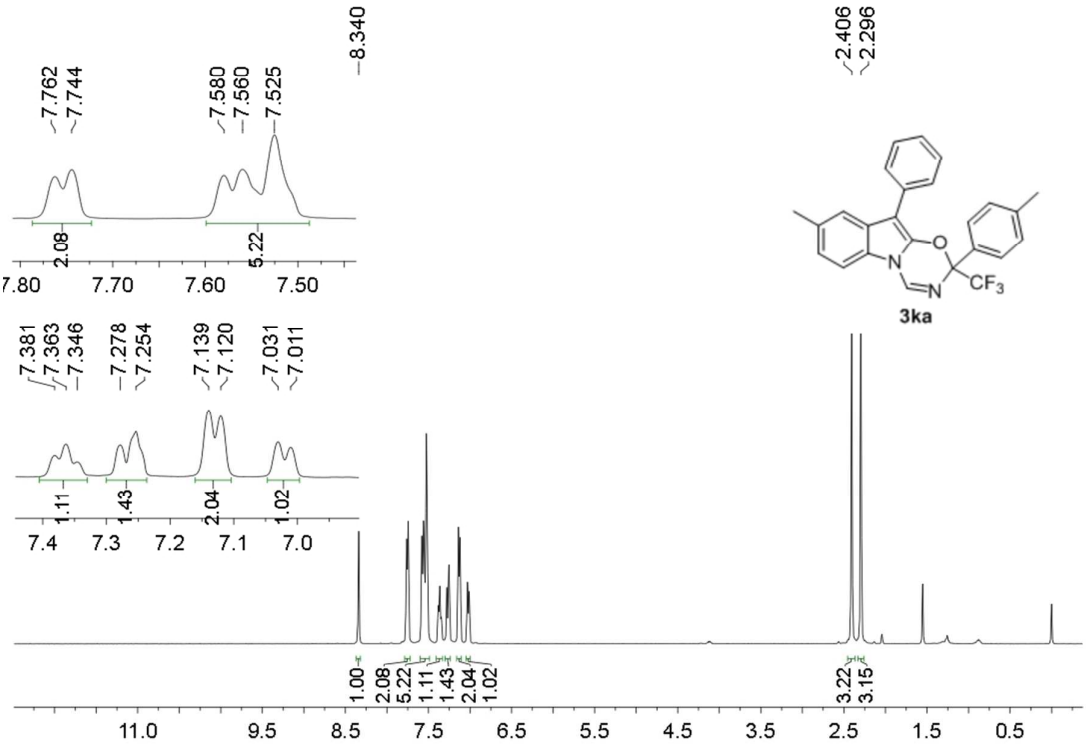
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7.744
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7.560
7.525
2.406
2.296
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7.363
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7.278
7.254
7.139
7.120
7.031
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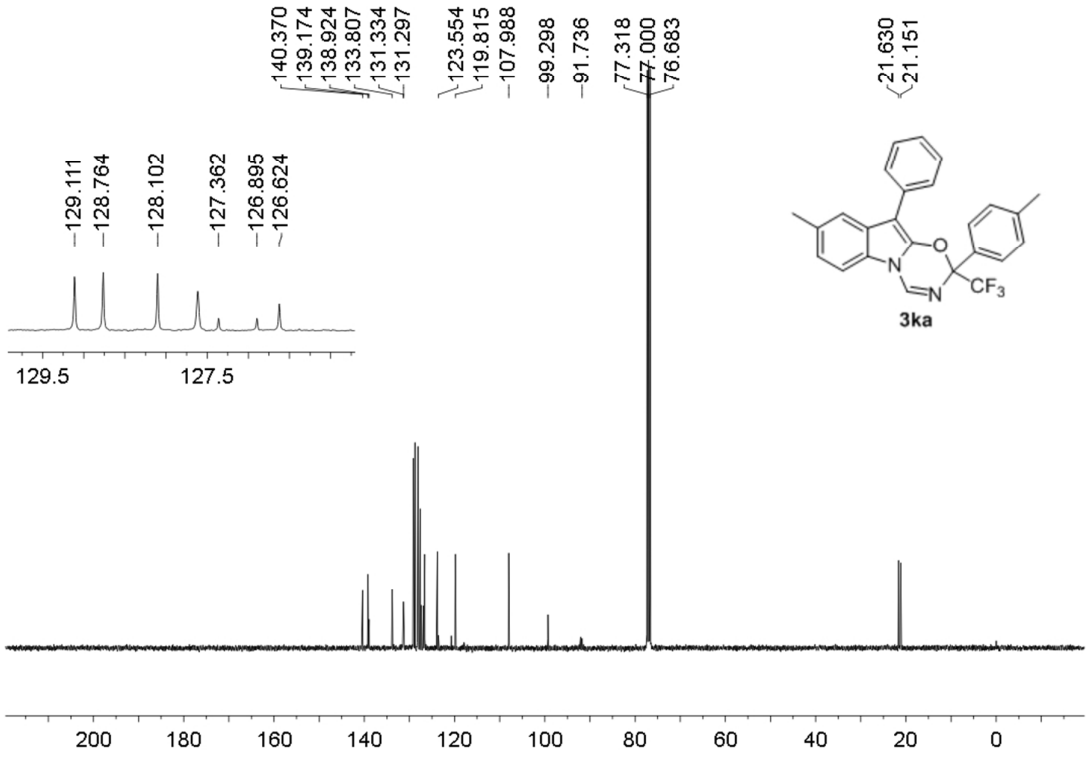
1.00
2.08
5.22
1.11
1.43
2.04
1.02
3.22
3.15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99.298
91.736
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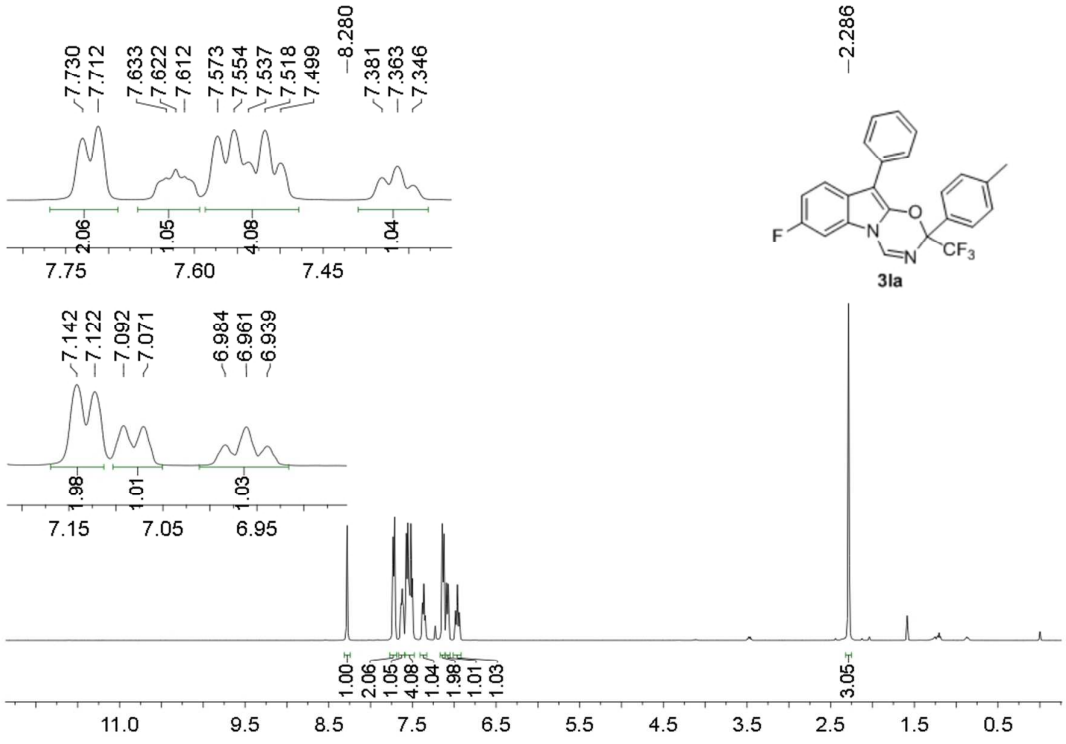
77.000
76.683
21.630
21.151
129.111
128.764
128.102
127.362
126.895
126.624
3ka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7.633
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7.612
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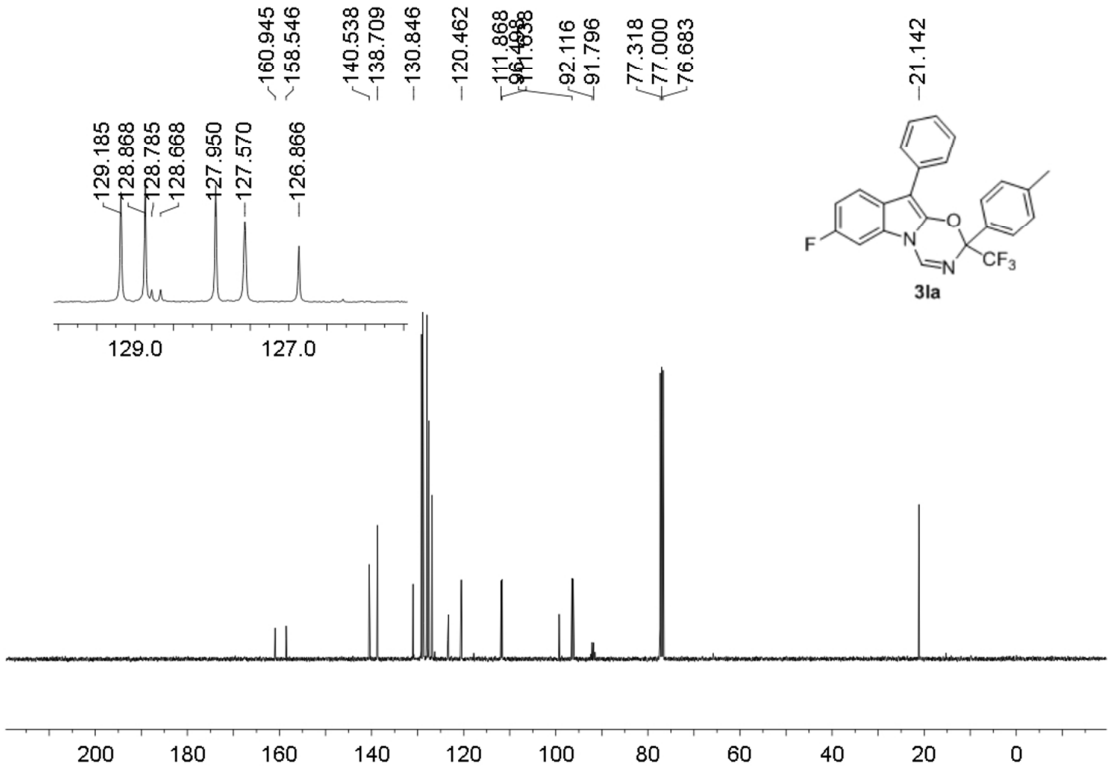
7.499
8.280
7.381
7.363
7.346
2.286
7.142
7.122
7.092
7.071
6.984
6.961
6.939
F
O
N
CF3
3la
1.00
2.06
1.05
4.08
1.04
1.98
1.01
1.03
3.05
11.0
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5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158.546
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127.0
200
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140
120
100
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20
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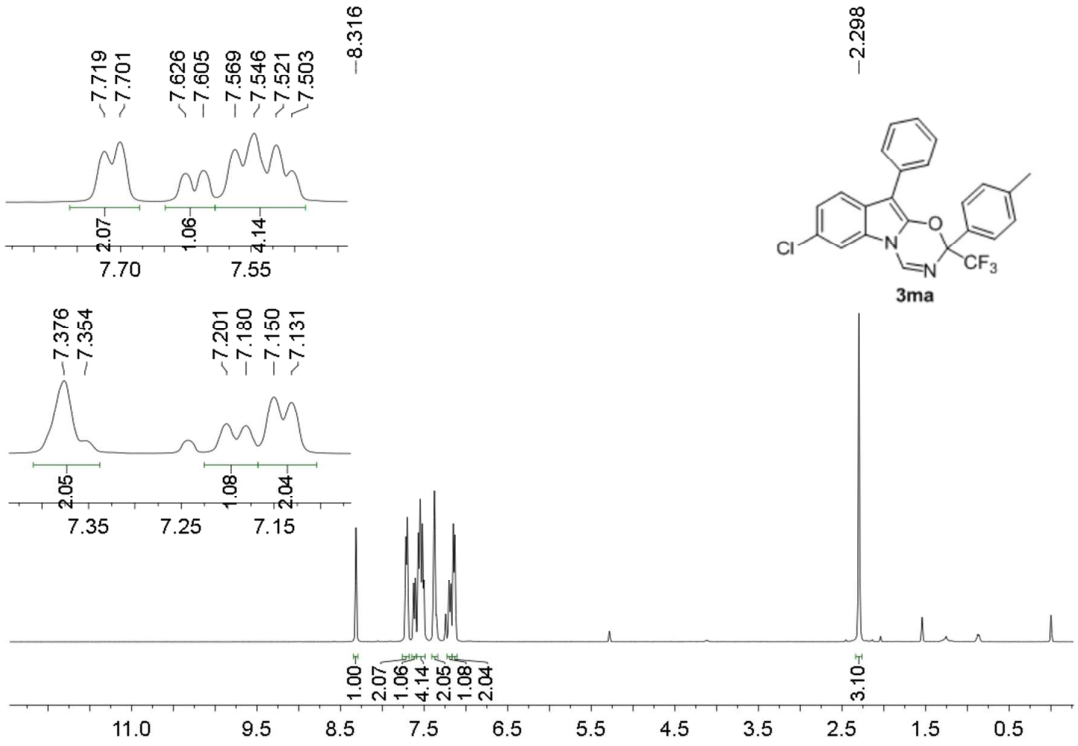
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7.521
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7.354
7.201
7.180
7.150
7.131
Cl
N
O
N
CF3
3ma
1.00
2.07
1.06
4.14
2.05
1.08
2.04
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4.5
3.5
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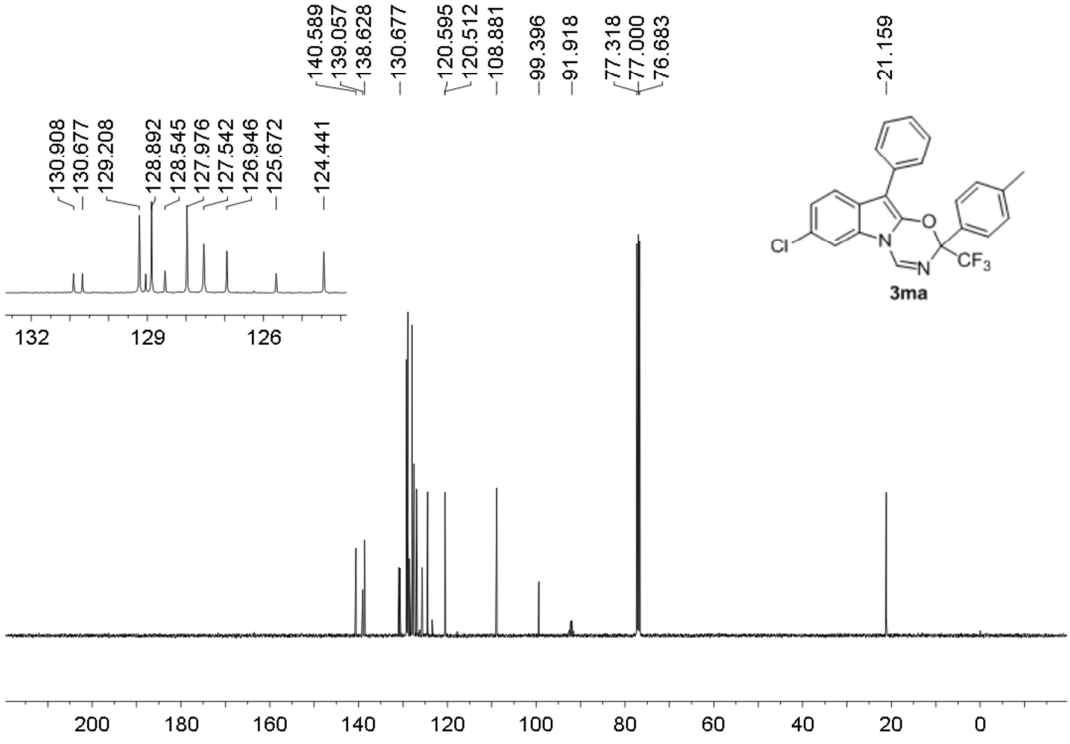
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128.892
128.545
127.976
127.542
126.946
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N
O
N
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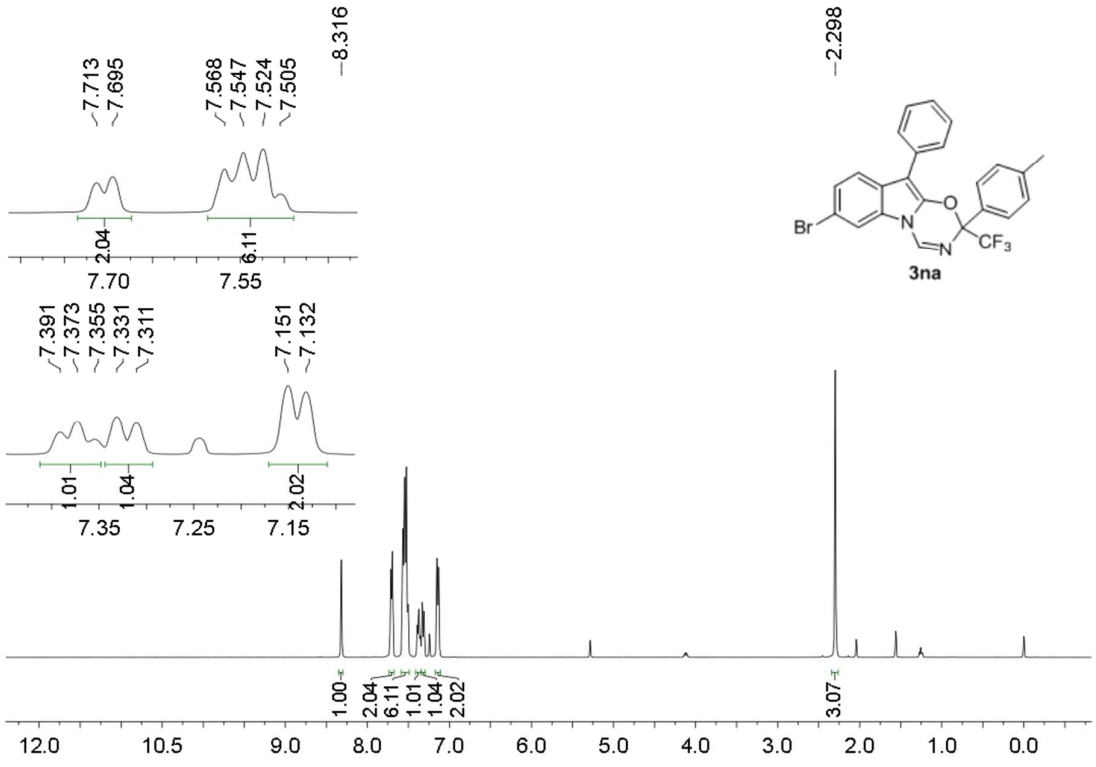
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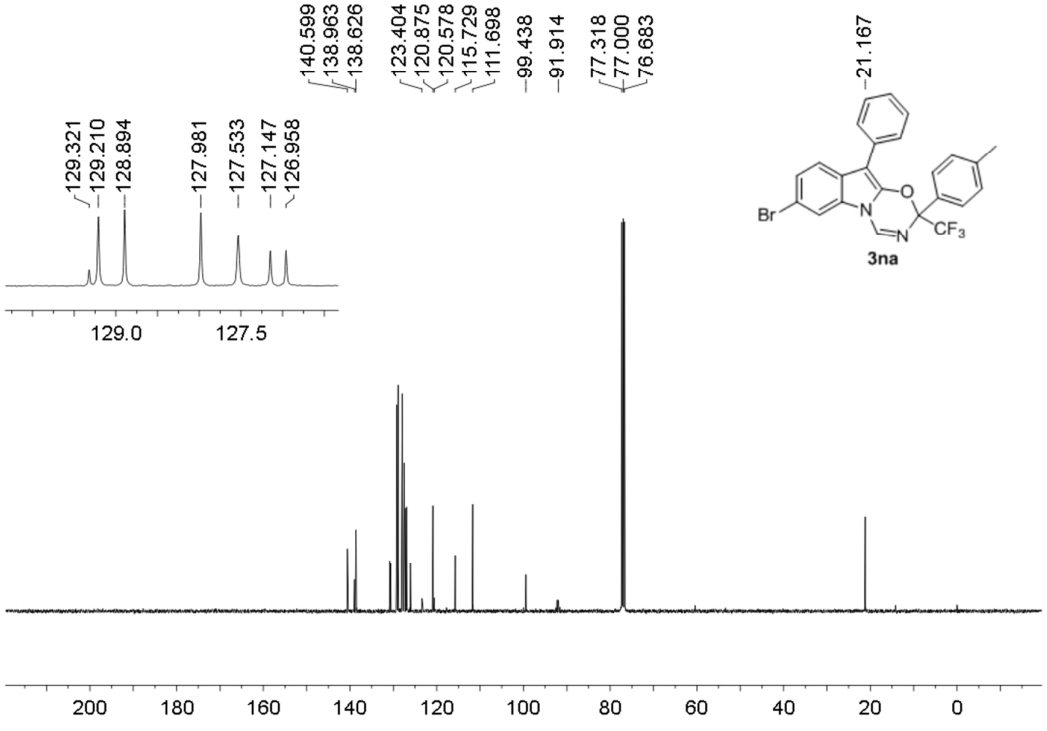
7.695
7.568
7.547
7.524
7.505
2.298
7.391
7.373
7.355
7.331
7.311
7.151
7.132
Br
O
N
N
CF3
3na
2.04
6.11
7.70
7.55
1.01
1.04
2.02
7.35
7.25
7.15
1.00
2.04
6.11
1.01
1.04
2.02
3.07
12.0
10.5
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0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111.698
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91.914
77.318
77.000
76.683
21.167
129.321
129.210
128.894
127.981
127.533
127.147
126.958
Br
O
N
N
CF3
3na
129.0
127.5
200
180
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140
120
100
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60
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20
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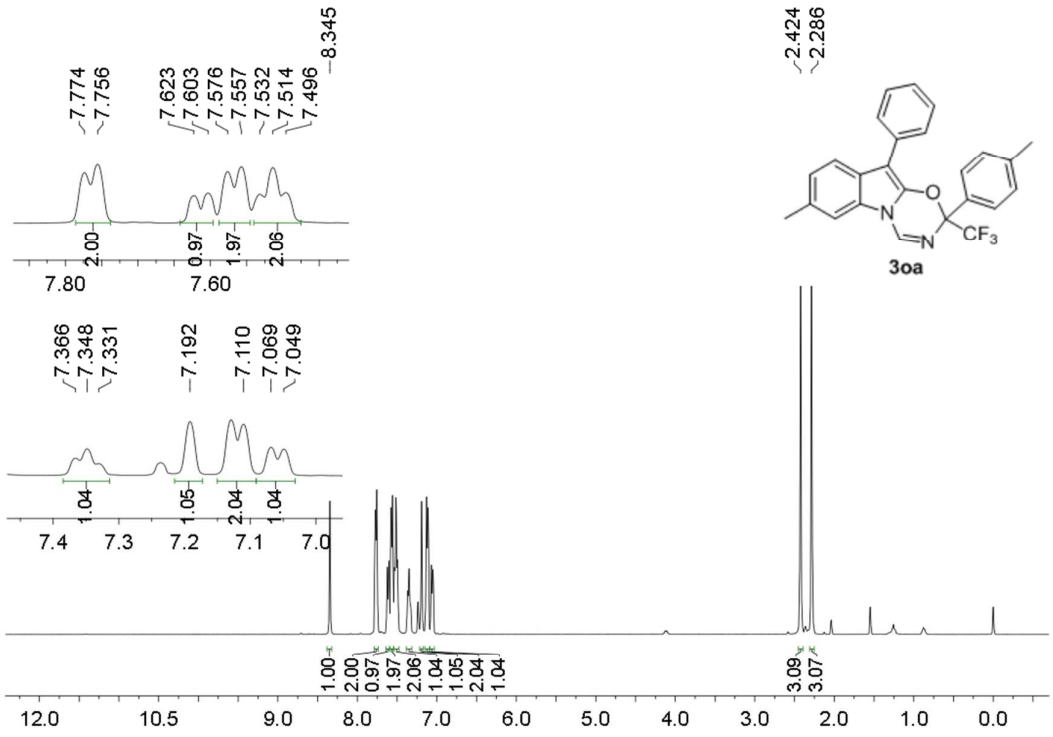
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7.348
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7.192
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7.049
3oa
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6.0
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4.0
3.0
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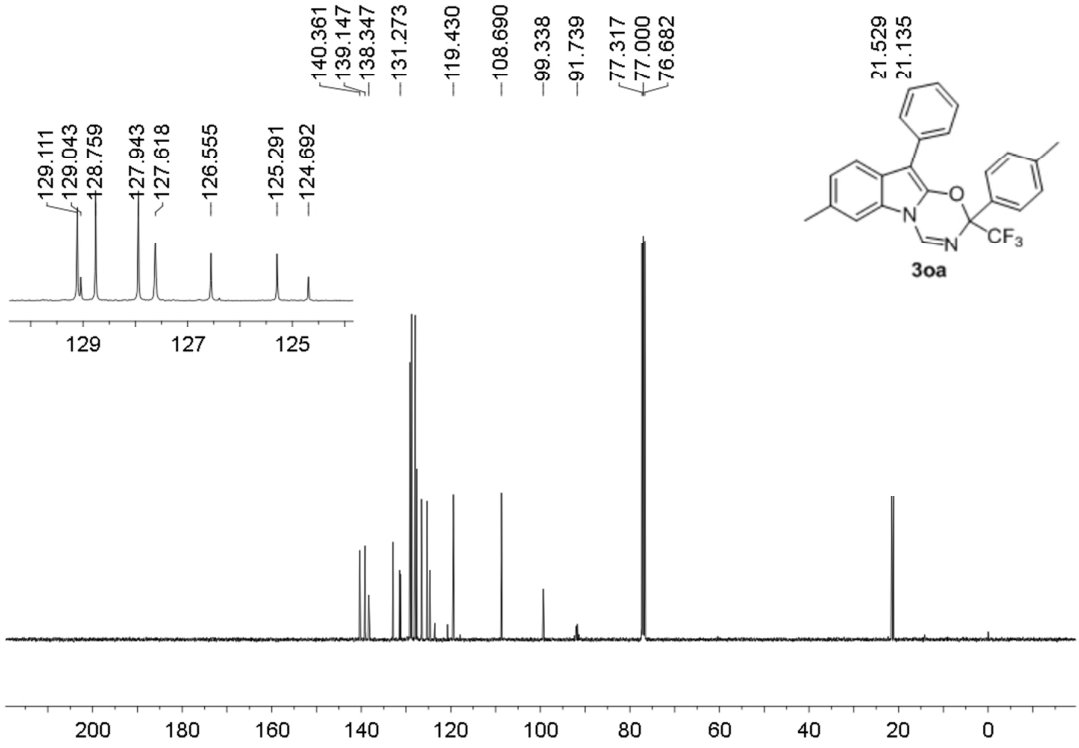
1.0
0.0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21.529
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129.111
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128.759
127.943
127.618
126.555
125.291
124.692
3oa
200
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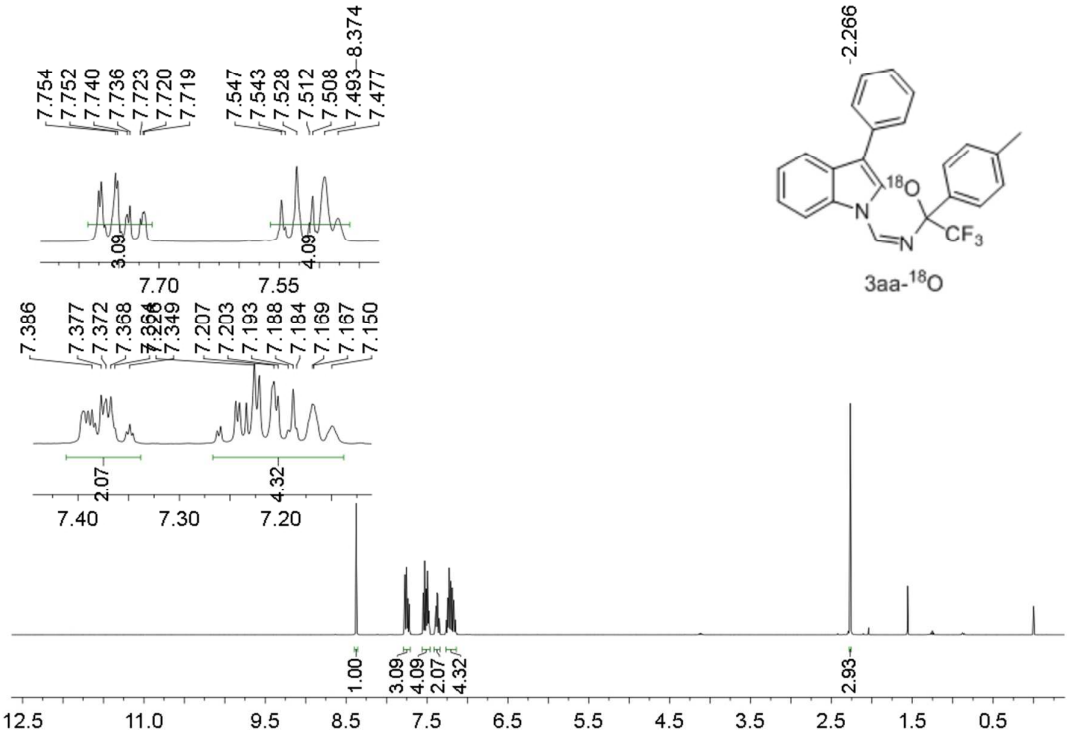
140
120
100
80
60
40
20
0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7.547
7.543
7.528
7.512
7.508
7.493
7.477
8.374
3.09
4.09
7.70
7.55
7.386
7.377
7.372
7.368
7.349
7.207
7.203
7.193
7.188
7.184
7.169
7.167
7.150
2.07
4.32
7.40
7.30
7.20
2.266
18O
N
N
CF3
3aa-18O
1.00
3.09
4.09
2.07
4.32
2.93
12.5
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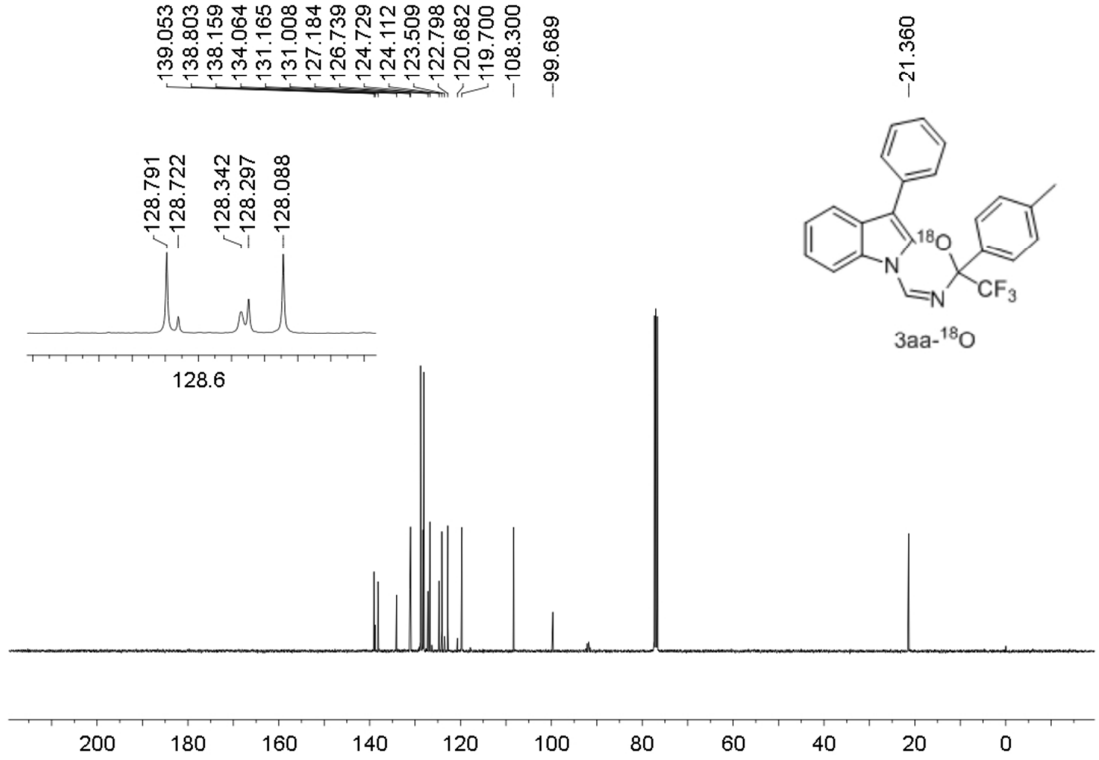
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5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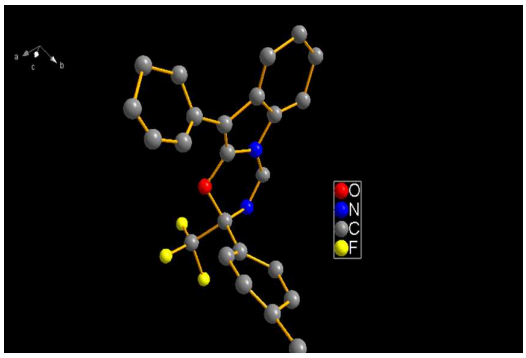
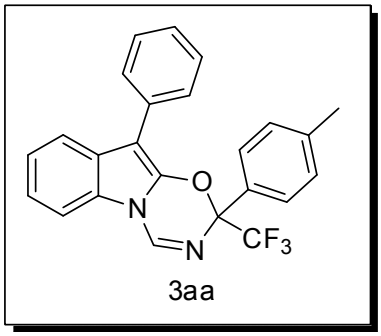
138.803
138.159
134.064
131.165
131.008
127.184
126.739
124.729
124.112
123.509
122.798
120.682
119.700
108.300
99.689
128.791
128.722
128.342
128.297
128.088
128.6
21.360
18O
N
N
CF3
3aa-18O
200
180
160
140
120
100
80
60
40
20
0

V. Crystal Data





Crystal data:	
Empirical formula	$C_{24}H_{17}F_3N_2O$
Formula weight	1699.70
Crystal system	Triclinic
Space group	-P 1
a (Å)	10.3304(12)
b (Å)	17.890(2)
c (Å)	23.784(3)
α (deg)	96.034(5)
β (deg)	99.172(5)
γ (deg)	99.186(5)
Volume ($Å^3$)	4245.1(9)
Z	2
Calculated density (mg/m^3)	1.330
Absorption coefficient (mm^{-1})	0.101
F(000)	1764
Theta range for data collection (deg)	2.351 to 28.275
Reflections collected/unique	83277/ 9757
Goodness-of-fit on F^2	1.041
Final R indices [$I > 2\sigma(I)$]	R1= 0.0729, WR2 = 0.1636
R indices (all data)	R1= 0.1776, WR2 = 0.2102