Supporting Information

for

Experimental and Computational Evidences on Gold-Catalyzed Regioselective Hydration of Phthalimido-Protected Propargylamines: An Entry to β-Amino Ketones.

Vincenzo Marsicano,[a,b] Antonio Arcadi,[a] Massimiliano Aschi, [a] and Véronique Michelet*[b]*

[a] *Dipartimento di Scienze Fisiche e Chimiche Università degli Studi di L'Aquila; Via Vetoio, 67100 Coppito (AQ), Italy*

[b] *University Côte d'Azur, Institut de Chimie de Nice, UMR 7272 CNRS, Parc Valrose, Faculté des Sciences, 06100 Nice, France*

CONTENTS

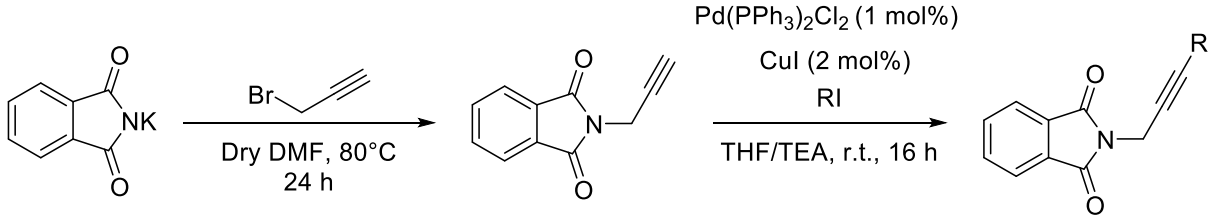
I. General Methods and Materials

Unless otherwise stated, commercial reagents and solvents were used without further purification. Solvents for chromatography [petroleum ether (PE), ethyl acetate (EtOAc), chloroform ($CHCl_3$) and acetone were used as received without further purification. Reactions were monitored by analytical thin layer chromatography (TLC), which was performed on 0.20-mm pre-coated silica plates (Kieselgel 60, F254; Macherey-Nagel GmbH & Co. KG, Düren, Germany). Products were purified by flash chromatography on 200-300 mesh silica gels, SiO_2. Solvents were freshly distilled [tetrahydrofuran (THF) was distilled from sodium/benzophenone ketyl]. NMR spectra (^1H, ^{13}C, and ^{19}F NMR spectra) were recorded on a Bruker Avance 400 MHz spectrometer (Bruker, Rheinstetten, Germany). All NMR spectra were recorded in $CDCl_3$ at room temperature (20 ± 3 °C). All chemical shifts are quoted in parts per million downfield from tetramethylsilane (TMS) as an internal standard. The peak patterns are indicated as follows: s, singlet; d, doublet; t, triplet; m, multiplet; q, quartet. The coupling constants, J, are reported in Hertz [Hz] and result from averaging the experimentally found values. ^{13}C and ^{19}F spectra were recorder with complete proton decoupling. Analytical GC/MS analyses were performed on a Shimdzu QP2010S- MS chromatograph (EI, 70 eV), equipped with an SLB-5ms capillary column (thickness 0.25 mm, length 30 m, and inside diameter 0.25 mm). High resolution mass spectroscopy (HRMS) analyses for new compounds were performed by Institut de Chimie de Nice using a Thermo Vanquish UHPLC-Q-Exactive Focus Mass Spectrometer equipped with H-ESI source operated in a positive mode.

The compounds **1a**, **1c**, **1i**, **1j**, **1k**, **1l, 1n, 3, 6, 7** and **8** have been obtained as already reported and their ^1H-NMR spectra are in accordance with those reported in literature. [1,2,3,4,5,6]

II. General Procedure for the Synthesis of N-propargylphthalimide Derivatives (1a-l) and Spectroscopic Characterization

General procedure for the synthesis of N-propargylphthalimide derivatives (1a-i, m) [1]

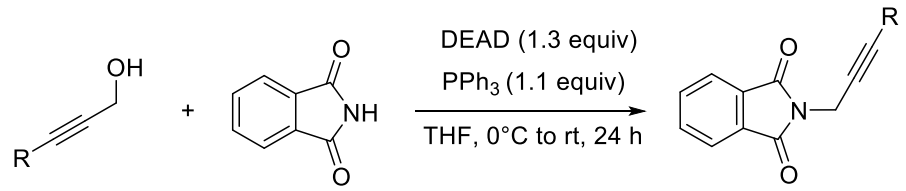


Step 1: To a stirred solution of potassium phthalimide (27 mmol) in dry DMF (40 mL) under nitrogen atmosphere at room temperature, propargyl bromide (80%) (32.4 mmol) was added and the resulting solution was heated to 80°C. The reaction mixture was maintained at 80°C for 24 hours and cooled to room temperature. The reaction mass was added to ice cold water and stirred for an additional hour. The obtained solid was filtered and dissolved in dichloromethane. The dichloromethane solution was dried using $MgSO_4$ and the organic layer was evaporated under high vacuum. N-propargyl phthalimide 1n was obtained as a white solid

in 64% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95-7.82 (m, 2H), 7.81-7.68 (m, 2H), 4.47 (d, J = 2.5 Hz, 2H), 2.24 (t, J = 2.5 Hz, 1H).

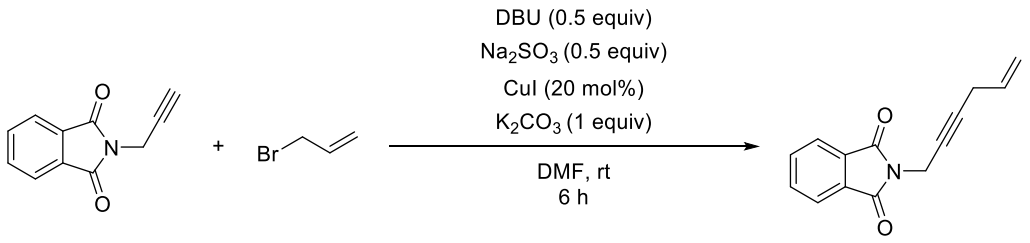
Step 2: To a stirring solution of *N*-propargyl phthalimide (10.8 mmol) in dry THF (15 mL), anhydrous triethylamine (15 mL), iodoaryl derivative (14.04 mmol, 1.30 equivalents) and $PdCl_2(PPh_3)_2$ (1 mol%) were added. After stirring for 15 min, CuI (2 mol%) was added and the reaction was stirred at room temperature overnight. After completion, as monitored by TLC and GC, the reaction mass was filtered through Celite bed, washed with ethyl acetate and the filtrate was evaporated under reduced pressure. The crude was purified by column chromatography over silica gel using PE/AcOEt 8:2.

General procedure for the synthesis of 1j-k [3]



To a solution of propargyl alcohol (4.46 mmol) in THF (10 mL) at 0°C were added triphenylphosphine (4.9 mmol), phthalimide (4.9 mmol) and DEAD (5.79 mmol). The reaction mixture was then stirred at room temperature for 24h. When the reaction was complete (as monitored by TLC), the solvent was evaporated and the triphenylphosphine oxide precipitated by addition of a mixture of PE/Et_2O 1:1 (40 mL). The precipitate was filtered through a plug of Celite and the solvent was evaporated under reduced pressure to afford a crude residue which was purified by column chromatography over silica gel with mixtures of PE/AcOEt from 98:2 to 9:1.

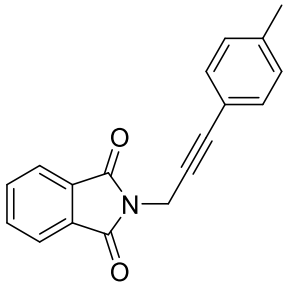
General procedure for the synthesis of 2-(hex-5-en-2-yn-1-yl)isoindoline-1,3-dione (1l) [4]



A mixture of propargyl phthalimide (3.78 mmol), allyl bromide (5.67 mmol), Na_2SO_3 (1.89 mmol), K_2CO_3 (3.78 mmol), DBU (2 mmol), and CuI (0.756 mmol) was stirred at room temperature in DMF (3 mL) for 4 h. The solution was then diluted with Et_2O (70 mL) and washed with H_2O (25 mL × 5). The organic phase was dried over dry $MgSO_4$, filtered, and evaporated, obtaining the desired product as a white solid in 56% of yield.

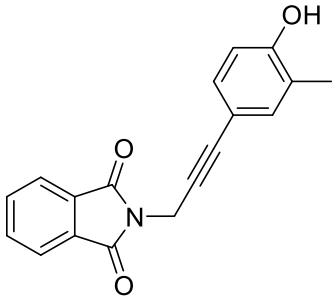
Spectroscopic characterization of new *N*-propargylphthalimide derivatives

2-(3-(*p*-Tolyl)prop-2-yn-1-yl)isoindoline-1,3-dione (1b):



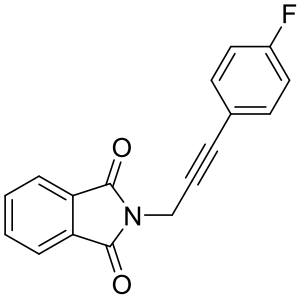
Pale brown solid (51% yield, 800 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 (dd, *J* = 5.5, 3.0 Hz, 2H), 7.74 (dd, *J* = 5.5, 3.0 Hz, 2H), 7.31 (d, *J* = 7.9 Hz, 2H), 7.07 (d, *J* = 7.9 Hz, 2H), 4.67 (s, 2H), 2.32 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 167.2, 138.6, 134.1, 132.2, 131.8, 129.0, 123.6, 119.3, 83.1, 81.9, 27.9, 21.5; GC-MS (EI, 70 eV): m/z(%) = 276 (43), 275 (M^+, 100), 247 (88), 246 (47), 233 (27), 232 (79), 218 (27), 204 (48), 115 (58), 102 (37).

2-(3-(4-hydroxy-3-methylphenyl)prop-2-yn-1-yl)isoindoline-1,3-dione (1d):



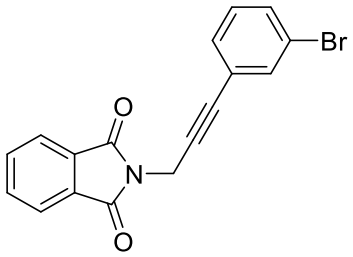
Pale brown solid (39% yield, 310 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 (dd, *J* = 5.4, 3.0 Hz, 2H), 7.74 (dd, *J* = 5.4, 3.0 Hz, 2H), 7.23 - 7.19 (m, 1H), 7.13 (dd, *J* = 8.2, 2.1 Hz, 1H), 6.66 (d, *J* = 8.2 Hz, 1H), 4.65 (s, 2H), 2.18 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 167.3, 154.3, 134.8, 134.2, 132.2, 131.1, 123.9, 123.5, 114.9, 114.4, 83.0, 28.0, 15.5; GC-MS (EI, 70 eV): m/z(%) = 291 (M^+, 100).

2-(3-(4-Fluorophenyl)prop-2-yn-1-yl)isoindoline-1,3-dione (1e):



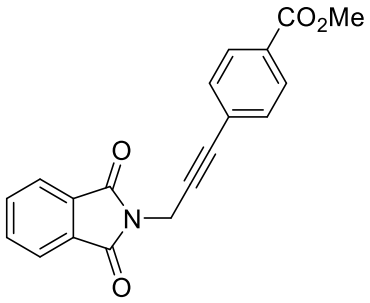
White solid (35% yield, 112 mg); ^{1}H NMR (400 MHz, CDCl3) δ 7.90 (dd, *J* = 5.6, 3.0 Hz, 2H), 7.75 (dd, *J* = 5.6, 3.0 Hz, 2H), 7.40 (dd, *J* = 8.8, 5.4 Hz, 2H), 6.97 (t, *J* = 8.8 Hz, 2H), 4.67 (s, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 167.2, 162.6 (d, *J* = 249.6 Hz), 134.2, 133.9 (d, *J* = 8.4 Hz), 132.1, 123.6, 118.4, 115.5 (d, *J* = 22.1 Hz), 82.4, 82.0, 27.8; GC-MS (EI, 70 eV): m/z(%) = 280 (28), 279 (M^+, 100), 252 (14), 251 (75), 250 (74), 249 (24), 223 (18), 222 (35), 221 (21), 196 (13).

2-(3-(3-Bromophenyl)prop-2-yn-1-yl)isoindoline-1,3-dione (1f):



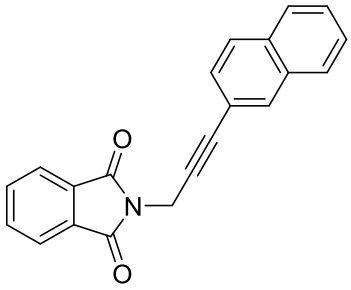
Brown solid (95% yield, 870 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 (dd, *J* = 5.5, 3.1 Hz, 2H), 7.75 (dd, *J* = 5.5, 3.1 Hz, 2H), 7.57 (t, *J* = 1.6 Hz, 1H), 7.43 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.34 (dd, *J* = 8.0, 1.1 Hz, 1H), 7.14 (t, *J* = 8.0 Hz, 1H), 4.67 (s, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 167.1, 134.7, 134.2, 132.1, 131.7, 130.5, 129.7, 124.3, 123.6, 122.0, 84.0, 81.5, 27.8; GC-MS (EI, 70 eV): m/z(%) = 342 (30), 341 (100), 340 (40), 339 (M^+, 93), 313 (32), 312 (29), 311 (36), 310 (22), 233 (15), 232 (51), 206 (14), 205 (43), 204 (73), 203 (44), 202 (20), 177 (15), 176 (25), 114 (13), 113 (29), 102 (23).

Methyl 4-(3-(1,3-dioxoisoindolin-2-yl)prop-1-yn-1-yl)benzoate (1g):



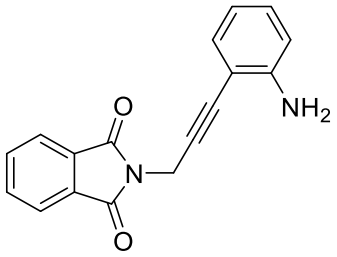
White solid (78% yield, 670 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 - 7.92 (m, 2H), 7.91 (dd, *J* = 5.5, 3.0 Hz, 2H), 7.76 (dd, *J* = 5.5, 3.0 Hz, 2H), 7.50 - 7.44 (m, 2H), 4.70 (s, 2H), 3.90 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 167.1, 166.5, 134.3, 132.1, 131.9, 129.8, 129.9, 127.0, 123.6, 85.6, 82.3, 52.2, 27.8; GC-MS (EI, 70 eV): m/z(%) = 320 (43), 319 (M^+, 100), 291 (46), 232 (58), 204 (39), 104 (32).

2-(3-(Naphthalen-2-yl)prop-2-yn-1-yl)isoindoline-1,3-dione (1h):



Pale brown solid (25% yield, 298 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 - 7.94 (m, 1H), 7.91 (dd, *J* = 5.5, 3.1 Hz, 2H), 7.80 - 7.71 (m, 5H), 7.49 - 7.43 (m, 3H), 4.73 (s, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 167.2, 134.2, 132.9, 132.8, 132.2, 132.0, 128.5, 127.9, 127.8, 127.7, 126.8, 126.5, 123.6, 119.6, 83.3, 83.0, 28.0; GC-MS (EI, 70 eV): m/z(%) = 311 (M^+, 100).

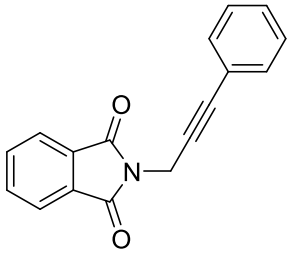
2-(3-(2-aminophenyl)prop-2-yn-1-yl)isoindoline-1,3-dione (1m):



Yellow solid (77% yield, 577 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 (dd, *J* = 5.4, 3.1 Hz, 2H), 7.74 (dd, *J* = 5.4, 3.1 Hz, 2H), 7.23 (dd, *J* = 7.7, 1.6 Hz, 1H), 7.09 (td, *J* = 8.2, 1.6 Hz, 1H), 6.64 (ddd, *J* = 8.2, 7.7, 1.6 Hz, 2H), 4.72 (s, 2H), 4.30 (s, 2H, broad); ^{13}C NMR (101 MHz, $CDCl_3$) δ 167.2, 148.7, 134.2, 132.2, 132.1, 130.0, 123.6, 117.6, 114.2, 106.7, 87.9, 80.3, 28.3; GC-MS (EI, 70 eV): m/z(%) = 277 (20), 276 (M^+, 100), 275 (26), 131 (16), 130 (47), 129 (12).

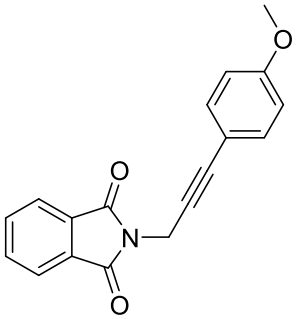
^{1}H NMR data of known *N*-propargylphthalimide derivatives:

2-(3-phenylprop-2-yn-1-yl)isoindoline-1,3-dione (1a):



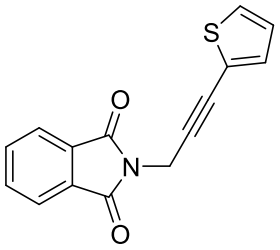
Light brown solid (88% yield, 2.48 g); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 (dd, *J* = 5.5, 3.1 Hz, 2H), 7.74 (dd, *J* = 5.4, 3.1 Hz, 2H), 7.42 (dd, *J* = 7.5, 2.1 Hz, 2H), 7.34-7.12 (m, 3H), 4.68 (s, 2H).

2-(3-(4-methoxyphenyl)prop-2-yn-1-yl)isoindoline-1,3-dione (1c):



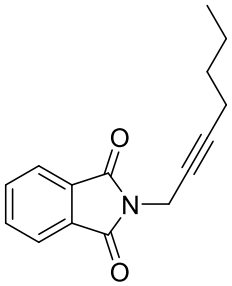
White solid (51% yield, 800 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 (dd, J = 5.5, 3.1 Hz, 2H), 7.74 (dd, J = 5.5, 3.0 Hz, 2H), 7.38 -7.31 (m, 2H), 6.82 -6.76 (m, 2H), 4.66 (s, 2H), 3.79 (s, 3H).

2-(3-(thiophen-2-yl)prop-2-yn-1-yl)isoindoline-1,3-dione (1i):



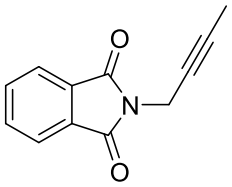
Brown solid (59% yield, 481 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92-7.87 (m, 2H), 7.78-7.72 (m, 2H), 7.23 (dd, J = 5.1, 1.2 Hz, 1H), 7.20 (dd, J = 3.7, 1.2 Hz, 1H), 6.93 (dd, J = 5.1, 3.7 Hz, 1H), 4.70 (s, 2H).

2-(hept-2-yn-1-yl)isoindoline-1,3-dione (1j):



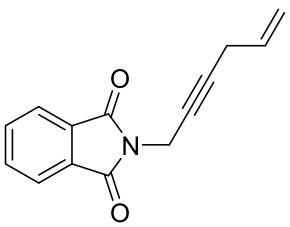
White solid (80% yield, 856 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 (dd, *J* = 5.4, 3.1 Hz, 2H), 7.73 (dd, *J* = 5.4, 3.1 Hz, 2H), 4.43 (t, *J* = 2.3 Hz, 2H), 2.14 (tt, *J* = 7.2, 2.3 Hz, 2H), 1.56-1.26 (m, 6H), 0.87 (t, *J* = 7.2 Hz, 3H).

2-(but-2-yn-1-yl)isoindoline-1,3-dione (1k):



White solid (27% yield, 390 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 (dd, J = 5.5, 3.1 Hz, 2H), 7.73 (dd, J = 5.5, 3.1 Hz, 2H), 4.41 (d, J = 2.4 Hz, 2H), 1.78 (t, J = 2.4 Hz, 3H).

2-(hex-5-en-2-yn-1-yl)isoindoline-1,3-dione (1l):



White solid (58% yield, 475 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 -7.86 (m, 2H), 7.77-7.70 (m, 2H), 5.76 (ddt, J = 17.0, 9.9, 5.3 Hz, 1H), 5.29 (dq, J = 17.0, 1.8 Hz, 1H), 5.09 (dq, J = 9.9, 1.8 Hz, 1H), 4.47 (t, J = 2.3 Hz, 2H), 2.94 (dt, J = 5.3, 2.0 Hz, 2H).

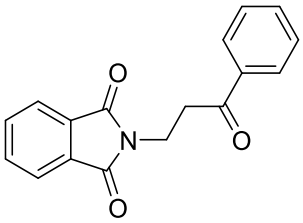
III. General Procedure for the Synthesis of Ketones (2a-l) and Spectroscopic Characterization

General procedure for the synthesis of Ketones (2a-l)

To a stirring solution of phthalimidic derivative **1** (0.191 mmol) in CH_3CN (3 mL), 0.3 mL of H_2O and $IPrAuNTf_2$ (5 mol%) were added. The reaction was stirred at 80°C for 24 h. Then, a saturated aqueous solution of NH_4Cl was added. The organic layer was separated and the aqueous phase was extracted with Et_2O. The combined organic layers were dried over anhydrous $MgSO_4$, filtered and concentrated under reduced pressure. The obtained crude was purified by column chromatography over silica gel using PE/AcOEt 9:1.

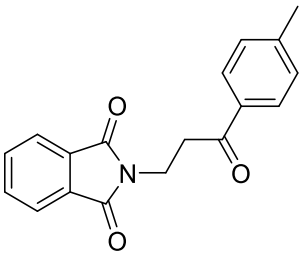
Spectroscopic characterization of new derivatives

2-(3-Oxo-3-phenylpropyl)isoindoline-1,3-dione (2a):



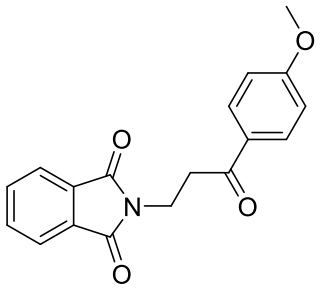
White solid (86% yield, 46 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94 (dt, *J* = 7.0, 1.4 Hz, 2H), 7.85 (dd, *J* = 5.4, 3.1 Hz, 2H), 7.72 (dd, *J* = 5.4, 3.1 Hz, 2H), 7.59 - 7.53 (m, 1H), 7.45 (dd, *J* = 8.4, 7.0 Hz, 2H), 4.15 (dd, *J* = 8.0, 6.8 Hz, 2H), 3.43 (dd, *J* = 8.0, 6.8 Hz, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 197.4, 168.2, 136.4, 134.0, 133.4, 132.1, 128.7, 128.1, 123.3, 36.8, 33.6; HRMS (H-ESI): m/z calculated for $C_{17}H_{14}NO_3$: $[M+H]^+$ 280.0974, Found: 280.0965.

2-(3-oxo-3-(p-Tolyl)propyl)isoindoline-1,3-dione (2b):



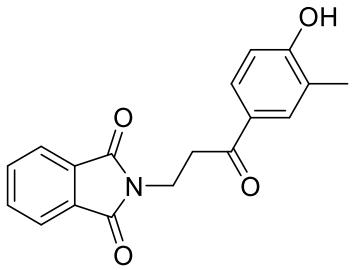
Pale brown solid (71% yield, 38 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88-7.81 (m, 4H), 7.72 (dd, *J* = 5.4, 3.1 Hz, 2H), 7.26-7.21 (m, 2H), 4.14 (dd, *J* = 8.0, 6.9 Hz 2H), 3.40 (dd, *J* = 8.0, 6.9 Hz, 2H), 2.40 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 197.0, 168.2, 144.2, 134.0, 132.2, 129.4, 128.2, 123.3, 36.7, 33.7, 21.7: HRMS (H-ESI): m/z calculated for $C_{18}H_{16}NO_3$: $[M+H]^+$ 294.1130, Found: 294.1120.

2-(3-(4-Methoxyphenyl)-3-oxopropyl)isoindoline-1,3-dione (2c):



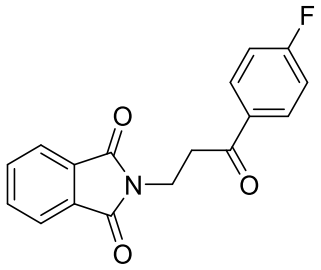
White solid (94% yield, 50 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92 (d, *J* = 8.9 Hz, 2H), 7.85 (dd, *J* = 5.4, 3.0 Hz, 2H), 7.72 (dd, *J* = 5.4, 3.0 Hz, 2H), 6.92 (d, *J* = 8.9 Hz, 2H), 4.13 (dd, *J* = 7.9, 6.8 Hz, 2H), 3.86 (s, 3H), 3.37 (dd, *J* = 7.9, 6.8 Hz, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.9, 168.2, 163.7, 134.0, 132.1, 130.3, 129.6, 123.3, 113.8, 55.5, 36.5, 33.7; HRMS (H-ESI): m/z calculated for $C_{18}H_{16}NO_4$: $[M+H]^+$ 310.1079, Found: 310.1066.

2-(3-(4-Hydroxy-3-methylphenyl)-3-oxopropyl)isoindoline-1,3-dione (2d):



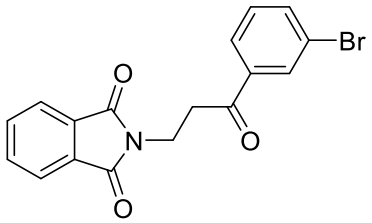
White solid (72% yield, 38 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 (dd, *J* = 5.4, 3.1 Hz, 2H), 7.77 - 7.66 (m, 3H), 7.68 (dd, *J* = 8.4, 2.6 Hz, 1H), 6.79 (d, *J* = 8.4 Hz, 1H), 4.13 (dd, *J* = 7.9, 6.8 Hz, 2H), 3.35 (dd, *J* = 7.9, 6.8 Hz, 2H), 2.25 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 193.5, 168.3, 167.5, 158.6, 134.4, 134.0, 132.1, 131.9, 131.6, 128.2, 123.7, 123.3, 114.8, 36.5, 33.8, 15.7; HRMS (H-ESI): m/z calculated for $C_{18}H_{16}NO_4$: $[M+H]^+$ 310.1079, Found: 310.1069.

2-(3-(4-Fluorophenyl)-3-oxopropyl)isoindoline-1,3-dione (2e):



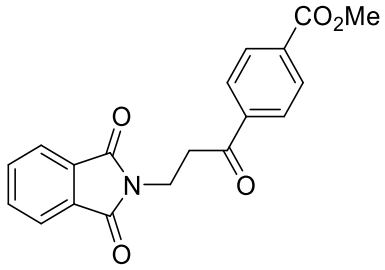
White solid (88% yield, 47 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 - 7.95 (m, 2H), 7.86 (dd, *J* = 5.5, 3.1 Hz, 2H), 7.73 (dd, *J* = 5.5, 3.1 Hz, 2H), 7.16 - 7.09 (m, 2H), 4.14 (dd, *J* = 8.0, 6.8 Hz, 2H), 3.40 (dd, *J* = 8.0, 6.8 Hz, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.7, 168.2, 165.92 (d, *J* = 255.2 Hz), 134.1, 132.9 (d, *J* = 3.0 Hz), 132.1, 130.8, 130.7 (d, *J* = 9.4 Hz), 123.3, 115.8 (d, *J* = 22.0 Hz), 36.8, 33.5; HRMS (H-ESI): m/z calculated for $C_{17}H_{13}FNO_3$: $[M+H]^+$ 298.0879, Found: 298.0871.

2-(3-(3-bromophenyl)-3-oxopropyl)isoindoline-1,3-dione (2f):



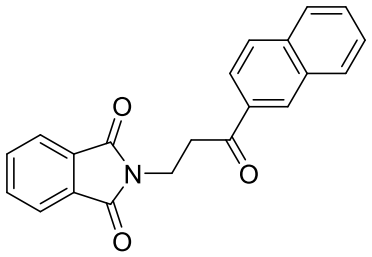
Brown solid (70% yield, 37 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (t, *J* = 1.8 Hz, 1H), 7.88 - 7.84 (m, 3H), 7.73 (dd, *J* = 5.5, 3.1 Hz, 2H), 7.69 (dq, *J* = 8.0, 1.0 Hz, 1H), 7.34 (t, *J* = 8.0 Hz, 1H), 4.14 (dd, *J* = 7.9, 6.8 Hz, 2H), 3.40 (dd, *J* = 7.9, 6.8 Hz, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 196.0, 168.2, 138.1, 136.3, 134.1, 132.1, 131.2, 130.3, 126.6, 123.6, 123.4, 123.1, 36.9, 33.4; HRMS (H-ESI): m/z calculated for $C_{17}H_{13}BrNO_3$: $[M+H]^+$ 358.0079, Found: 358.0070.

Methyl 4-(3-(1,3-dioxoisoindolin-2-yl)propanoyl)benzoate (2g):



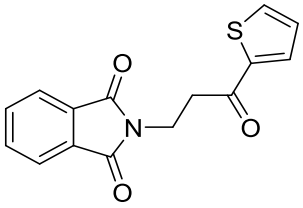
White solid (85% yield, 45 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14 - 8.08 (m, 2H), 8.02 - 7.96 (m, 2H), 7.85 (dd, *J* = 5.5, 3.1 Hz, 2H), 7.73 (dd, *J* = 5.5, 3.1 Hz, 2H), 4.15 (dd, *J* = 7.9, 6.8 Hz, 2H), 3.95 (s, 3H), 3.46 (dd, *J* = 7.9, 6.8 Hz, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 196.9, 168.2, 166.1, 139.5, 134.1, 134.0, 132.1, 129.9, 128.0, 123.3, 52.5, 37.2, 33.4; HRMS (H-ESI): m/z calculated for $C_{19}H_{16}NO_5$: $[M+H]^+$ 338.1028, Found: 338.1016.

2-(3-(Naphthalen-2-yl)-3-oxopropyl)isoindoline-1,3-dione (2h):



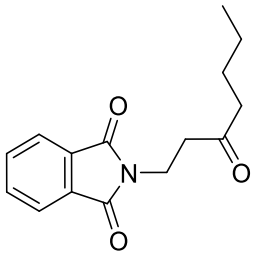
Pale brown solid (85% yield, 45 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.49 – 8.43 (m, 1H), 8.01 (dd, *J* = 8.6, 1.8 Hz, 1H), 7.94 (dd, *J* = 8.1, 1.4 Hz, 1H), 7.89 (d, *J* = 8.6 Hz, 2H), 7.86 (dd, *J* = 5.4, 3.1 Hz, 2H), 7.72 (dd, *J* = 5.4, 3.1 Hz, 2H), 7.57 (dtd, *J* = 24.6, 7,4, 1.4 Hz, 2H), 4.21 (dd, *J* = 8.0, 6.8 Hz, 2H), 3.57 (dd, *J* = 8.0, 6.8 Hz, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 197.3, 168.3, 135.7, 134.0, 133.8, 132.5, 132.1, 129.9, 129.6, 128.6, 127.8, 126.9, 123.6, 123.3, 36.9, 33.7; HRMS (H-ESI): m/z calculated for $C_{21}H_{16}NO_3$: $[M+H]^+$ 330.1130, Found: 330.1120.

2-(3-Oxo-3-(thiophen-2-yl)propyl)isoindoline-1,3-dione (2i):



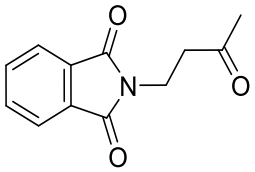
Brown solid (82% yield, 44 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 (dd, *J* = 5.4, 3.1 Hz, 2H), 7.75 - 7.70 (m, 3H), 7.64 (dd, *J* = 4.9, 1.1 Hz, 1H), 7.12 (dd, *J* = 4.9, 3.8 Hz, 1H), 4.13 (dd, *J* = 8.0, 6.8 Hz, 2H), 3.36 (dd, *J* = 8.0, 6.8 Hz, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 190.1, 168.1, 143.6, 134.0, 132.2, 132.1, 128.2, 123.3, 37.5, 33.6; HRMS (H-ESI): m/z calculated for $C_{15}H_{12}NO_3S$: $[M+H]^+$ 286.0538, Found: 286.0529.

2-(3-Oxoheptyl)isoindoline-1,3-dione (2j):



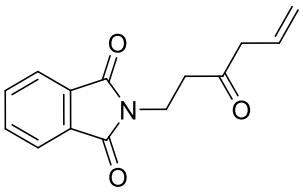
White solid (63% yield, 34 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84 (dd, *J* = 5.4, 3.1 Hz, 2H), 7.71 (dd, *J* = 5.4, 3.1 Hz, 2H), 3.96 (dd, *J* = 7.9, 6.9 Hz, 2H), 2.85 (dd, *J* = 7.9, 6.9 Hz, 2H), 2.43 (t, *J* = 7.5 Hz, 2H), 1.62 - 1.50 (m, 2H), 1.37 - 1.26 (m, 2H), 0.89 (t, *J* = 7.3 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 208.3, 168.1, 134.0, 132.1, 123.3, 42.6, 40.6, 33.1, 25.7, 22.3, 13.8; HRMS (H-ESI): m/z calculated for $C_{15}H_{18}NO_3$: $[M+H]^+$ 260.1287, Found: 260.1279.

2-(3-Oxobutyl)isoindoline-1,3-dione (2k):



White solid (72% yield, 39 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84 (dd, *J* = 5.4, 3.1 Hz, 2H), 7.72 (dd, *J* = 5.4, 3.1 Hz, 2H), 3.96 (dd, *J* = 7.9, 6.9 Hz, 2H), 2.88 (dd, *J* = 7.9, 6.9 Hz, 2H), 2.19 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 205.8, 168.1, 134.0, 132.0, 123.3, 41.6, 33.0, 29.9; HRMS (H-ESI): m/z calculated for $C_{12}H_{11}NO_3$: $[M+H]^+$ 218.0871, Found: 218.0810.

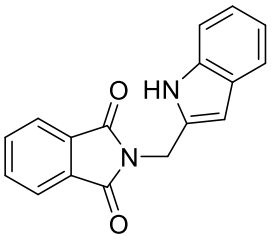
2-(3-Oxohex-5-en-1-yl)isoindoline-1,3-dione (2l):



White solid (54% yield, 29 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84 (dd, *J* = 5.5, 3.0 Hz, 2H), 7.72 (dd, *J* = 5.5, 3.0 Hz, 2H), 5.91 (ddt, *J* = 17.2, 10.2, 7.1 Hz, 1H), 5.23 – 5.10 (m, 2H), 3.96 (dd, *J* = 7.9, 6.9 Hz, 2H), 3.21 (dt, *J* = 7.0, 1.4 Hz,

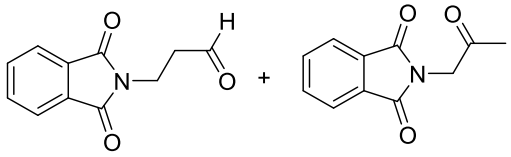
2H), 2.89 (dd, J = 7.9, 6.9 Hz, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 205.8, 168.1, 134.0, 132.1, 129.9, 123.3, 119.4, 47.7, 40.2, 33.0; HRMS (H-ESI): m/z calculated for $C_{14}H_{14}NO_3$: $[M+H]^+$ 244.0974, Found: 244.0965.

2-((1H-indol-2-yl)methyl)isoindoline-1,3-dione (2m):



White solid (52% yield, 26 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 (dd, J = 5.4, 3.0 Hz, 2H), 7.70 (dd, J = 5.4, 3.0 Hz, 2H), 7.55 (dd, J = 8.1, 1.1 Hz, 1H), 7.32 (dd, J = 8.1, 1.1 Hz, 2H), 7.15 (ddd, J = 8.1, 7.0, 1.1 Hz, 1H), 7.06 (ddd, J = 8.1, 7.0, 1.1 Hz, 2H), 6.55 (d, J = 2.1 Hz, 1H), 4.98 (s, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.4, 136.4, 134.3, 132.9, 131.9, 127.7, 123.5, 122.5, 120.8, 119.9, 111.0, 102.7, 34.9; HRMS (H-ESI): m/z calculated for $C_{17}H_{13}N_2O_2$: $[M+H]^+$ 277.0977, Found: 277.0968.

3-(1,3-dioxoisoindolin-2-yl)propanal (2n) and 2-(2oxopropyl)isoindoline-1,3-dione (2n') mixture:

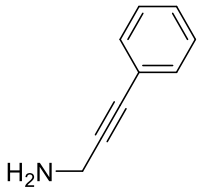


2n **2n'**

2n+**2n'** were obtained as an unresolved mixture (white solid, 66% cumulative yield, 36 mg); **2n**/**2n'** ratio (calculated by NMR) = 2.27/2.89 = 1/1.3; ^{1}H NMR (400 MHz, $CDCl_3$) Signals of **2n** δ 9.83 (s, 1H), 7.86 (m, 2H), 7.74 (m, 2H), 4.04 (t, J = 7.0 Hz, 2H), 2.88 (td, J = 7.0, 1.4 Hz, 2H); Signals of **2n'** δ 7.86 (m, 2H), 7.74 (m, 2H), 4.50 (s, 2H), 2.27 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) Signals of **2n** δ 199.6, 168.0, 134.1, 131.9 123.4, 42.4, 31.7; Signals of **2n'** δ 199.4, 167.7, 134.2, 132.1, 123.6, 47.1, 27.0.

IV. General Procedures for the Synthesis of the other Derivatives and Spectroscopic Characterization

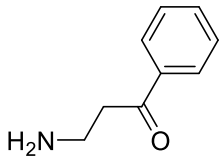
Synthesis of 3-phenylprop-2-yn-1-amine (3)



To a solution of phthalimide **1a** (7,65 mmol, 2 g) in EtOH (60 mL) was added hydrazine hydrate (45,93 mmol, 2,28 mL) drop wise and the resulting mixture was stirred at reflux for 4 hours. After completion of the reaction, as monitored by TLC, the reaction mass was filtered through a plug of Celite, washed with diethyl ether (20 mL) and the solvent was evaporated under reduced pressure. The obtained crude residue was finally purified by column chromatography over silica gel with a mixture of PE/AcOEt 5:5 and then 100% AcOEt, obtaining the product as a pale-yellow oil (624 mg, 62% yield). The spectra are in accordance with the data reported in literature.[**Erreur ! Signet non défini.**]

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48-7.36 (m, 2H), 7.35-7.18 (m, 3H), 3.65 (s, 2H).

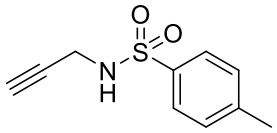
Synthesis of 3-amino-1-phenylpropan-1-one (4a)



To a stirring solution of 2-(3-oxo-3-phenylpropyl)isoindoline-1,3-dione **2a** (2.4 mmol, 0.7 g) in MeOH, ethylenediamine (4.8 mmol, 0.32 mL) was added. The obtained suspension was stirred at room temperature for 1 hour until complete homogenization. After completion (as shown by TLC analysis), the volatiles have been removed by concentration under reduced pressure and the crude has been further purified by column chromatography over silica gel with $CHCl_3$/Acetone 9:1 to give the (3-amino-1-phenylpropan-1-one) **4a** as a yellow oil (0.33 g, 86% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 – 7.93 (m, 2H), 7.68 - 7.56 (m, 1H), 7.52 – 7.45 (m, 2H), 3.79 (q, J = 5.9 Hz, 2H), 3.31 (t, J = 5.9 Hz, 2H). [7]

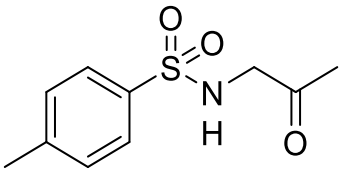
Synthesis of 4-methyl-N-(prop-2-yn-1-yl)benzenesulfonamide (6)



Propargylamine (18.16 mmol, 1.5 mL) was dissolved in DCE (40 mL) and the solution was cooled to 0 °C. To this solution were added triethylamine (43.21 mmol, 6.02 mL) and then p-toluenesulfonyl chloride (17.25 mmol, 3.29 g), previously dissolved in DCE (10 mL). The solution was stirred overnight while the ice bath was allowed to warm to room temperature. Then the reaction mixture was dissolved in Et_2O (200 mL), first washed with a solution of HCl (1M) and then with a satured solution of NH_4Cl. The organic layer was dried over $MgSO_4$, filtered and the solvent was evaporated, obtaining 3.31 g (87% yield) of the product as a white solid. The spectra are in accordance with the data reported in literature.[1]

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 (d, *J* = 8.3 Hz, 2H), 7.32 (d, *J* = 8.3 Hz, 2H), 3.83 (dd, *J* = 6.0, 2.5 Hz, 2H), 2.44 (s, 3H), 2.11 (t, *J* = 2.5 Hz, 1H).

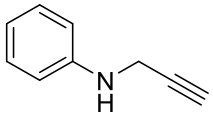
Synthesis of 4-methyl-N-(2-oxopropyl)benzenesulfonamide (7)



To a stirring solution of 4-methyl-N-(prop-2-yn-1-yl)benzenesulfonamide **6** (0.239 mmol, 0.05 g) in CH_3CN (3 mL), 0.3 mL of H_2O and $IPrAuNTf_2$ (0.012 mmol, 0.01 g) were added. The reaction was stirred at 80°C for 24 h. Then, a saturated aqueous solution of NH_4Cl was added. The organic layer was separated and the aqueous one was extracted with Et_2O. The combined organic layers were dried over anhydrous $MgSO_4$, filtered and concentrated under reduced pressure. The obtained crude was purified by column chromatography over silica gel using PE/AcOEt 8:2 to give the 4-methyl-*N*-(2-oxopropyl)benzenesulfonamide **7** as a white solid (42 mg, 77% yield). [4]

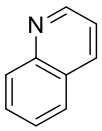
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 (d, *J* = 8.1 Hz, 2H), 7.30 (d, *J* = 8.1 Hz, 2H), 5.45 (t, *J* = 4.8 Hz, 1H), 3.85 (d, *J* = 4.8 Hz, 2H), 2.42 (s, 3H), 2.11 (s, 3H).

Synthesis of N-(prop-2-yn-1-yl)aniline (8)



To a stirred a solution of aniline (40.35 mmol, 3.68 mL) in DMF (11 mL) was added K_2CO_3 (20.17 mmol, 2.79 g). Five minutes later a solution of propargylbromide (10.09 mmol, 1.09 mL) in DMF (4 mL) was added dropwise. The reaction mixture was stirred at room temperature overnight. The mixture was diluted with H_2O and extracted with EtOAc, the combined extracts were washed with brine and dried over $MgSO_4$. After removal of the solvent, the residue was purified by column chromatography over silica gel with mixtures of PE/AcOEt from 99:1 to 80:20 to give the *N*-(prop-2-yn-1-yl)aniline **8** as a yellow oil (1.12 g, 85% yield). [5]
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.20 (td, *J* = 7.2, 1.8 Hz, 1H), 7.17-7.08 (m, 2H), 6.76 (t, *J* = 7.4 Hz, 2H), 3.90 (d, *J* = 1.9 Hz, 2H), 3.60 (s, 2H, broad), 2.20 (t, J = 1.9 Hz, 1H).

Synthesis of quinoline (9)



To a stirring solution of N-(prop-2-yn-1-yl)aniline **8** (0.381 mmol, 0.05 g) in CH_3CN (3 mL), 0.3 mL of H_2O and $IPrAuNTf_2$ (0.019 mmol, 0.017 g) were added. The reaction was stirred at 80°C for 24 h. Then, a saturated aqueous solution of NH_4Cl was added. The organic layer was separated and the aqueous one was extracted with Et_2O. The combined organic layers were dried over anhydrous $MgSO_4$, filtered and concentrated under reduced pressure. The obtained crude was purified by column chromatography over silica gel using PE/AcOEt 8:2. The product was obtained as a yellow oil (10 mg, 20% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.93 (dd, *J* = 4.2, 1.8 Hz, 1H), 8.17 (dd, *J* = 8.4, 1.8 Hz, 1H), 8.12 (d, *J* = 8.4 Hz, 1H), 7.83 (dd, *J* = 8.4, 1.4 Hz, 1H), 7.73 (ddd, *J* = 8.4, 6.9, 1.4 Hz, 1H), 7.56 (ddd, *J* = 8.4, 6.9, 1.2 Hz, 1H), 7.41 (dd, *J* = 8.4, 4.2 Hz, 1H).

V. Computational Details

In this section we report the cartesian coordinates and the harmonic frequencies of all the especies described in this study, indicated using the same acronyms and names of the figures in the main text,

A1

C	-0.790187	-1.989386	-0.182899
C	-1.923588	-2.855218	-0.026446
C	-1.797649	-4.214498	-0.348457
H	-0.842592	-4.600651	-0.689371
C	-2.901589	-5.049704	-0.241777
H	-2.808942	-6.100015	-0.498050
C	-4.125423	-4.538592	0.186519
H	-4.986464	-5.194838	0.265386
C	-4.251855	-3.187905	0.508338
H	-5.208187	-2.792860	0.835100
C	-3.155866	-2.342911	0.404419
H	-3.247030	-1.288753	0.645628
C	0.193620	-1.295723	-0.443918
C	1.154949	-0.507758	-1.258923
H	1.062381	0.552966	-1.013652
H	0.899274	-0.652770	-2.312519
N	2.530979	-0.903270	-1.086135
C	3.190282	-1.813095	-1.939634
O	2.659872	-2.384936	-2.860225
C	4.591748	-1.869967	-1.446350
C	5.671300	-2.592288	-1.918686
H	5.574689	-3.250242	-2.775974
C	6.888299	-2.434539	-1.248945
H	7.760885	-2.982166	-1.590225
C	7.003030	-1.580923	-0.150069
H	7.963347	-1.477683	0.344854
C	5.904525	-0.855061	0.319479
H	5.988472	-0.185815	1.169330
C	4.705207	-1.018616	-0.348675
C	3.378594	-0.395184	-0.103337

O	3.034714	0.390370	0.758147
Au	0.277208	-1.244596	1.790563
C	0.711150	-0.931027	3.742899
N	1.191360	0.208500	4.279826
C	1.359794	0.062922	5.641122
C	0.977868	-1.197942	5.951773
N	0.582717	-1.794986	4.771498
C	0.105298	-3.170160	4.683372
H	0.886723	-3.856361	5.016536
H	-0.148523	-3.388964	3.647049
H	-0.783173	-3.294284	5.305909
C	1.456293	1.444271	3.543138
H	1.909104	1.207957	2.580476
H	2.152808	2.049809	4.123755
H	1.735873	0.860996	6.262248
H	0.956395	-1.719739	6.896074
H	0.527331	2.000647	3.399343

Freq

7.3246	16.1568	18.1587
23.0753	26.7166	42.0452
45.9805	57.2481	61.0425
84.0585	94.3245	97.7141
123.7867	137.3030	144.8634
150.3344	164.6344	178.3763
213.4247	239.0197	249.3958
256.8128	276.1714	279.0451
295.4432	341.4958	350.7377
365.7251	391.7215	415.8154
423.3978	472.9354	475.1848
476.0559	527.7309	542.1217
550.9453	592.2543	627.5697
638.2608	638.9170	644.5472

688.7799	706.6324	707.4156
710.9200	731.6650	737.2702
763.8849	764.0604	767.8376
788.5077	806.7248	820.0719
860.9516	877.6092	883.0847
931.7907	962.7268	971.3038
973.2903	1008.9525	1018.4908
1027.2124	1028.5974	1046.6266
1046.6989	1050.3372	1057.8724
1067.7416	1068.4221	1116.3478
1121.9012	1125.2970	1126.8313
1163.5654	1170.3544	1175.4253
1181.8004	1200.4695	1203.9675
1211.9696	1220.0491	1240.0288
1269.5846	1273.2829	1333.7680
1341.0159	1375.0048	1375.7997

TSAbeta

C	-1.347621	3.398367	1.302182
C	-1.489229	2.958064	-0.022444
C	-2.642228	3.287486	-0.748666
C	-3.645109	4.040675	-0.150565
C	-3.500163	4.473157	1.166301
C	-2.353727	4.151310	1.892693
C	-0.449648	2.174416	-0.646857
C	0.029532	1.040183	-1.010169
C	1.283399	0.789518	-1.818551
N	2.412340	0.436037	-0.974792
C	3.194087	1.348794	-0.290755
C	4.240820	0.570825	0.413559
C	4.022802	-0.779569	0.147525
C	2.831268	-0.888356	-0.735338
C	4.843128	-1.760810	0.669406

C	5.905848	-1.342518	1.477219
C	6.123580	0.010215	1.742951
C	5.286347	0.995958	1.210910
O	3.018414	2.560583	-0.288046
O	2.281520	-1.866982	-1.184213
Au	-1.066894	-0.611852	-0.341157
C	-2.031309	-2.319153	0.230010
N	-1.658270	-3.586935	-0.049125
C	-2.567623	-4.486824	0.470794
C	-3.525013	-3.760748	1.091837
N	-3.178145	-2.432786	0.935914
C	-0.472048	-3.983429	-0.803048
C	-3.972548	-1.323460	1.446400
H	4.670969	-2.810642	0.456667
H	6.575504	-2.082248	1.903953
H	6.958748	0.301000	2.371869
H	5.450900	2.049486	1.410944
H	1.130885	-0.047848	-2.499773
H	1.554818	1.667926	-2.407854
H	-0.454032	3.137185	1.861071
H	-2.246643	4.487721	2.918905
H	-4.283891	5.064469	1.629671
H	-4.538483	4.293805	-0.712224
H	-2.743171	2.945882	-1.773770
H	-2.450415	-5.553587	0.357691
H	-4.410013	-4.066828	1.628106
H	-4.167559	-1.469264	2.510875
H	-3.412702	-0.399650	1.305968
H	-4.919810	-1.258306	0.905869
H	-0.764645	-4.379095	-1.778481
H	0.180858	-3.121639	-0.936509
H	0.070484	-4.750246	-0.246498
O	0.745954	3.566638	-1.251374

H	0.461013	4.427163	-0.902159
H	1.635966	3.340312	-0.860177

Freq

i290.6480	9.7201	19.3113
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122.4719	128.1573	137.3994
141.1134	153.9580	173.6202
175.7693	187.4851	206.4341
237.6268	252.7208	265.9493
273.7114	286.4047	332.0813
343.3884	345.5702	357.3423
390.9216	417.5915	422.5462
455.3542	462.1082	472.2034
477.1270	537.1720	545.6782
548.6126	590.3359	618.2677
627.5647	637.9060	638.9540
667.9771	689.2726	704.9136
708.5431	715.0408	719.2346
733.9595	750.5773	763.1360
766.0932	796.2558	804.5201
811.2271	820.7374	879.0158
880.3358	882.4333	932.0888
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1002.3611	1009.1590	1021.9111
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1047.4673	1048.3278	1057.6174
1064.4549	1068.3385	1115.9451
1116.9122	1121.4843	1122.5106
1165.9752	1169.9290	1172.9949
1175.2604	1201.2482	1202.8759

1212.8061	1217.7392	1238.0301
1259.8836	1264.1396	1334.5216
1337.5180	1367.3521	1371.8514
1400.7219	1405.7887	1406.3607
1411.7352	1464.2253	1468.5538
1470.1826	1490.6222	1504.6169
1518.8471	1522.5050	1523.9893
1529.9191	1530.8228	1531.2356
1539.4134	1546.9131	1550.2423
1653.1736	1659.0001	1682.5441
1684.8681	1695.0222	1695.6634
1789.5206	1872.5869	1900.9794
3104.6802	3105.4166	3132.5242
3179.6694	3180.8834	3186.7260
3209.5968	3215.1610	3224.7912
3230.2621	3232.5559	3237.2936
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TSA-alpha

N	2.183773	-3.291902	0.042809
C	2.591699	-2.005507	0.066681
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C	4.352552	-3.366448	0.369566
C	3.254727	-4.143555	0.227638
Au	1.470164	-0.318251	-0.155967
C	0.491850	1.561529	-0.335354
C	-0.590133	1.377633	-0.973556
O	-1.535074	3.154822	-1.274883
C	4.823329	-0.910489	0.365333
C	0.813044	-3.753528	-0.149852
C	1.162662	2.753404	0.209625

C	1.566926	2.789269	1.548378
C	2.172968	3.929421	2.064858
C	2.405786	5.032361	1.246595
C	2.025368	4.993153	-0.092417
C	1.403130	3.861900	-0.612115
C	-1.582460	0.565610	-1.703381
N	-2.712426	0.119337	-0.905749
C	-2.850853	-1.212039	-0.462563
C	-4.174467	-1.280891	0.205587
C	-4.760314	-0.018557	0.136530
C	-3.822937	0.887521	-0.567362
C	-6.008562	0.235066	0.672833
C	-6.665908	-0.834386	1.288698
C	-6.080175	-2.099581	1.357859
C	-4.815300	-2.343620	0.813415
O	-2.017272	-2.071465	-0.635203
O	-3.950367	2.075401	-0.812908
H	1.393375	1.927107	2.185108
H	2.469264	3.953905	3.108889
H	2.887209	5.917551	1.649897
H	2.213971	5.845156	-0.738167
H	1.117034	3.827926	-1.658920
H	-1.081956	-0.336915	-2.064056
H	-1.942418	1.120863	-2.573049
H	-4.356509	-3.325476	0.862284
H	-6.618192	-2.908197	1.841921
H	-7.649606	-0.679609	1.719875
H	-6.457732	1.220836	0.613844
H	5.387712	-3.625006	0.531273
H	3.140251	-5.216526	0.240333
H	5.581334	-0.964272	-0.418991
H	4.242394	0.002362	0.240693
H	5.307550	-0.899234	1.344207

H	0.759728	-4.388093	-1.037171
H	0.489186	-4.320702	0.725526
H	0.155930	-2.896847	-0.284274
H	-1.217069	3.815909	-0.638092
H	-2.496501	2.994807	-1.106093

Freq

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98.9587	124.9385	143.6177
148.3621	156.2708	170.2629
180.7705	191.5046	211.3717
222.8807	246.9277	248.7788
264.6932	274.1062	293.4422
323.4275	343.9846	365.8413
387.1740	418.8177	419.7963
430.3601	444.7679	469.4797
476.1866	497.6638	544.4623
559.9056	594.4886	610.1968
627.3195	637.6370	638.6952
641.2502	665.4074	689.0664
705.6935	714.9937	720.3789
732.6293	750.3024	766.2013
766.3763	781.1022	804.4529
805.8815	820.6991	866.3320
871.0632	881.8809	883.6483
932.6576	959.3479	972.4567
972.7454	1010.3653	1017.2234
1023.8663	1027.0620	1040.6565
1047.6329	1048.6866	1057.1574
1064.6919	1070.8736	1115.2636

1116.7449	1121.4430	1122.1208
1157.0262	1170.1216	1173.7976
1175.0133	1200.4402	1201.9350
1213.1269	1221.4442	1238.8799
1262.6836	1263.7470	1332.1405
1334.8391	1366.8627	1374.3499
1400.2702	1404.6314	1406.8023
1414.0932	1450.8942	1468.3783
1470.4292	1477.8906	1490.6232
1504.9526	1518.4206	1524.1814
1529.9798	1530.8955	1531.3102
1539.3629	1548.5949	1554.5059
1654.3802	1662.4210	1674.0700
1686.1328	1693.8318	1695.7065
1804.0113	1873.7190	1958.8136
3106.7599	3108.2053	3121.3335
3169.8472	3180.8791	3182.7897
3210.9063	3220.5336	3224.8812
3230.9960	3233.1702	3233.5018
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3251.9541	3256.0828	3315.1530
3334.3445	3430.7812	3793.6696

A2

N	-3.355913	-1.986874	1.128257
C	-2.293510	-2.059916	0.294197
N	-2.190225	-3.371243	-0.021747
C	-3.177464	-4.108482	0.603782
C	-3.911613	-3.235831	1.330384
Au	-1.100266	-0.515979	-0.366169
C	0.131419	0.986719	-1.040368
C	1.368099	0.599332	-1.829557
N	2.515405	0.248900	-0.962364

C	3.250823	1.074807	-0.223889
C	4.296618	0.330296	0.482719
C	4.135640	-1.014008	0.147287
C	2.984298	-1.111250	-0.784089
C	4.969993	-1.987927	0.654189
C	5.987117	-1.567212	1.521423
C	6.145907	-0.222815	1.856137
C	5.294043	0.759142	1.337709
O	3.107314	2.338573	-0.119297
O	2.482134	-2.053231	-1.325878
C	-1.198475	-3.947458	-0.920474
C	-3.856889	-0.769213	1.751341
C	-0.054273	2.291165	-0.806762
C	-1.200876	2.971434	-0.167973
C	-0.994088	3.949296	0.813869
C	-2.072844	4.603500	1.400174
C	-3.372531	4.295126	1.007176
C	-3.587469	3.330448	0.025326
C	-2.510420	2.674355	-0.561148
O	0.984934	3.192403	-1.182734
H	4.844548	-3.032762	0.390810
H	6.666343	-2.302175	1.940840
H	6.945124	0.067386	2.529966
H	5.414204	1.806041	1.594763
H	1.191855	-0.301246	-2.416939
H	1.709476	1.386623	-2.509348
H	0.014747	4.179854	1.147746
H	-1.897969	5.350982	2.167746
H	-4.214329	4.811013	1.458474
H	-4.598090	3.101266	-0.299141
H	-2.673546	1.939751	-1.342703
H	-3.268355	-5.176297	0.477024
H	-4.769176	-3.390210	1.967031

H	-3.760625	-0.836903	2.837578
H	-3.271558	0.075241	1.389446
H	-4.906278	-0.621186	1.486349
H	-1.677292	-4.289583	-1.841207
H	-0.457048	-3.186158	-1.159860
H	-0.704006	-4.789531	-0.431473
H	0.670239	4.110567	-1.205690
H	2.281793	2.753186	-0.588557

Freq

13.6627	17.9769	23.8223
27.8541	40.4639	47.2371
52.7695	64.5250	75.8395
79.7978	86.9477	128.2572
136.8229	143.6164	149.8735
165.5454	187.3168	193.7883
204.0021	222.5877	253.6340
268.8729	271.7406	287.3358
298.4566	339.7251	347.1903
368.6284	384.4684	410.2153
419.5066	422.3183	430.0288
459.9001	471.7175	475.2384
539.4101	544.5433	587.5919
613.9462	628.2401	637.2021
637.3326	670.2126	680.7662
695.3507	706.9127	711.1932
724.5274	732.8522	758.0689
761.7043	767.5534	792.4681
799.9089	802.8936	819.0454
875.4029	879.8138	882.0342
934.0597	962.0482	963.5931
979.3600	1010.8503	1012.1440
1013.5703	1027.1832	1038.8017

1045.8879	1051.5569	1053.1998
1062.9160	1069.6483	1073.2548
1102.5664	1115.2996	1116.4870
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1263.8273	1312.3225	1336.0847
1340.1157	1349.0182	1373.6104
1383.6832	1407.5621	1408.9210
1414.9619	1455.8096	1465.8061
1468.8172	1488.0235	1504.9729
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1525.7148	1529.0411	1532.4755
1539.6980	1544.8922	1556.6081
1596.0584	1653.4961	1663.0466
1680.8353	1689.5977	1690.5592
1704.4133	1728.4766	1913.5882
2546.8805	3102.2100	3103.0683
3105.9219	3175.3320	3176.6357
3184.8198	3204.7276	3209.5025
3210.3117	3220.6494	3230.5451
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3247.7081	3255.3824	3259.5070
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A3

Au	1.550614	-0.284789	-0.150136
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C	1.052569	2.724194	0.070858
C	1.223420	2.941472	1.445076
H	0.941376	2.158927	2.143954

C	1.751750	4.138232	1.915985
H	1.871724	4.289054	2.984745
C	2.132905	5.139890	1.024083
H	2.551781	6.070484	1.393831
C	1.981310	4.933807	-0.343000
H	2.287371	5.701165	-1.047777
C	1.443184	3.737603	-0.816800
H	1.354166	3.572596	-1.887910
C	-0.713636	1.511464	-1.042413
C	-1.499008	0.394616	-1.644893
H	-0.886958	-0.503572	-1.695316
H	-1.841264	0.647385	-2.654907
N	-2.695112	0.010114	-0.855431
C	-3.010673	-1.372843	-0.568940
O	-2.293799	-2.283517	-0.874002
C	-4.317346	-1.345451	0.131895
C	-5.095057	-2.370556	0.628075
H	-4.788818	-3.407357	0.538724
C	-6.298906	-2.012772	1.249711
H	-6.941757	-2.789660	1.650428
C	-6.689096	-0.678786	1.364159
H	-7.627946	-0.438572	1.851817
C	-5.891785	0.355834	0.861811
H	-6.190098	1.395009	0.949562
C	-4.710259	-0.011603	0.245926
C	-3.660537	0.800105	-0.373639
O	-3.685404	2.070105	-0.425122
C	2.710391	-1.964581	0.131840
N	4.018587	-1.996767	0.474225
C	4.474680	-3.298119	0.557828
C	3.424720	-4.096476	0.260496
N	2.353077	-3.262768	0.003578
H	5.494125	-3.536645	0.819374

H	3.344872	-5.171433	0.209319
C	4.856999	-0.831072	0.723484
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H	4.251723	0.066529	0.603794
H	5.252336	-0.867242	1.741113
C	1.030168	-3.744618	-0.369494
H	1.073181	-4.248510	-1.338061
H	0.662938	-4.440995	0.387727
H	0.350149	-2.897035	-0.435915
O	-1.439353	2.726858	-1.229873
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Freq

12.7595	19.5667	25.3383
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81.7108	84.5504	112.8809
129.4904	145.3945	156.4093
176.2646	179.4039	188.4122
197.1425	219.9382	255.9111
261.1447	265.2367	271.9044
274.1540	337.6343	344.0194
348.5369	387.2123	419.0087
420.4573	428.6638	468.4295
472.3764	498.0764	523.1966
545.7435	561.9653	579.8526
608.3159	628.2541	637.3704
638.3276	657.3609	681.5476
693.1069	707.5363	720.1304
729.9615	734.7939	760.2136
762.9878	767.1717	787.8105
796.5464	819.4928	854.2203

876.1630	885.2410	902.1437
919.0015	935.7772	958.1024
964.0863	994.6792	1013.8084
1014.0569	1024.9701	1035.0235
1045.6334	1052.9840	1053.3425
1062.4448	1069.2694	1085.6099
1109.9323	1114.4209	1117.6525
1119.9314	1121.4228	1167.4749
1170.2563	1174.1456	1197.0160
1198.8160	1205.5534	1211.3512
1218.3799	1230.2498	1255.7443
1263.5077	1294.1766	1325.1473
1334.3834	1336.6562	1371.4001
1390.7384	1408.0345	1408.7936
1415.2884	1465.6765	1467.3880
1473.4829	1486.6734	1500.5109
1511.8575	1519.6943	1521.3705
1528.3851	1529.3031	1532.2167
1539.2044	1545.1924	1551.7363
1645.3222	1654.1260	1657.6035
1670.1562	1685.8855	1689.5586
1707.4694	1737.7856	1907.8995
2221.1191	3097.6307	3103.9582
3104.1267	3175.3546	3178.3463
3206.4132	3209.6483	3210.5520
3213.1702	3218.2438	3224.5320
3231.5023	3239.1304	3243.4769
3248.4092	3255.8325	3260.0601
3313.1947	3332.7358	3650.1597

ATS1

Au -1.368053 -0.483197 -0.247642

C	-3.086205	-1.455304	0.292355
N	-3.614921	-2.589402	-0.244804
C	-4.793254	-2.943925	0.407148
C	-5.003762	-2.012207	1.367852
H	-5.367564	-3.809860	0.129006
C	-3.045892	-3.347609	-1.357085
H	-2.157992	-2.830079	-1.715145
H	-2.768719	-4.350294	-1.026616
H	-3.769870	-3.417995	-2.170633
H	-5.795107	-1.912483	2.089553
N	-3.951009	-1.104596	1.284594
C	-3.792519	0.042366	2.177354
H	-3.103666	0.753614	1.724533
H	-3.395602	-0.276778	3.143134
H	-4.759248	0.525876	2.323319
C	0.399457	0.464036	-0.850836
C	1.443636	-0.378843	-1.589989
H	1.752041	0.086058	-2.528319
H	1.061864	-1.379945	-1.802126
N	2.670402	-0.535818	-0.773518
C	2.735766	-0.369702	0.563017
O	1.727068	-0.035570	1.282139
C	3.964254	-0.878088	-1.302255
O	4.178689	-1.077141	-2.485925
C	4.864788	-0.921209	-0.124163
C	6.212255	-1.198317	-0.035769
H	6.796603	-1.436066	-0.916080
C	6.795859	-1.159680	1.240708
H	7.852193	-1.373603	1.348613
C	6.041210	-0.851311	2.372767
H	6.521286	-0.830270	3.343279
C	4.671318	-0.568139	2.275247
H	4.081631	-0.328098	3.151144

C	4.107816	-0.610051	1.014882
C	0.514930	1.816048	-1.013554
O	1.629350	2.281309	-1.681522
H	1.584762	3.233069	-1.890269
C	-0.367367	2.868507	-0.468963
C	0.209886	3.958968	0.201540
H	1.284402	3.995018	0.350757
C	-0.590971	4.973746	0.714981
H	-0.137297	5.802788	1.244739
C	-1.974587	4.921920	0.548648
H	-2.597387	5.717498	0.940233
C	-2.553974	3.852051	-0.132118
H	-3.626530	3.823625	-0.284610
C	-1.756994	2.828822	-0.639523
H	-2.203445	2.015236	-1.198198
H	0.837751	0.232713	0.552455

Freq

i968.5198	9.8466	14.8581
25.0574	31.4659	37.2612
45.4028	51.5470	62.5244
69.0682	77.7671	86.1854
109.5608	132.0923	135.5012
152.3208	165.9087	178.7893
199.1042	209.1408	224.8048
246.4133	264.2566	274.2062
289.9331	291.0669	348.8950
352.1182	357.0063	415.2232
434.7185	435.8248	458.5552
480.4032	482.2280	526.5595
552.0691	558.6270	575.1723
612.4042	632.8525	634.4229
656.5177	657.8068	687.4100

696.3449	728.1619	731.3901
737.3334	745.1468	750.5389
776.9829	795.2069	808.1035
809.2022	832.4564	841.8120
849.4816	905.4503	919.6891
923.1742	964.9100	995.2910
1001.9728	1008.9411	1042.1198
1042.6394	1051.6960	1058.4987
1064.7217	1067.1927	1077.5814
1079.8357	1087.5421	1090.1335
1109.3406	1126.3983	1135.0523
1141.0073	1141.8288	1156.0877
1174.1190	1188.0041	1190.7367
1193.9677	1226.0720	1234.8197
1236.0109	1242.8255	1247.1186
1250.8519	1281.6270	1316.7413
1341.1904	1362.5300	1371.1970
1387.7640	1400.0224	1400.7137
1405.6444	1435.8116	1462.8514
1472.6514	1493.7836	1514.8859
1522.9107	1532.7666	1538.8895
1541.1698	1543.9983	1545.2003
1547.4781	1557.1725	1559.6789
1570.4431	1618.8027	1657.3077
1665.2853	1681.3336	1699.5300
1704.6089	1710.3355	1733.8941
1842.4418	3106.5577	3107.0200
3115.2327	3176.2922	3188.8208
3190.0139	3215.4230	3219.0291
3223.1782	3235.0119	3245.2924
3248.4392	3253.3722	3257.9908
3263.8356	3266.2560	3273.1816
3341.4620	3364.1594	3701.5854

A4

C	4.870636	1.687200	4.429059
C	5.246854	0.839655	3.378345
C	6.581996	0.817103	2.953639
C	7.527185	1.614423	3.584922
C	7.148385	2.448632	4.634171
C	5.819122	2.487060	5.051283
C	4.255692	-0.003545	2.688890
C	3.027993	-0.406916	3.222650
C	1.871017	-0.796650	2.309217
N	0.760290	-1.370514	3.032300
C	0.504101	-2.737411	3.131399
C	-0.771553	-2.859312	3.885741
C	-1.209205	-1.577058	4.211913
C	-0.225903	-0.599848	3.673240
C	-2.379145	-1.367261	4.917078
C	-3.112007	-2.497957	5.290440
C	-2.675359	-3.782674	4.962087
C	-1.489323	-3.983365	4.249638
O	1.223429	-3.605080	2.676489
O	-0.205162	0.606967	3.738226
H	7.886623	3.078774	5.120086
Au	3.977280	-2.160314	4.185541
C	4.649790	-3.829096	5.133552
N	4.504124	-5.107139	4.726238
C	5.099736	-5.969278	5.623987
C	5.620982	-5.207188	6.613410
N	5.335377	-3.894664	6.295226
C	3.866782	-5.538032	3.483290
C	5.723117	-2.760807	7.125958
O	4.637410	-0.335267	1.456495
H	2.711097	0.148516	4.102588

H	-2.713695	-0.365215	5.164505
H	-4.038584	-2.376097	5.842161
H	-3.270077	-4.639231	5.262860
H	-1.147864	-4.978915	3.985960
H	1.496984	0.095244	1.793615
H	2.153557	-1.540833	1.557709
H	3.098312	-4.821421	3.195414
H	3.398908	-6.509605	3.648009
H	4.613538	-5.625050	2.690371
H	5.097986	-7.038878	5.481433
H	6.159471	-5.478937	7.508243
H	5.424578	-1.840760	6.625356
H	5.226826	-2.822670	8.096911
H	6.805969	-2.759367	7.266315
H	3.985669	-0.894539	1.003204
H	6.874437	0.173129	2.132289
H	8.559987	1.590001	3.252969
H	5.518001	3.153220	5.853164
H	3.835283	1.752801	4.745097

Freq

10.2789	17.4656	22.8164
25.9762	31.3538	42.0031
45.0355	59.0237	81.6653
85.6974	91.2946	96.8426
115.0459	130.1768	143.4416
153.0666	163.3888	184.4743
193.5768	209.5389	237.3724
246.4771	255.0054	275.2797
286.2021	297.6634	344.6835
356.7479	367.5819	415.5622
422.0306	426.2562	438.7812
472.8560	476.7470	509.2334

534.6338	542.4934	565.9626
617.4032	626.4009	634.9740
639.6727	661.3465	690.1922
692.7944	702.5430	712.0537
716.0777	734.8753	742.8856
763.6071	767.9604	808.6247
810.3684	818.3583	838.3868
862.8009	875.3815	882.7758
912.6492	932.4235	974.6406
976.7210	1009.0013	1020.0059
1020.8345	1027.5219	1039.2036
1046.6482	1047.1428	1049.3648
1059.4212	1066.6524	1071.9609
1116.3187	1120.7940	1121.9551
1123.6686	1134.8066	1169.7295
1173.4960	1176.3116	1179.5847
1200.6335	1204.3446	1212.2343
1220.5149	1233.1791	1240.2929
1267.2403	1327.1879	1334.6710
1355.4389	1381.2567	1390.2618
1406.2912	1406.5287	1413.5974
1432.9752	1451.1970	1460.8814
1467.1790	1471.4173	1494.1741
1496.5300	1511.9232	1518.5597
1523.5662	1529.0662	1530.7062
1534.4416	1541.8570	1548.3642
1554.3244	1599.1757	1650.9811
1671.2393	1687.6762	1693.7927
1696.4453	1814.7197	1879.3063
3083.2721	3107.5105	3107.5191
3130.1195	3183.9980	3187.2459
3203.6682	3211.9104	3218.6689
3228.4762	3231.1831	3236.6231

3241.3164	3244.5784	3249.6026
3251.6088	3254.2261	3259.0190
3315.8309	3334.8068	3764.0753

B1

N	-1.781701	2.976994	1.324892
C	-1.202329	2.460153	0.222023
N	-0.795277	3.516730	-0.508831
C	-1.121255	4.694352	0.130312
C	-1.742858	4.356049	1.284356
Au	-0.983887	0.508822	-0.272872
C	-0.180259	-1.536193	-1.086292
C	1.122524	-1.579331	-1.783284
N	2.249354	-1.267904	-0.943277
C	2.695999	0.025890	-0.677579
C	3.935829	-0.130279	0.124173
C	4.176207	-1.492795	0.299448
C	3.101532	-2.252213	-0.389840
C	5.271325	-1.951370	1.006839
C	6.133934	-0.990355	1.542623
C	5.895070	0.373788	1.366388
C	4.784005	0.827098	0.649316
O	2.126542	1.032374	-1.053515
O	2.925051	-3.438723	-0.507277
C	-0.126033	3.436706	-1.807278
C	-2.383920	2.219580	2.416465
C	-1.286017	-1.695060	-0.586528
H	-2.208814	-2.092246	-0.209356
H	5.451848	-3.013386	1.135839
H	7.006701	-1.309254	2.103174
H	6.586725	1.093709	1.791859
H	4.596401	1.885919	0.505085
H	1.256137	-2.602580	-2.151389

H	1.105225	-0.898679	-2.638677
H	-2.152815	4.966607	2.074014
H	-0.880682	5.660194	-0.286088
H	0.317876	4.408012	-2.026178
H	0.661669	2.684625	-1.766256
H	-0.849997	3.189037	-2.586619
H	-3.462170	2.391301	2.439981
H	-2.189793	1.159440	2.259453
H	-1.941447	2.528320	3.365440

Freq

10.2328	26.0448	36.1091
40.4405	51.6516	59.5749
80.7603	87.7261	106.7738
131.5649	141.9145	148.3329
167.8755	180.2272	211.0447
240.7525	256.3791	260.9410
276.8275	281.2855	301.4790
347.3307	349.7635	368.1240
407.0453	424.6045	474.6916
475.2533	541.7961	585.4611
628.3951	638.5797	646.1603
687.9832	697.8897	709.2133
711.5154	732.8274	748.1454
761.5004	766.9395	769.8862
805.3032	819.2173	861.4542
884.2493	923.4104	931.9815
965.6632	1009.9654	1026.5145
1048.5803	1051.2650	1059.3087
1068.6313	1116.2331	1122.5558
1128.2331	1164.6245	1169.5240
1176.5617	1184.1077	1201.6455
1211.9517	1241.4340	1271.6324

1334.2786	1371.1488	1402.8445
1407.8881	1413.8282	1416.6035
1453.2187	1469.5378	1470.9765
1473.8948	1495.9528	1516.6762
1526.2809	1528.3616	1530.9219
1534.8300	1545.7327	1550.8642
1649.3702	1692.7164	1694.7780
1817.3794	1889.1509	2151.3330
3104.2538	3109.6177	3112.9215
3157.7422	3187.6555	3195.8103
3212.2332	3219.6837	3232.8491
3242.5788	3250.4921	3255.3738
3318.2879	3337.0866	3435.9665

TSB-beta

C	-3.055682	-2.436285	1.194032
C	-1.936216	-2.331969	0.390498
C	-1.285861	-3.458289	-0.111444
C	-1.729686	-4.735664	0.171520
C	-2.860376	-4.853453	0.986492
C	-3.511232	-3.725305	1.488155
C	-0.134566	-2.999722	-0.931158
N	-0.137155	-1.594181	-0.836900
C	-1.217260	-1.130987	-0.097355
C	0.852574	-0.743422	-1.464585
C	0.372977	-0.212735	-2.789844
C	-0.232255	0.827146	-3.158735
H	-0.679357	1.504231	-3.858186
O	-1.487099	0.046446	0.078766
O	0.667090	-3.632832	-1.579014
Au	0.619980	-1.340005	-4.572634
C	0.984360	-2.599107	-6.132186
N	0.978085	-2.318944	-7.453236

C	1.288958	-3.445756	-8.188787
C	1.493812	-4.445177	-7.300771
N	1.302081	-3.908065	-6.043384
C	0.684476	-1.022274	-8.050496
C	1.447638	-4.676755	-4.810039
O	-0.602693	2.027663	-1.556394
H	-1.218354	-5.609205	-0.218968
H	-3.238640	-5.839632	1.235551
H	-4.385134	-3.852009	2.118848
H	-3.555441	-1.554867	1.581745
H	1.756491	-1.339395	-1.589705
H	1.069752	0.091919	-0.794498
H	1.758001	-5.480897	-7.449157
H	1.336511	-3.434793	-9.266835
H	-0.216517	-1.088811	-8.664318
H	0.525680	-0.297854	-7.252941
H	1.526132	-0.699373	-8.666691
H	2.477343	-5.027758	-4.713586
H	1.202299	-4.048312	-3.954992
H	0.769558	-5.532387	-4.830553
H	-1.191305	2.792704	-1.655761
H	-0.991633	1.426680	-0.873251

Freq

i313.5774	9.4981	20.9793
39.4999	44.4572	46.8384
64.3991	71.9629	90.9174
99.8220	123.9927	141.9147
147.5600	161.5315	175.4907
182.6988	193.5156	206.7823
225.7587	263.4868	270.2401
274.5212	302.9276	317.3935
344.9255	350.4739	380.7613

419.5029	428.5862	469.7966
476.0407	514.1445	544.7265
595.5071	626.7257	628.9582
638.5937	652.2233	660.6233
688.7471	706.5522	714.2226
733.4580	750.4016	765.4597
767.2766	805.6895	820.0034
850.6504	872.1166	882.9993
932.8540	955.6211	990.8587
1009.4869	1010.3365	1033.8282
1047.5147	1048.8031	1057.7942
1064.6404	1115.8643	1116.7319
1122.5784	1168.4393	1169.7598
1174.4121	1175.8686	1202.0075
1213.0965	1239.0825	1264.5035
1334.5814	1366.4996	1404.0698
1404.8578	1409.3059	1415.3418
1461.1904	1469.5537	1470.5130
1491.1323	1513.6331	1517.6175
1522.5451	1529.1488	1531.0468
1531.4586	1539.8104	1549.4604
1654.4202	1689.1656	1694.2851
1695.2500	1801.5352	1872.6864
1903.2929	3107.2900	3107.6304
3130.3683	3183.3977	3183.4644
3190.6418	3211.6323	3217.0286
3233.7096	3243.6139	3251.7234
3256.0962	3315.4801	3334.5799
3432.3817	3450.4871	3808.0519

TSB-alpha

C	-4.846949	-2.324020	0.799365
C	-4.213467	-1.257862	0.189938

C	-4.828795	-0.012345	0.075010
C	-6.100016	0.219286	0.565404
C	-6.750070	-0.854287	1.181952
C	-6.135003	-2.102011	1.296981
C	-3.891878	0.905168	-0.614172
N	-2.752299	0.156197	-0.901849
C	-2.870529	-1.169726	-0.435318
C	-1.616770	0.613365	-1.677545
C	-0.596203	1.347799	-0.910634
C	0.499318	1.488173	-0.301029
H	0.956801	2.366220	0.133805
O	-2.007756	-2.007781	-0.563325
O	-4.033123	2.085211	-0.884912
Au	1.555670	-0.331598	-0.139662
C	2.676027	-2.020406	0.067300
N	2.238989	-3.296695	0.112353
C	3.300054	-4.166531	0.266094
C	4.420878	-3.411110	0.316792
N	4.019106	-2.095979	0.192472
C	0.848671	-3.731207	0.019920
C	4.942519	-0.967764	0.203771
O	-1.576721	3.186147	-1.100522
H	-1.128969	-0.277177	-2.086110
H	-1.961100	1.223427	-2.516004
H	-4.365177	-3.292275	0.884609
H	-6.667853	-2.914281	1.780589
H	-7.751011	-0.716373	1.577657
H	-6.571995	1.191579	0.471255
H	5.457902	-3.688577	0.427105
H	3.163752	-5.235503	0.323040
H	5.681329	-1.086418	-0.591475
H	4.379038	-0.051096	0.035332
H	5.448205	-0.908909	1.170048

H	0.735956	-4.424037	-0.816596
H	0.554727	-4.226640	0.947876
H	0.206808	-2.867676	-0.144723
H	-1.330565	3.860078	-0.448036
H	-2.551074	3.038660	-1.032061

Freq

i250.6130	9.7174	20.9191
33.1833	42.4147	44.7956
63.5250	69.3365	97.4687
100.3583	120.4171	144.2694
149.6783	165.5497	176.4080
186.3244	204.7617	208.4994
236.1531	268.3709	272.4174
274.2931	285.4315	328.2907
344.6372	377.6565	393.7013
408.4331	424.3451	469.4240
474.9808	523.2724	543.7282
571.2126	588.2087	627.5004
638.7355	652.5701	688.5625
705.3512	713.9130	732.3582
751.1854	765.8054	765.8847
780.1981	803.7013	814.3903
821.1200	856.4330	881.8387
884.4737	933.0625	961.1290
972.8193	1011.1231	1025.0297
1047.6233	1049.8566	1058.1758
1064.5095	1115.4274	1116.6666
1121.6972	1158.5705	1169.7977
1174.5764	1175.1198	1202.4228
1213.1006	1240.3183	1263.8808
1335.2371	1366.8896	1400.8572
1404.5032	1408.9621	1415.0185

1448.3216	1469.0373	1469.4330
1469.9632	1490.3015	1517.8231
1523.3393	1529.4587	1530.9714
1531.0769	1539.6069	1549.1729
1654.3588	1683.3219	1693.2219
1695.0632	1807.3713	1873.9928
1939.3960	3107.3953	3108.2523
3116.2720	3167.6349	3182.0450
3183.7897	3211.6328	3225.7385
3234.5390	3244.3930	3252.5105
3256.7770	3303.3500	3315.2571
3334.3986	3459.8896	3818.1181

B3

N	2.425852	-3.283954	-0.013829
C	2.763335	-1.981535	0.123865
N	4.065098	-1.997927	0.491727
C	4.536224	-3.293449	0.581645
C	3.502807	-4.104659	0.262130
Au	1.578355	-0.321768	-0.172863
C	0.455807	1.363500	-0.459512
C	-0.729451	1.472724	-1.045718
O	-1.430564	2.710344	-1.217448
C	4.884028	-0.823094	0.759958
C	1.116624	-3.780827	-0.414459
H	0.875639	2.308174	-0.100107
C	-1.553056	0.388411	-1.662228
N	-2.744963	0.015060	-0.864448
C	-3.074630	-1.368532	-0.582176
C	-4.374304	-1.327889	0.130289
C	-4.750476	0.010324	0.253195
C	-3.696615	0.811250	-0.370953
C	-5.922494	0.389182	0.880469

C	-6.727538	-0.638101	1.385533
C	-6.353914	-1.976029	1.262739
C	-5.159689	-2.345674	0.629315
O	-2.369800	-2.283770	-0.898309
O	-3.707543	2.084055	-0.414719
H	-0.964023	-0.522980	-1.739560
H	-1.900366	0.672311	-2.662047
H	-4.866360	-3.385641	0.533724
H	-7.002259	-2.746863	1.666269
H	-7.659305	-0.388921	1.882159
H	-6.208142	1.431286	0.975205
H	5.553218	-3.519683	0.862965
H	3.437880	-5.180447	0.207527
H	5.725380	-0.787644	0.064145
H	4.270347	0.066889	0.627668
H	5.257471	-0.855171	1.785969
H	1.185185	-4.282193	-1.382862
H	0.741894	-4.482618	0.333991
H	0.429088	-2.939882	-0.492775
H	-2.813692	2.494181	-0.772724
H	-0.915279	3.446117	-0.846998

Freq

10.3595	18.0181	26.2001
37.0894	50.1836	70.4142
75.5950	83.0195	118.5621
136.2537	145.2212	161.3686
180.8230	196.9653	200.7680
210.2095	256.2376	267.9476
272.0151	292.7839	303.2927
332.1997	339.8095	382.6403
420.4509	437.0639	444.0358
469.8042	472.1566	484.7042

544.6305	588.0758	628.4102
637.4005	641.2928	680.1401
691.0384	706.0841	719.7963
733.5253	758.2469	760.5350
768.1033	794.3235	818.7737
840.6923	876.2691	899.3091
908.2983	935.3862	963.7590
991.3871	1014.0111	1045.5981
1052.8287	1053.1370	1061.1052
1062.8804	1093.2729	1113.1353
1115.7732	1120.0157	1134.3761
1168.1197	1170.5019	1174.4414
1199.3881	1206.0172	1211.7285
1230.3012	1263.6132	1319.8585
1336.2477	1336.8721	1399.3995
1408.3835	1409.2577	1416.5869
1466.3098	1467.9853	1472.5192
1487.2293	1511.6135	1519.6989
1521.4187	1528.5332	1528.8174
1531.6199	1539.3684	1545.2505
1639.1109	1654.2703	1674.1576
1688.7620	1706.9417	1738.2420
1910.9633	2394.9811	3100.3025
3103.3951	3104.2291	3124.4857
3175.6850	3178.3520	3210.9001
3212.9349	3214.0406	3239.5245
3248.7702	3256.1846	3260.3530
3313.7258	3333.2655	3765.6616

B2

C	5.439273	0.778611	1.219401
C	4.404153	0.341328	0.414906
C	4.243686	-1.003344	0.079310

C	5.116512	-1.968705	0.535028
C	6.172497	-1.539052	1.350020
C	6.330601	-0.194741	1.685103
C	3.045075	-1.111675	-0.788245
N	2.550754	0.244567	-0.934621
C	3.312494	1.075283	-0.229280
C	1.360480	0.585168	-1.742352
C	0.158712	0.943308	-0.885275
C	-0.012966	2.231111	-0.598414
O	0.942946	3.194981	-1.008788
O	3.157485	2.336643	-0.106982
O	2.522599	-2.056428	-1.304999
Au	-1.117439	-0.539196	-0.254143
C	-2.378558	-2.062732	0.322952
N	-3.546728	-1.968423	0.997789
C	-4.114110	-3.215252	1.179505
C	-3.278292	-4.108465	0.603587
N	-2.220893	-3.385115	0.085830
C	-4.148925	-0.730822	1.473727
C	-1.108258	-3.988257	-0.636292
H	-0.828141	2.655077	-0.023371
H	4.991332	-3.013691	0.272143
H	6.882690	-2.267101	1.728131
H	7.160193	0.102311	2.317967
H	5.558489	1.825351	1.477525
H	1.171197	-0.307063	-2.337926
H	1.653966	1.390260	-2.424317
H	-3.340704	-5.182322	0.516946
H	-5.050914	-3.353646	1.697037
H	-4.260883	-0.762751	2.559940
H	-3.496810	0.098230	1.202301
H	-5.126989	-0.587949	1.008599
H	-1.460328	-4.419567	-1.576404

H	-0.367407	-3.218350	-0.848676
H	-0.651047	-4.769226	-0.024751
H	0.626541	4.101179	-0.878025
H	2.302210	2.744672	-0.514709

Freq

11.4961	18.1279	29.1205
45.9983	54.6600	73.6966
82.7618	88.5207	126.0823
137.5526	145.1496	150.6823
189.2868	189.8281	200.4750
227.4779	233.6819	271.2318
272.1171	281.7223	300.3614
331.4260	339.4229	359.0015
392.7758	414.5543	422.9155
440.4838	470.5999	474.4266
544.1863	587.7659	628.6628
637.1072	645.4569	679.9983
703.6044	708.7756	729.7580
734.6517	758.9057	762.6842
767.8651	793.3274	818.9742
855.7657	872.9041	875.9038
934.2679	956.5561	966.4562
1011.7122	1012.8048	1045.9632
1049.9540	1052.5953	1054.3733
1062.9243	1087.0671	1114.7613
1115.8026	1120.3785	1125.2809
1168.3377	1170.3468	1174.2311
1205.2367	1211.4565	1228.5238
1253.0964	1263.6877	1336.4382
1340.7763	1370.3610	1388.2219
1408.5237	1409.2354	1415.8993
1449.9241	1466.6603	1468.2722

1487.4879	1519.2712	1521.0126
1523.2042	1526.0439	1528.9212
1533.8257	1539.6712	1545.2908
1593.6622	1654.1378	1680.7082
1689.8088	1702.1300	1719.9935
1914.4365	2624.1467	3103.0899
3103.2208	3103.4588	3176.8252
3177.1592	3188.5526	3209.6052
3209.9977	3238.5994	3247.9900
3255.5900	3257.2985	3259.7229
3313.5332	3333.0644	3806.6880

BTS1

C	3.948488	0.588083	1.222674
C	2.759478	0.433379	0.383656
N	3.080963	-0.258636	-0.727193
C	4.480225	-0.610951	-0.709451
C	5.005346	-0.051761	0.558671
C	4.126405	1.216058	2.440090
C	5.415586	1.188221	2.991121
C	6.467787	0.552299	2.331887
C	6.275259	-0.082004	1.093917
C	2.159168	-0.619168	-1.831401
C	0.836586	0.139086	-1.705700
C	0.647080	1.185397	-2.544656
H	-0.260750	1.782467	-2.531281
O	1.579558	0.879760	0.628855
O	5.023808	-1.241096	-1.599732
Au	-0.881091	-0.843334	-0.990935
C	-2.547762	-1.864450	-0.388913
N	-3.307068	-2.716474	-1.131880
C	-4.364248	-3.220446	-0.379671
C	-4.262274	-2.671666	0.854995

N	-3.144221	-1.842666	0.835156
C	-3.065490	-3.074293	-2.528868
C	-2.696239	-1.060890	1.986197
O	1.597529	1.562769	-3.450970
H	-5.081486	-3.912172	-0.784889
H	-2.204525	-2.515414	-2.890765
H	-2.859865	-4.142846	-2.612910
H	-3.936718	-2.820615	-3.135033
H	-4.874195	-2.792964	1.731306
H	-1.799311	-0.510590	1.708477
H	-2.466066	-1.724004	2.821894
H	-3.472347	-0.353614	2.283808
H	2.673893	-0.385195	-2.765648
H	2.001809	-1.699343	-1.783765
H	7.091297	-0.574373	0.579575
H	7.452435	0.548494	2.783135
H	5.597473	1.669335	3.944102
H	3.307462	1.710204	2.947669
H	1.349207	2.317990	-4.012053
H	0.910430	0.647263	-0.288229

Freq

i751.1065	3.4858	10.9314
30.0373	42.2128	56.2097
67.9189	73.2208	85.7641
99.6471	120.3720	141.3835
151.0943	167.5871	188.1826
202.8758	228.4178	248.8591
265.2061	281.9871	289.7681
309.4080	317.6799	345.0498
354.2077	425.6879	434.8463
478.8281	480.3097	489.8234
556.1215	591.7364	615.0108

634.1010	657.1323	679.6470
686.0508	716.9158	729.1151
742.8013	752.9660	777.0849
798.0245	805.6016	810.5402
839.9030	909.3106	925.6930
965.1380	988.2348	997.2813
1016.0921	1043.1512	1059.0570
1065.2837	1066.9540	1087.7367
1088.4298	1093.3140	1125.7138
1134.9309	1141.8251	1154.4374
1185.8970	1189.1146	1192.0663
1194.8759	1226.8340	1235.1537
1240.9011	1243.6716	1280.8236
1311.0134	1362.8555	1391.9507
1403.2011	1403.4279	1414.1919
1436.3438	1462.3040	1473.0585
1496.5128	1514.7090	1534.9558
1541.4900	1541.6145	1542.4275
1545.3629	1554.7811	1557.0724
1560.7593	1631.8649	1657.9619
1703.2397	1705.7611	1710.2857
1760.6772	1844.4512	3107.2967
3107.6339	3114.0861	3173.6051
3189.3423	3190.4375	3218.4174
3218.4782	3219.4516	3249.2695
3258.8594	3267.1609	3273.8430
3341.7437	3364.3145	3734.9869

BTS2

C	-3.511316	0.618544	0.105216
N	-2.970163	-0.448682	-0.518735
C	-3.974460	-1.481626	-0.706482
O	-3.734948	-2.548327	-1.240420

C	-5.211228	-0.926531	-0.118381
C	-4.922744	0.353179	0.378105
C	-5.887846	1.134406	0.984209
H	-5.660452	2.123323	1.361966
C	-7.176431	0.591437	1.088192
H	-7.961636	1.171026	1.557375
C	-7.464623	-0.681561	0.595354
H	-8.470304	-1.072440	0.689446
C	-6.476635	-1.465320	-0.022494
H	-6.699831	-2.451860	-0.409441
C	-1.566609	-0.614795	-0.929902
H	-1.536349	-1.497014	-1.570396
H	-0.950843	-0.783003	-0.044782
C	-1.099783	0.610748	-1.678250
O	-1.391478	0.467664	-3.011750
H	-1.112266	1.229789	-3.553840
C	-0.623930	1.721221	-1.070065
H	-0.453633	2.578400	-1.726658
Au	0.487600	1.807134	0.689283
C	1.714407	1.946283	2.322278
N	1.576886	2.764933	3.402084
C	0.493979	3.724620	3.609184
H	-0.225385	3.621858	2.799008
H	0.888234	4.742414	3.610548
H	-0.004525	3.524557	4.559118
C	2.628179	2.584917	4.296789
H	2.705963	3.141472	5.214011
C	3.435988	1.636091	3.765007
H	4.351543	1.205946	4.130814
N	2.864279	1.254200	2.554546
C	3.442589	0.243839	1.670245
H	4.471802	0.510404	1.424825
H	3.423797	-0.735465	2.152113

H	2.858619	0.204384	0.752625
O	-2.889272	1.703675	0.403164
H	-1.878254	1.820557	-0.049990

Freq

i319.2224	9.0979	21.2497
30.8003	53.3933	65.2902
69.6845	73.3699	81.1966
108.0104	132.7348	142.7459
156.5937	168.6448	196.9793
209.2009	232.7591	259.1141
283.6112	289.7766	294.5151
332.0375	351.6894	358.2517
435.2125	453.8098	471.6475
479.8022	480.6796	551.5493
560.1789	606.1563	634.1763
656.8998	666.7870	680.5697
686.8098	722.3131	732.5737
749.5918	774.0979	777.3293
797.8899	811.4965	840.9729
860.8233	891.6970	925.2956
929.7043	966.6335	969.4227
989.3736	1045.2911	1055.5391
1059.1689	1065.2939	1070.8489
1090.4265	1108.3709	1125.4480
1135.6863	1141.9926	1147.5373
1188.9453	1191.7242	1193.2188
1196.7103	1230.1324	1231.9058
1242.8439	1281.1381	1303.3709
1333.1069	1364.1606	1402.5646
1403.7352	1404.7450	1435.6450
1456.8718	1461.4702	1465.4460
1472.9185	1514.6999	1523.6299

1535.1647	1540.9371	1541.9898
1542.7566	1544.6847	1556.8445
1560.3659	1568.8623	1658.1166
1677.6016	1702.9249	1706.3903
1733.7327	1850.8475	3107.0636
3107.2805	3132.3292	3143.7226
3189.2310	3189.8800	3200.0106
3218.4548	3219.0925	3250.7691
3259.9568	3268.0573	3274.7710
3342.1582	3364.7684	3697.2647

B5

N	0.593736	3.827612	-0.659373
C	0.649085	2.687517	0.061255
N	0.434491	3.057233	1.341481
C	0.253056	4.422730	1.424394
C	0.351094	4.908092	0.164775
Au	1.036066	0.808999	-0.611118
C	1.730293	-1.164315	-1.292454
H	2.278125	-1.493846	-0.412097
C	0.453161	2.163237	2.497399
C	0.771697	3.937476	-2.103087
C	0.445862	-1.658607	-1.461178
O	-0.116236	-1.647513	-2.644324
C	-0.319295	-2.307957	-0.325959
N	-1.653029	-1.773361	-0.120707
C	-2.728439	-2.002763	-0.971790
C	-3.940207	-1.544060	-0.260751
C	-3.544691	-1.031748	0.974943
C	-2.069844	-1.168900	1.087306
C	-4.462296	-0.514126	1.868881
C	-5.807021	-0.527067	1.483593
C	-6.200948	-1.036569	0.245205

C	-5.264875	-1.553737	-0.655639
O	-2.608311	-2.466017	-2.096058
O	-1.319586	-0.852764	1.980070
H	-1.036862	-2.027223	-2.629904
H	-5.563292	-1.952119	-1.619607
H	-7.252814	-1.032879	-0.021188
H	-6.559737	-0.136369	2.160652
H	-4.151890	-0.122241	2.831738
H	-0.391552	-3.380928	-0.547370
H	0.221587	-2.182362	0.612252
H	0.082354	1.180139	2.208363
H	-0.200087	2.573432	3.268506
H	1.468514	2.076622	2.891084
H	0.069051	4.923100	2.362544
H	0.265961	5.914597	-0.215046
H	0.870517	2.937176	-2.522449
H	-0.096921	4.429377	-2.545301
H	1.672825	4.513214	-2.324776
H	2.314994	-0.984935	-2.191868

Freq

14.2396	23.4678	36.2202
45.2424	57.2517	66.9908
75.6192	78.0509	103.7523
127.0438	131.8164	147.2897
172.6249	182.3644	194.3867
208.5847	243.4334	253.9038
272.8732	276.6083	296.5322
345.2585	355.1812	378.3608
393.5298	423.1236	472.6614
474.8092	512.2521	526.0522
545.6449	605.2696	627.0960
638.7743	683.9666	689.3957

702.7804	715.8207	738.0128
757.3155	763.9904	767.4671
805.9417	818.3403	828.0458
866.5763	883.0173	908.5754
918.5342	934.2448	944.6083
990.0939	1012.0035	1019.6549
1048.9536	1050.6005	1057.0902
1065.3913	1066.9478	1116.1879
1121.1232	1122.3514	1156.8403
1168.8007	1172.6562	1178.1873
1202.7672	1213.3887	1238.8522
1267.5292	1314.2125	1334.8543
1354.7530	1406.7005	1407.3629
1413.2428	1418.5459	1455.7979
1466.3549	1471.4088	1477.7091
1492.9003	1494.2872	1499.0767
1517.9920	1519.8896	1528.7657
1531.0740	1533.7803	1540.9118
1548.0613	1647.2646	1650.2555
1692.1932	1694.0482	1796.7585
1874.5979	3083.0628	3108.7943
3109.7444	3167.6194	3186.0225
3189.6364	3190.2044	3212.6310
3214.3761	3234.8309	3244.5564
3252.2871	3256.8229	3258.2039
3275.5801	3316.3812	3335.2837

B4

C	-0.419958	3.532475	-0.875577
C	0.052808	2.529640	-0.050522
C	0.396429	2.775795	1.277844
C	0.277889	4.035887	1.834178
C	-0.200498	5.057723	1.008606

C	-0.542422	4.810658	-0.322176
C	0.859509	1.499827	1.882250
N	0.771600	0.543014	0.873344
C	0.282922	1.088583	-0.332297
C	1.024084	-0.865328	1.060959
C	2.452036	-1.266284	0.740055
H	2.859079	-0.865802	-0.187472
O	0.115894	0.449482	-1.342624
O	1.250668	1.268577	3.010654
Au	3.972102	-0.404150	2.175222
C	3.012036	-2.452052	1.162306
C	5.213225	0.655407	3.386102
N	6.488876	1.024262	3.143933
C	7.000721	1.718180	4.220972
C	6.016239	1.778909	5.148406
N	4.924986	1.124576	4.617245
C	7.249446	0.745490	1.930840
C	3.660619	0.929690	5.326165
O	2.515832	-3.313968	2.045124
H	-0.687548	3.331286	-1.907624
H	-0.912939	5.625274	-0.936036
H	-0.311727	6.060415	1.408589
H	0.539551	4.220757	2.870775
H	0.347025	-1.403176	0.387717
H	0.751903	-1.102454	2.094443
H	2.834590	0.954439	4.616128
H	3.535743	1.742347	6.042596
H	3.674073	-0.023485	5.859808
H	5.995517	2.229380	6.128687
H	8.007138	2.107560	4.229386
H	6.606260	0.221780	1.225180
H	7.588040	1.682055	1.483294
H	8.111398	0.118581	2.168538

H	3.923453	-2.836530	0.714067
H	1.650428	-3.045788	2.396984

Freq

8.2507	20.8861	35.2696
38.8721	45.6621	57.7919
67.1626	86.1478	106.4679
108.9937	130.3659	142.6822
154.7170	164.7759	192.7419
198.2501	211.0265	245.2218
253.7105	277.8949	283.3651
311.3387	345.5550	346.7627
366.3860	392.1746	424.6785
474.1232	475.8185	529.5889
542.2989	574.3129	610.0685
627.0530	639.8817	681.9177
688.8266	702.6730	712.7831
737.7691	753.1595	764.4593
769.6845	807.1437	818.9547
854.4106	885.3022	890.7945
931.9124	966.4578	1004.9833
1009.1442	1021.8224	1031.0080
1047.3191	1050.4891	1059.4860
1068.2755	1116.1266	1121.9740
1123.8878	1126.2917	1169.6707
1174.7207	1175.9601	1182.3176
1201.1482	1212.1393	1239.9735
1253.5342	1269.7584	1334.3936
1376.3657	1390.3632	1406.3582
1406.8664	1410.5937	1416.4118
1457.8363	1466.7065	1471.6787
1477.4358	1488.3646	1494.7890
1517.5047	1526.1106	1528.4810

1530.8769	1534.6001	1542.8011
1549.8677	1641.5026	1649.9628
1693.4958	1695.2534	1813.4004
1883.3556	3086.9459	3109.5790
3109.9514	3135.0668	3186.7976
3191.4036	3197.1420	3213.5954
3220.7540	3232.1571	3241.9115
3249.8694	3254.5945	3254.7484
3317.2653	3336.1292	3754.4032

C1

Au	-2.123105	2.109881	1.074568
C	-0.571838	1.763431	-0.175729
N	-0.580796	1.863508	-1.520642
C	-1.730700	2.224953	-2.348809
H	-2.484931	2.714543	-1.734559
H	-2.150755	1.328367	-2.810468
H	-1.402918	2.917713	-3.125546
C	0.657661	1.541634	-2.032936
H	0.863733	1.561291	-3.092015
C	1.452289	1.237795	-0.979699
H	2.489013	0.941239	-0.936798
N	0.680543	1.380724	0.154265
C	1.181825	1.144239	1.503497
H	1.482856	0.099981	1.610151
H	0.389398	1.366370	2.216618
H	2.036157	1.795415	1.698936
C	-3.780882	1.925618	2.579602
C	-3.809670	3.128397	2.358752
H	-3.956978	0.930814	2.940588
C	-4.005746	4.588970	2.267208
H	-3.065047	5.082976	1.996122
H	-4.269153	4.936099	3.270934

N	-5.116976	4.942252	1.378644
S	-4.699154	5.103657	-0.256872
C	-6.284068	5.246210	-1.016501
O	-3.942639	6.331226	-0.476133
O	-4.065692	3.821156	-0.580699
C	-6.646225	6.460982	-1.594259
C	-7.888746	6.563801	-2.205064
C	-8.767323	5.475935	-2.248276
C	-8.370449	4.268944	-1.661395
C	-7.133355	4.142687	-1.045652
H	-5.960749	7.301128	-1.570226
H	-8.180392	7.506017	-2.660173
C	-10.107267	5.608167	-2.920021
H	-9.040657	3.415157	-1.690028
H	-6.829599	3.202710	-0.597250
H	-10.694754	4.691369	-2.830598
H	-10.687012	6.426561	-2.480954
H	-9.988508	5.830288	-3.985886
H	-5.600317	5.780996	1.694102

Freq

7.8673	15.7780	18.1195
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41.3533	48.1091	66.9719
80.1617	103.6648	115.2588
132.1246	159.1898	167.6178
186.4257	206.1699	211.4702
253.1114	282.4946	283.5749
287.0985	305.1623	318.4403
334.3099	349.0407	364.9503
378.1819	421.3751	441.8096
475.6680	483.5483	513.7564
543.5353	590.7027	609.6301

629.8864	638.2435	651.7028
681.8789	697.5346	707.9583
733.9688	761.9250	765.6879
768.2274	799.7395	837.5469
846.3866	871.4829	881.7204
900.9964	999.4346	1002.0335
1017.9106	1027.4397	1043.5731
1052.1256	1069.1823	1087.4144
1106.6769	1122.2673	1128.8563
1138.1569	1159.4987	1161.5777
1170.0265	1176.7186	1185.0037
1228.3288	1257.9765	1272.3276
1289.3539	1319.8588	1351.8641
1357.1101	1392.2435	1408.9204
1418.1790	1452.4182	1464.4235
1468.7732	1474.7749	1475.7127
1482.6588	1494.7209	1515.7055
1515.9308	1522.2892	1522.6701
1534.2310	1546.7177	1551.7061
1560.5059	1648.4748	1661.5297
1686.2629	2135.6419	3082.2016
3109.8537	3110.0971	3111.5050
3142.1372	3166.9793	3175.4747
3187.8302	3195.9632	3211.0831
3214.0954	3223.1276	3227.4689
3248.5094	3254.6318	3318.5486
3337.3042	3436.2632	3579.9863

TSC-beta

C	-6.052995	0.583863	1.119962
C	-4.872441	-0.115221	0.934772
C	-3.934577	0.380185	0.028453
C	-4.163851	1.546937	-0.690234

C	-5.357357	2.233450	-0.487756
C	-6.315053	1.766957	0.413657
S	-2.437221	-0.511701	-0.245705
O	-1.680082	0.145531	-1.306625
C	-7.610876	2.502114	0.623916
N	-1.624499	-0.377773	1.222542
C	-0.743397	-1.479377	1.608806
C	0.386022	-1.750061	0.646161
C	0.625087	-2.628038	-0.225081
Au	2.010334	-0.418982	0.309181
C	3.459466	0.990930	0.053057
N	4.622645	1.120255	0.726778
C	5.336871	2.204265	0.257151
C	4.597738	2.759546	-0.730862
N	3.448759	2.002728	-0.841792
C	5.087530	0.252832	1.803161
C	2.393748	2.274658	-1.813117
O	-2.745050	-1.947367	-0.359947
H	1.199133	-3.120233	-0.984023
H	4.347434	-0.529128	1.967400
H	6.039664	-0.204275	1.525863
H	5.211397	0.832342	2.720446
H	6.297501	2.481313	0.663540
H	4.785940	3.616795	-1.358858
H	1.579669	1.566679	-1.661603
H	2.784591	2.163498	-2.826793
H	2.018618	3.290633	-1.674158
H	-1.348440	-2.380531	1.717510
H	-0.345932	-1.224572	2.592566
H	-1.192178	0.540699	1.295727
H	-3.427155	1.902727	-1.401874
H	-5.546930	3.144566	-1.047115
H	-7.769734	2.724584	1.684001

H	-7.632230	3.444834	0.072134
H	-8.459861	1.896502	0.288602
H	-6.791073	0.206061	1.821772
H	-4.681130	-1.033818	1.479069
O	-0.920596	-3.934992	-0.364113
H	-0.915855	-4.579260	-1.089910
H	-1.686173	-3.325061	-0.502002

Freq

-316.2094	4.4979	14.6395
17.2405	28.1786	35.5815
41.0624	43.7786	53.1104
75.7841	87.1073	97.8685
112.8790	131.5641	137.6812
155.4153	167.6531	191.3699
206.7201	212.4062	229.6707
258.6832	273.8272	291.0577
291.7668	303.0427	324.0517
340.1002	345.7639	358.4893
379.1452	421.9650	446.5679
469.9236	488.8394	503.9554
527.7238	547.5723	610.8598
626.9089	627.3229	639.2064
644.1280	652.4001	657.2978
693.9023	703.9870	731.5898
765.9361	768.3128	808.8532
839.1753	845.6186	851.4358
868.9974	884.4431	948.9643
1000.3997	1016.1368	1018.3896
1025.9431	1036.9055	1045.2128
1048.2681	1065.0633	1087.5513
1102.1400	1114.0321	1117.5509
1122.3461	1157.4859	1160.0751

1169.5555	1173.9381	1175.8823
1228.0568	1257.3766	1264.6846
1278.2525	1308.3793	1354.0220
1358.2320	1387.0750	1404.5066
1416.6451	1451.8034	1464.8196
1467.3614	1469.4314	1471.2202
1489.8345	1513.1487	1515.5148
1518.6633	1520.2242	1522.1289
1531.2348	1539.1669	1549.0928
1560.5747	1653.1194	1662.1682
1686.7500	1687.5268	1894.4710
3081.7287	3107.5435	3107.9333
3137.5885	3141.4848	3167.2381
3184.5496	3184.7647	3188.0555
3210.6691	3212.4185	3223.0978
3227.4367	3249.2091	3256.2311
3315.3118	3334.2852	3445.9968
3459.8973	3561.7502	3807.0499

TSC-alpha

C	-4.847353	0.365625	-0.936817
C	-4.643809	0.069908	0.411368
C	-5.316283	0.756994	1.416184
C	-6.201798	1.767881	1.057028
C	-6.424603	2.091428	-0.282621
C	-5.732795	1.376609	-1.271156
S	-3.549229	-1.235203	0.867183
O	-3.631196	-1.460435	2.303112
N	-2.045477	-0.581541	0.440408
C	-0.902167	-1.483149	0.615517
C	-0.075798	-1.604085	-0.592844
C	0.922346	-1.503856	-1.349166
Au	2.423794	-0.302658	-0.473404

C	3.981148	0.799231	0.241826
N	4.990805	0.368681	1.028561
C	5.873755	1.397244	1.290628
C	5.399558	2.490723	0.651047
N	4.237268	2.105317	0.012953
C	5.160565	-0.987176	1.539504
C	3.428803	3.005617	-0.800832
O	-3.701752	-2.387280	-0.032820
O	-1.517253	-2.916487	-1.569953
H	1.139144	-1.926632	-2.320167
H	4.326201	-1.598425	1.198502
H	6.094263	-1.410998	1.164012
H	5.176123	-0.972559	2.631249
H	6.752034	1.260383	1.902672
H	5.781696	3.498320	0.593042
H	2.554690	2.464145	-1.159875
H	4.010248	3.358387	-1.655309
H	3.105132	3.857890	-0.199734
H	-1.232422	-2.482656	0.914377
H	-0.244318	-1.131608	1.418006
H	-1.616288	-2.791970	-2.525522
H	-2.415683	-2.848426	-1.171160
H	-5.157921	0.493160	2.456175
H	-6.734811	2.306626	1.834503
C	-7.401065	3.168370	-0.670221
H	-5.901711	1.613178	-2.317852
H	-4.327106	-0.192861	-1.707375
H	-1.915535	0.323482	0.885708
H	-6.955056	3.869769	-1.382294
H	-8.284042	2.733669	-1.151752
H	-7.740574	3.735245	0.199855

Freq

i205.2605 10.3716 10.6743

20.4370 22.4457 30.6777

35.8867 42.1275 51.9465

63.0735 74.9277 80.2840

112.9645 127.3799 136.6933

149.2309 169.3134 181.6479

197.5395 206.8443 224.4110

251.5696 264.4762 272.3523

272.5581 289.7294 323.4377

340.0431 344.9595 366.5259

374.8104 422.0617 443.3580

469.8088 492.5853 501.3181

503.5154 532.1321 560.1986

574.1861 627.7007 638.5680

650.9166 667.7674 695.9238

703.5542 733.0965 748.8974

759.8494 768.1367 768.9577

787.8502 834.6947 845.0024

856.0666 872.2944 884.6661

960.1123 1000.6772 1006.3953

1019.6727 1027.1470 1044.6522

1048.1893 1065.0043 1087.3901

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1122.8794 1158.5430 1165.7671

1168.9351 1173.4411 1176.0166

1228.0389 1257.2431 1265.6825

1294.6865 1319.9006 1353.7932

1358.5171 1405.2353 1411.9643

1416.5139 1446.4673 1452.1480

1465.0293 1468.5592 1469.4341

1483.1178 1489.7595 1516.2139

1517.4755 1518.6403 1522.0239

1531.1109 1539.1918 1549.1977

1559.9848	1654.4286	1660.5414
1686.5174	1696.0711	1972.7404
3081.6265	3100.0416	3107.8224
3108.5213	3141.6905	3145.7561
3167.8906	3184.2352	3185.5477
3212.1637	3212.7932	3222.2453
3229.4519	3249.8040	3255.7178
3310.9126	3315.8031	3334.7919
3510.3064	3570.7601	3830.0857

C3

Au	-4.427038	-2.375591	1.238786
N	-4.127286	-0.745815	-1.358045
C	-5.523894	-0.331738	-1.360213
H	-5.591880	0.755014	-1.272270
H	-6.007260	-0.654919	-2.285030
H	-6.023933	-0.792820	-0.509480
C	-3.545401	-1.537381	-0.428223
C	-3.212465	-0.355669	-2.317201
H	-3.480631	0.281978	-3.145513
C	-2.031061	-0.918681	-1.977333
H	-1.061981	-0.870934	-2.449756
N	-2.254393	-1.638518	-0.819274
C	-1.216517	-2.384846	-0.121126
H	-1.663406	-2.873814	0.743446
H	-0.429642	-1.705998	0.215623
H	-0.789021	-3.139592	-0.785213
C	-5.277324	-3.130425	2.939319
H	-5.117851	-2.547746	3.852765
C	-6.018180	-4.220093	3.100024
O	-6.557812	-4.625019	4.355197
H	-6.955368	-6.044153	4.498737
H	-6.232892	-4.062093	5.075677

C	-6.420784	-5.220014	2.061343
H	-7.506094	-5.361877	2.019843
H	-6.093260	-4.875755	1.081305
N	-5.803517	-6.551413	2.282720
S	-6.472511	-7.725930	3.195671
O	-5.420866	-8.622407	3.615109
O	-7.286030	-7.017431	4.318148
C	-7.730762	-8.547101	2.294748
C	-9.057756	-8.119522	2.349538
C	-9.999955	-8.797818	1.591628
C	-9.641534	-9.888306	0.789350
C	-8.301872	-10.290837	0.763192
C	-7.337670	-9.630498	1.510278
H	-9.352227	-7.295729	2.989004
H	-11.038096	-8.481663	1.632663
C	-10.686328	-10.618010	-0.008149
H	-8.009624	-11.141463	0.155635
H	-6.304591	-9.961402	1.497331
H	-10.242013	-11.378512	-0.653987
H	-11.400760	-11.115810	0.656458
H	-11.255542	-9.925807	-0.636584
H	-4.789496	-6.562634	2.381909

Freq

4.1296	13.4045	16.0019
16.8322	24.4135	34.1116
49.5693	58.4627	78.4693
83.1763	89.7173	128.2611
138.0035	148.6741	174.4899
179.7073	201.2551	246.0519
248.0770	251.7767	271.4396
272.5155	296.1650	313.2012
334.0270	340.6155	343.4917

374.2325	399.2388	417.4046
424.4047	441.3232	463.0629
470.5503	509.6517	525.3459
555.7192	621.0043	629.0136
637.5333	648.6623	654.3846
697.0272	718.3834	729.9427
761.1597	767.9994	820.0994
845.5357	849.9437	865.7528
869.5452	876.8574	906.0866
931.9748	960.1864	1003.2155
1017.9127	1027.8388	1032.6164
1041.8626	1046.7030	1055.6229
1063.7707	1086.8049	1116.0268
1120.3322	1121.5906	1128.6368
1167.3839	1168.6076	1170.5511
1174.5329	1204.4195	1232.6815
1259.4254	1264.7809	1271.1920
1315.4759	1339.7262	1355.7791
1360.5045	1386.9843	1409.1383
1409.4813	1451.6450	1456.5927
1465.7392	1468.3812	1468.4636
1471.1442	1487.7876	1504.5369
1514.1223	1520.6332	1521.0541
1521.4134	1529.0532	1539.7411
1545.2047	1556.0738	1654.3236
1657.0625	1680.7935	1737.5155
2466.5093	3084.0069	3103.1596
3103.2876	3107.9784	3117.6388
3144.7392	3172.4505	3176.7246
3176.9771	3195.6084	3209.5951
3210.5232	3228.9172	3234.4547
3251.7107	3263.0813	3313.7699
3333.2742	3561.0569	3781.9691

C2

Au	-1.968137	-3.414465	-0.295895
C	-2.097005	-1.406751	0.134644
C	-1.344998	-6.345292	1.495998
H	-1.350605	-5.290147	1.766484
H	-0.368499	-6.775504	1.730330
H	-2.119815	-6.867789	2.062001
N	-1.607808	-6.457385	0.068356
C	-1.638321	-7.659367	-0.612650
H	-1.459515	-8.604989	-0.124374
C	-1.920903	-7.366255	-1.901987
H	-2.037122	-8.004998	-2.764049
N	-2.056572	-5.993248	-1.975411
C	-1.864796	-5.422311	-0.764056
C	-2.369811	-5.279595	-3.206411
H	-2.449264	-4.216973	-2.981053
H	-1.577783	-5.436767	-3.942275
H	-3.320511	-5.634445	-3.610592
C	-3.165506	-0.909043	0.751462
H	-4.032795	-1.469576	1.081274
O	-3.233239	0.467177	1.097097
H	-2.109968	0.856606	1.963853
H	-4.136476	0.749807	1.305203
C	-1.005348	-0.440580	-0.277593
H	-1.398951	0.550989	-0.530064
H	-0.478758	-0.800654	-1.161121
N	0.056168	-0.289888	0.777246
S	0.069953	1.079999	1.672557
C	1.350096	0.849510	2.838595
O	0.201626	2.322044	0.937826
O	-1.233405	0.993245	2.515612
H	0.999421	-0.521600	0.474282

C	2.351326	1.818365	2.895374
C	3.369005	1.656753	3.823402
C	3.395629	0.554812	4.686468
C	2.370561	-0.395810	4.599846
C	1.340621	-0.261338	3.681709
H	2.324728	2.677030	2.233132
H	4.155722	2.402915	3.882291
C	4.505284	0.407024	5.690016
H	2.377630	-1.251693	5.267394
H	0.544262	-0.995489	3.624139
H	4.406691	-0.514119	6.268601
H	5.481273	0.395179	5.194074
H	4.508113	1.248500	6.390830

Freq

8.7102	12.9275	20.8836
24.6764	33.0526	40.2170
50.7357	66.1486	77.9687
86.9097	96.3269	127.4726
137.6804	146.4991	158.0091
190.6139	202.6029	209.5445
232.5707	264.0260	270.8332
286.5279	290.9761	316.6723
324.9746	329.8400	338.9065
367.2710	380.1669	411.7282
412.6979	421.1743	469.0810
480.0450	516.2739	521.9844
554.0675	629.0443	637.2163
643.1351	648.6083	690.1622
704.4657	723.0200	731.2268
759.5953	768.3798	801.3904
835.4132	845.2094	858.1650
871.7863	875.8068	932.9542

979.9996	996.2907	1003.0067
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1043.9516	1046.4211	1054.2283
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1115.9693	1120.9986	1126.5718
1164.3062	1167.9041	1170.6506
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1257.9394	1264.0178	1296.6413
1306.6548	1357.7364	1361.4842
1374.1075	1403.2430	1408.5803
1409.5910	1423.0391	1442.4068
1452.5893	1465.3870	1468.0326
1468.2494	1487.2006	1514.5851
1520.4957	1521.2308	1522.3553
1528.5804	1534.6999	1539.5305
1544.8896	1556.2254	1654.1227
1657.2779	1680.5595	1708.8165
2425.4594	3084.6887	3091.7740
3101.9369	3103.5546	3145.3759
3171.6779	3171.9040	3175.0079
3177.5010	3208.7601	3210.3542
3230.5575	3232.7975	3253.1185
3254.3010	3254.9423	3313.1173
3332.6686	3572.4555	3801.9019

C5

C	0.552172	3.673164	-0.887077
H	0.814082	2.794797	-0.299466
H	0.329230	4.573781	-0.316912
Au	-1.371560	3.127822	-1.759887
C	1.267392	3.858249	-2.070004
O	1.305368	5.030948	-2.628944
H	1.876274	5.058091	-3.452614

C	2.071953	2.733257	-2.688608
H	1.769520	1.789315	-2.235501
H	3.125903	2.892299	-2.415689
C	-3.268092	2.683595	-2.357170
N	-3.933519	1.519280	-2.197339
C	-3.409473	0.314464	-1.565206
H	-3.996692	0.074922	-0.676156
H	-3.449622	-0.520570	-2.267809
H	-2.375258	0.493387	-1.274734
C	-5.213675	1.618055	-2.705985
H	-5.910925	0.794919	-2.675040
C	-5.343587	2.873322	-3.192647
H	-6.176996	3.364409	-3.671125
N	-4.140188	3.512932	-2.970185
C	-3.885082	4.900204	-3.341950
H	-4.558356	5.562202	-2.793260
H	-2.854532	5.148053	-3.091437
H	-4.037354	5.029134	-4.415509
N	1.893620	2.631086	-4.144787
S	3.103388	3.394772	-5.055730
C	2.575586	3.116510	-6.710583
O	2.932541	4.814305	-4.685572
O	4.399017	2.772767	-4.833819
H	1.782066	1.668137	-4.453603
C	3.277168	2.197832	-7.489673
C	2.873312	1.994173	-8.801478
C	1.790419	2.695687	-9.343737
C	1.113358	3.615720	-8.535566
C	1.498110	3.836400	-7.220566
H	4.131910	1.672090	-7.077944
H	3.416757	1.286344	-9.420653
C	1.380507	2.469843	-10.773491
H	0.280719	4.177424	-8.947917

H	0.983722	4.567163	-6.605951
H	0.504187	3.065149	-11.040412
H	2.192155	2.739331	-11.457498
H	1.143123	1.415944	-10.951855

Freq

10.5125	11.0999	13.5463
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74.7421	88.7078	103.2177
127.3565	153.2238	163.1821
171.7433	203.7176	206.7434
232.9878	250.2841	266.2821
272.3500	290.4034	331.5003
340.9774	344.2882	380.4199
404.3013	421.9153	444.7107
448.3438	469.4541	502.9613
523.4478	545.3554	573.2390
624.8451	628.2227	638.5383
650.8618	669.4435	701.8773
734.8354	739.0633	766.0149
767.4932	774.8742	824.6496
834.2416	845.3407	873.2531
884.1794	898.2284	903.1927
951.0197	1000.6275	1021.6393
1026.8902	1028.0661	1043.3946
1047.9134	1064.6781	1082.0073
1087.6065	1092.4682	1107.4076
1117.8647	1122.8342	1156.1374
1160.7851	1168.8532	1173.2373
1175.0638	1228.9747	1257.7204
1265.9121	1298.1283	1309.1623
1313.2293	1353.7948	1358.7602

1403.1776	1405.5224	1415.4579
1452.8233	1454.5257	1465.4089
1468.0151	1468.9522	1485.1949
1489.6422	1500.0196	1515.1010
1517.8883	1518.5593	1522.6081
1523.3763	1531.2649	1539.0989
1548.8997	1559.6911	1639.9886
1654.3297	1659.7527	1684.8259
3060.3426	3083.1331	3107.8715
3108.0891	3143.2448	3154.6884
3160.4174	3168.1490	3181.8766
3184.0845	3184.7794	3212.2430
3212.7569	3226.1397	3228.3815
3242.0305	3251.6072	3254.7693
3315.5591	3334.5961	3569.8147

C4

Au	-0.325829	3.599174	-1.158237
C	0.148186	1.484746	0.005676
O	0.634154	1.633049	1.240011
H	-0.039446	1.907129	1.884272
H	0.912972	1.120494	-0.672958
C	-1.160408	1.618776	-0.391598
H	-1.418534	1.194016	-1.359385
C	0.212023	5.417528	-1.896074
N	1.403858	5.770733	-2.423965
C	2.558183	4.898662	-2.603242
H	2.764474	4.765368	-3.667482
H	3.429693	5.335394	-2.111483
H	2.339871	3.931450	-2.153272
C	1.388028	7.098017	-2.802640
H	2.242595	7.577900	-3.254190
C	0.158497	7.574190	-2.498806

H	-0.272397	8.554941	-2.628078
N	-0.550849	6.528243	-1.946008
C	-1.918366	6.648106	-1.442388
H	-1.908916	6.998142	-0.407622
H	-2.457475	7.364250	-2.064072
H	-2.414105	5.680580	-1.502940
C	-2.303061	1.744813	0.599579
H	-2.199151	2.624772	1.250556
H	-2.297442	0.861547	1.249415
N	-3.608207	1.730713	-0.071673
S	-4.157318	3.232460	-0.629388
C	-5.751980	2.813361	-1.252743
O	-4.290132	4.171577	0.483627
O	-3.246283	3.592071	-1.721306
C	-6.880765	3.170300	-0.517290
C	-8.132717	2.842021	-1.018363
C	-8.271887	2.170006	-2.238305
C	-7.118317	1.832672	-2.954246
C	-5.855604	2.150704	-2.473019
H	-6.774200	3.706806	0.419480
H	-9.019736	3.118843	-0.455708
C	-9.639634	1.828822	-2.764495
H	-7.210950	1.318366	-3.905972
H	-4.964795	1.899029	-3.038543
H	-9.583326	1.296706	-3.716993
H	-10.185403	1.197480	-2.055603
H	-10.235775	2.734501	-2.917941
H	-4.329035	1.318110	0.517111

Freq

12.1669	13.6293	14.3063
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47.3712	55.2240	66.1371

73.5669	108.0059	110.1499
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166.7531	176.2364	208.2768
217.7433	224.4974	256.2633
274.0644	277.3083	306.1451
320.6015	339.0182	347.7409
365.3395	400.0275	421.5138
435.4185	457.6883	472.4174
506.8403	531.4594	551.1233
570.2538	626.4220	639.6992
644.8798	653.0427	672.8165
704.5274	728.3428	735.2763
764.0954	768.6928	799.0692
834.7782	848.0291	864.8604
874.7667	883.2008	1001.9239
1002.7304	1012.0502	1021.1141
1025.6537	1027.8156	1044.2280
1050.1288	1068.2797	1087.6375
1106.6911	1119.0657	1120.9662
1126.6885	1141.2115	1158.6405
1166.3353	1169.8173	1174.0515
1180.3304	1227.9533	1238.0520
1257.2943	1268.3262	1296.3613
1321.6304	1352.6358	1357.5459
1365.4482	1397.7757	1406.5780
1415.1420	1439.7244	1452.1480
1464.5718	1469.7402	1471.1469
1485.7370	1495.2654	1515.5640
1517.4314	1522.7084	1527.7258
1530.4937	1533.7446	1540.9248
1549.3034	1559.6571	1645.0033
1652.1488	1659.5412	1685.3662
3045.8368	3082.6043	3098.6463

3108.3919	3110.1571	3142.5399
3167.8891	3184.8231	3189.8552
3213.7913	3213.8835	3223.3945
3224.0538	3228.4911	3250.3000
3252.1349	3259.3009	3316.6791
3335.6296	3557.5735	3757.1697

CTS2

C	4.327586	0.116980	-1.129757
C	3.719952	-0.443436	-0.007427
C	4.409021	-1.286271	0.867297
C	5.741424	-1.557522	0.605356
C	6.389019	-1.008677	-0.510310
C	5.664161	-0.173775	-1.367093
S	2.049703	-0.095430	0.366444
O	1.354919	-1.178556	1.030992
C	7.830821	-1.334005	-0.783591
N	2.093422	1.209014	1.379699
C	0.783566	1.808772	1.732295
C	0.228638	2.619560	0.580823
O	0.789268	3.854905	0.608169
C	-0.553317	2.118963	-0.399904
Au	-1.900204	0.539466	-0.233109
C	-3.305265	-0.945876	-0.070809
N	-3.109896	-2.227174	0.313045
C	-4.299174	-2.929893	0.297580
C	-5.257200	-2.064491	-0.104600
N	-4.629991	-0.853609	-0.325024
C	-1.831160	-2.817592	0.689236
C	-5.326025	0.344598	-0.775821
O	1.425295	0.337968	-0.978632
H	-1.892056	-3.215251	1.704799
H	-1.058158	-2.051736	0.649981

H	-1.575692	-3.622605	-0.003705
H	-4.356610	-3.971842	0.572436
H	-6.317722	-2.199933	-0.251242
H	-5.762230	0.174685	-1.762777
H	-4.609750	1.163002	-0.834589
H	-6.114186	0.605877	-0.066290
H	-0.748064	2.816153	-1.220946
H	0.459756	4.397738	-0.127073
H	0.107636	1.001746	2.013571
H	0.957577	2.439202	2.606027
H	0.537181	1.005961	-0.805854
H	2.792861	1.890530	1.085711
H	3.908608	-1.722469	1.725432
H	6.291298	-2.211906	1.275074
H	6.150938	0.250730	-2.239450
H	3.766004	0.747598	-1.809788
H	8.243078	-0.705429	-1.575972
H	8.441822	-1.199845	0.114140
H	7.935706	-2.379334	-1.094855

Freq

-510.8478	11.0232	20.8173
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47.4699	50.7458	61.6486
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115.6900	138.5682	157.3536
165.2462	185.5276	202.6966
205.5079	262.4195	272.4922
273.8765	292.7480	297.2229
318.3397	342.8093	366.8899
380.8376	418.3501	447.2555
456.9370	470.3718	485.6433
520.4897	535.9147	555.2193

618.2120 628.1409 637.8015

648.3190 666.1413 689.2948

706.6797 721.6378 735.5389

760.7591 762.5127 767.3048

821.9092 845.4371 864.0270

868.2407 877.8646 904.1057

922.9856 936.9831 1005.5039

1009.1229 1019.7154 1029.2628

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1358.2033 1363.6393 1407.1436

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1520.9540 1523.9590 1530.0400

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1654.3904 1655.8056 1680.0781

1689.4959 3084.0759 3104.8081

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3146.4844 3173.3634 3177.2277

3179.8145 3207.7140 3210.6126

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E1

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C	-1.457034	-3.198575	0.033986
C	-0.373649	-4.032005	0.346236
H	0.627173	-3.616392	0.402667
C	-0.591968	-5.381244	0.590019
H	0.244687	-6.026290	0.837716
C	-1.882654	-5.903224	0.523513
H	-2.049297	-6.957813	0.719243
C	-2.961256	-5.076828	0.212547
H	-3.965641	-5.485158	0.168055
C	-2.754339	-3.726468	-0.035065
H	-3.589285	-3.074624	-0.271091
C	-1.079695	-0.576712	-0.253516
Au	-0.796600	-1.116474	-2.411140
C	-0.453575	-1.068671	-4.402652
N	0.109513	-0.046924	-5.079643
C	0.573835	1.212118	-4.502271
H	1.645481	1.323886	-4.680777
H	0.383493	1.209813	-3.428052
H	0.037401	2.044897	-4.961993
C	0.190696	-0.349650	-6.424382
H	0.609518	0.336912	-7.143981
C	-0.333992	-1.586811	-6.579473
H	-0.462970	-2.196065	-7.460826
N	-0.726548	-2.013436	-5.325746
C	-1.339675	-3.311614	-5.068822
H	-2.250279	-3.413773	-5.662539
H	-0.640929	-4.110578	-5.325662
H	-1.590530	-3.378803	-4.011018
C	-0.966563	0.856583	0.106660
H	-0.849252	0.908864	1.198408
H	-1.914789	1.343699	-0.139679
N	0.098169	1.517872	-0.646061
H	0.040774	2.524442	-0.513761

H 1.012343 1.225688 -0.308118

Freq

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163.8494	211.5328	226.2282
265.3665	276.2214	299.4791
328.8880	351.9523	357.9375
394.4512	416.3803	469.8770
522.6204	545.4007	590.9256
627.2463	638.3653	639.8033
707.4951	709.1351	735.4556
764.7259	768.0995	788.4165
877.3098	884.7003	889.4322
939.8035	971.4756	1013.7389
1017.7706	1028.6482	1046.6116
1049.0116	1066.6666	1066.8915
1107.7656	1120.7890	1124.7602
1124.8455	1170.2141	1176.2053
1179.8509	1203.7263	1207.4817
1220.1667	1264.9073	1273.2555
1338.8007	1340.0110	1374.4764
1402.5264	1417.7683	1438.1409
1471.8689	1473.6694	1495.9459
1506.1432	1517.5194	1518.3419
1527.7903	1533.6292	1541.9703
1551.9811	1552.9741	1654.2628
1660.3976	1684.1392	1709.9526
2244.6804	3052.7542	3100.8655
3108.5722	3129.4526	3182.9914
3185.9942	3196.4517	3211.9070

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3246.4197	3252.3902	3316.0727
3334.9903	3526.1182	3608.5072

TSE

C	-1.742620	1.607327	0.226450
C	-1.574723	0.362646	0.159455
Au	0.544799	0.175197	0.039779
C	2.538042	-0.229157	-0.072473
N	3.225056	-0.648194	-1.156145
C	2.669058	-0.891645	-2.481556
H	1.615675	-0.616221	-2.477530
H	2.764102	-1.948949	-2.736807
H	3.198092	-0.286806	-3.220496
C	4.555012	-0.840188	-0.841970
H	5.275658	-1.176185	-1.570926
C	4.694845	-0.532361	0.466426
H	5.562254	-0.544321	1.107570
N	3.446870	-0.160008	0.923201
H	3.455959	-0.560884	2.980880
H	2.119924	0.459960	2.403224
C	3.182248	0.245685	2.298003
H	3.758209	1.141349	2.539315
C	-2.413673	-0.841646	0.124169
C	-3.421697	-0.949993	-0.840071
H	-3.545859	-0.163338	-1.578406
C	-4.236676	-2.074569	-0.872078
H	-5.012654	-2.154518	-1.626392
C	-4.057011	-3.095008	0.056569
H	-4.697011	-3.970572	0.032288
C	-3.050131	-2.993109	1.010467
H	-2.904415	-3.787791	1.734604
C	-2.221854	-1.877845	1.039407

H	-1.434744	-1.800579	1.782506
C	-1.480484	3.057889	0.260998
O	-3.871611	2.050149	0.374729
H	-3.792723	2.728229	-0.331798
H	-4.408491	1.318430	0.035981
N	-2.174511	3.735062	-0.835464
H	-1.864596	3.452445	1.205822
H	-0.390662	3.196115	0.265715
H	-2.172462	4.739962	-0.684615
H	-1.716435	3.555701	-1.725230

Freq

i217.7854	11.2784	26.3225
29.9890	41.9652	51.1402
54.0688	63.0289	75.3247
85.3096	103.5005	129.5820
155.4442	171.5336	183.5674
216.9847	223.7579	258.6645
261.6432	269.4879	284.0099
317.8742	347.2699	355.6025
417.8190	454.5104	468.6345
479.1759	495.2889	543.8645
595.6018	607.6541	629.7287
637.9430	642.4351	700.2734
723.4424	764.0426	767.9432
768.9222	782.9979	797.4401
875.2560	875.5775	898.0495
937.3519	955.9436	1001.6372
1015.3095	1028.6904	1036.4980
1051.1411	1068.5692	1072.8092
1100.5732	1121.4884	1124.7076
1124.8638	1170.3616	1175.2745
1179.6300	1202.7774	1208.5215

1220.9408	1264.8593	1267.4281
1331.5995	1336.5307	1371.8830
1408.6876	1423.5263	1443.0214
1472.6987	1473.2499	1493.8068
1506.2786	1511.5305	1520.7865
1521.7938	1535.2874	1543.0728
1553.9789	1560.2487	1660.8192
1662.2306	1672.0468	1694.3374
1699.6695	2042.1843	3063.0590
3111.7432	3112.0727	3141.6343
3189.3518	3189.9740	3216.7388
3216.9359	3217.6881	3226.5861
3235.2202	3242.8651	3253.0981
3320.7932	3340.0111	3531.4135
3551.8214	3618.0746	3829.3627

E2

C	-0.841270	-1.971237	0.332170
C	-2.111656	-2.407792	-0.164596
C	-2.421366	-2.280090	-1.524555
H	-1.688524	-1.855118	-2.202052
C	-3.655484	-2.702783	-1.997588
H	-3.889596	-2.605379	-3.052455
C	-4.586960	-3.256520	-1.124039
H	-5.548684	-3.591178	-1.498953
C	-4.283918	-3.388884	0.228073
H	-5.006357	-3.830010	0.906938
C	-3.052986	-2.966621	0.710396
H	-2.804559	-3.079494	1.760695
C	0.223567	-1.599825	0.761724
C	1.506310	-1.146971	1.278318
H	2.336100	-1.603812	0.727952
H	1.614685	-1.419572	2.331266

N	1.617471	0.345988	1.192394
H	1.664987	0.612558	0.207894
H	2.503615	0.639695	1.605863
Au	-0.027215	1.395079	2.063579
C	-1.612475	2.343878	2.851728
N	-2.902766	1.963932	2.743135
C	-3.397304	0.793351	2.025218
H	-4.028706	0.199154	2.688041
H	-3.974493	1.106909	1.153095
C	-3.722913	2.858038	3.400227
H	-4.794186	2.736684	3.434364
C	-2.921309	3.809820	3.927566
H	-3.152545	4.684360	4.515158
N	-1.627250	3.478333	3.581181
C	-0.463800	4.268578	3.965033
H	-0.531581	5.266397	3.527195
H	0.433819	3.774060	3.597728
H	-0.413218	4.347035	5.052629
H	-2.553108	0.188129	1.698584

Freq

13.5922	15.2266	18.9023
29.2210	40.3540	44.4529
47.2115	91.2425	92.5801
127.5052	157.7352	172.5408
201.0528	219.0244	270.3872
270.5798	296.8383	351.7306
357.1068	399.2705	415.7947
427.1403	471.4477	522.5403
548.4447	583.1872	628.6593
637.7405	642.0515	686.4781
710.5704	712.2657	757.6650
766.9789	770.6430	787.4062

877.2076	883.9923	957.5862
963.5204	992.5166	1014.0600
1030.0233	1040.8376	1045.8636
1050.1139	1067.0114	1074.1775
1119.0679	1123.4742	1124.1492
1167.3179	1172.2128	1182.9417
1198.9022	1202.3145	1220.0576
1227.4345	1266.4139	1309.2147
1340.2976	1353.9368	1374.6875
1406.4670	1420.1065	1444.9193
1468.7907	1474.9411	1490.7180
1507.7662	1517.0031	1517.6737
1523.5982	1531.4687	1539.5981
1553.0570	1560.7196	1658.3534
1665.5825	1684.5759	1695.0355
2392.2272	3095.4632	3111.5635
3111.9296	3148.5871	3188.6268
3189.4037	3216.4820	3217.0114
3225.2449	3231.2144	3238.5329
3245.4640	3252.4366	3320.6732
3339.6481	3496.5954	3563.6889

TSA2

N	3.975663	0.116163	1.450162
C	3.218145	0.565183	0.411117
N	3.770384	1.762480	0.069554
C	4.858163	2.056777	0.886923
C	4.986815	1.023663	1.753969
Au	1.621512	-0.363634	-0.470855
C	0.093578	-1.405270	-1.467031
C	-0.842110	-2.138809	-0.805112
O	-1.560364	-3.182237	-1.324809

C	3.313235	2.632220	-1.013162
C	3.778447	-1.143861	2.164377
C	-1.362604	-1.794648	0.567355
N	-2.468130	-0.828803	0.457534
C	-2.471537	0.311928	-0.265813
C	-3.746722	1.001002	-0.069352
C	-4.515561	0.216955	0.803112
C	-3.723366	-0.976347	1.169220
C	-4.222990	2.186473	-0.595349
C	-5.514593	2.579872	-0.217119
C	-6.280568	1.800976	0.650747
C	-5.787319	0.596214	1.177047
O	-1.511457	0.718286	-1.015527
O	-3.966169	-1.920212	1.898307
H	-3.625696	2.786081	-1.270735
H	-5.925020	3.503206	-0.606538
H	-7.275515	2.131223	0.922932
H	-6.382038	-0.011430	1.847799
H	-1.773289	-2.678597	1.056974
H	-0.573735	-1.364975	1.187250
H	-1.268792	-3.420338	-2.229298
C	0.356590	-1.754704	-2.900252
H	2.427637	2.191940	-1.467405
H	4.092417	2.729195	-1.771227
H	3.061666	3.618211	-0.618872
H	5.434031	2.958681	0.777126
H	5.695212	0.853381	2.545350
H	4.695868	-1.734040	2.137603
H	3.499012	-0.950679	3.201784
H	2.983112	-1.703426	1.675546
H	-0.684015	-0.036237	-1.200642
C	-0.652649	-1.602177	-3.866802
C	-0.420284	-1.924703	-5.203154

C	0.823772	-2.410199	-5.598746
C	1.834014	-2.569130	-4.650607
C	1.604052	-2.243409	-3.316622
H	-1.620478	-1.206002	-3.572953
H	-1.210193	-1.792452	-5.933623
H	1.006041	-2.661322	-6.636849
H	2.803845	-2.948698	-4.951012
H	2.394652	-2.370734	-2.584955

Freq

i537.1236	11.3398	19.4976
24.4248	32.3358	36.2188
46.3630	58.8086	65.7333
72.0442	77.4211	85.2572
116.8830	131.0838	144.8006
154.2648	169.0573	184.6829
195.5003	209.1911	209.7154
251.8275	268.9461	284.8711
289.7649	294.9273	319.6414
352.9809	385.1154	412.5928
429.1365	436.3667	478.8944
480.4742	494.5982	515.9206
547.1244	558.0070	604.0081
630.0733	633.9522	647.3884
657.0140	660.1331	687.9328
696.3814	728.9980	730.4777
745.1880	748.6536	776.7831
780.9800	797.6267	809.4235
811.3630	841.7116	863.0331
900.6038	913.0801	914.5587
925.3050	962.0040	966.6441
988.1186	999.5473	1029.6030
1034.5028	1045.1903	1049.7199

1058.6648	1065.0682	1068.0709
1070.8576	1083.7453	1089.9672
1098.5745	1125.4172	1135.0049
1137.3370	1141.5937	1146.7280
1188.8803	1191.6308	1192.9080
1199.2362	1231.1416	1233.4981
1236.2350	1247.2154	1248.8950
1280.7966	1296.5412	1331.4186
1347.3477	1363.7929	1381.2278
1399.0617	1402.4406	1403.6195
1428.9865	1442.3940	1452.1273
1461.9391	1472.7659	1514.5115
1516.8413	1522.2755	1534.2263
1540.9003	1541.4502	1542.4319
1543.9792	1556.9185	1560.5031
1564.4434	1569.0605	1657.9950
1666.8275	1671.2098	1695.5810
1701.8365	1703.9221	1709.7870
1849.1423	3106.7358	3107.2593
3129.2904	3189.1014	3189.4032
3197.3525	3209.5063	3217.7598
3219.3046	3224.3649	3237.2049
3245.3945	3250.4171	3259.8443
3260.5018	3268.0691	3274.6548
3341.7141	3364.3267	3638.3890

D1

Au	0.039775	1.889404	-0.696129
C	2.028034	1.498553	-1.798075
C	1.419730	2.379565	-2.398468
H	1.092269	3.146328	-3.074256
C	-1.497949	1.818216	0.620943
N	-1.636040	2.539809	1.753395

C	-0.690659	3.525586	2.269288
H	-0.323766	3.209162	3.247700
H	0.147307	3.607392	1.578676
H	-1.181713	4.496727	2.356001
C	-2.819442	2.221048	2.384741
H	-3.122470	2.687429	3.309697
C	-3.427633	1.280316	1.624328
H	-4.366341	0.763840	1.754530
N	-2.602254	1.045441	0.545266
C	-2.913822	0.086414	-0.510482
H	-2.116183	0.104697	-1.251628
H	-2.991568	-0.916978	-0.087181
H	-3.856410	0.358724	-0.989214
C	3.003118	0.473663	-1.307878
H	2.511222	-0.501877	-1.281205
H	3.283984	0.712320	-0.277891
N	4.165181	0.385413	-2.141052
H	4.040259	-0.165024	-2.980086
C	5.075170	1.449762	-2.276027
C	5.147060	2.493010	-1.349784
H	4.472527	2.534779	-0.500825
C	6.104960	3.494284	-1.500521
H	6.152252	4.294351	-0.767865
C	6.992098	3.477204	-2.569639
H	7.734850	4.259879	-2.681373
C	6.914479	2.438877	-3.496692
H	7.599716	2.407390	-4.338172
C	5.966716	1.435304	-3.355065
H	5.922899	0.624235	-4.077964

Freq

7.1738	14.1591	22.8247
40.4263	45.5075	62.7009

66.9415	86.2347	107.7665
131.0300	166.5961	172.1116
210.8273	228.0285	261.0640
269.3492	275.2585	339.2434
349.0346	350.6230	409.0002
422.2465	470.9579	484.9663
522.5066	567.3907	615.2968
626.7450	639.1928	640.8408
671.2571	705.5776	710.3942
765.9540	772.0368	776.7021
780.1024	810.7782	842.7376
872.1050	891.2262	913.9168
995.5536	1017.2777	1021.2283
1024.5479	1049.7864	1067.0813
1071.4449	1118.7685	1123.3921
1124.8666	1160.1486	1168.0962
1172.9840	1181.3524	1198.0299
1225.3709	1266.4919	1291.8748
1310.1155	1364.0422	1379.9287
1402.5870	1403.3875	1423.3621
1464.9782	1469.2527	1490.0372
1492.9040	1502.8227	1516.7849
1517.4693	1532.1480	1537.4668
1551.1486	1558.9342	1573.9664
1652.5718	1682.9914	1696.2821
2118.5494	3108.8357	3111.3270
3111.4036	3155.0087	3190.0416
3190.1432	3203.7391	3214.6405
3214.8761	3217.2522	3229.4474
3234.5423	3248.4130	3316.1585
3334.7123	3433.3040	3630.9276

TSD-cycliz

C	5.186033	1.276920	-2.300388
C	6.202755	1.802242	-1.484518
H	6.397108	1.338680	-0.522918
C	6.968844	2.854022	-1.939194
H	7.774733	3.235717	-1.319966
C	6.740650	3.427767	-3.209123
H	7.379443	4.232947	-3.556731
C	5.737414	2.941486	-4.010790
H	5.579018	3.346323	-5.005697
C	4.894985	1.898244	-3.540195
N	4.339824	0.280766	-1.828431
C	3.291071	0.832819	-0.952571
H	3.714975	1.086624	0.023256
C	2.726112	2.088955	-1.574403
C	3.241521	2.778567	-2.523342
Au	0.943665	2.963791	-0.883370
C	-0.794522	3.743060	-0.141946
N	-0.926480	4.678977	0.823230
C	0.166140	5.337435	1.529179
H	0.115664	6.416252	1.367290
H	1.111374	4.959188	1.142391
H	0.101349	5.122982	2.598076
C	-2.259972	4.944393	1.065083
H	-2.579747	5.665510	1.801541
C	-2.971793	4.153954	0.229824
H	-4.036820	4.047079	0.092205
N	-2.056581	3.424354	-0.503122
C	-2.433497	2.446220	-1.516528
H	-1.528487	2.053058	-1.977508
H	-2.990319	1.627304	-1.055841
H	-3.049027	2.924358	-2.281291
H	2.528911	0.069103	-0.789988

H	3.899139	-0.213839	-2.599571
H	4.237351	1.395668	-4.244983
H	3.205260	3.693700	-3.084924

Freq

i282.6795	10.5124	26.4915
32.9133	66.9032	70.8648
72.1879	101.6652	129.7599
138.5982	157.3164	178.2697
197.1435	222.9639	226.8302
268.9052	271.9949	343.9136
384.1126	413.2968	421.4855
441.1157	471.5414	519.7140
597.4915	627.8605	628.2784
638.0789	651.8875	702.1952
730.7998	736.8860	765.9430
767.2636	796.7672	820.2753
856.6616	882.5886	891.1878
908.8001	935.4813	1009.1656
1012.9864	1025.7970	1047.5148
1048.0002	1053.7466	1057.2125
1064.8498	1071.9069	1114.4428
1117.7705	1122.6112	1169.2550
1173.5047	1174.3388	1205.4967
1210.9238	1255.5157	1265.4935
1300.6214	1346.9712	1377.7958
1397.8154	1406.3314	1414.9349
1468.5115	1469.1185	1482.0205
1489.4554	1502.6845	1518.4215
1518.9732	1530.8146	1534.5629
1539.3558	1548.1726	1559.6528
1640.4529	1654.3751	1689.9786
1766.2218	3107.1761	3107.4385

3121.0093	3179.1714	3183.2234
3183.5705	3211.7302	3211.8405
3212.1815	3229.9733	3235.5998
3246.1418	3252.8110	3315.1300
3334.2327	3396.3447	3554.3056

D2

C	4.045951	-0.753158	-0.868878
C	2.431460	-0.412936	-0.845334
C	1.637239	-0.548615	0.216018
C	2.192884	-0.928384	1.568797
H	1.614137	-1.710996	2.063086
H	2.218361	-0.063894	2.237723
N	3.591878	-1.444517	1.380565
H	3.510762	-2.357131	0.935454
C	4.263562	-0.576081	0.566978
C	4.844577	0.598339	1.061273
H	4.899752	0.750984	2.133680
C	5.398152	1.495352	0.176327
H	5.897172	2.379501	0.562668
C	5.353623	1.295896	-1.234558
H	5.839691	2.013380	-1.886821
C	4.736135	0.200423	-1.744300
H	4.726635	0.016790	-2.814862
H	4.114477	-1.786328	-1.223359
H	2.102861	-0.060704	-1.815463
Au	-0.401778	-0.246524	0.057029
C	-2.435041	0.053633	-0.081397
N	-3.112118	1.207037	0.115538
C	-2.517390	2.489883	0.466769
H	-2.750544	3.231099	-0.300896
H	-2.902080	2.828145	1.431547
H	-1.437210	2.366487	0.532248

C	-4.469090	1.017045	-0.061057
H	-5.183532	1.817990	0.051472
C	-4.640259	-0.286674	-0.376123
H	-5.534039	-0.851236	-0.593020
N	-3.383650	-0.860667	-0.384189
C	-3.142820	-2.267779	-0.676148
H	-3.626800	-2.894248	0.076589
H	-3.535058	-2.514238	-1.665202
H	-2.068823	-2.448066	-0.659622

Freq

8.2956	28.3247	34.6437
72.2494	75.1511	76.0488
111.4406	133.5926	147.2612
165.6335	183.4472	207.8638
223.7938	251.3269	271.1776
281.4292	339.8937	398.8176
423.4655	441.0952	458.6133
477.9399	500.3938	566.2935
607.2876	628.6664	637.4627
650.3636	703.4144	740.5574
762.3408	767.5799	779.0693
802.5426	825.4544	830.5917
878.6891	896.4093	918.6022
963.7429	981.8858	1003.5308
1026.7832	1037.9782	1047.0012
1059.2375	1063.8410	1064.6891
1086.8721	1103.2177	1116.8595
1121.7217	1169.8693	1170.4795
1174.1030	1198.0619	1216.4776
1235.0315	1264.8262	1272.8282
1313.3239	1340.2358	1389.0111
1408.3694	1411.3924	1426.6006

1467.5842	1468.7046	1481.9129
1488.3223	1501.1499	1519.4005
1519.8632	1526.3745	1529.6631
1539.6196	1542.3108	1546.1743
1606.0055	1631.0851	1654.6113
1704.8390	3104.5507	3105.0930
3118.2410	3123.3239	3175.7782
3179.0787	3179.7478	3210.2132
3210.8612	3230.9088	3236.0951
3251.7697	3256.1513	3258.8554
3314.1322	3333.4993	3526.9987

D-Adduct to nitrogen

C	5.180079	1.509872	-1.957504
C	5.188416	2.064705	-0.681790
H	4.679284	1.564408	0.137243
C	5.854994	3.264175	-0.464533
H	5.859205	3.702265	0.527887
C	6.518111	3.897555	-1.511406
H	7.040923	4.831660	-1.336855
C	6.507417	3.332223	-2.781023
H	7.018830	3.822982	-3.602077
C	5.830988	2.138606	-3.010057
H	5.808438	1.706980	-4.006896
N	4.473886	0.250226	-2.192237
H	4.685541	-0.033569	-3.149854
C	2.978132	0.392402	-2.122917
H	2.727945	0.762296	-1.126686
H	2.550935	-0.609435	-2.219329
C	2.458724	1.275201	-3.160488
C	2.037154	1.985944	-4.031900
H	1.652890	2.623492	-4.797846
Au	5.245437	-1.321340	-0.955018

C	6.007878	-2.785088	0.191822
N	7.107723	-2.708544	0.969841
C	7.975250	-1.545698	1.121380
H	7.513265	-0.690579	0.630259
H	8.105583	-1.323622	2.181920
H	8.947481	-1.742765	0.665124
C	7.331716	-3.912979	1.604811
H	8.164264	-4.063508	2.273968
C	6.347249	-4.751126	1.211734
H	6.146958	-5.778857	1.471024
N	5.542437	-4.042136	0.343374
C	4.360340	-4.606261	-0.297431
H	3.635245	-4.907228	0.461154
H	3.914811	-3.850998	-0.942486
H	4.643972	-5.471930	-0.898923

Freq

16.3387	19.0252	24.0965
32.5599	36.3306	38.3391
51.7418	84.1210	105.2970
131.9587	164.6299	169.0146
188.2377	214.8573	236.7605
269.3378	270.1049	322.0221
351.6673	357.0451	421.9090
471.4946	494.8790	524.5144
564.0705	628.7074	634.2327
637.7876	681.9436	691.4222
708.9840	717.9237	737.0591
766.7667	768.4747	791.2500
810.1094	860.8875	885.2015
944.9817	964.9223	1004.4716
1008.4042	1029.2092	1038.9993
1047.9745	1049.9325	1066.8620

1070.6192	1120.0329	1123.5875
1125.9932	1167.9779	1172.5392
1180.8630	1183.4466	1203.0582
1219.2695	1231.9972	1266.9253
1275.1777	1359.9680	1375.5609
1401.2121	1406.9878	1420.3502
1467.9626	1470.2030	1474.4692
1491.9822	1512.1003	1517.0554
1517.9065	1532.2479	1540.1069
1544.4388	1553.1388	1561.4858
1658.6304	1693.7345	1698.1136
2287.7556	3111.5652	3112.0646
3119.4361	3169.1320	3189.1938
3189.5567	3214.3942	3216.0493
3216.4211	3217.1481	3236.5257
3245.4279	3255.9330	3320.6950
3339.6368	3499.7651	3508.4890

Cyclization product from A1

N	2.322745	-2.017355	-1.511989
C	2.022435	-3.229125	-1.064396
O	0.845991	-3.601145	-0.754034
C	3.221761	-4.060965	-0.986890
C	4.283257	-3.260603	-1.420259
C	3.738464	-1.921457	-1.769189
O	4.261321	-0.924735	-2.176769
C	5.572623	-3.746359	-1.473812
H	6.395733	-3.125122	-1.810783
C	5.771773	-5.075076	-1.075557
H	6.772367	-5.493909	-1.103570
C	4.711117	-5.871621	-0.644830

H	4.902154	-6.896668	-0.345330
C	3.404704	-5.373728	-0.593240
H	2.576863	-5.991424	-0.261771
C	1.337787	-0.937732	-1.688026
H	1.648421	-0.093059	-1.066757
H	1.382752	-0.606417	-2.729482
C	-0.050547	-1.399944	-1.325201
C	-0.273542	-2.644607	-0.913429
C	-1.514937	-3.350489	-0.548153
C	-1.583720	-4.115297	0.621548
H	-0.716305	-4.189695	1.270459
C	-2.760604	-4.770058	0.965686
H	-2.804176	-5.355079	1.879064
C	-3.881212	-4.673483	0.143455
H	-4.797869	-5.190309	0.410227
C	-3.816993	-3.922959	-1.027356
H	-4.680247	-3.860987	-1.683035
C	-2.639235	-3.268651	-1.375213
H	-2.580886	-2.703364	-2.299647
Au	-1.552939	0.009944	-1.438038
C	-3.039934	1.428761	-1.496691
N	-4.198781	1.416945	-0.799911
C	-4.611441	0.383047	0.141110
H	-4.635067	0.787142	1.155870
H	-3.898137	-0.439003	0.096371
H	-5.602926	0.013495	-0.128945
C	-4.951088	2.541460	-1.078623
H	-5.911884	2.720882	-0.621200
C	-4.244360	3.269668	-1.972449
H	-4.465821	4.210259	-2.452845
N	-3.076952	2.572406	-2.216597

C	-2.042537	3.028770	-3.135218
H	-1.235684	2.297328	-3.140665
H	-1.652459	3.995144	-2.807867
H	-2.452859	3.121727	-4.143245

Frequencies

12.5842	20.8373	23.7972
38.3502	43.3757	53.7517
59.1971	71.3586	80.8623
90.4891	121.7812	133.7211
137.0347	140.3124	153.4174
167.4102	196.2751	208.1390
220.1101	240.2131	251.4324
269.4205	271.9912	302.7381
340.9979	359.2090	410.9484
421.0167	421.6035	461.6161
472.6839	477.4946	505.2665
561.8754	594.6089	623.9370
628.3580	633.9264	637.5626
645.7717	681.7713	685.1256
700.4340	706.6167	719.4244
731.6814	736.9838	761.7529
767.6177	791.2476	798.6219
814.0021	828.7947	877.0524
877.8118	891.8887	933.9458
934.4981	962.8339	1011.8726
1012.1123	1013.2317	1021.5845
1028.4904	1036.9549	1046.8270
1052.4201	1052.7793	1063.7697
1069.4147	1071.8682	1116.5642
1116.8774	1121.2188	1125.6220

1162.4624	1169.8176	1171.1123
1174.0126	1199.1699	1206.1705
1213.4488	1222.1686	1237.2072
1264.4440	1289.9572	1290.4301
1338.3173	1338.6784	1374.1189
1383.7477	1408.3879	1410.7796
1416.3755	1467.5665	1468.9006
1488.3648	1505.7892	1511.2006
1519.0042	1519.5207	1521.5817
1529.8818	1531.3644	1539.7790
1546.0500	1556.8053	1572.4379
1653.9202	1664.6439	1671.9812
1688.8538	1691.0598	1700.3362
1741.3952	1911.6016	3104.5951
3104.7534	3105.7539	3144.0521
3178.9012	3179.3548	3210.3611
3211.1485	3217.9443	3222.6425
3232.0386	3238.5687	3238.7414
3245.7068	3247.1421	3254.2745
3259.0026	3313.7634	3333.1588

Cyclization product from B1

C	-3.684131	0.052992	0.010530
N	-4.434659	1.070738	-0.468532
C	-3.925261	2.266213	-1.127394
H	-2.839447	2.200037	-1.179065
H	-4.206806	3.154623	-0.557663
H	-4.330682	2.335541	-2.139239
C	-5.778596	0.832640	-0.255336
H	-6.543900	1.527283	-0.565742

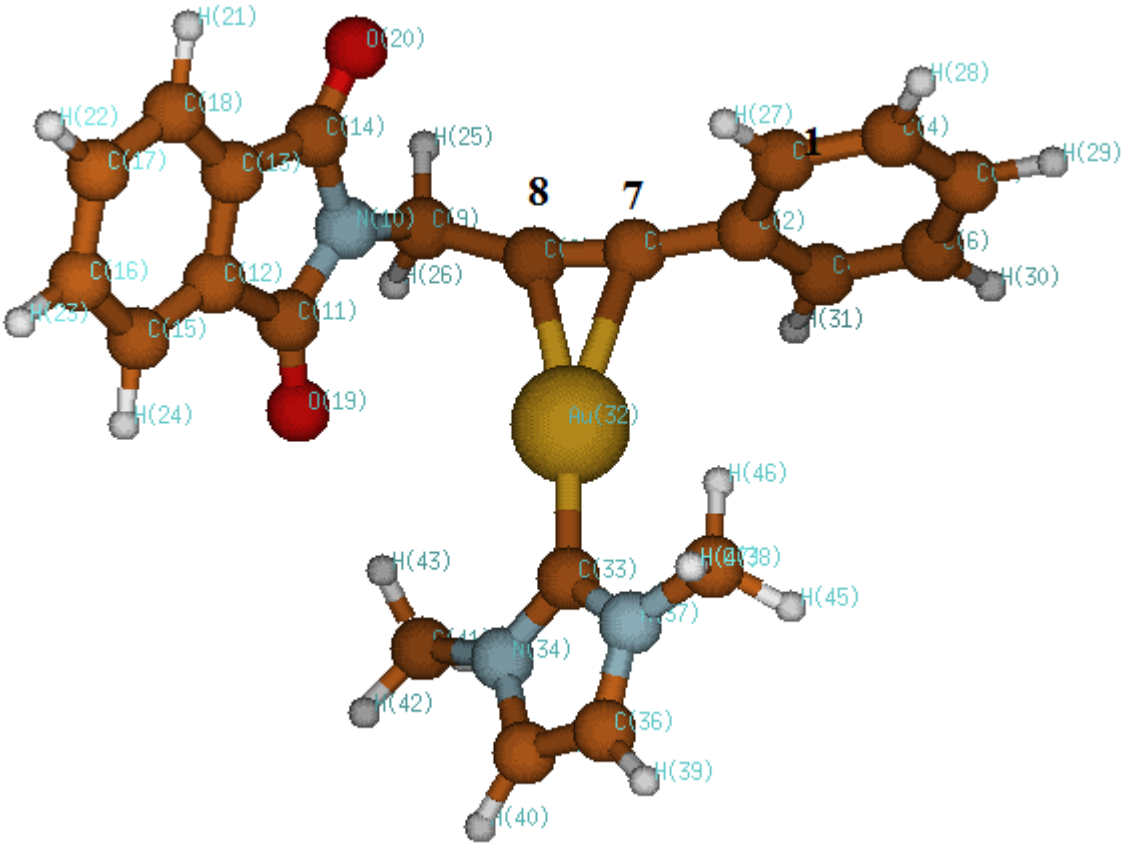
C	-5.866478	-0.363404	0.369303
H	-6.723445	-0.921019	0.714582
N	-4.574018	-0.826974	0.520852
C	-4.240777	-2.088051	1.170467
H	-4.549385	-2.061928	2.218032
H	-3.162701	-2.233782	1.117149
H	-4.743003	-2.913052	0.660645
Au	-1.635456	-0.120539	-0.041727
C	0.416596	-0.274876	-0.086099
C	1.260863	0.906034	0.322424
H	1.057041	1.199276	1.355889
H	1.062286	1.777386	-0.307665
C	1.002072	-1.398826	-0.480794
O	2.440808	-1.568497	-0.544556
C	3.175735	-0.582988	-0.198754
N	2.695676	0.581906	0.214116
C	3.784451	1.479250	0.525100
O	3.613681	2.596022	0.919429
C	5.017641	0.695043	0.251676
C	6.346390	1.040525	0.377666
H	6.642643	2.024254	0.726196
C	7.294845	0.066944	0.035847
H	8.350924	0.301024	0.121036
C	6.910635	-1.196679	-0.411872
H	7.672390	-1.925459	-0.667772
C	5.560891	-1.542638	-0.536796
H	5.259567	-2.525136	-0.883941
H	0.553639	-2.328110	-0.795222
C	4.634627	-0.573552	-0.196774

Frequencies

4.6207	20.2079	27.6950
53.3474	66.2948	70.5729
98.0613	109.2618	125.2577
138.5208	140.7578	153.4005
171.0188	205.7304	228.3570
241.5606	268.2029	271.1168
300.3721	306.9611	340.6949
419.8676	443.5643	459.9585
473.2435	500.1266	520.0642
582.6706	620.6109	628.7452
637.6738	682.3233	684.6416
705.6466	729.7939	733.7177
762.9111	767.8751	793.7221
813.9542	822.6238	827.6585
879.0728	890.1785	915.7345
934.3796	1010.3848	1012.7908
1021.4427	1044.7222	1047.3370
1053.5359	1059.8753	1064.2833
1115.9309	1116.8336	1121.6874
1162.7099	1169.6859	1172.0001
1173.8756	1206.8820	1212.1978
1238.3026	1264.9012	1288.3780
1334.3226	1339.2839	1398.7039
1408.4989	1411.7522	1419.0878
1468.1689	1468.8775	1488.3754
1511.0250	1518.7457	1519.2477
1521.4926	1529.6584	1531.3390
1539.4250	1546.3937	1573.1671
1649.5074	1654.6737	1687.7944
1691.2951	1711.9706	1913.2706
3104.9844	3105.1739	3109.8224

3149.4278	3179.7050	3179.7938
3210.4106	3211.2946	3239.5075
3248.1741	3255.3306	3259.8732
3314.5243	3324.9456	3333.8751

NBO natural charges



C -0.16020

C -0.20672

C -0.21189

C -0.18150

C -0.15495

C -0.19280

C 0.04615

C -0.12642

C -0.30921

N -0.53795

C 0.74433

C -0.13499

C -0.13050

C 0.72765

C -0.18561

C -0.21322

C -0.20994

C -0.18176

O -0.60355

O -0.54605

H 0.27548

H 0.26517

H 0.26381

H 0.26901

H 0.31093

H 0.29637

H 0.26255

H 0.24912

H 0.24626

H 0.24729

H 0.24835

Au 0.46318

C 0.14005

N -0.39296

C -0.05535

C -0.06532

N -0.39535

C -0.47139

H 0.27065

H 0.27057

C -0.48189

H 0.25618

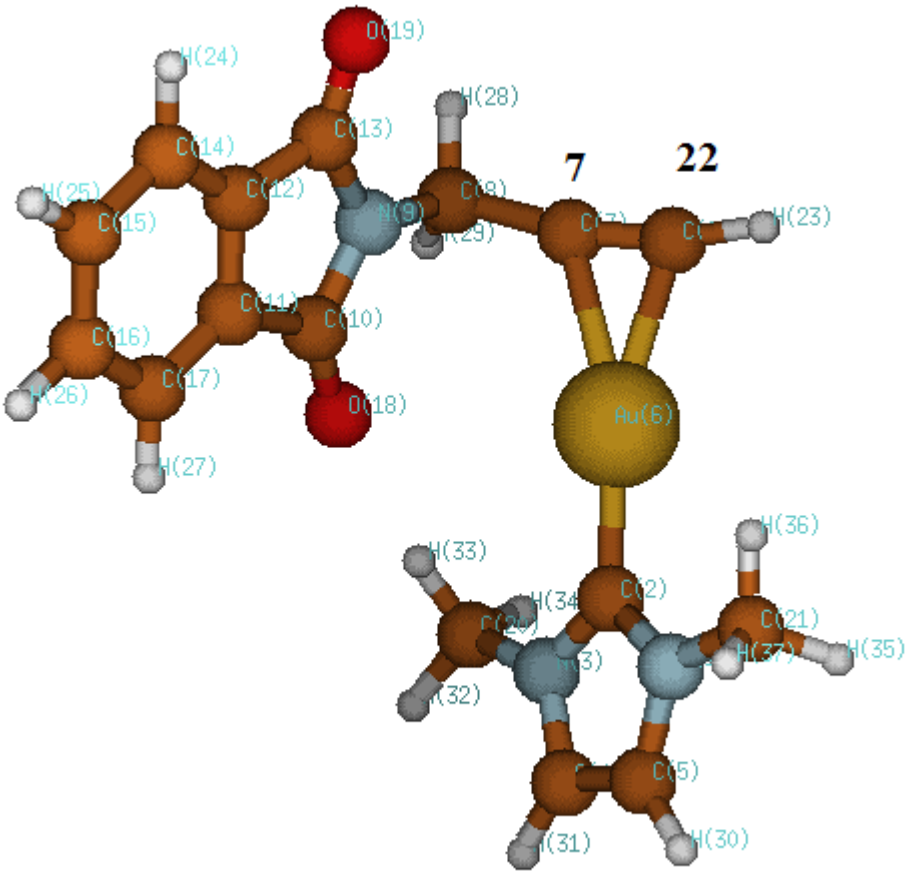
H 0.28098

H 0.25414

H 0.25899

H 0.25622

H 0.25872



N -0.39099

C 0.14003

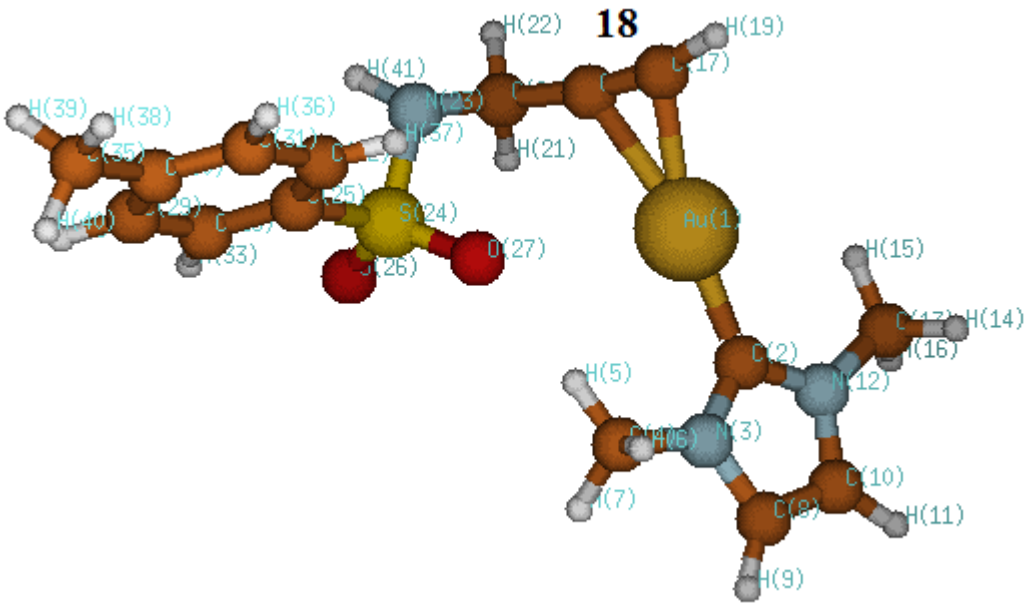
N	-0.38938
C	-0.05318
C	-0.06414
Au	0.46909
C	-0.00034
C	-0.33447
N	-0.54094
C	0.74520
C	-0.13687
C	-0.13240
C	0.73542
C	-0.17917
C	-0.20720
C	-0.21156
C	-0.18384
O	-0.60739
O	-0.54629
C	-0.48434
C	-0.47294
C	-0.28704
H	0.31297
H	0.27718
H	0.26686
H	0.26518
H	0.26950
H	0.32539
H	0.30152
H	0.27208
H	0.27161
H	0.25778
H	0.27999

H 0.25591

H 0.26090

H 0.25470

H 0.26118



Au 0.46988

C 0.13711

N -0.38562

C -0.48416

H 0.28076

H 0.25481

H 0.25770

C -0.05521

H 0.27169

C -0.06048

H 0.27121

N -0.39187

C -0.47361

H 0.25953

H 0.25692

H 0.26002

C -0.29801

C 0.01119

H 0.31069

C -0.35504

H 0.28531

H 0.30531

N -0.91703

S 2.35669

C -0.37587

O -0.94813

O -0.98610

C -0.19850

C -0.23081

C 0.01122

C -0.23387

C -0.19057

H 0.28206

H 0.25977

C -0.71546

H 0.25764

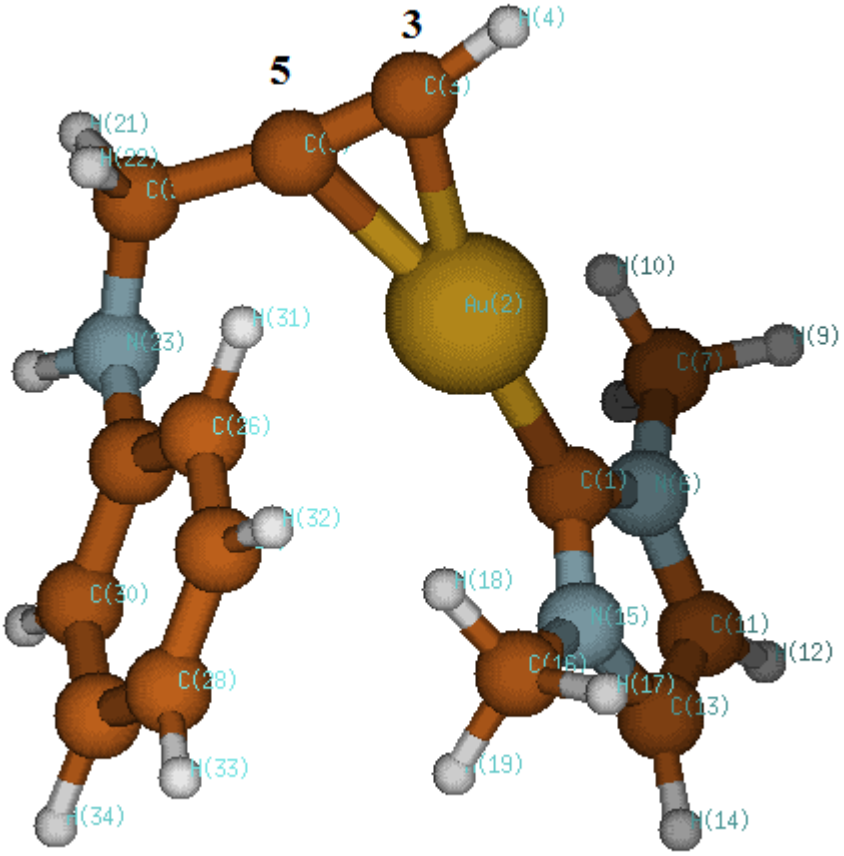
H 0.26922

H 0.25368

H 0.26462

H 0.26604

H 0.44727



C 0.13594

Au 0.47358

C -0.29343

H 0.31169

C -0.02918

N -0.39138

C -0.47304

H 0.26104

H 0.26106

H 0.25625

C -0.05814

H 0.27273

C -0.05583

H 0.27283

N -0.38897

C -0.47467

H 0.25852

H 0.26362

H 0.26171

C -0.33393

H 0.29807

H 0.27978

N -0.67182

H 0.43634

C 0.15752

C -0.31697

C -0.21601

C -0.27457

C -0.21629

C -0.28132

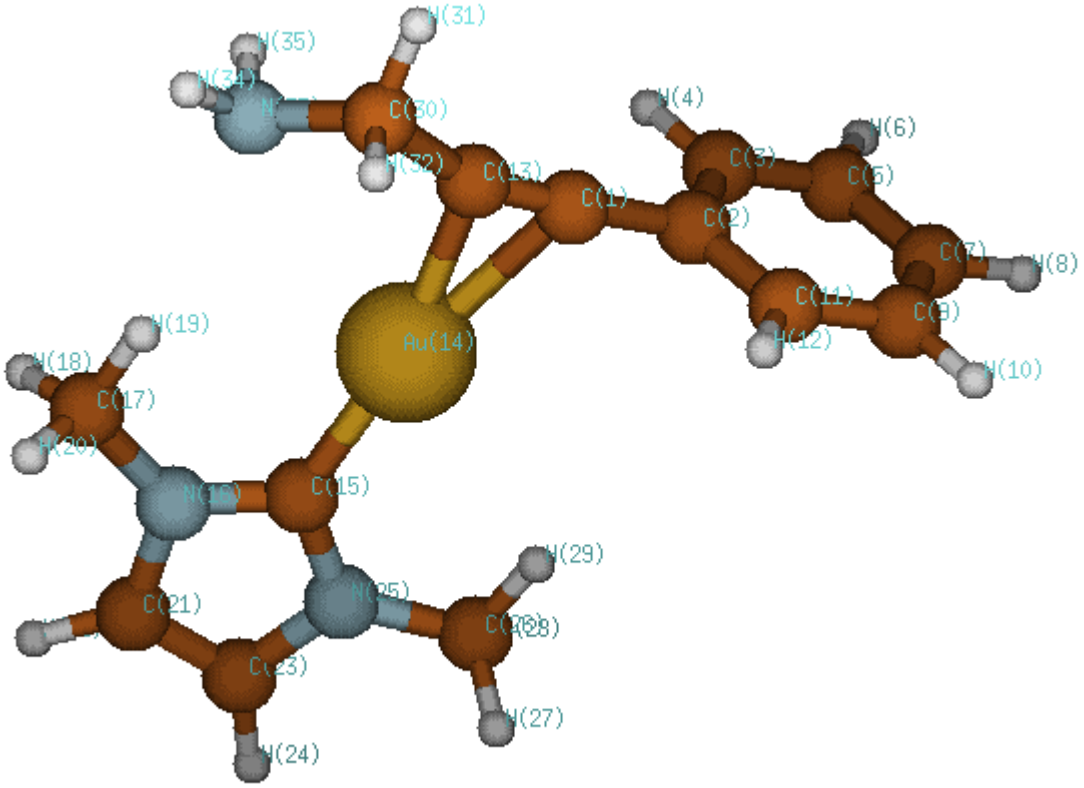
H 0.24289

H 0.25644

H 0.25779

H 0.25729

H 0.24647



C 0.03429

C -0.16344

C -0.18290

H 0.25938

C -0.23562

H 0.26402

C -0.19935

H 0.26314

C -0.23639

H 0.26388

C -0.18496

H 0.25977

C -0.12572

Au	0.46185
C	0.14560
N	-0.39460
C	-0.48141
H	0.25672
H	0.26979
H	0.25713
C	-0.05901
H	0.27155
C	-0.06057
H	0.27133
N	-0.39651
C	-0.47214
H	0.25937
H	0.25912
H	0.25683
C	-0.26443
H	0.25204
H	0.26707
N	-0.93664
H	0.41518
H	0.40599

QTAIMS ANALYSIS

The Quantum Theory of Atoms in Molecules is a density-based topological approach for studying the chemical bond representing, in the real space, the boundaries of the atoms forming a molecular system or a crystal. Within this theory an atom in a molecule is defined as that portion of the molecular space delimited by a surface S at any point of which the gradient of the electron density has zero flux. An atom in a molecule can be also defined as the union of a nucleus and the basin traversed by all the paths of *steepest ascent* along the electron density which terminate at the nucleus. These paths are called gradient paths (GP) which, hence, divide the molecule into *atomic basins*. Each GP is therefore characterized by initial and final points which are critical points in the density (i.e. points in which the density gradient is zero). Different critical points can be obviously defined depending on the density Hessian. In general they are defined in terms of the rank (r), i.e. the number of non-zero eigenvalues of the Hessian, and the signature (s), i.e. the sum of the signs of the Hessian eigenvalues. We can then classify the critical points (r,s) as:

- local maxima (3,-3) which corresponds to the position of an atom. The point therefore is also called an atomic critical point.

- local minima (3,+3) which lis located when several rings form a cage and is therefore called a cage critical point.

- saddle point (3,+1) which locates a point in the middle of several bonds forming a ring. It is also called a ring critical points.

- saddle points (3,-1)

The latter CP is of particular interest as it defines a CP between two neighboring atoms locating a *bond* between them. This point is therefore also called a *bond critical point (BCP) a*nd it is the focus of our investigation. It is important to remark that in this respect, the line of maximum density is called a *bond path* between two BCP which represents a topological proof that atoms are bonded to one another. The classification of the bond can be based on different observables, in this study we have followed the criterion based on the analysis of Laplacian of the density and the energy density (H_C) at the BCP. More precisely we can define as closed shell (non-covalent) the interactions showing $H_C > 0$ and Laplacian of the density > 0; we can define as transit the interactions showing $H_C < 0$ and Laplacian of the density > 0 and, finally, we can define as shared shell (covalent) the interactions showing $H_C < 0$ and Laplacian of the density < 0. Moreover the ratio between Hc and the density at the BCP can provide the covalent character of the bond. [8.9]

We report in the Figure below the representation of all the BCP (green balls) and bond paths (green sticks) which involve the atoms directly participating at the hydration process. For the sake of simplicity we did not report the whole repertoire of critical points.

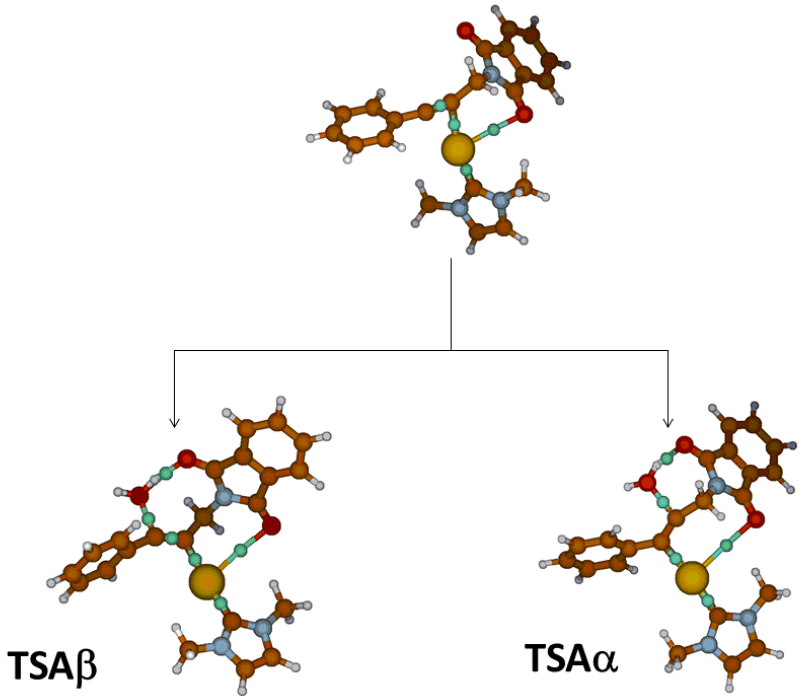


Figure S3. Bond critical points and Bond Paths for the initial adduct and the two hydration TSs for the hydration of *N*-propargylpthalimide (1a with R_2 = phenyl). (See Table SI for details)

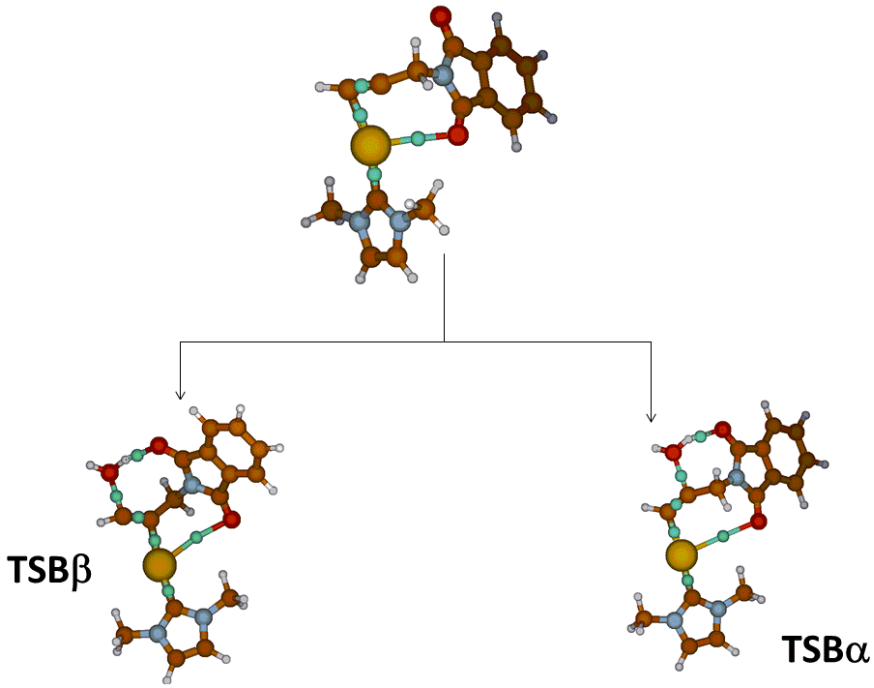


Figure S4. Bond critical points and Bond Paths for the initial adduct and the two hydration TSs for the hydration of *N*-propargylpthalimide (1n with R_2 = H). (See Table SI for details)

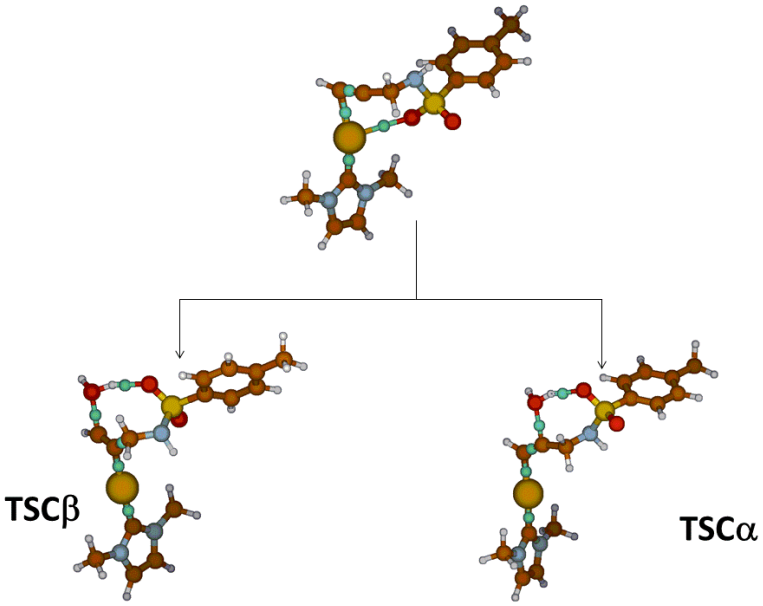


Figure S5. Bond critical points and Bond Paths for the initial adduct and the two hydration TSs for the hydration of *4*-methyl-N-(prop-2-yn-1-yl)benzenesulfonamide (See Table SI for details)

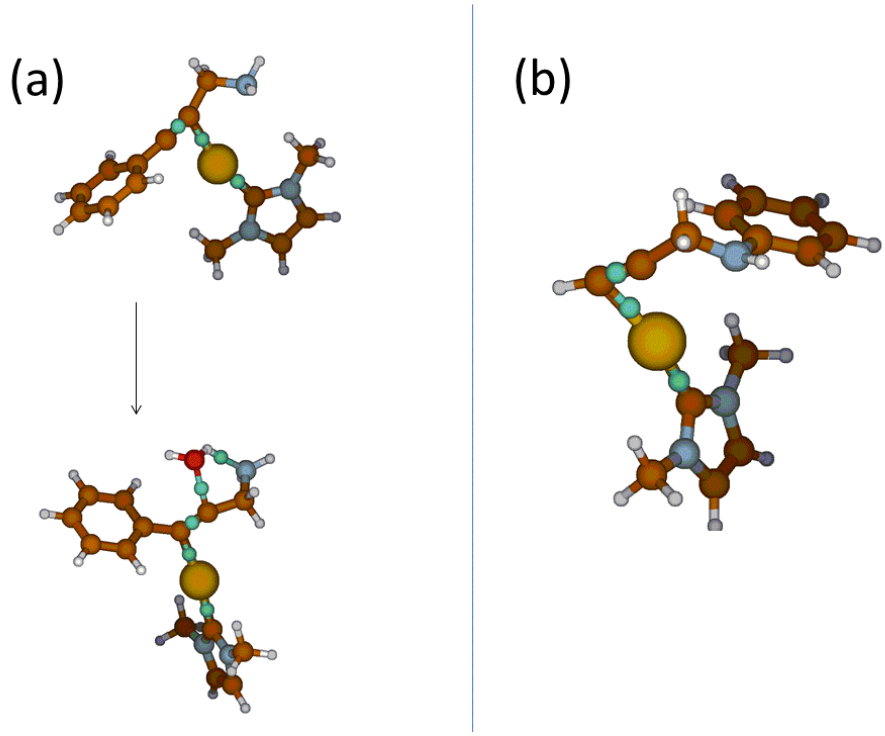


Figure S6. Bond critical points and Bond Paths for the initial adduct (upper side of inset a) and the hydration TS (lower side of inset a) for the hydration of 3-phenylprop-2-yn-1-amine *(inset a).* Bond critical points and Bond Paths for the initial adduct with N-(prop-2-yn-1-yl)aniline (inset b). See Table SI for details

In the Table SI below reported the above BCPs have quantified in terms of Laplacian of the density, energy density and the ratio between the energy density and the density itself. All the data reported in the table are in atomic units.

Table SI

Species	BCP	$\nabla^2\rho(r)$	H_C	H_C / ρ
Adduct (Fig. S3)	**Au-Cα** **Au-Cβ** **Au-O** **Cβ-Cα** **Au-C**	**0.20** **No BCP** **0.026** **-1.21** **0.31**	**-0.022** **No BCP** **0.00074** **-0.61** **-0.053**	**-0.27** **No BCP** **0.088** **-1.55** **-0.39**
Adduct (Fig. S4)	**Au-Cα** **Au-Cβ** **Au-O** **Cβ-Cα** **Au-C**	**No BCP** **0.22** **0.032** **-1.19** **0.31**	**No BCP** **-0.019** **0.00065** **-0.65** **-0.053**	**No BCP** **-0.25** **0.065** **-1.61** **-0.39**
Adduct (Fig. S5)	**Au-Cα** **Au-Cβ** **Au-O** **Cβ-Cα** **Au-C**	**No BCP** **0.21** **0.046** **-1.14** **0.31**	**No BCP** **-0.019** **0.00053** **-0.65** **-0.053**	**No BCP** **-0.25** **0.061** **-1.64** **-0.39**
Adduct (Fig. S6a)	**Au-Cα** **Au-Cβ** **Au-N** **Cβ-Cα** **Au-C**	**0.20** **No BCP** **No BCP** **-1.21** **0.31**	**-0.021** **No BCP** **No BCP** **-0.57** **-0.054**	**-0.27** **No BCP** **No BCP** **-1.46** **-0.40**
Adduct (Fig. S6b)	**Au-Cα** **Au-Cβ** **Au-N** **Cβ-Cα** **Au-C**	**No BCP** **0.23** **No BCP** **-1.21** **0.31**	**No BCP** **-0.017** **No BCP** **-0.62** **-0.054**	**No BCP** **-0.22** **No BCP** **-1.56** **-0.31**
TSAβ	**C-O** **Au-Cα** **Au-Cβ** **Au-O** **H-O** **Cβ-Cα** **Au-C**	**0.14** **0.25** **No BCP** **0.015** **0.15** **-1.08** **0.30**	**-0.014** **-0.039** **No BPC** **0.00060** **-0.0044** **-0.48** **-0.053**	**-0.19** **-0.35** **No BCP** **0.13** **-0.092** **-1.33** **-0.38**
TSAα	**C-O** **Au-Cα** **Au-Cβ** **Au-O** **H-O** **Cβ-Cα** **Au-C**	**0.14** **No BCP** **0.23** **0.0097** **0.14** **-1.09** **0.31**	**-0.065** **No BPC** **-0.034** **0.00051** **-0.0021** **-0.50** **-0.053**	**-0.11** **No BCP** **-0.33** **0.16** **-0.051** **-1.35** **-0.37**
TSBβ	**C-O** **Au-Cα**	**0.15** **0.23**	**-0.052** **-0.032**	**-0.092** **-0.34**

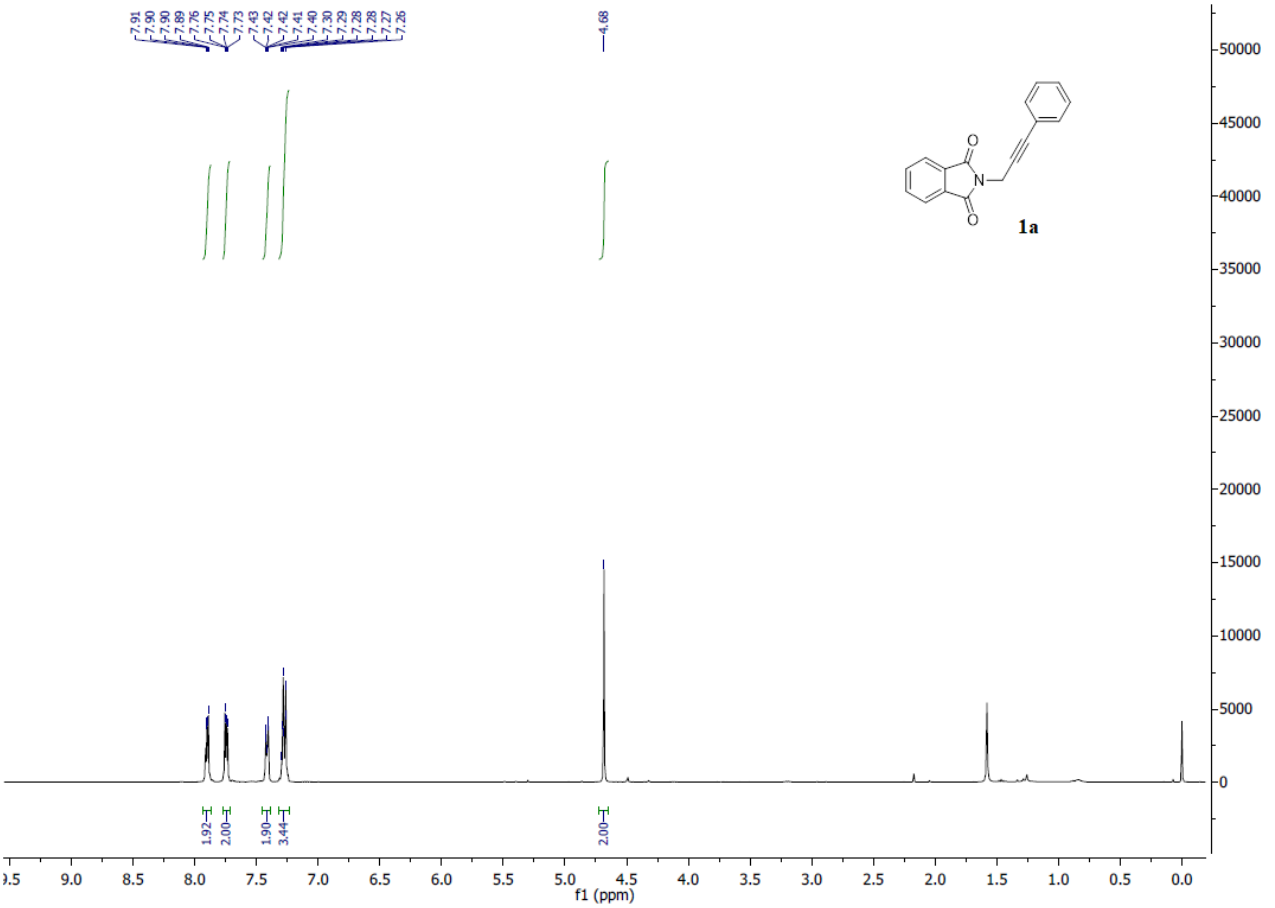
	Au-Cβ **Au-O** **H-O** **Cβ-Cα** **Au-C**	**No BCP** **0.0097** **0.14** **-1.09** **0.31**	**No BPC** **0.00057** **-0.0016** **-0.52** **-0.053**	**No BCP** **0.14** **-0.042** **-1.37** **-0.38**
TSBα	**C-O** **Au-Cα** **Au-Cβ** **Au-O** **H-O** **Cβ-Cα** **Au-C**	**0.13** **No BCP** **0.24** **0.0091** **0.143** **-1.11** **0.32**	**-0.0036** **No BPC** **-0.034** **0.00049** **-0.0012** **-0.52** **-0.051**	**-0.072** **No BCP** **-0.33** **0.17** **-0.033** **-1.40** **-0.37**
TSCβ	**C-O** **Au-Cα** **Au-Cβ** **Au-O** **H-O** **Cβ-Cα** **Au-C**	**0.15** **0.22** **No BCP** **No BCP** **0.14** **-0.56** **0.31**	**-0.0057** **-0.035** **No BPC** **No BCP** **-0.0015** **-0.19** **-0.053**	**-0.098** **-0.34** **No BCP** **No BCP** **-0.041** **-0.82** **-0.38**
TSCα	**C-O** **Au-Cα** **Au-Cβ** **Au-O** **H-O** **Cβ-Cα** **Au-C**	**0.12** **No BCP** **0.23** **No BCP** **0.13** **-1.12** **0.31**	**-0.0011** **No BPC** **-0.035** **No BCP** **-0.00081** **-0.54** **-0.051**	**-0.027** **No BCP** **-0.33** **No BCP** **-0.023** **-1.42** **-0.37**
TS **(Figure S6a)**	**C-O** **Au-Cα** **Au-Cβ** **Au-N** **H-N** **Cβ-Cα** **Au-C**	**0.12** **No BCP** **0.22** **No BCP** **0.10** **-1.12** **0.31**	**-0.0017** **No BPC** **-0.034** **No BCP** **0.00023** **-0.52** **-0.051**	**-0.039** **No BCP** **-0.34** **No BCP** **0.0041** **-1.38** **-0.37**

All the interactions turns out to be essentially non covalent with the obvious exception of the triple C□-C□ bond.

It is interesting to note that in the three cases where we were able of locating two possible hydration paths we systematically found that the carbon atom not interactiong with the gold(I) atom, is the one undergoing the kinetically more favorable water addition. In other words, defining in general with CX-CY the triple bond, gold cation, bound to CX atom, induces an electronic vacancy on the adiacent carbon (CY) atom which, hence, becomes more reactive toward entering water.

It is also important to note that when passing from the initial adduct to the TS we always observe a systematic Au-CY interaction increase which is obviously energetically less demanding when between these two atoms we do not observe any sort of interaction.

VI. Copies of ^{1}H Spectra of known derivatives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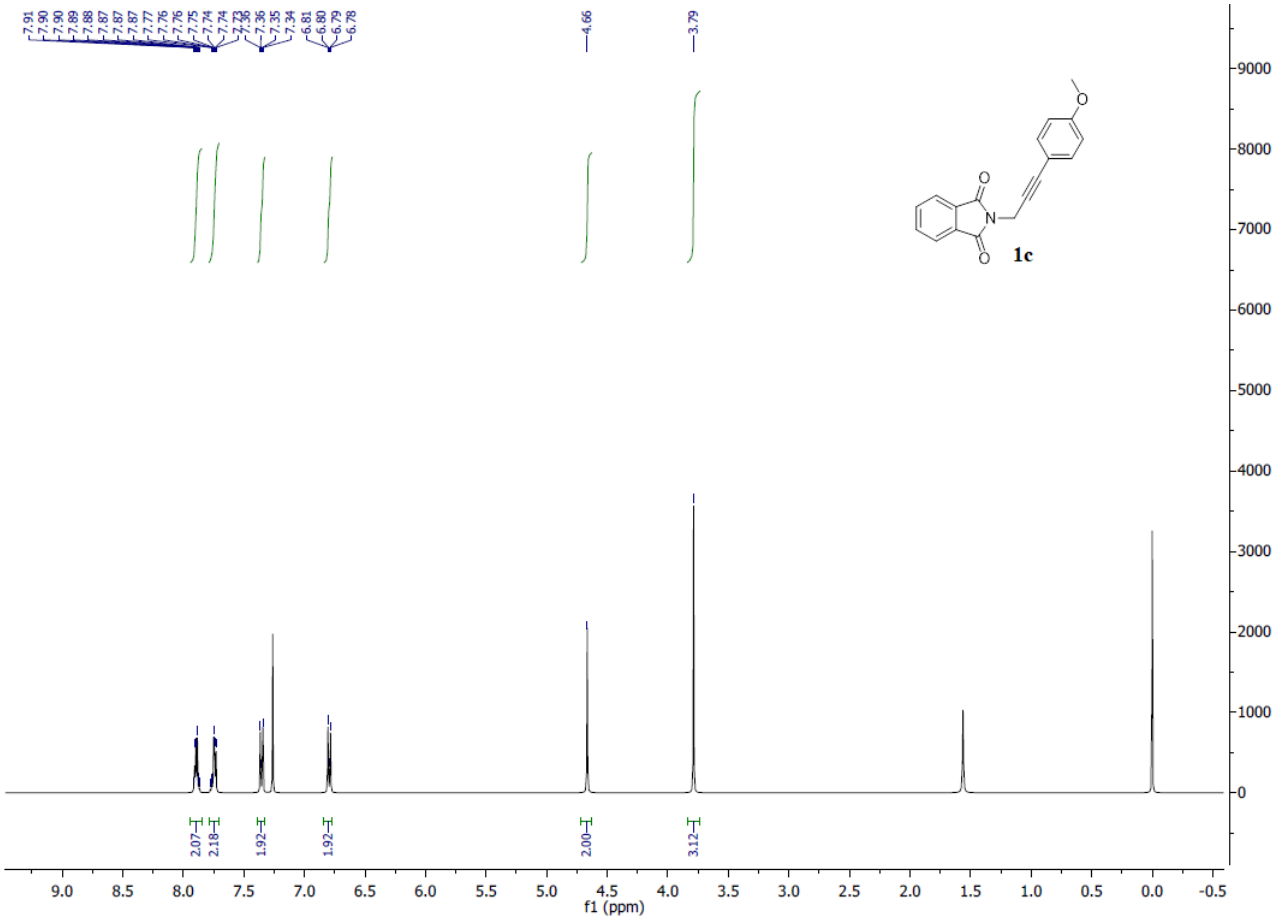
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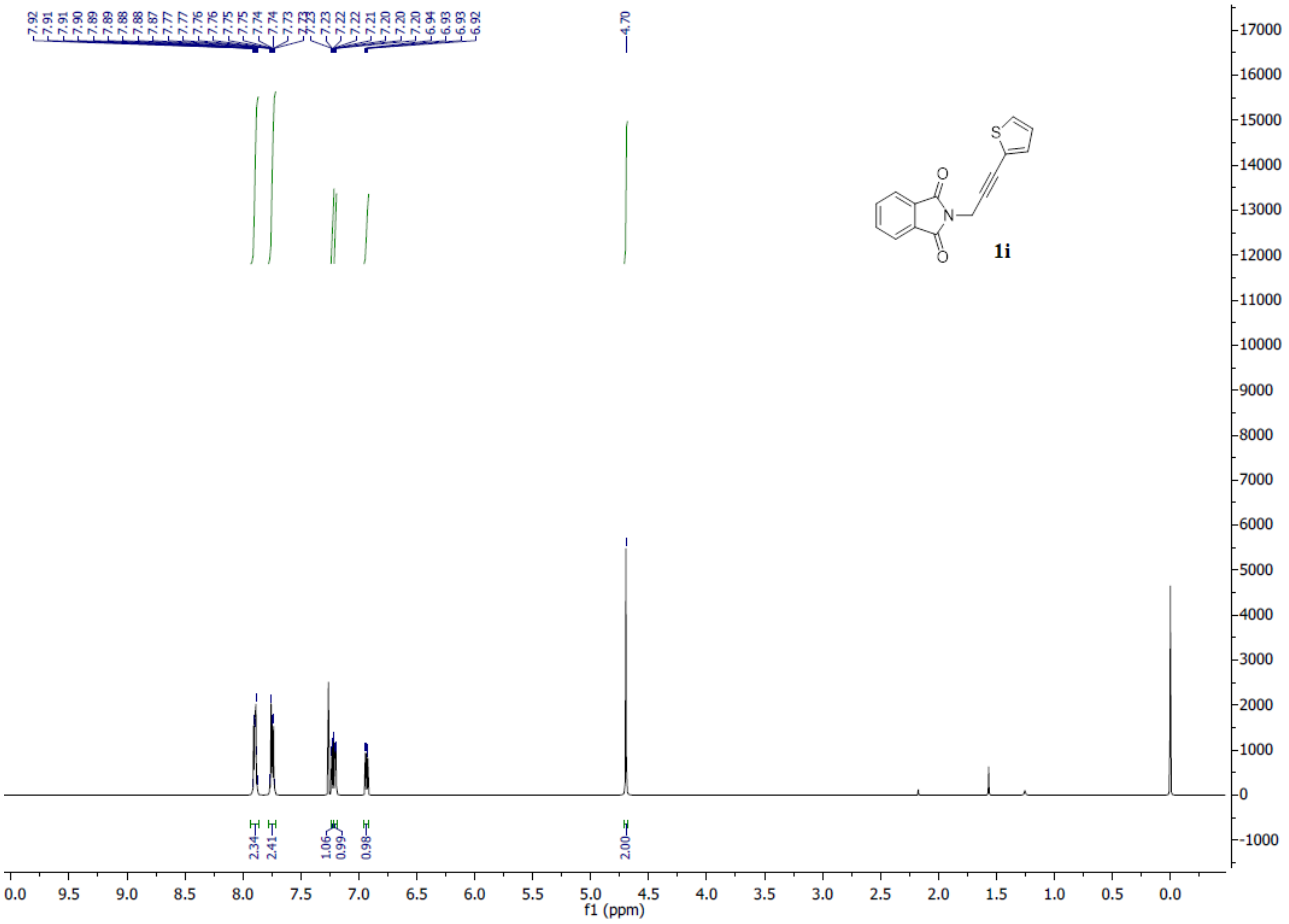
f1 (ppm)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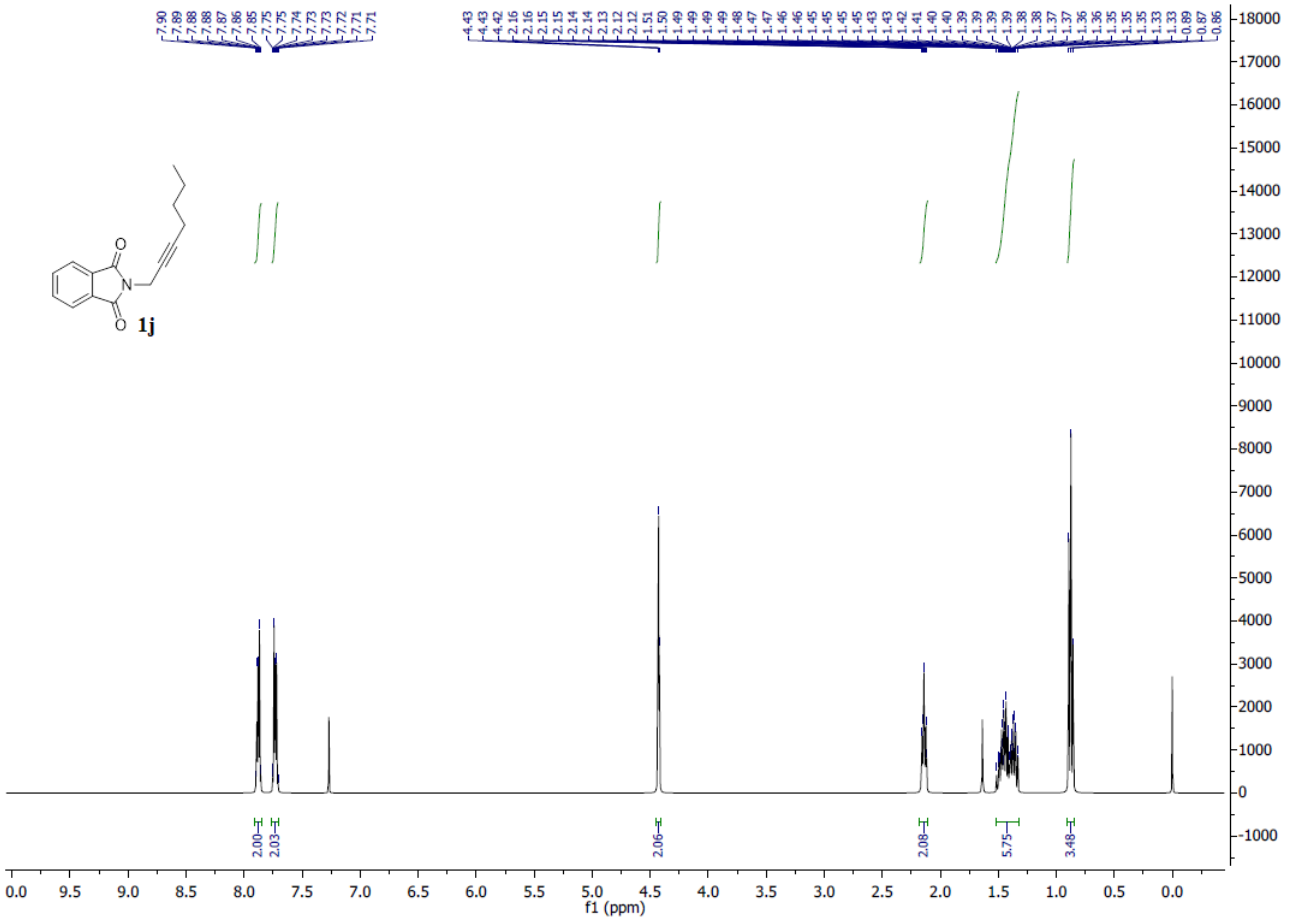
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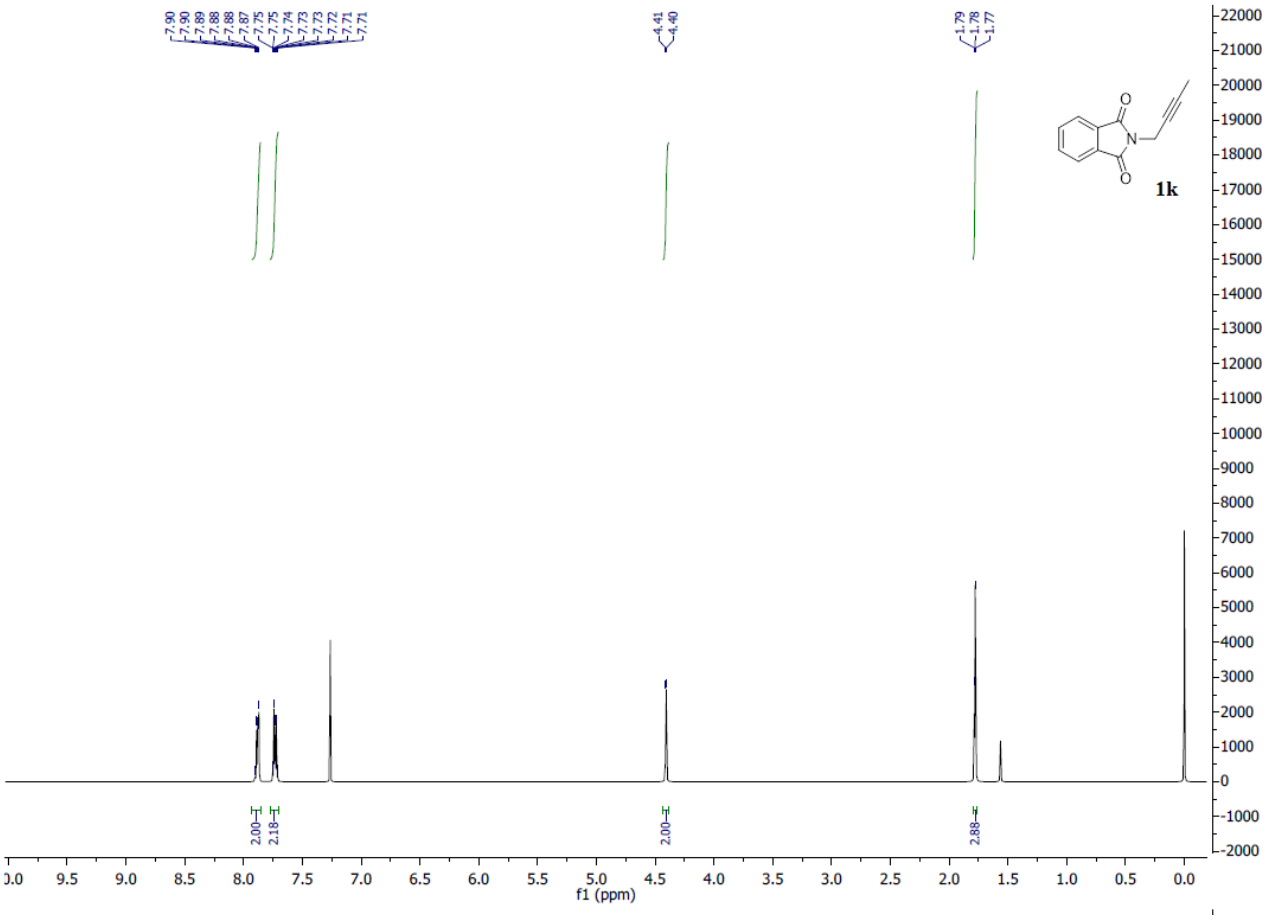
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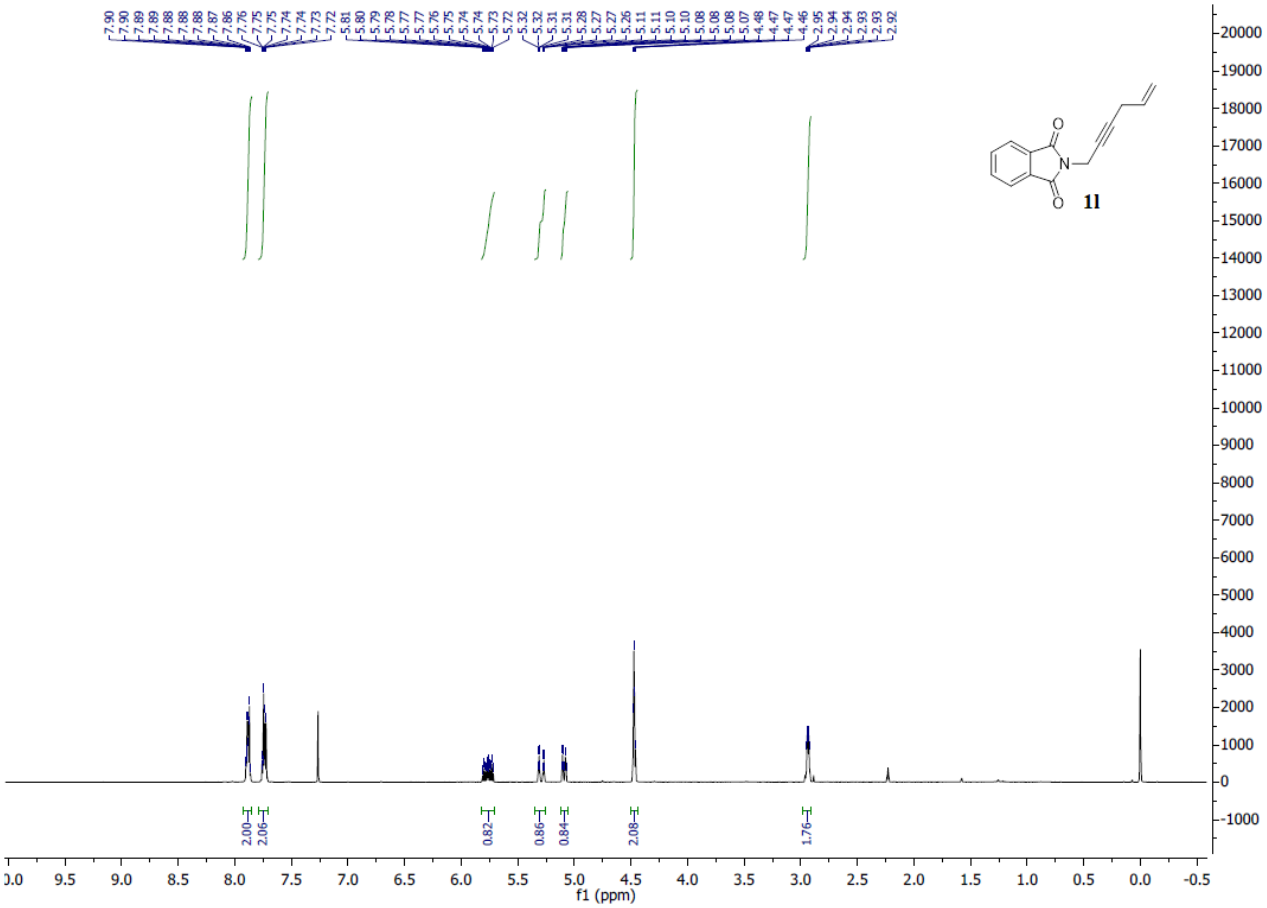
f1 (ppm)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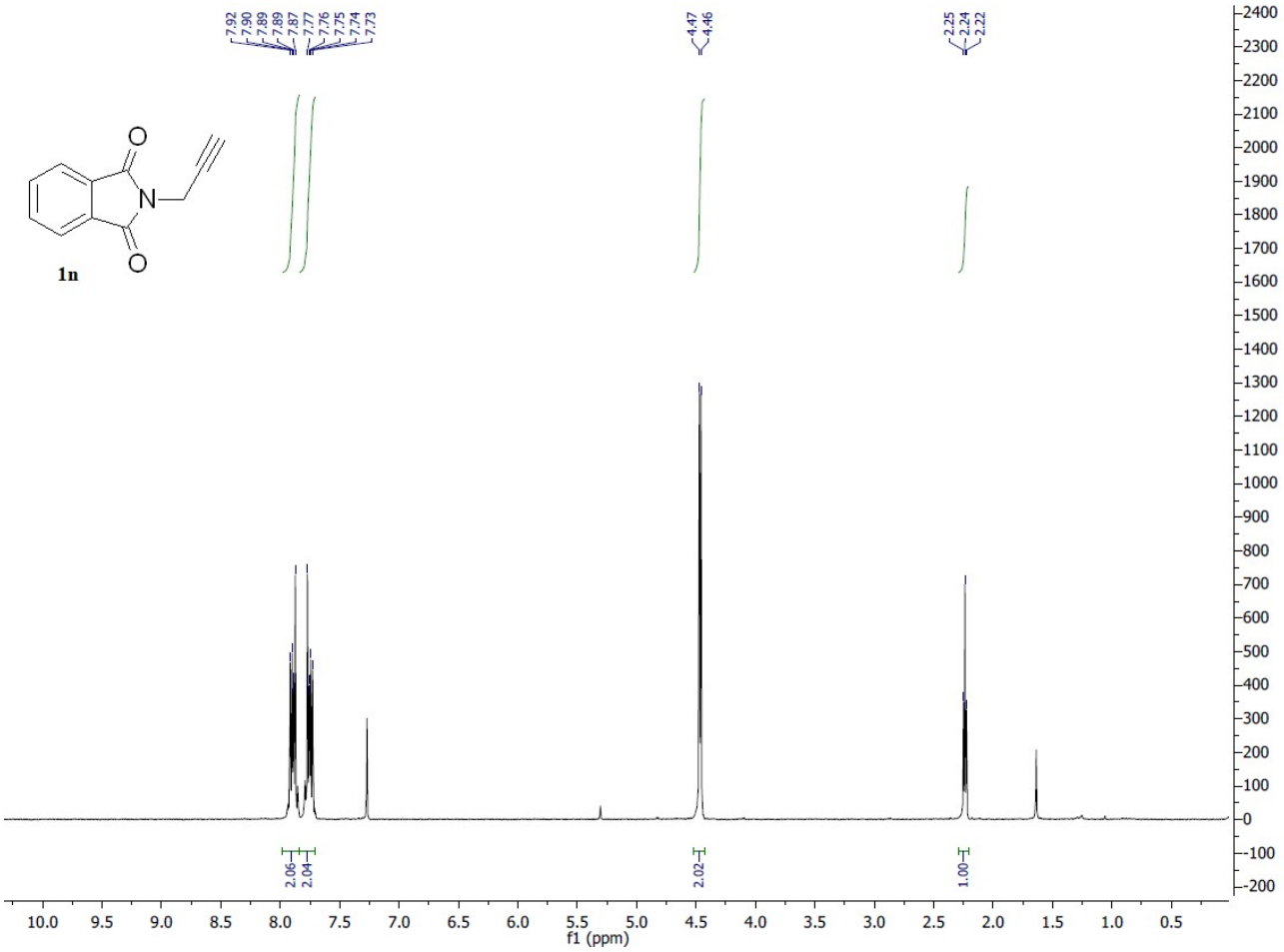
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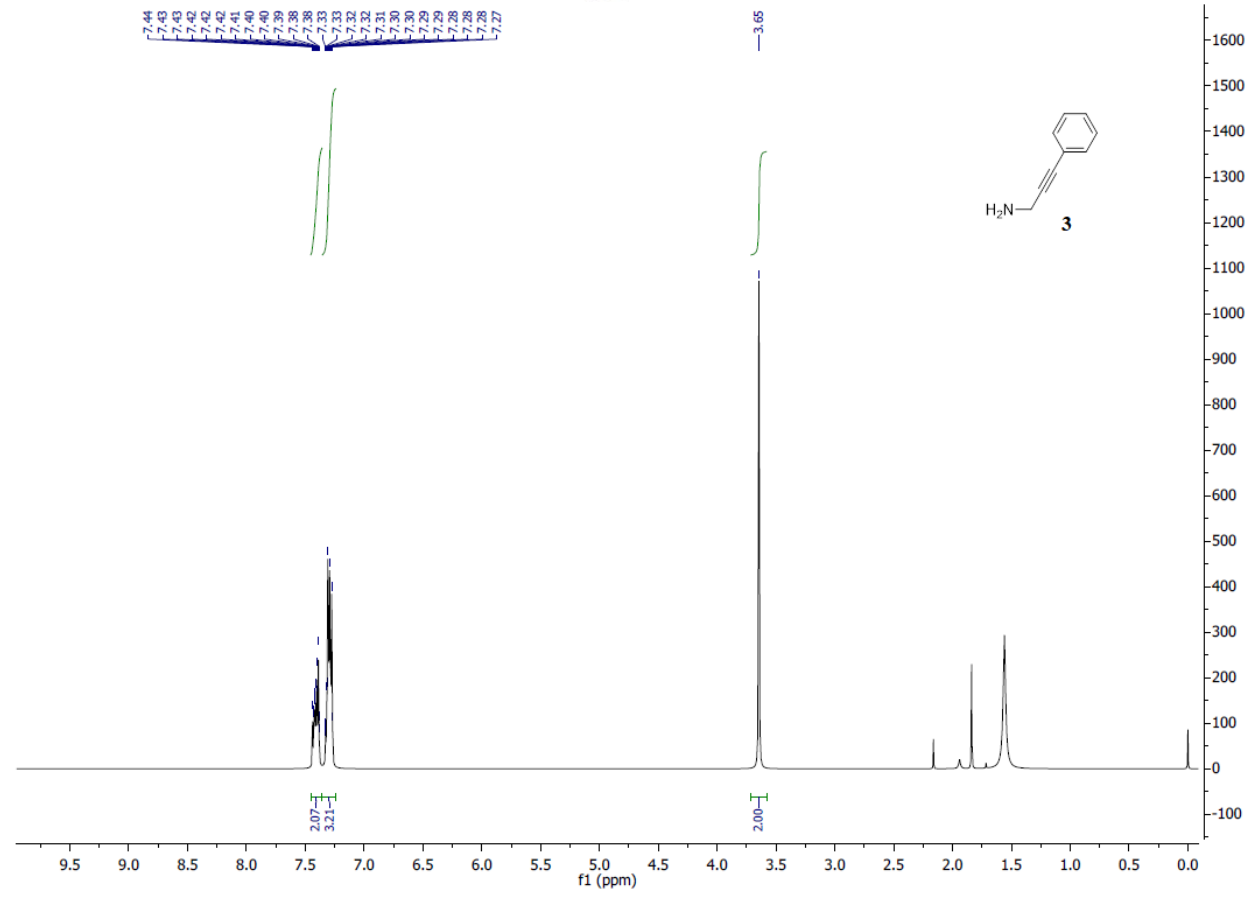
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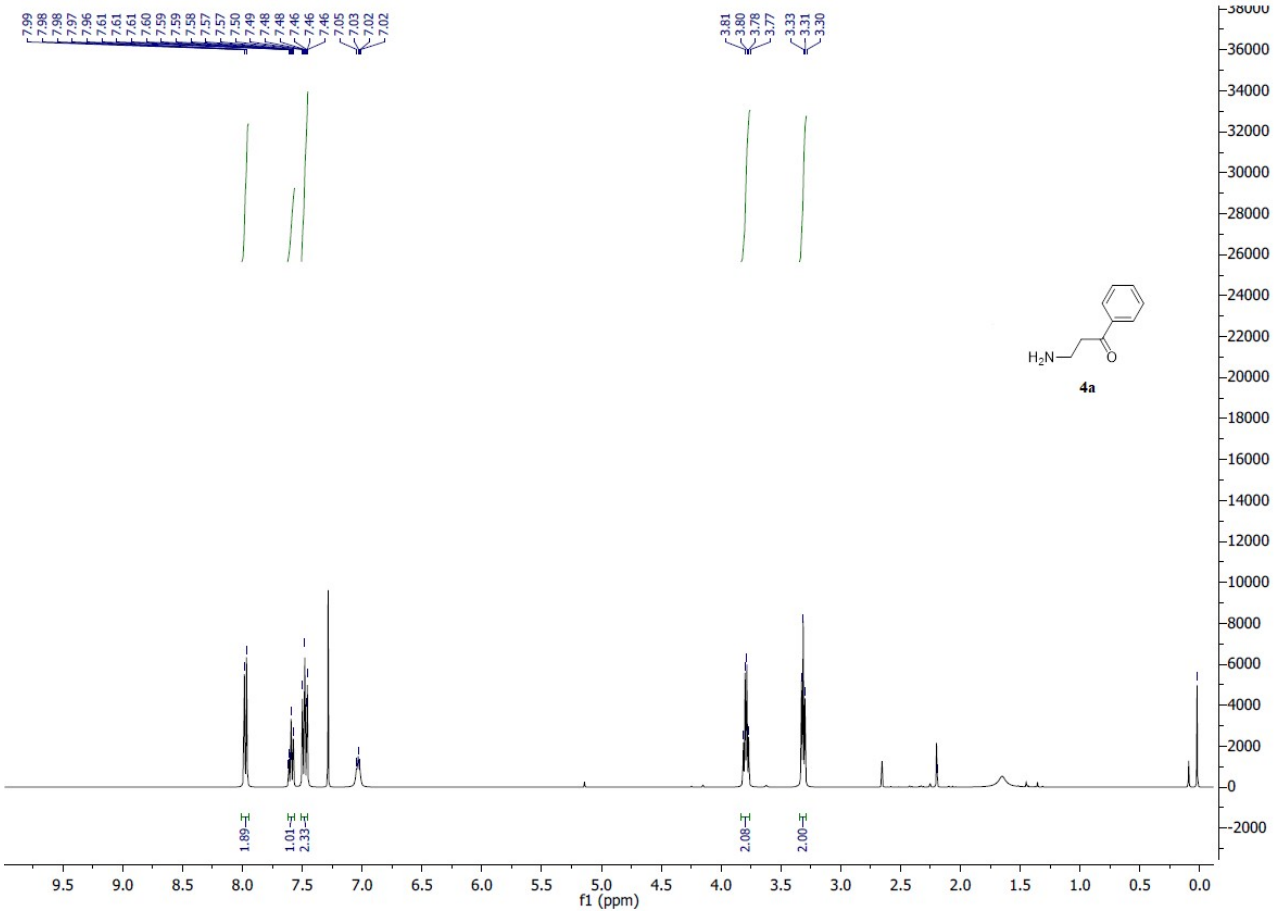
f1 (ppm)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3.78
3.77
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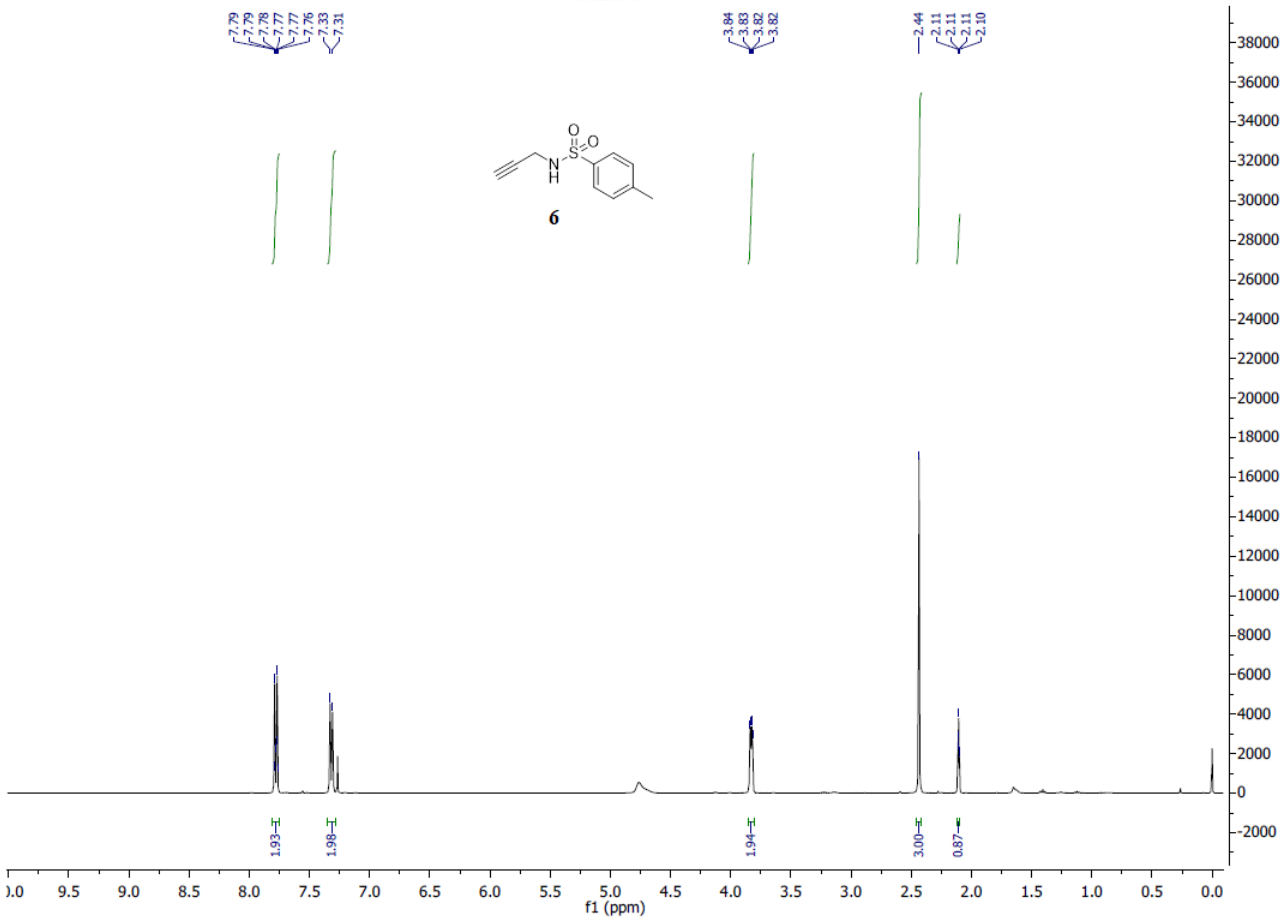
1.89
1.01
2.33
2.08
2.00
f1 (ppm)

H2N
O

4a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2.11
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1.98
1.94
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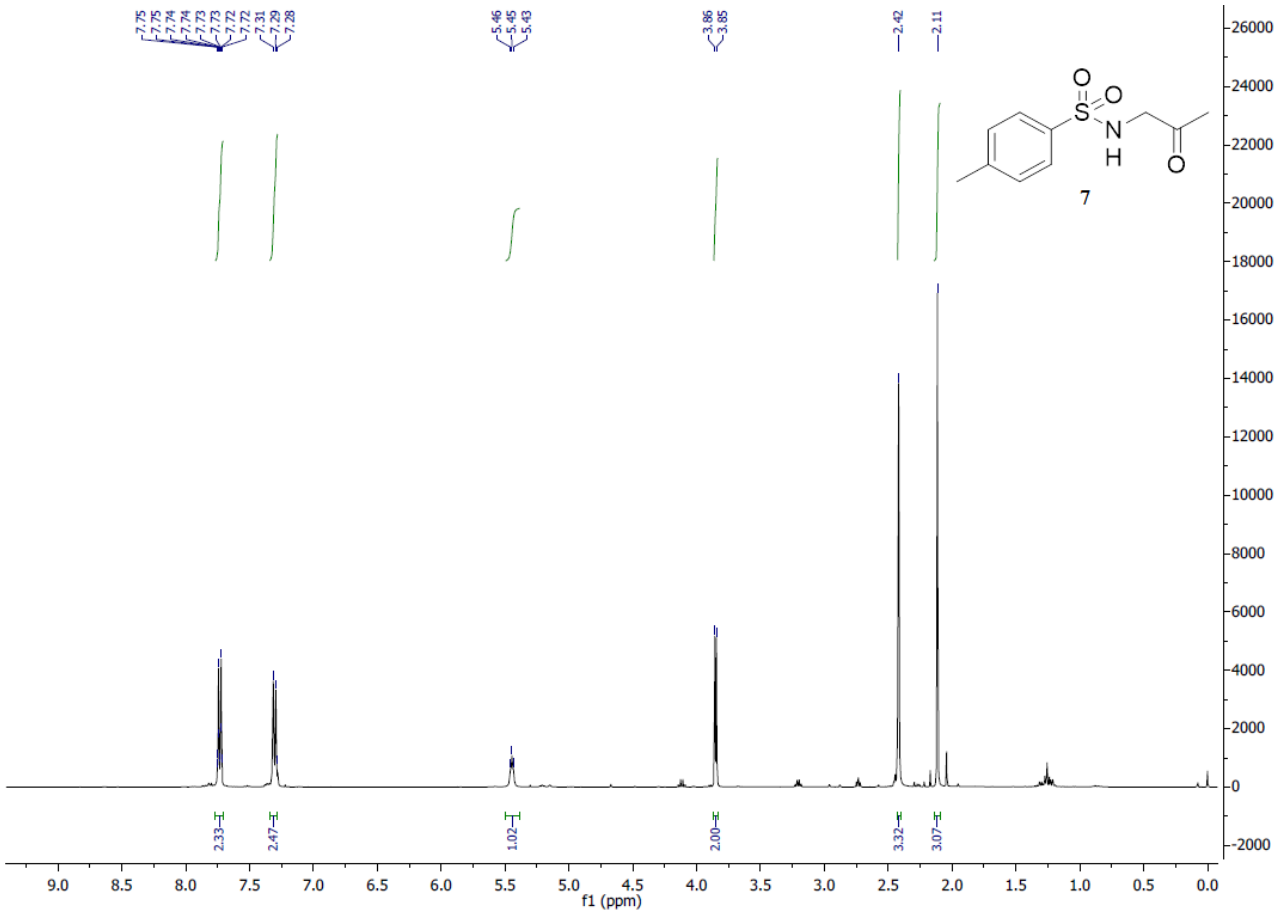
f1 (ppm)

O
S
O
N
H

6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3.85
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O
S
N
H
O
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24000
22000
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
-2000
2.33
2.47
1.02
2.00
3.32
3.07
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8.0
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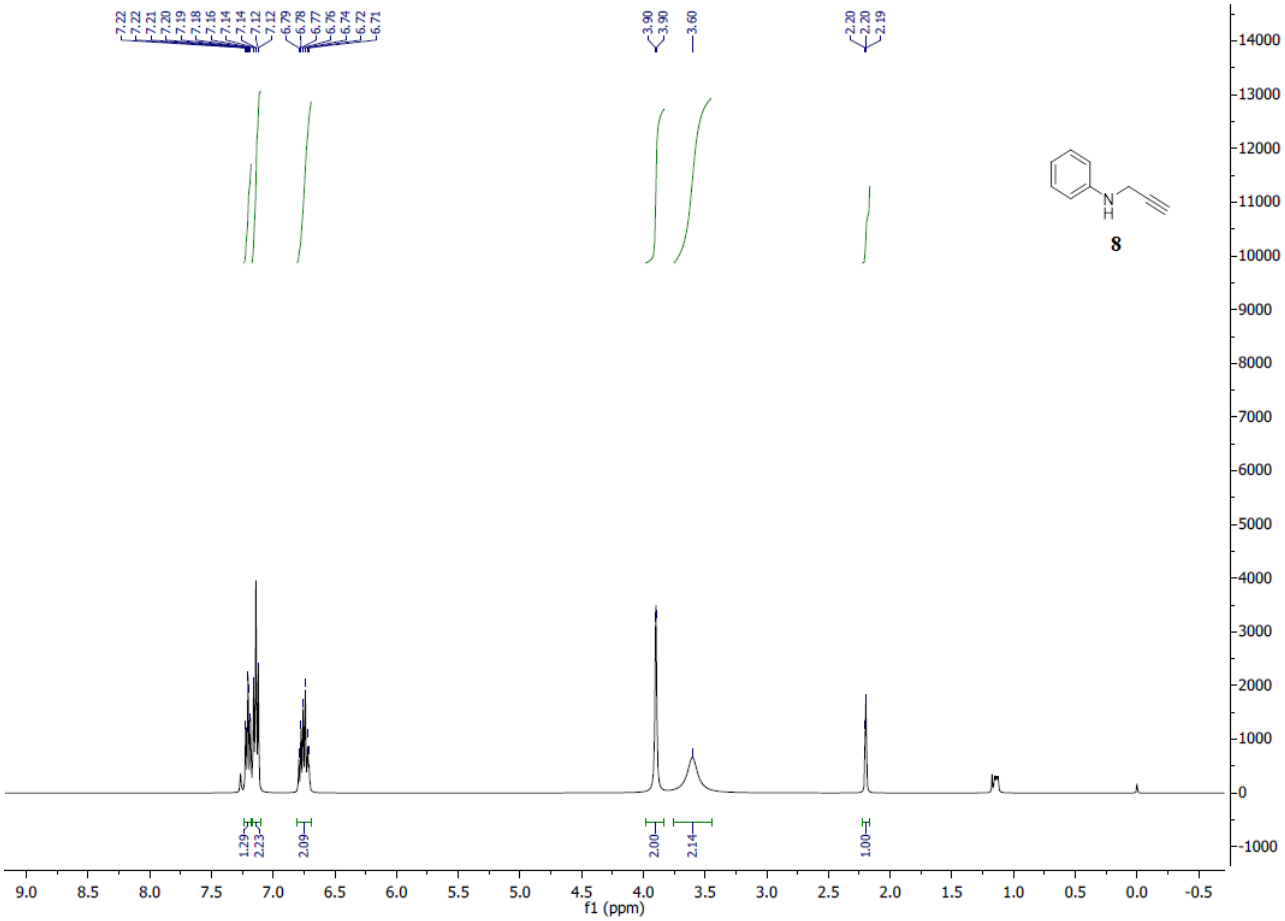
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2.20
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H
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12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
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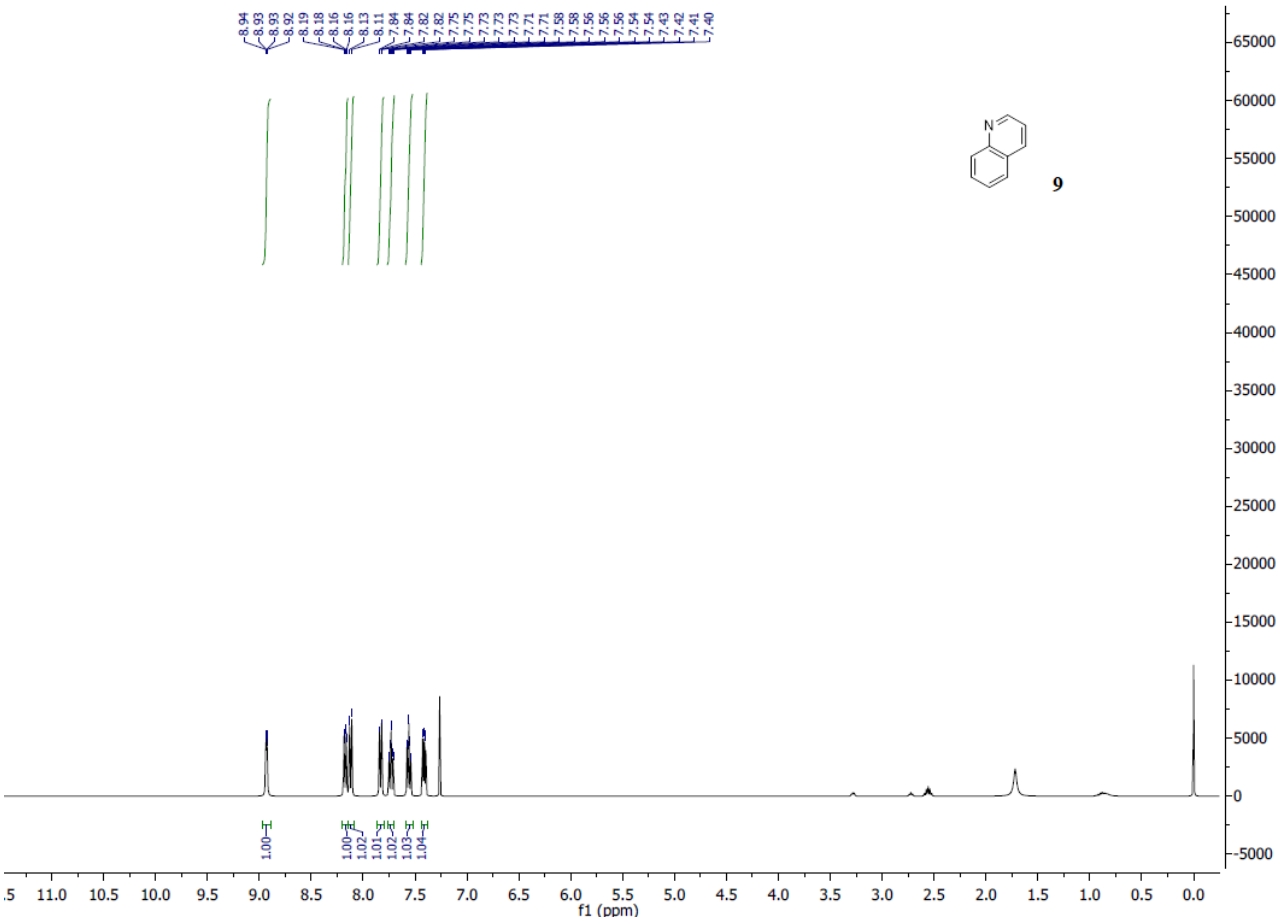
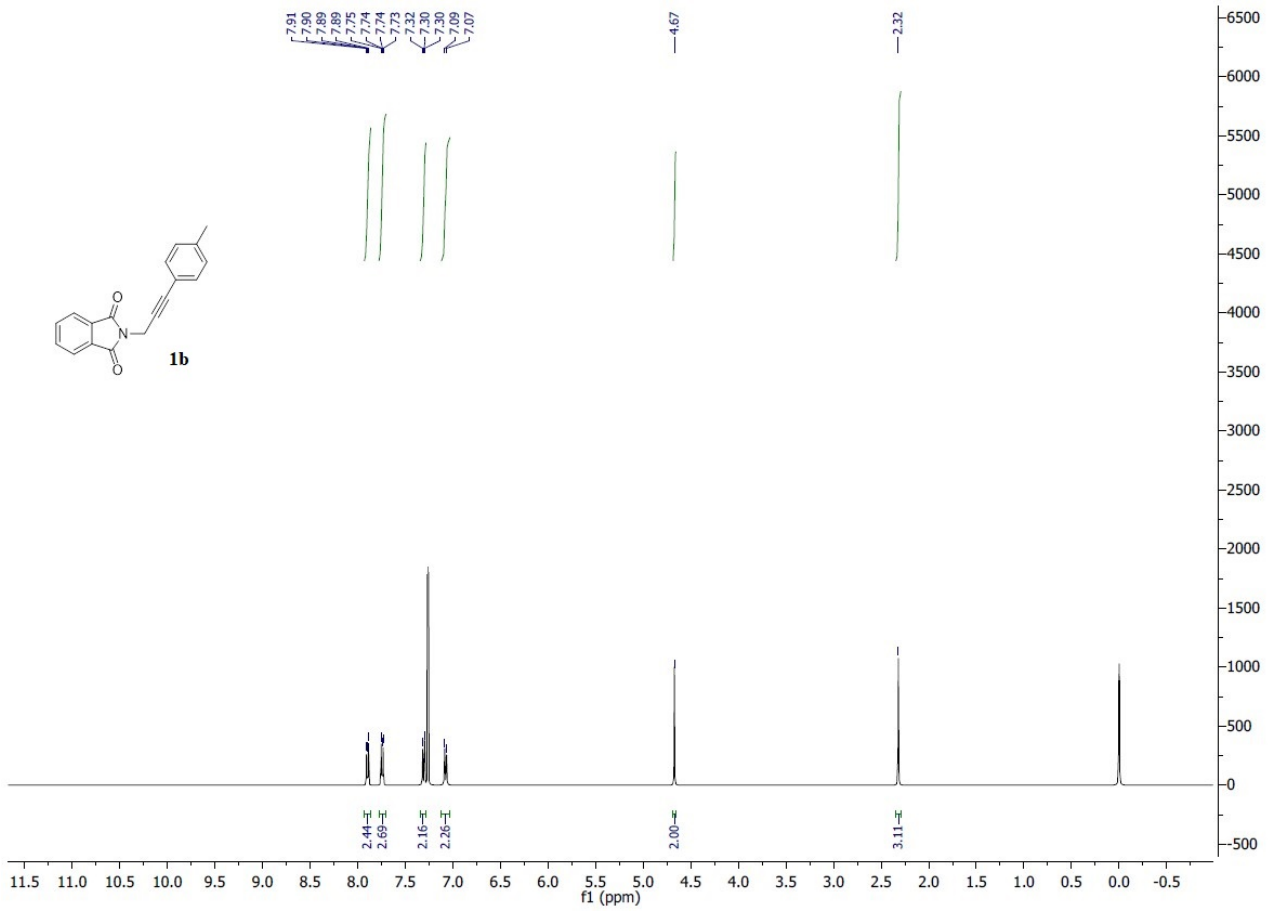


VII. Copies of ^{1}H and ^{13}C Spectra of new derivatives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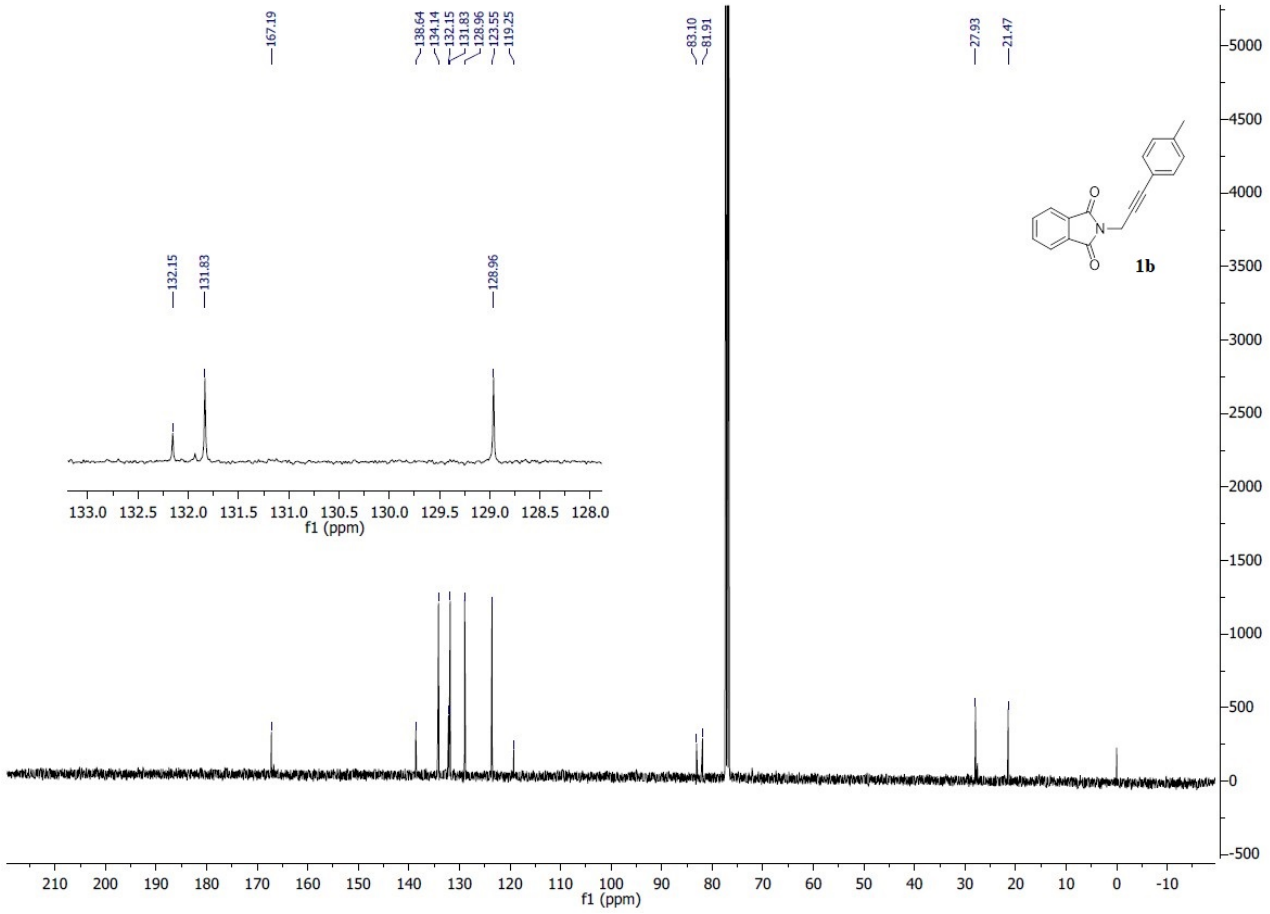
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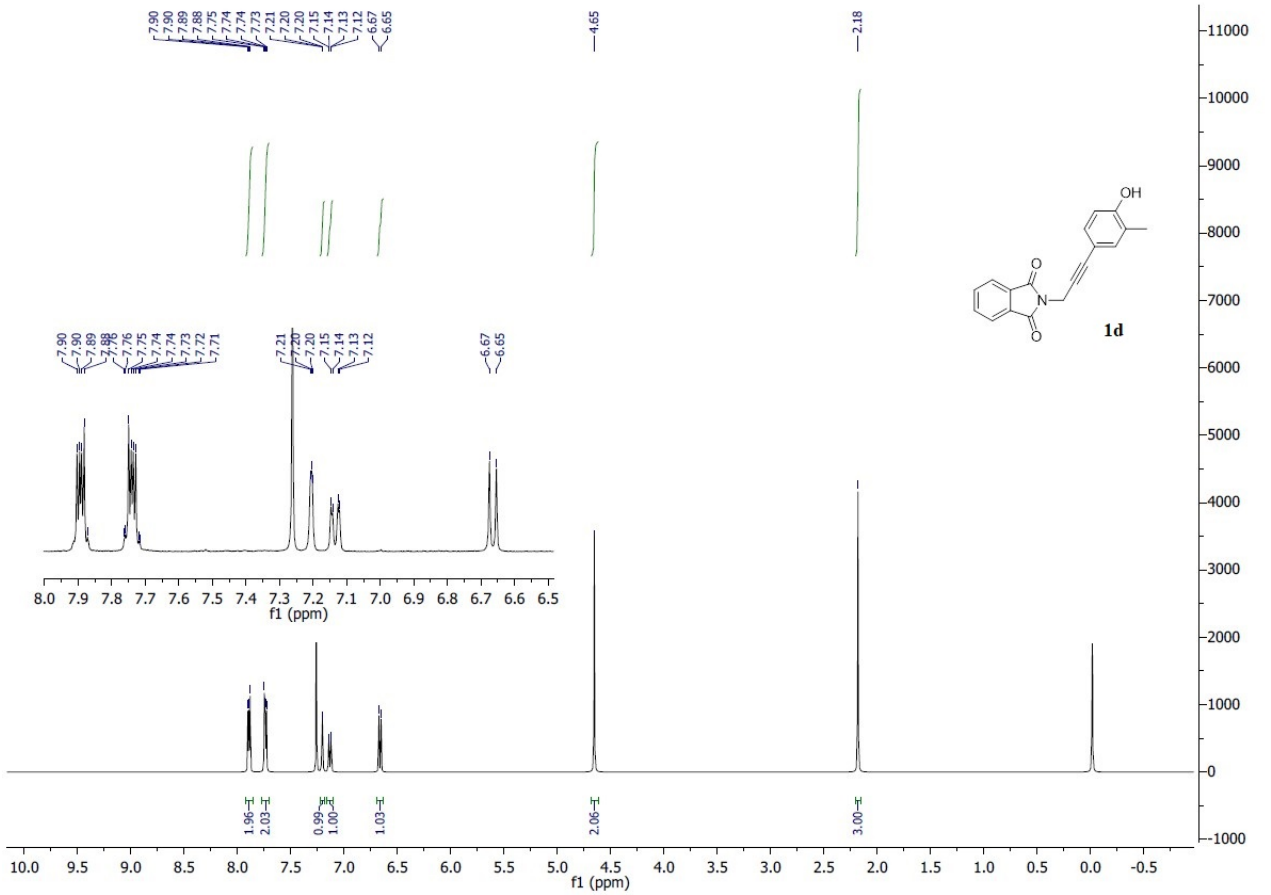
f1 (ppm)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f1 (ppm)
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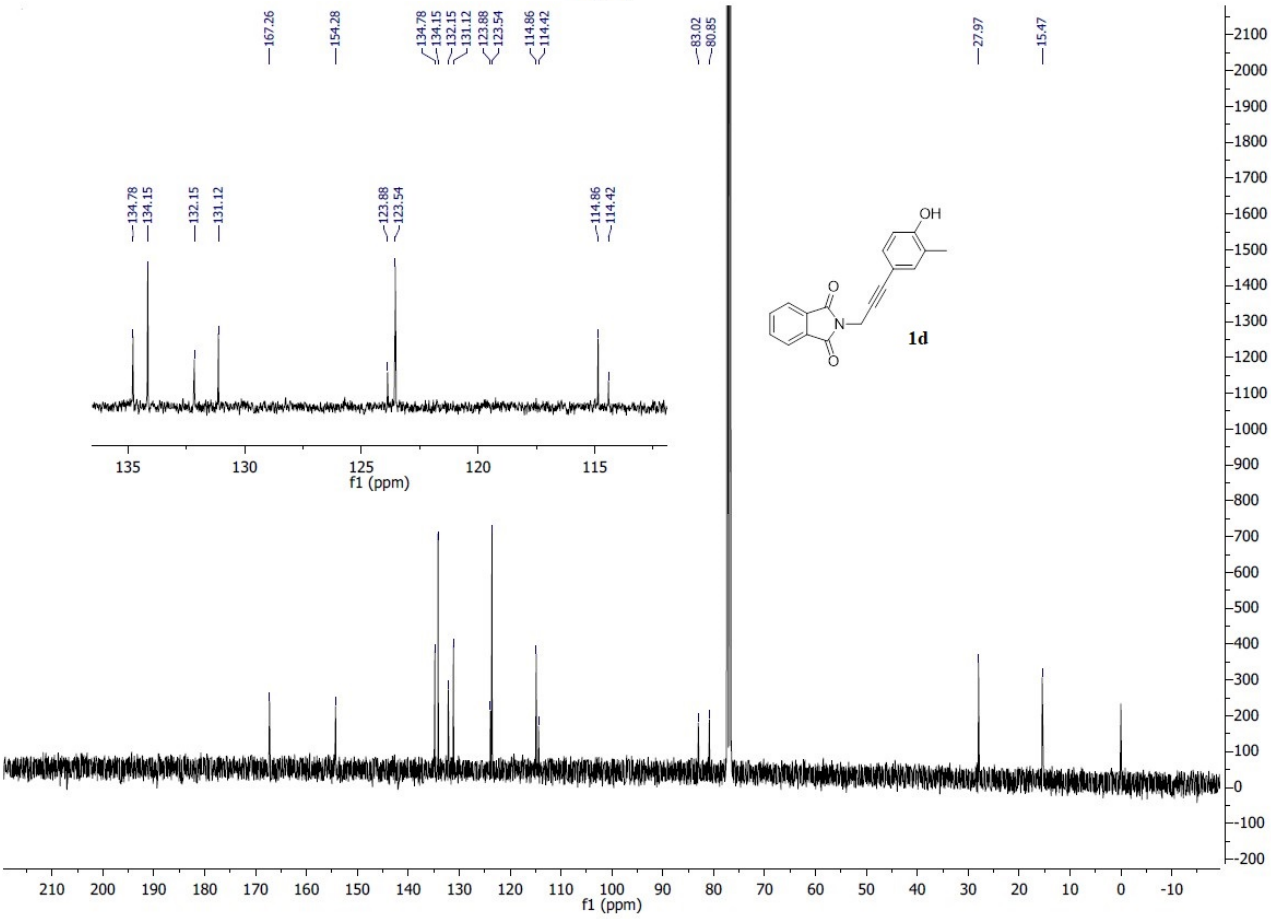
2.03
0.99
1.00
1.03
2.06
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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15.47
134.78
134.15
132.15
131.12
123.88
123.54
114.86
114.42
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N
O
1d
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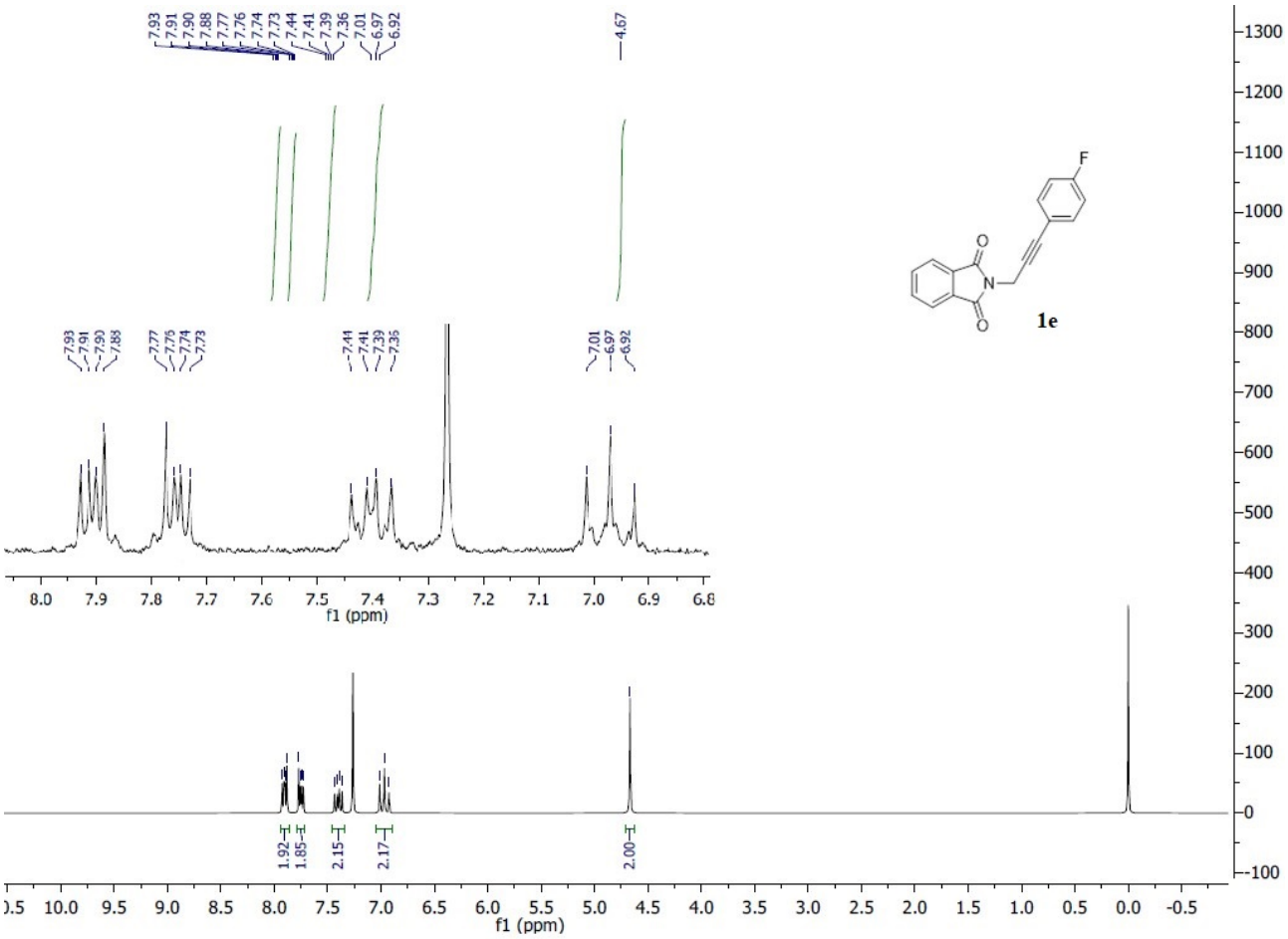
f1 (ppm)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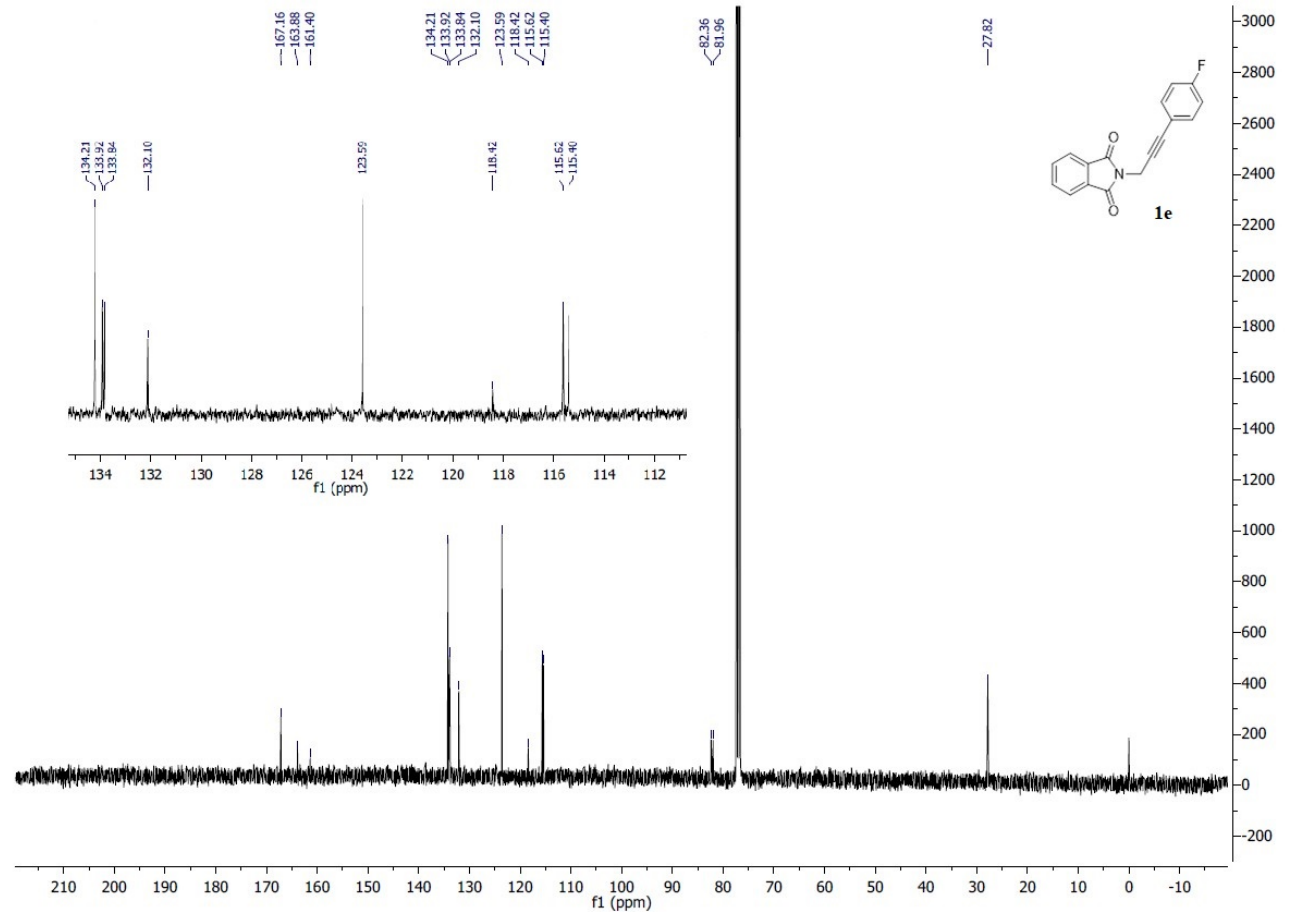
2.00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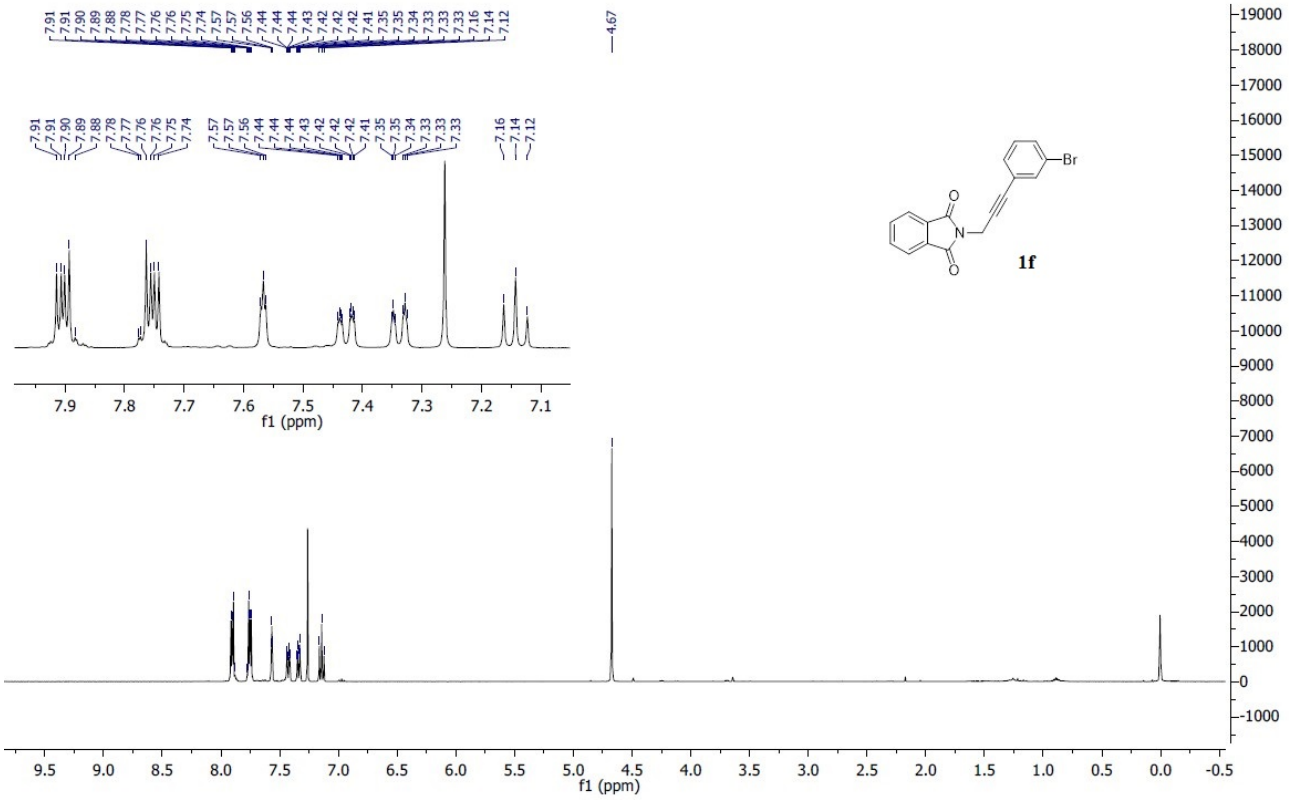
27.82
F
O
N
O
1e
f1 (ppm)


7.91
7.91
7.90
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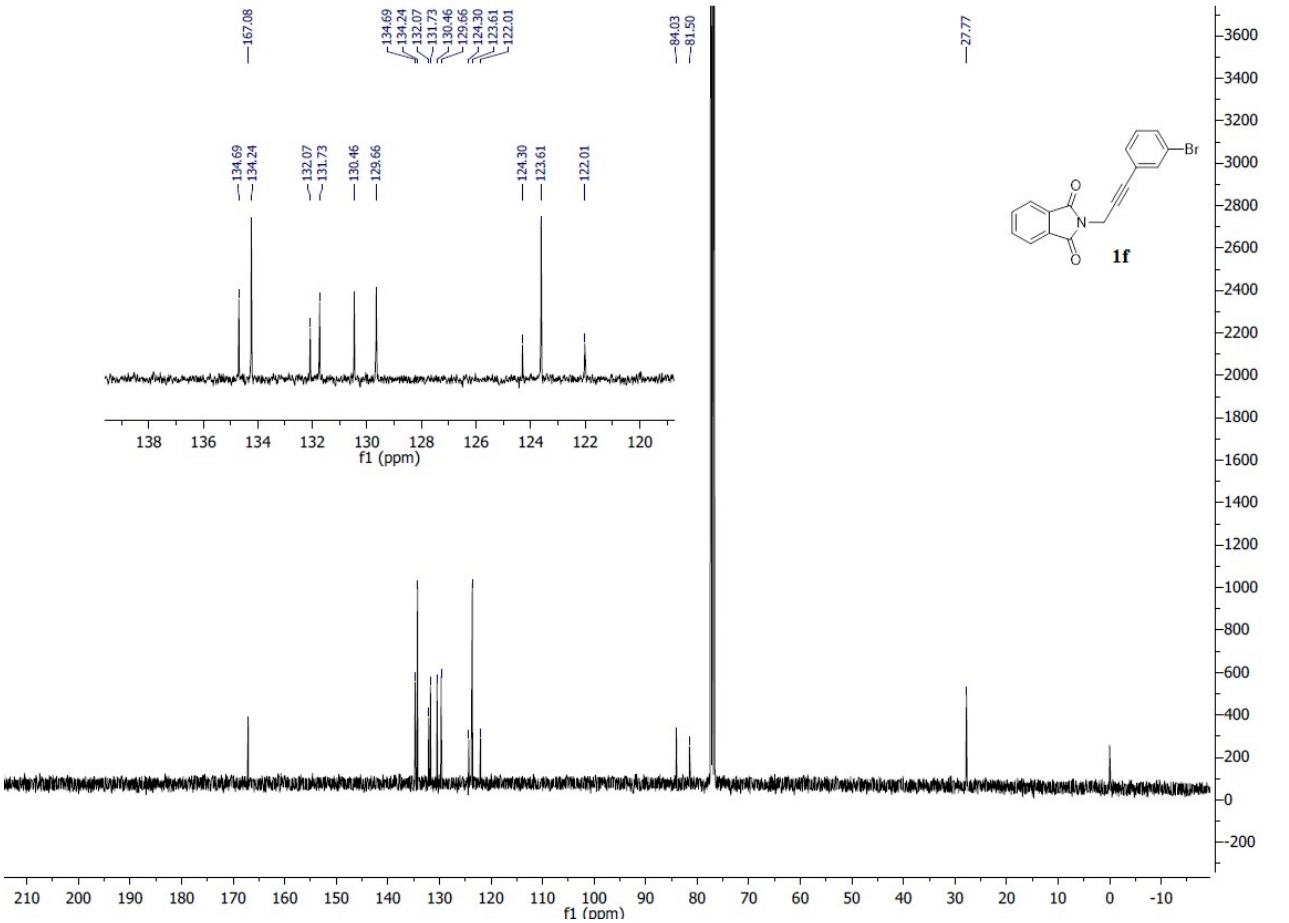
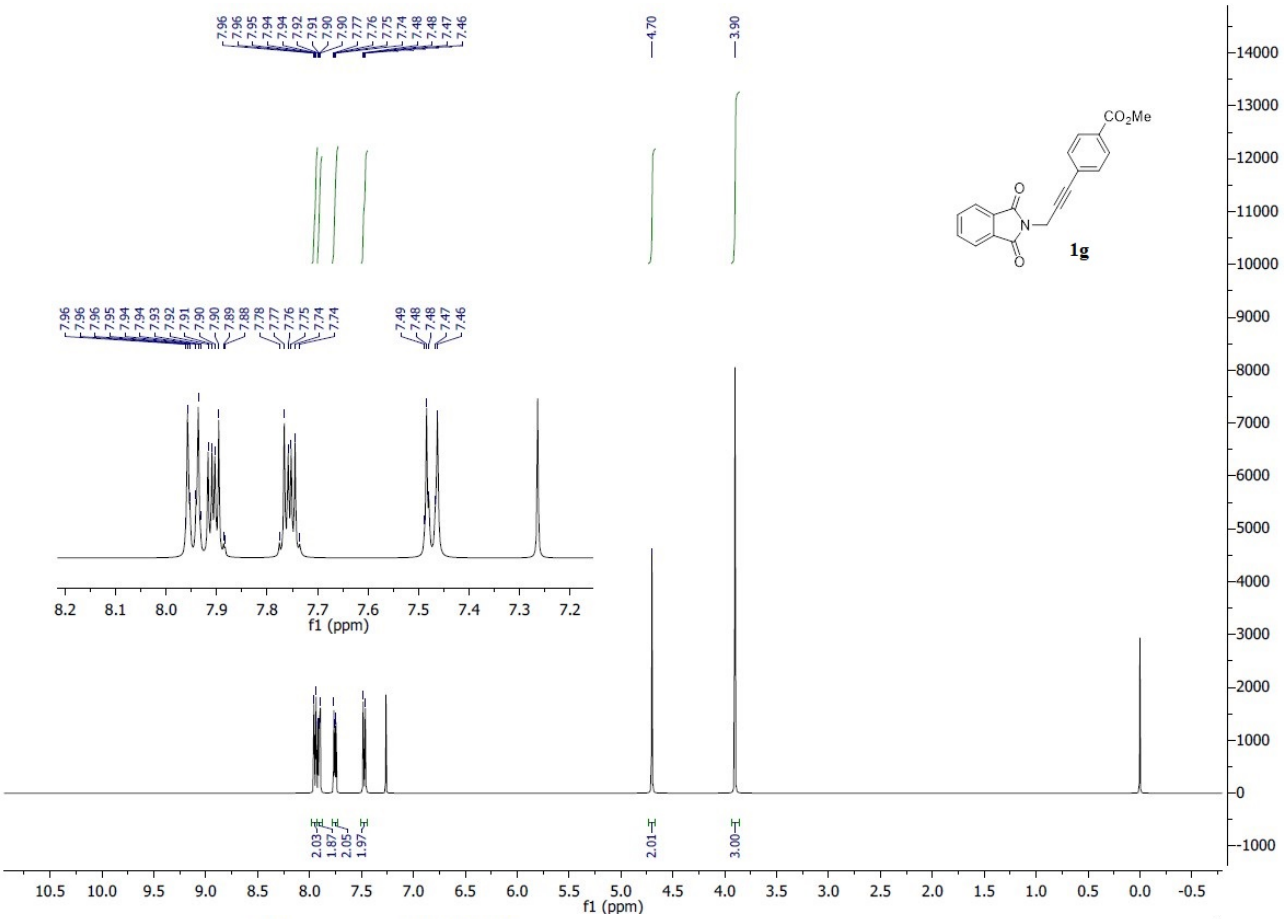
7.88
7.78
7.77
7.76
7.76
7.75
7.74
7.57
7.57
7.56
7.44
7.44
7.44
7.43
7.42
7.42
7.42
7.41
7.35
7.35
7.34
7.33
7.33
7.16
7.14
7.12
4.67
Br
O
N
O
1f
f1 (ppm)
f1 (ppm)


167.08
134.69
134.24
132.07
131.73
130.46
129.66
124.30
123.61
122.01
84.03
81.50
27.77
Br
O
N
O
1f
f1 (ppm)
f1 (ppm)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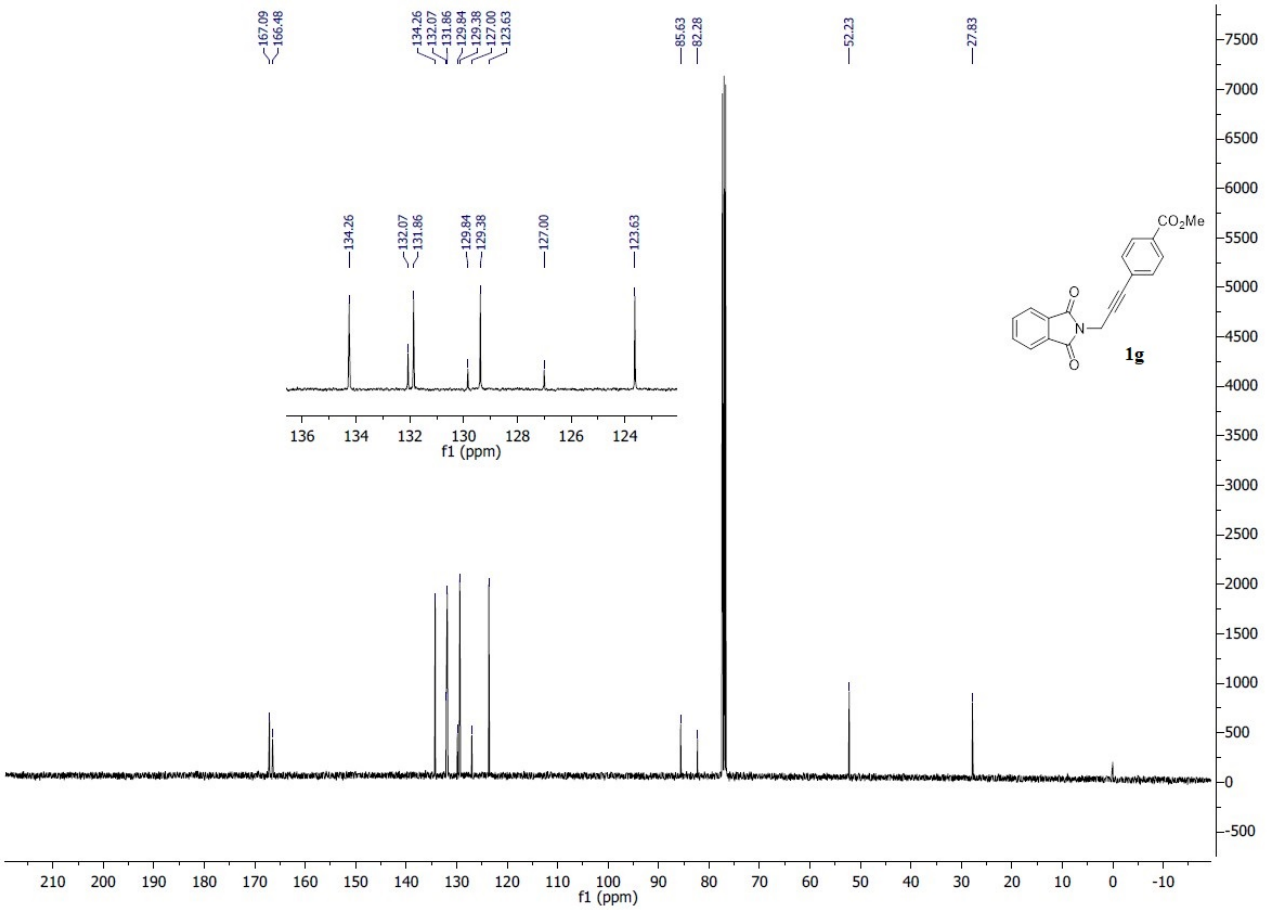
7.96
7.95
7.94
7.94
7.92
7.91
7.90
7.90
7.77
7.76
7.75
7.74
7.48
7.48
7.47
7.46
4.70
3.90
CO2Me
1g
7.96
7.96
7.96
7.95
7.94
7.94
7.93
7.92
7.91
7.90
7.90
7.89
7.88
7.78
7.77
7.76
7.75
7.74
7.74
7.49
7.48
7.48
7.47
7.46
8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2
f1 (ppm)
2.03
1.87
2.05
1.97
2.01
3.00
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 0.0 -0.5
f1 (ppm)


167.09
166.48
134.26
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129.38
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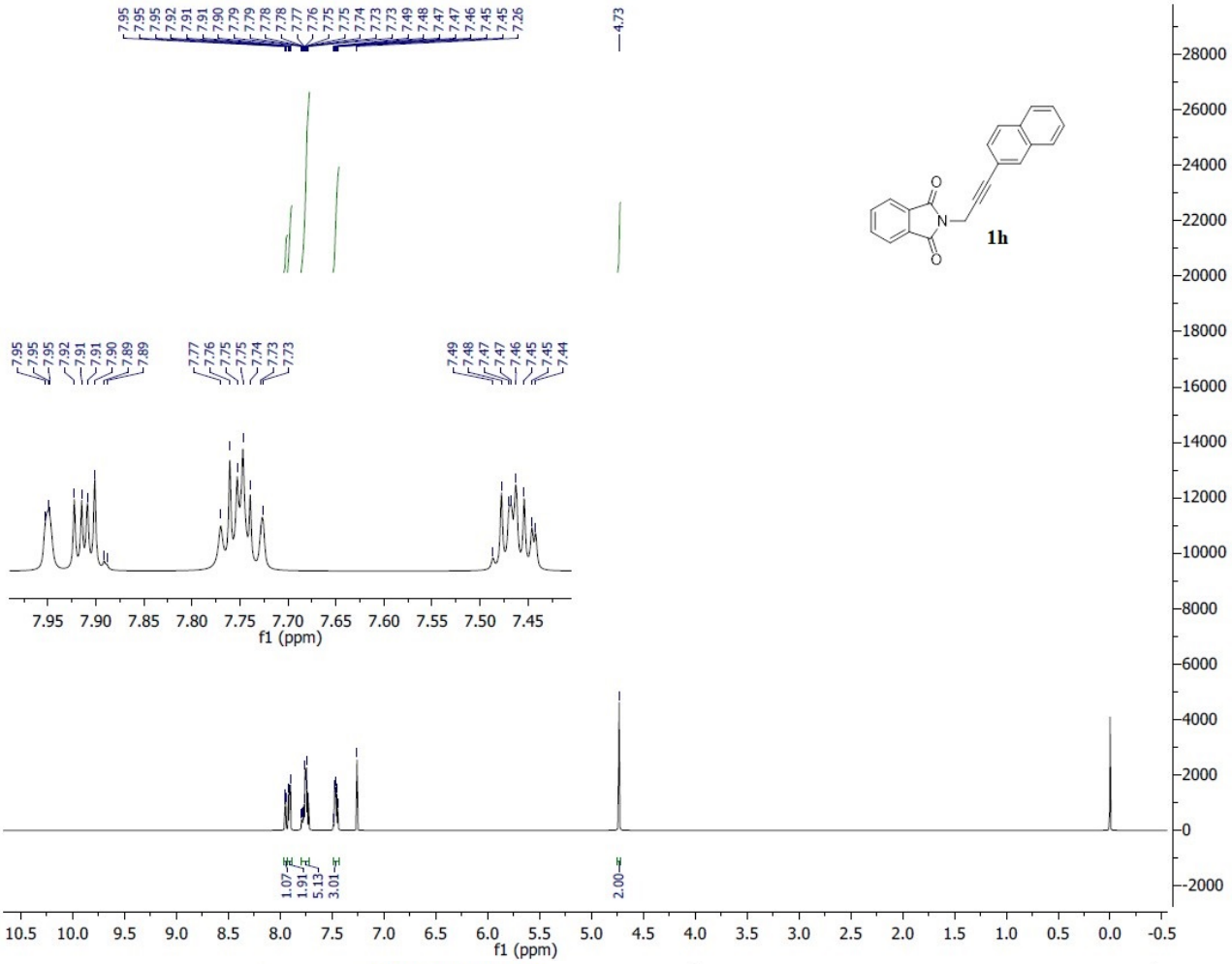
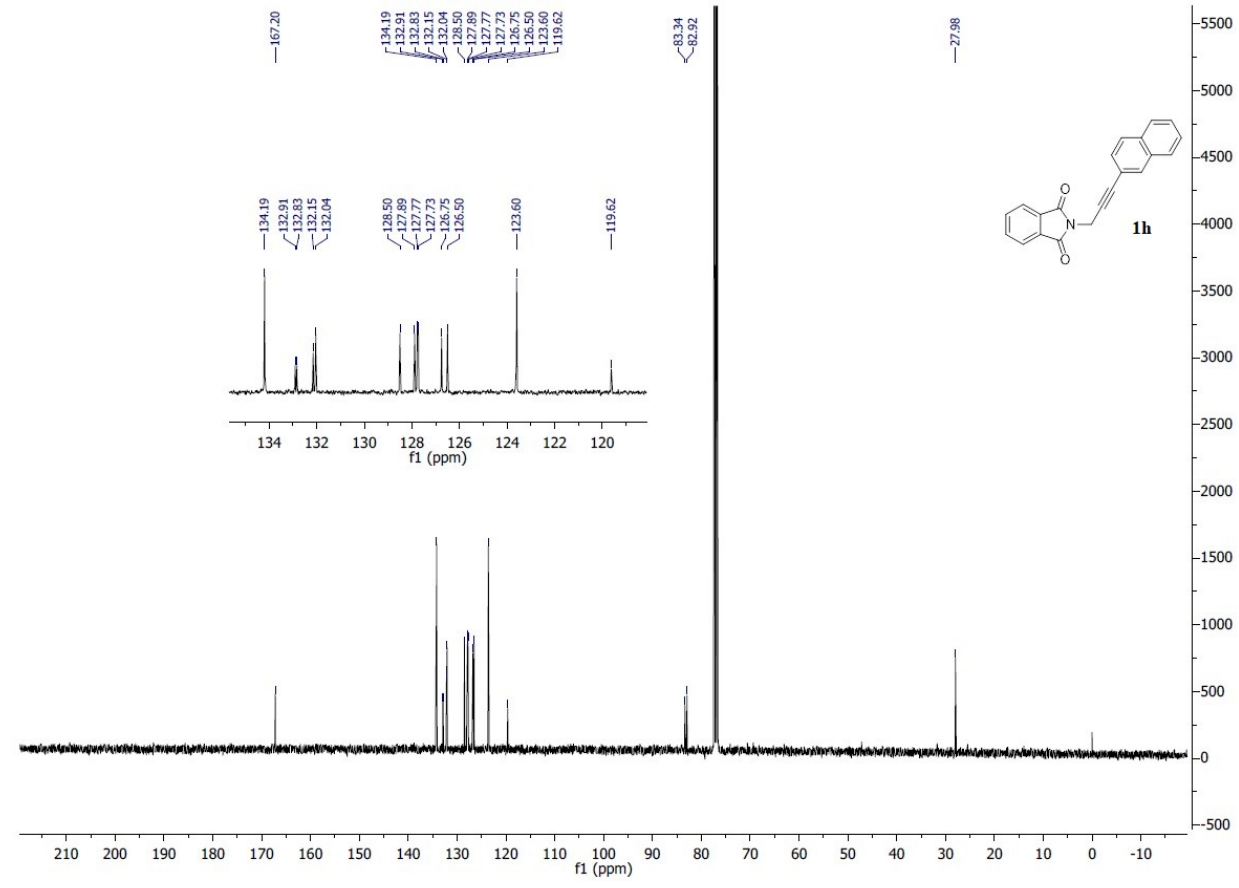
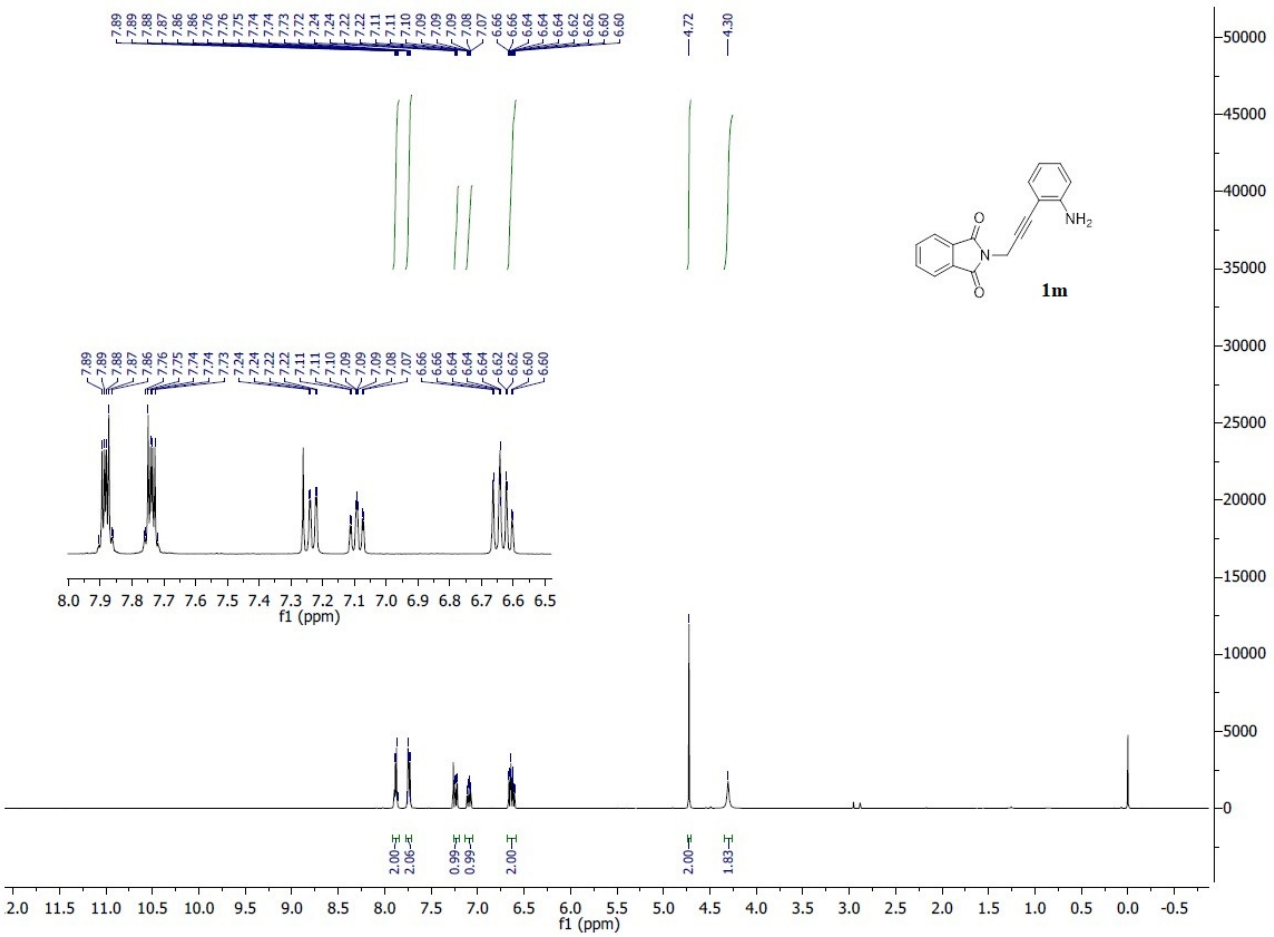
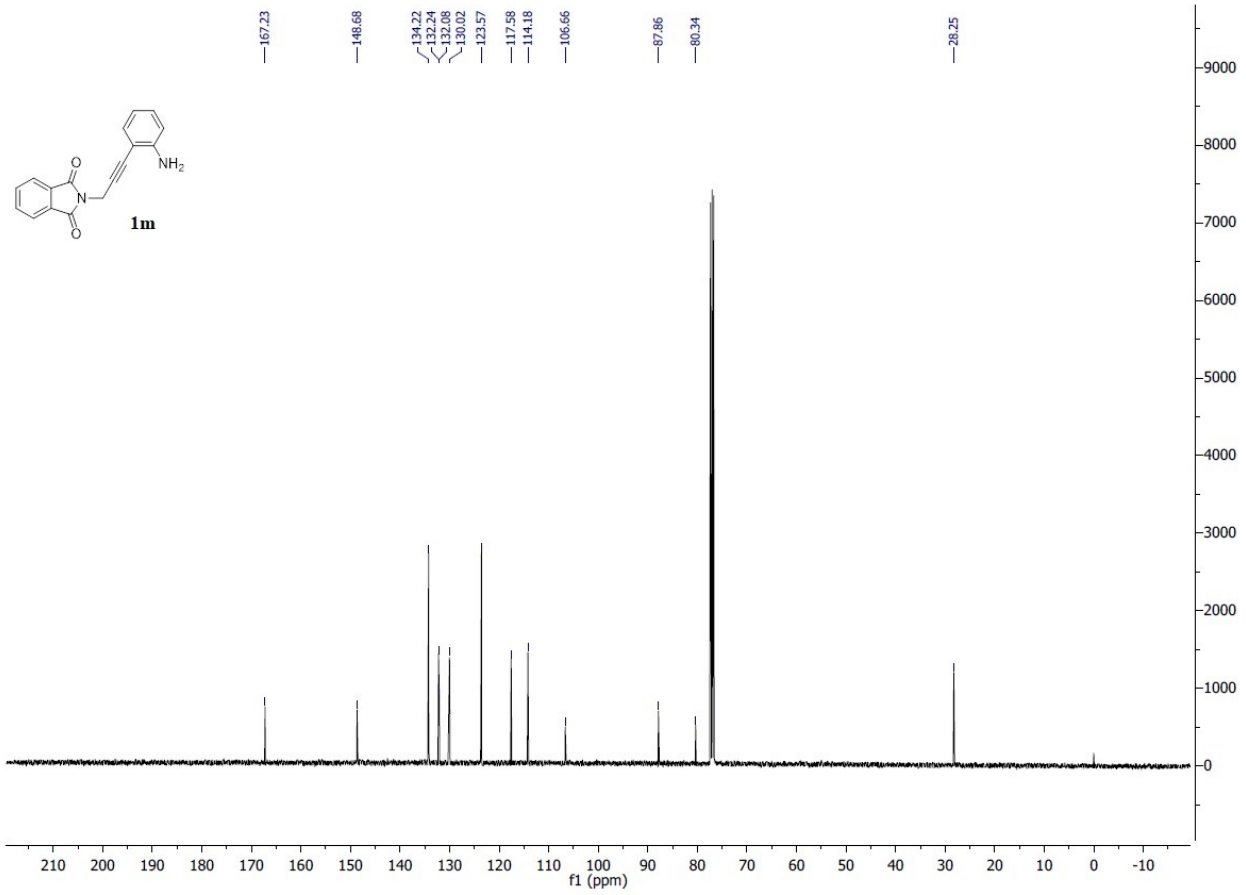
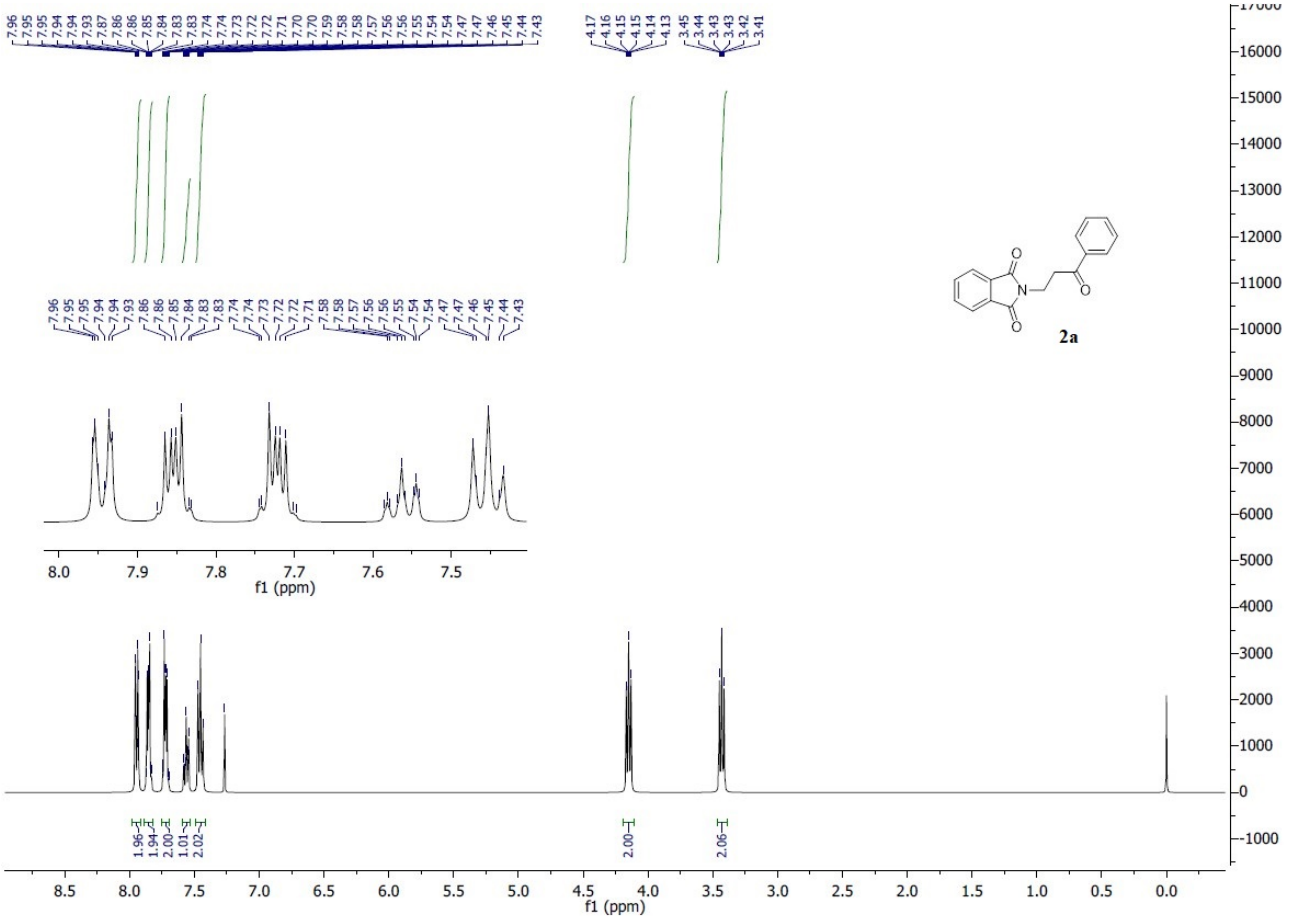
85.63
82.28
52.23
27.83
134.26
132.07
131.86
129.84
129.38
127.00
123.63
CO2Me
1g
136 134 132 130 128 126 124
f1 (ppm)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

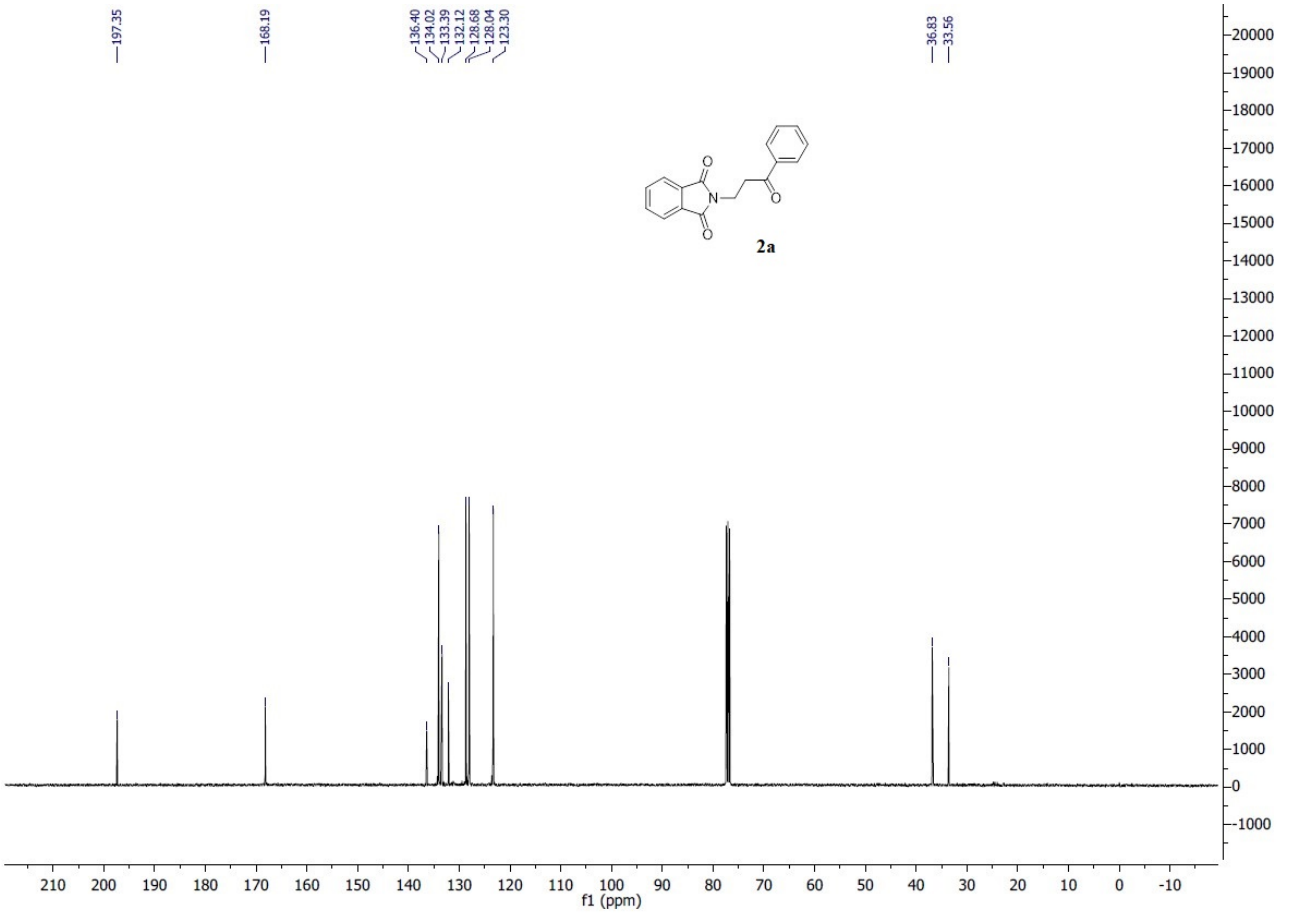

1h
f1 (ppm)

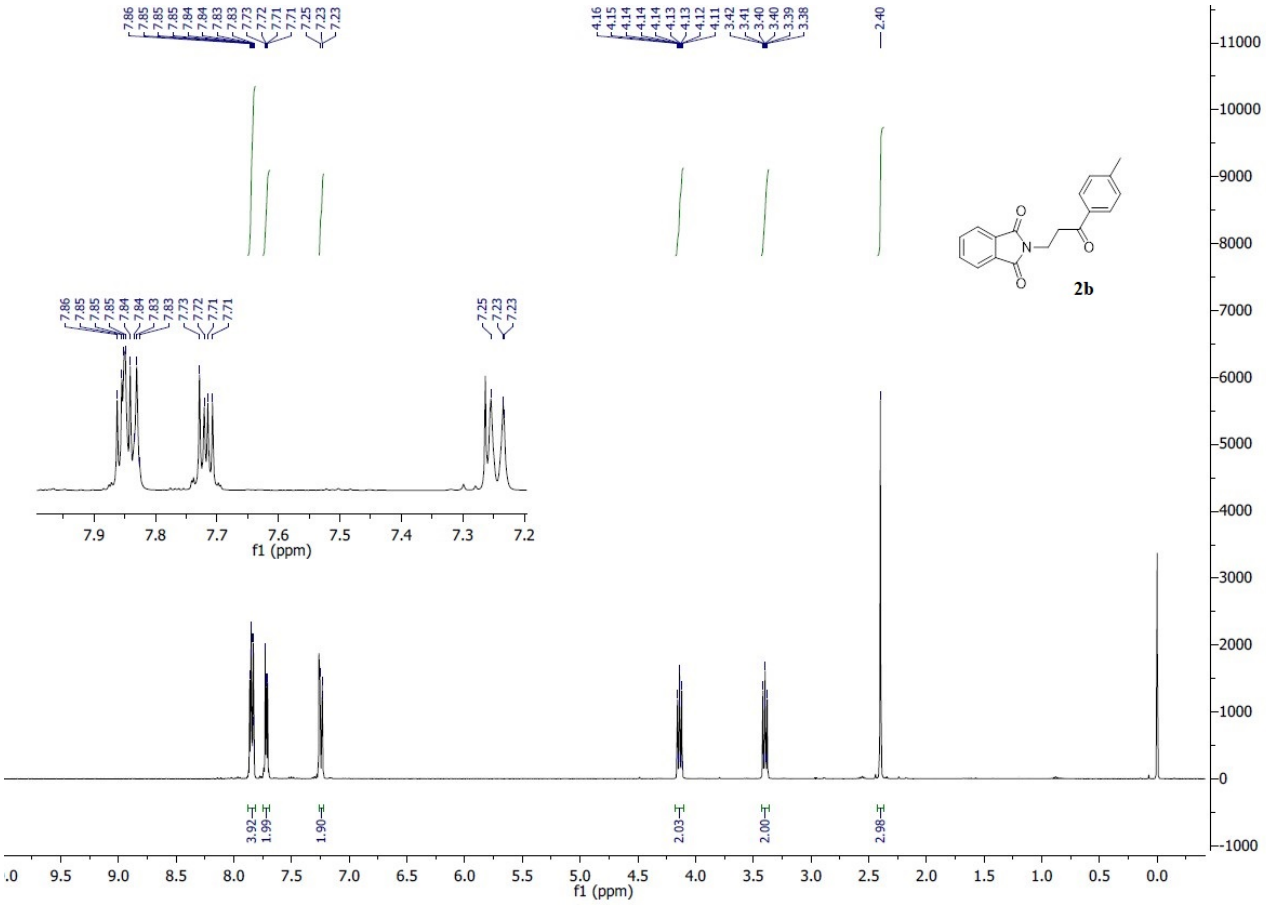

1h
f1 (ppm)

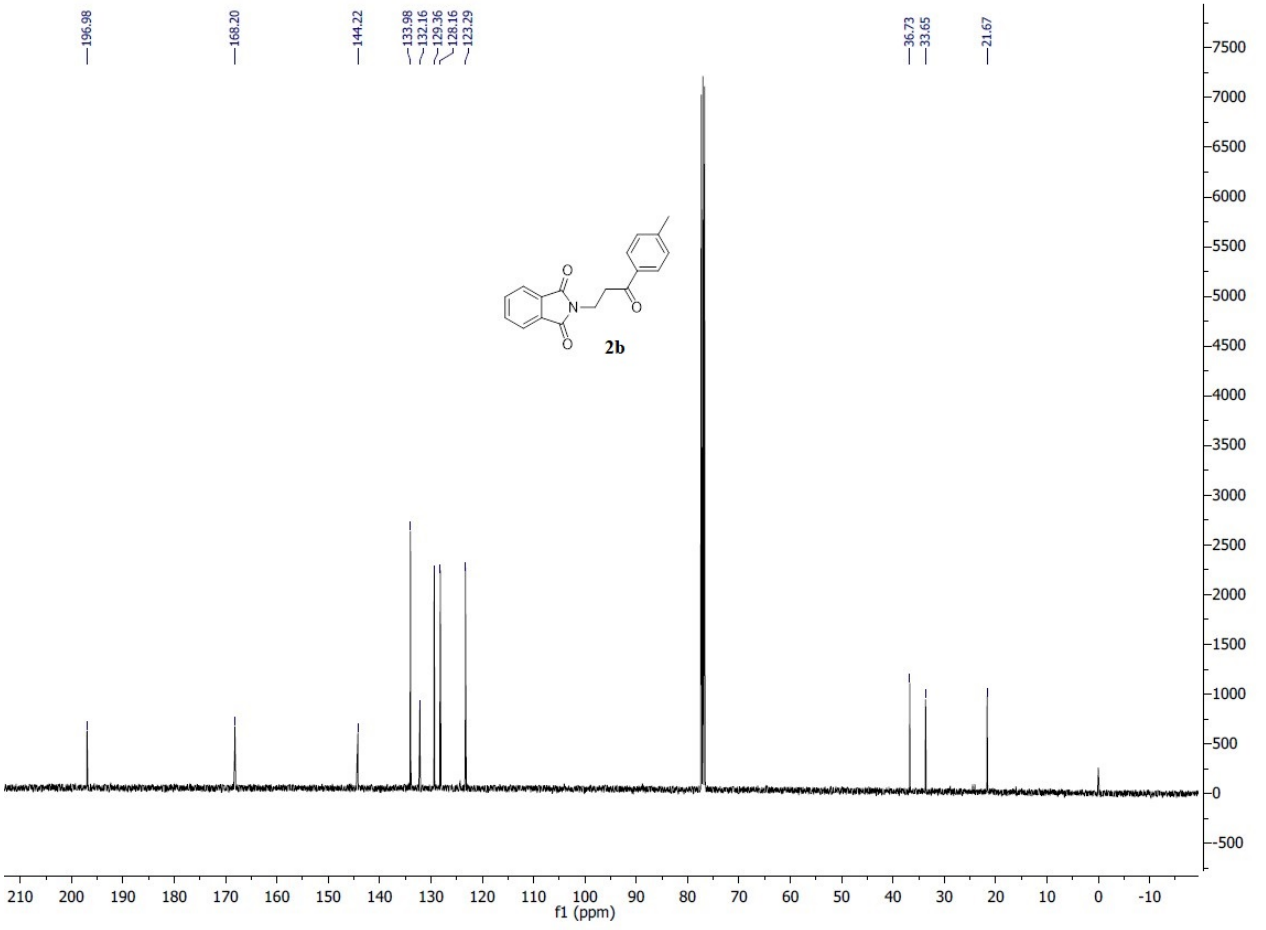

7.89
7.88
7.87
7.86
7.76
7.75
7.74
7.73
7.72
7.24
7.22
7.11
7.10
7.09
7.08
7.07
6.66
6.64
6.62
6.60
4.72
4.30
NH2
1m
8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7 6.6 6.5
f1 (ppm)
2.00
2.06
0.99
0.99
2.00
2.00
1.83
2.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

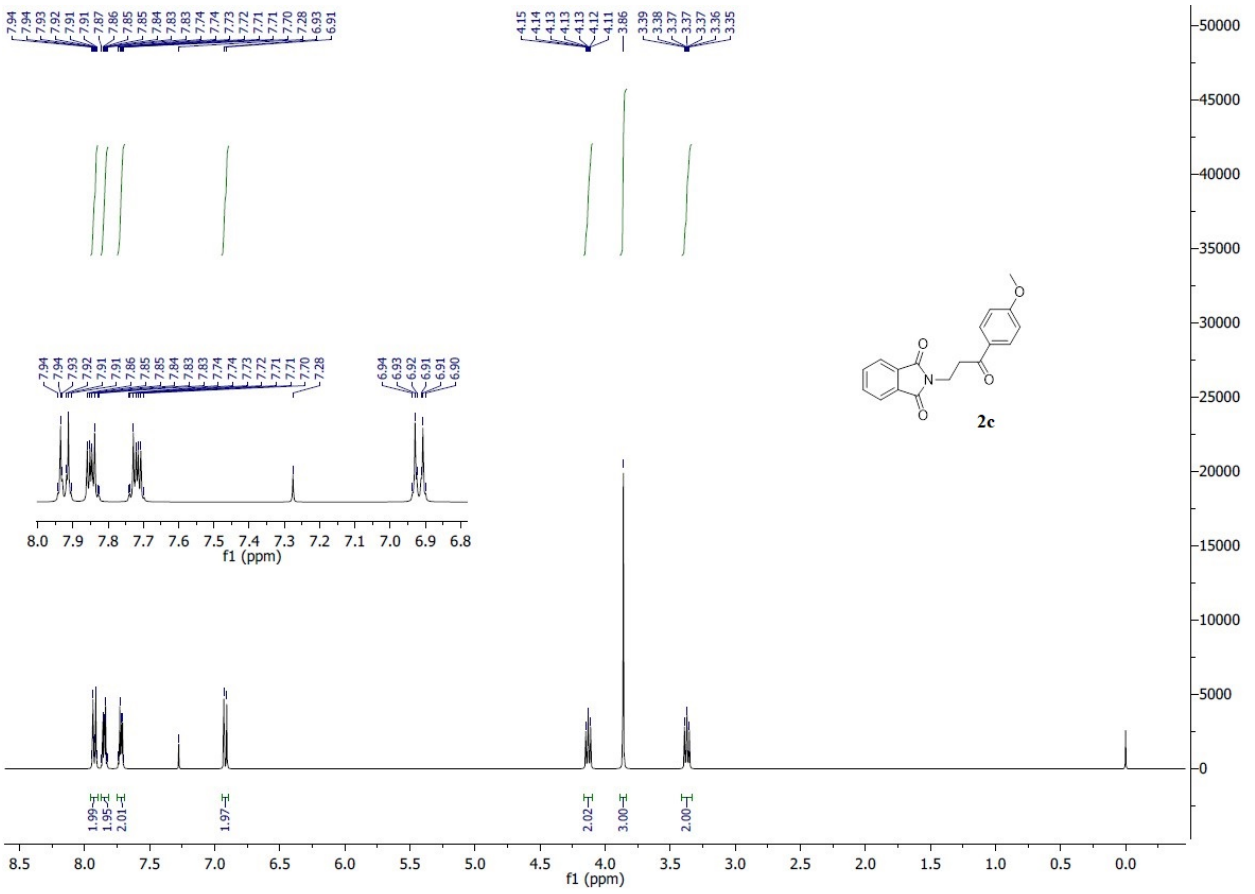

167.23
148.68
134.22
132.24
132.08
130.02
123.57
117.58
114.18
106.66
87.86
80.34
28.25
NH2
1m
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

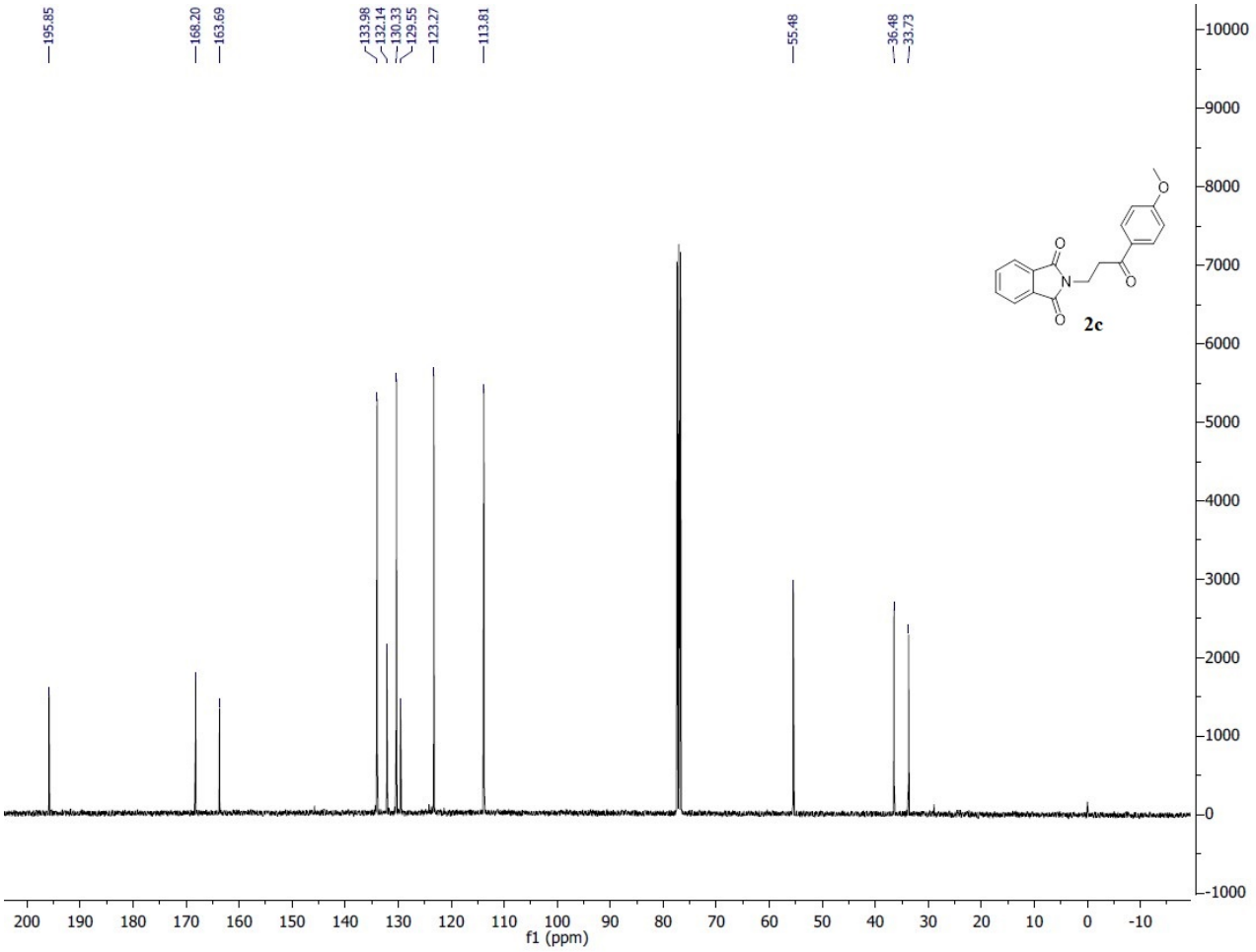

2a
f1 (ppm)

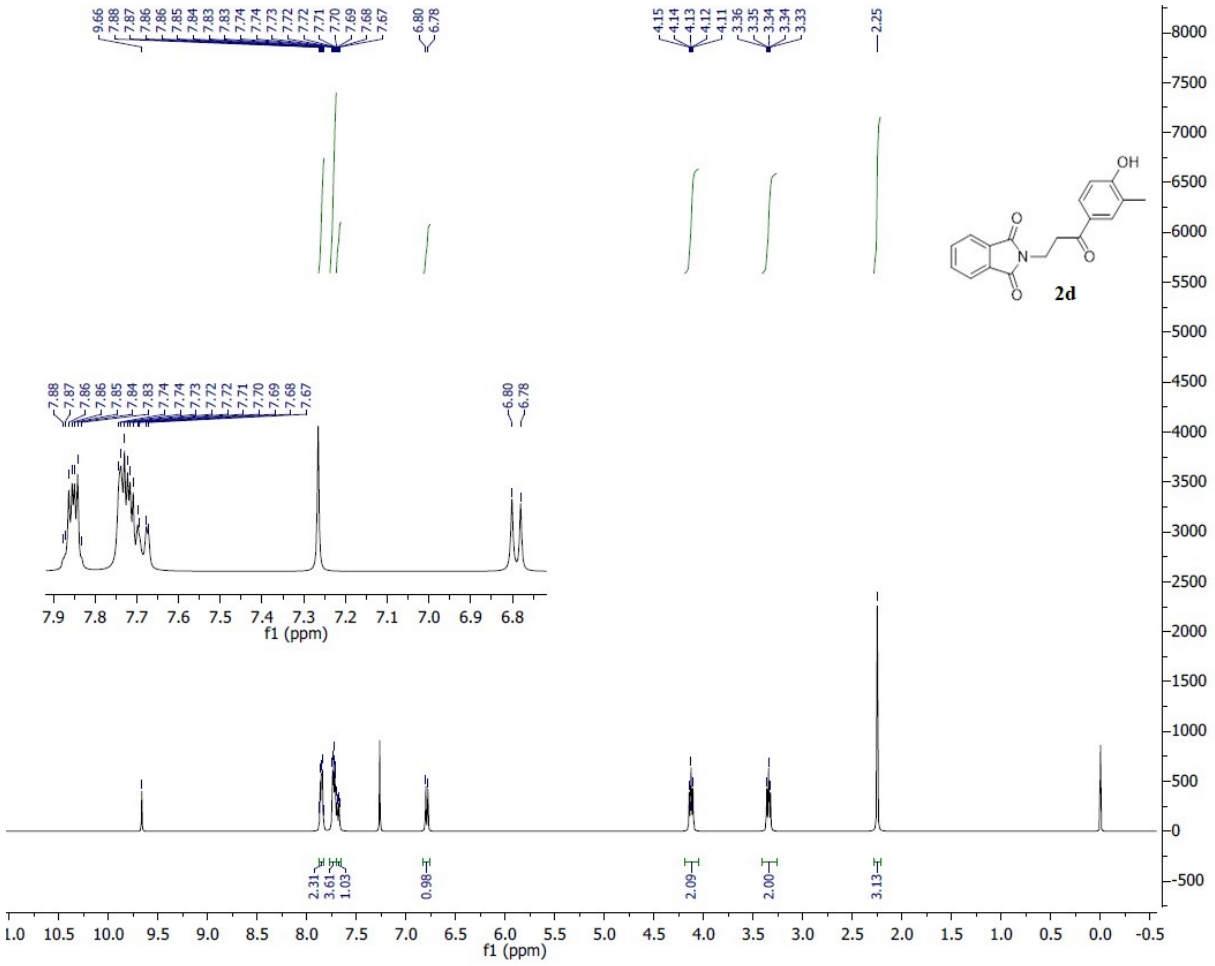

2a
f1 (ppm)

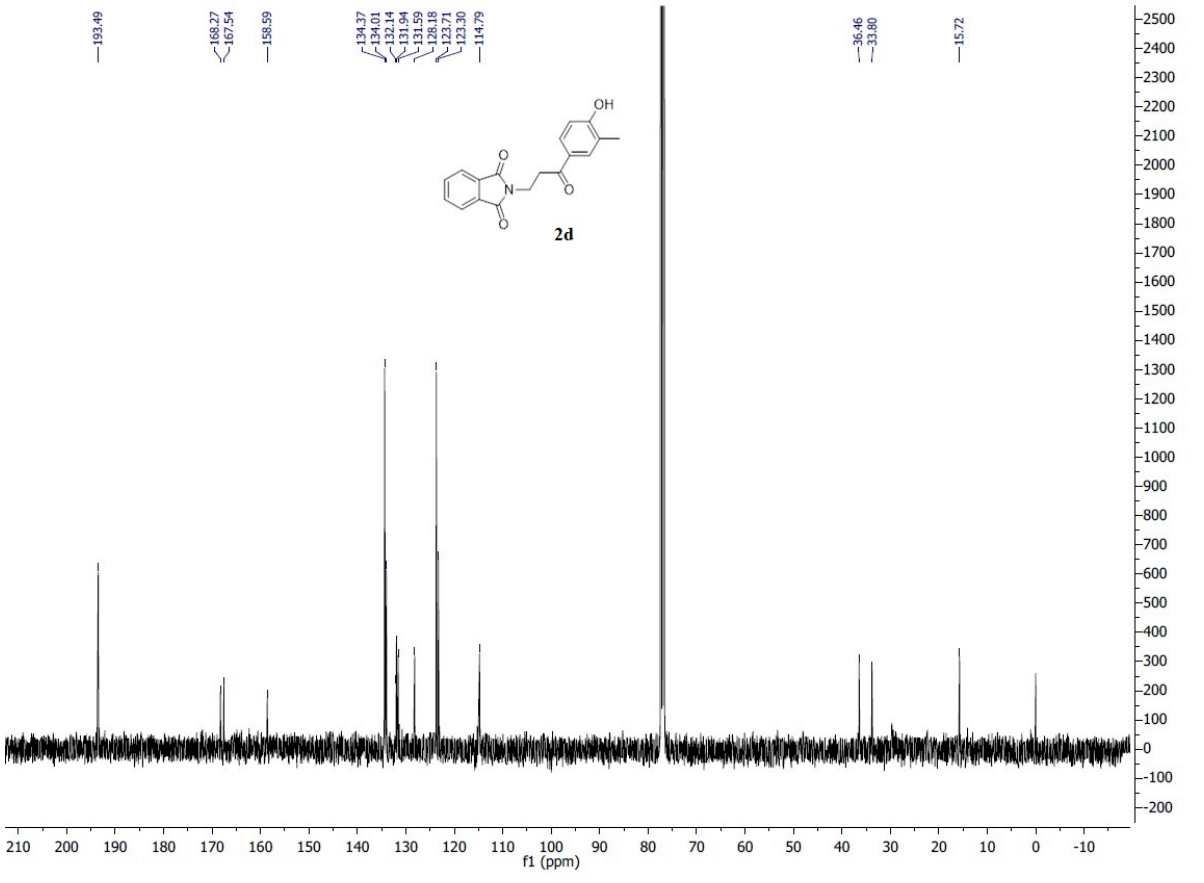

7.86
7.85
7.85
7.85
7.84
7.84
7.83
7.83
7.73
7.72
7.71
7.71
7.25
7.23
7.23
4.16
4.15
4.14
4.14
4.14
4.13
4.13
4.12
4.11
3.42
3.41
3.40
3.40
3.39
3.38
2.40
2b
f1 (ppm)
3.92
1.99
1.90
2.03
2.00
2.98

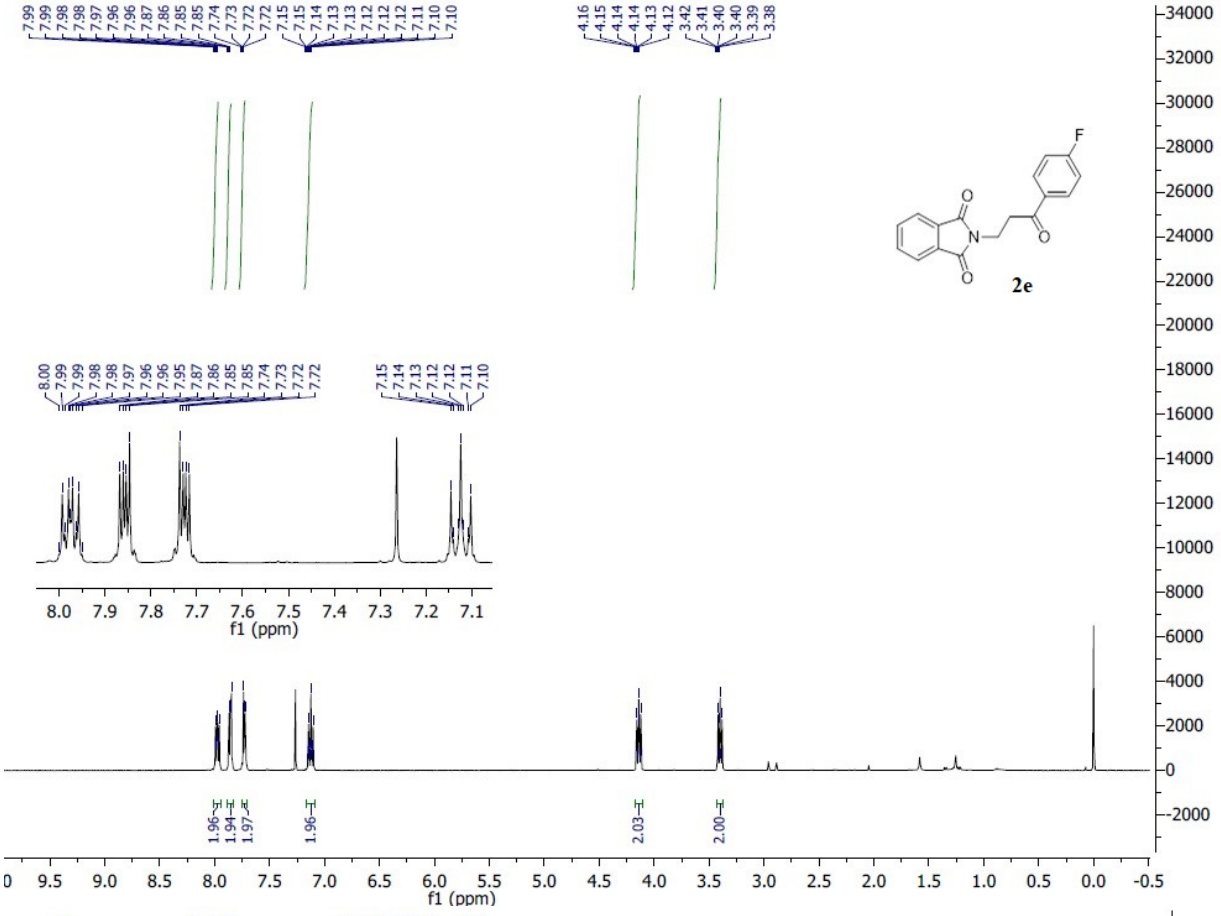

196.98
168.20
144.22
133.98
132.16
129.36
128.16
123.29
36.73
33.65
21.67
2b
f1 (ppm)

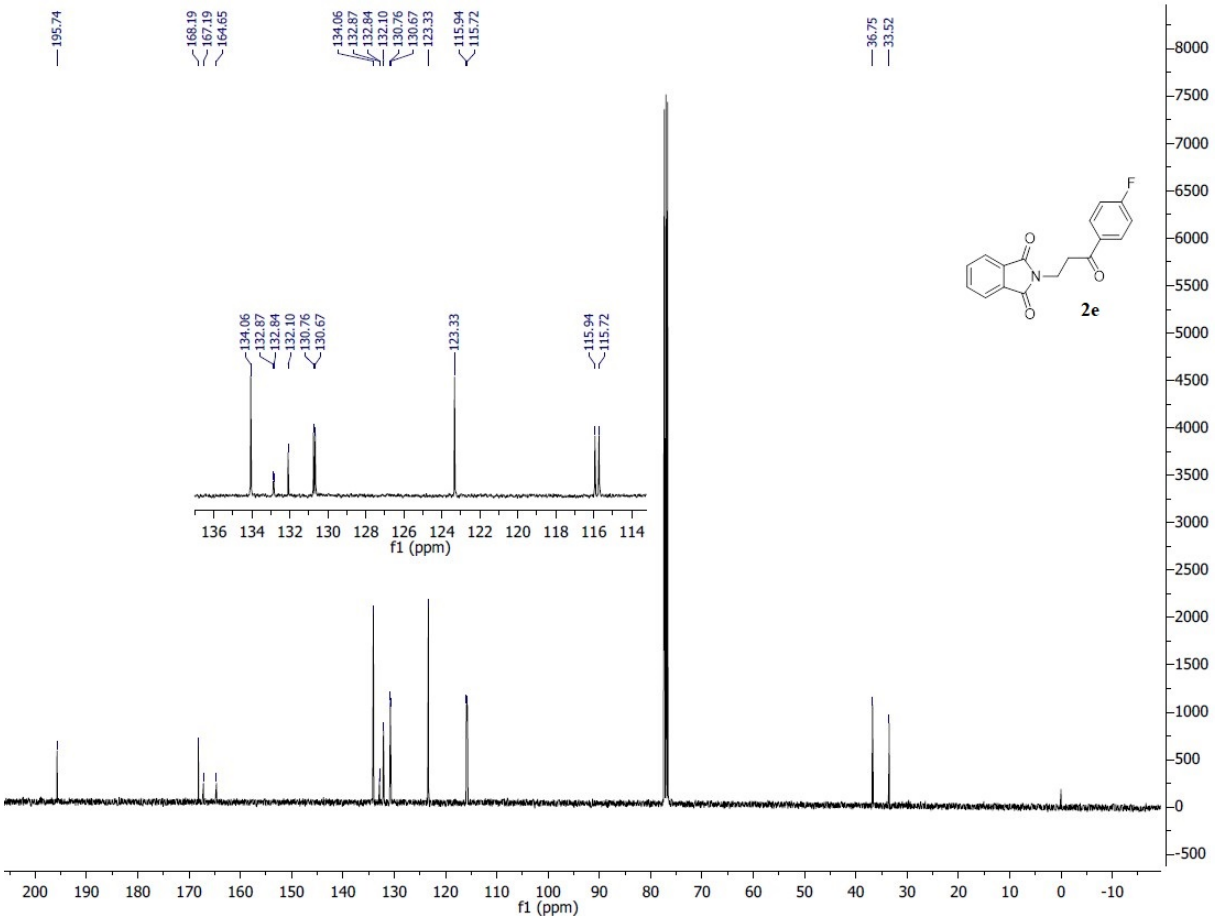

7.94 7.94 7.93 7.92 7.91 7.91 7.87 7.86 7.85 7.85 7.84 7.83 7.83 7.74 7.74 7.73 7.72 7.71 7.71 7.70 7.28 6.93 6.91
4.15 4.14 4.13 4.13 4.13 4.12 4.11 3.86 3.39 3.38 3.37 3.37 3.37 3.36 3.35
6.94 6.93 6.92 6.91 6.91 6.90
8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8
f1 (ppm)
1.99 1.95 2.01 1.97 2.02 3.00 2.00
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 0.0
f1 (ppm)
50000 45000 40000 35000 30000 25000 20000 15000 10000 5000 0
2c

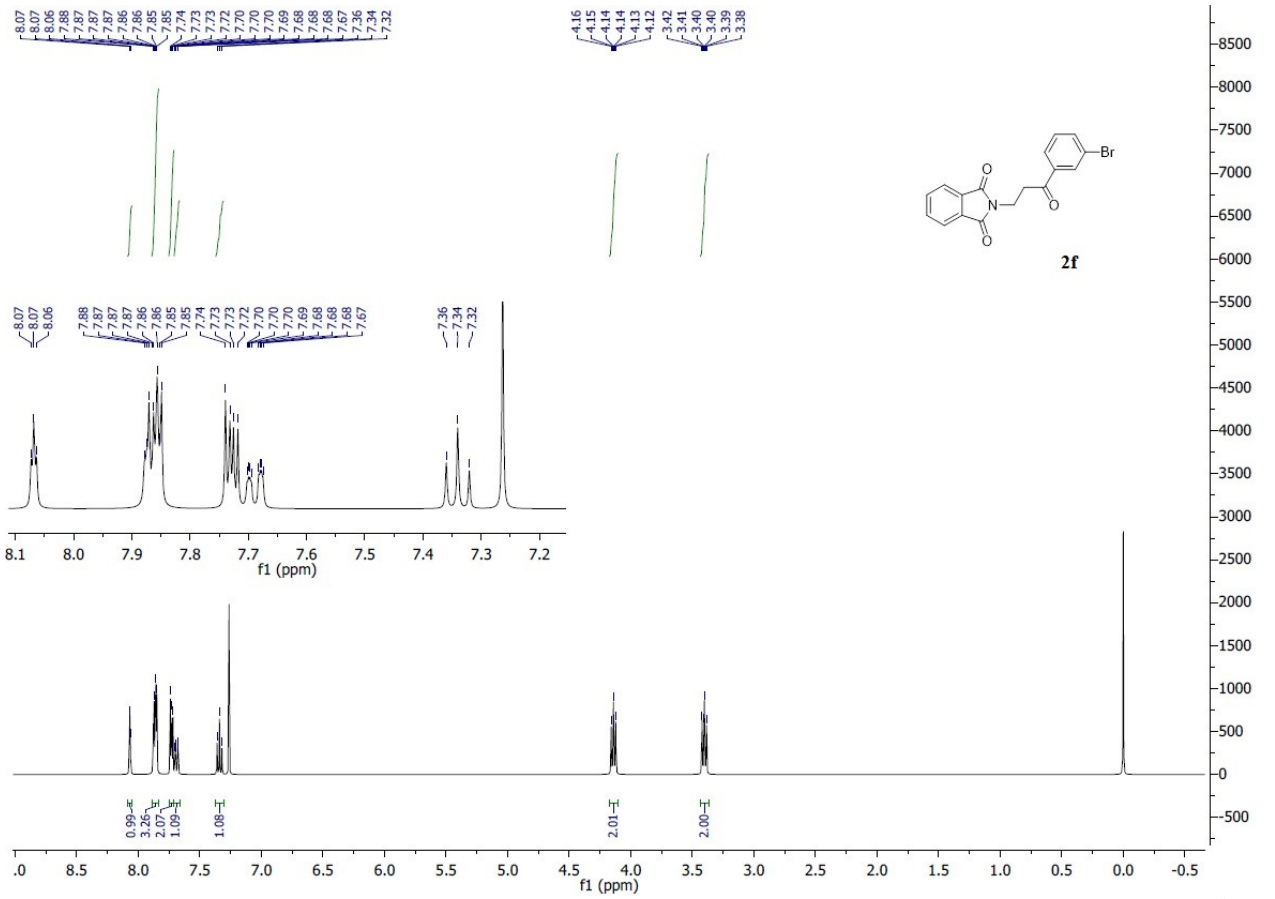

195.85 168.20 163.69 133.98 132.14 130.33 129.55 123.27 113.81 55.48 36.48 33.73
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)
10000 9000 8000 7000 6000 5000 4000 3000 2000 1000 0 -1000
2c

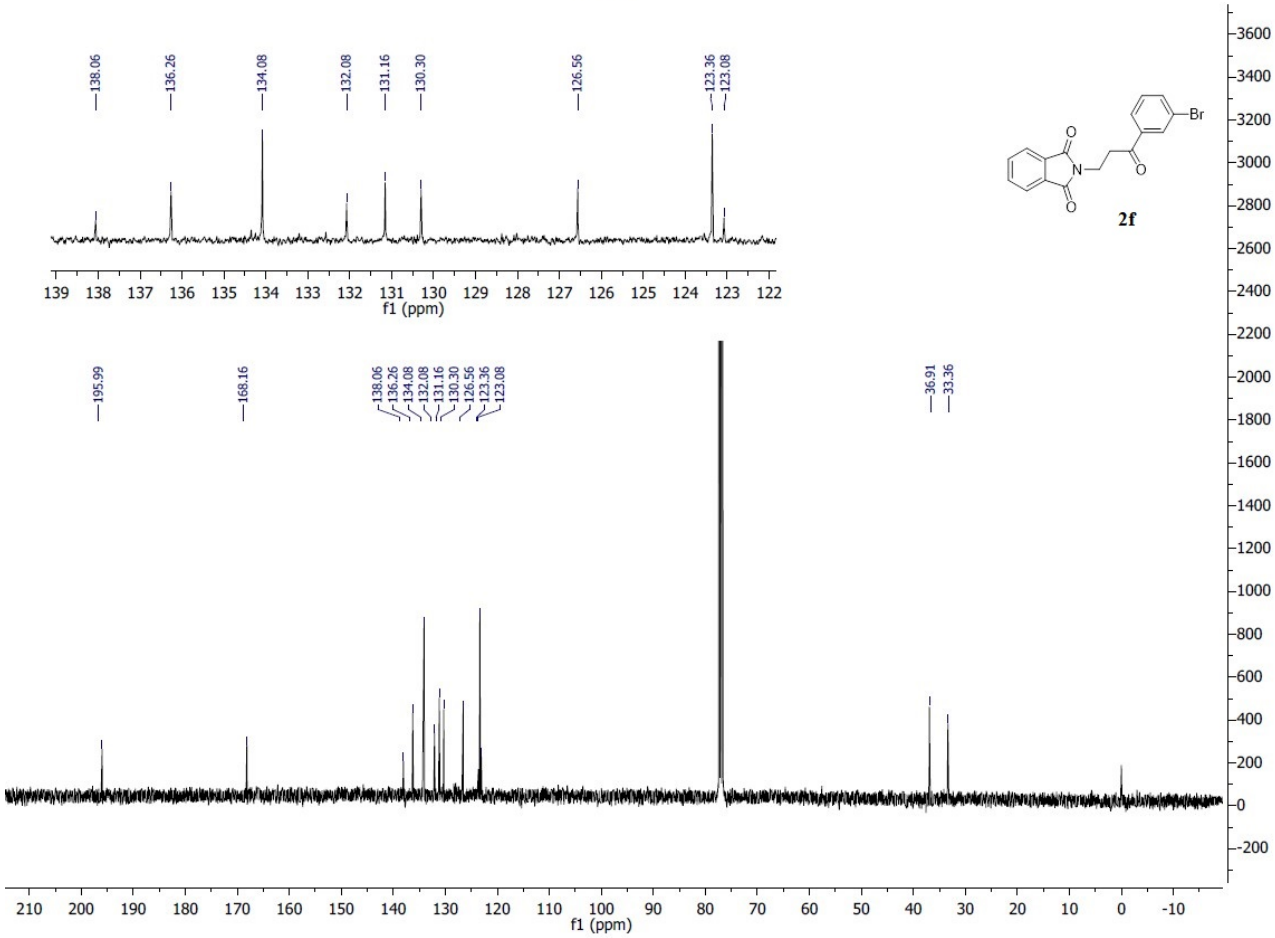

9.66
7.88
7.87
7.86
7.86
7.85
7.84
7.83
7.74
7.74
7.73
7.72
7.72
7.71
7.70
7.69
7.68
7.67
6.80
6.78
4.15
4.14
4.13
4.12
4.11
3.36
3.35
3.34
3.34
3.33
2.25
OH
O
N
O
O
2d
2.31
3.61
1.03
0.98
2.09
2.00
3.13
f1 (ppm)

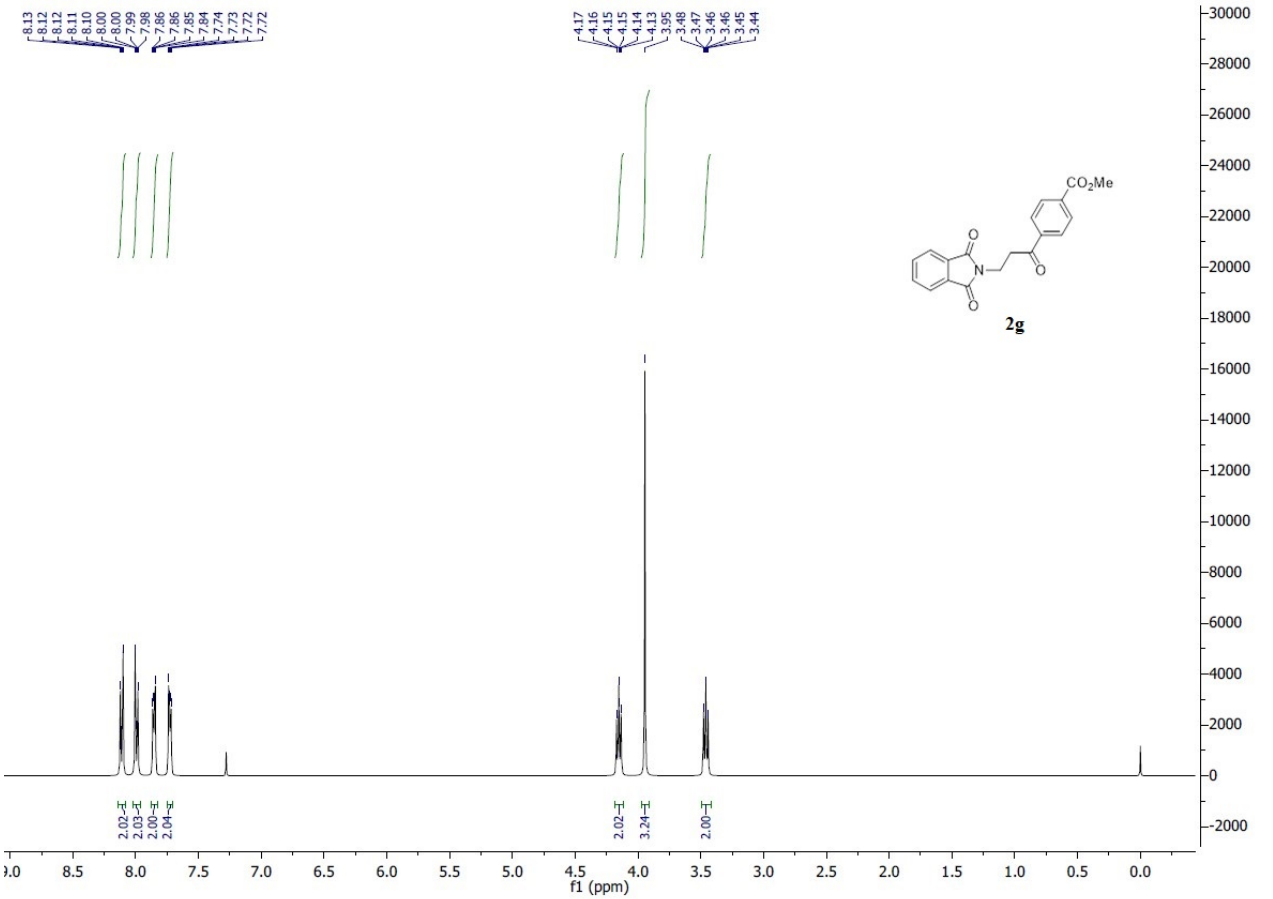

193.49
168.27
167.54
158.59
134.37
134.01
132.14
131.94
131.59
128.18
123.71
123.30
114.79
36.46
33.80
15.72
OH
O
N
O
O
2d
f1 (ppm)


2e
f1 (ppm)


2e
f1 (ppm)


8.07 8.07 8.06 7.88 7.87 7.87 7.87 7.86 7.86 7.85 7.85 7.74 7.73 7.73 7.72 7.70 7.70 7.70 7.69 7.68 7.68 7.68 7.67 7.36 7.34 7.32
4.16 4.15 4.14 4.14 4.13 4.12 3.42 3.41 3.40 3.40 3.39 3.38
Br
O
N
O
O
2f
f1 (ppm)
0.99 3.26 2.07 1.09 1.08 2.01 2.00


138.06 136.26 134.08 132.08 131.16 130.30 126.56 123.36 123.08
195.99 168.16 36.91 33.36
Br
O
N
O
O
2f
f1 (ppm)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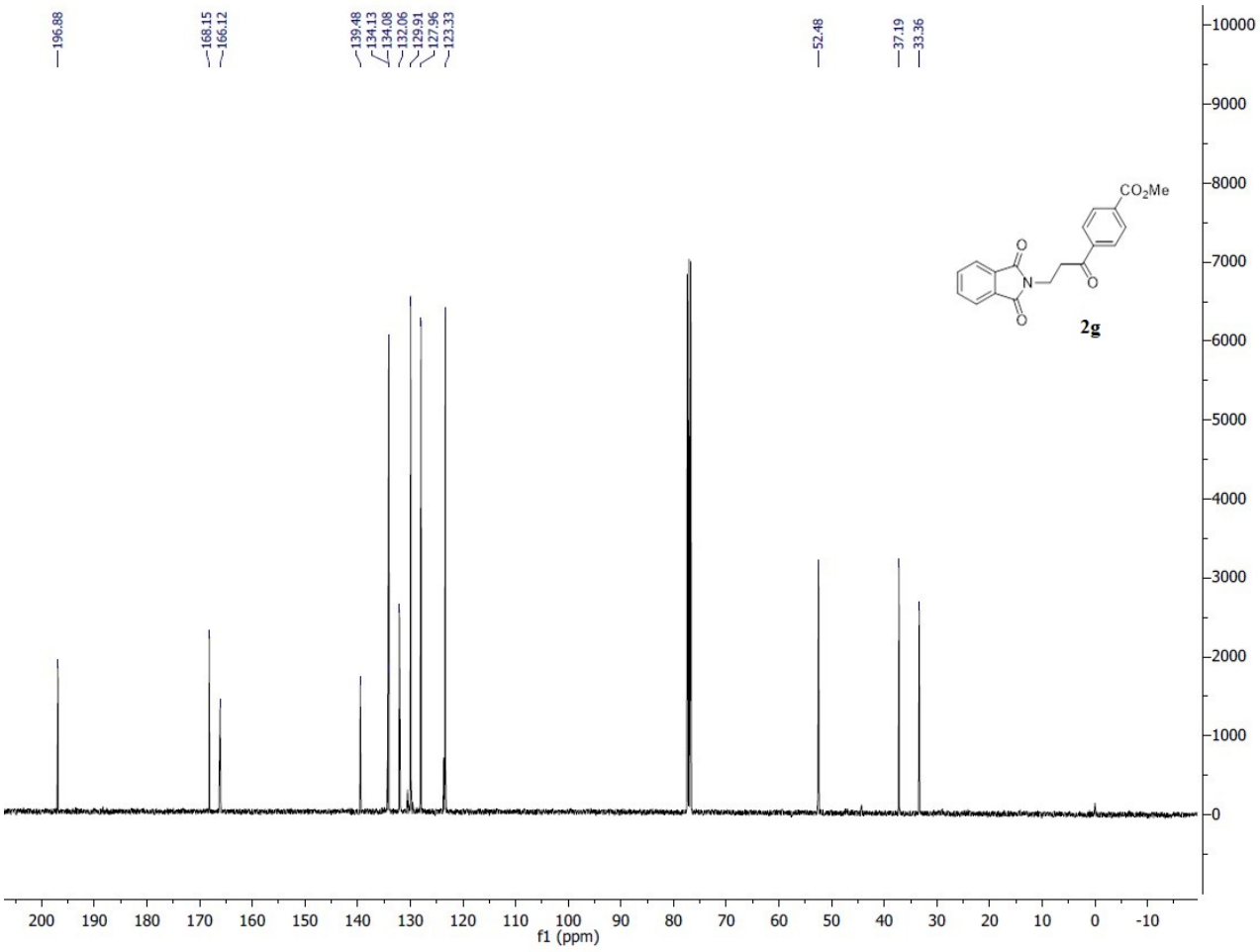
8.12
8.12
8.11
8.10
8.00
8.00
7.99
7.98
7.86
7.86
7.85
7.84
7.74
7.73
7.72
7.72
4.17
4.16
4.15
4.15
4.14
4.13
3.95
3.48
3.47
3.46
3.46
3.45
3.44
CO2Me
O
N
O
O
2g
2.02
2.03
2.00
2.04
2.02
3.24
2.00
f1 (ppm)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139.48
134.13
134.08
132.06
129.91
127.96
123.33
52.48
37.19
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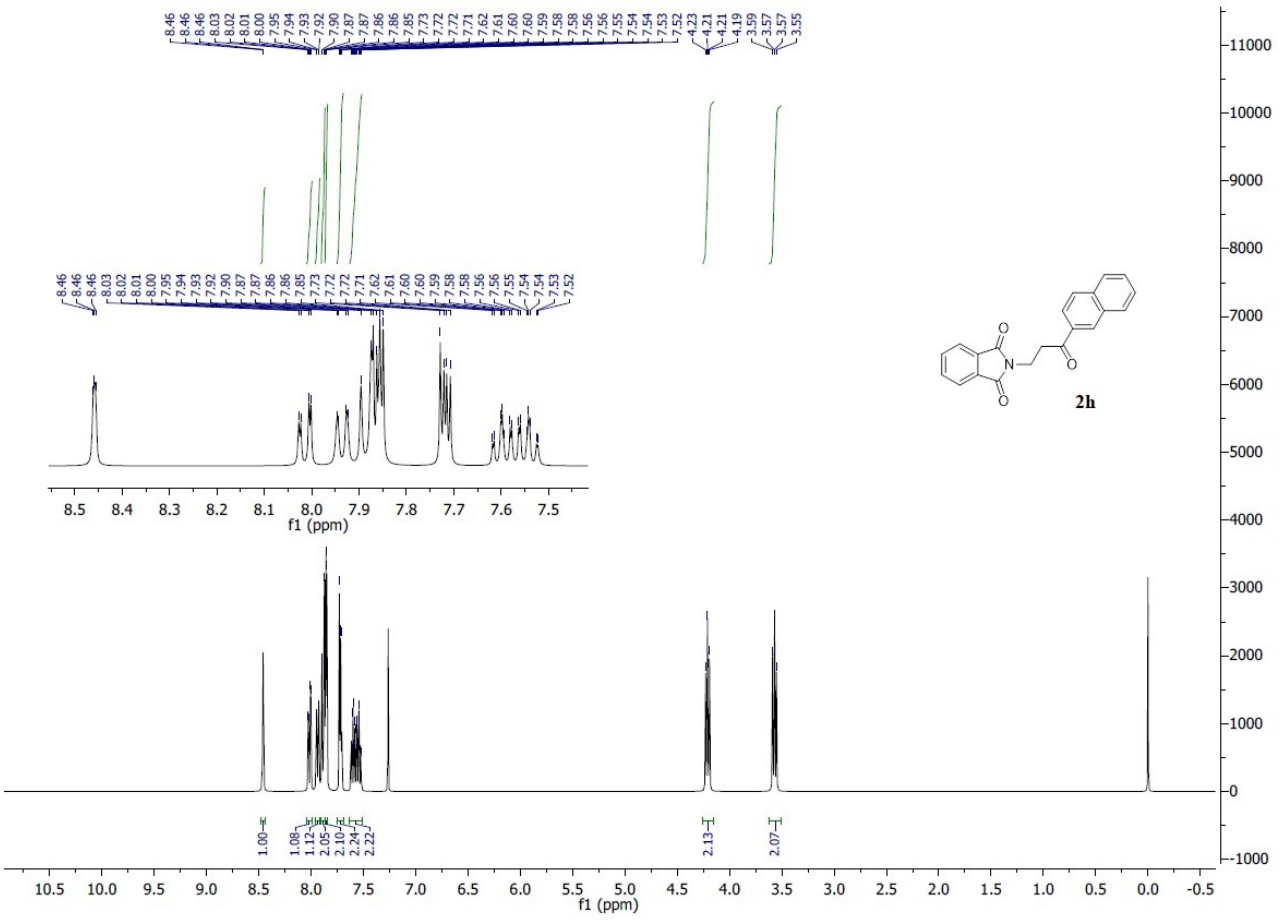
CO2Me
O
N
O
O
2g
f1 (ppm)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8.46
8.46
8.03
8.02
8.01
8.00
7.95
7.94
7.93
7.92
7.90
7.87
7.86
7.86
7.85
7.73
7.72
7.72
7.71
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7.60
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7.59
7.58
7.58
7.56
7.56
7.55
7.54
7.54
7.53
7.52
4.23
4.21
4.21
4.19
3.59
3.57
3.57
3.55
f1 (ppm)
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1.08
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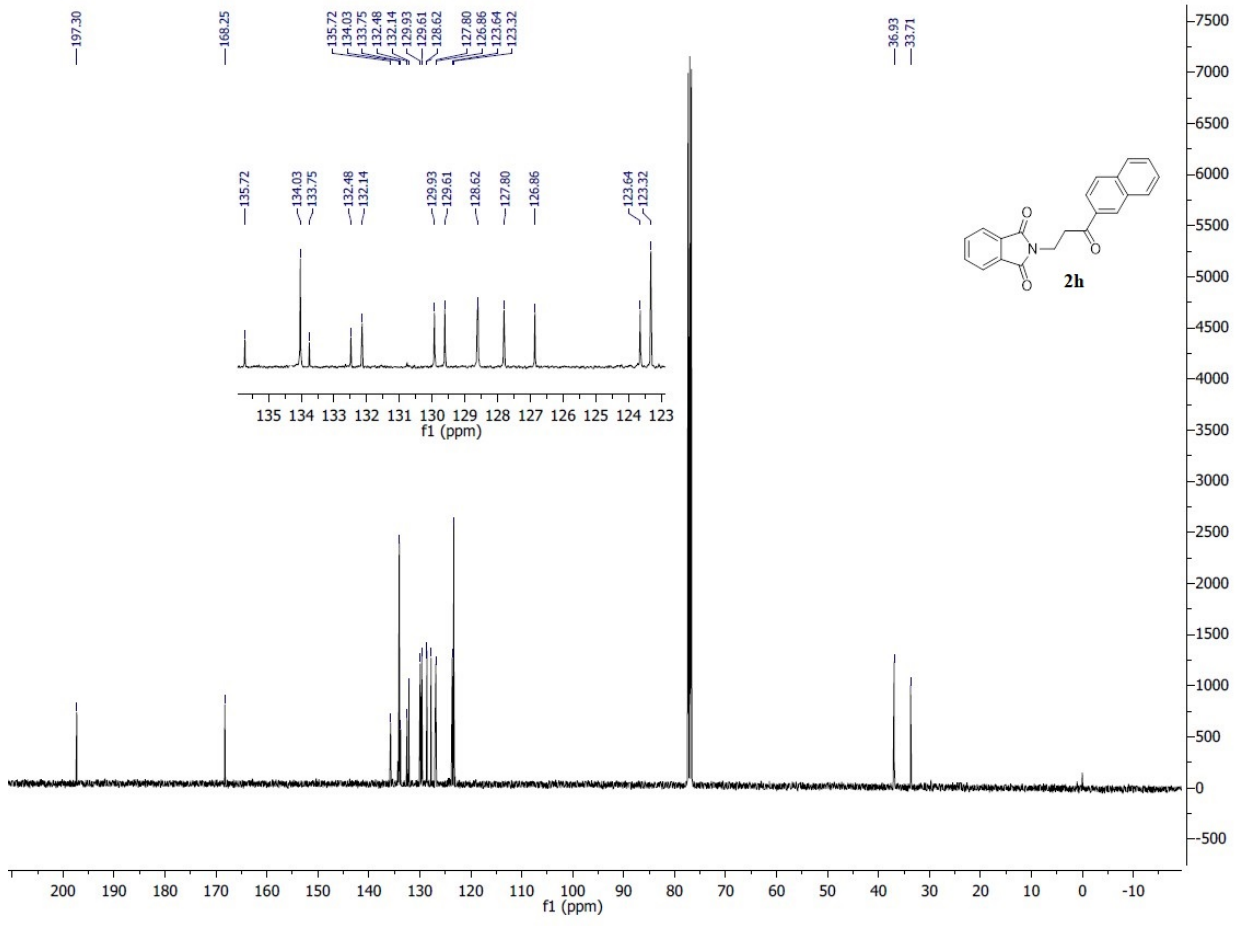
2.05
2.10
2.24
2.22
2.13
2.07
2h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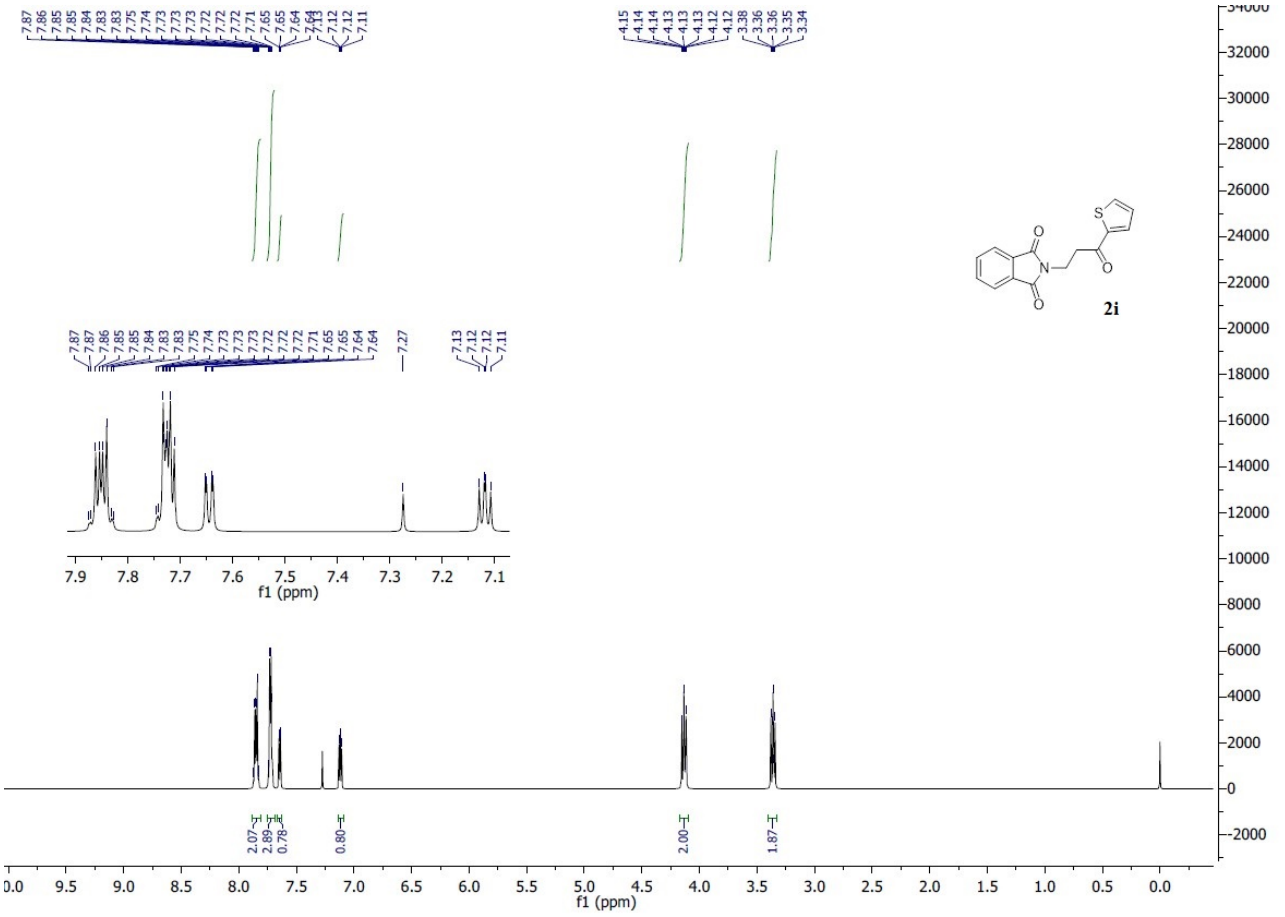
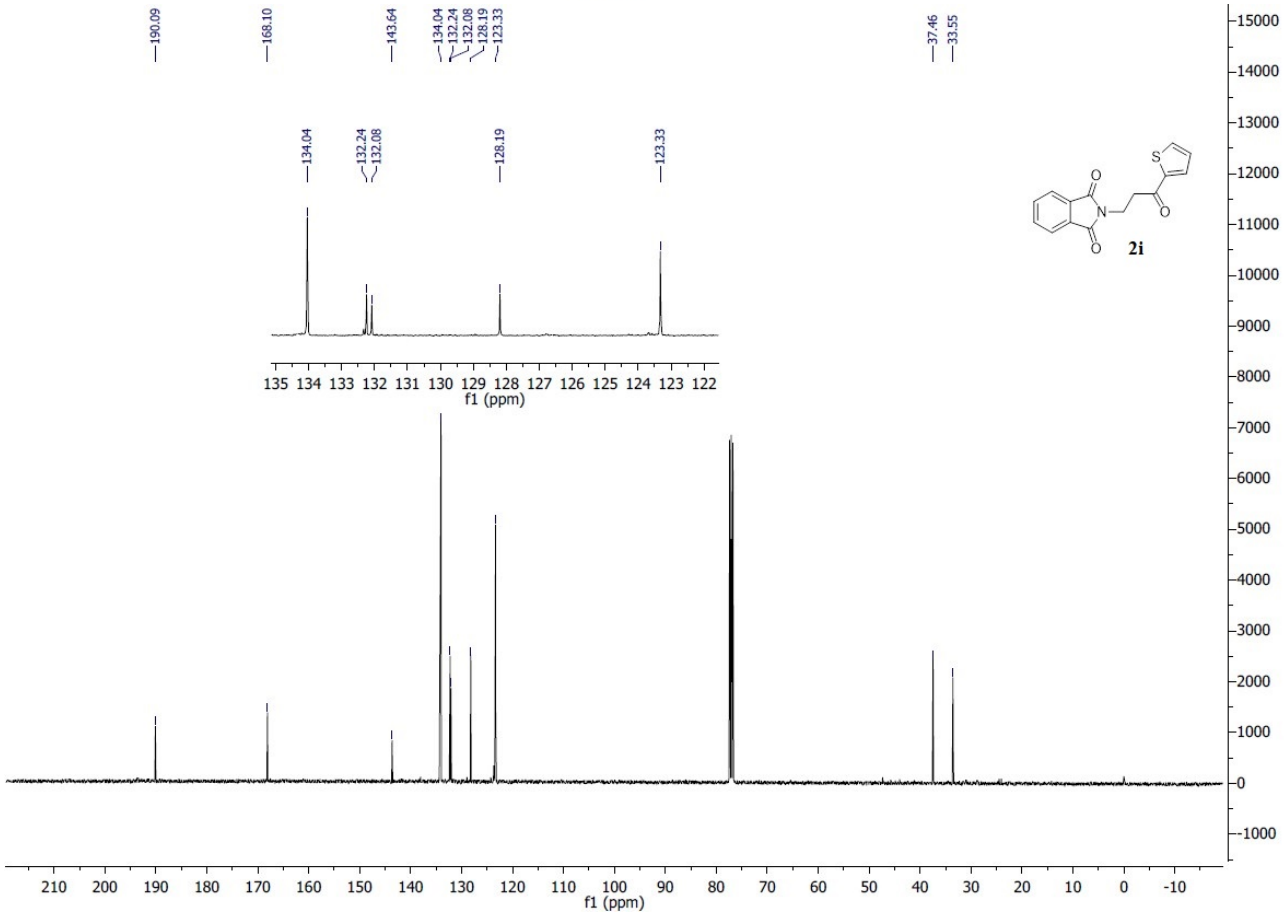
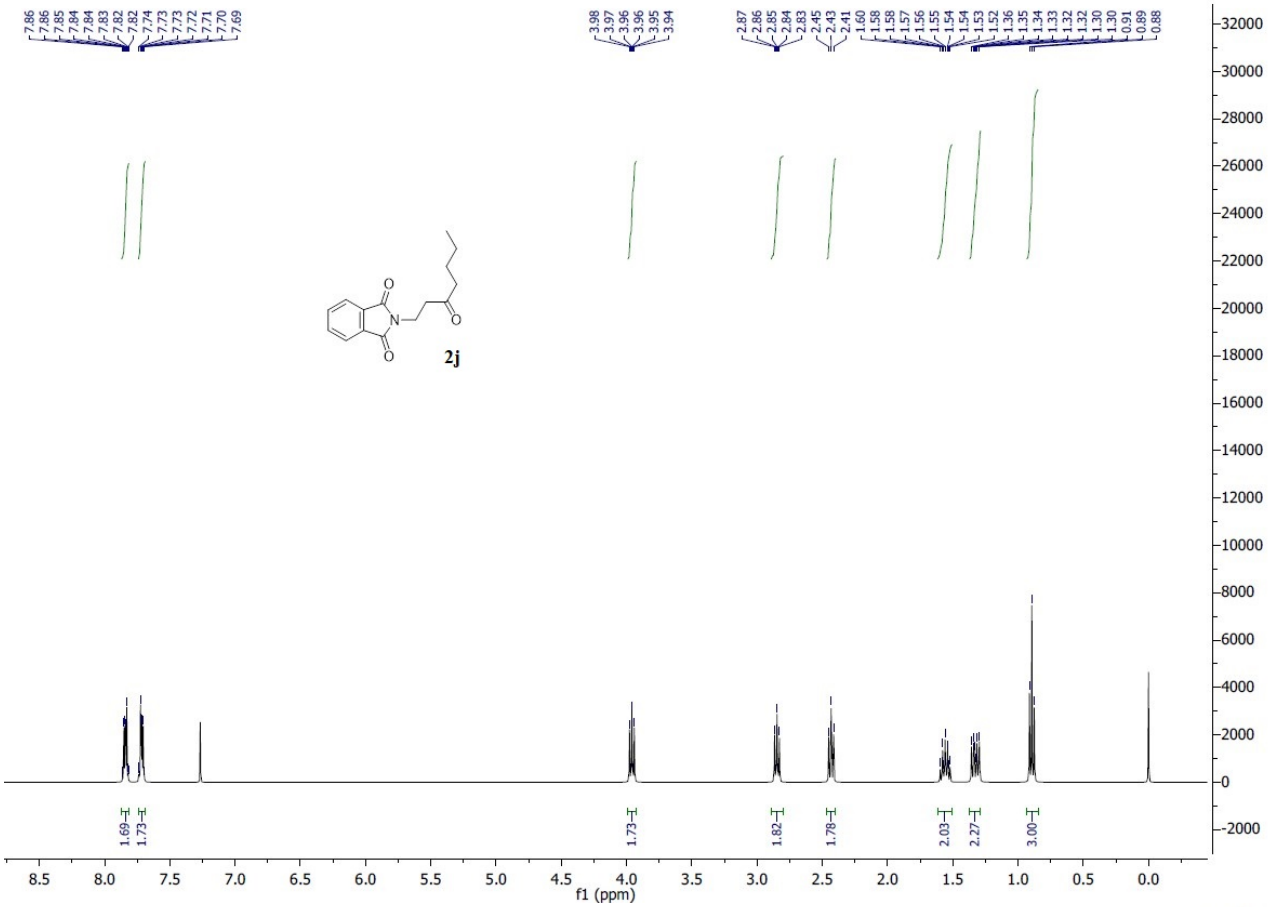
128.62
127.80
126.86
123.64
123.32
36.93
33.71
f1 (ppm)
2h


2i
f1 (ppm)


2i
f1 (ppm)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2.83
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1.54
1.54
1.53
1.52
1.36
1.35
1.34
1.33
1.32
1.32
1.30
1.30
0.91
0.89
0.88
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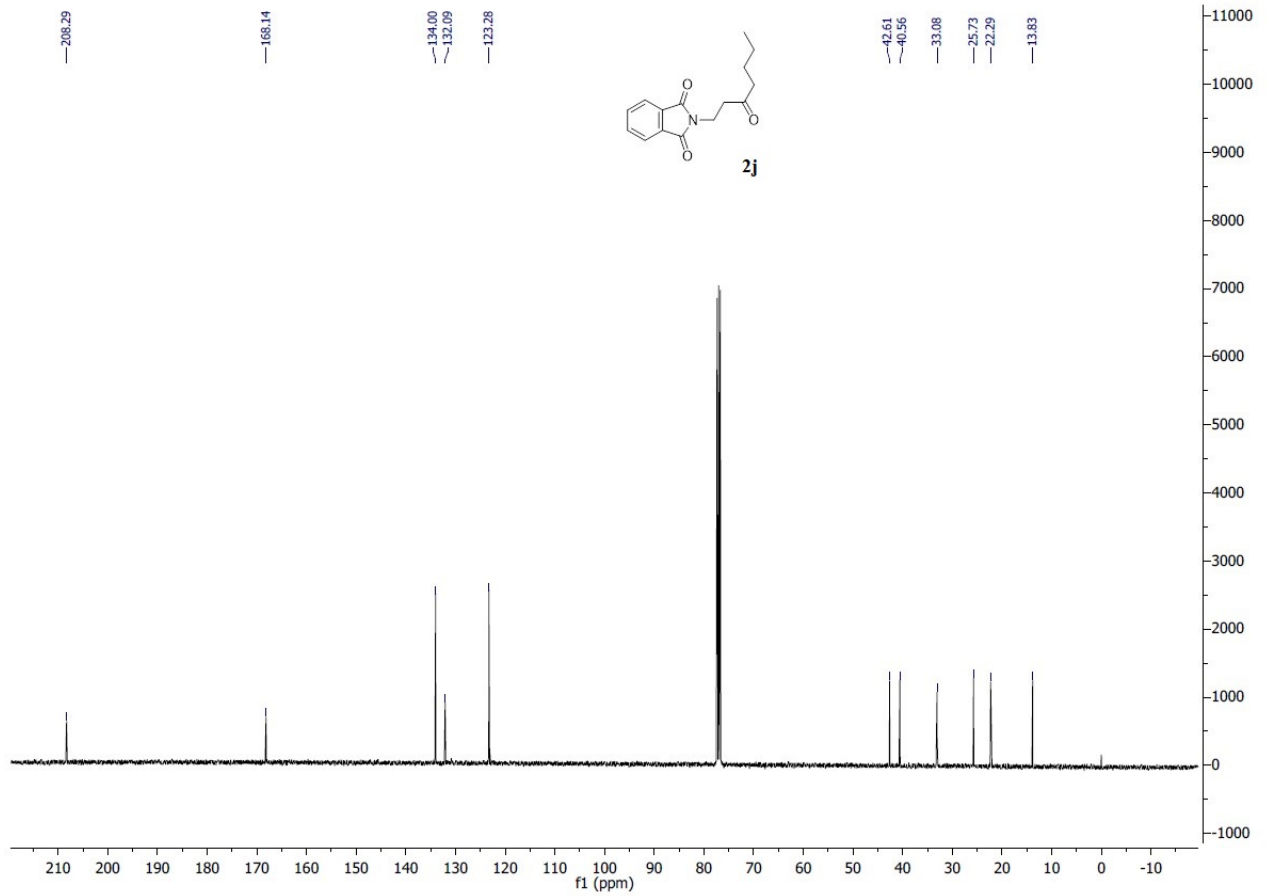
1.73
1.73
1.82
1.78
2.03
2.27
3.00
f1 (ppm)


208.29
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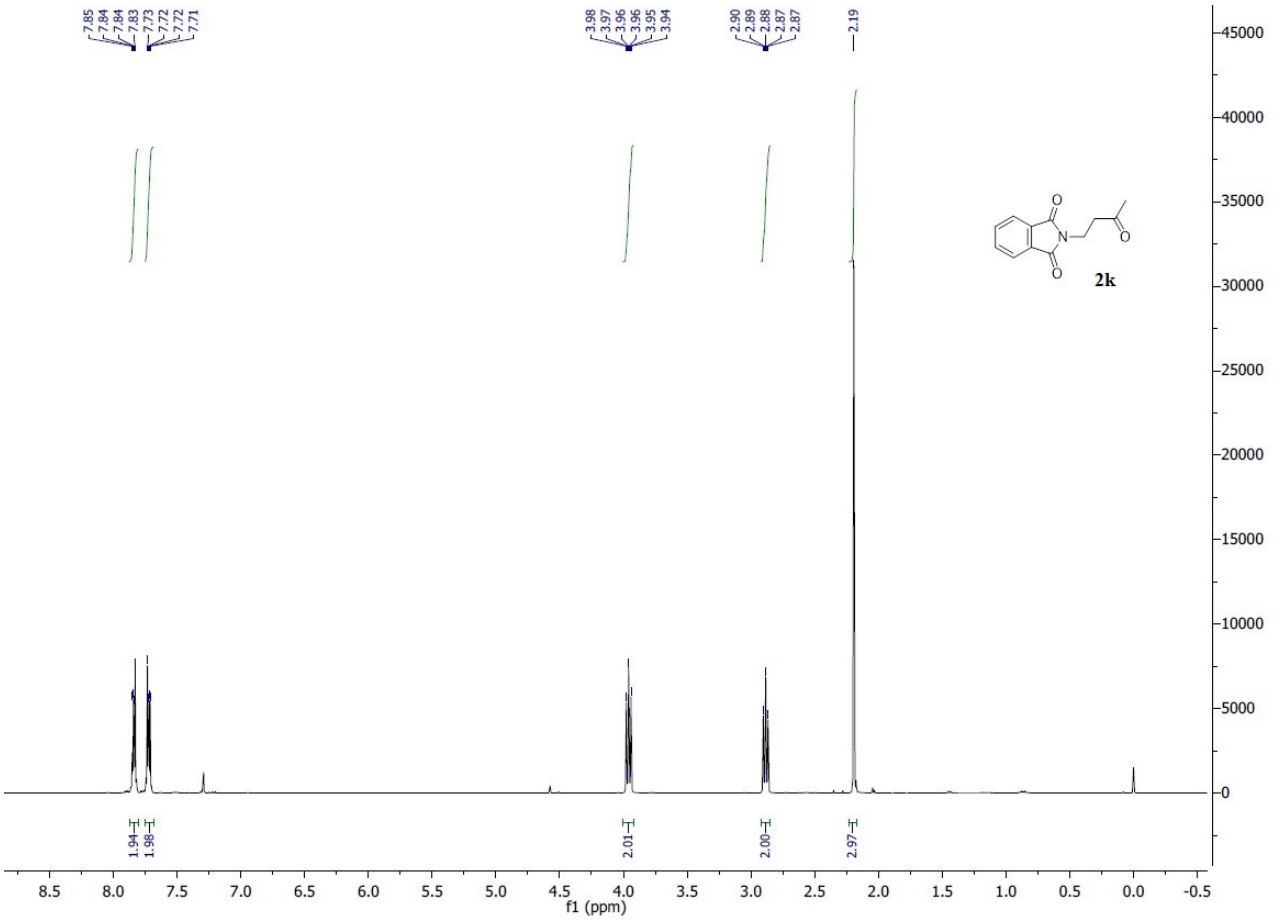
42.61
40.56
33.08
25.73
22.29
13.83
2j
f1 (ppm)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7.84
7.84
7.83
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7.72
7.72
7.71
3.98
3.97
3.96
3.96
3.95
3.94
2.90
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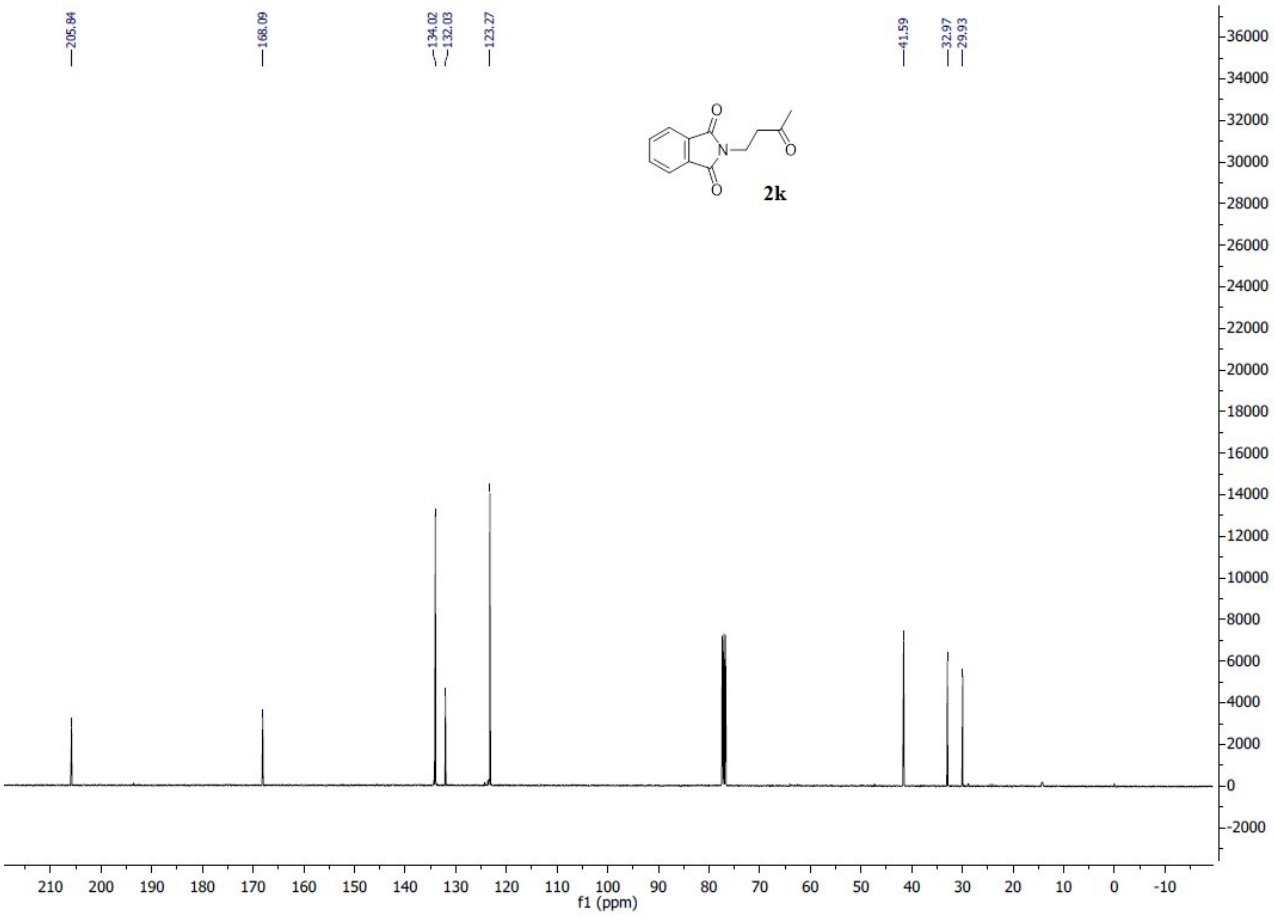
1.98
2.01
2.00
2.97
f1 (ppm)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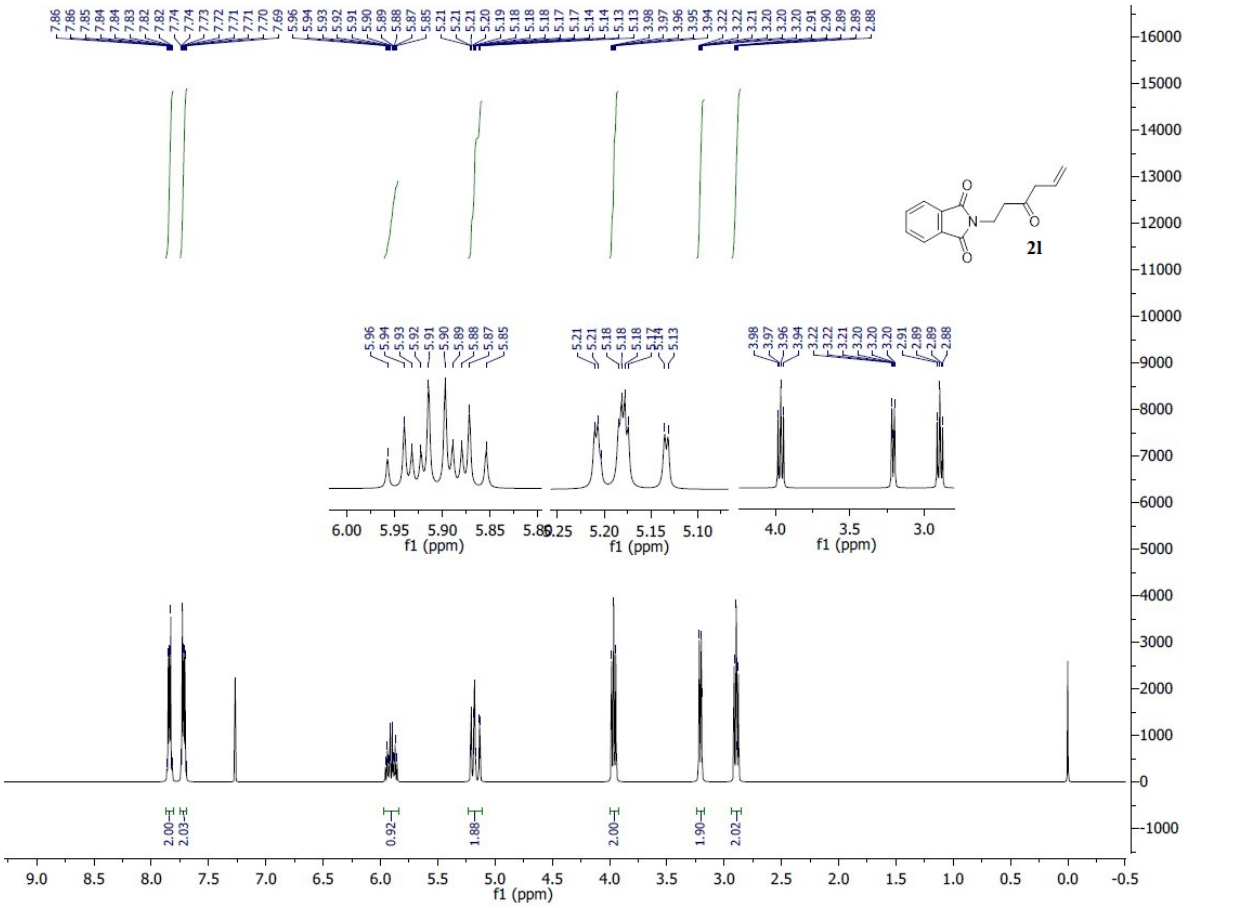
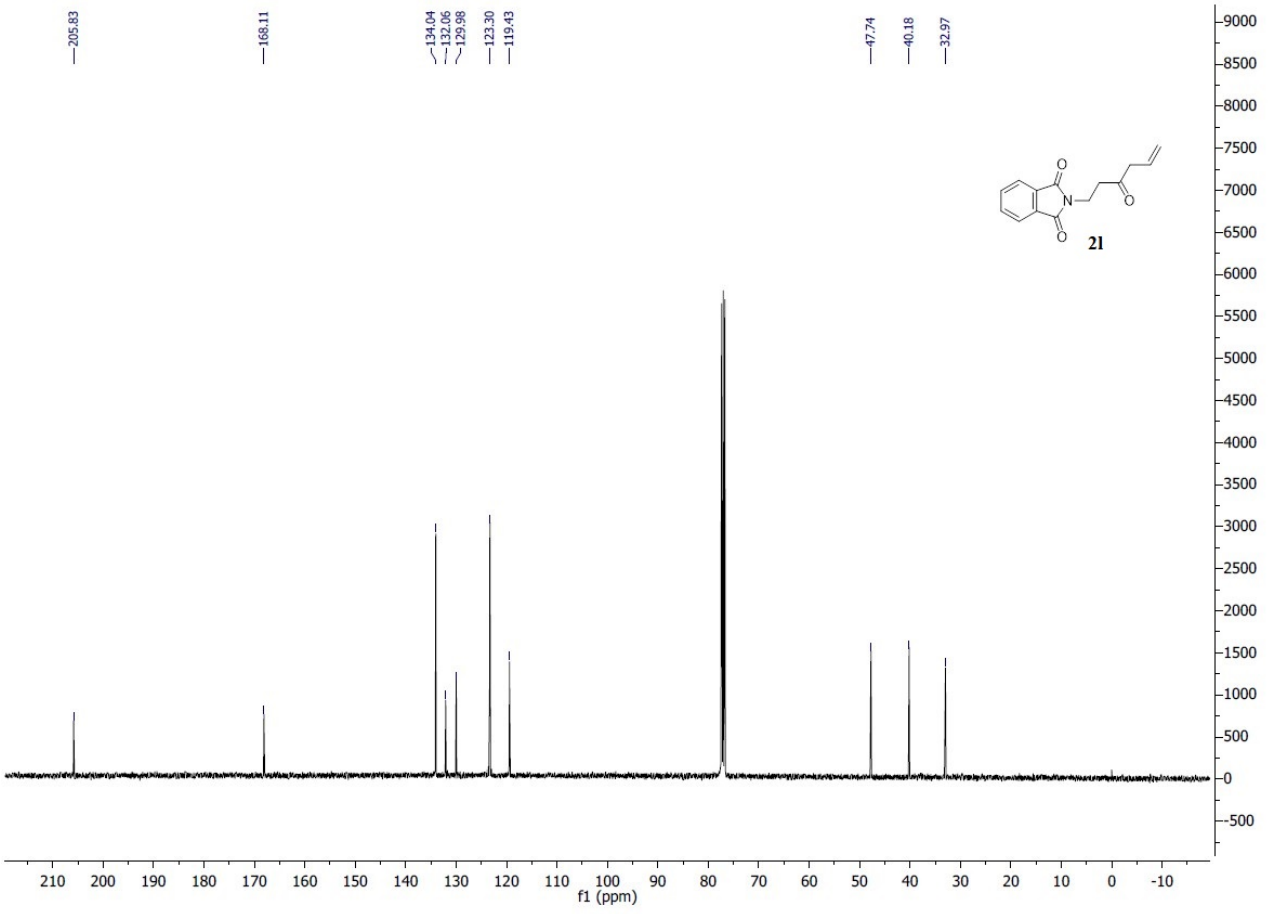
132.03
123.27
41.59
32.97
29.93
2k
f1 (ppm)


21
f1 (ppm)


205.83
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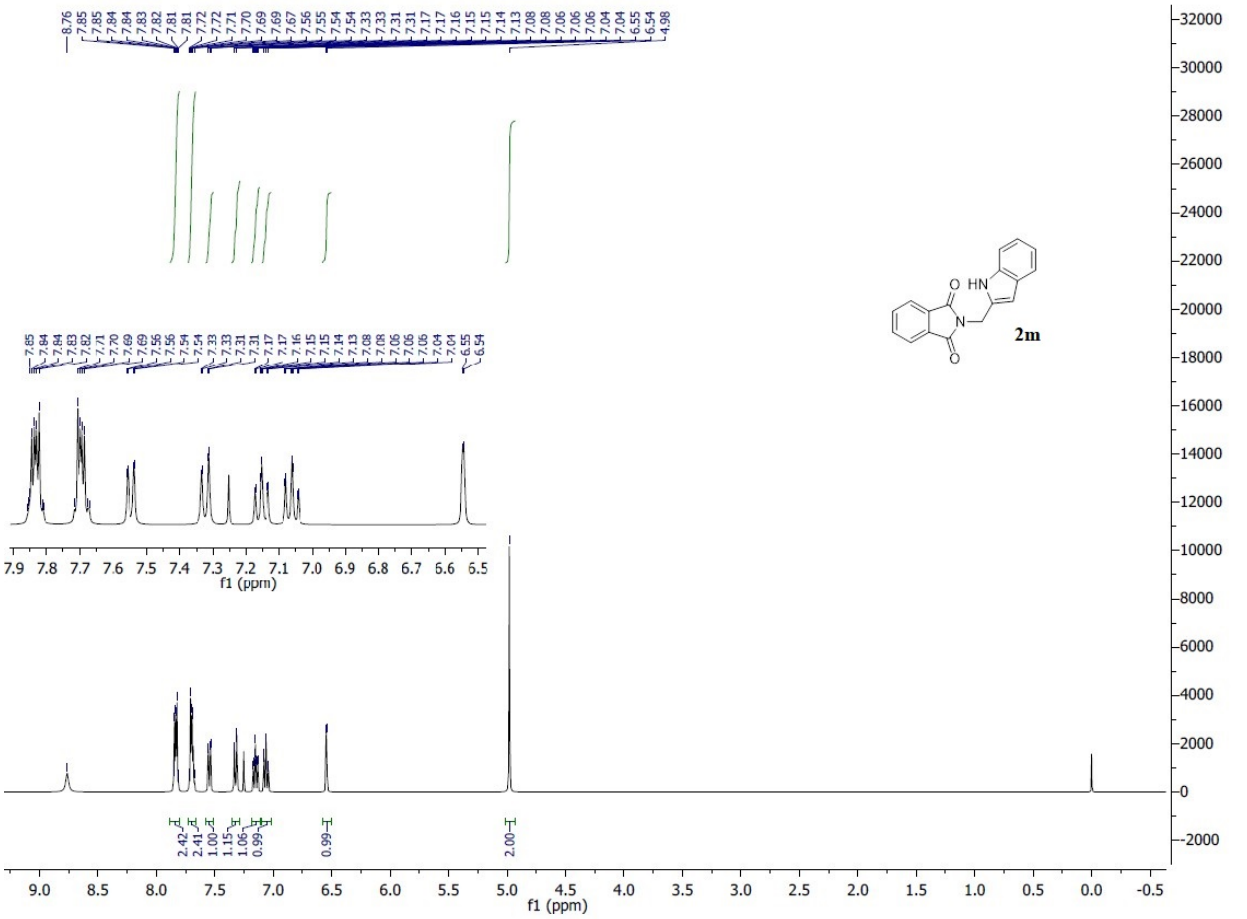
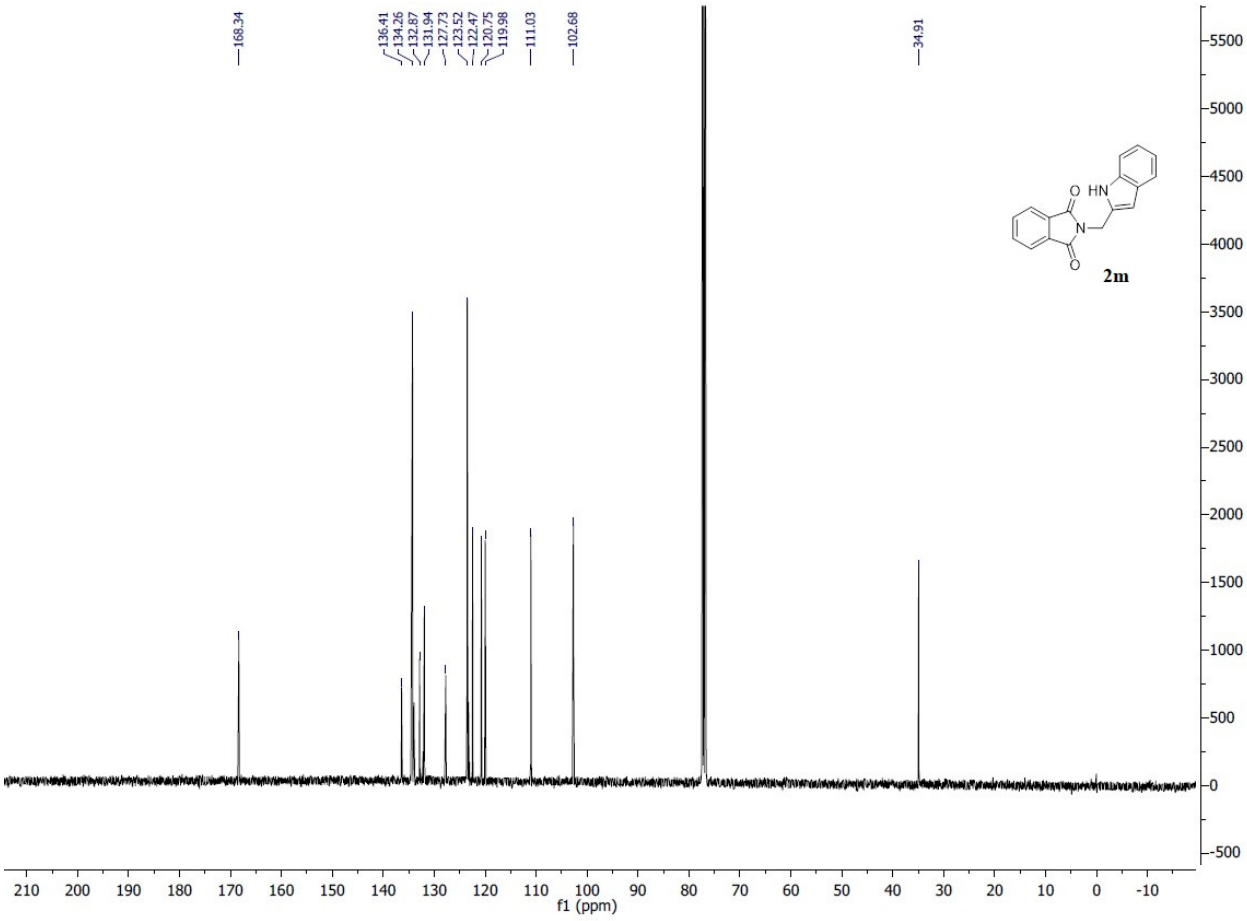
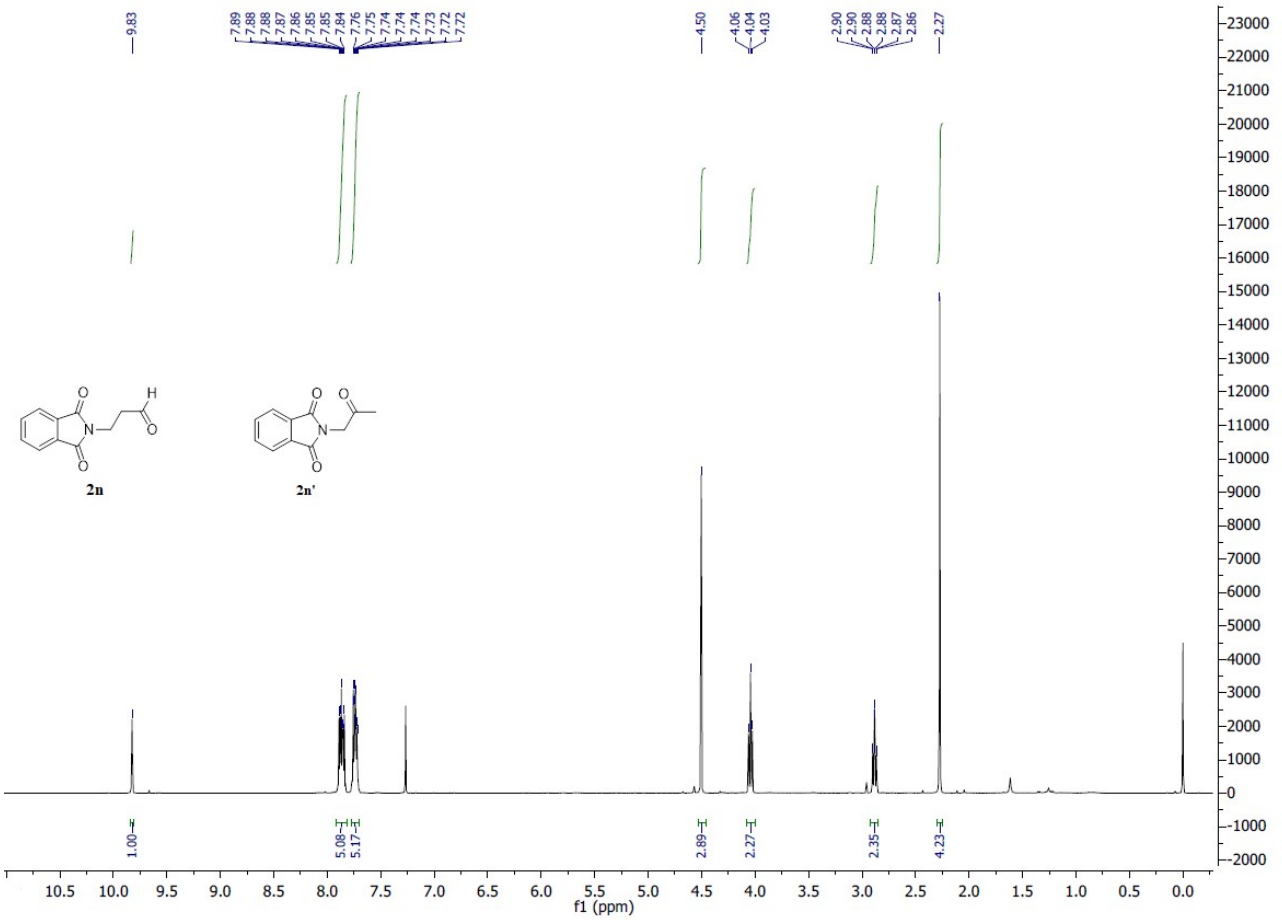
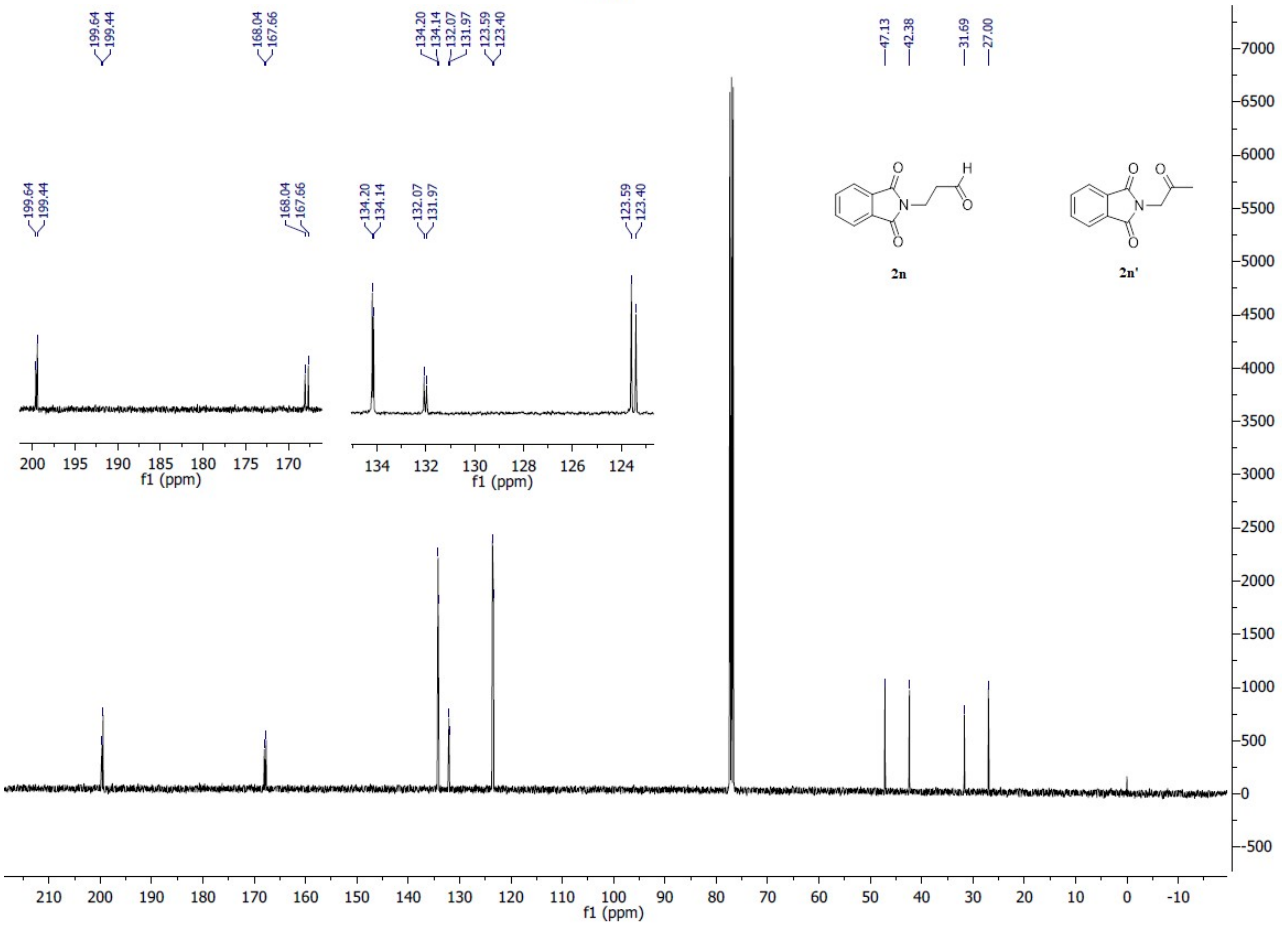
134.04
132.06
129.98
123.30
119.43
47.74
40.18
32.97
21
f1 (ppm)


2m
f1 (ppm)


2m
f1 (ppm)


9.83
7.89
7.88
7.88
7.87
7.86
7.85
7.85
7.84
7.76
7.75
7.74
7.74
7.74
7.73
7.72
7.72
4.50
4.06
4.04
4.03
2.90
2.90
2.88
2.88
2.87
2.86
2.27
1.00
5.08
5.17
2.89
2.27
2.35
4.23
f1 (ppm)
2n
2n'


199.64
199.44
168.04
167.66
134.20
134.14
132.07
131.97
123.59
123.40
47.13
42.38
31.69
27.00
f1 (ppm)
2n
2n'

VIII. References

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