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Supporting Information

Cu-Catalyzed Cycloaddition of Aryl Azides to 1-Iodobuta-1,3-diynes: An Experimental and Quantum Chemical Study of Unusual Regiochemistry

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1 General information

Solvents, reagents, and chemicals (2-methylbut-3-yn-2-ol, iodoarenes, ethynylbenzene) used for reactions were purchased from commercial suppliers. Solvents were dried under standard conditions; chemicals were used without further purification. 1-(4-Azidophenyl)ethan-1-one (**2a**),[1] 1-azido-4-methoxybenzene (**2b**),[1] 4-azidobenzonitrile (**2c**),[2] 1-azido-4-chlorobenzene (**2d**),[3] 1-azido-3-(trifluoromethyl)benzene (**2e**),[4] 1-azido-4-methylbenzene (**2f**),[5] 2-azido-1,3-dimethylbenzene (**2g**),[6] all 1-iodobuta-1,3-diynes (**1**),[7] 4-((4-chlorophenyl)ethynyl)-5-iodo-1-(4-methoxyphenyl)-1*H*-1,2,3-triazole (**3d**),[7] 1-(buta-1,3-diyn-1-yl)-4-methylbenzene (**8**),[7] 1,8-di-p-tolylocta-1,3,5,7-tetrayne (**9**),[7] (iodoethynyl)benzene (**5a**),[8] trimethyl((3-nitrophenyl)ethynyl)silane (**5´b**)[9] were synthesized using previously reported procedures. Evaporation of solvents and concentration of reaction mixtures were performed in vacuo at 35 °C on a rotary evaporator. Melting points (mp) determined are uncorrected. ^{1}H and ^{13}C NMR spectra were recorded at 400 and 100 MHz, respectively, at 25 °C in $CDCl_3$, DMSO-d_6 or acetone-d_6 without the internal standard. The ^{1}H NMR data are reported as chemical shifts (δ), multiplicity (s, singlet; d, doublet; t, triplet; q, quartet; m, multiplet; br, broad), coupling constants (*J*, given in Hz), and number of protons. The ^{13}C NMR data are reported as the chemical shifts (δ) and type of carbon (p, primary; s, secondary; t, tertiary; q, quaternary) determined from DEPT experiments with coupling constant $J_{(C-F)}$ for F-containing compounds. Chemical shifts for 1H and ^{13}C are reported as δ values (ppm) and referenced to residual solvent (δ = 7.26 ppm for ^{1}H; δ = 77.16 ppm for ^{13}C – for spectra recorded in $CDCl_3$ and δ = 2.50 ppm for ^{1}H; δ = 39.52 ppm for ^{13}C – for spectra in DMSO-d_6 and δ = 2.05 ppm for ^{1}H; δ = 29.84 ppm for ^{13}C – for spectra recorded in acetone-d_6). High resolution mass spectra (HRMS) were determined using electrospray ionization (ESI) in the mode of positive ion registration with a TOF mass analyzer. The single-crystal X-ray diffraction studies were carried out on a diffractometer at 100 K using Cu Kα radiation (λ = 1.54180 Å). Using Olex 2[10] the structure was solved with the Super flip structure solution program using Charge Flipping and refined with the ShelXL refinement package[11] using Least Squares minimization. Empirical absorption correction was applied in CrysAlisPro (Agilent Technologies, 2014)[12] program complex using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.

Accession Codes CCDC 2240443 (**3a**), 2240444 (**4a**), 2240445 (**3b**), 2240447 (**3d**), 2240446 (**4d**), 1869736 (**3m**), 2240448 [$CuI(PPh_3)_3$], 2240449 [$CuI(PPh_3)_3$·MeCN], and 2240450 [$Cu_2I_2(PPh_3)_3$] contain the supplementary crystallographic data for this paper. These data can be obtained free of charge via www.ccdc.cam.ac.uk/data_request/cif, or by emailing data_request@ccdc.cam.ac.uk, or by contacting The Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK; fax: +44 1223 336033.

2 Experimental section

2.1 Synthesis of complex [CuI(PPh_3)$_3$]

The synthesis of Cu-complex **[CuI(PPh_3)$_3$]** was carried out according to a slightly modified procedure published earlier.[13] A well stirred solution of CuI (0.380 g, 2.00 mmol, 1.00 equiv) and PPh_3 (1.57 g, 5.99 mmol, 3.00 equiv) in chloroform (40.0 mL) was heated under reflux in an oil bath (bath temperature – 85 °C) for 2 hours under argon atmosphere. Then the resulting solution was filtered hot through a pleated filter paper, and the clear filtrate was concentrated under reduced pressure to ~1/5 of the initial volume. The resulting crystalline precipitate was quickly filtered and dried in a vacuum to give complex **[CuI(PPh_3)$_3$]**, a as a white crystalline powder. Yield 1.27 g (65.4 %). The complex **[CuI(PPh_3)$_3$]** was stored under argon in a freezer. ^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ = 7.37 – 7.33 (m, 3H), 7.297– 7.23 (m, 2H, overlaps with solvent signal); ^{31}P NMR (162 MHz, $CDCl_3$, ppm) δ = −5.02. IR spectrum data (KBr, ν, cm^{-1}): 3050, 2955, 1479, 1433, 1308, 1182, 1155, 742, 693. Single crystals of complex **[CuI(PPh_3)$_3$]** for X-Ray studies were obtained from a solution of **[CuI(PPh_3)$_3$]** in chloroform by slow evaporation of the solvent at room temperature (see Table S3).

2.2 Synthesis of the mixture of complexes [CuI(PPh_3)$_3$]·CH_3CN and [Cu_2I_2(PPh_3)$_3$]

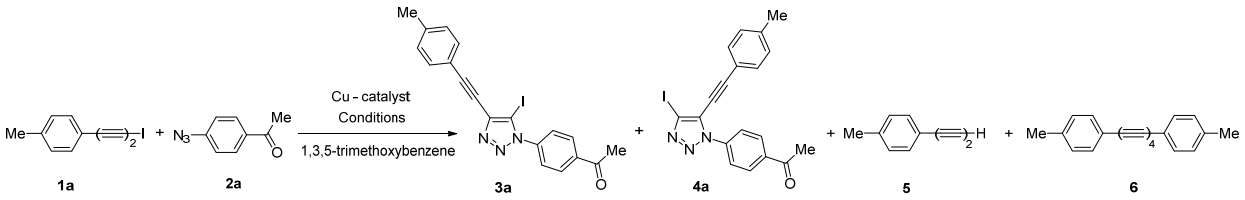
The mixture of complexes [CuI(PPh_3)$_3$]×CH_3CN and [Cu_2I_2(PPh_3)$_3$] was synthesized in accordance with the known procedure[13] that should have resulted in obtaining of an individual complex [Cu_2I_2(PPh_3)$_3$]. To a well-stirred solution of CuI (0.570 g, 3.00 mmol, 1.00 equiv) in boiling on an oil bath acetonitrile (60.0 mL) (bath temperature – 92 °C) a solution of triphenylphosphine (1.57 g, 6.00 mmol, 2.00 equiv.) in acetonitrile (60.0 mL) was added dropwise. The resulting mixture was refluxed overnight and the solution obtained was filtered hot through a pleated filter paper and was left at room temperature for slow crystallization of the product. After one week, a crystalline precipitate formed. The crystals were filtered off, dried in air and irradiated with a light (λ = 254 nm) that allowed observing two different types of crystals: a major fraction, long prisms with a blue-green fluorescence and a minor fraction, short prisms with a yellowish-orange fluorescence. The crystals were separated with tweezers under UV light. X-ray data for crystals of both types revealed that long prisms with a blue-green fluorescence correspond to complex **[CuI(PPh_3)$_3$]·CH_3CN**, while short prisms with a yellowish-orange fluorescence represent complex **[Cu_2I_2(PPh_3)$_3$]** (see Table S3)**.** Complete sorting of the crystals has not been done, so the yields have not been determined.

2.3 Test reaction between 1-iodobuta-1,3-diyne 1a and aryl azides 2a,b

Interaction of 1-(4-azidophenyl)ethan-1-one 2a with 1-(iodobuta-1,3-diyn-1-yl)-4-methylbenzene 1a (see Scheme 1). To 1-iodo-4-(*p*-tolyl)buta-1,3-diyne **1a** (133 mg, 0.500 mmol) in a crew vial was added 1-(4-azidophenyl)ethan-1-one **2a** (80.6 mg, 0.500 mmol), $CuI(PPh_3)_3$ (48.9 mg, 0.0500 mmol, 10.0 mol %) and 2,6-lutidine (4.30 mg, 0.0400 mmol, 8.0 mol %). The thick resulting mixture was vigorously stirred for 20 h at room temperature and 24 h at 40 °C. After completion of the reaction (TLC-control), the reaction mixture was diluted with DCM (20 – 30 mL) and saturated aqueous solution of NH_4Cl (2 × 10 mL). The reaction mixture was shacked; the organic layer was separated, dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The crude product was purified by column chromatography (eluent: hexane/acetone = 3:1) to give triazole **3a** (70.2 mg, 32.9%) and triazole **4a** (58.3 mg, 27.3%)

Interaction of 1-azido-4-methoxybenzene 2b with 1-(iodobuta-1,3-diyn-1-yl)-4-methylbenzene 1a (see Scheme 1). To iodobuta-1,3-diyne **1a** (51.0 mg, 0.192 mmol) in a crew vial was added azide **2b** (28.6 mg, 0.192 mmol), $CuI(PPh_3)_3$ (18.7 mg, 0.019 mmol, 10.0 mol %) and 2,6-lutidine (0.890 mg, 0.008 mmol, 4.00 mol %). The thick resulting mixture was vigorously stirred for 72 h at room temperature. After completion of the reaction (TLC-control), the reaction mixture was diluted with DCM (20 – 30 mL) and saturated aqueous solution of NH_4Cl (2 × 10 mL). The reaction mixture was shacked; the organic layer was separated, dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The crude product was purified by column chromatography (eluent: hexane/EtOAc = 10:1) to give pure triazole **3b** (11.0 mg, 13.8%) and a mixture triazoles **3b** and **4b** (12 mg, 15%, 5:1). The ratio of isomers **3b**:**4b** was calculated as 10.5:1.

2.4 Conditions Optimization for CuAAC of 1-Iodo-4-(*p*-tolyl)buta-1,3-diyne 1a and 1-(4-azidophenyl)ethan-1-one 2a



To 1-iodo-4-(*p*-tolyl)buta-1,3-diyne **1a** (26.6 mg, 0.100 mmol, 1.00 equiv) in a crew vial was added 1-(4-azidophenyl)ethan-1-one **2a** (16.1 mg, 0.100 mmol, 1.00 equiv) and other components (if needed) in according with Table 1: Cu-catalyst (5.00 mol %) and 2,6-lutidine (4.00 – 20.0 mol %). The thick resulting mixture was vigorously stirred for 18 h. Then 0.05 M solution of internal standard, 1,3,5-trimethoxybenzene (0.500 mL, 0.00333 mmol, 0.333 equiv, 1.00 equiv of [H standard]), was added to the reaction mixture, the resulting mixture was diluted with DCM (20 – 30 mL) and the resulting solution was washed with a saturated aqueous solution of NH_4Cl (2 × 10 mL) dried over anhydrous Na_2SO_4 and an aliquot of the solution was concentrated under reduced pressure. The conversion of starting materials and the analytical yields of triazoles **3a** and **4a** were determined by ^1H NMR spectroscopy (Figure S1).

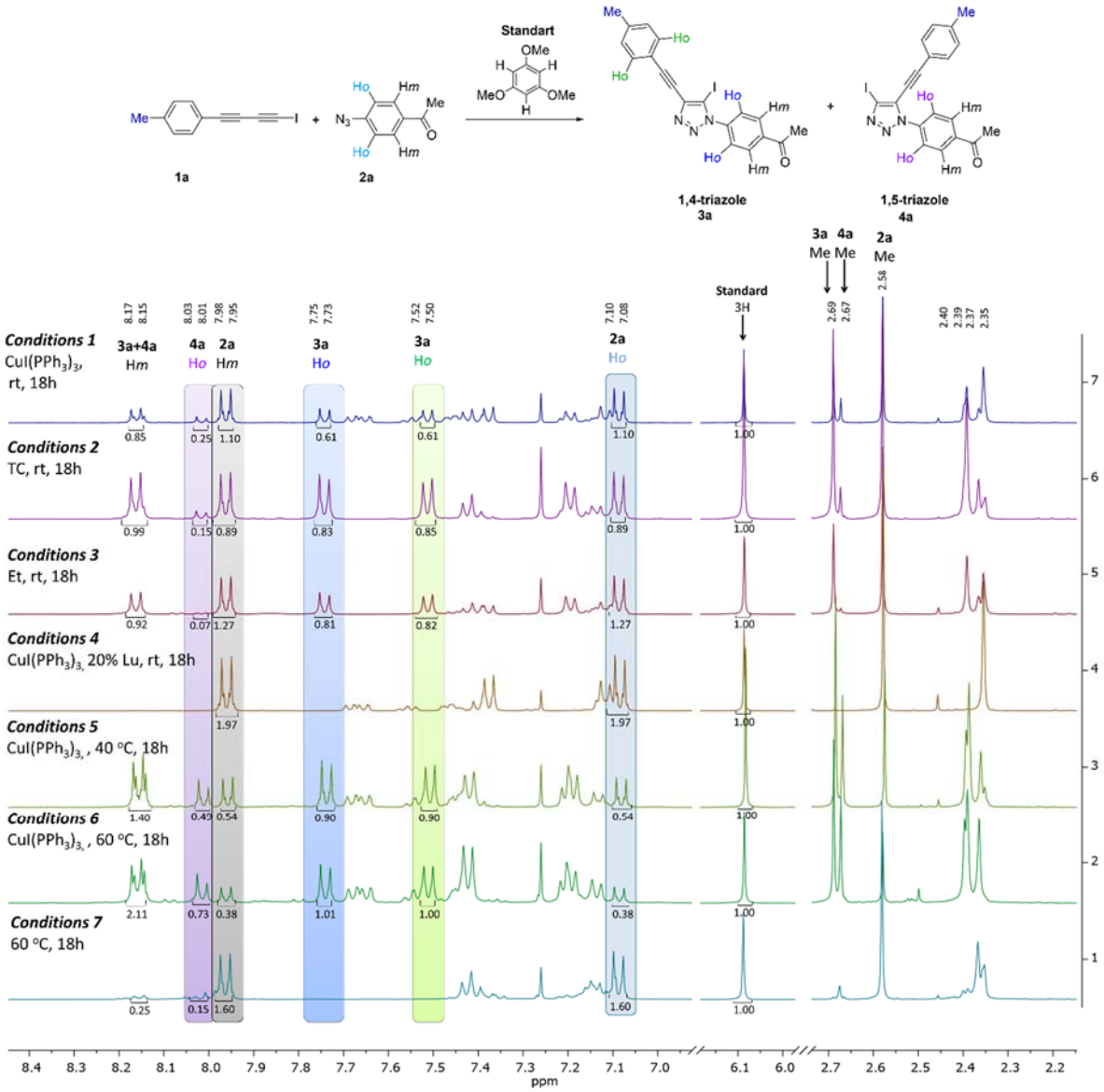


Figure S1. Analysis of the reaction mixtures obtained under different conditions in CuAAC of 1-iodobuta-1,3-diyne **1a** and aryl azide **2a** (see Table 1) by ^{1}H NMR spectra (400 MHz, 25 °C, $CDCl_3$)**.**

2.5 General procedure for the CuAAC of 1-iodobuta-1,3-diynes 1 and azides 2

General procedure for the interaction of 1-iodobuta-1,3-diynes 1 with azides 2. To an azide **2** (1.00 equiv) in a crew vial were added 1-iodobuta-1,3-diyne (1.00 equiv) **1**, [$CuI(PPh_3)_3$] (5.00 mol%), and 2,6-lutidine (4.00 mol %). The resulting thick mixture was vigorously stirred for 18 h at 60 °C (TLC control). Then the reaction mixture was diluted with DCM (20.0 mL) and the resulting solution was washed with a saturated aqueous solution of NH_4Cl (20.0 mL). The organic layer was separated, and the aqueous layer was extracted with DCM. The combined organic layers were dried over anhydrous Na_2SO_4, and concentrated under reduced pressure to yield the crude mixture of isomeric triazoles **3** and **4**, which were separated and purified by column chromatography on silica gel.

Synthesis of pair of triazoles (3a) / (4a). These compounds were prepared in accordance with the general procedure from 1-(iodobuta-1,3-diyn-1-yl)-4-methylbenzene (**1a**) (53.0 mg, 0.199 mmol), 1-(4-azidophenyl)ethan-1-one (**2a**) (32.1 mg, 0.199 mmol), $CuI(PPh_3)_3$ (9.70 mg, 0.010 mmol) and 2,6-lutidine (0.900 mg, 0.008 mmol). The crude mixture of products was separated by column chromatography (eluent: hexane/acetone = 3:1).

1-(4-(5-Iodo-4-(*p*-tolylethynyl)-1*H*-1,2,3-triazol-1-yl)phenyl)ethan-1-one (3a). A beige solid (27.3 mg, 32%), mp 156 − 157 °C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.30 – 8.01 (m, 2H, ArH), 7.82 – 7.65 (m, 2H, ArH), 7.57 – 7.40 (m, 2H, ArH), 7.19 (d, *J* = 7.8 Hz, 2H, ArH), 2.69 (s, 3H, CH_3), 2.39 (s, 3H, CH_3). ^{13}C NMR ($CDCl_3$, 101 MHz) *δ* 196.7 (q), 140.1 (q), 139.9 (q), 139.7 (q), 138.3 (q), 131.9 (t), 129.6 (t), 129.4 (t), 125.9 (t), 119.0 (q), 96.1 (q), 84.1 (q), 77.5 (q), 26.9 (p), 21.7 (p). HRMS ESI: $[M+H]^+$ calcd. for $C_{18}H_{15}IN_3O$+: 428.0254; found: 428.0268.

1-(4-(4-Iodo-5-(p-tolylethynyl)-1H-1,2,3-triazol-1-yl)phenyl)ethan-1-one (4a). A cream solid (12.3 mg, 14%), m.p. 181 − 183 °C. ^{1}H NMR ($CDCl_3$, 400 MHz) *δ* 8.30 – 8.08 (m, 2H, ArH), 8.08 – 7.92 (m, 2H, ArH), 7.42 (d, *J* = 8.0 Hz, 2H, ArH), 7.21 (d, *J* = 7.8 Hz, 2H, ArH), 2.67 (s, 3H, CH_3), 2.40 (s, 3H, CH_3). ^{13}C NMR ($CDCl_3$, 101 MHz) *δ* 196.8 (q), 140.9 (q), 139.8 (q), 137.7 (q), 131.8 (t), 129.7 (t), 129.6 (t), 126.6 (q), 123.0 (t), 117.8 (q), 104.2 (q), 95.7 (q), 73.9 (q), 26.9 (p), 21.8 (p). HRMS ESI: $[M+H]^+$ calcd. for $C_{19}H_{15}IN_3O^+$: 428.0254; found: 428.0264.

Synthesis of pair of triazoles (3b) / (4b). These compounds were prepared in accordance with the general procedure from 1-iodo(buta-1,3-diyne) **1a** (100.0 mg, 0.376 mmol), 1-azido-4-methoxybenzene **2b** (56.1 mg, 0.376 mmol), $CuI(PPh_3)_3$ (18.4 mg, 0.019 mmol) and 2,6-lutidine (1.61 mg, 0.015 mmol). The crude mixture of products was separated by column chromatography (eluent: hexane/EtOAc = 10:1).

5-Iodo-1-(4-methoxyphenyl)-4-(*p*-tolylethynyl)-1*H*-1,2,3-triazole (3b) colorless crystals (32.0 mg, 20%), m.p. 159 − 160 °C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.56 – 7.42 (m, 4H, Ar), 7.22 – 7.16 (m, 2H, Ar), 7.08 – 7.03 (m, 2H, Ar), 3.90 (s, 3H, OCH_3), 2.39 (s, 3H, CH_3). ^{13}C NMR (Acetone-d_6, 126 MHz) δ 161.9 (q), 140.4 (q), 138.9 (q), 132.4 (t), 130.8 (q), 130.4 (q), 128.5 (t), 127.4 (t), 115.4 (t), 95.1 (q), 88.8 (q), 79.3 (q), 56.1 (p), 21.5 (p). HRMS ESI: $[M+Na]^+$ calcd. for $C_{18}H_{14}IN_3ONa^+$: 438.0074; found: 438.0075.

4-Iodo-1-(4-methoxyphenyl)-5-(*p*-tolylethynyl)-1*H*-1,2,3-triazole (4b) a beige solid (6.0 mg, 4%). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.74 – 7.69 (m, 2H, Ar), 7.41 – 7.37 (m, 2H, Ar), 7.20 – 7.17 (m, 2H, Ar), 7.07 – 7.03 (m, 2H, Ar), 3.89 (s, 3H, OCH_3), 2.39 (s, 3H, CH_3). HR HPLCMS ESI: $[M+H]^+$ calcd. for $C_{18}H_{15}IN_3O^+$: 416.0254; found: 416.0246. Purity: 99.2% (HPLC analysis at 265 – 280 nm). Retention time HPLC in 9.0 min.

Synthesis of pair of triazoles (3c) / (4c). These compounds were prepared in accordance with the general procedure from 1-iodo(buta-1,3-diyne) **1b** (110.0 mg, 0.373 mmol), 1-(4-

azidophenyl)ethan-1-one **2a** (60.1 mg, 0.373 mmol), $CuI(PPh_3)_3$ (18.2 mg, 0.019 mmol) and 2,6-lutidine (1.6 mg, 0.015 mmol). The crude mixture of products was separated by column chromatography (eluent: hexane/acetone = 2:1).

1-(4-(4-((4-(Dimethylamino)phenyl)ethynyl)-5-iodo-1*H*-1,2,3-triazol-1-yl)phenyl)ethan-1-one (3c) a beige solid (47.6 mg, 28%), m.p. 173 – 175 °C (with decomposition). ^{1}H NMR (Acetone-d_6, 400 MHz) δ 8.30 – 8.27 (m, 2H, ArH), 7.91 – 7.85 (m, 2H, ArH), 7.48 – 7.41 (m, 2H, ArH), 6.80 – 6.76 (m, 2H, ArH), 3.03 (s, 6H, NMe_2), 2.71 (s, 3H, Me). ^{13}C NMR (Acetone-d_6, 101 MHz) δ 197.2 (q), 151.9 (q), 141.2 (q), 140.4 (q), 139.3 (q), 133.6 (t), 130.3 (t), 127.1 (t), 112.6 (t), 109.0 (q), 97.0 (q), 86.9 (q), 77.4 (q), 40.2 (p), 27.0 (p). HRMS ESI: $[M+H]^+$ calcd. for $C_{20}H_{18}IN_4ONa^+$: 457.0520; found: 457.0512.

1-(4-(5-((4-(Dimethylamino)phenyl)ethynyl)-4-iodo-1*H*-1,2,3-triazol-1-yl)phenyl)ethan-1-one (4c) a white solid (60.0 mg, 35%), m.p. 197 – 197.5 °C. ^{1}H NMR (Acetone-d_6, 400 MHz) δ 8.30 – 8.27 (m, 2H, ArH), 8.13 – 8.08 (m, 2H, ArH), 7.44 – 7.40 (m, 2H, ArH), 6.79 – 6.74 (m, 2H, ArH), 3.03 (s, 6H, NMe_2), 2.69 (s, 3H, Me). ^{13}C NMR (Acetone-d_6, 101 MHz) δ 197.0 (q), 152.4 (q), 140.5 (q), 138.7 (q), 133.8 (t), 130.5 (t), 127.9 (q), 124.1 (t), 112.7 (t), 107.3 (q), 106.4 (q), 95.4 (q), 73.4 (q), 40.1 (p), 26.9 (p). HRMS ESI: $[M+Na]^+$ calcd. for $C_{20}H_{17}IN_4ONa^+$: 479.0339; found: 479.0340.

Synthesis of pair of triazoles (3d) / (4d). These compounds were prepared in accordance with the general procedure from 1-iodo(buta-1,3-diyne) **1c** (92.3 mg, 0.327 mmol), 1-(4-azidophenyl)ethan-1-one **2a** (52.7 mg, 0.327 mmol), $CuI(PPh_3)_3$ (16.0 mg, 0.016 mmol) and 2,6-lutidine (1.40 mg, 0.013 mmol). The crude mixture of products was separated by column chromatography (eluent: hexane/acetone = 5:1).

1-(4-(5-Iodo-4-((4-methoxyphenyl)ethynyl)-1*H*-1,2,3-triazol-1-yl)phenyl)ethan-1-one (3d) a beige solid (36.3 mg, 25%), m.p. 177.5 – 179.5 °C (with decomposition). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.20 – 8.13 (m, 2H, ArH), 7.79 – 7.69 (m, 2H, ArH), 7.60 – 7.50 (m, 2H, ArH), 6.94 – 6.83 (m, 2H, ArH), 3.85 (s, 3H, OCH_3), 2.69 (s, 3H, CH_3).^{13}C NMR ($CDCl_3$, 101 MHz) δ 196.7 (q), 160.5 (q), 140.1 (q), 140.05 (q), 138.3 (q), 133.6 (t), 129.7 (t), 125.9 (t), 114.3 (t), 114.1 (q), 95.96 (q), 83.9 (q), 76.9 (q), 55.5 (p), 26.9 (p). HRMS ESI: $[M+Na]^+$ calcd. for $C_{19}H_{14}IN_3O_2Na^+$: 466.0023; found: 466.0009.

1-(4-(4-Iodo-5-((4-methoxyphenyl)ethynyl)-1*H*-1,2,3-triazol-1-yl)phenyl)ethan-1-one (4d) a white solid (33.4 mg, 23%), m.p. 153 − 154 °C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.18 – 8.13 (m, 2H, ArH), 8.05 – 7.98 (m, 2H, ArH), 7.51 – 7.43 (m, 2H, ArH), 6.94 – 6.88 (m, 2H, ArH), 3.85 (s, 3H, OCH_3), 2.67 (s, 3H, CH_3).^{13}C NMR ($CDCl_3$, 101 MHz) δ 196.8 (q), 161.3 (q), 139.8 (q), 137.7 (q), 133.6 (t), 129.7 (t), 126.7 (q), 123.0 (t), 114.6 (t), 112.8 (q), 104.2 (q), 95.5 (q), 73.4 (q), 55.6 (p), 26.9 (p). HRMS ESI: $[M+Na]^+$ calcd. for $C_{19}H_{14}IN_3O_2Na^+$: 466.0023; found: 466.0029.

Synthesis of pair of triazoles (3e) / (4e). These compounds were prepared in accordance with the general procedure from 1-iodo(buta-1,3-diyne) **1d** (100 mg, 0.349 mmol), 1-(4-azidophenyl)ethan-1-one **2a** (56.3 mg, 0.349 mmol), $CuI(PPh_3)_3$ (17.1 mg, 0.017 mmol) and 2,6-lutidine (1.50 mg, 0.014 mmol). The crude mixture of products was separated by column chromatography (eluent: hexane/EtOAc = 3:1).

1-(4-(4-((4-Chlorophenyl)ethynyl)-5-iodo-1*H*-1,2,3-triazol-1-yl)phenyl)ethan-1-one (3e) a beige solid (39.0 mg, 25%), m.p. 193−194 °C (with decomposition). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.19 – 8.13 (m, 2H, ArH), 7.78 – 7.70 (m, 2H, ArH), 7.56 – 7.51 (m, 2H, ArH), 7.40 – 7.33 (m, 2H, ArH), 2.69 (s, 3H, CH_3). ^{13}C NMR ($CDCl_3$, 101 MHz) δ 196.7 (q), 140.0 (q), 139.5 (q), 138.3 (q), 135.5 (q), 133.2 (t), 129.7 (t), 129.0 (t), 125.9 (t), 120.5 (q), 94.6 (q), 84.5 (q), 79.1 (q), 26.9 (p). HRMS ESI: $[M+H]^+$ calcd. for $C_{18}H_{12}ClIN_3O^+$: 447.9708; found: 447.9718.

1-(4-(5-((4-Chlorophenyl)ethynyl)-4-iodo-1*H*-1,2,3-triazol-1-yl)phenyl)ethan-1-one (4e) a beige solid (35.6 mg, 23%), m.p. 149.7−150 °C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.19 – 8.13 (m, 2H, ArH), 8.02 – 7.95 (m, 2H, ArH), 7.48 – 7.45 (m, 2H, ArH), 7.42 – 7.36 (m, 2H, ArH), 2.68 (s, 3H, CH_3). ^{13}C NMR ($CDCl_3$, 101 MHz) δ 196.7 (q), 139.6 (q), 137.9 (q), 136.7, 133.1 (t), 129.8 (t), 129.3 (t), 126.2 (q), 123.1 (t), 119.3 (q), 102.5 (q), 96.2 (q), 75.3 (q), 26.9 (p). HRMS ESI: $[M+Na]^+$ calcd. for $C_{18}H_{12}ClIN_3ONa^+$: 469.9528; found: 469.9537.

Synthesis of pair of triazoles (3f) / (4f). These compounds were prepared in accordance with the general procedure from 1-iodo(buta-1,3-diyne) **1e** (100.3 mg, 0.362 mmol), 1-(4-azidophenyl)ethan-1-one **2a**, (58.3 mg, 0.362 mmol) $CuI(PPh_3)_3$ (17.7 mg, 0.018 mmol) and 2,6-lutidine (1.60 mg, 0.015 mmol). The crude mixture of products was separated by column chromatography (eluent: hexane/EtOAc = 3:1→2:1).

4-((1-(4-Acetylphenyl)-5-iodo-1*H*-1,2,3-triazol-4-yl)ethynyl)benzonitrile (3f) a beige solid (66.6 mg, 42%), m.p. 189.5 − 190 °C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.17 (d, *J* = 8.3 Hz, 2H, ArH), 7.74 (d, *J* = 8.3 Hz, 2H, ArH), 7.72 – 7.66 (m, 2H, ArH), 2.69 (s, 3H, CH_3). ^{13}C NMR ($CDCl_3$, 101 MHz) δ 196.6 (q), 139.8 (q), 138.9 (q), 138.5 (q), 132.4 (t), 132.34 (q), 132.32 (t), 129.7 (t), 126.9 (q), 125.9 (t), 118.4 (q), 112.7 (q), 93.8 (q), 85.1 (q), 82.4 (q), 26.9 (p). HRMS ESI: $[M+Na]^+$ calcd. for $C_{19}H_{11}IN_4ONa^+$: 460.9870; found: 460.9881.

4-((1-(4-Acetylphenyl)-4-iodo-1*H*-1,2,3-triazol-5-yl)ethynyl)benzonitrile (4f) a beige solid (40.0 mg, 25%), m.p. 166.5 − 168 °C. ^{1}H NMR ($CDCl_3$, 400.13 MHz) δ 8.19 – 8.16 (m, 2H, ArH), 7.98 – 7.94 (m, 2H, ArH), 7.70 (d, *J* = 8.2 Hz, 2H, ArH), 7.62 (d, *J* = 8.2 Hz, 2H, ArH), 2.69 (s, 3H, CH_3).^{13}C NMR ($CDCl_3$, 101 MHz) δ 196.6 (q), 139.5 (q), 138.1 (q), 132.5 (t), 132.4 (t), 129.8 (t), 125.7 (q), 125.5 (q), 123.2 (t), 118.0 (q), 113.7 (q), 101.4 (q), 96.9 (q), 78.1 (q), 26.9 (p). HRMS ESI: $[M+Na]^+$ calcd. for $C_{19}H_{11}IN_4ONa^+$: 460.9870; found: 460.9874.

Synthesis of pair of triazoles (3g) / (4g). These compounds were prepared in accordance with the general procedure from 1-iodo(buta-1,3-diyne) **1f** (132 mg, 0.600 mmol), 1-(4-

azidophenyl)ethan-1-one **2a** (96.7 mg, 0.600 mmol), $CuI(PPh_3)_3$ (29.3 mg, 0.030 mmol) and 2,6-lutidine (2.57 mg, 0.024 mmol). The crude mixture of products was separated by column chromatography (eluent: hexane/acetone = 2:1).

1-(4-(4-(4-Hydroxybut-1-yn-1-yl)-5-iodo-1*H*-1,2,3-triazol-1-yl)phenyl)ethan-1-one (3g) a beige solid (69.0 mg, 30%), m.p. 156 − 157 °C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.16 – 8.12 (m, 2H, ArH), 7.73 – 7.68 (m, 2H, ArH), 3.89 (q, *J* = 6.3 Hz, 2H, CH_2), 2.81 (t, *J* = 6.3 Hz, 2H, CH_2), 2.68 (s, 3H, CH_3), 2.16 (br s, 1H, OH). ^{13}C NMR ($CDCl_3$, 101 MHz) δ 196.7 (q), 140.0 (q), 139.6 (q), 138.3 (q), 129.6 (t), 125.9 (t), 94.1 (q), 84.0 (q), 71.5 (q), 61.0 (s), 26.9 (p), 24.1 (s). HRMS ESI: $[M+Na]^+$ calcd. for $C_{14}H_{12}IN_3O_2Na^+$: 403.9866; found: 403.9872.

1-(4-(5-(4-Hydroxybut-1-yn-1-yl)-4-iodo-1*H*-1,2,3-triazol-1-yl)phenyl)ethan-1-one (4g) a light brown solid (25.0 mg, 10%), m.p. 133 – 135 °C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.15 – 8.11 (m, 2H, ArH), 7.98 – 7.93 (m, 2H, ArH), 3.90 – 3.83 (m, 2H, CH_2), 2.80 (t, *J* = 6.2 Hz, 2H, CH_2), 2.66 (s, 3H, CH_3), 1.88 (br s, 1H, OH). ^{13}C NMR ($CDCl_3$, 101 MHz) δ 196.8 (q), 139.6 (q), 137.7 (q), 129.7 (t), 126.3 (q), 123.0 (t), 103.2 (q), 95.9 (q), 68.0 (q), 60.6 (s), 26.9 (p), 24.3 (s). HRMS ESI: $[M+Na]^+$ calcd. for $C_{14}H_{12}IN_3O_2Na^+$: 403.9866; found: 403.9856.

Synthesis of pair of triazoles (3h) / (4h). These compounds were prepared in accordance with the general procedure from 1-iodo(buta-1,3-diyne) **1e** (101 mg, 0.365 mmol), azide **2c** (48.5 mg, 0.365 mmol), $CuI(PPh_3)_3$ (17.8 mg, 0.018 mmol) and 2,6-lutidine (1.56 mg, 0.015 mmol). The crude mixture of products was separated by column chromatography (eluent: benzene → benzene/EtOAc = 50:1).

4-((5-Iodo-1-(*p*-tolyl)-1*H*-1,2,3-triazol-4-yl)ethynyl)benzonitrile (3h) a white solid (55.0 mg, 37%), m.p. 178 − 179 °C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.72 – 7.66 (m, 4H, ArH), 7.46 – 7.41 (m, 2H, ArH), 7.40 – 7.36 (m, 2H), 2.48 (s, 3H, Me). ^{13}C NMR (DMSO-d_6, 101 MHz) δ 140.4 (q), 136.5 (q), 134.0 (q), 132.8 (t), 132.2 (t), 130.0 (t), 126.0 (q), 125.9 (t), 118.3 (q), 111.7 (q), 92.6 (q), 92.4 (q), 83.1 (q), 20.8 (p). HRMS ESI: $[M+Na]^+$ calcd. for $C_{18}H_{11}IN_4Na^+$: 432.9921; found: 432.9932.

4-((4-Iodo-1-(*p*-tolyl)-1*H*-1,2,3-triazol-5-yl)ethynyl)benzonitrile (4h) a beige solid (4.6 mg, 3%), m.p. 183 − 184 °C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.72 – 7.63 (m, 4H, ArH), 7.61 – 7.56 (m, 2H, ArH), 7.40 – 7.35 (m, 2H, ArH), 2.47 (s, 3H, Me). ^{13}C NMR ($CDCl_3$, 126 MHz) δ 140.6 (q), 133.9 (q), 132.4 (t), 132.3 (t), 130.2 (t), 126.0 (q), 125.7 (q), 123.3 (t), 118.2 (q), 113.4 (q), 100.5 (q), 96.0 (q), 78.6 (q), 21.5 (p). HRMS ESI: $[M+Na]^+$ calcd. for $C_{18}H_{11}IN_4Na^+$: 432.9921; found: 432.9922.

Synthesis of pair of triazoles (3i) / (4i). These compounds were prepared in accordance with the general procedure from 1-iodo(buta-1,3-diyne) **1e** (100 mg, 0.361 mmol), 1-azido-4-chlorobenzene **2d** (55.4 mg, 0.361 mmol), $CuI(PPh_3)_3$ (17.6 mg, 0.018 mmol) and 2,6-lutidine (1.55 mg, 0.014 mmol). The crude mixture of products was separated by column chromatography (eluent: hexane/acetone = 10:1→5:1).

4-((1-(4-Chlorophenyl)-5-iodo-1*H*-1,2,3-triazol-4-yl)ethynyl)benzonitrile (3i) a grey solid (106.5 mg, 69%), m.p. 209 − 211 °C (with decomposition). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.73 – 7.66 (m, 4H, ArH), 7.60 – 7.50 (m, 4H, ArH). ^{13}C NMR ($CDCl_3$, 101 MHz) δ 138.6 (q), 136.9 (q), 135.0, 132.4 (t), 132.3 (t), 130.0 (t), 127.2 (t), 127.0 (q), 118.4 (q), 112.6 (q), 93.7 (q), 85.7 (q), 82.5 (q). HRMS ESI: $[M+Na]^+$ calcd. for $C_{17}H_8ClIN_4Na^+$: 452.9374; found: 452.9374.

4-((1-(4-Chlorophenyl)-4-iodo-1*H*-1,2,3-triazol-5-yl)ethynyl)benzonitrile (4i) a beige solid (23.0 mg, 15%), m.p. 214 − 216 °C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.77 – 7.73 (m, 2H, ArH), 7.71 – 7.67 (m, 2H, ArH), 7.62 – 7.55 (m, 4H, ArH). ^{13}C NMR ($CDCl_3$, 101 MHz) δ 136.3 (q), 134.7 (q), 132.5 (t), 132.3 (t), 130.0 (t), 125.7 (q), 125.6 (q), 124.7 (t), 118.1 (q), 113.6 (q), 101.1 (q), 96.4 (q), 78.1 (q). HRMS ESI: $[M+Na]^+$ calcd. for $C_{17}H_8ClN_4INa^+$: 452.9374; found: 452.9374.

Synthesis of pair of triazoles (3j) / (4j). These compounds were prepared in accordance with the general procedure from 1-iodo(buta-1,3-diyne) **1e** (100 mg, 0.361 mmol), azide **2e** (67.5 mg, 0.361 mmol), $CuI(PPh_3)_3$ (17.6 mg, 0.018 mmol) and 2,6-lutidine (1.55 mg, 0.014 mmol). The crude mixture of products was separated by column chromatography (eluent: hexane/DCM = 1:2 → DCM).

4-((5-Iodo-1-(3-(trifluoromethyl)phenyl)-1*H*-1,2,3-triazol-4-yl)ethynyl)benzonitrile (3j) a beige solid (96.6 mg, 57%), m.p. 181.5 − 182 °C. ^{1}H NMR ($CDCl_3$, 400.13 MHz) δ 7.93 – 7.89 (m, 1H, ArH), 7.88 – 7.80 (m, 2H, ArH), 7.79 – 7.73 (m, 1H, ArH), 7.72 – 7.65 (m, 4H, ArH). ^{13}C NMR ($CDCl_3$, 101 MHz) δ 138.9 (q), 137.0 (q), 132.5 (q, $^{2}J_{C\text{-}F}$ = 35.5 Hz), 132.4 (t), 132.3 (t), 130.5 (t), 129.1 (t), 127.42 (q, t, $^{3}J_{C\text{-}F}$ = 3.8 Hz), 126.9 (q), 123.3 (q, $^{1}J_{C\text{-}F}$ = 272.6 Hz), 123.1 (t, q, $^{3}J_{C\text{-}F}$ = 3.8 Hz), 118.4 (q), 112.7 (q), 93.8 (q), 85.4 (q), 82.3 (q). HRMS ESI: $[M+Na]^+$ calcd. for $C_{18}H_8F_3IN_4Na^+$: 486.9638; found: 486.9647.

4-((4-Iodo-1-(3-(trifluoromethyl)phenyl)-1*H*-1,2,3-triazol-5-yl)ethynyl)benzonitrile (4j) a beige solid (23.7 mg, 14%), m.p. 185.5 – 186.5 °C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.18 (br.s, 1H, ArH), 8.08 – 8.04 (m, 1H, ArH), 7.85 – 7.81 (m, 1H, ArH), 7.78 – 7.73 (m, 1H, ArH), 7.72 – 7.68 (m, 2H, ArH), 7.63 – 7.59 (m, 2H, ArH). ^{13}C NMR ($CDCl_3$, 101 MHz) δ 136.7 (q), 132.4 (t), 132.3 (q, $^{2}J_{C\text{-}F}$ = 33.3 Hz), 132.27 (t), 130.7 (t), 126.8 (t, q, $^{3}J_{C\text{-}F}$ = 3.8 Hz), 126.5 (t), 125.77, 125.44, 123.4 (q, $^{1}J_{C\text{-}F}$ = 272.8 Hz), 120.1 (t, q, $^{3}J_{C\text{-}F}$ = 3.8 Hz), 118.0 (q), 113.8 (q), 101.6 (q), 96.6 (q), 77.9 (q). HRMS ESI: $[M+Na]^+$ calcd. for $C_{18}H_8F_3IN_4Na^+$: 486.9638; found: 486.9635.

4-((1-(2,6-Dimethylphenyl)-5-iodo-1*H*-1,2,3-triazol-4-yl)ethynyl)benzonitrile (3k). This compound was prepared in accordance with the general procedure from 1-iodo(buta-1,3-diyne) **1e** (101.5 mg, 0.366 mmol), 1-azido-2,6-dimethylbenzene **2f** (53.9 mg, 0.366 mmol), $CuI(PPh_3)_3$ (17.9 mg, 0.018 mmol) and 2,6-lutidine (1.57 mg, 0.015 mmol). The crude product was purified by column chromatography (eluent: benzene → benzene/EtOAc = 100:1) to afford a white solid (49.3 mg, 32%), m.p. 199 − 201 °C (with decomposition). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.74 – 7.65 (m, 4H, ArH), 7.42 – 7.35 (m, 1H, ArH), 7.26 – 7.22 (m, 2H, ArH), 1.98 (s, 6H, 2Me). ^{13}C NMR ($CDCl_3$,

101 MHz) δ 137.7 (q), 136.2 (q), 135.0 (q), 132.4 (t), 132.3 (t), 131.1 (t), 128.8 (t), 128.5 (q), 127.1 (q), 118.4 (q), 112.5 (q), 93.4 (q), 87.9 (q), 82.7 (q), 17.6 (p). HRMS ESI: $[M+Na]^+$ calcd. for $C_{19}H_{13}IN_4Na^+$: 447.0077; found: 447.0077.

Synthesis of pair of triazoles (3l) / (4l). These compounds were prepared in accordance with the general procedure from 1-iodo(buta-1,3-diyne) **1d** (124.7 mg, 0.435 mmol), 4-azidobenzonitrile **2g** (62.7 mg, 0.435 mmol), $CuI(PPh_3)_3$ (21.3 mg, 0.022 mmol) and 2,6-lutidine (1.86 mg, 0.017 mmol). The crude mixture of products was separated by column chromatography (eluent: hexane/acetone = 5:1).

4-(4-((4-Chlorophenyl)ethynyl)-5-iodo-1*H*-1,2,3-triazol-1-yl)benzonitrile (3l) a beige solid (99.7 mg, 53%), m.p. 181 − 182 °C (with decomposition). ^1H NMR ($CDCl_3$, 400 MHz) δ 7.93 – 7.88 (m, 2H, ArH), 7.84 – 7.77 (m, 2H, ArH), 7.58 – 7.53 (m, 2H, ArH), 7.40 – 7.35 (m, 2H, ArH). ^{13}C NMR ($CDCl_3$, 101 MHz) δ 139.8 (q), 135.7 (q), 133.6 (t), 133.2 (t), 129.1 (t), 126.4 (t), 120.4 (q), 117.5 (q), 114.5 (q), 94.9 (q), 84.1 (q), 78.9 (q). HRMS ESI: $[M+Na]^+$ calcd. for $C_{17}H_8ClIN_4Na^+$: 452.9374; found: 452.9370.

4-(5-((4-Chlorophenyl)ethynyl)-4-iodo-1*H*-1,2,3-triazol-1-yl)benzonitrile (4l) a beige solid (49.6 mg, 27%), m.p. 191 − 192 °C. ^1H NMR ($CDCl_3$, 400 MHz) δ 8.08 – 8.02 (m, 2H, ArH), 7.92 – 7.86 (m, 2H, ArH), 7.48 – 7.44 (m, 2H, ArH), 7.42 – 7.37 (m, 2H, ArH). ^{13}C NMR ($CDCl_3$, 100.6 MHz) δ 139.4 (q), 136.9 (q), 133.7 (t), 133.1 (t), 129.4 (t), 126.2 (q), 123.5 (t), 119.1 (q), 117.6 (q), 113.8 (q), 103.1 (q), 96.5 (q), 75.0 (q). HRMS ESI: $[M+Na]^+$ calcd. for $C_{17}H_8ClIN_4Na^+$: 452.9374; found: 452.9375.

Synthesis of pair of triazoles (3m) / (4m). These compounds were prepared in accordance with the general procedure from 1-iodo(buta-1,3-diyne) **1d** (100.0 mg, 0.349 mmol), azide **2b** (52.1 mg, 0.349 mmol), $CuI(PPh_3)_3$ (17.1 mg, 0.017 mmol) and 2,6-lutidine (1.55 mg, 0.014 mmol). The crude mixture of products was separated by column chromatography (eluent: hexane/acetone = 10:1).

4-((4-Chlorophenyl)ethynyl)-5-iodo-1-(4-methoxyphenyl)-1*H*-1,2,3-triazole[44] **(3m)** a beige solid (48.5 mg, 32%), m.p. 162 − 163 °C. ^1H NMR ($CDCl_3$, 400 MHz, δ) 7.56 – 7.51 (m, 2H, Ar), 7.49 – 7.43 (m, 2H, Ar), 7.38 – 7.33 (m, 2H, Ar), 7.08 – 7.01 (m, 2H, Ar), 3.90 (s, 3H, OCH_3).

5-((4-Chlorophenyl)ethynyl)-4-iodo-1-(4-methoxyphenyl)-1*H*-1,2,3-triazole (4m) a beige solid (7.0 mg, 5%). ^1H NMR ($CDCl_3$, 400.13 MHz, δ) 7.72 – 7.66 (m, 2H, Ar), 7.45 – 7.40 (m, 2H, Ar), 7.39 – 7.34 (m, 2H, Ar), 7.08 – 7.03 (m, 2H, Ar), 3.89 (s, 3H, OCH_3). HRMS ESI: $[M+Na]^+$ calcd. for $C_{17}H_{11}ClIN_3ONa^+$: 457.9528; found: 457.9519; HPLC-MS: m/z 435.9714 (calcd. $[M+H]^+$ = 435.9708), Purity: 90.5% (HPLC analysis at 270 – 280 nm). Retention time HPLC in 9.3 min.

1-(Iodoethynyl)-3-nitrobenzene (5b). To a solution of trimethyl((3-nitrophenyl)ethynyl)silane (176 mg, 0.803 mmol) in acetonitrile (10.0 mL) with an addition of H_2O (27.6 µL) under an

atmosphere of an Ar and in the dark was added AgF (102 mg, 0.803 mmol) and the mixture was stirred for 20 min. Then *N*-iodosuccinimide (NIS) (217 mg, 0.963 mmol) was added, and the mixture was stirred for two hours until the completion of the reaction (TLC control). Acetonitrile was removed under reduced pressure. EtOAc (15 – 20 mL) was added to the residue. The organic layer was separated, washed with H_2O (3 × 15 mL), and dried over anhydrous Na_2SO_4, and concentrated under reduced pressure to yield the crude product. Purification of the crude product by column chromatography (eluent: hexane/acetone = 50:1) gave **5b** (194.0 mg, 89%) as a yellowish powder. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.29 – 8.25 (m, 1H, ArH), 8.19 – 8.15 (m, 1H, ArH), 7.75 – 7.71 (m, 1H, ArH), 7.53 – 7.48 (m, 1H, ArH); ^{13}C NMR ($CDCl_3$, 101 MHz) δ 148.1 (q), 138.1 (t), 129.5 (t), 127.4 (t), 125.2 (q), 123.6 (t), 91.9 (q), 11.1 (q). HRMS ESI: $[M+H]^+$ calcd. for $C_8H_5INO_2^+$: 273.9359; found: 273.9353.

General Procedure for the Synthesis of 5-iodo-1*H*-1,2,3-triazole 6a,b. To a 1-iodoalkyne **5** (1.00 equiv) in a crew vial was added an azide (1.00 equiv), $CuI(PPh_3)_3$ (5.00 mol %) and 2,6-lutidine (4.00 mol %). The thick resulting mixture was vigorously stirred for 18 h at room temperature. The reaction mixture was diluted with DCM (20 – 30 mL) and saturated aqueous solution of NH_4Cl (2 × 15 mL). The reaction mixture was shacked; the organic layer was separated, dried over anhydrous Na_2SO_4 and concentrated under reduced pressure to yield the crude product, which was purified by column chromatography on silica gel.

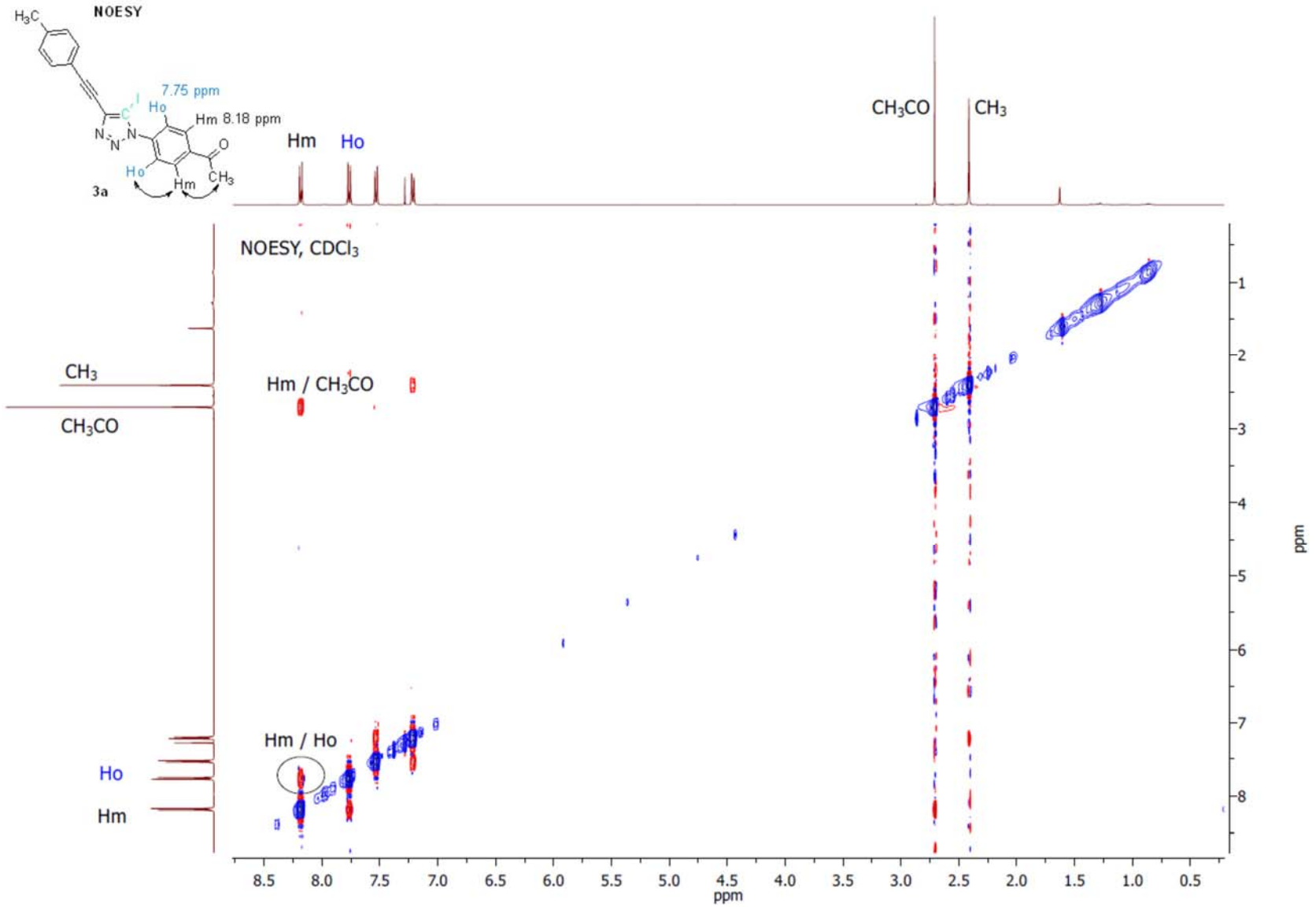
1-(4-(5-Iodo-4-phenyl-1*H*-1,2,3-triazol-1-yl)phenyl)ethan-1-one (6a). The triazole was prepared in accordance with the general procedure from iodoalkyne **5a** (130 mg, 0.570 mmol), 1-(4-azidophenyl)ethan-1-one **2a** (91.9 mg, 0.570 mmol), $CuI(PPh_3)_3$ (27.9 mg, 0.029 mmol) and 2,6-lutidine (2.40 mg, 0.023 mmol). The crude product was purified by column chromatography (eluent: hexane/acetone = 5:1→3:1) to afford a shiny yellow-beige solid (124.0 mg, 53%), m.p. 238 − 240 °C (with decomposition). ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.25 – 8.19 (m, 2H, Ar), 7.99 – 7.93 (m, 2H, Ar), 7.88 – 7.81 (m, 2H, Ar), 7.60 – 7.52 (m, 2H, Ar), 7.50 – 7.45 (m, 1H, Ar), 2.69 (s, 3H, Me). ^{13}C NMR (101 MHz, DMSO-d_6) δ 197.2 (q), 149.6 (q), 140.1 (q), 137.8 (q), 130.2 (q), 129.4 (t), 128.8 (t), 128.6 (t), 127.3 (t), 126.9 (t), 82.9 (q), 27.0 (p). HRMS ESI: $[M+Na]^+$ calcd. for $C_{16}H_{12}IN_3ONa^+$: 411.9917; found: 411.9905.

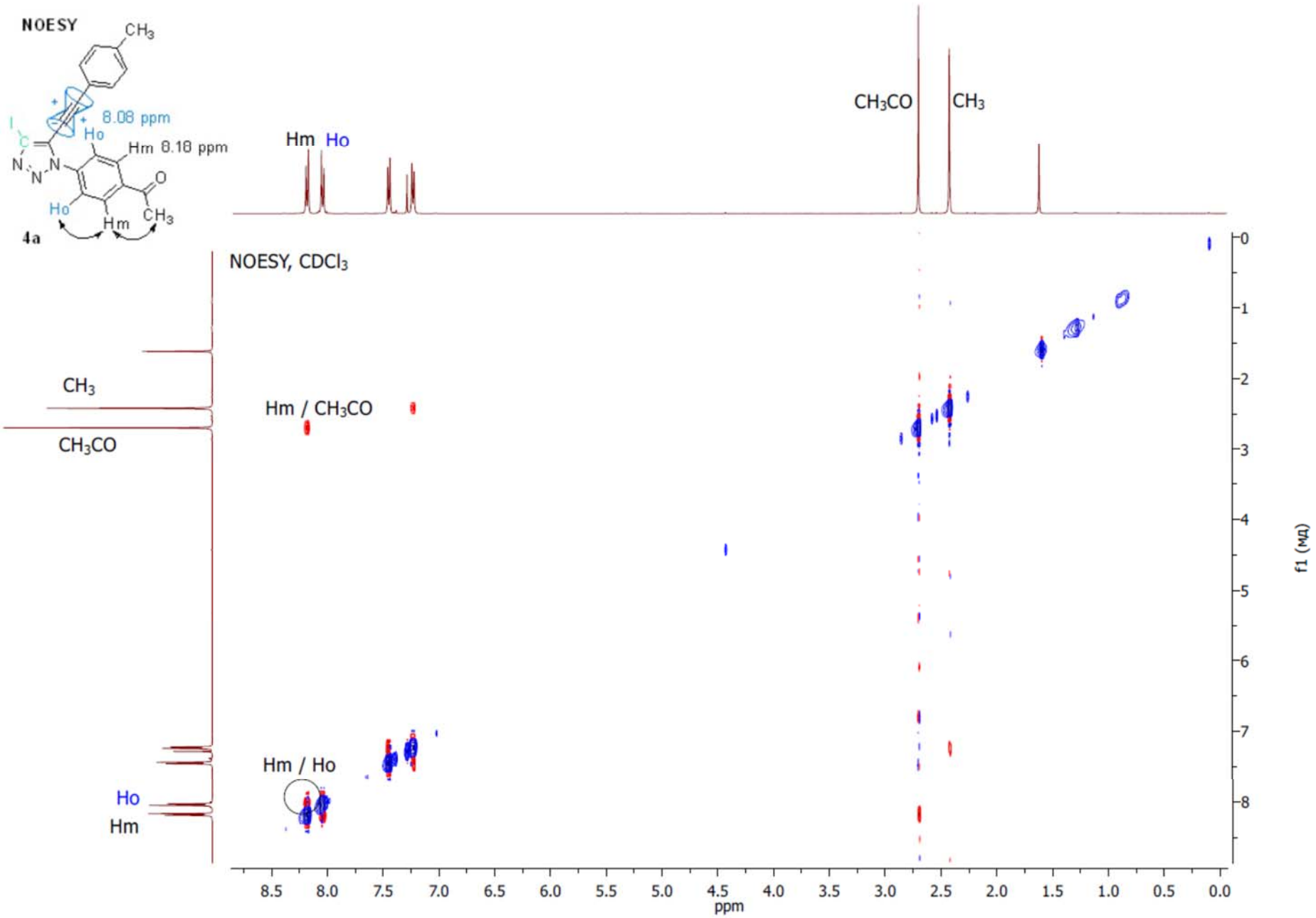
1-(4-(5-Iodo-4-(3-nitrophenyl)-1*H*-1,2,3-triazol-1-yl)phenyl)ethan-1-one (6b). The triazole was prepared in accordance with the general procedure from iodoalkyne **5b** (150.0 mg, 0.549 mmol), 1-(4-azidophenyl)ethan-1-one **2a** (88.5 mg, 0.549 mmol), $CuI(PPh_3)_3$ (26.9 mg, 0.028 mmol) and 2,6-lutidine (2.40 mg, 0.022 mmol). The crude product was purified by column chromatography (eluent: hexane/acetone = 3:1) to afford a shiny yellow solid (105.0 mg, 44%), m.p. 207 − 208 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.84 – 8.82 (m, 1H, Ar), 8.47 – 8.42 (m, 1H, Ar), 8.35 – 8.29 (m, 1H, Ar), 8.25 – 8.20 (m, 2H, Ar), 7.90 – 7.83 (m, 3H, Ar), 2.69 (s, 1H, Me). ^{13}C NMR (101 MHz, DMSO-d_6) δ 197.3 (q), 148.0 (q), 147.3 (q), 139.9 (q), 138.0 (q), 133.3 (t), 131.8 (q), 130.7 (t), 129.5

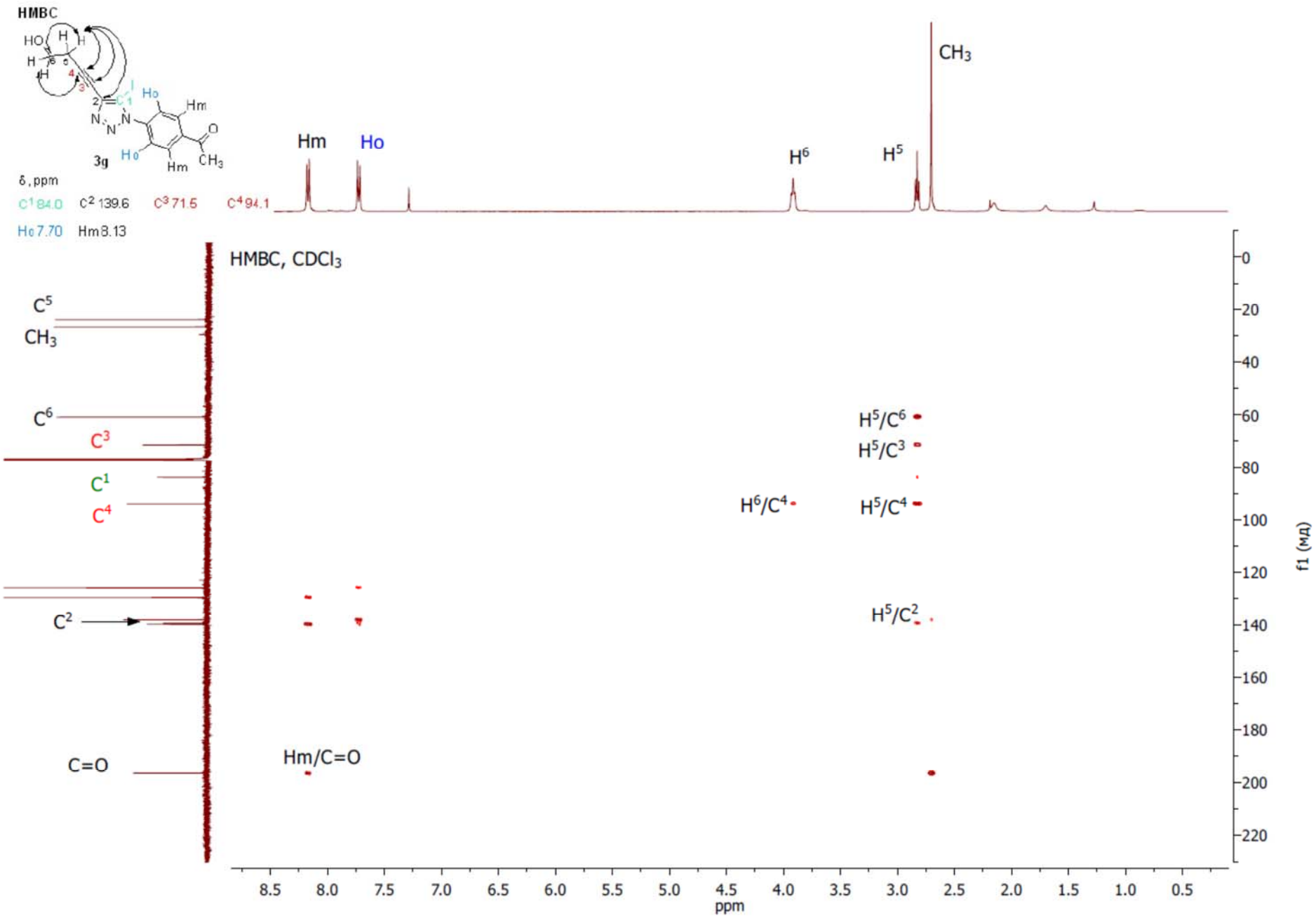
(t), 126.9 (t), 123.3 (t), 121.3 (t), 84.5 (q), 27.0 (p). HRMS ESI: $[M+H]^+$ calcd. for $C_{16}H_{12}IN_4O_3^+$: 434.9949; found: 434.9939.

3 Distinguishing between isomeric triazoles 3 and 4 by NMR

3.1 Copies of 2D NMR spectra for *N*-aryl substituted 5-iodo-4-ethynyltriazole 3g and 4-iodo-5-ethynyltriazoles 4g with an alkyl substituted triple bond




NOESY
8.08 ppm
Ho
Hm 8.18 ppm
Ho
Hm
CH3
O
CH3
4a
Hm Ho
CH3CO
CH3
NOESY, CDCl3
CH3
CH3CO
Hm / CH3CO
Hm / Ho
Ho
Hm
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
ppm
f1 (мд)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3g
δ, ppm
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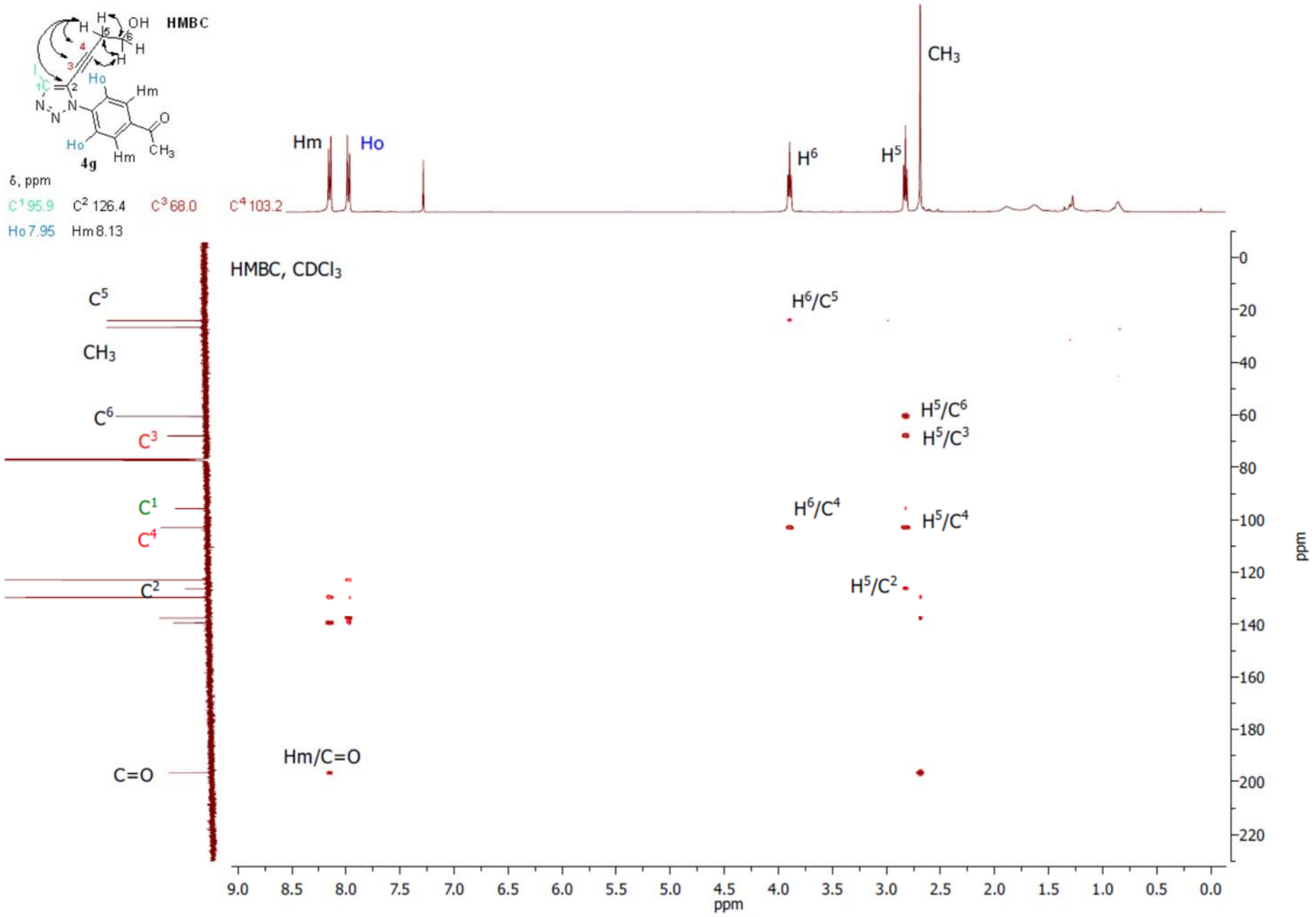
Ho 7.70 Hm 8.13
HMBC, CDCl3
Hm
Ho
H6
H5
CH3
C5
CH3
C6
C3
C1
C4
C2
C=O
H5/C6
H5/C3
H6/C4
H5/C4
H5/C2
Hm/C=O
ppm
f1 (мд)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δ, ppm
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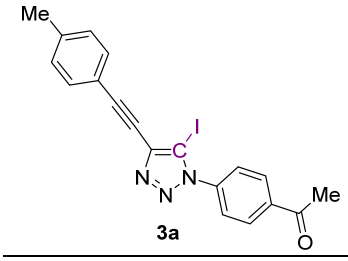
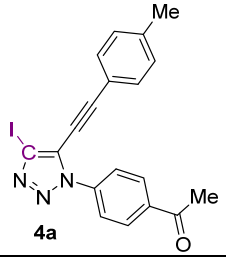
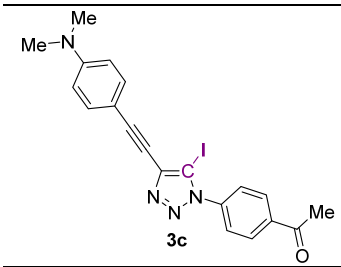
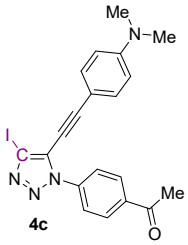
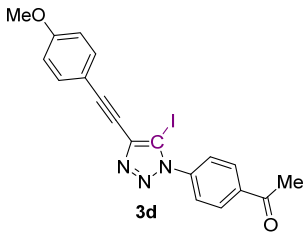
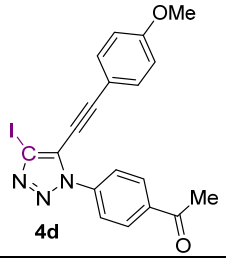
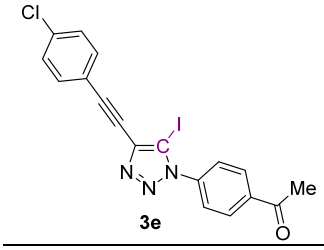
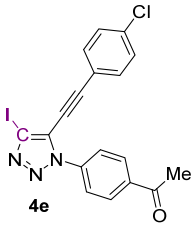
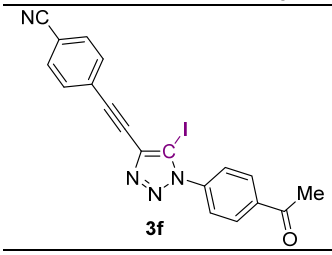
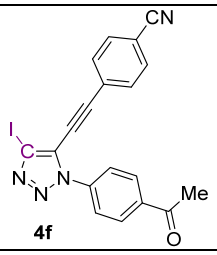
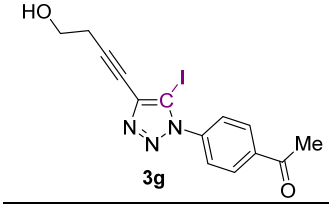
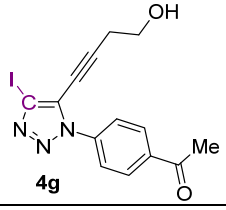
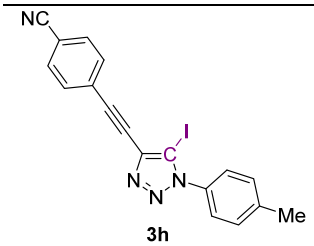
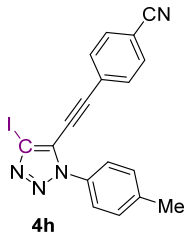
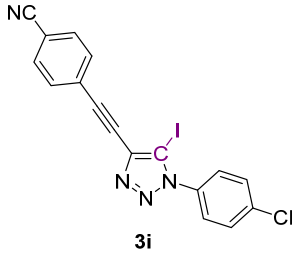
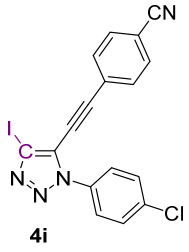
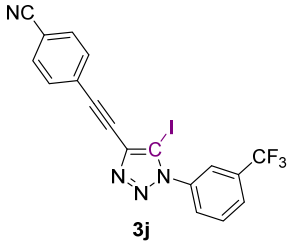
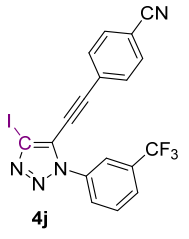
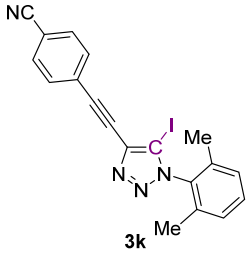
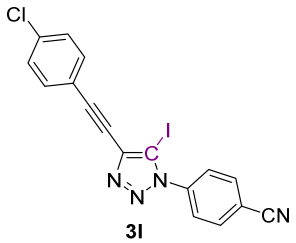
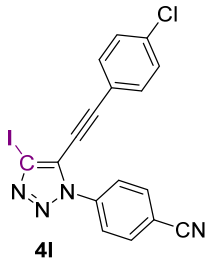
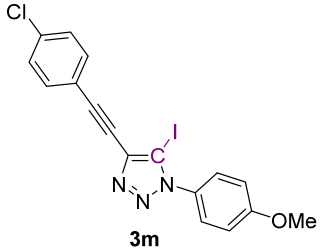
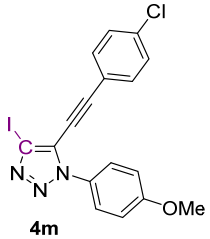
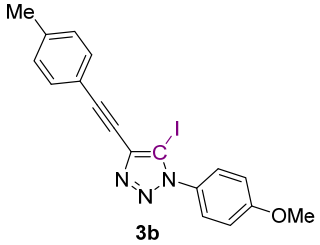
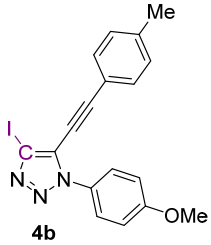
C2 126.4
C3 68.0
Ho 7.95
Hm 8.13
C4 103.2
Hm
Ho
H6
H5
CH3
HMBC, CDCl3
C5
CH3
C6
C3
C1
C4
C2
C=O
H6/C5
H5/C6
H5/C3
H6/C4
H5/C4
H5/C2
Hm/C=O
ppm

3.2 Characteristic chemical shift values

Table S1. Characteristic chemical shift values of C-I carbon atoms for triazoles 3 and 4 in ^{13}C NMR spectra[a]

1,4-Triazole	^{13}C NMR, δ (C-I), ppm	1,5-Triazole	^{13}C NMR, δ (C-I), ppm
 **3a**	84.1	 **4a**	95.7
 **3c**	86.9	 **4c**	95.4
 **3d**	83.9	 **4d**	95.5
 **3e**	84.5	 **4e**	96.2
 **3f**	85.1	 **4f**	96.9
 **3g**	84.0	 **4g**	95.9

 **3h**	92.5, 92.4, 83.1[b]	 **4h**	96.0
 **3i**	85.7	 **4i**	96.4
 **3j**	85.4	 **4j**	96.6
 **3k**	87.9	Not formed	
 **3l**	84.1	 **4l**	96.5
 **3m**	85.9	 **4m**	– [c]
 **3b**	88.8[d]	 **4b**	–

[a] ^{13}C NMR spectra were recorded in $CDCl_3$; [b] the signals cannot be distinguished in DMSO-d_6; [c] ^{13}C NMR was not measured; [d] ^{13}C NMR spectra were recorded in Acetone-d_6.

4 X-Ray diffraction studies

XRD measurements were performed using Rigaku (Oxford Diffraction) «XtaLAB SuperNova» in case of GAI-866-3, GAI-866-1, (Cu Kα, λ = 1.54184 Å, HyPix3000 type detector), Rigaku «XtaLAB Synergy» (Cu Kα, λ = 1.54184 Å, HyPix6000 type detector) in case of [$CuI(PPh_3)_3$], **3b**, **3d**, **4d, 3m** and Agilent Technologies (Oxford Diffraction) «Xcalibur Eos» diffractometer in case of [$CuI(PPh_3)_3$·MeCN] and [$Cu_2I_2(PPh_3)_3$] (Mo Kα, λ = 0.71073 Å, Atlas CCD type detector). All crystals were kept at 100(2) K during all experimental time. The unit cell parameters were refined by least square techniques. Using Olex2[2], the structure was solved with the ShelXT[3] structure solution program using Intrinsic Phasing and refined with the ShelXL[4] refinement package using CGLS minimization and refined by the full-matrix least squares technique against F2 in the anisotropic-isotropic approximation. Empirical absorption correction was applied in CrysAlisPro (Agilent Technologies, 2014) program complex using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.

All hydrogen atoms were placed in geometrically calculated positions and were refined in isotropic approximation in the riding model with the U_{iso}(H) parameters equal to $n \cdot U_{eq}(C_i)$ (n = 1.2 for CH and CH_2 groups and n = 1.5 for CH_3 groups), where $U(C_i)$ are respectively the equivalent thermal parameters of the atoms to which corresponding H atoms are bonded. The H(N) hydrogen atoms were found in the difference Fourier synthesis and refined in isotropic approximation.

Atomic coordinates, bond lengths, bond angles and thermal parameters have been deposited at the Cambridge Crystallographic Data Centre (CCDC). Accession Codes CCDC 2240443 (**3a**), 2240444 (**4a**), 2240445 (**3b**), 2240447 (**3d**), 2240446 (**4d**), 1869736 (**3m**), 2240448 [$CuI(PPh_3)_3$], 2240449 [$CuI(PPh_3)_3$•MeCN], and 2240450 [$Cu_2I_2(PPh_3)_3$] contain the supplementary crystallographic data for this paper. These data can be obtained free of charge via www.ccdc.cam.ac.uk/data_request/cif, or by emailing data_request@ccdc.cam.ac.uk, or by contacting The Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK; fax: +44 1223 336033.

Table S2. X-RAY diffraction data

Compound	**3a**	**4a**	**3b**	**4d**	**3a**	**3m**
Crystal Data						
Formula	$C_{19}H_{14}IN_3O$	$C_{19}H_{14}IN_3O$	$C_{18}H_{14}IN_3O$	$C_{19}H_{14}IN_3O_2$	$C_{19}H_{14}IN_3O_2$	$C_{17}H_{11}ClIN_3O$
Formula Weight	427.23	427.23	415.22	443.23	443.23	435.64
Space Group	$P2_1/c$	Pbca	P1	$P2_1/c$	$P2_1/c$	P1
Z	4	8	2	4	4	2
T, K	100(5)	100(6)	100.00(10)	100.00(10)	100.00(10)	100(2)
a, Å	14.5258(6)	4.7694(2)	7.2957(2)	10.40890(10)	14.2828(2)	7.21715(13)
b, Å	7.4296(3)	20.4826(12)	7.4157(2)	8.48620(10)	7.42180(10)	7.40565(11)
c, Å	15.9339(8)	35.0406(16)	15.3505(2)	19.6955(3)	16.4916(2)	15.40204(16)
α, °	90	90	98.052(2)	90	90	82.0610(11)
β, °	107.113(5)	90	101.391(2)	97.8050(10)	108.3930(10)	79.0302(12)
γ, °	90	90	90.231(2)	90	90	89.6967(13)
V, Å^3	1643.47(13)	3423.1(3)	805.69(3)	1723.63(4)	1658.87(4)	800.23(2)
μ, mm^{-1}	15.392	14.780	15.676	14.747	15.322	17.320
Data Collection						
Diffractometer	Rigaku (Oxford Diffraction) «XtaLAB SuperNova»	Rigaku (Oxford Diffraction) «XtaLAB SuperNova»	Rigaku «XtaLAB Synergy»	Rigaku «XtaLAB Synergy»	Rigaku «XtaLAB Synergy»	
Radiation type	CuKα (λ = 1.54184)	CuKα (λ = 1.54184)	Cu Kα (λ = 1.54184)	Cu Kα (λ = 1.54184)	Cu Kα (λ = 1.54184)	CuKα (λ = 1.54184)
Absorption correction	Multi-scan	Multi-scan	Multi-scan	Multi-scan	Multi-scan	Multi-scan
T_{min}, T_{max}	0.13406, 1.00000	0.40682, 1.00000	0.27079, 1.00000	0.48569, 1.00000	0.60604, 1.00000	0.397, 1.000
No. of measured, independent and observed [I > 2σ(I)] reflections	8335, 2662, 2403	21545, 3352, 2880	26330, 6284, 6011	33076, 3618, 3536	25287, 3475, 3384	
R_{int}	0.0727	0.0981	0.0866	0.0472	0.0429	0.0742
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.615	0.615	0.631	0.631	0.632	0.630
Refinement						
R[$F^2 > 2\sigma(F^2)$], wR(F^2), S	0.0633, 0.1722, 1.060	0.0519, 0.1247, 1.091	0.0418, 0.1095,1.092	0.0244, 0.0647, 1.098	0.0242, 0.0643, 1.060	0.0355, 0.0907, 1.050
No. of reflections	8335	21545	26330	33076	25287	13674
No. of parameters	2662	3352	6284	3618	3475	3015
H-atom treatment						
ρ_{max}, ρ_{min}, e/Å^3	2.37/-2.54	1.02/-0.98	0.96/-1.70	0.60/-0.78	0.72/-1.01	1.68/-1.61
CCDC	2240443	2240444	2240445	2240446	2240447	1869736

Table S3. X-RAY diffraction data

Compound	**$CuI(PPh_3)_3$**	**$CuI(PPh_3)_3$·MeCN**	**$Cu_2I_2(PPh_3)_3$**
Crystal Data			
Formula	$C_{52}H_{43}CuIP_3$	$C_{56}H_{48}CuINP_3$	$C_{54}H_{45}Cu_2I_2P_3$
Formula Weight	977.20	1018.30	1167.69

Space Group	P-1	$Pna2_1$	$P2_1$
Z	2	4	2
T, K	100.00(13)	100.00(10)	100.00(10)
a, Å	13.11763(14)	18.5498(2)	10.3589(4)
b, Å	14.31799(12)	20.2300(2)	20.5853(7)
c, Å	14.44658(10)	12.7711(2)	11.7439(6)
α, °	71.8942(7)	90	90
β, °	84.0976(8)	90	105.593(4)
γ, °	87.9689(8)	90	90
V, $Å^3$	2565.29(4)	4792.52(10)	2412.11(18)
μ, mm^{-1}	6.447	1.238	2.297
Data Collection			
Diffractometer	Rigaku «XtaLAB Synergy», Single source at offset/far, HyPix6000	«Xcalibur Eos»	«Xcalibur Eos»
Radiation type	Cu Kα (λ = 1.54184)	Mo Kα (λ = 0.71073)	Mo Kα (λ = 0.71073)
Absorption correction	Multi-scan	Multi-scan	Multi-scan
T_{min}, T_{max}	0.69391, 1.00000	0.96457, 1.00000	0.85190, 1.00000
No. of measured, independent and observed [I > 2σ(I)] reflections	49850, 10717, 10158	44915,17488, 15831	36890, 19480, 16801
R_{int}	0.0506	0.0300	0.0378
$(\sin \theta/\lambda)_{max}$ ($Å^{-1}$)	0.633	0.804	0.837
Refinement			
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.0329, 0.0824, 1.095	0.0262, 0.0511, 1.038	0.0415, 0.0635, 1.032
No. of reflections	49850	44915	36890
No. of parameters	562	560	550
H-atom treatment			
ρ_{max}, ρ_{min}, e/$Å^3$	0.49/-1.11	0.54/-0.43	1.32/-0.93
CCDC	2240448	2240449	2240450

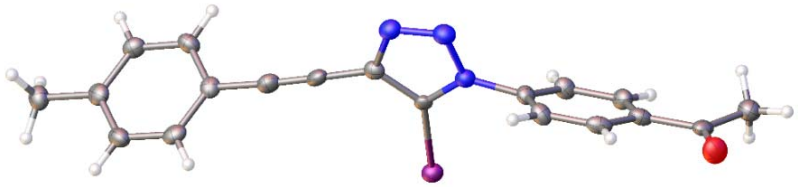


Figure S2. Molecular structure of compound **3a**, displacement parameters are drawn at 50% probability level

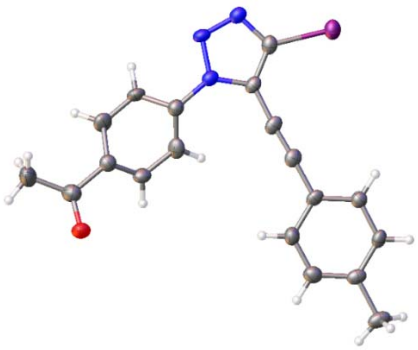


Figure S3. Molecular structure of compound **4a**, displacement parameters are drawn at 50% probability level

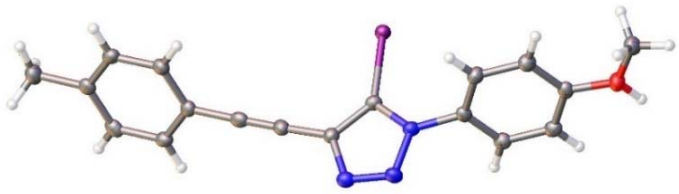


Figure S4. Molecular structure of compound **3b**, displacement parameters are drawn at 50% probability level

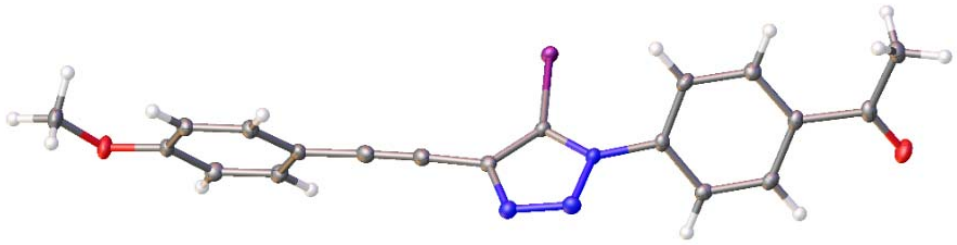


Figure S5. Molecular structure of compound **3d**, displacement parameters are drawn at 50% probability level

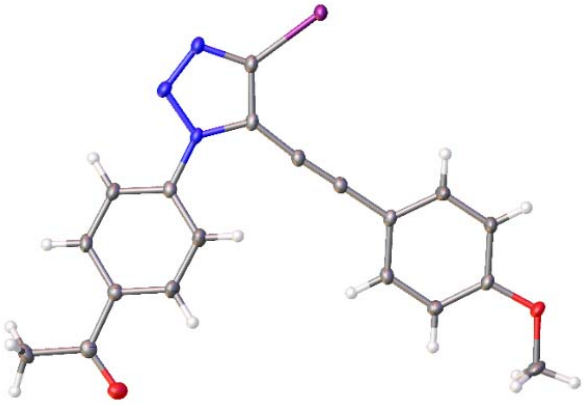


Figure S6. Molecular structure of compound **4d**, displacement parameters are drawn at 50% probability level

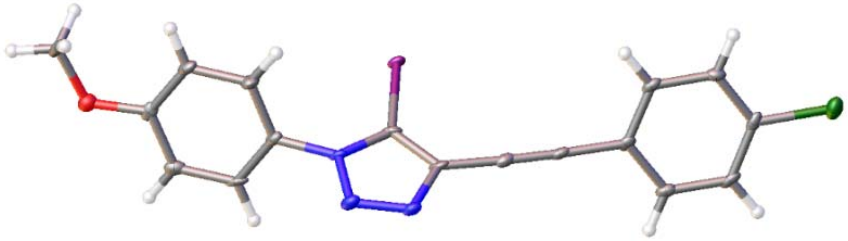


Figure S7. Molecular structure of compound **3m**, displacement parameters are drawn at 50% probability level

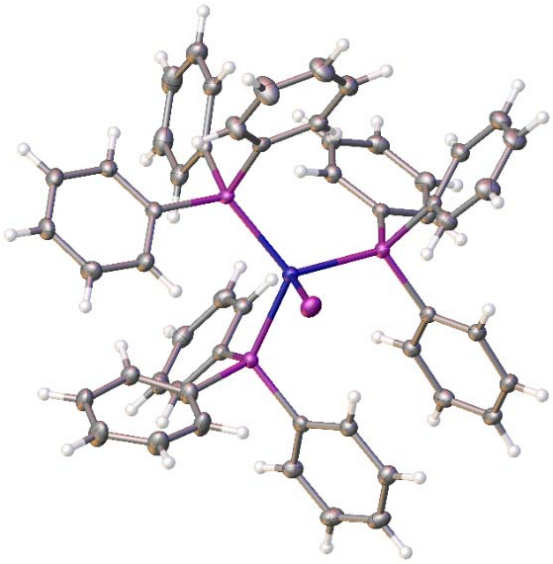


Figure S8. Molecular structure of complex $CuI(PPh_3)_3$, displacement parameters are drawn at 50% probability level

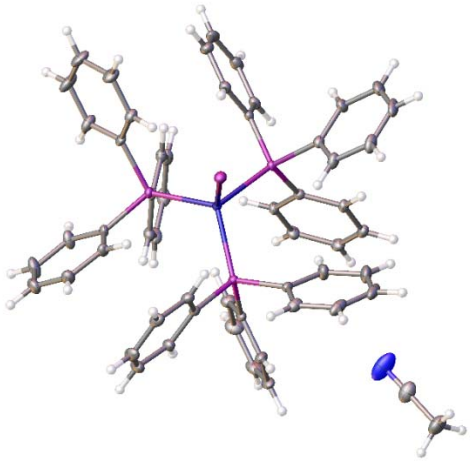


Figure S9. Molecular structure of complex $CuI(PPh_3)_3 \times MeCN$, displacement parameters are drawn at 50% probability level

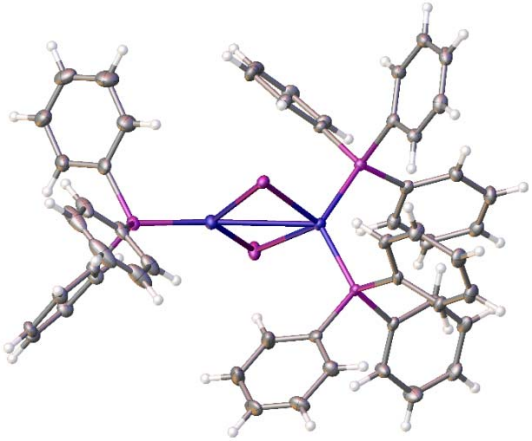


Figure S10. Molecular structure of complex $Cu_2I_2(PPh_3)_3$, displacement parameters are drawn at 50% probability level

5 Copies of thermogravimetry curves and derivative thermogravimetry curves of triazoles 3 and 4

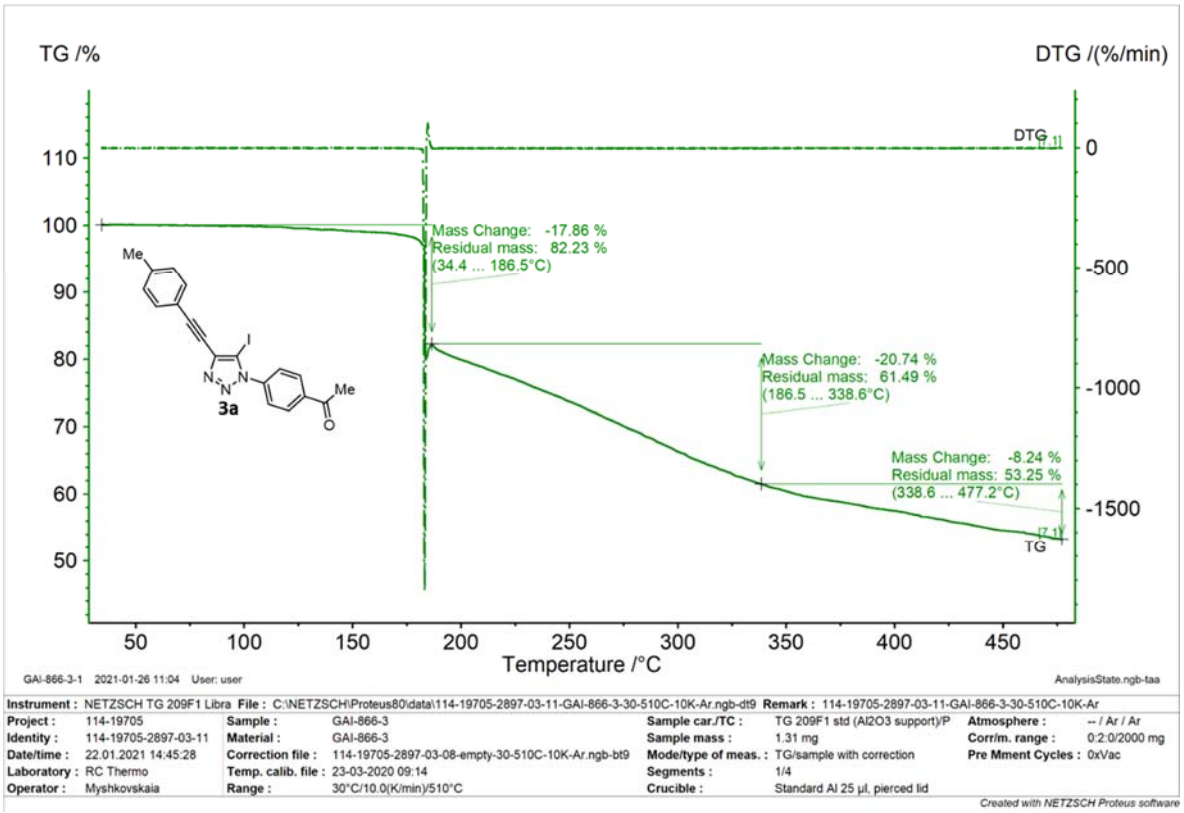


Figure S11. TG and DTG curves of triazole **3a**.

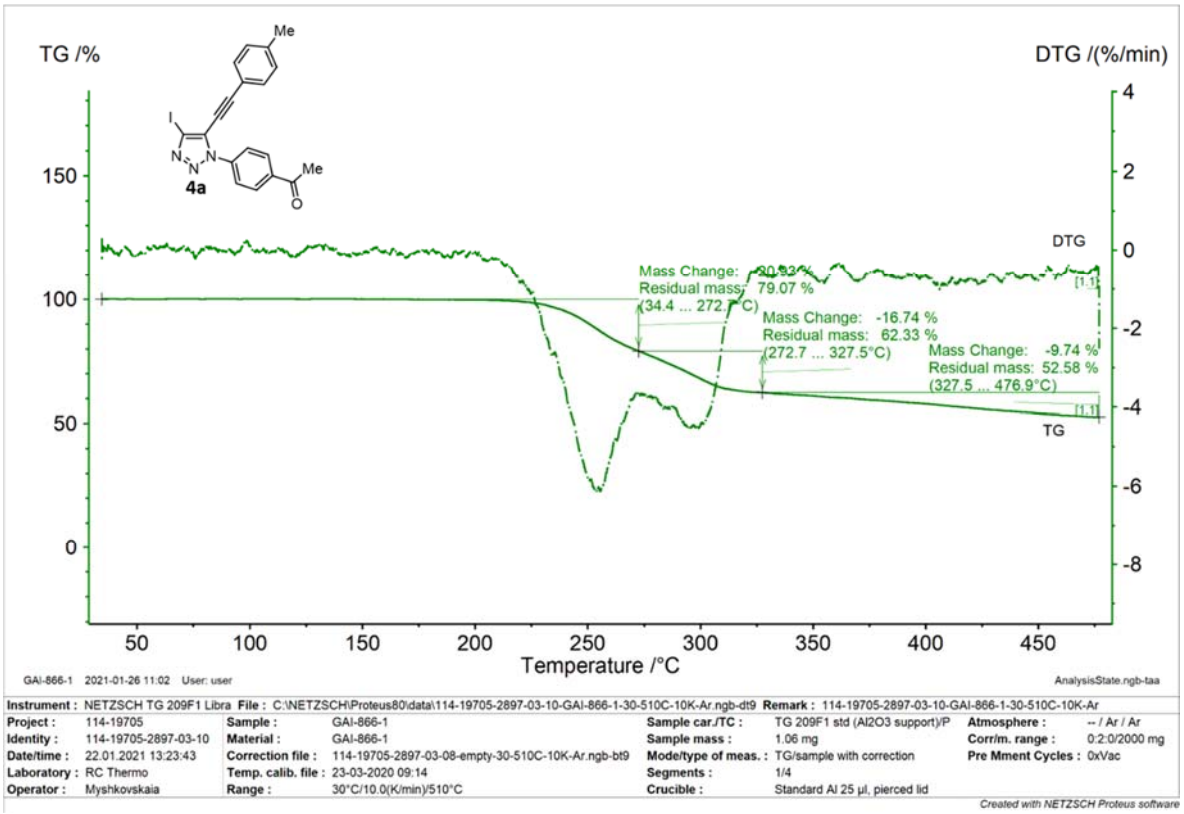


Figure S12. TG and DTG curves of triazole **4a**.

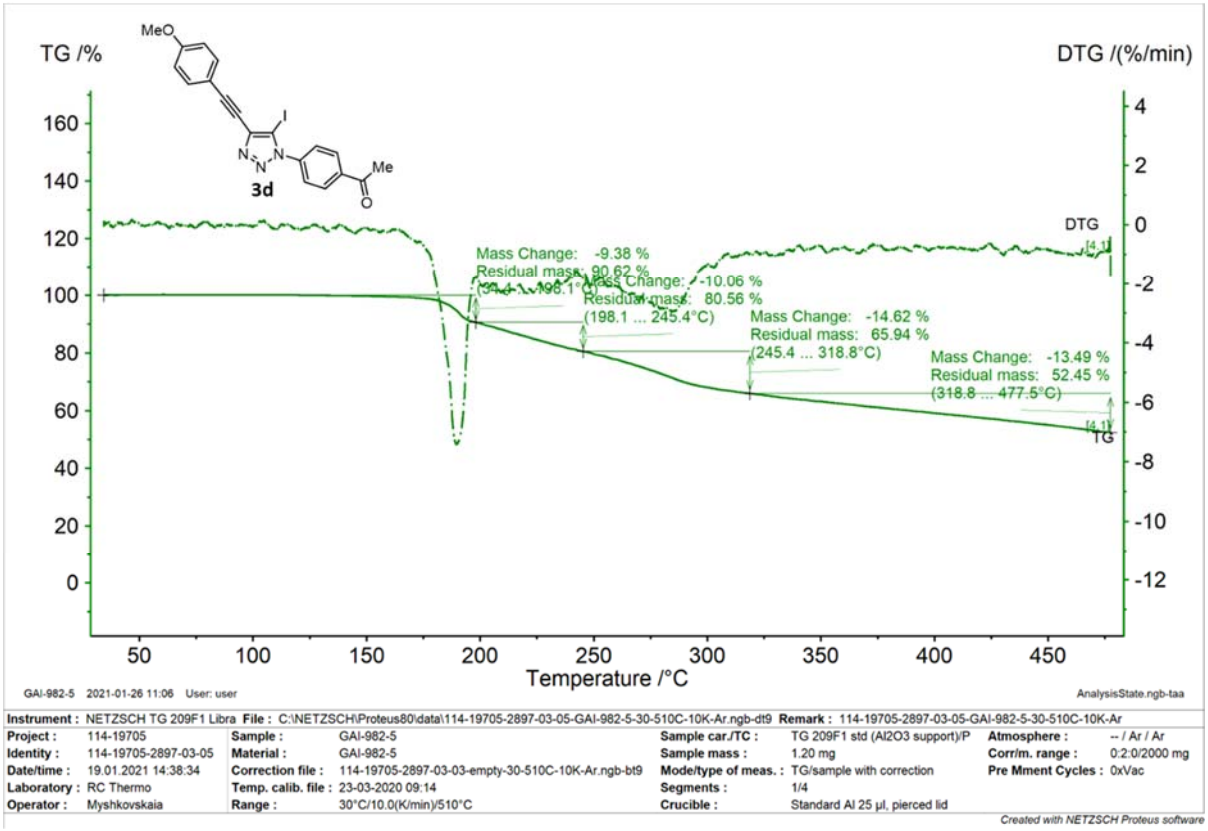


Figure S13. TG and DTG curves of triazole **3d**.

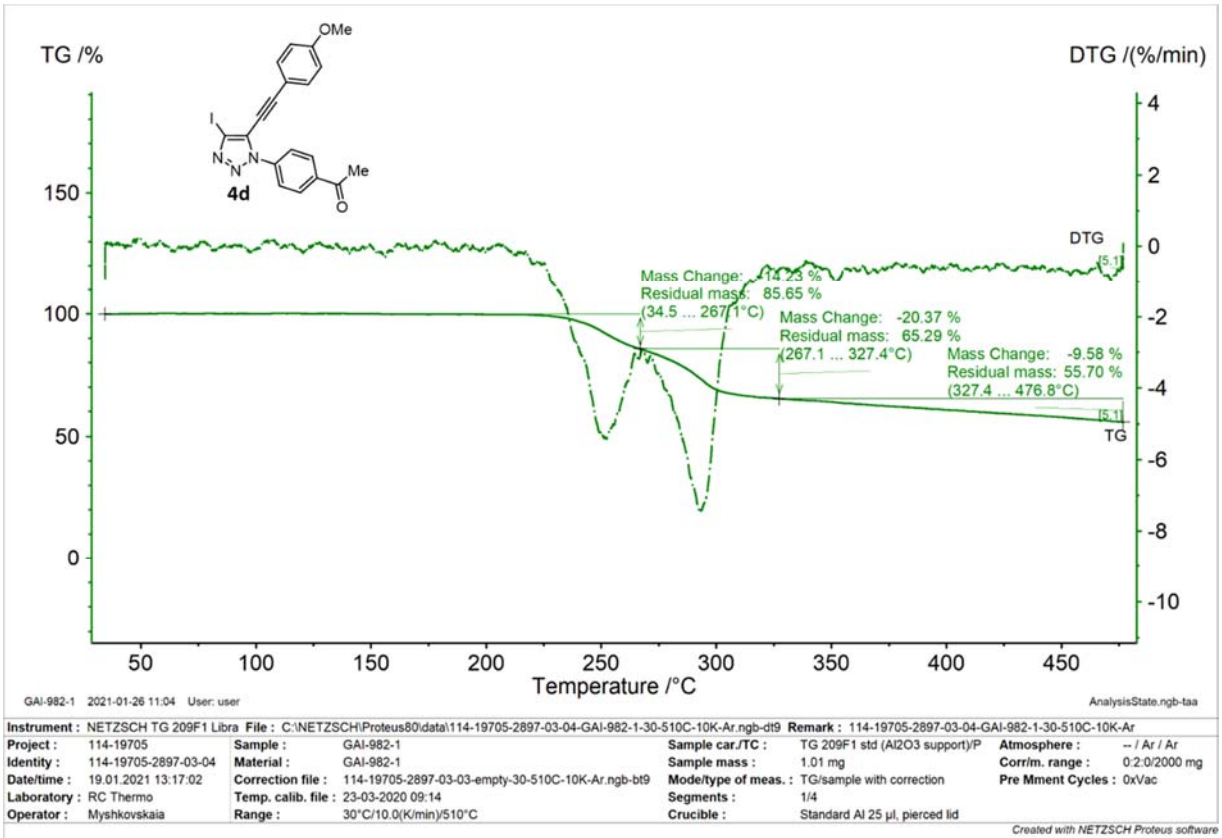


Figure S14. TG and DTG curves of triazole **4d**.

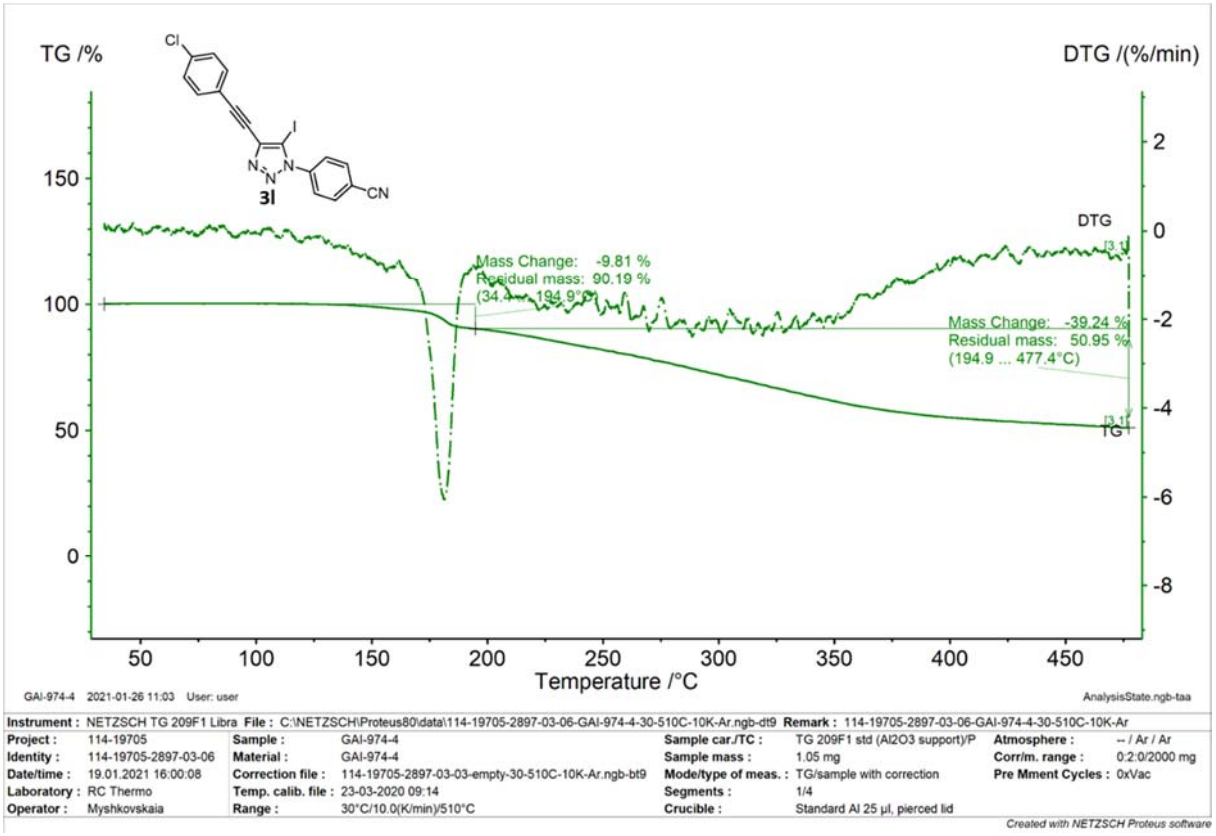


Figure S15. TG and DTG curves of triazole **3l**.

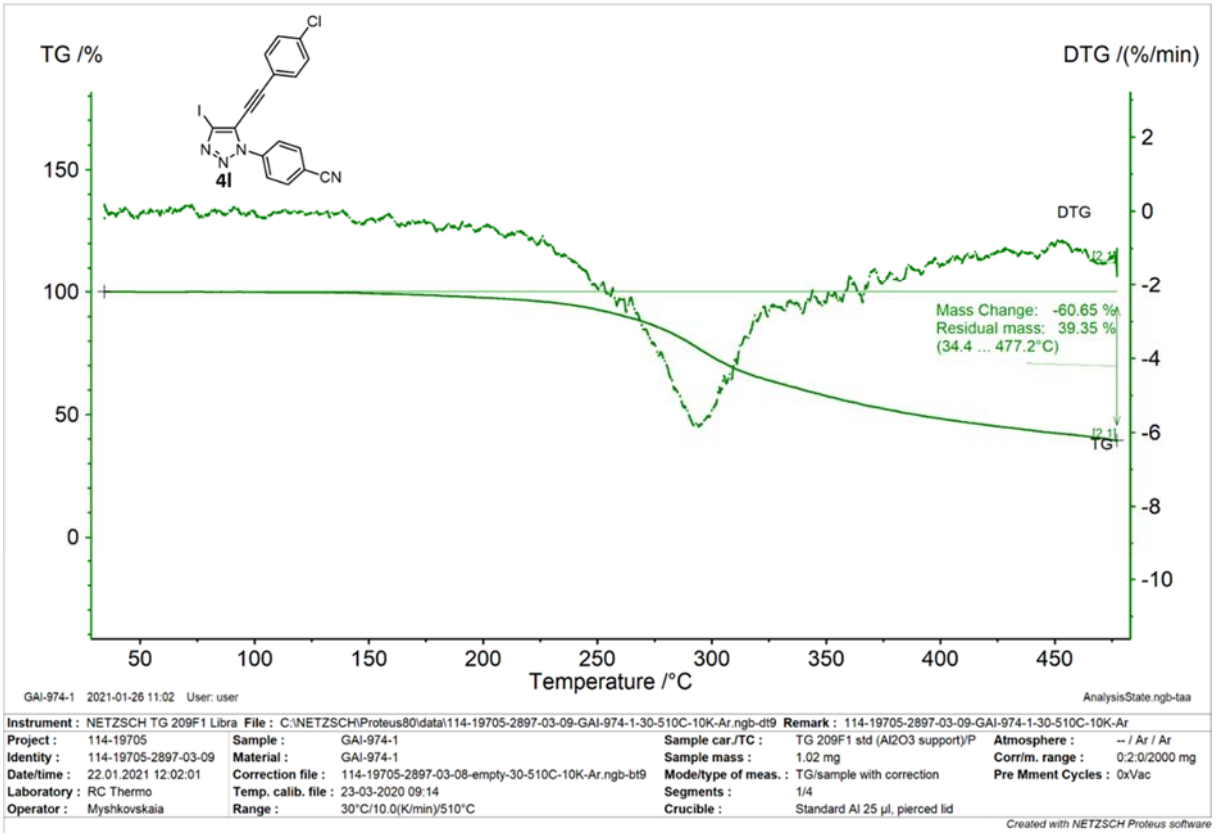


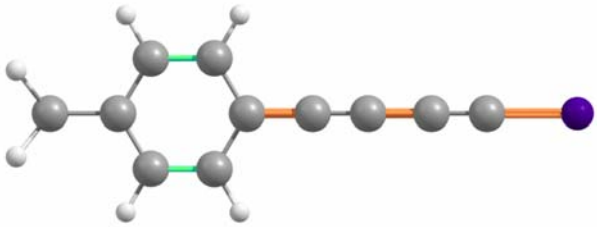
Figure S16. TG and DTG curves of triazole **4l**.

6 Computational details

6.1 Absolute Energies and Cartesian Coordinates of stationary points for starting materials, TSs and products

Table S4. Absolute Energies (au), Cartesian Coordinates of stationary points, M11/(Def2SVP for H,C,N,O,P; def2TZVP for I; LanL2DZ for Cu)

Alkyne 1a

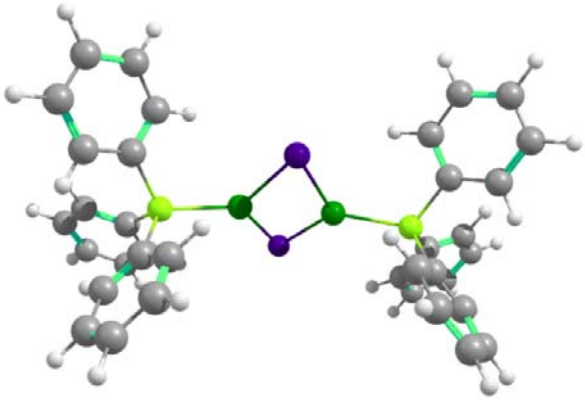


E= -720.244145
H (0K) = -720.105840
H (298K) = -720.093202
G (298K) = -720.147876

Imaginary frequency = 0.

C	-2.337016	-0.000138	-0.001108
C	-1.122218	-0.000237	-0.002590
I	-4.318992	0.000078	0.002196
C	0.261869	-0.000307	-0.003913
C	1.477396	-0.000329	-0.004544
C	2.914062	-0.000244	-0.004559
C	3.625402	1.209138	-0.006655
C	3.625723	-1.209407	-0.006650
C	5.015714	1.201600	-0.008657
C	5.016053	-1.201476	-0.008650
C	5.734318	0.000151	-0.006841
H	3.073601	2.156603	-0.009613
H	3.074210	-2.157039	-0.009602
H	5.561115	2.154649	-0.014390
H	5.561693	-2.154389	-0.014379
C	7.242362	0.000375	0.023171
H	7.609182	0.000541	1.066510
H	7.652513	-0.894670	-0.474373
H	7.652248	0.895435	-0.474566

$Cu_2I_2(PPh_3)_2$

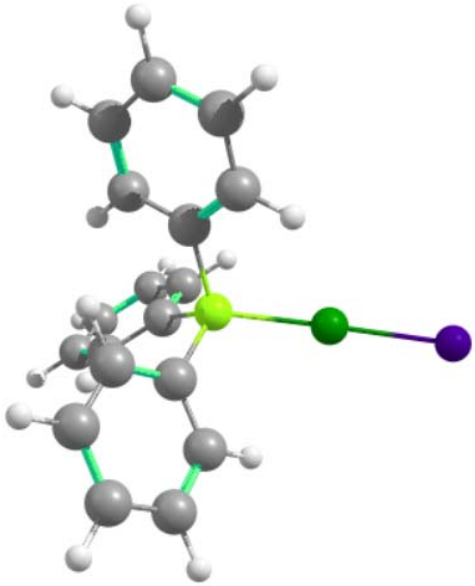
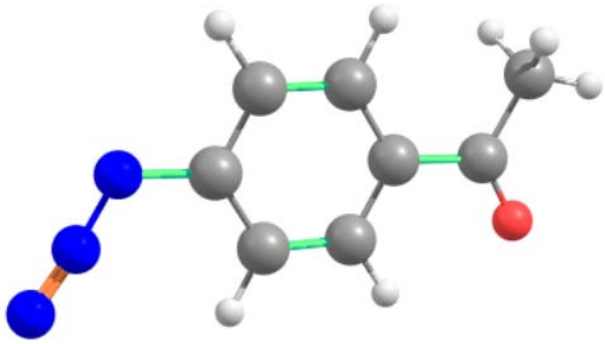


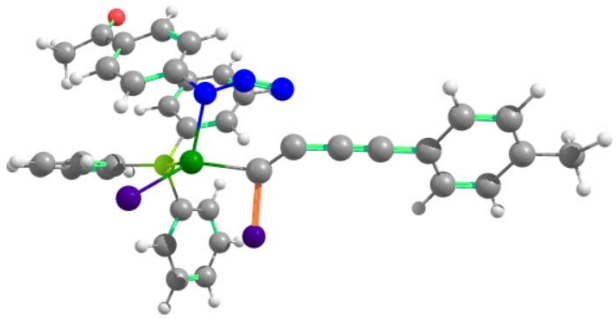
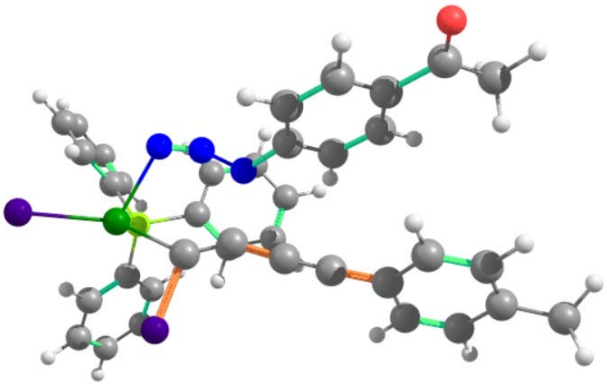
E= -3058.063508
H (0K) = -3057.510947
H (298K) = -3057.467419
G (298K) = -3057.600302

Imaginary frequency = 0.

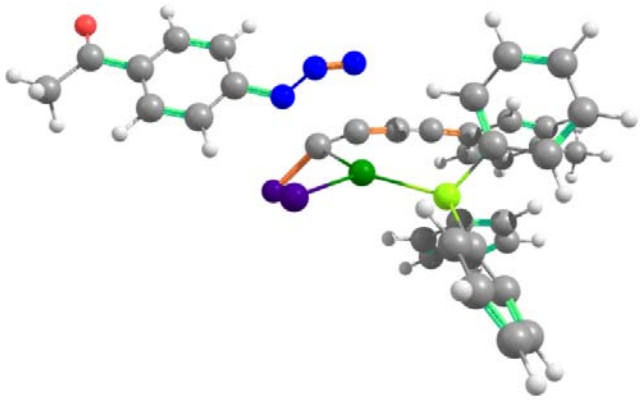
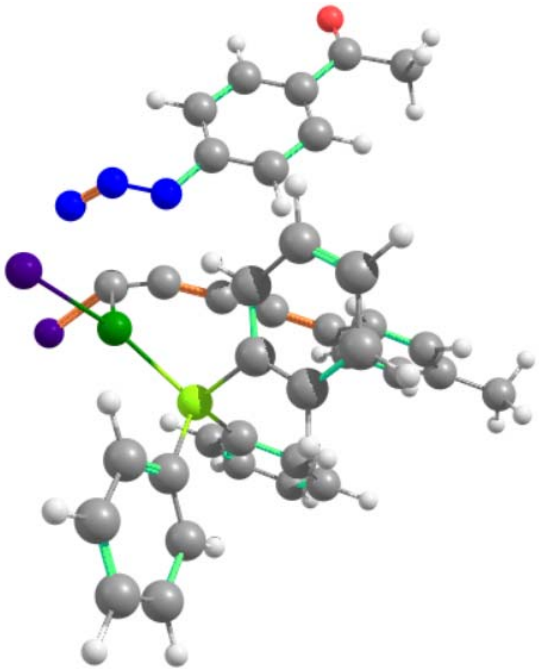
Cu	1.399678	-0.193321	-0.444612
P	3.695675	-0.029780	0.002524
C	4.003556	0.302809	1.779593
C	3.208147	1.282723	2.388857
C	4.987357	-0.355808	2.523462
C	3.410300	1.611440	3.727060
H	2.422946	1.788573	1.806026
C	5.179984	-0.027586	3.866270
H	5.604768	-1.132956	2.052848
C	4.396381	0.956089	4.466745
H	2.787162	2.381679	4.197822
H	5.951016	-0.547913	4.447914
H	4.550939	1.212338	5.522288
C	4.549587	1.362759	-0.822189
C	4.000581	1.880300	-1.999886
C	5.718042	1.926930	-0.294381
C	4.626912	2.939700	-2.656643
H	3.062654	1.463264	-2.393321
C	6.340708	2.984732	-0.951784
H	6.134887	1.538412	0.645675
C	5.796157	3.489495	-2.134241

	H 4.188210 3.345336 -3.576241 H 7.254034 3.425851 -0.534100 H 6.283535 4.328112 -2.647059 C 4.715618 -1.508911 -0.341066 C 5.994175 -1.456016 -0.904298 C 4.161336 -2.747800 0.009524 C 6.717345 -2.633383 -1.100990 H 6.427147 -0.490726 -1.197350 C 4.891814 -3.918770 -0.178167 H 3.143504 -2.794572 0.423951 C 6.170692 -3.862129 -0.733611 H 7.718377 -2.588041 -1.547410 H 4.451812 -4.884130 0.100094 H 6.742681 -4.785400 -0.889042 I 0.021117 -2.434415 -0.709606 Cu -1.404457 -0.225504 -0.454187 I -0.019264 2.066892 -0.547687 P -3.699437 -0.038608 -0.006350 C -4.770486 -1.461288 -0.427662 C -6.107356 -1.327415 -0.818654 C -4.208240 -2.737984 -0.301789 C -6.878241 -2.463342 -1.063418 C -4.984514 -3.870341 -0.541926 C -6.320093 -3.733471 -0.920305 H -6.547991 -0.329130 -0.939059 H -3.150033 -2.844405 -0.021474 H -7.925152 -2.353856 -1.372266 H -4.537349 -4.866805 -0.441494 H -6.929391 -4.625183 -1.113931 C -3.992880 0.210889 1.786383 C -4.950580 -0.501371 2.514082 C -3.203756 1.174510 2.429744 C -5.123887 -0.243248 3.875075 C -3.387030 1.433409 3.785584 C -4.347327 0.723929 4.509698 H -5.563610 -1.265593 2.017765 H -2.438465 1.723297 1.859213 H -5.874430 -0.806395 4.443462 H -2.768969 2.191036 4.282761 H -4.486590 0.924994 5.579228 C -4.507041 1.422852 -0.753415 C -3.970146 1.946978 -1.934109 C -5.628692 2.028595 -0.172864 C -4.564353 3.052182 -2.542870 C -6.220513 3.131838 -0.783470 C -5.690081 3.641468 -1.969940 H -3.065627 1.497655 -2.367917 H -6.033304 1.636268 0.770991 H -4.134763 3.461904 -3.464941

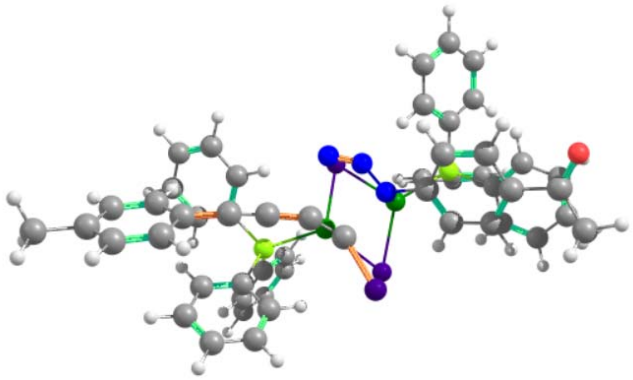
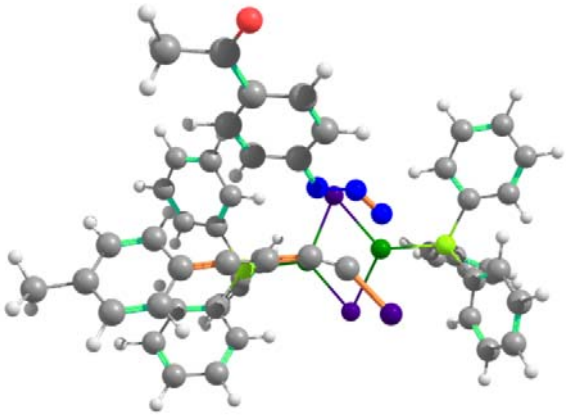
	H -7.098774 3.603496 -0.325835 H -6.153262 4.514774 -2.445870
$CuI(PPh_3)_3$  E= -1529.005482 H (0K) = -1528.729680 H (298K) = -1528.709402 G (298K) = -1528.783478 Imaginary frequency = 0. Cu 1.589924 -0.071940 0.108779 P -0.710628 -0.009956 0.016583 C -1.581517 -0.287005 1.600731 C -1.157925 -1.360536 2.395600 C -2.647032 0.512258 2.025390 C -1.808054 -1.642437 3.594215 H -0.308857 -1.980557 2.073111 C -3.289521 0.231469 3.231962 H -2.975864 1.362782 1.414124 C -2.874832 -0.845432 4.012994 H -1.472155 -2.484680 4.211165 H -4.121972 0.863783 3.564073 H -3.381408 -1.062886 4.961366 C -1.439130 -1.248459 -1.115263 C -0.746624 -1.530234 -2.299524 C -2.651629 -1.893614 -0.848178 C -1.270558 -2.438386 -3.216508 H 0.216310 -1.039202 -2.502590 C -3.168983 -2.806995 -1.766296 H -3.190213 -1.686498 0.086784	**Azide 2a**  E= -547.756116 H (0K) = -547.614200 H (298K) = -547.602920 G (298K) = -547.650869 Imaginary frequency = 0. N -4.363291 -1.069306 -0.189454 N -3.586089 -0.261375 -0.108341 N -2.827872 0.698008 -0.016649 C -1.439676 0.460326 0.020741 C -0.611658 1.581593 0.139339 C -0.880043 -0.823460 -0.053943 C 0.767001 1.419415 0.183634 C 0.499348 -0.971758 -0.009145 C 1.335951 0.142426 0.110242 H -1.076277 2.572188 0.195515 H -1.527580 -1.705160 -0.147671 H 1.405315 2.306710 0.277817 H 0.969294 -1.961585 -0.065286 C 2.820449 -0.099698 0.153252 O 3.257586 -1.224890 0.083152 C 3.737073 1.098473 0.285883 H 4.777993 0.743038 0.303909 H 3.516310 1.653267 1.215092 H 3.594117 1.790627 -0.562992

C -2.481761 -3.077117 -2.949481 H -0.723512 -2.655724 -4.141779 H -4.117277 -3.315084 -1.552561 H -2.890484 -3.798651 -3.667711 C -1.349981 1.594230 -0.584425 C -2.531884 1.695784 -1.327028 C -0.637407 2.751206 -0.247759 C -3.001832 2.948934 -1.716642 H -3.083827 0.787845 -1.606062 C -1.113501 4.002503 -0.635270 H 0.302909 2.672113 0.317192 C -2.296101 4.100872 -1.367969 H -3.926869 3.026317 -2.301012 H -0.551086 4.905847 -0.370072 H -2.667517 5.085503 -1.677871 I 4.032700 -0.050709 0.095646	
1,4-Ts (1a + 2a) Path A  E= -2796.992726 H (0K) = -2796.435085 H (298K) = -2796.389807 G (298K) = -2796.522004 Imaginary frequency = 1. Cu -0.417650 -2.459938 1.338202 C 0.211734 -0.487329 1.194302 C 1.064164 0.255350 1.783025 N 0.874551 -2.605753 3.040859 N 1.995293 -0.589710 3.084850 N 1.586851 -1.645433 3.337063 C 2.491485 4.050819 1.857605 C 3.732559 4.341646 2.443666 C 1.742028 5.093629 1.292891 C 4.205543 5.648530 2.463282	**1,5-Ts (1a + 2a) Path A**  E= -2796.992522 H (0K) = -2796.435373 H (298K) = -2796.389548 G (298K) = -2796.524819 Imaginary frequency = 1. Cu 1.919445 0.918371 -0.835690 C 0.123708 -0.071761 -1.335795 C -1.076488 -0.171259 -0.920586 N 0.571847 2.297111 0.402505 N -1.455492 1.157298 0.479969 N -0.482154 1.916267 0.544770 C -4.732039 -1.900947 -0.941390 C -4.918132 -3.261679 -0.655473 C -5.854472 -1.090740 -1.177270 C -6.200744 -3.795708 -0.608862

H	4.324477	3.528123	2.879697	H	-4.042918	-3.896610	-0.472270
C	2.227954	6.395844	1.319783	C	-7.131682	-1.638952	-1.124042
H	0.774522	4.869057	0.828453	H	-5.708734	-0.026598	-1.404332
C	3.462906	6.697015	1.906514	C	-7.327141	-2.997305	-0.842427
H	5.180497	5.863759	2.920250	H	-6.334936	-4.862025	-0.384049
H	1.634729	7.203433	0.870731	H	-8.003802	-0.999030	-1.315598
P	-2.784599	-2.496411	2.345118	P	2.508061	-0.308023	1.195543
C	-3.896048	-1.402803	1.371975	C	3.394007	-1.884600	0.932468
C	-4.192894	-1.834961	0.070875	C	4.282785	-1.913236	-0.150600
C	-4.370318	-0.167244	1.815673	C	3.253221	-3.012837	1.749001
C	-4.955023	-1.035238	-0.774436	C	5.035449	-3.059182	-0.403009
H	-3.800665	-2.799853	-0.286283	H	4.381480	-1.026991	-0.797953
C	-5.126464	0.637271	0.959259	C	4.000711	-4.159452	1.485434
H	-4.146938	0.178324	2.833337	H	2.546016	-2.997352	2.590486
C	-5.417277	0.207739	-0.332965	C	4.893197	-4.181228	0.412566
H	-5.182882	-1.380103	-1.790637	H	5.732933	-3.075257	-1.249366
H	-5.491893	1.610034	1.311028	H	3.886414	-5.044311	2.123897
H	-6.010549	0.842423	-1.003017	H	5.480815	-5.085214	0.208876
C	-2.757512	-1.736824	4.015645	C	0.989711	-0.747858	2.124029
C	-1.970352	-0.580206	4.147825	C	0.167596	-1.782576	1.653034
C	-3.382617	-2.263186	5.149568	C	0.547101	0.043802	3.192107
C	-1.835561	0.047839	5.383047	C	-1.060617	-2.037859	2.259931
H	-1.457800	-0.167188	3.264939	H	0.493452	-2.391244	0.795856
C	-3.238220	-1.638938	6.390996	C	-0.688418	-0.206478	3.789999
H	-3.969755	-3.188041	5.076725	H	1.180283	0.860969	3.564677
C	-2.470375	-0.482949	6.509001	C	-1.488563	-1.252790	3.332620
H	-1.226508	0.956735	5.468052	H	-1.691049	-2.855377	1.887013
H	-3.715143	-2.079703	7.275714	H	-1.021155	0.414612	4.631098
H	-2.359644	0.005971	7.484924	H	-2.451095	-1.461219	3.817645
C	-3.833958	-3.995850	2.492747	C	3.514292	0.609051	2.415397
C	-3.338001	-5.226697	2.052253	C	3.872931	1.924759	2.107665
C	-5.146559	-3.914965	2.981367	C	3.917411	0.039258	3.630912
C	-4.129284	-6.374377	2.145194	C	4.622845	2.671931	3.019442
H	-2.334698	-5.280927	1.605749	H	3.583541	2.357899	1.138068
C	-5.929685	-5.061789	3.083216	C	4.663061	0.787237	4.536060
H	-5.557119	-2.938171	3.275792	H	3.641883	-0.998653	3.866360
C	-5.416680	-6.295109	2.672035	C	5.013620	2.105851	4.229801
H	-3.736189	-7.334001	1.787117	H	4.908842	3.701141	2.770973
H	-6.952948	-4.992584	3.472458	H	4.978618	0.340623	5.487062
H	-6.036776	-7.197549	2.745073	H	5.604719	2.692828	4.944123
I	-0.237866	-4.404964	-0.372420	I	3.742435	2.207681	-2.049471
I	-0.960717	-0.090973	-0.446438	I	0.975155	-1.355015	-2.717530
C	3.968915	8.116689	1.960419	C	-8.712238	-3.593186	-0.826707
H	5.071368	8.149414	1.936337	H	-8.975466	-3.982469	-1.827741
H	3.583188	8.711482	1.115332	H	-8.778475	-4.433256	-0.114775
H	3.640354	8.609800	2.894238	H	-9.470261	-2.840394	-0.552100
C	1.996283	2.702181	1.834284	C	-2.315334	-0.811807	-0.959940
C	1.576959	1.563019	1.814492	C	-3.414455	-1.331260	-0.967823
C	0.227091	-3.361594	4.054061	C	-2.786312	1.655485	0.598572

C -0.401180 -4.538090 3.648976 H -0.272135 -4.885085 2.613270 C -1.215555 -5.210726 4.556261 H -1.755805 -6.104058 4.221482 C -1.375793 -4.724550 5.854443 C -2.416701 -5.275184 6.792120 O -2.560720 -4.792979 7.892719 C -3.318045 -6.374003 6.273220 H -2.729178 -7.267851 6.000406 H -3.844523 -6.031393 5.360622 H -4.047932 -6.633853 7.054178 C -0.645488 -3.604762 6.274425 H -0.779291 -3.259280 7.306897 C 0.151433 -2.911180 5.379490 H 0.677097 -1.997152 5.684103	C -3.171045 2.853392 -0.011011 C -4.500468 3.248160 0.063690 H -4.849622 4.178042 -0.401778 C -5.441400 2.449330 0.723558 C -5.037772 1.257558 1.332503 C -3.706371 0.857418 1.275557 H -3.360022 -0.074707 1.735404 H -5.764702 0.621483 1.852157 C -6.876983 2.917334 0.728266 O -7.173890 3.964131 0.204871 C -7.911207 2.031629 1.388667 H -7.679877 1.901639 2.460973 H -7.915283 1.029323 0.922782 H -8.899639 2.501351 1.277787 H -2.432686 3.459638 -0.552163
1,4-Ts (1a + 2a) Path B  E= -2797.005220 H (0K) = -2796.447598 H (298K) = -2796.401887 G (298K) = -2796.535716 Imaginary frequency = 1. Cu 0.244928 0.802232 -0.156502 C 1.447091 -1.247342 -0.451504 C 0.410850 -1.571720 0.183908 I 2.417291 -1.253710 -2.224438 P -2.108575 1.106929 -0.124413 C -2.624944 2.786477 -0.643916 C -1.866789 3.859231 -0.157442	**1,5-Ts (1a + 2a) Path B**  E= -2797.005824 H (0K) = -2796.447646 H (298K) = -2796.402280 G (298K) = -2796.534946 Imaginary frequency = 1. Cu -1.689935 -0.954001 -0.088511 C -0.526275 -2.192380 1.661941 C 0.349829 -1.373147 1.283813 I -2.055232 -2.618878 2.905944 P -1.637859 1.390026 -0.316511 C -3.200957 2.147706 -0.897174 C -3.844808 1.508731 -1.966740

C	-3.722379	3.032151	-1.476051	C	-3.761634	3.295522	-0.330371
C	-2.219685	5.166704	-0.482458	C	-5.028438	2.033461	-2.477157
H	-0.977687	3.667017	0.460244	H	-3.419267	0.587411	-2.393734
C	-4.069344	4.343765	-1.800690	C	-4.953586	3.811525	-0.843124
H	-4.304735	2.195451	-1.883875	H	-3.270751	3.788946	0.518585
C	-3.322398	5.410008	-1.301691	C	-5.582824	3.186483	-1.917384
H	-1.616471	6.000422	-0.103177	H	-5.526899	1.530220	-3.314489
H	-4.928849	4.532357	-2.455891	H	-5.392916	4.711298	-0.394963
H	-3.595174	6.440055	-1.563280	H	-6.518421	3.595696	-2.318477
C	-2.893277	0.930759	1.525332	C	-0.517109	1.695910	-1.739973
C	-2.174839	0.284004	2.537337	C	0.316965	0.653552	-2.161766
C	-4.168694	1.439081	1.803165	C	-0.502832	2.910808	-2.439411
C	-2.740115	0.114067	3.801920	C	1.189191	0.839861	-3.236180
H	-1.164310	-0.096242	2.336705	H	0.278576	-0.326712	-1.660902
C	-4.737769	1.255737	3.061762	C	0.382439	3.102463	-3.497857
H	-4.712071	2.002017	1.030828	H	-1.213021	3.705124	-2.169327
C	-4.025196	0.588585	4.060516	C	1.235625	2.069130	-3.891727
H	-2.167085	-0.392252	4.588177	H	1.826518	0.010229	-3.567805
H	-5.738648	1.652651	3.271632	H	0.391109	4.058523	-4.035727
H	-4.470346	0.453600	5.054242	H	1.920643	2.215663	-4.736237
C	-3.034753	-0.011843	-1.243072	C	-1.071154	2.487541	1.037890
C	-4.387132	-0.333126	-1.079898	C	-0.534164	3.763861	0.830116
C	-2.326181	-0.556192	-2.320656	C	-1.192911	2.001835	2.344608
C	-5.024774	-1.172950	-1.991679	C	-0.135917	4.545029	1.912729
H	-4.948130	0.056464	-0.220641	H	-0.404933	4.150989	-0.187888
C	-2.963471	-1.397428	-3.231211	C	-0.792820	2.782799	3.428508
H	-1.255553	-0.328070	-2.440211	H	-1.585103	0.987051	2.510688
C	-4.314779	-1.702514	-3.068690	C	-0.267382	4.056013	3.212545
H	-6.082295	-1.428485	-1.848385	H	0.291989	5.540047	1.737362
H	-2.398006	-1.819045	-4.071181	H	-0.889561	2.390036	4.448076
H	-4.816761	-2.367432	-3.782941	H	0.051829	4.669723	4.064492
I	1.946869	2.664939	-0.478601	I	-2.667542	-2.574995	-1.749112
C	-0.851908	-2.122808	0.371712	C	1.103148	-0.206147	1.248806
C	-1.981243	-2.555893	0.502145	C	1.731467	0.832604	1.178034
C	-3.338209	-3.025089	0.543151	C	2.398260	2.101142	1.104631
C	-4.260366	-2.484360	1.452951	C	2.551919	2.757103	-0.128458
C	-3.775147	-3.980186	-0.386571	C	2.846527	2.727333	2.276148
C	-5.591067	-2.885499	1.415274	C	3.133262	4.019306	-0.172646
C	-5.106308	-4.379902	-0.404341	C	3.433564	3.985821	2.213275
C	-6.037062	-3.838344	0.490856	C	3.584755	4.653911	0.992106
H	-3.929297	-1.729275	2.176393	H	2.188139	2.282157	-1.049664
H	-3.058830	-4.391644	-1.108068	H	2.712905	2.220142	3.239315
H	-6.305263	-2.445178	2.124215	H	3.236688	4.529516	-1.139929
H	-5.437759	-5.125453	-1.139643	H	3.777264	4.469643	3.137281
C	-7.475566	-4.291826	0.478335	N	1.230448	-2.463692	-0.401006
H	-7.611498	-5.169439	1.137550	N	0.617717	-3.515576	-0.127039
H	-8.149637	-3.496802	0.839867	N	-0.232160	-3.922972	0.528784
H	-7.794329	-4.586572	-0.536004	C	2.631411	-2.465657	-0.547640
N	1.078380	-1.129350	2.315583	C	3.233530	-1.267213	-0.944002

N 2.132502 -0.839667 1.965796 N 2.825784 -0.601502 0.975115 C 4.225803 -0.763902 0.904143 C 4.920837 0.067554 0.025106 C 4.889056 -1.746539 1.651401 C 6.296704 -0.096159 -0.112733 C 6.261805 -1.886243 1.514827 C 6.973658 -1.068293 0.628629 H 4.366554 0.847066 -0.514406 H 4.321594 -2.388442 2.337416 H 6.842195 0.561179 -0.800673 H 6.822783 -2.636434 2.085622 C 8.463316 -1.280965 0.527198 O 9.001335 -2.136869 1.189465 C 9.248400 -0.397394 -0.418051 H 9.129876 0.665289 -0.141324 H 10.309944 -0.680430 -0.362448 H 8.883701 -0.518461 -1.453560	C 3.416117 -3.597329 -0.279246 C 4.618462 -1.195176 -1.048772 C 4.794554 -3.515963 -0.404465 C 5.409398 -2.316163 -0.781820 H 2.605266 -0.396709 -1.158289 H 2.934986 -4.537992 0.016544 H 5.078038 -0.245386 -1.349010 H 5.438110 -4.382728 -0.208941 C 6.911833 -2.301511 -0.884731 O 7.548477 -3.301076 -0.646967 C 7.587492 -1.008082 -1.288914 H 8.675302 -1.171149 -1.306734 H 7.242360 -0.688962 -2.288477 H 7.341293 -0.202968 -0.573957 C 4.243205 6.009340 0.926665 H 3.817621 6.622344 0.113945 H 4.127842 6.558208 1.876507 H 5.326704 5.904700 0.731133
1,4-Ts (1a + 2a) Path C  E= -4326.078048 H (0K) = -4325.244027 H (298K) = -4325.176233 G (298K) = -4325.365866 Imaginary frequency = 1. Cu 1.024125 -0.725193 -0.435185 C 0.830811 2.201268 -0.284302 C 1.727901 1.960664 0.555385 I 0.357378 3.135546 -2.000052 P 3.322824 -1.189226 -0.664587 C 3.513169 -2.642922 -1.761761 C 2.527546 -3.634217 -1.665584 C 4.565682 -2.794884 -2.669985 C 2.609267 -4.777833 -2.456016 H 1.682232 -3.501567 -0.972415 C 4.640378 -3.940686 -3.462734 H 5.324966 -2.006125 -2.766057	**1,5-Ts (1a + 2a) Path C**  E= -4326.076476 H (0K) = -4325.241735 H (298K) = -4325.174055 G (298K) = -4325.362823 Imaginary frequency = 1. Cu -0.530808 -0.894778 -0.234580 C 0.211755 1.569588 1.447165 C -0.969207 1.710344 1.053003 I 1.506403 1.146514 2.928537 P -2.748227 -1.639059 -0.411027 C -2.718348 -3.391873 -0.952558 C -1.818188 -3.714316 -1.978181 C -3.510766 -4.393565 -0.385358 C -1.733575 -5.022588 -2.445772

C	3.665926	-4.932300	-3.353540	H	-1.170490	-2.933165	-2.405924
H	1.832510	-5.548247	-2.378569	C	-3.416874	-5.705240	-0.854199
H	5.465354	-4.055928	-4.176759	H	-4.197675	-4.154725	0.436944
H	3.725551	-5.830021	-3.981597	C	-2.534039	-6.019620	-1.884901
C	4.173023	-1.696023	0.878104	H	-1.026173	-5.267652	-3.247360
C	3.596373	-1.320872	2.097444	H	-4.037187	-6.489217	-0.402273
C	5.346949	-2.460765	0.876018	H	-2.459743	-7.052136	-2.248443
C	4.193233	-1.696021	3.301432	C	-3.688746	-0.821220	-1.757933
H	2.663935	-0.739762	2.104898	C	-3.199270	0.396291	-2.244629
C	5.952107	-2.818841	2.079545	C	-4.828144	-1.389356	-2.342919
H	5.782081	-2.790585	-0.078388	C	-3.863222	1.056503	-3.280382
C	5.373650	-2.438078	3.292817	H	-2.277465	0.822120	-1.818271
H	3.726371	-1.407015	4.250654	C	-5.503064	-0.718060	-3.359962
H	6.872747	-3.415460	2.071423	H	-5.174055	-2.380225	-2.015914
H	5.842660	-2.733778	4.239712	C	-5.022722	0.507822	-3.826667
C	4.373781	0.106029	-1.414280	H	-3.461296	2.001661	-3.667576
C	5.720551	0.300405	-1.096837	H	-6.397622	-1.165791	-3.810243
C	3.735595	0.987644	-2.296803	H	-5.543906	1.025659	-4.641707
C	6.418633	1.379583	-1.638856	C	-3.828473	-1.647886	1.069005
H	6.225218	-0.368559	-0.387982	C	-5.223967	-1.750473	1.014137
C	4.436653	2.059417	-2.843703	C	-3.191039	-1.579786	2.313032
H	2.670556	0.839562	-2.535588	C	-5.970448	-1.803329	2.188871
C	5.776827	2.261168	-2.507091	H	-5.740154	-1.772723	0.046200
H	7.467214	1.542764	-1.356520	C	-3.941211	-1.629413	3.488473
H	3.927382	2.751842	-3.525864	H	-2.095053	-1.481999	2.357492
H	6.323560	3.116781	-2.923008	C	-5.328885	-1.747282	3.426709
I	-0.642415	-0.755752	-2.556987	H	-7.064284	-1.876973	2.135949
C	3.041172	2.000776	1.016934	H	-3.432935	-1.577714	4.459084
C	4.206674	2.061029	1.358621	H	-5.917491	-1.787647	4.352161
C	5.608118	2.172996	1.659213	I	1.174402	-2.422652	1.152535
C	6.339522	1.071338	2.128956	C	-2.357669	1.665010	1.082137
C	6.276880	3.380552	1.412285	C	-3.573435	1.636621	1.111605
C	7.710133	1.182756	2.333262	C	-5.005024	1.563665	1.190936
C	7.647200	3.479626	1.630976	C	-5.789232	1.425314	0.034343
C	8.387615	2.385182	2.092576	C	-5.633719	1.593415	2.444589
H	5.827608	0.119611	2.313570	C	-7.169775	1.297414	0.142544
H	5.709836	4.238282	1.031120	C	-7.015440	1.477578	2.535020
H	8.271174	0.308918	2.691795	C	-7.805647	1.317062	1.390118
H	8.159637	4.430231	1.431682	H	-5.308429	1.397426	-0.951828
C	9.869650	2.499609	2.349976	H	-5.020761	1.696598	3.348281
H	10.303655	3.362781	1.817926	H	-7.771500	1.180943	-0.769107
H	10.067715	2.635933	3.429359	H	-7.496974	1.504255	3.521870
H	10.402366	1.587889	2.028637	C	-9.299884	1.146739	1.501752
N	0.597459	1.286136	2.294178	H	-9.702423	1.690043	2.373739
N	-0.430757	1.337485	1.792239	H	-9.812244	1.513725	0.596155
N	-0.992099	1.470655	0.679931	H	-9.561886	0.079206	1.624635
C	-2.193195	2.209540	0.557629	N	-0.663906	2.831517	-0.830013
C	-2.769640	2.264259	-0.715004	N	0.569139	2.861544	-0.688243
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C -3.891705 3.060921 -0.918942	Cu 2.131712 -0.427526 -0.361320
C -3.935770 3.618178 1.432094	I 0.662637 -0.176217 -2.569209
C -4.477103 3.745980 0.148014	P 4.390512 0.124413 -0.128654
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H -2.343838 2.789872 2.643503	C 5.155263 1.925537 1.915881
H -4.333310 3.108180 -1.922202	C 4.834605 -0.385776 2.560556
H -4.438683 4.134896 2.258827	C 5.355054 2.266303 3.254865
C -5.707738 4.596720 -0.012672	C 5.036176 -0.041651 3.894728
O -6.341917 4.941761 0.958327	C 5.292870 1.286811 4.244564
C -6.097585 5.025773 -1.410817	H 5.186277 2.704122 1.142136
H -6.337312 4.145320 -2.031668	H 4.605711 -1.426678 2.287960
H -6.975876 5.685413 -1.345921	H 5.554395 3.310373 3.526033
H -5.258183 5.557683 -1.893149	H 4.985704 -0.816936 4.669350
Cu -1.732180 -0.873508 -0.134277	H 5.447603 1.558148 5.296355
I -0.096402 -2.203477 1.557586	C 5.381271 -1.378149 -0.476269
P -4.005112 -1.100810 0.436516	C 6.672157 -1.572216 0.030978
C -5.259458 -0.024145 -0.354342	C 4.802512 -2.359694 -1.289186
C -6.144356 0.790374 0.354920	C 7.380499 -2.728541 -0.285719
C -5.291014 -0.026048 -1.757831	C 5.516262 -3.514713 -1.608075
C -7.076595 1.574061 -0.331589	C 6.804064 -3.698061 -1.108628
C -6.227445 0.745892 -2.438273	H 7.118518 -0.820485 0.696880
C -7.128833 1.541154 -1.723346	H 3.777197 -2.225411 -1.666690
H -6.107308 0.822413 1.451803	H 8.389979 -2.878157 0.116735
H -4.576170 -0.648219 -2.318320	H 5.054014 -4.281008 -2.241900
H -7.765263 2.215713 0.233532	H 7.362079 -4.610520 -1.353236
H -6.258519 0.723923 -3.534889	C 5.086825 1.418259 -1.218860
H -7.878044 2.138818 -2.258926	C 4.234479 2.012143 -2.154206
C -4.583261 -2.777777 -0.038600	C 6.433733 1.801814 -1.164306
C -5.909736 -3.053018 -0.393579	C 4.725226 2.983951 -3.028841
C -3.638550 -3.811381 -0.034562	C 6.918619 2.773826 -2.034187
C -6.287616 -4.352023 -0.728468	C 6.063155 3.364707 -2.967822
C -4.022531 -5.109851 -0.366544	H 3.180211 1.702886 -2.202114
C -5.345191 -5.380799 -0.713159	H 7.106537 1.337416 -0.429867
H -6.651158 -2.242052 -0.421565	H 4.053068 3.441559 -3.765002
H -2.592034 -3.596657 0.228351	H 7.973202 3.072317 -1.987477
H -7.327162 -4.561692 -1.009384	H 6.448205 4.128672 -3.654967
H -3.276198 -5.913525 -0.361475	C -1.388796 4.007560 -1.101283
H -5.644780 -6.401663 -0.981324	C -0.780870 5.272381 -1.126161
C -4.369934 -0.992664 2.227149	C -2.765247 3.883962 -1.313635
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C -5.582526 -1.438497 2.768803	C -3.531937 5.023309 -1.534086
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C -5.824059 -1.318743 4.134376	H 0.300822 5.360704 -0.964894
C -4.853409 -0.760063 4.969731	H -3.223779 2.891191 -1.292502
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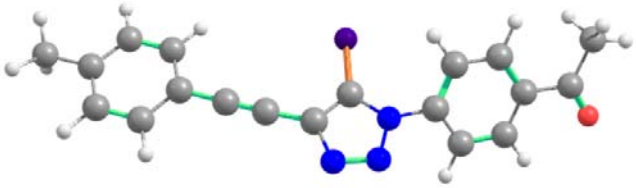
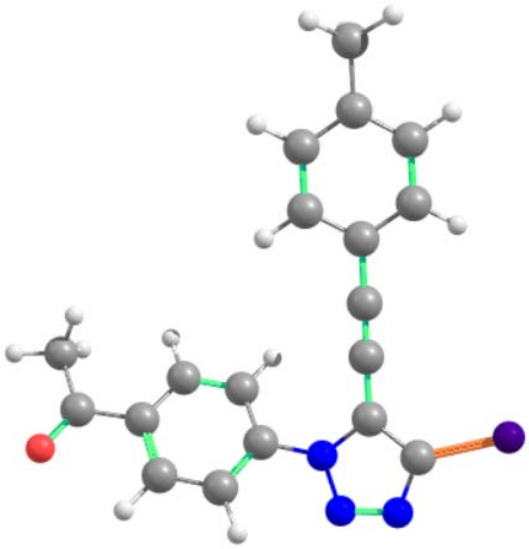
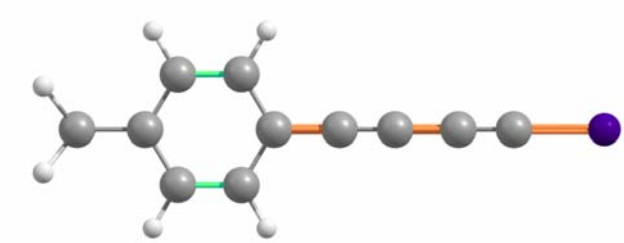
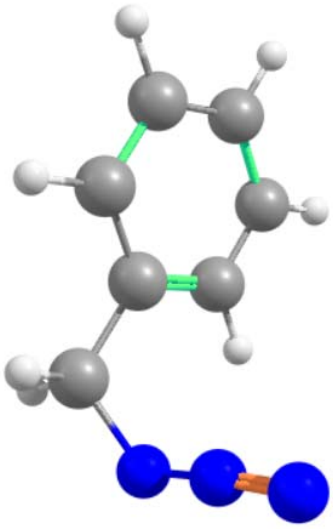
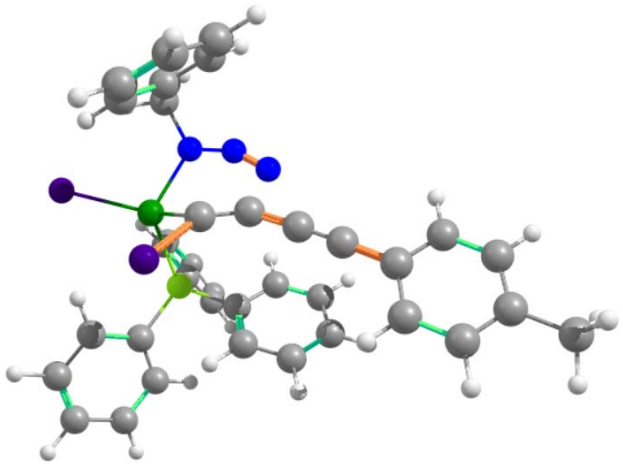
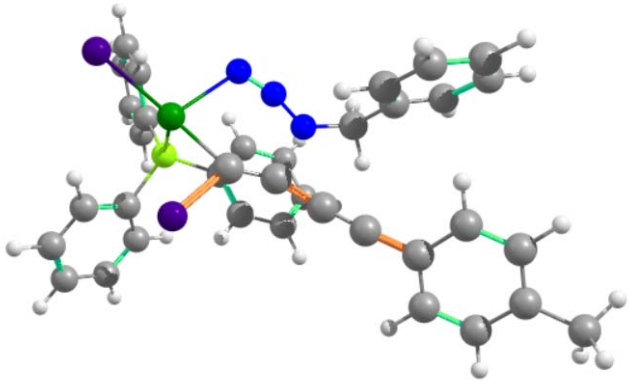
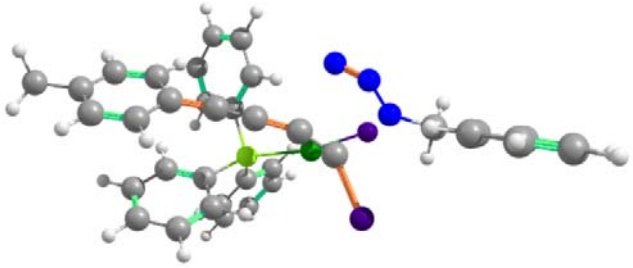
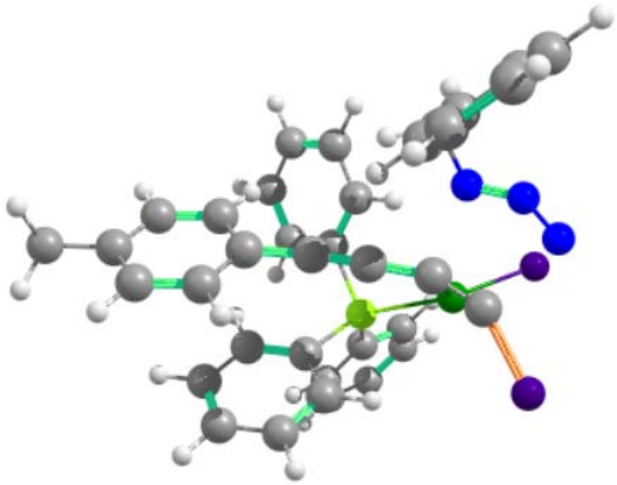
H -5.044311 -0.671266 6.046535	C -5.212010 7.445517 -1.995719

	H -5.621133 8.456004 -2.142876 H -5.444050 6.818767 -2.875302 H -5.682005 6.975734 -1.113641
1,4-Triazole 3a  E= -1268.115553 H (0K) = -1267.829386 H (298K) = -1267.807669 G (298K) = -1267.883630 Imaginary frequency = 0. C -0.267439 0.435998 0.125675 C 0.750284 1.377416 0.168420 I -0.109680 -1.589764 -0.133083 C 2.156668 1.139713 0.127893 C 3.339581 0.877158 0.089437 C 4.738988 0.548126 0.045281 C 5.715783 1.554152 0.029728 C 5.144254 -0.794491 0.022859 C 7.064488 1.217013 -0.009389 C 6.495719 -1.116983 -0.016302 C 7.478323 -0.119764 -0.035983 H 5.403745 2.605094 0.051896 H 4.383543 -1.584364 0.039838 H 7.819988 2.013999 -0.017194 H 6.800315 -2.172060 -0.029659 C 8.941783 -0.477002 -0.111890 H 9.146431 -1.435515 0.394609 H 9.262138 -0.581096 -1.165380 H 9.568775 0.303232 0.351863 N 0.169819 2.607721 0.242137 N -1.102989 2.477495 0.246230 N -1.405788 1.175311 0.181324 C -2.775717 0.780321 0.163564 C -3.217053 -0.268603 0.967627 C -3.658529 1.492907 -0.649891 C -4.561845 -0.628277 0.932502 C -4.998260 1.130802 -0.667535 C -5.457107 0.065513 0.114694 H -2.515477 -0.789012 1.629013 H -3.276028 2.326478 -1.249498	**1,5-Triazole 4a**  E= -1268.120066 H (0K) = -1267.833796 H (298K) = -1267.811193 G (298K) = -1267.890625 Imaginary frequency = 0. C 1.625698 -2.272194 -0.032146 C 0.662696 -1.273724 -0.068725 I 3.665200 -2.044865 0.037137 C 0.782641 0.140548 -0.033543 C 0.906075 1.346685 0.006911 C 1.023037 2.778012 0.054310 C -0.119596 3.572179 0.230798 C 2.275267 3.397710 -0.069067 C -0.005709 4.956844 0.278045 C 2.373452 4.783040 -0.018432 C 1.238572 5.585992 0.152376 H -1.098331 3.088460 0.338730 H 3.170877 2.779020 -0.201328 H -0.905860 5.568972 0.422140 H 3.358996 5.258218 -0.110967 C 1.353034 7.089501 0.175308 H 2.302824 7.410689 0.635497 H 1.326585 7.495517 -0.853020 H 0.520751 7.545870 0.737047 N -0.507936 -1.980692 -0.087338

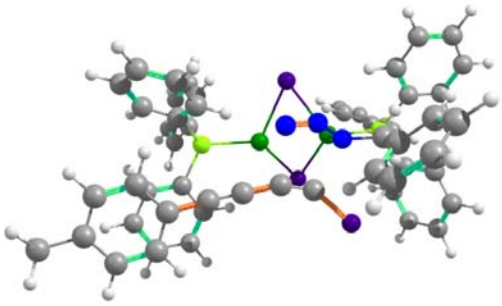
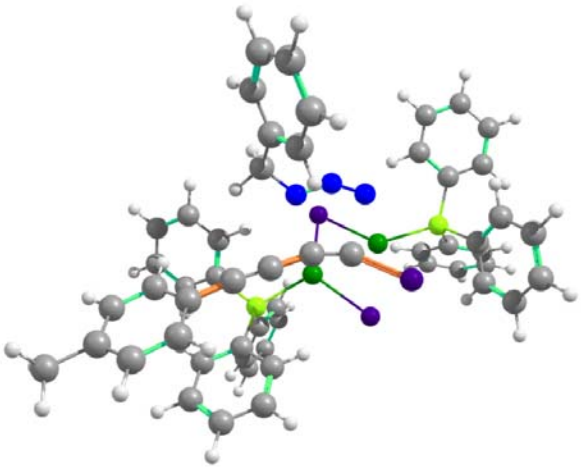
H -4.909289 -1.454092 1.564954 H -5.727003 1.660682 -1.293041 C -6.925320 -0.278654 0.036401 O -7.655852 0.351916 -0.689550 C -7.438283 -1.420938 0.886366 H -8.517216 -1.536171 0.705530 H -7.259980 -1.215381 1.956939 H -6.915308 -2.359528 0.630519	N -0.263008 -3.287432 -0.056356 N 1.009038 -3.470614 -0.025542 C -1.853671 -1.513421 -0.102160 C -2.818275 -2.252533 0.586932 H -2.515051 -3.164220 1.112832 C -4.134720 -1.813994 0.577532 H -4.923771 -2.362109 1.106778 C -4.491977 -0.647084 -0.106504 C -5.940740 -0.226981 -0.065599 O -6.745921 -0.887070 0.546341 C -6.342136 1.030143 -0.807316 H -6.116110 0.931765 -1.884132 H -5.783940 1.902295 -0.422957 H -7.421572 1.190059 -0.668273 C -3.515142 0.074039 -0.797597 H -3.781309 0.981496 -1.353210 C -2.190873 -0.357776 -0.805359 H -1.426527 0.191608 -1.365519
Alkyne 1a  E= -720.244145 H (0K) = -720.105840 H (298K) = -720.093202 G (298K) = -720.147876 Imaginary frequency = 0. C -2.337016 -0.000138 -0.001108 C -1.122218 -0.000237 -0.002590 I -4.318992 0.000078 0.002196 C 0.261869 -0.000307 -0.003913 C 1.477396 -0.000329 -0.004544 C 2.914062 -0.000244 -0.004559 C 3.625402 1.209138 -0.006655 C 3.625723 -1.209407 -0.006650 C 5.015714 1.201600 -0.008657 C 5.016053 -1.201476 -0.008650 C 5.734318 0.000151 -0.006841 H 3.073601 2.156603 -0.009613 H 3.074210 -2.157039 -0.009602	**Azide 8**  E= -434.549496 H (0K) = -434.416646 H (298K) = -434.407352 G (298K) = -434.451565 Imaginary frequency = 0. N 2.674374 1.073842 1.236025 N 2.439537 0.399786 0.364964 N 2.269393 -0.279784 -0.638729 C 1.142823 -1.215260 -0.618105 H 1.121030 -1.673776 -1.621644

H 5.561115 2.154649 -0.014390 H 5.561693 -2.154389 -0.014379 C 7.242362 0.000375 0.023171 H 7.609182 0.000541 1.066510 H 7.652513 -0.894670 -0.474373 H 7.652248 0.895435 -0.474566	H 1.331459 -2.032726 0.106888 C -0.191335 -0.558750 -0.312157 C -0.478365 0.721826 -0.795609 C -1.155719 -1.233327 0.440344 C -1.712382 1.313835 -0.534624 C -2.393336 -0.644176 0.697911 C -2.673702 0.631320 0.211067 H 0.280594 1.256935 -1.382079 H -0.932676 -2.234412 0.834199 H -1.926160 2.319664 -0.916867 H -3.141276 -1.184137 1.291709 H -3.644010 1.098741 0.419010
1,4-Ts (8 + 1a) Path A  E= -2683.796297 H (0K) = -2683.247405 H (298K) = -2683.204951 G (298K) = -2683.335675 Imaginary frequency = 1. Cu 1.926152 1.557714 -0.312890 C 0.056254 0.885261 -1.037312 C -1.071382 0.853474 -0.451424 N 0.723884 3.215050 0.141126 N -1.271066 2.240692 0.764809 N -0.390960 2.981618 0.613452 C -4.535909 -1.209108 -0.082612 C -4.596857 -2.534950 -0.538863 C -5.655523 -0.658377 0.558850 C -5.753423 -3.285083 -0.356144 H -3.721089 -2.968340 -1.037631 C -6.805656 -1.419581 0.733765 H -5.610343 0.375410 0.921615	**1,5-Ts (8 + 1a) Path A**  E= -2683.796837 H (0K) = -2683.248314 H (298K) = -2683.204598 G (298K) = -2683.335052 Imaginary frequency = 1. Cu 1.929741 0.915137 -0.822746 C 0.150442 -0.105424 -1.423873 C -1.057573 -0.196496 -1.052619 N 0.551225 2.357826 0.471735 N -1.435415 1.151256 0.423157 N -0.478720 1.898105 0.556339 C -4.885686 -1.473463 -1.214834 C -5.295102 -2.798846 -1.005721 C -5.848445 -0.489490 -1.490965 C -6.642864 -3.128971 -1.078763 H -4.543733 -3.567690 -0.789342 C -7.193551 -0.835848 -1.553938 H -5.527652 0.547916 -1.653743 C -7.613020 -2.156936 -1.355863

C	-6.877159	-2.741986	0.278709	H	-6.955112	-4.169039	-0.916126
H	-5.788362	-4.322112	-0.715887	H	-7.939818	-0.059012	-1.767209
H	-7.674618	-0.977960	1.239589	P	2.447408	-0.319497	1.209034
P	2.208505	-0.325728	1.218829	C	3.280150	-1.932007	0.985718
C	3.350707	-1.653877	0.680762	C	4.185980	-2.013866	-0.080184
C	4.149749	-1.424877	-0.443157	C	3.080813	-3.041295	1.816241
C	3.461788	-2.865229	1.377876	C	4.898003	-3.191988	-0.300667
C	5.052926	-2.401743	-0.867947	H	4.328928	-1.143674	-0.740495
H	4.074679	-0.469076	-0.981900	C	3.787327	-4.220351	1.584874
C	4.359493	-3.837645	0.948741	H	2.359594	-2.985242	2.643858
H	2.830573	-3.051574	2.257971	C	4.697624	-4.294401	0.529761
C	5.156013	-3.605288	-0.175920	H	5.608990	-3.249257	-1.133926
H	5.680451	-2.212683	-1.747402	H	3.626618	-5.089531	2.234767
H	4.441942	-4.784977	1.495732	H	5.253069	-5.223568	0.350739
H	5.864758	-4.372937	-0.511366	C	0.900460	-0.699035	2.117406
C	0.653963	-1.209113	1.617363	C	0.048608	-1.702174	1.631420
C	0.265615	-2.337662	0.885031	C	0.468117	0.109178	3.176999
C	-0.232840	-0.669227	2.559659	C	-1.204343	-1.904346	2.206860
C	-0.973714	-2.934754	1.117646	H	0.370481	-2.326786	0.784501
H	0.941153	-2.758209	0.127548	C	-0.790672	-0.090342	3.746278
C	-1.469064	-1.269897	2.789791	H	1.126011	0.900091	3.563242
H	0.050646	0.229308	3.126464	C	-1.626474	-1.098831	3.266583
C	-1.839454	-2.408832	2.074674	H	-1.858786	-2.695512	1.819421
H	-1.263637	-3.822983	0.541976	H	-1.113274	0.540014	4.584962
H	-2.152302	-0.839344	3.532188	H	-2.610381	-1.263579	3.724343
H	-2.816247	-2.877175	2.251526	C	3.459636	0.578092	2.438430
C	2.861062	0.209465	2.847087	C	3.825311	1.895299	2.145581
C	3.575555	1.412636	2.885868	C	3.854873	-0.006005	3.649712
C	2.702334	-0.540852	4.019888	C	4.574278	2.629486	3.068587
C	4.130909	1.857518	4.086392	H	3.541284	2.340243	1.179745
H	3.708008	2.000988	1.965010	C	4.600683	0.728904	4.565494
C	3.254163	-0.090727	5.216281	H	3.574631	-1.045263	3.873016
H	2.128932	-1.477946	3.999044	C	4.958072	2.049023	4.274541
C	3.969481	1.108496	5.249800	H	4.865536	3.660018	2.831962
H	4.693201	2.798984	4.107370	H	4.911000	0.270660	5.512691
H	3.124727	-0.679873	6.132633	H	5.549327	2.625873	4.996966
H	4.403701	1.460080	6.194137	I	3.727489	2.258729	-2.008883
I	4.151263	2.585122	-1.160260	I	1.084788	-1.311651	-2.811567
I	0.857952	-0.237126	-2.548677	C	-9.069162	-2.532810	-1.466763
C	-8.140738	-3.548941	0.443716	H	-9.327770	-3.344299	-0.765423
H	-8.677099	-3.267879	1.365951	H	-9.723018	-1.669173	-1.259309
H	-8.825765	-3.374835	-0.406974	H	-9.298976	-2.889484	-2.488009
H	-7.923775	-4.629824	0.481643	C	-2.346965	-0.719486	-1.103595
C	-2.296876	0.179093	-0.358993	C	-3.500351	-1.103084	-1.147188
C	-3.334437	-0.440747	-0.247143	C	-3.693502	2.150505	0.078584
C	0.858731	4.425282	-0.713979	C	-3.342285	2.492597	-1.228512
H	0.509051	5.296031	-0.130383	C	-4.255303	3.156557	-2.049957
H	1.938127	4.521661	-0.912281	H	-3.967342	3.419399	-3.075066
C	0.061554	4.231615	-1.982087	C	-5.522681	3.483485	-1.571885

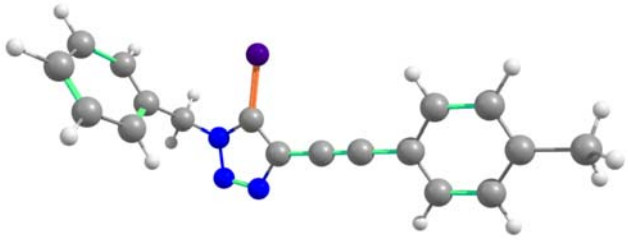
C 0.667329 3.636662 -3.092959 H 1.737957 3.385134 -3.052057 C -0.090356 3.348671 -4.226012 H 0.388231 2.881712 -5.095814 C -1.453663 3.645378 -4.252931 H -2.048303 3.412997 -5.145094 C -2.060534 4.239248 -3.146761 H -3.131388 4.476092 -3.166283 C -1.302954 4.532647 -2.013857 H -1.778932 5.000984 -1.140164	C -5.876516 3.145689 -0.263971 C -4.966267 2.482068 0.555154 H -5.250220 2.212777 1.581870 H -6.870660 3.402624 0.122057 H -2.350924 2.229098 -1.620481 H -6.237209 4.007756 -2.218197 C -2.752633 1.388940 0.995389 H -3.168330 0.387679 1.208261 H -2.635234 1.904238 1.967031
1,4-Ts (8 + 1a) Path B  E= -2683.808580 H (0K) = -2683.259240 H (298K) = -2683.216000 G (298K) = -2683.342824 Imaginary frequency = 1. Cu 0.570356 0.815407 -0.042623 C 1.807655 -1.232195 -0.259002 C 0.746138 -1.552337 0.331304 I 2.779951 -1.103821 -2.041244 P -1.747440 1.098717 -0.426483 C -2.235128 2.694134 -1.182803 C -1.630670 3.846047 -0.659028 C -3.140056 2.804060 -2.242592 C -1.947151 5.096680 -1.181534 H -0.896070 3.757005 0.155709 C -3.448645 4.061575 -2.765570 H -3.603859 1.905202 -2.668942 C -2.857450 5.206001 -2.234768 H -1.468837 5.992945 -0.768212 H -4.157195 4.143609 -3.599186 H -3.101517 6.192119 -2.649240 C -2.507358 1.200707 1.241855 C -1.773308 0.720189 2.333263 C -3.775372 1.756954 1.457491 C -2.319463 0.751348 3.616692	**1,5-Ts (8 + 1a) Path B**  E= -2683.804499 H (0K) = -2683.255138 H (298K) = -2683.211795 G (298K) = -2683.341472 Imaginary frequency = 1. Cu 0.790516 -1.410144 -0.016630 C 2.237453 0.170367 1.204290 C 1.413702 0.888527 0.583326 I 2.798249 -0.804808 2.871003 P -1.570527 -1.280364 -0.003718 C -2.443700 -2.890997 0.023807 C -1.862179 -3.929125 -0.717790 C -3.630223 -3.118657 0.728726 C -2.479174 -5.176385 -0.769015 H -0.909530 -3.763746 -1.244087 C -4.240220 -4.372898 0.676432 H -4.077276 -2.318042 1.332417 C -3.669363 -5.398941 -0.074562 H -2.017215 -5.984471 -1.349168 H -5.168888 -4.548951 1.233402

H	-0.761694	0.314899	2.190002	H	-4.150209	-6.384496	-0.111034
C	-4.325135	1.774724	2.737559	C	-2.049569	-0.592198	-1.638286
H	-4.327366	2.200175	0.616283	C	-1.054642	0.033068	-2.400728
C	-3.599947	1.264151	3.816885	C	-3.347752	-0.694469	-2.155149
H	-1.733469	0.373362	4.463008	C	-1.366413	0.593561	-3.639848
H	-5.320566	2.206777	2.898435	H	-0.018942	0.072077	-2.030245
H	-4.030703	1.286352	4.825760	C	-3.660838	-0.121238	-3.386279
C	-2.708093	-0.152983	-1.358545	H	-4.115168	-1.251039	-1.598442
C	-4.087216	-0.337986	-1.205357	C	-2.672055	0.531220	-4.125701
C	-2.008458	-0.944278	-2.276348	H	-0.578644	1.072402	-4.234778
C	-4.758688	-1.288150	-1.971799	H	-4.680710	-0.201650	-3.782327
H	-4.645250	0.253196	-0.468274	H	-2.917414	0.972093	-5.099960
C	-2.680002	-1.896341	-3.042372	C	-2.438786	-0.266622	1.253596
H	-0.919010	-0.824004	-2.375393	C	-3.708657	0.293615	1.069023
C	-4.055968	-2.064870	-2.893308	C	-1.769343	-0.058034	2.464789
H	-5.837964	-1.432708	-1.836608	C	-4.306058	1.033414	2.087712
H	-2.121785	-2.512818	-3.757614	H	-4.235710	0.169455	0.114697
H	-4.584728	-2.816648	-3.492950	C	-2.365246	0.685370	3.482814
I	2.024282	2.681483	0.897528	H	-0.757030	-0.468041	2.600892
C	-0.533888	-2.029794	0.569759	C	-3.636534	1.226739	3.296081
C	-1.680002	-2.395169	0.757166	H	-5.298297	1.474414	1.929299
C	-3.056069	-2.793994	0.857471	H	-1.829238	0.843986	4.426575
C	-3.957814	-2.081565	1.664882	H	-4.105813	1.814067	4.095578
C	-3.529466	-3.868730	0.090466	I	2.186742	-3.098591	-1.270101
C	-5.301865	-2.435351	1.683935	C	0.275811	1.674813	0.404697
C	-4.874230	-4.219672	0.131780	C	-0.742363	2.322983	0.251106
C	-5.783642	-3.508638	0.923473	C	-1.996836	3.018496	0.172261
H	-3.598745	-1.235876	2.264086	C	-2.844326	2.854519	-0.934689
H	-2.828813	-4.417145	-0.550983	C	-2.418271	3.815528	1.246700
H	-5.998982	-1.862523	2.310607	C	-4.091953	3.468502	-0.949141
H	-5.232786	-5.062383	-0.474563	C	-3.664211	4.430218	1.212608
C	-7.237650	-3.905961	0.982528	C	-4.523307	4.265196	0.118808
H	-7.414449	-4.608598	1.818166	H	-2.525927	2.224776	-1.774791
H	-7.886179	-3.028074	1.145403	H	-1.763265	3.929184	2.119244
H	-7.554975	-4.407709	0.052623	H	-4.751767	3.323251	-1.815241
N	1.459125	-0.971455	2.542427	H	-3.986979	5.047417	2.061854
N	2.495061	-0.765827	2.106561	C	-5.866032	4.951435	0.081824
N	3.210797	-0.796779	1.107685	H	-6.576465	4.408173	-0.563923
C	4.431520	-0.028978	0.910964	H	-6.302402	5.032016	1.092079
H	4.270258	0.605736	0.017450	H	-5.766800	5.977043	-0.319843
H	4.558781	0.672736	1.753804	N	2.232938	0.918295	-1.397977
C	5.651788	-0.908646	0.723611	N	3.323013	0.440597	-1.046262
C	5.551686	-2.288944	0.545120	N	3.868775	-0.096493	-0.194495
C	6.914922	-0.307235	0.700539	C	2.172211	2.188933	-2.121980
C	6.698778	-3.058390	0.343605	H	1.124565	2.524242	-2.008225
C	8.059331	-1.074782	0.501142	H	2.348819	1.992931	-3.196733
C	7.953933	-2.454868	0.321034	C	3.138459	3.222195	-1.588213
H	4.563009	-2.765249	0.566538	C	2.764528	4.070341	-0.541466
H	7.000492	0.778933	0.842812	C	4.439195	3.292686	-2.096046

H 6.607068 -4.142824 0.204454 H 9.044103 -0.591505 0.488253 H 8.855185 -3.060455 0.165068	C 3.678244 4.982119 -0.015867 C 5.354025 4.203193 -1.570034 C 4.973402 5.049441 -0.529112 H 1.743891 4.012873 -0.139013 H 4.738256 2.625244 -2.916643 H 3.375834 5.646931 0.802557 H 6.371636 4.252318 -1.976442 H 5.692133 5.767074 -0.114474
1,4-Ts (8 + 1a) Path C  E= -4212.876345 H (0K) = -4212.050581 H (298K) = -4211.986036 G (298K) = -4212.164737 Imaginary frequency = 1. Cu 1.083721 -1.097779 0.092246 C -0.423561 2.116031 -0.743324 C 0.746518 2.164451 -0.304166 I -1.718017 2.265333 -2.284844 P 3.411819 -1.263176 0.262124 C 3.897715 -3.020761 0.467777 C 3.386453 -3.689583 1.589784 C 4.687167 -3.715359 -0.452018 C 3.680941 -5.033866 1.795918 H 2.747582 -3.147661 2.303834 C 4.975220 -5.065972 -0.242662 H 5.077563 -3.202485 -1.340532 C 4.477654 -5.724133 0.879461 H 3.278684 -5.549405 2.676611 H 5.594640 -5.606981 -0.968808 H 4.706741 -6.784986 1.040353 C 4.105094 -0.506825 1.780890 C 3.314548 0.419606 2.468707 C 5.364332 -0.852181 2.290379 C 3.793680 1.029253 3.629206 H 2.310788 0.663464 2.098572	**1,5-Ts (8 + 1a) Path C**  E= -4212.869562 H (0K) = -4212.044012 H (298K) = -4211.978343 G (298K) = -4212.160123 Imaginary frequency = 1. Cu -0.432449 -0.276861 -0.411440 C 0.171008 0.286197 2.454392 C -1.025137 0.548981 2.191124 I 1.589646 -0.822295 3.342433 P -2.548518 -1.012907 -1.125260 C -2.352493 -1.962671 -2.681634 C -1.360036 -1.518419 -3.565709 C -3.112017 -3.091743 -3.003368 C -1.149296 -2.184447 -4.770325 H -0.735241 -0.652121 -3.299302 C -2.893037 -3.758616 -4.209452 H -3.868658 -3.465623 -2.300625 C -1.915973 -3.304157 -5.093744 H -0.367753 -1.832475 -5.454552 H -3.486810 -4.648050 -4.454375 H -1.741724 -3.834755 -6.038171 C -3.681874 0.349507 -1.595471 C -3.380492 1.630851 -1.117728

C	5.847967	-0.232484	3.440303	C	-4.798269	0.166813	-2.420457
H	5.959240	-1.634275	1.798102	C	-4.216579	2.706624	-1.419809
C	5.064595	0.713828	4.107013	H	-2.471164	1.779324	-0.515745
H	3.160931	1.751739	4.159076	C	-5.639139	1.239718	-2.711157
H	6.836211	-0.503168	3.832374	H	-4.998945	-0.822088	-2.856682
H	5.443426	1.193208	5.018498	C	-5.352972	2.508765	-2.203509
C	4.422603	-0.691910	-1.153639	H	-3.972806	3.710370	-1.049228
C	5.814924	-0.546290	-1.095519	H	-6.515526	1.089051	-3.353669
C	3.752130	-0.449398	-2.357072	H	-6.010414	3.354652	-2.440602
C	6.528266	-0.186622	-2.234821	C	-3.510240	-2.132901	-0.039092
H	6.349416	-0.706442	-0.150688	C	-4.894342	-2.317274	-0.135865
C	4.471061	-0.086902	-3.498138	C	-2.784797	-2.850213	0.920506
H	2.656711	-0.546571	-2.400703	C	-5.543263	-3.222090	0.701560
C	5.857007	0.037662	-3.438783	H	-5.481365	-1.735744	-0.857759
H	7.618299	-0.069908	-2.180719	C	-3.437173	-3.752581	1.760225
H	3.937345	0.096241	-4.438742	H	-1.698732	-2.691475	1.012065
H	6.421604	0.321284	-4.336256	C	-4.814122	-3.943056	1.647474
I	-0.409856	-1.499954	-2.043622	H	-6.630056	-3.353214	0.623395
C	2.130978	2.286623	-0.337611	H	-2.860716	-4.311063	2.507917
C	3.340271	2.425949	-0.354566	H	-5.325721	-4.653605	2.309272
C	4.763115	2.608015	-0.452490	I	1.393543	-2.264791	-0.403567
C	5.607894	2.395571	0.649450	C	-2.411177	0.402395	2.181987
C	5.326884	2.997320	-1.676717	C	-3.621217	0.274230	2.182386
C	6.982444	2.552256	0.512305	C	-5.033496	0.009946	2.208631
C	6.702022	3.164577	-1.794289	C	-5.895743	0.548187	1.240353
C	7.553713	2.935632	-0.707610	C	-5.556210	-0.845004	3.189761
H	5.180177	2.098997	1.614600	C	-7.246332	0.219366	1.254034
H	4.668936	3.159266	-2.539387	C	-6.911350	-1.155401	3.196832
H	7.630809	2.377650	1.382023	C	-7.778264	-0.633149	2.229897
H	7.129185	3.471620	-2.758630	H	-5.496692	1.210745	0.462612
C	9.049038	3.069460	-0.854022	H	-4.880443	-1.276786	3.937925
H	9.518274	3.382579	0.094185	H	-7.907995	0.637248	0.483070
H	9.500189	2.101525	-1.144031	H	-7.307727	-1.829778	3.967808
H	9.311763	3.805160	-1.633089	C	-9.251678	-0.955256	2.254897
N	0.379703	2.156930	1.903336	H	-9.675711	-0.970200	1.236314
N	-0.750022	2.022663	1.786914	H	-9.440784	-1.934333	2.726885
N	-1.642931	1.786330	0.943060	H	-9.805492	-0.193221	2.834423
Cu	-1.621676	-0.466162	0.222723	N	-0.903804	2.518128	1.334520
I	-0.284893	-1.438751	2.383889	N	0.301938	2.652002	1.537616
P	-3.913715	-0.975953	-0.088491	N	1.254896	2.083697	1.844727
C	-4.677807	-0.079827	-1.489889	Cu	2.177728	0.310663	-0.216159
C	-5.453832	1.070221	-1.301842	I	0.666147	1.803039	-1.819392
C	-4.310765	-0.456072	-2.790470	P	4.448673	0.501433	0.290213
C	-5.853886	1.836830	-2.396924	C	4.957780	-0.301512	1.851514
C	-4.717702	0.308778	-3.881682	C	5.276171	0.438688	2.993920
C	-5.485080	1.458999	-3.687551	C	4.846891	-1.697122	1.937928
H	-5.747600	1.375980	-0.287922	C	5.481821	-0.209667	4.212609
H	-3.682573	-1.345477	-2.944775	C	5.057972	-2.340166	3.155210
H	-6.459936	2.737348	-2.237955	C	5.370553	-1.596575	4.296370

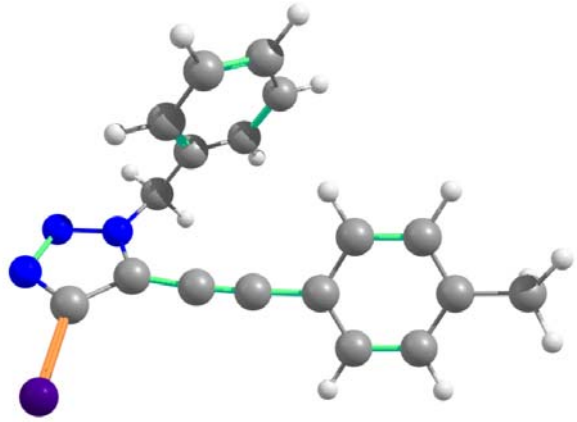
H -4.424078 0.005390 -4.894227 H -5.802082 2.061177 -4.548159 C -4.119617 -2.742012 -0.524744 C -5.254500 -3.225988 -1.187873 C -3.104380 -3.626477 -0.146047 C -5.373890 -4.585750 -1.462003 C -3.230367 -4.989001 -0.418631 C -4.362036 -5.467460 -1.074933 H -6.042994 -2.530344 -1.508070 H -2.202044 -3.244664 0.354687 H -6.261511 -4.961880 -1.985528 H -2.428117 -5.675999 -0.123741 H -4.456381 -6.538099 -1.296025 C -5.057445 -0.736554 1.325060 C -4.483287 -0.544033 2.587008 C -6.451570 -0.796911 1.202264 C -5.295036 -0.400570 3.713786 C -7.259485 -0.649163 2.326888 C -6.681358 -0.449613 3.582646 H -3.386167 -0.516324 2.684193 H -6.907901 -0.955564 0.215157 H -4.836503 -0.255099 4.699537 H -8.350872 -0.694418 2.224856 H -7.320486 -0.336393 4.467357 C -2.939829 3.863416 1.471112 C -2.959735 2.406874 1.062211 H -3.580147 1.811531 1.758790 H -3.411135 2.286530 0.058137 C -1.954817 4.735326 0.994762 H -1.161669 4.359233 0.333819 C -1.972081 6.079942 1.361039 H -1.192293 6.753477 0.985053 C -2.973187 6.566760 2.200675 H -2.984191 7.625293 2.488406 C -3.956095 5.701443 2.679686 H -4.742481 6.075583 3.346799 C -3.935510 4.355187 2.319612 H -4.703105 3.670573 2.706343	H 5.347476 1.532922 2.937172 H 4.565023 -2.279562 1.048507 H 5.725327 0.378029 5.106321 H 4.967541 -3.431972 3.214757 H 5.531557 -2.104151 5.255691 C 5.394941 -0.396875 -0.996770 C 6.662495 -0.946525 -0.768906 C 4.805954 -0.515871 -2.261096 C 7.340109 -1.590665 -1.801324 C 5.489463 -1.156657 -3.293758 C 6.755823 -1.690993 -3.065083 H 7.114409 -0.888005 0.231231 H 3.795796 -0.114970 -2.436512 H 8.331338 -2.023044 -1.617084 H 5.019868 -1.248134 -4.280498 H 7.290258 -2.201493 -3.876075 C 5.195858 2.169536 0.347898 C 4.360832 3.272881 0.147908 C 6.566136 2.363845 0.566853 C 4.894160 4.563788 0.171928 C 7.093744 3.650901 0.593014 C 6.255779 4.751763 0.395366 H 3.287483 3.114221 -0.034318 H 7.224163 1.497324 0.721208 H 4.236455 5.426661 0.010905 H 8.166893 3.799659 0.765053 H 6.673170 5.766428 0.412966 C -1.888385 3.555787 1.575795 H -1.900052 4.255671 0.717577 H -2.858722 3.020053 1.575094 C -1.698010 4.301674 2.881137 C -1.259816 3.629720 4.027114 H -1.028919 2.556319 3.976135 C -1.112224 4.317477 5.229999 H -0.764980 3.781844 6.122008 C -1.403694 5.679695 5.300720 H -1.285546 6.219739 6.248150 C -1.839985 6.353828 4.161199 H -2.065148 7.426518 4.207730 C -1.982183 5.667382 2.956218 H -2.316102 6.202148 2.056591
1,4-Triazole 9	**1,4-Triazole 10**



E= -1154.922709
H (0K) = -1154.645010
H (298K) = -1154.626375
G (298K) = -1154.695875

Imaginary frequency = 0.

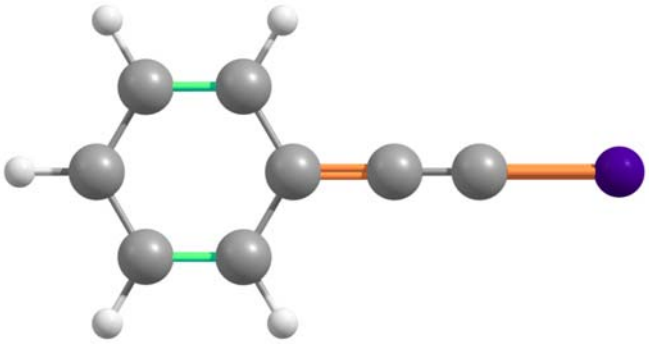
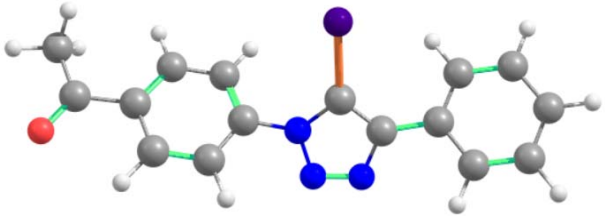
C	0.975688	0.549512	-0.763067
C	-0.101728	1.404984	-0.575336
I	1.088071	-1.492952	-0.744164
C	-1.465412	1.067164	-0.323330
C	-2.618049	0.757155	-0.111447
C	-3.991866	0.412070	0.138736
C	-4.978914	1.408577	0.160625
C	-4.367372	-0.921126	0.359047
C	-6.306641	1.072550	0.399794
C	-5.698951	-1.242903	0.596884
C	-6.690405	-0.254850	0.624051
H	-4.690185	2.451534	-0.015896
H	-3.600454	-1.704721	0.339121
H	-7.069946	1.862120	0.410052
H	-5.980379	-2.291233	0.763878
C	-8.128216	-0.607747	0.912805
H	-8.325327	-0.578641	2.000751
H	-8.819088	0.104062	0.429957
H	-8.370061	-1.623728	0.557303
N	0.369214	2.678005	-0.678680
N	1.631668	2.645934	-0.912896
N	2.023351	1.375635	-0.975264
C	3.425955	1.047623	-1.166131
H	3.507726	0.291408	-1.967262
H	3.893838	1.983702	-1.517209
C	4.075204	0.551749	0.111175
C	3.751991	1.138768	1.337643
C	5.011026	-0.483237	0.068783
C	4.362961	0.694317	2.508249
C	5.626399	-0.924075	1.239745
C	5.302270	-0.336265	2.461492
H	3.013970	1.952300	1.372568
H	5.256396	-0.955693	-0.892265

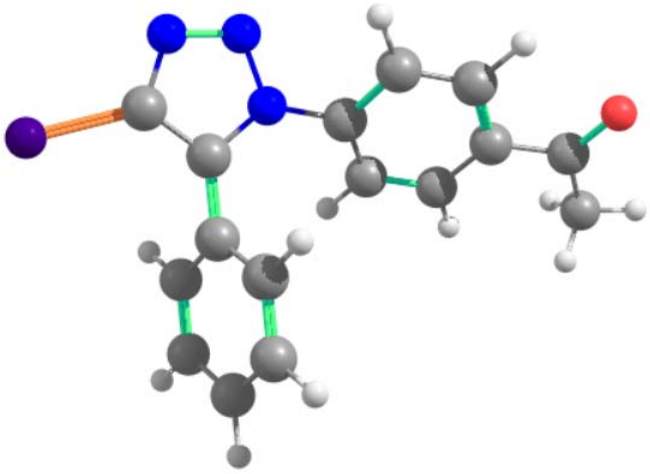
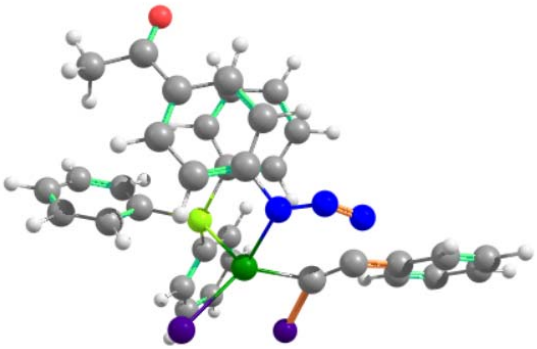


E= -1154.925960
H (0K) = -1154.648207
H (298K) = -1154.628732
G (298K) = -1154.700373

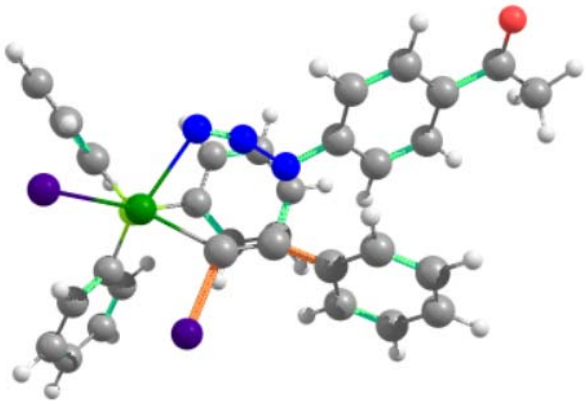
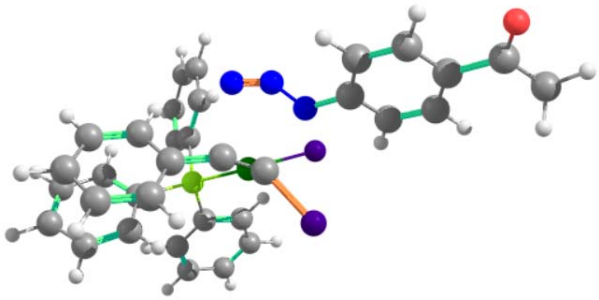
Imaginary frequency = 0.

C	-2.758075	0.117904	-0.289851
C	-1.443118	0.425238	-0.610746
I	-3.493167	-1.647397	0.463553
C	-0.206166	-0.266687	-0.518604
C	0.896968	-0.762979	-0.431972
C	2.232586	-1.277111	-0.295510
C	3.203714	-0.494006	0.347890
C	2.585274	-2.538279	-0.793672
C	4.503022	-0.969834	0.478867
C	3.889503	-3.001088	-0.652682
C	4.869005	-2.226512	-0.020425
H	2.919367	0.490276	0.742751
H	1.825812	-3.153156	-1.291049
H	5.256142	-0.352763	0.987006
H	4.156906	-3.992134	-1.042487
C	6.289543	-2.719130	0.101144
H	6.910398	-2.319871	-0.722425
H	6.745884	-2.391162	1.050692
H	6.337530	-3.820024	0.053217
N	-3.526813	1.194293	-0.543961
N	-2.779869	2.144047	-0.998288
N	-1.532631	1.709070	-1.052882
C	-0.454800	2.564123	-1.518775
H	0.021114	2.089191	-2.395487
H	-0.949880	3.493881	-1.849805
C	0.581399	2.842290	-0.447606
C	0.218913	2.930578	0.898604
C	1.915484	3.036459	-0.812525
C	1.180757	3.214098	1.866486

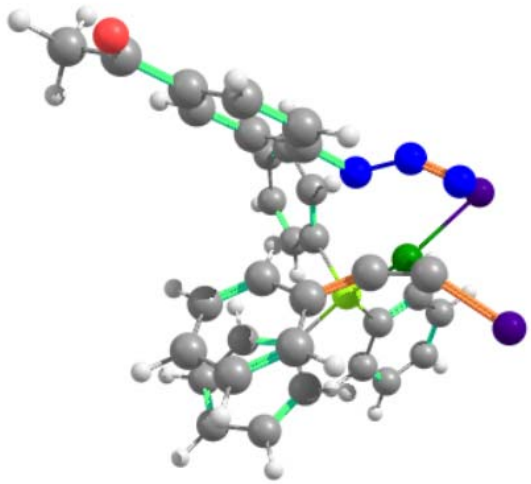
H 4.102406 1.158260 3.467405 H 6.358925 -1.739557 1.197571 H 5.781155 -0.685981 3.384292	C 2.875600 3.335216 0.153624 C 2.510155 3.421936 1.496548 H -0.827656 2.771572 1.192915 H 2.208774 2.950753 -1.867648 H 0.886739 3.277389 2.921368 H 3.919398 3.491234 -0.145933 H 3.263919 3.651689 2.259757
Alkyne 5a  E= -604.938449 H (0K) = -604.837691 H (298K) = -604.828872 G (298K) = -604.873199 Imaginary frequency = 0. C 1.121295 0.000049 -0.002139 C -0.090983 0.000091 -0.004470 I 3.108327 0.000089 0.002834 C -1.531889 0.000037 -0.006797 C -2.238718 1.211959 -0.008133 C -2.238627 -1.211938 -0.007528 C -3.630703 1.207742 -0.009977 C -3.630614 -1.207824 -0.009372 C -4.328693 -0.000067 -0.010514 H -1.682013 2.156541 -0.007611 H -1.681852 -2.156481 -0.006522 H -4.177013 2.158862 -0.010938 H -4.176854 -2.158985 -0.009848 H -5.425771 -0.000106 -0.011912	**1,4-Triazole 6a**  E= -1152.814721 H (0K) = -1152.565814 H (298K) = -1152.547200 G (298K) = -1152.614823 Imaginary frequency = 0. C -0.559992 0.182879 -0.131155 C -1.647166 1.028255 -0.290164 I -0.468133 -1.774293 0.491927 C -3.101303 0.789123 -0.210984 C -3.923528 1.829761 0.239961 C -3.680697 -0.424338 -0.597225 C -5.300425 1.648686 0.326369 C -5.060044 -0.603078 -0.507511 C -5.871824 0.429420 -0.040586 H -3.458855 2.784144 0.515225 H -3.051539 -1.229062 -0.995652 H -5.935704 2.468091 0.684598 H -5.505255 -1.557244 -0.815065 N -1.151918 2.276710 -0.506514 N 0.128539 2.250632 -0.501650 N 0.524397 0.997015 -0.282092 C 1.921290 0.715588 -0.224283 C 2.452592 -0.378962 -0.903516 C 2.739873 1.591784 0.490976 C 3.823549 -0.615046 -0.838967 C 4.106181 1.351601 0.538202 C 4.655748 0.245339 -0.118316 H 1.799632 -1.032707 -1.492432 H 2.286603 2.455967 0.989400

	H 4.241046 -1.476920 -1.373161 H 4.785904 2.013370 1.088840 C 6.148370 0.041451 -0.016902 O 6.821871 0.812769 0.623331 C 6.759250 -1.142648 -0.734599 H 7.844351 -1.140291 -0.554265 H 6.322053 -2.087283 -0.365250 H 6.561860 -1.079863 -1.819640 H -6.957204 0.286070 0.029977
1,5-Triazole 7a  E= -1152.817470 H (0K) = -1152.568620 H (298K) = -1152.549997 G (298K) = -1152.617508 Imaginary frequency = 0. C 1.904641 -1.379985 -0.171596 C 0.839609 -0.498321 -0.111674 I 3.918930 -0.957400 -0.114017 C 0.779433 0.967769 0.045367 C 0.032180 1.534557 1.086008 C 1.480110 1.797695 -0.836108 C -0.018880 2.917111 1.235197 C 1.427820 3.182101 -0.681749 C 0.677468 3.742567 0.350912 H -0.509444 0.880919 1.782514 H 2.066524 1.348478 -1.647805 H -0.603006 3.355032 2.053652 H 1.978454 3.827947 -1.376406 N -0.238565 -1.334992 -0.140526 N 0.148945 -2.610257 -0.203728 N 1.431400 -2.644326 -0.222152	**1,4-Ts (2a + 5a) Path A**  E= -2681.693404 H (0K) = -2681.173096 H (298K) = -2681.131838 G (298K) = -2681.252709 Imaginary frequency = 1. Cu -0.430092 -2.479990 1.327716 C 0.221932 -0.486972 1.140904 C 1.040962 0.265902 1.747515 N 0.870067 -2.633027 3.019308 N 1.978132 -0.610624 3.057107 N 1.578981 -1.667232 3.309153 C 1.519049 1.647408 1.844596 C 2.814327 1.981273 2.257859 C 0.625804 2.663352 1.473169 C 3.210950 3.315322 2.285258 H 3.510841 1.189561 2.552941 C 1.028893 3.995324 1.506993 H -0.392623 2.398084 1.162489 C 2.321994 4.323875 1.912047 H 4.229220 3.570854 2.602657 H 0.323734 4.783831 1.217258 P -2.744709 -2.463779 2.431320 C -3.839815 -1.328738 1.488774

C -1.630404 -1.026601 -0.151129 C -2.499721 -1.853590 0.562876 C -2.103922 0.061875 -0.882570 C -3.859176 -1.570787 0.552928 C -3.468080 0.338315 -0.876360 C -4.352018 -0.471854 -0.158190 H -2.090800 -2.712838 1.106090 H -1.408804 0.683634 -1.457864 H -4.577579 -2.192478 1.101261 H -3.838914 1.195034 -1.451630 C -5.838979 -0.216879 -0.114460 O -6.558386 -0.940210 0.532186 C -6.386262 0.957800 -0.896737 H -5.926033 1.901245 -0.553296 H -6.159548 0.843483 -1.971848 H -7.475591 1.001125 -0.749841 H 0.637717 4.832225 0.471466	C -4.202688 -1.763233 0.204999 C -4.236485 -0.064622 1.928596 C -4.953265 -0.938706 -0.626631 H -3.871835 -2.752201 -0.149453 C -4.981773 0.764173 1.085599 H -3.964618 0.282062 2.934123 C -5.338446 0.331627 -0.189258 H -5.233267 -1.286254 -1.628802 H -5.289158 1.757639 1.435226 H -5.923489 0.985473 -0.848017 C -2.639935 -1.717069 4.104836 C -1.819015 -0.582326 4.221123 C -3.233196 -2.243747 5.255332 C -1.621598 0.025919 5.457695 H -1.328225 -0.173446 3.324149 C -3.025899 -1.639886 6.497766 H -3.844374 -3.153545 5.193740 C -2.226520 -0.504046 6.600576 H -0.986092 0.917747 5.530571 H -3.479204 -2.081187 7.394616 H -2.065843 -0.031361 7.577538 C -3.840707 -3.925931 2.601344 C -3.401593 -5.165895 2.127402 C -5.132915 -3.808438 3.135283 C -4.228274 -6.287377 2.228586 H -2.415630 -5.246613 1.647561 C -5.950801 -4.929730 3.245551 H -5.499906 -2.823468 3.458560 C -5.494650 -6.172818 2.798150 H -3.880311 -7.253839 1.843316 H -6.957779 -4.832529 3.669733 H -6.143245 -7.054440 2.877624 I -0.335764 -4.446198 -0.374929 I -0.929474 -0.211789 -0.537804 C 0.273222 -3.415600 4.043221 C -0.387341 -4.575550 3.641496 H -0.307835 -4.903208 2.594641 C -1.175127 -5.254131 4.567563 H -1.744345 -6.130657 4.235798 C -1.276828 -4.792411 5.880908 C -2.293628 -5.339361 6.845537 O -2.387371 -4.878001 7.960561 C -3.238505 -6.407158 6.338592 H -2.681360 -7.307995 6.025233 H -3.791208 -6.033549 5.454044 H -3.944379 -6.667027 7.141333 C -0.507985 -3.696295 6.293616 H -0.593353 -3.369608 7.337362 C 0.263801 -2.997130 5.380855

	H 0.816574 -2.097789 5.681224 H 2.640077 5.373376 1.939048
1,5-Ts (2a + 5a) Path A  E= -2681.688143 H (0K) = -2681.168211 H (298K) = -2681.126383 G (298K) = -2681.250526 Imaginary frequency = 1. Cu 1.908346 0.965858 -0.825872 C 0.109781 -0.026528 -1.304177 C -1.106835 -0.111045 -0.950028 N 0.538546 2.332548 0.457035 N -1.466698 1.151648 0.531982 N -0.499339 1.916666 0.612947 C -2.405915 -0.750100 -1.088224 C -2.546599 -2.089517 -0.699897 C -3.499567 -0.062814 -1.632326 C -3.780051 -2.724091 -0.827401 H -1.672060 -2.623000 -0.306796 C -4.729129 -0.701509 -1.757826 H -3.377148 0.981944 -1.945789 C -4.872753 -2.027659 -1.345867 H -3.888706 -3.773173 -0.526223 H -5.583836 -0.160387 -2.181417 P 2.580851 -0.137285 1.238748 C 3.446597 -1.732370 1.016818 C 4.185846 -1.874741 -0.164371 C 3.422978 -2.774442 1.952686 C 4.906855 -3.045289 -0.399438 H 4.194651 -1.057082 -0.902434 C 4.139777 -3.944141 1.710507 H 2.826707 -2.674766 2.870859	**1,4-Ts (2a + 5a) Path B**  E= -2681.697383 H (0K) = -2681.177642 H (298K) = -2681.135707 G (298K) = -2681.260749 Imaginary frequency = 1. Cu -1.116516 -0.892632 -0.102738 C 0.141264 -2.232011 1.264148 C 0.770456 -1.148803 1.145622 I -0.994768 -3.475339 2.385412 P -1.675875 1.410358 -0.343318 C -3.469139 1.785236 -0.212450 C -4.357114 0.895817 -0.832960 C -3.965912 2.915710 0.446073 C -5.727494 1.142474 -0.797743 H -3.972303 0.001076 -1.343842 C -5.341037 3.151656 0.483919 H -3.279229 3.619229 0.934632 C -6.221639 2.268352 -0.138182 H -6.414275 0.441049 -1.287111 H -5.725005 4.038138 1.003810 H -7.301996 2.457734 -0.106961 C -1.281778 1.858899 -2.073666 C -0.277160 1.143489 -2.734162 C -1.958066 2.884848 -2.745588 C 0.067290 1.468566 -4.045902 H 0.228295 0.305845 -2.229136 C -1.613736 3.205324 -4.056349 H -2.766943 3.428986 -2.237587 C -0.598643 2.499883 -4.705056 H 0.850250 0.897993 -4.559630 H -2.148478 4.006989 -4.580494 H -0.333975 2.749228 -5.740192

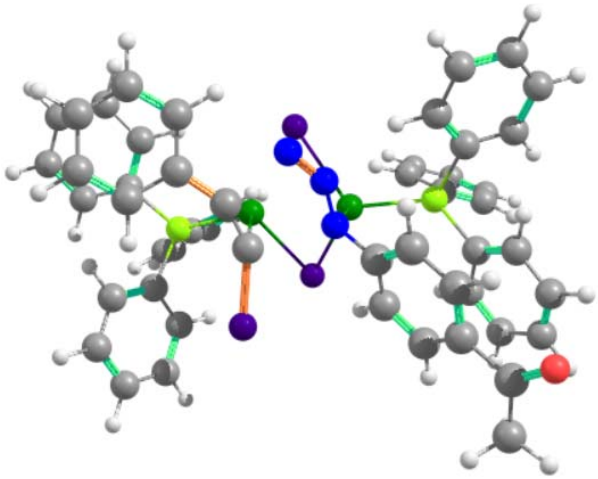
C 4.883443 -4.078113 0.536166 H 5.487174 -3.149554 -1.324260 H 4.118604 -4.759747 2.444005 H 5.447118 -5.000668 0.348742 C 1.098109 -0.538973 2.240909 C 0.301009 -1.634999 1.880724 C 0.654036 0.324164 3.251326 C -0.904095 -1.876212 2.538352 H 0.638966 -2.309437 1.078912 C -0.562260 0.090947 3.894822 H 1.270296 1.187433 3.539580 C -1.339146 -1.012663 3.545284 H -1.509974 -2.750556 2.266448 H -0.897335 0.771471 4.687578 H -2.287026 -1.203893 4.064339 C 3.622669 0.846018 2.375761 C 4.013244 2.119794 1.951322 C 4.027226 0.372711 3.631603 C 4.803065 2.918008 2.782552 H 3.715101 2.479090 0.954359 C 4.811725 1.171823 4.456638 H 3.722963 -0.629472 3.964805 C 5.199389 2.446179 4.030728 H 5.113450 3.913005 2.441360 H 5.128588 0.799910 5.438813 H 5.821743 3.073018 4.681857 I 3.635160 2.285273 -2.151268 I 0.923955 -1.298296 -2.730462 C -2.767127 1.593515 0.904797 C -3.151469 2.927916 0.732765 C -4.446964 3.306637 1.057642 H -4.787789 4.342686 0.939988 C -5.363117 2.363458 1.534531 C -4.963450 1.034048 1.700835 C -3.663460 0.644159 1.394448 H -3.330500 -0.393177 1.512745 H -5.669096 0.282366 2.075010 C -6.759208 2.843198 1.849574 O -7.046411 4.006430 1.698366 C -7.766936 1.831539 2.350046 H -7.419982 1.375417 3.294343 H -7.900547 1.020295 1.612450 H -8.725662 2.344191 2.517011 H -2.436395 3.661783 0.337995 H -5.843558 -2.529185 -1.444357	C -0.920115 2.737618 0.668684 C -0.368282 3.899048 0.122883 C -0.927768 2.564259 2.059731 C 0.157543 4.884087 0.962087 H -0.347272 4.038954 -0.965593 C -0.412369 3.551578 2.893699 H -1.337963 1.639346 2.492009 C 0.130510 4.715221 2.344582 H 0.588298 5.794415 0.526733 H -0.421665 3.405675 3.981102 H 0.540085 5.493191 3.001178 I -2.360467 -2.437042 -1.737312 C 1.409939 0.048553 1.675563 C 1.862198 1.084682 0.848700 C 1.601409 0.137557 3.063162 C 2.500512 2.190076 1.402368 C 2.252411 1.239978 3.609671 C 2.704872 2.266422 2.780025 H 1.703191 1.016930 -0.235282 H 1.246399 -0.678533 3.705380 H 2.840519 3.003081 0.749158 H 2.410348 1.296196 4.693865 N 1.821573 -1.454335 -0.775498 N 1.508878 -2.559003 -0.876898 N 0.762917 -3.410501 -0.399865 C 0.940009 -4.805429 -0.454478 C 2.214872 -5.387066 -0.412362 C -0.210600 -5.594528 -0.502931 C 2.327941 -6.768819 -0.425737 C -0.081336 -6.980606 -0.501922 C 1.183284 -7.574940 -0.464300 H 3.105102 -4.746555 -0.372023 H -1.187203 -5.097984 -0.567760 H 3.305391 -7.266106 -0.400207 H -0.986596 -7.598162 -0.546552 C 1.383571 -9.069436 -0.467461 O 2.499217 -9.532921 -0.431147 C 0.156920 -9.954938 -0.516842 H 0.482232 -11.005752 -0.511797 H -0.495138 -9.761693 0.353421 H -0.430334 -9.750157 -1.429601 H 3.214697 3.137347 3.210833
1,5-Ts (2a + 5a) Path B	**1,4-Ts (2a + 5a) Path C**



E= -2681.694452
H (0K) = -2681.174571
H (298K) = -2681.132744
G (298K) = -2681.257964

Imaginary frequency = 1.

Cu	-1.108715	-0.903851	-0.143329
C	0.198407	-2.226965	1.208679
C	0.831538	-1.142384	1.095423
I	-1.012398	-3.390114	2.335555
P	-1.819821	1.355600	-0.154111
C	-3.633142	1.619921	-0.136146
C	-4.395629	0.818626	-0.997540
C	-4.262928	2.568646	0.675463
C	-5.777741	0.977356	-1.050269
H	-3.901693	0.059459	-1.622548
C	-5.650088	2.716755	0.621108
H	-3.671736	3.194930	1.356609
C	-6.406449	1.925102	-0.241340
H	-6.368112	0.346587	-1.726004
H	-6.141983	3.460072	1.260736
H	-7.496464	2.044787	-0.280727
C	-1.326887	2.024501	-1.787439
C	-0.341687	1.342361	-2.511786
C	-1.931229	3.159341	-2.344040
C	0.065565	1.814652	-3.759726
H	0.087281	0.407603	-2.115789
C	-1.521040	3.630351	-3.589055
H	-2.742600	3.665176	-1.800563
C	-0.517747	2.962122	-4.293772
H	0.825396	1.264441	-4.328951
H	-1.998220	4.518565	-4.021035



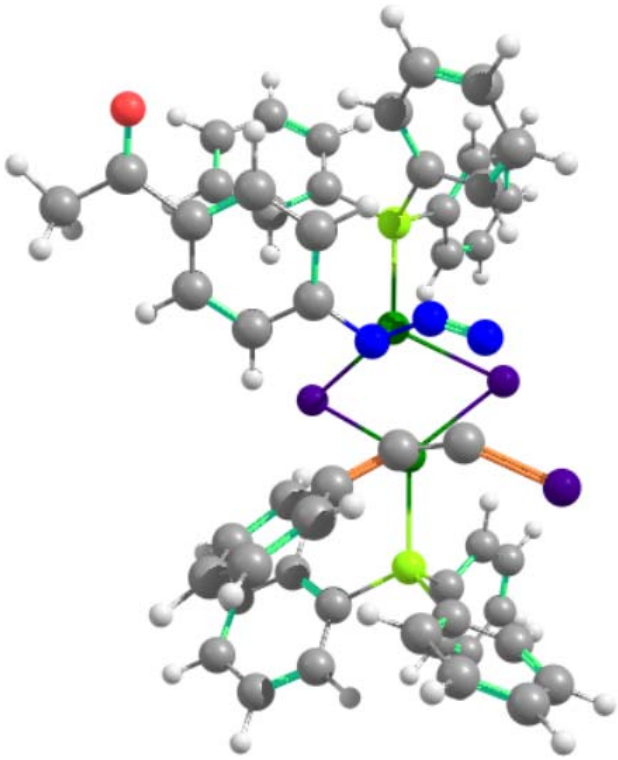
E= -4210.779433
H (0K) = -4209.982155
H (298K) = -4209.918723
G (298K) = -4210.090546

Imaginary frequency = 1.

Cu	-0.678823	0.770960	0.807996
C	-0.316035	-1.682130	0.058375
C	-1.540836	-1.725198	0.305361
I	1.189566	-1.615801	-1.271340
P	-1.457751	2.004309	-1.051633
C	-1.023982	3.770846	-0.812804
C	-0.785720	4.222908	0.488539
C	-0.974602	4.672769	-1.882993
C	-0.501651	5.569948	0.717198
H	-0.810095	3.513075	1.329042
C	-0.687428	6.014804	-1.651701
H	-1.152487	4.316875	-2.907837
C	-0.451797	6.463571	-0.349884
H	-0.308392	5.916928	1.739403
H	-0.645631	6.717986	-2.492697
H	-0.221810	7.521132	-0.169177
C	-3.252424	2.090960	-1.404709
C	-4.107568	1.832637	-0.328428
C	-3.787429	2.491934	-2.635592
C	-5.485935	1.982077	-0.479520
H	-3.686125	1.510360	0.636383
C	-5.166510	2.610654	-2.790379
H	-3.120505	2.715909	-3.479702
C	-6.016329	2.360958	-1.710453
H	-6.148688	1.785103	0.372498
H	-5.582388	2.917318	-3.758233
H	-7.101634	2.469071	-1.832126

H	-0.205297	3.328215	-5.279698	C	-0.621086	1.566867	-2.619696
C	-1.203859	2.555996	1.087629	C	-1.210996	0.747023	-3.589097
C	-0.817859	3.863675	0.782541	C	0.725816	1.933686	-2.759034
C	-1.117864	2.103012	2.411255	C	-0.465518	0.298214	-4.679850
C	-0.359174	4.711151	1.792778	H	-2.265073	0.456100	-3.491053
H	-0.862990	4.224025	-0.253024	C	1.465439	1.485657	-3.850660
C	-0.665326	2.951164	3.418134	H	1.203061	2.561536	-1.992807
H	-1.392724	1.064124	2.648960	C	0.873220	0.663879	-4.811487
C	-0.285283	4.258323	3.108625	H	-0.938234	-0.342540	-5.434647
H	-0.056319	5.736454	1.545957	H	2.517985	1.779176	-3.948178
H	-0.595170	2.584613	4.449794	H	1.457649	0.310578	-5.670220
H	0.077036	4.926178	3.900272	I	1.977393	1.563500	1.132431
I	-2.149878	-2.376765	-1.951430	C	-2.918978	-1.573812	-0.141732
C	1.481834	0.048208	1.617048	C	-4.020083	-1.549413	0.723311
C	1.646291	1.209855	0.854493	C	-3.118198	-1.434150	-1.524313
C	1.948066	0.018375	2.940667	C	-5.302356	-1.399596	0.200079
C	2.268884	2.325890	1.403790	C	-4.400698	-1.270742	-2.038040
C	2.570415	1.137668	3.485704	C	-5.495916	-1.260462	-1.174458
C	2.733657	2.291535	2.718173	H	-3.861722	-1.637220	1.803641
H	1.256377	1.234796	-0.171654	H	-2.242517	-1.463944	-2.186736
H	1.816811	-0.895226	3.534004	H	-6.163516	-1.383076	0.879672
H	2.378927	3.236720	0.802367	H	-4.548969	-1.154553	-3.119585
H	2.934883	1.106911	4.519828	N	-1.683062	-2.566714	2.238580
N	1.738550	-1.435877	-0.885194	N	-0.567957	-2.561769	2.508566
N	1.460755	-2.658407	-0.902391	N	0.538623	-2.126164	2.114464
N	0.809931	-3.436823	-0.363050	Cu	0.816748	0.051613	3.003621
C	3.091200	-1.039054	-1.045247	I	-1.806535	0.777954	3.244644
C	3.351973	0.180762	-1.671490	P	2.072307	-0.272260	4.974970
C	4.143732	-1.818361	-0.546421	C	3.732816	-1.048607	4.893417
C	4.665183	0.625959	-1.793654	C	4.015507	-2.296361	5.454509
C	5.449366	-1.370566	-0.679621	C	4.738941	-0.360225	4.197140
C	5.720684	-0.145192	-1.300104	C	5.301027	-2.835624	5.358383
H	2.516803	0.767899	-2.071904	C	6.021028	-0.895809	4.111340
H	3.925940	-2.776459	-0.056646	C	6.306826	-2.130558	4.702291
H	4.860400	1.583998	-2.290597	H	3.229746	-2.856690	5.978014
H	6.298279	-1.954813	-0.303612	H	4.513450	0.611295	3.731861
C	7.163290	0.279569	-1.410932	H	5.512314	-3.819142	5.797485
O	8.039174	-0.425234	-0.968548	H	6.807098	-0.339718	3.584831
C	7.470717	1.598919	-2.087012	H	7.322337	-2.544584	4.650432
H	8.560353	1.750066	-2.083272	C	2.434127	1.368511	5.713363
H	7.098896	1.596353	-3.127109	C	3.515037	1.597671	6.574344
H	6.977365	2.431112	-1.554007	C	1.568805	2.421624	5.394581
H	3.222925	3.173669	3.149646	C	3.715857	2.862314	7.122428
				C	1.770996	3.685150	5.948556
				C	2.842086	3.905794	6.812251
				H	4.216927	0.783682	6.803901
				H	0.731560	2.252566	4.700569
				H	4.565856	3.036994	7.793680
				H	1.088217	4.504408	5.692670

	H 3.004904 4.902121 7.242031 C 1.215518 -1.193759 6.308859 C -0.009361 -1.798849 6.013900 C 1.740993 -1.294225 7.604181 C -0.696367 -2.512717 6.998130 C 1.055885 -2.005279 8.584125 C -0.162971 -2.617733 8.280044 H -0.443506 -1.684627 5.010586 H 2.698347 -0.811814 7.845152 H -1.660320 -2.978173 6.759388 H 1.471966 -2.080503 9.596307 H -0.703134 -3.175977 9.054990 C 1.721618 -2.871879 2.322262 C 1.727403 -4.112222 2.975505 H 0.791940 -4.529802 3.368747 C 2.929650 -4.787892 3.129805 H 2.979868 -5.751063 3.652741 C 4.117682 -4.254943 2.617366 C 4.097163 -3.013162 1.978003 C 2.907307 -2.305741 1.847510 H 2.881588 -1.306457 1.392246 H 5.023051 -2.563584 1.598961 C 5.387179 -5.033795 2.825014 O 5.409548 -5.976930 3.583056 C 6.615334 -4.610943 2.047693 H 6.907774 -3.582105 2.320985 H 7.436862 -5.305179 2.279595 H 6.404237 -4.621893 0.963508 H -6.508863 -1.130455 -1.575810
1,5-Ts (2a + 5a) Path C	



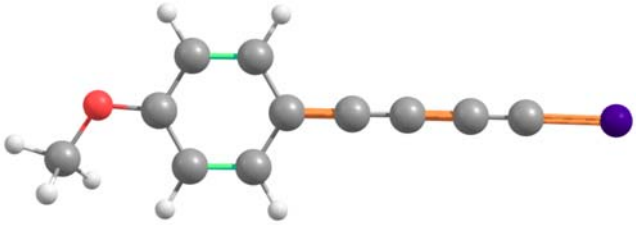
E= -4210.771945
H (0K) = -4209.974647
H (298K) = -4209.910883
G (298K) = -4210.085934

Imaginary frequency = 1.

Cu	-0.745940	-0.645701	0.726462
C	-0.189697	-0.423598	3.949639
C	-0.617818	0.650235	3.480946
I	-0.563657	-2.202455	4.814408
P	-3.080955	-1.147543	0.997995
C	-3.482304	-2.600602	-0.046918
C	-2.441146	-3.434917	-0.464887
C	-4.802123	-2.898641	-0.410539
C	-2.719183	-4.566463	-1.234191
H	-1.402472	-3.200756	-0.188789
C	-5.074612	-4.025585	-1.180561
H	-5.619429	-2.237119	-0.091057
C	-4.032670	-4.861047	-1.591097
H	-1.897104	-5.215551	-1.559389
H	-6.108475	-4.253851	-1.467640
H	-4.249820	-5.747543	-2.200176
C	-4.281417	0.118504	0.413790
C	-3.930725	0.836687	-0.736962
C	-5.500059	0.389006	1.046133

C -4.778957 1.822874 -1.237575 H -2.976148 0.629633 -1.240074 C -6.341475 1.384778 0.549184 H -5.797511 -0.175027 1.938911 C -5.981717 2.105850 -0.588497 H -4.490436 2.377650 -2.138922 H -7.291335 1.594513 1.056482 H -6.645528 2.888882 -0.976108 C -3.718413 -1.629189 2.651160 C -3.938275 -0.639407 3.621139 C -3.920423 -2.972049 2.986661 C -4.353462 -0.990272 4.902873 H -3.805078 0.421260 3.367942 C -4.336169 -3.318947 4.273299 H -3.751937 -3.756946 2.237645 C -4.552086 -2.332026 5.232650 H -4.523691 -0.203457 5.648802 H -4.493542 -4.375173 4.524774 H -4.879072 -2.608269 6.242802 I 1.333296 -2.307950 0.952237 C -1.578426 1.724662 3.331949 C -2.104362 2.113654 2.092800 C -2.099949 2.291650 4.507951 C -3.165734 3.014591 2.032374 C -3.151943 3.200252 4.440357 C -3.697106 3.553153 3.203732 H -1.694459 1.696077 1.163167 H -1.684071 1.986211 5.475875 H -3.591200 3.276271 1.054450 H -3.557979 3.630603 5.364162 N 1.326984 1.373897 2.516117 N 2.001061 0.547940 3.177521 N 1.867914 -0.389116 3.830152 Cu 1.886620 0.238774 0.233918 I -0.073737 1.211528 -1.241557 P 4.167602 0.690754 -0.068043 C 5.154584 0.802331 1.471422 C 6.020102 1.862986 1.756476 C 4.945858 -0.201245 2.427874 C 6.661835 1.924901 2.994895 C 5.587609 -0.135459 3.662474 C 6.442935 0.931554 3.948684 H 6.175086 2.661651 1.018730 H 4.253013 -1.029812 2.209316 H 7.334122 2.763172 3.216813 H 5.408569 -0.918717 4.409441 H 6.942524 0.987342 4.923899 C 4.954602 -0.685408 -0.981447 C 6.290305 -1.055896 -0.786484	

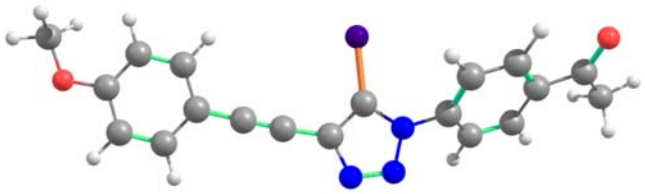
C 4.165600 -1.385878 -1.901919 C 6.835866 -2.106837 -1.521591 C 4.715918 -2.433942 -2.637349 C 6.050156 -2.792935 -2.448586 H 6.903074 -0.524143 -0.044736 H 3.105710 -1.117887 -2.028360 H 7.881956 -2.397541 -1.364650 H 4.091726 -2.981989 -3.353406 H 6.480221 -3.623685 -3.021979 C 4.618078 2.204327 -0.986427 C 3.729091 3.281191 -0.918200 C 5.818903 2.335161 -1.694755 C 4.052854 4.492480 -1.529395 C 6.134103 3.544079 -2.311060 C 5.254506 4.625082 -2.222846 H 2.773644 3.164710 -0.385961 H 6.508887 1.483110 -1.766259 H 3.351670 5.334769 -1.468543 H 7.074651 3.644764 -2.866552 H 5.507344 5.577095 -2.705868 C 1.815161 2.684322 2.332520 C 3.072384 3.086687 2.811328 C 1.008622 3.579604 1.621534 C 3.517473 4.374840 2.552998 C 1.458567 4.875963 1.395350 C 2.718234 5.282447 1.848285 H 3.703092 2.373957 3.359978 H 0.043553 3.241383 1.232778 H 4.505407 4.712299 2.891921 H 0.814445 5.567762 0.838568 C 3.271588 6.658272 1.600282 O 4.383593 6.950119 1.975711 C 2.394803 7.661851 0.878405 H 1.457801 7.827178 1.439446 H 2.946693 8.609165 0.787683 H 2.120531 7.293440 -0.126129 H -4.538917 4.254714 3.153320	
Alkyne 1c	1,4-Triazole 3d



E= -795.371600
H (0K) = -795.227686
H (298K) = -795.214356
G (298K) = -795.270255

Imaginary frequency = 0.

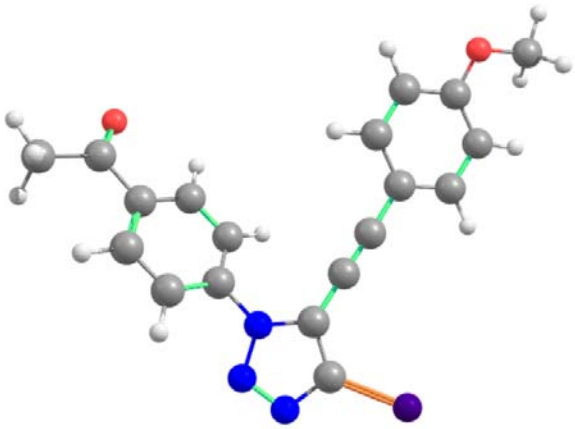
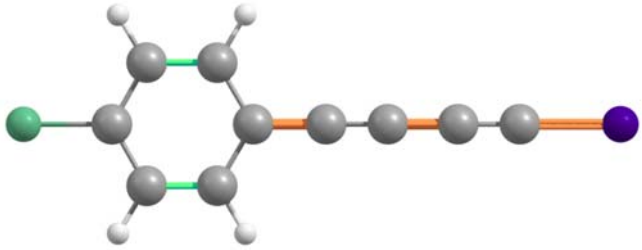
C	-2.794542	0.011720	-0.000155
C	-1.580182	0.049022	-0.000204
I	-4.775153	-0.062376	0.000081
C	-0.196779	0.087077	-0.000244
C	1.018787	0.116128	-0.000252
C	2.453383	0.150740	-0.000157
C	3.141065	1.379675	-0.000047
C	3.195451	-1.035918	-0.000176
C	4.523618	1.411699	0.000044
C	4.588601	-1.012368	-0.000083
C	5.260473	0.215921	0.000031
H	2.568351	2.314681	-0.000032
H	2.667661	-1.997027	-0.000269
H	5.077489	2.357208	0.000132
H	5.140442	-1.957511	-0.000108
O	6.601356	0.338074	0.000125
C	7.387448	-0.828018	0.000258
H	7.197034	-1.442707	0.902813
H	7.197355	-1.442703	-0.902369
H	8.439972	-0.504689	0.000444

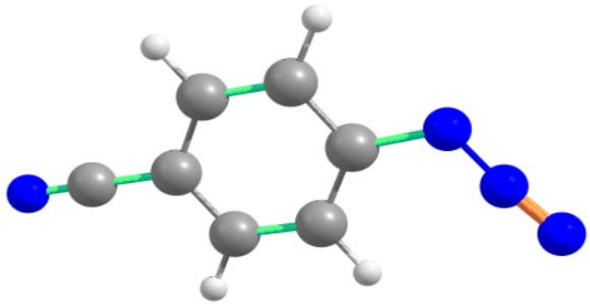
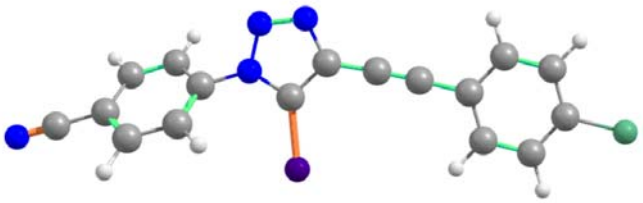


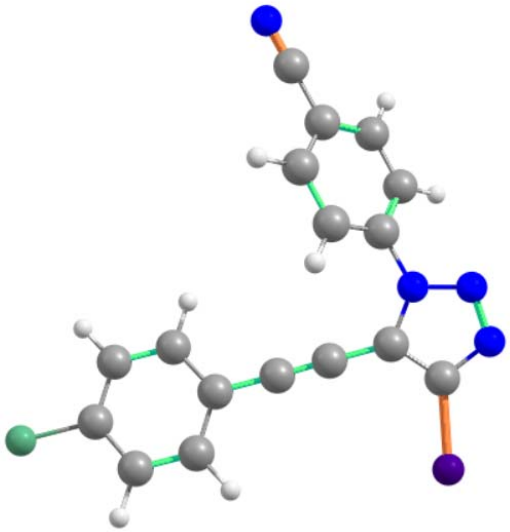
E= -1343.243023
H (0K) = -1342.951156
H (298K) = -1342.927914
G (298K) = -1343.008121

Imaginary frequency = 0.

C	-0.627958	0.520615	0.124004
C	0.365625	1.486263	0.189276
I	-0.419817	-1.495904	-0.170010
C	1.777400	1.283047	0.151163
C	2.965478	1.043802	0.111382
C	4.368753	0.738191	0.063293
C	5.337615	1.759008	0.084821
C	4.795150	-0.592300	-0.006744
C	6.685209	1.449396	0.037890
C	6.150379	-0.912847	-0.054995
C	7.104397	0.111293	-0.033113
H	5.012927	2.804862	0.140466
H	4.046207	-1.393424	-0.023304
H	7.455324	2.228965	0.053955
H	6.451747	-1.963715	-0.110414
N	-0.246366	2.700201	0.281042
N	-1.515731	2.537745	0.275239
N	-1.785212	1.230182	0.185747
C	-3.144114	0.801149	0.146450
C	-3.567784	-0.281064	0.918912
C	-4.035427	1.512020	-0.655516
C	-4.899224	-0.672225	0.856617
C	-5.369054	1.117861	-0.698496
C	-5.805703	0.019044	0.047700
H	-2.859530	-0.800064	1.574501
H	-3.668759	2.371275	-1.227732
H	-5.275277	-1.518544	1.444151
H	-6.070298	1.676809	-1.329843
C	-7.235960	-0.464852	0.030195
O	-7.557624	-1.423180	0.691515
C	-8.232412	0.280450	-0.830612
H	-9.214296	-0.205605	-0.732696
H	-7.914324	0.269136	-1.888328

	H -8.305182 1.335295 -0.510916 O 8.434870 -0.098293 -0.076424 C 8.909165 -1.419690 -0.147770 H 8.595130 -2.009394 0.736805 H 8.551851 -1.927837 -1.065979 H 10.008757 -1.364923 -0.171801
1,5-Triazole 4d  E= -1343.248355 H (0K) = -1342.956198 H (298K) = -1342.933967 G (298K) = -1343.010186 Imaginary frequency = 0. C -0.152772 -2.977756 -0.031012 C -0.400322 -1.612889 -0.059430 I 1.670066 -3.920770 0.008837 C 0.484234 -0.503252 -0.023179 C 1.254950 0.433202 0.016225 C 2.140516 1.561783 0.059052 C 1.632245 2.853112 0.298673 C 3.516129 1.401709 -0.139247 C 2.479785 3.944592 0.335407 C 4.376352 2.496653 -0.102391 C 3.860242 3.776910 0.134974 H 0.555047 2.985875 0.458742 H 3.917882 0.398816 -0.326901 H 2.106080 4.957758 0.521128 H 5.448100 2.341156 -0.260811 N -1.766771 -1.552278 -0.072192 N -2.287671 -2.776840 -0.044668 N -1.330334 -3.633533 -0.022427 C -2.627562 -0.417518 -0.084629 C -3.847853 -0.508379 0.585456 H -4.106825 -1.442103 1.095764	**Alkyne 1d**  E= -1140.422354 H (0K) = -1140.320807 H (298K) = -1140.308802 G (298K) = -1140.362288 Imaginary frequency = 0. C -2.783072 0.000673 -0.000079 C -1.568365 0.001066 -0.000304 I -4.764596 -0.000356 0.000170 C -0.184357 0.001277 -0.000593 C 1.030829 0.001220 -0.000856 C 2.467264 0.000875 -0.000473 C 3.176224 1.212338 -0.000312 C 3.175231 -1.211205 -0.000314 C 4.566361 1.214633 -0.000013 C 4.565353 -1.214705 -0.000014 C 5.249852 -0.000312 0.000140 H 2.623731 2.159123 -0.000449 H 2.621909 -2.157508 -0.000452 H 5.131184 2.153705 0.000098 H 5.129386 -2.154253 0.000096

C -4.707420 0.584961 0.576897 H -5.666581 0.511582 1.103608 C -4.349539 1.762575 -0.086855 C -5.235913 2.983015 -0.121511 O -4.874669 3.977919 -0.704055 C -6.570833 2.916613 0.588160 H -6.426976 2.708856 1.663504 H -7.191739 2.105338 0.168249 H -7.084622 3.881013 0.461930 C -3.126076 1.829946 -0.759828 H -2.879368 2.760281 -1.286005 C -2.261516 0.742372 -0.770951 H -1.313884 0.784437 -1.318665 O 4.611987 4.891265 0.187191 C 6.002239 4.780587 0.000997 H 6.462083 4.136314 0.776870 H 6.243028 4.370479 -1.000117 H 6.417832 5.796662 0.083450	
Azide 2g  E= -487.423888 H (0K) = -487.320617 H (298K) = -487.310998 G (298K) = -487.355124 Imaginary frequency = 0. N -3.972968 -0.913453 0.000294 N -3.147135 -0.151858 0.000117 N -2.327584 0.761858 -0.000137 C -0.958870 0.436947 0.000178 C -0.055932 1.507007 -0.000076 C -0.485652 -0.881892 -0.000318 C 1.308546 1.262126 -0.000077 C 0.882176 -1.125131 -0.000199 C 1.786201 -0.056430 0.000009 H -0.453515 2.527795 -0.000176 H -1.189367 -1.724071 -0.000755	**1,4-Triazole 3l**  E= -1627.961139 H (0K) = -1627.750075 H (298K) = -1627.729944 G (298K) = -1627.802649 Imaginary frequency = 0. C -0.997992 0.471667 0.077427 C 0.006240 1.427450 0.118142 I -0.813943 -1.553996 -0.163773 C 1.415480 1.205998 0.091438 C 2.600298 0.951874 0.067174 C 3.999341 0.621084 0.042305 C 4.978810 1.625613 0.048778 C 4.394488 -0.725031 0.013952 C 6.328727 1.292160 0.028984 C 5.741696 -1.063837 -0.006368 C 6.699561 -0.051099 0.001805 H 4.670502 2.677418 0.071089 H 3.628971 -1.509993 0.009190 H 7.103345 2.067497 0.035210

H 2.019779 2.096179 -0.000130 H 1.259573 -2.154287 -0.000492 C 3.206893 -0.311813 0.000137 N 4.342453 -0.515191 0.000244	H 6.063673 -2.110826 -0.028138 N -0.589941 2.651316 0.175374 N -1.860070 2.505365 0.172245 N -2.145833 1.197717 0.118604 C -3.509850 0.788125 0.096855 C -3.943265 -0.268574 0.896593 C -4.396804 1.495414 -0.714732 C -5.280713 -0.644765 0.858868 C -5.735094 1.125810 -0.741543 C -6.177117 0.049010 0.037898 H -3.239711 -0.784462 1.559176 H -4.022362 2.335959 -1.309205 H -5.640326 -1.473424 1.479200 H -6.447503 1.668166 -1.373466 Cl 8.387450 -0.477021 -0.019902 C -7.567388 -0.344033 0.000998 N -8.675979 -0.660168 -0.028536
1,5-Triazole 4l  E= -1627.965189 H (0K) = -1627.754284 H (298K) = -1627.734945 G (298K) = -1627.806117 Imaginary frequency = 0. C 2.443906 -1.514261 0.017716 C 1.549702 -0.454749 0.061400 I 2.011489 -3.520332 -0.019566 C 0.130438 -0.429679 0.048975 C -1.082116 -0.428435 0.024287 C -2.518082 -0.394002 -0.007738 C -3.180464 0.802105 -0.324651	

C -3.266956 -1.546233 0.275600 C -4.568875 0.848928 -0.356176 C -4.655915 -1.504308 0.243828 C -5.296135 -0.306344 -0.071834 H -2.593646 1.700487 -0.551306 H -2.748462 -2.480181 0.521736 H -5.099473 1.775428 -0.602764 H -5.253794 -2.396523 0.461532 N 2.371971 0.639085 0.053311 N 3.647207 0.261918 0.000272 N 3.698418 -1.021474 -0.018635 C 2.044472 2.023873 0.064352 C 2.866959 2.902273 -0.643064 H 3.734336 2.504657 -1.180724 C 2.572979 4.259224 -0.640679 H 3.206617 4.963527 -1.191634 C 1.457133 4.731588 0.062217 C 0.646124 3.842378 0.776760 H -0.213673 4.223256 1.339647 C 0.942807 2.484182 0.785711 H 0.328791 1.785678 1.364083 C 1.142624 6.141862 0.055485 N 0.887177 7.266429 0.049824	

6.2 Details for the NBO Analysis

NBO analysis was performed with the NBO6 program package.[14]

Table S5. Values of delocalization energy E(2) obtained by NBO

	1a	5a	2a	8	1a+2a (5-I-TS)	1a+2a (4-I-TS)	5a+2a (5-I-TS)	5a+2a (4-I-TS)	1a+8 (5-I-TS)	1a+8 (4-I-TS)
σC2-N->πBin	---	---	---	---	---	---	---	---	---	---
π*Bin->σC2-N	---	---	---	---	14,42	8,67	---	---	22,54	13,55
σ*C2-N->πBin	---	---	---	---	11,17	18,41	---	---	13,27	14,06
σ*C2-N->π*Bin	---	---	---	---	9,87	23,93	---	---	13,00	24,56
σC-N->πBout	---	---	---	---	---	---	---	---	---	---
π*Bout->σC-N	---	---	---	---	4,03	1,17	---	---	---	0,93
σ*C-N->πBout	---	---	---	---	3,25	2,41	---	---	---	0,90
σ*C-N->π*Bout*	---	---	---	---	2,72	3,35	---	---	---	1,74
πAryne->πCCout	---	---	---	---	---	---	---	---	---	---
π*Aryne->πCCout	---	11,43	---	---	---	---	9,06	1,40	---	---
π*CCout->πAryne	---	21,09	---	---	---	---	20,70	2,86	---	---
π*CCout->π*Aryne	---	26,51	---	---	---	---	36,51	3,44	---	---
πAryne->πCCin	---	---	---	---	---	---	---	---	---	---
π*Aryne->πCCin	---	---	---	---	---	---	---	---	---	---
π*CCin->πAryne	---	---	---	---	---	---	---	---	---	---
π*CCin->π*Aryne	---	---	---	---	---	---	---	---	---	---
πAryne->σC-N	---	---	---	---	---	---	---	---	---	---
π*Aryne->σC-N	---	---	---	---	---	---	---	7,19	---	---
σ*C-N->πAryne	---	---	---	---	---	---	---	29	---	---
π*Aryne->σ*C-N	---	---	---	---	---	---	1,19	45,3	---	---
σC-N->πAraz	---	---	---	---	---	---	---	---	---	---
π*Araz->σC-N	---	---	---	---	2,02	1,40	1,76	1,41	---	---
σ*C-N->πAraz	---	---	---	---	1,78	1,13	1,62	0,85	---	---
π*Araz->σ*C-N	---	---	---	---	1,46	0,64	1,11	1,42	---	---
πBout->πAryne	---	---	---	---	---	---	---	---	---	---
π*Aryne->πBout	12,44	---	---	---	11,06	11,94	---	---	11,85	11,59
π*Bout->πAryne	20,88	---	---	---	18,50	21,44	---	---	21,42	21,22
π*Bout->π*Aryne	20,74	---	---	---	18,30	21,79	---	---	20,94	21,74
nN->πAraz	---	---	---	---	---	---	---	---	---	---
nN->π*Araz	---	---	55,59	---	37,08	43,84	36,97	39,88	---	---

7 References

1. I. Ugi, H. Perlinger, L. Behringer, *Chem. Ber.,* **1958**, 91, 2330–2336.
2. T. Slagbrand, A. Volkov, P. Trillo, F. Tinnis, H. Adolfsson, *ACS Catalysis*, **2017**, 7, 1771–1775.
3. M. K. Zilla, D. Nayak, R. A. Vishwakarma, P. R. Sharma, A. Goswami, A. Ali, *Eur. J. Med. Chem.,* **2014**, 77, 47–55.
4. Y. Lu, L. Wang, X. Wang, T. Xi, J. Liao, Z. Wang, F. Jiang, *Eur. J. Med. Chem.*, **2017**, 135, 125–141.
5. Q.-K. Shen, C.-F. Liu, H.-J. Zhang, Y.-S. Tian, Z.-S. Quan, *Bioorg. Med. Chem. Lett.*, **2017**, 27, 4871–4875.
6. M. Liu, Y. Hou, W. Yin, S. Zhou, P. Qian, Z. Guo, L. Xu, Y. Zhao, *Eur. J. Med. Chem.*, **2016**, 119, 96–108.
7. A. I. Govdi, N. A. Danilkina, A. V Ponomarev and I. A. Balova, *J. Org. Chem.*, **2019**, 84, 1925–1940.
8. F. Zhao, M. Abdellaoui, W. Hagui, M. Ballarin-Marion, J. Berthet, V. Corcé, S. Delbaere, H. Dossmann, A. Espagne, J. Forté, L. Jullien, T. Le Saux, V. Mouriès-Mansuy, C. Ollivier, L. Fensterbank, *Nat. Commun.*, **2022**, 13, 2295.
9. Y. Jeong, J. Lee, J.-S. Ryu, *Bioorg. Med. Chem.*, **2016**, 24, 2114–2124.
10. O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard, H. Puschmann, *J. Appl. Crystallogr.,* **2009**, 42, 339–341.
11. G. M. Sheldrick, *Acta Crystallogr. Sect. A Found. Adv.,* **2015**, 71, 3–8.
12. Agilent. CrysAlis PRO. Agilent Technologies Ltd, Yarnton, Oxfordshire, England, **2014**
13. L. Maini, D. Braga, P. P. Mazzeo, B. Ventura, *Dalt. Trans.* **2012**, 41, 531–539.
14. NBO 6.0. E. D. Glendening, J. K. Badenhoop, A. E. Reed, J. E. Carpenter, J. A. Bohmann, C. M. Morales, C. R. Landis, and F. Weinhold (Theoretical Chemistry Institute, University of Wisconsin, Madison, WI, 2013); http://nbo6.chem.wisc.edu/
15. T. Lu, F. Chen, *J. Comp. Chem.*, **2012**, 33(5), 580–592.
16. W. Humphrey, A. Dalke, K. Schulten, *J. Mol. Graph.*, **1996**, 14(1), 33–38

8 Copies of NMR ^{1}H, ^{13}C

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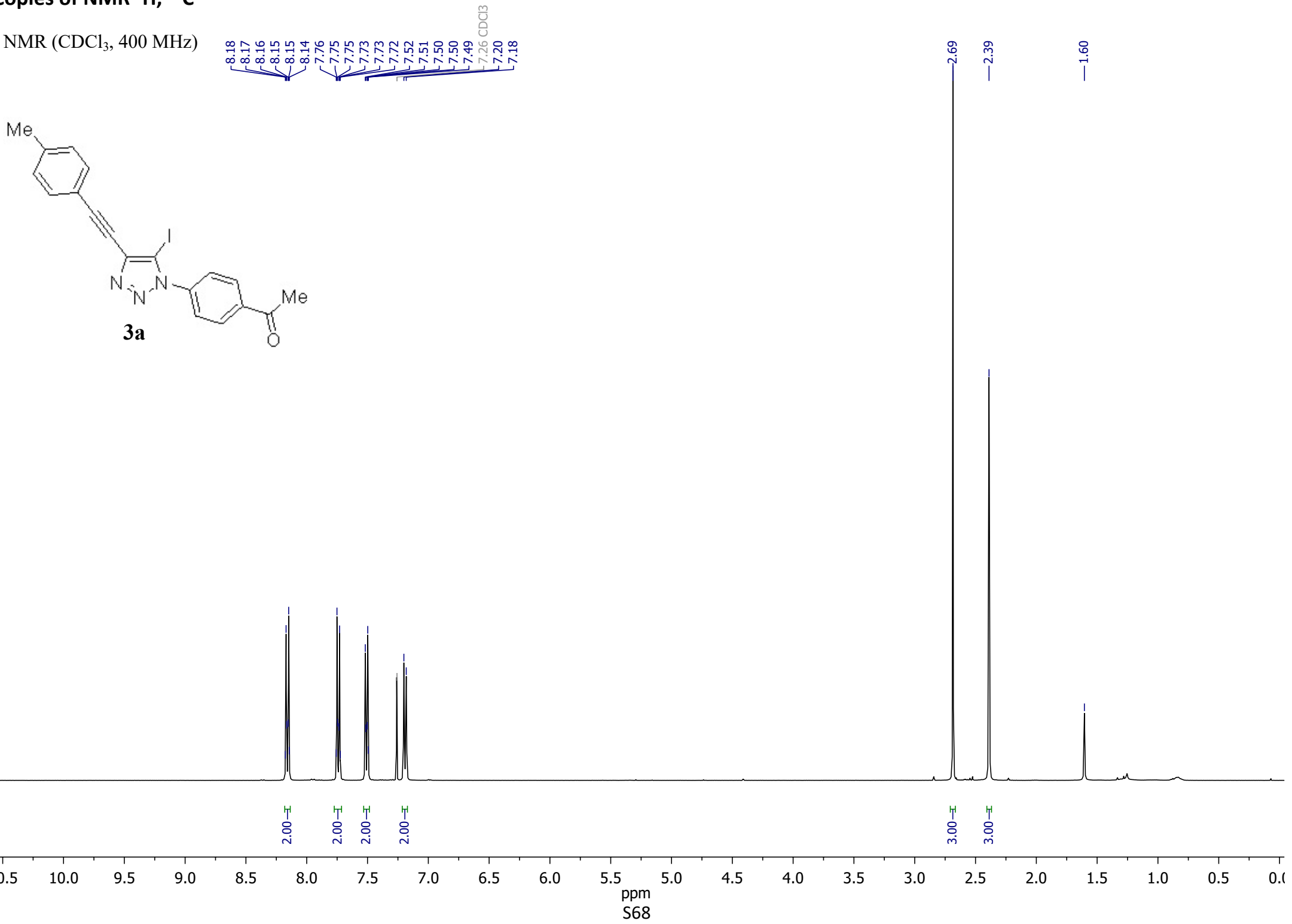
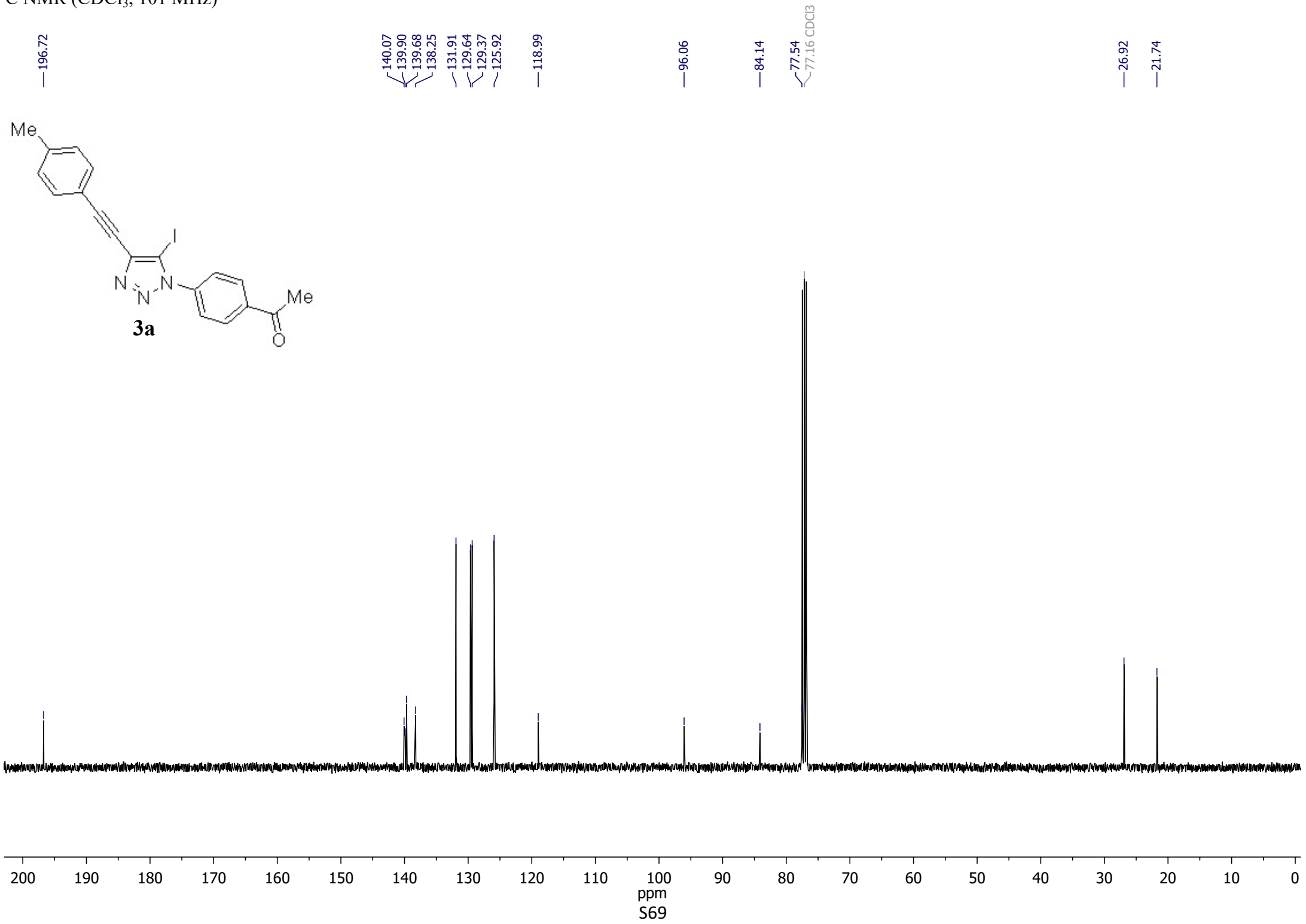


^{13}C NMR ($CDCl_3$, 101 MHz)



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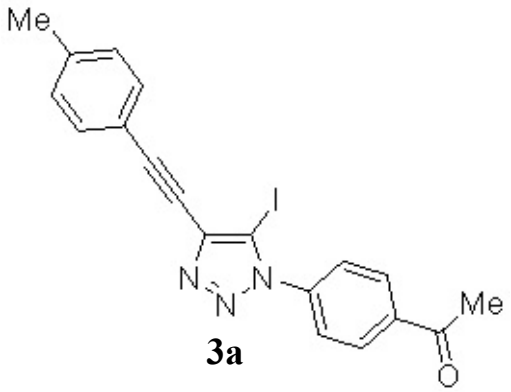
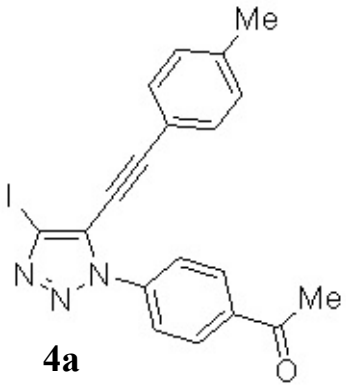


3a

^{1}H NMR ($CDCl_3$, 400 MHz)



4a

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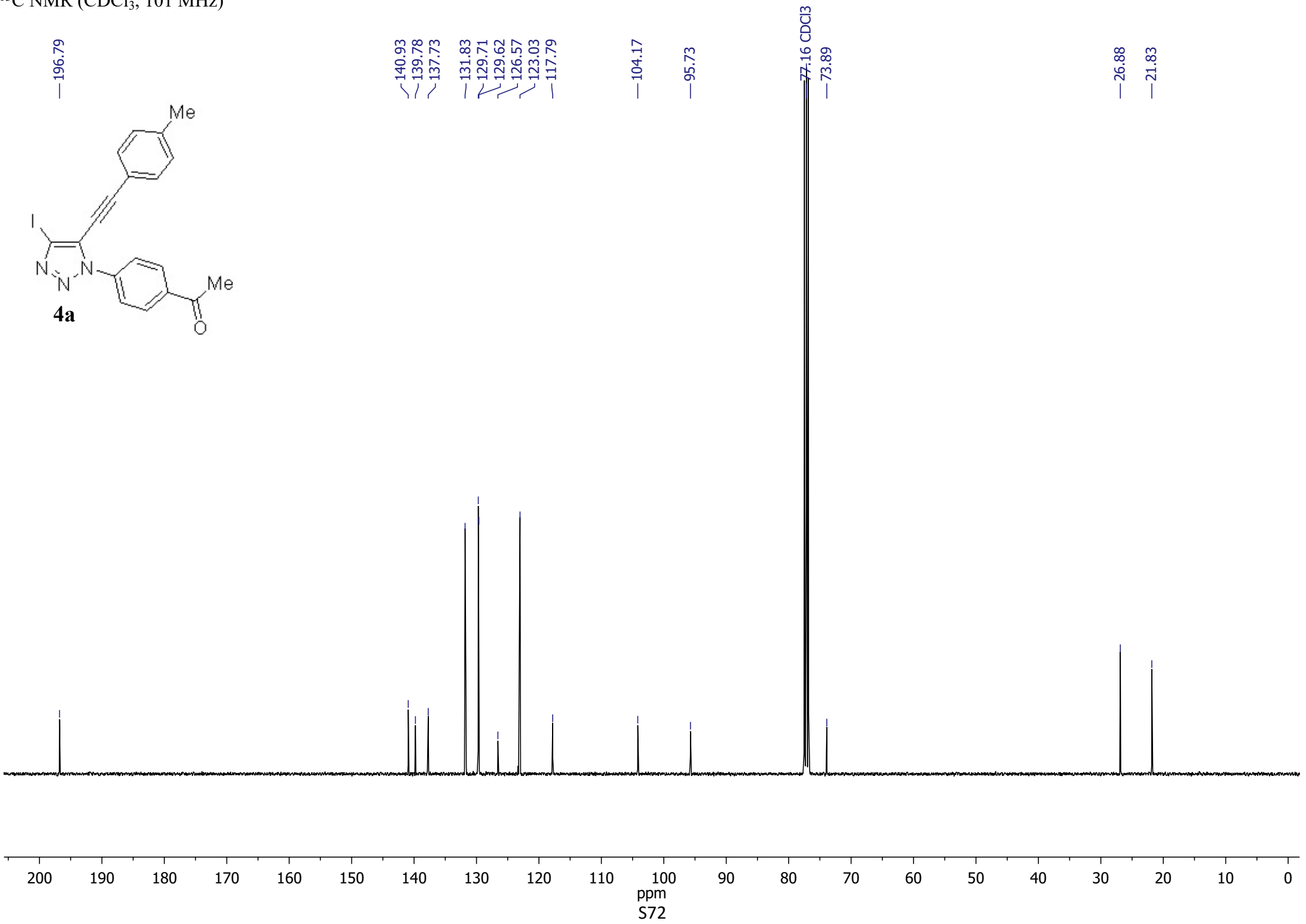
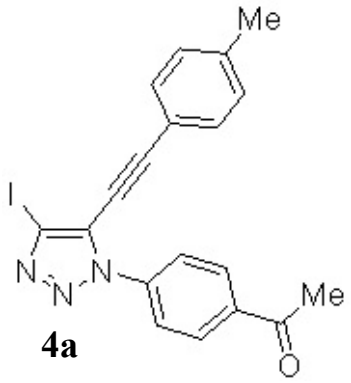
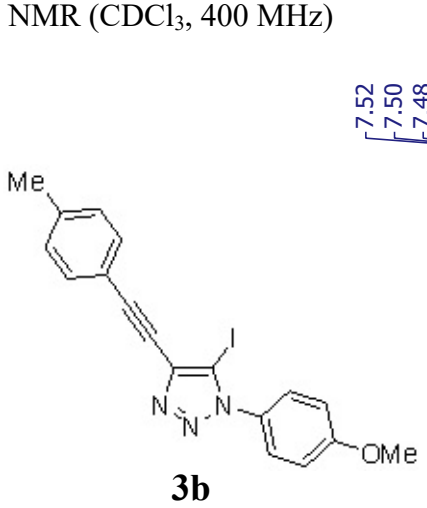


^{13}C NMR ($CDCl_3$, 101 MHz)



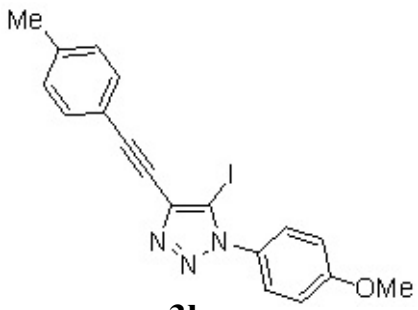
4a

^{1}H NMR ($CDCl_3$, 400 MHz)



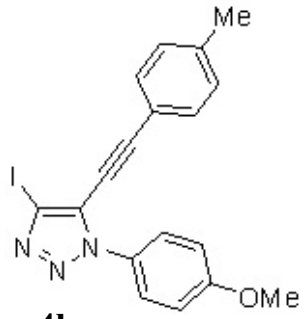
3b

^{13}C NMR (Acetone-d_6, 126 MHz)



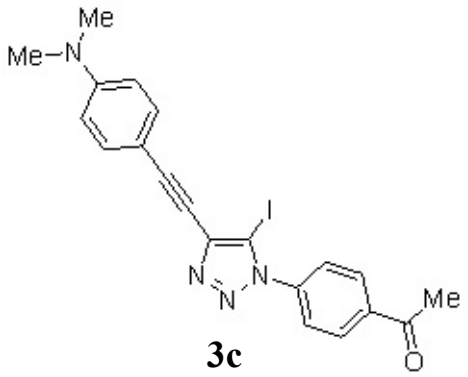
3b

^{1}H NMR ($CDCl_3$, 400 MHz)



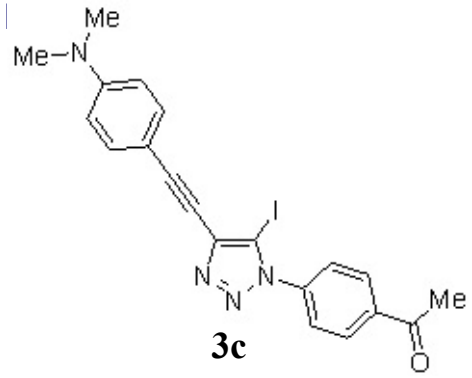
4b

^{1}H NMR (Acetone-d_6, 400 MHz)



3c

^{13}C NMR (Acetone-d_6, 101 MHz)

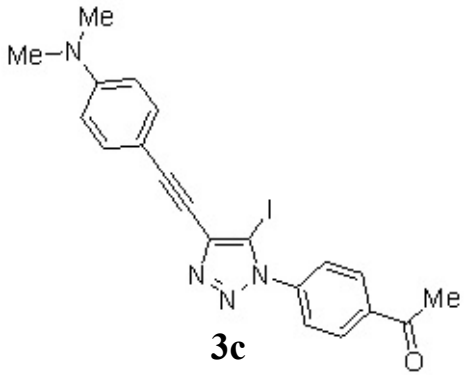


3c

197.15
151.90
141.19
140.44
139.25
133.62
130.33
127.07
112.75
109.00
97.04
86.87
77.41
40.17
29.84 (CD3)2CO
26.95

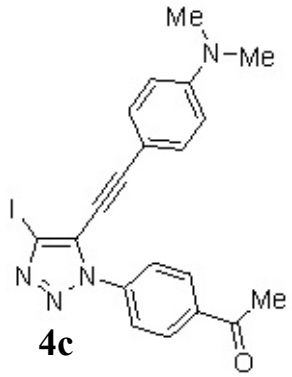
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm

^{13}C NMR (Acetone-d_6, 101 MHz)



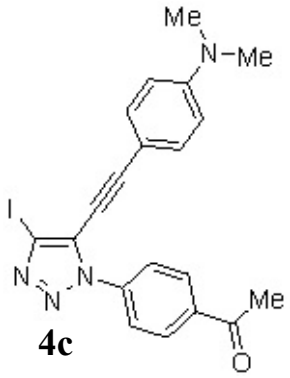
3c

^{1}H NMR (Acetone-d_6, 400 MHz)



4c

^{13}C NMR (Acetone-d_6, 101 MHz)



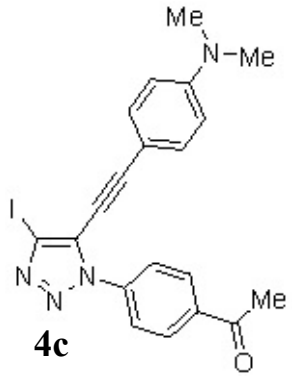
4c

197.03
152.44
140.53
138.74
133.82
130.45
127.92
124.06
112.67
107.28
106.40
95.39
73.44
40.08
29.84 ((CD3)2CO)
26.89

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

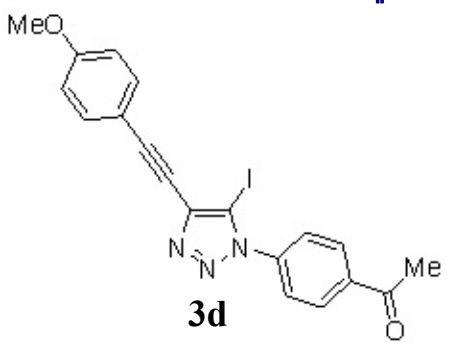
ppm

^{13}C NMR (Acetone-d_6, 101 MHz)



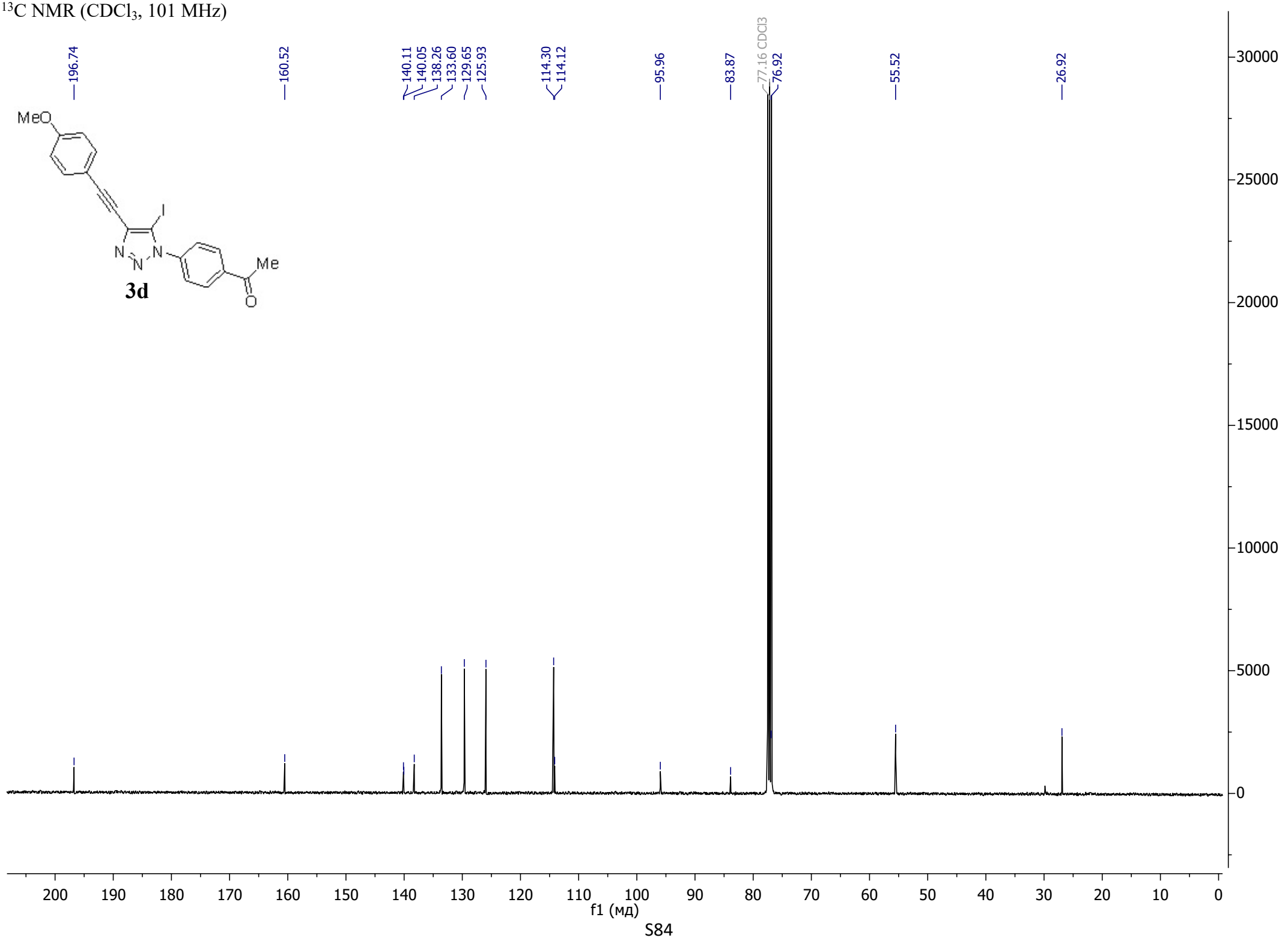
4c

^{1}H NMR ($CDCl_3$, 400 MHz)

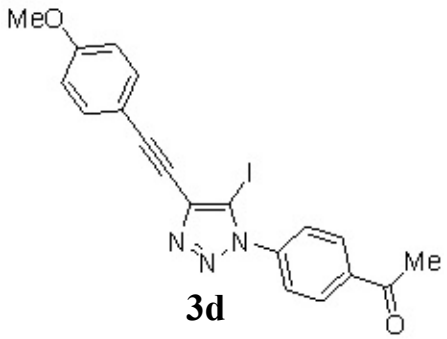


3d

^{13}C NMR ($CDCl_3$, 101 MHz)

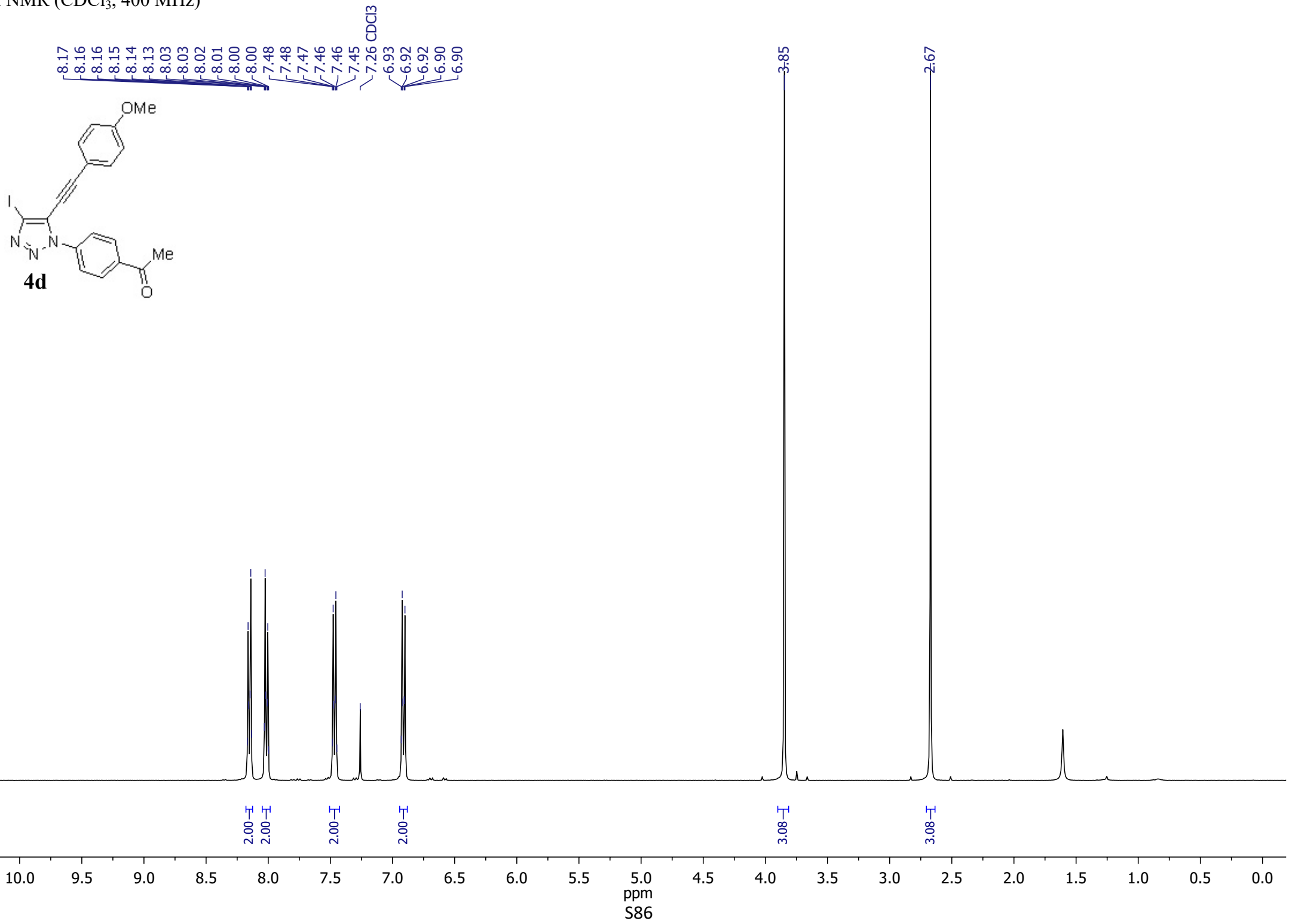


^{13}C NMR ($CDCl_3$, 101 MHz)



3d

^{1}H NMR ($CDCl_3$, 400 MHz)



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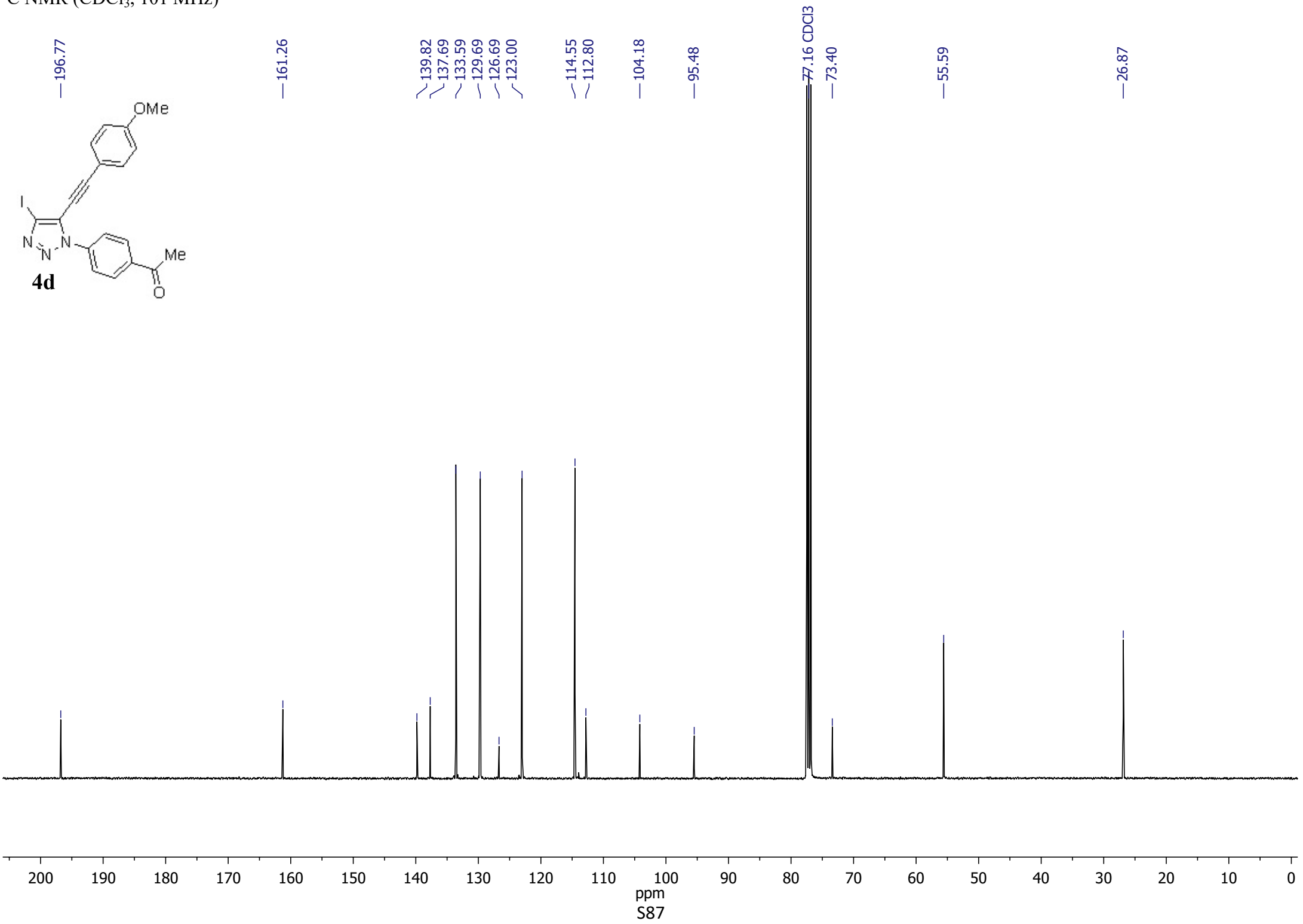
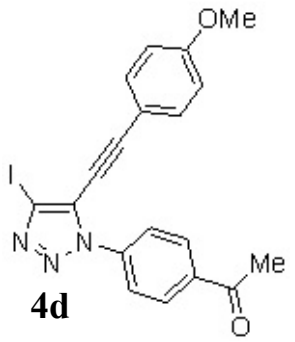
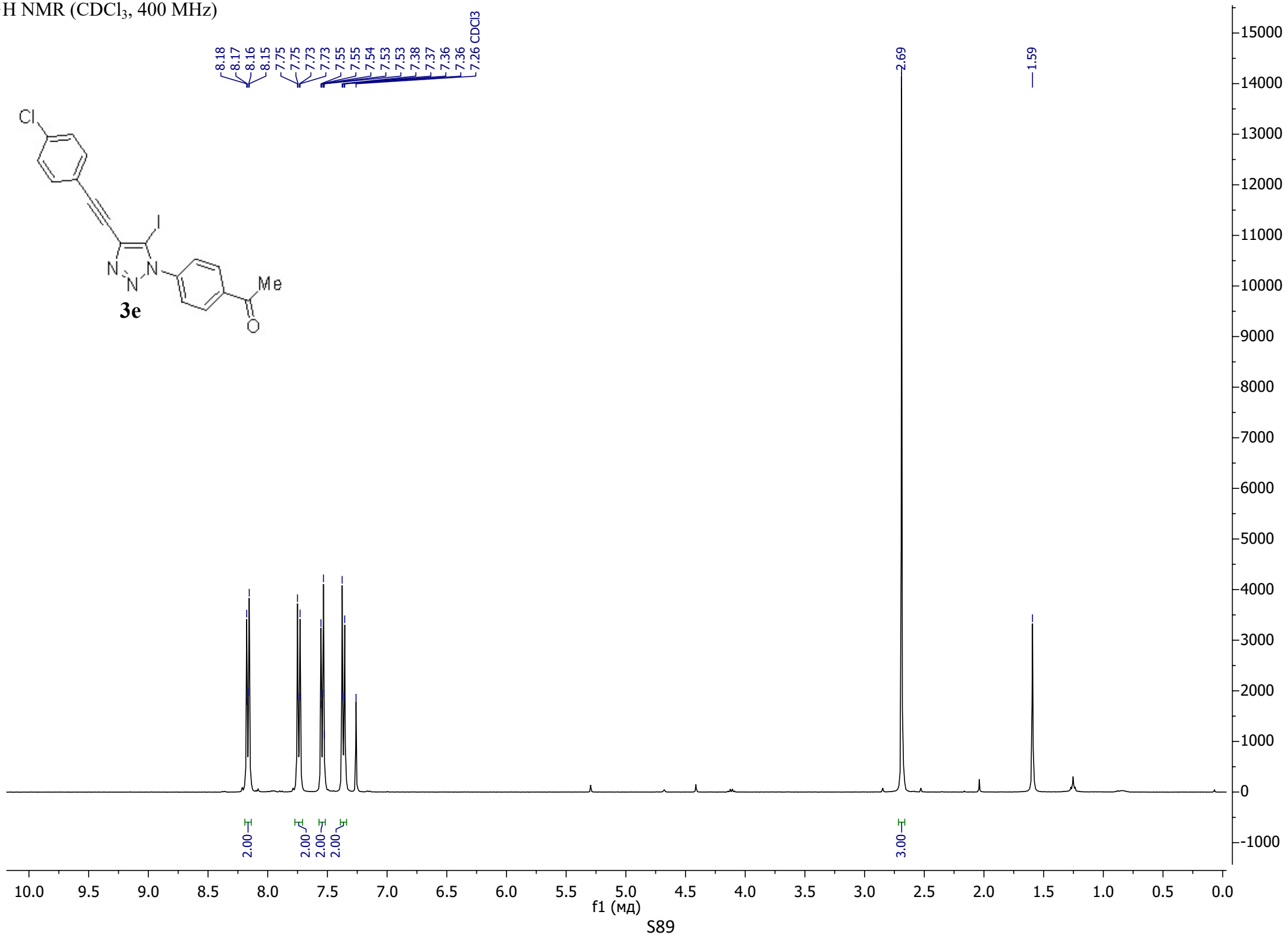


^{13}C NMR ($CDCl_3$, 101 MHz)

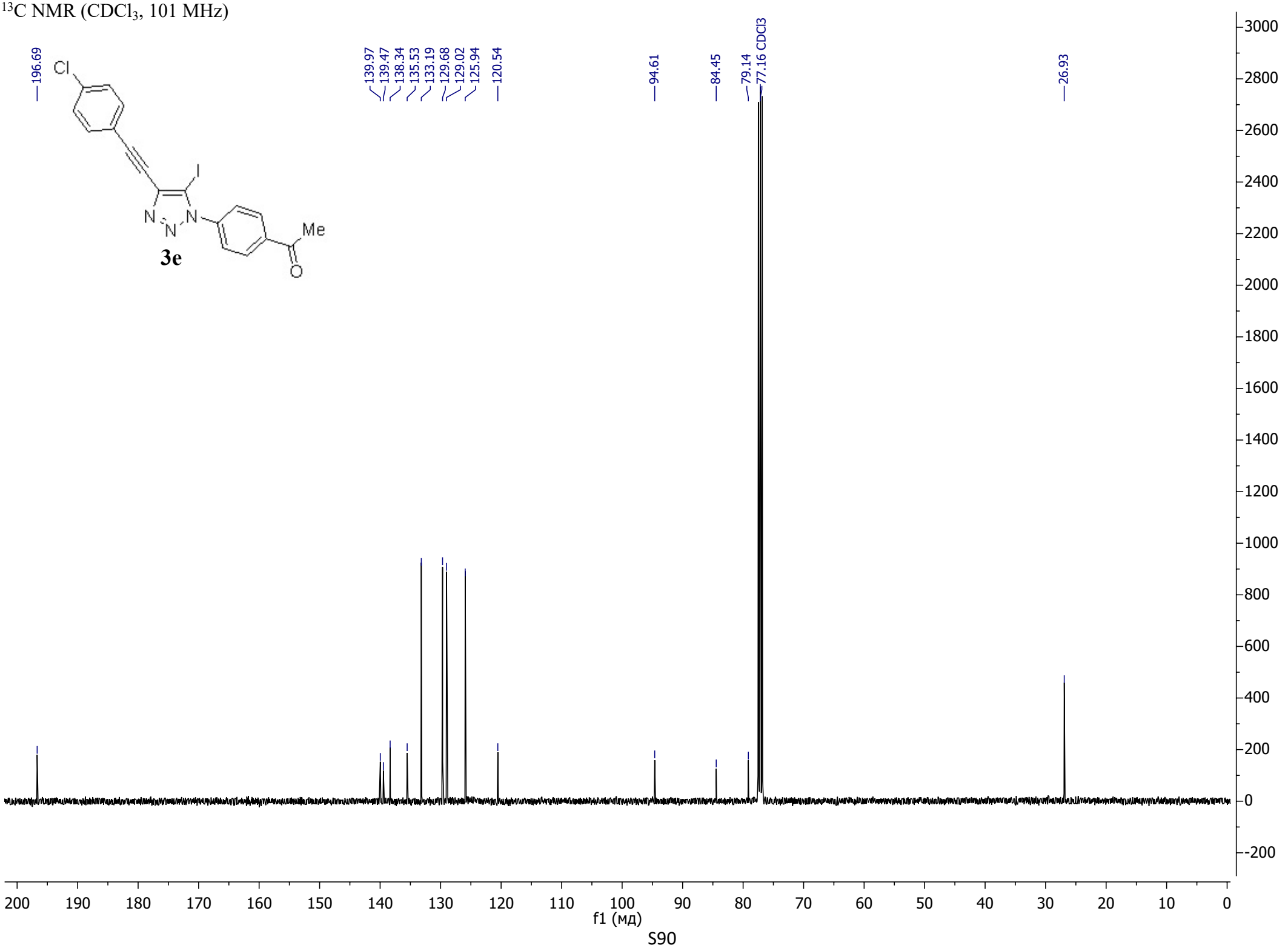


4d

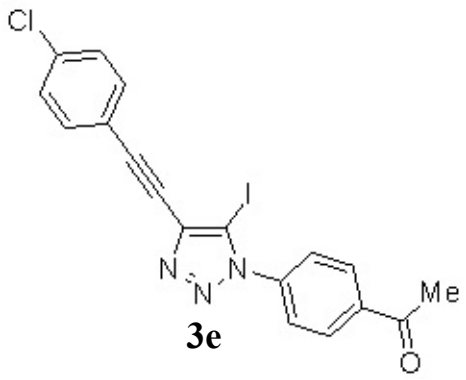
^{1}H NMR ($CDCl_3$, 400 MHz)



^{13}C NMR ($CDCl_3$, 101 MHz)

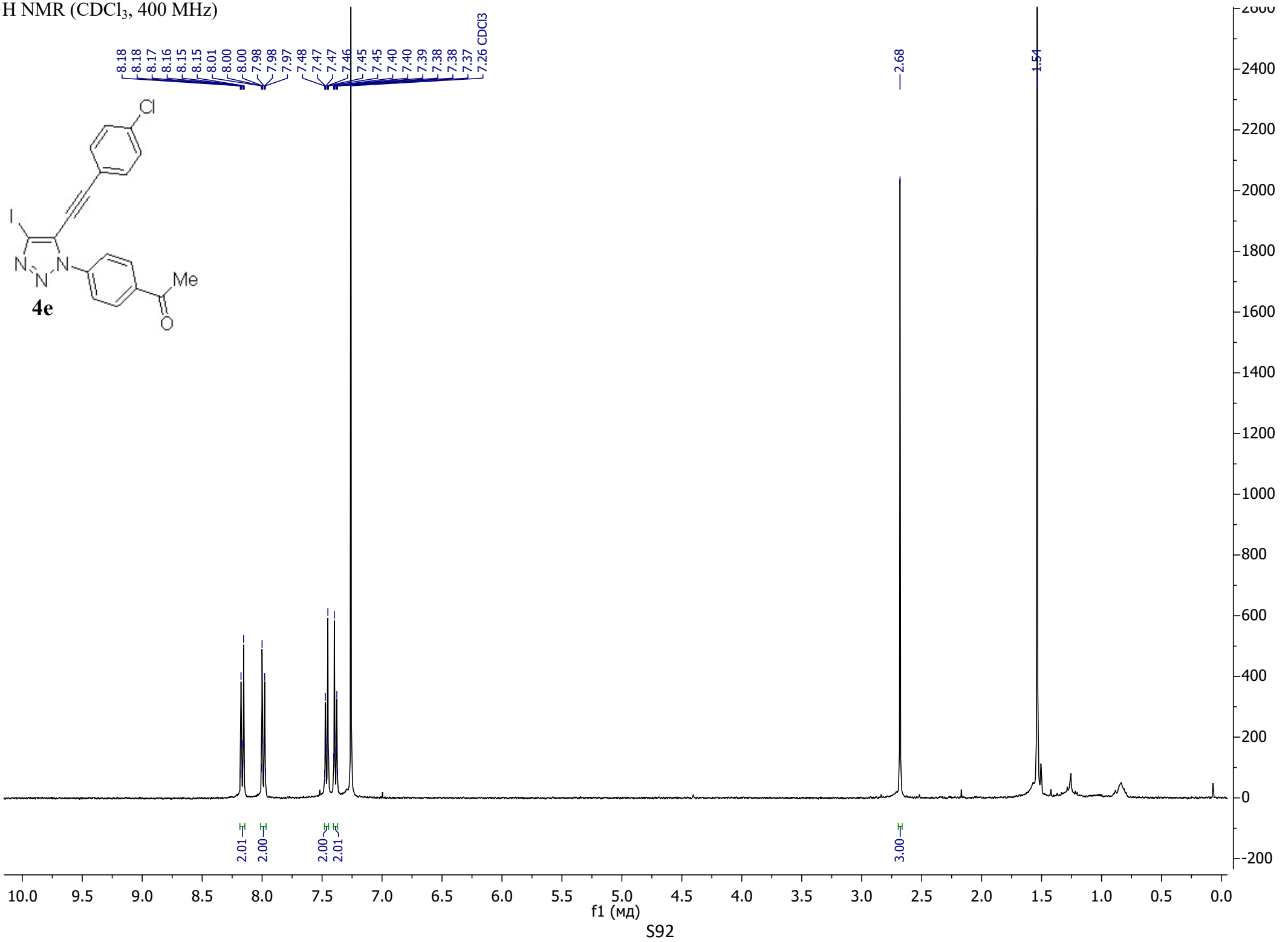


^{13}C NMR ($CDCl_3$, 101 MHz)

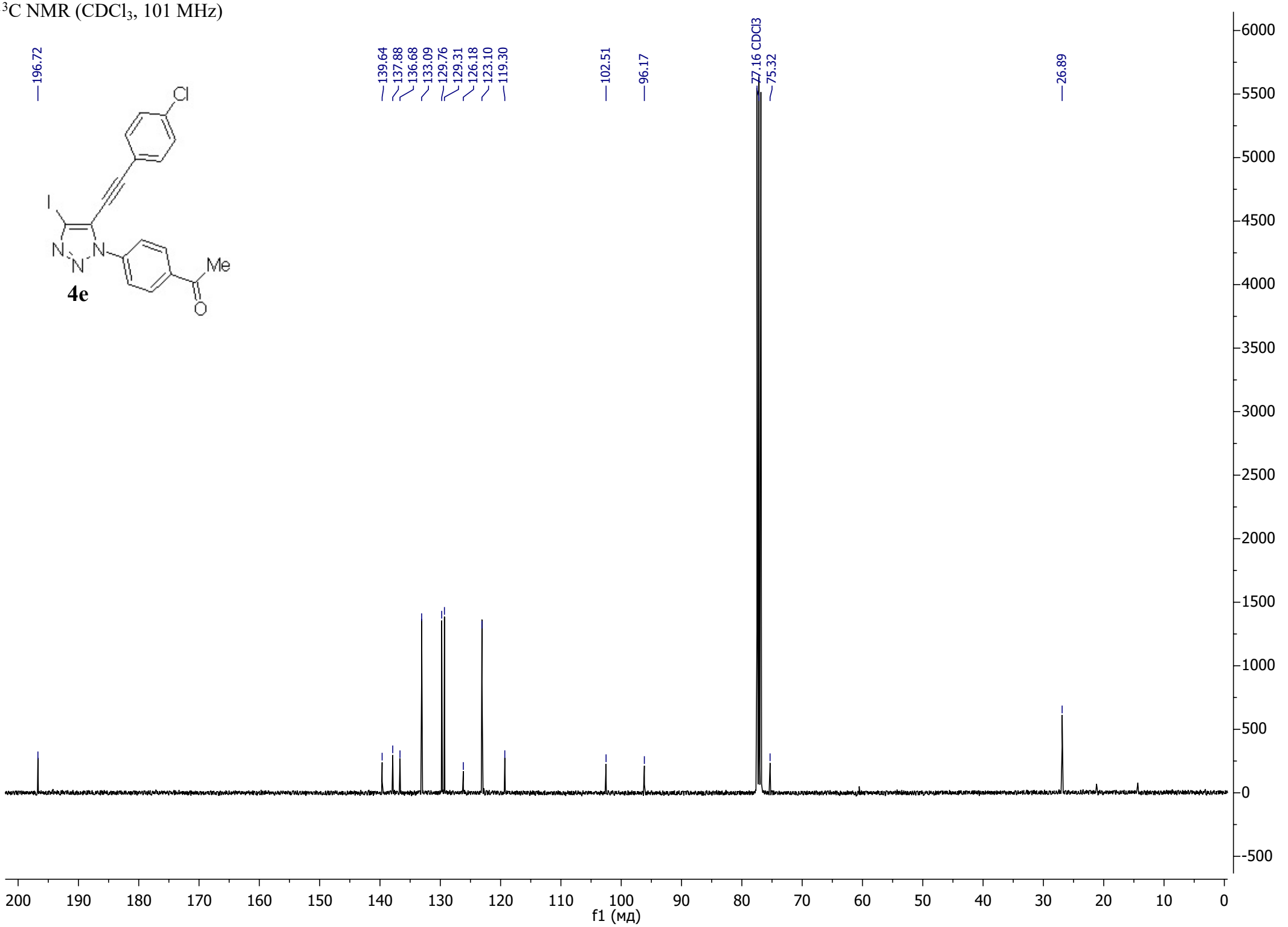


3e

^{1}H NMR ($CDCl_3$, 400 MHz)



^{13}C NMR ($CDCl_3$, 101 MHz)



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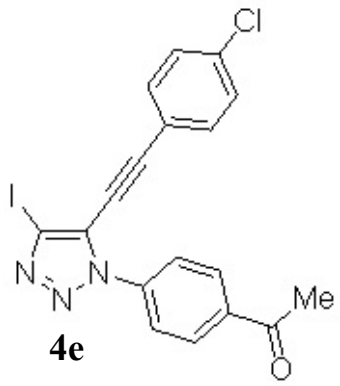
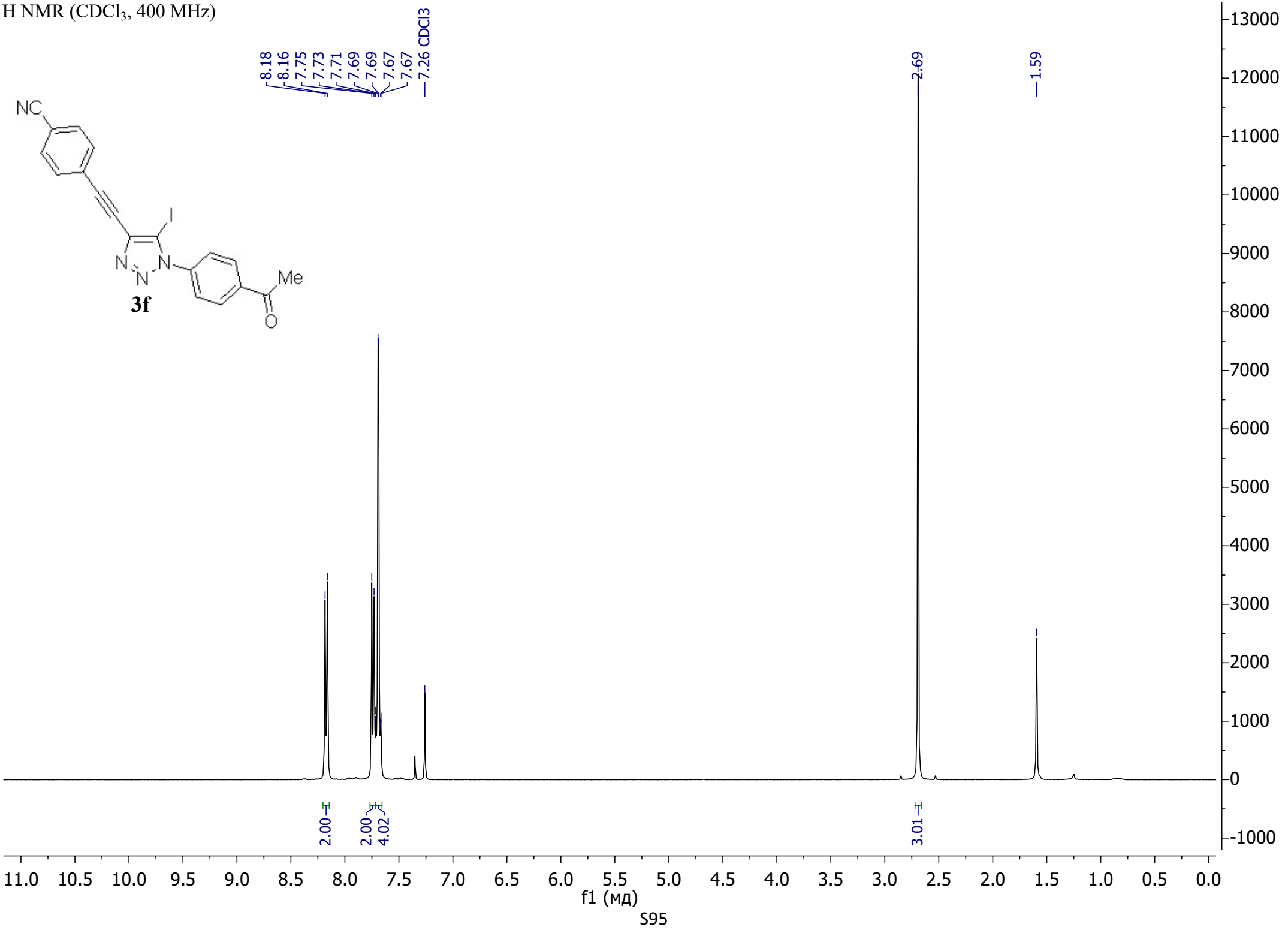
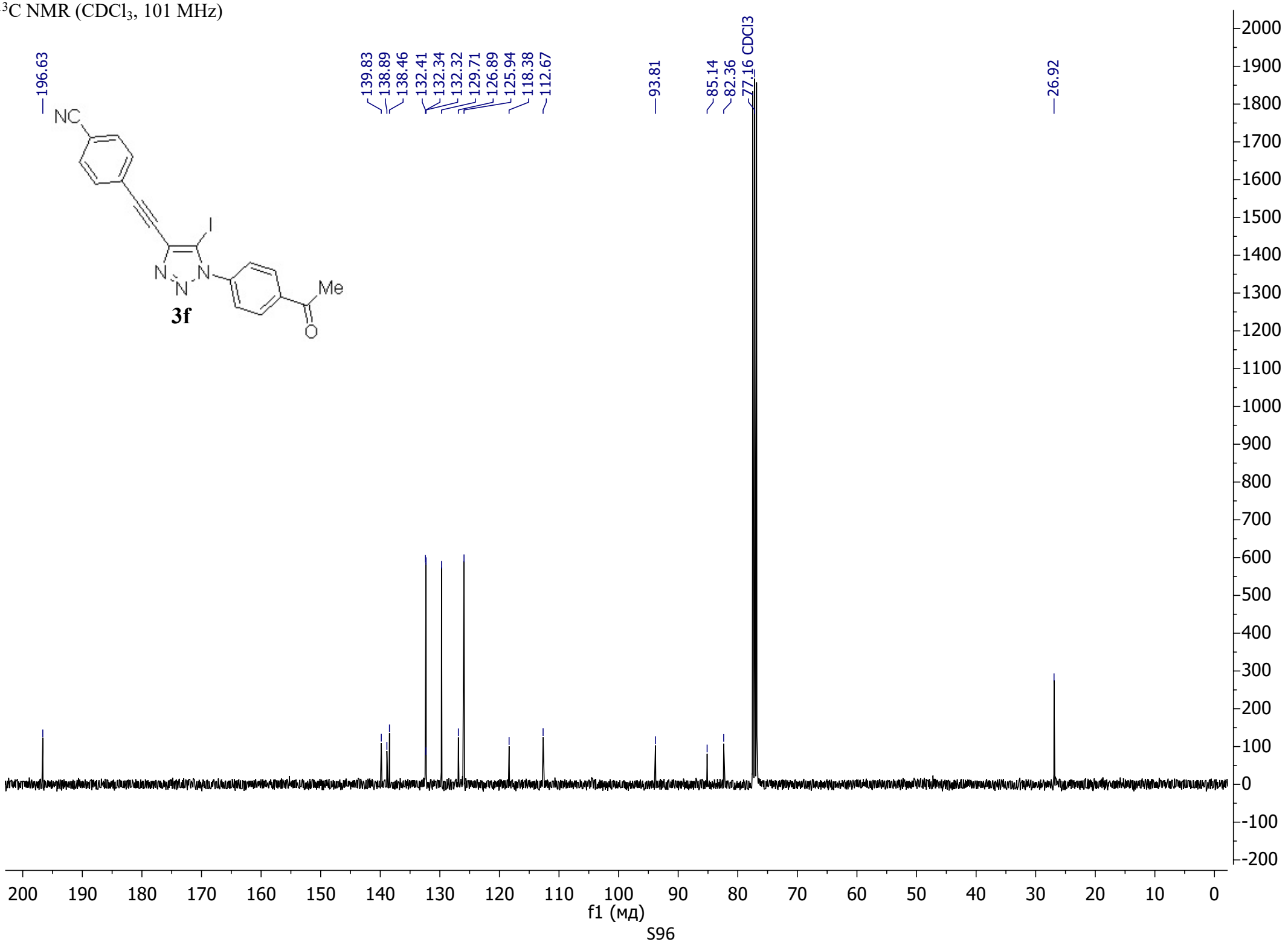


4e

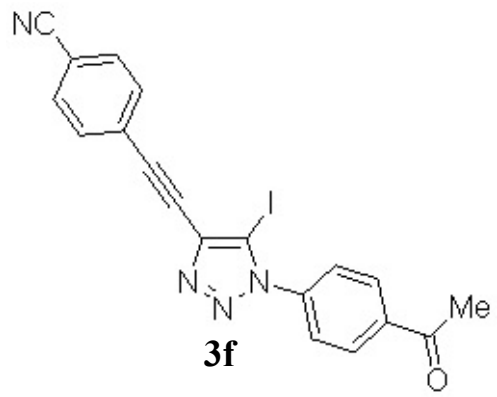
^{1}H NMR ($CDCl_3$, 400 MHz)



^{13}C NMR ($CDCl_3$, 101 MHz)

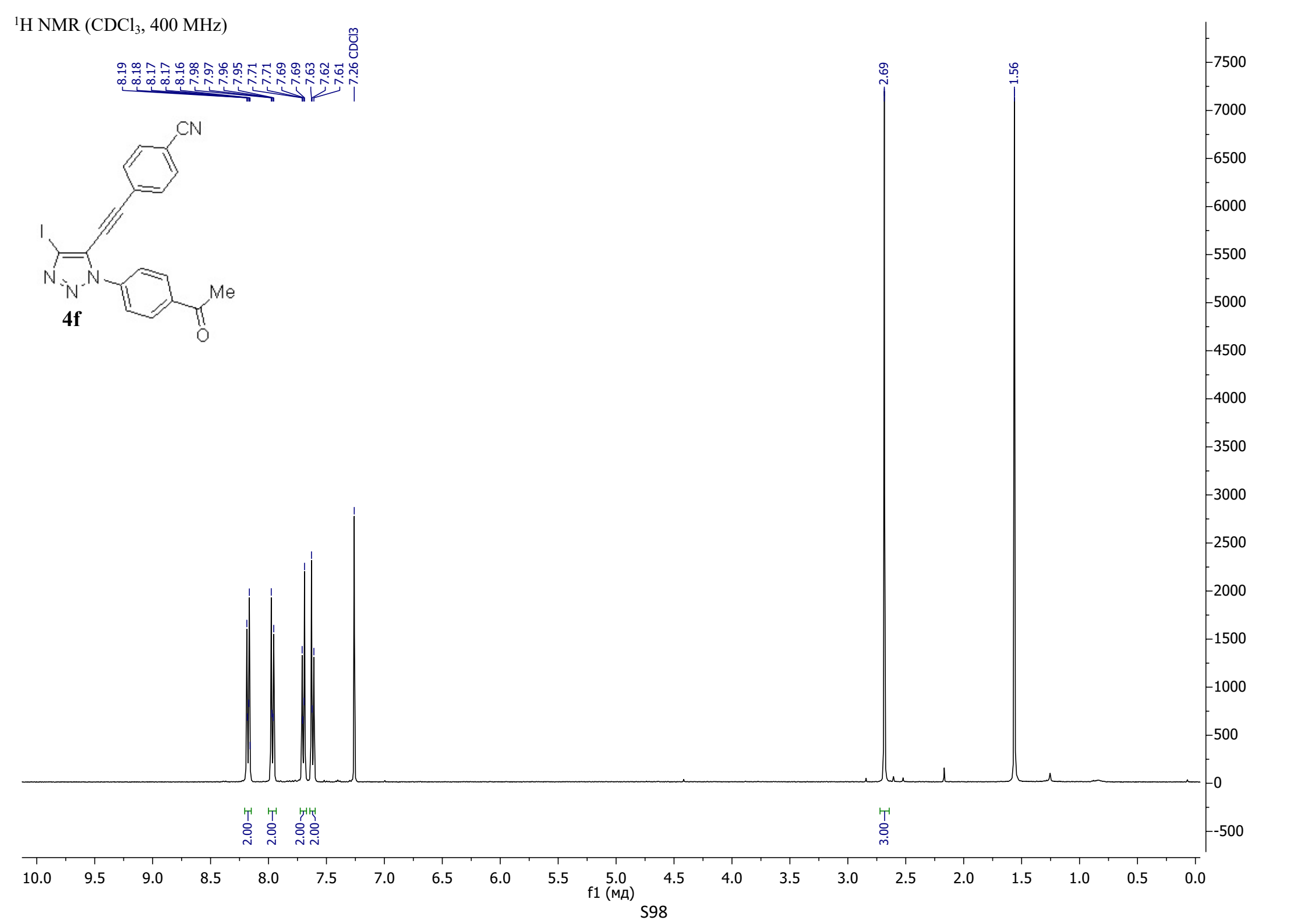


^{13}C NMR ($CDCl_3$, 101 MHz)

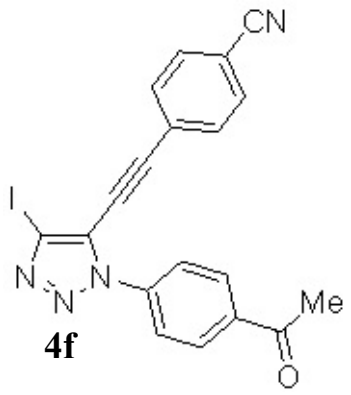


3f

^{1}H NMR ($CDCl_3$, 400 MHz)

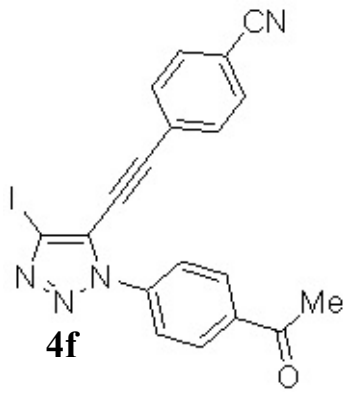


^{13}C NMR ($CDCl_3$, 101 MHz)



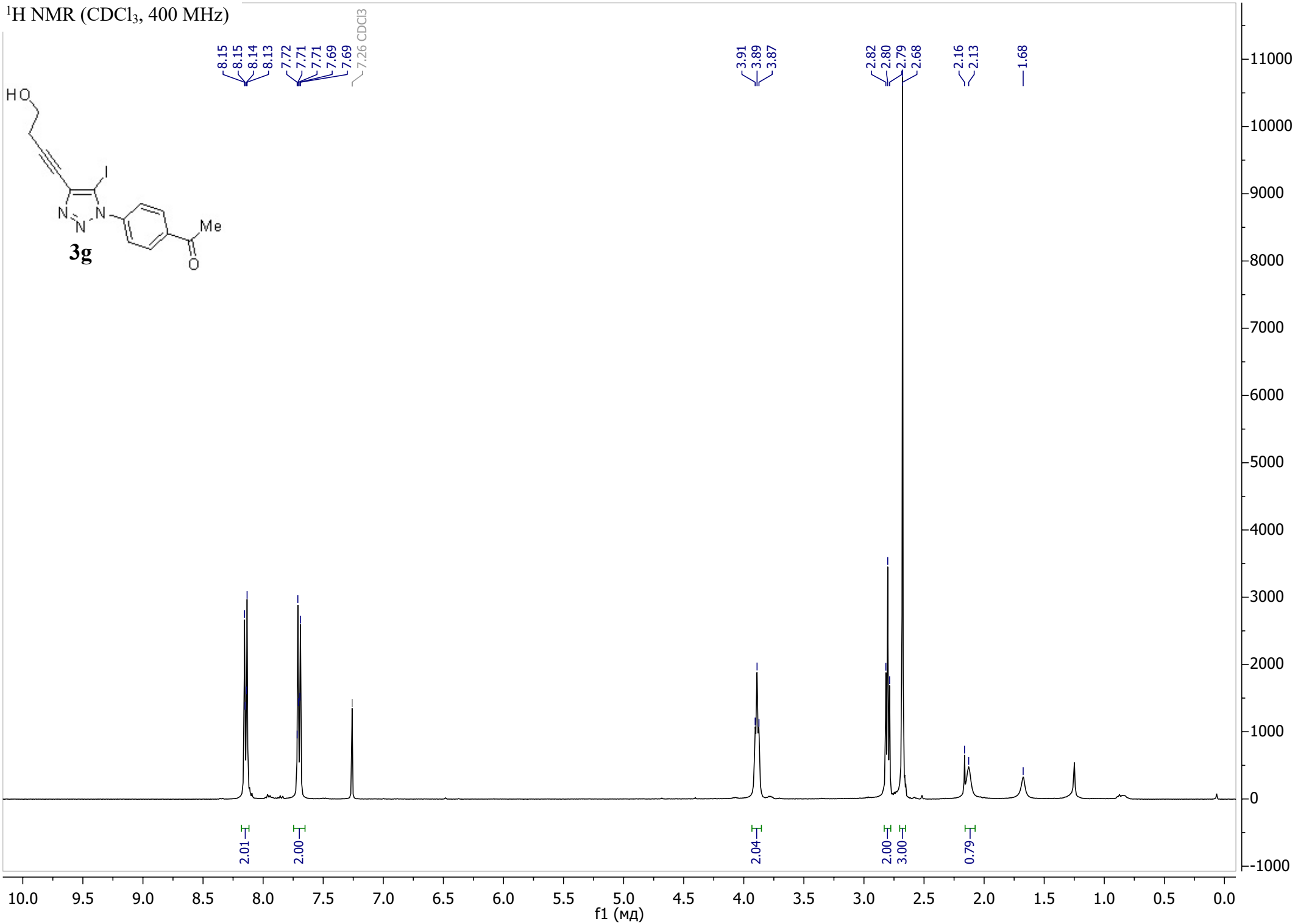
4f

^{13}C NMR ($CDCl_3$, 101 MHz)

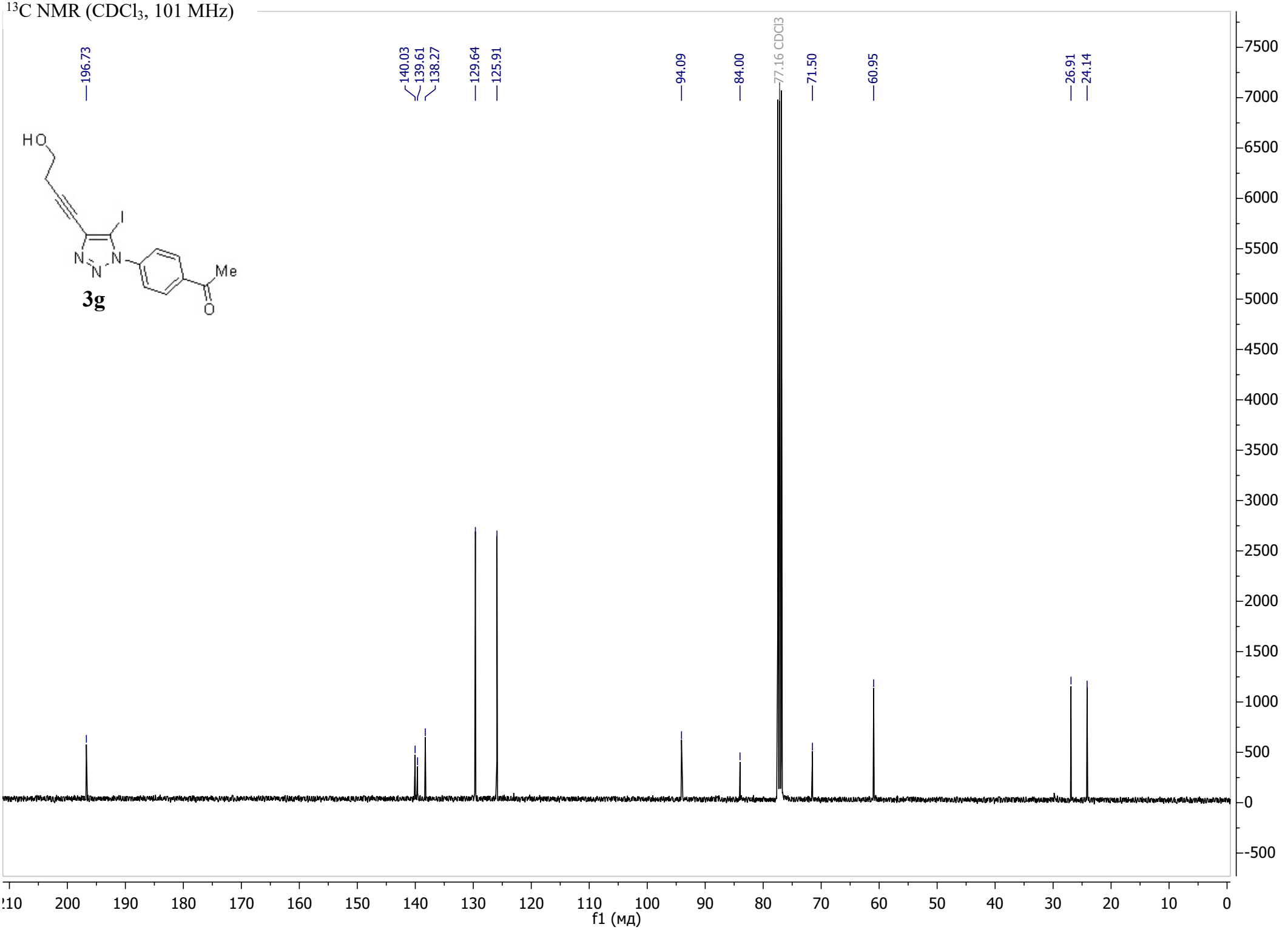


4f

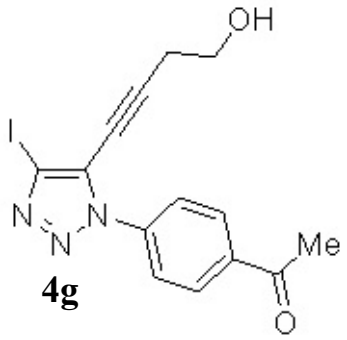
^{1}H NMR ($CDCl_3$, 400 MHz)



^{13}C NMR ($CDCl_3$, 101 MHz)



^{1}H NMR ($CDCl_3$, 400 MHz)



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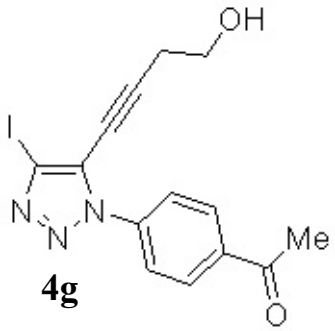
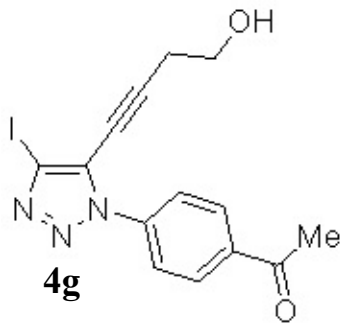
^{13}C NMR ($CDCl_3$, 101 MHz)



4g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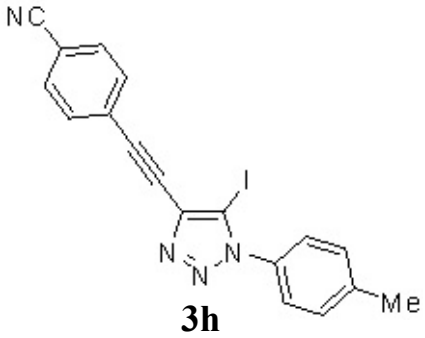
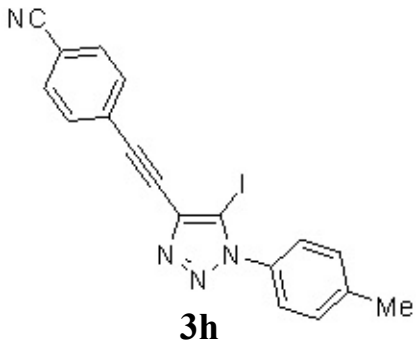
^{1}H NMR ($CDCl_3$, 400 MHz)



3h

^{13}C NMR (DMSO-d_6, 101 MHz)



3h

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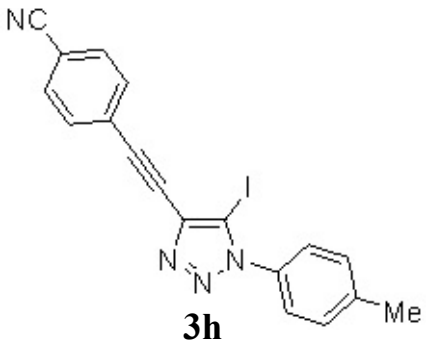

3h

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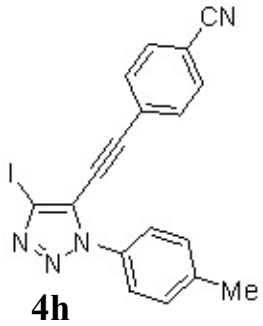

4h

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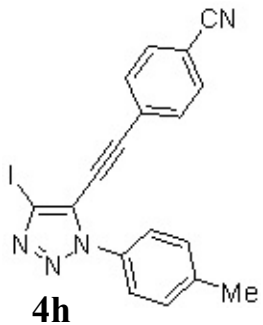

4h

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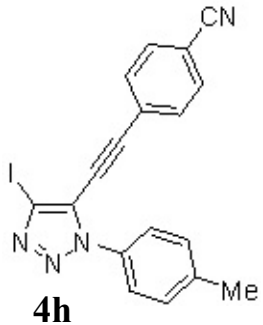

4h

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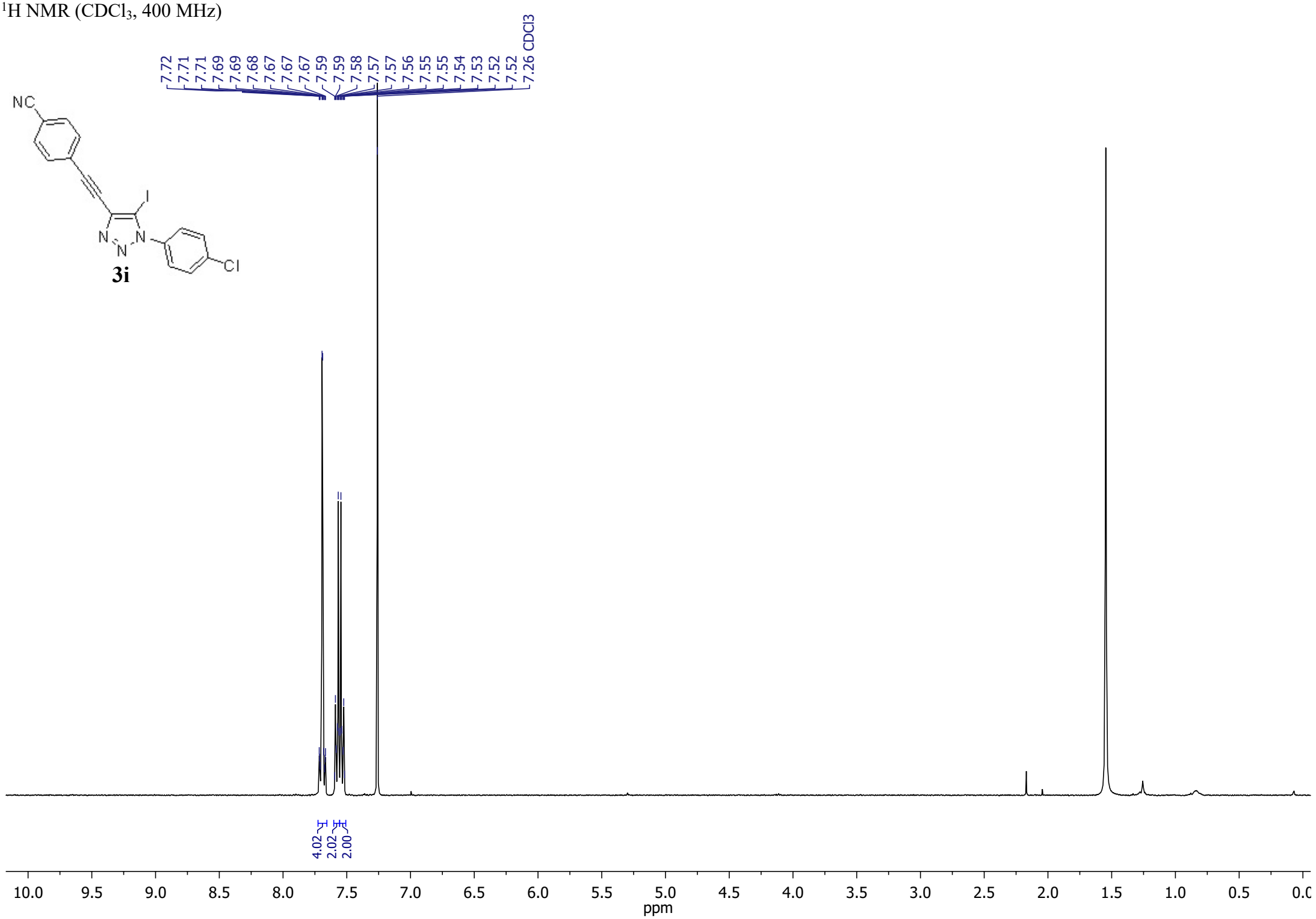

3i

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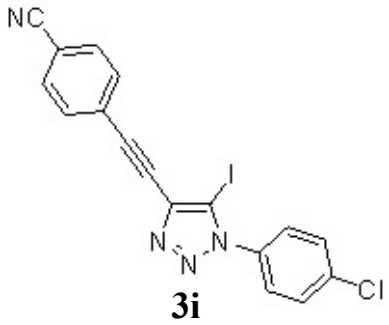
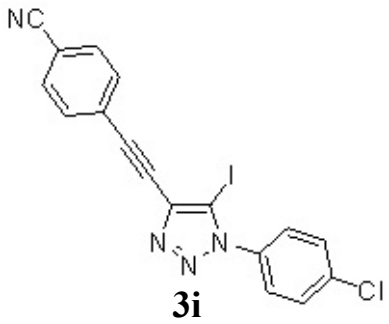


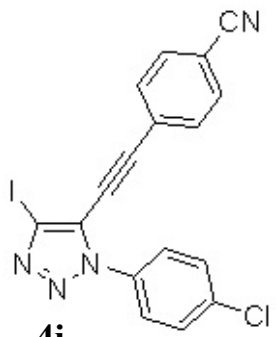
3i

^{13}C NMR ($CDCl_3$, 101 MHz)



3i

^{1}H NMR ($CDCl_3$, 400 MHz)



4i

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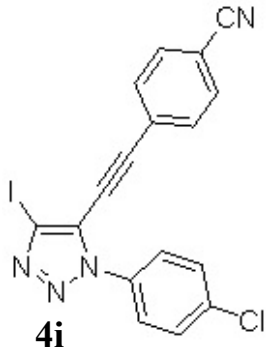

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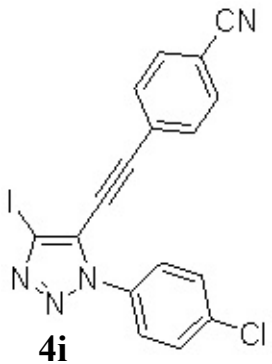

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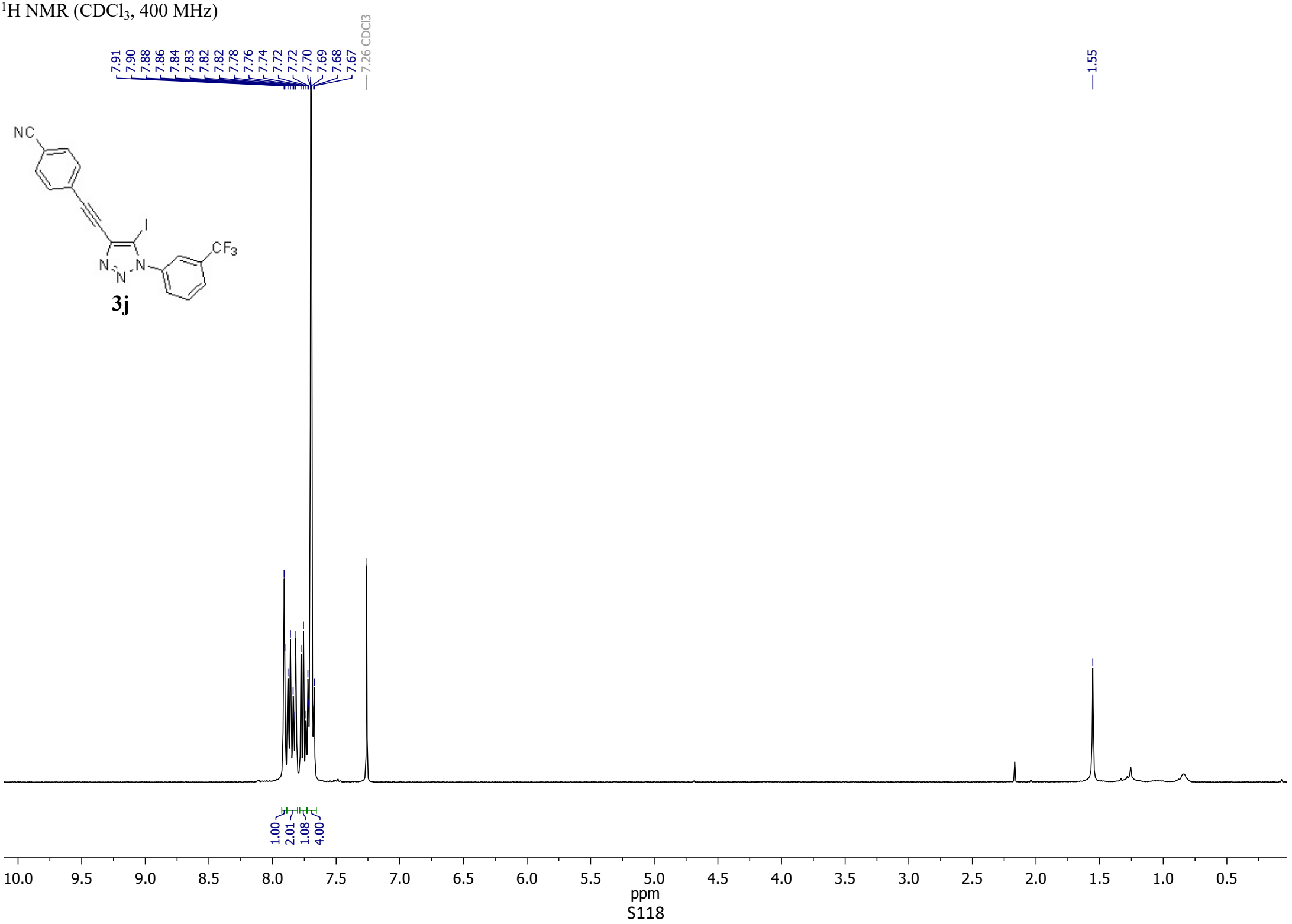

3j

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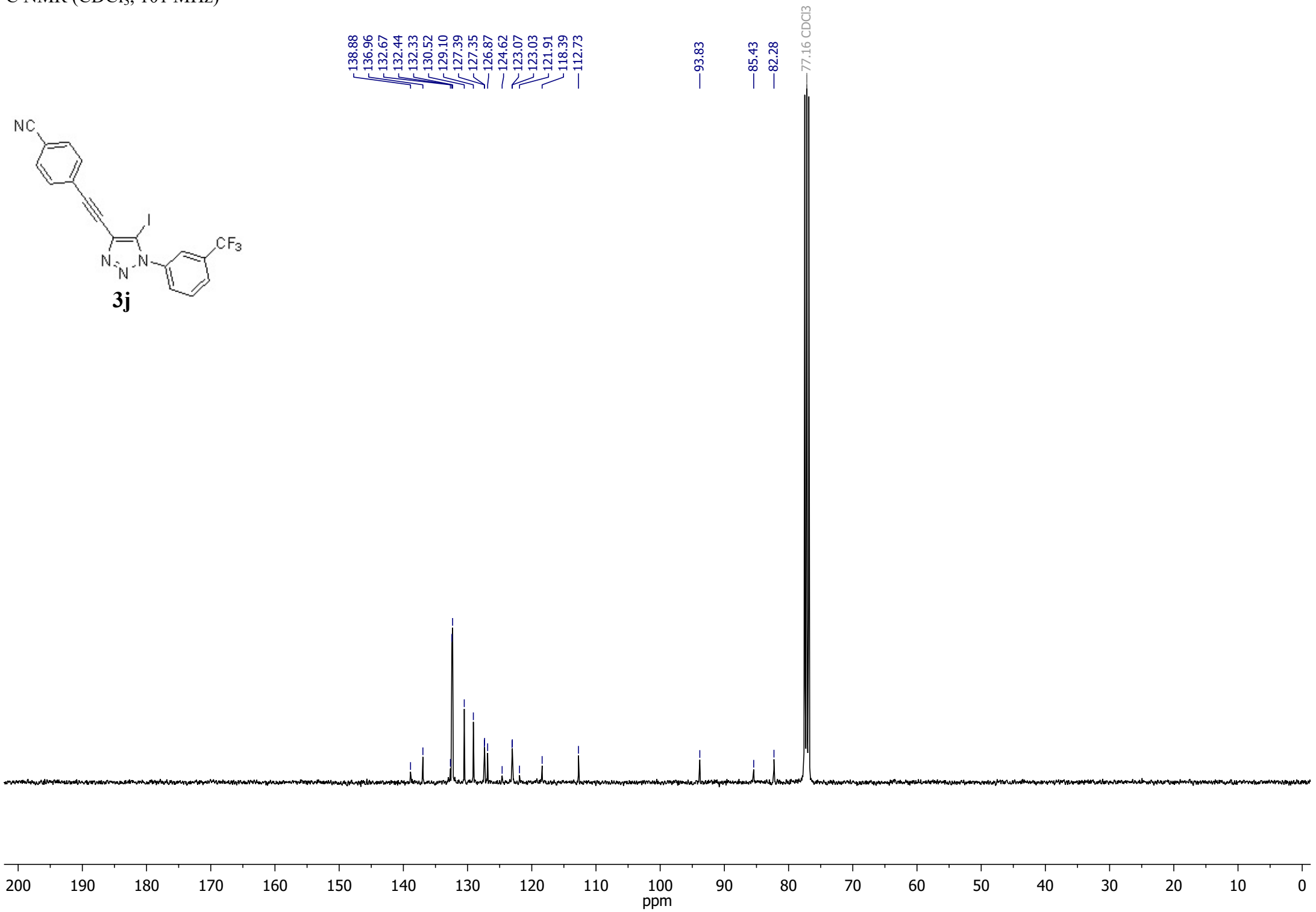

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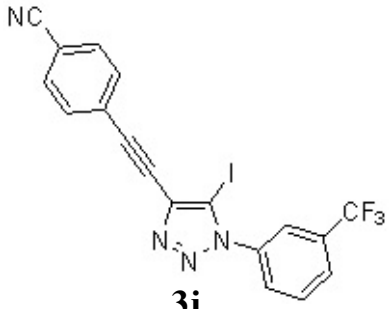

3j

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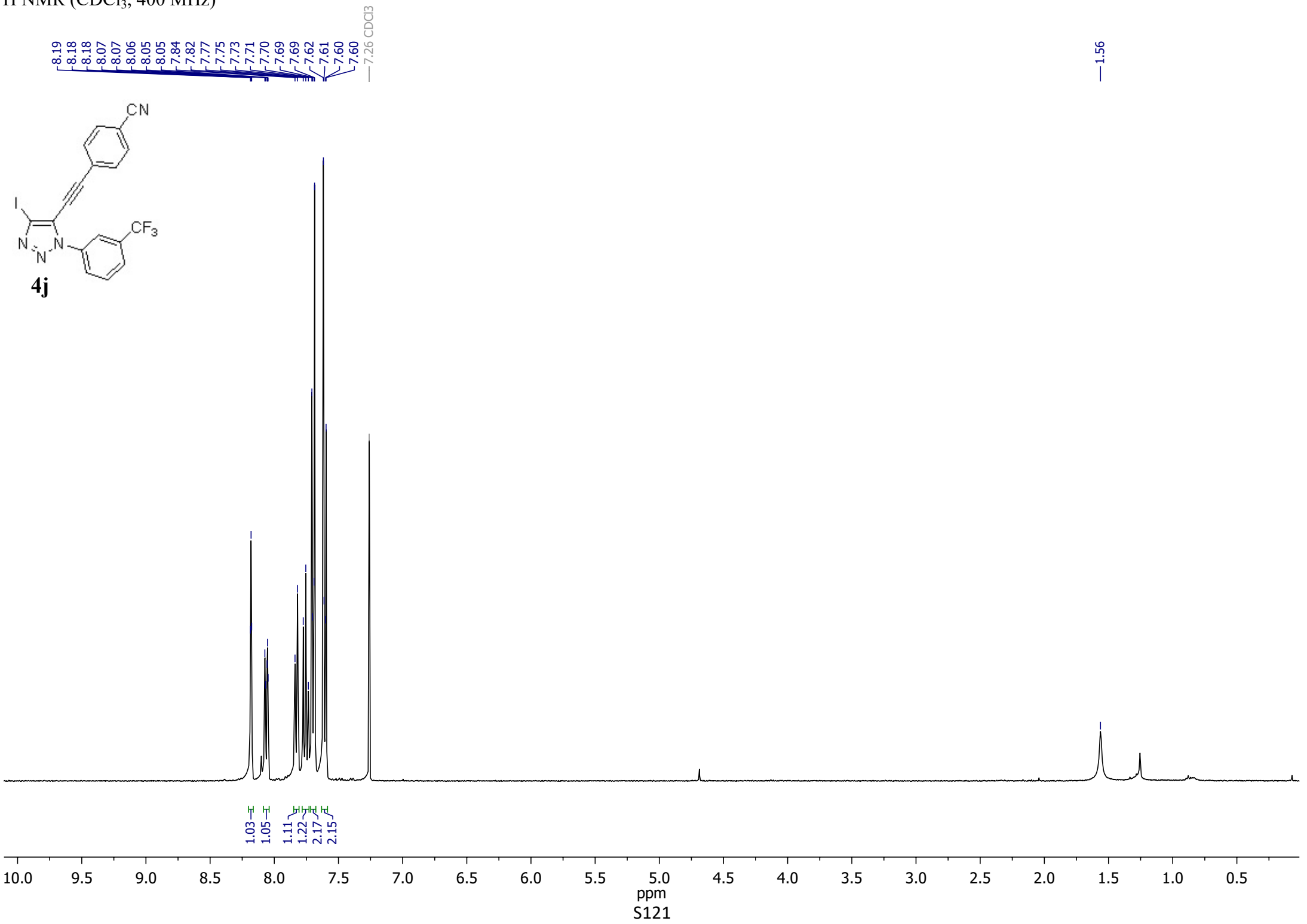
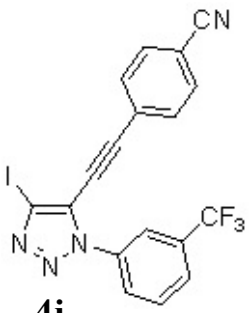


^{13}C NMR ($CDCl_3$, 101 MHz)



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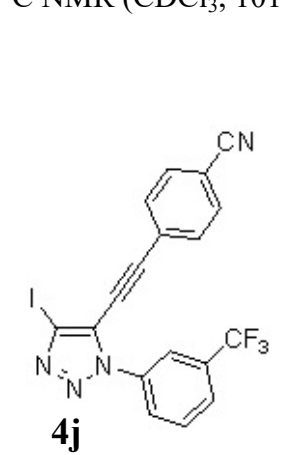

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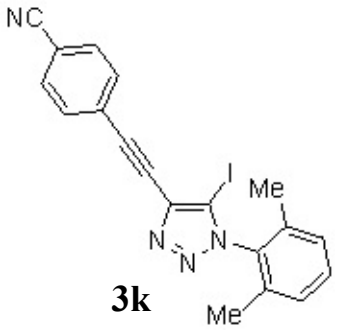

3k

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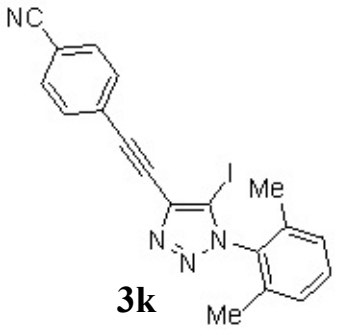

3k

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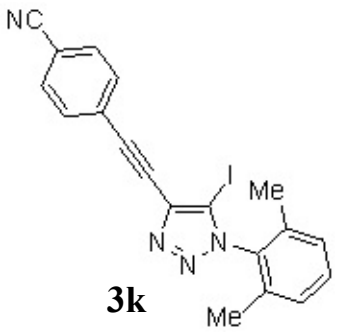

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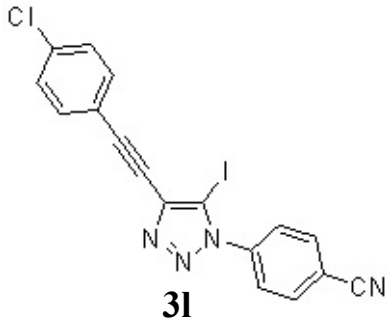

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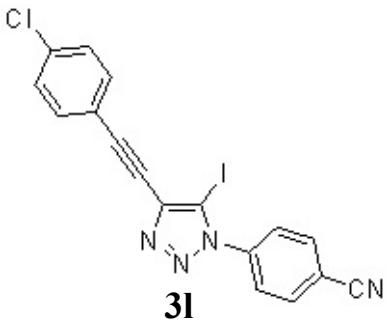

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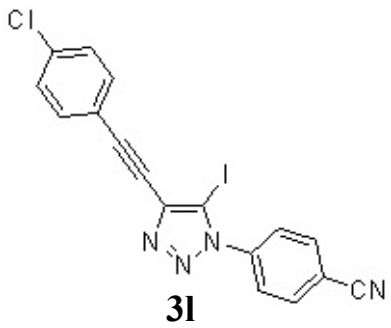

3l

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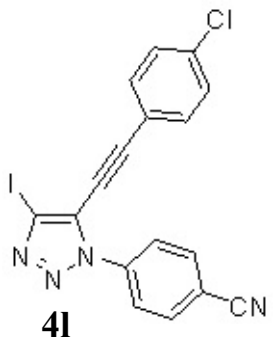

4l

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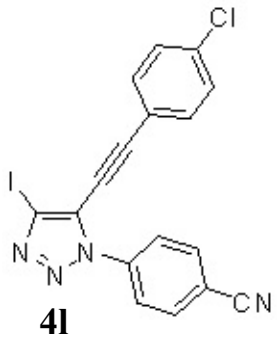

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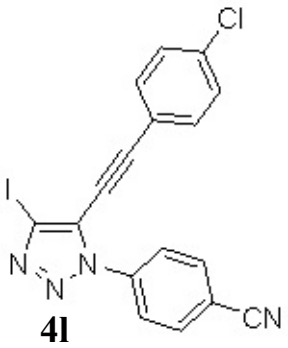
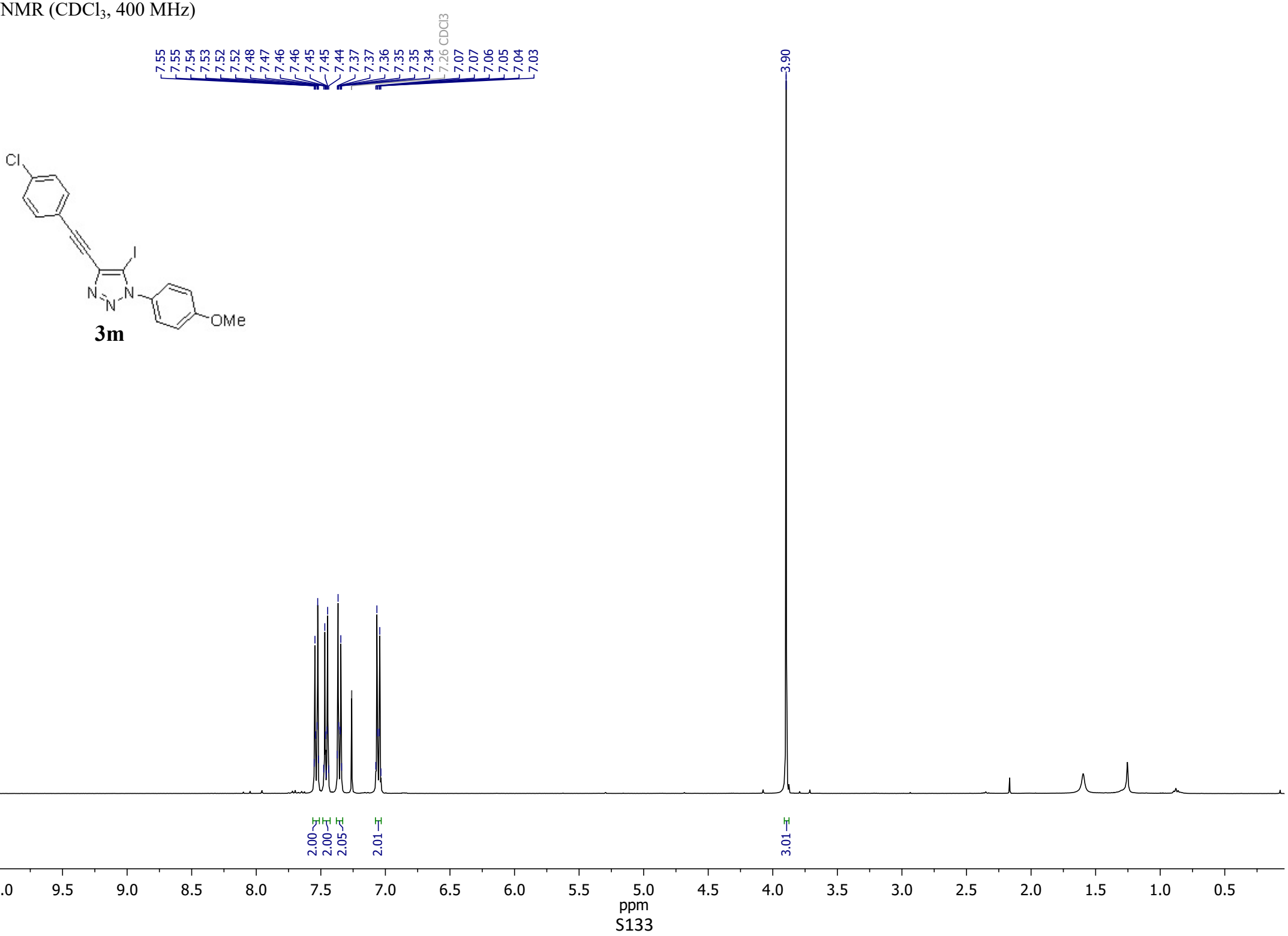
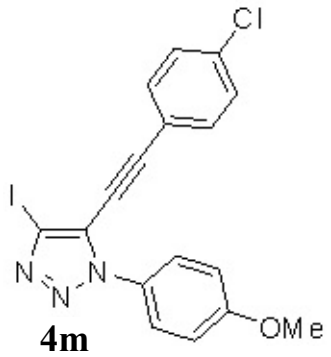


4l

^{1}H NMR ($CDCl_3$, 400 MHz)

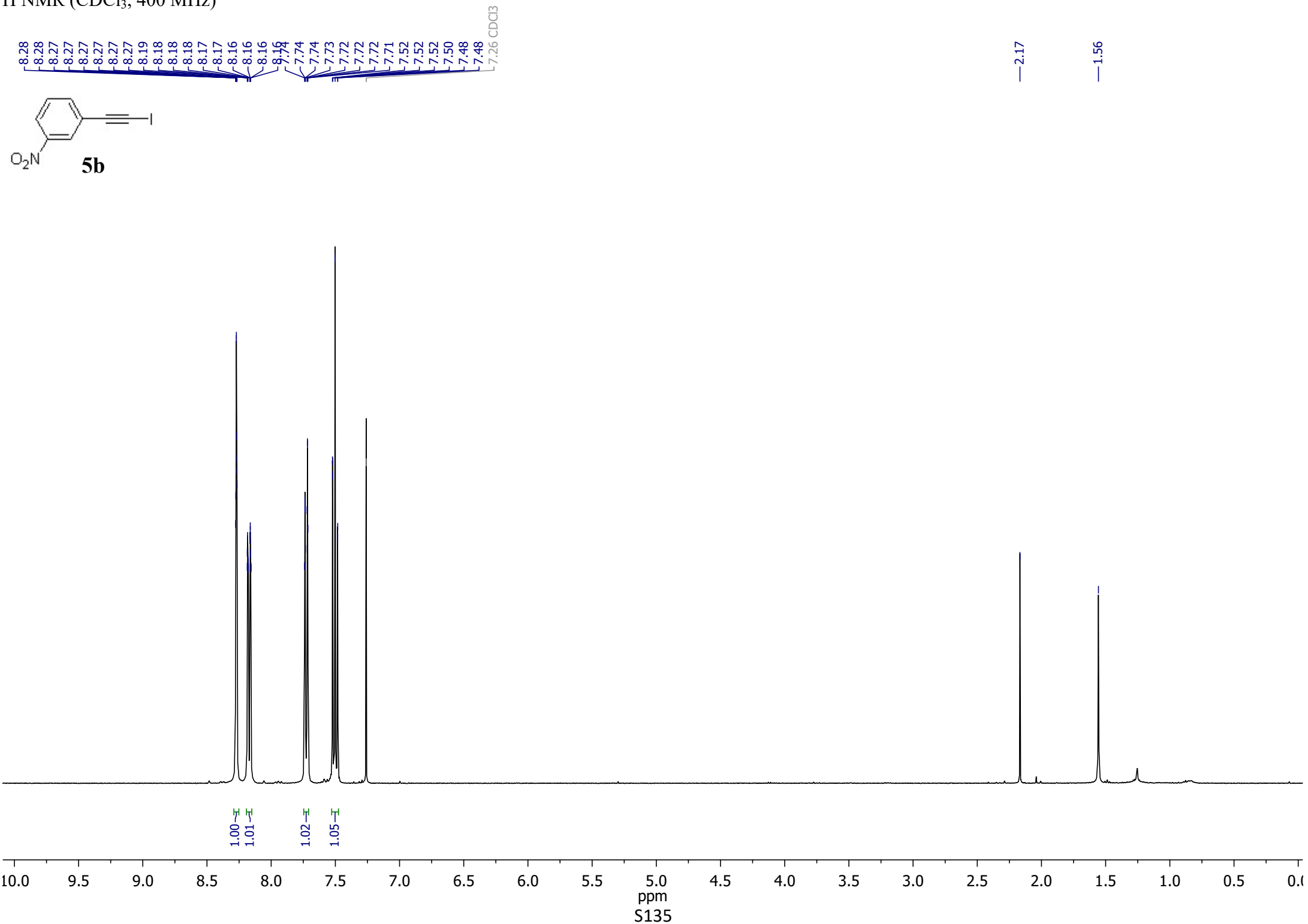


^{1}H NMR ($CDCl_3$, 400 MHz)



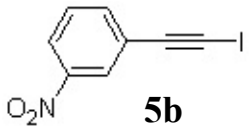
4m

^{1}H NMR ($CDCl_3$, 400 MHz)



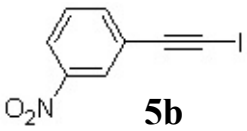
5b

^{13}C NMR ($CDCl_3$, 101 MHz)



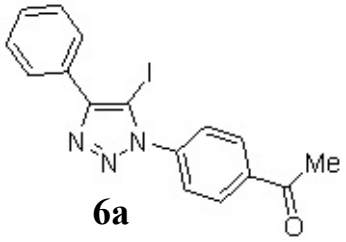
5b

^{13}C NMR ($CDCl_3$, 101 MHz)



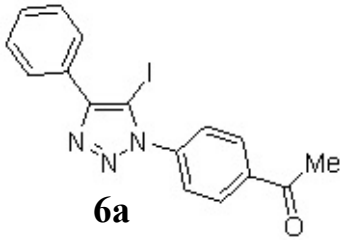
5b

^{1}H NMR (DMSO-d_6, 400 MHz)



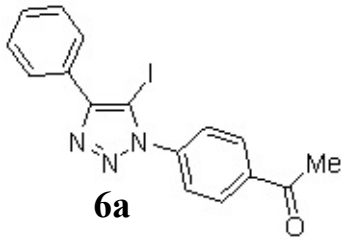
6a

^{13}C NMR (DMSO-d_6, 101 MHz)



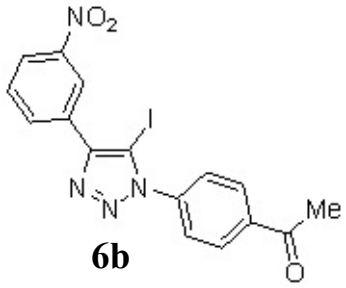
6a

^{13}C NMR (DMSO-d_6, 101 MHz)



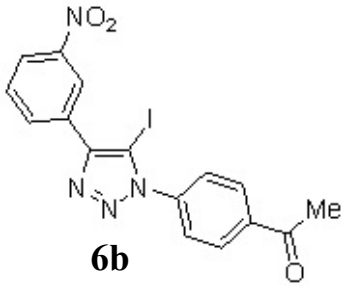
6a

^{1}H NMR (DMSO-d_6, 400 MHz)



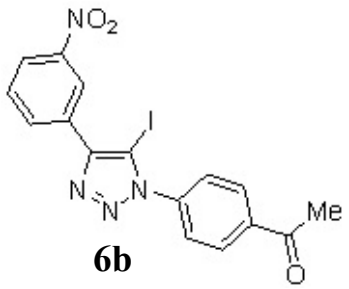
6b

^{1}H NMR (DMSO-d_6, 400 MHz)



6b

^{1}H NMR (DMSO-d_6, 400 MHz)



6b