Supplementary Materials

Design and synthesis of imidazoles linearly connected to carbocyclic and heterocyclic rings via a 1,2,3-triazole linker. Reactivity of β-azolyl enamines towards heteroaromatic azides

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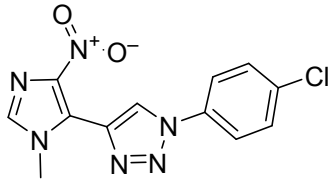
General experimental information

All melting points were determined with a Stuart SMP3 apparatus and are uncorrected. IR spectra were obtained with Bruker Alpha (NPVO, ZnSe) IR-Fur spectrometer. ^{1}H NMR and ^{13}C NMR spectra were recorded on a Bruker Avance II spectrometer with DMSO-d_6 or $CDCl_3$ as the solvent (400 and 100 MHz, respectively) using Me_4Si as an internal standard. ^{1}H NMR data are reported as the chemical shift in parts per million, multiplicity (s, singlet; d, doublet; t, triplet; m, multiplet), coupling constant in hertz, and number of protons. High-resolution mass spectra (HRMS) were obtained on Bruker impact HD Q-TOF analyser in the ESI mode. Mass spectra were recorded with Shimadzu GCMS-QP2010 Ultra instrument in electron ionization (EI) mode. Electron energy - 70eV. The reactions were monitored by analytical TLC on aluminium foil plates with 0.2 mm silica gel with a fluorescent indicator visualed under UV light. The column chromatography was performed with 60−120 mesh silica gel.

The calculations were conducted utilizing Gaussian 09 D.01[1] code with DFT approach using mPW1K density functional,[2,3] specially designed for kinetics by Truhlar group, with 6-311++(d,p) basis set on all atoms and superfine density grid. Conductor-like polarizable continuum solvation model C-PCM[4,5] was applied to simulate the solvation effect of *N*,*N*-dimethyformamide (DMF) – the solvent used in the experimental work. The geometry optimization procedures were performed with "tight" optimization criteria. Vibrational analysis proved that each of the obtained relaxed geometry represents a minimum and each transition state geometry represents a first-order saddle point on the potential energy surface. Calculation of internal reaction coordinates (IRC) with the transition state geometries proved them connecting respective starting materials with products as reported. NBO analyses of the calculated structures was carried out with NBO 6.0 software.[6]

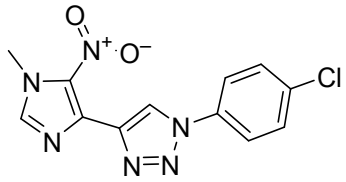
General method for synthesis of triazoles 3a-f.

A mixture of enamine **1** (1 mmol), appropriate azide **2** (1 mmol) and DMF (0.6 mL) was stirred for 1–2 h at 100 °C (for compounds **3e** and **3f** – 3 hours at 130–140 °C). After cooling ethanol (5 mL) was added to the reaction mixture and after 10 min of stirring the precipitate was filtered off, washed with ethanol and dried.

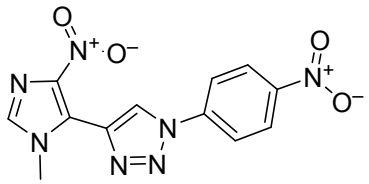


1-(4-Chlorophenyl)-4-(1-methyl-4-nitro-1H-imidazol-5-yl)-1H-1,2,3-triazole (3a). Synthesized from enamine **1c** and azide **2a**. Reaction's time is 1.5 h Yellowish powder; yield 0.176 g (58%); m. p. 236–237 °C;

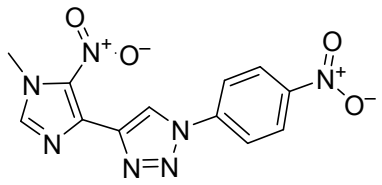
IR (ν/cm^{-1}) 1500; ^{1}H NMR (400 MHz, DMSO-d_6) δ 3.85–3.99 (s, 3H, NCH_3), 7.60–7.71 (m, 2H, *J* 9.0 Hz, HAr), 7.98 (s, 1H, CH), 8.02–8.11 (m, 2H, *J* 9.0, HAr), 9.35 (s, 1H, CH); ^{13}C NMR (100 MHz, DMSO-d_6) δ 34.3 (NCH_3), 122.1 ($2C^{Ar}$), 122.2 (C-5^{imidaz}), 125.9 (C-5^{triaz}), 130.0 ($2C^{Ar}$), 133.56 (C^{Ar}), 134.8 (C-4^{triaz}), 134.9 (C^{Ar}), 138.5 (C-2^{imidaz}), 144.1 (C-4^{imidaz}); MS-EI (*m/z*) 304 $[M]^+$; Anal. Calcd (%) for $C_{12}H_9ClN_6O_2$: C, 47.30; H, 2.98; N, 27.58. Found: C, 47.19; H, 3.37; N, 27.96. Supplementary crystallographic data for the compound **3a** (CCDC 1580078) can be obtained free of charge from The Cambridge Crystallographic Data Center via www.ccdc.cam.ac.uk/data_request/cif.



1-(4-Chlorophenyl)-4-(1-methyl-5-nitro-1H-imidazol-4-yl)-1H-1,2,3-triazole (3b). Synthesized from enamine **1d** and azide **2a**. Reaction's time is 1.5 h Pink powder; yield 0.267 g (88%); m. p. 249–250°C; IR (ν/cm^{-1}) 3181, 3094, 3042, 3013, 1587, 1494; ^{1}H NMR (400 MHz, DMSO-d_6) δ 4.01 (s, 3H, NCH_3), 7.57–7.68 (m, 2H, *J* 9.0 Hz, HAr), 7.98–8.07 (m, 2H, *J* 9.0 Hz, HAr), 8.12 (s, 1H, CH), 9.14 (s, 1 H, CH); ^{13}C NMR (100 MHz, DMSO-d_6) δ 35.6 (NCH_3), 122.7 ($2C^{Ar}$), 124.1 (C-5^{triaz}), 130.3 ($2C^{Ar}$), 133.9 (C^{Ar}), 134.0 (C^{Ar}), 135.6 (C-4^{imidaz}), 135.8 (C-4^{triaz}), 140.7 (C-2^{imidaz}), 142.3 (C-5^{imidaz}); MS-EI (*m/z*) 304 $[M]^+$; Anal. Calcd (%) for $C_{12}H_9ClN_6O_2$: C, 47.30; H, 2.98; N, 27.58. Found: C, 47.24; H, 2.73; N, 27.73.

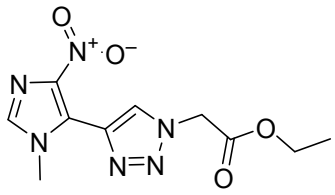


4-(1-Methyl-4-nitro-1H-imidazol-5-yl)-1-(4-nitrophenyl)-1H-1,2,3-triazole (3c). Synthesized from enamine **1c** and azide **2b**. Reaction's time is 1.2 h . Yellowish powder; yield 0.277 g (88%); m. p. Calcd (%) for $C_{12}H_9N_7O_4$: C, 45.72; H, 2.88; N, 31.10. Found: C, 46.08; H, 3.15; N, 30.95.

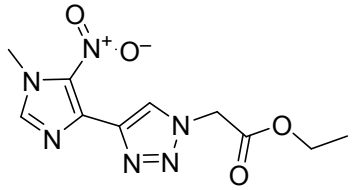


4-(1-Methyl-5-nitro-1H-imidazol-4-yl)-1-(4-nitrophenyl)-1H-1,2,3-triazole (3d). Synthesized from enamine **1d** and azide **2b**. Reaction's time is 1.0 h. Pink powder; yield 0.214 (68%); m. p. > 300 °C; IR (ν/cm^{-1}) 1497, 1335; ^{1}H NMR (400 MHz, DMSO-d_6) δ 4.02 (s, 3H, CH_3), 8.13 (s, 1H, CH), 8.31–8.41 (m,

2H, *J* 9.3 Hz, HAr), 8.41–8.51 (m, 2H, *J* 9.3 Hz, HAr), 9.36 (s, 1H, H-5); ^{13}C NMR (101 MHz, DMSO-d_6) δ 35.3 (NCH_3), 121.1 ($2C^{Ar}$), 123.9 (C-5^{triaz}), 125.4 ($2C^{Ar}$), 133.1 (C-4^{imidaz}), 135.2 (C-5^{imidaz}), 140.6 (C-4^{triaz}), 140.7 (C^{Ar}), 141.9 (C-2^{imidaz}), 147.06 (C^{Ar}); MS-EI (*m/z*) 315 $[M]^+$; Anal. Calcd (%) for $C_{12}H_9N_7O_4$: C, 45.72; H, 2.88; N, 31.10. Found: C, 45.42; H, 3.08; N, 30.83.



Ethyl 2-(4-(1-methyl-4-nitro-1H-imidazol-5-yl)-1H-1,2,3-triazol-1-yl)acetate (3e). Synthesized from enamine **1c** and azide **2c**. Reaction's time is 3h. Pink powder; yield 0.126 g (45%); m. p. 133–135 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 1.30 (t, 3H, *J* 7.1 Hz, $OCH_2C\underline{H}_3$), 3.92 (s, 3H, NCH_3), 4.24 (q, 2H, *J* 7.1 Hz, $OC\underline{H}_2CH_3$), 5.47 (s, 2H, CH_2), 7.91 (s, 1H, CH), 8.75 (s, 1H, CH); ^{13}C NMR (100 MHz, DMSO-d_6) δ 13.9 (CH_3), 34.6 (NCH_3), 50.6 (NCH_2), 61.6 (OCH_2), 122.8 (C-5^{imidaz}), 129.4 (C-5^{triaz}), 133.7 (C-4^{triaz}), 138.3 (C-4^{imidaz}), 138.3 (C-2^{imidaz}), 166.9 (C=O); MS-EI (*m/z*) 280 $[M]^+$; Anal. Calcd (%) for $C_{10}H_{12}N_6O_4$: C, 42.86; H, 4.32; N, 29.99. Found: C, 43.05; H, 4.47; N, 30.18.



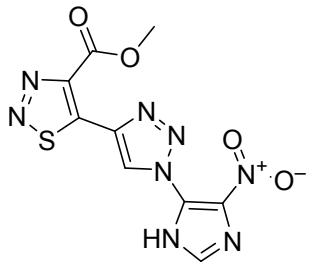
Ethyl 2-(4-(1-methyl-5-nitro-1H-imidazol-4-yl)-1H-1,2,3-triazol-1-yl)acetate (3f). Synthesized from enamine **1d** and azide **2c**. Reaction's time is 3h. Pink powder; yield 0.148 g (53%); m. p. 185–186 °C; IR (ν/cm^{-1}) 1736, 1503, 1356, 1268; ^{1}H NMR (400 MHz, DMSO-d_6) δ 1.27 (t, 3H, *J* 7.1 Hz, $OCH_2C\underline{H}_3$), 3.98 (s, 3H, NCH_3), 4.22 (q, 2H, *J* 7.1 Hz, $OC\underline{H}_2CH_3$), 5.44 (s, 2H, CH_2), 8.09 (s, 1H, CH), 8.64 (s, 1H, CH); ^{13}C NMR (100 MHz, DMSO-d_6) δ 13.9 (CH_3), 35.4 (NCH_3), 50.4 (NCH_2), 61.5 (OCH_2), 127.4 (C-4^{triaz}), 134.2 (C-5^{triaz}), 134.6 (C-4^{imidaz}), 138.8 (C-5^{imidaz}), 142.0 (C-2^{imidaz}), 167.1 (C=O); MS-EI (*m/z*) 280 $[M]^+$; Anal. Calcd (%) for $C_{10}H_{12}N_6O_4$: C, 42.86; H, 4.32; N, 29.99. Found: C, 43.12; H, 4.01; N, 30.34.

General method for synthesis of 1,2,3-triazoles 4a, d, g, i.

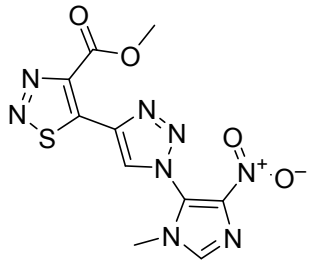
A mixture of enamine **1** (1 mmol), appropriate azide **2** (1 mmol) and DMF (0.4 mL) was stirred for 12-16 h at room temperature. Ethanol (5 mL) was added to the reaction mixture and after 10 min of stirring the formed precipitate of dimethylammonium salt of compound **4** was filtered off, washed with ethanol and dried. This salt was suspended in 1% nitric acid solution in water (10 mL) and stirred for 10 min. The solids were filtered off and washed with water. Crude products were crystallized from ethanol (**4a, d**) or refluxed in ethanol (10 mL) for 10 min and filtered off (**4g, i**).

General method for synthesis of 1,2,3-triazoles 4b, c, f.

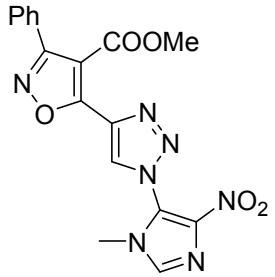
A mixture of enamine **1** (1 mmol), appropriate azide **2** (1 mmol) and DMF (0.4 mL) was stirred for 13-16 h at room temperature. Ethanol (5 mL) was added to the reaction mixture and after 10 min of stirring the formed precipitate was filtered off, washed with ethanol and dried.



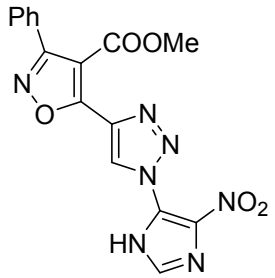
Methyl 5-[1-(4-nitro-1H-imidazol-5-yl)-1H-1,2,3-triazol-4-yl]-1,2,3-thiadiazole-4-carboxylate (4a). Synthesized from enamine **1a** and azide **2e**; reaction's time is 14 h. Yellowish powder. Yield 0.171 g (53%); m.p. 241–242 °C; IR (ν/cm^{-1}) 3155, 2952, 2552, 1741, 1499, 1358; ^{1}H NMR (400 MHz, DMSO-d_6) δ 4.03 (s, 3H, OCH_3), 7.08 (s, 1H, CH^{imidaz}), 9.04 (s, 1H, H-5); ^{13}C NMR (100 MHz, DMSO-d_6) δ 53.0 (OCH_3), 127.3 (C-5^{imidaz}), 128.6 (C-5^{triaz}), 133.7 (C-4^{imidaz}), 134.9 (C-4^{triaz}), 135.3 (C-2^{imidaz}), 146.6 (C-5^{thiadiaz}), 151.1 (C-4^{thiadiaz}), 160.7 (C=O). HRMS (ESI) $[M+H]^+$ found *m/z* 323.0308, calcd for $C_9H_6N_8O_4S$ 323.0305; Anal. Calcd (%): C, 33.54; H, 1.88; N, 34.77. Found: C, 33.39; H, 1.50; N, 34.66.



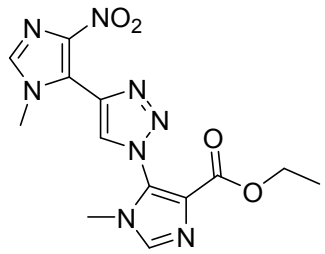
Methyl 5-[1-(1-methyl-4-nitro-1H-imidazol-5-yl)-1H-1,2,3-triazol-4-yl]-1,2,3-thiadiazole-4-carboxylate (4b). Synthesized from enamine **1a** and azide **2d**; reaction's time is 14 h. Yellowish powder. Yield 0.275 g (82%), m. p. 230 °C (decomp.); IR (ν/cm^{-1}) 1727, 1608, 1525, 1514, 1338; ^{1}H NMR (400 MHz, DMSO-d_6) δ 3.64 (s, 1H, NCH_3), 4.04 (s, 3H, OCH_3), 8.14 (s, 1H, CH^{imid}), 9.49 (s, 1H, H-5); ^{13}C NMR (100 MHz, DMSO-d_6) δ 32.4 (NCH_3), 53.0 (OCH_3), 122.4 (C-5^{imidaz}), 130.1 (C-5^{triaz}), 135.3 (C-4^{triaz}), 136.3 (C-2^{imidaz}), 139.5 (C-4^{imidaz}), 146.7 (C-5^{thiadiaz}), 150.8 (C-4^{thiadiz}), 160.6 (C=O). HRMS (ESI) $[M+H^+]$ found *m/z* 337.0460, calcd for $C_{10}H_8N_8O_4S$ 337.0462; Anal. Calcd (%): C, 35.72; H, 2.40; N, 33.32. Found: C, 35.89; H, 2.58; N, 33.02.



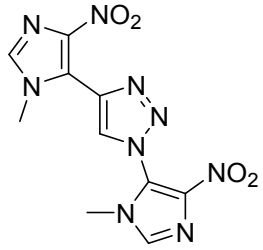
Methyl 5-(1-(1-methyl-4-nitro-1H-imidazol-5-yl)-1H-1,2,3-triazol-4-yl)-3-phenylisoxazole-4-carboxylate (4c). Synthesized from enamine **1b** and azide **2d**; reaction's time is 16 h. Yellow powder. Yield 0.182 g (46%); m. p. 187–188 °C; IR (ν/cm^{-1}) 1718, 1609, 1511, 1337; ^{1}H NMR (400 MHz, DMSO-d_6) δ 3.66 (s, 3H, NCH_3), 3.77 (s, 3H, OCH_3), 7.45–7.59 (m, 3H, HAr), 7.66 (m, 2H, HAr), 8.14 (s, 1H, CH^{imidaz}), 9.46 (s, 1H, H-5); ^{13}C NMR (100 MHz, DMSO-d_6) δ 32.5 (NCH_3), 52.3 (OCH_3), 108.5 (C-4^{izoxaz}), 122.5 (C-5^{imidaz}), 127.4 (C^{Ph}), 128.3 ($2C^{Ph}$), 129.0 ($2C^{Ph}$), 130.2 (C^{Ph}), 131.5 (C-5^{triaz}), 134.6 (C-4^{triaz}), 136.3 (C-2^{imidaz}), 139.4 (C-4^{imidaz}), 161.0 (C=O), 162.4 (C-3^{izoxaz}), 163.1 (C-5^{izoxaz}). HRMS (ESI) $[M+H]^+$ found *m/z* 396.1053, calcd for $C_{17}H_{13}N_7O_5$ 396.1051; Anal. Calcd (%): C, 51.65; H, 3.31; N, 24.80. Found: C, 51.31; H, 2.97; N, 24.86.



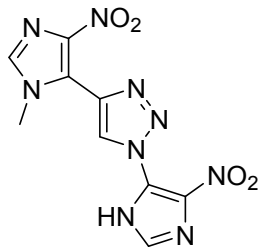
Methyl 5-(1-(4-nitro-1H-imidazol-5-yl)-1H-1,2,3-triazol-4-yl)-3-phenylisoxazole-4-carboxylate (4d). Synthesized from enamine **1b** and azide **2e**; reaction's time is 16 h. White powder. Yield 0.198 g (52%), m. p. 219 °C (decomp.); IR (ν/cm^{-1}) 1736, 1613, 1524, 1361; ^{1}H NMR (400 MHz, DMSO-d_6) δ 3.78 (s, 3H, OCH_3), 7.43–7.59 (m, 3H, HAr), 7.60–7.71 (m, 2H, HAr), 7.96 (s, 1H, CH^{imid}), 9.40 (s, 1H, H-5); ^{13}C NMR (100 MHz, DMSO-d_6) δ 52.2 (OCH_3), 108.3 (C-4^{isoxaz}), 127.3 (C-5^{isoxaz}), 127.4 (C-5^{imidaz}), 128.3 ($2C^{Ph}$), 129.0 ($2C^{Ph}$), 129.9 (C-5^{triaz}), 130.2 (C^{Ph}), 134.0 (C-4^{imidaz}), 134.2 (C-4^{triaz}), 135.6 (C-2^{imidaz}), 161.1 (C=O), 162.4 (C^{Ph}), 163.4 (C-3^{isoxaz}). HRMS (ESI) $[M+H]^+$ found *m/z* 382.0896, calcd for $C_{16}H_{11}N_7O_5$ 382.0894; Anal. Calcd (%): C, 50.40; H, 2.91; N, 25.71. Found: C, 50.54; H, 2.65; N, 25.54.



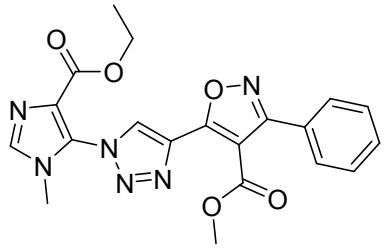
Ethyl 1-methyl-5-[4-(1-methyl-4-nitro-1*H*-imidazol-5-yl)-1*H*-1,2,3-triazol-1-yl]-1*H*-imidazole-4-carboxylate (4e). A mixture of azide **2f** (1 mmol), enamine **1c** (1 mmol) and DMF (0.4 mL) was stirred at 100°C for 12 h. Ethanol (5 ml) was added to the cooled reaction mixture and the formed precipitate was filtered off, washed with ethanol and dried. Pink powder. Yield 0.087 g (25%), m. p. 230–232 °C; IR (ν/cm^{-1}) 3108, 1703, 1511, 1330; ^{1}H NMR (400 MHz, DMSO-d_6) δ 1.01 (t, *J* 7.0 Hz, 3H, CH_3), 3.85 (s, 3H, CH_3), 3.97, (s, 3H, CH_3), 4.13 (q, *J* 7.0 Hz, 2H, OCH_2) 8.06 (s, 1H, CH^{imid}), 8.15 (s, 1H, CH^{imid}), 9.02 (s, 1H, CH^{triaz}); ^{13}C NMR (100 MHz, DMSO-d_6) δ 13.5 (CH_3), 34.3 (NCH_3), 34.9 (NCH_3), 60.7 (OCH_2), 116.4 (C-5^{imidaz}), 122.4 (C-5^{imidaz}), 130.0 (C-5^{triaz}), 133.1 (C-4^{triaz}), 138.4 (C-4^{imidaz}), 138.5 (C-2^{imidaz}), 140.6 (C-2^{imidaz}), 144.0 (C-4^{imidaz}), 158.0 (C=O). HRMS (ESI) $[M+H]^+$ found *m/z* 347.1212, calcd for $C_{13}H_{14}N_8O_4$ 347.1211.



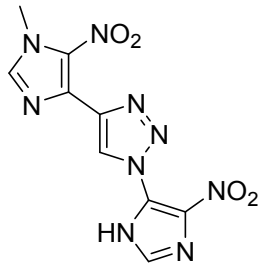
1,4-Bis(1-methyl-4-nitro-1H-imidazol-5-yl)-1H-1,2,3-triazole (4f). Synthesized from enamine **1c** and azide **2d**; reaction's time is 13 h. Orange powder. Yield 0.198 g (62%); m. p. 207 °C (decopm. with explosion); IR (ν/cm^{-1}) 1608, 1516, 1326; ^{1}H NMR (400 MHz, DMSO-d_6) δ 3.65 (s, 3H, NCH_3), 3.96 (s, 3H, NCH_3), 7.99 (s, 1H, CH^{imid}), 8.11 (s, 1H, CH^{imid}), 9.26 (s, 1H, CH^{triaz}); ^{13}C NMR (100 MHz, DMSO-d_6) δ 32.4 (NCH_3), 34.5 (NCH_3), 121.7 (C-5^{imidaz}), 122.7 (C-5^{imidaz}), 131.7 (C-5^{triaz}), 134.1 (C-4^{triaz}), 136.3 (C-2^{imidaz}), 138.7 (C-2^{imidaz}), 139.3 (C-4^{imidaz}), 144.3 (C-4^{imidaz}). HRMS (ESI) $[M+H]^+$ found *m/z* 320.0851, calcd for $C_{10}H_9N_9O_4$ 320.0850; Anal. Calcd (%): C, 37.62; H, 2.84; N, 39.49. Found: C, 37.82; H, 3.10; N, 39.44.



4-(1-Methyl-4-nitro-1H-imidazol-5-yl)-1-(4-nitro-1H-imidazol-5-yl)-1H-1,2,3-triazole (4g). Synthesized from enamine **1c** and azide **2e**; reaction's time is 12 h. White powder. Yield 0.156 g (51%), m. p. 217 °C (decopm. with explosion); IR (ν/cm^{-1}) 1587, 1524, 1360; ^{1}H NMR (400 MHz, DMSO-d_6) δ 3.94 (s, 3H, NCH_3), 7.97 (s, 1H, CH^{imid}), 8.01 (s, 1H, CH^{imid}), 9.18 (s, 1H, CH^{triaz}); ^{13}C NMR (100 MHz, DMSO-d_6) δ 34.4 (NCH_3), 121.8 (C-5^{imidaz}), 127.0 (C-5^{imidaz}), 130.3 (C-5^{triaz}), 133.4 (C-4^{imidaz}), 133.7 (C-4^{triaz}), 135.2 (C-2^{imidaz}), 138.6 (C-2^{imidaz}), 144.2 (C-4^{imidaz}). HRMS (ESI) $[M+H]^+$ found *m/z* 306.0696, calcd for $C_9H_7N_9O_4$ 306.0694; Anal. Calcd (%): C, 35.42; H, 2.31; N, 41.30. Found: C, 35.06; H, 2.44; N, 41.42.

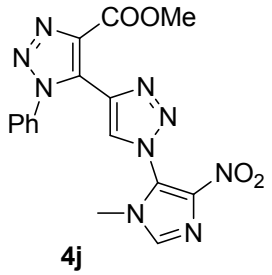


Methyl 5-(1-(4-(ethoxycarbonyl)-1-methyl-1H-imidazol-5-yl)-1H-1,2,3-triazol-4-yl)-3-phenylisoxazole-4-carboxylate (4h). A mixture of enamine **2f** (1 mmol), enamine **1b** (1 mmol) and DMF (0.4 mL) was stirred at 100°C for 12 h. After cooling, the reaction mixture was separated by column chromatography (silica gel, ethyl acetate). The fraction containing substance with R_f 0.36 was collected. Yellowish powder; yield 0.173 g (41%); m. p.145–148 °C; IR (ν/cm^{-1}) 3119, 1720, 1446, 1226, 1131; ^{1}H NMR (400 MHz, DMSO-d_6) δ 1.06 (t, *J* 7.0 Hz, 3H, CH_3), 3.74 (s, 3H, CH_3), 3.98 (s, 3H, CH_3), 4.14 (q, *J* 7.0 Hz, 2H, OCH_2), 7.40–7.60 (m, 3H, HPh), 7.60–7.75 (m, 2H, HPh), 8.11 (s, 1H, CH^{imid}), 9.16 (s, 1H, CH^{triaz}); ^{13}C NMR (100 MHz, DMSO-d_6) δ 13.4 (CH_3), 34.9 (NCH_3), 52.2 (OCH_3), 60.8 (OCH_2), 107.9 (C-4^{isoxaz}), 116.4 (C-5^{imidaz}), 127.5 (C^{Ph}), 128.4 (C^{Ph}), 128.9 (C^{Ph}), 129.6 (C-5^{triaz}), 130.2 (C^{Ph}), 133.7 (C-4^{triaz}), 138.3 (C-5^{imidaz}), 140.6 (C-2^{imidaz}), 158.0 (C=O^{imidaz}), 161.3 (C=O^{isoxaz}), 162.2 (C-3^{isoxaz}), 163.8 (C-5^{isoxaz}). MS-EI (*m/z*) 422 $[M]^+$; Anal. Calcd (%) for $C_{20}H_{18}N_6O_5$: C, 56.87; H, 4.30; N, 19.90. Found: C, 59.94; H, 4.26; N, 19.89.

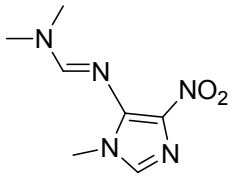


4-(1-Methyl-5-nitro-1H-imidazol-4-yl)-1-(4-nitro-1H-imidazol-5-yl)-1H-1,2,3-triazole (4i). Synthesized from enamine **1d** and azide **2e**; reaction's time is 12 h. White powder. Yield 0.201 g (66%); 290 °C (decopm. with explosion); IR (ν/cm^{-1}) 1533, 1523, 1371, 1356; ^{1}H NMR (400 MHz, DMSO-d_6) δ 4.02 (s, 3H, NCH_3), 7.99 (s, 1H, CH), 8.13 (s, 1H, CH), 9.09 (s, 1H), 14.88 (NH); ^{13}C NMR (100 MHz, DMSO-d_6) δ 35.7 (NCH_3), 127.3 (C-5^{imidaz}), 128.4 (C-5^{triaz}), 133.6 (C-4^{triaz}), 134.8 (C-4^{imidaz}), 135.1 (C-5^{imidaz}), 135.7 (C-

2^{imidaz}), 139.5 (C-4^{imidaz}), 142.4 (C-2^{imidaz}); HRMS (ESI) $[M+H]^+$ found *m/z* 306.0696, calcd for $C_9H_7N_9O_4$ 306.0694; Anal. Calcd (%): C, 35.42; H, 2.31; N, 41.30. Found: C, 35.42; H, 2.31; N, 41.30.



4j

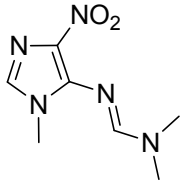


5a

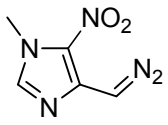
Methyl 1-(1-methyl-4-nitro-1H-imidazol-5-yl)-3'-phenyl-1H,3'H-[4,4'-bi(1,2,3-triazole)]-5'-carboxylate (4j) and N,N-dimethyl-N'-(1-methyl-4-nitro-1H-imidazol-5-yl)formimidamide (5a). A mixture of 5-azido-1-methyl-4-nitro-1*H*-imidazole (**2d**) (1 mmol), methyl 5-[(*E*)-2-(dimethylamino)ethenyl]-1-phenyl-1*H*-1,2,3-triazole-4-carboxylate (**1e**) (1 mmol) and DMF (0.2 mL) was stirred for 16 h at room temperature. The reaction mixture was diluted with water (5 mL), the precipitate was filtered off, washed with water, dried and purified by column chromatography (EtOAc/EtOH 9:1). Two compounds (**4j** (major, R_f 0.41) and **5a** (minor, R_f 0.27)) were separated.

4j: white powder; yield 0.130 g (33%); m.p.187–189 °C; IR (ν/cm^{-1}): 3153, 3111, 2918, 1736, 1513, 1204; ^{1}H NMR (400 MHz, DMSO-d_6) δ 3.57 (s, 3H, NCH_3), 3.88 (s, 3H, OCH_3), 7.44–7.58 (m, 5H, HPh), 8.08 (s, 1H, CH^{imid}), 9.12 (s, 1H, CH^{triaz}); ^{13}C NMR (100 MHz, DMSO) δ 32.3, 39.5, 52.1, 122.6, 125.6, 129.4, 130.2, 130.8, 131.9, 132.8, 135.7, 136.3, 137.2, 139.3, 160.5; HRMS (ESI) $[M+H]^+$ found *m/z* 396.1162, calcd for $C_{16}H_{13}N_9O_4$ 396.1163; Anal. Calcd (%): C, 48.61; H, 3.31; N, 31.89. Found: C, 48.39; H, 3.42; N, 31.73.

5a: yellow crystals; yield 0.020 g (10%), m. p.142–144 °C. Spectral data of compound **5a** see below.



5a



6a

N,N-Dimethyl-N'-(1-methyl-4-nitro-1H-imidazol-5-yl)formimidamide (5a). A mixture of 5-azido-1-methyl-4-nitro-1*H*-imidazole (**2d**) (1 mmol), (*E*)-*N*,*N*-dimethyl-2-(1-methyl-5-nitro-1*H*-imidazol-4-yl)ethenamine **1d** (1 mmol) and DMF (0.4 mL) was stirred for 48 h at room temperature. The reaction mixture was diluted with ethanol (10 mL) and insoluble part was filtered off, washed with ethanol and dried to give compound **6** as a mixture with 20–30% of unknown impurities. The filtrate was evaporated in vacuum to dryness and the residue was separated by column chromatography (silica gel, EtOAc–ethanol 9:1).

Fractions with R_f 0.27 were collected and the solvent was evaporated in vacuum to dryness to give amidine **5a**.

5a: Yield 0.110 g (56%). Yellow crystals; m. p.142–144 °C; IR (ν/cm^{-1}): 3105, 2916, 2808, 1631, 1523; ^{1}H NMR (400 MHz, DMSO-d_6) δ 3.04 (s, 3H, NCH_3), 3.11 (s, 3H, NCH_3), 3.39 (s, 3H, NCH_3), 7.46 (s, 1H, CH^{imid}), 8.33 (s, 1H, CH=); ^{13}C NMR (100 MHz, DMSO-d_6) δ 30.6 ($N(CH_3)_2$), 34.2 ($N(CH_3)_2$), 40.6 (NCH_3), 132.9 (C-2^{imidaz}), 133.4 (C-5^{imidaz}), 144.6 (C-4^{imidaz}), 159.6 ($CH^{amidine}$); HRMS (ESI) $[M+H]^+$ found *m/z* 198.0986, calcd for $C_7H_{11}N_5O_2$ 198.0986; Anal. Calcd (%): C, 42.64; H, 5.62; N, 35.52. Found: C, 42.68; H, 5.91; N, 35.35.

6a: Yellow solid, m. p. 130–135 °C (decopm.), yield 0.060 g (36%). IR (ν/cm^{-1}): 1140, 1189, 1354, 1444, 1513, 1554, 1603, 2081, 3100; ^{1}H NMR (400 MHz, DMSO-d_6) δ 3.91 (s, 3H, NCH_3); 6.21 (s, 1H, CH); 7.91 (s, 1H, $CH^{imid.}$).

The structure of diazo compound **6a** was also confirmed by X-ray diffraction analysis for monocrystal of **6a**.

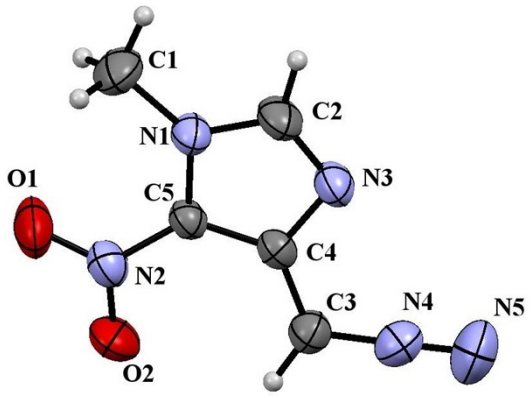
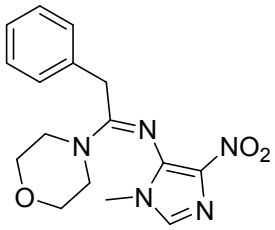


Fig. S1. Perspective view of compound **6a** (50% probability thermal ellipsoids) as determined by X-ray diffraction analysis.

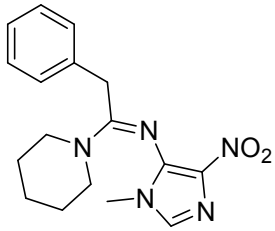
Supplementary crystallographic data for the compound **6a** (CCDC 1826375) can be obtained free of charge from The Cambridge Crystallographic Data Center via www.ccdc.cam.ac.uk/data_request/cif.

General method for synthesis of amidines 8a-c.[7]

A mixture of phenylacetaldehyde (1 mmol), secondary amine **7a-c** (1 mmol), azide **2d** (1 mmol) and CH_3OH (2 mL) was stirred at 50 °C for 2 h. Then reaction mixture was evaporated in vacuum to dryness and purified by column chromatography (silica gel, ethyl acetate).

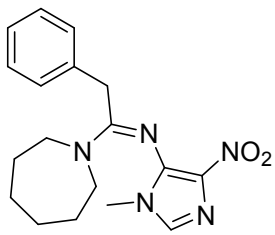


***(Z)-N*-(1-Methyl-4-nitro-1H-imidazol-5-yl)-1-morpholino-2-phenylethan-1-imine (8a).** Yellow powder; m. p. 133–137 °C; yield 0.370 g (89%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.26 (s, 3H, NCH_3), 3.67 (br. s, 6H, $4H^{morph}$ + CH_2), 3.88 (s, 4H, H^{morph}), 6.98 (d, 2H, *J* 7.2, HPh), 7.09 (s, 1H, CH^{imidaz}), 7.20 (t, 1H, *J* 7.3, HPh), 7.26 (dd, 2H, *J* 7.9, 6.6, HPh); ^{13}C NMR (100 MHz, $CDCl_3$) δ 30.4 (NCH_3), 36.3 (CH_2), 45.2 (C^{morph}), 47.6 (C^{morph}), 66.5 (C^{morph}), 127.3 (C^{Ph}), 127.6 ($2C^{Ph}$), 129.2 ($2C^{Ph}$), 132.0 (C-2^{imidaz}), 133.4 (C-4^{imidaz}), 134.9 (C^{Ph}), 142.2 (C-5^{imidaz}), 164.6 ($C{=}N^{amid}$); HRMS (ESI) $[M+H]^+$ found *m/z* 330.1561, calcd for $C_{16}H_{19}N_5O_3$ 330.1561; Anal. Calcd (%): C, 58.35; H, 5.81; N, 21.26. Found: C, 58.19; H, 6.0; N, 20.86.



***(Z)-N*-(1-Methyl-4-nitro-1H-imidazol-5-yl)-1-piperidiino-2-phenylethan-1-imine (8b).** Yellow prisms; yield 0.137 g (42%); m. p. 90–93 °C; IR (ν/cm^{-1}) 3407, 3030, 2941, 2855, 1583, 1352, 1252; ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.37 (br. s, 1H, H^{piper}), 1.63 (br. s, 5H, H^{piper}), 3.27 (s, 3H, NCH_3), 3.25–4.15 (m, 6H, $4H^{piper}$ + CH_2), 7.02 (d, *J* 7.0 Hz, 2H, H^{Ph}), 7.08 (s, 1H, CH^{imidaz}), 7.17–7.24 (m, 1H, H^{Ph}), 7.24–7.32 (m, 2H, H^{Ph}); ^{13}C NMR (100 MHz, $CDCl_3$) δ 24.4 (C^{piper}), 25.0 (C^{piper}), 26.5 (C^{piper}), 30.2 (NCH_3), 36.5 (CH_2), 46.0 (C^{piper}), 48.6 (C^{piper}), 126.9 (C^{Ph}), 127.6 ($2C^{Ph}$), 128.9 ($2C^{Ph}$), 131.8 (C-2^{imidaz}), 133.1 (C-4^{imidaz}), 135.4 (C^{Ph}), 143.0 (C-5^{imidaz}), 164.2 ($C{=}N^{amid}$); MS-EI (*m/z*) 327 $[M]^+$; Anal. Calcd (%) for $C_{17}H_{21}N_5O_2$: C, 62.37; H, 6.47; N, 21.39. Found: C, 62.03; H, 6.66; N, 21.24.

Supplementary crystallographic data for the compound **8b** (CCDC 1580079) can be obtained free of charge from The Cambridge Crystallographic Data Center via www.ccdc.cam.ac.uk/data_request/cif.



(*Z*)-1-(Azepan-1-yl)-N-(1-methyl-4-nitro-1H-imidazol-5-yl)-2-phenylethan-1-imine (8c). Yellow powder; yield 0.174 g (51%); m. p. 80–82 °C; IR (ν/cm^{-1}) 3445, 3115, 3029, 2931, 2851, 1580, 1355, 1267;

^{1}H NMR (400 MHz, $CDCl_3$) δ 1.52–1.82 (m, 6H, CH_2^{azep}), 1.92 (br. s, 2H, CH_2^{azep}), 3.17 (s, 3H, NCH_3), 3.36 (br. s, 1H, CH_2^{azep}), 3.43 (br. s, 1H, CH^{azep}), 3.59–3.88 (m, 3H, CH^{azep} + CH_2), 4.18 (br. s, 1H, CH^{azep}), 7.00 (d, *J* 7.0 Hz, 2H, CHPh), 7.04 (s, 1H, CH^{imidaz}), 7.16–7.32 (m, 3H,CHPh); ^{13}C NMR (100 MHz, $CDCl_3$) δ 26.0 (C^{azep}), 26.2 (C^{azep}), 26.9 (C^{azep}), 29.3 (C^{azep}), 30.0 (NCH_3), 36.6 (CH_2), 49.3 (C^{azep}), 50.1 (C^{azep}), 126.9 (C^{Ph}), 127.8 ($2C^{Ph}$), 128.9 ($2C^{Ph}$), 131.5 (C-2^{imidaz}), 133.3 (C-4^{imidaz}), 135.5 (C^{Ph}), 143.0 (C-5^{imidaz}), 165.0 ($C{=}N^{amid}$); MS-EI (*m/z*) 341 $[M]^+$; Anal. Calcd (%) for $C_{18}H_{23}N_5O_2$: C, 63.32; H, 6.79; N, 20.51. Found: C, 63.23; H, 7.17; N, 20.53.

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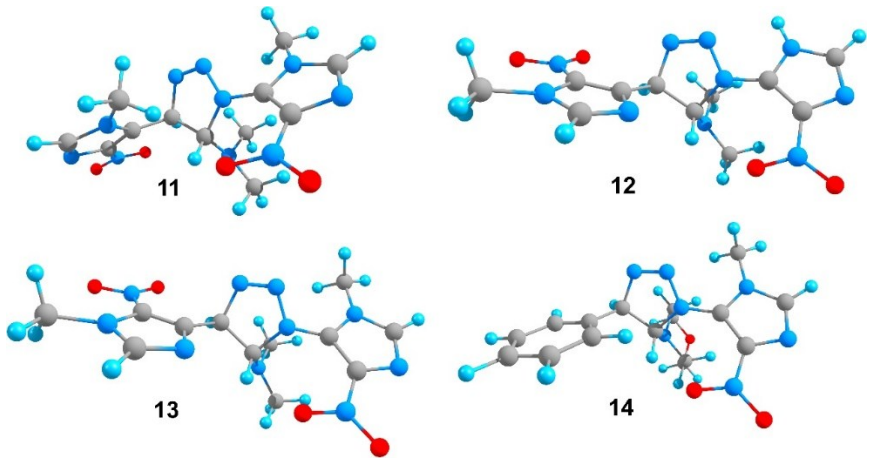


Fig. S2 Calculated geometries of triazolines **11** - **14** corresponding to the lowest free energy conformations.

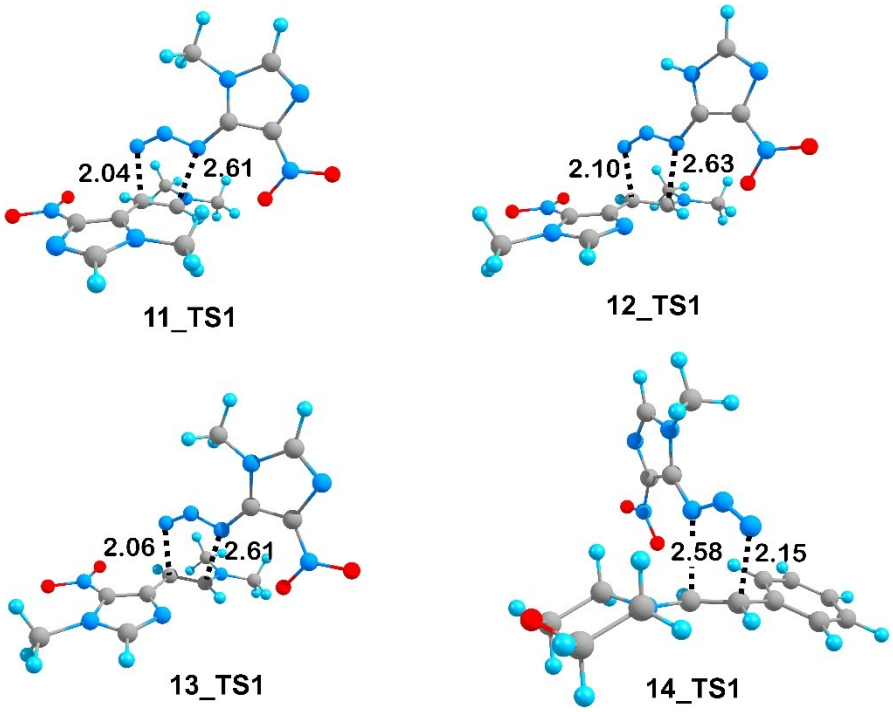


Fig. S3 Calculated transition state geometries corresponding to formation of triazolines **11** – **14** by 1,3-dipolar cycloaddition of enamines with azides. The shown numbers are the interatomic distances given in angströms.

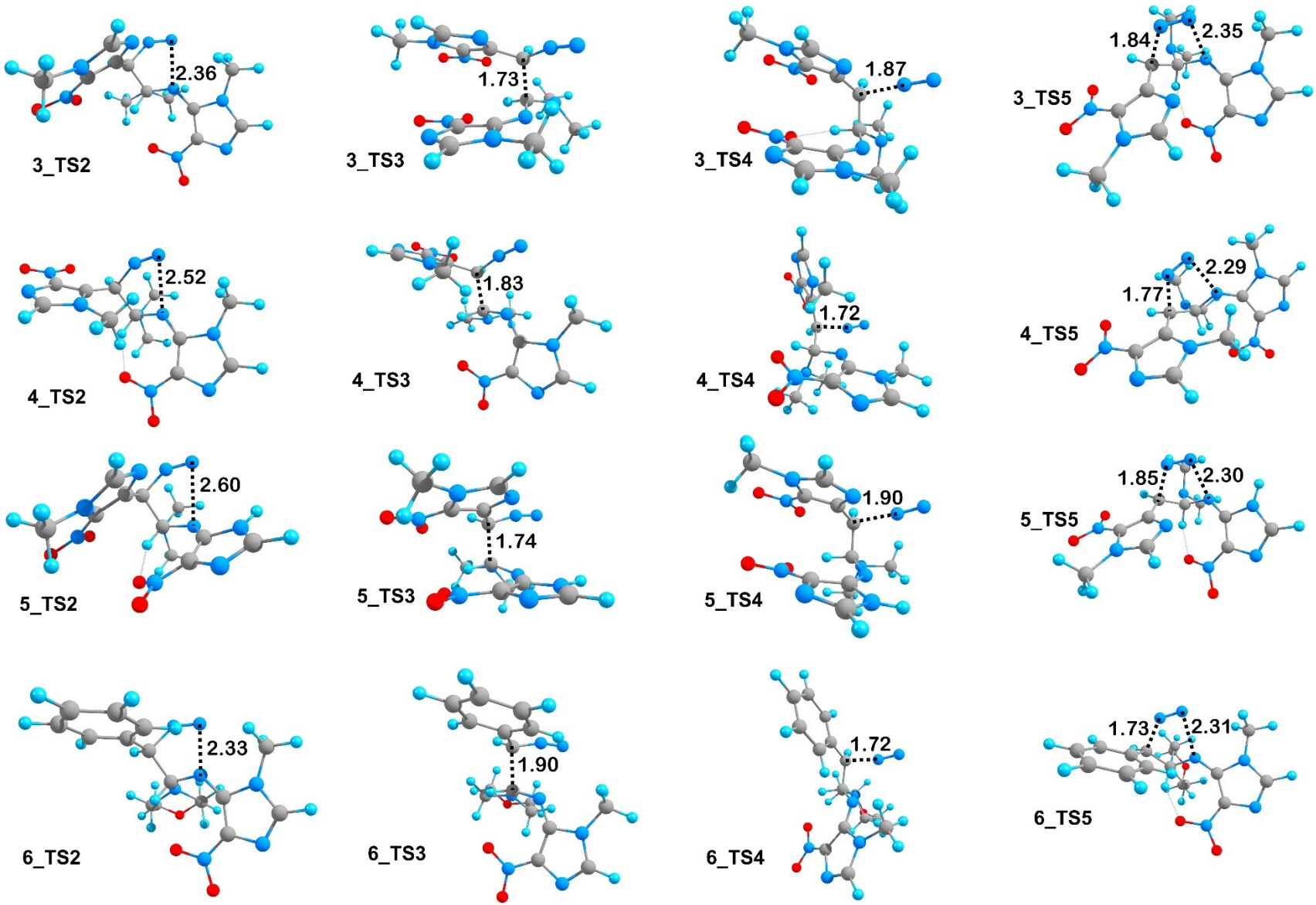


Fig. S4 Calculated transition state geometries corresponding to the degradation pathways of the triazolines **11** – **14** shown in Scheme 8. The shown numbers are the interatomic distances given in angströms

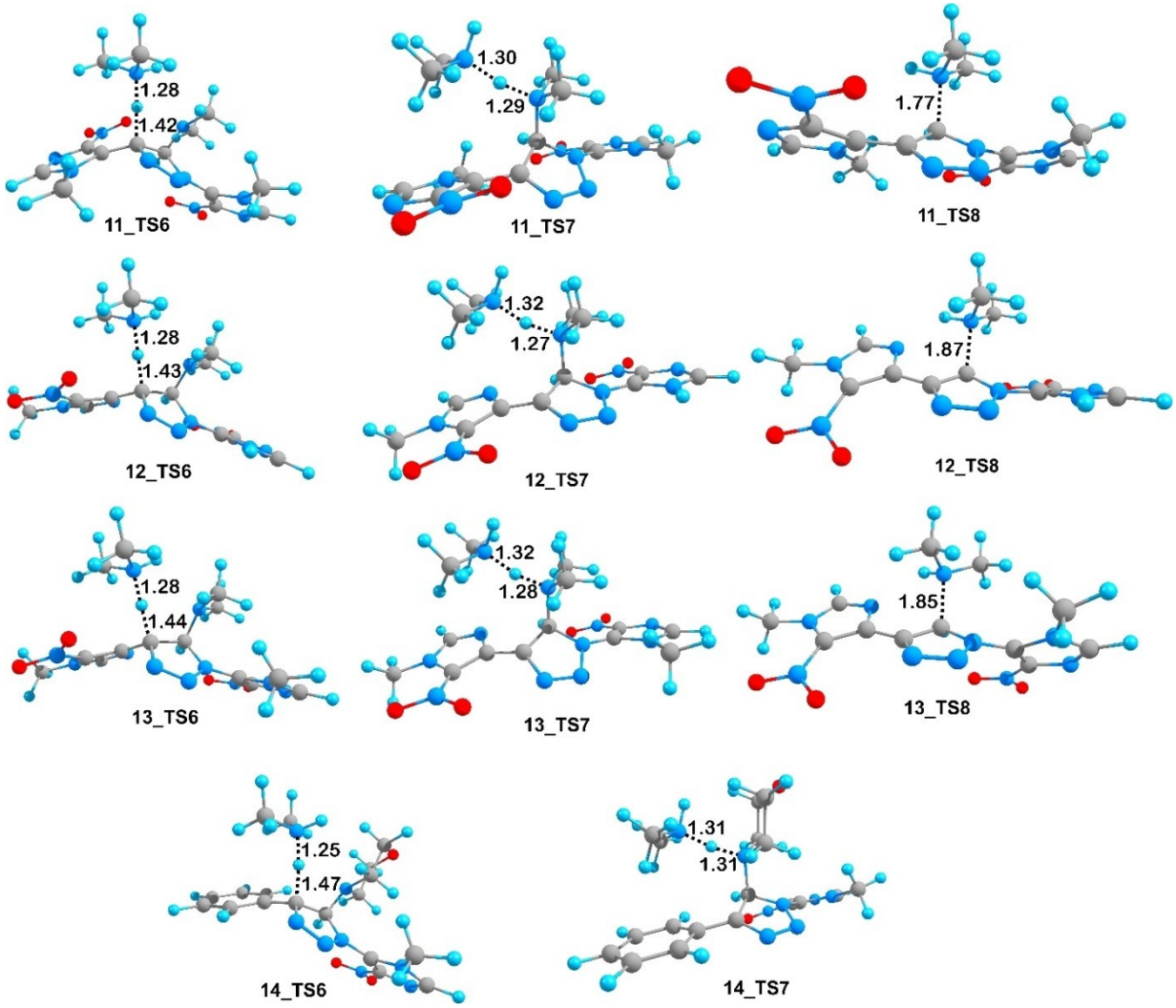
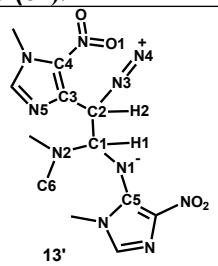


Fig. S5 Calculated transition state geometries corresponding to the base-catalyzed transformation of triazolines **11** – **14** to the corresponding triazoles as shown in Scheme 9. The base-catalyst is represented by dimethylamine (dma). The shown numbers are the interatomic distances given in angströms.

Table S1 Second order perturbation analysis of **13'** in the NBO basis. The presented results are related to the antibonding orbitals **C1–C2 (σ*)** and **C2–N3 (σ*)**.

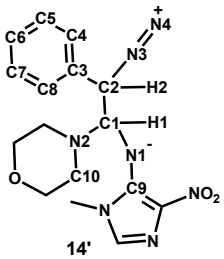


13'

C1–C2 (σ*) (acceptor), population = **0.08416**				**C2–N3 (σ*)** (acceptor), population = **0.04212**			
NBO (donor)	***E*** *kcal·mol^{-1}*	***ΔE*** *a. u.*	***F*** *a. u.*	*NBO (donor)*	***E*** *kcal·mol^{-1}*	***ΔE*** *a. u.*	***F*** *a. u.*
N2 (LP)	6.17	0.63	0.056	**O1 (LP)**	1.85	0.71	0.032
C3–C4 (π)	3.34	0.67	0.042	**N4 (LP)**	8.64	0.97	0.082
C2–C3 (σ)	1.16	1.01	0.031	**N5–C3 (σ)**	0.52	1.13	0.022
C1–C2 (σ)	0.56	0.91	0.020	**C3–C4 (σ)**	1.39	1.06	0.034
N1–C5 (π)	10.85	0.67	0.076	**C3–C4 (π)**	0.84	0.68	0.021
N3–N4 (π)	1.42	0.94	0.033	**C1–H1 (σ)**	4.39	0.87	0.055
N2–C6 (σ)	1.65	1.00	0.036	**N3–N4 (σ)**	2.20	1.56	0.052
total (net)	**25.15**			**total (net)**	**19.83**		

σ - sigma bonding orbital; **π** - pi bonding orbital; **σ*** - sigma antibonding orbital; **LP** - lone pair. ***E*** - the energy of delocalization (conjugation) of the donor orbital over (with) the acceptor orbital. ***ΔE*** - the energy gap between the donor and acceptor orbitals. ***F*** - the element of the Kohn-Sham matrix describing the donor-acceptor interaction (represents spatial overlap).

Table S2 Second order perturbation analysis of **14'** in the NBO basis. The presented results are related to the antibonding orbitals **C1–C2 (σ*)** and **C2–N3 (σ*)**.



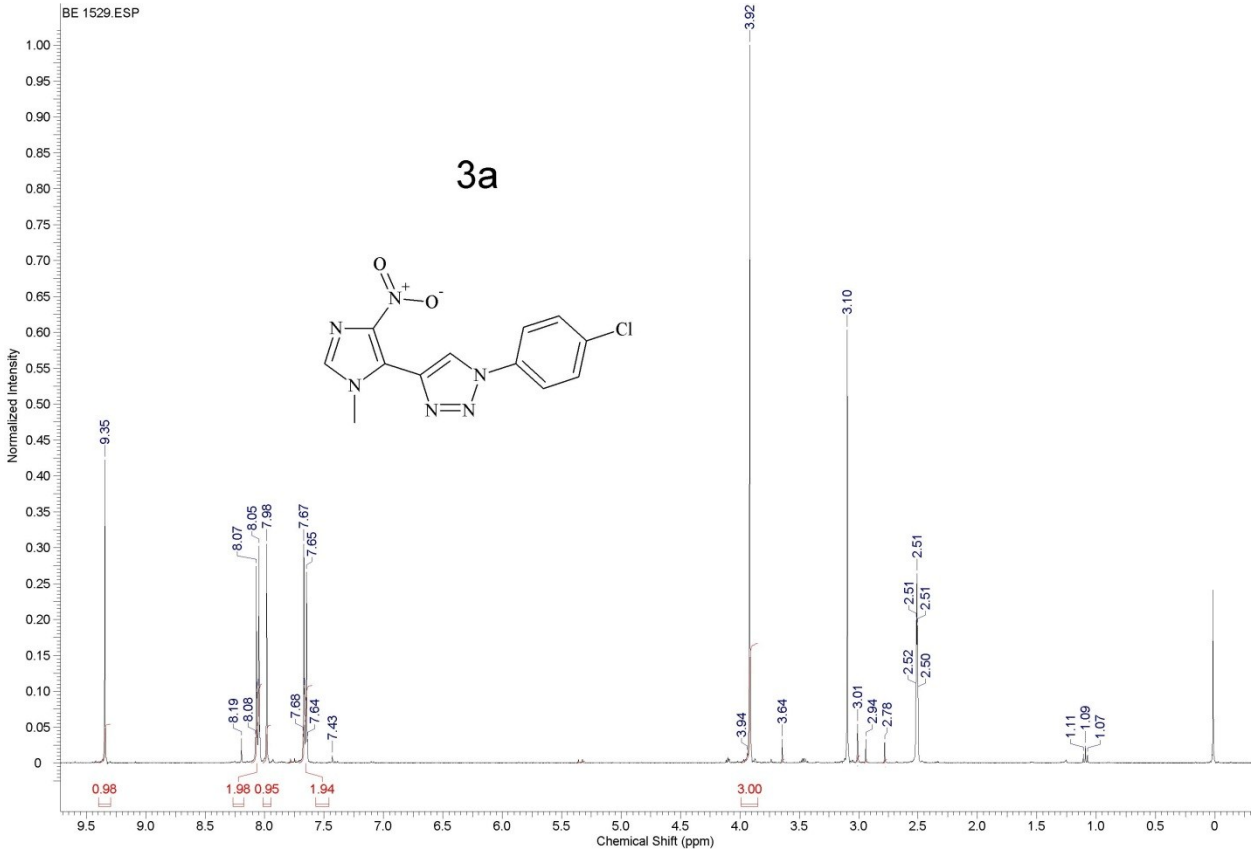
14'

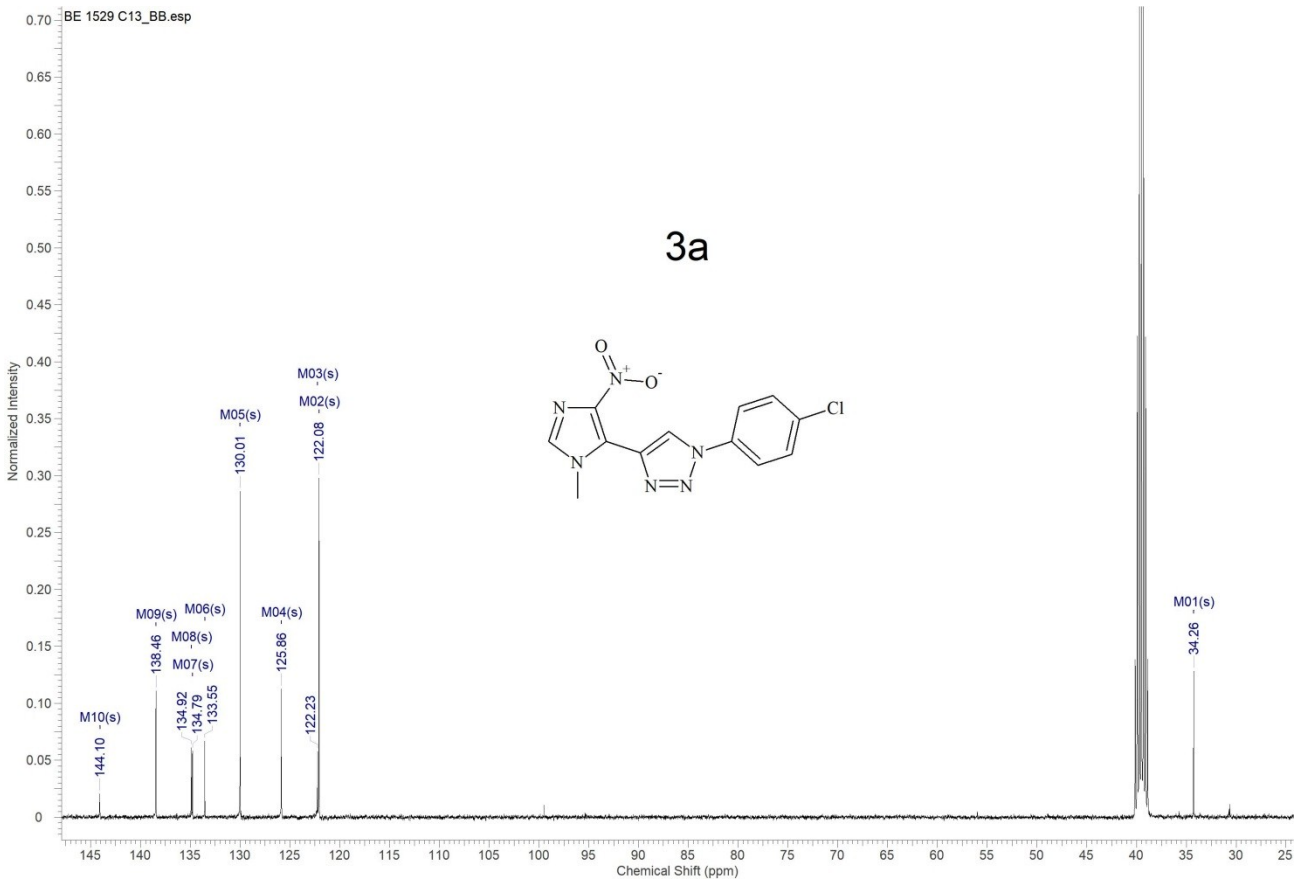
C1–C2 (σ*) (acceptor), population = **0.05896**				**C2–N3 (σ*)** (acceptor), population = **0.05776**			
NBO (donor)	***E*** *kcal·mol^{-1}*	***ΔE*** *a. u.*	***F*** *a. u.*	*NBO (donor)*	***E*** *kcal·mol^{-1}*	***ΔE*** *a. u.*	***F*** *a. u.*
N1 (LP)	4.50	0.70	0.050				
O1 (LP)	1.10	0.70	0.025				
N2 (LP)	5.23	0.68	0.053	**N4 (LP)**	8.52	0.93	0.079
C3–C4 (σ)	0.55	1.04	0.021	**C3–C4 (σ)**	1.35	0.97	0.032
C3–C4 (π)	4.53	0.66	0.049	**C3–C4 (π)**	7.64	0.59	0.060
C2–C3 (σ)	1.52	1.02	0.035	**C1–H1 (σ)**	5.21	0.83	0.059
N1–C9 (σ)	0.94	1.17	0.030	**N3–N4 (π)**	1.95	1.53	0.049
N1–C9 (π)	1.90	0.72	0.033				
N3–N4 (π)	0.97	0.99	0.028				
N2–C10 (σ)	1.26	1.05	0.032				

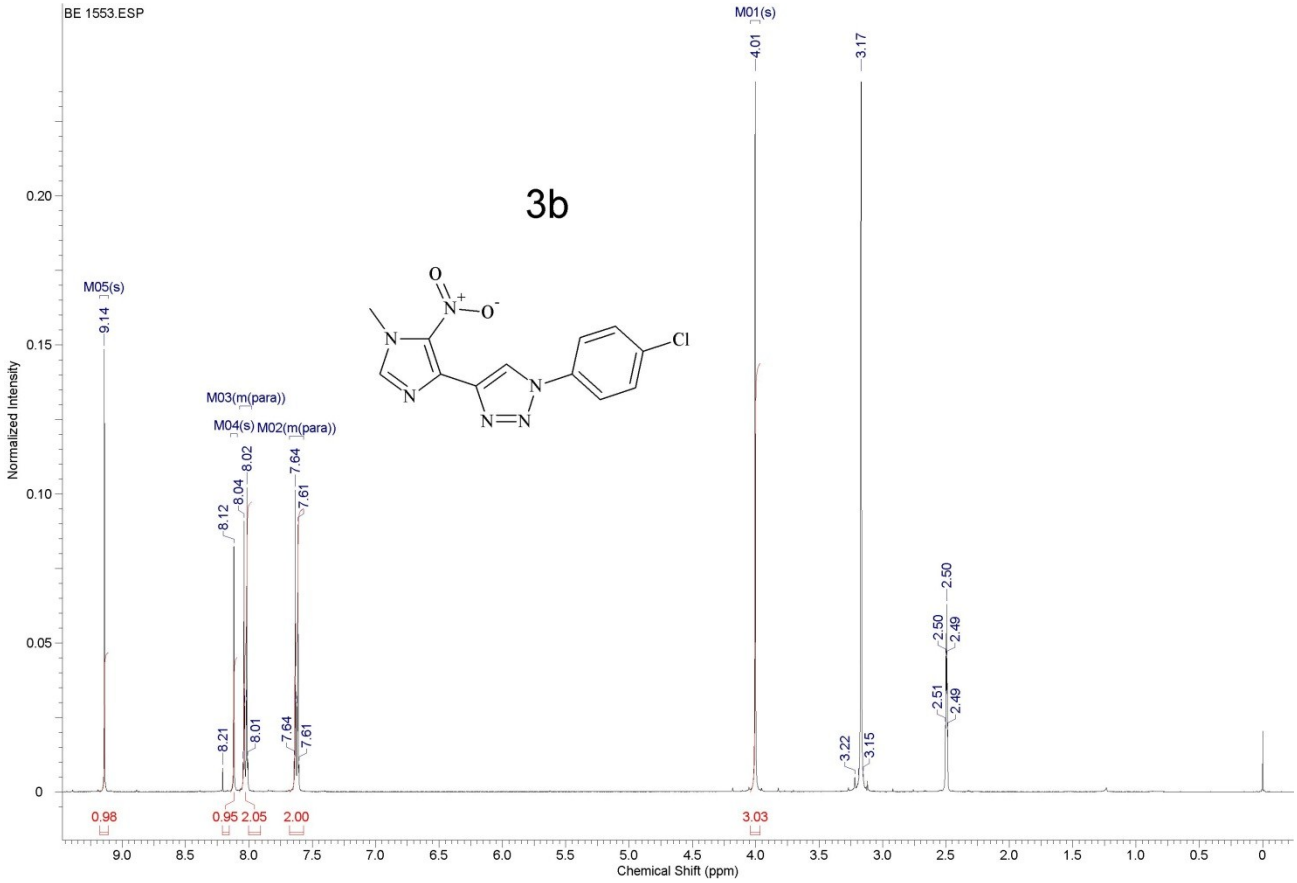
total (net)	**22.50**	**total (net)**	**24.67**

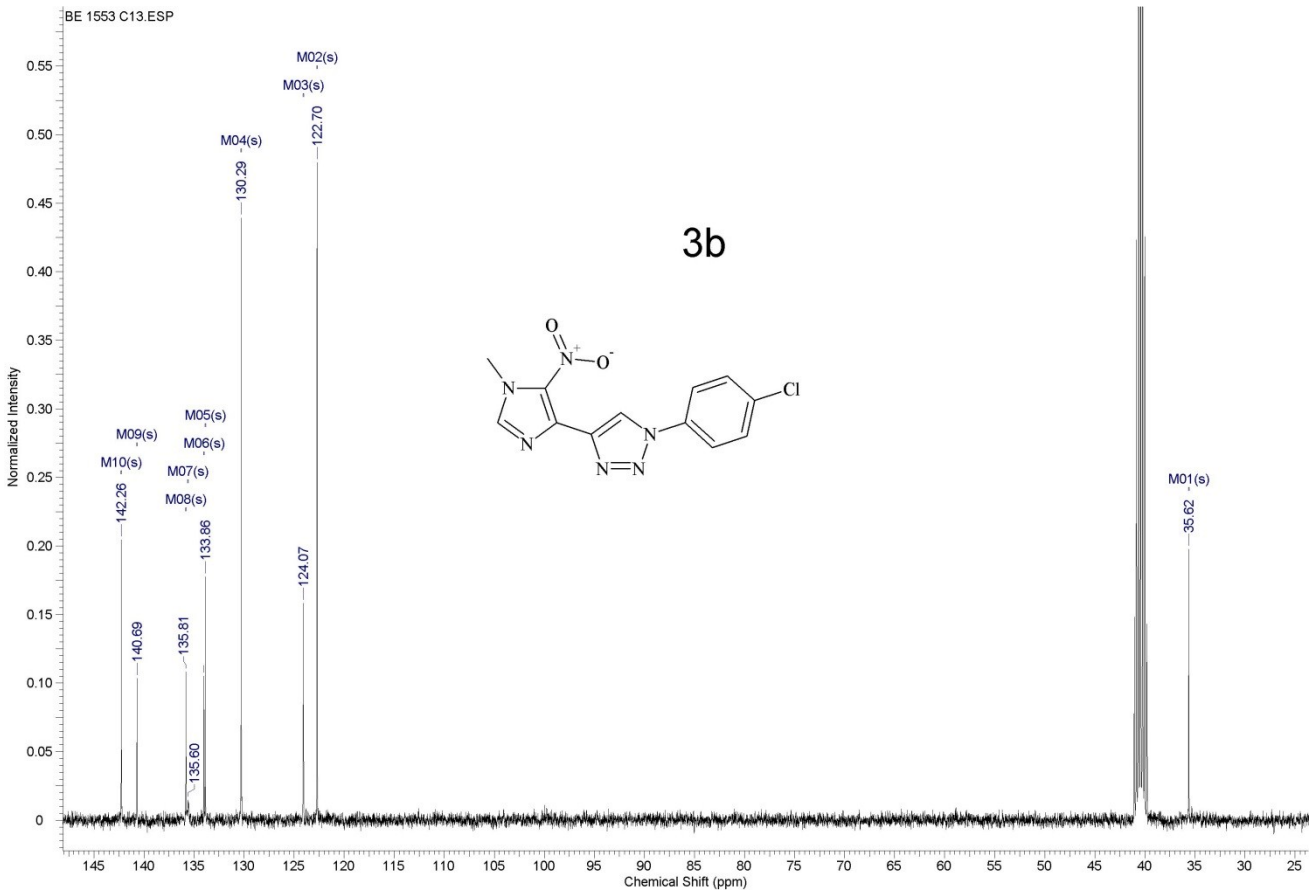
σ - sigma bonding orbital; **π** - pi bonding orbital; **σ*** - sigma antibonding orbital; **LP** - lone pair. ***E*** - the energy of delocalization (conjugation) of the donor orbital over (with) the acceptor orbital. ***ΔE*** - the energy gap between the donor and acceptor orbitals. ***F*** - the element of the Kohn-Sham matrix describing the donor-acceptor interaction (represents spatial overlap).

NMR spectra of triazoles 3a-f




BE 1529 C13_BB.esp
3a
Normalized Intensity
Chemical Shift (ppm)
M01(s)
34.26
M02(s)
122.08
M03(s)
M04(s)
125.86
M05(s)
130.01
M06(s)
134.92
M07(s)
134.79
M08(s)
133.55
M09(s)
138.46
M10(s)
144.10
122.23
Cl


BE 1553.ESP
3b
Normalized Intensity
Chemical Shift (ppm)
M01(s)
4.01
3.17
M05(s)
9.14
M03(m(para))
M04(s)
M02(m(para))
8.12
8.04
8.02
8.21
8.01
7.64
7.61
7.64
7.61
3.22
3.15
2.50
2.50
2.49
2.51
2.49
0.98
0.95
2.05
2.00
3.03
Cl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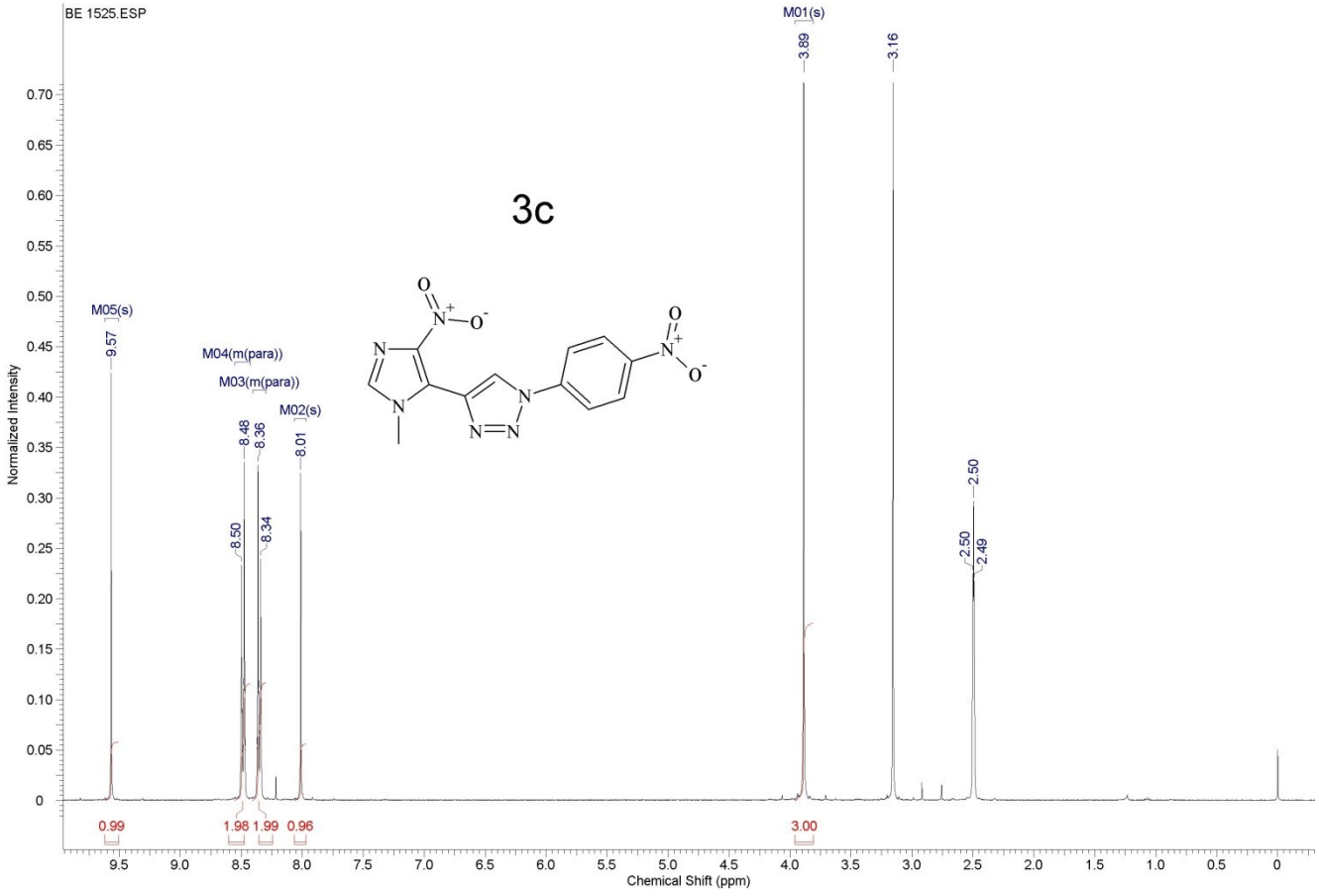
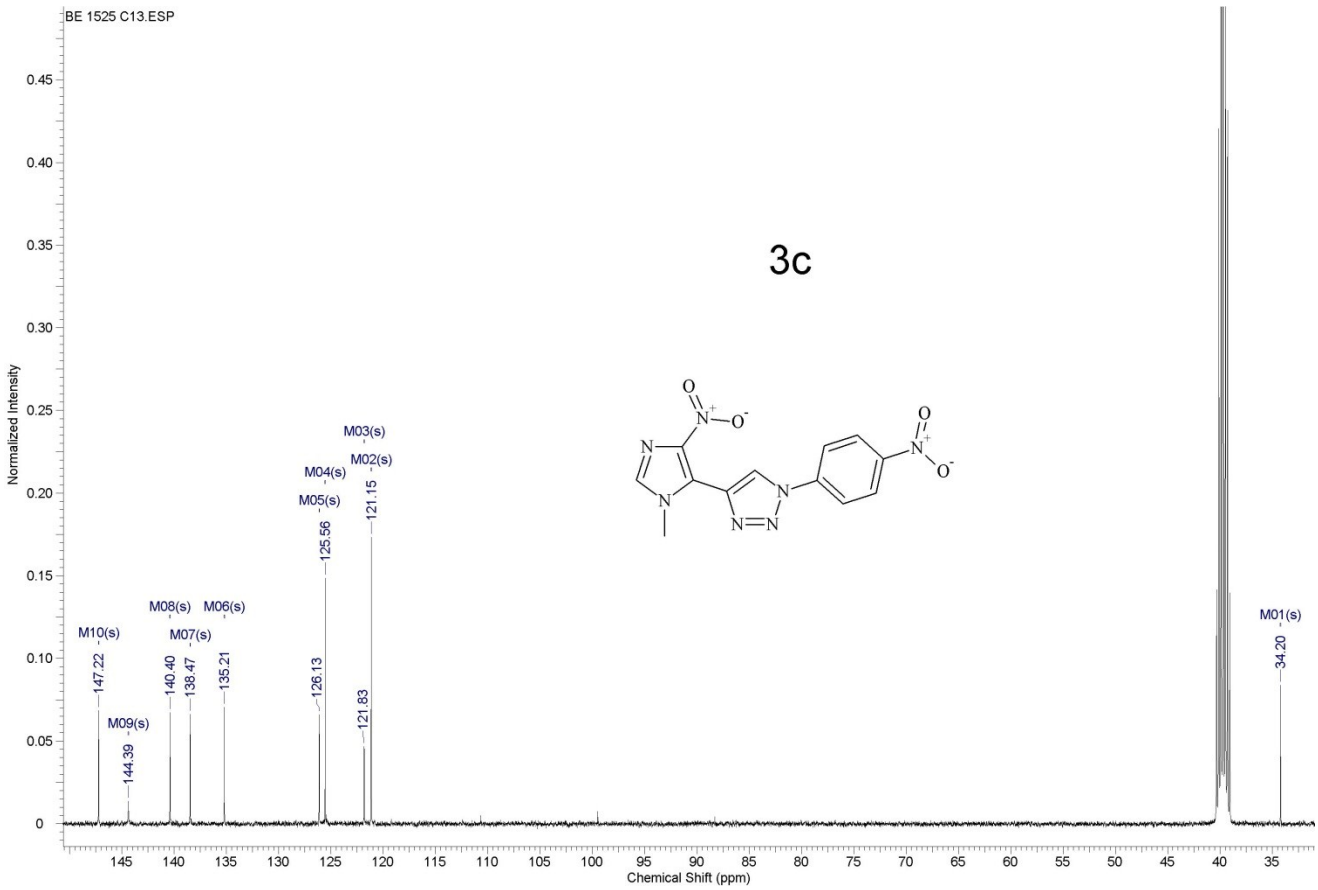
3b
M02(s)
M03(s)
122.70
M04(s)
130.29
M05(s)
M06(s)
M09(s)
M10(s)
M07(s)
M08(s)
142.26
140.69
135.81
135.60
133.86
124.07
M01(s)
35.62
Cl
Normalized Intensity
Chemical Shift (ppm)


BE 1525.ESP
3c
M01(s)
3.89
3.16
M05(s)
9.57
M04(m(para))
M03(m(para))
M02(s)
8.48
8.36
8.01
8.50
8.34
2.50
2.50
2.49
0.99
1.98
1.99
0.96
3.00
Normalized Intensity
Chemical Shift (ppm)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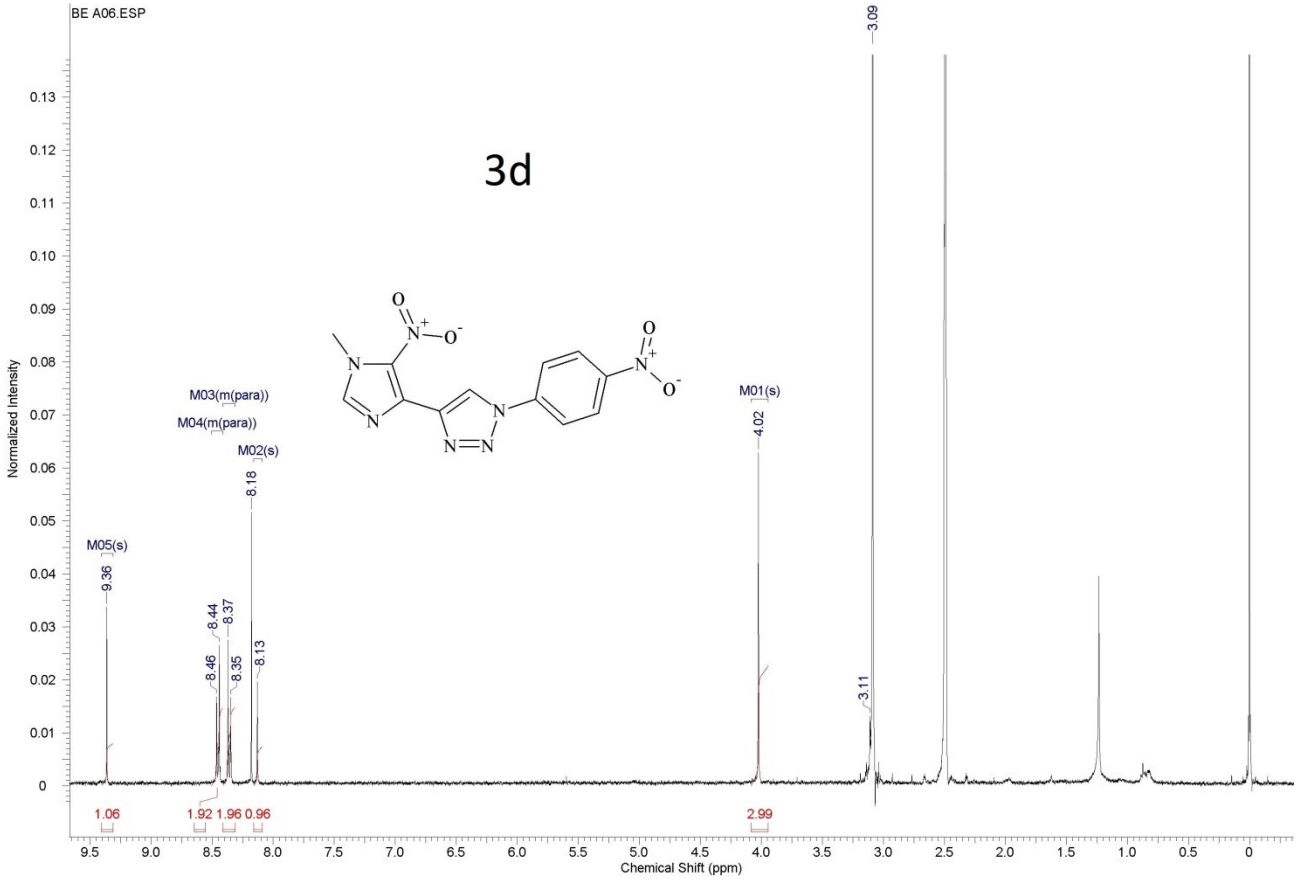
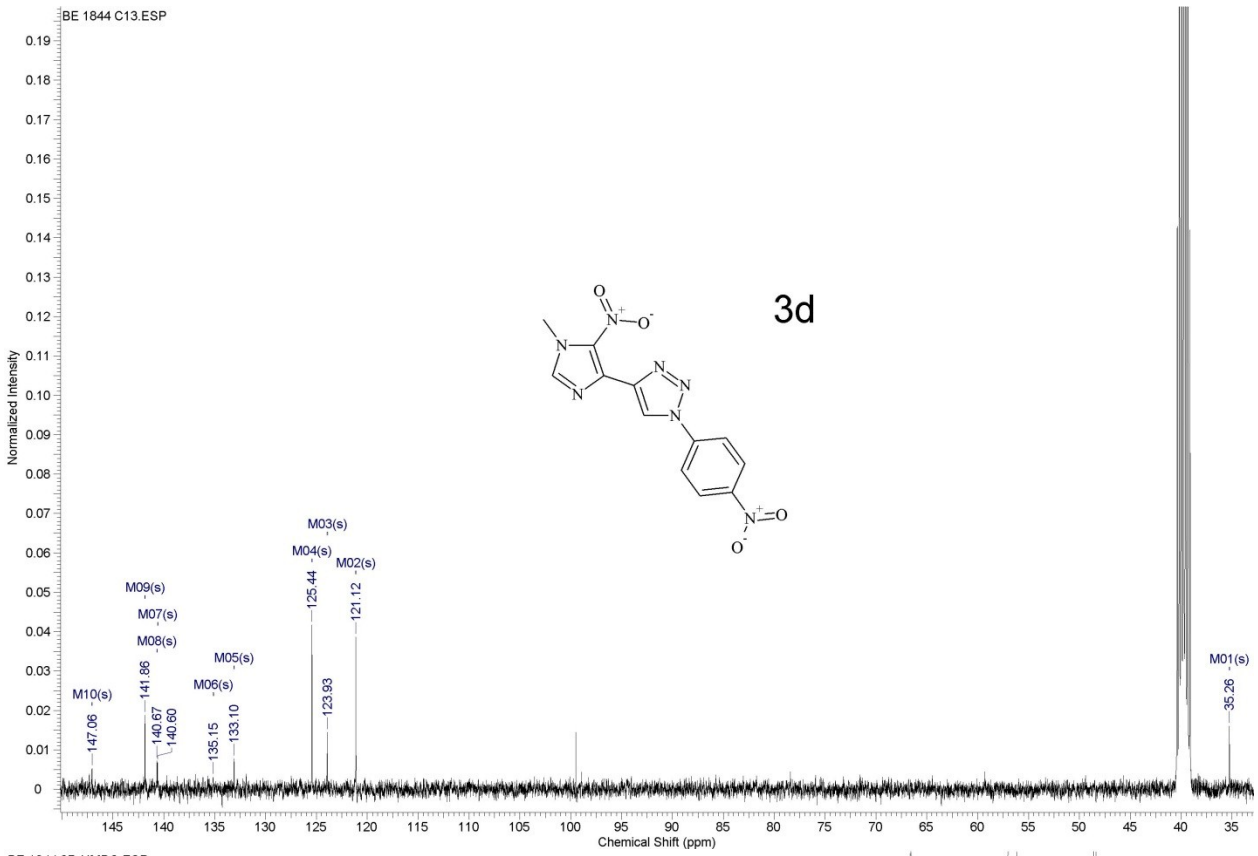
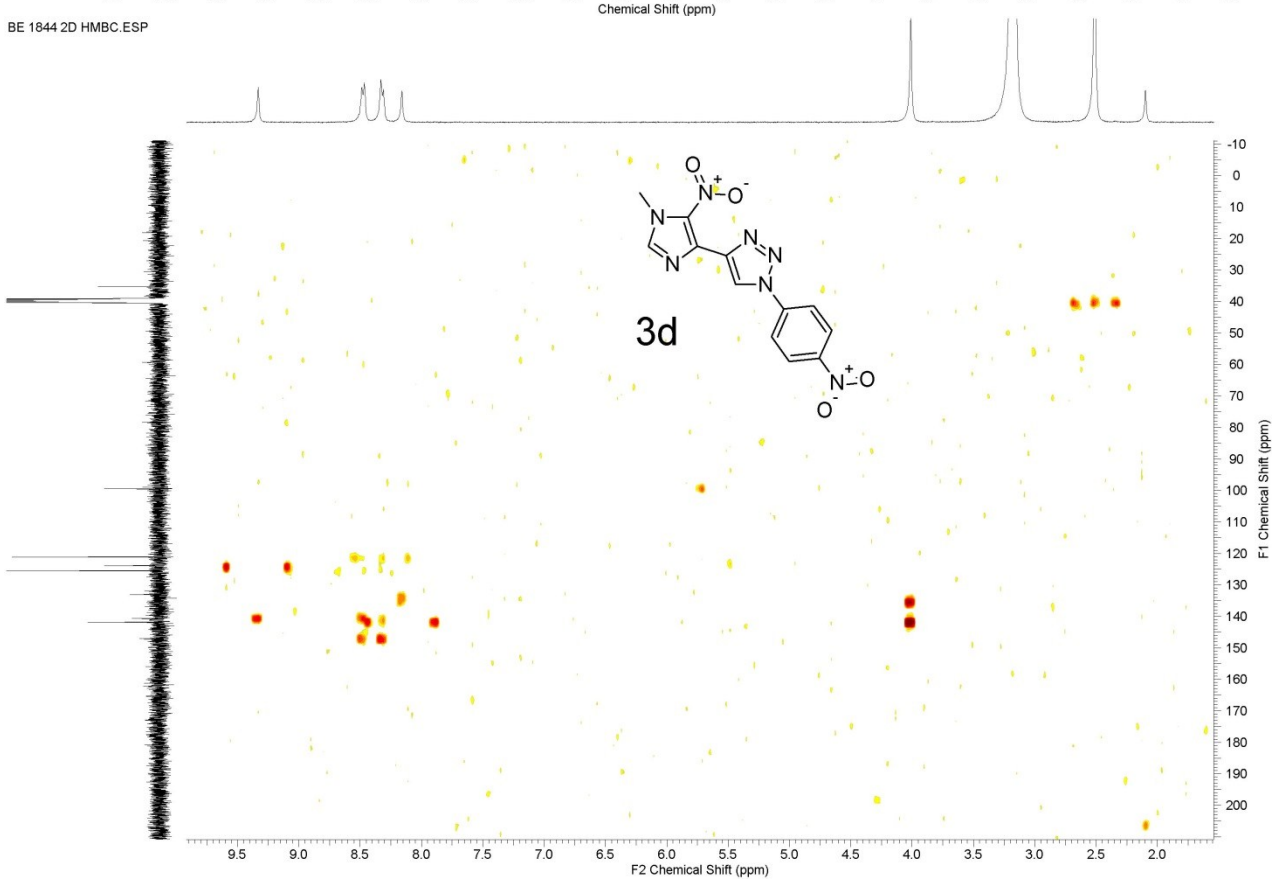
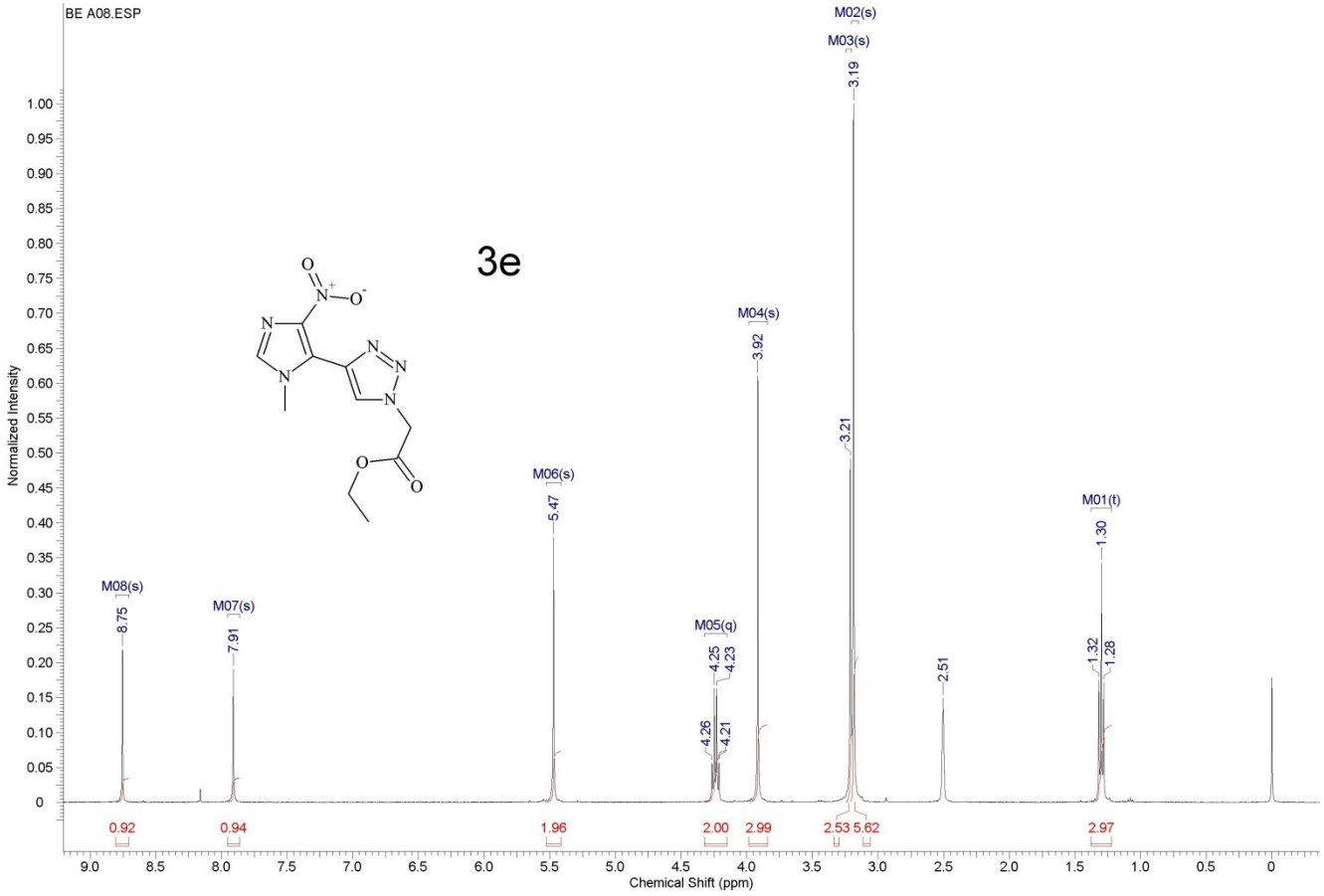
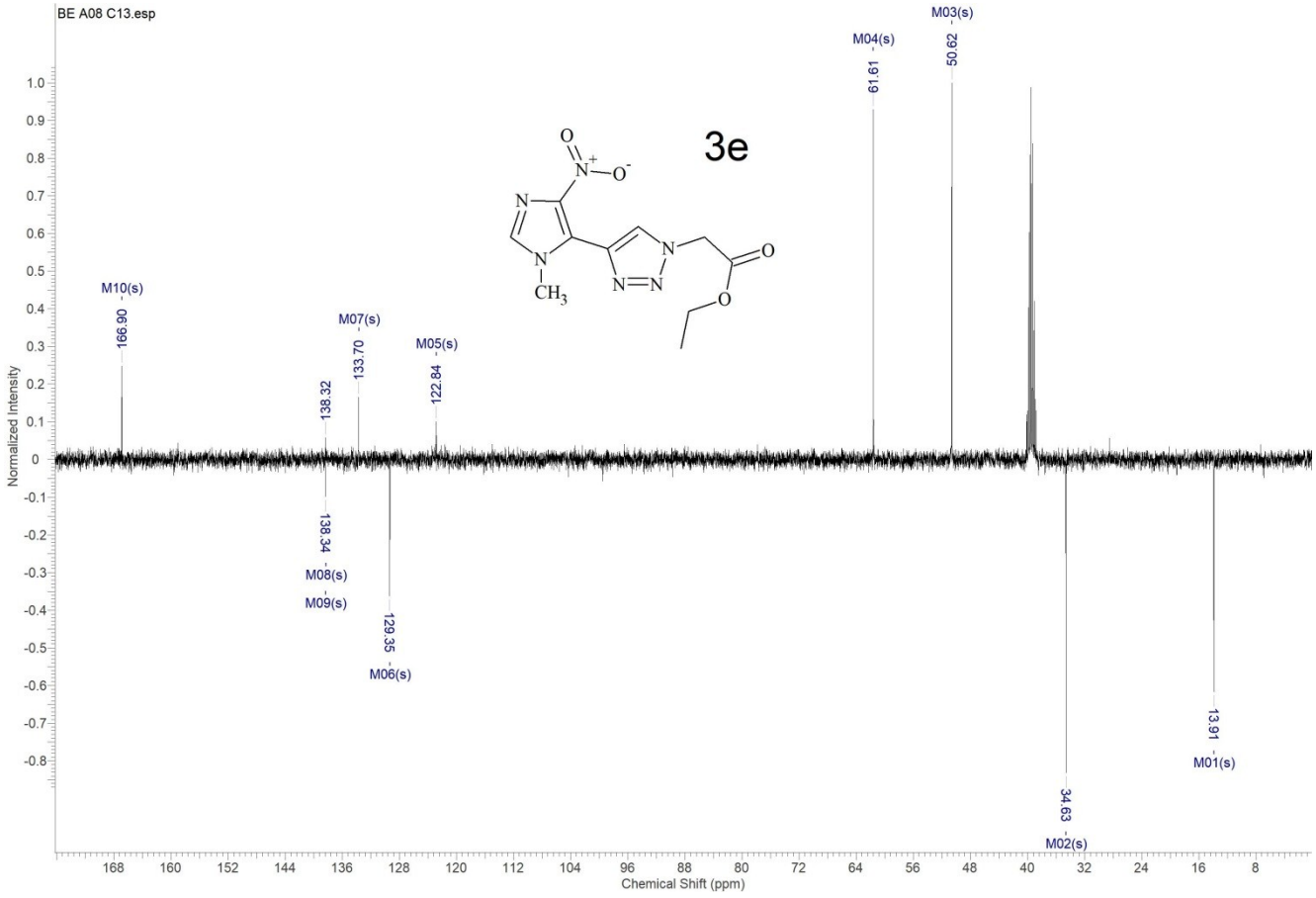
3c
Normalized Intensity
Chemical Shift (ppm)
M10(s)
M09(s)
M08(s)
M07(s)
M06(s)
M05(s)
M04(s)
M03(s)
M02(s)
M01(s)
147.22
144.39
140.40
138.47
135.21
126.13
125.56
121.83
121.15
34.20

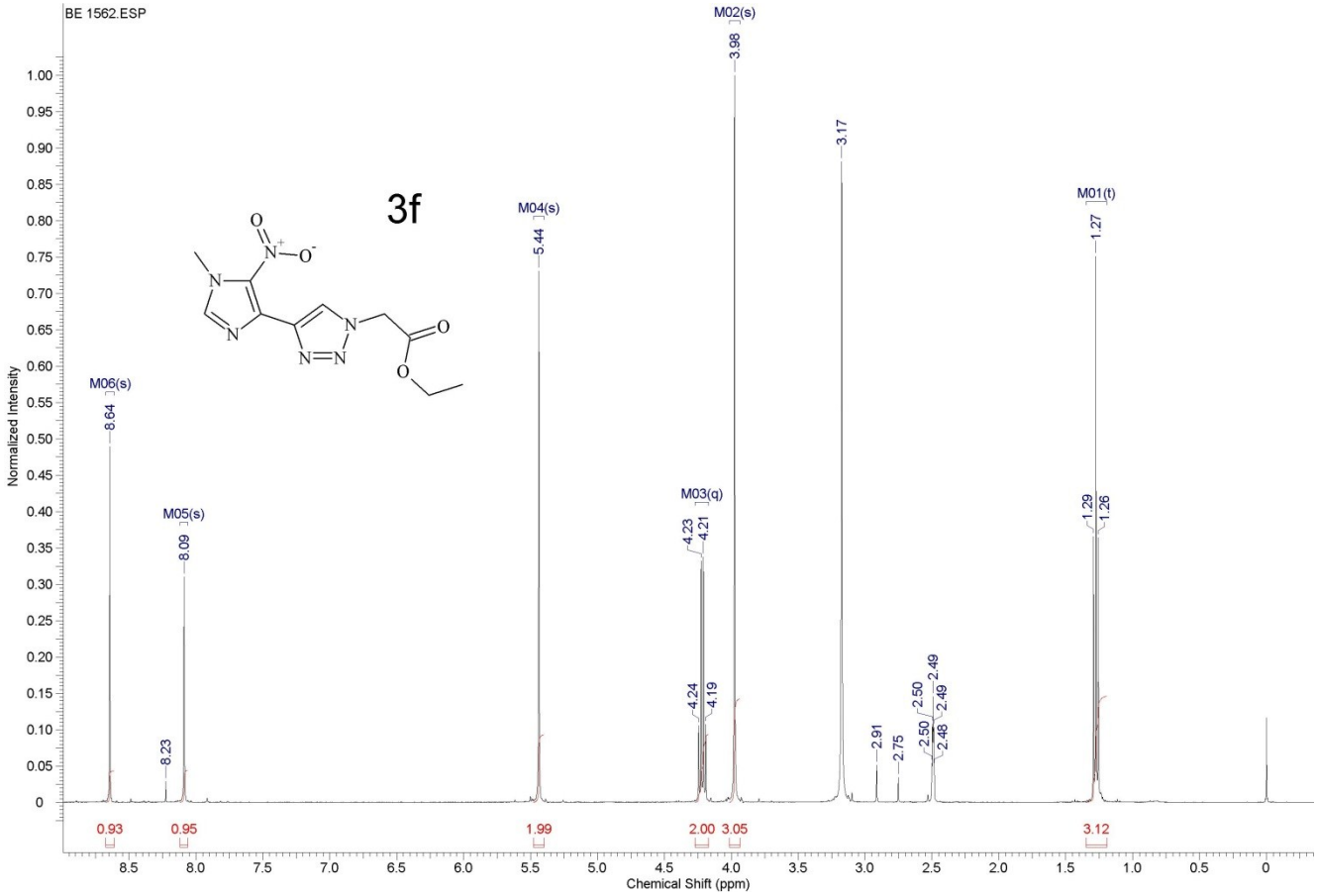

BE A06.ESP
3d
Normalized Intensity
Chemical Shift (ppm)
M05(s)
M04(m(para))
M03(m(para))
M02(s)
M01(s)
9.36
8.46
8.44
8.37
8.35
8.18
8.13
4.02
3.11
3.09
1.06
1.92
1.96
0.96
2.99


BE 1844 C13.ESP
Normalized Intensity
Chemical Shift (ppm)
3d
M01(s)
M02(s)
M03(s)
M04(s)
M05(s)
M06(s)
M07(s)
M08(s)
M09(s)
M10(s)
147.06
141.86
140.67
140.60
135.15
133.10
125.44
123.93
121.12
35.26


BE 1844 2D HMBC.ESP
3d
F2 Chemical Shift (ppm)
F1 Chemical Shift (ppm)


BE A08.ESP
3e
M02(s)
M03(s)
3.19
M04(s)
3.92
3.21
M06(s)
5.47
M01(t)
1.30
M08(s)
8.75
M07(s)
7.91
M05(q)
4.25
4.23
4.26
4.21
2.51
1.32
1.28
0.92
0.94
1.96
2.00
2.99
2.53
5.62
2.97
Normalized Intensity
Chemical Shift (ppm)


BE A08 C13.esp
3e
M10(s)
166.90
M07(s)
133.70
M05(s)
122.84
138.32
M04(s)
61.61
M03(s)
50.62
138.34
M08(s)
M09(s)
129.35
M06(s)
34.63
M02(s)
13.91
M01(s)
Normalized Intensity
Chemical Shift (ppm)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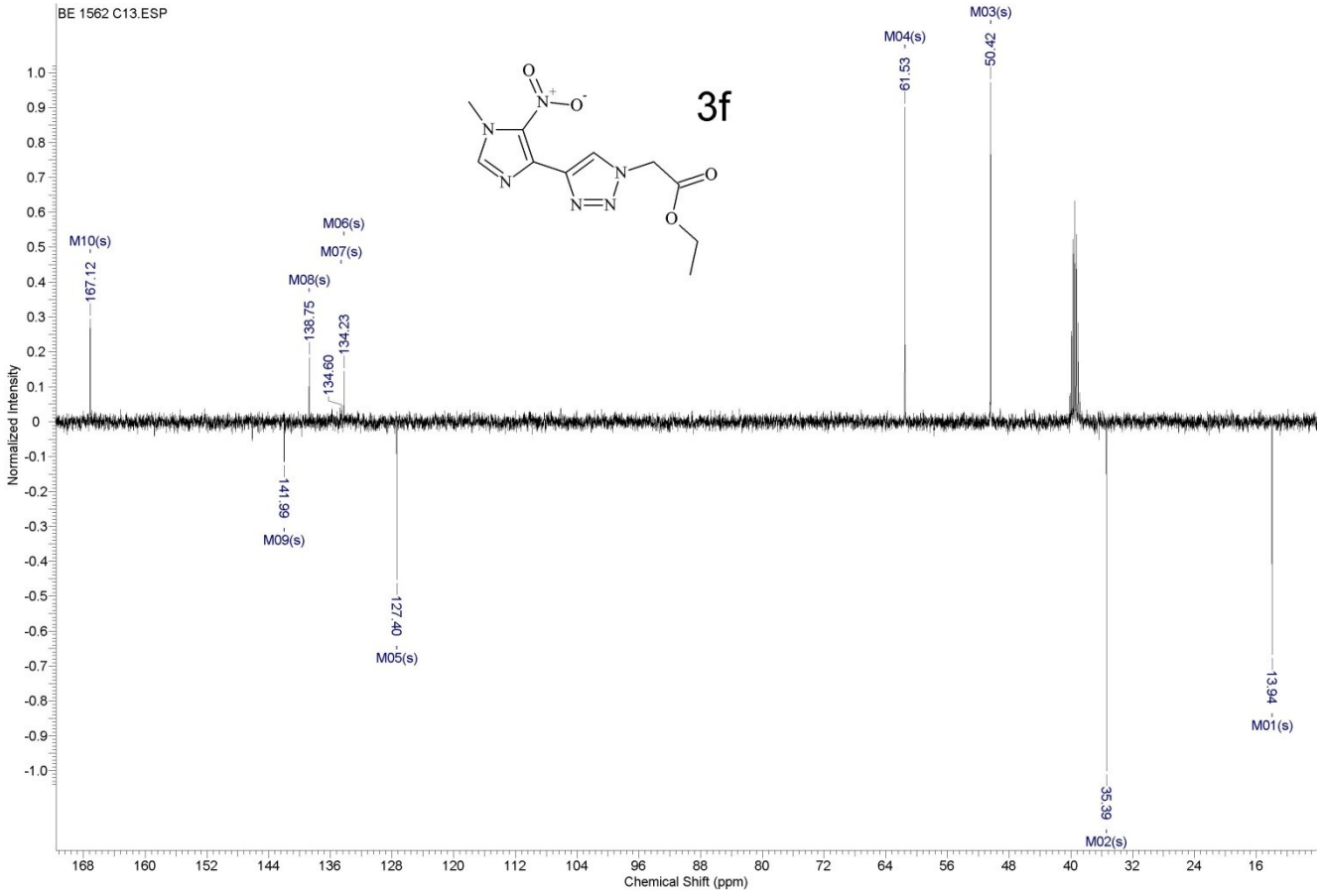
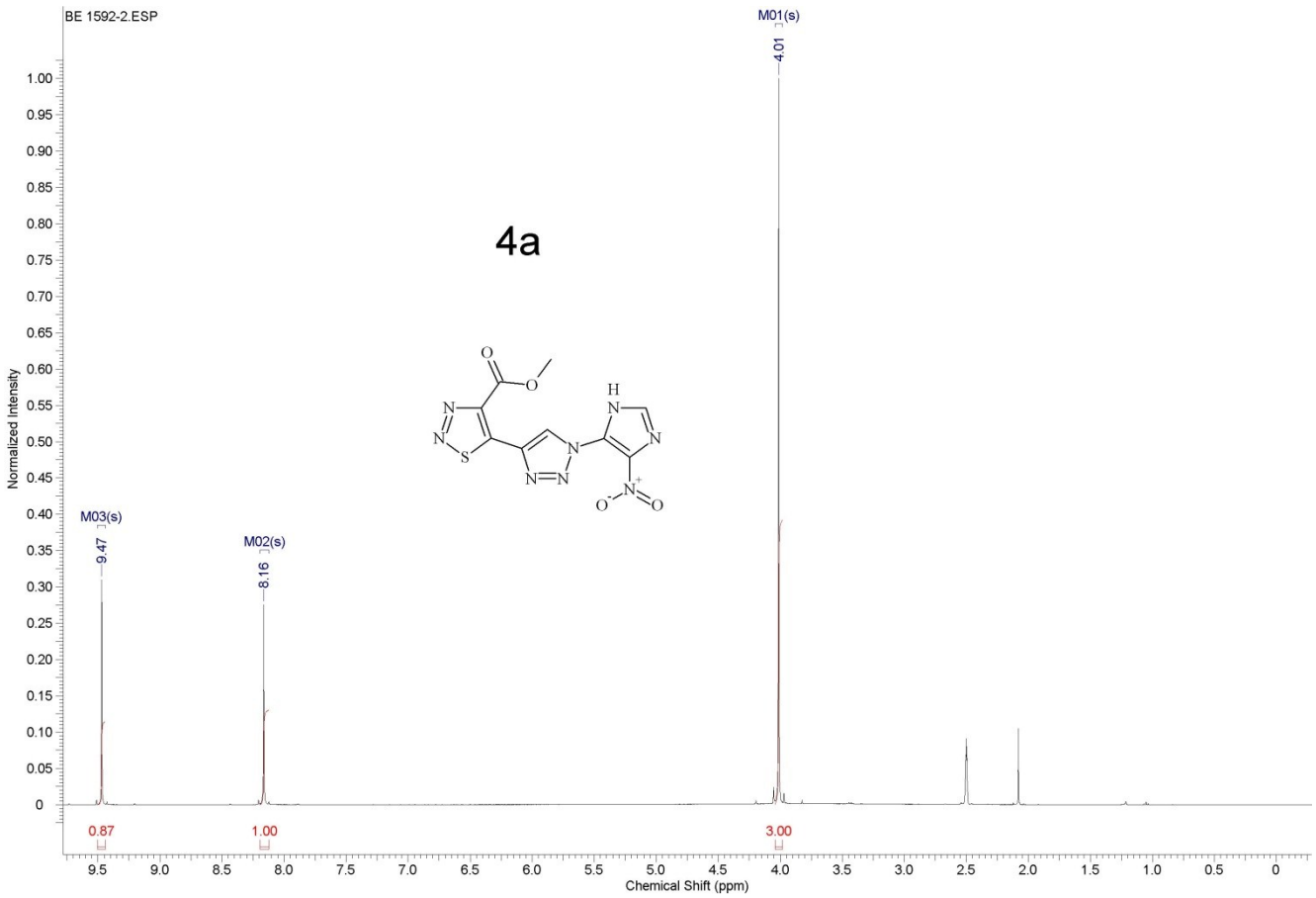
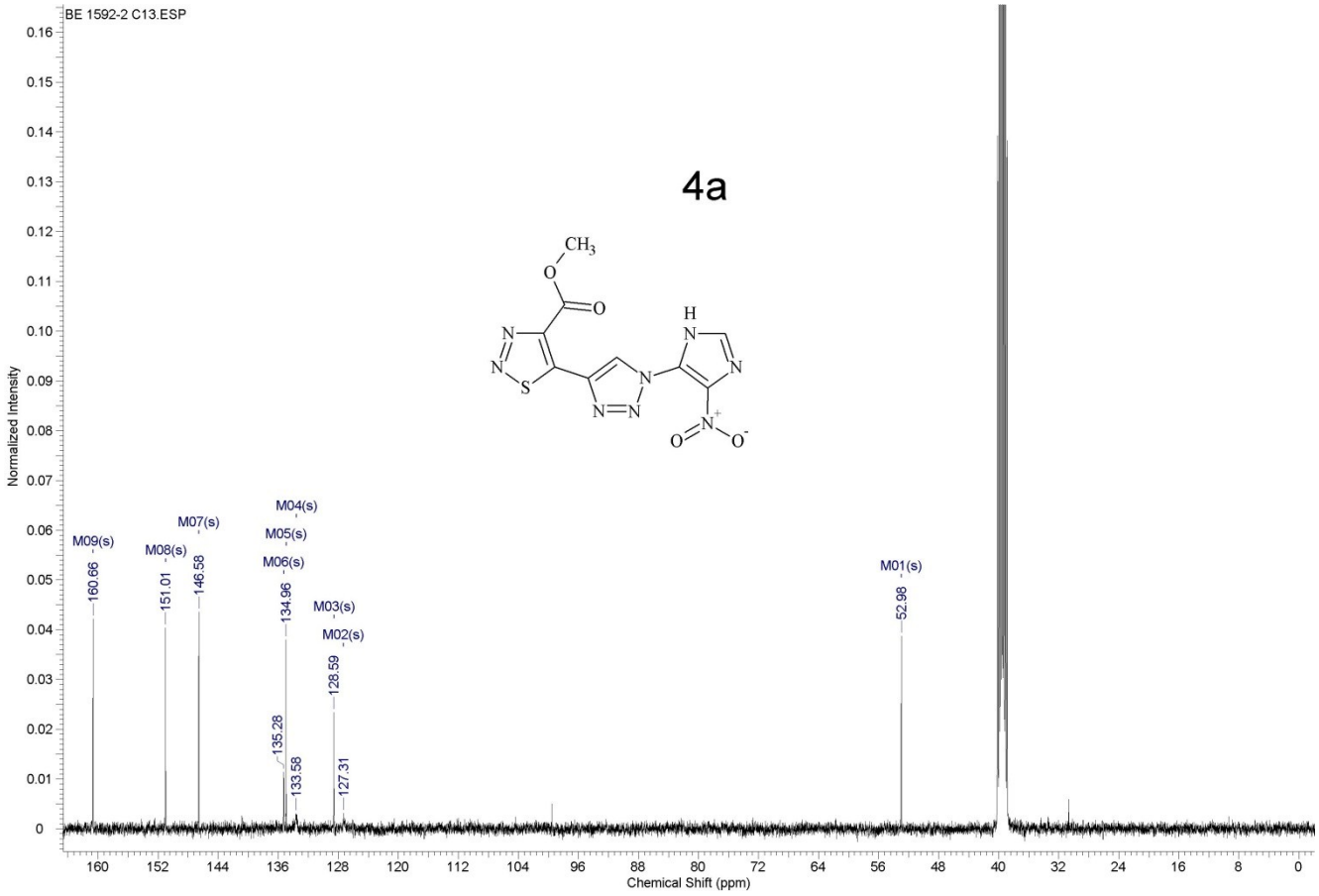
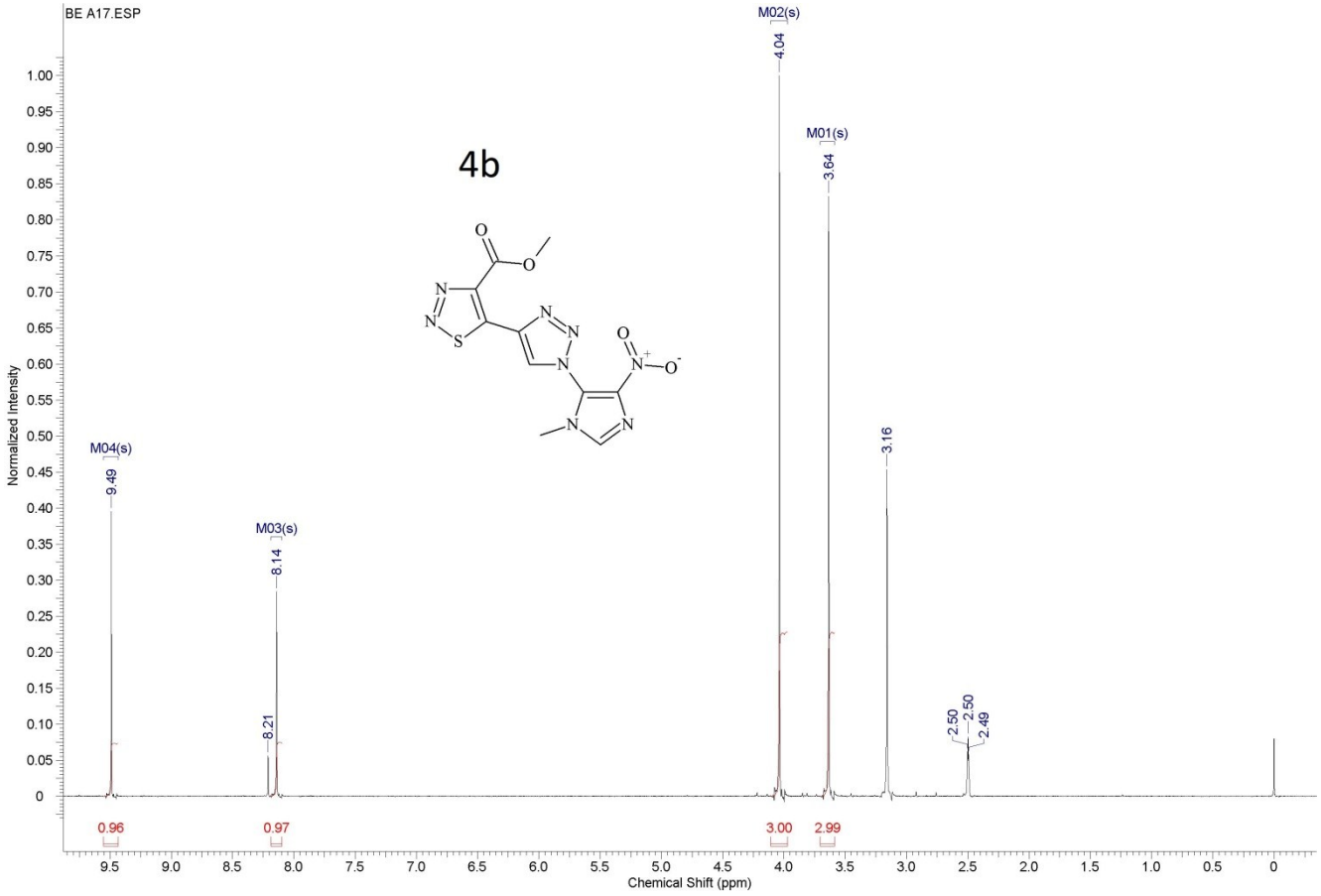
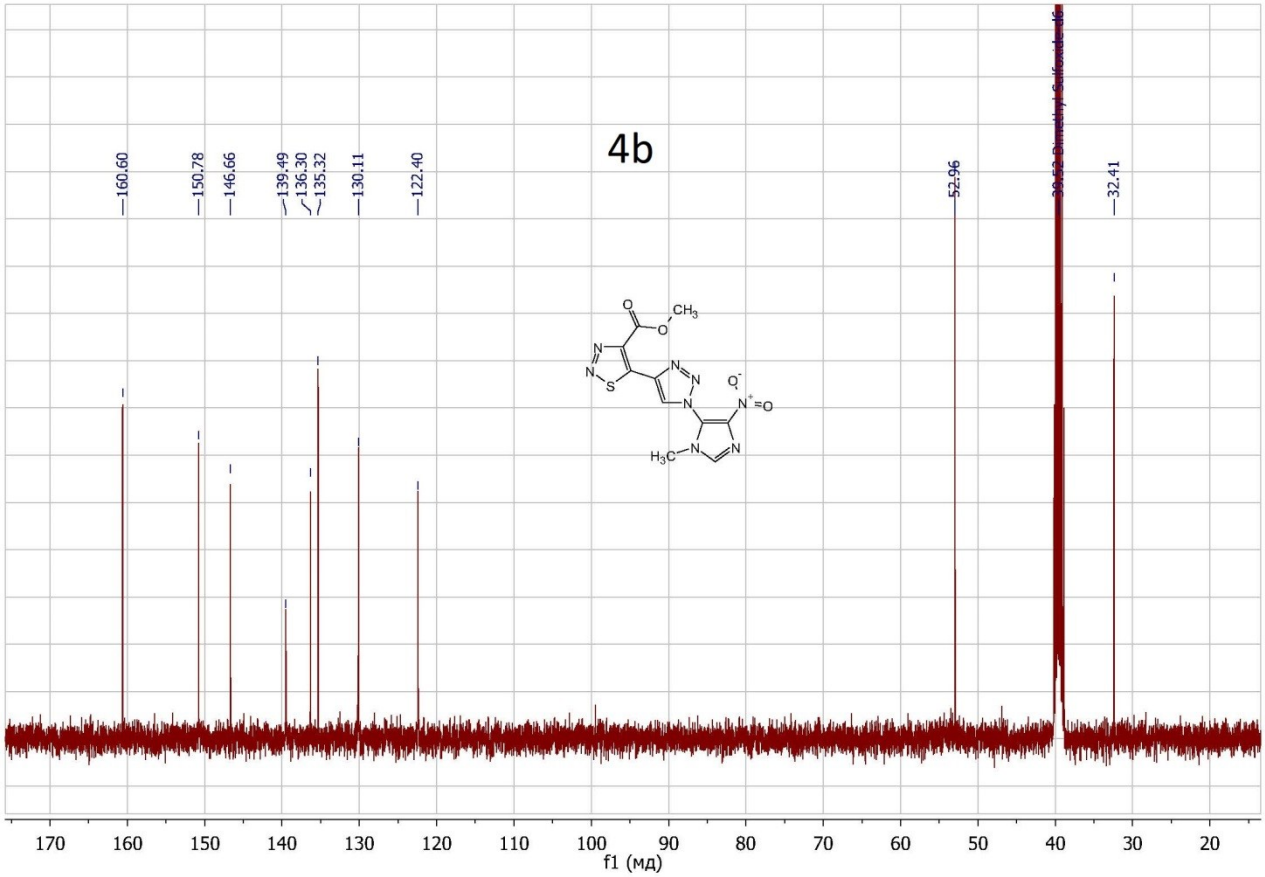
3f
M02(s)
3.98
3.17
M04(s)
5.44
M01(t)
1.27
M06(s)
8.64
M05(s)
8.09
8.23
M03(q)
4.23
4.21
4.24
4.19
1.29
1.26
2.91
2.75
2.50
2.49
2.50
2.49
2.48
0.93
0.95
1.99
2.00
3.05
3.12
Normalized Intensity
Chemical Shift (ppm)

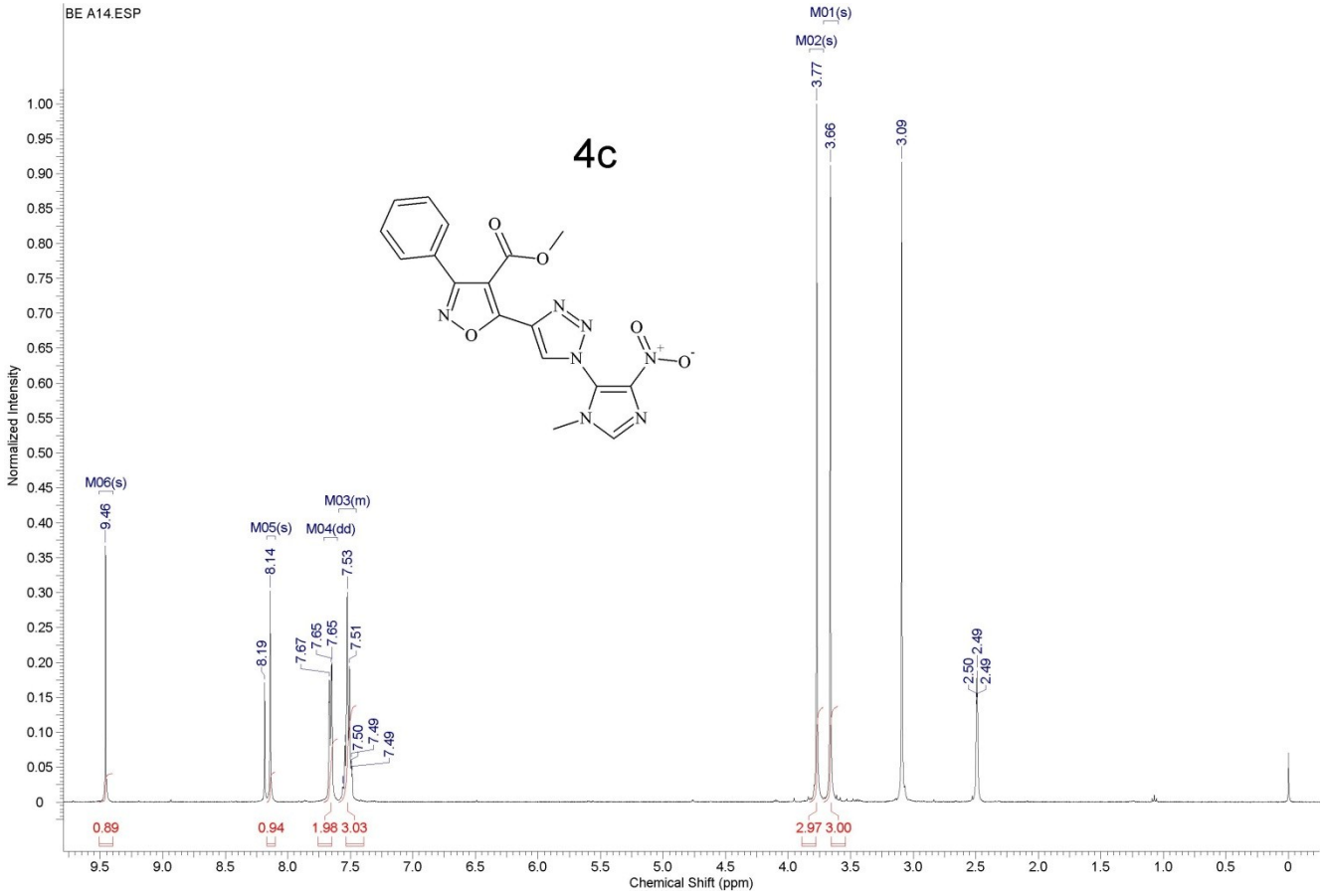

BE 1562 C13.ESP
3f
M03(s)
50.42
M04(s)
61.53
M10(s)
167.12
M06(s)
M07(s)
M08(s)
138.75
134.23
134.60
141.99
M09(s)
127.40
M05(s)
35.39
M02(s)
13.94
M01(s)
Normalized Intensity
Chemical Shift (ppm)

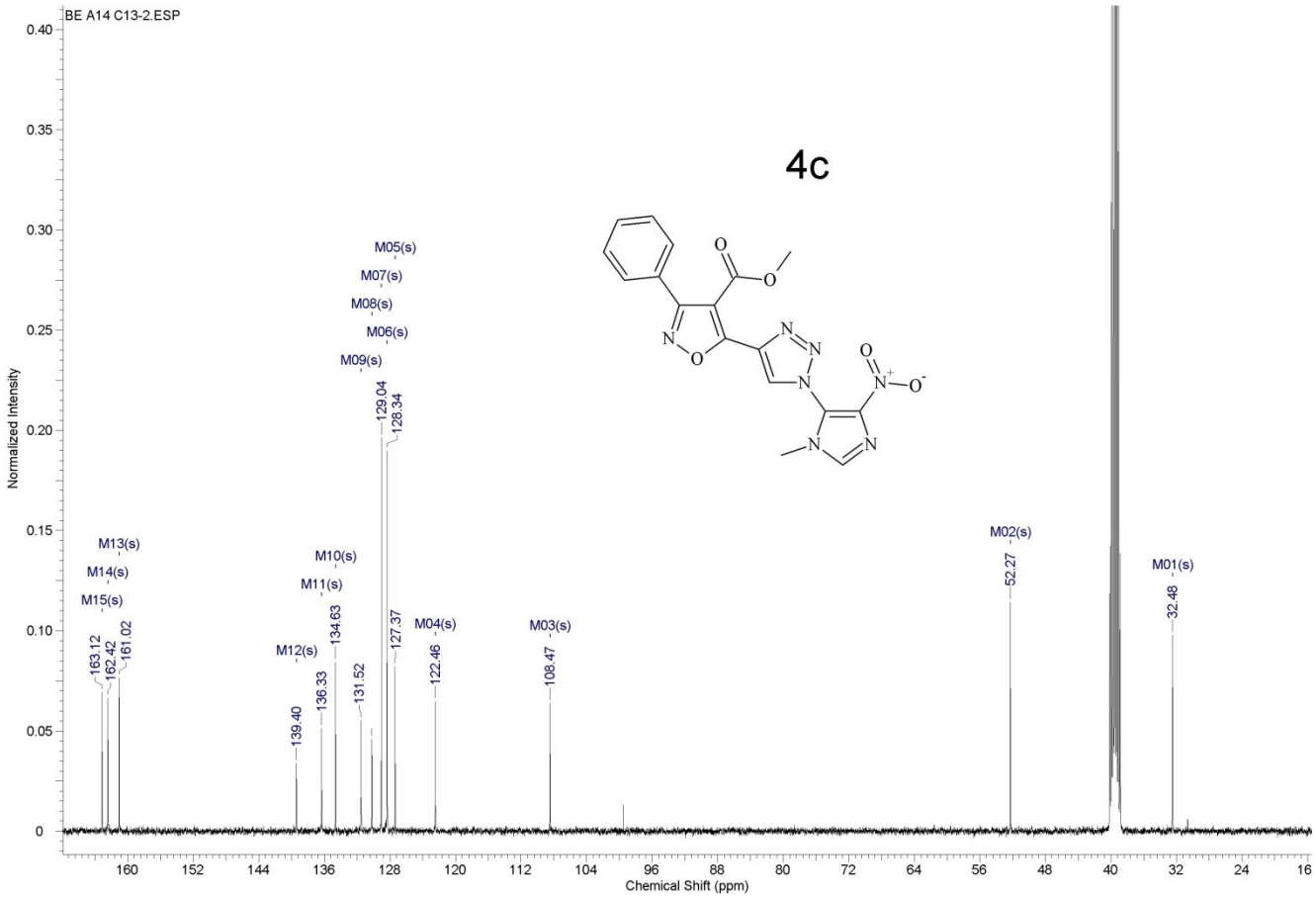

BE 1592-2.ESP
4a
M01(s)
4.01
M03(s)
9.47
M02(s)
8.16
0.87
1.00
3.00
Normalized Intensity
Chemical Shift (ppm)

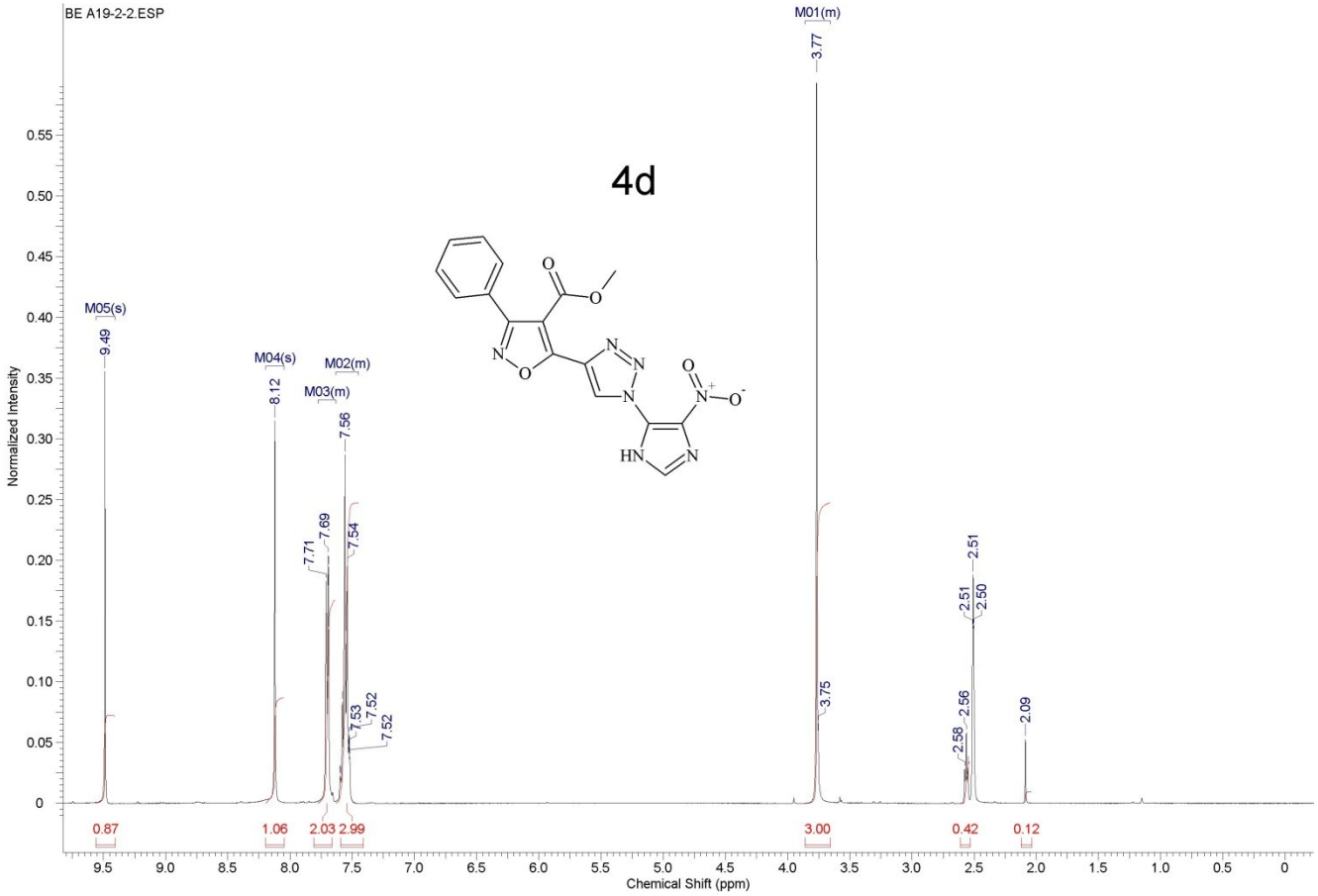

BE 1592-2 C13.ESP
4a
M09(s)
160.66
M08(s)
151.01
M07(s)
146.58
M04(s)
M05(s)
M06(s)
134.96
M03(s)
M02(s)
128.59
135.28
133.58
127.31
M01(s)
52.98
Normalized Intensity
Chemical Shift (ppm)

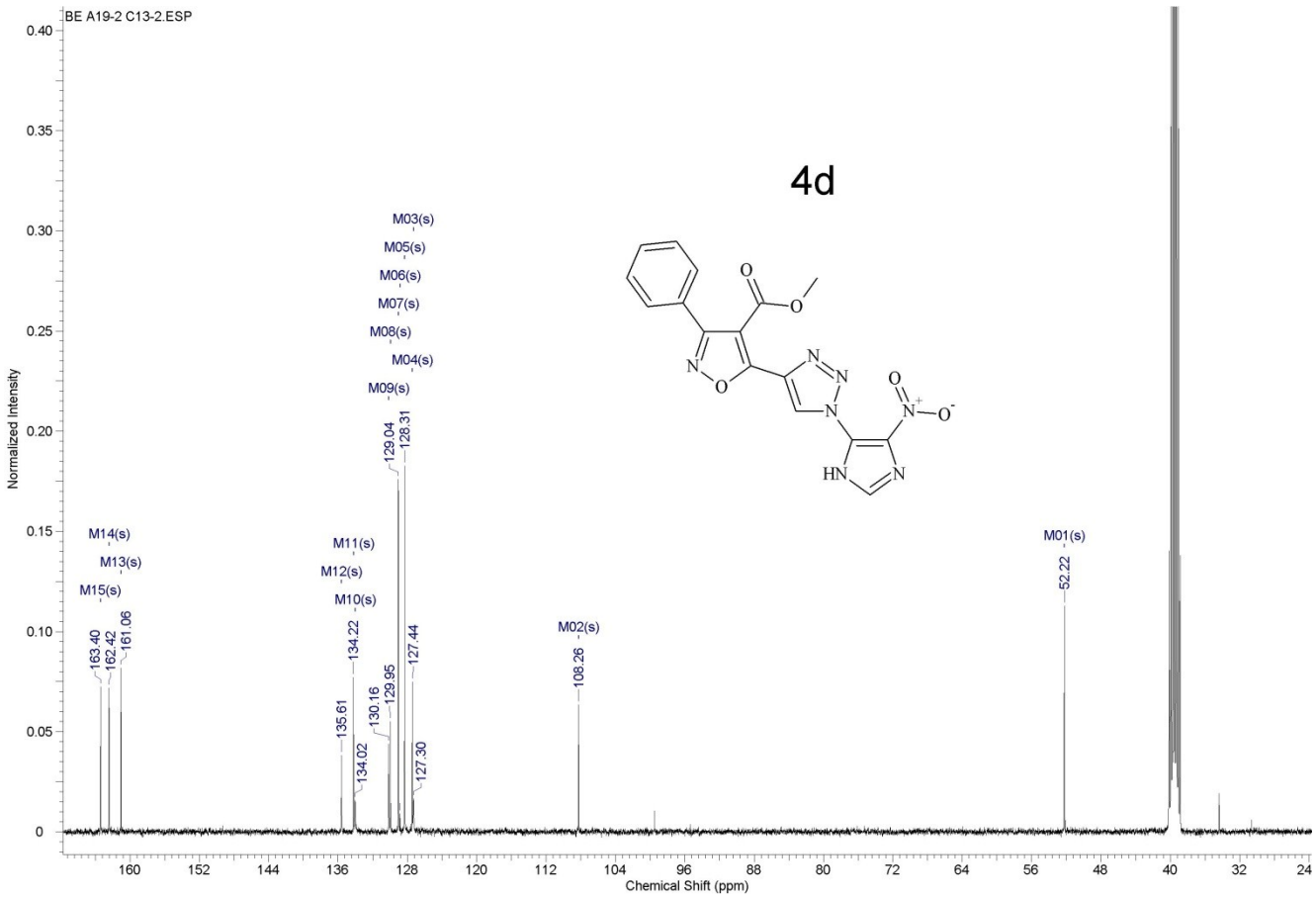

BE A17.ESP
4b
M02(s)
4.04
M01(s)
3.64
3.16
M04(s)
9.49
M03(s)
8.14
8.21
2.50
2.50
2.49
0.96
0.97
3.00
2.99
Normalized Intensity
Chemical Shift (ppm)

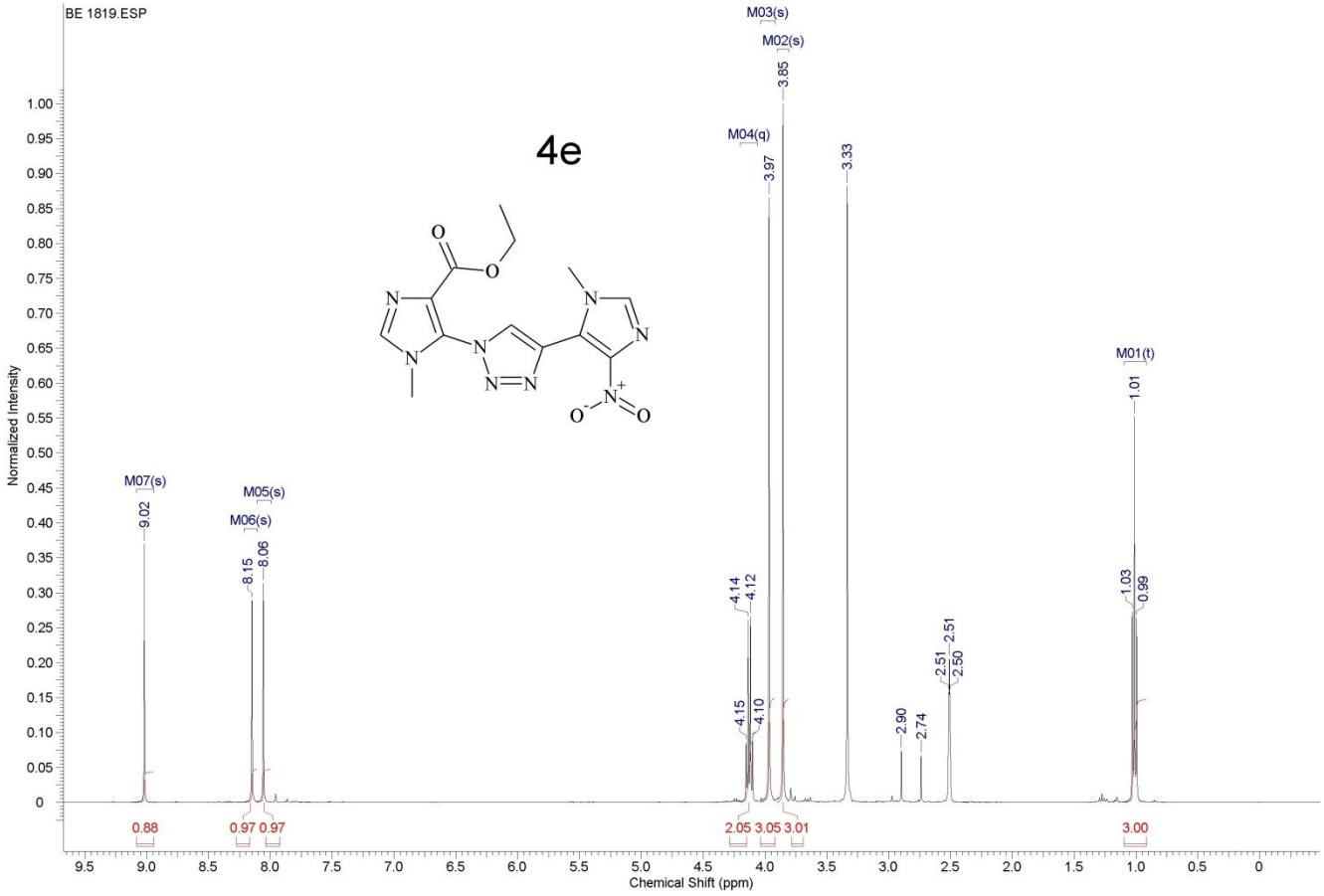

4b
160.60
150.78
146.66
139.49
136.30
135.32
130.11
122.40
52.96
39.52
32.41
f1 (мд)

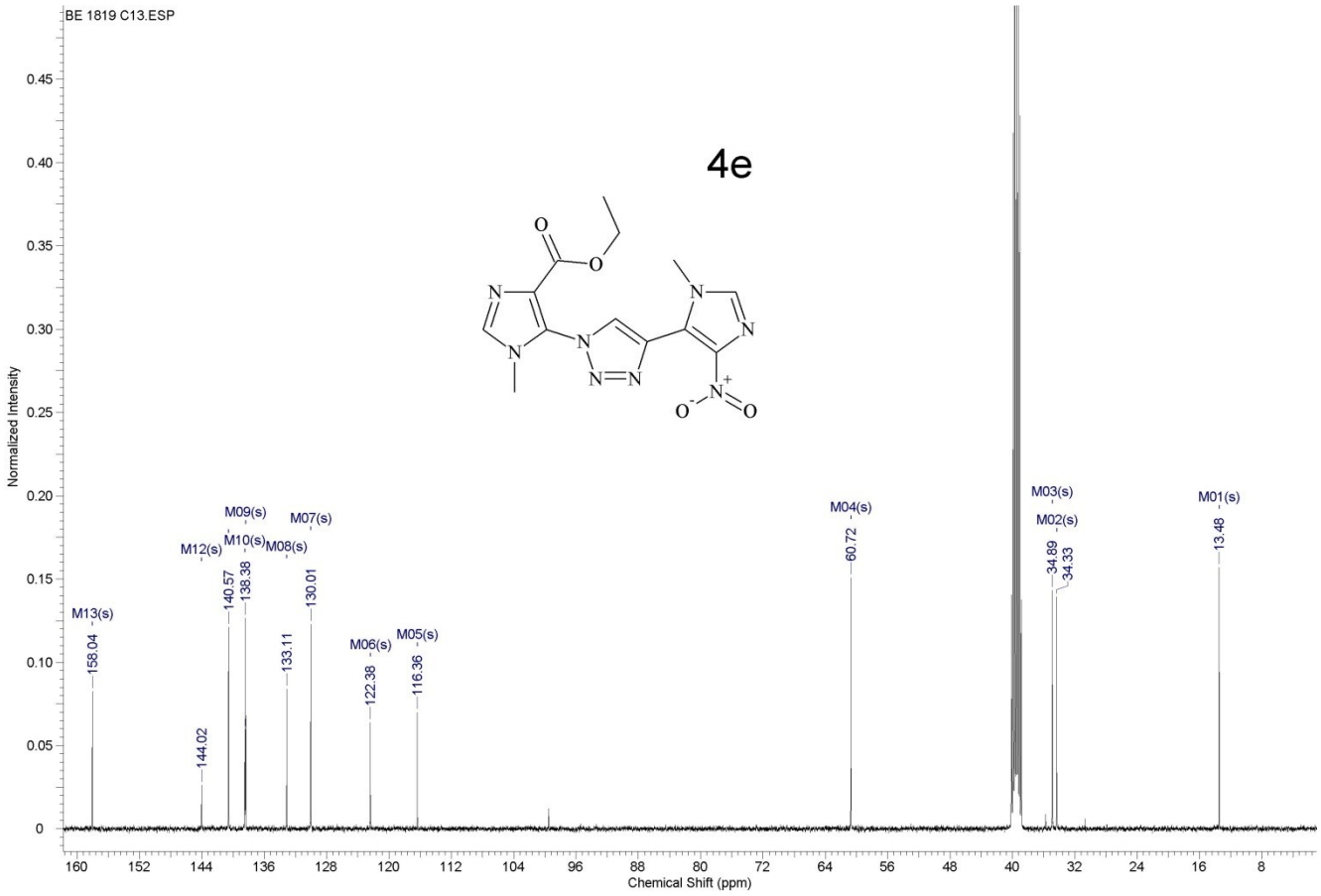

BE A14.ESP
4c
M01(s)
M02(s)
3.77
3.66
3.09
M06(s)
9.46
M05(s)
8.14
M04(dd)
M03(m)
7.53
8.19
7.67
7.65
7.65
7.51
7.50
7.49
7.49
2.50
2.49
2.49
0.89
0.94
1.98
3.03
2.97
3.00
Normalized Intensity
Chemical Shift (ppm)

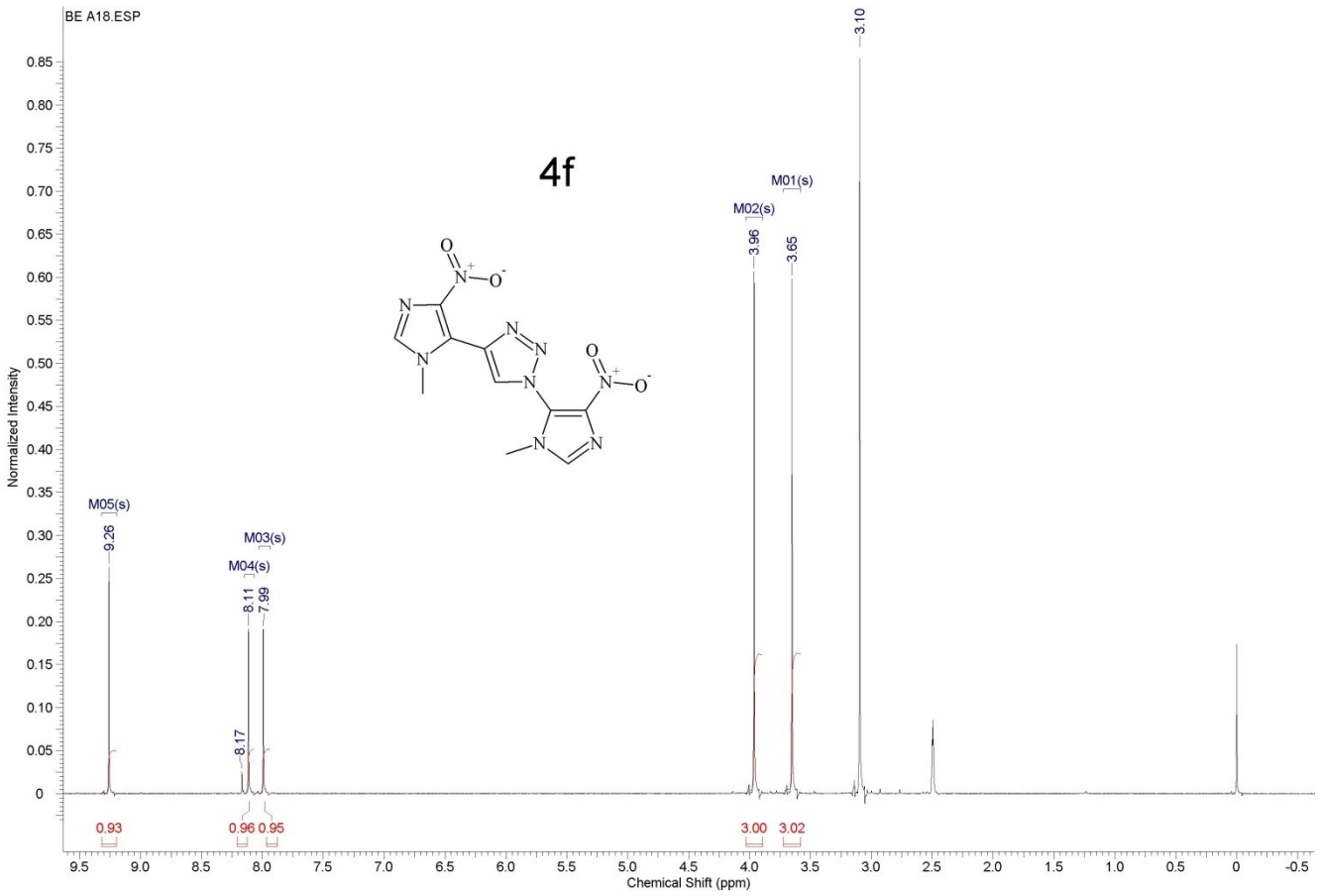

BE A14 C13-2.ESP
4c
M05(s)
M07(s)
M08(s)
M06(s)
M09(s)
129.04
128.34
M13(s)
M14(s)
M15(s)
M10(s)
M11(s)
134.63
127.37
M04(s)
M03(s)
M12(s)
163.12
162.42
161.02
136.33
131.52
139.40
122.46
108.47
M02(s)
52.27
M01(s)
32.48
Normalized Intensity
Chemical Shift (ppm)

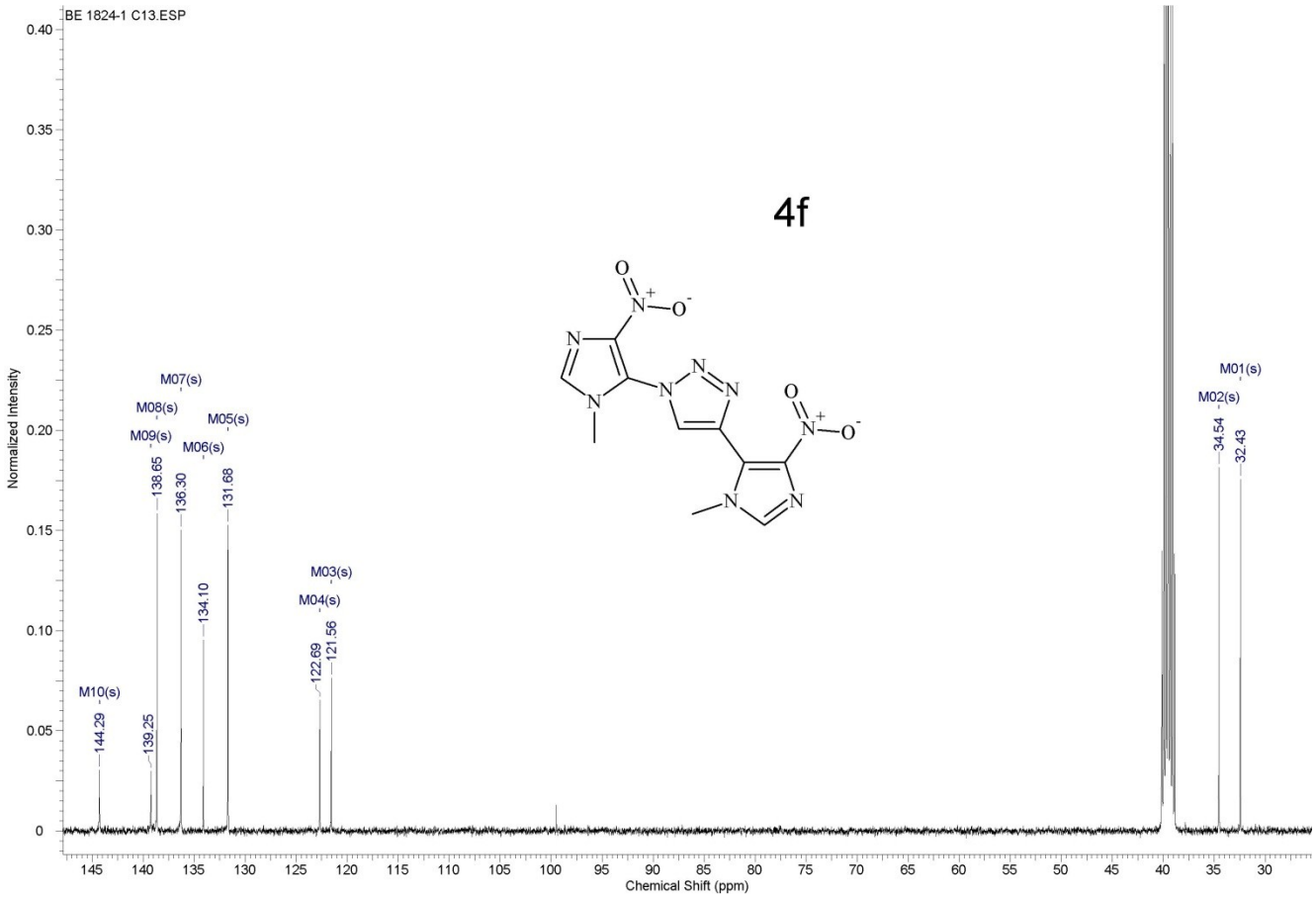

BE A19-2-2.ESP
4d
M01(m)
3.77
M05(s)
9.49
M04(s)
8.12
M02(m)
M03(m)
7.56
7.71
7.69
7.54
7.53
7.52
7.52
3.75
2.51
2.51
2.50
2.58
2.56
2.09
0.87
1.06
2.03
2.99
3.00
0.42
0.12
Normalized Intensity
Chemical Shift (ppm)

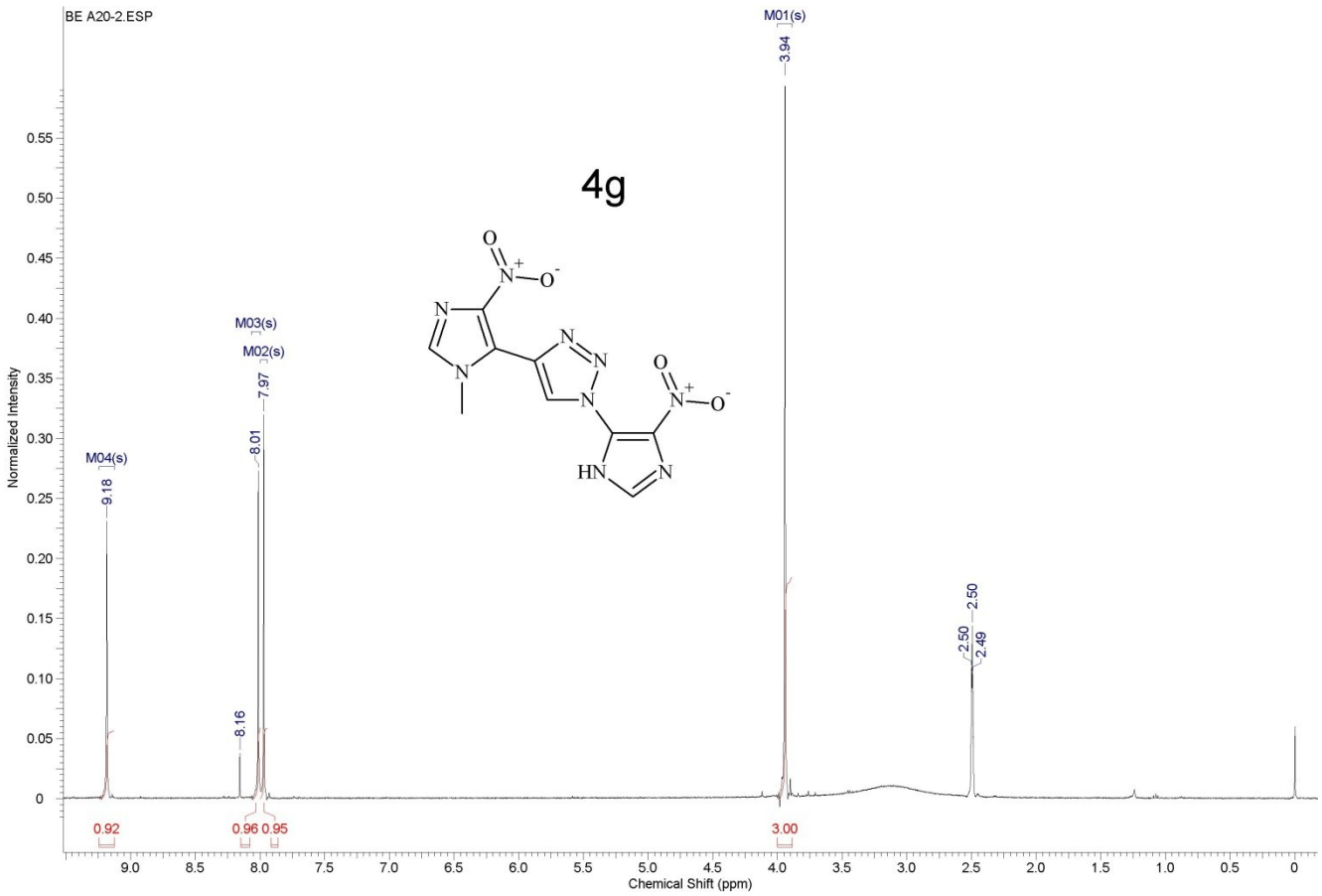

BE A19-2 C13-2.ESP
4d
M03(s)
M05(s)
M06(s)
M07(s)
M08(s)
M04(s)
M09(s)
129.04
128.31
M14(s)
M13(s)
M15(s)
163.40
162.42
161.06
M11(s)
M12(s)
M10(s)
134.22
135.61
130.16
129.95
134.02
127.44
127.30
M02(s)
108.26
M01(s)
52.22
Normalized Intensity
Chemical Shift (ppm)

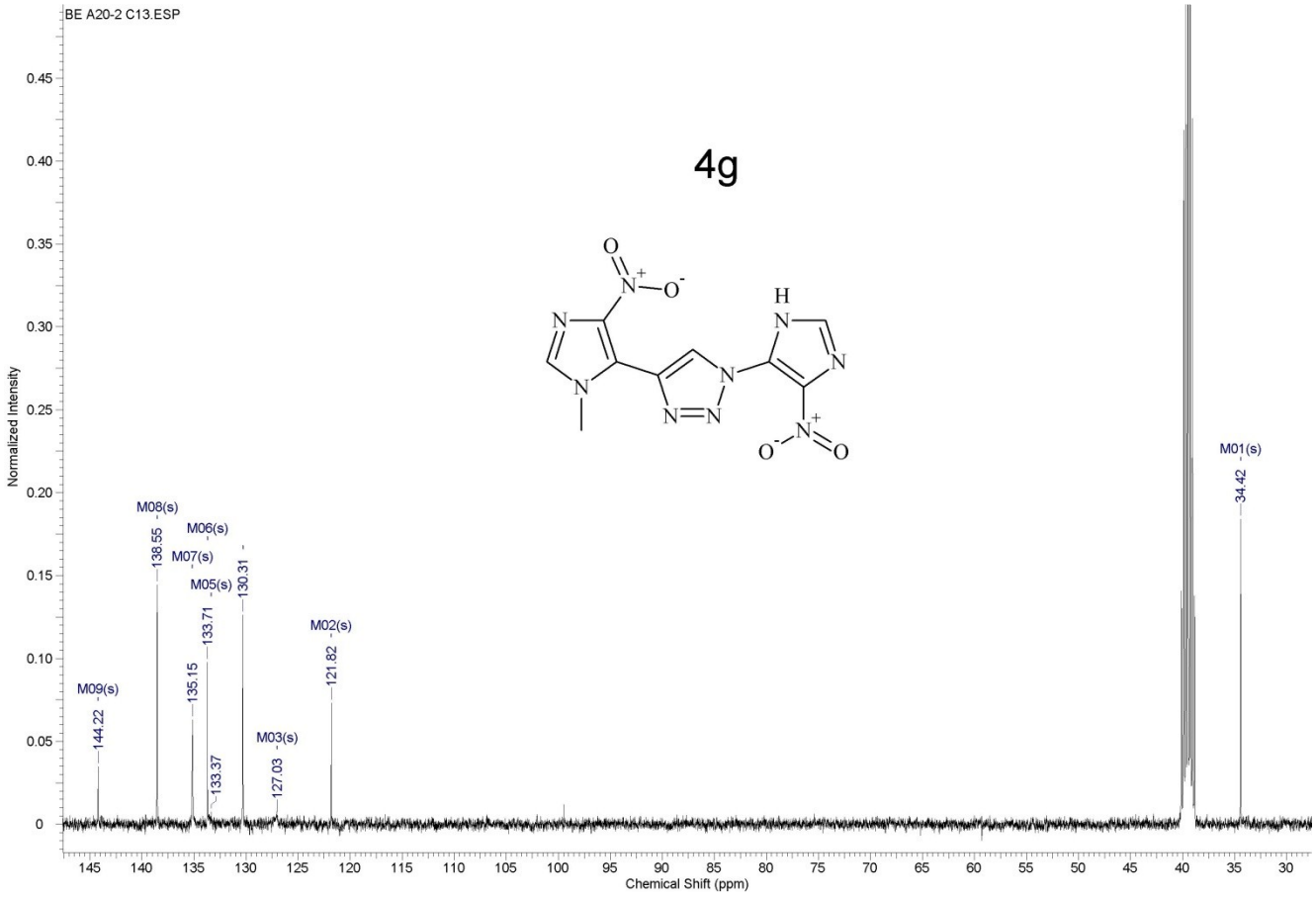

BE 1819.ESP
4e
M03(s)
M02(s)
3.85
M04(q)
3.97
3.33
M01(t)
1.01
M07(s)
9.02
M05(s)
M06(s)
8.15
8.06
4.14
4.12
1.03
0.99
2.51
2.50
4.15
4.10
2.90
2.74
0.88
0.97 0.97
2.05 3.05 3.01
3.00
Normalized Intensity
Chemical Shift (ppm)

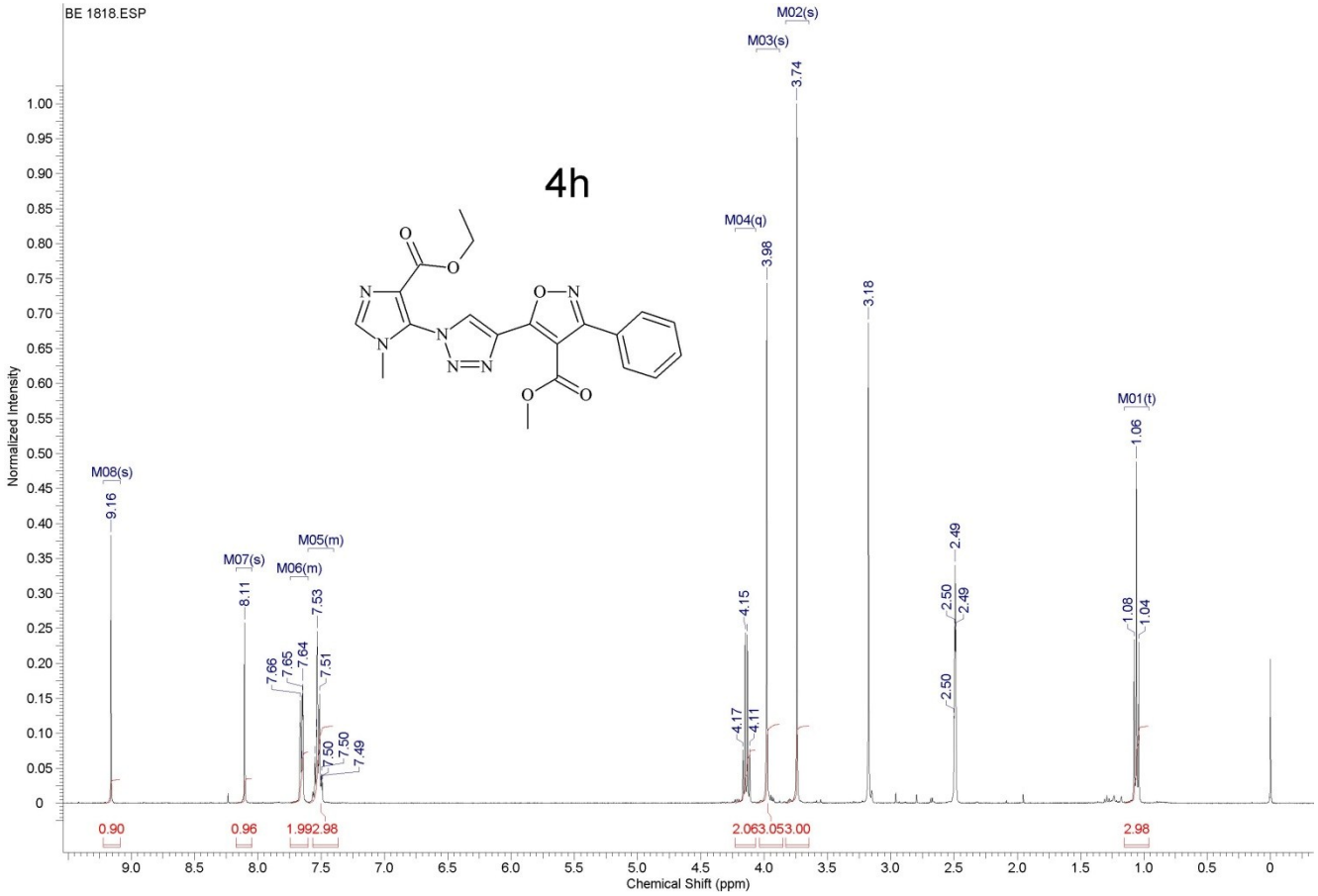

BE 1819 C13.ESP
4e
M09(s)
M07(s)
M12(s)
M10(s)
M08(s)
M13(s)
158.04
140.57
138.38
130.01
133.11
144.02
M06(s)
M05(s)
122.38
116.36
M04(s)
60.72
M03(s)
M02(s)
34.89
34.33
M01(s)
13.48
Normalized Intensity
Chemical Shift (ppm)

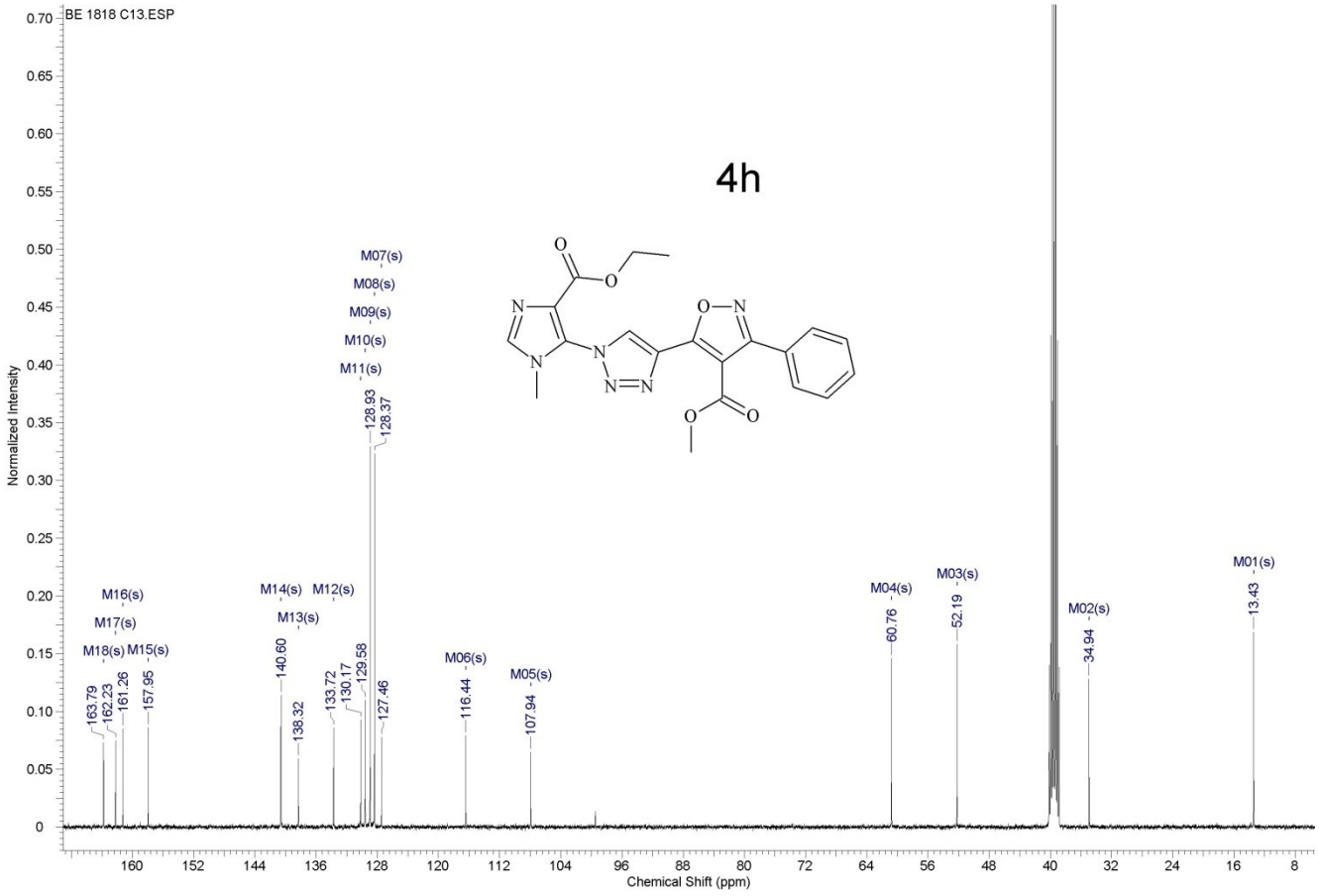

BE A18.ESP
4f
Normalized Intensity
Chemical Shift (ppm)
M05(s)
9.26
M03(s)
M04(s)
8.11
7.99
8.17
M02(s)
3.96
M01(s)
3.65
3.10
0.93
0.96
0.95
3.00
3.02

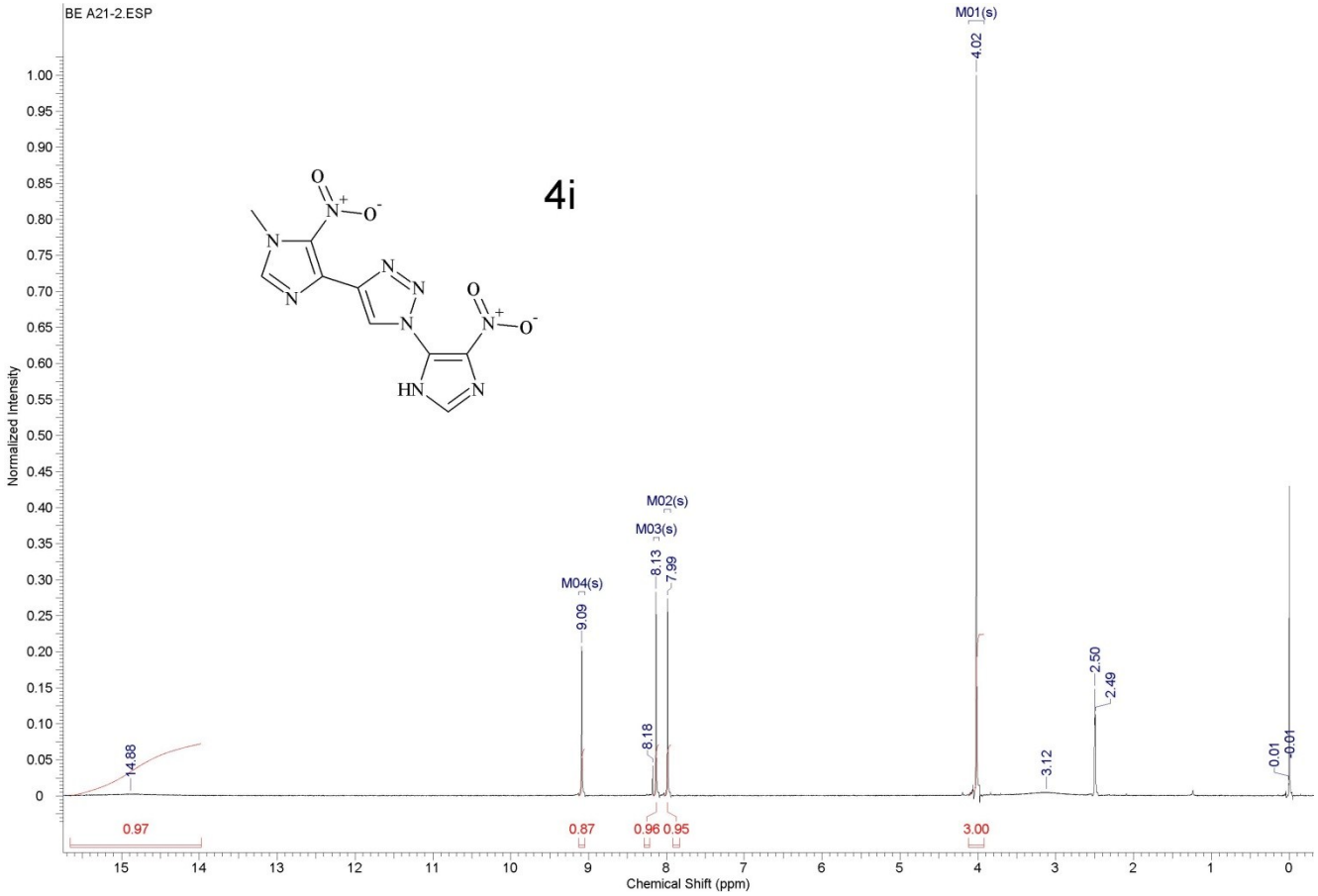

BE 1824-1 C13.ESP
4f
Normalized Intensity
Chemical Shift (ppm)
M07(s)
M08(s)
M09(s)
M05(s)
M06(s)
138.65
136.30
131.68
134.10
M03(s)
M04(s)
122.69
121.56
M10(s)
144.29
139.25
M01(s)
M02(s)
34.54
32.43

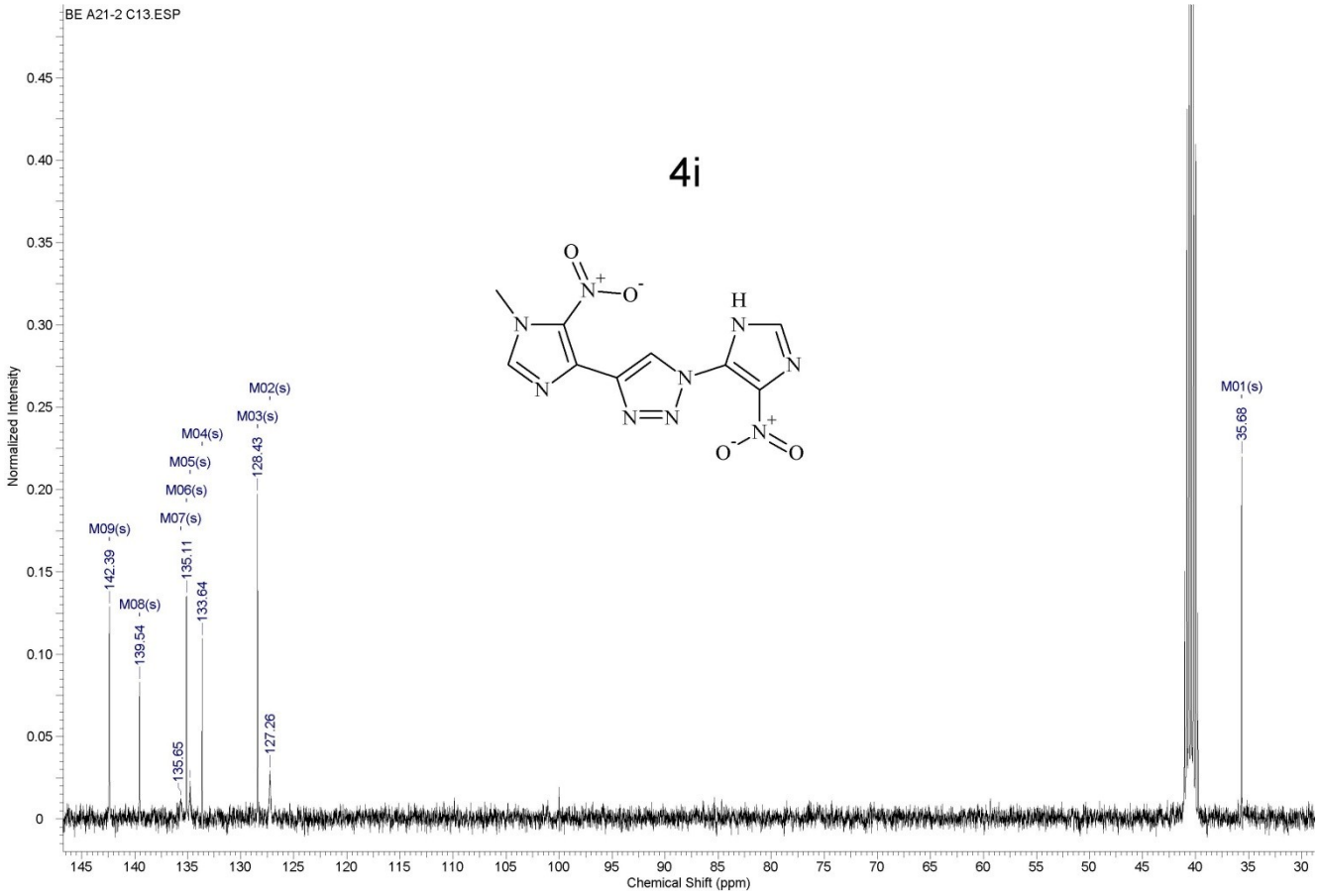

BE A20-2.ESP
4g
M01(s)
3.94
M03(s)
M02(s)
7.97
8.01
M04(s)
9.18
8.16
2.50
2.50
2.49
0.92
0.96
0.95
3.00
Normalized Intensity
Chemical Shift (ppm)

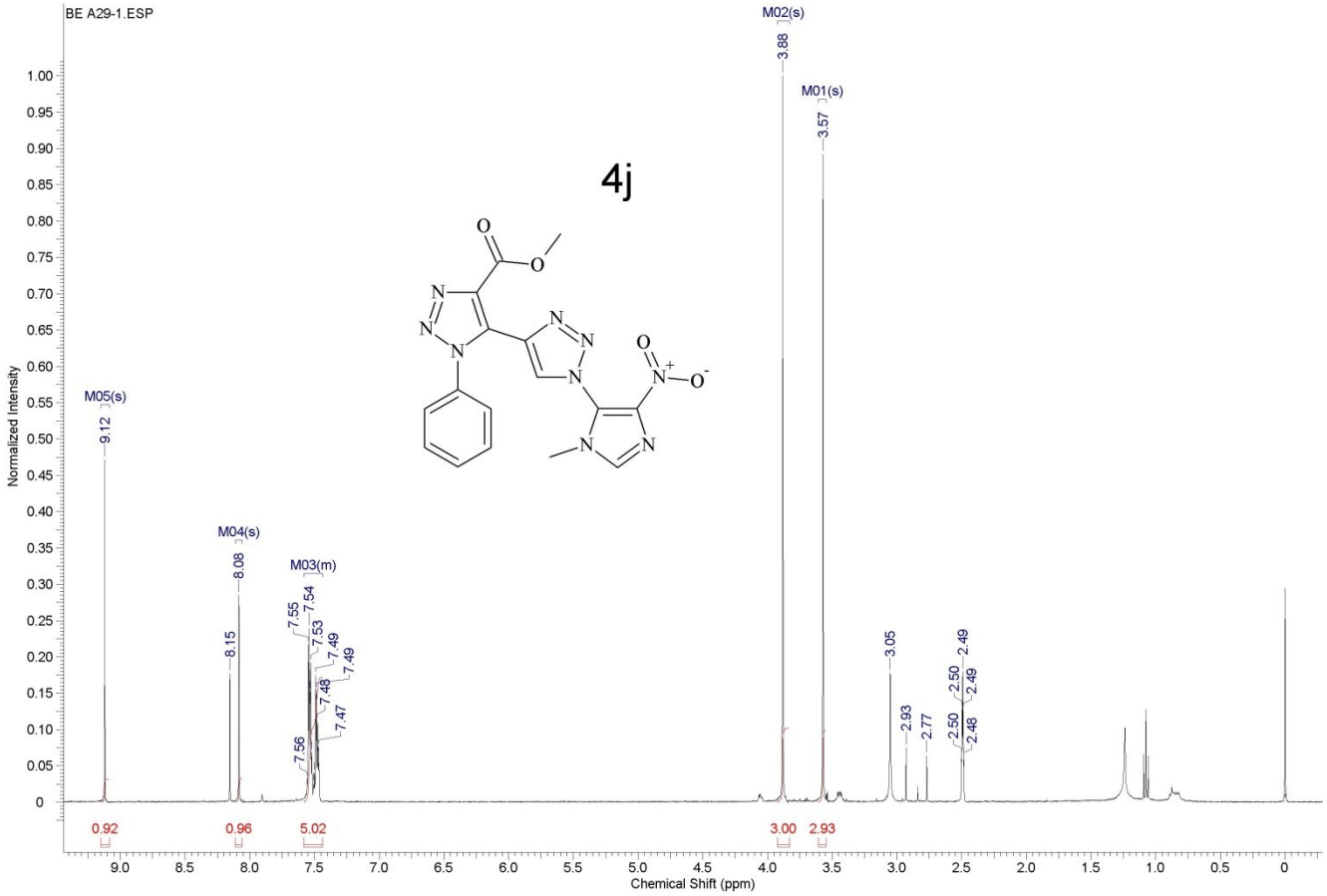

BE A20-2 C13.ESP
4g
M08(s)
138.55
M06(s)
M07(s)
M05(s)
130.31
133.71
M02(s)
121.82
M09(s)
144.22
135.15
133.37
M03(s)
127.03
M01(s)
34.42
Normalized Intensity
Chemical Shift (ppm)

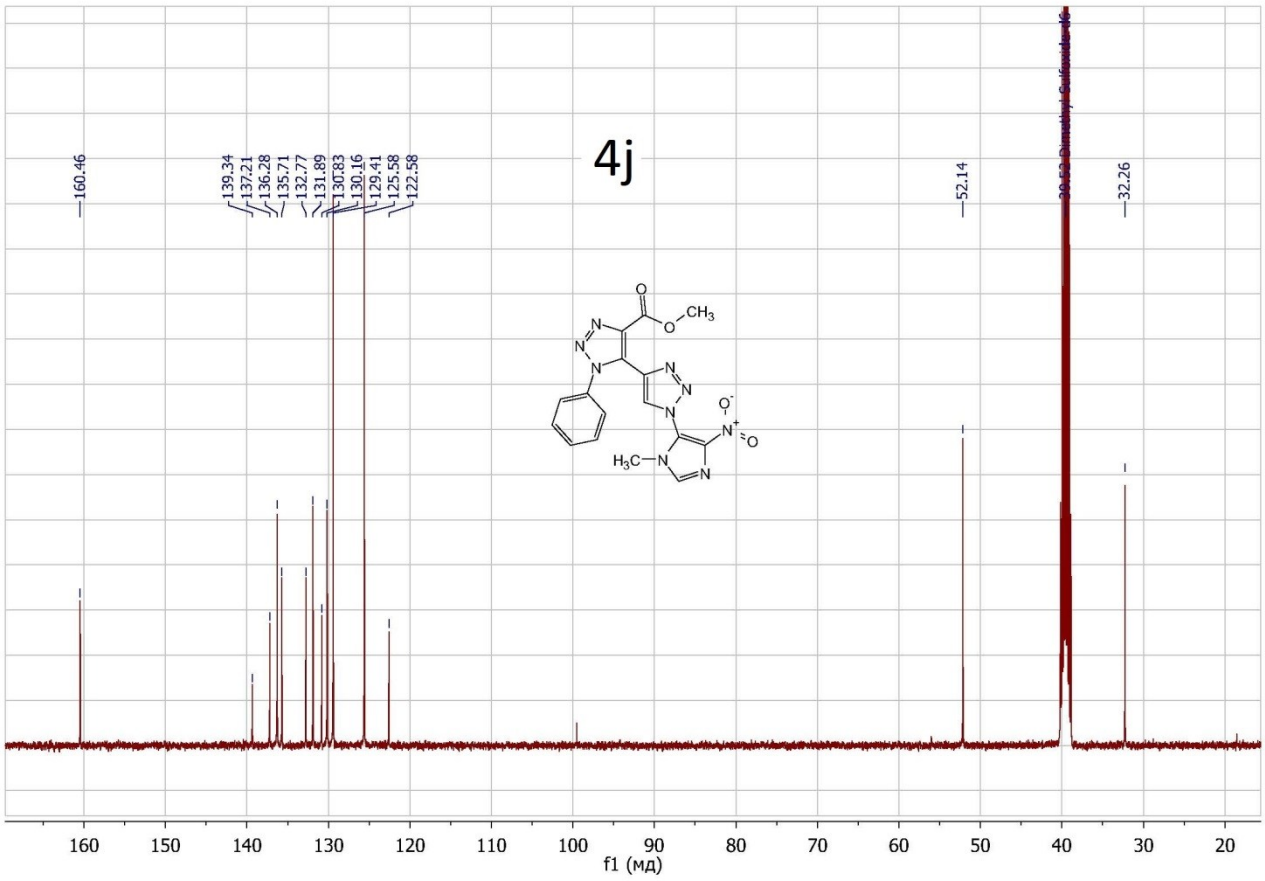

BE 1818.ESP
4h
M02(s)
M03(s)
3.74
M04(q)
3.98
3.18
M01(t)
1.06
M08(s)
9.16
M07(s)
8.11
M05(m)
M06(m)
7.53
7.66
7.65
7.64
7.51
7.50
7.49
4.15
4.17
4.11
2.49
2.50
2.49
2.50
1.08
1.04
0.90
0.96
1.99
2.98
2.06
3.05
3.00
2.98
Normalized Intensity
Chemical Shift (ppm)

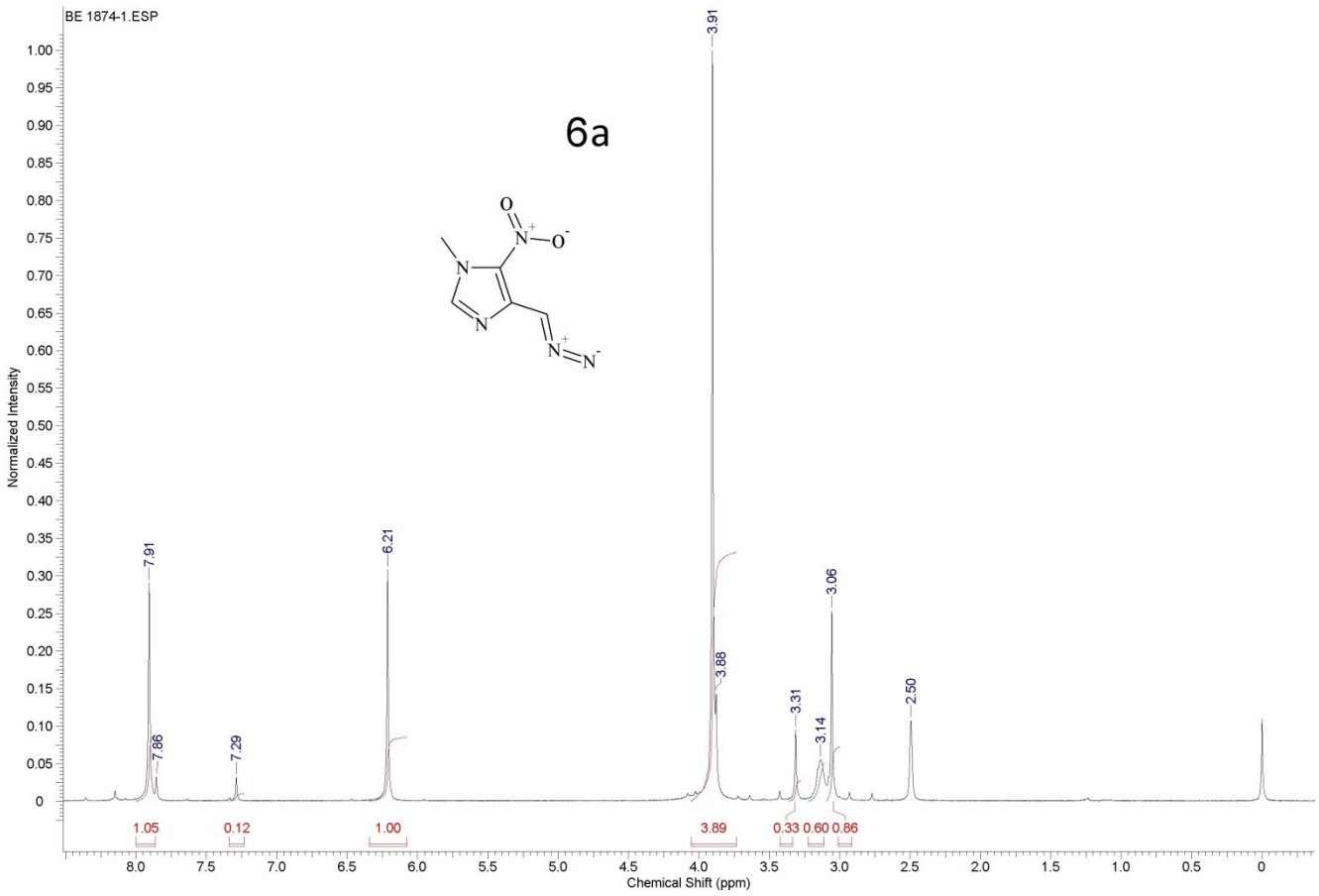

BE 1818 C13.ESP
4h
M07(s)
M08(s)
M09(s)
M10(s)
M11(s)
128.93
128.37
M16(s)
M17(s)
M18(s)
M15(s)
163.79
162.23
161.26
157.95
M14(s)
M12(s)
M13(s)
140.60
138.32
133.72
130.17
129.58
127.46
M06(s)
116.44
M05(s)
107.94
M04(s)
60.76
M03(s)
52.19
M02(s)
34.94
M01(s)
13.43
Normalized Intensity
Chemical Shift (ppm)

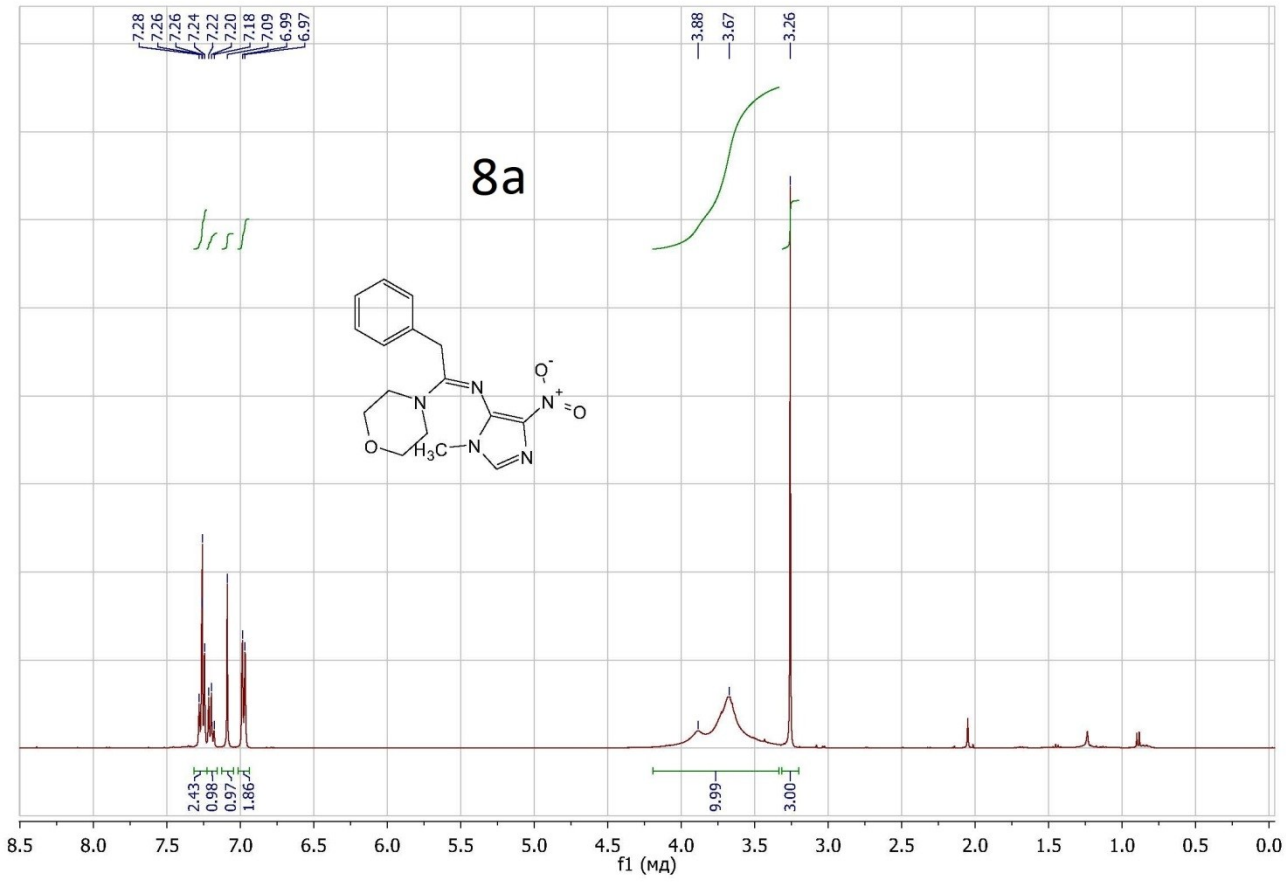

BE A21-2.ESP
4i
M01(s)
4.02
M02(s)
M03(s)
8.13
7.99
M04(s)
9.09
8.18
14.88
3.12
2.50
2.49
0.01
0.01
0.97
0.87
0.96
0.95
3.00
Normalized Intensity
Chemical Shift (ppm)

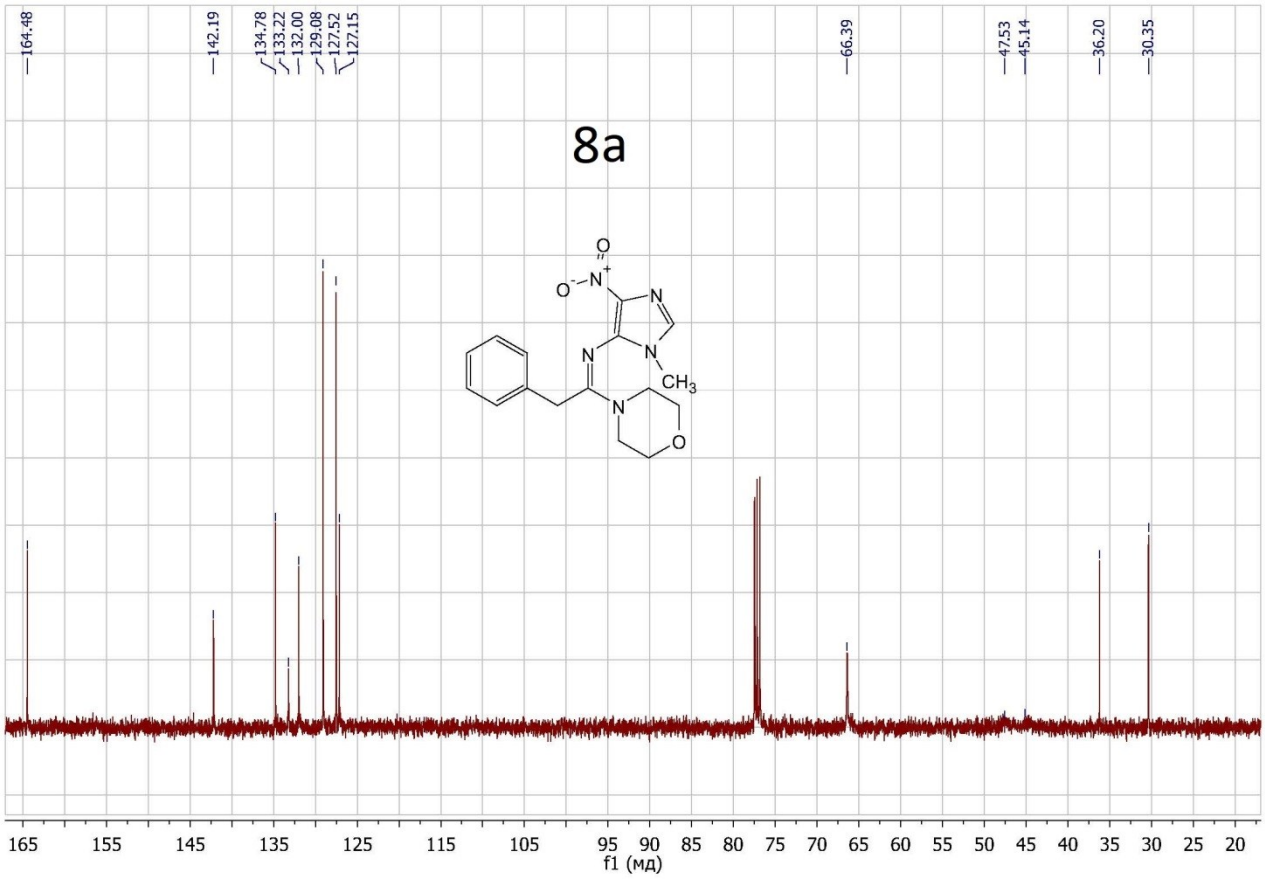

BE A21-2 C13.ESP
4i
M01(s)
35.68
M02(s)
M03(s)
M04(s)
M05(s)
M06(s)
M07(s)
M08(s)
M09(s)
128.43
142.39
139.54
135.11
133.64
135.65
127.26
Normalized Intensity
Chemical Shift (ppm)

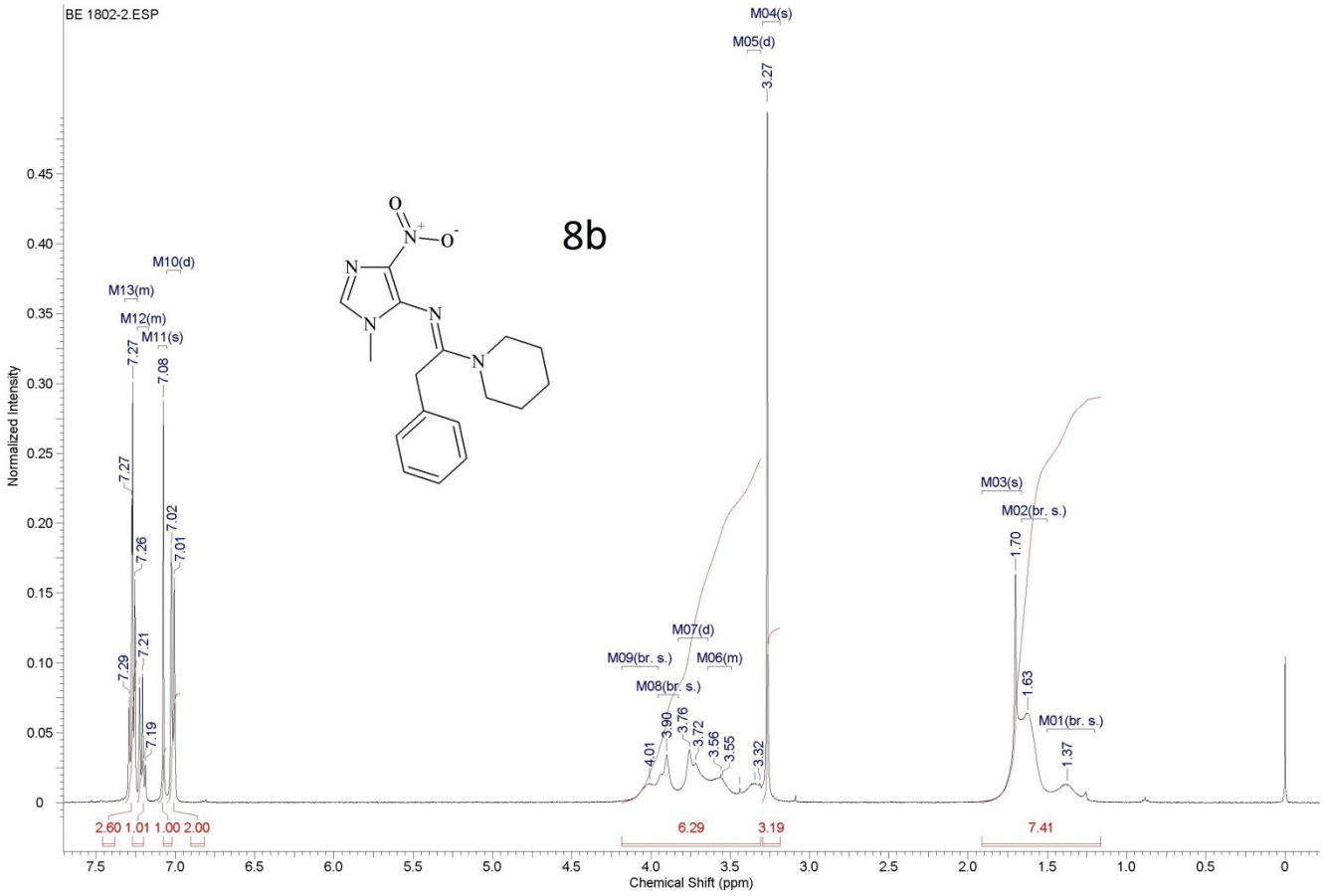

BE A29-1.ESP
4j
M05(s)
9.12
M04(s)
8.08
8.15
M03(m)
7.55
7.54
7.53
7.49
7.49
7.48
7.47
7.56
M02(s)
3.88
M01(s)
3.57
3.05
2.93
2.77
2.50
2.49
2.50
2.49
2.48
0.92
0.96
5.02
3.00
2.93
Normalized Intensity
Chemical Shift (ppm)

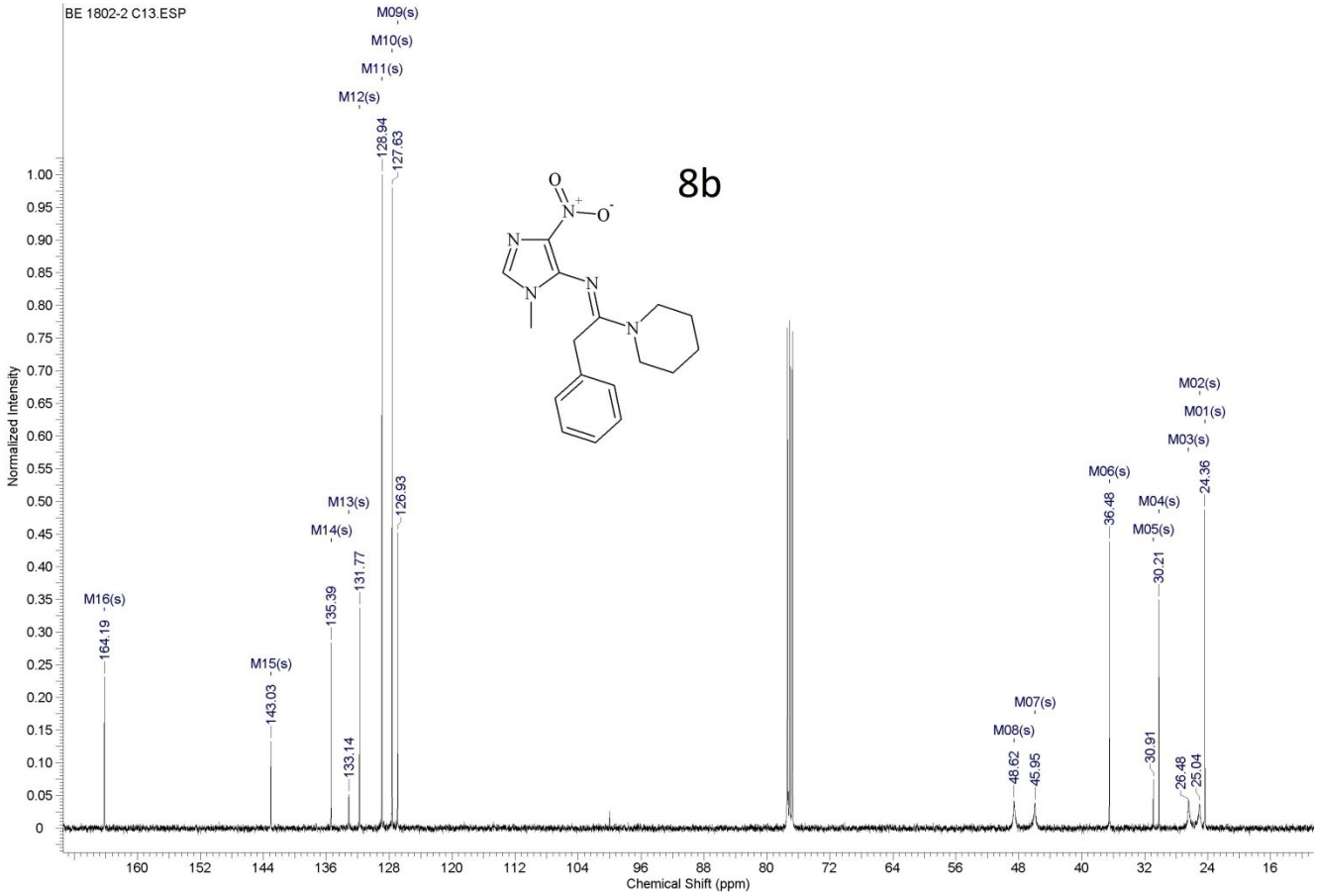

4j
160.46
139.34
137.21
136.28
135.71
132.77
131.89
130.83
130.16
129.41
125.58
122.58
52.14
32.26
f1 (мд)

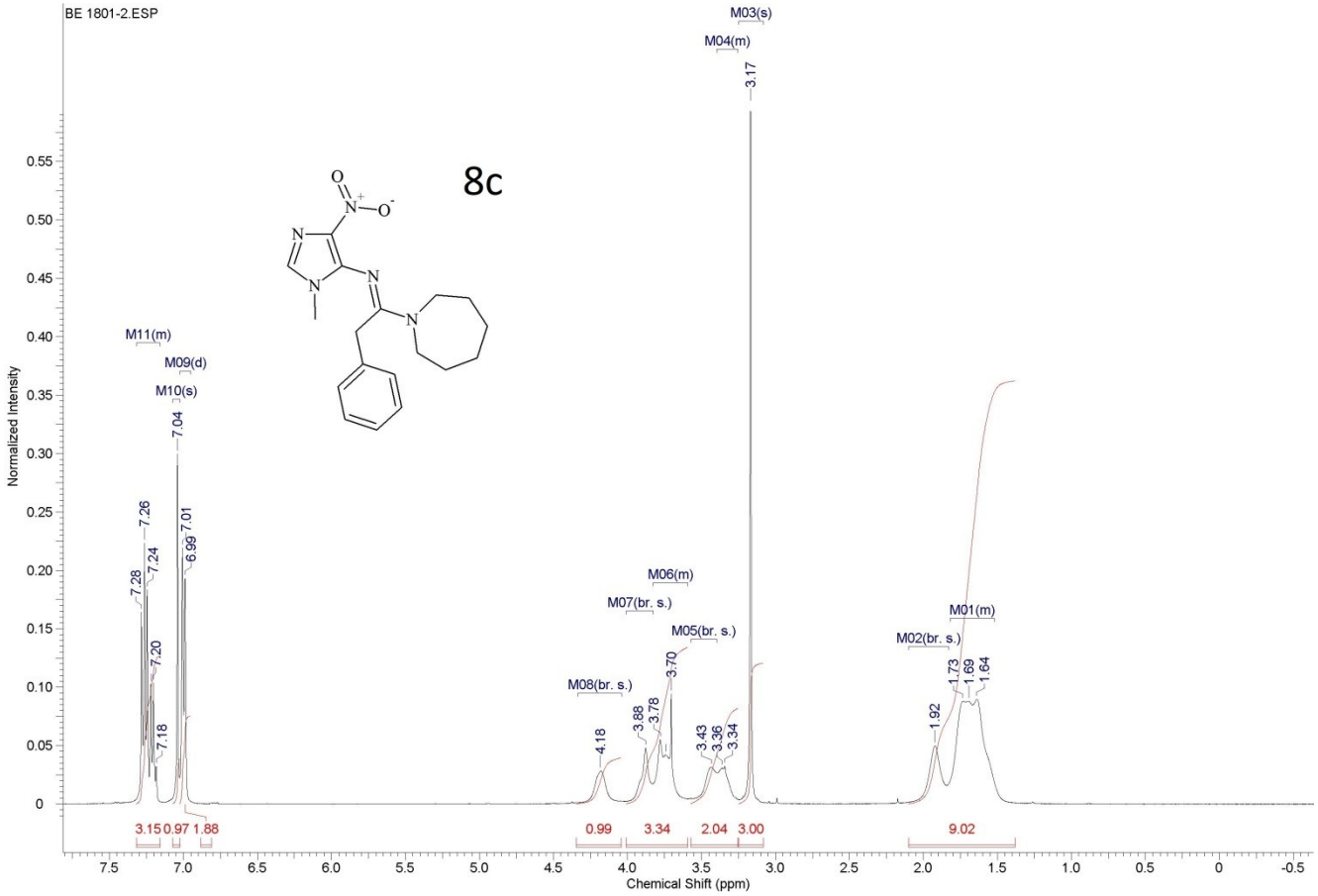

BE 1874-1.ESP
6a
Normalized Intensity
Chemical Shift (ppm)
7.91
7.86
7.29
6.21
3.91
3.88
3.31
3.14
3.06
2.50
1.05
0.12
1.00
3.89
0.33
0.60
0.86

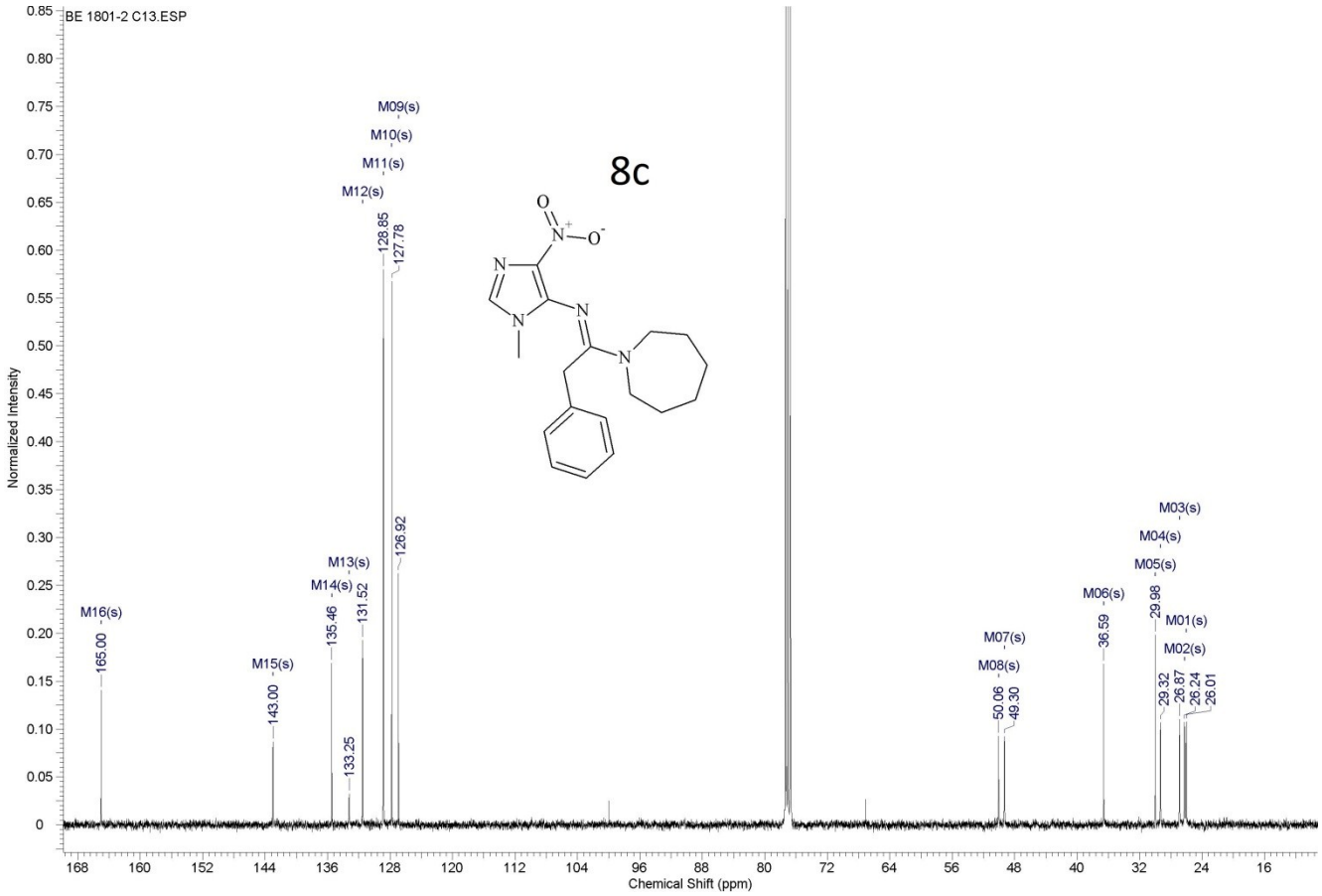

8a
7.28
7.26
7.26
7.24
7.22
7.20
7.18
7.09
6.99
6.97
3.88
3.67
3.26
2.43
0.98
0.97
1.86
9.99
3.00
f1 (мд)


8a
164.48
142.19
134.78
133.22
132.00
129.08
127.52
127.15
66.39
47.53
45.14
36.20
30.35
f1 (мд)


BE 1802-2.ESP
8b
M04(s)
M05(d)
M10(d)
M13(m)
M12(m)
M11(s)
M03(s)
M02(br. s.)
M07(d)
M09(br. s.)
M06(m)
M08(br. s.)
M01(br. s.)
Normalized Intensity
Chemical Shift (ppm)
2.60 1.01 1.00 2.00
6.29
3.19
7.41


BE 1802-2 C13.ESP
8b
M09(s)
M10(s)
M11(s)
M12(s)
128.94
127.63
M13(s)
M14(s)
131.77
135.39
126.93
M16(s)
164.19
M15(s)
143.03
133.14
M07(s)
M08(s)
48.62
45.95
M06(s)
36.48
M02(s)
M01(s)
M03(s)
24.36
M04(s)
M05(s)
30.21
30.91
26.48
25.04
Normalized Intensity
Chemical Shift (ppm)


BE 1801-2.ESP
8c
M03(s)
M04(m)
3.17
M11(m)
M09(d)
M10(s)
7.04
7.26
7.01
6.99
7.28
7.24
7.20
7.18
M06(m)
M07(br. s.)
M05(br. s.)
M08(br. s.)
3.70
3.88
3.78
4.18
3.43
3.36
3.34
M01(m)
M02(br. s.)
1.73
1.69
1.64
1.92
3.15
0.97
1.88
0.99
3.34
2.04
3.00
9.02
Normalized Intensity
Chemical Shift (ppm)


BE 1801-2 C13.ESP
8c
Normalized Intensity
Chemical Shift (ppm)
M09(s)
M10(s)
M11(s)
M12(s)
128.85
127.78
126.92
M13(s)
M14(s)
135.46
131.52
133.25
M15(s)
143.00
M16(s)
165.00
M03(s)
M04(s)
M05(s)
M06(s)
29.98
36.59
M01(s)
M02(s)
M07(s)
M08(s)
50.06
49.30
29.32
26.87
26.24
26.01