SUPPORTING INFORMATION

Taming Ambident Triazole Anions: Regioselective Ion-Pairing Catalyzes Direct N-Alkylation with Atypical Regioselectivity

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General Experimental

NMR spectroscopy

Unless otherwise stated, all ^{1}H, $^{13}C\{^{1}H\}$, ^{11}B, ^{19}F and ^{31}P NMR spectra were acquired on a Bruker Ascend 400 MHz NMR spectrometer at 300 K (27 °C) (^{1}H 400 MHz; $^{13}C\{^{1}H\}$ 101 MHz; ^{11}B 126 MHz, ^{19}F 377 MHz, ^{31}P 162 MHz). All ^{1}H chemical shifts are quoted in parts per million (ppm) relative to the residual solvent peak: MeCN-d_2 (δ_H = 1.94 ppm) , DMSO-d_5 (δ_H = 2.50 ppm), $CHCl_3$ (δ_H = 7.26 ppm) $CDHCl_2$ (δ_H = 5.32 ppm), Me_2CO-d_5 (δ_H = 2.05 ppm), MeOD-d_3 (δ_H = 4.87 ppm), HDO (δ_H = 4.79 ppm). All ^{13}C chemical shifts are quoted in parts per million (ppm) relative to the deuterated solvent peak: MeCN-d_3 (δ_C = 118.3 ppm), DMSO-d_6 (δ_C = 39.5 ppm), $CDCl_3$ (δ_C = 77.2 ppm) CD_2Cl_2 (δ_C = 53.8 ppm), Me_2CO-d_6 (δ_C = 29.8 ppm), MeOD-d_4 (δ_C = 49.0 ppm). All coupling constants, J, are quoted in Hz. Multiplicities are indicated as s (singlet), d (doublet), t (triplet), q (quartet), quint. (quintet), m (multiplet), and multiples thereof. ^{1}H and $^{13}C\{^{1}H\}$ NMR assignments were confirmed using 2D ^{1}H correlated spectroscopy (COSY), 2D ^{1}H–^{13}C heteronuclear multiple-bond correlation spectroscopy (HMBC) and 2D ^{1}H–^{13}C heteronuclear single quantum coherence (HSQC) where necessary. ^{19}F and ^{11}B NMR spectra are reported in ppm relative to $BF_3{\cdot}OEt_2$ as an external standard; ^{31}P NMR spectra are reported relative to phosphoric acid (85 % H_3PO_4) as an external standard. Coupling constants, *J*, are reported in Hertz (Hz), were calculated using MestReNova 11 to the nearest 0.1 Hz. Coupling constants that did not match as a result of digitisation are reported as rounded averages.

Chromatography

Analytical thin-layer chromatography was performed on precoated aluminium-backed plates (Silica Gel 60 F254; Merck), and visualisation was achieved using ultraviolet light (254 nm) and/or staining with either aqueous basic potassium permanganate ($KMnO_4$) solution or ethanolic phosphomolybdic acid followed by heating. Column chromatography was performed using Geduran® Silica Gel 60 (40-63 µm; Merck).

Solvents

Anhydrous ethereal solvents (THF, Et_2O) were obtained by passing solvent through a column of anhydrous alumina using an Anhydrous Engineering Grubbs-type system and storing over 3 Å molecular sieves. Anhydrous non-ethereal organic solvents (MeCN, MeCN-d_3, CH_2Cl_2, CD_2Cl_2, $CHCl_3$, $CDCl_3$, MeOH, MeOD-d_4, DMSO, DMSO-d_6, Me_2CO, Me_2CO-d_6) were obtained by drying over activated 3 Å molecular sieves (dried at 2 mbar, 220 °C, 16 h) for a minimum of 48 h.

Infrared spectroscopy

Infrared (IR) spectra of neat compounds were recorded over the range 4000-400 cm^{-1} using a Bruker APLHA^{TM} ATR-FTIR spectrometer, peaks are reported in cm^{-1}.

Mass spectrometry

Electrospray ionisation (ESI^+) spectra were recorded on a Bruker ESI Micro-Tof mass spectrometer using a time-of-flight mass analyser. Data are reported in the form of m/z.

Melting points

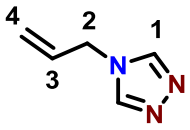
Melting points (mp) were determined on a Griffin capillary apparatus in capillary melting point tubes and are uncorrected.

Miscellaneous

Room temperature (rt) refers to 20 ± 2 °C. Temperatures of -20 °C to 0 °C for overnight reactions were obtained using an immersion cooler (LabPlant AP100). Reactions involving heating were performed using DrySyn blocks and a contact thermocouple. Unless stated otherwise, reagents were purchased from commercial sources (Sigma Aldrich, Alfa Aesar, or Acros Organics) at the highest available grade, and were used without purification.

Synthetic Procedures

N-Alkyl-triazoles

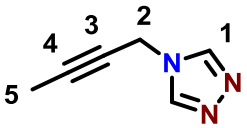


Potassium 1,2,4-triazolate (0.129 g, 1.2 mmol, 1.2 equiv.) and catalytic $PMDH^+BPh_4^-$ (0.053 g, 0.10 mmol, 10 mol%) were suspended in anhydrous CH_2Cl_2 (5 mL), and the resulting suspension was stirred for 10 min under ambient conditions (rt, air); allyl bromide (1.0 mmol, 1.0 equiv., 0.20 M) was then dispensed to this suspension as a solution in CH_2Cl_2. The fully assembled suspension was subsequently stirred vigorously for a further 48 h at 30 °C. After this time the suspension was filtered, the CH_2Cl_2 solvent evaporated under reduced pressure and the crude product purified by flash column chromatography (silica, EtOAc:MeOH, 75:25, R_f = 0.34) to yield a pale yellow oil (0.095g, 88 %, [M] = $C_5H_7N_3$).

^{1}H NMR (400 MHz, $CDCl_3$) δ_H / ppm: 4.63 (2H, dt, *J* = 5.9, 1.5 Hz, C(2)*H*), 5.24 (1H, dt, *J* = 17.1, 1.7 Hz, C(4)H_{trans}), 5.36 (1H, dt, *J* = 10.2, 1.7 Hz, C(4)H_{cis}), 5.95 (1H, ddt, *J* = 17.1, 10.2, 5.9 Hz, C(3)*H*), 8.14 (2H, s, C(1)*H*).**^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$)** δ_C / ppm: 47.6, 120.2, 131.2, 142.8.

HRMS (ESI^+): $[MH]^+$ Found 110.07100; Required 110.07127 (-0.27 ppm).

IR υ_{film} / cm^{-1}: 3107, 2928, 1646, 1530, 1181, 1456, 1422, 1181, 1074, 990, 975, 938.

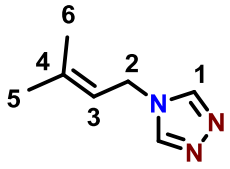


Potassium 1,2,4-triazolate (0.129 g, 1.2 mmol, 1.2 equiv.) and catalytic $PMDH^+BPh_4^-$ (0.053 g, 0.10 mmol, 10 mol%) were suspended in anhydrous CH_2Cl_2 (5 mL), and the resulting suspension was stirred for 10 min under ambient conditions (rt, air); propargyl bromide (1.0 mmol, 1.0 equiv., 0.20 M) was then dispensed to this suspension as a solution in CH_2Cl_2. The fully assembled suspension was subsequently stirred vigorously for a further 48 h at 30 °C. After this time the suspension was filtered, the CH_2Cl_2 solvent evaporated under reduced pressure and the crude product purified by flash column chromatography (silica, EtOAc:MeOH, 75:25, R_f = 0.43) to yield a pale yellow crystalline solid (0.097 G, 80 %, m.p. 64 – 66 °C, [M] = $C_6H_7N_3$).

^{1}H NMR (400 MHz, $CDCl_3$) δ_H / ppm: 1.87 (3H, t, *J* = 2.5 Hz, C(5)H_3), 4.75 (2H, q, *J* = 2.5 Hz, C(2)H_2), 8.25 (2H, s, C(1)*H*). **^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$)** δ_C / ppm: 3.6, 35.5, 70.5, 84.4, 142.4

HRMS (ESI^+): $[MH]^+$ Found 122.07160; Required 122.07127 (0.33 ppm).

IR υ_{film} / cm^{-1}: 3111, 2970, 2921, 2851, 2304, 2237, 1537, 1523, 1464, 1445, 1388, 1338, 1178, 1144, 1077, 964.

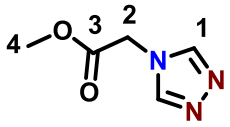


Potassium 1,2,4-triazolate (0.129 g, 1.2 mmol, 1.2 equiv.) and catalytic $PMDH^+BPh_4^-$ (0.053 g, 0.10 mmol, 10 mol%) were suspended in anhydrous CH_2Cl_2 (5 mL), and the resulting suspension was stirred for 10 min under ambient conditions (rt, air); 3,3-dimethylallyl bromide (1.0 mmol, 1.0 equiv., 0.20 M) was then dispensed to this suspension as a solution in CH_2Cl_2. The fully assembled suspension was subsequently stirred vigorously for a further 48 h at 30 °C. After this time the suspension was filtered, the CH_2Cl_2 solvent evaporated under reduced pressure and the crude product purified by flash column chromatography (silica, EtOAc:MeOH, 75:25, R_f = 0.43) to yield a pale yellow oil (0.108 g, 79 %, [M] = $C_7H_{11}N_3$).

^{1}H NMR (400 MHz, $CDCl_3$) δ_H / ppm: 1.78 (3H, s, CH_3), 1.81 (3H, s, CH_3), 4.58 (2H, d, J = 7.3 Hz, C(2)H_2), 5.36 (1H, m, C(3)H), 8.12 (2H, s, C(1)H). **^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$)** δ_C / ppm: 18.2, 25.8, 43.1, 117.1, 140.5, 142.6.

HRMS (ESI$^+$): $[MH]^+$ Found 138.10290; Required 138.10257 (0.33 ppm).

IR υ_{film} / cm^{-1}: 3105, 2972, 2916, 2861, 1674, 1529, 1451, 1379, 1319, 1174, 1073, 976.

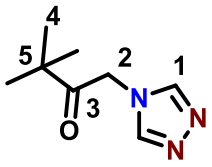


Potassium 1,2,4-triazolate (0.129 g, 1.2 mmol, 1.2 equiv.) and catalytic $PMDH^+BPh_4^-$ (0.053 g, 0.10 mmol, 10 mol%) were suspended in anhydrous CH_2Cl_2 (5 mL), and the resulting suspension was stirred for 10 min under ambient conditions (rt, air); methyl bromoacetate (1.0 mmol, 1.0 equiv., 0.20 M) was then dispensed to this suspension as a solution in CH_2Cl_2. The fully assembled suspension was subsequently stirred vigorously for a further 48 h at 20 °C. After this time the suspension was filtered, the CH_2Cl_2 solvent evaporated under reduced pressure and the crude product purified by flash column chromatography (silica, EtOAc:MeOH, 75:25, R_f = 0.40) to yield a white crystalline solid (0.109 g, 77 %, m.p. 80 – 82 °, [M] = $C_5H_7N_3O_2$).

^{1}H NMR (400 MHz, $CDCl_3$) δ_H / ppm: 3.83 (3H, s, C(4)H_3), 4.81 (2H, s, C(2)H_2), 8.21 (2H, s, C(1)H). **^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$)** δ_C / ppm: 46.0, 53.4, 143.3, 166.7.

HRMS (ESI$^+$): $[MH]^+$ Found 142.06090; Required 142.06110 (-0.20 ppm).

IR υ_{film} / cm^{-1}: 3115, 3095, 2992, 2955, 1729, 1537, 1520, 1459, 1416, 1351, 1215, 1188, 1071, 989, 965.

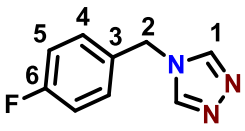


Potassium 1,2,4-triazolate (0.129 g, 1.2 mmol, 1.2 equiv.) and catalytic $PMDH^+BPh_4^-$ (0.053 g, 0.10 mmol, 10 mol%) were suspended in anhydrous CH_2Cl_2 (5 mL), and the resulting suspension was stirred for 10 min under ambient conditions (rt, air); 1-bromopinacolone (1.0 mmol, 1.0 equiv., 0.20 M) was then dispensed to this suspension as a solution in CH_2Cl_2. The fully assembled suspension was subsequently stirred vigorously for a further 48 h at 20 °C. After this time the suspension was filtered, the CH_2Cl_2 solvent evaporated under reduced pressure and the crude product purified by flash column chromatography (silica, EtOAc:MeOH, 75:25, Rf = 0.34) to yield a white crystalline solid (0.124 g, 74 %, m.p. 174 – 177 °C, [M] = $C_8H_{13}N_3O$).

^{1}H NMR (400 MHz, $CDCl_3$) δ_H / ppm: 1.27 (9H, s, C(4)*H*$_3$), 5.03 (2H, s, C(2)*H*$_2$), 8.10 (2H, s, C(1)*H*).
^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ_C / ppm: 26.3, 43.6, 48.8, 143.5, 206.0.

HRMS (ESI$^+$): $[MH]^+$ Found 168.11290; Required 168.11314 (-0.24 ppm).

IR υ_{film} / cm^{-1}: 3095, 3044, 2968, 2869, 1713, 1537, 1479, 1459, 1383, 1364, 1229, 1194, 1080, 1064, 1015, 969.

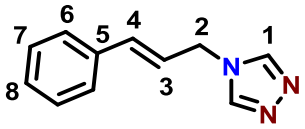


Potassium 1,2,4-triazolate (0.129 g, 1.2 mmol, 1.2 equiv.) and catalytic $PMDH^+BPh_4^-$ (0.053 g, 0.10 mmol, 10 mol%) were suspended in anhydrous CH_2Cl_2 (5 mL), and the resulting suspension was stirred for 10 min under ambient conditions (rt, air); 4-fluorobenzyl bromide (1.0 mmol, 1.0 equiv., 0.20 M) was then dispensed to this suspension as a solution in CH_2Cl_2. The fully assembled suspension was subsequently stirred vigorously for a further 48 h at 30 °C. After this time the suspension was filtered, the CH_2Cl_2 solvent evaporated under reduced pressure and the crude product purified by flash column chromatography (silica, EtOAc:MeOH, 75:25, R_f = 0.37) to yield a white crystalline solid (0.152 g, 86 %, m.p. 99 – 101 °C, [M] = $C_9H_8FN_3$).

^{1}H NMR (400 MHz, $CDCl_3$) δ_H / ppm: 5.16 (2H, s, C(2)*H*$_2$), 6.91 – 7.13 (2H, m, C(5)*H*), 7.13 – 7.23 (2H, m, C(4)*H*), 8.14 (2H, s, C(1)*H*). **^{13}C NMR (101 MHz, $CDCl_3$)** δ_C / ppm: 48.4, 116.5 (d, *J* = 21.9 Hz), 129.7 (d, *J* = 8.4 Hz), 130.2 (d, *J* = 3.4 Hz), 142.8, 163.0 (d, *J* = 248.8 Hz).**^{19}F NMR (377 MHz, $CDCl_3$)** δ_F / ppm: -112.18 (m).

HRMS (ESI$^+$): $[MH]^+$ Found 178.07750; Required 178.07750 (0 ppm).

IR υ_{film} / cm^{-1}: 3124, 2996, 2956, 2923, 1603, 1529, 1505, 1455, 1445, 1381, 1329, 1210, 1161, 1074, 970.

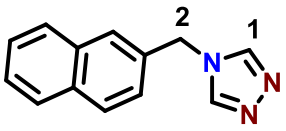


Potassium 1,2,4-triazolate (0.129 g, 1.2 mmol, 1.2 equiv.) and catalytic $PMDH^{+}BPh_4^{-}$ (0.053 g, 0.10 mmol, 10 mol%) were suspended in anhydrous CH_2Cl_2 (5 mL), and the resulting suspension was stirred for 10 min under ambient conditions (rt, air); cinnamyl bromide (1.0 mmol, 1.0 equiv., 0.20 M) was then dispensed to this suspension as a solution in CH_2Cl_2. The fully assembled suspension was subsequently stirred vigorously for a further 48 h at 30 °C. After this time the suspension was filtered, the CH_2Cl_2 solvent evaporated under reduced pressure and the crude product purified by flash column chromatography (silica, EtOAc:MeOH, 75:25, R_f = 0.40) to yield a white crystalline solid (0.137 g, 74 %, m.p. 92 – 94 °C, [M] = $C_{11}H_{11}N_3$).

^{1}H NMR (400 MHz, $CDCl_3$) δ_H / ppm: 4.79 (2H, dd, *J* = 6.4, 1.5 Hz, C(2)*H*$_2$), 6.26 (1H, dt, *J* = 15.9, 6.4 Hz, C(3)*H*), 6.60 (1H, dt, *J* = 15.9, 1.5 Hz, C(4)*H*), 7.09 – 7.55 (5H, m, Ar-*H*), 8.21 (2H, s,C(1)*H*).
^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ_C / ppm: 47.4, 121.6, 126.8, 128.9, 129.0, 135.2, 135.5, 142.8.

HRMS (ESI$^+$): $[MH]^+$ Found 186.10310; Required 186.10257 (0.53 ppm).

IR υ_{film} / cm^{-1}: 3108, 3025, 2927, 2852, 1531, 1512, 1449, 1435, 1360, 1177, 1062, 969.

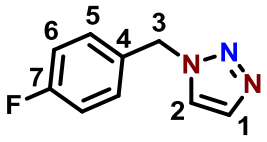


Potassium 1,2,4-triazolate (0.129 g, 1.2 mmol, 1.2 equiv.) and catalytic $PMDH^{+}BPh_4^{-}$ (0.053 g, 0.10 mmol, 10 mol%) were suspended in anhydrous CH_2Cl_2 (5 mL), and the resulting suspension was stirred for 10 min under ambient conditions (rt, air); 2-(bromomethyl)napthalene (1.0 mmol, 1.0 equiv., 0.20 M) was then dispensed to this suspension as a solution in CH_2Cl_2. The fully assembled suspension was subsequently stirred vigorously for a further 48 h at 30 °C. After this time the suspension was filtered, the CH_2Cl_2 solvent evaporated under reduced pressure and the crude product purified by flash column chromatography (silica, EtOAc:MeOH, 75:25, R_f = 0.43) to yield a white crystalline solid (0.163 g, 78 %, m.p. 172 – 174 °C, [M] = $C_{13}H_{11}N_3$).

^{1}H NMR (400 MHz, $CDCl_3$) δ_H / ppm: 5.34 (2H, s, C(2)*H*$_2$), 7.27 (1H, dd, J = 8.5, 1.9 Hz, Ar-*H*), 7.51 – 7.56 (2H, m, Ar-*H*), 7.64 (1H, s, Ar-*H*), 7.78 – 7.91 (3H, m, Ar-*H*), 8.22 (2H, s, C(1)*H*). **^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$)** δ_C / ppm: 49.4, 124.8, 127.0, 127.1, 127.2, 128.0, 129.6, 131.6, 133.3, 143.1.

HRMS (ESI$^+$): $[MH]^+$ Found 210.10390; Required 210.10257 (1.33 ppm).

IR υ_{film} / cm^{-1}: 3088, 3054, 1600, 1526, 1507, 1442, 1379, 1322, 1191, 1122, 1075, 978.

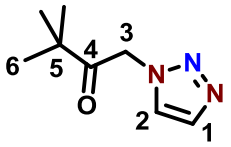


Potassium 1,2,3-triazolate (0.129 g, 1.2 mmol, 1.2 equiv.) and catalytic $PMDH^+BPh_4^-$ (0.053 g, 0.10 mmol, 10 mol%) were suspended in anhydrous CH_2Cl_2 (5 mL), and the resulting suspension was stirred for 10 min under ambient conditions (rt, air); 4-fluorobenzyl bromide (1.0 mmol, 1.0 equiv., 0.20 M) was then dispensed to this suspension as a solution in CH_2Cl_2. The fully assembled suspension was subsequently stirred vigorously for a further 48 h at 30 °C. After this time the suspension was filtered, the CH_2Cl_2 solvent evaporated under reduced pressure and the crude product purified by flash column chromatography (silica, EtOAc, R_f = 0.44) to yield a white crystalline solid (0.159 g, 90 %, m.p. 42 – 44 °C, [M] = $C_9H_8FN_3$).

^{1}H NMR (400 MHz, $CDCl_3$) δ_H / ppm: 5.55 (2H, s, C(3)H_2), 7.03 – 7.10 (2H, m, C(6)*H*), 7.24 – 7.31 (2H, m, C(5)*H*), 7.50 (1H, d, *J* = 1.0 Hz, C(2)*H*), 7.72 (1H, d, *J* = 1.0 Hz, C(1)*H*). **^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$)** δ_C / ppm: 53.3, 116.2 (d, *J* = 21.7 Hz), 123.3, 130.0 (d, *J* = 8.4 Hz), 130.7, 134.4, 162.9 (d, *J* = 248.1 Hz). **^{19}F NMR (377 MHz, $CDCl_3$)** δ_F / ppm: -112.8.

HRMS (ESI$^+$): $[MH]^+$ Found 178.07970; Required 178.07750 (1.20 ppm).

IR υ_{film} / cm^{-1}: 3132, 3104, 2354, 1606, 1509, 1486, 1438, 1222, 1212, 1075.

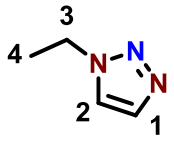


Potassium 1,2,3-triazolate (0.129 g, 1.2 mmol, 1.2 equiv.) and catalytic $PMDH^+BPh_4^-$ (0.053 g, 0.10 mmol, 10 mol%) were suspended in anhydrous CH_2Cl_2 (5 mL), and the resulting suspension was stirred for 10 min under ambient conditions (rt, air); 1-bromopinacolone (1.0 mmol, 1.0 equiv., 0.20 M) was then dispensed to this suspension as a solution in CH_2Cl_2. The fully assembled suspension was subsequently stirred vigorously for a further 48 h at 20 °C. After this time the suspension was filtered, the CH_2Cl_2 solvent evaporated under reduced pressure and the crude product purified by flash column chromatography (silica, EtOAc, R_f = 0.44) to yield a white crystalline solid (0.142 g, 85 %, m.p. 92 – 94 °C, [M] = $C_8H_{13}N_3O$).

^{1}H NMR (400 MHz, $CDCl_3$) δ_H / ppm: 1.28 (9H, s, C(6)H_3), 5.41 (2H, s, C(3)H_2), 7.63 (1H, d, *J* = 1.0 Hz, C(2)*H*), 7.73 (1H, d, *J* = 1.0 Hz, C(1)*H*). **^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$)** δ_C / ppm: 26.3, 43.8, 53.5, 125.3, 134.1, 206.1.

HRMS (ESI$^+$): $[MH]^+$ Found 168.11350; Required 168.11314 (0.36 ppm).

IR υ_{film} / cm^{-1}: 3102, 2976, 1716, 1479, 1365, 1341, 1291, 1219, 1062, 1036, 1014.



Potassium 1,2,3-triazolate (0.258 g, 2.4 mmol, 1.2 equiv.) and catalytic $PMDH^+BPh_4^-$ (0.216 g, 0.40 mmol, 20 mol%) were suspended in anhydrous CH_2Cl_2 (5 mL), and the resulting suspension was stirred for 10 min under ambient conditions (rt, air); ethyl iodide (2.0 mmol, 1.0 equiv., 0.20 M) was then dispensed to this suspension as a solution in CH_2Cl_2. The fully assembled suspension was subsequently stirred vigorously for a further 48 h at 40 °C. After this time the suspension was filtered, the CH_2Cl_2 solvent evaporated under reduced pressure and the crude product purified by flash column chromatography (silica, EtOAc, R_f = 0.34) to yield a pale yellow oil (0.173 g, 89 %, [M] = $C_4H_7N_3$).

^{1}H NMR (400 MHz, $CDCl_3$) δ_H / ppm: 1.56 (3H, t, *J* = 7.4 Hz, C(4)*H*$_3$), 4.44 (2H, q, *J* = 7.4 Hz, C(3)*H*$_2$), 7.55 (1H, d, *J* = 1.0 Hz, C(2)*H*), 7.70 (1H, d, *J* = 1.0 Hz, C(1)*H*). **^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$)** δ_C / ppm: 15.7, 45.3, 122.7, 134.0.

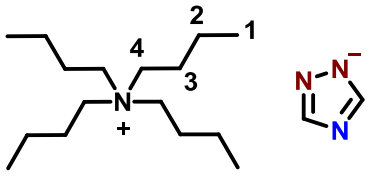
HRMS (ESI$^+$): [MH]+ Found 98.07050; Required 98.07127 (-0.77 ppm).

IR υ_{film} / cm^{-1}: 3123, 2984, 2942, 1640, 1466, 1444, 1284, 1223, 1206, 1115, 1066.

Triazolate salts

General procedure

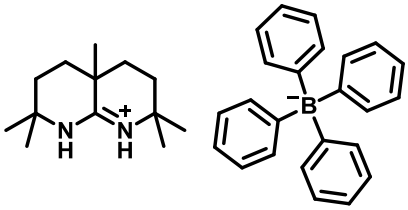
1,2,4-Triazole or 1,2,3-triazole (2.0 g, 28.9 mmol, 1.05 equiv.) and metal (Li^+, Na^+, K^+, Cs^+) or organic ($^nBu_4N^+$) hydroxide (27.5 mmol, 1.00 equiv.) were dissolved in H_2O (7 ml) and dispensed to a flask with PhMe (70 mL). The salt was dried azeotropically for 16 h using a standard Dean-Stark apparatus and the PhMe solvent subsequently removed under reduced pressure. The crude solid was suspended in anhydrous THF, triturated to remove the small excess of 1,2,4-triazole and filtered to afford a white crystalline solid, which was then dried *in vacuo* for 24 h at 40 °C. The trituration procedure was skipped in the case of $^nBu_4N^+Trz^-$, which was used without further purification.



^{1}H NMR (400 MHz, DMSO-d_6) δ_H / ppm: 0.93 (12H, t, *J* = 7.4 Hz, C(1)*H*$_3$), 1.31 (8H , sext., *J* = 7.4 Hz, C(2)*H*$_2$), 1.50 – 1.64 (8H, m, C(3)*H*$_2$), 3.11 – 3.24(8H, m, C(4)*H*$_2$), 7.54 (2H, s, Trz-*H*).

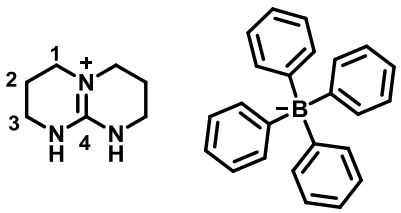
^{13}C NMR (101 MHz, DMSO-d_6) δ_C / ppm: 13.4, 19.2, 23.1, 57.5 148.9.

Amidinium and guanidinium salts



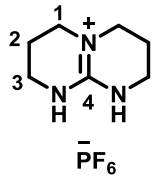
An aqueous solution of sodium tetraphenylborate (2.4 g, 7.0 mmol, 0.140 M) was added to a solution of 3,3,6,9,9-pentamethyl-2,10-diazabicyclo[4.4.0]dec-1-ene (PMD, 1.50 g, 7.2 mmol, 0.144 M) in 10 % $HCl_{(aq).}$, immediately affording a white precipitate. The resulting suspension was stirred vigorously for 1 h under ambient conditions and then filtered. The crude precipitate was washed extensively with H_2O and dried *in vacuo* for 24 h at 40 °C. No further purification was required (3.03 g, 82 %, m.p. 220 – 225 °C).

^{1}H NMR (400 MHz, DMSO-d$_6$) δ_H / ppm: 1.25 (s, 6H, gem-C*H*$_3$), 1.29 (3H, s, CH_3), 1.31 (6H, s, gem-C*H*$_3$), 1.50 – 1.60 (2H, m, CH_2), 1.84 – 1.67 (4H, m, CH_2), 1.97 (2H, td, *J* = 13.7, 3.9 Hz, CH_2), 6.69 – 6.85 (4H, m, Ar-H), 6.92 (8H, t, *J* = 7.4 Hz, Ar-H), 7.15-7.21 (8H, m, Ar-H), 8.10 (2H, s, NH). **^{13}C{^{1}H} NMR (101 MHz, DMSO-d$_6$)** δ_C / ppm: 168.44, 163.32 (q, $^{1}J_{C\text{-}B}$ = 49.3 Hz), 135.4-135.6 (q, $^{3}J_{C\text{-}B}$ = 1.2 Hz), 126.2 (q, $^{2}J_{C\text{-}B}$ = 2.7 Hz), 121.46, 54.27, 32.0, 30.37, 30.21, 29.56, 24.14. **^{11}B NMR (126 MHz, DMSO-d$_6$)** δ_B / ppm: -6.7 (*B*Ph$_4$).



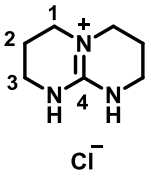
TBD·HBPh$_4$: An aqueous solution of sodium tetraphenylborate (2.4 g, 7.0 mmol, 0.140 M) was added dropwise to a solution of 1,5,7-triazabicyclo[4.4.0]dec-5-ene (1.0 g, 7.2 mmol, 0.144 M) in 10 % $HCl_{(aq).}$ (50 mL), immediately affording a white precipitate. The resulting suspension was stirred vigorously for 1 hr under ambient conditions and then filtered. The crude precipitate was washed extensively with H_2O and recrystallised (4:1 MeOH: $CHCl_3$) to afford a white crystalline solid (1.9 g, 0.42 mmol, 57 %). The ^{1}H, ^{13}C and ^{11}B NMR spectra are consistent with the literature.[1,2]

^{1}H NMR (400 MHz, DMSO-d$_6$) δ_H / ppm: 1.86 (4H, quint, *J* = 5.8 Hz, [C2]-*H*), 3.17 (4H, t, *J* = 5.8 Hz, [C3]-*H*), 3.25 (4H, t, *J* = 5.8 Hz, [C1]-*H*), 6.80 (4H, tt, 3J = 7.3 Hz, 4J = 1.5 Hz, Ar-*H*), 6.93 (8H, t, J = 7.3 Hz, Ar-*H*), 7.19 (8H, m, Ar-*H*), 7.40 (2H, s, N*H*).**^{13}C{^{1}H} NMR (101 MHz, DMSO-d$_6$)** δ_C / ppm: 20.7, 38.1, 46.7, 122.0, 125.8 (q, $^{2}J_{C\text{-}B}$ = 2.7 Hz), 136.0 (q, $^{3}J_{C\text{-}B}$ = 1.2 Hz), 151.0, 163.8 (q, $^{1}J_{C\text{-}B}$ = 49.3 Hz). **^{11}B NMR (126 MHz, DMSO-d$_6$)** δ_B / ppm: -6.7 (*B*Ph$_4$).



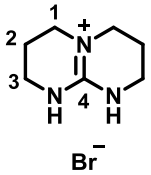
TBD.HPF$_6$ (285.2 g mol^{-1}): An aqueous solution (10 mL) of $NaPF_6$ (0.13 g, 0.80 mmol) and TBD·HCl (0.13 g, 0.72 mmol) was added to CH_2Cl_2 (15 mL) and the resulting mixture was vigorously stirred for 16 h. The aqueous layer was extracted with CH_2Cl_2 and the combined organic extracts evaporated under reduced pressure to afford a white crystalline solid (0.14 g, 0.49 mmol, 68 %). The ^{1}H, ^{13}C and ^{31}P NMR spectra are consistent with the literature.[4]

^{1}H NMR (400 MHz, DMSO-d$_6$) δ_H / ppm: 1.88 (4H, quint, *J* = 5.8 Hz, [C2]-*H*), 3.18 (4H, t, *J* = 5.8 Hz, [C3]-*H*), 3.27 (4H, t, *J* = 5.8 Hz, [C1]-*H*), 7.40 (2H, s, N*H*). **^{13}C{^{1}H} NMR (101 MHz, DMSO-d$_6$)** δ_C / ppm: 20.7 (s, *C*2), 38.1 (s, *C*3), 46.7 (s, *C*1), 151.0 (s, *C*4). **^{19}F NMR (377 MHz, DMSO-d$_6$)** δ_F / ppm: -70.2 (d, $^1J_{P\text{-}F}$ = 706 Hz, P*F*$_6$). **^{31}P NMR (162 MHz, DMSO-d$_6$)** δ_P / ppm: -144.2 (m, $^1J_{P\text{-}F}$ = 706 Hz, *P*F$_6$).



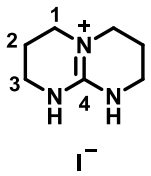
TBD·HCl: A solution of 1,5,7-triazabicyclo[4.4.0]dec-5-ene (1.0 g, 7.2 mmol) and NH_4Cl (0.42 g, 7.9 mmol) in MeOH (20 ml) was stirred under ambient conditions for 1 hr, after which time the solvent was removed *in vacuo* to give a white crude solid. This solid was dissolved in CH_2Cl_2 and filtered; evaporation of the filtrate *in vacuo* afforded a white crystalline solid (0.82 g, 4.7 mmol, 65 %). The ^{1}H and ^{13}C NMR spectra are consistent with the literature.[1]

^{1}H NMR (400 MHz, DMSO-d$_6$) δ_H / ppm: 1.87 (4H, quint, *J* = 5.8 Hz, [C2]-*H*), 3.16 – 3.22 (4H, m, [C3]-*H*), 3.27 (4H, t, *J* = 5.8 Hz, [C1]-*H*), 8.06 (2H, s, N*H*). **^{13}C{^{1}H} NMR (101 MHz, DMSO-d$_6$)** δ_C / ppm: 20.7, 37.9, 46.6, 151.4.



TBD·HBr: A solution of 1,5,7-triazabicyclo[4.4.0]dec-5-ene (1.0 g, 7.2 mmol) and NH_4Br (0.77 g, 7.9 mmol) in MeOH (20 ml) was stirred under ambient conditions for 1 hr, after which time the solvent was removed *in vacuo* to give a white crude solid. This solid was dissolved in CH_2Cl_2 and filtered; evaporation of the filtrate *in vacuo* afforded a white crystalline solid (0.94 g, 4.3 mmol, 60 %). The ^1H and ^{13}C NMR spectra are consistent with the literature.[1]

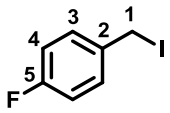
^{1}H NMR (400 MHz, DMSO-d$_6$) δ_H / ppm: 1.87 (4H, quint, *J* = 5.8 Hz, [C2]-*H*), 3.16 – 3.22 (4H, m, [C3]-*H*), 3.28 (4H, t, *J* = 5.8 Hz, [C1]-*H*), 7.54 (2H, s, N*H*). **^{13}C{^{1}H} NMR (101 MHz, DMSO-d$_6$)** δ_C / ppm: 20.7, 38.0, 46.7, 151.1.



TBD·HI: NaI (0.82 g, 5.4 mmol) was added to a solution of TBD·HCl (0.23 g, 1.3 mmol) in anhydrous CH_2Cl_2 and the resulting suspension was vigorous stirred for 16 hr under ambident conditions. The reaction mixture was filtered through a pad of Celite, and concentrated *in vacuo* to afford a yellow crystalline solid (0.19 g, 0.71 mmol, 56 %). The ^1H and ^{13}C NMR spectra are consistent with the literature.[3]

^{1}H NMR (400 MHz, DMSO-d$_6$) δ_H / ppm: 1.88 (4H, quint, *J* = 5.8 Hz, [C2]-*H*), 3.19 (4H, t, *J* = 5.8 Hz, [C3]-*H*), 3.28 (4H, t, *J* = 5.8 Hz, [C1]-*H*), 7.39 (2H, s, N*H*).**^{13}C{^{1}H} NMR (101 MHz, DMSO-d$_6$)** δ_C / ppm: 20.7, 38.1, 46.8, 151.0.

Miscellaneous



4-Fluorobenzyl iodide: 4-Fluorobenzyl bromide (0.65 mL, 5.3 mmol) was dissolved in $(CH_3)_2CO$ (10 mL) and added to an excess of NaI (1.5 g, 10 mmol). The resulting suspension was stirred in the dark for 16 hr, after which time the reaction was quenched with H_2O and the aqueous layer extracted with Et_2O (3 x 20 mL). The combined ethereal extracts were washed with saturated aqueous NaCl (2 x 20 mL), dried over anhydrous Mg_2SO_4 and evaporated under reduced pressure to afford a pale orange solid that was used without further purification (0.82 g, 66 %). The ^{1}H, ^{13}C and ^{19}F NMR spectra are consistent with the literature.[5]

^{1}H NMR (400 MHz, $CDCl_3$) δ_H / ppm: 4.46 (2H, s, [C]-*H*), 7.01 (2H, m, [C4]-*H*), 7.38 (2H, m, [C3]-*H*).**^{13}C NMR (101 MHz, $CDCl_3$)** δ_C / ppm: 4.6, 115.9 (d, *J* = 21.8 Hz), 130.6 (d, *J* = 8.3 Hz), 135.3 (d, *J* = 3.3 Hz), 162.3 (d, *J* = 247.8 Hz). **^{19}F NMR (377 MHz, $CDCl_3$)** δ_F / ppm: -113.5 (m).

Regioselectivity determination by ^{1}H NMR spectroscopy

General procedure I: Stoichiometric conditions

1,2,4-Triazole (0.0069 g, 0.10 mmol, 1.0 equiv.) and organic base (0.10 mmol, 1.0 equiv.) were dissolved in anhydrous deuterated (CD_2Cl_2, $CDCl_3$, Me_2CO-d_6, DMSO-d_6, MeCN-d_3, MeOD-d_4) or protic (THF-h_8) solvent (0.50 mL) within a glass V-shaped vial (3 mL). The alkylating agent RX (0.10 mmol, 1.0 equiv., 0.20 M) was dissolved in the same solvent and added to the first solution in one portion. The vial was then sealed and the solution stirred for a further 24 h at room temperature. After this time the solution was dispensed to a borosilicate NMR tube (Norrell, 5 mm) for analysis by ^{1}H and ^{19}F (*p*-F-BnBr) NMR spectroscopy. For a few combinations of organic base and solvent (*e.g.*, *p*-F-BnBr and MTBD in THF) the formation of a white precipitate (*e.g.* MTBDH^{+}Br^{-}) was observed; in such cases the precipitate was removed *via* filtration and the filtrate dispensed to the NMR tube. Regioselectivities were determined by integration, using an extended relaxation delay of D1 = 10.0 seconds.

General procedure II: Catalytic conditions

A metal (M^{+} = Li^{+}, Na^{+}, K^{+}, Cs^{+}) or organic ($^{n}Bu_4N^{+}$) salt of 1,2,3- or 1,2,4-triazolate (0.12 mmol, 1.2 equiv.), phase transfer organocatalyst (0.010 mmol, 10 mol%) and 1,3,5-trimethoxybenzene (0.033 mmol) were weighed directly into a glass V-shaped vial (3 mL) and suspended in anhydrous deuterated (CD_2Cl_2, $CDCl_3$, Me_2CO-d_6, DMSO-d_6, MeCN-d_3, MeOD-d_4) or protic (THF-h_8) solvent (0.5 mL); the resulting suspension or solution was then stirred vigorously under ambient conditions (rt, air). The alkylating agent RX (0.10 mmol, 1.0 equiv., 0.20 M) was dissolved in the same solvent and added to the catalytic mixture in one portion after 10 min of stirring. The vial was then sealed and the suspension stirred vigorously for a further 48 h at the appropriate temperature (20 – 40 °C). After this time the suspension was filtered and the filtrate dispensed to a borosilicate NMR tube (Norrell, 5 mm) for analysis by ^{1}H and ^{19}F (*p*-F-BnBr) NMR spectroscopy. ^{1}H NMR yields were determined by integration with respect to the 1,3,5-trimethoxybenzene standard, using an extended relaxation delay of D1 = 10.0 seconds.

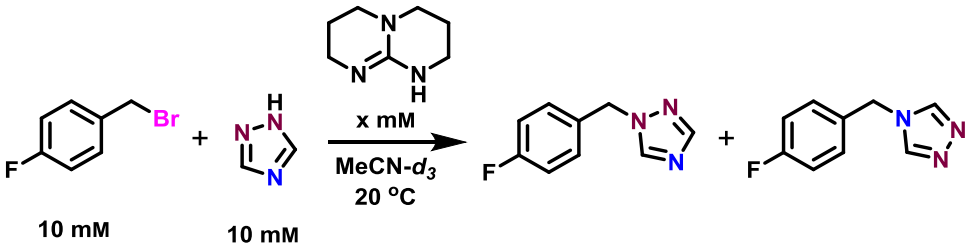
In Situ Reaction Monitoring by ^{1}H NMR Spectroscopy

General considerations

All kinetic studies were performed at 293 K (20 °C) with *in situ* reaction monitoring by ^{1}H NMR spectroscopy, using anhydrous MeCN-d_3 (3 Å MS) and 1,3,5-trimethoxybenzene (> 99.9 %) as an internal standard. All *in situ* monitoring was conducted by manual assembly with a Bruker Ascend 400 MHz NMR spectrometer; a typical ^{1}H NMR monitoring experiment involved a relaxation delay of 1.0 s and acquisition time of 3.9 s (4 scans, 1 dummy scan). All NMR spectra were processed using standard MestReNova software (Version 11).

Solid compounds were weighed using a high precision analytical balance (resolution = 0.01 mg) and neat liquids were dispensed with gas-tight microsyringes. All stock solutions were prepared in volumetric glassware and used on the day of their preparation, and all reactions remained visibly homogeneous throughout the course of monitoring.

Representative experiment



In a typical kinetic experiment, a stock solution of 4-fluorobenzyl bromide (0.10 M), 1,2,4-triazole (0.10 M) and 1,3,5-trimethoxybenzene (0.033 M) was freshly prepared in MeCN-d_3 [Stock *A*] using a volumetric flask. 1,2,4-Triazole and 1,3,5-trimethoxybenzene were weighed into a vial, dissolved in MeCN-d_3 and transferred to a volumetric flask with three washes; 4-fluorobenzyl bromide was added directly to the volumetric flask by microsyringe. Stock A was subsequently diluted to 0.010 M [Stock *B1*] or 0.050 M [Stock *B2*]. A stock solution of organic base (TMG, DBU, TMGN, MTBD, TBD, P_1-^{t}Bu) was also prepared at a concentration of either 0.20 M [Stock *C1*] or 1.0 M [Stock *C2*]. In the absence of base, mixed solutions of 4-fluorobenzyl bromide and 1,2,4-triazole (0.10 M) were found to be stable on the timescale of days.

Stock *B1* (700 µL) was dispensed to a borosilicate glass NMR tube (Norell, 5 mm) and the sample loaded into a Bruker Ascend 400 MHz NMR spectrometer with a probe temperature of 293 K (20°C). After locking (^{1}H, MeCN-d_2), tuning, shimming and spectrum acquisition (t = 0), the sample was ejected from the spectrometer; an appropriate volume of stock *C1* was then added directly to the sample by microsyringe (e.g., 1.0 eq = 35 µL).

In quick succession, the sample was inverted three times, shaken vigorously for ten seconds and re-injected into the spectrometer, whereupon monitoring was commenced. The time between the addition of stock C1 and the first spectrum was measured manually with a stopwatch. For 3,3,6,9,9-pentamethyl-2,10-diazabicyclo[4.4.0]dec-1-ene (PMD), higher concentrations were used (stock B2, stock C2).

For kinetics experiments in which variable concentrations of 4-fluorobenzyl bromide were required, 1,2,4-triazole (0.10 M), organic base (0.10 M) and 1,3,5-trimethoxybenzene (0.033 M) were pre-mixed in a stock solution (MeCN-d_3). Following an analogous procedure to that outlined above, 4-fluorobenzyl bromide was added directly by microsyringe to initiate the reaction.

Free energies of activation and binding

Experimental free energies of activation ($\Delta^{\ddagger}G_i$) were obtained in accordance with classical transition state theory, using the Eyring-Polanyi equation and bimolecular rate coefficients (k_i) obtained from kinetic modelling. Boltzmann's constant $k_B = 1.38 \times 10^{-23}$ J K^{-1}, the molar gas constant $R = 8.314$ J K^{-1} mol^{-1}, the temperature $T = 293.15$ K, Planck's constant $h = 6.626 \times 10^{-34}$ J s, the transmission coefficient $\kappa = 1$ and the standard concentration $c° = 1$ mol dm^{-3}.

$$\Delta^{\ddagger}G_i = -RT \ln\left(\frac{hc°k_i}{\kappa k_B T}\right) \quad [SE1]$$

Experimental free energies of binding ($\Delta_{Bind}G_i$) were obtained in accordance with classical thermodynamics, using binding equilibrium constants (K_i) obtained from kinetic modelling. The molar gas constant $R = 8.314$ J K^{-1} mol^{-1} and the temperature $T = 293.15$ K.

$$\Delta_{Bind}G_i = -RT \ln K_i \quad [SE2]$$

Supplementary Figures

Figure S1: *N*-Benzylation of 1,2,4-triazole

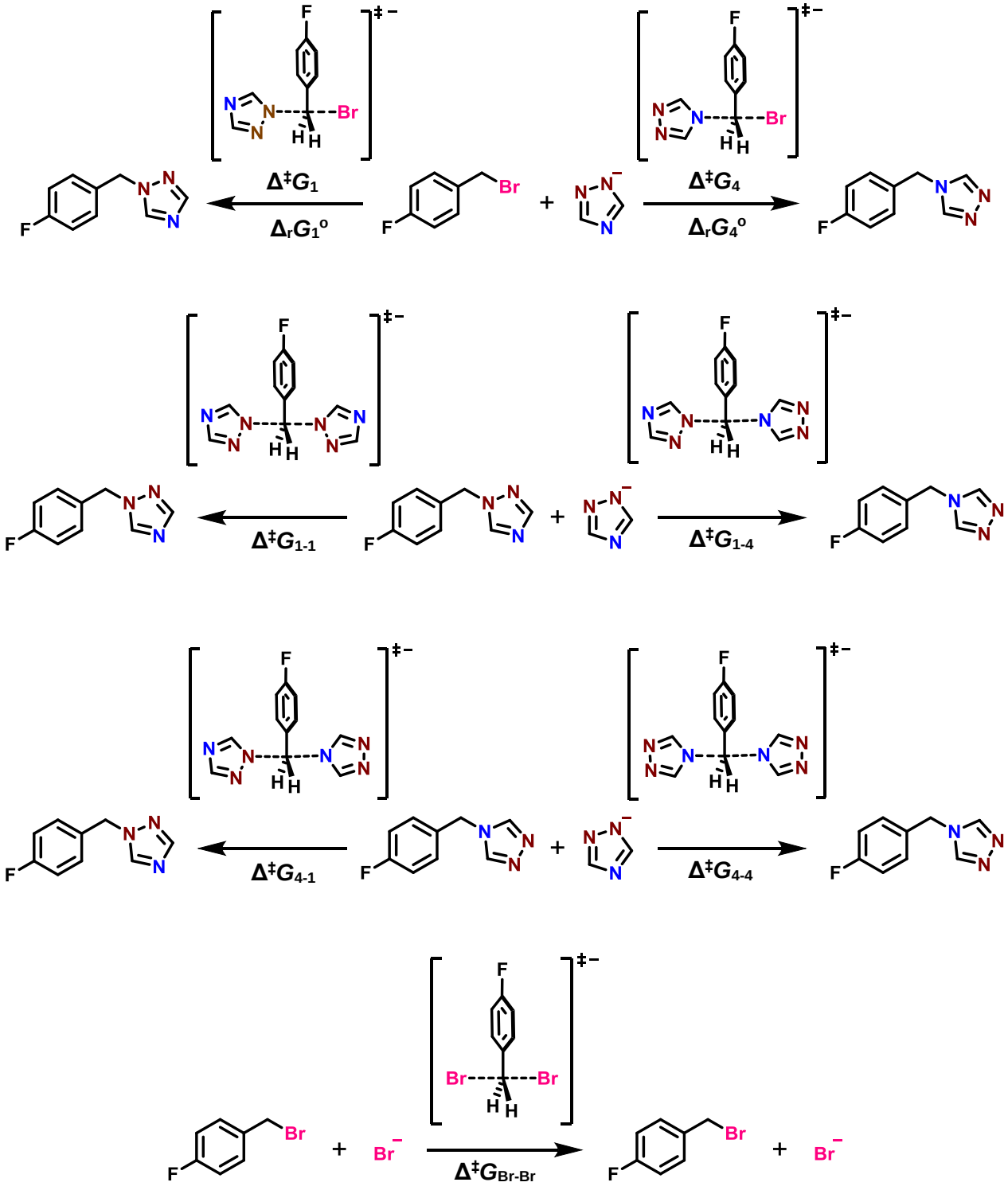


Figure S1a: Summary of key transition states and free energy changes for the *N*-benzylation of 1,2,4-triazolate with *p*-F-BnBr.

Free energy difference	kJ mol^{-1}
$\Delta^{\ddagger}G_1$	81.1
$\Delta^{\ddagger}G_4$	86.5
$\Delta^{\ddagger}G_{1\text{-}1}$	170.1
$\Delta^{\ddagger}G_{4\text{-}4}$	160.3
$\Delta^{\ddagger}G_{1\text{-}4}$	175.2
$\Delta^{\ddagger}G_{4\text{-}1}$	153.3
$\Delta^{\ddagger}G_{\text{Br-Br}}$	91.0

Table S1b: Computed free energies of activation for the *N*-benzylation of 1,2,4-triazolate with *p*-F-BnBr in MeCN, using a combined KS-DFT/DLPNO-CCSD(T) methodology and the ideal-gas rigid-rotor harmonic-oscillator (IGRRHO) approximation (f_s = 0.95).

Figure S2: Marcus theory

According to Marcus theory, the free energy of activation $\Delta^{\ddagger}G_i^M$ of an elementary group-transfer reaction can be expressed as a function of the intrinsic free energy barrier $\Delta^{\ddagger}G_i^o$ and the free energy of reaction $\Delta_rG_i^o$ [SE3].

$$\Delta^{\ddagger}G_i^M = \Delta^{\ddagger}G_i^o + \frac{1}{2}\Delta_rG_i^o + \frac{(\Delta_rG_i^o)^2}{16\Delta^{\ddagger}G_i^o} \quad [\mathrm{SE3}]$$

The intrinsic free energy barrier $\Delta^{\ddagger}G_i^o$ is defined as the arithmetic mean [3] of the free energy barriers for the two corresponding identity reactions ($\Delta^{\ddagger}G_{i\text{-}i}$, $\Delta^{\ddagger}G_{Br\text{-}Br}$, Figure S1), in which there is no thermodynamic contribution to the overall free energy of activation.

$$\Delta^{\ddagger}G_i^o = \frac{\Delta^{\ddagger}G_{i-i} + \Delta^{\ddagger}G_{Br-Br}}{2} \quad [\mathrm{SE4}]$$

Using a combined KS-DFT/DLPNO-CCSD(T) methodology (*vide infra*), the free energies of reaction $\Delta_rG_i^o$ (i = 1, 4), intrinsic free energies of activation $\Delta^{\ddagger}G_i^o$ (i = 1, 4) and overall free energies of activation $\Delta^{\ddagger}G_i^M$ (i = 1, 4) were computed for the *N*-benzylation of 1,2,4-triazolate with *p*-F-BnBr. The results of these computations are shown in **Table S2a**, in which the Marcus free energies of activation ($\Delta^{\ddagger}G_i^M$) are compared with the directly computed barriers ($\Delta^{\ddagger}G_i$). The agreement between Marcus theory and the directly computed free energy barriers is very good (< 1 kJ mol^{-1}).

It can be seen that intrinsic free energy of substitution at the N-1 site $\Delta^{\ddagger}G_1^o$ is larger than that for the N-4 site $\Delta^{\ddagger}G_4^o$, whereas the free energy of reaction $\Delta_rG_1^o$ is more exergonic than $\Delta_rG_4^o$. These two factors serve to affect the overall free energies of activation in opposite directions. The relative thermodynamic stability of the *N*-1 product is the dominant term, however, such that $\Delta^{\ddagger}G_1^M < \Delta^{\ddagger}G_4^M$.

Free energy difference	***i* = 1**	***i* = 4**
$\Delta^{\ddagger}G_i°$	130.6	125.6
Δ_rG_i	-109.8	-88.1
$\Delta^{\ddagger}G_i^M$	**81.4**	**85.5**
$\Delta^{\ddagger}G_i$	***81.1***	***86.5***

Table S2a: Assorted kinetic and thermodynamic parameters for the *N*-benzylation of 1,2,4-triazolate with *p*-F-BnBr, as computed using a combined KS-DFT/DLPNO-CCSD(T) methodology. See below for further computational details.

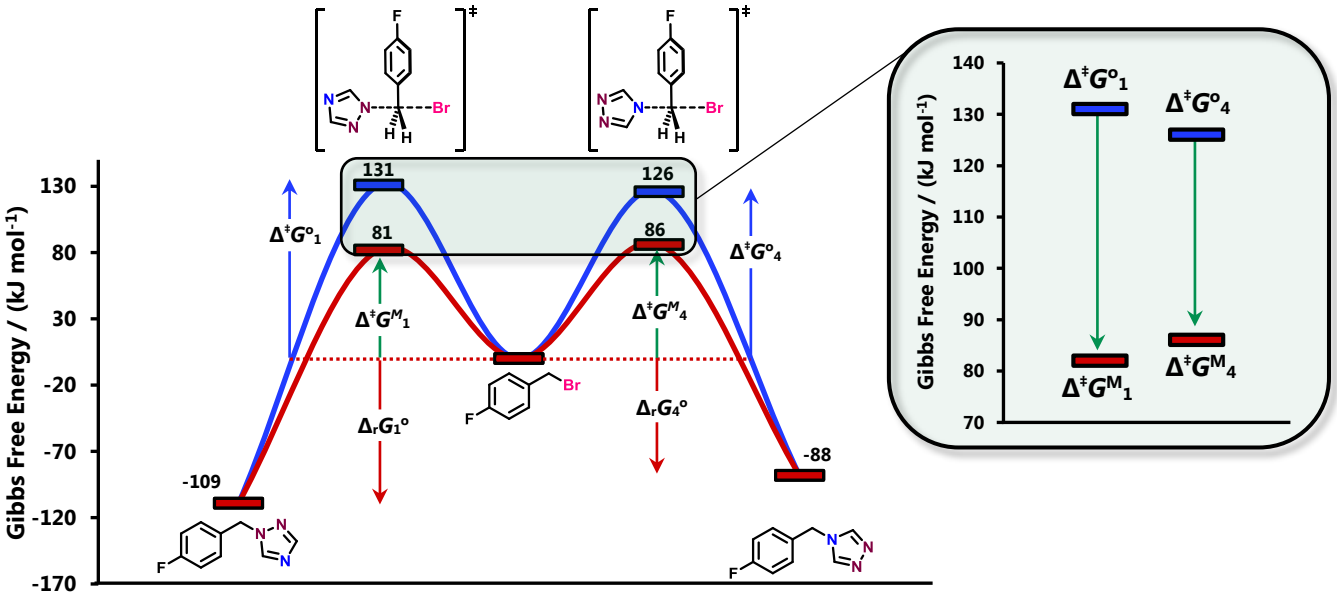
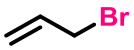


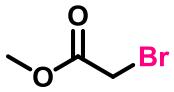
Figure S2a: Assorted kinetic and thermodynamic parameters for the *N*-benzylation of 1,2,4-triazolate with *p*-F-BnBr, as computed using a combined KS-DFT/DLPNO-CCSD(T) methodology.

This analysis was replicated for three other alkylating agents of varying reactivities (**Tables S2b-d**) – allyl bromide, methyl bromoacetate and phenacyl bromide – and in all three cases the intrinsic free energy of activation for substitution at the *N*-1 site is higher than or equal to that for substitution at the *N*-4 site. Moreover, in all three cases the thermodynamic stability of the *N*-1 product is sufficiently great to reverse the intrinsic selectivity, leading to $\Delta^{\ddagger}G_1^M < \Delta^{\ddagger}G_4^M$. It is also important to note that in all three cases Marcus theory is able to reproduce the directly computed free energies of activation to within 1 kJ mol^{-1}.



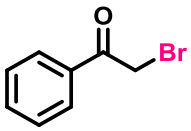
Free energy difference	i = 1	i = 4
$\Delta^{\ddagger}G_i°$	138.4	138.1
Δ_rG_i	-109.7	-97.4
$\Delta^{\ddagger}G_i^M$	**88.7**	**94.0**
$\Delta^{\ddagger}G_i$	89.1	94.2

Table S2b: Marcus analysis of the allylation of 1,2,4-triazolate with allyl bromide, as computed using a combined KS-DFT/DLPNO-CCSD(T) methodology.



Free energy difference	***i* = 1**	***i* = 4**
$\Delta^{\ddagger}G_i°$	131.9	131.7
$\Delta_r G_i$	-120.6	-109.4
$\boldsymbol{\Delta^{\ddagger}G_i^M}$	**78.5**	**82.6**
$\boldsymbol{\Delta^{\ddagger}G_i}$	***77.8***	***82.7***

Table S2c: Marcus analysis of the α-carbonylation of 1,2,4-triazolate with methyl bromoacetate, as computed using a combined KS-DFT/DLPNO-CCSD(T) methodology.



Free energy difference	***i* = 1**	***i* = 4**
$\Delta^{\ddagger}G_i°$	117.8	116.9
$\Delta_r G_i$	-109.4	-94.0
$\boldsymbol{\Delta^{\ddagger}G_i^M}$	**69.5**	**74.7**
$\boldsymbol{\Delta^{\ddagger}G_i}$	***69.7***	***73.8***

Table S2d: Marcus analysis of the α-carbonylation of 1,2,4-triazolate with phenylacyl bromdide, as computed using a combined KS-DFT/DLPNO-CCSD(T) methodology.

Figure S3: Solvent effects

End-point regioselectivities were determined for the *N*-benzylation of 1,2,4-triazole with p-F-BnBr in a range of solvents of varying ionising strengths (H_2O, MeOH, DMSO, MeCN, Me_2CO, CH_2Cl_2, $CHCl_3$, THF), as quantified by the normalised Dimroth-Reichardt $E_T(30)$ parameter. Selectivities were determined using both the MTBDH$^+$ (F_{N1}(MTBDH$^+$)) and ^{n}Bu$_4$N$^+$ (F_{N1}(^{n}Bu$_4$N$^+$)) salts of 1,2,4-triazolate (**Figure S3a**) in order to explore the effect of ion-pairing on the ambident reactivity of the 1,2,4-triazolate anion. Combined KS-DFT and CCSD(T)-F12 computations (*vide infra*) were employed to predict the regioselectivity of the naked anion (F_{N1}(CCSD(T)-F12)) in accordance with equation [SE5]:

$$F_{N_1}(CCSD(T)-F12) = \frac{100\, e^{\frac{(\Delta^{\ddagger}G_4 - \Delta^{\ddagger}G_1)}{RT}}}{1 + e^{\frac{(\Delta^{\ddagger}G_4 - \Delta^{\ddagger}G_1)}{RT}}}\ \%\quad [SE5]$$

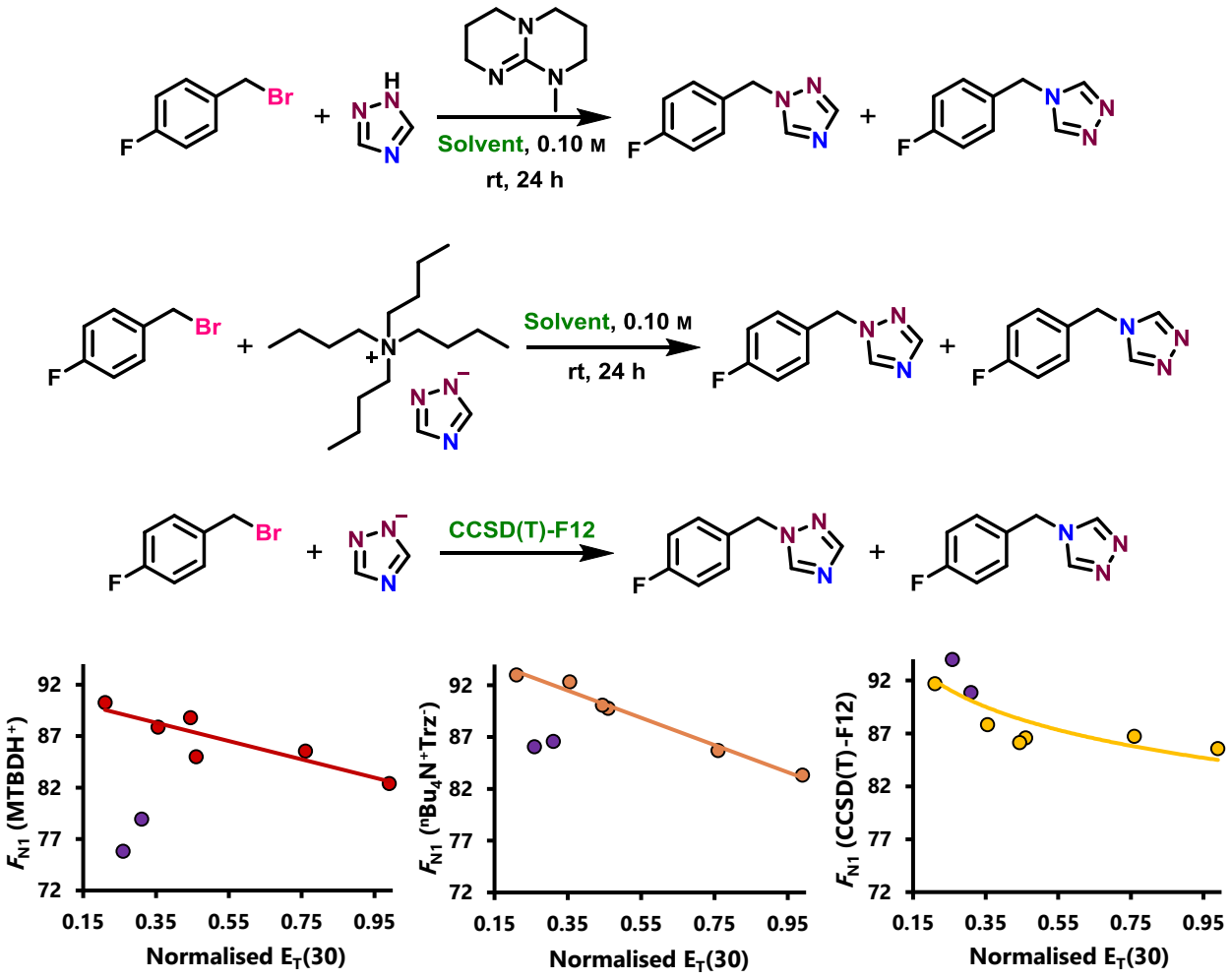


Figure S3a: Experimental selectivities determined with ^{1}H NMR spectroscopy after full conversion of p-F-BnBr. Equimolar quantities of 1,2,4-triazole, p-F-BnBr and MTBD (or ^{n}Bu$_4$N$^+$Trz$^-$) were used (0.10 M). Computed selectivities determined using free energies obtained from a KS-DFT/CCSD(T)-F12 methodology, with the solvent simulated using the IEFPCM model. Experimental and computational selectivities plotted as a function of the normalised Dimroth-Reichardt $E_T(30)$ parameter. Chlorinated solvents ($CHCl_3$, CH_2Cl_2) highlighted in purple (●).

The *difference* in selectivity ΔF_{N1} [SE6] obtained with the MTBDH$^+$ and ^{n}Bu$_4$N$^+$ salts of 1,2,4-triazolate was calculated for each solvent to differentiate the effects of *direct solvation* and *ion-pairing* on selectivity. In **Figure S3b** the selectivity differential ΔF_{N1} is plotted as a function of two parameters: (i) the normalised Dimroth-Reichardt $E_T(30)$ parameter; and (ii) the Kamlet-Taft β parameter (hydrogen-bond basicity).

$$\Delta F_{N1} = F_{N1}(\mathrm{Bu_4N^+}) - F_{N1}(\mathrm{MTBDH^+}) \quad [\mathrm{SE6}]$$

There is a strong inverse relationship between ΔF_{N1} and both of these two parameters. This suggests that ion-pairing between MTBDH$^+$ and the 1,2,4-triazolate anion – which will be promoted by solvents of low ionising strength and low hydrogen-bond basicity – serves to enhance N-4 selectivity.

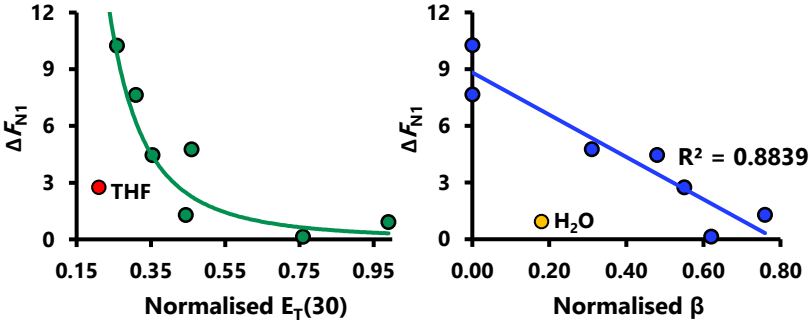


Figure S3b: Selectivity differential ΔF_{N1} plotted as a function of the normalised Dimroth-Reichardt $E_T(30)$ and Kamlet-Taft β parameters. For each solvent descriptor there is one outlier: THF (red, ●), H_2O (yellow, ●). THF is unique among the solvents studied for having a very low ionising strength (low $E_T(30)$) but comparitvely high hydrogen-bond basicity (high β); water is unique for the opposite reason.

Solvent	$E_T(30)$[6]	β[7]
THF	0.21	0.55
$CHCl_3$	0.26	0
CH_2Cl_2	0.31	0
Me_2CO	0.36	0.48
DMSO	0.44	0.76
MeCN	0.46	0.31
MeOH	0.76	0.62
H_2O	0.99	0.18

Table S3c: Literature solvent parameters ($E_T(30)$, β) for the solvents considered in this work.

Figure S4: Leaving group effects

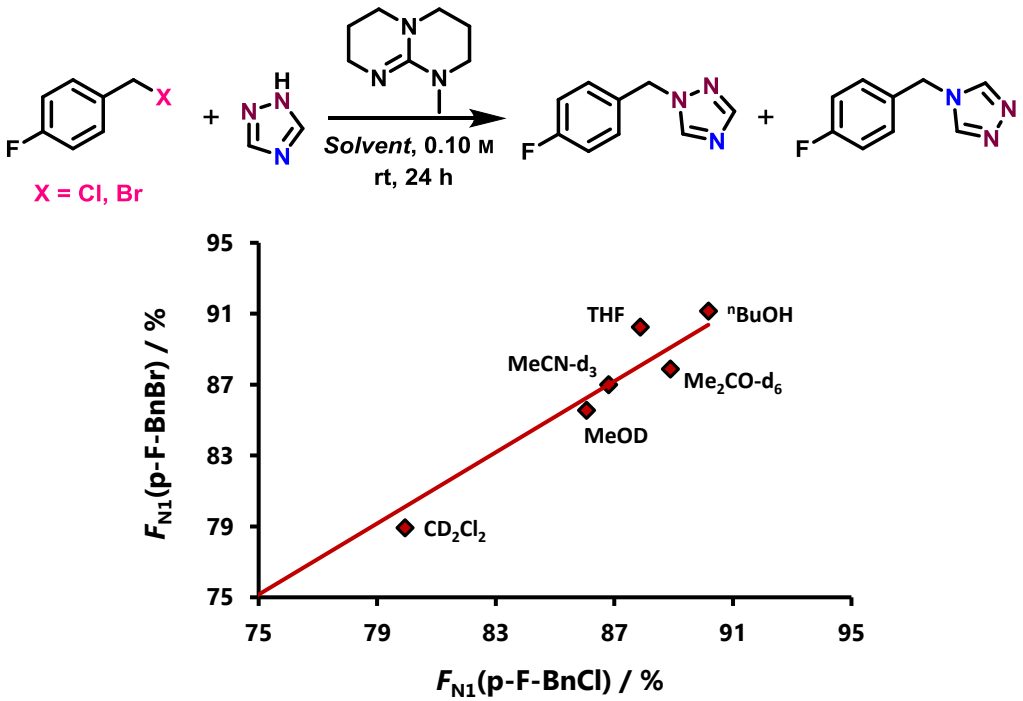


Figure S4a: Experimental selectivities determined with ^{1}H NMR spectroscopy after full conversion of *p*-F-BnCl or *p*-F-BnBr, using a range of solvents. Equimolar quantities of 1,2,4-triazole, *p*-F-BnX and MTBD were used (0.10 M). Selectivity was found to be independent of the charge density of the leaving group when MTBD was used as a base.

Figure S5: Base kinetics

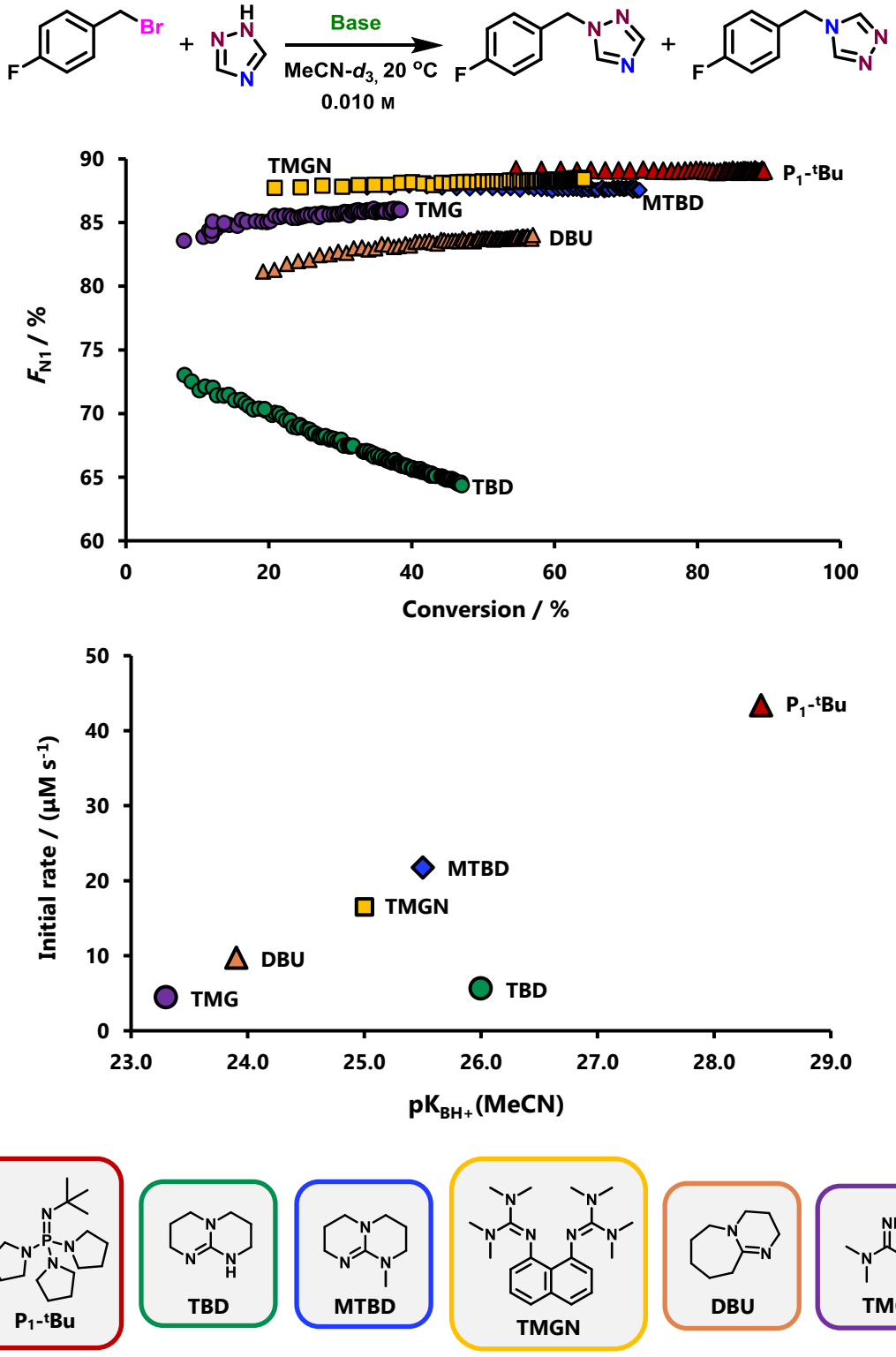


Figure S5a: Selectivity-conversion profiles for the *N*-benzylation of 1,2,4-triazole (10.0 mM) with *p*-F-BnBr (10.0 mM) and six different organic bases (10.0 mM) in MeCN-d_3 (20°C). Initial rate–pK_{BH+} plot obtained under the same conditions for all six bases. Kinetic data obtained from *in situ* ^{1}H NMR spectroscopy, using 1,3,5-trimethoxybenzene as an internal standard. pK_{BH+}(MeCN) data obtained from the literature.

Figure S6: ^{1}H NMR-DOSY

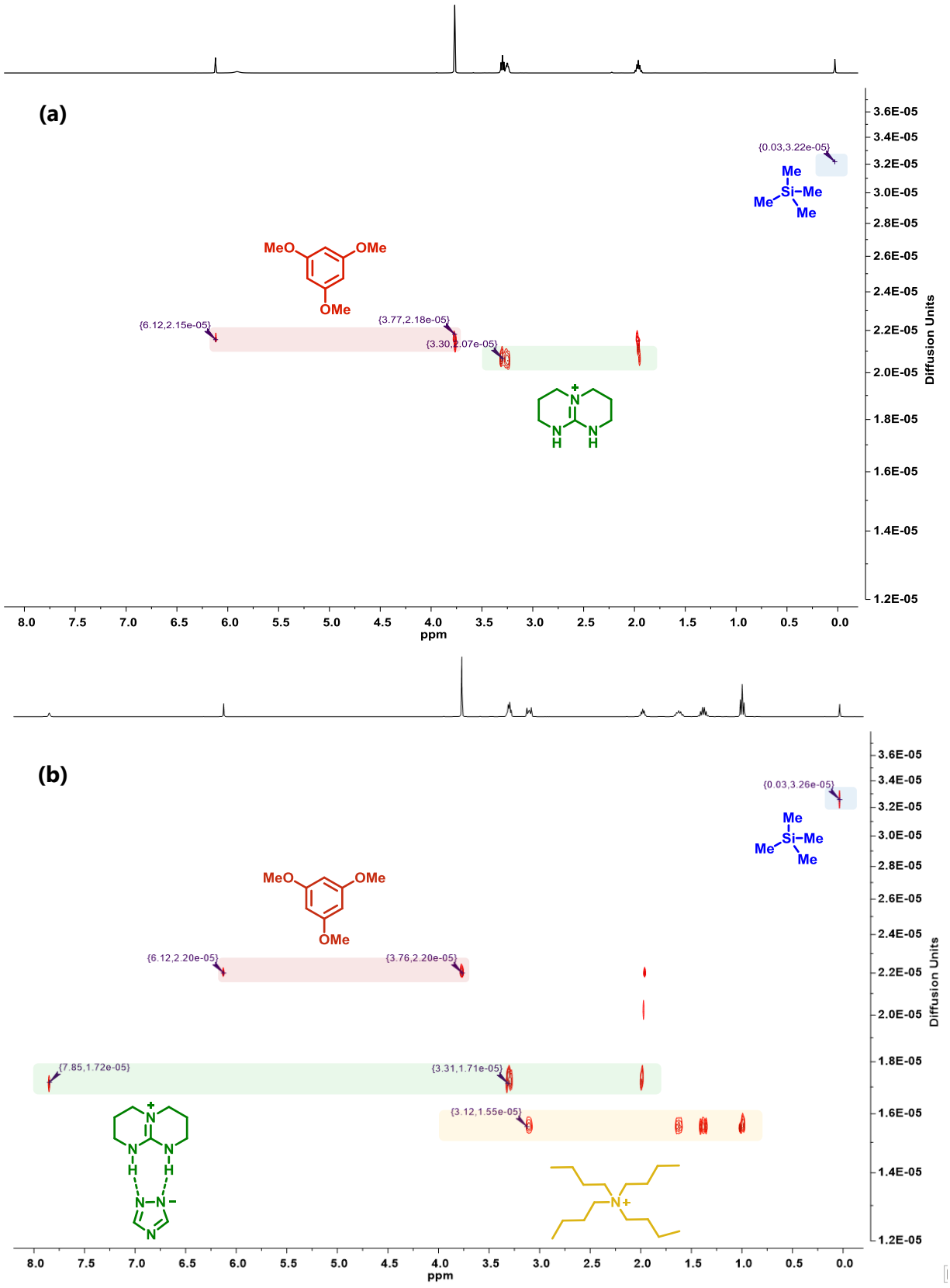


Figure S6a: ^{1}H NMR-DOSY spectra obtained in MeCN-d_3 (20 °C) with 1,3,5-trimethoxybenzene (0.10 M) and TMS as internal standards. (a) $TBDH^{+}PF_6^{-}$ (0.10 M). (b) $TBDH^{+}PF_6^{-}$ (0.10 M) + $^{n}Bu_4N^{+}Trz^{-}$ (0.10 M).

^{1}H NMR-DOSY spectra (MeCN-d_3, 20 °C) were obtained separately for $TBDH^+PF_6^-$ (0.10 M) and an equimolar mixture of $TBDH^+PF_6^-$ (0.10 M) and $^nBu_4N^+Trz^-$ (0.10 M) in an attempt to characterise the $TBDH^+Trz^-$ ion-pair in the solution phase. TMS and 1,3,5-trimethoxybenzene were used as internal standards.

$TBDH^+PF_6^-$ (a): In the absence of the 1,2,4-triazolate anion, a diffusion constant of D_{TBDH+} = 2.07 × 10^{-5} cm^2 s^{-1} was measured for the unassociated $TBDH^+$ cation (in the presence of the diffuse, non-coordinating PF_6^- anion). Diffusion constants of D_{TMS} = 3.22 × 10^{-5} cm^2 s^{-1} and $D_{1,3,5\text{-}TMB}$ = 2.18 × 10^{-5} cm^2 s^{-1} were measured for TMS and 1,3,5-trimethoxybenzene, respectively.

$TBDH^+PF_6^-$ + $^nBu_4N^+Trz^-$ (b): In the presence of the 1,2,4-triazolate anion (Trz^-), the same diffusion constant – $D_{Complex}$ = 1.70 × 10^{-5} cm^2 s^{-1} – was measured for both the $TBDH^+$ cation and the 1,2,4-triazolate anion (δ_H = 7.85 ppm), indicating the formation of the $TBDH^+Trz^-$ complex. Diffusion constants of D_{TMS} = 3.26 × 10^{-5} cm^2 s^{-1} and $D_{1,3,5\text{-}TMB}$ = 2.20 × 10^{-5} cm^2 s^{-1} were measured for TMS and 1,3,5-trimethoxybenzene, respectively.

The decrease in the $TBDH^+$ diffusion constant upon the addition of the 1,2,4-triazolate anion – and the observation that both the cation and anion share a single, common diffusion constant – are suggestive of solution-phase association between $TBDH^+$ and T^-. Assuming strong association, the relative radii of the complex and naked $TBDH^+$ cation can be approximated from the Stokes-Einstein equation [SE7], where in general R_i denotes the radius of a molecular species, k_B = 1.38 x 10^{-23} J K^{-1}, T = 293 K and η denotes the dynamic viscosity of the medium.

$$D_i = \frac{k_B T}{8\pi\eta R_i^3} \quad [SE7]$$

The relative ratios of the diffusion constants of TMS and $TBDH^+$, and of TMS and the complex, are thus given by:

$$\frac{D_{Complex}}{D_{TMS}} = \left(\frac{R_{TMS}}{R_{Complex}}\right)^3 = \frac{1.70}{3.26} = 0.521 \quad [SE8]$$

$$\frac{D_{TBDH^+}}{D_{TMS}} = \left(\frac{R_{TMS}}{R_{TBDH^+}}\right)^3 = \frac{2.07}{3.22} = 0.643 \quad [SE9]$$

As such, the relative volumes V_i of the complex and the naked $TBDH^+$ cation may be approximated from:

$$\frac{V_{Complex}}{V_{TBDH^+}} = \left(\frac{R_{Complex}}{R_{TBDH^+}}\right)^3 = \frac{D_{TBDH^+}}{D_{TMS}} . \frac{D_{TMS}}{D_{Complex}} = \frac{0.643}{0.521} = 1.23 \quad [SE10]$$

The magnitude of $V_{Complex}/V_{TBDH+}$ suggests that the complex is monomeric in nature, with a 1:1 stoichiometry between the $TBDH^+$ cation and 1,2,4-triazolate anion. To confirm this conclusion, KS-DFT computations (PBE0+GD3BJ/6-311+G(d,p)/Ultrafine/Tight) were used to calculate the molecular volume – defined as the volume inside an electron density contour of 10^{-3} electrons $Bohr^{-3}$ – of $TBDH^+$ (V_{TBDH+}(KS-DFT)) and the simple ion-paired monomer $TBDH^+Trz^-$ ($V_{TBDH+Trz-}$(KS-DFT)). Indeed, the ratio of computed molecular volumes is in *quantitative* agreement with ^{1}H NMR-DOSY data, strongly suggesting the the presence of a monomeric ion-pair in solution.

$$V_{TBDH^+}^{(KS-DFT)} = 115.2 \text{ cm}^3 \text{ mol}^{-1}$$

$$V_{TBDH^+Trz^-}^{(KS-DFT)} = 143.1 \text{ cm}^3 \text{ mol}^{-1}$$

$$\frac{V_{TBDH^+Trz^-}^{(KS-DFT)}}{V_{TBDH^+}^{(KS-DFT)}} = 1.24 \quad [SE11]$$

As the above ^{1}H NMR-DOSY analysis is strictly only valid in the limit of strong association, the fraction of 1,2,4-triazolate that is expected to be bound under the DOSY conditions ($[Trz^-]_0 = [TBDH^+]_0$ = 0.10 M, MeCN-d_3, 20 °C), denoted f_{Bound}, was calculated in accordance with the ion-pairing binding constant K_{Trz} = 9,800, obtained from ^{1}H NMR reaction monitoring and kinetic modelling (see main text). For 1:1 association the equilibrium constant for ion-pairing between $TBDH^+$ and Trz^-, K_{Trz}, may be expressed as below, where $[TBDH^+]_0$ = 0.10 M denotes the *total* concentration of $TBDH^+$ cations in solution and $[TBDH^+Trz^-]$, $[TBDH^+]$ and $[Trz^-]$ denote the *equilibrium* concentrations of the ion pair, $TBDH^+$ cation and 1,2,4-triazolate anion, respectively.

$$K_{Trz} = \frac{[\text{TBDH}^+\ \text{Trz}^-]}{[\text{Trz}^-][\text{TBDH}^+]} = \frac{[\text{TBDH}^+\ \text{Trz}^-]}{[\text{TBDH}^+]^2} = \frac{[\text{TBDH}^+\ \text{Trz}^-]}{([\text{TBDH}^+]_0 - [\text{TBDH}^+\ \text{Trz}^-])^2} \quad [SE12]$$

Following rearrangement and solving the resulting quadratic, the fraction of 1,2,4-triazolate that ought to be bound at equilibrium f_{Bound} was calculated as 97 %, supporting the assumption of strong association.

$$f_{Bound} = \frac{[\text{TBDH}^+\ \text{Trz}^-]}{[\text{TBDH}^+]_0} = \frac{2K_{Trz}[\text{TBDH}^+]_0 + 1 - \sqrt{4K_{Trz}[\text{TBDH}^+]_0 + 1}}{2K_{Trz}[\text{TBDH}^+]_0} = 0.97 \quad [SE13]$$

Figure S7: Full modelling results: TBD

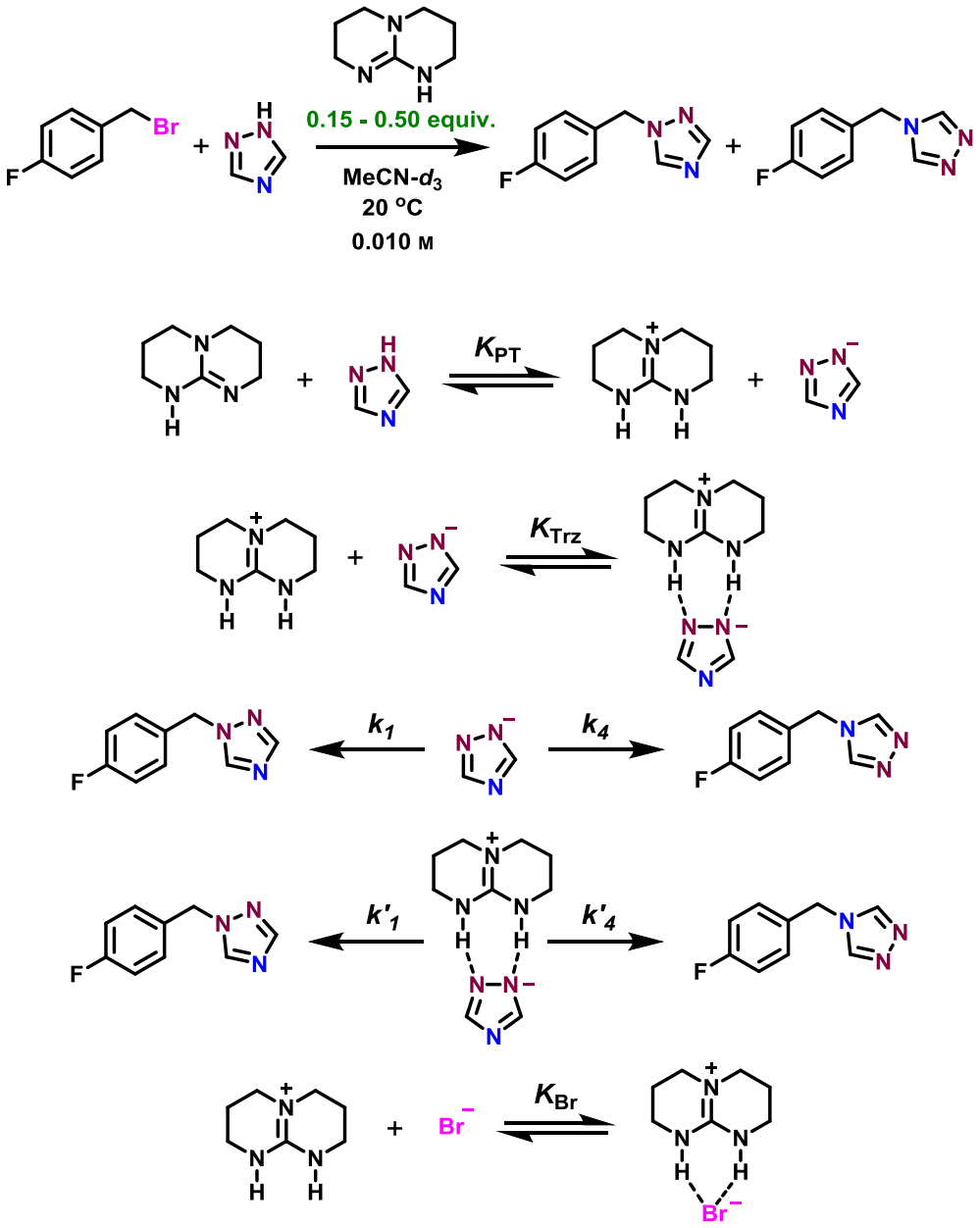


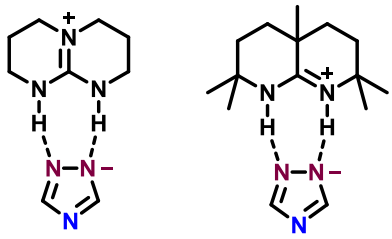
Figure S7a: Formal kinetic model (Model 1) for the N-benzylation of 1,2,4-triazole with *p*-F-BnBr and TBD in MeCN. In accordance with experimental pK_a data, the equilibrium constant for proton transfer K_{PT} >> 100. For Model 2 the binding constant for bromide was set to K_{Br} = 0.

	Experiment		DLPNO-CCSD(T)	
	Model 1	**Model 2**	**IGRRHO**	**qRRHO**
k_1 / M^{-1} s^{-1}	0.30	0.30	-	-
k_4 / M^{-1} s^{-1}	0.044	0.044	**-**	**-**
$\Delta^{\ddagger}G_1$ / kJ mol^{-1}	74.7	74.7	81.1	87.6
$\Delta^{\ddagger}G_4$ / kJ mol^{-1}	79.4	79.4	86.5	92.4
$\Delta\Delta^{\ddagger}G$ / kJ mol^{-1}	4.7	4.7	5.4	4.8
k_1' / M^{-1} s^{-1}	0.0035	0.0061	-	-
k_4' / M^{-1} s^{-1}	0.013	0.013	-	-
$\Delta^{\ddagger}G_1(\mathrm{TBD})$ / kJ mol^{-1}	85.5	84.2	87.2	96.0
$\Delta^{\ddagger}G_4(\mathrm{TBD})$ / kJ mol^{-1}	82.3	82.3	80.1	90.2
$\Delta\Delta^{\ddagger}G(\mathrm{TBD})$ / kJ mol^{-1}	3.2	1.9	7.1	5.8
$\Delta\Delta^{\ddagger}G_1(\mathrm{TBD})$ / kJ mol^{-1}	10.8	9.5	6.1	8.4
$\Delta\Delta^{\ddagger}G_4(\mathrm{TBD})$ / kJ mol^{-1}	3.0	1.9	-6.4	-2.2
K_{Trz}	9800	10000	-	-
$\Delta_{\mathrm{Bind}}G_{\mathrm{Trz}}$ / kJ mol^{-1}	-22.4	-22	-22.0	-18.0
K_{Br}	185	-	-	-
$\Delta_{\mathrm{Bind}}G_{Br}$ / kJ mol^{-1}	-12.7	-	-18.0	-15.3
$\Delta\Delta_{\mathrm{Bind}}G(\mathrm{TBD})$ / kJ mol^{-1}	9.7	-	4.0	2.7

Table S7b: Experimental rate coefficients and binding constants obtained from *in situ* ^{1}H NMR reaction monitoring (MeCN-d_3, 0.010 M, 20 °C) and kinetic modelling. Equimolar concentraitons of *p*-F-BnBr (10.0 mM) and 1,2,4-triazole (10.0 mM) were used for all kinetic runs; [TBD] = 1.5 – 5.0 mM. The rate coefficients k_1 = 0.30 M^{-1} s^{-1} and k_4 = 0.044 M^{-1} s^{-1} were obtained from separate reaction monitoring experiments with MTBD. Experimental free energies of activation obtained in accordance with classical transition state theory, using the Eyring-Polanyi equation and a transmission coefficient of κ = 1. Experimental binding free energies calculated in accordance with classical thermodynamics. Theoretical free energies of activation and binding free energies computed using a combined KS-DFT/DLPNO-CCSD(T) methodology (*vide infra*) and the IEFPCM(MeCN,UFF) model. Theoretical free energy corrections were obtained in accordance with two separate statistical mechanical approximations: (i) the ideal-gas rigid-rotor harmonic-oscillator approximation (IGRRHO); and (ii) Grimme's quasi rigid-rotor harmonic-oscillator approximation (qRRHO). See below for further computational details.

Figure S8: DLPNO-LED analysis

A DLPNO local energy decomposition (DLPNO-LED) analysis (ORCA 4.0.1) was employed to explore the interactions of the 1,2,4-triazolate anion with the $TBDH^+$ and $PMDH^+$ cations, and rationalise the relative affinities of the two cations for 1,2,4-triazolate.



$TBDH^+Trz^-$ **$PMDH^+Trz^-$**

Under the LED scheme the gas-phase DLPNO-CCSD(T) binding energy of two fragments associated by virtue of non-covalent interactions, $\Delta_{Bind}E_{(g)}$, is decomposed into arbitrary but nevertheless chemically intuitive contributions. In the simplest form of the analysis $\Delta_{Bind}E$ can be segmented into contributions from: (i) *intramolecular* distortion energies (or *preparation* energies), which describe the energy input required to distort the molecular ($\Delta E_{(G\text{-}Prep)}$) and electronic structures ($\Delta E_{(E\text{-}Prep)}$) of the two fragments, relative to their relaxed structures, in order to optimise the overall binding energy; and (ii) genuine *intermolecular* interaction energies between the two distorted fragments ($\Delta E_{(E\text{-}Int)}$).

$$\Delta_{\mathrm{Bind}}E_{(g)} = \Delta E_{(\mathrm{E-Int})} + \Delta E_{(\mathrm{G-Prep})} + \Delta E_{(\mathrm{E-Prep})} \quad [SE14]$$

The intermolecular interaction energy term $\Delta E_{(E\text{-}Int)}$ can in turn be further decomposed into contributions from: (i) permanent electrostatic interactions and interactions induced by charge-transfer between the two fragments, $\Delta E_{(Es)}$; (ii) the quantum-mechanical exchange interaction, $\Delta E_{(Ex)}$; (iii) London dispersion interactions, $\Delta E_{(Disp)}$; and (iv) a chemically nebulous triples correction, $\Delta E_{(T)}$.

$$\Delta E_{(\mathrm{E-Im})} = \Delta E_{(\mathrm{Es})} + \Delta E_{(\mathrm{Ex})} + \Delta E_{(\mathrm{Disp})} + \Delta E_{(\mathrm{T})} \quad [SE15]$$

Before undertaking a DLPNO-LED analysis, the solution-phase binding free energy of each ion-pair, $\Delta_{Bind}G$, was decomposed into its constituent parts: (i) the gas-phase DLPNO-CCSD(T) binding energy, $\Delta_{Bind}E_{(g)}$, to be taken forward for the LED analysis; (ii) the *change* in the overall solvation energy of the two fragments that accompanies binding, $\Delta_{Bind}\delta E_{solv}$; and (iii) the *change* in the free energy correction of the two fragments, $\Delta_{Bind}\delta G$. This preliminary analysis was conducted using both the ideal-gas rigid-rotor harmonic-oscillator (IGRRHO) and quasi rigid-rotor harmonic-oscillator (qRRHO) approximations **Tables S8a/b**).

$$\Delta_{\mathrm{Bind}}G = \Delta_{\mathrm{Bind}}E_{(g)} + \Delta_{\mathrm{Bind}}\delta E_{solv} + \Delta_{\mathrm{Bind}}\delta G \quad [SE16]$$

It can be seen that $\Delta_{Bind}E_{(g)}$ *and* $\Delta_{Bind}\delta E_{solv}$, acting to favour and disfavour binding, respectively, are the primary contributors to $\Delta_{Bind}G$ for both ion-pairs. The *differential* binding affinities of $PMDH^+Trz^-$ and $TBDH^+Trz^-$ are also largely governed by these two terms, with the entropic penalty of binding essentially invariant between the two cations.

IGRRHO	$\Delta_{Bind}G$	$\Delta_{Bind}E_{(g)}$	$\Delta_{Bind}\delta E_{solv}$	$\Delta_{Bind}\delta G$
$TBDH^+Trz^-$	-22.0	-441.9	380.4	47.4
$PMDH^+Trz^-$	-35.9	-451.8	376.3	47.6
	-13.9	**-9.9**	**-4.1**	**0.2**

Table S8a: Theoretical binding energies (kJ mol^{-1}) computed using a combined KS-DFT/DLPNO-CCSD(T) methodology (*vide infra*). Solvation energies computed at the PBE0+GD3BJ/6-311+G(d,p)/IEFPCM(MeCN,UFF) level of theory. Theoretical free energy corrections were obtained in accordance with the ideal-gas rigid-rotor harmonic-oscillator approximation (IGRRHO). See below for further computational details.

qRRHO	$\Delta_{Bind}G$	$\Delta_{Bind}E_{(g)}$	$\Delta_{Bind}\delta E_{solv}$	$\Delta_{Bind}\delta G$
$TBDH^+Trz^-$	-18.0	**-441.9**	380.4	51.5
$PMDH^+Trz^-$	-30.8	**-451.8**	376.3	52.7
	-12.8	**-9.9**	**-4.1**	**1.2**

Table S8b: Theoretical binding energies (kJ mol^{-1}) computed using a combined KS-DFT/DLPNO-CCSD(T) methodology (*vide infra*). Solvation energies computed at the PBE0+GD3BJ/6-311+G(d,p)/IEFPCM(MeCN,UFF) level of theory. Theoretical free energy corrections were obtained in accordance with Grimme's quasi rigid-rotor harmonic-oscillator approximation (qRRHO). See below for further computational details.

Regardless of the statistical mechanical approximation used to treat vibrational entropies, the increase in the gas-phase DLPNO-CCSD(T) binding energy accounts for more than 70 % of the increase in the solution-phase binding free energy upon exchanging $TBDH^+$ for $PMDH^+$. The results of a DLPNO-LED analysis, which decomposes $\Delta_{Bind}E_{(g)}$ further, are shown in **Table S8c**.

Ion-pair	$TBDH^+Trz^-$	$PMDH^+Trz^-$	$\Delta\Delta E$
$\Delta_{Bind}E_{(g)}$	**-441.9**	**-451.8**	**-9.9**
$\Delta E_{(E\text{-}Im)}$	-1549.3	-1537.0	12.3
$\Delta E_{(Es)}$	-1390.6	-1374.2	16.4
$\Delta E_{(Disp)}$	-30.1	-35.3	-5.2
$\Delta E_{(Ex)}$	-116.7	-114.2	2.5
$\Delta E_{(E\text{-}Prep)}$	1081.5	1067.3	-14.2
$\Delta E_{(G\text{-}Prep)}$	26.0	17.9	-8.1
$\Delta E_{(T)}$	-11.9	-13.2	-1.3

Table S8c: DLPNO-LED analysis of the binding between $TBDH^+$ and 1,2,4-triazolate, and $PMDH^+$ and 1,2,4-triazolate (kJ mol^{-1}). The energy difference between the two cations for each contribution is denoted $\Delta\Delta E$, with a negative term favouring $PMDH^+$. Gas-phase energies computed at the DLPNO-CCSD(T)/ma-def2-TZVPP/TightSCF/TightPNO level of theory (*ORCA 4.0*). Geometries obtained at the PBE0+GD3BJ/6-311+G(d,p)/Tight/Ultrafine level (*Gaussian09*).

The results in **Table S8c** highlight a number of interesting findings: (i) the genuine *intermolecular* interactions between $PMDH^+$ and 1,2,4-triazolate are in fact *weaker* than between $TBDH^+$ and 1,2,4-triazolate ($\Delta\Delta E_{(E\text{-}Int)}$ = +12.3 kj mol-1), primarly due to weaker electrostatic and exchange interactions ($\Delta\Delta E_{(Es)}$ = +12.3 kJ mol^{-1}; $\Delta\Delta E_{(Ex)}$ = +2.5 kJ mol^{-1}); (ii) the weakened electrostatic and exchange interactions are partially offset by stronger London dispersion interactions ($\Delta\Delta E_{(Disp)}$ = -5.2 kJ mol^{-1}); and (iii) both the electronic and geometric preparation energies are smaller for $PMDH^+$ ($\Delta\Delta E_{(E\text{-}Prep)}$ = -14.2 kJ mol^{-1}, $\Delta\Delta E_{(G\text{-}Prep)}$ = -8.1 kJ mol-1), suggesting that its superior binding affinity for 1,2,4-triazolate is almost exclusively because the relaxed geometric and electronic structures of the $PMDH^+$ cation are more closely aligned to those of the paired state than $TBDH^+$.

Figure S9: PMD kinetics

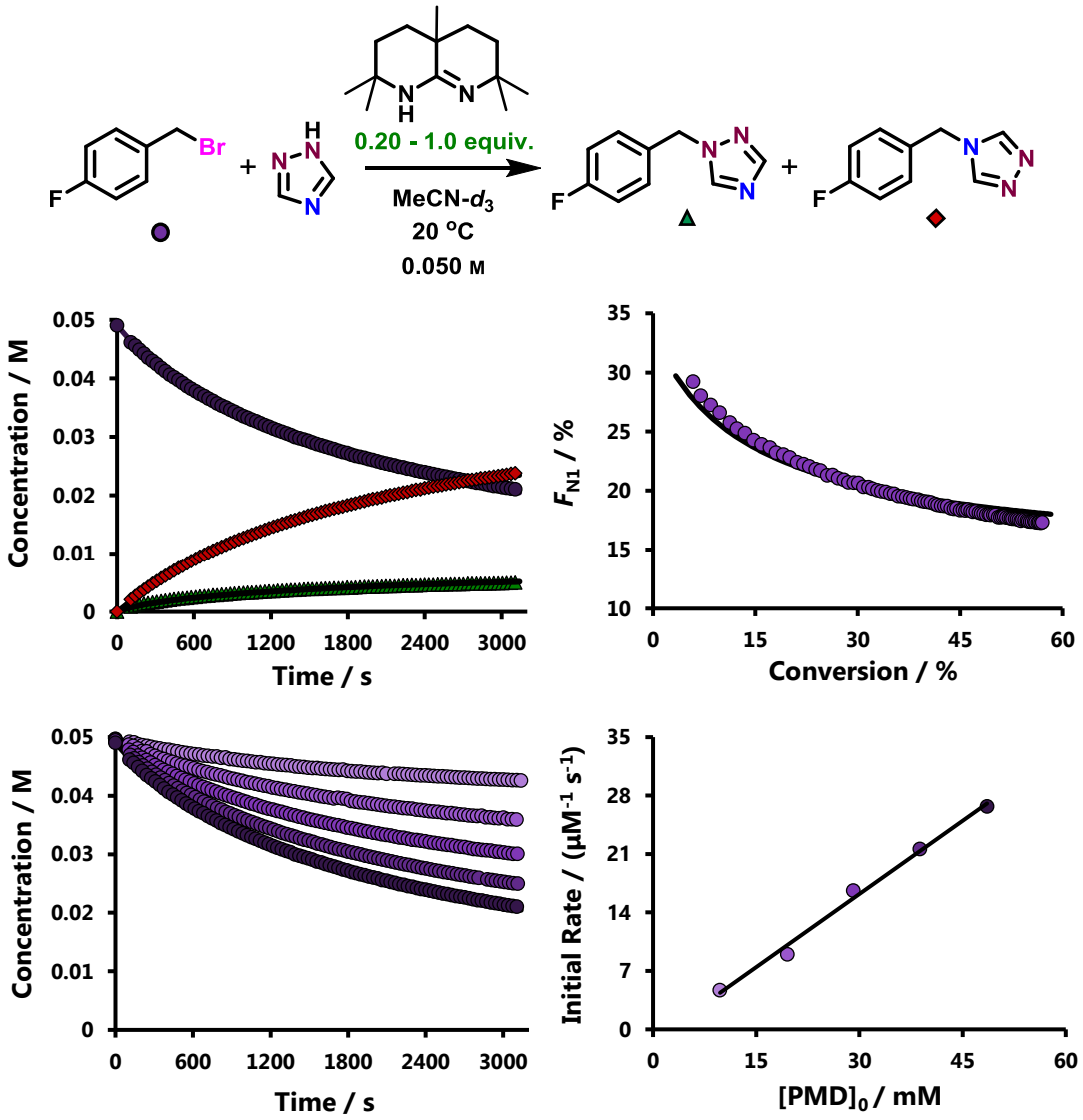


Figure S9a: Kinetic profiles obtained by *in situ* ^{1}H NMR spectroscopy, using 1,3,5-trimethoxybenzene as an internal standard under the following conditions (MeCN-d_3, 20°C): p-F-BnBr (50.0 mM), 1,2,4-triazole (50.0 mM), PMD (10.0 – 50.0 mM). Time evolution of products and selectivity-conversion profile shown for $[PMD]_0$ = 50.0 mM. Kinetic fits shown as black lines.

Figure S10: PMD concentration dependence

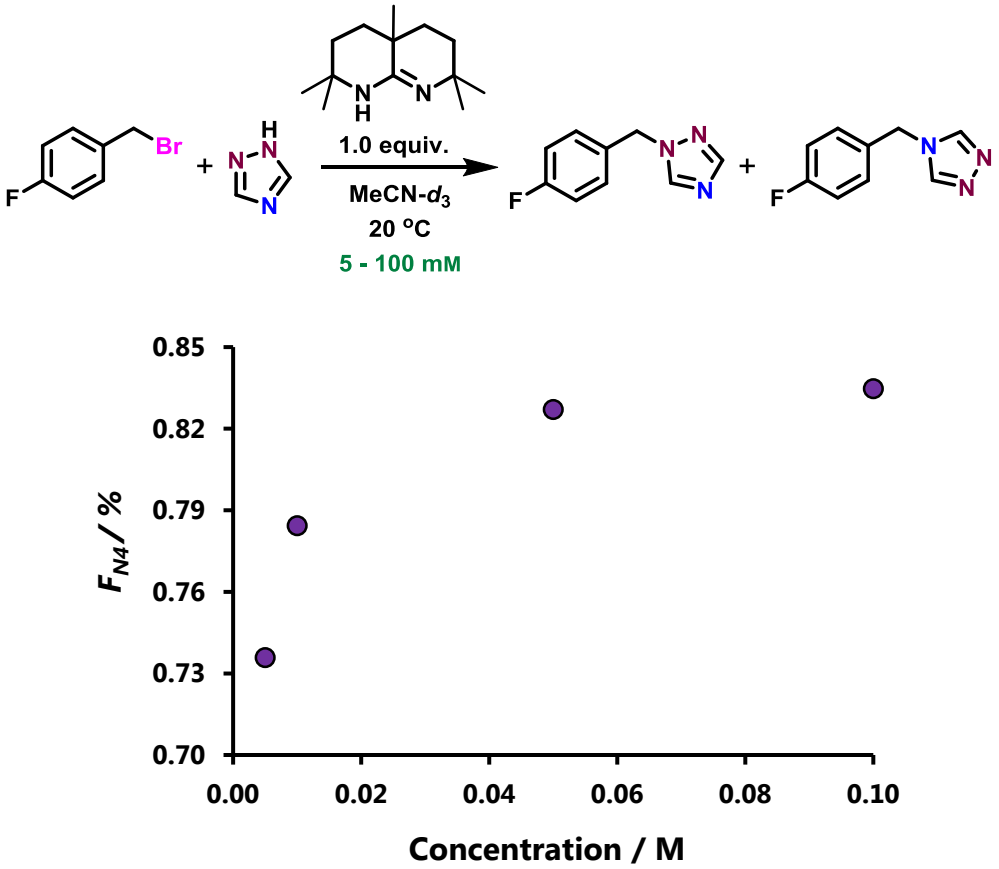


Figure S10a: End-point regioselectivities observed for the *N*-benzylation of 1,2,4-triazole with *p*-F-BnBr in the presence of PMD (MeCN-d_3, 20 °C); regioselectivity reported as final mole fraction of N-4 regioisomer, F_{N4} = $[N_4]/([N_1]+[N_4])$, after full conversion of *p*-F-BnBr. Equimolar concentrations (5, 10, 50, 100 mM) of 1,2,4-triazole, *p*-F-BnBr and PMD used for all four runs. The increase in *N*-4 selectivity at higher reaction concentrations is indicative of bimolecular association.

Figure S11: PMD temperature dependence

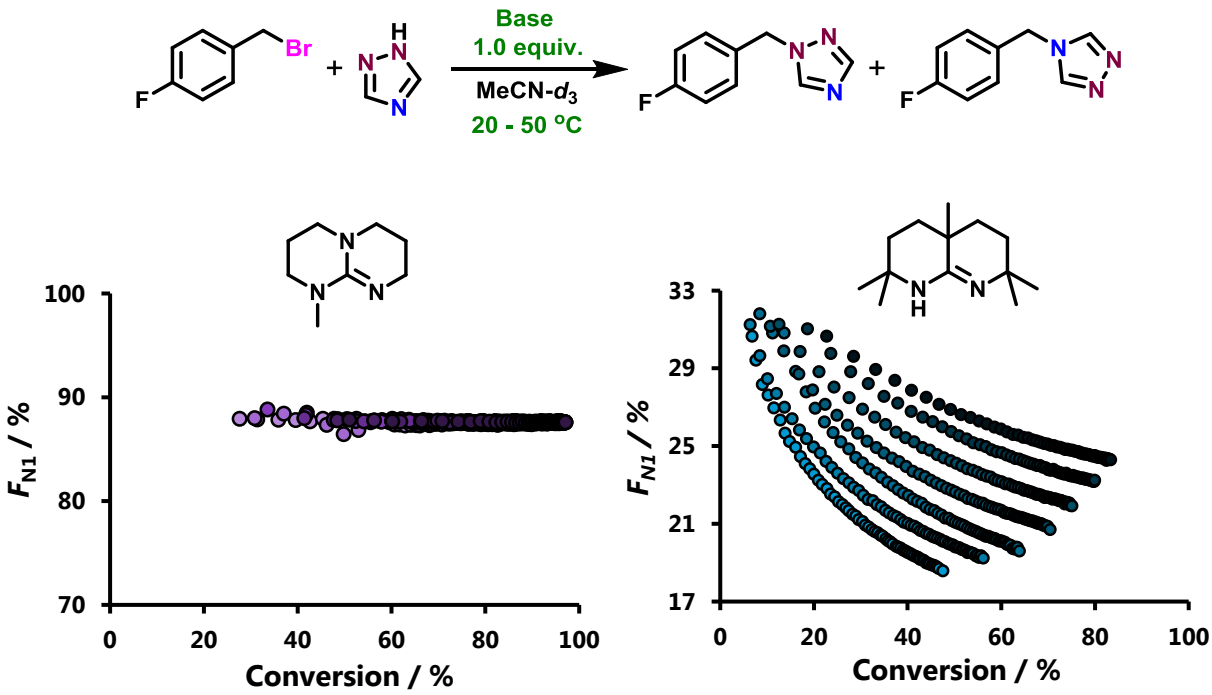


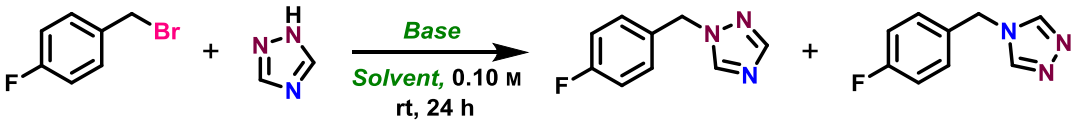
Figure S11a: Selectivity-conversion profiles for the *N*-benzylation of 1,2,4-triazole with *p*-F-BnBr in the presence of two distinct organic bases: MTBD and PMD. Kinetic runs monitored by *in situ* ^{1}H NMR spectroscopy over a range of temperatures (20 – 50 °C), with 1,3,5-trimethoxybenzene used as an internal standard. For kinetic runs with MTBD, equimolar quantities of 1,2,4-triazole (10.0 mM), p-F-BnBr (10.0 mM) and MTBD (10.0 mM) were used; for kinetic runs with PMD, higher equimolar concencentrations were used (50.0 mM).

The temperature dependence of regioselectivity was observed to be strikingly different for MTBD and PMD in the *N*-benzylation of 1,2,-triazole. In the case of MTBD the observed regioselectivity remained constant over all conversions and a range of temperatures (20 – 50 °C). Under a non-associative regime, it should be expected that N-1 selectivity will change by less than 2 % upon increasing the temperature from 20 °C to 50 °C ($F_{N1}(T_\beta)$ = 0.89; T_α = 323.15 K, T_β = 293.15 K; $\Delta\Delta^\ddagger G = \Delta^\ddagger G_4 - \Delta^\ddagger G_1$ = 4.7 kJ mol^{-1}). The selectivity-conversion profiles with MTBD are consistent with this regime.

$$\frac{F_1(T_\alpha)}{F_1(T_\beta)} = \frac{e^{\frac{(\Delta^\ddagger G_4 - \Delta^\ddagger G_1)}{RT_\alpha}}\left(1 + e^{\frac{(\Delta^\ddagger G_4 - \Delta^\ddagger G_1)}{RT_\beta}}\right)}{e^{\frac{(\Delta^\ddagger G_4 - \Delta^\ddagger G_1)}{RT_\beta}}\left(1 + e^{\frac{(\Delta^\ddagger G_4 - \Delta^\ddagger G_1)}{RT_\alpha}}\right)} = 0.98 \quad [SE17]$$

In the case of PMD, *N*-1 selectivity decreased significantly at higher conversions and lower temperatures, as shown in **Figure S11a**. The decrease in *N*-1 selectivity at lower temperatures in the case of PMD is consistent with the *exothermic* association of PMDH$^+$ and 1,2,4-triazolate, for lower temperatures will favour ion-pairing and thereby promote *N*-4 substitution in accordance with the findings laid out in the main text.

Figure S12: PMD solvent dependence



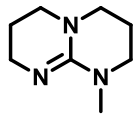
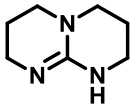
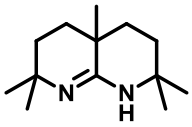
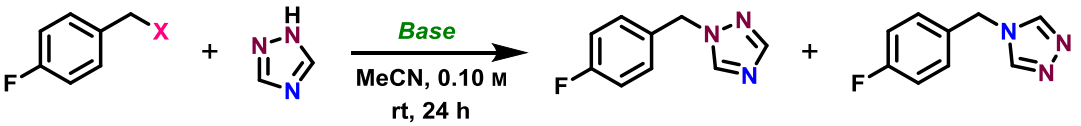
F_{N1} / %	DMSO	MeOH	MeCN	Me_2CO	THF	CH_2Cl_2
	89	86	85	88	90	79
	85	83	48	49	38	38
	62	79	16	16	7	6

Figure S12a: End-point regioselectivities, F_{N1} = $[N_1]/([N_1]+[N_4])$, obtained for the N-benzylation of 1,2,4-triazole with p-F-BnBr in the presence of MTBD, TBD or PMD as the base. Regioselectivities obtained over a range of solvents after full consumption of p-F-BnBr. Equimolar quantities of 1,2,4-triazole (0.10 M), p-F-BnBr (0.10 M) and base (0.10 M) were used throughout.

Figure S13: PMD leaving group dependence



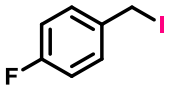
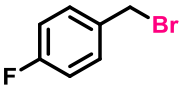
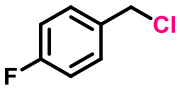
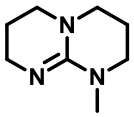
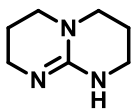
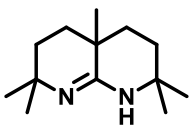
F_{N1} / %			
	84	85	87
	40	48	60
	10	17	29

Figure S13a: End-point regioselectivities, F_{N1} = $[N_1]/([N_1]+[N_4])$, obtained for the N-benzylation of 1,2,4-triazole with p-F-BnX in the presence of MTBD, TBD or PMD as the base. Regioselectivities obtained in MeCN-d_3 with X = Cl, Br, I. Equimolar quantities of 1,2,4-triazole (0.10 M), p-F-BnX (0.10 M) and base (0.10 M) were used throughout.

Figure S14: PMD computations

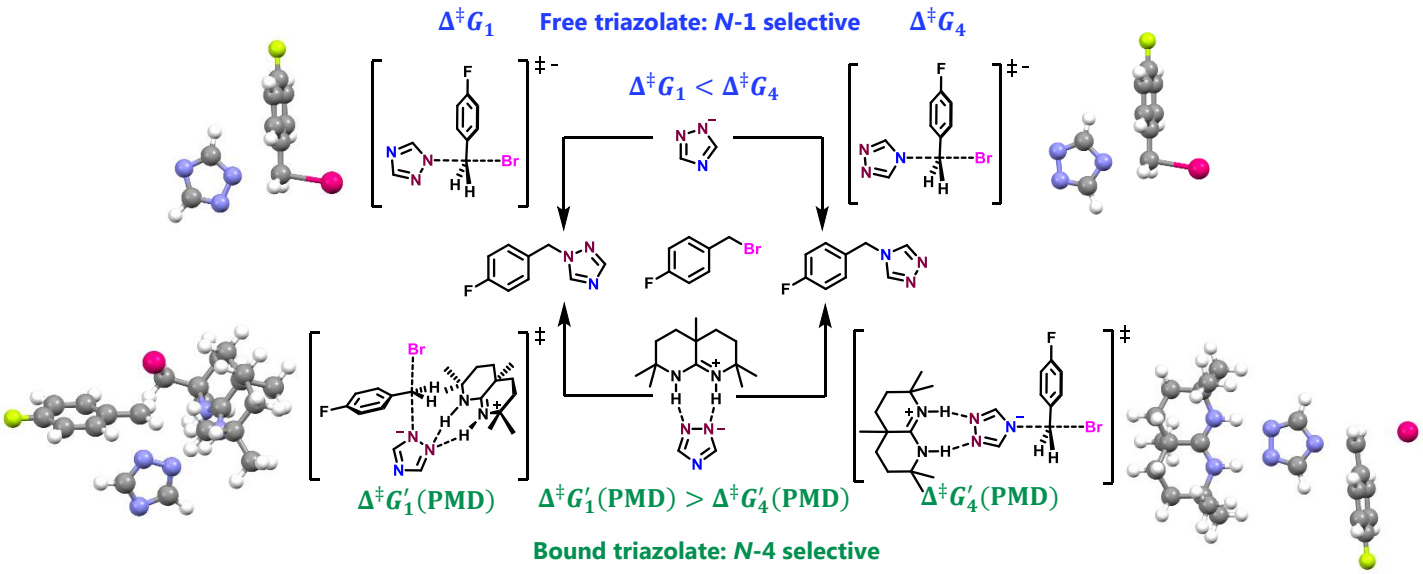


Figure S14a: Computed transition states for the *N*-benzylation of the 1,2,4-triazolate anion (free and bound to $PMDH^+$). $\Delta^{\ddagger}G_1$ = 82 kJ mol^{-1} and $\Delta^{\ddagger}G_4$ = 87 kJ mol^{-1} denote the free energies of activation for the *N*-benzylation of liberated 1,2,4-triazolate anions; $\Delta^{\ddagger}G'_1$ = 94 kJ mol^{-1} and $\Delta^{\ddagger}G'_4$ = 80 kJ mol^{-1} denote the free energy barriers for the bound anion. Free energies computed using a combined KS-DFT/DLPNO-CCSD(T) methodology and the ideal-gas rigid-rotor harmonic-oscillator approximation (f_S = 0.95). See below for for further computational details.

Figure S15: Full modelling results: PMD

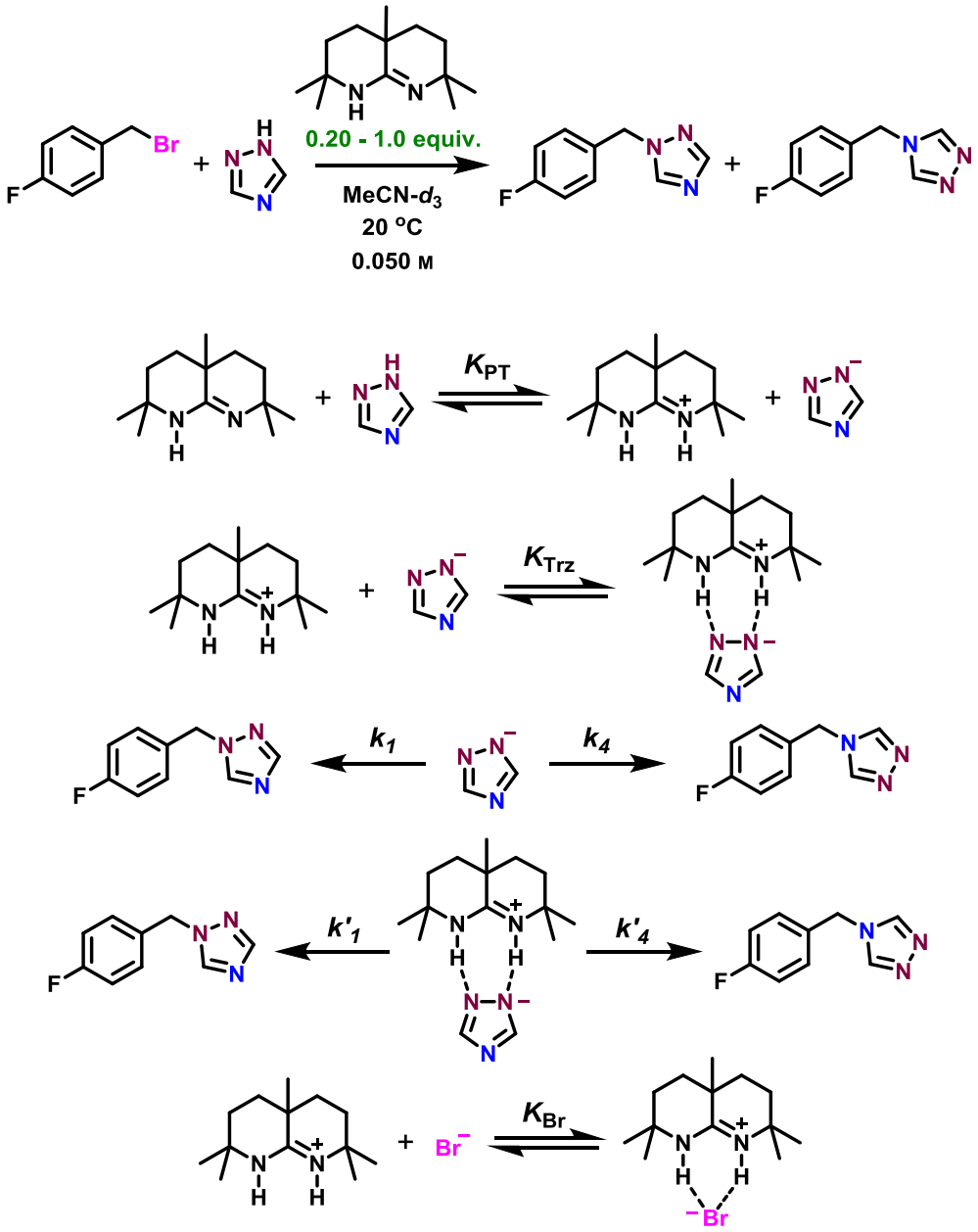


Figure S15a: Formal kinetic model (Model 1) for the *N*-benzylation of 1,2,4-triazole with *p*-F-BnBr and PMD in MeCN. In accordance with experimental pK_a data, the equilibrium constant for proton transfer K_{PT} >> 100. For Model 2 the binding constant for bromide was set to K_{Br} = 0

	Experiment		DLPNO-CCSD(T)	
	Model 1	**Model 2**	**IGRRHO**	**qRRHO**
k_1 / M^{-1} s^{-1}	0.30	0.30	-	-
k_4 / M^{-1} s^{-1}	0.044	0.044	**-**	**-**
$\Delta^{\ddagger}G_1$ / kJ mol^{-1}	74.7	74.7	81.1	87.6
$\Delta^{\ddagger}G_4$ / kJ mol^{-1}	79.4	79.4	86.5	92.4
$\Delta\Delta^{\ddagger}G$ / kJ mol^{-1}	4.7	4.7	5.4	4.8
k_1' / M^{-1} s^{-1}	0.00012	0.00073	-	-
k_4' / M^{-1} s^{-1}	0.0074	0.0074	-	-
$\Delta^{\ddagger}G_1(\mathrm{PMD})$ / kJ mol^{-1}	93.8	89.4	93.5	101.1
$\Delta^{\ddagger}G_4(\mathrm{PMD})$ / kJ mol^{-1}	83.7	83.7	80.0	90.9
$\Delta\Delta^{\ddagger}G(\mathrm{PMD})$ / kJ mol^{-1}	10.1	5.7	13.5	10.2
$\Delta\Delta^{\ddagger}G_1(\mathrm{PMD})$ / kJ mol^{-1}	19.1	14.7	12.4	13.5
$\Delta\Delta^{\ddagger}G_4(\mathrm{PMD})$ / kJ mol^{-1}	4.3	4.3	-6.5	-1.5
K_{Trz}	130,000	180,000	-	-
$\Delta_{\mathrm{Bind}}G_{\mathrm{Trz}}$ / kJ mol^{-1}	-28.7	-29.5	-35.9	-30.8
K_{Br}	74	-	-	-
$\Delta_{\mathrm{Bind}}G_{Br}$ / kJ mol^{-1}	-10.5	-	-27.8	-24.4
$\Delta\Delta_{\mathrm{Bind}}G(\mathrm{PMD})$ / kJ mol^{-1}	-18.2	-	-8.1	-6.4

Table S15b: Experimental rate coefficients and binding constants obtained from *in situ* ^{1}H NMR reaction monitoring (MeCN-d_3, 20 °C) and kinetic modelling. Equimolar concentraitons of *p*-F-BnBr (50.0 mM) and 1,2,4-triazole (50.0 mM) were used for all kinetic runs; [PMD] = 10.0 – 50.0 mM. The rate coefficients k_1 = 0.30 M^{-1} s^{-1} and k_4 = 0.044 M^{-1} s^{-1} were obtained from separate reaction monitoring experiments with MTBD. Experimental free energies of activation obtained in accordance with classical transition state theory, using the Eyring-Polanyi equation and a transmission coefficient of κ = 1. Experimental binding free energies calculated in accordance with classical thermodynamics. Theoretical free energies of activation and binding free energies computed using a combined KS-DFT/DLPNO-CCSD(T) methodology (*vide infra*) and the IEFPCM(MeCN,UFF) model. Theoretical free energy corrections were obtained in accordance with two separate statistical mechanical approximations: (i) the ideal-gas rigid-rotor harmonic-oscillator approximation (IGRRHO); and (ii) Grimme's quasi rigid-rotor harmonic-oscillator approximation (qRRHO). See below for further computational details.

Figure S16: 1,2,3-Triazoles

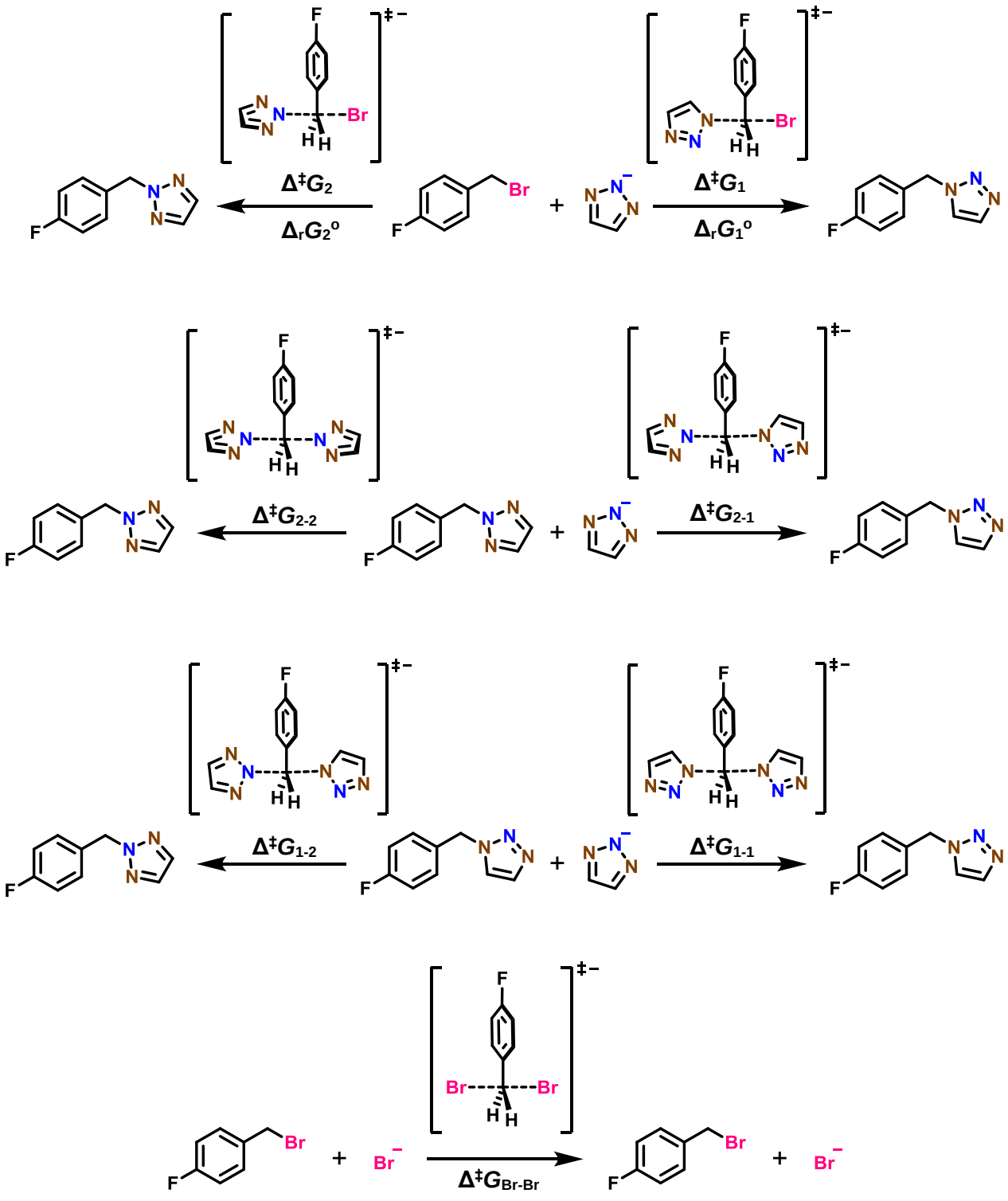


Figure S16a: Summary of key transition states and free energy changes for the *N*-benzylation of 1,2,3-triazolate with *p*-F-BnBr.

Free energy difference	kJ mol^{-1}
$\Delta^{\ddagger}G_1$	83.4
$\Delta^{\ddagger}G_2$	82.8
$\Delta^{\ddagger}G_{1\text{-}1}$	178.3
$\Delta^{\ddagger}G_{2\text{-}2}$	175.8
$\Delta^{\ddagger}G_{\text{Br-Br}}$	91.0

Table S16b: Computed free energies of activation for the *N*-benzylation of 1,2,3-triazolate with *p*-F-BnBr in MeCN. Free energies obtained using a combined KS-DFT/DLPNO-CCSD(T) methodology and the ideal-gas rigid-rotor harmonic-oscillator (IGRRHO) approximation (f_s = 0.95).

Free energy difference	***i* = 1**	***i* = 2**
$\Delta^{\ddagger}G_i^{\circ}$	134.6	133.4
$\Delta_r G_i$	-104.3	-112.8
$\boldsymbol{\Delta^{\ddagger}G_i^{M}}$	**87.5**	**83.0**
$\boldsymbol{\Delta^{\ddagger}G_i}$	***85.8***	***86.5***

Table S16c: Assorted kinetic and thermodynamic parameters for the N-benzylation of 1,2,3-triazolate with *p*-F-BnBr. Free energies obtained using a combined KS-DFT/DLPNO-CCSD(T) methodology and the ideal-gas rigid-rotor harmonic-oscillator (IGRRHO) approximation (f_s = 0.95).

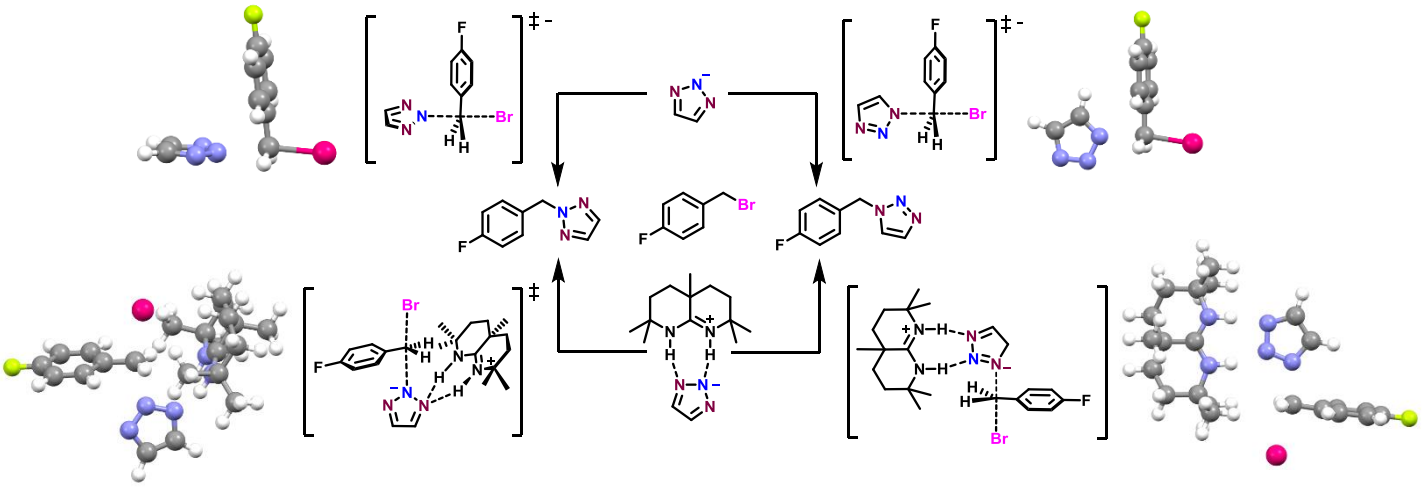
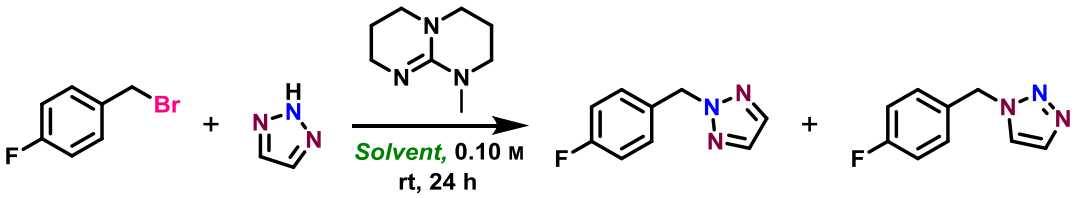


Figure S16d: Computed transition states for the *N*-benzylation of the 1,2,3-triazolate anion (free and bound to PMDH$^+$). $\Delta^{\ddagger}G_1$ = 83 kJ mol^{-1} and $\Delta^{\ddagger}G_2$ = 83 kJ mol^{-1} denote the free energies of activation for the *N*-benzylation of liberated 1,2,3-triazolate anions; $\Delta^{\ddagger}G'_1$ = 83 kJ mol^{-1} and $\Delta^{\ddagger}G_2$ = 93 kJ mol^{-1} denote the free energy barriers for the bound anion. Free energies computed using a combined KS-DFT/DLPNO-CCSD(T) methodology and the ideal-gas rigid-rotor harmonic-oscillator approximation (f_s = 0.95). See below for for further computational details.



	DMSO	MeOH	MeCN	Me_2CO	THF	CH_2Cl_2	$CHCl_3$
F_{N1} / %	67	67	68	69	77	77	80

Table S16e: Solvent dependence of regioselectivity in the *N*-benzylation of 1,2,3-triazole with *p*-F-BnBr in the presence of MTBD. Regioselectivities reported a the final mole fraction of the *N*-1 regioisomer, F_{N1} = $[N_1]/([N_1]+[N_2])$, after full consumption of *p*-F-BnBr. The increase in *N*-1 selectivity observed with non-polar chlorinated solvents mirrors the trend with 1,2,4-triazole: enhanced ion-pairing between MTBDH$^+$ and 1,2,3-triazolate in these solvents protects the two adjacent nitrogen atoms, promoting *N*-1 substitution.

Mathematical Proofs

Proof S1: Increasing [TBDH$^+$Trz$^-$]/[Trz$^-$]

For the ratio of bound to liberated 1,2,4-triazolate anions [TBDH$^+$Trz$^-$]/[Trz$^-$] to increase over time, the temporal derivative of the ratio of concentrations must remain positive under all conditions, such that:

$$\frac{d}{dt}\left(\frac{[\mathrm{TBDH^+Trz^-}]}{[\mathrm{Trz^-}]}\right) > 0 \quad [SE18]$$

By standard differential calculus and algebraic manipulation – and noting that the concentration of free 1,2,4-triazolate anions must decrease over the course of the reaction – it can be shown that condition [SE18] is equivalent to [SE23].

$$\frac{d}{dt}\left(\frac{[\mathrm{TBDH^+Trz^-}]}{[\mathrm{Trz^-}]}\right) = \frac{[\mathrm{Trz^-}]\frac{d[\mathrm{TBDH^+Trz^-}]}{dt} - [\mathrm{TBDH^+Trz^-}]\frac{d[\mathrm{Trz^-}]}{dt}}{[\mathrm{Trz^-}]^2} > 0 \quad [SE19]$$

$$[\mathrm{Trz^-}]\frac{d[\mathrm{TBDH^+Trz^-}]}{dt} - [\mathrm{TBDH^+Trz^-}]\frac{d[\mathrm{Trz^-}]}{dt} > 0 \quad [SE20]$$

$$\frac{1}{[\mathrm{TBDH^+Trz^-}]}\frac{d[\mathrm{TBDH^+Trz^-}]}{dt} > \frac{1}{[\mathrm{Trz^-}]}\frac{d[\mathrm{Trz^-}]}{dt} \quad [SE21]$$

$$\frac{d\ln[\mathrm{TBDH^+Trz^-}]}{dt} > \frac{d\ln[\mathrm{Trz^-}]}{dt} \quad [SE22]$$

$$\frac{\frac{d\ln[\mathrm{TBDH^+Trz^-}]}{dt}}{\frac{d\ln[\mathrm{Trz^-}]}{dt}} = \frac{d\ln[\mathrm{TBDH^+Trz^-}]}{d\ln[\mathrm{Trz^-}]} < 1 \quad [SE23]$$

At any point in time the equilibrium constant K_{Trz} for ion-pairing between the TBDH$^+$ cation and 1,2,4-triazolate anion is given by the expression:

$$K_{Trz} = \frac{[\mathrm{TBDH^+Trz^-}]}{[\mathrm{TBDH^+}][\mathrm{Trz^-}]} \quad [SE24]$$

The concentration of free $TBDH^+$ at any time, $[TBDH^+]$, is equal to the initial concentration $[TBDH]^+_0$ (i.e. $[TBD]_0$, a constant) *minus* the concentration of the ion-pair $[TBDH^+Trz^-]$, such that:

$$[\mathrm{TBDH^+}] = [\mathrm{TBDH^+}]_0 - [\mathrm{TBDH^+Trz^-}] \quad [SE25]$$

$$K_{Trz} = \frac{[\mathrm{TBDH^+Trz^-}]}{[\mathrm{Trz^-}]([\mathrm{TBDH^+}]_0 - [\mathrm{TBDH^+Trz^-}])} \quad [SE26]$$

$$K_{Trz}[\mathrm{Trz^-}][\mathrm{TBDH^+}]_0 - K_{Trz}[\mathrm{Trz^-}][\mathrm{TBDH^+Trz^-}] = [\mathrm{TBDH^+Trz^-}] \quad [SE27]$$

$$[\mathrm{TBDH^+Trz^-}] = \frac{K_{Trz}[\mathrm{Trz^-}][\mathrm{TBDH^+}]_0}{1 + K_{Trz}[\mathrm{Trz^-}]} \quad [SE28]$$

$$\ln[\mathrm{TBDH^+Trz^-}] = \ln[\mathrm{Trz^-}] + \ln K_{Trz}[\mathrm{TBDH^+}]_0 - \ln(1 + K_{Trz}[\mathrm{Trz^-}]) \quad [SE29]$$

Combining these results confirms that condition [SE23] – and by equivalence, the initial condition [SE18] – remains true for all values of *t* (that is, throughout the whole duration of the reaction):

$$\frac{d\ln[\mathrm{TBDH^+Trz^-}]}{d\ln[\mathrm{Trz^-}]} = 1 - \frac{d}{d\ln[\mathrm{Trz^-}]}\{\ln(1 + K_{Trz}[\mathrm{Trz^-}])\} \quad [SE30]$$

$$= 1 - \frac{d[\mathrm{Trz^-}]}{d\ln[\mathrm{Trz^-}]} \cdot \frac{d}{d[\mathrm{Trz^-}]}\{\ln(1 + K_{Trz}[\mathrm{Trz^-}])\} \quad [SE31]$$

$$= 1 - [\mathrm{Trz^-}]\frac{d}{d[\mathrm{Trz^-}]}\{\ln(1 + K_{Trz}[\mathrm{Trz^-}])\} \quad [SE32]$$

$$\frac{d\ln[\mathrm{TBDH^+Trz^-}]}{d\ln[\mathrm{Trz^-}]} = 1 - \frac{K_{Trz}[\mathrm{Trz^-}]}{1 + K_{Trz}[\mathrm{Trz^-}]} < 1 \quad [SE33]$$

Proof S2: S_1 and k_1'/k_4'

In the presence of TBD, the rate equations for the *N*-1 and *N*-4 benzylated regioisomers (N_1, N_4) each have two components: one for the *N*-benzylation of the free 1,2,4-triazolate anion (k_1, k_4), and one for the *N*-benzylation of the bound anion (k_1', k_4'):

$$\frac{d[\mathrm{N_1}]}{dt} = k_1[\mathrm{Trz^-}][\mathrm{pFBnBr}] + k_1'[\mathrm{TBDH^+Trz^-}][\mathrm{pFBnBr}] \quad [SE34]$$

$$\frac{d[N_4]}{dt} = k_4[\mathrm{Trz^-}][\mathrm{pFBnBr}] + k_4'[\mathrm{TBDH^+Trz^-}][\mathrm{pFBnBr}] \quad [SE35]$$

The instantaneous selectivity S_1 is defined as the fractional rate of *N*-1 substitution, such that:

$$S_1 = \frac{\frac{d[\mathrm{N_1}]}{dt}}{\frac{d[\mathrm{N_1}]}{dt} + \frac{d[\mathrm{N_4}]}{dt}} = \frac{k_1 + k_1'[\mathrm{TBDH^+Trz^-}]/[\mathrm{Trz^-}]}{k_1 + k_4 + (k_1' + k_4')[\mathrm{TBDH^+Trz^-}]/[\mathrm{Trz^-}]} \quad [SE36]$$

The derivative of S_1 with respect to *R,* the ratio of bound to free 1,2,4-triazolate, is given by:

$$S_1 = \frac{\frac{d[\mathrm{N_1}]}{dt}}{\frac{d[\mathrm{N_1}]}{dt} + \frac{d[\mathrm{N_4}]}{dt}} = \frac{k_1 + k_1'R}{k_1 + k_4 + (k_1' + k_4')R}, \qquad R = \frac{[\mathrm{TBDH^+Trz^-}]}{[\mathrm{Trz^-}]} \quad SE37]$$

$$\frac{dS_1}{dR} = \frac{\left[[k_1 + k_4 + (k_1' + k_4')R]k_1' - [k_1 + k_1'R](k_1' + k_4')\right]}{[k_1 + k_4 + (k_1' + k_4')\mathrm{R}]^2} \quad [SE38]$$

For S_1 to be a monotone decreasing function in *R* – that is, for *N*-1 selectivity to decrease as more of the remaining 1,2,4-triazolate becomes bound – it must be so that the derivative $dS_1/dR < 0$:

$$\frac{dS_1}{dR} < 0 \quad [SE39]$$

$$k_1k_1' + k_4k_1' + {k_1'}^2R + k_4'k_1'R - k_1k_1' - k_1k_4' - {k_1'}^2R - k_1'k_4'R < 0 \quad [SE40]$$

$$k_4k_1' - k_1k_4' < 0 \quad [SE41]$$

$$\frac{k_1'}{k_4'} < \frac{k_1}{k_4} \quad [SE42]$$

Given that *R* is a monotone increasing function in time and S_1 is a monotone decreasing function in *R* if $k_1'/k_4' < k_1/k_4$, S_1 must be a monotone decreasing function in time under conditions where substitution at the *N*-1 site of the anion is selectively inhibited by non-covalent interactions with the conjugate acid (i.e. regioselective ion-pairing). This conclusion is in accordance with experimental kinetics, which show that the mole fraction of the *N*-1 regioisomer decreases over time when TBD or PMD is used as the base.

Computational Details

General methodology

KS-DFT

Kohn-Sham density functional theory (KS-DFT) calculations were conducted with the *Gaussian09* (E.01) suite of programs.[9] *Ab initio* wavefunction-based calculations were carried out with the *Molpro* (2015.1)[8] (CCSD(T)-F12, DF-LCCSD(T)-F12) and *ORCA* (4.0.1)[10,11] (DLPNO-CCSD(T)) packages.

Optimised geometries and harmonic vibrational frequencies for all species were computed with restricted KS-DFT (RKS-DFT), using an ultrafine integration grid and tight optimisation criteria as implemented in *Gaussian09*. The hybrid variant of the Perdew-Burke-Ernzerhof functional [PBE0],[12] in combination with Grimme's D3 empirical dispersion correction [GD3BJ][13] and Becke-Johnson damping, was employed alongside a polarised triple-zeta basis set [6-311+G(d,p) (5d,7f)]. All optimised stationary points were characterised as minimum-energy structures or transition states in accordance with a harmonic frequency analysis. Single-point gas-phase potential energies $E^{(1)}_{(g)}$ were obtained at the optimisation level of theory [PBE0+GD3BJ/6-311+G(d,p)/Ultrafine/Tight], which is denoted **1**.

Molecular partition functions were first computed at T = 298.15 K (25.0 °C) and p = 1 atm (0.041 mol dm^{-3}), with all harmonic vibrational frequencies scaled by a linear factor [f_s = 0.95]. Gas-phase free energies $G^{(1)}_{(g)}$ at the optimisation level of theory **1,** corresponding to a standard state of 1 atm, were obtained from molecular partition functions in accordance with one of two statistical mechanical approximations: (i) the ideal-gas rigid-rotor harmonic-oscillator approximation [$G^{(1)}_{(g)}$(IGRRHO)], as implemented in *Gaussian09*; and (ii) the quasi rigid-rotor harmonic-oscillator approximation disclosed by Grimme[14] and implemented in *Python*,[15] in which the contributions to the vibrational entropy made by normal modes with frequencies below a cutoff of ω_c = 100 cm^{-1} were obtained from the free-rotor approximation [$G^{(1)}_{(g)}$(qRRHO)].

Solvated free energies $G_{(solv)}$ corresponding to a standard state of 1 mol dm^{-3} were obtained from a hybrid approach. For RKS-DFT methods [$G^{DFT}_{(solv)}$] separate, single-point calculations at a level of theory **2**, including implicit solvation, were conducted on the gas-phase optimised structures to obtain solvated potential energies $E^{(2)}_{(solv)}$. Solvated geometry optimisations were attempted, but in several structures this approach lead to multiple spurious low vibrational frequencies and thus artificial perturbations in the vibrational entropy. Benchmarking studies established that the integral equation formalism of the polarisable continuum model (IEFPCM(16)) in conjunction with universal force-field (UFF) radii offered the closest agreement with experimental kinetic data in MeCN.

Benchmarking work (*vide infra*) also suggested that Dunning's minimally-augmented quadruple-zeta basis set [spaug-cc-pVQZ] was more than sufficient to eliminate a large degree of systematic error arising from basis-set incompleteness. Thus, level **2** corresponds to [PBE0+GD3BJ/spaug-cc-pvQZ/IEFPCM(UFF)/Ultrafine].

$$\boldsymbol{G}^{\boldsymbol{DFT}}_{(\boldsymbol{solv})}(\boldsymbol{IGRRHO}) = E^{(\mathbf{2})}_{(solv)} + \left[G^{(\mathbf{1})}_{(g)}(IGRRHO) - E^{(\mathbf{1})}_{(g)}\right] + RT\ln\left(\frac{1\ \mathrm{mol\ dm^{-3}}}{0.041\ \mathrm{mol\ dm^{-3}}}\right) \quad [SE43]$$

$$\boldsymbol{G}^{\boldsymbol{DFT}}_{(\boldsymbol{solv})}(\boldsymbol{qRRHO}) = E^{(\mathbf{2})}_{(solv)} + \left[G^{(\mathbf{1})}_{(g)}(qRRHO) - E^{(\mathbf{1})}_{(g)}\right] + RT\ln\left(\frac{1\ \mathrm{mol\ dm^{-3}}}{0.041\ \mathrm{mol\ dm^{-3}}}\right) \quad [SE44]$$

Coupled-cluster computations

For *ab-initio* wavefunction-based methods (CCSD(T)-F12, DF-LCCSD(T)-F12, DLPNO-CCSD(T)), the approach adopted to compute $G^{\mathbf{WF}}_{(\mathrm{solv})}$ was slightly different. As before, gas-phase RKS-DFT optimised structures were used. However, two further single-point calculations were then carried out on each structure. First, the solvated potential energy of each structure was recomputed with RKS-DFT using the optimisation level of theory **1**, with the *sole addition* of implicit solvation to the method; this energy is denoted $E^{(\mathbf{1})}_{(solv)}$, such that $E^{(\mathbf{1})}_{(\mathrm{solv})} - E^{(\mathbf{1})}_{(\mathrm{g})}$ approximates the solvation energy of a given species. Secondly, the gas-phase potential energy $E^{(\mathbf{3})}_{(\mathrm{g})}$ of each optimised structure was computed using a given wavefunction-based method (denoted **3**). With these energies in hand, the solvated free energies $G^{\mathbf{WF}}_{(\mathrm{solv})}$(IGRRHO) and $G^{\mathbf{WF}}_{(\mathrm{solv})}$(qRRHO) were obtained from:

$$\boldsymbol{G}^{\boldsymbol{WF}}_{(\boldsymbol{solv})}(\boldsymbol{IGRRHO}) = E^{(3)}_{(g)} + \left[E^{(1)}_{(solv)} - E^{(1)}_{(g)}\right] + \left[G^{(1)}_{(g)}(IGRRHO) - E^{(1)}_{(g)}\right] + RT\ln\left(\frac{1\ \mathrm{mol\ dm^{-3}}}{0.041\ \mathrm{mol\ dm^{-3}}}\right) \quad [SE45]$$

$$\boldsymbol{G}^{\boldsymbol{WF}}_{(\boldsymbol{solv})}(\boldsymbol{qRRHO}) = E^{(3)}_{(g)} + \left[E^{(1)}_{(solv)} - E^{(1)}_{(g)}\right] + \left[G^{(1)}_{(g)}(qRRHO) - E^{(1)}_{(g)}\right] + RT\ln\left(\frac{1\ \mathrm{mol\ dm^{-3}}}{0.041\ \mathrm{mol\ dm^{-3}}}\right) \quad [SE46]$$

CCSD(T)-F12 *(Molpro 2015.1)*

Canonical CCSD(T)-F12[17,18] energies were computed using the 3C(FIX) wavefunction ansatz and the specially optimised correlation consistent cc-pVDZ-F12[19] basis set for all atoms except bromine, for which the def2-TZVPP basis was applied. With the exception of bromine, the optimised CABS basis set of Peterson was used for the resolution of identity (RI), the aug-cc-pVDZ basis for density fitting (DF) and the cc-pVDZ basis for density fitting in the calculation of the Fock and exchange operators (JK); for bromine the def2-TZVPP (RI, JK) def2-ATZVPP (DF) basis sets were employed instead. Unless specified otherwise, default options were used throughout and all energies correspond to the CCSD(T)-F12b approximation.

```
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ANGSTROM
C,      0.2533850000,      0.8465700000,      0.0000010000,
Br,     2.5260270000,      1.4223380000,     -0.0000030000,
C,     -3.9048280000,      1.5025180000,      0.0000070000,
C,     -2.8371160000,     -0.2759410000,     -0.0000050000,
N,     -1.9443860000,      0.7136270000,     -0.0000020000,
N,     -4.1025170000,      0.1671350000,      0.0000010000,
N,     -2.6288090000,      1.8750640000,      0.0000060000,
H,     -4.7138260000,      2.2233590000,      0.0000130000,
H,     -2.5494660000,     -1.3195470000,     -0.0000110000,
H,      0.3748530000,     -0.7775850000,     -2.1364600000,
C,      0.4088950000,     -1.3258220000,     -1.2007450000,
C,      0.4816780000,     -2.7112720000,     -1.2020120000,
H,      0.5045600000,     -3.2489470000,     -2.1450760000,
C,      0.5184450000,     -3.4115680000,      0.0000010000,
H,      0.5716780000,     -4.4959560000,      0.0000020000,
C,      0.4816990000,     -2.7112700000,      1.2020150000,
H,      0.5045980000,     -3.2489430000,      2.1450790000,
C,      0.4089160000,     -1.3258200000,      1.2007470000,
H,      0.3748920000,     -0.7775820000,      2.1364610000,
C,      0.3729390000,     -0.6167170000,      0.0000000000,
H,      0.0738290000,      1.3742650000,     -0.9196560000,
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hf

basis={
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set,df
default=avdz/mp2fit,Br=def2-atzvpp/mp2fit
set,jk
default=vdz/jkfit,Br=def2-tzvpp/jkfit
set,rib
default=vdz-f12/optri,Br=def2-tzvpp/jkfit
}

ccsd(t)-f12,df_basis=df,df_basis_exch=jk,ri_basis=rib,ansatz=3C(FIX)
```

DF-LCCSD(T)-F12 *(Molpro 2015.1)*

Local DF-LCCSD(T)-F12[20] energies were computed using the 3*A(LOC) wavefunction ansatz and the specially optimised correlation consistent cc-pVDZ-F12 basis set for all atoms except bromine, for which the def2-TZVPP basis was applied. A similar combination of auxiliary basis sets were used as for CCSD(T)-F12 calculations. Valence orbitals were localised using the default Pipek-Mizey procedure, with the orbital domains determined in accordance with the method of Boughton and Pulay with a completeness criterion of 0.980. Localisation was improved by removing the contribution of the two most diffuse basis functions for each angular momentum type. Unless specified otherwise, default options were used throughout and all energies correspond to the DF-LCCSD(T)-F12b approximation.

```
memory,750,M
gdirect ! direct integral evaluations
symmetry,nosym,noorient ! recommended for local calculations

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ANGSTROM
C,      0.2533850000,      0.8465700000,      0.0000010000,
Br,     2.5260270000,      1.4223380000,     -0.0000030000,
C,     -3.9048280000,      1.5025180000,      0.0000070000,
C,     -2.8371160000,     -0.2759410000,     -0.0000050000,
N,     -1.9443860000,      0.7136270000,     -0.0000020000,
N,     -4.1025170000,      0.1671350000,      0.0000010000,
N,     -2.6288090000,      1.8750640000,      0.0000060000,
H,     -4.7138260000,      2.2233590000,      0.0000130000,
H,     -2.5494660000,     -1.3195470000,     -0.0000110000,
H,      0.3748530000,     -0.7775850000,     -2.1364600000,
C,      0.4088950000,     -1.3258220000,     -1.2007450000,
C,      0.4816780000,     -2.7112720000,     -1.2020120000,
H,      0.5045600000,     -3.2489470000,     -2.1450760000,
C,      0.5184450000,     -3.4115680000,      0.0000010000,
H,      0.5716780000,     -4.4959560000,      0.0000020000,
C,      0.4816990000,     -2.7112700000,      1.2020150000,
H,      0.5045980000,     -3.2489430000,      2.1450790000,
C,      0.4089160000,     -1.3258200000,      1.2007470000,
H,      0.3748920000,     -0.7775820000,      2.1364610000,
C,      0.3729390000,     -0.6167170000,      0.0000000000,
H,      0.0738290000,      1.3742650000,     -0.9196560000,
H,      0.0738310000,      1.3742620000,      0.9196600000,
}

set,charge=-1

basis=vdz-f12,Br=def2-tzvpp
hf

basis={
default=vdz-f12,Br=def2-tzvpp
set,hf
default=avdz/jkfit,Br=def2-atzvpp/jkfit
set,df
default=avdz/mp2fit,Br=def2-atzvpp/mp2fit
set,jk
default=vdz/jkfit,Br=def2-tzvpp/jkfit
set,rib
default=vdz-f12/optri,Br=def2-tzvpp/jkfit
}

df-hf,df_basis=hf
locali,pipek;pipek,delete=2
df-lccsd(t)-f12,df_basis=df,df_basis_exch=jk,ri_basis=rib,ansatz=3*A(loc)
```

DLPNO-CCSD(T) ***(ORCA 4.0.1)***

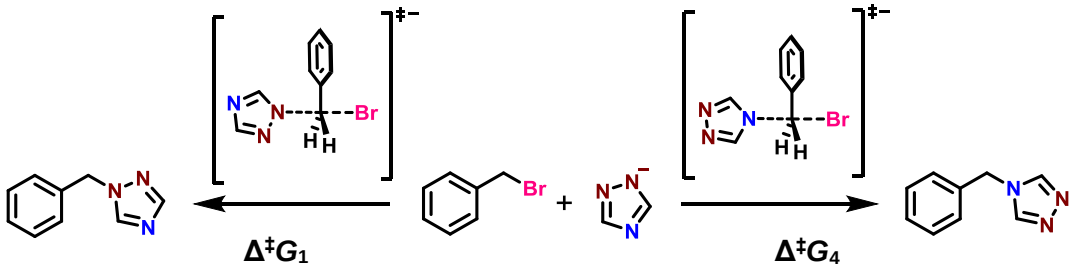
Domain-based local pair natural orbital coupled-cluster (DLPNO-CCSD(T)[21-24] computations were conducted with the minimally augmented Karlsruhe basis set ma-def2-TZVPP,[25] with the unaugmented version of this basis (def2-TZVPP) employed for the resolution of identity approximation. In accordance with the standard defintions in ORCA 4.0, tight SCF convergence criteria and PNO theshholds were imposed for all calculations ($T_{CutPairs} = 10^{-5}$, $T_{CutDO} = 5 \times 10^{-3}$, $T_{CutPNO} = 10^{-7}$, $T_{CutMKN} = 10^{-3}$), with the MP2 part of the calculation treated in a fully iterative manner (DLPNO-MP2). All Local Energy Decomposition calculations (DLPNO-CCSD(T)-LED) were carried out with the same basis sets and settings.

```
! DLPNO-CCSD(T) ma-def2-tzvpp def2-tzvpp/C TIGHTSCF TightPNO PAL4
%maxcore 3684
*xyz -1 1
C       0.2533850000     0.8465700000     0.0000010000
Br      2.5260270000     1.4223380000    -0.0000030000
C      -3.9048280000     1.5025180000     0.0000070000
C      -2.8371160000    -0.2759410000    -0.0000050000
N      -1.9443860000     0.7136270000    -0.0000020000
N      -4.1025170000     0.1671350000     0.0000010000
N      -2.6288090000     1.8750640000     0.0000060000
H      -4.7138260000     2.2233590000     0.0000130000
H      -2.5494660000    -1.3195470000    -0.0000110000
H       0.3748530000    -0.7775850000    -2.1364600000
C       0.4088950000    -1.3258220000    -1.2007450000
C       0.4816780000    -2.7112720000    -1.2020120000
H       0.5045600000    -3.2489470000    -2.1450760000
C       0.5184450000    -3.4115680000     0.0000010000
H       0.5716780000    -4.4959560000     0.0000020000
C       0.4816990000    -2.7112700000     1.2020150000
H       0.5045980000    -3.2489430000     2.1450790000
C       0.4089160000    -1.3258200000     1.2007470000
H       0.3748920000    -0.7775820000     2.1364610000
C       0.3729390000    -0.6167170000     0.0000000000
H       0.0738290000     1.3742650000    -0.9196560000
H       0.0738310000     1.3742620000     0.9196600000
*
```

Benchmarking

General considerations

In the early stages of the project, benchmarking calculations were conducted with various electronic structure methods, continuum solvation treatments and statistical mechanics appoximations in pursuit of a robust computational methodology. To this end, the *N*-benzylation (BnBr) of the 1,2,4-triazolate anion was selected as a model reaction. Computational methodologies were judged on their ability to reproduce the experimentally observed regioselectivity F_{N1} = 87 % and the experimental free energies of activation $\Delta^{\ddagger}G_1$ = 74.7 kJ mol^{-1} (k_1 = 0.30 dm^3 mol^{-1} s^{-1}) and $\Delta^{\ddagger}G_4$ = 79.4 kJ mol^{-1} (k_1 = 0.044 dm^3 mol^{-1} s^{-1}), as determined from kinetic modelling studies with 1,2,4-triazole, *p*-F-BnBr and MTBD (10.0 mM, MeCN-d_3, 20°C). Although changes in the *para*-substitutent and structure of the organic base (i.e. P$_1$-^{t}Bu vs MTBD) led to experimentally observable perturbations in the rate of substitution, in terms of free energies of activation these perturbations were very small, and in any case easily fall within the error typically associated with chemical accuracy (< 4 kJ mol^{-1}).



$$F_{N_1} = \frac{k_1}{k_1 + k_4} = \frac{e^{-\frac{\Delta^{\ddagger}G_1}{RT}}}{e^{-\frac{\Delta^{\ddagger}G_1}{RT}} + e^{-\frac{\Delta^{\ddagger}G_4}{RT}}} = \frac{e^{\left(\frac{\Delta^{\ddagger}G_4 - \Delta^{\ddagger}G_1}{RT}\right)}}{e^{\left(\frac{\Delta^{\ddagger}G_4 - \Delta^{\ddagger}G_1}{RT}\right)} + 1} = \frac{e^{\left(\frac{\Delta\Delta^{\ddagger}G}{RT}\right)}}{e^{\left(\frac{\Delta\Delta^{\ddagger}G}{RT}\right)} + 1} \quad [SE47]$$

To account for the anionic nature of the model reaction, throughout all calculations atomic orbital basis sets were either augmented with diffuse functions (e.g. aug-cc-pVTZ, spaug-cc-pVQZ, ma-def2-TZVPP) or specially optimised for explicitly correlated methodologies (e.g. cc-pVDZ-F12). Extensive basis set benchmarking was not carried out: instead, for each electronic structure method the largest feasible basis set was used, taking into account time/resource constraints and the prospect of needing to extend the method to larger systems (> 50 atoms).

Vibrational entropies and solvation

To identify an appropriate continuum solvation model and statistical mechanical treatment of vibrational entropies, $\Delta^{\ddagger}G_1$, $\Delta^{\ddagger}G_4$ and F_{N1} were computed using the highly correlated CCSD(T)-F12 method (see above for basis sets and details). This approach was pursued to obtain highly accurate gas-phase potential energies and thereby avoid fortuitous error cancellations that might arise when comparing solvation/vibrational entropy treatments using less robust electronic structure theories.

For all combinations of solvent models and statistical mechanical approximations the computed free energies of activation were found to *overestimate* the experimental values. Nevertheless, chemical accuracy was attained by invoking a combination of: (i) the integral equation formalism of the polarisable continuum model (IEFPCM, MeCN, UFF radii) for solvation; and (ii) the standard ideal-gas rigid-rotor harmonic-oscillator (IGRRHO) approximation with linearly scaled harmonic frequencies for vibrational entropies (f_s = 0.95).

Method	$\Delta^{\ddagger}G_1$ / kJ mol^{-1}	$\Delta^{\ddagger}G_4$ / kJ mol^{-1}	$\Delta\Delta^{\ddagger}G$ / kJ mol^{-1}	F_{N1} / %
CCSD(T)-F12/IEFPCM/IGRRHO	**77.0**	**81.6**	**4.6**	**87**
CCSD(T)-F12/SMD/IGRRHO	92.7	98.8	6.1	92
CCSD(T)-F12/IEFPCM/IGRRHO(f_s = 1)	77.6	82.2	4.6	86
CCSD(T)-F12/IEFPCM/qRRHO	83.4	87.5	4.1	84
Exp.	***74.7***	***79.4***	***4.7***	***87***

Using unscaled harmonic frequencies (f_s = 1) had a very minor effect on the individual free energies of activation (< 1 kJ mol^{-1}) and a negligible effect on the computed selectivity, but ultimately led to slightly poorer agreement with experiment. Whilst the quasi rigid-rotor harmonic-oscillator (qRRHO) approximation proposed by Grimme also afforded a favourable description of the kinetic selectivity, invoking the free-rotor approximation to treat small vibrational frequencies (< 100 cm^{-1}) lead to more significant deviations from experiment in the individual free energies of activation $\Delta^{\ddagger}G_1$ and $\Delta^{\ddagger}G_4$. In contrast, the SMD solvation model of Cramer and Truhlar[26,27] significantly overestimated both $\Delta^{\ddagger}G_1$ and $\Delta^{\ddagger}G_4$ (> 15 kJ mol^{-1}), seemingly due to overly enthusiastic solvation of the free 1,2,4-triazolate anion.

Electronic structure theories

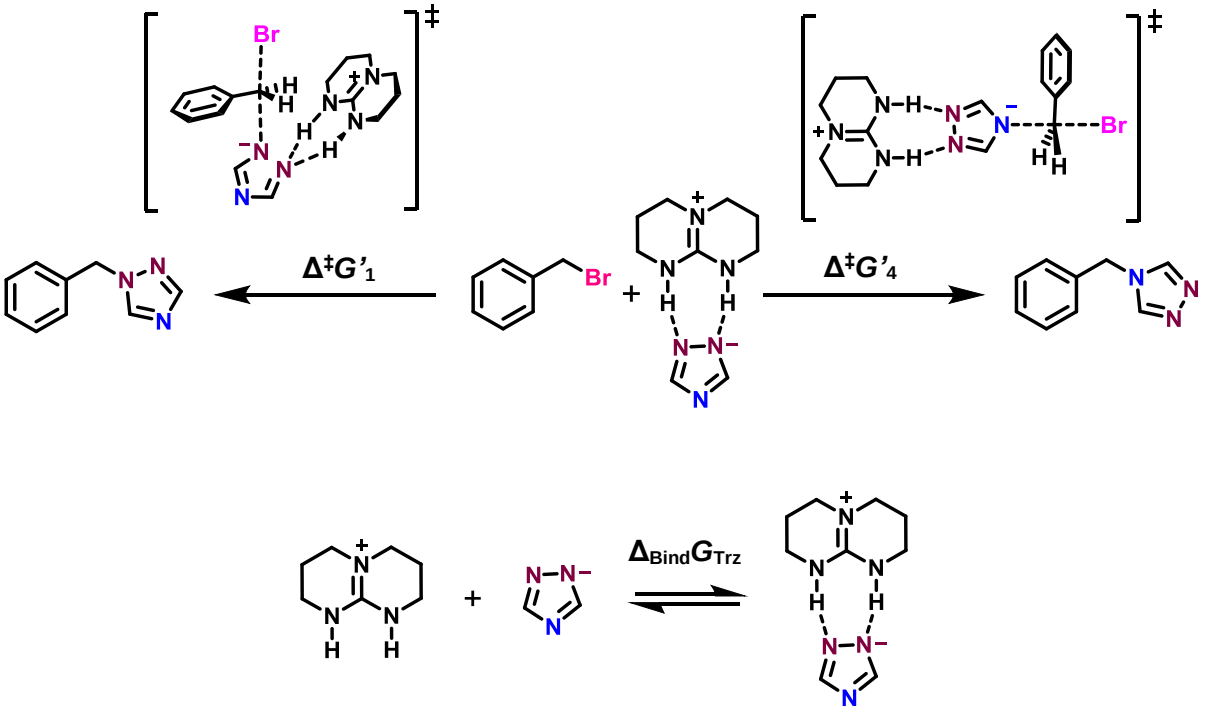
Although highly accurate gas-phase potential energies can be computed using the CCSD(T)-F12 method, this approach becomes impracticable for larger molecular systems. Having established that the IGRRHO approximation and IEFPCM solvation model offer the best description of the three kinetic parameters $\Delta^{\ddagger}G_1$, $\Delta^{\ddagger}G_4$ and F_{N1}, a range of alternative, more efficient electronic structure theories were therefore tested. These included: (i) local implementations of coupled-cluster theory with (DF-LCCSD(T)-F12) and without (DLPNO-CCSD(T)) explicit correlation; (ii) second-order Møller-Plesset perturbation theory (MP2) and the spin-component scaled variant (SCS-MP2),[28] and their various local and explicitly correlated implementations (e.g. MP2-F12, DF-LMP2-F12, DF-SCS-LMP2-F12; and (iii) a double-hybrid KS-DFT functional (B2PLYPD3).[29] In all cases, optimised geometries, harmonic frequencies, free energy corrections (IGRRHO) and solvation energies (IEFPCM(MeCN,UFF)) were computed as outlined above.

Method (IEFPCM, IGRRHO)	**$\Delta^{\ddagger}G_1$ / kJ mol^{-1}**	**$\Delta^{\ddagger}G_4$ / kJ mol^{-1}**	**$\Delta\Delta^{\ddagger}G$ / kJ mol^{-1}**	**F_{N1} / %**
CCSD(T)-F12/cc-pVDZ-F12	**76.9**	**81.6**	**4.7**	**87**
DF-LCCSD(T)-F12/cc-pVDZ-F12	**79.6**	**84.8**	**5.2**	**89**
DLPNO-CCSD(T)/ma-def2-TZVPP	**80.9**	**86.2**	**5.3**	**89**
MP2-F12/cc-pVDZ-F12	76.3	83.3	7.0	94
SCS-MP2-F12/cc-pVDZ-F12	86.1	92.3	6.2	92
DF-LMP2/aug-pVTZ	81.0	87.6	6.6	93
DF-SCS-LMP2/aug-pVTZ	90.6	96.4	5.8	91
DF-LMP2-F12/cc-pVDZ-F12	79.2	85.6	6.4	93
DF-SCS-LMP2-F12/cc-pVDZ-F12	88.5	94.1	5.6	91
PBE0+GD3BJ/6-311+G(d,p)	61.9	67.3	5.4	90
PBE0+GD3BJ/spaug-cc-pVQZ	**67.9**	**72.9**	**5.0**	**88**
B2PLYPD3/spaug-cc-pVQZ	84.8	87.6	2.8	75
Exp	***74.7***	***79.4***	***4.7***	***87***

As might be expected, all electronic structure methods offered poorer agreement with experiment than the CCSD(T)-F12 benchmark. Correspondence with experiment was closest for DF-LCCSD(T)-F12 and DLPNO-CCSD(T), although reasonable agreement was also reached with PBE0+GD3BJ, provided and an enlarged basis set (spaug-cc-pVQZ) was employed; presumably the improvement in performance in the latter case is due to a significant reduction in basis set superposition error. All implementations of MP2 theory overestimated the N-1 selectivity, whilst the double-hybrid functional B2PLYPD3 significantly underestimated it. The spin-component scaled variant SCS-MP2 offered a poor performance on all fronts.

Ion-pairing benchmark

To distinguish DF-LCCSD(T)-F12, DLPNO-CCSD(T) and dispersion-corrected KS-DFT (PBE0+GD3BJ/spaug-cc-pVQZ), all three methods were challenged with a more difficult experimental benchmark: reproducing the binding free energy of 1,2,4-triazolate and TBDH$^+$ ($\Delta_{Bind}G_{Trz}$), the free energies of activation for the *N*-benzylation of bound 1,2,4-triazolate ($\Delta^{\ddagger}G'_1$, $\Delta^{\ddagger}G'_4$) and the kinetic selectivity of the TBDH$^+$Trz$^-$ ion pair ($\Delta\Delta^{\ddagger}G = \Delta^{\ddagger}G'_4 - \Delta^{\ddagger}G'_1$). Experimental values of $\Delta_{Bind}G_{Trz}$ = -22.4 kJ mol^{-1} (K_{Trz} = 9,800), $\Delta^{\ddagger}G'_1$ = 85.5 kJ mol^{-1} (k'_1 = 0.0035 dm^3 mol^{-1} s^{-1}), $\Delta^{\ddagger}G'_4$ = 82.3 kJ mol^{-1} (k'_4 = 0.013 dm^3 mol^{-1} s^{-1}) and $\Delta\Delta^{\ddagger}G$ = -3.2 kJ mol^{-1} were determined from kinetic modelling studies with 1,2,4-triazole, *p*-F-BnBr and TBD (10.0 mM, MeCN-d_3, 20°C). In all cases, optimised geometries, harmonic frequencies, free energy corrections and solvation energies (IEFPCM(MeCN,UFF)) were computed as outlined above.



Reproducing all of these parameters poses a more challenging task for an electronic structure method, for in addition to describing the formation and cleavage of two covalent bonds it must also be able to accurately account for the stabilisation afforded by myriad *non-covalent* interactions, including contributions from ion-pairing, hydrogen bonding, and London dispersion interactions.

Pleasingly, DLPNO-CCSD(T)-F12/IGRRHO was able to reproduce all four parameters $\Delta_{Bind}G_{Trz}$, $\Delta^{\ddagger}G'_1$, $\Delta^{\ddagger}G'_4$ and $\Delta\Delta^{\ddagger}G$ to within chemical accuracy (< 4 kJ mol^{-1}). Whilst DF-LCCSD(T)-F12/IGRRHO was also able to predict the binding free energy $\Delta_{Bind}G_{Trz}$ with near quantitative accuracy, it failed to reproduce $\Delta^{\ddagger}G'_4$ and thereby $\Delta\Delta^{\ddagger}G$ to the same level of accuracy. Unlike the coupled-cluster theories, KS-DFT (PBE0+GD3BJ) fails badly in every respect, for it significantly overbinds the two ionic fragments and grossly overestimates the *N*-4 selectivity of the ion-pair. Indeed, according to the KS-DFT results 1,2,4-triazolate and $TBDH^+$ should be completely bound in MeCN, and the $TBDH^+Trz^-$ ion-pair exclusively selective towards *N*-4 benzylation, contrary to experimental findings.

Method	$\Delta_{Bind}G_{Trz}$ / kJ mol^{-1}	$\Delta^{\ddagger}G'_1$ / kJ mol^{-1}	$\Delta^{\ddagger}G'_4$ / kJ mol^{-1}	$\Delta\Delta^{\ddagger}G'$ / kJ mol^{-1}
DLPNO-CCSD(T)/IGRRHO	**-22.0**	**87.6**	**80.8**	**-6.8**
DLPNO-CCSD(T)/qRRHO	**-18.0**	**96.1**	**90.8**	**-5.3**
DF-LCCSD(T)-F12/IGRRHO	-21.1	87.7	77.1	-10.6
DF-LCCSD(T)-F12/qRRHO	-17.1	96.1	87.1	-9.0
PBE0+GD3BJ/IGRRHO	-34.3	87.1	67.3	-19.8
PBE0+GD3BJ/qRRHO	-30.3	95.6	77.4	-18.2
Exp (Model 1)	***-22.4***	***85.5***	***82.3***	***-3.2***

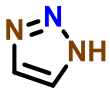
KS-DFT Optimised Structures

Optimised structures obtained at the PBE0+GD3BJ/6-311+G(d,p)/Ultrafine/Tight level of theory (Gaussian09). Potential energies (E), enthalpies (H) and Gibbs free energies (G) quoted in Hartree. Cartesian atomic coordinates (x,y,z) reported in Å.

Triazoles

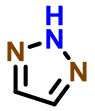
E = -241.463277
H = -241.413138
G = -241.443521

C	1.11038	0.26198	0.00004
N	-1.09435	0.27477	-0.00003
N	0.68064	-1.01592	-0.00002
H	2.16471	0.50965	0.00007
H	-0.10057	2.15685	0.00006
N	-0.64874	-0.97827	-0.00003
C	-0.01116	1.07751	0.00003



E = -242.022375
H = -241.958138
G = -241.988783

C	1.08140	0.27080	0.00003
N	-1.05238	0.28686	-0.00002
N	0.62051	-1.00672	-0.00001
H	2.13620	0.49356	0.00007
H	-0.08637	2.19582	0.00006
H	-2.03516	0.50857	-0.00004
N	-0.67139	-0.99280	-0.00005
C	0.00718	1.12257	0.00003



E = -242.030301
H = -241.96532
G = -241.995893

C	1.10910	0.24531	0.00003
N	-1.10624	0.28788	-0.00002
N	0.71323	-1.02357	-0.00001
H	2.15692	0.50129	0.00007
H	-0.11610	2.13964	0.00006
N	-0.59917	-0.92649	-0.00004
C	-0.02763	1.06465	0.00003
H	-1.18818	-1.74367	-0.00008

E = -241.487494
H = -241.436634
G = -241.466936

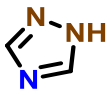
C	1.03174	0.26633	0.00003
C	-1.03181	0.26610	-0.00002
N	0.68085	-1.01790	-0.00001
H	2.07090	0.58053	0.00006
H	-2.07103	0.58006	-0.00004
N	-0.68062	-1.01805	-0.00005
N	-0.00013	1.13396	0.00003

E = -242.03842

H = -241.97422

G = -242.004927

C	-0.35086	-0.98425	0.00003
C	1.38629	0.28887	-0.00002
N	-0.76859	0.25015	-0.00001
H	-0.97539	-1.86448	0.00007
H	1.60490	-1.83115	0.00006
H	2.41373	0.61933	-0.00004
N	0.33499	1.05894	-0.00005
N	1.00992	-1.01931	0.00003



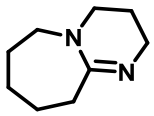
E = -242.050014

H = -241.985027

G = -242.015613

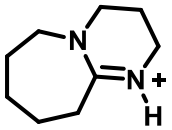
C	-0.31913	-1.01056	0.00005
C	1.32028	0.28134	-0.00002
N	-0.74728	0.26365	0.00001
H	-0.98128	-1.86406	0.00009
H	2.33871	0.64047	-0.00004
N	0.29519	1.10971	-0.00003
N	0.99532	-1.03659	0.00003
H	-1.68802	0.62282	0.00001

Organic bases



E = -461.681018
H = -461.423703
G = -461.469691

H	1.86240	-0.19466	2.45844
C	1.44662	-0.31068	1.45727
H	1.52200	-1.38070	1.22571
C	-0.01086	0.13443	1.40789
H	-0.49105	-0.07251	2.36894
H	-0.04957	1.22270	1.27995
C	-0.78554	-0.55322	0.28817
H	-1.71900	-0.01247	0.09383
H	-1.07200	-1.56394	0.60110
C	0.03462	-0.64345	-0.99425
H	0.77531	-1.44725	-0.92723
H	-0.62108	-0.90570	-1.83072
C	0.74900	0.64908	-1.34963
H	1.00774	0.61547	-2.41561
H	0.05651	1.49987	-1.23349
N	1.99677	0.92621	-0.65326
C	2.40971	0.45381	0.57466
N	3.58511	0.62138	1.06631
C	4.55330	1.32054	0.25449
C	2.80187	1.91065	-1.36480
C	3.90574	2.47188	-0.49534
H	5.01385	0.62584	-0.46620
H	5.35946	1.67635	0.90263
H	4.62250	3.01887	-1.11485
H	3.48879	3.17600	0.23289
H	3.22385	1.44615	-2.26848
H	2.13648	2.71620	-1.70390

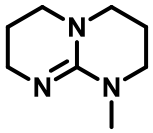


E = -462.099086

H = -461.826581

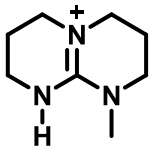
G = -461.872433

H	1.83593	-0.04583	2.51015
C	1.44417	-0.21086	1.50273
H	1.58229	-1.27958	1.29829
C	-0.03571	0.16171	1.45532
H	-0.48395	-0.07577	2.42263
H	-0.13026	1.24745	1.34279
C	-0.78112	-0.56437	0.34197
H	-1.74004	-0.06797	0.16608
H	-1.01576	-1.58659	0.65448
C	0.02591	-0.61253	-0.94999
H	0.78642	-1.40077	-0.91640
H	-0.62973	-0.87715	-1.78387
C	0.69630	0.70146	-1.30467
H	0.95599	0.69296	-2.36603
H	0.02017	1.55055	-1.14952
N	1.97149	0.99533	-0.61820
C	2.33787	0.56221	0.57273
N	3.56179	0.80569	1.03148
C	4.59154	1.53547	0.30662
C	2.86080	1.84990	-1.42260
C	3.90175	2.55107	-0.57868
H	5.19477	0.83724	-0.28338
H	5.24565	2.01348	1.03688
H	4.62391	3.04551	-1.23037
H	3.43073	3.32061	0.04009
H	3.32555	1.22527	-2.19369
H	2.22498	2.57971	-1.92903
H	3.76936	0.47209	1.95943



E = -477.716874
H = -477.471625
G = -477.518766

H	-2.49821	0.44614	-1.42627
H	2.59884	-0.56058	-1.35363
H	1.48382	1.84183	-0.98671
H	-1.10573	2.28464	-0.68725
H	-0.32926	-3.27456	-0.44643
H	-2.09964	-3.25770	-0.20855
C	-2.43567	0.62124	-0.34785
C	2.37936	-0.76680	-0.29282
N	0.00765	0.62735	-0.12625
N	1.12456	-1.46263	-0.16476
C	0.05177	-0.75420	-0.11530
C	1.23609	1.39523	-0.01229
N	-1.17049	-1.41063	-0.09403
C	-1.14623	-2.83832	0.12429
C	-1.19741	1.42147	-0.01530
H	-3.32655	1.17448	-0.03831
H	3.17828	-1.42603	0.06116
H	-3.21766	-1.33390	0.12006
H	3.32687	1.08255	0.36601
C	-2.34976	-0.71316	0.35934
C	2.38372	0.54011	0.48209
H	1.05206	2.22619	0.68112
H	-1.27982	1.82538	1.00794
H	-0.99291	-3.09716	1.18252
H	-2.34965	-0.56664	1.45488
H	2.25043	0.32149	1.54745

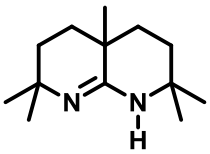


E = -478.138622

H = -477.878079

G = -477.925922

H	-2.33762	0.48285	-1.48636
H	2.65690	-0.59261	-1.37051
H	1.41362	1.75717	-1.04702
H	-1.06379	2.30752	-0.52457
H	-0.71229	-3.29726	-0.76513
H	-2.14979	-3.21216	0.24435
H	1.09790	-2.39063	-0.18803
C	-2.40268	0.62381	-0.40323
C	2.44557	-0.75035	-0.30680
N	0.00873	0.62409	0.01595
N	1.14685	-1.38775	-0.14309
C	-0.00508	-0.71240	-0.01715
C	1.25640	1.38954	-0.02581
N	-1.15034	-1.40595	0.08027
C	-1.12545	-2.85785	0.14908
C	-1.21607	1.41705	0.09087
H	-3.32505	1.16803	-0.19263
H	3.20208	-1.42854	0.09046
H	-3.20747	-1.35494	-0.13751
H	3.36040	1.11230	0.26170
C	-2.42569	-0.72193	0.28489
C	2.43431	0.56398	0.44265
H	1.11822	2.26006	0.62049
H	-1.36346	1.74978	1.12538
H	-0.56795	-3.21496	1.02163
H	-2.62407	-0.61390	1.35854
H	2.36020	0.37654	1.51806

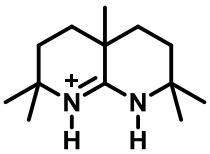


E = -618.824099

H = -618.450742

G = -618.507543

N	-0.94884	-0.93410	1.41789
C	-2.32441	-0.55869	1.06015
C	-2.41121	0.96844	1.02822
C	-1.30549	1.58719	0.18786
H	-1.43982	1.31257	-0.86491
H	-1.36179	2.68133	0.22984
C	0.09339	1.14589	0.63997
C	0.12804	-0.37150	0.74225
N	1.05889	-1.14902	0.35184
C	2.28007	-0.64952	-0.26830
C	1.14085	1.59815	-0.37730
C	2.45590	0.87236	-0.16094
C	2.23587	-1.08063	-1.73753
C	3.45263	-1.34709	0.41898
H	3.20583	1.20379	-0.88704
H	2.85640	1.11843	0.82885
H	0.76835	1.39705	-1.38895
H	1.27282	2.68369	-0.30366
H	-3.39285	1.25901	0.63984
H	-2.35565	1.34314	2.05548
C	-3.24814	-1.10828	2.13949
C	-2.70574	-1.15984	-0.29790
H	-0.82217	-1.94007	1.45306
H	-2.97210	-0.70690	3.11786
H	-3.18535	-2.20058	2.18742
H	-4.28813	-0.84218	1.92906
H	-2.03037	-0.82359	-1.08879
H	-3.72870	-0.88732	-0.57629
H	-2.64458	-2.25195	-0.25873
H	3.35769	-2.43150	0.32079
H	3.46855	-1.10262	1.48511
H	4.40433	-1.03411	-0.02322
H	2.04517	-2.15467	-1.80195
H	3.18588	-0.86089	-2.23507
H	1.43451	-0.56666	-2.27628
C	0.40357	1.73333	2.02487
H	1.41371	1.47382	2.34881
H	-0.28496	1.35628	2.78239
H	0.32436	2.82536	1.98976

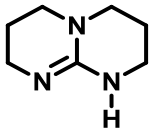


E = -619.237369

H = -618.849339

G = -618.9073

N	1.13437	-1.00051	-0.35334
C	2.49266	-0.57870	0.08031
C	2.50491	0.92803	0.34011
C	1.22332	1.41763	0.99099
H	1.09437	0.96209	1.97926
H	1.27072	2.49814	1.15243
C	-0.00698	1.11244	0.13098
C	-0.00856	-0.35202	-0.21609
N	-1.15020	-0.97605	-0.44613
C	-2.52985	-0.52493	-0.12367
C	-1.29616	1.44459	0.88868
C	-2.53093	0.98194	0.13561
C	-2.97486	-1.30048	1.11599
C	-3.41424	-0.87050	-1.31448
H	-3.43331	1.22273	0.70281
H	-2.61564	1.51708	-0.81374
H	-1.25751	0.98725	1.88375
H	-1.33338	2.52601	1.04669
H	3.36328	1.14997	0.97881
H	2.67773	1.46040	-0.59878
C	3.46310	-0.94415	-1.03516
C	2.81900	-1.36250	1.35131
H	1.08152	-1.97917	-0.61125
H	3.19816	-0.44020	-1.96785
H	3.48108	-2.02424	-1.21276
H	4.47494	-0.64113	-0.75643
H	2.14939	-1.09462	2.17242
H	3.84538	-1.15367	1.66158
H	2.73825	-2.44071	1.18263
H	-3.44086	-1.95011	-1.49390
H	-3.06383	-0.37313	-2.22216
H	-4.43864	-0.54568	-1.11844
H	-2.90376	-2.38031	0.95346
H	-4.01832	-1.06950	1.34220
H	-2.36846	-1.04627	1.98893
C	0.05534	1.88959	-1.19887
H	-0.79990	1.67472	-1.84051
H	0.95500	1.65594	-1.76925
H	0.05785	2.96044	-0.97846
H	-1.09755	-1.95585	-0.69973

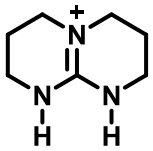


E = -438.448768

H = -438.232629

G = -438.276013

N	1.37605	-0.04734	1.39296
C	-0.02083	0.05735	1.04932
C	-0.15132	-0.27470	-0.42377
C	0.69270	0.69777	-1.22266
H	0.79838	0.34621	-2.25641
H	0.18455	1.67567	-1.27141
N	2.02009	0.86891	-0.66407
C	2.34484	0.60138	0.64709
N	3.46935	0.84442	1.21898
C	4.51164	1.42490	0.40946
C	2.94533	1.62297	-1.49281
C	3.95779	2.36921	-0.64631
H	5.10038	0.63323	-0.08250
H	5.20696	1.95577	1.06743
H	4.74881	2.77338	-1.28520
H	3.46698	3.21196	-0.14663
H	3.45485	0.94407	-2.19187
H	2.36152	2.32707	-2.09861
H	0.19689	-1.29928	-0.58621
H	-1.19170	-0.20901	-0.75353
H	-0.43453	1.06192	1.24375
H	-0.58277	-0.65330	1.66067
H	1.62630	-0.04251	2.36985

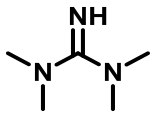


E = -438.868213

H = -438.637166

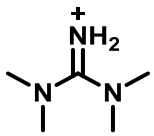
G = -438.681447

N	1.26889	0.31547	1.49546
C	-0.10332	0.07051	1.07221
C	-0.09123	-0.31326	-0.39269
C	0.64086	0.74817	-1.18615
H	0.82330	0.40505	-2.20758
H	0.05550	1.67320	-1.24585
N	1.94623	1.05367	-0.59624
C	2.21375	0.80722	0.68369
N	3.43282	1.04635	1.18391
C	4.54864	1.52752	0.38045
C	2.94066	1.64562	-1.49402
C	3.99950	2.40604	-0.72409
H	5.10904	0.68100	-0.03194
H	5.21631	2.08787	1.03623
H	4.80028	2.70395	-1.40310
H	3.57056	3.31569	-0.29330
H	3.38675	0.84893	-2.10079
H	2.40346	2.31555	-2.16998
H	0.40189	-1.28205	-0.51633
H	-1.11209	-0.40840	-0.76665
H	-0.71488	0.96415	1.23985
H	-0.50510	-0.73480	1.68855
H	1.51052	0.16378	2.46104
H	3.59549	0.82559	2.15270



E = -362.275815
H = -362.076184
G = -362.121562

N	1.08454	1.23866	0.21069
C	0.71859	-0.11124	0.21386
N	1.75828	-0.97386	-0.10196
N	-0.44274	-0.58222	0.48214
C	1.40112	-2.36427	-0.27848
C	3.04333	-0.78621	0.54353
C	1.80286	1.75406	-0.94080
C	0.13291	2.17348	0.75778
H	0.49693	-2.43729	-0.88075
H	1.20651	-2.86731	0.67923
H	2.22497	-2.87321	-0.78695
H	3.22104	0.26941	0.74100
H	3.84250	-1.16638	-0.10030
H	3.08901	-1.32580	1.50199
H	2.43248	0.97611	-1.36865
H	2.43317	2.59799	-0.64300
H	1.10967	2.10095	-1.72280
H	-0.24360	1.80942	1.71565
H	-0.72338	2.36045	0.08795
H	0.63563	3.12879	0.92938
H	-1.13639	0.15753	0.52709



E = -362.685035

H = -362.470997

G = -362.516753

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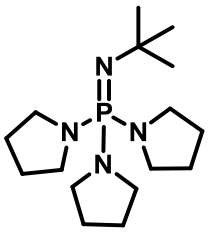
C	0.70153	-0.13127	0.20856
N	1.68887	-1.02227	0.06728
N	-0.53401	-0.56250	0.49687
C	1.40724	-2.42354	-0.21443
C	3.06510	-0.72019	0.44594
C	1.91306	1.70542	-0.86305
C	0.00320	2.16357	0.62979
H	0.49827	-2.51812	-0.80858
H	1.31661	-3.01247	0.70551
H	2.23524	-2.82935	-0.79749
H	3.11816	0.24384	0.94768
H	3.72662	-0.71777	-0.42405
H	3.40791	-1.48828	1.14377
H	2.32321	0.90308	-1.47291
H	2.72295	2.21652	-0.33642
H	1.42045	2.42125	-1.52591
H	-0.45373	1.78143	1.54268
H	-0.77475	2.44929	-0.08749
H	0.57352	3.05747	0.88652
H	-1.34014	0.01417	0.32364
H	-0.68759	-1.47416	0.89397



E = -1189.093945
H = -1188.579667
G = -1188.656981

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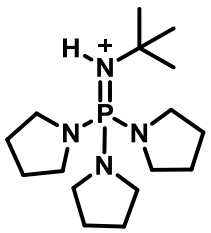
H	-2.58109	-2.29986	3.45869
H	-0.87565	-0.21420	2.97088
H	3.14239	-0.93075	1.65637
C	2.63688	1.57934	2.63544
H	3.66452	1.95030	2.71461
H	-0.40239	-1.84674	2.50192
C	-2.55876	-1.59504	2.62440
C	-1.15772	-1.06296	2.34711
H	-3.23343	-0.76550	2.86318
H	1.94837	2.39628	2.86861
H	4.35815	0.20646	1.03044
C	3.31460	-0.11703	0.94620
N	0.98017	0.55582	1.25229
C	2.34344	1.03557	1.23456
H	1.08418	-2.38591	0.42443
H	3.16199	-0.50871	-0.06375
H	-2.45519	-3.18921	1.17194
C	-2.95454	-2.22134	1.29026
N	-1.22924	-0.66838	0.94048
H	-0.17865	-2.99927	-0.65372
H	-4.02960	-2.38050	1.17858
C	0.72618	-2.37917	-0.61096
H	-1.52611	2.27875	0.84551
P	0.01055	0.10317	0.13352
C	2.57884	2.15732	0.21586
H	3.62266	2.48932	0.23000
C	-2.39960	-1.22627	0.27394
H	-0.20578	3.19396	0.11323
H	1.72023	-3.95760	-1.76114
H	1.94732	3.01927	0.44724
N	0.42091	-1.01323	-1.06787
H	-3.14167	-0.44561	0.05182
C	-1.05518	2.54578	-0.11012
C	1.79452	-2.88286	-1.58128

H	2.79085	-2.67965	-1.17582
H	2.33775	1.82657	-0.79900
H	-2.12956	-1.70450	-0.67482
N	-0.62279	1.33258	-0.82610
H	-2.79113	3.81393	-0.51062
H	-3.40183	1.50793	-1.13390
C	-2.06284	3.20335	-1.04877
H	0.71061	-2.42106	-3.39912
C	1.56477	-2.03778	-2.83050
C	1.22429	-0.67534	-2.24310
C	-2.67811	2.01596	-1.78064
C	-1.46515	1.12436	-2.01067
H	-1.71361	0.06927	-2.14007
H	2.14568	-0.13636	-1.97837
H	-1.54430	3.85133	-1.76373
H	0.66202	-0.04541	-2.93527
H	2.42950	-2.00246	-3.49716
H	-3.18456	2.28837	-2.70992
H	-0.93128	1.45223	-2.91416



E = -1189.532361
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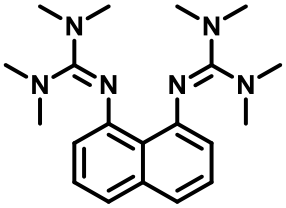
H	-2.56913	-3.00261	2.91885
H	-0.68152	-1.06497	2.96581
H	3.06597	-1.31233	1.61311
C	2.84455	1.18962	2.67955
H	3.90551	1.44559	2.70820
H	-0.45651	-2.44918	1.88596
H	0.58108	0.58517	2.24692
C	-2.53660	-2.05561	2.37828
C	-1.10829	-1.59806	2.11398
H	-3.06389	-1.30629	2.97660
H	2.27817	2.07681	2.97982
H	4.32195	-0.28374	0.90319

C	3.25214	-0.50696	0.89818
N	1.00799	0.39644	1.35118
C	2.45316	0.73783	1.27669
H	1.05676	-2.59715	0.04821
H	2.99120	-0.86377	-0.10013
H	-2.79844	-3.04415	0.47469
C	-3.13884	-2.13514	0.98053
N	-1.25598	-0.71116	0.94317
H	-0.41872	-2.73447	-0.92719
H	-4.22967	-2.13821	0.97616
C	0.59406	-2.31945	-0.90351
H	-1.56733	2.22150	1.16026
P	-0.05505	0.07605	0.14422
C	2.70271	1.86982	0.28373
H	3.77092	2.09501	0.23633
C	-2.56466	-0.90473	0.28705
H	-0.09529	3.09268	0.68748
H	1.11761	-3.77220	-2.44672
H	2.17937	2.77919	0.58882
N	0.53255	-0.84909	-1.06886
H	-3.19713	-0.02396	0.44356
C	-0.98137	2.58258	0.30513
C	1.42552	-2.78583	-2.09749
H	2.48142	-2.84671	-1.81720
H	2.37281	1.61005	-0.72485
H	-2.45157	-1.05696	-0.79095
N	-0.59809	1.45031	-0.57005
H	-2.55448	4.05675	-0.02649
H	-3.30000	1.94961	-1.07333
C	-1.83255	3.47063	-0.59661
H	0.25248	-1.78442	-3.62255
C	1.22631	-1.68382	-3.13308
C	1.25233	-0.42528	-2.28089
C	-2.47567	2.48003	-1.56087
C	-1.33028	1.52238	-1.85104
H	-1.65539	0.53430	-2.18214
H	2.28631	-0.14358	-2.04800
H	-1.19337	4.16797	-1.14637
H	0.76545	0.42777	-2.75127
H	1.99650	-1.67489	-3.90571
H	-2.86320	2.94734	-2.46753
H	-0.67519	1.94161	-2.62336



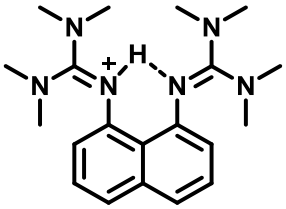
E = -1107.71152

H = -1107.198518

G = -1107.284678

H	0.16566	4.64411	-0.98480
H	-1.08378	2.52791	-1.87739
C	1.09809	4.06083	-0.98022
H	1.68672	4.35901	-0.11294
C	-0.05996	2.13963	-1.95741
H	1.65854	4.31139	-1.88944
H	2.54676	-0.51260	-2.18161
H	0.35054	2.43489	-2.92977
N	0.81362	2.64552	-0.92250
H	-0.08461	1.05031	-1.90806
H	1.42363	-1.73784	-2.78708
C	2.33926	-1.59211	-2.21549
H	3.16961	-2.09527	-2.71976
H	-5.12348	-1.15007	-0.37599
H	-5.12352	1.14992	0.37598
C	-4.03842	1.16330	0.39546
C	-4.03839	-1.16342	-0.39546
H	-3.89642	-3.17384	-1.09639
H	-3.89652	3.17372	1.09639
C	-3.35549	-2.28100	-0.79796
C	-3.35556	2.28091	0.79796
C	-3.33629	-0.00005	-0.00000
H	3.19894	2.48904	-0.90355
C	-1.95391	2.27005	0.86684
C	-1.95384	-2.27010	-0.86684
C	-1.90788	-0.00003	-0.00000
H	-1.41942	-3.12988	-1.25886
H	-1.41952	3.12985	1.25887
C	0.97452	1.94134	0.25662
C	-1.22138	1.15223	0.50205
C	-1.22134	-1.15226	-0.50205
H	3.89199	-1.20275	-0.10063
N	0.14144	1.10921	0.76670
N	0.14147	-1.10920	-0.76670
C	0.97457	-1.94130	-0.25662

N	2.18491	-2.15670	-0.89466
H	1.68682	-4.35896	0.11293
N	2.18484	2.15676	0.89467
C	3.40928	2.19133	0.12212
C	3.40934	-2.19124	-0.12212
H	4.11513	-2.90413	-0.56064
H	3.89193	1.20284	0.10061
C	1.09821	-4.06080	0.98021
H	4.11506	2.90421	0.56067
N	0.81368	-2.64550	0.92249
H	1.65869	-4.31134	1.88943
H	3.19899	-2.48893	0.90356
C	2.33920	1.59218	2.21549
H	1.42357	1.73790	2.78708
H	0.16579	-4.64410	0.98482
H	2.54672	0.51268	2.18161
H	3.16954	2.09535	2.71976
C	-0.05990	-2.13964	1.95740
H	-0.08459	-1.05032	1.90806
H	0.35061	-2.43489	2.92976
H	-1.08371	-2.52795	1.87739



E = -1108.144472

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G = -1107.703023

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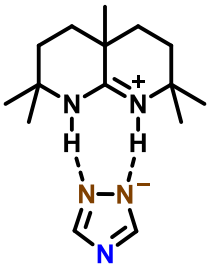
C	4.80253	-0.90335	-0.06605
H	4.74089	-1.52997	0.82230
C	3.42068	0.53823	-1.50313
H	5.34197	-1.44176	-0.85114
H	-0.71222	-3.22716	-1.33527
H	4.07730	0.25564	-2.33040
N	3.47248	-0.51188	-0.50089
H	2.40589	0.64972	-1.88153
H	-1.34360	-1.87256	-2.29370
C	-1.62705	-2.72012	-1.67264

H	-2.20893	-3.43015	-2.26675
H	-1.18292	4.96839	-0.57274
H	0.97344	5.01327	0.52225
C	1.02529	3.92982	0.51219
C	-1.17602	3.88399	-0.57823
H	-3.06785	3.69627	-1.54505
H	2.91764	3.84105	1.49399
C	-2.22355	3.17589	-1.10564
C	2.10805	3.28029	1.04041
C	-0.05813	3.20600	-0.04152
H	3.47593	-2.93846	-1.12140
C	2.18657	1.87864	0.98365
C	-2.22705	1.77360	-1.06557
C	-0.02230	1.77904	-0.05437
H	-3.07505	1.22714	-1.46565
H	3.05559	1.36907	1.38630
C	2.35807	-0.98584	0.08556
C	1.17177	1.14747	0.40894
C	-1.17903	1.06159	-0.50835
H	-2.37854	-4.12177	0.39243
N	1.26158	-0.25005	0.26386
N	-1.19993	-0.33034	-0.40818
C	-2.29612	-0.98656	-0.10440
N	-2.42861	-2.26266	-0.55942
H	0.30675	-0.66548	0.04739
H	-4.79003	-1.39611	-0.49669
N	2.31642	-2.27021	0.49111
C	3.02932	-3.32642	-0.20771
C	-3.08334	-3.30225	0.21012
H	-3.94933	-3.71308	-0.31916
H	2.31998	-4.11407	-0.47840
C	-4.69966	-0.76033	0.38270
H	3.81124	-3.76667	0.41815
N	-3.30282	-0.51392	0.68647
H	-5.21597	-1.23803	1.22212
H	-3.41010	-2.90938	1.17139
C	1.35328	-2.70924	1.48600
H	1.07210	-1.87384	2.12551
H	-5.19958	0.19254	0.17117
H	0.45053	-3.11959	1.01854
H	1.81132	-3.48910	2.09867
C	-3.06070	0.50779	1.68297
H	-2.00376	0.53248	1.94623
H	-3.63909	0.26425	2.57927
H	-3.35313	1.50411	1.33283

Ion-pairs



E = -860.900672
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G = -860.531896

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C	2.47524	-0.51101	-0.00816
C	2.49995	0.97206	0.36508
C	1.21499	1.41149	1.04420
H	1.08744	0.87899	1.99398
H	1.25427	2.47857	1.28777
C	-0.00862	1.15283	0.16166
C	0.00408	-0.28907	-0.29068
N	-1.12534	-0.91113	-0.56847
C	-2.48323	-0.49306	-0.20455
C	-1.29629	1.42058	0.94474
C	-2.52666	0.99026	0.16600
C	-2.91854	-1.36306	0.97965
C	-3.38633	-0.76918	-1.40348
H	-3.43301	1.17300	0.75076
H	-2.62137	1.59176	-0.74307
H	-1.24811	0.88744	1.90148
H	-1.34700	2.48798	1.18475
H	3.35851	1.14843	1.01974
H	2.67060	1.57260	-0.53348
C	3.46831	-0.79400	-1.13199
C	2.80924	-1.38378	1.20652
H	1.09385	-1.94335	-0.78885
H	3.21462	-0.21458	-2.02371
H	3.45713	-1.85392	-1.39958
H	4.48152	-0.52715	-0.81817
H	2.14108	-1.16588	2.04436
H	3.84018	-1.21094	1.52881
H	2.69453	-2.44125	0.95530
H	-3.36168	-1.82923	-1.66966
H	-3.05873	-0.19186	-2.27218
H	-4.41924	-0.49493	-1.17069

H	-2.79196	-2.42140	0.73798
H	-3.97046	-1.18268	1.21945
H	-2.31718	-1.14975	1.86777
C	0.04445	2.03461	-1.09773
H	-0.80797	1.85327	-1.75374
H	0.94475	1.84693	-1.68432
H	0.03660	3.08886	-0.80331
N	0.04369	-5.54943	-1.77167
C	-0.99833	-4.72471	-1.59816
H	-2.03089	-5.02505	-1.72024
C	1.07465	-4.73221	-1.51606
N	-0.64883	-3.48715	-1.25917
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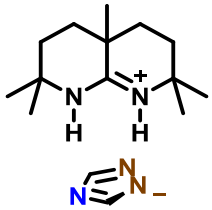
N	0.70838	-3.49206	-1.20541
H	-1.05481	-1.93556	-0.87396



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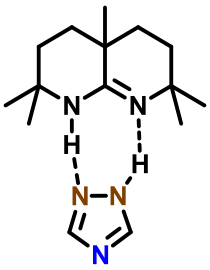
C	-2.03249	2.49911	-0.07647
C	-2.58424	1.24911	0.58639
H	-2.29716	1.22143	1.64399
H	-3.67875	1.25216	0.55950
C	-2.08070	-0.02392	-0.09825
C	-0.57380	0.02486	-0.17122
N	0.11646	-1.09990	-0.20301
C	-0.32741	-2.44494	0.21536
C	-2.51171	-1.26401	0.69014
C	-1.85172	-2.52805	0.16599
C	0.19907	-2.67931	1.63351
C	0.31029	-3.44320	-0.74406
H	-2.16392	-3.39288	0.75782
H	-2.17541	-2.72356	-0.86089
H	-2.26206	-1.11873	1.74721

H	-3.60215	-1.34818	0.63536
H	-2.39267	3.39506	0.43698
H	-2.39810	2.56742	-1.10523
C	0.02597	3.41438	-1.19584
C	0.03418	3.02498	1.27290
H	1.09603	1.16017	-0.27791
H	-0.30806	3.04416	-2.16895
H	1.11927	3.43051	-1.18810
H	-0.33652	4.43841	-1.06999
H	-0.35275	2.42322	2.09985
H	-0.25600	4.06702	1.43350
H	1.12540	2.96235	1.28885
H	1.39985	-3.34612	-0.72520
H	-0.03618	-3.27161	-1.76739
H	0.04174	-4.46192	-0.45177
H	1.27987	-2.51294	1.66722
H	-0.01630	-3.70625	1.94261
H	-0.27073	-1.99647	2.34795
C	-2.60650	-0.10303	-1.54266
H	-2.25589	-1.00307	-2.04914
H	-2.28326	0.74982	-2.14122
H	-3.70061	-0.11911	-1.52661
N	2.83585	0.86468	-0.10424
C	3.03282	-0.11978	-1.01141
H	3.04671	0.04918	-2.08116
C	2.92091	0.16109	1.05075
N	3.19404	-1.32458	-0.47244
H	2.81955	0.61202	2.03030
N	3.12645	-1.13632	0.87881
H	1.13115	-1.04058	-0.32589



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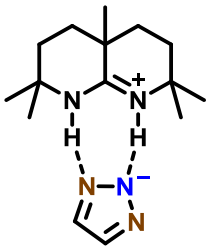
C	-0.59171	2.44272	0.02253
C	-2.11788	2.50454	0.06033
C	-2.72589	1.22428	0.60807
H	-2.45456	1.10163	1.66310
H	-3.82039	1.27490	0.57515
C	-2.26835	-0.01705	-0.16845
C	-0.74985	-0.02627	-0.24767
N	-0.00239	-1.06431	-0.10791
C	-0.52534	-2.40539	0.14524
C	-2.74445	-1.28259	0.54288
C	-2.04719	-2.51093	-0.00936
C	-0.10996	-2.78274	1.57143
C	0.15361	-3.35464	-0.84173
H	-2.39730	-3.41725	0.49530
H	-2.29505	-2.63396	-1.06896
H	-2.54148	-1.18874	1.61641
H	-3.83168	-1.36769	0.43756
H	-2.42010	3.36165	0.67052
H	-2.49108	2.69348	-0.95128
C	-0.03976	3.56259	-0.85079
C	0.00229	2.55288	1.43196
H	0.84445	1.12061	-0.66916
H	-0.43162	3.48244	-1.86815
H	1.05207	3.51001	-0.89807
H	-0.31715	4.53867	-0.44247
H	-0.36451	1.75477	2.08349
H	-0.25028	3.51480	1.88896
H	1.09140	2.46653	1.38463
H	1.24021	-3.33768	-0.71566
H	-0.07178	-3.06021	-1.87043
H	-0.19254	-4.38194	-0.69021
H	0.96825	-2.65470	1.70185
H	-0.36047	-3.82658	1.78392

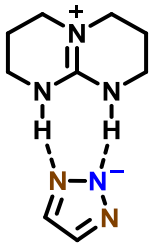
H	-0.60883	-2.14783	2.30872
C	-2.82064	0.03039	-1.60185
H	-2.54389	-0.86160	-2.16746
H	-2.43587	0.89092	-2.15029
H	-3.91366	0.09274	-1.57269
N	4.84947	-0.19409	0.07491
C	3.86219	-1.06369	0.21914
H	3.96610	-2.09840	0.51218
C	4.19429	0.92812	-0.29623
N	2.68541	-0.49101	-0.04973
H	4.68939	1.86500	-0.50704
N	2.88166	0.79491	-0.38451
H	1.68714	-0.85128	-0.04907



E = -860.878539
H = -860.439483
G = -860.510484

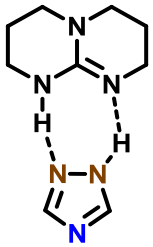
N	-0.01740	1.09825	-0.13354
C	-0.51244	2.45570	0.11101
C	-2.03950	2.51250	0.03324
C	-2.68544	1.26215	0.60417
H	-2.44572	1.16684	1.66977
H	-3.77654	1.32541	0.53344
C	-2.21659	0.00036	-0.12450
C	-0.70587	-0.01688	-0.15403
N	-0.06156	-1.17220	-0.27203
C	-0.58144	-2.50105	0.07398
C	-2.71748	-1.25233	0.59985
C	-2.10925	-2.51881	0.02280
C	-0.07616	-2.83905	1.48092
C	-0.00366	-3.49336	-0.93022
H	-2.46189	-3.39662	0.57238
H	-2.43696	-2.65165	-1.01272
H	-2.47537	-1.16745	1.66562
H	-3.81011	-1.28518	0.53069

H	-2.38053	3.40038	0.57364
H	-2.34865	2.64936	-1.00748
C	0.11588	3.36960	-0.93830
C	-0.01914	2.86041	1.50411
H	1.07048	1.00284	-0.11887
H	-0.18347	3.06220	-1.94414
H	1.20700	3.33271	-0.87810
H	-0.20549	4.40308	-0.77953
H	-0.48514	2.24734	2.28080
H	-0.25601	3.91026	1.69940
H	1.06377	2.72974	1.57523
H	1.08920	-3.48087	-0.89840
H	-0.31901	-3.23968	-1.94577
H	-0.34425	-4.50697	-0.70051
H	1.01100	-2.73484	1.52517
H	-0.34018	-3.86702	1.74626
H	-0.50538	-2.16568	2.22802
C	-2.71086	0.00699	-1.58109
H	-2.36663	-0.87171	-2.12804
H	-2.35350	0.88287	-2.12454
H	-3.80539	0.01619	-1.59271
C	4.66774	0.18688	0.01914
C	4.00407	-1.02218	-0.13426
H	4.38213	-2.03098	-0.20896
N	3.74632	1.16464	0.05691
N	2.69239	-0.74590	-0.18537
N	2.57871	0.57396	-0.06780
H	0.98925	-1.13255	-0.29066
H	5.72326	0.39940	0.10093



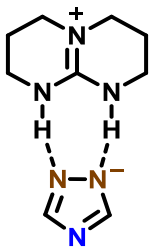
E = -680.507005
H = -680.225569
G = -680.282204

H	-3.82328	-1.11396	-0.65479
H	-3.86295	1.06855	0.65145
H	-3.35831	-1.42828	1.02027
H	-3.39919	1.38393	-1.02350
C	-2.96307	-1.24394	0.01129
C	-3.00346	1.22067	-0.01089
H	-2.64870	-3.34624	-0.27231
H	-2.76002	3.33491	0.25140
N	-2.21094	0.00148	0.00721
C	-2.11119	-2.41084	-0.44558
C	-2.19418	2.41947	0.44022
H	-1.91177	-2.32869	-1.51875
H	-2.00059	2.35573	1.51563
H	-0.97038	-2.58959	1.37734
H	-1.04661	2.61011	-1.37661
C	-0.85560	0.01833	0.01381
C	-0.79735	-2.38620	0.31084
C	-0.87443	2.42916	-0.30560
N	-0.16143	-1.10492	0.12799
N	-0.19835	1.17365	-0.09319
H	-0.11222	-3.15305	-0.05693
H	-0.22103	3.22575	0.05684
H	0.92440	-1.02906	0.10923
H	0.86152	1.14695	-0.08902
N	2.43128	-0.58068	0.04962
N	2.49482	0.74364	-0.05932
N	3.62362	-1.13089	0.08112
C	3.79616	1.06539	-0.10069
H	4.13295	2.08751	-0.18820
C	4.50737	-0.12215	-0.01158
H	5.57236	-0.30039	-0.00895



E = -680.531195
H = -680.248654
G = -680.305895

H	-1.83049	-2.27810	-1.53164
H	-1.11904	2.53202	-1.37124
H	-3.45446	1.31749	-0.99462
H	-3.78861	-1.10305	-0.74960
C	-2.07690	-2.38894	-0.47027
C	-0.95686	2.43368	-0.28570
H	-2.59863	-3.34172	-0.34298
H	4.47312	1.84958	-0.25771
N	-0.25704	1.22078	0.04835
H	0.76167	1.21406	-0.00534
C	3.99894	0.88487	-0.14896
H	-0.10856	-3.12629	0.02658
N	2.68472	0.75360	-0.07876
C	-3.05699	1.19180	0.02484
C	-0.86771	0.00583	0.09831
N	-2.23745	-0.00511	0.07779
N	4.68192	-0.27745	-0.07316
C	-2.97474	-1.25216	-0.02889
N	2.51505	-0.57268	0.05003
H	-0.33982	3.27857	0.02836
C	3.70938	-1.16870	0.05147
N	-0.12852	-1.06359	0.18812
H	1.50196	-0.92171	0.12432
H	3.83872	-2.23718	0.14389
H	-2.87508	3.32085	0.19117
C	-0.79524	-2.33444	0.34285
C	-2.28932	2.43091	0.43567
H	-3.91985	1.04049	0.68519
H	-3.44191	-1.48567	0.93894
H	-1.02647	-2.52970	1.40276
H	-2.11117	2.42432	1.51545

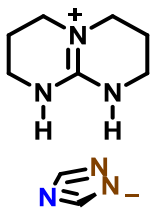


E = -680.530114

H = -680.248221

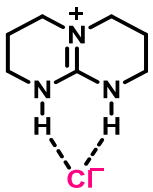
G = -680.30472

H	-2.33866	0.55025	-1.52457
H	2.60378	-0.39995	-1.39248
H	1.40835	1.96274	-0.99584
H	-1.09014	2.42063	-0.62112
C	-2.41406	0.72597	-0.44681
C	2.40842	-0.59308	-0.32768
N	-0.67545	-3.89631	-0.03081
H	-3.34016	1.27388	-0.25709
N	0.67727	-3.89398	-0.14381
C	-1.03280	-5.17688	-0.02512
H	1.08923	-2.32743	-0.15628
H	-2.06469	-5.49218	0.05546
C	1.03496	-5.17331	-0.19829
N	1.13983	-1.25331	-0.14564
H	-3.18906	-1.26682	-0.10160
H	2.06693	-5.48504	-0.29082
N	0.00119	-6.02318	-0.12787
C	1.23260	1.54851	0.00713
C	0.00047	-0.57945	-0.02411
N	0.00029	0.77575	0.00172
C	-1.23222	1.54783	0.02581
H	3.19016	-1.26846	0.02718
N	-1.13873	-1.25775	0.07163
H	-1.08784	-2.33149	0.04134
H	3.34061	1.26450	0.27943
C	-2.40748	-0.60526	0.27874
C	2.41464	0.70952	0.44810
H	1.09028	2.39596	0.68686
H	-1.40804	1.92348	1.04384
H	-2.60285	-0.45292	1.35014
H	2.33927	0.49282	1.51837



E = -680.508994
H = -680.226168
G = -680.282938

H	-1.97419	-2.43665	-1.44001
H	-1.17190	2.68349	-1.50345
H	-3.46082	1.40872	-0.93473
H	-3.80435	-1.13821	-0.53831
C	-2.07617	-2.41982	-0.35059
C	-0.89317	2.48209	-0.46053
H	-2.58437	-3.33736	-0.04578
H	0.85459	1.22454	-0.20673
N	-0.18903	1.22475	-0.35636
H	-0.03219	-3.10910	-0.07440
C	-2.96689	1.24117	0.03209
C	-0.82127	0.06985	-0.16514
N	-2.16463	0.02814	-0.04321
C	-2.90263	-1.22340	0.07798
H	-0.20514	3.26979	-0.14849
N	-0.11713	-1.05768	-0.10391
H	0.89565	-1.02187	-0.23275
H	-2.72184	3.35369	0.30260
C	-0.70042	-2.32282	0.27754
C	-2.12902	2.44328	0.41723
H	-3.75424	1.06951	0.77367
H	-3.22987	-1.33854	1.12020
H	-0.75626	-2.40607	1.37047
H	-1.82551	2.36607	1.46600
H	2.94952	-0.09009	-1.67054
C	2.80593	-0.20958	-0.60350
N	2.94179	-1.37914	0.01464
N	2.46294	0.80796	0.22075
N	2.70237	-1.13029	1.33531
C	2.43047	0.16305	1.41282
H	2.19232	0.65662	2.34690

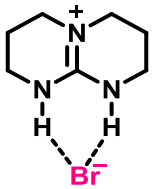


E = -899.163542

H = -898.931722

G = -898.981382

H	-2.35260	0.41290	-1.47597
H	2.62106	-0.63569	-1.33044
H	1.40401	1.76425	-1.13932
H	-1.11162	2.32349	-0.64711
C	-2.42200	0.62732	-0.40487
C	2.40776	-0.72748	-0.25649
H	-3.34646	1.18280	-0.23089
H	0.99540	-2.38140	0.01252
N	1.12217	-1.34201	-0.03996
H	-3.19041	-1.35799	-0.00489
C	1.24254	1.45209	-0.09814
C	-0.00686	-0.64725	0.05347
N	-0.00044	0.70125	-0.00371
C	-1.23620	1.46917	0.02629
H	3.16981	-1.38071	0.17309
N	-1.14240	-1.32085	0.20491
H	-1.02554	-2.36210	0.24066
H	3.35008	1.16850	0.18322
C	-2.42201	-0.67801	0.36813
C	2.42046	0.63855	0.40323
H	1.12635	2.36151	0.50047
H	-1.39428	1.86988	1.03723
H	-2.63398	-0.49359	1.43038
H	2.34946	0.51625	1.48861
Cl	-0.02334	-4.10923	0.20026

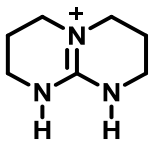


E = -3012.92876

H = -3012.696853

G = -3012.748085

H	-2.35365	0.41869	-1.47544
H	2.61947	-0.63436	-1.33319
H	1.40514	1.76531	-1.14480
H	-1.10652	2.32899	-0.65351
C	-2.42158	0.63740	-0.40515
C	2.40817	-0.72379	-0.25892
H	-3.34447	1.19575	-0.23255
H	1.00782	-2.37271	0.01395
N	1.12120	-1.33649	-0.04011
H	-3.19356	-1.34526	0.00348
C	1.24482	1.45574	-0.10282
C	-0.00784	-0.64164	0.05479
N	0.00081	0.70606	-0.00588
C	-1.23343	1.47729	0.02262
H	3.16863	-1.37855	0.17102
N	-1.14563	-1.31064	0.21107
H	-1.04556	-2.34889	0.25039
H	3.35222	1.17124	0.17789
C	-2.42451	-0.66431	0.37326
C	2.42235	0.64252	0.39940
H	1.12920	2.36629	0.49397
H	-1.38915	1.88127	1.03247
H	-2.63398	-0.47602	1.43504
H	2.35220	0.52174	1.48497
Br	-0.03122	-4.28395	0.21872



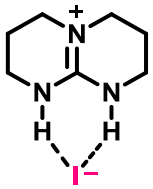
$^{-}PF_6$

E = -1379.193599

H = -1378.934576

G = -1378.999585

P	1.52082	-2.18022	0.10440
F	2.74907	-1.47535	0.99737
F	1.55953	-3.45382	1.07610
F	0.45363	-1.42754	1.15070
F	1.49025	-0.79984	-0.79600
F	2.60675	-2.82078	-0.88783
F	0.28652	-2.77198	-0.73246
H	4.18082	1.63281	-0.75191
H	-0.52912	2.44539	-1.12478
H	2.99887	4.03208	-1.07681
C	4.10138	1.82580	0.32596
N	2.86501	1.28775	0.85079
C	-0.69393	2.95216	-0.16896
H	2.81192	0.27644	0.98208
C	1.71025	1.94718	0.74723
N	0.58300	1.33021	1.09441
H	-1.43067	1.12097	0.72375
H	0.61863	0.31596	1.20252
H	0.58789	4.58021	-0.76784
H	4.92529	1.30600	0.81695
N	1.68934	3.22693	0.33673
C	2.90564	3.96378	0.01513
C	-0.72946	1.92694	0.94545
H	-1.64170	3.49136	-0.22826
C	0.43373	3.92754	0.09674
C	4.13515	3.31225	0.61449
H	5.03129	3.77061	0.19105
H	2.78568	4.98247	0.39804
H	-1.04228	2.39269	1.88819
H	0.20175	4.56949	0.95684
H	4.15466	3.47023	1.69712



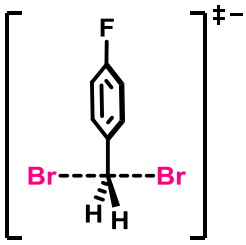
E = -734.830827

H = -734.598878

G = -734.651459

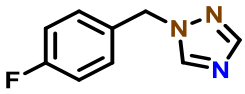
H	-2.35071	0.41665	-1.48517
H	2.62846	-0.61449	-1.32408
H	1.40158	1.77912	-1.14081
H	-1.11257	2.33208	-0.66089
C	-2.42319	0.63665	-0.41548
C	2.41383	-0.70386	-0.25071
H	-3.34852	1.19215	-0.24704
H	1.03150	-2.35585	0.01769
N	1.12777	-1.32152	-0.03692
H	-3.18855	-1.34921	-0.00703
C	1.23928	1.46944	-0.09930
C	-0.00547	-0.63306	0.05490
N	-0.00206	0.71406	-0.00683
C	-1.23956	1.48099	0.01585
H	3.17398	-1.35659	0.18283
N	-1.14213	-1.30451	0.20904
H	-1.05111	-2.33997	0.24929
H	3.34682	1.19524	0.18941
C	-2.42501	-0.66340	0.36516
C	2.41873	0.66214	0.40773
H	1.11675	2.37951	0.49671
H	-1.40006	1.88547	1.02462
H	-2.63893	-0.47514	1.42581
H	2.34540	0.54129	1.49305
I	-0.01528	-4.51551	0.23282

p-F-BnBr + 1,2,4-triazole derivatives



E = -5517.627109
H = -5517.506176
G = -5517.556726

C	0.00002	-0.81199	0.00001
Br	2.50948	-1.15122	-0.00007
Br	-2.50944	-1.15131	0.00008
H	0.00005	0.81076	2.13754
C	0.00001	1.35719	1.20100
C	-0.00001	2.74321	1.21075
H	0.00001	3.30674	2.13676
C	-0.00006	3.41103	-0.00000
F	-0.00008	4.76546	-0.00001
C	-0.00008	2.74320	-1.21075
H	-0.00012	3.30673	-2.13676
C	-0.00006	1.35719	-1.20100
H	-0.00008	0.81075	-2.13754
C	-0.00001	0.64519	0.00000
H	0.00005	-1.36088	0.92343
H	-0.00000	-1.36089	-0.92342

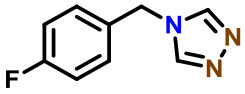


E = -611.346349

H = -611.173252

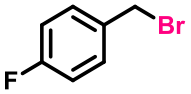
G = -611.222787

C	-0.46274	1.14022	-0.70453
C	-3.50589	-0.34067	0.06783
C	-1.57710	-0.54321	0.83515
N	-1.55808	0.33749	-0.18212
N	-2.80078	-0.99787	1.01893
N	-2.79671	0.48068	-0.68340
H	-4.56759	-0.47173	-0.08286
H	-0.69449	-0.82312	1.39009
H	0.69506	-1.05565	-1.79852
C	1.31858	-0.60138	-1.03452
C	2.54365	-1.17246	-0.72549
H	2.90278	-2.06114	-1.23092
C	3.32145	-0.57812	0.25434
F	4.50812	-1.12377	0.55657
C	2.91650	0.55835	0.92818
H	3.55710	0.99189	1.68692
C	1.68366	1.11392	0.60611
H	1.34861	2.00510	1.12791
C	0.87484	0.54474	-0.37356
H	-0.61482	1.20243	-1.78429
H	-0.54381	2.15309	-0.29961



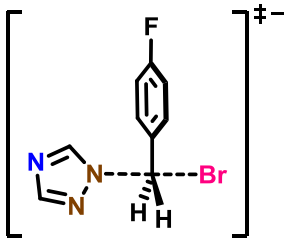
E = -611.331974
H = -611.160488
G = -611.206566

C	0.11646	2.10817	0.66640
N	1.16622	1.57164	4.05979
C	1.83804	0.95941	2.10759
N	0.77567	1.78999	1.91183
N	2.08785	0.82346	3.38083
C	0.39154	2.13369	3.17322
H	2.38345	0.49470	1.29942
H	-0.75301	-0.16134	1.98700
C	-1.28553	0.02378	1.06031
C	-2.28823	-0.85763	0.67062
H	-2.54614	-1.72124	1.27215
C	-2.96273	-0.61691	-0.51004
F	-3.93130	-1.46235	-0.89302
C	-2.67030	0.47228	-1.31325
H	-3.22237	0.62682	-2.23279
C	-1.66772	1.34122	-0.90999
H	-1.42973	2.19932	-1.53248
C	-0.96671	1.12767	0.27670
H	-0.30110	3.11535	0.75623
H	0.88102	2.15557	-0.11466
H	-0.44199	2.78841	3.38092



E = -2943.714584
H = -2943.594372
G = -2943.638156

C	-0.75193	-1.13620	-0.00000
Br	1.07726	-1.87861	-0.00000
H	-0.74343	0.51866	2.14266
C	-0.74941	1.05903	1.20118
C	-0.74848	2.44630	1.21134
H	-0.74968	3.01015	2.13666
C	-0.74757	3.11469	0.00000
F	-0.74900	4.45640	0.00000
C	-0.74848	2.44630	-1.21134
H	-0.74968	3.01015	-2.13666
C	-0.74941	1.05903	-1.20118
H	-0.74343	0.51866	-2.14266
C	-0.75107	0.34985	-0.00000
H	-1.21963	-1.55125	0.89031
H	-1.21963	-1.55125	-0.89031

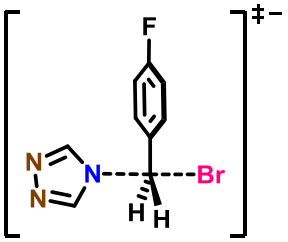


E = -3185.217658

H = -3185.045753

G = -3185.103467

C	0.24373	0.85517	-0.00000
Br	2.51625	1.43758	-0.00001
C	-3.90878	1.52198	0.00001
C	-2.85076	-0.26197	0.00001
N	-1.95241	0.72292	0.00000
N	-4.11346	0.18772	0.00001
N	-2.63085	1.88772	0.00001
H	-4.71396	2.24695	0.00001
H	-2.57011	-1.30754	0.00001
H	0.37059	-0.77202	-2.13675
C	0.40806	-1.31656	-1.19959
C	0.49250	-2.70168	-1.20994
H	0.52147	-3.26365	-2.13645
C	0.53420	-3.36888	-0.00000
F	0.61569	-4.72045	0.00000
C	0.49251	-2.70168	1.20994
H	0.52148	-3.26365	2.13645
C	0.40806	-1.31656	1.19959
H	0.37060	-0.77202	2.13675
C	0.36782	-0.60665	-0.00000
H	0.06333	1.38272	-0.91940
H	0.06333	1.38272	0.91939

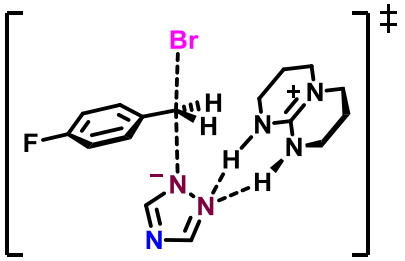


E = -3185.212404

H = -3185.04064

G = -3185.097987

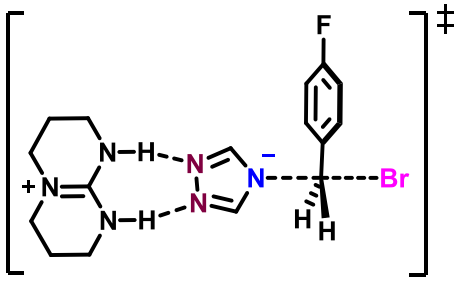
C	0.26034	0.85650	0.00000
Br	2.58788	1.37501	0.00000
N	-4.07295	0.20975	0.00000
C	-2.75079	1.89980	0.00000
N	-1.93046	0.82764	0.00000
N	-4.03329	1.57342	0.00000
C	-2.81211	-0.19396	0.00000
H	-2.39558	2.92313	0.00000
H	0.33890	-0.77027	-2.13755
C	0.36162	-1.31537	-1.20031
C	0.40654	-2.70186	-1.21038
H	0.41861	-3.26473	-2.13656
C	0.42953	-3.36958	-0.00000
F	0.47272	-4.72139	-0.00000
C	0.40654	-2.70186	1.21037
H	0.41861	-3.26473	2.13656
C	0.36162	-1.31537	1.20031
H	0.33890	-0.77028	2.13755
C	0.34216	-0.60577	0.00000
H	0.13370	1.38972	-0.92412
H	0.13370	1.38972	0.92413
H	-2.51531	-1.23493	0.00000



E = -3624.236249
H = -3623.831006
G = -3623.912393

H	-1.39213	-1.02004	2.24654
H	-1.43975	-0.28209	-2.45426
H	-3.03885	-1.84556	-1.04750
C	-2.31412	-0.50086	2.52615
H	-3.38804	-1.93130	1.34170
C	-2.18387	0.51229	-2.31000
C	2.49092	2.69288	-0.16559
N	-1.91129	1.25461	-1.09681
N	1.40011	1.94114	-0.10849
C	-3.64382	-0.93711	-0.93883
C	-2.28953	0.79960	0.10381
C	-3.38992	-0.85188	1.51797
H	-2.61734	-0.84539	3.51735
N	-3.15288	-0.21138	0.22733
N	2.22000	4.00802	-0.19894
C	0.88386	4.01095	-0.16070
N	0.34159	2.79045	-0.10726
H	3.48662	2.27094	-0.18128
N	-1.80045	1.43062	1.17379
H	-1.14553	1.93887	-1.05262
H	-1.23012	1.26991	3.14986
C	-2.08364	0.99835	2.52522
H	-2.12162	1.20488	-3.15147
H	-1.03879	2.09379	0.95666
C	-3.56980	-0.09230	-2.19503
H	0.28179	4.91033	-0.17075
H	-3.78550	-0.72054	-3.06192
H	-4.67818	-1.22830	-0.73085
H	-4.38558	-0.56662	1.88096
H	-2.96139	1.52688	2.91914
H	-4.31635	0.70767	-2.16254
H	0.55016	0.05099	-1.11526
H	0.39258	0.05924	0.72838
C	0.95974	-0.18132	-0.15044

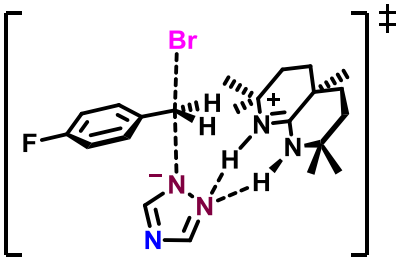
C	2.33389	-0.65020	-0.03496
C	3.10526	-0.86423	-1.17826
C	2.90991	-0.85279	1.22010
C	4.42503	-1.27473	-1.07834
C	4.22760	-1.26343	1.33925
C	4.96155	-1.46670	0.18306
H	2.66226	-0.71104	-2.15653
H	2.31511	-0.68922	2.11245
H	5.03801	-1.44684	-1.95504
H	4.69089	-1.42623	2.30508
F	6.23931	-1.86359	0.28958
Br	-0.27025	-2.28058	-0.24030



E = -3624.224959
H = -3623.820542
G = -3623.903437

C	-3.17361	-0.82668	-0.02916
Br	-5.59291	-1.65620	-0.06545
H	-3.58102	0.83783	-2.10205
C	-3.66870	1.33627	-1.14264
C	-3.93365	2.69677	-1.09552
H	-4.05113	3.28609	-1.99738
C	-4.05921	3.30262	0.14214
F	-4.31126	4.62401	0.19694
C	-3.93477	2.59614	1.32536
H	-4.05301	3.10862	2.27289
C	-3.66984	1.23639	1.25971
H	-3.58296	0.66010	2.17455
C	-3.53712	0.59102	0.02970
H	-3.14185	-1.33849	-0.97493
H	-3.14287	-1.41547	0.87075
H	5.12904	2.28424	-1.62583
H	4.64636	-2.73231	-1.25838
H	6.88334	-1.28165	-0.98078
C	5.30316	2.42491	-0.55449

H	7.11823	1.26682	-0.68522
C	4.46085	-2.50249	-0.20012
C	-0.28358	-1.57885	-0.05998
N	3.68657	-1.29060	-0.06529
N	0.94450	-1.09257	-0.04050
C	6.48138	-1.10550	0.02632
C	4.24807	-0.08486	-0.00580
C	6.23906	1.35147	-0.03808
H	5.75937	3.40713	-0.41279
N	5.59158	0.04711	-0.00557
N	-1.20617	-0.60360	-0.01899
C	-0.47491	0.52166	0.02711
N	0.82052	0.26118	0.01545
H	-0.51906	-2.63257	-0.10362
N	3.46218	0.98712	0.05357
H	2.63600	-1.34689	-0.06074
H	3.24549	3.01579	-0.22871
C	3.98446	2.32725	0.18610
H	3.87096	-3.32306	0.21331
H	2.41895	0.83586	0.04485
C	5.77302	-2.34161	0.54108
H	-0.90154	1.51299	0.06846
H	6.41221	-3.21569	0.39828
H	7.32676	-0.85144	0.67416
H	6.59809	1.60356	0.96907
H	4.12064	2.59067	1.24400
H	5.57449	-2.23911	1.61250



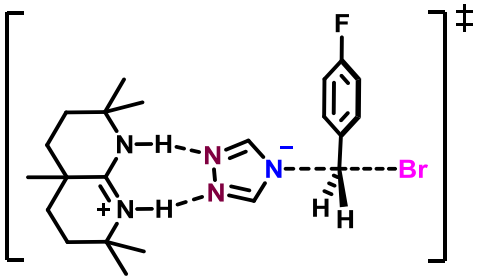
E = -3804.60569908

H = -3804.042955

G = -3804.137327

C	-2.181966	3.010211	0.165617
N	-1.285369	2.038774	0.061983
N	-1.625012	4.219257	0.346477
C	-0.322159	3.920712	0.347671
N	-0.065298	2.619235	0.180448
H	-3.246188	2.826487	0.109031
H	0.464472	4.653955	0.471741
H	-0.708696	-0.067969	0.706391
H	-0.816548	0.124432	-1.128689
C	-1.291182	-0.095060	-0.192240
C	-2.734356	-0.287206	-0.129846
C	-3.368984	-0.495677	1.095720
C	-3.505137	-0.225375	-1.291478
C	-4.744767	-0.642041	1.167333
C	-4.882604	-0.369502	-1.238963
C	-5.476710	-0.575226	-0.005968
H	-2.774574	-0.550347	2.001465
H	-3.016674	-0.067908	-2.247255
H	-5.254159	-0.806419	2.109428
H	-5.496406	-0.326241	-2.130813
F	-6.810574	-0.714990	0.054838
Br	-0.503846	-2.388682	-0.446740
H	2.714257	-1.809385	3.336456
H	2.386654	0.631137	4.607199
C	2.956397	-1.094580	2.545333
H	3.940518	-0.686141	2.793753
H	3.769367	-2.582405	1.209808
H	0.541339	-0.960345	3.936349
C	3.005538	-1.798222	1.199307
C	2.303066	1.084513	3.615758
C	0.532032	-0.542392	2.926081
C	1.911650	0.026101	2.588706
H	2.047056	-2.280834	0.978178
H	3.264320	1.537825	3.359003

H	0.245598	-1.331835	2.224495
H	1.550219	1.876794	3.668514
H	5.472122	-1.013101	0.211575
H	-0.225785	0.247591	2.900019
H	4.831313	0.304225	1.207008
C	3.326928	-0.817407	0.068181
C	4.729435	-0.210567	0.250516
H	3.969742	-2.270716	-1.377140
N	1.815605	0.694271	1.279528
C	3.199139	-1.497154	-1.297708
H	2.226623	-1.999554	-1.345183
C	2.329043	0.304083	0.125239
H	4.966210	0.513196	-0.530732
H	1.133499	1.463838	1.194486
C	3.342062	-0.494277	-2.430193
N	1.979071	0.957577	-0.965696
H	4.345187	-0.057426	-2.423063
H	3.235431	-0.997128	-3.395165
H	0.617140	-0.743580	-2.601639
C	2.295796	0.624465	-2.364631
H	1.267681	1.693071	-0.803646
C	0.997159	0.183295	-3.041395
H	3.724698	2.250478	-2.522492
C	2.824618	1.892197	-3.029523
H	0.231962	0.960768	-2.947414
H	1.173451	0.018362	-4.107766
H	3.072421	1.690418	-4.075197
H	2.074546	2.688381	-3.006631



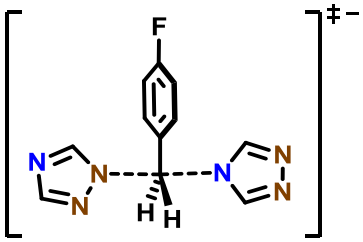
E = -3804.59503592

H = -3804.033198

G = -3804.130884

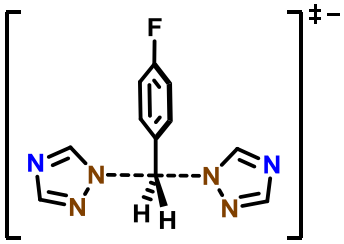
C	-3.630677	-1.193370	-0.034740
Br	-5.999442	-2.161774	0.031043
H	-4.182865	0.360355	-2.159729
C	-4.277441	0.890946	-1.218382
C	-4.618120	2.235376	-1.217350
H	-4.789350	2.780555	-2.138163
C	-4.749704	2.882401	-0.001337
F	-5.074581	4.188775	0.008646
C	-4.559074	2.231710	1.204924
H	-4.685811	2.774075	2.134568
C	-4.218855	0.887342	1.185358
H	-4.079580	0.353575	2.119342
C	-4.076914	0.201842	-0.021735
H	-3.594874	-1.741398	-0.959935
H	-3.545316	-1.742684	0.886397
C	-0.702798	-1.771404	-0.113056
N	0.492731	-1.209296	-0.137172
N	-1.684497	-0.854943	-0.085974
C	-1.025020	0.314678	-0.095652
N	0.284038	0.135713	-0.125918
H	-0.872980	-2.838684	-0.115400
H	-1.513543	1.277979	-0.080919
H	5.490612	-0.566242	-2.123533
H	3.810844	-3.137250	-1.951865
H	5.204476	1.164751	-2.119527
C	5.699065	0.356102	-1.579887
H	2.773005	3.035107	-1.940427
H	6.778418	0.534667	-1.603518
C	3.567939	-3.480985	-0.943013
H	5.847767	-2.303033	-1.015844
H	2.489527	-3.653398	-0.890299
C	2.433323	3.282890	-0.931357
H	4.075905	-4.433139	-0.767431
H	4.972235	2.916693	-1.006059

H	1.357529	3.095582	-0.876346
H	2.604233	4.348837	-0.758113
N	3.273579	-1.207062	-0.178258
C	3.741573	0.026448	-0.130721
C	5.230330	0.275230	-0.116375
C	5.515779	-2.228143	0.023770
N	2.897131	1.038569	-0.162826
C	4.004892	-2.452930	0.095997
H	2.229351	-1.324775	-0.186965
H	1.869168	0.806575	-0.169510
C	4.684862	2.734605	0.033568
C	3.183229	2.455035	0.107918
C	5.923775	-0.884972	0.602251
H	6.009155	-3.042038	0.562470
C	5.508840	1.595391	0.606776
H	7.007220	-0.747702	0.525279
H	6.577833	1.818795	0.529555
H	4.887787	3.663064	0.574681
C	3.588796	-2.919343	1.494423
C	2.639265	2.762272	1.506464
H	2.500217	-2.988668	1.565085
H	4.012414	-3.904613	1.707717
H	5.678824	-0.840580	1.669846
H	5.292727	1.469703	1.674118
H	1.587548	2.473415	1.578863
H	2.718709	3.832207	1.717560
H	3.930239	-2.220291	2.262724
H	3.190983	2.214061	2.275012



E = -852.808963
H = -852.585619
G = -852.649433

C	-0.01598	-0.78897	-0.00000
C	-3.83357	-1.96280	0.00000
C	-3.03708	-0.04589	0.00000
N	-2.01419	-0.90199	0.00000
N	-4.22032	-0.66950	0.00000
N	-2.51869	-2.14887	-0.00000
H	-4.53003	-2.79192	0.00000
H	-2.90215	1.02743	0.00000
H	0.01508	0.84929	2.13688
C	0.02120	1.39438	1.19911
C	0.04136	2.78312	1.20972
H	0.05081	3.34542	2.13630
C	0.05055	3.45163	0.00000
F	0.06952	4.80356	0.00000
C	0.04136	2.78313	-1.20972
H	0.05080	3.34543	-2.13630
C	0.02120	1.39438	-1.19911
H	0.01508	0.84929	-2.13687
C	0.01048	0.68564	0.00000
H	-0.05092	-1.33768	0.92449
H	-0.05092	-1.33768	-0.92449
H	2.84337	0.96515	-0.00000
C	2.98308	-0.10733	-0.00000
N	4.16473	-0.69897	-0.00000
N	1.96037	-0.98980	-0.00000
N	3.92041	-2.04112	-0.00000
C	2.60620	-2.17574	-0.00000
H	2.09614	-3.13060	-0.00000

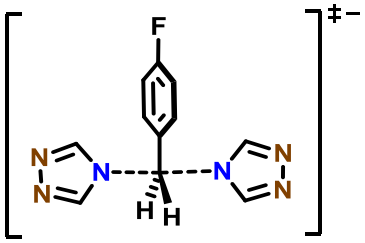


E = -852.815327

H = -852.59175

G = -852.655856

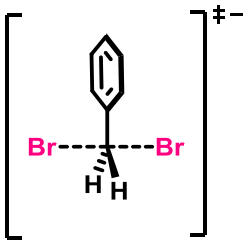
C	-0.02247	-0.80356	0.11832
C	3.82892	-1.27117	-0.77666
C	2.90273	-0.88216	1.03832
N	1.94405	-0.99290	0.12049
N	4.12458	-1.05486	0.52206
N	2.53206	-1.24155	-1.06236
H	4.57941	-1.45876	-1.53414
H	2.69767	-0.67240	2.07994
H	0.63129	0.65141	-2.04629
C	0.35024	1.27728	-1.20650
C	0.37095	2.66101	-1.32999
H	0.63698	3.14397	-2.26340
C	0.05438	3.42828	-0.22546
F	0.07340	4.77806	-0.33688
C	-0.28211	2.86344	0.99035
H	-0.53044	3.50125	1.83102
C	-0.30476	1.47879	1.09301
H	-0.59483	1.01288	2.02896
C	0.01345	0.67202	0.00272
H	0.00485	-1.41664	-0.76693
H	-0.08220	-1.28684	1.07991
H	-2.83060	0.69413	-0.98562
C	-2.99333	-0.22223	-0.43416
N	-4.18798	-0.77858	-0.20502
N	-1.99760	-0.92013	0.11233
C	-3.83608	-1.86201	0.51933
N	-2.53132	-1.98689	0.73317
H	-4.55124	-2.57861	0.90351



E = -852.801206
H = -852.578211
G = -852.642204

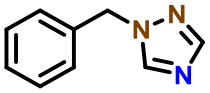
C	-0.00000	-0.81235	0.00000
N	3.99542	-1.97158	0.00000
C	3.00604	-0.06387	0.00000
N	2.00685	-0.97278	0.00000
N	4.20327	-0.62364	0.00000
C	2.68528	-2.14071	0.00000
H	2.83801	1.00458	0.00000
H	0.00000	0.82398	-2.13768
C	0.00000	1.36857	-1.19967
C	0.00000	2.75702	-1.20998
H	0.00000	3.31946	-2.13639
C	0.00000	3.42544	-0.00000
F	0.00000	4.77621	-0.00000
C	0.00000	2.75702	1.20998
H	0.00000	3.31946	2.13639
C	0.00000	1.36857	1.19967
H	0.00000	0.82398	2.13768
C	0.00000	0.66092	0.00000
H	-0.00000	-1.35402	-0.92862
H	-0.00000	-1.35402	0.92862
H	-2.83801	1.00458	0.00000
C	-3.00604	-0.06387	0.00000
N	-4.20327	-0.62364	0.00000
N	-2.00685	-0.97278	0.00000
N	-3.99542	-1.97158	0.00000
C	-2.68528	-2.14071	0.00000
H	-2.20417	-3.11082	0.00000
H	2.20416	-3.11082	0.00000

BnBr + 1,2,4-triazole derivatives



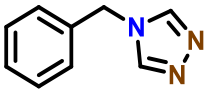
E = -5418.444028
H = -5418.315774
G = -5418.364173

C	0.16309	0.79232	-0.00348
Br	2.62359	1.38971	0.00112
Br	-2.36751	0.87626	-0.00867
H	0.33326	-0.82041	-2.13922
C	0.38758	-1.36672	-1.20360
C	0.52938	-2.74524	-1.20309
H	0.58646	-3.28183	-2.14537
C	0.59861	-3.44165	0.00026
H	0.70971	-4.52178	0.00121
C	0.52440	-2.74363	1.20237
H	0.57758	-3.27895	2.14560
C	0.38261	-1.36511	1.20045
H	0.32441	-0.81755	2.13511
C	0.31233	-0.65858	-0.00220
H	0.10880	1.33762	-0.92762
H	0.10504	1.33886	0.91969



E = -512.167287
H = -511.986799
G = -512.034394

C	0.44509	-1.09886	-0.76982
C	3.49551	0.29905	0.12097
C	1.55787	0.48821	0.86911
N	1.54361	-0.34057	-0.19058
N	2.78439	0.91722	1.09342
N	2.78776	-0.47458	-0.68063
H	4.56096	0.42340	-0.00755
H	0.66981	0.75111	1.42362
H	-0.69155	1.16090	-1.74012
C	-1.32126	0.67224	-1.00227
C	-2.54350	1.22916	-0.65364
H	-2.87102	2.15047	-1.12345
C	-3.34908	0.60484	0.29418
H	-4.30526	1.03953	0.56544
C	-2.92743	-0.57697	0.88948
H	-3.55215	-1.06870	1.62749
C	-1.70060	-1.13172	0.54026
H	-1.36930	-2.05427	1.00807
C	-0.88913	-0.51297	-0.40653
H	0.60090	-1.09159	-1.85087
H	0.51641	-2.13604	-0.42983

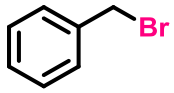


E = -512.153177

H = -511.974273

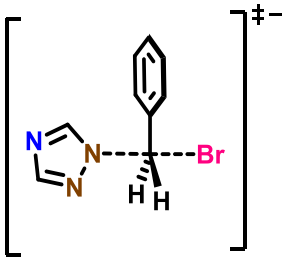
G = -512.018325

C	0.33811	1.37213	-0.00000
N	3.21555	-0.66789	0.68378
C	2.21918	0.07931	-1.07286
N	1.55399	0.59147	-0.00000
N	3.21555	-0.66790	-0.68377
C	2.21918	0.07931	1.07286
H	1.93977	0.28437	-2.09578
H	0.04120	-1.37580	-0.00001
C	-0.90519	-0.84522	-0.00000
C	-2.09658	-1.56452	-0.00000
H	-2.06583	-2.64889	-0.00000
C	-3.31622	-0.90194	0.00000
H	-4.24339	-1.46484	0.00000
C	-3.34295	0.48933	0.00000
H	-4.29134	1.01616	0.00001
C	-2.15552	1.20694	0.00000
H	-2.18277	2.29354	0.00000
C	-0.92771	0.54515	-0.00000
H	0.35946	2.02587	0.87695
H	0.35946	2.02586	-0.87696
H	1.93976	0.28437	2.09578



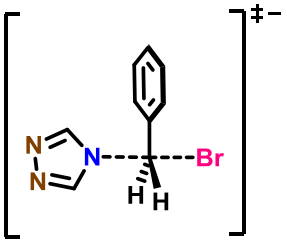
E = -2844.535141
H = -2844.407542
G = -2844.449276

C	-0.76588	-1.09287	0.00000
Br	1.04919	-1.86740	0.00000
H	-0.72724	0.55661	2.14209
C	-0.72337	1.10077	1.20227
C	-0.69934	2.48881	1.20324
H	-0.69162	3.02813	2.14451
C	-0.68687	3.18582	0.00000
H	-0.66877	4.27053	0.00000
C	-0.69934	2.48881	-1.20324
H	-0.69162	3.02813	-2.14451
C	-0.72337	1.10077	-1.20227
H	-0.72724	0.55661	-2.14209
C	-0.73599	0.39391	0.00000
H	-1.24073	-1.49864	0.89092
H	-1.24073	-1.49864	-0.89092



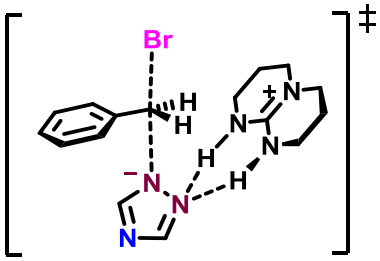
E = -3086.035143
H = -3085.855911
G = -3085.911542

C	0.95005	-0.81066	-0.53689
Br	3.21827	-0.60962	-1.09472
C	-2.81471	-2.67251	-0.25213
C	-2.21097	-0.78730	0.36787
N	-1.14789	-1.37553	-0.17990
N	-3.30176	-1.56667	0.34971
N	-1.53006	-2.60270	-0.58654
H	-3.41343	-3.55321	-0.45211
H	-2.17557	0.21394	0.77791
H	1.23790	-0.15325	2.05194
C	0.90997	0.68671	1.44844
C	0.66644	1.91966	2.03607
H	0.80499	2.04366	3.10585
C	0.23953	2.99304	1.26006
H	0.04516	3.95728	1.71962
C	0.05919	2.81954	-0.10887
H	-0.27870	3.64956	-0.72196
C	0.30335	1.58564	-0.69424
H	0.15856	1.44620	-1.76049
C	0.73267	0.50528	0.07674
H	1.13237	-1.67175	0.08098
H	0.66775	-0.98325	-1.56011



E = -3086.030102
H = -3085.851005
G = -3085.906336

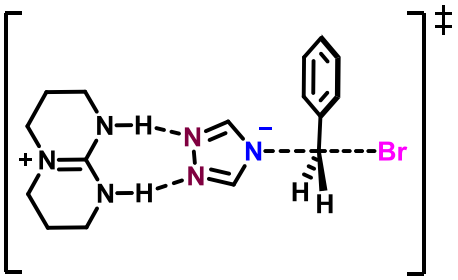
C	1.04872	-0.92072	0.07630
Br	3.42916	-0.82729	0.01170
N	-3.30675	-1.38747	0.16776
C	-1.60602	-2.68495	-0.00172
N	-1.07910	-1.44584	0.09412
N	-2.92889	-2.69220	0.03822
C	-2.18655	-0.68213	0.19714
H	-1.00724	-3.58217	-0.10120
H	0.77892	0.46984	2.35723
C	0.63143	1.08755	1.47756
C	0.31658	2.43193	1.60974
H	0.21711	2.86751	2.59916
C	0.12100	3.21910	0.47903
H	-0.12970	4.27033	0.58176
C	0.24312	2.64836	-0.78419
H	0.08606	3.25362	-1.67163
C	0.55803	1.30380	-0.91442
H	0.64835	0.85452	-1.89785
C	0.75733	0.50914	0.21451
H	1.08879	-1.54952	0.94678
H	1.03232	-1.38314	-0.89356
H	-2.15672	0.39555	0.29364



E = -3525.056194
H = -3524.643598
G = -3524.722839

H	-1.32521	-1.04564	2.29068
H	-1.47335	-0.29878	-2.38967
H	-3.06394	-1.84320	-0.95820
C	-2.23386	-0.51793	2.59694
H	-3.35464	-1.93109	1.43554
C	-2.20435	0.50547	-2.23353
C	2.54336	2.59934	-0.18556
N	-1.90018	1.24635	-1.02693
N	1.43863	1.87067	-0.10709
C	-3.65376	-0.92677	-0.83459
C	-2.25630	0.79253	0.18101
C	-3.33923	-0.85238	1.61549
H	-2.51469	-0.86431	3.59409
N	-3.12681	-0.21013	0.32143
N	2.29882	3.92009	-0.21325
C	0.96405	3.95054	-0.14858
N	0.39788	2.74139	-0.08472
H	3.52904	2.15569	-0.22093
N	-1.73677	1.41603	1.24097
H	-1.12229	1.91796	-0.99794
H	-1.11482	1.23814	3.19980
C	-1.98781	0.97881	2.59725
H	-2.14889	1.19571	-3.07736
H	-0.96907	2.06688	1.00733
C	-3.59531	-0.08141	-2.09123
H	0.38044	4.86211	-0.14658
H	-3.83654	-0.70615	-2.95394
H	-4.68725	-1.20399	-0.60410
H	-4.32185	-0.55649	2.00469
H	-2.84903	1.51427	3.01744
H	-4.33080	0.72796	-2.04297
H	0.54132	-0.00276	-1.10102
H	0.41613	0.00382	0.74604
C	0.96419	-0.24202	-0.14352

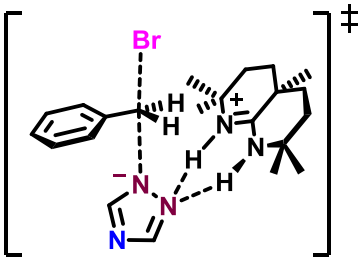
C	2.33777	-0.72459	-0.05182
C	3.08407	-0.94906	-1.20933
C	2.93488	-0.92101	1.19407
C	4.40436	-1.36426	-1.12269
C	4.25467	-1.33615	1.28161
C	4.99293	-1.55819	0.12302
H	2.61968	-0.79888	-2.17861
H	2.35528	-0.74630	2.09489
H	4.97740	-1.53713	-2.02744
H	4.71152	-1.48617	2.25407
H	6.02597	-1.88268	0.19114
Br	-0.28566	-2.32468	-0.21528



E = -3525.044483
H = -3524.632771
G = -3524.713763

C	0.07007	0.81374	-0.10075
Br	2.56107	1.37839	-0.15852
H	0.27634	-0.90251	-2.15760
C	0.31777	-1.40131	-1.19474
C	0.43056	-2.78222	-1.12538
H	0.47125	-3.36650	-2.03894
C	0.50125	-3.41653	0.11138
H	0.59578	-4.49615	0.16568
C	0.46235	-2.65862	1.27798
H	0.52790	-3.14619	2.24525
C	0.34959	-1.27770	1.20840
H	0.33332	-0.68273	2.11579
C	0.28076	-0.63553	-0.02868
H	0.08524	1.31623	-1.05211
H	0.10607	1.41130	0.79334
H	-8.48969	-1.46688	-1.65261
H	-7.51270	3.48096	-1.34580
H	-9.88283	2.26305	-1.06050
C	-8.68057	-1.57602	-0.58044
H	-10.37123	-0.24525	-0.73390

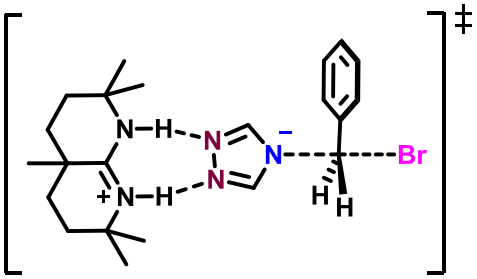
C	-7.35419	3.24719	-0.28397
C	-2.72848	1.85558	-0.13082
N	-6.70450	1.96638	-0.13075
N	-3.99918	1.49554	-0.10102
C	-9.50418	2.06081	-0.04923
C	-7.38304	0.82325	-0.05834
C	-9.50703	-0.40852	-0.08162
H	-9.23254	-2.50627	-0.42875
N	-8.73333	0.82528	-0.06197
N	-1.90857	0.79333	-0.07821
C	-2.74831	-0.25230	-0.01396
N	-4.01121	0.13691	-0.02587
H	-2.38852	2.87958	-0.19037
N	-6.70774	-0.32048	0.01805
H	-5.65272	1.91763	-0.12504
H	-6.69278	-2.36392	-0.23753
C	-7.36115	-1.60000	0.16496
H	-6.68703	4.01042	0.12182
H	-5.65340	-0.27390	0.00996
C	-8.67821	3.22691	0.45337
H	-2.42133	-1.28029	0.04033
H	-9.22693	4.15831	0.29704
H	-10.37313	1.90069	0.59749
H	-9.89292	-0.61117	0.92681
H	-7.52660	-1.83486	1.22546
H	-8.49420	3.11871	1.52682



E = -3705.425589
H = -3704.855514
G = -3704.947674

C	-2.54003	2.86147	0.19206
N	-1.59531	1.93979	0.06722
N	-2.04502	4.09179	0.40829
C	-0.72884	3.85894	0.40879
N	-0.40627	2.57686	0.20836
H	-3.59309	2.62467	0.12531
H	0.01958	4.62696	0.55680
H	-0.90714	-0.14734	0.65469
H	-1.06057	0.07232	-1.17427
C	-1.50616	-0.18372	-0.23255
C	-2.94121	-0.43542	-0.14572
C	-3.54131	-0.69007	1.08828
C	-3.73529	-0.37692	-1.29144
C	-4.91129	-0.88350	1.17497
C	-5.10608	-0.57011	-1.20558
C	-5.69742	-0.82288	0.02809
H	-2.92415	-0.74099	1.97939
H	-3.26860	-0.18237	-2.25179
H	-5.36986	-1.08213	2.13790
H	-5.71607	-0.52407	-2.10153
H	-6.76963	-0.97428	0.09586
Br	-0.63405	-2.43581	-0.53475
H	2.50347	-1.80695	3.31489
H	2.06409	0.58826	4.63770
C	2.72958	-1.06427	2.54499
H	3.69351	-0.62471	2.81839
H	3.61834	-2.48714	1.18700
H	0.29104	-1.05361	3.90341
C	2.82545	-1.73226	1.18347
C	1.97686	1.06182	3.65604
C	0.28058	-0.61519	2.90184
C	1.64158	0.01408	2.59866
H	1.88935	-2.24501	0.93560
H	2.92319	1.55809	3.42446

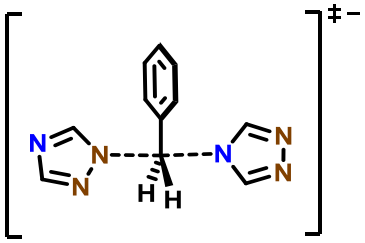
H	0.03616	-1.40058	2.18014
H	1.19288	1.82277	3.71607
H	5.27437	-0.82718	0.25930
H	-0.50785	0.14419	2.87898
H	4.56496	0.44206	1.27067
C	3.12594	-0.71242	0.08146
C	4.49997	-0.05536	0.30184
H	3.85098	-2.10244	-1.38699
N	1.53848	0.70926	1.30407
C	3.04745	-1.36374	-1.30187
H	2.09777	-1.90486	-1.37693
C	2.08291	0.36675	0.14840
H	4.72119	0.69393	-0.45966
H	0.82686	1.45196	1.22652
C	3.16470	-0.32880	-2.40811
N	1.72092	1.03004	-0.93217
H	4.14799	0.15002	-2.37448
H	3.09429	-0.81234	-3.38620
H	0.45491	-0.68982	-2.62321
C	2.07044	0.74233	-2.33322
H	0.97559	1.73086	-0.76384
C	0.80119	0.26148	-3.03794
H	3.43047	2.43079	-2.43483
C	2.55333	2.04613	-2.96236
H	0.00225	1.00335	-2.93824
H	0.99886	0.12739	-4.10491
H	2.82330	1.87871	-4.00863
H	1.76956	2.80890	-2.93248



E = -3705.414638
H = -3704.845477
G = -3704.940742

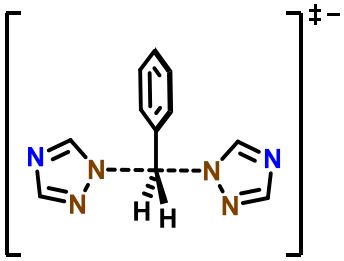
C	-3.85091	-0.85797	-0.03967
Br	-6.26760	-1.68882	0.04349
H	-4.32661	0.72446	-2.15858
C	-4.38353	1.26194	-1.21758
C	-4.64167	2.62495	-1.20379
H	-4.78145	3.15674	-2.13935
C	-4.73113	3.30730	0.00588
H	-4.93948	4.37215	0.01694
C	-4.56499	2.61493	1.20175
H	-4.64531	3.13885	2.14869
C	-4.30677	1.25196	1.18774
H	-4.19112	0.70643	2.11870
C	-4.21770	0.56173	-0.02191
H	-3.85138	-1.40548	-0.96603
H	-3.78786	-1.41207	0.88060
C	-0.95765	-1.58646	-0.13642
N	0.26476	-1.08552	-0.16393
N	-1.89139	-0.62162	-0.10485
C	-1.17432	0.51340	-0.11514
N	0.12407	0.26848	-0.15019
H	-1.18161	-2.64376	-0.13953
H	-1.61538	1.49938	-0.09715
H	5.30959	-0.69440	-2.10676
H	3.49752	-3.17618	-1.95938
H	5.10853	1.04859	-2.10290
C	5.55645	0.21595	-1.55897
H	2.77204	3.03917	-1.94593
H	6.64348	0.34139	-1.56959
C	3.22610	-3.50921	-0.95421
H	5.56307	-2.44875	-0.99869
H	2.13981	-3.62674	-0.91408
C	2.43431	3.30241	-0.94011
H	3.68318	-4.48624	-0.77536
H	4.95262	2.80860	-0.98805

H	1.34994	3.16934	-0.89711
H	2.65709	4.35811	-0.76282
N	3.03855	-1.22494	-0.18695
C	3.56789	-0.01683	-0.13234
C	5.06712	0.15636	-0.10125
C	5.22379	-2.35855	0.03735
N	2.77584	1.03656	-0.17146
C	3.70272	-2.50657	0.09222
H	1.98904	-1.28934	-0.20505
H	1.73662	0.85649	-0.18653
C	4.64476	2.63981	0.04799
C	3.13016	2.43602	0.10538
C	5.69279	-1.03850	0.62283
H	5.66935	-3.19712	0.57989
C	5.40368	1.45957	0.62797
H	6.78263	-0.95624	0.55839
H	6.48342	1.62883	0.56346
H	4.88824	3.55607	0.59321
C	3.24782	-2.95422	1.48470
C	2.58725	2.76811	1.49870
H	2.15641	-2.96835	1.54300
H	3.61866	-3.96010	1.70012
H	5.43826	-0.98320	1.68767
H	5.16906	1.34315	1.69247
H	1.52178	2.53179	1.55940
H	2.71784	3.83245	1.71280
H	3.61539	-2.27483	2.25855
H	3.10278	2.19189	2.27188



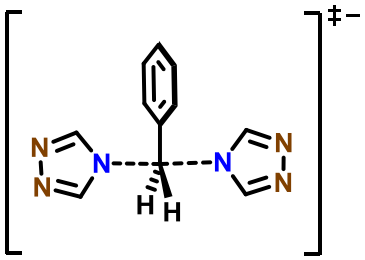
E = -753.62715
H = -753.396453
G = -753.458267

C	-0.11215	0.74809	-0.11944
C	-3.99222	-0.14244	0.22636
C	-2.35138	-1.40275	0.05624
N	-1.89517	-0.14987	0.03234
N	-3.68255	-1.45551	0.17856
N	-2.95058	0.67699	0.14200
H	-5.00546	0.22660	0.32544
H	-1.69995	-2.26326	-0.01656
H	0.52349	-0.62410	-2.34410
C	0.88580	-1.11080	-1.44440
C	1.58813	-2.30583	-1.52828
H	1.77459	-2.75445	-2.49908
C	2.05294	-2.92622	-0.37320
H	2.60277	-3.85994	-0.43766
C	1.80942	-2.34072	0.86494
H	2.16950	-2.81671	1.77173
C	1.10681	-1.14564	0.94582
H	0.91689	-0.68612	1.91038
C	0.63815	-0.51941	-0.20729
H	-0.49811	1.22040	-1.00560
H	-0.32785	1.19356	0.83574
H	3.22340	0.63597	-0.42948
C	2.81968	1.63797	-0.37756
N	3.55344	2.73602	-0.42941
N	1.50081	1.90035	-0.25179
N	2.68316	3.78251	-0.33370
C	1.47838	3.25028	-0.23006
H	0.56785	3.82846	-0.13744



E = -753.632821
H = -753.401894
G = -753.463985

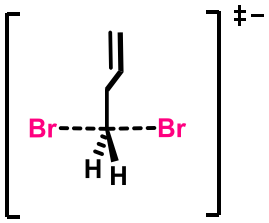
C	-0.00303	-0.79479	-0.00187
C	-3.82398	-1.89943	0.25751
C	-2.98252	-0.08551	-0.29850
N	-1.98187	-0.91004	0.01482
N	-4.17968	-0.66616	-0.16180
N	-2.51548	-2.08965	0.37748
H	-4.53947	-2.68031	0.48343
H	-2.82079	0.93593	-0.61556
H	-0.14999	0.84127	2.12927
C	-0.06723	1.39085	1.19711
C	-0.05059	2.77955	1.20035
H	-0.11371	3.31726	2.14149
C	0.04120	3.48086	0.00241
H	0.05242	4.56639	0.00350
C	0.11848	2.78021	-1.19693
H	0.19273	3.31838	-2.13700
C	0.10640	1.39145	-1.19647
H	0.17779	0.84215	-2.12974
C	0.01225	0.68241	-0.00039
H	-0.02225	-1.35196	0.91933
H	0.00469	-1.35039	-0.92419
H	2.84992	0.87604	0.61523
C	2.99049	-0.14788	0.29612
N	4.17539	-0.75290	0.15823
N	1.97301	-0.95091	-0.01883
C	3.79427	-1.97770	-0.26354
N	2.48211	-2.14058	-0.38386
H	4.49346	-2.77276	-0.49104



E = -753.619623
H = -753.389258
G = -753.450927

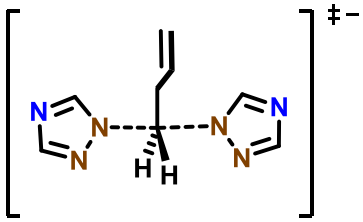
C	0.00574	-0.80771	-0.00991
N	-3.99863	-1.93690	-0.02379
C	-2.99378	-0.03692	-0.01387
N	-2.00222	-0.95383	-0.01520
N	-4.19563	-0.58710	-0.01888
C	-2.68976	-2.11629	-0.02144
H	-2.81568	1.02985	-0.00921
H	0.00894	0.81590	2.13388
C	0.01389	1.36785	1.19965
C	0.02088	2.75621	1.20638
H	0.02138	3.29050	2.15119
C	0.02722	3.46091	0.00711
H	0.03269	4.54628	0.01144
C	0.02652	2.76577	-1.19774
H	0.03144	3.30755	-2.13827
C	0.01953	1.37739	-1.20208
H	0.01897	0.83288	-2.14068
C	0.01316	0.66636	-0.00403
H	0.00083	-1.35310	0.91674
H	0.00519	-1.34572	-0.94087
H	2.84551	1.00130	0.00396
C	3.01286	-0.06722	0.00010
N	4.20911	-0.62949	0.00068
N	2.01212	-0.97408	-0.00586
N	3.99853	-1.97724	-0.00518
C	2.68792	-2.14341	-0.00893
H	2.20462	-3.11244	-0.01392
H	-2.21624	-3.09015	-0.02420

AllyBr + 1,2,4-triazole derivatives



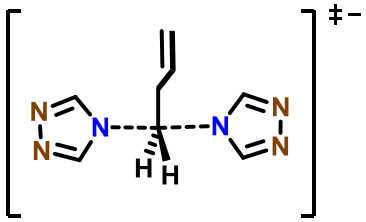
E = -5264.920078
H = -5264.84218
G = -5264.884559

C	-0.31356	-0.01284	0.02034
Br	-2.81267	-0.48081	0.10146
Br	2.21947	-0.24318	-0.02230
C	-0.42567	2.44090	0.17348
H	-0.39746	2.40905	1.25826
C	-0.39060	1.32113	-0.55022
H	-0.28783	-0.88374	-0.60555
H	-0.28079	-0.15078	1.08801
H	-0.41974	1.37282	-1.63463
H	-0.48331	3.41582	-0.29792



E = -600.107977
H = -599.927543
G = -599.982047

C	-0.35071	0.04338	0.25118
C	3.43898	-1.15299	-0.05650
C	2.63890	0.75575	0.09160
N	1.61845	-0.10153	0.05761
N	3.82392	0.13907	0.02289
N	2.12532	-1.34309	-0.03891
H	4.13644	-1.97805	-0.13130
H	2.49935	1.82604	0.15530
C	-0.38487	2.51240	0.05206
H	-0.27923	2.63344	1.12696
C	-0.43283	1.30468	-0.50421
H	-0.39259	-0.92089	-0.22918
H	-0.24475	0.06815	1.32360
H	-0.53877	1.20286	-1.58092
H	-0.44944	3.41477	-0.54710
N	-4.48996	0.09037	0.84547
C	-3.32168	0.72083	0.68135
H	-3.18478	1.79274	0.71770
C	-4.11308	-1.19723	0.69069
N	-2.31781	-0.12459	0.44707
N	-2.81932	-1.37206	0.45030
H	-4.80205	-2.03041	0.75305

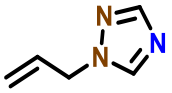


E = -600.094816
H = -599.914931
G = -599.969857

C	-0.35284	0.01733	0.22646
N	3.63239	-1.15103	0.02492
C	2.64807	0.75874	0.06784
N	1.64676	-0.14572	0.05891
N	3.84423	0.19625	0.04726
C	2.32154	-1.31517	0.03316
H	2.48067	1.82689	0.07870
C	-0.37344	2.48412	0.08321
H	-0.27298	2.57924	1.16077
C	-0.42474	1.29174	-0.50283
H	-0.39928	-0.91952	-0.29961
H	-0.25262	0.00954	1.29825
H	-0.52536	1.21434	-1.58160
H	-0.43020	3.39987	-0.49537
N	-4.51136	0.17184	0.82839
C	-3.33539	0.74126	0.62721
H	-3.17507	1.81036	0.60744
N	-4.29953	-1.17421	0.76644
N	-2.34787	-0.15739	0.43235
C	-3.00894	-1.33075	0.53147
H	-2.52931	-2.29655	0.43199
H	1.83738	-2.28379	0.02377

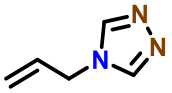
E = -2691.01318
H = -2690.936164
G = -2690.971174

C	0.53707	0.85307	0.05076
Br	2.30801	1.58586	-0.39854
C	0.34610	-1.33642	1.18766
H	0.14471	-0.85557	2.14097
C	0.56936	-0.62706	0.08585
H	-0.12021	1.23804	-0.72828
H	0.26846	1.28551	1.01309
H	0.78238	-1.12782	-0.85563
H	0.35734	-2.42069	1.17365



E = -358.644979
H = -358.515149
G = -358.555608

C	0.33347	0.10141	0.16987
C	3.52156	-1.23544	-0.17200
C	2.79090	0.69599	0.11334
N	1.75569	-0.15921	0.03071
N	3.93028	0.04649	-0.01473
N	2.21388	-1.41007	-0.15059
H	4.20122	-2.06340	-0.31148
H	2.66518	1.75898	0.25694
C	-0.66533	2.38109	0.12092
H	-0.88915	2.33610	1.18345
C	-0.06263	1.37580	-0.50276
H	-0.16581	-0.75603	-0.28867
H	0.06358	0.12016	1.23063
H	0.15889	1.44235	-1.56626
H	-0.96325	3.27936	-0.40869

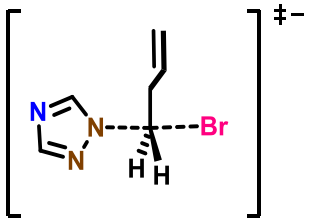


E = -358.630517

H = -358.501297

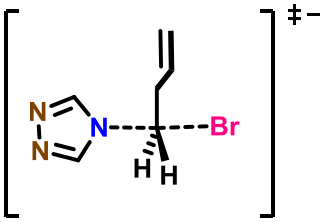
G = -358.542099

C	0.36790	0.09223	0.27773
N	3.63845	-1.25603	-0.41719
C	2.83592	0.64445	0.20217
N	1.77489	-0.19618	0.04991
N	3.95352	0.02845	-0.07248
C	2.34162	-1.37184	-0.33875
H	2.73616	1.67702	0.50086
C	-0.65737	2.35316	0.08982
H	-0.82198	2.39794	1.16320
C	-0.08333	1.30074	-0.48010
H	-0.19032	-0.79122	-0.04738
H	0.18632	0.21950	1.34941
H	0.08282	1.27719	-1.55531
H	-0.98760	3.20404	-0.49566
H	1.77032	-2.26436	-0.54795



E = -2932.510569
H = -2932.381803
G = -2932.430814

C	0.26050	0.86064	0.12089
Br	2.51754	1.49158	0.02506
C	-3.89205	1.46233	-0.25800
C	-2.86204	-0.19675	0.43907
N	-1.94794	0.70000	0.07433
N	-4.11874	0.23332	0.25196
N	-2.60803	1.78330	-0.38225
H	-4.68522	2.14136	-0.54785
H	-2.59736	-1.16814	0.83603
C	0.43943	-1.44564	0.98450
H	0.32702	-1.10613	2.01005
C	0.43154	-0.58443	-0.03134
H	0.02731	1.48241	-0.72466
H	0.10928	1.28012	1.10160
H	0.54907	-0.94194	-1.05048
H	0.56199	-2.51092	0.82064



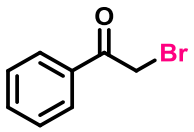
E = -2932.505628

H = -2932.376996

G = -2932.42603

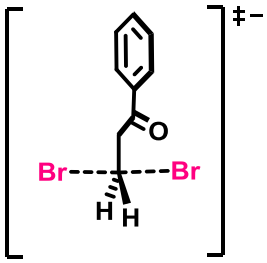
C	0.27392	0.86896	0.11683
Br	2.58058	1.47378	0.09766
N	-4.03558	1.47432	-0.20595
C	-2.80685	-0.20669	0.32134
N	-1.92889	0.77126	0.02280
N	-4.07036	0.17184	0.19749
C	-2.75327	1.79069	-0.29765
H	-2.50461	-1.20036	0.62511
C	0.38651	-1.42012	1.02424
H	0.22192	-1.06239	2.03623
C	0.43813	-0.57735	-0.00551
H	0.13075	1.47726	-0.75613
H	0.11541	1.31590	1.08328
H	0.60403	-0.95232	-1.01127
H	0.50940	-2.48870	0.88505
H	-2.40194	2.77093	-0.59663

PhCOCH$_2$Br + 1,2,4-triazole derivatives



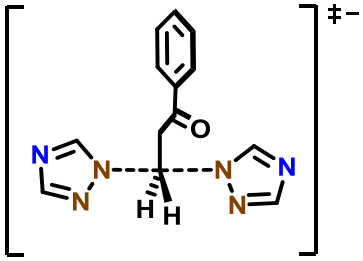
E = -2957.773678
H = -2957.634314
G = -2957.680461

C	-0.39536	0.88289	0.34596
O	-0.36707	1.28406	1.48804
C	-0.41193	-0.61355	0.09860
H	0.30507	-0.92887	-0.65834
Br	-2.16966	-1.18478	-0.52181
H	-0.23167	-1.12348	1.04088
H	-0.44970	3.50816	0.48836
C	-0.40906	3.18605	-0.54614
C	-0.38513	1.81454	-0.81271
C	-0.33124	1.37416	-2.13698
H	-0.33080	0.31498	-2.36750
C	-0.29892	2.29255	-3.17733
H	-0.25904	1.94423	-4.20362
C	-0.32323	3.65510	-2.90302
H	-0.30010	4.37146	-3.71770
C	-0.37955	4.10133	-1.58530
H	-0.40010	5.16462	-1.37187



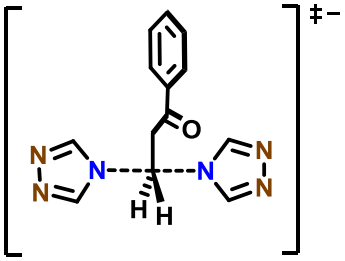
E = -5531.690864
H = -5531.550803
G = -5531.603195

C	-0.21028	-0.24593	0.91301
O	-0.27767	-0.46020	2.10489
C	0.16448	-1.31795	-0.04999
H	0.20795	-1.15842	-1.11047
Br	-2.20578	-1.87663	-0.40783
H	0.36177	-2.29671	0.35143
H	-1.73271	1.55284	2.07016
C	-1.36515	1.93383	1.12378
C	-0.54054	1.10839	0.36163
C	-0.04425	1.57322	-0.85457
H	0.63682	0.95570	-1.42859
C	-0.37715	2.84488	-1.30393
H	0.02365	3.20376	-2.24688
C	-1.21433	3.65799	-0.54793
H	-1.47890	4.64900	-0.90502
C	-1.70874	3.19867	0.66943
H	-2.36462	3.82856	1.26292
Br	2.56166	-0.77403	0.02516



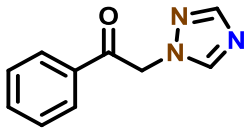
E = -866.88486
H = -866.641833
G = -866.706147

C	-0.02492	-0.17424	0.96498
O	-0.09538	-0.35886	2.16536
C	0.08773	-1.32425	0.02551
H	0.10516	-1.22229	-1.04930
H	0.12020	-2.30766	0.46431
C	2.99349	-1.28012	0.90983
C	3.89751	-1.01724	-0.94118
N	2.59740	-1.00722	-1.20449
N	4.20803	-1.18573	0.36242
N	2.02359	-1.18136	-0.00056
H	2.79112	-1.40947	1.96418
H	4.64075	-0.89897	-1.71925
H	-0.92538	1.96419	2.20011
C	-0.59271	2.22179	1.20047
C	-0.08107	1.20441	0.39478
C	0.36530	1.50267	-0.89210
H	0.80413	0.72752	-1.51039
C	0.29445	2.80791	-1.36333
H	0.65370	3.03678	-2.36156
C	-0.23117	3.81579	-0.56321
H	-0.29300	4.83257	-0.93987
C	-0.67621	3.52063	0.72267
H	-1.08929	4.30487	1.34965
H	-2.72655	-1.51683	1.80590
N	-4.04669	-1.54226	0.10803
C	-2.86899	-1.48491	0.73450
C	-3.66289	-1.44230	-1.18402
N	-1.85212	-1.36442	-0.12145
H	-4.35891	-1.44983	-2.01310
N	-2.35410	-1.33166	-1.36754



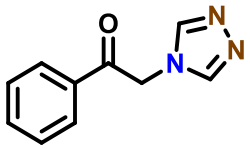
E = -866.867078
H = -866.624827
G = -866.69054

C	0.02091	-0.17783	0.88800
O	0.00830	-0.41264	2.07847
C	0.15848	-1.28113	-0.10442
H	0.15771	-1.11003	-1.16805
H	0.22773	-2.28771	0.27016
C	3.04089	-0.94634	0.84587
N	4.17252	-1.10089	-0.97629
C	2.88327	-1.19372	-1.23941
N	4.27432	-0.93958	0.37497
N	2.11792	-1.10396	-0.12900
H	2.78341	-0.83023	1.88939
H	-1.21821	1.78711	2.12289
C	-0.82553	2.12848	1.17156
C	-0.13732	1.21482	0.37456
C	0.38601	1.62761	-0.84957
H	0.96229	0.93534	-1.45231
C	0.21876	2.94030	-1.27159
H	0.64431	3.26015	-2.21723
C	-0.48548	3.84246	-0.48230
H	-0.62408	4.86535	-0.81863
C	-1.00867	3.43391	0.74097
H	-1.56213	4.13513	1.35741
H	-2.42582	-2.08370	1.73996
N	-3.92868	-1.81612	0.25874
C	-2.69739	-1.80305	0.73165
N	-3.85077	-1.37468	-1.03227
N	-1.79896	-1.37732	-0.18404
C	-2.57711	-1.12172	-1.25914
H	-2.19272	-0.74625	-2.19873
H	2.47989	-1.33769	-2.23429



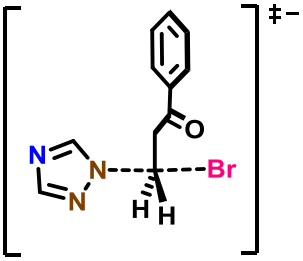
E = -625.407755
H = -625.215629
G = -625.267038

C	-0.31354	-0.35926	0.83753
O	-0.88662	-0.79040	1.81364
C	0.64650	-1.28344	0.08697
H	0.29912	-1.45622	-0.93369
H	0.66242	-2.23604	0.61908
C	2.80690	-0.32602	0.96034
C	3.73193	-0.02650	-0.88423
N	2.56587	-0.54628	-1.21619
N	3.93008	0.12952	0.44698
N	1.98056	-0.73838	-0.01890
H	2.55066	-0.37951	2.00897
H	4.46367	0.24656	-1.63034
H	-1.62053	1.53568	2.11073
C	-1.24846	1.90169	1.16025
C	-0.51785	1.02705	0.34992
C	-0.03288	1.47040	-0.88361
H	0.54296	0.81262	-1.52508
C	-0.28036	2.77255	-1.29746
H	0.09577	3.11245	-2.25617
C	-1.00269	3.63780	-0.48437
H	-1.18941	4.65615	-0.80928
C	-1.48659	3.20131	0.74666
H	-2.05001	3.87776	1.38030



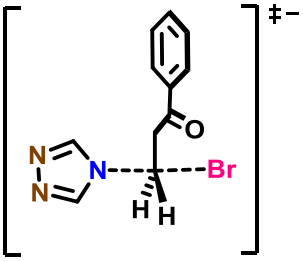
E = -625.391334
H = -625.199901
G = -625.251631

C	-0.15204	-0.12711	1.09748
O	-0.55926	-0.30435	2.22358
C	0.09186	-1.35535	0.21745
H	-0.65692	-1.37994	-0.58024
H	-0.05669	-2.23145	0.85154
C	2.60227	-1.08731	0.18349
N	3.00866	-1.56919	-1.87621
C	1.72318	-1.67184	-1.68632
N	3.56868	-1.19671	-0.68597
N	1.40220	-1.37634	-0.39486
H	2.71039	-0.80295	1.21985
H	-0.09053	2.08916	2.50662
C	0.08820	2.30028	1.45821
C	0.09947	1.23167	0.55661
C	0.31877	1.48039	-0.80075
H	0.33448	0.66978	-1.51930
C	0.52296	2.77812	-1.24755
H	0.69308	2.96438	-2.30209
C	0.51876	3.83351	-0.34297
H	0.68768	4.84629	-0.69351
C	0.30108	3.59346	1.01123
H	0.29825	4.41788	1.71594
H	0.99135	-1.95464	-2.42924



E = -3199.285735
H = -3199.094441
G = -3199.152759

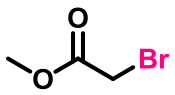
C	-0.25770	0.93486	0.43310
O	-0.21087	1.38974	1.55777
C	-0.32683	-0.53381	0.19749
H	-0.22944	-0.97050	-0.78153
Br	-2.63621	-0.61520	0.11067
H	-0.24505	-1.16757	1.06438
C	2.83075	-0.19604	0.83374
C	3.57932	-1.05931	-0.90022
N	2.26261	-1.04864	-1.07256
N	3.99675	-0.54056	0.27391
N	1.78829	-0.48798	0.05722
H	2.72065	0.27772	1.79973
H	4.25377	-1.45530	-1.64922
H	-1.09626	3.42662	0.39569
C	-0.74458	3.13635	-0.58834
C	-0.26572	1.83828	-0.75965
C	0.20797	1.43738	-2.00813
H	0.63411	0.44764	-2.13633
C	0.19445	2.33106	-3.07229
H	0.58074	2.01936	-4.03772
C	-0.30315	3.61837	-2.90331
H	-0.31973	4.30996	-3.74063
C	-0.77387	4.02076	-1.65650
H	-1.16319	5.02512	-1.51941



E = -3199.277345
H = -3199.086441
G = -3199.145819

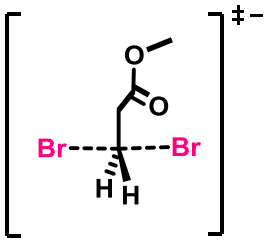
C	-0.43092	0.72191	0.29258
O	-0.52753	1.12570	1.43200
C	-0.30365	-0.73352	-0.00206
H	-0.07723	-1.09816	-0.98797
Br	-2.57044	-1.18001	-0.26549
H	-0.19340	-1.39643	0.83889
C	2.56254	0.03363	1.13340
N	3.93500	-0.43175	-0.45548
C	2.69171	-0.60600	-0.86481
N	3.85090	-0.01541	0.84362
N	1.78152	-0.32960	0.09384
H	2.16401	0.34448	2.08974
H	0.29583	3.24362	0.41212
C	0.03238	2.97986	-0.60608
C	-0.38133	1.67362	-0.86086
C	-0.72855	1.30550	-2.15954
H	-1.09415	0.30380	-2.35599
C	-0.65808	2.23440	-3.19011
H	-0.94152	1.94399	-4.19690
C	-0.22892	3.53180	-2.93351
H	-0.16419	4.25332	-3.74241
C	0.11704	3.90317	-1.63763
H	0.45854	4.91331	-1.43403
H	2.42818	-0.93038	-1.86363

MeOCOCH$_2$Br +1,2,4-triazole derivatives



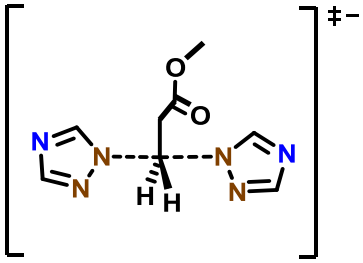
E = -2841.385864
H = -2841.296495
G = -2841.337764

C	-6.11115	-0.97759	-3.65666
O	-5.02404	-1.71864	-3.87403
O	-6.43050	-0.02588	-4.31714
C	-6.88331	-1.48211	-2.46730
C	-4.25128	-1.35425	-5.01819
H	-3.42077	-2.05636	-5.04672
H	-3.88739	-0.32963	-4.92232
H	-4.85527	-1.43610	-5.92374
H	-6.22160	-1.80145	-1.66509
Br	-7.93586	-3.03771	-2.97461
H	-7.58145	-0.71878	-2.13681



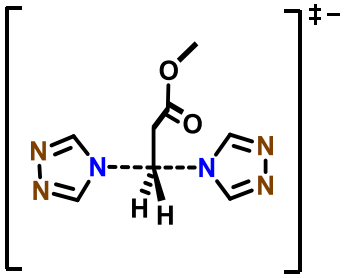
E = -5415.300295
H = -5415.210159
G = -5415.257069

C	-0.27120	0.86203	0.32556
O	-0.26852	1.53425	-0.83977
O	-0.28823	1.40183	1.40230
C	-0.25064	-0.59971	0.09112
C	-0.28742	2.94179	-0.70705
H	-0.28270	3.33671	-1.72309
H	0.59248	3.29088	-0.15963
H	-1.18606	3.26859	-0.17656
H	-0.23621	-0.99117	-0.90804
Br	-2.71118	-0.74042	0.01233
H	-0.25068	-1.24668	0.94785
Br	2.21372	-0.67863	0.05925



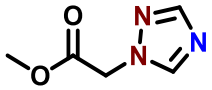
E = -750.491689
H = -750.298745
G = -750.358188

C	-0.32109	0.88455	0.29145
O	-0.34323	1.49324	-0.89887
O	-0.34448	1.47953	1.34352
C	-0.26510	-0.58957	0.15478
C	-0.39694	2.90881	-0.84661
H	-0.40875	3.24194	-1.88381
H	0.47737	3.31067	-0.32806
H	-1.29998	3.24329	-0.32947
H	-0.24637	-1.06338	-0.81507
H	-0.24371	-1.17243	1.05782
C	2.61485	-0.05500	0.93864
C	3.58963	-1.05221	-0.59916
N	2.30124	-1.18035	-0.88870
N	3.85010	-0.35831	0.53044
N	1.68220	-0.53218	0.11177
H	2.37072	0.51719	1.82334
H	4.36224	-1.47596	-1.22812
H	-2.97977	0.31436	1.81910
C	-3.17849	-0.27464	0.93405
N	-4.38657	-0.67058	0.52393
N	-2.21107	-0.67978	0.10869
C	-4.07253	-1.34271	-0.60521
N	-2.77768	-1.37292	-0.89271
H	-4.80984	-1.82371	-1.23536



E = -750.478183
H = -750.285843
G = -750.346892

C	0.00000	0.85597	-0.27773
O	0.00000	1.50919	0.89024
O	0.00000	1.40159	-1.35272
C	-0.00000	-0.61252	-0.07487
C	0.00001	2.92515	0.78210
H	0.00001	3.29937	1.80501
H	-0.88995	3.26975	0.25017
H	0.88996	3.26975	0.25017
H	-0.00000	-1.03130	0.91695
H	-0.00000	-1.24946	-0.94017
C	-2.85878	-0.36240	-1.02579
N	-4.03545	-1.00129	0.65604
C	-2.75562	-1.00972	0.97534
N	-4.10230	-0.58072	-0.64140
N	-1.96366	-0.61730	-0.04590
H	-2.57638	-0.00375	-2.00615
H	2.57637	-0.00376	-2.00616
C	2.85878	-0.36241	-1.02580
N	4.10230	-0.58074	-0.64141
N	1.96366	-0.61731	-0.04590
N	4.03545	-1.00131	0.65604
C	2.75562	-1.00973	0.97533
H	2.37720	-1.29613	1.94810
H	-2.37720	-1.29612	1.94811

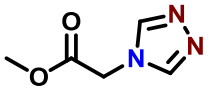


E = -509.020492

H = -508.878537

G = -508.925476

C	0.43879	1.28860	-0.13007
O	-0.72655	1.66601	-0.65775
O	1.26320	2.03194	0.32072
C	0.54178	-0.22574	-0.15283
C	-0.97320	3.07501	-0.65948
H	-1.95241	3.20050	-1.11635
H	-0.20770	3.59152	-1.24071
H	-0.97102	3.46235	0.36090
H	0.21948	-0.60582	-1.12228
H	-0.13591	-0.62772	0.60600
C	2.53192	-0.83368	1.25872
C	3.83646	-1.23355	-0.31682
N	2.71326	-0.92796	-0.93381
N	3.77668	-1.19318	1.03770
N	1.87704	-0.68329	0.09269
H	2.06852	-0.67201	2.22115
H	4.72850	-1.50087	-0.86395

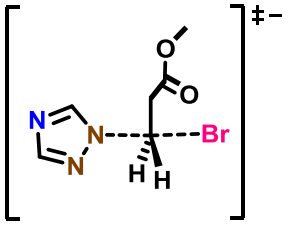


E = -509.005541

H = -508.86421

G = -508.912206

C	1.57391	0.38495	0.16299
O	1.28305	-0.88573	-0.12082
O	2.66402	0.79959	0.43354
C	0.30726	1.22007	0.08861
C	2.38965	-1.79287	-0.08865
H	1.97685	-2.76729	-0.34018
H	2.83734	-1.80872	0.90637
H	3.14519	-1.49425	-0.81715
H	-0.42690	0.80896	0.78596
H	-0.12330	1.11821	-0.91070
C	0.90668	3.59533	-0.47877
N	0.83819	4.47638	1.48423
C	0.52591	3.21749	1.60051
N	1.08085	4.71716	0.15923
N	0.53835	2.60470	0.38259
H	1.02555	3.44393	-1.54148
H	0.28155	2.70597	2.51978

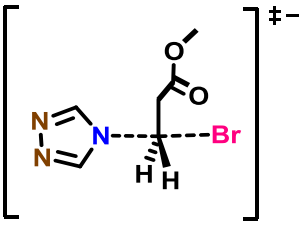


E = -3082.89305401

H = -3082.751816

G = -3082.805270

C	-0.301070	0.851453	0.319293
O	-0.324786	1.528137	-0.838728
O	-0.251848	1.386045	1.399814
C	-0.327066	-0.611117	0.088969
C	-0.258395	2.935758	-0.704652
H	-0.293164	3.332249	-1.719177
H	0.671739	3.233586	-0.213168
H	-1.102823	3.310536	-0.120069
H	-0.164193	-1.005978	-0.899248
Br	-2.625933	-0.832492	-0.011960
H	-0.233827	-1.243456	0.952425
C	2.747968	-0.014692	0.901867
C	3.699838	-1.030776	-0.637693
N	2.405697	-1.139649	-0.915750
N	3.979296	-0.337287	0.486873
N	1.799819	-0.477610	0.086923
H	2.520043	0.562669	1.787735
H	4.461622	-1.467775	-1.271601



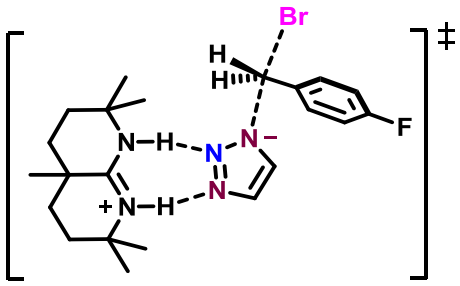
E = -3082.887293

H = -3082.746274

G = -3082.80023

C	-0.30247	0.86518	0.32882
O	-0.34971	1.49353	-0.85548
O	-0.21260	1.43764	1.38534
C	-0.36157	-0.60497	0.15621
C	-0.25167	2.90514	-0.78097
H	-0.30677	3.26093	-1.80942
H	0.69751	3.20128	-0.32701
H	-1.07256	3.31926	-0.18986
H	-0.31080	-1.03381	-0.82793
Br	-2.68698	-0.77192	0.20469
H	-0.24069	-1.21656	1.03062
C	2.68246	-0.14288	0.96643
N	3.82127	-0.97983	-0.65348
C	2.53024	-1.03241	-0.93003
N	3.92017	-0.40059	0.57942
N	1.76164	-0.51861	0.05337
H	2.42416	0.33206	1.90335
H	2.12989	-1.44101	-1.84931

p-F-BnBr +1,2,3-triazole derivatives



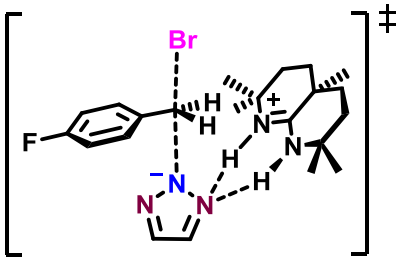
E = -3804.57995478

H = -3804.018239

G = -3804.114769

F	7.432808	-1.978747	0.042763
H	6.213505	-1.230337	-2.105756
C	6.211131	-1.417438	0.025549
H	6.028725	-1.502421	2.155598
C	5.657215	-1.060793	-1.191414
C	5.552264	-1.215328	1.225653
C	4.396140	-0.484968	-1.199996
C	4.292042	-0.638384	1.198449
H	3.947094	-0.186463	-2.141258
H	2.564064	-3.140320	-0.208917
C	3.701704	-0.265637	-0.009753
H	3.762254	-0.458258	2.127754
Br	2.931474	2.723380	0.168915
C	1.557086	-2.753672	-0.229469
C	2.349192	0.286199	-0.033158
H	0.073393	-4.429089	-0.340997
H	1.904082	0.591940	-0.962407
C	0.323711	-3.380291	-0.293726
N	1.300837	-1.437858	-0.192321
H	1.821226	0.467892	0.884995
N	-0.618518	-2.419407	-0.290709
N	0.002777	-1.255709	-0.228279
H	0.159599	2.120047	-1.163834
H	-0.117026	1.734166	1.301159
H	-1.148589	0.109191	-0.254394
H	-2.276734	-1.744102	-0.273472
H	-3.397409	-3.826277	-0.753440
H	-2.947344	-3.084023	1.631526
C	-0.821398	2.595335	-1.229462
C	-1.015948	2.351554	1.251130
H	-0.647323	3.672769	-1.172967
N	-1.999287	0.716290	-0.234570

H	-0.692699	3.389532	1.358100
H	-1.276410	2.361833	-2.196289
N	-3.182990	-1.234527	-0.198713
C	-4.344775	-3.280442	-0.745752
C	-3.937745	-2.621414	1.632099
H	-1.666394	2.090334	2.090997
C	-1.732604	2.160778	-0.086637
H	-4.544819	-2.926118	-1.760373
H	-4.669009	-3.366724	1.957454
H	-5.139148	-3.973308	-0.455107
H	-3.925954	-1.805412	2.359830
C	-3.152566	0.089429	-0.152393
C	-4.285531	-2.110112	0.230481
C	-3.039573	2.955181	-0.121925
H	-2.858895	3.921474	0.356323
H	-3.307835	3.173365	-1.159826
C	-4.445595	0.864762	-0.080742
C	-5.612750	-1.352085	0.238813
H	-4.246618	1.595783	-2.137134
H	-3.946905	2.076704	1.627110
H	-5.130219	0.084579	-2.011054
H	-5.134537	0.065524	1.796073
H	-6.034382	-1.342545	-0.770582
C	-4.178043	2.225264	0.565857
H	-6.319951	-1.906853	0.862089
C	-4.957242	1.043509	-1.520944
C	-5.457737	0.069470	0.748668
H	-5.096954	2.819240	0.525877
H	-5.900382	1.598150	-1.501641
H	-6.418890	0.593123	0.721841



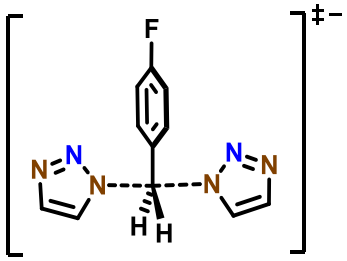
E = -3804.58137532

H = -3804.019186

G = -3804.113965

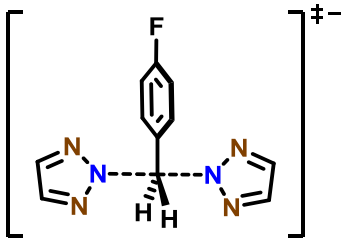
F	-6.782983	-0.766527	-0.009823
H	-5.601323	0.387580	-1.991281
C	-5.454655	-0.585017	-0.091969
H	-5.110323	-1.526420	1.798575
C	-4.935409	0.046381	-1.207791
C	-4.656083	-1.037268	0.945125
C	-3.564319	0.229203	-1.282165
C	-3.288354	-0.845440	0.853757
H	-3.133962	0.726244	-2.144618
C	-2.727121	-0.215016	-0.258339
H	-2.642130	-1.197847	1.650183
H	-2.210019	4.852130	1.444999
N	-2.189044	2.888020	0.638574
C	-1.642363	3.953030	1.259142
N	-1.257421	1.979938	0.575556
C	-1.294867	0.014570	-0.335014
H	-0.877336	0.519058	-1.185096
H	-0.659180	-0.219299	0.495395
C	-0.329955	3.638639	1.564293
H	-0.382549	-0.723350	2.749449
N	-0.109531	2.384760	1.119602
Br	-0.468766	-2.082659	-1.300457
H	0.439390	4.212776	2.059427
H	0.120004	-1.985759	1.599091
H	0.363596	1.894508	-2.480416
H	0.327000	-2.227911	3.347529
C	0.370920	-1.490016	2.541891
H	0.741028	0.168192	-2.697650
H	1.050497	0.972751	1.624265
C	1.136614	1.183854	-2.790594
H	1.308426	1.862856	-0.176055
H	1.346962	0.516270	4.108935
H	1.362917	1.377923	-3.842510
N	1.734733	0.207292	1.478086

C	1.766498	-0.866083	2.486393
N	2.021287	1.214239	-0.532840
H	2.194178	3.525640	-1.874984
C	2.102710	-0.223722	3.829021
H	2.134867	-0.987189	4.611071
H	1.991860	-2.493451	0.197170
C	2.310519	0.222160	0.290528
C	2.400193	1.363840	-1.948781
H	2.295587	-1.448110	-1.880363
H	2.529743	-2.860034	2.605467
C	2.949978	2.775928	-2.128190
C	2.813476	-1.923309	2.118118
H	3.075775	0.273412	3.789079
C	2.935828	-2.129115	0.617581
H	3.244845	2.932409	-3.169342
C	3.260995	-1.002785	-1.615652
C	3.313336	-0.827664	-0.095478
H	3.403751	0.176152	-3.415609
C	3.456505	0.322074	-2.333370
H	3.824353	2.936934	-1.491672
H	3.782398	-1.640665	2.540608
H	3.700722	-2.881434	0.399694
H	4.039695	-1.712775	-1.912393
H	4.454582	0.720353	-2.127171
C	4.702235	-0.339089	0.353083
H	4.751181	-0.179107	1.431209
H	4.978682	0.602101	-0.124541
H	5.448162	-1.092803	0.083576



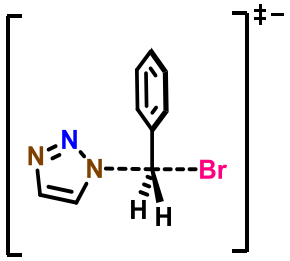
E = -852.766068
H = -852.543685
G = -852.606548

C	0.00000	-0.86715	-0.00001
N	3.90148	-1.36683	0.74669
C	2.86171	-0.75956	-1.10883
N	1.96554	-1.02156	-0.14274
C	4.09835	-0.98642	-0.53379
N	2.60089	-1.37850	0.96031
H	2.56978	-0.43418	-2.09611
H	-1.00299	0.77422	-1.88544
C	-0.54268	1.32418	-1.07124
C	-0.54289	2.71308	-1.08109
H	-0.96802	3.27521	-1.90484
C	0.00000	3.38109	0.00002
F	0.00000	4.73611	0.00003
C	0.54289	2.71307	1.08113
H	0.96802	3.27519	1.90488
C	0.54268	1.32417	1.07126
H	1.00299	0.77419	1.88545
C	0.00000	0.61734	0.00000
H	-0.12026	-1.41264	-0.92237
H	0.12026	-1.41265	0.92235
H	5.08987	-0.90055	-0.95514
C	-2.86171	-0.75957	1.10882
H	-2.56977	-0.43419	2.09610
N	-1.96553	-1.02157	0.14272
C	-4.09835	-0.98643	0.53378
N	-2.60089	-1.37851	-0.96032
N	-3.90148	-1.36684	-0.74670
H	-5.08987	-0.90056	0.95513



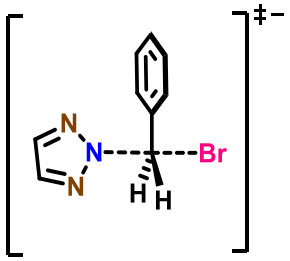
E = -852.771487
H = -852.548833
G = -852.612798

C	-0.00000	-0.89854	-0.00000
C	3.94911	-1.14066	-0.69491
N	2.67079	-1.07547	1.10401
N	1.95723	-1.04141	0.00000
C	3.94911	-1.14066	0.69491
N	2.67079	-1.07547	-1.10401
H	4.76700	-1.18326	-1.40021
H	0.00000	0.74106	-2.13615
C	0.00000	1.28792	-1.20033
C	0.00001	2.67662	-1.20944
H	0.00001	3.23909	-2.13628
C	0.00001	3.34438	0.00001
F	0.00001	4.70171	0.00001
C	0.00000	2.67662	1.20944
H	0.00001	3.23909	2.13629
C	0.00000	1.28792	1.20033
H	0.00000	0.74105	2.13616
C	0.00000	0.58092	0.00000
H	-0.00000	-1.43486	-0.93567
H	-0.00000	-1.43486	0.93567
H	4.76700	-1.18326	1.40021
H	-4.76700	-1.18325	1.40020
N	-2.67079	-1.07546	1.10401
C	-3.94911	-1.14065	0.69490
N	-1.95723	-1.04141	-0.00000
C	-3.94911	-1.14064	-0.69491
N	-2.67079	-1.07546	-1.10402
H	-4.76700	-1.18324	-1.40021



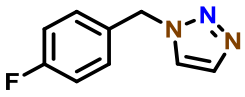
E = -3185.192837
H = -3185.021598
G = -3185.079422

C	0.24671	-0.86120	0.00000
Br	2.54297	-1.40251	0.00000
N	-3.90831	-1.66170	0.00000
C	-2.82169	0.26452	0.00000
N	-1.94260	-0.75496	0.00000
C	-4.07452	-0.32131	0.00000
N	-2.60843	-1.89848	0.00000
H	-2.50490	1.29731	0.00000
H	0.35558	0.76665	2.13683
C	0.38446	1.31179	1.19975
C	0.44847	2.69799	1.21002
H	0.47034	3.26023	2.13657
C	0.47962	3.36575	-0.00000
F	0.53981	4.71851	-0.00000
C	0.44847	2.69799	-1.21002
H	0.47034	3.26022	-2.13657
C	0.38446	1.31178	-1.19975
H	0.35558	0.76665	-2.13683
C	0.35357	0.60141	0.00000
H	0.08535	-1.39359	0.92007
H	0.08535	-1.39359	-0.92007
H	-5.05748	0.12912	0.00000



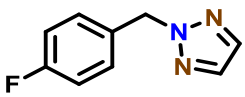
E = -3185.195024
H = -3185.023687
G = -3185.082136

C	-0.37548	-0.90767	0.00000
Br	-2.69804	-1.20634	0.00000
C	3.82362	-0.87489	-0.69454
N	2.54637	-0.98950	1.10193
N	1.82639	-1.06252	0.00000
C	3.82362	-0.87489	0.69454
N	2.54637	-0.98950	-1.10193
H	4.63954	-0.80029	-1.40009
H	-0.25921	0.71679	-2.13679
C	-0.23697	1.26330	-1.20075
C	-0.14092	2.64714	-1.21033
H	-0.09241	3.20824	-2.13657
C	-0.09784	3.31321	-0.00000
F	-0.00458	4.66560	-0.00000
C	-0.14092	2.64714	1.21032
H	-0.09241	3.20824	2.13657
C	-0.23697	1.26330	1.20075
H	-0.25921	0.71679	2.13679
C	-0.29058	0.55621	0.00000
H	-0.26432	-1.44795	-0.92369
H	-0.26432	-1.44795	0.92370
H	4.63954	-0.80029	1.40009



E = -611.320236
H = -611.147923
G = -611.197641

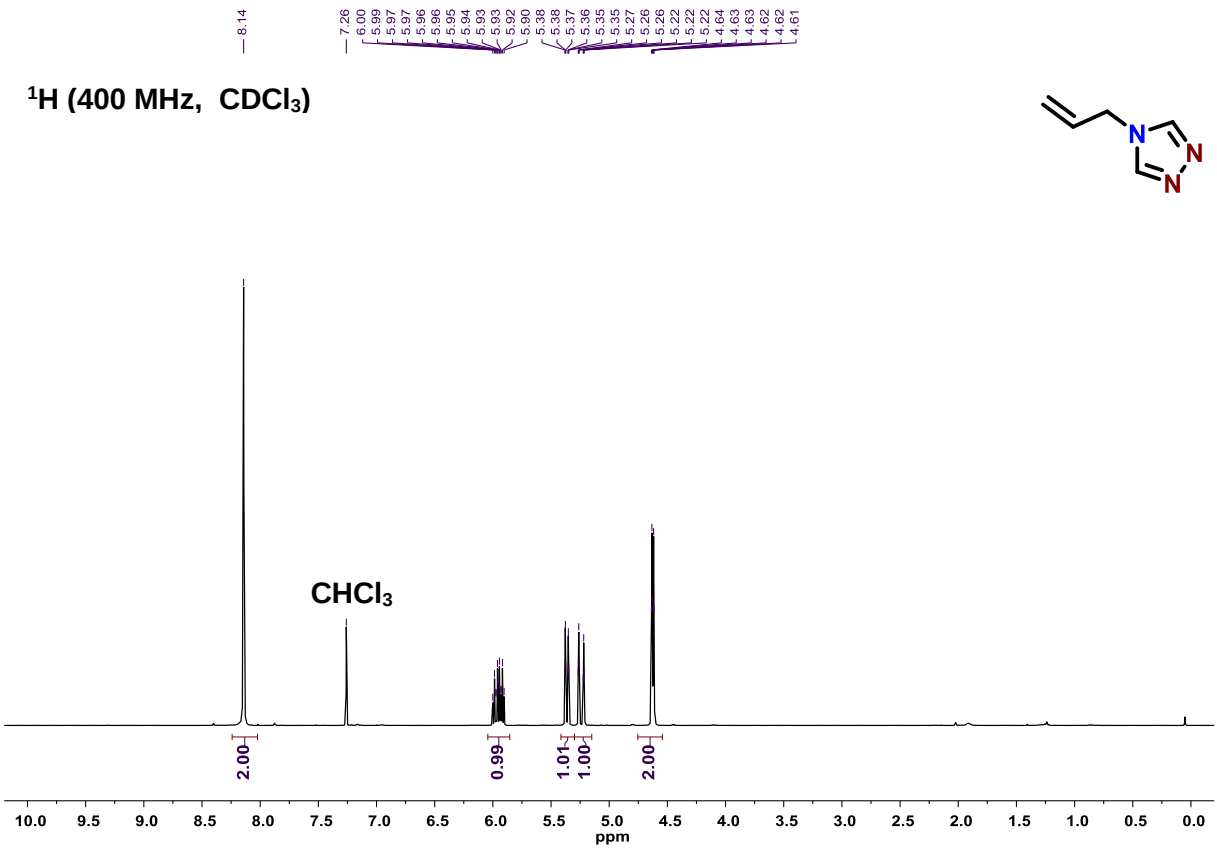
C	-0.39793	-1.18255	-0.68499
C	-3.03747	0.47208	1.06083
N	-2.38482	0.16021	-0.97129
N	-1.55215	-0.48953	-0.14950
N	-3.28527	0.73945	-0.24530
C	-1.91762	-0.31663	1.13841
H	0.21025	1.44593	-0.96189
C	1.04242	0.87556	-0.56043
C	2.23589	1.51664	-0.26566
H	2.36567	2.58013	-0.42838
C	3.28201	0.76795	0.24738
F	4.43905	1.38376	0.53494
C	3.17216	-0.58994	0.47657
H	4.01380	-1.13778	0.88356
C	1.96596	-1.21519	0.18025
H	1.86232	-2.28128	0.35967
C	0.89660	-0.49436	-0.34084
H	-0.39690	-2.21179	-0.31725
H	-0.55760	-1.21183	-1.76562
H	-1.36913	-0.74321	1.96208
H	-3.66729	0.85326	1.84885

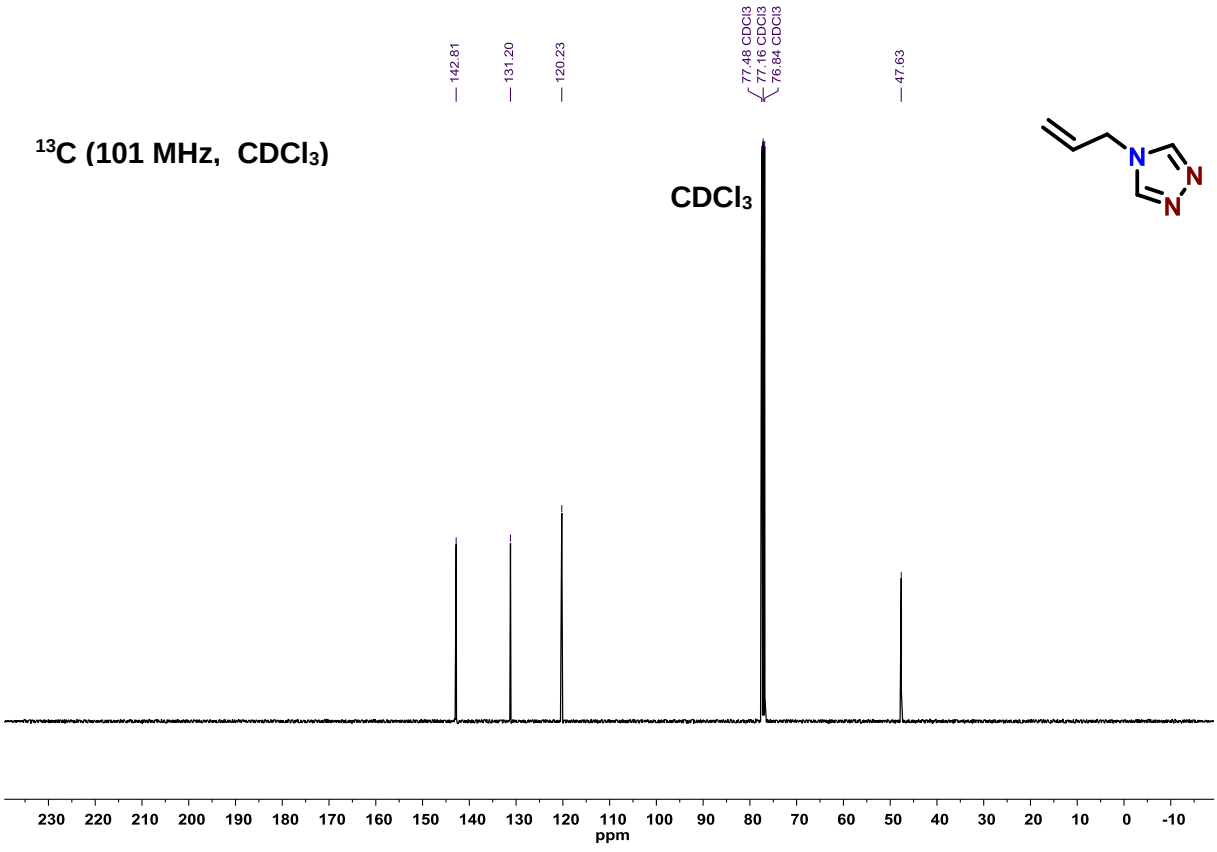


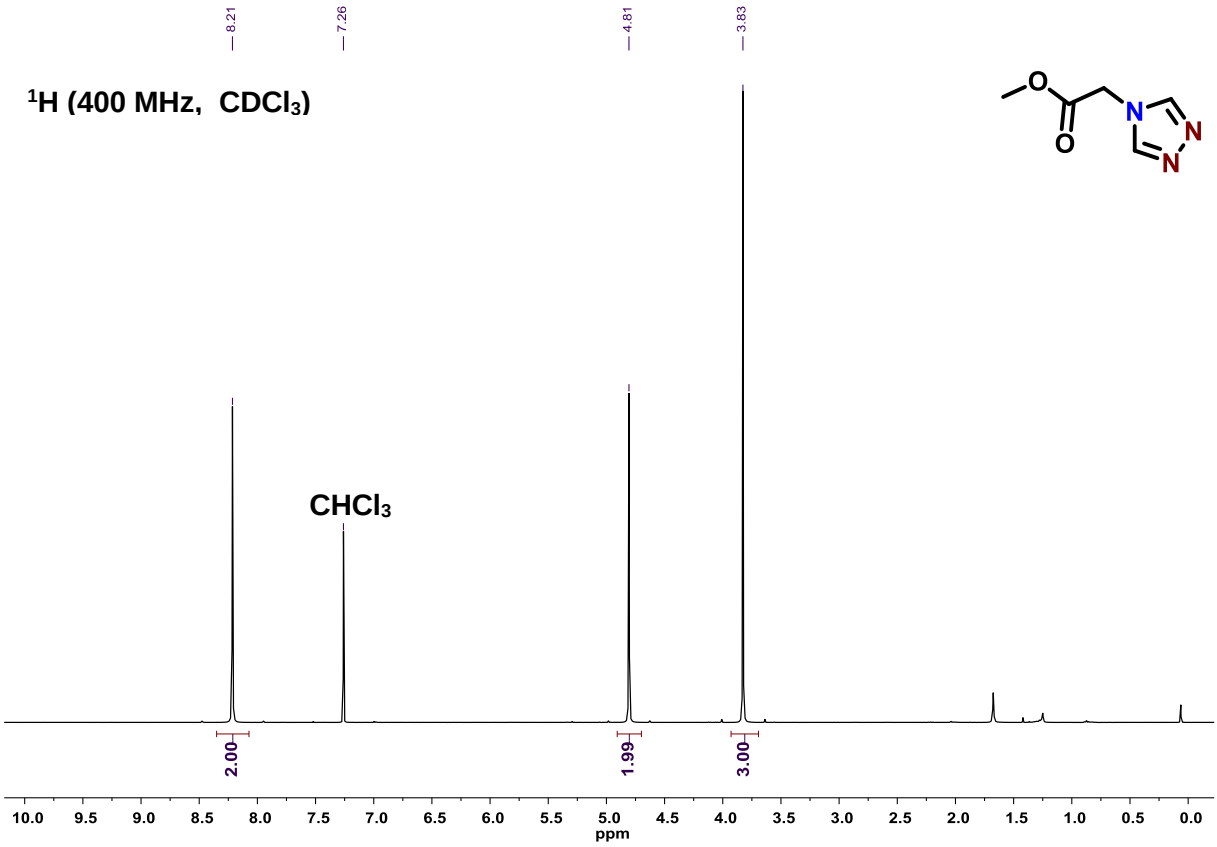
E = -611.328346
H = -611.155468
G = -611.206216

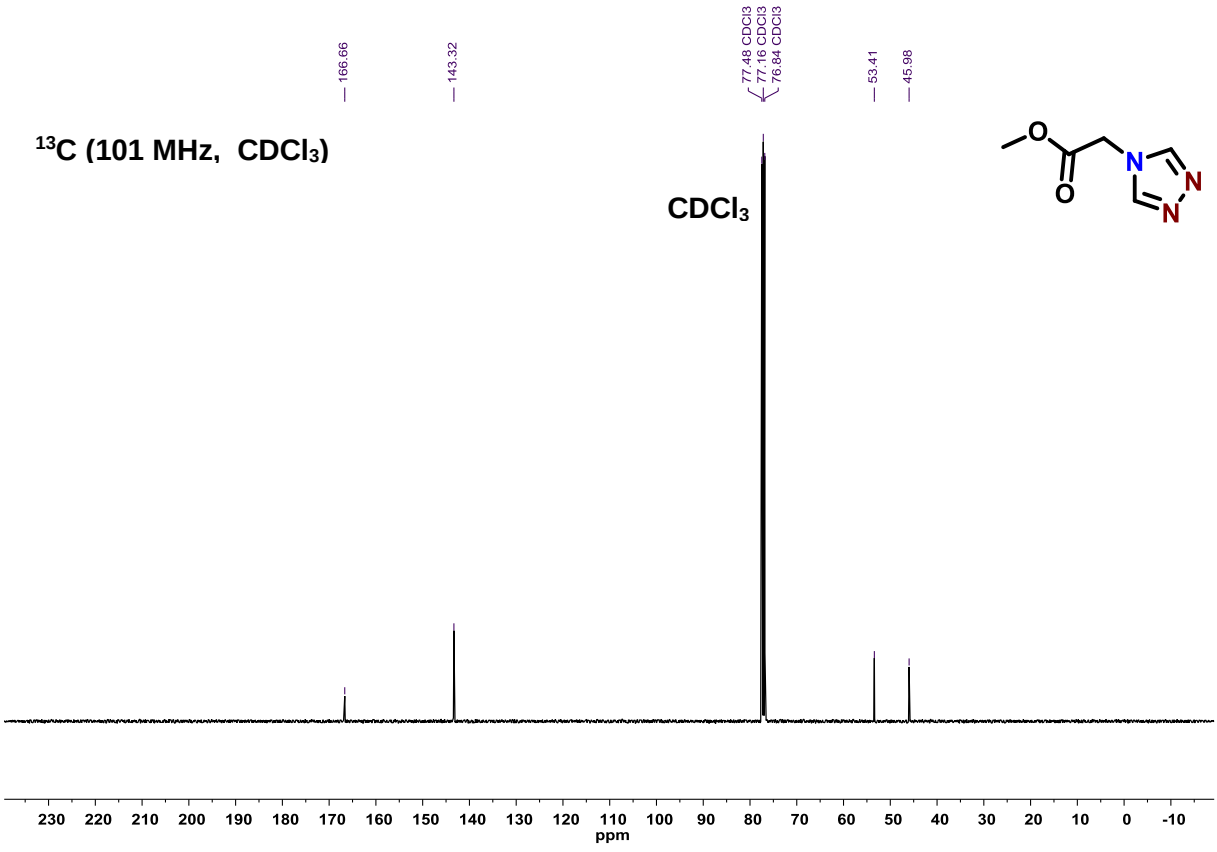
C	0.44089	0.40696	1.35314
C	3.04229	-0.78883	-0.62849
N	2.04645	1.15919	-0.29729
N	1.58141	0.20066	0.47766
C	2.99017	0.55423	-1.01435
N	2.12993	-0.98712	0.31978
H	3.67641	-1.59242	-0.96902
H	-0.80871	-1.96880	0.96781
C	-1.36275	-1.14199	0.53485
C	-2.55056	-1.39003	-0.13892
H	-2.95226	-2.39160	-0.23771
C	-3.23039	-0.31991	-0.69300
F	-4.38239	-0.55092	-1.34301
C	-2.76559	0.97893	-0.59894
H	-3.33034	1.78669	-1.04926
C	-1.57438	1.20751	0.07760
H	-1.18793	2.21891	0.15339
C	-0.86585	0.15486	0.65117
H	0.57309	-0.27053	2.19748
H	0.50370	1.43552	1.70920
H	3.57209	1.09808	-1.74195

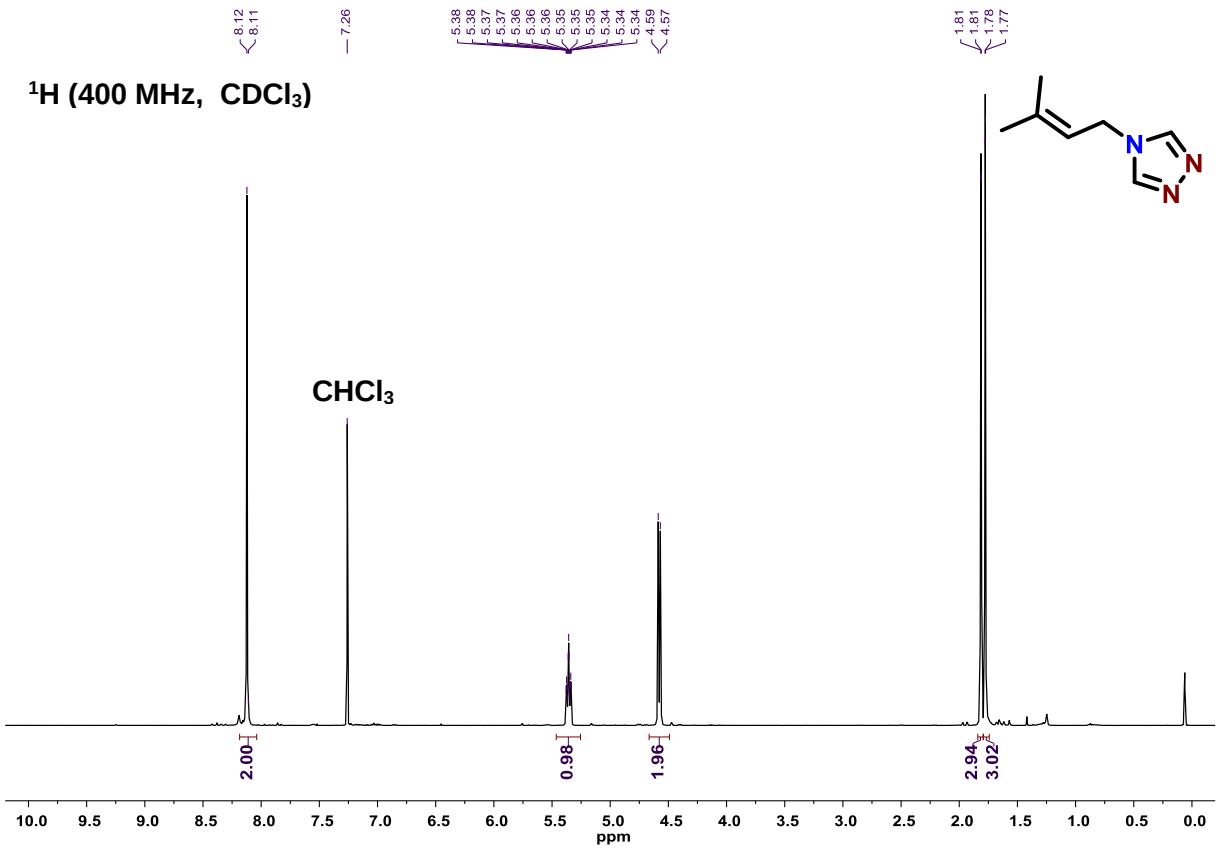
NMR Spectra of *N*-Alkyl Triazoles

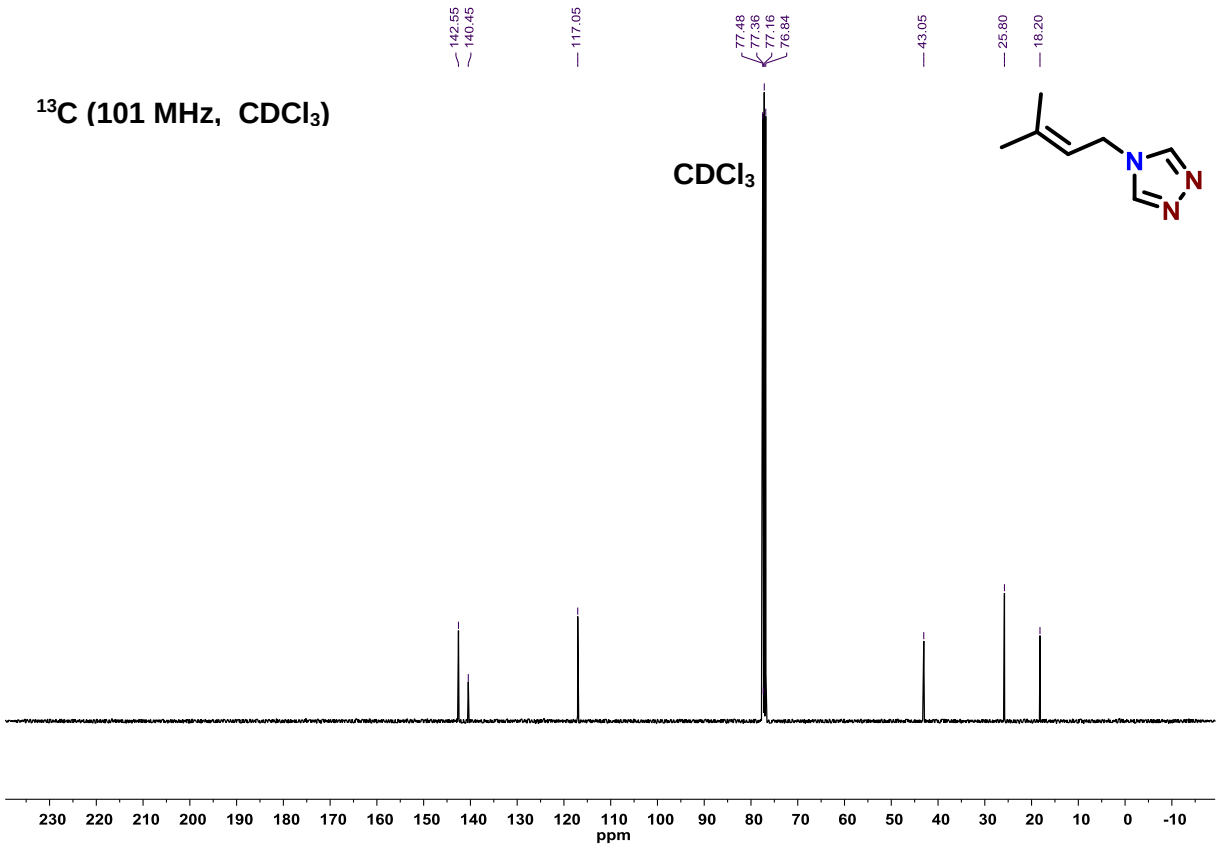

8.14
7.26
6.00
5.99
5.97
5.97
5.96
5.96
5.95
5.94
5.93
5.93
5.92
5.90
5.38
5.38
5.37
5.36
5.35
5.35
5.27
5.26
5.26
5.22
5.22
5.22
4.64
4.63
4.63
4.62
4.62
4.61
1H (400 MHz, CDCl3)
N
N
N
CHCl3
2.00
0.99
1.01
1.00
2.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
ppm

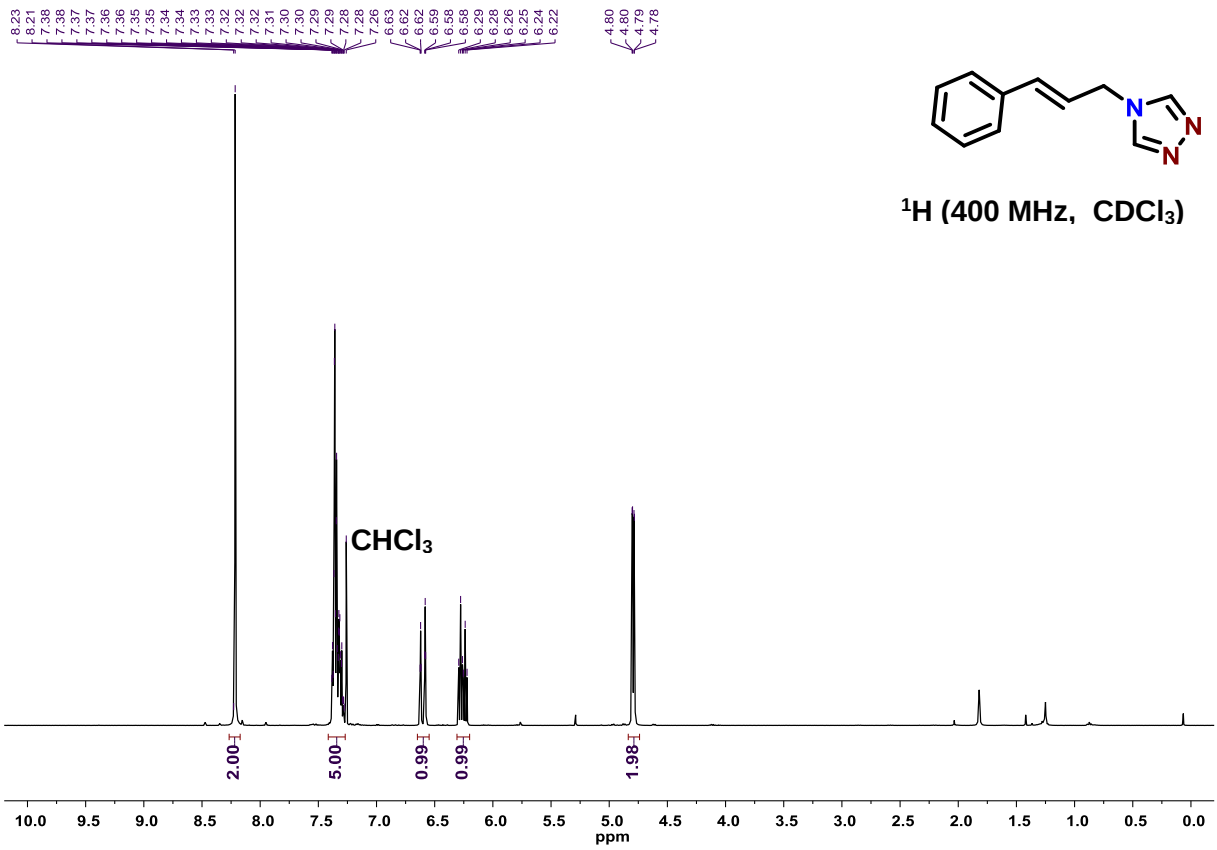

142.81
131.20
120.23
77.48 CDCl3
77.16 CDCl3
76.84 CDCl3
47.63
13C (101 MHz, CDCl3)
N
N
N
CDCl3
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
ppm


8.21
7.26
4.81
3.83
1H (400 MHz, CDCl3)
CHCl3
2.00
1.99
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
ppm

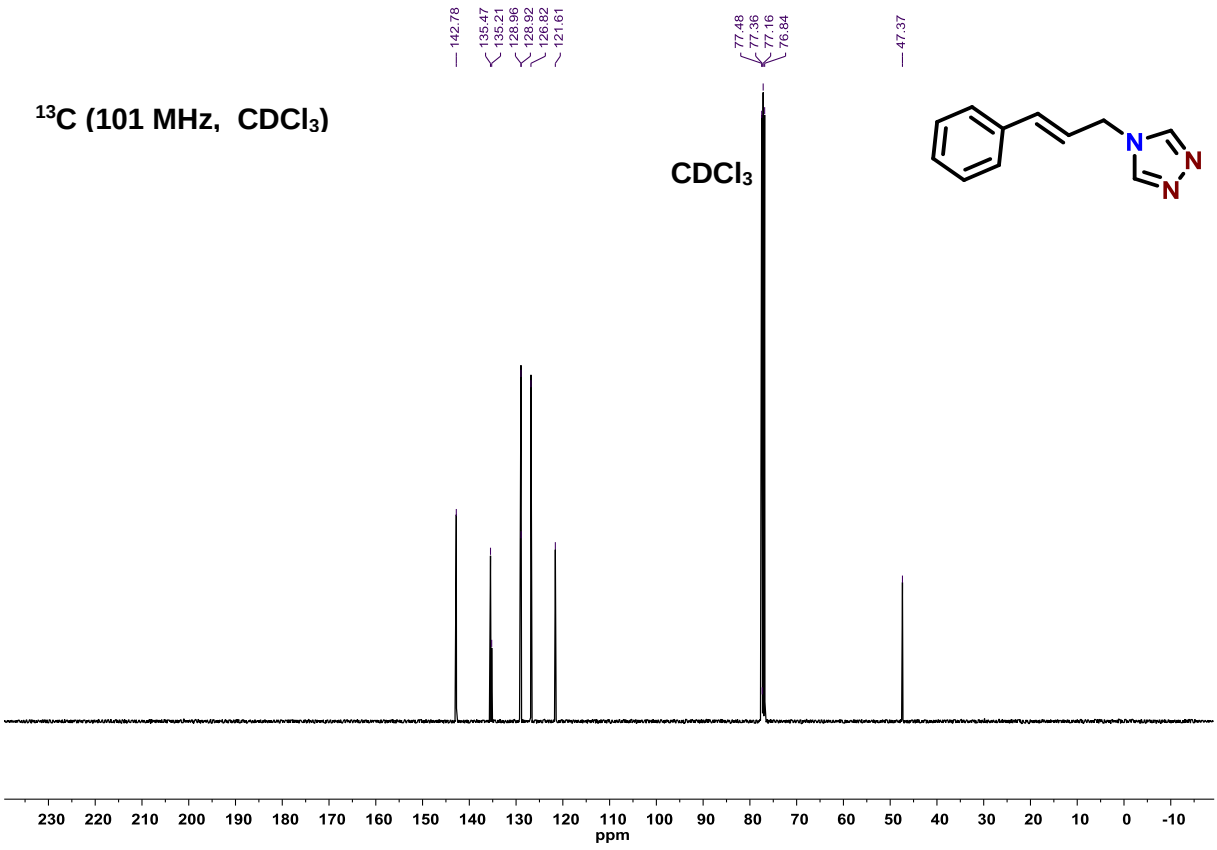

166.66
143.32
77.48 CDCl3
77.16 CDCl3
76.84 CDCl3
53.41
45.98
13C (101 MHz, CDCl3)
CDCl3
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
ppm


8.12
8.11
7.26
5.38
5.38
5.37
5.37
5.36
5.36
5.36
5.35
5.35
5.35
5.34
5.34
5.34
4.59
4.57
1.81
1.81
1.78
1.77
1H (400 MHz, CDCl3)
CHCl3
N
N
N
2.00
0.98
1.96
2.94
3.02
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
ppm

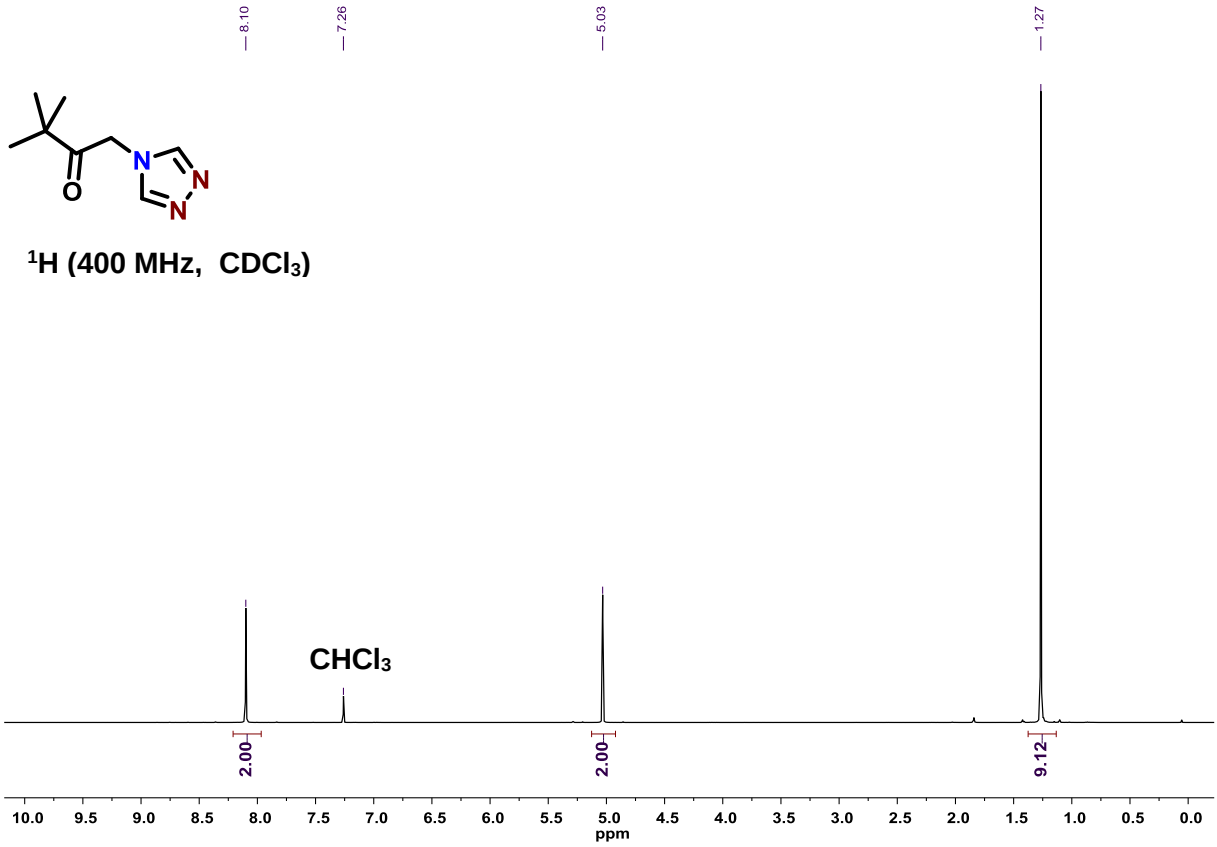

142.55
140.45
117.05
77.48
77.36
77.16
76.84
43.05
25.80
18.20
13C (101 MHz, CDCl3)
CDCl3
N
N
N
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
ppm



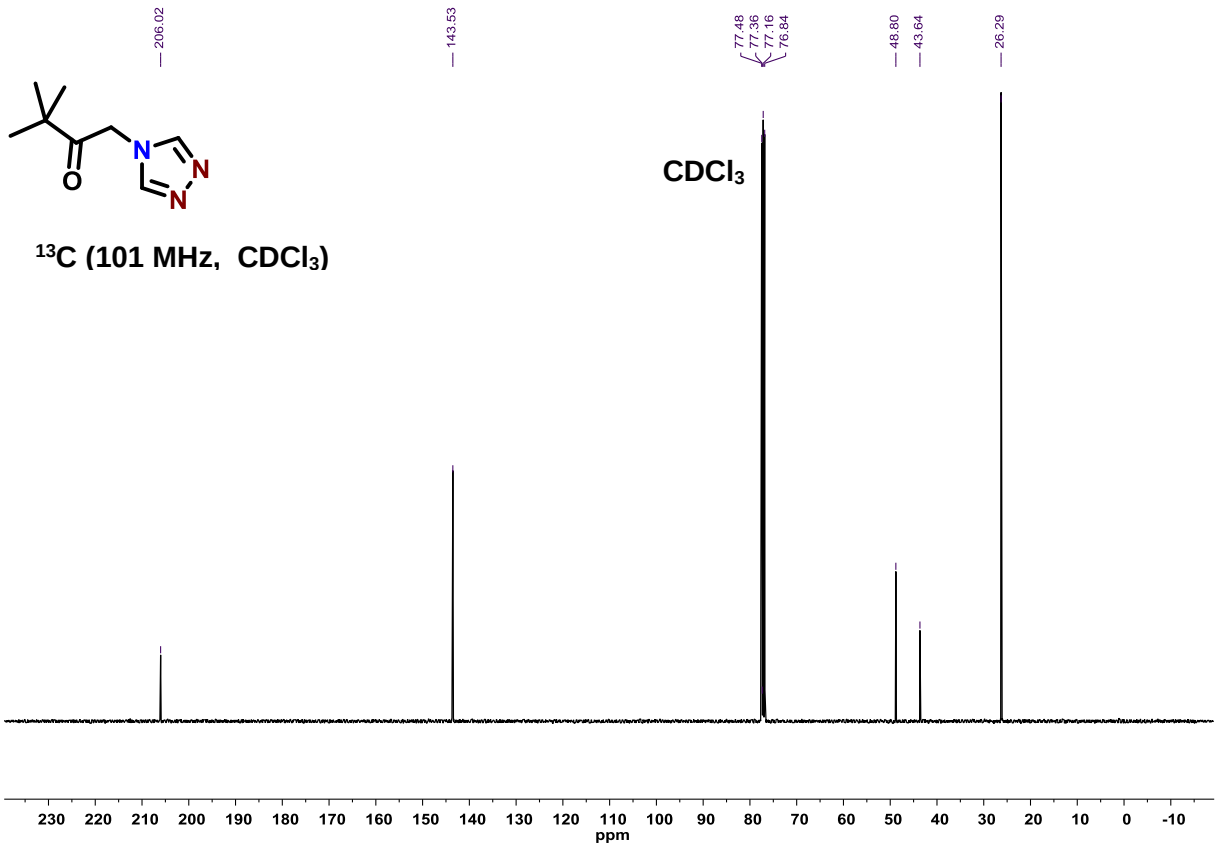
^{1}H (400 MHz, $CDCl_3$)



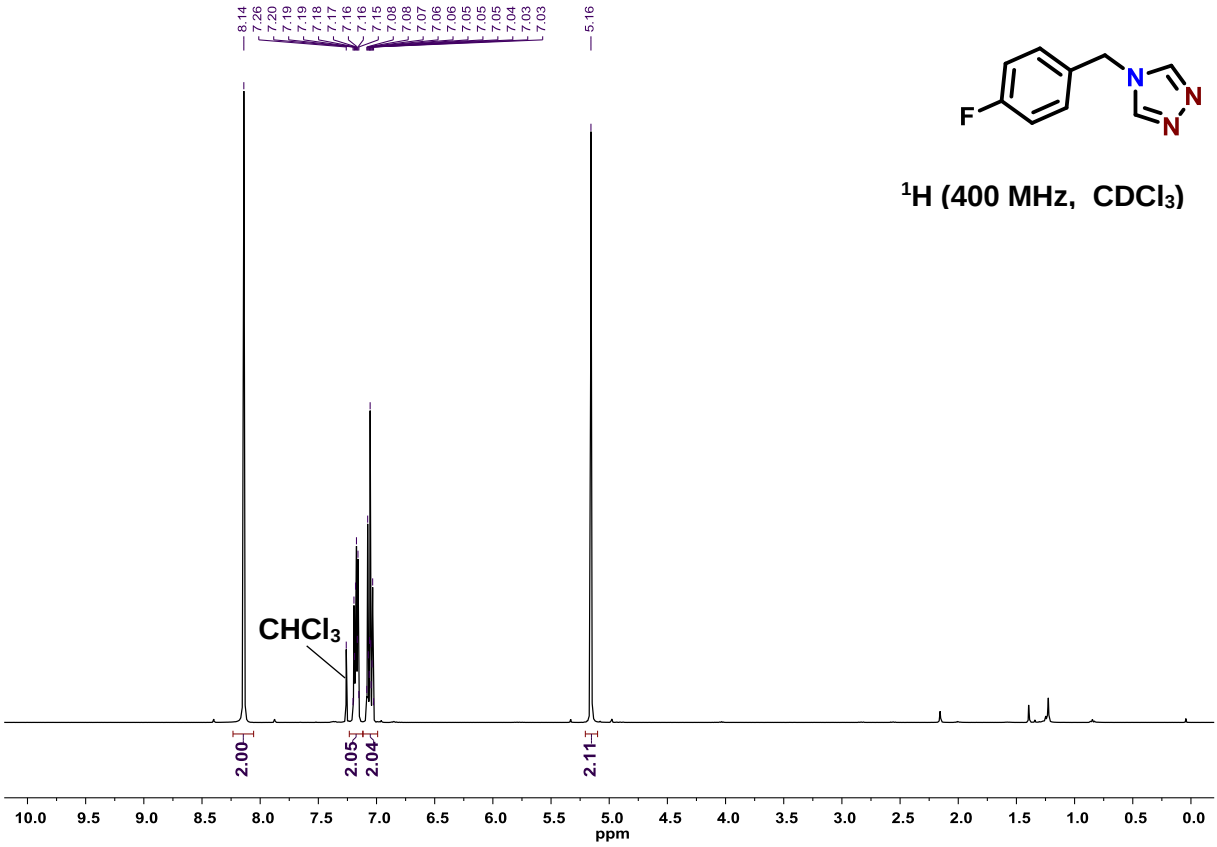
^{13}C (101 MHz, $CDCl_3$)



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

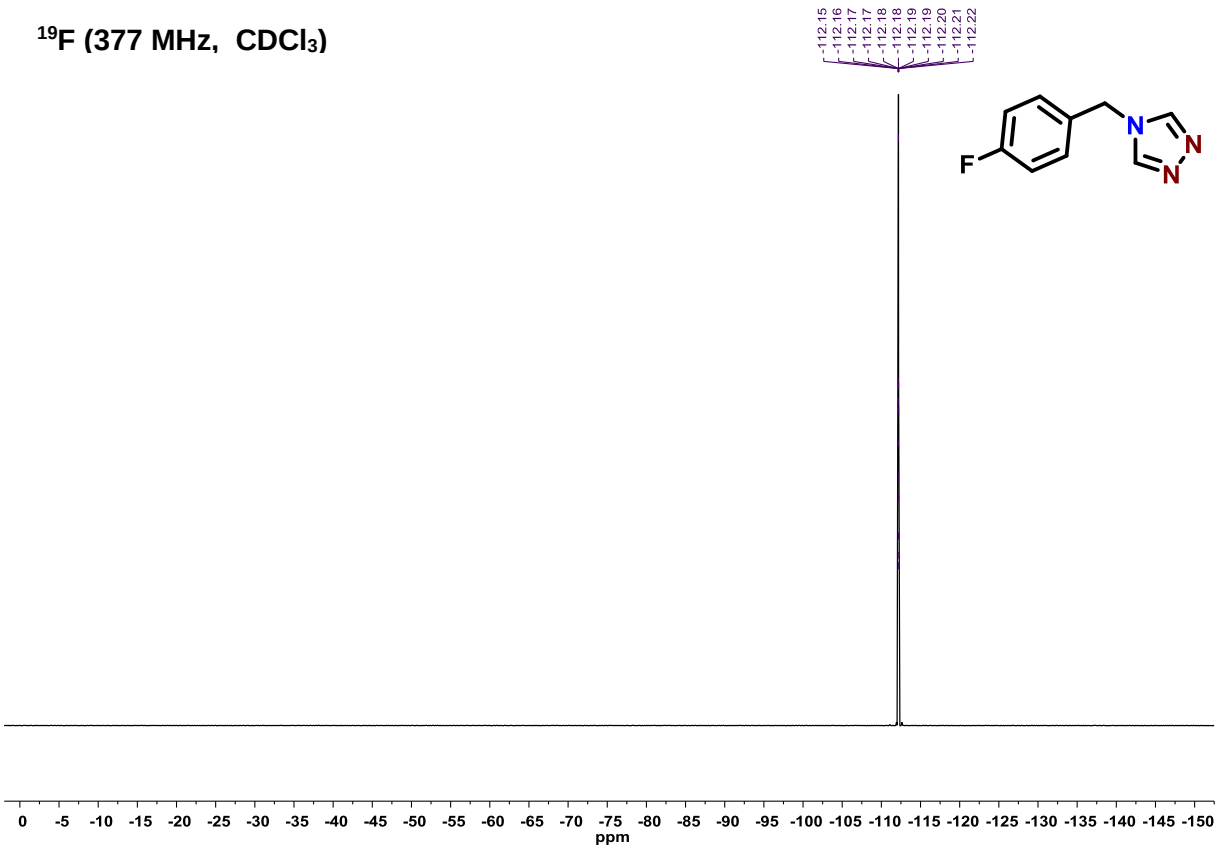


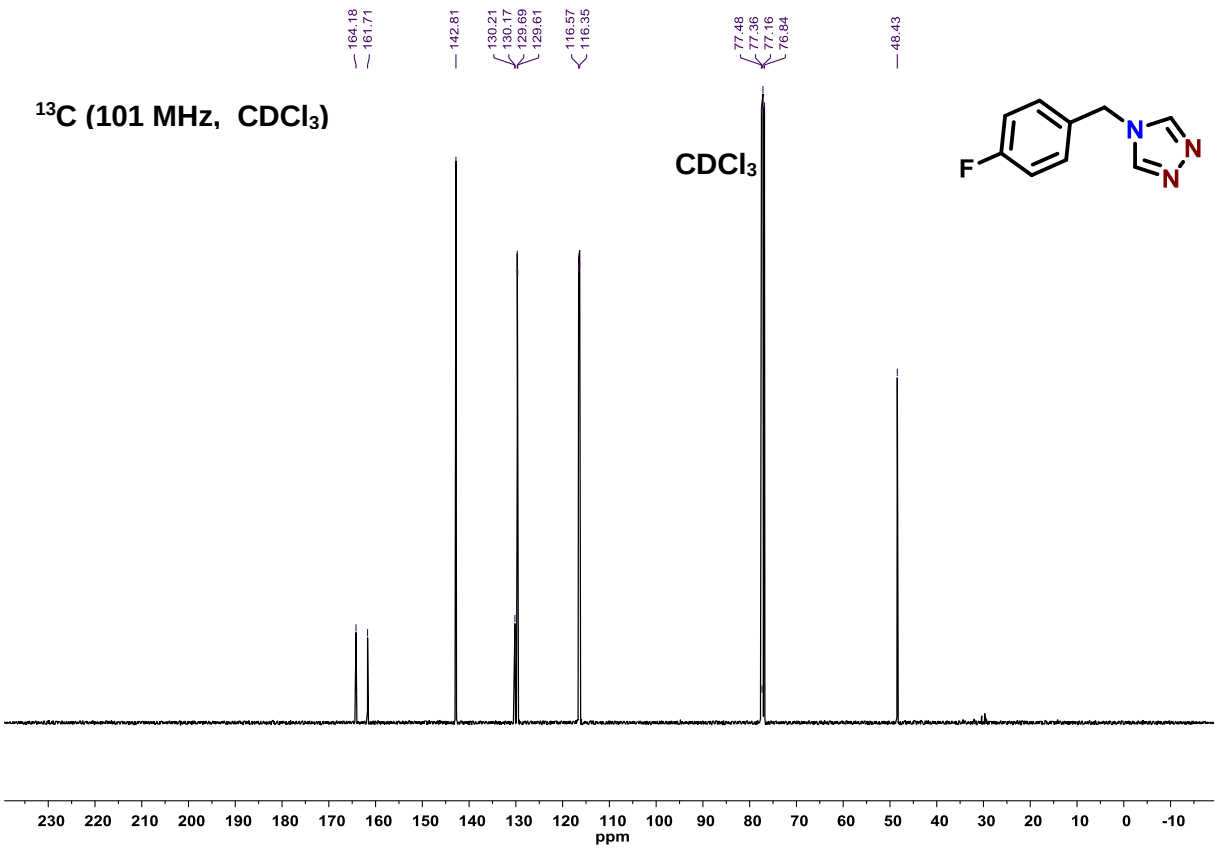
^{13}C (101 MHz, $CDCl_3$)

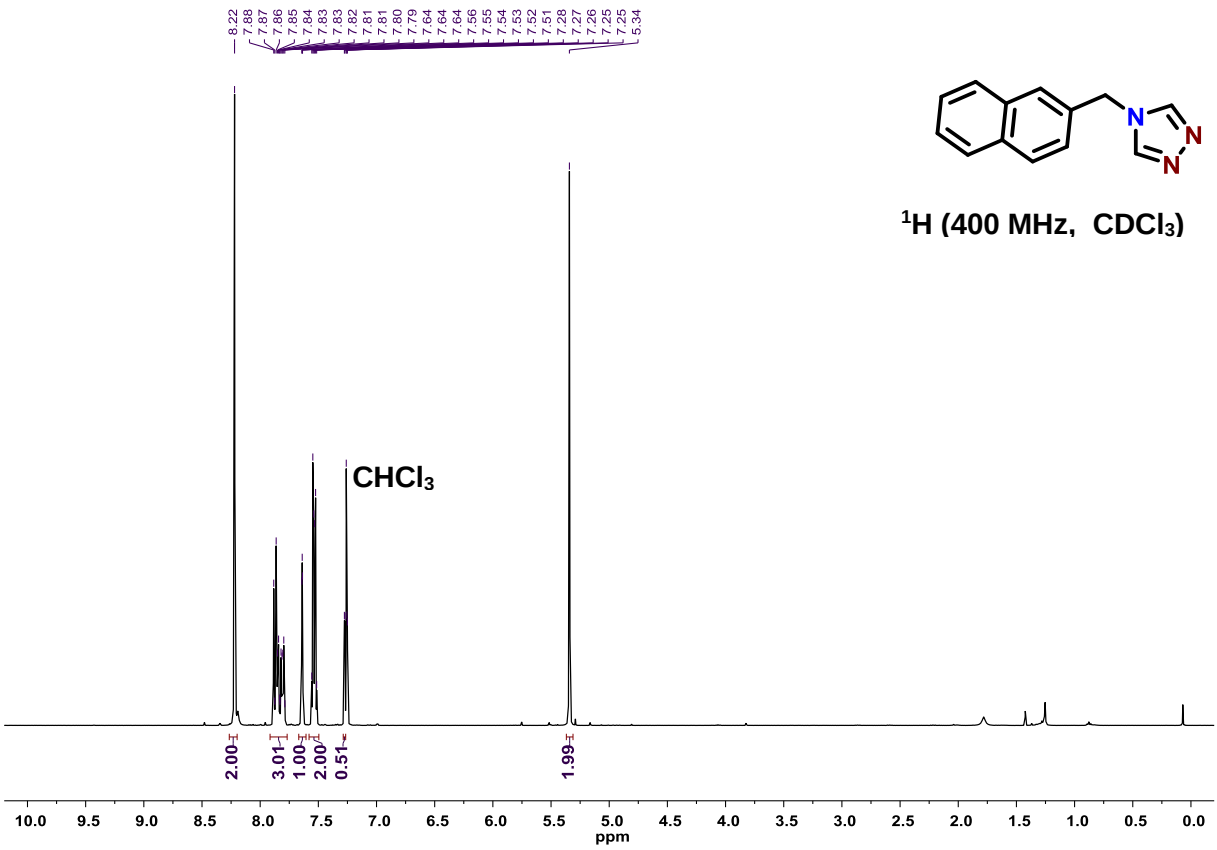


^{1}H (400 MHz, $CDCl_3$)

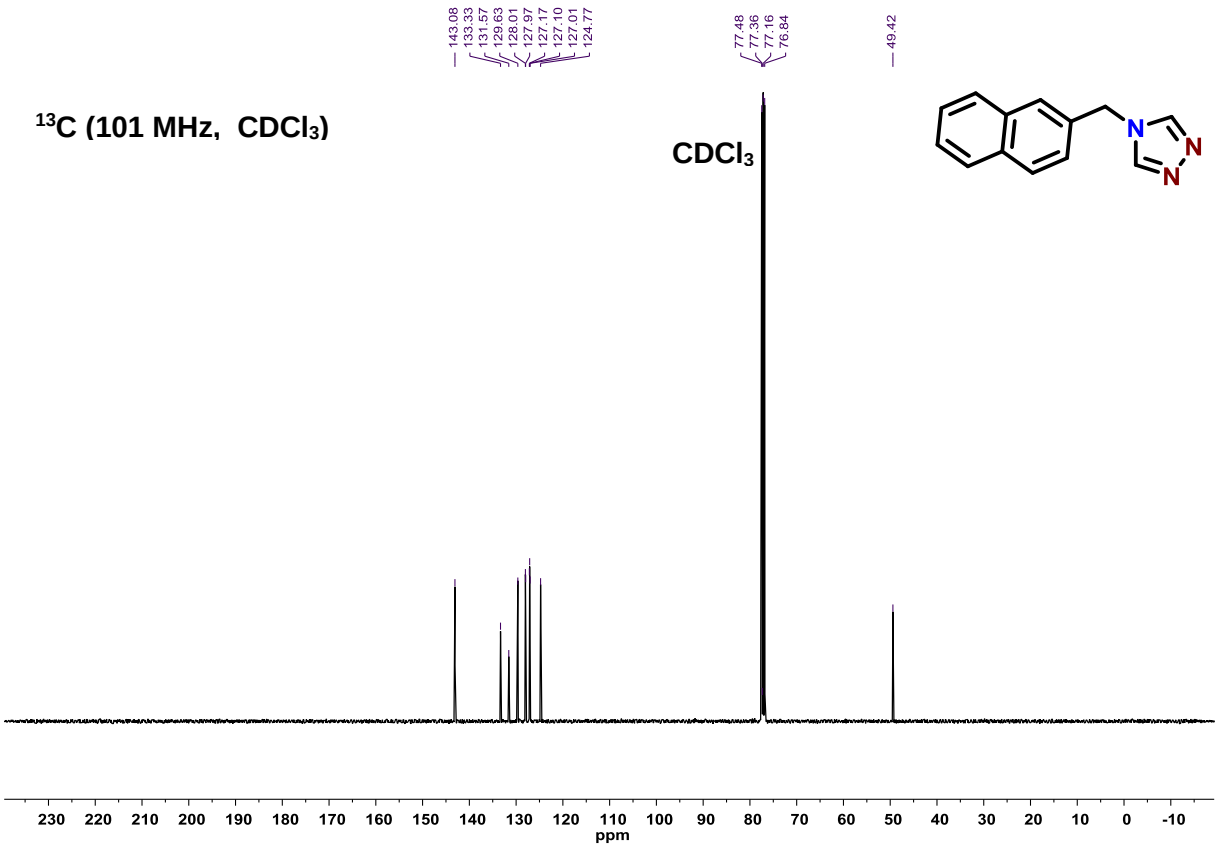
^{19}F (377 MHz, $CDCl_3$)



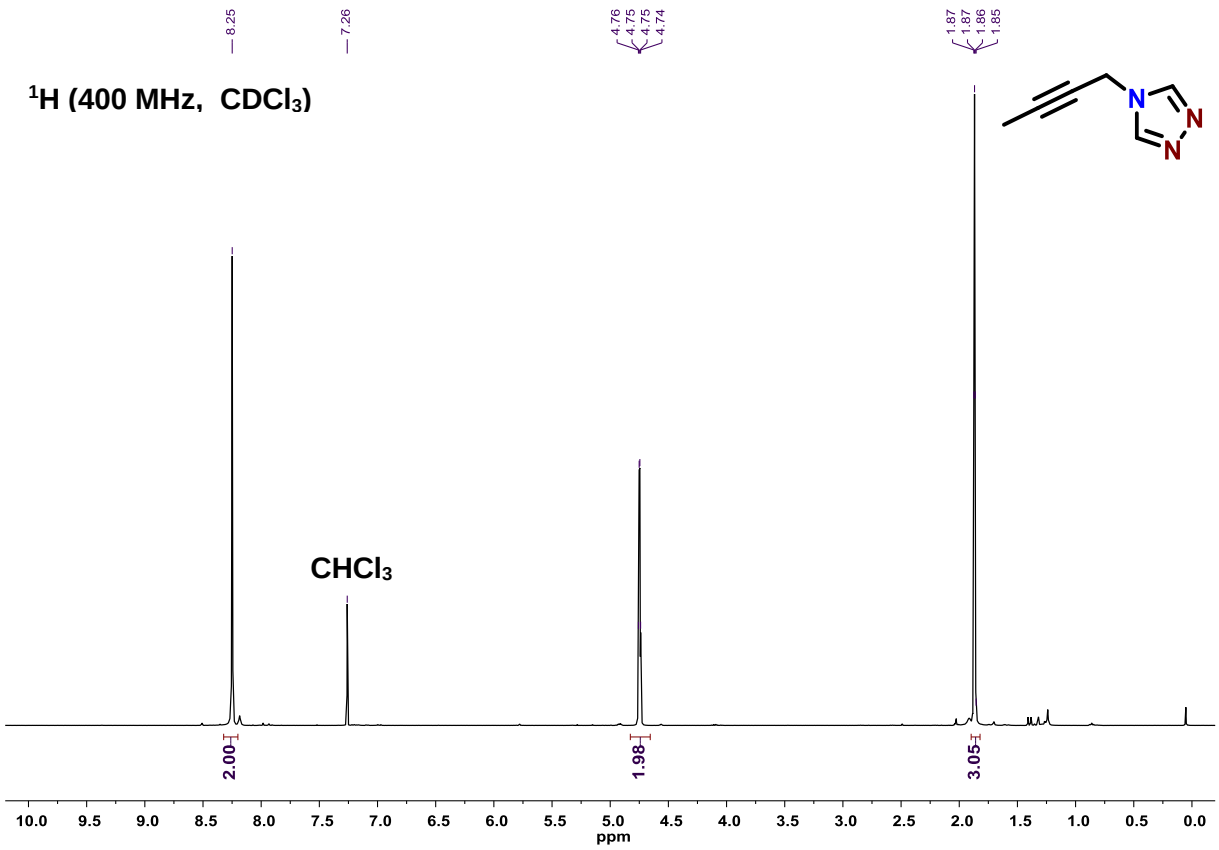

164.18
161.71
142.81
130.21
130.17
129.69
129.61
116.57
116.35
77.48
77.36
77.16
76.84
48.43
13C (101 MHz, CDCl3)
CDCl3
F
N
N
N
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
ppm

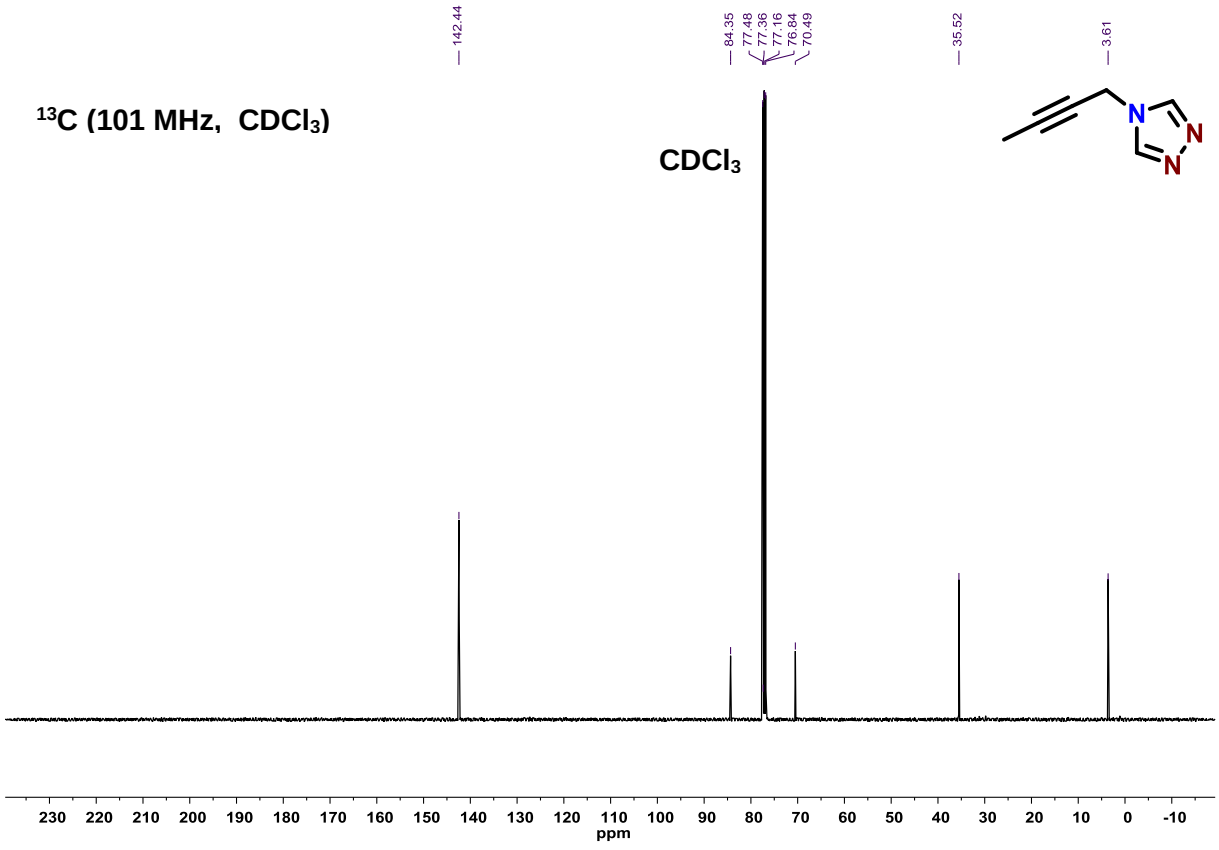


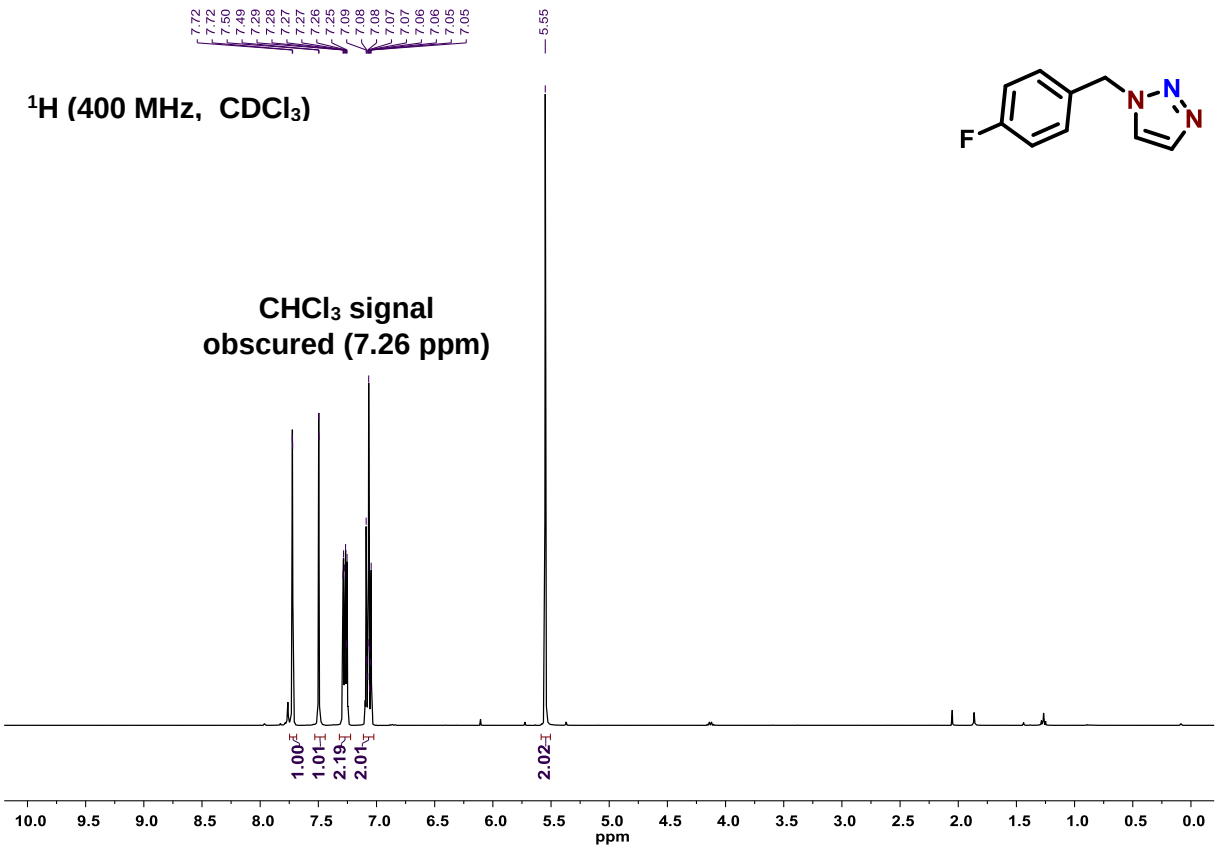
^{1}H (400 MHz, $CDCl_3$)

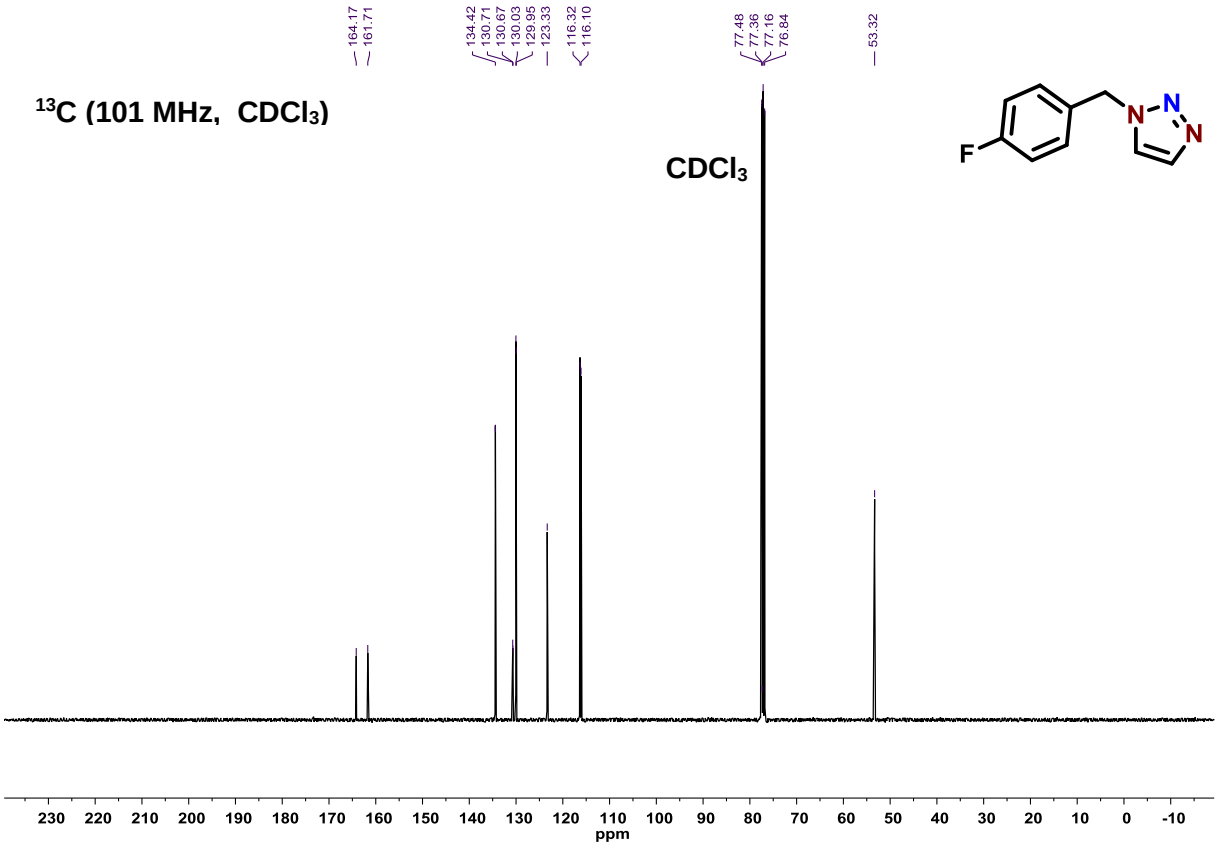


^{13}C (101 MHz, $CDCl_3$)

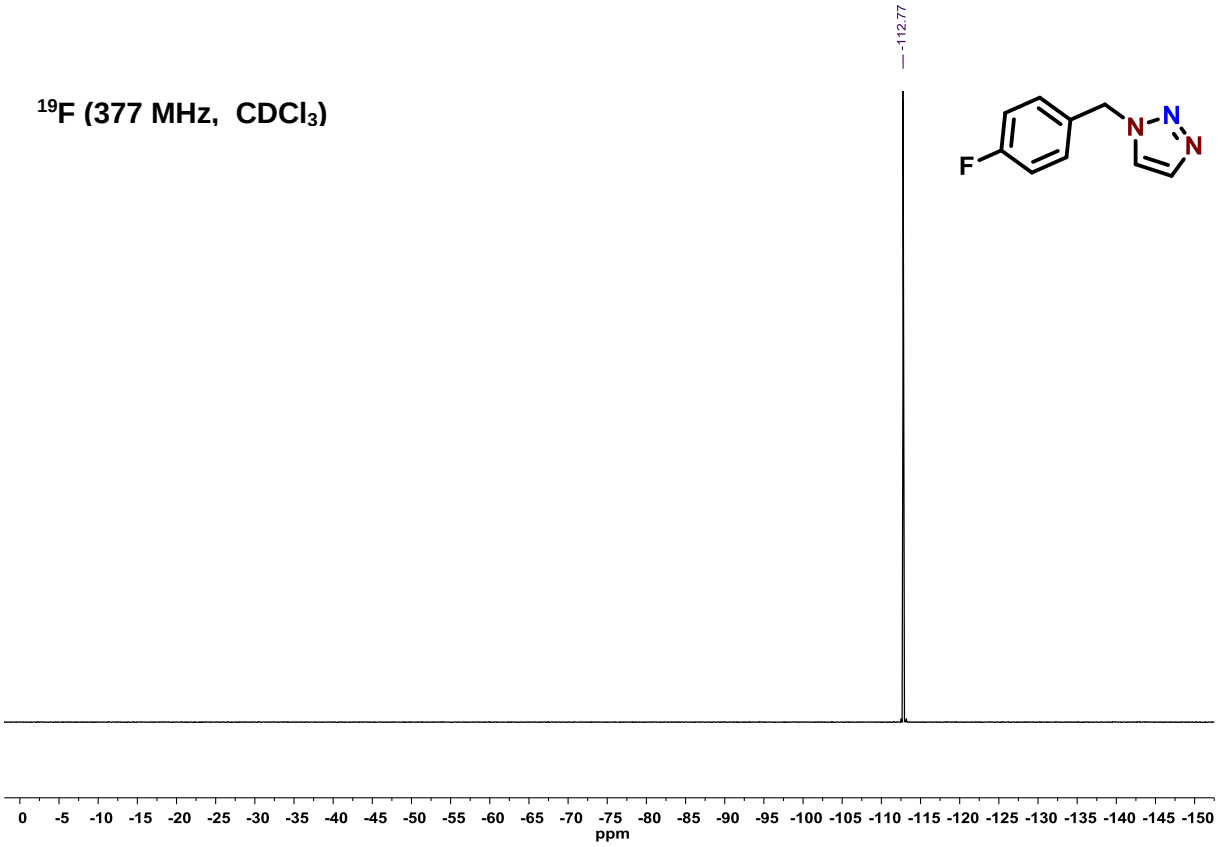

8.25
7.26
4.76
4.75
4.75
4.74
1.87
1.87
1.86
1.85
^{1}H (400 MHz, CDCl$_3$)
CHCl$_3$
2.00
1.98
3.05
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
ppm

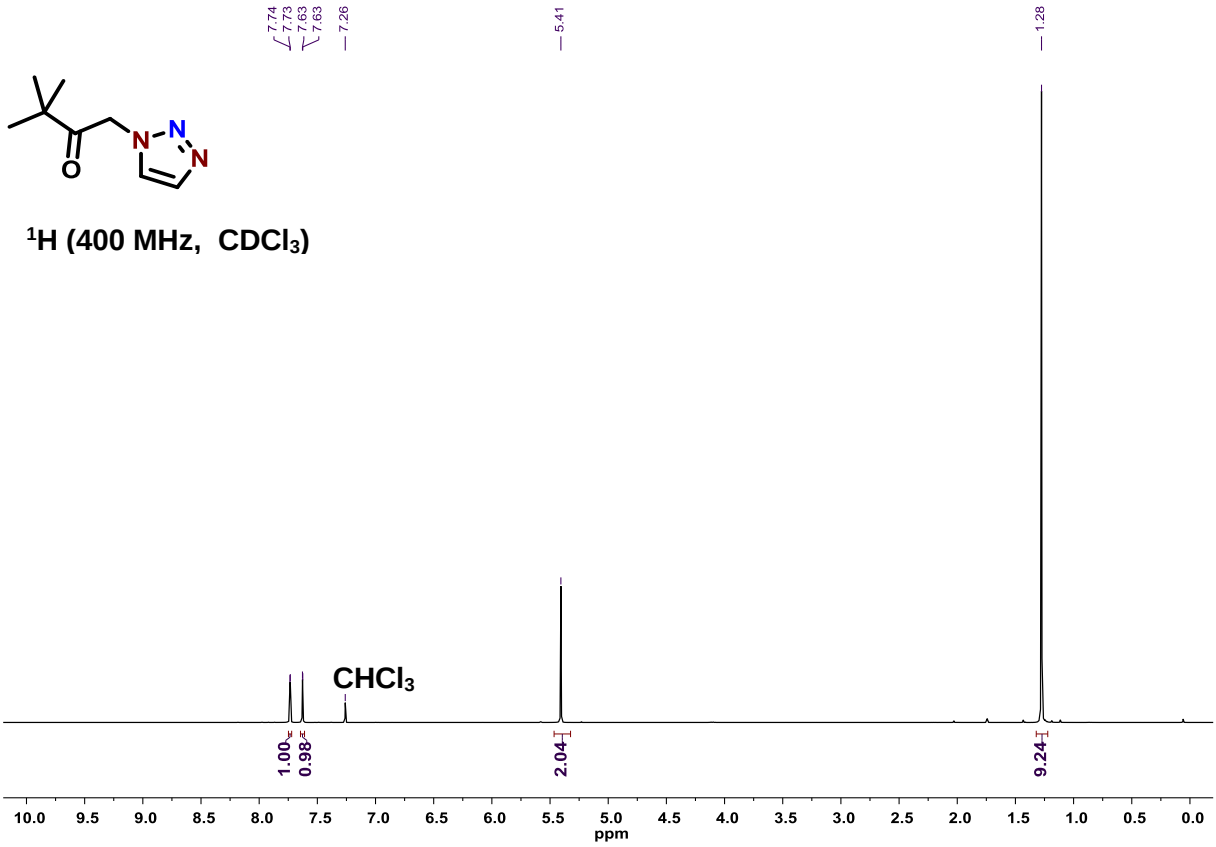

142.44
84.35
77.48
77.36
77.16
76.84
70.49
35.52
3.61
^{13}C (101 MHz, CDCl$_3$)
CDCl$_3$
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
ppm


7.72
7.72
7.50
7.49
7.29
7.28
7.27
7.27
7.26
7.25
7.09
7.08
7.08
7.07
7.07
7.06
7.06
7.05
7.05
5.55
1H (400 MHz, CDCl3)
CHCl3 signal
obscured (7.26 ppm)
1.00
1.01
2.19
2.01
2.02
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
ppm

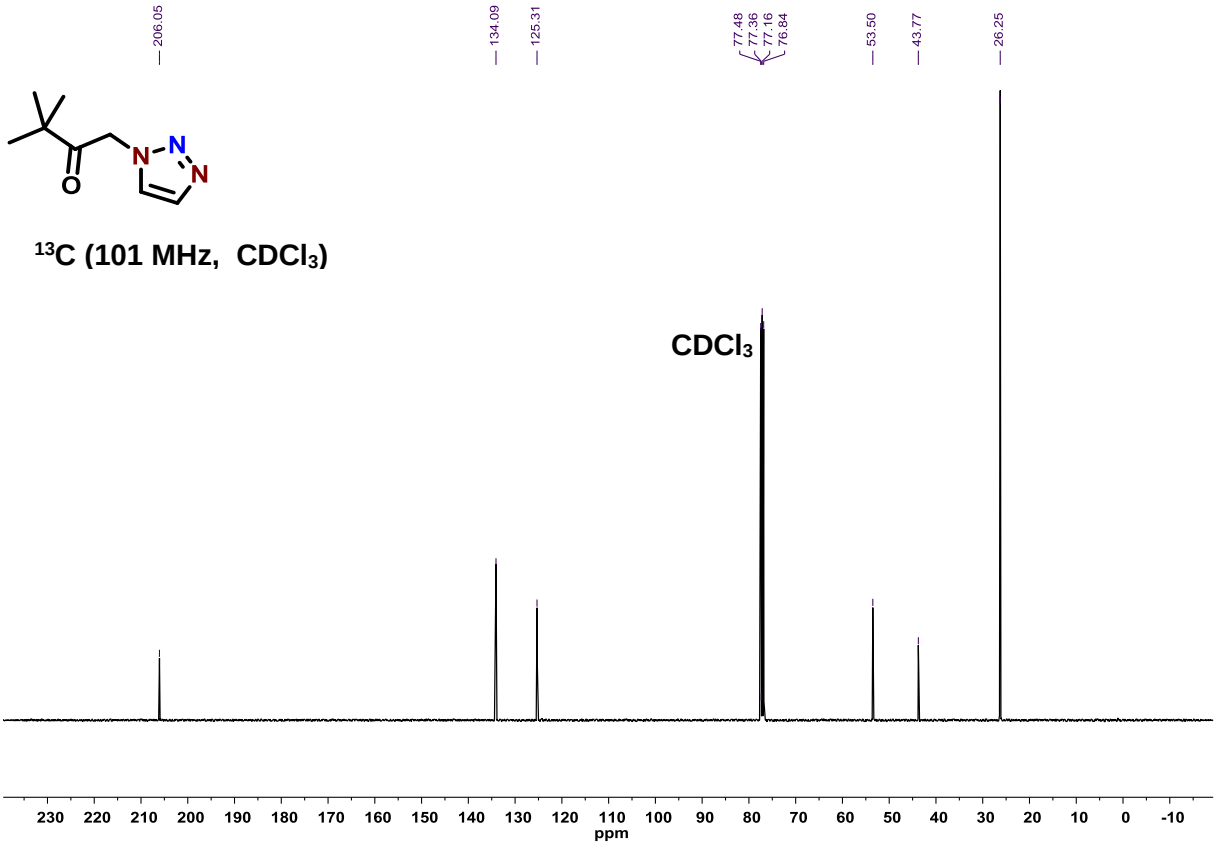

164.17
161.71
134.42
130.71
130.67
130.03
129.95
123.33
116.32
116.10
77.48
77.36
77.16
76.84
53.32
13C (101 MHz, CDCl3)
CDCl3
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
ppm

^{19}F (377 MHz, $CDCl_3$)

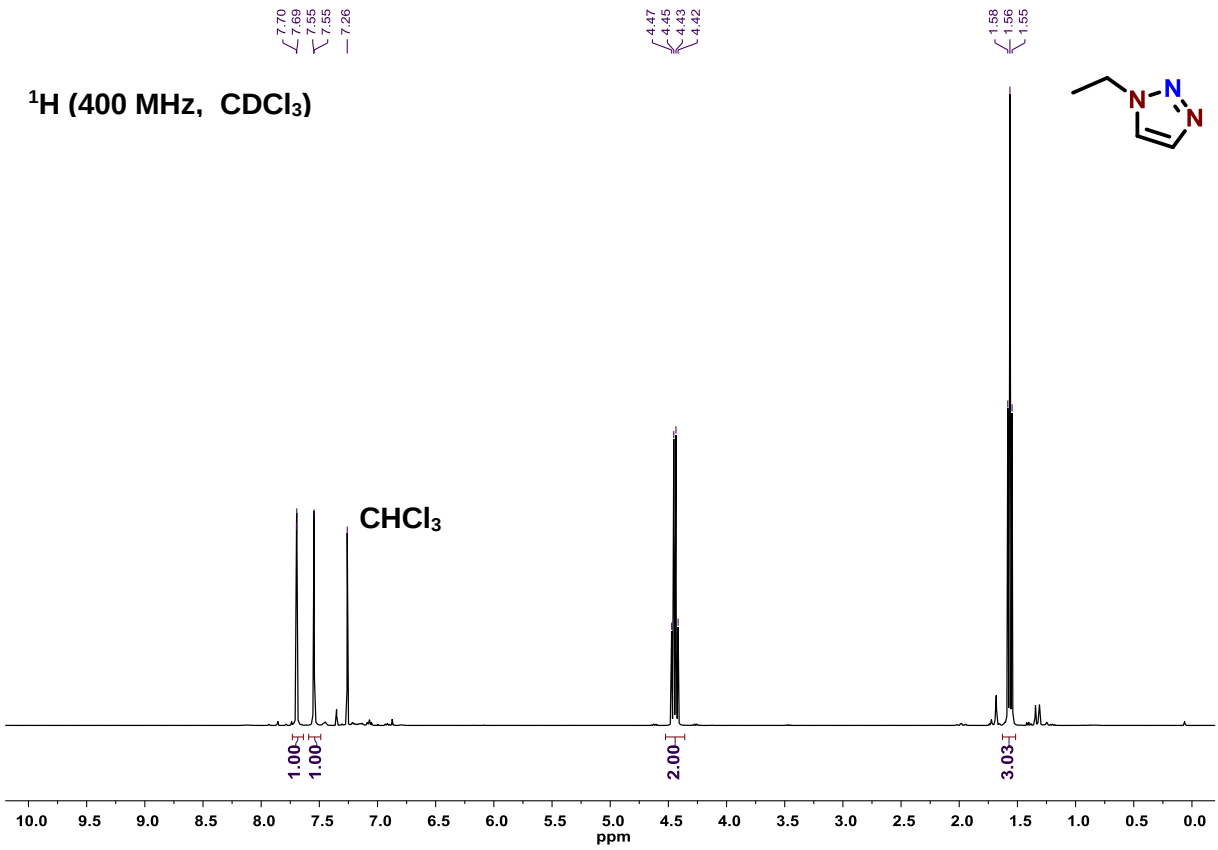


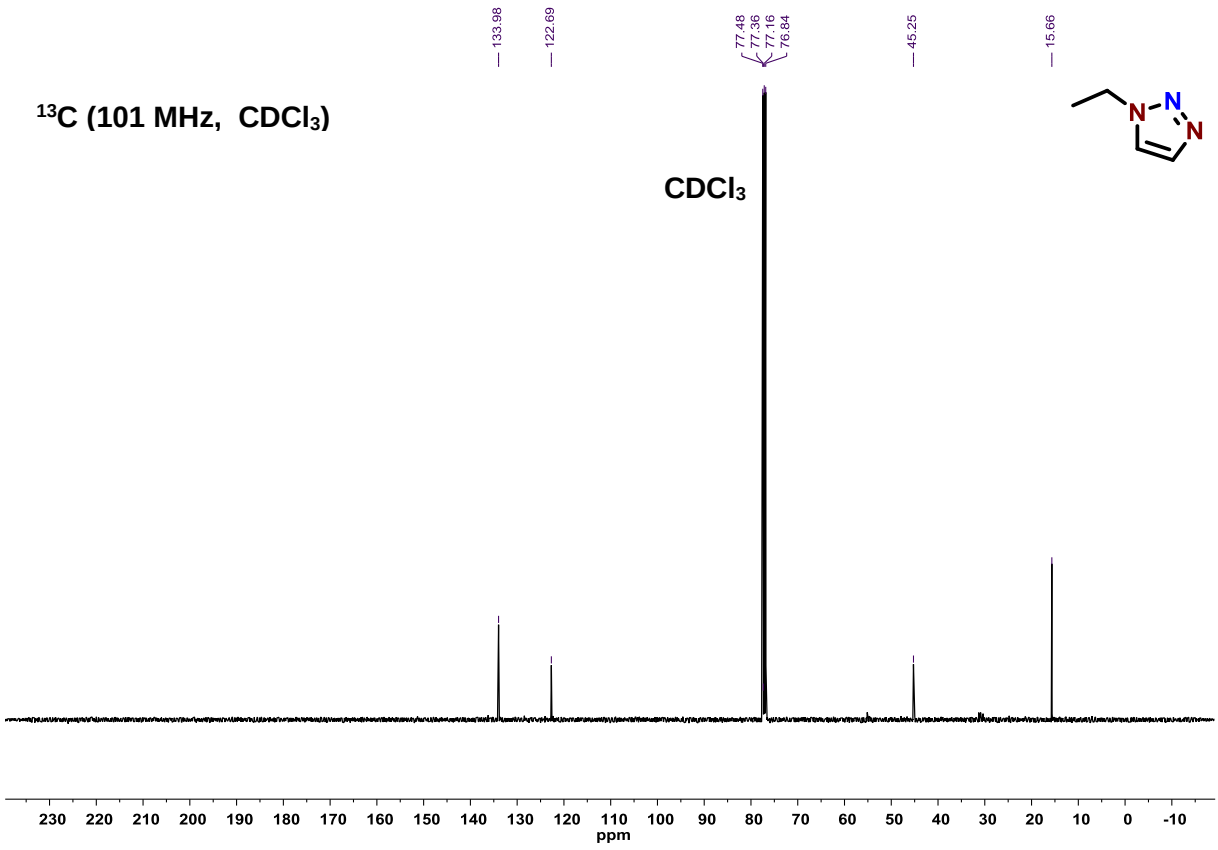


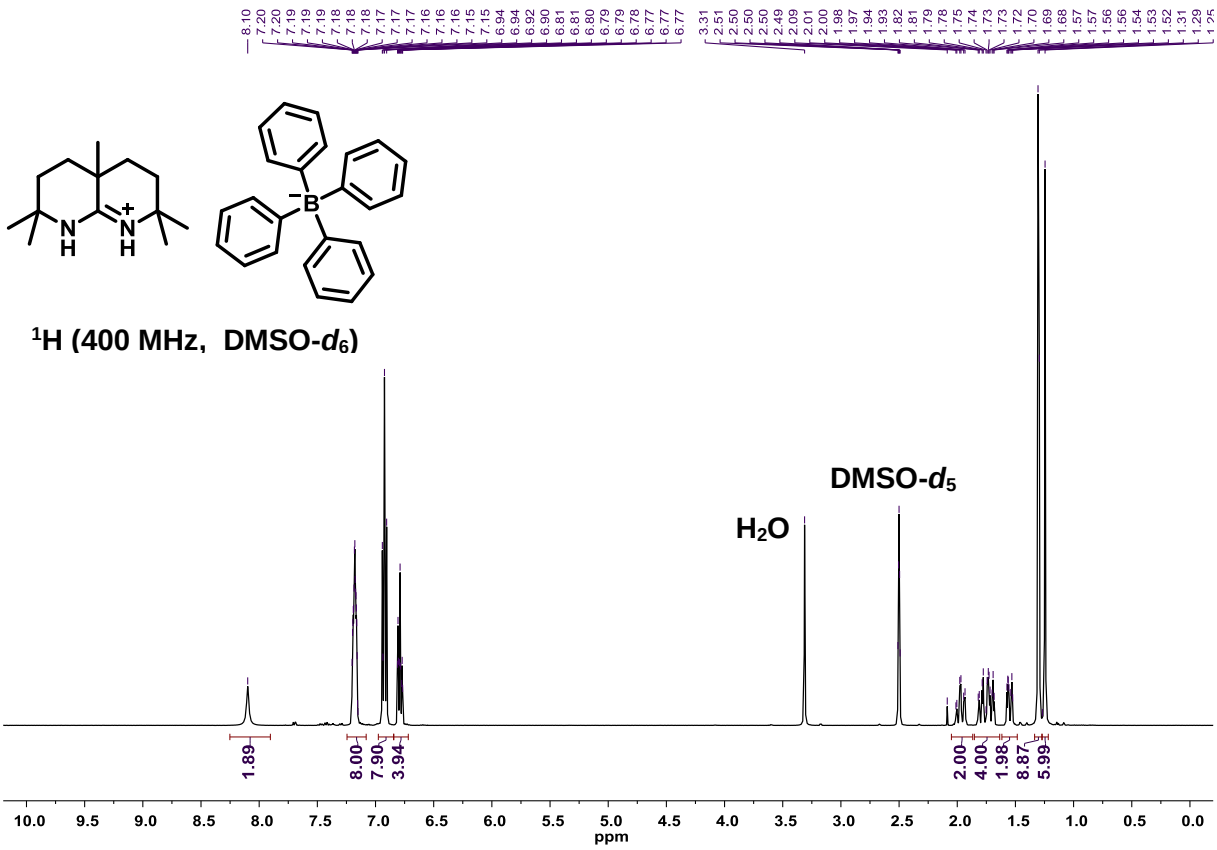
^{1}H (400 MHz, $CDCl_3$)



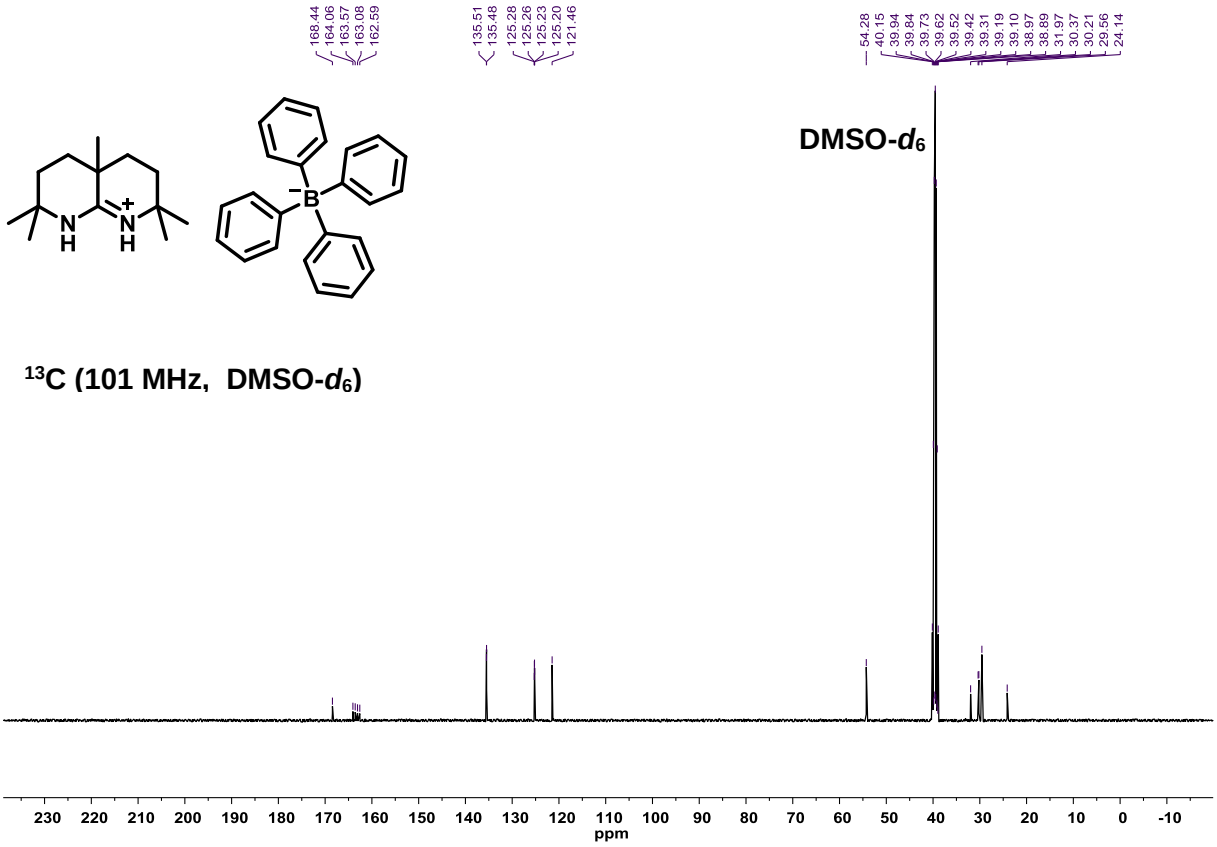
^{13}C (101 MHz, $CDCl_3$)


^{1}H (400 MHz, CDCl$_3$)
7.70
7.69
7.55
7.55
7.26
4.47
4.45
4.43
4.42
1.58
1.56
1.55
CHCl$_3$
1.00
1.00
2.00
3.03
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
ppm

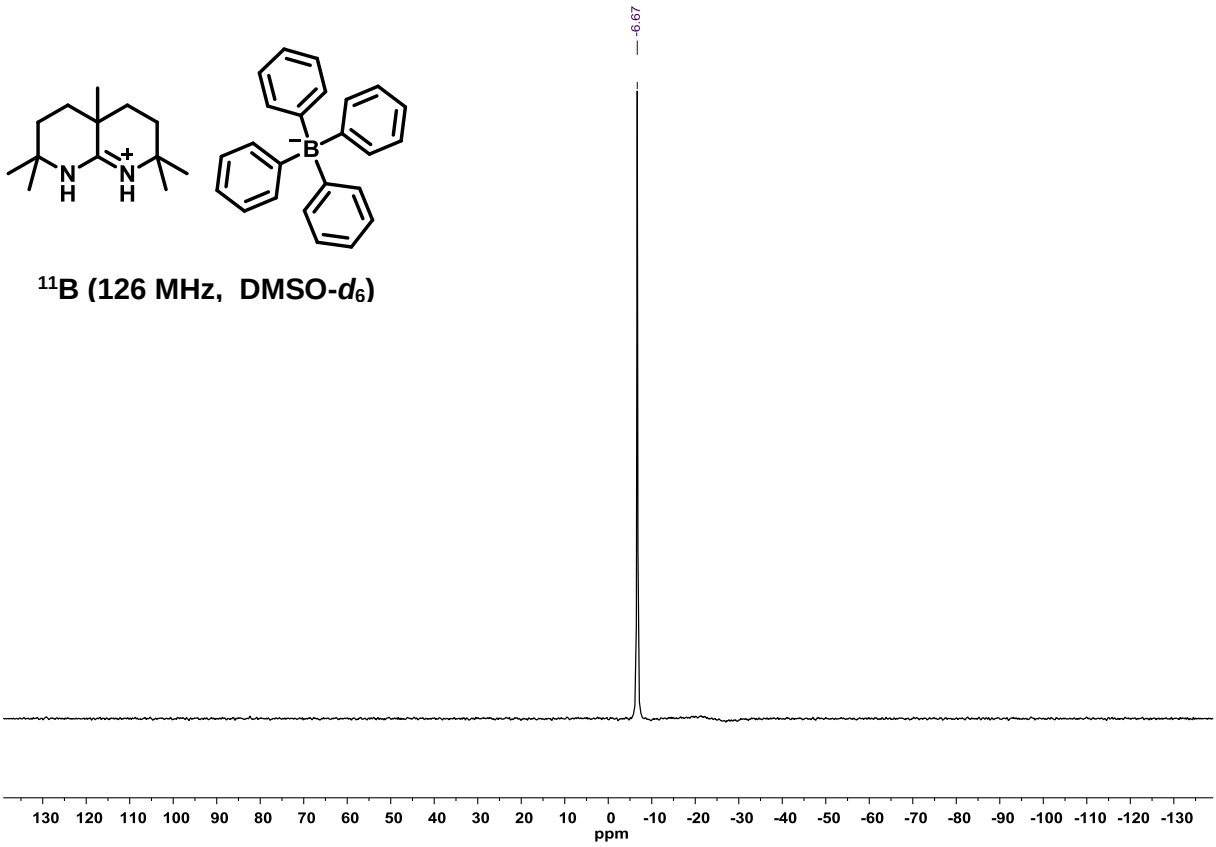

^{13}C (101 MHz, CDCl$_3$)
133.98
122.69
77.48
77.36
77.16
76.84
45.25
15.66
CDCl$_3$
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
ppm



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



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



^{11}B (126 MHz, DMSO-d_6)

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