Supplementary information

DES as solvent and catalyst: One-pot synthesis of 1,3-dinitropropanes via tandem Henry reaction/Michael addition

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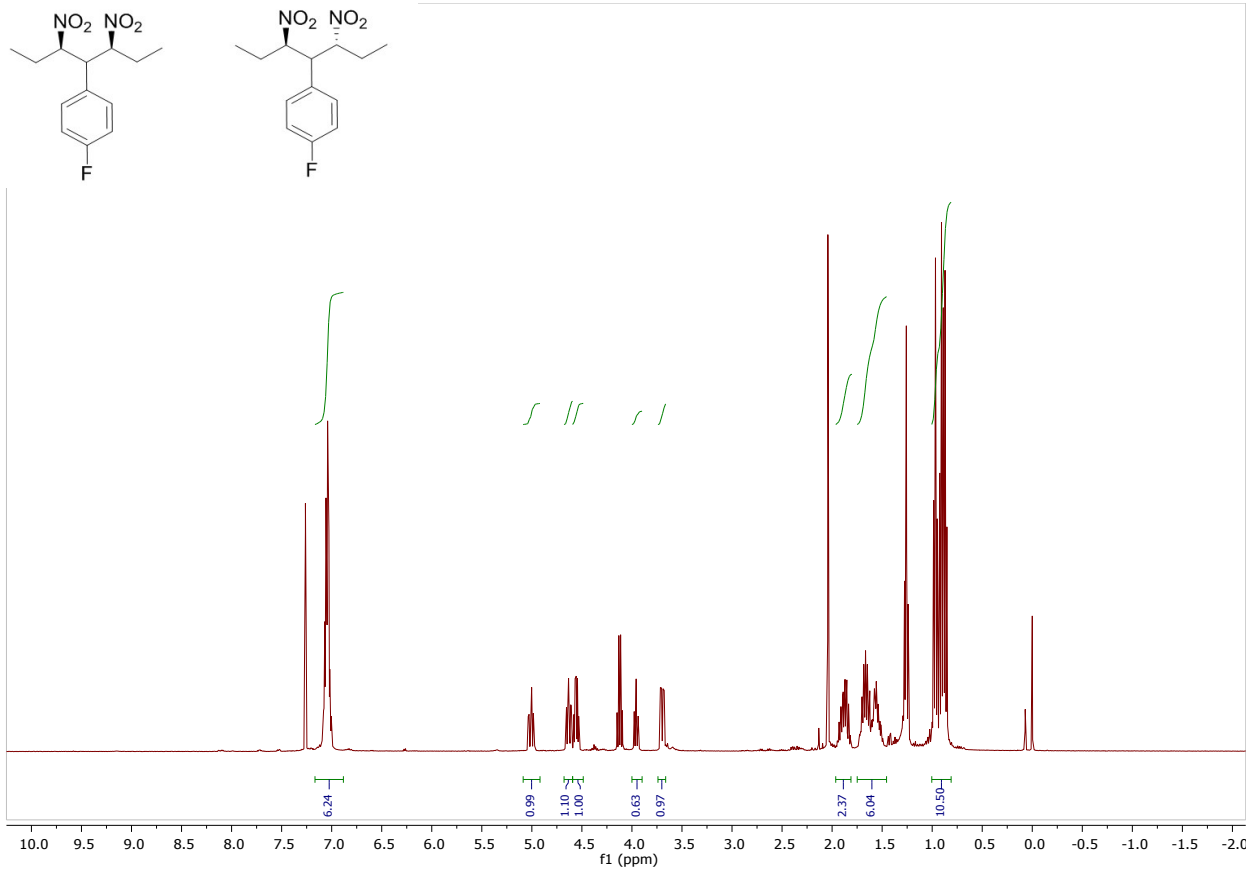
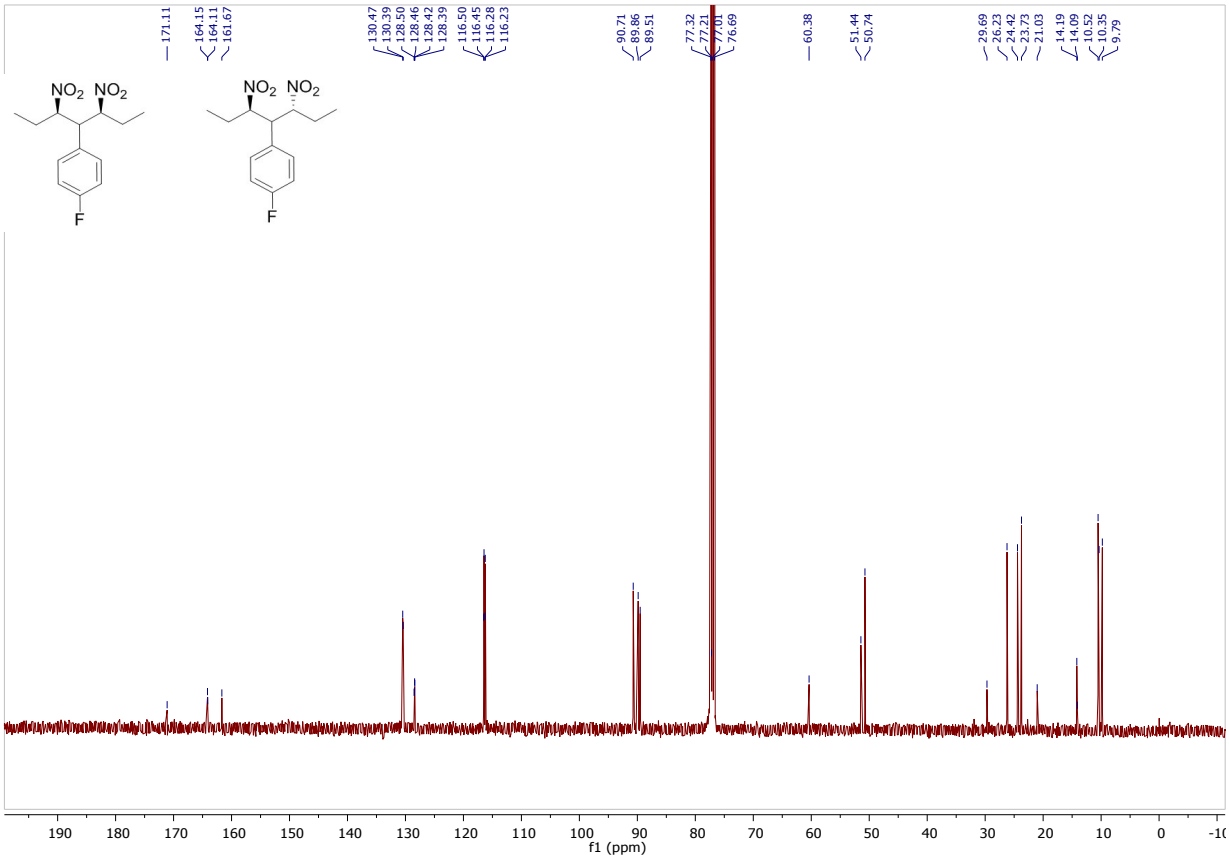
Copy of the ^{1}H-NMR spectrum of new compound **4**

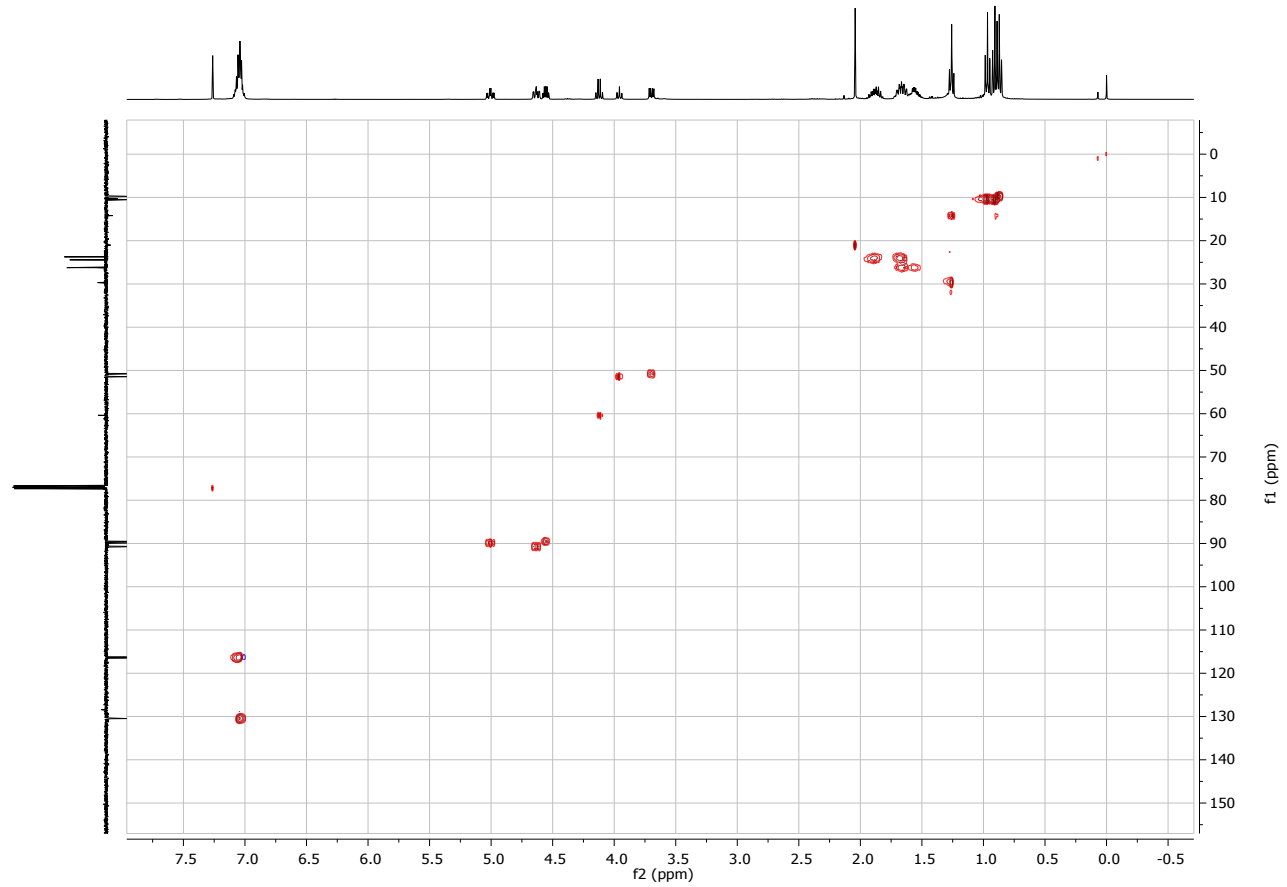


Copy of the ^{13}C-NMR spectrum of new compound **4**



Copy of the COSY spectrum of new compound **4**

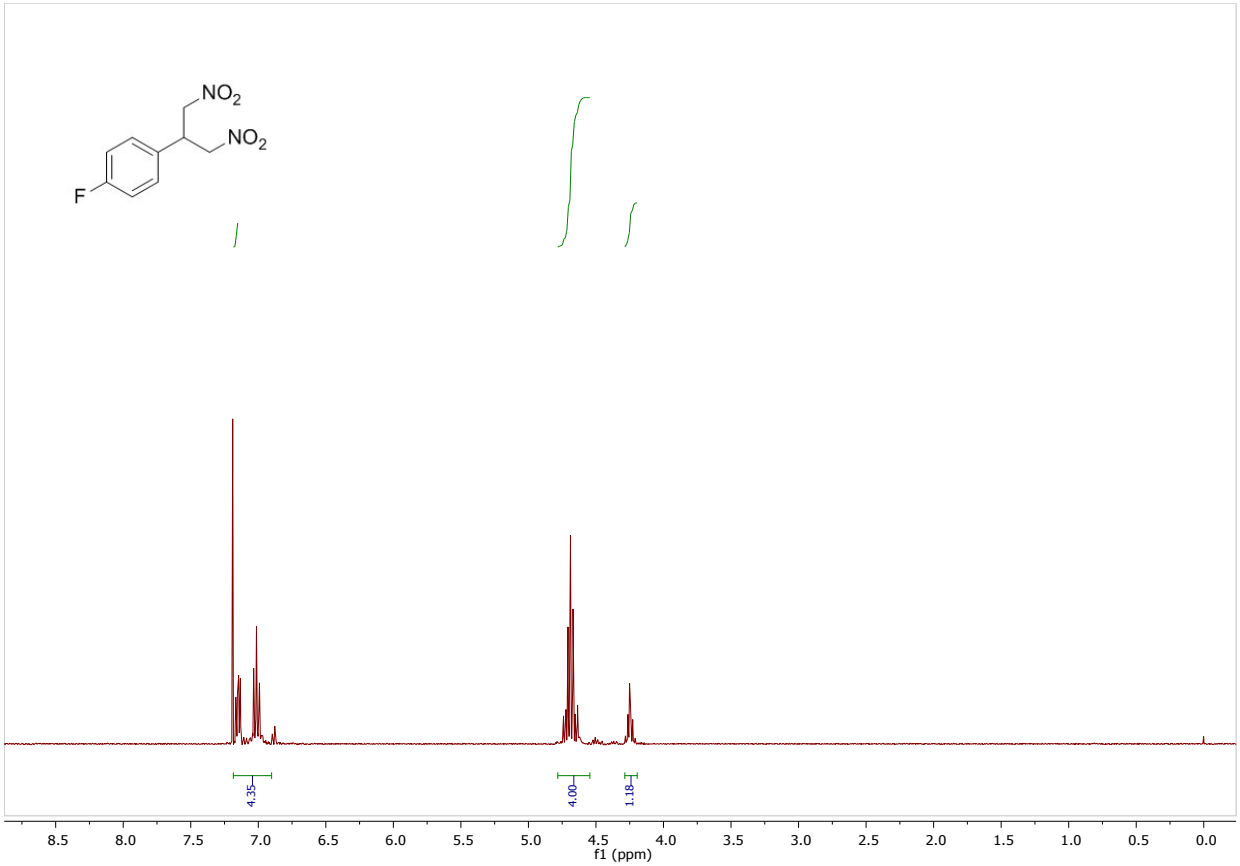
Copy of the HSQC spectrum of new compound **4**



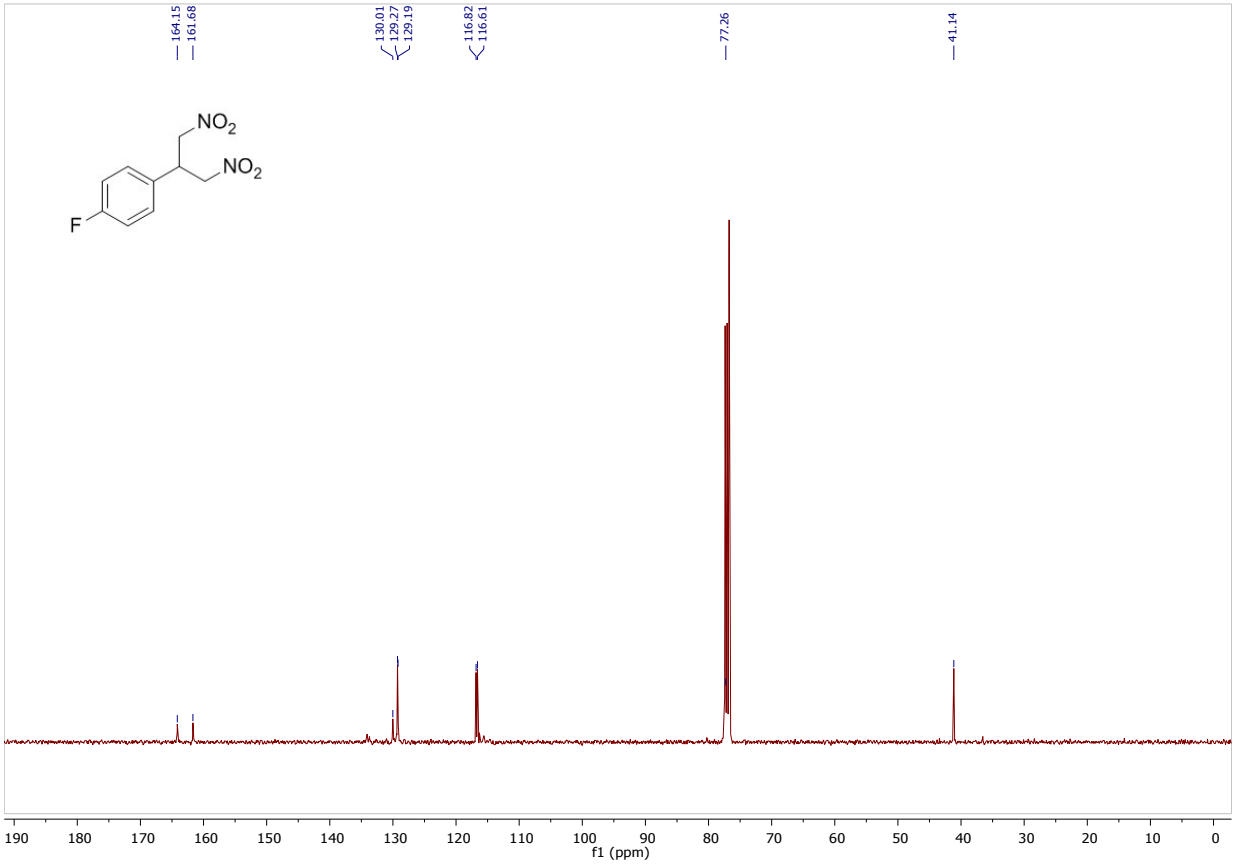
Characterization of known compounds **3a-3h** and **5a,b**

1-(1,3-dinitropropan-2-yl)-4-fluorobenzene 3a. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.18 – 7.12 (m, 2H), 7.01 (t, *J* = 8.5 Hz, 2H), 4.77 – 4.64 (m, 2H), 4.30 – 4.19 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.92 (d, *J* = 248 Hz), 130.01, 129.23 (d, *J* = 8.3 Hz, 2C), 116.71 (d, *J* = 21.8 Hz, 2C), 77.26, 41.14.
1-bromo-4-(1,3-dinitropropan-2-yl)benzene 3b. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52 (d, *J* = 8.4 Hz, 2H), 7.11 (d, *J* = 8.5 Hz, 2H), 4.93 – 4.64 (m, 2H), 4.28 (p, *J* = 6.9 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 132.8 (2C), 131.0, 129.1 (2C), 123.4, 76.5, 41.3.
4-(1,3-dinitropropan-2-yl)phenol 3c. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.10 (d, *J* = 8.6 Hz, 2H), 6.83 (d, *J* = 8.6 Hz, 2H), 4.90 – 4.60 (m, 4H), 4.25 (p, *J* = 7.3 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 156.2, 128.8 (2C), 126.2, 116.5 (2C), 77.2, 41.2.
(1,3-dinitropropan-2-yl)benzene 3d. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 – 7.32 (m, 3H), 7.22 (dd, *J* = 7.7, 1.8 Hz, 2H), 4.86 – 4.65 (m, 4H), 4.41 – 4.21 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 134.3, 129.6 (2C), 129.1, 127.4 (2C), 76.8, 41.8.
1-(1,3-dinitropropan-2-yl)-4-methylbenzene 3e. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.17 (d, *J* = 8.0 Hz, 2H), 7.09 (d, *J* = 8.2 Hz, 2H), 4.99 – 4.62 (m, 4H), 4.26 (p, *J* = 7.2 Hz, 1H), 2.33 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 139.1, 131.1, 130.3 (2C), 127.2 (2C), 76.9, 41.5, 21.1.
1-chloro-4-(1,3-dinitropropan-2-yl)benzene 3f. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 (d, *J* = 8.8 Hz, 2H), 7.18 (d, *J* = 8.8 Hz, 2H), 4.99 – 4.59 (m, 4H), 4.30 (p, *J* = 7.1 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 135.3, 132.6, 129.9 (2C), 128.8 (2C), 76.5, 41.2.
1-(1,3-dinitropropan-2-yl)-4-methoxybenzene 3g. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.14 (d, *J* = 8.8 Hz, 1H), 6.89 (d, *J* = 8.8 Hz, 1H), 4.96 – 4.57 (m, 4H), 4.26 (p, *J* = 7.2 Hz, 1H), 3.79 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.6, 128.3 (2C), 127.2, 114.8 (2C), 76.9, 55.2, 41.2.
1-bromo-2-(1,3-dinitropropan-2-yl)benzene 3h. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66 (dd, *J* = 8.0, 1.4 Hz, 1H), 7.33 (dd, *J* = 7.6, 1.3 Hz, 1H), 7.26 – 7.15 (m, 2H), 4.89 (d, *J* = 5.6 Hz, 4H), 4.87 – 4.76 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 134.1, 133.2, 130.4, 128.4, 127.9, 124.3, 75.3, 40.6.
1,1,1-trifluoro-3-nitro-2-phenylpropan-2-ol 5a. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 – 7.44 (m, 2H), 7.41 – 7.29 (m, 3H), 5.00 (d, *J* = 13.6 Hz, 1H), 4.92 (d, *J* = 13.6 Hz, 1H), 4.57 (s,1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 132.54, 129.52, 128.50, 125.65, 122.98 (d, *J* = 284.6 Hz), 75.74 (d, *J* = 29.7 Hz).
1,1,1-trifluoro-2-(nitromethyl)butan-2-ol 5b. ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.67 (d, *J* = 12.8 Hz, 1H), 4.57 (d, *J* = 12.8 Hz, 1H), 3.95 (s, 1H), 2.03 – 1.87 (m, 1H), 1.88 – 1.74 (m, 1H), 1.07 (t, *J* = 7.6, Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 124.57 (q, *J* = 286.0 Hz), 76.08, 74.84 (q, *J* = 27.7 Hz), 26.20, 6.76.

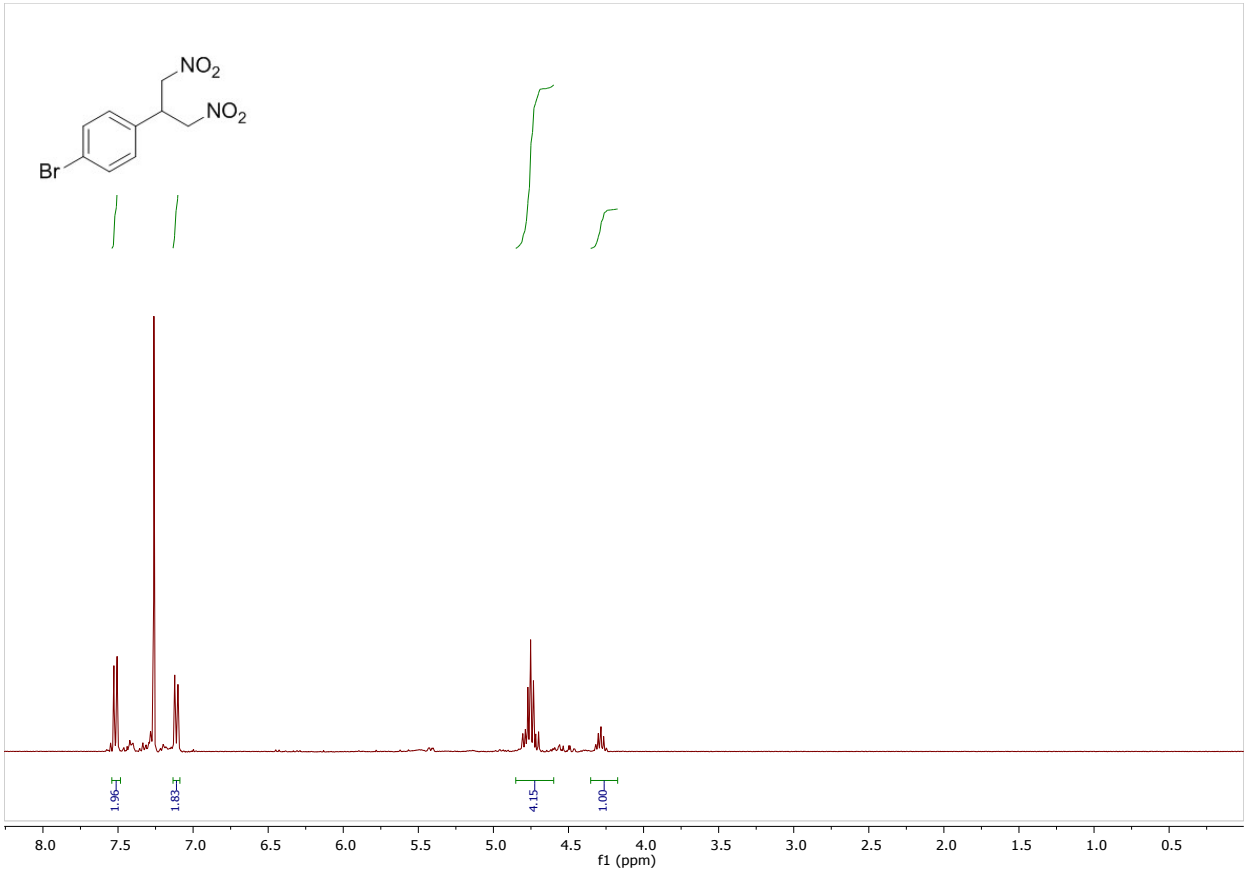
Copy of the ^{1}H-NMR spectrum of compound **3a**



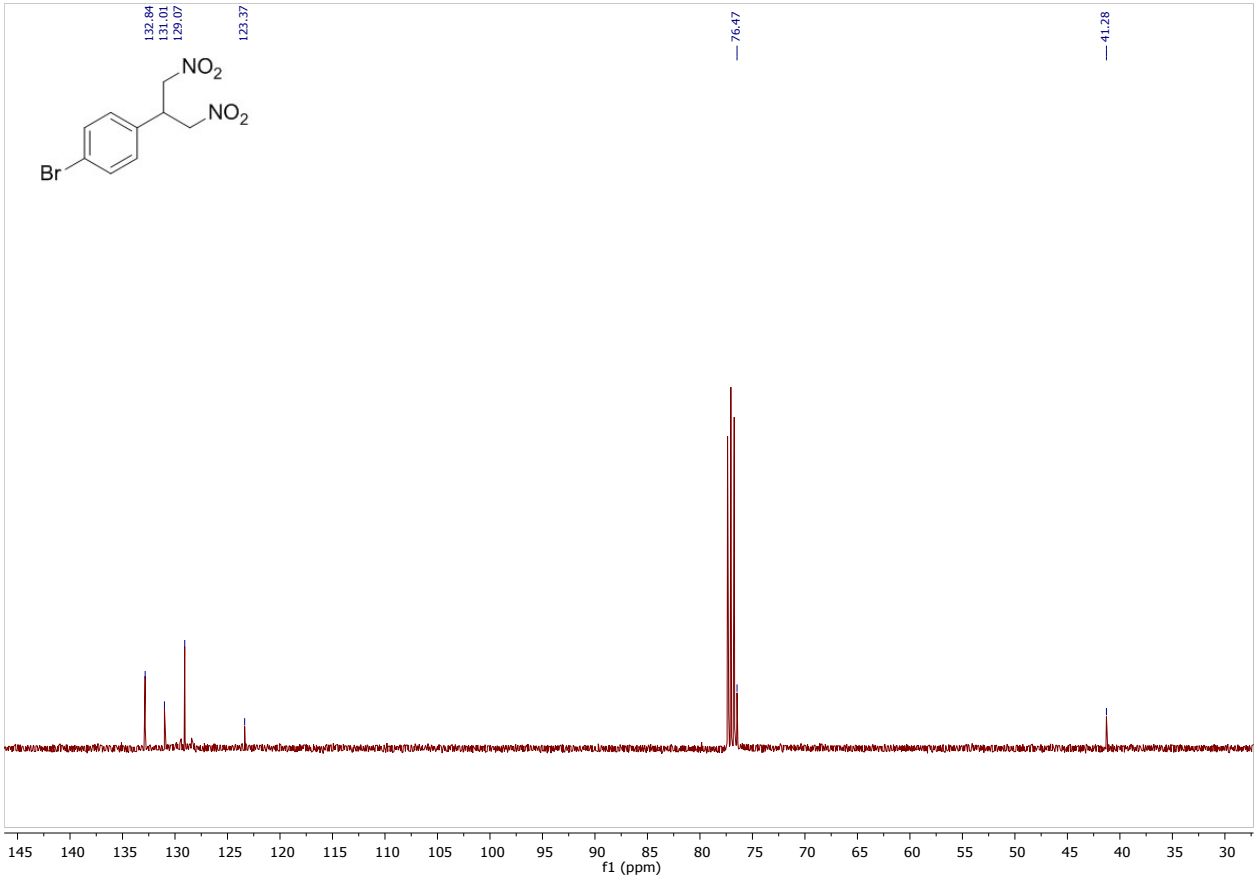
Copy of the ^{13}C-NMR spectrum of new compound **3a**



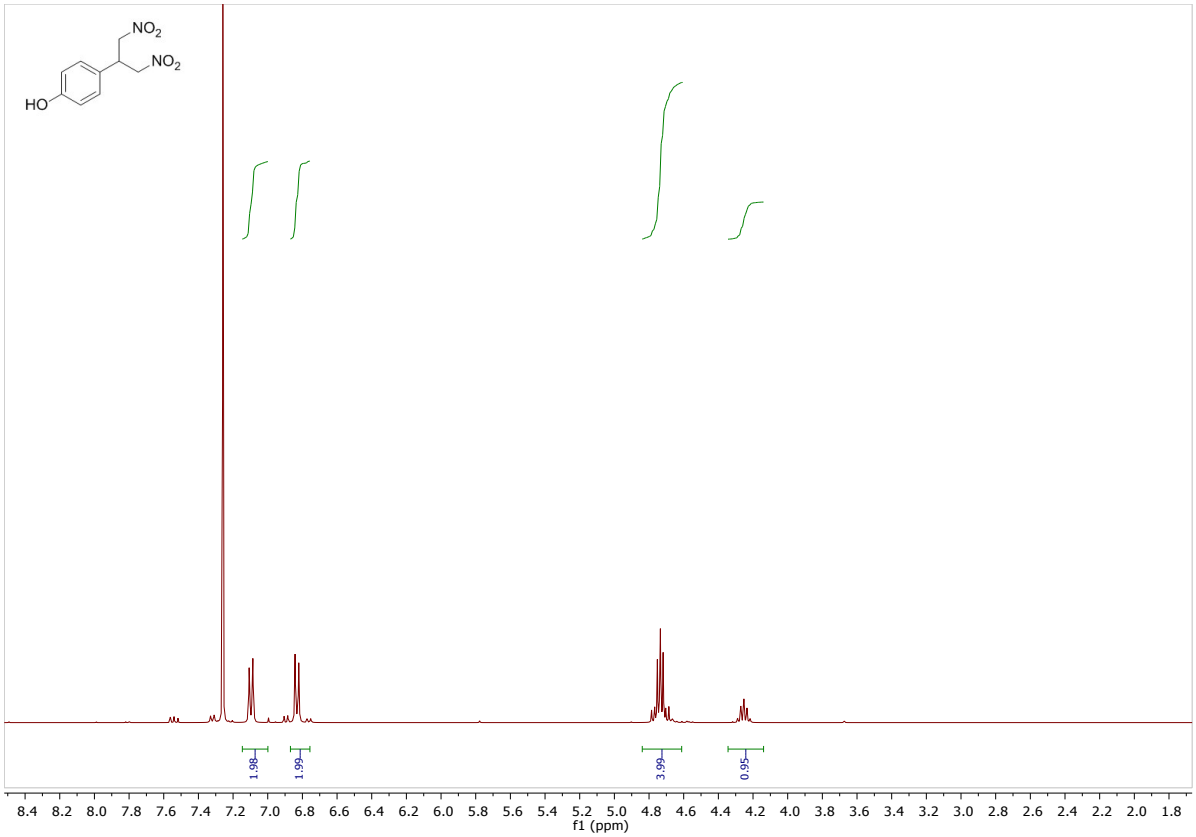
Copy of the ^{1}H-NMR spectrum of compound **3b**



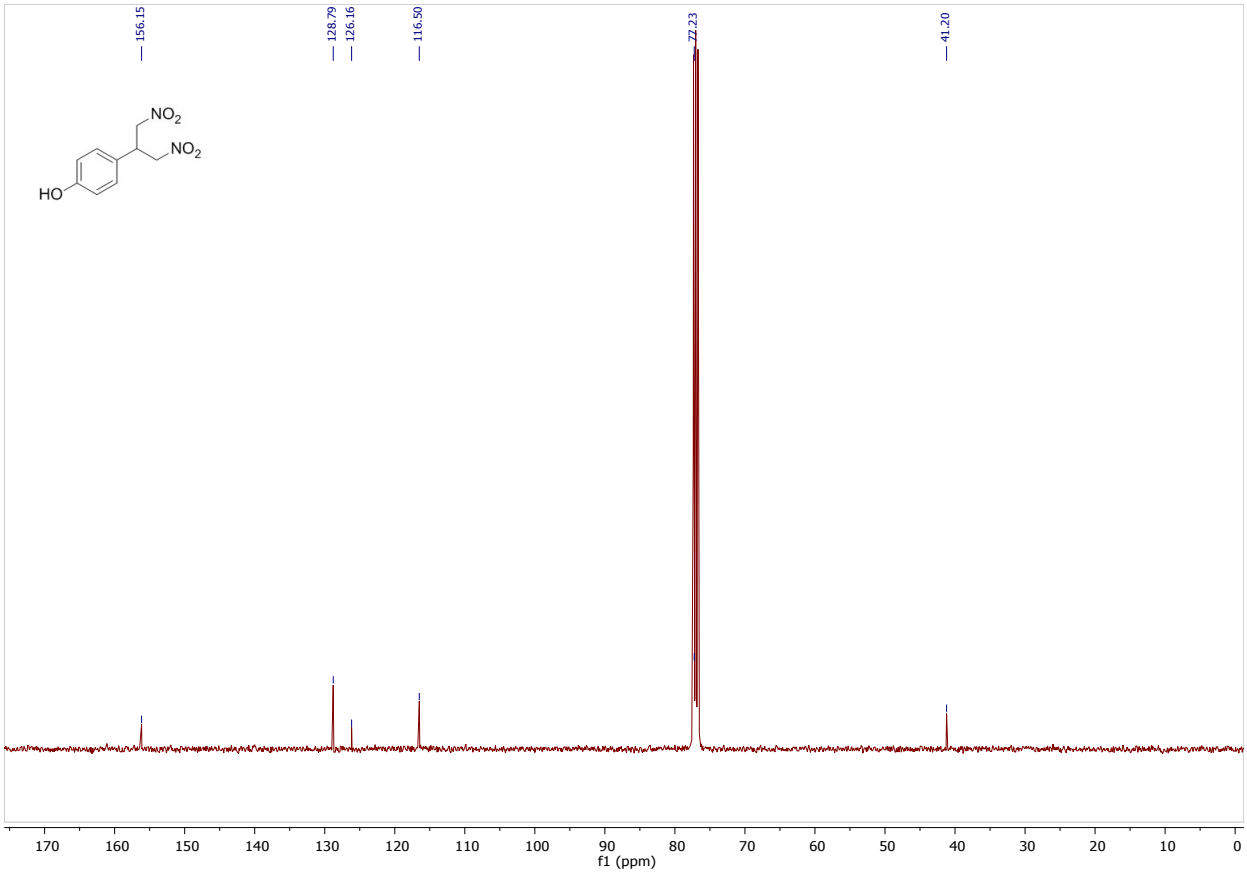
Copy of the ^{13}C-NMR spectrum of new compound **3b**



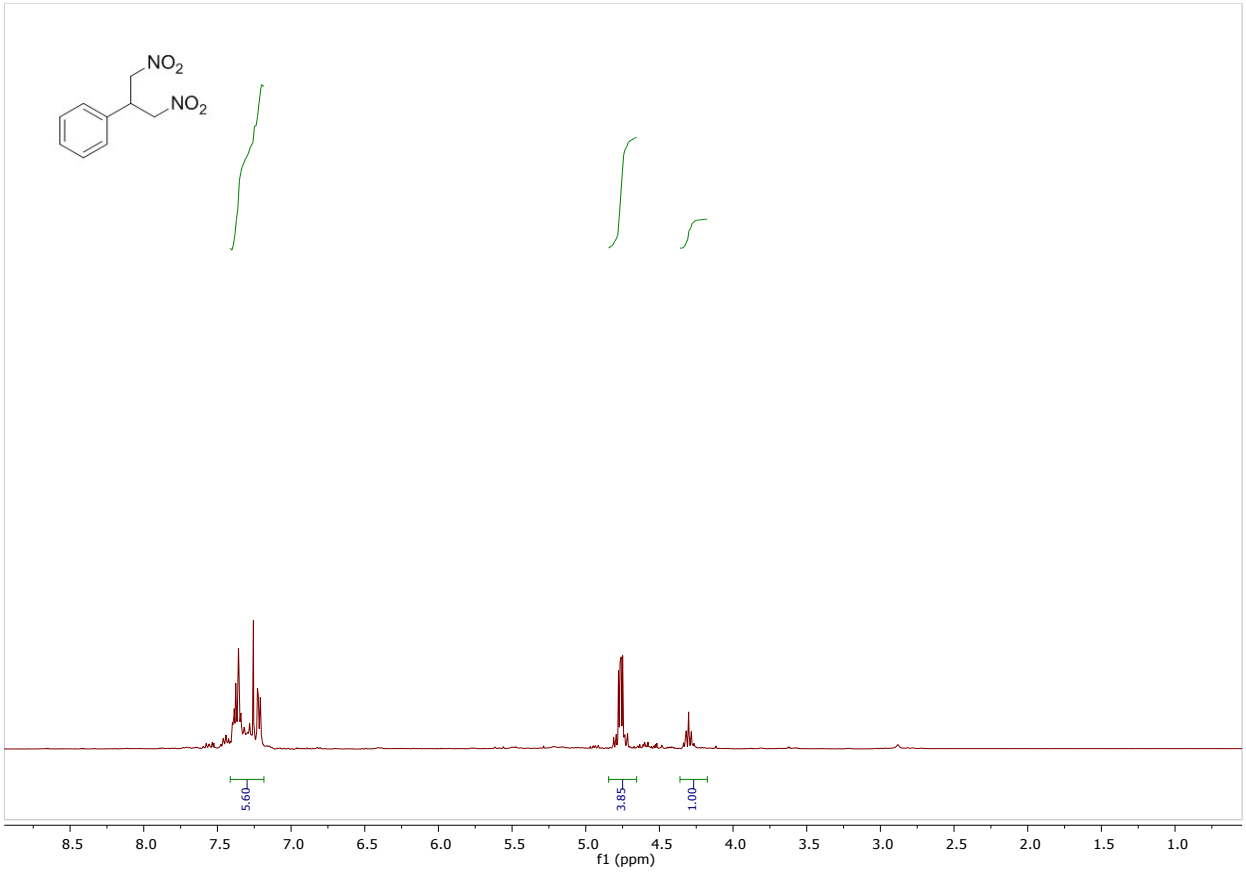
Copy of the ^{1}H-NMR spectrum of compound **3c**



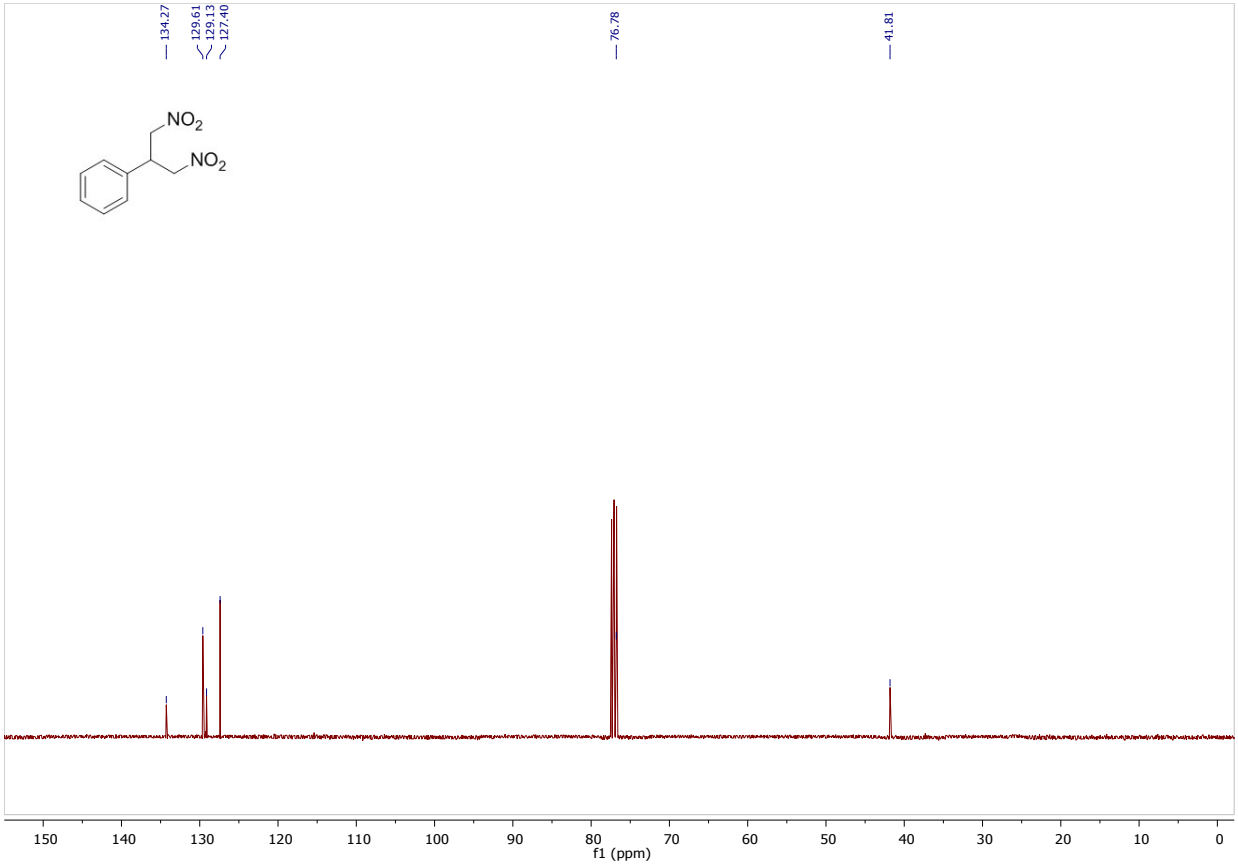
Copy of the ^{13}C-NMR spectrum of new compound **3c**



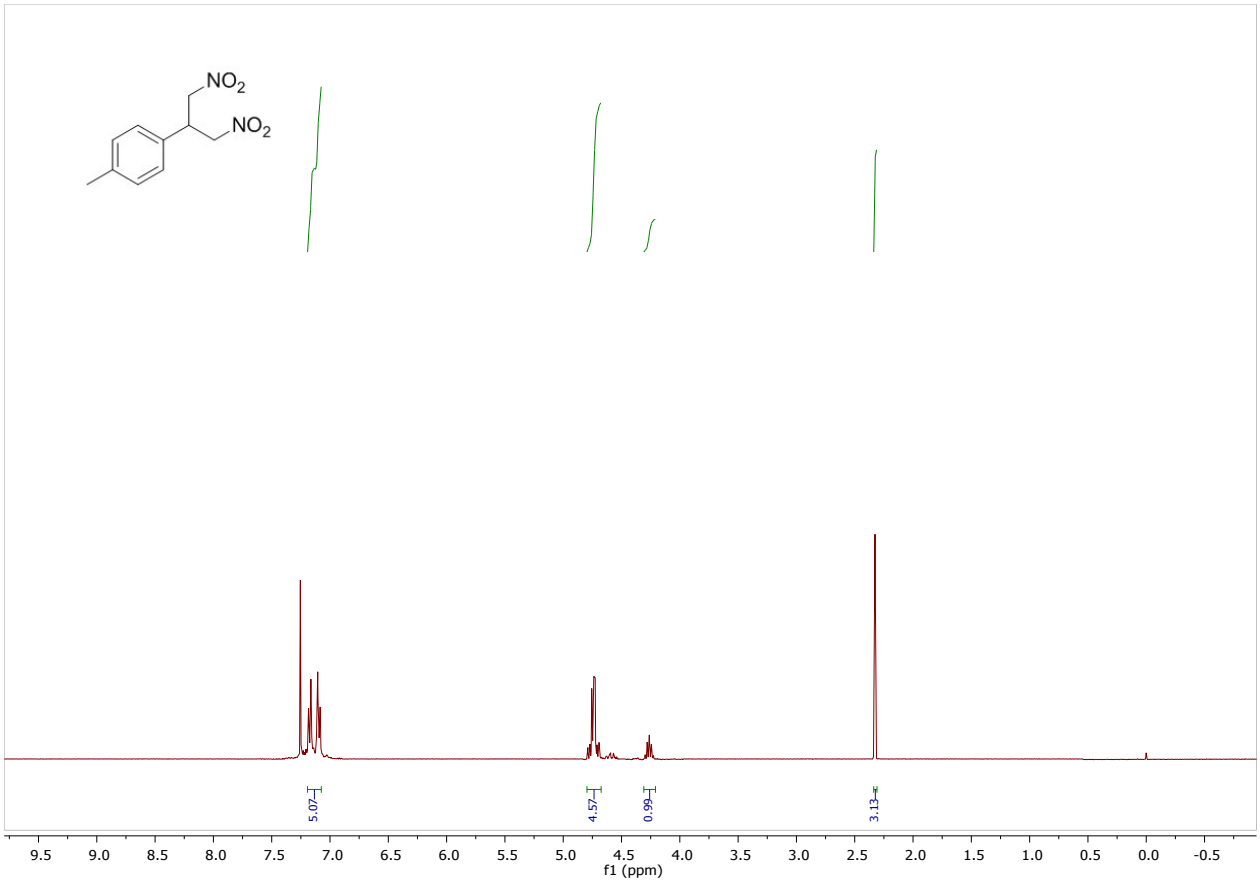
Copy of the ^{1}H-NMR spectrum of compound **3d**



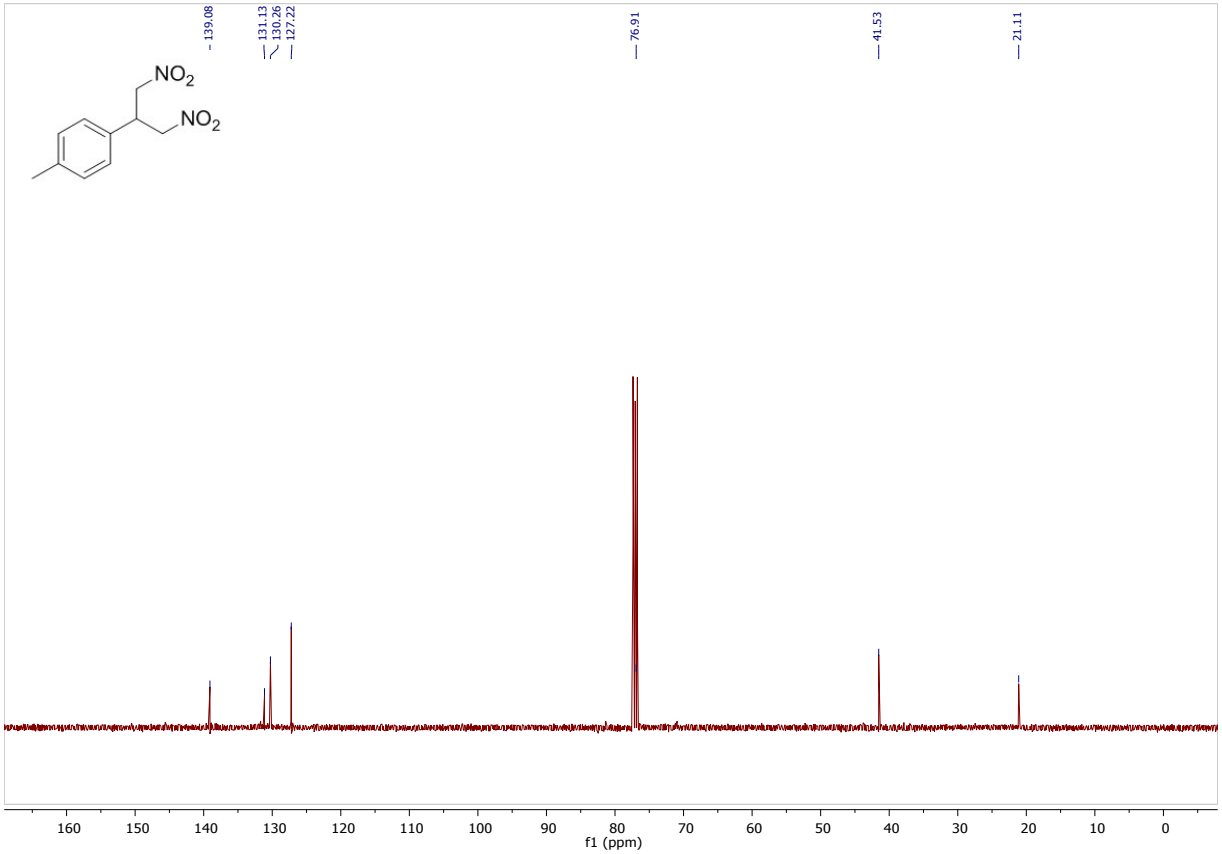
Copy of the ^{13}C-NMR spectrum of new compound **3d**



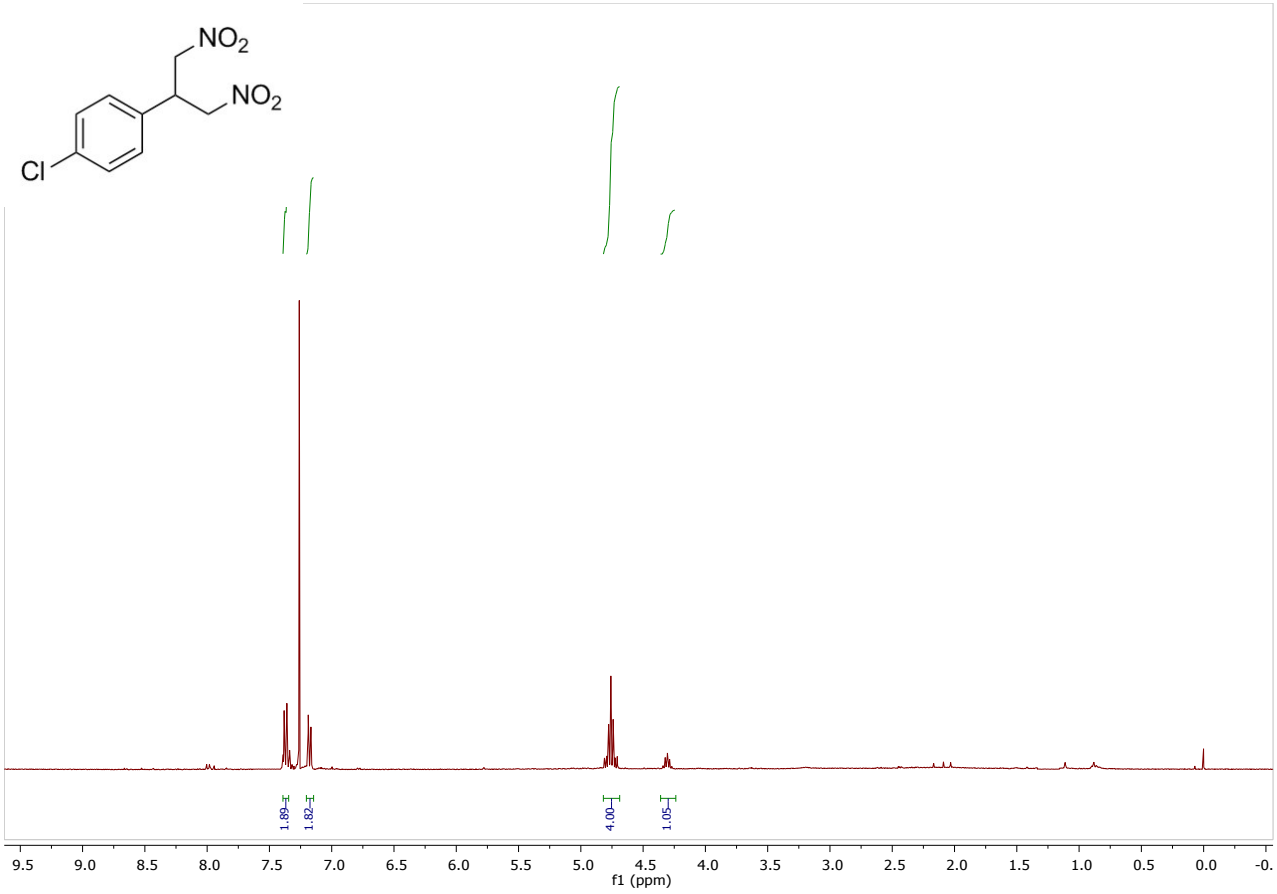
Copy of the ^{1}H-NMR spectrum of compound **3e**



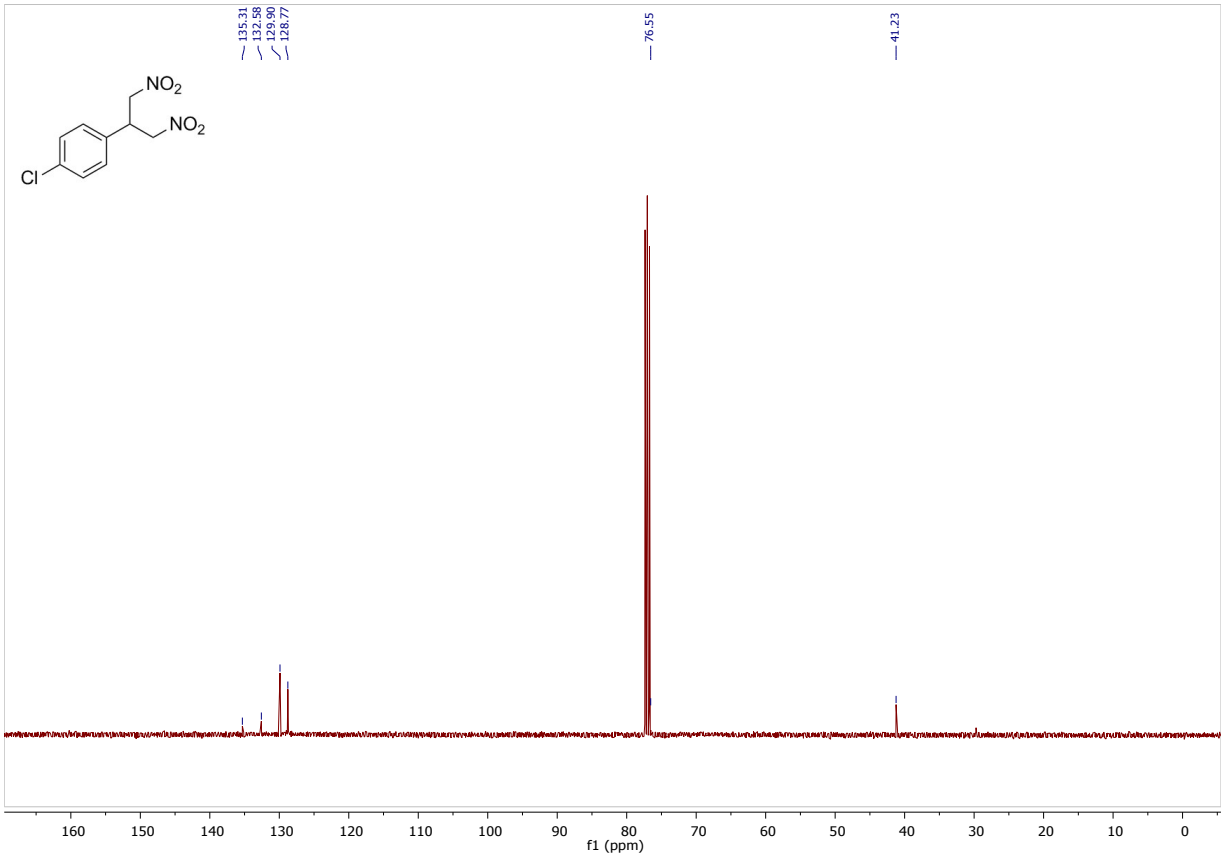
Copy of the ^{13}C-NMR spectrum of new compound **3e**



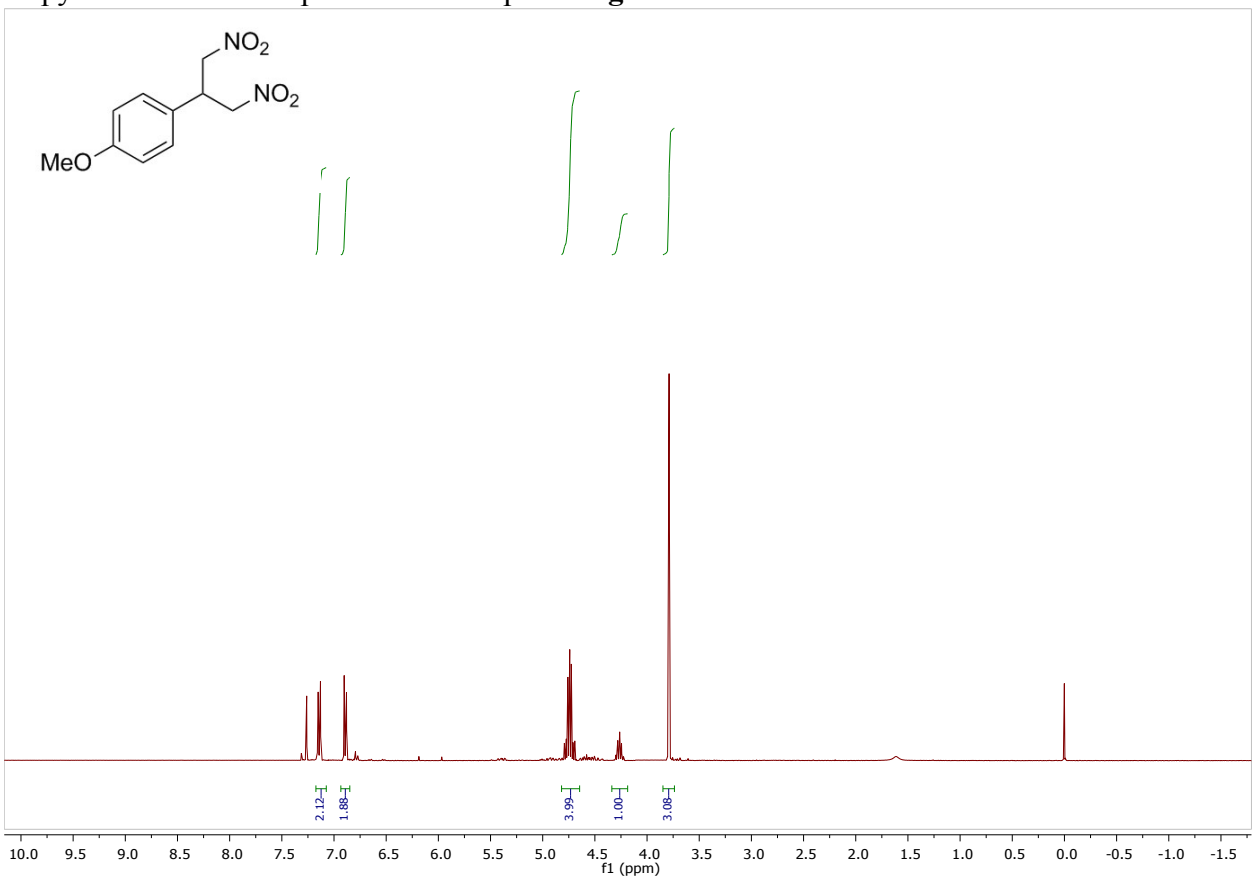
Copy of the ^{1}H-NMR spectrum of compound **3f**



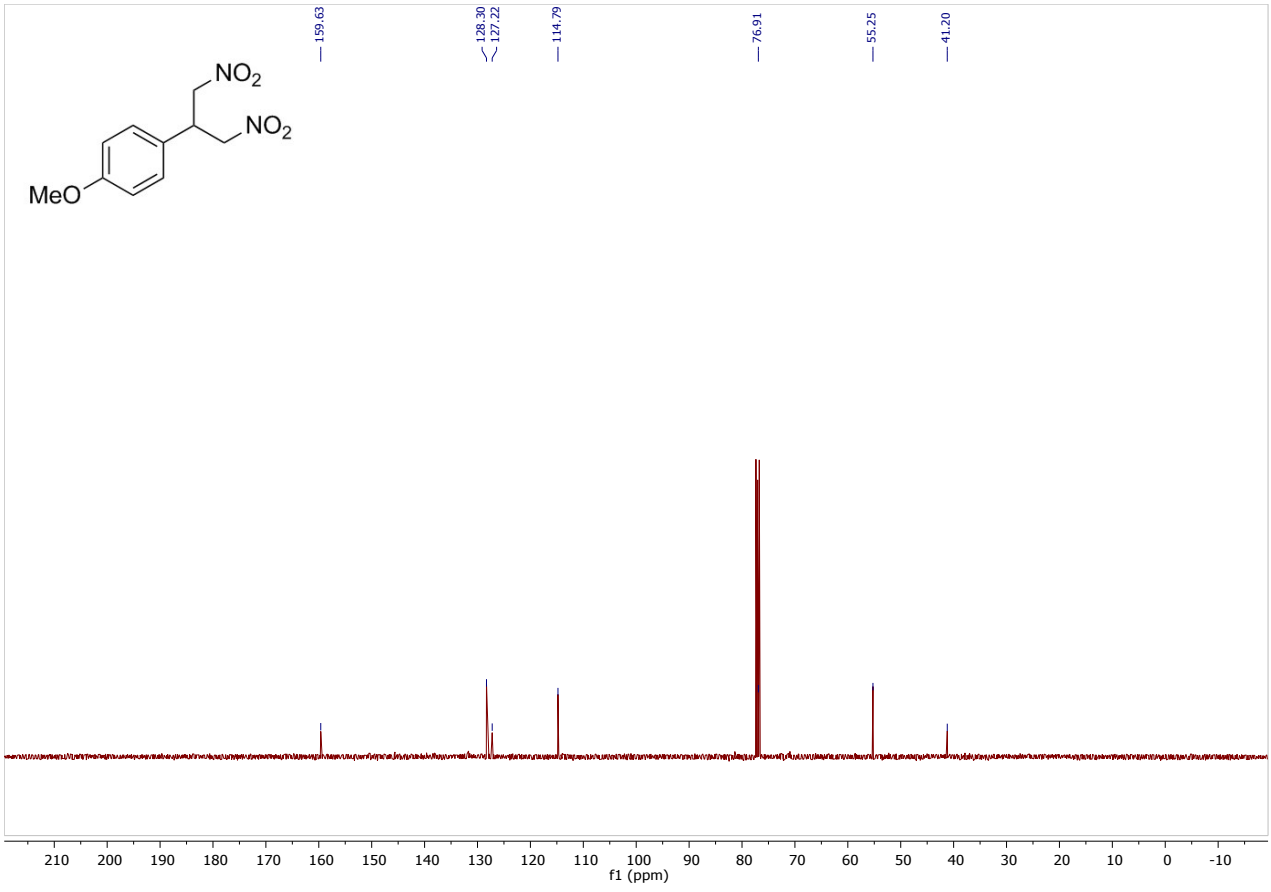
Copy of the ^{13}C-NMR spectrum of new compound **3f**



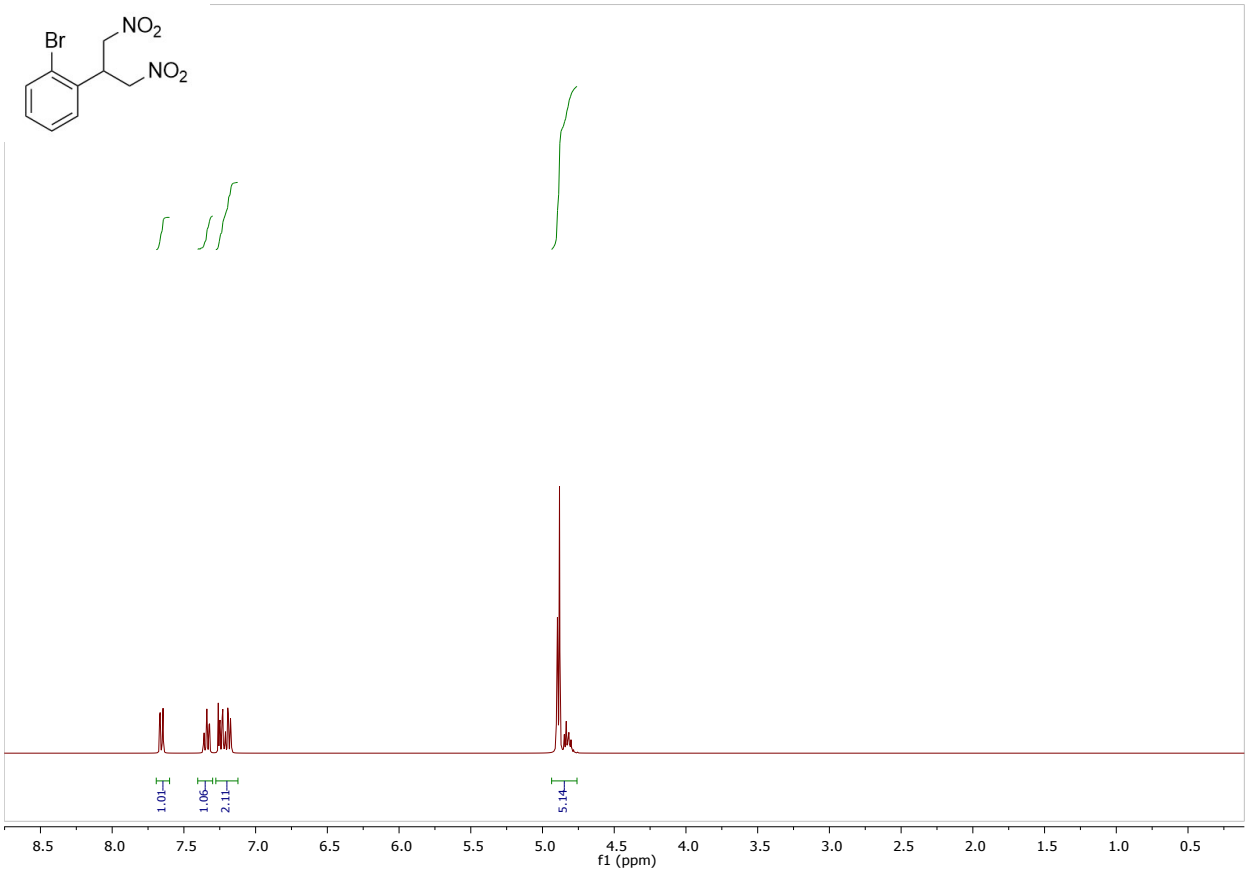
Copy of the ^{1}H-NMR spectrum of compound **3g**



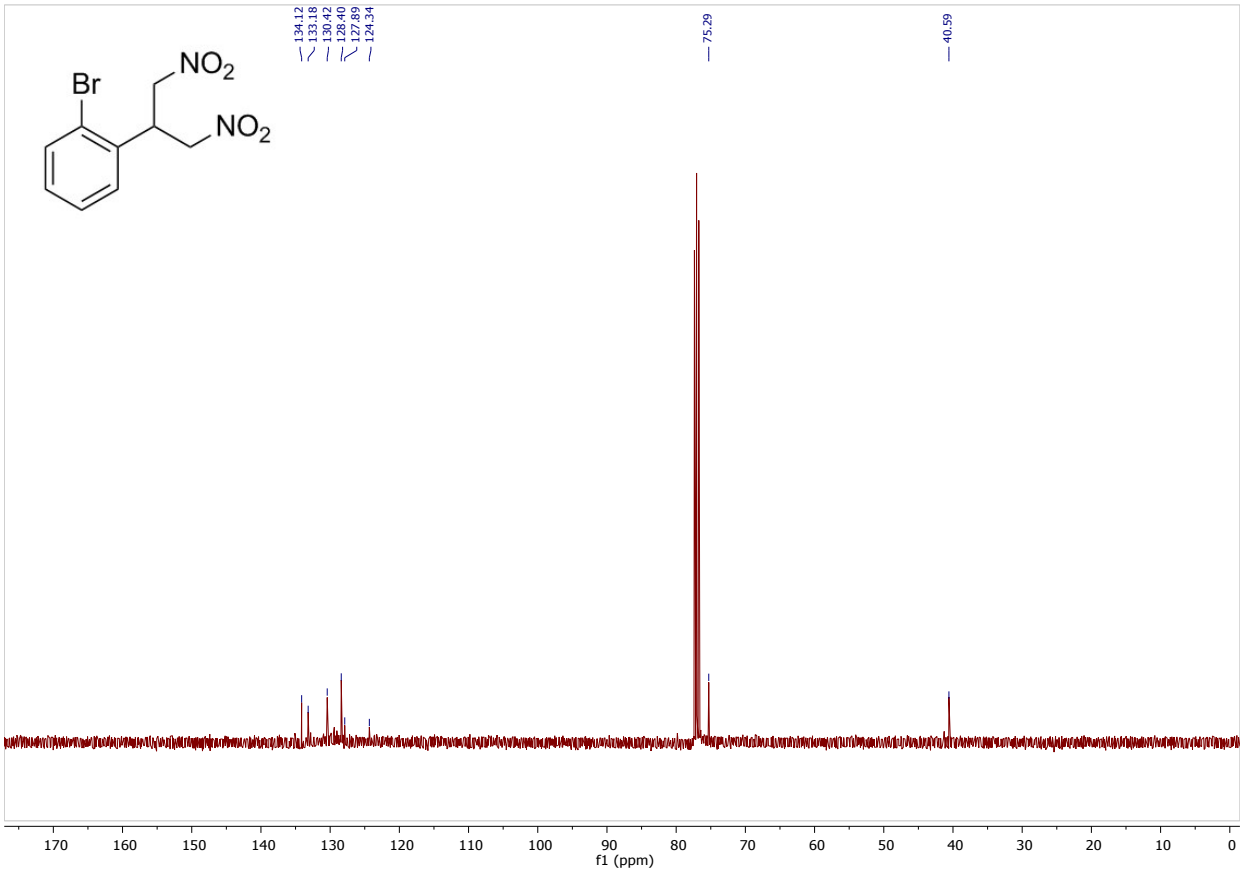
Copy of the ^{13}C-NMR spectrum of new compound **3g**



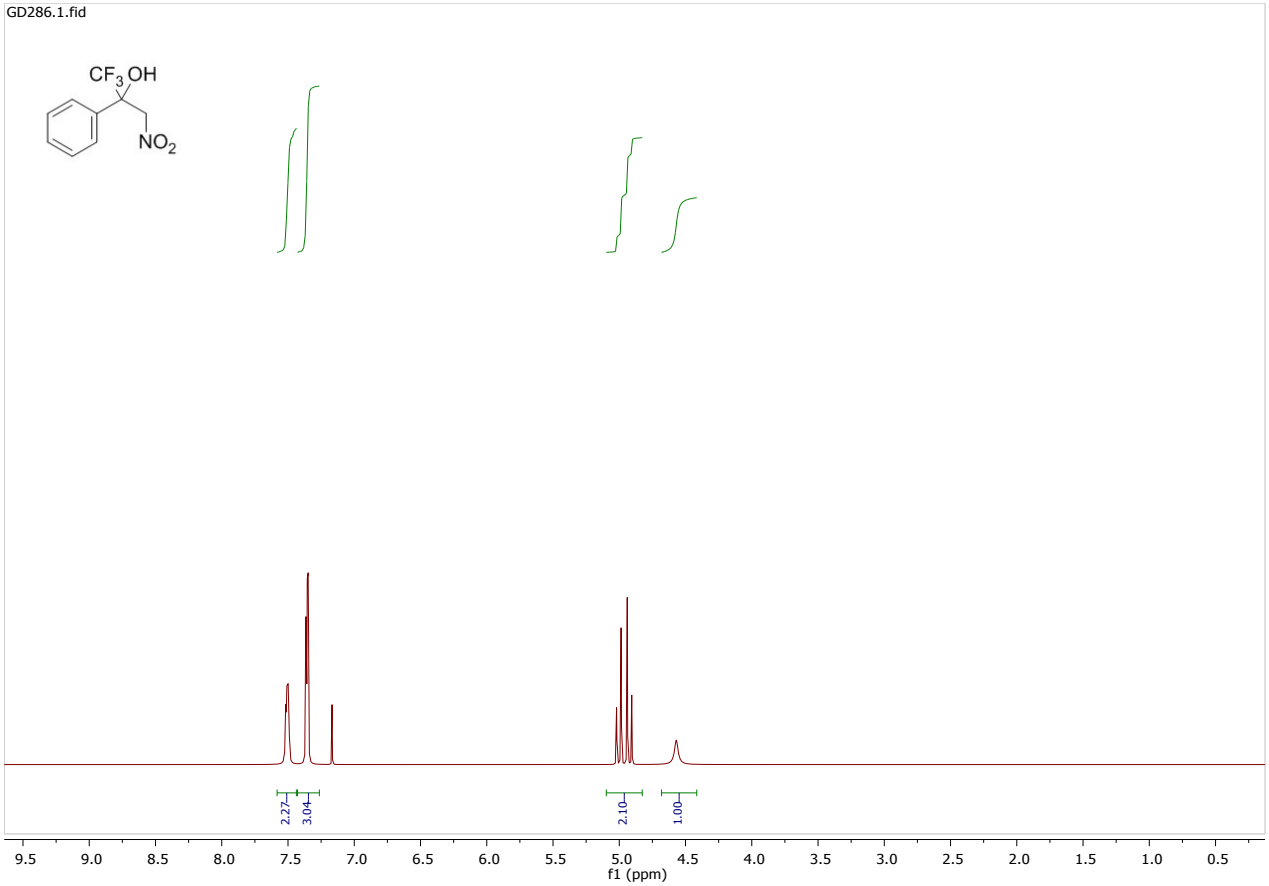
Copy of the ^{1}H-NMR spectrum of compound **3h**



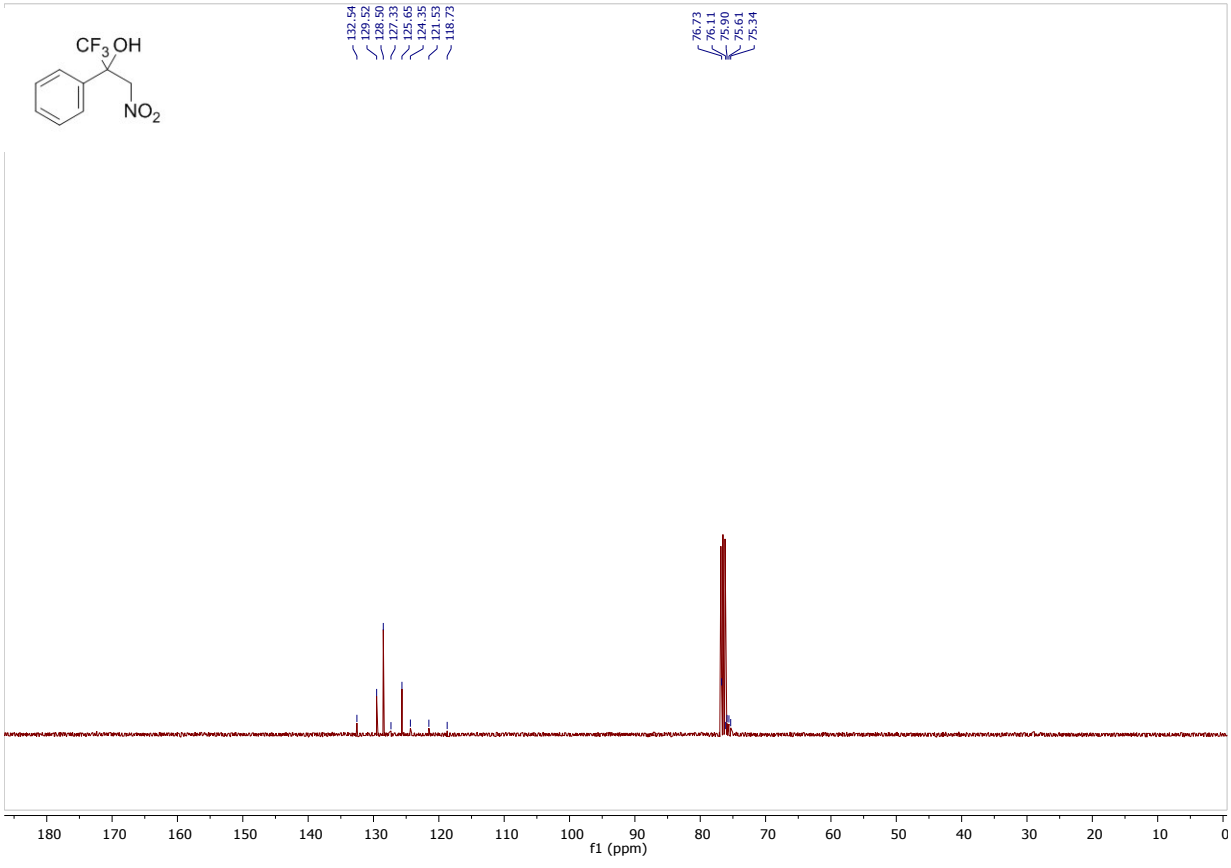
Copy of the ^{13}C-NMR spectrum of new compound **3h**



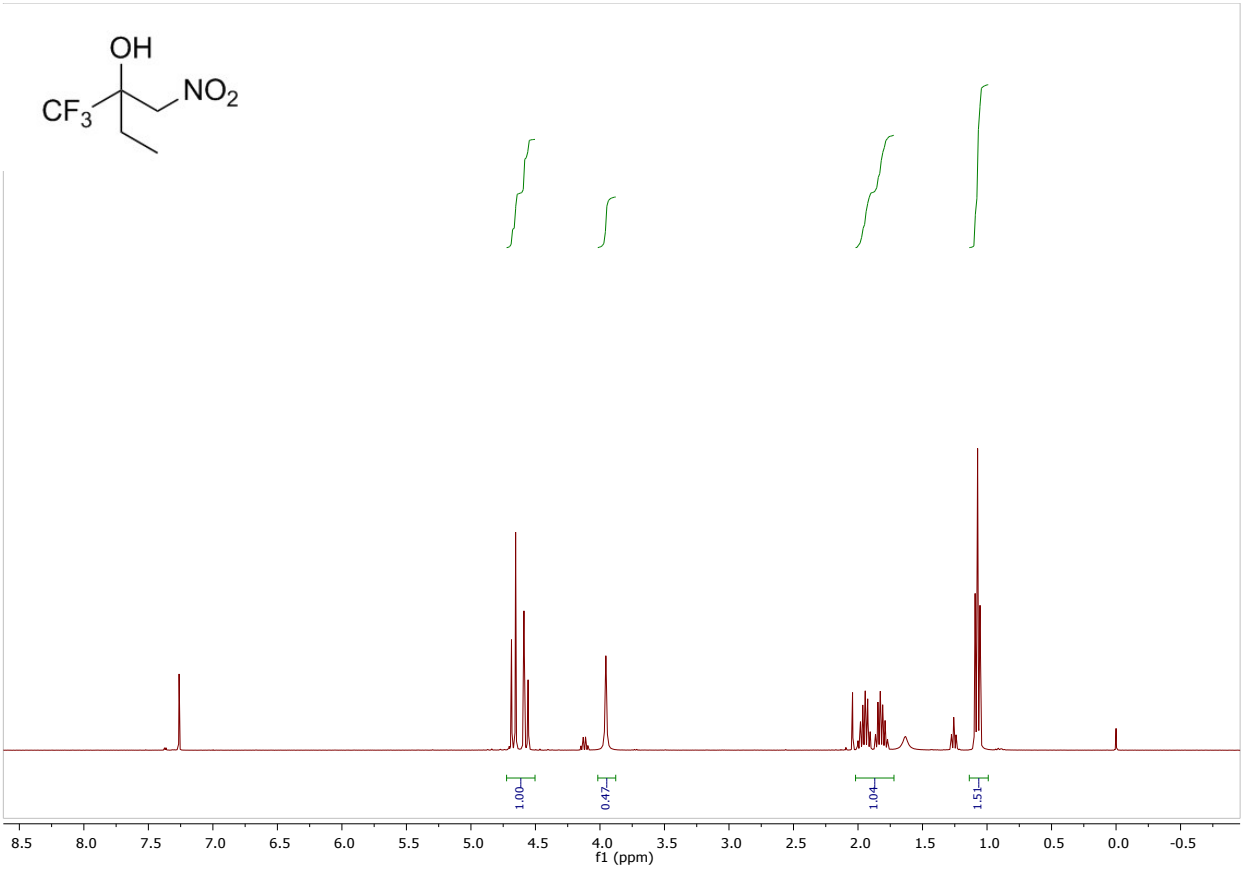
Copy of the ^{1}H-NMR spectrum of compound **5a**



Copy of the ^{13}C-NMR spectrum of new compound **5a**



Copy of the ^{1}H-NMR spectrum of compound **5b**



Copy of the ^{13}C-NMR spectrum of new compound **5b**