Supplementary information

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

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**General information**

Copy of NMR spectra for new compound 4 S2
Characterization of compounds 3a-3h and 5a,b S4
Copy of \textsuperscript{1}H and \textsuperscript{13}C NMR spectra for known compounds 3a-3h and 5a,b S5
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\(_3\)) \(\delta\) 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\(_3\)) \(\delta\) 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\(_3\)) \(\delta\) 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\(_3\)) \(\delta\) 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\(_3\)) \(\delta\) 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\(_3\)) \(\delta\) 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\(_3\)) \(\delta\) 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\(_3\)) \(\delta\) 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\(_3\)) \(\delta\) 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). \(^{13}^C\)NMR (101 MHz, CDCl\(_3\)) \(\delta\) 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\(_3\)) \(\delta\) 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\(_3\)) \(\delta\) 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\(_3\)) \(\delta\) 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\(_3\)) \(\delta\) 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\(_3\)) \(\delta\) 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\(_3\)) \(\delta\) 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\(_3\)) \(\delta\) 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\(_3\)) \(\delta\) 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\(_3\)) \(\delta\) 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, \(J = 7.6, 3\)H). \(^{13}^C\)NMR (101 MHz, CDCl\(_3\)) \(\delta\) 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 3e

Copy of the $^{13}$C-NMR spectrum of new compound 3e
Copy of the $^1\text{H}$-NMR spectrum of compound 3d

Copy of the $^{13}\text{C}$-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