

Supporting information

1. Experimental details

1.1. Materials

All materials were used as obtained commercially.

1.2. Product analysis and identification

Crude reaction mixtures were analyzed by gas chromatography (GC) (quantitative, internal standard in the reaction mixture) and nuclear magnetic resonance (NMR) spectroscopy (qualitative; amine, amide, carboxylic acid region between 2.0 and 3.0 ppm). NMR samples were prepared by mixing 300 μL of the reaction mixture with 300 μL methanol- d_4 . ^1H -NMR spectra, as well as ^1H , ^1H -COSY and ^1H , ^{13}C -HSQC spectra, were recorded on a Bruker Ascend 400 MHz spectrometer equipped with a BBO 5 mm atma probe and a sample case. One of the signals of CPME was suppressed by applying an adapted zgpr pulse program: p1 9.75 μs ; plw1 15W; plw9 5.7-05W; o1P on the resonance signal of CPME (around 3.27 ppm). Besides GC and NMR, the products were also identified by gas chromatography coupled to mass spectrometry (GC-MS) with an Agilent 6890 GC, equipped with a HP-5ms column, coupled to a 5973 MSD mass spectrometer.

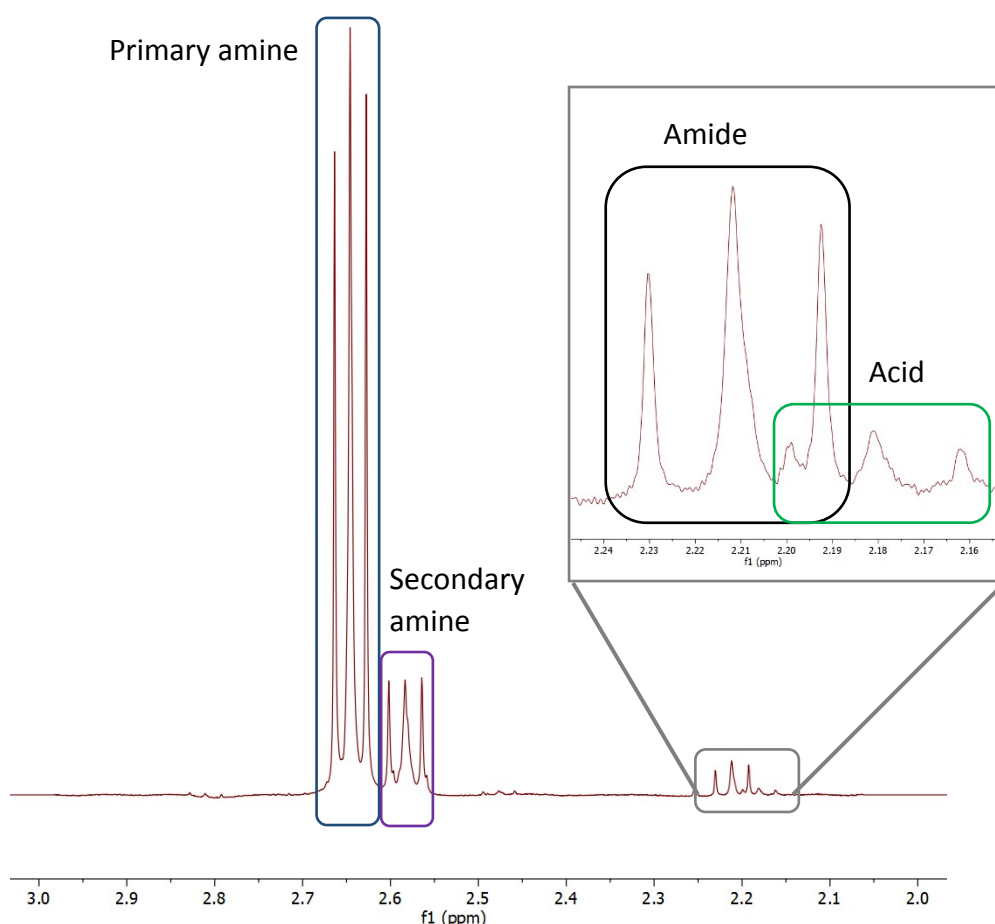


Figure S 1 – ^1H NMR spectrum of reaction mixture after reductive amination of octanoic acid

1.3. Catalyst synthesis and characterization

The catalysts were prepared as described by Coeck *et al.* (2019).¹ Although the catalyst was already characterized extensively, additional inductively coupled plasma optical emission spectrometry measurements (ICP-OES) were performed to check the catalysts' stability. Possible Ru, W and Mg leaching was measured by ICP using a Varian 720-ES with the Varian SPS3 sample preparation system and applying the calibration curve method. For 1 mL of the supernatant of the reaction mixture, the solvent was evaporated and residual ions were redissolved in 20 mL aqua regia.

1.4. NH₃- and CO₂-TPD measurements

Ammonia (NH₃) and carbon dioxide (CO₂) temperature programmed desorption (TPD) experiments were performed using a Quantachrome ChemBET pulsar equipped with a TCD. Prior to each measurement, the catalyst (300 mg) was dried at 450 °C for 1 h under flowing He (20 mL/min) and cooled to 30 °C. The catalyst was then exposed to either NH₃ or CO₂ (20 mL/min) for 45 min, followed by purging the physisorbed NH₃ and CO₂ with He for 1 h. Finally, the catalyst was heated gradually (10 °C/min) in a He flow (20 mL/min).

2. Dehydration of ammonium octanoate

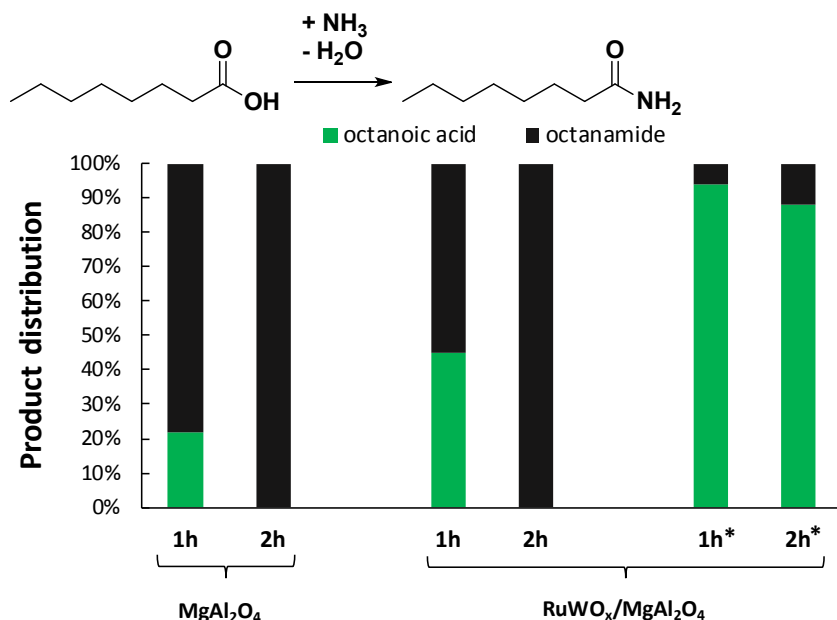


Figure S 2 – Dehydration of ammonium octanoate with RuWO_x/MgAl₂O₄ (left) and pure MgAl₂O₄ (right). The dehydration occurs faster with the pure MgAl₂O₄, due to a partial coverage of MgAl₂O₄ with RuWO_x. Reaction conditions: octanoic acid (1 mmol), 200°C, 6 bar NH₃, no additional H₂, 0.126 g catalyst, undecane (20 µL), CPME (10 mL). *reaction performed in dimethoxyethane, with 3 bar NH₃ (at 3 bar an equal amount of NH₃ is dissolved in comparison with 6 bar NH₃ over CPME)

3. Influence of low quantities of water

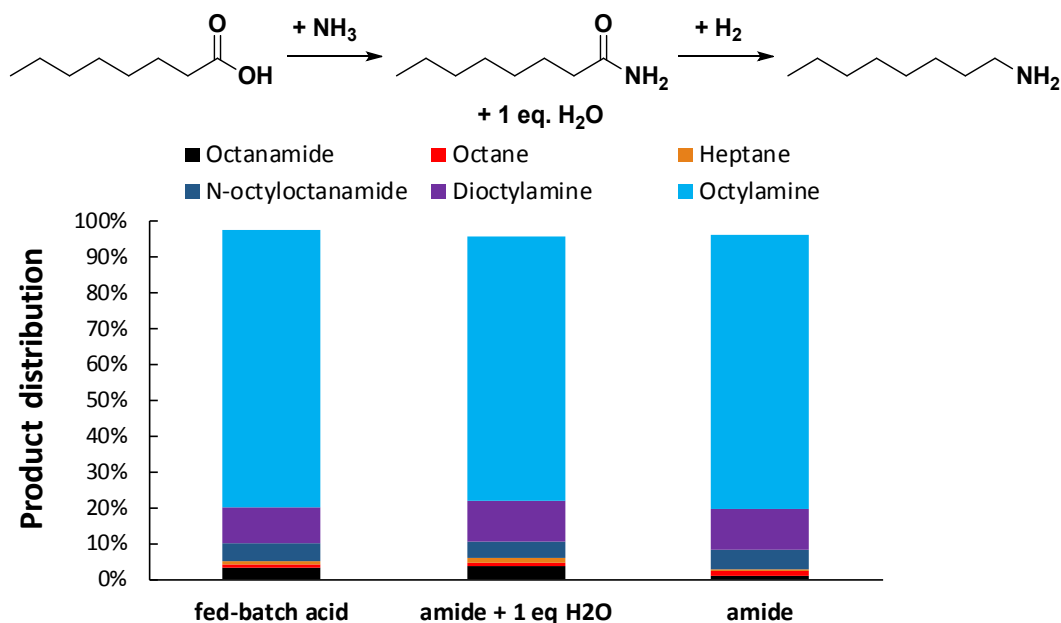


Figure S 3 – Synthesis of octylamine from octanoic acid (left, fed batch, initial 2h with 6 bar NH₃), octanamide with 1 eq. water (middle) and octanamide (right, no addition of water). Reaction conditions: substrate (1 mmol), 200°C, 6 bar NH₃, 50 bar H₂, 5 mol% Ru (4 wt% Ru on RuWO_x/MgAl₂O₄), undecane (20 µL), CPME (10 mL).

4. Recycling and characterization of catalyst

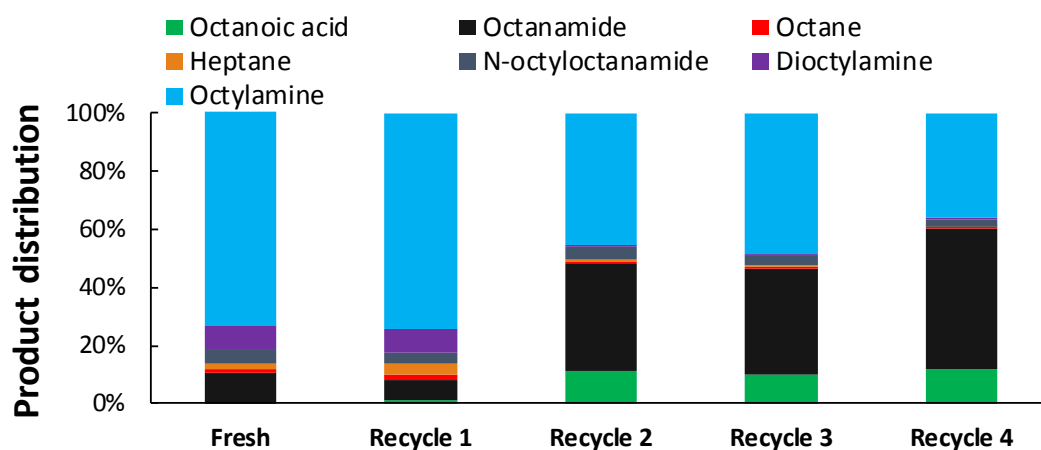


Figure S 4 – Recycling test of RuWO_x/MgAl₂O₄. Reaction conditions: octanoic acid (1 mmol), 200°C, 6 bar NH₃, 50 bar H₂, 5 mol% Ru (4 wt% Ru on RuWO_x/MgAl₂O₄), undecane (20 µL), CPME (10 mL), for 4 h.

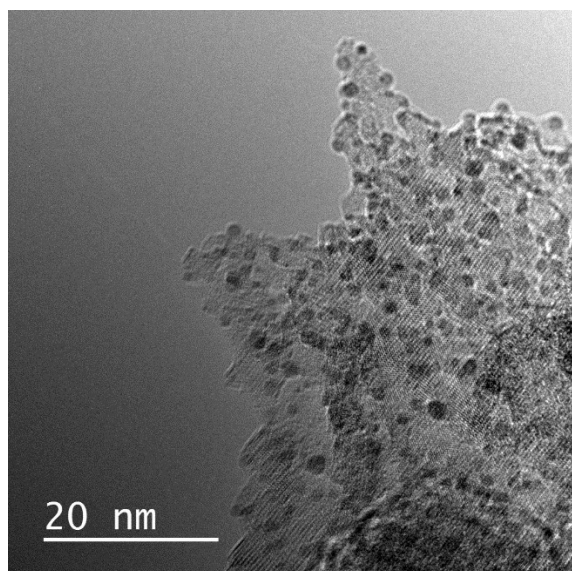


Figure S 5 – TEM images of RuWO_x/MgAl₂O₄ catalyst (black dots are Ru particles).

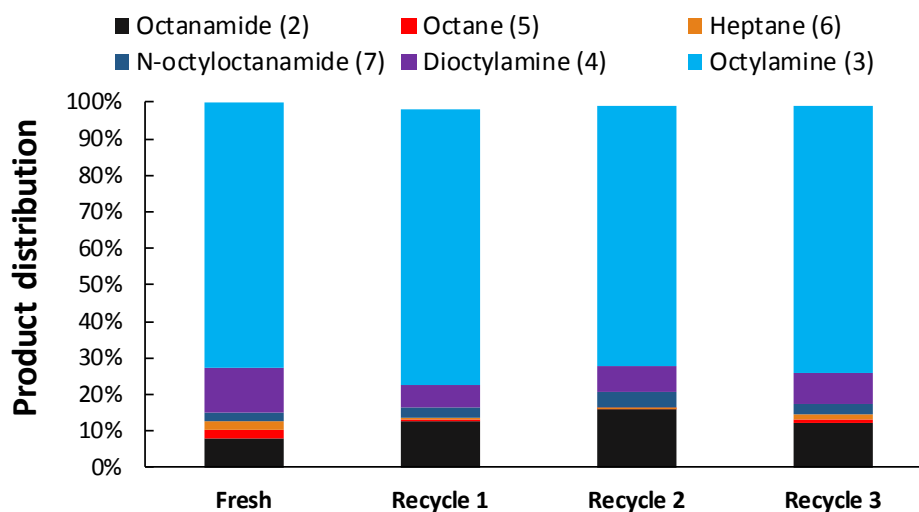


Figure S 6 – Recycling test of RuWO_x/ZrO₂. Reaction conditions: fed-batch reaction, octanoic acid (1 mmol), 200°C, 6 bar NH₃ (initial 2 h), 6 bar NH₃ + 50 bar H₂ (5 h), 7.5 mol% Ru, undecane (20 µL), CPME (10 mL).

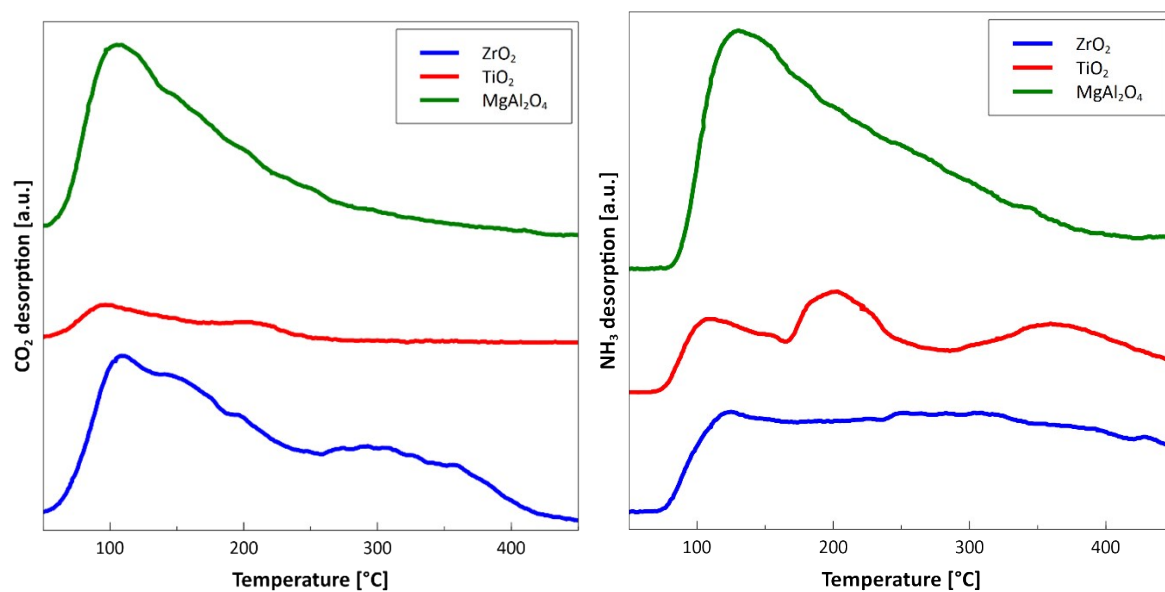


Figure S 7 – TPD experiments for ZrO₂, TiO₂ and MgAl₂O₄. CO₂ desorption (left) and NH₃ desorption (right) normalized by the weight of the materials.

Table S 1 – Acidic and basic properties of ZrO₂, TiO₂ and MgAl₂O₄ as determined by TPD experiments.

Support	BET surface ^a [m ² /g]	Acid amount ^b [μmol/g]	Base amount ^c [μmol/g]	Acid density ^d [μmol/m ²]	Base density ^d [μmol/m ²]
ZrO ₂	25	140.7	106.8	5.6	4.3
TiO ₂	50	95.1	16.1	1.9	0.3
MgAl ₂ O ₄	177	173.7	97.8	1.0	0.6

^a Specific surface area determined by N₂ physisorption or specified by the supplier. ^b Amount of acidic sites determined by NH₃-TPD. ^c Amount of basic sites determined by CO₂-TPD. ^d Density of sites determined via TPD results and specific surface area of the support.

5. Substrate scope investigation

Table S 2 – Full list of substrate scope investigation

Substrate	Products distribution (yield)
Butyric acid	Butylamine (80%), Dibutylamine (5%), Butyramide (6%), <i>N</i> -Butylbutyramide (4%)
Hexanoic acid	Hexylamine (75%), Dihexylamine (13%), Pentane (1%), Hexane (1%), Hexanamide (1%), <i>N</i> -Hexylhexanamide (6%), Hexylhexanoate (1%), <i>N</i> -Hexylcyclopentanamine (1%)
Octanoic acid	Octylamine (76%), Dioctylamine (8%), Octanamide (5%), Octane (2%), <i>N</i> -Octyloctanamide (4%), Heptane (4%)
Methyl octanoate	Octylamine (73%), Dioctylamine (13%), Octanamide (5%), Octane (1%), <i>N</i> -Octyloctanamide (7%), <i>N</i> -Octyloctanoate (1%).
Undecylenic acid	Undecylamine (70%), Diundecylamine (7%), Undecanamide (13%), <i>N</i> -Undecylundecanamide (6%), <i>N</i> -Undecylcyclopentanamine (1%), Decane (1%),
Lauric acid	Dodecylamine (74%), Didodecylamine (15%), Dodecanamide (3%), <i>N</i> -Dodecylundecanamide (5%), Undecane (1%), Dodecane (1%), <i>N</i> -Dodecylcyclopentanamine (1%)
Myristic acid	Tetradecylamine (70%), Ditetradecylamine (20%), Tetradecane (1%), Tridecane (1%), <i>N</i> -Tetradecyltetradecanamide (6%), <i>N</i> -Tetradecylcyclopentanamine (2%)
3,5,5-Trimethylhexanoic acid	3,5,5-Trimethylhexylamine (60%), 3,5,5-Trimethylhexanamide (21%), 3,5,5-Trimethyl- <i>N</i> -(3,5,5-trimethylhexyl)hexanamide (1%), Bis(3,5,5-trimethylhexyl)amine (14%), 2,2,4-Trimethylpentane (1%)
Benzoic acid	Cyclohexylmethylamine (78%), Dicyclohexylmethylamine (7%), Cyclohexane (5%), Cyclohexanecarboxamide (4%), <i>N</i> -(cyclohexylmethyl)cyclopentanamine (1%), <i>N</i> -(cyclohexylmethyl)cyclohexanecarboxamide (2%),
p-Toluic acid	(4-methylcyclohexyl)methanamine (80%), 1,4-Dimethylcyclohexane (4%), p-Xylene (1%), Bis((4-methylcyclohexyl)methyl)amine (11%), 4-Methyl- <i>N</i> -((4-methylcyclohexyl)methyl)cyclohexanecarboxamide (2%), 4-Methylcyclohexanecarboxamide (1%)
2-Methylbutanoic acid	2-Methylbutylamine (90%), Bis(2-methylbutyl)amine (1%), 2-Methylbutanamide (10%)
2-Methylpentanoic acid	2-Methylpentylamine (74%), 2-Methylpentanamide (24%)
2-Ethylbutanoic acid	2-Ethylbutylamine (43%), 2-Ethylbutanamide (53%), 2-Ethylbutanol (2%)
2-Ethylbutanoic acid ^a	2-Ethylbutylamine (85%), 2-Ethylbutanamide (9%), 2-Ethyl- <i>N</i> -(2-ethylbutyl)butanamide (1%), Bis(2-ethylbutyl)amine (3%), <i>N</i> -(2-ethylbutyl)cyclopentanamine (1%)
2-Propylpentanoic acid	2-Propylpentylamine (17%), 2-Propylpentanamide (82%), 2-Propylpentanol (1%)
2-Propylpentanoic acid ^b	2-Propylpentylamine (83%), 2-Propylpentanamide (6%), Bis(2-propylpentyl)amine (8%), <i>N</i> -(2-propylpentyl)cyclopentanamine (4%), 2-Propyl- <i>N</i> -(2-propylpentyl)pentanamide (1%)
Pivalic acid	Neopentylamine (74%), Pivalamide (26%)
(<i>S</i>)-2-Phenylpropanoic acid	3-Cyclohexyl-2-methylpropylamine (46%), Isopropylbenzene (1%), 3-Cyclohexyl-2-methylpropanamide (47%), Ethylbenzene (2%), Ethylcyclohexane (3%), Isopropylcyclohexane (1%)
Isophthalic acid	3-Azabicyclo[3.3.1]nonane (57%), (3-methylcyclohexyl)methanamine (11%), 3-Azabicyclo[3.3.1]nonan-2-one (21%), 1,3-Dimethylcyclohexane (1%), o-Xylene (1%), Cyclohexanemethylamine (3%)
Adipic acid	Azepane (53%), Caprolactam (39%), 6-(azepan-1-yl)hexan-1-amine (4%), Hexylamine (2%), Pentylamine (2%)
Sebacic acid	Decamethylenediamine (30%), Decylamine (11%), Nonylamine (4%), <i>N</i> ¹ -(10-aminodecyl)decane-1,10-diamine (55%)
L-Valine	Isobutylamine (50%), Valine (6%), 2-Amino-3-methylbutane (7%), Diisobutylamine (5%), 3,6-Diisopropylpiperazine-2,5-dione (2%)
Salicylic acid	Cyclohexylamine (50%), 2-Methylcyclohexylamine (11%), o-Cresol (5%), Cyclohexanemethylamine (10%), Cyclohexanecarboxamide (11%)

Substrate	Products distribution (yield)
2-Octanol	2-Octylamine (98%), octane (1%).
Pentafluorobenzoic acid	Cyclohexane (55%), the remaining 45% is mainly a complex mixture of mono-, di- and trifluorinated aromatic compounds.
5-Chlorovaleric acid	Piperidine (85%), 2-Piperidinone (9%), butylamine (2%), pentylamine (2%)
Furoic acid	Tetrahydrofuran (13%), Methyltetrahydrofuran (5%), Butylamine (10%), Piperidine (9%), Tetrahydrofurfurylamine (43%), Pentylamine (6%).
m-Anisic acid	Cyclohexane (2%), methylcyclohexane (3%), methoxycyclohexane (2%), 1-methoxy-3-methylcyclohexane (1%), Cyclohexanemethylamine (44%), (3-methoxycyclohexyl)methanamine (29%) cyclohexanecarboxamide (6%).
4-Methoxycyclohexane-carboxylic acid	Methoxycyclohexane (1%), 1-methoxy-4-methylcyclohexane (1%), 4-methoxy-N-((4-methoxycyclohexyl)methyl)cyclohexanecarboxamide (3%), (4-methoxycyclohexyl)methanamine (81%), 4-methoxycyclohexanecarboxamide (4%), bis((4-methoxycyclohexyl)methyl)amine (9%).
BOC-Valine-OH	Degradation of protecting group: 0.07M tert-butylalcohol in reaction mixture. 3-methyl-1,2-butanediamine (20%), 2-amino-3-methylbutanamide (37%), remaining 43% is a complex mixture of non-volatile compounds.
a longer reaction time (48h). b longer reaction time (120h).	

6. Raw isolated product NMR spectra

Due to an intense ^1H -signal for the solvent (CPME) located between 1.4 and 1.8 ppm, a NMR spectrum of the crude reaction mixture did not yield a clean spectrum for the amine products. In order to obtain clean NMR spectra for at least a number of crude amine products, a few drops of H_2SO_4 were added to 5 randomly selected samples (2.5 mL each). Doing so, an ammonium. HSO_4 salt was formed and precipitated out of the apolar CPME solution. This precipitate was washed with diethyl ether to remove leftover CPME and dried afterwards at 60°C overnight. The obtained white powders were redissolved in D_2O after which NMR spectra were recorded (the sample of tetradecylammonium. HSO_4 did not dissolve in D_2O and was recorded in MeOH-d_4 instead).

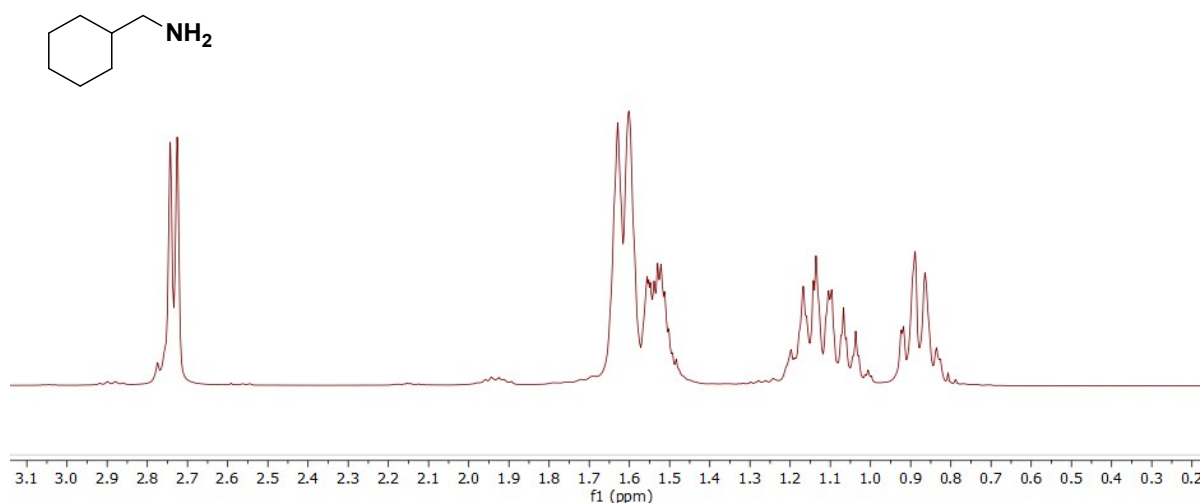


Figure S 8 – NMR spectrum of cyclohexylmethanamine (hydrogensulfate salt) in D_2O with impurities of bis(cyclohexylmethyl)amine and cyclohexanecarboxamide.

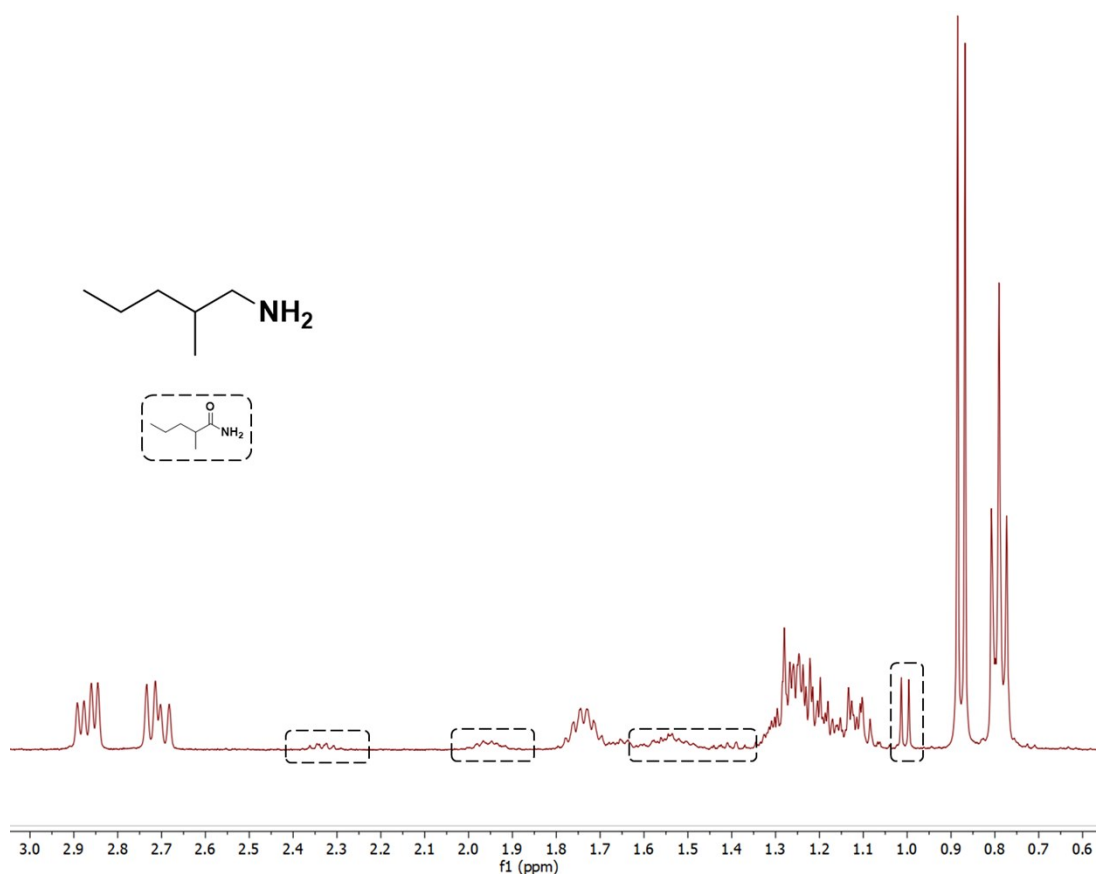


Figure S 9 – NMR spectrum of 2-methylpentylamine (hydrogensulfate salt) in D₂O with impurities of 2-methylpentanamide.

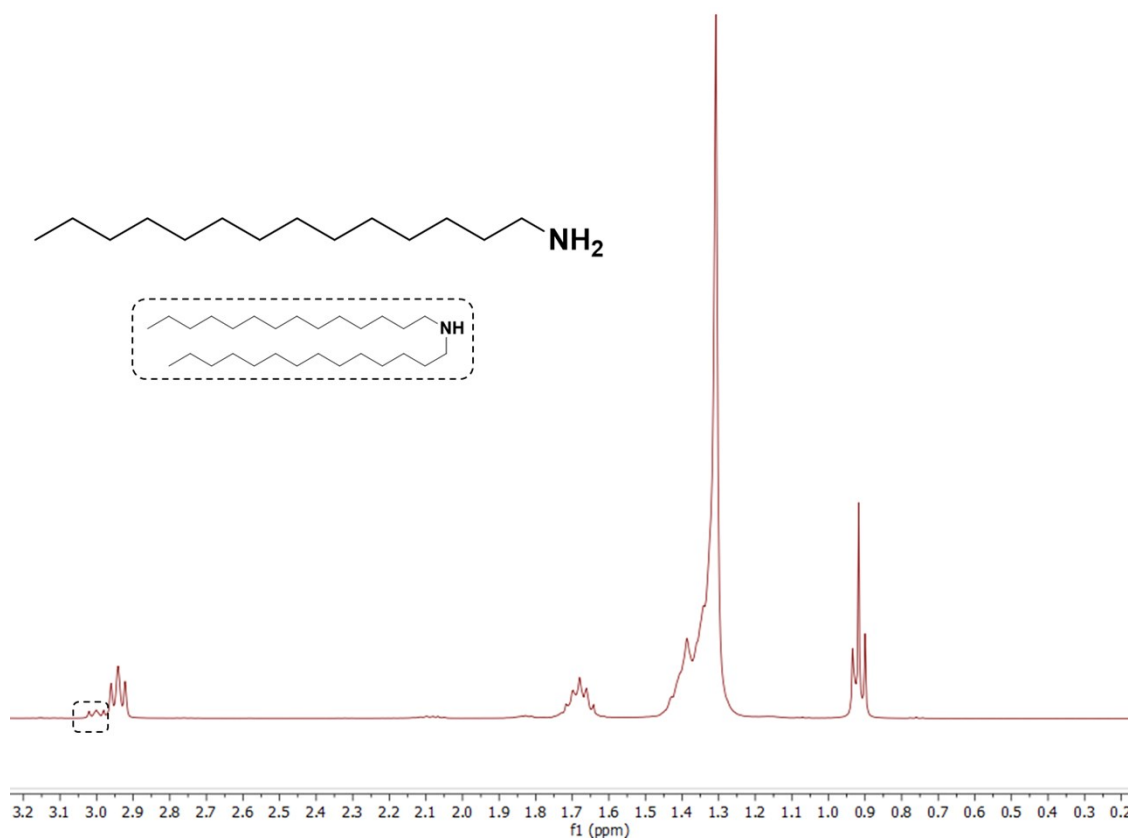


Figure S 10 – NMR spectrum of tetradecylamine (hydrogensulfate salt) in MeOH-d₄ with impurities of ditetradecylamine.

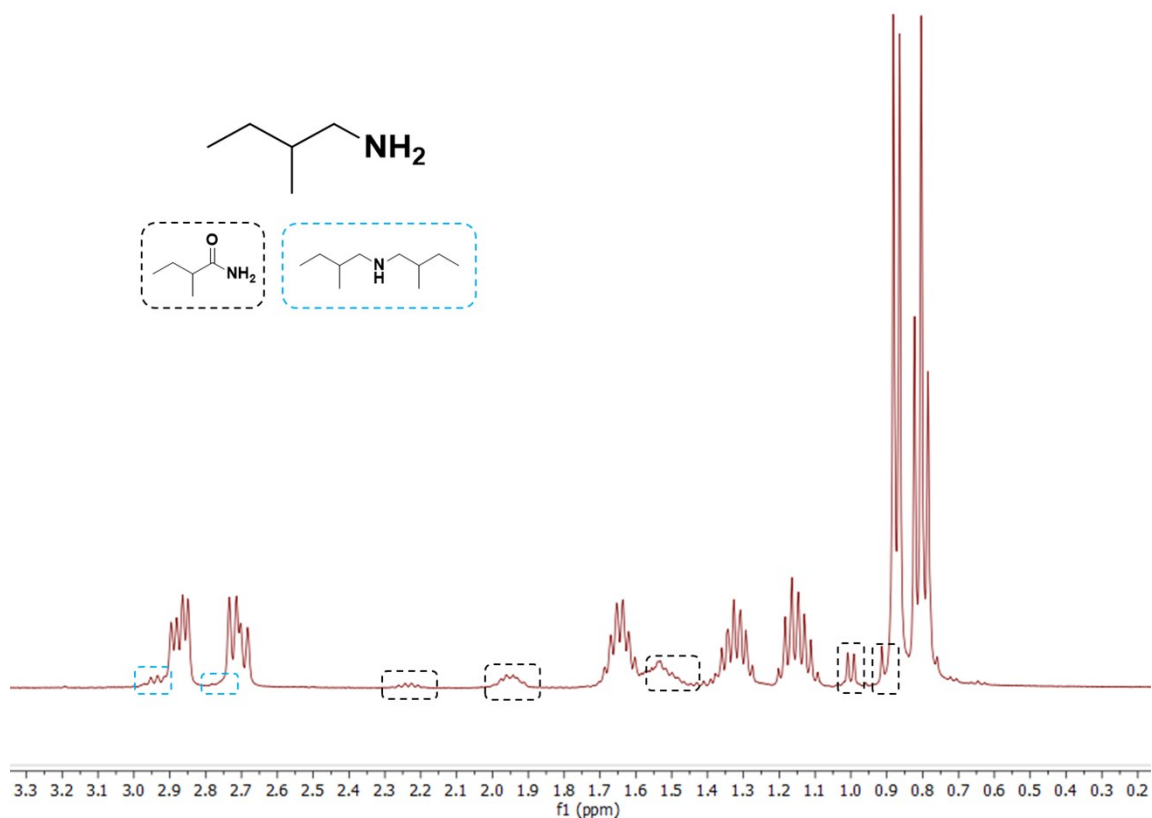


Figure S 11 – NMR spectrum of 2-methylbutylamine (hydrogensulfate salt) in D₂O with impurities of bis(2-methylbutyl)amine and 2-methylbutyramide.

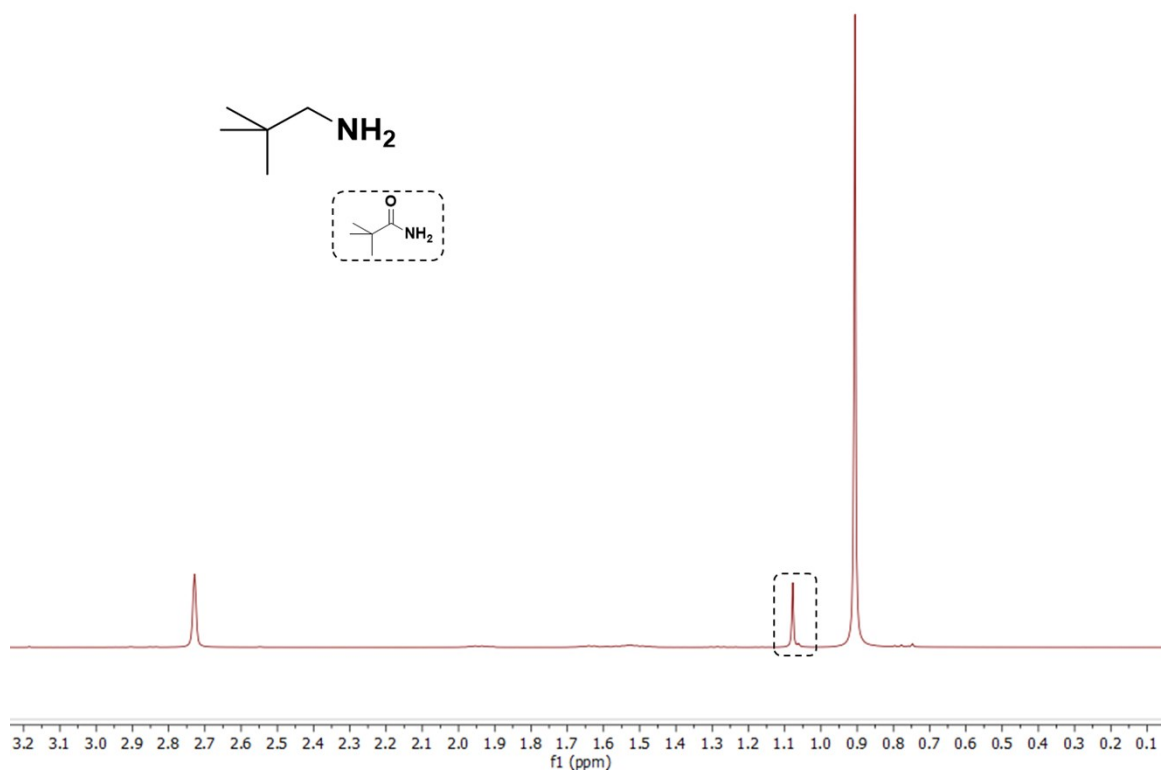
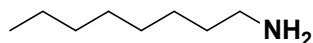


Figure S 12 – NMR spectrum of neopentylamine (hydrogensulfate salt) in D₂O with impurities of trimethylacetamide.

7. Product identification

General information: ^1H -NMR spectra were calibrated by setting the singlet signal of the external standard (benzyl alcohol) to 4.59 ppm.²

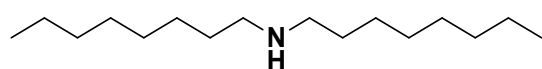
Octylamine (1, MW = 129 g/mol)



^1H -NMR (400 MHz, methanol- d_4): δ (ppm) = 2.62 (t, 2H, $\text{NH}_2\text{-CH}_2\text{-}$), 1.46 (quint, 2H, $\text{NH}_2\text{-CH}_2\text{-CH}_2\text{-}$), 1.39-1.25 (m, 10H, $-(\text{CH}_2)_5\text{-CH}_3$), 0.91 (t, 3H, $-\text{CH}_3$).

GC-MS (EI, 70eV): m/z (rel. int, %): 129 (13), 128 (8), 114 (5), 100 (26), 87 (5), 86 (52), 84 (8), 83 (12), 73 (6), 72 (17), 70 (16), 69 (33), 68 (5), 67 (6), 59 (15), 57 (9), 56 (40), 55 (48), 54 (7), 53 (10), 45 (62), 44 (75), 43 (47), 42 (39), 41 (100), 40 (8), 39 (42).

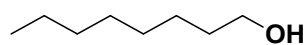
Dioctylamine (2, MW = 241 g/mol)



^1H -NMR (400 MHz, methanol- d_4): δ (ppm) = 2.56 (t, 4H, $-\text{NH-CH}_2\text{-}$), 1.46 (quint, 4H, $-\text{NH-CH}_2\text{-CH}_2\text{-}$), 1.39-1.25 (m, 20H, $-(\text{CH}_2)_5\text{-CH}_3$), 0.91 (t, 6H, $-\text{CH}_3$).

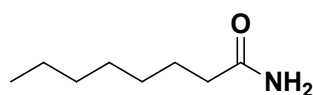
GC-MS (EI, 70eV): m/z (rel. int, %): 241 (5), 143 (11), 142 (100), 57 (6), 44 (32), 43 (10), 41 (8).

Octanol (3, MW = 130 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 39 (21), 41 (86), 42 (49), 43 (63), 44 (5), 53 (6), 54 (6), 55 (91), 56 (100), 57 (38), 67 (7), 68 (20), 69 (68), 70 (67), 71 (9), 82 (10), 83 (44), 84 (51).

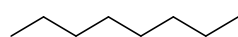
Octanamide (4, MW = 143 g/mol)



^1H -NMR (400 MHz, methanol- d_4): δ (ppm) = 2.18 (t, 2H, $-\text{C(=O)-CH}_2\text{-}$), 1.78-1.47 (m, 4H, $-\text{C(=O)-CH}_2\text{-CH}_2\text{-CH}_2\text{-}$), 1.38-1.23 (m, 4H, $-\text{CH}_2\text{-CH}_2\text{-CH}_3$), 0.90 (t, 3H, $-\text{CH}_3$).

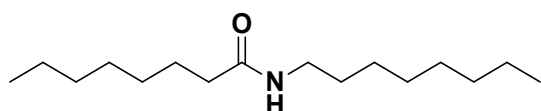
GC-MS (EI, 70eV): m/z (rel. int, %): 86 (9), 73 (5), 72 (29), 59 (100), 57 (8), 55 (9), 44 (20), 43 (14), 42 (5), 41 (14), 39 (5).

Octanol (5, MW = 114 g/mol)



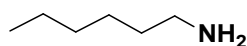
GC-MS (EI, 70eV): m/z (rel. int, %): 39 (13), 41 (46), 42 (15), 43 (100), 55 (13), 56 (22), 57 (42), 70 (17), 71 (31), 84 (11), 85 (52), 114 (7).

N-Octyloctanamide (6, MW = 255 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 255 (16), 226 (20), 212 (20), 198 (25), 185 (13), 184 (100), 172 (7), 171 (55), 170 (6), 157 (16), 156 (49), 144 (13), 142 (17), 130 (7), 129 (8), 128 (29), 127 (39), 115 (10), 114 (44), 101 (19), 100 (38), 98 (5), 87 (30), 86 (47), 84 (8), 83 (5), 73 (63), 72 (21), 71 (17), 70 (5), 69 (12), 67 (5), 60 (9), 59 (5), 58 (15), 57 (87), 56 (11), 55 (37), 44 (41), 43 (60), 42 (12), 41 (51), 39 (8).

Hexylamine (7, MW = 101 g/mol)

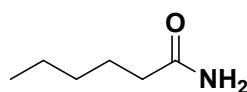


$^1\text{H-NMR}$ (400 MHz, methanol- d_4): δ (ppm) = 2.63 (t, 2H, $\text{NH}_2\text{-CH}_2\text{-}$), 1.47 (quint, 2H, $\text{NH}_2\text{-CH}_2\text{-CH}_2\text{-}$), 1.40-1.26 (m, 6H, $-(\text{CH}_2)_3\text{-CH}_3$), 0.92 (t, 3H, $-\text{CH}_3$).

$^{13}\text{C-NMR}$ (400 MHz, $\text{H}_2\text{O/D}_2\text{O}$): δ (ppm) = 41.3 ($\text{NH}_2\text{-CH}_2\text{-}$), 32.5 ($\text{NH}_2\text{-CH}_2\text{-CH}_2\text{-}$), 31.5 ($-(\text{CH}_2)_2\text{-CH}_2\text{-}$), 26.3 ($-\text{CH}_2\text{-CH}_2\text{-CH}_3$), 22.4 ($-\text{CH}_2\text{-CH}_3$), 13.6 ($-\text{CH}_3$).

GC-MS (EI, 70eV): m/z (rel. int, %): 55 (3), 45 (5), 44 (9), 43 (4), 42 (5), 41 (8), 39 (6), 30 (100), 28 (8), 27 (7).

Hexanamide (8, MW = 115 g/mol)

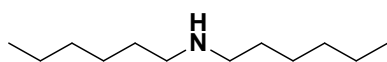


$^1\text{H-NMR}$ (400 MHz, methanol- d_4): δ (ppm) = 2.19 (t, 2H, $-\text{C}(=\text{O})\text{-CH}_2\text{-}$), 1.61 (quint, 2H, $-\text{C}(=\text{O})\text{-CH}_2\text{-CH}_2\text{-}$), 1.41-1.26 (m, 4H, $-\text{CH}_2\text{-CH}_2\text{-CH}_3$), 0.91 (t, 3H, $-\text{CH}_3$).

$^{13}\text{C-NMR}$ (400 MHz, $\text{H}_2\text{O/D}_2\text{O}$): δ (ppm) = 178.0 ($-\text{C}(=\text{O})\text{-}$), 35.3 ($-\text{C}(=\text{O})\text{-CH}_2\text{-}$), 31.2 ($-\text{CH}_2\text{-CH}_3$), 25.3 ($-\text{C}(=\text{O})\text{-CH}_2\text{-CH}_2\text{-}$), 22.2 ($-\text{CH}_2\text{-CH}_2\text{-CH}_3$), 13.4 ($-\text{CH}_3$).

GC-MS (EI, 70 eV): m/z (rel. int., %): 39 (19), 41 (24), 42 (14), 43 (29), 44 (52), 55 (14), 59 (100), 72 (33), 73 (8), 86 (23).

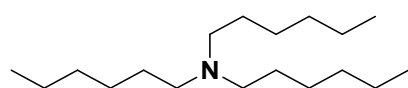
Dihexylamine (9, MW = 185 g/mol)



$^1\text{H-NMR}$ (400 MHz, methanol- d_4): δ (ppm) = 2.57 (t, 4H, $-\text{CH}_2\text{-NH-CH}_2\text{-}$), 1.47 (quint, 4H, $-\text{NH-CH}_2\text{-CH}_2\text{-}$), 1.40-1.26 (m, 12H, $-(\text{CH}_2)_3\text{-CH}_3$), 0.92 (t, 6H, $-\text{CH}_3$).

GC-MS (EI, 70eV): m/z (rel. int, %): 185 (6), 115 (9), 114 (100), 56 (5), 55 (6), 44 (53), 43 (21), 41 (11), 30 (9), 29 (6).

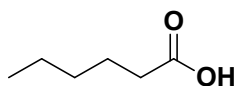
Trihexylamine (10, MW = 269 g/mol)



$^1\text{H-NMR}$ (400 MHz, methanol- d_4): δ (ppm) = 2.43 (t, 6H, $-\text{CH}_2-\text{NH}-\text{CH}_2-$), 1.47 (quint, 6H, $-\text{NH}-\text{CH}_2-\text{CH}_2-$), 1.40-1.26 (m, 18H, $-(\text{CH}_2)_3-\text{CH}_3$), 0.92 (t, 9H, $-\text{CH}_3$).

GC-MS (EI, 70eV): m/z (rel. int, %): 200 (15), 199 (100), 128 (13), 98 (5), 58 (5), 44 (5), 43 (12), 41 (5).

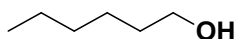
Hexanoic acid (11, MW = 116 g/mol)



$^1\text{H-NMR}$ (400 MHz, methanol- d_4): δ (ppm) = 2.16 (t, 2H, $-\text{C}(=\text{O})-\text{CH}_2-$), 1.61 (quint, 2H, $-\text{C}(=\text{O})-\text{CH}_2-\text{CH}_2-$), 1.41-1.26 (m, 4H, $-\text{CH}_2-\text{CH}_2-\text{CH}_3$), 0.91 (t, 3H, $-\text{CH}_3$).

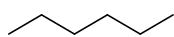
GC-MS (EI, 70eV): m/z (rel. int, %): 87 (16), 74 (8), 73 (53), 70 (6), 61 (10), 60 (100), 57 (11), 56 (10), 55 (15), 45 (16), 43 (20), 42 (14), 41 (29), 39 (14).

Hexanol (12, MW = 102 g/mol)



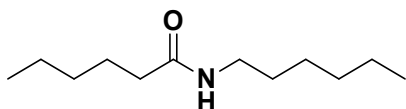
GC-MS (EI, 70eV): m/z (rel. int, %): 84 (5), 69 (31), 57 (9), 56 (100), 55 (52), 44 (5), 43 (54), 42 (39), 41 (42), 39 (13).

Hexane (13, MW = 72 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 39 (26), 41 (77), 42 (27), 43 (51), 55 (8), 56 (52), 57 (100).

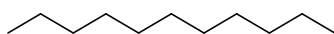
N-Hexylhexanamide (14, MW = 199 g/mol)



$^1\text{H-NMR}$ (400 MHz, methanol- d_4): δ (ppm) = 7.29 (s, 1H, $-\text{NH}-$), 3.15 (t, 2H, $-\text{NH}-\text{CH}_2-$), 2.16 (t, 2H, $-\text{C}(=\text{O})-\text{CH}_2-$), 1.60 (quint, 2H, $-\text{C}(=\text{O})-\text{CH}_2-\text{CH}_2-$), 1.49 (quint, 2H, $-\text{NH}-\text{CH}_2-\text{CH}_2-$), 1.38-1.25 (m, 10H, $-\text{CH}_3-(\text{CH}_2)_2-\text{R}-\text{C}(=\text{O})-\text{NH}-\text{R}'-(\text{CH}_2)_3-\text{CH}_3$), 0.91 (t, 6H, $-\text{CH}_3$).

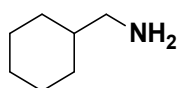
GC-MS (EI, 70eV): m/z (rel. int, %): 199 (8), 170 (31), 157 (10), 156 (86), 144 (7), 143 (71), 142 (6), 129 (18), 128 (52), 116 (16), 115 (5), 114 (35), 101 (29), 100 (43), 99 (62), 87 (37), 86 (54), 85 (12), 73 (53), 72 (24), 71 (35), 69 (5), 60 (9), 59 (5), 58 (15), 57 (10), 56 (10), 55 (27), 44 (40), 43 (100), 42 (13), 41 (42), 39 (11).

Undecane (15, MW = 156 g/mol)



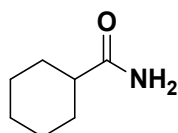
GC-MS (EI, 70eV): m/z (rel. int, %): 156 (6), 99 (5), 98 (7), 85 (32), 84 (9), 71 (51), 70 (14), 69 (6), 58 (5), 57 (100), 56 (18), 55 (16), 43 (81), 42 (12), 41 (40), 39 (9).

Cyclohexylmethanamine (16, MW = 113 g/mol)



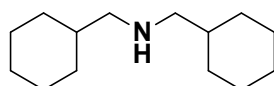
GC-MS (EI, 70eV): m/z (rel. int, %): 114 (12), 113 (100), 96 (43), 95 (11), 83 (5), 82 (16), 81 (38), 79 (9), 77 (8), 70 (6), 68 (18), 67 (73), 66 (5), 65 (7), 56 (23), 55 (70), 54 (43), 53 (21), 52 (5), 51 (8), 43 (10), 42 (19), 41 (77), 39 (53).

Cyclohexanecarboxamide (17, MW = 127 g/mol)



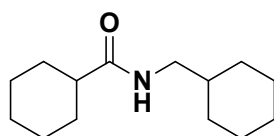
GC-MS (EI, 70eV): m/z (rel. int, %): 127 (39), 126 (13), 112 (15), 99 (9), 98 (40), 86 (18), 85 (10), 84 (5), 83 (38), 82 (6), 81 (7), 79 (5), 73 (10), 72 (96), 69 (5), 67 (14), 59 (64), 56 (16), 55 (100), 54 (11), 53 (11), 44 (31), 43 (7), 42 (7), 41 (50), 39 (25).

Bis(cyclohexylmethyl)amine (18, MW = 209 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 209 (5), 127 (9), 126 (100), 97 (6), 55 (23), 44 (33), 43 (7), 41 (11).

N-(cyclohexylmethyl)cyclohexanecarboxamide (19, MW = 223 g/mol)



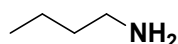
GC-MS (EI, 70eV): m/z (rel. int, %): 223 (10), 168 (17), 141 (20), 140 (8), 129 (8), 128 (100), 112 (10), 111 (17), 97 (6), 86 (9), 83 (43), 81 (7), 73 (8), 67 (9), 55 (42), 44 (11), 41 (19), 39 (5).

Cyclohexane (20, MW = 84 g/mol)



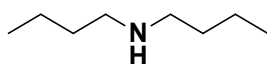
GC-MS (EI, 70eV): m/z (rel. int, %): 39 (28), 40 (6), 41 (53), 42 (20), 43 (11), 51 (5), 53 (6), 54 (7), 55 (35), 56 (100), 57 (5), 67 (5), 69 (34), 83 (5), 84 (92), 85 (6).

Butylamine (21, MW = 73 g/mol)



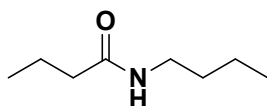
GC-MS (EI, 70eV): m/z (rel. int, %): 38 (6), 39 (31), 40 (13), 41 (64), 42 (100), 43 (25), 44 (6), 71 (55), 72 (57).

Dibutylamine (22, MW = 129 g/mol)



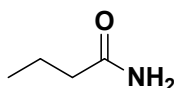
GC-MS (EI, 70eV): m/z (rel. int, %): 39 (10), 41 (22), 42 (8), 43 (10), 44 (90), 56 (7), 57 (17), 59 (8), 72 (5), 86 (100), 87 (6), 129 (12).

N-butylbutyramide (23, MW = 143 g/mol)



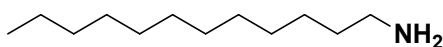
GC-MS (EI, 70eV): m/z (rel. int, %): 39 (26), 41 (65), 42 (17), 43 (100), 44 (70), 55 (13), 56 (9), 57 (41), 58 (19), 59 (10), 60 (7), 70 (6), 71 (98), 72 (19), 73 (63), 86 (22), 87 (7), 88 (28), 100 (67), 101 (29), 114 (12), 115 (52), 128 (35), 143 (34).

Butyramide (24, MW = 87 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 39 (16), 41 (26), 42 (13), 43 (36), 44 (69), 55 (10), 59 (100), 71 (9), 72 (24).

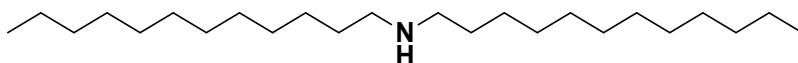
Dodecylamine (25, MW = 185 g/mol)



¹H-NMR (400 MHz, methanol-d₄): δ (ppm) = 2.62 (t, 2H, NH₂-CH₂-), 1.47 (quint, 2H, NH₂-CH₂-CH₂-), 1.40-1.25 (m, 18H, -(CH₂)₉-CH₃), 0.92 (t, 3H, -CH₃).

GC-MS (EI, 70eV): m/z (rel. int, %): 185 (12), 184 (9), 170 (5), 156 (14), 142 (15), 128 (12), 114 (15), 111 (6), 100 (34), 98 (6), 97 (13), 87 (7), 86 (59), 84 (10), 83 (18), 82 (6), 73 (9), 72 (21), 71 (5), 70 (16), 69 (36), 68 (6), 67 (8), 59 (20), 57 (23), 56 (41), 55 (67), 54 (7), 53 (8), 45 (59), 44 (78), 43 (71), 42 (27), 41 (100), 39 (21)

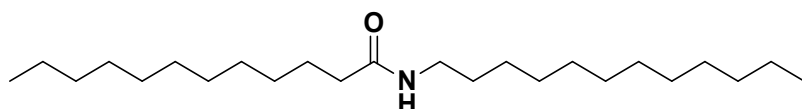
Didodecylamine (26, MW = 354 g/mol)



¹H-NMR (400 MHz, methanol-d₄): δ (ppm) = 2.56 (t, 4H, -NH-CH₂-), 1.47 (quint, 4H, -NH-CH₂-CH₂-), 1.40-1.25 (m, 36H, -(CH₂)₉-CH₃), 0.92 (t, 6H, -CH₃).

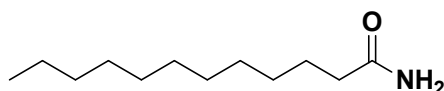
GC-MS (EI, 70eV): m/z (rel. int, %): 199 (15), 198 (100), 196 (5), 57 (8), 56 (5), 55 (7), 44 (19), 43 (9), 41 (7), 30 (5).

N-Dodecyl dodecanamide (27, MW = 368 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 368 (5), 367 (18), 338 (10), 324 (15), 310 (9), 296 (20), 282 (19), 268 (12), 254 (22), 241 (17), 240 (100), 228 (12), 227 (61), 213 (14), 212 (55), 207 (5), 200 (9), 198 (11), 186 (14), 184 (20), 183 (15), 170 (13), 156 (12), 142 (16), 129 (5), 128 (18), 115 (9), 114 (36), 101 (16), 100 (27), 98 (8), 97 (7), 87 (23), 86 (34), 85 (13), 84 (8), 83 (11), 81 (5), 73 (47), 72 (16), 71 (21), 70 (6), 69 (19), 60 (8), 58 (9), 57 (55), 55 (39), 44 (27), 43 (71), 42 (8), 41 (37).

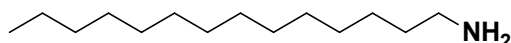
Dodecanamide (28, MW = 199 g/mol)



$^1\text{H-NMR}$ (400 MHz, methanol- d_4): δ (ppm) = 2.19 (t, 2H, $-\text{C}(=\text{O})-\text{CH}_2-$), 1.60 (quint, 2H, $-\text{C}(=\text{O})-\text{CH}_2-\text{CH}_2-$), 1.38-1.22 (m, 16H, $-(\text{CH}_2)_8-\text{CH}_3$), 0.90 (t, 3H, $-\text{CH}_3$).

GC-MS (EI, 70eV): m/z (rel. int, %): 128 (5), 114 (5), 86 (8), 73 (6), 72 (40), 60 (6), 59 (100), 57 (7), 55 (11), 44 (15), 43 (17), 41 (15).

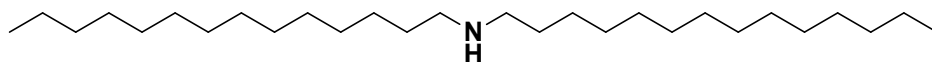
Tetradecylamine (29, MW = 213 g/mol)



$^1\text{H-NMR}$ (400 MHz, methanol- d_4): δ (ppm) = 2.63 (t, 2H, NH_2-CH_2-), 1.47 (quint, 2H, $\text{NH}_2-\text{CH}_2-\text{CH}_2-$), 1.40-1.24 (m, 22H, $-(\text{CH}_2)_{11}-\text{CH}_3$), 0.91 (t, 3H, $-\text{CH}_3$).

GC-MS (EI, 70eV): m/z (rel. int, %): 39 (19), 40 (5), 41 (100), 42 (24), 43 (81), 44 (85), 45 (48), 53 (8), 54 (8), 55 (71), 56 (40), 57 (31), 58 (5), 59 (19), 67 (11), 68 (7), 69 (40), 70 (15), 71 (8), 72 (21), 73 (9), 82 (7), 83 (23), 84 (9), 86 (58), 87 (8), 97 (17), 98 (6), 100 (36), 111 (8), 114 (18), 128 (15), 142 (19), 156 (18), 170 (13), 184 (13), 198 (8), 212 (15), 213 (18), 214 (9).

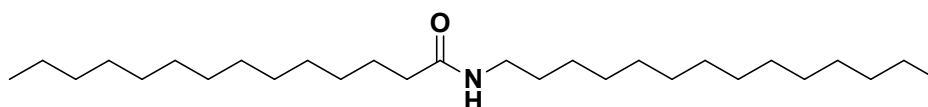
Ditetradecylamine (30, MW = 409 g/mol)



$^1\text{H-NMR}$ (400 MHz, methanol- d_4): δ (ppm) = 2.56 (t, 4H, $-\text{NH}-\text{CH}_2-$), 1.47 (quint, 4H, $-\text{NH}-\text{CH}_2-\text{CH}_2-$), 1.40-1.24 (m, 44H, $-(\text{CH}_2)_{11}-\text{CH}_3$), 0.91 (t, 6H, $-\text{CH}_3$).

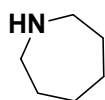
GC-MS (EI, 70eV): m/z (rel. int, %): 41 (8), 43 (12), 44 (21), 55 (5), 57 (6), 73 (18), 96 (8), 133 (7), 147 (7), 177 (6), 191 (12), 193 (5), 207 (100), 208 (21), 209 (12), 224 (19), 226 (95), 227 (16), 267 (6), 281 (52), 282 (14), 283 (9), 341 (9), 355 (9).

N-tetradecyltetradecanamide (31, MW = 423 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 41 (27), 42 (6), 43 (47), 44 (19), 55 (27), 56 (10), 57 (43), 58 (8), 60 (5), 67 (5), 69 (18), 70 (6), 71 (18), 72 (11), 73 (44), 83 (9), 84 (7), 85 (12), 86 (23), 87 (13), 95 (5), 96 (8), 97 (8), 98 (8), 100 (18), 101 (10), 114 (28), 115 (9), 128 (14), 133 (8), 142 (13), 147 (6), 156 (10), 170 (9), 177 (5), 184 (9), 191 (11), 193 (7), 198 (13), 207 (98), 208 (19), 209 (14), 211 (12), 212 (21), 213 (6), 214 (17), 226 (8), 228 (7), 240 (57), 241 (14), 255 (75), 256 (17), 267 (7), 268 (100), 269 (23), 281 (49), 282 (37), 283 (13), 296 (13), 297 (5), 310 (18), 311 (8), 324 (26), 325 (6), 338 (13), 341 (10), 352 (7), 355 (8), 366 (8), 380 (21), 381 (6), 394 (13), 422 (7), 423 (25), 424 (8).

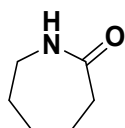
Azepane (32, MW = 99 g/mol)



$^1\text{H-NMR}$ (400 MHz, methanol- d_4): δ (ppm) = 2.87-2.71 (m, 4H, $-\text{CH}_2-\text{NH}-\text{CH}_2-$), 1.74-1.49 (m, 8H, $-\text{NH}-\text{CH}_2-\text{CH}_2-\text{CH}_2-$).

GC-MS (EI, 70eV): m/z (rel. int, %): 99 (64), 98 (28), 84 (15), 71 (9), 70 (100), 68 (6), 57 (39), 56 (51), 55 (8), 44 (25), 43 (66), 42 (24), 41 (25), 39 (17).

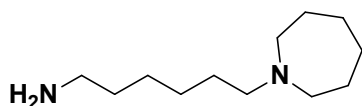
Caprolactam (33, MW = 113 g/mol)



$^1\text{H-NMR}$ (400 MHz, methanol- d_4): δ (ppm) = 3.22-3.15 (m, 2H, $-\text{NH}-\text{CH}_2-$), 2.48-2.39 (m, 2H, $-\text{C}(=\text{O})-\text{CH}_2-$), 1.82-1.48 (m, 6H, $-\text{NH}-\text{CH}_2-(\text{CH}_2)_3-\text{CH}_2-\text{C}(=\text{O})-$).

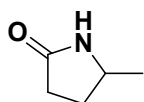
GC-MS (EI, 70eV): m/z (rel. int, %): 114 (7), 113 (100), 86 (5), 85 (60), 84 (54), 83 (10), 69 (5), 68 (8), 67 (13), 59 (13), 57 (11), 56 (84), 55 (84), 55 (25), 54 (6), 53 (5), 44 (17), 43 (21), 42 (56), 41 (54), 40 (11), 39 (31).

6-(azepan-1-yl)hexan-1-amine (34, MW = 198 g/mol)



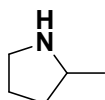
GC-MS (EI, 70eV): m/z (rel. int, %): 41 (6), 42 (5), 55 (6), 58 (8), 112 (100), 113 (8).

5-Methyl-2-pyrrolidone (35, MW = 99 g/mol)



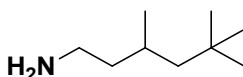
GC-MS (EI, 70eV): m/z (rel. int, %): 39 (7), 40 (5), 41 (44), 42 (14), 43 (5), 44 (25), 55 (11), 56 (19), 84 (100), 85 (5), 99 (26).

2-Methylpyrrolidine (36, MW = 85 g/mol)



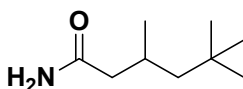
GC-MS (EI, 70eV): m/z (rel. int, %): 39 (9), 41 (15), 42 (14), 43 (11), 56 (23), 57 (44), 68 (8), 70 (100), 71 (5), 84 (10), 85 (9).

3,5,5-Trimethylhexylamine (37, MW = 143 g/mol)



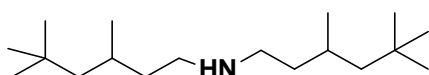
GC-MS (EI, 70eV): m/z (rel. int, %): 39 (36), 40 (10), 41 (100), 42 (20), 43 (41), 44 (38), 45 (50), 53 (11), 54 (6), 55 (50), 56 (36), 57 (77), 58 (7), 67 (9), 68 (5), 69 (46), 70 (57), 71 (21), 72 (5), 83 (22), 84 (8), 86 (82), 87 (7), 128 (36).

3,5,5-Trimethylhexylamide (38, MW = 157 g/mol)



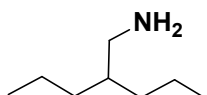
GC-MS (EI, 70eV): m/z (rel. int, %): 39 (8), 41 (21), 43 (10), 44 (14), 55 (11), 56 (5), 57 (25), 59 (100), 60 (5), 83 (23), 86 (7), 100 (18), 101 (5), 142 (9).

Bis(3,5,5-trimethylhexyl)amine (39, MW = 269 g/mol)



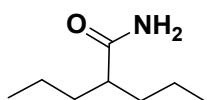
GC-MS (EI, 70eV): m/z (rel. int, %): 39 (6), 41 (23), 42 (6), 43 (18), 44 (100), 55 (11), 56 (18), 57 (37), 60 (17), 69 (12), 70 (7), 83 (5), 84 (7), 86 (6), 98 (7), 127 (21), 154 (7), 156 (27), 210 (6), 212 (27), 254 (30).

2-Propylpentylamine (40, MW = 129 g/mol)



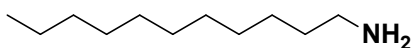
GC-MS (EI, 70eV): m/z (rel. int, %): 39 (38), 40 (6), 41 (100), 42 (34), 43 (32), 44 (25), 53 (11), 54 (10), 55 (50), 56 (54), 57 (25), 58 (9), 67 (9), 68 (6), 69 (29), 70 (33), 72 (7), 83 (9), 84 (7), 86 (22), 87 (14), 98 (5), 100 (5), 112 (40), 129 (29).

2-Propylpentanamide (41, MW = 143 g/mol)



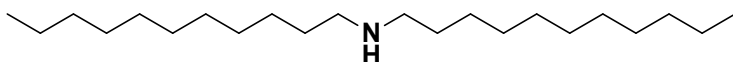
GC-MS (EI, 70eV): m/z (rel. int, %): 39 (6), 41 (17), 43 (12), 44 (13), 55 (13), 57 (17), 72 (100), 73 (5), 100 (14), 101 (40), 114 (12).

Undecylamine (42, MW = 171 g/mol)



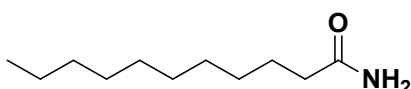
GC-MS (EI, 70eV): m/z (rel. int, %): 39 (26), 40 (6), 41 (100), 42 (29), 43 (62), 44 (71), 45 (51), 53 (8), 54 (7), 55 (59), 56 (39), 57 (17), 59 (17), 67 (7), 68 (5), 69 (32), 70 (15), 72 (17), 73 (7), 82 (5), 83 (15), 84 (8), 86 (50), 87 (6), 97 (10), 100 (27), 111 (5), 114 (12), 128 (9), 142 (13), 156 (5), 170 (7), 171 (9).

Diundecylamine (43, MW = 326 g/mol)



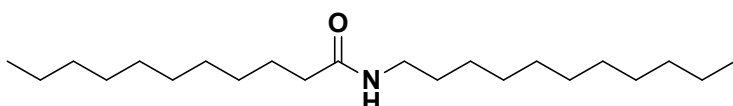
GC-MS (EI, 70eV): m/z (rel. int, %): 41 (7), 43 (10), 44 (26), 55 (6), 57 (6), 182 (7), 184 (100), 185 (14).

Undecanamide (44, MW = 185 g/mol)



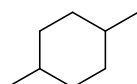
GC-MS (EI, 70eV): m/z (rel. int, %): 41 (16), 43 (16), 44 (15), 55 (11), 57 (6), 59 (100), 60 (6), 72 (38), 73 (6), 86 (9), 114 (5).

N-undecylundecanamide (45, MW = 340 g/mol)



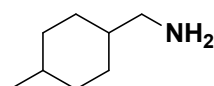
GC-MS (EI, 70eV): m/z (rel. int, %): 41 (35), 42 (8), 43 (62), 44 (22), 55 (33), 56 (10), 57 (43), 58 (8), 60 (7), 67 (5), 69 (16), 70 (5), 71 (16), 72 (15), 73 (43), 83 (8), 84 (8), 85 (14), 86 (32), 87 (21), 95 (6), 97 (5), 98 (7), 100 (26), 101 (15), 114 (35), 115 (8), 128 (18), 129 (5), 142 (15), 156 (16), 169 (17), 170 (20), 171 (5), 172 (12), 184 (10), 186 (10), 198 (53), 199 (13), 212 (6), 213 (61), 214 (9), 226 (100), 227 (16), 240 (24), 241 (5), 254 (13), 268 (19), 282 (21), 283 (5), 296 (19), 297 (5), 310 (11), 339 (19), 340 (5).

1,4-Dimethylcyclohexane (46, MW = 112 g/mol)



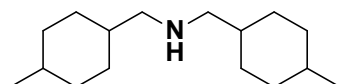
GC-MS (EI, 70eV): m/z (rel. int, %): 39 (15), 41 (28), 42 (10), 43 (5), 53 (6), 55 (73), 56 (18), 67 (5), 69 (16), 70 (9), 83 (9), 84 (6), 96 (10), 97 (100), 98 (8), 112 (35).

(4-methylcyclohexyl)methanamine (47, MW = 127 g/mol)



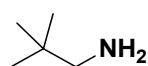
GC-MS (EI, 70eV): m/z (rel. int, %): 39 (54), 40 (9), 41 (69), 42 (20), 43 (15), 51 (8), 52 (5), 53 (26), 54 (37), 55 (100), 56 (28), 65 (9), 67 (51), 68 (29), 69 (12), 70 (11), 77 (10), 79 (14), 80 (6), 81 (78), 82 (23), 95 (40), 96 (9), 109 (9), 110 (50), 111 (5), 126 (5), 127 (73), 128 (8).

Bis((4-methylcyclohexyl)methyl)amine (48, MW = 237 g/mol)



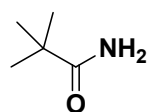
GC-MS (EI, 70eV): m/z (rel. int, %): 41 (9), 43 (6), 44 (28), 55 (16), 69 (11), 140 (100), 141 (10).

Neopenylamine (49, MW = 87 g/mol)



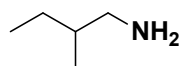
GC-MS (EI, 70eV): m/z (rel. int, %): 38 (5), 39 (46), 40 (7), 41 (88), 42 (14), 43 (8), 44 (7), 53 (7), 54 (7), 55 (100), 56 (38), 57 (54), 70 (8), 72 (81), 87 (43).

Trimethylacetamide (50, MW = 101 g/mol)



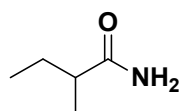
GC-MS (EI, 70eV): m/z (rel. int, %): 39 (23), 41 (66), 42 (7), 44 (24), 46 (17), 55 (5), 56 (7), 57 (100), 58 (19), 59 (5), 69 (5), 86 (13), 101 (18).

2-Methylbutylamine (51, MW = 87 g/mol)



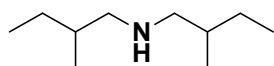
GC-MS (EI, 70eV): m/z (rel. int, %): 38 (7), 39 (64), 40 (9), 41 (100), 42 (31), 43 (19), 44 (35), 50 (6), 51 (8), 52 (5), 53 (9), 54 (12), 55 (29), 56 (45), 57 (16), 58 (33), 69 (8), 70 (18), 86 (5), 87 (69), 88 (5).

2-Methylbutyramide (52, MW = 101 g/mol)



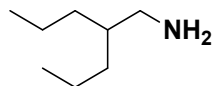
GC-MS (EI, 70eV): m/z (rel. int, %): 39 (13), 41 (37), 43 (6), 44 (44), 55 (10), 56 (10), 57 (33), 69 (9), 72 (17), 73 (100), 86 (29).

Bis(2-methylbutyl)amine (53, MW = 157 g/mol)



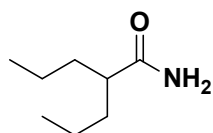
GC-MS (EI, 70eV): m/z (rel. int, %): 39 (6), 41 (16), 42 (7), 43 (30), 44 (46), 55 (5), 70 (5), 71 (14), 100 (100), 101 (7), 157 (5).

2-Propylpentylamine (54, MW = 129 g/mol)



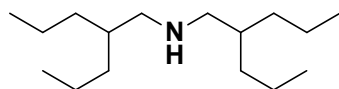
GC-MS (EI, 70eV): m/z (rel. int, %): 39 (39), 40 (8), 41 (100), 42 (34), 43 (32), 44 (25), 53 (11), 54 (10), 55 (49), 56 (53), 57 (24), 58 (8), 67 (9), 68 (6), 69 (28), 70 (32), 72 (6), 83 (9), 84 (6), 86 (21), 87 (12), 98 (5), 112 (36), 129 (27).

2-Propylpentanamide (55, MW = 143 g/mol)



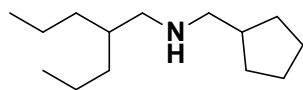
GC-MS (EI, 70eV): m/z (rel. int, %): 39 (6), 41 (17), 43 (12), 44 (13), 55 (13), 57 (17), 72 (100), 73 (5), 100 (13), 101 (40), 114 (12).

Bis(2-propylpentyl)amine (56, MW = 241 g/mol)



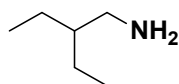
GC-MS (EI, 70eV): m/z (rel. int, %): 41 (16), 42 (5), 43 (20), 44 (58), 55 (7), 57 (15), 71 (9), 142 (100), 143 (10).

N-(cyclopentylmethyl)-2-propylpentan-1-amine (57, MW = 211 g/mol)



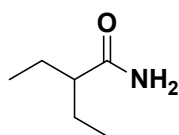
GC-MS (EI, 70eV): m/z (rel. int, %): 41 (14), 43 (5), 56 (7), 69 (6), 98 (100), 99 (7).

2-Ethylbutylamine (58, MW = 101 g/mol)



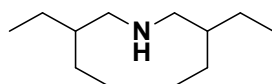
GC-MS (EI, 70eV): m/z (rel. int, %): 38 (7), 39 (77), 40 (12), 41 (100), 42 (47), 43 (66), 44 (29), 50 (6), 51 (10), 52 (6), 53 (21), 54 (18), 55 (99), 56 (82), 57 (6), 58 (22), 67 (6), 68 (5), 69 (17), 70 (24), 71 (5), 72 (36), 73 (5), 84 (42), 100 (5), 101 (74), 102 (9).

2-Ethylbutanamide (59, MW = 115 g/mol)



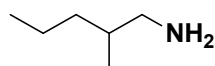
GC-MS (EI, 70eV): m/z (rel. int, %): 39 (19), 41 (30), 42 (8), 43 (64), 44 (41), 55 (26), 57 (5), 69 (19), 70 (5), 71 (16), 72 (99), 73 (6), 86 (50), 87 (100), 88 (5), 100 (9).

Bis(2-ethylbutyl)amine (60, MW = 185 g/mol)



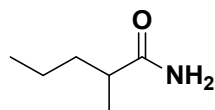
GC-MS (EI, 70eV): m/z (rel. int, %): 41 (14), 42 (5), 43 (34), 44 (57), 55 (7), 56 (5), 57 (5), 85 (7), 114 (100), 115 (8), 185 (4).

2-Methylpentylamine (61, MW = 101 g/mol)



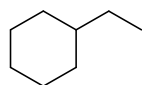
GC-MS (EI, 70eV): m/z (rel. int, %): 38 (6), 39 (70), 40 (11), 41 (100), 42 (45), 43 (51), 44 (22), 51 (6), 53 (12), 54 (11), 55 (51), 56 (45), 57 (9), 58 (34), 59 (35), 67 (5), 69 (13), 70 (11), 72 (6), 84 (22), 100 (5), 101 (58), 102 (9).

2-Methylpentanamide (62, MW = 115 g/mol)



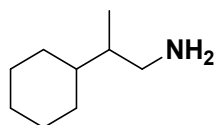
GC-MS (EI, 70eV): m/z (rel. int, %): 39 (10), 41 (18), 42 (6), 43 (35), 44 (29), 55 (12), 57 (7), 71 (7), 72 (21), 73 (100), 86 (21), 100 (6).

Ethylcyclohexane (63, MW = 112 g/mol)



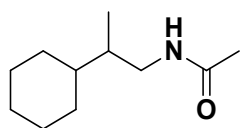
GC-MS (EI, 70eV): m/z (rel. int, %): 39 (17), 41 (36), 42 (9), 43 (6), 53 (6), 54 (7), 55 (77), 56 (10), 67 (15), 69 (8), 82 (48), 83 (100), 84 (7), 112 (23).

2-Cyclohexylpropanamine (64, MW = 141 g/mol)



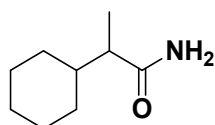
GC-MS (EI, 70eV): m/z (rel. int, %): 39 (33), 40 (7), 41 (73), 42 (15), 43 (11), 53 (17), 54 (17), 55 (54), 56 (16), 57 (9), 58 (13), 59 (32), 65 (5), 66 (5), 67 (41), 68 (17), 69 (34), 77 (6), 79 (10), 80 (6), 81 (38), 82 (42), 83 (6), 95 (11), 96 (6), 109 (7), 110 (9), 124 (100), 125 (10).

***N*-(2-cyclohexylpropyl)acetamide (65, MW = 183 g/mol)**



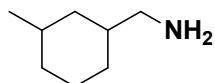
GC-MS (EI, 70eV): *m/z* (rel. int, %): 39 (10), 41 (31), 42 (7), 43 (36), 44 (6), 45 (6), 53 (6), 54 (5), 55 (28), 56 (6), 57 (5), 58 (15), 60 (39), 67 (17), 68 (7), 69 (30), 72 (31), 73 (100), 74 (9), 79 (5), 81 (22), 82 (19), 86 (9), 95 (6), 100 (25), 101 (8), 109 (6), 124 (13), 168 (15), 183 (4).

2-Cyclohexylpropanamide (66, MW = 155 g/mol)



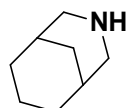
GC-MS (EI, 70eV): *m/z* (rel. int, %): 39 (6), 41 (12), 44 (10), 55 (11), 69 (6), 72 (10), 73 (100), 140 (5).

(3-methylcyclohexyl)methanamine (67, MW = 127 g/mol)



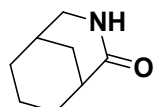
GC-MS (EI, 70eV): *m/z* (rel. int, %): 39 (53), 40 (10), 41 (72), 42 (17), 43 (15), 51 (8), 52 (5), 53 (24), 54 (31), 55 (100), 56 (29), 65 (9), 66 (5), 67 (50), 68 (27), 69 (13), 70 (5), 77 (10), 79 (14), 80 (6), 81 (62), 82 (41), 84 (7), 95 (37), 96 (9), 109 (10), 110 (37), 127 (67), 128 (6).

3-Azabicyclo[3.2.2]nonane (68, MW = 125 g/mol)



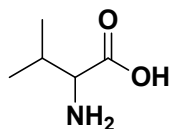
GC-MS (EI, 70eV): *m/z* (rel. int, %): 39 (20), 41 (21), 42 (10), 43 (14), 44 (100), 53 (9), 54 (14), 55 (15), 56 (9), 67 (18), 68 (14), 70 (6), 77 (5), 79 (10), 80 (7), 81 (7), 82 (61), 83 (6), 96 (7), 124 (30), 125 (53), 126 (5).

3-Azabicyclo[3.2.2]nonan-2-one (69, MW = 139 g/mol)



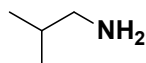
GC-MS (EI, 70eV): *m/z* (rel. int, %): 39 (28), 40 (6), 41 (25), 43 (16), 44 (5), 51 (6), 53 (15), 54 (28), 55 (26), 56 (12), 65 (5), 66 (7), 67 (57), 68 (90), 69 (10), 77 (10), 79 (23), 80 (11), 81 (26), 82 (33), 83 (7), 84 (15), 94 (12), 95 (5), 96 (13), 97 (6), 110 (15), 111 (7), 138 (10), 139 (100), 140 (9).

L-Valine (70, MW = 117 g/mol)



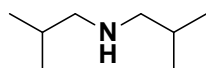
GC-MS (EI, 70eV): m/z (rel. int, %): 39 (13), 41 (12), 42 (6), 43 (8), 44 (5), 45 (13), 46 (13), 54 (6), 55 (39), 56 (30), 57 (37), 72 (100), 73 (6), 74 (34), 75 (13).

Isobutylamine (71, MW = 73 g/mol)



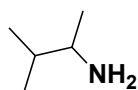
GC-MS (EI, 70eV): m/z (rel. int, %): 31 (11), 37 (8), 38 (100), 40 (14), 41 (74), 42 (26), 43 (24), 51 (7), 52 (9), 53 (5), 54 (20), 55 (28), 56 (53), 57 (20), 58 (18), 72 (13), 73 (87).

Diisobutylamine (72, MW = 129 g/mol)



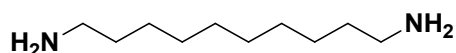
GC-MS (EI, 70eV): m/z (rel. int, %): 39 (8), 40 (6), 41 (29), 42 (16), 43 (15), 44 (17), 54 (5), 55 (7), 56 (12), 57 (27), 58 (9), 72 (7), 86 (100), 87 (12), 129 (23).

2-Amino-3-methylbutane (73, MW = 87 g/mol)



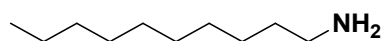
GC-MS (EI, 70eV): m/z (rel. int, %): 39 (11), 41 (10), 42 (11), 43 (13), 44 (100), 55 (17), 56 (12), 70 (7), 72 (11).

1,10-Diaminodecane (74, MW = 172 g/mol)



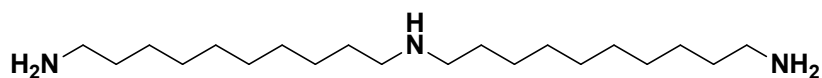
GC-MS (EI, 70eV): m/z (rel. int, %): 39 (12), 41 (40), 42 (17), 43 (23), 44 (75), 45 (38), 53 (5), 54 (6), 55 (44), 56 (60), 57 (8), 59 (27), 67 (10), 68 (6), 69 (32), 70 (20), 72 (26), 73 (11), 81 (7), 82 (6), 83 (12), 86 (45), 87 (11), 95 (5), 97 (9), 98 (6), 100 (45), 101 (5), 114 (31), 128 (36), 129 (5), 142 (21), 143 (72), 144 (8), 156 (100), 157 (12).

Decylamine (75, MW = 157 g/mol)



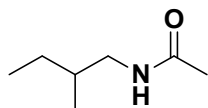
GC-MS (EI, 70eV): m/z (rel. int, %): 39 (31), 40 (7), 41 (100), 42 (30), 43 (54), 44 (67), 45 (50), 53 (9), 54 (7), 56 (37), 57 (13), 59 (15), 67 (7), 69 (27), 70 (15), 72 (16), 73 (6), 83 (13), 84 (7), 86 (46), 87 (5), 97 (8), 100 (25), 114 (10), 128 (9), 156 (7), 157 (10).

***N*¹-(10-aminodecyl)decane-1,10-diamine (76, MW = 327 g/mol)**



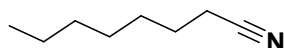
GC-MS (EI, 70eV): m/z (rel. int, %): 44 (11), 55 (7), 56 (6), 156 (6), 171 (6), 185 (100), 186 (13).

***N*-(2-methylbutyl)acetamide (77, MW = 129 g/mol)**



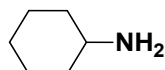
GC-MS (EI, 70eV): m/z (rel. int, %): 39 (16), 40 (5), 41 (32), 42 (18), 43 (95), 44 (9), 45 (10), 55 (15), 56 (12), 57 (9), 58 (36), 60 (61), 70 (11), 72 (100), 73 (64), 74 (10), 100 (51), 114 (10), 129 (9).

Octanenitrile (78, MW = 125 g/mol)



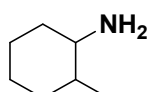
GC-MS (EI, 70eV): m/z (rel. int, %): 39 (22), 40 (5), 41 (62), 42 (10), 43 (26), 53 (5), 54 (37), 55 (34), 56 (7), 57 (9), 68 (8), 69 (35), 82 (100), 83 (40), 96 (52), 97 (22), 110 (13).

Cyclohexylamine (79, MW = 99 g/mol)



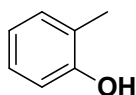
GC-MS (EI, 70eV): 39 (6), 41 (6), 42 (8), 43 (25), 56 (100), 57 (5), 70 (10), 99 (18).

2-Methylcyclohexylamine (80, MW = 113 g/mol)



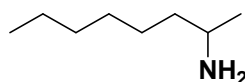
GC-MS (EI, 70eV): 39 (8), 41 (11), 42 (7), 43 (23), 55 (5), 56 (100), 57 (14), 67 (5), 70 (49), 71 (5), 84 (5), 113 (21).

O-Cresol (81, MW = 108 g/mol)



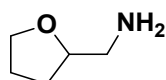
GC-MS (EI, 70eV): 39 (12), 50 (8), 51 (13), 52 (6), 53 (10), 63 (7), 77 (37), 78 (9), 79 (36), 80 (14), 89 (14), 90 (23), 91 (7), 107 (88), 108 (100), 109 (8).

2-Octylamine (82, MW = 129 g/mol)



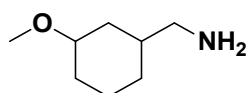
GC-MS (EI, 70eV): 39 (5), 41 (10), 42 (8), 43 (8), 44 (100), 55 (5), 56 (5), 114 (8).

Tetrahydrofurfurylamine (83, MW = 101 g/mol)



GC-MS (EI, 70eV): 39 (20), 40 (5), 41 (45), 42 (20), 43 (88), 44 (7), 56 (8), 58 (19), 70 (12), 71 (100), 72 (6), 84 (16), 101 (2).

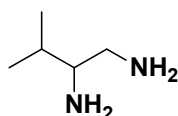
(3-methoxycyclohexyl)methanamine (84, MW = 143 g/mol)



GC-MS (trans) (EI, 70eV): 39 (33), 40 (5), 41 (57), 42 (12), 43 (35), 44 (8), 45 (26), 51 (5), 53 (19), 54 (35), 55 (27), 56 (43), 57 (8), 58 (20), 65 (6), 66 (5), 67 (100), 68 (35), 69 (15), 70 (8), 71 (41), 77 (13), 79 (27), 80 (14), 81 (42), 82 (48), 83 (9), 84 (10), 85 (6), 91 (7), 93 (9), 94 (21), 95 (10), 96 (7), 97 (9), 98 (5), 100 (17), 110 (6), 111 (24), 112 (44), 113 (69), 114 (6), 128 (14).

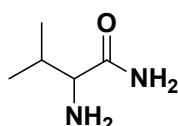
GC-MS (cis) (EI, 70eV): 39 (22), 41 (37), 42 (9), 43 (20), 45 (17), 53 (13), 54 (19), 55 (19), 56 (21), 57 (5), 58 (15), 67 (54), 68 (19), 69 (10), 70 (5), 71 (30), 72 (10), 77 (9), 79 (20), 80 (9), 81 (29), 82 (24), 83 (6), 84 (8), 85 (5), 91 (5), 93 (8), 94 (10), 95 (9), 97 (7), 98 (12), 110 (5), 111 (36), 112 (15), 113 (5), 126 (12), 128 (100), 129 (8), 143 (2).

3-Methyl-1,2-butanediamine (85, MW = 102 g/mol)



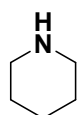
GC-MS (EI, 70eV): 39 (7), 41 (8), 42 (8), 43 (6), 44 (5), 55 (52), 56 (12), 57 (9), 59 (18), 72 (100), 73 (5).

2-Amino-3-methylbutanamide (86, MW = 116 g/mol)



GC-MS (EI, 70eV): 39 (8), 41 (7), 43 (5), 44 (12), 55 (50), 56 (15), 57 (16), 72 (100), 73 (14), 116 (0.02).

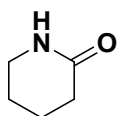
Piperidine (87, MW = 85 g/mol)



GC-MS (EI, 70eV): 39 (11), 41 (12), 42 (19), 43 (14), 44 (18), 55 (8), 56 (48), 57 (32), 70 (11), 84 (100), 85 (51).

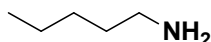
¹H-NMR (400 MHz, methanol-d₄): δ (ppm) = 2.78 (t, 4H, -NH-CH₂-), 1.34 (s, 6H, -NH-CH₂-CH₂-CH₂-).

2-Piperidinone (88, MW = 99 g/mol)



GC-MS (EI, 70eV): 39 (22), 40 (7), 41 (42), 42 (52), 43 (45), 44 (5), 55 (27), 56 (11), 70 (20), 71 (10), 98 (20), 99 (100).

Pentylamine (89, MW = 87 g/mol)



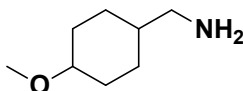
GC-MS (EI, 70eV): 38 (11), 39 (85), 40 (15), 41 (92), 42 (65), 43 (34), 44 (33), 45 (62), 50 (7), 51 (8), 52 (6), 53 (9), 54 (12), 55 (22), 56 (27), 58 (5), 69 (9), 70 (5), 86 (12), 87 (100), 88 (10).

Tetrahydrofuran (90, MW = 72 g/mol)



GC-MS (EI, 70eV): 38 (6), 39 (30), 40 (13), 41 (61), 42 (100), 43 (24), 44 (6), 71 (45), 72 (46).

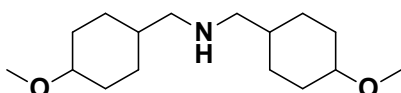
(4-methoxycyclohexyl)methylamine (91, MW = 143 g/mol)



GC-MS (cis) (EI, 70eV): 39 (46), 40 (7), 41 (68), 42 (17), 43 (44), 44 (6), 45 (24), 51 (8), 52 (5), 53 (26), 54 (38), 55 (39), 56 (51), 57 (12), 58 (84), 59 (8), 60 (15), 65 (9), 66 (8), 67 (100), 68 (16), 69 (9), 70 (15), 71 (35), 72 (6), 77 (21), 78 (5), 79 (50), 80 (38), 81 (55), 82 (43), 83 (11), 84 (10), 91 (12), 93 (14), 94 (68), 95 (22), 96 (6), 97 (71), 98 (14), 110 (15), 111 (21), 112 (99), 113 (11), 126 (80), 127 (8), 128 (51), 143 (6).

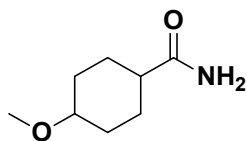
GC-MS (trans) (EI, 70eV): 39 (32), 40 (5), 41 (50), 42 (12), 43 (31), 44 (5), 45 (15), 51 (6), 53 (19), 54 (37), 55 (25), 56 (35), 57 (8), 58 (52), 59 (5), 60 (6), 65 (7), 66 (7), 67 (91), 68 (12), 69 (6), 70 (15), 71 (20), 77 (14), 79 (42), 80 (30), 81 (40), 82 (36), 83 (7), 91 (7), 93 (8), 94 (79), 95 (17), 96 (5), 97 (15), 98 (5), 110 (7), 111 (63), 112 (100), 113 (10).

Bis((4-methoxycyclohexyl)methyl)amine (92, MW = 269 g/mol)



GC-MS (EI, 70eV): 41 (12), 43 (6), 44 (20), 45 (6), 55 (7), 58 (5), 67 (11), 71 (7), 81 (6), 93 (7), 95 (20), 124 (48), 125 (5), 156 (100), 157 (10), 238 (10), 254 (8), 269 (2).

4-Methoxycyclohexanecarboxamide (93, MW = 157 g/mol)



GC-MS (EI, 70eV): 39 (21), 40 (6), 41 (31), 42 (5), 43 (23), 44 (36), 45 (10), 53 (12), 54 (11), 55 (24), 56 (6), 57 (4), 58 (100), 59 (9), 67 (15), 68 (5), 69 (7), 71 (41), 72 (15), 77 (7), 79 (17), 80 (8), 81 (34), 82 (16), 83 (6), 85 (7), 86 (5), 96 (17), 97 (16), 98 (5), 108 (5), 111 (7), 112 (6), 114 (9), 125 (47), 126 (10), 127 (14), 128 (7), 129 (42), 140 (18), 142 (14), 157 (5).

8. References supporting information

- (1) Coeck, R., et al. *Green Chemistry*, **2019**, 21, 5326–5335.
- (2) Babij, N. R., et al. *Organic Process Research and Development*, **2016**, 20, 661–667.