Supporting Information

The Sustainable and Catalytic Synthesis of N,N-alkylated Fatty Amines from Fatty Acids and Esters

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1. Experimental details

1.1. Materials

Most materials were used as obtained commercially. *N*,*N*-dimethylpalmitamide was produced and kindly provided by Eastman, Taminco. Before use, the sample was rotary evaporated to remove any leftover methylamines and methanol from their production process. An ¹H-NMR measurement confirmed the high purity of the final product.

Due to the inaccessibility of pure TMA (trimethylamine), the majority of the experiments were performed with the commercially available saturated solutions of 1M TMA in THF. A small quantity of TMA was produced by reacting TMA.HCl with very concentrated NaOH (in water) in a closed reactor system. The reactor system was connected to a cooled stainless steel gas cylinder, in which a noticeable amount of TMA was condensed.

1.2. Reactions

Reactions were performed in a 50 mL pressure Parr batch reactor. In a typical reaction, the reactor is filled with an substrate (i.e. fatty acid (FA)/fatty acid methyl ester (FAME)/fatty amide/fatty amine), catalyst (e.g. Nb₂O₅/Pt-base catalyst), dodecane (internal standard, 100 μ L) and cyclopentyl methyl ether (CPME, 18.5 mL). Next, the reactor is sealed, purged with H₂ and DMA (dimethylamine) was added to the reactor in the liquid phase via a mass flow controller. After the addition of DMA, the reactor was pressurized with additional H₂, if required. After an appropriate reaction time at a temperature of typically 200°C, the reactor is cooled down in an ice bath until room temperature and the pressure is released and passed through a scrubbing solution (15% H₂SO₄ in water) to capture all amines in the gas/vapor phase. The reaction mixture is transferred to one or more glass reaction vials (11 mL) which is/are then sealed and centrifuged. The mixture, with a typically clear, is analyzed via GC, GC-MS and/or ¹H-NMR.

1.3. Product analysis and identification

The crude and acetic anhydride treated reaction mixtures (described in section 1.2) were quantitatively analysed by gas chromatography (GC, see Figures S1 - S3). A few samples were additionally checked via nuclear magnetic resonance (NMR) spectroscopy. NMR samples were prepared by mixing 275 µL of the reaction mixture with 275 µL methanol-d4. ¹H-NMR spectra were recorded on a Bruker Ascend 400 MHz spectrometer equipped with a Bruker Ascend[™] 400 magnet, a 5 mm PABBO BB/19F-1H/D probe and a sample case. Aside from 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 — Chromatogram of a crude reaction mixture after the amidation of methyl palmitate with dimethylamine (DMA).



Figure S 2 — Chromatogram of a crude reaction mixture after the reductive amination of palmitic acid (DMA and H₂). The chromatogram of a crude reaction mixture after the hydrogenation of *N*,*N*-dimethylpalmitamide looks similar.



Figure S 3 — Chromatogram of a crude reaction mixture after the reductive amination of palmitic acid (DMA and H₂) which is treated with acetic anhydride and triethylamine.

1.4. Catalyst synthesis

 Nb_2O_5 was hydrothermally (HT) synthesized as described in a previous report by Coeck *et al.*^[1] To a glass-lined Parr reactor (600 mL) 15 g ammonium niobium oxalate hydrate (C₄H₄NNbO₉.xH₂O) was added along with 300 mL deionized water. The reactor was sealed and stirred (500 rpm) for 3 days at 175°C. The resulting precipitate was isolated via filtration and excessively washed with deionized water. Instead of pure white, the precipitate had a very light pale yellow color due to some metal ions leaching from the stirrer and being incorporated into the Nb_2O_5 structure. This HT synthesis method was repeated 2 more times and the crude Nb_2O_5 from all three runs was combined. Any metal ions on the outer surface of the crude Nb_2O_5 were leached off by stirring the powder in a solution of 5 g citric acid in 250 mL deionized water at 80°C overnight. The wet powder was isolated via centrifugation, decanted and excessively washed with deionized water. After drying the powder overnight at 80°C, the material was calcined in air at 400°C for 4 h after which the *ortho*-Nb₂O₅ was ready to use.

 $Na^{+}/Nb_{2}O_{5}$ was prepared by Na^{+} -exchange via an adapted method as described by Nakajima *et al.*^[2] 2 g of *ortho*-Nb₂O₅ was added to and stirred vigorously in a 0.2 M NaCl solution in water (4.68 g NaCl and 400 mL water). Upon addition of the solid Nb₂O₅, the pH of the liquid dropped to ± 4. The pH was adjusted to ± 6 by addition of 0.05 M NaOH in water (0.02 g NaOH added in total). The suspension was stirred for 24 hours after which the material was filtered off, washed with a large quantity of distilled water and dried at 100°C overnight.

Simple unpromoted noble metal catalysts on an oxide support (e.g. Pt/Nb_2O_5 , Pd/ZrO_2 or Ru/Nb_2O_5) were prepared via incipient wetness impregnation. In a typical synthesis, the appropriate amount of metal precursor (i.e. $[Pt(NH_3)_4](NO_3)_2$, $[Pd(NH_3)_4]Cl_2 H_2O$ or $RuCl_3 xH_2O$) was dissolved in water and mixed into the catalyst support (e.g. *ortho*-Nb₂O₅ or ZrO₂). Next, the resulting pre-catalyst is dried overnight in an oven at 80°C, after which the material is granulated (250-500 µm). Finally, in a quartz U-tube, the material is calcined in oxygen at 400°C (2°C min⁻¹, 100 mL min⁻¹ O₂, for 1 h; only for Pt and Pd-based catalysts) followed by a reduction at the same temperature (400°C, 2°C min⁻¹, 100 mL min⁻¹ H₂, for 1 h).

Promoted noble metal catalysts were prepared via an adapted method as described by Mitsudome *et al.*^[3] In a typically synthesis of $PtVO_x/SiO_2$ (7 wt% Pt, molar ratio Pt - V = 1), 0.0787 g $Pt(acac)_2$ and 0.0531 g $VO(acac)_2$ were dissolved in 45 mL acetone in a 100 mL round-bottom flask. After shaking the solution for 30 minutes, the support (i.e. 0.5 g of fumed SiO₂) was added to the solution. After shaking the suspension for an additional 4 hours, the acetone was removed via rotary evaporation under reduced pressure. The temperature of the water bath was kept to a maximum of 60°C to prevent any condensation reactions of the ketone (e.g. aldol reactions). Next, the obtained powder was dried in a muffle furnace at 85°C for 9 hours after which it was calcined in air at 300°C for 4 hours (heat rate of 5°C/min).

1.5. Catalyst characterization

Ortho-Nb₂O₅ was characterized with X-ray powder diffraction (XRD). Any XRD measurements were performed with the Malvern PANalytical Empyrean equipped with a Cu X-ray tube and a Pixcel3D detector. Additional characterization of Nb₂O₅ can be found in our previous report.^[1]

CO adsorption experiments were performed to determine the dispersion of the supported Pt nanoparticles. The experiments were performed with a ChemBet Pulsar TPR/TPD. Before every measurement, the catalyst was first pre-treated with H₂ at 200°C for approximately an hour. Next, the samples were cooled to room temperature and CO and He were then alternately pulsed over the sample. An adsorption stoichiometry of 1 molecules of CO per Pt atom is assumed.^[4]

High resolution scanning transmission electron microscopy (HRSTEM) images were acquired with an aberration-corrected Thermo Fisher Scientific Titan microscope operated at 300 kV and 50 pA beam current. The sample was deposited on a graphene grid in order to improve the contrast and the stability of the particles. 150 particles were measured to obtain the particle size distributions. Energy dispersive X-ray spectroscopy (EDX) measurements were carried out using a ChemiSTEM system and analyzed using the Bruker Esprit software. The EDX-STEM datasets were acquired with a 150 pA beam current and the total acquisition time was limited to approximately 3 minutes to reduce beam damage on the sample.

1.6. Recycling test

After each reaction, the catalyst was separated from the reaction mixture and washed 4 times with the reaction solvent. The catalyst was dried in an oven at 120°C for 4 hours and was reused afterwards. Small quantities of catalyst (< 5%) that were lost in the process, were replenished with fresh catalyst.

2. Additional experiments – Amidation of FA(ME)



Figure S 4 — Influence of DMA concentration on the amidation of methyl palmitate and palmitic acid. Reaction conditions: substrate (5 mmol), 200°C, variable amount of dimethylamine, 0.25 g ZrO₂, dodecane standard (100 μL), CPME (18.5 mL), 5 h reaction time, batch setup.



Figure S 5 — Influence of reaction solvent on the amidation of methyl palmitate. Reaction conditions: methyl palmitate (5 mmol), 200°C, 2 g dimethylamine, 0.25 g Nb₂O₅, dodecane standard (100 μL), solvent (18.5 mL), 5 h reaction time, batch setup. *DEGDBE : Diethylene glycol dibutyl ether.

3. Additional experiments – Hydrogenation of amides



Figure S 6 — Variation of the hydrogen pressure during the hydrogenation of *N*,*N*-dimethylpalmitamide to *N*,*N*-dimethylpalmitylamine. Reaction conditions: *N*,*N*-dimethylpalmitamide (5 mmol), 200°C, 2 g DMA, 0.0714 g catalyst (PtVOx/SiO₂(gel), 7% Pt), dodecane standard (100 μ L), CPME (18.5 mL), 16 h.



Figure S 7 — The influence of the reaction solvent on the hydrogenation of *N*,*N*-dimethylpalmitamide to *N*,*N*-dimethylpalmitylamine. Reaction conditions: *N*,*N*-dimethylpalmitamide (5 mmol), 200°C, 1 g DMA, 60 bar H₂, 0.5 mol% Pt (PtVO_x/SiO₂, 7 wt% Pt), dodecane standard (100 μ L), solvent (18.5 mL), 16 h. The poor result in glyme is most likely due to partial degradation of the solvent and water abstraction from the air.



Figure S 8 — The influence of temperature on the initial hydrogenation reaction rate of *N*,*N*-dimethylpalmitamide to *N*,*N*-dimethylpalmitylamine. Reaction conditions: *N*,*N*-dimethylpalmitamide (5 mmol), 200°C, 1 g DMA, 60 bar H₂, 0.5 mol% Pt (PtVO_x/SiO₂, 7 wt% Pt), dodecane standard (100 μ L), CPME (18.5 mL), 1 h.



Figure S 9 — Time profile for the hydrogenation of *N*,*N*-dimethylpalmitamide to *N*,*N*-dimethylpalmitylamine with **20 bar H₂ (top)**, **40 bar H₂ (middle)**, **60 bar H₂** (**bottom**). Reaction conditions: *N*,*N*-dimethylpalmitamide (5 mmol; 0.25 M), 1 g DMA, 200°C, 20-60 bar H₂, 0.5 mol% Pt (PtVO_x/SiO₂, 7 wt% Pt), dodecane (100 µL), CPME (18.5 mL), variable reaction time.

4. Kinetics – competitive adsorption

The experimental data for the hydrogenation of amides does not fit with a simple 1e order kinetics in amide concentration:

$$rate = -\frac{\partial [amide]}{\partial t} \neq k[amide]$$

For this reason, a model was built where the amide hydrogenation reaction was hindered by the competitive adsorption of amines and water to the catalytic surface.^[5]

Adsorption-desorption:rate of adsorption= rate of desorptionAmide + *
$$\frac{k_{a,amide}}{k_{d,amide}}$$
 Amide* $k_{a,amide} \cdot [Amide] \cdot = k_{d,amide} \cdot \theta_{amide} \rightarrow \theta_{amide} = b_{amide} \cdot [Amide] \cdot = k_{d,amide} \cdot \theta_{amide} \rightarrow \theta_{amide} = b_{amide} \cdot [Amide] \cdot = k_{d,amide} \cdot Amide \cdot$

with * = 1 - $\theta_{amide} - \theta_{H_2} - \theta_{dma} - \theta_{water} - \theta_{amine}$ and $b_X = \frac{k_{a,X}}{k_{d,X}}$

where *: relative amount of available adsorption sites, θ_X : relative surface coverage of compound X, [X]: concentration of compound X and X^{*}: chemisorbed compound X. Only dissolved H₂ is able to adsorb to the catalytic surface. However, this derivation assumes a linear correlation between the H₂ pressure and the concentration of H₂ in solution (Henry's Law), so the statements above remain valid.

Surface reactions:

$$\begin{array}{c} \mathbf{O} \\ R_{1} \\ R_{3} \\ R_{3} \\ Amide^{*} \\ R_{1} \\ R_{3} \\ Amide^{*} \\ R_{1} \\ R_{3} \\ R_{1} \\ R_{3} \\ R_{1} \\ R_{3} \\ R_{3} \\ R_{1} \\ R_{3} \\ R_{1} \\ R_{3} \\ R_{3} \\ R_{1} \\ R_{3} \\ R_{3} \\ R_{1} \\ R_{3} \\ R_{3} \\ R_{3} \\ R_{3} \\ R_{3} \\ R_{3} \\ R_{1} \\ R_{3} \\ R_{3} \\ R_{3} \\ R_{1} \\ R_{3} \\$$

This adsorption-desorption-reaction model is based on a Langmuir-Hinshelwood mechanism. In this reaction, the surface bound amide reacts with 2 surface bound hydrides to an hemiaminal. This initial hydrogenation is thermodynamically unfavourable. In order to complete the reaction, the now available surface sites are quickly refilled with 2 new hydrides so that a second hydrogenation can take place. Otherwise, the hemiaminal reconverts to the original surface bound amide and hydrides. The reaction therefore requires 1 amide molecule, 2 H₂ molecules and 3 surface sites. Therefore:

Reaction rate
$$= -\frac{\partial [Amide]}{\partial t} = k. [Amide]. (P_{H_2})^2.*^3$$

 $= \frac{k[Amide](P_{H_2})^2}{(1+b_{Amide}[Amide]+\sqrt{b_{H_2}P_{H_2}}+b_{dma}[DMA]+b_{water}[H_2O]+b_{amine}[Amine])^3}$
Neglectable ~ weak amide adsorption
Neglectable ~ relatively weak H₂ adsorption
Neglectable ~ constant
No nett DMA consumption

The equation can be reduced to the following:

$$rate = -\frac{\partial [amide]}{\partial t} = \frac{k_1 \cdot [amide] \cdot (P_{H_2})^2}{(1+k_2 \cdot [H_2O])^3} \quad \text{or} \quad \frac{w \cdot [amide]}{(1+k_2 \cdot [H_2O])^3} \text{ at a constant } H_2 \text{ pressure}$$

with $w = k_1 \cdot (P_{H_2})^2 \text{ or } \sqrt{w} = k_3 \cdot P_{H_2}$

These equations are true, as long as:

(1) water and the dimethylalkylamine are generated/present in equimolar concentrations.

(2) no secondary products are generated with significantly different adsorption/desorption rate constants.

In Figure S 10 - Figure S 12 and Figure 10 (main text) the model is fit with the experimental data. [Amide] is expressed as relative remaining concentration of amide (ranging from 0% to 100%) and $[H_2O]$ in equivalents of water (and amine product) in comparison to the original amount of amide. With $k_1 = 0.001$ and $k_2 = 1.58$, the graphs predict the experimental data nicely. Only at very long reaction times and/or low H_2 pressures, the simplified equation breaks down due to the generation of a lot of secondary product, e.g. disproportionation of DMA.



Figure S 10 — Kinetic profile for the hydrogenation of a fatty amide with competitive adsorption of water and amines in comparison with regular first order kinetics. Experimental conditions: *N*,*N*-dimethylpalmitamide (5 mmol; 0.25 M), 1 g DMA, 200°C, 60 bar H₂, 0.5 mol% Pt (PtVO_x/SiO₂, 7 wt% Pt), dodecane (100 μL), CPME (18.5 mL), variable reaction time.



Figure S 11 — Kinetic profile for the hydrogenation of *N*,*N*-dimethylpalmitamide with competitive adsorption of water and amines, with variable hydrogen pressure. The fitted values for *v* are linearly correlated to $(P_{H2})^2$, proving a second order relationship between the hydrogen pressure and the reaction rate. Experimental conditions: *N*,*N*-dimethylpalmitamide (5 mmol; 0.25 M), 1 g DMA, 200°C, variable pressure of H₂, 0.5 mol% Pt (PtVO_x/SiO₂, 7 wt% Pt), dodecane (100 µL), CPME (18.5 mL), variable reaction time.

With a proper equation for the reaction rate, we can determine the apparent activation energy E_a . Under the assumption that k_2 , a constant determined by the adsorption equilibrium constants, remains constant over a short temperature window, we can rewrite the equation for the reaction rate as follow:

$$rate = \mathbf{k_1} \cdot \frac{[amide] \cdot (P_{H_2})^2}{(1 + k_2 \cdot [H_2O])^3} = \mathbf{k_0} \cdot e^{\frac{-Ea}{R.T}} \frac{[amide] \cdot (P_{H_2})^2}{(1 + k_2 \cdot [H_2O])^3}$$

Next, the amide hydrogenation was performed at different reaction temperatures and k_1 was determined for each temperature (Figure S 12).



Figure S 12 — Kinetic profile for the hydrogenation of *N*,*N*-dimethylpalmitamide with competitive adsorption of water and amines, with variable reaction temperature. Experimental conditions: *N*,*N*-dimethylpalmitamide (5 mmol; 0.25 M), 1 g DMA, 160-200°C, 60 bar H₂, 0.5 mol% Pt (PtVO_x/SiO₂, 7 wt% Pt), dodecane (100 μL), CPME (18.5 mL), variable reaction time.

Plotting ln(**k**₁) (or ln(w); $w = k_1 \cdot (P_{H_2})^2$) in function of T⁻¹, should give a straight curve if all previously made assumptions are correct. This indeed appeared to be the case (Figure S 13). **E**_a was determined as **103 kJ/mol**.



Figure S 13 — Arrhenius plot for the hydrogenation of of N,N-dimethylpalmitamide with competitive adsorption of water and amines.

5. Substrate scope investigation and range of applicability

Table S 1 – Full list of substrate	scope	investigation.
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	Substrate	Amine	Stage	Products distribution (yield)	
			Α	N,N-dimethyloctanamide (76%), N-methyloctanamide (3%), Octanoic acid (20%).	
1	Octanoic acid	DMA	Н	Octylamine (9%), N-methyl-octylamine (23%), N,N-dimethyl-octylamine (54%),	
				Octane (4%), N,N-dimethyloctanamide (5%), N-methyl-dioctylamine (3%).	
			Α	N,N-dimethyldecanamide (89%), N-methyldecanamide (3%), Decanoic acid (8%).	
2	Decanoic acid ^f	DMA	Н	Decylamine (8%), N-methyl-decylamine (22%), N,N-methyl-decylamine (55%),	
				Decane (6%), N,N-dimethyldecanamide (2%), N-methyl-didecylamine (5%).	
			Α	N,N-dimethyllauramide (92%), N-methyllauramide (2%),Lauric acid (6%).	
3	Lauric acid (C12) ^f	DMA	Н	Laurylamine (8%), N-methyllaurylamine (22%), N,N-dimethyllaurylamine (56%),	
				Dodecane (5%), N,N-dimethyllauramide (3%), N-methyldilaurylamine (4%).	
			^	N,N-dimethyltetradecanamide (84%), N-methyltetradecanamide (3%),	
				Myristic acid (12%).	
4	Myristic acid (C14)	DMA		Tetradecylamine (7%), N-methyl-tetradecylamine (19%), Tetradecane (6%),	
			Н	N,N-dimethyl-tetradecylamine (54%), N-methyltetradecanamide (1%)	
				,N,N-dimethyltetradecanamide (7%), N-methyl-ditetradecylamine (3%).	
			А	<i>N</i> , <i>N</i> -dimethylpalmitamide (80%), <i>N</i> -methylpalmitamide (2%), Palmitic acid (17%).	
5	Palmitic acid (C16)	DMA		Palmitylamine (8%), N-methylpalmitylamine (20%), Hexadecane (6%),	
		DIVIN	Н	N,N-dimethylpalmitylamine (55%), N-methylpalmitamide (1%),	
				N,N-dimethylpalmitamide (3%), N-methyldipalmitylamine (3%).	
			A	N,N-dimethylstearamide (80%), N-methylstearamide (3%), Stearic acid (16%).	
6	Stearic acid (C18)	DMA	н	Stearylamine (6%), <i>N</i> -methylstearylamine (20%), <i>N</i> , <i>N</i> -dimethylstearylamine(55%),	
				Octadecane (5%), N,N-dimethylstearamide (10%), N-methylstearamide (2%).	
	Arachidic acid (C20)	DMA		A	<i>N,N</i> -dimethylicosanamide (83%), <i>N</i> -methylicosanamide (3%), Arachidic acid (14%)
7				N-methyl-icosanylamine (19%), N,N-dimethyl-icosanylamine (50%),	
′			Н	Icosanylamine (7%), Icosane (6%), <i>N</i> , <i>N</i> -dimethylicosanamide (9%),	
			-	N-methylicosanamide (1%).	
	Behenic acid (C22)		А	N,N-dimethyldocosanamide (81%), N-methyldocosanamide (3%),	
			-	-	Behenic acid (16%).
8		DMA		N-methyl-docosylamine (19%), N,N-dimethyl-docosylamine (56%),	
			H	Docosane (8%), Docosylamine (7%), N,N-dimethyldocosanamide (8%),	
				N-methyldocosanamide (1%).	
			А	<i>N</i> , <i>N</i> -dimethyltetracosanamide (69%), <i>N</i> -dimethyltetracosanamide (1%),	
					Lignoceric acid (30%).
9	Lignoceric acid (C24)	DIMA		N-methyl-tetracosylamine (21%), N,N-dimethyl-tetracosylamine (53%),	
			н	i etracosylamine (7%), i etracosane (7%), /v/v-dimetnyitetracosanamide (7%),	
			^	N-Qimethylelacosanamue (1%),	
10	Obio soid $(C10,1)$		A	/////-dimethyloleamide (83%), //-methyloleamide (4%), Oleic acid (13%).	
10	Oleic acid (C18:1)	DIVIA	Н	Stearylamine (7%), N-methylstearylamine (17%), N/N-dimethylstearylamine(51%),	
			^	Octadecalle (0%), N , N -differing steal affiliae (14%), N -fileting steal affiliae (2%).	
			A	N/N-ullitethylinoleannae (78%), N-methylinoleannae (5%), Linoleic acia (19%).	
11	Linoleic acid (C18:2)	DMA	ц	Steal yiannie (8%), N-methylsteal yiannie (16%), N, N-uniethylsteal yiannie (46%), (2%)	
	. ,			N methyldictearylamine (2%)	
<u> </u>				NV-memyulsied ylamine (270). N N. dimethylaalmitamide (70%). N. methylaalmitamide (1%)	
			А	Methyl nalmitate (20%). Nethol nalmitate (20%). Nethol nalmitate (20%).	
12	Methyl nalmitate ^a			Palmitulamine (1%) N-methylnalmitulamine (13%) Hevadecane (10%)	
12		DIVIA	н	N N-dimethylpalmitylamine (62%) N N-dimethylpalmitamide (1%)	
				N-methyldinalmitylamine (6%)	
	1		<u> </u>		

Each entry consists of a stage **A** (amidation) and/or stage **H** (hydrogenation). General reaction conditions (unless stated otherwise): FA(ME) (5 mmol), 200°C, 1 g of amine, 0.2 g Nb₂O₅, dodecane standard (100 μ L), CPME (18.5mL). Stage **A**: reaction time of 2 hours. Stage **H**: follows directly after stage A, addition of 60 bar H₂, 2.5 mol% Pt (PtVO_x/SiO₂, 7wt% Pt), reaction time of 16 hours. ^a 5 mol% Pt instead of 2.5 mol% Pt. ^bN-methylethanolamine, 1 equivalents added (0.38 g). ^cDiethylamine. ^dN-methylbutylamine, 2 eq. added (0.87 g) along with 3 eq. of *N*,*N*-dimethylbutylamine (1.52 g). ^eNo Nb₂O₅ added. ^fNonane instead of dodecane as internal standard.

Table S 1 - Full list of substrate scope investigation. (Continued)

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13	Decanoic acid	MEA ^b	А	N-(2-hydroxyethyl)-N-methyldecanamide (5%), N-(2-((2-hydroxyethyl)(methyl)amino)ethyl)-N-methyldecanamide (4%), 2-(N-methyldecanamido)ethyl decanoate (71%).
			Н	n-Decanol (1%), N-methyl-decylamine (5%), N,N-dimethyl-decylamine (9%), Decane (19%), N-ethyl-decylamine (4%), N-ethyl-N-methyldecan-1-amine (21%), 2-(decyl(methyl)amino)ethanol (1%), N^1 -decyl- N^2 -(2-(diethylamino)ethyl)- N^1 , N^2 -dimethylethane-1,2-diamine (2%),
				N^1 -decyl- N^2 -(2-(ethylamino)ethyl)- N^1 , N^2 -dimethylethane-1,2-diamine (4%), N^1 -decyl- N^2 -ethyl- N^1 , N^2 -dimethylethane-1,2-diamine (1%), N^1 -decyl- N^2 -(2-(ethyl(methyl)amino)ethyl)- N^1 , N^2 -dimethylethane-1,2-diamine (12%).
14	<i>N,N</i> -Diethyl- lauramide ^{e,f}	DEA ^c	Н	Dodecane (5%), <i>N</i> -ethyldodecylamine (17%), <i>N</i> , <i>N</i> -diethyldodecylamine (65%), Dodecylamine (1%), <i>N</i> , <i>N</i> -diethyldodecanamide (5%).
	Lauric acid (C12) ^f	DEA ^c	А	N,N-diethyl-dodecanamide (25%), Lauric acid (56%), N-ethyl-dodecanamide (19%)
15			Н	Dodecane (21%), <i>N</i> -ethyl-dodecylamine (30%), <i>N</i> , <i>N</i> -diethyl-dodecylamine (27%), <i>N</i> , <i>N</i> -diethyl-dodecanamide (10%), <i>N</i> -ethyl-didodecylamine (6%), Dodecylamine (3%).
	Palmitic acid (C16)		А	Palmitic acid (5%), N,N-dimethylpalmitamide (1%), N-methylpalmitamide (2%), N-butylpalmitamide (7%), N-methyl-N-butylpalmitamide (84%).
16		tic acid (C16) MBA ^d	MBA ^d	Н

Each entry consists of a stage **A** (amidation) and/or stage **H** (hydrogenation). General reaction conditions (unless stated otherwise): FA(ME) (5 mmol), 200°C, 1 g of amine, 0.2 g Nb₂O₅, dodecane standard (100 μ L), CPME (18.5mL). Stage **A**: reaction time of 2 hours. Stage **H**: follows directly after stage A, addition of 60 bar H₂, 2.5 mol% Pt (PtVO_x/SiO₂, 7wt% Pt), reaction time of 16 hours. ^a 5 mol% Pt instead of 2.5 mol% Pt. ^bN-methylethanolamine, 1 equivalents added (0.38 g). ^cDiethylamine. ^dN-Methylbutylamine, 2 eq. added (0.87 g) along with 3 eq. of *N*,*N*-dimethylbutylamine (1.52 g). ^eNo Nb₂O₅ added. ^fNonane instead of dodecane as internal standard.



6. Additional experiments – Industrialization and further improvements

Figure S 14 — Improved reductive amination of FAs with DMA by addition of TMA. Each run consists of a stage **A** (amidation) and stage **H** (hydrogenation). Reaction conditions (unless stated otherwise): Palmitic acid (5 mmol), 200°C, DMA and/or TMA, 2.5 mol% Pt (PtVOx/SiO₂, 7wt% Pt), 0.2 g Nb₂O₅, dodecane standard (100 μ L), THF (18.5mL). [postponed addition of Pt]: the PtVOx catalyst added in stage H (not at the start of stage A). Side-note: THF is a worse solvent than CPME. Reactions in THF generally lead to more defunctionalized product and side products. However, we resorted to utilizing THF as the reaction solvent in order to apply TMA via a commercial TMA in THF solution.



Figure S 15 — Reductive amination of palmitic acid with increasing substrate concentration. Reaction conditions: *N*,*N*-dimethylpalmitamide (substrate), 200°C, 1 g DMA, 60 bar H₂, 0.5 mol% Pt (PtVO_x/SiO₂ fumed 7wt% Pt), dodecane standard (100 μL), CPME, total liquid volume of 20 mL, 16 hours.

 Table S 2 – Solventless hydrogenation of N,N-dimethylpalmitamide.

DMA	ТМА	Water	Hexadecane	N,N-dimethyl- palmitylamine	N,N-dimethyl- palmitamide	Palmitylamine	N-methyl palmitylamine	Dipalmityl- methylamine	Hexadecanol
1	1	1	2,2%	35,6%	56%	0,1%	1,8%	0,36%	1,73%
1	0.5 g	1	1,8%	<u>35,8%</u>	58%	0%	1,16%	0,12%	0,57%
1	1 g	1	1,8%	<u>35,8%</u>	59%	0%	0,85%	0,08%	0,79%
0.4 g	1	1	1,2%	28%	62%	0,3%	6,7%	0,54%	0,80%
1 g	1	1	0,6%	18,2%	76%	0,3%	3,6%	0,05%	1,04%
2 g	1	1	0,6%	17,0%	77%	0,3%	3,3%	0,05%	1,02%
1 g	1	0.125 eq.	0,5%	14,4%	81%	0,3%	3,4%	0,06%	0,54%
1 g	1	0.25 eq.	0,3%	6,7%	90%	0,2%	1,9%	0,03%	0,32%

Reaction conditions: N,N-dimethylpalmitamide (9.47g), 200°C; DMA, TMA and/or water; 60 bar H₂, 0.5 mol% Pt (PtVO_x/SiO₂, 7 wt% Pt), dodecane (333 µL), 1 hour reaction time.

7. Additional experiments – Transalkylation and alkylation of amines

7.1. Transalkylation of amines



Figure S 16 — Catalyst evaluation for the transalkylation of *N*,*N*-dimethylpalmitylamine with DMA. Reaction conditions: *N*,*N*-dimethylpalmitylamine (5 mmol; 0.25 M), 200°C, 1 g DMA, 60 bar H₂, 1 mol% noble metal or 15 mol% Ni, dodecane (100 μL), CPME (18.5 mL), 16 h.



Figure S 17 — Variation of the reaction conditions for the transalkylation of *N*,*N*dimethylpalmitylamine with DMA with Ni/SiO₂ (left) and Pt/C (right). Reaction conditions: *N*,*N*-dimethylpalmitylamine (5 mmol; 0.25 M), 200°C, 1 g DMA, H₂, 1 mol% noble metal or 15 mol% Ni, dodecane (100 μL), CPME (18.5 mL).



Figure \$ 18 — Transalkylation of different alkylamines. Reaction conditions: substrate, 200°C, 5 bar H₂, Pt/C (5 wt% Pt), nonane (100 µL), solvent (18.5 mL).



Figure S 19 — Transalkylation of tertiary amines, i.e. DAMAs in ADMAs and vice versa, catalysed by a metal catalyst and traces of secondary amine.

Table S 3 – Synthesis of tertiary fatty amines via transalkylations with a different tertiary amine.

	Substrate	Stage	Reagent	Products distribution (yield)	
1	<i>N,N</i> -dimethyl- decylamine	Т	<i>N,N-</i> dimethyl- butylamine ^a	n-Decane (1%), Decylamine (3%), <i>N</i> , <i>N</i> -dimethyl-decylamine (23%), <i>N</i> -methyl- decylamine (3%), <i>N</i> -butyl- <i>N</i> -methyl-decylamine (25%), <i>N</i> -butyldecylamine (10%), <i>N</i> , <i>N</i> -dibutyl-decylamine (4%), <i>N</i> -methyl-didecylamine (14%), Didecylamine (6%), <i>N</i> -butyl-didecylamine (5%), Tridecylamine (1%).	
2	<i>N,N</i> -dimethyl- decylamine	Tb	<i>N,N</i> -dimethyl- butylamine ^a	n-Decane (<1%), Decylamine (3%), N,N-dimethyl-decylamine (41%), N-methyl- decylamine (4%), N-butyl-N-methyl-decylamine (20%), N-butyldecylamine (10%), N,N-dibutyl-decylamine (1%), N-methyl-didecylamine (9%), Didecylamine (6%), N-butyl-didecylamine (1%).	
Sta	Stage T (transalkylations): Reactions were performed at 200°C, with fatty amine (5 mmol), 5 bar H ₂ , 1 mol% Pt (Pt/C, 5 wt% Pt), dodecane				

standard (100 μL), CPME (18.5mL)., 4 hours. ^a 2 eq. added (1.01 g) along with 2 mol% of *N*-methylbutylamine (9 μL). ^b With 15 mol% Ni instead of Pt (Ni/SiO₂ catalyst; 64 wt% Ni).

8. Catalyst characterization

8.1. General catalyst characterization via XRD, TEM and CO chemisorption



Figure S 20 — XRD diffractogram for ortho-Nb₂O₅.

Table S 4 –	co	chemisorption	of	different Pt	based	catal	/sts.
	co	chemisorption	01	uniciciitit	buscu	cutur	1313.

Catalyst	Pt/C	Pt/Nb₂O₅	Pt/Nb ₂ O ₅	PtVO _x /SiO ₂
Pt content	5 wt%	1 wt%	4 wt%	7 wt%
Average crystal size	3.3 nm	4.1 nm	4.6 nm	/
Dispersion	35%	28%	25%	9%

CO chemisorption could not be employed to estimate the average crystal size for PtVO_x/SiO₂. (Pt is partially covered by VO_x)

Table S 5 – Size distribution of Pt nanoparticles of PtVO_x/SiO₂ catalysts (7 wt% Pt, Pt-V ratio of 1), determined by TEM analysis.

Catalyst	PtVO _x /SiO ₂ (Fresh)	PtVO _x /SiO ₂ (1x use)	PtVO _x /SiO ₂ (5x used)
Average crystal size	1.70 nm	2.14 nm	2.28 nm
Standard deviation	0.53 nm	1.13 nm	0.63 nm

Size distributions based on 150 particles for each sample

8.2. TEM analysis of fresh PtVO_x/SiO₂

See also main text for HAADF-STEM imaging and EDX elemental mapping of fresh PtVO_x/SiO₂. Elemental mapping of Si, O, Pt and V.



Figure S 21 — High resolution scanning transmission electron microscopy (HRSTEM) images of a fresh PtVO_x/SiO₂ catalyst (7 wt% Pt, molar Pt-V ratio of 1-1).



Figure S 22 — EDX analysis of fresh PtVO_x/SiO₂ catalyst (7 wt% Pt, molar Pt-V ratio of 1-1).

8.3. TEM analysis of PtVO_x/SiO₂ (1x used)



Figure S 23 — High resolution scanning transmission electron microscopy (HRSTEM) images of a PtVO_x/SiO₂ catalyst after a single use.



Figure S 24 — HAADF-STEM imaging and EDX elemental mapping of PtVO_x/SiO₂ after a single use. Elemental mapping of Si, O, Pt and V.



Figure S 25 — EDX analysis of of $PtVO_x/SiO_2$ after a single use.

8.4. TEM analysis of PtVO_x/SiO₂ (5x used)



Figure S 26 — High resolution scanning transmission electron microscopy (HRSTEM) images of a PtVO_x/SiO₂ after being used 5 times.



Figure S 27 — High resolution scanning transmission electron microscopy (HRSTEM) images of a PtVO_x/SiO₂ after being used 5 times.



 $\label{eq:Figure S28} \textbf{Figure S28} - \textbf{HAADF-STEM} imaging and \textbf{EDX} elemental mapping of 5 times used PtVO_x/SiO_2. Elemental mapping of Si, O, Pt and V.$

9. Product identification

Amine reagents

Dimethylamine (1, MW = 45 g/mol)

GC-MS (EI, 70eV): m/z (rel. int, %): 40 (8), 41 (7), 42 (25), 43 (15), 44 (100), 45 (61).

Trimethylamine (2, MW = 59 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 40 (5), 41 (7), 42 (40), 43 (18), 45 (54), 46 (18), 58 (100), 59 (52).

Di-ethylamine (3, MW = 73 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 42 (10), 44 (22), 58 (100), 72 (15), 73 (24).

Tri-ethylamine (4, MW = 101 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 42 (9), 44 (8), 56 (7), 58 (27), 86 (100), 87 (6), 100 (6), 101 (16).

N,N-Dimethylbutylamine (5, MW = 101 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 56 (3), 58 (100), 59 (3), 101 (9).

N-Methyldibutylamine (6, MW = 143 g/mol)

`N´

GC-MS (EI, 70eV): m/z (rel. int, %): 57 (10), 58 (89), 100 (100), 101 (7), 143 (11).

1,4-Dimethylpiperazine (7, MW = 114 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 54 (8), 55 (6), 56 (24), 57 (13), 58 (15), 70 (35), 71 (48), 72 (6), 99 (8), 113 (5), 114 (100), 115 (7).

C8 alkyl products

Octane (8, MW = 114 g/mol)

$$\sim \sim \sim$$

GC-MS (EI, 70eV): m/z (rel. int, %): 39 (20), 41 (57), 42 (18), 43 (100), 55 (16), 56 (26), 57 (44), 70 (20), 71 (32), 84 (15), 85 (64), 114 (10).

Octylamine (9, MW = 129 g/mol)

GC-MS (EI, 70eV): m/z (rel. int, %): 39 (49), 40 (9), 41 (100), 42 (40), 43 (48), 44 (74), 45 (50), 53 (11), 54 (8), 55 (40), 56 (35), 57 (9), 59 (12), 67 (6), 69 (27), 70 (13), 72 (13), 83 (9), 84 (6), 86 (45), 100 (22), 128 (7), 129 (10).

N-Methyloctylamine (10, MW = 143 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 41 (9), 42 (5), 43 (5), 44 (100), 143 (7).

N,N-Dimethyloctylamine (11, MW = 157 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 41 (6), 42 (7), 43 (3), 44 (3), 58 (100), 59 (4), 157 (6).

N,N-Diethyloctylamine (12, MW = 185 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 55 (3), 56 (4), 57 (3), 58 (11), 72 (12), 86 (100), 87 (9), 170 (7), 185 (6).

N-Isopropyloctylamine (13, MW = 171 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 55 (5), 56 (7), 57 (14), 58 (10), 69 (3), 70 (6), 71 (9), 72 (100), 73 (5), 84 (3), 85 (3), 128 (5), 156 (70), 157 (8), 170 (3), 171 (5).

N-Propyloctylamine (14, MW = 171 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 55 (4), 56 (5), 57 (5), 58 (3), 70 (4), 72 (100), 73 (5), 128 (3), 142 (34), 143 (3), 171 (7).

N,N-Dipropyloctylamine (15, MW = 213 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 55 (4), 56 (3), 57 (4), 58 (4), 70 (4), 72 (10), 84 (5), 86 (46), 87 (3), 98 (3), 112 (4), 114 (100), 115 (8), 184 (88), 185 (12), 213 (6).

N-Butyloctylamine (16, MW = 185 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 55 (8), 56 (8), 57 (12), 69 (4), 70 (6), 71 (3), 72 (3), 84 (4), 86 (100), 87 (6), 128 (3), 142 (61), 143 (6), 185 (9).

N,N-Dibutyloctylamine (17, MW = 241 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 55 (5), 57 (7), 58 (9), 84 (4), 98 (5), 100 (37), 101 (3), 112 (3), 142 (72), 143 (7), 156 (6), 198 (100), 199 (14), 241 (5).

N-Methyloctanamide (18, MW = 157 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 39 (7), 41 (17), 42 (5), 43 (10), 45 (9), 55 (12), 57 (13), 58 (46), 73 (100), 86 (25), 87 (5), 100 (8), 114 (5), 128 (5), 157 (1).

N,N-Dimethyloctanamide (19, MW = 171 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 39 (6), 41 (16), 42 (11), 43 (11), 44 (16), 45 (35), 46 (7), 55 (12), 57 (14), 72 (51), 87 (100), 88 (5), 100 (28), 101 (6), 114 (8), 142 (6), 171 (5).

Dioctylamine (20, MW = 241 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 41 (7), 43 (9), 44 (33), 57 (5), 142 (100), 143 (13), 241 (5).

N-Methyldioctylamine (21, MW = 255 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 41 (6), 42 (3), 43 (7), 44 (6), 55 (3), 57 (4), 58 (30), 84 (4), 156 (100), 157 (11), 255 (3).

N-Ethyldioctylamine (22, MW = 270 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 55 (3), 57 (4), 58 (6), 72 (29), 98 (3), 112 (3), 170 (100), 171 (14), 254 (3), 269 (3), 270 (0.6).

N-Isopropyldioctylamine (23, MW = 284 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 55 (3), 57 (3), 86 (10), 126 (3), 170 (3), 184 (100), 185 (14), 268 (27), 269 (5), 283 (3), 284 (0.5).

N-Propyldioctylamine (24, MW = 284 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 55 (4), 57 (4), 58 (4), 72 (3), 84 (3), 86 (25), 98 (3), 112 (4), 156 (6), 184 (100), 185 (16), 254 (42), 255 (8), 282 (3), 283 (3), 284 (0.7).

N-Butyldioctylamine (25, MW = 298 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 55 (4), 57 (5), 58 (7), 84 (3), 98 (4), 100 (15), 112 (5), 154 (3), 156 (11), 198 (100), 199 (19), 254 (52), 255 (10), 296 (3), 297 (4), 298 (0.8).

C9 products

n-Nonane (26, MW = 128 g/mol)

 \sim

GC-MS (EI, 70eV): m/z (rel. int, %): 39 (23), 41 (70), 42 (20), 43 (99), 53 (5), 55 (22), 56 (24), 57 (100), 69 (5), 70 (20), 71 (28), 84 (14), 85 (47), 98 (7), 99 (13), 128 (11).

C10 alkyl products

Decane (27, MW = 142 g/mol)

$$\sim$$

GC-MS (EI, 70eV): m/z (rel. int, %): 39 (16), 41 (57), 42 (16), 43 (85), 55 (19), 56 (20), 57 (100), 58 (5), 69 (6), 70 (16), 71 (43), 84 (12), 85 (32), 98 (8), 99 (9), 113 (5), 142 (9).

Decylamine (28, MW = 157 g/mol)

MH₂

GC-MS (EI, 70eV): m/z (rel. int, %): 39 (33), 40 (5), 41 (100), 42 (28), 43 (48), 44 (52), 45 (44), 53 (10), 54 (8), 55 (51), 56 (39), 57 (11), 59 (14), 67 (7), 69 (27), 70 (15), 72 (16), 83 (11), 86 (45), 87 (5), 97 (7), 100 (24), 114 (11), 128 (9), 142 (6), 156 (7), 157 (11).

N-Methyldecylamine (29, MW = 171 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 39 (3), 41 (10), 42 (5), 43 (6), 44 (100), 45 (3), 55 (4), 171 (6).

N,*N*-Dimethyldecylamine (30, MW = 185 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 41 (7), 42 (6), 43 (4), 44 (3), 55 (3), 58 (100), 59 (4), 185 (5).

N-Butyldecylamine (31, MW = 213 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 55 (9), 56 (7), 57 (11), 58 (6), 69 (3), 70 (6), 84 (5), 86 (100), 87 (5), 100 (9), 142 (3), 156 (4), 170 (80), 171 (9), 184 (7), 212 (4), 213 (11).

N-Butyl-N-methyldecylamine (32, MW = 227 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 55 (7), 57 (10), 58 (63), 59 (3), 70 (4), 84 (6), 98 (4), 100 (100), 101 (8), 184 (59), 185 (9), 227 (5).

N,N-Dibutyldecylamine (33, MW = 270 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 55 (5), 57 (6), 58 (7), 84 (4), 98 (5), 100 (28), 140 (3), 142 (64), 143 (7), 184 (4), 226 (100), 227 (17), 269 (4), 270 (0.7).

2-(decyl(methyl)amino)ethanol (34, MW = 215 g/mol)

GC-MS (EI, 70eV): m/z (rel. int, %): 55 (8), 56 (3), 57 (11), 58 (70), 59 (3), 70 (5), 71 (3), 84 (6), 88 (70), 89 (4), 98 (3), 184 (100), 185 (15), 214 (1), 215 (0.9).

 N^{1} -decyl- N^{2} -(2-(ethyl(methyl)amino)ethyl)- N^{1} , N^{2} -dimethylethane-1,2-diamine (35, MW = 314 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 55 (3), 57 (4), 58 (21), 70 (2), 84 (3), 98 (2), 184 (100), 185 (15), 310 (2), 311 (3), 313 (0.06), 314 (0.004).

N-(2-hydroxyethyl)-N-methyldecanamide (36, MW = 229 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 53 (6), 55 (59), 56 (20), 57 (56), 58 (39), 67 (8), 68 (5), 69 (17), 70 (6), 71 (32), 72 (5), 73 (34), 74 (45), 75 (7), 76 (23), 81 (9), 83 (6), 84 (5), 85 (18), 86 (15), 87 (7), 95 (9), 98 (5), 99 (18), 100 (7), 102 (32), 112 (23), 113 (5), 117 (100), 118 (6), 130 (25), 144 (5), 155 (13), 168 (6), 186 (21), 198 (6), 229 (5).

N-(2-((2-hydroxyethyl)(methyl)amino)ethyl)-N-methyldecanamide (37, MW = 286 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 55 (4), 56 (2), 57 (6), 58 (8), 70 (5), 71 (2), 83 (2), 86 (2), 88 (100), 89 (5), 99 (2), 101 (12), 102 (2), 112 (3), 210 (2), 212 (12), 213 (2), 285 (0.03), 286 (0.006).

2-(N-methyldecanamido)ethyl decanoate (38, MW = 384 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 55 (29), 56 (10), 57 (100), 58 (44), 69 (11), 71 (23), 73 (10), 74 (18), 76 (15), 81 (6), 83 (5), 85 (14), 86 (6), 87 (5), 95 (6), 98 (7), 99 (36), 100 (82), 101 (10), 102 (11), 112 (47), 113 (8), 116 (8), 117 (9), 118 (17), 126 (9), 130 (9), 154 (7), 155 (20), 159 (35), 168 (18), 172 (8), 182 (7), 186 (8), 196 (36), 197 (5), 199 (5), 210 (7), 211 (12), 212 (61), 213 (9), 228 (22), 230 (11), 271 (28), 272 (5), 284 (5), 383 (5), 384 (2).

N-Methyldecanamide (39, MW = 185 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 39 (4), 41 (15), 42 (3), 43 (9), 55 (10), 56 (3), 57 (5), 58 (37), 69 (3), 71 (3), 73 (100), 74 (4), 84 (3), 86 (26), 100 (5), 128 (5), 142 (5), 155 (3), 185 (3).

N,N-Dimethyldecanamide (40, MW = 199 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 41 (16), 42 (8), 43 (13), 44 (12), 45 (28), 46 (7), 55 (11), 57 (5), 72 (42), 87 (100), 88 (5), 100 (28), 101 (5), 114 (7), 142 (5), 156 (5), 199 (6).

Didecylamine (41, MW = 298 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 41 (3), 43 (4), 44 (14), 55 (3), 56 (3), 57 (3), 70 (3), 156 (4), 168 (4), 170 (100), 171 (13), 297 (3), 298 (0.2).

N-Methyldidecylamine (42, MW = 312 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 41 (5), 43 (7), 44 (5), 58 (22), 184 (100), 185 (14), 311 (2), 312 (0.4).

N-Butyldidecylamine (43, MW = 354 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 55 (3), 57 (4), 58 (5), 98 (3), 100 (7), 140 (3), 184 (5), 226 (100), 227 (16), 310 (41), 311 (9), 352 (3), 353 (2), 354 (0.5).

C12 alkyl products

Dodecane (44, MW = 170 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 39 (27), 40 (6), 41 (100), 42 (23), 43 (99), 44 (3), 53 (8), 54 (5), 55 (34), 56 (22), 57 (93), 58 (4), 67 (4), 69 (10), 70 (14), 71 (54), 72 (3), 83 (4), 84 (8), 85 (33), 98 (6), 99 (6), 112 (4), 113 (4), 127 (3), 170 (4).

Dodecylamine (45, MW = 185 g/mol)

NH2

GC-MS (EI, 70eV): m/z (rel. int, %): 39 (25), 41 (100), 42 (27), 43 (63), 44 (73), 45 (41), 53 (9), 54 (7), 55 (59), 56 (37), 57 (18), 59 (15), 67 (9), 68 (5), 69 (31), 70 (13), 72 (16), 73 (7), 82 (5), 83 (15), 84 (8), 86 (47), 87 (7), 97 (11), 100 (28), 111 (5), 114 (13), 128 (11), 142 (15), 156 (13), 170 (5), 184 (9), 185 (12).

N-Dodecylacetamide (46, MW = 227 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 39 (11), 41 (45), 42 (15), 43 (85), 44 (26), 45 (6), 55 (25), 56 (13), 57 (10), 58 (13), 60 (32), 69 (10), 70 (6), 72 (79), 73 (100), 74 (5), 83 (5), 86 (51), 87 (25), 100 (49), 101 (15), 114 (49), 115 (8), 128 (22), 129 (6), 142 (20), 156 (22), 170 (13), 184 (28), 199 (24).

N-Methyldodecylamine (47, MW = 199 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 41 (11), 43 (8), 44 (100), 55 (6), 199 (7).

N-Dodecyl-N-methylacetamide (48, MW = 241 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 39 (5), 41 (20), 42 (12), 43 (34), 44 (100), 45 (6), 55 (9), 56 (6), 57 (6), 58 (11), 73 (6), 74 (8), 86 (59), 87 (37), 100 (15), 101 (5), 114 (15), 128 (7), 142 (6), 156 (7), 170 (9), 198 (99), 199 (13), 240 (0.001).

N,N-Dimethyldodecylamine (49, MW = 213 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 41 (7), 43 (5), 58 (100), 213 (6).

Dodecanoic acid (Lauric acid) (50, MW = 200 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 39 (20), 41 (76), 42 (18), 43 (60), 45 (17), 53 (7), 54 (5), 55 (63), 56 (14), 57 (44), 59 (5), 60 (80), 61 (14), 67 (7), 68 (5), 69 (31), 70 (9), 71 (29), 73 (100), 74 (9), 82 (5), 83 (20), 84 (11), 85 (31), 87 (21), 96 (5), 97 (16), 98 (10), 99 (8), 101 (18), 111 (8), 112 (5), 115 (25), 129 (58), 130 (5), 138 (6), 143 (17), 157 (52), 158 (5), 171 (20), 200 (21).

N,N-Dimethyldodecanamide (51, MW = 227 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 41 (16), 42 (6), 43 (13), 44 (10), 45 (23), 46 (7), 55 (11), 57 (6), 72 (36), 87 (100), 88 (5), 100 (26), 101 (5), 114 (6), 142 (5), 227 (5).

Didodecylamine (52, MW = 354 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 43 (8), 44 (18), 198 (100), 199 (15), 353 (3), 354 (0.7).

N-Methyldidodecylamine (53, MW = 368 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 41 (3), 43 (5), 44 (3), 57 (3), 58 (12), 212 (100), 213 (16), 366 (3), 367 (2), 368 (0.4).

Tridodecylamine (54, MW = 522 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 41 (3), 43 (4), 58 (3), 72 (10), 226 (100), 227 (17), 380 (3).

N-Ethyldodecylamine (55, MW = 213 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 41 (9), 42 (3), 43 (7), 44 (7), 55 (5), 56 (4), 58 (100), 59 (4), 184 (3), 198 (3), 212 (3), 213 (7).

N,N-Diethyldodecylamine (56, MW = 241 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 41 (5), 58 (5), 72 (6), 86 (100), 87 (6), 226 (8), 241 (4).

N-Ethyldodecanamide (57, MW = 227 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 41 (13), 43 (11), 44 (11), 46 (5), 55 (10), 57 (6), 72 (32), 87 (100), 88 (5), 100 (27), 101 (5), 114 (6), 142 (5), 227 (5).

N,N-Diethyldodecanamide (58, MW = 255 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 41 (12), 43 (11), 44 (9), 55 (10), 57 (6), 58 (25), 72 (20), 73 (5), 86 (8), 87 (5), 100 (42), 115 (100), 116 (7), 128 (37), 129 (6), 142 (7), 170 (6), 255 (8).

N-Ethyldidodecylamine (59, MW = 382 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 43 (3), 58 (3), 84 (3), 212 (100), 213 (16), 381 (0.01), 382 (0.006).

C14 alkyl products

Tetradecane (60, MW = 198 g/mol)

GC-MS (EI, 70eV): m/z (rel. int, %): 39 (9), 41 (52), 42 (12), 43 (76), 55 (24), 56 (17), 57 (100), 69 (10), 70 (13), 71 (69), 83 (6), 84 (8), 85 (48), 98 (7), 99 (12), 112 (6), 113 (6), 127 (5), 198 (7).

Tetradecylamine (61, MW = 213 g/mol)

MH₂

GC-MS (EI, 70eV): m/z (rel. int, %): 39 (19), 41 (100), 42 (25), 43 (79), 44 (97), 45 (45), 53 (9), 54 (8), 55 (69), 56 (38), 57 (29), 58 (5), 59 (18), 67 (10), 68 (6), 69 (36), 70 (14), 71 (8), 72 (19), 73 (8), 82 (6), 83 (20), 84 (9), 86 (52), 87 (8), 97 (15), 98 (8), 100 (31), 111 (8), 114 (15), 128 (14), 142 (17), 156 (15), 170 (11), 184 (12), 198 (7), 212 (11), 213 (14).

N-Methyltetradecylamine (62, MW = 227g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 41 (11), 42 (4), 43 (9), 44 (100), 45 (3), 55 (7), 57 (4), 58 (3), 70 (3), 227 (7).

N,N-Dimethyltetradecylamine (63, MW = 241 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 41 (7), 43 (6), 58 (100), 241 (6).

Tetradecanoic acid (Myristic acid) (64, MW = 228g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 39 (18), 41 (80), 42 (20), 43 (87), 45 (16), 53 (8), 54 (6), 55 (83), 56 (17), 57 (64), 59 (6), 60 (96), 61 (22), 67 (9), 68 (8), 69 (44), 70 (13), 71 (37), 73 (100), 74 (14), 81 (5), 82 (7), 83 (29), 84 (14), 85 (29), 87 (27), 97 (22), 98 (15), 99 (14), 101 (12), 111 (11), 112 (5), 113 (7), 115 (22), 116 (6), 125 (6), 129 (86), 130 (9), 143 (24), 157 (10), 166 (6), 171 (25), 185 (73), 186 (10), 199 (15), 228 (36), 229 (6).

N-Methyltetradecanamide (65, MW = 241g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 41 (14), 43 (13), 55 (10), 57 (7), 58 (26), 73 (100), 74 (5), 86 (26), 87 (5), 100 (7), 128 (5), 142 (5), 198 (5), 241 (3).

N,N-Dimethyltetradecanamide (66, MW = 255 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 41 (13), 42 (5), 43 (12), 44 (7), 45 (18), 46 (6), 55 (10), 57 (5), 69 (3), 72 (29), 87 (100), 88 (5), 100 (25), 101 (5), 114 (6), 142 (5), 156 (3), 212 (3), 255 (5).

Ditetradecylamine (67, MW = 410 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 41 (3), 43 (7), 44 (13), 55 (3), 57 (4), 212 (4), 224 (3), 226 (100), 227 (17), 408 (4), 409 (3), 410 (0.7).

N-Methylditetradecylamine (68, MW = 428 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 58 (9), 240 (100), 241 (18), 428 (0.001).

C16 alkyl products

Hexadecane (69, MW = 226 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 39 (15), 41 (87), 42 (18), 43 (100), 53 (6), 55 (38), 56 (18), 57 (83), 67 (5), 69 (14), 70 (11), 71 (52), 83 (6), 84 (6), 85 (36), 99 (10), 113 (5), 226 (2).

Palmitylamine (70, MW = 241 g/mol)

GC-MS (EI, 70eV): m/z (rel. int, %): 39 (12), 41 (85), 42 (20), 43 (86), 44 (100), 45 (50), 53 (6), 54 (7), 55 (69), 56 (37), 57 (36), 58 (6), 59 (19), 67 (10), 68 (6), 69 (37), 70 (15), 71 (10), 72 (19), 73 (10), 82 (6), 83 (21), 84 (7), 85 (5), 86 (47), 87 (7), 97 (16), 98 (6), 100 (27), 111 (7), 114 (13), 128 (12), 142 (14), 156 (12), 170 (10), 184 (9), 198 (9), 212 (9), 226 (5), 240 (7), 241 (8).

N-Hexadecylacetamide (71, MW = 283 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 39 (5), 41 (38), 42 (10), 43 (70), 44 (19), 45 (5), 55 (30), 56 (12), 57 (20), 58 (9), 60 (32), 67 (5), 69 (15), 70 (6), 71 (6), 72 (69), 73 (100), 74 (5), 83 (8), 86 (49), 87 (30), 97 (5), 100 (47), 101 (19), 114 (59), 115 (11), 128 (28), 129 (7), 142 (22), 143 (5), 156 (22), 170 (18), 184 (14), 198 (15), 212 (14), 226 (15), 240 (19), 254 (11), 268 (40), 269 (8), 283 (39), 284 (8).

Hexadecyl acetate (72, MW = 284 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 39 (6), 41 (38), 42 (11), 43 (100), 54 (7), 55 (48), 56 (24), 57 (38), 61 (31), 67 (11), 68 (13), 69 (43), 70 (26), 71 (19), 81 (7), 82 (24), 83 (50), 84 (19), 85 (11), 96 (11), 97 (47), 98 (15), 110 (5), 111 (27), 112 (9), 125 (13), 126 (6), 196 (7), 224 (5), 284 (0.06).

N-Methylpalmitylamine (73, MW = 255 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 41 (8), 43 (8), 44 (100), 55 (6), 255 (3).

N-Hexadecyl-N-methylacetamide (74, MW = 298 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %):41 (9), 42 (4), 43 (16), 44 (39), 55 (7), 56 (3), 57 (6), 58 (4), 69 (3), 73 (3), 74 (5), 86 (33), 87 (25), 100 (9), 101 (3), 114 (9), 128 (5), 142 (4), 156 (5), 170 (5), 184 (4), 198 (3), 212 (4), 226 (4), 240 (4), 254 (6), 268 (3), 282 (100), 283 (20), 297 (3), 298 (1).

N,N-Dimethylpalmitylamine (75, MW = 270 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 41 (9), 43 (9), 44 (6), 55 (5), 58 (100), 59 (5), 269 (2), 270 (0.4).

N-Butyl-N-methylhexadecylamine (76, MW = 312 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 41 (8), 43 (10), 44 (8), 55 (5), 57 (7), 58 (30), 100 (89), 101 (6), 268 (100), 269 (21), 310 (5), 311 (5), 312 (1).

N,N-Dibutylhexadecylamine (77, MW = 354 g/mol)

N N

GC-MS (EI, 70eV): m/z (rel. int, %): 55 (5), 57 (7), 58 (5), 84 (3), 98 (4), 100 (15), 142 (59), 143 (6), 310 (100), 311 (23), 312 (3), 352 (4), 353 (3), 354 (0.6).

Palmitamide (78, MW = 255 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 39 (6), 41 (44), 43 (13), 55 (23), 57 (17), 59 (100), 69 (8), 72 (52), 73 (5), 86 (8), 114 (6), 128 (7), 212 (5), 255 (2).

N-Methylpalmitamide (79, MW = 269 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 39 (4), 41 (25), 42 (6), 43 (25), 45 (5), 55 (18), 56 (4), 57 (11), 58 (36), 69 (6), 71 (3), 73 (100), 74 (5), 83 (3), 84 (3), 86 (29), 87 (6), 100 (7), 114 (3), 128 (5), 142 (4), 226 (3), 269 (2).

N,N-Dimethylpalmitamide (80, MW = 283 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 41 (12), 42 (4), 43 (13), 44 (7), 45 (17), 46 (6), 55 (10), 57 (6), 69 (3), 72 (24), 87 (100), 88 (6), 100 (24), 101 (5), 114 (5), 142 (4), 283 (2).

¹H-NMR (400 MHz, methanol-d4): δ (ppm) = 3.08 (s, 3H, >N-C<u>H₃</u>), 2.94 (s, 3H, >N-C<u>H₃</u>), 2.39 (t, 2H, -C<u>H₂</u>-C(=O)-N<), 1.61 (quint, 2H, -(O=)C-CH₂-C<u>H₂-</u>), 1.40-1.26 (m, 24H, -(C<u>H₂)₁₂-</u>CH₃), 0.92 (t, 3H, -C<u>H₃</u>).

Methyl palmitate (81, MW = 270 g/mol)



¹H-NMR (400 MHz, methanol-d4): δ (ppm) = 3.64 (s, 3H, -O-C<u>H₃</u>), 2.30 (t, 2H, -C<u>H₂</u>-C(=O)-), 1.61 (quint, 2H, -(O=)C-CH₂-C(H₂-), 1.37-1.25 (m, 24H, -(C<u>H₂)₁₂-CH₃</u>), 0.92 (t, 3H, -C<u>H₃</u>).

Dipalmitylamine (82, MW = 466 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 43 (6), 57 (5), 70 (3), 240 (5), 252 (4), 254 (100), 255 (19), 268 (6), 464 (3), 465 (1), 466 (0.04).

N-Methylpalmitylamine (83, MW = 480 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 41 (3), 43 (7), 44 (4), 55 (3), 57 (5), 58 (11), 268 (100), 269 (20), 479 (1), 480 (0.2)

N-Palmitylpalmitamide (84, MW = 480 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 39 (5), 41 (47), 42 (13), 43 (100), 44 (12), 55 (35), 56 (14), 57 (67), 58 (7), 67 (5), 69 (19), 70 (7), 71 (21), 72 (10), 73 (18), 83 (11), 84 (7), 85 (11), 86 (15), 87 (9), 97 (7), 98 (6), 100 (13), 101 (6), 114 (18), 128 (8), 142 (7), 156 (6), 170 (5), 184 (5), 198 (5), 226 (5), 239 (6), 240 (9), 242 (8), 268 (23), 269 (6), 283 (28), 284 (7), 296 (40), 297 (9), 310 (9), 324 (6), 338 (8), 352 (9), 436 (6), 480 (8).

N-Butylpalmitamide (85, MW = 312 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 55 (14), 57 (23), 69 (6), 71 (5), 72 (6), 73 (23), 74 (8), 86 (8), 100 (18), 115 (100), 116 (8), 128 (30), 142 (6), 170 (6), 184 (6), 239 (5), 268 (8), 311 (8), 312 (2).

N,N-Dibutylpalmitamide (86, MW = 368 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 55 (12), 57 (19), 58 (10), 69 (5), 73 (6), 86 (7), 87 (24), 88 (5), 100 (6), 114 (100), 115 (7), 129 (30), 142 (26), 156 (5), 325 (6), 367 (0.0016975).

C18 alkyl products

Octadecane (87, MW = 254 g/mol)

GC-MS (EI, 70eV): m/z (rel. int, %): 39 (6), 41 (45), 42 (10), 43 (77), 55 (28), 56 (15), 57 (100), 58 (5), 69 (14), 70 (12), 71 (75), 83 (9), 84 (8), 85 (56), 97 (7), 98 (6), 99 (18), 112 (5), 113 (12), 127 (8), 141 (6), 254 (6).

Octadecylamine (88, MW = 270 g/mol)

GC-MS (EI, 70eV): m/z (rel. int, %): 39 (9), 41 (63), 42 (15), 43 (72), 44 (100), 45 (34), 54 (5), 55 (55), 56 (28), 57 (36), 58 (6), 59 (14), 67 (9), 68 (5), 69 (32), 70 (12), 71 (11), 72 (15), 73 (8), 82 (6), 83 (20), 84 (7), 85 (6), 86 (37), 87 (7), 97 (17), 100 (26), 111 (8), 114 (12), 128 (12), 142 (14), 156 (14), 170 (11), 184 (11), 198 (13), 212 (13), 226 (12), 240 (14), 254 (8), 268 (12), 269 (13), 270 (2).

N-Methyloctadecylamine (89, MW = 284 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 41 (8), 43 (11), 44 (100), 55 (7), 57 (6), 283 (5), 284 (1).

N,N-Dimethyloctadecylamine (90, MW = 298 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 41 (6), 43 (8), 55 (5), 58 (100), 296 (5), 297 (5), 298 (1).

Stearic acid (91, MW = 284 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 39 (11), 41 (77), 42 (17), 43 (95), 45 (10), 53 (6), 54 (6), 55 (81), 56 (19), 57 (76), 60 (83), 61 (23), 67 (11), 68 (8), 69 (49), 70 (13), 71 (45), 73 (100), 74 (10), 81 (9), 82 (8), 83 (38), 84 (15), 85 (32), 87 (26), 95 (6), 96 (8), 97 (33), 98 (17), 99 (13), 101 (10), 111 (15), 112 (6), 113 (7), 115 (21), 116 (10), 125 (7), 127 (5), 129 (69), 130 (8), 143 (12), 157 (7), 171 (17), 185 (46), 186 (7), 199 (16), 213 (6), 227 (15), 241 (53), 242 (10), 255 (9), 284 (70), 285 (15).

N-Methylstearamide (92, MW = 298 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 41 (12), 43 (15), 55 (11), 57 (9), 58 (21), 73 (100), 74 (6), 86 (28), 87 (6), 100 (7), 128 (6), 142 (6), 254 (5), 297 (4), 298 (0.8).

N,N-Dimethylstearamide (93, MW = 312 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 41 (10), 42 (3), 43 (13), 44 (5), 45 (13), 46 (6), 55 (9), 57 (6), 69 (3), 72 (21), 87 (100), 88 (5), 100 (23), 101 (4), 114 (5), 142 (4), 156 (3), 268 (3), 311 (5), 312 (2).

N-Methyloleamide (94, MW = 296 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 41 (23), 43 (15), 54 (6), 55 (27), 56 (5), 57 (9), 58 (40), 67 (11), 69 (12), 73 (100), 74 (6), 81 (8), 83 (7), 86 (78), 87 (13), 95 (5), 100 (12), 114 (7), 126 (7), 128 (12), 140 (14), 142 (11), 154 (7), 168 (8), 252 (5), 295 (15), 296 (3).

N,N-Dimethyloleamide (95, MW = 310 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 41 (18), 42 (5), 43 (13), 44 (9), 45 (17), 46 (17), 55 (21), 57 (6), 67 (9), 69 (8), 72 (46), 81 (6), 87 (100), 88 (6), 100 (77), 101 (13), 114 (12), 128 (5), 142 (12), 154 (5), 156 (16), 168 (5), 170 (5), 182 (7), 196 (7), 210 (10), 224 (10), 238 (6), 252 (5), 266 (6), 309 (42), 310 (11).

N-Methyllinoleamide (96, MW = 294 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 39 (8), 41 (34), 42 (5), 43 (12), 45 (5), 53 (7), 54 (12), 55 (37), 56 (5), 57 (7), 58 (60), 65 (5), 67 (41), 68 (9), 69 (16), 73 (100), 74 (8), 77 (11), 79 (27), 80 (11), 81 (29), 82 (8), 83 (8), 86 (62), 87 (11), 91 (9), 93 (10), 95 (18), 96 (7), 97 (5), 100 (12), 107 (6), 109 (10), 110 (5), 112 (5), 114 (11), 121 (6), 123 (5), 126 (7), 128 (13), 135 (6), 140 (16), 142 (10), 154 (6), 156 (6), 166 (5), 168 (5), 170 (5), 180 (5), 184 (6), 194 (5), 207 (5), 293 (26), 294 (6).

N,N-Dimethyllinoleamide (97, MW = 308 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 41 (19), 42 (5), 43 (7), 44 (12), 45 (19), 46 (29), 54 (5), 55 (22), 67 (22), 69 (7), 72 (52), 77 (6), 79 (15), 80 (6), 81 (14), 87 (100), 88 (6), 91 (5), 93 (5), 95 (8), 100 (64), 101 (10), 114 (11), 128 (7), 142 (11), 154 (5), 156 (10), 196 (11), 210 (6), 307 (39), 308 (10), 309 (5).

C20 alkyl products

Icosane (98, MW = 283 g/mol)

GC-MS (EI, 70eV): m/z (rel. int, %): 41 (39), 42 (9), 43 (73), 55 (27), 56 (14), 57 (100), 69 (15), 70 (12), 71 (76), 83 (11), 84 (8), 85 (57), 97 (9), 98 (6), 99 (21), 111 (5), 112 (5), 113 (13), 126 (5), 127 (10), 141 (7), 155 (5), 282 (6), 283 (1).

lcosanylamine (99, MW = 298 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 39 (7), 41 (46), 42 (11), 43 (65), 44 (100), 45 (33), 54 (5), 55 (50), 56 (26), 57 (41), 58 (5), 59 (14), 65 (7), 67 (7), 69 (29), 70 (13), 71 (12), 72 (17), 73 (5), 83 (20), 84 (6), 86 (39), 87 (7), 91 (45), 92 (6), 100 (26), 111 (5), 114 (13), 128 (12), 142 (16), 156 (14), 170 (13), 184 (14), 196 (12), 198 (17), 210 (16), 212 (16), 226 (17), 240 (16), 254 (16), 268 (16), 282 (6), 287 (13), 296 (15), 297 (17), 298 (3).

N-Methylicosanylamine (100, MW = 312 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 41 (8), 43 (11), 44 (100), 55 (7), 57 (7), 58 (6), 311 (5), 312 (1).

N,N-Dimethylicosanylamine (101, MW = 326 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 41 (6), 43 (9), 44 (6), 55 (5), 57 (5), 58 (100), 324 (6), 325 (5), 326 (1).

Eicosanoic acid (Arachidic acid) (102, MW = 313 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 39 (8), 41 (66), 42 (15), 43 (99), 45 (6), 54 (6), 55 (81), 56 (19), 57 (85), 58 (5), 60 (81), 61 (25), 67 (12), 68 (8), 69 (53), 70 (13), 71 (53), 73 (99), 74 (10), 81 (13), 82 (10), 83 (46), 84 (15), 85 (36), 87 (18), 95 (7), 96 (9), 97 (39), 98 (19), 99 (13), 101 (12), 111 (18), 112 (6), 113 (7), 115 (21), 116 (11), 125 (10), 127 (5), 129 (70), 130 (8), 143 (9), 157 (13), 171 (21), 185 (26), 199 (9), 213 (29), 227 (22), 241 (12), 255 (10), 269 (52), 270 (9), 281 (10), 283 (10), 312 (100), 313 (21).

N-Methylicosanamide (103, MW = 326 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 41 (9), 43 (15), 55 (9), 57 (9), 58 (18), 69 (4), 71 (4), 73 (100), 74 (6), 83 (3), 84 (3), 86 (28), 100 (6), 114 (3), 128 (6), 142 (7), 296 (3), 325 (6), 326 (1).

N,N-Dimethylicosanamide (104, MW = 340 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 41 (9), 42 (3), 43 (13), 44 (5), 45 (12), 46 (6), 55 (9), 57 (7), 69 (4), 72 (19), 87 (100), 88 (5), 100 (22), 101 (4), 114 (5), 142 (4), 156 (3), 296 (3), 338 (3), 339 (5), 340 (2).

C22 alkyl products

Docosane (105, MW = 311 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 41 (36), 42 (8), 43 (72), 55 (27), 56 (14), 57 (100), 58 (5), 69 (16), 70 (12), 71 (76), 83 (13), 84 (8), 85 (61), 97 (11), 98 (6), 99 (23), 111 (6), 112 (5), 113 (15), 126 (5), 127 (11), 141 (9), 155 (7), 169 (5), 310 (6), 311 (2).

N-Methyldocosanylamine (106, MW = 340 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 41 (12), 42 (5), 43 (17), 44 (100), 45 (3), 55 (11), 56 (4), 57 (10), 58 (75), 59 (4), 69 (5), 70 (3), 71 (6), 281 (3), 283 (3), 338 (4), 339 (6), 340 (1).

N,N-Dimethyldocosanylamine (107, MW = 354 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 41 (6), 43 (10), 44 (14), 55 (6), 57 (7), 58 (100), 352 (10), 353 (7), 354 (2).

N-Methyldocosanamide (108, MW = 354 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 41 (10), 43 (16), 55 (10), 57 (11), 58 (16), 69 (5), 71 (4), 73 (100), 74 (6), 83 (3), 86 (28), 87 (5), 100 (6), 114 (3), 128 (6), 142 (7), 207 (4), 310 (7), 324 (4), 353 (8), 354 (2).

N,N-Dimethyldocosanamide (109, MW = 368 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 41 (7), 43 (12), 44 (4), 45 (10), 46 (6), 55 (8), 57 (8), 69 (4), 71 (3), 72 (17), 87 (100), 88 (5), 100 (21), 101 (4), 114 (5), 142 (4), 156 (3), 324 (4), 366 (4), 367 (6), 368 (2).

C24 alkyl products

Tetracosane (110, MW = 339 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 41 (32), 42 (8), 43 (70), 55 (28), 56 (14), 57 (100), 69 (18), 70 (11), 71 (77), 83 (14), 84 (8), 85 (61), 97 (13), 98 (6), 99 (22), 111 (7), 112 (5), 113 (15), 126 (5), 127 (11), 141 (9), 155 (7), 169 (6), 281 (5), 338 (5), 339 (1).

N,N-Dimethyltetracosanylamine (111, MW = 382 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 41 (6), 43 (10), 44 (17), 55 (6), 57 (8), 58 (100), 59 (4), 69 (3), 71 (3), 366 (3), 380 (12), 381 (7), 382 (2).

N-Methyltetracosanamide (112, MW = 382 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 41 (8), 43 (16), 55 (11), 56 (3), 57 (14), 58 (16), 69 (6), 71 (5), 73 (100), 74 (6), 83 (4), 85 (3), 86 (31), 87 (6), 100 (7), 114 (3), 128 (6), 142 (8), 338 (8), 352 (4), 381 (10), 382 (3).

N,N-Dimethyltetracosanamide (113, MW = 396 g/mol)



GC-MS (EI, 70eV): m/z (rel. int, %): 41 (6), 43 (12), 44 (4), 45 (9), 46 (6), 55 (8), 57 (9), 69 (4), 71 (3), 72 (15), 87 (100), 88 (5), 100 (20), 101 (4), 114 (4), 142 (4), 156 (3), 352 (4), 394 (4), 395 (6), 396 (2).

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