Supplementary information

Direct electrochemical amidation of fatty acids with ammonia in liquefied ammonia

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1. *Experimental*

All reagents used in this work were purchased from Tokyo Chemical Industry and Fujifilm Wako Pure Chemicals. Liquefied ammonia was purchased from Resonac. The electrolysis in liquefied ammonia was carried out in a pressure-resistant undivided electrochemical cell (HPG-96-1, Taiatsu Techno Inc., Figure S1(a)) at ambient temperature. First, the substrates and supporting electrolyte were added into the cell, and the cell was sealed up. After N_2 purging, liquefied ammonia was transferred into the cell from the liquefied ammonia cylinder by partially vaporizing liquefied ammonia in the cell and reducing the cell pressure. The electrolyte was stirred during electrolysis. The electrolyte temperature was not controlled in this work. The cell pressure before the electrolysis was approximately 0.85 MPa. An H-type cell, which is the stainless cell we originally produced, was also used to investigate the reaction pathway, as illustrated in Figure S1(b). In the cell, the anolyte and catholyte were fully separated by a 0.5 µm-pore filter (SS-4FWS-05, Swagelok). The anode and cathode were platinum (Pt) mesh electrodes (Nilaco, 99.95%). The Pt mesh was cut into 2 cm × 1 cm pieces and positioned such that the immersed geometric area was 2 cm^2. For electrochemical measurements, the working electrode, counter electrode, and quasi-reference electrode were a Pt disk electrode ($\phi = 3$ mm, Pt-6380, EC Frontier), Pt mesh, and Pt wire ($\phi = 0.3$ mm, Nilaco, 99.95%), respectively. All electrodes were sonicated in ultrapure water (Milli-Q) and acetone before use. A DC power supply (PWR-401MH, Kikusui Electronics) was used for electrolysis, and a potentio-galvanostat (SP-50, Bio-Logic) was used for electrochemical measurements. After electrolysis, the cell was gradually vented to the atmosphere to evaporate ammonia. The products were extracted with ethyl acetate according to the procedure reported in our previous paper[1]. The products were analysed by GC-MS (GCMS-QP2010 SE, Shimadzu) with a DB-5MS column (30 m × 0.25 mm × 0.25µm, Agilent Technologies).

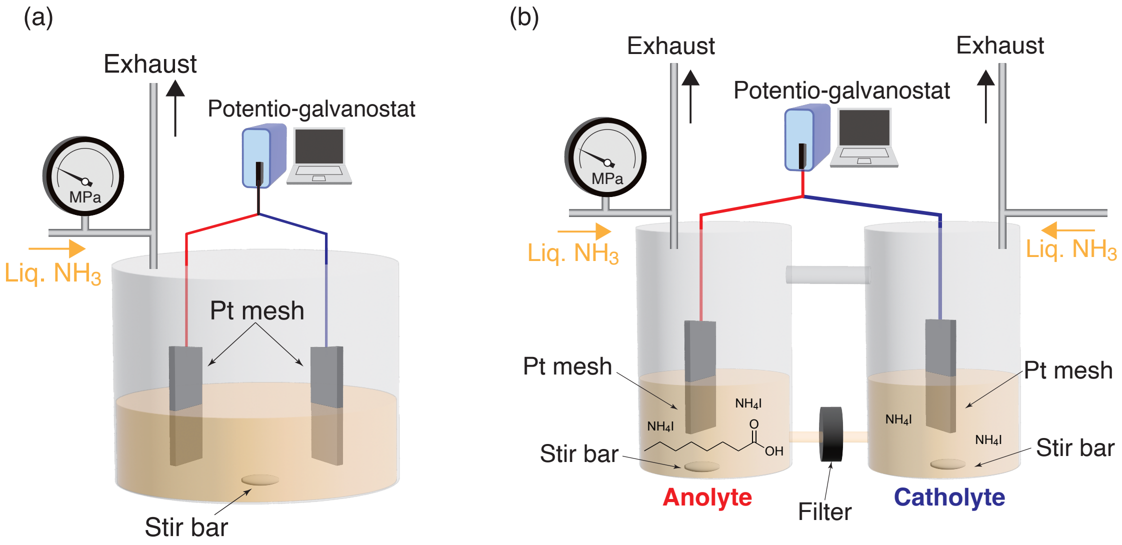

Figure S1 Schematics of pressure-resistance (a) undivided electrochemical cell and (b) H-type cell for liquefied ammonia.

2. *Electrolysis products in various conditions*

To confirm the effects of solvents, constant-voltage electrolysis was conducted in 0.1 M octanoic acid. The applied voltage was 5 V in aqueous solutions (aq. NaOH), whereas 50 V was applied in liquefied ammonia (liq. NH_3) owing to the low conductivity of the electrolyte.

The obtained products were summarised in Table S1. The peaks other than amide and nitriles were also detected in GC-MS, but the peaks could not be identified since the intensity was quite low. The investigation of such minor side reactions will be discussed in future works.

Table S1. The experimental details and products by the electrolysis of octanoic acid. All experiments were conducted as a constant-voltage electrolysis. The electrolyte was 0.1 M octanoic acid without supporting electrolytes.

Solvents	Applied voltage / V	Current / mA	Products
Aq. NaOH	5	37	Heptanal 1-heptanol Tetradecane
Liq. NH_3	50	89	Octanamide Octanenitrile Heptanenitrile

The obtained products by the electrolysis in various substrates and supporting electrolytes were summarised in Table S2. Constant-current electrolysis was conducted in 0.1 M substrates + 0.2 M supporting electrolytes.

Table S2 Electrolysis products in various conditions. The electrolysis was conducted as a constant-current electrolysis in an undivided cell shown in Figure S1(a). The concentrations of substrates and supporting electrolytes were 0.1 M and 0.2 M, respectively.

Entry	Electrolyte			Applied current / mA	Products
	Solvent	Substrate	Supporting electrolyte		
1	Liq. NH_3	Octanamide	NH_4I	300	Not detected
2	Liq. NH_3	Octanenitrile	NH_4I	300	Not detected
3	Liq. NH_3	Octanoic acid	KI	50	Octanamide Octanenitrile Heptanenitrile
4	Liq. NH_3	Octanoic acid	Cs_2CO_3	300	Octanamide Octanenitrile Heptanenitrile
5	Liq. NH_3	Octanoic acid	–	50	Octanamide Octanenitrile Heptanenitrile

3. Calculation of selectivity and production rate of the electrolysis products

The moles of the electrolysis products were calculated from the GC-MS results. The calibration curves were measured using the purchased standard samples. The geometric surface area of the electrode was 2 cm^2. The duration of the electrolysis was 2 h.

Selectivity / % =

(moles of the product) × 100 / (total moles of products)

Production rate / $\mu mol\ cm^{-2}\ h^{-1}$ =

(moles of the product) / [(surface area of the electrode) × (duration of the electrolysis)]

4. Voltage-time and current-time curves of the electrolysis

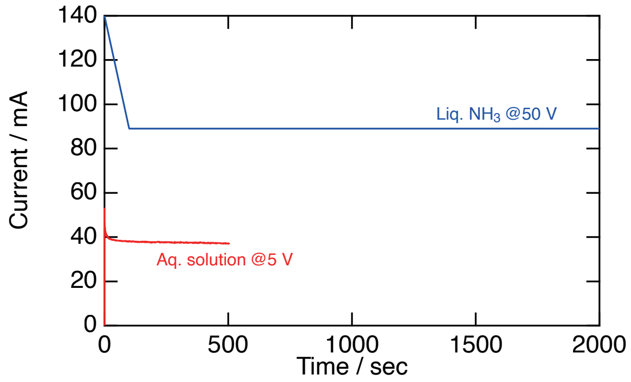

Figure S2 Current-time curve of the constant-voltage electrolysis in aqueous solution and liquefied ammonia. The electrolytes were 0.1 M octanoic acid in 0.1 M NaOH aqueous solution and 0.1 M octanoic acid in liquefied ammonia. Due to the high solution resistance of liquefied ammonia, the applied voltage was set to 50 V to obtain enough current.

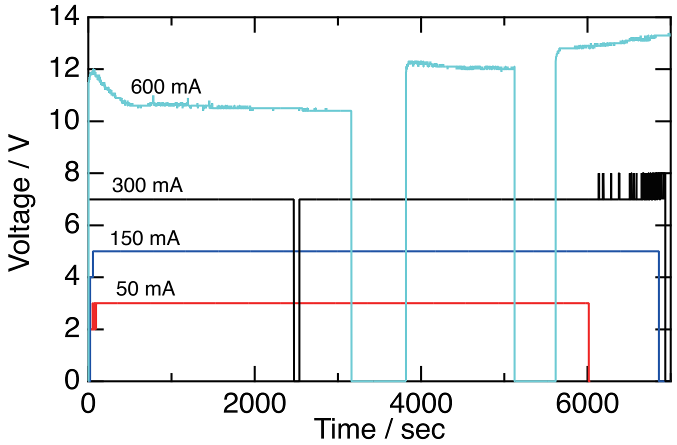

Figure S3 Voltage-time curve of the constant-current electrolysis in Figure 1. During the electrolysis, the cell pressure gradually increased due to the increment of the electrolyte temperature. When the cell pressure was over 1 MPa, the electrolysis was temporarily stopped, and the pressure was released.

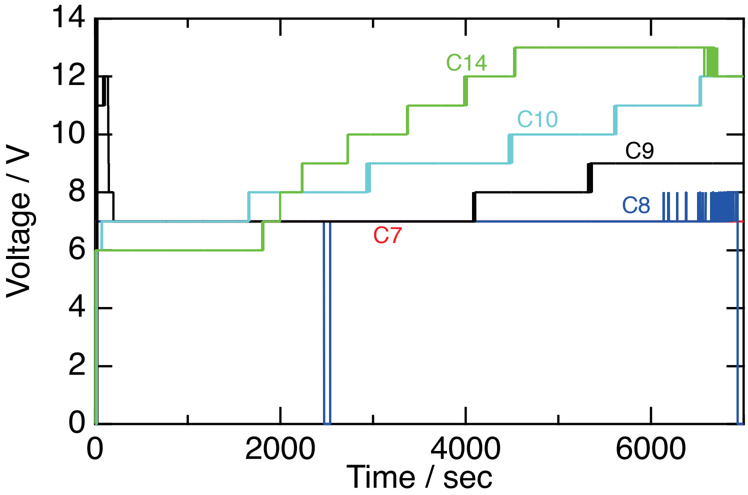

Figure S4 Voltage-time curve of the constant-current electrolysis in Figure 3. In the case of C7, the applied voltage was 7 V. The applied voltage gradually increases during the electrolysis with an increment in the number of carbon atoms in fatty acid. The reason for this increase remains unknown. This should be due to the higher viscosity and lower conductivity of fatty acids with longer carbon chain lengths.

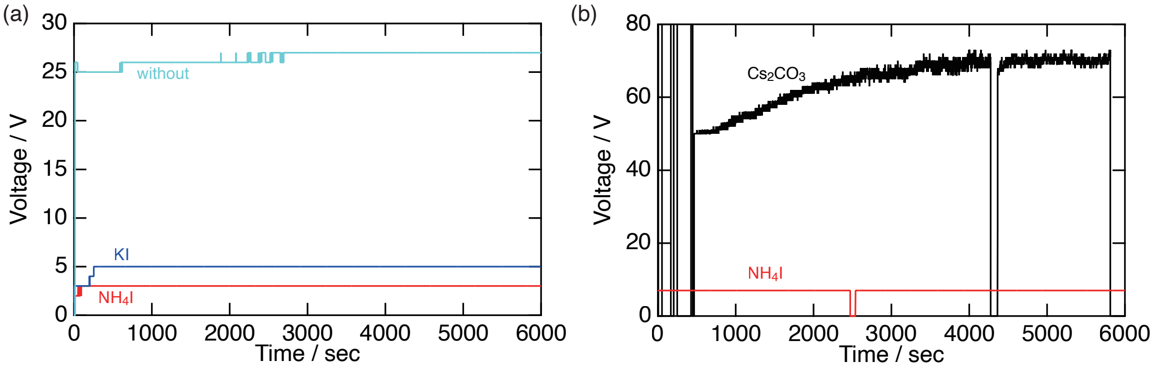

Figure S5 Voltage-time curve of the constant-current electrolysis at (a) 50 mA and (b) 300 mA with various supporting electrolytes. Since Cs_2CO_3 was not soluble enough in liquefied ammonia, the applied voltage was high due to its low conductivity.

5. The reaction of octanoyl chloride in liquefied ammonia

Octanoyl chloride is often used as a carboxylic acid derivative to produce an amide via nucleophilic substitution. We confirmed the reaction of acid chloride in liquefied ammonia in the following conditions: 1. Electrolysis in liquefied ammonia, 2. Stirring in liquefied ammonia without electrolysis, and 3. Stirring in aqueous ammonia without electrolysis. Table S3 indicates that octanenitrile was obtained in liquefied ammonia, but not in aqueous ammonia.

In addition, heptanenitrile, which is detected in the electrolysis of octanoic acid in liquefied ammonia, was not obtained in all conditions. Thus, octanamide is synthesised from acid chloride in both aqueous and liquefied ammonia via nucleophilic substitution. Octanenitrile is chemically produced only in liquefied ammonia. Heptanenitrile is produced only by the electrolysis of octanoic acid in liquefied ammonia, which suggests that heptanenitrile comes from Kolbe reaction in liquefied ammonia (detailed discussion is shown in Figure 3). These results are summarised in Figure S3.

Table S3 The reaction of octanoyl chloride in aqueous and liquefied ammonia. The electrolyte contains 0.1 M octanoly chloride.

Entry	Solvents	Supporting electrolyte	Applied current / mA	Selectivity / %	
				octanamide	octanenitrile
1	Liq. NH_3	NH_4I	300	90.3	9.7
2	Liq. NH_3	NH_4I	–	94.0	6.0
3	Aq. NH_3	NH_4I	–	100	Not detected

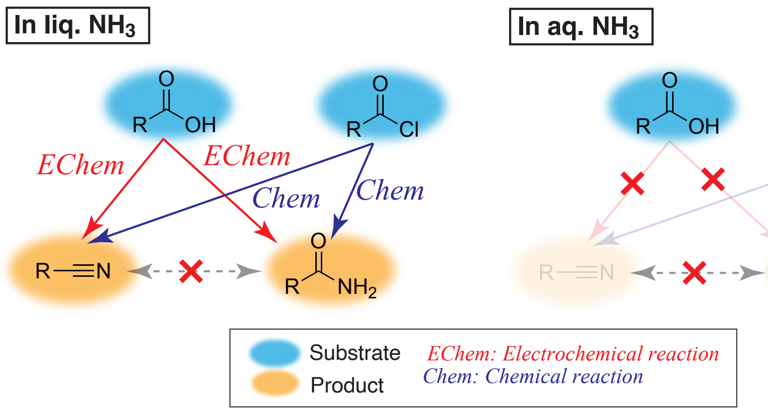

Figure S6 Summary of the octanoyl chloride reactions in liquefied and aqueous ammonia.

6. *Electrochemical reactions on the anode and cathode*

Anode

$$R_n\text{-}COOH + 4NH_3 \rightarrow R_n\text{-}CONH_2 + NH_2OH + 2NH_4^+ + 2e^- \quad (1)$$

$$R_n\text{-}COOH + 4NH_3 \rightarrow R_n\text{-}CN + NH_2OH + H_2O + 2NH_4^+ + 2e^- \quad (2)$$

$$R_{n-1}\text{-}CH_2COOH + 7NH_3 \rightarrow R_{n-1}\text{-}CN + 6NH_4^+ + CO_2 + 6e^- \quad (3)$$

$$8NH_3 \rightarrow N_2 + 6NH_4^+ + 6e^- \quad (4)$$

Cathode

$$2NH_4^+ + 2e^- \rightarrow H_2 + 2NH_3 \quad (5)$$

Hydroxylamine, water, and carbon dioxide are produced in addition to nitriles and amides in liquefied ammonia.

7. *Cyclic voltammograms (CVs) of octanoic acid in liquefied ammonia*

CVs were measured in the electrolyte with and without octanoic acid. The electrolytes were 0.1 M octanoic acid + 0.2 M tetrabutylammonium perchlorate ($TBAClO_4$), 0.2 M $TBAClO_4$, and 0.2 M NH_4I. Scan rate was 100 mV s^{-1}. Only in the case that NH_4I was a supporting electrolyte, redox reaction of I^-/I_2 additionally occurred.

Although the onset potential of H_2 evolution was positively shifted with an increment of NH_4^+ concentration from Nernst equation, that of N_2 evolution was not. This is because the overpotential of N_2 evolution on the Pt electrode was effectively higher than the concentration effect[2].

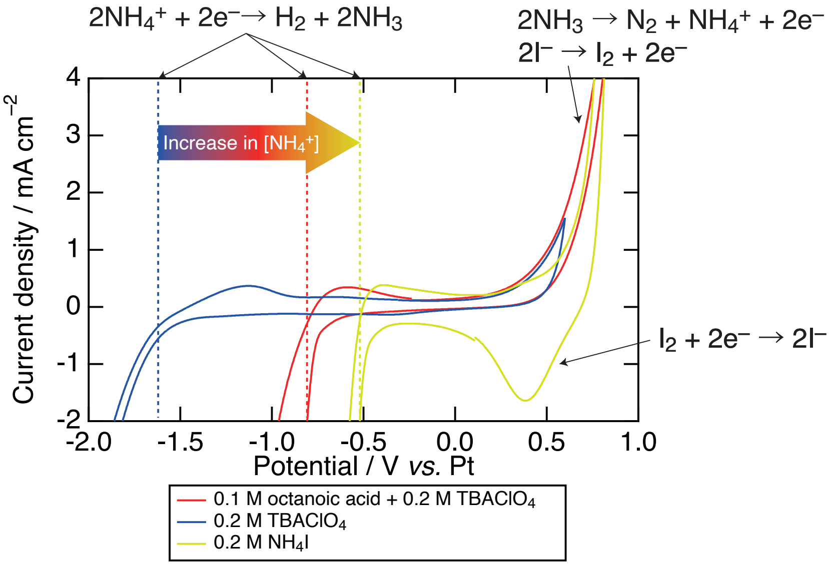

Figure S7 CVs of the electrolyte with and without octanoic acid. The electrolytes were 0.1 M octanoic acid + 0.2 M tetrabutylammonium perchlorate ($TBAClO_4$), 0.2 M $TBAClO_4$, and 0.2 M NH_4I. Scan rate was 100 mV s^{-1}.

8. *Effective utilisation of hydroxylamine*

Constant-current electrolysis of 300 mA was conducted for 2h in the electrolyte, which consisted of 0.1 M octanoic acid, 0.2 M acetone, and 0.2 M NH_4I in liquefied ammonia. Triacetoneamine is formed through the aldol condensation of acetone and ammonia[3]. Figure S4 shows the overall reaction of fatty acids with acetone in liquefied ammonia. Hydrogen evolution occurred at the cathode. In the anodic reaction, nitrile **3b** and *O*-acyl hydroxylamine **5** were produced through radical coupling, followed by the formation of amide **3a** and nitrile

3c through nucleophilic ammonia addition and hydroxylamine elimination. In parallel with this reaction, triacetoneamine **(6)** was synthesised from acetone and ammonia. Through the reaction of 6 with hydroxylamine, oxime **7** was also obtained. This result suggests that hydroxylamine, a byproduct of fatty acid electrolysis, can be used effectively as a reactive reagent in organic synthesis.

Thus, oxime **7** was synthesised from triacetoneamine using acetone, ammonia, and hydroxylamine derived from the electrolysis of octanoic acid in liquefied ammonia.

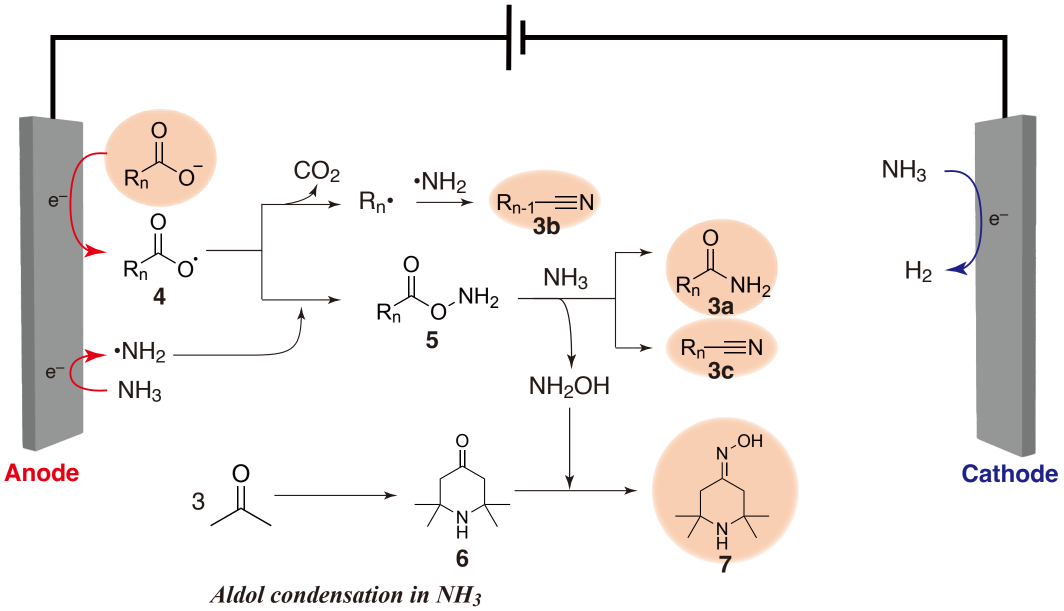

Figure S8 Overall reaction of the electrolysis of fatty acid and acetone. By the effective use of hydroxylamine produced by the electrolysis of fatty acid, oxime **7** is obtained in addition to amide and nitriles. The numbering of compounds is shown in Figure 2.

9. Faradaic efficiency of this reaction

From the overall reaction discussed above, the amidation of fatty acid should be a 2-electron reaction (Equation 1). Thus, the Faradaic efficiency of the amidation is described as follows (F means Faraday constant).

Faradaic efficiency / % =

$2F$ × (moles of amide) × 100 / (total charge passed)

The effects of the applied current, supporting electrolytes, and the number of carbon atoms in fatty acids on Faradaic efficiency are summarised in Tables S4, S5, and S6, respectively.

Table S4 Faradaic efficiency of the electrochemical amidation of octanoic acid. The electrolyte was 0.1 M octanoic acid and 0.2 M NH_4I.

Applied current / mA	Faradaic efficiency / %
0	–
50	0.30
150	0.19
300	0.27
600	0.44

Table S5 Faradaic efficiency of the electrochemical amidation of octanoic acid with various supporting electrolytes. The electrolyte was 0.1 M octanoic acid and 0.2 M supporting electrolytes.

Supporting electrolytes	Applied current / mA	Faradaic efficiency / %
–	50	0.30
NH_4I	300	0.27
KI	50	0.49
Cs_2CO_3	300	0.24

Table S6 Faradaic efficiency of the electrochemical amidation of fatty acids with various carbon chain length. Applied current was set to 300 mA.

Number of carbon atoms in fatty acids	Faradaic efficiency / %
C7	0.35
C8	0.27
C9	0.25
C10	0.22
C14	0.28

Since the ammonia oxidation to N_2 inevitably occurs to produce NH_2 radical, Faradaic efficiency of this reaction is low. To improve the efficiency, the detailed investigation of applied voltage and temperature should be conducted to control the radical production and reaction in future work. In addition, the actual efficiency should be improved by the effective utilization of H_2 evolved from cathode.

Table S5 suggests that supporting electrolytes has little effects on Faradaic efficiency. In the case with iodide as a supporting electrolyte, iodide oxidation and reduction should occurs in addition to the H_2 and N_2 evolution from NH_3. However, there is no difference with Faradaic efficiency among the supporting electrolytes. This also suggests that iodine-related reaction has no impact on this reaction.

Moreover, the carbon chain length of fatty acids has also little effects on Faradaic efficiency. Thus, this reaction can be effectively applied to longer fatty acids, up to C14.

10. Estimation of the energy consumption of this reaction

The energy consumption (P) of the amide synthesis is calculated the following equation.

$$P = \frac{1}{n_p} \int VIdt$$

where, V, I, t, and n_p are applied voltage, applied current, time, and mole of the produced fatty amide, respectively. In addition, n_p is described as the following equation.

$$n_p = \frac{\alpha \int Idt}{2F}$$

α means the Faradaic efficiency. Thus,

$$P = \frac{2F \int Vdt}{\alpha \int dt}$$

since I was constant in the constant-current electrolysis. Table S7, S8, and S9 summarises the energy consumption.

The high energy consumption of the amidation comes from the low Faradaic efficiency, high applied current and voltage. The current and voltage strongly depends on the solution resistance, the distance between anode and cathode, and so on. To improve the energy consumption, the optimisation of the experimental setup should be conducted. This point is our future work.

Table S7 Energy consumption of the electrochemical amidation of octanoic acid. The electrolyte was 0.1 M octanoic acid and 0.2 M NH_4I.

Applied current / mA	Energy consumption / kWh mol^{-1}
0	–
50	54.5
150	135.4
300	133.7
600	126.0

Table S8 Energy consumption of the electrochemical amidation of octanoic acid with various supporting electrolytes. The electrolyte was 0.1 M octanoic acid and 0.2 M supporting electrolytes.

Supporting electrolytes	Applied current / mA	Energy consumption / kWh mol^{-1}
–	50	474.6
NH_4I	300	133.7
KI	50	54.3
Cs_2CO_3	300	1219.4

Table S9 Energy consumption of the electrochemical amidation of fatty acids with various carbon chain length.

Number of carbon atoms in fatty acids	Energy consumption / kWh mol^{-1}
C7	105.9
C8	133.7
C9	166.8
C10	228.1
C14	194.2

11. Computational details

The quantum chemical studies were conducted by density functional theory (DFT) using quantum chemical calculation software GAMESS[4]. The DFT functional used was B3LYP. The basis set was 6-31+G**. The geometries of all species were optimized, and vibrational frequencies analysis was conducted to confirm all stable species have no imaginary frequency and all transition states (TSs) have one imaginary frequency. In addition, to verify the route from reactant to TS and from TS to product, the intrinsic reaction coordinate (IRC) calculation was also conducted. Solvent effects were evaluated by using a polarizable continuum model (PCM). Since the dataset of liquefied ammonia for PCM was not installed in the software, we employed the static dielectric constant of 16.6 and the solvent radium of 2.5 Å[5].

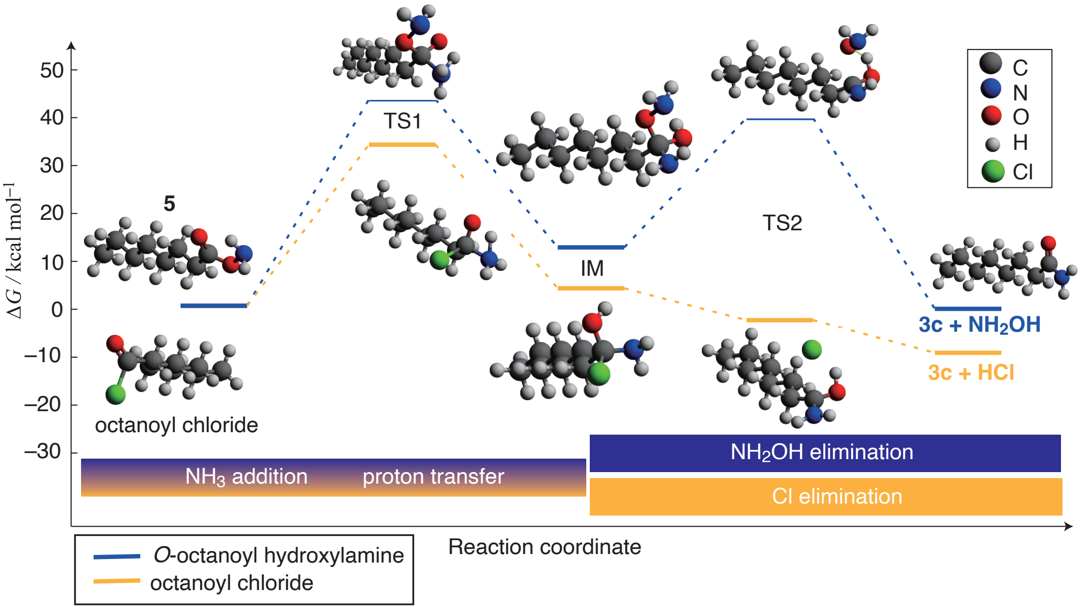

Figure S9 Calculated free energy diagram of octanamide synthesis from O-octanoyl hydroxylamine and octanoyl chloride. TS and IM indicate transition state and intermediate, respectively. The suggested route was verified by the intrinsic reaction coordinate (IRC) calculation. This calculation confirmed that the amide synthesis from *O*-octanoyl hydroxylamine occurred via NH_3 addition, proton transfer, and elimination of the leaving group in the same with octanoyl chloride.

Optimized geometries

O-octanoyl hydroxylamine

ATOM	CHARGE	X	Y	Z
C	6	-10.898596	2.39727478	-0.0562493
C	6	-9.3653677	2.38993906	-0.022411
H	1	-11.278336	1.85994364	-0.9353258
H	1	-11.294366	3.41980973	-0.0942836
H	1	-11.317555	1.91191447	0.83522198
H	1	-8.977799	2.9125506	-0.9096232
C	6	-8.7687815	0.97641563	0.03455812
H	1	-9.0164349	2.9662162	0.8474414
H	1	-9.1199052	0.39973083	-0.8353262
H	1	-9.1595751	0.45547959	0.92280386
C	6	-7.2342193	0.95364488	0.06953932
H	1	-6.8428244	1.46935781	-0.8208547
C	6	-6.6476558	-0.4639698	0.13378308
H	1	-6.8819849	1.53258295	0.93704935
H	1	-7.0064084	-1.0438967	-0.7306526
H	1	-7.0363285	-0.9766001	1.02773364
C	6	-5.1133638	-0.4877829	0.16216823
H	1	-4.7178298	0.01721387	-0.7300368
C	6	-4.5574697	-1.9171361	0.22107289
H	1	-4.7437766	0.07966109	1.02503763
H	1	-4.8888864	-2.5120419	-0.6379322
H	1	-4.9358249	-2.4346164	1.11596742
C	6	-3.0468426	-1.9690876	0.29284225
O	8	-2.5842864	-3.1493825	-0.1939223
O	8	-2.3117445	-1.1027029	0.72755511
N	7	-1.1390431	-3.277707	-0.2024991
H	1	-0.9850002	-4.0472838	0.45233031
H	1	-0.8100828	-2.420613	0.25779267

TS1 of *O*-octanoyl hydroxylamine

ATOM	CHARGE	X	Y	Z
C	6	-5.0949766	3.80996182	0.34424179
C	6	-3.5922574	3.54625053	0.18017158
H	1	-5.6735476	3.31616964	-0.4484765
H	1	-5.3202459	4.88297127	0.30302972
H	1	-5.4612891	3.42842762	1.30716184
H	1	-3.2464952	3.97559257	-0.7725164

C	6	-3.2296881	2.05495643	0.22037748
H	1	-3.0397648	4.07520181	0.97190093
H	1	-3.7716762	1.52927542	-0.5823427
H	1	-3.5903002	1.62035497	1.16676451
C	6	-1.7241786	1.78548725	0.0776705
H	1	-1.3594755	2.24098271	-0.8564835
C	6	-1.360935	0.29390293	0.08099543
H	1	-1.186371	2.29282659	0.8943076
H	1	-1.8899095	-0.2080432	-0.7450261
H	1	-1.7330923	-0.1686853	1.00934284
C	6	0.14788702	0.04151336	-0.0543949
H	1	0.52578348	0.50891071	-0.9729772
C	6	0.50091443	-1.4510865	-0.0981095
H	1	0.67844611	0.51462669	0.78245601
H	1	-0.0669701	-1.9319416	-0.9069257
H	1	0.22591519	-1.9437547	0.84485679
C	6	1.98398444	-1.6906314	-0.3919381
O	8	2.6916613	-1.3414909	0.78543865
O	8	2.48316906	-1.19881	-1.5473465
N	7	4.1131182	-1.5687529	0.57518512
H	1	4.49250015	-1.2453719	1.46536411
H	1	4.37252487	-0.8728126	-0.1317444
N	7	2.28674307	-3.2052684	-0.7429653
H	1	1.48908709	-3.8418341	-0.7750614
H	1	3.04650124	-3.5755345	-0.1673994
H	1	2.63979597	-2.5296786	-1.7138438

IM of *O*-octanoyl hydroxylamine

ATOM	CHARGE	X	Y	Z
C	6	-10.680419	2.64339503	0.3487394
C	6	-9.1587308	2.47338743	0.25767579
H	1	-11.176889	2.26374055	-0.5540409
H	1	-10.958742	3.69840305	0.46350042
H	1	-11.090723	2.09560005	1.20744743
H	1	-8.7761298	3.06293736	-0.588813
C	6	-8.7201061	1.01121317	0.09587303
H	1	-8.6889165	2.89351715	1.15945686
H	1	-9.1870104	0.58978705	-0.8078031

H	1	-9.1085713	0.42224256	0.94150111
C	6	-7.1979428	0.82910295	0.01415362
H	1	-6.8088541	1.40254198	-0.8415237
C	6	-6.7647729	-0.6378083	-0.1147713
H	1	-6.7324872	1.26558378	0.91134612
H	1	-7.214385	-1.07358	-1.0198666
H	1	-7.1716076	-1.2087079	0.73419962
C	6	-5.2401104	-0.8248386	-0.1574381
H	1	-4.8454409	-0.2701872	-1.0234762
C	6	-4.8354392	-2.3031469	-0.2537911
H	1	-4.7935079	-0.3751548	0.73831401
H	1	-5.2322129	-2.7449276	-1.1745798
H	1	-5.2776942	-2.8524231	0.58845461
C	6	-3.3251024	-2.5863227	-0.2572516
O	8	-2.8467496	-1.9968747	0.99166314
O	8	-2.6431214	-1.977114	-1.3337987
N	7	-1.4729149	-2.3674589	1.23084151
H	1	-1.4599805	-2.5372021	2.23717308
H	1	-0.940699	-1.5081909	1.07726616
N	7	-3.0681804	-3.9857034	-0.3874524
H	1	-3.4984328	-4.4902556	0.38445012
H	1	-2.0620619	-4.14084	-0.3458617
H	1	-2.7672704	-1.0179265	-1.253226

TS2 of *O*-octanoyl hydroxylamine

ATOM	CHARGE	X	Y	Z
C	6	-5.2357659	3.53913732	0.42222429
C	6	-3.7197341	3.32915605	0.32190165
H	1	-5.7417842	3.2310756	-0.5026635
H	1	-5.483926	4.59287706	0.60152916
H	1	-5.6637475	2.95156517	1.24540529
H	1	-3.3162407	3.95984665	-0.4842676
C	6	-3.3264003	1.86715871	0.06704159
H	1	-3.2414986	3.67723275	1.24974907
H	1	-3.7972471	1.52332067	-0.8674377
H	1	-3.7430262	1.23629456	0.86799623
C	6	-1.810503	1.63922134	-0.0156452
H	1	-1.391025	2.26531912	-0.8179859
C	6	-1.4279844	0.17296293	-0.2631512
H	1	-1.3404958	1.98396862	0.91806874
H	1	-1.8830908	-0.1658851	-1.2073899

H	1	-1.8687706	-0.4518119	0.52976247
C	6	0.08838341	-0.059248	-0.3110447
H	1	0.53299349	0.54718972	-1.1100287
C	6	0.43629414	-1.5342237	-0.5516995
H	1	0.55314716	0.26280386	0.62799347
H	1	-0.0086573	-1.8648527	-1.505319
H	1	-0.0019098	-2.1642353	0.23337134
C	6	1.90997662	-1.8279322	-0.664483
O	8	2.82308658	-0.6854214	0.92252868
O	8	2.69737551	-1.0303093	-1.3797698
N	7	3.81971046	-1.5457839	1.46804444
H	1	3.67186409	-1.524384	2.48042977
H	1	4.71935801	-1.0796477	1.32196615
N	7	2.33837547	-3.0740806	-0.4243079
H	1	1.79885792	-3.6350468	0.22490664
H	1	3.34530259	-3.1669679	-0.3064327
H	1	3.06078273	-0.5277986	-0.4830118

octanamide

ATOM	CHARGE	X	Y	Z
C	6	-10.939725	2.50558319	0.00016043
C	6	-9.4072959	2.46731933	0.04391127
H	1	-11.323119	2.02613491	-0.9102791
H	1	-11.317151	3.53568539	0.01667965
H	1	-11.374228	1.97860603	0.85999233
H	1	-9.0036447	3.03019622	-0.810858
C	6	-8.8371362	1.04177614	0.0269573
H	1	-9.054576	2.98884502	0.94615691
H	1	-9.1932536	0.5217528	-0.8763338
H	1	-9.2438961	0.47961949	0.88218983
C	6	-7.3040415	0.98694833	0.07027224
H	1	-6.8956945	1.54710663	-0.7848878
C	6	-6.7441533	-0.4429677	0.05252572
H	1	-6.9473788	1.50609727	0.97311991
H	1	-7.1034735	-0.9595982	-0.8515359
H	1	-7.1566577	-1.0025008	0.90703023
C	6	-5.2116203	-0.500121	0.09740255
H	1	-4.7881504	0.04991863	-0.7519772
C	6	-4.6793289	-1.9358925	0.07919786
H	1	-4.8447357	0.00864626	0.99858813
H	1	-5.0305244	-2.4570112	-0.8250738

H	1	-5.0818508	-2.5046476	0.93043419
C	6	-3.1534229	-2.0253254	0.10653187
N	7	-2.653692	-3.2924156	0.27612161
O	8	-2.4155165	-1.054038	-0.0072638
H	1	-1.6525549	-3.4266216	0.21426709
H	1	-3.2460913	-4.1104206	0.28163482

ammonia

ATOM	CHARGE	X	Y	Z
N	7	-8.9592584	0.97606925	0.0027518
H	1	-7.9412766	0.94555998	-0.001472
H	1	-9.2840655	0.36274356	0.74810282
H	1	-9.2840695	0.58781061	-0.8809913

hydroxylamine

ATOM	CHARGE	X	Y	Z
N	7	-4.5412685	1.62890299	0.10525305
O	8	-3.1103801	1.53978914	0.30750277
H	1	-4.9305783	1.19436208	0.94389543
H	1	-4.716481	0.97552288	-0.6603249
H	1	-2.8258632	2.46363104	0.2251913

Octanoyl chloride

ATOM	CHARGE	X	Y	Z
C	6	-5.0402136	3.79529802	0.38589704
C	6	-3.5249656	3.55874218	0.37798461
H	1	-5.4858564	3.5495309	-0.5871457
H	1	-5.280167	4.84263314	0.60644637
H	1	-5.5350145	3.1736066	1.14379176
H	1	-3.0566951	4.21841001	-0.3674897
C	6	-3.1408558	2.1032171	0.07754894
H	1	-3.1043332	3.85158533	1.35159015
H	1	-3.5702444	1.80821198	-0.8927248
H	1	-3.6028731	1.44438077	0.82888059
C	6	-1.6255819	1.85999139	0.05331067
H	1	-1.1658937	2.5119698	-0.7050111
C	6	-1.2485602	0.40011446	-0.2362408
H	1	-1.1938375	2.16210671	1.01973418
H	1	-1.6912893	0.09236313	-1.1956484

H	1	-1.692713	-0.2505885	0.53201982
C	6	0.26851587	0.16836367	-0.2788516
H	1	0.71689141	0.79206758	-1.0639511
C	6	0.61493548	-1.3129673	-0.5495391
H	1	0.71770682	0.47892432	0.67242473
H	1	0.18440817	-1.6365097	-1.503945
H	1	0.21218149	-1.9415531	0.25186649
C	6	2.10213738	-1.5483968	-0.6499343
CL	17	2.93863254	-1.5045128	0.98337665
O	8	2.7457221	-1.7296852	-1.6351042

TS1 of octanoyl chloride

ATOM	CHARGE	X	Y	Z
C	6	-4.9703367	3.87120543	0.28103811
C	6	-3.4647616	3.58073253	0.29839367
H	1	-5.4218834	3.57303015	-0.6738342
H	1	-5.1752848	4.93919367	0.42664975
H	1	-5.4879419	3.32189024	1.07743882
H	1	-2.9676762	4.17068038	-0.4862475
C	6	-3.132368	2.09511172	0.0985342
H	1	-3.0378158	3.92257848	1.25345228
H	1	-3.56955	1.75215572	-0.8526167
H	1	-3.6231131	1.50616159	0.88959783
C	6	-1.6263355	1.79611507	0.0978914
H	1	-1.1379778	2.39257946	-0.6880372
C	6	-1.2953271	0.31285301	-0.1213024
H	1	-1.1877964	2.12971175	1.05095214
H	1	-1.7625983	-0.0259903	-1.0594112
H	1	-1.7530151	-0.2838493	0.68304069
C	6	0.21361594	0.03517166	-0.1759061
H	1	0.67359286	0.62044755	-0.982215
C	6	0.52878049	-1.4479404	-0.409648
H	1	0.68666603	0.35822721	0.76014826
H	1	0.03366619	-1.7788165	-1.3372458
H	1	0.14654333	-2.0630691	0.4127048
C	6	2.01260899	-1.7163579	-0.6115179
CL	17	2.86359101	-1.5612599	1.17148498
O	8	2.66280512	-1.0918441	-1.5601836
N	7	2.40002141	-3.1519996	-1.0116012
H	1	1.65050054	-3.6689654	-1.477779
H	1	2.82915145	-3.7142615	-0.2742492

H	1	3.05666442	-2.3629496	-1.743378

IM of octanoyl chloride

ATOM	CHARGE	X	Y	Z
C	6	-6.0762829	1.89802261	-0.3073748
C	6	-4.5424162	1.89215929	-0.305829
H	1	-6.4753973	1.04680738	-0.8749462
H	1	-6.4723338	2.81498603	-0.7614799
H	1	-6.4760265	1.83230812	0.7132541
H	1	-4.1746451	1.99925011	-1.3372549
C	6	-3.941689	0.62204072	0.31415179
H	1	-4.1743321	2.77210283	0.24276082
H	1	-4.3122381	-0.2574671	-0.2353707
H	1	-4.3108036	0.51543689	1.34630238
C	6	-2.4062517	0.60604464	0.31927187
H	1	-2.0377908	0.72264328	-0.7118693
C	6	-1.8090858	-0.6722418	0.92590216
H	1	-2.0357111	1.48027788	0.87656511
H	1	-2.1843893	-1.5452603	0.36983372
H	1	-2.1727419	-0.7886014	1.95827972
C	6	-0.2732262	-0.6886477	0.9224682
H	1	0.09421085	-0.5581909	-0.1044265
C	6	0.29238627	-1.9884685	1.51814334
H	1	0.101619	0.1658083	1.50226251
H	1	-0.0642261	-2.857881	0.95053962
H	1	-0.0633554	-2.11347	2.54625742
C	6	1.82249605	-2.0295291	1.56492477
N	7	2.42363492	-1.9385753	0.28017641
CL	17	2.27138678	-3.6887529	2.41055731
O	8	2.36213586	-1.060178	2.41386155
H	1	2.73664254	-0.3630507	1.84792998
H	1	1.96880877	-2.5406256	-0.4006874
H	1	3.41225933	-2.1800827	0.31374197

TS2 of octanoyl chloride

ATOM	CHARGE	X	Y	Z
C	6	-5.1075716	3.50174627	0.51417795
C	6	-3.6105943	3.26609445	0.27774601
H	1	-5.7118023	3.0331822	-0.2735374
H	1	-5.3467483	4.57238924	0.52423823

H	1	-5.4304615	3.07979201	1.47494174
H	1	-3.3150026	3.73180817	-0.6745567
C	6	-3.2251873	1.78059183	0.25481087
H	1	-3.0315278	3.7781428	1.06057304
H	1	-3.8171139	1.26512057	-0.516991
H	1	-3.5059355	1.31966275	1.21422698
C	6	-1.7319861	1.53965919	-0.008298
H	1	-1.459136	1.98746997	-0.9769662
C	6	-1.3431302	0.05458963	-0.0101771
H	1	-1.1371745	2.06784412	0.75203357
H	1	-1.9576125	-0.4803769	-0.751819
H	1	-1.5869631	-0.3850085	0.96906425
C	6	0.14527344	-0.1711595	-0.3136845
H	1	0.38663375	0.26059872	-1.2946994
C	6	0.50184959	-1.6618486	-0.3107703
H	1	0.76353786	0.33857139	0.43256029
H	1	-0.1512042	-2.1940696	-1.0244102
H	1	0.3238093	-2.0992513	0.67725037
C	6	1.91229337	-2.0051495	-0.7301465
CL	17	3.01890365	-0.8940257	1.48935939
O	8	2.73108884	-1.1450254	-1.3123522
N	7	2.24476323	-3.2759936	-0.8749319
H	1	1.65969495	-4.0125012	-0.5003274
H	1	3.20358602	-3.5022303	-1.116517
H	1	2.96085271	-0.4953313	-0.5747129

hydrogen chloride

ATOM	CHARGE	X	Y	Z
CL	17	-3.81155	7.41844117	1.31728523
H	1	-2.5205723	7.41844117	1.31728523

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