Supplementary Information

Rhodium Hydroformylation of Linseed Oil: from Rhodium Catalyst Stability Study to Machine Learning Data Analysis

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Number of figures: 9

Number of schemes: 4

Number of tables: 3

Table of contents

I) General purpose

All manipulations involving metal-amine catalysts precursors were typically performed under air atmosphere. The catalytic precursor $Rh(acac)(CO)_2$ was purchased from Merck and used as received. All chemicals were purchased from Fisher Scientific or Merck and were used without prior purification. Syngas ($CO:H_2$ / 1:1) and dihydrogen were provided by the Linde Group in cylinders pressurized at 150 and 200 bar, respectively.

Hydroformylation experiments were conducted under a fume hood in a room equipped with a CO detector and an explosimeter, both connected to an alarm and were carried out in a 25 mL autoclave (Parr instrument company) equipped with a mechanical stirrer

The NMR spectra were recorded at 298 K on a Bruker Avance Neo 400 spectrometer operating at 9.4 T field strength (400 MHz for ^{1}H nuclei and 100 MHz for ^{13}C nuclei) equipped with a 5 mm BBFO SmartProbe ($^{1}H/^{19}F/^{31}P$ - ^{109}Ag) and an automatic sample loading system.

Flow Injection Analyses (FIA) were performed using an Acquity UPLC H-Class chromatographic system (Waters, Milford, MA, USA) hyphenated with a Synapt-G2-Si Q-TOF (Waters, Manchester, UK) high resolution mass spectrometer (HRMS). The electrospray ionisation (ESI) source was operated mainly in the positive ion mode and if necessary, in the negative ion mode using a capillary voltage of ± 2.5 kV and the following conditions: cone voltage / source offset 40 V / 80 V for the positive ion mode and 20 V / 20 V for the negative ion mode; source temperature, 120 °C; desolvation gas temperature, 450 °C; desolvation gas flow, 600 $L \cdot h^{-1}$; and cone gas flow, 50 $L \cdot h^{-1}$. Nitrogen (>99.5%) was employed as the desolvation gas. Mass calibration was carried out using a sodium formate solution (10 mM NaOH in isopropanol/water/formic acid 49.9:49.9:0.2, v/v/v), and a lock mass correction was applied for accurate mass measurements using the ions of Leu-enkephalin solution (m/z 556.2771 for ESI^+ and m/z 554.2615 for ESI^-). The scan range was m/z 50–2000 at 0.20 $s \cdot scan^{-1}$. The time of flight (TOF) was operated in the resolution mode providing an average resolution power of 20,000 (FWHM). The HRMS spectrum were recorded either in the centroid or in the continuum mode. For MS/MS experiments the precursor ions were selected with the quadrupole (Q) and their fragmentations were performed in the trap cell, using variable collision energies (specified for each spectrum) and Argon (99.9999%) as the collision gas mode. Data acquisition and processing were performed with MassLynx™ software (V4.2, Waters). Direct introduction conditions: linseed oil, methyl oleate and crude HHM reaction mixtures were solubilised at a concentration of 5 $mg \cdot mL^{-1}$ in i-PrOH and 0.2 µL was injected in the mass spectrometer source using an isocratic flux composed of 10% H_2O and 90% CH_3OH and the flow rate was set at 0.4 $mL \cdot min^{-1}$.

II) Standard protocol for linseed oil reductive hydroformylation reactions catalysed by the rhodium/triethylamine system

In a typical catalytic experiment, a mixture of $Rh(acac)(CO)_2$ (6 mg, 23.3 µmol, 1 eq.), triethylamine, linseed oil (860 mg, 5.81 mmol of C=C bonds, 250 equiv. of C=C bonds), and toluene (to reach a total volume of 10.2 mL) were transferred into an autoclave of 25 mL (Parr instrument company) equipped with a mechanical stirrer.

The autoclave was then heated under stirring and, once a temperature of 80 °C was reached, the autoclave was charged with 80 bar of CO/H_2 (1:1).

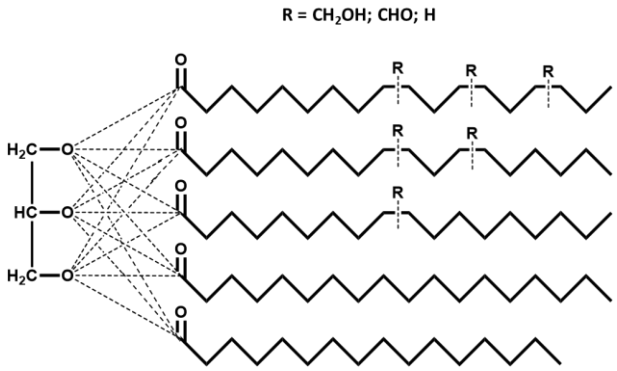
After 24 h, the autoclave was allowed to cool down to room temperature and depressurized. Triethylamine and toluene were removed by rotary evaporator and the obtained mixture was analysed by ^1H NMR spectroscopy giving access, after integration of the characteristic signals for each type of compound, to the exact overall composition of the medium as described in a previous work.[1]

III) Characterization of crude reaction mixture obtained from linseed oil in reductive hydroformylation conditions

1) Crude reaction mixture analyses

- **^{1}H NMR**

^1H NMR spectrum of a typical crude product obtained by linseed oil reductive hydroformylation (**Scheme S1**) is shown below (**Figure S1**).



Scheme S1. Crude product derived from linseed oil in reductive hydroformylation conditions

[1] W. Abdallah, M. Ferreira, C. Becquet, J. Ternel, H. Bricout, E. Monflier, S. Tilloy, *ChemCatChem* **2025**, *17*, e202401677.

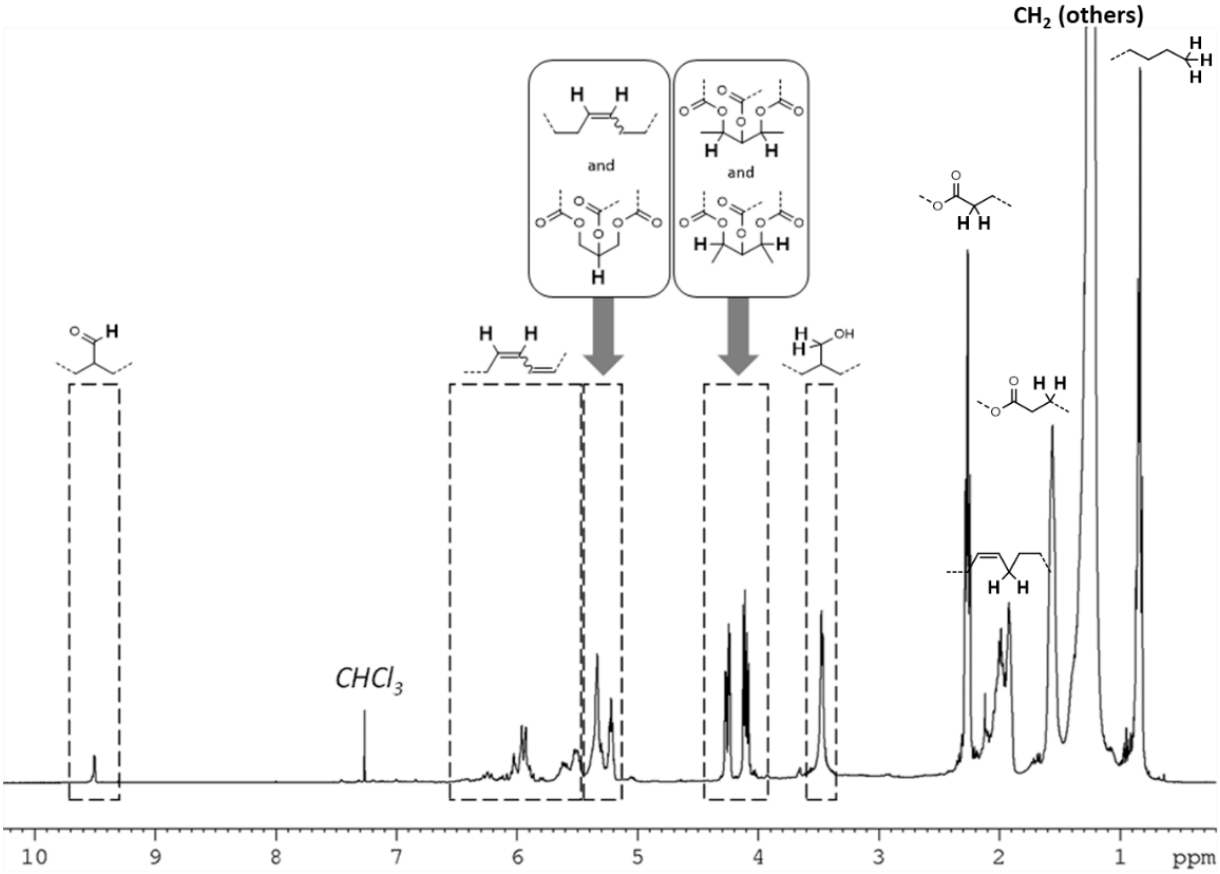


Figure S1. Typical ^{1}H NMR spectrum of the crude mixture obtained after linseed oil reductive hydroformylation, and after concentration (400 MHz, $CDCl_3$, 25 °C)

- **ESI$^+$-HRMS**

The positive electrospray ionization high-resolution mass spectrometry (ESI$^+$-HRMS) spectrum of the sample obtained from the reductive hydroformylation of linseed oil after 24 h (**Figure S2a**; see exact catalytic conditions in the title) was compared with that one of the reductive hydroformylation of linseed oil after 66 h (**Figure S2b**)

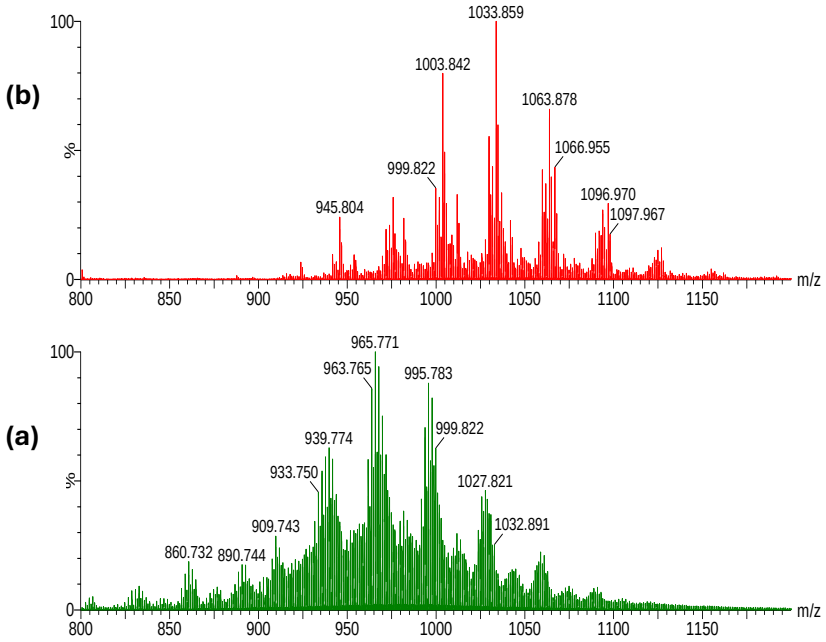
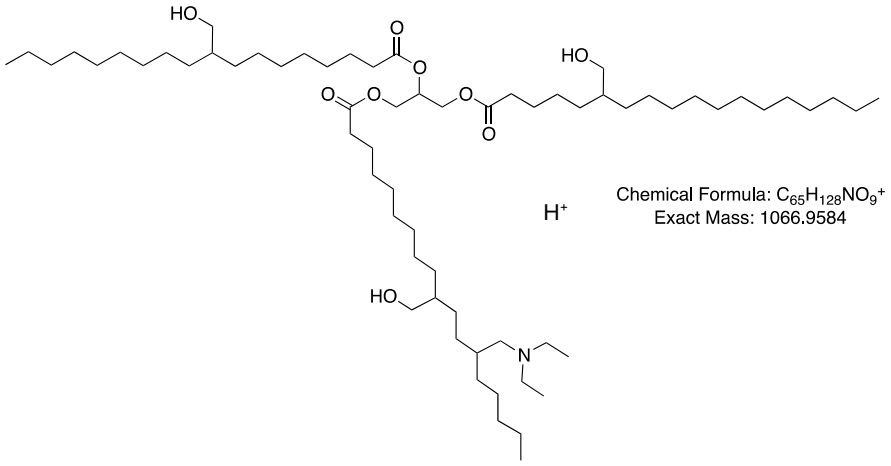


Figure S2. ESI$^+$-HRMS spectrum of the crude reaction mixture obtained by linseed oil reductive hydroformylation: **(a)** after 24 h, **(b)** after 66 h. Experimental conditions: $Rh(acac)(CO)_2$ (6 mg, 23.3 µmol, 1 equiv.), linseed oil (250 equiv. of C=C bonds, i.e., 5.81 mmol), NEt_3 (23.3 mmol, 1000 equiv.), toluene (amount to reach a total volume of 10.2 mL in the autoclave), 80 bar of CO/H_2 (1:1).

After 24 h, a Gaussian distribution of sodium adducts [M, Na^+] is observed, corresponding to the different reductive hydroformylation species, with mass differences of 30 Da (CH_2O units) (**Figure S2a**). Additionally, numerous ions differing by 2 Da (H_2) are detected, indicating that formyl groups and C=C double bonds are still present due to incomplete hydrogenation. The distribution is centered (i.e., the most abundant ion of the Gaussian distribution) at m/z 965.771, corresponding to $C_{57}(CH_2OH)_2$ with four residual double bonds on the aliphatic chains of the triglyceride [$C_{59}H_{106}O_8$, Na^+].

When the reductive hydroformylation reaction time is extended to 66 h (**Figure S2b**), the distribution shifts toward higher masses, centered on $C_{57}(CH_2OH)_4$ at m/z 1033.8558 [$C_{61}H_{118}O_{10}$, Na^+], reflecting a more advanced reaction progress characterized by a reduced number of residual double bonds (-CH=O and C=C). Moreover, the ESI$^+$-HRMS analysis of the reductive hydroformylation reaction mixture after 66 h (**Figure S2b**) revealed the presence of several even ions (i.e., m/z 1066.955 and m/z 1096.970) which were attributed to aminated products as exemplified for m/z 1066.955 corresponding to the H^+ adduct of $C_{57}(CH_2OH)_3(CH_2N(CH_2CH_3)_2$ on **Scheme S2** (1096.970 corresponding to the H^+ adduct of $C_{57}(CH_2OH)_4(CH_2N(CH_2CH_3)_2$).



Scheme S2. Hypothetical structure of an aminated product detected at m/z 1066.955 in the crude linseed oil reductive hydroformylation mixture after 66 h, in the experimental conditions of Figure S2.

This side reaction, formally resulting in the grafting of a $–CH_2–N(CH_2CH_3)_2$ group, was unambiguously confirmed by MS/MS (**Figure S3**), with two fragment ions generated at m/z 752.676 and 382.369.

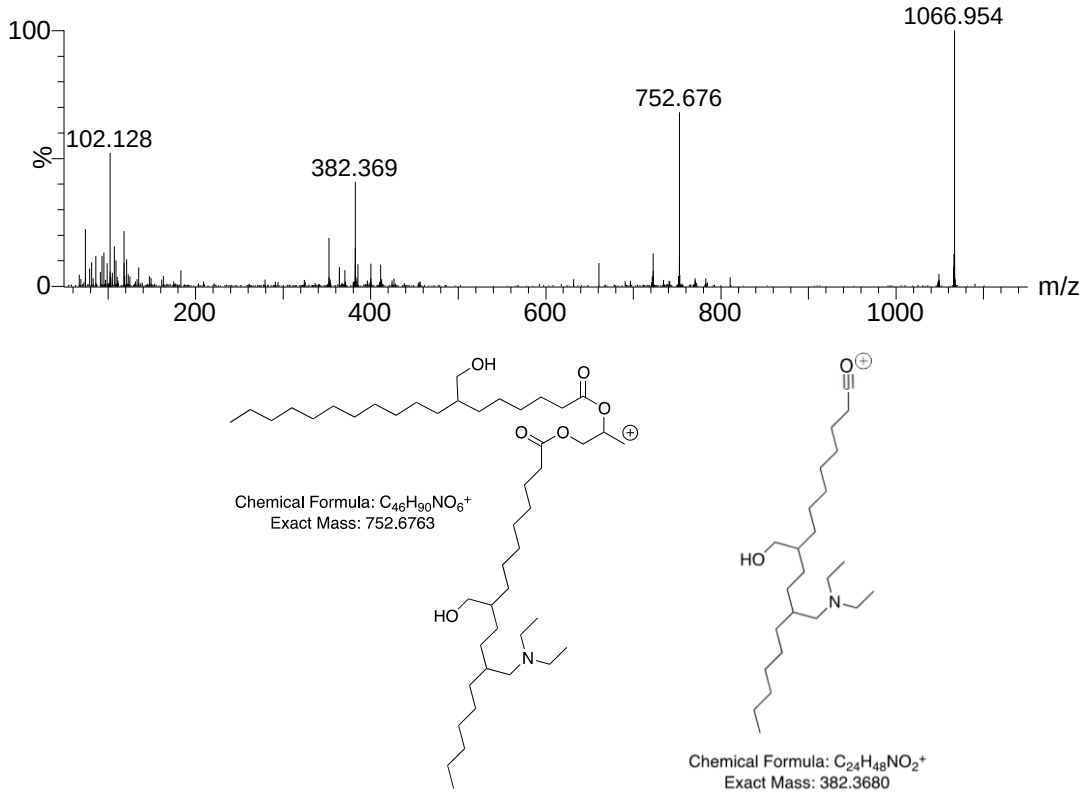


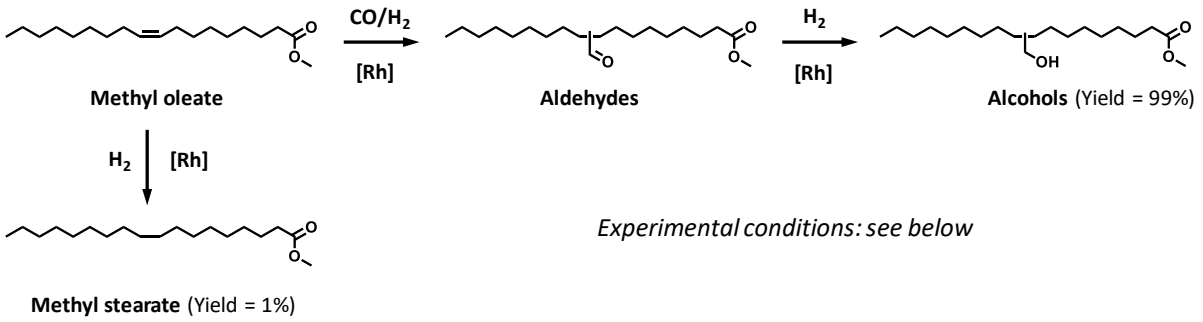
Figure S3. MS/MS spectrum (70 eV) of the ion at m/z 1066.954 observed in the crude reaction mixture of linseed oil reductive hydroformylation after 66 h; experimental conditions of Figure S2. The hypothetical structure of the daughter ions at m/z 752.676 and m/z 382.369 is also presented.

The yield of these aminated compounds was estimated to be below the micromolar range, as no corresponding signals were detected in the ^{1}H NMR spectra.

2) Reactions with methyl oleate as substrate

- **Methyl oleate HHM** (HHM = hydrohydroxymethylation = reductive hydroformylation)

To understand the aminated products formation during the reductive hydroformylation of linseed oil, the reductive hydroformylation of methyl oleate was subsequently performed using the Rh/triethylamine catalytic system (**Scheme S3**).



Scheme S3. Reductive hydroformylation of methyl oleate. Experimental conditions: $Rh(acac)(CO)_2$ (6 mg, 23.3 µmol, 1 equiv), methyl oleate (5.81 mmol, 250 equiv.), NEt_3 (23.3 mmol, 1000 equiv.), toluene (amount to reach a total volume of 10.2 mL in the autoclave), 80 bar of CO/H_2 (1:1), 24 h, leading to 99% of alcohol isomers and 1% of methyl stearate (100% conversion), determined by ^{1}H NMR.

Mass spectrometric analysis (ESI^{+}-HRMS) demonstrates a similar aminated product formation (**Figure S4**).

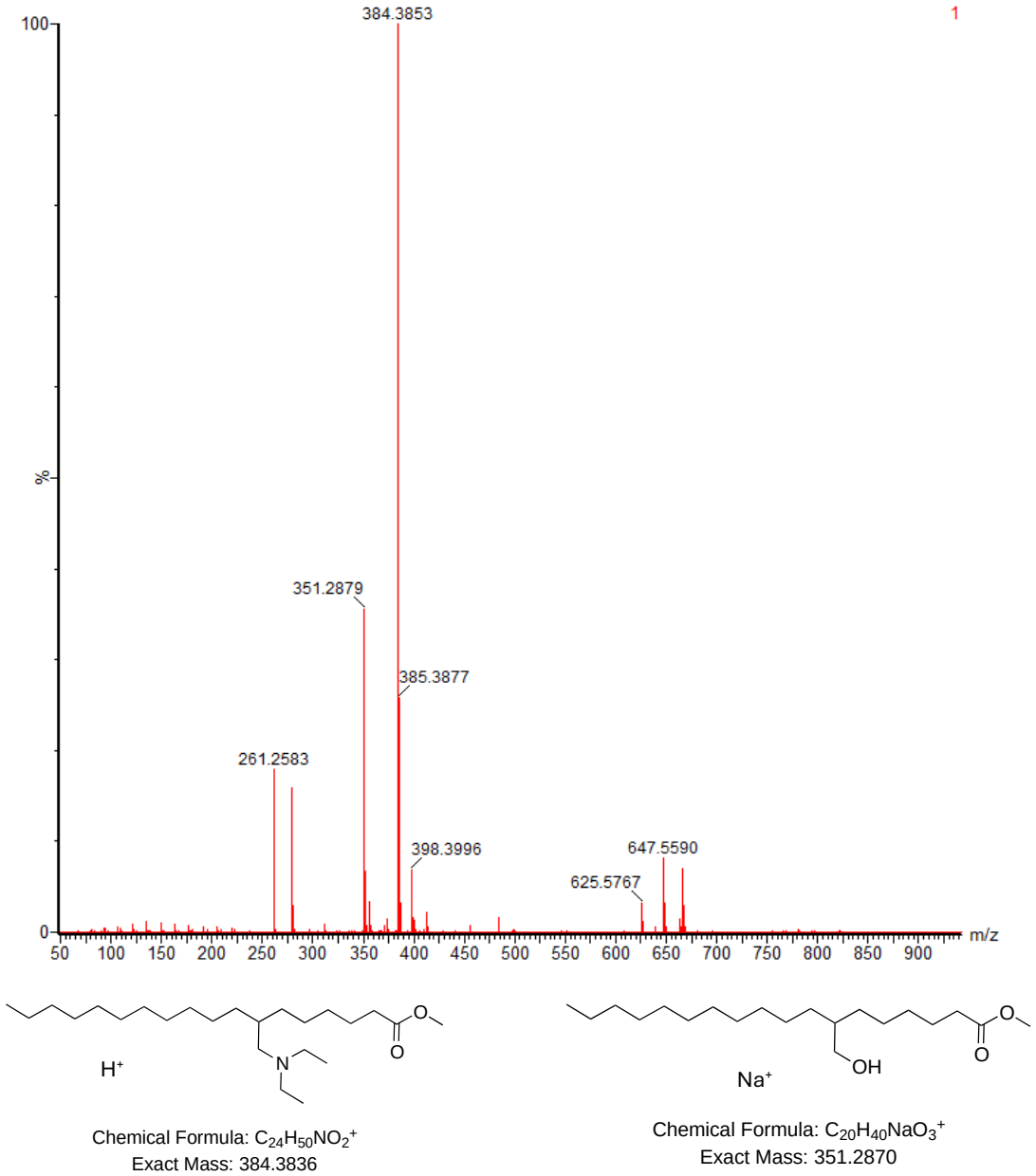
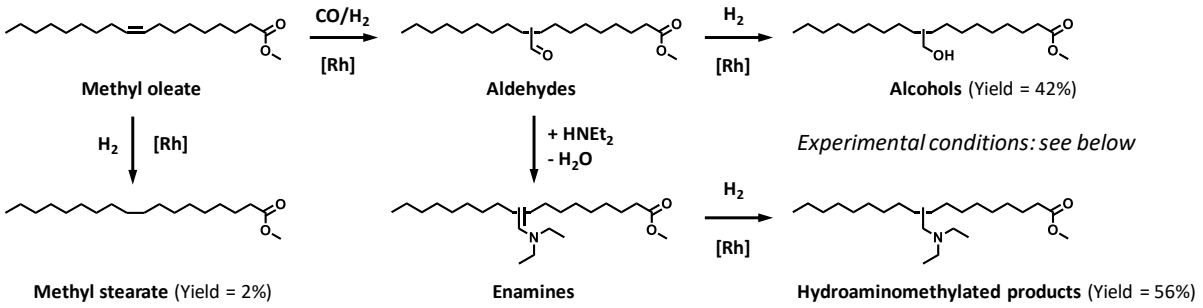


Figure S4. ESI$^+$-HRMS spectrum of the crude reductive hydroformylation reaction mixture of methyl oleate obtained in the experimental conditions of Scheme S3 and showing two compounds at m/z 384.385 and m/z 351.288 and their hypothetical structures.

- **Methyl oleate HAM** (Hydroaminomethylation)

To validate these findings, the aminated derivative of methyl oleate was independently synthesized via HydroAminoMethylation (HAM). Under these hydroaminomethylation conditions, the aminated product was obtained in 56% yield, whereas the corresponding alcohols accounted for 42% (**Scheme S4**).



Scheme S4. Methyl oleate hydroaminomethylation test (HAM); Experimental conditions: $Rh(acac)(CO)_2$ (3.9 mg, 15.1 µmol, 1 equiv.), methyl oleate (3 mmol, 200 equiv.), $HNEt_2$ (6 mmol, 400 equiv.), toluene (5 mL), 80 bar of CO/H_2 (1:1), 24 h, leading to 56% of isomeric aminated compounds, 42% of isomeric alcohol compounds and 2% of methyl stearate (100% conversion), determined by ^1H NMR.

ESI$^+$-HRMS analysis of the resulting hydroaminomethylation mixture revealed the same aminated species at m/z 384.384 as that formed during the reductive hydroformylation of methyl oleate, thus confirming the proposed hypothesis (**Figure S5**).

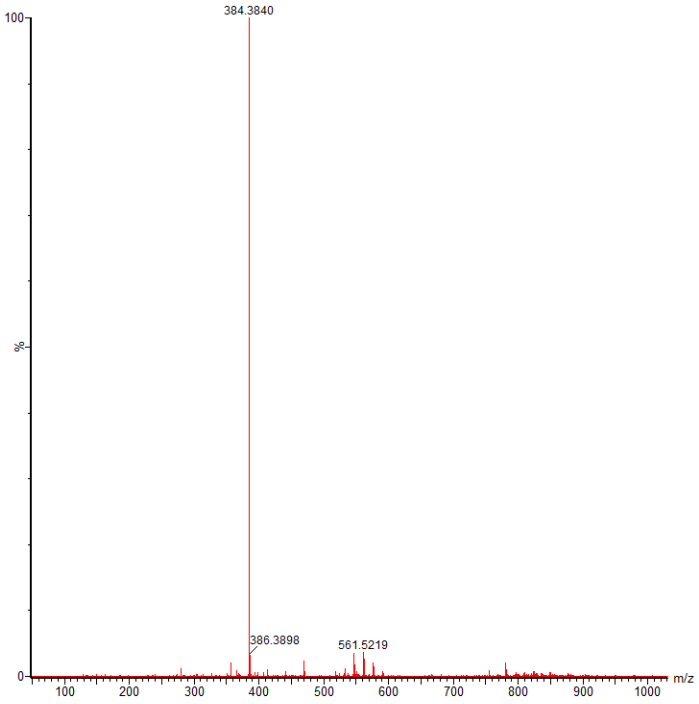


Figure S5. ESI$^+$-HRMS spectra of HAM reaction mixture of methyl oleate showing mainly the m/z 384.385 (see Scheme S3 for obtention).

The mass spectrometric signal of the aminated compound was approximately 2000 times more intense than that of the alcohol, reflecting a markedly higher MS response factor. This difference accounts for the apparent prominence of the aminated species H^+ adduct in HRMS analyses, despite the aminated compound formation in only trace amounts under reductive hydroformylation conditions.

Further investigations led us to conclude that the minor formation of the aminated product under Rh/triethylamine reductive hydroformylation conditions originates from trace amounts of diethylamine ($HNEt_2$, DEA) present as an impurity in the triethylamine (TEA) reagent. This hypothesis was confirmed by ^1H NMR analysis of the used TEA (**Figure S6**) which demonstrated the presence of DEA signals (a TEA/DEA mixture (**Figure S7** and **S8**) was also prepared as reference).

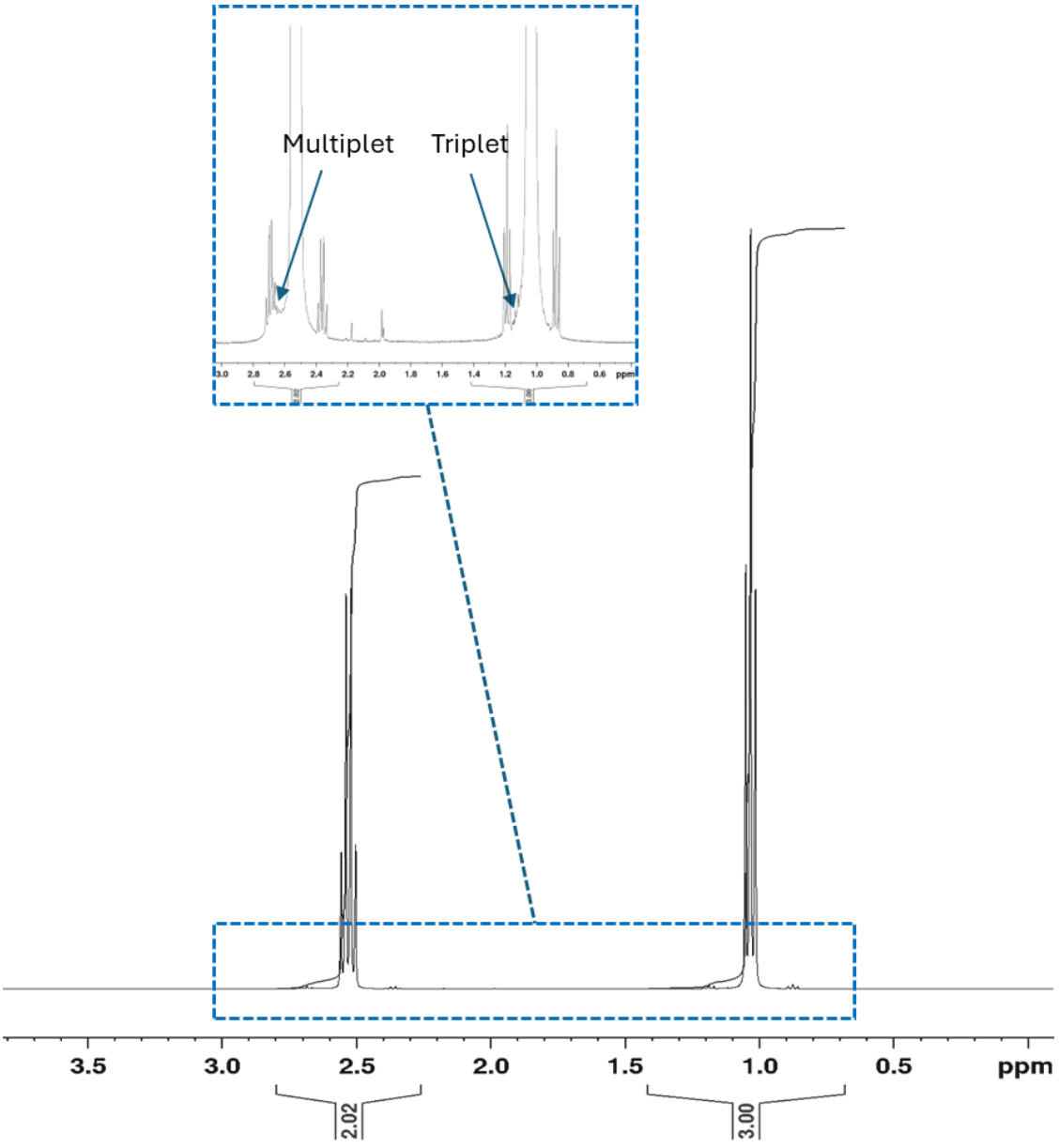


Figure S6. ^1H NMR (400 MHz, 25 °C, $CDCl_3$) spectrum of the 99% triethylamine (TEA) used in this study

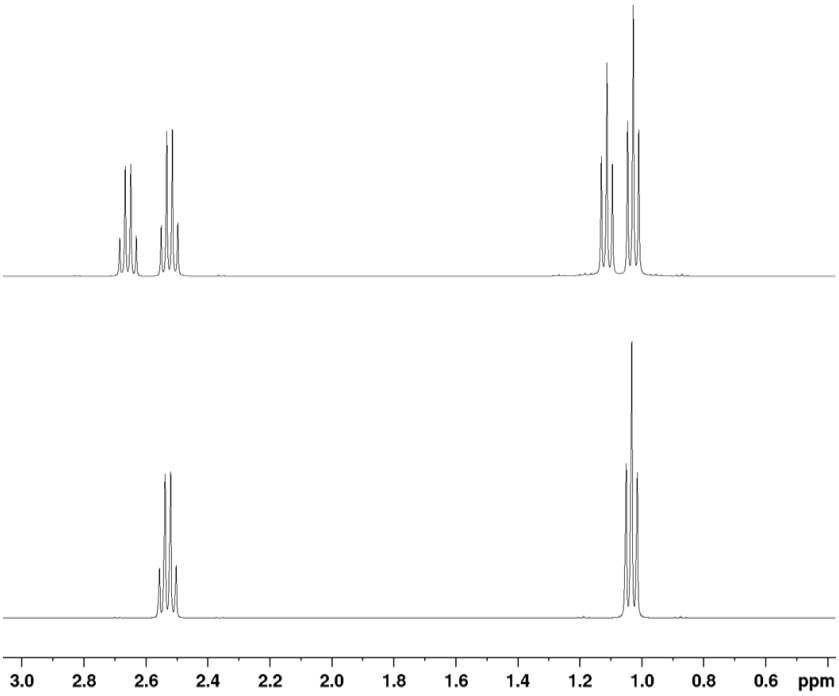


Figure S7. Overlay of ^{1}H NMR spectra (400 MHz, 25 °C, $CDCl_3$) of the TEA/DEA mixture (top) and TEA (bottom).

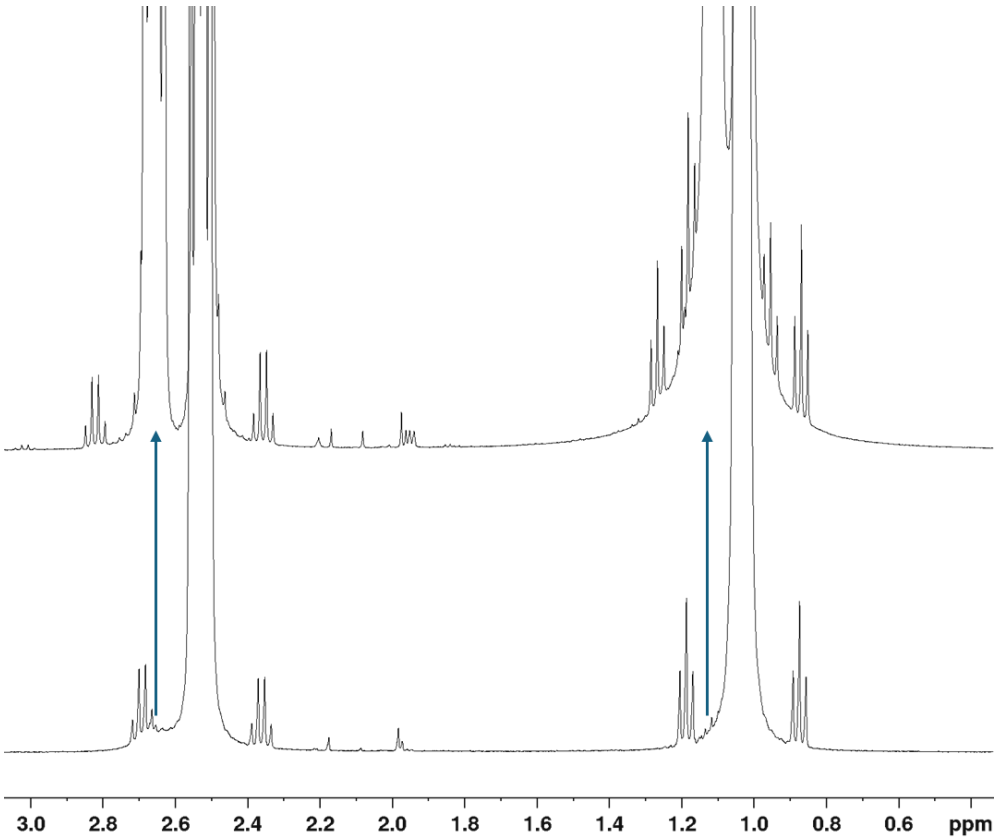


Figure S8. Zoom region overlay of ^{1}H NMR spectra (400 MHz, 25 °C, $CDCl_3$) of the TEA/DEA mixture (top) and TEA (bottom).

The presence of traces of diethylamine in the triethylamine used to conduct the catalytic tests of reductive hydroformylation was confirmed by an ESI$^+$-HRMS analysis of the triethylamine (**Figure S9a**; see also **Figure S9b** for a zoom). Indeed, in addition to the [NEt_3, H^+] adduct detected at m/z 102.1265, a small signal corresponding to the [$HNEt_2$, H^+] adduct was seen at m/z 74.0963 (see also **Figure S9c** for the ESI$^+$-HRMS spectrum of diethylamine).

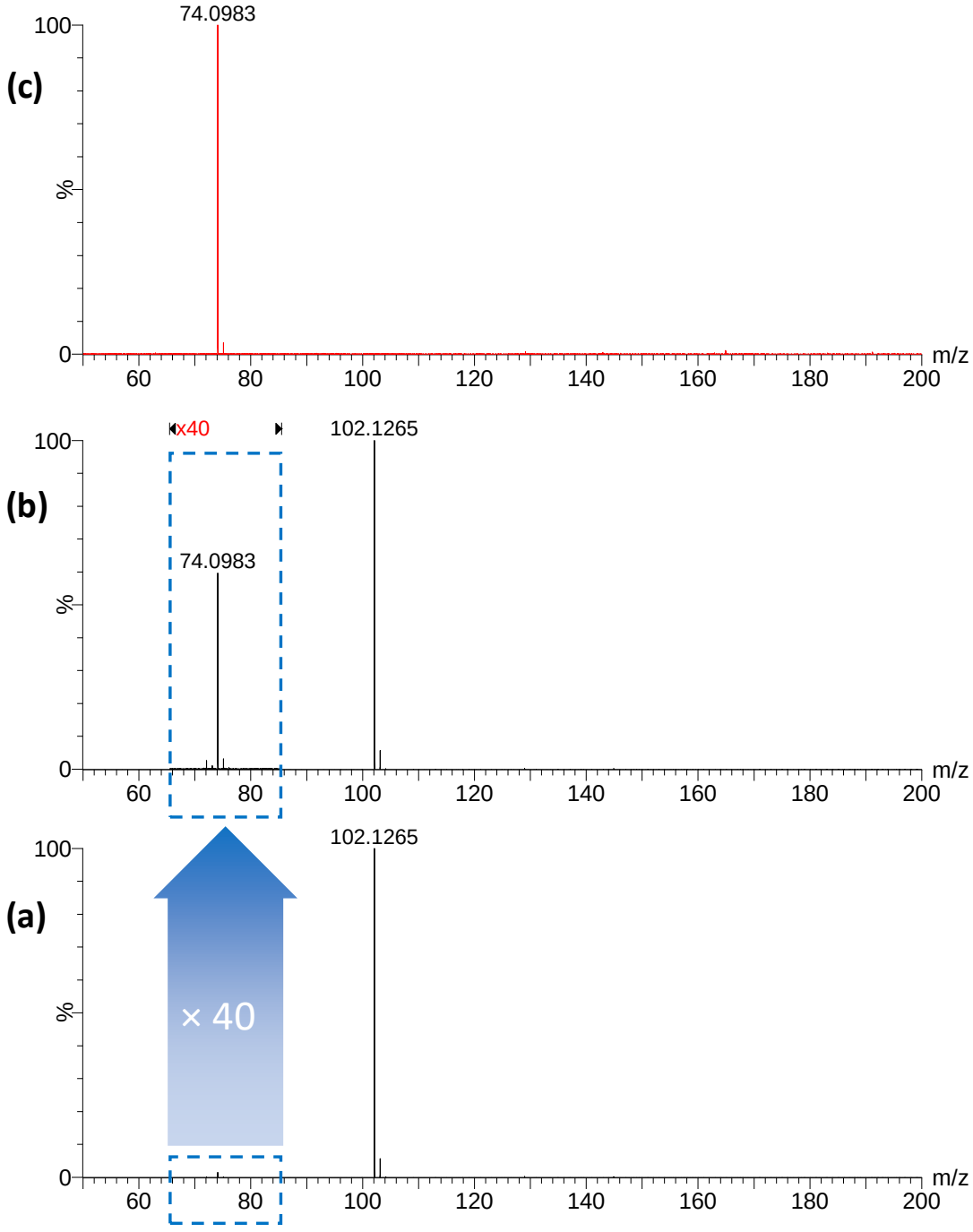


Figure S9. (a) ESI$^+$-HRMS spectrum of triethylamine (TEA) used in this study, **(b)** previous spectrum with a zoom of ×40 in the 65-85 Da zone, and **(c)** ESI$^+$-HRMS spectrum of diethylamine (DEA).

IV) Raw data

Table S1.

	EXPERIMENTAL CONDITIONS							EXPERIMENTAL RESULTS			
Data n°	**Rh** (µmol)	**C=C** (µmol)	**TEA** (µmol)	**T** (°C)	**t** (h)	**CO** (bar)	**H_2** (bar)	**ALD** (µmol)	**ALC** (µmol)	**CONJ** (µmol)	**SAT** (µmol)
1	23.30	5825	23300	80	24.0	53	27	350	990	2913	175
2	23.60	5900	23600	70	24.0	45	45	413	885	2714	0
3	23.30	5825	0	80	24.0	40	40	1282	0	2097	1282
4	23.30	5825	5825	80	24.0	40	40	466	816	2447	757
5	23.30	5825	11650	80	24.0	40	40	408	1049	2505	641
6	23.30	5825	23300	80	24.0	40	40	233	1223	2388	932
7	23.30	5825	65240	80	24.0	40	40	175	1107	2330	932
8	23.30	5825	117	80	24.0	40	40	990	117	2155	1107
9	23.30	5825	1165	80	24.0	40	40	990	291	2330	816
10	23.30	5825	2913	80	24.0	40	40	816	816	2214	641
11	23.30	5825	23300	70	24.0	40	40	466	874	2680	0
12	23.30	5825	23300	100	24.0	40	40	0	2621	0	3204
13	23.30	5825	23300	120	24.0	40	40	0	2563	0	3262
14	23.30	5825	23300	140	24.0	40	40	175	2621	0	3029
15	23.30	5825	11650	80	66.0	40	40	0	3379	0	2447
16	23.30	5825	23300	70	66.0	40	40	0	2272	1689	932
17	23.30	5825	23300	80	66.0	40	40	0	3262	0	2563
18	11.65	5825	23300	80	24.0	40	40	699	350	2680	233
19	23.30	2912.5	23300	70	24.0	40	40	58	961	1049	320
20	46.60	11650	46600	80	24.0	40	40	117	3728	3495	1515
21	46.60	5825	46600	80	24.0	40	40	0	3379	0	2039
22	23.30	1456	23300	80	24.0	40	40	0	684	0	772
23	23.30	1456	23300	60	24.0	40	40	0	524	597	87
24	23.30	1456	23300	120	6.0	40	40	44	699	0	714
25	23.30	1456	23300	70	24.0	40	40	15	743	306	233
26	23.30	5825	23300	80	0.4	40	40	204	117	1398	0
27	23.30	5825	23300	80	0.8	40	40	291	117	1485	0
28	23.30	5825	23300	80	1.5	40	40	320	117	1893	29
29	23.30	5825	23300	80	3.0	40	40	466	117	2126	87
30	23.30	5825	23300	80	4.5	40	40	553	146	2388	175
31	23.30	5825	23300	80	5.8	40	40	583	175	2476	233
32	23.30	5825	23300	80	8.0	40	40	583	350	2563	291
33	23.30	5825	23300	80	10.0	40	40	583	466	2621	350
34	23.30	5825	23300	80	12.0	40	40	553	524	2650	466
35	23.30	5825	23300	80	14.0	40	40	524	612	2650	553
36	23.30	5825	23300	80	16.0	40	40	466	728	2621	641
37	23.30	5825	23300	80	18.0	40	40	408	845	2592	728
38	23.30	5825	23300	80	21.0	40	40	320	1019	2505	845
39	23.30	5825	23300	80	27.5	40	40	204	1398	2214	1165
40	23.30	5825	23300	80	30.5	40	40	175	1544	2039	1311

	EXPERIMENTAL CONDITIONS							EXPERIMENTAL RESULTS			
Data n°	**Rh** (µmol)	**C=C** (µmol)	**TEA** (µmol)	**T** (°C)	**t** (h)	**CO** (bar)	**H_2** (bar)	**ALD** (µmol)	**ALC** (µmol)	**CONJ** (µmol)	**SAT** (µmol)
41	23.30	5825	23300	80	33.5	40	40	175	1689	1806	1515
42	23.30	5825	23300	80	36.0	40	40	146	1835	1631	1631
43	23.30	5825	23300	80	38.5	40	40	146	1922	1456	1777
44	23.30	5825	23300	80	41.0	40	40	117	2097	1223	1922
45	23.30	5825	23300	80	44.5	40	40	87	2301	990	2097
46	23.30	5825	23300	80	48.0	40	40	58	2505	757	2243
47	23.30	5825	23300	80	51.5	40	40	58	2680	524	2388
48	23.30	5825	23300	80	54.5	40	40	29	2913	291	2476
49	23.30	5825	23300	80	57.5	40	40	29	3116	87	2534
50	23.30	5825	23300	80	60.0	40	40	0	3262	0	2563
51	46.60	2913	46600	80	2.0	40	40	58	320	1252	29
52	46.60	2913	46600	80	6.0	40	40	58	699	1165	146
53	46.60	2913	46600	80	24.0	40	40	29	1689	0	1194
54	23.30	5825	2330	80	7.0	40	40	641	0	2796	0
55	23.30	5825	2330	80	24.0	40	40	932	641	2330	699
56	23.30	5825	583	80	6.0	40	40	641	0	2680	0
57	23.30	5825	583	80	24.0	40	40	1165	175	2330	1049
58	23.30	5825	1748	80	3.5	40	40	524	0	2214	0
59	23.30	5825	1748	80	24.0	40	40	874	350	2447	757
60	23.30	5825	233	80	6.0	40	40	699	0	2913	0
61	23.30	5825	233	80	24.0	40	40	1282	0	2097	1223
62	23.60	5900	23600	60	66.0	40	40	0	2183	2301	0
63	23.60	5900	23600	80	24.0	30	30	118	944	2832	295
64	23.30	5825	23300	80	24.0	27	53	0	2330	816	1515
65	23.30	5825	23300	100	24.0	27	53	0	2913	0	2913
66	23.30	5825	23300	80	66.0	27	53	0	3728	0	2097
67	23.30	5825	23300	100	66.0	27	53	0	3204	0	2621
68	46.60	2913	46600	80	2.5	27	53	58	320	1136	87
69	46.60	2913	46600	80	6.0	27	53	29	350	1165	117
70	46.60	2913	46600	80	24.0	27	53	0	1806	0	1019
71	46.60	2913	13980	80	6.0	27	53	29	1107	175	1078
72	46.60	2913	13980	80	22.0	27	53	0	1631	0	1223
73	46.60	2913	13980	80	6.0	20	60	29	553	0	1893
74	23.60	5900	2360	80	24.0	20	60	177	1239	1180	1711
75	23.60	5900	23600	80	24.0	20	20	0	472	3127	236
76	23.60	5900	23600	100	24.0	20	20	295	1475	0	2773
77	23.30	5825	23300	80	24.0	16	64	0	1049	1049	1340

V) Machine learning code explanation

Follow the following link for more information concerning the machine learning part of the manuscript and the corresponding used data:

https://github.com/LAREFRACHID/Rhodium-Catalyzed-Reductive-Hydroformylation-of-Linseed-Oil

This machine learning pipeline predicts four chemical outputs: ALD, ALC, CONJ, and SAT, from experimental reaction conditions. It also explains the predictions using SHAP analysis in order to identify the most influential experimental parameters.

Input file. exp_data.xlsx

Output folder. results_regression

1) Models used

- Linear Regression
- Support Vector Regression (SVR)
- Random Forest (RF)
- XGBoost
- Multi-Layer Perceptron (MLP)

2) Pipeline organization

- **Data loading:** Experimental conditions and target outputs are loaded from the Excel file.
- **Train/test split:** The dataset is divided into training and test subsets to evaluate model generalization.
- **Scaling:** Input features are standardized. Output variables are also scaled during training and converted back to original units for evaluation.
- **Hyperparameter tuning:** For SVR, Random Forest, XGBoost, and MLP, optimized hyperparameters are selected using randomized search and cross-validation.
- **Multi-output prediction:** Each optimized model predicts the four outputs: ALD, ALC, CONJ, and SAT.
- **Model comparison:** Models are compared using R^2, RMSE, and MAE.
- **SHAP interpretation:** The best-performing model is interpreted using SHAP to identify the most important variables controlling the predicted outputs.

3) Optimized hyperparameters

Table S2.

Model	Best hyperparameters
SVR	C = 26.67; epsilon = 0.048; gamma = 0.06; kernel = rbf
Random Forest	max_depth = 16; min_samples_leaf = 1; min_samples_split = 2; n_estimators = 774
XGBoost	colsample_bytree = 0.96; learning_rate = 0.025; max_depth = 4; n_estimators = 932; subsample = 0.92
MLP	activation = tanh; alpha = 0.0002342; hidden_layer_sizes = [128, 64, 32]; learning_rate_init = 0.0052

4) Evaluation metrics

- **R^2:** Coefficient of determination. Higher values indicate better predictive performance.
- **RMSE:** Root-mean-square error, expressed in µmol. Lower values indicate better prediction accuracy.
- **MAE:** Mean absolute error, expressed in µmol. Lower values indicate better average prediction accuracy.

5) Model comparison results

Random Forest and XGBoost provided the best average predictive performances, with average R^2 values close to 0.86.

XGBoost showed the lowest average RMSE, indicating the smallest global prediction error among the tested models.

The SHAP analysis was applied to the best-performing model “XGBoost” to interpret the influence of experimental variables on the four predicted outputs.

Table S3.

Model	**Output**	**R^2**	**RMSE** (μmol)	**MAE** (μmol)
Linear Regression	ALD(μmol)	0.61	169	150
Linear Regression	ALC(μmol)	0.82	424	293
Linear Regression	CONJ(μmol)	0.62	657	543
Linear Regression	SAT(μmol)	0.74	535	416
Linear Regression	**AVG**	**0.70**	**446**	**350**
SVR	ALD(μmol)	0.84	108	82
SVR	ALC(μmol)	0.85	394	273
SVR	CONJ(μmol)	0.72	563	377
SVR	SAT(μmol)	0.87	375	248
SVR	**AVG**	**0.82**	**360**	**245**
Random Forest	ALD(μmol)	0.85	103	67
Random Forest	ALC(μmol)	0.92	285	195
Random Forest	CONJ(μmol)	0.77	511	328
Random Forest	SAT(μmol)	0.91	307	208
Random Forest	**AVG**	**0.86**	**301**	**199**
XGBoost	ALD(μmol)	0.82	112	78
XGBoost	ALC(μmol)	0.93	256	195
XGBoost	CONJ(μmol)	0.76	519	313
XGBoost	SAT(μmol)	0.93	277	210
XGBoost	**AVG**	**0.86**	**291**	**199**
MLP	ALD(μmol)	0.72	143	126
MLP	ALC(μmol)	0.94	233	153
MLP	CONJ(μmol)	0.85	411	366
MLP	SAT(μmol)	0.81	454	377
MLP	**AVG**	**0.83**	**310**	**256**