Electronic Supplementary Material (ESI) for Green Chemistry.

Rationally designed acidic deep eutectic solvent induced catalysis and spontaneous catalyst recycling of Pd-catalyzed ethylene alkoxycarbonylation

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Content

1. Calculation methods

For alkoxycarbonylation, the specific calculation methods for conversion and selectivity are as follows:

Since the equimolar mixture of ethylene and CO is the reactant and they will react equimolarly, the molar ratio of ethylene to CO in the gas mixture will remain equimolar throughout the process, according to the literature,[1] the conversion of ethylene was gauged and correlated to the pressure drop of the gas mixture:

$$X_{ethylene} = \frac{p^0 - p - p^a}{p^0 - p^a} \times 100\%$$

Where p^0 is the initial pressure at 80 °C, p is the pressure after reaction at 80 °C, p^a is the pressure of pure alcohol at 80 °C.

Distillation results revealed that the distillate of the lower DES phase contains predominantly reactant alcohol without noticeable product or by-products, suggesting that the product and by-products are concentrated in the upper product phase. The selectivity of esters was calculated by:

$$S_{ester} = \frac{n_{ester}}{n_{ester} + n_b} \times 100\%$$

Where n_{ester} is the quantity of the generated ester, n_b is the quantity of the generated by-products.

2. Details of HBD and HBAs

Table S1. Details of HBD and HBAs.

Entry	Reagent	Purity	Supplier	CAS Number
1	L-carnitine	≥98%	Macklin	541-15-1
2	4-Picolinic acid	≥98%	Macklin	55-22-1
3	Nicotinic acid	≥98%	Macklin	59-67-6
4	Histidine	≥99%	Macklin	71-00-1
5	Urea	≥99%	Macklin	57-13-6
6	Lidocaine	≥98%	Macklin	137-58-6
7	p-Toluidine-2-sulfonic acid	≥98%	Macklin	88-44-8
8	Benzamide	≥99%	Macklin	55-21-0
9	Betaine	≥98%	Macklin	107-43-7
10	Dimethylglycine	≥98%	Macklin	1118-68-9
11	N-(2-Hydroxyethyl)piperazine	≥99%	Macklin	103-76-4
12	Choline chloride	≥99%	Macklin	67-48-1
13	p-Toluenesulfonic acid	≥99%	Macklin	6192-52-5

3. Details of ligands

Table S2. Details of ligands.

Entry	Reagent	Abbreviation	Purity	Supplier	CAS Number
L1	1,2-Bis(di-tert-butylphosphinomethyl)-benzene	1,2-DTBPMB	≥97%	Aladdin	121954-50-5
L2	1,2-Bis(diphenylphosphanyl)benzene	DPPBE	≥98%	Aladdin	13991-08-7
L3	1,2-Bis(diphenylphosphino)ethane	DPPE	≥98%	Aladdin	1663-45-2
L4	1,3-Bis(diphenylphosphino)propane	DPPP	≥98%	Aladdin	6737-42-4
L5	1,4-Bis(diphenylphosphino)butane	DPPB	≥96%	Aladdin	231-698-7
L6	1,5-Bis(diphenylphosphino)pentane	DPPPE	≥98%	Aladdin	27721-02-4
L7	1,1-Bis(diphenylphosphino)ferrocene	DPPF	≥98%	Aladdin	12150-46-8
L8	Triphenylphosphine	PPh_3	≥99%	Aladdin	603-35-0
L9	2-Diphenylphosphinopyridine	Ph2P(2-py)	≥95%	Aladdin	37943-90-1
L10	Cyclohexyldiphenylphosphine	Ph_2Pcy	≥95%	Aladdin	6372-42-5
L11	Dimethylphenylphosphine	Me_2PPh	≥98%	Aladdin	672-66-2
L12	Tripropylphosphine	TPPhos	≥98%	Aladdin	2234-97-1
L13	Bis(2-diphenylphosphinophenyl)ether	DPEPhos	≥98%	Aladdin	166330-10-5
L14	1,1'-Binaphthyl-2,2'-diphemyl phosphine	BINAP	≥97%	Aladdin	98327-87-8
L15	9,9-Dimethyl-4,5-bis(diphenylphosphino)xanthene	Xantphos	≥98%	Aladdin	1265-03-8

4. Details of alcohols

Table S3. Details of alcohols.

Entry	Reagent	Purity	Supplier	CAS Number
1	Methanol	≥99.5%	Titan	67-56-1
2	Ethanol	≥99.5%	Titan	64-17-5
3	n-Propanol	≥99.5%	Titan	71-23-8
4	iso-Propanol	≥99.5%	Titan	67-63-0
5	n-Butanol	≥99%	Titan	71-36-3
6	iso-Butanol	≥99%	Titan	78-83-1
7	n-Pentanol	≥99%	Titan	71-41-0
8	iso-Pentanol	≥99%	Titan	23-51-3
9	n-Hexanol	≥98%	Titan	111-27-3

5. Details of DES preparation

Entry	DES	HBD/g	HBD/mol	HBA/g	HBA/mol
1	2PTSA:L-carnitine	8.00	0.0465	3.74	0.0232
2	2PTSA:4-Picolinic acid	8.00	0.0465	2.86	0.0232
3	2PTSA:Nicotinic acid	8.00	0.0465	2.86	0.0232
4	2PTSA:Histidine	8.00	0.0465	3.60	0.0232
5	2PTSA:Urea	8.00	0.0465	1.40	0.0232
6	2PTSA:Lidocaine	8.00	0.0465	4.44	0.0232
7	2PTSA:p-Toluidine-2-sulfonic acid	8.00	0.0465	4.35	0.0232
8	2PTSA:Benzamide	8.00	0.0465	2.81	0.0232
9	2PTSA:Betaine	8.00	0.0465	4.47	0.0232
10	2PTSA:Dimethylglycine	8.00	0.0465	2.40	0.0232
11	2PTSA:N-(2-Hydroxyethyl)piperazine	8.00	0.0465	3.02	0.0232
12	2PTSA:Choline chloride	8.00	0.0465	3.24	0.0232

Table S4. Details of DES screening.

Table S5. Details of HBD to HBA ratio screening.

Entry	DES	PTSA/g	HBD/mol	L-carnitine/g	HBA/mol
1	2.00PTSA:L-carnitine	8.00	0.0465	3.74	0.0232
2	1.02PTSA:L-carnitine	8.00	0.0465	3.82	0.0237
3	PTSA:L-carnitine	8.00	0.0465	7.50	0.0465
4	PTSA:2.00L-carnitine	4.00	0.0232	7.50	0.0465
5	PTSA:3.00L-carnitine	4.00	0.0232	11.24	0.0697

6	PTSA:4.00L-carnitine	4.00	0.0232	14.98	0.0929

6. NCI diagrams of interactions in DESs

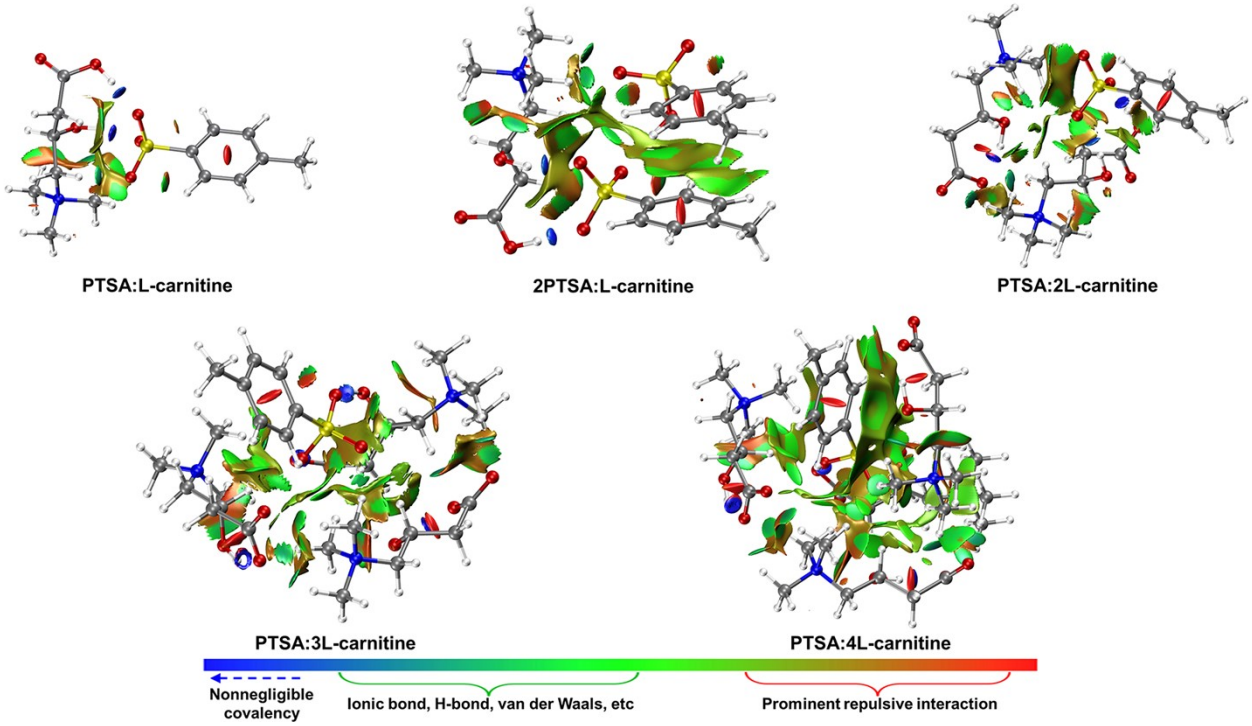


Fig. S1. NCI diagrams of interactions in DESs.

7. ESP penetration schematic of DES formation

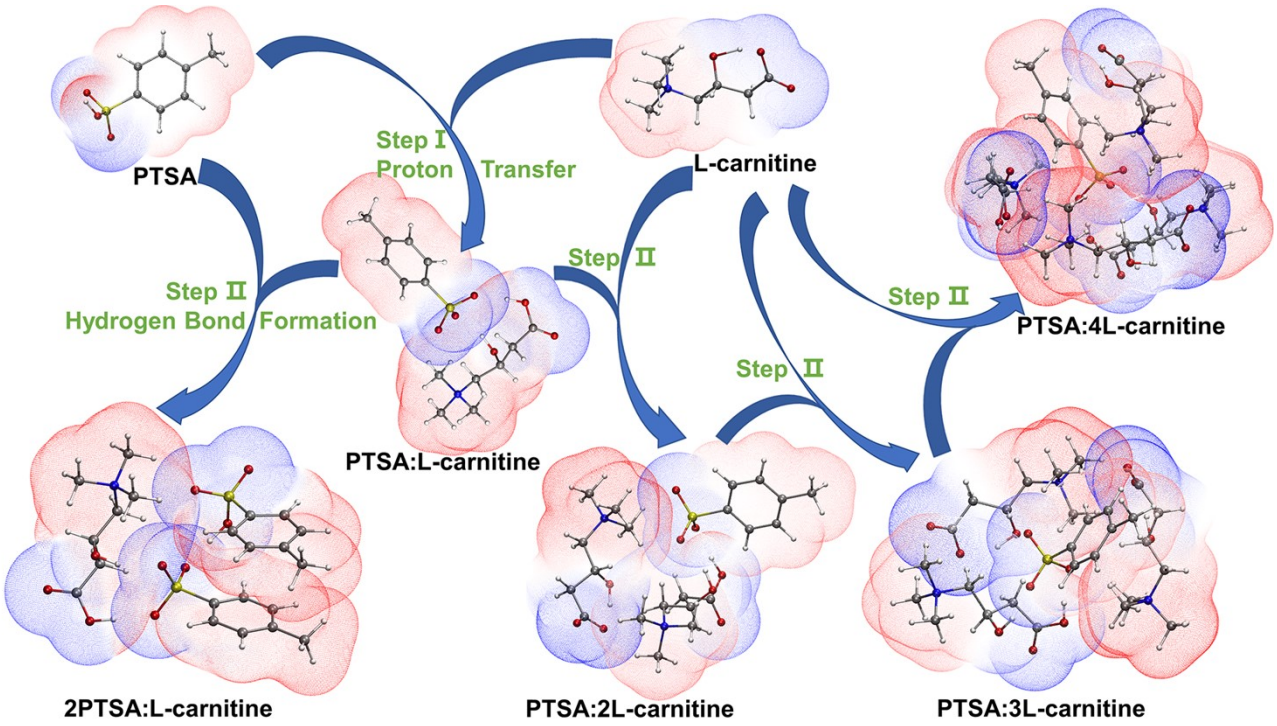


Fig. S2. ESP penetration schematic of DES formation.

8. Evaluation of ligands

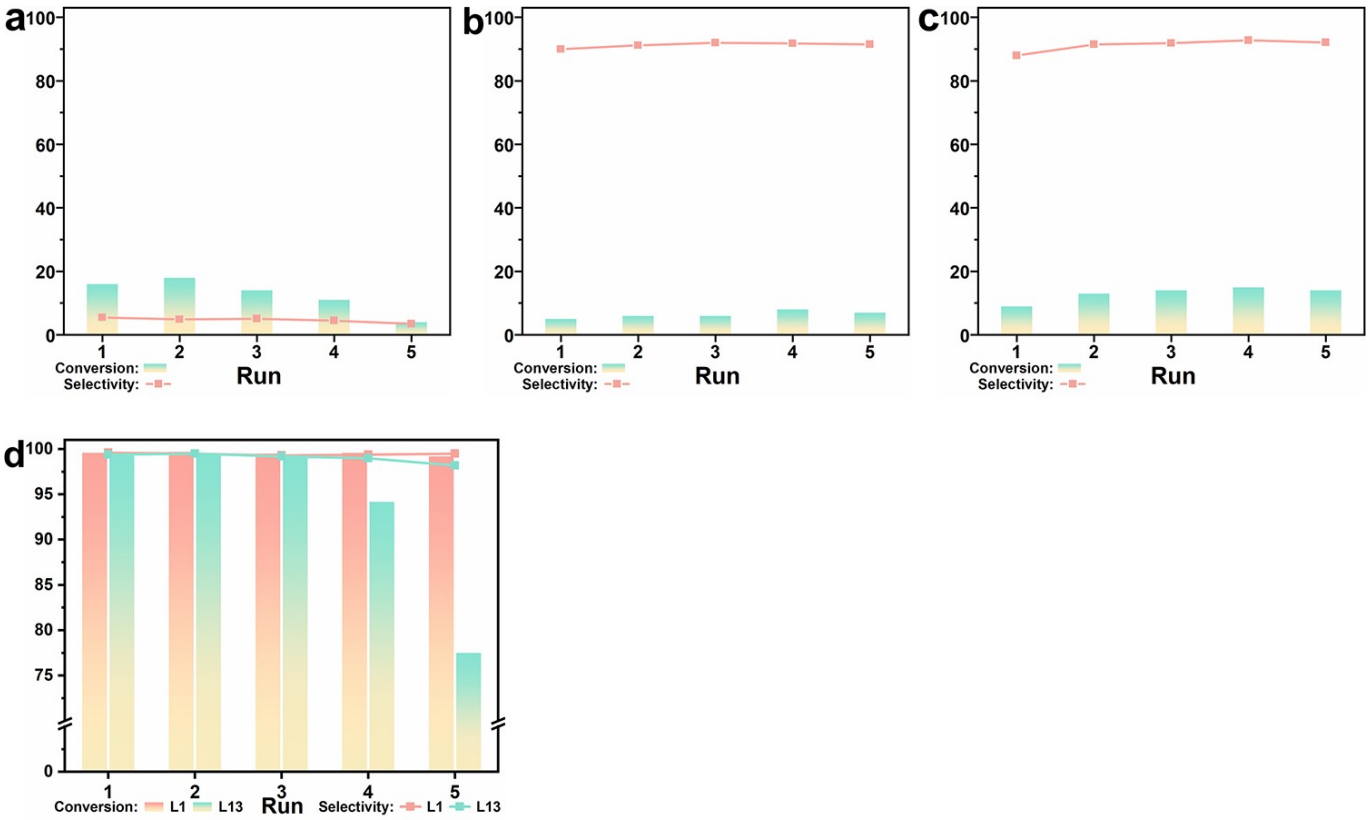


Fig. S3. Evaluation of ligands. (a) L5 (1,4-bis(diphenylphosphino)butane, DPPB). (b) L7 (1,1-Bis(diphenylphosphino)ferrocene, DPPF). (c) L10 (Cyclohexyldiphenylphosphine, Ph_2Pcy). (d) Comparison of the reactivity of L1 and L13 in five consecutive runs. Reaction condition: $Pd(OAc)_2$ (0.013 mmol, 2.9 mg), monodentate ligand (8 equivalents, 0.104 mmol) or bidentate ligand (4 equivalents, 0.052 mmol), n-pentanol (6 mL), PTSA (16 equivalents, 0.208 mmol, 39.6 mg), 10 bar mixed gas, T = 80 °C, t = 2 h.

9. Evaluation of HBD to HBA molar ratio

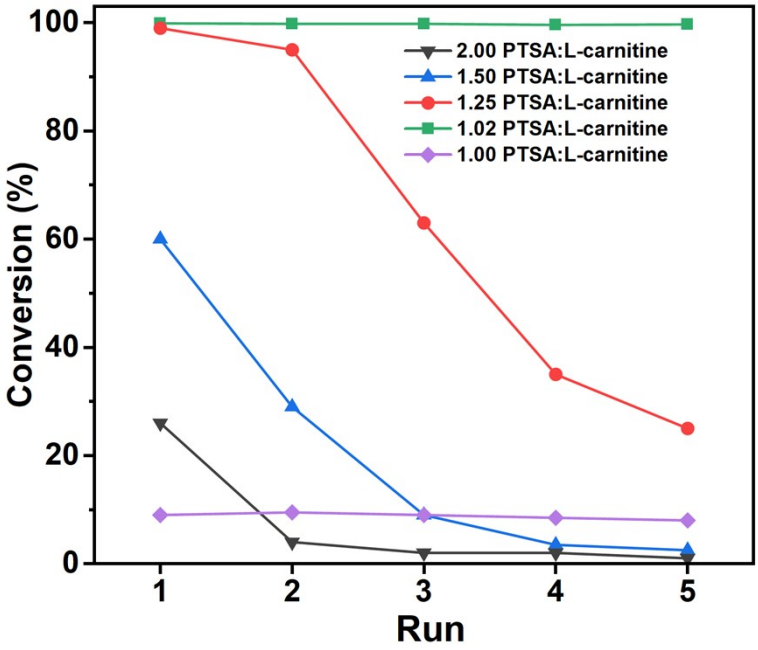


Fig. S4. Evaluation of HBD to HBA Molar Ratio. Reaction condition: $Pd(OAc)_2$ (0.013 mmol, 2.9 mg), 1,2-DTBPMB (4 equivalents, 0.052 mmol), n-pentanol (6 mL), DES (50 vol% of n-pentanol), 10 bar mixed gas, T = 80 °C, t = 2 h.

10. Comparison of catalytic performance with DES composed of halogen-containing HBA or weakly acidic HBD

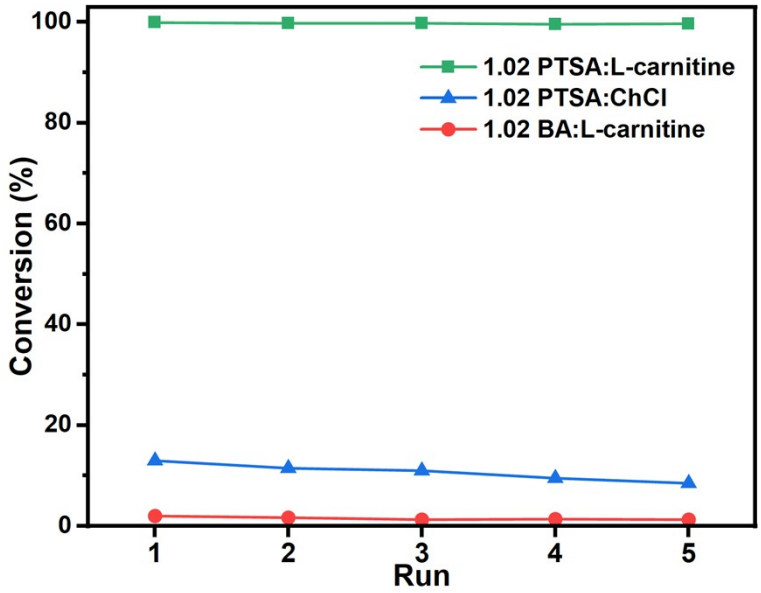


Fig. S5. Comparison of catalytic performance with DES composed of halogen-containing HBA or weakly acidic HBD. Reaction condition: $Pd(OAc)_2$ (0.013 mmol, 2.9 mg), 1,2-DTBPMB (4 equivalents, 0.052 mmol), n-pentanol (6 mL), DES (50 vol% of n-pentanol), 10 bar mixed gas, T = 80 °C, t = 2 h.

11. Concentrations of Pd and P in DES phase and product phase after reaction

Table S6. ICP-OES results of Pd and P in product and DES phase.

Entry	Pd in ester phase (μg/g)	Pd in DES phase (μg/g)	P from 1,2-DTBPMB in ester phase (μg/g)	P from 1,2-DTBPMB in DES phase (μg/g)
1	5	335	10	788

12. NCI diagrams of ligand-DES interactions

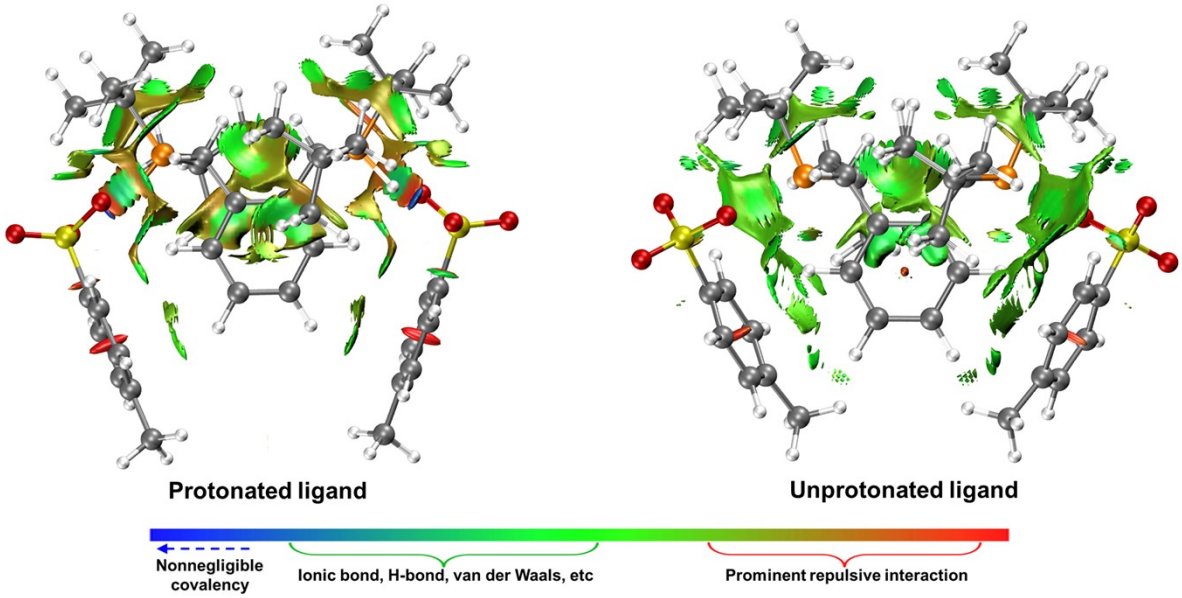


Fig. S6. NCI diagrams of ligand-DES interactions.

13. Evaluation of nucleophiles

Table S7. Details of nucleophile evaluation.

Entry	Nucleophile	Volume/mL	Mass/g	Quantity/mol
1	Methanol	6.0	4.75	0.1481
2	Ethanol	6.0	4.74	0.1028
3	n-Propanol	6.0	4.82	0.0803
4	iso-Propanol	6.0	4.71	0.0785
5	n-Butanol	6.0	4.86	0.0656
6	iso-Butanol	6.0	4.82	0.0650
7	n-Pentanol	6.0	4.87	0.0552
8	iso-Pentanol	6.0	4.85	0.0551
9	n-Hexanol	6.0	4.88	0.0478

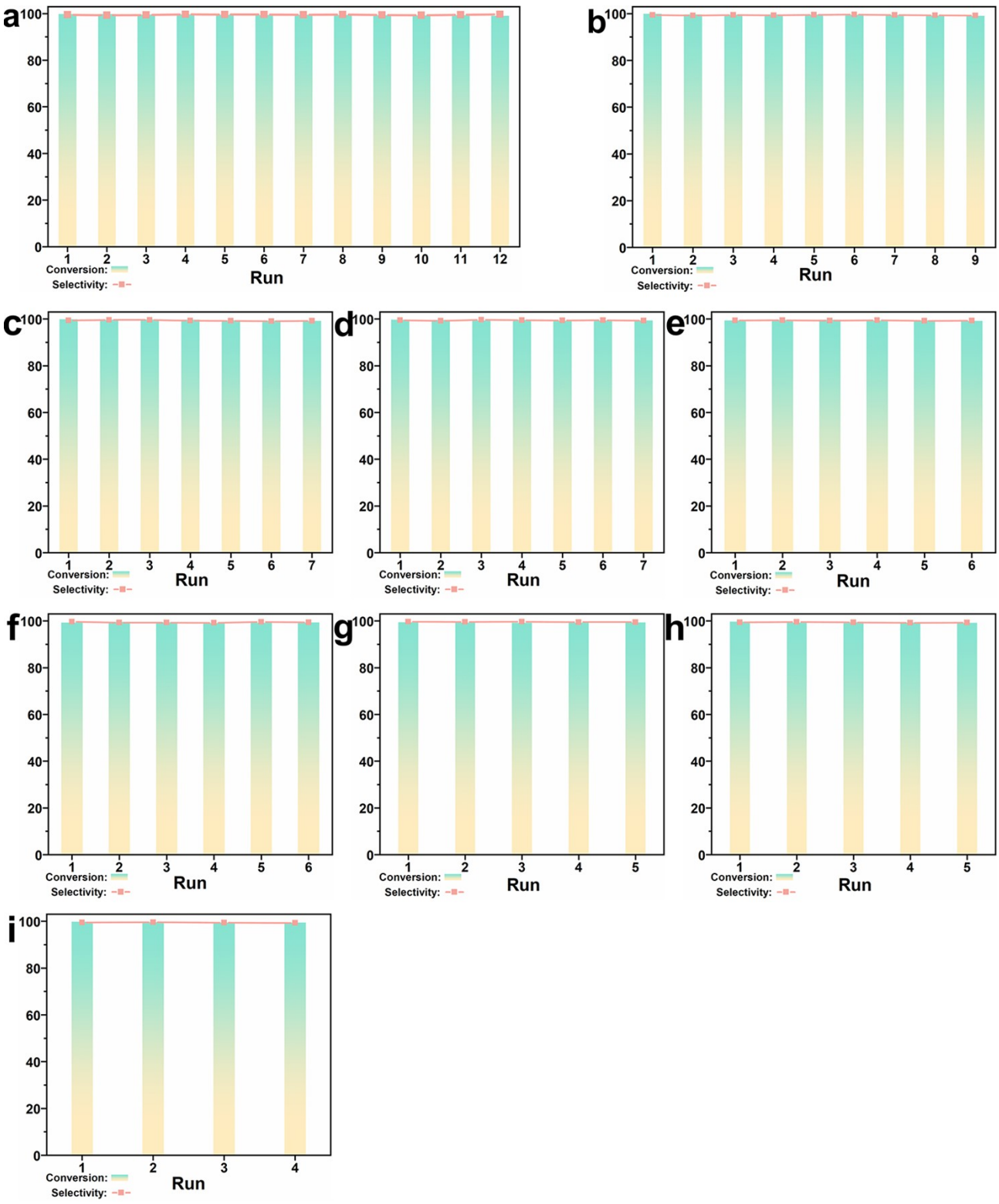


Fig. S7. Evaluation of nucleophiles. (a) methanol. (b) ethanol. (c) n-propanol. (d) iso-propanol. (e) n-butanol. (f) iso-butanol. (g) n-pentanol. (h) iso-pentanol. (i) n-hexanol. Reaction condition: $Pd(OAc)_2$ (0.013 mmol, 2.9 mg), L1 (4 equivalents, 0.052 mmol), nucleophile (6 mL), DES (50 vol% of alcohol), 10 bar mixed gas, T = 80 °C, t = 2 h, for iso-propanol, iso-butanol and iso-pentanol, T = 90 °C. Conversion of ethylene was determined by the pressure

drop of the gas mixture. Selectivity was determined by analyzing the product mixture using GC-FID with toluene as the internal standard.

14. Energy profile under implicit solvent model

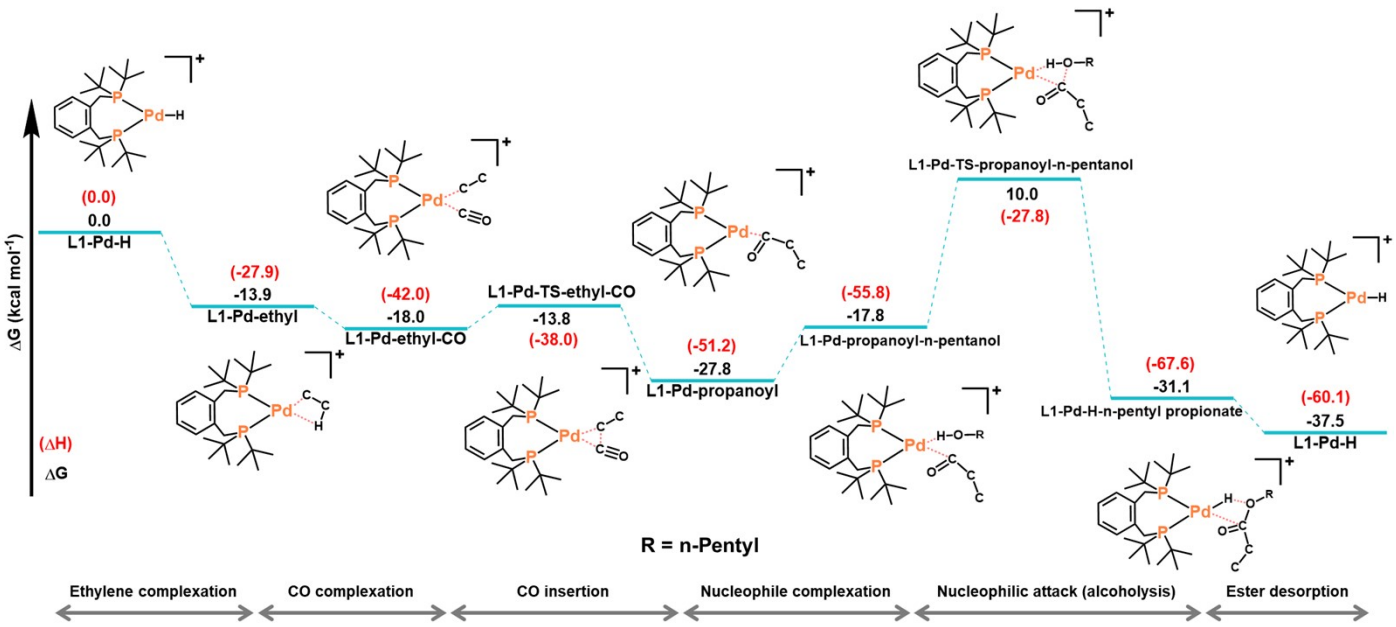


Fig. S8. Energy profile using L1 as ligand, ethylene as olefin substrate and n-pentanol as a nucleophile at PBE0-D3(BJ)/def2-TZVP-SCRF//PBE0-D3(BJ)/def2-SVP level.

Self-consistent reaction field (SCRF) single-point energies were calculated on the PBE0-D3(BJ)/def2-SVP optimized geometries at the PBE0-D3(BJ)/def2-TZVP-SCRF level by using the solvation model based on density (SMD) and n-pentanol was applied as the solvent to estimate the solvation influence (PBE0-D3(BJ)/def2-TZVP-SCRF//PBE0-D3(BJ)/def2-SVP). The thermal corrections to Gibbs free energy and enthalpy at 298 K from the frequency analysis at PBE0-D3(BJ)/def2-SVP level were added to the energy calculations.

Compared to the calculated energy in the gas phase, the Gibbs free energy (ΔG) of ethylene insertion is 4.1 kcal mol^{-1} lower in gas phase. There is a major difference in the Gibbs free energy (ΔG) from that in the gas phase, where the Gibbs free energy (ΔG) of CO insertion is <0 when applying the solvent model, which indicate that the CO insertion is a spontaneous process. While the calculated results in the gas phase indicate that the Gibbs free energy (ΔG) of CO insertion is slightly >0. From intermediate L1-Pd-ethyl-CO to transition state L1-Pd-TS-ethyl-CO, the Gibbs free energy (ΔG) applied the solvent model is 0.5 kcal mol^{-1} lower than that in the gas phase. In the generation of intermediate L1-Pd-propanoyl, the Gibbs free energy (ΔG) calculated by applying the solvent model is 3.7 kcal mol^{-1} lower than that in the gas phase. The Gibbs free energy (ΔG) of the subsequent insertion of n-

pentanol is 3.7 kcal mol^{-1} in the gas phase and 10 kcal mol^{-1} in the solvent. Alcoholysis, the rate-limiting step of alkoxycarbonylation, requires a heat uptake of 27.0 kcal mol^{-1} in the gas phase and 28.0 kcal mol^{-1} in the solvent, the Gibbs free energy (ΔG) is 26.8 kcal mol^{-1} in the gas phase compared to 27.8 kcal mol^{-1} in the solvent. Whether in the gas phase or in solution, the alcoholysis presents the greatest energy barrier. In the following n-pentyl propionate formation, the Gibbs free energy (ΔG) in the gas phase is -37.6 kcal mol^{-1}, while in solution is -41.1 kcal mol^{-1}. Finally, the desorption of the product and regeneration of the reactive intermediate L1-Pd-H, the Gibbs free energy (ΔG) is -2.8 kcal mol^{-1} in the gas phase and -6.4 kcal mol^{-1} in the solution. In general, ethylene alkoxycarbonylation with n-pentanol is an exothermic reaction and alcoholysis is the rate-limiting step.

15. Energy profile of alcoholysis under explicit solvent

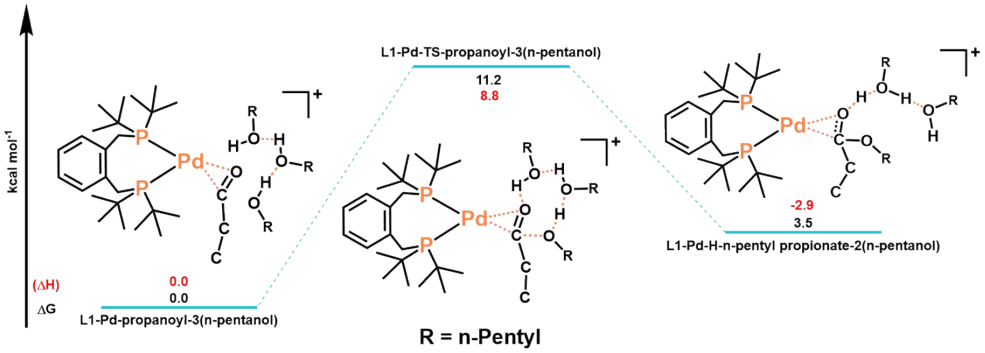


Fig. S9. Energy profile of alcoholysis under explicit solvent using L1 as ligand, ethylene as olefin substrate and n-pentanol as a nucleophile at PBE0-D3(BJ)/def2-TZVP//PBE0-D3(BJ)/def2-SVP level.

16. CHEM21 green metrics toolkit analysis

The following formulas were used for calculating Atom Economy (AE), Reaction Mass Efficiency (RME), Optimum Efficiency (OE) and Process Mass Intensity (PMI).[2, 3]

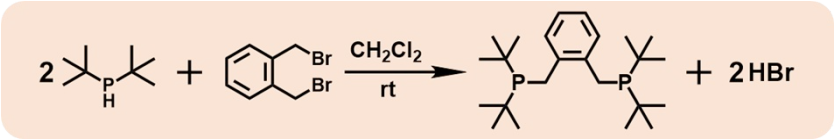
$$AE = \frac{\textit{Molecular weight of product}}{\textit{Total molecular weight of reactants}} \times 100$$

$$RME = \frac{\textit{Mass of isolated product}}{\textit{Total mass of reactants}} \times 100$$

$$OE = \frac{RME}{AE} \times 100$$

$$PMI = \frac{\textit{Total mass in a process or process step}}{\textit{Mass of product}}$$

Synthesis of Ligand L1:



Experimental procedure: Di-tert-butylphosphine (4.15 mmol, 0.6 g) and ortho-xylylene-dibromide (1.98 mmol, 0.52 g) were dissolved in 5 mL CH_2Cl_2 and stirred at room temperature overnight in a Schlenk tube. triethylamine (1.7 mL, 12.5 mmol, 1.25 g) was added and the solution was stirred for 0.5 h. The solvent was pumped off in vacuo to get a white residue. The product was extracted with n-hexane and flushed over a small column with silica gel (6 x 2 mL). Evaporation of the solvent in vacuo yielded the product as white powder (5-10%).[4]

Green chemistry metrics of Ligand L1 Synthesis (Based on 7.5% yield)

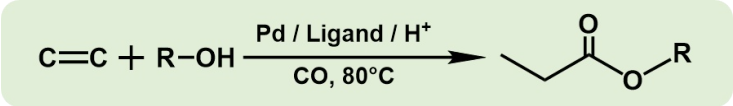
$$AE = \frac{394.55}{146.21 \times 2 + 263.96} \times 100 = 70.9$$

$$RME = \frac{0.059}{0.600 + 0.520} \times 100 = 5.3$$

$$OE = \frac{5.3}{70.9} \times 100 = 7.5$$

$$PMI = \frac{0.6 + 0.52 + 5 \times 1.325 + 1.25 + 6 \times 2 \times 0.659}{0.059} = 286.5$$

Alkoxycarbonylation：



Experimental procedure: Take the synthesis of n-pentyl propionate as an example. An autoclave was charged with the corresponding $Pd(OAc)_2$ (0.013 mmol, 2.9 mg), 1,2-DTBPMB (4 equivalents, 0.052 mmol, 20.5 mg), DES (3 mL, 3.765 g), ethylene (5 bar, 0.00887 mol, 0.248 g), CO (5 bar, 0.00887 mol, 0.248 g) and n-pentanol (6 mL, 0.0552 mol, 4.866 g). Then, it was heated and stirred at 80 °C for 2 h and repeat the procedure of feeding the gas mixture 5 times. The upper product phase was decanted and evaporated to afford 6.242 g of n-Pentyl propionate in 99.4% yield.

Green chemistry metrics of alkoxycarbonylation

$$AE = \frac{144.25}{28.05 + 28.01 + 88.15} \times 100 = 100$$

$$RME = \frac{6.242}{0.248 \times 5 + 0.248 \times 5 + 4.866} \times 100 = 85.0$$

$$OE = \frac{85.0}{100} \times 100 = 85.0$$

$$PMI(\text{without DES recycled}) = \frac{0.0029 + 0.0205 + 3.765 + 1.240 + 1.240 + 4.866}{6.242} = 1.784$$

$$PMI(\text{with DES recycled}) = \frac{1.240 + 1.240 + 4.866}{6.242} = 1.177$$

Table S8. Qualitative appraisal of solvents used, inherent hazards of reagents and reactants, reagent used, energy and work up methods for the synthesis of pentyl propionate through alkoxycarbonylation.

Solvents	Flag	Health and safety	Flag	Reagent used	Flag	Energy	Flag	Work up	Flag
None		Ethylene, CO, n-pentanol, H220		Pd, phosphine ligand, PTSA, L-carnitine		80 °C		High temperature distillation	

As a key component of the catalyst for alkoxycarbonylation, the ligand can directly affect the efficiency of this reaction, while the synthesis of these ligands is notoriously difficult. According to the synthetic procedure reported by Scherer and co-workers,[4] the synthesis of ligand L1 requires the use of excessive hazardous solvents and reagents. It needs chromatography to obtain a pure product and suffers from its low yield (5-10%). The use of DES allows the spontaneous separation of ligand as well as the noble metal, avoiding catalyst deactivation during

high temperature distillation. Moreover, DES and the catalysts in DES can be reused without treatment. The use of DES to separate catalysts can result in more than four times the catalyst lifespan of homogeneous system, which can significantly reduce the use of hazardous solvents and reagents as well as energy in ligand synthesis by reducing ligand consumption.

In high temperature distillation, the catalyst will be deactivated and Pd will aggregate into bulk palladium black, which makes it difficult to regenerate the catalyst. If the aggregation of Pd occurs, it is necessary to add excessive ligand and heat for a long period of time in order to regenerate the catalyst.[5] In the case of DES, the catalyst can be spontaneously separated and recovered before distillation, thus avoiding the deactivation of the catalyst and the aggregation of Pd under high temperature distillation. Even if the catalyst is deactivated after a long period of operation, the unaggregated Pd can be reactivated by the addition of a small amount of ligand without additional heating. Overall, the DES participated alkoxycarbonylation is a green, sustainable and promising protocol for ester synthesis.

17. Variation of density and PH with HBD:HBA ratio

Table S9. Variation of density and PH with HBD:HBA ratio

Entry	Density (g/cm^3)	PH
2.5 PTSA:L-carnitine	1.271	1.05
2.0 PTSA:L-carnitine	1.268	1.07
1.5 PTSA:L-carnitine	1.256	1.17
1.0 PTSA:L-carnitine	1.255	2.27
PTSA:1.5 L-carnitine	1.238	3.59
PTSA:2.0 L-carnitine	1.227	3.86
PTSA:2.5 L-carnitine	1.230	4.01
PTSA:3.0 L-carnitine	1.236	4.25
PTSA:3.5 L-carnitine	1.222	4.45
PTSA:4.0 L-carnitine	1.225	4.65

PH was measured by dissolving 1g DES in 10mL deionized water at 25 °C.

18. ^{1}H and ^{13}C NMR spectra of the formed DESs

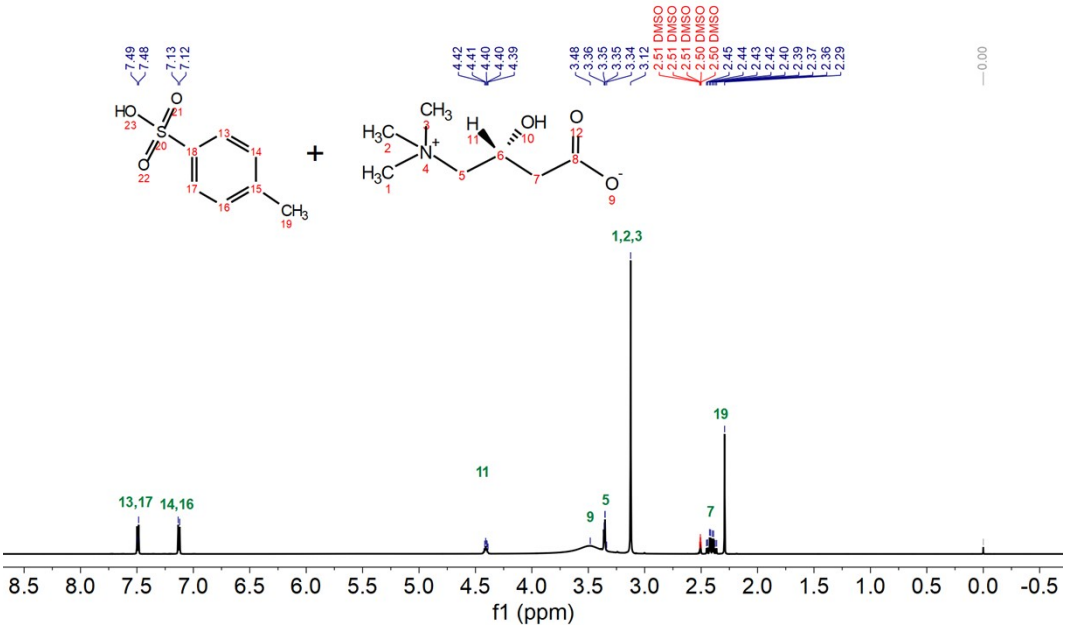


Fig. S10. ^{1}H NMR spectra of PTSA:L-carnitine.

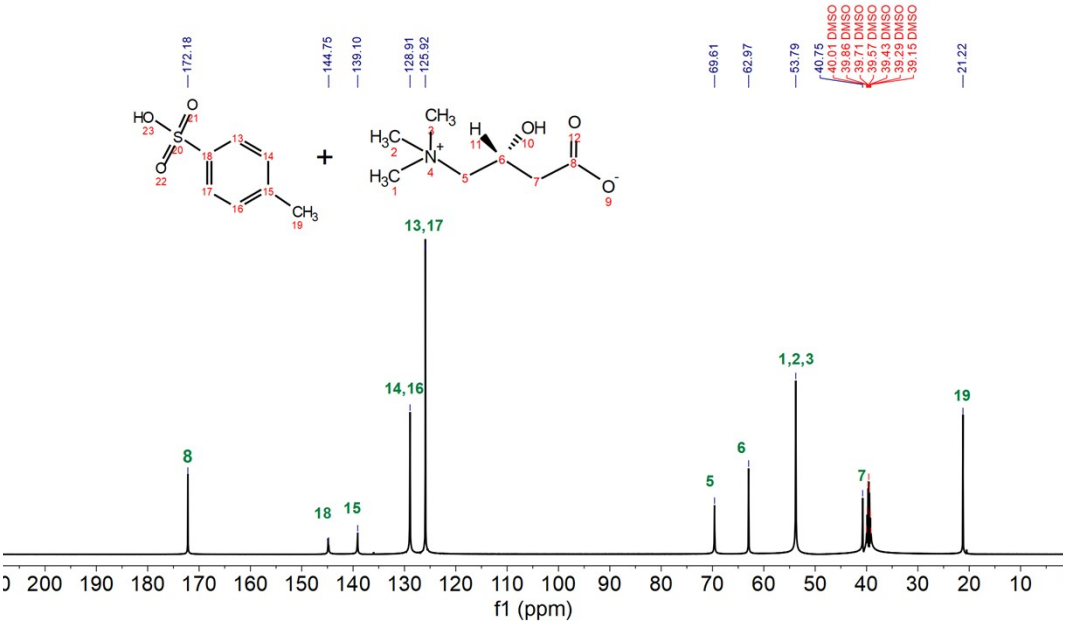


Fig. S11. ^{13}C NMR spectra of PTSA:L-carnitine.

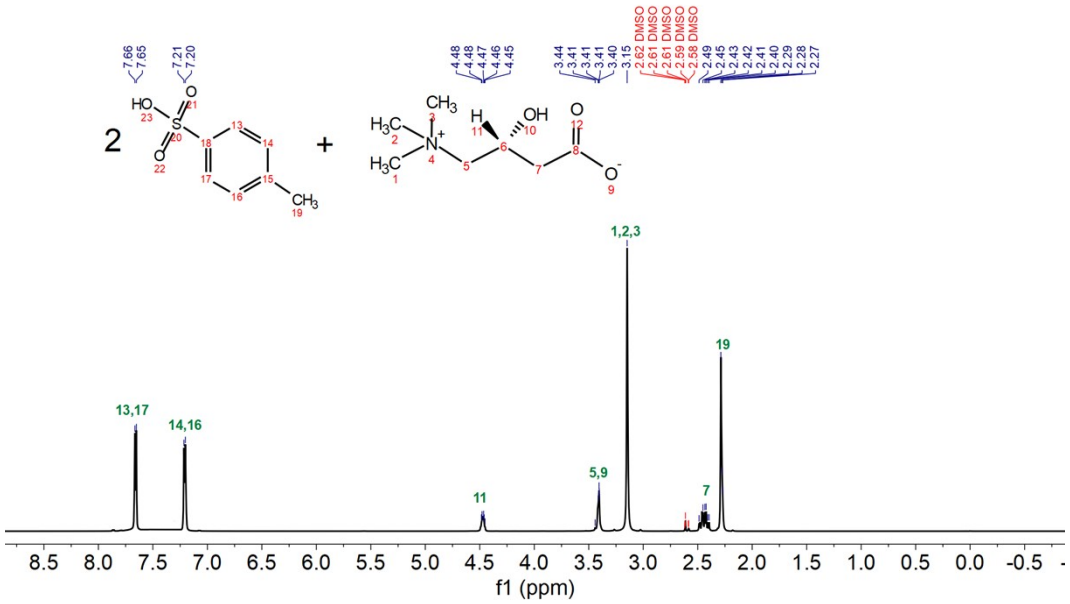


Fig. S12. ^{1}H NMR spectra of 2PTSA:L-carnitine.

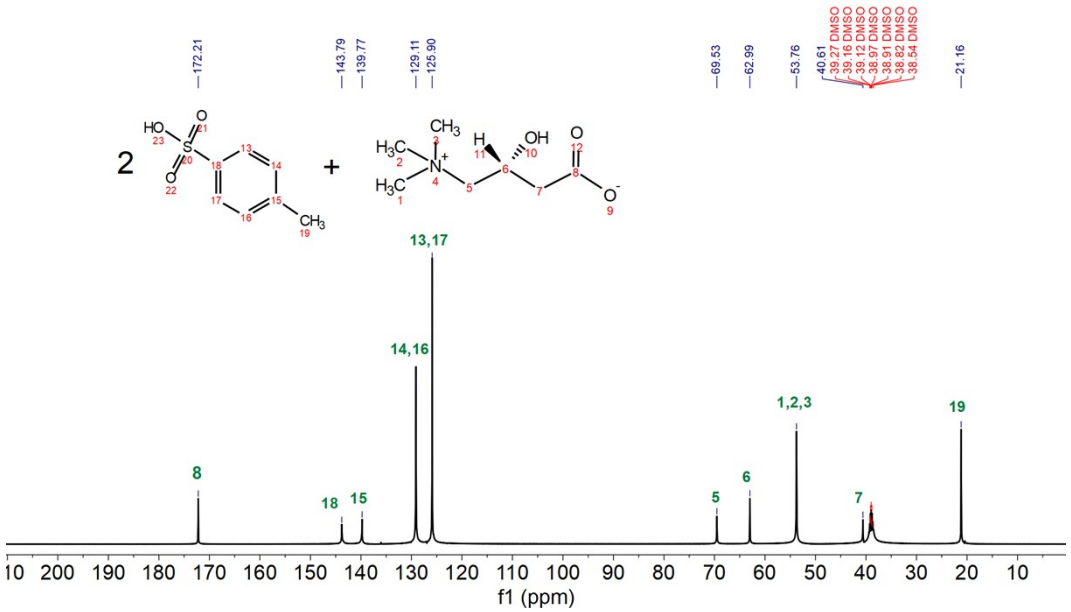


Fig. S13. ^{13}C NMR spectra of 2PTSA:L-carnitine.

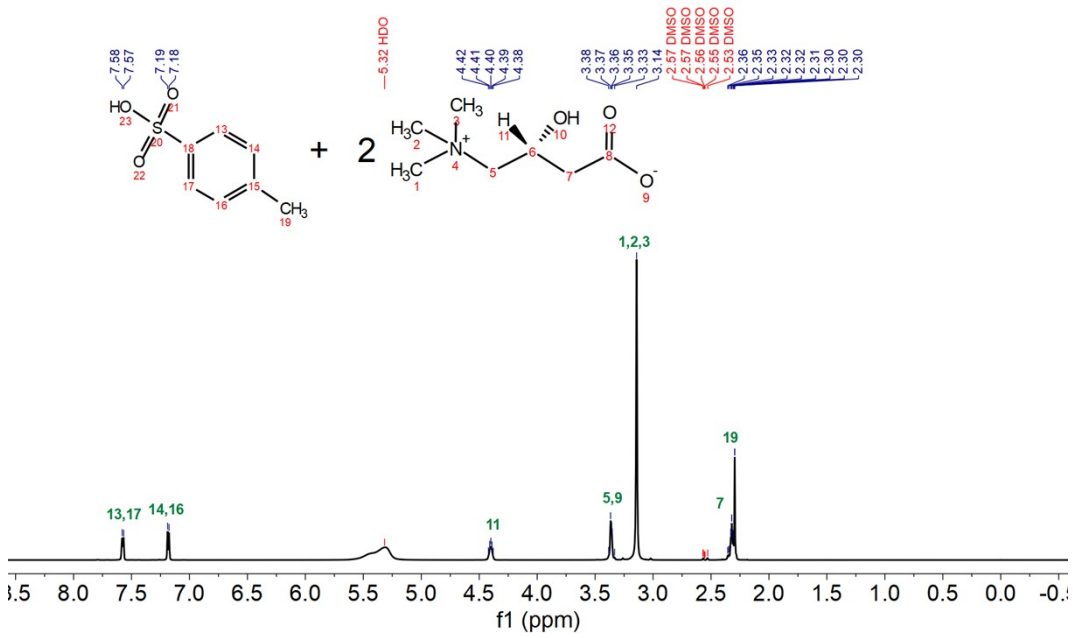


Fig. S14. [1]H NMR spectra of PTSA:2L-carnitine.

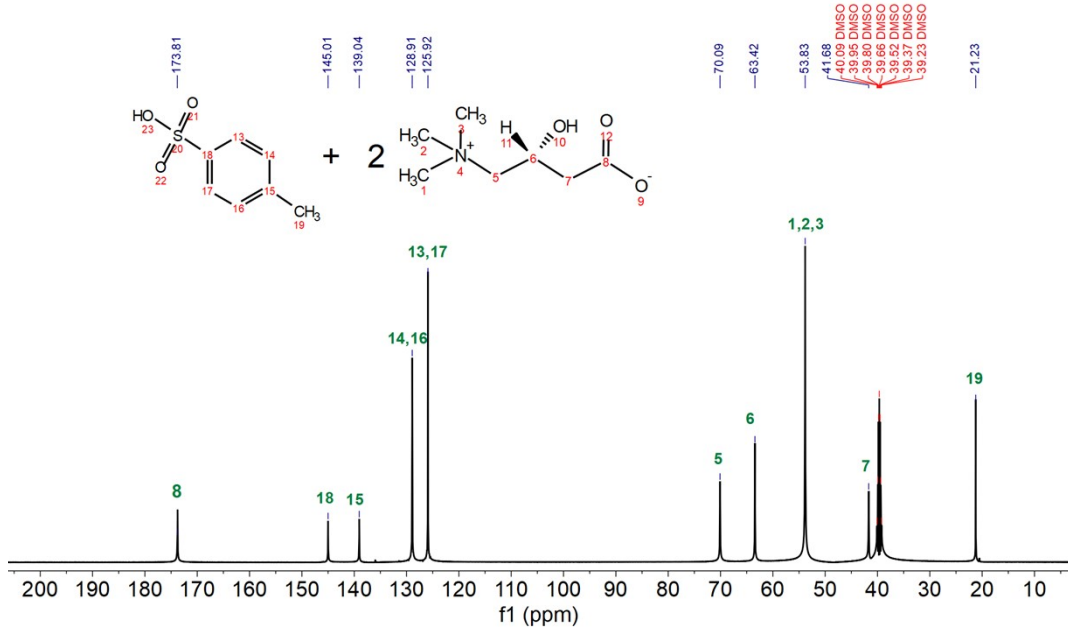


Fig. S15. [13]C NMR spectra of PTSA:2L-carnitine.

19. ^{1}H, ^{13}C NMR and FT-IR spectra of the upper product phase

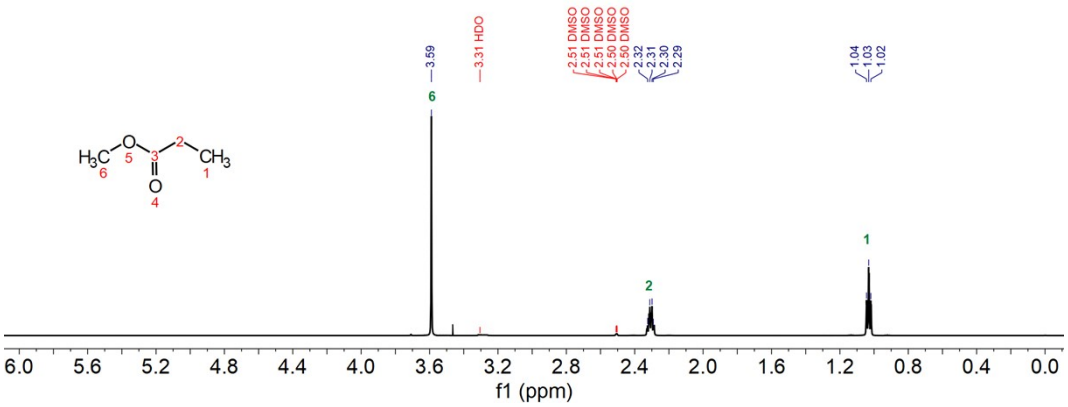


Fig. S16. ^{1}H NMR spectra of the upper product phase with methanol as the nucleophile.

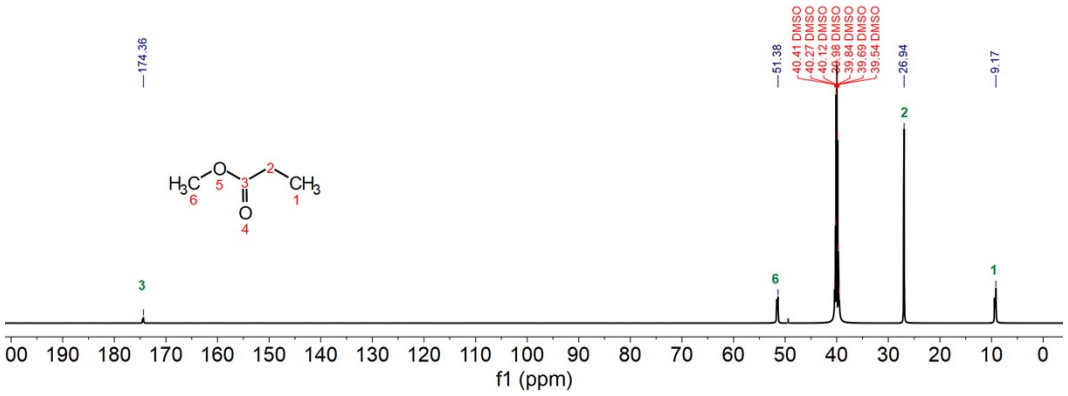


Fig. S17. ^{13}C NMR spectra of the upper product phase with methanol as the nucleophile.

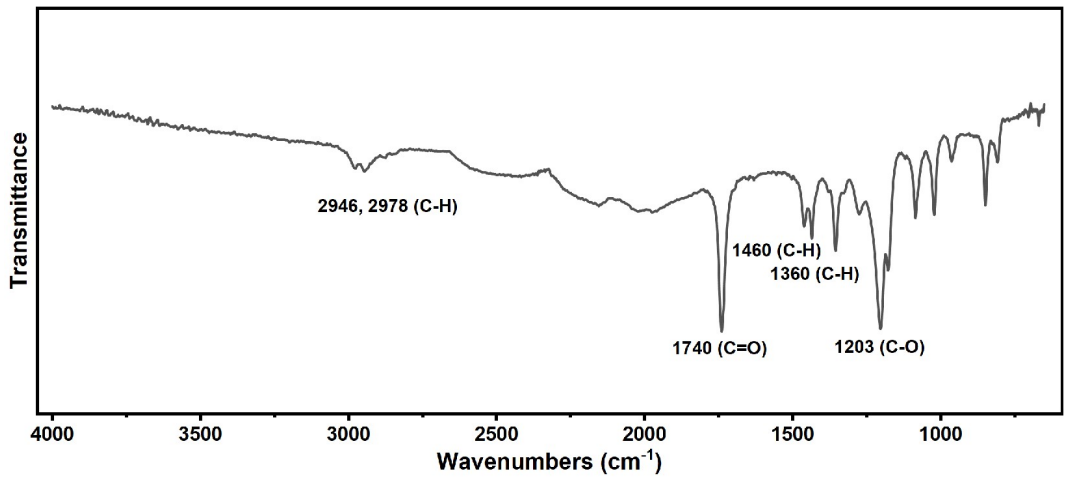


Fig. S18. FT-IR spectra of the upper product phase with methanol as the nucleophile.

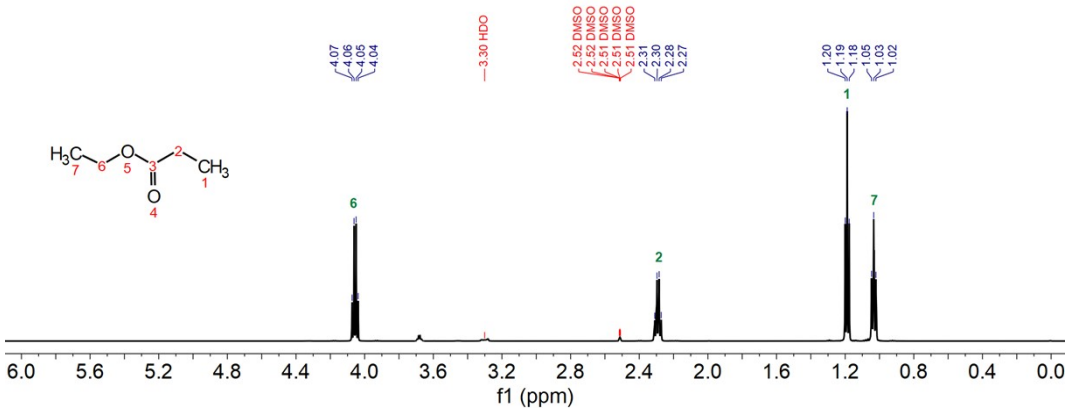


Fig. S19. ^{1}H NMR spectra of the upper product phase with ethanol as the nucleophile.

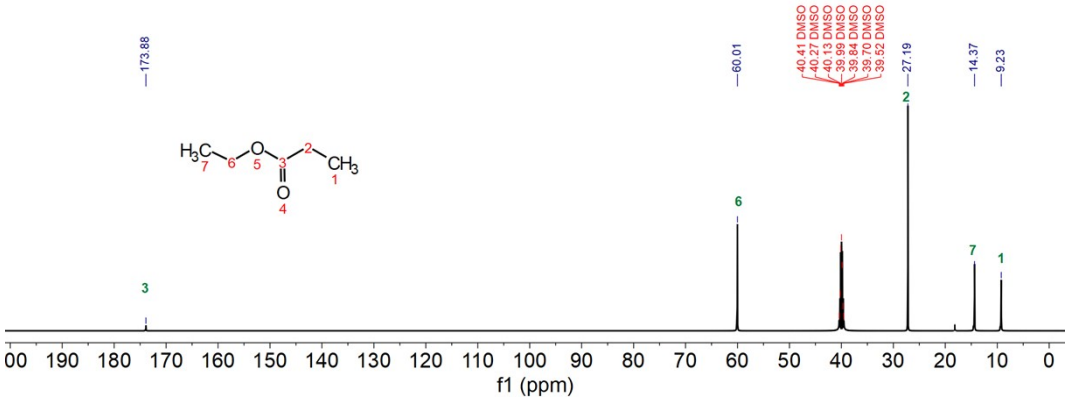


Fig. S20. ^{13}C NMR spectra of the upper product phase with ethanol as the nucleophile.

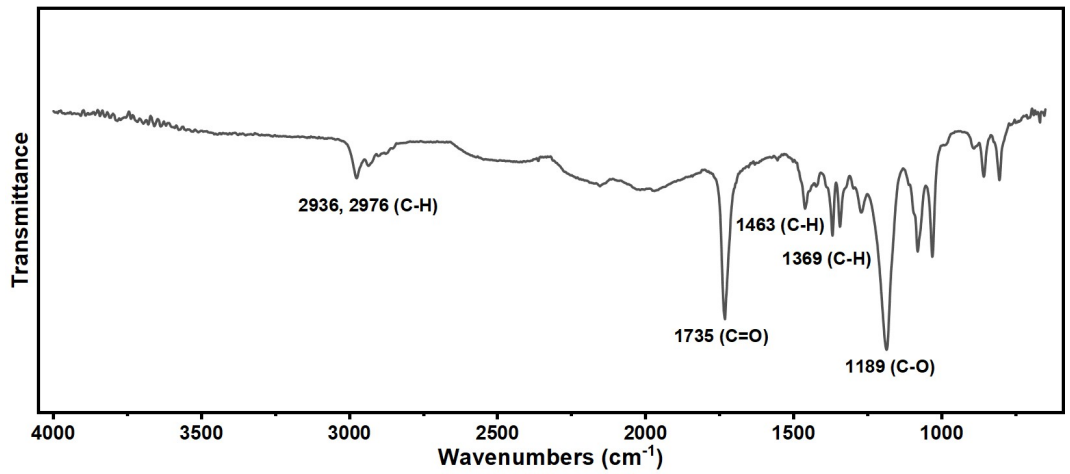


Fig. S21. FT-IR spectra of the upper product phase with ethanol as the nucleophile.

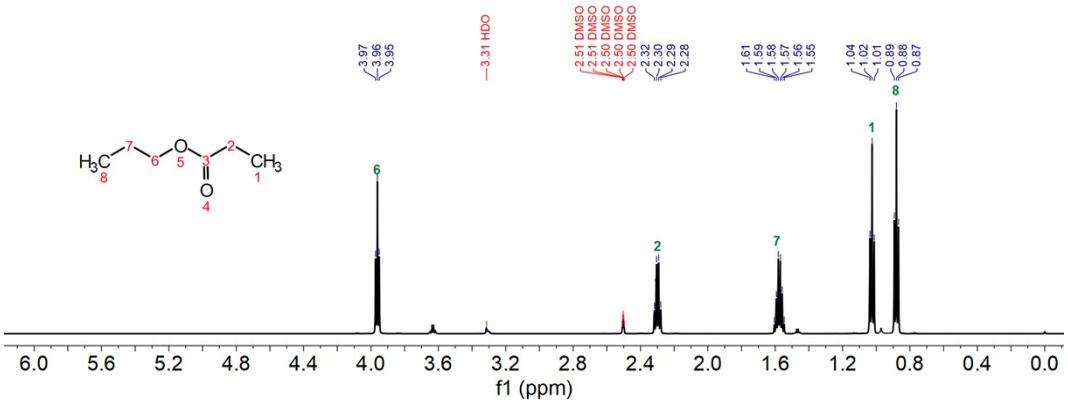


Fig. S22. [1]H NMR spectra of the upper product phase with n-propanol as the nucleophile.

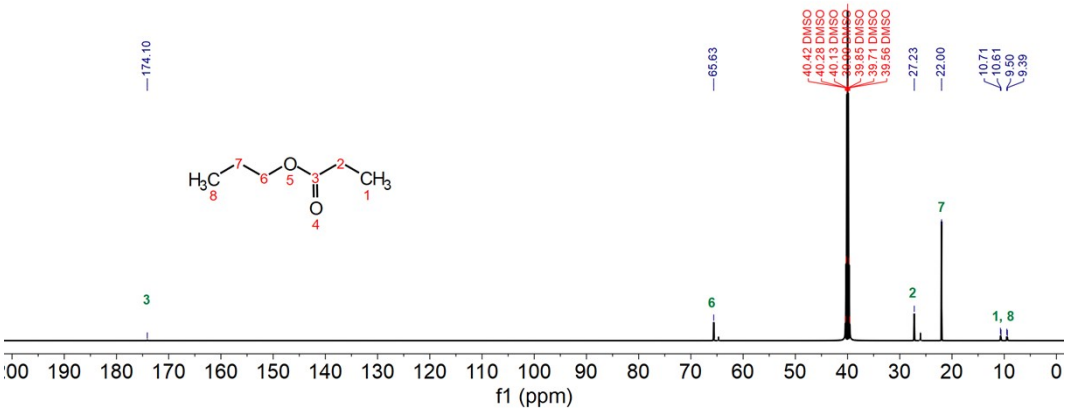


Fig. S23. [13]C NMR spectra of the upper product phase with n-propanol as the nucleophile.

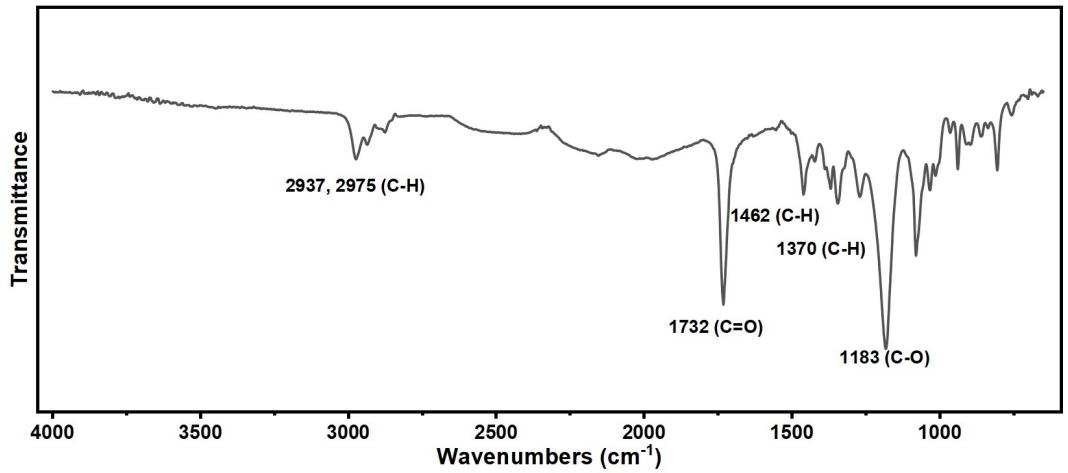


Fig. S24. FT-IR spectra of the upper product phase with n-propanol as the nucleophile.

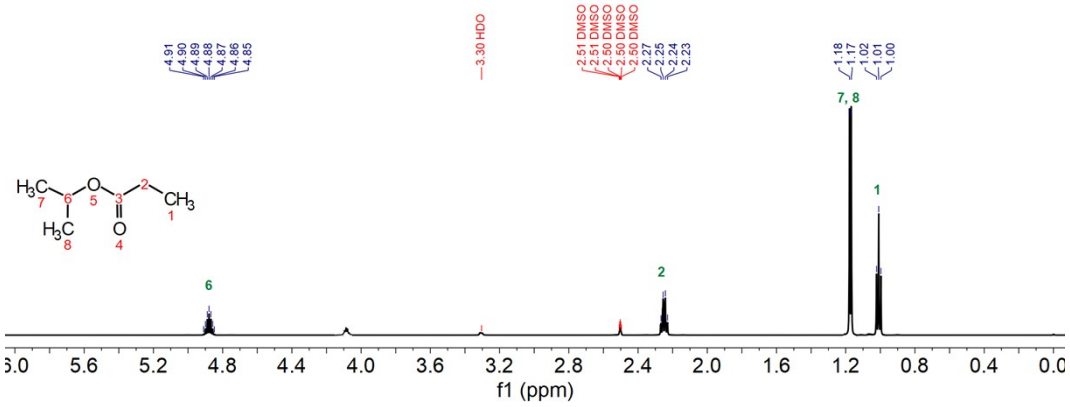


Fig. S25. ^{1}H NMR spectra of the upper product phase with iso-propanol as the nucleophile.

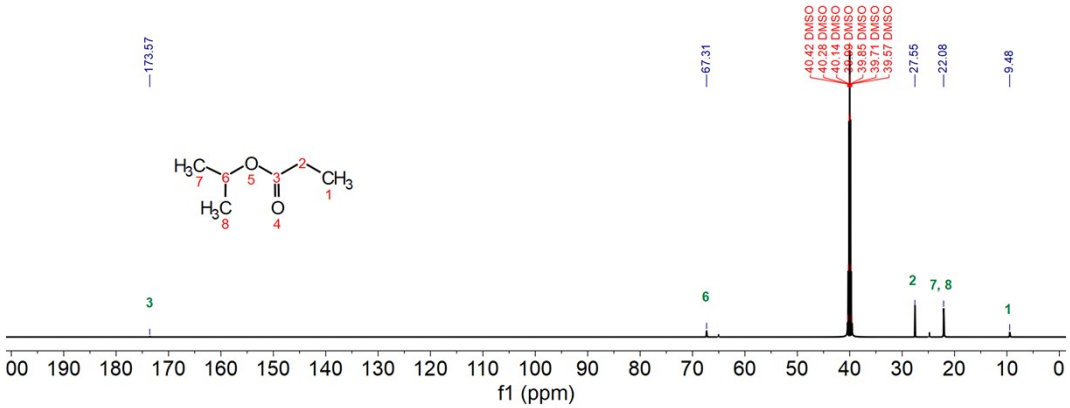


Fig. S26. ^{13}C NMR spectra of the upper product phase with iso-propanol as the nucleophile.

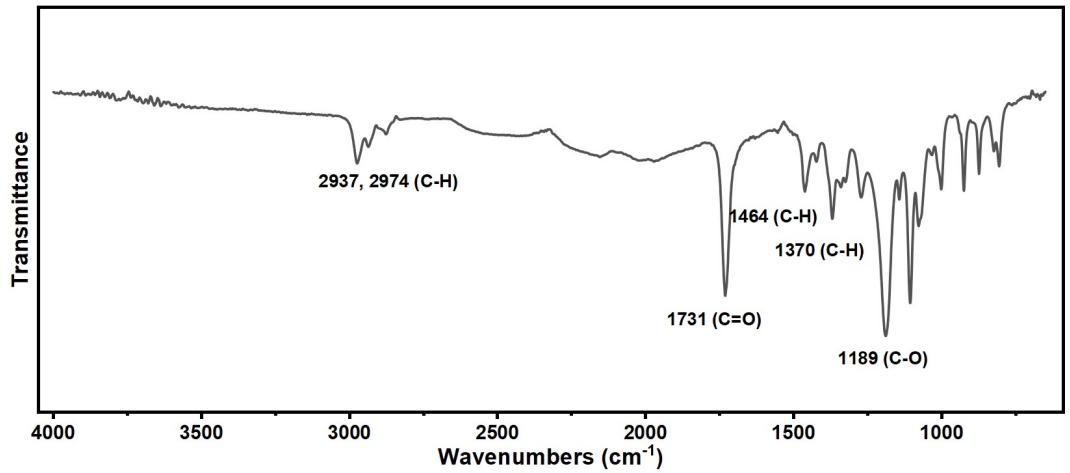


Fig. S27. FT-IR spectra of the upper product phase with iso-propanol as the nucleophile.

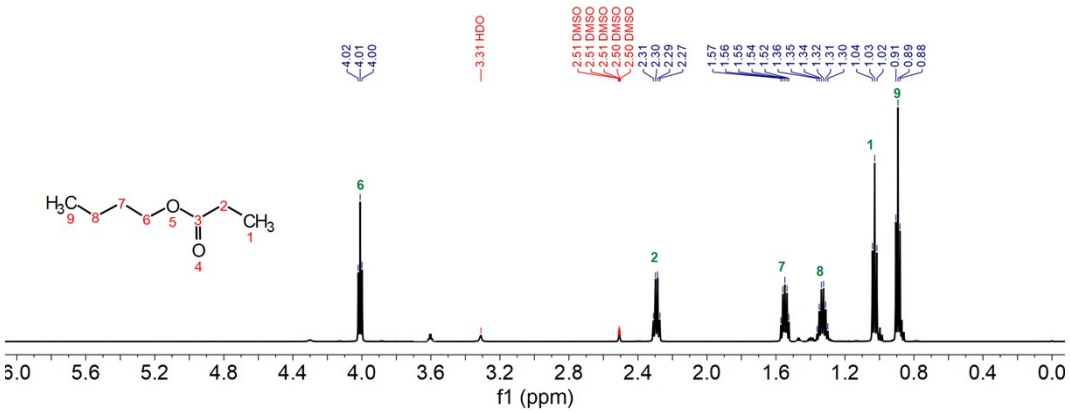


Fig. S28. ^{1}H NMR spectra of the upper product phase with n-butanol as the nucleophile.

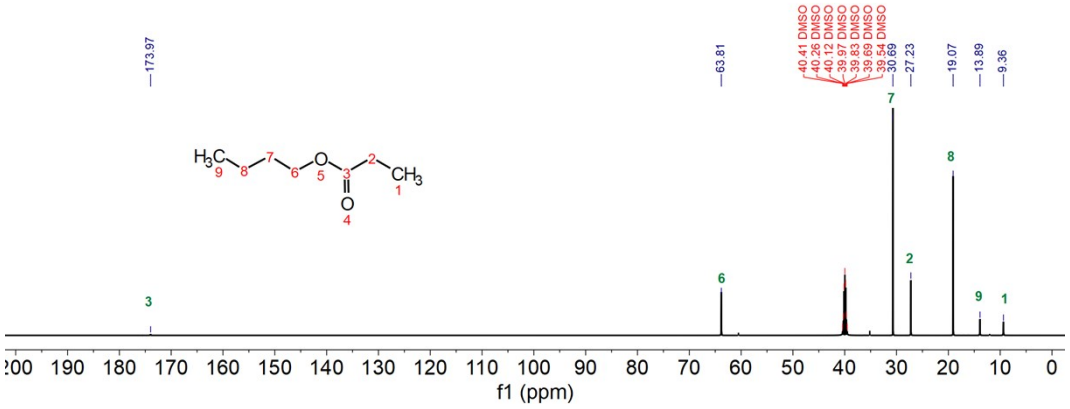


Fig. S29. ^{13}C NMR spectra of the upper product phase with n-butanol as the nucleophile.

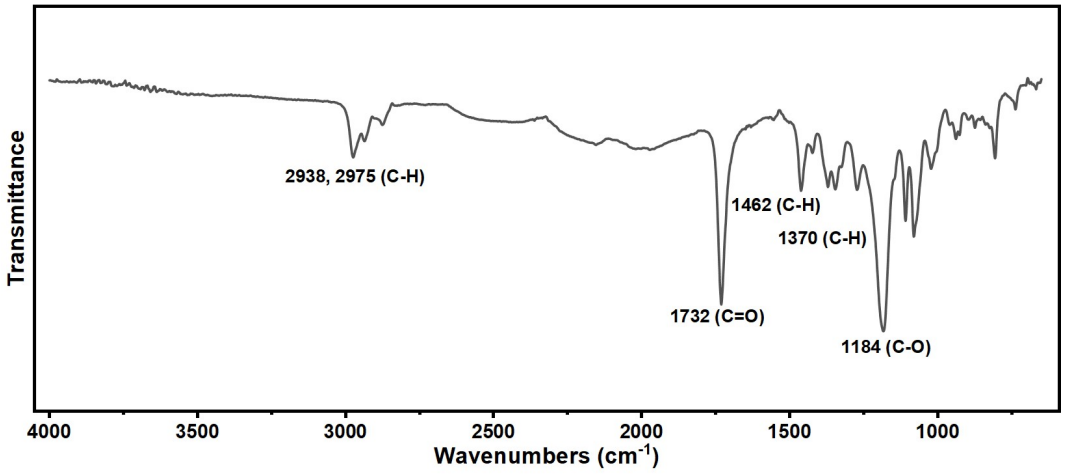


Fig. S30. FT-IR spectra of the upper product phase with n-butanol as the nucleophile.

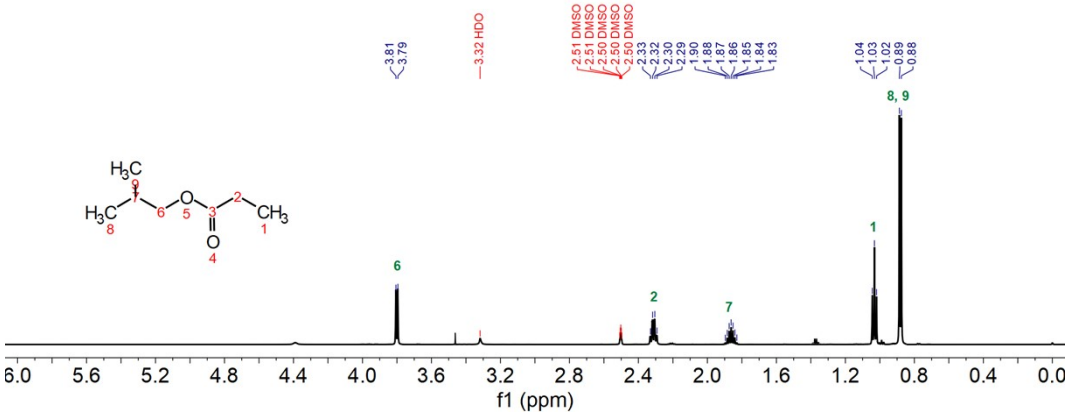


Fig. S31. ^{1}H NMR spectra of the upper product phase with iso-butanol as the nucleophile.

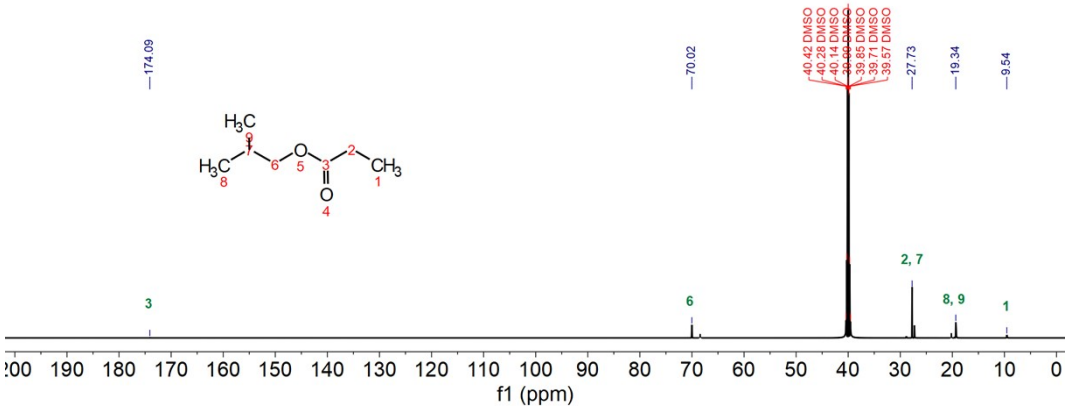


Fig. S32. ^{13}C NMR spectra of the upper product phase with iso-butanol as the nucleophile.

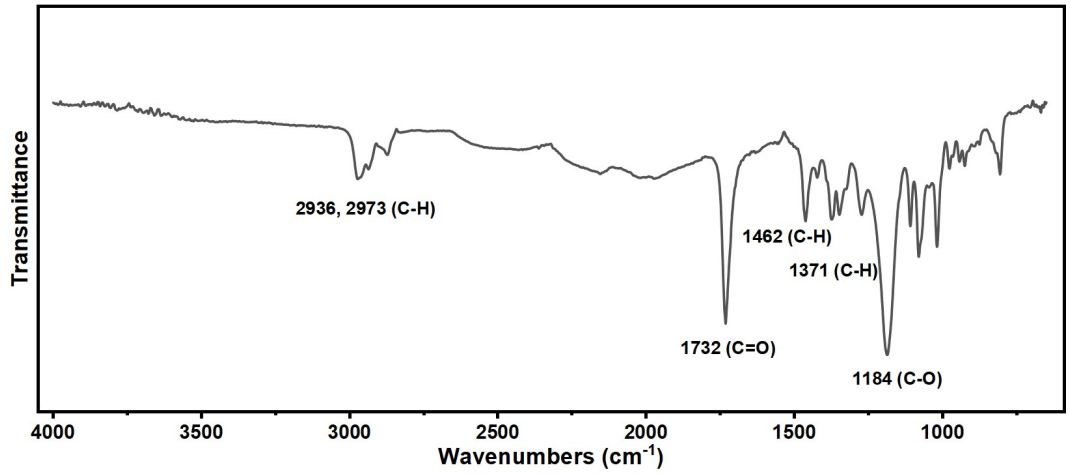


Fig. S33. FT-IR spectra of the upper product phase with iso-butanol as the nucleophile.

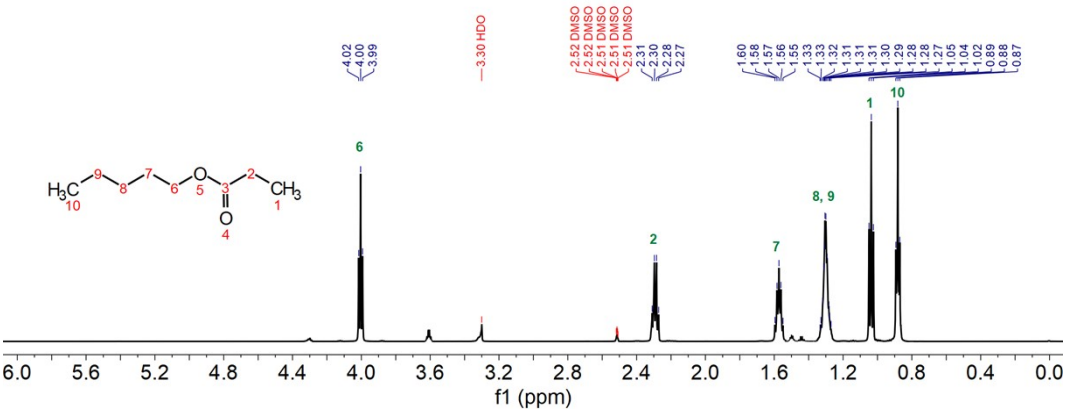


Fig. S34. [1]H NMR spectra of the upper product phase with n-pentanol as the nucleophile.

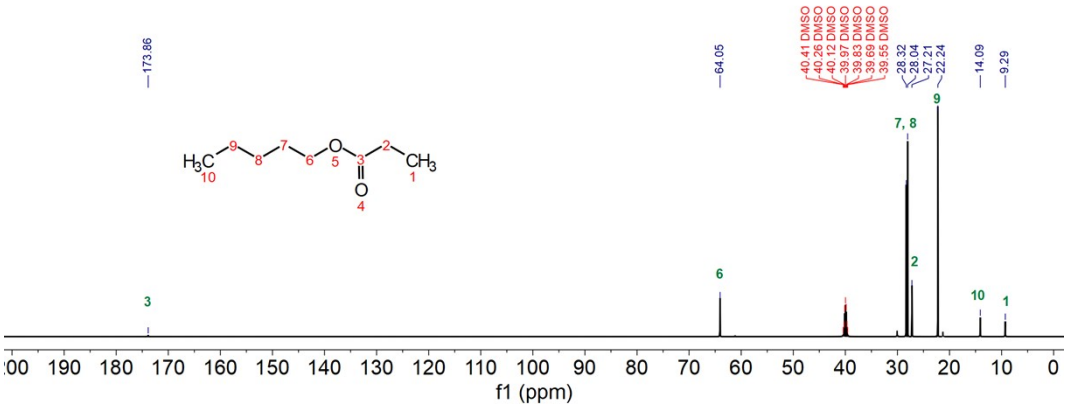


Fig. S35. [13]C NMR spectra of the upper product phase with n-pentanol as the nucleophile.

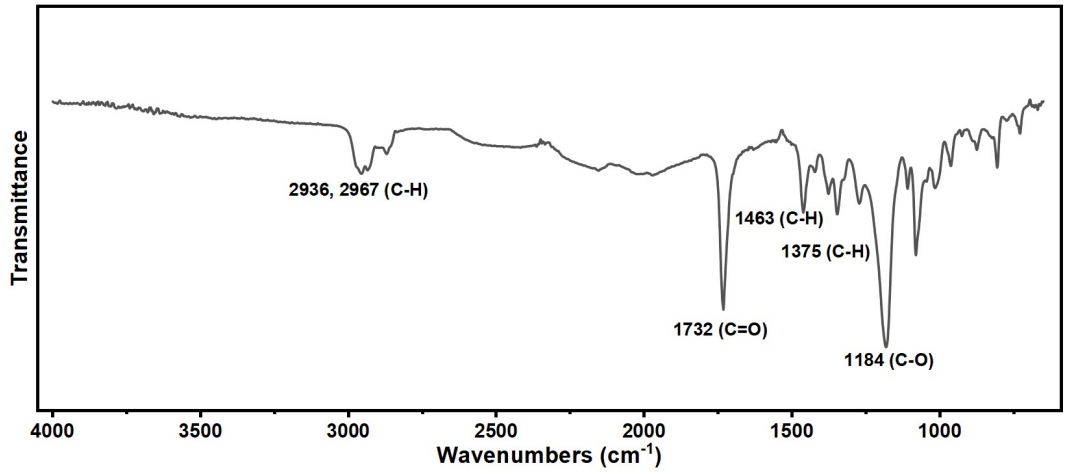


Fig. S36. FT-IR spectra of the upper product phase with n-pentanol as the nucleophile.

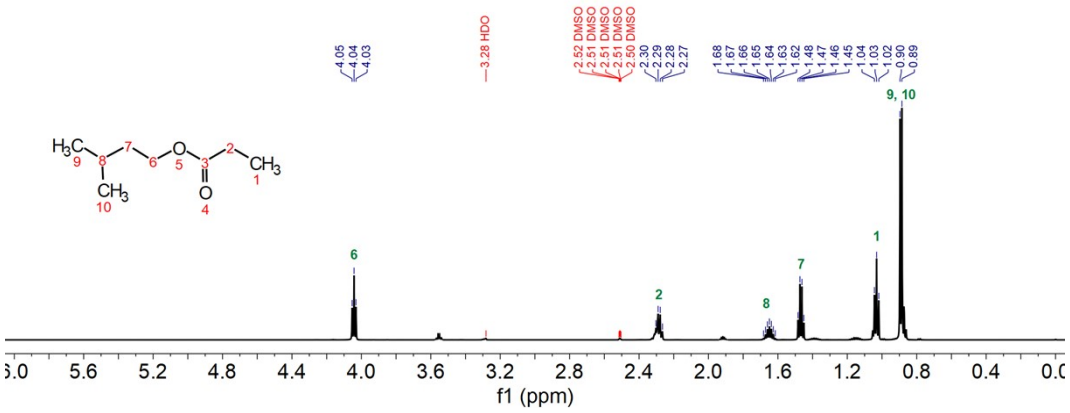


Fig. S37. ^{1}H NMR spectra of the upper product phase with iso-pentanol as the nucleophile.

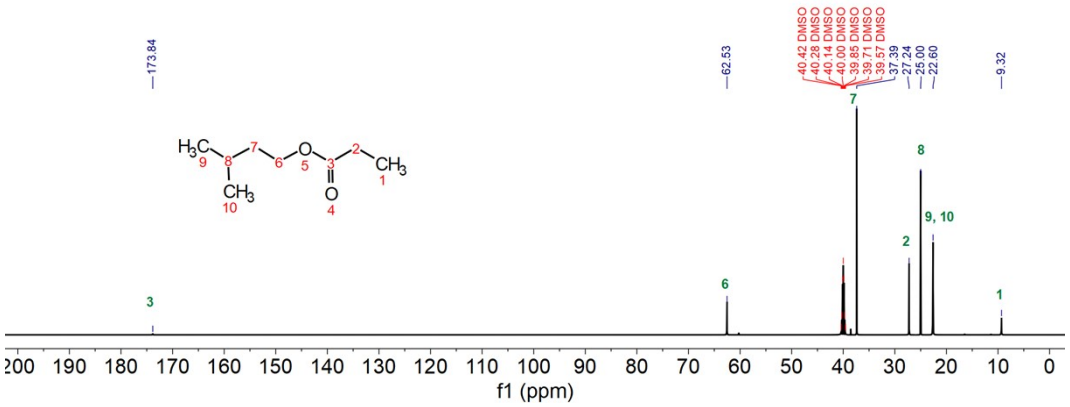


Fig. S38. ^{13}C NMR spectra of the upper product phase with iso-pentanol as the nucleophile.

Fig. S39. FT-IR spectra of the upper product phase with iso-pentanol as the nucleophile.

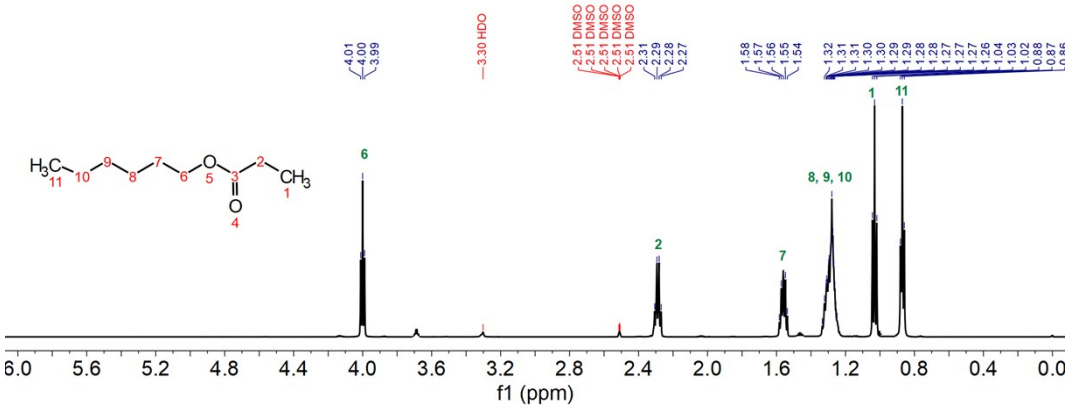


Fig. S40. [1]H NMR spectra of the upper product phase with n-hexanol as the nucleophile.

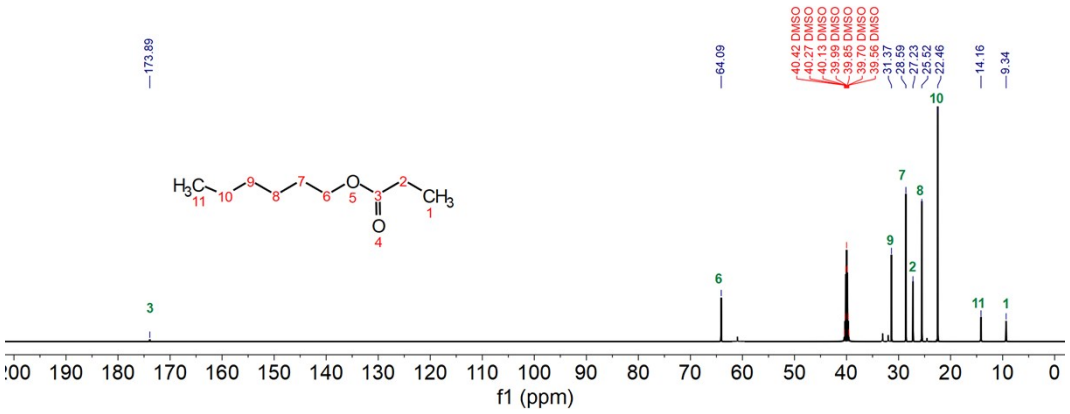


Fig. S41. [13]C NMR spectra of the upper product phase with n-hexanol as the nucleophile.

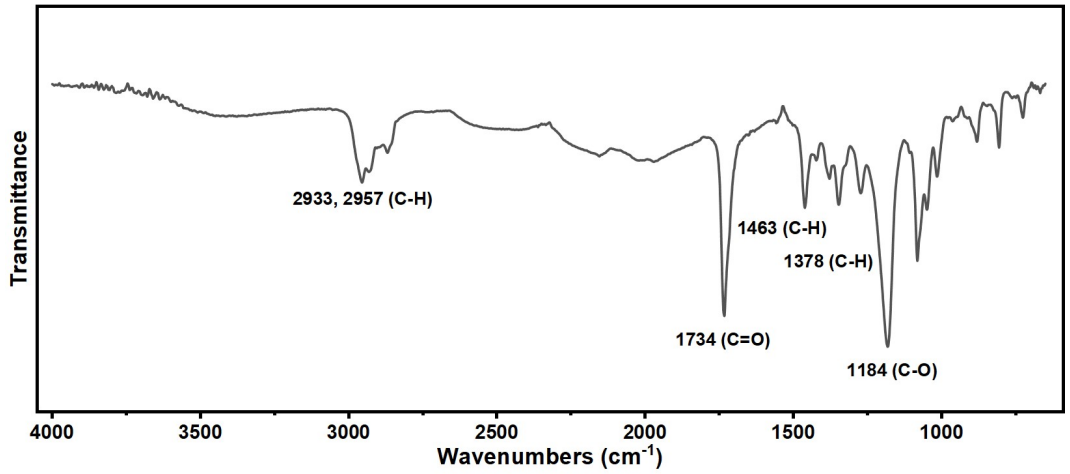


Fig. S42. FT-IR spectra of the upper product phase with hexanol as the nucleophile.

The unlabeled peaks in the ^{1}H and ^{13}C NMR spectra are attributed to the reactant alcohol, and some of the peaks are overlapped with those of the ester.

20. GC spectra of the upper product phase

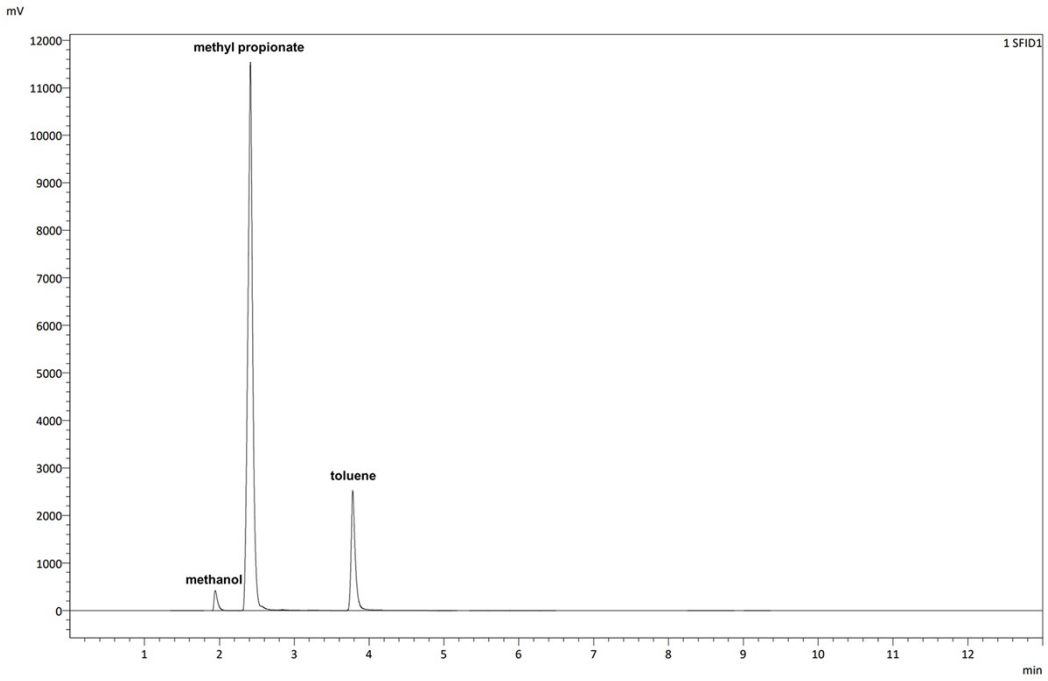


Fig. S43. GC spectra of the upper product phase with methanol as the nucleophile.

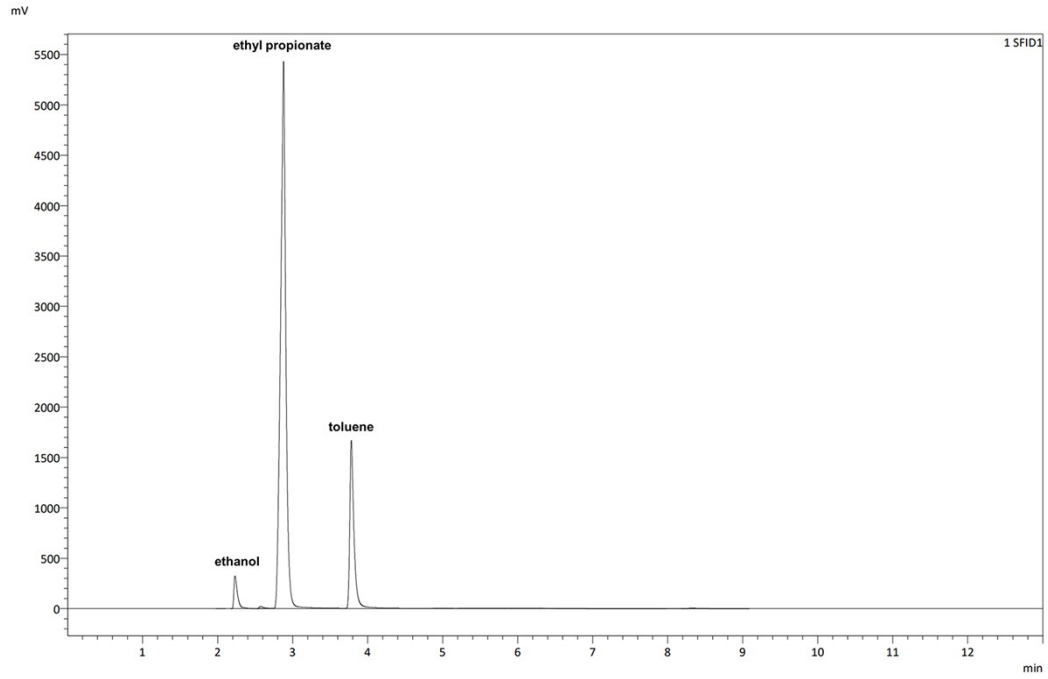


Fig. S44. GC spectra of the upper product phase with ethanol as the nucleophile.

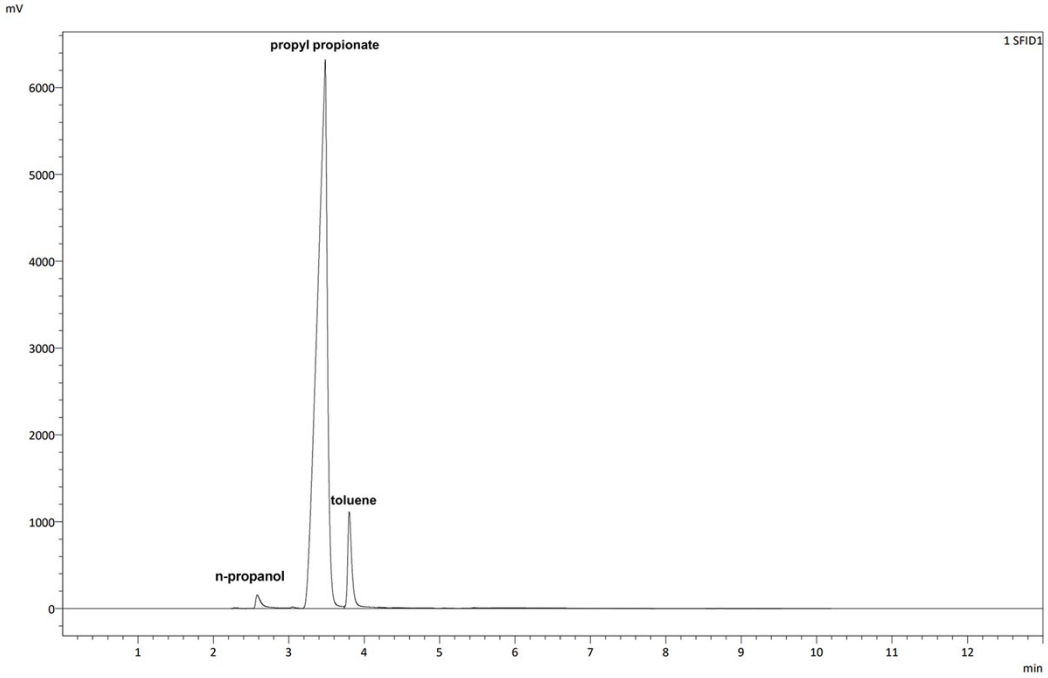


Fig. S45. GC spectra of the upper product phase with n-propanol as the nucleophile.

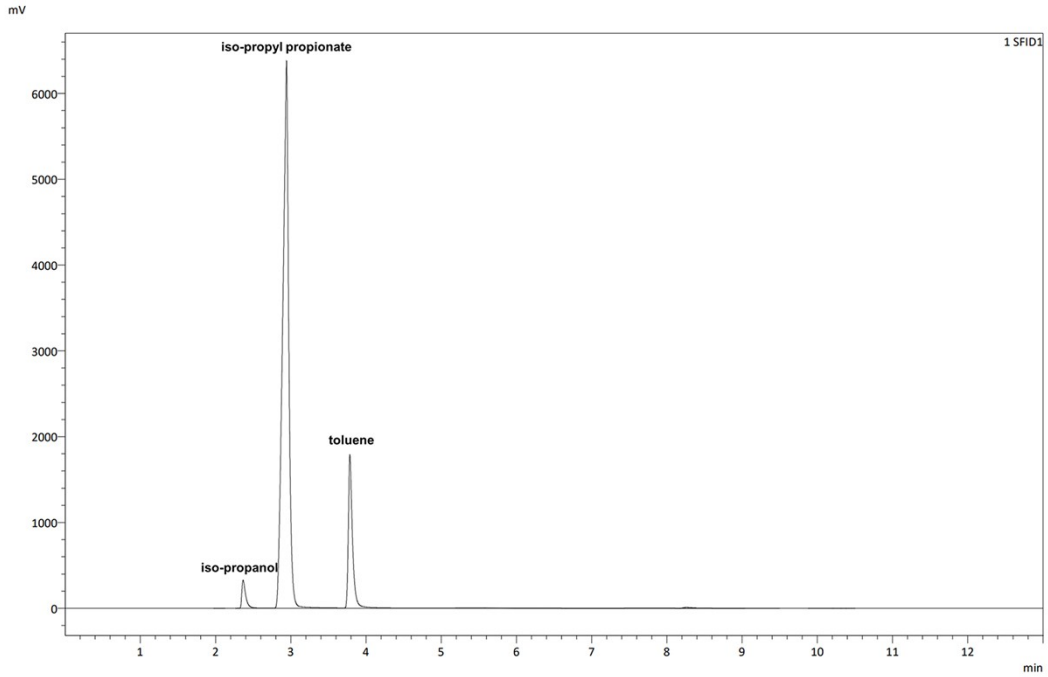


Fig. S46. GC spectra of the upper product phase with iso-propanol as the nucleophile.

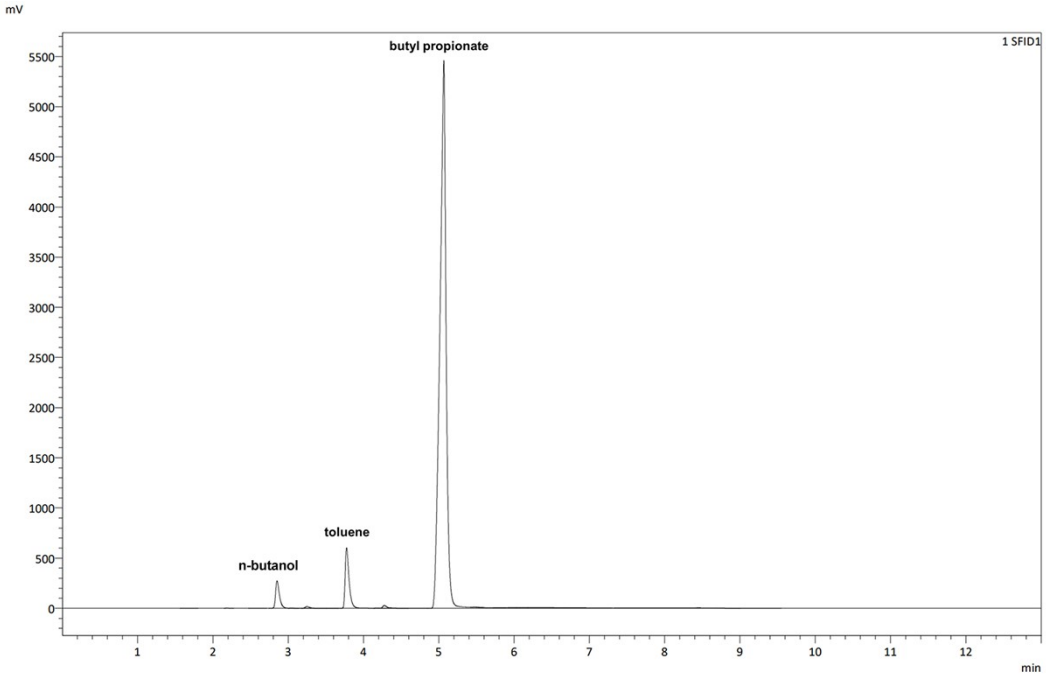


Fig. S47. GC spectra of the upper product phase with n-butanol as the nucleophile.

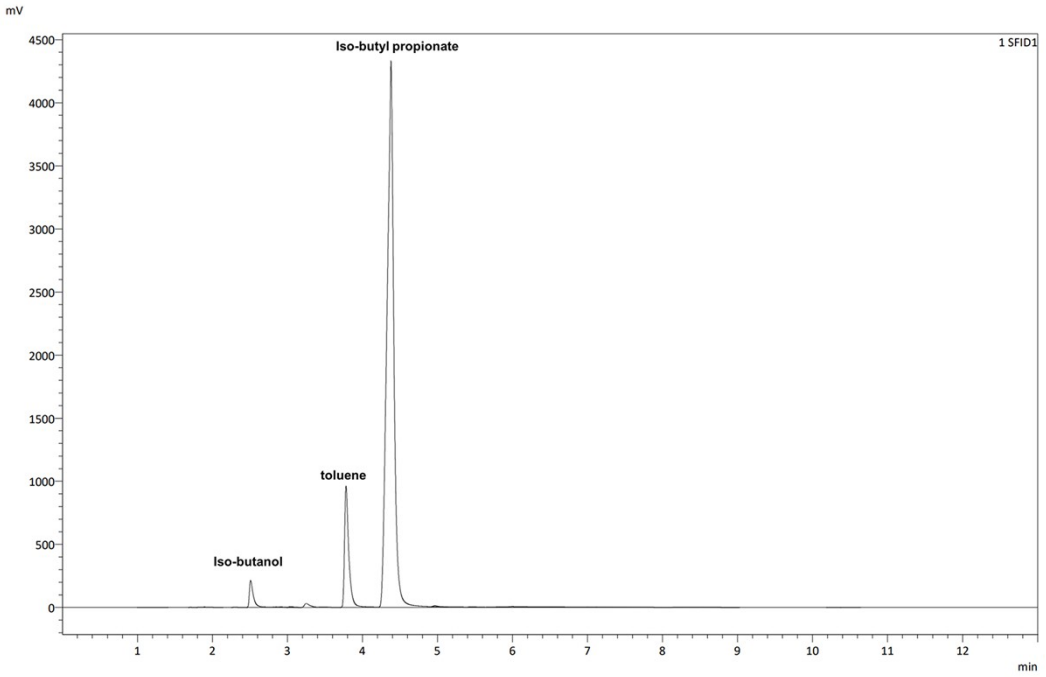


Fig. S48. GC spectra of the upper product phase with iso-butanol as the nucleophile.

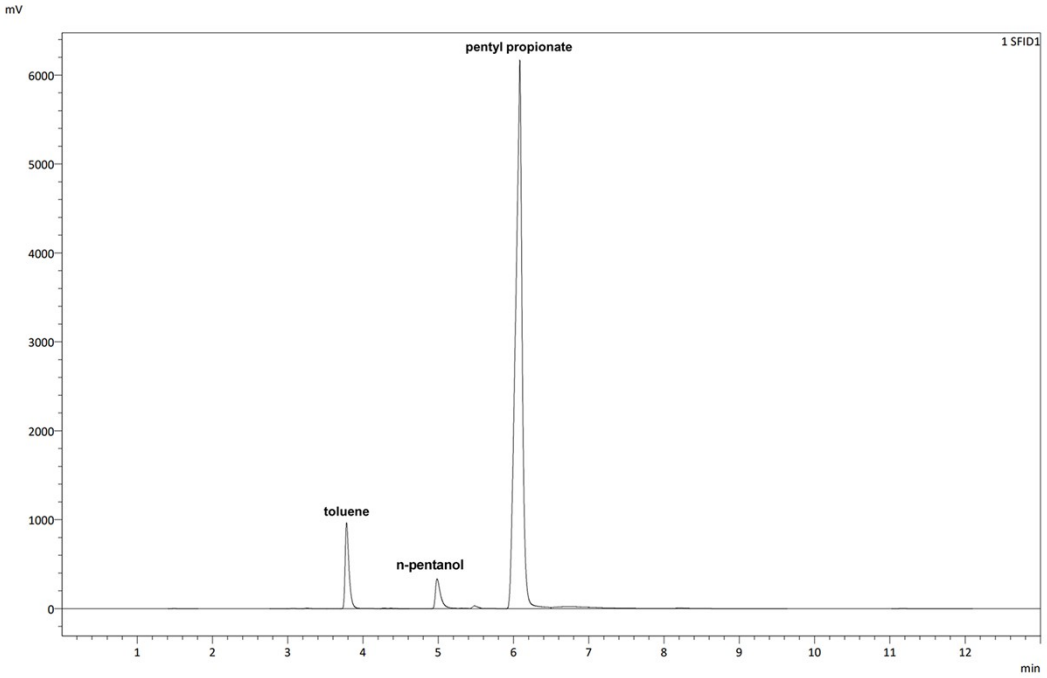


Fig. S49. GC spectra of the upper product phase with n-pentanol as the nucleophile.

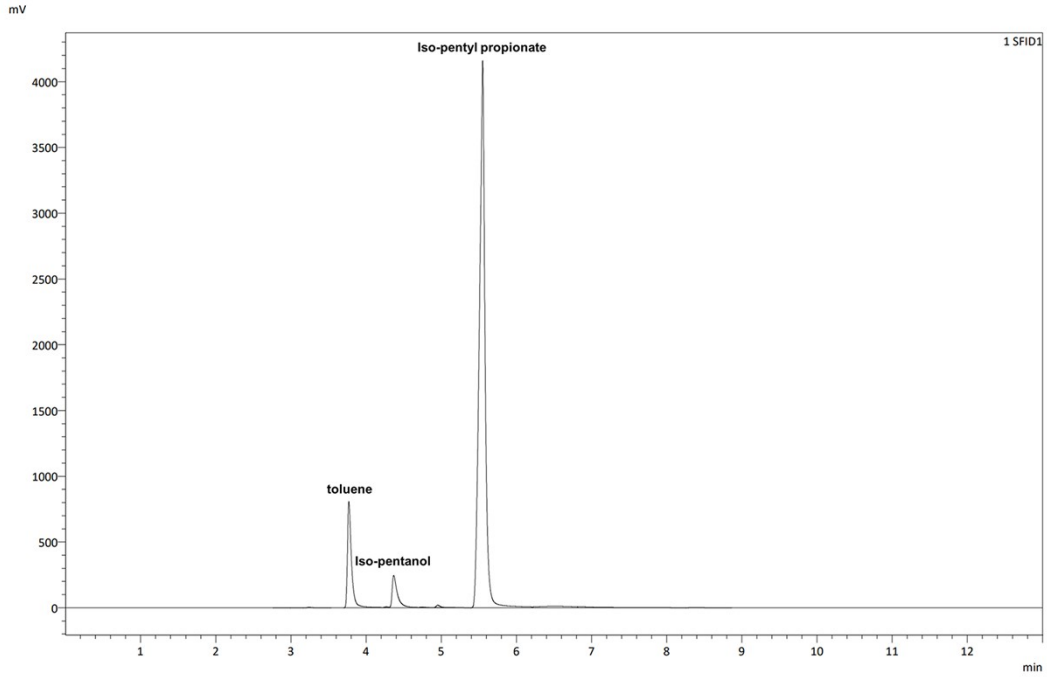


Fig. S50. GC spectra of the upper product phase with iso-pentanol as the nucleophile.

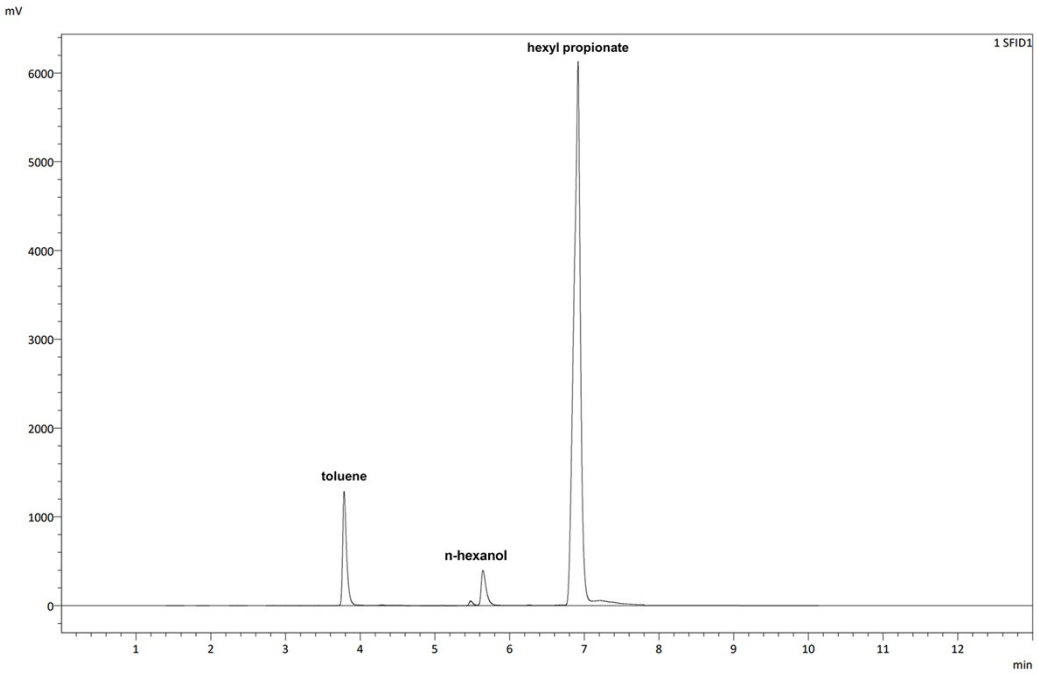


Fig. S51. GC spectra of the upper product phase with n-hexanol as the nucleophile.

21. Atomic coordinates of HBDs, HBAs, formed DESs, and ligand-DES pairs optimized at M06-2X-D3(0)/6-311+G** level

p-Toluenesulfonic acid

C	1.940611	-1.199367	0.023691
C	0.554912	-1.214706	-0.038161
C	-0.122680	-0.002417	-0.089917
C	0.550121	1.212097	-0.088822
C	1.937915	1.204958	-0.030037
C	2.649431	0.005290	0.028090
H	2.483085	-2.137473	0.064630
H	0.000596	-2.145330	-0.055912
H	-0.006350	2.139562	-0.152149
H	2.476751	2.145892	-0.034000
C	4.154277	0.004674	0.058494
H	4.541583	0.936616	0.471311
H	4.535249	-0.824292	0.656441
H	4.553370	-0.104597	-0.953599
S	-1.893079	-0.011167	-0.129583
O	-2.356757	1.280452	-0.583760
O	-2.338777	-1.242712	-0.718521
O	-2.282703	-0.120281	1.440930
H	-2.456659	0.765442	1.787383

L-carnitine

C	-3.305185	-1.017455	-0.045939
H	-3.280249	-1.546300	-0.997894
H	-3.238927	-1.729293	0.775631
H	-4.224508	-0.437525	0.033851
C	-2.097106	0.560242	1.363708
C	-2.305822	0.970743	-1.032708
H	-1.288577	1.290804	1.342589
H	-3.062383	1.033946	1.541695
H	-1.911714	-0.207117	2.114508
H	-3.188124	1.559548	-0.780152
H	-1.386532	1.558261	-1.026040
H	-2.447744	0.474473	-1.992331
N	-2.142908	-0.091784	0.017384
C	-0.866208	-0.882818	-0.240636
H	-0.838001	-1.045149	-1.321078
H	-0.984242	-1.842447	0.270074
C	0.395116	-0.144402	0.233429
C	1.622325	-0.898274	-0.315674
H	1.545632	-0.943780	-1.408556
H	1.716031	-1.914486	0.071837
C	2.925814	-0.148488	-0.003766
O	2.808024	1.157200	0.003207
O	3.958653	-0.744681	0.185443
O	0.380318	1.166460	-0.154754
H	1.772232	1.375741	-0.106944
H	0.427899	-0.253307	1.339472

4-Picolinicacid

C	1.698073	0.123826	-0.000032
O	2.312414	1.154199	-0.000195
C	0.207568	0.030596	0.000074
C	-0.530865	1.208315	0.000144
C	-0.462915	-1.187342	0.000006
C	-1.917349	1.112471	0.000007
C	-1.854237	-1.166306	-0.000025
H	-0.026839	2.166479	0.000234
H	0.080743	-2.122640	0.000269
H	-2.528627	2.008926	0.000439
H	-2.414191	-2.095819	-0.000289
N	-2.575779	-0.046820	-0.000138
O	2.291469	-1.082187	0.000090
H	3.246643	-0.934663	0.000116

Nicotinicacid

C	0.536336	1.223393	0.000021
C	-0.202625	0.043640	0.000001
C	1.918344	1.133487	0.000014
C	0.475691	-1.175699	-0.000028
C	-1.686505	0.129719	0.000007
C	2.498699	-0.133189	-0.000011
N	1.803136	-1.269915	-0.000033

O	-2.278722	-1.077816	0.000001
O	-2.307025	1.158181	0.000023
H	0.018178	2.175250	0.000041
H	2.540720	2.018932	0.000029
H	-0.079962	-2.106868	-0.000042
H	3.579216	-0.238786	-0.000019
H	-3.233762	-0.930153	0.000010

Histidine

C	1.262861	-0.302602	0.293272
C	-0.182510	-0.522166	0.602664
C	-1.119021	0.112071	-0.439813
N	-1.039439	1.572949	-0.392219
C	-2.547879	-0.342537	-0.107048
O	-3.307389	0.603670	0.441277
O	-2.924982	-1.465234	-0.291090
C	2.211453	-1.225918	-0.052424
N	1.825609	0.956302	0.322715
C	3.084046	0.795583	0.001984
N	3.372104	-0.510031	-0.234690
H	-0.415916	-0.093045	1.583191
H	-0.395874	-1.591212	0.645724
H	2.163955	-2.294501	-0.176006
H	4.271899	-0.885417	-0.487234
H	3.825054	1.576392	-0.070552
H	-0.877163	-0.305200	-1.422522
H	-2.750425	1.409932	0.456045
H	-0.116948	1.874605	-0.087040
H	-1.207231	1.979826	-1.305550

Urea

N	-1.156674	-0.609342	-0.070319
C	0.000000	0.145429	0.000022
N	1.156665	-0.609361	0.070314
O	0.000013	1.354922	-0.000006
H	-1.996194	-0.070075	0.076256
H	-1.153967	-1.520421	0.361425
H	1.153929	-1.520436	-0.361439
H	1.996189	-0.070106	-0.076290

Lidocaine

C	3.374481	1.712248	-0.093961
C	2.021656	1.391494	-0.020918
C	4.326490	0.724679	-0.312540
C	3.927506	-0.594451	-0.472777
C	2.580925	-0.955433	-0.417764
C	1.637046	0.053279	-0.181403
C	2.175891	-2.388941	-0.621407
N	0.252403	-0.272813	-0.120130
C	0.991989	2.461231	0.224416
C	-0.284544	-1.135611	0.788422
C	-1.771545	-1.413999	0.593308
O	0.348604	-1.700646	1.655033
N	-2.505925	-0.335355	-0.056216
C	-2.707549	2.156549	0.247575
C	-2.720233	0.772545	0.890815
C	-3.750147	-0.873023	-0.617864
C	-4.597961	0.138908	-1.374206
H	3.680513	2.744821	0.033356
H	5.377335	0.984305	-0.361104
H	4.668067	-1.365790	-0.653900
H	1.250042	-2.457424	-1.197231
H	2.957101	-2.931318	-1.154795
H	1.998287	-2.874639	0.340422
H	-0.415217	0.199599	-0.719402
H	1.470206	3.388952	0.539058
H	0.420032	2.676211	-0.683706
H	0.281709	2.155706	0.996413
H	-1.824975	-2.310047	-0.032856
H	-2.178886	-1.682163	1.578581
H	-2.693052	2.924938	1.024396
H	-1.811130	2.274842	-0.362516
H	-3.571432	2.339060	-0.388158
H	-1.908035	0.737626	1.623141
H	-3.651735	0.613311	1.457733
H	-3.466834	-1.676387	-1.302455
H	-4.359762	-1.330319	0.181371
H	-5.395186	-0.385130	-1.904794

H	-5.070562	0.858301	-0.704317
H	-3.994702	0.681028	-2.105268

p-Toluidine-2-sulfonic acid

C	2.387552	-0.488376	-0.017734
C	1.069725	-0.931723	-0.074421
C	0.024644	-0.018288	-0.080650
C	0.236752	1.364499	-0.044102
C	1.559303	1.801790	0.025422
C	2.605664	0.889952	0.039199
H	0.834827	-1.990231	-0.101406
H	1.764720	2.866273	0.059033
S	-1.644130	-0.610275	-0.089283
O	-2.363619	0.076648	-1.143808
O	-1.661618	-2.041816	0.012976
O	-2.189033	-0.055100	1.318768
H	-2.141951	0.918280	1.304515
C	3.538399	-1.459625	0.015403
H	4.367163	-1.105791	-0.600271
H	3.910943	-1.584672	1.035434
H	3.234757	-2.440104	-0.352026
H	3.623887	1.262196	0.086664
N	-0.856418	2.249950	0.004324
H	-0.574791	3.220901	0.016633
H	-1.536633	2.080673	-0.732506

Benzamide

N	2.403887	1.005666	0.265347
C	1.714809	-0.137532	-0.040156
O	2.276978	-1.172161	-0.327637
C	0.216824	-0.026276	-0.019379
C	-0.512418	-1.204875	0.131143
C	-0.453200	1.188550	-0.165758
C	-1.900031	-1.166409	0.161093
C	-2.566808	0.048458	0.024682
C	-1.843297	1.224204	-0.145481
H	1.961489	1.744567	0.785684
H	3.403601	0.907952	0.355563
H	0.029011	-2.138978	0.219784
H	0.101365	2.105200	-0.332498
H	-2.463316	-2.083271	0.286374
H	-3.649838	0.077735	0.043011
H	-2.360621	2.167696	-0.271123

Betaine

C	-0.307332	-0.867961	0.000093
N	0.979833	-0.060991	-0.000002
C	-1.660840	-0.047566	0.000081
C	2.137024	-0.995646	0.000255
C	1.045291	0.798574	-1.223402
C	1.045142	0.799072	1.223055
O	-2.619674	-0.810646	-0.000034
O	-1.560453	1.192333	-0.000021
H	-0.279032	-1.501523	0.887808
H	-0.279072	-1.501636	-0.887542
H	3.062432	-0.419065	0.000183
H	2.085737	-1.619669	0.891125
H	2.085829	-1.620038	-0.890362
H	1.993766	1.335993	-1.215256
H	0.192645	1.473476	-1.193838
H	0.989162	0.147880	-2.095696
H	0.988877	0.148738	2.095609
H	1.993627	1.336471	1.214824
H	0.192516	1.473984	1.193095

Dimethylglycine

C	1.199309	-0.000179	-0.178255
O	0.956656	-0.000691	-1.346106
O	2.483636	0.000173	0.252518
H	2.521992	0.000550	1.214660
C	-1.639071	1.213196	-0.161178
H	-1.203536	1.306862	-1.164041
H	-2.727374	1.212851	-0.249501
H	-1.352126	2.084887	0.431873
C	-1.639494	-1.213050	-0.160263
H	-1.352333	-2.084420	0.433147
H	-2.727839	-1.212675	-0.248093
H	-1.204454	-1.307380	-1.163278

N	-1.226035	0.000251	0.531267
C	0.150237	0.000200	0.939814
H	0.339919	0.880501	1.566933
H	0.339768	-0.879788	1.567419

N-(2-Hydroxyethyl)piperazine

C	2.457603	0.427176	0.331517
C	1.414389	-0.501113	-0.282409
N	0.063060	-0.215414	0.174555
O	3.769903	0.035595	-0.030768
C	-0.436729	1.053965	-0.351814
C	-0.846605	-1.299420	-0.188946
C	-1.837356	1.331920	0.174086
C	-2.244519	-1.023197	0.342553
N	-2.719295	0.237977	-0.215163
H	2.350371	1.446583	-0.039305
H	2.325866	0.445205	1.419564
H	1.656517	-1.526070	0.021767
H	1.496296	-0.462721	-1.383089
H	3.939291	-0.838486	0.329083
H	0.226778	1.861168	-0.036944
H	-0.461979	1.036077	-1.456036
H	-0.465912	-2.229405	0.241015
H	-0.898937	-1.420272	-1.285460
H	-1.778527	1.453582	1.267643
H	-2.209083	2.262669	-0.259277
H	-2.917095	-1.826443	0.034601
H	-2.200705	-1.004705	1.443388
H	-3.669160	0.424133	0.083526

Choline chloride

C	0.492379	-0.538262	-0.469534
N	0.630883	0.896592	-0.016758
C	1.286256	-1.456206	0.371825
C	-0.200511	1.758394	-0.917052
C	0.128899	1.037301	1.392633
C	2.054710	1.323493	-0.084256
H	0.740253	-0.588099	-1.534714
H	-0.602050	-0.782789	-0.350801
H	-0.114626	2.788682	-0.572721
H	0.187928	1.667824	-1.931256
H	-1.232373	1.402058	-0.859791
H	0.223454	2.086007	1.673533
H	0.743065	0.406207	2.031067
H	-0.914894	0.714332	1.403069
H	2.405770	1.209802	-1.109811
H	2.120855	2.367789	0.219568
H	2.635688	0.691406	0.585239
O	1.273709	-2.616719	-0.220899
H	1.737527	-3.260860	0.327167
Cl	-2.653344	-0.399592	0.014250

2PTSA:L-carnitine

C	-3.123496	3.482341	0.564032
H	-2.223307	3.486509	-0.048405
H	-4.003189	3.730524	-0.028450
H	-3.022515	4.181864	1.393194
C	-4.566621	2.058132	1.915340
C	-2.140915	1.817943	2.036661
H	-4.640691	1.085391	2.397368
H	-4.529481	2.851296	2.661265
H	-5.409424	2.219457	1.243627
H	-2.130548	2.588457	2.807930
H	-2.279467	0.833850	2.471809
H	-1.233866	1.852629	1.437903
N	-3.302114	2.106621	1.126560
C	-3.333073	1.127108	-0.038691
H	-2.293426	0.999704	-0.350471
H	-3.885884	1.623270	-0.839514
C	-4.004095	-0.210614	0.275977
C	-3.937442	-1.098162	-0.972346
H	-2.913608	-1.209116	-1.329046
H	-4.530075	-0.642759	-1.768964
C	-4.592209	-2.433988	-0.639029
O	-3.786896	-3.476070	-0.481448
O	-5.783313	-2.522380	-0.512438
O	-3.472950	-0.826648	1.422983
H	-2.523978	-1.004219	1.277446

H	-5.065070	-0.057562	0.491461
C	3.582078	-1.690358	-1.029945
C	2.229949	-1.425718	-1.201152
C	1.331562	-1.871701	-0.239802
C	1.760523	-2.584277	0.872315
C	3.117055	-2.844693	1.024620
C	4.044095	-2.401066	0.079004
H	4.291163	-1.334177	-1.769913
H	1.881663	-0.873000	-2.064736
H	1.041444	-2.923698	1.609184
H	3.460226	-3.402666	1.889541
C	5.513564	-2.696107	0.225737
H	5.754893	-3.034316	1.234422
H	5.817951	-3.479696	-0.473051
H	6.111165	-1.808344	0.005963
S	-0.402591	-1.499473	-0.388944
O	-0.788793	-0.746914	0.832626
O	-0.547439	-0.654173	-1.608216
O	-1.125188	-2.772110	-0.507692
H	-2.842130	-3.228682	-0.539636
C	4.516429	1.632608	0.071763
C	3.471830	2.148964	-0.685157
C	2.166477	1.886264	-0.288787
C	1.886223	1.130795	0.843577
C	2.943977	0.630765	1.589298
C	4.267260	0.871050	1.215658
H	5.540240	1.828715	-0.227849
H	3.658189	2.753077	-1.565188
H	0.861975	0.906830	1.117706
H	2.736974	0.026518	2.466149
C	5.392755	0.322327	2.050624
H	5.192534	-0.715383	2.327965
H	6.343516	0.363347	1.517790
H	5.499644	0.897104	2.974456
S	0.834454	2.497616	-1.289390
O	-0.371579	2.508250	-0.461435
O	1.256947	3.711948	-1.939510
O	0.649458	1.411329	-2.408342
H	0.142531	0.592893	-2.062945

PTSA:L-carnitine

C	3.064499	-3.325326	-0.767219
H	2.212251	-3.334278	-1.445896
H	3.991800	-3.218775	-1.328042
H	3.085081	-4.241243	-0.178140
C	4.098166	-2.077804	1.058356
C	1.666828	-2.380137	0.968618
H	3.932168	-1.263315	1.760645
H	4.195363	-3.026593	1.585502
H	4.987114	-1.891476	0.455635
H	1.762027	-3.349342	1.458658
H	1.573631	-1.580394	1.694280
H	0.810991	-2.353686	0.294085
N	2.914998	-2.161976	0.154312
C	2.791195	-0.916471	-0.706792
H	1.784901	-0.956408	-1.131537
H	3.527011	-1.022798	-1.508267
C	3.039318	0.415859	0.015742
C	2.604559	1.525440	-0.958348
H	1.645652	1.284714	-1.420050
H	3.357011	1.631718	-1.742578
C	2.537048	2.849622	-0.207435
O	1.321163	3.300608	0.076157
O	3.532325	3.435474	0.119621
O	2.431617	0.487166	1.275555
H	1.451085	0.494577	1.198144
H	4.109035	0.541109	0.206792
C	-4.642254	-0.909848	-0.846974
C	-3.265700	-0.785190	-1.012870
C	-2.548943	-0.008381	-0.116787
C	-3.178486	0.641373	0.939697
C	-4.549898	0.506012	1.090992
C	-5.300904	-0.267684	0.199855
H	-5.211114	-1.518039	-1.542001
H	-2.744609	-1.286480	-1.819295
H	-2.592455	1.233220	1.633075
H	-5.049589	1.005426	1.914490
C	-6.793482	-0.383083	0.367377

H	-7.285777	0.547239	0.071928
H	-7.199224	-1.187747	-0.246640
H	-7.056906	-0.578738	1.408684
S	-0.795144	0.204038	-0.331806
O	-0.195792	0.073175	1.023690
O	-0.342019	-0.868609	-1.241655
O	-0.586138	1.563189	-0.876394
H	0.610954	2.706212	-0.251807

PTSA:2L-carnitine

C	2.521224	-2.510096	-2.339731
H	1.864670	-1.846836	-2.901582
H	3.422593	-1.993157	-2.006678
H	2.802680	-3.363443	-2.956736
C	2.694714	-3.888648	-0.356359
C	0.596730	-3.816972	-1.632460
H	2.162425	-4.271336	0.512371
H	3.013734	-4.716244	-0.989334
H	3.544737	-3.270868	-0.056683
H	0.972704	-4.609049	-2.279286
H	0.063021	-4.235060	-0.783341
H	-0.074311	-3.155798	-2.177398
N	1.766251	-3.023471	-1.153357
C	1.331256	-1.842650	-0.304351
H	0.914098	-1.093646	-0.981851
H	2.251217	-1.461134	0.138172
C	0.273032	-2.185578	0.741968
C	0.357333	-1.210865	1.917769
H	0.210661	-0.189149	1.568919
H	1.339120	-1.287928	2.390478
C	-0.686509	-1.631475	2.944832
O	-1.698335	-0.798517	3.160806
O	-0.599497	-2.684496	3.517614
O	-1.015360	-2.197181	0.163492
H	-1.159647	-1.306263	-0.205351
H	0.428962	-3.187273	1.153795
C	-5.464037	0.819600	-1.658306
C	-4.225542	1.361172	-1.330225
C	-3.452064	0.735315	-0.364099
C	-3.894237	-0.415582	0.281176
C	-5.131196	-0.942841	-0.061083
C	-5.932774	-0.334329	-1.030975
H	-6.077061	1.304775	-2.410328
H	-3.859275	2.263906	-1.803551
H	-3.288551	-0.892606	1.044527
H	-5.483017	-1.839102	0.438535
C	-7.288783	-0.900149	-1.362356
H	-8.021909	-0.602512	-0.607735
H	-7.640870	-0.542308	-2.330595
H	-7.263978	-1.990987	-1.385421
S	-1.839909	1.386617	0.028199
O	-0.851150	0.478609	-0.632949
O	-1.781974	2.757382	-0.493765
O	-1.700726	1.313960	1.502891
H	-1.660991	-0.004669	2.581636
C	1.850851	4.908277	0.197055
H	2.330903	5.130884	1.148840
H	2.421620	5.342946	-0.622941
H	0.832359	5.293076	0.191896
C	1.109647	3.130793	-1.278705
C	1.004559	2.838323	1.150303
H	0.931817	2.060206	-1.355474
H	0.137211	3.618420	-1.272184
H	1.742443	3.492482	-2.089254
H	0.023748	3.309441	1.162379
H	0.902898	1.772009	0.976864
H	1.552158	3.004378	2.076629
N	1.797002	3.429592	0.020494
C	3.215405	2.904959	0.010441
H	3.692085	3.264886	0.924847
H	3.694945	3.363526	-0.856512
C	3.354244	1.391188	-0.039278
C	4.764627	1.003797	-0.499668
H	5.484158	1.316859	0.264012
H	5.017655	1.473204	-1.451222
C	4.823535	-0.529827	-0.675322
O	4.329331	-1.196916	0.289570
O	5.256293	-0.979639	-1.737221

O	3.083194	0.874368	1.242744
H	3.525861	-0.009973	1.230944
H	2.638603	0.982575	-0.771739

PTSA:3L-carnitine

C	-5.055029	-1.012165	2.471097
H	-4.183286	-1.377960	3.012091
H	-5.036879	0.074298	2.370170
H	-5.970750	-1.338518	2.964438
C	-6.238267	-1.116591	0.353250
C	-5.048695	-3.089730	1.198674
H	-6.212170	-1.513015	-0.659583
H	-7.123718	-1.481546	0.873995
H	-6.204194	-0.025597	0.339942
H	-5.928914	-3.376733	1.773763
H	-5.078491	-3.523800	0.202600
H	-4.136443	-3.414917	1.695806
N	-5.031192	-1.603535	1.094785
C	-3.780302	-1.106190	0.401486
H	-2.956042	-1.213999	1.109281
H	-3.964457	-0.053232	0.201710
C	-3.416904	-1.835449	-0.890688
C	-2.546943	-0.875754	-1.722907
H	-1.844912	-0.331395	-1.085511
H	-3.199158	-0.138099	-2.193359
C	-1.828566	-1.656114	-2.809161
O	-0.514542	-1.857624	-2.614027
O	-2.383091	-2.086312	-3.779927
O	-2.794109	-3.075262	-0.638680
H	-1.987759	-2.904600	-0.120698
H	-4.303112	-2.068066	-1.487344
C	2.994074	-2.804394	2.977869
C	1.802045	-2.571261	2.298113
C	1.503690	-1.276845	1.892746
C	2.373156	-0.223878	2.151738
C	3.556621	-0.469953	2.834079
C	3.881992	-1.762896	3.255766
H	3.233631	-3.811290	3.303920
H	1.103092	-3.371289	2.085972
H	2.144053	0.785856	1.831905
H	4.221069	0.368488	3.017794
C	5.152912	-2.013717	4.024384
H	5.012346	-1.770100	5.080928
H	5.457040	-3.059469	3.960553
H	5.966227	-1.389207	3.651107
S	0.037909	-0.961717	0.930177
O	-0.746530	-2.213998	0.969761
O	-0.652388	0.203524	1.494662
O	0.549406	-0.682551	-0.451677
H	-0.207268	-1.432336	-1.782123
C	1.036685	4.882845	-0.372310
H	0.770050	5.190317	-1.382888
H	0.790424	5.674442	0.335812
H	2.092084	4.610443	-0.311903
C	0.663769	3.195136	1.328487
C	0.502003	2.596168	-1.030587
H	0.119862	2.281934	1.570181
H	1.741896	3.021573	1.296935
H	0.446010	3.980235	2.052703
H	1.580736	2.464994	-1.069630
H	0.010778	1.680167	-0.709505
H	0.096500	2.912038	-1.989476
N	0.228394	3.674270	-0.023021
C	-1.233076	4.057324	-0.005957
H	-1.402675	4.696643	-0.874573
H	-1.379743	4.638202	0.906467
C	-2.217435	2.898133	-0.093811
C	-3.592332	3.350950	0.419533
H	-3.935802	4.196297	-0.186876
H	-3.535099	3.653869	1.465626
C	-4.604082	2.198034	0.285033
O	-4.665764	1.652964	-0.855424
O	-5.231124	1.840469	1.296351
O	-2.286967	2.507124	-1.449696
H	-3.188780	2.117006	-1.547024
H	-1.869911	2.058942	0.529306
C	4.180599	-2.677416	-3.342205
H	4.577018	-2.091489	-4.169845

H	4.993761	-3.156635	-2.797857
H	3.483765	-3.427429	-3.714182
C	2.791373	-2.586285	-1.351225
C	2.400745	-1.025378	-3.193082
H	2.371246	-1.915187	-0.607701
H	1.986070	-3.162643	-1.807527
H	3.539218	-3.243534	-0.908152
H	1.763926	-1.760030	-3.683292
H	1.809755	-0.435052	-2.497708
H	2.898338	-0.367146	-3.901306
N	3.452078	-1.767101	-2.416488
C	4.453461	-0.820129	-1.777983
H	5.154007	-0.520988	-2.559950
H	4.973752	-1.407511	-1.018717
C	3.841109	0.443321	-1.189669
C	4.776115	1.064196	-0.145765
H	5.709445	1.362625	-0.635630
H	4.995544	0.353997	0.652322
C	4.098244	2.318481	0.456542
O	3.619231	3.122576	-0.403703
O	4.021969	2.418408	1.683276
O	3.618932	1.335709	-2.260693
H	3.606357	2.224950	-1.822330
H	2.888115	0.194656	-0.692876

PTSA:4L-carnitine

C	4.645715	1.662148	-1.371719
H	3.706671	2.215222	-1.337689
H	4.907243	1.274851	-0.383344
H	5.441808	2.302984	-1.751558
C	5.761711	-0.227588	-2.402204
C	4.102081	1.061917	-3.667666
H	5.638352	-1.072974	-3.076317
H	6.522698	0.446648	-2.794583
H	6.010430	-0.558959	-1.392254
H	4.877570	1.766166	-3.968223
H	4.021535	0.244651	-4.379389
H	3.135777	1.557995	-3.591239
N	4.469062	0.521984	-2.325492
C	3.386518	-0.380044	-1.768274
H	2.564372	0.269859	-1.463139
H	3.827057	-0.834879	-0.880913
C	2.841503	-1.428804	-2.737307
C	2.177233	-2.530443	-1.893346
H	1.592413	-2.089921	-1.083249
H	2.946412	-3.154819	-1.436433
C	1.324487	-3.407477	-2.795681
O	0.002069	-3.216346	-2.717408
O	1.799895	-4.214533	-3.543011
O	1.965328	-0.868557	-3.686867
H	1.252117	-0.403094	-3.213973
H	3.640675	-1.898679	-3.318346
C	-3.316146	2.602372	-0.968616
C	-2.195291	1.851497	-1.293028
C	-1.661880	0.994091	-0.332944
C	-2.248353	0.852058	0.918527
C	-3.363589	1.620742	1.231706
C	-3.895595	2.517863	0.302110
H	-3.697369	3.318339	-1.689453
H	-1.723027	1.953406	-2.263483
H	-1.850026	0.162855	1.656021
H	-3.799002	1.516076	2.220462
C	-5.026711	3.443581	0.650011
H	-4.683671	4.474208	0.518293
H	-5.876182	3.295464	-0.021410
H	-5.362907	3.298572	1.676974
S	-0.254219	-0.006864	-0.730145
O	0.306167	0.531032	-1.988922
O	0.703523	0.078295	0.400022
O	-0.771063	-1.399581	-0.893891
H	-0.215137	-2.514387	-2.066127
C	0.213241	-3.516651	4.158723
H	0.645775	-4.497582	3.964295
H	0.496488	-3.173018	5.153839
H	-0.872090	-3.529214	4.042269
C	0.129410	-1.216059	3.391105
C	0.410525	-3.027977	1.775155
H	0.408730	-0.558929	2.570158

H	-0.953421	-1.342378	3.435219
H	0.492494	-0.832382	4.345412
H	-0.671036	-3.151679	1.744067
H	0.729181	-2.274635	1.059324
H	0.935817	-3.964803	1.593195
N	0.763076	-2.553760	3.155318
C	2.255864	-2.461580	3.331451
H	2.642984	-3.481984	3.351839
H	2.411811	-1.997379	4.306934
C	2.987410	-1.702609	2.227631
C	4.250186	-1.029311	2.780559
H	4.928961	-1.797634	3.164760
H	3.989593	-0.339495	3.585412
C	4.937683	-0.252213	1.643864
O	5.286676	-0.956460	0.648701
O	5.031393	0.980060	1.743481
O	3.303355	-2.631754	1.209013
H	4.128918	-2.291078	0.802278
H	2.334556	-0.919046	1.815757
C	-5.308871	-2.680718	-3.059515
H	-5.695916	-3.678763	-2.860599
H	-6.096656	-1.939260	-2.930526
H	-4.909206	-2.629134	-4.071353
C	-3.614781	-1.057397	-2.423755
C	-3.148392	-3.442042	-2.219942
H	-2.827518	-0.850305	-1.706784
H	-3.191415	-1.105296	-3.426771
H	-4.392313	-0.295815	-2.370902
H	-2.804078	-3.456816	-3.253292
H	-2.328878	-3.185952	-1.555463
H	-3.570206	-4.398748	-1.919733
N	-4.212063	-2.389831	-2.095940
C	-4.798778	-2.353727	-0.695507
H	-5.463676	-3.215430	-0.608131
H	-5.378898	-1.430495	-0.642810
C	-3.771109	-2.430217	0.423134
C	-4.350842	-1.865443	1.723625
H	-5.189537	-2.492904	2.045169
H	-4.698842	-0.840854	1.586298
C	-3.266553	-1.878965	2.821453
O	-2.579434	-2.948955	2.888315
O	-3.107759	-0.865293	3.507911
O	-3.412324	-3.787865	0.572489
H	-3.015130	-3.819828	1.475010
H	-2.886004	-1.833498	0.156447
C	2.648955	2.413286	1.869755
H	2.444541	1.538549	1.252285
H	3.475402	2.986309	1.454265
H	2.904748	2.106594	2.882283
C	1.665128	4.515328	2.650540
C	0.334433	2.471871	2.596375
H	0.725270	5.058746	2.733996
H	2.049606	4.254550	3.636083
H	2.404136	5.104729	2.108340
H	0.677850	2.274488	3.612831
H	-0.583707	3.051758	2.577548
H	0.207469	1.543978	2.043355
N	1.410759	3.255552	1.901111
C	1.021987	3.551666	0.464079
H	0.637629	2.610137	0.069376
H	1.950071	3.805882	-0.055333
C	0.005934	4.669611	0.269566
C	-0.365003	4.699855	-1.227843
H	-0.233328	3.712474	-1.680367
H	0.292711	5.383821	-1.769902
C	-1.830741	5.119111	-1.554365
O	-2.554093	5.474699	-0.572251
O	-2.159515	5.020548	-2.732944
O	-1.092205	4.443880	1.107164
H	-1.859414	4.904445	0.594164
H	0.480079	5.630765	0.526103

Protonated ligand-PTSA anions

C	3.724221	3.612844	2.542700
C	4.264251	2.363689	2.274586
C	4.618476	2.037625	0.968006
C	4.437915	2.949116	-0.061121
C	3.899619	4.203368	0.222930

C	3.535032	4.551639	1.521817	H	5.702939	-4.029010	-1.410914
H	3.441877	3.868598	3.558996	H	5.052731	-3.019956	-2.703264
H	4.403734	1.634128	3.064348	H	5.606781	-2.270243	-1.197006
H	4.714887	2.667747	-1.069946	C	2.985613	-4.546000	-1.593378
H	3.758737	4.918904	-0.580677	H	2.906189	-4.492964	-2.679546
C	2.966910	5.911736	1.834797	H	3.555423	-5.446393	-1.347405
H	2.662352	6.431671	0.925642	H	1.982244	-4.670491	-1.174843
H	2.099631	5.833656	2.493844	C	0.683706	-2.362840	-3.035757
H	3.710594	6.531813	2.342387	H	0.252511	-2.154610	-4.019087
S	5.254716	0.393906	0.623755	H	0.884258	-3.433939	-2.979867
O	5.263465	0.298605	-0.860589	H	-0.070273	-2.100877	-2.290980
O	6.556053	0.274946	1.262383	C	2.981109	-1.835692	-3.955631
O	4.216484	-0.519571	1.186754	H	3.239299	-2.893760	-3.997700
H	3.675201	-0.708381	-1.114715	H	2.549011	-1.561713	-4.921879
C	0.674052	2.017470	0.177700	H	3.896745	-1.252922	-3.822639
C	-0.674067	2.017531	-0.177387	C	1.590179	-0.018744	-2.985607
C	-1.343520	0.810883	-0.316424	H	0.763743	0.271833	-2.337812
C	-0.688414	-0.412246	-0.129960	H	2.449540	0.620420	-2.765753
C	0.688235	-0.412303	0.130072	H	1.286516	0.166626	-4.019967
C	1.343426	0.810764	0.316635	C	-3.714603	-3.341444	0.985583
H	1.217117	2.943791	0.330177	C	-1.947350	-1.515172	2.864617
H	-1.217069	2.943900	-0.329800	C	-3.899332	-3.582857	-0.524284
H	-2.396262	0.796838	-0.573432	H	-4.327457	-2.713220	-1.026342
H	2.396173	0.796630	0.573621	H	-2.957590	-3.851555	-1.009345
C	-1.545057	-1.656122	-0.176383	H	-4.581464	-4.429571	-0.639215
H	-0.978087	-2.588549	-0.183792	C	-5.100577	-3.140941	1.620886
H	-2.195017	-1.630845	-1.055987	H	-5.703271	-4.028861	1.410716
C	1.544791	-1.656238	0.176330	H	-5.053021	-3.020035	2.703216
H	2.194719	-1.631154	1.055959	H	-5.607033	-2.270078	1.197057
H	0.977750	-2.588627	0.183560	C	-2.985956	-4.545981	1.593201
P	2.747416	-1.764082	-1.206252	H	-3.555819	-5.446328	1.347182
P	-2.747654	-1.764023	1.206229	H	-1.982602	-4.670491	1.174632
C	3.714313	-3.341539	-0.985663	H	-2.906500	-4.493021	2.679369
C	1.947108	-1.515155	-2.864627	C	-0.683991	-2.362939	3.035685
C	3.899023	-3.583078	0.524182	H	-0.252759	-2.154792	4.019017
H	4.327189	-2.713500	1.026304	H	-0.884599	-3.434024	2.979735
H	2.957272	-3.851759	1.009234	H	0.069975	-2.100968	2.290898
H	4.581101	-4.429846	0.639041	C	-1.590366	-0.018782	2.985697
C	5.100289	-3.141029	-1.620950	H	-0.763884	0.271799	2.337962

H	-2.449693	0.620425	2.765830
H	-1.286744	0.166517	4.020082
C	-2.981364	-1.835717	3.955603
H	-3.239577	-2.893780	3.997646
H	-2.549264	-1.561773	4.921860
H	-3.896985	-1.252922	3.822616
C	-3.723465	3.612964	-2.542667
C	-4.263674	2.363884	-2.274562
C	-4.618217	2.037964	-0.968033
C	-4.437826	2.949540	0.061054
C	-3.899369	4.203722	-0.222994
C	-3.534441	4.551839	-1.521830
H	-3.440849	3.868599	-3.558916
H	-4.403013	1.634242	-3.064275
H	-4.715018	2.668286	1.069850
H	-3.758613	4.919317	0.580583
C	-2.966163	5.911882	-1.834766
H	-2.099513	5.833816	-2.494634
H	-3.710107	6.532407	-2.341430
H	-2.660629	6.431352	-0.925668
S	-5.254640	0.394321	-0.623741
O	-5.263331	0.299063	0.860609
O	-6.556013	0.275466	-1.262306
O	-4.216514	-0.519254	-1.186779
H	-3.675404	-0.708295	1.114659

Unprotonated ligand-PTSA anions

C	3.967714	3.887519	0.568950
C	4.500015	2.844591	1.317689
C	4.998167	1.716420	0.674735
C	4.995906	1.644618	-0.711039
C	4.464594	2.696508	-1.452384
C	3.925525	3.819257	-0.825755
H	3.559585	4.759575	1.072386
H	4.520116	2.882154	2.401177
H	5.379096	0.750832	-1.187294
H	4.443596	2.632655	-2.536591
C	3.253526	4.901156	-1.632110
H	3.738539	5.032607	-2.601954
H	2.207047	4.638366	-1.818476
H	3.269904	5.857906	-1.105405
S	5.485589	0.293877	1.670773
O	6.243178	-0.582110	0.756953
O	6.274039	0.857245	2.777705
O	4.190730	-0.280886	2.097067
C	0.674014	2.343828	0.183977
C	-0.673343	2.344259	-0.180861
C	-1.343001	1.140051	-0.326201
C	-0.690783	-0.088852	-0.131270
C	0.690334	-0.089252	0.132651
C	1.343129	1.139219	0.328469
H	1.210085	3.273744	0.340391
H	-1.208989	3.274524	-0.336634
H	-2.398742	1.125762	-0.582023
H	2.398869	1.124253	0.584290
C	-1.553225	-1.328221	-0.197326
H	-0.976916	-2.250824	-0.113373
H	-2.086275	-1.331854	-1.153532
C	1.552267	-1.329044	0.197695
H	2.085292	-1.333730	1.153900
H	0.975625	-2.251367	0.112924
P	2.958120	-1.304809	-1.047717
P	-2.959162	-1.304759	1.048038
C	3.665153	-3.055885	-0.780071
C	2.062144	-1.270607	-2.733346
C	3.827281	-3.248510	0.737698
H	4.295552	-2.382727	1.210290
H	2.866008	-3.433731	1.224509
H	4.462529	-4.126186	0.908882
C	5.079601	-3.059723	-1.383652
H	5.548276	-4.035534	-1.201991
H	5.074802	-2.887217	-2.462406
H	5.687786	-2.288353	-0.901935
C	2.848891	-4.233311	-1.319879
H	2.802480	-4.252942	-2.410299
H	3.319148	-5.169920	-0.992938
H	1.825976	-4.226815	-0.932193
C	0.774882	-2.088886	-2.860287

H	0.339453	-1.932724	-3.855473
H	0.938955	-3.159013	-2.733506
H	0.030641	-1.763587	-2.133298
C	3.059741	-1.692126	-3.821279
H	3.299855	-2.755877	-3.780539
H	2.624532	-1.485570	-4.806563
H	3.994146	-1.127323	-3.739792
C	1.713145	0.208616	-2.996271
H	0.921406	0.569773	-2.338476
H	2.586316	0.851681	-2.856067
H	1.361903	0.312881	-4.030372
C	-3.665989	-3.055784	0.779399
C	-2.063461	-1.271341	2.733826
C	-3.828151	-3.247536	-0.738443
H	-4.297871	-2.381998	-1.210043
H	-2.866872	-3.431182	-1.225782
H	-4.462385	-4.125872	-0.910086
C	-5.080582	-3.060170	1.382668
H	-5.548754	-4.036230	1.201046
H	-5.076294	-2.887360	2.461365
H	-5.688863	-2.289198	0.900440
C	-2.849545	-4.233315	1.318662
H	-3.319481	-5.169856	0.991071
H	-1.826538	-4.226322	0.931219
H	-2.803363	-4.253590	2.409077
C	-0.776209	-2.089645	2.860690
H	-0.340706	-1.933433	3.855835
H	-0.940321	-3.159770	2.734001
H	-0.032013	-1.764422	2.133629
C	-1.714534	0.207757	2.997516
H	-0.922505	0.569149	2.340199
H	-2.587628	0.850909	2.857231
H	-1.363720	0.311573	4.031808
C	-3.061277	-1.693379	3.821363
H	-3.301470	-2.757086	3.779999
H	-2.626223	-1.487392	4.806836
H	-3.995620	-1.128454	3.740018
C	-3.965582	3.887900	-0.568216
C	-4.497903	2.845460	-1.317585
C	-4.997045	1.717332	-0.675274
C	-4.995780	1.645168	0.710460
C	-4.464425	2.696598	1.452461
C	-3.924346	3.819224	0.826515
H	-3.556676	4.759892	-1.071134
H	-4.517242	2.883330	-2.401077
H	-5.379724	0.751446	1.186222
H	-4.444206	2.632427	2.536664
C	-3.252264	4.900548	1.633563
H	-2.205651	4.637808	1.819263
H	-3.269047	5.857774	1.107731
H	-3.736901	5.031007	2.603724
S	-5.484594	0.295401	-1.672125
O	-6.242752	-0.580697	-0.758849
O	-6.272558	0.859662	-2.778964
O	-4.189923	-0.279733	-2.098471

22. Atomic coordinates of intermediates and transition states optimized at PBE0-D3(BJ)/def2-SVP (SDD for Pd) level

CO

C	0.000000	0.000000	-0.644610
O	0.000000	0.000000	0.483457

Ethylene

C	0.000000	0.000000	0.665295
H	0.000000	0.931325	1.239867
H	0.000000	-0.931325	1.239867
C	0.000000	0.000000	-0.665295
H	0.000000	0.931325	-1.239867
H	0.000000	-0.931325	-1.239867

n-Pentanol

C	0.738705	0.841125	-0.139430
C	-0.426093	-0.055374	0.251700
C	-1.770170	0.407158	-0.291726
C	2.089729	0.314284	0.318724
C	-2.924568	-0.496964	0.109493
O	2.383819	-0.965804	-0.178477
H	0.595602	1.857215	0.269364
H	0.756730	0.964311	-1.239856
H	-0.212362	-1.080284	-0.096205
H	-0.477532	-0.121517	1.354004
H	-1.968450	1.438049	0.052530
H	-1.713023	0.468679	-1.393361
H	2.098319	0.222039	1.417482
H	2.882390	1.044218	0.057422
H	-2.765523	-1.527010	-0.248153
H	-3.031884	-0.544690	1.205156
H	-3.882039	-0.144545	-0.303305
H	2.401606	-0.911409	-1.139829

n-Pentyl propionate

O	1.204943	1.094271	-0.163761
C	2.014248	0.079122	0.167155
C	3.338526	0.189545	-0.542106
O	1.707361	-0.796880	0.933854
C	-0.092775	1.102757	0.425170
C	4.302052	-0.920928	-0.177089
C	-1.066607	0.229948	-0.340211
C	-2.474990	0.292788	0.231596
C	-3.472907	-0.577301	-0.520544
C	-4.878291	-0.518436	0.055291
H	3.125097	0.210718	-1.624105
H	3.749994	1.186914	-0.314171
H	-0.017371	0.769073	1.471766
H	-0.409953	2.155806	0.408941
H	5.252282	-0.808613	-0.718503
H	4.515806	-0.919274	0.901380
H	3.878494	-1.905847	-0.420392
H	-1.071887	0.544765	-1.397942
H	-0.700690	-0.809583	-0.315324
H	-2.454046	-0.013808	1.293199
H	-2.830748	1.339697	0.228774
H	-3.491769	-0.270416	-1.581278
H	-3.112600	-1.621027	-0.518572
H	-5.575364	-1.156543	-0.508581
H	-4.894490	-0.854782	1.104512
H	-5.276719	0.508830	0.033986

L1-Pd-H

Pd	-0.023398	-1.142397	0.909850
P	1.937999	-0.274283	-0.109517
P	-1.870324	-0.393355	-0.063071
H	-1.318081	-1.642868	1.636674
C	2.957838	-1.537634	-1.078059
C	1.973162	-2.246721	-2.014665
H	1.466195	-1.557840	-2.707613
H	1.205743	-2.792994	-1.446098
H	2.520222	-2.977607	-2.631154
C	4.079067	-0.905324	-1.905018
H	3.695126	-0.245196	-2.695629
H	4.646777	-1.705507	-2.406469

H	4.789628	-0.334963	-1.293077
C	3.535058	-2.583984	-0.123387
H	2.758540	-3.029853	0.518631
H	4.330455	-2.179387	0.516738
H	3.978122	-3.401114	-0.714382
C	2.868283	0.422980	1.374223
C	2.741257	-0.630323	2.484484
H	1.676587	-0.857770	2.704360
H	3.167116	-0.233442	3.420001
H	3.254161	-1.572625	2.259355
C	4.330026	0.774940	1.118226
H	4.945146	-0.107602	0.895542
H	4.753786	1.249356	2.018202
H	4.441005	1.492870	0.291400
C	2.111237	1.672586	1.837101
H	1.025122	1.500517	1.901736
H	2.274754	2.530964	1.176350
H	2.468197	1.951561	2.841396
C	1.703777	1.059774	-1.367701
H	2.694298	1.477691	-1.599619
H	1.390198	0.514164	-2.273368
C	0.750890	2.193846	-1.099016
C	1.314713	3.465719	-0.919988
H	2.404070	3.559210	-0.920453
C	0.540737	4.608799	-0.770500
H	1.018447	5.580598	-0.630697
C	-0.844456	4.500874	-0.845791
H	-1.477863	5.387377	-0.775143
C	-1.418032	3.252297	-1.048355
H	-2.500387	3.194396	-1.169589
C	-0.656177	2.077525	-1.143255
C	-1.370782	0.780006	-1.427368
H	-0.752699	0.145081	-2.077169
H	-2.295434	0.989786	-1.989951
C	-2.989970	0.515539	1.152614
C	-4.054442	1.367473	0.455163
H	-4.790943	0.765847	-0.089079
H	-3.628240	2.102024	-0.234258
H	-4.600766	1.932351	1.226467
C	-2.064464	1.412875	1.985304
H	-1.342393	0.813554	2.561060
H	-2.675989	1.983100	2.702242
H	-1.508298	2.134047	1.370502
C	-3.692251	-0.471993	2.085285
H	-2.985530	-1.142125	2.597441
H	-4.445352	-1.080883	1.566630
H	-4.218171	0.104591	2.862270
C	-2.751364	-1.778642	-1.005756
C	-1.887317	-2.151295	-2.216118
H	-1.905411	-1.386575	-3.005009
H	-2.286693	-3.077731	-2.656792
H	-0.843368	-2.344758	-1.931079
C	-4.135537	-1.343814	-1.493189
H	-4.111961	-0.410449	-2.074940
H	-4.851471	-1.226538	-0.669108
H	-4.532103	-2.127813	-2.157304
C	-2.878605	-3.016781	-0.114182
H	-3.434077	-2.825738	0.812338
H	-1.891955	-3.419942	0.156918
H	-3.421218	-3.795268	-0.672873

L1-Pd-ethyl

Pd	-0.090537	-1.207766	-0.671802
P	-1.859583	-0.081069	0.260659
P	1.864013	-0.221567	0.277276
C	-1.161359	-2.391240	-1.978180
H	-1.902327	-3.055430	-1.526462
H	-1.567134	-1.815005	-2.816353
C	0.189743	-2.950683	-2.183733
H	0.603331	-2.817467	-3.193051
H	0.331559	-3.979750	-1.827976
H	1.010744	-2.377129	-1.548754
C	-2.732824	-1.185230	1.539295
C	-1.755571	-1.425246	2.694652
H	-1.596349	-0.537618	3.322466
H	-0.783146	-1.781099	2.323527
H	-2.166656	-2.209924	3.348561
C	-4.016402	-0.559105	2.086716

H	-3.861885	0.451703	2.491417
H	-4.386615	-1.184137	2.915043
H	-4.814685	-0.517146	1.333998
C	-3.045425	-2.553317	0.927929
H	-2.122149	-3.085975	0.659537
H	-3.686664	-2.496986	0.040351
H	-3.574285	-3.160159	1.679447
C	-3.078675	0.625685	-1.004804
C	-3.959101	-0.472511	-1.605398
H	-3.385848	-1.324702	-1.984978
H	-4.514855	-0.044253	-2.454629
H	-4.704437	-0.843482	-0.888555
C	-4.008266	1.694986	-0.424728
H	-4.664760	1.307591	0.362974
H	-4.655992	2.063091	-1.236093
H	-3.473343	2.562976	-0.029056
C	-2.208465	1.245225	-2.106497
H	-1.598997	0.483958	-2.614075
H	-1.529235	2.017840	-1.718835
H	-2.859624	1.717210	-2.859342
C	-1.335984	1.359308	1.316997
H	-2.259267	1.789265	1.733189
H	-0.821516	0.878683	2.159332
C	-0.468450	2.473758	0.787755
C	-1.067759	3.659963	0.340873
H	-2.154983	3.734547	0.318030
C	-0.326445	4.773551	-0.036391
H	-0.835638	5.675272	-0.382527
C	1.059025	4.740852	0.080474
H	1.661330	5.616981	-0.168094
C	1.669769	3.586246	0.553877
H	2.751489	3.586181	0.701056
C	0.940059	2.434903	0.880614
C	1.683864	1.238932	1.405440
H	1.176037	0.838349	2.294868
H	2.690509	1.538790	1.733381
C	2.888067	0.379007	-1.204588
C	4.021089	1.336095	-0.833160
H	4.763167	0.884688	-0.164182
H	3.649901	2.257683	-0.373601
H	4.548309	1.630086	-1.755005
C	1.895869	1.099779	-2.129566
H	1.107792	0.417396	-2.487440
H	2.436069	1.482591	-3.010455
H	1.405981	1.952230	-1.639343
C	3.480951	-0.809579	-1.964763
H	2.721464	-1.545966	-2.262906
H	4.265279	-1.329133	-1.398538
H	3.943653	-0.435346	-2.891695
C	2.849923	-1.440578	1.348747
C	2.192941	-1.492774	2.732424
H	2.382072	-0.586886	3.324941
H	2.616749	-2.339636	3.294579
H	1.107173	-1.652625	2.671523
C	4.318654	-1.056086	1.525990
H	4.439750	-0.042631	1.936263
H	4.891411	-1.124155	0.591984
H	4.784150	-1.751456	2.242986
C	2.739135	-2.835148	0.724281
H	3.146698	-2.883251	-0.294158
H	1.692375	-3.176505	0.696953
H	3.305471	-3.553243	1.338019

L1-Pd-ethyl-CO

Pd	-0.116033	-1.273213	-0.494873
P	-1.867162	0.189598	0.200602
P	1.847225	-0.095765	0.341378
C	0.879798	-2.524988	-1.550112
C	-1.573203	-2.738847	-1.031266
H	-2.559690	-2.300919	-0.888618
H	-1.496709	-2.962699	-2.105881
C	-1.400179	-3.990737	-0.192342
H	-2.215499	-4.704207	-0.404963
H	-1.432577	-3.787857	0.888568
H	-0.456965	-4.521215	-0.392797
O	1.327483	-3.290046	-2.257544
C	-3.039121	-0.504020	1.553537
C	-2.133657	-1.277190	2.516957

H	-1.381538	-0.628409	2.990578
H	-1.608880	-2.101211	2.013916
H	-2.743347	-1.707800	3.327055
C	-3.764033	0.593558	2.345331
H	-3.089399	1.202132	2.960468
H	-4.463525	0.101911	3.039301
H	-4.359783	1.261717	1.708899
C	-4.114966	-1.444475	1.004052
H	-3.709575	-2.315022	0.477098
H	-4.823477	-0.926061	0.344126
H	-4.695950	-1.830796	1.856218
C	-2.786169	0.818102	-1.336233
C	-3.414225	-0.307682	-2.162120
H	-2.654417	-0.982986	-2.573362
H	-3.934701	0.154858	-3.015482
H	-4.156369	-0.899726	-1.613265
C	-3.881905	1.819055	-0.966866
H	-4.283966	2.261249	-1.892252
H	-3.526287	2.648803	-0.342908
H	-4.721988	1.333989	-0.449869
C	-1.718610	1.469045	-2.226281
H	-0.935687	0.742205	-2.492959
H	-1.234480	2.338678	-1.768982
H	-2.194875	1.802580	-3.161965
C	-1.331314	1.727773	1.101508
H	-2.263506	2.246421	1.354317
H	-0.943900	1.336919	2.055712
C	-0.382005	2.755860	0.555656
C	-0.916582	3.940431	0.027976
H	-2.000498	4.039752	-0.063115
C	-0.111770	5.005449	-0.356941
H	-0.562100	5.910493	-0.769503
C	1.263848	4.922006	-0.162321
H	1.913102	5.763980	-0.410773
C	1.804890	3.766140	0.387857
H	2.875079	3.738914	0.599783
C	1.012540	2.657769	0.718551
C	1.647809	1.451834	1.349784
H	1.055516	1.136500	2.220676
H	2.644154	1.713797	1.734158
C	3.062447	0.366915	-1.040563
C	4.129431	1.369305	-0.596089
H	4.733234	1.009569	0.246267
H	3.701813	2.340906	-0.335110
H	4.816622	1.540640	-1.439799
C	2.199821	0.995016	-2.143082
H	1.486242	0.268515	-2.561131
H	2.850874	1.336640	-2.963512
H	1.630931	1.864587	-1.783040
C	3.782292	-0.859620	-1.602031
H	3.105156	-1.645204	-1.953433
H	4.485512	-1.300297	-0.882686
H	4.372077	-0.540361	-2.475783
C	2.641164	-1.259166	1.620561
C	1.726410	-1.274017	2.851453
H	1.776765	-0.343810	3.434303
H	2.045423	-2.088036	3.521155
H	0.678219	-1.466357	2.577674
C	4.043867	-0.818264	2.040825
H	4.072232	0.216557	2.412001
H	4.776219	-0.917537	1.228663
H	4.385719	-1.463856	2.865719
C	2.694329	-2.690163	1.075769
H	3.248068	-2.778254	0.132888
H	1.684869	-3.103556	0.931332
H	3.203090	-3.329988	1.813694

L1-Pd-TS-ethyl-CO

Pd	0.055049	-1.218571	-0.449009
P	-1.884873	0.053283	0.268487
P	1.842058	0.110684	0.354994
C	1.022661	-2.497971	-1.417301
C	-0.982706	-3.119490	-1.279873
H	-1.945065	-2.672091	-1.030387
H	-0.944315	-3.236552	-2.370838
C	-0.753225	-4.407635	-0.519766
H	-1.596826	-5.095943	-0.695071
H	-0.689861	-4.245047	0.566784

H	0.161778	-4.930320	-0.833165
O	1.708171	-3.186105	-2.025007
C	-3.012687	-0.826253	1.527671
C	-2.292069	-0.806845	2.881862
H	-2.289504	0.185250	3.353332
H	-1.253715	-1.162697	2.800974
H	-2.816498	-1.487543	3.570362
C	-4.381735	-0.163165	1.678175
H	-4.320580	0.913253	1.893676
H	-4.907661	-0.631579	2.525628
H	-5.011406	-0.306385	0.789976
C	-3.204127	-2.292450	1.138653
H	-2.250784	-2.836748	1.142195
H	-3.681983	-2.421589	0.158639
H	-3.858987	-2.772233	1.882901
C	-2.819381	0.554202	-1.308561
C	-3.495961	-0.652611	-1.960517
H	-2.784116	-1.443818	-2.225536
H	-3.966616	-0.318598	-2.898826
H	-4.293232	-1.080540	-1.337285
C	-3.881052	1.632082	-1.089353
H	-4.287127	1.920903	-2.072050
H	-3.476795	2.540739	-0.635024
H	-4.723081	1.282560	-0.481408
C	-1.739023	1.081729	-2.262931
H	-0.995673	0.302572	-2.496000
H	-1.206537	1.953129	-1.857710
H	-2.212076	1.387608	-3.209794
C	-1.570180	1.642591	1.185462
H	-2.557021	2.031004	1.476774
H	-1.087978	1.316452	2.117763
C	-0.765412	2.756790	0.575098
C	-1.434296	3.890364	0.092046
H	-2.523616	3.927201	0.141514
C	-0.756560	4.995445	-0.408201
H	-1.315041	5.856631	-0.780518
C	0.633825	5.006975	-0.382917
H	1.191085	5.877155	-0.735615
C	1.311664	3.915122	0.146052
H	2.396572	3.974954	0.240365
C	0.645134	2.771250	0.606908
C	1.437698	1.675706	1.267531
H	0.902037	1.329524	2.162261
H	2.395098	2.082470	1.625214
C	3.035413	0.616047	-1.028420
C	4.007304	1.721729	-0.610624
H	4.637757	1.440614	0.241599
H	3.499923	2.661375	-0.376605
H	4.679374	1.926759	-1.458874
C	2.145433	1.121447	-2.171079
H	1.506560	0.318876	-2.569487
H	2.783600	1.481825	-2.993535
H	1.498057	1.954321	-1.860609
C	3.862678	-0.571806	-1.522158
H	3.256645	-1.430138	-1.829930
H	4.596531	-0.908379	-0.777276
H	4.430310	-0.246859	-2.408413
C	2.709394	-0.902844	1.709186
C	1.769566	-0.953737	2.919555
H	1.707205	0.001755	3.458620
H	2.150726	-1.700267	3.633609
H	0.753994	-1.265235	2.630155
C	4.048235	-0.298994	2.135660
H	3.962433	0.752737	2.445554
H	4.809383	-0.370681	1.347475
H	4.428133	-0.859930	3.004528
C	2.919948	-2.344131	1.234491
H	3.496942	-2.419024	0.305267
H	1.960158	-2.861749	1.088944
H	3.473157	-2.893368	2.012161

L1-Pd-propanoyl

Pd	0.217824	-1.082609	-0.419192
P	-1.932398	-0.174024	0.329996
P	1.828927	0.366302	0.354364
C	1.330691	-2.392836	-1.343710
C	0.053665	-3.198083	-1.634444
H	-0.876908	-2.723344	-1.232344

H	-0.069638	-3.169697	-2.728977
C	0.172953	-4.614622	-1.089077
H	-0.715680	-5.205873	-1.349692
H	0.277113	-4.615779	0.005397
H	1.060771	-5.101954	-1.516885
O	2.429737	-2.700197	-1.653209
C	-2.816726	-1.364365	1.514594
C	-2.193089	-1.185594	2.903564
H	-2.494446	-0.244886	3.384754
H	-1.094186	-1.228820	2.873793
H	-2.534811	-2.004944	3.555339
C	-4.322853	-1.130122	1.619692
H	-4.565896	-0.095908	1.905187
H	-4.733915	-1.786572	2.403700
H	-4.854001	-1.366875	0.688323
C	-2.531381	-2.799346	1.059795
H	-1.451364	-3.015967	1.086287
H	-2.906717	-3.014847	0.050618
H	-3.023095	-3.504633	1.748333
C	-2.946597	0.129988	-1.243012
C	-3.358807	-1.204619	-1.867977
H	-2.500832	-1.868098	-2.049684
H	-3.819206	-1.005697	-2.848749
H	-4.099842	-1.747698	-1.266372
C	-4.195499	0.984857	-1.032028
H	-4.707915	1.106756	-2.000056
H	-3.952016	1.990426	-0.673423
H	-4.912877	0.529853	-0.338577
C	-1.993264	0.840669	-2.215362
H	-1.115474	0.215325	-2.448847
H	-1.628169	1.799666	-1.823630
H	-2.523127	1.042096	-3.160329
C	-1.946135	1.418199	1.279889
H	-2.987093	1.650626	1.550380
H	-1.426020	1.184786	2.220401
C	-1.312704	2.607222	0.614952
C	-2.151040	3.624983	0.138935
H	-3.228856	3.532805	0.286890
C	-1.655077	4.761027	-0.487713
H	-2.339260	5.531120	-0.849624
C	-0.278718	4.914153	-0.615286
H	0.142084	5.805995	-1.084014
C	0.566447	3.941818	-0.093888
H	1.639797	4.122750	-0.136037
C	0.086800	2.772813	0.514717
C	1.056661	1.838204	1.197994
H	0.564482	1.392410	2.072080
H	1.897232	2.427252	1.596087
C	2.984240	1.059698	-0.973880
C	3.743514	2.307222	-0.513867
H	4.449538	2.093651	0.297096
H	3.095105	3.126907	-0.193100
H	4.332713	2.679521	-1.366882
C	2.072280	1.399794	-2.160124
H	1.606946	0.492241	-2.573663
H	2.675367	1.861490	-2.957834
H	1.272095	2.104851	-1.893052
C	4.022907	0.027453	-1.417457
H	3.582917	-0.927930	-1.720774
H	4.773135	-0.164167	-0.637749
H	4.561671	0.440990	-2.284852
C	2.774966	-0.450094	1.781004
C	1.796965	-0.646430	2.944123
H	1.532521	0.291015	3.453123
H	2.269209	-1.297984	3.695615
H	0.874105	-1.144963	2.609937
C	3.962042	0.390329	2.254896
H	3.680341	1.420544	2.517774
H	4.769875	0.425508	1.512309
H	4.378430	-0.072304	3.163942
C	3.257367	-1.837796	1.350213
H	3.870266	-1.828813	0.441981
H	2.409089	-2.514968	1.175553
H	3.863153	-2.265583	2.164137

L1-Pd-propanoyl-n-pentanol

Pd	0.426865	-0.063724	0.615187
P	-0.322474	-1.812228	-0.699712

P	-0.838267	1.957355	-0.252789
C	-0.812018	-3.505262	0.024894
C	1.019033	-2.023124	-2.034092
C	0.058031	3.370120	-1.176474
C	-1.633032	2.618937	1.347016
C	-1.796422	-1.300610	-1.712433
C	-2.260862	1.657307	-1.415346
C	-3.286284	0.640151	-1.004361
C	-4.551808	1.088364	-0.601134
C	-5.550073	0.213313	-0.191785
C	-5.299114	-1.154705	-0.210611
C	-4.071060	-1.616581	-0.670158
C	-3.045376	-0.749018	-1.071378
H	-2.751646	2.624329	-1.600815
H	-1.791706	1.363494	-2.365433
H	-1.385247	-0.549906	-2.398113
H	-2.062942	-2.163548	-2.339194
H	-4.767281	2.158311	-0.628187
H	-6.522995	0.598511	0.120036
H	-6.068731	-1.866647	0.094498
H	-3.923062	-2.693390	-0.742593
C	1.193282	-1.335895	1.939692
C	0.563749	-1.062068	3.301926
C	1.100734	-1.969392	4.395847
H	0.758642	0.001422	3.527188
H	-0.529933	-1.137376	3.205281
O	2.137131	-2.054237	1.795111
H	2.046476	2.052228	0.941577
H	0.885574	-3.025132	4.175658
H	2.190429	-1.870638	4.496153
C	0.691347	-3.109454	-3.058179
C	1.167608	-0.680827	-2.756185
C	2.363781	-2.318982	-1.365334
C	-1.668539	-4.328399	-0.945265
C	0.397704	-4.369621	0.392605
C	-1.617495	-3.206369	1.295584
C	-2.790734	3.596127	1.147117
C	-2.155294	1.382869	2.092680
C	-0.562564	3.285421	2.215096
C	-0.680959	4.707371	-1.142551
C	1.458143	3.552164	-0.585393
C	0.229550	2.950265	-2.641484
H	2.042874	-0.731665	-3.422650
H	0.302753	-0.423172	-3.384057
H	1.341228	0.133450	-2.036663
H	3.136273	-2.381640	-2.148170
H	2.645503	-1.518473	-0.669483
H	2.376825	-3.259944	-0.806370
H	1.451648	-3.080067	-3.855398
H	0.723452	-4.117223	-2.623845
H	-0.286525	-2.963713	-3.540426
H	-2.108798	-4.130576	1.638870
H	-0.964502	-2.865142	2.107848
H	-2.397097	-2.446400	1.143600
H	-1.885210	-5.296357	-0.466552
H	-2.633711	-3.870659	-1.183597
H	-1.154157	-4.543739	-1.889184
H	0.029140	-5.243825	0.952965
H	0.912677	-4.756273	-0.497307
H	1.129410	-3.854533	1.023726
H	-1.002806	3.520418	3.197451
H	0.302326	2.629898	2.389481
H	-0.209347	4.235672	1.790142
H	-2.591485	1.700210	3.053589
H	-2.930281	0.844729	1.531112
H	-1.342586	0.673735	2.311260
H	-3.199970	3.854719	2.137304
H	-2.488371	4.533441	0.668151
H	-3.612455	3.158326	0.571317
H	0.922011	3.652095	-3.132870
H	0.657785	1.943653	-2.742473
H	-0.714137	2.988561	-3.202423
H	1.970870	4.382179	-1.096905
H	1.439501	3.808492	0.484427
H	2.077534	2.658208	-0.758155
H	-0.160968	5.416655	-1.806998
H	-1.715975	4.627195	-1.504803
H	-0.696334	5.155000	-0.140270

H	0.638056	-1.718256	5.360546
C	4.221073	0.344855	1.071798
C	4.299697	1.010927	-0.293477
C	5.315735	0.365669	-1.225945
C	3.309077	1.038982	2.063753
C	5.301959	0.958595	-2.624741
O	1.991690	1.313146	1.561241
H	5.224172	0.310724	1.530092
H	3.904099	-0.702243	0.954296
H	3.307297	0.959357	-0.778414
H	4.536251	2.086210	-0.183714
H	6.323109	0.461710	-0.786207
H	5.115193	-0.718538	-1.277056
H	3.739558	2.000557	2.391561
H	3.170817	0.421894	2.962134
H	4.317050	0.829873	-3.103638
H	5.520736	2.038213	-2.606067
H	6.050528	0.481936	-3.274226

L1-Pd-TS-propanoyl-n-pentanol

Pd	0.290992	-0.011548	0.274786
P	-0.575987	-2.099572	-0.250015
P	-0.399068	2.086961	-0.318431
C	-1.467514	-3.088254	1.088252
C	0.575981	-3.188260	-1.289909
C	0.702798	3.190563	-1.403319
C	-1.273331	3.080051	1.035936
C	-1.861112	-1.577366	-1.514831
C	-1.695583	1.556814	-1.580996
C	-2.915966	0.766559	-1.180446
C	-4.095897	1.495318	-0.953713
C	-5.305190	0.893741	-0.636194
C	-5.372407	-0.495118	-0.578328
C	-4.231046	-1.236234	-0.849675
C	-2.987825	-0.647941	-1.137179
H	-2.027888	2.469608	-2.100960
H	-1.103355	0.985281	-2.309093
H	-1.253436	-1.111473	-2.302491
H	-2.291092	-2.490593	-1.956372
H	-4.065302	2.581886	-1.052596
H	-6.193659	1.505167	-0.465710
H	-6.314706	-1.001281	-0.358813
H	-4.309490	-2.324679	-0.866856
C	1.822859	-0.465563	2.344884
C	0.854706	0.043249	3.359576
C	1.600791	0.493616	4.617252
H	0.263424	0.864411	2.938050
H	0.177184	-0.792883	3.579506
O	2.408366	-1.486257	2.271531
H	1.899072	1.035668	0.928081
H	2.189871	-0.328503	5.047697
H	2.273978	1.336255	4.403215
C	0.003625	-4.551683	-1.669748
C	0.898068	-2.402536	-2.566622
C	1.881745	-3.360593	-0.508778
C	-2.450902	-4.138455	0.572788
C	-0.416781	-3.764751	1.972894
C	-2.222084	-2.052604	1.932313
C	-2.180450	4.209299	0.545350
C	-2.115748	2.067163	1.824411
C	-0.208360	3.665953	1.968282
C	0.057522	4.504290	-1.842612
C	2.000225	3.490309	-0.649635
C	1.057327	2.362498	-2.645581
H	1.762963	-2.866673	-3.066225
H	0.068201	-2.405931	-3.287032
H	1.164856	-1.356934	-2.340930
H	2.599149	-3.930032	-1.121835
H	2.329114	-2.384622	-0.274104
H	1.750728	-3.900896	0.436410
H	0.686295	-5.043690	-2.381810
H	-0.090676	-5.218395	-0.801926
H	-0.978570	-4.476532	-2.160012
H	-2.702743	-2.560935	2.783855
H	-1.539203	-1.287117	2.327887
H	-3.004647	-1.533151	1.363961
H	-2.976511	-4.587070	1.431506
H	-3.217957	-3.711418	-0.084304

H	-1.955135	-4.953139	0.032807
H	-0.907995	-4.154327	2.879272
H	0.060406	-4.618688	1.472122
H	0.374713	-3.068592	2.288785
H	-0.695494	4.039859	2.883105
H	0.542566	2.919358	2.271015
H	0.318946	4.516057	1.514004
H	-2.513063	2.556774	2.728062
H	-2.965864	1.689776	1.243392
H	-1.525337	1.192930	2.133567
H	-2.776642	4.580393	1.394693
H	-1.617326	5.061397	0.148864
H	-2.888522	3.881202	-0.224658
H	1.907046	2.833841	-3.164386
H	1.356623	1.336112	-2.381813
H	0.228038	2.310298	-3.364202
H	2.660324	4.097297	-1.290091
H	1.839601	4.048024	0.281270
H	2.543585	2.565057	-0.414729
H	0.681420	4.966820	-2.624494
H	-0.946621	4.365937	-2.269355
H	-0.013502	5.226575	-1.018957
H	0.873420	0.825108	5.371150
C	4.370312	-0.200056	0.265365
C	3.811066	0.178526	-1.096464
C	4.341365	-0.700586	-2.221460
C	3.977782	0.706678	1.407207
C	3.871413	-0.266772	-3.599810
O	2.544866	0.790602	1.704540
H	5.473124	-0.154545	0.234574
H	4.117629	-1.240690	0.513947
H	2.703641	0.116431	-1.070219
H	4.054938	1.232565	-1.318339
H	5.444742	-0.692653	-2.190331
H	4.045925	-1.746802	-2.033115
H	4.264465	1.752636	1.226437
H	4.424242	0.380913	2.355977
H	2.774333	-0.302200	-3.685105
H	4.186483	0.764793	-3.823377
H	4.283669	-0.915496	-4.386277

L1-Pd-n-pentyl propionate

Pd	-0.298121	-0.183448	0.221116
P	0.569651	1.903043	-0.538003
P	1.043829	-1.899416	-0.239137
C	0.873610	3.125466	0.867716
C	-0.641638	2.581807	-1.820589
C	0.287948	-3.102113	-1.493630
C	1.620631	-2.742686	1.346741
C	2.161550	1.738663	-1.477963
C	2.544583	-1.278527	-1.151736
C	3.492163	-0.261935	-0.568434
C	4.666479	-0.718937	0.048025
C	5.648958	0.145056	0.514772
C	5.494937	1.514251	0.323137
C	4.358373	1.983479	-0.322852
C	3.332778	1.130162	-0.755087
H	3.111414	-2.181899	-1.428922
H	2.119045	-0.888022	-2.085781
H	1.896631	1.124787	-2.351027
H	2.439408	2.729651	-1.867474
H	4.837891	-1.792509	0.135995
H	6.545880	-0.254528	0.992156
H	6.268234	2.213599	0.647399
H	4.271551	3.053165	-0.521813
C	-3.116369	0.668641	2.279495
C	-1.837302	0.300539	2.991207
C	-1.858572	-0.969545	3.816455
H	-1.055020	0.217261	2.194804
H	-1.538450	1.179111	3.580291
O	-3.389632	1.794414	1.938648
H	-0.835831	-1.591369	0.653890
H	-2.579710	-0.890450	4.642325
H	-2.149639	-1.835069	3.205986
C	-0.425615	4.048805	-2.183812
C	-0.499119	1.725730	-3.083918
C	-2.051801	2.360099	-1.262840
C	1.723826	4.329082	0.462418

C	-0.466661	3.616990	1.420085
C	1.592167	2.332969	1.968634
C	2.837957	-3.646332	1.134405
C	1.979028	-1.608081	2.315639
C	0.492700	-3.577236	1.953843
C	1.127480	-4.372374	-1.650127
C	-1.136593	-3.476968	-1.078057
C	0.216627	-2.376538	-2.842670
H	-1.344838	1.937786	-3.756655
H	0.422441	1.941786	-3.642857
H	-0.528961	0.649644	-2.852369
H	-2.795190	2.701708	-2.000894
H	-2.239290	1.286833	-1.087652
H	-2.247064	2.889972	-0.323558
H	-1.111758	4.321033	-3.002082
H	-0.638772	4.724590	-1.345071
H	0.596807	4.245264	-2.539740
H	1.807578	3.007835	2.812651
H	0.964417	1.512879	2.347259
H	2.545215	1.903708	1.631014
H	1.833001	4.993273	1.334972
H	2.734930	4.041518	0.152836
H	1.268371	4.920026	-0.341625
H	-0.278521	4.160423	2.359884
H	-0.967911	4.318896	0.739665
H	-1.174661	2.807009	1.648215
H	0.812414	-3.918407	2.951104
H	-0.432294	-2.997868	2.087290
H	0.267094	-4.473926	1.360354
H	2.345133	-2.047400	3.257106
H	2.764566	-0.947579	1.923444
H	1.098687	-0.991434	2.549960
H	3.159059	-4.026352	2.116849
H	2.617931	-4.516699	0.506262
H	3.692902	-3.115848	0.704248
H	-0.427589	-2.955543	-3.521495
H	-0.229028	-1.375424	-2.745015
H	1.197620	-2.282296	-3.328518
H	-1.536984	-4.192924	-1.812852
H	-1.185187	-3.954165	-0.091560
H	-1.800224	-2.602082	-1.068357
H	0.730889	-4.948957	-2.500460
H	2.185815	-4.166322	-1.867243
H	1.069715	-5.020914	-0.766066
H	-0.868572	-1.164096	4.253512
C	-5.104067	0.180840	-0.035488
C	-4.285768	-0.771683	-0.893923
C	-4.414687	-0.466887	-2.380401
C	-5.166889	-0.169461	1.437260
C	-3.511685	-1.307646	-3.264956
O	-3.884219	-0.389010	2.040654
H	-6.147130	0.196226	-0.396945
H	-4.725771	1.208141	-0.149288
H	-3.221159	-0.718529	-0.591491
H	-4.590994	-1.816485	-0.702025
H	-5.466582	-0.608845	-2.681847
H	-4.203566	0.603405	-2.548701
H	-5.695303	-1.119739	1.594704
H	-5.685273	0.622916	1.998327
H	-2.450626	-1.121710	-3.037616
H	-3.695674	-2.384820	-3.123279
H	-3.665072	-1.083061	-4.330991

L1-Pd-propanoyl-3(n-pentanol)

Pd	1.42126	-0.032662	-0.433805
P	3.147969	1.451489	-0.432712
P	2.126817	-1.740882	1.076104
C	-0.023674	0.58689	-1.6429
C	-0.683256	1.613159	-2.493721
H	-0.490299	2.59138	-2.032325
H	-0.115121	1.621211	-3.441734
C	-2.163503	1.354838	-2.726237
H	-2.608684	2.186562	-3.289277
H	-2.694547	1.253762	-1.768939
H	-2.321304	0.432042	-3.303561
O	-0.514099	-0.502034	-1.390449
C	2.638109	3.073758	0.410349
C	2.205682	2.708125	1.835401

H	3.027973	2.334428	2.461795	C	2.757787	-4.534366	0.796914
H	1.390368	1.969375	1.817571	H	2.263591	-4.784261	1.743104
H	1.820534	3.615148	2.32746	H	3.823274	-4.368021	0.992397
C	3.757297	4.11432	0.452058	H	2.687311	-5.421057	0.146209
H	4.687882	3.738531	0.900896	C	0.914145	-1.807076	2.532525
H	3.422802	4.962257	1.070914	C	1.312846	-0.698418	3.513983
H	3.986643	4.516217	-0.543756	H	2.226053	-0.936545	4.077766
C	1.41101	3.663866	-0.28626	H	0.502882	-0.573237	4.249739
H	0.5734	2.954682	-0.26044	H	1.445653	0.269801	3.010199
H	1.608439	3.96774	-1.320451	C	0.918727	-3.144237	3.271559
H	1.101467	4.566883	0.263825	H	1.92191	-3.433519	3.619435
C	3.849568	1.706548	-2.173037	H	0.509955	-3.962138	2.663622
C	2.864731	2.46991	-3.056274	H	0.280155	-3.055459	4.165439
H	1.849674	2.063676	-2.980814	C	-0.490946	-1.483823	2.013694
H	3.187037	2.37555	-4.105353	H	-0.846555	-2.173172	1.238332
H	2.834791	3.541985	-2.82089	H	-0.543368	-0.457962	1.621441
C	5.183944	2.454011	-2.192304	H	-1.201281	-1.544246	2.854159
H	5.089435	3.490091	-1.845777	C	-1.598087	2.830039	1.479255
H	5.547189	2.489912	-3.231828	H	-2.098495	2.497544	2.410232
H	5.962902	1.965307	-1.599122	H	-0.755566	3.467398	1.79506
C	4.022917	0.295621	-2.750635	O	-1.0622	1.72962	0.785576
H	3.050883	-0.211163	-2.846693	C	-3.739986	-2.586052	-1.615113
H	4.678003	-0.339191	-2.139207	H	-3.401156	-3.307222	-2.38067
H	4.46872	0.371218	-3.755283	H	-4.141984	-1.704636	-2.15231
C	4.596933	0.942659	0.623474	O	-2.656481	-2.202187	-0.78576
H	5.307926	1.780251	0.575774	H	-1.955124	-1.801164	-1.318403
H	4.182875	0.95664	1.641181	C	-4.402745	0.143741	1.141309
C	5.354469	-0.343624	0.411724	H	-4.381349	0.980239	1.859257
C	6.553915	-0.317975	-0.314532	H	-4.536819	-0.777155	1.740131
H	6.889273	0.619897	-0.758695	O	-3.154761	0.117849	0.485238
C	7.358992	-1.441289	-0.461905	H	-1.804803	1.093731	0.663137
H	8.282716	-1.377644	-1.040633	H	-3.009148	-0.769219	0.082011
C	5.833216	-2.661067	0.927759	C	0.669918	-3.703765	-0.294674
H	5.581575	-3.575704	1.46859	H	0.142776	-2.861071	-0.762721
C	4.987617	-1.549734	1.046188	H	0.688528	-4.529817	-1.023566
C	3.77134	-1.660625	1.919976	H	0.07766	-4.041679	0.565965
H	3.702081	-0.783299	2.579514	C	6.996806	-2.626995	0.169169
H	3.860728	-2.53673	2.579547	H	7.629739	-3.513757	0.096401
C	2.111109	-3.350453	0.078908	C	2.88445	-3.056358	-1.214064

H	2.387489	-2.273447	-1.807079
H	3.918658	-2.736939	-1.026124
H	2.920901	-3.972013	-1.826229
C	-4.82502	-3.198722	-0.757256
H	-4.993773	-2.537046	0.109419
H	-4.465573	-4.154776	-0.341439
C	-6.13824	-3.394687	-1.499106
H	-5.995237	-4.093413	-2.342888
H	-6.444001	-2.434951	-1.955455
C	-7.265084	-3.897356	-0.606791
H	-7.37615	-3.208116	0.249471
H	-6.978281	-4.870467	-0.171462
C	-8.594858	-4.026157	-1.330616
H	-8.524869	-4.725974	-2.178475
H	-9.385536	-4.394987	-0.660677
H	-8.926723	-3.0546	-1.73126
C	-5.564978	0.308811	0.177394
H	-5.444853	-0.419847	-0.642581
H	-5.507515	1.305131	-0.294707
C	-6.924657	0.103859	0.826765
H	-7.074958	0.847384	1.630341
H	-6.94071	-0.881952	1.32769
C	-8.083836	0.177377	-0.157988
H	-7.902608	-0.541947	-0.976792
H	-8.094385	1.173781	-0.633533
C	-9.434667	-0.107111	0.476963
H	-9.65714	0.607449	1.285346
H	-10.249881	-0.040076	-0.258637
H	-9.464515	-1.118515	0.913612
C	-2.568579	3.639346	0.63671
H	-2.044812	3.984444	-0.27295
H	-3.376284	2.971853	0.287287
C	-3.168064	4.827352	1.371971
H	-2.358164	5.495999	1.717268
H	-3.672744	4.474403	2.289983
C	-4.156545	5.626379	0.533394
H	-4.962026	4.953249	0.189399
H	-3.650841	5.97778	-0.383565
C	-4.758247	6.80993	1.272751
H	-5.467486	7.364711	0.640808
H	-5.301332	6.484261	2.174311
H	-3.978627	7.517735	1.596905

L1-Pd-TS-propanoyl-3(n-pentanol)

Pd	1.292835	0.146001	-0.04368
P	3.013352	1.63412	0.194861
P	2.233414	-1.9162	0.700121
C	-0.3786	0.898389	-0.95969
C	-0.77204	1.606992	-2.22433
H	-0.81326	2.691235	-2.0563
H	0.065126	1.450007	-2.92417
C	-2.06734	1.070807	-2.81849
H	-2.36207	1.653769	-3.70232
H	-2.88918	1.11507	-2.08903
H	-1.9501	0.021633	-3.12526
O	-0.6362	-0.31662	-0.79265
C	2.74283	2.80757	1.667497
C	2.869017	1.980684	2.950988
H	3.903981	1.694065	3.183513
H	2.249587	1.073823	2.901566
H	2.50544	2.582993	3.798096
C	3.727952	3.974034	1.722827
H	4.778475	3.648543	1.703213
H	3.577481	4.520028	2.668324
H	3.569617	4.693101	0.907915
C	1.309612	3.333161	1.613641
H	0.590276	2.502559	1.601021
H	1.125465	3.960842	0.734534
H	1.118276	3.94938	2.506859
C	3.32641	2.595709	-1.40678
C	2.194793	3.597384	-1.6337
H	1.211485	3.135439	-1.48075
H	2.240192	3.962803	-2.67217
H	2.278166	4.473395	-0.9756
C	4.65873	3.344939	-1.45369
H	4.738625	4.124106	-0.68698
H	4.745736	3.841094	-2.43379
H	5.524206	2.680813	-1.3575

C	3.294236	1.543465	-2.52318
H	2.320517	1.032873	-2.56036
H	4.069058	0.774201	-2.39739
H	3.463352	2.037707	-3.49353
C	4.655409	0.8881	0.65255
H	5.368922	1.723477	0.716766
H	4.499467	0.546801	1.684237
C	5.282631	-0.23318	-0.13404
C	6.268386	0.064508	-1.08525
H	6.508313	1.107784	-1.29467
C	6.9875	-0.92496	-1.74582
H	7.744318	-0.6494	-2.48313
C	5.811821	-2.57207	-0.45942
H	5.678363	-3.61626	-0.16997
C	5.034074	-1.58988	0.168933
C	4.020745	-2.01713	1.194199
H	4.096688	-1.3834	2.090113
H	4.230546	-3.04641	1.522329
C	2.025799	-3.12505	-0.74925
C	2.808661	-4.42867	-0.59646
H	2.516057	-5.00333	0.290224
H	3.890491	-4.26261	-0.56435
H	2.609548	-5.06161	-1.47662
C	1.334607	-2.54794	2.2487
C	1.932161	-1.82972	3.46265
H	2.945282	-2.17805	3.708684
H	1.298029	-2.03078	4.3404
H	1.958179	-0.73995	3.323459
C	1.460488	-4.05462	2.470646
H	2.508447	-4.3872	2.515589
H	0.94157	-4.63977	1.70052
H	0.998685	-4.31042	3.438209
C	-0.14004	-2.14531	2.143795
H	-0.65697	-2.58688	1.283617
H	-0.25215	-1.05219	2.075598
H	-0.66791	-2.47794	3.052087
C	-1.73014	3.102703	0.382971
H	-1.64445	3.419874	1.436568
H	-0.95796	3.657799	-0.17063
O	-1.3829	1.729327	0.308532
C	-3.57529	-2.41429	-1.19267
H	-3.03719	-2.95616	-1.99176
H	-4.06384	-1.54026	-1.66667
O	-2.66377	-1.99389	-0.19646
H	-1.93539	-1.48675	-0.59997
C	-4.37944	0.440393	1.692739
H	-4.35138	1.446142	2.143827
H	-4.71378	-0.24809	2.489212
O	-3.05309	0.123955	1.316911
H	-2.09146	1.093746	0.705304
H	-3.02121	-0.75211	0.848229
C	0.543375	-3.45088	-0.94245
H	-0.06921	-2.5453	-1.023
H	0.430785	-4.01598	-1.88189
H	0.136052	-4.07557	-0.13662
C	6.76638	-2.25902	-1.41961
H	7.349216	-3.0528	-1.89133
C	2.517771	-2.37857	-1.99801
H	1.910399	-1.48073	-2.19007
H	3.568897	-2.06907	-1.9205
H	2.426664	-3.04397	-2.872
C	-4.61993	-3.31347	-0.57155
H	-5.06136	-2.7939	0.297486
H	-4.12164	-4.20968	-0.16523
C	-5.72022	-3.70993	-1.54343
H	-5.27724	-4.21784	-2.41933
H	-6.20494	-2.79864	-1.94043
C	-6.78076	-4.60954	-0.92351
H	-7.21606	-4.10028	-0.04533
H	-6.29655	-5.52033	-0.52977
C	-7.88584	-4.99342	-1.89342
H	-7.48391	-5.53589	-2.764
H	-8.6354	-5.64187	-1.41631
H	-8.41147	-4.10317	-2.27462
C	-5.35193	0.410474	0.528073
H	-5.41973	-0.61974	0.139638
H	-4.94378	1.021101	-0.29639
C	-6.74334	0.904999	0.89104

H	-6.68097	1.948769	1.250549
H	-7.13473	0.318895	1.742052
C	-7.72804	0.829832	-0.26809
H	-7.78756	-0.21498	-0.62209
H	-7.328	1.410643	-1.11837
C	-9.1176	1.331434	0.087401
H	-9.09258	2.384772	0.409373
H	-9.80378	1.262916	-0.76953
H	-9.55564	0.745942	0.911259
C	-3.10941	3.425345	-0.15212
H	-3.18331	3.116802	-1.20758
H	-3.85801	2.831759	0.396592
C	-3.45496	4.901737	-0.02434
H	-2.72203	5.505915	-0.58949
H	-3.35255	5.2154	1.030326
C	-4.86111	5.227019	-0.51119
H	-5.58687	4.615491	0.054447
H	-4.96081	4.909338	-1.56416
C	-5.21845	6.698168	-0.38217
H	-6.23867	6.898144	-0.74098
H	-5.16338	7.033338	0.665749
H	-4.53136	7.329991	-0.96718

L1-Pd-n-pentyl propionate-2(n-pentanol)

Pd	-1.20987	0.237914	-0.34911
P	-1.84552	-1.91262	0.106148
P	-2.90493	1.572095	0.746847
C	0.421191	0.298932	-1.65606
C	0.177707	0.032284	-3.12664
H	0.224148	-1.04323	-3.34266
H	-0.86232	0.332621	-3.31965
C	1.107875	0.826711	-4.03932
H	0.84033	0.666531	-5.09352
H	2.162654	0.539243	-3.91866
H	1.025549	1.902418	-3.82792
O	0.138453	1.599134	-1.3481
C	-0.74413	-2.62643	1.487215
C	-0.8053	-1.6281	2.648166
H	-1.80489	-1.54317	3.096677
H	-0.47772	-0.62825	2.325473
H	-0.12817	-1.96861	3.447912
C	-1.1657	-4.01024	1.978481
H	-2.20778	-4.04378	2.326481
H	-0.53186	-4.29195	2.835104
H	-1.02968	-4.78363	1.211159
C	0.71024	-2.67043	1.019422
H	1.003283	-1.70836	0.579104
H	0.89814	-3.46163	0.285093
H	1.361961	-2.86678	1.885889
C	-1.93784	-3.06693	-1.39422
C	-0.53081	-3.37244	-1.90864
H	0.11704	-2.48776	-1.88044
H	-0.59368	-3.71539	-2.95389
H	-0.0479	-4.17365	-1.33321
C	-2.65532	-4.39345	-1.14234
H	-2.1405	-5.01881	-0.40236
H	-2.68252	-4.96208	-2.08594
H	-3.69413	-4.26845	-0.81694
C	-2.69723	-2.26202	-2.45786
H	-2.16287	-1.33727	-2.71245
H	-3.70812	-1.98214	-2.13272
H	-2.79236	-2.86842	-3.37312
C	-3.51848	-2.06358	0.915719
H	-3.69096	-3.13844	1.068098
H	-3.36000	-1.63911	1.916461
C	-4.76146	-1.45864	0.315866
C	-5.60092	-2.26416	-0.46698
H	-5.30218	-3.29054	-0.68479
C	-6.82418	-1.81485	-0.95046
H	-7.44524	-2.47386	-1.56065
C	-6.45825	0.262546	0.189819
H	-6.82843	1.243093	0.495867
C	-5.19756	-0.15546	0.638176
C	-4.39817	0.77167	1.508918
H	-4.00588	0.224987	2.379039
H	-5.04961	1.563357	1.908923
C	-3.56864	2.667591	-0.656
C	-4.86142	3.411858	-0.32469

H	-4.75165	4.110594	0.512618	H	-4.55948	0.945938	-1.61849
H	-5.68939	2.729467	-0.10319	H	-4.20103	2.316551	-2.69404
H	-5.16208	4.002317	-1.20559	C	4.299718	2.939785	-0.04095
C	-2.24632	2.628645	2.181322	H	4.262714	2.003996	0.543619
C	-2.22637	1.757616	3.44226	H	4.315102	3.761821	0.694492
H	-3.23177	1.576211	3.847905	C	5.569136	2.948828	-0.87908
H	-1.65318	2.281956	4.223401	H	5.652854	3.905646	-1.4241
H	-1.73406	0.791102	3.269571	H	5.497983	2.166044	-1.65595
C	-3.07555	3.877998	2.474217	C	6.830767	2.716367	-0.05862
H	-4.13218	3.644241	2.673033	H	6.721323	1.771611	0.505103
H	-3.02869	4.616548	1.663468	H	6.920576	3.508989	0.704361
H	-2.67645	4.364646	3.379224	C	8.094146	2.663485	-0.90099
C	-0.80061	3.010627	1.853237	H	8.244847	3.602876	-1.45591
H	-0.70584	3.588138	0.925703	H	8.987405	2.498291	-0.28082
H	-0.16489	2.116893	1.766754	H	8.046475	1.847623	-1.64032
H	-0.39429	3.629368	2.66988	C	3.933546	-0.65352	1.995031
C	2.490953	-1.06455	-1.67583	H	4.593613	0.074362	1.49268
H	2.39703	-1.95623	-1.03388	H	3.606003	-1.3634	1.213466
H	2.155636	-1.35357	-2.68117	C	4.725611	-1.41085	3.048514
O	1.66487	-0.03475	-1.14076	H	4.070351	-2.14693	3.548926
C	3.036124	3.021782	-0.86998	H	5.051988	-0.7126	3.839752
H	2.94263	4.003431	-1.35889	C	5.941122	-2.12499	2.470812
H	3.064728	2.25607	-1.66541	H	6.587932	-1.38367	1.968294
O	1.865749	2.833568	-0.07907	H	5.608245	-2.81595	1.675147
H	0.870471	2.115517	-0.77821	C	6.746417	-2.88803	3.508851
C	2.718018	0.072779	2.53479	H	6.135212	-3.66088	4.001483
H	2.053115	-0.63789	3.058571	H	7.614784	-3.38968	3.057098
H	3.015764	0.833628	3.272522	H	7.123766	-2.21558	4.295338
O	1.993611	0.753191	1.527393	C	3.924552	-0.57427	-1.69199
H	1.872664	0.192577	0.740412	H	4.058016	0.150258	-2.51272
H	2.063763	2.216822	0.667371	H	4.099732	-0.01472	-0.76046
C	-2.49351	3.676409	-1.06935	C	4.952633	-1.68888	-1.79913
H	-1.53718	3.188214	-1.30166	H	4.807924	-2.25547	-2.73643
H	-2.83245	4.193756	-1.98153	H	4.788366	-2.41369	-0.98052
H	-2.32171	4.447575	-0.30636	C	6.384695	-1.17467	-1.72727
C	-7.26322	-0.53939	-0.60989	H	6.502325	-0.57747	-0.80517
H	-8.2377	-0.17714	-0.94378	H	6.56023	-0.47225	-2.56106
C	-3.82069	1.726666	-1.84427	C	7.426277	-2.28007	-1.75502
H	-2.8911	1.230867	-2.16584	H	8.446815	-1.87283	-1.70705

H	7.301918	-2.96614	-0.90176
H	7.351221	-2.88001	-2.67568

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