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Electronic Supplementary Information

Runge-Kutta Analysis for Optimizing the Zn-Catalyzed Transesterification Conditions of MA and MMA with Diols to Maximize Monoesterified Products

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1. Experimental section

General:

All manipulations involving air- and moisture-sensitive organometallic compounds were handled under argon atmosphere using the standard Schlenk technique or an argon-filled glovebox. In all kinetic studies of the transesterification, the raw materials (complex, ligand, solvent and substrate) were weighed using an electronic balance in an argon-filled glovebox, and the samples for GC analysis were weighted using an electronic balance under atmosphere. Argon was used after purification by passing it through a gas clean CC-X(Ar) column (Nikka Seiko). Toluene and diglyme were distilled under an argon atmosphere over CaH_2. Methanol was distilled under an argon atmosphere over the corresponding magnesium alkoxide. THF and CPME were distilled over sodium benzophenone ketyl. $CDCl_3$ was dried over MS3A&4A in a J-Young Schlenk under an argon atmosphere. All other reagents were purchased from commercial resources and used without further purification. These compounds mentioned above were used after the Freeze-Pump-Thaw (FPT) cycling. NMR spectra were recorded on a Bruker AV 600M spectrometer operating at 600 MHz (^{1}H NMR) and at 150 MHz (^{13}C{^{1}H} NMR) in 5 mm NMR tubes. All ^{1}H NMR chemical shifts were reported in ppm relative to the residual solvent proton in chloroform-d_1 at δ 7.26. All ^{13}C{^{1}H} NMR chemical shifts were reported in ppm relative to carbon resonance of chloroform-d_1 at δ 77.16. DART-mass spectra (DART-MS) and high resolution mass spectra (HRMS) were recorded using a JEOL JMS-T100LP spectrometer. GC analyses were recorded on a Shimadzu GC-2010 gas chromatograph with J&W Scientific DB-1 and all samples were preliminary washed through Celite® to remove the catalysts. Flash column chromatography was performed using silica gel 60 (0.063–0.200 mm, 70-230 mesh ASTM).

Preparation of alkoxy-bridged tetranuclear complexes

Synthesis of [Zn(tmhd)(OMe)(MeOH)]$_4$ (1a)[S1]

[Zn(tmhd)(OMe)(MeOH)]$_4$ was prepared according to the literature. $ZnCl_2$ (1.36 g, 10.0 mmol) and 2,2,6,6-tetramethylheptanedione (2.08 mL, 10.0 mmol, 1.0 equiv.) were dissolved in 20 mL of methanol. In another flask, KOMe (1.40 g, 20.0 mmol, 2.0 equiv.) was dissolved in 20 mL of methanol. The two solutions were slowly mixed to form a white precipitate. The supernatant was removed by using a cannula, and the residues were extracted with toluene, and layered with methanol to induce recrystallization to give **1a** as a white solid in 77% yield (2.40 g, 1.92 mmol).

Synthesis of [M(tmhd)(OMe)(MeOH)]$_4$ (M = Mn,[S1-2] Fe,[S2a] Co,[S3] Ni[S4]) and [Cu(tmhd)(OMe)]$_4$.[S5]

[M(tmhd)(OMe)(MeOH)]$_4$ was prepared according to the literature. MCl_2 (10.0 mmol) and 2,2,6,6-tetramethylheptanedione (1.0 equiv.) were dissolved in methanol. In another flask, KOMe (2.0 equiv.) was dissolved in methanol. The two solutions were slowly mixed to form a precipitate. The supernatant was removed by using a cannula, and the residues were extracted with toluene, and layered with methanol to induce recrystallization. Mn: yellow solid 2.17 g, 1.80 mmol, 72% yield, Fe: deep red solid, 2.57 g, 2.13 mmol, 85% yield, Co: burgundy solid, 1.99 g, 1.63 mmol, 65% yield, Ni: emerald green solid, 2.29 g, 1.88 mmol, 75% yield, Cu: deep blue solid, 0.36 g, 0.33 mmol, 13% yield.

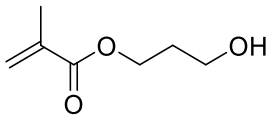
General procedure for catalytic transesterification of methyl (meth)acrylate.

The catalyst precursor (9.0 μmol based on metal atoms) and the ligand (36.0 μmol) were charged into a Schlenk tube in a glovebox. Then, methyl (meth)acrylate (18.0 mmol), 1,4-butanediol (27.0 mmol) and toluene (0.41 mL) were added and the mixture was stirred at 85 °C for 3 hours under an argon atmosphere. After addition of a few drops of acetone and cooling to room temperature, yields were

determined using the following procedures. GC yield: metal salts were removed by filtration through Celite® with EtOH. The yield was determined by GC analysis with triphenylmethane as an internal standard.

2. Spectral data

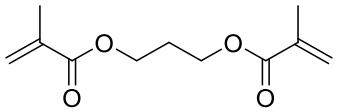
3-hydroxypropyl methacrylate (**3c**)



Colorless oil

^{1}H NMR (600 MHz, $CDCl_3$, 30 °C): δ 6.10 (s, 1H), 5.56 (s, 1H), 4.30 (t, J = 6.0 Hz, 2H), 3.70 (t, J = 6.0 Hz, 2H), 1.93 (s, 3H), 1.92-1.89 (m, 2H); ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$, 30 °C): δ 167.9, 136.3, 125.8, 61.7, 59.3, 31.9, 18.4; HRMS (DART+) m/z ($C_7H_{12}O_3$+H^+) calcd. for 145.08592, found 145.08643; Anal. Calcd for $C_7H_{12}O_3$: C, 58.32; H, 8.39. Found: C, 58.00; H, 8.36.

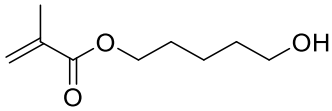
propane-1,3-diyl bis(2-methylacrylate) (**4c**)



pale yellow oil

^{1}H NMR (600 MHz, $CDCl_3$, 30 °C): δ 6.10 (s, 2H), 5.56 (s, 2H), 4.25 (t, J = 6.6 Hz, 4H), 2.07 (quint, J = 6.3 Hz, 2H), 1.94 (s, 6H); ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$, 30 °C): δ 167.4, 136.3, 125.8, 61.5, 28.2, 18.4; HRMS (DART+) m/z ($C_{11}H_{16}O_4$+H^+) calcd. for 213.11214, found 213.11222; Anal. Calcd for $C_{11}H_{16}O_4$: C, 62.25; H, 7.60. Found: C, 62.36; H, 7.81.

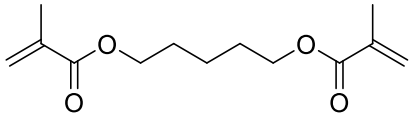
5-hydroxypentyl methacrylate (**3d**)



colorless oil

^{1}H NMR (600 MHz, $CDCl_3$, 30 °C): δ 6.09 (s, 1H), 5.54 (s, 1H), 4.15 (t, *J* = 6.7 Hz, 2H), 3.65 (t, *J* = 5.7 Hz, 2H), 1.93 (s, 3H), 1.73-1.68 (m, 2H), 1.63-1.57 (m, 2H), 1.48-1.42 (m, 2H); ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$, 30 °C): δ 167.7, 136.6, 125.4, 64.7, 62.8, 32.4, 28.6, 22.4, 18.5; HRMS (DART+) *m/z* ($C_9H_{16}O_3$+H^+) calcd. for 173.11772, found 173.11778; Anal. Calcd for $C_9H_{16}O_3$: C, 62.77; H, 9.36. Found: C, 62.89; H, 9.14.

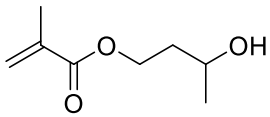
pentane-1,5-diyl bis(2-methylacrylate) (**4d**)



pale yellow oil

^{1}H NMR (600 MHz, $CDCl_3$, 30 °C): δ 6.09 (s, 2H), 5.55 (s, 1H), 4.16 (t, *J* = 6.6 Hz, 4H), 1.94 (s, 6H), 1.73 (tt, *J* = 7.6, 6.6 Hz, 4H), 1.48 (tt, *J* = 7.5, 6.7 Hz, 2H); ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$, 30 °C): δ 167.6, 136.6, 125.4, 64.6, 28.4, 22.7, 18.5; HRMS (DART+) *m/z* ($C_{13}H_{20}O_4$+H^+) calcd. for 241.14344, found 241.14433; Anal. Calcd for $C_{13}H_{20}O_4$: C, 64.98; H, 8.39. Found: C, 64.66; H, 8.85.

3-hydroxybutyl methacrylate (**3e**)

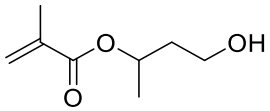


colorless oil

^{1}H NMR (600 MHz, $CDCl_3$, 30 °C): δ 6.07 (s, 1H), 5.54 (s, 1H), 4.37 (ddd, *J* = 11.1, 5.6, 3.6 Hz, 1H), 4.19 (dt, *J* = 11.3, 5.6 Hz, 1H), 3.88 (br, 1H), 1.91 (s, 3H), 1.86-1.79 (m, 1H), 1.78-1.72 (m, 1H), 1.21 (d, *J* = 6.2 Hz, 3H); ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$, 30 °C): δ 167.9, 136.4, 125.8, 65.0, 62.1, 38.2,

23.6, 18.4; HRMS (DART+) *m/z* ($C_8H_{14}O_3$+H^+) calcd. for 159.10157, found 159.10220; Anal. Calcd for $C_8H_{14}O_3$: C, 60.74; H, 8.92. Found: C, 60.45; H, 8.89.

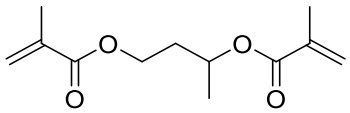
4-hydroxybutan-2-yl methacrylate (**3e'**)



colorless oil

^{1}H NMR (600 MHz, $CDCl_3$, 30 °C): δ 6.10 (s, 1H), 5.57 (s, 1H), 5.21-5.15 (ddq, *J* = 2.8, 8.8, 6.3 Hz, 1H), 3.69-3.64 (m, 1H), 3.61-3.56 (m, 1H), 1.94 (s, 3H), 1.89-1.81 (m, 1H), 1.80-1.73 (m, 1H), 1.32 (d, *J* = 6.3 Hz, 3H); ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$, 30 °C): δ 167.9, 136.6, 125.8, 68.6, 59.0, 39.4, 20.6, 18.5; HRMS (DART+) *m/z* ($C_8H_{14}O_3$+H^+) calcd. for 159.10157, found 159.10104.

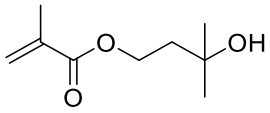
butane-1,3-diyl bis(2-methylacrylate) (**4e**)



pale yellow oil

^{1}H NMR (600 MHz, $CDCl_3$, 30 °C): δ 6.09 (s, 1H), 6.08 (s, 1H), 5.55 (t, 1H), 5.54 (t, 1H), 5.10 (ddq, *J* = 7.9, 4.7, 6.1 Hz, 1H), 4.24 (dt, *J* = 11.0, 6.1 Hz, 1H), 4.18 (ddd, *J* = 11.2, 3.7, 2.7 Hz, 1H), 2.05-1.95 (m, 2H), 1.931 (s, 3H), 1.930 (s, 3H), 1.31 (d, *J* = 6.3 Hz, 3H); ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$, 30 °C): δ 167.5, 167.0, 136.7, 136.4, 125.8, 125.4, 68.4, 61.2, 35.0, 20.2, 18.5, 18.4; HRMS (DART+) *m/z* ($C_{12}H_{18}O_4$+H^+) calcd. for 227.12779, found 227.12822; Anal. Calcd for $C_{12}H_{18}O_4$: C, 63.70; H, 8.02. Found: C, 63.80; H, 8.18.

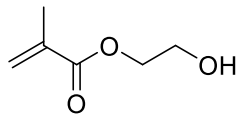
3-hydroxy-3-methylbutyl methacrylate (**3f**)



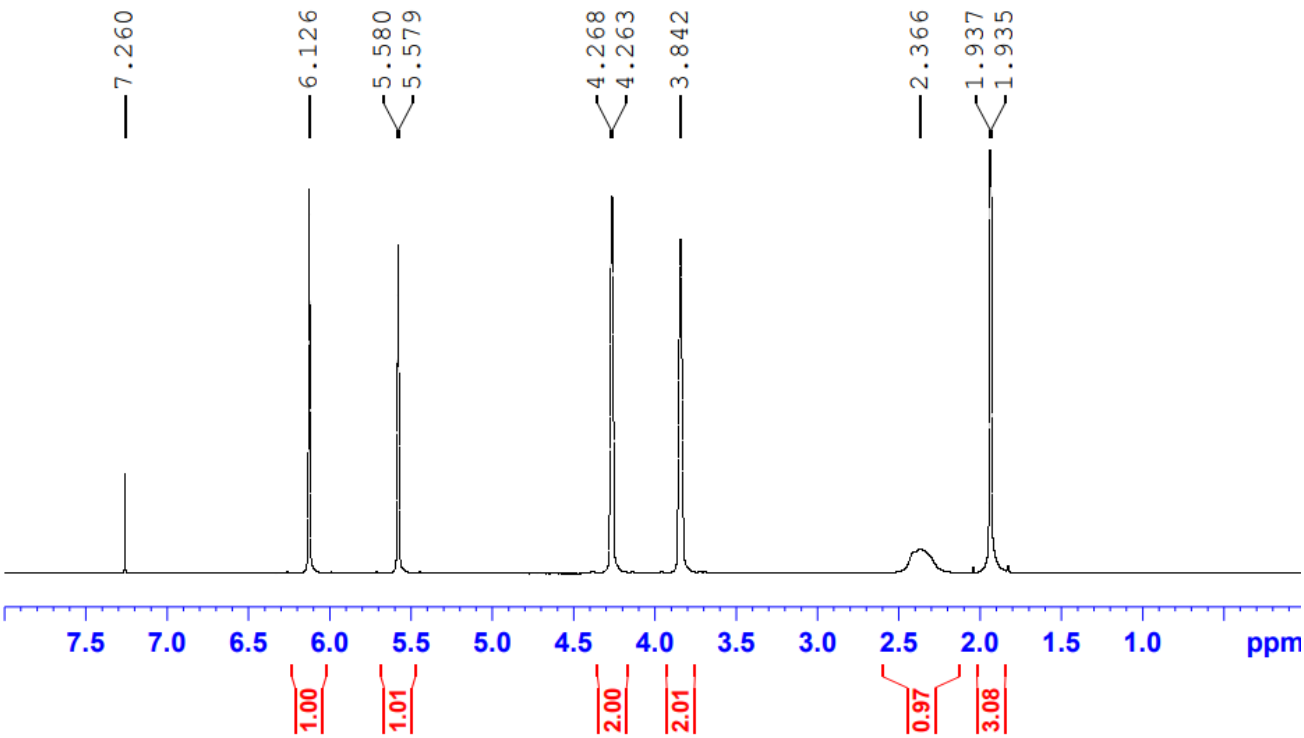
colorless oil

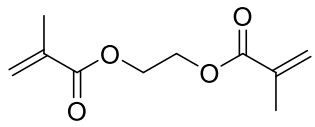
^{1}H NMR (600 MHz, $CDCl_3$, 30 °C): δ 6.08 (s, 1H), 5.55 (s, 1H), 4.32 (t, J = 6.6 Hz, 2H), 1.93 (s, 3H), 1.88 (t, J = 6.6 Hz, 2H), 1.27 (s, 6H); ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$, 30 °C): δ 167.5, 136.5, 125.6, 70.2, 61.8, 41.7, 29.8, 18.5; HRMS (DART+) *m/z* ($C_9H_{16}O_3$+H^+) calcd. for 173.11722, found 173.11709; Anal. Calcd for $C_9H_{16}O_3$: C, 62.77; H, 9.36. Found: C, 62.49; H, 9.17.

3. ^{1}H and ^{13}C{^{1}H} NMR chart of products



(3b)





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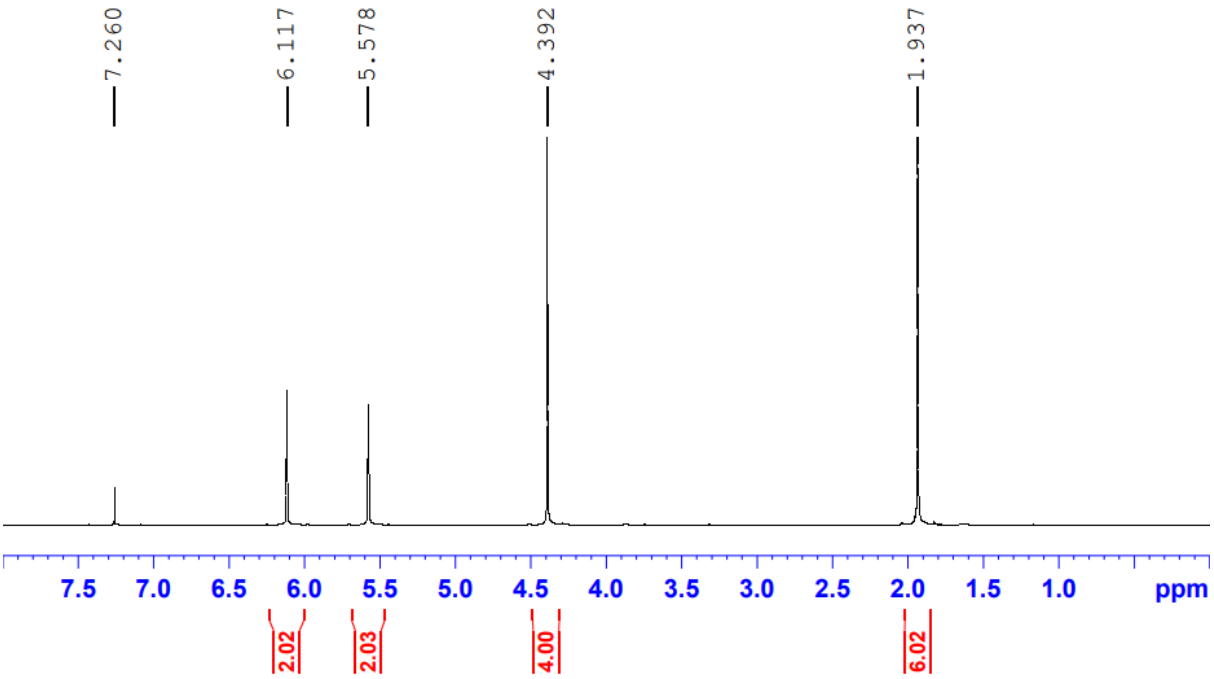
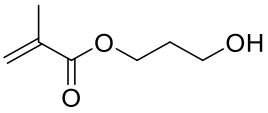
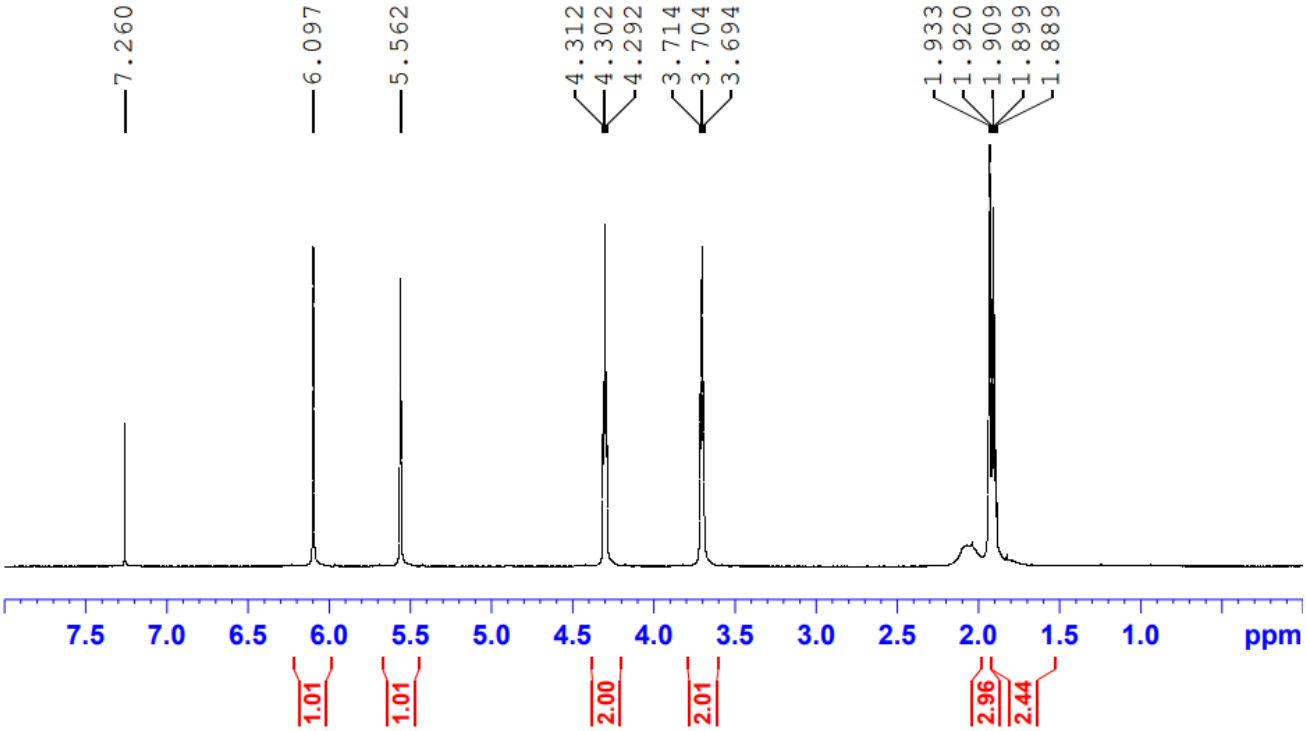


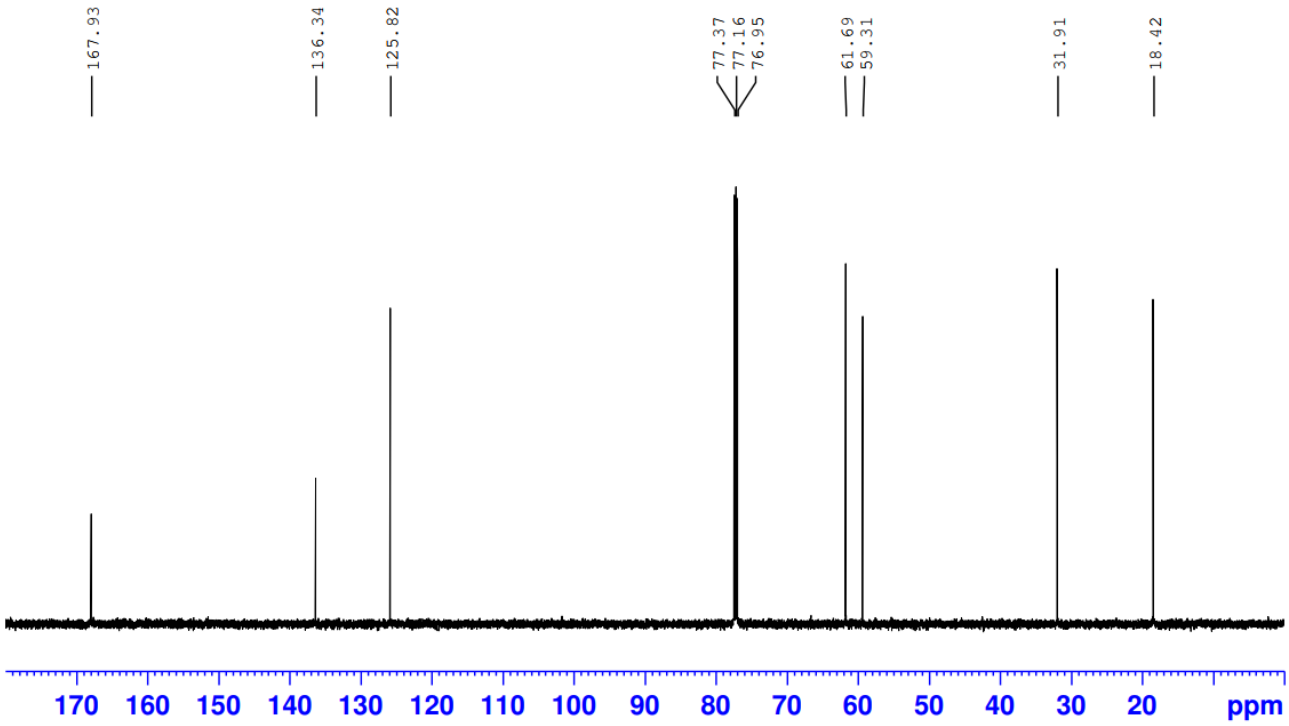


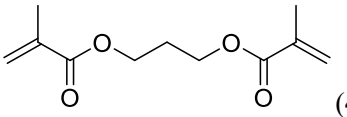
(**3c**)

^{1}H NMR



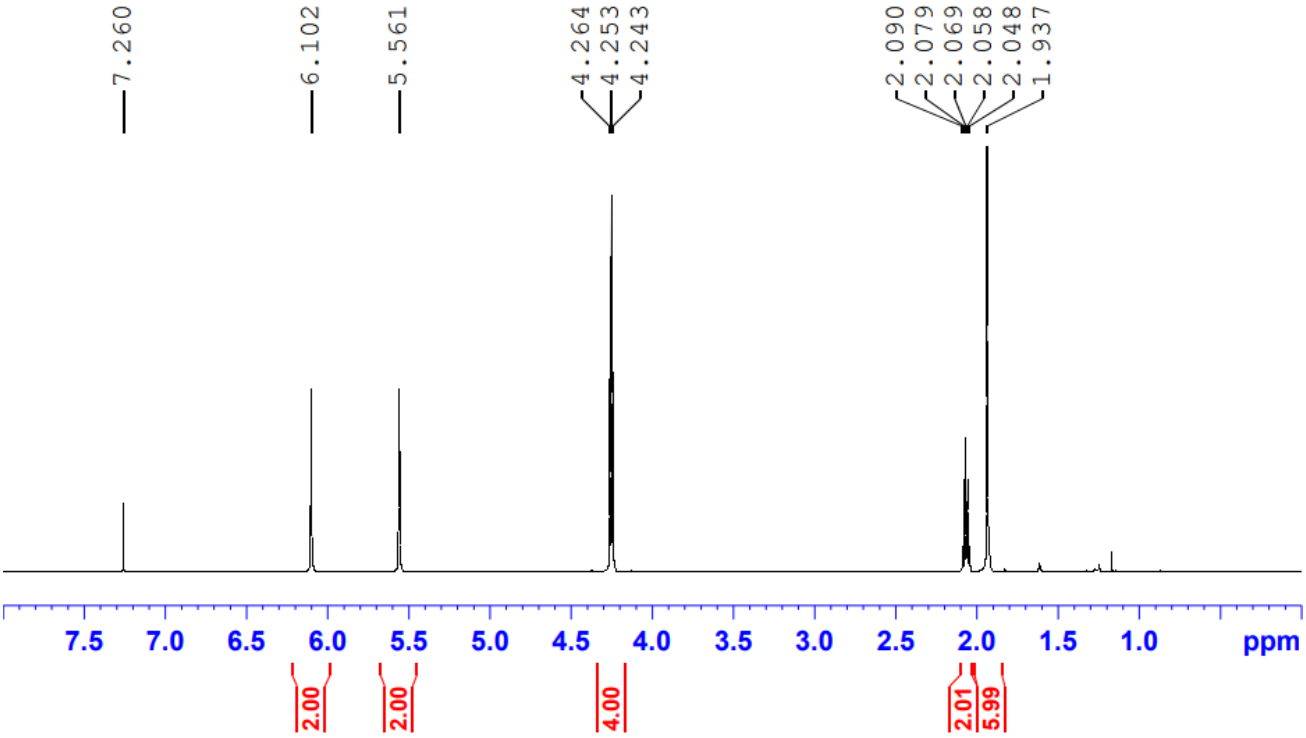
^{13}C{^{1}H} NMR



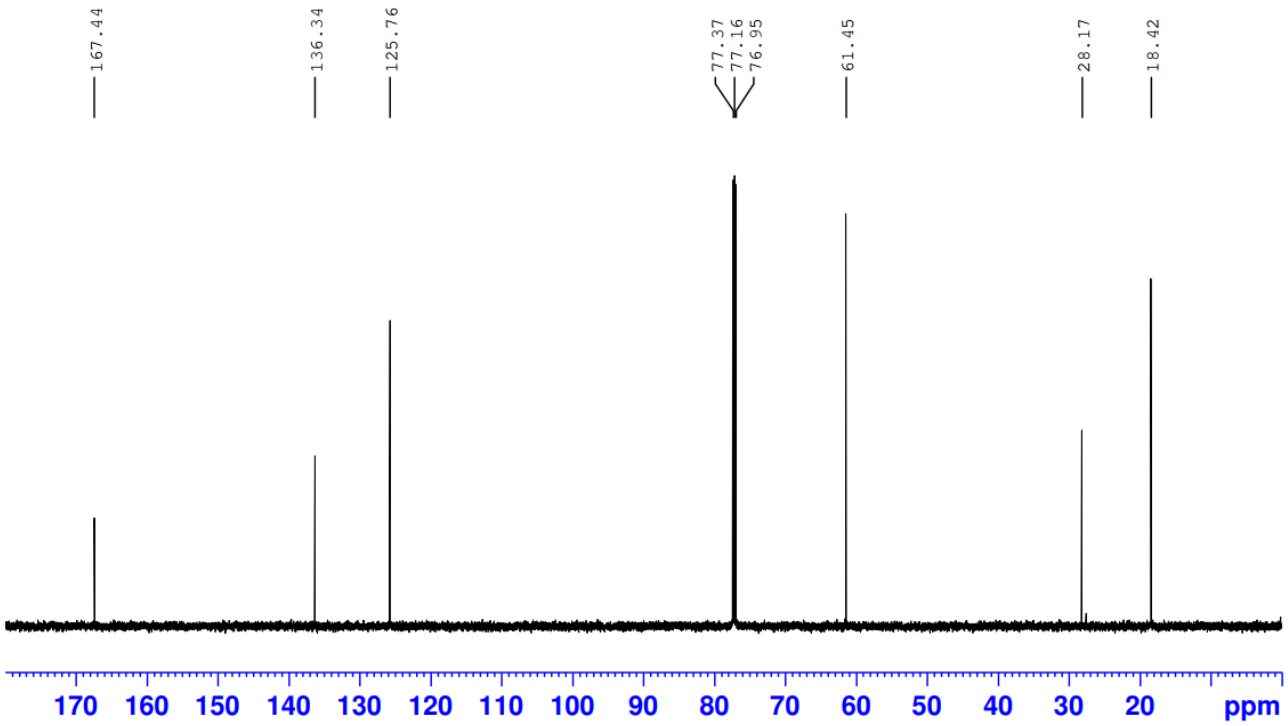


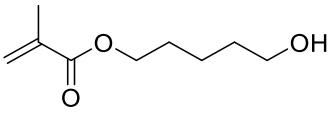
(4c)

^{1}H NMR



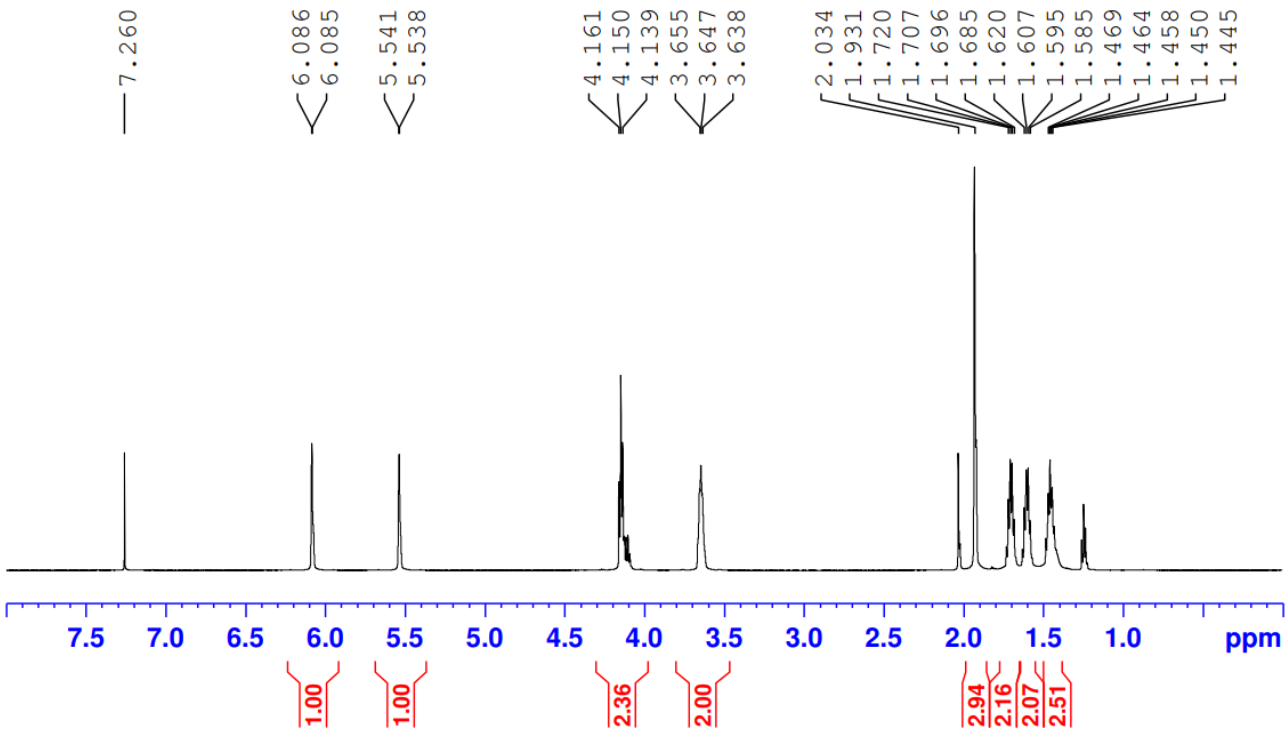
^{13}C{^{1}H} NMR



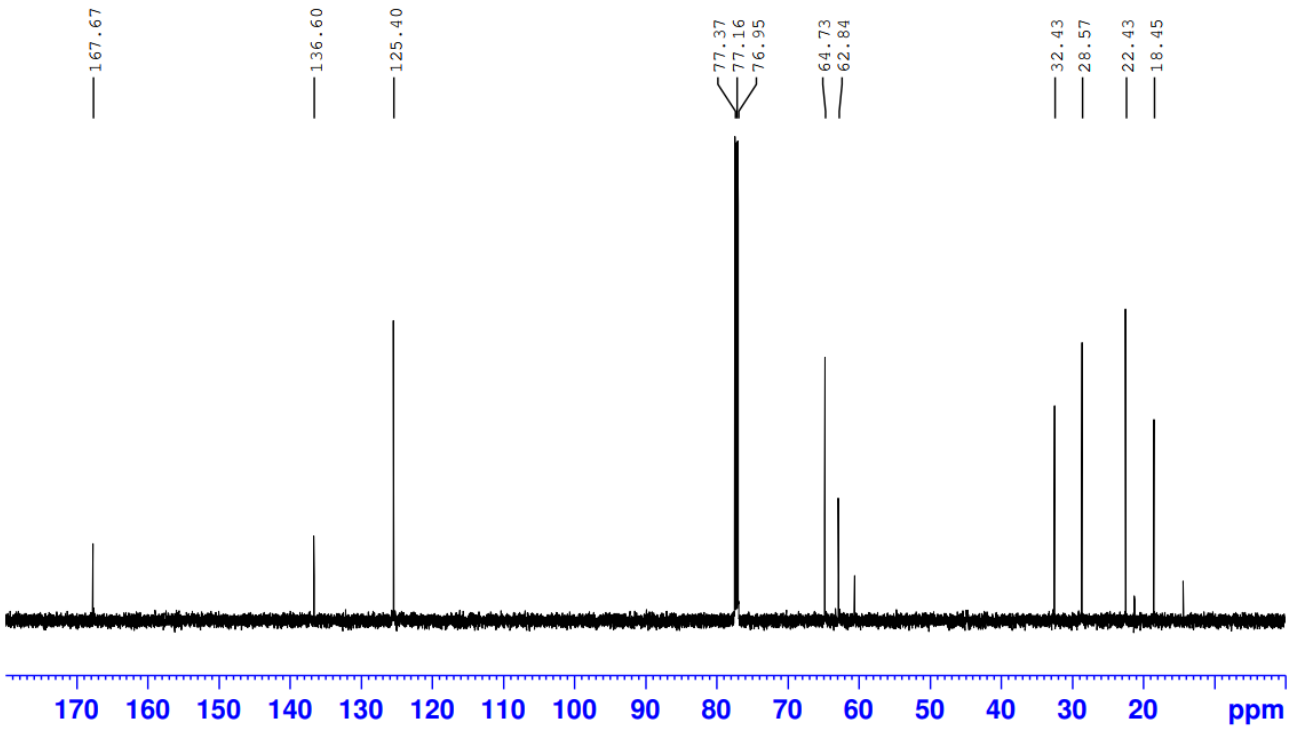


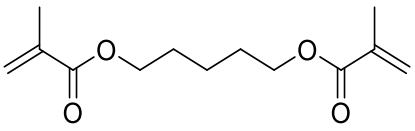
(3d)

^{1}H NMR



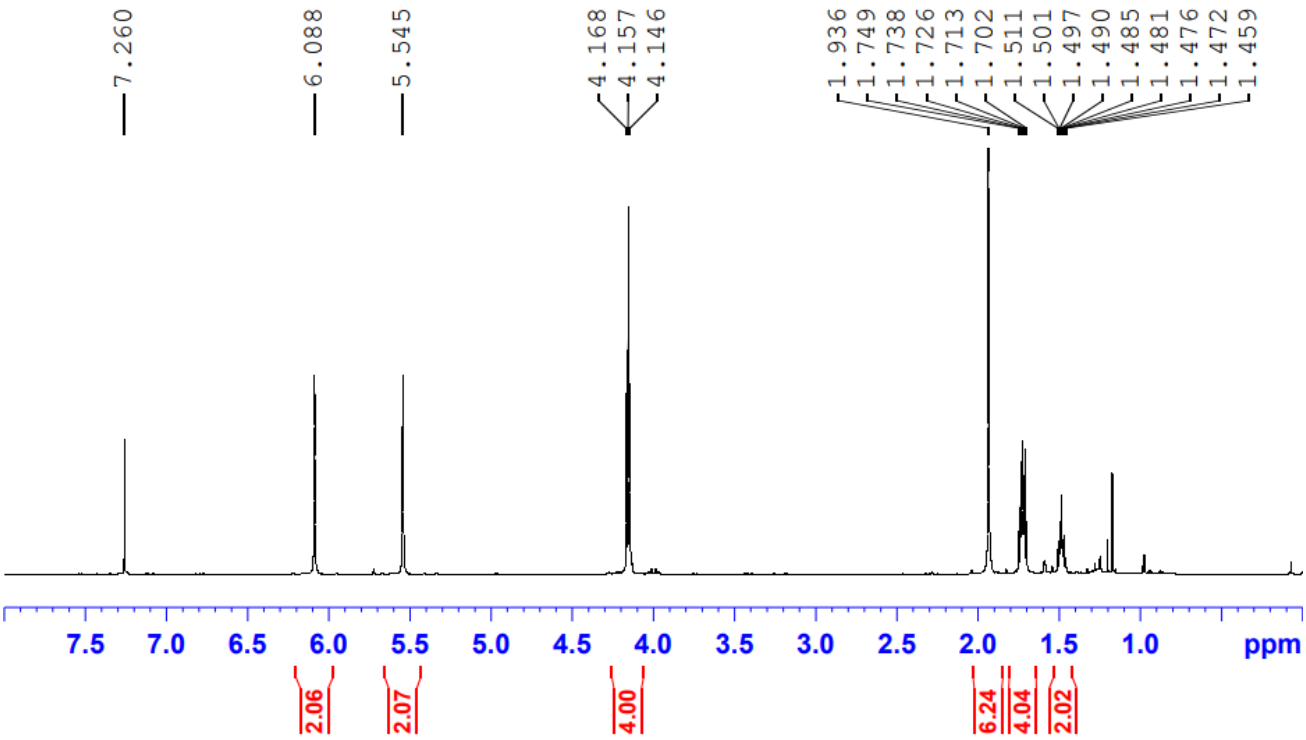
^{13}C{^{1}H} NMR



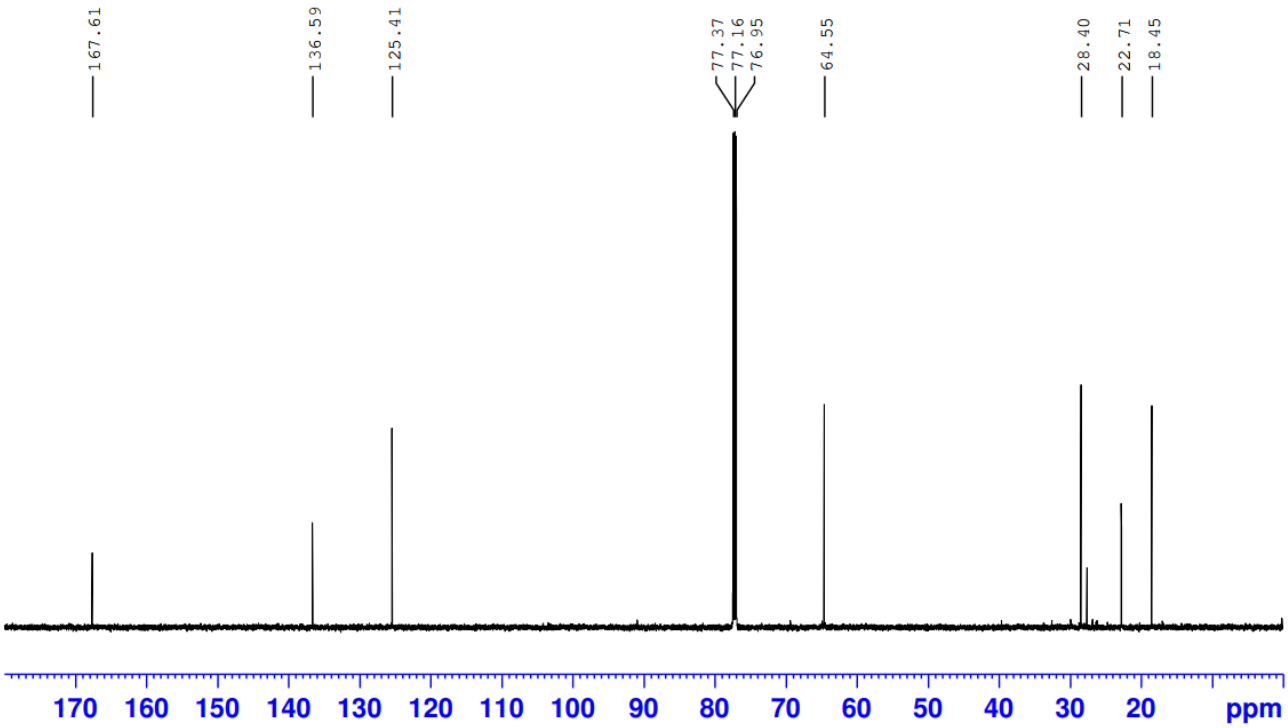


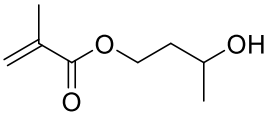
(4d)

^{1}H NMR



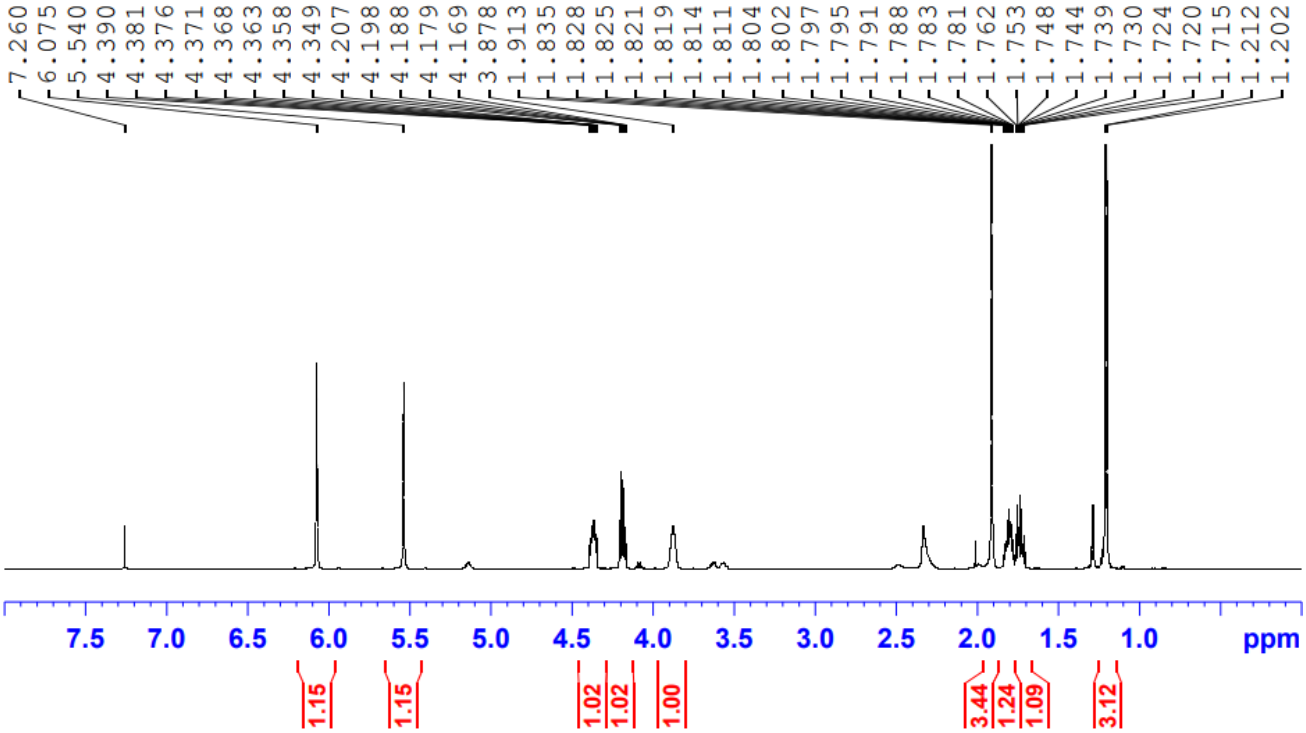
^{13}C{^{1}H} NMR



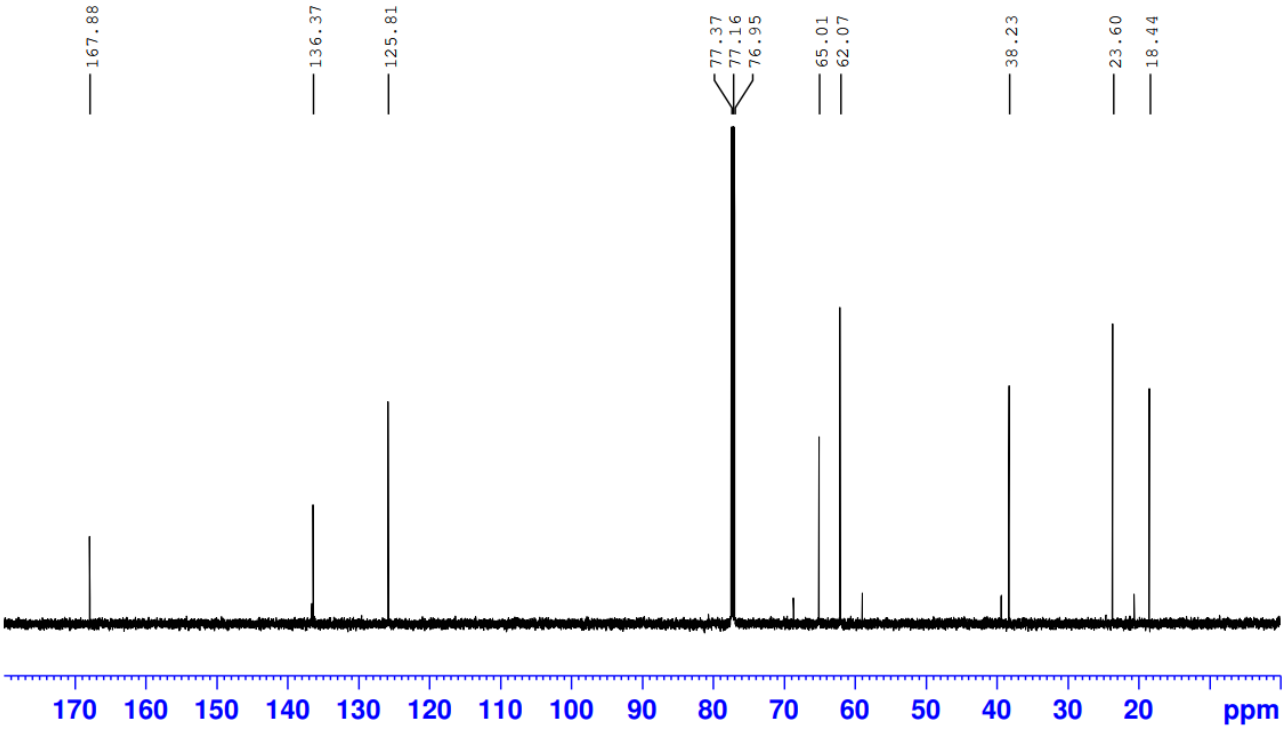


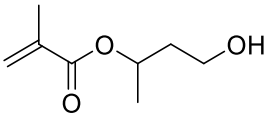
(**3e**)

^{1}H NMR



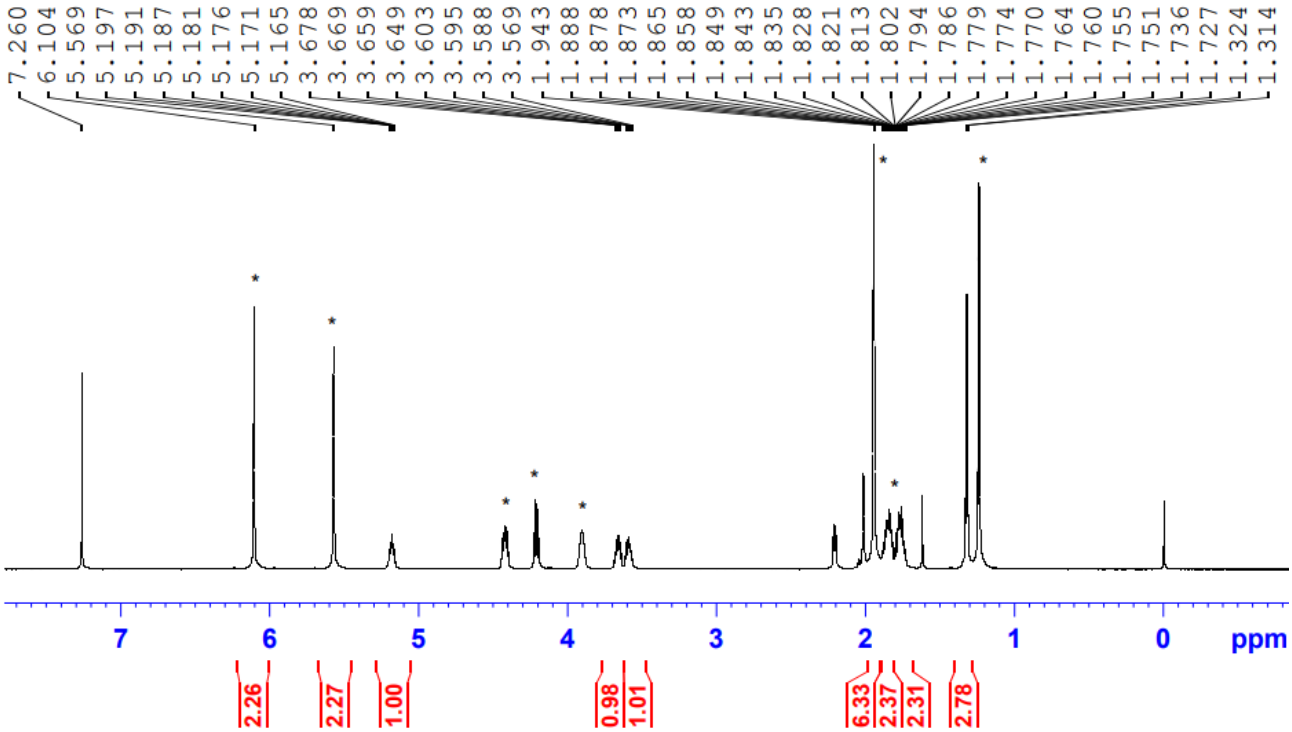
^{13}C{^{1}H} NMR



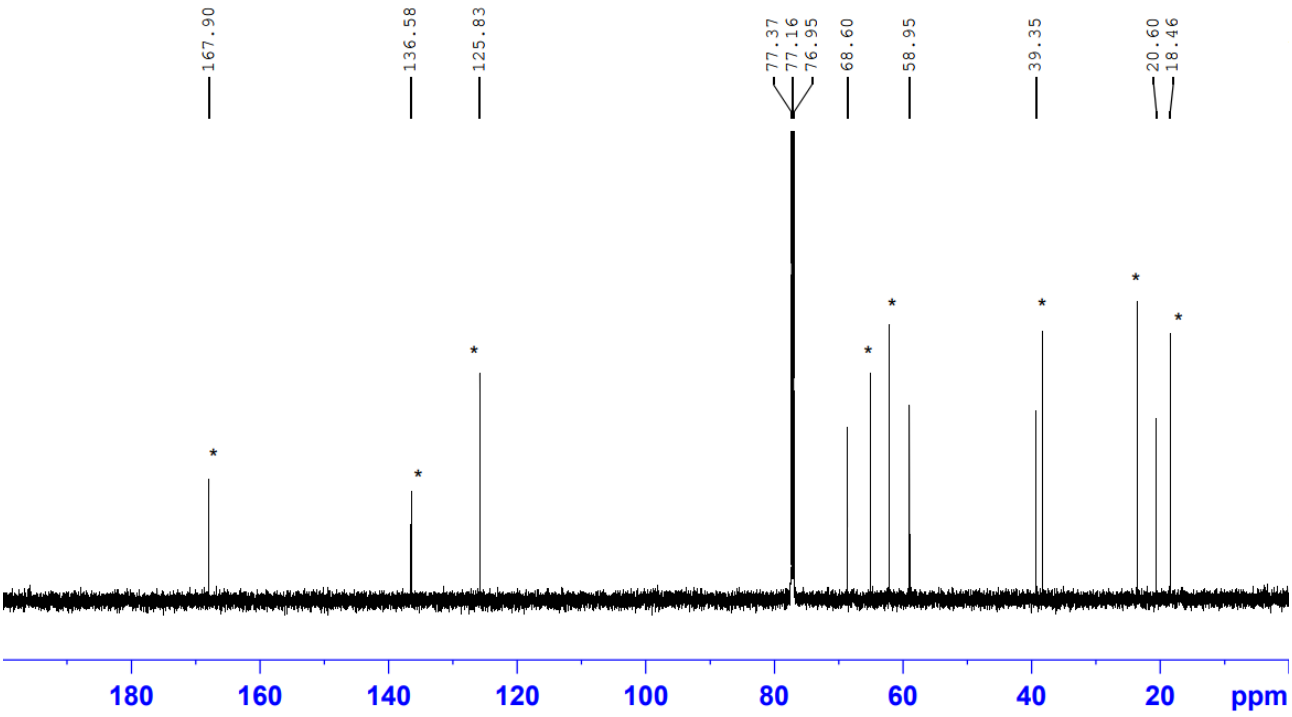


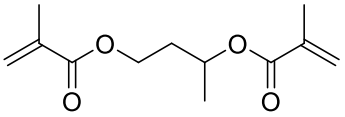
(**3e'**)

^{1}H NMR * marks express the overlapping of the peaks of compound **3e** (mixture).



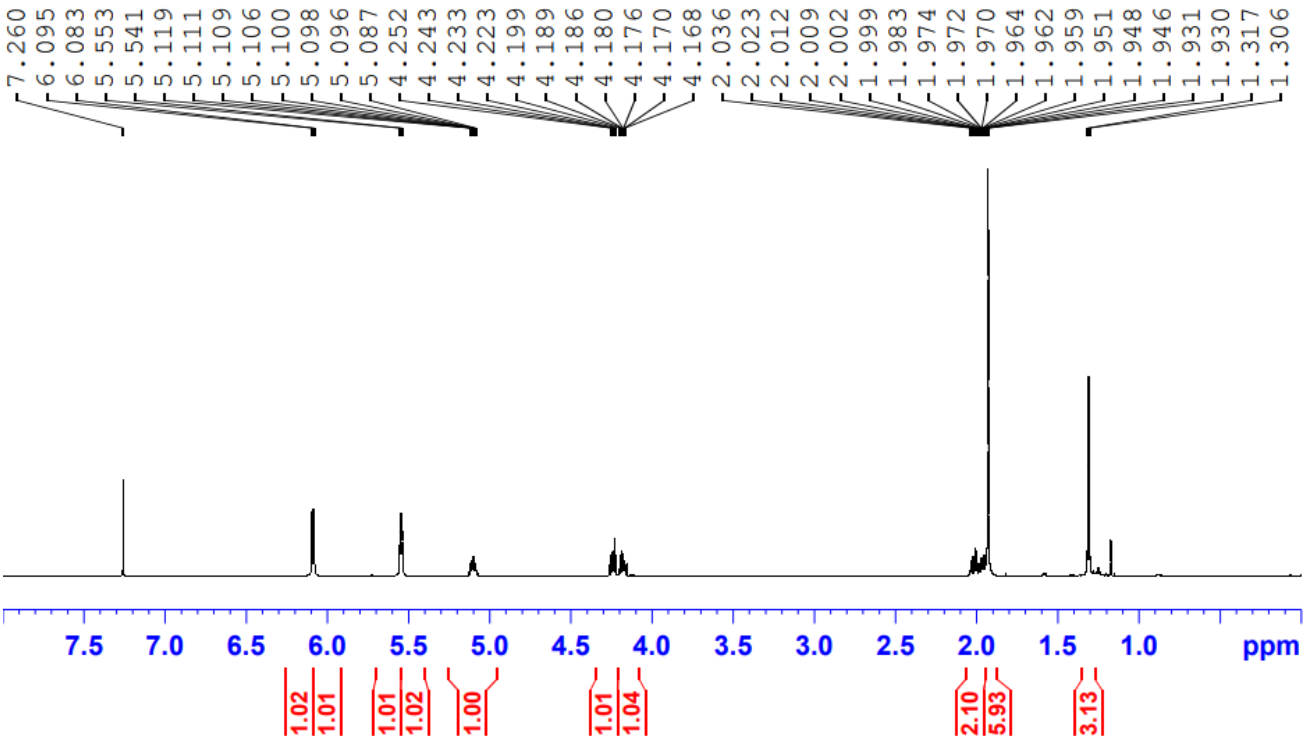
^{13}C{^{1}H} NMR



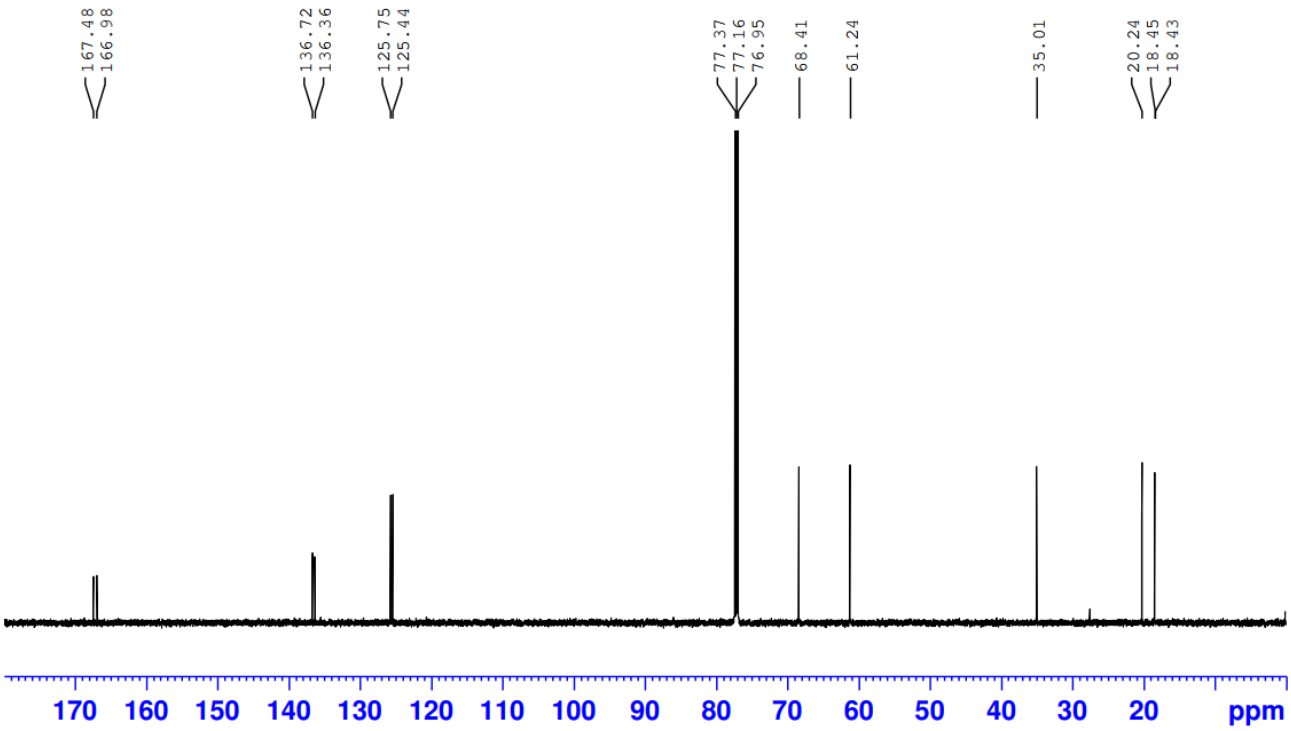


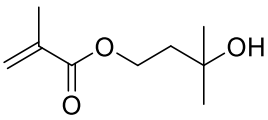
(4e)

^{1}H NMR



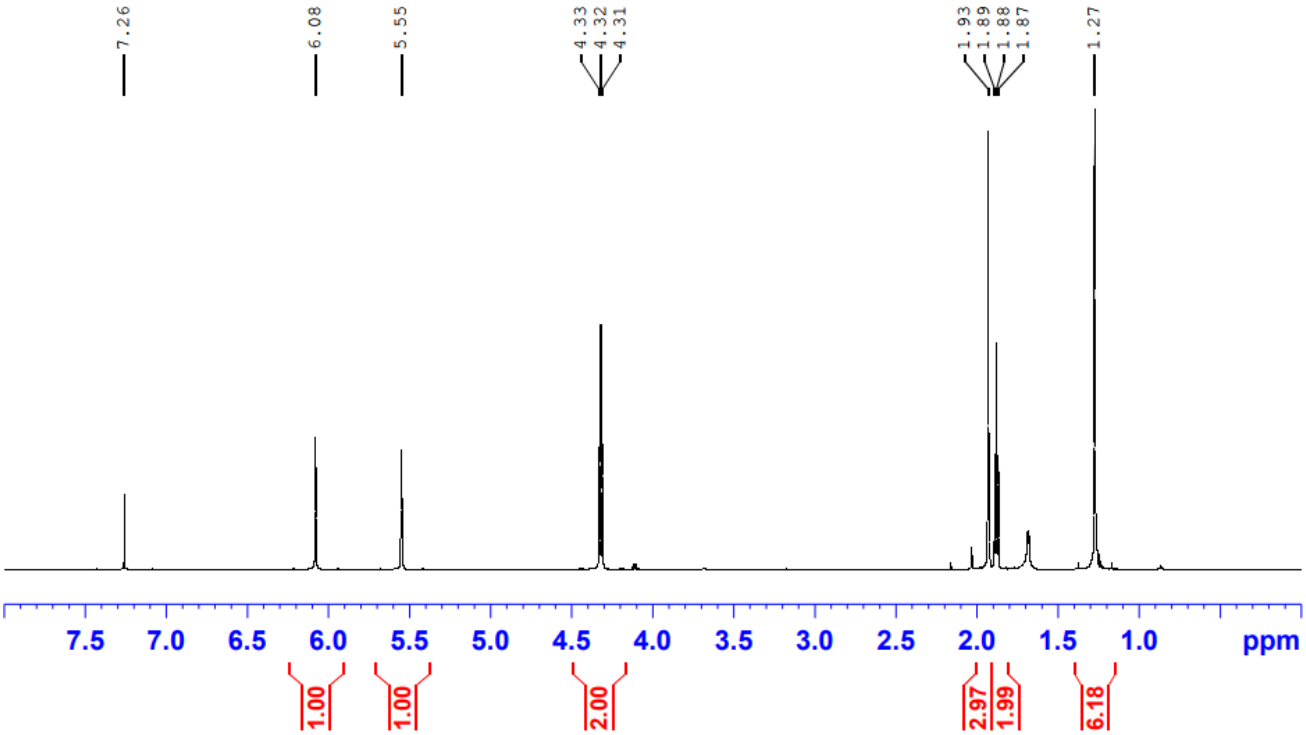
^{13}C{^{1}H} NMR



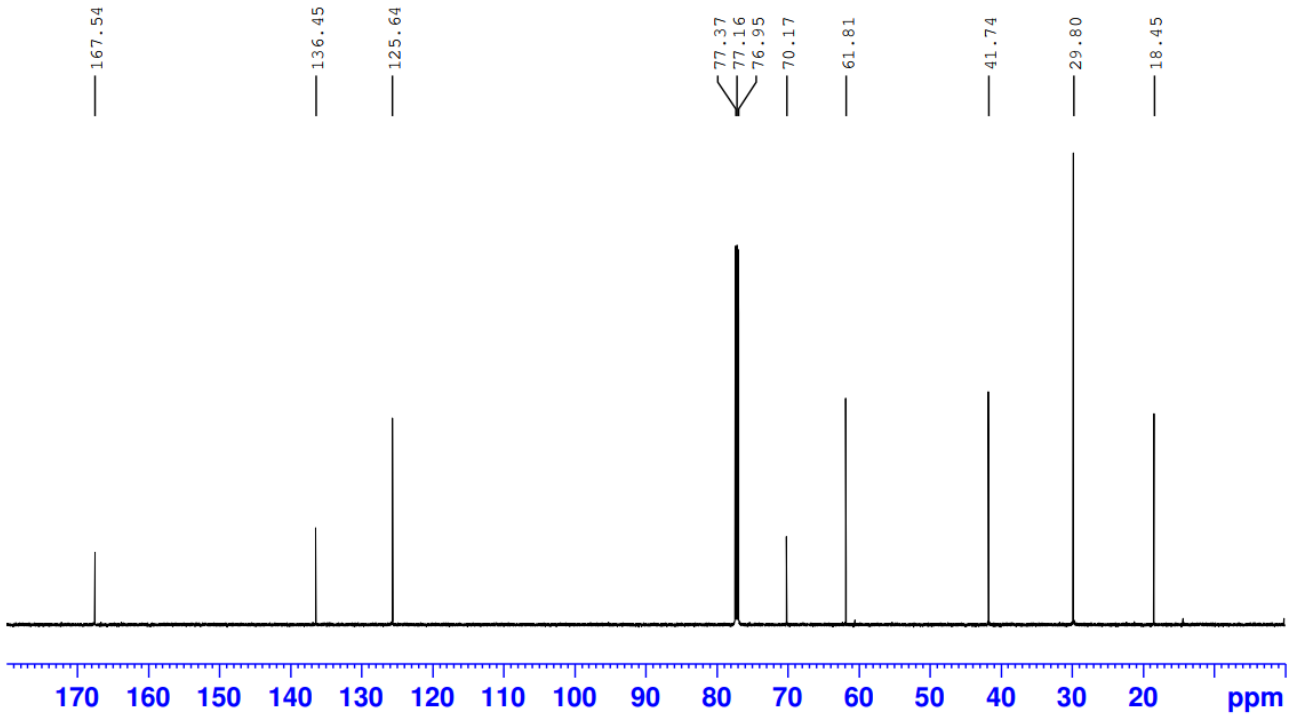


(**3f**)

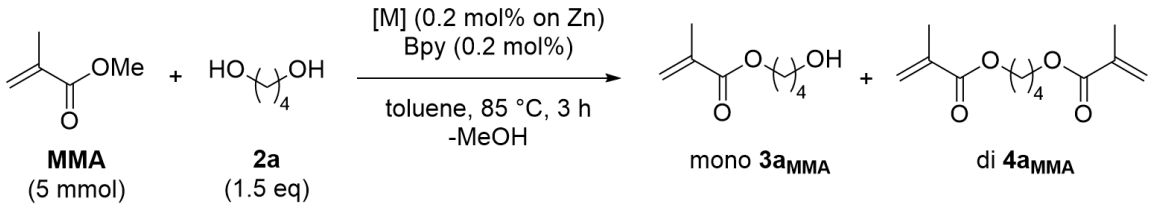
^{1}H NMR



^{13}C{^{1}H} NMR



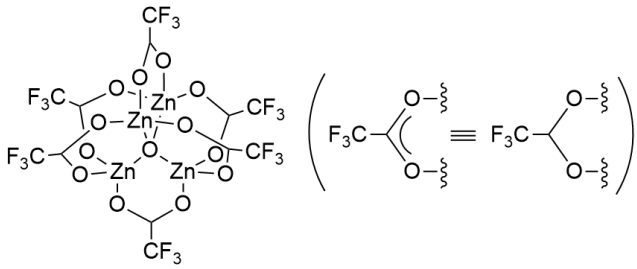
4. Comparison of catalytic transesterification activities among several zinc precursors with MMA and 1,4-butanediol

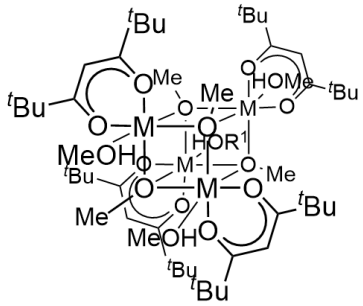


Entry	[M]	Conv. [%][a] MMA	Conv. [%][a] **2a**	chemoselectivity [%][b]	Yield [%][a] mono **3a**	Yield [%][a] di **4a**
1	ZnTAC24®	38	15	95	30	6
2	$Zn(OAc)_2$	18	8	68	11	1
3	$Zn(acac)_2$	gel.	gel.	gel.	–	–
4	$Zn(tmhd)_2$	47	19	93	36	8
5	$Zn(hfac)_2 \cdot 2H_2O$	10	3	49	5	0
6	$[Zn(tmhd)(OMe)(MeOH)]_4$ (**1a**)	65	35	100	51	16

[a] Determined by GC analysis with triphenylmethane as an internal standard.

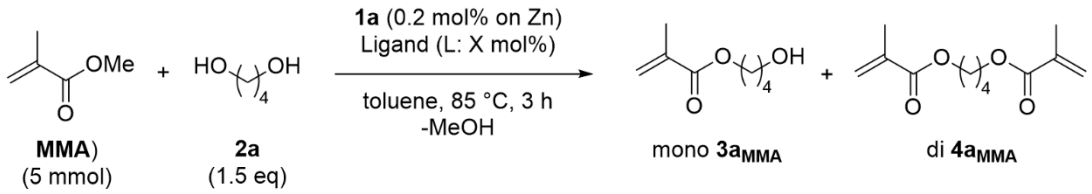
[b] The chemoselectivity of transesterification reaction was calculated as dividing the provided amounts of the monoesters **3a** and diesters **4a** by the converted amounts of MMA.





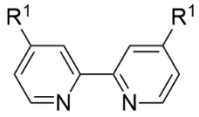
M = Zn (**1a**)

5. Screening of ligands in catalytic transesterification with MMA and 1,4-butanediol

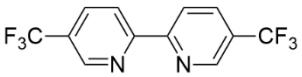


Entry	Ligand	X [mol%]	Conv. [%][a] (meth)acrylate	Conv. [%][a] **2a**	chemoselectivity [%][b]	Yield [%][a] mono $\mathbf{3a_{MMA}}$	Yield [%][a] di $\mathbf{4a_{MMA}}$
20	**L6**	0.2	65	35	100	51	16
21	**L6**	0.4	62	26	100	50	14
22	**L7**	0.2	50	20	98	39	9
23	**L8**	0.2	49	26	100	40	10
24	**L9**	0.2	46	22	91	34	8
25	**L10**	0.2	36	20	97	30	6
26	**L11**	0.2	37	13	100	33	6
27	**L12**	0.2	43	20	87	32	6
28	**L13**	0.2	n.r.[c]	n.r.[c]	n.r.[c]	n.r.[c]	n.r.[c]
29	**L14**	0.2	57	30	91	41	11
30	**L15**	0.2	40	19	90	30	5
31	**L16**	0.2	32	16	100	28	5
32	**L17**	0.2	48	28	96	37	8

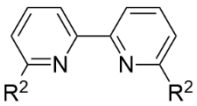
[a] Determined by GC analysis with triphenylmethane as an internal standard.
[b] The chemoselectivity of transesterification reaction was calculated as dividing the provided amounts of the monoesters **3a** and diesters **4a** by the converted amounts of MA or MMA.
[c] No reaction.



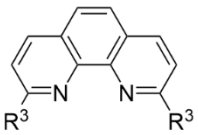
L6: R^1 = H
L7: R^1 = Me
L8: R^1 = OMe
L9: R^1 = ^{t}Bu
L10: R^1 = Br



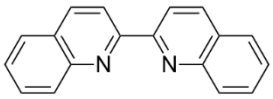
L11



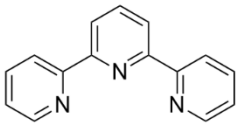
L12: R^2 = Me
L13: R^2 = OH



L14: R^3 = H
L15: R^3 = Me (1/2 H_2O)

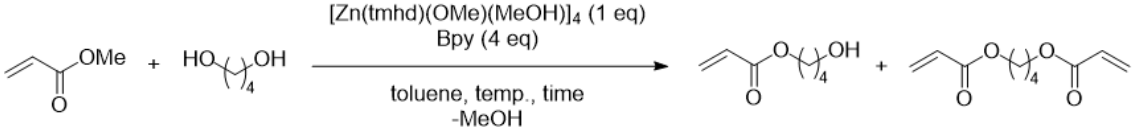


L16



L17

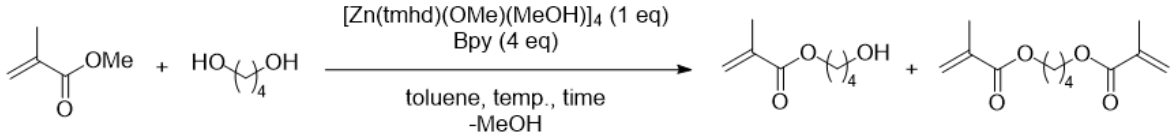
6. Experimental results of transesterification with MA and 1,4-butanediol



			initial condition [mol/kg]						
Entry	temperature[°C]	cat.[mmol/kg]	$[MA]_0$	$[BD]_0$	time[min]	[MA]	[BD]	[mono]	[di]
1	85	8.26	3.72	5.58	30	2.07	4.01	1.30	0.130
2					60	1.35	3.57	1.71	0.210
3					90	1.06	3.38	1.87	0.241
4					120	0.941	3.28	1.92	0.242
5					180	0.812	3.19	1.93	0.250
6					240	0.740	3.14	1.98	0.263
7	85	8.26	3.10	6.19	30	1.81	5.01	1.03	0.0839
8					60	1.08	4.44	1.42	0.131
9					90	0.841	4.06	1.60	0.162
10					120	0.694	4.15	1.72	0.171
11					180	0.597	4.13	1.78	0.174
12					240	0.556	3.99	1.79	0.168
13	85	8.26	2.64	6.61	30	1.25	5.75	1.00	0.0654
14					60	0.778	5.23	1.39	0.100
15					90	0.581	4.84	1.51	0.124
16					120	0.474	4.88	1.63	0.128
17					180	0.391	4.85	1.61	0.126
18					240	0.379	4.78	1.61	0.126
19	85	12.4	3.10	6.19	30	1.22	4.63	1.44	0.130
20					60	0.761	4.17	1.67	0.153
21					90	0.671	4.09	1.71	0.169
22					120	0.631	3.99	1.71	0.161
23					180	0.556	3.96	1.64	0.162
24					240	0.530	3.90	1.69	0.164
25	85	16.5	3.10	6.19	30	1.07	4.58	1.55	0.136
26					60	0.740	4.24	1.70	0.162
27					90	0.687	4.12	1.74	0.173
28					120	0.636	4.05	1.75	0.171
29					180	0.592	4.00	1.77	0.169
30					240	0.575	3.96	1.75	0.165

31	65	8.26	3.10	6.19	30	2.51	5.75	0.491	0.00
32					60	2.04	5.46	0.857	0.0551
33					90	1.49	5.20	1.17	0.0860
34					120	1.37	4.84	1.27	0.107
35					180	1.11	4.71	1.57	0.141
36					240	1.07	4.67	1.65	0.149
37	75	8.26	3.10	6.19	30	1.86	5.48	0.834	0.0607
38					60	1.17	5.00	1.22	0.0923
39					90	1.03	4.60	1.47	0.131
40					120	0.909	4.37	1.53	0.144
41					180	0.634	4.24	1.61	0.141
42					240	0.631	4.14	1.69	0.159

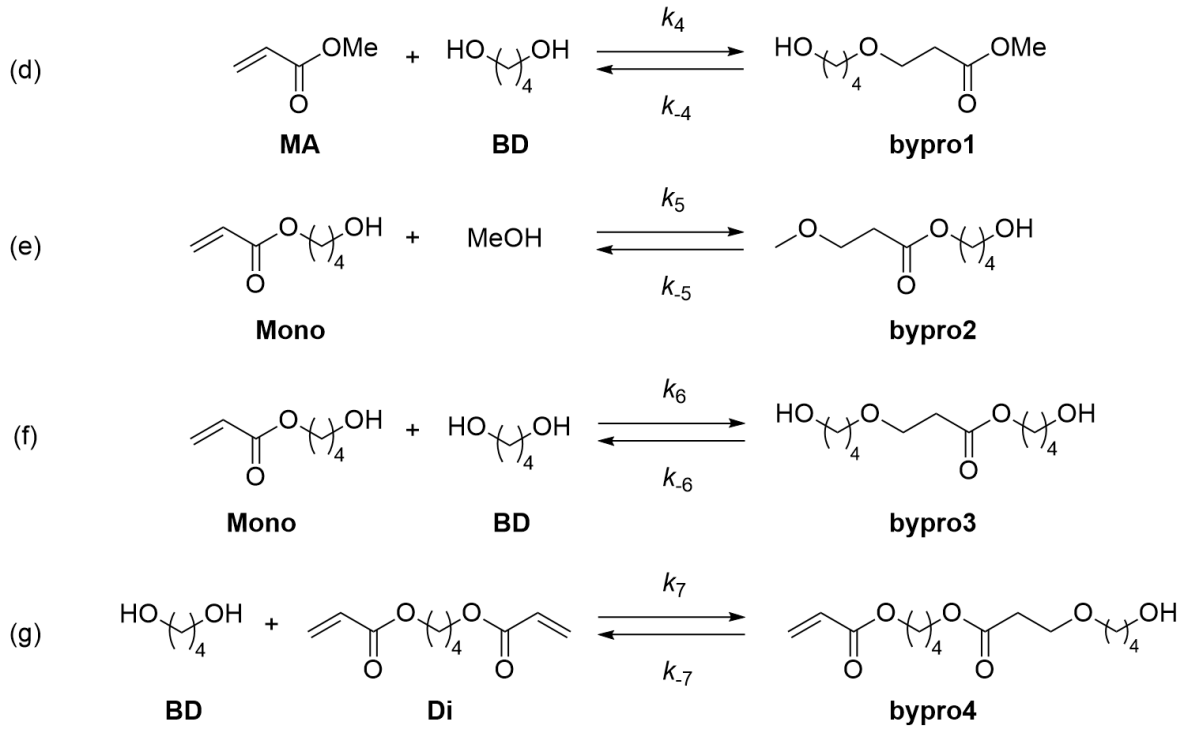
7. Experimental results of transesterification with MMA and 1,4-butanediol



Entry	temperature[°C]	cat.[mmol/kg]	initial condition [mol/kg] $[MMA]_0$	$[BD]_0$	time[min]	[MMA]	[BD]	[mono]	[di]
1	85	7.82	4.30	4.30	60	3.29	3.52	1.30	0.130
2					90	2.86	3.24	1.71	0.210
3					120	2.44	2.79	1.87	0.241
4					180	2.05	2.52	1.92	0.242
5					240	1.82	2.30	1.93	0.250
6	85	7.82	3.91	5.86	30	3.14	5.35	0.672	0.0665
7					60	2.30	4.69	1.14	0.127
8					90	1.82	4.34	1.47	0.185
9					120	1.54	4.01	1.72	0.220
10					180	1.35	3.80	1.98	0.286
11					240	1.16	3.79	2.12	0.317
12	85	7.82	3.28	6.57	30	2.32	6.07	0.564	0.0513
13					60	1.93	5.51	0.961	0.117
14					90	1.55	5,24	1.30	0.126
15					120	1.33	5.03	1.52	0.165
16					180	0.946	4.60	1.75	0.204
17					240	0.795	4.43	1.97	0.220
18	85	11.7	3.91	5.86	30	2.99	5.30	0.766	0.0746
19					60	2.30	4.90	1.35	0.152
20					90	1.60	4.50	1.73	0.204
21					120	1.37	4.19	1.89	0.259
22					180	0.991	3.94	2.19	0.312
23					240	0.910	3.86	2.29	0.323
24	85	15.6	3.91	5.86	30	2.44	5.20	0.931	0.107
25					60	1.97	4.73	1.62	0.195
26					90	1.49	4.30	2.02	0.234
27					120	1.13	4.10	2.21	0.303
28					180	1.09	3.95	2.39	0.354
29					240	0.980	3.91	2.47	0.355

30	65	7.82	3.91	5.86	180	3.01	5.12	0.789	0.0763
31					240	2.86	5.19	1.10	0.108
32					360	2.42	4.78	1.34	0.172
33					480	2.16	4.56	1.59	0.210
34					600	1.92	4.30	1.75	0.228
35					720	1.72	4.06	1.89	0.257
36	75	7.82	3.91	5.86	180	2.08	4.66	1.58	0.178
37					240	1.84	4.44	1.84	0.226
38					360	1.51	4.02	2.12	0.289
39					480	1.32	3.89	2.27	0.337
40					600	1.19	3.73	2.38	0.346
41					720	1.12	3.66	2.40	0.357

8. The scheme of Michael addition reaction in case of MA



Each byproduct was detected by DART-MS analysis as described below,

Bypro1: m/z = 177.11317 [$C_8H_{16}O_4$+H^+]

Bypro2: m/z = 177.11224 [$C_8H_{16}O_4$+H^+]

Bypro3: m/z = 235.15447 [$C_{11}H_{22}O_5$+H^+]

Bypro4: m/z = 289.16299 [$C_{14}H_{24}O_6$+H^+]

$$\frac{d[\boldsymbol{MA}]}{dt} = [cat](-k_1[\boldsymbol{MA}][\boldsymbol{2a}] + k_{-1}[\boldsymbol{Mono}][MeOH] - k_2[\boldsymbol{MA}][\boldsymbol{Mono}] + k_{-2}[\boldsymbol{Di}][MeOH] - k_4[MA][\boldsymbol{2a}])$$

(7)

$$\frac{d[\boldsymbol{2a}]}{dt} = [cat](-k_1[\boldsymbol{MA}][\boldsymbol{2a}] + k_{-1}[\boldsymbol{Mono}][MeOH] - k_3[\boldsymbol{2a}][\boldsymbol{Di}] + k_{-3}[\boldsymbol{Mono}]^2 - k_4[\boldsymbol{MA}][\boldsymbol{2a}] - k_6[\boldsymbol{2a}][\boldsymbol{Mono}] - k_7[\boldsymbol{2a}][\boldsymbol{Di}])$$ (8)

$$\frac{d[\boldsymbol{Mono}]}{dt} = [cat](k_1[\boldsymbol{MA}][\boldsymbol{2a}] - k_{-1}[\boldsymbol{Mono}][MeOH] - k_2[\boldsymbol{MA}][\boldsymbol{Mono}] + k_{-2}[\boldsymbol{Di}][MeOH] + 2(k_3[\boldsymbol{2a}][\boldsymbol{Di}] - k_{-3}[\boldsymbol{Mono}]^2) - k_5[\boldsymbol{Mono}][MeOH] - k_6[\boldsymbol{2a}][\boldsymbol{Mono}])$$ (9)

$$\frac{d[\boldsymbol{Di}]}{dt} = [cat](k_2[\boldsymbol{MA}][\boldsymbol{Mono}] - k_{-2}[\boldsymbol{Di}][MeOH] - k_3[\boldsymbol{2a}][\boldsymbol{Di}] + k_{-3}[\boldsymbol{Mono}]^2 - k_7[\boldsymbol{2a}][\boldsymbol{Di}]) \quad (10)$$

$$\frac{d[MeOH]}{dt} = [cat](k_1[\boldsymbol{MA}][\boldsymbol{2a}] - k_{-1}[\boldsymbol{Mono}][MeOH] + k_2[\boldsymbol{MA}][\boldsymbol{Mono}] - k_{-2}[\boldsymbol{Di}][MeOH] - k_5[\boldsymbol{Mono}][MeOH]) \quad (11)$$

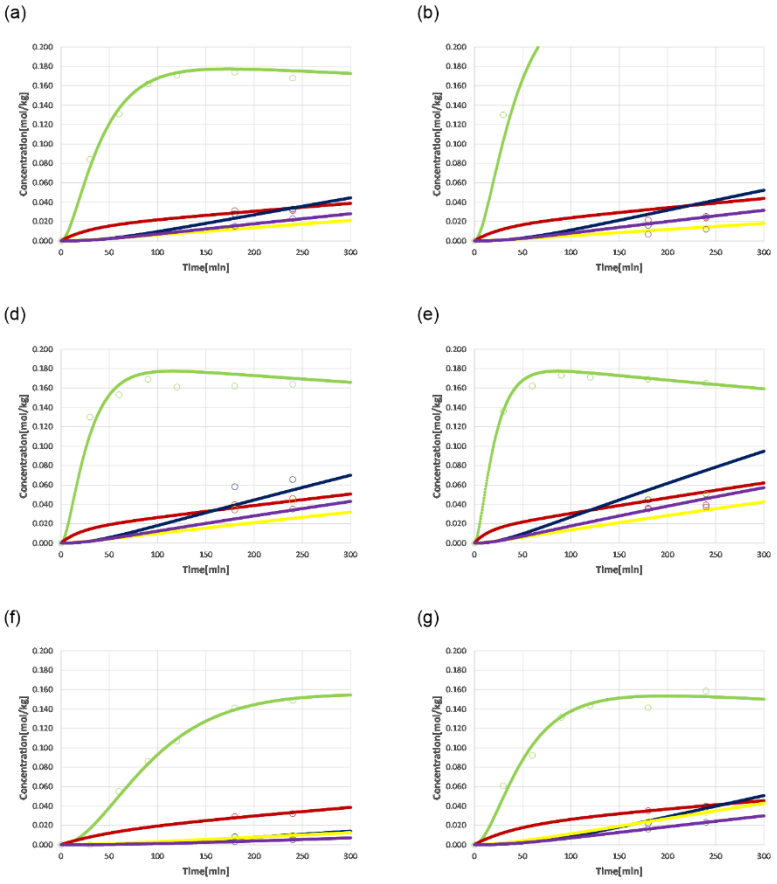
$$\frac{d[\boldsymbol{bypro1}]}{dt} = [cat](k_4[\boldsymbol{MA}][\boldsymbol{2a}]) \quad (12)$$

$$\frac{d[\boldsymbol{bypro2}]}{dt} = [cat](k_5[\boldsymbol{Mono}][MeOH]) \quad (13)$$

$$\frac{d[\boldsymbol{bypro3}]}{dt} = [cat](k_6[\boldsymbol{2a}][\boldsymbol{Mono}]) \quad (14)$$

$$\frac{d[\boldsymbol{bypro4}]}{dt} = [cat](k_7[\boldsymbol{2a}][\boldsymbol{Di}]) \quad (15)$$

9. A curve fitting of byproducts in case of MA



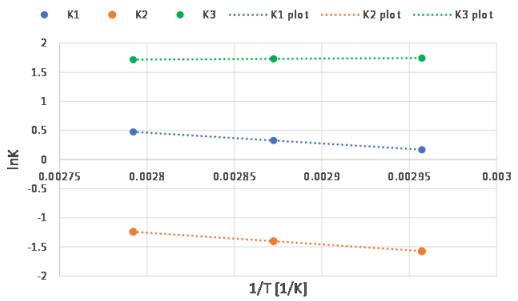
Conditions: $[MA]_0$ / $[BD]_0$ / [cat.] / Temp.
(a) 3.10 mol kg^{-1} / 6.19 mol kg^{-1} / 8.26 mmol kg^{-1} / 85 °C
(b) 3.72 mol kg^{-1} / 5.58 mol kg^{-1} / 8.26 mmol kg^{-1} / 85 °C
(c) 2.64 mol kg^{-1} / 6.61 mol kg^{-1} / 8.26 mmol kg^{-1} / 85 °C
(d) 3.10 mol kg^{-1} / 6.19 mol kg^{-1} / 12.4 mmol kg^{-1} / 85 °C
(e) 3.10 mol kg^{-1} / 6.19 mol kg^{-1} / 16.5 mmol kg^{-1} / 85 °C
(f) 3.10 mol kg^{-1} / 6.19 mol kg^{-1} / 8.26 mmol kg^{-1} / 65 °C
(g) 3.10 mol kg^{-1} / 6.19 mol kg^{-1} / 8.26 mmol kg^{-1} / 75 °C

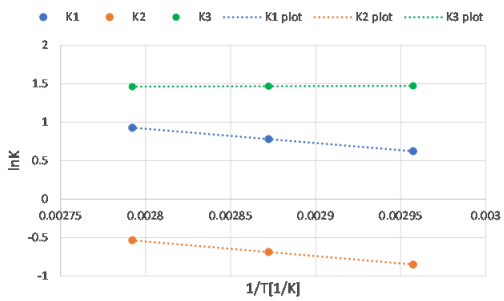
kinetic parameters[a]	Unit	Value
k_4	$kg^2\ mol^{-2}\ hr^{-1}$	0.206
k_5	$kg^2\ mol^{-2}\ hr^{-1}$	0.292
k_6	$kg^2\ mol^{-2}\ hr^{-1}$	0.072
k_7	$kg^2\ mol^{-2}\ hr^{-1}$	1.08
E_4	kJ mol^{-1}	30.1
E_5	kJ mol^{-1}	31.7
E_6	kJ mol^{-1}	23.3
E_7	kJ mol^{-1}	21.9

[a] $k_{-4} = k_{-5} = k_{-6} = k_{-7} = 0$ [kg/(mol*hr)]

Di: Green / BP1: Brown / BP2: Navy / BP3: Yellow / BP4:Purple

10. The van't Hoff plot of MA and MMA





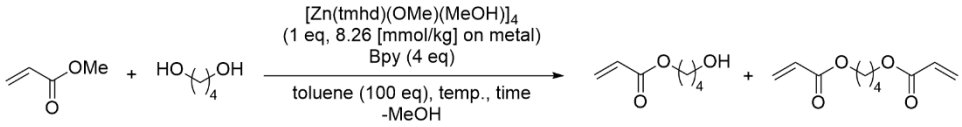
MA / T = 65, 75, 85 °C

$\ln K_1 = -1847/T+5.63$
$\ln K_2 = -2010/T+4.37$
$\ln K_3 = 164/T+1.26$

MMA / T = 65, 75, 85 °C

$\ln K_1 = -1847/T+6.09$
$\ln K_2 = -1908/T+4.79$
$\ln K_3 = 61/T+1.30$

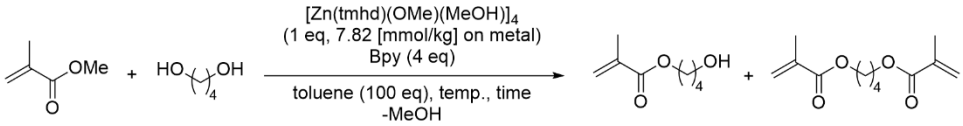
11. Simulated results of temperature effect and equivalent effect of 1,4-butanediol to MA



Entry	temperature[°C]	BD [eq]	initial condition [mol/kg]			conversion [%]		yield [%]		productivity [mol/(kg*hr)]	mono / di ratio
			$[MA]_0$	$[BD]_0$	time[min]	MA	BD	mono	di	mono	
1	60	2.0	3.45	6.91	461	71.0	34.1	56.6	8.53	0.254	13.3
2	65				363	72.2	34.5	57.7	8.99	0.329	12.8
3	70				288	73.4	34.9	58.7	9.44	0.423	12.4
4	75				229	74.4	35.3	59.7	9.89	0.541	12.1
5	80				184	75.5	35.6	60.7	10.3	0.683	11.8
6	85				148	76.5	36.0	61.5	10.7	0.862	11.5
7	90				119	77.4	36.3	62.3	11.2	1.09	11.2
8	95				97	78.4	36.6	63.1	11.6	1.35	10.9
9	100				79	79.2	36.9	63.8	11.9	1.67	10.7
10	105				65	80.1	37.2	64.4	12.3	2.05	10.5
11	110				54	80.9	37.5	65.0	12.7	2.50	10.3
12	115				45	81.6	37.8	65.6	13.0	3.02	10.1
13	120				37	82.3	38.1	66.2	13.4	3.71	9.90

Entry	temperature[°C]	BD [eq]	initial condition [mol/kg]			conversion [%]		yield [%]		yield [mol/kg]
			$[MA]_0$	$[BD]_0$	time[min]	MA	BD	mono	di	mono
14	85	1.0	5.22	5.22	157	61.7	53.8	43.4	16.0	2.27
15		1.1	4.97	5.47	157	63.9	51.2	46.0	15.5	2.29
16		1.2	4.74	5.69	157	65.8	48.8	48.4	14.9	2.29
17		1.3	4.53	5.89	157	67.5	46.6	50.5	14.4	2.29
18		1.4	4.34	6.07	157	69.1	44.6	52.5	13.9	2.28
19		1.5	4.16	6.24	157	70.5	42.7	54.3	13.4	2.26
20		1.6	4.00	6.19	157	71.8	41.0	56.0	13.0	2.24
21		1.7	3.85	6.54	157	73.0	39.4	57.5	12.6	2.21
22		1.8	3.71	6.67	157	74.0	38.0	59.0	12.2	2.18
23		1.9	3.58	6.79	157	75.0	36.6	60.3	11.8	2.16
24		2.0	3.45	6.91	157	76.0	35.3	61.6	11.4	2.13
25		2.1	3.34	7.02	157	76.9	34.1	62.7	11.1	2.10
26		2.2	3.24	7.12	157	77.6	33.1	63.8	10.8	2.06
27		2.3	3.14	7.21	157	78.4	32.0	64.8	10.5	2.03
28		2.4	3.04	7.30	157	79.1	31.0	65.8	10.2	2.00
28		2.5	2.96	7.39	157	79.7	30.1	66.7	9.90	1.97

12. Simulated results of temperature effect and equivalent effect of 1,4-butanediol to MMA



			initial condition [mol/kg]			conversion [%]		yield [%]		productivity [mol/(kg*hr)]	mono / di ratio
Entry	temperature[°C]	BD [eq]	$[MMA]_0$	$[BD]_0$	time[min]	MMA	BD	mono	di	mono	
1	60	1.5	3.93	5.89	3591	72.4	42.8	55.8	16.6	0.0365	6.72
2	65				2407	73.7	43.4	56.5	17.2	0.0550	6.56
3	70				1711	74.8	44.0	57.0	17.8	0.0782	6.42
4	75				1376	75.9	44.5	57.6	18.3	0.0980	6.28
5	80				974	77.0	45.0	58.1	18.9	0.140	6.16
6	85				576	77.9	45.5	58.6	19.4	0.238	6.04
7	90				486	78.9	46.0	59.0	19.9	0.285	5.93
8	95				333	79.8	46.4	59.4	20.4	0.418	5.83
9	100				271	80.6	46.8	59.8	20.8	0.517	5.74
10	105				207	81.4	47.2	60.1	21.3	0.681	5.65
11	110				124	82.1	47.5	60.5	21.6	1.14	5.59
12	115				70	82.6	47.8	60.8	21.7	2.04	5.60
13	120				43	82.7	48.0	61.3	21.4	3.34	5.73

			initial condition [mol/kg]			conversion [%]		yield [%]		yield [mol/kg]
Entry	temperature[°C]	BD [eq]	$[MMA]_0$	$[BD]_0$	time[min]	MMA	BD	mono	di	mono
14	85	1.0	4.86	4.86	439	63.9	54.0	44.2	19.8	2.15
15		1.1	4.64	5.10	442	66.0	51.3	46.9	19.2	2.17
16		1.2	4.44	5.33	443	67.9	48.8	49.4	18.5	2.19
17		1.3	4.25	5.53	445	69.6	46.6	51.7	17.9	2.20
18		1.4	4.08	5.72	446	71.1	44.5	53.8	17.3	2.20
19		1.5	3.93	5.89	446	72.3	42.7	55.6	16.8	2.18
20		1.6	3.78	6.05	447	73.6	40.9	57.4	16.3	2.17
21		1.7	3.65	6.20	447	74.7	39.3	59.0	15.8	2.15
22		1.8	3.52	6.34	449	75.8	37.9	60.6	15.3	2.13
23		1.9	3.41	6.47	448	76.7	36.5	61.9	14.8	2.11
24		2.0	3.30	6.59	449	77.7	35.3	63.3	14.4	2.09
25		2.1	3.19	6.71	448	78.6	34.0	64.6	14.0	2.06
26		2.2	3.10	6.81	448	79.2	32.9	65.6	13.6	2.03
27		2.3	3.01	6.91	448	79.9	31.9	66.7	13.3	2.00
28		2.4	2.92	7.01	448	80.7	30.9	67.8	12.9	1.98
28		2.5	2.84	7.10	448	81.2	30.0	68.7	12.6	1.95

29	105	1.0	4.86	4.86	206	73.6	60.4	47.3	26.3	2.30
30		1.1	4.64	5.10	209	75.6	57.3	50.4	25.2	2.34
31		1.2	4.44	5.33	210	77.4	54.4	53.2	24.1	2.36
32		1.3	4.25	5.53	210	78.9	51.8	55.8	23.1	2.37
33		1.4	4.08	5.72	209	80.3	49.3	58.1	22.2	2.37
34		1.5	3.93	5.89	207	81.4	47.2	60.1	21.3	2.36
35		1.6	3.78	6.05	205	82.5	45.1	62.0	20.4	2.35
36		1.7	3.65	6.20	202	83.4	43.3	63.7	19.7	2.33
37		1.8	3.52	6.34	201	84.3	41.5	65.4	18.9	2.30
38		1.9	3.41	6.47	200	85.0	40.0	66.8	18.3	2.27
39		2.0	3.30	6.59	199	85.7	38.5	68.1	17.6	2.24
40		2.1	3.19	6.71	197	86.4	37.0	69.4	17.0	2.22
41		2.2	3.10	6.81	195	86.9	35.8	70.5	16.4	2.18
42		2.3	3.01	6.91	193	87.5	34.6	71.6	15.9	2.15
43		2.4	2.92	7.01	191	88.0	33.4	72.6	15.4	2.12
44		2.5	2.84	7.10	189	88.4	32.4	73.5	14.9	2.09

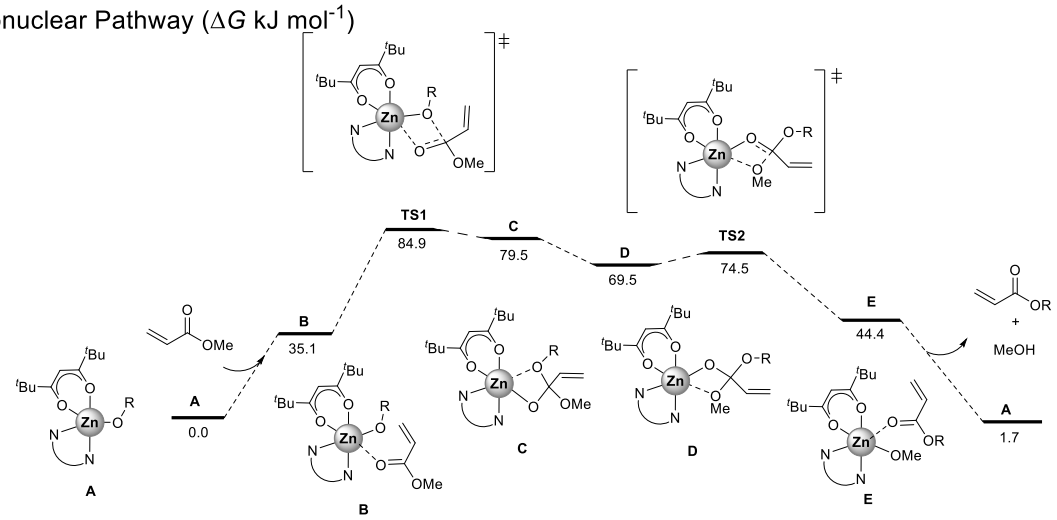
13. Computational studies

The calculations were performed using the Gaussian 16[S6] program employing B3LYP-GD3 functional, and using a LANL2DZ[S7] set for zinc with a solvation of toluene by means of the SMD model at 358 K. All stationary points were fully characterized *via* analytical frequency calculations as either true minima (all positive eigenvalues) or transition states (one imaginary eigenvalue). The IRC procedure was used to confirm the nature of each transition state connecting two minima. Thermal corrections to Energy, Enthalpy, and Gibbs Energy were estimated by a frequency calculation the same level of theory, to be considered for the calculation of the total energy values.

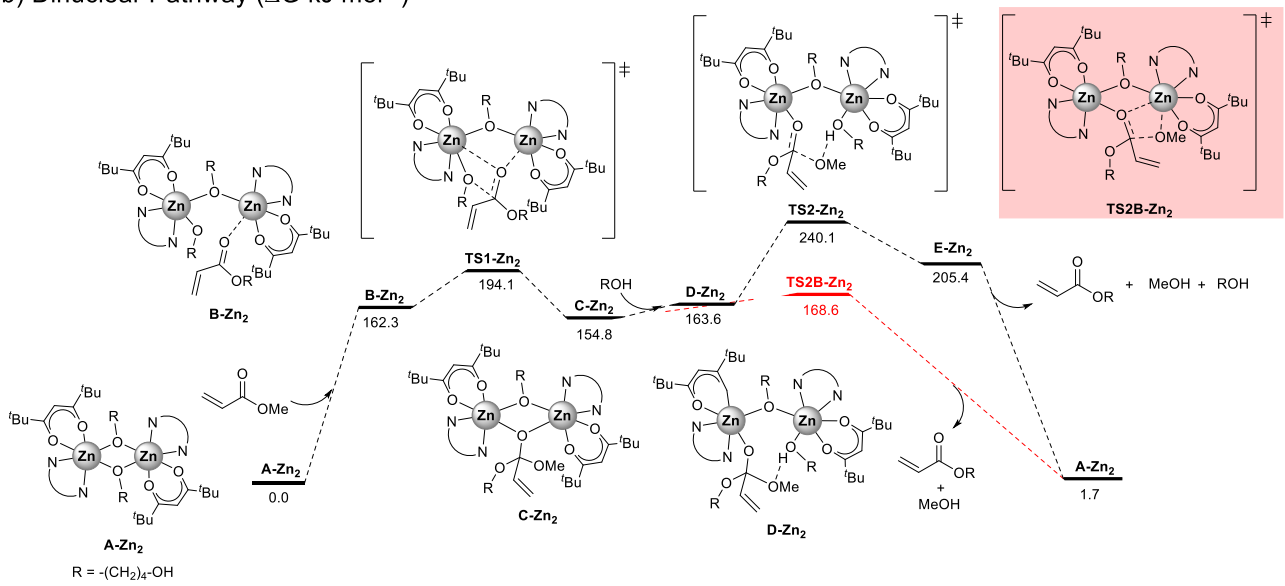
Reaction pathway mediated by dinuclear complexes.

We first check energies for two reaction pathways, one is a mononuclear complex catalyzed pathway and the other is dinuclear complex catalyzed pathway,[S8] using B3LYP/6-31G(d,p), LANL2DZ without solvation. As the result, mononuclear pathway (a) requires much lower activation energy than that of dinuclear pathway (b). Accordingly, we proposed the mononuclear pathway in the main text and reoptimized the mononuclear pathway using B3LYP-GD3/6-31G(d,p), LANL2DZ with solvation (SMD=toluene).

(a) Mononuclear Pathway (ΔG kJ mol^{-1})

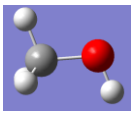


(b) Dinuclear Pathway (ΔG kJ mol^{-1})



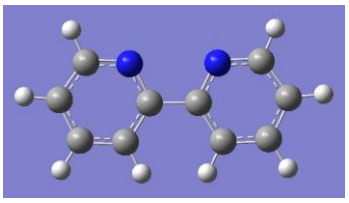
Cartesian coordinates

MeOH



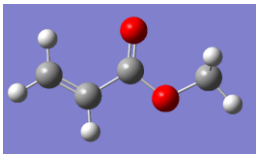
C	-0.04697900	0.66127700	0.00000000
H	-1.09294000	0.98298600	0.00000000
H	0.43764200	1.08890800	0.89181800
H	0.43764200	1.08890800	-0.89181800
O	-0.04697900	-0.75998700	0.00000000
H	0.87535600	-1.04856600	0.00000000

L1 (bpy)



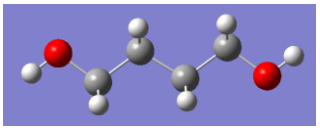
C	0.00000000	3.50381400	-0.09688900
C	0.00000000	2.88599900	1.15150600
C	0.00000000	1.49534100	1.21686800
C	0.00000000	0.74934300	0.02548200
C	0.00000000	2.68319500	-1.22660200
C	0.00000000	-0.74934300	0.02548200
C	0.00000000	-1.49534100	1.21686800
C	0.00000000	-2.88599900	1.15150600
C	0.00000000	-3.50381400	-0.09688900
C	0.00000000	-2.68319500	-1.22660200
H	0.00000000	4.58426400	-0.19755300
H	0.00000000	3.12354500	-2.22259200
H	0.00000000	-4.58426400	-0.19755300
H	0.00000000	-3.12354500	-2.22259200
N	0.00000000	-1.34989500	-1.17876500
N	0.00000000	1.34989500	-1.17876500
H	0.00000000	3.47487800	2.06405500
H	0.00000000	1.00977500	2.18525800
H	0.00000000	-1.00977500	2.18525800
H	0.00000000	-3.47487800	2.06405500

MA



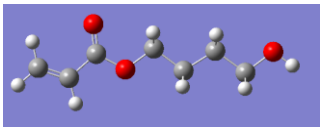
O	1.01423300	-0.72401700	0.00009000
C	2.30535100	-0.08912300	0.00004400
H	2.43094700	0.53403200	0.89004200
H	3.03434500	-0.90023000	0.00009200
H	2.43093800	0.53392900	-0.89002700
C	-0.04394900	0.11623000	-0.00012700
O	0.05977900	1.32870300	-0.00020700
C	-1.31719600	-0.64640600	0.00007600
C	-2.49131500	-0.01287800	0.00008300
H	-1.24172000	-1.72947300	0.00021100
H	-3.43154600	-0.55544100	0.00022300
H	-2.53240100	1.07276500	-0.00005500

2a



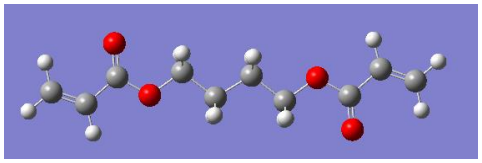
C	-1.88195200	-0.50574500	0.00000900
H	-1.86098700	-1.16140200	-0.88674600
H	-1.86104100	-1.16142100	0.88674500
C	-0.65540900	0.39539400	0.00005500
H	-0.70628100	1.04850800	0.88060500
H	-0.70632200	1.04864200	-0.88039600
C	0.65540900	-0.39539400	-0.00004300
H	0.70627800	-1.04850800	-0.88059300
H	0.70632500	-1.04864100	0.88040800
C	1.88195200	0.50574500	-0.00000400
H	1.86101200	1.16137500	0.88677000
H	1.86101600	1.16144800	-0.88672100
O	3.04038700	-0.32671000	-0.00003100
H	3.81694800	0.24867100	-0.00029100
O	-3.04038700	0.32671000	-0.00002800
H	-3.81694800	-0.24867100	0.00058900

Monoester



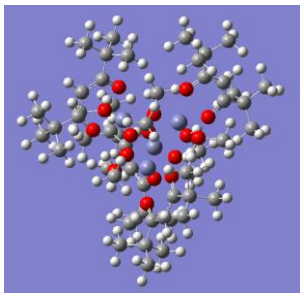
O	-1.14915700	-0.42652900	0.00037400
C	0.02100500	0.42446300	0.00036400
H	-0.00767000	1.07121100	0.88422000
H	-0.00790800	1.07155100	-0.88323000
C	-2.34134800	0.20725100	0.00002600
O	-2.46244100	1.41837300	-0.00015600
C	-3.45561300	-0.77413300	-0.00001200
C	-4.72534400	-0.36476200	-0.00030800
H	-3.18466000	-1.82551900	0.00020700
H	-5.55156600	-1.06890500	-0.00034500
H	-4.96239300	0.69545200	-0.00051700
C	1.24248100	-0.47782800	0.00004400
H	1.20195500	-1.12996100	-0.88123800
H	1.20213500	-1.13035200	0.88104500
C	2.54291500	0.33192100	0.00009200
H	2.58424100	0.98503800	0.88069000
H	2.58407300	0.98541400	-0.88023400
C	3.77999200	-0.55492000	-0.00021500
H	3.76724100	-1.21022400	-0.88731800
H	3.76742400	-1.21058100	0.88662600
O	4.92558700	0.29375000	-0.00016500
H	5.71068900	-0.26983100	-0.00026400

Diester



O	0.02802000	3.05978800	-0.00001100
C	0.72690300	1.79425500	-0.00002400
H	1.37223800	1.74131000	0.88379500
H	1.37224000	1.74132700	-0.88384200
C	0.80624200	4.16403500	0.00002200
O	2.02282800	4.13115000	0.00003600
C	-0.02802000	5.39188800	0.00000300
C	0.53716500	6.60039500	0.00001600
H	-1.10500700	5.25453500	-0.00001900
H	-0.05823400	7.50808600	0.00000600
H	1.61869800	6.70303200	0.00003900
C	-0.32176600	0.69554900	-0.00003400
H	-0.96379600	0.81552100	-0.88113900
H	-0.96380300	0.81551500	0.88106600
C	0.32176600	-0.69554900	-0.00003400
H	0.96380300	-0.81551500	0.88106600
H	0.96379600	-0.81552100	-0.88113900
C	-0.72690300	-1.79425500	-0.00002400
H	-1.37224000	-1.74132700	-0.88384200
H	-1.37223800	-1.74131000	0.88379500
O	-0.02802000	-3.05978800	-0.00001100
C	-0.80624200	-4.16403500	0.00002200
O	-2.02282800	-4.13115000	0.00003600
C	0.02802000	-5.39188800	0.00000300
C	-0.53716500	-6.60039500	0.00001600
H	1.10500700	-5.25453500	-0.00001900
H	0.05823400	-7.50808600	0.00000600
H	-1.61869800	-6.70303200	0.00003900

1a



Zn	-1.07666900	-0.13660700	1.54219200
Zn	0.83170100	1.76483900	-0.15359100
Zn	1.41675400	-1.38413400	-0.00954400
Zn	-1.05551700	-0.27873900	-1.66221300
O	-3.06268300	-0.49719100	1.98648000
O	-0.66147100	-1.55032500	3.06935000
O	-1.12797100	1.68967700	2.79200000
O	1.01494000	0.22192100	1.29779300
O	2.78552800	2.37604200	-0.05743600
O	0.41693700	3.33938200	1.21324400
O	0.43191900	2.90216600	-1.99496500
O	1.00523200	0.10100200	-1.46420400
O	1.50465500	-2.95000400	-1.43721800
O	3.47544600	-1.41254900	-0.05732900
O	1.45540500	-2.63129100	1.80097900
O	-0.71900600	-1.54879500	0.00773100
O	-3.05713100	-0.63288000	-1.89650400
O	-1.25639200	1.16338500	-3.19706400
O	-0.50177400	-1.96920800	-2.96539400
O	-1.20917000	1.17353400	-0.10306900
C	-3.55223900	-0.97134200	3.05402600
C	-2.80440900	-1.59811400	4.08486800
H	-3.34733100	-1.93852200	4.95028500
C	-1.43716300	-1.90208100	4.02968000
C	-5.09394000	-0.88398600	3.15632200
C	-5.52298300	0.54865200	2.77822900
H	-5.13441500	0.82796700	1.79794300
H	-6.61594100	0.62399700	2.75678800
H	-5.14831200	1.27474500	3.50934900
C	-5.65680300	-1.88933400	2.12541800
H	-5.38009400	-2.91656100	2.38975000
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H	-5.27083500	-1.68025800	1.12564200
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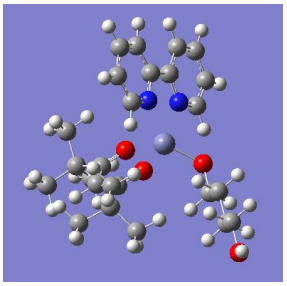

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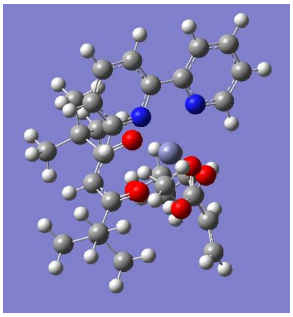

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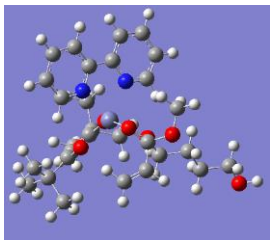

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H	2.47482000	0.97217300	0.58210200
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O	2.32657800	-1.44866700	-2.74601800
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H	1.12931200	-3.07684900	-2.23975300
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C	1.65382600	0.74162900	-3.16134900
C	0.68993000	1.58406200	-3.52351300
H	2.69073100	0.89990000	-3.45005400
H	0.89558000	2.46922800	-4.11993000
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H	6.54358100	-0.72199100	0.58577800
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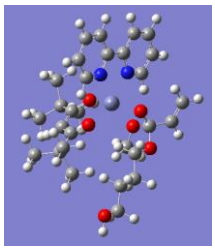

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C	4.89036000	-1.50962600	0.75907900
C	5.36873900	-1.96681700	-0.46814800
C	4.53358500	-1.93884400	-1.58346100
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C	-4.06290900	-2.13399700	-0.61156300
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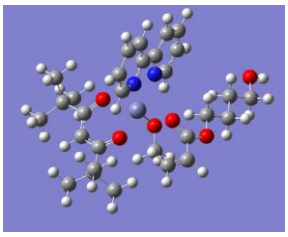

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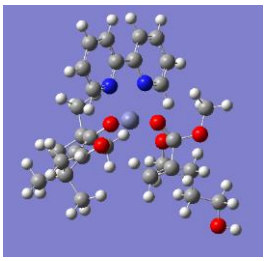
TS1



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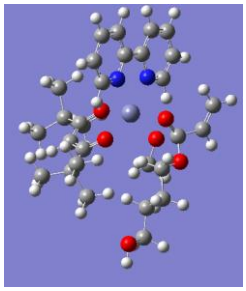
TS2



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C	5.37908200	-1.85625500	-0.55075500
C	4.53638300	-1.87053800	-1.66080700
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C	0.74477100	2.58551500	-0.88101600
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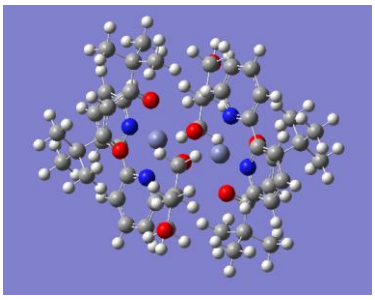
Dinuclear Pathway

A-Zn_2



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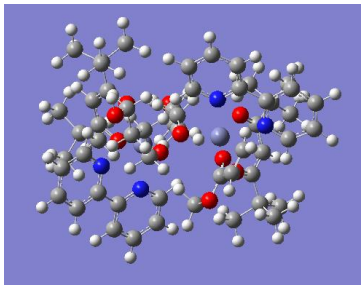
B-Zn_2



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C	2.21854900	4.97984000	1.74027200
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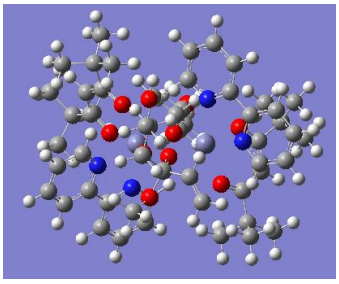
C-Zn_2



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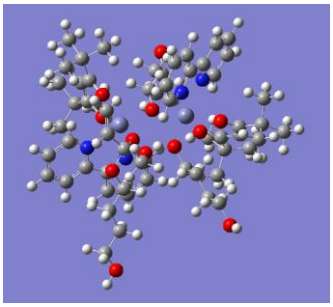

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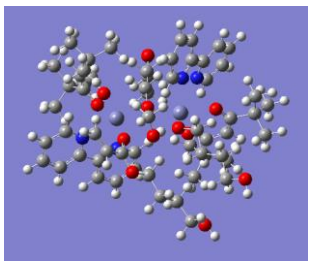
E-Zn_2



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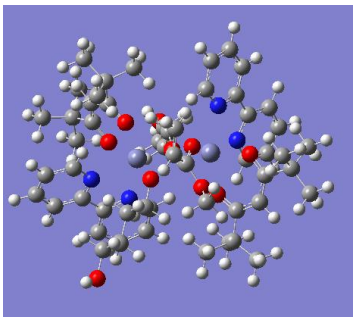
TS1-Zn_2



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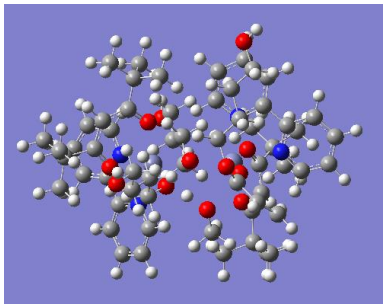

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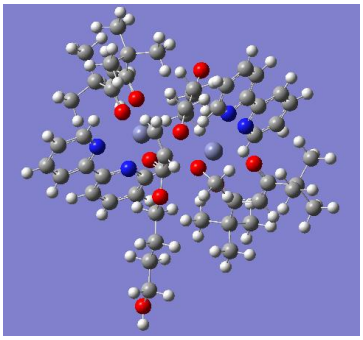
TS2B-Zn_2



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