Supplementary Materials

Application of Phase Transfer Catalysis in the Esterification of Organic acids: the Primary Products from Ring Hydrocarbon Oxidation Processes

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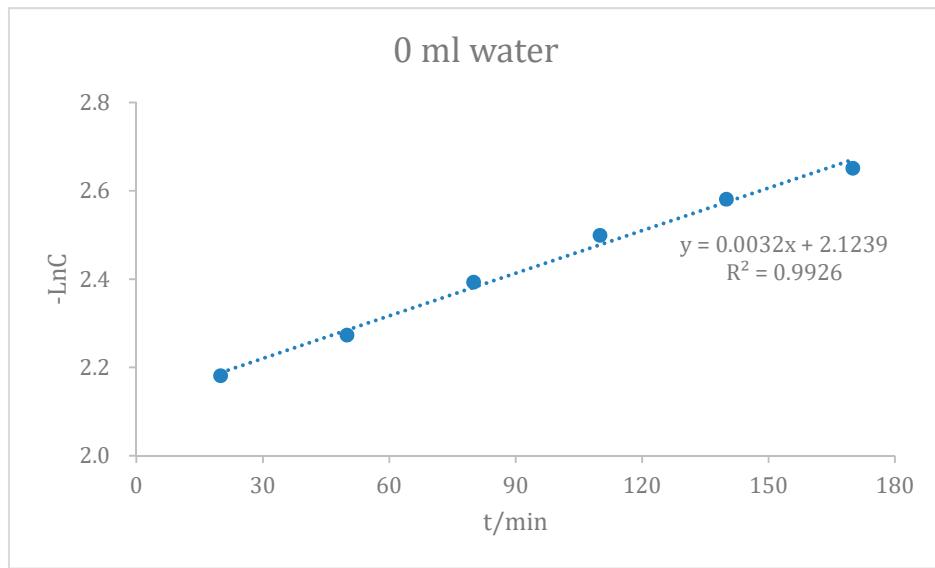
Figure S1 First-order reaction curve without water
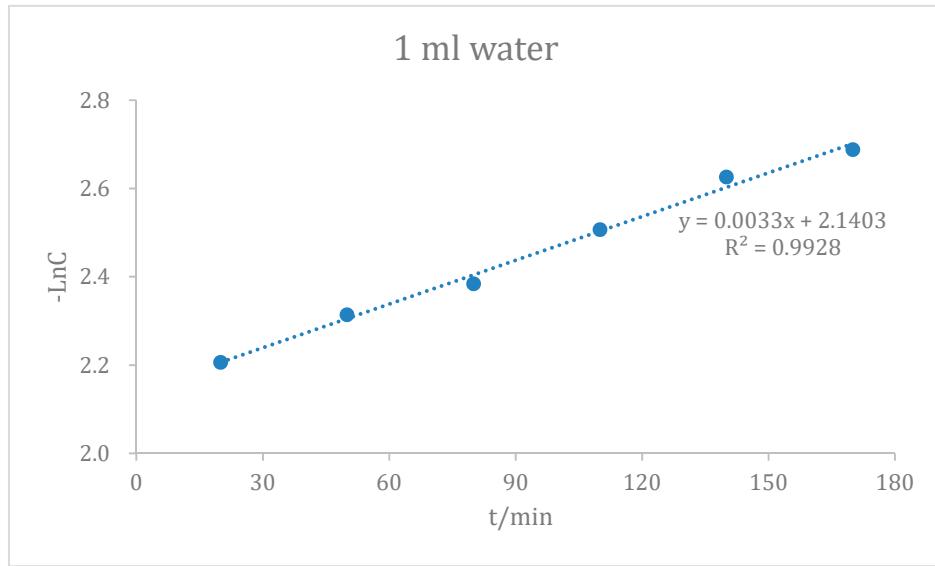
Figure S2 First-order reaction curve with 1 ml water
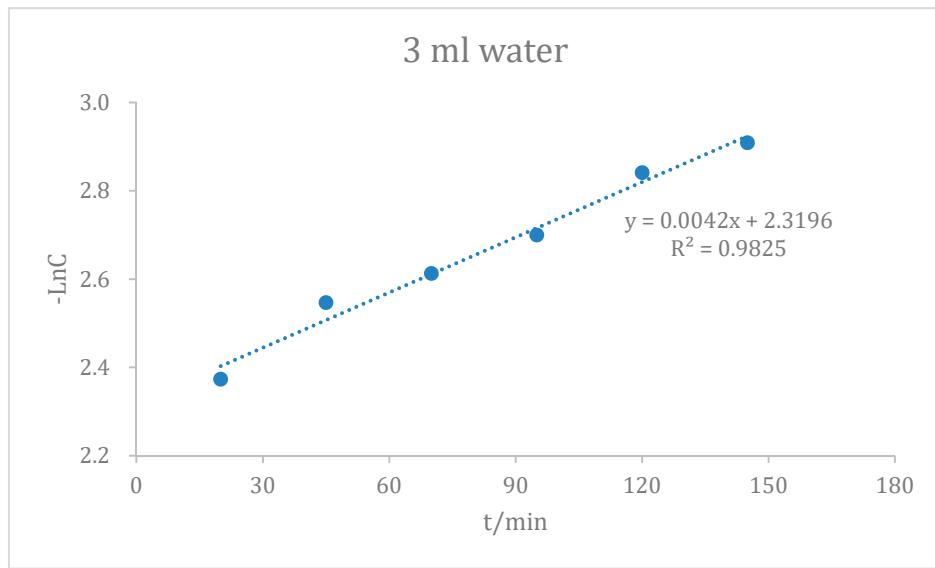
Figure S3 First-order reaction curve with 3 ml water
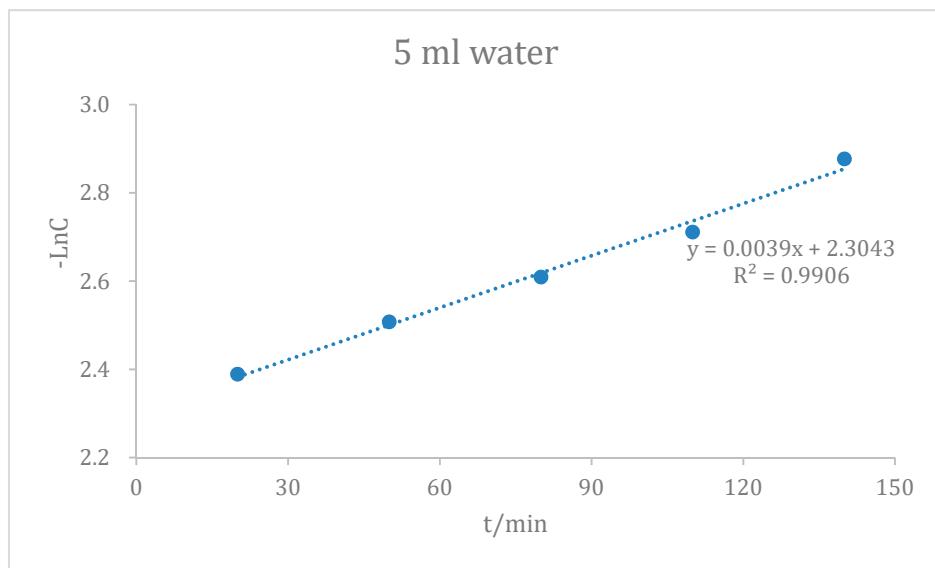
Figure S4 First-order reaction curve with 5 ml water
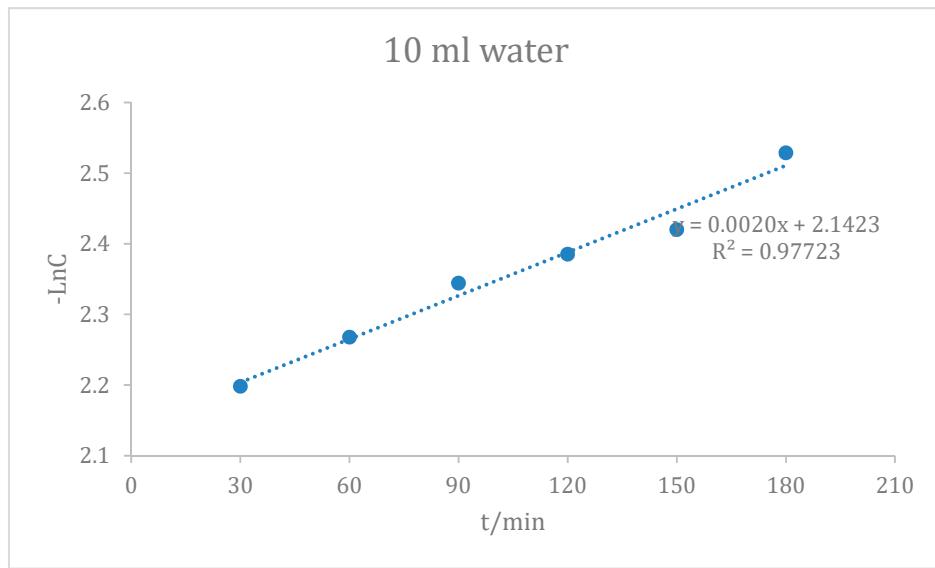
Figure S5 First-order reaction curve with 10 ml water
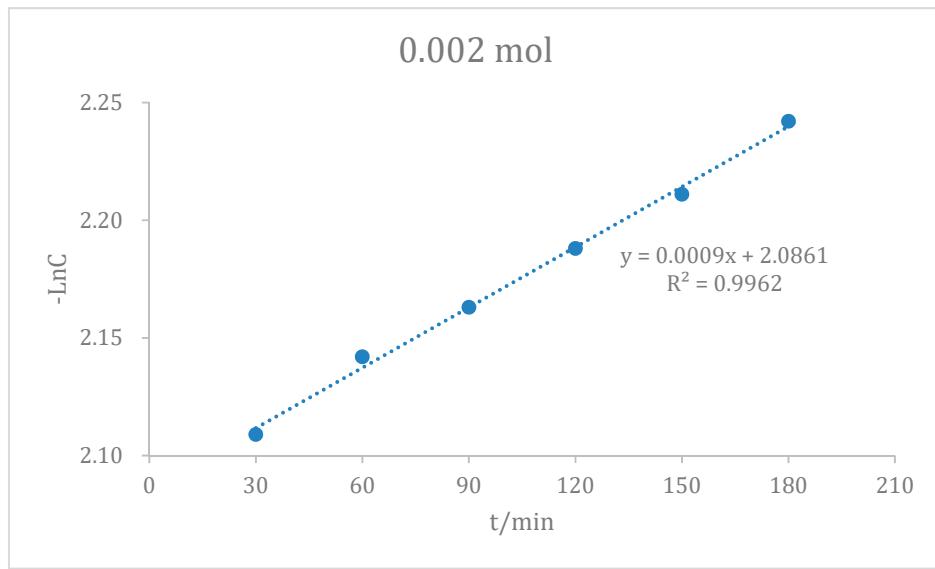
Figure S6 First-order reaction curve with 0.002 mol TBAB
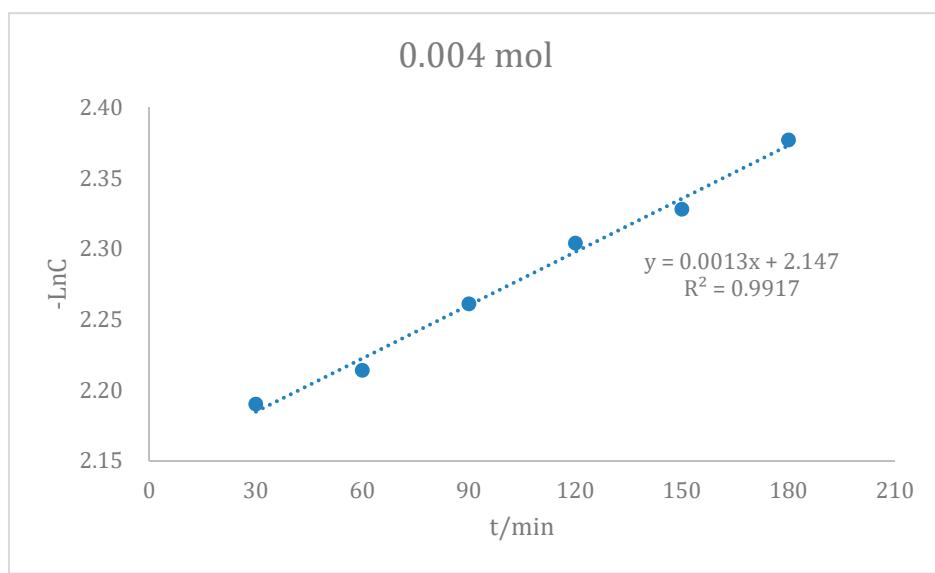
Figure S7 First-order reaction curve with 0.004 mol TBAB
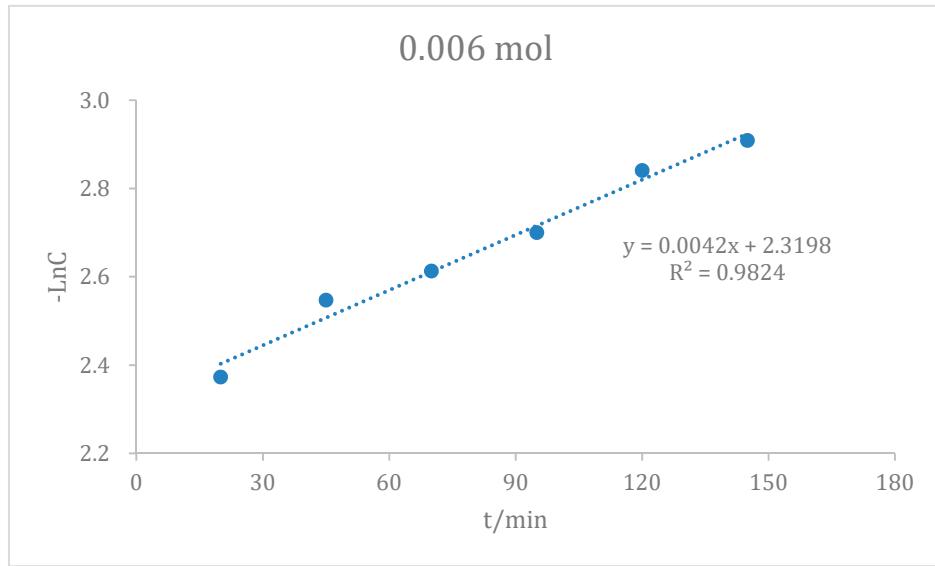
Figure S8 First-order reaction curve with 0.006 mol TBAB

0.008 mol

$y = 0.0046x + 2.2014$
$R^2 = 0.9943$
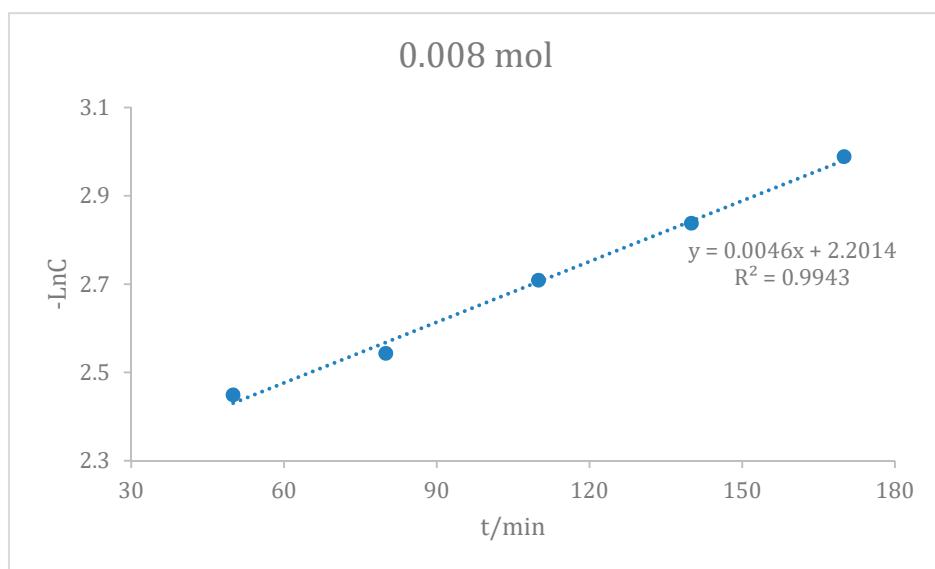
Figure S9 First-order reaction curve with 0.008 mol TBAB

THAB

$y = 0.0046x + 2.0668$
$R^2 = 0.9857$
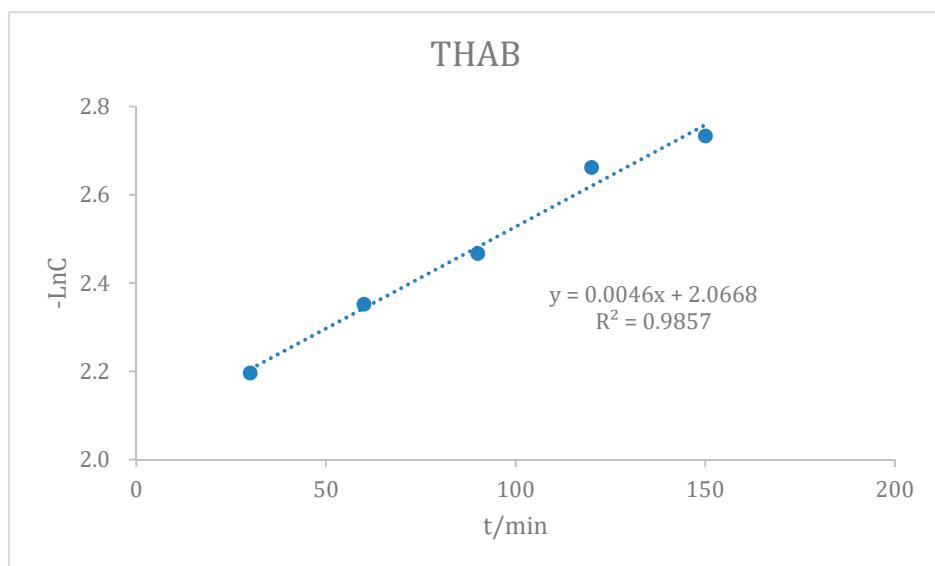
Figure S10 First-order reaction curve with THAB as PTC catalyst
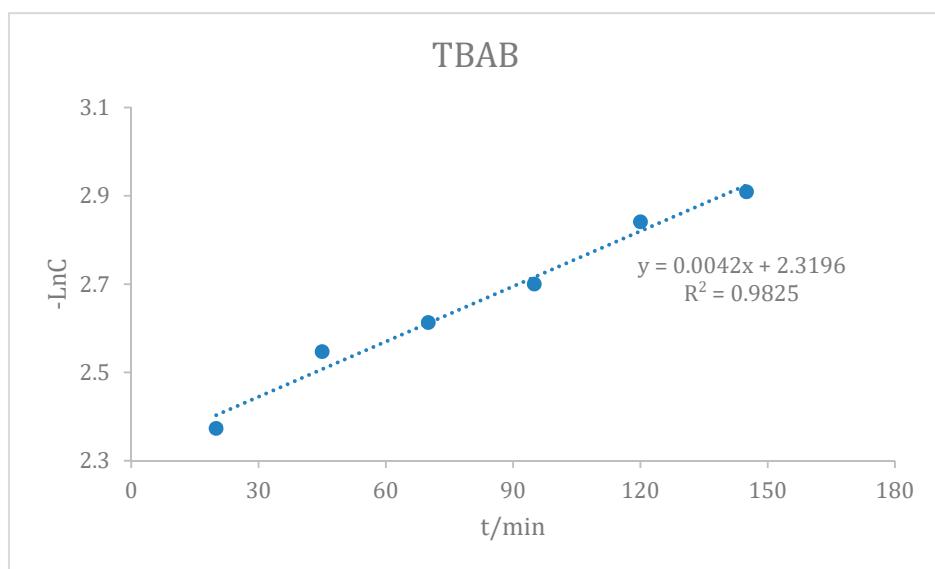
Figure S11 First-order reaction curve with TBAB as PTC catalyst
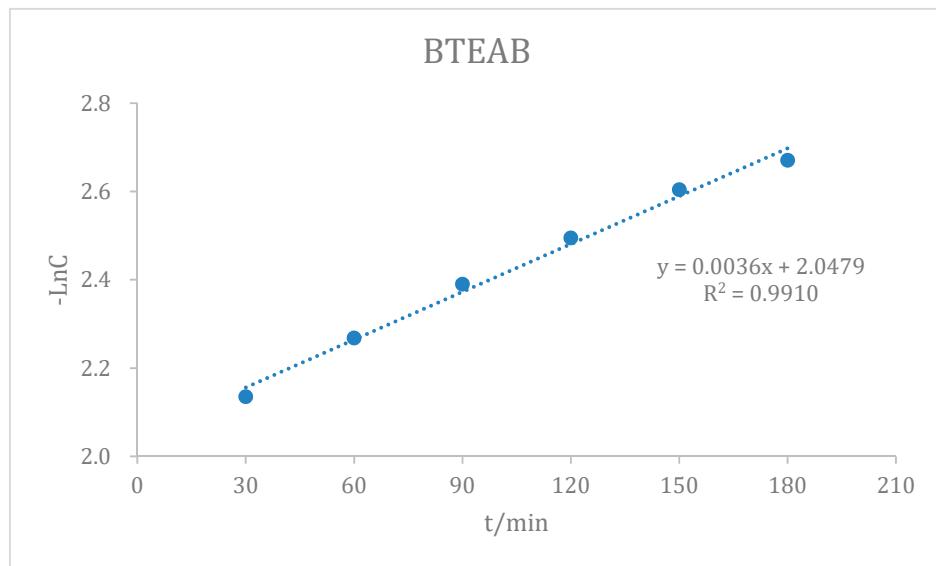
Figure S12 First-order reaction curve with BTEAB as PTC catalyst
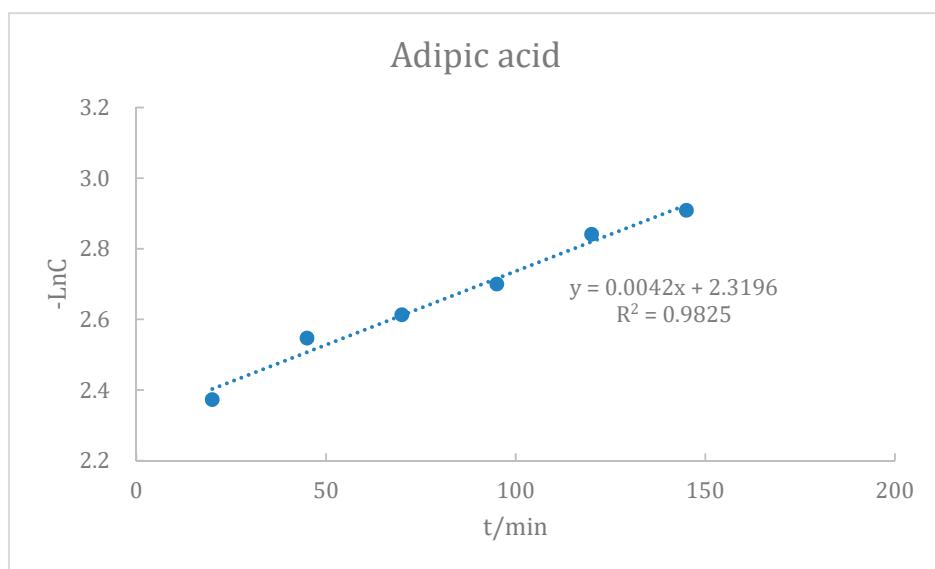
Figure S13 First-order reaction curve for adipic acid
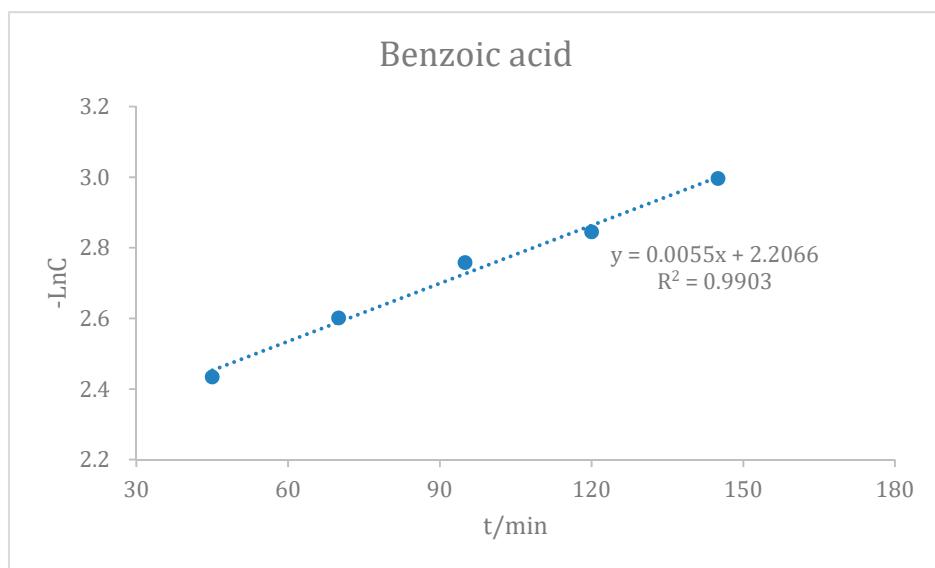
Figure S14 First-order reaction curve for benzoic acid
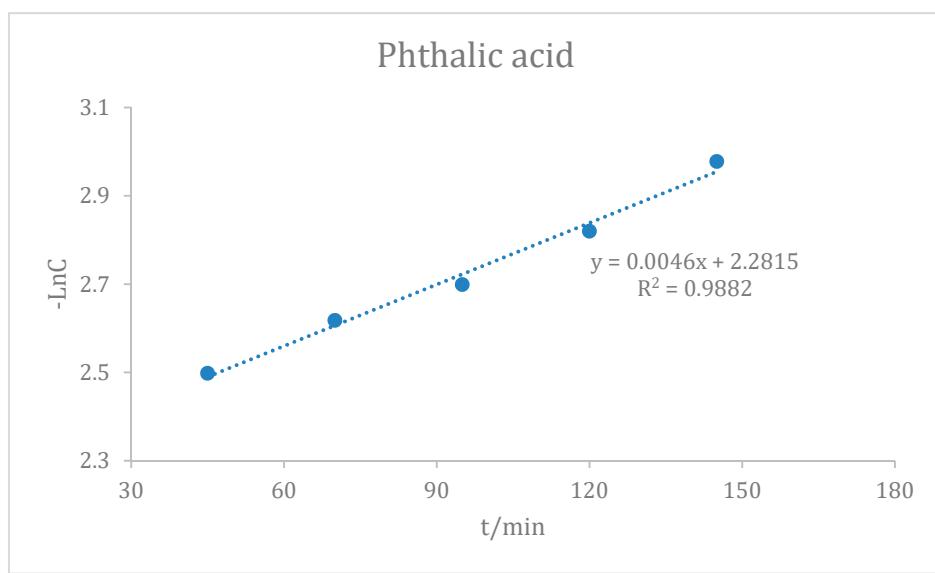
Figure S15 First-order reaction curve for phthalic acid

Table S1 Orthogonal experimental factors and levels for the esterification of adipic acid

No.	Factors				Conversion (%)
	Water (ml)	TBAB (mol)	Temperature (°C)	Time (h)	
1	V1 (3)	n1 (0.002)	T1 (90)	t1(1)	15
2	V1(3)	n2 (0.004)	T2 (105)	t2(2)	28
3	V1 (3)	n3(0.006)	T3 (115)	t3(4)	79
4	V2 (5)	n1 (0.002)	T2 (105)	t3(4)	42
5	V2 (5)	n2 (0.004)	T3 (115)	t1(1)	44
6	V2 (5)	n3 (0.006)	T1 (90)	t2(2)	28
7	V3 (10)	n1 (0.002)	T3 (115)	t2(2)	9
8	V3 (10)	n2(0.004)	T1 (90)	t3(4)	7
9	V3 (10)	n3(0.006)	T2 (105)	t1(1)	14
K1	121	65	49	73	
K2	113	79	84	65	

K3	30	121	132	127
k1	41	22	16	24
k2	38	26	28	22
k3	10	40	44	42
R	31	18	28	21

Table S2 Orthogonal experimental factors and levels for the esterification of

phthalic acid

No.	Factors				Conversion (%)
	Water (ml)	TBAB (mol)	Temperature (°C)	Time (h)	
1	V1 (3)	n1 (0.002)	T1 (90)	t1(1)	0
2	V1(3)	n2 (0.004)	T2 (105)	t2(2)	28
3	V1 (3)	n3(0.006)	T3 (115)	t3(4)	86
4	V2 (5)	n1 (0.002)	T2 (105)	t3(4)	29
5	V2 (5)	n2 (0.004)	T3 (115)	t1(1)	23
6	V2 (5)	n3 (0.006)	T1 (90)	t2(2)	21
7	V3 (10)	n1 (0.002)	T3 (115)	t2(2)	0
8	V3 (10)	n2(0.004)	T1 (90)	t3(4)	9
9	V3 (10)	n3(0.006)	T2 (105)	t1(1)	9
K1	114	29	30	32	
K2	73	61	66	49	

K3	18	116	109	125
k1	38	10	10	11
k2	24	20	22	16
k3	6	39	36	42
R	32	29	26	31

Table S3 Orthogonal experimental factors and levels for the esterification of benzoic acid

No.	Factors				Conversion (%)
	Water (ml)	TBAB (mol)	Temperature (°C)	Time (h)	
1	V1 (3)	n1 (0.002)	T1 (90)	t1(1)	5
2	V1(3)	n2 (0.004)	T2 (105)	t2(2)	51
3	V1 (3)	n3(0.006)	T3 (115)	t3(4)	97
4	V2 (5)	n1 (0.002)	T2 (105)	t3(4)	23
5	V2 (5)	n2 (0.004)	T3 (115)	t1(1)	24
6	V2 (5)	n3 (0.006)	T1 (90)	t2(2)	27
7	V3 (10)	n1 (0.002)	T3 (115)	t2(2)	6
8	V3 (10)	n2(0.004)	T1 (90)	t3(4)	9
9	V3 (10)	n3(0.006)	T2 (105)	t1(1)	14
K1	152	33	41	42	
K2	73	84	87	83	

K3	29	138	127	129
k1	51	11	14	14
k2	24	28	29	28
k3	10	46	42	43
R	41	35	29	29

Table S4 Effects of reaction time on the concentration of 1-bromobutane at 96 ºC

Reaction time (min)	Concentration (mol/L)
20	0.1011
60	0.0908
100	0.0845
140	0.0801
180	0.0732
220	0.0680

Table S5 Effects of reaction time on the concentration of 1-bromobutane at 103 °C

Reaction time (min)	Concentration (mol/L)
30	0.1049
60	0.0951
90	0.0887
120	0.0796
150	0.0721
180	0.0680

Table S6 Effects of reaction time on the concentration of 1-bromobutane at 107

ºC

Reaction time (min)	Concentration (mol/L)
30	0.1022
60	0.0918
90	0.0815
120	0.0726
150	0.0665

Table S7 Effects of reaction time on the concentration of 1-bromobutane at 110 °C

Reaction time (min)	Concentration (mol/L)
20	0.0932
45	0.0783
70	0.0733
95	0.0672
120	0.0584
145	0.0545

Table S8 The rate constant of 1-bromobutane at different temperatures

T (°C)	K_{obs} (min^{-1})
96	0.0019
103	0.0030
107	0.0036
110	0.0042