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The first two-fold interpenetrating polyoxometalate-base coordination polymer with helical channels: Structure and catalytic activities

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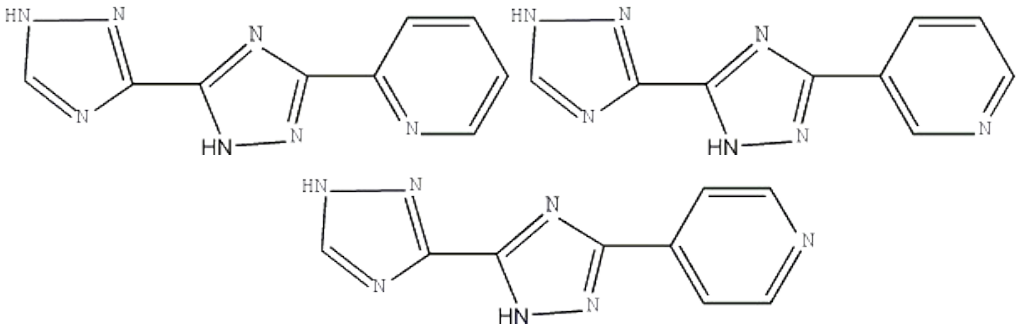

Fig.S1 Representations of the ligand H_2pyttz- I, H_2pyttz- II and H_2pyttz- III.

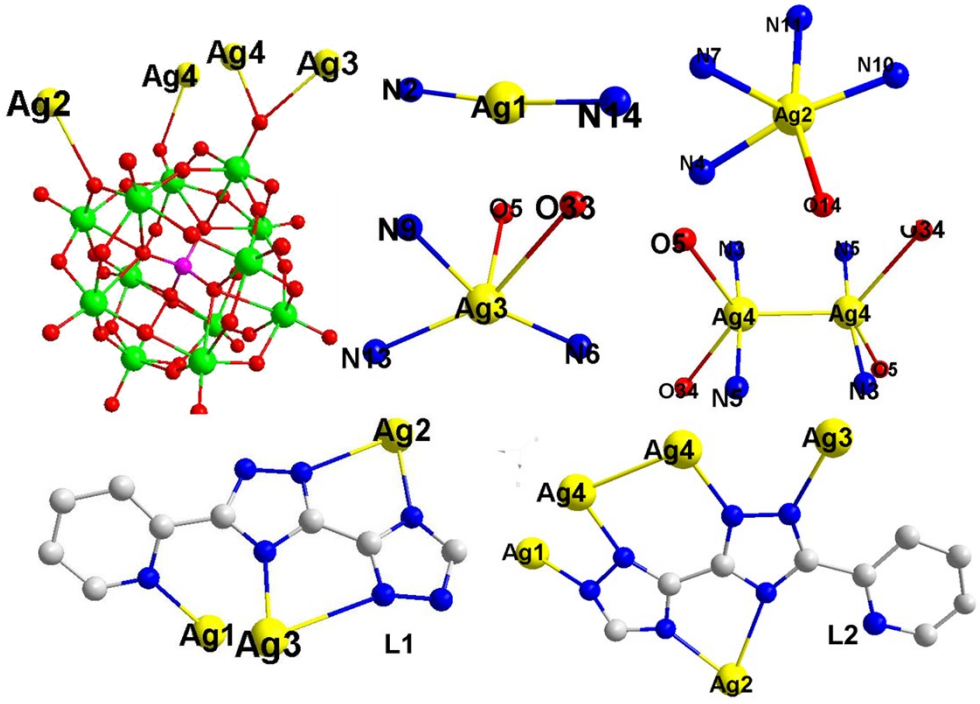

Fig.S2 The coordination modes of POMs, Ag ions and pyttz ligands: Ag1 ions adopt two coordinated mode completed by two N atoms from two pyttz ligands with Ag-N bond distances of

2.149 Å and 2.221Å; Ag2 ions are five coordinated by four N atoms from two ligands and one O atom from PMo_{12} with 2.199 Å-2.662 Å for Ag-N and 2.826 Å for Ag-O. Ag3 ions are five coordinated by three N atoms from two ligands and two O atoms from PMo_{12}, with distances of 2.164Å-2.572 Å for Ag-N and 2.661 Å-2.891 Å for Ag-O. Ag4 ions adopts four coordinated mode completed by two N atoms from two pyttz ligands with Ag-N bond distances of 2.089 Å and 2.104Å, and two oxygen atoms from two POMs with Ag-O bond distances of 2.733-2.801 Å.

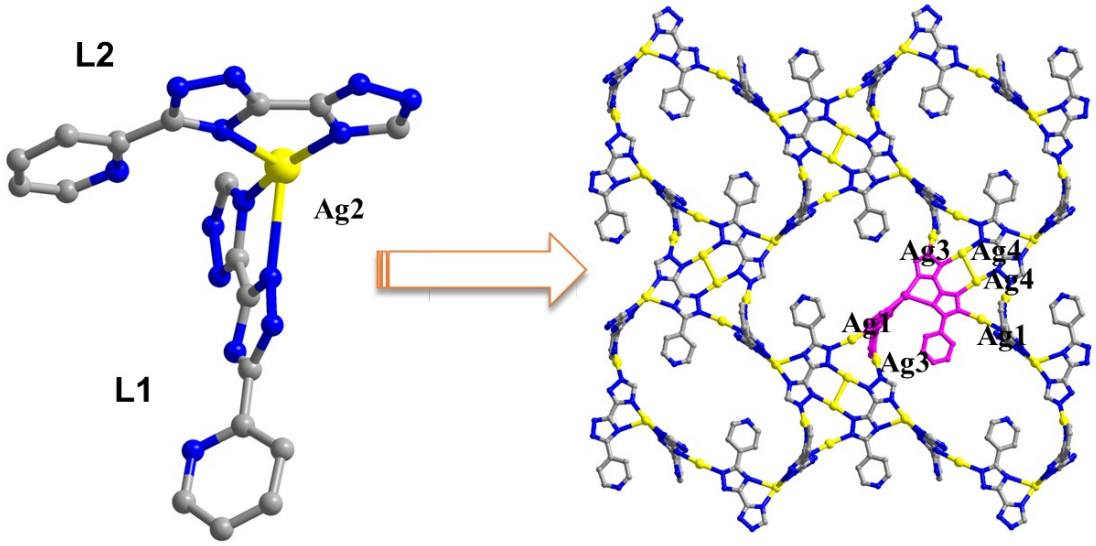

Fig.S3 Ball/stick representation of "T"-type subunit formed by Ag2 ion links with L1 and L2 ligands and infinite 2D CPs layer formed by Ag1, Ag3 and Ag4 ions and"T"-type subunit.

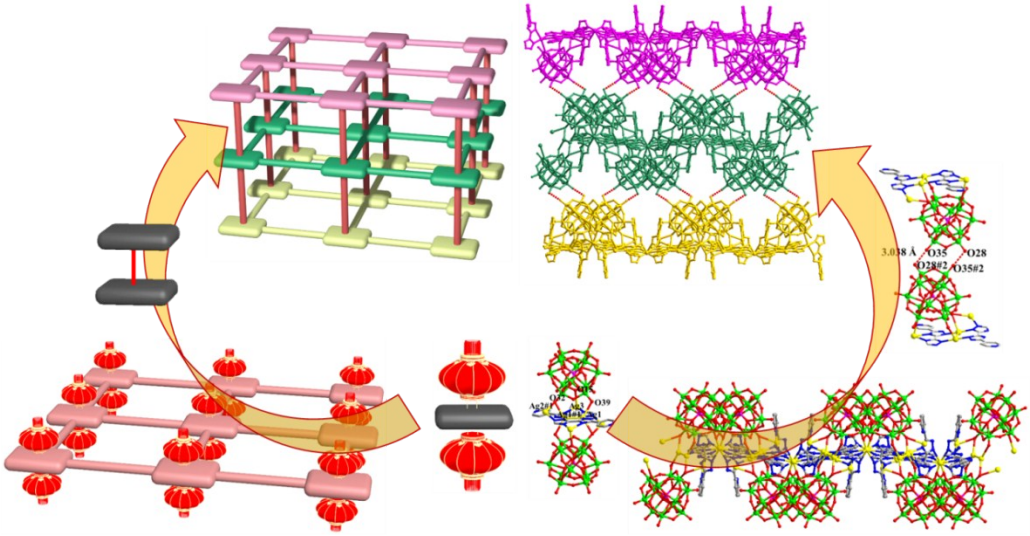

Fig.S4 Ball/stick representation and scheme about the formation of 3D POMCPs.

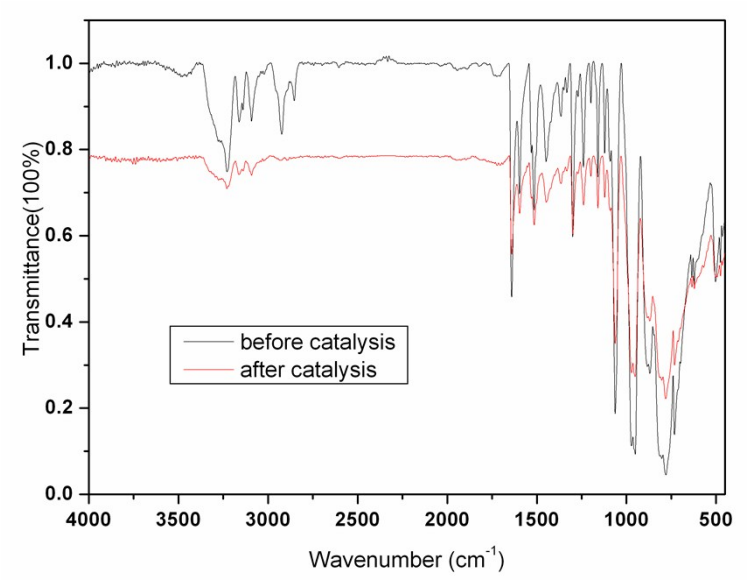

Fig.S5 Comparison IR chart for POMCP-**1** before and after catalysis.

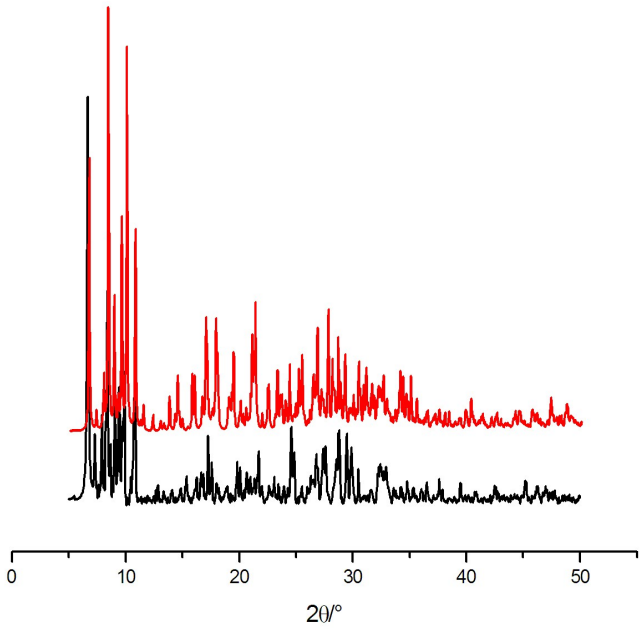

Fig.S6 The simulated (top) and experimental (below) XRPD pattern for the POMCP-**1.**

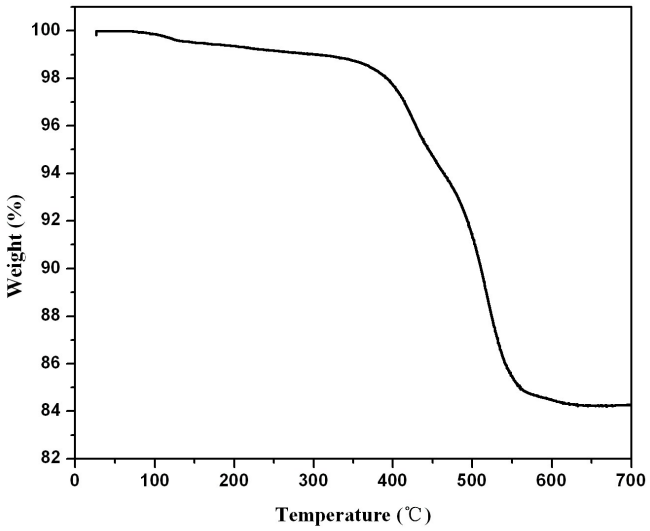

Fig.S7 The TG curve for the POMCP-**1.**

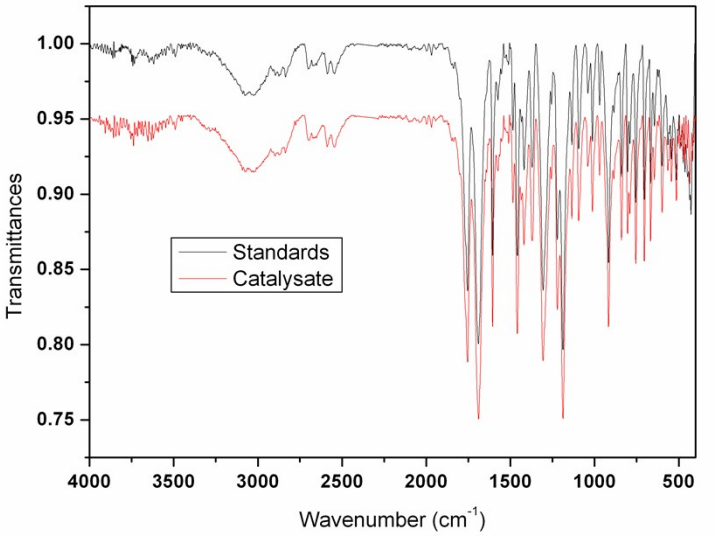

Fig.S8 The IR spectra about catalysate and Aspirin standard.

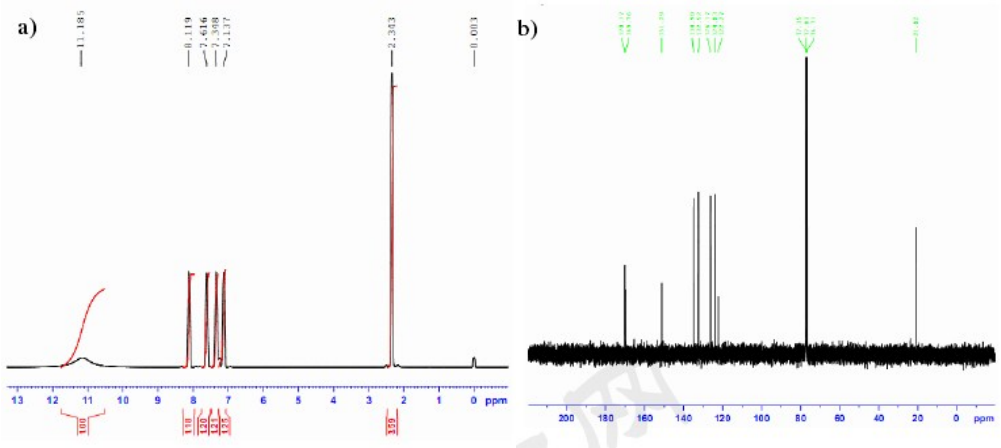

Fig.S9 ^{1}H-NMR and ^{13}C-NMR spectroscopy of catalysate.

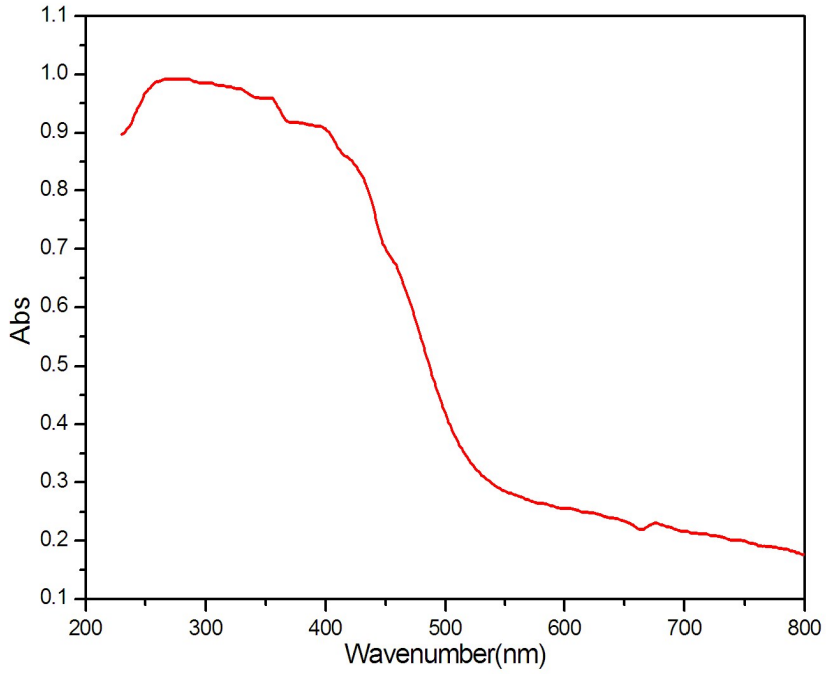

Fig.S10 Solid state UV-vis spectra of POMCP-**1**

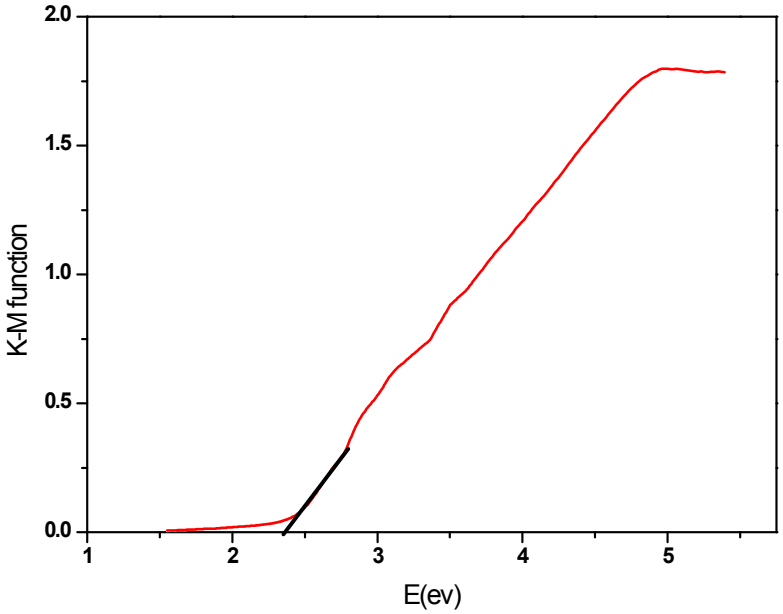

Fig.S11 The diffuse reflectance spectra of POMCP-**1.**

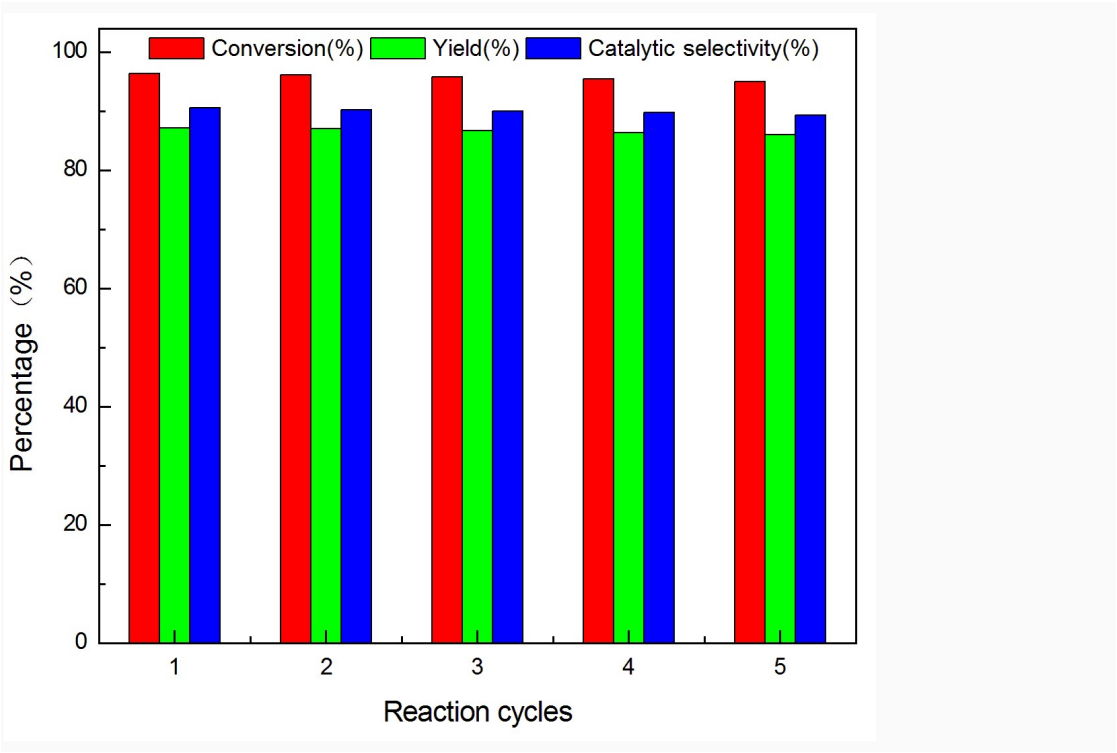

Fig.S12 Results of recycle of POMCP-**1** as catalyst.

Table S1 Selected bond length (Å) and angle (°) for POMCP-**1.**

N(1)-Ag(2)	2.102(12)	O(16)-Mo(1)	1.955(11)
N(26)-Ag(2)	2.160(13)	O(17)-Mo(1)	1.849(9)
N(4)-Ag(3)	2.621(12)	O(17)-Mo(8)	1.974(10)
N(5)-Ag(4)	2.100(12)	O(18)-Mo(10)	1.885(10)
O(1)-P(1)	1.538(10)	O(18)-Mo(9)	1.956(10)
O(1)-Mo(3)	2.408(9)	O(19)-Mo(8)	1.845(10)
O(1)-Mo(1)	2.436(9)	O(19)-Mo(9)	1.976(10)
O(1)-Mo(2)	2.440(9)	O(20)-Mo(8)	1.879(10)
O(2)-P(1)	1.542(9)	O(20)-Mo(12)	1.966(10)
O(2)-Mo(10)	2.415(9)	O(21)-Mo(10)	1.687(10)
O(2)-Mo(4)	2.424(9)	O(22)-Mo(10)	1.846(10)
O(2)-Mo(9)	2.437(9)	O(22)-Mo(12)	1.979(10)
O(3)-P(1)	1.526(10)	O(23)-Mo(7)	1.871(10)
O(3)-Mo(12)	2.435(9)	O(23)-Mo(8)	1.972(11)
O(3)-Mo(8)	2.447(9)	O(24)-Mo(4)	1.872(10)
O(3)-Mo(7)	2.447(9)	O(24)-Mo(10)	2.005(10)
O(4)-P(1)	1.544(9)	O(25)-Mo(11)	1.892(10)
O(4)-Mo(5)	2.415(9)	O(25)-Mo(10)	1.941(10)
O(4)-Mo(11)	2.421(9)	O(26)-Mo(7)	1.839(10)
O(4)-Mo(6)	2.447(9)	O(26)-Mo(2)	1.990(10)
O(5)-Mo(5)	1.860(10)	O(28)-Mo(11)	1.679(10)
O(5)-Mo(6)	2.002(10)	O(29)-Mo(12)	1.855(10)
O(6)-Mo(2)	1.876(10)	O(29)-Mo(11)	1.971(10)

O(6)-Mo(6)	1.948(10)	O(30)-Mo(12)	1.835(10)
O(7)-Mo(6)	1.884(10)	O(30)-Mo(7)	2.001(10)
O(7)-Mo(11)	1.941(10)	O(31)-Mo(12)	1.687(10)
O(8)-Mo(6)	1.853(10)	O(32)-Mo(3)	1.684(10)
O(8)-Mo(7)	1.960(10)	O(33)-Mo(5)	1.671(10)
O(9)-Mo(11)	1.857(10)	O(34)-Mo(4)	1.688(10)
O(9)-Mo(5)	1.969(10)	O(27)-Mo(4)	1.858(10)
O(10)-Mo(5)	1.855(10)	O(27)-Mo(5)	1.979(10)
O(10)-Mo(3)	1.969(10)	O(35)-Mo(6)	1.674(10)
O(11)-Mo(2)	1.846(10)	O(36)-Mo(7)	1.667(10)
O(11)-Mo(3)	1.971(10)	O(37)-Mo(8)	1.675(10)
O(12)-Mo(3)	1.848(10)	O(38)-Mo(9)	1.680(11)
O(12)-Mo(4)	1.968(10)	O(39)-Mo(1)	1.675(10)
O(13)-Mo(3)	1.858(10)	O(40)-Mo(2)	1.684(10)
O(13)-Mo(1)	2.002(10)	Ag(1)-N(99)#1	2.153(12)
O(14)-Mo(1)	1.881(10)	Ag(1)-N(12)	2.231(12)
O(14)-Mo(2)	1.946(10)	Ag(1)-Ag(2)	3.112(3)
O(15)-Mo(9)	1.867(10)	Ag(1)-Ag(4)	3.346(2)
O(15)-Mo(4)	1.958(9)	Ag(2)-Ag(4)	3.355(2)
O(16)-Mo(9)	1.873(11)	Ag(3)-O(6W)#2	1.509(16)
N(98)-Ag(4)#1	2.098(12)	Ag(3)-O(2W)	1.89(2)
N(99)-Ag(1)#1	2.153(12)	Ag(3)-N(96)#2	2.204(13)
N(96)-Ag(3)#3	2.204(13)	Ag(3)-N(22)	2.206(13)
O(6W)-Ag(3)#3	1.509(16)	Ag(4)-N(98)#1	2.098(12)
O(3)-P(1)-O(1)	109.6(5)	O(17)-Mo(8)-O(3)	82.1(4)
O(3)-P(1)-O(2)	109.5(5)	O(38)-Mo(9)-O(15)	102.7(5)
O(1)-P(1)-O(2)	110.0(5)	O(38)-Mo(9)-O(16)	103.1(5)
O(3)-P(1)-O(4)	109.5(5)	O(15)-Mo(9)-O(16)	93.9(4)
O(1)-P(1)-O(4)	109.5(5)	O(38)-Mo(9)-O(18)	100.8(5)
O(2)-P(1)-O(4)	108.8(5)	O(15)-Mo(9)-O(18)	87.8(4)
O(39)-Mo(1)-O(17)	102.7(5)	O(16)-Mo(9)-O(18)	155.0(4)
O(39)-Mo(1)-O(14)	102.4(5)	O(38)-Mo(9)-O(19)	101.1(5)
O(17)-Mo(1)-O(14)	94.2(5)	O(15)-Mo(9)-O(19)	156.0(4)
O(39)-Mo(1)-O(16)	101.9(5)	O(16)-Mo(9)-O(19)	83.9(4)
O(17)-Mo(1)-O(16)	86.5(4)	O(18)-Mo(9)-O(19)	84.6(4)
O(14)-Mo(1)-O(16)	154.9(4)	O(38)-Mo(9)-O(2)	171.5(5)
O(39)-Mo(1)-O(13)	99.7(5)	O(15)-Mo(9)-O(2)	73.7(3)
O(17)-Mo(1)-O(13)	157.1(4)	O(16)-Mo(9)-O(2)	85.0(4)
O(14)-Mo(1)-O(13)	85.4(4)	O(18)-Mo(9)-O(2)	71.6(4)
O(16)-Mo(1)-O(13)	84.5(4)	O(19)-Mo(9)-O(2)	82.3(3)
O(39)-Mo(1)-O(1)	170.1(4)	O(21)-Mo(10)-O(22)	102.8(5)
O(17)-Mo(1)-O(1)	86.4(4)	O(21)-Mo(10)-O(18)	102.0(5)
O(14)-Mo(1)-O(1)	72.9(4)	O(22)-Mo(10)-O(18)	93.7(4)
O(16)-Mo(1)-O(1)	82.2(4)	O(21)-Mo(10)-O(25)	101.6(5)

O(13)-Mo(1)-O(1)	71.6(4)	O(22)-Mo(10)-O(25)	86.5(4)
O(40)-Mo(2)-O(11)	103.7(5)	O(18)-Mo(10)-O(25)	155.7(4)
O(40)-Mo(2)-O(6)	103.7(5)	O(21)-Mo(10)-O(24)	99.6(5)
O(11)-Mo(2)-O(6)	94.0(4)	O(22)-Mo(10)-O(24)	157.3(4)
O(40)-Mo(2)-O(14)	100.5(5)	O(18)-Mo(10)-O(24)	85.3(4)
O(11)-Mo(2)-O(14)	88.2(4)	O(25)-Mo(10)-O(24)	85.3(4)
O(6)-Mo(2)-O(14)	154.5(4)	O(21)-Mo(10)-O(2)	170.7(4)
O(40)-Mo(2)-O(26)	100.6(5)	O(22)-Mo(10)-O(2)	85.6(4)
O(11)-Mo(2)-O(26)	155.5(4)	O(18)-Mo(10)-O(2)	73.2(4)
O(6)-Mo(2)-O(26)	83.0(4)	O(25)-Mo(10)-O(2)	82.7(4)
O(14)-Mo(2)-O(26)	84.6(4)	O(24)-Mo(10)-O(2)	72.4(4)
O(40)-Mo(2)-O(1)	171.6(4)	O(28)-Mo(11)-O(9)	104.5(5)
O(11)-Mo(2)-O(1)	73.2(4)	O(28)-Mo(11)-O(25)	103.1(5)
O(6)-Mo(2)-O(1)	84.5(4)	O(9)-Mo(11)-O(25)	92.8(4)
O(14)-Mo(2)-O(1)	71.8(4)	O(28)-Mo(11)-O(7)	100.3(5)
O(26)-Mo(2)-O(1)	82.3(4)	O(9)-Mo(11)-O(7)	88.5(4)
O(32)-Mo(3)-O(12)	104.3(5)	O(25)-Mo(11)-O(7)	155.4(4)
O(32)-Mo(3)-O(13)	102.4(5)	O(28)-Mo(11)-O(29)	99.6(5)
O(12)-Mo(3)-O(13)	94.9(5)	O(9)-Mo(11)-O(29)	155.7(4)
O(32)-Mo(3)-O(10)	100.6(5)	O(25)-Mo(11)-O(29)	83.8(4)
O(12)-Mo(3)-O(10)	86.0(4)	O(7)-Mo(11)-O(29)	85.0(4)
O(13)-Mo(3)-O(10)	156.0(4)	O(28)-Mo(11)-O(4)	172.3(4)
O(32)-Mo(3)-O(11)	98.0(5)	O(9)-Mo(11)-O(4)	74.1(4)
O(12)-Mo(3)-O(11)	156.8(4)	O(25)-Mo(11)-O(4)	84.5(4)
O(13)-Mo(3)-O(11)	86.6(5)	O(7)-Mo(11)-O(4)	72.2(4)
O(10)-Mo(3)-O(11)	83.5(4)	O(29)-Mo(11)-O(4)	81.7(4)
O(32)-Mo(3)-O(1)	169.5(5)	O(31)-Mo(12)-O(30)	103.6(5)
O(12)-Mo(3)-O(1)	86.0(4)	O(31)-Mo(12)-O(29)	103.2(5)
O(13)-Mo(3)-O(1)	74.5(4)	O(30)-Mo(12)-O(29)	95.6(4)
O(10)-Mo(3)-O(1)	81.7(4)	O(31)-Mo(12)-O(20)	99.7(5)
O(11)-Mo(3)-O(1)	72.0(4)	O(30)-Mo(12)-O(20)	87.5(4)
O(34)-Mo(4)-O(27)	103.0(5)	O(29)-Mo(12)-O(20)	155.4(4)
O(34)-Mo(4)-O(24)	101.9(5)	O(31)-Mo(12)-O(22)	100.3(5)
O(27)-Mo(4)-O(24)	94.6(4)	O(30)-Mo(12)-O(22)	155.5(4)
O(34)-Mo(4)-O(15)	100.0(5)	O(29)-Mo(12)-O(22)	84.2(4)
O(27)-Mo(4)-O(15)	156.1(4)	O(20)-Mo(12)-O(22)	83.1(4)
O(24)-Mo(4)-O(15)	87.0(4)	O(31)-Mo(12)-O(3)	171.8(4)
O(34)-Mo(4)-O(12)	101.1(5)	O(30)-Mo(12)-O(3)	74.1(4)
O(27)-Mo(4)-O(12)	85.6(4)	O(29)-Mo(12)-O(3)	84.9(4)
O(24)-Mo(4)-O(12)	156.4(4)	O(20)-Mo(12)-O(3)	72.5(4)
O(15)-Mo(4)-O(12)	83.7(4)	O(22)-Mo(12)-O(3)	81.5(4)
O(34)-Mo(4)-O(2)	171.7(4)	N(99)#1-Ag(1)-N(12)	162.0(5)
O(27)-Mo(4)-O(2)	84.8(4)	N(99)#1-Ag(1)-Ag(2)	115.7(3)
O(24)-Mo(4)-O(2)	74.3(4)	N(12)-Ag(1)-Ag(2)	63.9(3)

O(15)-Mo(4)-O(2)	72.6(3)	N(99)#1-Ag(1)-Ag(4)	61.0(3)
O(12)-Mo(4)-O(2)	82.2(4)	N(12)-Ag(1)-Ag(4)	125.4(4)
O(33)-Mo(5)-O(10)	104.4(5)	Ag(2)-Ag(1)-Ag(4)	62.47(5)
O(33)-Mo(5)-O(5)	102.0(5)	N(1)-Ag(2)-N(26)	163.6(5)
O(10)-Mo(5)-O(5)	93.9(4)	N(1)-Ag(2)-Ag(1)	105.2(4)
O(33)-Mo(5)-O(9)	98.7(5)	N(26)-Ag(2)-Ag(1)	89.4(4)
O(10)-Mo(5)-O(9)	155.9(4)	N(1)-Ag(2)-Ag(4)	59.1(4)
O(5)-Mo(5)-O(9)	87.9(4)	N(26)-Ag(2)-Ag(4)	124.7(3)
O(33)-Mo(5)-O(27)	100.9(5)	Ag(1)-Ag(2)-Ag(4)	62.19(5)
O(10)-Mo(5)-O(27)	84.8(4)	O(6W)#2-Ag(3)-O(2W)	108.5(8)
O(5)-Mo(5)-O(27)	156.7(4)	O(6W)#2-Ag(3)-N(96)#2	114.3(7)
O(9)-Mo(5)-O(27)	84.2(4)	O(2W)-Ag(3)-N(96)#2	69.1(7)
O(33)-Mo(5)-O(4)	170.3(5)	O(6W)#2-Ag(3)-N(22)	65.5(6)
O(10)-Mo(5)-O(4)	84.8(4)	O(2W)-Ag(3)-N(22)	124.7(6)
O(5)-Mo(5)-O(4)	74.4(4)	N(96)#2-Ag(3)-N(22)	166.0(5)
O(9)-Mo(5)-O(4)	72.5(4)	O(6W)#2-Ag(3)-N(4)	85.3(6)
O(27)-Mo(5)-O(4)	82.3(4)	O(2W)-Ag(3)-N(4)	53.2(6)
O(35)-Mo(6)-O(8)	103.7(5)	N(96)#2-Ag(3)-N(4)	122.3(5)
O(35)-Mo(6)-O(7)	102.3(5)	N(22)-Ag(3)-N(4)	71.6(4)
O(8)-Mo(6)-O(7)	93.8(4)	N(98)#1-Ag(4)-N(5)	173.4(5)
O(35)-Mo(6)-O(6)	102.3(5)	O(23)-Mo(7)-O(3)	73.2(4)
O(8)-Mo(6)-O(6)	85.8(4)	O(8)-Mo(7)-O(3)	81.3(4)
O(7)-Mo(6)-O(6)	154.7(4)	O(30)-Mo(7)-O(3)	71.3(4)
O(35)-Mo(6)-O(5)	100.7(5)	O(37)-Mo(8)-O(19)	103.6(5)
O(8)-Mo(6)-O(5)	155.2(4)	O(37)-Mo(8)-O(20)	102.2(5)
O(7)-Mo(6)-O(5)	85.4(4)	O(19)-Mo(8)-O(20)	94.6(4)
O(6)-Mo(6)-O(5)	84.6(4)	O(37)-Mo(8)-O(23)	100.2(5)
O(35)-Mo(6)-O(4)	170.6(5)	O(19)-Mo(8)-O(23)	155.4(4)
O(8)-Mo(6)-O(4)	84.7(4)	O(20)-Mo(8)-O(23)	86.8(4)
O(7)-Mo(6)-O(4)	72.4(4)	O(37)-Mo(8)-O(17)	101.6(5)
O(6)-Mo(6)-O(4)	82.5(4)	O(19)-Mo(8)-O(17)	85.5(4)
O(5)-Mo(6)-O(4)	71.4(4)	O(20)-Mo(8)-O(17)	155.5(4)
O(36)-Mo(7)-O(26)	103.3(5)	O(23)-Mo(8)-O(17)	83.3(4)
O(36)-Mo(7)-O(23)	103.6(5)	O(37)-Mo(8)-O(3)	170.7(5)
O(26)-Mo(7)-O(23)	96.4(4)	O(19)-Mo(8)-O(3)	85.1(4)
O(36)-Mo(7)-O(8)	101.1(5)	O(20)-Mo(8)-O(3)	73.5(4)
O(26)-Mo(7)-O(8)	84.9(4)	O(23)-Mo(8)-O(3)	71.7(4)

Symmetry transformations used to generate equivalent atoms: #1 -x,-y+1,-z+1; #2 x-1/2,-y+1/2,z-1/2 ; #3 x+1/2,-y+1/2,z+1/2

Table S2 Summary of POMCPs based on PYTTZ by altering POM and PYTTZ

No	compounds	Orgainc ligands	POMs	Structure	Ref
1	$K[Ag_{14}(pyttz)_4(H_2O)_2][PW_{12}O_{40}]_2\cdot(OH)\cdot 5H_2O$	PYTTZ-2	$[PW_{12}O_{40}]^{3-}$	close inorganic helix	5b
2	$K[Ag_{14}(pyttz)_4(H_2O)_4][HSiW_{12}O_{40}]_2\cdot H_2O$	PYTTZ-2	$[SiW_{12}O_{40}]^{4-}$	close inorganic helix	5b
3	$[Ag_3(Hpyttz)_2][H_2PMo_{12}O_{40}]$	PYTTZ-3	$[PMo_{12}O_{40}]^{3-}$	close hybrid helix	5e
4	$[Ag_6(Hpyttz)_2(H_2pyttz\text{-}II)_2][H_2CoW_{12}O_{40}]\cdot 4H_2O$	PYTTZ-2	$[CoW_{12}O_{40}]^{6-}$	open hybrid helix	5e
5	$[Ag_7(Hpyttz\text{-}II)_2(H_2pyttz\text{-}II)_2][GeW_{12}O_{40}]\cdot(OH)\cdot 6H_2O$	PYTTZ-2	$[GeW_{12}O_{40}]^{4-}$	open hybrid helix	5e
6	$Na_2[Ag_6(pyttz)_2(H_2O)][PMo_{12}O_{40}]\cdot(OH)$	PYTTZ-2	$[PMo_{12}O_{40}]^{3-}$	close imorganic helix	5c

PYTTZ-1= 3-(pyrid-2-yl)-5-(1H-1,2,4-triazol-3-yl)- 1,2,4-triazolyl; PYTTZ-2= 3-(pyrid-3-yl) -53-(1H-1,2,4-triazol-3-yl)- 1,2,4-triazolyl; PYTTZ-3= 3-(pyrid-3-yl)-5-(1H-1,2,4-triazol-3-yl)-1,24,4-triazolyl

Table S3 Comparison of salicylic acid conversion, yield of aspirin and catalytic selectivity catalyzed by POMCP-**1.**

Catalyst (40mg)		Time (min)											
		5	10	15	20	25	30	35	40	45	50	55	60
Yield	70	19.83	31.19	39.30	47.66	57.68	65.45	70.77	72.75	73.03	75.15	77.87	78.77
	75	25.31	35.53	46.44	52.45	60.49	70.21	72.22	76.87	79.53	80.02	81.79	83.26
	80	27.68	47.83	58.71	65.54	73.29	79.71	80.70	81.43	82.29	82.78	83.20	83.46
	85	31.72	49.46	63.73	67.83	75.66	79.87	85.28	85.63	87.20	87.16	86.69	86.83
	90	34.25	58.47	67.09	70.60	81.23	73.91	71.49	70.77	66.39	63.37	59.96	51.18
Conversion	70	38.60	52.18	60.25	67.35	71.32	76.08	79.11	82.20	85.16	86.66	88.55	89.26
	75	49.36	62.61	72.49	79.59	84.22	87.98	88.42	89.19	90.77	92.04	93.17	93.97
	80	61.64	68.62	78.48	85.14	88.32	90.51	92.67	93.82	94.78	95.22	95.75	96.17
	85	63.98	81.80	88.77	93.23	94.62	95.51	95.93	96.13	96.30	96.53	96.63	96.70
	90	71.40	86.10	90.67	93.76	95.16	95.42	95.49	96.10	96.14	96.35	96.73	96.72
Selectivity	70	51.38	59.78	65.22	70.76	80.87	86.03	89.46	88.50	85.76	86.72	87.94	88.25
	75	51.28	56.75	64.07	65.90	71.82	79.80	81.67	86.19	87.62	86.94	87.79	88.61
	80	44.91	69.70	74.81	76.98	82.98	88.07	87.08	86.79	86.82	86.94	86.90	86.78
	85	49.59	60.46	71.79	72.76	79.96	83.63	88.91	89.08	90.55	90.29	89.72	89.79
	90	47.96	67.91	73.99	75.30	85.37	77.46	74.87	73.64	69.05	65.77	61.99	52.81

ESI† The establishment of the detection method of ultraviolet two-wavelength isoabsorption spectrophotometry.

The standard curve equation

The precision amount of SA standard was dissolved in0.002M phosphate buffer solution, then making into a certain mass concentration as the reference substance solution: 8ug.ml^{-1}, 16ug.ml^{-1}, 24ug.ml^{-1}, 32ug.ml^{-1} and 40ug.ml^{-1}; According to the same method, the Aspirin reference substance solution, 60ug.ml^{-1}, 120ug.ml^{-1}, 180ug.ml^{-1}, 240ug.ml^{-1} and 300ug.ml^{-1}, are obtained. According to the UV spectrophotometry of SA, ASP and their mixture, the measure wavelength is determined to be 270nm and 297nm (Fig. S12 and S13). The process of standard curve equation is as follows:

$A_{270}=A_{ASP270}+A_{SA270}$

$A_{297}=A_{ASP297}+A_{SA297}$

$A_{ASP270}=0.0029C_{ASP}-0.0039(R^2=0.9999)$ (1)

$A_{ASP297}=0.0003C_{ASP}-0.0025(R^2=0.9998)$ (2)

$A_{SA270}=0.0059C_{SA}-0.0208$ ($R^2=0.9997$) (3)

$A_{SA297}=0.0256C_{SA}-0.0172(R^2=0.9999)$ (4)

The final equation can be worked out by equations 1, 2, 3 and 4.

$C_{SA}=40.0166A_{297}-4.138A_{270}+0.686$ (5)

$C_{ASP}=353.25A_{270}-81.390A_{297}+7.122$ (6)

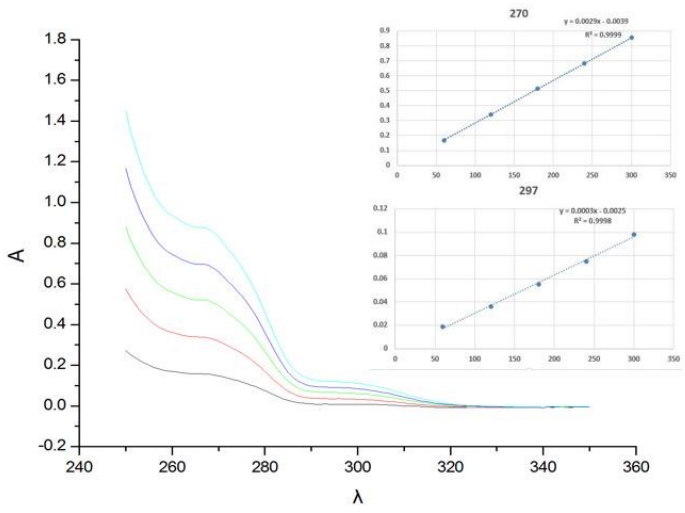

Fig.S12 The UV and standard curve of Aspirin.

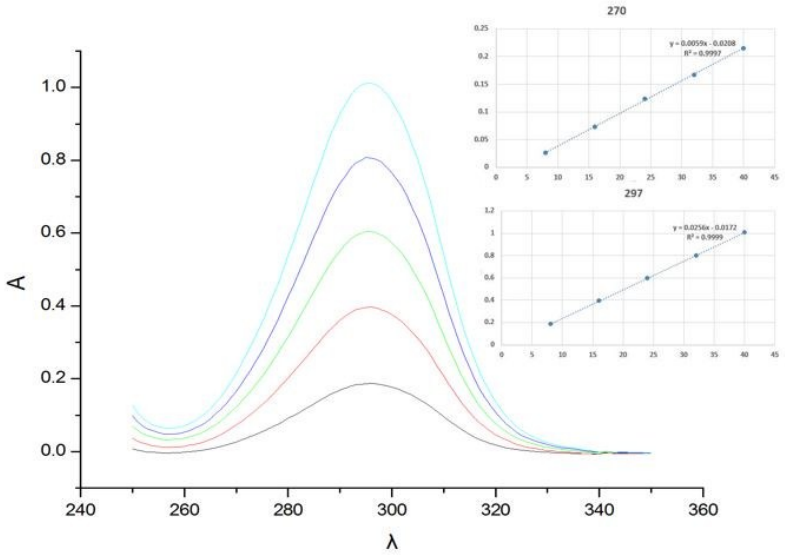

Fig.S13 The UV and standard curve of SA.

The measure about recovery

The absorbance value of mixture of SA and ASP is measured at 270 nm and 297nm, respectively. Then the recovery rate of SA and ASP is calculated by the equation 5 and 6. The results show that this test method is of high reliability, accurate, reproducible and easy (table S4 and S5).

Table S4 Recovery rate of ASP (100%)

SA(ug.ml^{-1})	ASP(ug.ml^{-1})		
	60	180	300
8	100.03	99.97	100.20
24	100.04	100.72	100.49
40	99.30	99.67	101.55
mean of ASP (100%)	99.91	100.12	100.75
SD	0.5529	0.5437	0.7114
RSD	0.5534	0.5430	0.7061
mean recovery rate of ASP (100%)		100.26	

Table S5 Recovery rate of SA (100%)

SA ($ug.ml^{-1}$)	ASP($ug.ml^{-1}$)		
	8	24	40
60	99.50	101.15	100.92
180	98.00	100.15	99.65
300	100.25	99.42	99.13
mean of ASP (100%)	99.25	100.24	99.90
SD	1.1456	0.8725	0.9243
RSD	1.1543	0.8704	0.9252
mean recovery rate of ASP (100%)		99.80	

Table S6 Concentration and conversation of SA at 70°C

Time (min)	C_{AS} ($mol \cdot L^{-1}$)	Conversion (%)	Ln C_{SA}	Ln($\Delta C_{SA}/\Delta t$)
5	2.670	38.60	0.98	-1.06
10	2.083	52.18	0.73	-2.14
15	1.735	60.25	0.55	-2.66
20	1.428	67.35	0.36	-2.79
25	1.257	71.32	0.23	-3.78
30	1.051	76.08	0.05	-3.19
35	0.920	79.11	-0.08	-3.64
40	0.785	82.20	-0.24	-3.62
45	0.656	85.16	-0.42	-3.66
50	0.591	86.66	-0.53	-4.34
55	0.508	88.55	-0.68	-4.10
60	0.478	89.26	-0.74	-5.10

Table S7 Concentration and conversation of SA at 75°C

Time (min)	C_{SA} ($mol \cdot L^{-1}$)	Conversion (%)	Ln C_{SA}	Ln($\Delta C_{SA}/\Delta t$)
5	2.202	49.36	0.79	-0.82
10	1.629	62.61	0.49	-2.17
15	1.201	72.49	0.18	-2.46
20	0.893	79.59	-0.11	-2.79
25	0.692	84.22	-0.37	-3.21
30	0.528	87.98	-0.64	-3.42
35	0.509	88.42	-0.67	-5.60
40	0.476	89.19	-0.74	-5.02
45	0.408	90.77	-0.90	-4.29
50	0.352	92.04	-1.04	-4.50
55	0.303	93.17	-1.19	-4.62
60	0.268	93.97	-1.32	-4.96

Table S8 Concentration and conversation of SA at 80°C

Time (min)	C_{SA} ($mol \cdot L^{-1}$)	Conversion (%)	Ln C_{SA}	Ln($\Delta C_{SA}/\Delta t$)
5	1.668	61.64	0.51	-0.60
10	1.367	68.62	0.31	-2.81
15	0.939	78.48	-0.06	-2.46
20	0.650	85.14	-0.43	-2.85
25	0.512	88.32	-0.67	-3.59
30	0.417	90.51	-0.88	-3.96
35	0.323	92.67	-1.13	-3.97
40	0.272	93.82	-1.30	-4.60
45	0.231	94.78	-1.47	-4.79
50	0.212	95.22	-1.55	-5.58
55	0.189	95.75	-1.67	-5.38
60	0.170	96.17	-1.77	-5.59

Table S9 Concentration and conversation of SA at 85°C

Time (min)	C_{SA} ($mol \cdot L^{-1}$)	Conversion (%)	Ln C_{SA}	Ln($\Delta C_{SA}/\Delta t$)
5	1.567	63.98	0.45	-0.57
10	0.793	81.80	-0.23	-1.59
15	0.490	88.77	-0.71	-2.80
20	0.296	93.23	-1.22	-3.25
25	0.236	94.62	-1.45	-4.41
30	0.197	95.51	-1.62	-4.87
35	0.179	95.93	-1.72	-5.63
40	0.170	96.13	-1.77	-6.34
45	0.164	96.30	-1.81	-6.59
50	0.154	96.53	-1.87	-6.21
55	0.150	96.63	-1.90	-7.12
60	0.147	96.70	-1.92	-7.40