Supporting information

Methods for Predicting Ethylene/cyclic Copolymerization Rates promoted by Single-sight Metallocene: Kinetics is the Key

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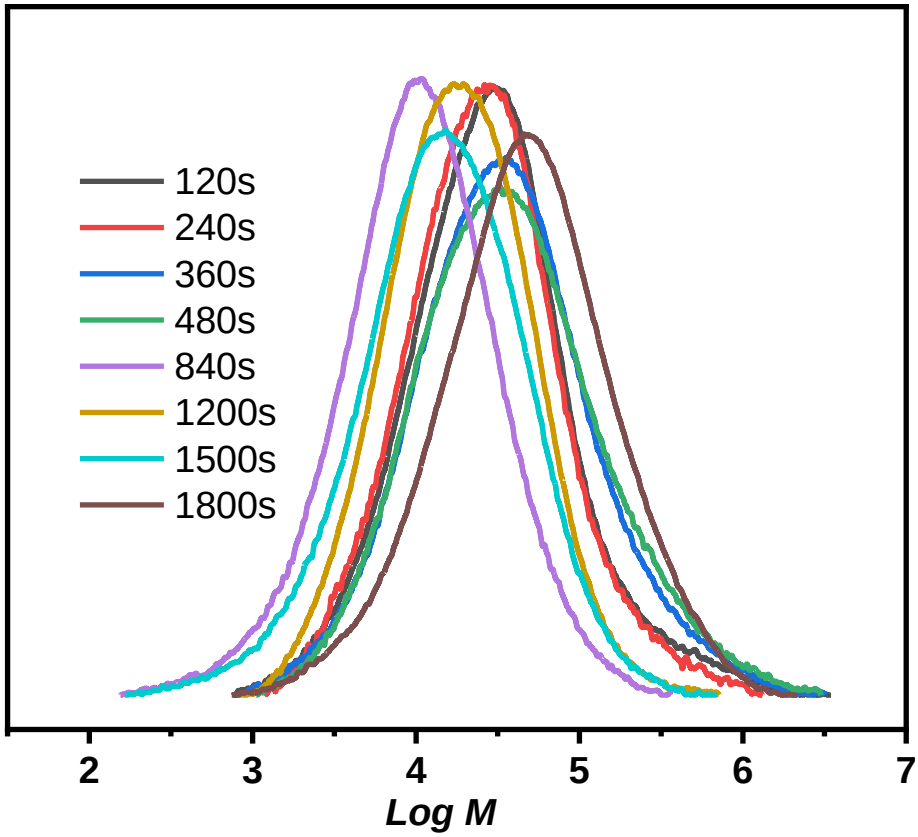
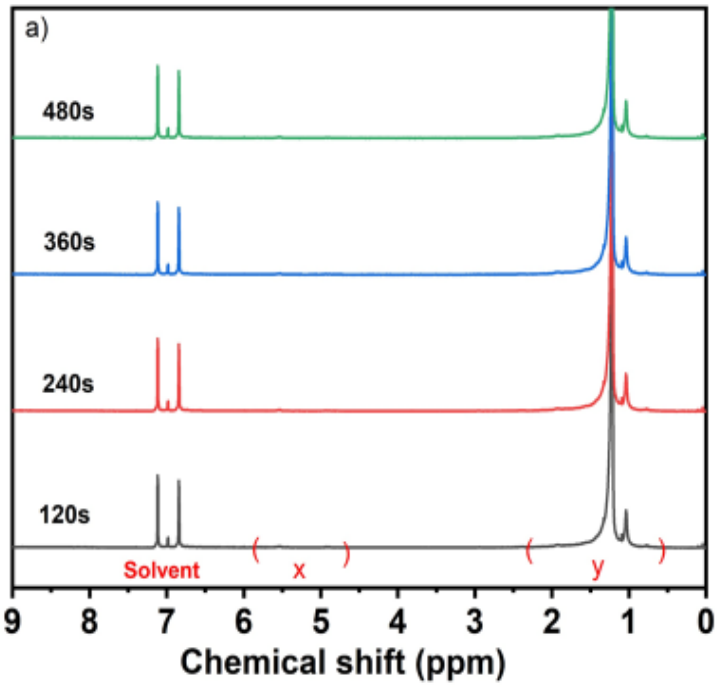
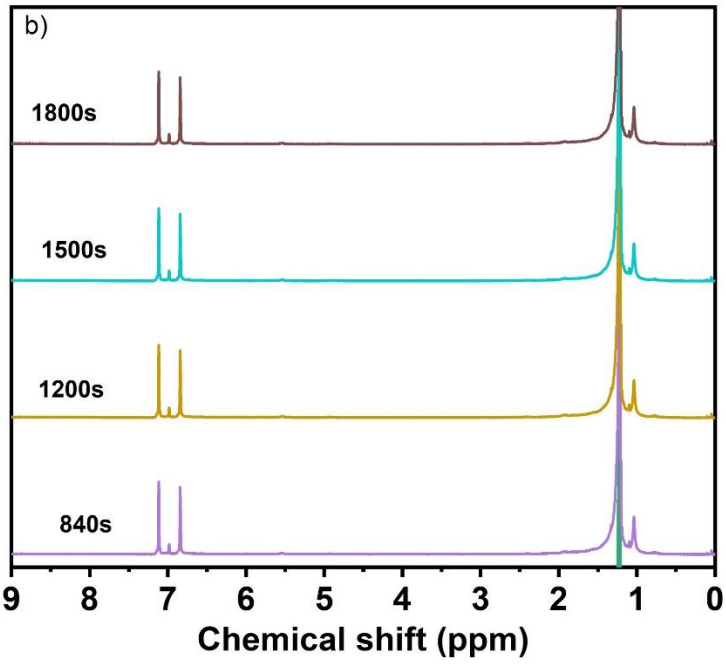


Figure S1. Change of molecular distribution of E/VCH copolymers with polymerization time


a)
480s
360s
240s
120s
Solvent
x
y
9
8
7
6
5
4
3
2
1
0
Chemical shift (ppm)


b)
1800s
1500s
1200s
840s
9
8
7
6
5
4
3
2
1
0
Chemical shift (ppm)

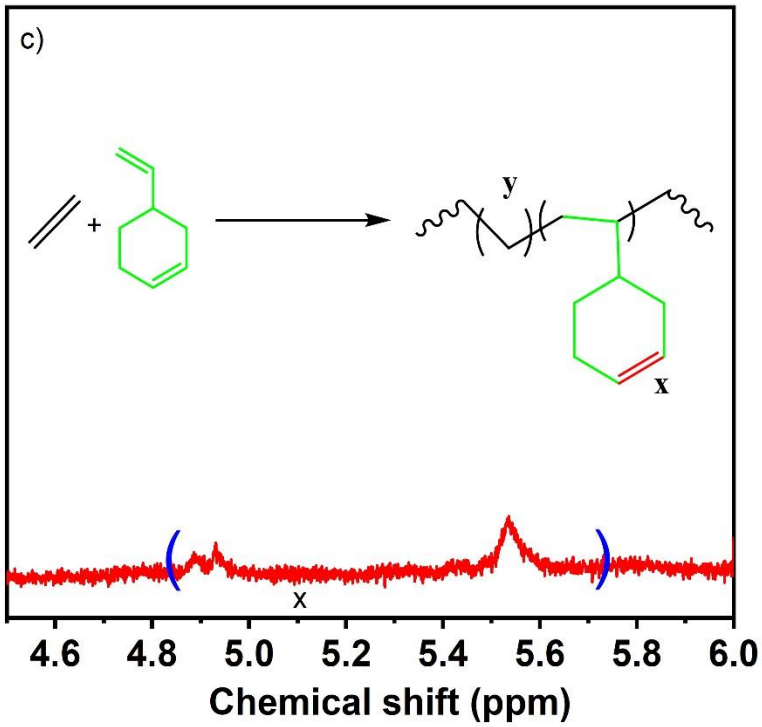
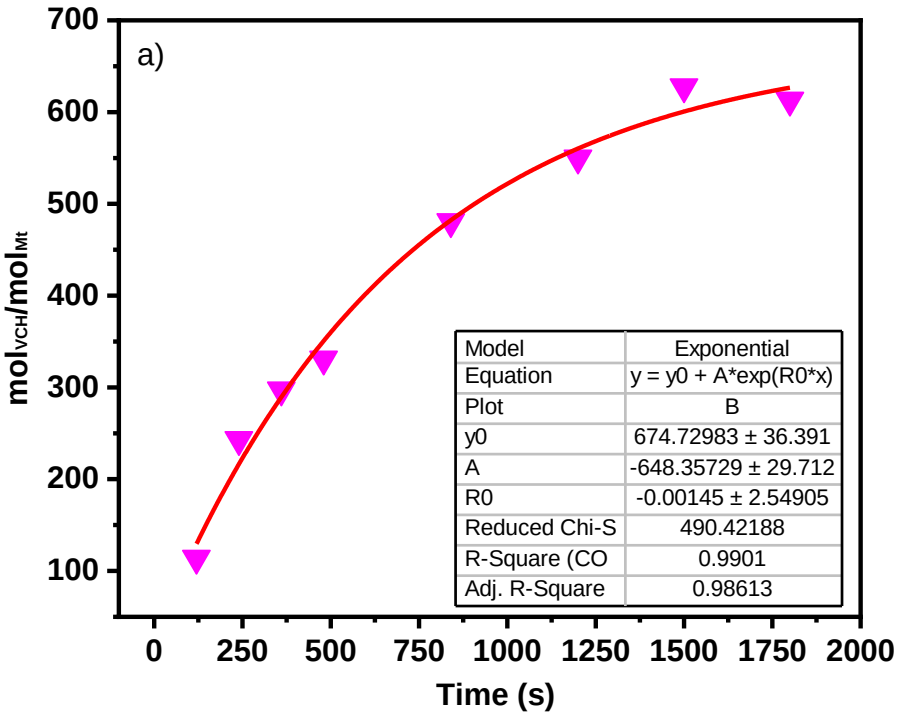


Figure S2 HNMR Spectra's of the E/VCH copolymer

Table S1 Calculation of R_P^{VCH} and K_P^{VCH} in the ethylene-VNB copolymerization.

RUN	Time see	VCH In polymer	VCH in Pol wt%	Mol_{VCH}/mol_{cat}	R_P^{VCH}/mol_{cat} molVNB/molcats	S Ppm	*C %	[VCH] mol/L	*kp* VCH L/mols
1.1	120	1.43	0.053	114	0.78	14.23	14.72	0.0572	93
1.2	240	1.56	0.058	243	0.66	12.63	25.68	0.0539	48
1.3	360	1.65	0.061	297	0.55	16.09	37.89	0.0526	28
1.4	480	1.53	0.057	331	0.46	19.97	49.16	0.0517	18.1
1.5	840	1.46	0.054	481	0.27	14.31	61.27	0.0480	9.18
1.6	1200	1.41	0.052	550	0.16	13.06	66.17	0.0463	5.228
1.7	1500	1.35	0.050	628	0.1	11.54	69.58	0.0443	3.244
1.8	1800	1.22	0.046	613	0.069	11.30	73.38	0.0447	2.1048


a)
700
600
500
400
300
200
100
0
250
500
750
1000
1250
1500
1750
2000
Time (s)
molVCH/molMt
Model | Exponential
Equation | y = y0 + A*exp(R0*x)
Plot | B
y0 | 674.72983 ± 36.391
A | -648.35729 ± 29.712
R0 | -0.00145 ± 2.54905
Reduced Chi-S | 490.42188
R-Square (CO | 0.9901
Adj. R-Square | 0.98613

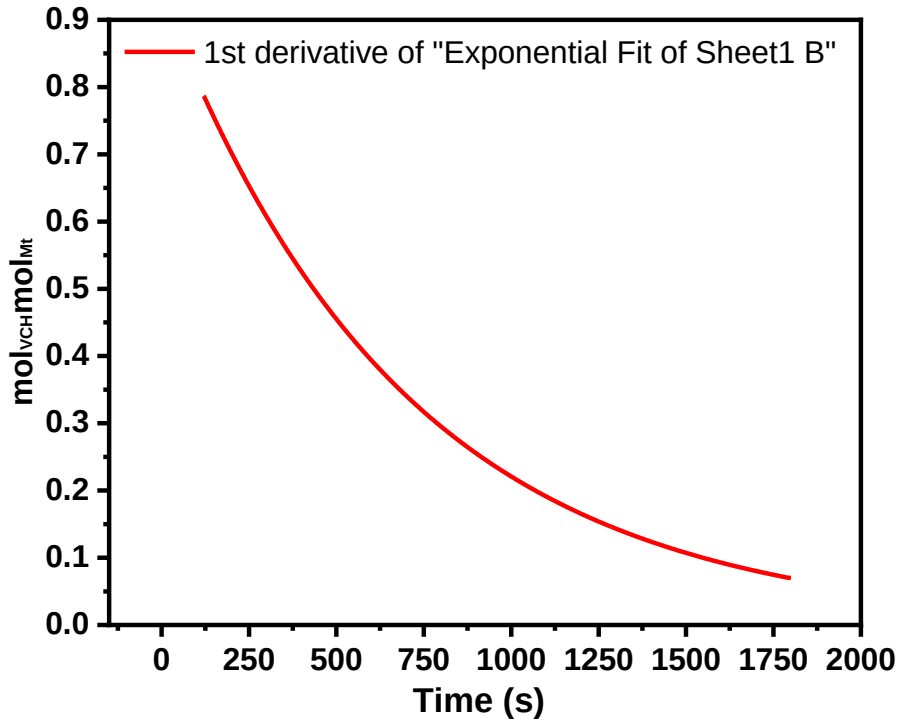
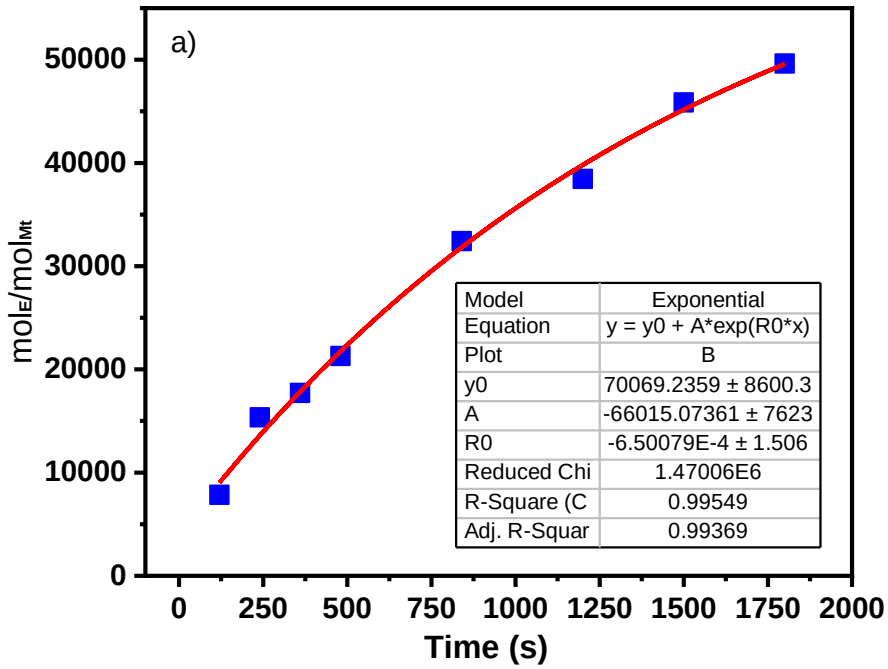

1st derivative of "Exponential Fit of Sheet1 B"
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
0
250
500
750
1000
1250
1500
1750
2000
Time (s)
molVCHmolMt

Figure S3.The plot of mol_{VCH}/mol_{cat} vs. time, and Differentiate.

Table S2. Calculation of R_P^E and K_P^E in the ethylene-VCH copolymerization.

RUN	Time see	VCH In polymer	VCH In Pol wt%	S Ppm	*C %	mE g	mol_E/mol_{cat}	R_P^E molE/molcat s	*kp* E L/mol s
1.1	120	1.43	0.053	14.23	14.72	0.275	7846	39.63	6410
1.2	240	1.56	0.058	12.63	25.68	0.537	15347	36.72	3405
1.3	360	1.65	0.061	16.09	37.89	0.620	17710	33.94	2133
1.4	480	1.53	0.057	19.97	49.16	0.745	21294	31.41	1521
1.5	840	1.46	0.054	14.31	61.27	1.135	32431	24.86	966
1.6	1200	1.41	0.052	13.06	66.17	1.346	38449	19.67	708
1.7	1500	1.35	0.050	11.54	69.58	1.605	45863	16.17	553
1.8	1800	1.22	0.046	11.30	73.38	1.737	49634	13.32	432



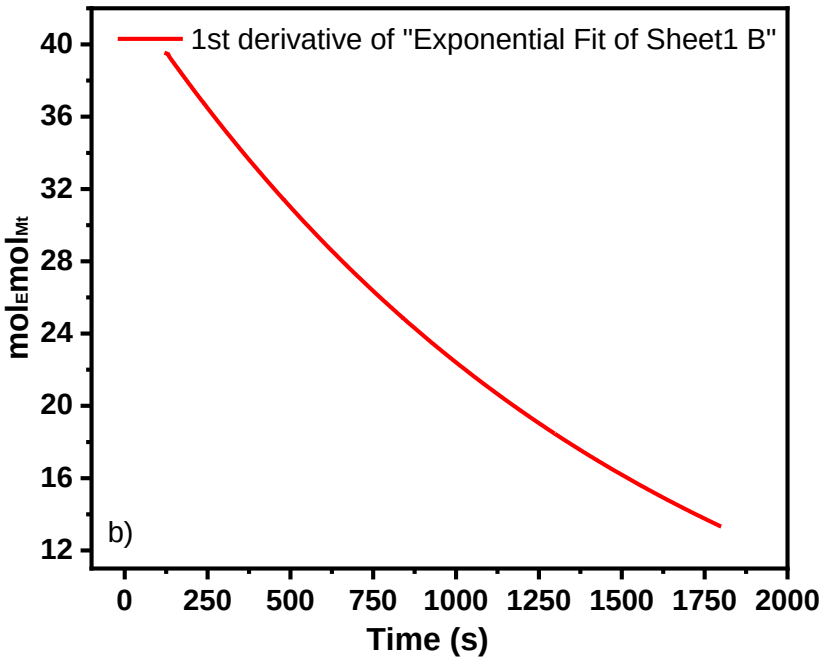


Figure S4.The plot of mol_E/mol_{cat} vs. time, and Differentiate