Upgrading Process of 4-Methylanisole as a Lignin-Derived Bio-Oil Catalyzed by Pt/γ-Al_2O_3: Kinetic Investigation and Reaction Network Development

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This document includes the following Table and Figures:

Table S-1: Overall mass balance closure data.

Figure S-1: Selectivity for the formation of the following products in the conversion of 4-methylanisole catalyzed by Pt/γAl_2O_3 in the presence of H_2 at T = 623 K and P = 8 bar. Data for each main product were fitted with a straight line and extrapolated to zero conversion; intercepts of regression lines significantly different from zero selectivity at zero conversion indicate primary products.

Figure S-2: Selectivity for the formation of the following products in the conversion of 4-methylanisole catalyzed by Pt/γAl_2O_3 in the presence of H_2 at T = 673 K and P = 8

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bar. Data for each main product were fitted with a straight line and extrapolated to zero conversion; intercepts of regression lines significantly different from zero selectivity at zero conversion indicate primary products.

Figure S-3: Conversion to each of the main products as a function of inverse space velocity at 623 K and 8 bar; the term X_i represents the conversion to product i.

Figure S-4: Conversion to each of the main products as a function of inverse space velocity at 673 K and 8 bar; the term X_i represents the conversion to product i.

Figure S-5: Conversion of 4-methylanisole in the presence of H_2 at T=623 K and P=8 bar to give main products, where X_i is conversion of 4-methylanisole on a logarithmic scale.

Figure S-6: Conversion of 4-methylanisole in the presence of H_2 at T=673 K and P=8 bar to give main products, where X_i is conversion of 4-methylanisole on a logarithmic scale.

Table S-1

Experiment number	Mass balance closure (%)	Time on stream (min)	Liquid flow rate (mL/min)	Mass of liquid fed (g)	Mass of liquid collected from condenser (g)	Mass of reactant leaving condenser as vapor (g)	Approximate mass of liquid remaining in condenser (g)
1	97.56	150	0.1	14.54	12.97	0.21	1
2	98.04	150	0.1	14.54	13.02	0.23	1
3	97.49	150	0.1	14.54	12.98	0.19	1
4	99.90	150	0.1	14.54	13.29	0.23	1
5	98.86	150	0.1	14.54	13.15	0.22	1
6	96.80	150	0.1	14.54	12.87	0.2	1
7	100.38	150	0.1	14.54	13.38	0.21	1
8	97.81	180	0.05	8.72	7.38	0.15	1
9	98.38	180	0.05	8.72	7.43	0.15	1
10	97.24	180	0.05	8.72	7.35	0.13	1
11	99.87	180	0.05	8.72	7.57	0.14	1
12	98.73	180	0.05	8.72	7.46	0.15	1
13	99.07	180	0.05	8.72	7.49	0.15	1
14	95.98	180	0.05	8.72	7.21	0.16	1
15	97.24	180	0.05	8.72	7.34	0.14	1
16	98.61	360	0.03	10.47	9.16	0.16	1
17	97.94	360	0.03	10.47	9.08	0.17	1
18	98.71	360	0.03	10.47	9.16	0.17	1
19	97.94	360	0.03	10.47	9.09	0.16	1
20	100.24	360	0.03	10.47	9.31	0.18	1

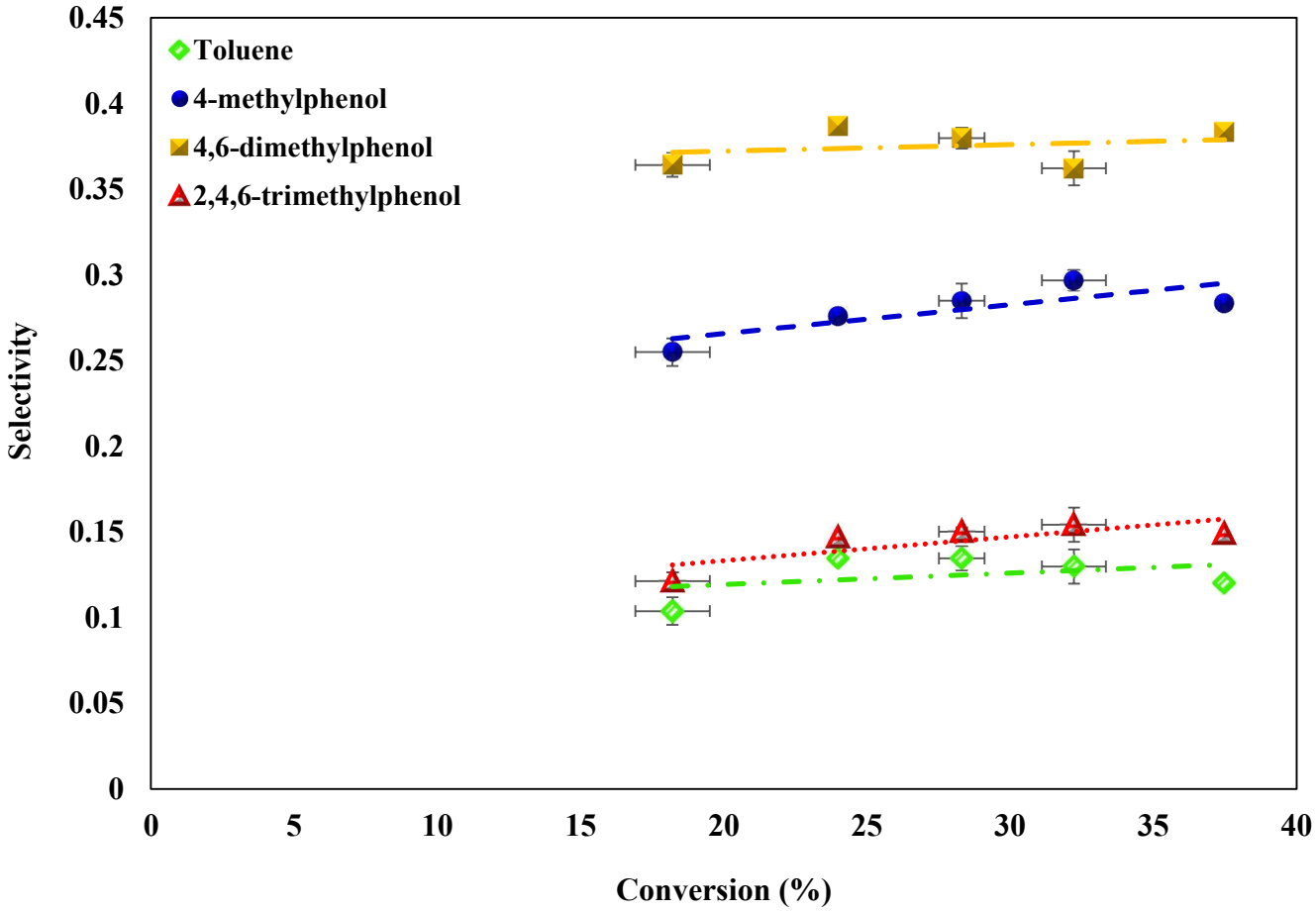
Toluene
4-methylphenol
4,6-dimethylphenol
2,4,6-trimethylphenol
Selectivity
0.45
0.4
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
0
5
10
15
20
25
30
35
40
Conversion (%)

Figure S-1(a)

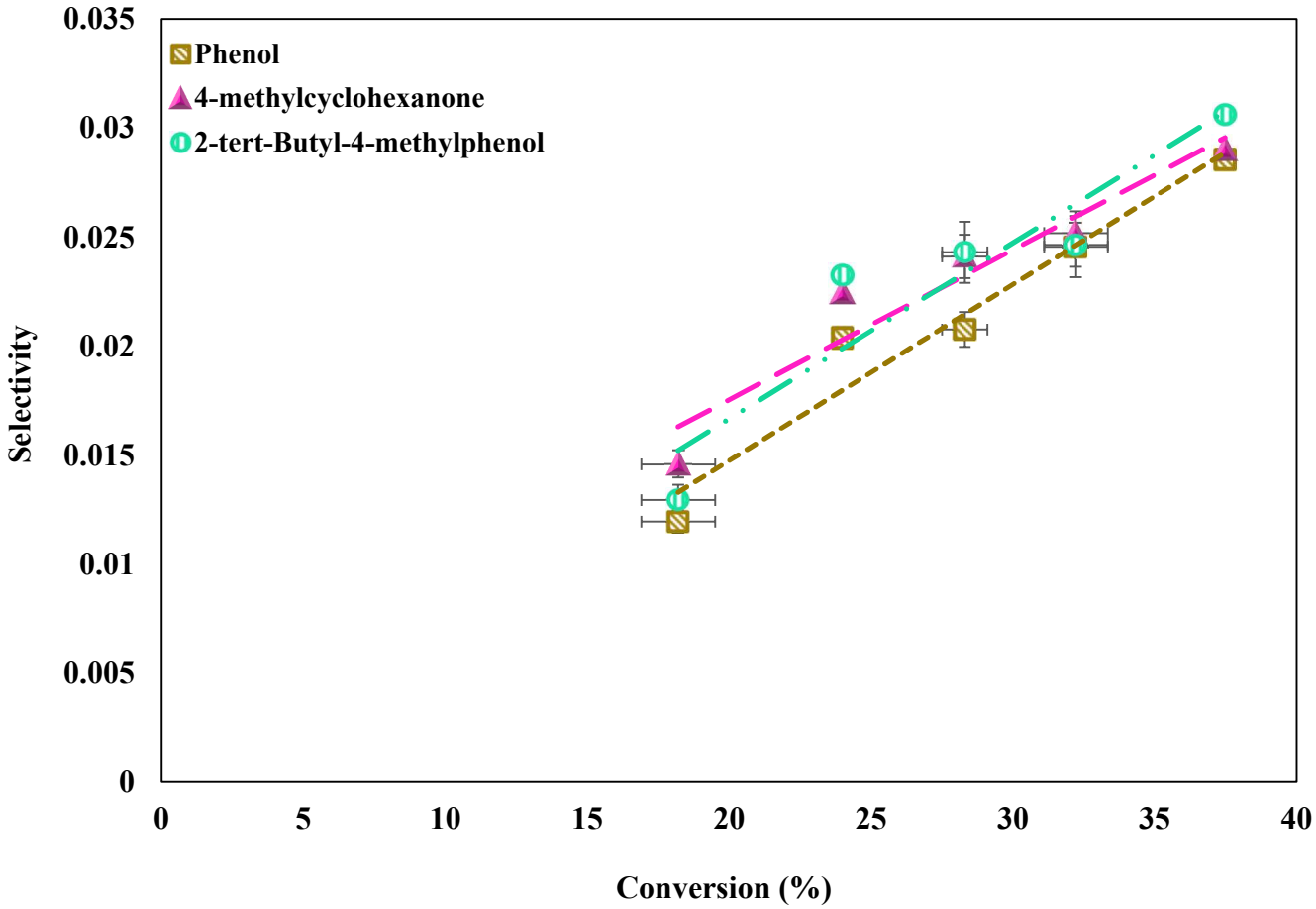
Phenol
4-methylcyclohexanone
2-tert-Butyl-4-methylphenol
Selectivity
0.035
0.03
0.025
0.02
0.015
0.01
0.005
0
0
5
10
15
20
25
30
35
40
Conversion (%)

Figure S-1(b)

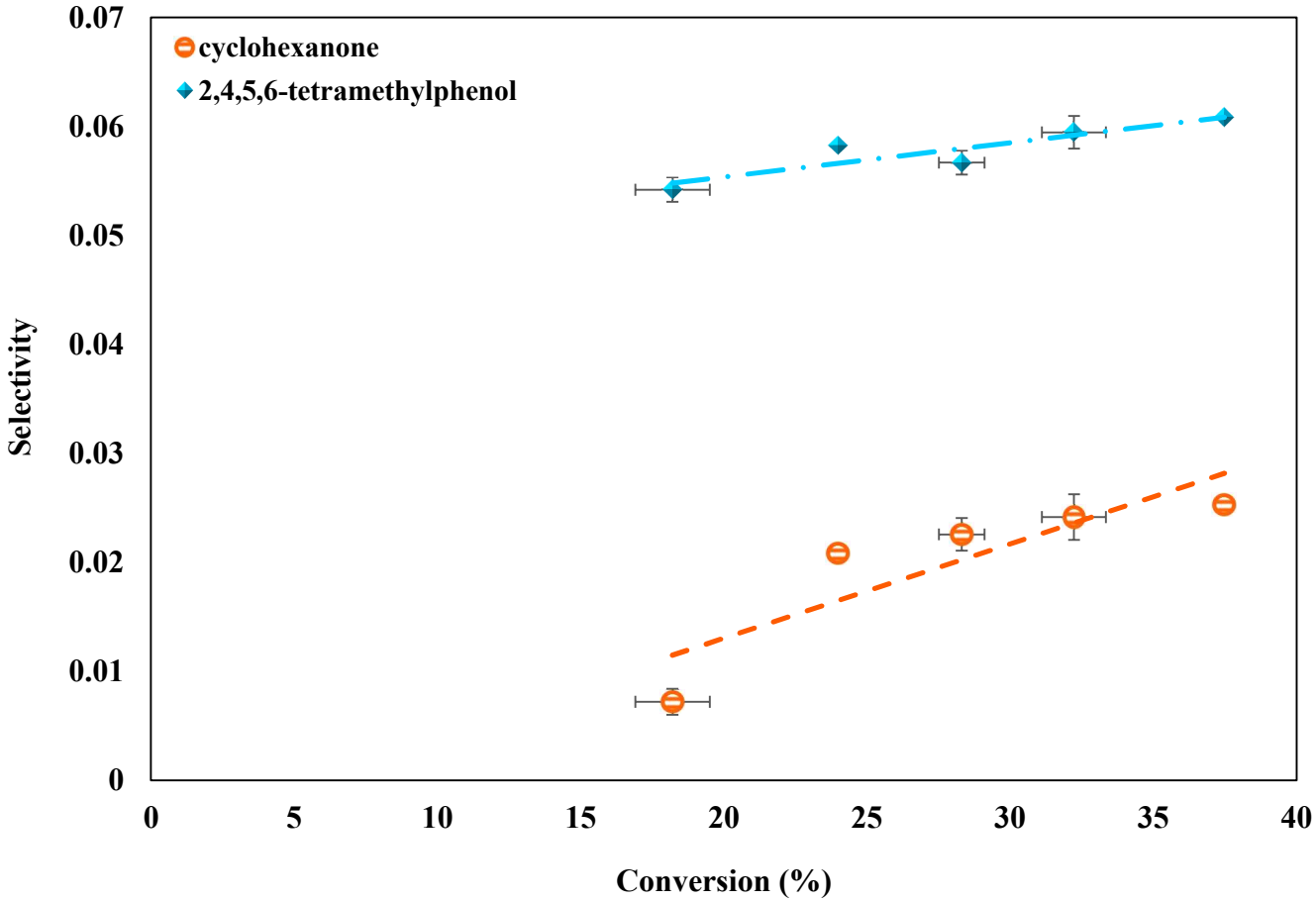
cyclohexanone
2,4,5,6-tetramethylphenol
Selectivity
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0
0
5
10
15
20
25
30
35
40
Conversion (%)

Figure S-1(c)

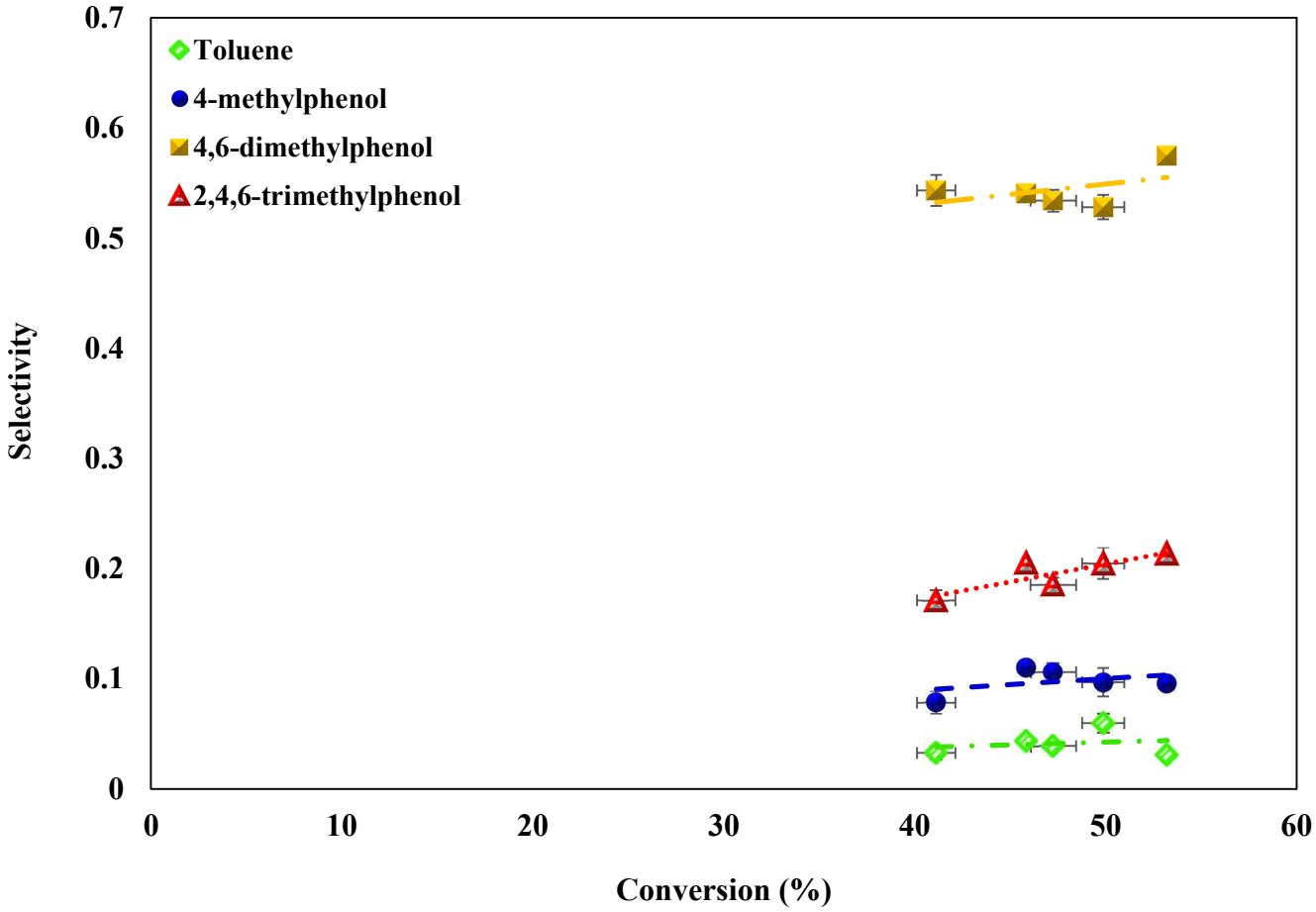
Toluene
4-methylphenol
4,6-dimethylphenol
2,4,6-trimethylphenol
Selectivity
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0
10
20
30
40
50
60
Conversion (%)

Figure S-2(a)

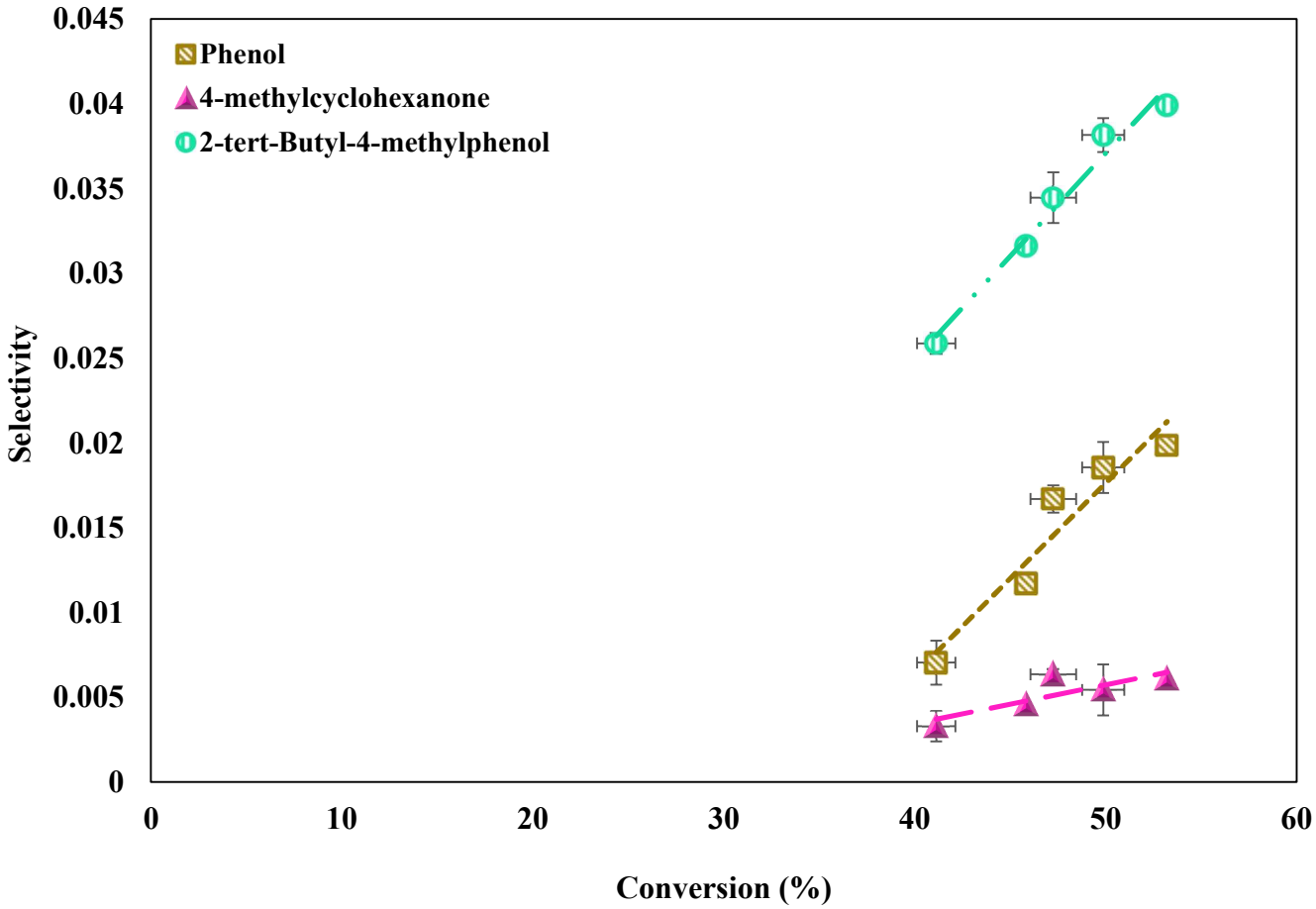
Phenol
4-methylcyclohexanone
2-tert-Butyl-4-methylphenol
Selectivity
0.045
0.04
0.035
0.03
0.025
0.02
0.015
0.01
0.005
0
0
10
20
30
40
50
60
Conversion (%)

Figure S-2(b)

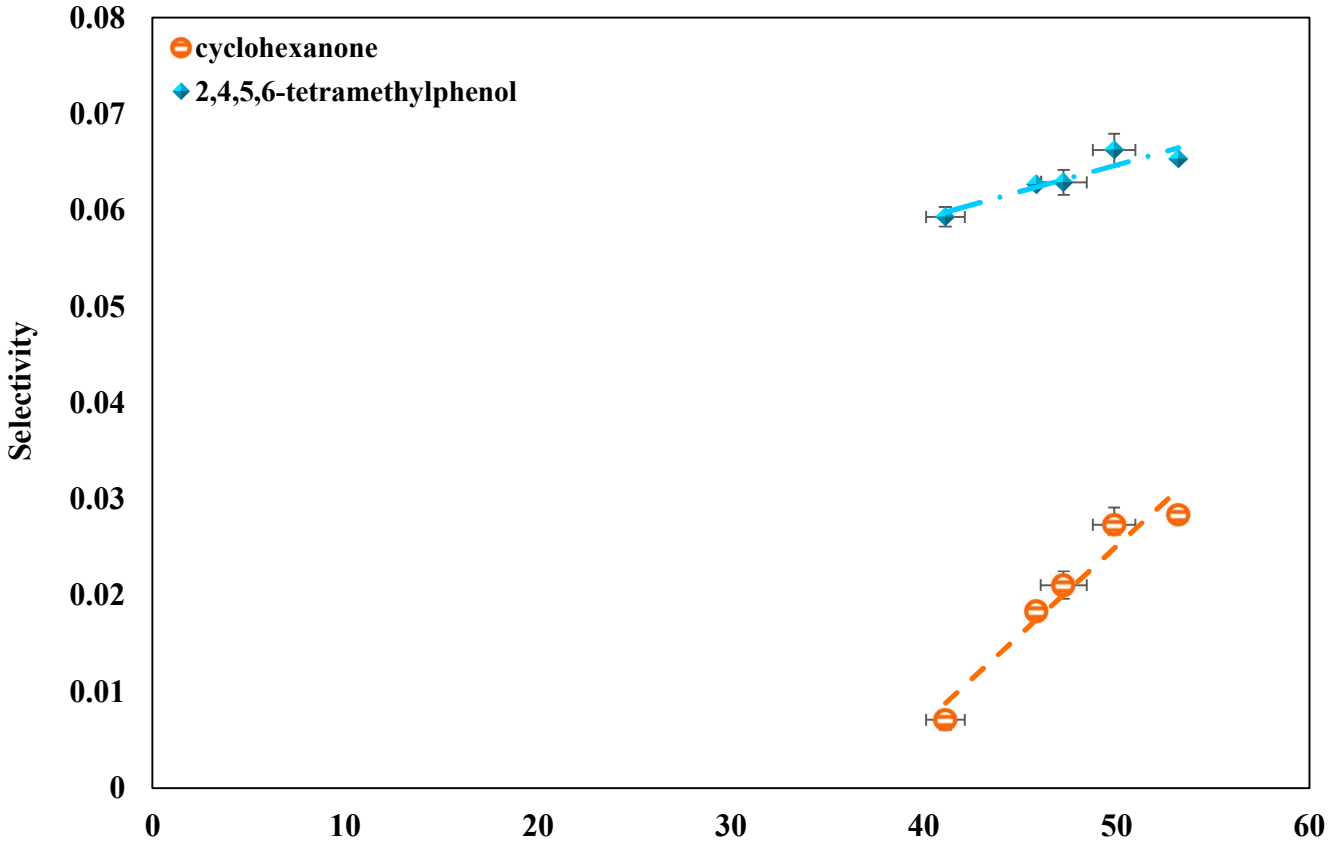
cyclohexanone
2,4,5,6-tetramethylphenol
Selectivity
0.08
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0
0
10
20
30
40
50
60
Conversion (%)

Figure S-2(c)

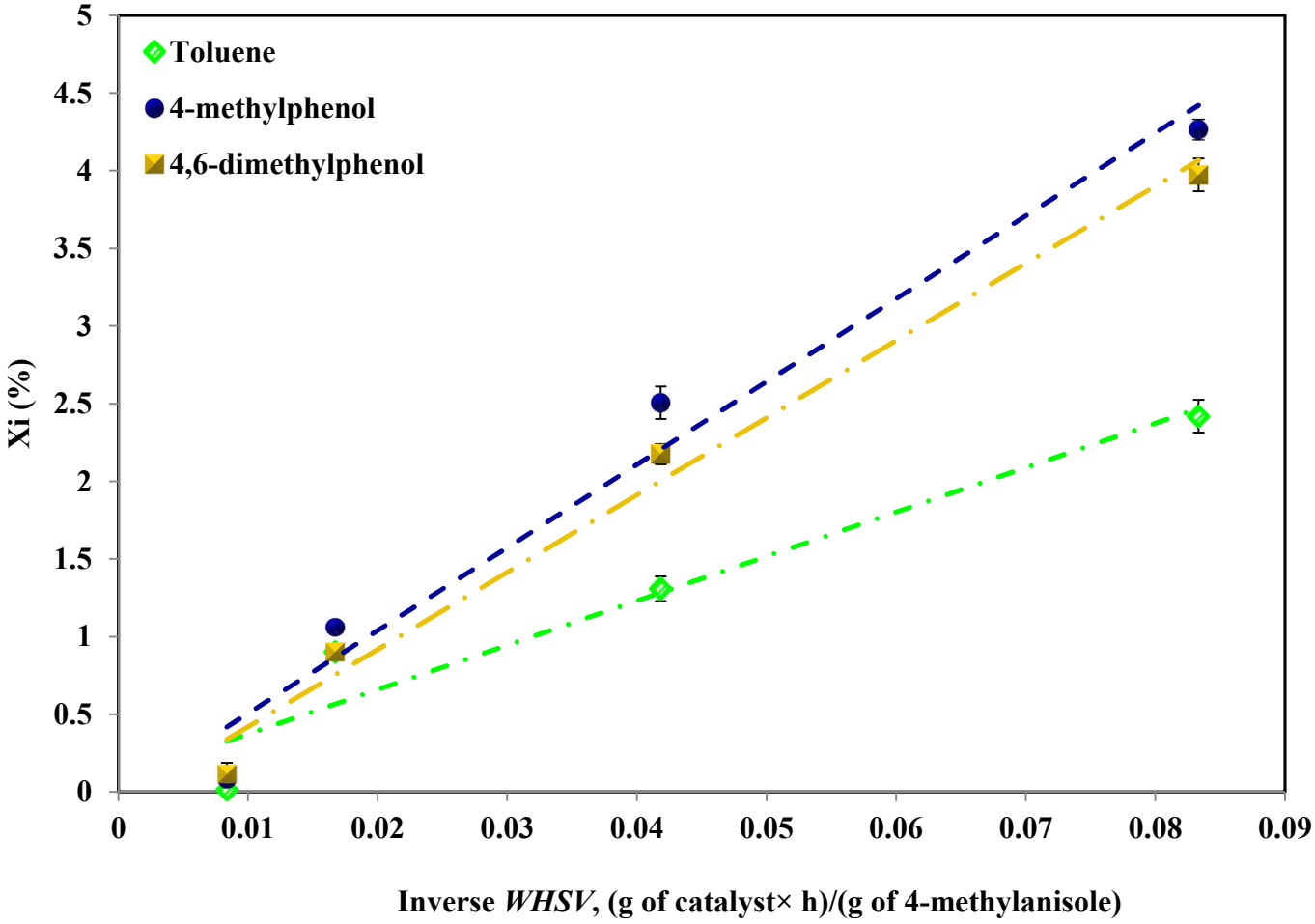
Toluene
4-methylphenol
4,6-dimethylphenol
Xi (%)
0
0.5
1
1.5
2
2.5
3
3.5
4
4.5
5
0
0.01
0.02
0.03
0.04
0.05
0.06
0.07
0.08
0.09
Inverse *WHSV*, (g of catalyst× h)/(g of 4-methylanisole)

Figure S-3(a)

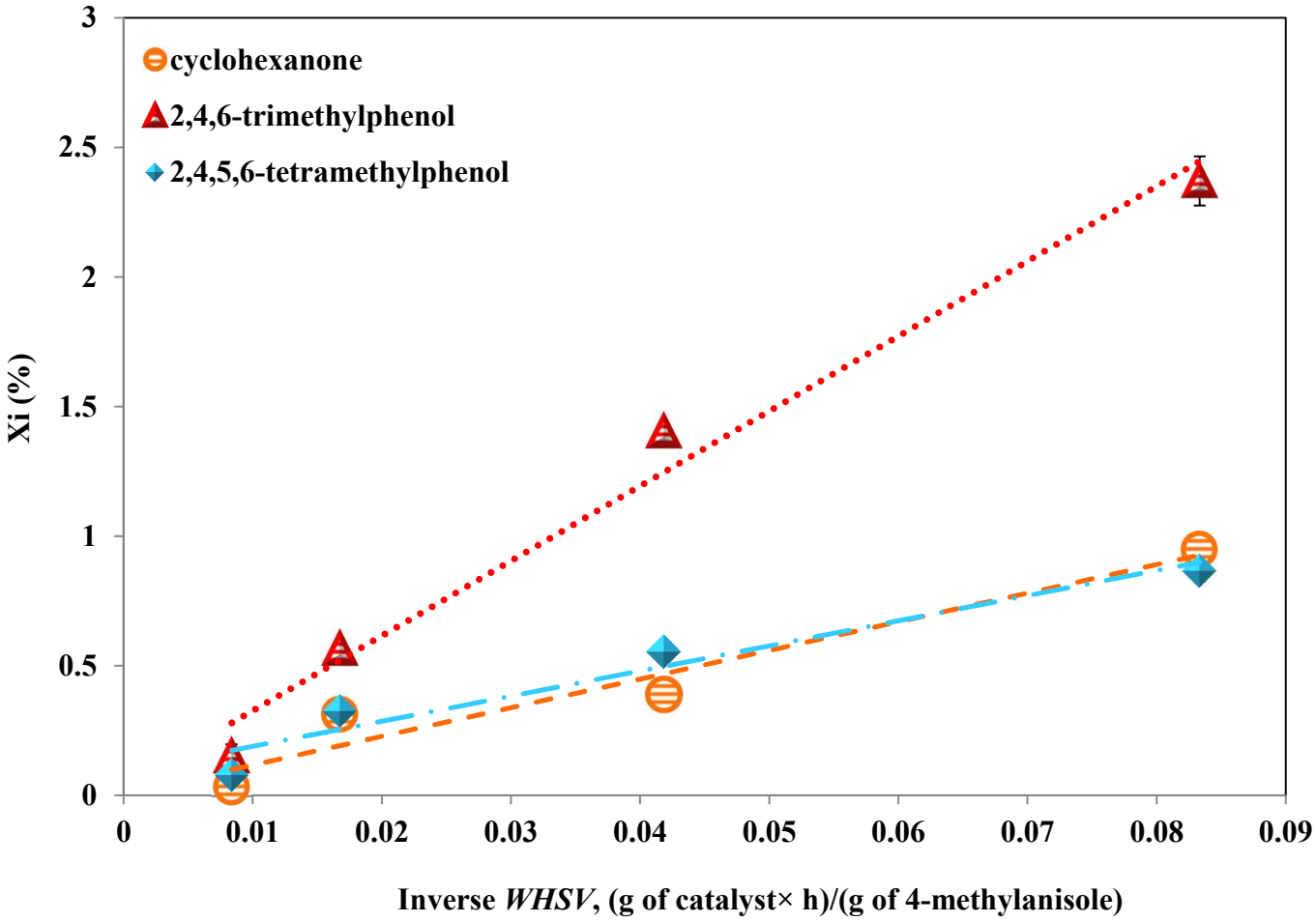
cyclohexanone
2,4,6-trimethylphenol
2,4,5,6-tetramethylphenol
Xi (%)
3
2.5
2
1.5
1
0.5
0
0
0.01
0.02
0.03
0.04
0.05
0.06
0.07
0.08
0.09
Inverse *WHSV*, (g of catalyst× h)/(g of 4-methylanisole)

Figure S-3(b)

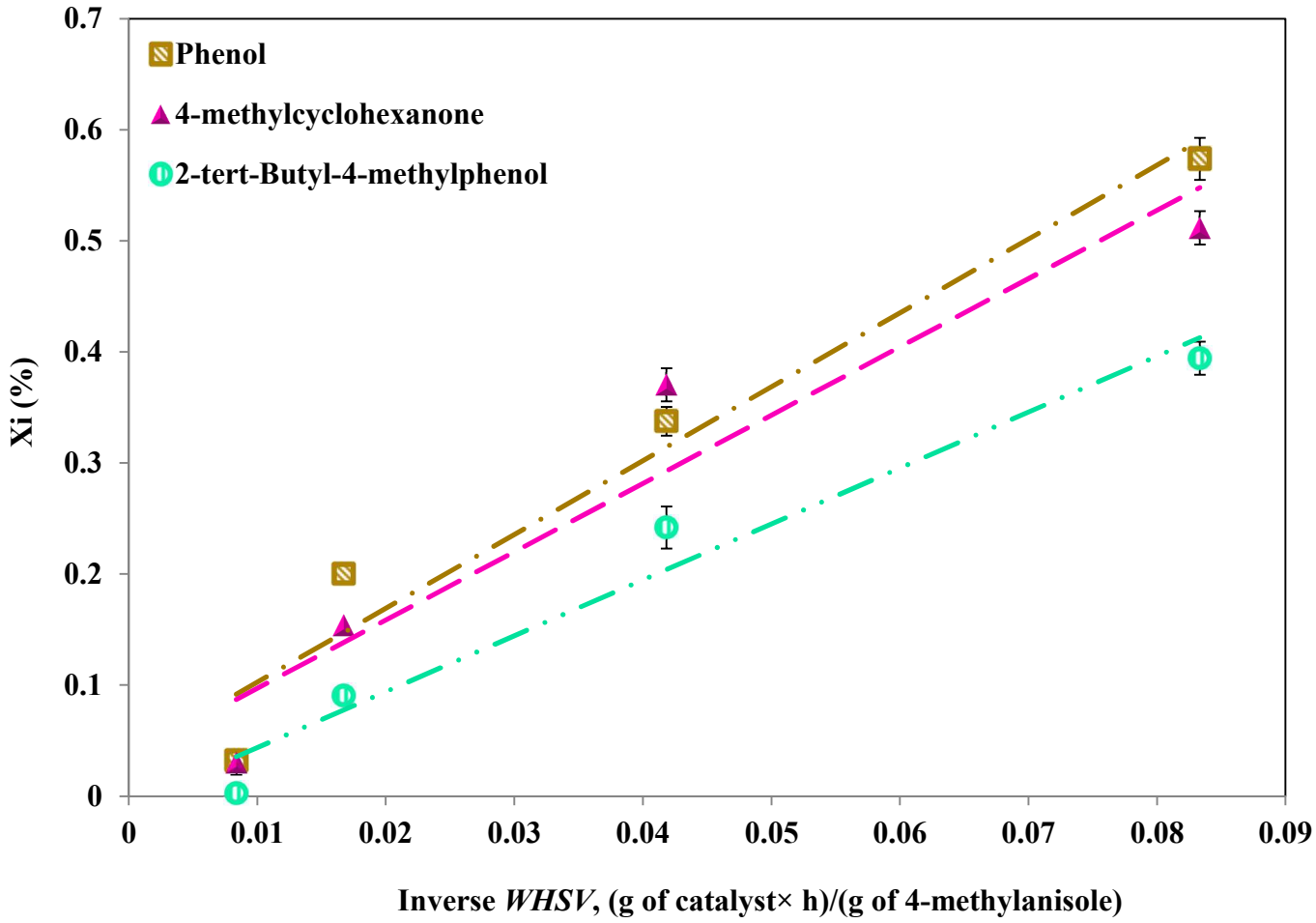
Phenol
4-methylcyclohexanone
2-tert-Butyl-4-methylphenol
Xi (%)
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0
0.01
0.02
0.03
0.04
0.05
0.06
0.07
0.08
0.09
Inverse *WHSV*, (g of catalyst× h)/(g of 4-methylanisole)

Figure S-3(c)

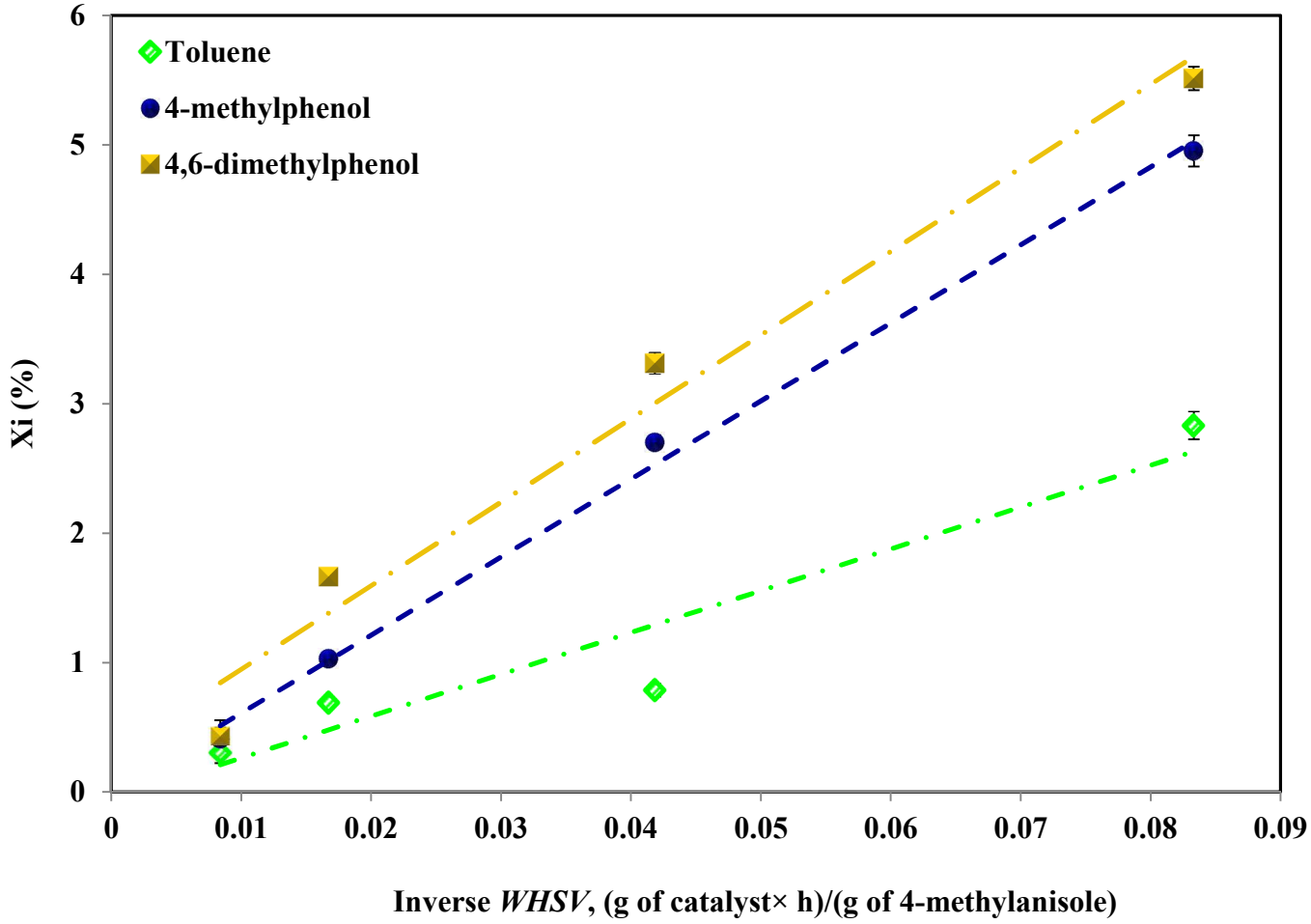
Toluene
4-methylphenol
4,6-dimethylphenol
Xi (%)
0
1
2
3
4
5
6
0
0.01
0.02
0.03
0.04
0.05
0.06
0.07
0.08
0.09
Inverse *WHSV*, (g of catalyst× h)/(g of 4-methylanisole)

Figure S-4(a)

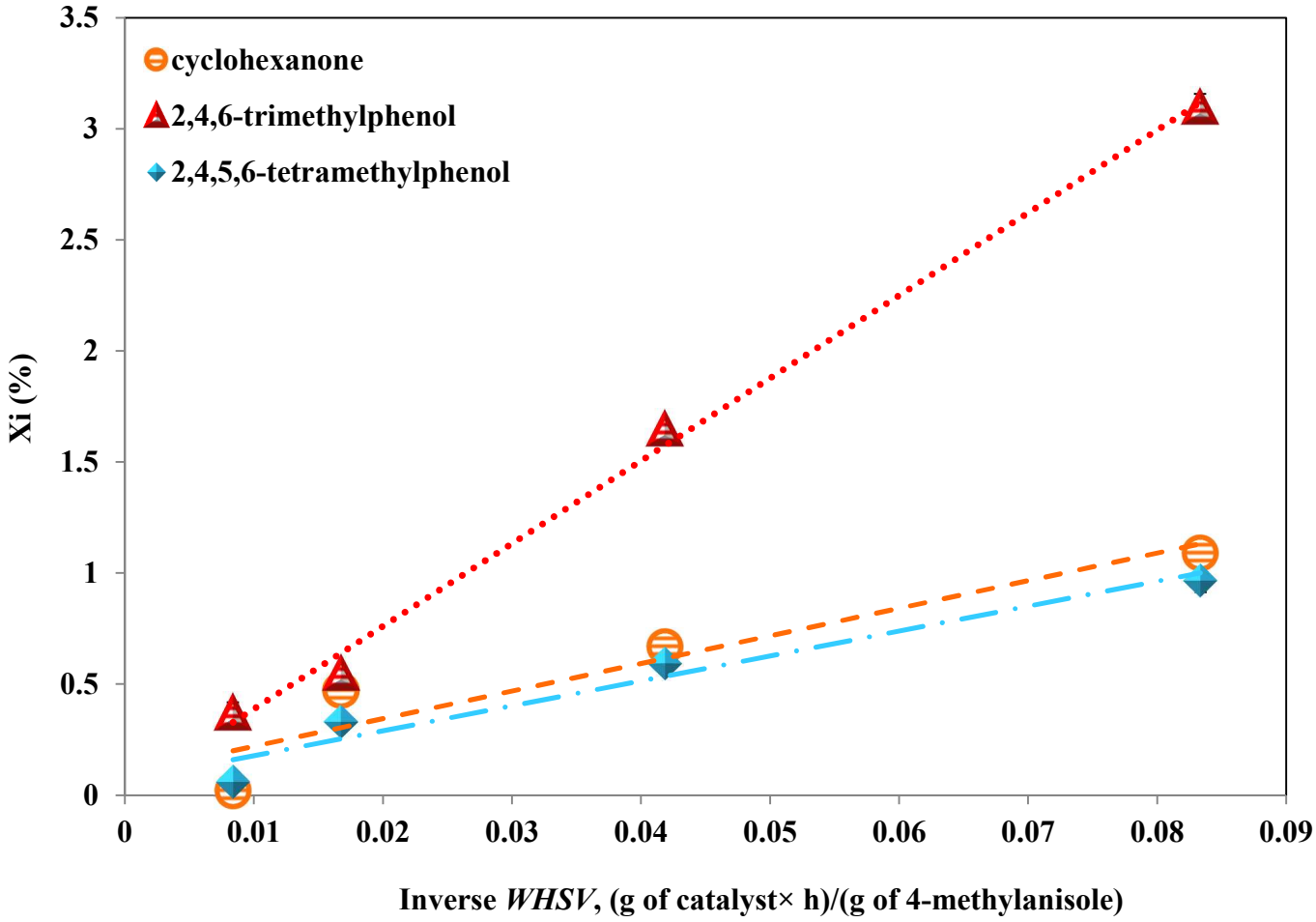
cyclohexanone
2,4,6-trimethylphenol
2,4,5,6-tetramethylphenol
Xi (%)
3.5
3
2.5
2
1.5
1
0.5
0
0
0.01
0.02
0.03
0.04
0.05
0.06
0.07
0.08
0.09
Inverse *WHSV*, (g of catalyst× h)/(g of 4-methylanisole)

Figure S-4(b)

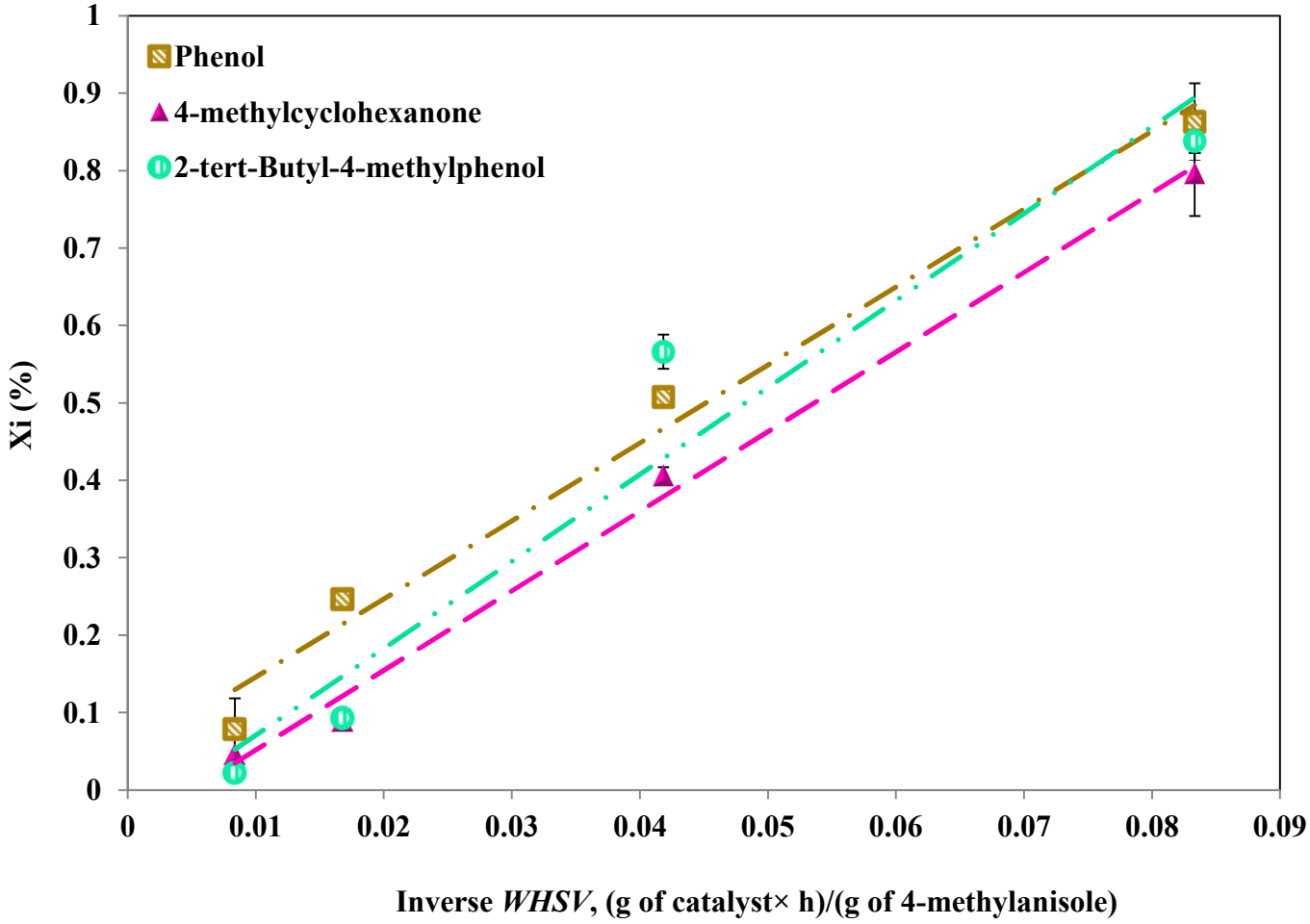
Phenol
4-methylcyclohexanone
2-tert-Butyl-4-methylphenol
Xi (%)
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0
0.01
0.02
0.03
0.04
0.05
0.06
0.07
0.08
0.09
Inverse *WHSV*, (g of catalyst× h)/(g of 4-methylanisole)

Figure S-4(c)

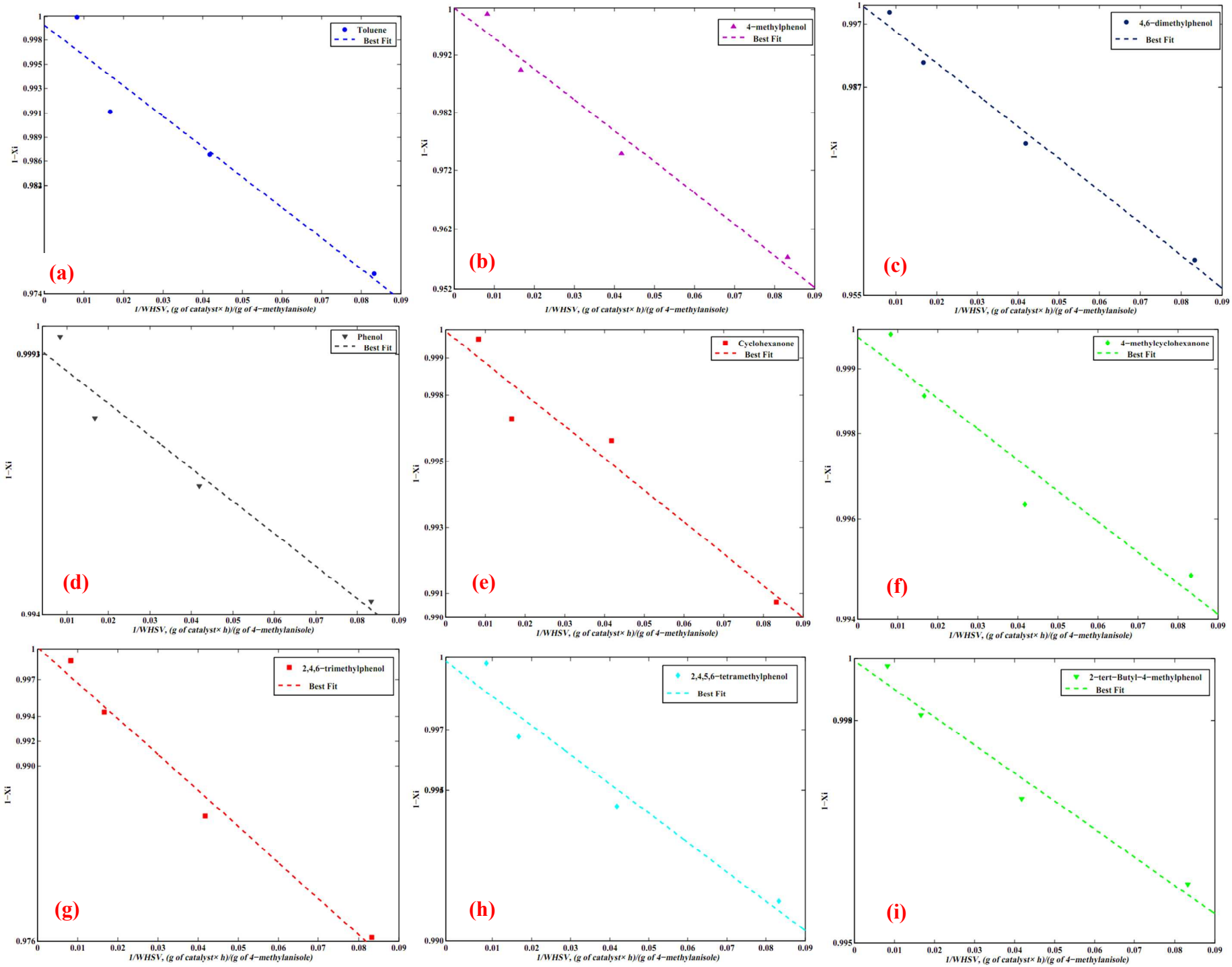
(a)
Toluene
Best Fit
(b)
4−methylphenol
Best Fit
(c)
4,6−dimethylphenol
Best Fit
(d)
Phenol
Best Fit
(e)
Cyclohexanone
Best Fit
(f)
4−methylcyclohexanone
Best Fit
(g)
2,4,6−trimethylphenol
Best Fit
(h)
2,4,5,6−tetramethylphenol
Best Fit
(i)
2−tert−Butyl−4−methylphenol
Best Fit
1−Xi
1/WHSV, (g of catalyst× h)/(g of 4−methylanisole)

Figure S-5

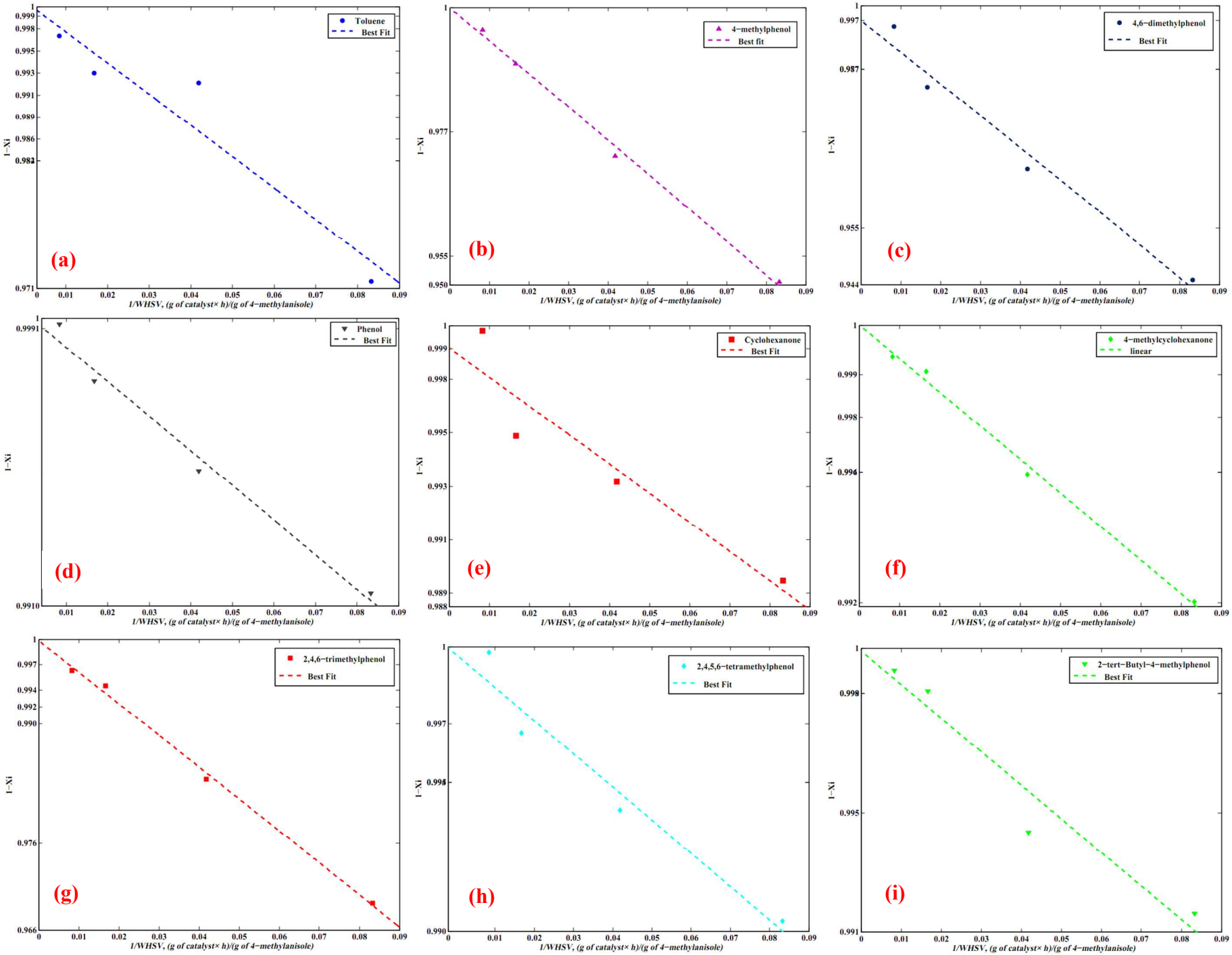
(a)
Toluene
Best Fit
(b)
4−methylphenol
Best fit
(c)
4,6−dimethylphenol
Best Fit
(d)
Phenol
Best Fit
(e)
Cyclohexanone
Best Fit
(f)
4−methylcyclohexanone
linear
(g)
2,4,6−trimethylphenol
Best Fit
(h)
2,4,5,6−tetramethylphenol
Best Fit
(i)
2−tert−Butyl−4−methylphenol
Best Fit
1−Xi
1/WHSV, (g of catalyst× h)/(g of 4−methylanisole)

Figure S-6