Copper(II) induced oxidative modification and complexation of a Schiff base Ligand: synthesis, crystal structure, catalytic oxidation of aromatic hydrocarbons and DFT calculation†

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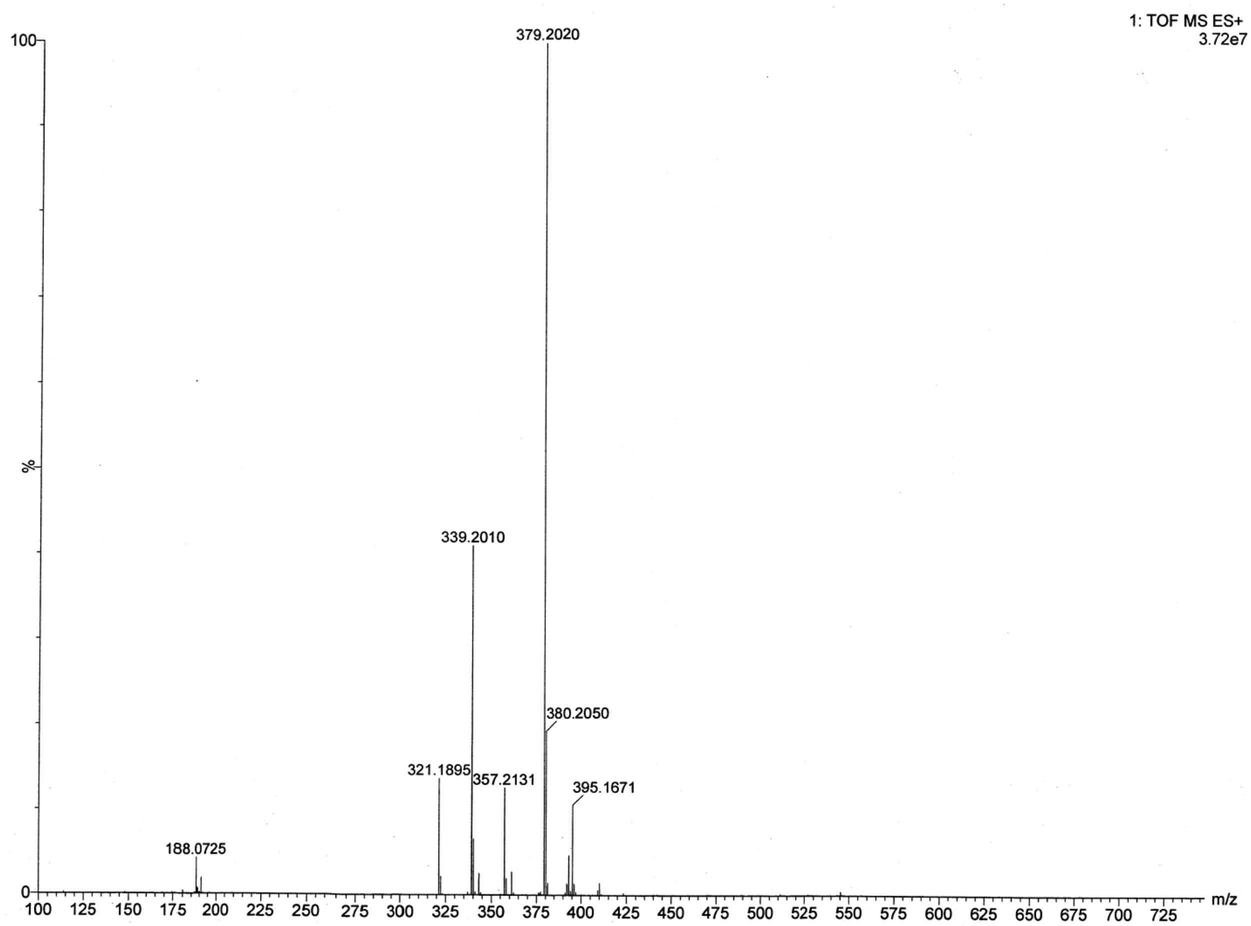


Fig.S1HRMS spectra of [H_2L^a].

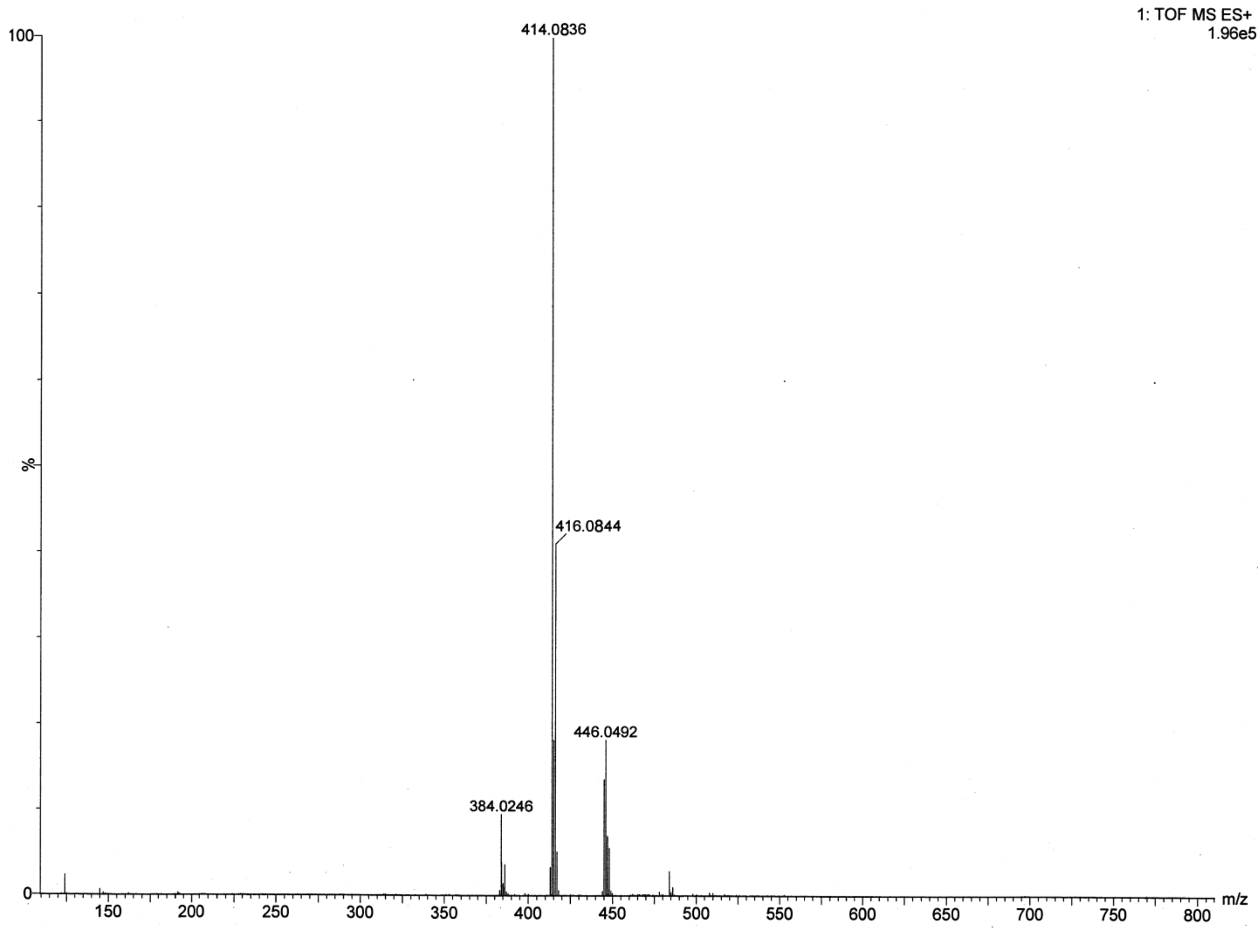


Fig.S2 HRMS spectra of [Cu(L^f)].

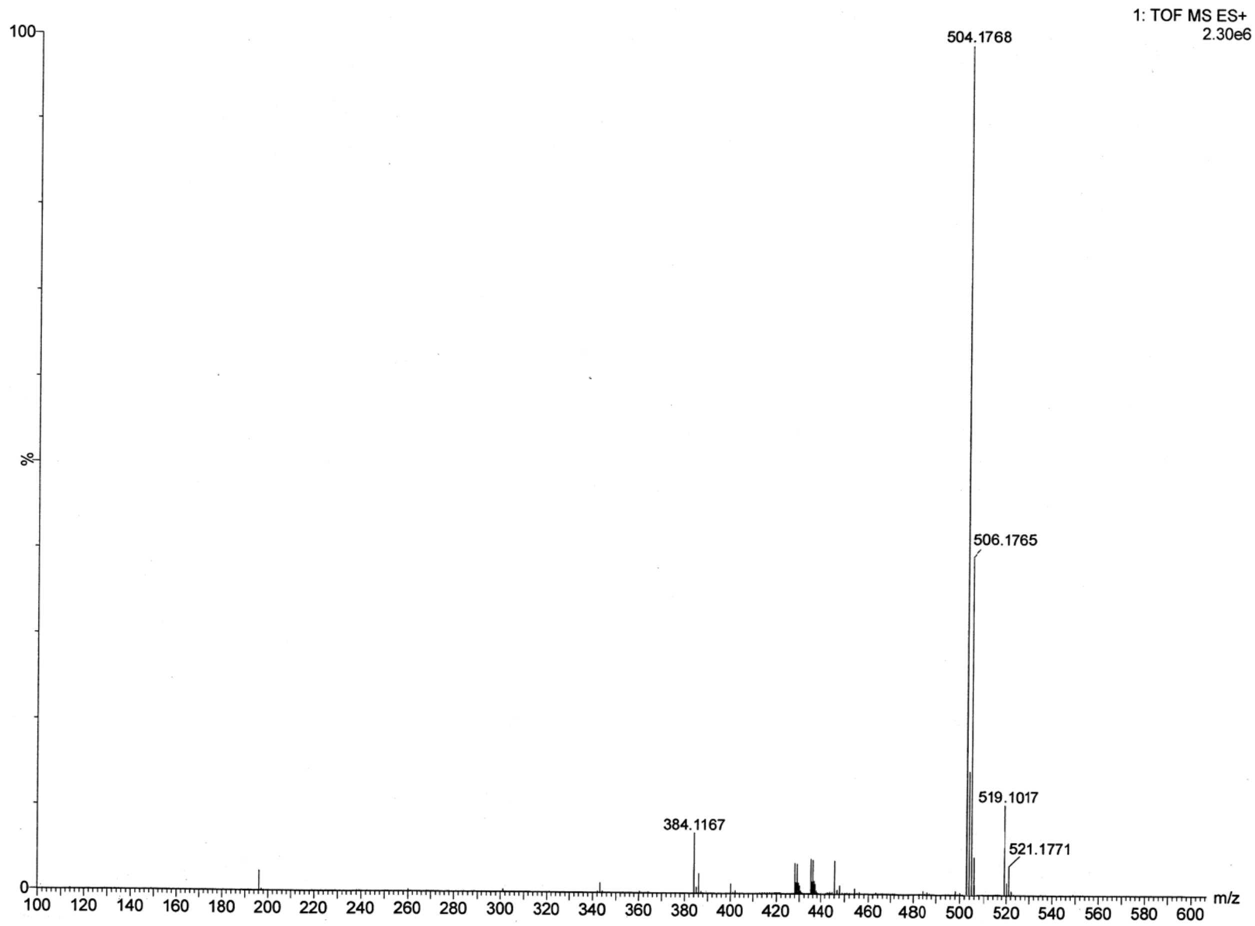


Fig.S3 HRMS spectra of [Cu(L^g)].

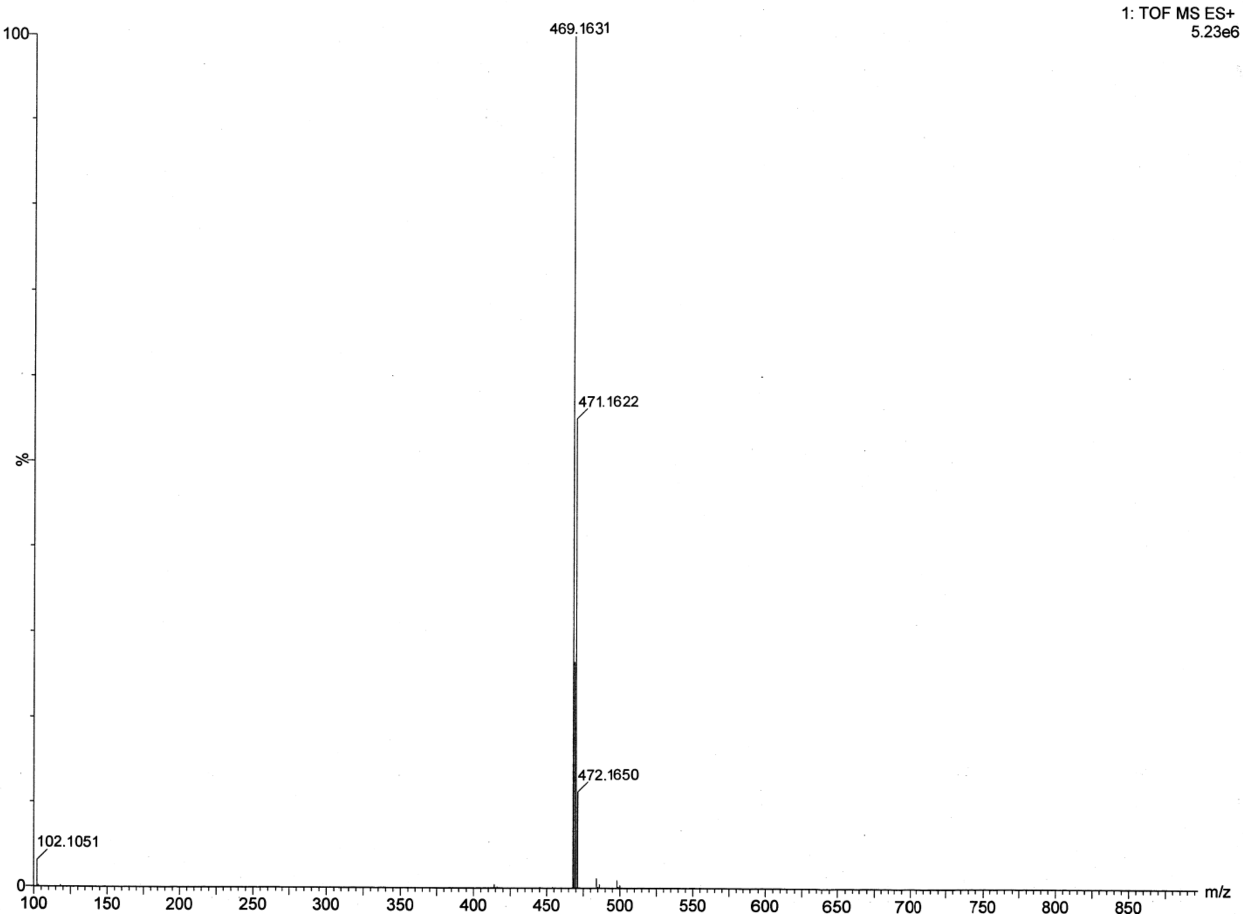


Fig. S4 HRMS spectra of [Cu(L^h)].

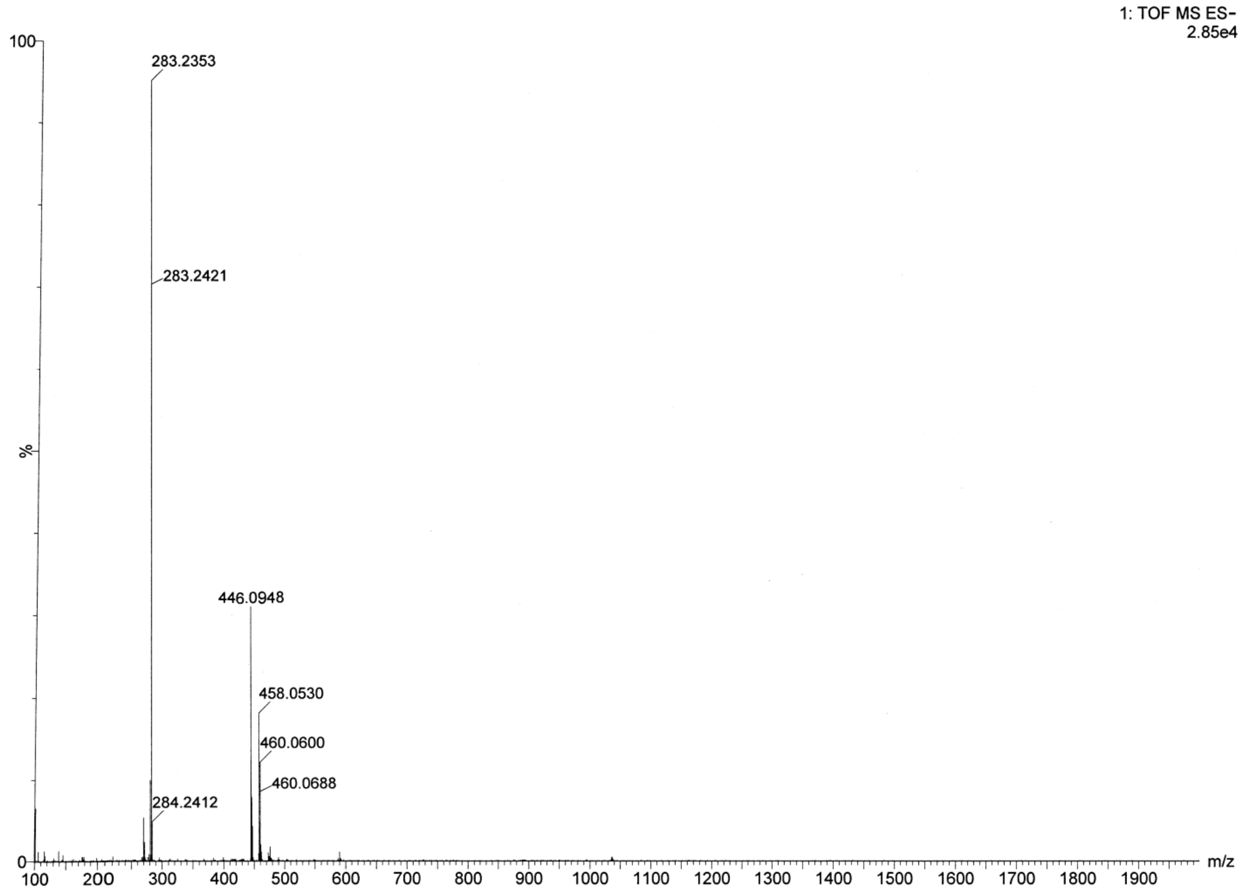


Fig. S5HRMS spectra of $[Cu(L^{f})(OOH)]^{-}$ generated *in situ* by the reaction between $[Cu(L^{2f})]$ and H_2O_2 in presence of **1** and equivalent amount of TEA.

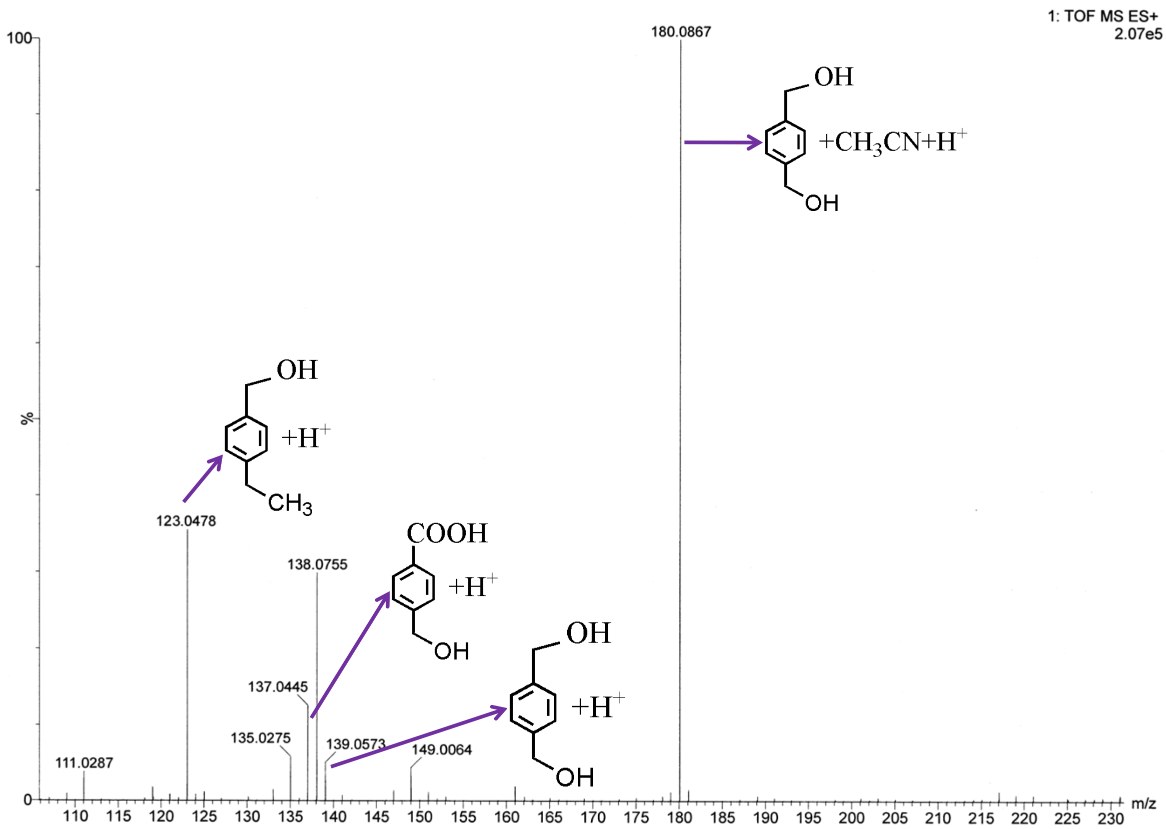
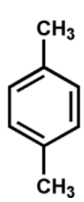
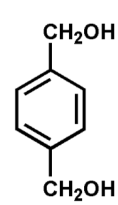


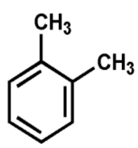
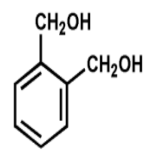
Fig.S6HRMS spectra of [Cu(L^{f})(OOH)] generated *in situ* by the reaction between [Cu(L^{2f})] and H_2O_2 in presence of **1** and equivalent amount of TEA.

Table S1. Oxidation of *p*-xyleneby complex **1**, catalyst = 0.055 mmol.

Catalyst	**Substrate**	**n(H_2O_2)/n(Catalyst)**	**Reaction time (h)**	**Conversion**	**Yield**		**Major product**	**TON**	**Rate constant (h^{-1})**
					Major	**Minor**			
1		150	3 6 9 12 24	15 33 51 66 72	13 02 27 06 43 08 54 12 56 16			254	
		300	3 6 9 12 24	19 36 53 70 78	16 03 29 07 44 09			272	

					57 13 60 18			
		500	3 6 9 12 24	22 40 59 73 83	17 05 32 08 48 11 59 14 62 21		287	0.107 ± 0.02

Table S2. Oxidation of *o*-xyleneby complex **1**, catalyst = 0.055 mmol.

Catalyst	Substrate	$n(H_2O_2)/n(Catalyst)$	Reaction time (Hr.)	Conversion	Yield		Major product	TON	Rate constant (h^{-1})
					Major	Minor			
1		150	3 6 9 12 24	17 31 50 65 71	14 26 41 52 55	03 05 09 13 16		236	
		300	3 6 9 12 24	19 35 54 68 76	15 28 44 53 57	04 07 10 15 19		250	
		500	3 6 9 12 24	22 39 56 72 80	16 31 45 55 59	06 08 11 17 21		280	0.109 ± 0.02

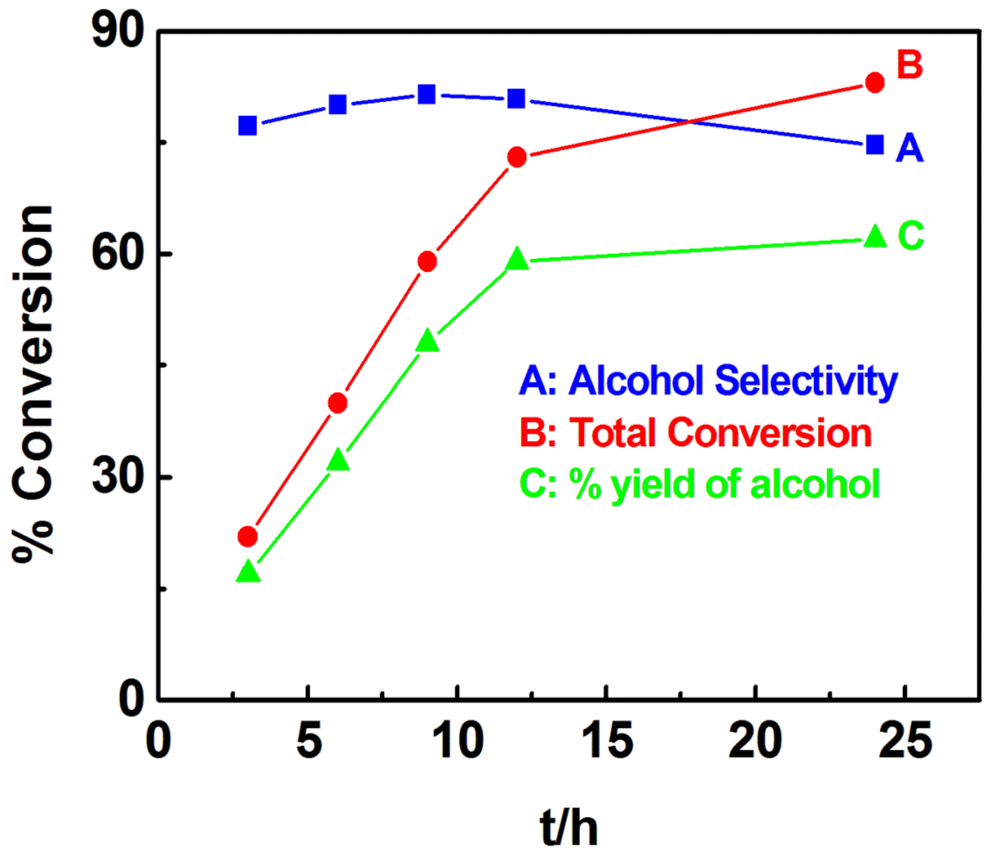


Fig. S7 Liquid phase partial oxidation of *p*-xylene by H_2O_2 using complex **1** as catalysts.

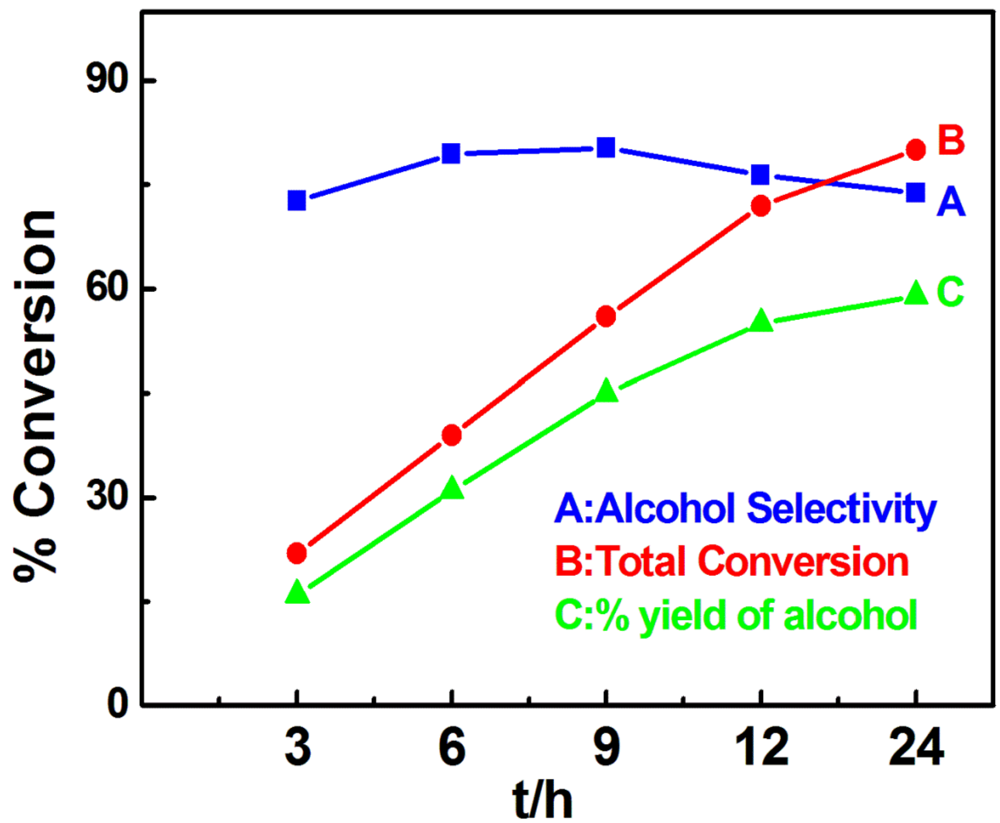
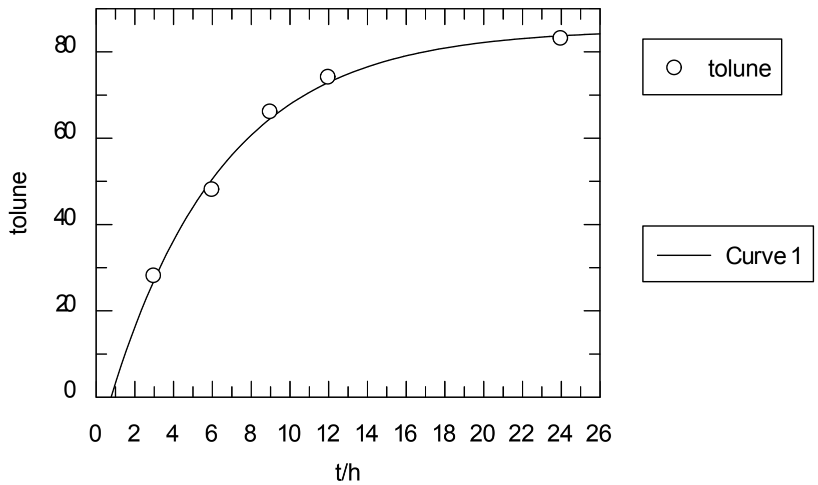


Fig. S8 Liquid phase partial oxidation of *o*-Xylene by H_2O_2 using complex **1** as catalysts.

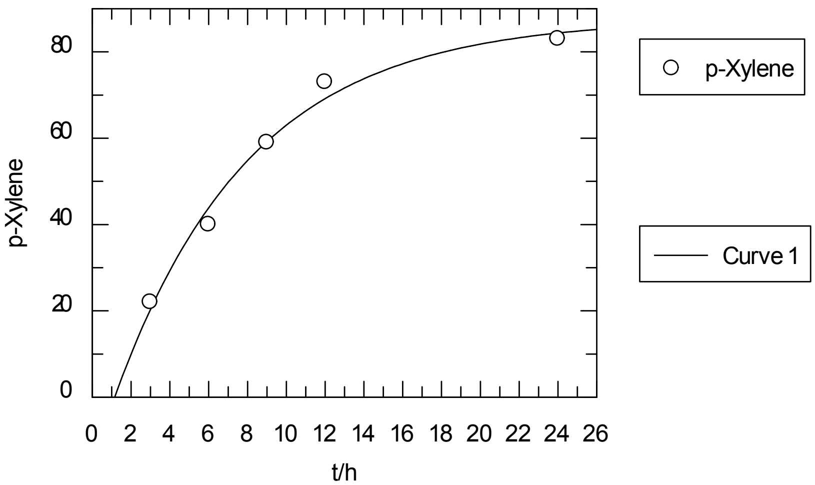


File : (untitled)
Thursday 17-04-14 12:30
y = A+B*(1-exp(-k*t))
Simple weighting
Reduced Chi squared =
5.557

Variable	Value	Std. Err.
A	-1.2081e+001	8.0725e+000
B	9.7380e+001	7.0378e+000
k	1.7195e-001	2.3630e-002

	t t/h	Y tolune	Calculated
1	3.0000e+000	2.8000e+001	2.7164e+001
2	6.0000e+000	4.8000e+001	5.0593e+001
3	9.0000e+000	6.6000e+001	6.4580e+001
4	1.2000e+001	7.4000e+001	7.2930e+001
5	2.4000e+001	8.3000e+001	8.3728e+001

Fig. S9a Evaluation of rate constant from the non-linear fit of % conversion of toluene with time in h using equation y = *A**(1-exp(-*k*t).



File : (untitled)
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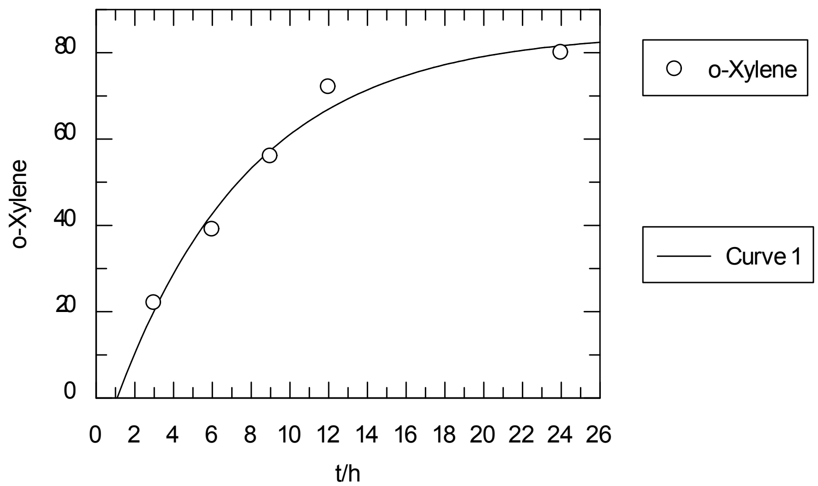
y = A+B*(1-exp(-k*t))
Simple weighting
Reduced Chi squared =
17.26

Variable	Value	Std. Err.
A	-1.5803e+001	1.2053e+001
B	1.0349e+002	1.0186e+001
k	1.4334e-001	3.2589e-002

	t t/h	Y p-Xylene	Calculated
1	3.0000e+000	2.2000e+001	2.0368e+001
2	6.0000e+000	4.0000e+001	4.3897e+001
3	9.0000e+000	5.9000e+001	5.9203e+001
4	1.2000e+001	7.3000e+001	6.9159e+001
5	2.4000e+001	8.3000e+001	8.4371e+001

Fig. S9b Evaluation of rate constant from the non-linear fit of % conversion of p-xylene with time in h using equation y = A*(1-exp(-kt).



File : (untitled)
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y = A+B*(1-exp(-k*t))
Simple weighting
Reduced Chi squared =
23.53

Variable	Value	Std. Err.
A	-1.4193e+001	1.4030e+001
B	9.9043e+001	1.1848e+001
k	1.4258e-001	3.9619e-002

	t t/h	Y o-Xylene	Calculated
1	3.0000e+000	2.2000e+001	2.0276e+001
2	6.0000e+000	3.9000e+001	4.2750e+001
3	9.0000e+000	5.6000e+001	5.7401e+001
4	1.2000e+001	7.2000e+001	6.6954e+001
5	2.4000e+001	8.0000e+001	8.1616e+001

Fig. S9c Evaluation of rate constant from the non-linear fit of % conversion of o-xylene with time in h using equation y = A*(1-exp(-kt)).