

*ESI for*

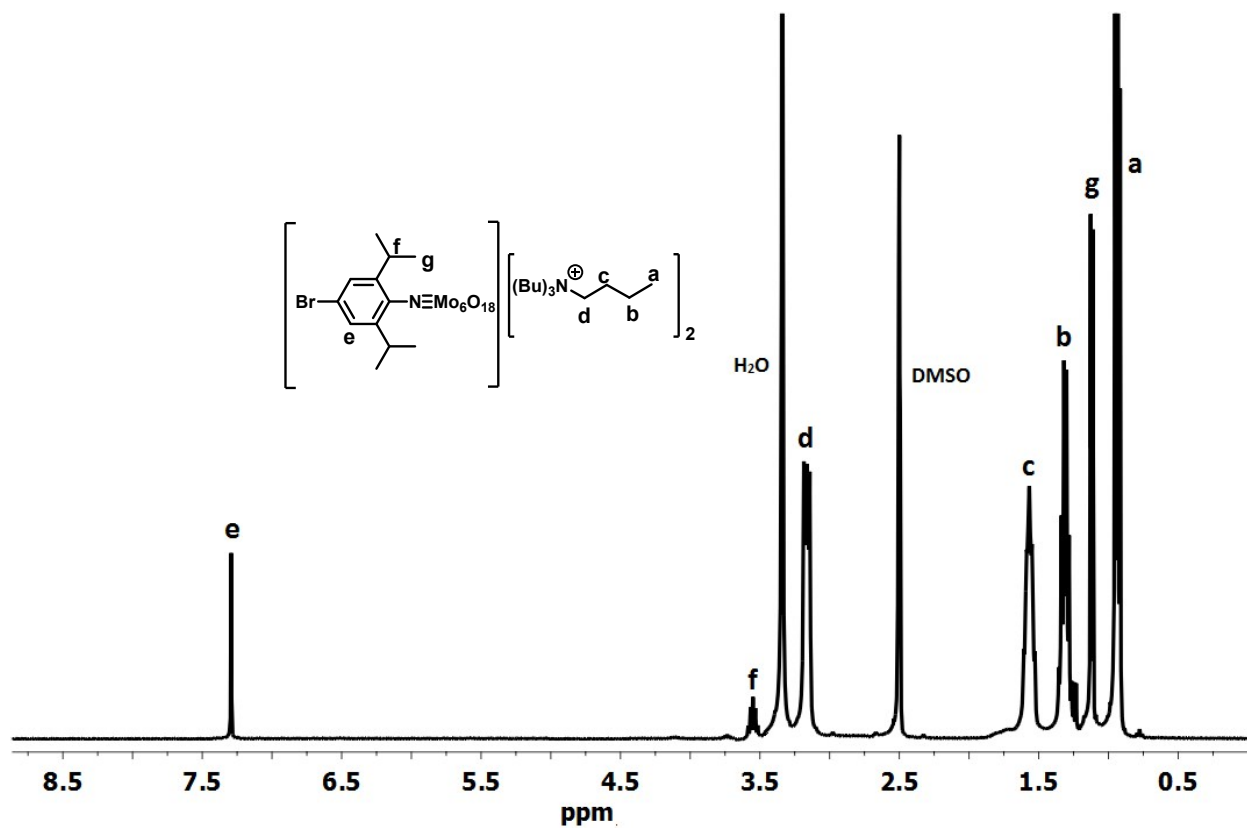
**New sterically encumbered arylimido hexamolybdates for organic oxidation reactions**

Ritambhara Jangir, Rajendran Antony, Ramaswamy Murugavel\*

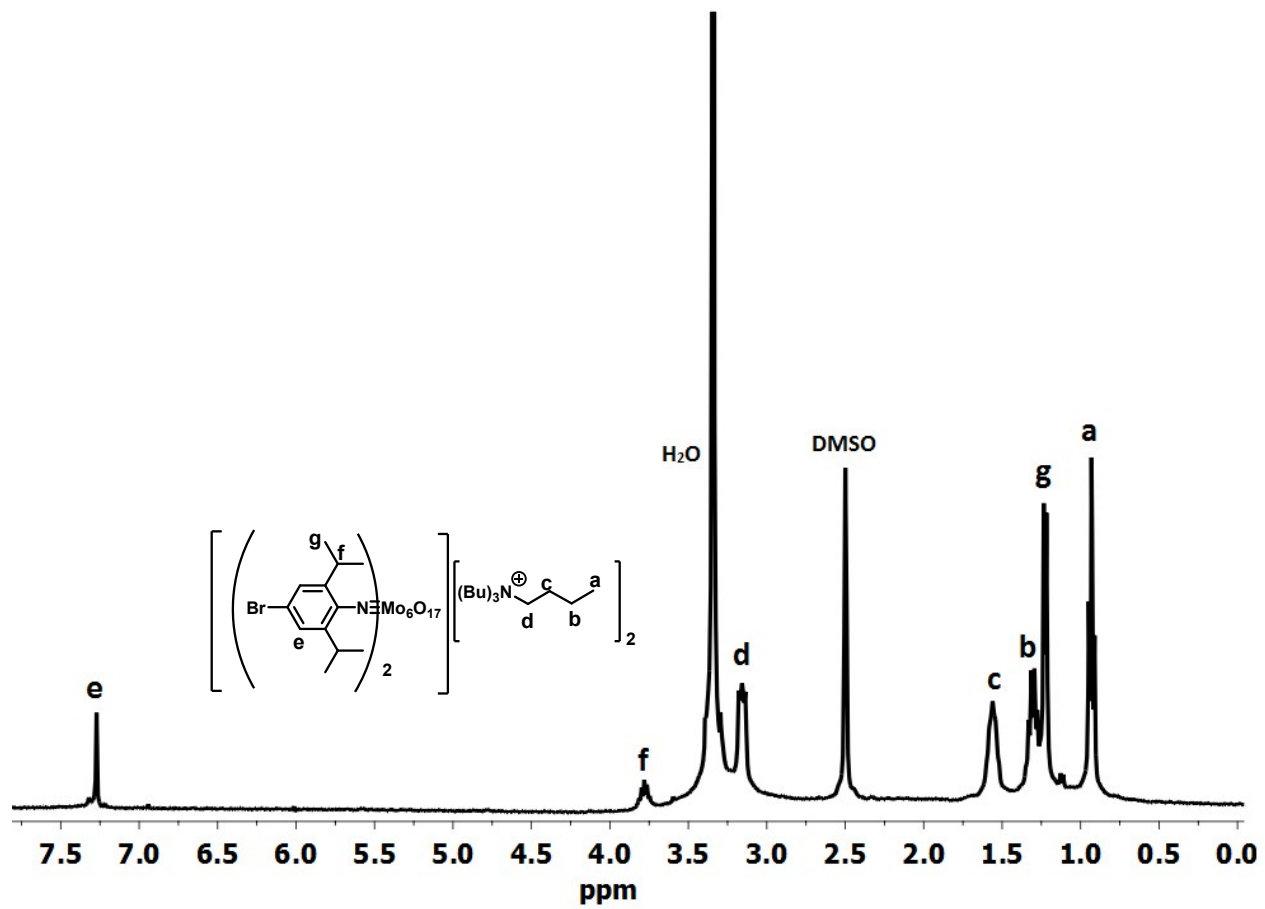
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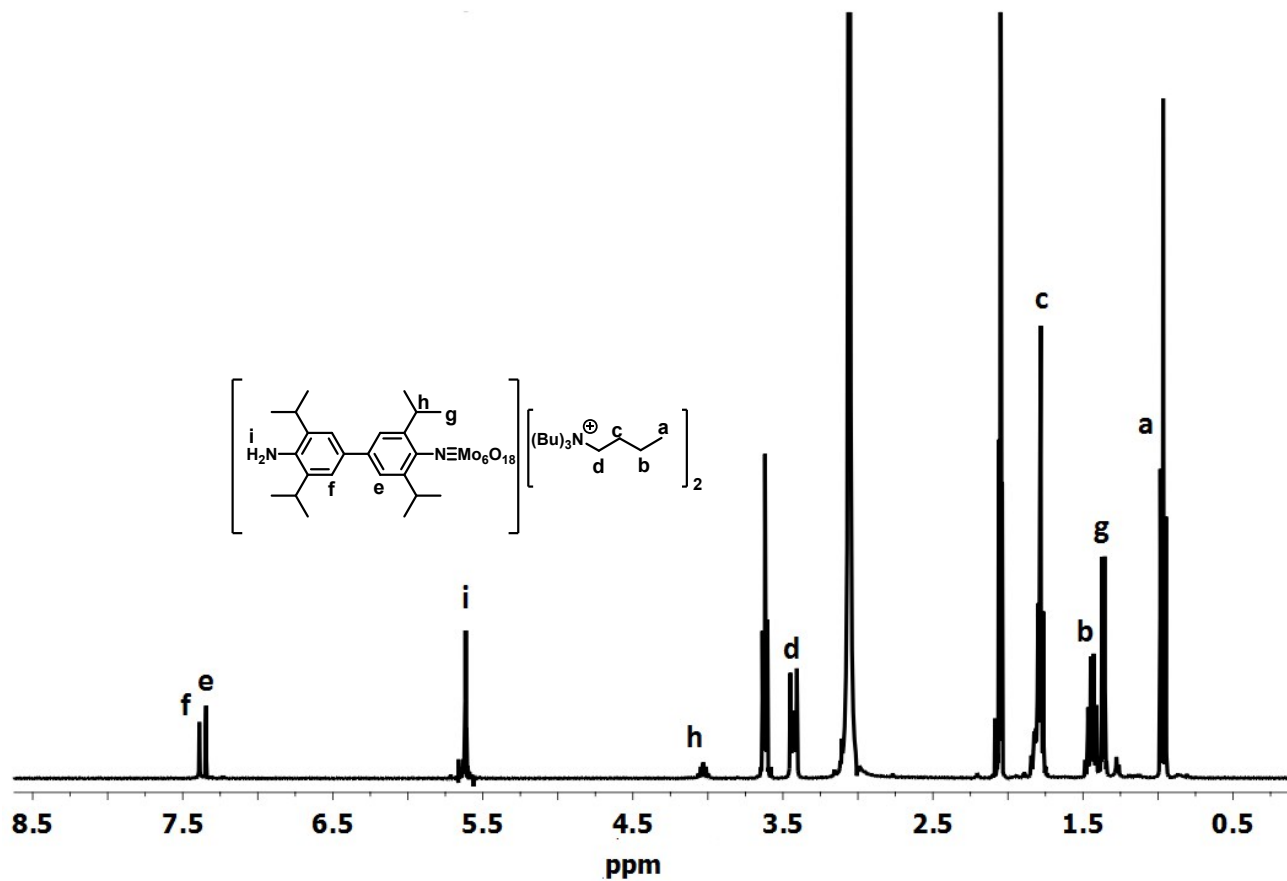
1. Figure S1. <sup>1</sup>H NMR spectrum of compound **1** in DMSO-*d*<sub>6</sub> (400 MHz).
2. Figure S2. <sup>1</sup>H NMR spectrum of compound **2** in DMSO-*d*<sub>6</sub> (400 MHz).
3. Figure S3. <sup>1</sup>H NMR spectrum of compound **3** in Acetone-*d*<sub>6</sub> (400 MHz).
4. Figure S4. TGA curves of **1-3** (10 °C/min, N<sub>2</sub> atm).
5. Figure S6. . Effect of time on selectivity and conversion % in cyclohexene oxidation catalysed by **2**.
6. Figure S7. Effect of time on selectivity and conversion % in cyclohexene oxidation catalysed by **3**.
7. Effect of time on selectivity and conversion % in benzyl alcohol oxidation catalysed by **1**.
8. Effect of time on selectivity and conversion % in benzyl alcohol oxidation catalysed by **2**.
9. Figure S9. ESI-MS spectrum of reaction mixture after benzyl alcohol oxidation catalysed by **1**.



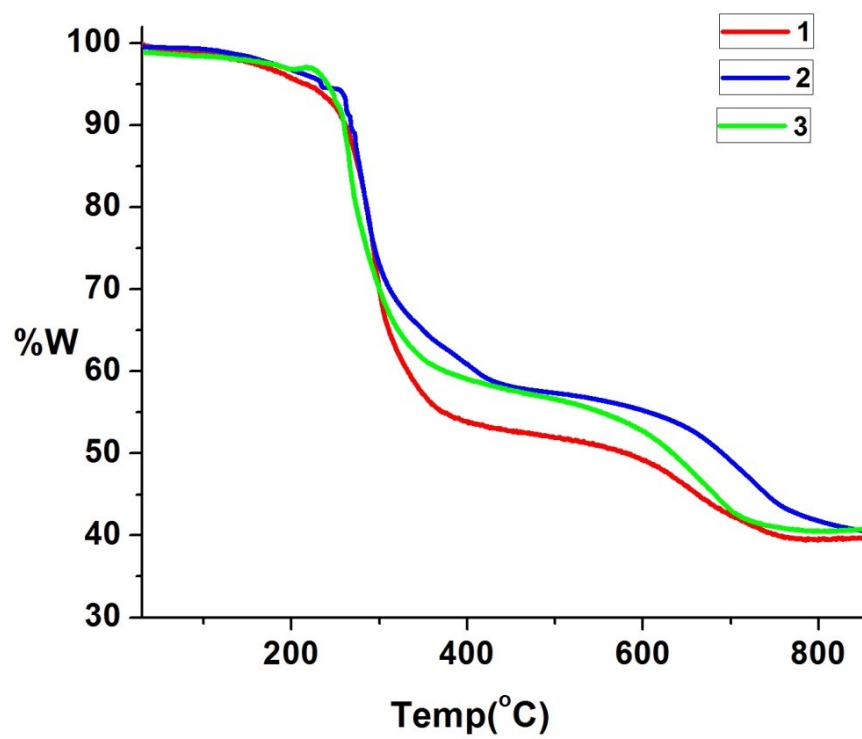
**Figure S1.**  $^1\text{H}$  NMR spectrum of compound **1** in  $\text{DMSO-}d_6$  (400 MHz).



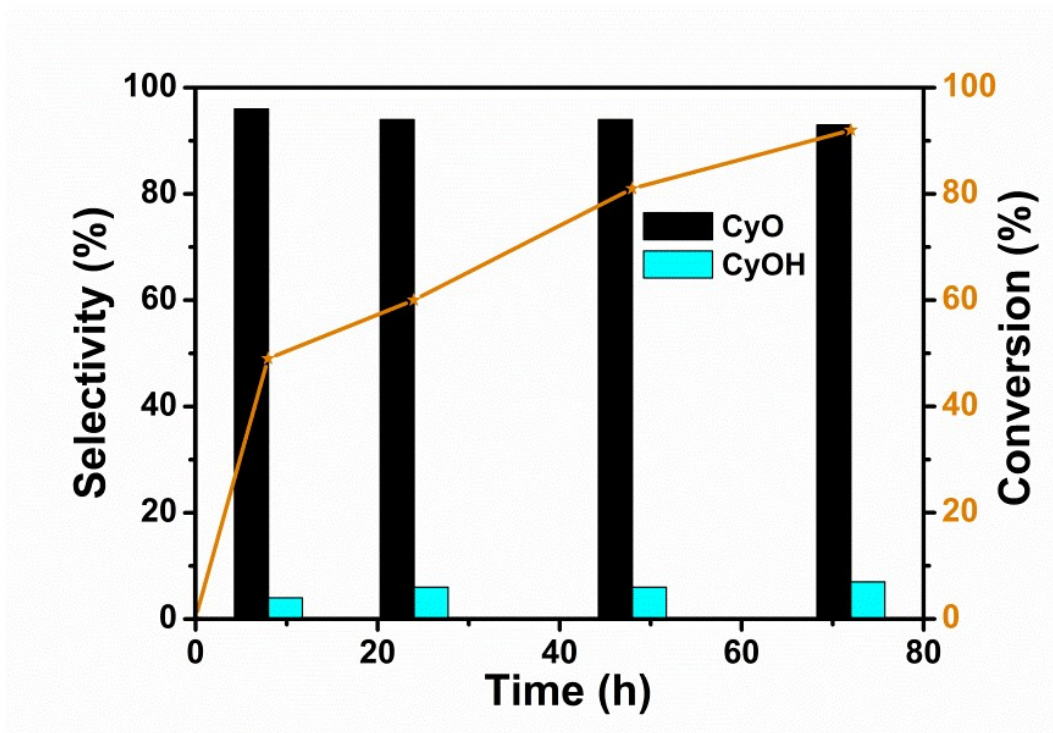
**Figure S2.** <sup>1</sup>H NMR spectrum of compound 2 in DMSO-*d*<sub>6</sub> (400 MHz).



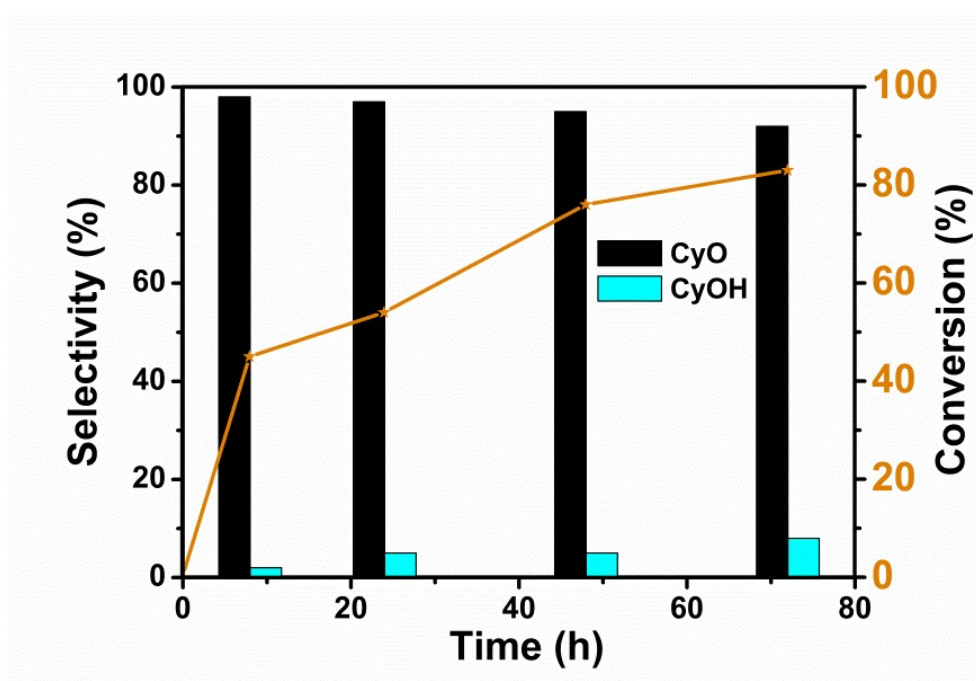
**Figure S3.**  $^1\text{H}$  NMR spectrum of compound **3** in  $\text{Acetone-}d_6$  (400 MHz).



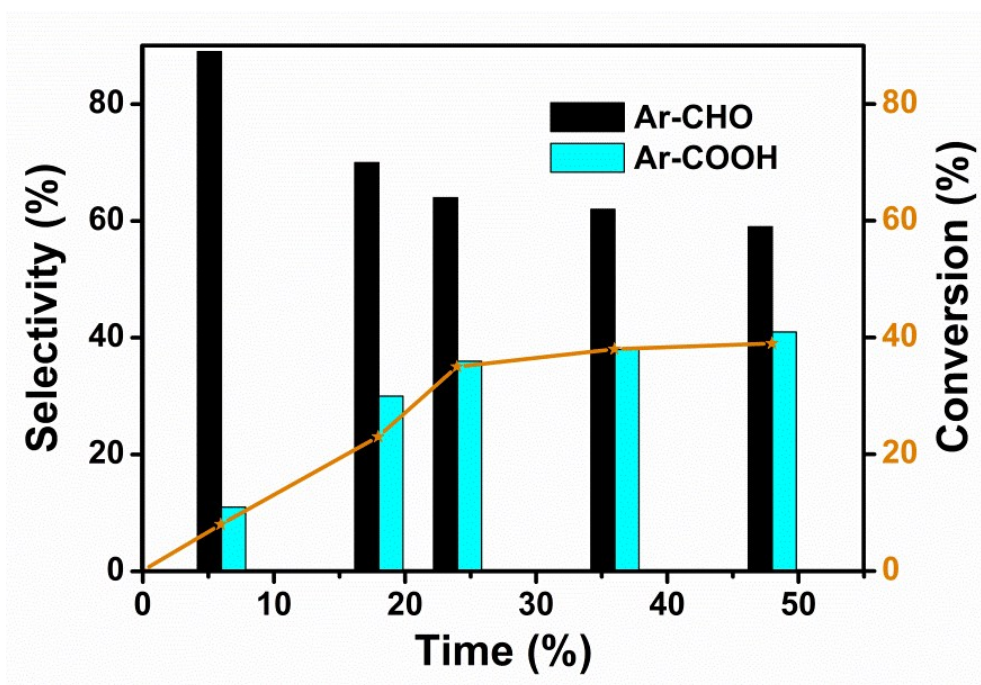
**Figure S4.** TGA cures of 1-3 (10 °C/min, N<sub>2</sub> atm).



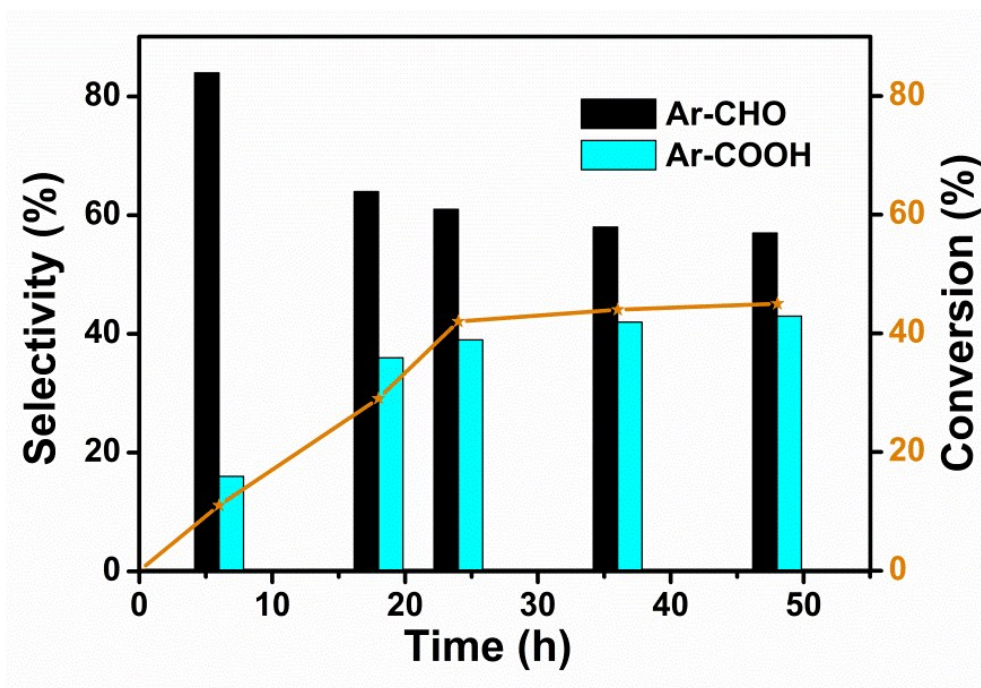
**Figure S5.** Effect of time on selectivity and conversion % in cyclohexene oxidation catalysed by 2.



**Figure S6.** Effect of time on selectivity and conversion % in cyclohexene oxidation catalysed by 3.



**Figure S7.** Effect of time on selectivity and conversion % in benzyl alcohol oxidation catalysed by 1.



**Figure S8.** Effect of time on selectivity and conversion % in benzyl alcohol oxidation catalysed by 2.

# Display Report

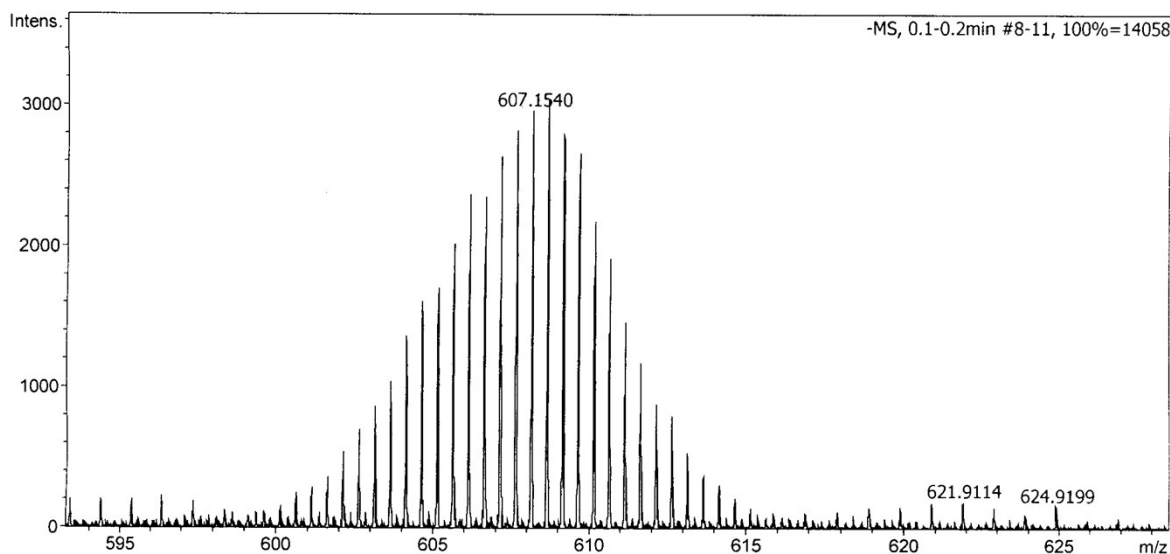
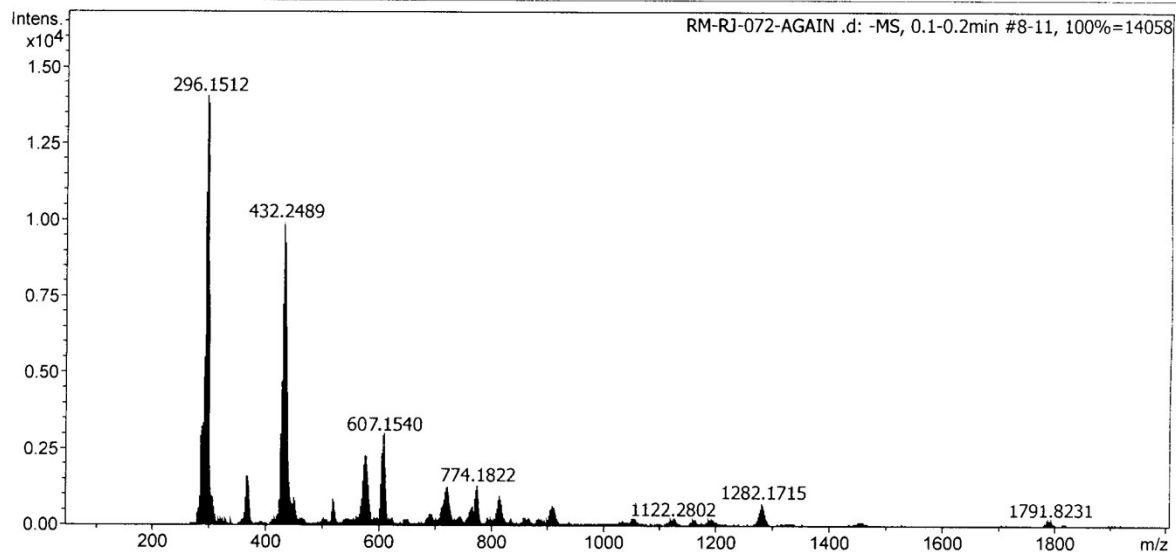
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Comment LRMS

Acquisition Date 11/5/2015 9:17:12 PM  
Operator SSK OUT  
Instrument maXis impact 282001.00081

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RM-RJ-072-AGAIN.d

Bruker Compass DataAnalysis 4.1

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**Figure S9.** ESI-MS spectrum of reaction mixture after benzyl alcohol oxidation catalysed by **1**. The peak centered at  $m/z$  607 corresponds to the molecular ion of **1**.