

Supporting Information

Insertion of Organometallic Moieties into Peptides and Peptide Nucleic Acids using Alternative “Click” Strategies

Cristina Mari,^a Sandro Mosberger,^a Nuria Llorente,^a Sarah Spreckelmeyer,^a Gilles Gasser^{a,*}

University of Zurich, Department of Chemistry, Winterthurerstrasse 190, 8050, Zurich, Switzerland. Tel: +41 44 635 46 30; Email: gilles.gasser@chem.uzh.ch; WWW: www.gassergroup.com.

Figure S 2 – ¹³ C-NMR spectrum of 2A.....	2
Figure S 3 – UPLC-MS analysis of 2A.....	2
Figure S 4 – HR ESI-MS of 2A	3
Figure S 5 – IR spectrum of 2A.....	3
Figure S 6 – UPLC-MS analysis of 3A.....	4
Figure S 7 – MALDI spectrum of 3A.....	4
Figure S 8 – IR spectrum of 3A.....	5
Figure S 9 – ¹ H-NMR of 2B	6
Figure S 10 – ¹³ C-NMR of 2B	6
Figure S 11–HSQC of 2B.....	7
Figure S 12 – HSQC of 2B	7
Figure S 13 – DEPT of 2B.....	8
Figure S 14 – UPLC-MS analysis of 2B.....	8
Figure S 15 – HR ESI-MS of 2B	9
Figure S 16 – UPLC-MS analysis of 3B.....	9
Figure S 17 – MALDI spectrum of 3B	10
Figure S 18 – UPLC-MS analysis of 5A.....	10
Figure S 19 – IR spectrum of 5A.....	11
Figure S 20- -UPLC-MS analysis of byproduct of 5A	11
Figure S 21 – IR spectrum of byproduct of 5A.....	12
Figure S 22 – ¹³ C-NMR of 5B.....	13
Figure S 23 – UPLC-MS analysis of 5B.....	13
Figure S 24 – HR ESI-MS analysis of 5B.....	14
Figure S 25 – UPLC-MS analysis of 6B.....	14
Figure S 26 – MALDI of 6B	15
Figure S 27 – UPLC-MS analysis of 11.....	15
Figure S 28 – MALDI spectrum of 11	16
Figure S 29 – UPLC-MS analysis of 12.....	16
Figure S 30 – MALDI analysis of 12	17
Figure S 31 – UPLC-MS analysis of 13	17
Figure S 32 – MALDI of 13	18
Figure S 33 – UPLC-MS analysis of 14	18

Figure S 1 – ^{13}C -NMR spectrum of 2A

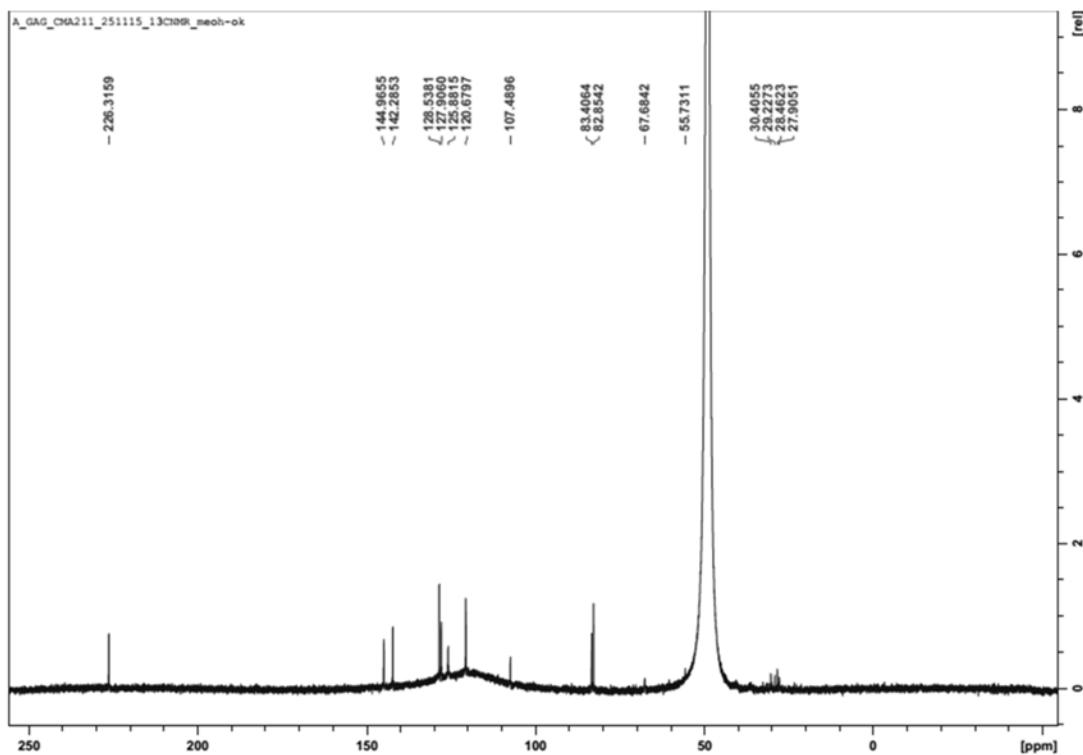


Figure S 2 – UPLC-MS analysis of 2A

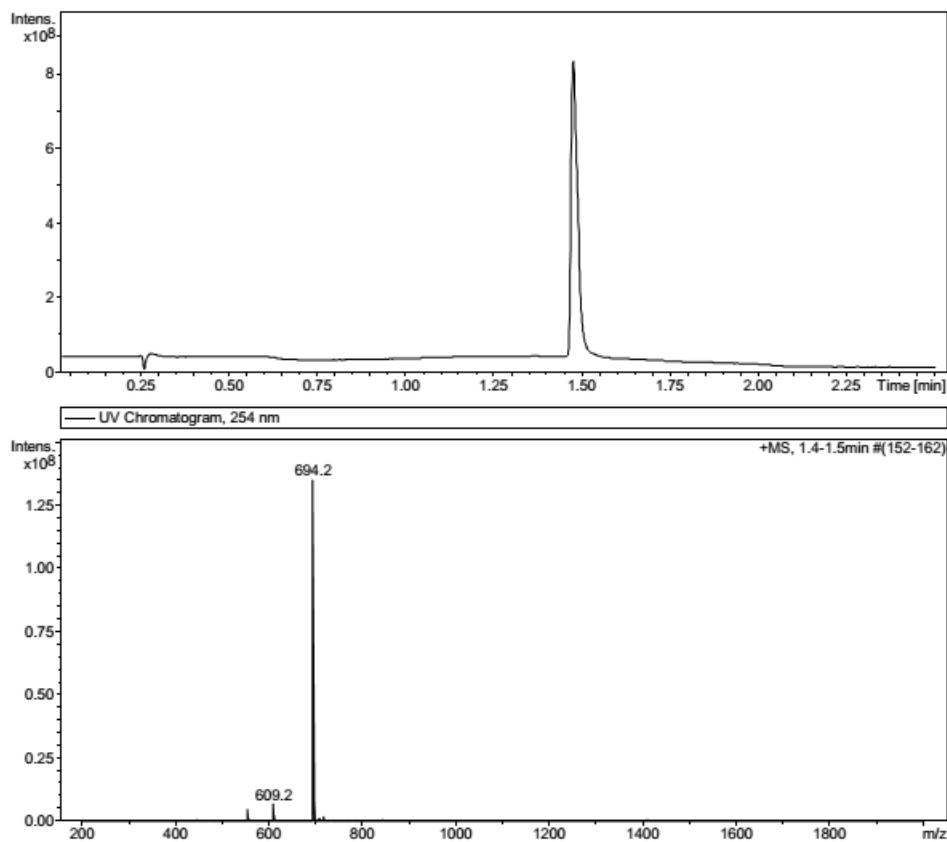


Figure S 3 – HR ESI-MS of 2A

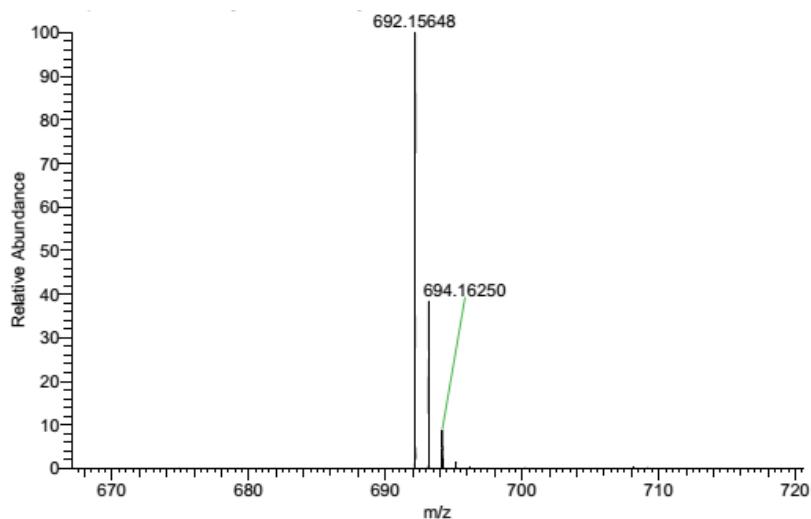


Figure S 4 – IR spectrum of 2A

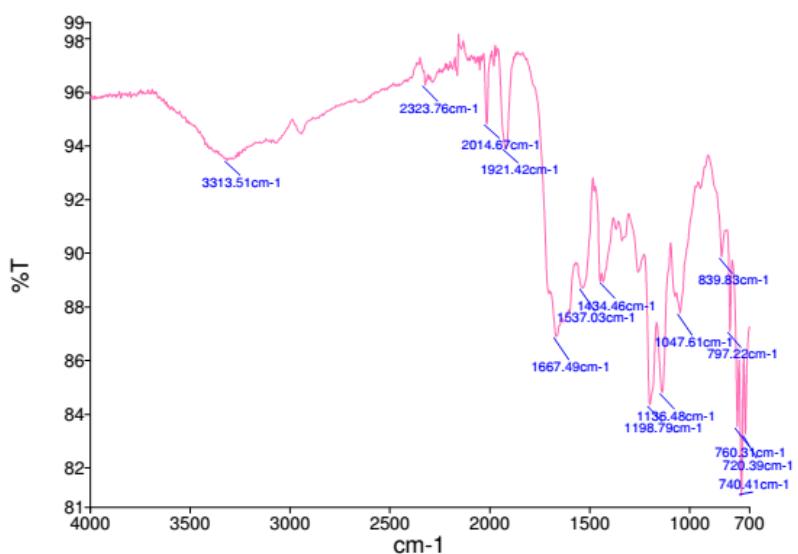


Figure S 5 – UPLC-MS analysis of 3A

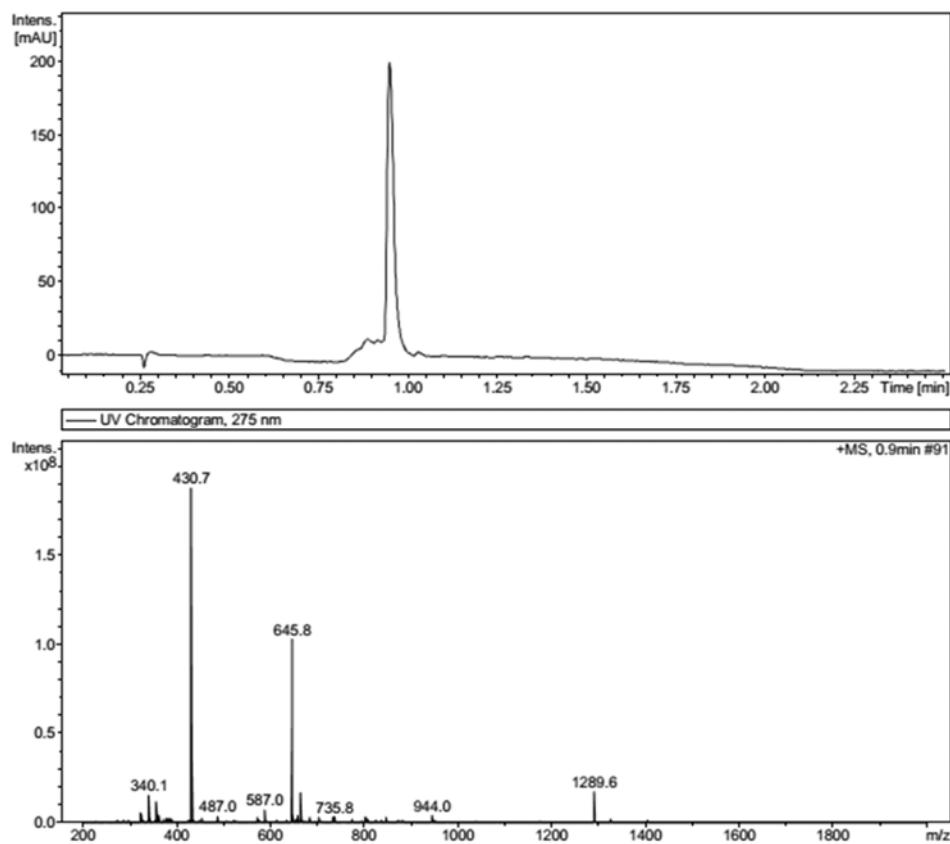


Figure S 6 – MALDI spectrum of 3A

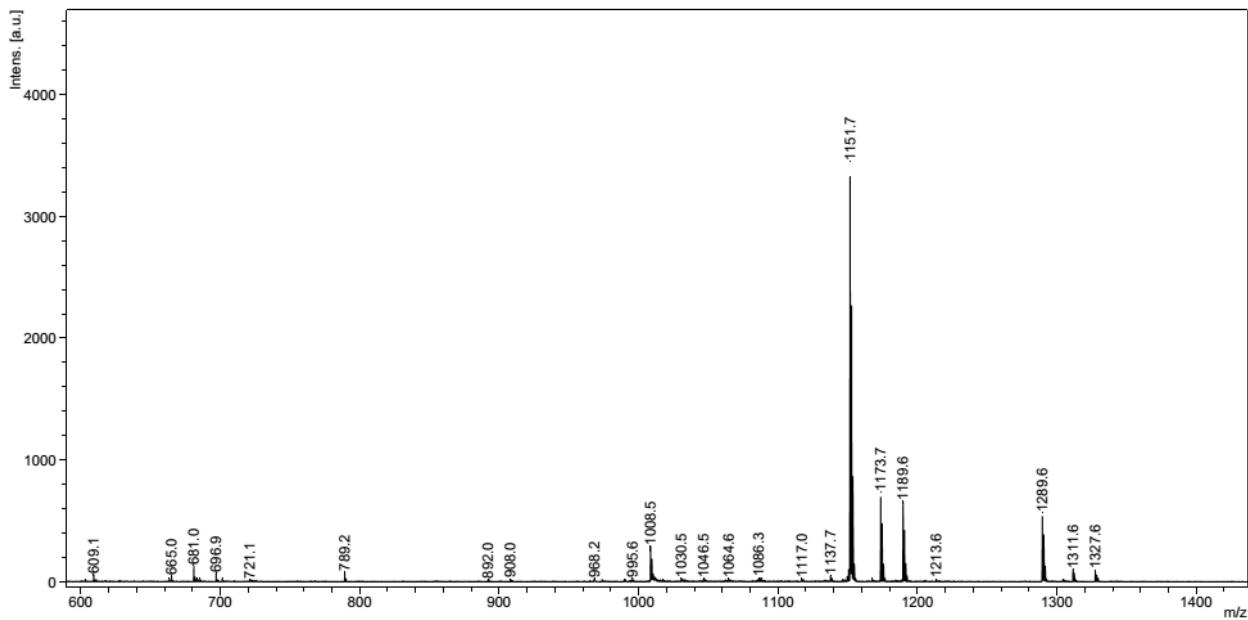


Figure S 7 – IR spectrum of 3A

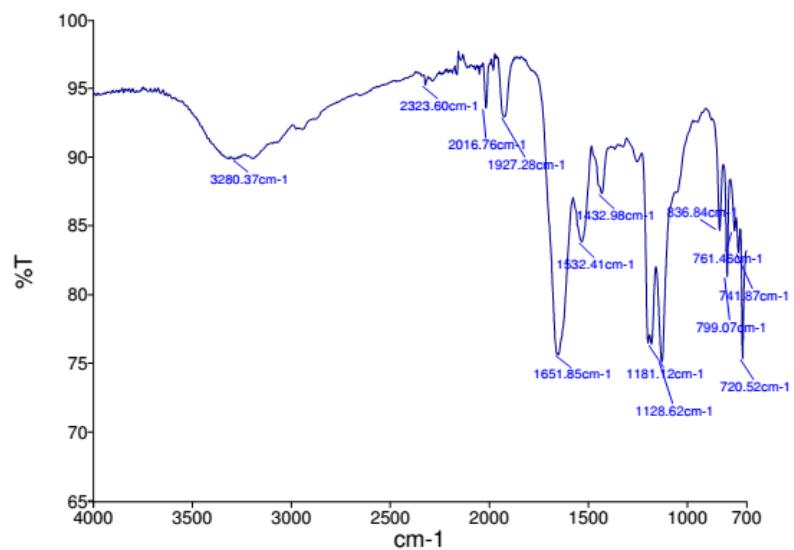


Figure S 8 – ^1H -NMR of 2B

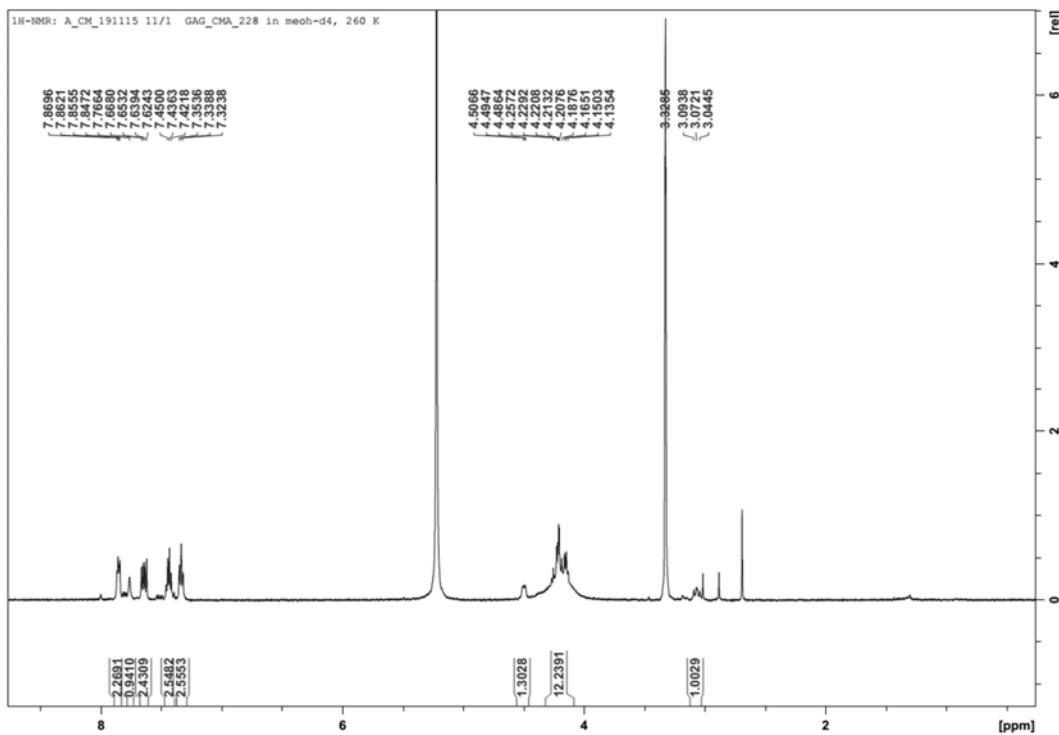


Figure S 9 – ^{13}C -NMR of 2B

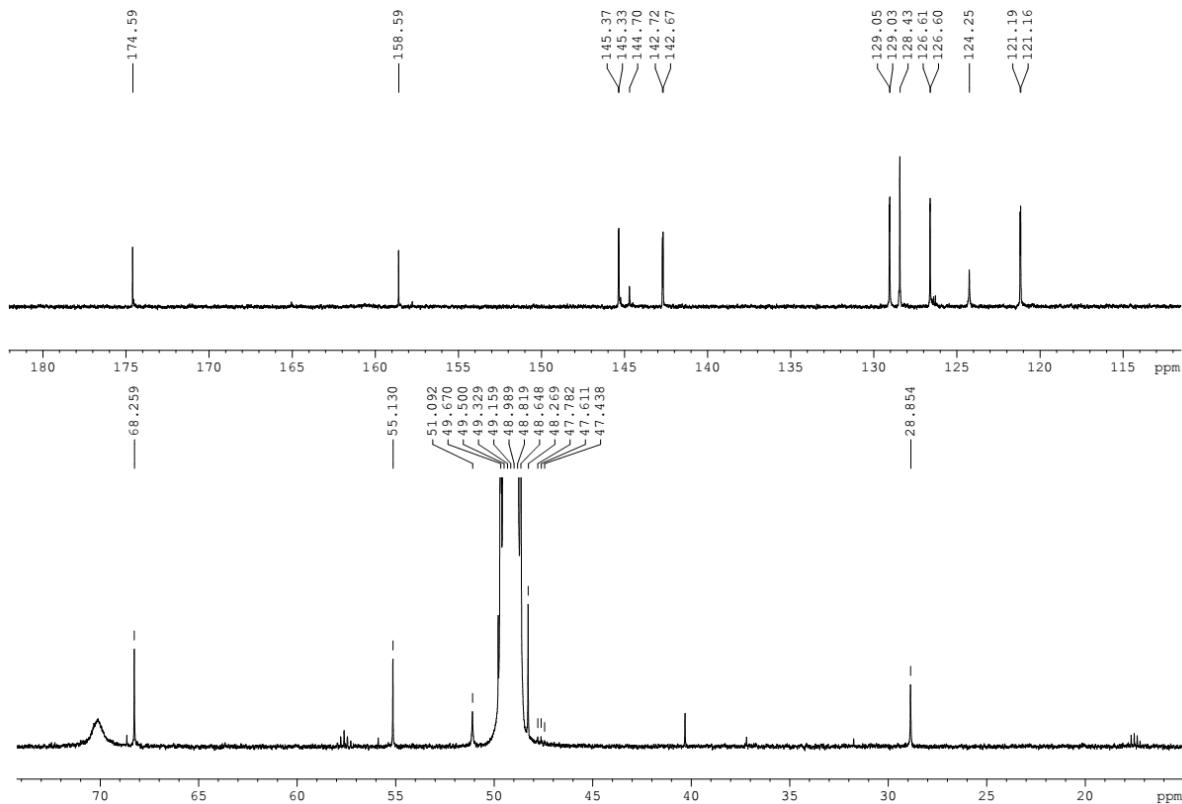


Figure S 10—HSQC of 2B

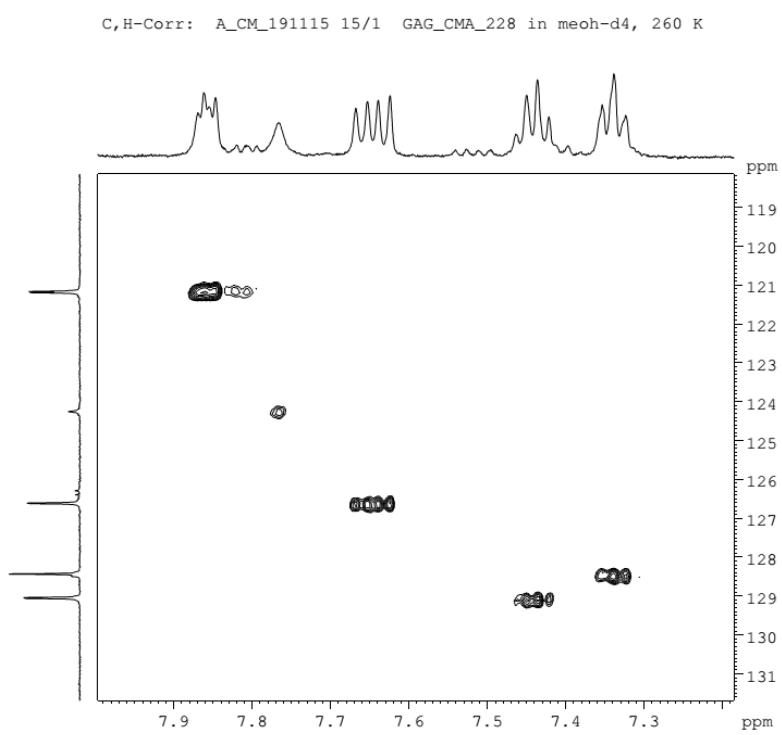


Figure S 11 – HSQC of 2B

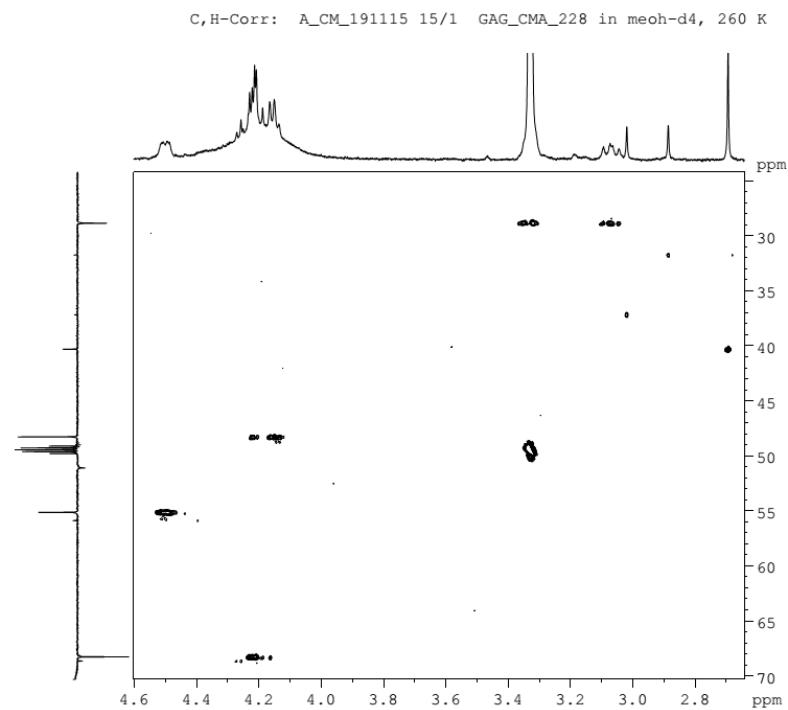


Figure S 12 – DEPT of 2B

¹³C (DEPT): A_CM_191115 19/1 GAG_CMA_228 in meoh-d₄, 260 K
CH, CH₃ up; CH₂ down; C(q) zero

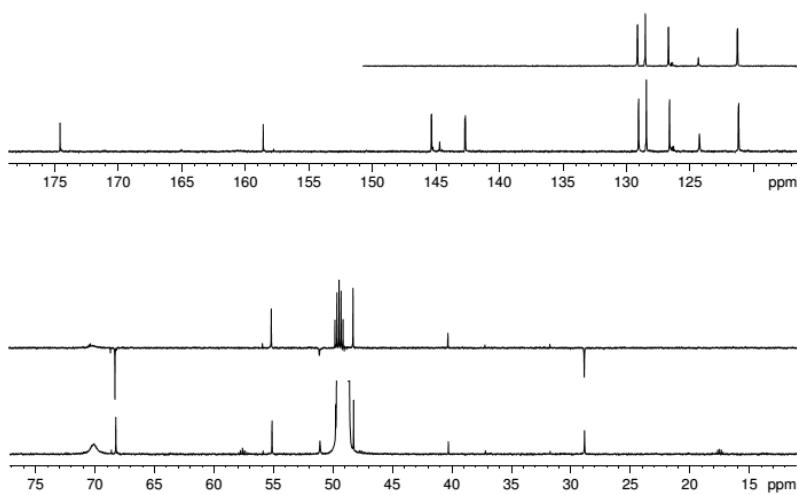


Figure S 13 – UPLC-MS analysis of 2B

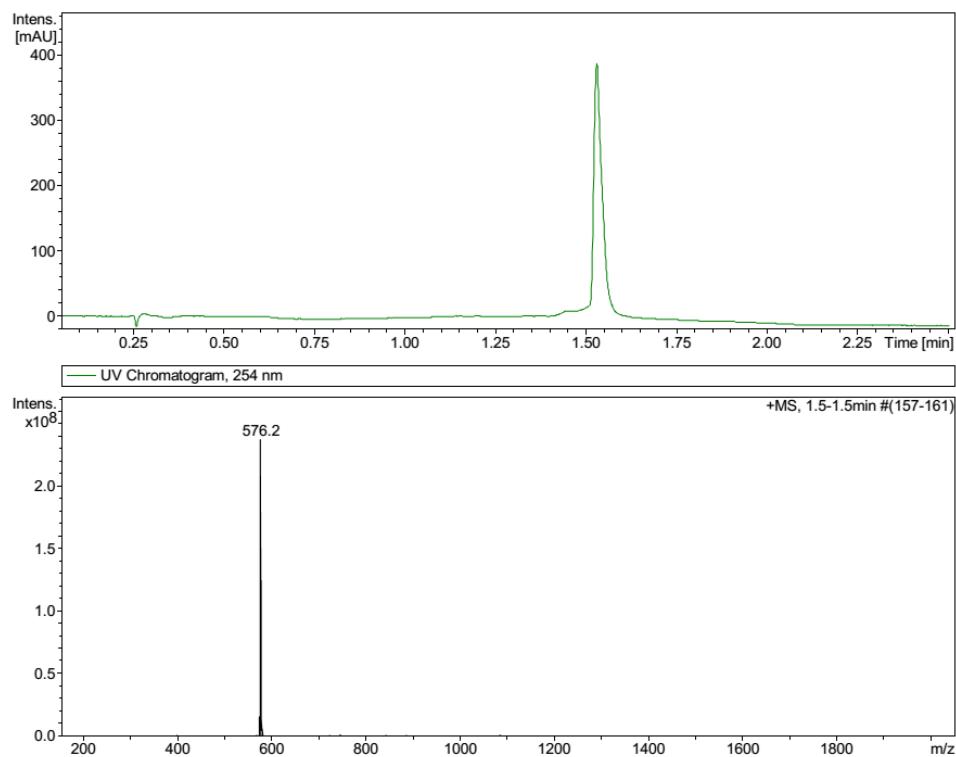


Figure S 14 – HR ESI-MS of 2B

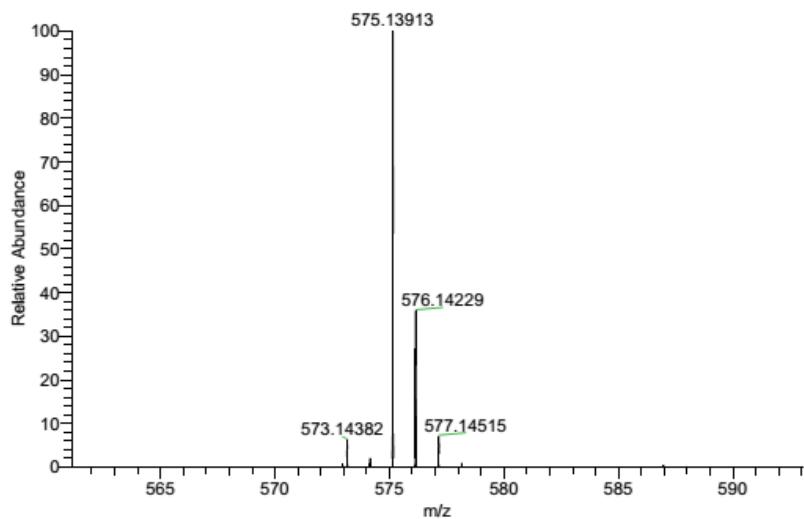


Figure S 15 – UPLC-MS analysis of 3B

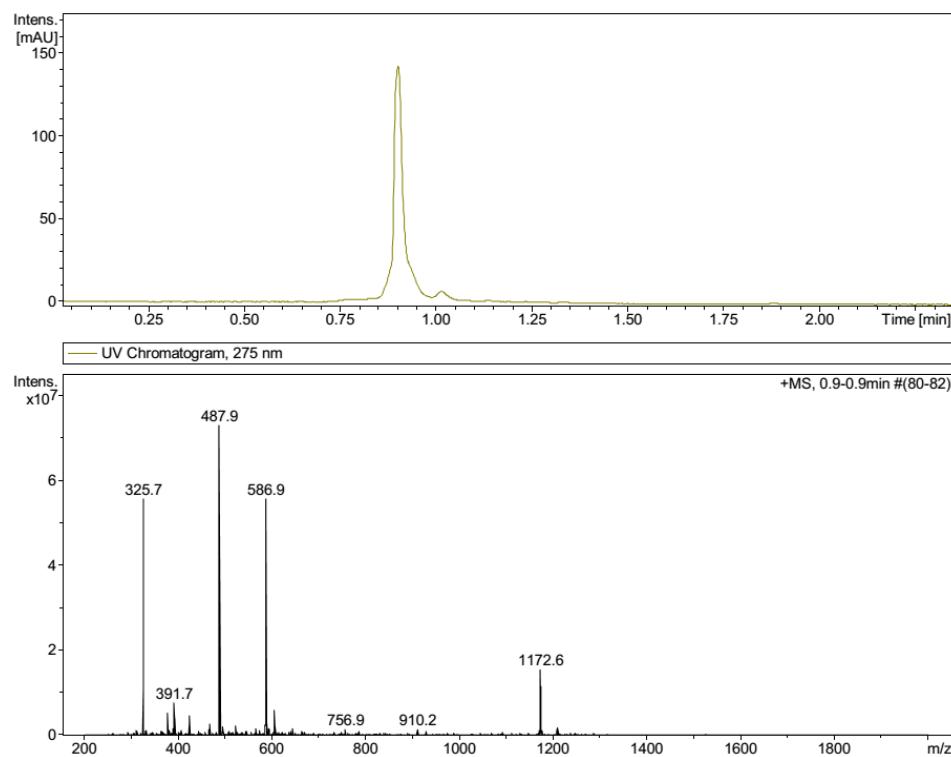


Figure S 16 – MALDI spectrum of 3B

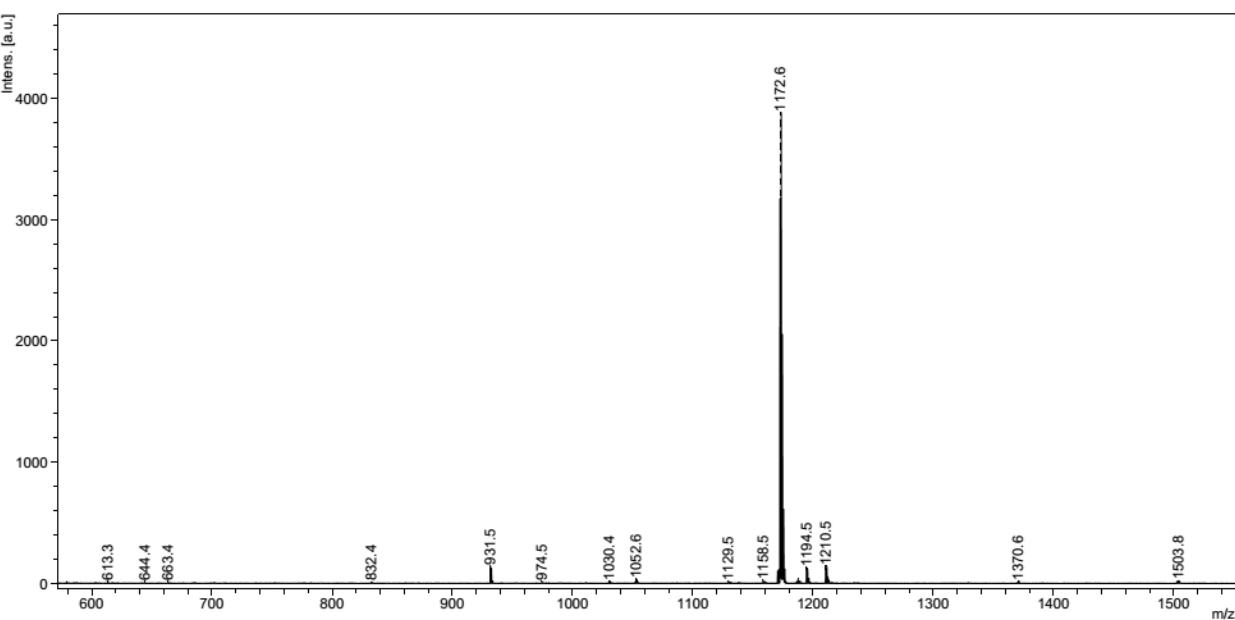


Figure S 17 – UPLC-MS analysis of 5A

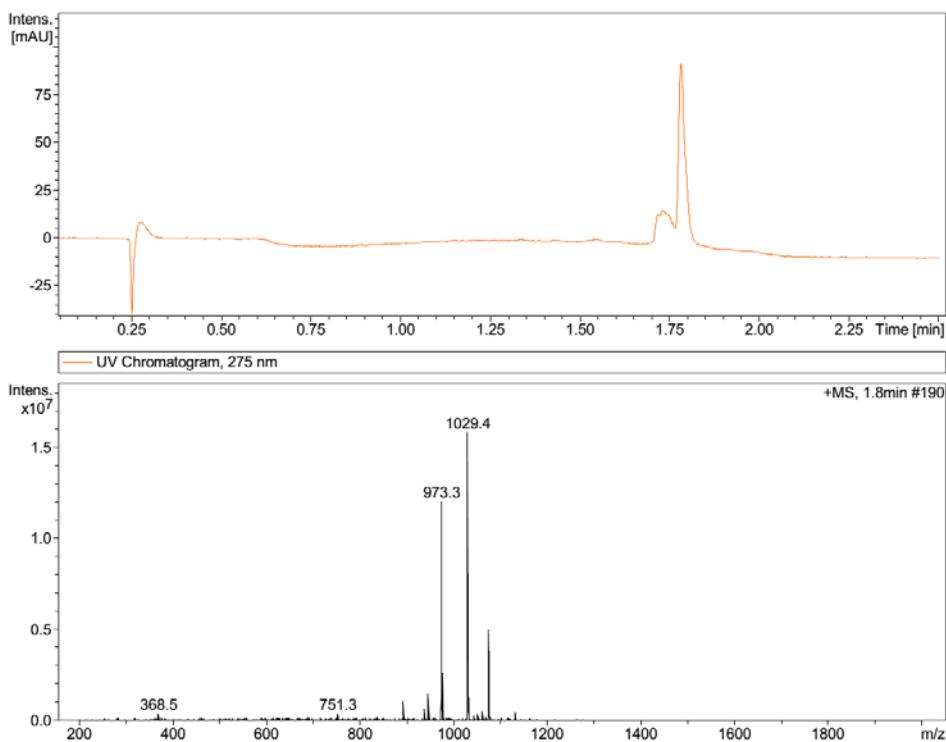


Figure S 18 – IR spectrum of 5A

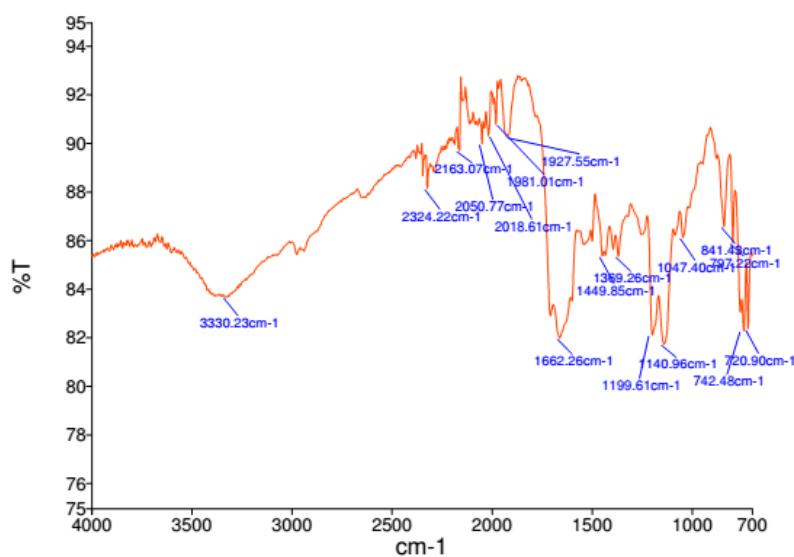


Figure S 19- -UPLC-MS analysis of byproduct of 5A

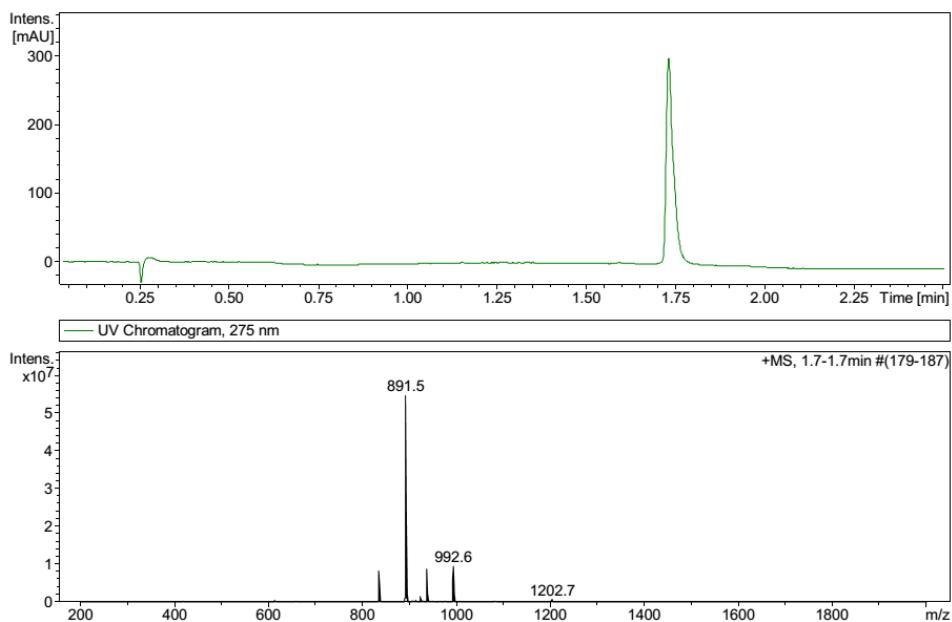


Figure S 20 – IR spectrum of byproduct of 5A

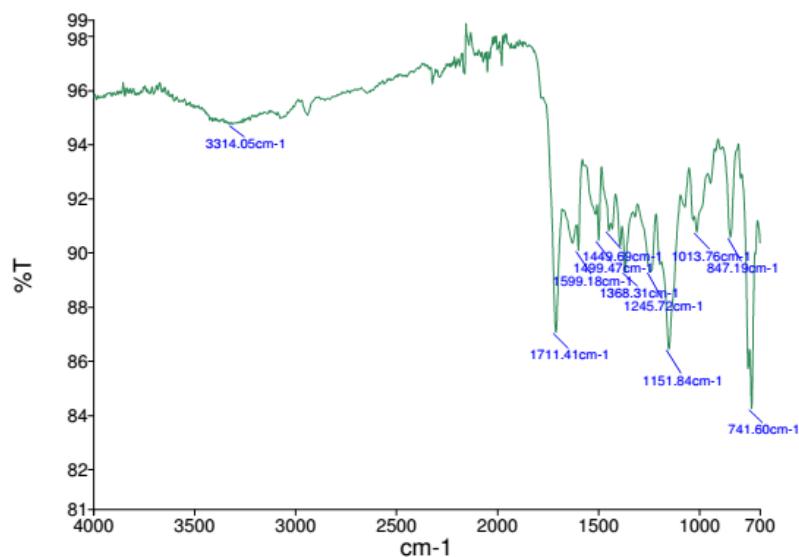


Figure S 21 – ^{13}C -NMR of 5B

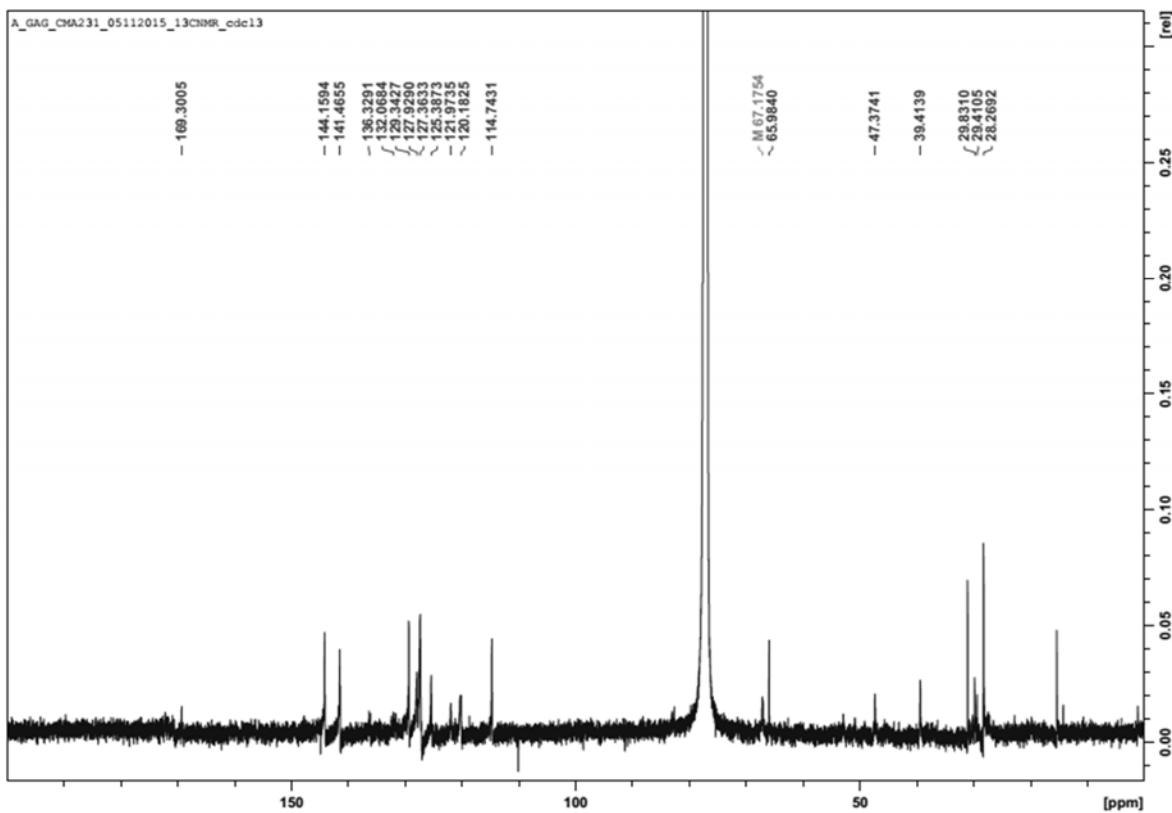


Figure S 22 – UPLC-MS analysis of 5B

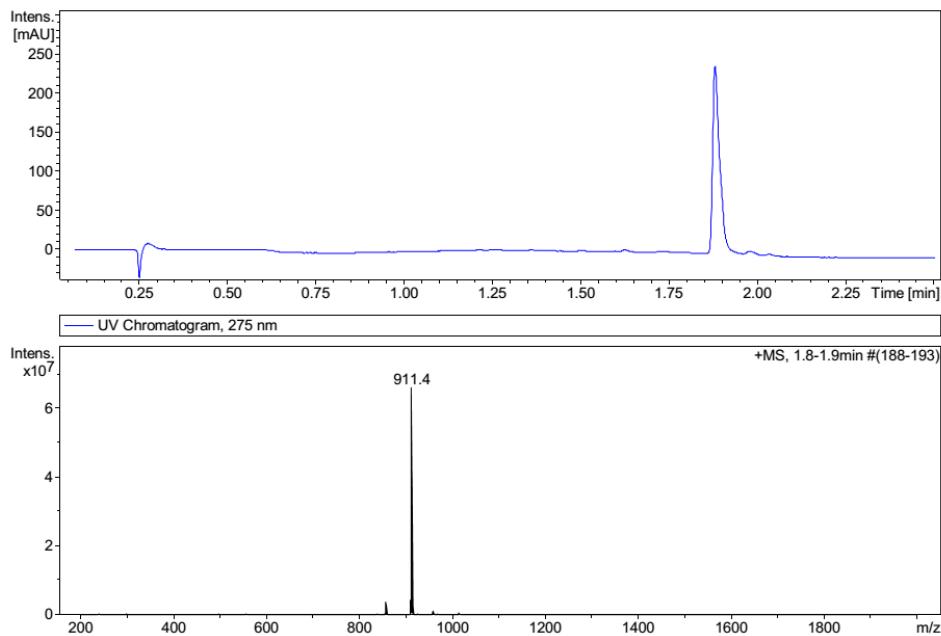


Figure S 23 – HR ESI-MS analysis of 5B

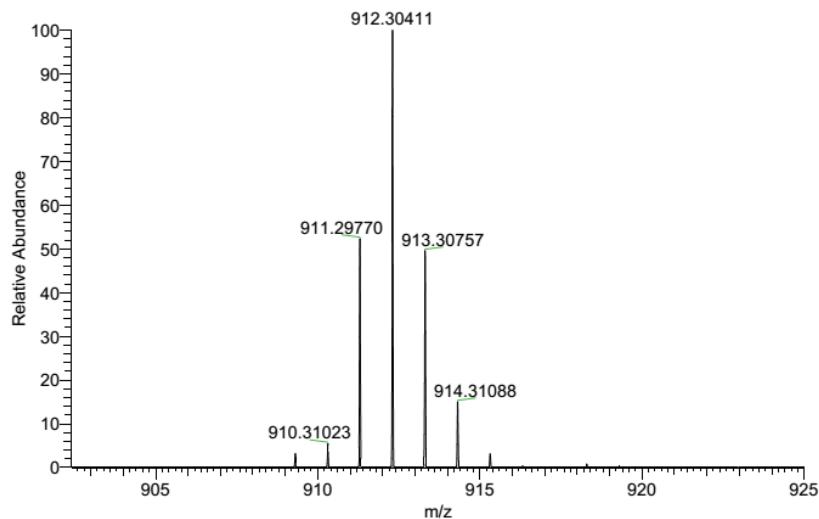


Figure S 24 – UPLC-MS analysis of 6B

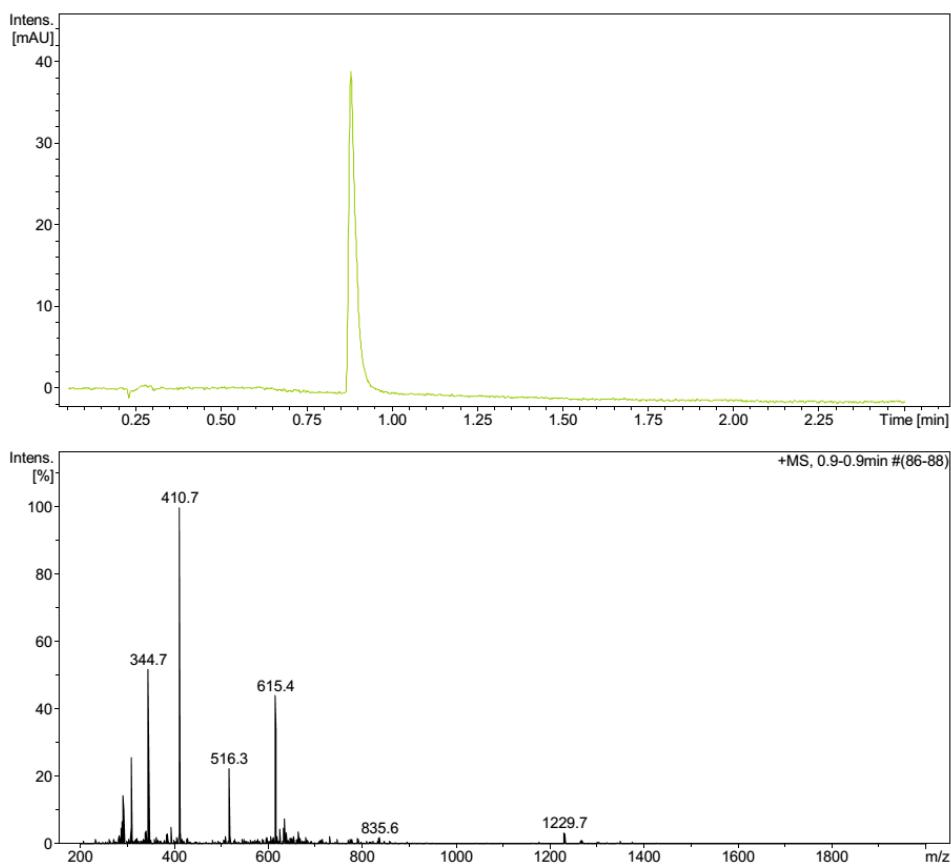


Figure S 25 – MALDI of 6B

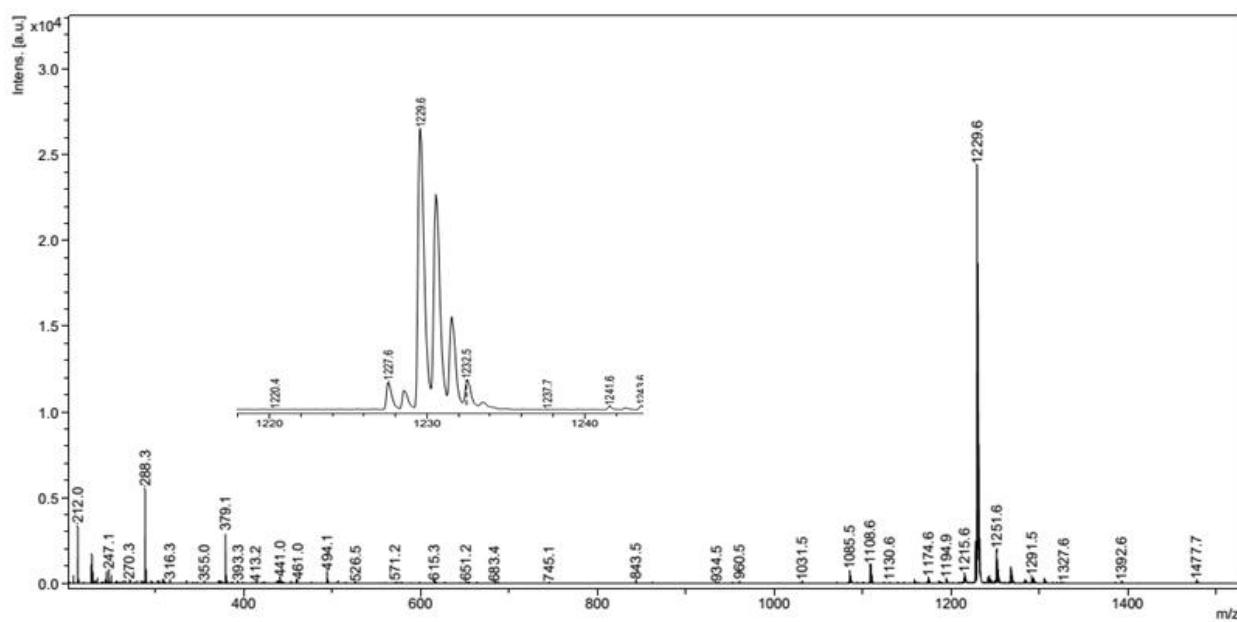


Figure S 26 – UPLC-MS analysis of 11

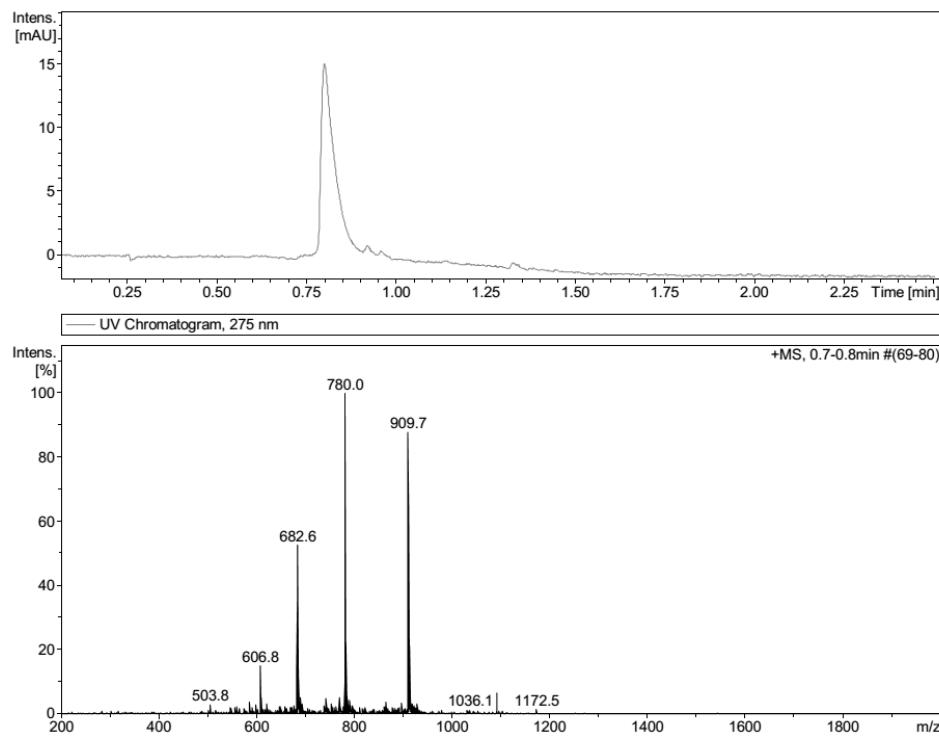


Figure S 27 – MALDI spectrum of 11

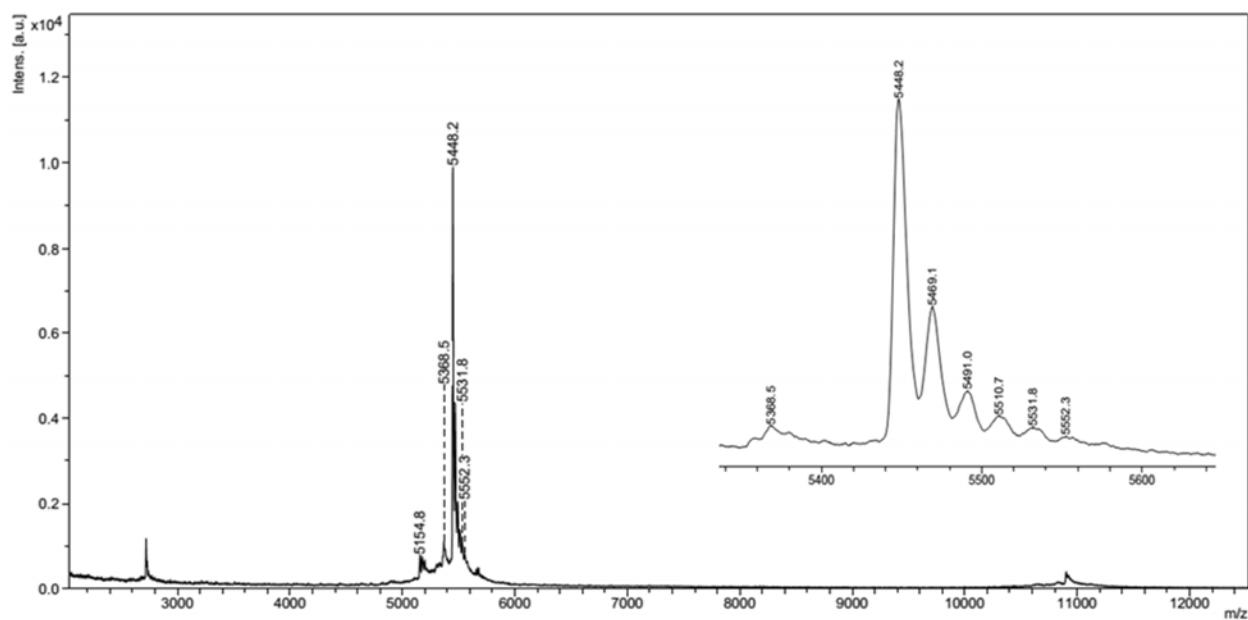


Figure S 28 – UPLC-MS analysis of 12

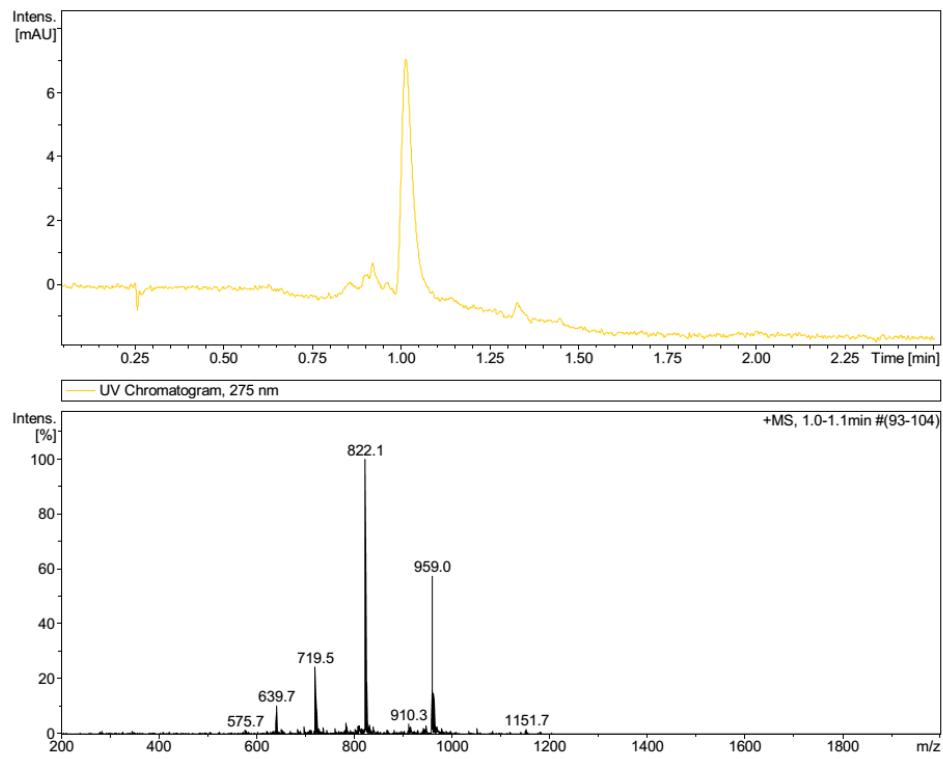


Figure S 29 – MALDI analysis of 12

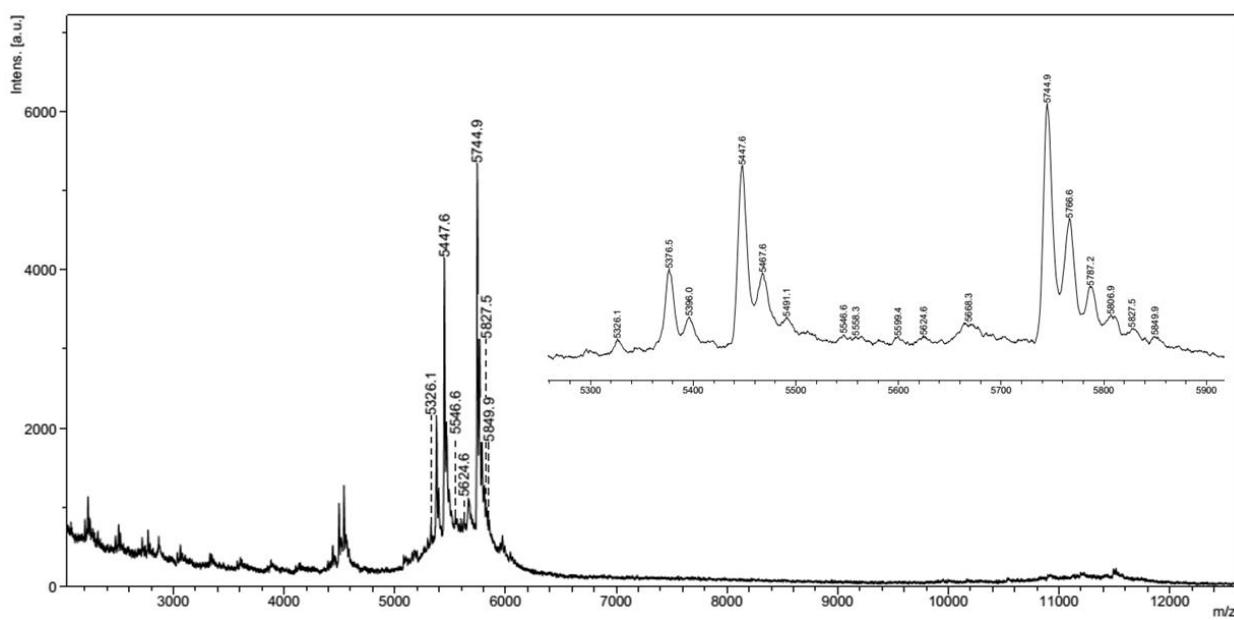


Figure S 30 – UPLC-MS analysis of 13

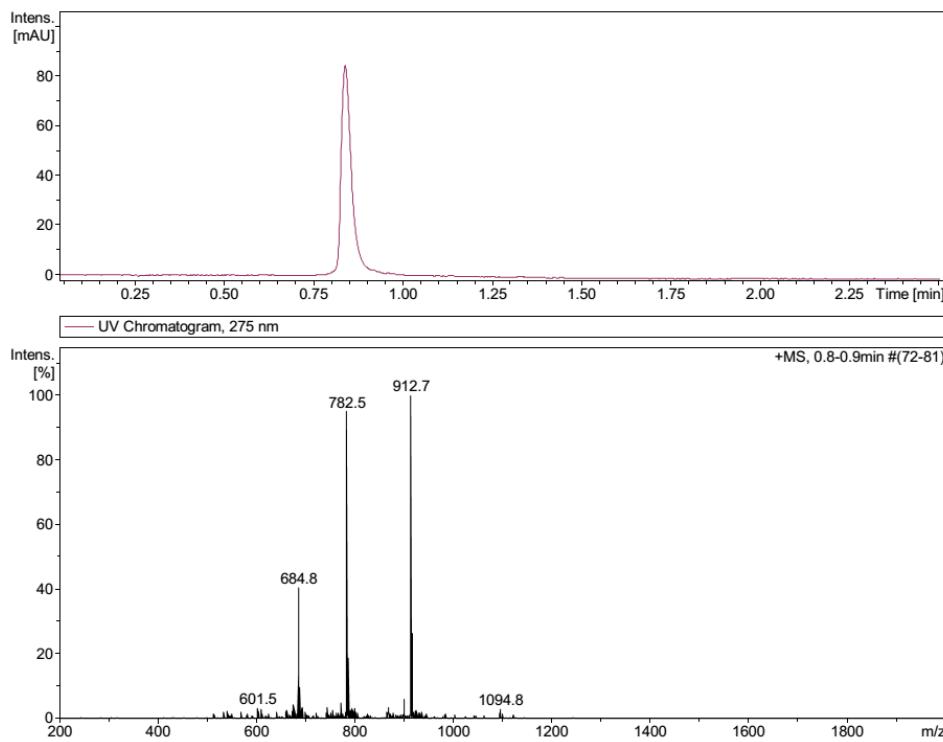


Figure S 31 – MALDI of 13

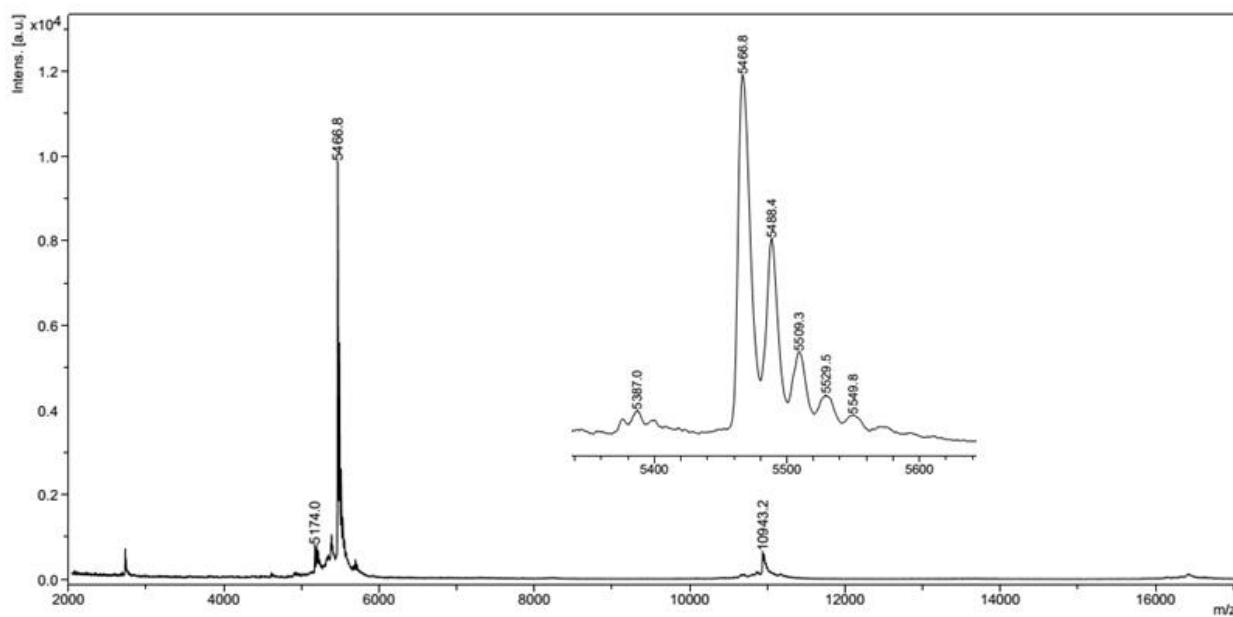


Figure S 32 – UPLC-MS analysis of 14

