

Supporting information for:

First results of transfer of 8 organic UV filters from sediment to the common ragworm *Hediste diversicolor*: bioaccumulation of benzophenone-3 and further proof of octocrylene metabolism

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Table S1. List of OC metabolites

Cmpd. #	Acyl chain	Formula	t_R (min)	Exp. <i>m/z</i> ([M+Na]⁺)	Calcd. <i>m/z</i> ([M+Na]⁺)
1	C16:0	C ₄₀ H ₅₇ O ₄ N	15.44	638.4177	638.418
2	C18:0	C ₄₂ H ₆₁ O ₄ N	16.46	666.45	666.4498
3	C18:1	C ₄₂ H ₅₉ O ₄ N	15.52	664.4338	664.4336
4	C18:1	C ₄₂ H ₅₉ O ₄ N	15.67	664.4330	664.4336
5	C20:1	C ₄₄ H ₆₃ O ₄ N	16.51	692.4647	692.4654
6	C20:2	C ₄₄ H ₆₁ O ₄ N	15.67	690.4496	690.4498
7	C20:2	C ₄₄ H ₆₁ O ₄ N	15.77	690.4495	690.4498
8	C20:3	C ₄₄ H ₅₉ O ₄ N	14.99	688.4339	688.4336
9	C20:5	C ₄₄ H ₅₅ O ₄ N	13.71	684.4025	684.4023
10	C22:2	C ₄₆ H ₆₅ O ₄ N	16.63	718.4806	718.4811
11	C22:6	C ₄₆ H ₅₇ O ₄ N	14.05	710.4181	710.418

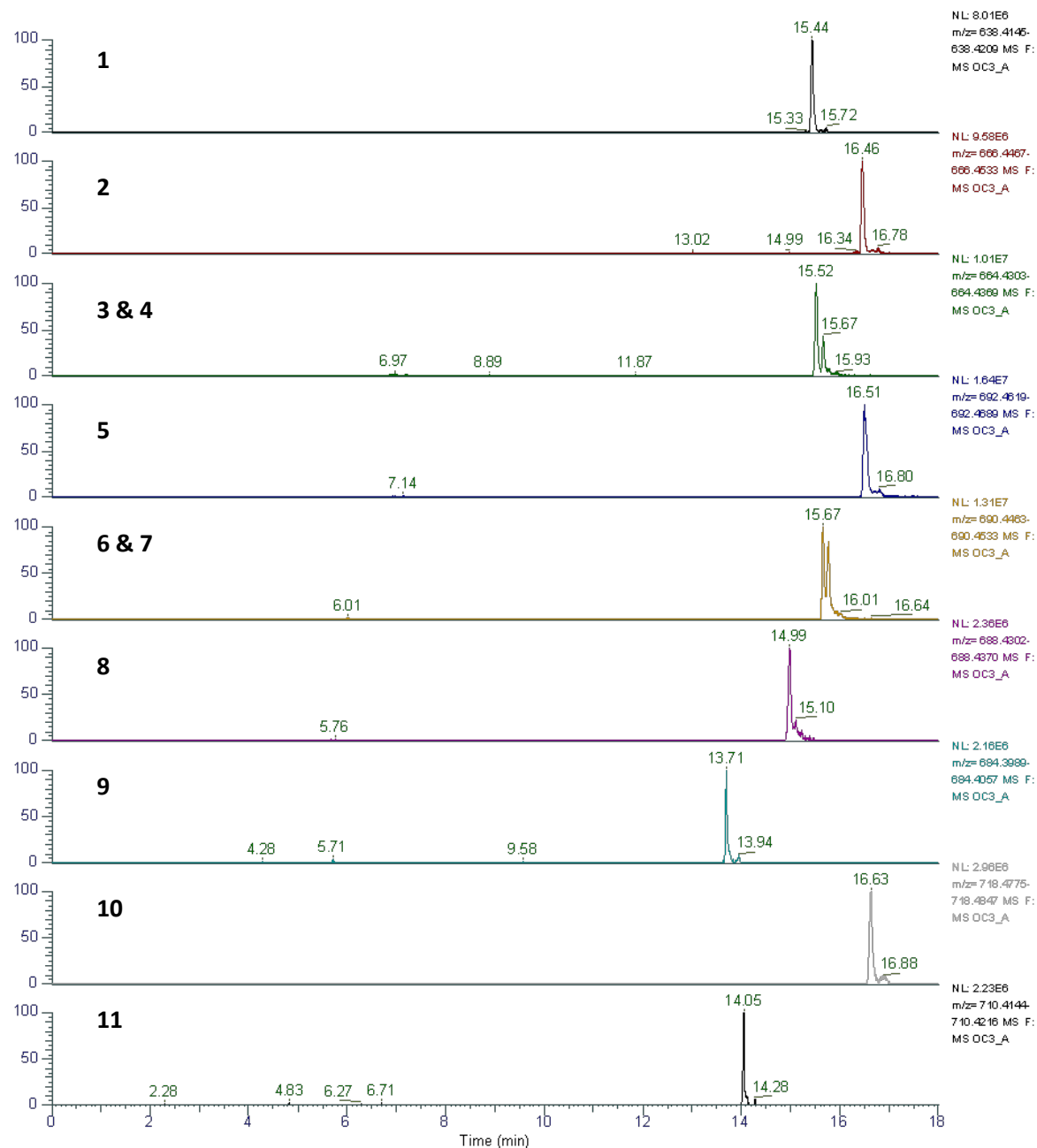


Figure S1. Extracted ion chromatograms for compounds **1** to **11** ($[M+Na]^+$) in the profile of worms *Hediste diversicolor* exposed to OC.

OC3_A #4207-4222 RT: 15.41-15.46 AV: 8 SB: 21 15.56-15.70 NL: 6.36E+007
T: FTMS + c ESI Full lock ms [133.4000-2000.0000]

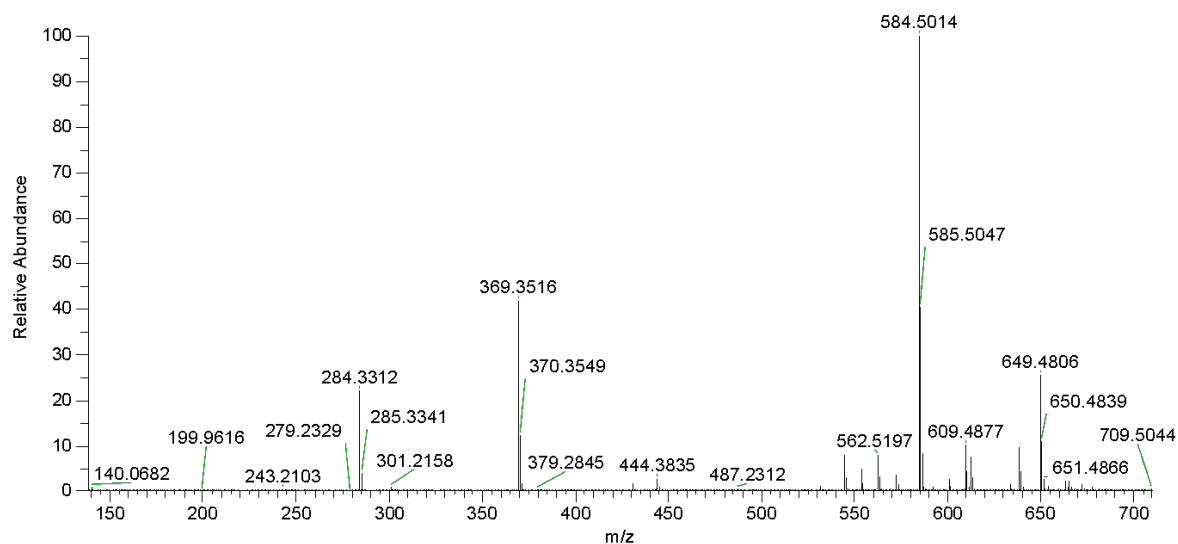


Figure S2. MS spectrum of compound 1

OC3_A #4207-4222 RT: 15.41-15.46 AV: 8 SB: 21 15.56-15.70 NL: 1.62E+007
T: FTMS + c ESI Full lock ms [133.4000-2000.0000]

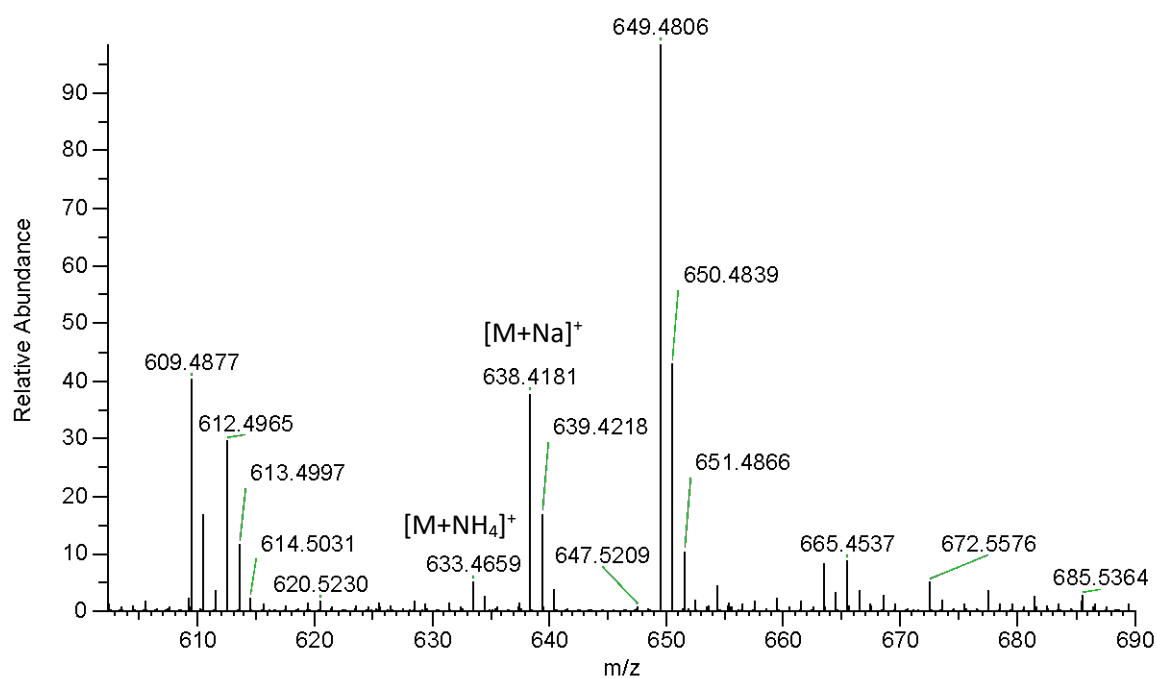


Figure S3. Expanded MS spectrum of compound 1

OC3_A #4210 RT: 15.42 AV: 1 NL: 8.04E+005
T: FTMS + c ESI d Full ms2 638.4180@hcd30.00 [50.0000-670.0000]

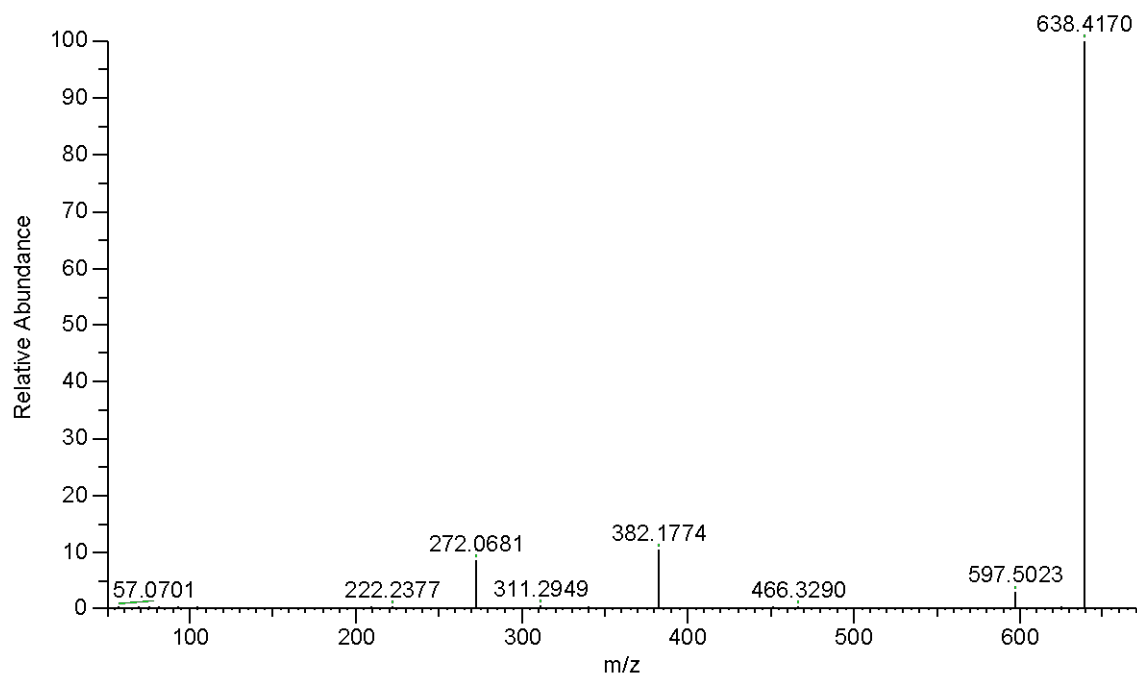


Figure S4. MS/MS spectrum of ion at m/z 638.4180 $[(1+Na)^+]$

OC3_A #4513-4528 RT: 16.44-16.49 AV: 8 SB: 24 16.21-16.37 NL: 7.75E+006
T: FTMS + c ESI Full lock ms [133.4000-2000.0000]

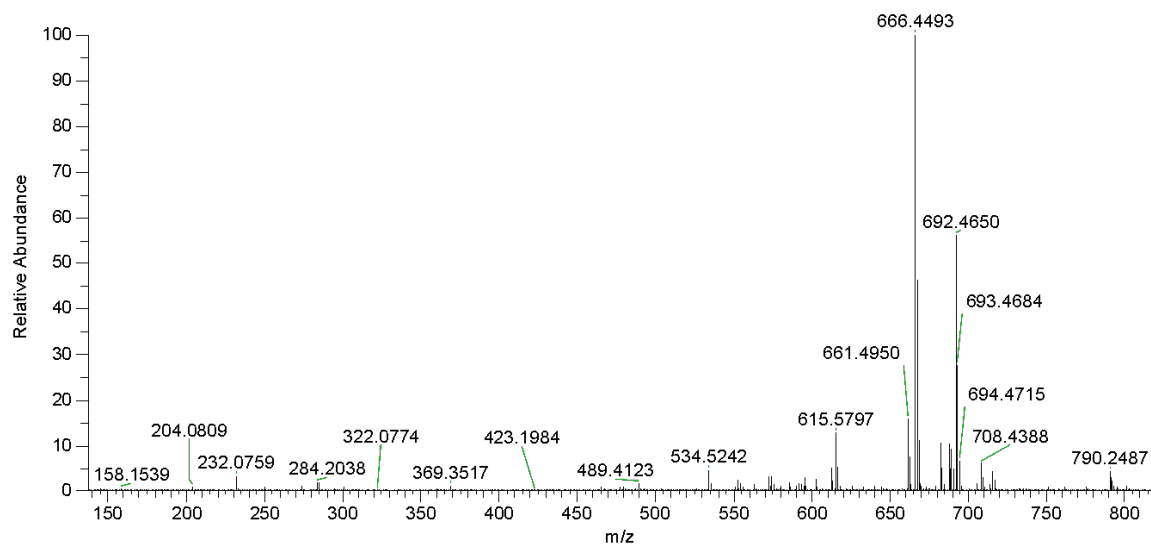


Figure S5. MS spectrum of compound **2**

OC3_A #4513-4528 RT: 16.44-16.49 AV: 8 SB: 24 16.21-16.37 NL: 7.75E+006
T: FTMS + c ESI Full lock ms [133.4000-2000.0000]

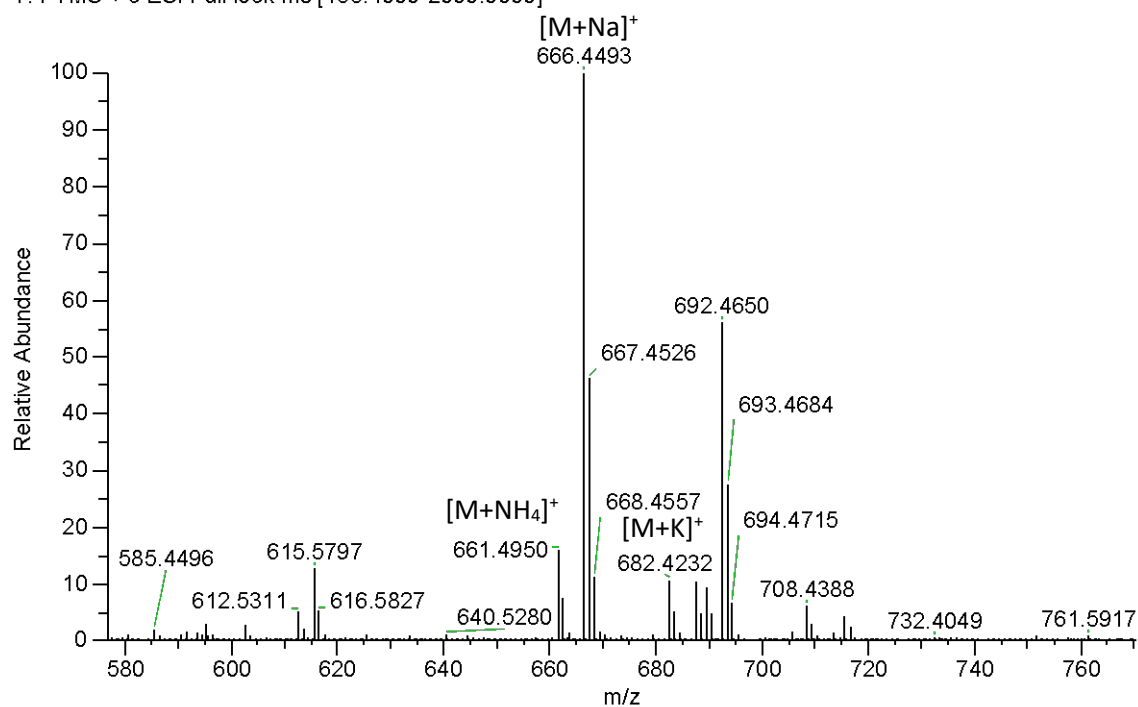


Figure S6. Expanded MS spectrum of compound 2

OC3_A #4514 RT: 16.44 AV: 1 NL: 7.06E+005
T: FTMS + c ESI d Full ms2 666.4493@hcd30.00 [50.0000-695.0000]

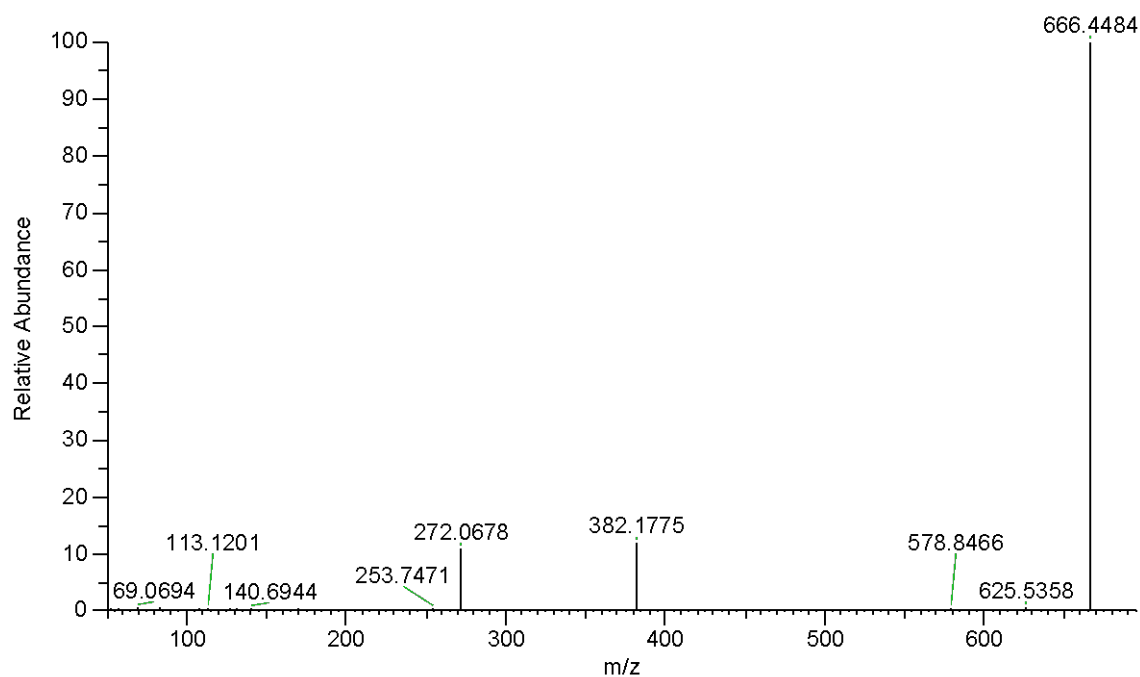


Figure S7. MS/MS spectrum of ion at m/z 666.4498 $[(2+Na)^+]$

OC3_A #4231-4246 RT: 15.49-15.54 AV: 8 SB: 23 15.30-15.45 NL: 7.77E+006
T: FTMS + c ESI Full lock ms [133.4000-2000.0000]

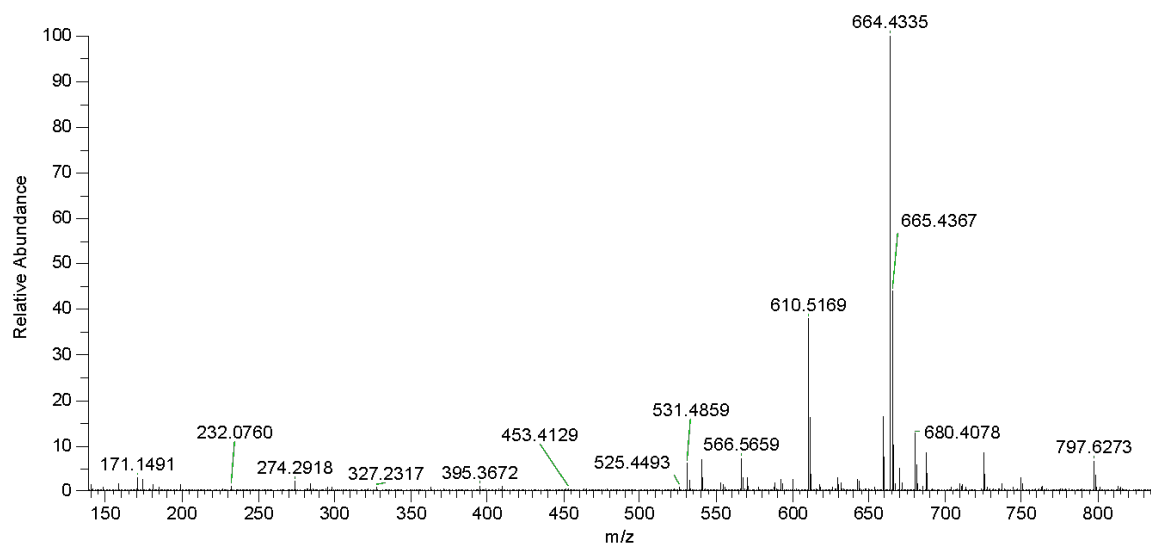


Figure S8. MS spectrum of compound 3

OC3_A #4231-4246 RT: 15.49-15.54 AV: 8 SB: 23 15.30-15.45 NL: 7.77E+006
T: FTMS + c ESI Full lock ms [133.4000-2000.0000]

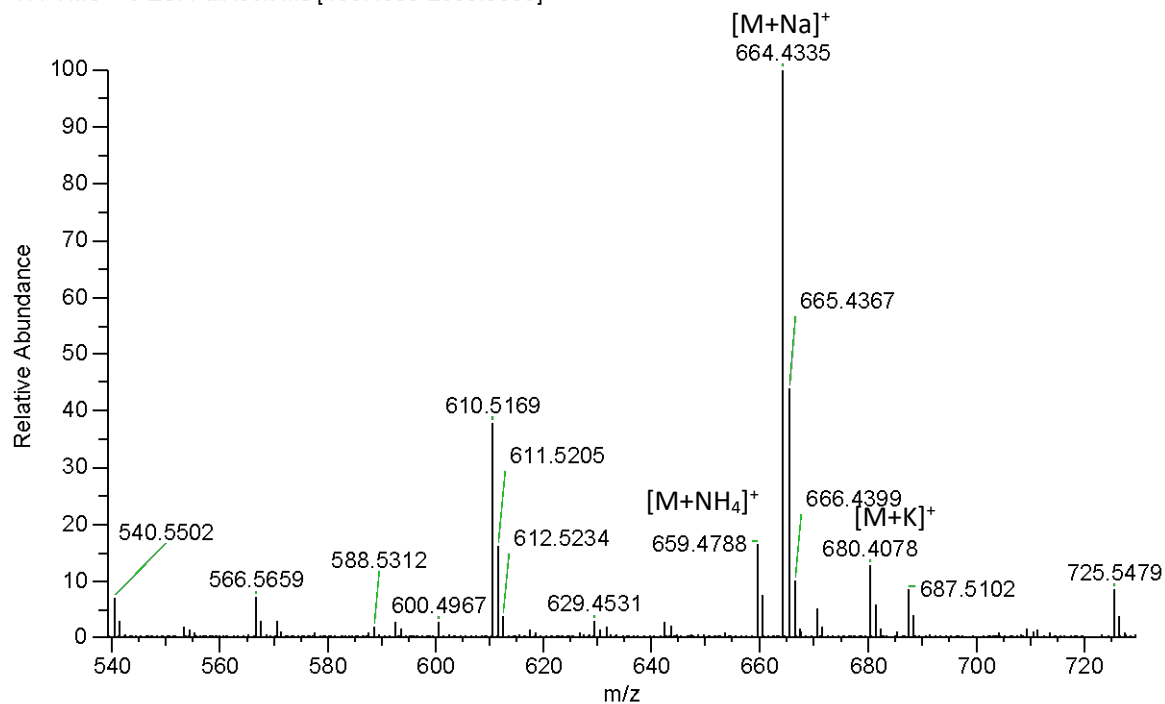


Figure S9. Expanded MS spectrum of compound 3

OC3_A #4236 RT: 15.51 AV: 1 NL: 1.30E+006
T: FTMS + c ESI d Full ms2 664.4334@hcd30.00 [50.0000-695.0000]

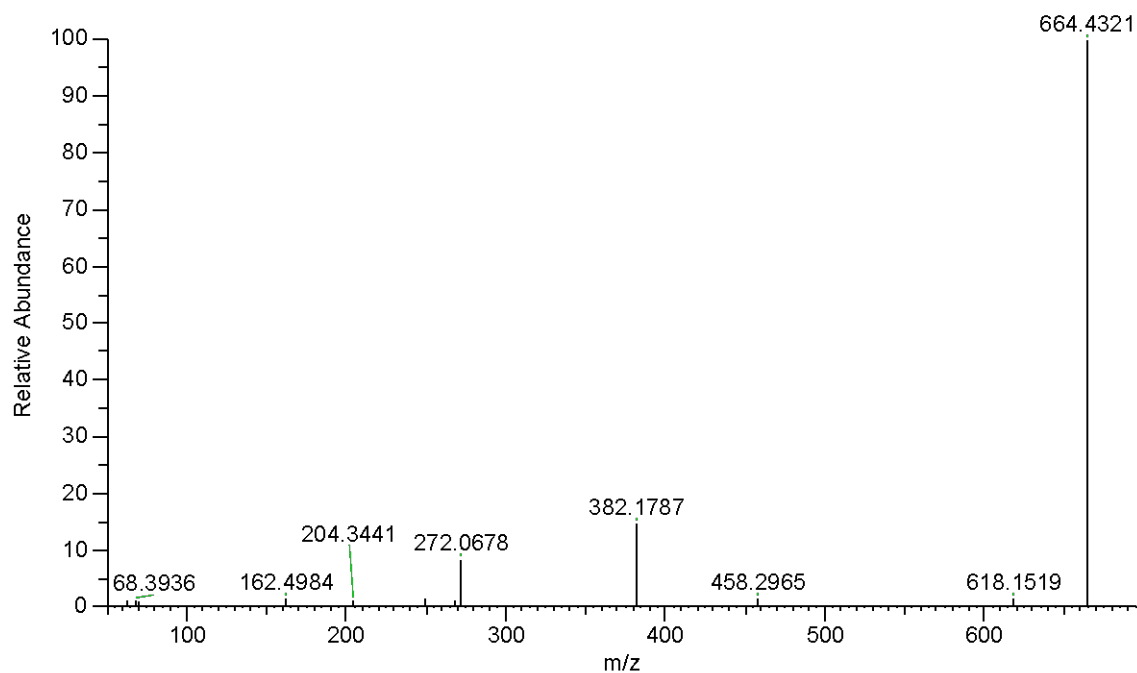


Figure S10. MS/MS spectrum of ion at m/z 664.4336 $[(3+Na)^+]$ and $[(4+Na)^+]$

OC3_A #4278-4290 RT: 15.65-15.69 AV: 6 SB: 28 15.78-15.96 NL: 2.95E7
T: FTMS + c ESI Full lock ms [133.4000-2000.0000]

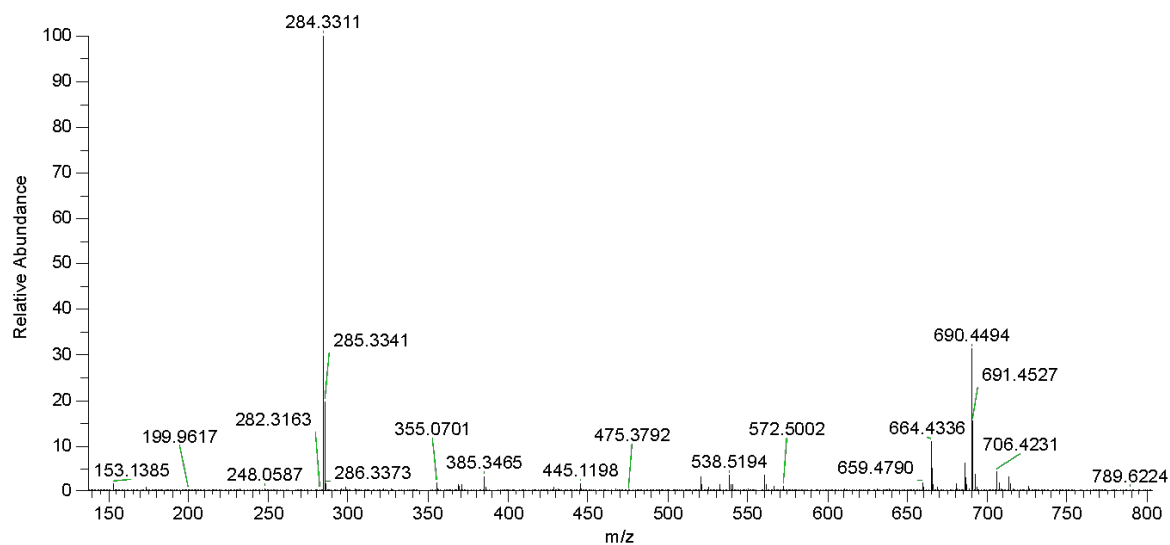


Figure S11. MS spectrum of compound 4

OC3_A #4278-4290 RT: 15.65-15.69 AV: 6 SB: 28 15.78-15.96 NL: 3.23E+006
T: FTMS + c ESI Full lock ms [133.4000-2000.0000]

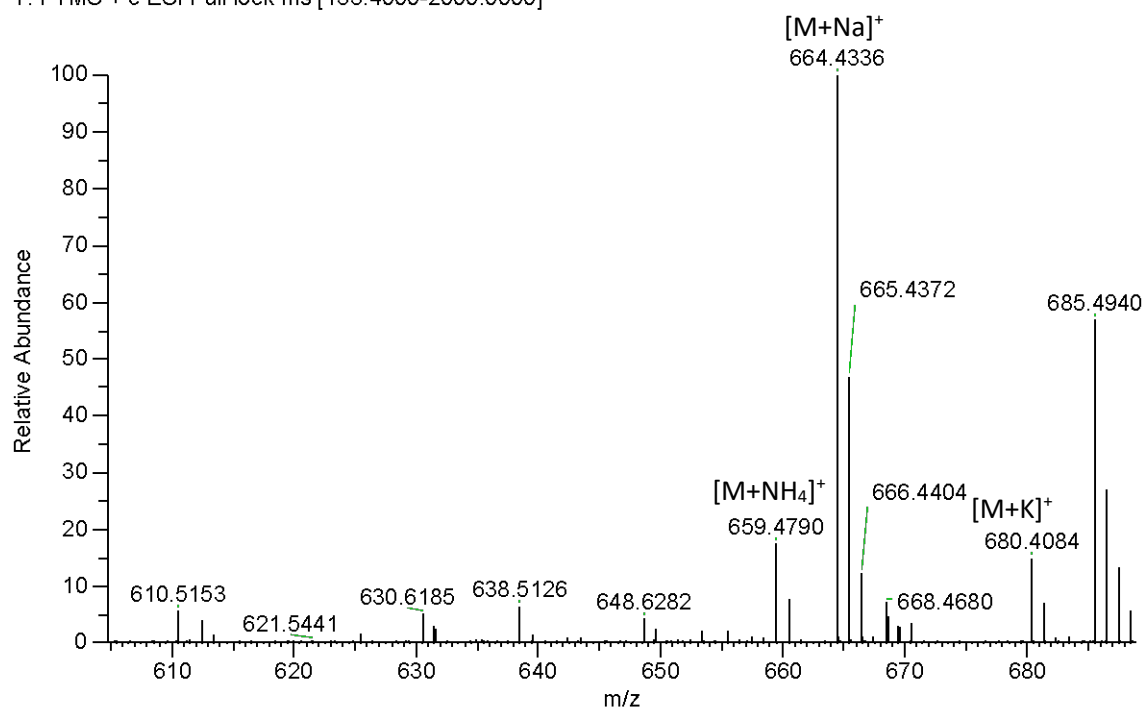


Figure S12. Expanded MS spectrum of compound 4

OC3_A #4522-4552 RT: 16.47-16.57 AV: 15 SB: 12 16.34-16.42 NL: 1.18E+007
T: FTMS + c ESI Full lock ms [133.4000-2000.0000]

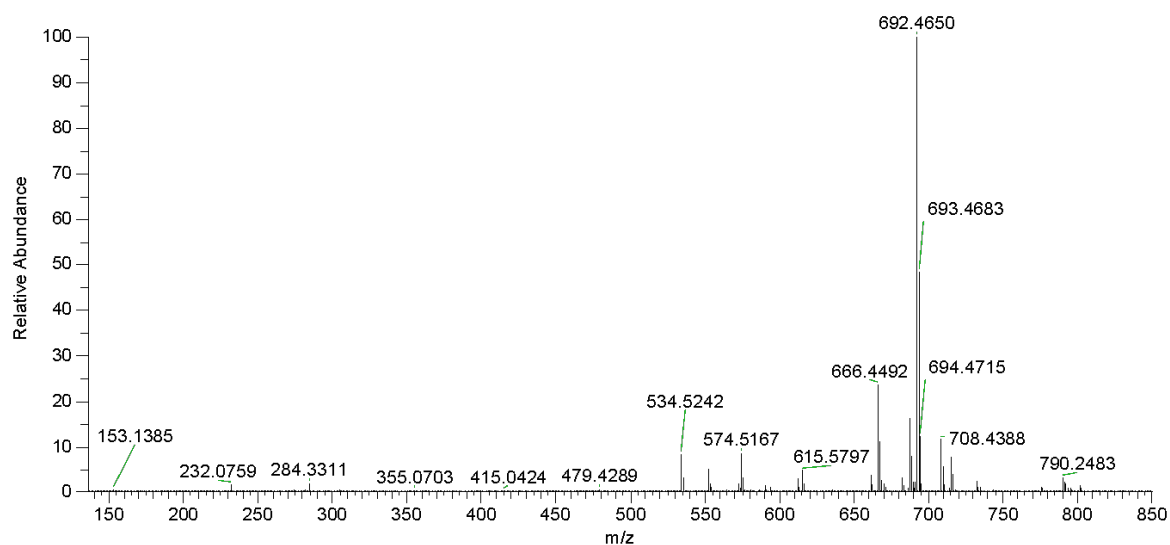


Figure S13. MS spectrum of compound 5

OC3_A #4522-4552 RT: 16.47-16.57 AV: 15 SB: 12 16.34-16.42 NL: 1.18E+007
T: FTMS + c ESI Full lock ms [133.4000-2000.0000]

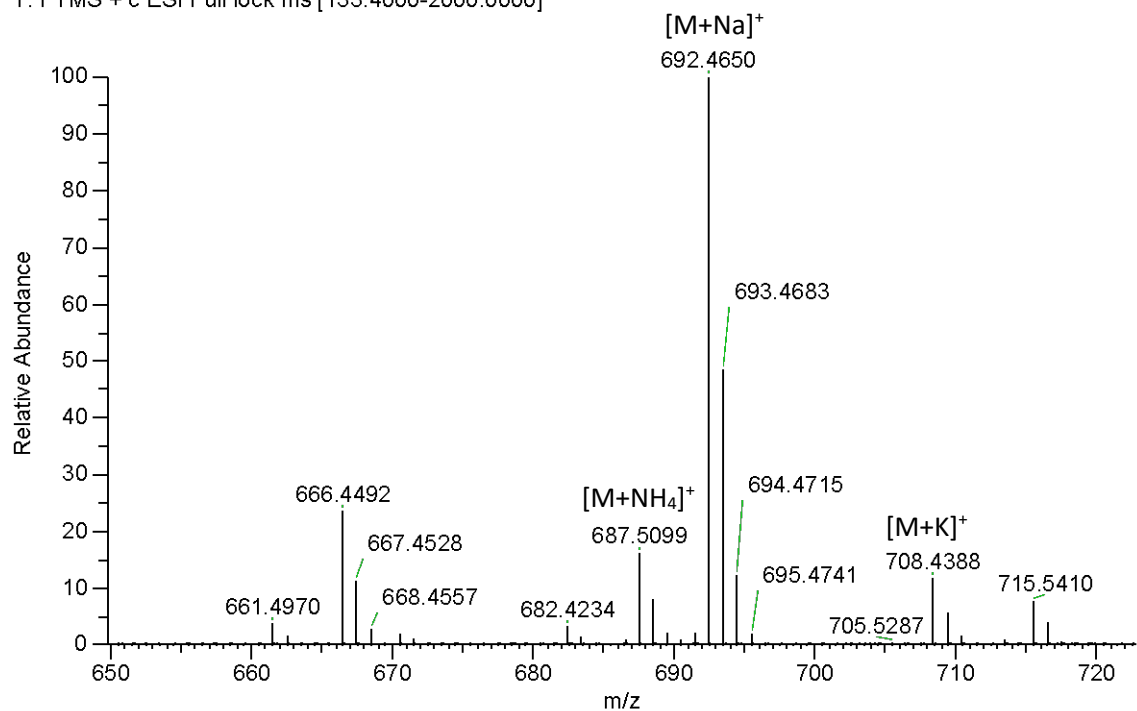


Figure S14. Expanded MS spectrum of compound **5**

OC3_A #4522 RT: 16.47 AV: 1 NL: 6.10E+005
T: FTMS + c ESI d Full ms2 692.4650@hcd30.00 [50.0000-725.0000]

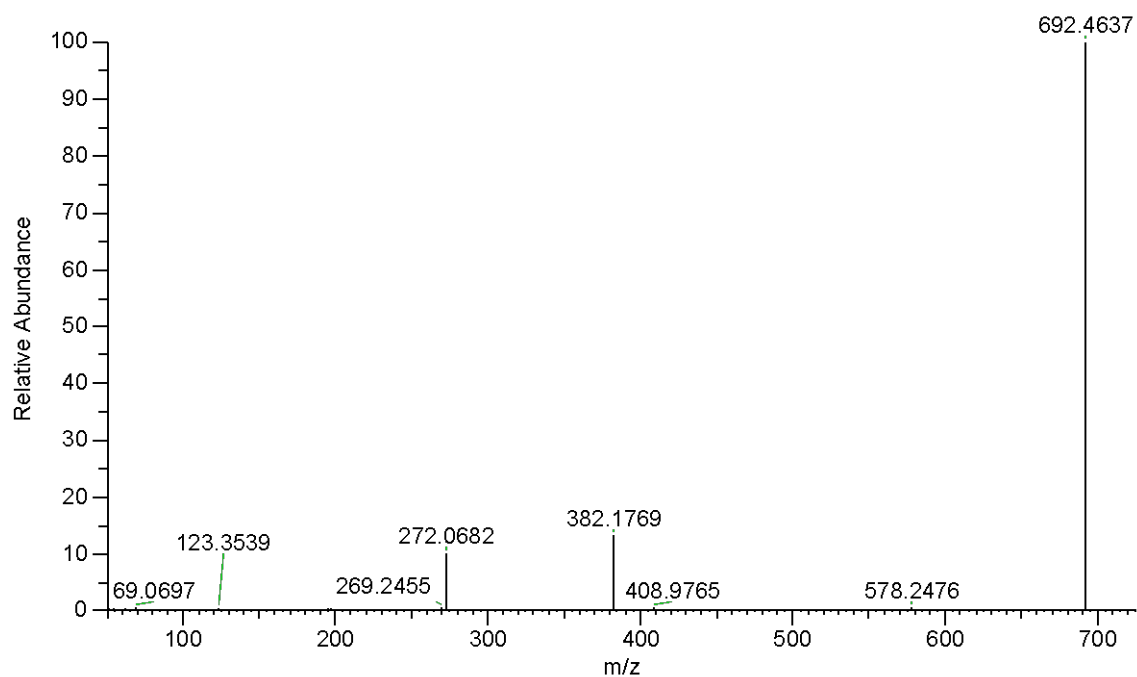


Figure S15. MS/MS spectrum of ion at m/z 692.4654 $[(5+Na)^+]$

OC3_A #4530 RT: 16.50 AV: 1 NL: 8.16E+005
T: FTMS + c ESI d Full ms2 687.5099@hcd30.00 [50.0000-720.0000]

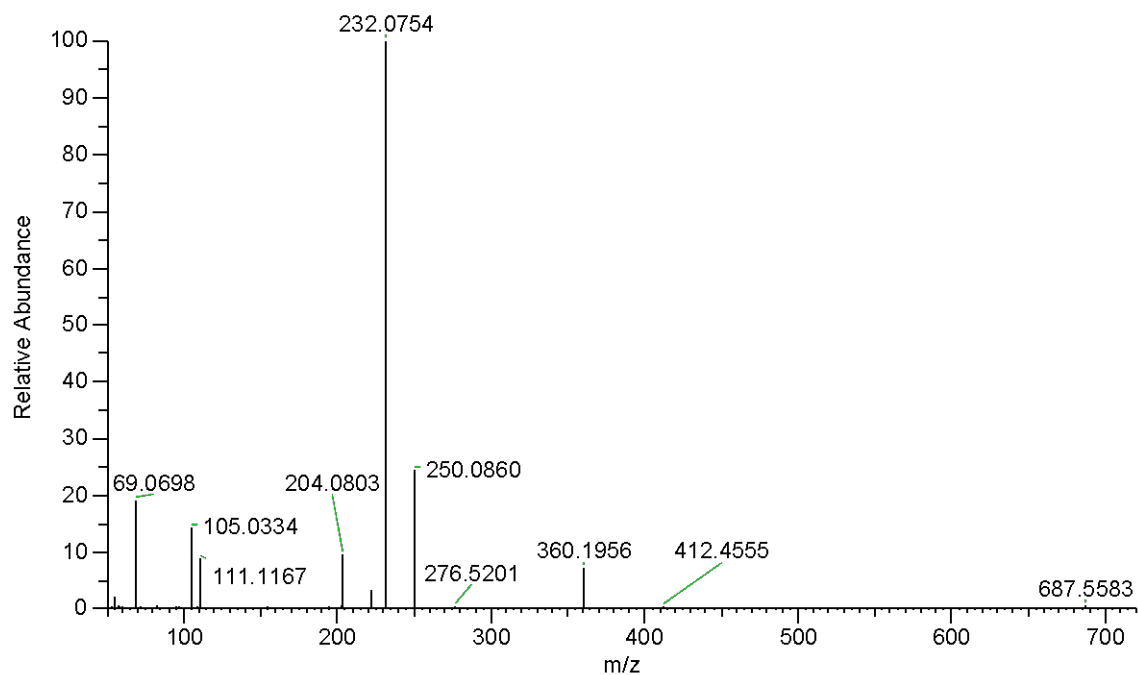


Figure S16. MS/MS spectrum of ion at m/z 687.5099 [(5+NH₄)⁺]

OC3_A #4278-4290 RT: 15.65-15.69 AV: 6 SB: 10 15.55-15.61 NL: 1.65E+007
T: FTMS + c ESI Full lock ms [133.4000-2000.0000]

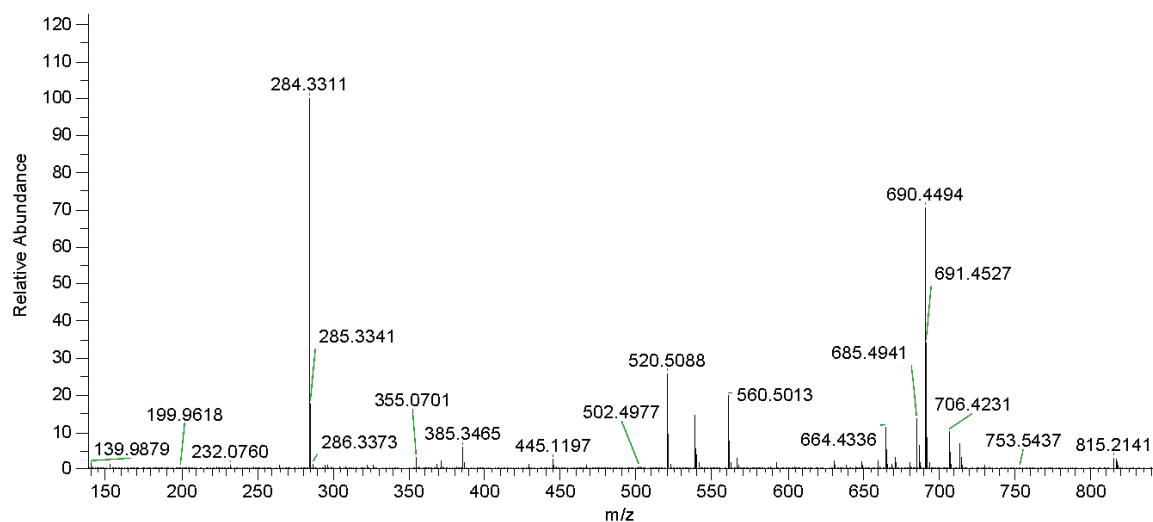


Figure S17. MS spectrum of compound **6**

OC3_A #4278-4290 RT: 15.65-15.69 AV: 6 SB: 10 15.55-15.61 NL: 1.16E+007
T: FTMS + c ESI Full lock ms [133.4000-2000.0000]

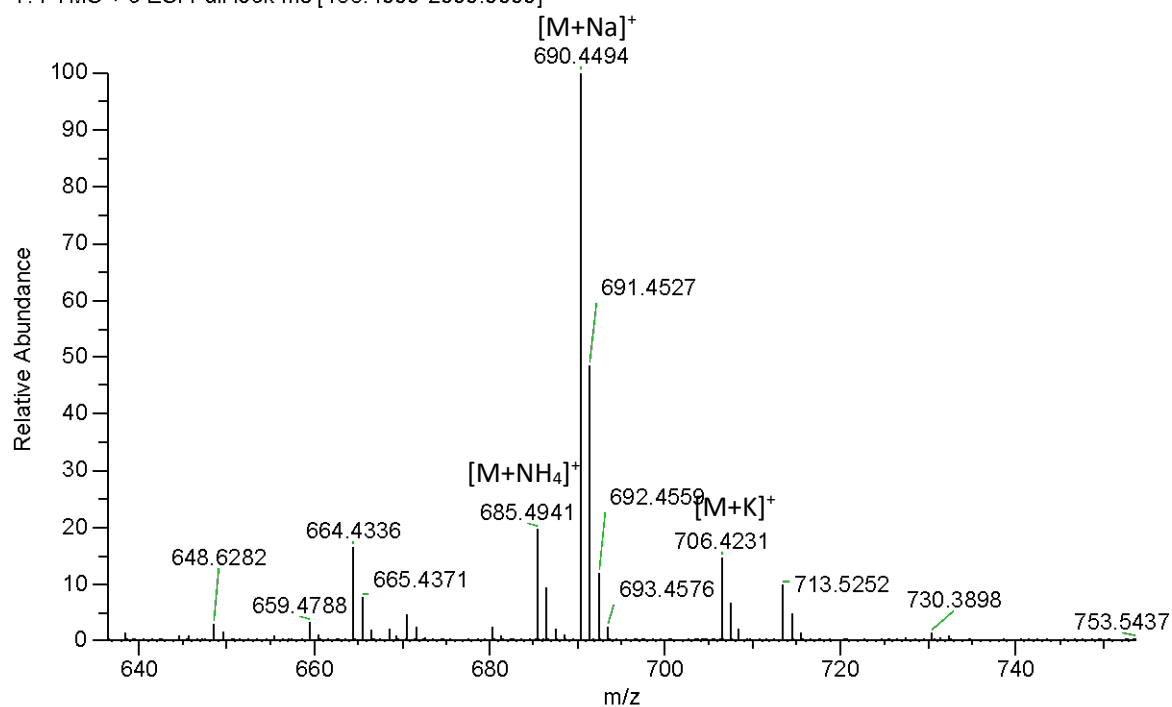


Figure S18. Expanded MS spectrum of compound 6

OC3_A #4280 RT: 15.66 AV: 1 NL: 1.44E+006
T: FTMS + c ESI d Full ms2 690.4494@hcd30.00 [50.0000-720.0000]

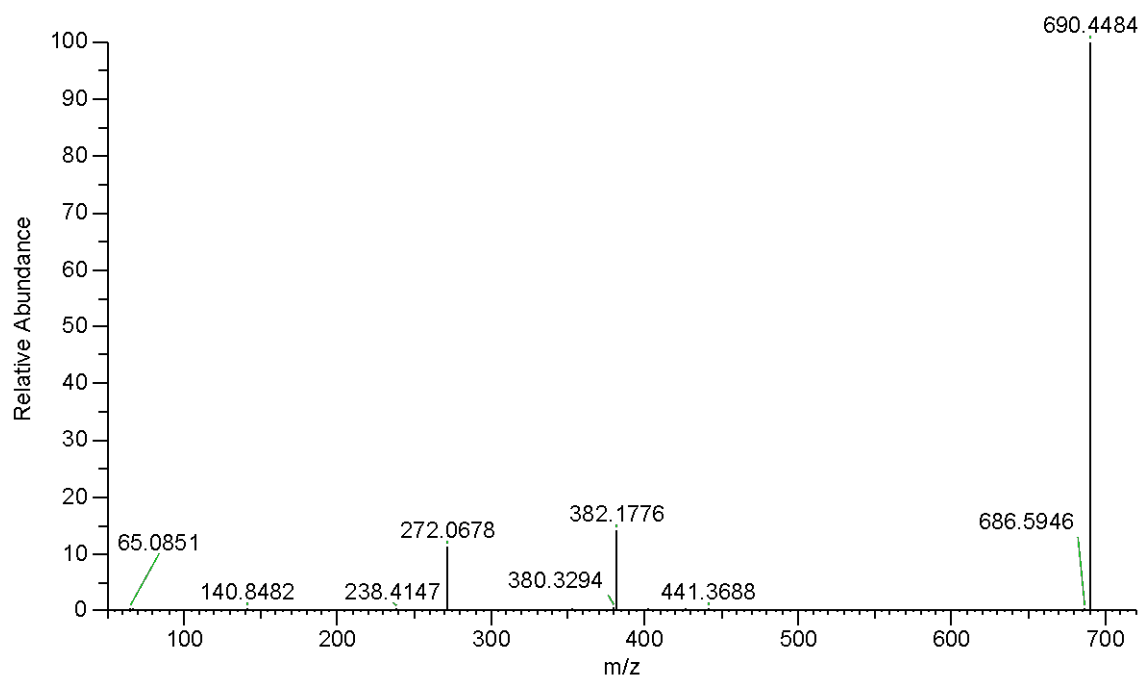


Figure S19. MS/MS spectrum of ion at m/z 690.4498 $[(6+Na)^+]$

OC3_A #4309-4321 RT: 15.75-15.79 AV: 7 SB: 3 15.71-15.73 NL: 5.71E+006
T: FTMS + c ESI Full lock ms [133.4000-2000.0000]

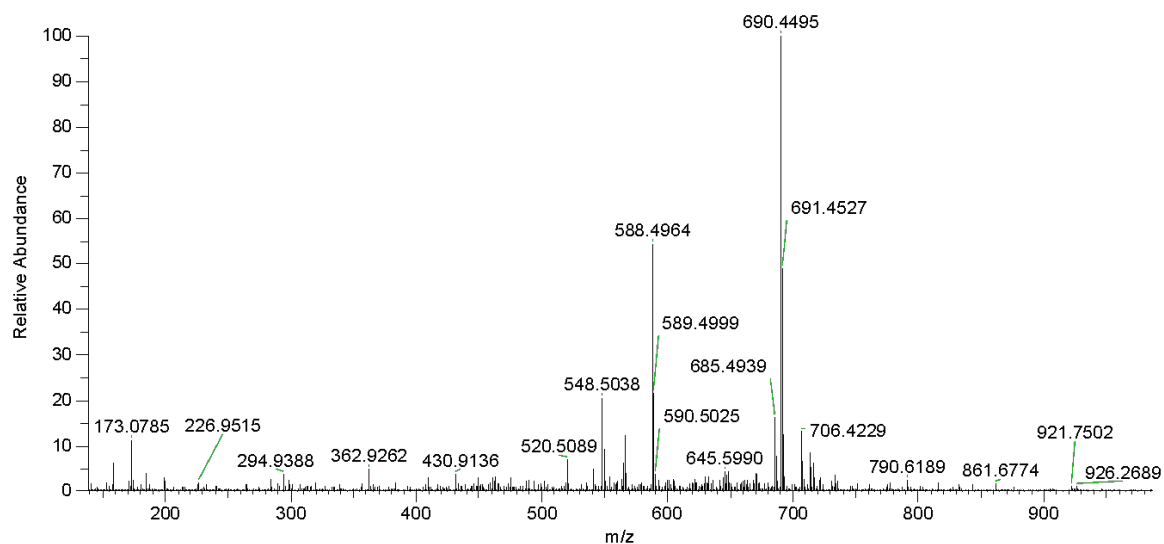


Figure S20. MS spectrum of compound 7

OC3_A #4309-4321 RT: 15.75-15.79 AV: 7 SB: 3 15.71-15.73 NL: 5.71E+006
T: FTMS + c ESI Full lock ms [133.4000-2000.0000]

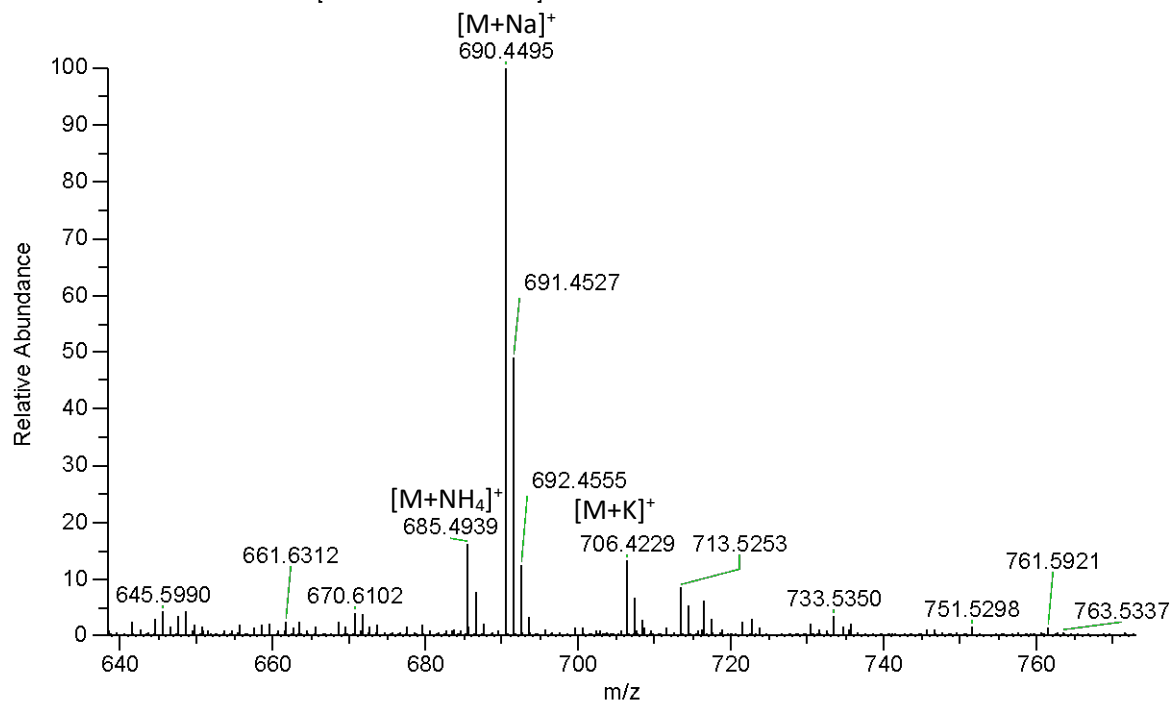


Figure S21. Expanded MS spectrum of compound 7

OC3_A #4073-4091 RT: 14.96-15.02 AV: 10 SB: 19 14.76-14.89 NL: 1.67E+006
T: FTMS + c ESI Full lock ms [133.4000-2000.0000]

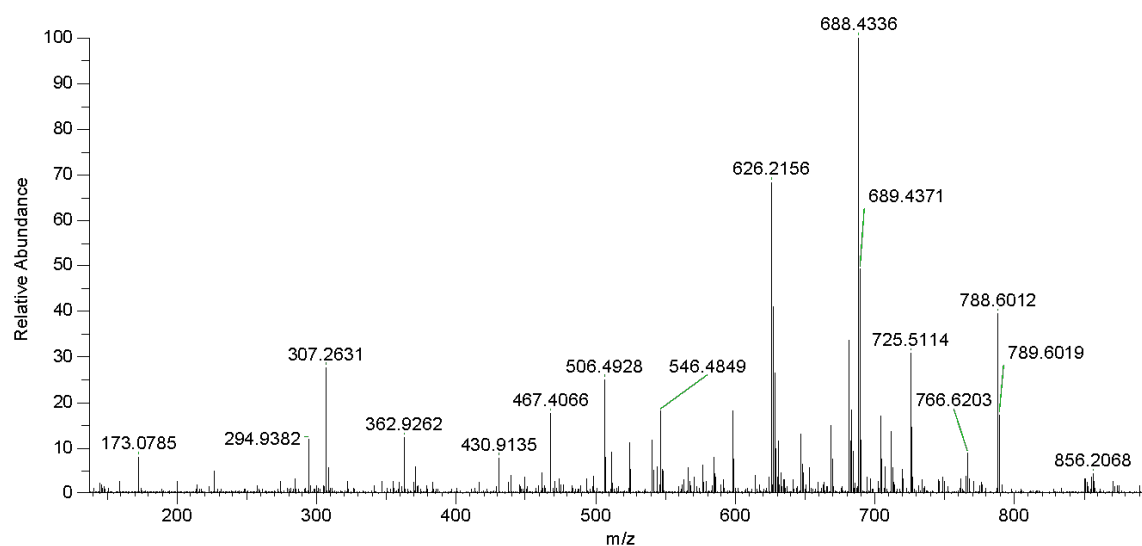


Figure S22. MS spectrum of compound **8**

OC3_A #4073-4091 RT: 14.96-15.02 AV: 10 SB: 19 14.76-14.89 NL: 1.67E+006
T: FTMS + c ESI Full lock ms [133.4000-2000.0000]

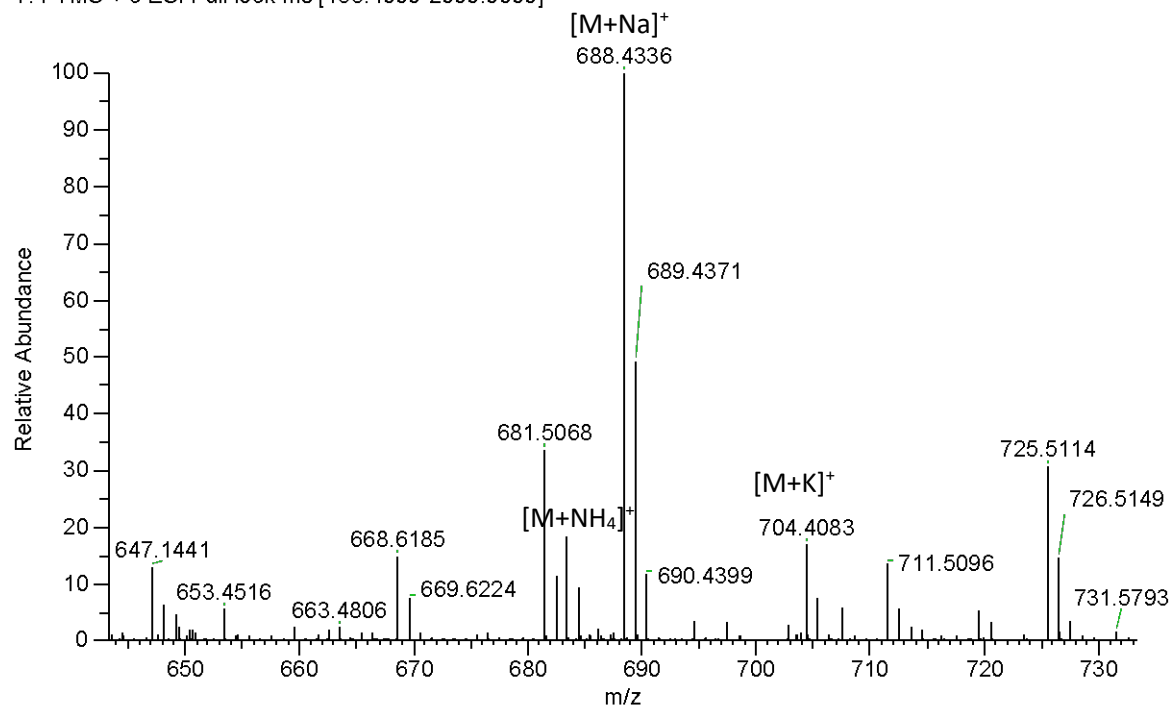


Figure S23. Expanded MS spectrum of compound **8**

OC3_A #4086 RT: 15.00 AV: 1 NL: 2.00E+005
T: FTMS + c ESI d Full ms2 688.4336@hcd30.00 [50.0000-720.0000]

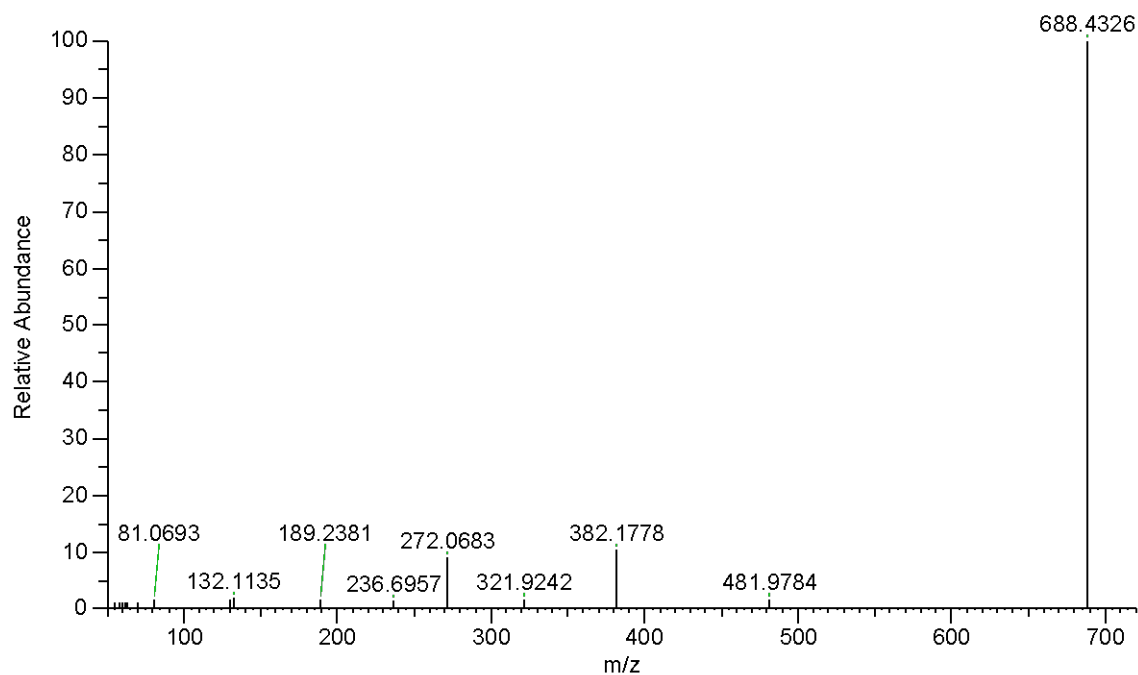


Figure S24. MS/MS spectrum of ion at m/z 688.4336 [(8+Na)⁺]

OC3_A #3688-3709 RT: 13.67-13.74 AV: 11 SB: 12 13.56-13.64 NL: 2.37E+006
T: FTMS + c ESI Full lock ms [133.4000-2000.0000]

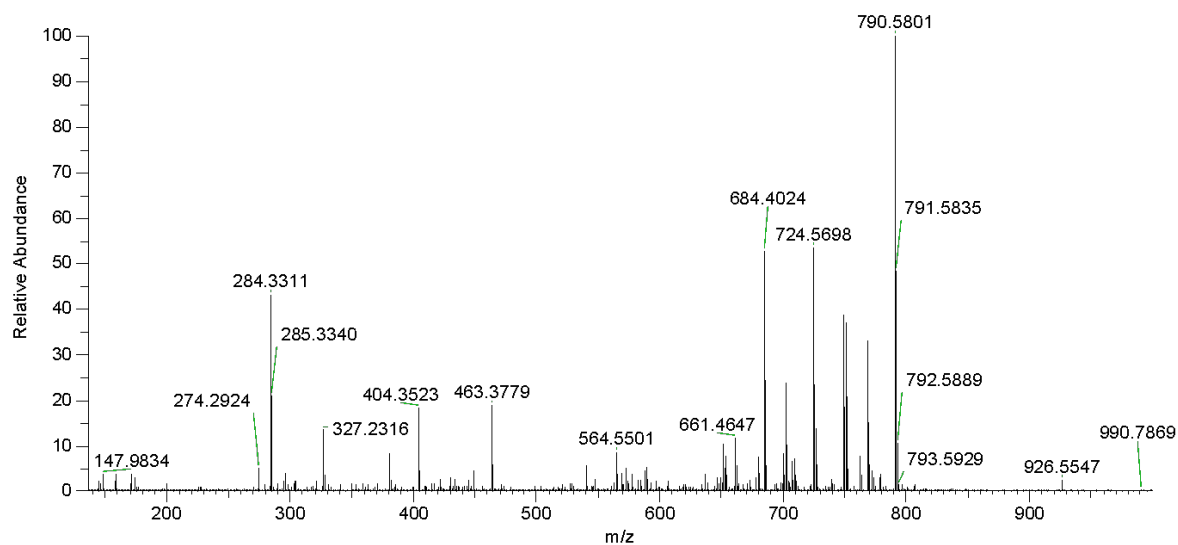


Figure S25. MS spectrum of compound **9**

OC3_A #3688-3709 RT: 13.67-13.74 AV: 11 SB: 12 13.56-13.64 NL: 1.25E+006
T: FTMS + c ESI Full lock ms [133.4000-2000.0000]

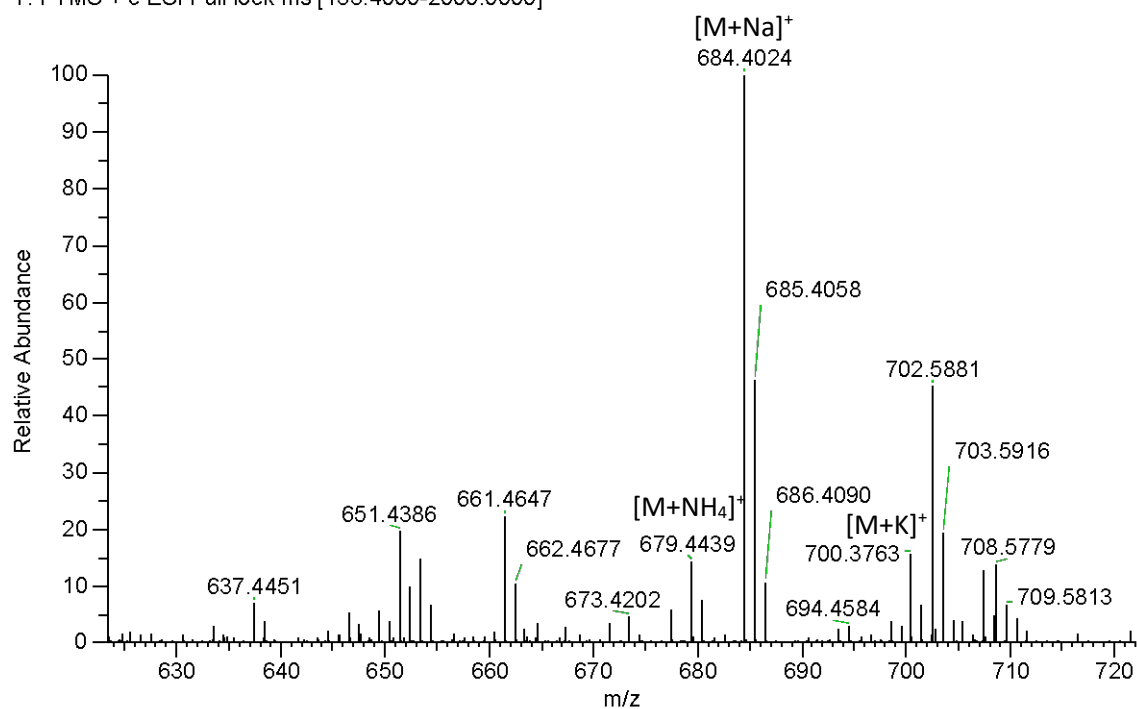


Figure S26. Expanded MS spectrum of compound **9**

OC3_A #3700 RT: 13.71 AV: 1 NL: 2.20E+005
T: FTMS + c ESI d Full ms2 684.4025@hcd30.00 [50.0000-715.0000]

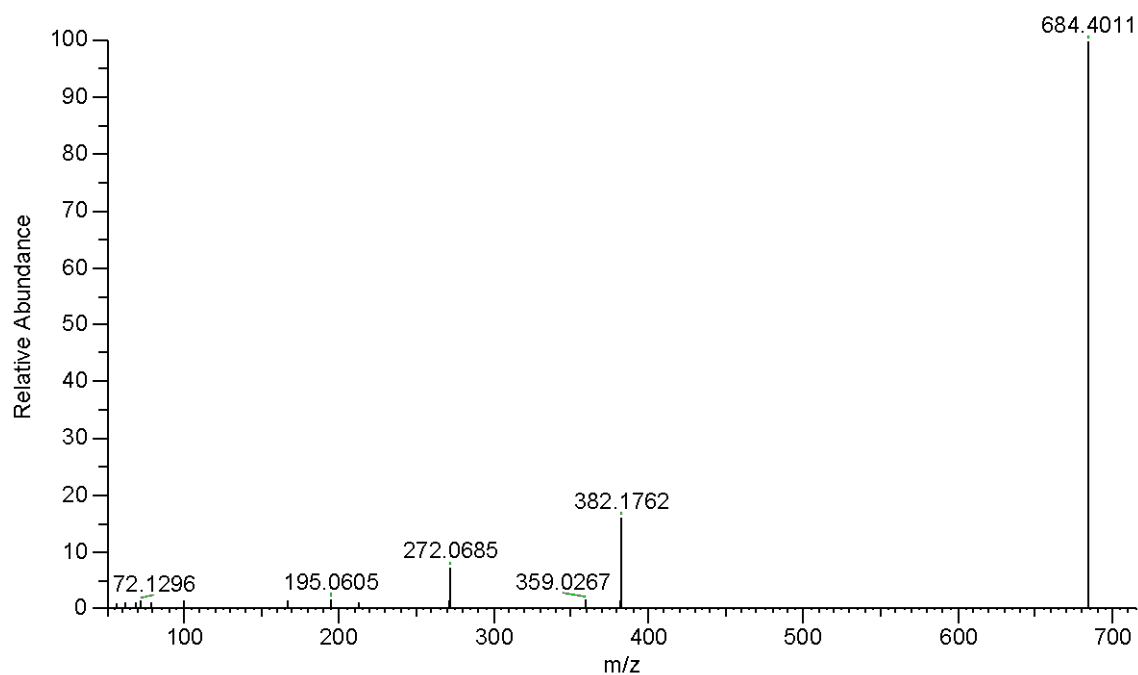


Figure S27. MS/MS spectrum of ion at m/z 684.4023 $[(9+Na)^+]$

OC3_A #4560-4578 RT: 16.6-16.66 AV: 9 SB: 31 16.36-16.56 NL: 2.39E+006
T: FTMS + c ESI Full lock ms [133.4000-2000.0000]

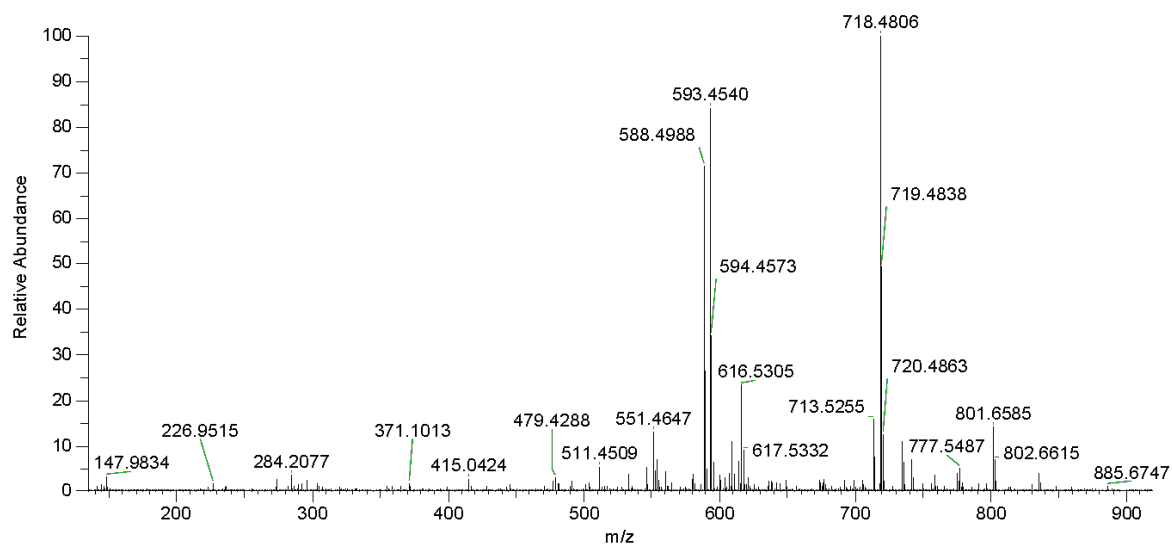


Figure S28. MS spectrum of compound **10**

OC3_A #4560-4578 RT: 16.6-16.66 AV: 9 SB: 31 16.36-16.56 NL: 2.39E+006
T: FTMS + c ESI Full lock ms [133.4000-2000.0000]

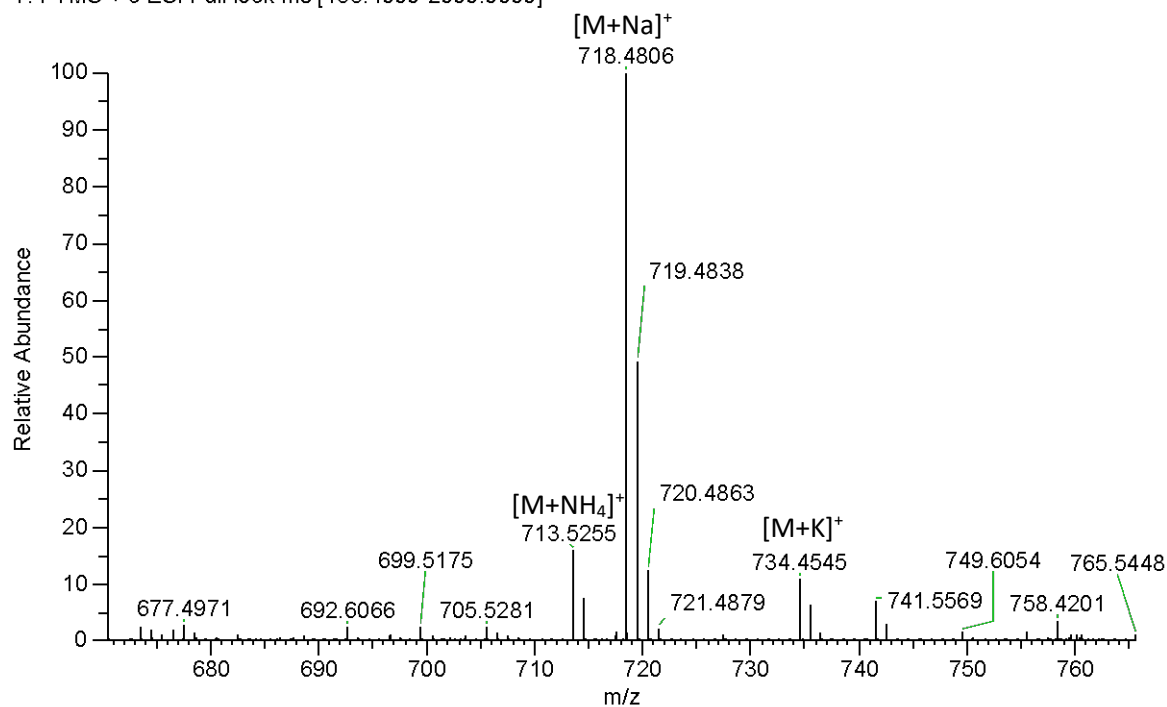


Figure S29. Expanded MS spectrum of compound **10**

OC3_A #4570 RT: 16.63 AV: 1 NL: 4.19E+005
T: FTMS + c ESI d Full ms2 718.4804@hcd30.00 [50.0000-750.0000]

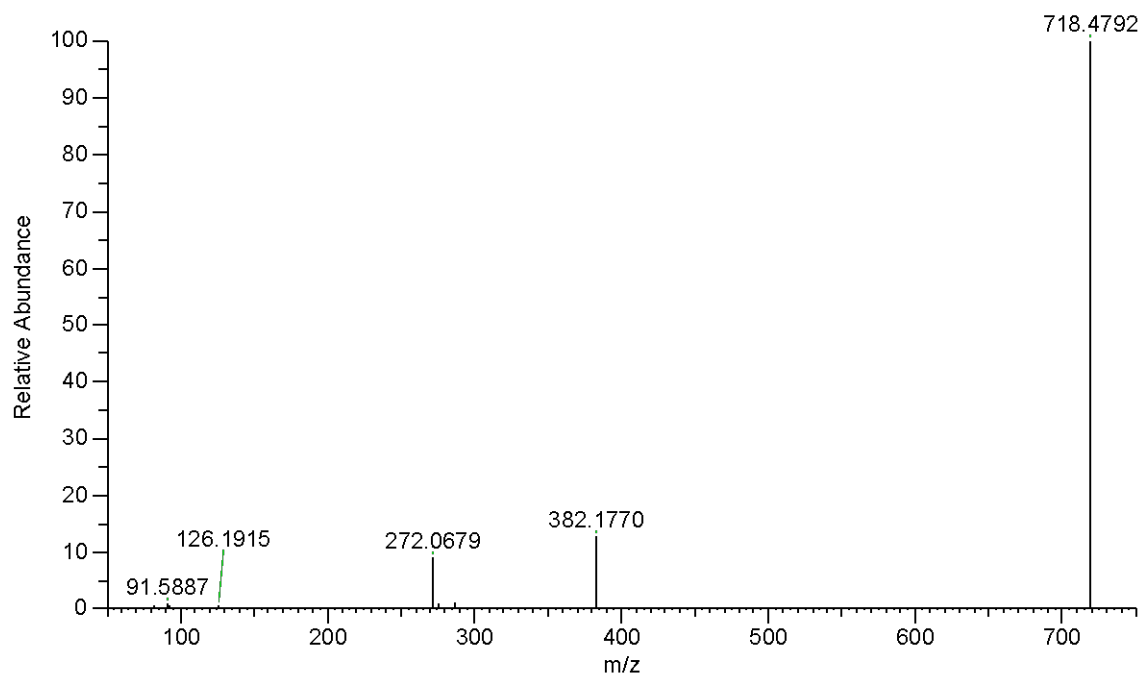


Figure S30. MS/MS spectrum of ion at m/z 718.4811 [(10+Na)⁺]

OC3_A #3792-3807 RT: 14.02-14.07 AV: 8 SB: 17 13.88-14.00 NL: 3.30E+007
T: FTMS + c ESI Full lock ms [133.4000-2000.0000]

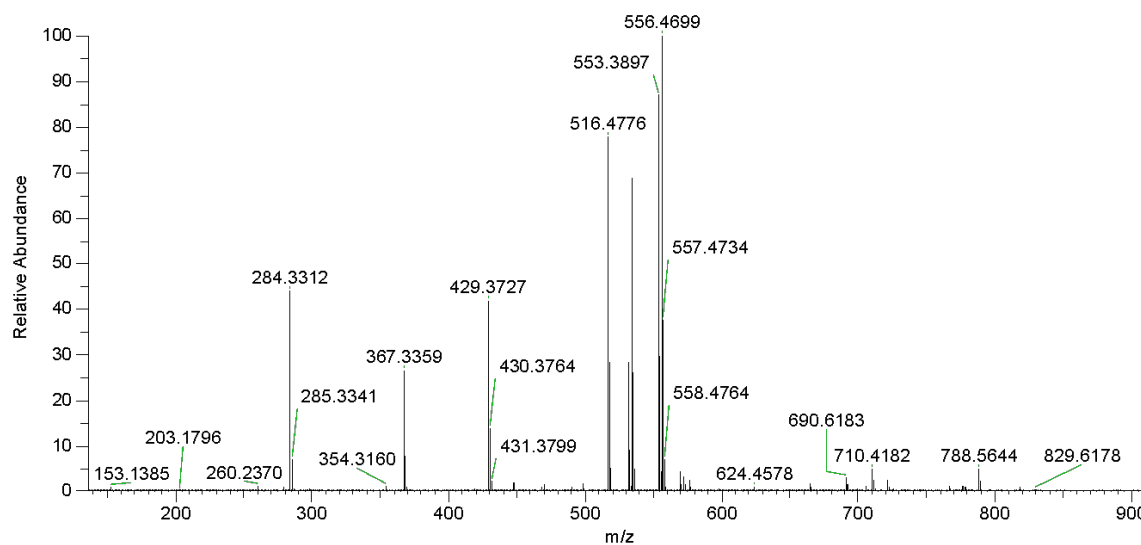


Figure S31. MS spectrum of compound **11**

OC3_A #3792-3807 RT: 14.02-14.07 AV: 8 SB: 17 13.88-14.00 NL: 1.60E+006
T: FTMS + c ESI Full lock ms [133.4000-2000.0000]

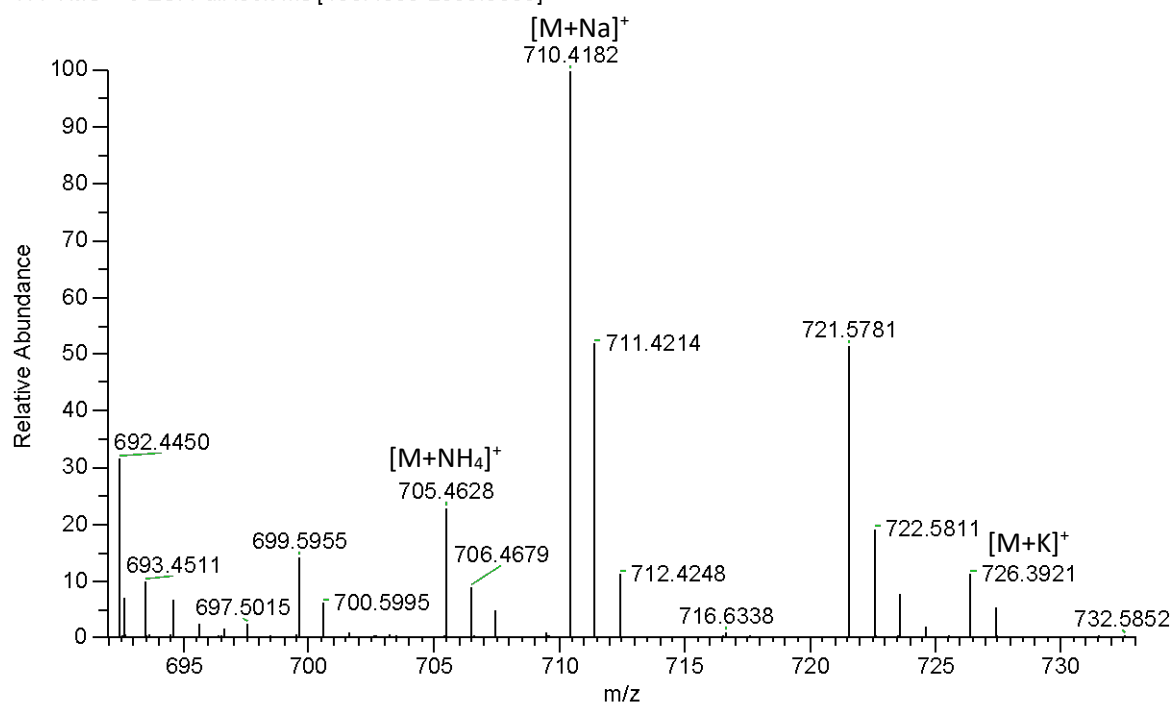


Figure S32. Expanded MS spectrum of compound **11**