

Supporting Information.

Stable Helical Peptoids via Covalent Side Chain to Side Chain Cyclization

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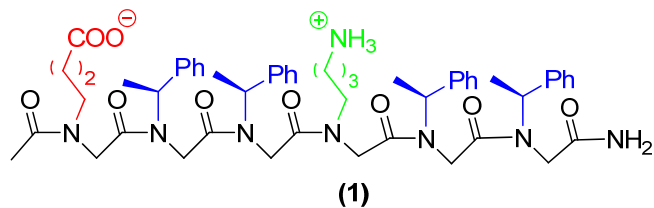
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1. General information.

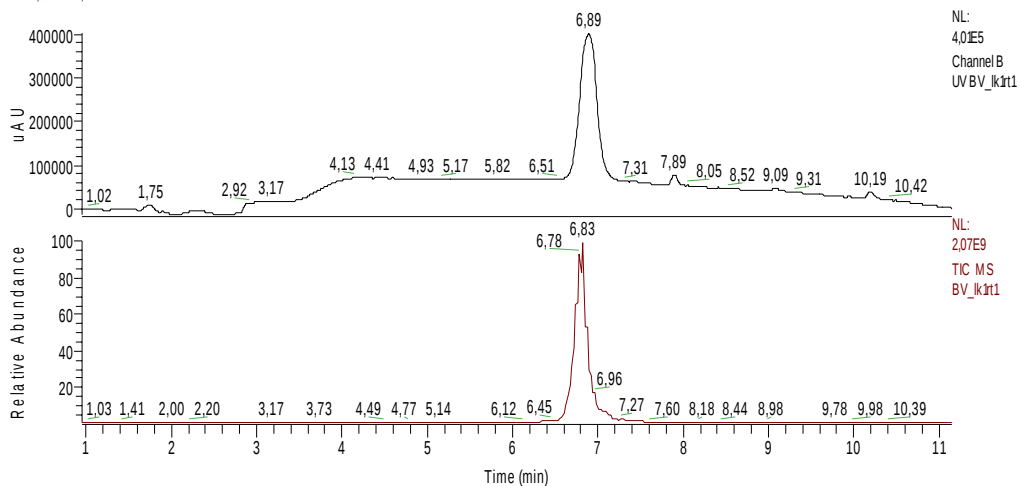
The crude reaction mixture of each peptoid was analyzed by LC-ESI-MS, carried on an Agilent 1100 series binary pump together with a reversed-phase HPLC column (Macherey-Nagel) and a Finnigan Thermoquest LCQ. Peptoids were subsequently purified by reverse-phase HPLC on a Nucleodur C4 Gravity column (125 x 21 mm, Macherey-Nagel) with a linear gradient of A (0.1% HCOOH in H₂O) and B (0.1% HCOOH in MeCN) from 20% of A to 40% of B and a flow rate of 25 mL min⁻¹ and were detected at 210 nm using a diode array UV/VIS detector. The identities and purities of the purified peptoids were assessed by LC-ESI-MS. In order to assess the purity of purified peptoids, either UV detector at 210 nm or Corona® Charged Aerosol Detector coupled to the LC-ESI-MS were employed. Following purification, all peptoids were lyophilized and kept at -20 °C.

2. LC-MS characterization.

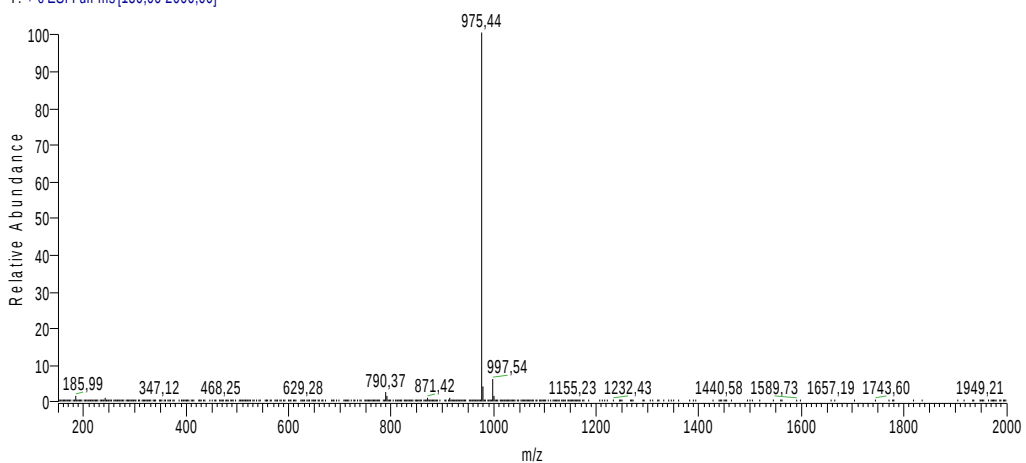


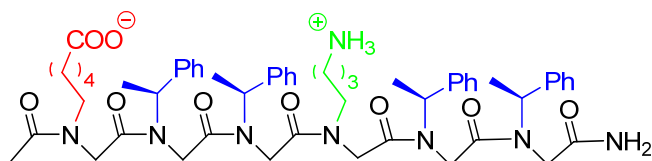
Calculated mass	Observed mass
$[M + H]^+$	$[M + H]^+$
975.5	975.4

RT: 0.94 - 11.14



BV_k11 #261-275 RT: 6.65-6.96 AV: 15 NL: 4.86E8
T: + c ESI Full ms[150,00-2000,00]

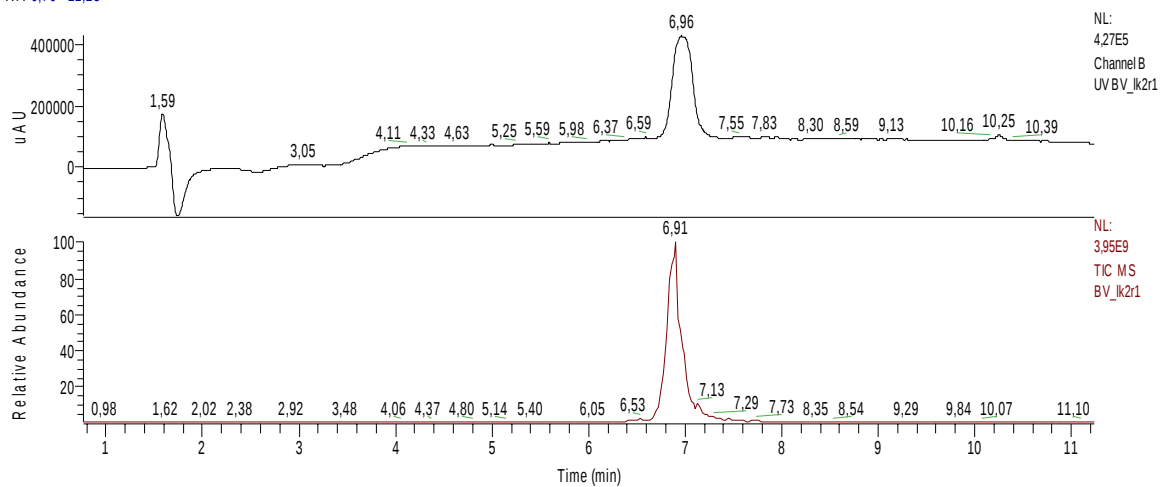




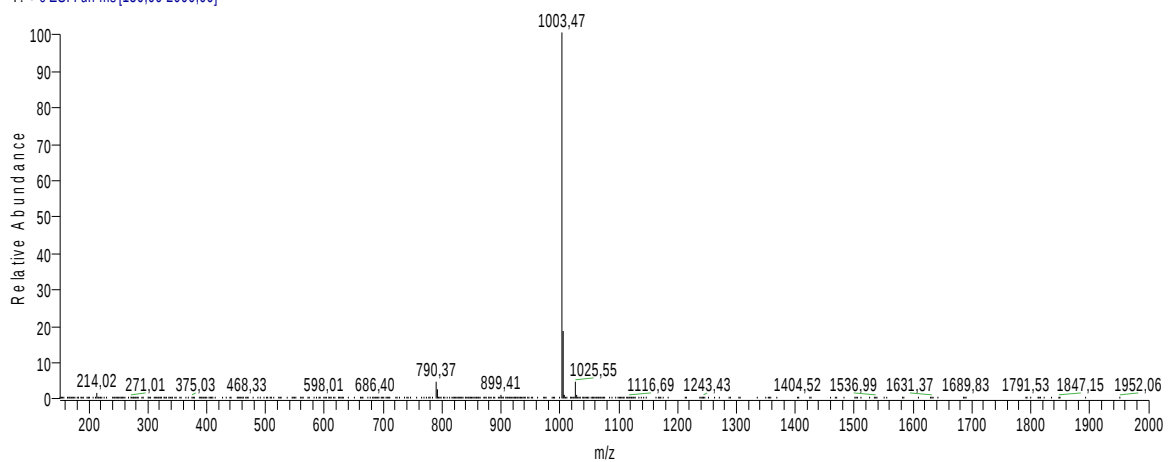
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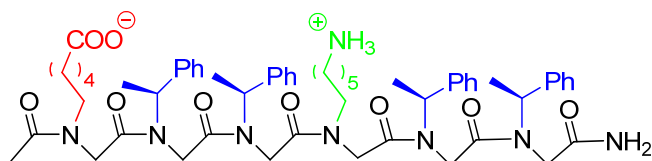
Calculated mass	Observed mass
$[M + H]^+$	$[M + H]^+$
1003.6	1003.5

RT: 0,76 - 11,23



BV_ik2r1 #265-276 RT: 6,75-7,00 AV: 12 NL: 1,08E9
T: + c ESI Full ms [150,00-2000,00]



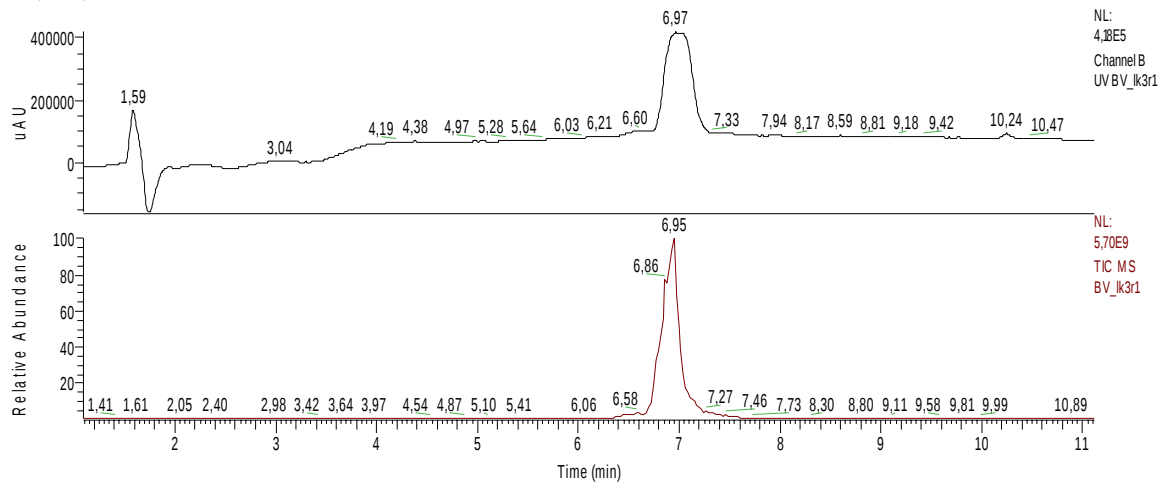


(3)

Calculated mass
[M + H]⁺
1031.6

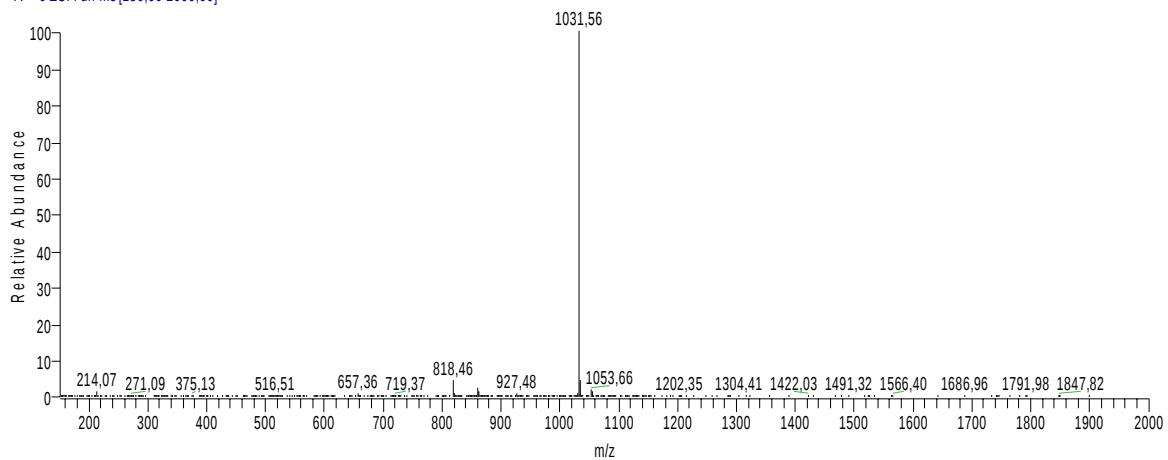
Observed mass
[M + H]⁺
1031.6

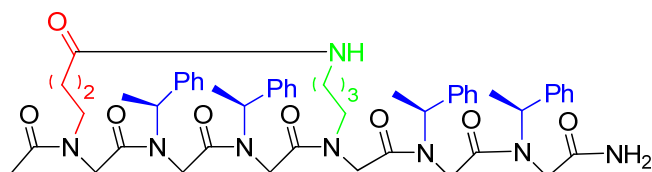
RT: 1.09 - 11.11



BV Ik3r1 #267-279 RT: 6.77-7.04 AV: 13 NL: 1.66E9

T: + c ESI Full ms [150,00-2000,00]

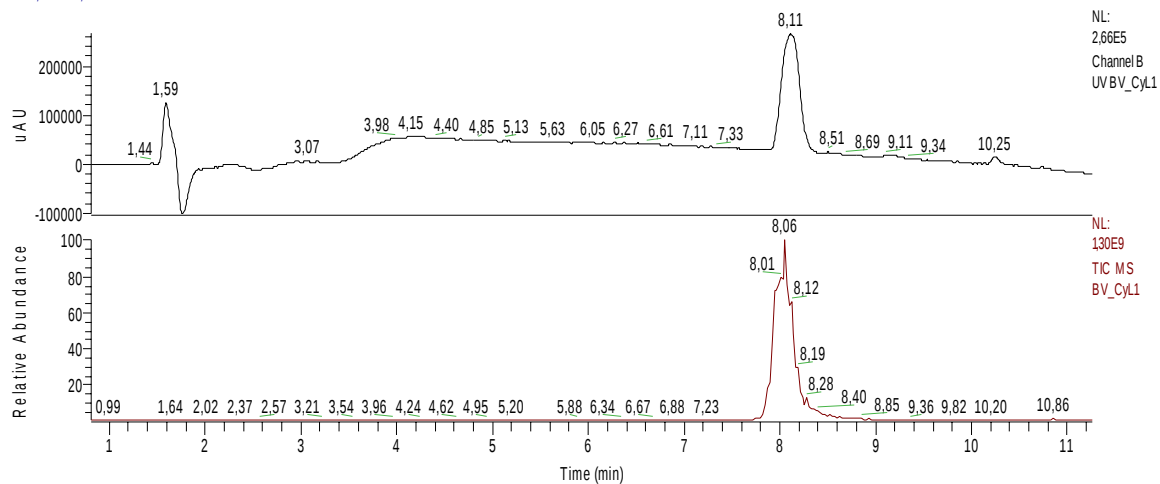




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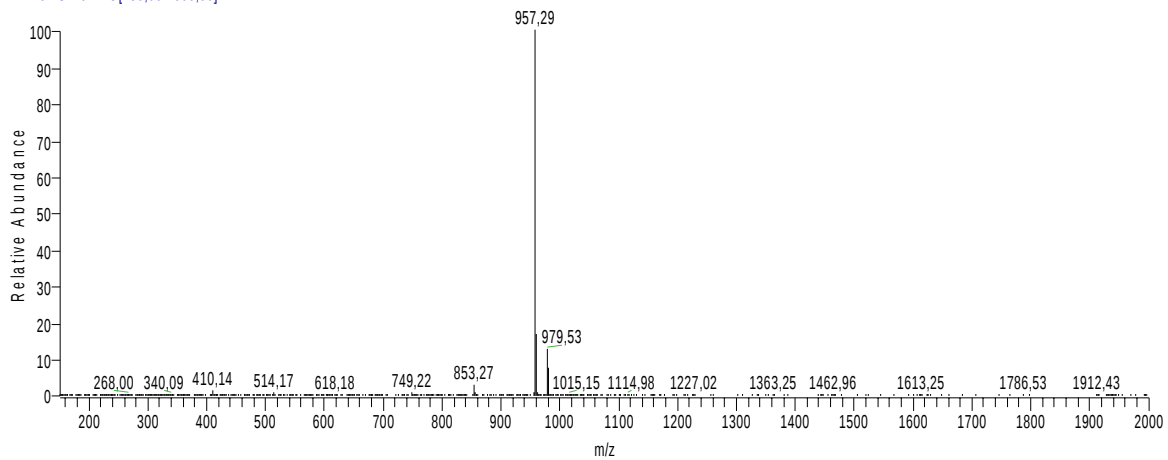
Calculated mass	Observed mass
[M + H]⁺	[M + H⁺]⁺
957.5	957.3

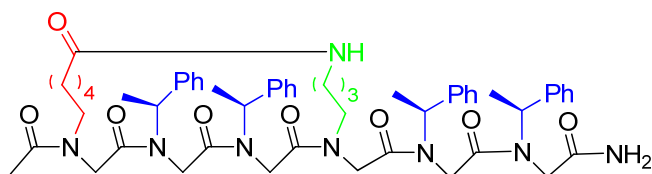
RT: 0,81 - 11,26



BV_Cyl1 #314-327 RT: 7,90-8,19 AV: 14 NL: 3,63E8

T: + c ESI Full ms [150,00-2000,00]

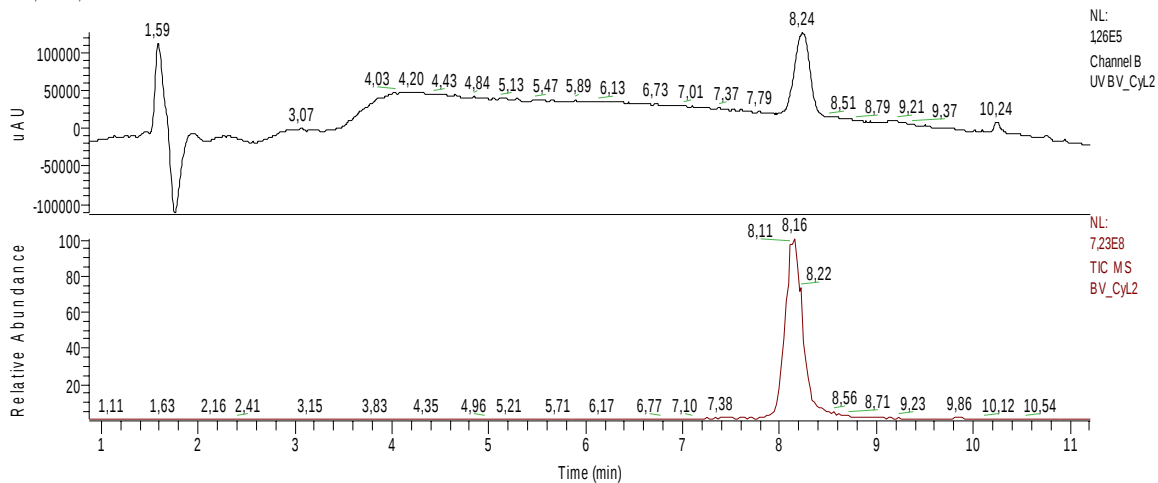




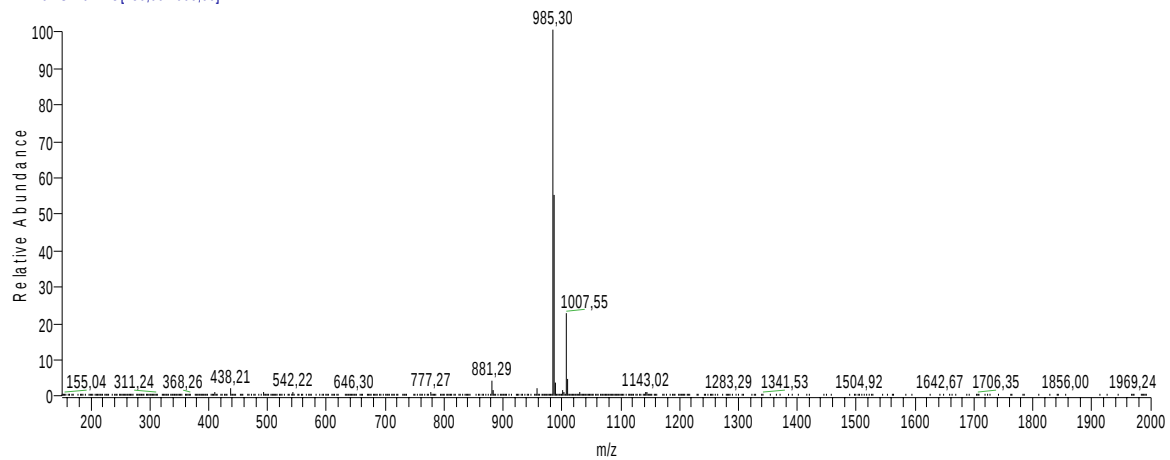
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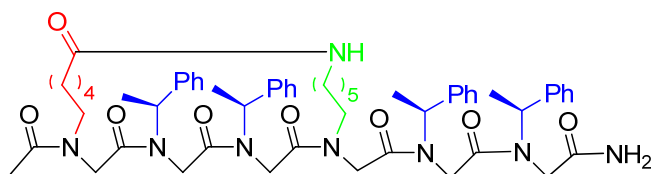
Calculated mass	Observed mass
[M + H]⁺	[M + H]⁺
985.6	985.3

RT: 0.87 - 11.20



BV_Cyl2 #320-330 RT: 8.02-8.25 AV: 11 NL: 2,00E8
T: + c ESI Full ms[150.00-2000.00]

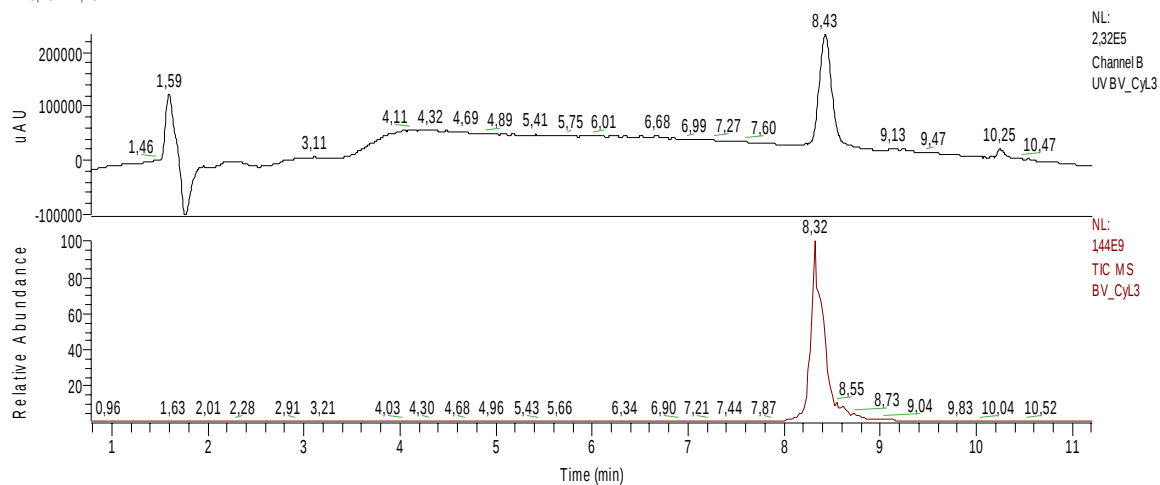




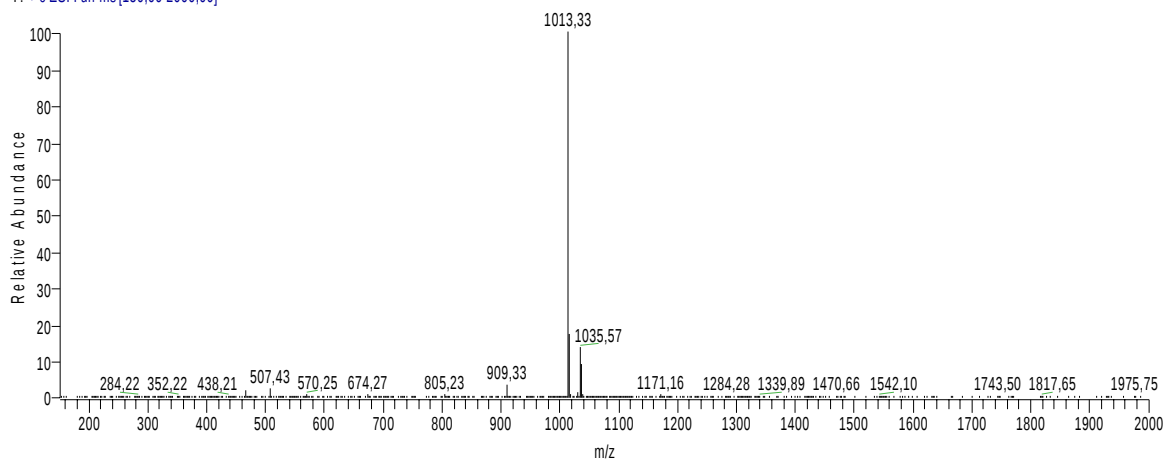
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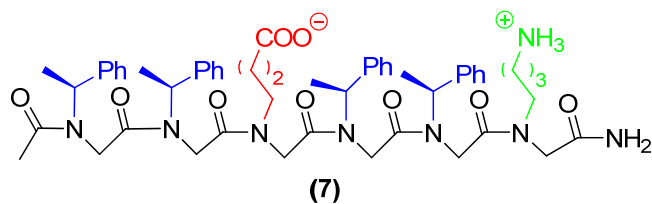
Calculated mass	Observed mass
[M + H]⁺	[M + H]⁺
1013.6	1013.3

RT: 0,78 - 11,20



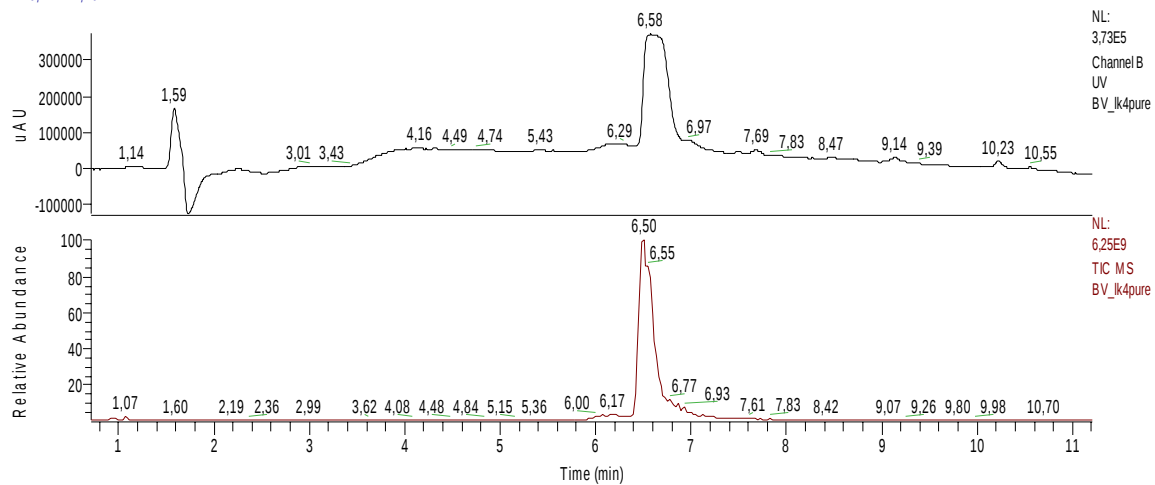
BV_Cyl3 #329-338 RT: 8,25-8,45 AV: 10 NL: 3,41E8
T: + c ESI Full ms [150,00-2000,00]



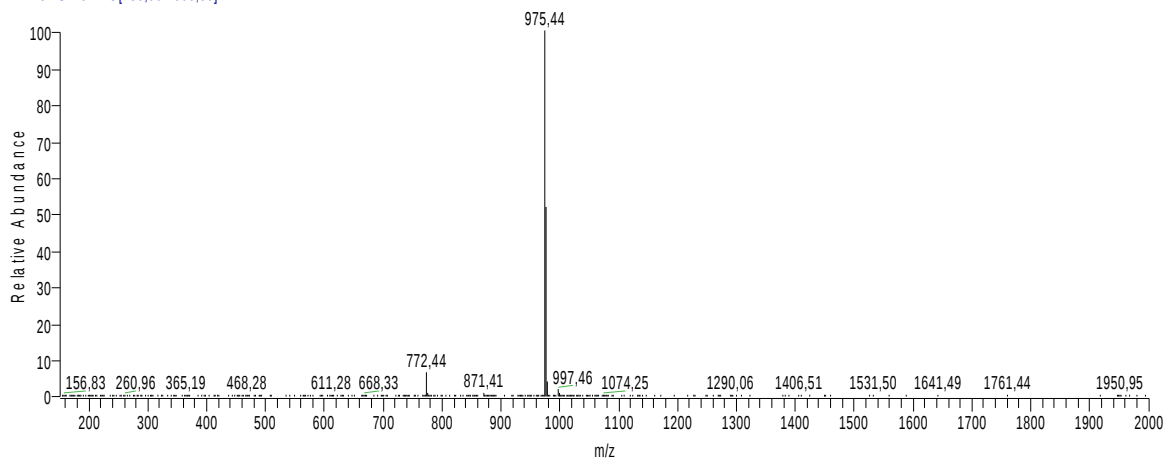


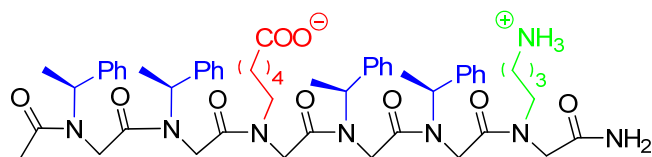
Calculated mass	Observed mass
$[M + H]^+$	$[M + H]^+$
975.5	975.4

RT: 0,71 - 11,20



BV_ik4pure #255-263 RT: 6,44-6,62 AV: 9 NL: 2,34E9
 T: + c ESI Full ms [150,00-2000,00]

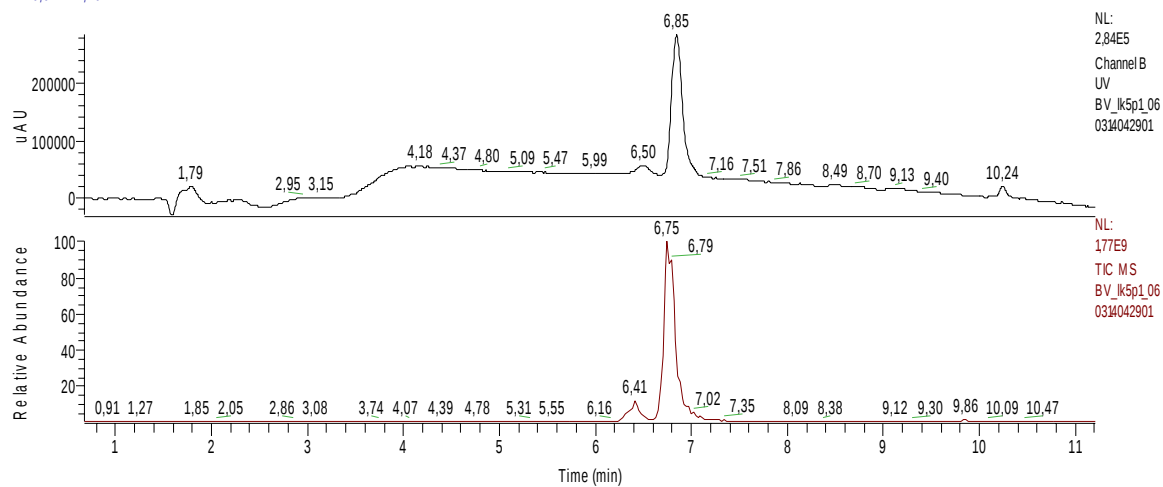




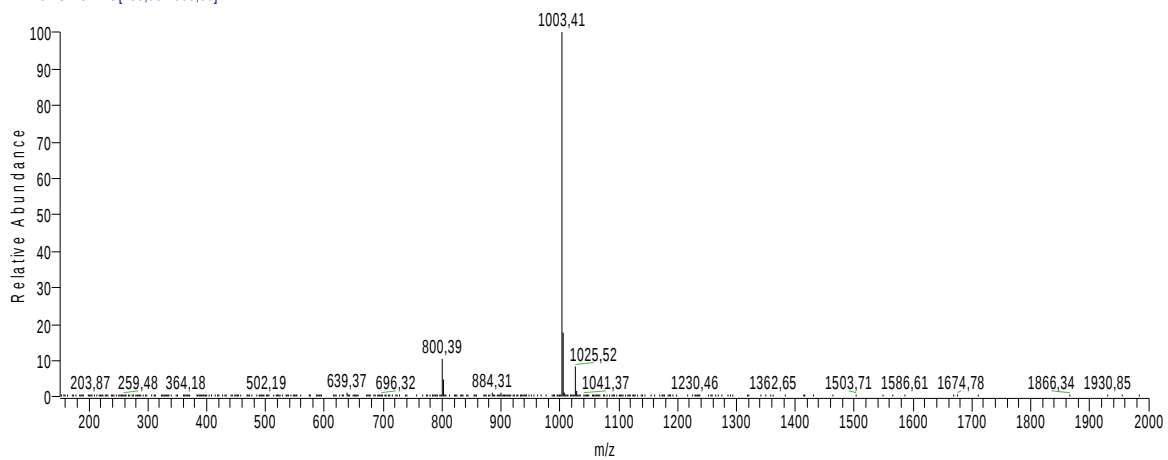
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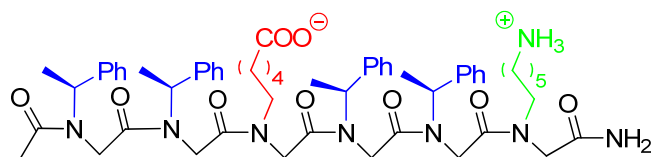
Calculated mass	Observed mass
$[\text{M} + \text{H}]^+$	$[\text{M} + \text{H}]^+$
1003.6	1003.4

RT: 0,67 - 11,20



BV_ik5p1_060314042901 #265-273 RT: 6,68-6,86 AV: 9 NL: 4,85E8
T: + c ESI Full ms [150,00-2000,00]

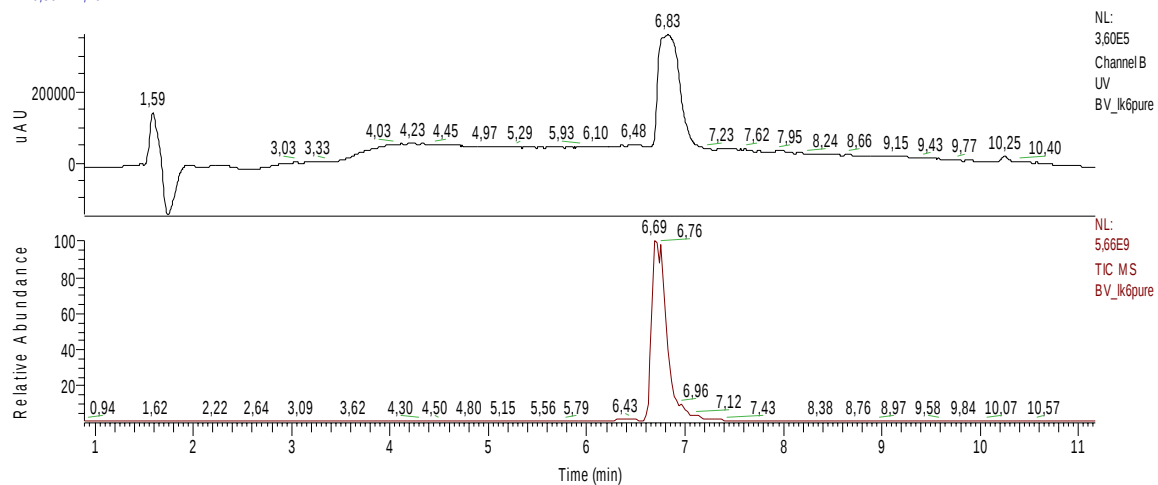




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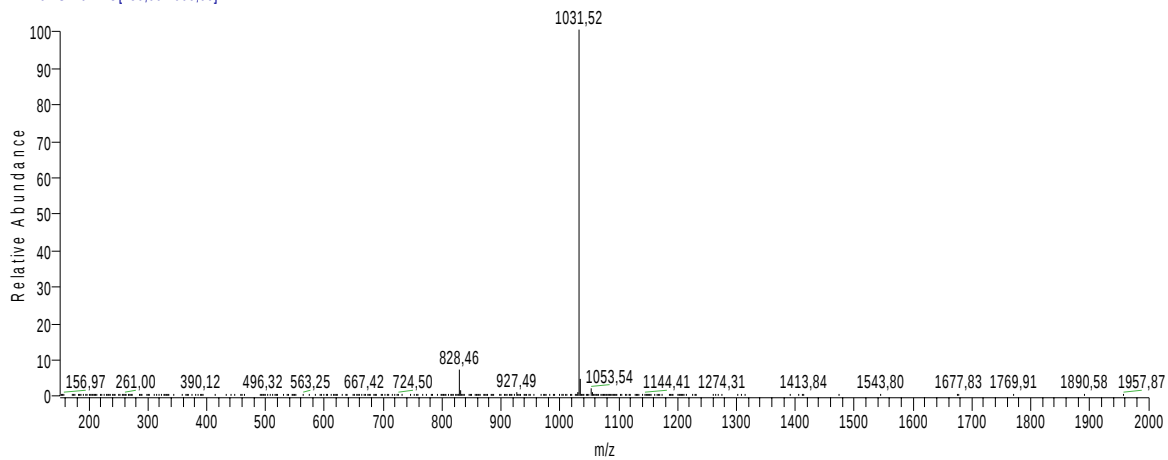
Calculated mass	Observed mass
$[\text{M} + \text{H}]^+$	$[\text{M} + \text{H}]^+$
1031.6	1031.5

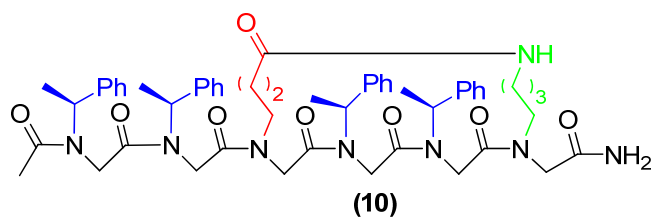
RT: 0.89 - 11.16



BV_ik6pure #264-273 RT: 6.62-6.82 AV: 10 NL: 1,86E9

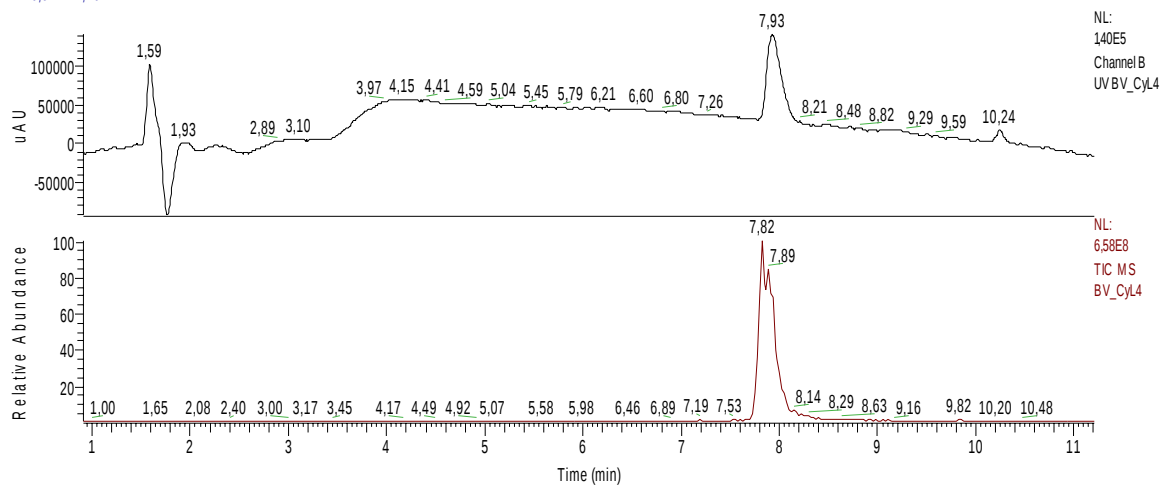
T: + c ESI Full ms [150,00-2000,00]



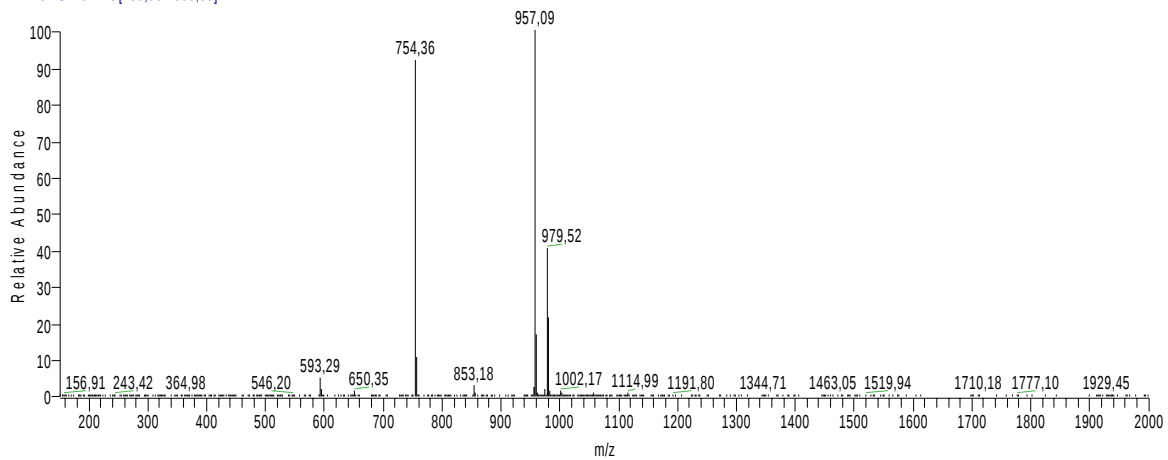


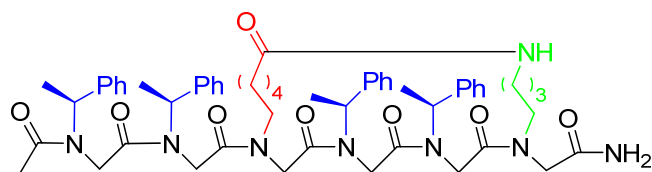
Calculated mass	Observed mass
$[M + H]^+$	$[M + H]^+$
957.5	957.1

RT: 0,91 - 11,20



BV_Cyl4 #311-321 RT: 7,78-8,00 AV: 11 NL: 9,40E7
T: + c ESI Full ms [150,00-2000,00]

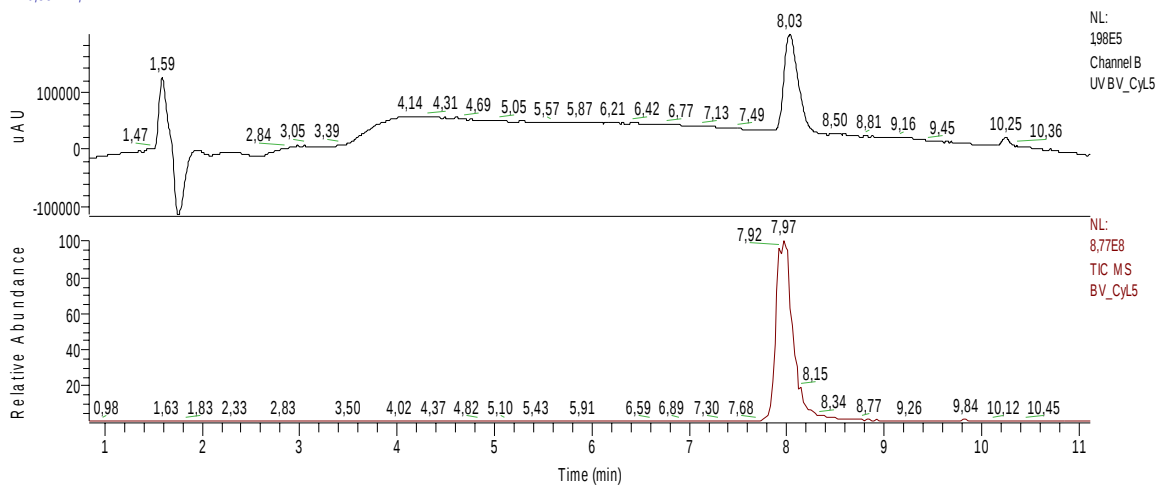




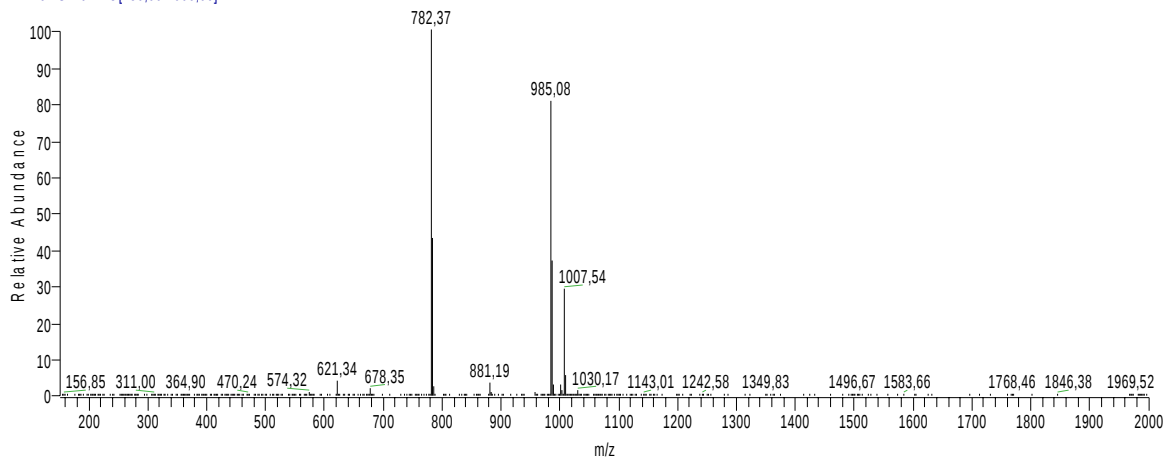
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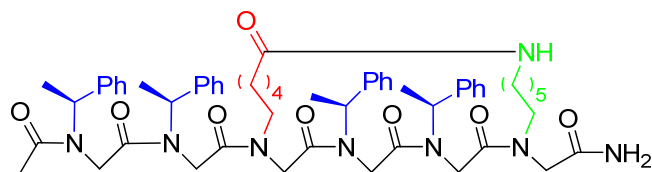
Calculated mass	Observed mass
[M + H]⁺	[M + H]⁺
985.6	985.1

RT: 0.83 - 11.11



BV_Cyl5 #315-324 RT: 7.88-8.08 AV: 10 NL: 1.69E8
T: + c ESI Full ms [150,00-2000,00]

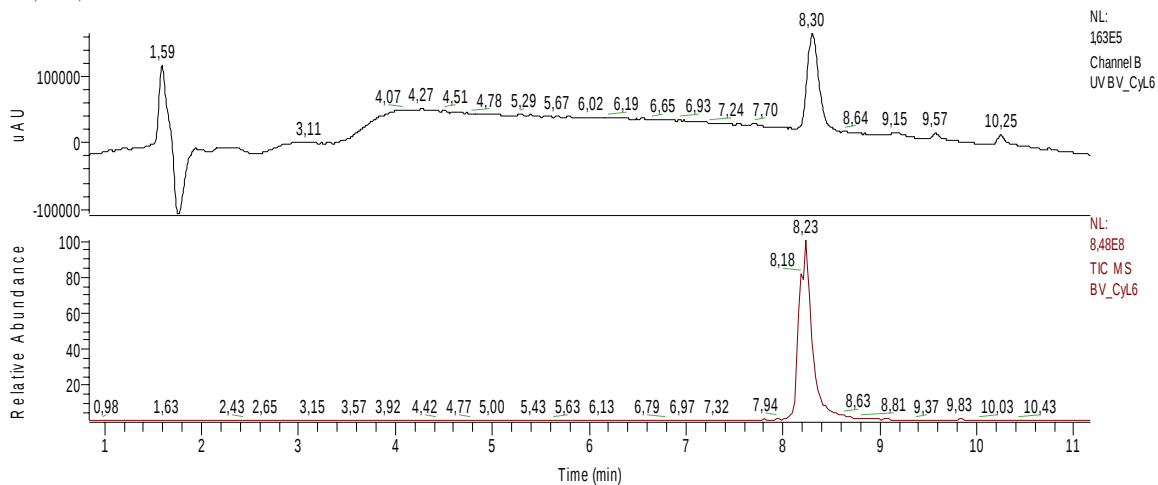




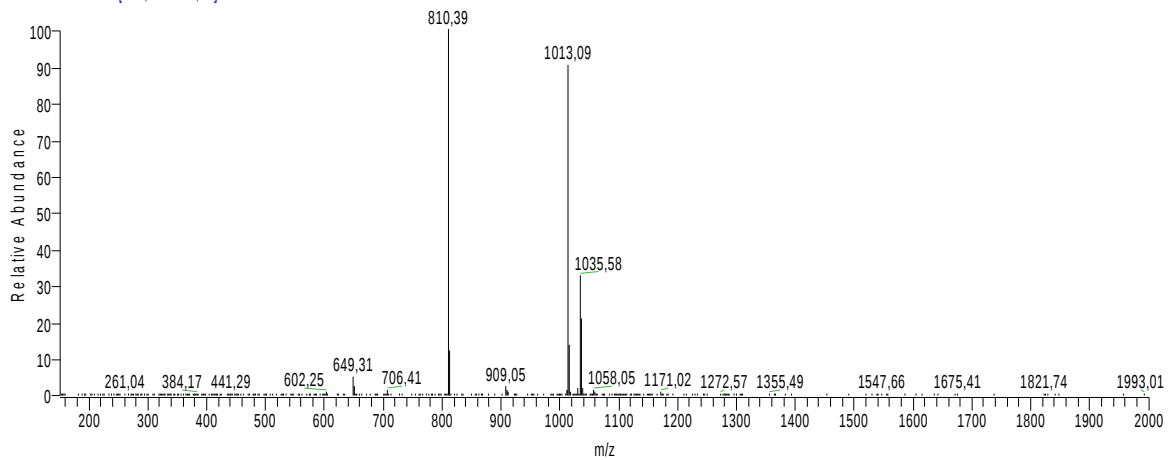
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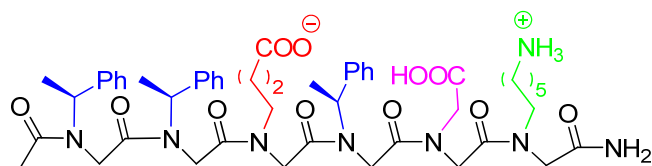
Calculated mass	Observed mass
[M + H]⁺	[M + H]⁺
1013.6	1013.1

RT: 0.83 - 11.16



BV_Cyl6 #325-332 RT: 8.14-8.30 AV: 8 NL: 1,35E8
T: + c ESI Full ms [150,00-2000,00]

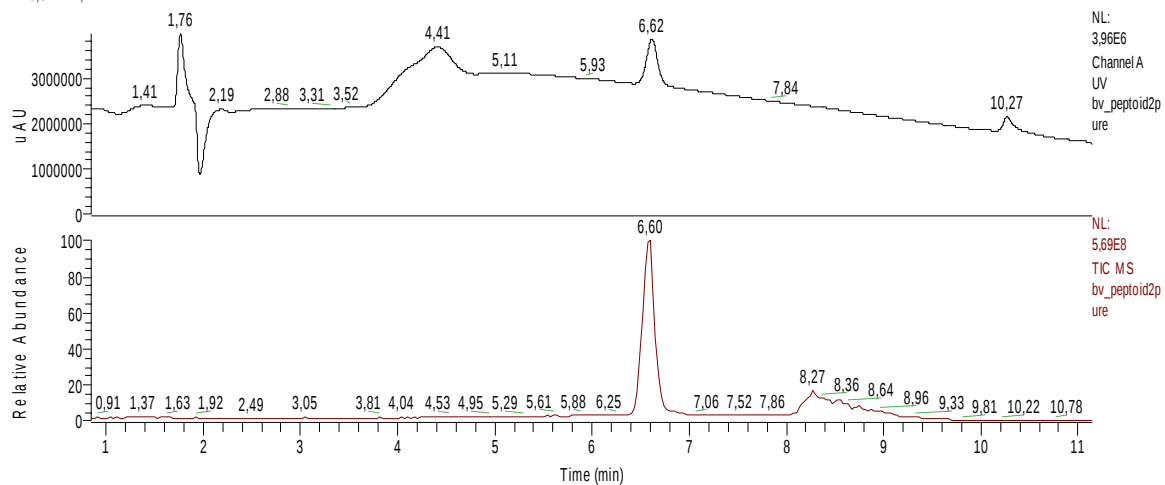




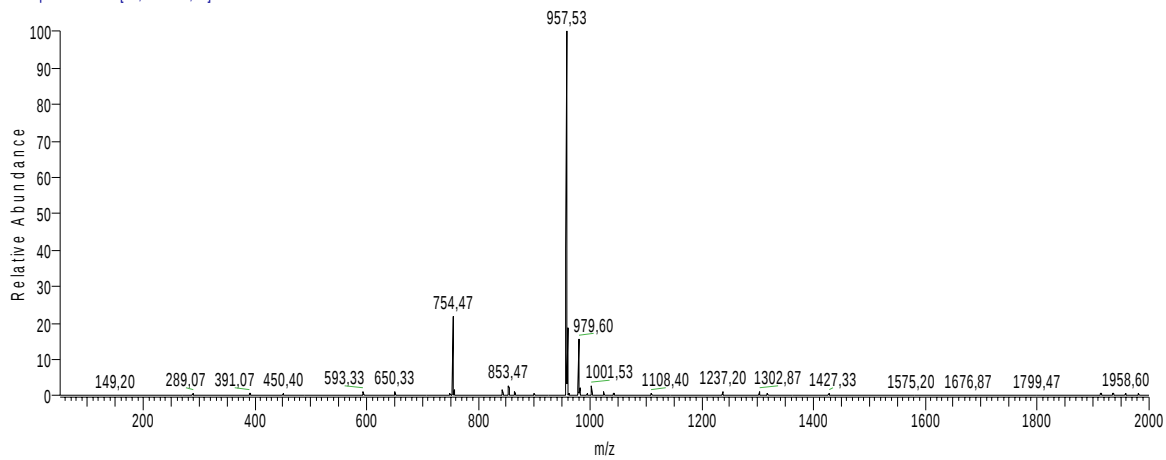
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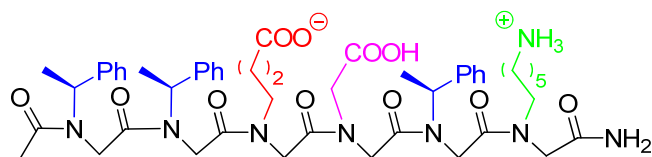
Calculated mass	Observed mass
[M + H]⁺	[M + H⁺]⁺
957.5	957.5

RT: 0.84 - 11.14



bv_peptoid2pure #202-208 RT: 6.49-6.66 AV: 7 NL: 1.60E7
T: + p ESI Full ms [50,00-2000,00]

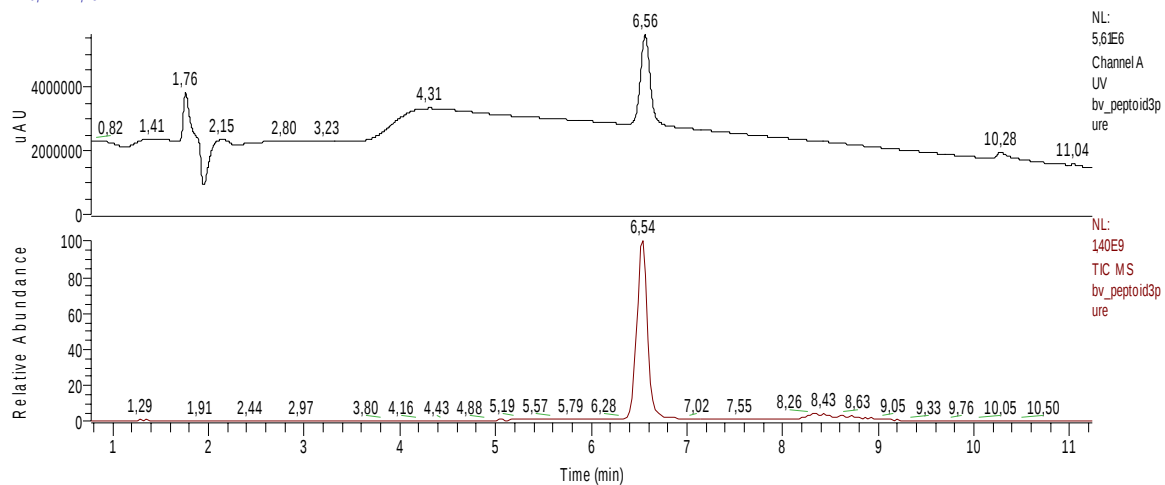




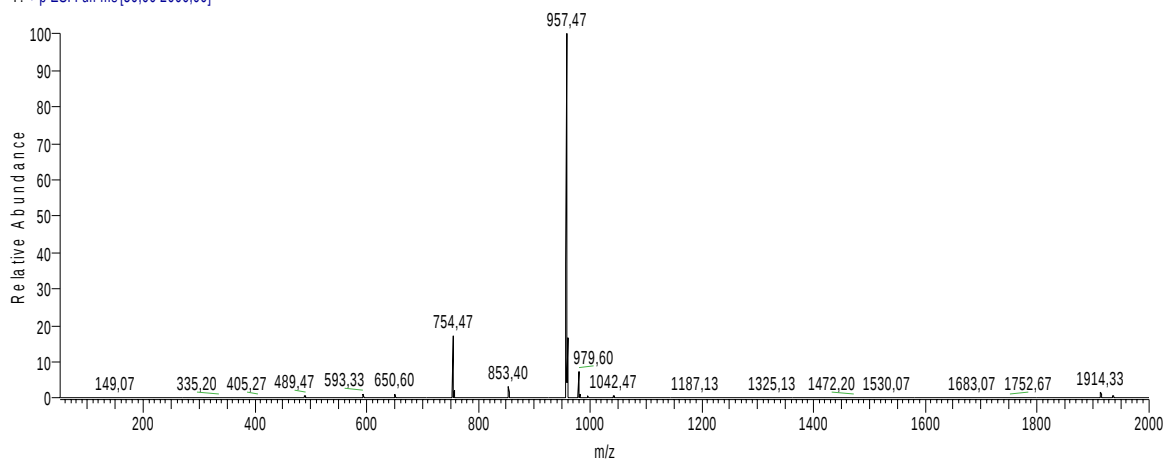
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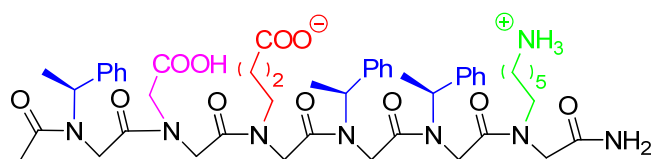
Calculated mass	Observed mass
$[M + H]^+$	$[M + H]^+$
957.5	957.5

RT: 0,77 - 11,23



bv_peptoid3pure #200-206 RT: 6,46-6,62 AV: 7 NL: 4,46E7
T: + p ESI Full ms [50,00-2000,00]

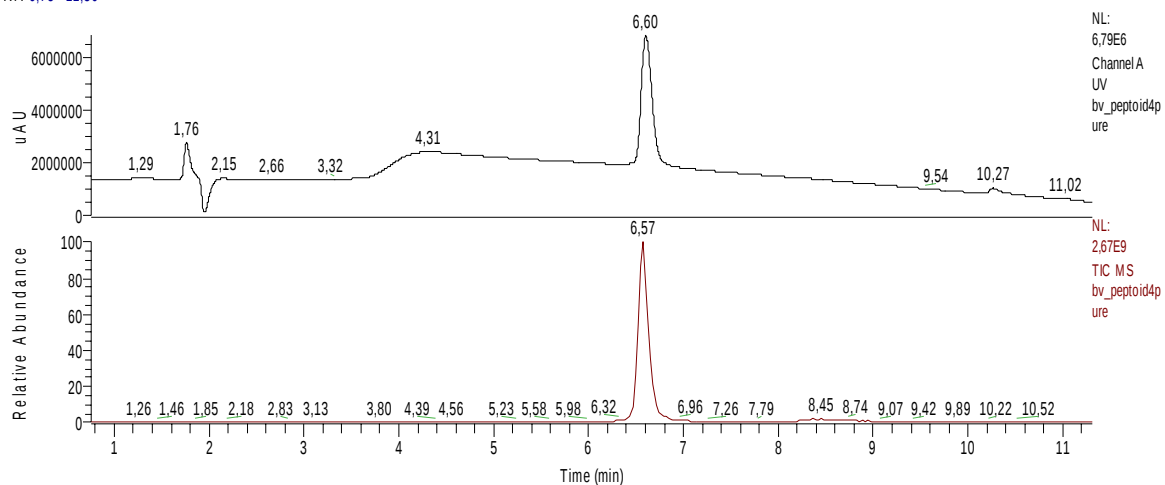




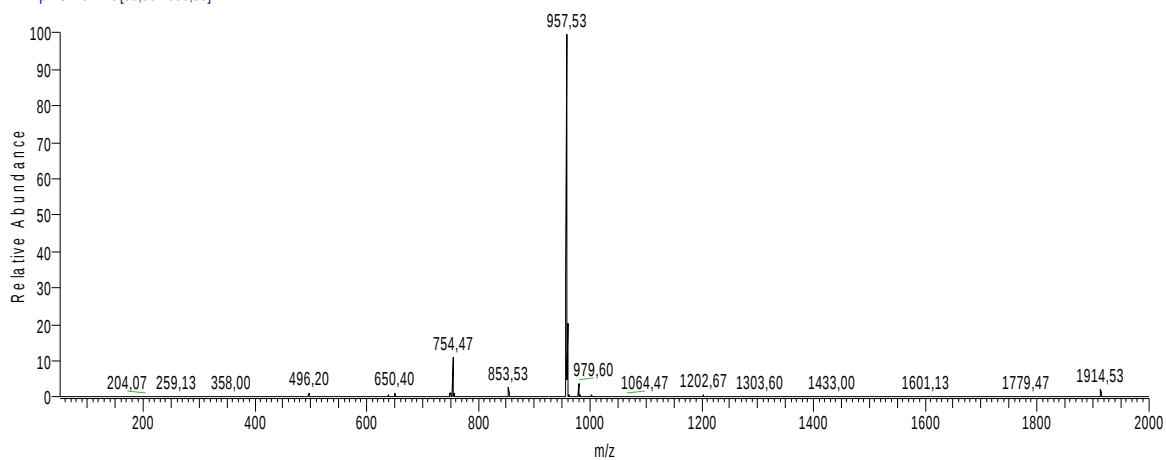
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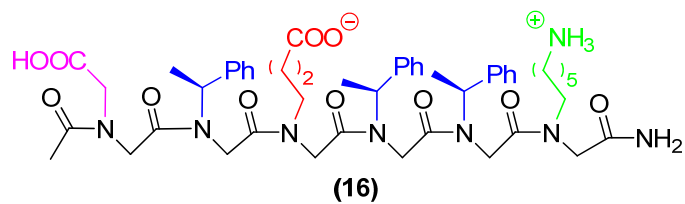
Calculated mass	Observed mass
$[M + H]^+$	$[M + H]^+$
957.5	957.4

RT: 0,75 - 11,30



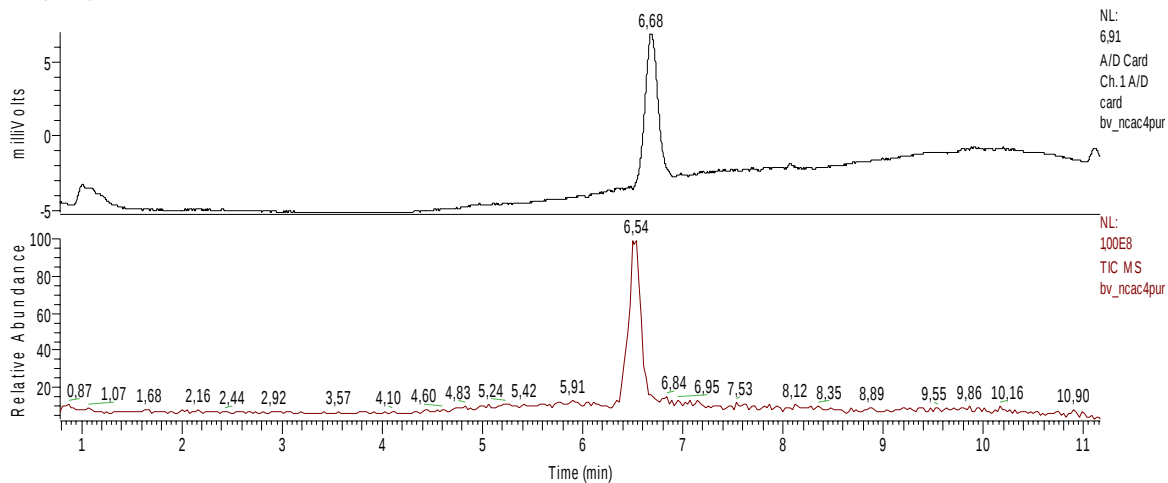
bv_peptoid4pure #200-206 RT: 6,49-6,66 AV: 7 NL: 8,67E7
T: + p ESI Full ms [50,00-2000,00]



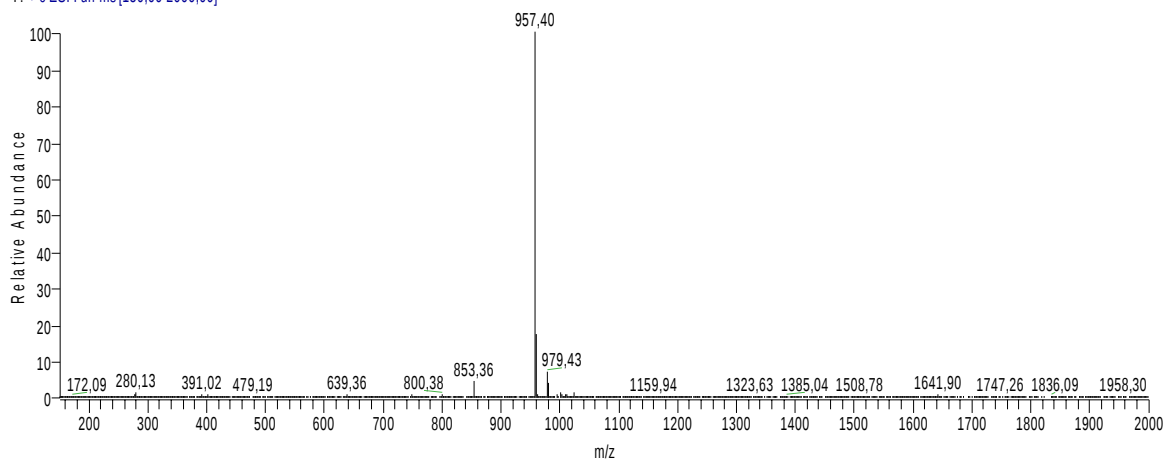


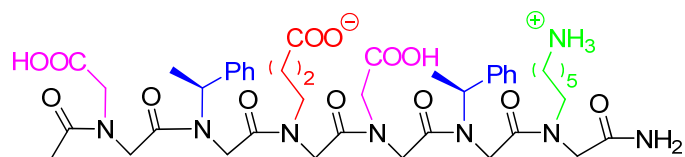
Calculated mass	Observed mass
$[M + H]^+$	$[M + H]^+$
957.5	957.4

RT: 0,78 - 11,16



bv_ncac4pur #254-262 RT: 6,42-6,61 AV: 9 NL: 2,50E7
 T: + c ESI Full ms [150,00-2000,00]

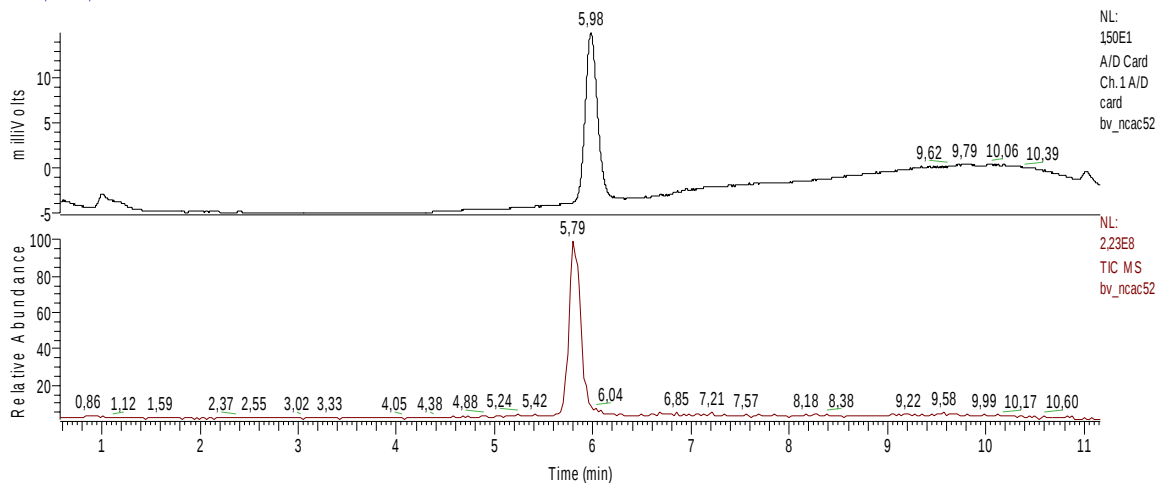




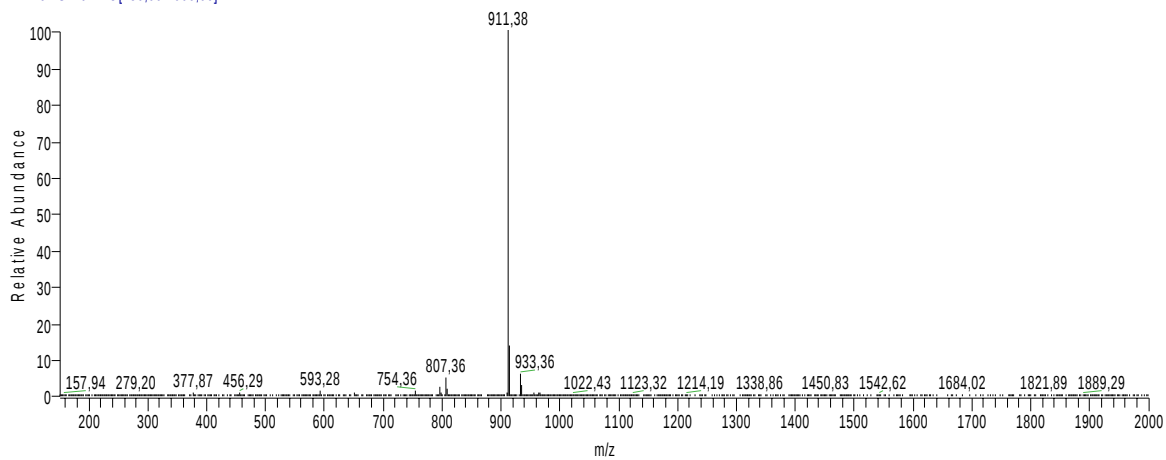
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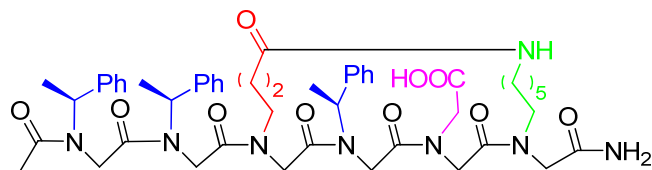
Calculated mass	Observed mass
[M + H]⁺	[M + H]⁺
911.4	911.4

RT: 0.57 - 11.16



bv_ncac52 #229-235 RT: 5.75-5.89 AV: 7 NL: 7.31E7
T: + c ESI Full ms[150.00-2000.00]

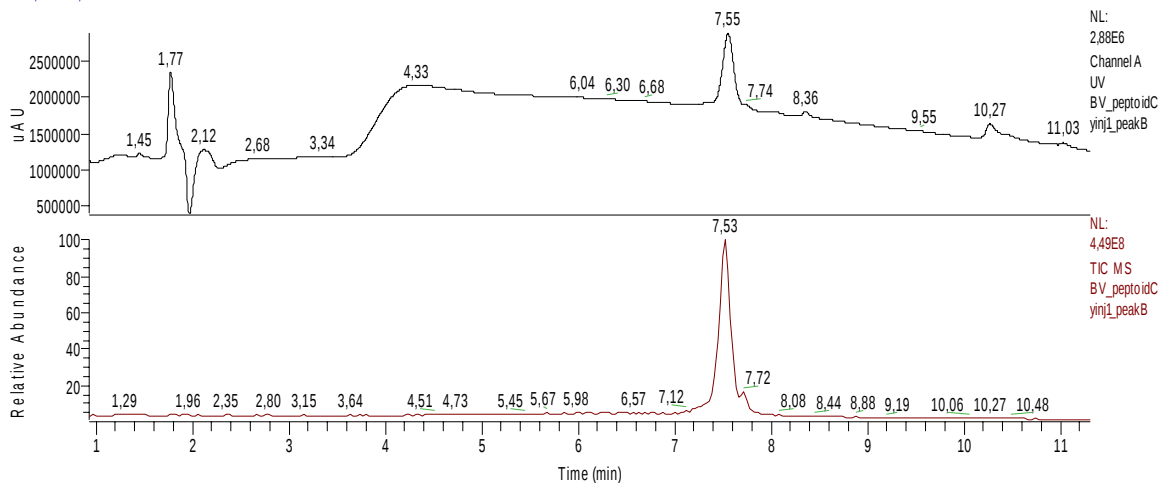




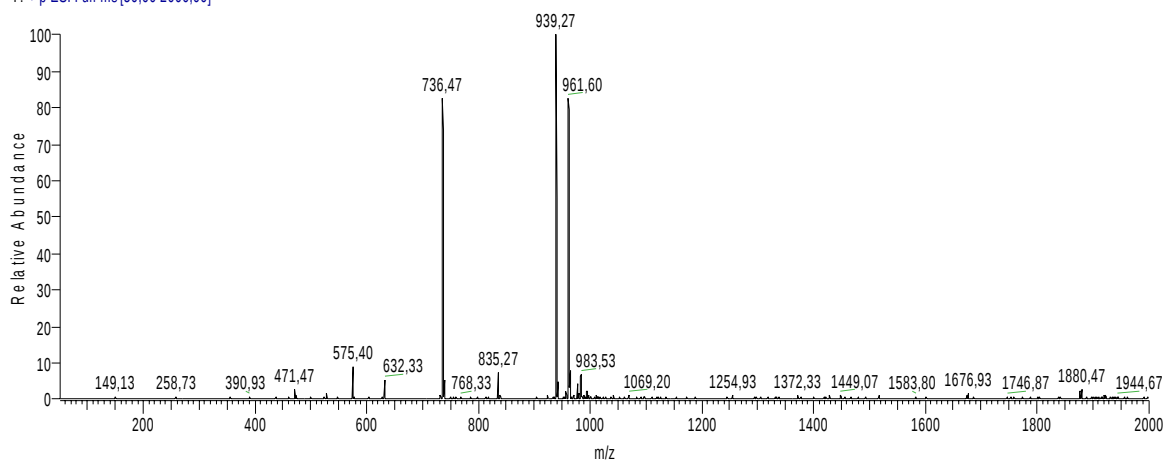
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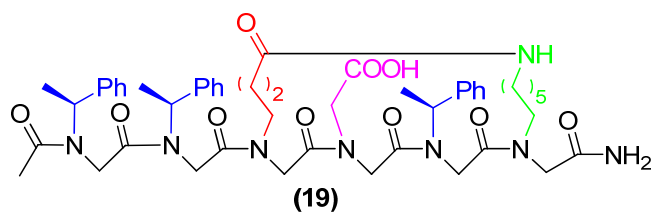
Calculated mass	Observed mass
[M + H]⁺	[M + H]⁺
939.5	939.3

RT: 0,92 - 11,30



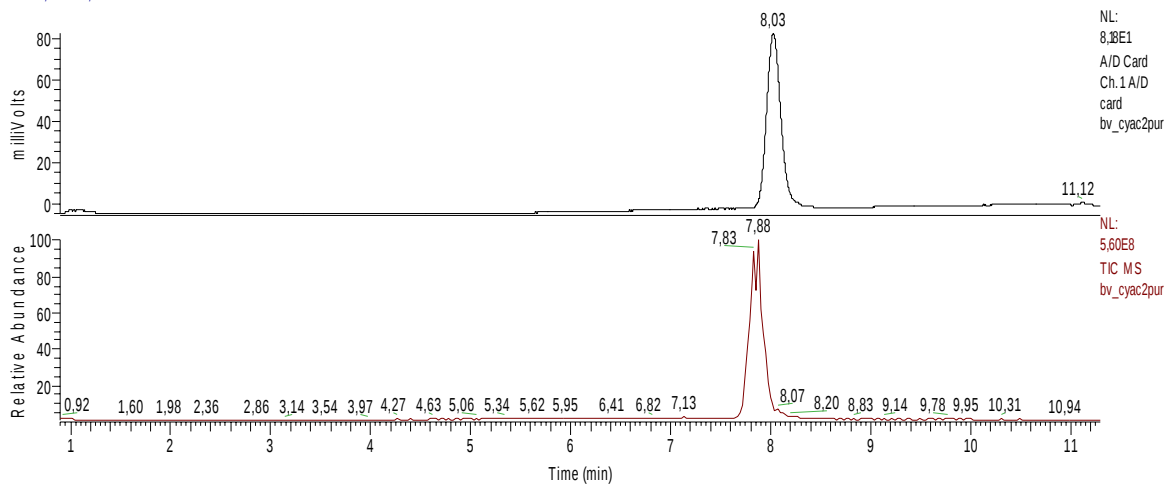
BV_peptoidC yinj1_peakB #235-243 RT: 7,42-7,63 AV: 9 NL: 4,63E6
T: + p ESI Full ms [50,00-2000,00]



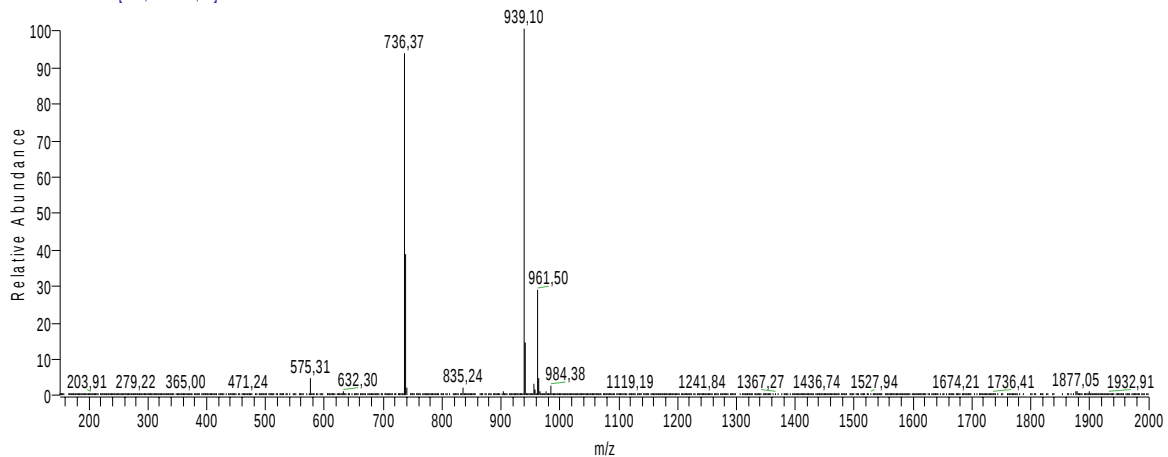


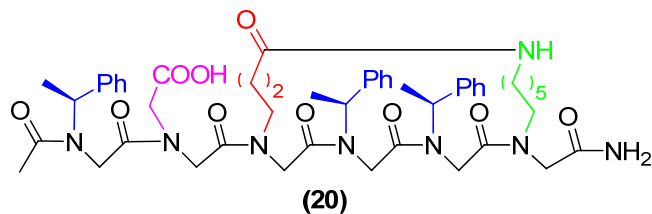
Calculated mass	Observed mass
$[M + H]^+$	$[M + H]^+$
939.5	939.1

RT: 0,89 - 11,29



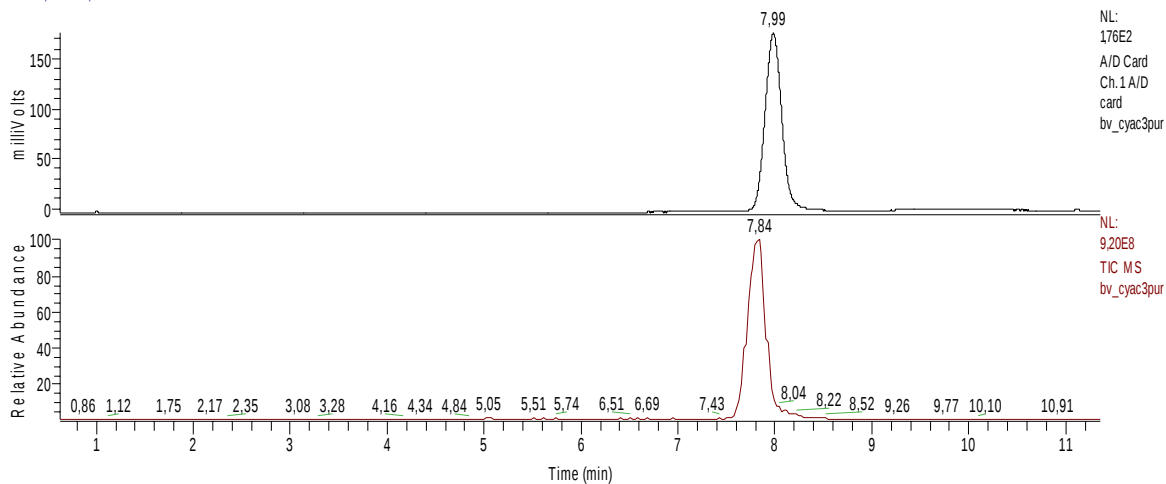
bv_cyac2pur #305-316 RT: 7,72-7,97 AV: 12 NL: 6,99E7
T: + c ESI Full ms [150,00-2000,00]



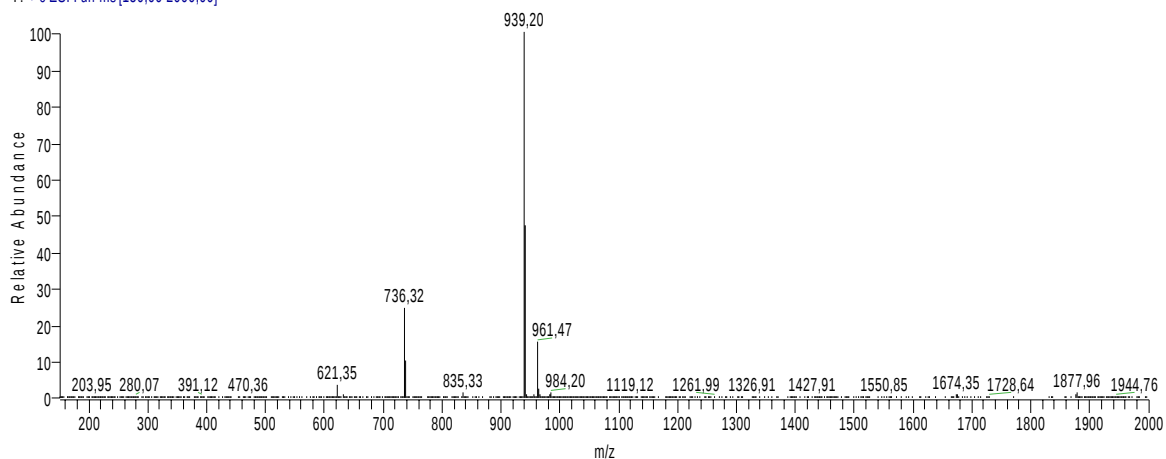


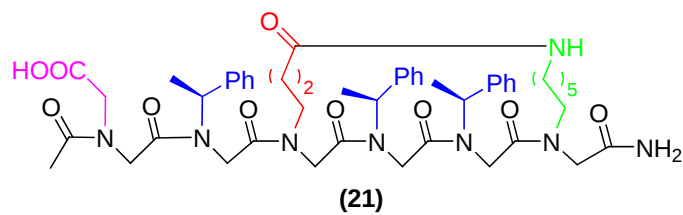
Calculated mass	Observed mass
$[M + H]^+$	$[M + H]^+$
939.5	939.2

RT: 0.62 - 11.35



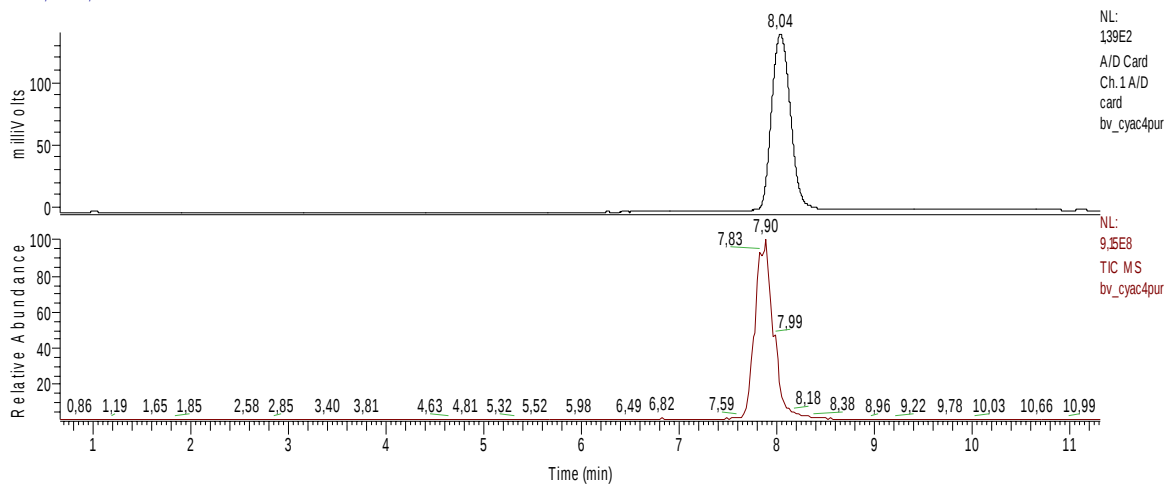
bv_cyac3pur #303-316 RT: 7.66-7.95 AV: 14 NL: 2,19E8
T: + c ESI Full ms [150,00-2000,00]



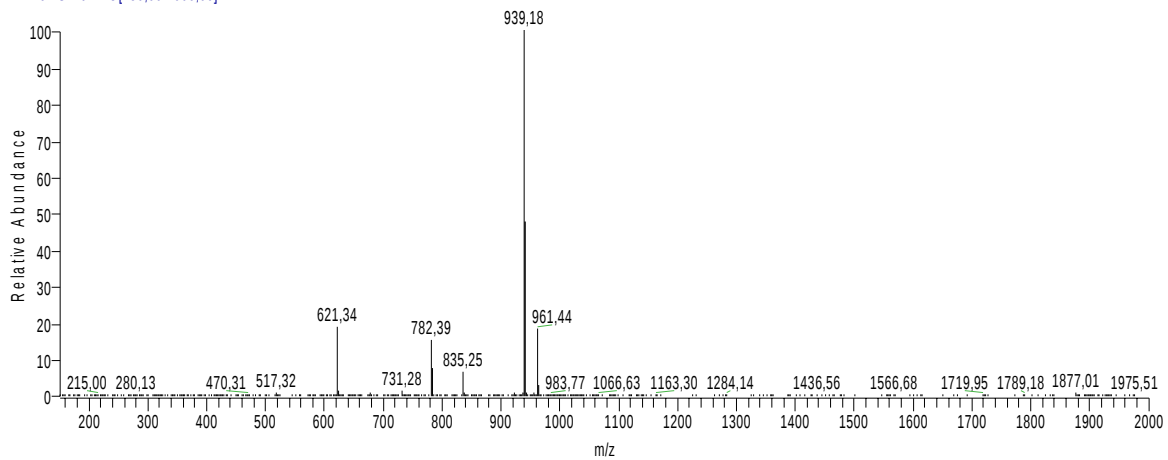


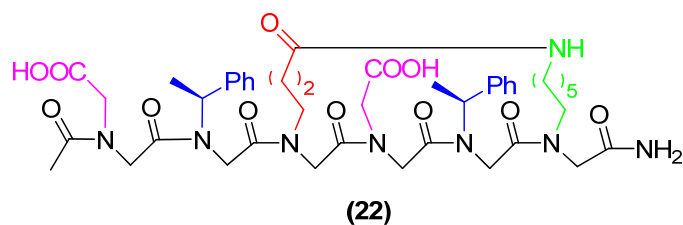
Calculated mass	Observed mass
[M + H]⁺	[M + H]⁺
939.5	939.2

RT: 0.66 - 11.31



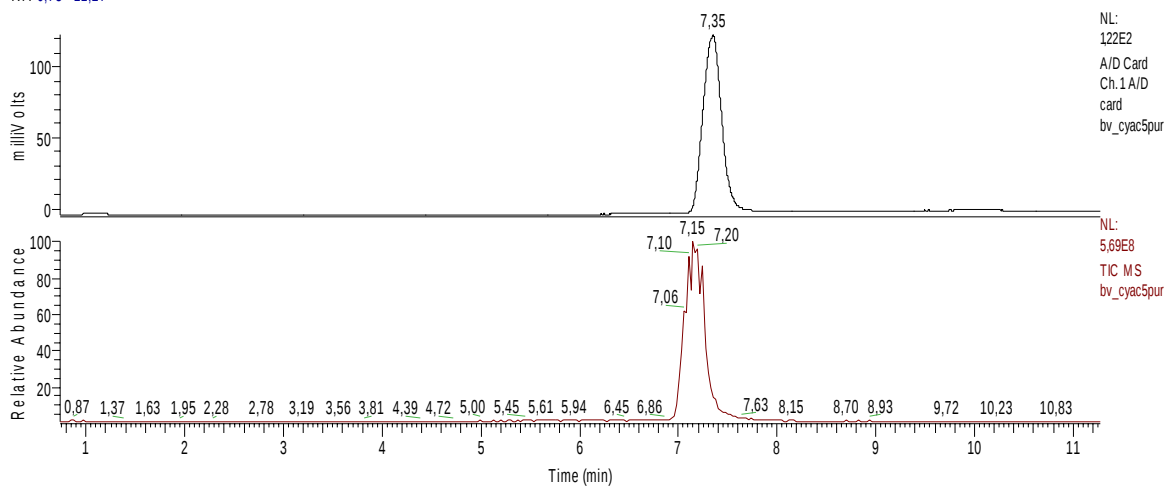
bv_cyac4pur #308-316 RT: 7.76-7.94 AV: 9 NL: 2.45E8
T: + c ESI Full ms [150,00-2000,00]





Calculated mass	Observed mass
[M + H]⁺	[M + H]⁺
893.4	893.1

RT: 0,73 - 11,27



bv_cyac5pur #279-289 RT: 7,04-7,26 AV: 11 NL: 1,39E8
T: + c ESI Full ms [150,00-2000,00]

