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Impact of Substituent Effects in the Design of β-Sheet Mimetic and β-Double Helix from (E)-Vinylogous γ-Amino Acid Oligomers

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1. ORTEP diagrams of peptides

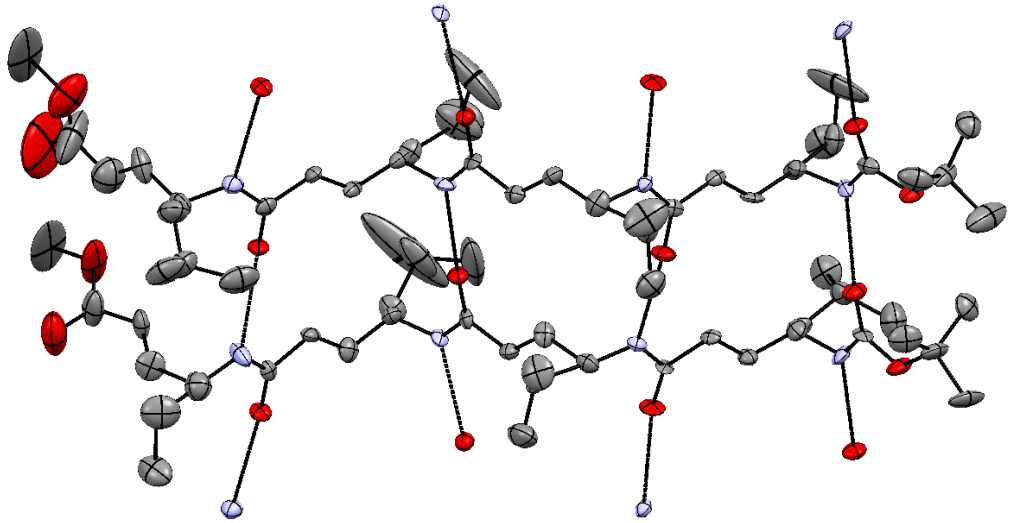


Figure S1: ORTEP diagramof**P1**(BocNH-((*S*,*E*)d^{2,3}γLue)$_4$-OMe)Ellipsoids are drawn to 50% probability and hydrogen atoms are not shown for clarity.(CCDC 1907413)

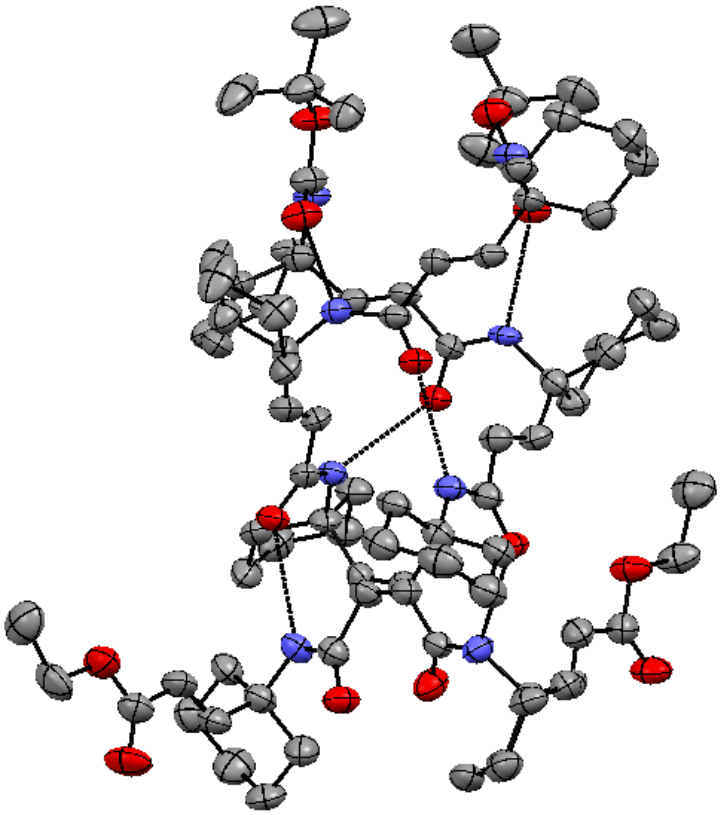


Figure S2: ORTEP diagramof**P2 (**BocNH–((*E*)d^{2,3}γAc$_6$c)$_4$-OEt) Ellipsoids are drawn to 50% probability and hydrogen atoms are not shown for clarity.(CCDC 1912116)

2. Crystallographic Information of Peptides

The X-ray dataof **P1** and **P2** was collected at 100 K on diffractometer using Mo K_α radiation (λ = 0.71073 Å). The structures were obtained by direct methods using the SHELXS-97 program.

	P1	**P2[(a)]**
Chemical formula	C_{38} H_{64} N_4 O_7	C_{43} H_{66} N_4 O_7
Molecular weight	688.9510	751.022
Crystal habit	Clear	Clear
Crystal size (nm)	0.2× 0.2× 0.3	0.3× 0.3× 0.4
Crystallization solvent	ethyl acetate/n-hexane	ethyl acetate/n-hexane
Space group	P 1	P -1
a (Å)	10.0311(19)	15.8190(9)
b (Å)	13.762(3)	15.8231(10)
c (Å)	14.965(3)	21.9625(13)
α (dge)	92.146(5)	71.776(4)
β (dge)	95.340(5)	84.613(4)
γ (dge)	97.624(5)	63.813(4)
Volume $(Å)^3$	2036.1(7)	4679.4(5)
Z	2	2
Molecules/asym.unit	2	2
Density (g/cm^3)(cal)	1.124	1.163
F (000)	1752.33	751.0
Radiation	Mo K_α	Mo K_α
2θ Max. (°)	56.924	155.702
μ mm^{-1}	0.077	0.656
Reflections (cal)	20574	19967
Parameters	907	1065
R (reflections)	0.1362(6570)	0.1122(7584)
wR2 (Reflections)	0.3810(20311)	0.3551(19967)
Goodness-of- fit (S)	0.977	1.031

[(a)]Option SQUEEZE of PLATON program was used to remove disordered solvent molecules. SQUEEZE Output CIF was submitted to CCDC.

3. Torsion angles and H-bond parameters of peptides

Table1.Torsion angles of peptide **P1** and **P2.**

Residue	ϕ °	θ_1°	θ_2°	ψ°
BocNH-((*S,E*)d^{2,3}γLue)$_4$-OMe (P1)				
β-Sheet strand a				
(*S,E*)d^{2,3}γLue (1)	-96.59	114.97	-179.56	171.94
(*S,E*)d^{2,3}γLue (2)	-109.15	116.15	-178.54	168.54
(*S,E*)d^{2,3}γLue (3)	-118.06	111.60	179.14	176.31
(*S,E*)d^{2,3}γLue (3)	-112.40	116.90	-179.64	-10.97
β-Sheet strand b				
(*S,E*)d^{2,3}γLue (1)	-100.88	112.67	-177.95	169.06
(*S,E*)d^{2,3}γLue (2)	-104.01	111.86	177.63	172.30
(*S,E*)d^{2,3}γLue (3)	-108.51	114.93	179.27	166.99
(*S,E*)d^{2,3}γLue (3)	137.20	-15.24	176.76	178.77
BocNH–((*E*)d^{2,3}γAc$_6$c)$_4$-OEt(P2)				
β-double helical Strand a				
E-d^{2},^{3}γAc$_6$c (1)	65.50	17.72	169.10	-167.56
E-d^{2},^{3}γAc$_6$c (2)	79.61	15.46	173.89	-170.96
E-d^{2},^{3}γAc$_6$c (3)	66.11	14.26	173.05	-173.77
E-d^{2},^{3}γAc$_6$c (4)	-62.58	-17.43	177.65	175.34
β-double helical Strand b				
E-d^{2},^{3}γAc$_6$c (1)	72.41	5.81	173.97	-167.10
E-d^{2},^{3}γAc$_6$c (2)	65.25	27.69	172.38	-172.65
E-d^{2},^{3}γAc$_6$c (3)	68.42	21.02	172.86	-174.16
E-d^{2},^{3}γAc$_6$c (4)	-65.76	-15.31	-176.50	168.39

Table 2: Hydrogen Bond Parameters of **P1**

Donor (D)	**Acceptor (A)**	**DH….A (Å)**	**D….A (Å)**	**NH….O (deg)**
N1	O9	2.073	2.854	150.68
N3	O11	2.086	2.882	153.77
N6	O3	2.040	2.881	165.33
N8	O5	2.15	2.996	167.37

Table 3: Hydrogen Bond Parameters of **P2**

Donor (D)	**Acceptor (A)**	**DH….A (Å)**	**D….A (Å)**	**NH….O (deg)**
N2	O9	2.041	2.879	172.21
N3	O10	2.13	2.819	155.59
N4	O11	2.11	2.857	145.60
N6	O2	2.073	2.930	175.03
N7	O3	2.059	2.883	160.22
N8	O4	2.130	2.995	160.80

4. C-H···O H-bonding in Parameters of peptide P1 and P2

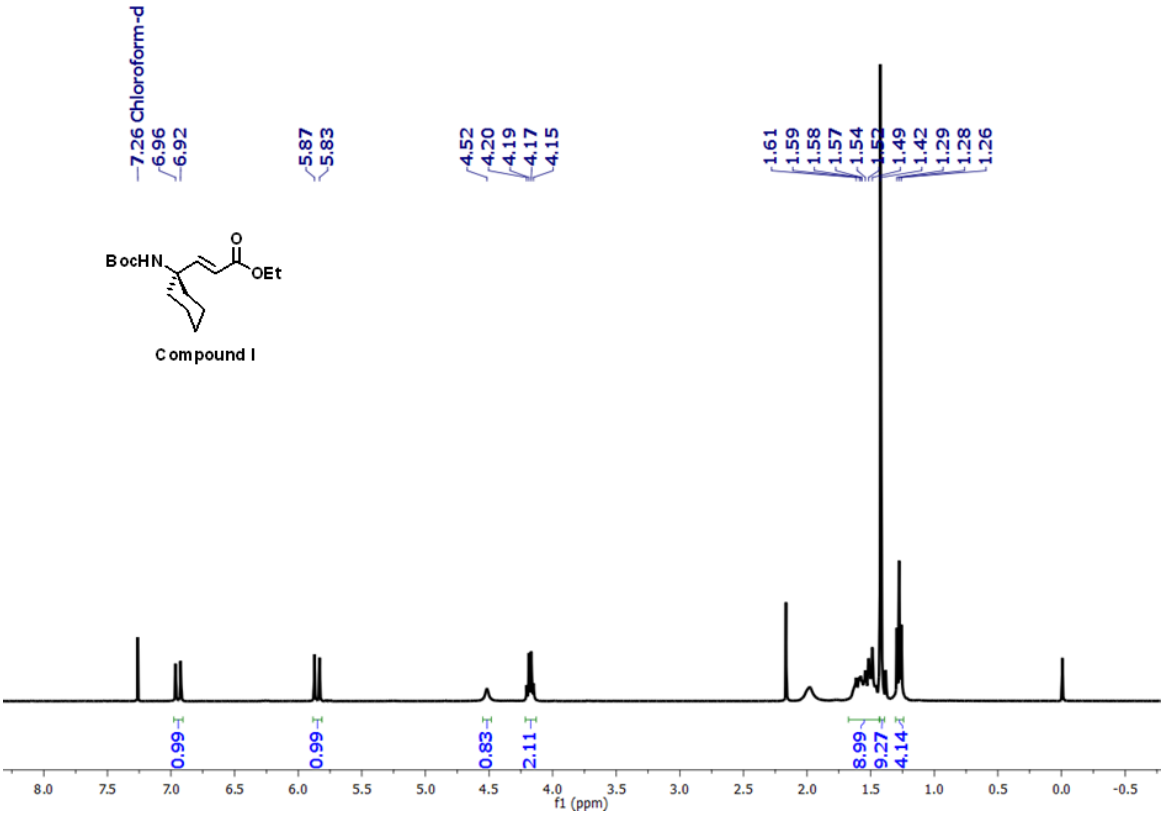
Table 4: C-H···O H-bond parameters **P1**

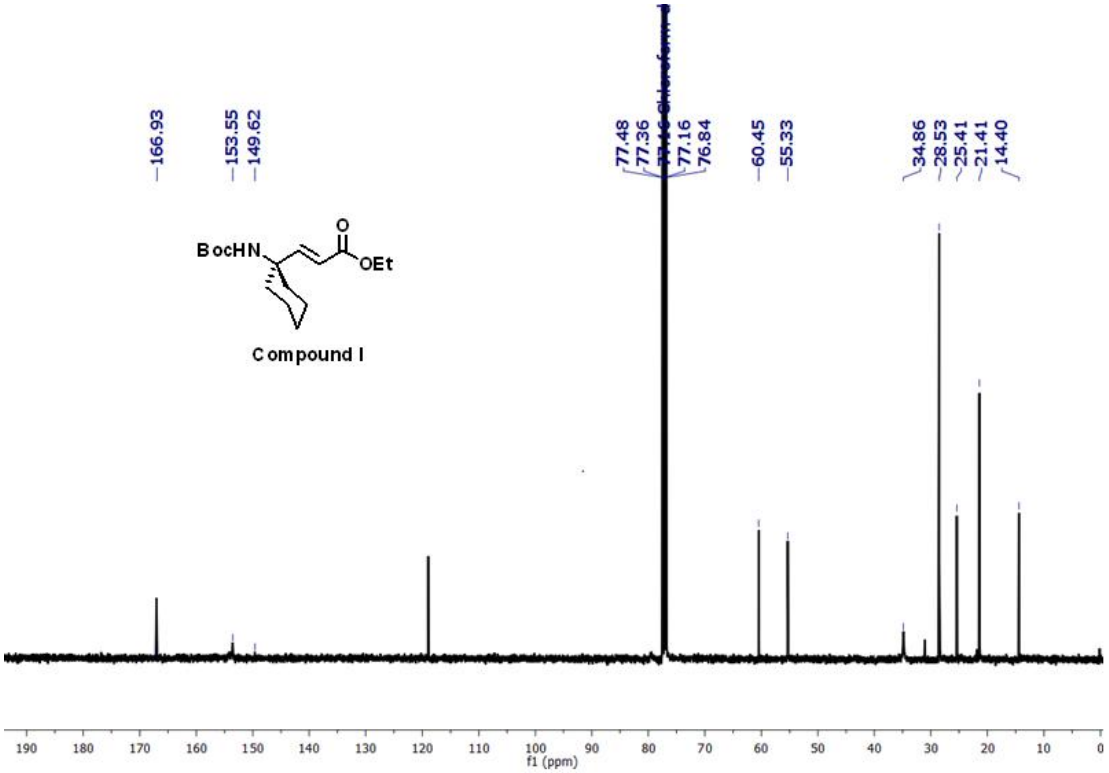
Donor (D)	**Acceptor (A)**	**DH….A (Å)**	**D….A (Å)**	**CH….O (deg)**
C66	O5	2.825	3.561	136.88
C23	O11	2.783	3.482	129.61
C53	O3	2.740	3.489	134.47

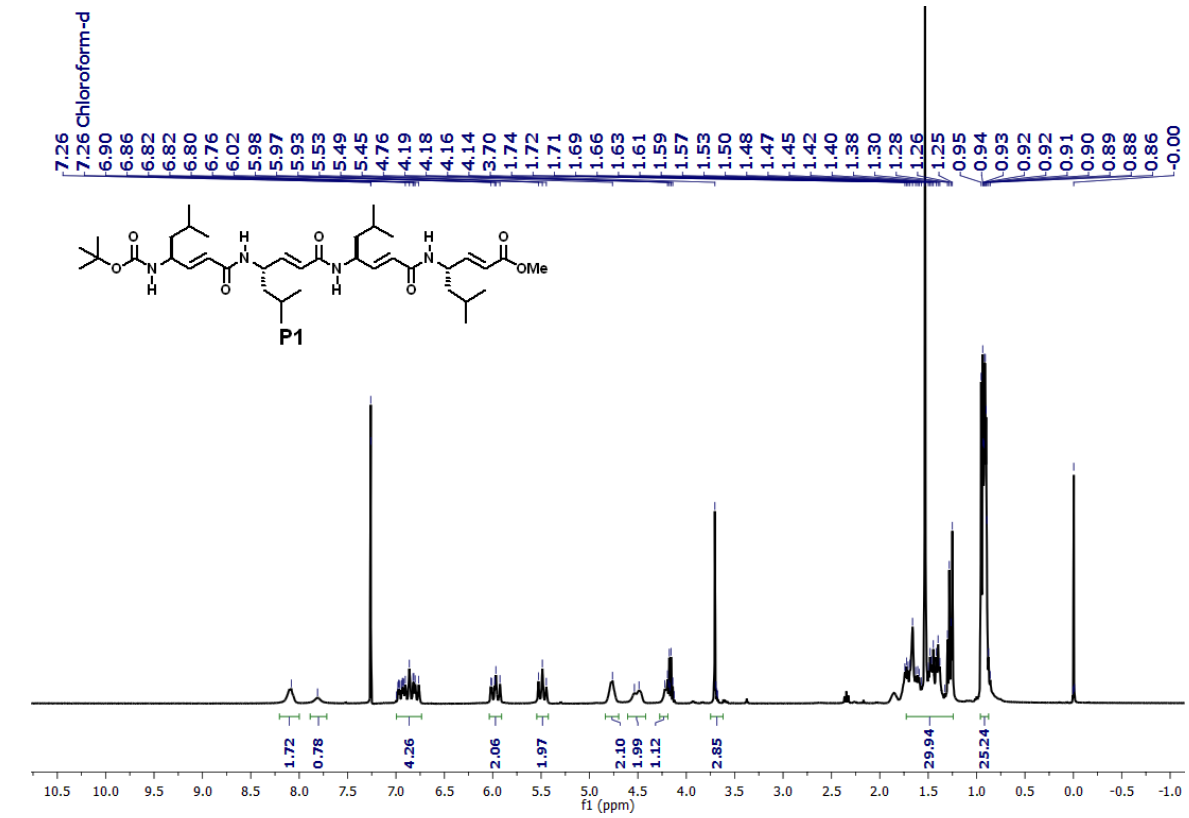
Table 5: C-H···O H-bond parameters **P2**

Donor (D)	**Acceptor (A)**	**DH….A (Å)**	**D….A (Å)**	**NH….O (deg)**
C19	O9	2.257	3.357	143.59
C59	O6	2.702	3.392	128.56
C71	O5	2.684	3.372	128.29
C22	O10	2.678	3.404	135.50
C31	O11	2.642	3.371	135.22
C80	O4	2.662	3.384	131.52

5. ^{1}H, ^{13}C and mass spectra of compounds



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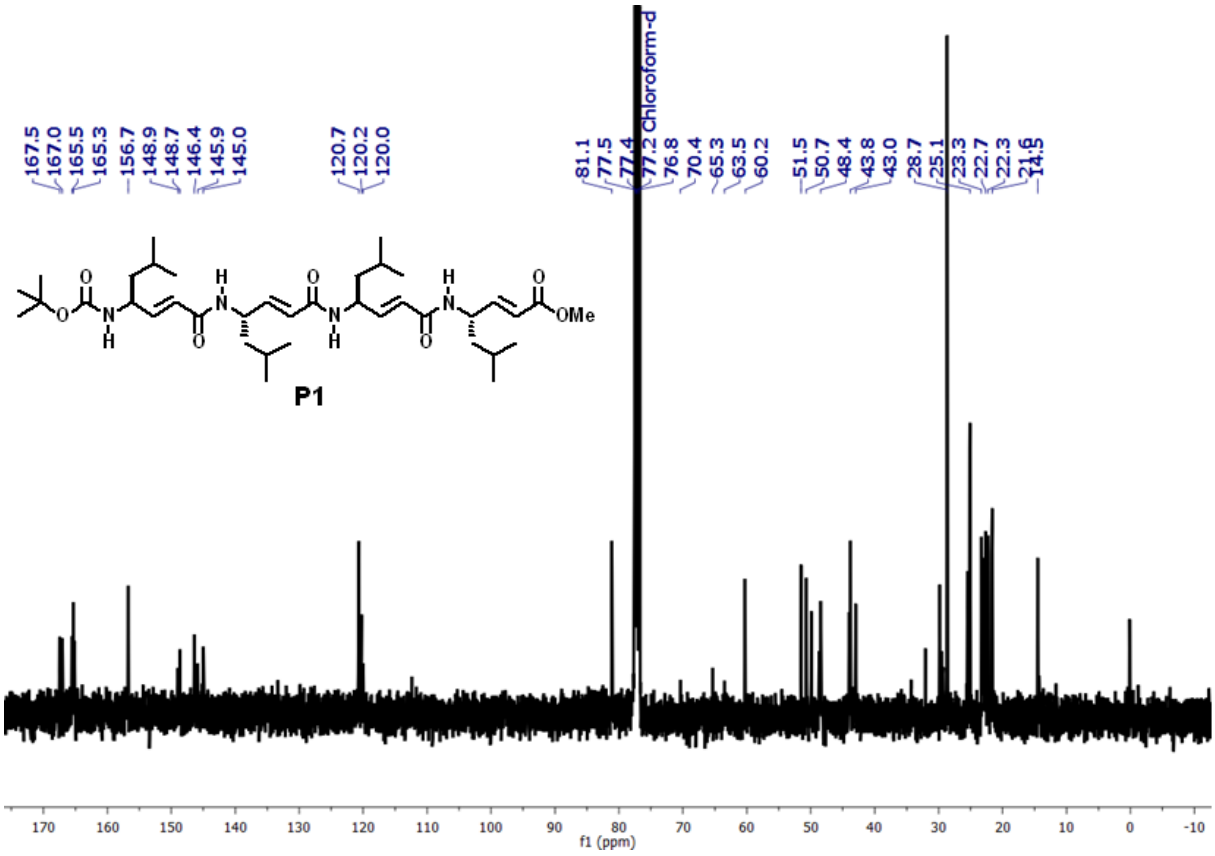
7.26 6.90 6.86 6.82 6.82 6.80 6.76 6.02 5.98 5.97 5.93 5.53 5.49 5.45 4.76 4.19 4.18 4.16 4.14 3.70 1.74 1.72 1.71 1.69 1.66 1.63 1.61 1.59 1.57 1.53 1.50 1.48 1.47 1.45 1.42 1.40 1.38 1.30 1.28 1.26 1.25 0.95 0.94 0.93 0.92 0.92 0.91 0.90 0.89 0.88 0.86 -0.00
OMe
P1
1.72 0.78 4.26 2.06 1.97 2.10 1.99 1.12 2.85 29.94 25.24
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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81.1 77.5 77.4 77.2 Chloroform-d 76.8 70.4 65.3 63.5 60.2 51.5 50.7 48.4 43.8 43.0 28.7 25.1 23.3 22.7 22.3 21.6 14.5
OMe
P1
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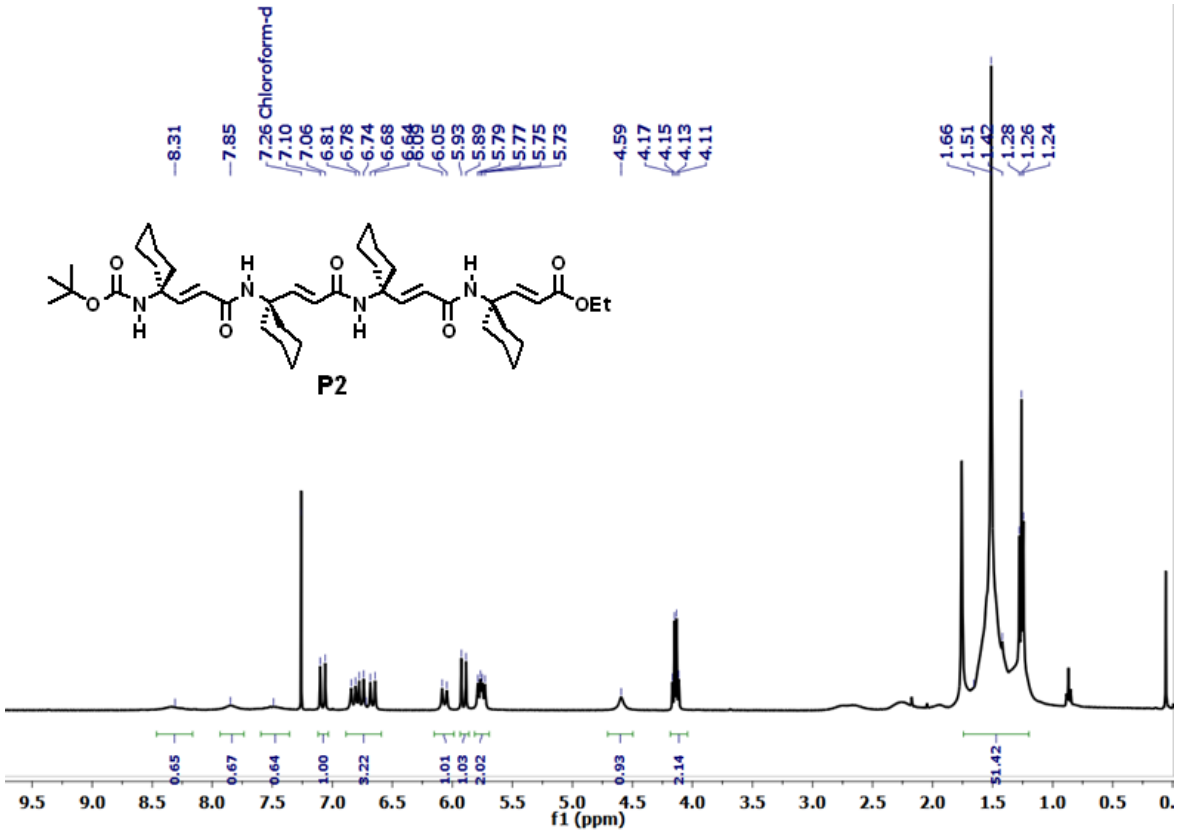
f1 (ppm)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7.10
7.06
6.81
6.78
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6.68
6.64
6.09
6.05
5.93
5.89
5.79
5.77
5.75
5.73
4.59
4.17
4.15
4.13
4.11
1.66
1.51
1.42
1.28
1.26
1.24
OEt
P2
0.65
0.67
0.64
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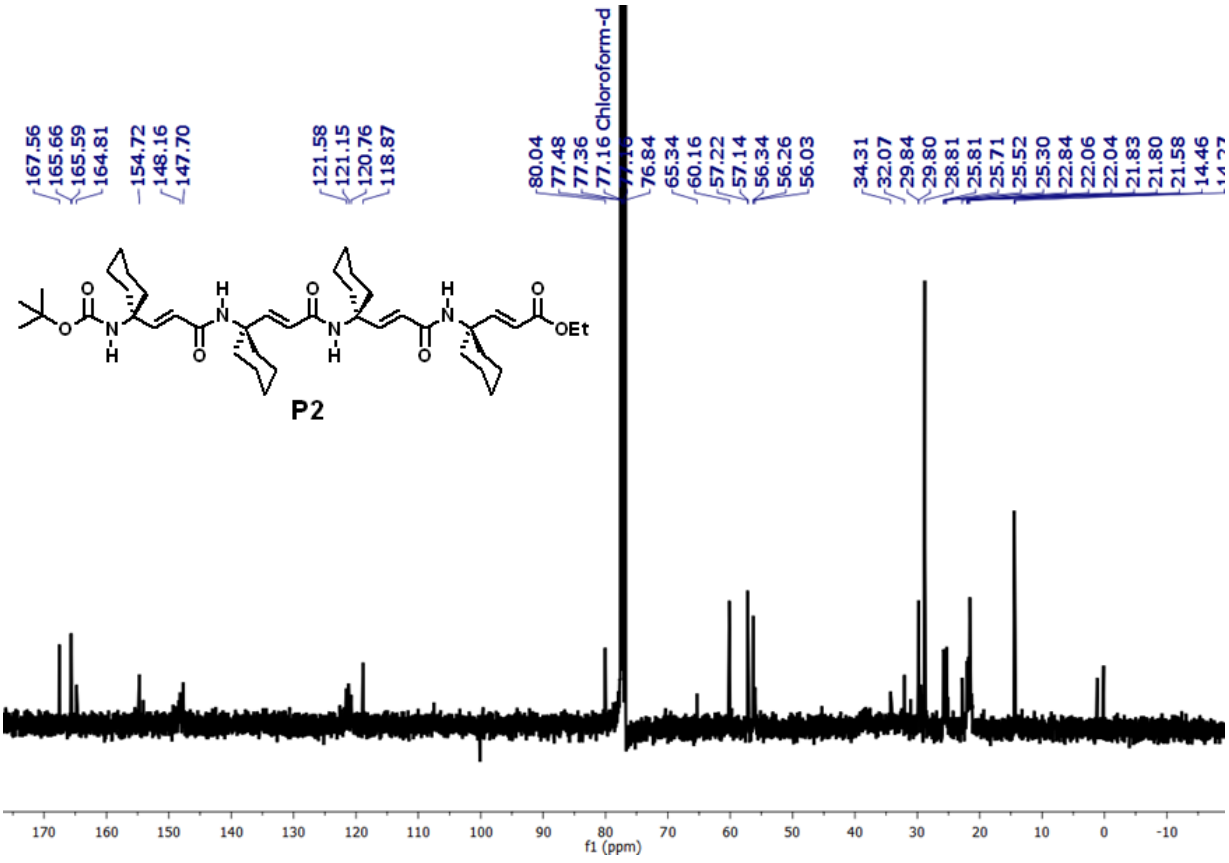
3.22
1.01
1.03
2.02
0.93
2.14
51.42
f1 (ppm)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165.59
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147.70
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120.76
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80.04
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77.36
77.16 Chloroform-d
76.84
65.34
60.16
57.22
57.14
56.34
56.26
56.03
34.31
32.07
29.84
29.80
28.81
25.81
25.71
25.52
25.30
22.84
22.06
22.04
21.83
21.80
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14.46
OEt
P2
f1 (ppm)

Spectrum Report

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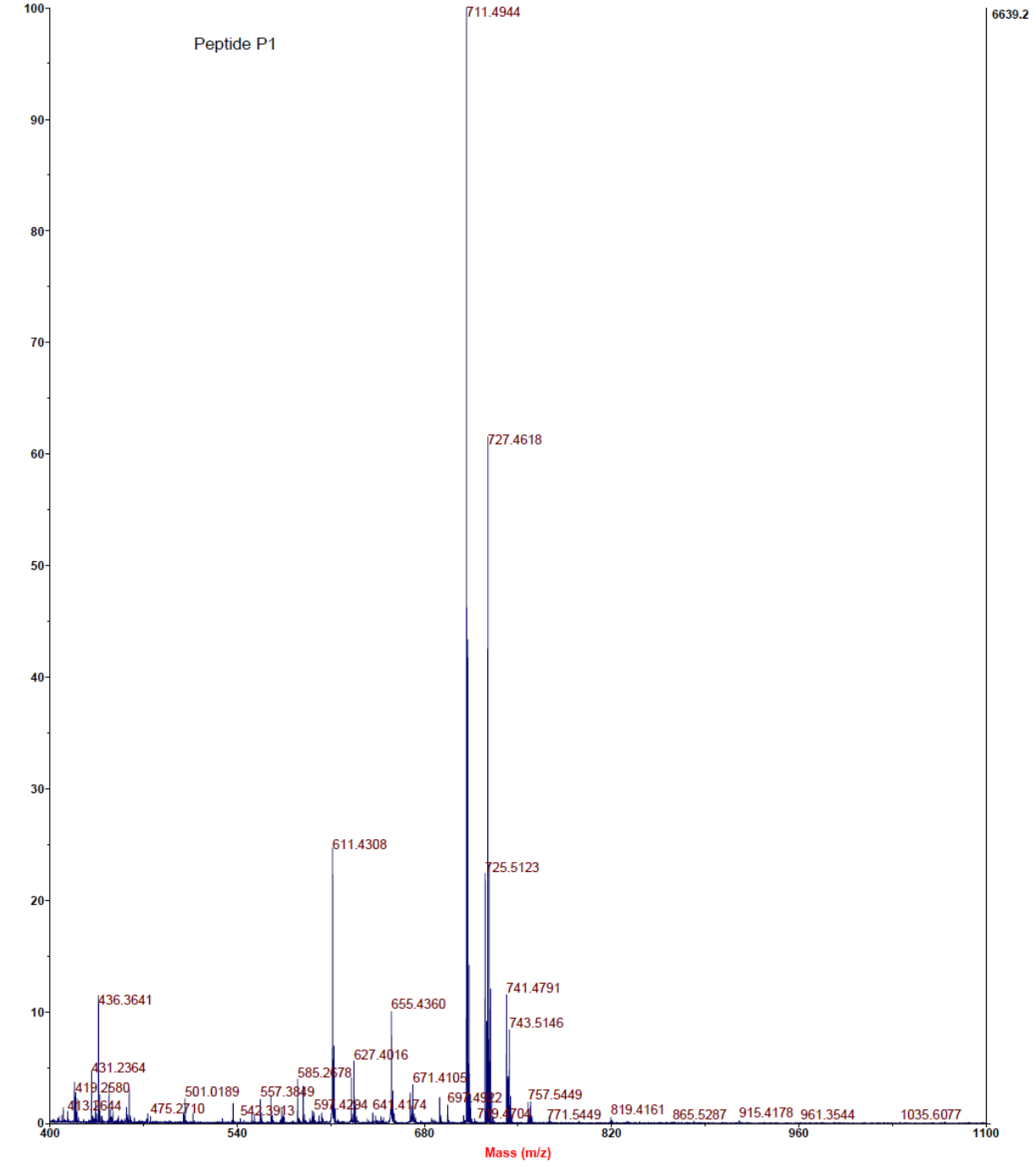

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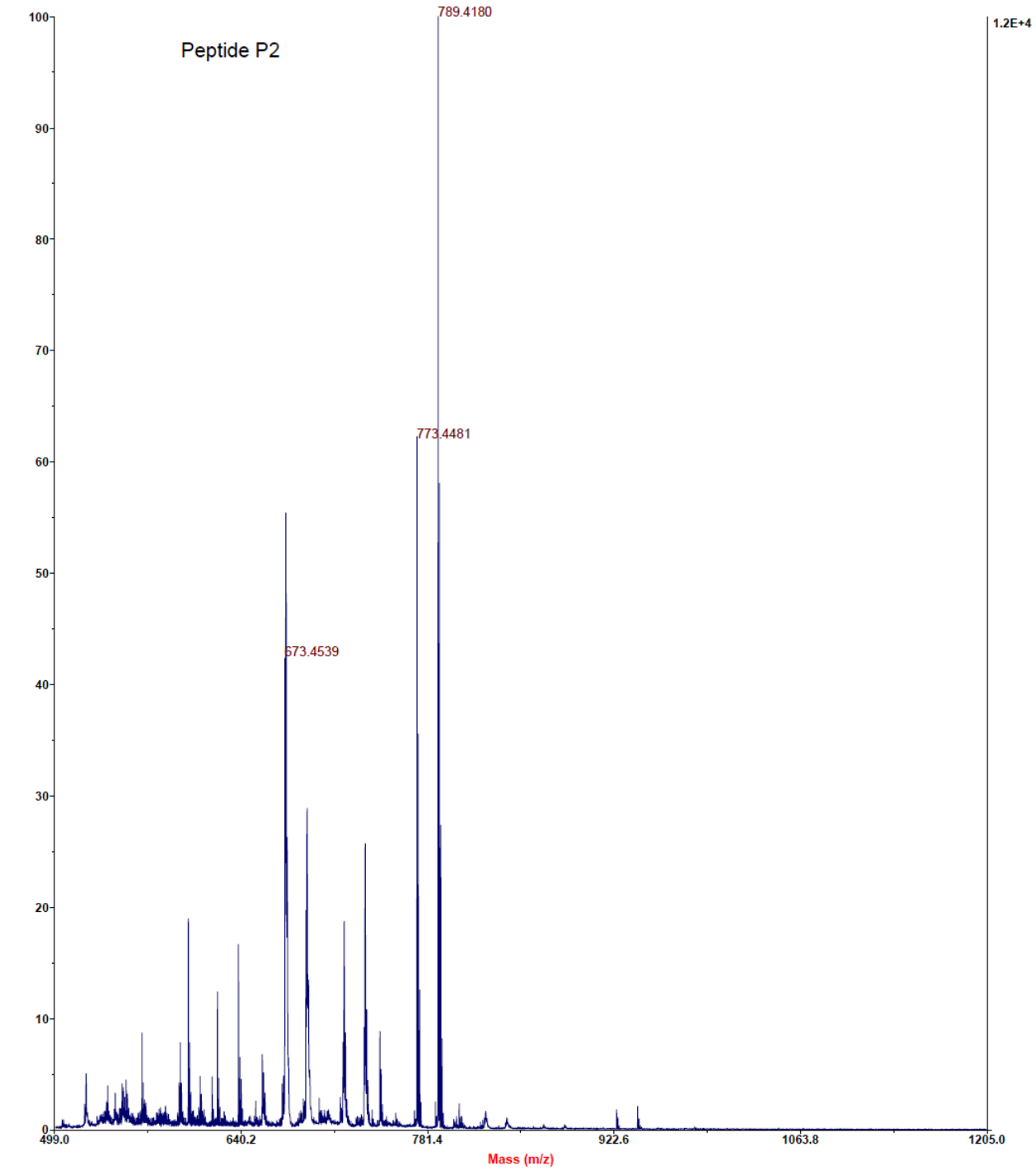

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