Electronic Supporting Information

Weak backbone CH···O=C and side chain *t*Bu···*t*Bu London interactions help promote helix folding of achiral N*t*Bu peptoids

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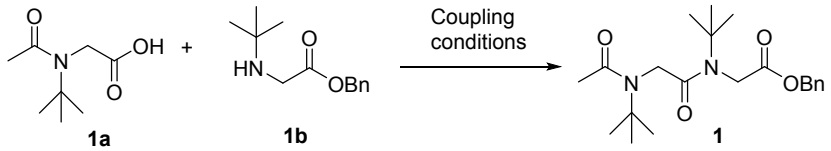
Peptoid segment coupling.

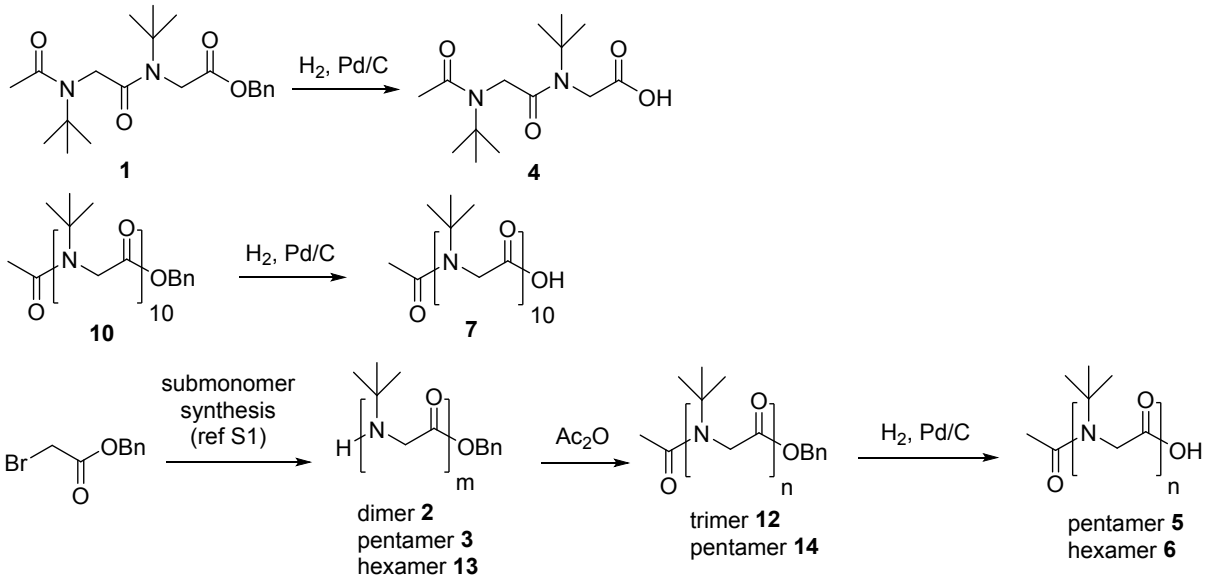
*Coupling conditions optimization on dimer **1***



	Coupling Reagent (equiv.)	Base (equiv.)	Solvent, Temperature	Conversion after 48h
A	HATU (1.2)	DIPEA (5)	DCM/DMF (4:1), r.t.	No reaction
B	HATU (1.2)	DBU (3)	DMF, r.t.	Traces of product
C	HATU (1.2)	DBU (3)	DCM, r.t.	Traces of product
D	DCC (1.2), HOBt	DBU (3)	DCM, r.t.	No reaction
E	DIC (1.2), DMAP (0.2)	-	DMF, r.t.	No reaction
F	EEDQ (1.2)	-	THF, r.t.	No reaction
G	EDCI (1.2), DMAP (0.2)	-	DCM/DMF (4:1), r.t.	Traces of product
H	PyBrOP	DIPEA (3)	DCM/DMF (4:1), r.t	No reaction
I	PyBOP (1.2)	DBU (3)	DMF, r.t.	No reaction
L	Ghosez reag.	DBU (2)	DCM, r.t.	No reaction
M	Ghosez reag.	DBU (2)	DMF, r.t.	No reaction
N	FDPP (1.2)	DIPEA (3)	DCM, r.t.	No reaction
O	FDPP (1.2)	DBU (3)	DCM, r.t.	Formation of the product

Table 1. Initial coupling conditions test on the synthesis of dimer **1**. Reactions progress were followed by TLC.

Preparation of peptoid amine and acid blocks for segment coupling



General procedure of coupling with pentafluorophenyl diphenylphosphinate (FDPP).

To a solution of free-acid block NtBu peptoid oligomer (1.0 equiv., 0.4M) in dry CH_2Cl_2 at rt under argon, was added FDPP (1.2 equiv). The mixture was stirred for 5 min. Separately, a solution of the free-amine block NtBu peptoid oligomer (1.0 equiv., 0.4M) and DBU (3 equiv.) in CH_2Cl_2 was prepared and was slowly dropped into the first solution containing the free-acid block. The mixture was left stirring at rt for 48h. The resulting solution was diluted with CH_2Cl_2 and subsequently washed with aqueous HCl (1N) solution and saturated aqueous $NaHCO_3$ solution. The organic fraction was then dried over sodium sulfate and concentrated in vacuo, to give the crude product. Products were purified and isolated by column chromatography.

General procedure of coupling with pentafluorophenyl trifluoroacetate (TFAPfp).

To a solution of free-acid block NtBu peptoid oligomer (1.0 equiv., 0.3M) in dry CH_2Cl_2 at rt under Ar, was added pentafluorophenyl trifluoroacetate (1.5 equiv.) and Pyridine (1.5 equiv.). The mixture was stirred for 1 h. Afterwards diluted with CH_2Cl_2 and washed with 1N aqueous HCl solution and saturated aqueous $NaHCO_3$ solution. The organic fraction was then dried over sodium sulfate and concentrated in vacuo, to give the crude activated ester, which was immediately used in the next step. To the solution of the activated ester (1.0 equiv., 0.2 M) in dry CH_2Cl_2 at r.t. under Ar, was slowly added a previously prepared solution of free-amine block NtBu peptoid oligomer (1.0 equiv., 0.2M) and DBU (3 equiv.) in CH_2Cl_2. The mixture was left stirring for 48h. It was then diluted with CH_2Cl_2 and subsequently washed with 1N aqueous HCl solution and saturated aqueous $NaHCO_3$ solution. The organic fraction was dried over sodium sulfate and concentrated in vacuo, to give the crude product. Products were purified and isolated by chromatography column.

*Dimer **1** (FDPP conditions)*

Free-acid block unit monomer **1a**, (200 mg, 1.23 mmol), was dissolved in 3 mL of dry CH_2Cl_2 under argon, and 567 mg of FDPP (1.48 mmol) were added in the solution. Free-amine block unit monomer **1b**, (272 mg of 1.23 mmol) was dissolved in 3 mL of dry CH_2Cl_2 with DBU (552 μL, 3.7 mmol). The obtained mixture was dropped in the initial solution, and let stirring for 48h at r.t. The resulting solution was washed two times, with aqueous HCl solution (1N) and saturated aqueous $NaHCO_3$ solution, dried over sodium sulfate and concentrated in *vacuo*. Crude product was purified by flash chromatography on silica gel using a gradient of cyclohexane/EtOAc, from 70:30 to 50:50, affording dimer **1** (277 mg, 0.73 mmol, 60%) as a white powder. Complete characterization in Ref. S1.

*Dimer **1** (TFA-Pfp conditions)*

Free-acid block unit monomer **1a**, (50 mg, 0.30 mmol), was dissolved in 1 mL of dry CH_2Cl_2. TFAPfp (80 μL, 0.46 mmol), and pyridine (37 μL, 0.46 mmol) were added, and the reaction was let stirring for 1h at r.t. The solution was washed two times, with 1N aqueous HCl solution and saturated aqueous $NaHCO_3$ solution, dried over sodium sulfate and concentrated in *vacuo*. The reaction crude was re-dissolved in 2 mL of dry CH_2Cl_2, under argon, and a solution of free-amine block unit monomer **1b** (68 mg, 0.30 mmol, in 2 mL of dichloromethane) was added. DBU (135 μL, 0.9 mmol) were dropped in, and the reaction was let stirring at rt for 48h. The resulting solution was washed two times, with aqueous solution of HCl (1N) and saturated aqueous $NaHCO_3$ solution, dried over sodium sulfate and concentrated in *vacuo*. Crude product was purified by flash chromatography on silica gel using a gradient of cyclohexane/EtOAc, from 50:50 to 30:70, affording dimer **1** (62 mg, 0.17 mmol, 55%) as a white powder. Complete characterization on Ref. S1

*15-mer **11***

According to the procedure used to synthesise dimer **1**, 50 mg of free-acid block unit decamer **7** (0.042 mmol) were coupled to 28 mg of fee-amine block unit pentamer **3** to obtain the penta-decamer oligomer **11**. Crude product was purified by flash chromatography on silica gel using a gradient of cyclohexane/EtOAc, from 50:50 to 30:70, affording the product **11** (40 mg, 0.022 mmol, 52%) as a white powder.

Mp = 172°C (dec.); Rf = 0.30 (cyclohexane/EtOAc 30:70); IR (ATR) ν (cm^{-1}): 2974, 2929, 1663, 1458, 1437, 1391, 1362, 1327, 1269, 1198, 991, 837, 733; ^{1}HNMR (400 MHz, CD_2Cl_2) δ (ppm): 1.38-1.48 (bs, m, 135H), 1.87 (s, 3H), 3.46-4.35 (bs, m, 30H), 5.24 (s, 2H), 7.35-7.40 (m, 5H); HRMS (TOF MS ES+): calcd for $C_{99}H_{175}N_{15}O_{17}$ $[M + H]^+$ *m/z* 1847.3369, found 1847.3427.

*Tetramer **8***

To a solution of fully protected dimer **1** (958 mg, 2.55 mmol) in methanol (60 mL), was added 10% palladium on charcoal (96 mg). The mixture was stirred under a hydrogen atmosphere for 24 h. The catalyst was then filtered through a celite pad, and the solution was concentrated under reduced pressure, giving the free-acid dimer **4**, as a white powder, with complete conversion. The product was controlled by TLC and ^{1}H NMR and used for the following step without further purification. Afterwards, free-acid block unit dimer **4**, (200 mg,

0.70 mmol), was dissolved in 2 mL of dry CH_2Cl_2. TFAPfp (180 µL, 1.05 mmol), and pyridine (85 µL, 1.05 mmol) were added, and the reaction was let stirring for 1h at r.t. The solution was washed two times, with 1N aqueous HCl solution and saturated aqueous $NaHCO_3$ solution, dried over sodium sulfate and concentrated in *vacuo*. The reaction crude was re-dissolved in 3 mL of dry CH_2Cl_2, under argon, and a solution of free-amine block unit dimer **2** (233 mg, 0.70 mmol, in 2 mL of dichloromethane) was added. DBU (313 µL, 2.1 mmol) were dropped in, and the reaction was let stirring at rt for 48h. The resulting solution was washed two times, with aqueous solution of HCl (1N) and saturated aqueous $NaHCO_3$ solution, dried over sodium sulfate and concentrated in *vacuo*. Crude product was purified by flash chromatography on silica gel using a gradient of cyclohexane/EtOAc, from 50:50 to 30:70, affording the tetramer **8** (236 mg, 0.4 mmol, 70%) as a white powder. Complete characterization on Ref. S1

*Octamer **9***

According to the procedure used to synthesise the tetramer **8**, 500 mg of fully protected hexamer oligomer **13** (0.6 mmol) were deprotected through hydrogenolysis to afford the free-acid hexamer unit **6**, with complete conversion, as a white powder. Afterwards, 427 mg of free-acid hexamer unit **6** (0.47 mmol) were coupled to 157 mg of free-amine dimer unit **2** (0.47 mmol) following the already described procedure for the tetramer **8**. The reaction crude was purified by flash chromatography on silica gel using a gradient of cyclohexane:EtOAc, from 60:40 to 30:70, affording the octamer **9** (358 mg, 0.34 mmol, 68%) as a white powder, with a 68% yield.

Mp = 138°C; Rf = 0.50 (cyclohexane/EtOAc 30:70); IR (ATR) ν (cm^{-1}): 2972, 2930, 2359, 1742, 1667, 1391, 1362, 1327, 1269, 1198, 991, 837; ^{1}HNMR (400 MHz, CD_2Cl_2) δ (ppm): 1.36-1.40 (bs, m, 72H), 1.88 (s, 3H), 3.70-4.28 (bs, m, 16H), 5.23 (s, 2H), 7.37-7.40 (m, 5H); ^{13}CNMR (100 MHz, CD_2Cl_2) δ (ppm): 27.2-29.42, 46.7, 57.3, 57.9-59.1, 60.6, 68.1, 129.0, 129.2, 135.5, 170.5-171.2, 172.7; HRMS (TOF MS ES+): calcd for $C_{57}H_{98}N_8O_{10}$ $[M + H]^+$ *m/z* 1055.7484, found 1055.7451.

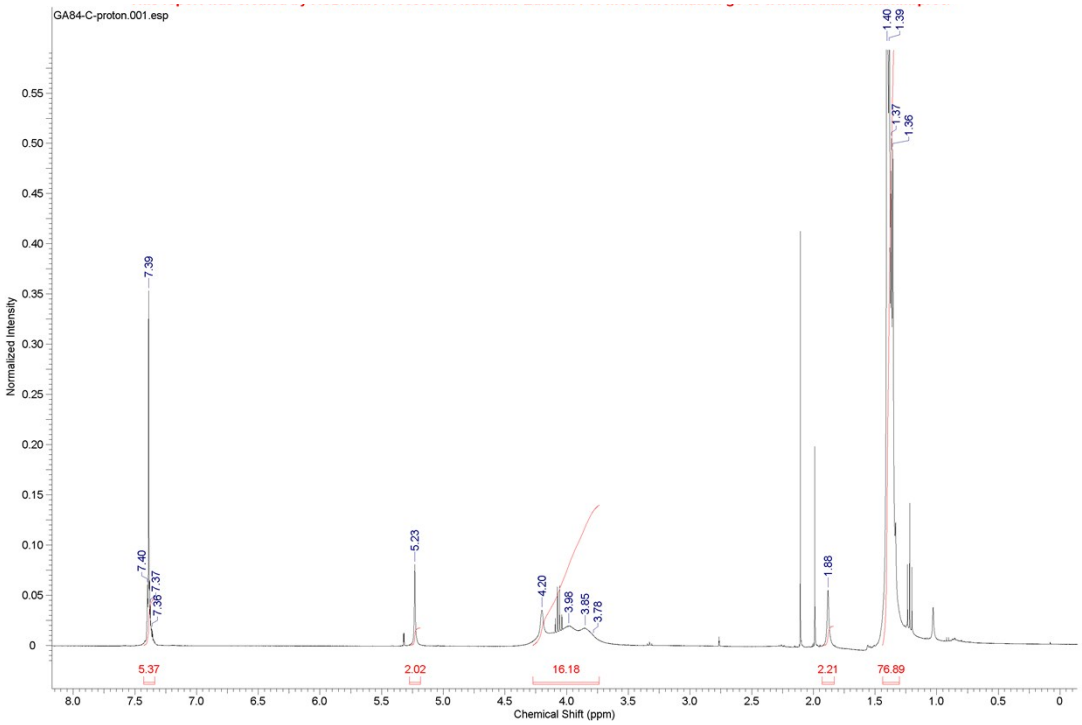
*Decamer **10***

According to the same procedure used to synthesise tetramer **8**, fully protected pentamer **14** (1.58 g, 2.21 mmol) was deprotected through hydrogenolysis to afford with complete conversion the free-acid pentamer **5**, as a white powder. Afterwards, free-acid block pentamer **5**, (400 mg, 0.64 mmol), was coupled to free-amine pentamer **3**, (472 mg, 0.70 mmol), following the already described procedure for the tetramer **8**. Crude product was purified by flash chromatography on silica gel using a gradient of cyclohexane/EtOAc, from 50:50 to 30:70, affording decamer **10** (602 mg, 0.47 mmol, 73%) as a white powder.

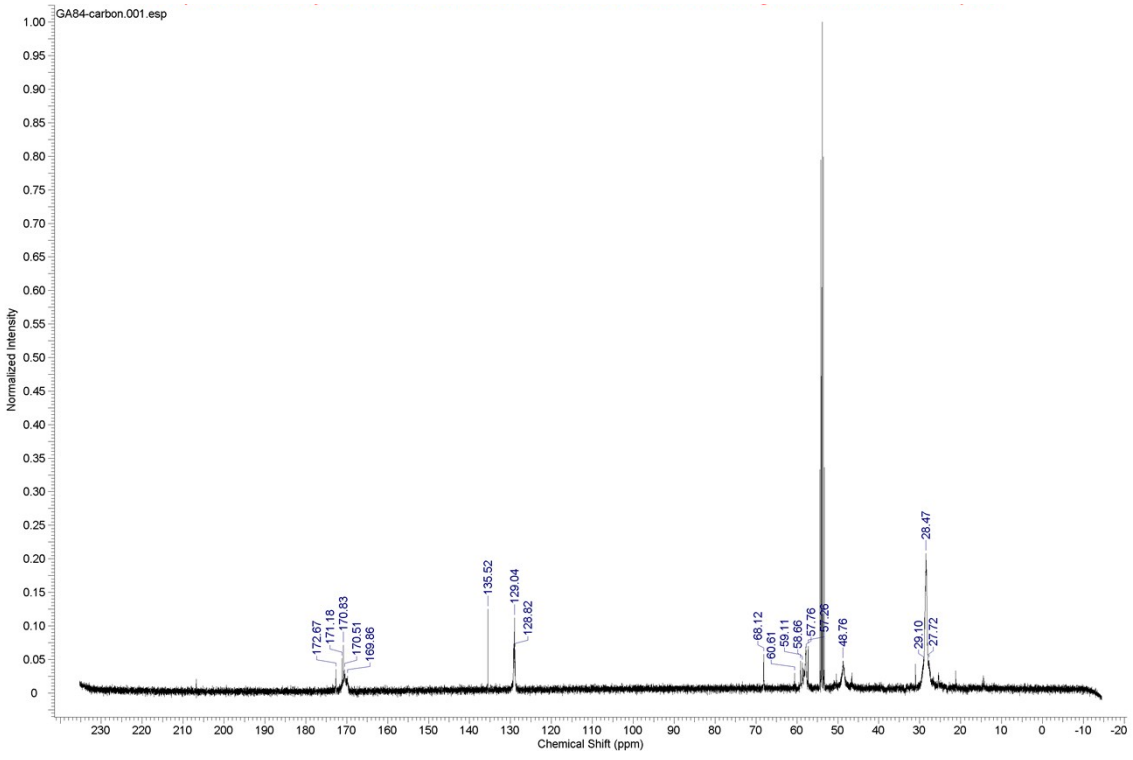
Mp = 158°C; Rf = 0.48 (cyclohexane/EtOAc 30:70); IR (ATR) ν (cm^{-1}): 2977, 2916, 2849, 1747, 1652, 1463, 1436, 1390, 1362, 1323, 1269, 1198, 1050, 991, 878, 838; ^{1}HNMR (400 MHz, $CDCl_3$) δ (ppm): 1.36-1.48 (bs, m, 90H), 1.99 (s, 3H), 3.60-4.40 (bs, m, 20H), 5.25 (s, 2H), 7.37-7.43 (m, 5H); ^{13}CNMR (100 MHz, CD_2Cl_2) δ (ppm): 28.1-28.9, 46.6, 48.3-49.1, 57.3, 57.6-58.8, 59.1, 68.1, 128.9, 129.1, 129.2, 135.5, 169.7-171.4, 172.7; HRMS (TOF MS ES+): calcd for $C_{69}H_{120}N_{10}O_{12}$ $[M + H]^+$ *m/z* 1281.9165, found 1281.8976.

Analysis of the products (9), (10), (11), at room temperature (298K)

*^{1}HNMR of the Octamer Ac-(NtBu)$_{8}$-OBn (**9**)*



*^{13}CNMR of the Octamer Ac-(NtBu)$_{8}$-OBn (**9**)*



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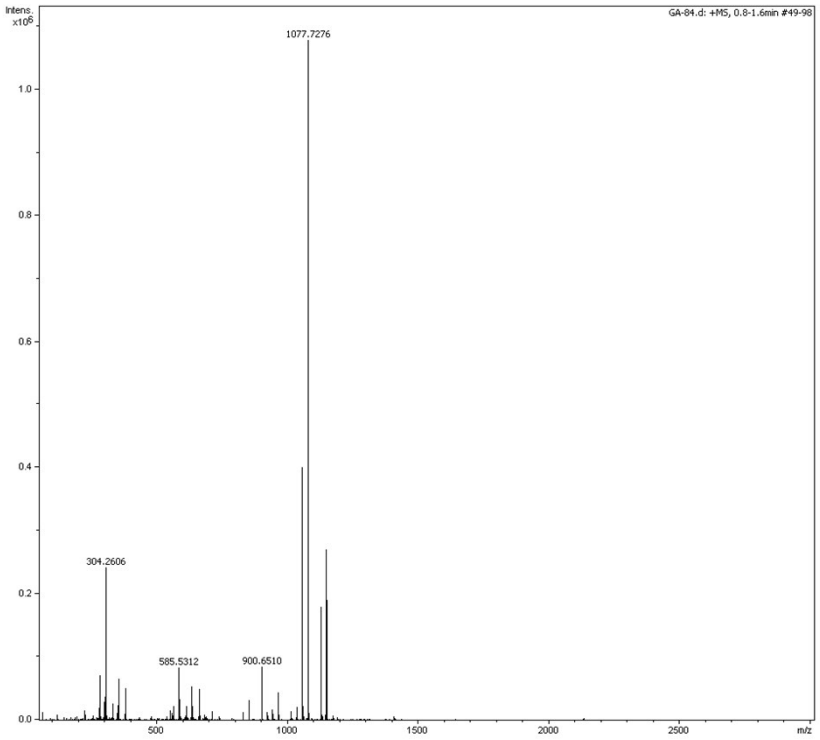
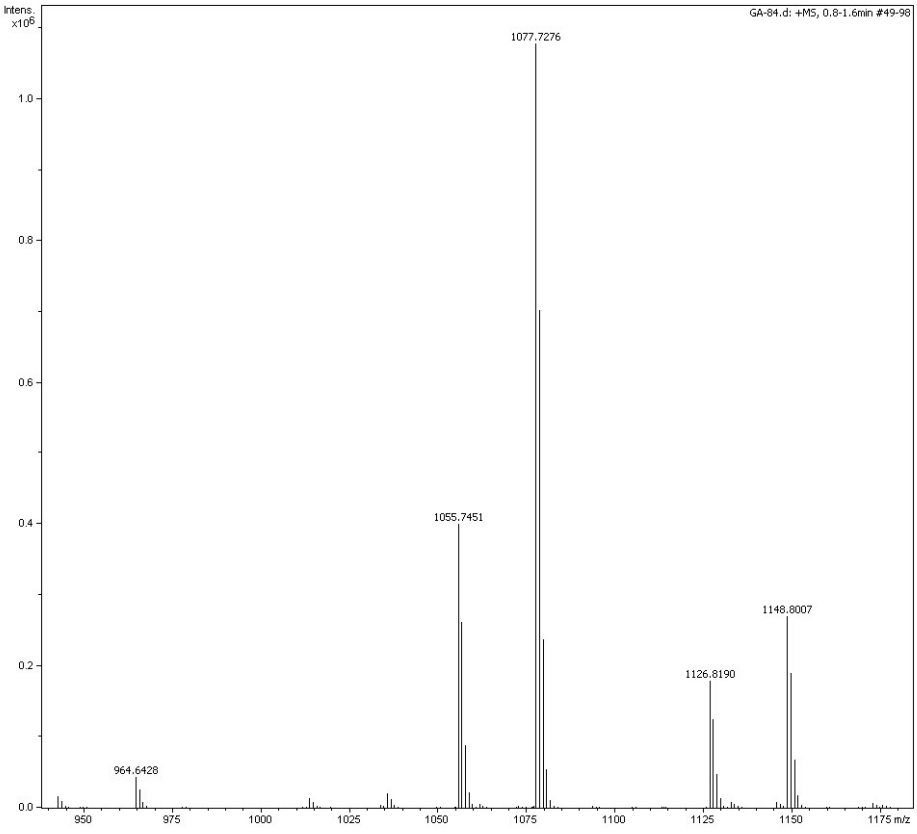
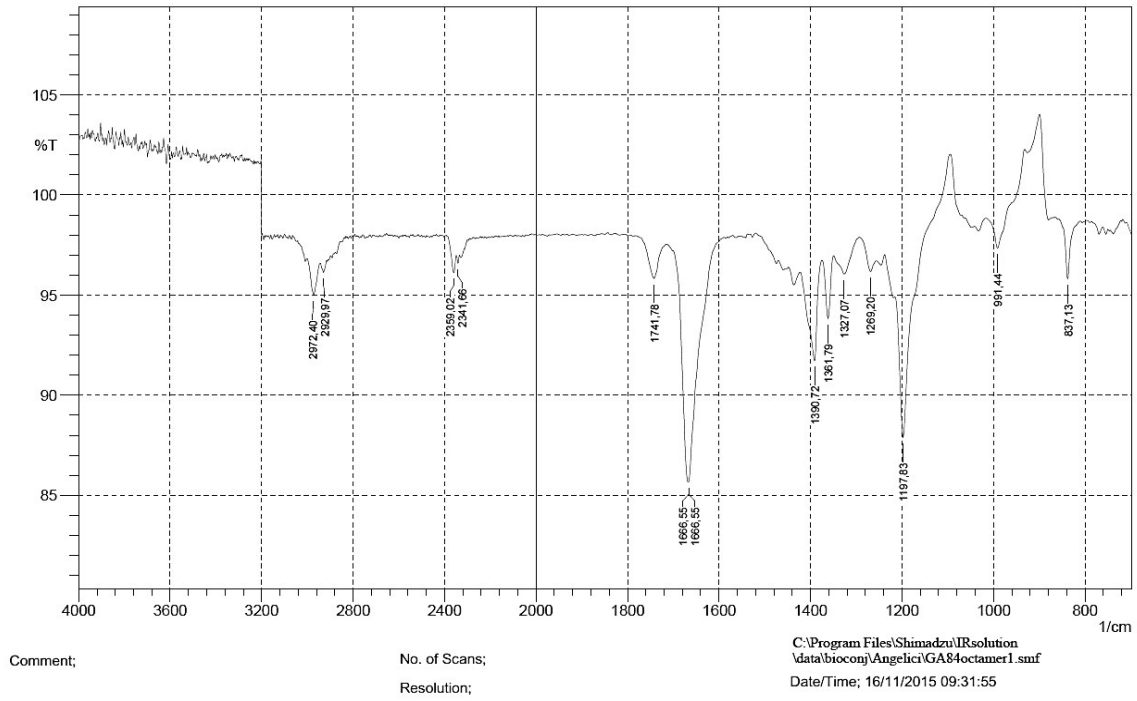


*HR-MS of octamer Ac-(NtBu)$_8$-OBn (**9**) zoom*



*Infra-Red spectra of octamer Ac-(NtBu)$_8$-OBn (**9**)*



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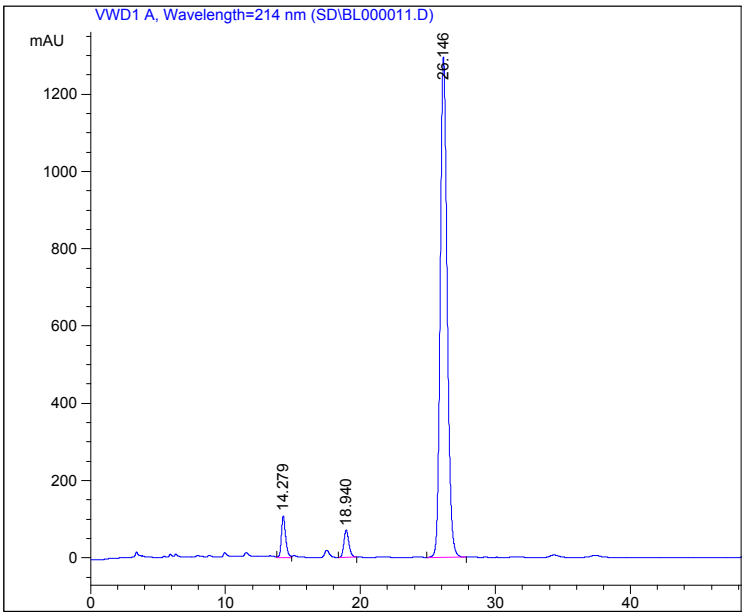


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Use Multiplier & Dilution Factor with ISTDs


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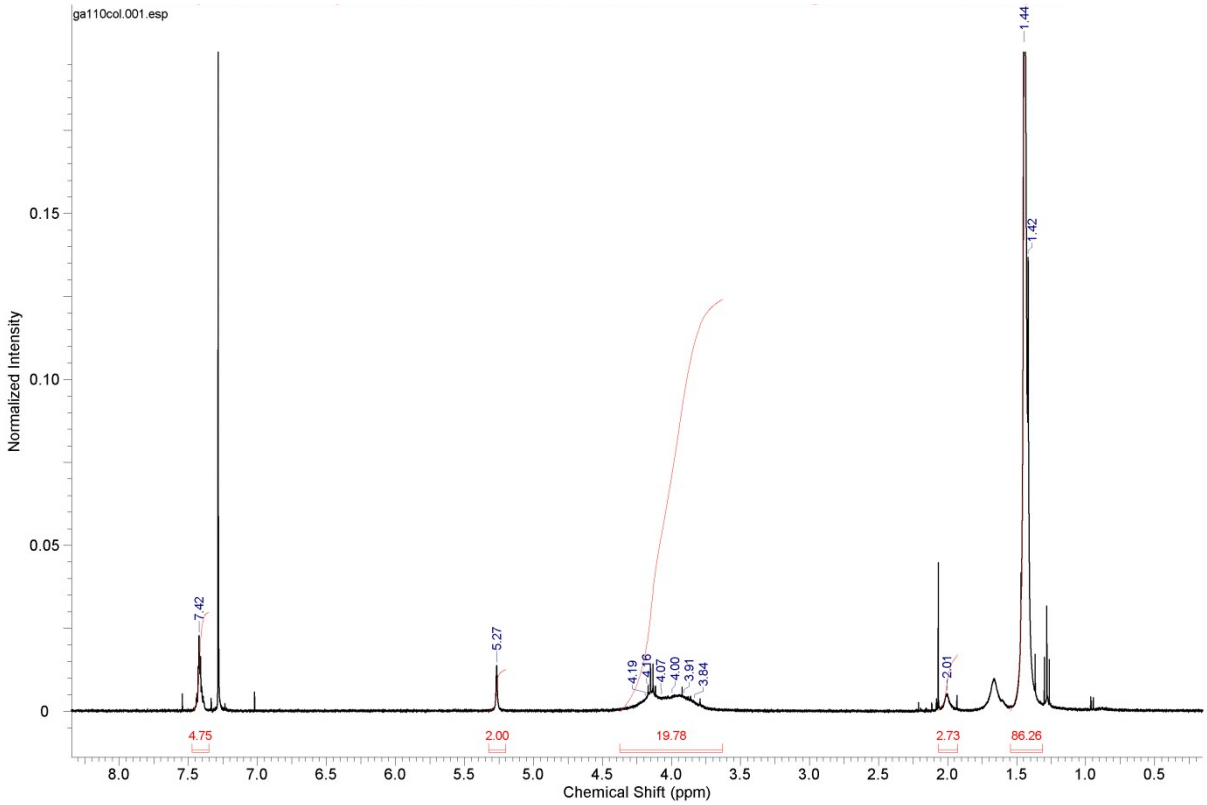
*^{1}HNMR of the Decamer Ac-(NtBu)$_{10}$-OBn (**10**)*



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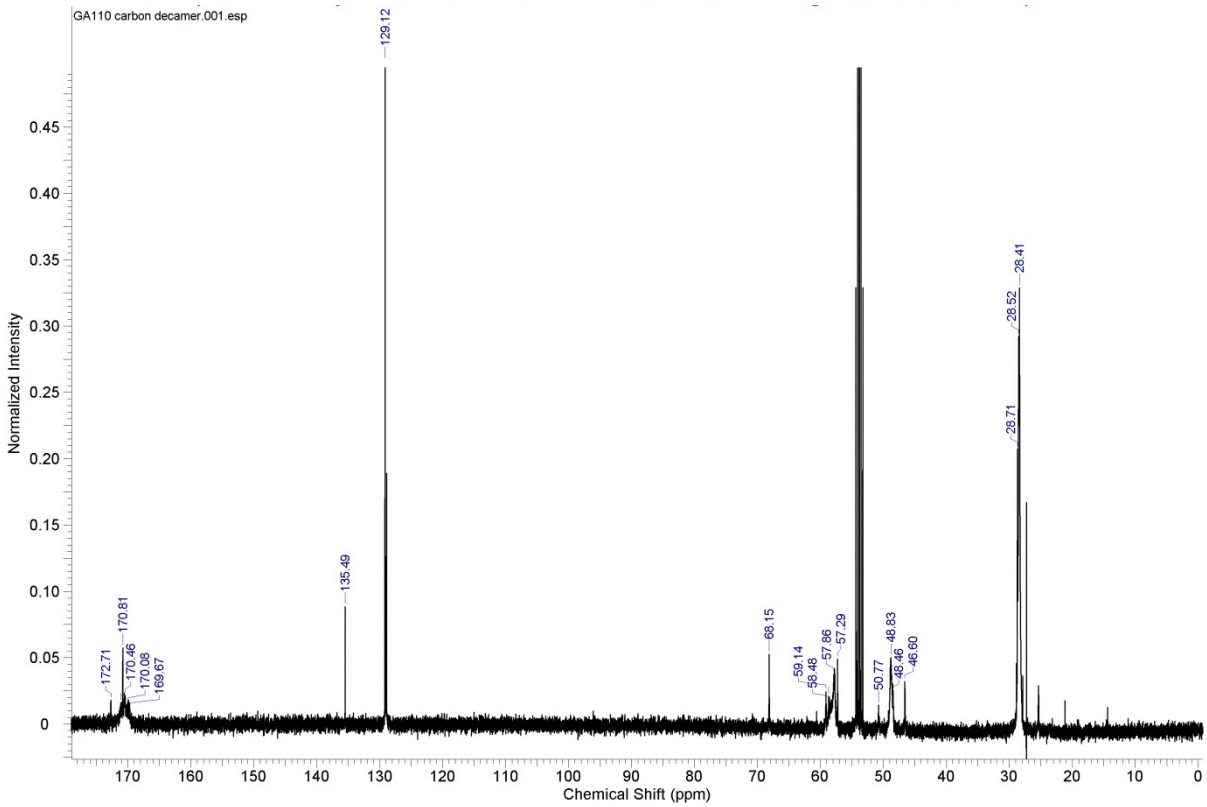

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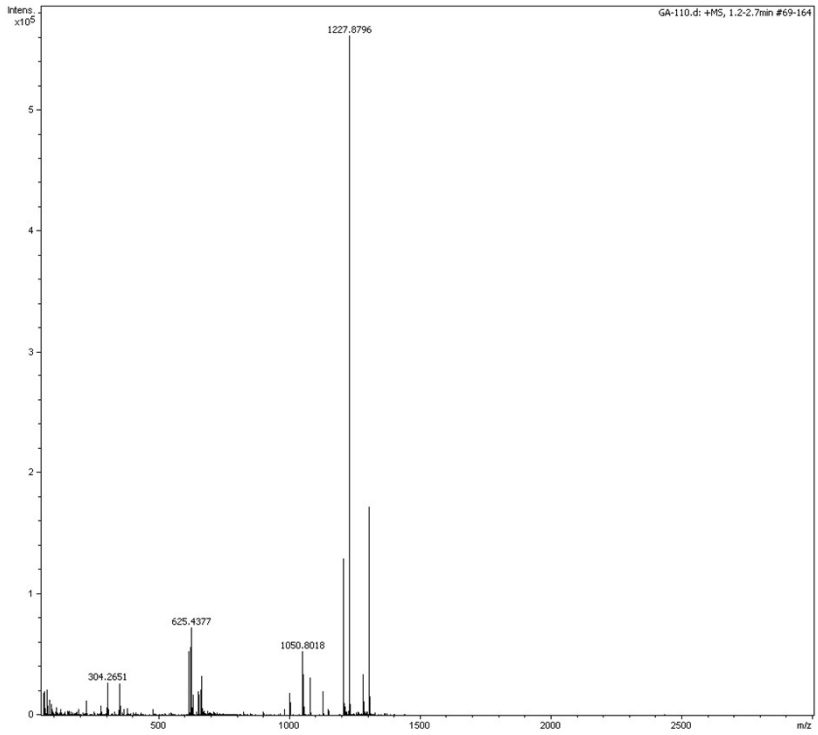

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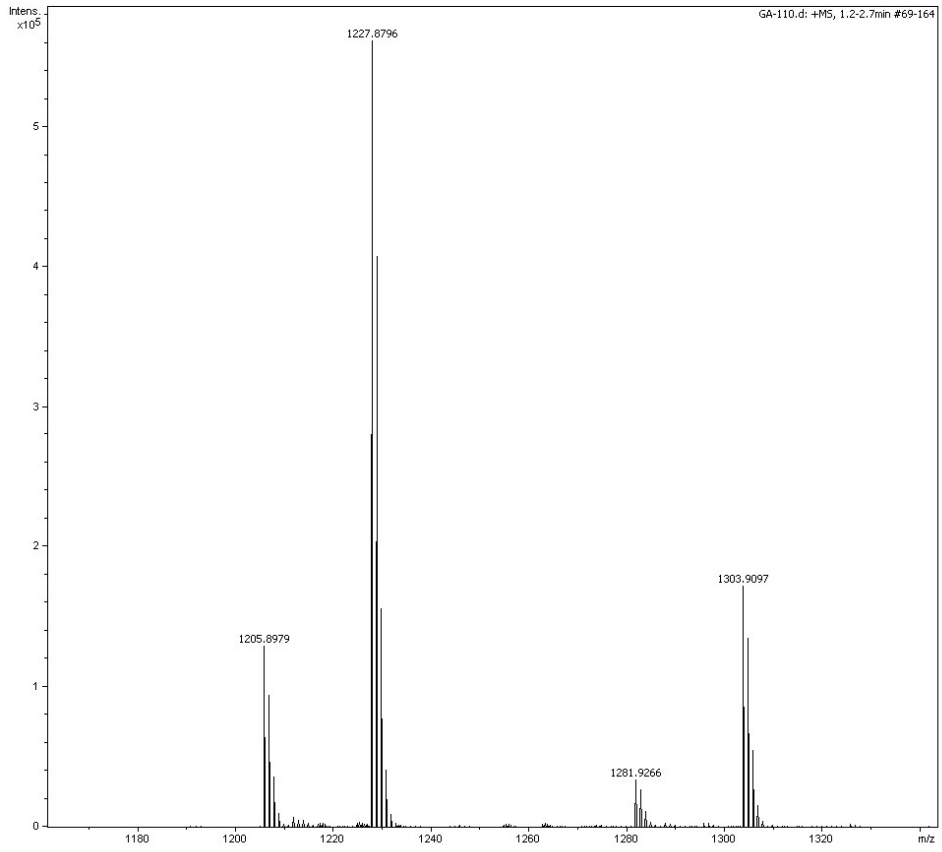
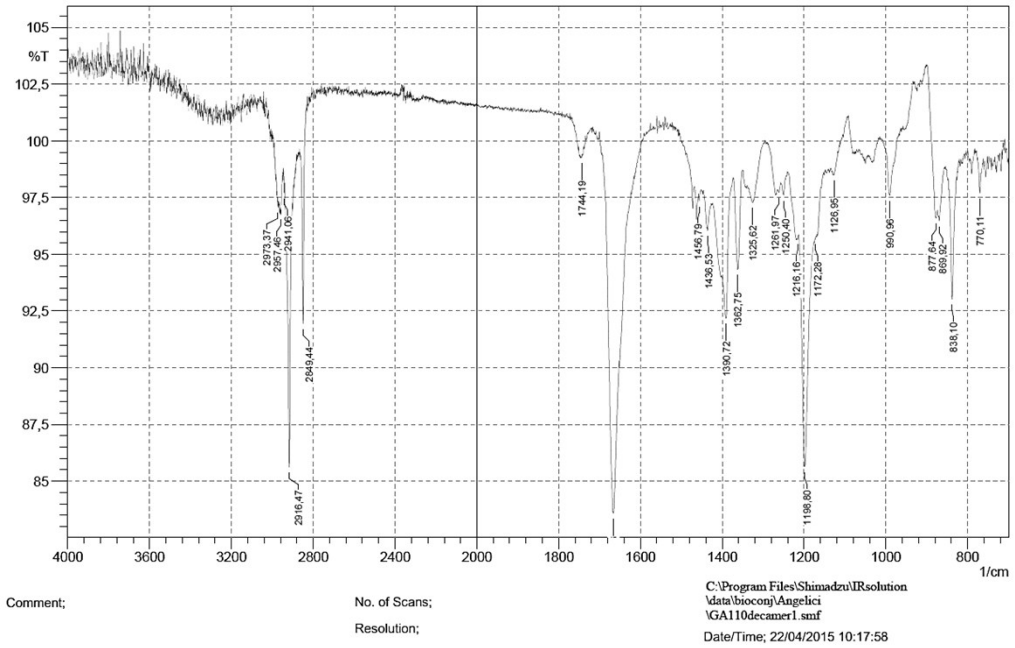
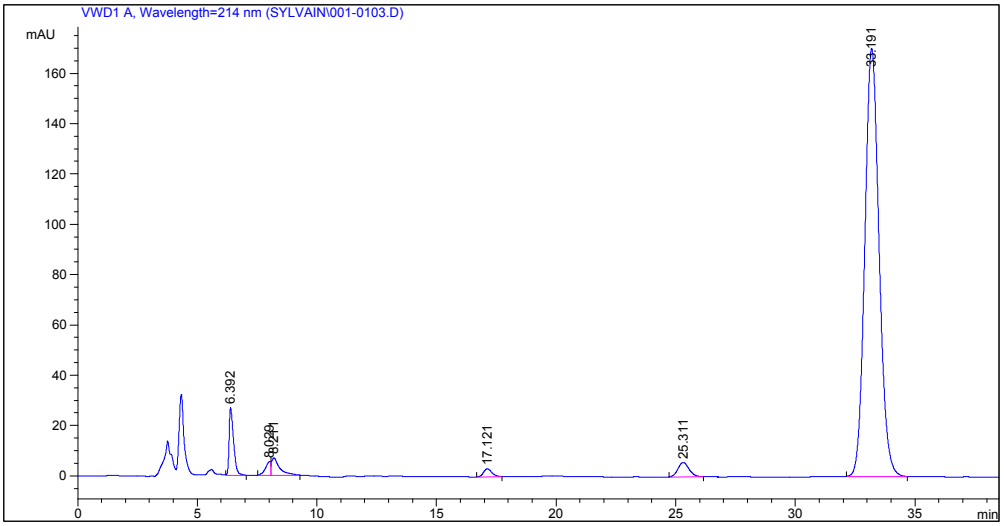


*Infra-Red spectra of decamer Ac-(NtBu)$_{10}$-OBn (**10**)*



*HPLC spectra of decamer Ac-(NtBu)$_{10}$-OBn (**10**)*

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 Results obtained with enhanced integrator!
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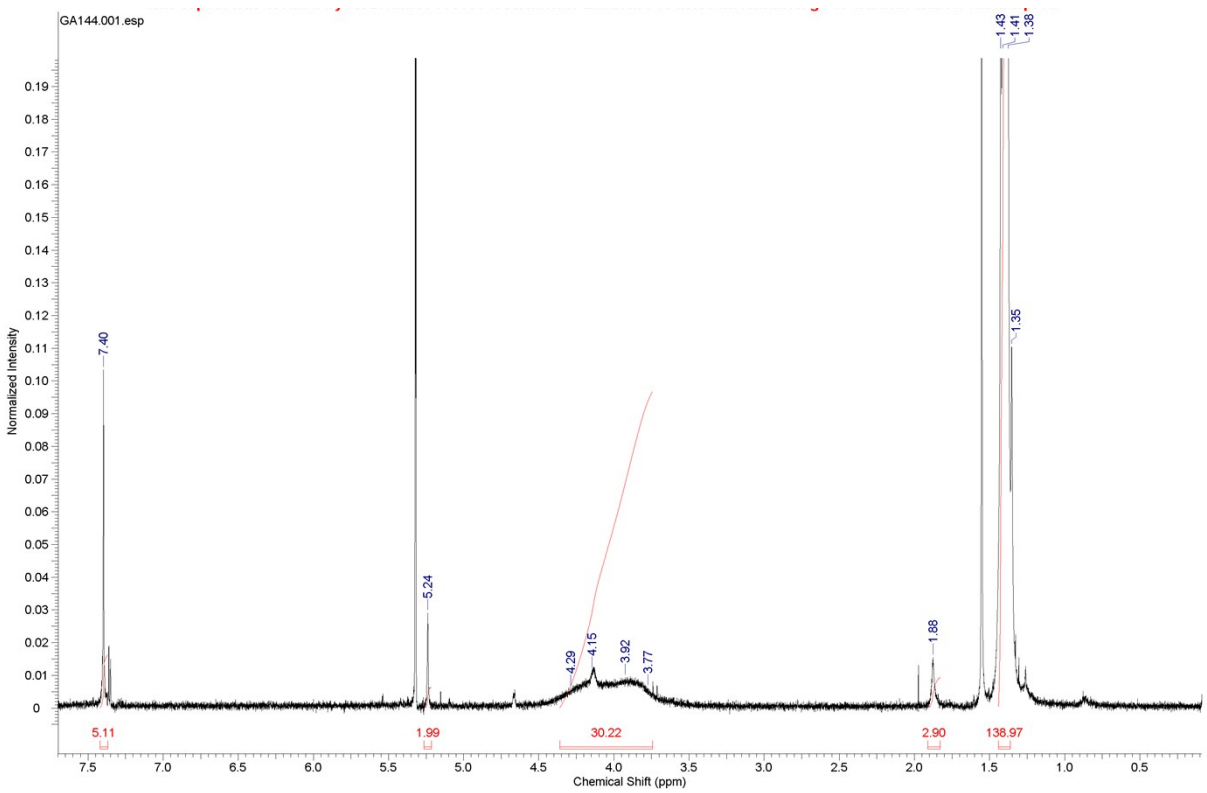
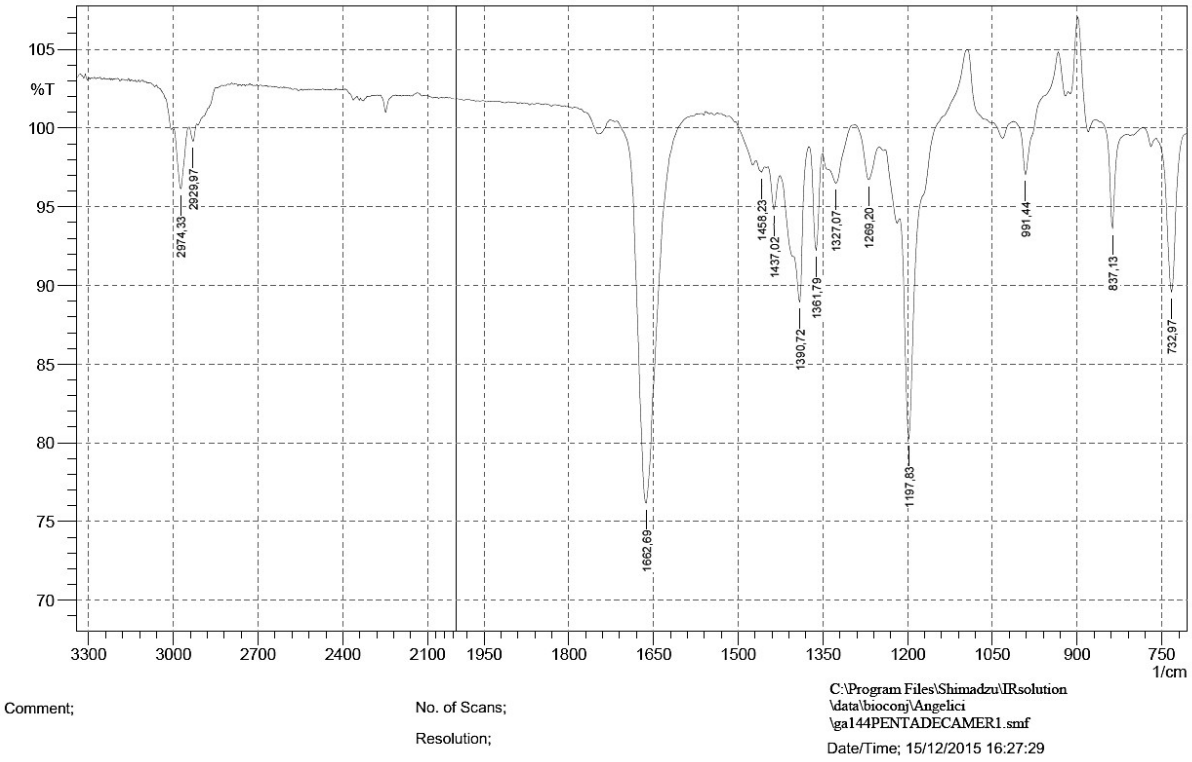
*^{1}HNMR of Pentadecamer Ac-(NtBu)$_{15}$-OBn (**11**)*



*Infra-Red spectra of pentadecamer Ac-(NtBu)$_{15}$-OBn (**11**)*



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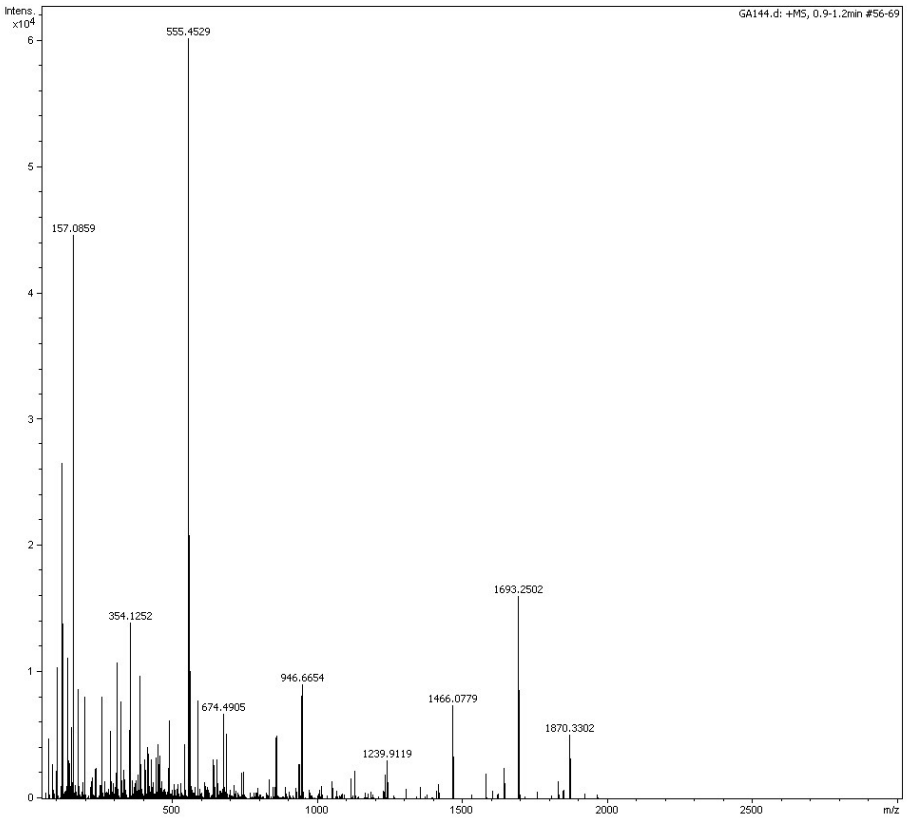
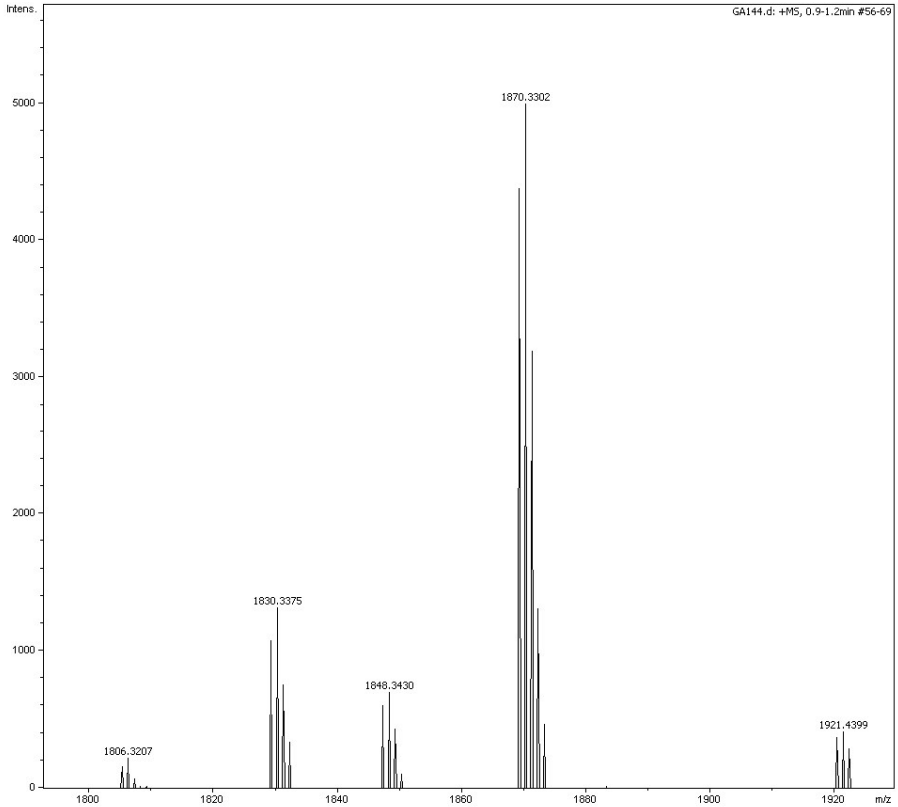
*HR-MS of pentadecamer Ac-(NtBu)$_{15}$-OBn (**11**)*

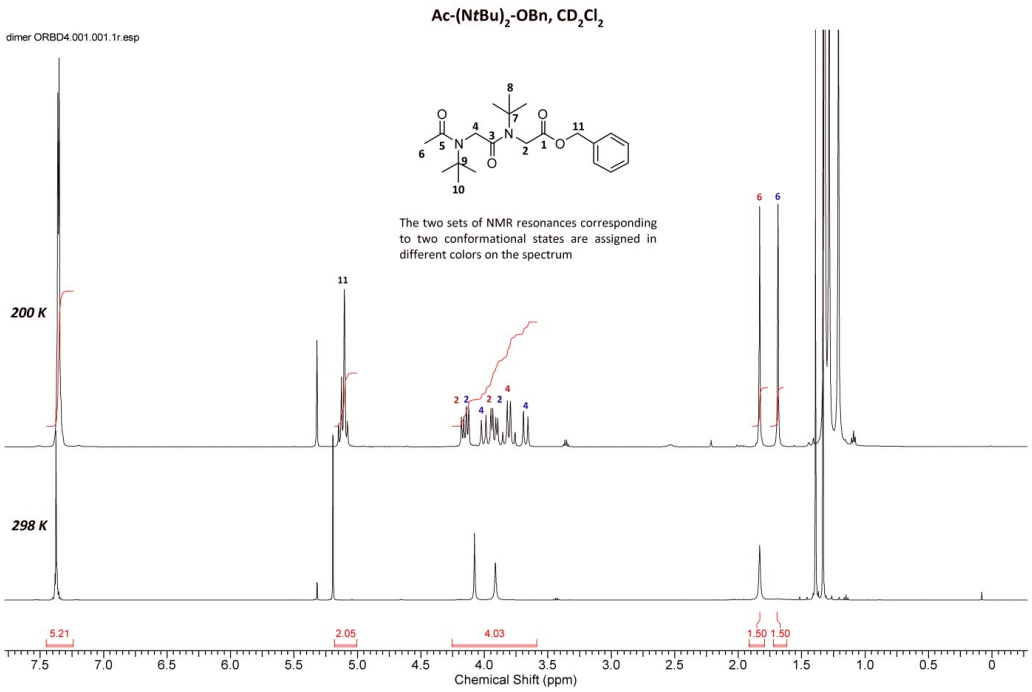


*HR-MS of pentadecamer Ac-(NtBu)$_{15}$-OBn (**11**) zoom*

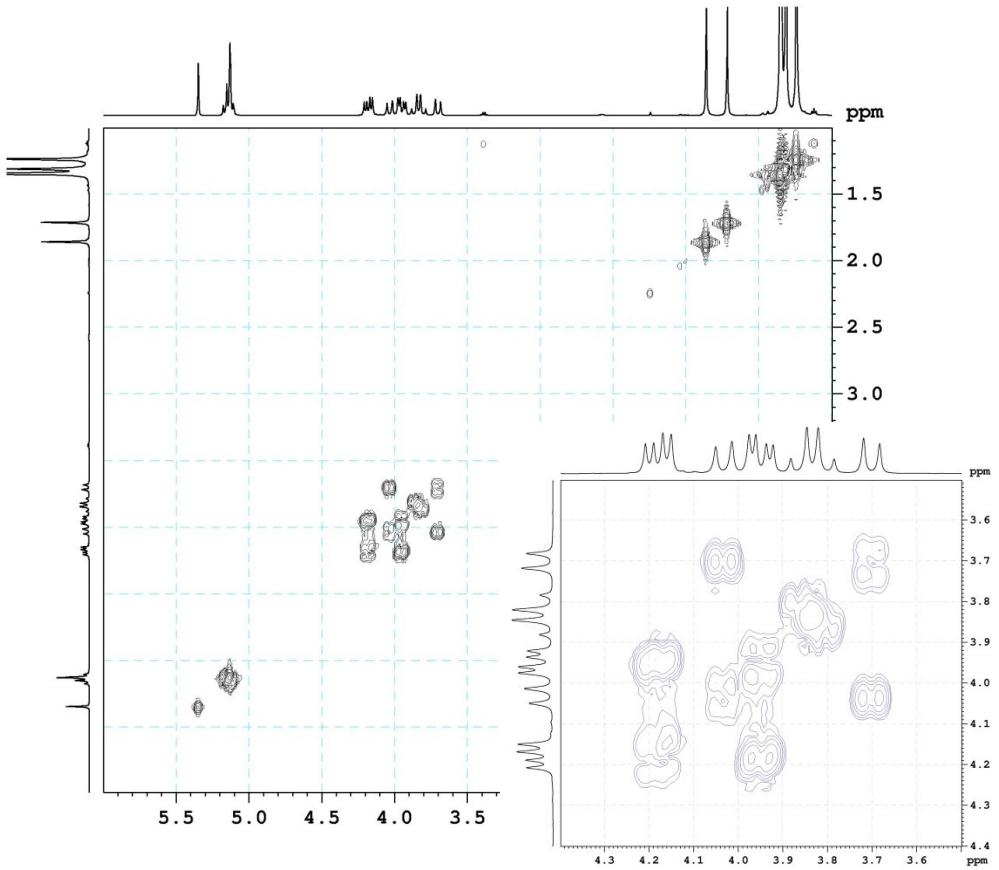


Variable temperature NMR studies

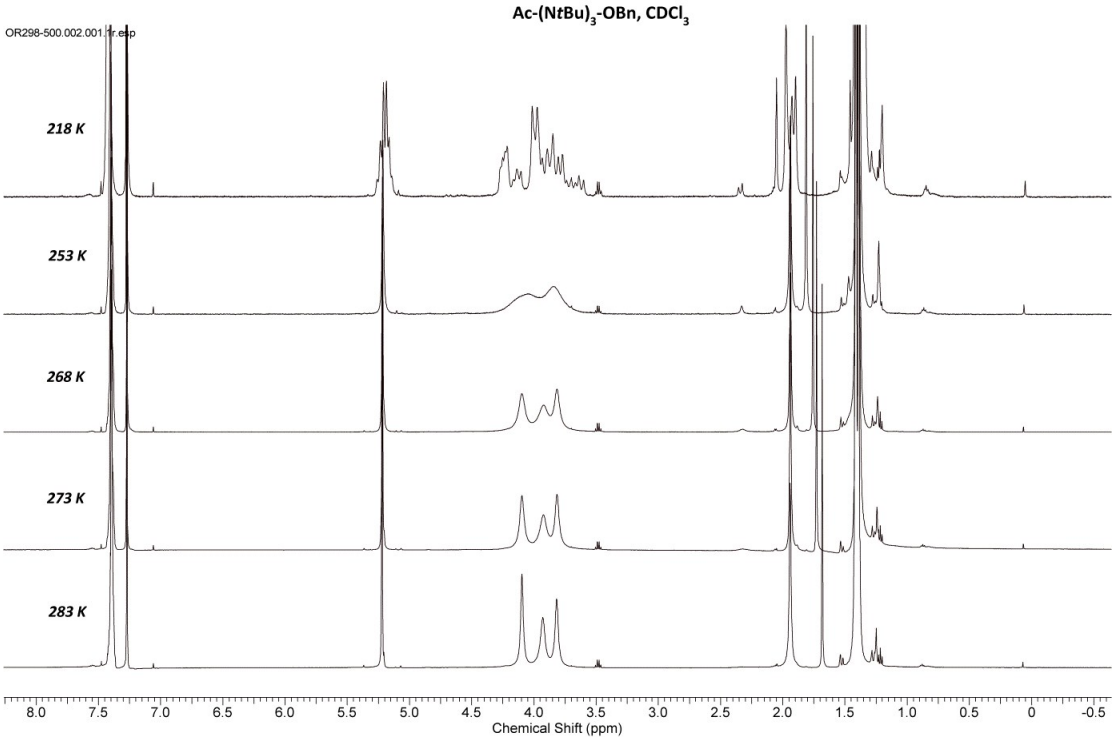
*Dimer Ac-(NtBu)$_2$-OBn (**1**)*



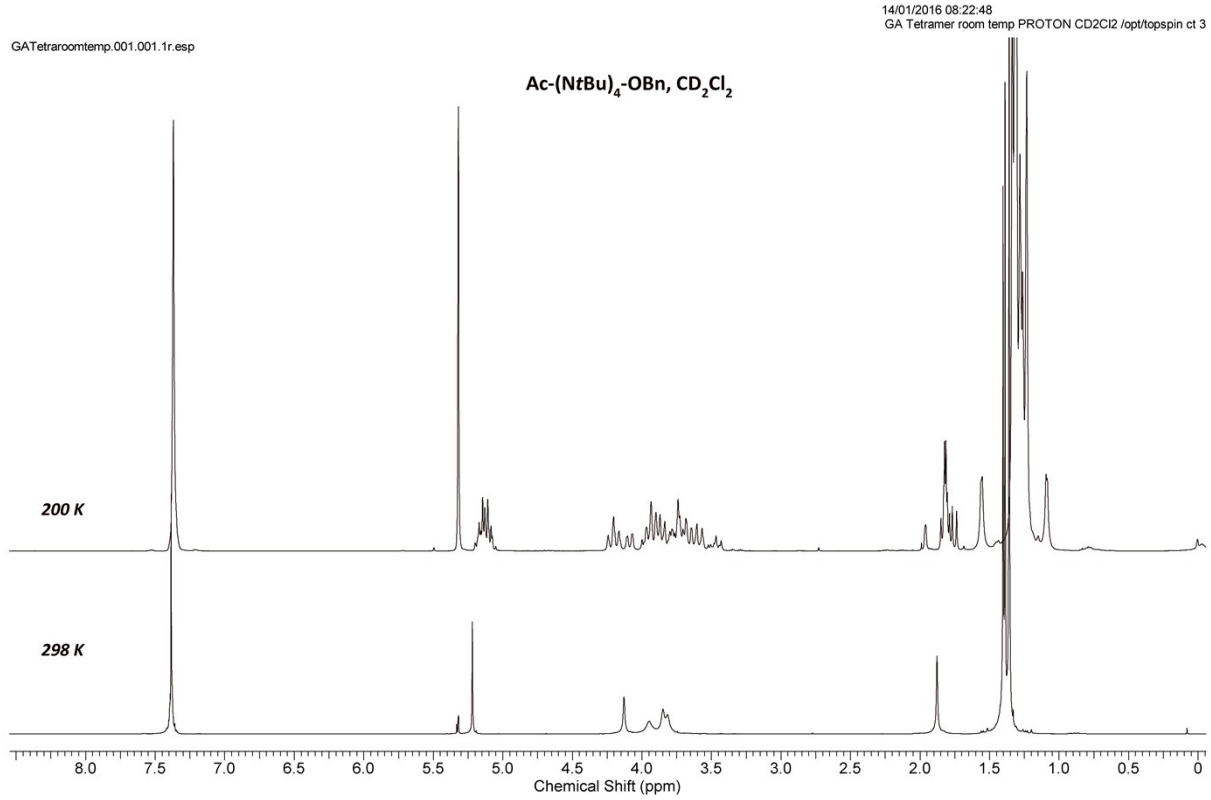
*COSY NMR experiment of dimer (**1**) at 200K in CD_2Cl_2*



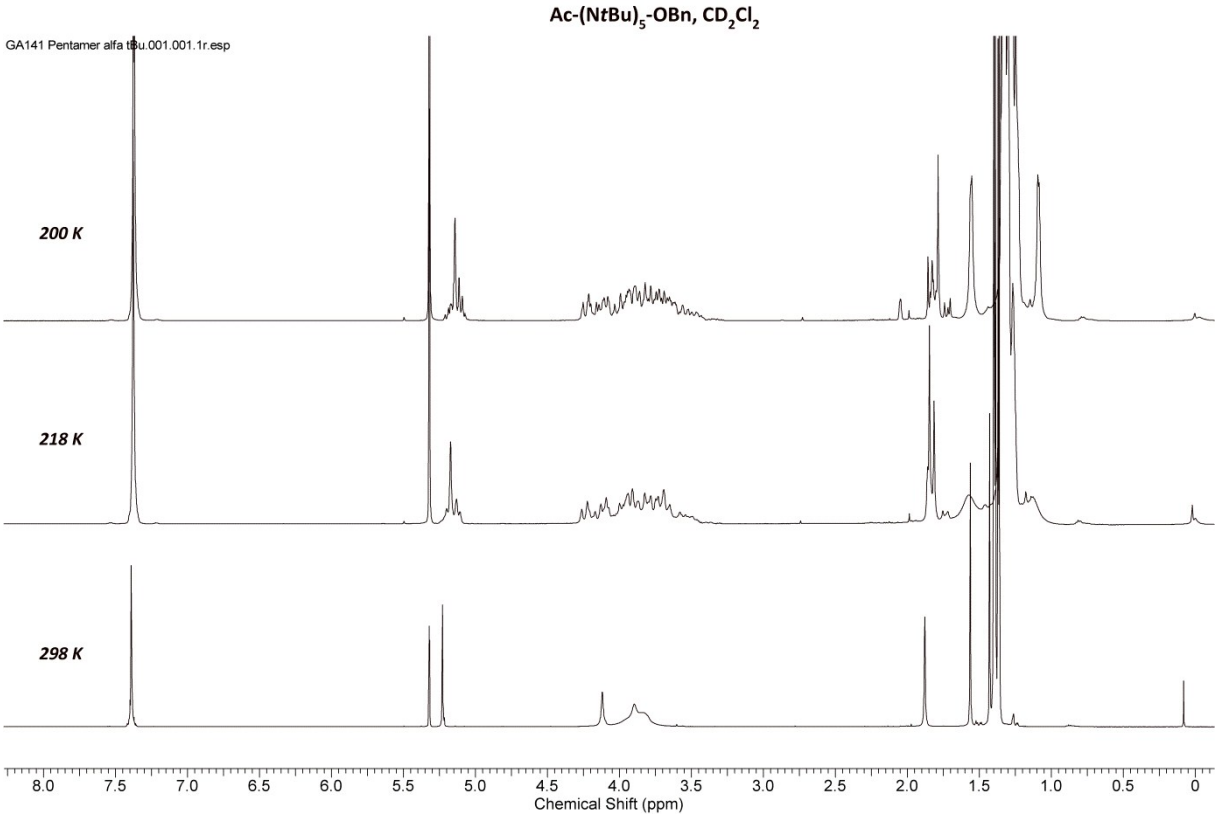
*Trimer Ac-(NtBu)$_3$-OBn (**12**)*



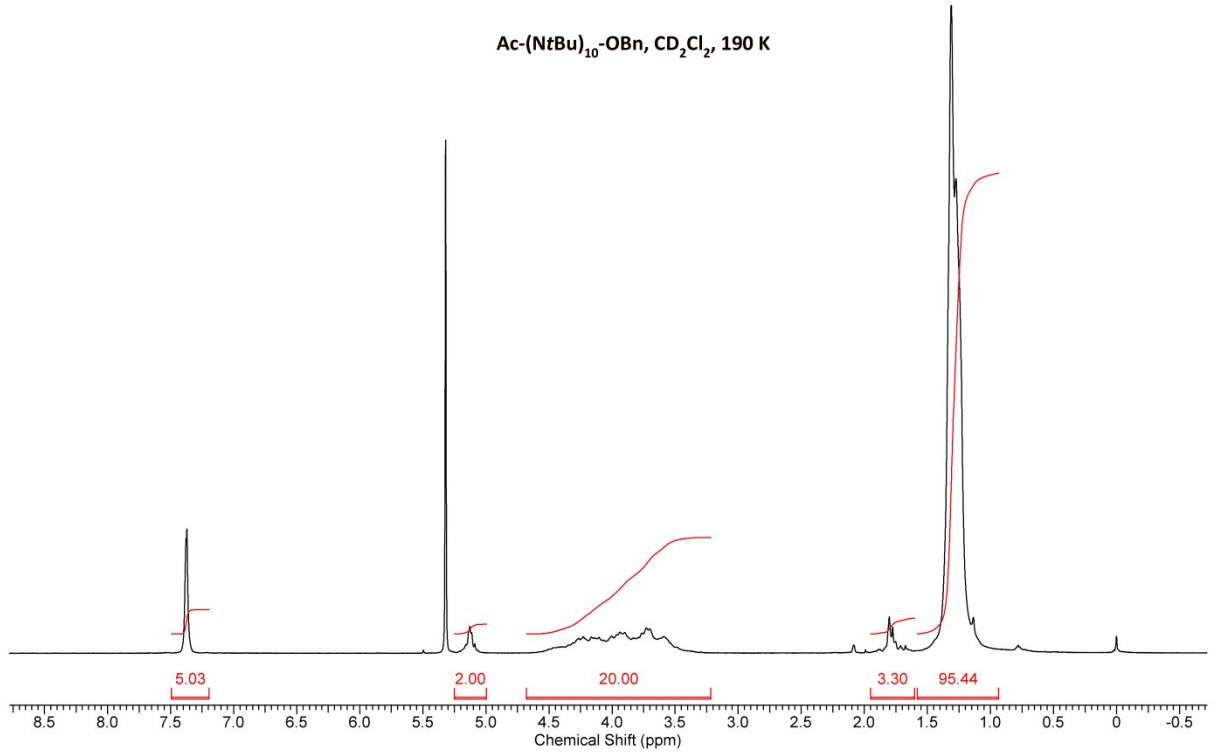
*Tetramer Ac-(NtBu)$_4$-OBn (**8**)*



*Pentamer Ac-(NtBu)$_5$-OBn (**14**)*



*Decamer Ac-(NtBu)$_{10}$-OBn (**10**)*



Crystallographic data

Dihedral angles for the crystal conformations of dipeptoid **1** (Ac-(N*t*Bu)$_2$-OBn), tripeptoid **12** (Ac-(N*t*Bu)$_3$-OBn) and pentapeptoid **3** (H-(N*t*Bu)$_5$-OBn).

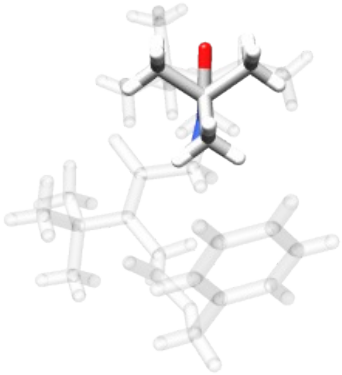
The relevant backbone dihedral angles are ω [C_α(*i*-1); C(*i*-1); N; C_α], ϕ [C(*i*-1); N; C_α; C], ψ [N; C_α; C; N(*i*+1)], χ1 [C_α; N; NCα; Cβ]

Crystals of dimer **1** were obtained by slow evaporation in Et_2O.[S1]

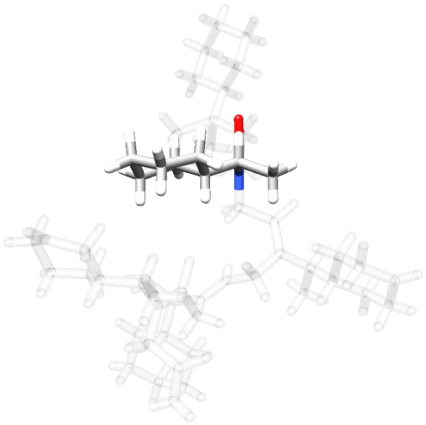
Crystals of trimer **12** were obtained by slow evaporation in EtOAc. The unit cell includes two different molecules in a monoclinic system with a P 21/c space group

Crystals of pentamer **3** were obtained by slow evaporation in EtOAc. The unit cell includes two identical molecules in a triclinic system with a P 1 space group.

Residue	*cis/trans*	ω		φ		ψ		χ1 **(measured for the three Me groups of *t*Bu**	
Dimer (**1**)									
1 (*N*-term)	*cis*	+13.3		+77.8		+170.3		-15.2, -132.9, +104.4	
2 (*C*-term)	*cis*	+3.5		-97.4		-		-3.9, -122.7, +114.7	
Trimer (**12**) (Values in bracket correspond to the second molecule in the unit cell)									
1 (*N*-term)	*cis*	+0.5	(+0.5)	+83.1	(+84.1)	+178.7	(+179.3)	+2.87 -116.5 +121.9	(+3.5) (-115.6) (+122.2)
2	*cis*	-16.3	(-16.9)	-77.1	(-72.4)	-174.0	(+178.3)	+14.9 -105.0 +133.2	+17.9 -102.2 +135.3
3 (*C*-term)	*cis*	+2.7	(+10.6)	+89.1	(+82.1)	-	-	-2.4 -121.5 +116.2	-11.6 -130.0 +108.2
Pentamer (**3**)									
1 (*N*-term)	-	-		-		-176.21		-	
2	*cis*	-4.54		-82.77		174.06		-0.1, -119.5, +118.8	
3	*cis*	-4.81		-85.01		-177.51		+3.5, -115.9, +122.6	
4	*cis*	-23.88		-68.41		-176.50		+22.2, -98.4, +139.5	
5 (*C*-term)	*cis*	17.46		+76.56		-		-20.4, -138.2, +100.5	



View of the crystal structure of trimer **12** showing the positioning of the tBu Me groups relative to the peptoid backbone (χ1 torsional angles)



View of the crystal structure of pentamer H-(*N*rch)$_5$-NH$_2$ showing the positioning of the NCα substituents relative to the peptoid backbone ((χ1 torsional angles)

Computational Methods

Preparation of structures for quantum calculations: The structures for quantum calculations were prepared with the help of gauss view package[S2]. Structures were prepared from dimer to decamer. The ω dihedral angle was considered to be in *cis* conformations while ψ dihedral angle was considered to be around ±180º. For each polymer two different conformations were prepared depending on the sign of φ dihedral angle. First called similar φ angle conformation has positive φ angle (~ 75º) for the first residue and negative value (~ -75º) for all subsequent residues. Second one called alternate φ angle conformation has alternate sign of φ angle starting from positive value for the first residue. Only deviation from this is the dimer where similar φ angle conformation has positive φ angle for both the residues. φ angle sign for all polymers are tabulated below. All polymers were capped with acyl and o-benzyl group at N- and C- termini respectively.

Polymer	φ angle sign	
	Similar φ angle conformation	Alternate φ angle conformation
Dimer	+ +	+ –
Trimer	+ – –	+ – +
Tetramer	+ – – –	+ – + –
Pentamer	+ – – – –	+ – + – +
Hexamer	+ – – – – –	+ – + – + –
Heptamer	+ – – – – – –	+ – + – + – +
Octemer	+ – – – – – – –	+ – + – + – + –
Nonamer	+ – – – – – – – –	+ – + – + – + – +
Decamer	+ – – – – – – – – –	+ – + – + – + – + –

Quantum calculation: All quantum calculations were performed with Gaussian09 package[S3]. All optimization as well as frequency calculations were performed at Density Functional Theory (DFT) level M06-2X hybrid meta-GGA functional[S4]. Carbon and hydrogen atoms were represented with 6-311G** basis set while nitrogen and oxygen atoms were represented with 6-311++G** basis set[S5]. No symmetry or geometry constrain was included during the optimization. Implicit solvent environment was consider with SMD solvent model for dichloromethane[S6].

To access the energetics related to φ dihedral angle sign change a relaxed energy scan was performed for this angle. Inner 4th residue (residues from termini avoided for being flexible) of $(+)_8$ octamer was subjected to dihedral scan from 90º to –90º with increment of 5º. The scan was performed at restricted Hartee Fock level using Ahlrichs split valence basis set. A single point calculation was performed on the resultant trajectory at DFT level using above mentioned functional and basis set. All minima and transition states are optimized M06-2X and 6-311G** basis set.

Setup for Molecular Dynamics (MD) simulation: The Generalized AMBER Force Field (GAFF)[S7] parameters were used to describe the potential of tertiary butyl peptoid monomers. The RESP charges were generated using RED server[S8] followed by the antechamber module[S9] of AMBER to make the parameter/topology (parm) file. The peptoid polymers were capped by acetyl group at N-terminus and N,N-dimethyl at C-terminus. Initially the ω dihedral angle describing the peptide bond was kept at *trans* configuration. The φ dihedral angle was kept at positive value. The peptoid polymer was solvated in acetonitrile box with a buffer of 16 Å towards each direction.

Molecular Dynamics simulation: All Molecular Dynamics simulations were performed using NAMD software package[S10]. Timestep of 1 femtosecond was applied for each simulation. A cutoff of 14Å was applied for non-bonded interactions while Particle Mesh Ewald summation was applied for electrostatic interactions. The system was initially minimized for 200 steps. This was followed by equilibration at NVT ensemble. During this NVT equilibration the temperature was gradually raised from 5K to 315K with an increment of 10K. At each temperature 5000 steps (5 picoseconds) of simulation was performed. This was followed by 200 picoseconds of NVT equilibration at 300K. Thereafter the system was subjected to 400 picoseconds of equilibration at NPT ensemble. The temperature was kept fixed at 300K through Langevin dynamics with a damping coefficient of 5/ps while the pressure was controlled at 1 atm using Nose-Hoover Langevin piston.

From the equilibrated system two initial production runs of each 10 nanoseconds were performed. The resultant snapshots were subjected to another two similar production run each. Conversion of ω dihedral angle from *trans* to *cis* is observed during these production runs (results not shown). A final production run of 50 nanoseconds was performed from the final snapshot of the initial production run. The trajectory was stored for every 2 picoseconds. The trajectory from this final production run was used for calculation of all equilibrium properties. A similar protocol was followed for peptoid polymer with alternate positive and negative φ dihedral angle.

Replica Exchange Molecular Dynamics simulation: The REMD simulations[S11] were performed for a temperature range of 300-600K. The generation of temperature series was done using scheme developed by Patrikson *et.al.*[S12] This allows an uniform exchange probability for all replicas during REMD simulation. The targeted exchange probability, P_{exch}, was set at a value of 0.3. The final production snapshot for both all positive and alternate signed φ angle conformations were used as input structure. 42 number of replicas were used with 50 nanosecond of trajectory for each replica.

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Supplementary figures.

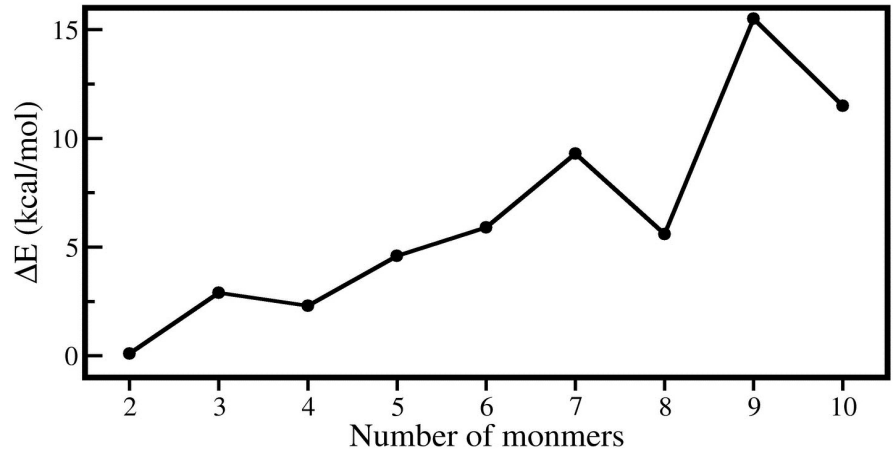

Figure S1. Difference in energy between similar and alternate φ angle conformation obtained from quantum calculations.

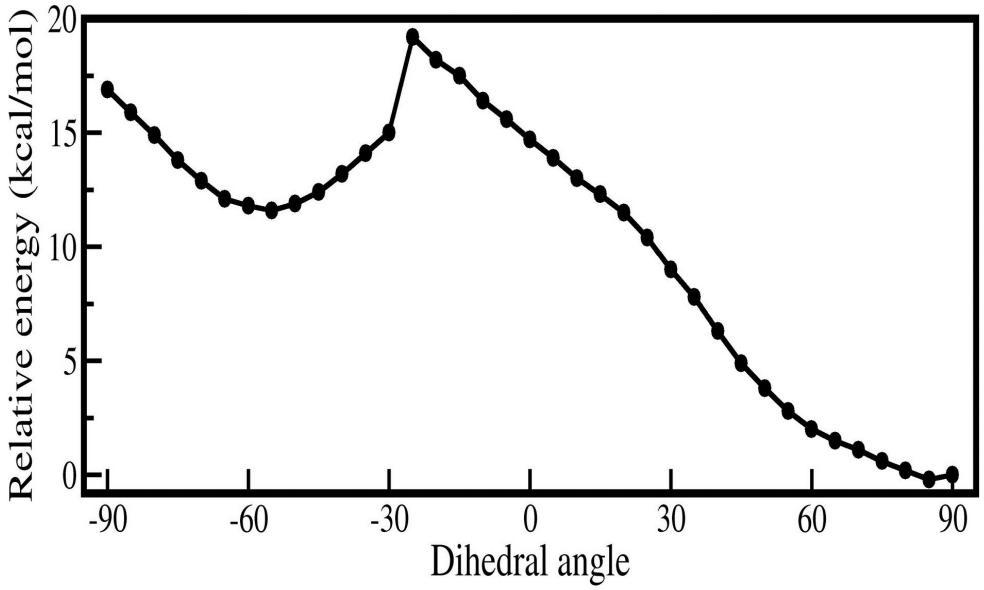

Figure S2. Relative energy from φ dihedral angle rotation of 4th residue from N-terminus in the $(+)_8$ octamer conformation.

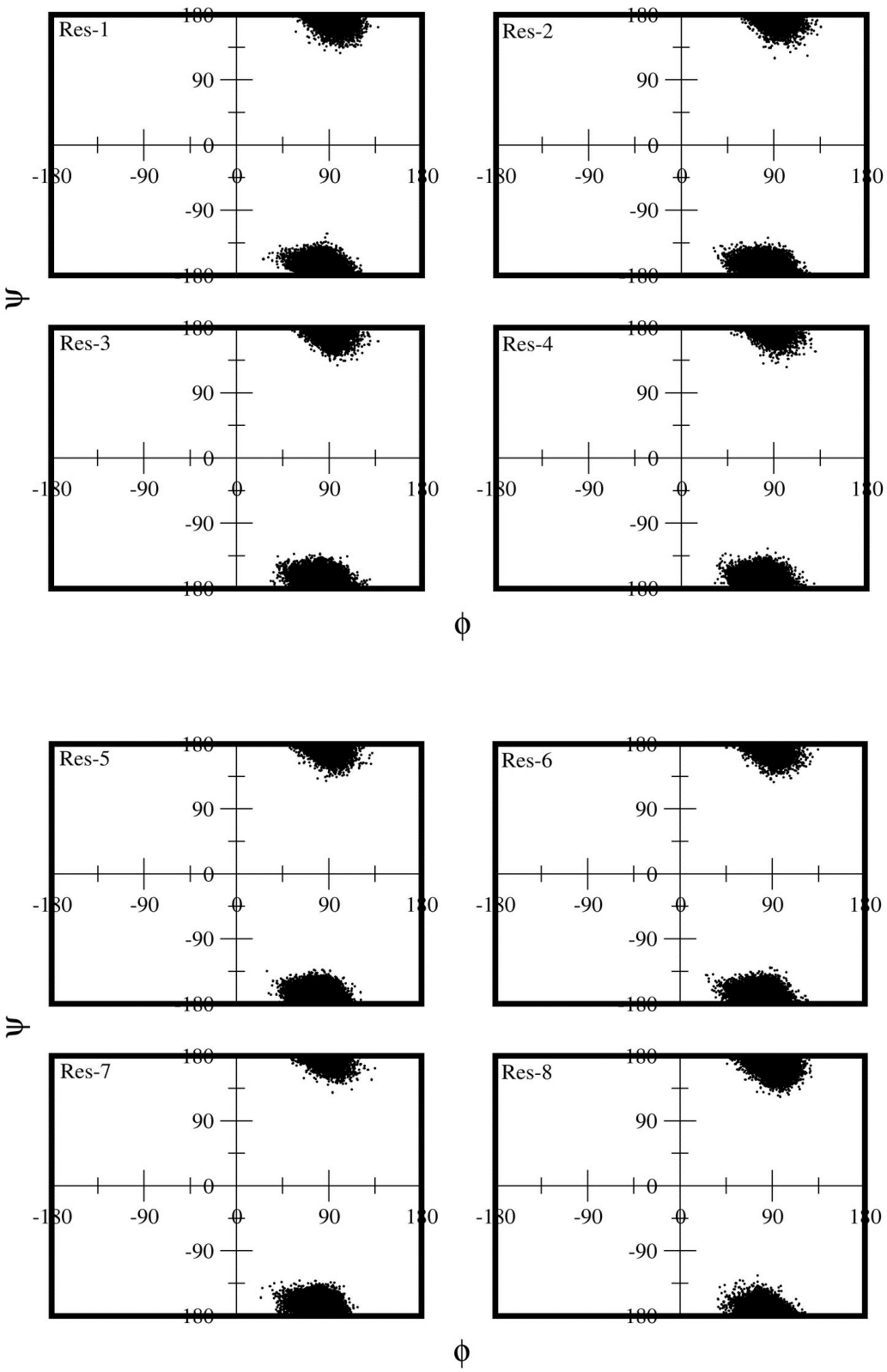

Figure S3. Ramachandran (φ, ψ) distribution plot from 50 ns production run of $(+)_8$ octamer conformation.

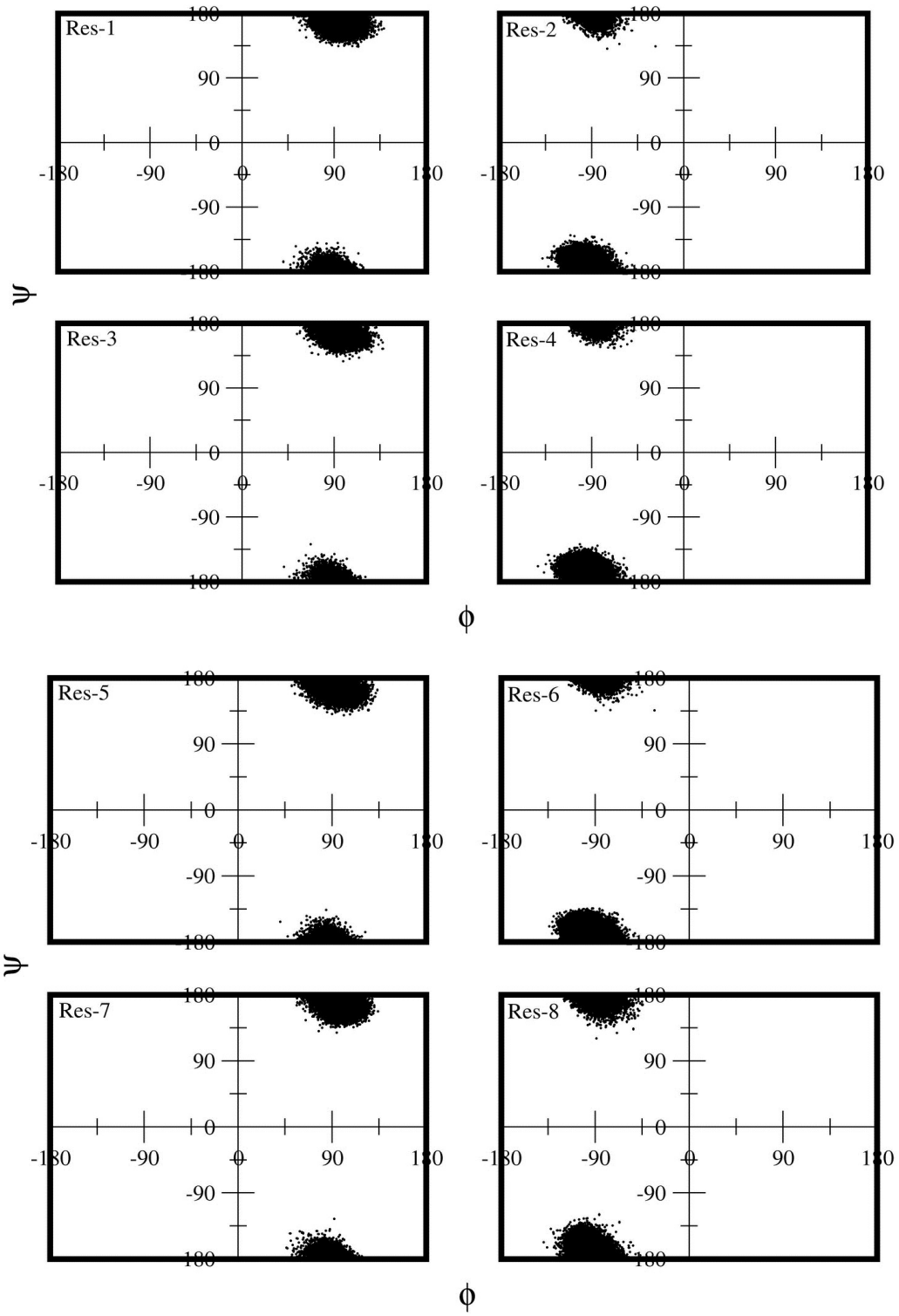

Figure S4. Ramachandran (φ, ψ) distribution plot from 50 ns production run of $(+-)_4$ octamer conformation.

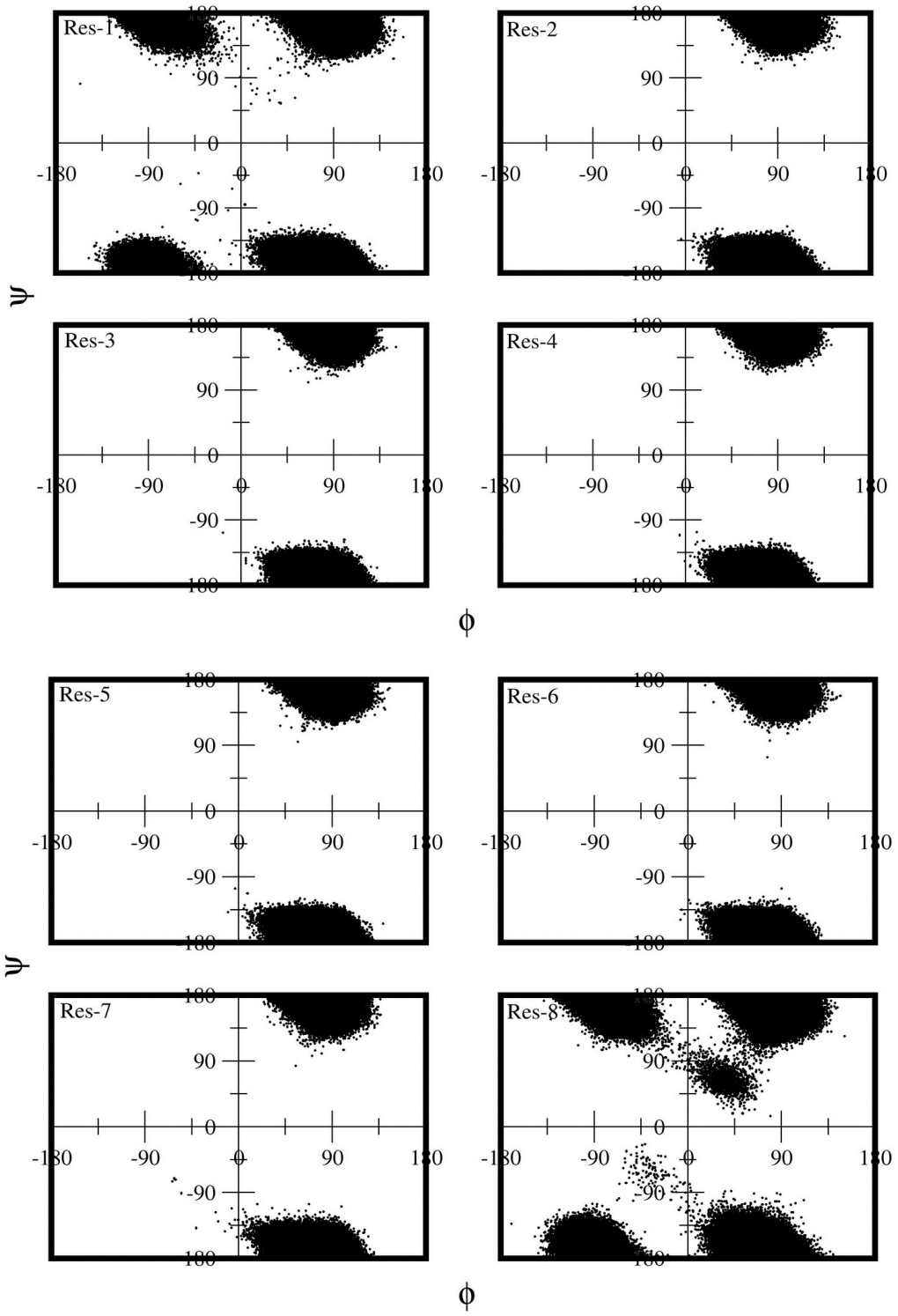

Figure S5. Ramachandran (φ, ψ) distribution plot from 50 ns REMD simulation of $(+)_8$ octamer conformation.

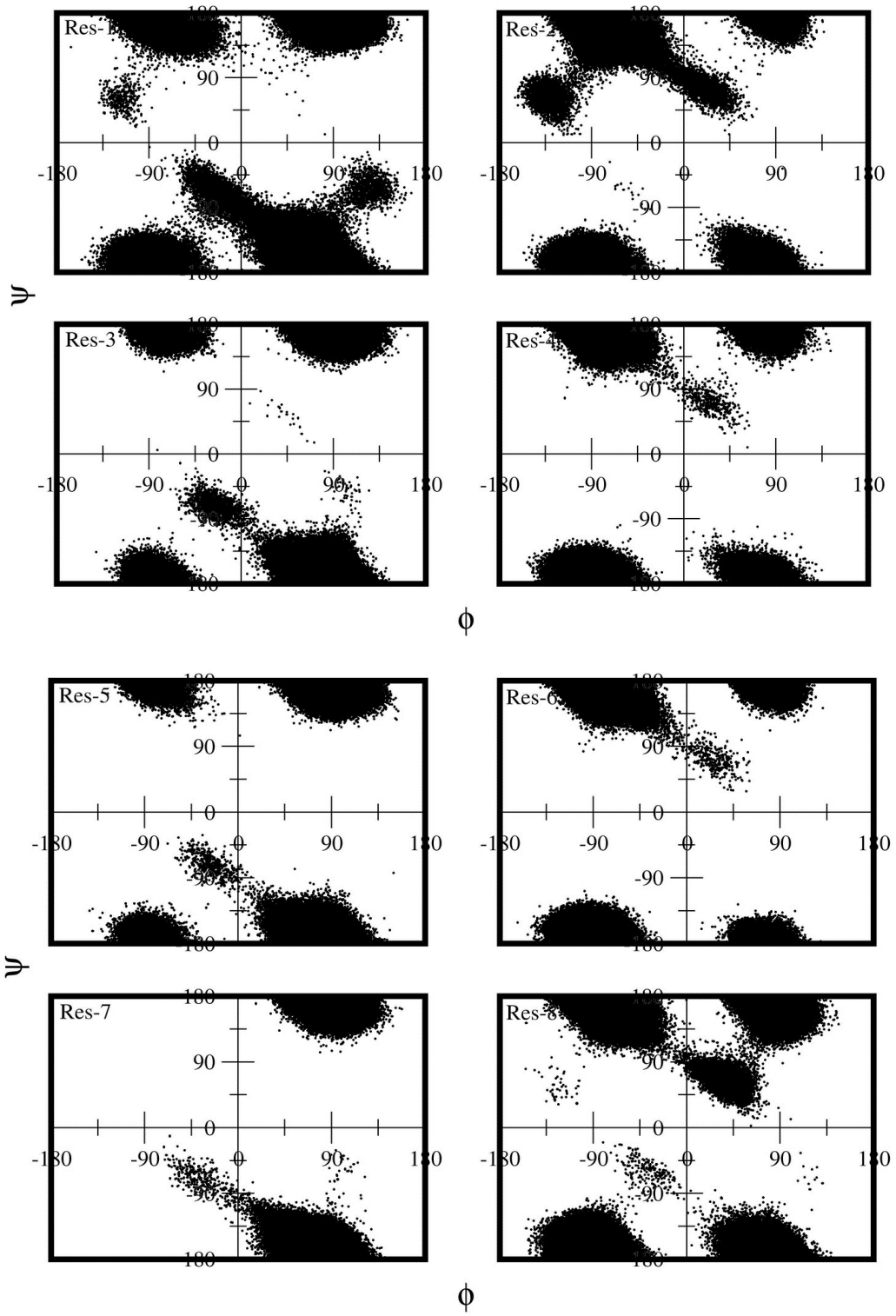

Figure S6. Ramachandran (φ, ψ) distribution plot from 50 ns REMD simulation of $(+-)_4$ octamer conformation.

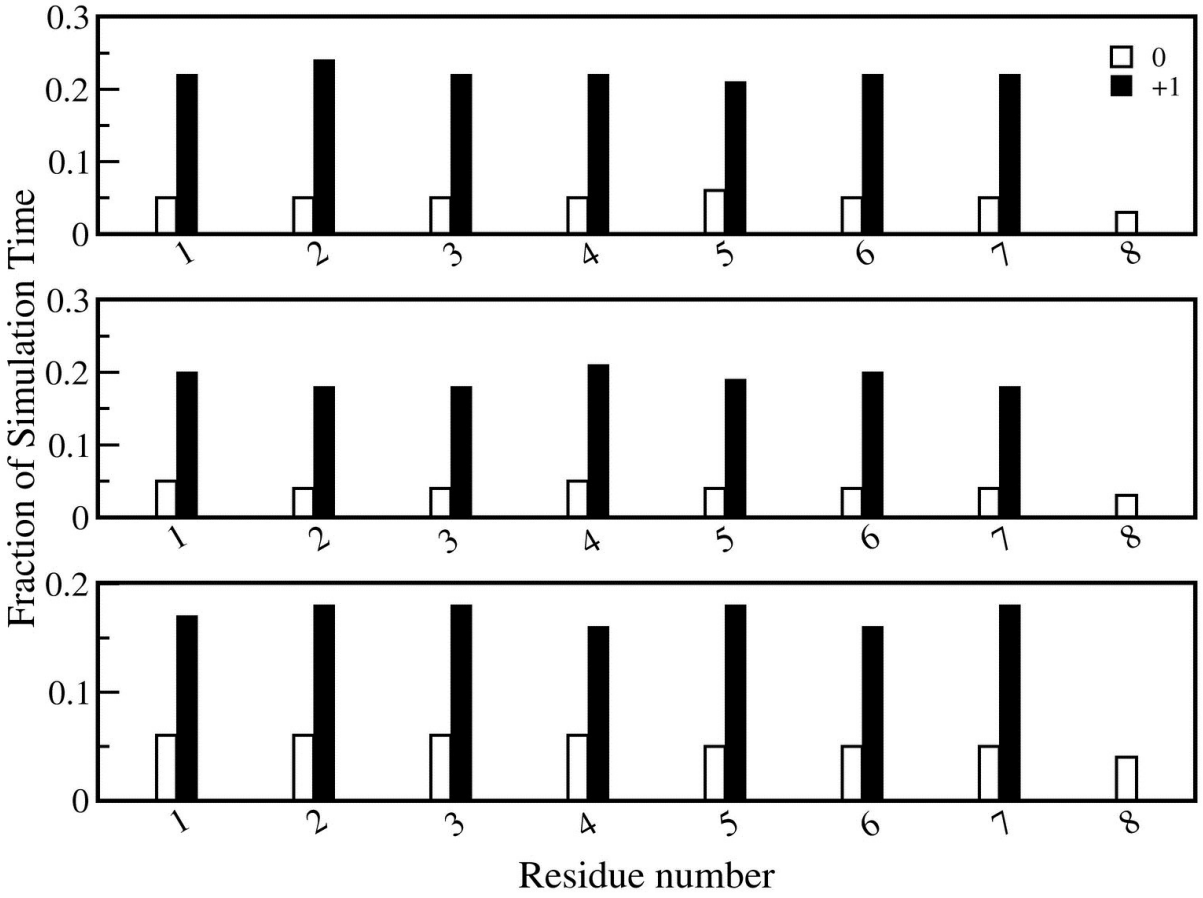

Figure S7. Hydrogen bonding probabilities between carbonyl oxygen and methyl side chain (i and i+1 residue) obtained from MD simulation of $(+)_8$ octamer conformation. Result for each methyl group is plotted separately.

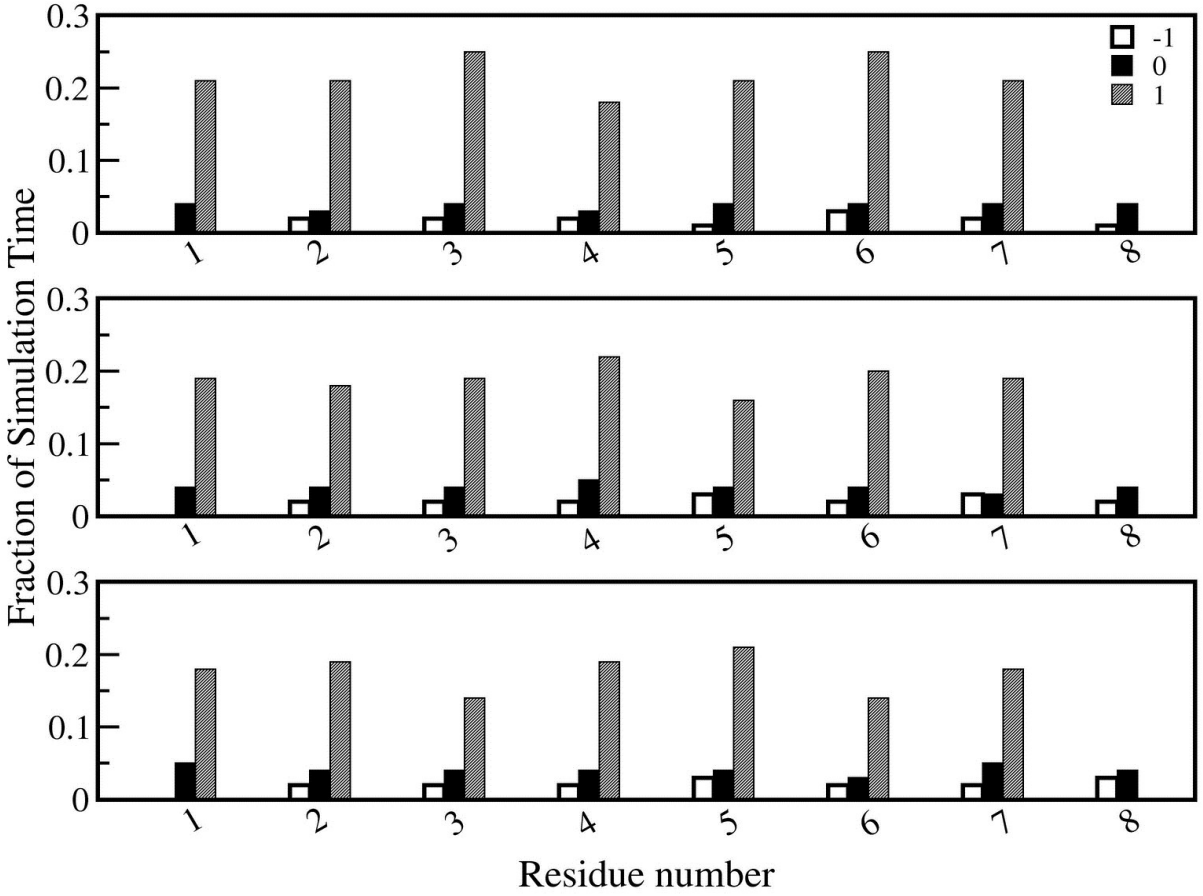

Figure S8. Hydrogen bonding probabilities between carbonyl oxygen and methyl side chain (i-1, i and i+1 residue) obtained from MD simulation of (+-)4 octamer conformation. Result for each methyl group is plotted separately.

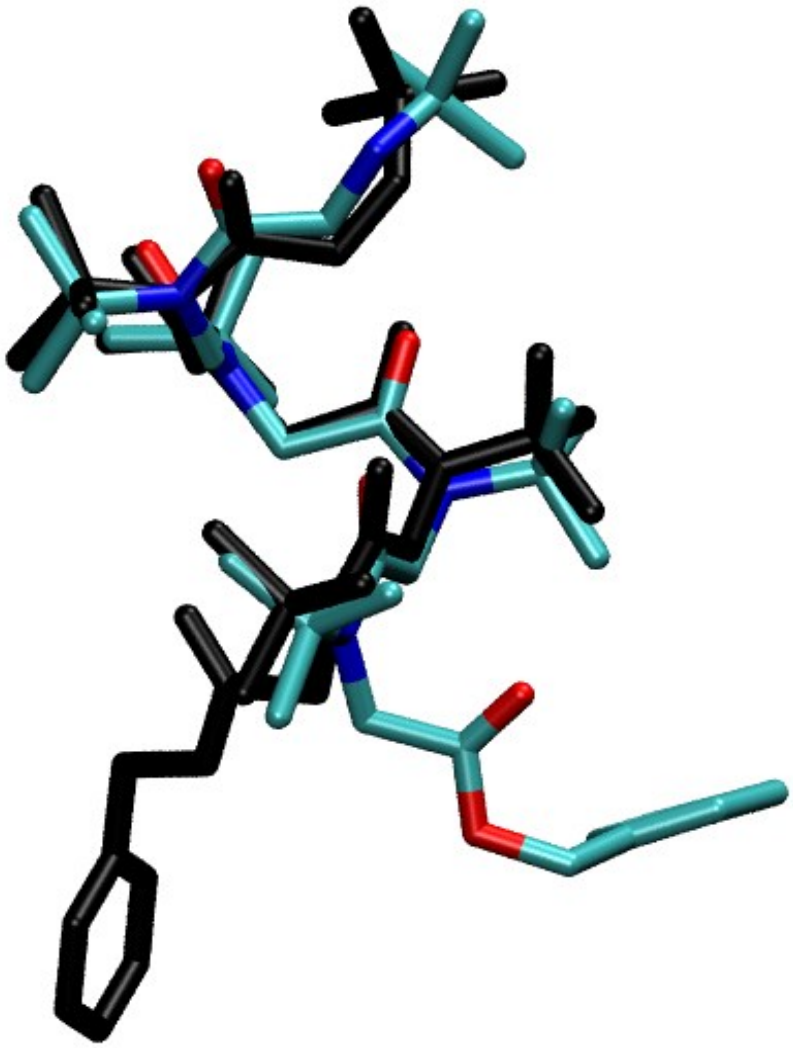

Figure S9. Superimposed crystal structure of pentamer (colored) with quantum optimized structure (black) neglecting the C-terminus.

Cartesian coordinates and energy of optimized structures.

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C	-5.38133456	7.19985403	6.72771155
H	-4.46336190	7.03205644	7.29330494
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H	-5.29602017	6.72284844	5.75383718
C	-5.63770049	8.67513303	6.48504049
O	-5.86677763	9.06709399	5.34617234
N	-5.61779524	9.51386747	7.56333504
C	-5.68859744	11.00226836	7.35597471
C	-4.56421663	11.46404752	6.41861240
H	-3.59416445	11.19609223	6.84195399
H	-4.65614650	11.01665975	5.43059214
H	-4.61452008	12.55114237	6.31363862
C	-7.06408157	11.37317876	6.79006054
H	-7.85487429	11.02404892	7.46005445
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(++)
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C	-10.13200575	7.24159014	11.51805278
C	-10.76492155	8.69226485	13.80650313
C	-11.13244161	6.78849828	12.37388112
C	-11.44798275	7.51234185	13.51912315
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(+—)
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N	10.20132090	25.42311000	2.50312880
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N	6.66788788	22.49548510	-0.88889438
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H	8.47807807	23.29358769	3.30193757
H	7.60538598	24.81885454	3.15260893
H	8.06437260	24.20928858	4.76172348
C	9.70921058	25.01851893	3.71131871
C	11.44509026	26.26356394	2.44228650
C	11.27905337	27.52634576	3.29885595
H	10.40314856	28.08617295	2.96500709
H	12.16555326	28.15458921	3.17961955
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C	12.64313271	25.43196374	2.91399255
H	12.52606779	25.12649299	3.95268544
H	13.55795653	26.02412165	2.82349086
H	12.75094485	24.53919345	2.29128572
C	11.71743595	26.72048563	1.00554606
H	11.96609467	25.88937508	0.34161393
H	12.58098630	27.38783819	1.02782613
H	10.87641057	27.28014065	0.58759545
C	9.43299751	25.14540774	1.30520464
H	8.95911988	24.16800203	1.38850185
H	10.10215975	25.08489305	0.45002174
C	8.35678148	26.21626906	1.03528612
C	6.35326009	26.92536911	-0.24504405
C	6.86364578	28.33214663	-0.57509066
H	7.41120192	28.76525886	0.25991390
H	6.01331468	28.97838978	-0.80834054
H	7.51781725	28.30054573	-1.45091821
C	5.45239127	26.93888708	0.99698326
H	5.06450393	25.93675623	1.18964020
H	4.61034078	27.61159656	0.81399004
H	5.98623756	27.28830031	1.87865786
C	5.50625082	26.43993569	-1.42496901
H	6.04509760	26.49230005	-2.37433155
H	4.64217317	27.10256541	-1.50244451
H	5.13078820	25.42289504	-1.28455446
C	7.64102838	24.78069317	-0.79244789
H	8.68647109	24.48355861	-0.87812354
H	7.30403699	24.96156466	-1.80950807
C	6.83728111	23.62900739	-0.15201428
C	5.74667487	21.41185515	-0.38850233
C	6.31850159	20.80547286	0.89712336
H	7.33124714	20.43260409	0.72016129
H	5.69526030	19.96183697	1.20490016
H	6.34360331	21.53276704	1.70638471
C	4.34506108	21.99101711	-0.15984385
H	4.34974885	22.77133503	0.59899826
H	3.67952508	21.19054053	0.17278448
H	3.95469106	22.40200943	-1.09383175
C	5.62474078	20.29197831	-1.42622107
H	5.25963087	20.65394341	-2.39140539
H	4.89378776	19.57454271	-1.04923648
H	6.56386083	19.75444757	-1.57280379
C	7.26188070	22.39521052	-2.20600698
H	7.53558982	21.36648099	-2.43051875
H	8.19504901	22.95472089	-2.26501842
C	6.35048738	22.89726674	-3.31323217
C	6.13803970	23.08784819	-5.64764788
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H	5.15896943	22.60127373	-5.62410483
C	6.88333712	22.72812440	-6.90519087
C	7.97951500	21.86930851	-6.90978074
H	8.34252568	21.45309030	-5.97819509
C	8.61382674	21.55192623	-8.10956951
H	9.46991659	20.88686831	-8.10255458
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C	7.05524290	22.93835641	-9.30791267
H	6.69015912	23.35734796	-10.23865390
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O	6.18192483	36.98513546	3.56628034
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N	6.62294290	29.42778098	1.72958921
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C	6.39721818	28.56550041	4.03444859
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H	6.54727643	27.61163580	4.53533230
C	6.62836677	28.33801724	2.55233960
C	6.99625945	29.27224358	0.28069737
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H	9.12821644	29.27716764	0.65807650
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H	8.42709802	27.64849391	0.57876633
C	5.94422435	28.41114971	-0.42858222
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H	6.17410259	28.36824762	-1.49671239
H	4.95151448	28.85527579	-0.31216524
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H	6.04361970	31.10245080	-0.46441654
H	7.37459778	30.48166146	-1.43569417
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H	5.98505078	31.40870725	1.57844881
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H	9.06499878	32.78768266	5.51492704
H	10.64558499	33.32479854	4.92647178
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C	8.83947817	34.85455297	3.71755396
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H	9.81237163	35.33275709	3.84833980
H	8.27302598	35.01510212	4.63782713
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H	10.92723389	33.83605951	2.40729444
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C	6.54840395	33.40765489	3.16339061
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H	5.71195358	32.74997699	3.40096046
C	6.26996582	34.09685959	1.81056950
C	5.04020869	35.82918140	0.52819076
C	4.61277170	34.89905213	-0.61305506
H	5.40926512	34.20759221	-0.88276635
H	4.35863408	35.49899751	-1.49068814
H	3.72672912	34.32695014	-0.32370559
C	6.32106523	36.59423397	0.17178245
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H	6.13569888	37.20231747	-0.71741331
H	7.14777549	35.91811309	-0.04024803
C	3.92776161	36.85624198	0.75014820

H	2.95558667	36.38797865	0.92050041
H	3.84760085	37.45437048	-0.15917962
H	4.15315990	37.53766159	1.57431738
C	4.53839019	35.29957846	3.00140810
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H	3.55227277	35.70483470	2.78333633
C	5.25566051	36.29572741	3.89915649
C	5.35554983	37.15259764	6.09540451
H	4.63563439	37.20993023	6.91099496
H	5.50345032	38.14571554	5.67054081
C	6.66158388	36.55977007	6.55899783
C	6.68813228	35.27622346	7.10909366
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H	7.90094346	33.73233699	7.98091923
C	9.06782494	35.46283430	7.45731138
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C	9.04550200	36.74204880	6.91147942
H	9.96262563	37.31402551	6.82958343
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H	7.82855145	38.27542770	6.01500720

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C	3.65543163	-0.72771457	-4.17802593
C	5.17787049	2.64400455	-4.90478406
C	5.62205929	3.83681945	-4.02811428
N	6.07116465	4.95400332	-4.83860980
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C	5.13725852	5.78049671	-5.38990379
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C	2.68949358	4.34739516	-7.17769111
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C	4.58248909	4.89958723	-9.10741371
C	1.12526968	3.41478170	-8.79404192
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O	0.76763244	3.10231674	-9.92567902
O	1.45007446	6.34344178	-7.62318401
C	0.91388037	7.91814295	-5.14141744
C	2.84164730	8.70816502	-6.57516327
O	5.40341680	6.66864609	-6.18425133
C	7.61263255	4.84863923	-6.81174211
C	8.06592025	6.41633877	-4.88191304
O	5.28364576	2.73404457	-6.11810889
C	3.00728970	0.85275042	-5.97723938
C	5.30767247	-0.20024023	-5.93981620
O	2.45173411	2.92770314	-3.34841142
C	3.68149539	2.98786518	-10.39739591
C	2.64213766	5.28700484	-10.59976779
H	-0.76465998	2.84687726	-8.03498705
H	0.01555276	4.11548694	-7.06409612
H	0.57188971	2.43682385	-6.94371234
H	4.13096340	2.27280250	-9.70216767
H	4.42113877	3.22564320	-11.16672378
H	2.81923100	2.52459413	-10.87349250
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H	3.34698891	5.53714668	-11.39729687
H	2.39211030	6.19856925	-10.05287439
H	5.14823708	4.20387766	-8.48225547
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H	5.21073606	5.16373928	-9.96077411
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H	0.32445210	7.66226913	-6.02036284
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H	4.25165589	8.13562743	-4.27880986
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H	8.66739956	4.89318994	-7.09631876
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H	2.21653111	1.28402482	-5.35868649
H	2.59700527	-0.00815773	-6.51150299
H	5.68461823	0.51709723	-6.66588105
H	4.93511163	-1.07508063	-6.47842767
H	6.13099137	-0.52163214	-5.29618546
H	4.44386253	-1.13505439	-3.54098092
H	3.29405193	-1.53656941	-4.81494326
H	2.81813671	-0.40558809	-3.55262954
H	5.17465236	2.18114832	-2.32393784
H	4.43599838	0.61890148	-2.39639750
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H	0.64757795	2.28684727	-1.56137203
H	1.54183366	3.72197245	-1.01425526
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C	0.29463848	0.69811830	2.14361086
H	0.16364607	0.43767271	0.01154162
C	1.41288325	2.69980907	2.88946322
H	2.15307689	3.99315049	1.33698217
C	0.74222776	1.51487524	3.17871559
H	-0.23230609	-0.22239851	2.36655235
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H	0.56457739	1.23026804	4.20945720

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O	2.58960290	1.95206167	-0.79872521
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N	4.91558787	1.08006074	-3.44235121
C	4.60862380	-0.24460702	-4.09425229
C	3.92698838	-1.18691116	-3.09830389
C	5.48052090	2.07587461	-4.18169197
C	5.64063272	3.45624723	-3.51082142
N	6.05199290	4.47619060	-4.45743999
C	5.02275011	5.18272188	-5.30258297

C	3.61373335	4.70939074	-4.93570382
C	7.37314676	4.67184715	-4.71490708
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N	9.73951079	3.96371063	-4.44694852
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C	10.48959458	5.00576938	-3.99145386
C	9.87752537	5.88222697	-2.87903160
N	10.70596310	7.02925004	-2.55870043
C	10.57714795	8.30276502	-3.34899671
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C	11.52104813	2.43606472	-5.24925983
C	10.44554291	4.08560996	-6.83748597
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C	5.10478007	6.69115498	-5.04480213
C	5.24586061	4.86044986	-6.78615201
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H	11.08492980	5.30169024	-0.33312678
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H	8.46019958	8.09890559	-3.88824082
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H	9.43070208	9.10745747	-4.95706359
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H	6.05510758	7.10158358	-5.38258888
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H	3.32237473	5.00151336	-3.92415729
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H	4.70952589	3.76158041	-3.03964835
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H	2.72095236	0.42368974	-4.92067129
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H	6.60308661	-1.00039291	-3.70549332
H	4.58082250	-1.45634936	-2.26563119
H	3.68139411	-2.10560535	-3.63382153
H	2.99148482	-0.77982650	-2.70493260
H	5.08669255	2.08632650	-1.60077921
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C	1.25688303	2.48782544	-0.61129824
H	0.55213580	1.87242450	-1.17231204
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C	0.18041564	1.44832091	1.40665660
C	1.48215240	3.45439359	1.69411372
C	-0.07777947	1.41935326	2.77421266
H	-0.22846455	0.68115413	0.75722939
C	1.22940354	3.42477522	3.06057501
H	2.08452331	4.25030943	1.26762631
C	0.44735769	2.40672182	3.60168020
H	-0.68987113	0.62860168	3.19219828
H	1.63495274	4.19728661	3.70361025
H	0.24488756	2.38674776	4.66632346

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E: -2325.43255697

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C	4.829628	1.069707	-3.151214
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C	4.858776	-0.103492	-5.444463
C	4.065783	-1.158192	-4.668953
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