Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Supporting Information

For

Tuning the biomimetic performances of 4-hydroxyproline-containing cyclic peptoids

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List of abbreviations

DCM: dichloromethane

DIC: *N*,*N′*-diisopropylcarbodiimide

DIPEA: *N*,*N*-diisopropylethylamine

DMF: *N*,*N*-dimethylformamide

HFIP: 1,1,1,3,3,3-hexafluoro-2-propanol

HATU: *O*-(7-azabenzotriazol-1-yl)-*N*,*N*,*N′*,*N′*-tetramethyluronium hexafluorophosphate

RP HPLC: reversed-phase high-performance liquid chromatography

TCDE: tetrachloro dideuteroethane

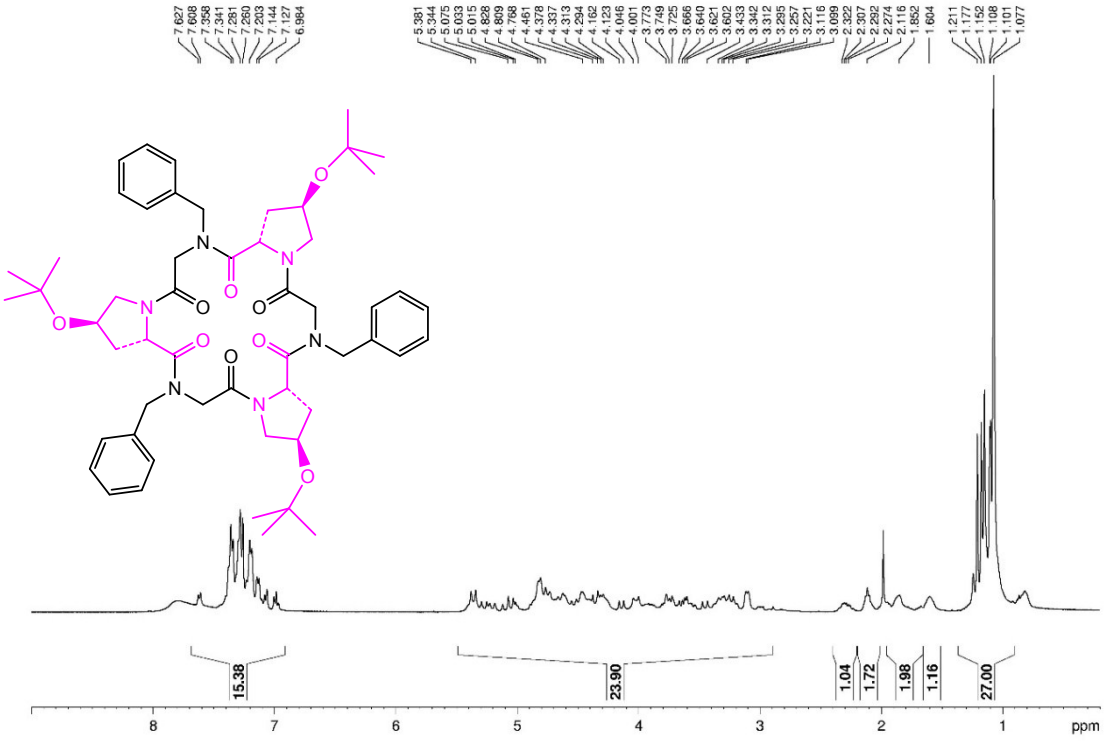
TFA: trifluoroacetic acid

TFPB: tetrakis[3,5-bis(trifluoromethyl)phenyl]borate

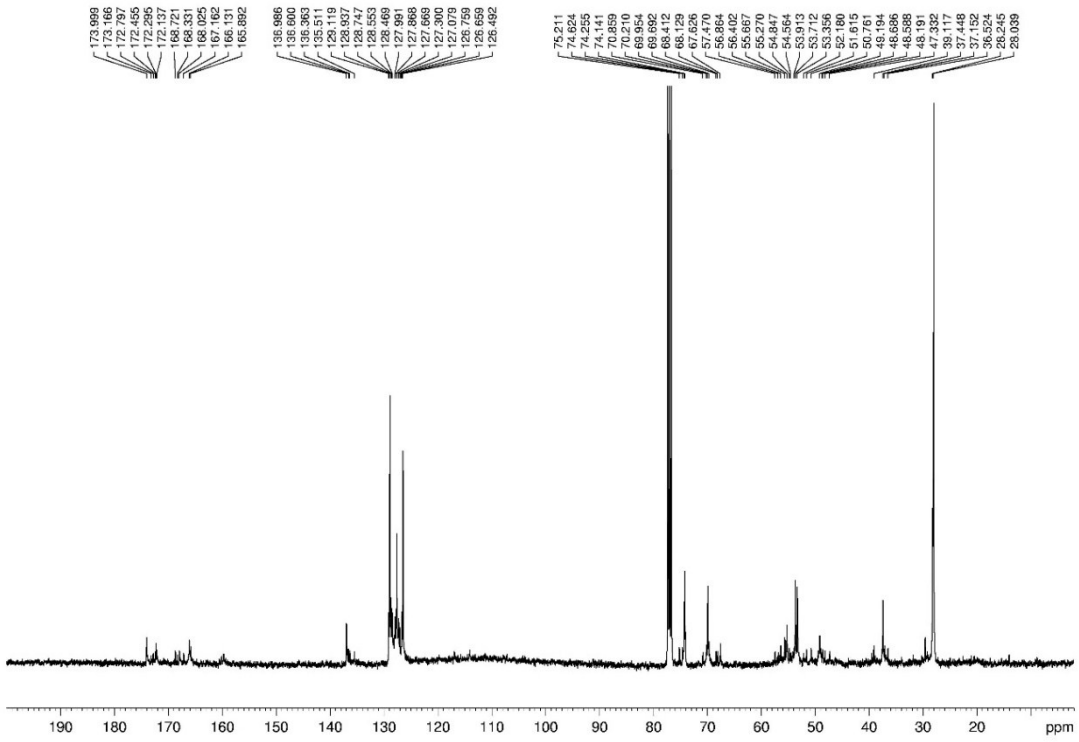
DMAP: 4-dimethylaminopyridine

1.0 ^{1}H and ^{13}C NMR spectra

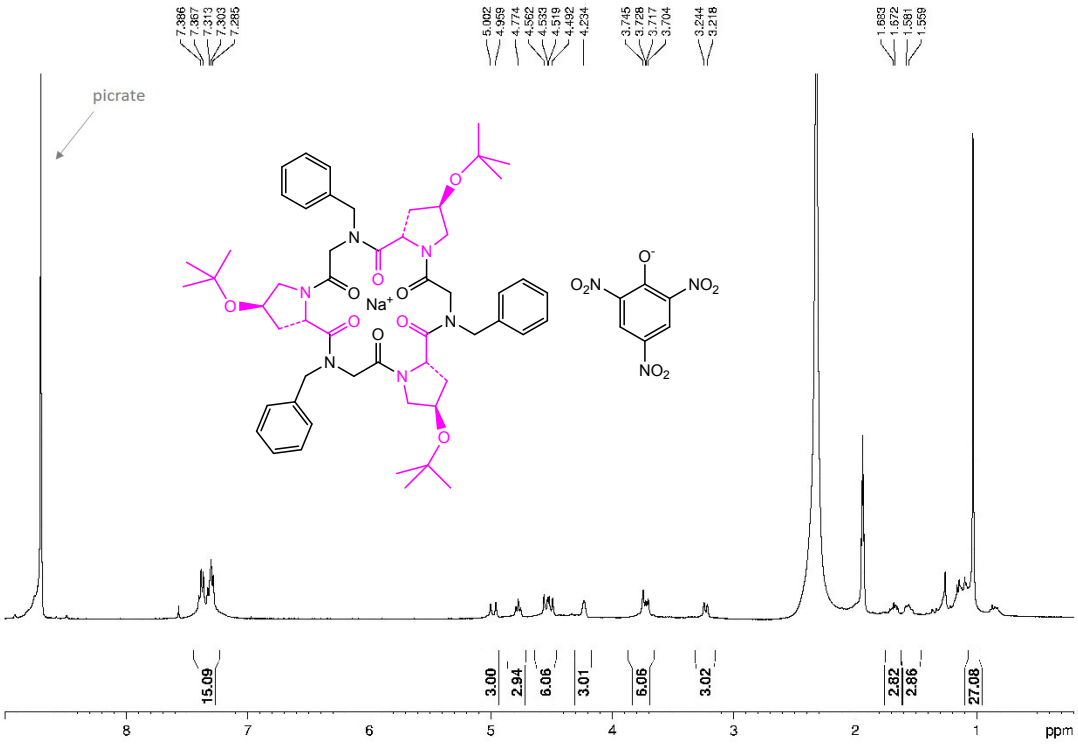
1.1 1D and 2D spectra of cyclic peptoids **1**-**5** and their complexed forms



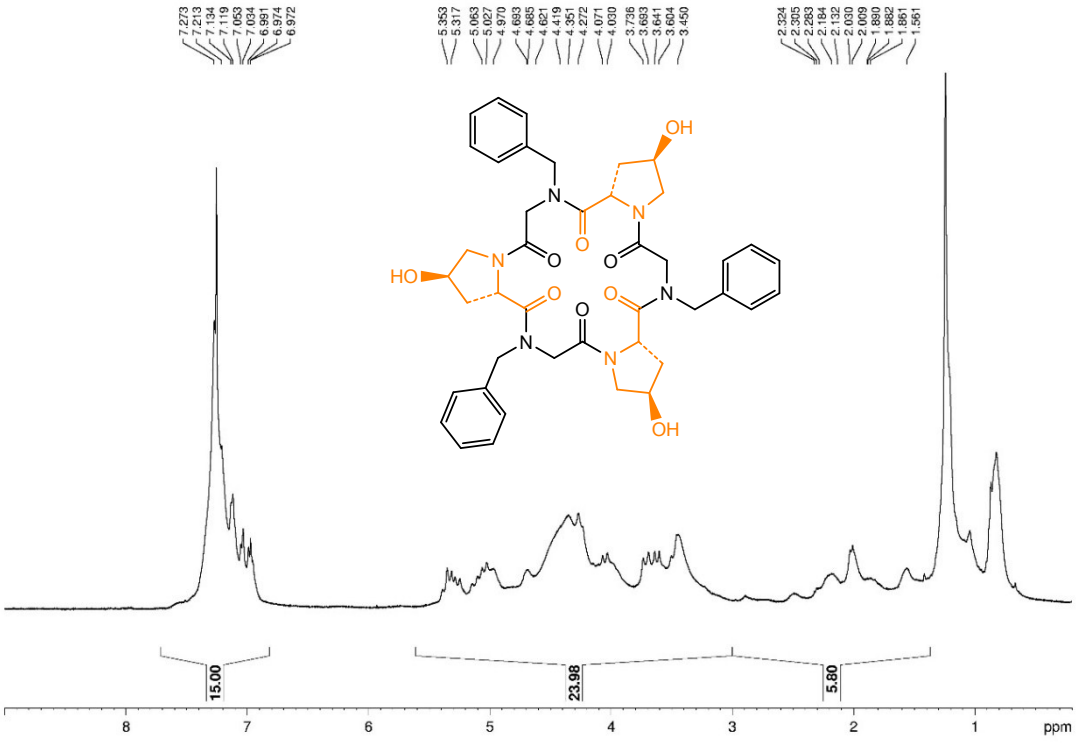
1: ^{1}H NMR (400 MHz, $CDCl_3$)



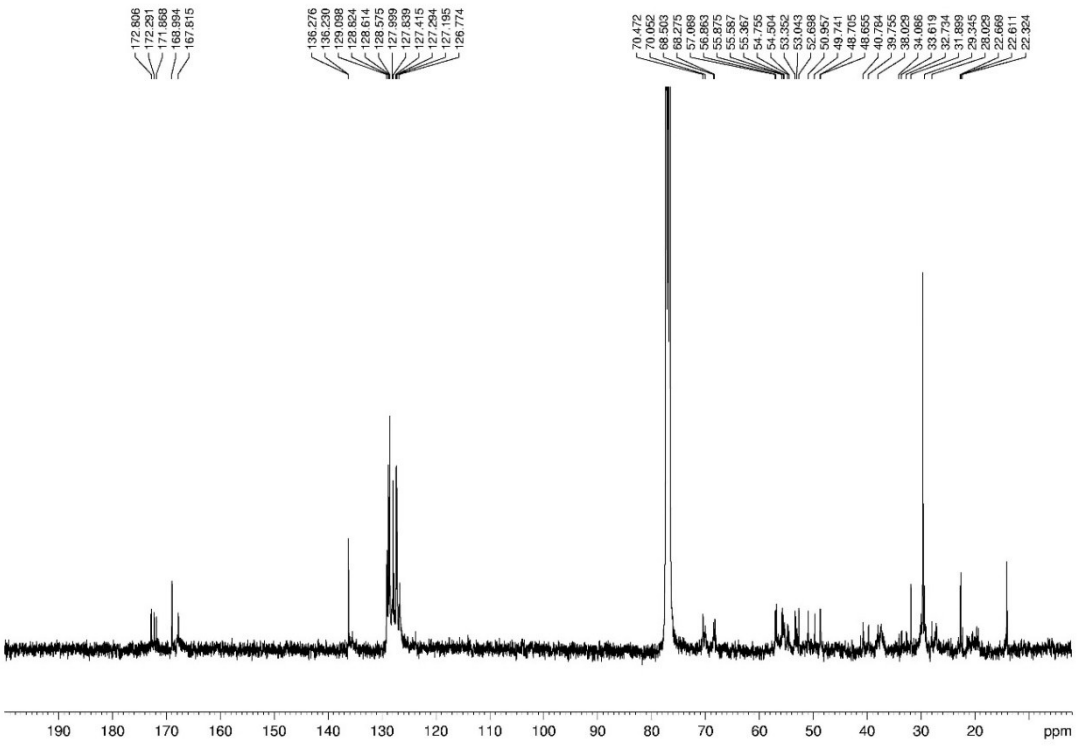
1: ^{13}C NMR (100 MHz, $CDCl_3$)



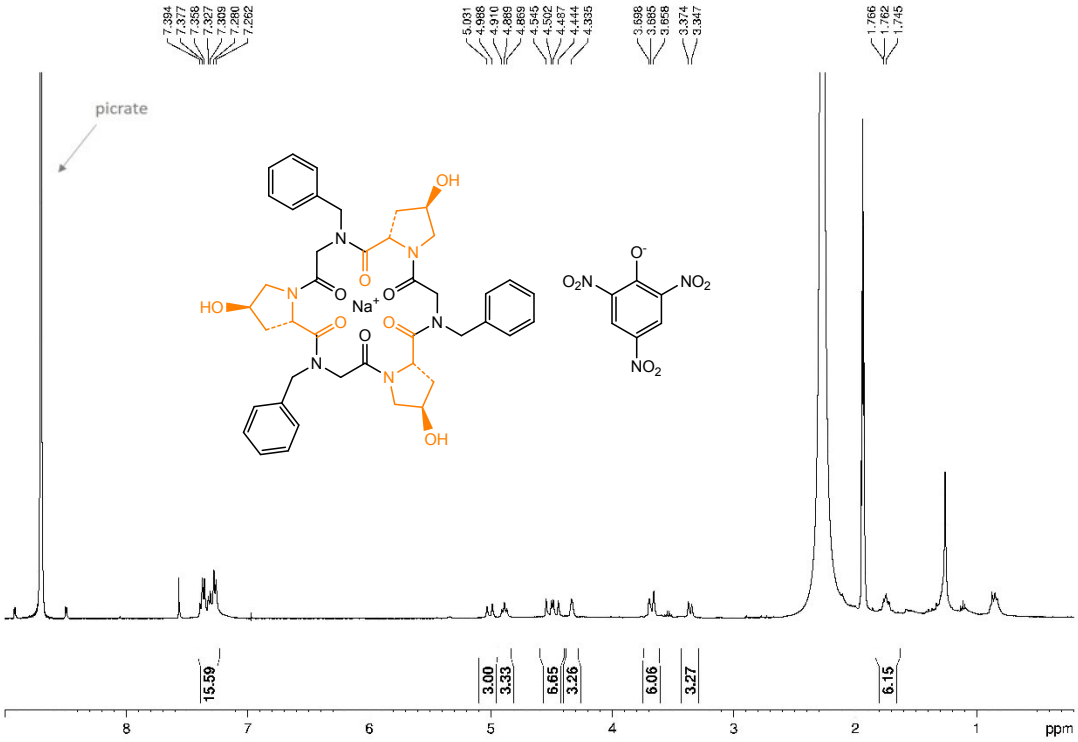
[**1**·Na]$^{+}$Pic^{-}: ^{1}H NMR (400 MHz, $CD_3CN/CDCl_3$ 9/1)



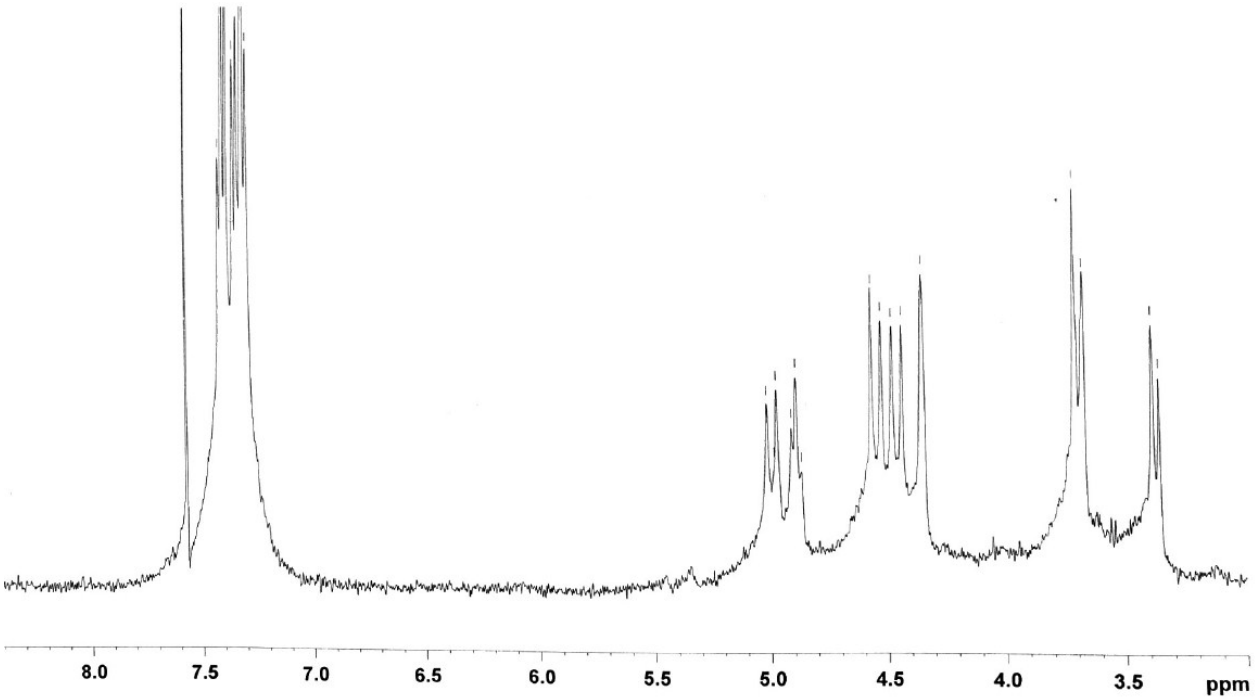
2: ^{1}H NMR (400 MHz, $CDCl_3$)



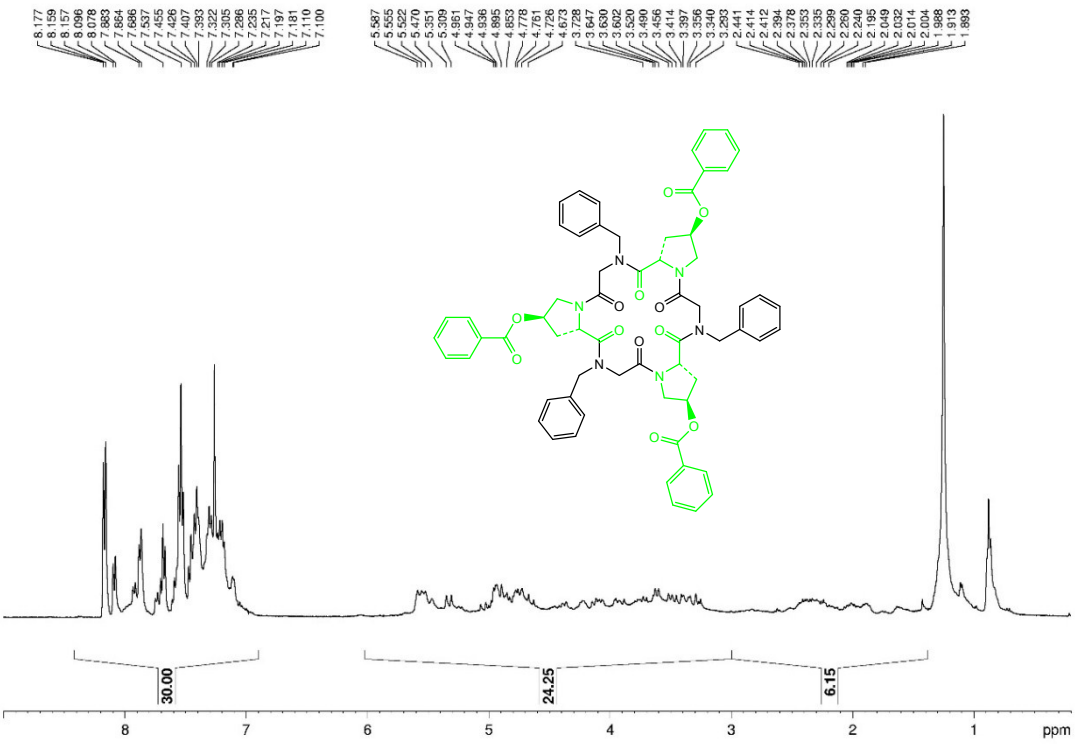
2: ^{13}C NMR (100 MHz, $CDCl_3$)



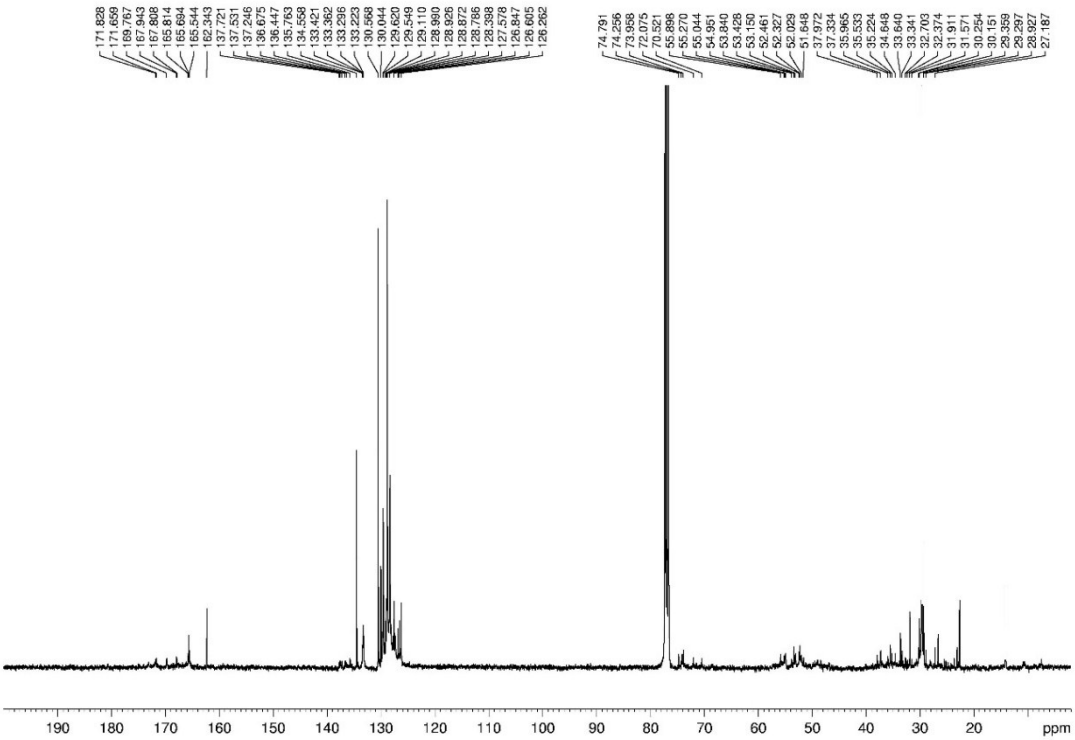
[**2**·Na]$^+$Pic$^-$: ^{1}H NMR (400 MHz, $CD_3CN/CDCl_3$ 9/1)



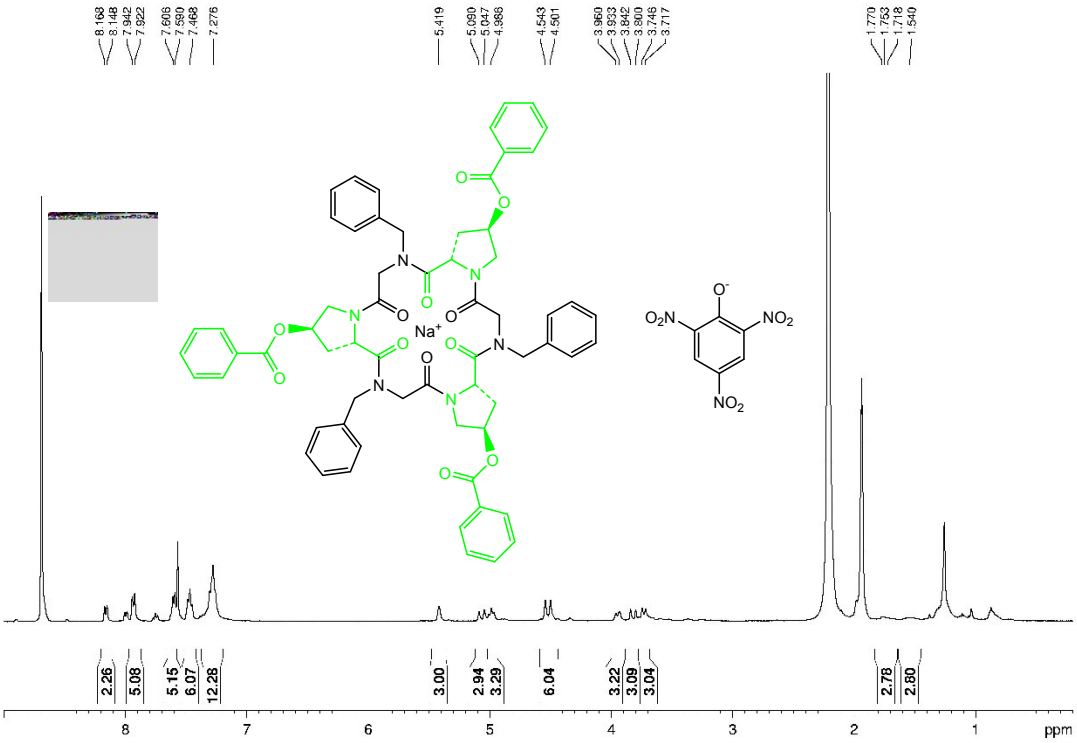
Expansion of [**1**·Na]$^+$Pic$^-$: ^{1}H NMR (400 MHz, $CD_3CN/CDCl_3$ 9/1).



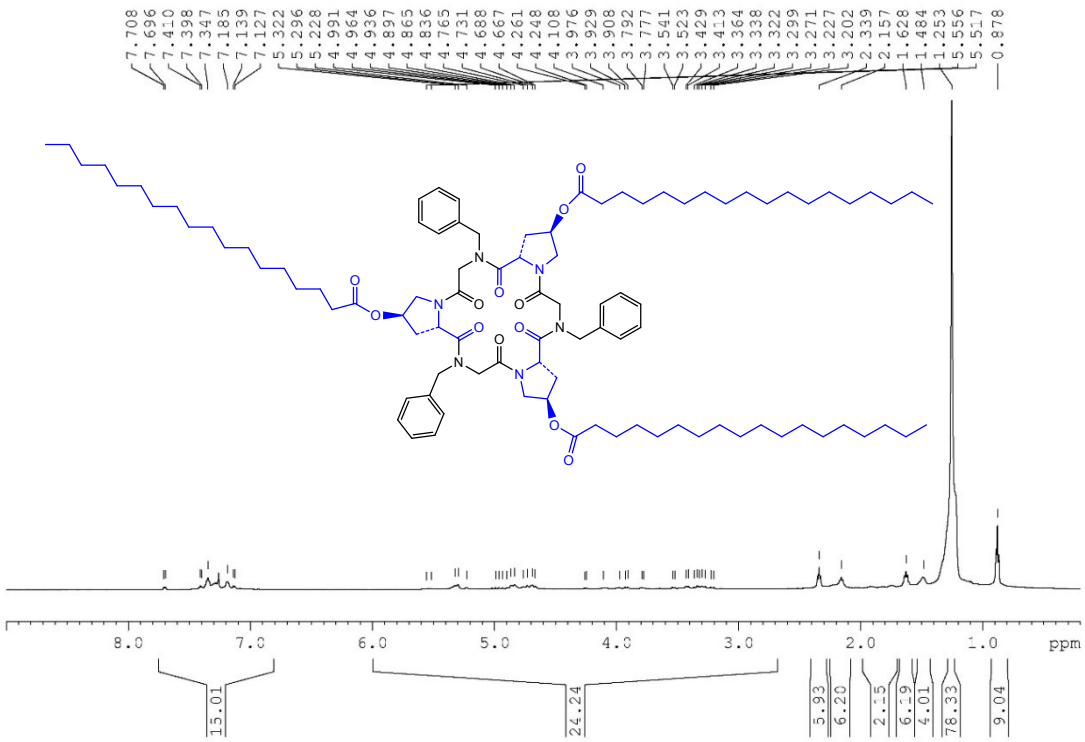
3: ^{1}H NMR (400 MHz, $CDCl_3$)



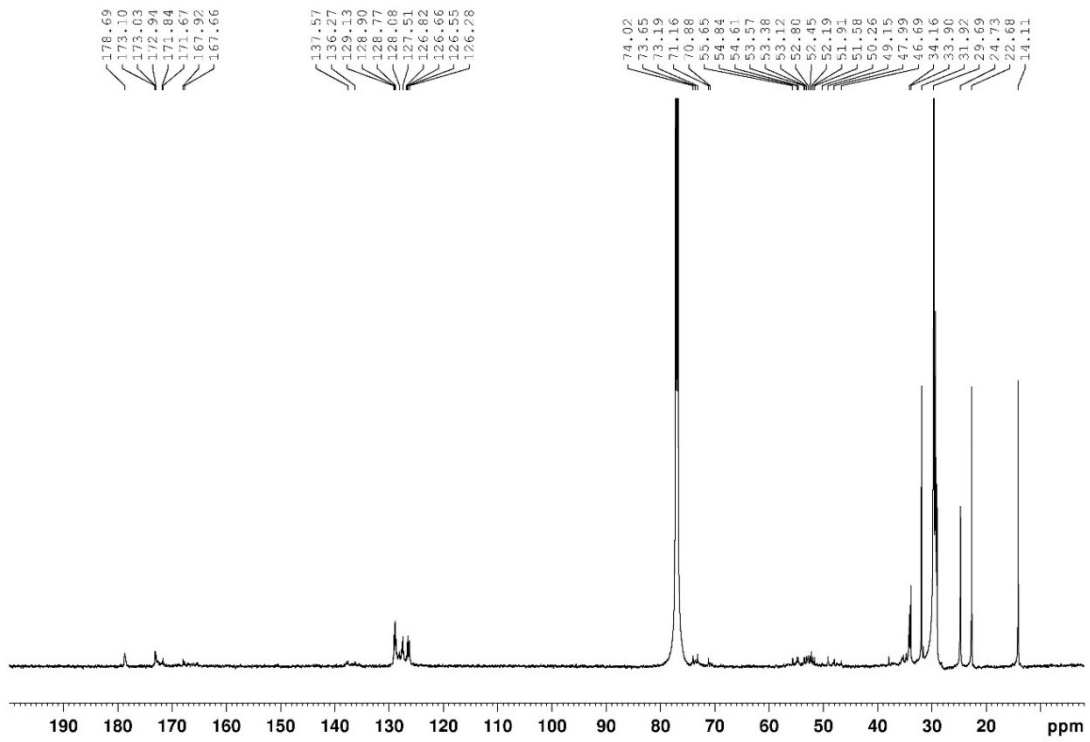
3: ^{13}C NMR (100 MHz, $CDCl_3$)



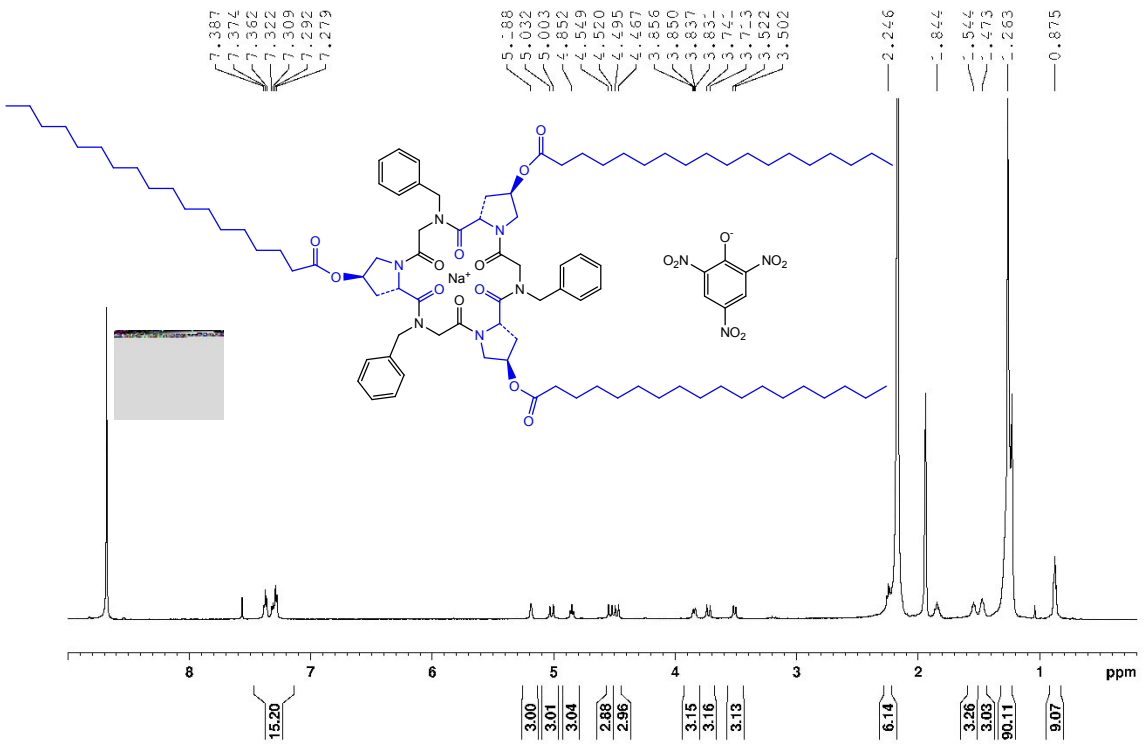
[**3**·Na]$^{+}$Pic^{-}: ^{1}H NMR (400 MHz, $CD_3CN/CDCl_3$ 9/1)



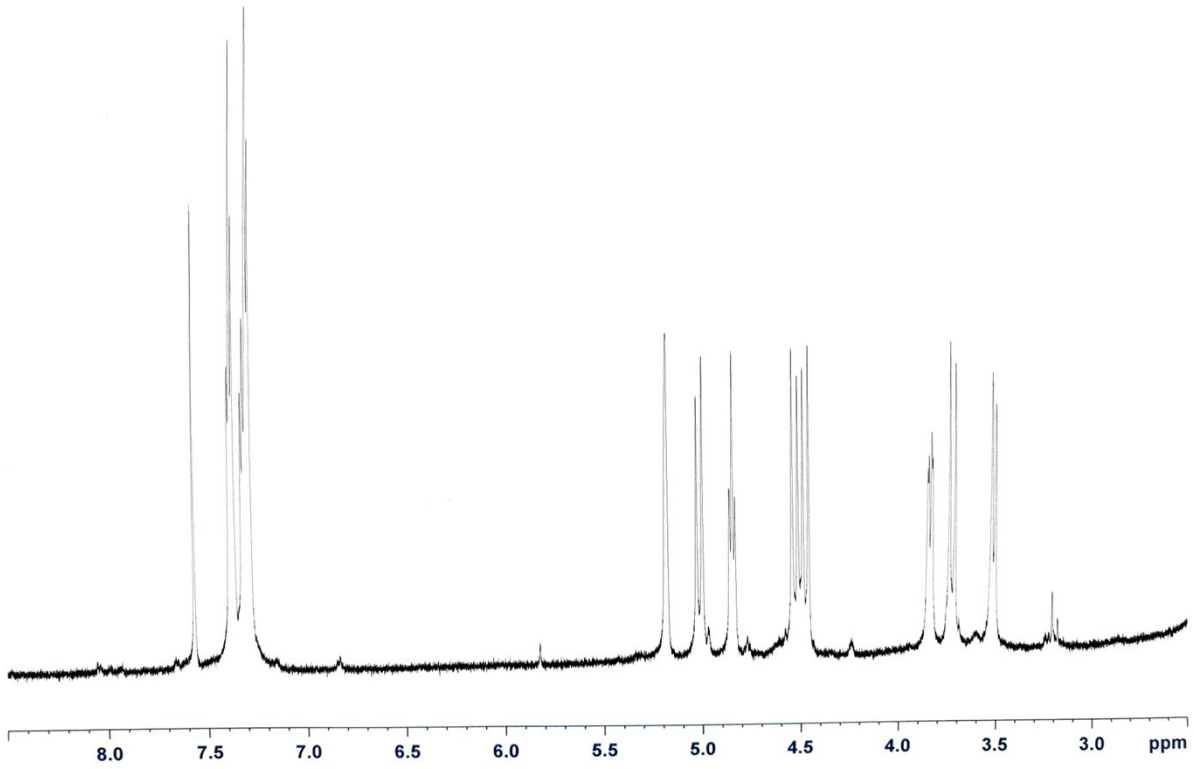
4: ^{1}H NMR (600 MHz, $CDCl_3$)



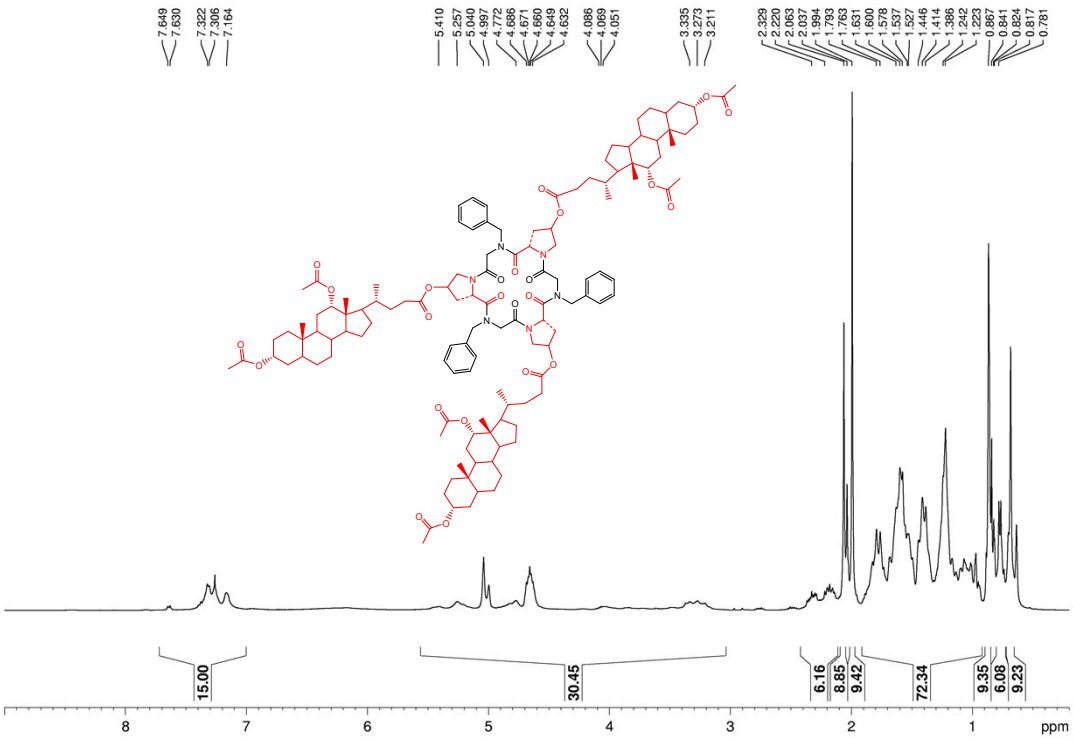
4: ^{13}C NMR (150 MHz, $CDCl_3$)



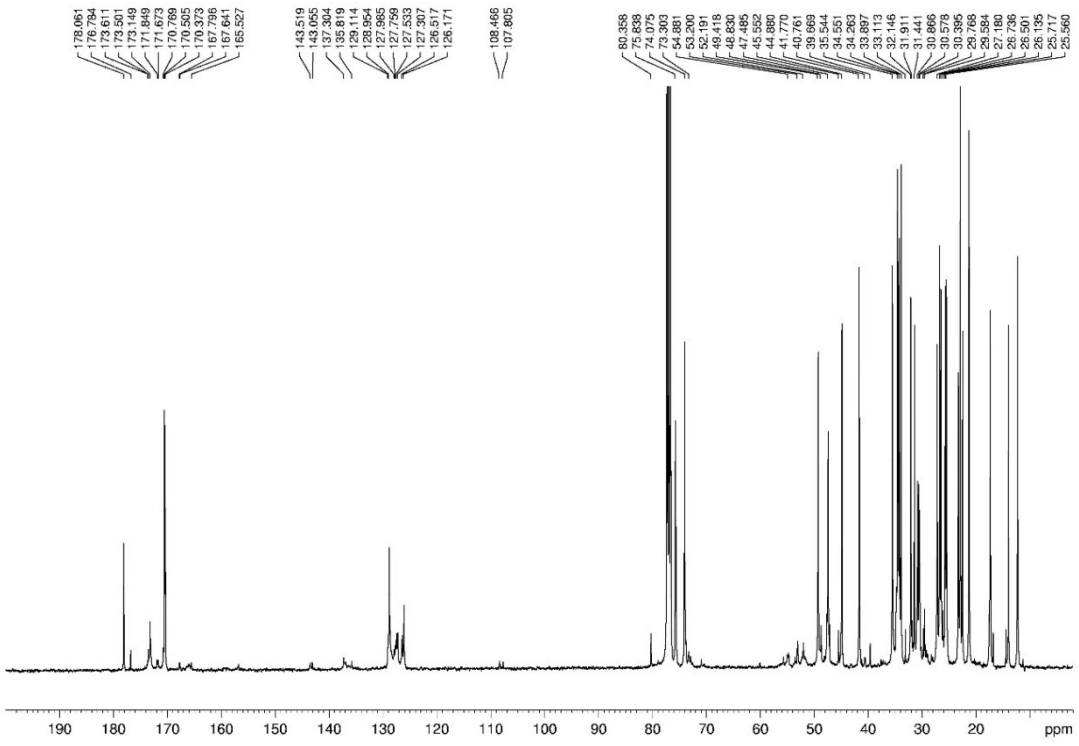
[**4**·Na]$^+$Pic$^-$: ^{1}H NMR (600 MHz, $CD_3CN/CDCl_3$ 9/1)



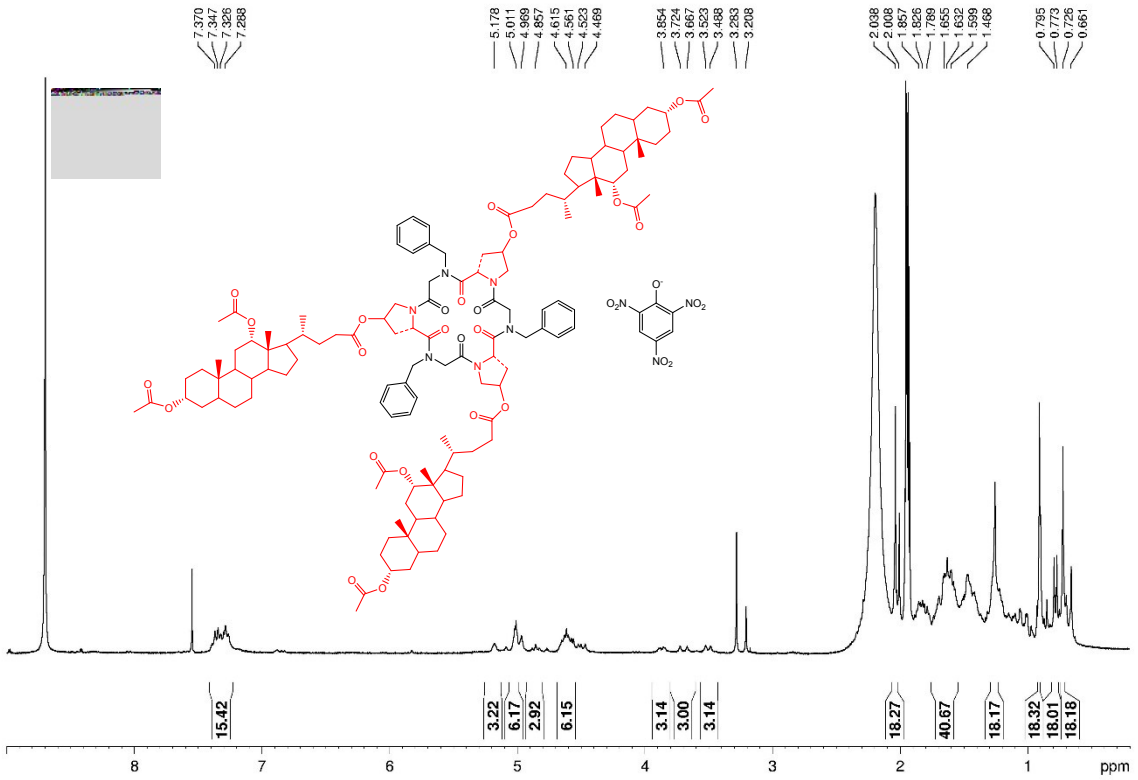
Expansion of [**4**·Na]$^+$Pic$^-$: ^{1}H NMR (600 MHz, $CD_3CN/CDCl_3$ 9/1).



5: ^{1}H NMR (400 MHz, $CDCl_3$)



5: ^{13}C NMR (100 MHz, $CDCl_3$)



[**5**·Na]$^+$Pic$^-$: ^{1}H NMR (400 MHz, $CD_3CN/CDCl_3$ 9/1)

1.2 Titration of cyclic peptoids **1**-**5** with NaPic

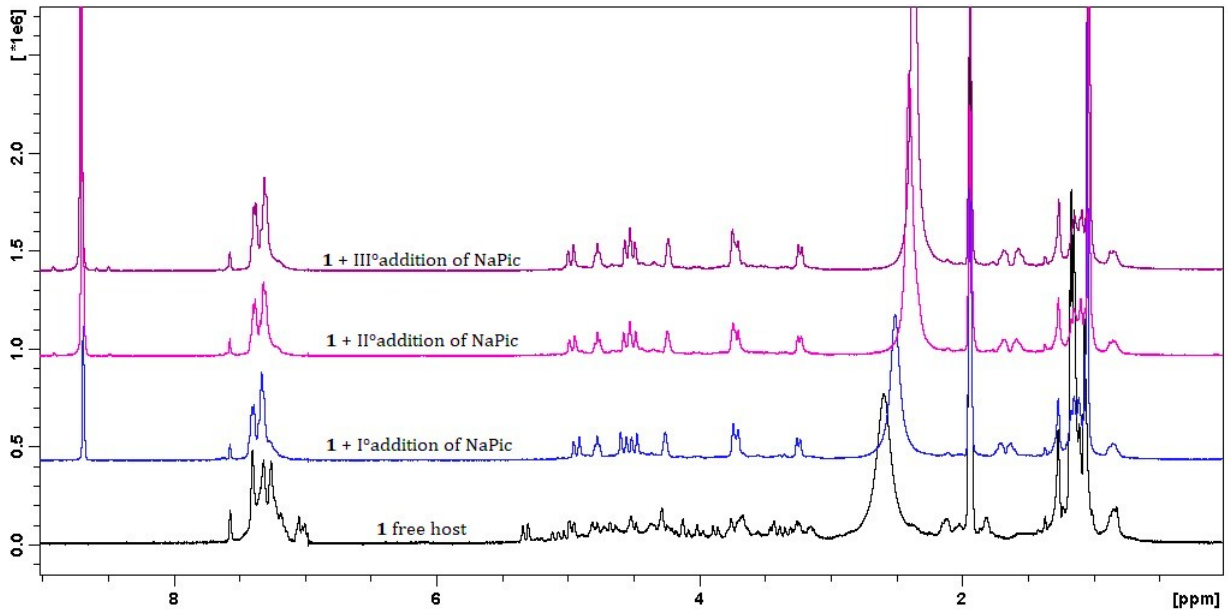


Figure S1. Step-wise addition of NaPic to **1**. ^{1}H NMR (400 MHz, $CD_3CN/CDCl_3$ 9/1, 298 K)

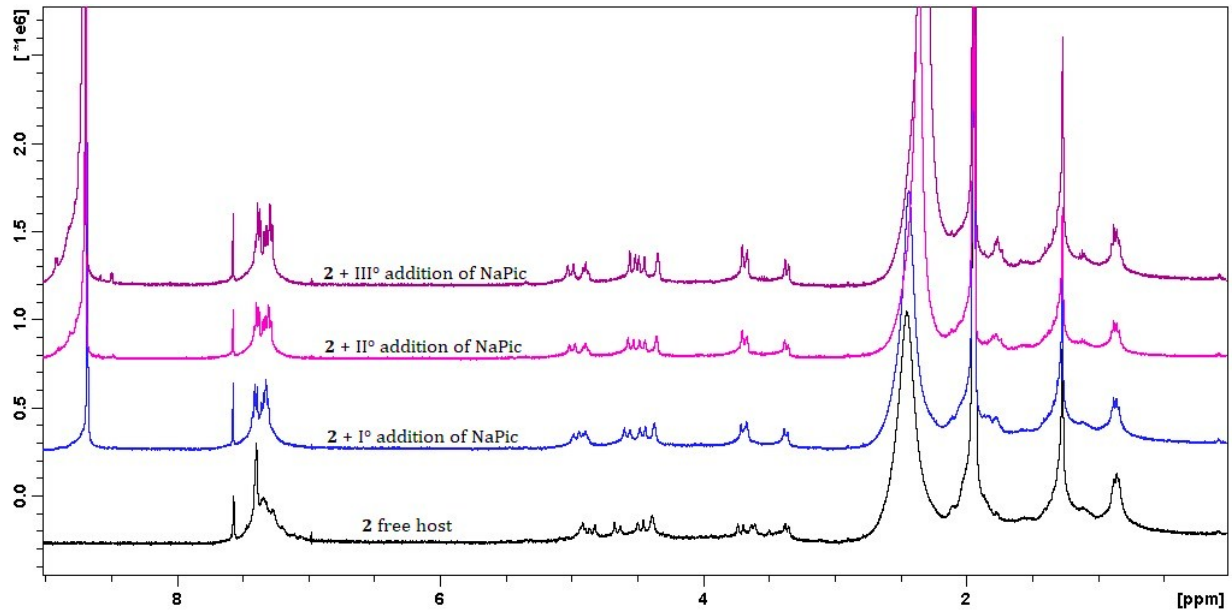


Figure S2. Step-wise addition of NaPic to **2**. ^{1}H NMR (400 MHz, $CD_3CN/CDCl_3$ 9/1, 298 K)

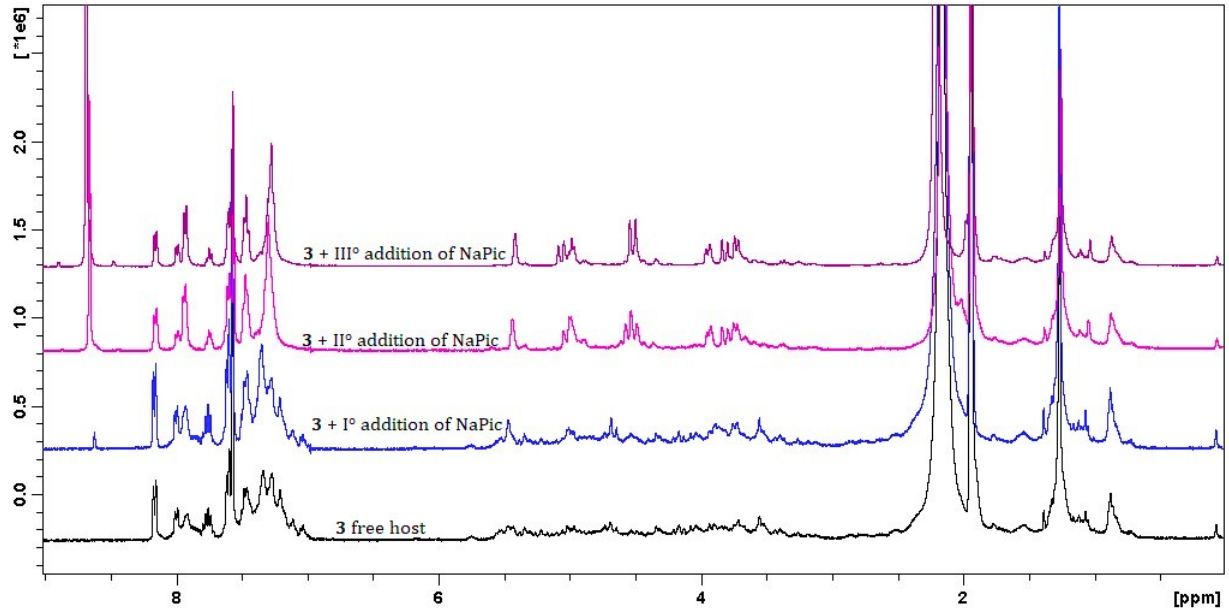


Figure S3. Step-wise addition of NaPic to **3**. ^{1}H NMR (400 MHz, $CD_3CN/CDCl_3$ 9/1, 298 K)

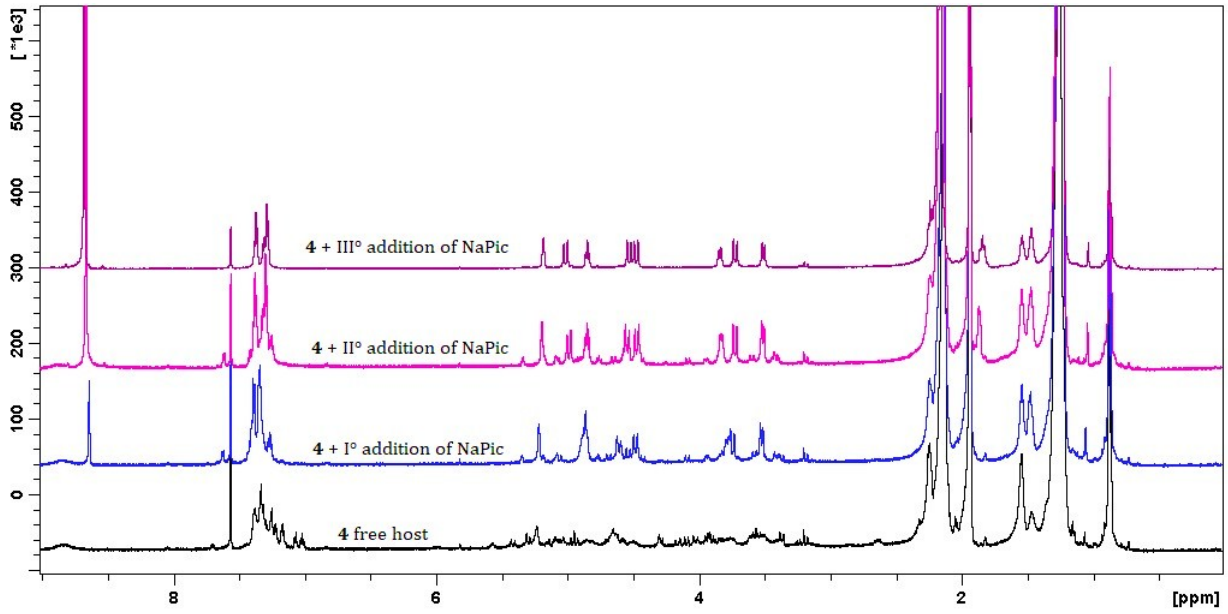


Figure S4. Step-wise addition of NaPic to **4**. ^{1}H NMR (600 MHz, $CD_3CN/CDCl_3$ 9/1, 298 K)

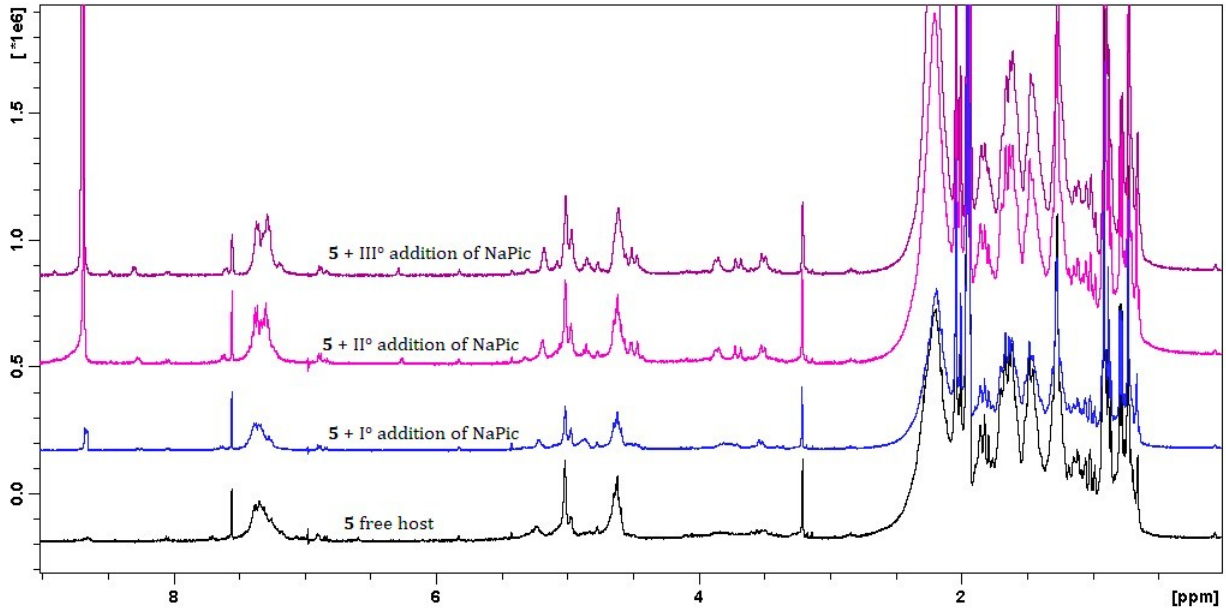
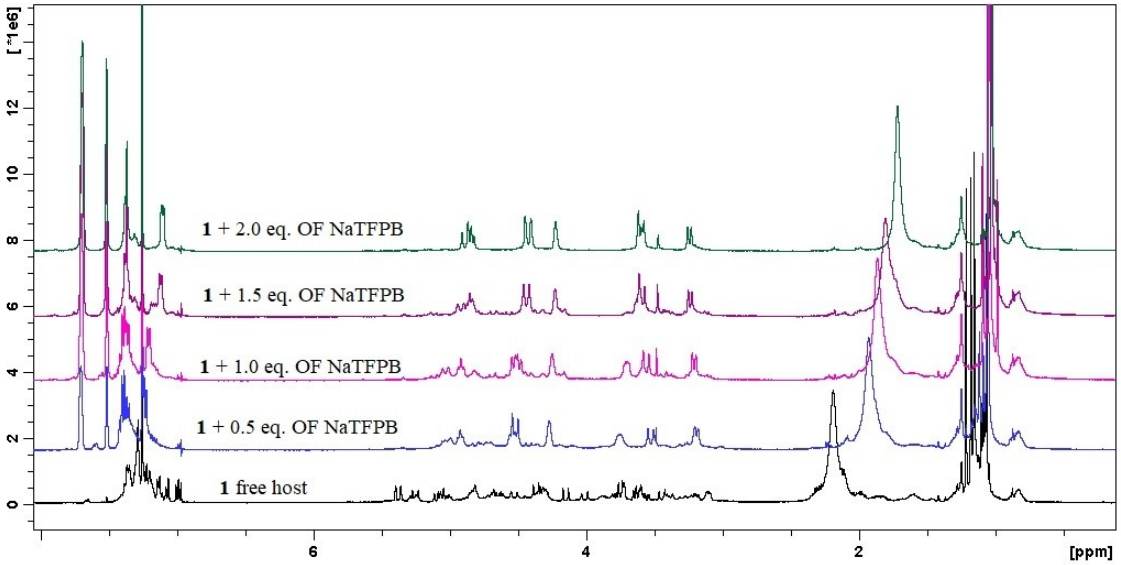
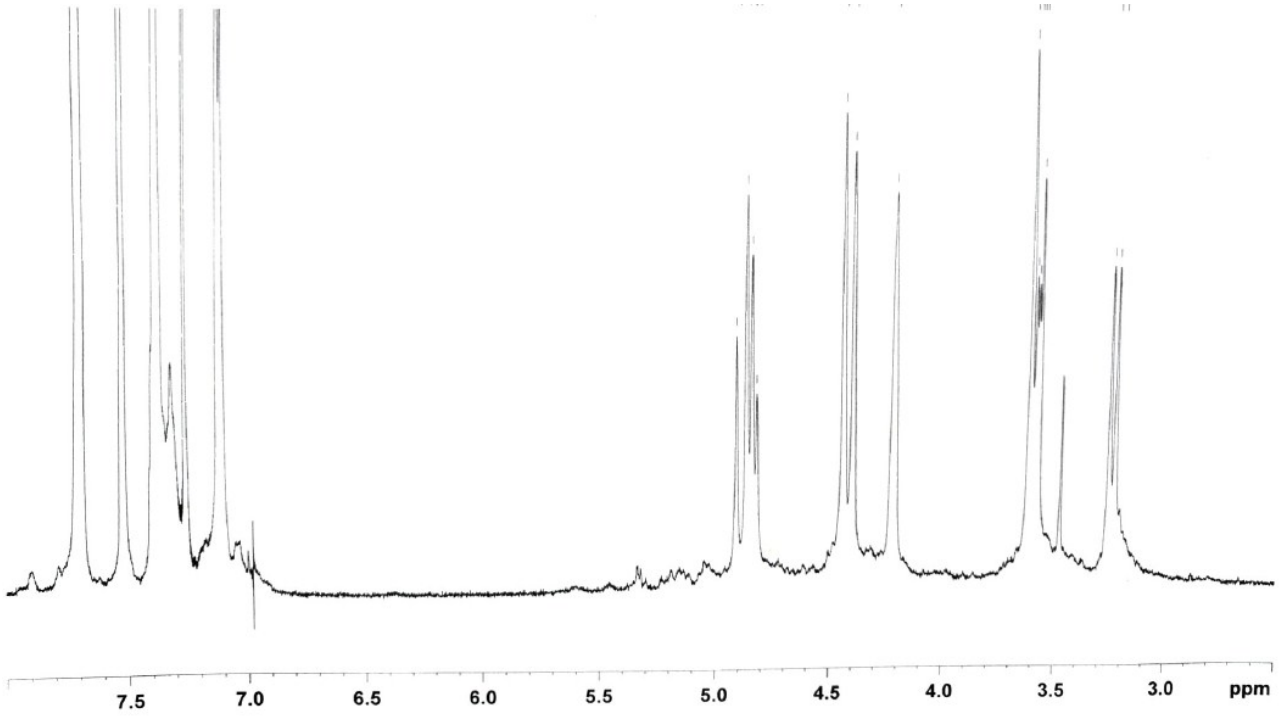


Figure S5. Step-wise addition of NaPic to **5**. ^{1}H NMR (400 MHz, $CD_3CN/CDCl_3$ 9/1, 298 K)

1.3 Titration of cyclic peptoids **1**-**5** with NaTFPB



a)



b)

Figure S6. a) Quantitative step-wise addition of NaTFPB to **1** ^{1}H NMR (400 MHz, $CDCl_3$, 298 K); b) Expansion of spectrum obtained after addition of 2.0 eq of NaTFPB

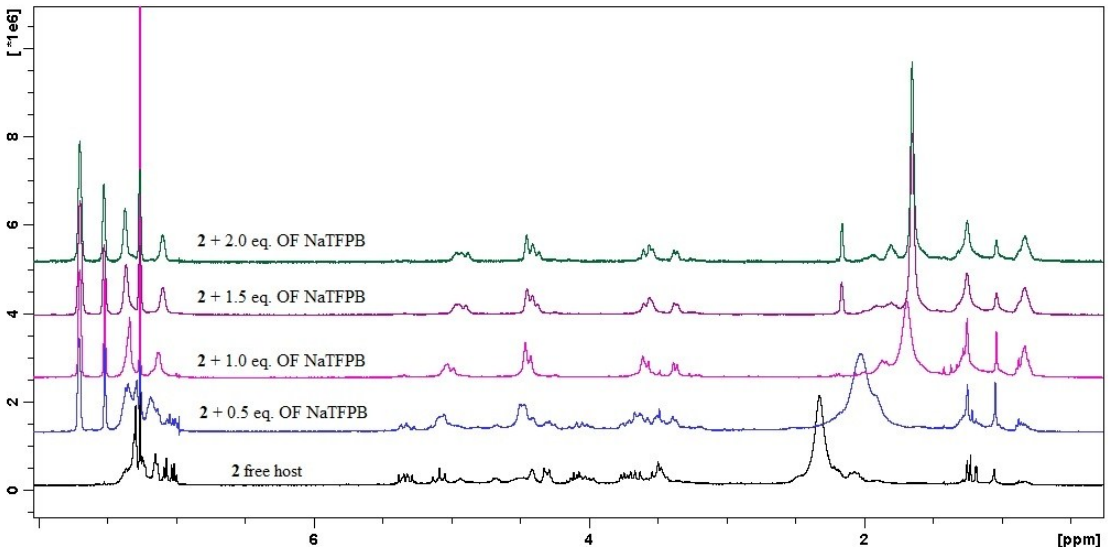
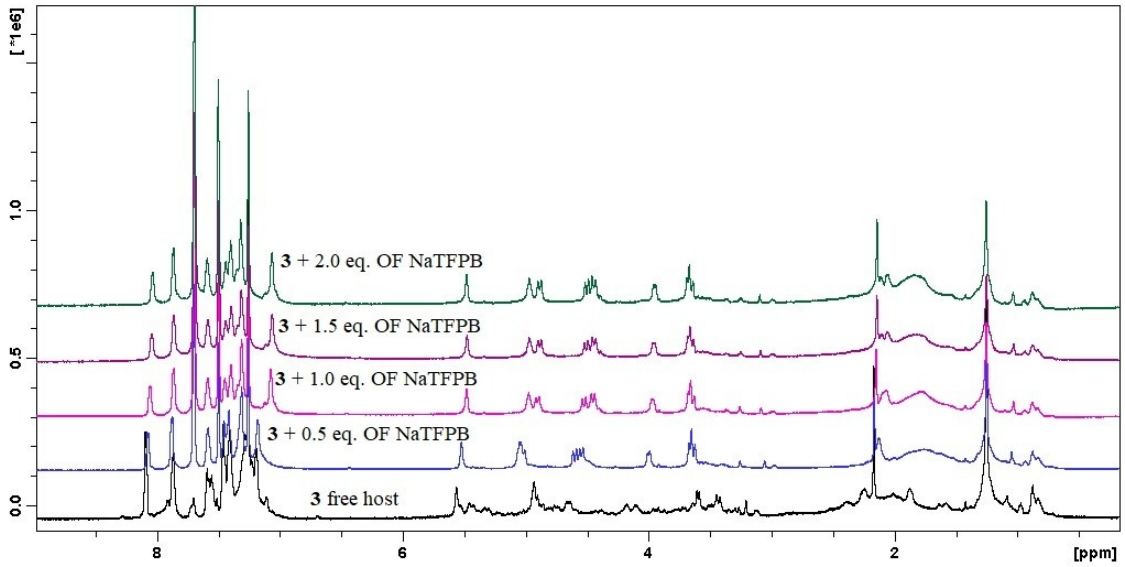
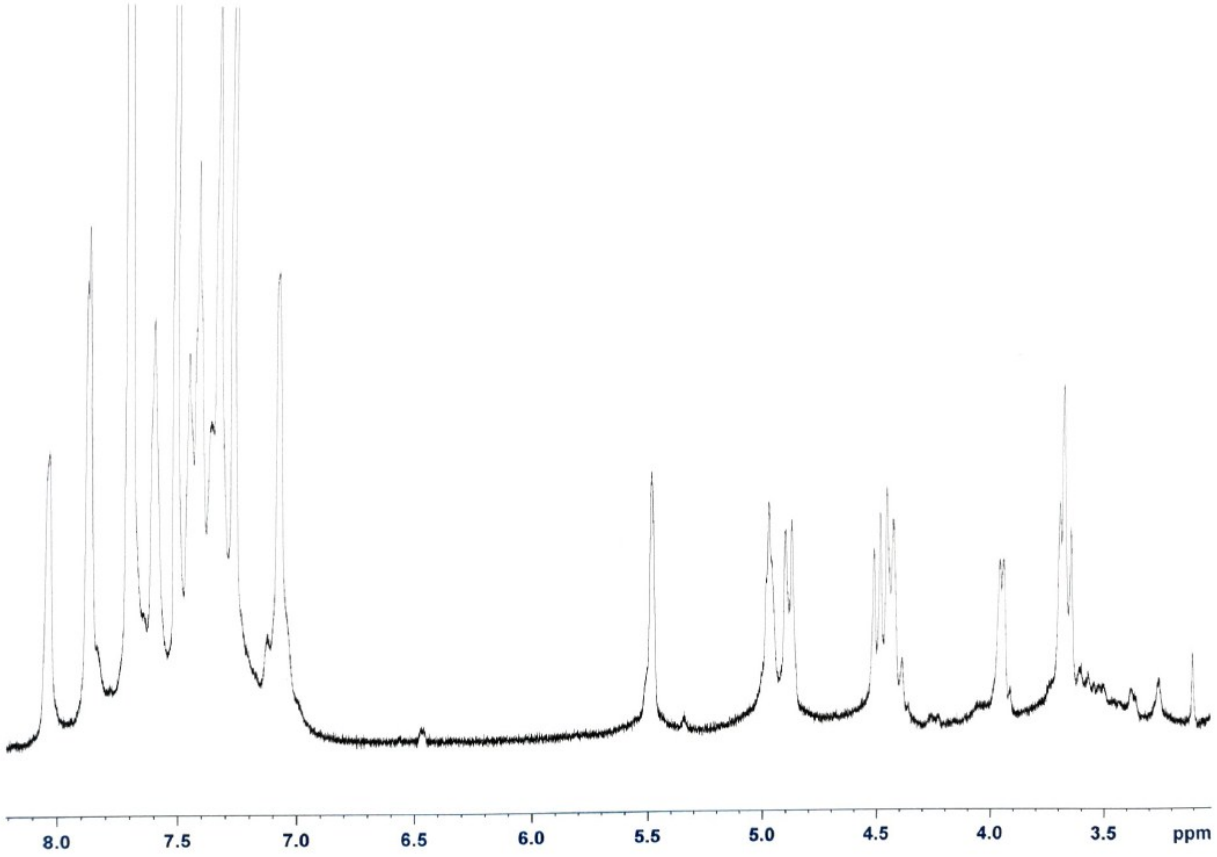


Figure S7. Quantitative step-wise addition of NaTFPB to **2**. ^{1}H NMR (400 MHz, $CDCl_3$, 298 K)



a)



b)

Figure S8. Quantitative step-wise addition of NaTFPB to **3**. ^{1}H NMR (600 MHz, $CDCl_3$, 298 K); b) Expansion of ^{1}H NMR spectrum obtained after addition of 2.0 eq of NaTFPB

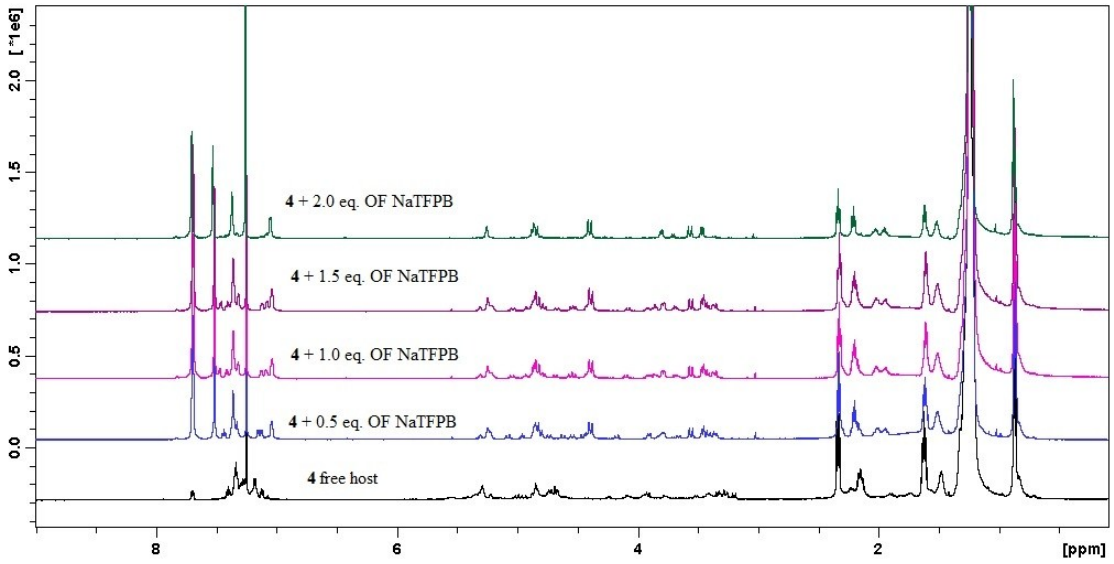


Figure S9. Quantitative step-wise addition of NaTFPB to **4**. ^{1}H NMR (600 MHz, $CDCl_3$, 298 K)

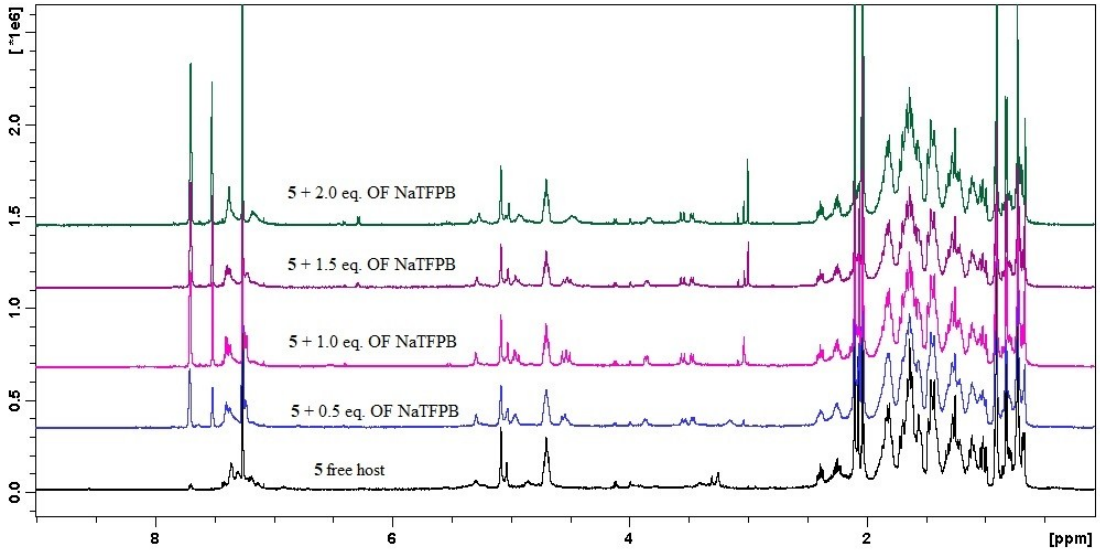
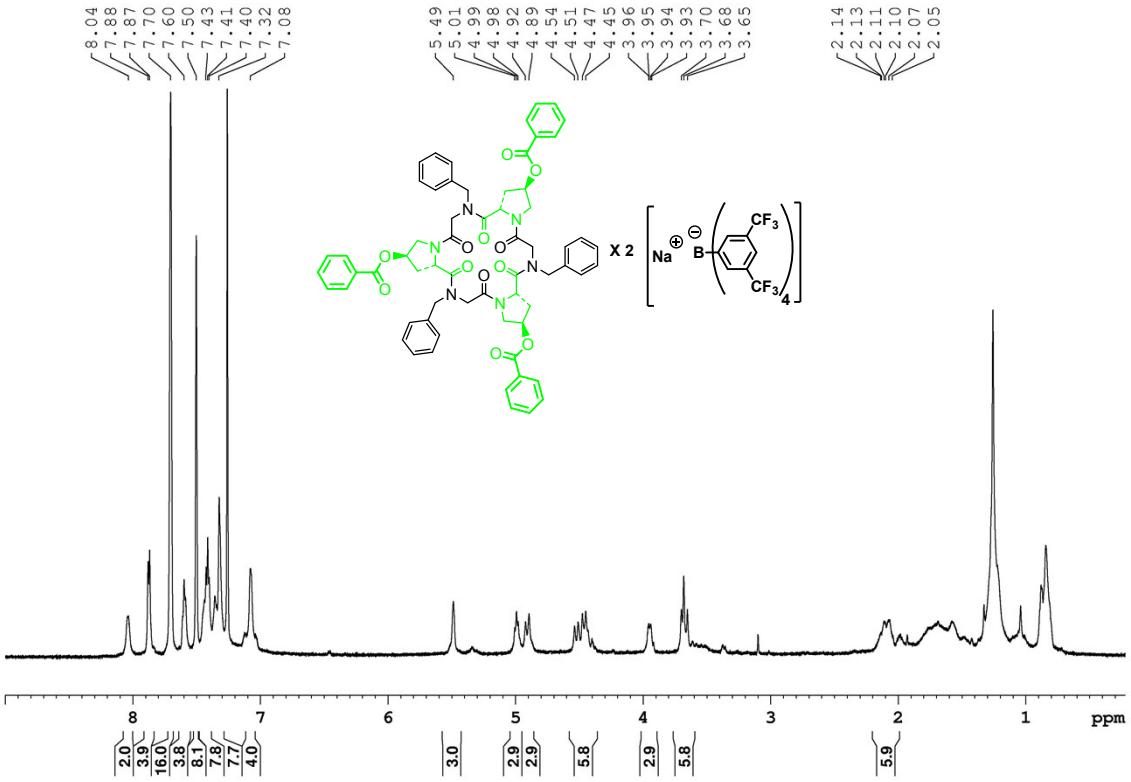
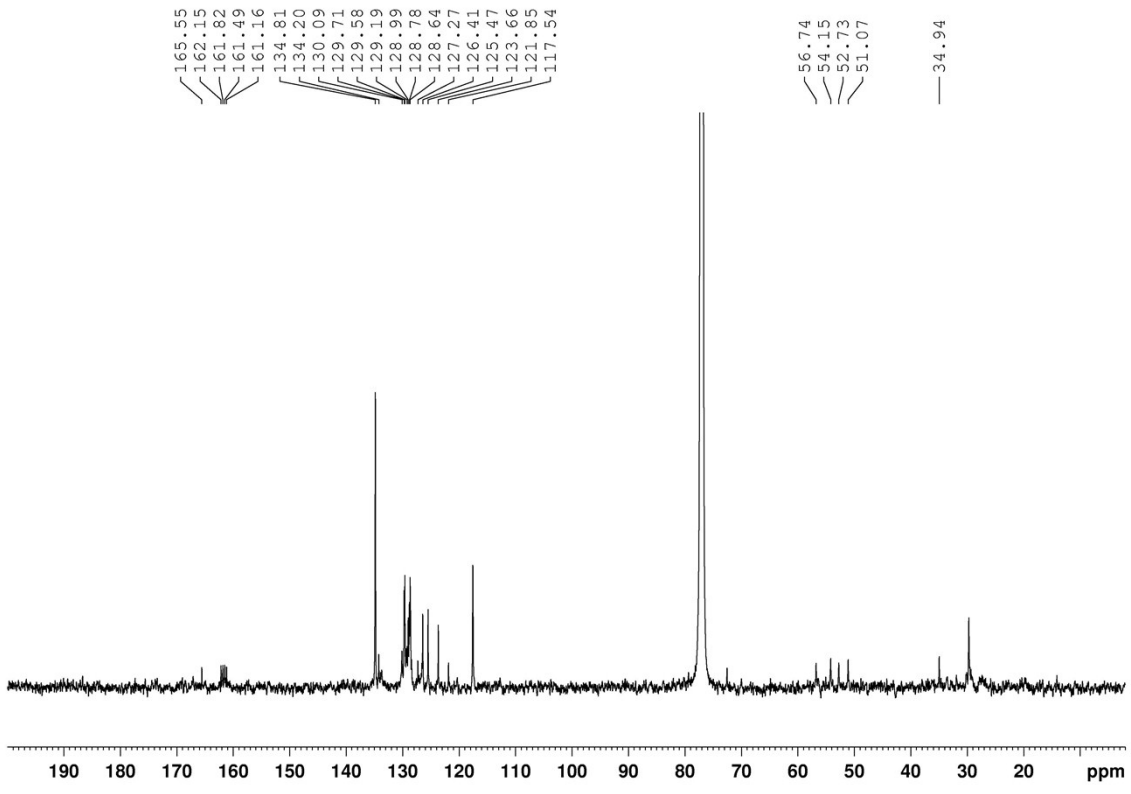


Figure S10. Quantitative step-wise addition of NaTFPB to **5**. ^{1}H NMR (600 MHz, $CDCl_3$, 298 K)

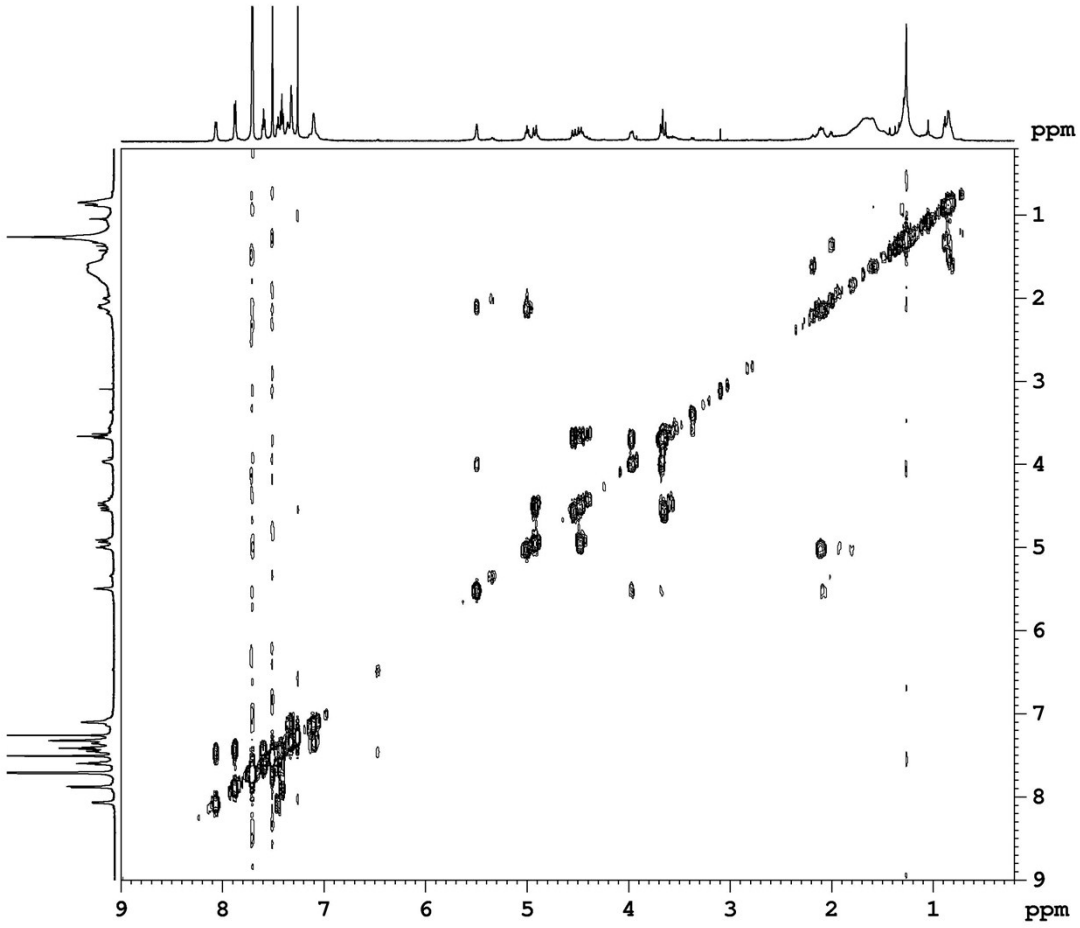
1.4 NMR spectra (1 and 2D) of **[3·2Na]$^{2+}$2TFPB^{-}**



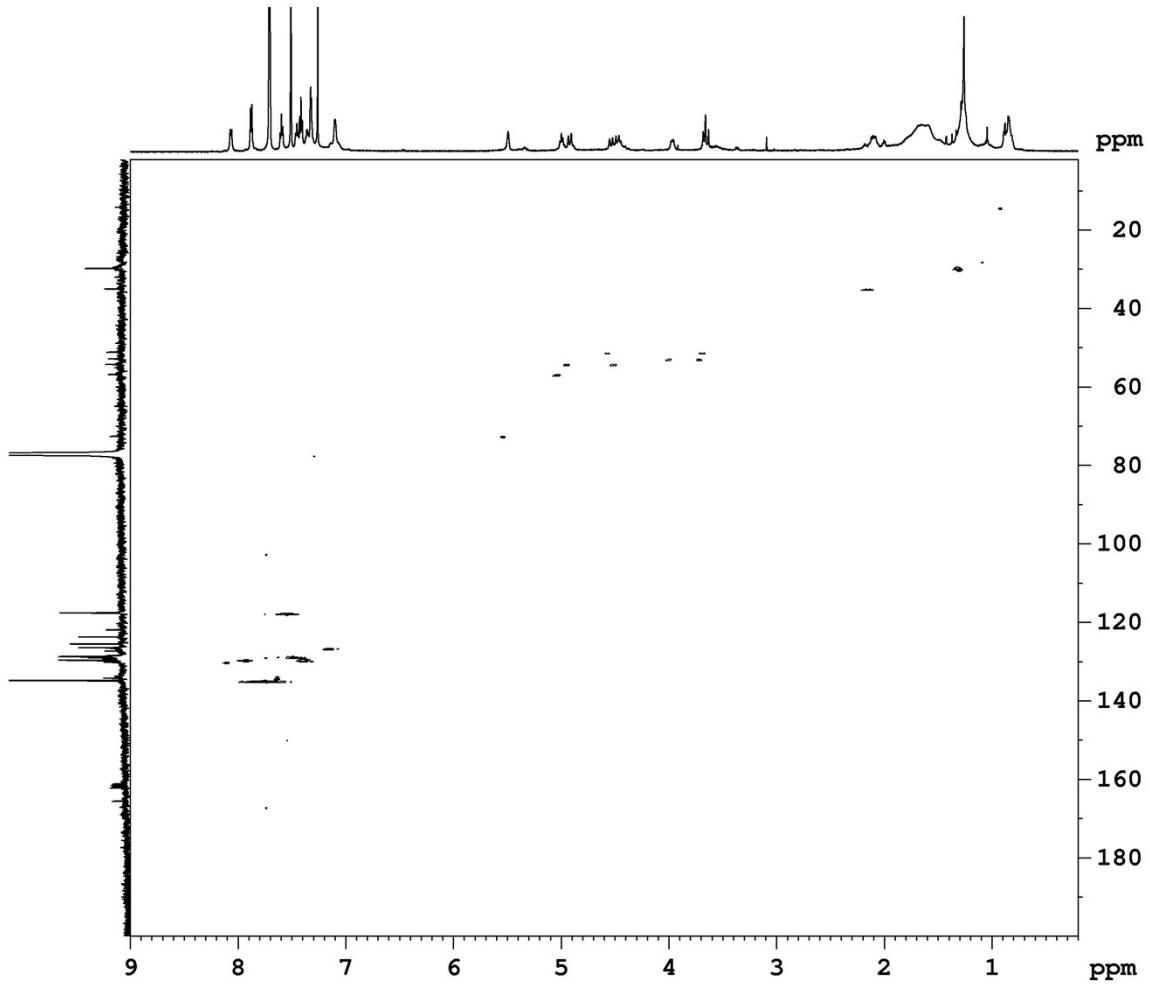
[3·2 Na+]$^{2+}$2TFPB^{-}: ^{1}H-NMR (600 MHz, $CDCl_3$)



[3·2 Na+]$^{2+}$2TFPB^{-}: ^{13}C-NMR (600 MHz, $CDCl_3$)

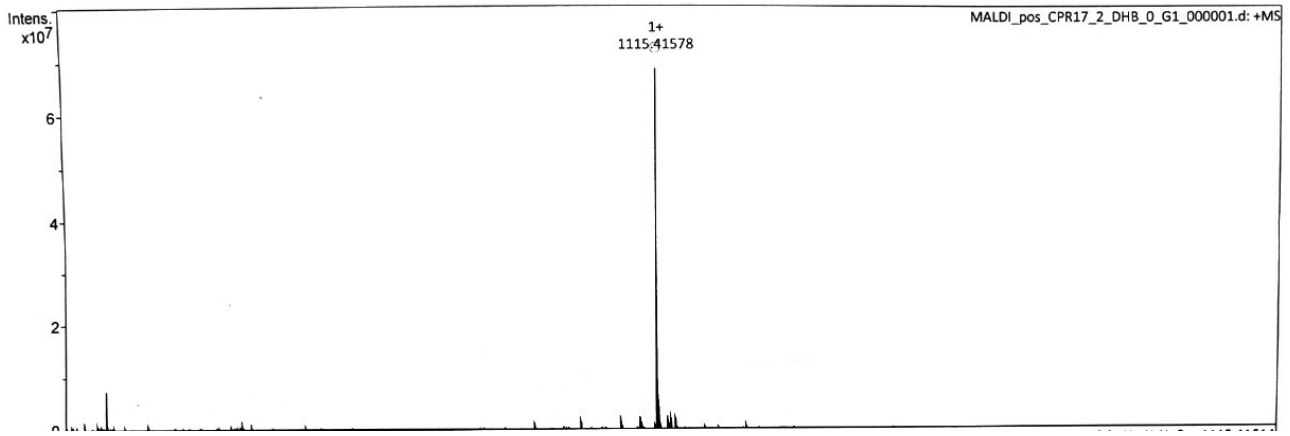


[3·2 Na+]$^{2+}$2TFPB^{-}: ^{1}H-^{1}H COSY NMR (600 MHz, $CDCl_3$)

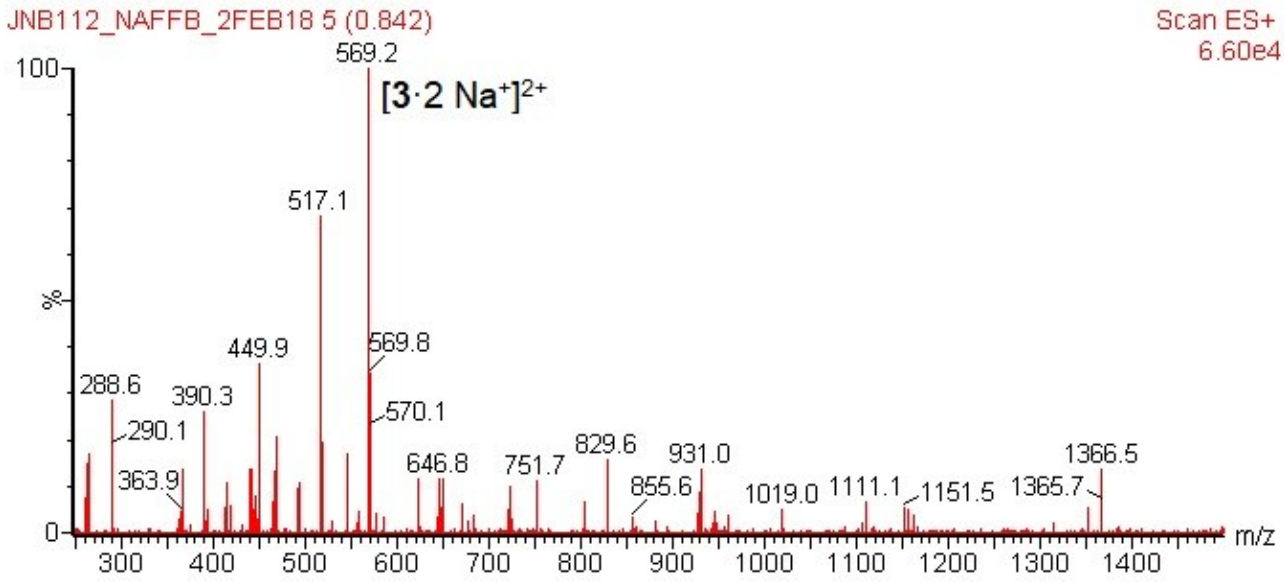


[3·2 Na+]$^{2+}$2TFPB^{-}: ^{1}H-^{13}C HSQC NMR (600 MHz, $CDCl_3$)

1.5 MS spectra of free and complexed **3**



a)



b)

Figure S11. a) HRMS spectrum of **3**; b) ESI MS spectrum of **3** treated with two equivalents of NaTFPB (presence of the [**3**·2 Na+]$^{2+}$ peak 100%).

2.0 HPLC analysis

2.1 HPLC chromatograms of linear peptoid (**6**) as crude mixture

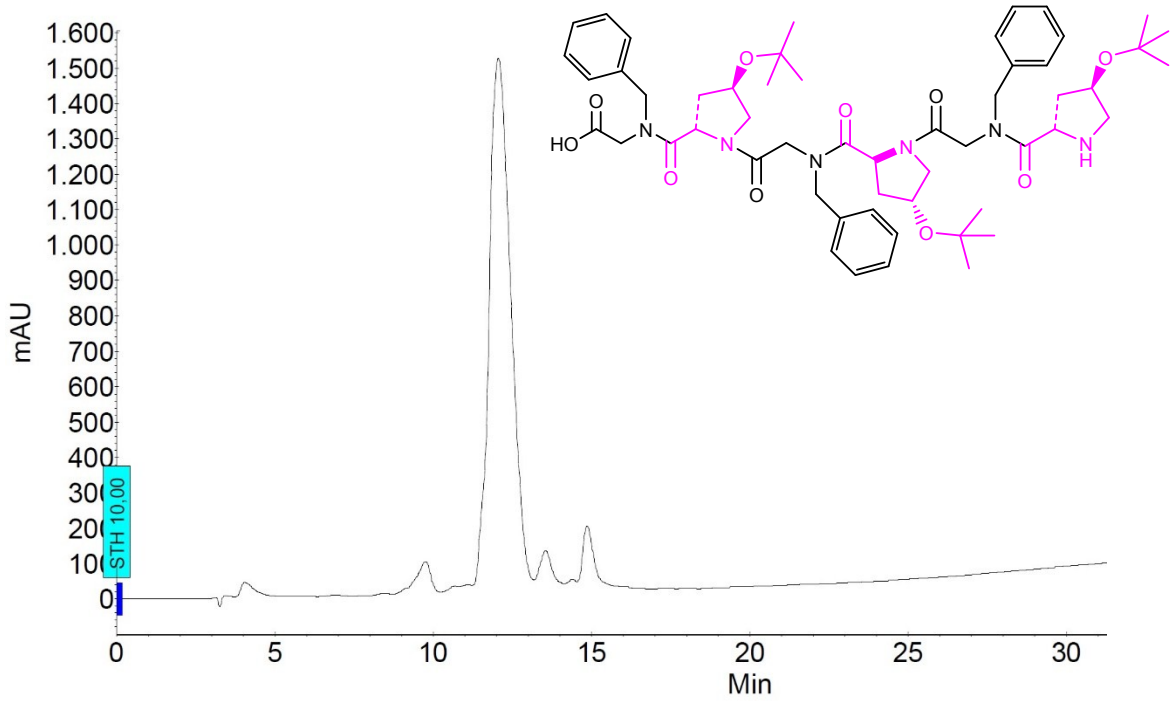


Figure S12. HPLC analysis of **6**.

2.2 HPLC chromatograms of cyclic peptoids

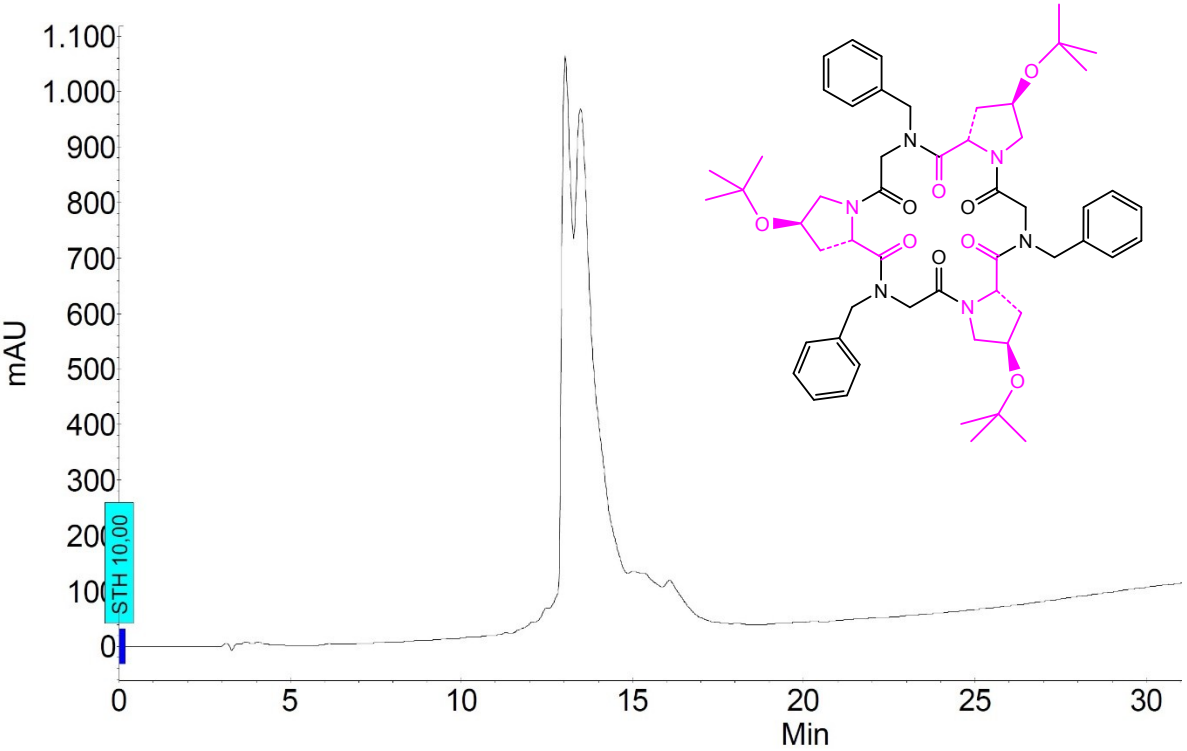


Figure S13. HPLC analysis of **1**.

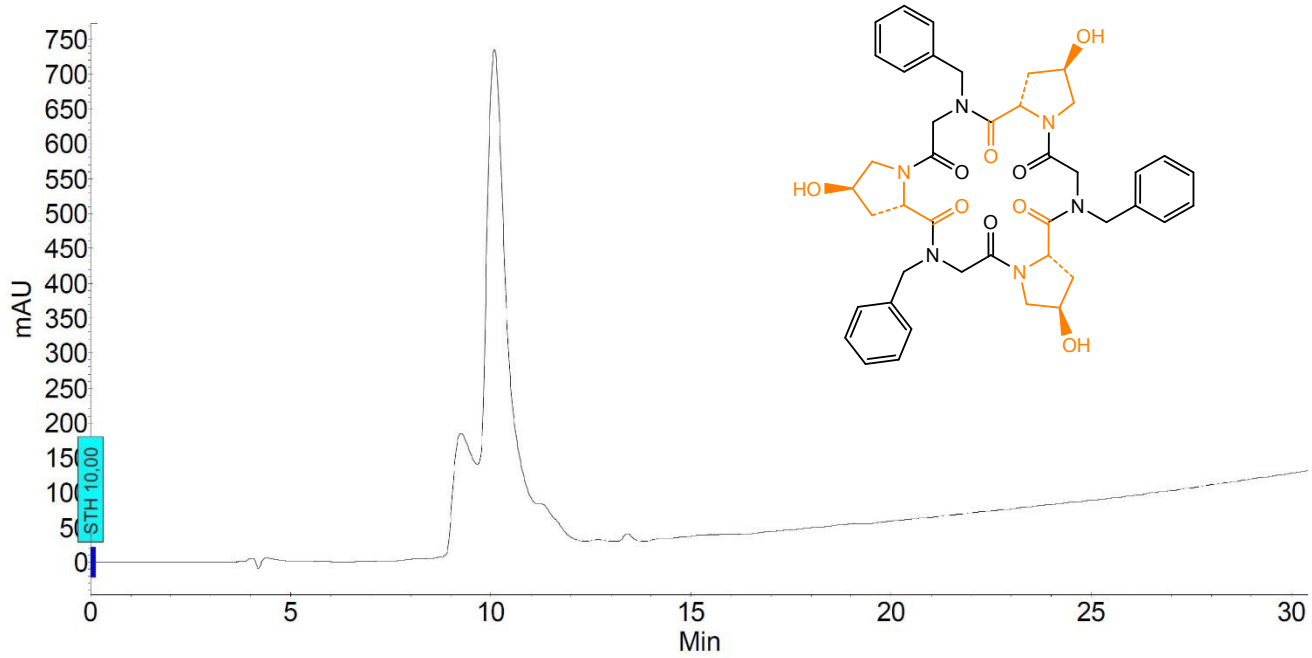


Figure S14. HPLC analysis of **2**.

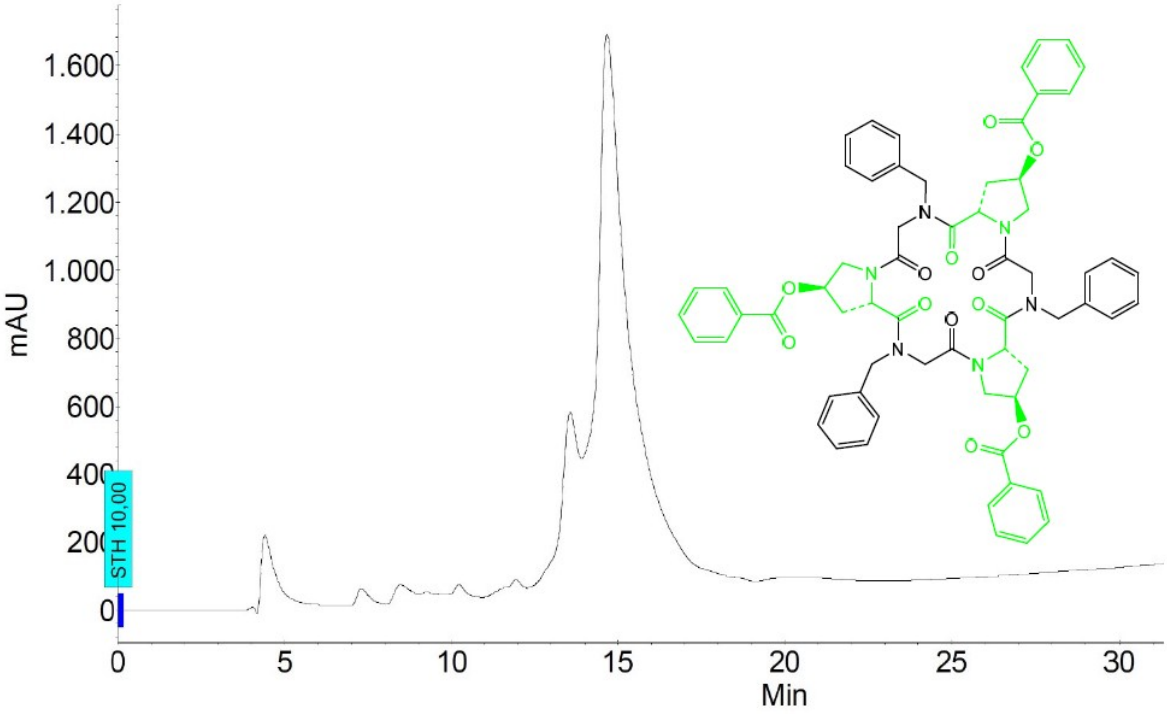


Figure S15. HPLC analysis of **3**.

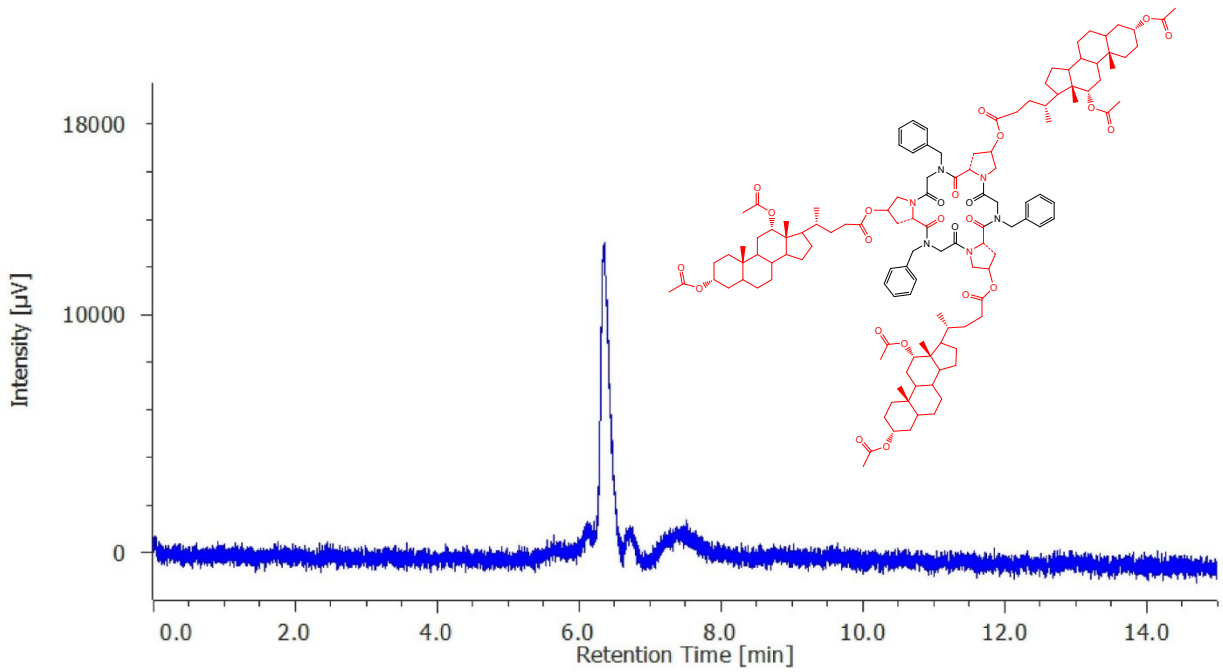


Figure S16. HPLC analysis of **5**.

3.0 Computational details

The DFT calculations were performed with the Gaussian09 set of programs,[1] using the BP86 functional of Becke and Perdew.[2] The electronic configuration of the molecular systems was described with the standard triple zeta valence basis set with a polarization function of Ahlrichs and co-workers for H, B, C, N, O, F, Na, K (TZVP keyword in Gaussian).[3] The geometry optimizations were performed without symmetry constraints. Solvent effects including contributions of non electrostatic terms have been estimated in single-point calculations on the gas phase optimized structures, based on the polarizable continuous solvation model PCM using $CHCl_3$ as a solvent.[4]

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[1] Gaussian 09, Revision A.02, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; N. Kudin, K.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, **2009**.

[2] a) Becke, A. *Phys. Rev. A* **1988**, *38*, 3098– 3100. b) Perdew, J. P. *Phys. Rev. B* **1986**, *33*, 8822– 8824. c) Perdew, J. P. *Phys. Rev. B* **1986**, *34*, 7406– 7406.

[3] Schaefer, A., Horn, H. and Ahlrichs, R. *J. Chem. Phys.* **1994**, *100*, 5829– 5835.

[4] a) Barone, V. and Cossi, M. *J. Phys. Chem. A* **1998**, *102*, 1995– 2001. b) Tomasi, J. and Persico, M. *Chem. Rev.* **1994**, *94*, 2027– 2094.

Cartesian coordinates and energies of calculated structures

69

TFPB$^-$ E(gas)=-3649.30702872 G(gas)=-3649.025082 E($CHCl_3$)=-3649.34095198

B	-0.000042	0.003641	0.001022
C	-0.978000	1.294977	-0.328960
C	0.988269	0.314987	1.289886
C	1.001489	-0.330080	-1.271401
C	-1.010962	-1.267319	0.314882
C	-0.916032	2.063565	-1.503913
C	-1.795610	3.133626	-1.744675
C	-2.771340	3.479236	-0.809661
C	-2.857748	2.726540	0.369078
C	-1.986501	1.655335	0.594785
H	-0.169963	1.820633	-2.263932
C	-1.648551	3.928371	-3.018234
H	-3.450124	4.311724	-0.992537
C	-3.952872	3.043266	1.357046
H	-2.096551	1.074605	1.513974
C	1.981477	-0.625958	1.647597
C	2.859516	-0.415841	2.716756
C	2.796471	0.764816	3.468247
C	1.836206	1.716933	3.125364
C	0.948344	1.490547	2.059137
H	2.073104	-1.547260	1.066886
C	3.937301	-1.424042	3.028616
H	3.480958	0.935757	4.298652
C	1.713677	2.991596	3.922668
H	0.214341	2.262940	1.818854
C	0.948650	-1.505545	-2.039195
C	1.845953	-1.750804	-3.093837
C	2.829669	-0.819316	-3.424057
C	2.907874	0.360021	-2.670515
C	2.019337	0.590114	-1.615240
H	0.196755	-2.262983	-1.806756
C	1.705117	-3.021361	-3.894431
H	3.522134	-1.006229	-4.244646
C	4.009635	1.342573	-2.980721
H	2.123465	1.509521	-1.034102
C	-2.016981	-1.605030	-0.621313
C	-2.912736	-2.657134	-0.407462
C	-2.853186	-3.414981	0.770368
C	-1.882705	-3.091367	1.717209
C	-0.978062	-2.038907	1.488276
H	-2.106116	-1.020487	-1.540037
C	-3.998812	-2.969672	-1.406251
H	-3.552415	-4.232612	0.945080
C	-1.766134	-3.892500	2.989930
H	-0.236858	-1.811741	2.257871
F	3.769743	2.584432	-2.476292
F	5.218289	0.938934	-2.468759

F	4.202574	1.491435	-4.330161
F	2.788464	-3.266574	-4.692724
F	1.545882	-4.120409	-3.097190
F	0.613399	-2.988495	-4.724025
F	4.221983	-1.482018	4.367708
F	3.605278	-2.687444	2.640103
F	5.121359	-1.122611	2.402160
F	1.596026	4.093079	3.121355
F	0.608530	2.988733	4.734738
F	2.790207	3.211034	4.737566
F	-2.700574	4.774186	-3.239519
F	-0.520310	4.707706	-3.011738
F	-1.551078	3.125047	-4.120444
F	-3.653985	2.638681	2.623407
F	-4.220299	4.385854	1.421736
F	-5.138420	2.435641	1.024029
F	-4.122075	-4.318237	-1.625783
F	-5.231387	-2.544232	-0.975575
F	-3.788526	-2.389189	-2.619370
F	-1.654825	-3.094201	4.094447
F	-2.842537	-4.709479	3.201358
F	-0.659394	-4.702089	2.990274

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NaTFPB E(gas)=-3811.52239772 G(gas)=-3811.23723 E($CHCl_3$)=-3811.54853395

B	0.410027	0.160580	0.030594
C	-0.498064	1.432672	-0.508734
C	2.028508	0.414842	-0.012140
C	0.046235	-1.144225	-0.924046
C	-0.164453	-0.162022	1.554899
C	-1.492686	1.287247	-1.489106
C	-2.455605	2.283255	-1.742256
C	-2.403844	3.507868	-1.081304
C	-1.373731	3.708882	-0.148354
C	-0.467745	2.687541	0.150245
H	-1.530391	0.367284	-2.081826
C	-3.590692	1.932859	-2.659941
H	-3.146557	4.283148	-1.272083
C	-1.312992	5.046707	0.561632
H	0.262535	2.857926	0.943735
C	2.914211	-0.659935	0.216967
C	4.306038	-0.500778	0.191962
C	4.873636	0.747409	-0.078025
C	4.018916	1.823031	-0.330938
C	2.626830	1.654894	-0.302963
H	2.511464	-1.661032	0.393625
C	5.182262	-1.698900	0.477660
H	5.955022	0.875918	-0.099931
C	4.586629	3.175854	-0.695602
H	2.001341	2.521102	-0.526835
C	-0.921067	-2.105089	-0.589063
C	-1.357786	-3.086352	-1.501895

C	-0.791819	-3.179070	-2.771261
C	0.223296	-2.269445	-3.108122
C	0.620151	-1.272792	-2.212639
H	-1.336077	-2.112937	0.425317
C	-2.498405	-3.972182	-1.088269
H	-1.121980	-3.938095	-3.481090
C	0.840416	-2.375521	-4.488874
H	1.395193	-0.567581	-2.519650
C	-1.522422	0.064808	1.848258
C	-2.143740	-0.401483	3.014044
C	-1.398597	-1.057235	3.996691
C	-0.026938	-1.221514	3.772497
C	0.570960	-0.798334	2.575082
H	-2.116072	0.664043	1.150033
C	-3.623141	-0.183633	3.154409
H	-1.864311	-1.422316	4.911308
C	0.832805	-1.915836	4.810212
H	1.641076	-0.970497	2.438749
F	1.862898	-1.504789	-4.673088
F	1.321975	-3.630469	-4.723848
F	-0.088296	-2.124089	-5.463175
F	-2.893466	-4.847976	-2.027459
F	-2.278158	-4.646067	0.061348
F	-3.640113	-3.156816	-0.818448
F	6.500212	-1.453943	0.243314
F	5.076813	-2.101233	1.782158
F	4.830909	-2.776736	-0.287372
F	3.918906	4.192754	-0.073747
F	5.901787	3.297199	-0.364110
F	4.492621	3.416852	-2.040936
F	-4.507114	2.903692	-2.811501
F	-3.199914	1.516715	-3.884008
F	-4.299591	0.818337	-2.108856
F	-0.296263	5.118734	1.456082
F	-1.151120	6.071280	-0.325812
F	-2.472767	5.299045	1.242983
F	-4.195987	-0.901982	4.136289
F	-3.969923	1.115092	3.322161
F	-4.279963	-0.577170	1.953362
F	1.250460	-3.140680	4.371540
F	1.951842	-1.195693	5.097794
F	0.167493	-2.117633	5.982138
Na	-3.499411	-0.768256	-0.400163

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Free Ideal Cyclopeptoid E(gas)=-2753.77277239 G(gas)=-2752.951847 E(CHCl3)=-2753.79304473

O	1.202184	-2.511586	1.828075
O	2.793356	-0.195696	-1.455674
N	1.082132	-3.163128	-0.355247
N	3.324378	-0.648912	0.715722
C	1.728614	-2.585531	0.707889

C	3.388519	1.700144	-0.090861
H	3.719213	1.913177	0.931303
H	4.172999	2.008117	-0.798871
C	1.509681	-3.102446	-1.759832
H	2.165369	-2.226492	-1.884867
H	0.607274	-2.873122	-2.349114
C	2.166487	-4.369805	-2.284416
C	3.133256	0.201420	-0.328226
C	3.192155	-2.111133	0.522998
H	3.579435	-2.372577	-0.469072
C	3.783266	-0.293706	2.075099
H	4.772138	0.192574	2.043079
H	3.060740	0.374003	2.563190
C	3.940200	-1.642434	2.799224
H	3.043448	-1.861125	3.402434
O	5.091908	-1.554096	3.642422
C	4.067802	-2.678096	1.657101
H	3.759511	-3.688555	1.954251
H	5.118246	-2.707503	1.326255
O	1.575520	2.295840	1.819841
O	-1.226839	2.508371	-1.460359
N	2.196505	2.516055	-0.363358
N	-1.102917	3.200567	0.709569
C	1.372165	2.785778	0.699137
C	-3.169924	2.082225	-0.097219
H	-3.521451	2.267505	0.923364
H	-3.827428	2.604917	-0.808530
C	1.932324	2.859223	-1.767387
H	0.845983	2.990227	-1.892178
H	2.185304	1.964772	-2.358440
C	2.704369	4.061892	-2.287191
C	-1.742594	2.607534	-0.334090
C	0.230217	3.816984	0.517129
H	0.260550	4.284832	-0.474275
C	-1.642699	3.424359	2.066470
H	-2.555001	4.042473	2.031138
H	-1.865832	2.465707	2.553723
C	-0.551242	4.229136	2.793733
H	0.085069	3.557955	3.394229
O	-1.200682	5.181369	3.639758
C	0.283866	4.857302	1.653025
H	1.313041	5.094703	1.951109
H	-0.215181	5.782771	1.323716
O	-2.778991	0.218718	1.820436
O	-1.562642	-2.320743	-1.452333
N	-3.284719	0.641613	-0.363998
N	-2.225867	-2.553479	0.717557
C	-3.105418	-0.203847	0.701188
C	-0.221788	-3.783921	-0.083836
H	-0.204183	-4.175843	0.938797
H	-0.347716	-4.618034	-0.791173

C	-3.445672	0.235174	-1.766926
H	-3.016103	-0.772079	-1.885712
H	-2.795102	0.897997	-2.359274
C	-4.871469	0.300436	-2.292491
C	-1.390493	-2.812000	-0.323839
C	-3.426354	-1.709050	0.520697
H	-3.844038	-1.918553	-0.471386
C	-2.153127	-3.131071	2.075739
H	-2.235978	-4.229981	2.042136
H	-1.211195	-2.847536	2.563982
C	-3.394369	-2.581453	2.799553
H	-3.129547	-1.690137	3.392607
O	-3.896304	-3.612161	3.654093
C	-4.355876	-2.180559	1.655666
H	-5.077888	-1.408057	1.949488
H	-4.905224	-3.077952	1.329234
C	-5.081836	0.258118	-3.682547
C	-6.373771	0.282679	-4.212454
C	-7.483306	0.359218	-3.360650
C	-7.285386	0.408457	-1.978141
C	-5.988561	0.377881	-1.449116
H	-4.219972	0.204819	-4.353894
H	-6.516456	0.248030	-5.295078
H	-8.493983	0.383604	-3.773877
H	-8.143227	0.473145	-1.304485
H	-5.842671	0.422415	-0.367291
C	2.318435	-4.525184	-3.673796
C	2.948792	-5.653318	-4.203460
C	3.432611	-6.654923	-3.352123
C	3.279700	-6.514609	-1.970151
C	2.652588	-5.379065	-1.441149
H	1.938396	-3.749821	-4.345163
H	3.058691	-5.754985	-5.285697
H	3.921653	-7.539641	-3.765540
H	3.648912	-7.292079	-1.297013
H	2.534089	-5.279445	-0.359482
C	2.794605	4.258317	-3.676696
C	3.463603	5.366522	-4.201194
C	4.065650	6.296636	-3.343943
C	3.990024	6.105721	-1.961478
C	3.312456	4.997013	-1.438156
H	2.332650	3.532534	-4.352163
H	3.520702	5.503054	-5.283657
H	4.592814	7.161231	-3.753035
H	4.460421	6.821861	-1.283401
H	3.262851	4.852527	-0.356071
C	-0.313709	5.787061	4.578131
H	-0.927921	6.424590	5.227577
H	0.199314	5.026628	5.197338
H	0.451003	6.415753	4.084643
C	-4.857251	-3.135061	4.593634

H	-5.104354	-3.979808	5.250017
H	-4.447478	-2.308949	5.205569
H	-5.784397	-2.784648	4.102334
C	5.176437	-2.625346	4.580050
H	6.036626	-2.411547	5.228093
H	4.262695	-2.691039	5.201110
H	5.338673	-3.601591	4.085688

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[Ciclopeptoid·Na]$^+$ E(gas)=-2915.99721926 G(gas)=-2915.176358 E(CHCl3)=-2916.04848691

O	-1.439012	1.601274	1.168080
O	-2.039931	-0.446535	-1.161959
N	-1.465956	3.411963	-0.203010
N	-3.660114	0.402706	0.179747
C	-2.013895	2.255464	0.283029
C	-3.193955	-2.025973	0.282578
H	-3.122038	-1.978661	1.378684
H	-4.208451	-2.363535	0.022535
C	-1.935417	4.128719	-1.402970
H	-2.943109	3.767286	-1.646540
H	-1.285540	3.859787	-2.253512
C	-1.973714	5.638524	-1.235389
C	-2.917885	-0.625470	-0.300910
C	-3.386591	1.778183	-0.276073
H	-3.341398	1.777868	-1.373975
C	-4.673643	0.338915	1.244916
H	-5.603641	-0.136048	0.890396
H	-4.300162	-0.209259	2.121454
C	-4.964228	1.814073	1.575871
H	-4.309223	2.150677	2.403460
O	-6.324771	1.919489	1.959908
C	-4.591681	2.568011	0.275269
H	-4.362486	3.628219	0.442329
H	-5.439109	2.499367	-0.424688
O	-0.682870	-2.102590	1.168346
O	1.363106	-1.591906	-1.187606
N	-2.237810	-3.015110	-0.214813
N	1.464792	-3.412682	0.162255
C	-0.963269	-2.919626	0.276014
C	3.328142	-1.788016	0.233678
H	3.265135	-1.747145	1.330667
H	4.126262	-2.496906	-0.033724
C	-2.614264	-3.750416	-1.439921
H	-1.825482	-4.483275	-1.654085
H	-2.636582	-3.041673	-2.285462
C	-3.947430	-4.469503	-1.331558
C	1.971136	-2.255514	-0.331182
C	0.134873	-3.875284	-0.276053
H	0.106897	-3.860179	-1.374067
C	2.036478	-4.235874	1.240036
H	2.912325	-4.808168	0.891449
H	2.327505	-3.619611	2.102442

C	0.910048	-5.222176	1.598664
H	0.297156	-4.810620	2.424281
O	1.506861	-6.444015	1.999415
C	0.060354	-5.302330	0.305810
H	-0.971234	-5.629189	0.487864
H	0.537770	-6.015841	-0.383817
O	2.147317	0.431211	1.120238
O	0.640339	1.951559	-1.178338
N	3.698036	-0.466954	-0.274057
N	2.212286	2.944943	0.120651
C	2.986687	0.592512	0.219225
C	-0.124807	3.743313	0.277442
H	-0.101292	3.649437	1.372825
H	0.086076	4.792681	0.022030
C	4.548194	-0.434247	-1.477331
H	4.709633	0.615459	-1.756006
H	3.998767	-0.903458	-2.311490
C	5.893252	-1.118361	-1.292955
C	0.940438	2.806668	-0.328523
C	3.257524	2.017119	-0.349035
H	3.218667	1.975318	-1.446352
C	2.684329	3.862474	1.170227
H	2.740102	4.901418	0.804266
H	2.035241	3.827446	2.056538
C	4.108972	3.371408	1.484921
H	4.080813	2.639966	2.316419
O	4.890317	4.495487	1.853040
C	4.553756	2.665016	0.180529
H	5.359104	1.936103	0.336535
H	4.907531	3.430129	-0.528141
Na	-0.001759	-0.028187	0.042952
C	6.422359	-1.894685	-2.335214
C	7.685742	-2.484204	-2.214197
C	8.430279	-2.312518	-1.042964
C	7.905624	-1.548960	0.006388
C	6.646618	-0.954057	-0.119372
H	5.842062	-2.036833	-3.251341
H	8.085230	-3.083954	-3.034523
H	9.413936	-2.775876	-0.945210
H	8.479993	-1.415909	0.925653
H	6.238383	-0.369717	0.709457
C	-1.565047	6.461991	-2.295425
C	-1.649100	7.854737	-2.189327
C	-2.133804	8.440443	-1.015623
C	-2.534457	7.627106	0.050978
C	-2.457314	6.235498	-0.059621
H	-1.180076	6.009808	-3.213800
H	-1.329043	8.482644	-3.023327
H	-2.195156	9.527026	-0.929445
H	-2.909441	8.078871	0.971823
H	-2.761635	5.607010	0.781546

C	-4.889802	-4.344345	-2.363206
C	-6.102034	-5.042181	-2.310391
C	-6.388436	-5.866597	-1.218302
C	-5.457538	-5.991116	-0.179419
C	-4.244474	-5.299692	-0.237803
H	-4.671273	-3.698372	-3.218141
H	-6.824458	-4.937242	-3.122401
H	-7.334528	-6.409544	-1.173901
H	-5.676722	-6.632973	0.676486
H	-3.526269	-5.396033	0.580934
C	0.593890	-7.348715	2.629334
H	1.190476	-8.199842	2.979264
H	0.094942	-6.875293	3.495342
H	-0.174768	-7.717755	1.926505
C	6.153326	4.149874	2.431312
H	6.614544	5.090050	2.757004
H	6.023940	3.487152	3.307110
H	6.822035	3.658767	1.701582
C	-6.654802	3.177445	2.557988
H	-7.696948	3.100158	2.890724
H	-6.010055	3.386498	3.431887
H	-6.571126	4.012154	1.838914

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[Ciclopeptoid·2Na]$^{2+}$ E(gas)=-3078.12039958 G(gas)=-3077.299614 E(CHCl3)=-3078.27655927

O	-1.324209	1.716299	1.135291
O	-2.092440	-0.318737	-1.279750
N	-1.346961	3.446810	-0.331620
N	-3.597008	0.533468	0.190821
C	-1.916256	2.353519	0.237993
C	-3.294817	-1.902288	0.132192
H	-3.340155	-1.898434	1.230207
H	-4.290888	-2.192672	-0.236714
C	-1.913927	4.232469	-1.456889
H	-2.967630	3.950163	-1.572661
H	-1.391666	3.943736	-2.384669
C	-1.805164	5.733107	-1.256301
C	-2.938723	-0.497537	-0.377884
C	-3.324795	1.917473	-0.240593
H	-3.349800	1.948158	-1.338625
C	-4.620930	0.452107	1.250696
H	-5.566219	0.037275	0.864372
H	-4.277444	-0.162417	2.094211
C	-4.856206	1.916042	1.664041
H	-4.175203	2.190774	2.494274
O	-6.201682	2.035332	2.071394
C	-4.482675	2.720889	0.392764
H	-4.209223	3.761285	0.608382
H	-5.349999	2.723298	-0.285197
O	-0.834497	-2.040405	1.150800
O	1.276404	-1.671687	-1.304460
N	-2.337521	-2.911739	-0.310422

N	1.316442	-3.402846	0.163748
C	-1.100071	-2.862611	0.247810
C	3.275236	-1.927467	0.070680
H	3.316469	-1.977291	1.167838
H	4.017800	-2.642735	-0.316158
C	-2.731135	-3.769303	-1.459738
H	-1.985199	-4.567400	-1.559907
H	-2.693539	-3.161724	-2.379698
C	-4.110733	-4.381892	-1.310264
C	1.870150	-2.317494	-0.414742
C	-0.023669	-3.861838	-0.246705
H	-0.052617	-3.901106	-1.344168
C	1.920737	-4.250167	1.210155
H	2.749459	-4.854776	0.807167
H	2.291916	-3.646932	2.050050
C	0.784149	-5.194512	1.640506
H	0.224110	-4.754539	2.489633
O	1.369030	-6.421226	2.019965
C	-0.130719	-5.265928	0.390213
H	-1.164784	-5.541101	0.631996
H	0.278768	-6.020923	-0.298321
O	2.172387	0.268439	1.104525
O	0.761895	1.923751	-1.308750
N	3.663741	-0.591610	-0.372319
N	2.271422	2.818380	0.131977
C	3.009543	0.454131	0.195379
C	0.011297	3.774269	0.091796
H	0.051854	3.823610	1.189012
H	0.253853	4.778463	-0.289235
C	4.628132	-0.506865	-1.496145
H	4.885940	0.548828	-1.647052
H	4.128333	-0.857208	-2.414948
C	5.893630	-1.314026	-1.265569
C	1.042330	2.757012	-0.420793
C	3.328972	1.886926	-0.302643
H	3.352227	1.881063	-1.401159
C	2.730003	3.770664	1.161970
H	2.835901	4.787190	0.749109
H	2.040704	3.801280	2.017005
C	4.123047	3.255183	1.564371
H	4.038376	2.552080	2.416951
O	4.904251	4.373512	1.925548
C	4.613317	2.496320	0.304081
H	5.376012	1.740470	0.528769
H	5.045773	3.227889	-0.395622
Na	0.010639	-0.016514	1.718009
Na	-0.022740	-0.024018	-2.097543
C	6.366635	-2.163971	-2.276711
C	7.563933	-2.869576	-2.109124
C	8.293776	-2.738641	-0.924074
C	7.824606	-1.898761	0.093749

C	6.633350	-1.188582	-0.077450
H	5.801658	-2.268958	-3.207396
H	7.924738	-3.522975	-2.905638
H	9.226624	-3.289582	-0.791778
H	8.392636	-1.793607	1.020146
H	6.274247	-0.538410	0.725290
C	-1.248018	6.530391	-2.267493
C	-1.187384	7.921572	-2.123566
C	-1.675203	8.526397	-0.961637
C	-2.226600	7.737474	0.055986
C	-2.294417	6.349844	-0.092037
H	-0.867594	6.063181	-3.180349
H	-0.758056	8.531646	-2.920439
H	-1.628362	9.610860	-0.847469
H	-2.611142	8.207524	0.963241
H	-2.724925	5.743500	0.709926
C	-5.068288	-4.195476	-2.318751
C	-6.328607	-4.797349	-2.222490
C	-6.644244	-5.585143	-1.111882
C	-5.696345	-5.772127	-0.097541
C	-4.436249	-5.177284	-0.197992
H	-4.824601	-3.585479	-3.193312
H	-7.062418	-4.650995	-3.017267
H	-7.625962	-6.056036	-1.035767
H	-5.938443	-6.391401	0.768352
H	-3.702847	-5.331829	0.598530
C	0.478830	-7.302191	2.723039
H	1.081057	-8.162887	3.035469
H	0.056906	-6.809433	3.617566
H	-0.343199	-7.657008	2.077016
C	6.125094	4.040586	2.605040
H	6.579490	4.991773	2.904777
H	5.924905	3.433370	3.506240
H	6.827984	3.500566	1.946772
C	-6.496211	3.255600	2.769432
H	-7.535564	3.173676	3.107240
H	-5.836976	3.379155	3.647576
H	-6.402388	4.137753	2.112251

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1 E(gas)=-3107.71501253

O	0.902406	-2.647727	1.003655
O	2.723763	-0.508952	-2.276386
N	0.709047	-3.266407	-1.182597
N	3.222414	-1.022651	-0.110482
C	1.417695	-2.769638	-0.118702
C	3.558840	1.301125	-0.920104
H	3.923794	1.470896	0.098324
H	4.367209	1.514637	-1.636199
C	1.142852	-3.256315	-2.586585
H	1.897042	-2.463212	-2.709408
H	0.275369	-2.922560	-3.177685

C	1.645959	-4.592672	-3.109573
C	3.123069	-0.156386	-1.153759
C	2.925671	-2.463155	-0.303509
H	3.280152	-2.765001	-1.296433
C	3.760436	-0.729796	1.233936
H	4.815206	-0.413015	1.176227
H	3.165862	0.052870	1.725281
C	3.707081	-2.083881	1.973283
H	2.755440	-2.167825	2.514394
O	4.829868	-2.196469	2.850551
C	3.734518	-3.121223	0.830544
H	3.327624	-4.094407	1.133773
H	4.777910	-3.259522	0.506792
O	1.846597	2.093579	1.007641
O	-0.925925	2.633967	-2.255175
N	2.470758	2.254235	-1.179215
N	-0.723313	3.305923	-0.084897
C	1.690862	2.611395	-0.109323
C	-2.907052	2.440894	-0.894833
H	-3.234438	2.662718	0.126360
H	-3.497902	3.040198	-1.604395
C	2.237280	2.632065	-2.579878
H	1.172685	2.889419	-2.694873
H	2.378091	1.716903	-3.176456
C	3.140471	3.738405	-3.102207
C	-1.427496	2.794489	-1.129658
C	0.672876	3.767664	-0.279483
H	0.753943	4.234258	-1.268625
C	-1.241359	3.618229	1.262941
H	-2.038934	4.378182	1.212605
H	-1.625982	2.710323	1.748030
C	-0.036801	4.236710	2.004202
H	0.510175	3.446779	2.535535
O	-0.491674	5.259480	2.892941
C	0.846185	4.786058	0.863436
H	1.894129	4.912940	1.164014
H	0.447343	5.763572	0.550302
O	-2.747162	0.542781	1.017586
O	-1.814521	-2.105637	-2.268285
N	-3.188684	1.024305	-1.167101
N	-2.501431	-2.276533	-0.099899
C	-3.113069	0.160155	-0.104819
C	-0.658881	-3.730842	-0.912786
H	-0.687839	-4.127158	0.107652
H	-0.882795	-4.540647	-1.624096
C	-3.395402	0.646806	-2.572086
H	-3.086193	-0.402811	-2.696523
H	-2.671438	1.231919	-3.161028
C	-4.803549	0.881892	-3.095990
C	-1.704330	-2.625092	-1.144836
C	-3.600848	-1.299103	-0.291488

H	-4.039840	-1.454398	-1.284390
C	-2.515313	-2.889242	1.244371
H	-2.768418	-3.961025	1.186715
H	-1.539657	-2.765968	1.734684
C	-3.660590	-2.166168	1.984958
H	-3.257346	-1.299700	2.525387
O	-4.318454	-3.082088	2.863117
C	-4.574103	-1.671906	0.842926
H	-5.214157	-0.833536	1.146390
H	-5.214739	-2.507001	0.519155
C	-5.015503	0.882357	-4.486217
C	-6.296236	1.057126	-5.015352
C	-7.391296	1.244915	-4.162200
C	-7.190672	1.254251	-2.779172
C	-5.905953	1.072604	-2.251071
H	-4.164037	0.742936	-5.158520
H	-6.440643	1.053326	-6.098312
H	-8.392540	1.386648	-4.574799
H	-8.036837	1.404670	-2.104396
H	-5.757315	1.086801	-1.168676
C	1.766737	-4.771473	-4.499238
C	2.259576	-5.966917	-5.027246
C	2.632599	-7.013199	-4.173739
C	2.508526	-6.849286	-2.791434
C	2.019997	-5.646805	-2.264338
H	1.471395	-3.961118	-5.171950
H	2.347416	-6.086051	-6.109729
H	3.013343	-7.950333	-4.585608
H	2.791862	-7.660491	-2.116445
H	1.921551	-5.529149	-1.182520
C	3.237449	3.931684	-4.491764
C	4.023711	4.958742	-5.018878
C	4.738069	5.808370	-4.164432
C	4.655651	5.619663	-2.782153
C	3.861284	4.592736	-2.256027
H	2.687439	3.267995	-5.165155
H	4.084980	5.093636	-6.101340
H	5.357123	6.608751	-4.575488
H	5.212375	6.273360	-2.106374
H	3.806596	4.449447	-1.174183
C	0.019035	5.248124	4.262961
C	-0.601248	6.506317	4.879573
C	-0.466978	3.992409	5.005905
C	1.553591	5.343040	4.280948
C	-4.575477	-2.646009	4.234835
C	-5.355513	-3.820011	4.835957
C	-3.251285	-2.441578	4.989978
C	-5.429700	-1.367722	4.257136
C	4.582736	-2.645695	4.219807
C	5.989640	-2.728683	4.821313
C	3.736362	-1.610571	4.979731

C 3.911407 -4.028955 4.234314
H 3.805395 -4.390679 5.268656
H 2.904981 -3.998553 3.789976
H 4.519926 -4.756389 3.676342
H 3.619060 -1.908867 6.032926
H 4.224787 -0.625335 4.950799
H 2.727961 -1.511566 4.550642
H 5.943336 -3.049517 5.872631
H 6.603183 -3.448814 4.260715
H 6.482347 -1.746618 4.775748
H 1.919109 5.417547 5.316686
H 2.021877 4.456069 3.828125
H 1.888852 6.236093 3.732574
H -0.300440 6.610400 5.932682
H -0.274894 7.401594 4.330698
H -1.698609 6.453321 4.831938
H -0.148969 4.022608 6.059425
H -1.565113 3.934275 4.976872
H -0.058136 3.071334 4.563944
H -5.683854 -1.096428 5.293334
H -4.896469 -0.513634 3.812991
H -6.367051 -1.523800 3.702460
H -3.445391 -2.192595 6.044602
H -2.648504 -3.361199 4.956484
H -2.657062 -1.620640 4.561141
H -5.604556 -3.621062 5.888932
H -6.289290 -3.983490 4.278633
H -4.757253 -4.741303 4.785145
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3 E(Gas)=-3669.37561419
O 2.089462 -1.730264 0.321415
O 2.635443 1.013936 -2.922374
N 2.307311 -2.421999 -1.842347
N 3.300386 0.802190 -0.753142
C 2.628976 -1.606773 -0.787575
C 2.375489 2.972174 -1.539327
H 2.578976 3.292503 -0.511690
H 2.966061 3.587967 -2.234852
C 2.684840 -2.199236 -3.244878
H 2.920590 -1.131117 -3.372764
H 1.774601 -2.367069 -3.842208
C 3.811983 -3.085552 -3.752373
C 2.770597 1.506407 -1.790184
C 3.776679 -0.582215 -0.959958
H 4.243838 -0.651695 -1.949291
C 3.516147 1.276614 0.630323
H 4.174622 2.159851 0.642420
H 2.557882 1.530172 1.103836
C 4.236935 0.105395 1.323114
H 3.555237 -0.483419 1.946583
O 5.279819 0.674963 2.167690

C	4.800795	-0.754356	0.178960
H	4.944539	-1.797998	0.481232
H	5.768612	-0.338135	-0.141980
O	0.457857	2.681174	0.338785
O	-2.174177	1.789649	-2.926503
N	0.955582	3.223982	-1.820617
N	-2.335819	2.456008	-0.753170
C	0.084145	3.088459	-0.770524
C	-3.755283	0.583061	-1.561831
H	-4.141017	0.596216	-0.536656
H	-4.578093	0.794097	-2.261908
C	0.580658	3.446668	-3.224154
H	-0.462353	3.119388	-3.358196
H	1.182236	2.744193	-3.822605
C	0.789905	4.868048	-3.723736
C	-2.676902	1.654391	-1.798853
C	-1.378213	3.565576	-0.946992
H	-1.548425	4.010693	-1.934275
C	-2.866566	2.397468	0.625302
H	-3.960609	2.528212	0.628681
H	-2.613460	1.437162	1.094794
C	-2.217637	3.602046	1.331382
H	-1.367945	3.302136	1.954492
O	-3.237163	4.207701	2.178690
C	-1.751991	4.530098	0.196384
H	-0.925071	5.178204	0.508305
H	-2.596926	5.158600	-0.126268
O	-2.557877	-0.942783	0.315283
O	-0.449607	-2.756757	-2.941275
N	-3.267453	-0.773368	-1.846297
N	-0.962213	-3.244074	-0.775062
C	-2.720383	-1.465585	-0.796768
C	1.376788	-3.524856	-1.566561
H	1.553021	-3.867326	-0.541095
H	1.611271	-4.341110	-2.266971
C	-3.271002	-1.203962	-3.251439
H	-2.466603	-1.943857	-3.386900
H	-2.961168	-0.329756	-3.845823
C	-4.606103	-1.729958	-3.755273
C	-0.089182	-3.129086	-1.812511
C	-2.400832	-2.969918	-0.978423
H	-2.694161	-3.335473	-1.969556
C	-0.655864	-3.679182	0.603983
H	-0.223018	-4.692521	0.607007
H	0.045849	-2.981418	1.081037
C	-2.028685	-3.721063	1.299677
H	-2.199735	-2.835746	1.921953
O	-2.048337	-4.907936	2.145293
C	-3.056583	-3.780988	0.156864
H	-4.033836	-3.390599	0.462952
H	-3.175063	-4.826198	-0.169556

C	-4.813388	-1.829887	-5.142500
C	-6.007976	-2.343726	-5.652311
C	-7.024137	-2.759187	-4.782251
C	-6.831862	-2.655753	-3.401851
C	-5.630438	-2.145763	-2.893157
H	-4.026829	-1.501206	-5.827881
H	-6.150136	-2.414707	-6.733218
H	-7.960480	-3.156654	-5.179794
H	-7.619606	-2.971803	-2.713870
H	-5.491333	-2.062863	-1.812619
C	4.016363	-3.190940	-5.139688
C	5.060077	-3.964563	-5.652502
C	5.915529	-4.656693	-4.785610
C	5.716264	-4.565057	-3.405446
C	4.672264	-3.783707	-2.893526
H	3.348383	-2.658246	-5.822703
H	5.203784	-4.033103	-6.733359
H	6.729159	-5.265668	-5.185500
H	6.374635	-5.104081	-2.720053
H	4.520807	-3.721679	-1.813226
C	0.797087	5.103446	-5.109983
C	0.949342	6.396656	-5.615388
C	1.107390	7.480242	-4.741905
C	1.110016	7.256196	-3.362412
C	0.950960	5.959016	-2.858083
H	0.680766	4.261257	-5.798188
H	0.951287	6.559792	-6.695661
H	1.231424	8.491180	-5.136097
H	1.237352	8.093197	-2.671782
H	0.960669	5.792176	-1.778337
C	-2.785479	5.085657	3.126405
C	-3.893292	5.602239	3.986143
O	-1.612557	5.401090	3.245742
C	-3.046627	-4.962916	3.079942
C	-2.941892	-6.180088	3.940659
O	-3.914596	-4.111720	3.187261
C	5.817266	-0.165735	3.104439
C	6.836365	0.520038	3.955507
O	5.494275	-1.336899	3.221176
C	-3.561159	6.522204	4.995870
C	-4.553973	7.033990	5.832360
C	-5.885580	6.632440	5.667162
C	-6.221301	5.716634	4.662729
C	-5.230988	5.201076	3.823166
H	-2.516998	6.819476	5.108088
H	-4.290467	7.747353	6.616134
H	-6.662454	7.032785	6.322504
H	-7.259232	5.401999	4.534512
H	-5.486576	4.486001	3.041086
C	7.476998	-0.242022	4.947906
C	8.437285	0.345576	5.772484

C	8.765512	1.697809	5.612940
C	8.129587	2.461067	4.626343
C	7.167725	1.877392	3.798317
H	7.204681	-1.293438	5.055499
H	8.931682	-0.250723	6.542293
H	9.516968	2.157681	6.258769
H	8.383773	3.515991	4.502845
H	6.668528	2.467156	3.029320
C	-3.930232	-6.374136	4.921430
C	-3.880041	-7.491614	5.755727
C	-2.843290	-8.423320	5.618217
C	-1.856072	-8.233670	4.643684
C	-1.902389	-7.117127	3.805571
H	-4.727191	-5.634064	5.012847
H	-4.650010	-7.637621	6.516279
H	-2.803770	-9.297490	6.272079
H	-1.046100	-8.958534	4.537645
H	-1.135212	-6.963227	3.046581

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[1-K]$^{+}$ E(gas)=-3707.60773977

O	-2.573748	0.458572	1.034788
O	-1.367293	-1.487931	-1.467343
N	-3.215127	1.674392	-0.776307
N	-3.138480	-1.986926	-0.147401
C	-3.151932	0.505288	-0.068407
C	-1.201657	-3.551181	-0.188522
H	-1.145644	-3.569631	0.908751
H	-1.770264	-4.435063	-0.516567
C	-3.756998	1.835403	-2.141419
H	-4.281129	0.912711	-2.416965
H	-2.911699	1.949175	-2.839196
C	-4.709187	3.012828	-2.269169
C	-1.909030	-2.258979	-0.661717
C	-3.856283	-0.771442	-0.601841
H	-3.868111	-0.776014	-1.698261
C	-3.883493	-2.754163	0.861259
H	-4.330948	-3.666705	0.431722
H	-3.239490	-3.034017	1.707367
C	-5.017281	-1.794940	1.288360
H	-4.648747	-1.142724	2.095583
O	-6.161138	-2.532829	1.685398
C	-5.260206	-0.954644	0.013460
H	-5.761094	-0.001713	0.228184
H	-5.900670	-1.534880	-0.667882
O	0.920805	-2.476399	1.068898
O	1.952769	-0.482654	-1.472869
N	0.158090	-3.646511	-0.728427
N	3.302704	-1.750135	-0.168641
C	1.150019	-3.005642	-0.035945
C	3.695763	0.706791	-0.262133
H	3.720578	0.779525	0.833841

H	4.733872	0.649440	-0.624137
C	0.270902	-4.164053	-2.110337
H	1.334966	-4.240443	-2.363480
H	-0.179392	-3.426694	-2.794369
C	-0.381030	-5.522444	-2.296344
C	2.913474	-0.556968	-0.692484
C	2.599924	-2.987652	-0.588827
H	2.597167	-3.017905	-1.684730
C	4.379578	-1.999813	0.800895
H	5.374170	-1.957253	0.324702
H	4.348544	-1.278392	1.629930
C	4.114357	-3.447710	1.275128
H	3.389753	-3.426561	2.104039
O	5.319672	-4.099884	1.637965
C	3.464521	-4.103869	0.037305
H	2.885804	-4.999839	0.297485
H	4.264895	-4.401413	-0.657020
O	1.723194	2.010668	1.021293
O	-0.581239	1.901062	-1.509941
N	3.084645	1.925372	-0.800478
N	-0.126787	3.689858	-0.195151
C	2.045486	2.467092	-0.093084
C	-2.455151	2.813411	-0.254291
H	-2.509036	2.802452	0.843022
H	-2.930773	3.740723	-0.609492
C	3.452707	2.272333	-2.191679
H	2.966506	3.220182	-2.450462
H	3.043828	1.498644	-2.861532
C	4.951450	2.409793	-2.392797
C	-0.978000	2.763676	-0.713258
C	1.287306	3.705363	-0.642023
H	1.294248	3.709311	-1.738215
C	-0.427404	4.724642	0.805534
H	-0.996415	5.562137	0.366965
H	-0.994257	4.311264	1.652204
C	0.965046	5.238463	1.234204
H	1.345881	4.605176	2.050648
O	0.883380	6.601891	1.615121
C	1.822097	5.020917	-0.034127
H	2.896984	4.984162	0.186211
H	1.639365	5.858718	-0.723946
K	0.020009	-0.004926	0.574652
C	5.599844	1.659996	-3.385152
C	6.974658	1.807508	-3.606397
C	7.716444	2.703418	-2.830924
C	7.078519	3.453253	-1.834550
C	5.705513	3.309193	-1.620115
H	5.022531	0.958868	-3.994347
H	7.465423	1.220106	-4.385185
H	8.788544	2.819461	-3.001556
H	7.652748	4.157597	-1.228905

H	5.213862	3.897466	-0.840532
C	-4.530088	3.952357	-3.295489
C	-5.426800	5.016195	-3.452904
C	-6.508406	5.155675	-2.578286
C	-6.692150	4.225859	-1.547192
C	-5.800310	3.160967	-1.396740
H	-3.684196	3.847263	-3.980762
H	-5.276665	5.737986	-4.258428
H	-7.207169	5.985936	-2.698137
H	-7.537172	4.328661	-0.863090
H	-5.949789	2.440884	-0.587922
C	-1.316512	-5.713623	-3.324043
C	-1.892141	-6.971402	-3.540139
C	-1.543247	-8.050605	-2.722961
C	-0.614116	-7.868269	-1.690762
C	-0.034557	-6.614086	-1.482274
H	-1.592274	-4.871348	-3.964708
H	-2.615137	-7.106179	-4.347315
H	-1.991850	-9.032050	-2.888810
H	-0.335171	-8.709079	-1.052082
H	0.690118	-6.479550	-0.674833
C	5.460064	-4.596860	3.015622
C	6.859545	-5.217441	3.019309
C	5.381831	-3.434276	4.016516
C	4.396518	-5.664699	3.312141
C	1.501144	7.010098	2.886807
C	1.265579	8.522450	2.916697
C	0.789360	6.329814	4.066206
C	3.004425	6.696473	2.884824
C	-6.804023	-2.185844	2.962257
C	-8.008665	-3.129309	3.012226
C	-5.849790	-2.468333	4.132620
C	-7.266600	-0.721139	2.957956
H	-7.814090	-0.493431	3.884723
H	-6.418216	-0.021446	2.900777
H	-7.939752	-0.532233	2.108595
H	-6.359596	-2.290256	5.091216
H	-5.517052	-3.516528	4.110404
H	-4.962058	-1.817013	4.111109
H	-8.581013	-2.972853	3.937969
H	-8.672886	-2.948532	2.155173
H	-7.677272	-4.176944	2.979085
H	4.553754	-6.091037	4.314147
H	3.377327	-5.248732	3.291704
H	4.458965	-6.481708	2.578362
H	7.093987	-5.631849	4.010550
H	6.922246	-6.027483	2.278719
H	7.616711	-4.460669	2.769152
H	5.575004	-3.796391	5.037354
H	6.135025	-2.669108	3.776816
H	4.387216	-2.961882	4.022272

H 3.472796 7.075396 3.805470
H 3.196981 5.613134 2.843145
H 3.497779 7.177587 2.027356
H 1.194796 6.698583 5.020238
H -0.287734 6.551186 4.042713
H 0.924979 5.237012 4.056453
H 1.674574 8.957978 3.839915
H 1.752397 9.004763 2.057096
H 0.189629 8.744114 2.873742
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[3-K]$^{+}$ E(gas)=-4269.26675816
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O 0.121813 -1.993321 1.683113
N 3.612297 -0.655760 0.970351
N 1.260367 -3.488676 0.420517
C 2.815620 -1.543391 0.300304
C -1.233466 -3.549501 0.396410
H -1.274611 -3.520569 -0.701633
H -1.321096 -4.599809 0.713707
C 4.143347 -0.851024 2.337463
H 4.085758 -1.919736 2.577644
H 3.490886 -0.316587 3.047388
C 5.581156 -0.387746 2.491047
C 0.103185 -2.947262 0.893670
C 2.556647 -2.955650 0.897624
H 2.520134 -2.904810 1.992380
C 1.405385 -4.568518 -0.569497
H 1.143860 -5.549914 -0.138287
H 0.779751 -4.389201 -1.455451
C 2.905111 -4.530922 -0.906222
H 3.107595 -3.850955 -1.745429
O 3.320058 -5.864368 -1.265168
C 3.567764 -4.000700 0.377589
H 4.563632 -3.586139 0.182362
H 3.663566 -4.823570 1.102787
O -2.233214 -1.365765 -0.825484
O -1.788277 0.888910 1.673790
N -2.377098 -2.805935 0.931023
N -3.648735 0.653957 0.404431
C -2.741245 -1.664220 0.270707
C -2.454996 2.844447 0.392274
H -2.404316 2.870157 -0.705468
H -3.322034 3.444626 0.707845
C -2.824702 -3.181934 2.290349
H -3.723952 -2.600352 2.527623
H -2.042748 -2.891717 3.011230
C -3.143897 -4.660330 2.424355
C -2.603254 1.384164 0.883726
C -3.834925 -0.737533 0.873799
H -3.769716 -0.737454 1.968432
C -4.653294 1.072977 -0.586665

H	-5.367395	1.795998	-0.157009
H	-4.181198	1.520171	-1.473136
C	-5.380348	-0.239864	-0.922514
H	-4.904490	-0.753993	-1.769114
O	-6.744903	0.075798	-1.265361
C	-5.247288	-1.086018	0.356033
H	-5.388484	-2.154530	0.155405
H	-6.004863	-0.760754	1.085715
O	-0.059928	2.624596	-0.821928
O	1.656362	1.111207	1.697175
N	-1.241374	3.460839	0.934321
N	2.392275	2.832799	0.423594
C	-0.068210	3.208576	0.277152
C	3.693300	0.704750	0.432250
H	3.705846	0.650819	-0.665466
H	4.642330	1.154121	0.762488
C	-1.348504	4.031672	2.295442
H	-0.398105	4.523915	2.535529
H	-1.485491	3.206558	3.013532
C	-2.474975	5.040860	2.430264
C	2.498068	1.564449	0.910022
C	1.279114	3.693497	0.883684
H	1.242893	3.644680	1.978542
C	3.259570	3.485799	-0.570445
H	4.242231	3.745233	-0.141040
H	3.411372	2.846924	-1.452159
C	2.487325	4.769514	-0.917454
H	1.805162	4.607625	-1.763618
O	3.444555	5.789235	-1.268652
C	1.685508	5.087285	0.357363
H	0.831261	5.742457	0.150199
H	2.344383	5.585688	1.085155
K	0.007240	0.000400	-0.414081
C	-3.430928	4.891611	3.445979
C	-4.450368	5.837271	3.609921
C	-4.527759	6.938299	2.752016
C	-3.580330	7.092940	1.731844
C	-2.558833	6.152647	1.574685
H	-3.372823	4.031306	4.118705
H	-5.184777	5.711417	4.408195
H	-5.322475	7.676411	2.877205
H	-3.633662	7.953554	1.061787
H	-1.824172	6.280258	0.775153
C	5.923444	0.498339	3.523244
C	7.252643	0.897048	3.709069
C	8.252206	0.418750	2.856747
C	7.918717	-0.461276	1.819228
C	6.592924	-0.864530	1.640083
H	5.143864	0.873998	4.191929
H	7.505603	1.582734	4.520416
H	9.289318	0.728755	2.999347

H	8.696029	-0.840397	1.152483
H	6.341318	-1.550519	0.826843
C	-2.545583	-5.416367	3.443228
C	-2.865208	-6.769566	3.608104
C	-3.781679	-7.381705	2.748056
C	-4.379839	-6.635970	1.724227
C	-4.065689	-5.283711	1.565916
H	-1.828518	-4.940092	4.117774
H	-2.395983	-7.344920	4.408875
H	-4.031915	-8.436928	2.874318
H	-5.099322	-7.108373	1.052173
H	-4.536205	-4.709219	0.763480
C	-7.437212	-0.930959	-1.911874
C	-8.821099	-0.523020	-2.269941
O	-6.937204	-2.019085	-2.143424
C	2.919341	6.889686	-1.919795
C	3.966760	7.873778	-2.299495
O	1.725508	7.005757	-2.141202
C	4.541673	-5.946678	-1.906791
C	4.881104	-7.340005	-2.298067
O	5.235491	-4.964754	-2.112199
C	-9.622039	-1.459548	-2.948897
C	-10.928845	-1.130572	-3.308987
C	-11.446098	0.132174	-2.993095
C	-10.652973	1.067144	-2.316588
C	-9.343566	0.744941	-1.954900
H	-9.200780	-2.437909	-3.185955
H	-11.547206	-1.858929	-3.837128
H	-12.469549	0.388461	-3.275054
H	-11.057733	2.051033	-2.071237
H	-8.723169	1.470394	-1.428557
C	6.102955	-7.550765	-2.963185
C	6.471547	-8.837200	-3.356479
C	5.626065	-9.921350	-3.088543
C	4.409377	-9.716537	-2.426261
C	4.033951	-8.431299	-2.030797
H	6.747270	-6.693101	-3.163403
H	7.419571	-8.997217	-3.873630
H	5.915654	-10.928102	-3.397129
H	3.751323	-10.562679	-2.218741
H	3.087225	-8.268016	-1.515768
C	3.553027	9.041439	-2.966592
C	4.493379	9.998123	-3.348692
C	5.850980	9.797769	-3.067996
C	6.267394	8.637275	-2.404121
C	5.331390	7.675468	-2.019434
H	2.491121	9.178316	-3.177450
H	4.169288	10.902561	-3.867114
H	6.586322	10.547430	-3.367861
H	7.326090	8.482409	-2.186765
H	5.651857	6.770432	-1.503308

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[1-K-1]$^{+}$ E(gas)=-6815.32879160

O	3.005064	-1.561570	-1.211593
O	5.037321	-1.393063	1.754027
N	5.007475	-1.364970	-2.281794
N	3.965234	-3.156678	0.799821
C	4.191946	-1.914546	-1.328083
C	3.286603	-2.447168	3.069200
H	2.235826	-2.554910	2.769681
H	3.582939	-3.352568	3.620534
C	6.468503	-1.595561	-2.362574
H	6.688449	-2.556047	-1.880340
H	6.979496	-0.802800	-1.793263
C	6.987338	-1.639749	-3.787999
C	4.177424	-2.273947	1.821255
C	4.767980	-3.035221	-0.420228
H	5.789803	-2.768061	-0.122173
C	3.035318	-4.292315	0.777794
H	3.263140	-5.015382	1.577996
H	1.989453	-3.961071	0.877045
C	3.284365	-4.976858	-0.589979
H	2.508552	-4.657003	-1.304754
O	3.262952	-6.389552	-0.405791
C	4.668994	-4.444768	-1.037012
H	4.791854	-4.450595	-2.128045
H	5.440264	-5.095811	-0.598333
O	1.779016	-0.241545	2.748592
O	4.271674	2.257410	2.328694
N	3.403464	-1.293935	3.958708
N	2.419754	2.273425	3.647715
C	2.659310	-0.190017	3.624952
C	2.595639	3.943875	1.832363
H	1.547884	3.751585	1.568302
H	2.629051	4.856396	2.447021
C	4.615014	-1.226016	4.819050
H	4.455261	-0.439931	5.566982
H	5.470394	-0.939379	4.187020
C	4.911373	-2.523943	5.543413
C	3.178583	2.748833	2.616382
C	2.908653	1.123736	4.413261
H	3.988267	1.253963	4.559836
C	1.149203	2.812335	4.146491
H	1.265701	3.847000	4.509237
H	0.365689	2.787633	3.373054
C	0.776094	1.906103	5.344539
H	0.036844	1.157778	5.017116
O	0.256936	2.722850	6.390464
C	2.108473	1.214283	5.729167
H	1.952475	0.238236	6.207241
H	2.635888	1.868463	6.439919
O	2.152315	2.534143	-0.413860

O	5.434408	1.098606	-1.143303
N	3.359284	4.177651	0.608554
N	3.926286	2.169840	-2.470263
C	3.113294	3.321854	-0.433389
C	4.491620	-0.185086	-2.973501
H	3.431828	-0.349187	-3.207121
H	5.041785	-0.064049	-3.919653
C	4.597600	4.973916	0.753455
H	5.019756	5.137942	-0.245999
H	5.326996	4.383314	1.331713
C	4.374475	6.322446	1.413897
C	4.663237	1.078819	-2.103797
C	4.032346	3.402638	-1.682981
H	5.076965	3.506502	-1.364669
C	3.045617	2.303279	-3.636976
H	3.593383	2.140684	-4.579537
H	2.196175	1.603560	-3.587306
C	2.560327	3.774591	-3.595457
H	1.561604	3.812343	-3.131672
O	2.534539	4.295195	-4.921511
C	3.592944	4.485766	-2.688032
H	3.186116	5.384287	-2.205927
H	4.449040	4.783411	-3.312414
K	0.977675	-0.020795	0.034302
C	5.171751	6.702460	2.503854
C	5.021350	7.962633	3.094393
C	4.063638	8.855381	2.604210
C	3.257590	8.482522	1.521291
C	3.414171	7.226450	0.929162
H	5.919030	6.004668	2.891441
H	5.651581	8.244547	3.940571
H	3.943578	9.838629	3.063737
H	2.508296	9.176277	1.133772
H	2.777778	6.939059	0.087810
C	8.010699	-0.768180	-4.189871
C	8.534622	-0.831766	-5.486821
C	8.034863	-1.765786	-6.399006
C	7.009159	-2.636788	-6.009198
C	6.491796	-2.574775	-4.712730
H	8.403105	-0.037340	-3.477581
H	9.334702	-0.150096	-5.783178
H	8.443481	-1.818497	-7.410227
H	6.620308	-3.373500	-6.715760
H	5.692766	-3.258672	-4.413560
C	6.023595	-3.298662	5.179712
C	6.321681	-4.483902	5.862639
C	5.509434	-4.906853	6.919232
C	4.399783	-4.138414	7.293538
C	4.104967	-2.955477	6.610443
H	6.662362	-2.964252	4.357810
H	7.193081	-5.074324	5.571611

H	5.743273	-5.828362	7.456310
H	3.772158	-4.457615	8.128577
H	3.245667	-2.351111	6.914449
C	-0.873604	2.224329	7.183479
C	-0.983587	3.250703	8.315373
C	-2.150365	2.227133	6.329577
C	-0.588613	0.827891	7.756654
C	1.395201	5.120538	-5.331357
C	1.792430	5.595818	-6.732189
C	0.121103	4.263506	-5.399467
C	1.209034	6.321152	-4.390687
C	2.636056	-7.227902	-1.432140
C	2.957806	-8.650962	-0.966345
C	1.116585	-6.998857	-1.439180
C	3.243821	-6.967092	-2.818999
O	-3.103079	-1.722631	-2.360868
O	-0.688494	-2.292381	0.272678
N	-1.136051	-1.421447	-3.448017
N	-2.110667	-3.749468	-0.747582
C	-1.969911	-2.137544	-2.618440
C	-2.239023	-3.485237	1.704174
H	-3.087839	-4.169074	1.591559
H	-1.453335	-3.996195	2.281956
C	0.222224	-1.771120	-3.862774
H	0.552006	-2.647512	-3.289637
H	0.903071	-0.953169	-3.571807
C	0.369896	-2.047490	-5.355320
C	-1.631936	-3.104779	0.344069
C	-1.507857	-3.508027	-2.070704
H	-0.416658	-3.554191	-1.963389
C	-3.302752	-4.621224	-0.818946
H	-3.119844	-5.587877	-0.321898
H	-4.161692	-4.114234	-0.358415
C	-3.493015	-4.882470	-2.335063
H	-4.186393	-4.134261	-2.747258
O	-3.926128	-6.209819	-2.612986
C	-2.083885	-4.660055	-2.916390
H	-2.099377	-4.443731	-3.992681
H	-1.494395	-5.576078	-2.758159
O	-4.608852	-2.324555	1.295141
O	-2.578588	1.204192	2.652613
N	-2.670718	-2.319714	2.481763
N	-4.735794	0.531543	2.342299
C	-3.925361	-1.836814	2.206921
C	-4.044118	2.773041	1.545361
H	-5.073834	2.824615	1.178511
H	-3.893101	3.559819	2.301017
C	-1.710826	-1.779449	3.452730
H	-1.994476	-0.739403	3.667204
H	-0.733579	-1.710376	2.950495
C	-1.581838	-2.615422	4.718049

C	-3.724651	1.426396	2.215699
C	-4.532165	-0.727358	3.101254
H	-3.897743	-0.510513	3.968869
C	-6.139554	0.716328	1.916952
H	-6.603455	1.563230	2.448552
H	-6.195804	0.883889	0.832509
C	-6.855603	-0.577780	2.361962
H	-6.849688	-1.302636	1.536792
O	-8.179513	-0.262828	2.785871
C	-5.967930	-1.105084	3.512022
H	-6.093482	-2.182776	3.677121
H	-6.241834	-0.571563	4.435416
O	-4.653925	2.060719	-0.971288
O	-0.913354	0.937400	-1.894797
N	-3.143234	3.049925	0.418562
N	-2.667822	1.887045	-3.002309
C	-3.575663	2.651313	-0.821867
C	-1.683451	-0.157868	-3.931406
H	-2.689767	-0.330860	-4.333368
H	-1.047098	0.202113	-4.754990
C	-1.839654	3.648783	0.767225
H	-1.158966	3.541427	-0.085489
H	-1.425281	3.038549	1.584222
C	-1.944709	5.100838	1.205481
C	-1.729302	0.922517	-2.832489
C	-2.758121	3.033738	-2.076468
H	-1.740025	3.358393	-1.834962
C	-3.685018	1.939848	-4.069946
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H	-4.333351	1.051951	-4.035800
C	-4.481997	3.239013	-3.794551
H	-5.387770	2.988666	-3.226396
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C	-3.532018	4.074569	-2.910999
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H	-2.836563	4.617904	-3.569179
C	-1.724011	5.456068	2.545238
C	-1.826062	6.789418	2.960784
C	-2.150413	7.786347	2.036674
C	-2.370426	7.444754	0.695994
C	-2.269320	6.113002	0.286449
H	-1.472600	4.678616	3.271999
H	-1.653618	7.047435	4.008028
H	-2.232970	8.826753	2.357739
H	-2.621415	8.220650	-0.030833
H	-2.444114	5.857336	-0.761999
C	1.607418	-1.820387	-5.978819
C	1.788308	-2.105373	-7.335516
C	0.727004	-2.612956	-8.093389
C	-0.512494	-2.832864	-7.484246
C	-0.688609	-2.552351	-6.124727

H	2.440152	-1.416770	-5.395298
H	2.756851	-1.920358	-7.805057
H	0.864134	-2.829590	-9.154667
H	-1.348268	-3.222379	-8.069822
H	-1.663796	-2.714751	-5.659772
C	-0.326125	-2.766212	5.328024
C	-0.187975	-3.498396	6.512423
C	-1.305461	-4.096465	7.103707
C	-2.560139	-3.960291	6.499500
C	-2.695118	-3.227501	5.316041
H	0.553350	-2.309149	4.864870
H	0.798743	-3.615975	6.965556
H	-1.198511	-4.674702	8.023796
H	-3.437334	-4.430527	6.949644
H	-3.676489	-3.144901	4.842830
C	-9.275721	-1.106851	2.300479
C	-10.503335	-0.530637	3.012683
C	-9.424966	-0.966012	0.777180
C	-9.058491	-2.573723	2.705022
C	-6.202968	4.149635	-5.330760
C	-6.140542	4.886477	-6.671978
C	-6.947405	2.813701	-5.484469
C	-6.861567	5.035311	-4.261801
C	-5.324684	-6.411994	-3.010416
C	-5.445622	-7.936237	-3.097041
C	-6.285994	-5.853423	-1.950128
C	-5.583106	-5.774555	-4.385553
H	-0.163696	3.873738	-4.409634
H	0.272520	3.411911	-6.078893
H	-0.724315	4.858577	-5.776216
H	0.409011	6.976831	-4.766397
H	0.925818	6.007081	-3.373929
H	2.134702	6.912427	-4.331581
H	0.996626	6.216515	-7.169176
H	2.716313	6.189899	-6.688012
H	1.966595	4.734015	-7.392265
H	-7.153178	5.120690	-7.031393
H	-5.581440	5.827465	-6.566301
H	-5.636370	4.266906	-7.427587
H	-7.899436	5.267186	-4.545178
H	-6.893505	4.539000	-3.279917
H	-6.313529	5.983827	-4.159399
H	-7.988335	2.989302	-5.795275
H	-6.462178	2.189564	-6.249717
H	-6.978636	2.249267	-4.539720
H	-6.458567	-8.226509	-3.412643
H	-4.724583	-8.336433	-3.824390
H	-5.239602	-8.393131	-2.118286
H	-6.606877	-5.995197	-4.723830
H	-5.477856	-4.679003	-4.357250
H	-4.879989	-6.175739	-5.130593

H	-7.327631	-6.076903	-2.226628
H	-6.088612	-6.311172	-0.969171
H	-6.199190	-4.760560	-1.852696
H	2.510316	-9.390674	-1.646172
H	4.045321	-8.809570	-0.942320
H	2.561814	-8.821049	0.044992
H	0.627358	-7.677132	-2.154222
H	0.698066	-7.187734	-0.440035
H	0.860943	-5.969241	-1.734732
H	2.818787	-7.665461	-3.555424
H	3.031569	-5.947104	-3.174939
H	4.333714	-7.114363	-2.798427
H	-11.410917	-1.081994	2.725904
H	-10.381234	-0.599807	4.103165
H	-10.638580	0.527579	2.746454
H	-9.923167	-3.184927	2.404517
H	-8.167364	-3.003023	2.221872
H	-8.942532	-2.657955	3.795990
H	-10.298133	-1.536360	0.425434
H	-9.570272	0.089686	0.504312
H	-8.543803	-1.348082	0.239524
H	-1.832427	3.010094	8.972120
H	-0.064356	3.258230	8.918546
H	-1.135298	4.259275	7.904548
H	-1.404899	0.524163	8.429043
H	-0.516899	0.061874	6.969684
H	0.345926	0.830944	8.337213
H	-3.007683	1.871525	6.921657
H	-2.371919	3.247228	5.982896
H	-2.061291	1.577614	5.445674

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[3-K-3]$^{+}$ E(gas)=-7938.66746135

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N	3.965989	-3.361359	-1.345428
C	4.239297	-1.180147	-2.491795
C	4.103198	-3.938060	1.053786
H	3.011700	-4.025232	0.997026
H	4.532997	-4.952482	1.091373
C	6.615591	-0.634325	-3.213634
H	6.783783	-1.701544	-3.030520
H	7.173615	-0.091245	-2.436215
C	7.128581	-0.256890	-4.593009
C	4.662628	-3.211009	-0.180658
C	4.480250	-2.706477	-2.557212
H	5.544331	-2.945681	-2.653085
C	2.690904	-4.066447	-1.553160
H	2.813026	-5.158457	-1.454220
H	1.915487	-3.716732	-0.856149
C	2.313711	-3.706753	-2.997234

H	1.617235	-2.860834	-3.007333
O	1.676553	-4.864117	-3.600612
C	3.639911	-3.344489	-3.684785
H	3.493415	-2.682856	-4.547628
H	4.128261	-4.268527	-4.030374
O	2.667279	-1.870701	1.969641
O	5.563990	0.170645	2.928111
N	4.449133	-3.255243	2.300484
N	3.578894	-0.124712	3.982738
C	3.630843	-2.224125	2.673242
C	4.243726	2.168453	3.328172
H	3.166994	2.374040	3.334678
H	4.695770	2.638747	4.217083
C	5.794934	-3.554975	2.835604
H	5.999758	-2.883724	3.676921
H	6.519547	-3.295358	2.048835
C	5.967367	-5.002726	3.260259
C	4.521629	0.656057	3.377140
C	3.820914	-1.572384	4.062223
H	4.830795	-1.734215	4.452803
C	2.278383	0.287530	4.533305
H	2.400773	0.906711	5.438014
H	1.680376	0.833582	3.789570
C	1.597455	-1.041801	4.894766
H	0.900022	-1.341763	4.104303
O	0.862619	-0.851084	6.133231
C	2.741356	-2.056670	5.053281
H	2.410913	-3.086173	4.867237
H	3.132051	-1.996148	6.080742
O	2.969757	2.195856	0.965116
O	6.009731	1.481775	-0.992255
N	4.825191	2.801656	2.144257
N	4.282157	2.875463	-1.461479
C	4.070228	2.776092	1.005419
C	4.822123	1.081927	-3.072798
H	3.767327	1.156325	-3.361219
H	5.435299	1.551316	-3.859255
C	6.260189	3.140646	2.243302
H	6.629126	3.400582	1.244825
H	6.788198	2.218414	2.529717
C	6.554805	4.252749	3.234424
C	5.089008	1.811129	-1.746035
C	4.515828	3.617933	-0.212343
H	5.576379	3.885105	-0.156355
C	3.127577	3.361054	-2.232114
H	3.440339	3.822089	-3.184537
H	2.406539	2.555623	-2.433199
C	2.499618	4.423485	-1.318476
H	1.656076	4.000887	-0.761259
O	2.026815	5.515302	-2.151901
C	3.628242	4.871034	-0.375341

H	3.244511	5.257981	0.576976
H	4.208434	5.666986	-0.866495
K	1.206619	-0.059980	0.123772
C	7.596941	4.099455	4.161191
C	7.919688	5.130752	5.051117
C	7.195808	6.326798	5.029263
C	6.148225	6.487027	4.113651
C	5.833178	5.458126	3.221752
H	8.163185	3.164128	4.181824
H	8.735210	4.996527	5.764963
H	7.444878	7.132006	5.723543
H	5.580199	7.419740	4.091111
H	5.011279	5.590061	2.513127
C	8.326549	0.464381	-4.712852
C	8.854859	0.769919	-5.972353
C	8.184048	0.363658	-7.129969
C	6.983449	-0.348796	-7.021866
C	6.461444	-0.658256	-5.762397
H	8.851059	0.786015	-3.809070
H	9.790473	1.328065	-6.048257
H	8.593208	0.601232	-8.114100
H	6.455811	-0.669878	-7.922797
H	5.523560	-1.214531	-5.686198
C	7.059749	-5.743349	2.784124
C	7.261978	-7.065481	3.197282
C	6.367475	-7.665014	4.088874
C	5.270701	-6.936166	4.566764
C	5.074446	-5.614763	4.155799
H	7.761425	-5.276684	2.087291
H	8.118880	-7.627487	2.819721
H	6.523292	-8.696165	4.412727
H	4.570889	-7.397806	5.266894
H	4.216031	-5.051938	4.531685
C	-0.127992	-1.757417	6.395477
C	-0.789777	-1.508582	7.705818
O	-0.421638	-2.664235	5.625712
C	1.092782	6.342860	-1.591710
C	0.704797	7.457431	-2.499231
O	0.638023	6.168209	-0.467678
C	0.876985	-4.618128	-4.684143
C	0.325286	-5.867685	-5.275701
O	0.654031	-3.489334	-5.104150
O	-2.921127	-0.008617	-2.546809
O	-0.349252	-2.229968	-0.976856
N	-1.036948	0.413727	-3.735658
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C	-1.941890	-0.446201	-3.161636
C	-1.926129	-3.771655	0.032481
H	-2.985828	-4.026309	-0.088059
H	-1.340948	-4.698068	-0.074952
C	0.182185	0.061847	-4.476842

H	0.248462	-1.031434	-4.552001
H	1.063519	0.390819	-3.900279
C	0.236994	0.654000	-5.878125
C	-1.454512	-2.800259	-1.062128
C	-1.779039	-1.968490	-3.359009
H	-0.742668	-2.254991	-3.567706
C	-3.636901	-3.163540	-2.286655
H	-3.697917	-4.263234	-2.255902
H	-4.248942	-2.730800	-1.483462
C	-4.065708	-2.674200	-3.680940
H	-4.621628	-1.730607	-3.621126
O	-4.925339	-3.689726	-4.259359
C	-2.747806	-2.475634	-4.447292
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H	-2.393916	-3.445456	-4.829716
O	-3.365893	-1.778567	0.942513
O	-0.569275	0.266035	2.413877
N	-1.707202	-3.258639	1.385169
N	-2.677624	-0.184142	3.163294
C	-2.526860	-2.214133	1.739757
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H	-2.988215	2.362268	3.270996
H	-1.366121	2.422416	3.995758
C	-0.631985	-3.865272	2.179025
H	-0.588994	-3.372931	3.159244
H	0.332351	-3.661498	1.683585
C	-0.798974	-5.364340	2.384062
C	-1.678989	0.665375	2.820087
C	-2.462543	-1.643201	3.170773
H	-1.509371	-1.852325	3.665939
C	-4.078662	0.184965	3.459144
H	-4.153044	0.749112	4.403163
H	-4.493455	0.779026	2.633624
C	-4.786143	-1.171032	3.622959
H	-5.272400	-1.481692	2.690412
O	-5.792584	-1.026016	4.658915
C	-3.662837	-2.150291	3.997423
H	-3.930582	-3.191981	3.786751
H	-3.432142	-2.055521	5.069444
O	-3.172947	2.200418	0.774543
O	-0.129058	1.997099	-1.452222
N	-1.452765	3.022184	2.003008
N	-2.062577	3.190568	-1.622978
C	-2.192272	2.950321	0.847340
C	-1.342118	1.833503	-3.549509
H	-2.362977	2.031112	-3.897429
H	-0.650737	2.409870	-4.182946
C	-0.246255	3.828789	2.245668
H	-0.036868	4.430306	1.352215
H	0.617640	3.155431	2.380952
C	-0.370630	4.760898	3.441664

C	-1.144713	2.314423	-2.101975
C	-1.851933	3.878905	-0.335139
H	-0.820631	4.243957	-0.303236
C	-3.385095	3.488159	-2.214551
H	-3.284662	4.014807	-3.177047
H	-3.952932	2.557979	-2.352721
C	-4.043984	4.428894	-1.191269
H	-4.717906	3.883722	-0.519182
O	-4.807695	5.422476	-1.923382
C	-2.869701	5.035508	-0.407074
H	-3.177597	5.408392	0.577020
H	-2.435823	5.868953	-0.979984
C	0.698729	4.895759	4.338892
C	0.626441	5.790934	5.412537
C	-0.526370	6.557708	5.607298
C	-1.603117	6.425769	4.721687
C	-1.524099	5.535916	3.646899
H	1.603426	4.299557	4.189720
H	1.469931	5.885164	6.100101
H	-0.587966	7.253918	6.446278
H	-2.506408	7.022298	4.866563
H	-2.368861	5.436911	2.960710
C	1.447135	1.167836	-6.367975
C	1.539582	1.669848	-7.670798
C	0.413541	1.672819	-8.500187
C	-0.800408	1.167991	-8.019418
C	-0.887008	0.660207	-6.719576
H	2.330103	1.168894	-5.722292
H	2.490622	2.063592	-8.036095
H	0.479640	2.067803	-9.516053
H	-1.684162	1.166151	-8.661231
H	-1.839789	0.271534	-6.352108
C	0.320427	-6.206680	2.310146
C	0.201572	-7.580889	2.547449
C	-1.046141	-8.132680	2.854281
C	-2.171243	-7.302397	2.922243
C	-2.047652	-5.929666	2.689297
H	1.299481	-5.781459	2.070573
H	1.084289	-8.221246	2.486345
H	-1.143371	-9.205064	3.035575
H	-3.150032	-7.725602	3.158506
H	-2.933443	-5.291806	2.736569
C	-6.730142	-2.027579	4.718287
C	-7.752426	-1.778724	5.774775
O	-6.709723	-3.001153	3.981887
C	-5.693442	6.156407	-1.173057
C	-6.459851	7.133220	-1.999252
O	-5.816972	6.013715	0.032854
C	-5.647501	-3.301021	-5.361151
C	-6.575257	-4.369871	-5.830673
O	-5.532032	-2.199620	-5.874152

C	-7.373998	-4.096760	-6.955565
C	-8.268821	-5.057560	-7.427998
C	-8.372511	-6.296865	-6.783590
C	-7.578200	-6.573860	-5.664266
C	-6.681869	-5.615599	-5.186318
H	-7.280147	-3.124215	-7.441827
H	-8.889355	-4.840607	-8.299831
H	-9.074888	-7.047089	-7.153414
H	-7.660817	-7.539390	-5.160932
H	-6.065714	-5.824486	-4.311868
C	-0.438622	-5.756960	-6.452037
C	-0.981726	-6.898183	-7.043017
C	-0.768556	-8.155826	-6.464547
C	-0.007963	-8.270938	-5.294327
C	0.541239	-7.133154	-4.699928
H	-0.591788	-4.768667	-6.888949
H	-1.572560	-6.808856	-7.956673
H	-1.194718	-9.048404	-6.927524
H	0.157689	-9.251928	-4.844555
H	1.135179	-7.218127	-3.789747
C	-1.755351	-2.434355	8.142154
C	-2.400742	-2.247519	9.364722
C	-2.090251	-1.135999	10.158561
C	-1.130031	-0.211909	9.728582
C	-0.477862	-0.395393	8.507964
H	-1.978933	-3.297792	7.513216
H	-3.146171	-2.970046	9.702576
H	-2.595555	-0.991352	11.115893
H	-0.887756	0.653172	10.349108
H	0.272649	0.319652	8.170848
C	-8.770105	-2.735772	5.936805
C	-9.751755	-2.556410	6.911835
C	-9.725015	-1.421791	7.732725
C	-8.714027	-0.465876	7.574730
C	-7.729253	-0.639910	6.599953
H	-8.773436	-3.611850	5.286024
H	-10.540679	-3.301455	7.033090
H	-10.493770	-1.281214	8.495705
H	-8.694824	0.419515	8.213681
H	-6.940721	0.102095	6.473328
C	-0.176475	8.433662	-1.999429
C	-0.569485	9.501120	-2.806920
C	-0.085912	9.603181	-4.117410
C	0.793487	8.635622	-4.618778
C	1.192068	7.566024	-3.814873
H	-0.535977	8.343022	-0.973003
H	-1.252844	10.256998	-2.415118
H	-0.392923	10.439924	-4.748512
H	1.171453	8.717330	-5.639838
H	1.877657	6.811682	-4.201100
C	-7.384716	7.961129	-1.338658

C	-8.123481	8.900559	-2.058662
C	-7.945562	9.020737	-3.442733
C	-7.027429	8.197112	-4.105406
C	-6.284534	7.255536	-3.389562
H	-7.509315	7.850465	-0.260115
H	-8.840784	9.540831	-1.541235
H	-8.524536	9.755990	-4.005884
H	-6.891649	8.288494	-5.185081
H	-5.569425	6.611798	-3.901935

4.0 Ionophoric activities

4.1 Ion selectivity with the HPTS assay

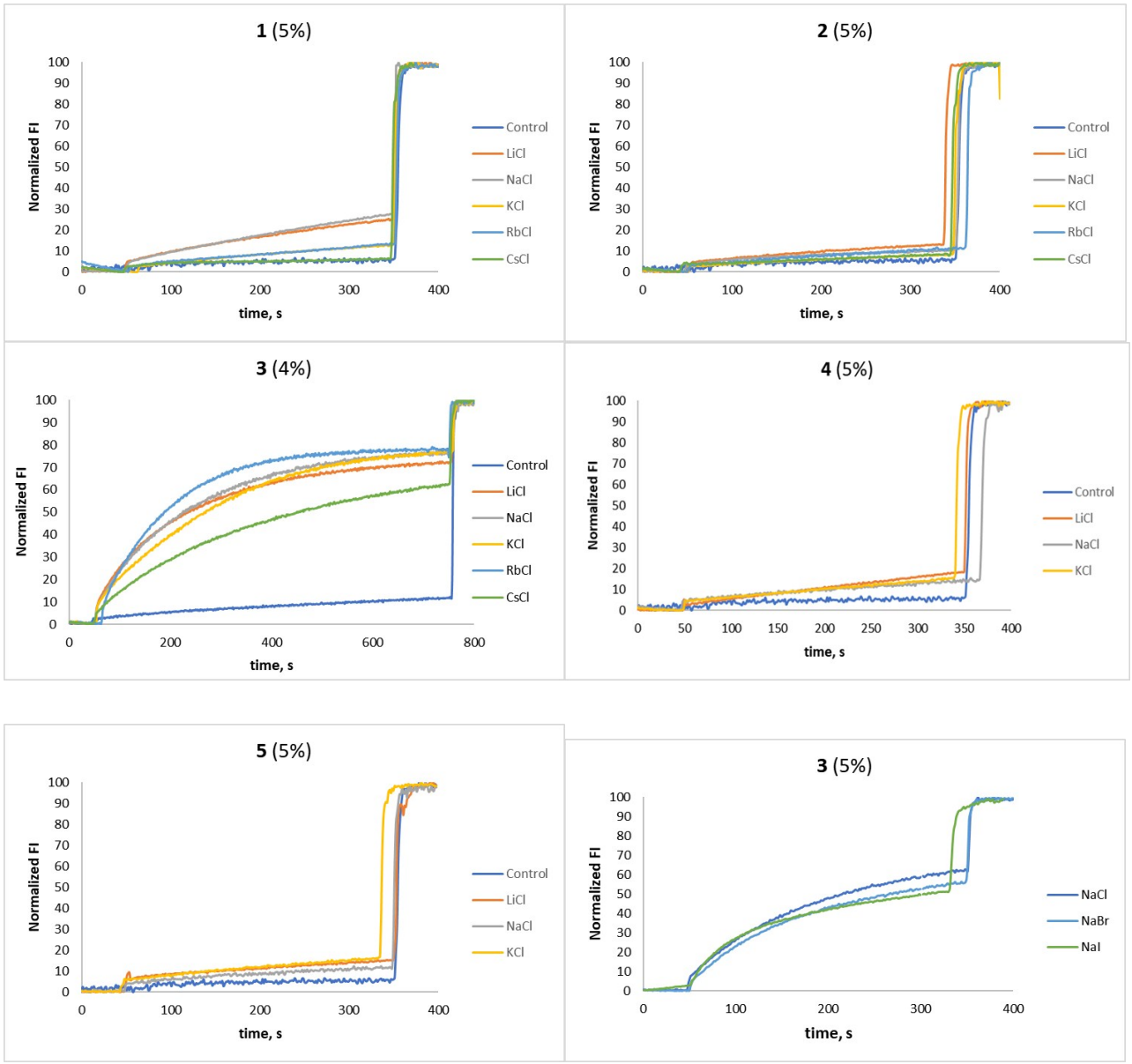

Figure S17. Normalized fluorescence time courses for cyclopeptoids **1**-**5** in the HPTS assay in the presence of the different alkaline metal ions (100 mM MCl, pH 7.0, base pulse by addition of 50 µL of 0.5M MOH) or

different halide anions (100 mM NaX, pH 7.0, base pulse by addition of 50 µL of 0.5M NaOH). The liposomes were made of 95:5 EYPC/EYPG (100 nm diameter), loaded with HPTS (0.1 mM HPTS, 25 mM HEPES, 100 mM NaCl, pH 7.0) and diluted to 0.17 mM total lipid concentration with the appropriate buffer solution. The concentration of the ionophores is showed in each figure and it is expressed in mol% with respect to the total concentration of lipids. The control trace is recorded in the absence of ionophore. The kinetic experiments were performed at 25 °C. Base pulse at 50 s and addition of TRITON X-100 (40 µL of 5% aqueous solution) to lyse the liposomes at 350 s.

4.2 Ion selectivity with the HPTS assay and the protonophore CCCP

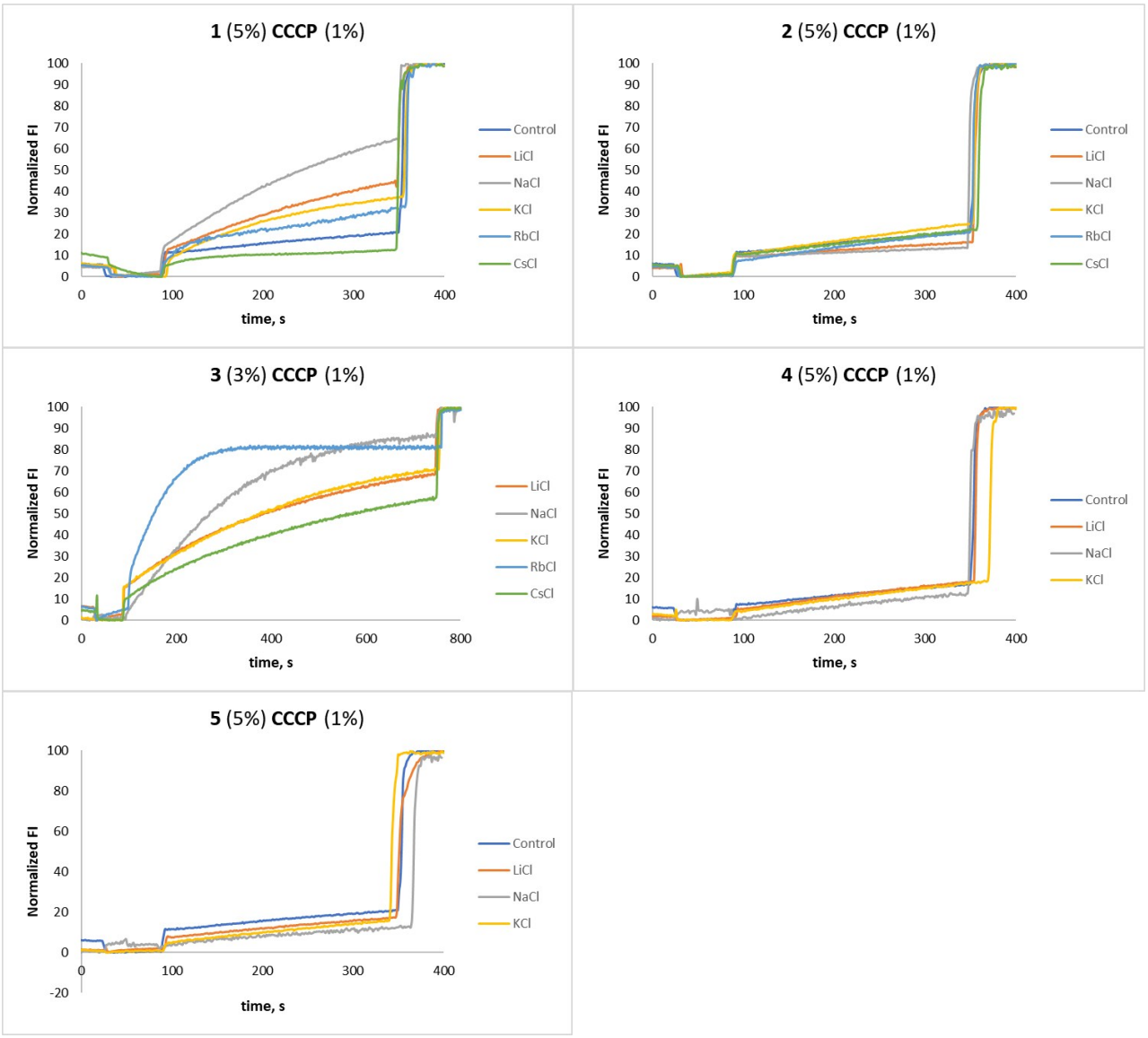

Figure S18. Normalized fluorescence time courses for cyclopeptoids **1**-**5** in the HPTS assay with 1 mol% of the CCCP protonophore in the presence of the different alkaline metal ions (100 mM MCl, pH 7.0, base pulse by addition of 50 µL of 0.5M MOH). The liposomes were made of 95:5 EYPC/EYPG (100 nm diameter), loaded with HPTS (0.1 mM HPTS, 25 mM HEPES, 100 mM NaCl, pH 7.0) and diluted to 0.17 mM total lipid concentration with the appropriate buffer solution. The concentration of the ionophores is showed in each figure and it is expressed in mol% with respect to the total concentration of lipids. The control trace is

recorded in the absence of ionophore. The kinetic experiments were performed at 25 °C. Base pulse at 25 s, addition of CCCP at 50s, addition of the ionophore at 90s, and addition of TRITON X-100 (40 µL of 5% aqueous solution) to lyse the liposomes at 350 s.

4.3 LogP values

Compound	**1**	**2**	**3**	**4**	**5**
LogP	4.63	0.59	4.46	8.55	6.34

Table S1. LogP values of compounds **1**-**5** were calculated using ALOGPs 2.1 software (VCCLAB, V. C. C. L., http://www.vcclab.org 2005.).

4.4 Kinetic profiles of compounds **3** at different ionophore concentration in the HPTS assay with added cholesterol

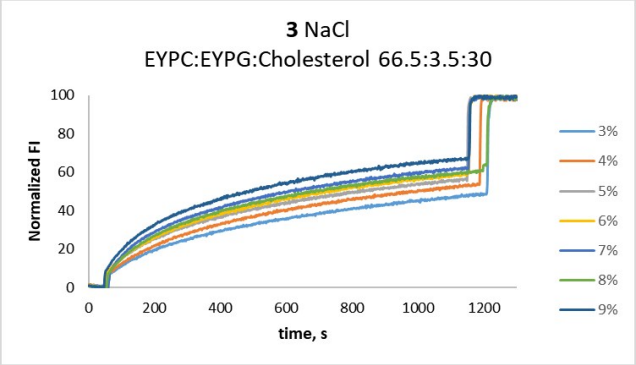

Figure S19. Normalized fluorescence time courses for cyclopeptoid **3** in the HPTS assay in the presence of NaCl (100 mM NaCl, pH 7.0, base pulse by addition of 50 µL of 0.5M NaOH). The liposomes were made of 66.5:3.5:30 EYPC/EYPG/Cholesterol (100 nm diameter), loaded with HPTS (0.1 mM HPTS, 25 mM HEPES, 100 mM NaCl, pH 7.0) and diluted to 0.17 mM total lipid concentration with the appropriate buffer solution. The concentration of the ionophores is showed in the figure and it is expressed in mol% with respect to the total concentration of lipids. The kinetic experiments were performed at 25 °C. Base pulse at 50 s and addition of TRITON X-100 (40 µL of 5% aqueous solution) to lyse the liposomes at 1150 s.

4.5 Kinetic profiles of compounds **1** and **3** at different ionophore concentration in the HPTS assay

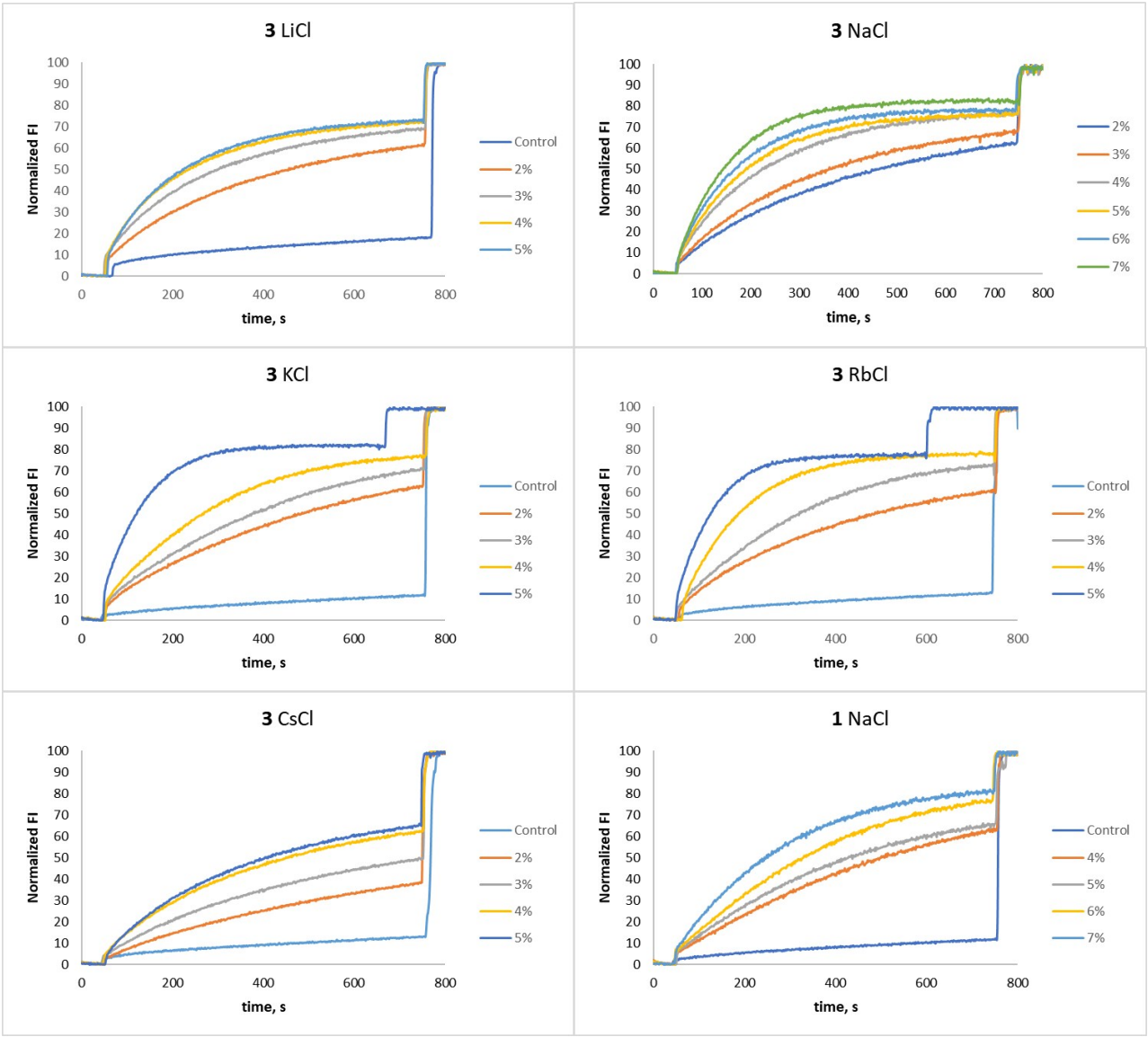

Figure S20. Normalized fluorescence time courses for cyclopeptoids **1, 3** in the HPTS assay in the presence of the different alkaline metal ions (100 mM MCl, pH 7.0, base pulse by addition of 50 µL of 0.5M MOH). The liposomes were made of 95:5 EYPC/EYPG (100 nm diameter), loaded with HPTS (0.1 mM HPTS, 25 mM HEPES, 100 mM MCl, pH 7.0) and diluted to 0.17 mM total lipid concentration with the appropriate buffer solution. The concentration of the ionophores is showed in each figure and it is expressed in mol% with respect to the total concentration of lipids. The control trace is recorded in the absence of ionophore. The kinetic experiments were performed at 25 °C. Base pulse at 50 s and addition of TRITON X-100 (40 µL of 5% aqueous solution) to lyse the liposomes at 750 s.

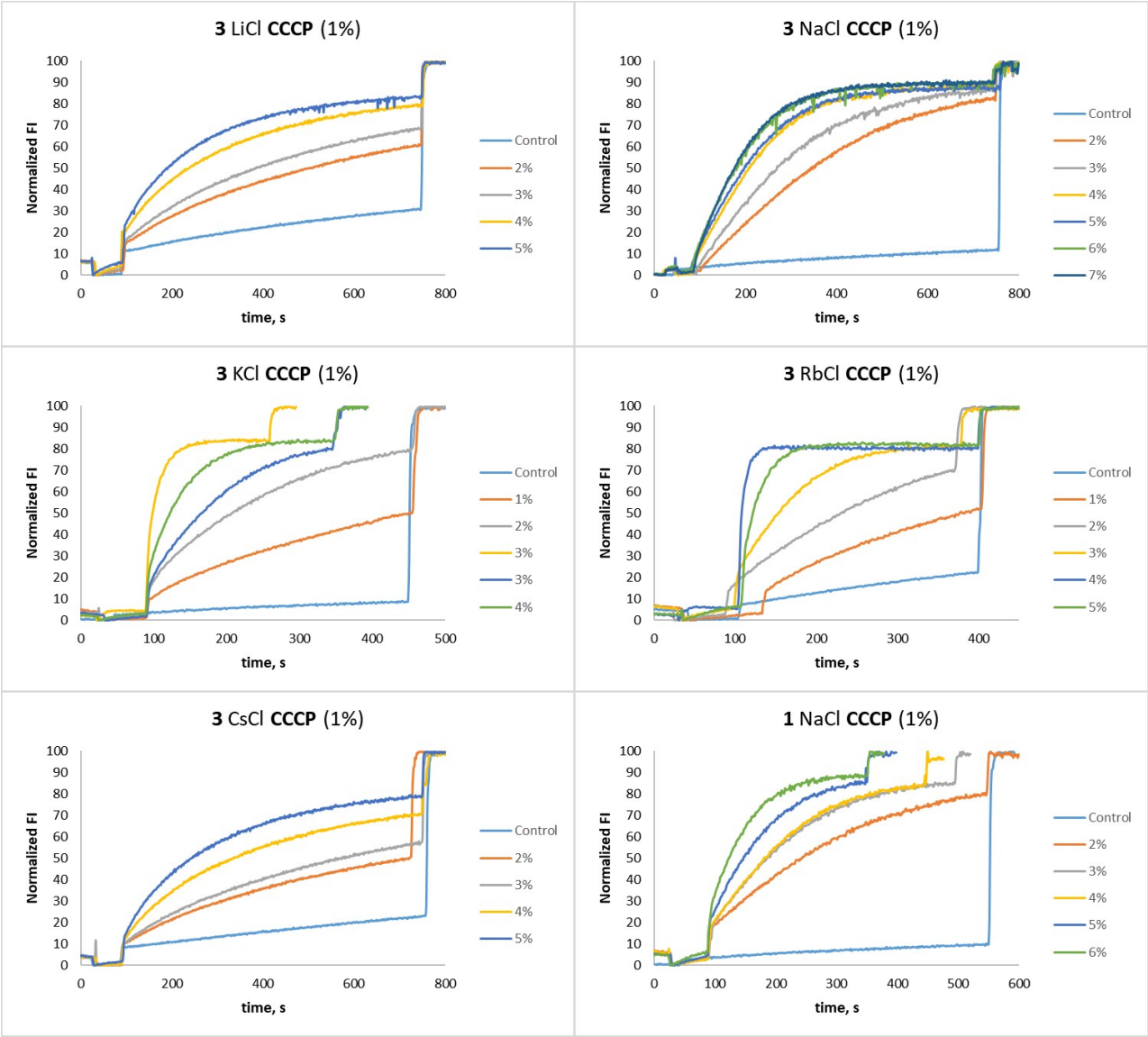

Figure S21. Normalized fluorescence time courses for cyclopeptoids **1,3** in the HPTS assay with 1 mol% of the CCCP protonophore in the presence of the different alkaline (100 mM MCl, pH 7.0, base pulse by addition of 50 µL of 0.5M MOH). The liposomes were made of 95:5 EYPC/EYPG (100 nm diameter), loaded with HPTS (0.1 mM HPTS, 25 mM HEPES, 100 mM MCl, pH 7.0) and diluted to 0.17 mM total lipid concentration with the appropriate buffer solution. The concentration of the ionophores is showed in each figure and it is expressed in mol% with respect to the total concentration of lipids. The control trace is recorded in the absence of ionophore. The kinetic experiments were performed at 25 °C. Base pulse at 25 s, addition of CCCP at 50s, addition of the ionophore at 90s, and addition of TRITON X-100 (40 µL of 5% aqueous solution) to lyse the liposomes at 750 s.

4.6 First-order rate constants of compounds **1** and **3** in the HPTS assay

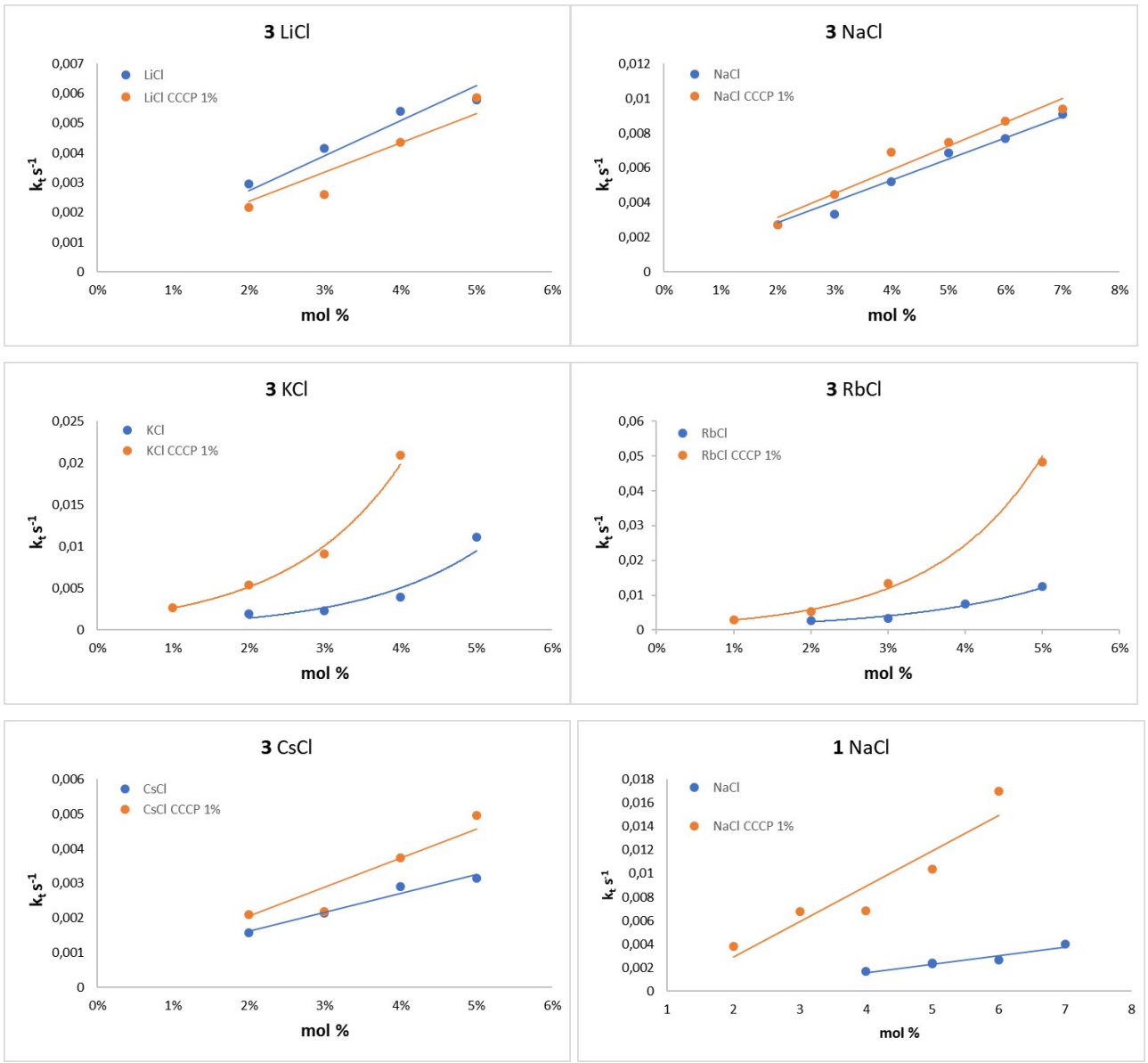

Figure S22. Dependence of the first order rate constant of the cation transport process (k_t, s^{-1}) on the concentration of cyclopeptoids **1** and **3** in the presence and in the absence of CCCP. The Figures report the first order rate constants obtained by the fitting of the kinetic profiles reported in Fig. S20 e S21.

4.7 Fitting of the kinetic profiles with the Regen equation.

The rate data obtained with cyclic peptoid **3** in the transport of K^+ and Rb^+ in the presence of CCCP (Figure S22) were fitted with the equation proposed by S. Regen,[5] which is used to describe cooperative association phenomena between monomers forming higher order ionophoric active structures:

[5] M. Merritt, M. Lanier, G. Deng and S. T. Regen, *J. Am. Chem. Soc.*, **1998**, *120*, 8494.

$$k_t = k_2/K \times [monomer]^n$$

In this equation, K is the dissociation constant of the higher order species formed, k_2 is the intrinsic rate constant for the transport process, and n is the number of monomers which self-assemble forming the higher order species. The fitting of the data is shown in Figure S23 and gives n=2.4 and n=2.5 respectively for K^+ and Rb^+, suggesting that **3** may act as a dimeric species.

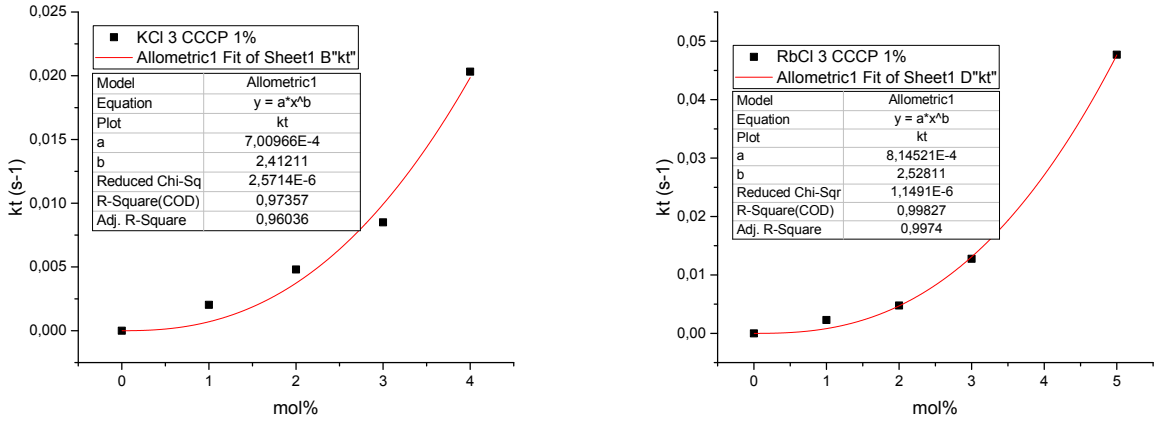

Figure S23. Dependence of the observed rate constant for the transport process (k_t, s^{-1}) vs concentration of **3** in the transport of K^+ and Rb^+ in the presence of CCCP (1%). The red line is the fitting of the data with the Regen's equation.