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

Supporting information for

Application of optically active chiral bis(imidazolium) salts as potential receptors of chiral dicarboxylate salts of biological relevance

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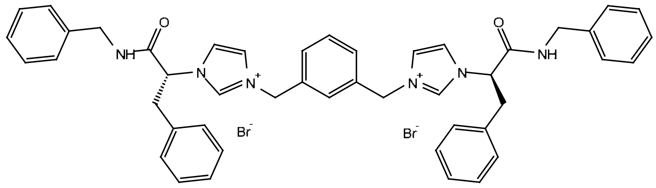
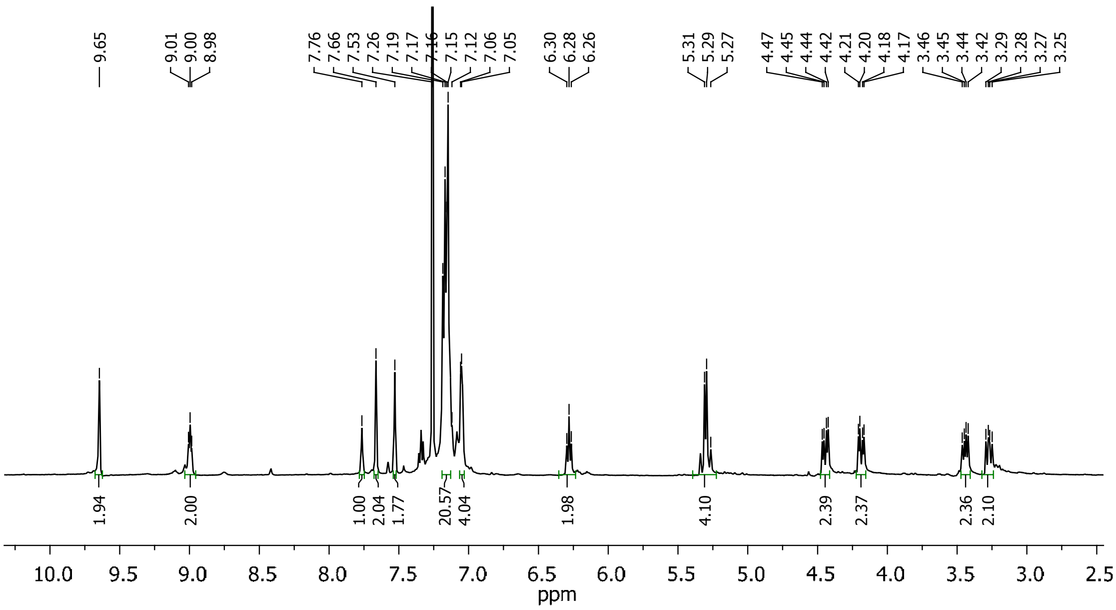
Copies of the NMR spectra of all the described compounds

5a





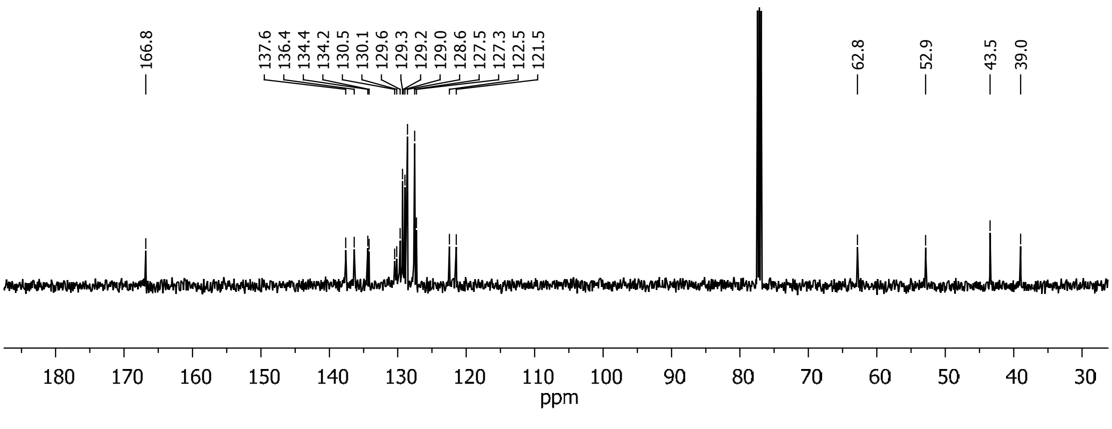
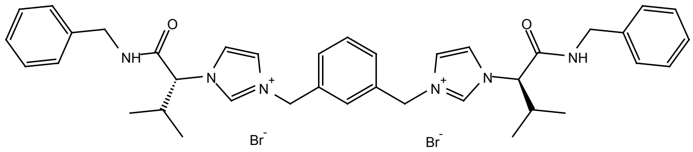
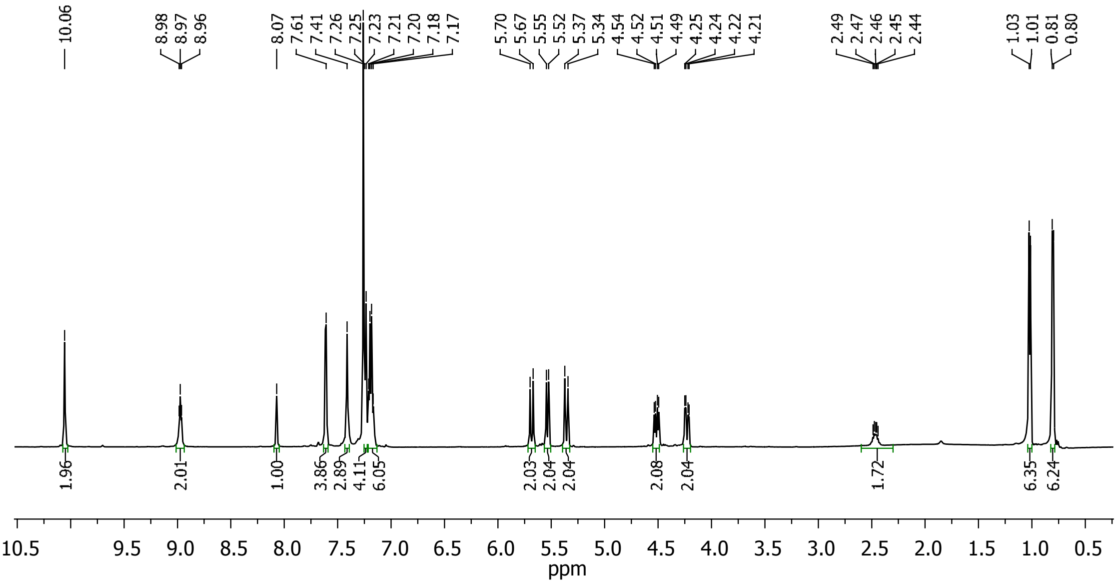


Figure S1. ^{1}H NMR spectra (upper trace) and ^{13}C NMR spectra (lower trace) for the bis(imidazolium) salt **5a** (10 mM, $CDCl_3$, 303 K).

5b





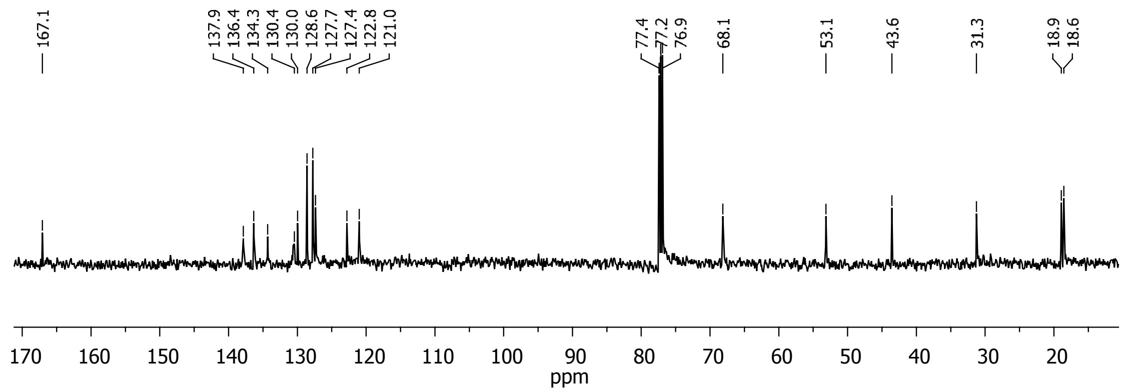
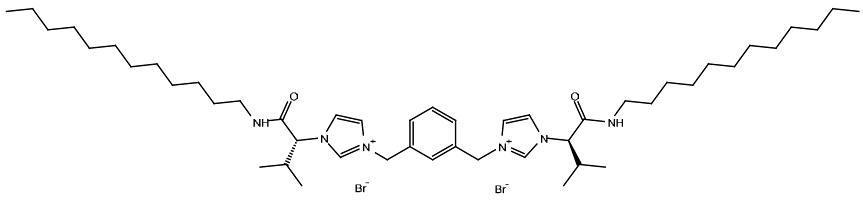
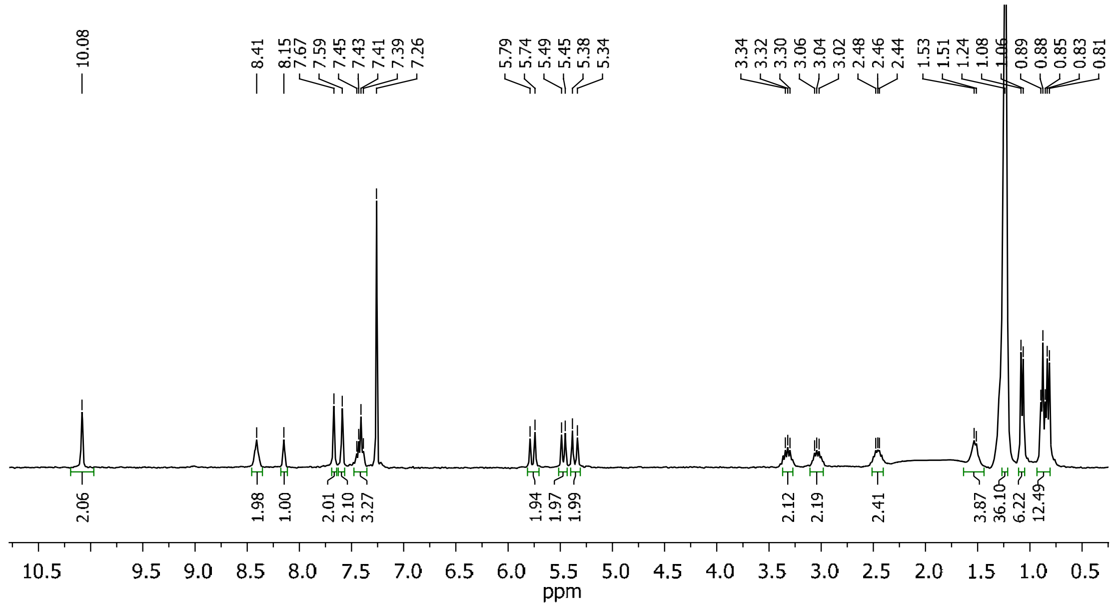


Figure S2. ^{1}H NMR spectra (upper trace) and ^{13}C NMR spectra (lower trace) for the bis(imidazolium) salt **5b** (10 mM, $CDCl_3$, 303 K).

5c





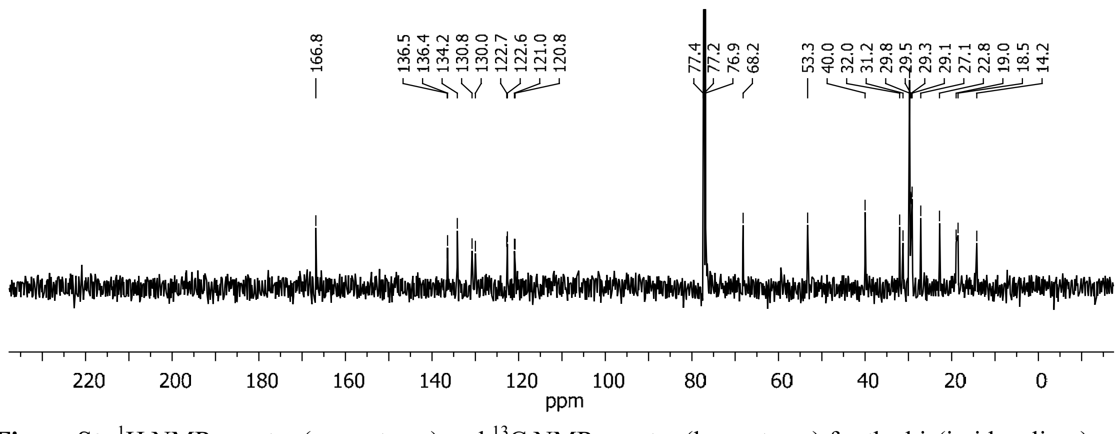
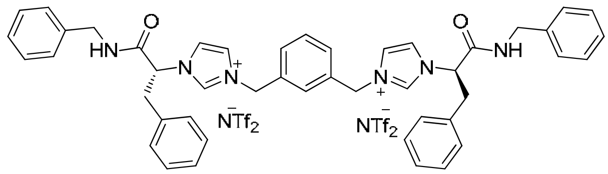


Figure S3. ^{1}H NMR spectra (upper trace) and ^{13}C NMR spectra (lower trace) for the bis(imidazolium) salt **5c** (10 mM, $CDCl_3$, 303 K).

3a



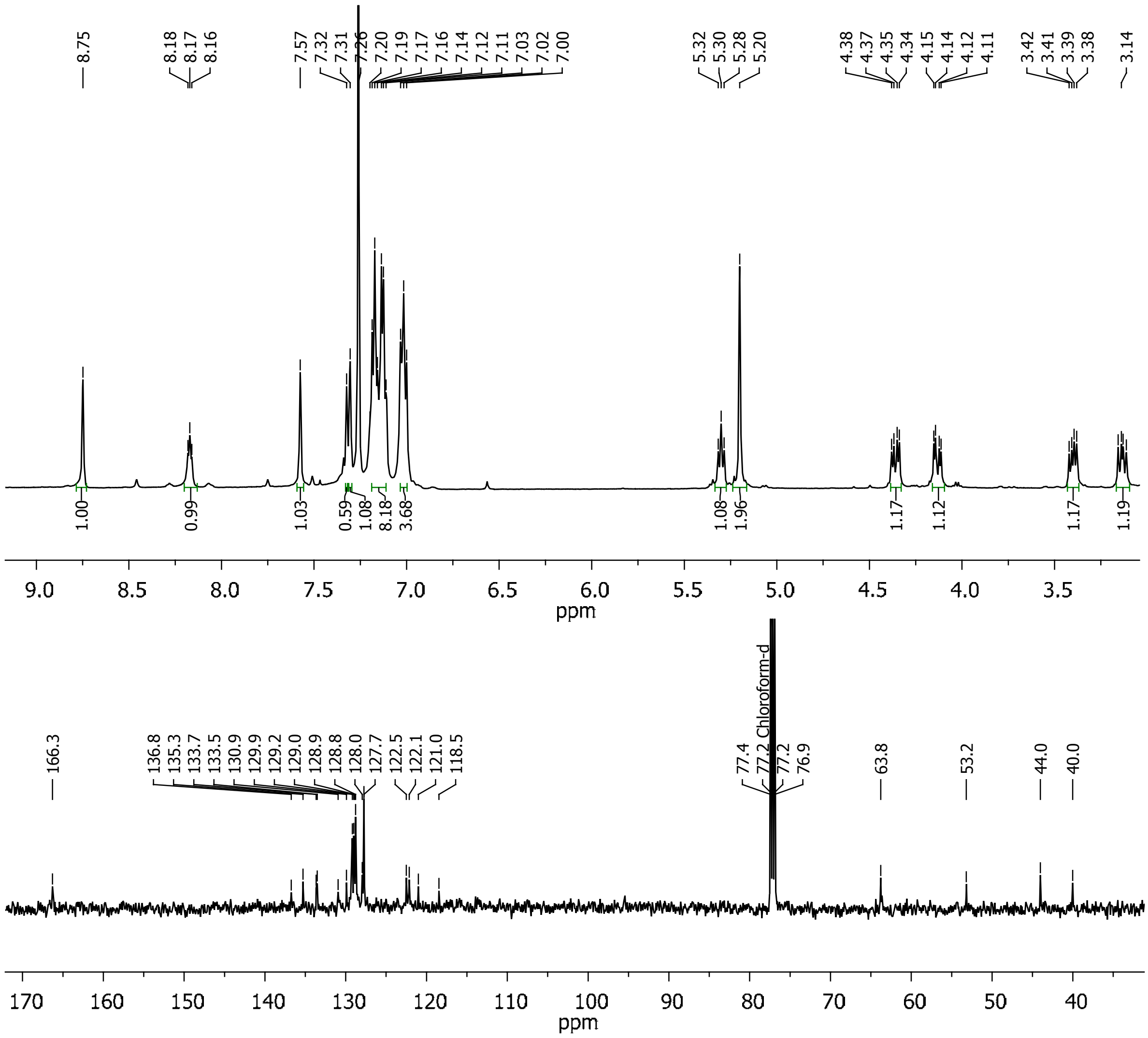
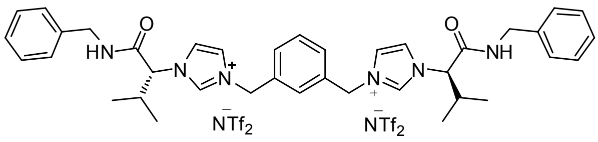
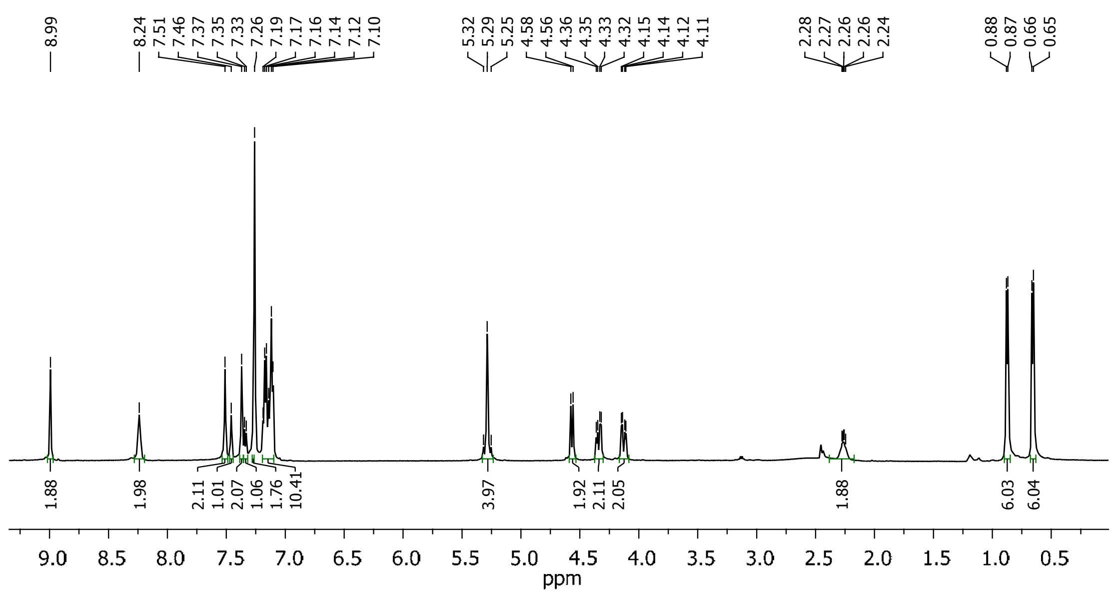


Figure S4. ^{1}H NMR spectra (upper trace) and ^{13}C NMR spectra (lower trace) for the bis(imidazolium) salt **3a** (10 mM, $CDCl_3$, 303 K).

3b





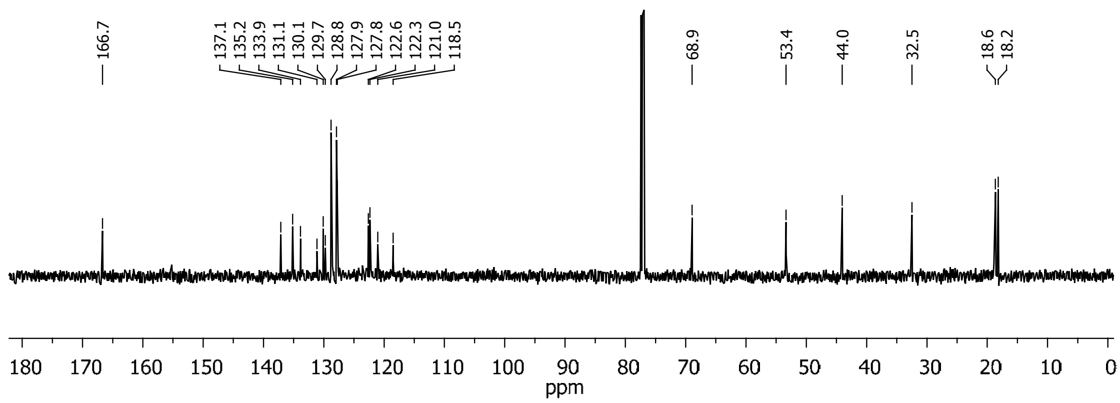
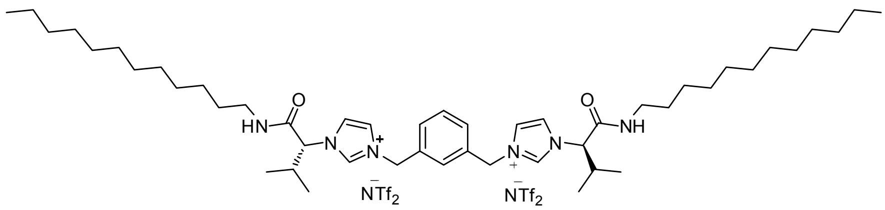


Figure S5. ^{1}H NMR spectra (upper trace) and ^{13}C NMR spectra (lower trace) for the bis(imidazolium) salt **3b** (10 mM, $CDCl_3$, 303 K).

3c



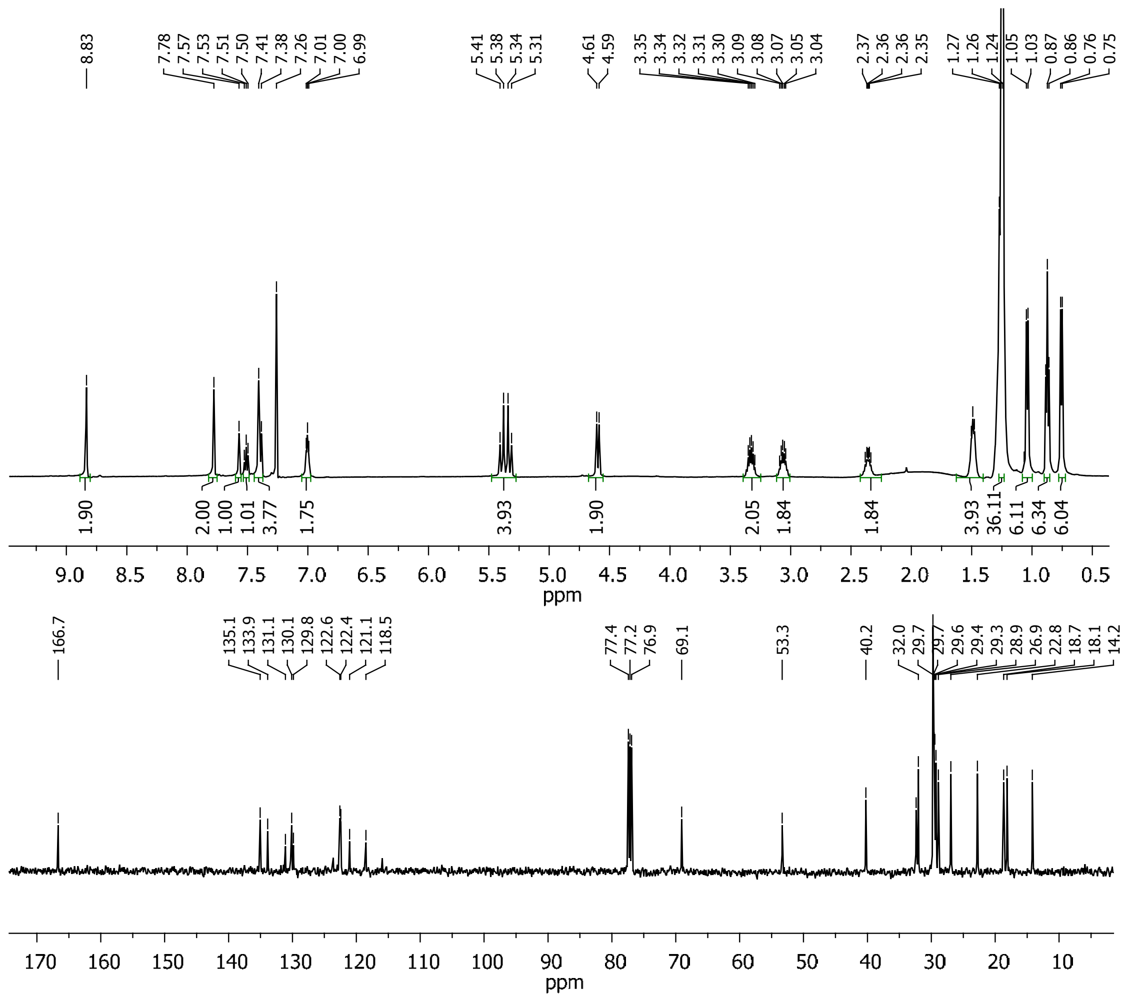


Figure S6. ^{1}H NMR spectra (upper trace) and ^{13}C NMR spectra (lower trace) for the bis(imidazolium) salt **3c** (10 mM, $CDCl_3$, 303 K).

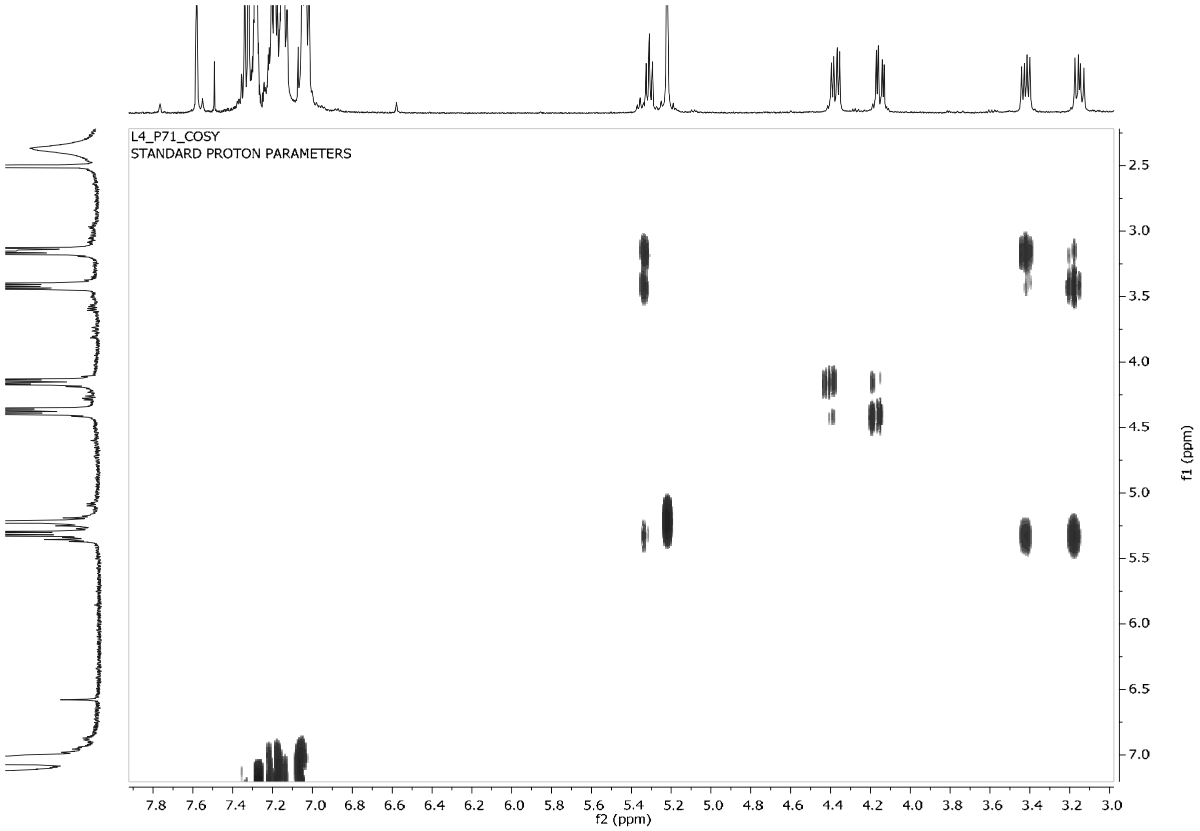


Figure S7. gCOSY spectra for the bis(imidazolium) salt **3a**

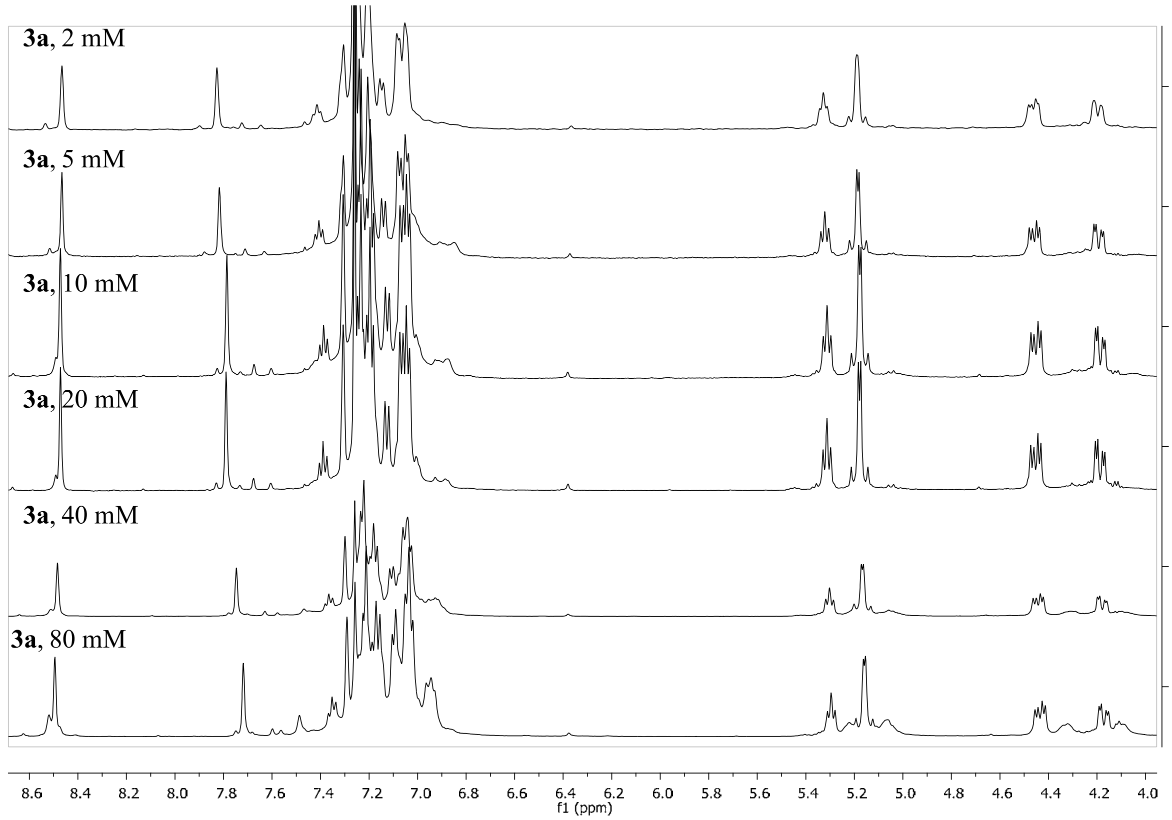


Figure S8. ^{1}H NMR spectra in $CDCl_3$ of **3a** at different concentrations.

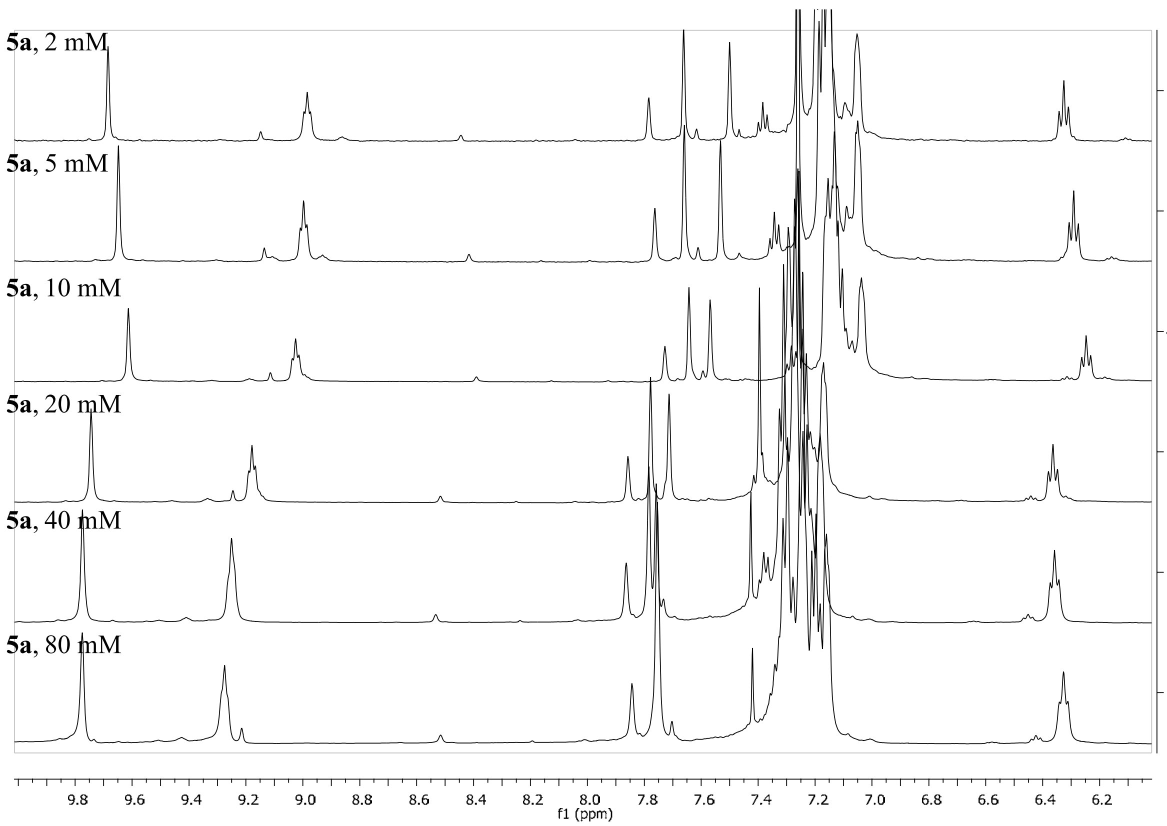


Figure S9. ^{1}H NMR spectra in $CDCl_3$ of **5a** at different concentrations.

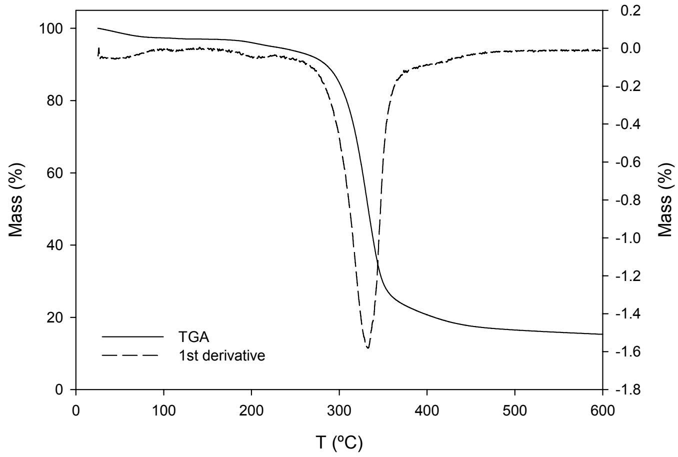


Figure S10. TGA and first derivative for the (bis)imidazolium salt **5a**.

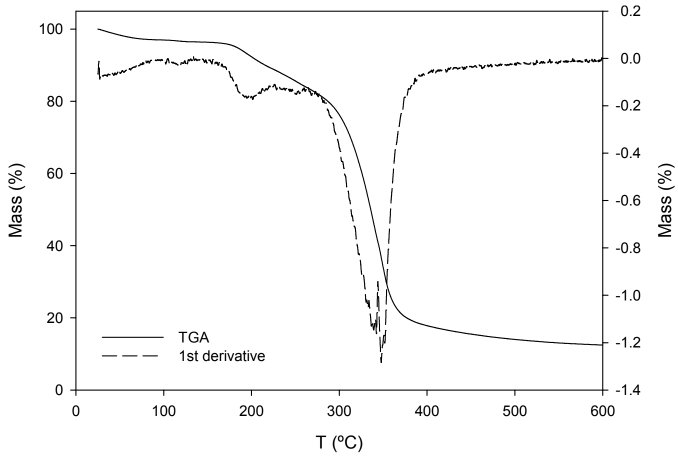


Figure S11. TGA and first derivative for the (bis)imidazolium salt **5b**.

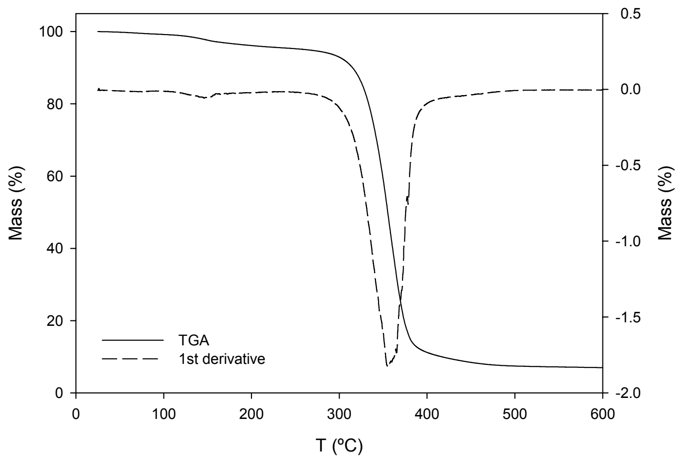


Figure S12. TGA and first derivative for the bis(imidazolium) salt **5c**.

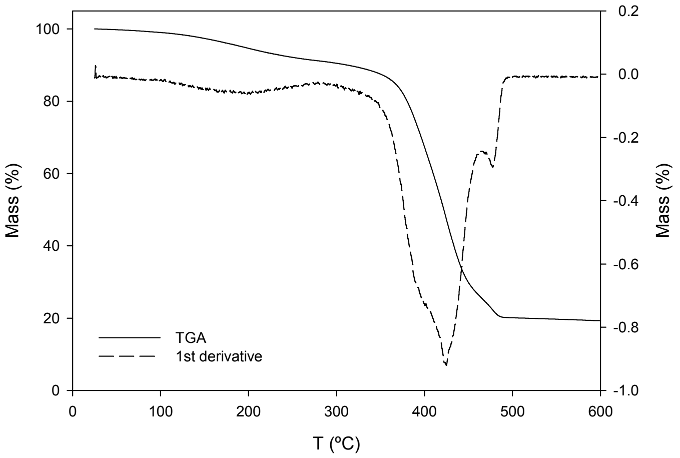


Figure S13. TGA and first derivative for the bis(imidazolium) salt **3a**.

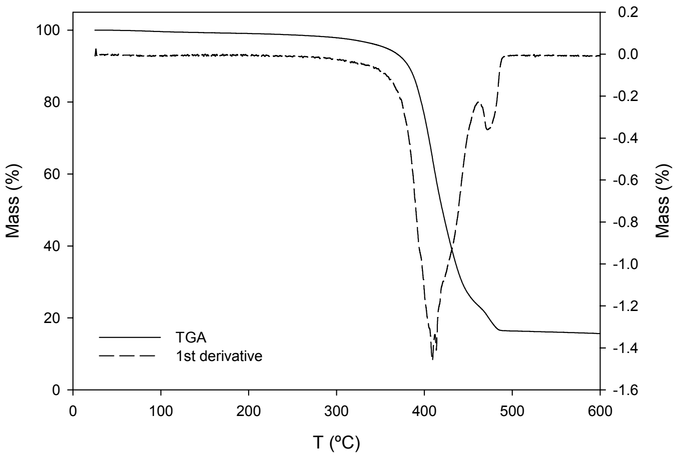


Figure S14. TGA and first derivative for the bis(imidazolium) salt **3b**.

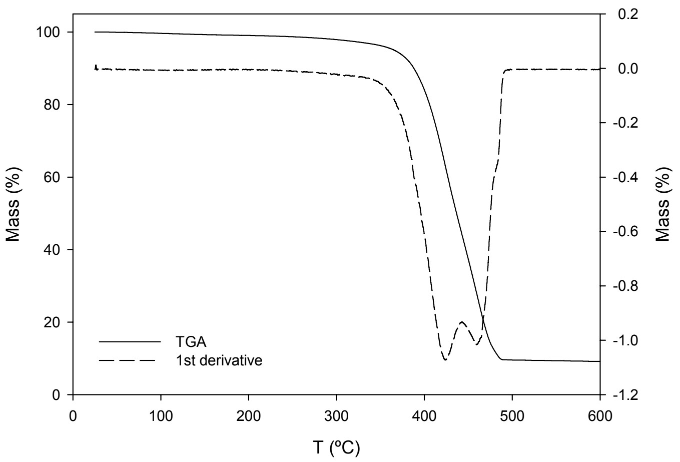


Figure S15. TGA and first derivative for the bis(imidazolium) salt **3c**.

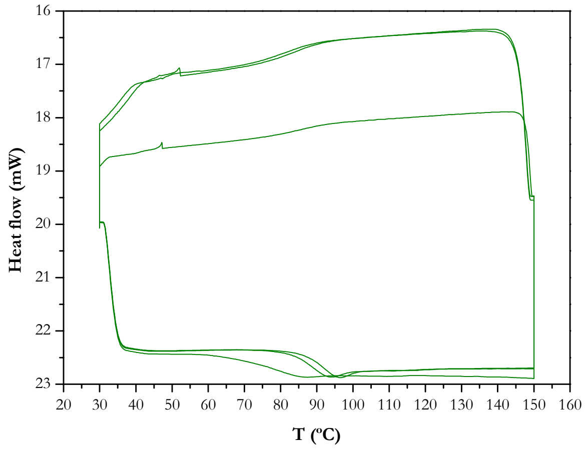


Figure S16. DSC for the bis(imidazolium) salt **5a**.

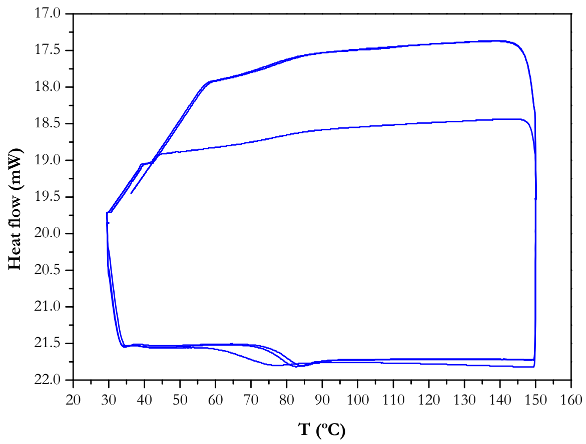


Figure S17. DSC for the bis(imidazolium) salt **5b**.

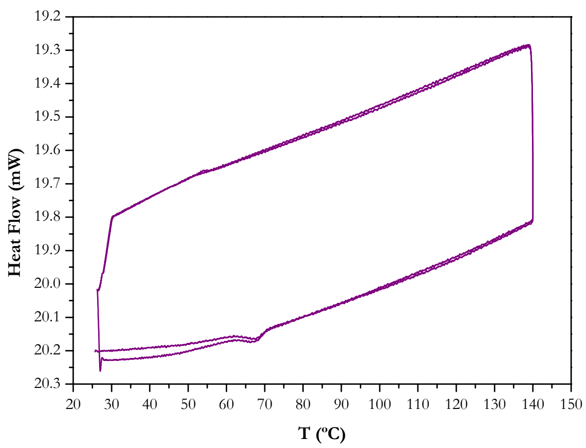


Figure S18. DSC for the bis(imidazolium) salt **5c**.

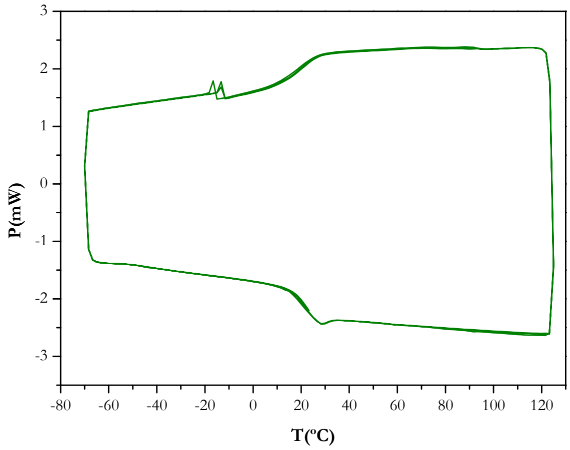


Figure S19. DSC for the bis(imidazolium) salt **3a**.

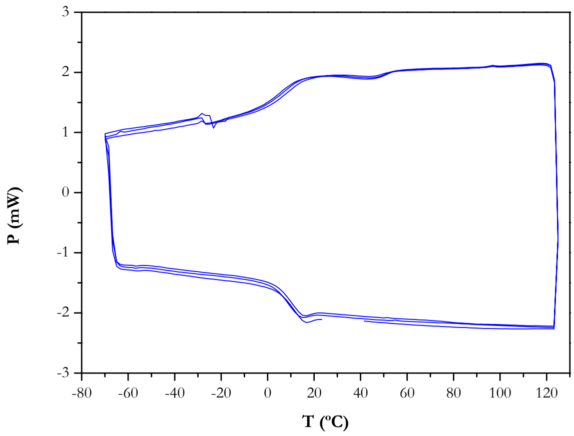


Figure S20. DSC for the bis(imidazolium) salt **3b**.

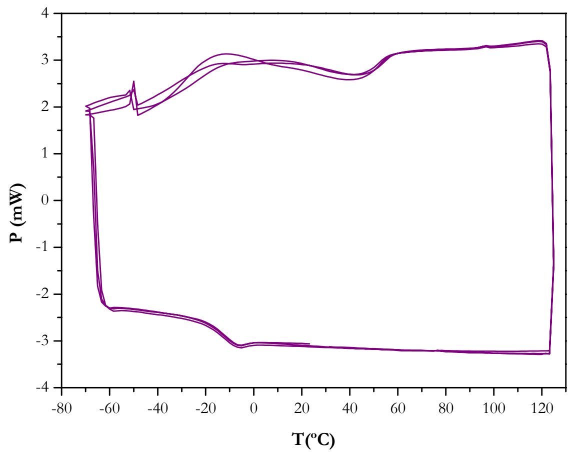


Figure S21. DSC for the bis(imidazolium) salt **3c**.

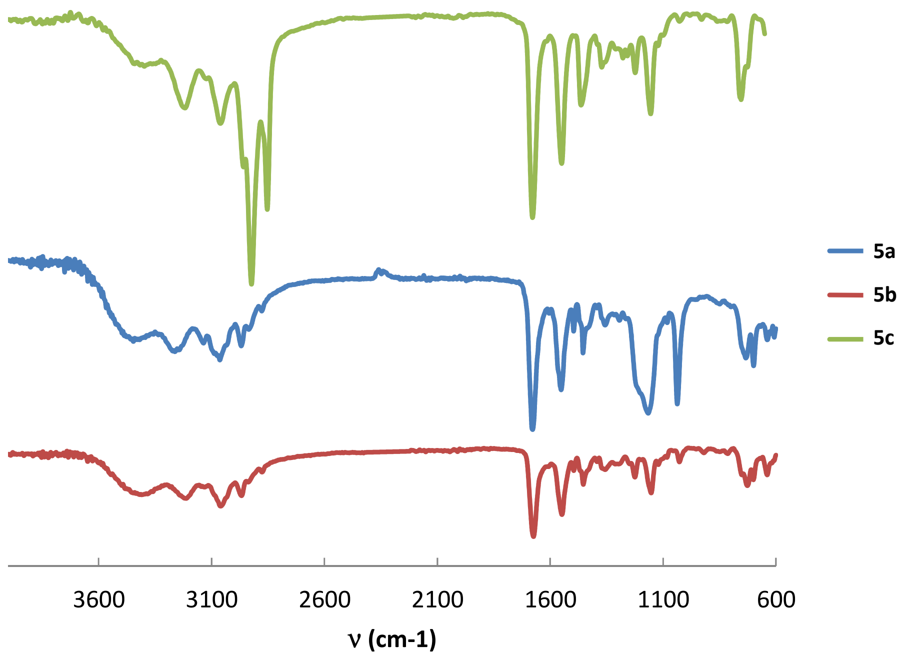


Figure S22. ATR-FTIR spectra for **5a-c** at 25 °C.

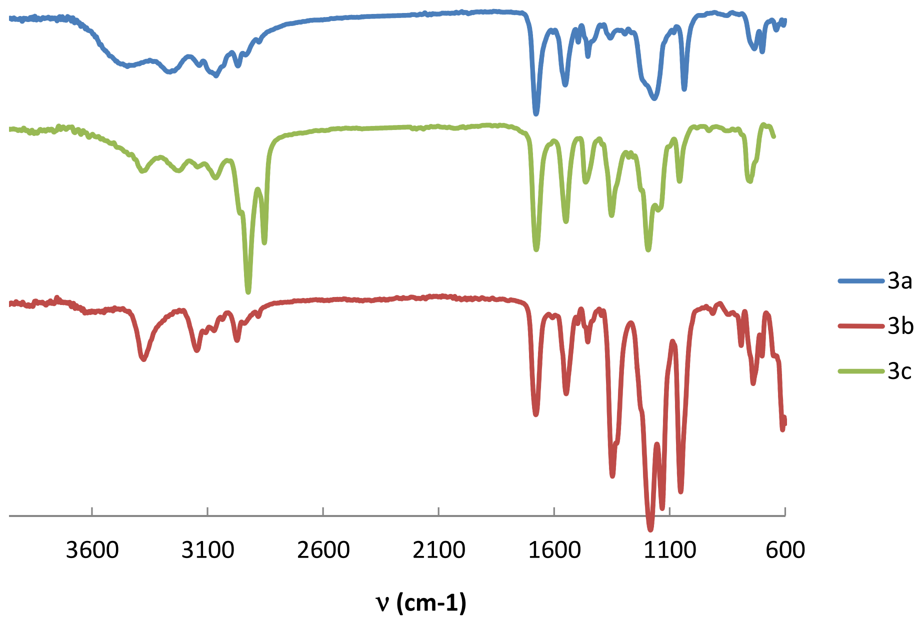


Figure S23. ATR-FTIR spectra for **3a-c** at 25 °C.

Table S1. Maximum chemical induced shifts ($\Delta\delta_{max}$, ppm) of selected receptor signals of **3a** in the presence of L- and D-TEA salts ($CDCl_3$/DMSO-d_6 5%, 303 K, 500 MHz).

Proton signal	$\Delta\delta_{max}$ L-AspTEA (ppm)	$\Delta\delta_{max}$ D-AspTEA (ppm)	$\Delta\delta_{max}$ L-GluTEA (ppm)	$\Delta\delta_{max}$ D-GluTEA (ppm)
Ha	1.268	1.193	1.100	1.073
NH	2.698	2.681	2.623	2.718
Hd	0.776	0.771	0.926	0.880

Table S2. Maximum chemical induced shifts ($\Delta\delta_{max}$, ppm) of selected receptor signals of **3b** in the presence of L- and D-TEA salts ($CDCl_3$/DMSO-d_6 5%, 303 K, 500 MHz).

Proton signal	$\Delta\delta_{max}$ L-AspTEA (ppm)	$\Delta\delta_{max}$ D-AspTEA (ppm)	$\Delta\delta_{max}$ L-GluTEA (ppm)	$\Delta\delta_{max}$ D-GluTEA (ppm)
Ha	1.241	1.114	1.365	1.330
NH	2.644	2.604	2.781	2.782
Hd	0.694	0.700	0.858	0.836

Table S3. Maximum chemical induced shifts ($\Delta\delta_{max}$, ppm) of selected receptor signals of **3c** in the presence of L- and D-TEA salts ($CDCl_3$/DMSO-d_6 5%, 303 K, 500 MHz).

Proton signal	$\Delta\delta_{max}$ L-AspTEA (ppm)	$\Delta\delta_{max}$ D-AspTEA (ppm)	$\Delta\delta_{max}$ L-GluTEA (ppm)	$\Delta\delta_{max}$ D-GluTEA (ppm)
Ha	1.490	1.424	1.388	1.431
NH	2.934	2.798	2.572	2.656
Hd	0.766	0.717	0.885	0.863

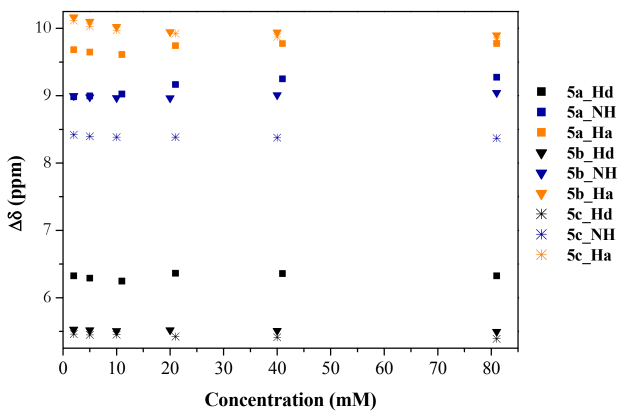


Figure S24. Observed chemical shift changes with changing concentration for a Ha, NH and Hd signals in the ^{1}H NMR spectra of **5a-c** in $CDCl_3$.

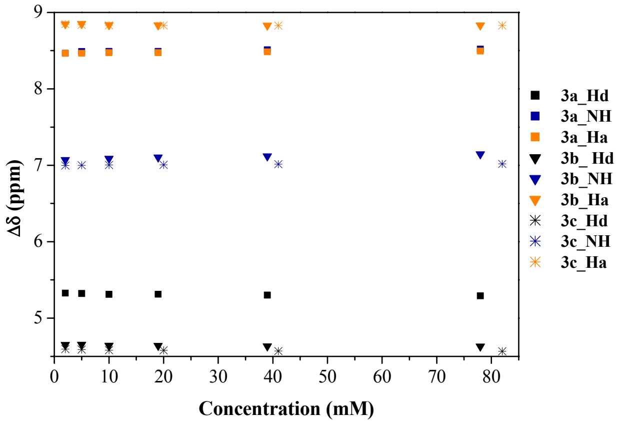


Figure S25. Observed chemical shift changes with changing concentration for a Ha, NH and Hd signals in the ^{1}H NMR spectra of **3a-c** in $CDCl_3$.

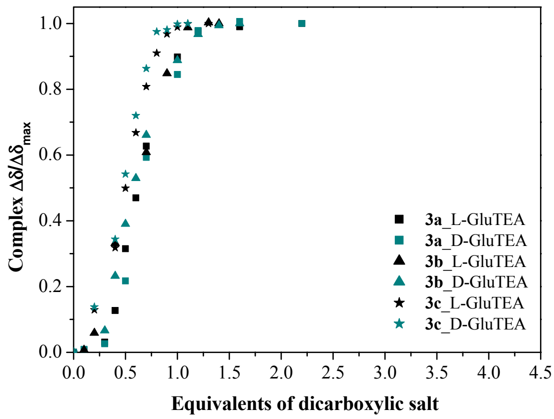


Figure S26. Complexation curve for the receptors **3a-c** (8mM) in the presence of L- or D- GluTEA (variation of Hd proton signal).

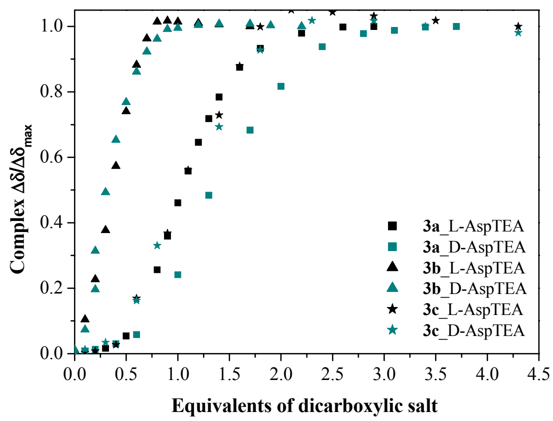


Figure S27. Complexation curve for the receptors **3a-c** (8mM) in the presence of L- or D- AspTEA (variation of Ha proton signal).

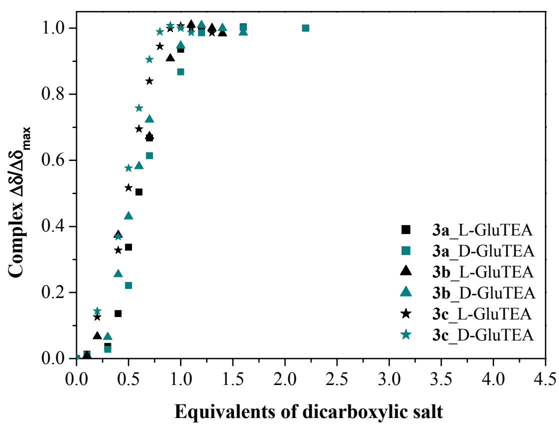


Figure S28. Complexation curve for the receptors **3a-c** (8mM) in the presence of L- or D- GluTEA (variation of Ha proton signal).

Fitting of the titration data

We were unable to perform an acceptable fitting to the 1:1 bindig mode (receptor:guest), and we could only get a rough estimation of the binding interaction by manual fitting, and considering a complex model of equilibria, using the variation of the chemical shifts of the Ha, Hd and NH proton signals

For the complexes **3a**, **3b** and **3c** with Asp:

3a + L-Asp = [**3a**·L-Asp] logβ = 3.73

3a + 2L-Asp = [**3a**·L-Asp$_2$] logβ = 6.34

2**3a** + L-Asp = [**3a**$_2$·L-Asp] logβ = 6.94

2**3a** + 2L-Asp = [**3a**$_2$·L-Asp$_2$] logβ = 9.17

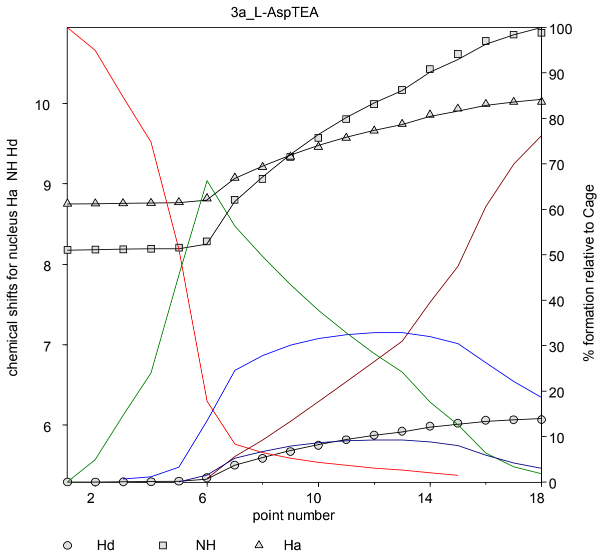


Figure S29. Plot of the experimental and calculated chemical shifts (manual fit) of the **3a**/L-Asp titration experiments, including a more complex binding mode. The obtained binding constants for the corresponding equilibria are shown.

3a + D-Asp = [**3a**·D-Asp] logβ = 3.32

3a + 2D-Asp = [**3a**·D-Asp$_2$] logβ = 6.14

2**3a** + D-Asp = [**3a**$_2$·D-Asp] logβ = 7.36

2**3a** + 2D-Asp = [**3a**$_2$·D-Asp$_2$] logβ = 8.95

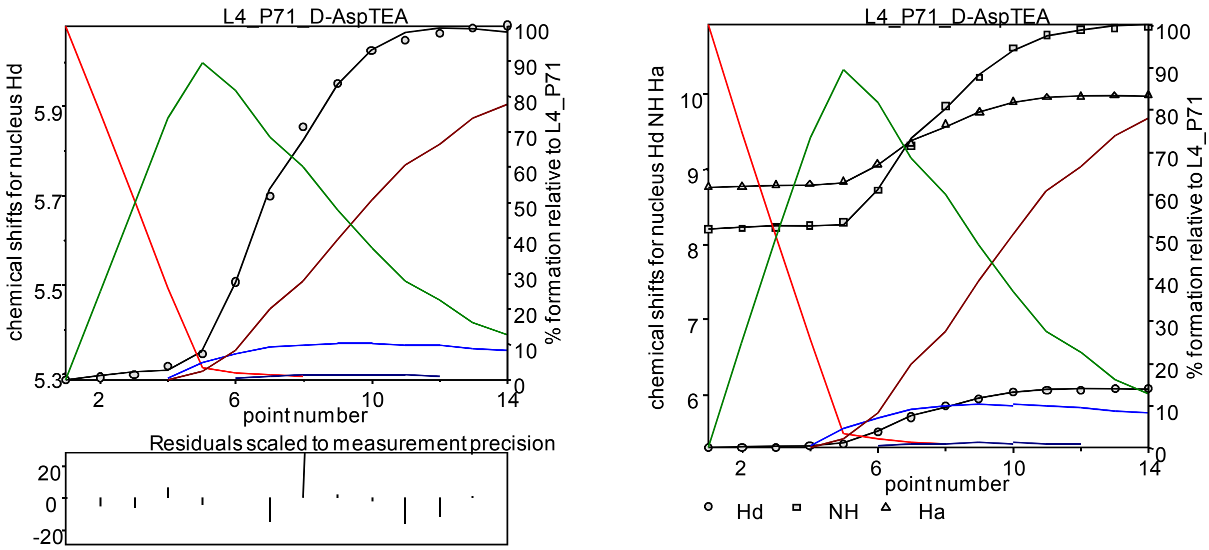


Figure S30. Plot of the experimental and calculated chemical shifts (manual fit) of the **3a**/D-Asp titration experiments, including a more complex binding mode. The obtained binding constants for the corresponding equilibria are shown

3b + D-Asp = [**3b**·D-Asp] logβ = 4.45

3b + 2D-Asp = [**3b**·D-Asp$_2$] logβ = 7.12

2**3b** + D-Asp = [**3b**$_2$·D-Asp] logβ = 9.37

2**3b** + 2D-Asp = [**3b**$_2$·D-Asp$_2$] logβ = 12.02

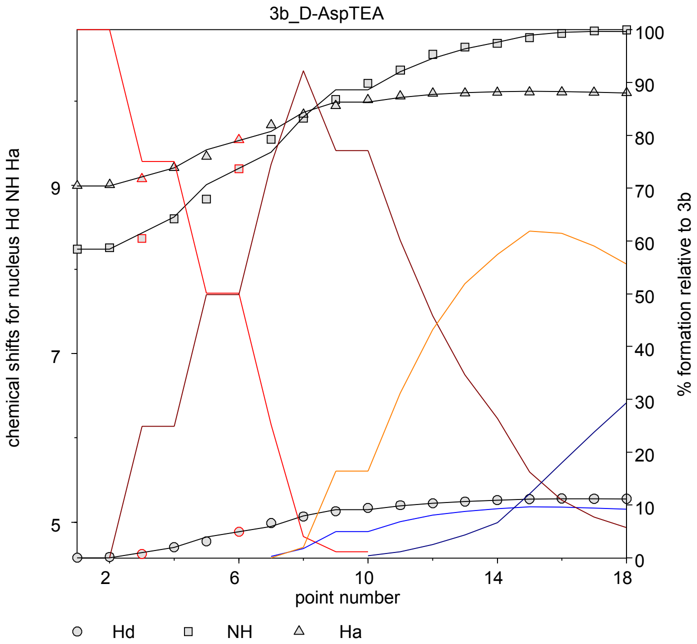


Figure S31. Plot of the experimental and calculated chemical shifts (manual fit) of the **3b**/D-Asp titration experiments, including a more complex binding mode. The obtained binding constants for the corresponding equilibria are shown

3b + L-Asp = [**3b**·L-Asp] logβ = 4.42

3b + 2L-Asp = [**3b**·L-Asp$_2$] logβ = 6.85

2**3b** + L-Asp = [**3b**$_2$·L-Asp] logβ = 9.55

2**3b** + 2L-Asp = [**3b**$_2$·L-Asp$_2$] logβ = 10.74

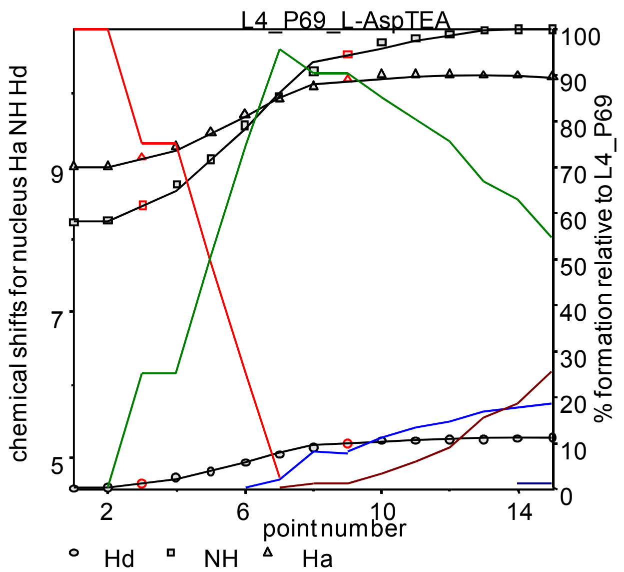


Figure S32. Plot of the experimental and calculated chemical shifts (manual fit) of the **3b**/L-Asp titration experiments, including a more complex binding mode. The obtained binding constants for the corresponding equilibria are shown

3c + D-Asp = [**3c**·D-Asp] logβ = 3.62
3c + 2D-Asp = [**3c**·D-Asp$_2$] logβ = 4.68
2**3c** + D-Asp = [**3c**$_2$·D-Asp] logβ = 6.75
2**3c** + 2D-Asp = [**3c**$_2$·D-Asp$_2$] logβ = 8.45

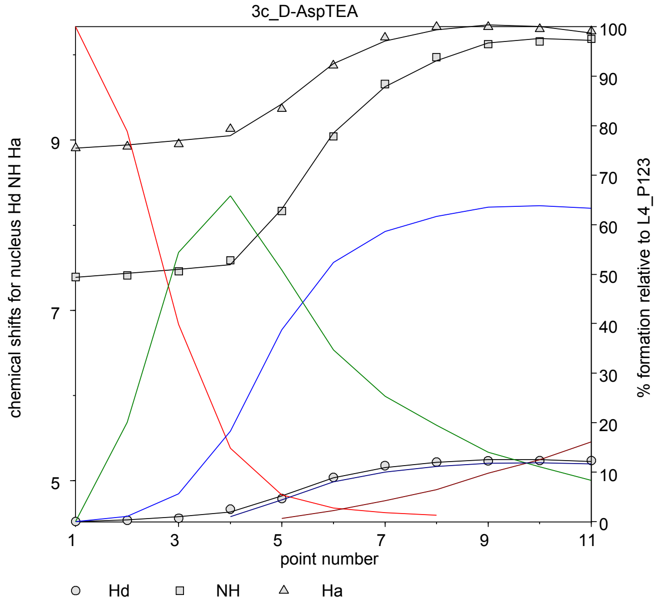


Figure S33. Plot of the experimental and calculated chemical shifts (manual fit) of the **3c**/D-Asp titration experiments, including a more complex binding mode. The obtained binding constants for the corresponding equilibria are shown

3c + L-Asp = [**3c**·L-Asp] logβ = 3.52
3c + 2L-Asp = [**3c**·L-Asp$_2$] logβ = 4.98
2**3c** + L-Asp = [**3c**$_2$·L-Asp] logβ = 6.54
2**3c** + 2L-Asp = [**3c**$_2$·L-Asp$_2$] logβ = 8.78

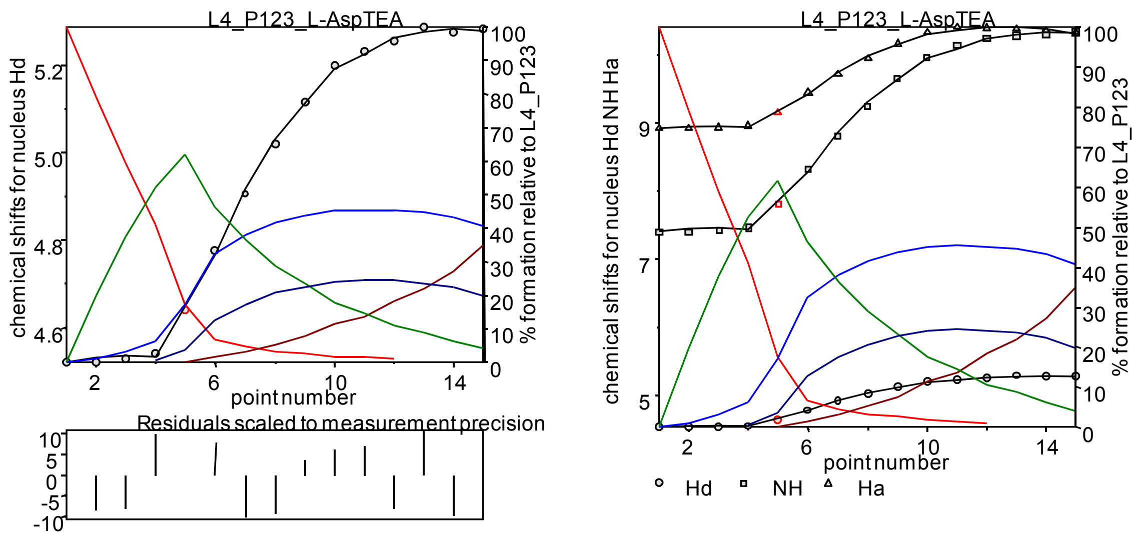


Figure S34. Plot of the experimental and calculated chemical shifts (manual fit) of the **3c**/L-Asp titration experiments, including a more complex binding mode. The obtained binding constants for the corresponding equilibria are shown

For the complexes **3a**, **3b** and **3c** with Glu

3a + D-Glu = [**3a**·D-Glu] logβ = 4.38
3a + 2D-Glu = [**3a**·D-Glu_2] logβ = 7.51
3a + 3D-Glu = [**3a**·D-Glu_3] logβ = 8.86
2**3a** + 2D-Glu = [$\mathbf{3a}_2$·D-Glu_2] logβ = 9,54
2**3a** + 3D-Glu = [$\mathbf{3a}_2$·D-Glu_3] logβ = 12.96

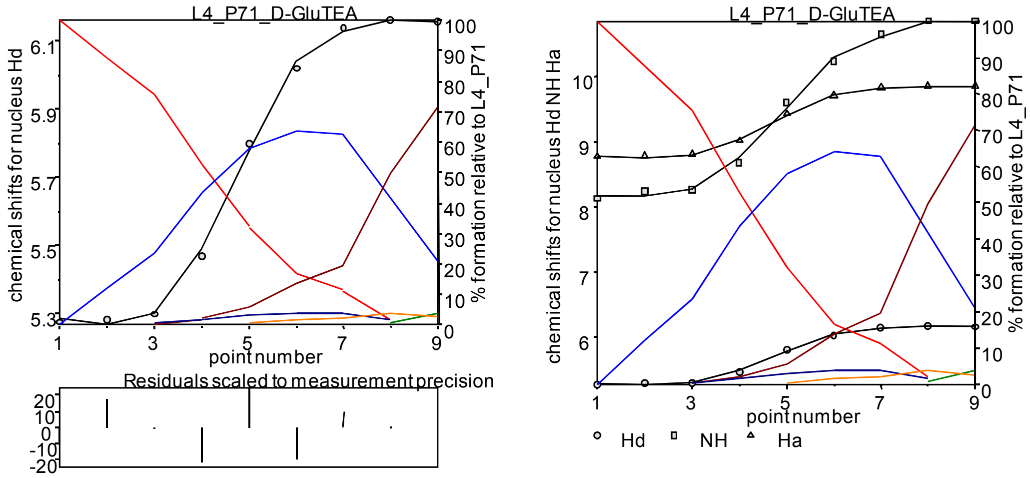


Figure S35. Plot of the experimental and calculated chemical shifts (manual fit) of the **3a**/L-Glu titration experiments, including a more complex binding mode. The obtained binding constants for the corresponding equilibria are shown.

3a + L-Glu = [**3a**·L-Glu] logβ = 4.29
3a + 2L-Glu = [**3a**·L-Glu_2] logβ = 7.21
3a + 3L-Glu = [**3a**·L-Glu_3] logβ = 9.12
2**3a** + 2L-Glu = [$\mathbf{3a}_2$·L-Glu_2] logβ = 10.84
2**3a** + 3L-Glu = [$\mathbf{3a}_2$·L-Glu_3] logβ = 12.80

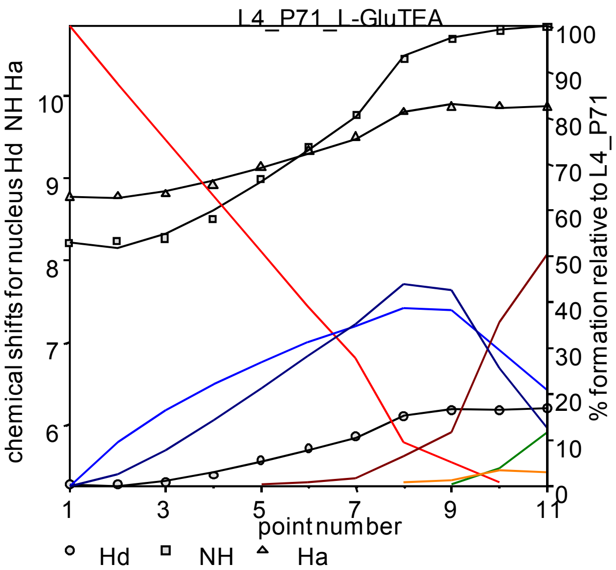


Figure S36. Plot of the experimental and calculated chemical shifts (manual fit) of the **3a**/D-Glu titration experiments, including a more complex binding mode. The obtained binding constants for the corresponding equilibria are shown

3b+ D-Glu = [**3b**·D-Glu] logβ = 4.96

3b + 2D-Glu = [**3b**·D-Glu_2] logβ = 11.01

2**3b** + D-Glu = [$\mathbf{3b}_2$·D-Glu] logβ = 7.62

2**3b** + 2D-Glu = [$\mathbf{3b}_2$·D-Glu_2] logβ = 14.54

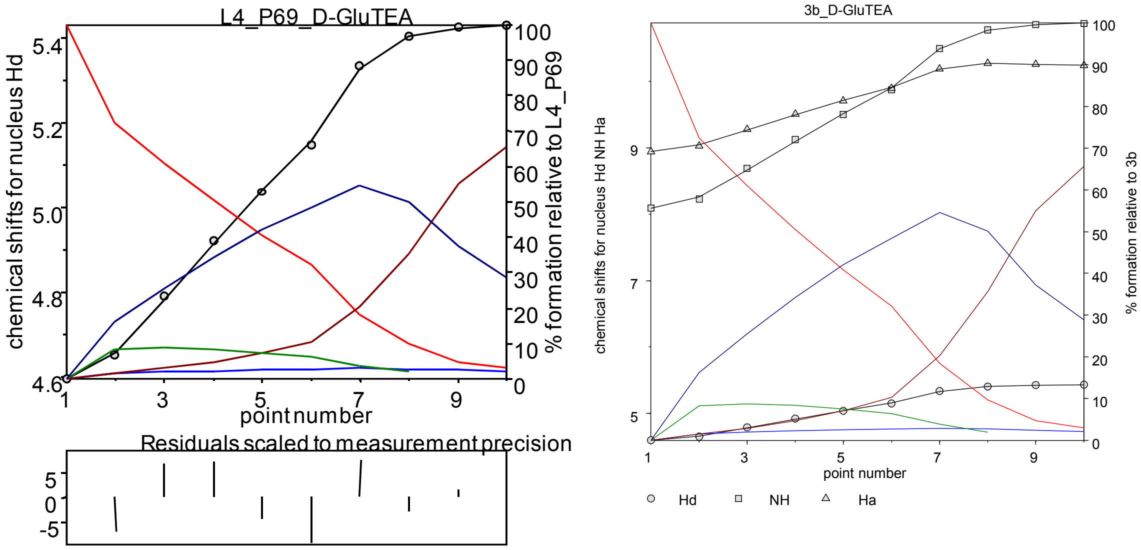


Figure S37. Plot of the experimental and calculated chemical shifts (manual fit) of the **3b**/D-Glu titration experiments, including a more complex binding mode. The obtained binding constants for the corresponding equilibria are shown

3b+ L-Glu = [**3b**·L-Glu] logβ = 4.95

3b + 2L-Glu = [**3b**·L-Glu_2] logβ = 8.93

2**3b** + L-Glu = [$\mathbf{3b}_2$·L-Glu] logβ = 7.41

2**3b** + 2L-Glu = [$\mathbf{3b}_2$·L-Glu_2] logβ = 13.69

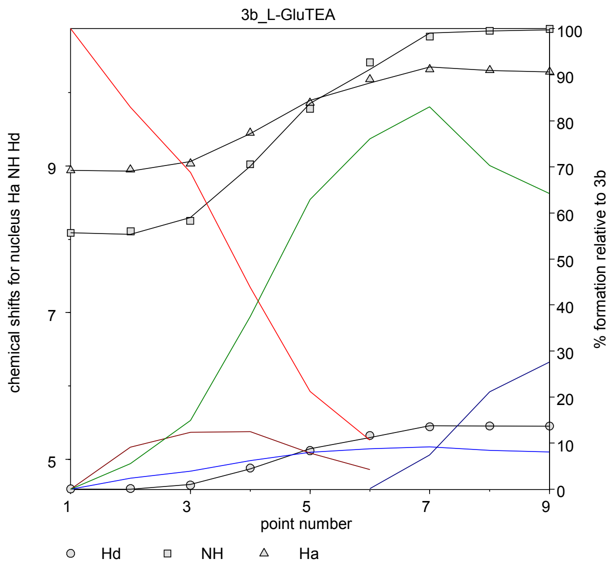


Figure S38. Plot of the experimental and calculated chemical shifts (manual fit) of the **3b**/L-Glu titration experiments, including a more complex binding mode. The obtained binding constants for the corresponding equilibria are shown

3c + D-Glu = [**3c**·D-Glu] logβ = 4.86
3c + 2D-Glu = [**3c**·D-Glu$_2$] logβ = 9.65
2**3c** + D-Glu = [**3c**$_2$·D-Glu] logβ = 7.45
2**3c** + 2D-Glu = [**3c**$_2$·D-Glu$_2$] logβ = 10.94

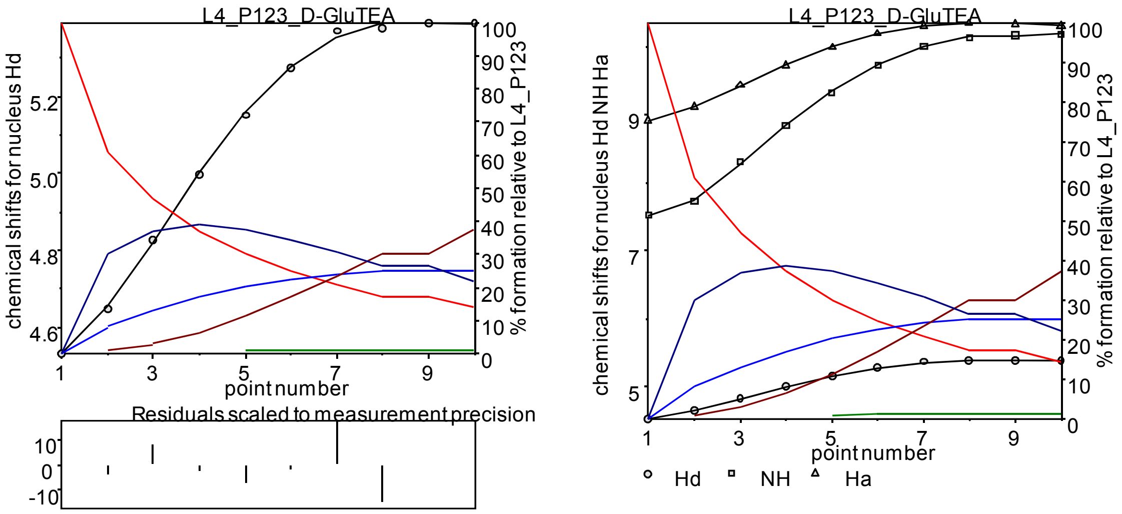


Figure S39. Plot of the experimental and calculated chemical shifts (manual fit) of the **3c**/L-Glu titration experiments, including a more complex binding mode. The obtained binding constants for the corresponding equilibria are shown

3c + L-Glu = [**3c**·L-Glu] logβ = 4.79
3c + 2L-Glu = [**3c**·L-Glu$_2$] logβ = 9.62
2**3c** + L-Glu = [**3c**$_2$·L-Glu] logβ = 7.06
2**3c** + 2L-Glu = [**3c**$_2$·L-Glu$_2$] logβ = 12.00

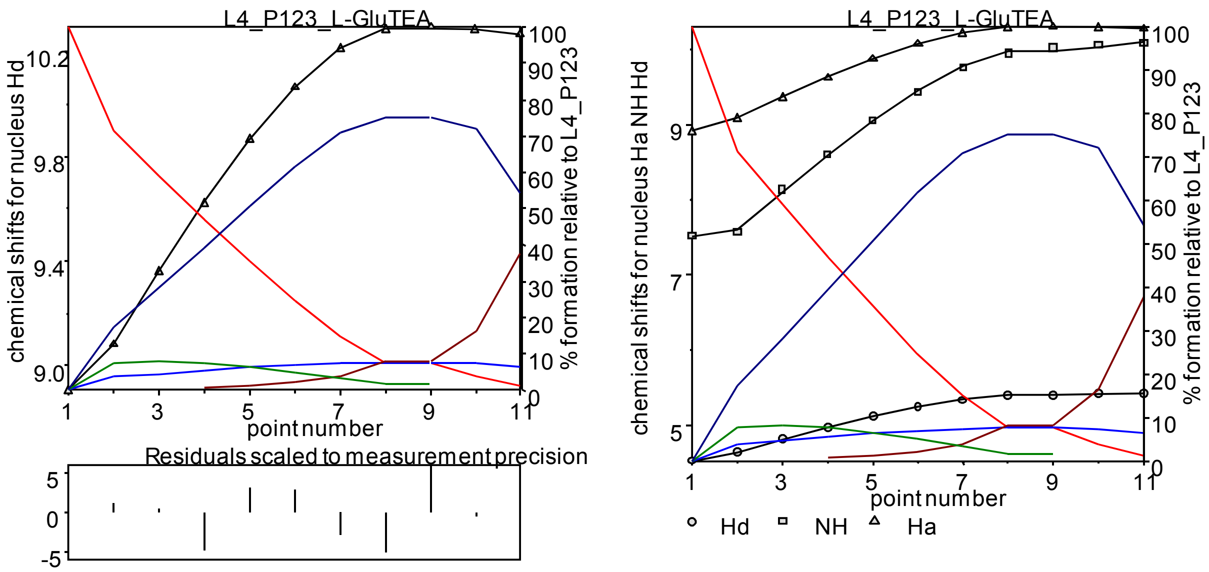


Figure S40. Plot of the experimental and calculated chemical shifts (manual fit) of the **3c**/D-Glu titration experiments, including a more complex binding mode. The obtained binding constants for the corresponding equilibria are shown

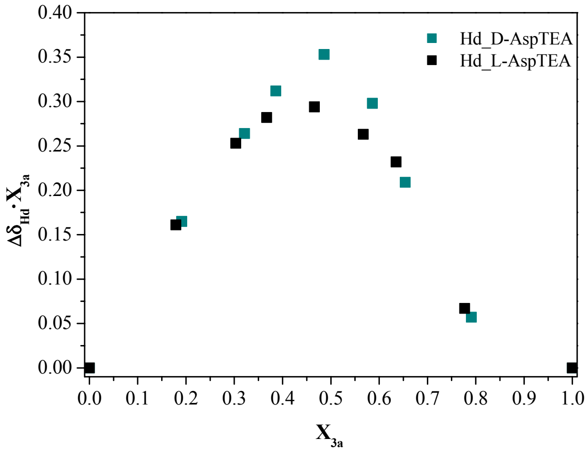


Figure S41. Job plots of **3a** with L-aspartate and with D-aspartate. The Δδ stands for the chemical shift change of the Hd (chiral proton) proton of **3a** in the presence of guest. Total concentration is 8 mM, $CDCl_3$/DMSO-d_6 (5%).

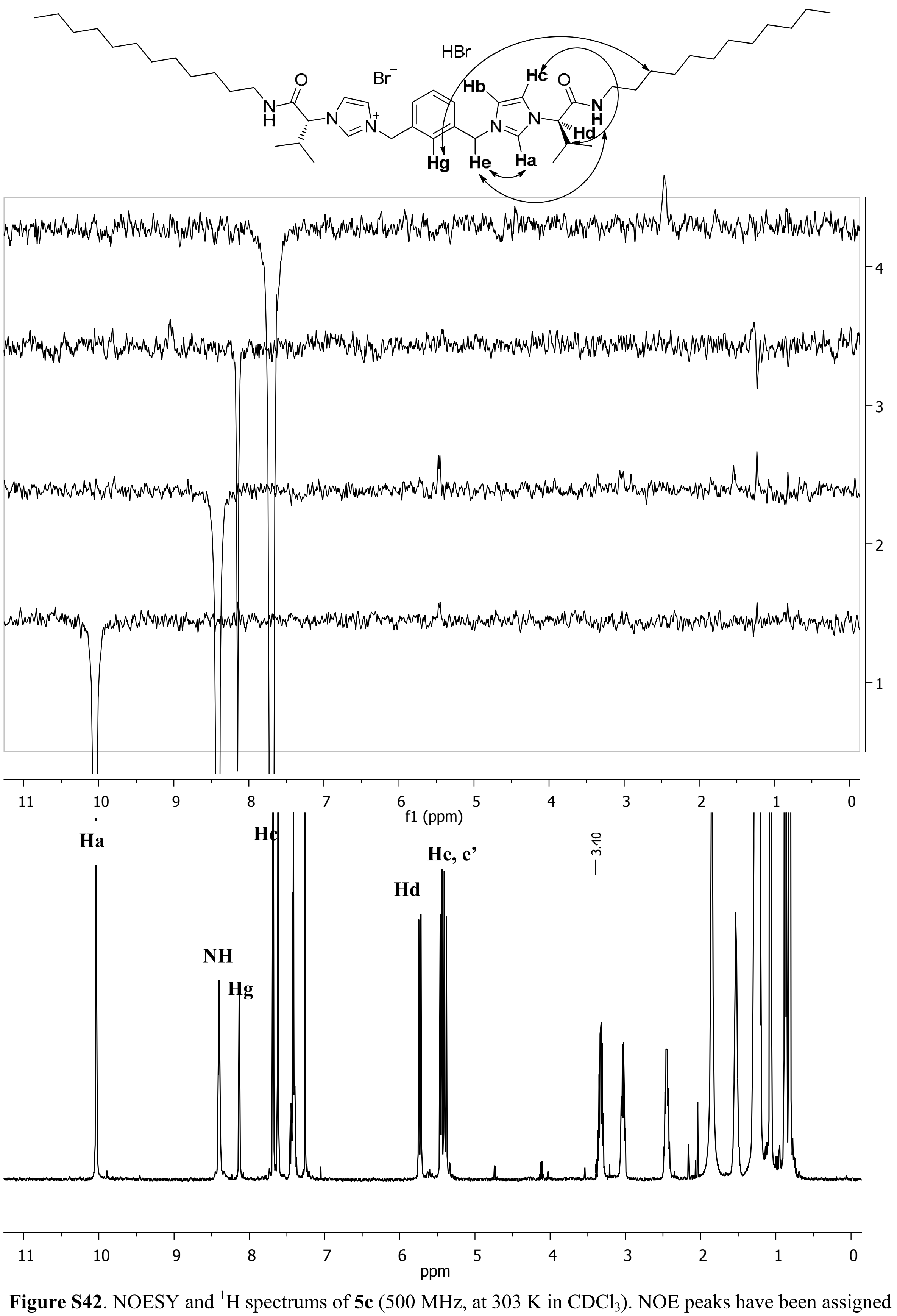


Figure S42. NOESY and [1]H spectrums of **5c** (500 MHz, at 303 K in $CDCl_3$). NOE peaks have been assigned with double-headed arrows (NOESY spectrum 500 MHz, at 303 K in $CDCl_3$).

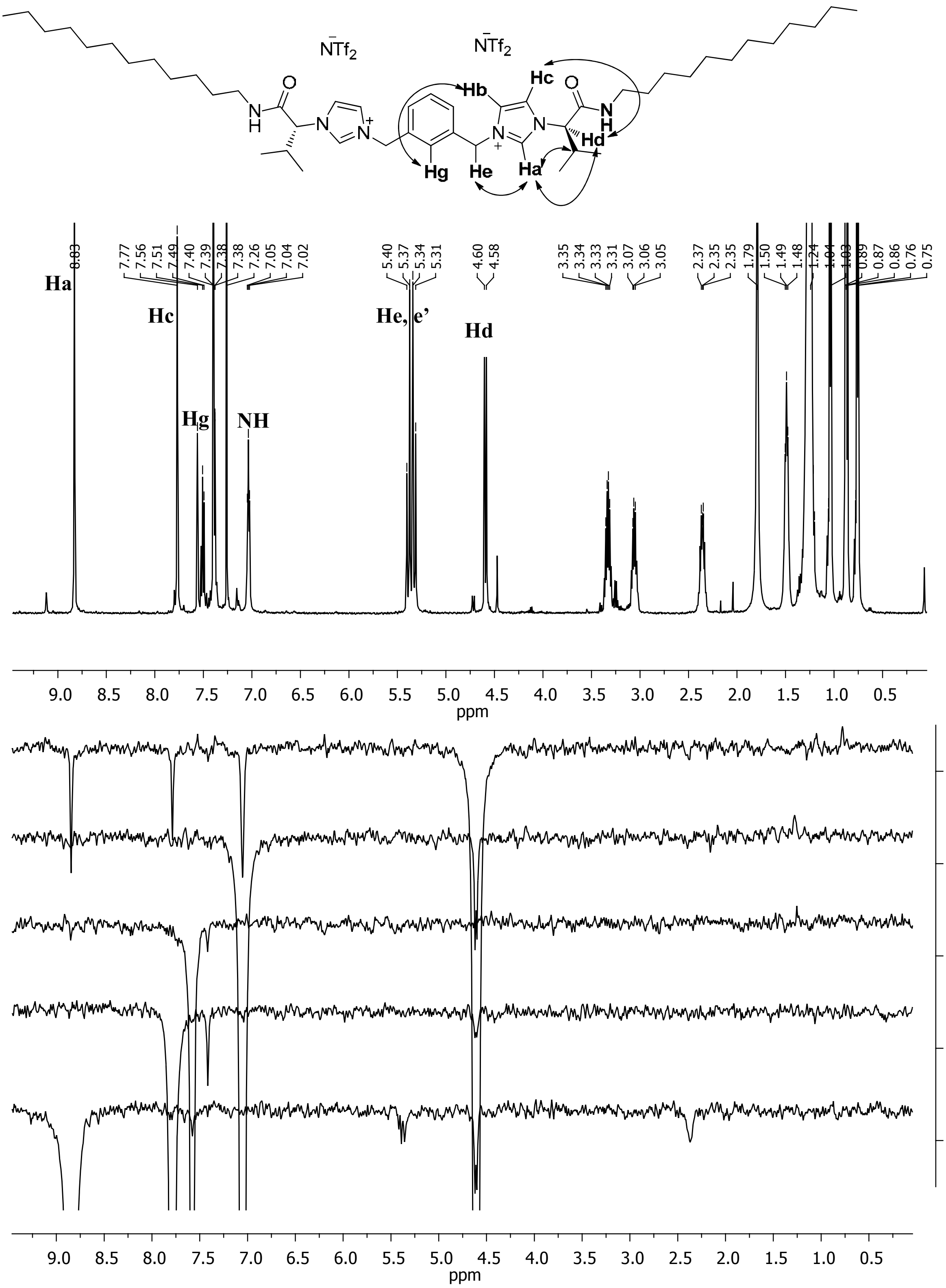


Figure S43. NOESY and ^{1}H spectrums of **3c** (500 MHz, at 303 K in $CDCl_3$). NOE peaks have been assigned with double-headed arrows (NOESY spectrum 500 MHz, at 303 K in $CDCl_3$).

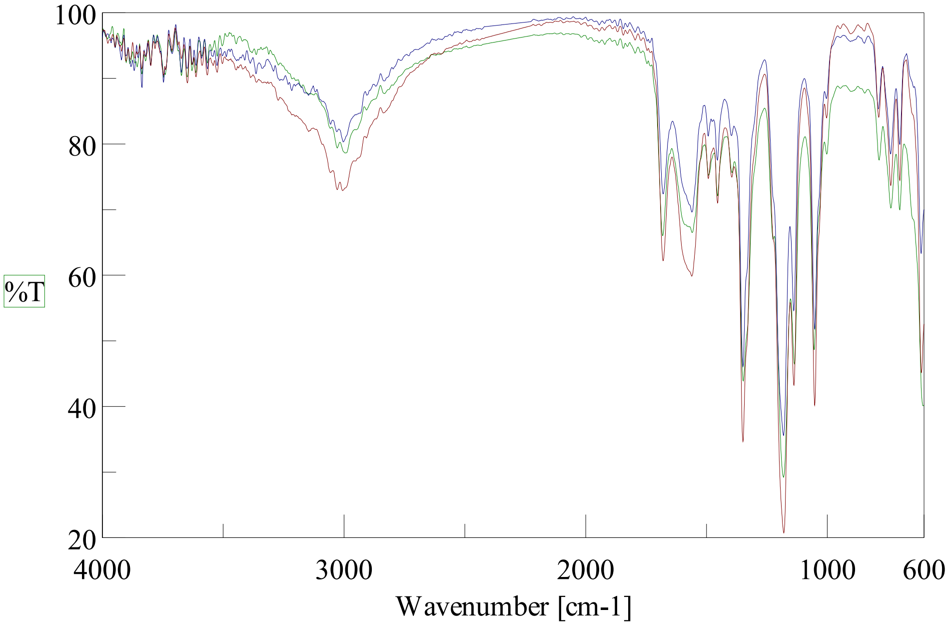


Figure S44. ATR-FTIR spectra of the 1:1 mixture **3a**:L-AspTEA at 25 °C (blue line); **3a**:L-AspTEA at 55 °C (red line) and **3a**:L-AspTEA at 94 °C (green line).

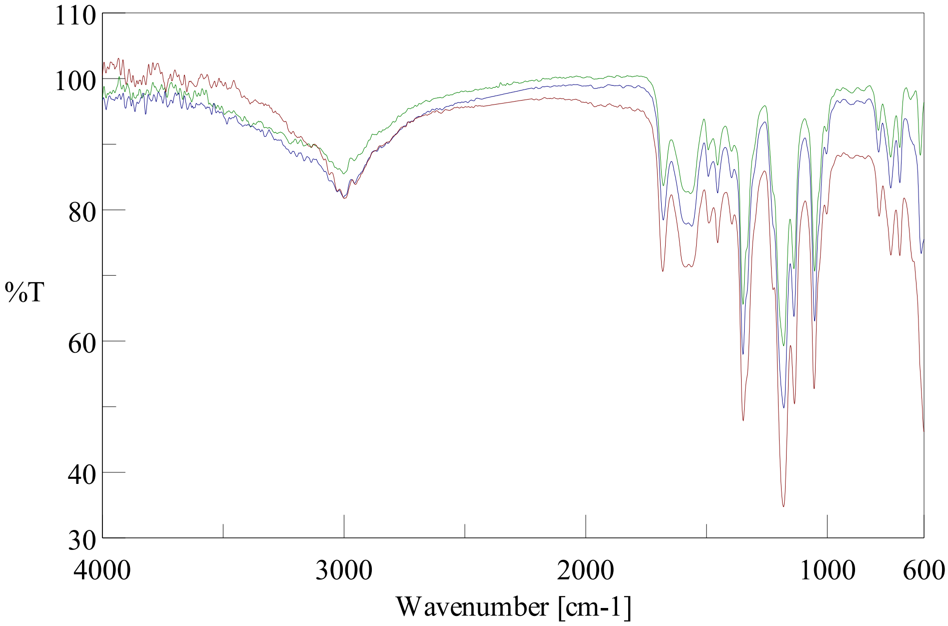


Figure S45. ATR-FTIR spectra of the 1:1 mixture **3a**:D-AspTEA at 30 °C (green line); **3a**:D-AspTEA at 55 °C (blue line) and **3a**:D-AspTEA at 94 °C (red line).

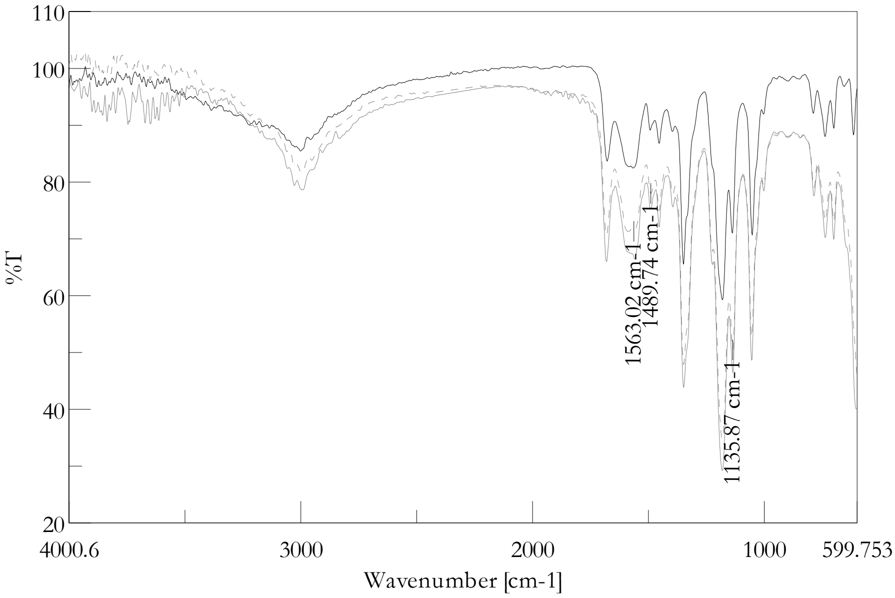


Figure S46. ATR-FTIR spectra of the 1:1 mixture **3a**:D-AspTEA at 25 °C (black line); **3a**:D-AspTEA at 94 °C (dotted grey line) and **3a**:L-AspTEA at 94 °C (grey line).

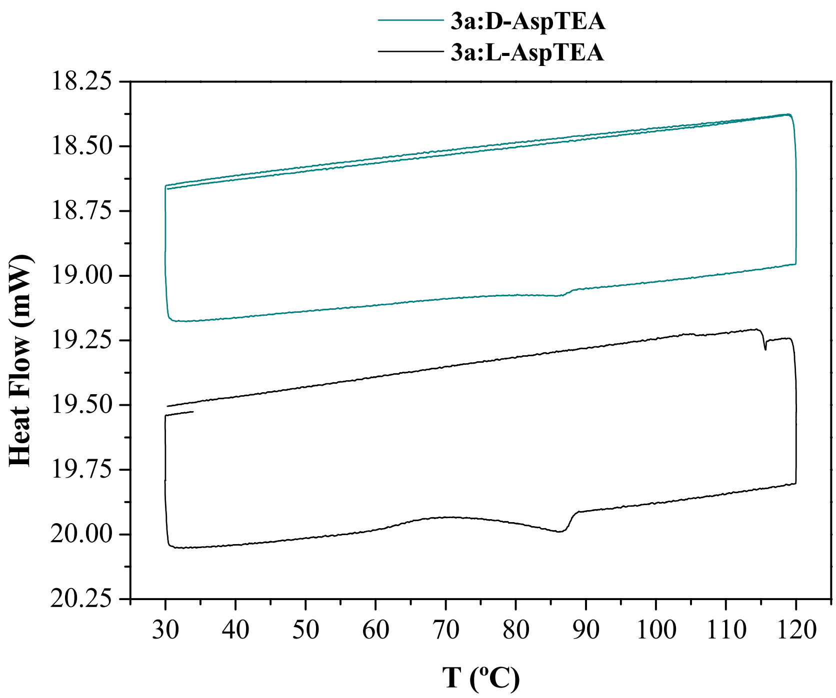


Figure S47. DSC of **3a**:D-aspTEA complex and **3a**:L-AspTEA complex.

Theoretical calculations

Optimized structure for 5a

C	-1.398158000	-2.954080000	1.914275000
H	-2.195135000	-3.570525000	2.342607000
H	-0.666161000	-2.704213000	2.692429000
C	1.365712000	-2.668410000	-2.244764000
H	0.581115000	-2.303075000	-2.922278000
H	2.126695000	-3.214160000	-2.811917000
N	1.991803000	-1.453591000	-1.672848000
N	3.006255000	-0.085877000	-0.319662000
N	-1.972072000	-1.662102000	1.491696000
N	-2.980929000	-0.137471000	0.313495000
C	2.048783000	-0.221633000	-2.303160000
H	1.564832000	-0.057595000	-3.252964000
C	2.690272000	0.636145000	-1.459796000
H	2.900708000	1.689615000	-1.538477000
C	2.574513000	-1.342559000	-0.471639000
H	2.618852000	-2.098477000	0.297502000
C	-2.684700000	-1.438505000	0.379215000
H	-2.927189000	-2.163952000	-0.379804000
C	-1.797026000	-0.456290000	2.150961000
H	-1.165283000	-0.387348000	3.023191000
C	-2.441481000	0.498393000	1.421774000
H	-2.537806000	1.562242000	1.562928000
C	0.733527000	-3.534537000	-1.182723000
C	-0.581567000	-5.061269000	0.760027000
C	0.849529000	-4.926375000	-1.192283000
C	-0.036517000	-2.921282000	-0.194792000
C	-0.684389000	-3.666263000	0.786495000
C	0.183321000	-5.684856000	-0.226574000
H	1.447560000	-5.419426000	-1.954818000
H	-0.122845000	-1.842385000	-0.194959000
H	0.266678000	-6.767850000	-0.239975000
H	-1.082805000	-5.659827000	1.516969000
Br	-1.460668000	-0.857945000	-3.015378000
Br	1.523590000	-1.366487000	2.966865000
C	3.720433000	0.378393000	0.885572000
H	3.532696000	-0.393208000	1.635779000
C	-3.731694000	0.455569000	-0.813277000
C	-3.236628000	1.889612000	-1.102062000
C	3.154216000	1.730365000	1.372375000
N	2.510891000	1.659856000	2.551655000
H	2.214378000	0.728919000	2.887854000
N	-2.640014000	2.029332000	-2.301690000
H	-2.280574000	1.175592000	-2.759692000
O	-3.475897000	2.803051000	-0.305739000
O	3.383332000	2.763333000	0.734073000
C	-2.259667000	3.334479000	-2.833203000
H	-2.644662000	3.408339000	-3.857117000
H	-2.783208000	4.075413000	-2.221698000
C	2.080438000	2.851324000	3.281827000
H	2.627118000	3.694352000	2.853236000
H	2.402057000	2.730143000	4.322817000

C	5.234494000	0.526332000	0.612423000
H	5.684698000	0.873477000	1.550992000
H	5.378784000	1.328988000	-0.117165000
C	-5.248014000	0.489673000	-0.515154000
H	-5.725465000	0.947064000	-1.390894000
H	-5.419717000	1.167322000	0.326615000
H	-3.508710000	-0.190565000	-1.668410000
C	-0.768698000	3.620405000	-2.838981000
C	1.968168000	4.252949000	-2.858034000
C	-0.039495000	3.660217000	-1.643300000
C	-0.106737000	3.886728000	-4.042161000
C	1.253840000	4.203519000	-4.055168000
C	1.319496000	3.976484000	-1.649610000
H	-0.542250000	3.444358000	-0.704264000
H	-0.661484000	3.845692000	-4.977148000
H	1.751788000	4.411085000	-4.999002000
H	1.880874000	3.991293000	-0.719397000
H	3.025366000	4.506873000	-2.860841000
C	0.586882000	3.121169000	3.244724000
C	-2.172111000	3.663135000	3.211366000
C	0.030477000	3.930995000	2.246509000
C	-0.257151000	2.584088000	4.224783000
C	-1.627517000	2.853513000	4.210977000
C	-1.339596000	4.198354000	2.224866000
H	0.678116000	4.364073000	1.488327000
H	0.162855000	1.956114000	5.007608000
H	-2.266881000	2.438076000	4.986019000
H	-1.760283000	4.817621000	1.438131000
H	-3.237342000	3.877428000	3.197098000
C	-5.839492000	-0.878067000	-0.251642000
C	-6.895754000	-3.440013000	0.239113000
C	-5.989103000	-1.803527000	-1.295744000
C	-6.227041000	-1.257724000	1.039727000
C	-6.752833000	-2.528317000	1.285425000
C	-6.512197000	-3.073636000	-1.053672000
H	-5.692970000	-1.526524000	-2.305122000
H	-6.119833000	-0.549032000	1.858024000
H	-7.052402000	-2.802632000	2.293650000
H	-6.623418000	-3.775972000	-1.875394000
H	-7.306261000	-4.428411000	0.427494000
C	5.893329000	-0.757626000	0.157924000
C	7.077536000	-3.166001000	-0.687358000
C	6.280009000	-0.935469000	-1.176518000
C	6.108779000	-1.806863000	1.063842000
C	6.695398000	-3.001078000	0.646249000
C	6.869351000	-2.129571000	-1.597794000
H	6.124706000	-0.128930000	-1.889745000
H	5.813831000	-1.686624000	2.104086000
H	6.856540000	-3.801426000	1.363398000
H	7.167338000	-2.246852000	-2.636494000
H	7.537871000	-4.095055000	-1.012685000

Optimized structure for 3c

C	-2.249842000	-0.010792000	-2.198060000
H	-2.241379000	1.117102000	-2.047742000
H	-3.116224000	-0.214351000	-2.870553000
C	2.775680000	-0.166970000	-2.097175000
H	3.624497000	-0.804182000	-2.449169000
H	2.701648000	-0.413541000	-0.991606000
N	3.116186000	1.263190000	-2.240265000
N	3.220535000	3.456761000	-1.844413000
N	-2.497955000	-0.651640000	-0.888949000
N	-2.622325000	-0.962195000	1.317399000
C	3.898898000	1.836021000	-3.254029000
H	4.340108000	1.264966000	-4.056215000
C	3.969552000	3.201744000	-3.003833000
H	4.463586000	4.000897000	-3.563038000
C	2.703105000	2.260065000	-1.381790000
H	2.087205000	2.106122000	-0.477636000
C	-2.237443000	-0.069899000	0.333990000
H	-1.843003000	0.953100000	0.484891000
C	-3.034288000	-1.932452000	-0.673790000
H	-3.302040000	-2.604905000	-1.473857000
C	-3.123679000	-2.120241000	0.700354000
H	-3.498319000	-2.970679000	1.271997000
C	1.478677000	-0.495375000	-2.788248000
C	-0.946152000	-1.167812000	-4.015205000
C	1.479022000	-1.201107000	-3.998720000
C	0.266891000	-0.121537000	-2.190697000
C	-0.945070000	-0.455239000	-2.807143000
C	0.265274000	-1.536279000	-4.606022000
H	2.418204000	-1.500624000	-4.462842000
H	0.278211000	0.421250000	-1.238140000
H	0.264138000	-2.090815000	-5.545046000
H	-1.884788000	-1.433315000	-4.499799000
C	3.015981000	4.777724000	-1.206947000
H	2.099127000	4.716644000	-0.533352000
C	-2.515366000	-0.698263000	2.771177000
C	-2.365627000	-2.047950000	3.521916000
C	2.803748000	5.826346000	-2.333188000
N	1.670272000	6.583935000	-2.217408000
H	1.005176000	6.441656000	-1.436450000
N	-1.194835000	-2.206734000	4.219180000
O	-3.266866000	-2.879273000	3.508771000
O	3.619861000	5.946060000	-3.242628000
C	-1.009157000	-3.347423000	5.153778000
H	-2.002803000	-3.822275000	5.346498000
C	1.342176000	7.629711000	-3.219780000
H	2.284785000	8.136570000	-3.538253000
H	0.703100000	8.393581000	-2.723870000
C	4.244494000	5.185160000	-0.338269000
H	5.145899000	5.226914000	-1.001924000
C	-3.780796000	0.037671000	3.312433000
H	-4.667746000	-0.625597000	3.137183000
H	-1.602575000	-0.039545000	2.934830000
H	-0.645701000	-2.938998000	6.123737000
C	0.639772000	7.044086000	-4.454215000
H	1.239661000	6.201882000	-4.855721000
H	0.633625000	7.810759000	-5.254579000

C	-0.791280000	6.580548000	-4.165933000
H	-0.797186000	5.798430000	-3.374810000
H	-1.390913000	7.415123000	-3.756184000
C	-0.037693000	-4.403822000	4.612458000
H	-0.345031000	-4.711648000	3.593147000
C	1.420278000	-3.930707000	4.597460000
H	1.697958000	-3.506094000	5.580514000
H	1.534964000	-3.100896000	3.870764000
H	-0.127182000	-5.318000000	5.234405000
C	2.391233000	-5.057798000	4.220385000
H	1.970025000	-5.668905000	3.399575000
H	3.316668000	-4.613575000	3.790569000
C	-1.463121000	6.025845000	-5.430104000
H	-1.527427000	6.811782000	-6.205479000
H	-0.839236000	5.220075000	-5.862172000
C	2.744184000	-5.954372000	5.413856000
H	3.209200000	-5.347454000	6.214186000
H	1.821736000	-6.379104000	5.853027000
C	3.695292000	-7.085096000	4.998775000
H	3.232526000	-7.689912000	4.195363000
H	4.615165000	-6.655778000	4.555039000
C	4.056718000	-7.983352000	6.189055000
H	3.136140000	-8.407725000	6.633433000
H	4.526025000	-7.377523000	6.987882000
C	5.003592000	-9.115667000	5.768918000
H	5.925201000	-8.689616000	5.327226000
H	4.536601000	-9.717619000	4.965703000
C	-2.862777000	5.484114000	-5.110820000
H	-3.513510000	6.305719000	-4.757071000
H	-2.798201000	4.774723000	-4.255181000
C	-3.493804000	4.795154000	-6.326854000
H	-2.841854000	3.969272000	-6.669774000
H	-3.553666000	5.504982000	-7.173879000
C	-4.892430000	4.254785000	-5.999073000
H	-5.551515000	5.087452000	-5.685434000
H	-4.836792000	3.575133000	-5.127086000
C	-5.508705000	3.521974000	-7.198127000
H	-4.847231000	2.692422000	-7.512670000
H	-5.566546000	4.206112000	-8.066694000
C	-6.906072000	2.980458000	-6.867737000
H	-7.570199000	3.814813000	-6.569244000
H	-6.852347000	2.311347000	-5.987808000
C	-7.514396000	2.229875000	-8.059677000
H	-6.851158000	1.396680000	-8.360498000
H	-7.569991000	2.900450000	-8.938816000
C	-8.912845000	1.689219000	-7.730165000
H	-8.860529000	1.021699000	-6.848095000
H	-9.578771000	2.524559000	-7.436897000
C	-9.521216000	0.936356000	-8.911263000
H	-10.519622000	0.556796000	-8.667077000
H	-9.622413000	1.581608000	-9.791467000
C	5.362616000	-10.018554000	6.956660000
H	5.830113000	-9.415732000	7.758889000
H	4.440623000	-10.443783000	7.397670000
C	6.309474000	-11.149923000	6.534926000
H	5.844473000	-11.751226000	5.730289000

H	7.232566000	-10.725236000	6.095697000
C	6.667212000	-12.056426000	7.720997000
H	7.132847000	-11.455400000	8.526422000
H	5.744318000	-12.484677000	8.158664000
C	7.611816000	-13.182719000	7.307158000
H	8.552835000	-12.791772000	6.903791000
H	7.165438000	-13.820351000	6.535698000
H	7.861200000	-13.824011000	8.159643000
H	-8.905774000	0.078370000	-9.203905000
C	-3.993748000	1.368255000	2.594848000
H	-3.118249000	2.027627000	2.660930000
H	-4.830298000	1.924547000	3.040466000
H	-4.238010000	1.244678000	1.534162000
C	-3.619854000	0.257527000	4.818707000
H	-2.716331000	0.829557000	5.061917000
H	-3.581301000	-0.688202000	5.373584000
H	-4.470356000	0.822648000	5.222523000
C	3.992353000	6.575683000	0.247627000
H	4.772898000	6.849183000	0.968121000
H	3.032020000	6.631194000	0.780084000
H	3.985940000	7.354964000	-0.524461000
C	4.482239000	4.164215000	0.774309000
H	5.316981000	4.474770000	1.417433000
H	4.736042000	3.171161000	0.391257000
H	3.608624000	4.060090000	1.431113000
S	2.996239000	-2.790151000	0.825830000
S	1.626598000	-0.279689000	1.918049000
N	2.219582000	-1.720800000	1.733490000
C	2.819096000	0.577207000	3.032415000
C	1.592936000	-3.763300000	0.093120000
F	0.689382000	-2.997821000	-0.536730000
F	0.878713000	-4.477235000	0.964558000
F	2.486571000	1.849507000	3.274887000
F	2.950705000	0.017019000	4.236194000
F	4.060230000	0.638580000	2.535651000
F	1.990974000	-4.642626000	-0.831011000
O	1.632295000	0.523923000	0.688698000
O	0.364660000	-0.271371000	2.653213000
O	3.582878000	-2.136360000	-0.335889000
O	3.772944000	-3.731289000	1.576622000
H	-0.407969000	-1.553502000	4.102637000
S	-2.600027000	3.931109000	-0.790877000
S	-0.827734000	5.747549000	0.876677000
N	-1.964239000	4.733225000	0.414201000
C	-0.461043000	5.131249000	2.575351000
C	-4.407546000	4.245884000	-0.600226000
F	-4.765958000	5.511878000	-0.823999000
F	-4.907908000	3.946707000	0.601131000
F	0.542202000	5.798512000	3.158299000
F	-1.478911000	5.219426000	3.433595000
F	-0.082002000	3.848876000	2.615412000
F	-5.138701000	3.523441000	-1.460374000
O	0.425581000	5.524324000	0.133954000
O	-1.231694000	7.116785000	1.015677000
O	-2.245708000	4.417945000	-2.104606000
O	-2.493628000	2.471786000	-0.624388000

Optimized structure for 5c

C	0.663594000	-0.133211000	2.469995000
H	1.729482000	0.082012000	2.546803000
H	0.192686000	0.313606000	3.353757000
C	1.013024000	0.636342000	-2.501726000
H	0.523111000	1.187184000	-3.314307000
H	1.019297000	-0.411489000	-2.797181000
N	2.383986000	1.138563000	-2.396608000
N	4.536129000	1.150084000	-2.166285000
N	0.438849000	-1.576550000	2.490602000
N	0.725643000	-3.686929000	2.109195000
C	2.808933000	2.420704000	-2.684476000
H	2.082162000	3.164555000	-2.956897000
C	4.167021000	2.425721000	-2.558639000
H	4.922917000	3.180688000	-2.691168000
C	3.439323000	0.382184000	-2.039328000
H	3.421938000	-0.655912000	-1.728394000
C	1.202620000	-2.463265000	1.824262000
H	2.042978000	-2.244243000	1.177771000
C	-0.545864000	-2.246555000	3.189331000
H	-1.254223000	-1.682662000	3.768546000
C	-0.365512000	-3.577529000	2.952379000
H	-0.880221000	-4.468920000	3.267155000
C	0.265558000	0.836578000	-1.205350000
C	-1.190031000	1.045308000	1.196497000
C	-1.001341000	1.434134000	-1.188641000
C	0.782667000	0.347878000	0.002258000
C	0.072601000	0.443552000	1.208264000
C	-1.721378000	1.540525000	0.004301000
H	-1.450948000	1.805708000	-2.107087000
H	1.753067000	-0.142684000	0.005362000
H	-2.706736000	2.001275000	0.001302000
H	-1.773123000	1.129393000	2.110344000
Br	4.449265000	-0.608418000	1.528845000
Br	1.762061000	-3.083735000	-1.890354000
C	5.915290000	0.679071000	-1.839138000
H	5.830685000	-0.230393000	-1.235828000
C	1.257283000	-4.938227000	1.497018000
C	0.059392000	-5.661356000	0.823198000
C	6.613977000	1.783574000	-0.997355000
N	6.355267000	1.731657000	0.351883000
H	5.749987000	0.980215000	0.722137000
N	-0.219630000	-5.239037000	-0.456102000
H	0.396160000	-4.542904000	-0.907034000
O	-0.657876000	-6.455548000	1.434844000
O	7.251510000	2.701978000	-1.516423000
C	-1.445728000	-5.569838000	-1.145021000
H	-1.672569000	-6.626762000	-0.967503000
C	6.680413000	2.808087000	1.260544000
H	7.696661000	3.154750000	1.043661000
H	6.669263000	2.396418000	2.274991000
C	6.706511000	0.356642000	-3.129326000
H	6.855463000	1.277663000	-3.707256000

C	1.953637000	-5.822755000	2.556291000
H	1.219008000	-6.153341000	3.301386000
H	1.988608000	-4.662894000	0.731553000
H	-1.270359000	-5.433723000	-2.217103000
C	5.702485000	3.981010000	1.145688000
H	5.780670000	4.428602000	0.147353000
H	5.994468000	4.754595000	1.865830000
C	4.249294000	3.567102000	1.397436000
H	3.946407000	2.811775000	0.663610000
H	4.161936000	3.108743000	2.389818000
C	-2.622246000	-4.708011000	-0.675785000
H	-2.791838000	-4.864194000	0.396400000
C	-2.403655000	-3.213733000	-0.941421000
H	-2.281010000	-3.042928000	-2.017678000
H	-1.473740000	-2.888617000	-0.460634000
H	-3.522483000	-5.050455000	-1.197644000
C	-3.528617000	-2.326065000	-0.402575000
H	-3.649297000	-2.497972000	0.673970000
H	-3.221588000	-1.279884000	-0.521602000
C	3.296659000	4.758847000	1.298503000
H	3.523899000	5.478475000	2.094007000
H	3.446183000	5.273655000	0.341634000
C	-4.865857000	-2.535207000	-1.114709000
H	-4.728819000	-2.419783000	-2.196590000
H	-5.230578000	-3.553263000	-0.938852000
C	-5.914573000	-1.535268000	-0.622021000
H	-6.049561000	-1.648590000	0.460563000
H	-5.558886000	-0.512732000	-0.798291000
C	-7.254783000	-1.739651000	-1.330136000
H	-7.611948000	-2.761412000	-1.152919000
H	-7.119044000	-1.627627000	-2.412727000
C	-8.301549000	-0.738453000	-0.838710000
H	-7.944151000	0.283280000	-1.015755000
H	-8.437242000	-0.850539000	0.243890000
C	1.840344000	4.303432000	1.405857000
H	1.690784000	3.758678000	2.346066000
H	1.617317000	3.605173000	0.589800000
C	0.876402000	5.488573000	1.341981000
H	1.056051000	6.062539000	0.424832000
H	1.064769000	6.160920000	2.187612000
C	-0.577016000	5.015447000	1.370409000
H	-0.752694000	4.414954000	2.271205000
H	-0.762222000	4.367493000	0.506211000
C	-1.553397000	6.191216000	1.339195000
H	-1.373945000	6.794886000	0.441275000
H	-1.376808000	6.839337000	2.206106000
C	-3.003478000	5.703866000	1.348214000
H	-3.182367000	5.099787000	2.246089000
H	-3.177834000	5.053959000	0.481921000
C	-3.985449000	6.875799000	1.314947000
H	-3.806237000	7.480138000	0.417336000
H	-3.812156000	7.525281000	2.181654000
C	-5.433693000	6.387115000	1.322449000
H	-5.613100000	5.740329000	0.455720000
H	-5.619286000	5.785762000	2.220026000
C	-6.413848000	7.548842000	1.289081000
H	-7.443094000	7.176645000	1.295049000
H	-6.282352000	8.198240000	2.160473000
C	-9.641938000	-0.942175000	-1.546843000
H	-9.506180000	-0.830221000	-2.629452000
H	-9.999440000	-1.963843000	-1.369664000
C	-10.688570000	0.059219000	-1.055570000
H	-10.824361000	-0.052507000	0.027089000
H	-10.331114000	1.080976000	-1.232527000
C	-12.027965000	-0.144342000	-1.763237000
H	-11.898578000	-0.029590000	-2.845732000
H	-12.391857000	-1.163112000	-1.586049000
C	-13.071240000	0.849289000	-1.277661000
H	-12.751973000	1.878629000	-1.469661000
H	-13.248000000	0.738818000	-0.203003000
H	-14.020876000	0.685787000	-1.796669000
H	-6.276123000	8.152534000	0.386350000
C	3.051917000	-5.048114000	3.293442000
H	3.797076000	-4.654400000	2.593780000
H	3.569624000	-5.695121000	4.009851000
H	2.637044000	-4.207210000	3.857773000
C	2.569896000	-7.069859000	1.911834000
H	3.308776000	-6.797950000	1.150169000
H	1.807751000	-7.694524000	1.436140000
H	3.073126000	-7.686429000	2.664519000
C	8.085813000	-0.225090000	-2.796557000
H	8.638678000	-0.459901000	-3.712625000
H	7.995649000	-1.147012000	-2.211787000
H	8.693198000	0.481363000	-2.222772000
C	5.952267000	-0.635121000	-4.021987000
H	6.550759000	-0.901165000	-4.900063000
H	5.014713000	-0.206780000	-4.389587000
H	5.718138000	-1.557878000	-3.480310000