Efficient microwave-assisted synthetic protocols and *in silico* behaviour prediction of *per*-substituted β-cyclodextrins.

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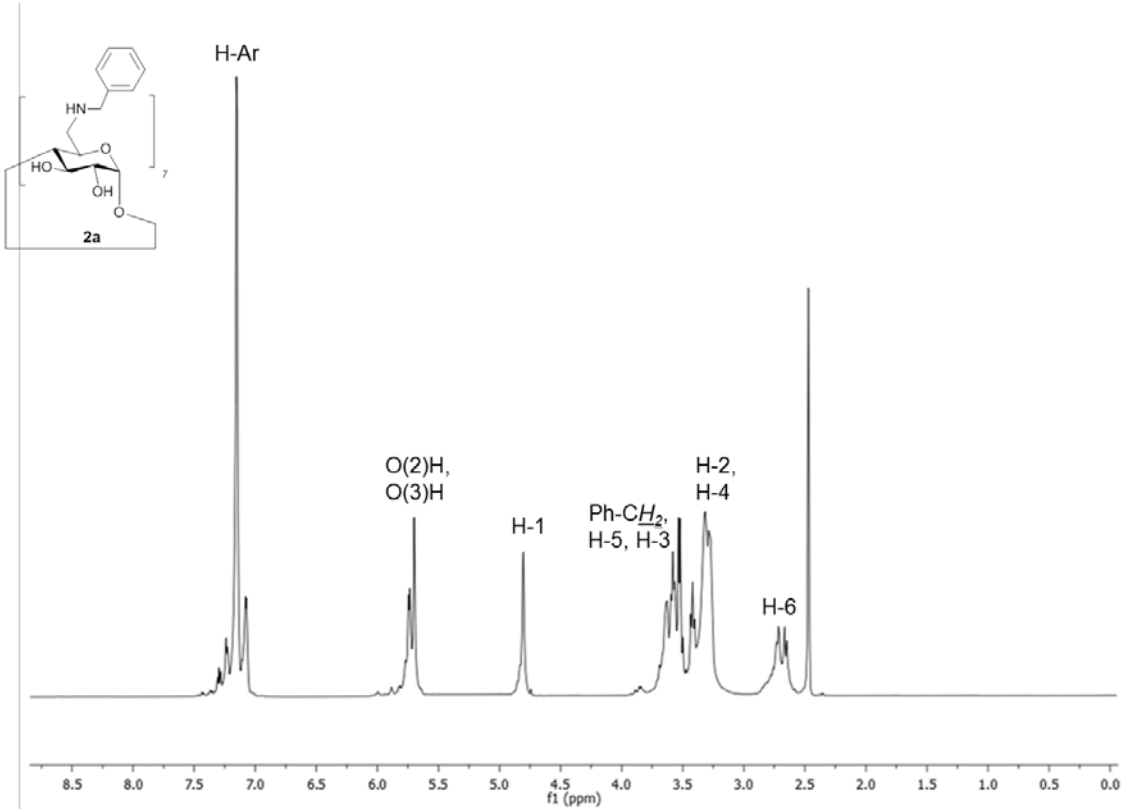


Fig 1. ^{1}H-NMR of *per*-(6-benzylamino-6-deoxy)-β-CD **(2a)**

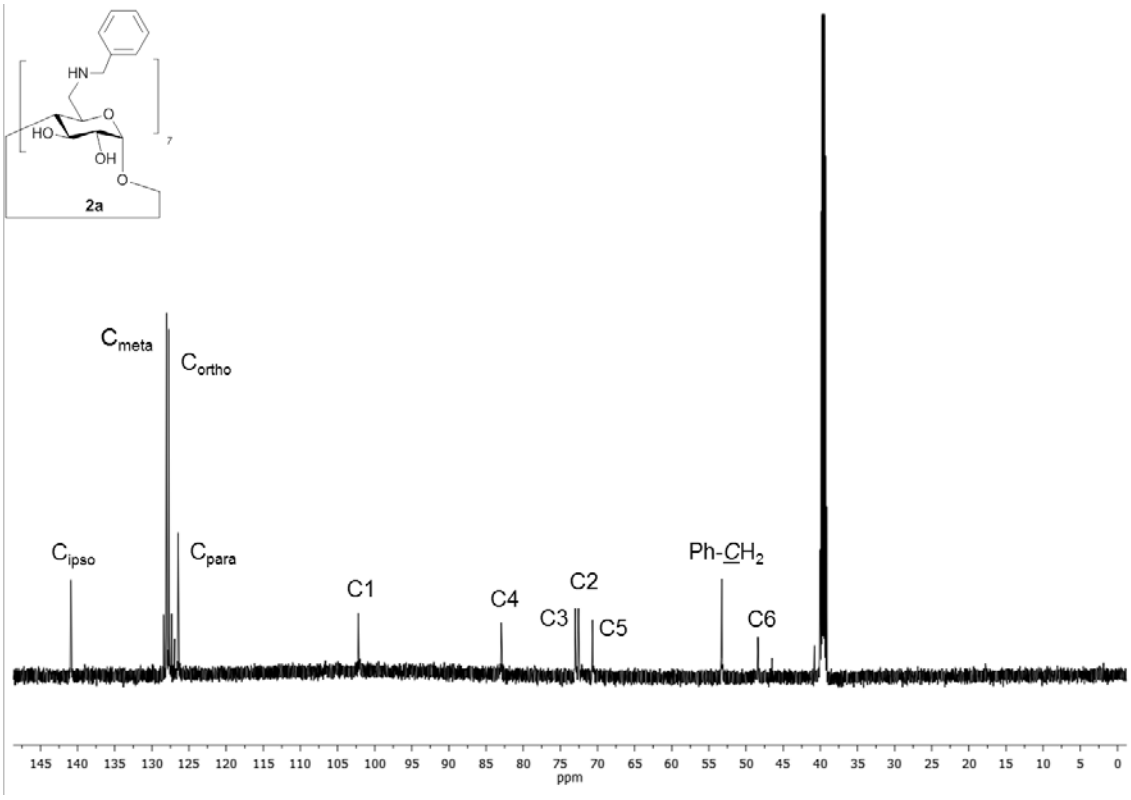


Fig 2. ^{13}C NMR of *per*-(6-benzylamino-6-deoxy)-β-CD **(2a)**

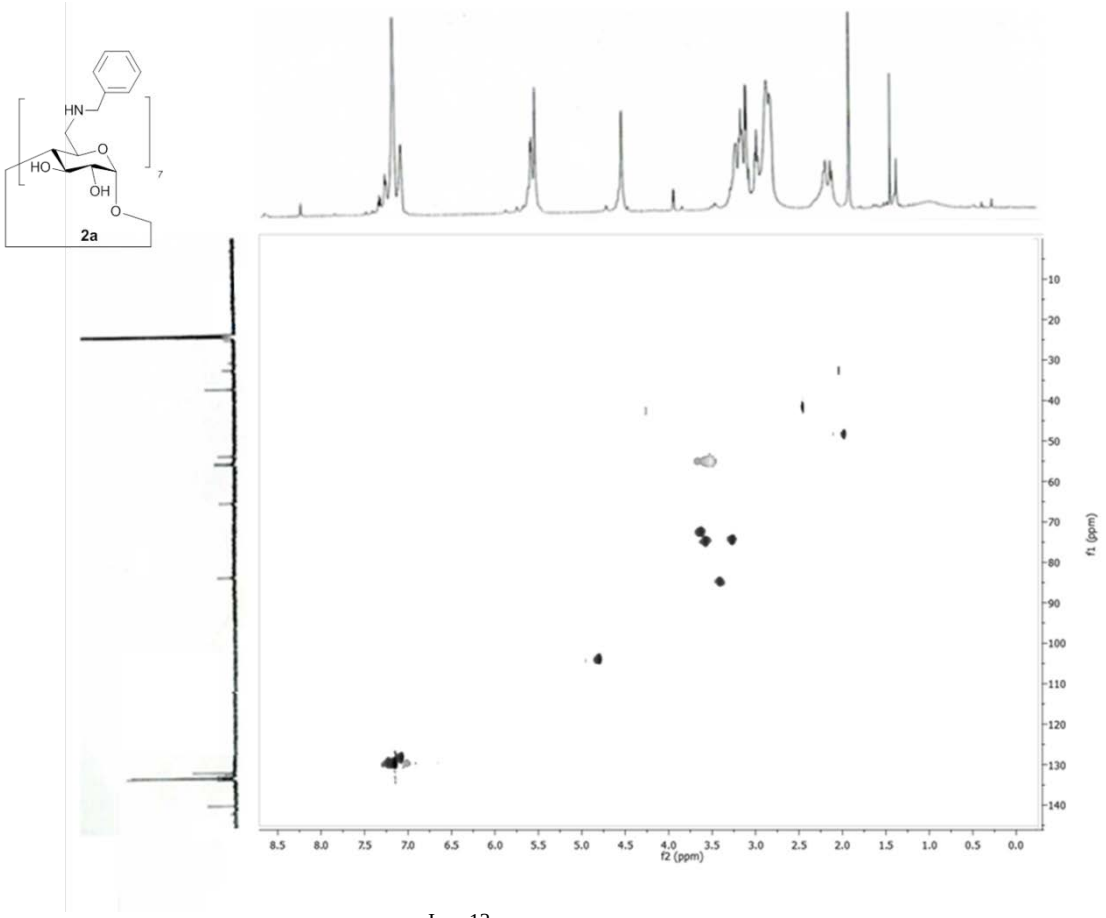


Fig 3. HMQC spectrum (300 MHz for ^{1}H-^{13}C, in DMSO-d_6) of *per*-(6-benzylamino-6-deoxy)-β-CD **(2a)**

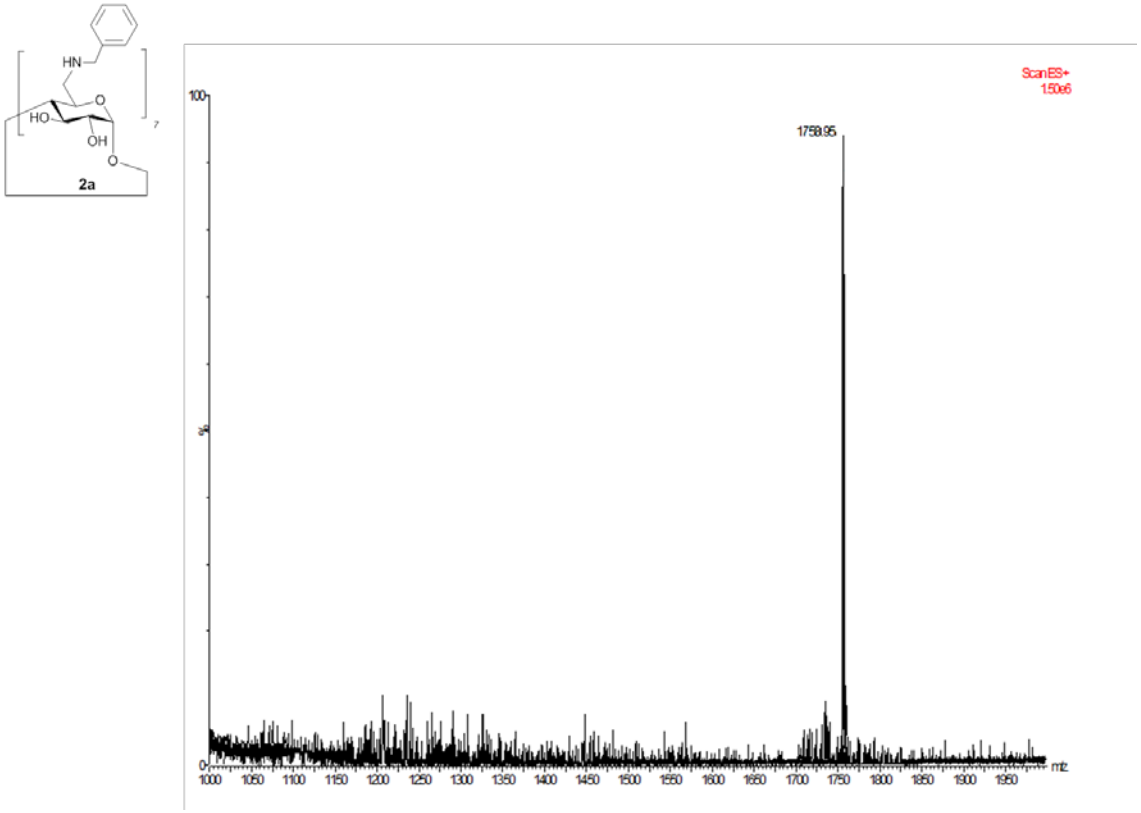


Fig 4. MS (ESI) spectrum of *per*-(6-benzylamino-6-deoxy)-β-CD **(2a)**

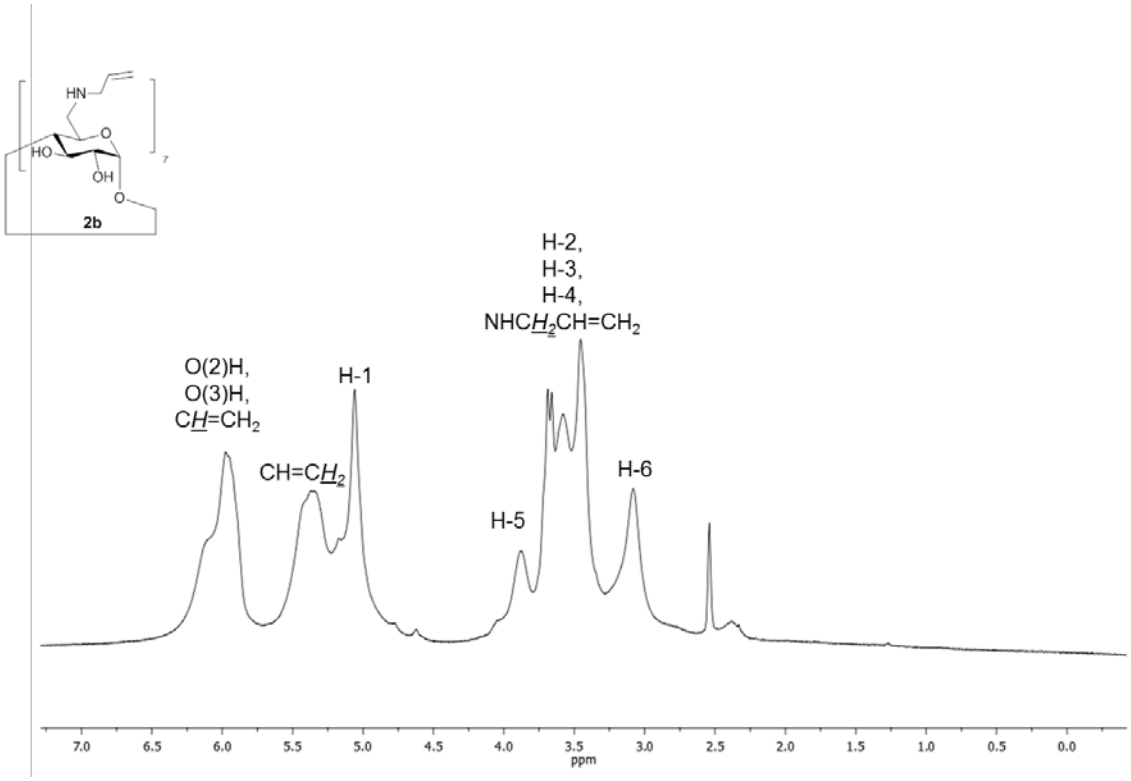
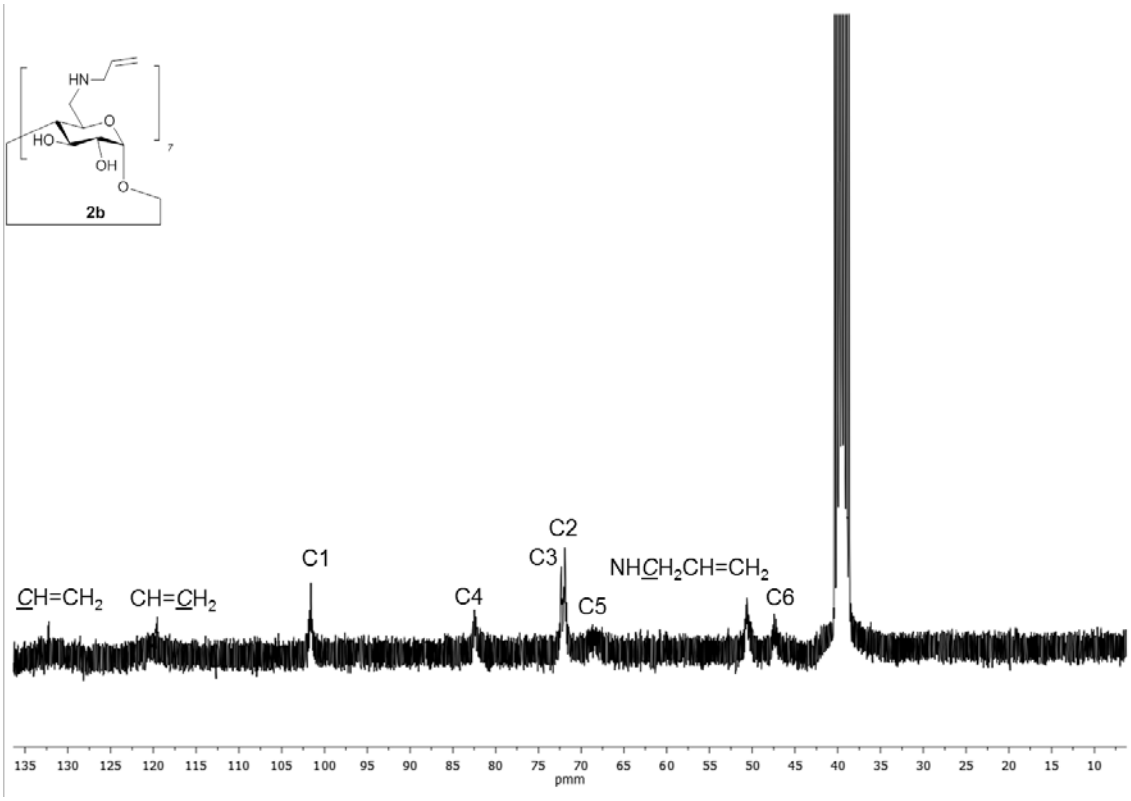


Fig 5. ^{1}H-NMR of *per*-(6-allylamino-6-deoxy)-β-CD **(2b)**



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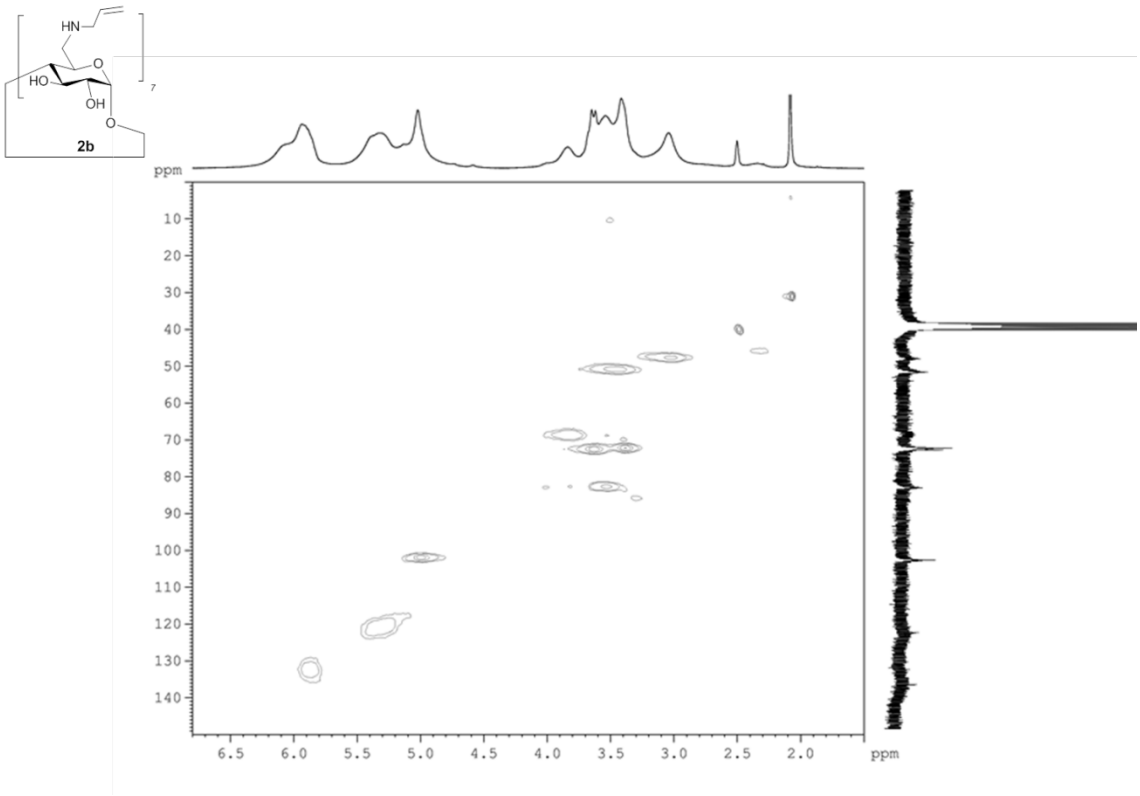
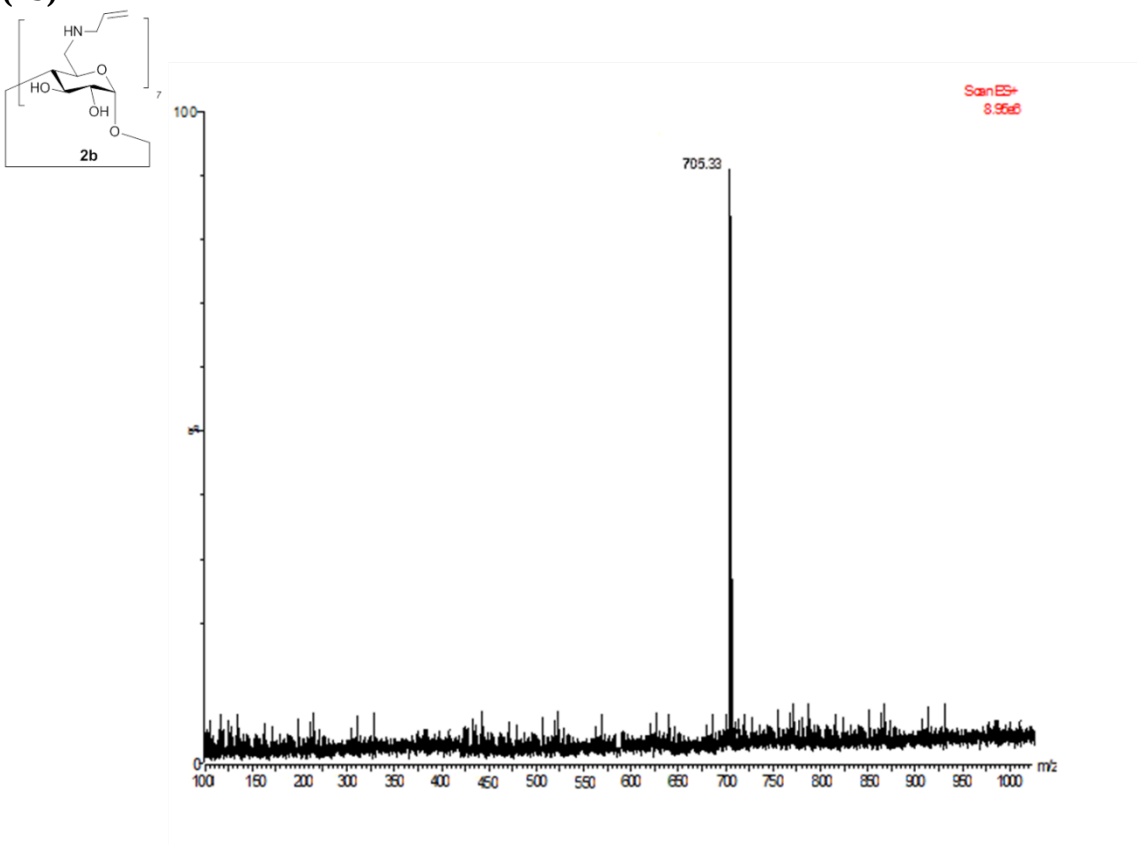


Fig 7. HMQC spectrum (300 MHz for ^{1}H-^{13}C, in DMSO-d_6) of *per*-(6-allylamino-6-deoxy)-β-CD **(2b)**



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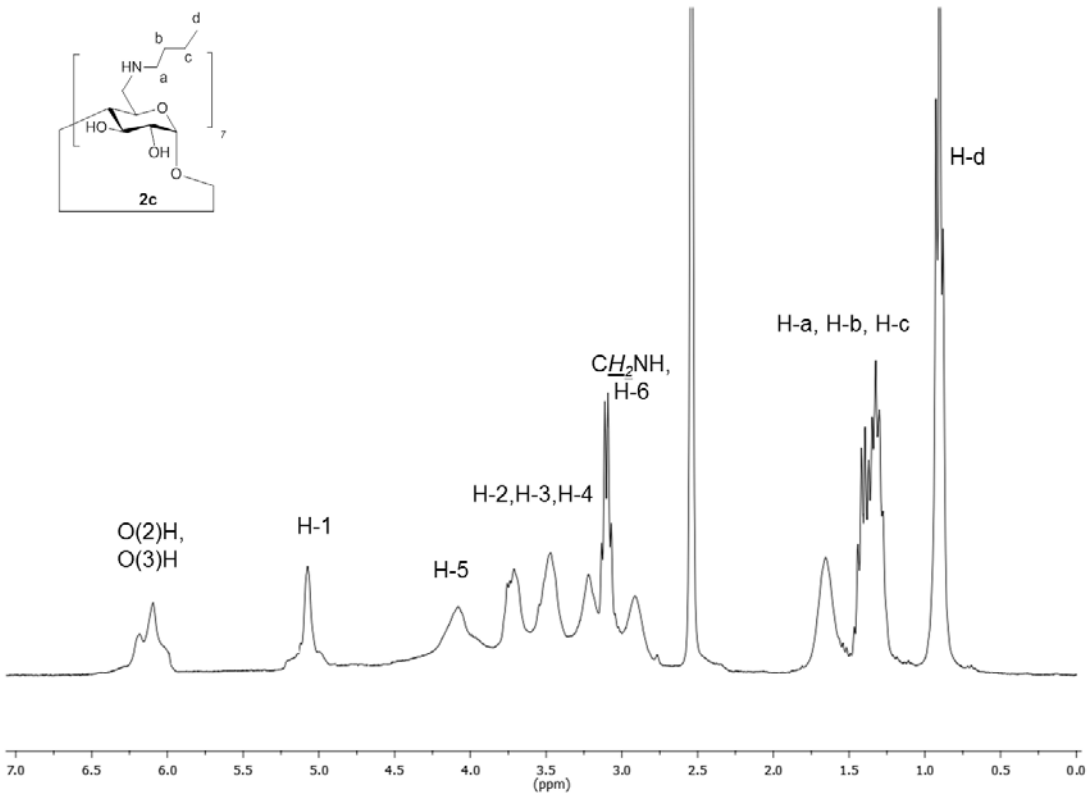
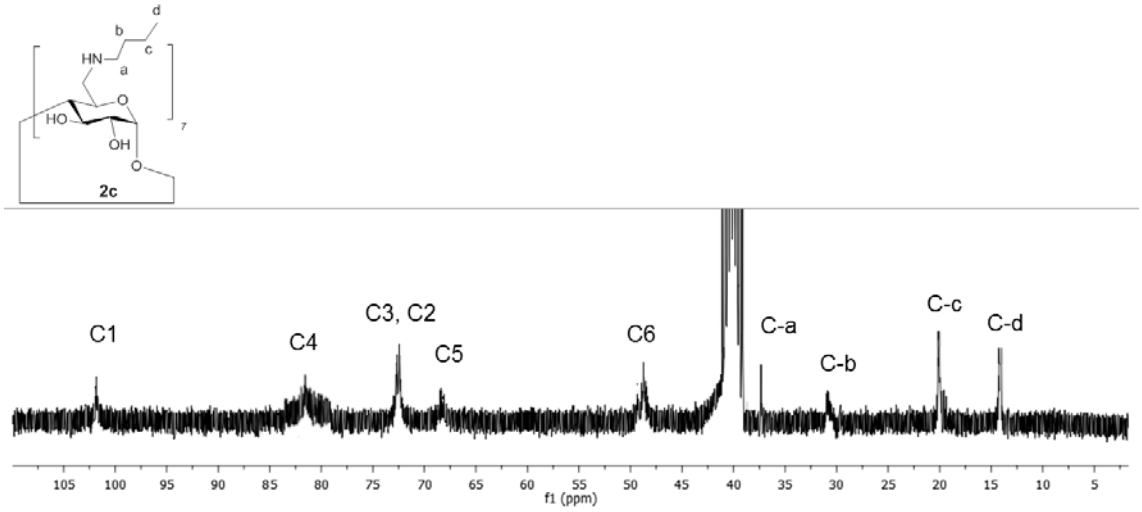


Fig 9. ^{1}H-NMR of *per*-(6-butylamino-6-deoxy)-β-CD **(2c)**



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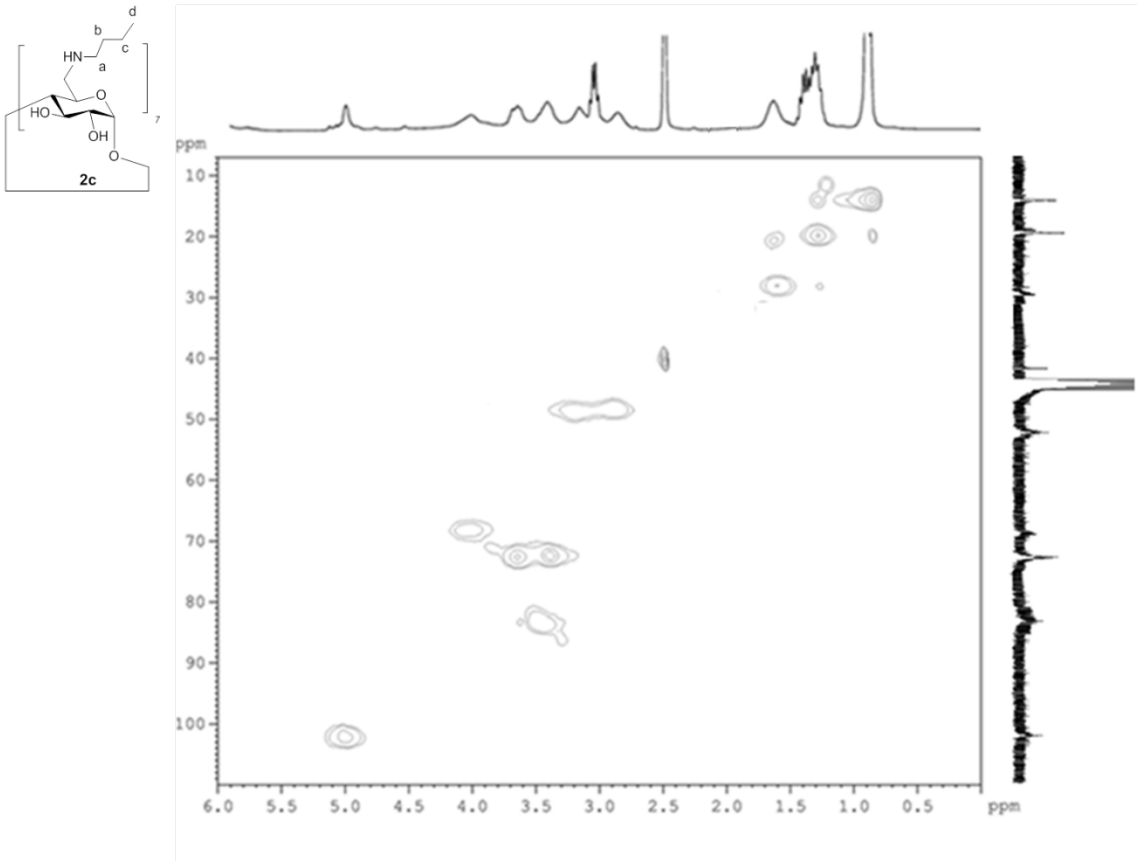

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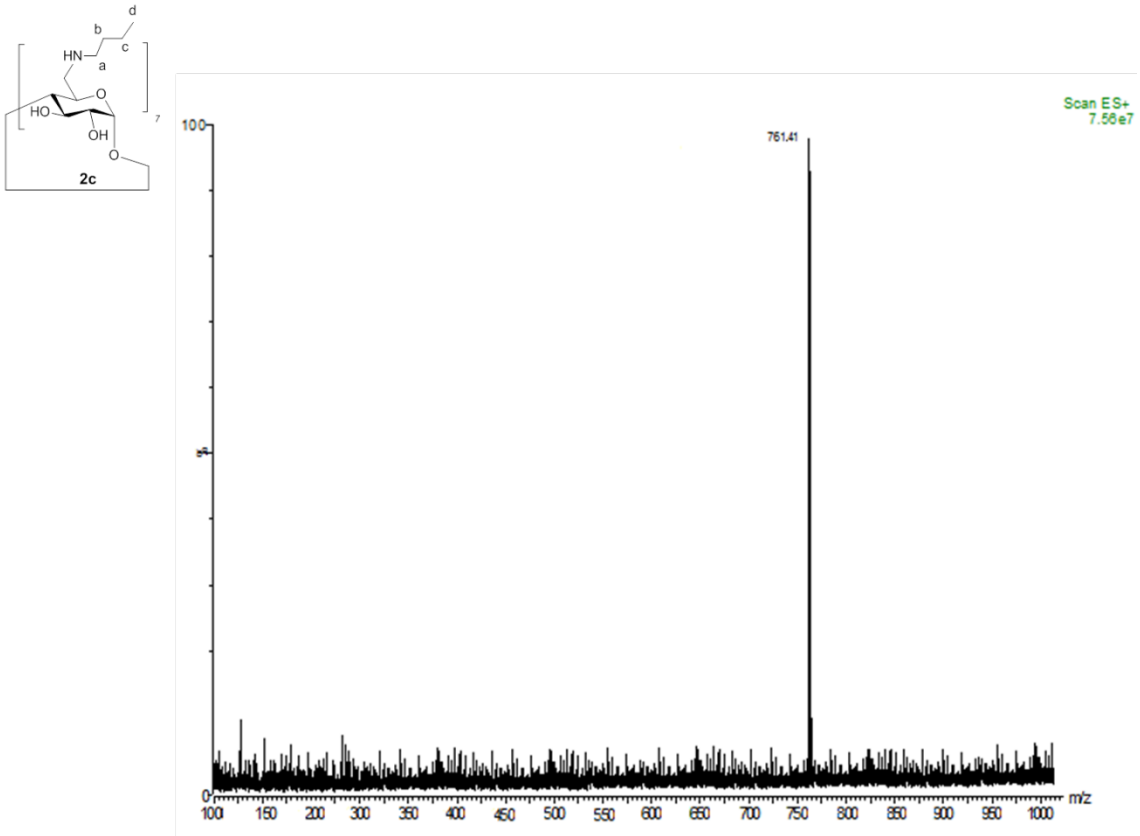

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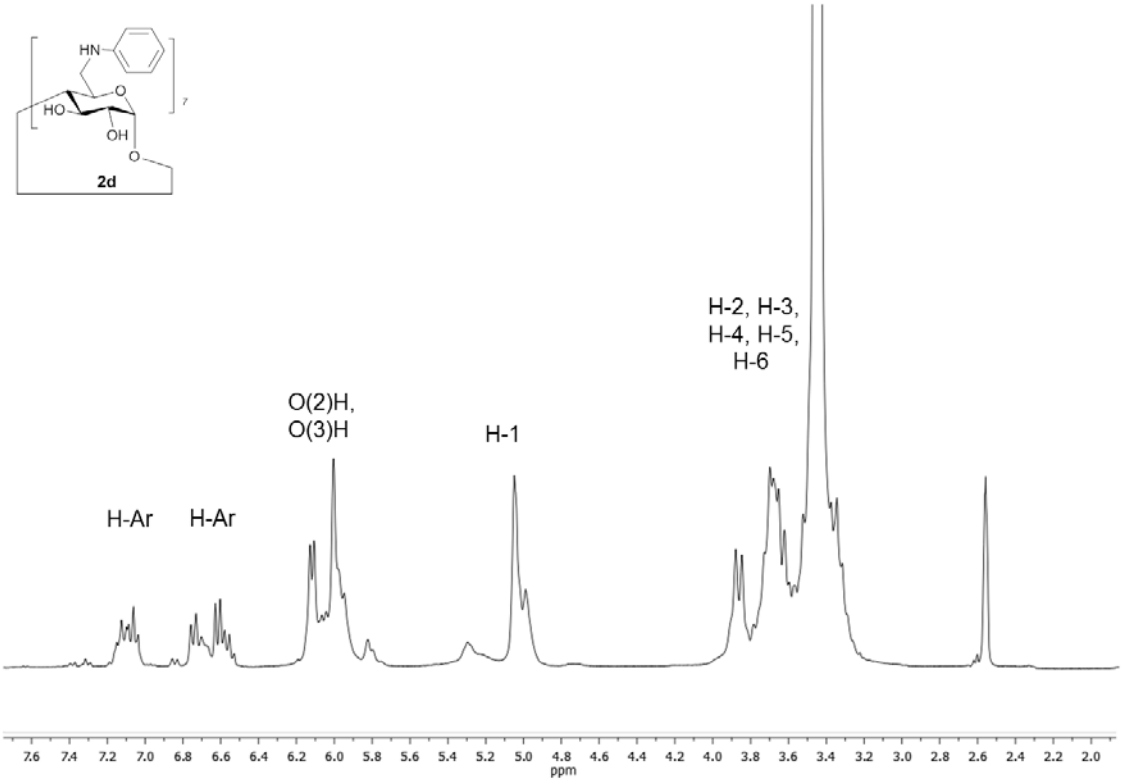
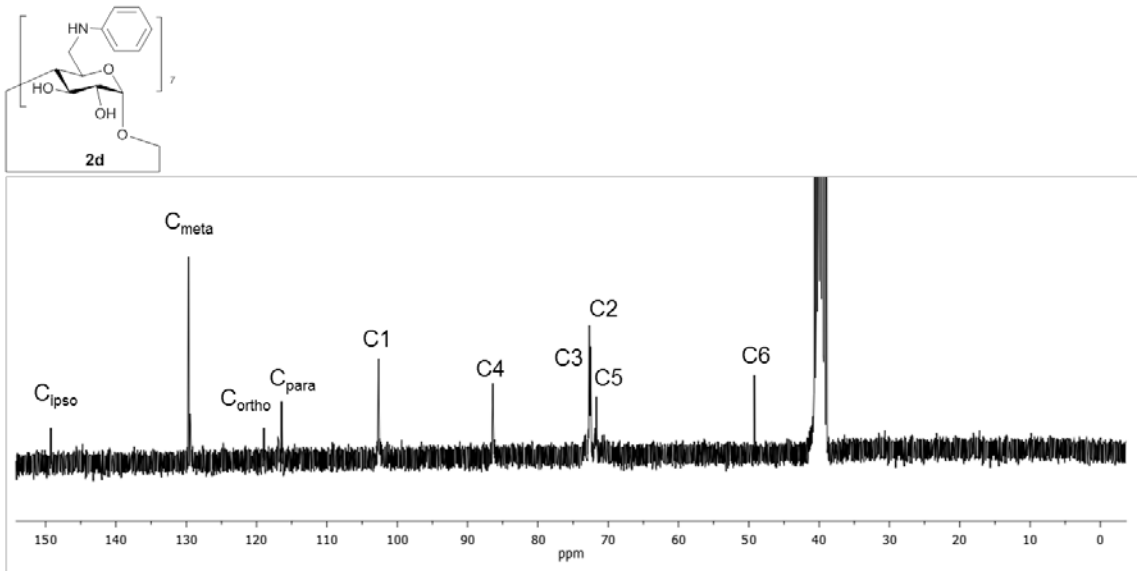


Fig 13. ^{1}H-NMR of *per*-(6-anilino-6-deoxy)-β-CD **(2d)**



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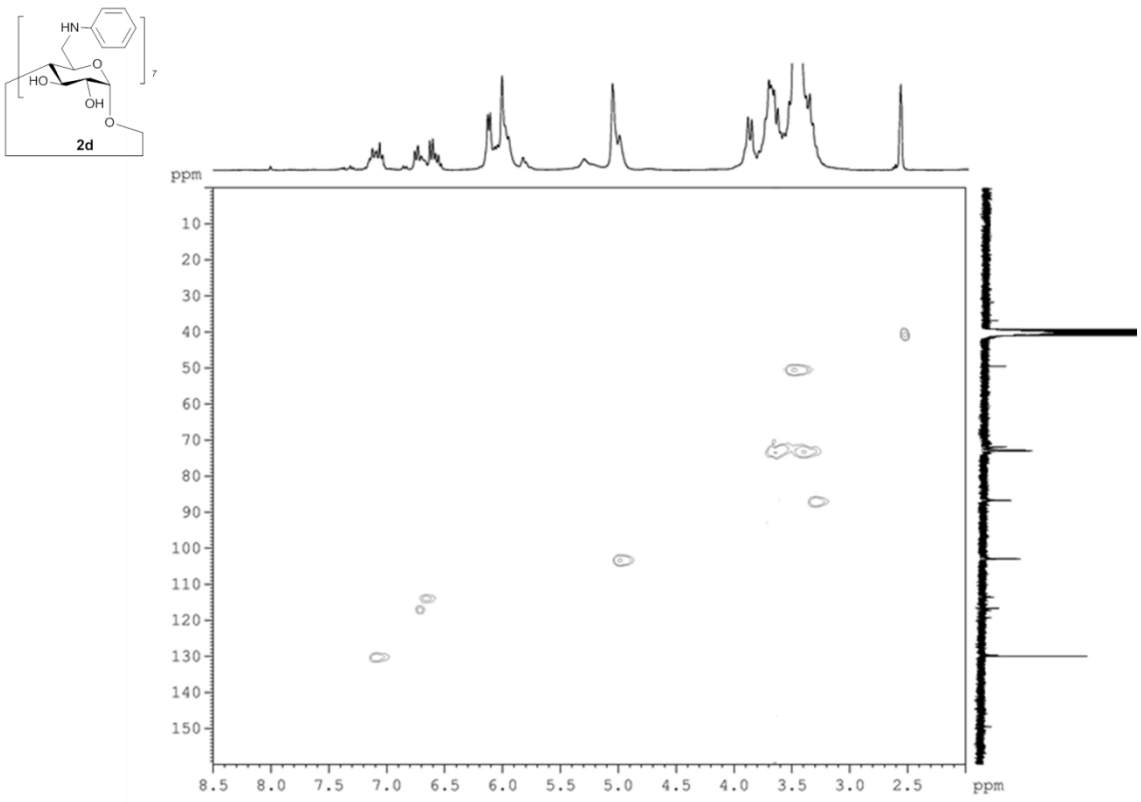

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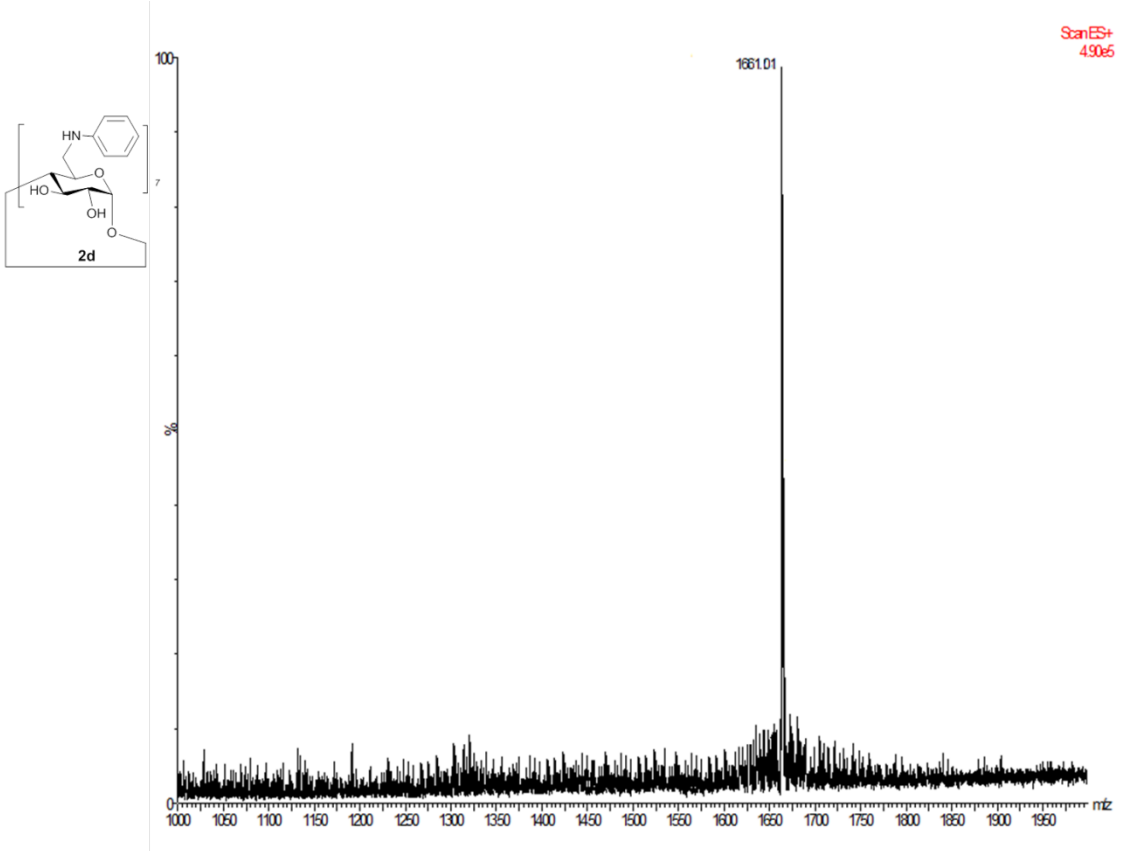

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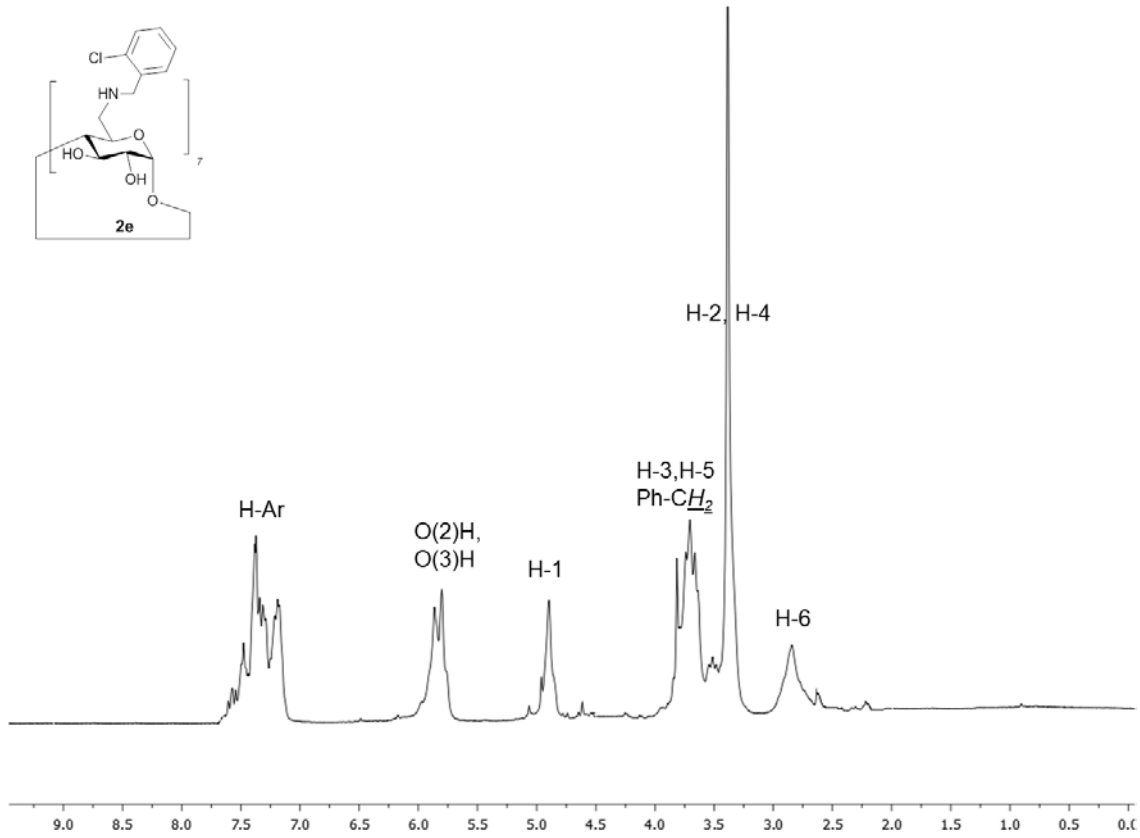

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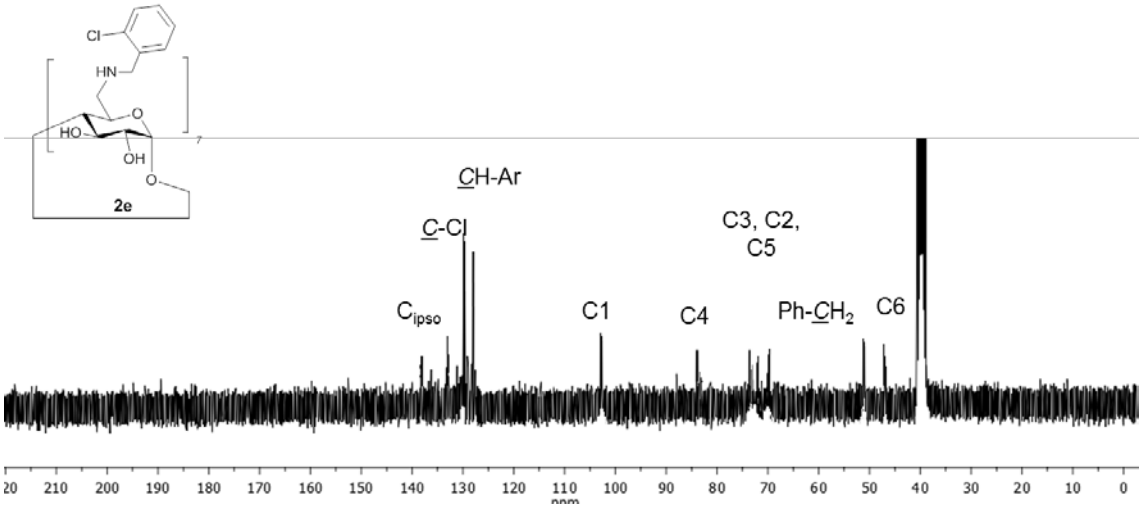

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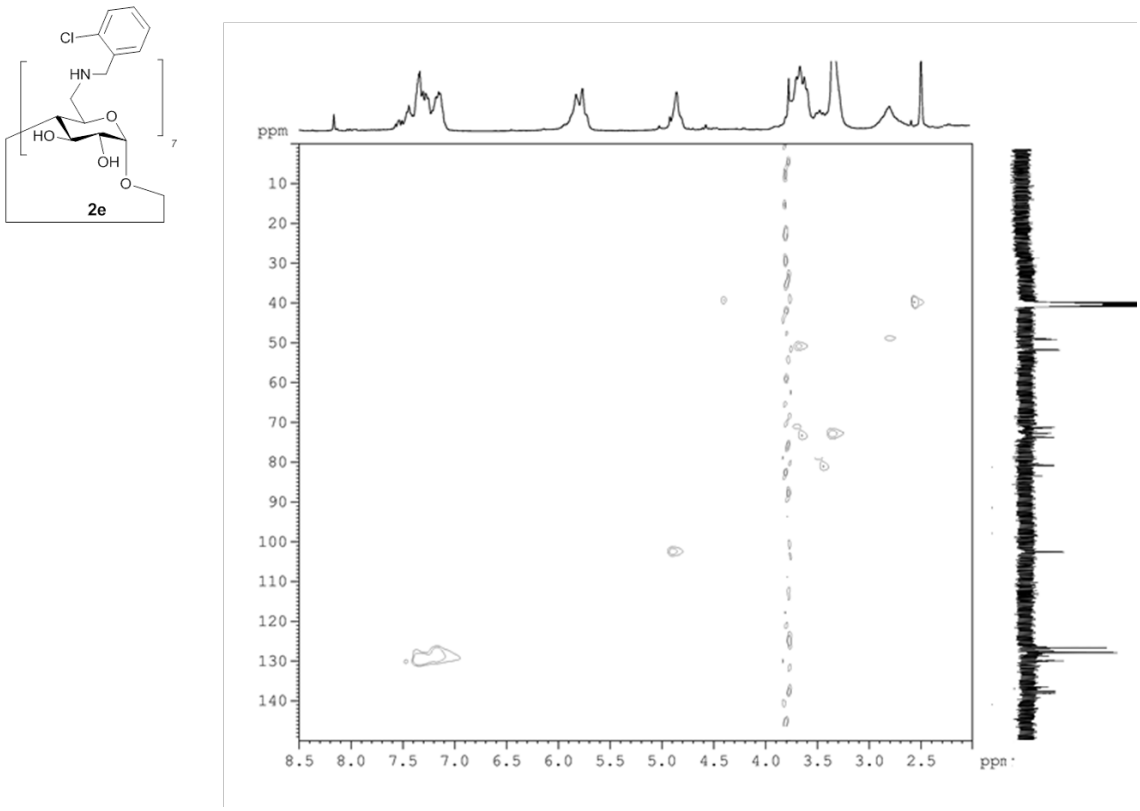

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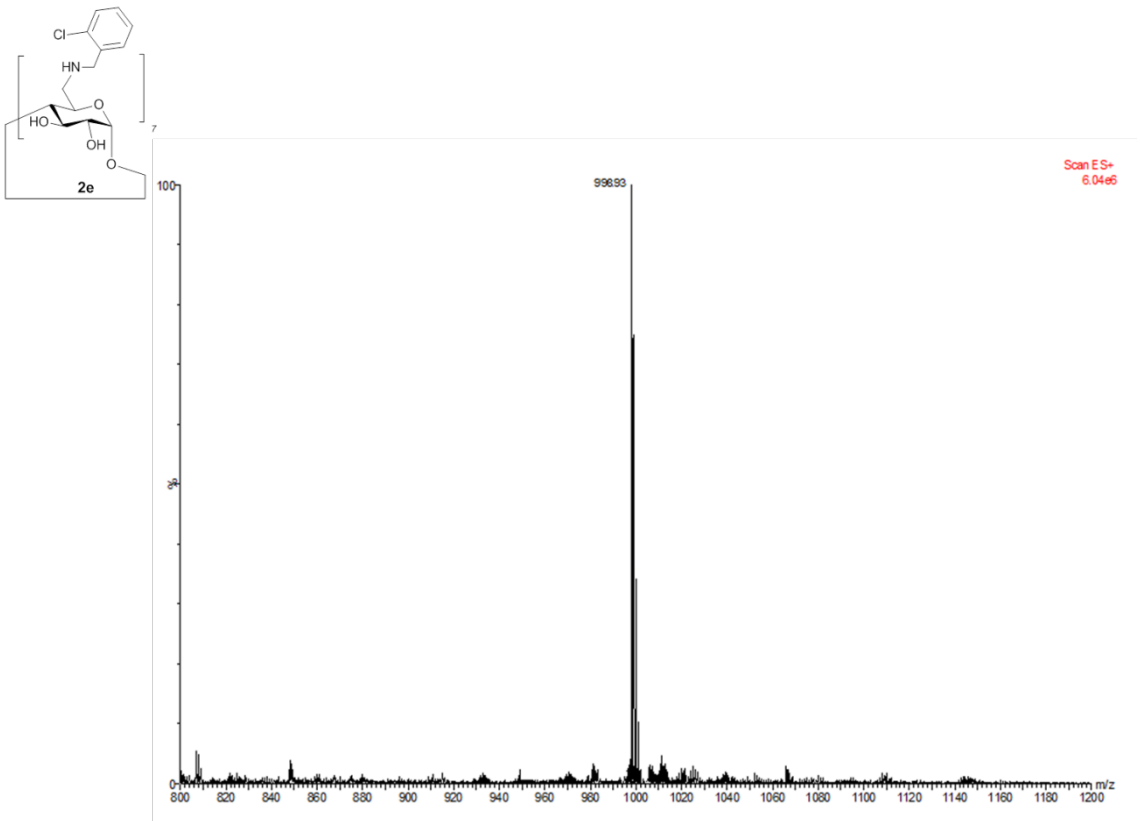

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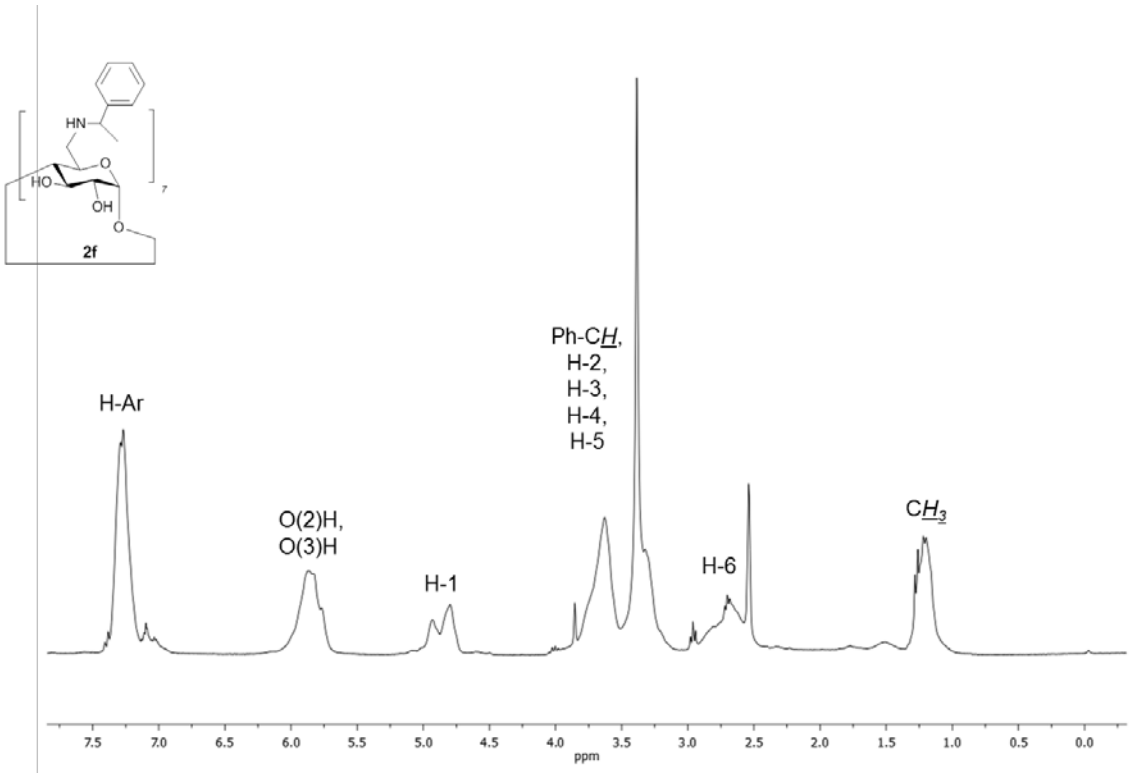

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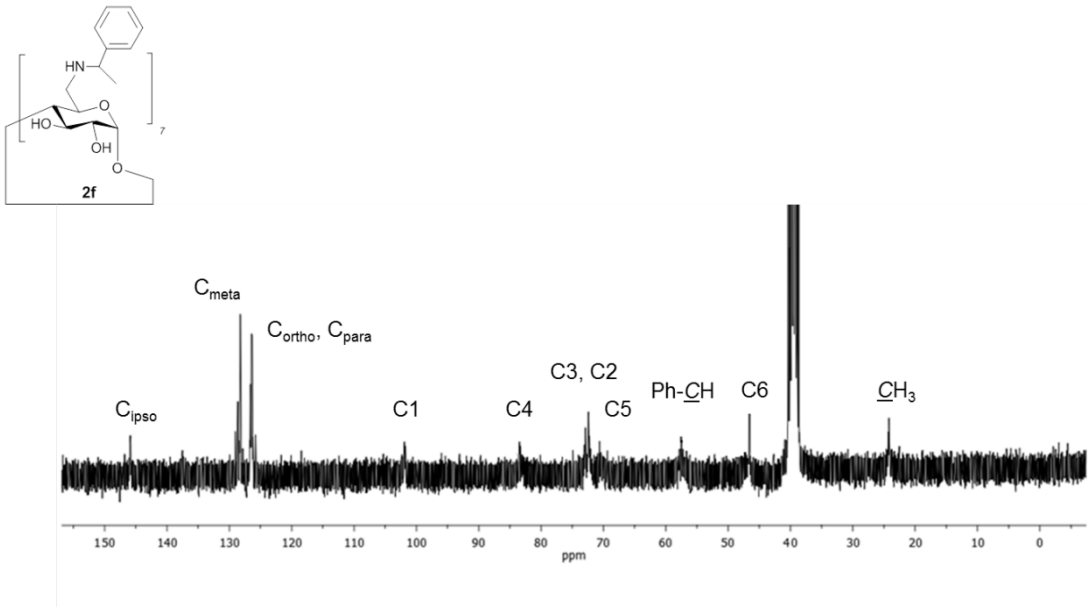

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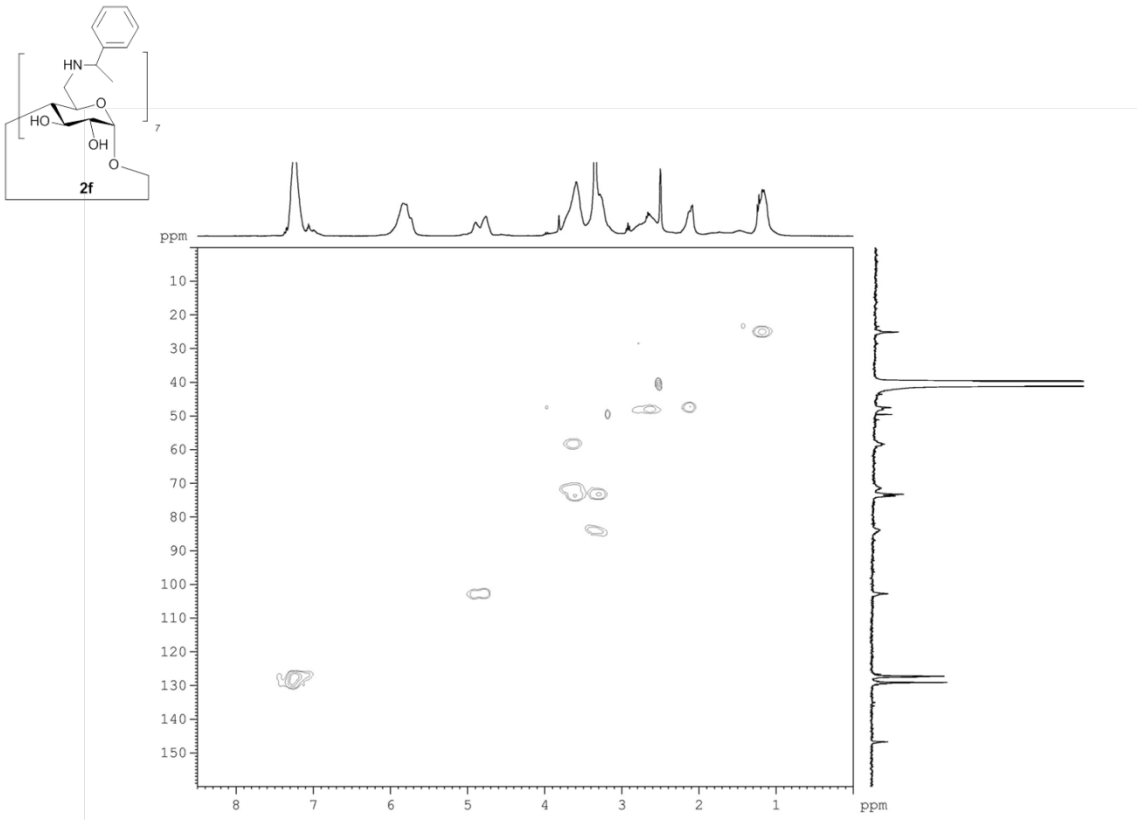
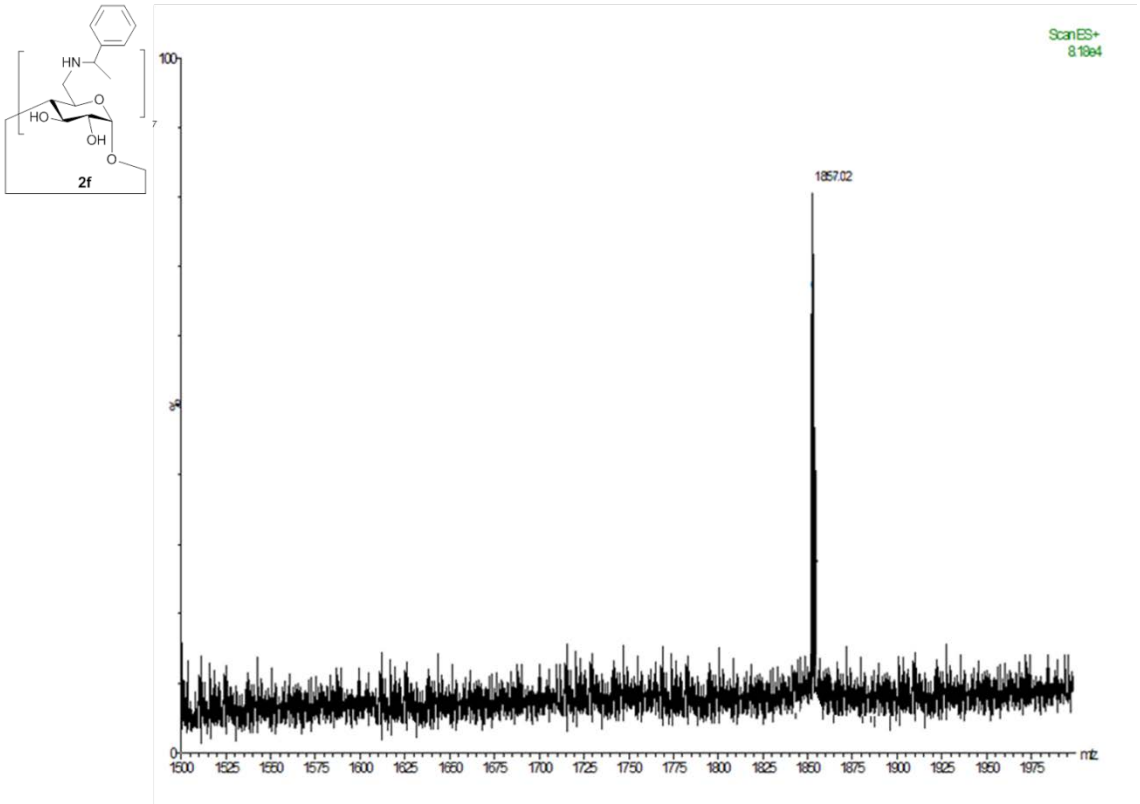


Fig 23. HMQC spectrum (300 MHz for ^{1}H-^{13}C, in DMSO-d_6) of *per*-(6-phenylethylamino-6-deoxy)-β-CD **(2f)**



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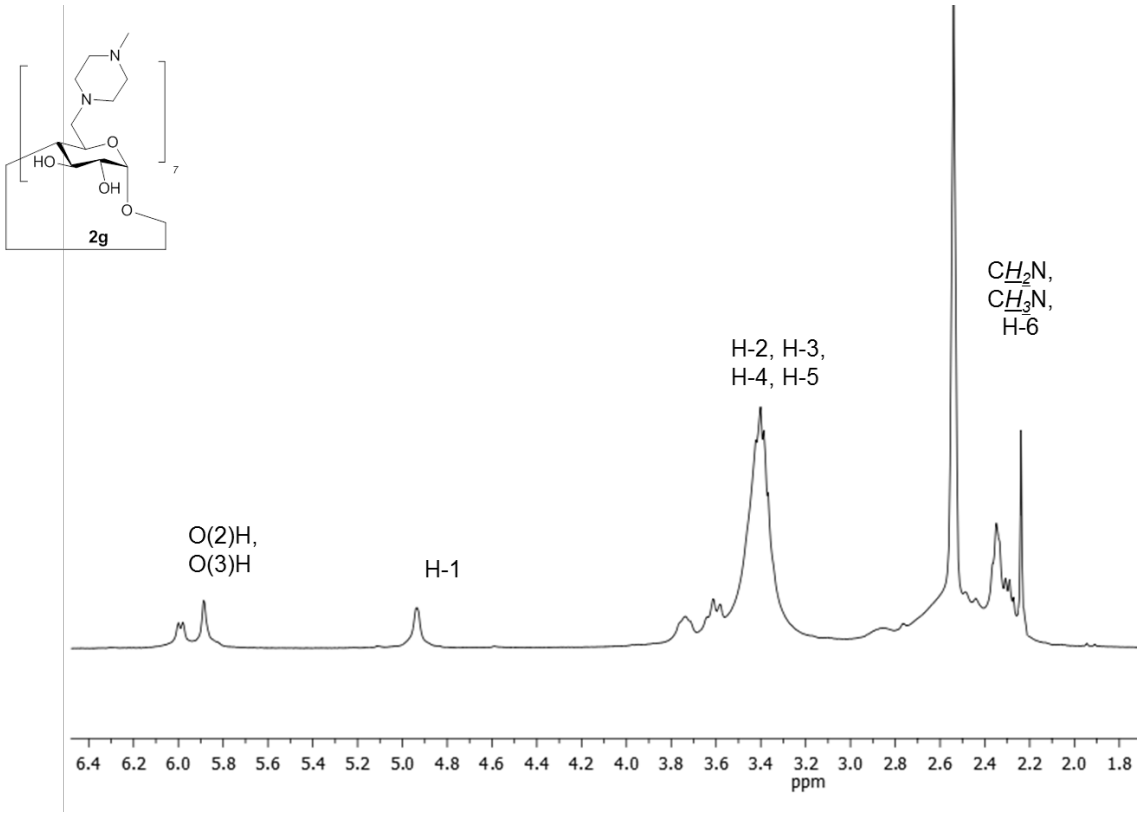


Fig 25. ^{1}H-NMR of *per*-(6-methyl piperazino-6-deoxy)-β-CD **(2g)**

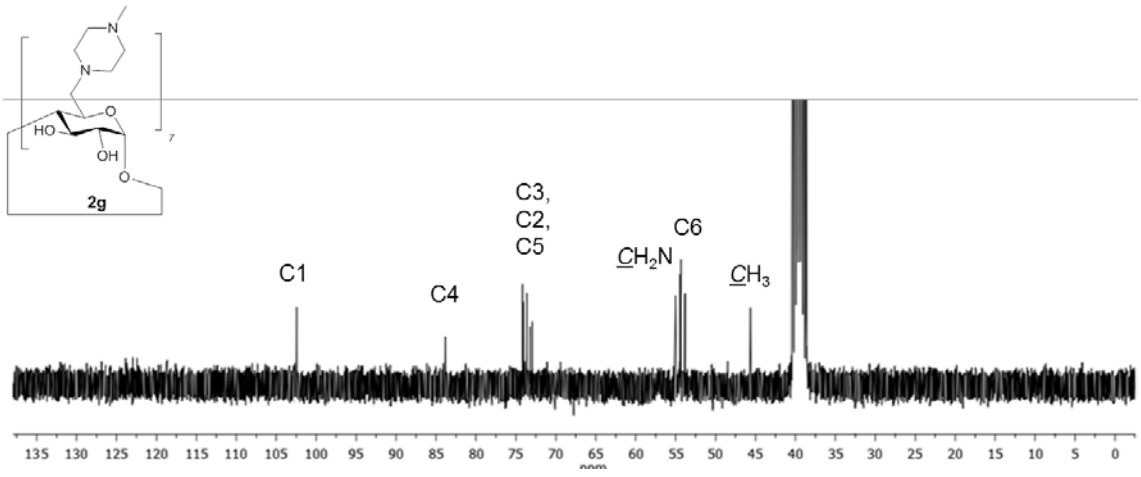


Fig. 26. ^{13}C-NMR of *per*-(6-methyl piperazino-6-deoxy)-β-CD **(2g)**

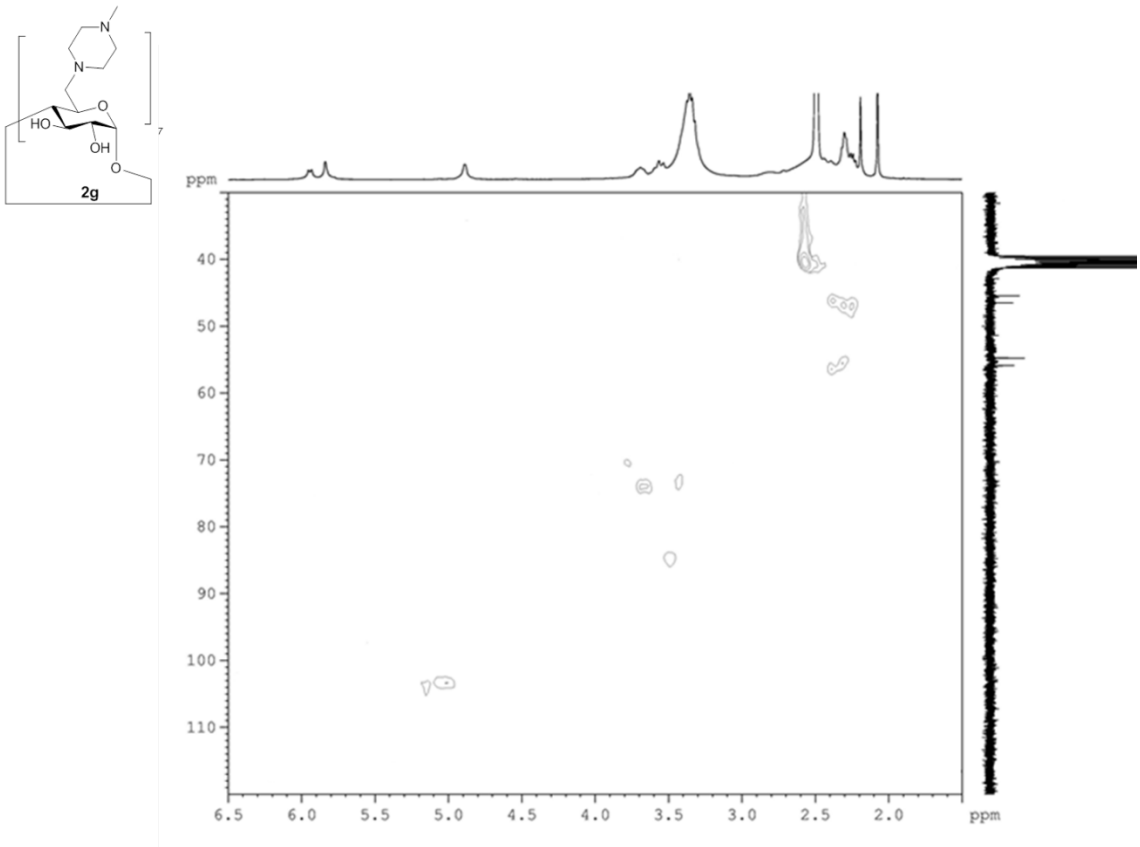


Fig 27. HMQC spectrum (300 MHz for ^{1}H-^{13}C, in DMSO-d_6) of *per*-(6-methyl piperazino-6-deoxy)-β-CD **(2g)**

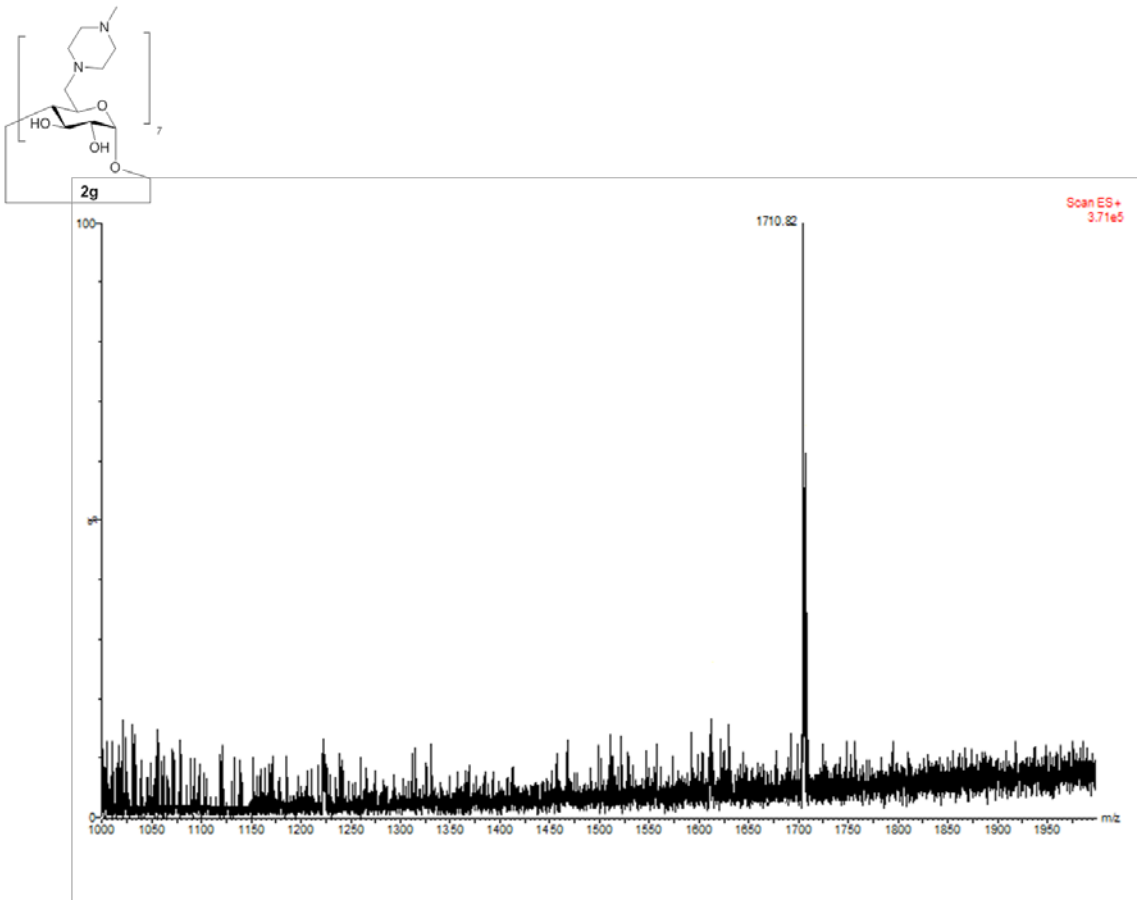


Fig 28. MS (ESI) spectrum of *per*-(6-methyl piperazino-6-deoxy)-β-CD **(2g)**

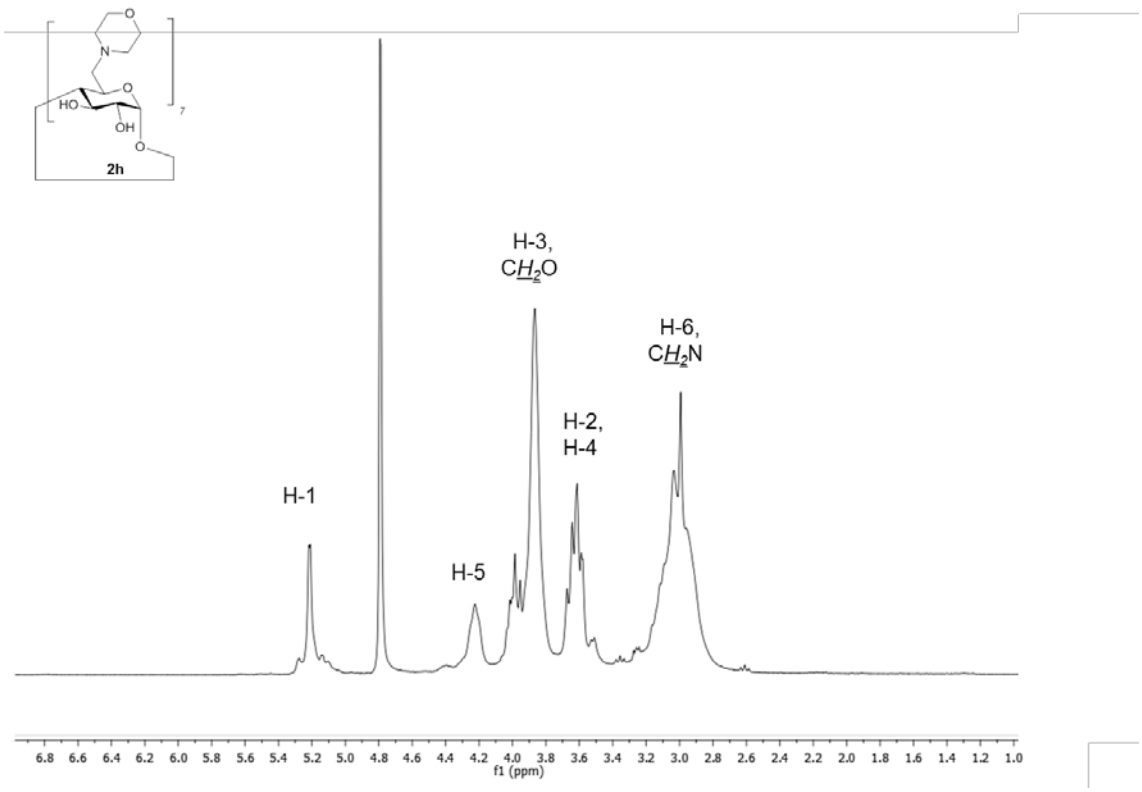
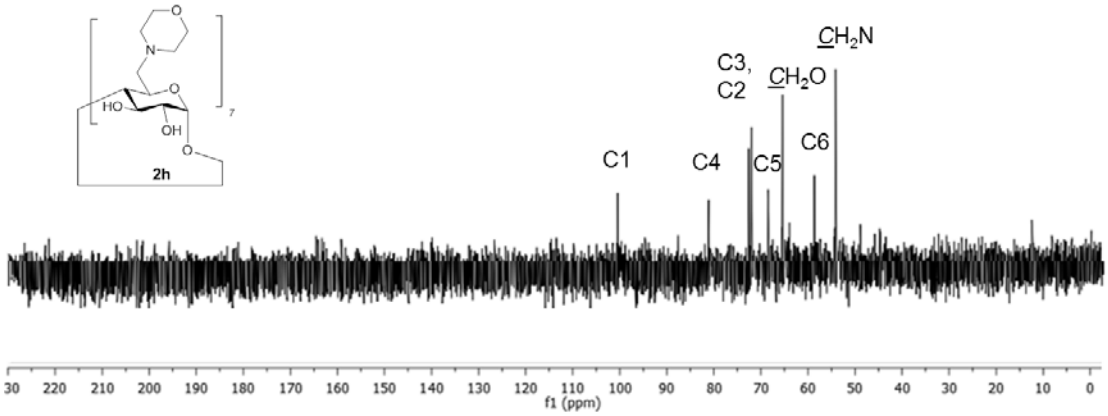


Fig 29. ^{1}H-NMR of *per*-(6-morpholino-6-deoxy)-β-CD **(2h)**



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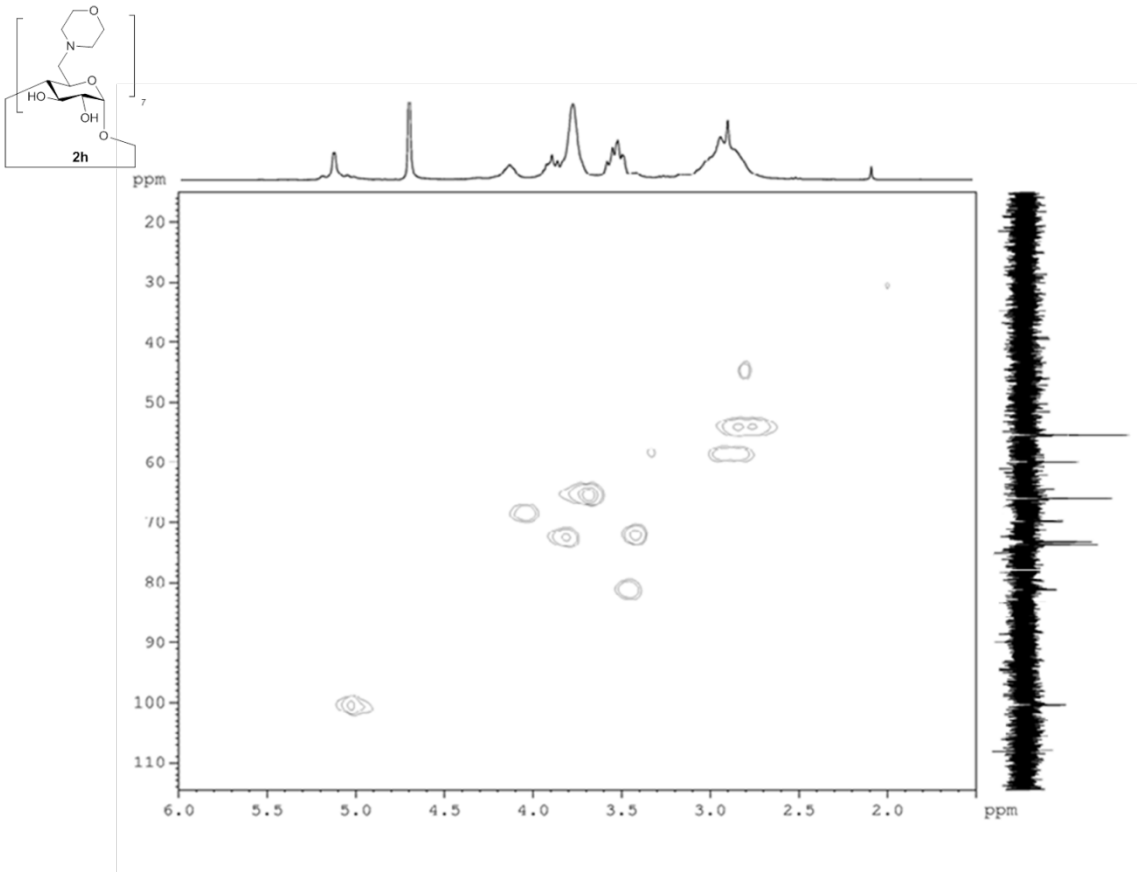
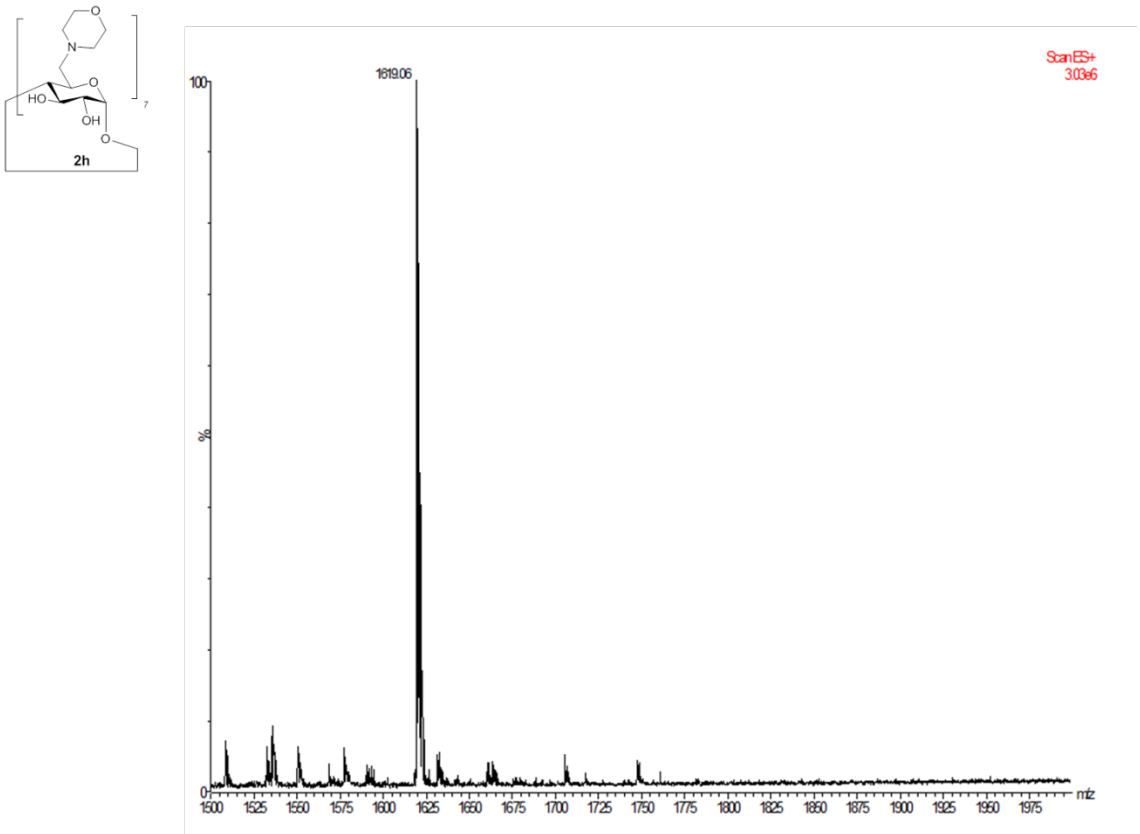


Fig 31. HMQC spectrum (300 MHz for ^{1}H-^{13}C, in D_2O) of *per*-(6-morpholino-6-deoxy)-β-CD **(2h)**



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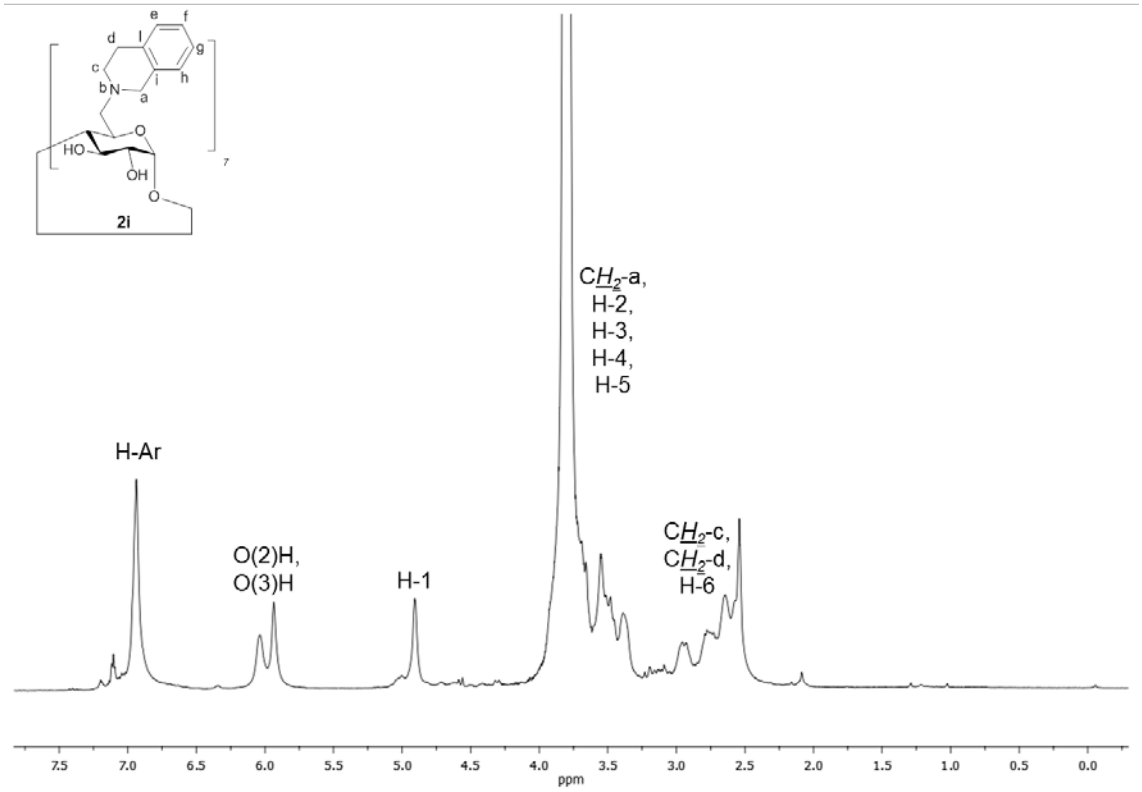

Fig 33. ^{1}H-NMR of *per*-(6-tetrahydroisoquinolino-6-deoxy)-β-CD **(2i)**

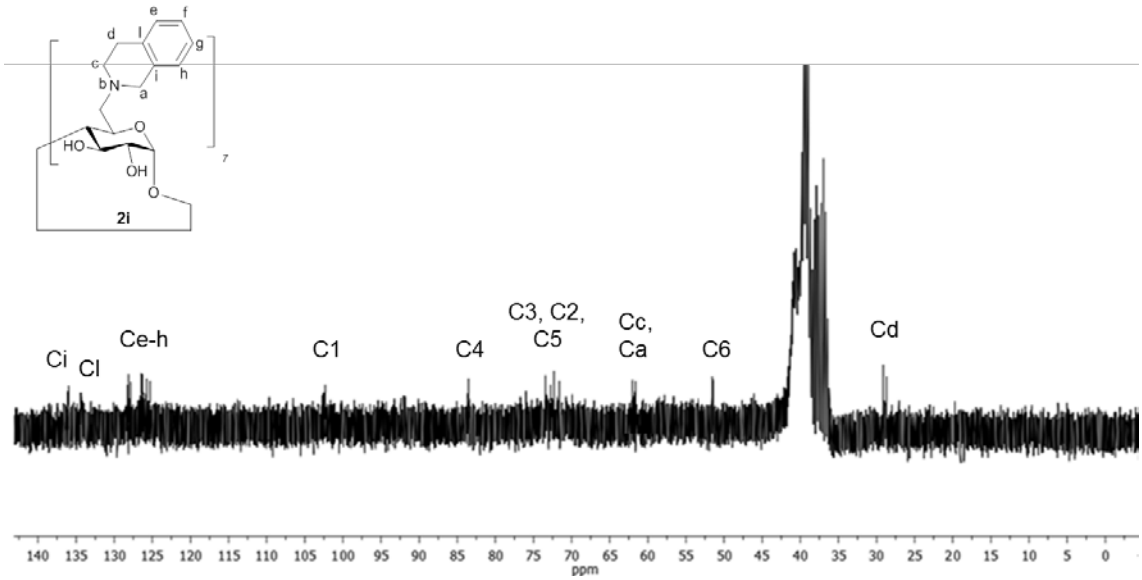

Fig 34. ^{13}C NMR of *per*-(6-tetrahydroisoquinolino-6-deoxy)-β-CD **(2i)**

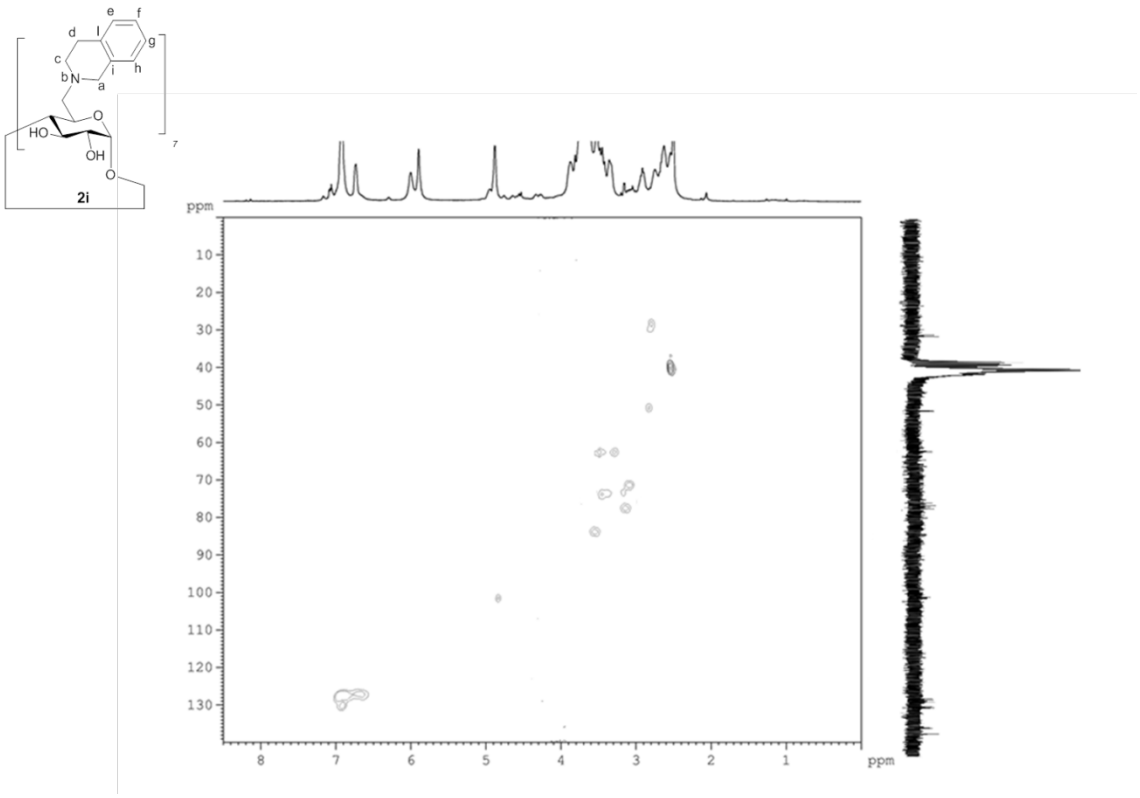

Fig 35. HMQC spectrum (300 MHz for ^{I}H-^{13}C, in DMSO-d_6) of *per*-(6-tetrahydroisoquinolino-6-deoxy)-β-CD **(2i)**

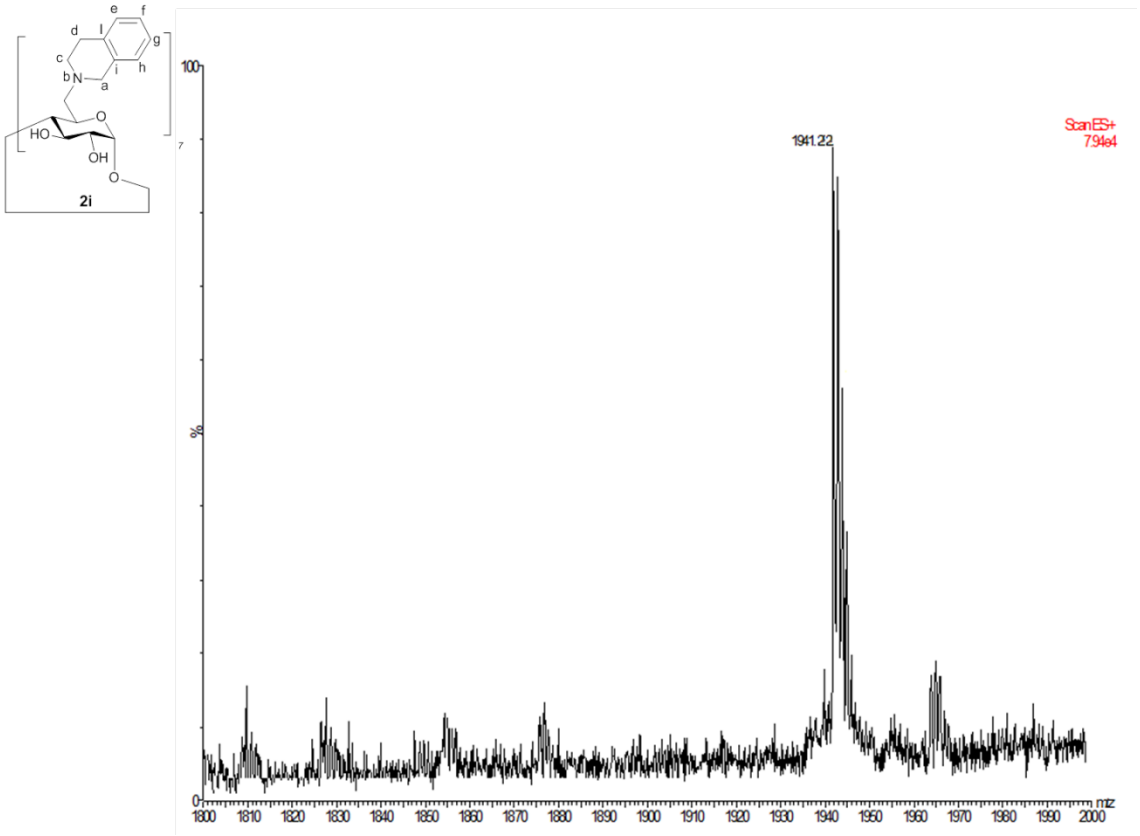

Fig 36. MS (ESI) spectrum of **2i**

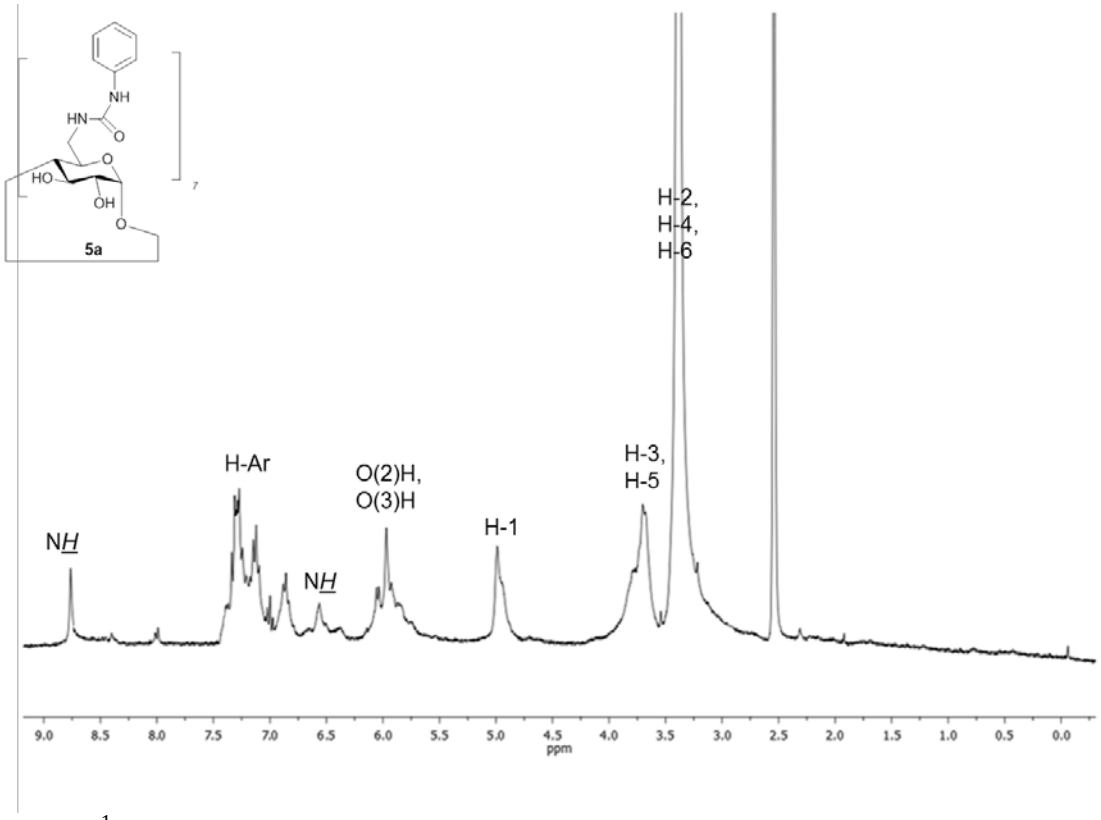

Fig 37. [1]H-NMR of *per*-(6(3-phenylureido)-6-deoxy)-β-CD **(5a)**

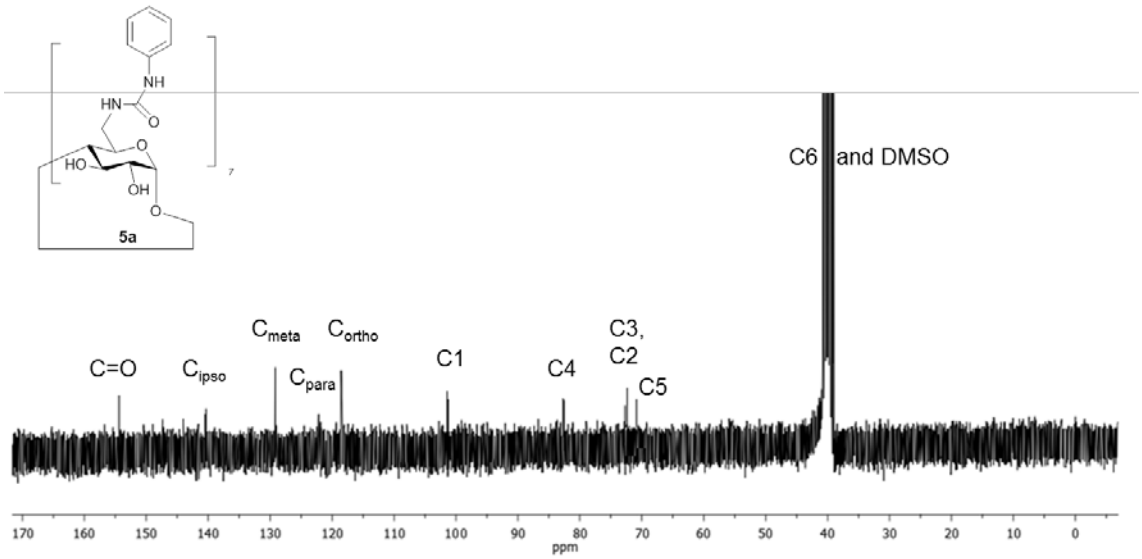

Fig 38. [13]C NMR of *per*-(6(3-phenylureido)-6-deoxy)-β-CD **(5a)**

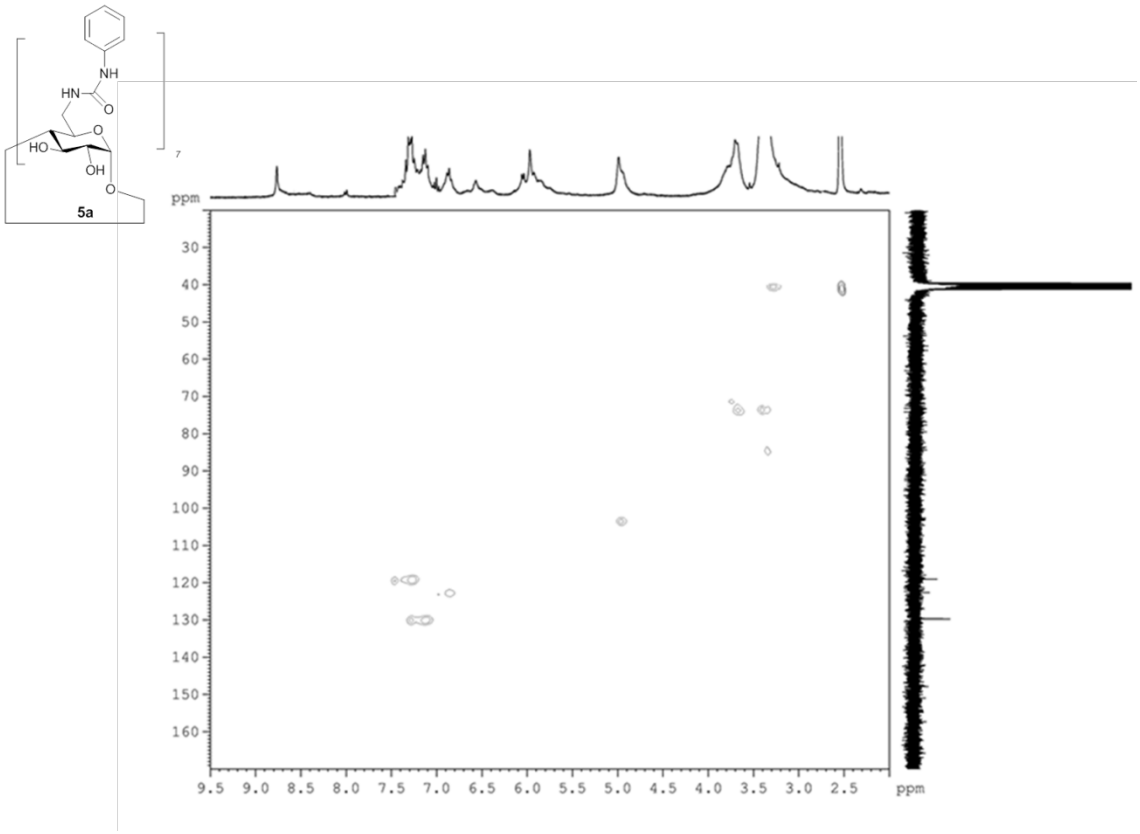

Fig 39. HMQC spectrum (300 MHz for ^{I}H-^{13}C, in DMSO-d_6) of *per*-(6(3-phenylureido)-6-deoxy)-β-CD **(5a)**

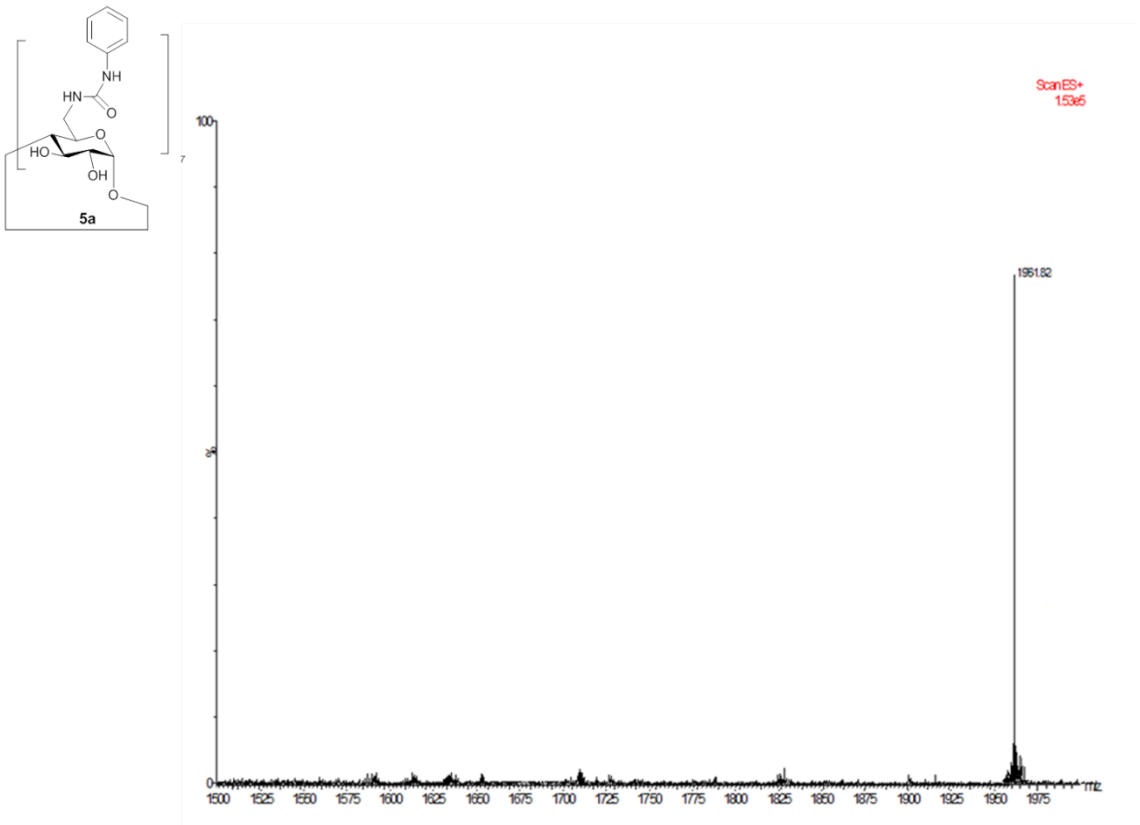

Fig 40. MS (ESI) spectrum of *per*-(6(3-phenylureido)-6-deoxy)-β-CD **(5a)**

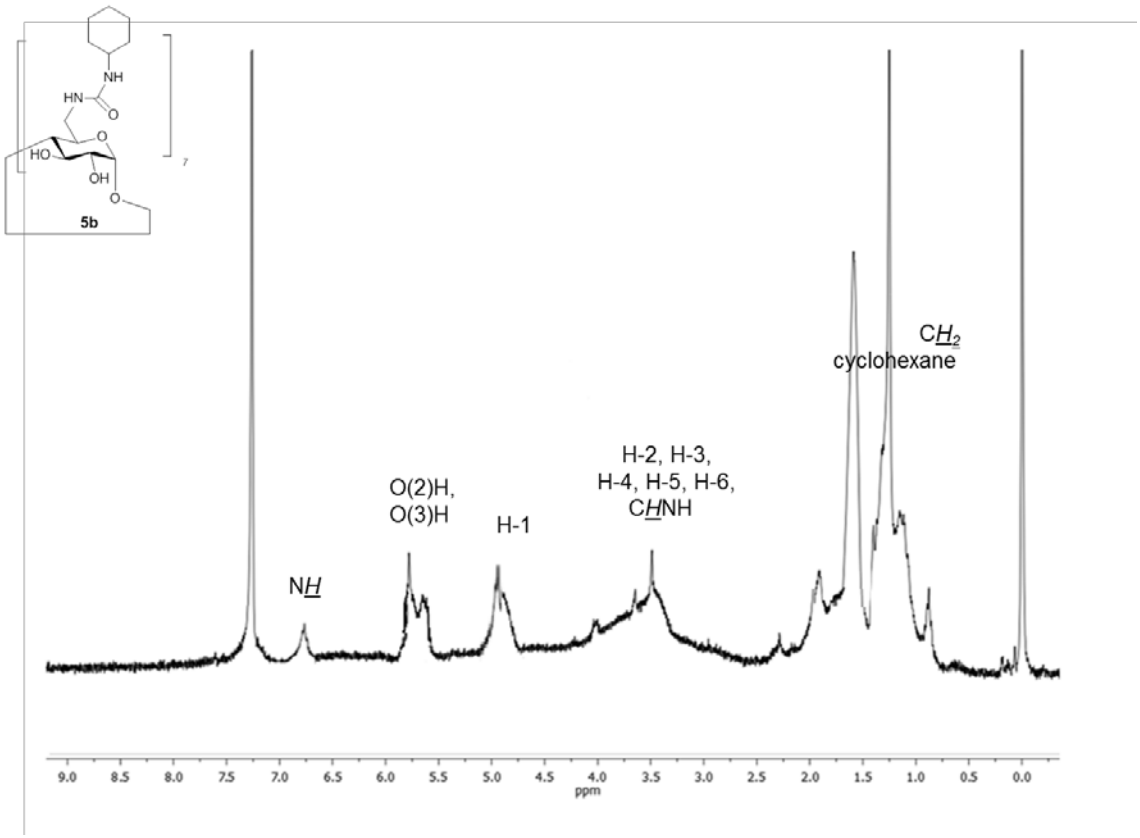

Fig 41. ^{1}H-NMR of *per*-(6(3-cyclohexylureido)-6-deoxy)-β-CD **(5b)**

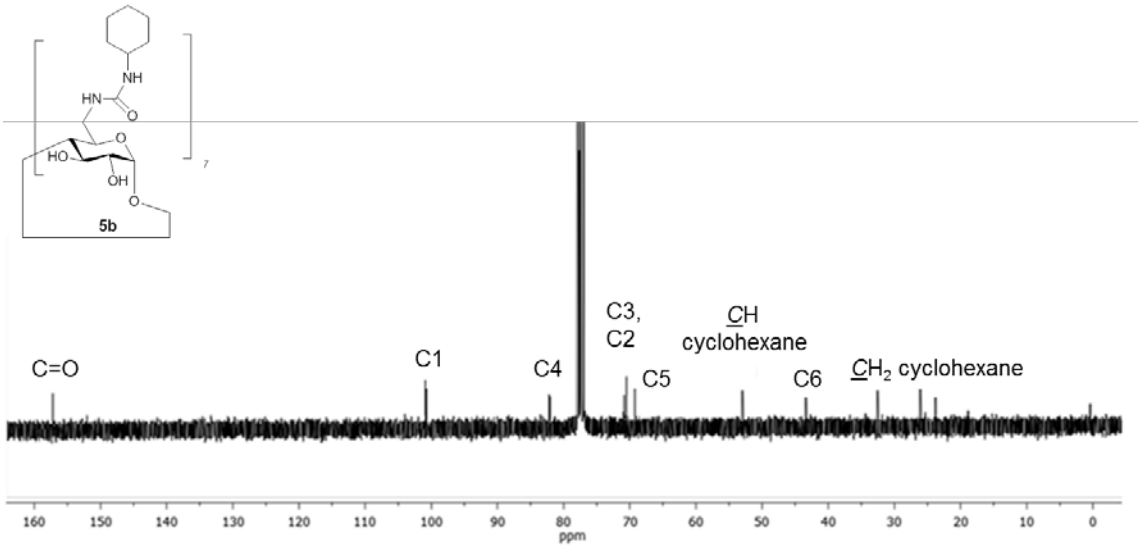

Fig 42. ^{13}C NMR of *per*-(6(3-cyclohexylureido)-6-deoxy)-β-CD **(5b)**

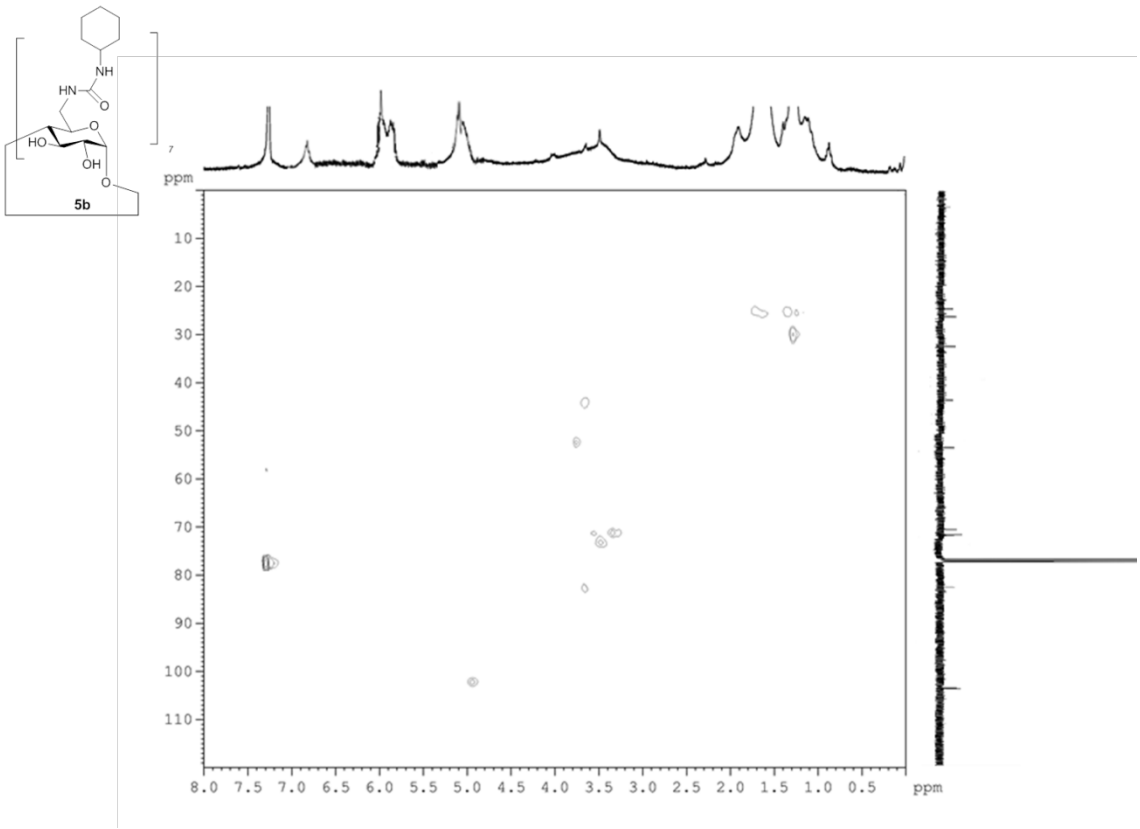

Fig 43. HMQC spectrum (300 MHz for ^{I}H-^{13}C, in $CDCl_3$) of *per*-(6(3-cyclohexylureido)-6-deoxy)-β-CD **(5b)**

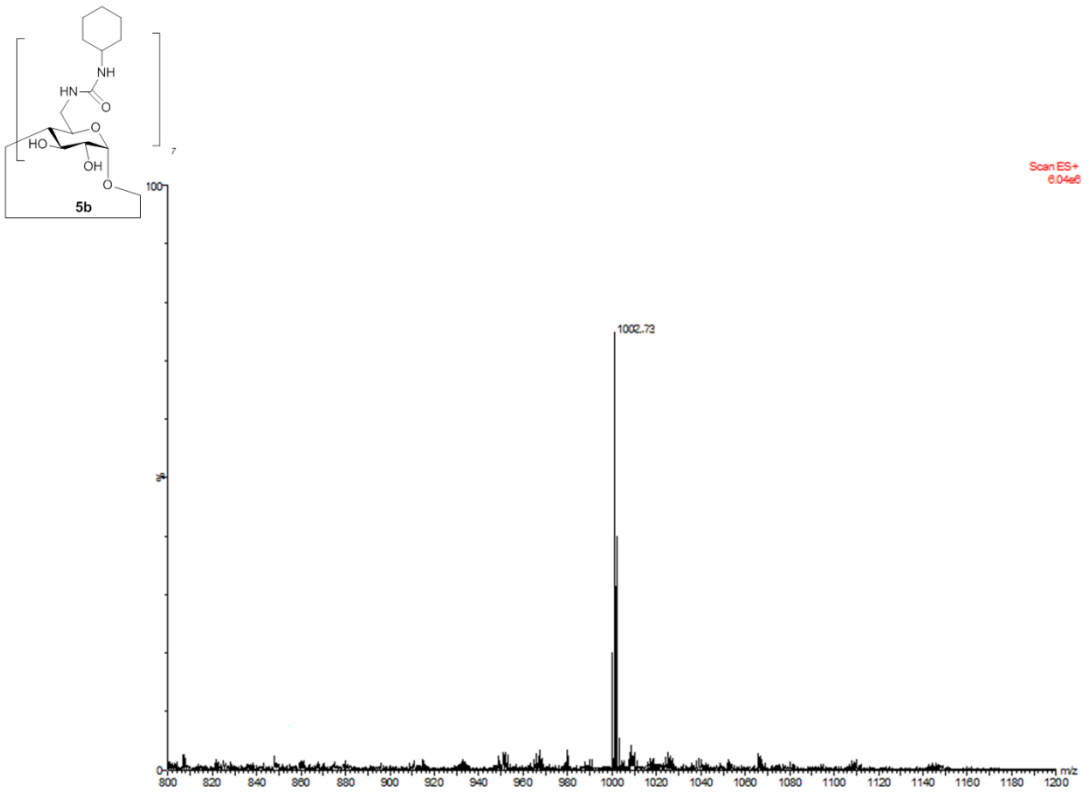

Fig 44. MS (ESI) spectrum of *per*-(6(3-cyclohexylureido)-6-deoxy)-β-CD **(5b)**

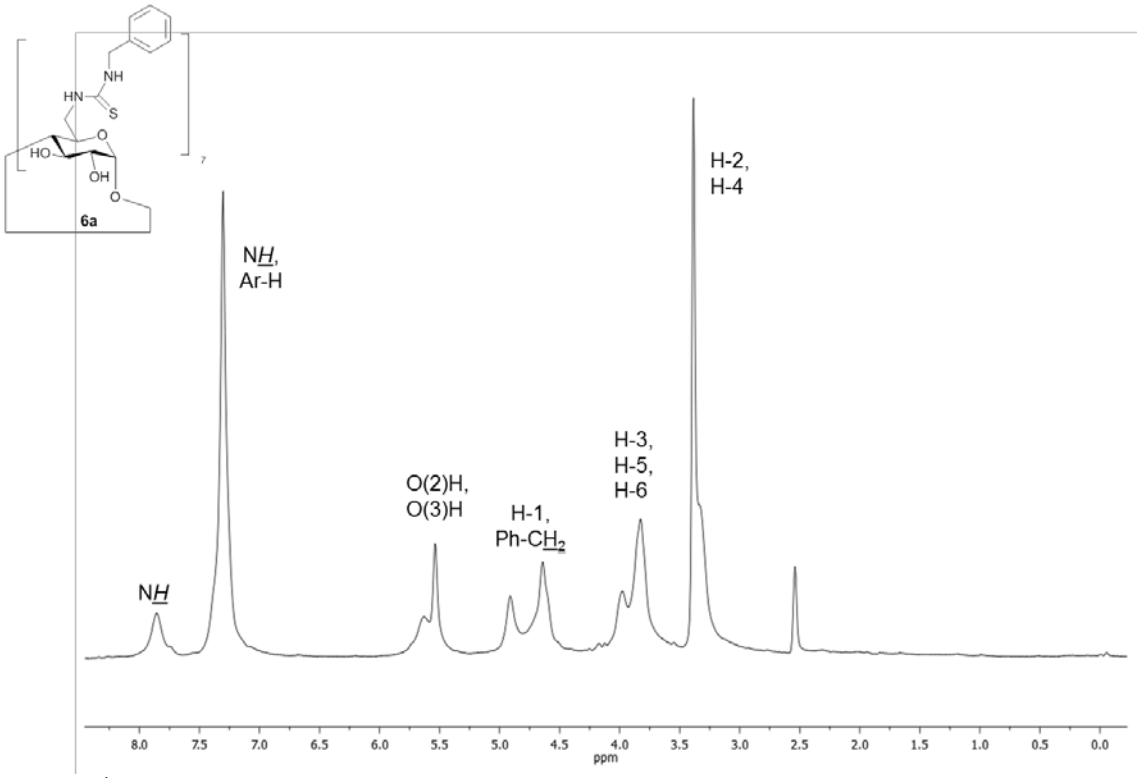

Fig 45. ^{1}H-NMR of *per*-(6(3-benzylthioureido)-6-deoxy)-β-CD **(6a)**

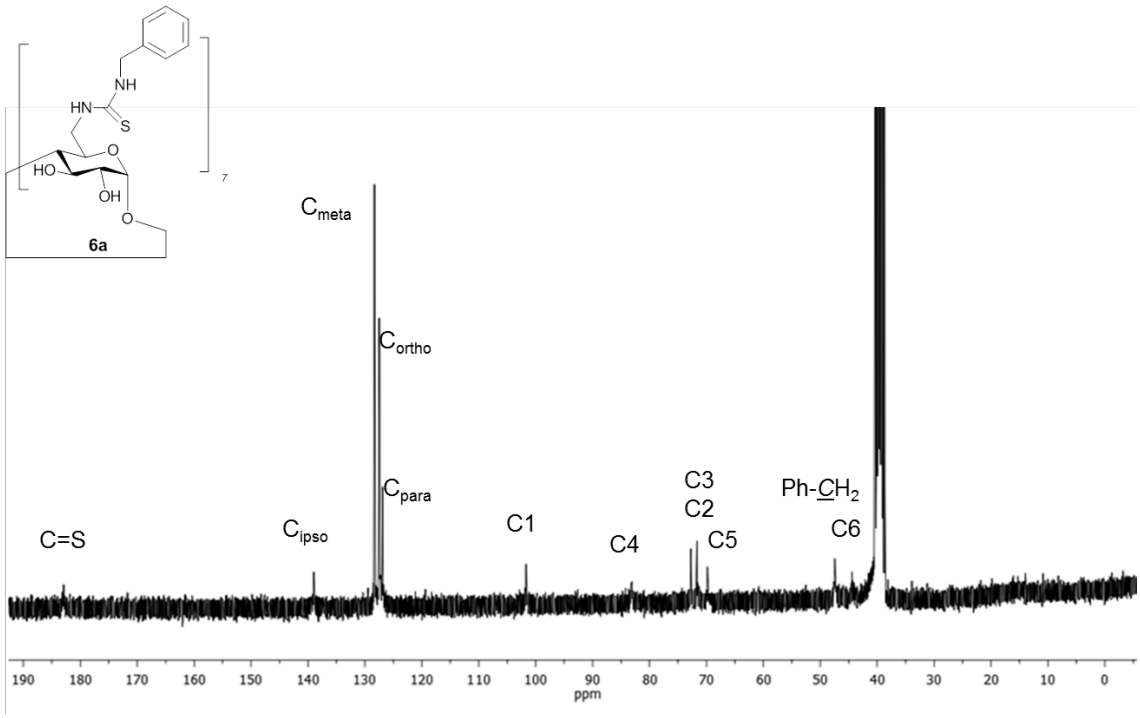

Fig 46. ^{13}C NMR of *per*-(6(3-benzylthioureido)-6-deoxy)-β-CD **(6a)**

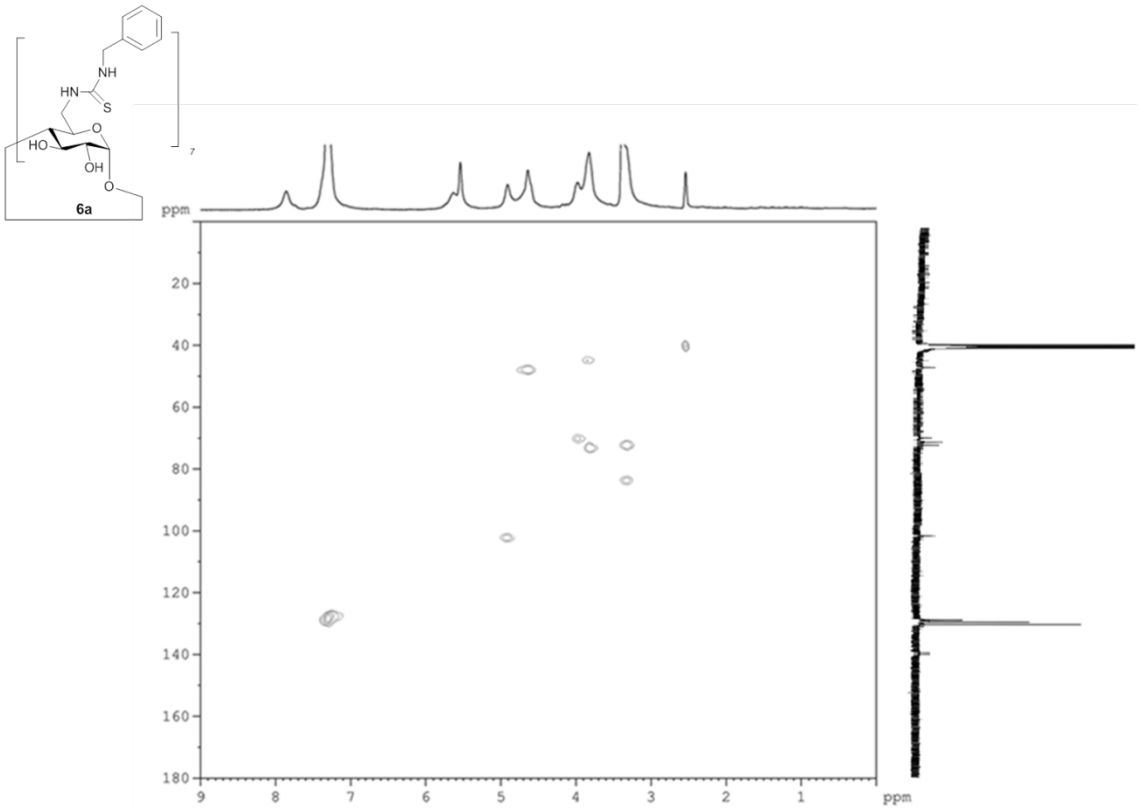

Fig 47. HMQC spectrum (300 MHz for ^{I}H-^{13}C, in DMSO-d_6) of *per*-(6(3-benzylthioureido)-6-deoxy)-β-CD **(6a)**

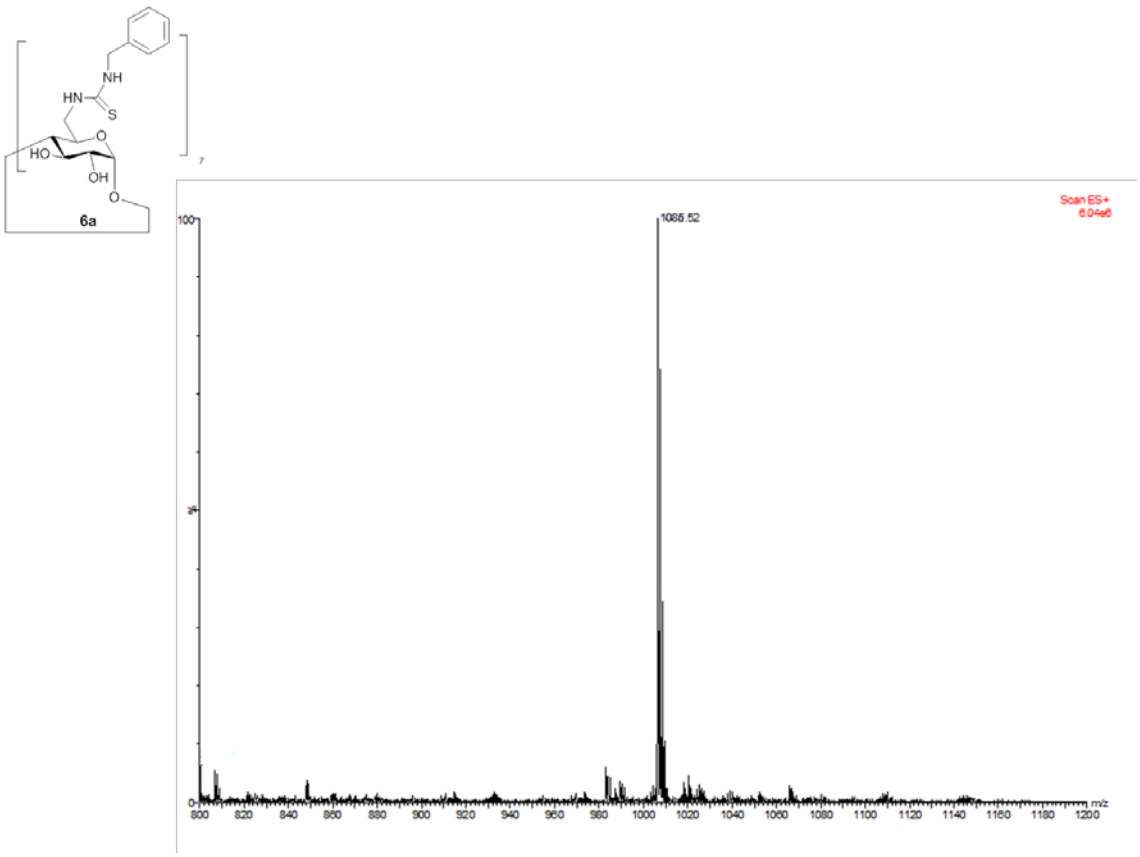

Fig 48. MS (ESI) spectrum of *per*-(6(3-benzylthioureido)-6-deoxy)-β-CD **(6a)**

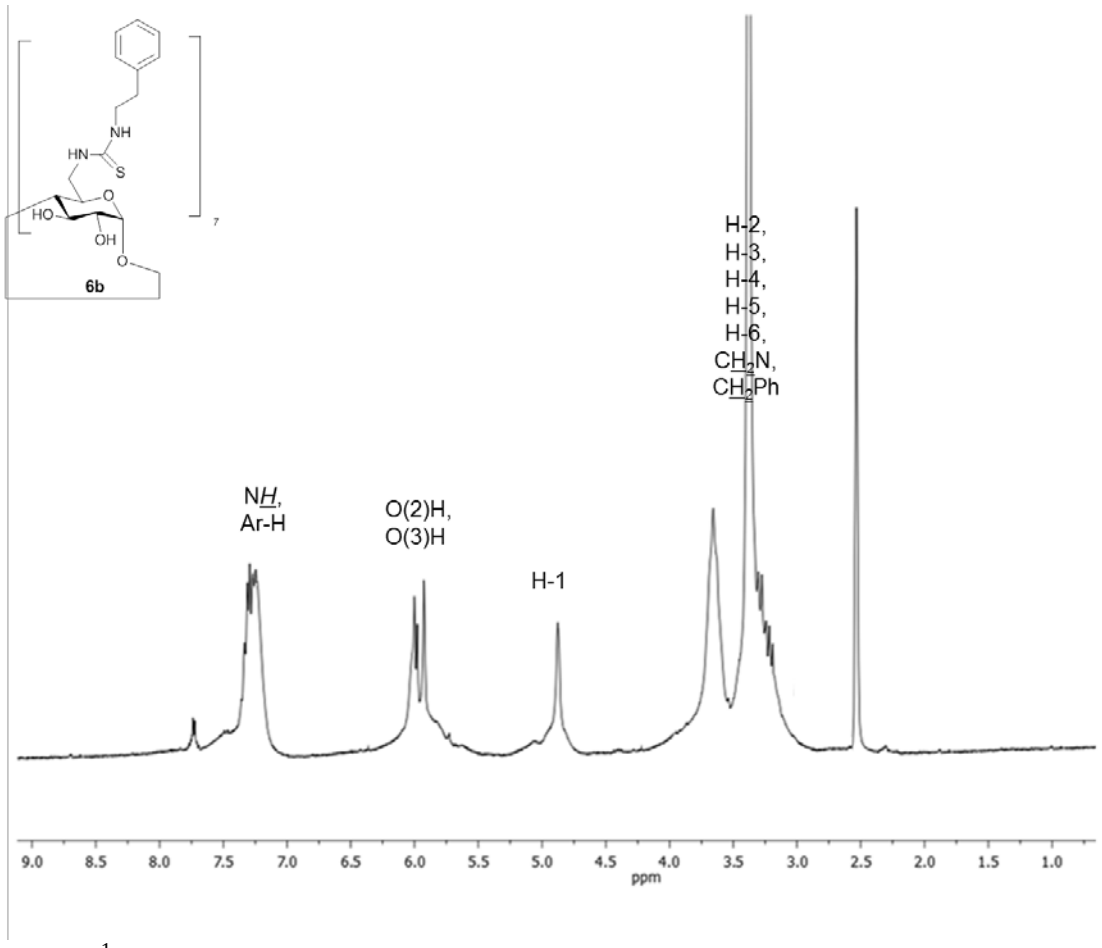

Fig 49. ^{1}H-NMR of *per*-(6(3-phenylethylthioureido)-6-deoxy)-β-CD **(6b)**

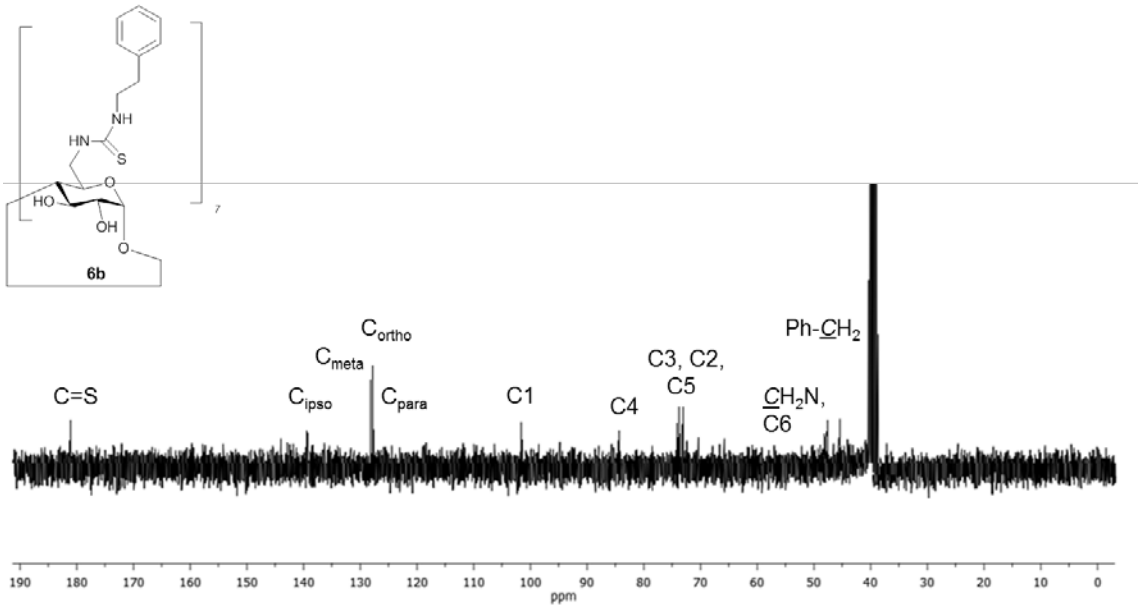

Fig 50. ^{13}C NMR of *per*-(6(3-phenylethylthioureido)-6-deoxy)-β-CD **(6b)**

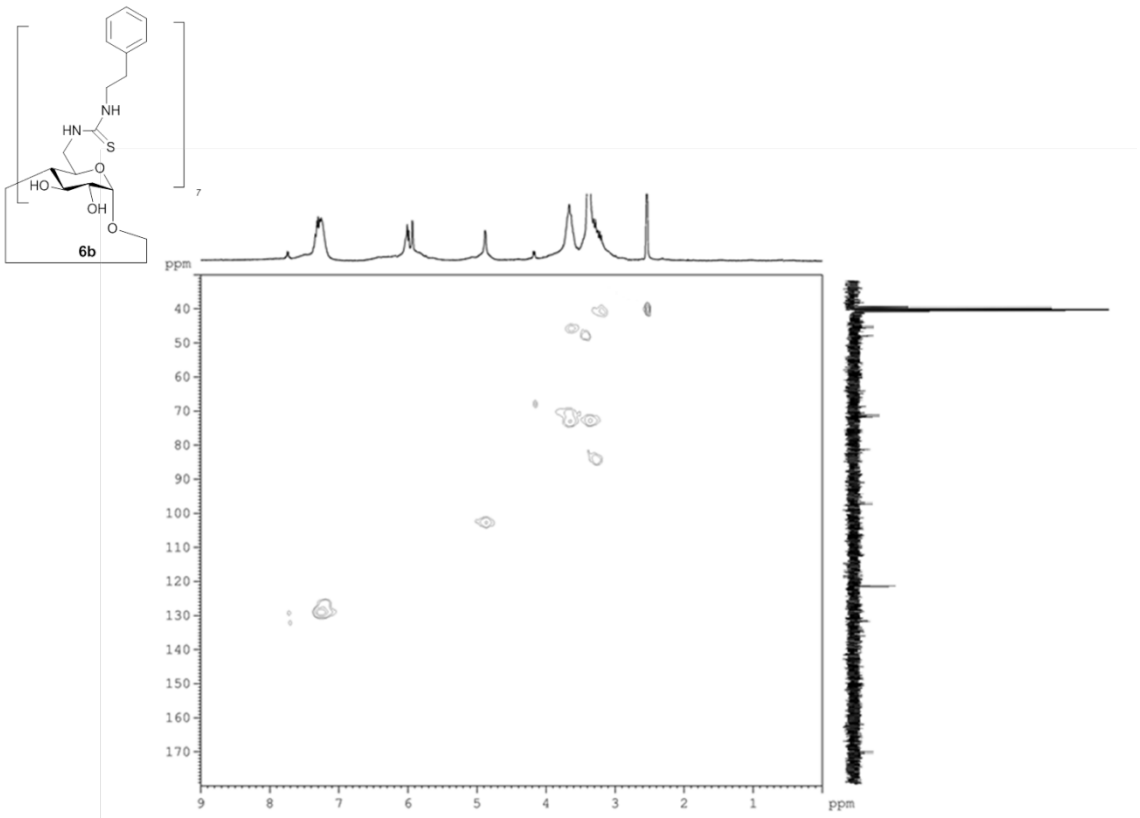

Fig 51. HMQC spectrum (300 MHz for ^{I}H-^{13}C, in DMSO-d_6) of *per*-(6(3-phenylethylthioureido)-6-deoxy)-β-CD **(6b)**

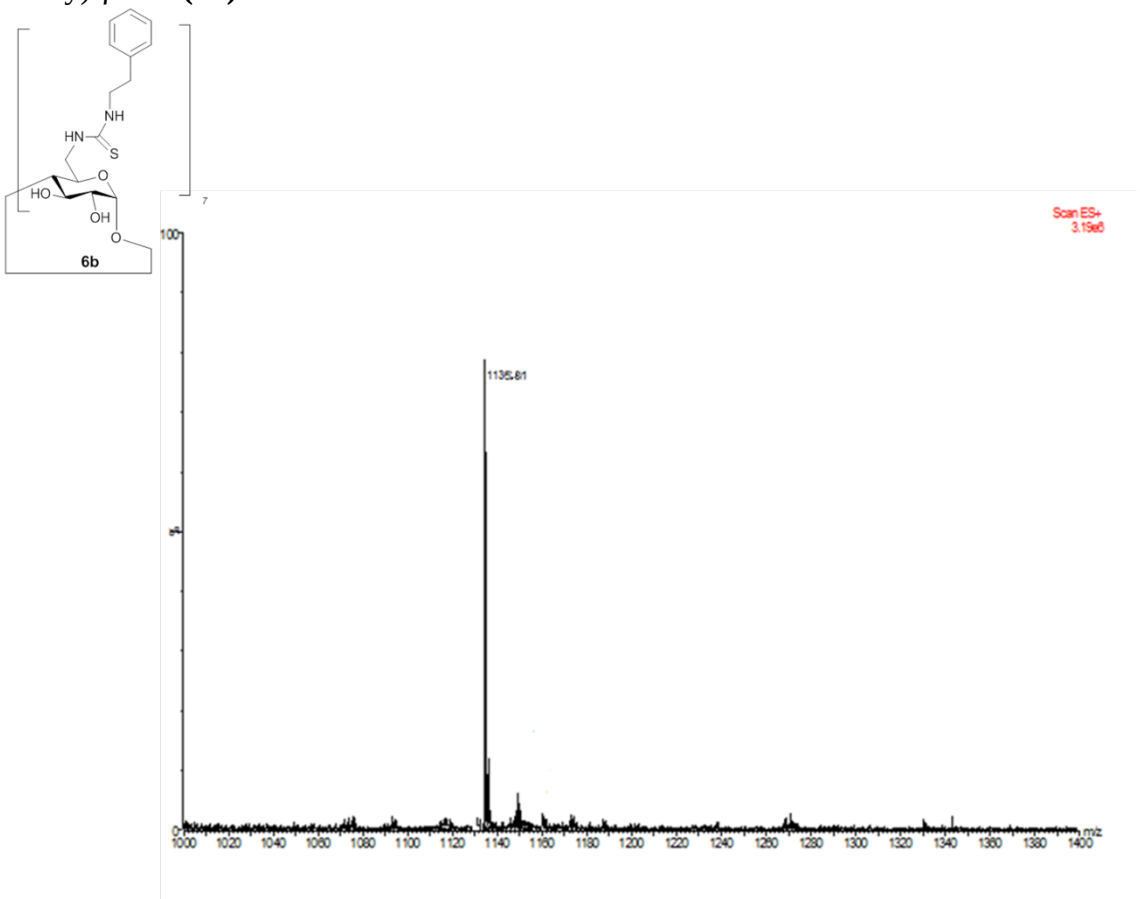

Fig 52. MS (ESI) spectrum of *per*-(6(3-phenylethylthioureido)-6-deoxy)-β-CD **(6b)**

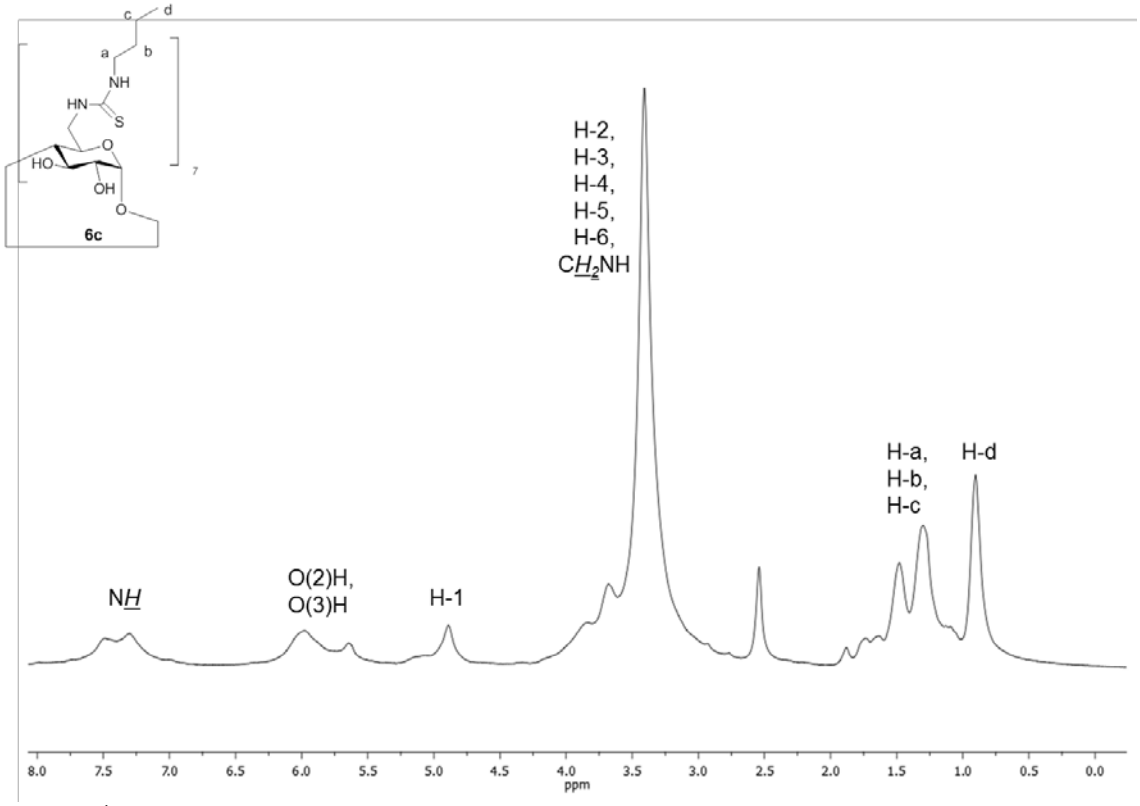

Fig 53. ^{1}H-NMR of *per*-(6(3-butylthioureido)-6-deoxy)-β-CD **(6c)**

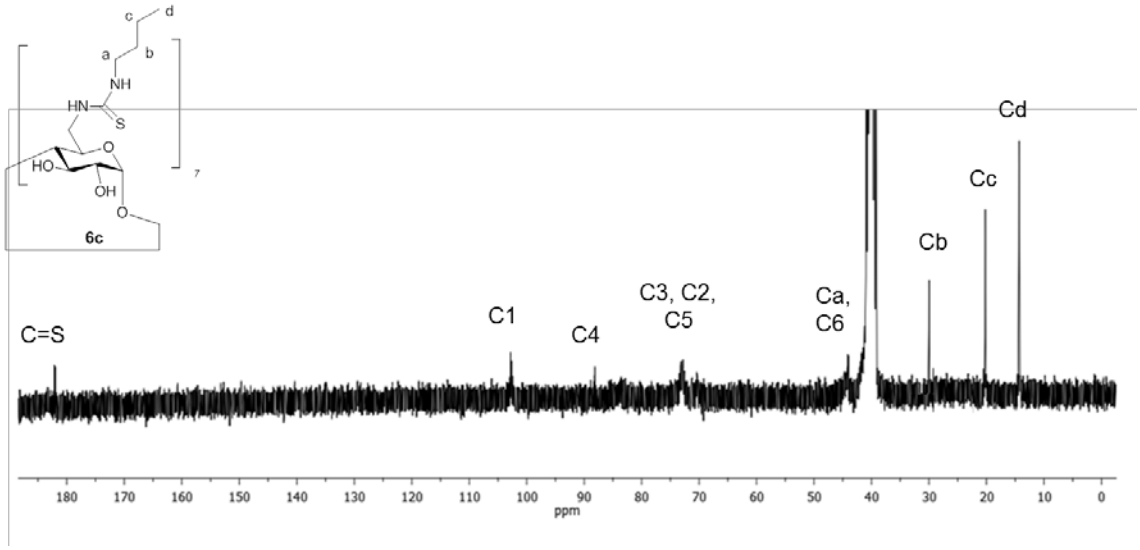

Fig 54. ^{13}C NMR of *per*-(6(3-butylthioureido)-6-deoxy)-β-CD **(6c)**

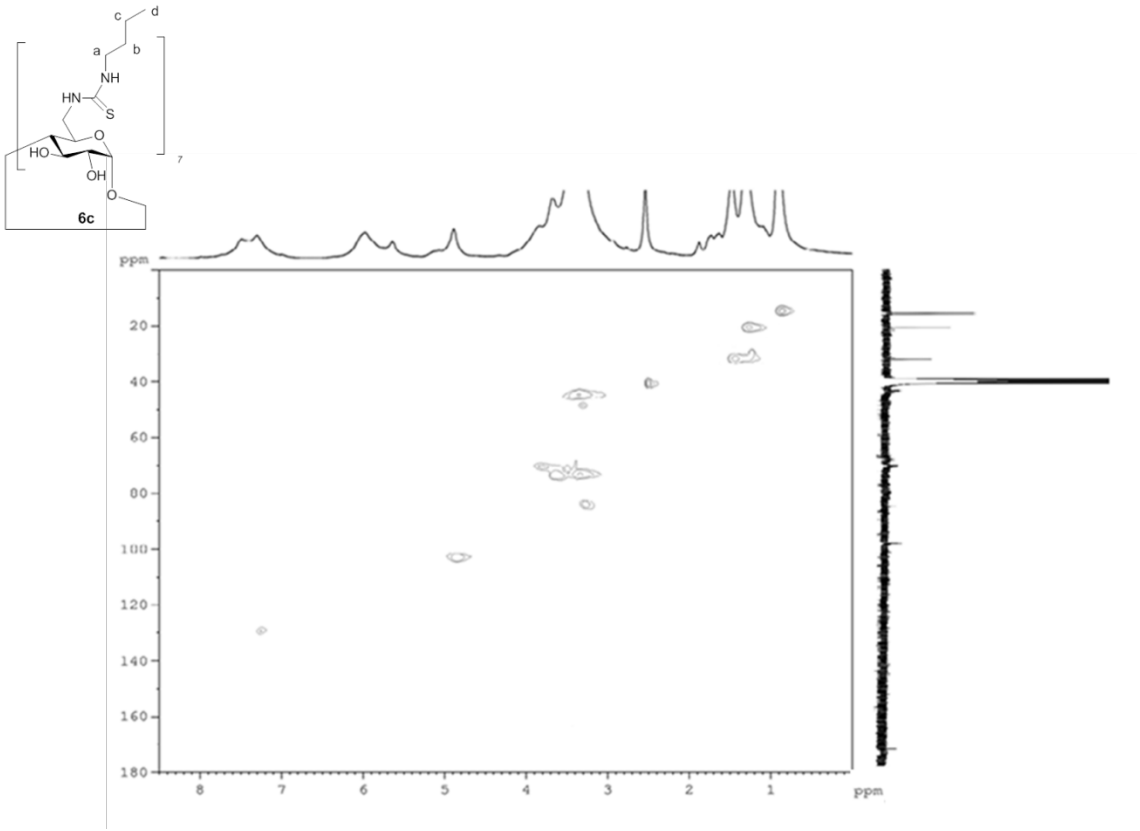

Fig 55. HMQC spectrum (300 MHz for ^{I}H-^{13}C, in DMSO-d_6) of *per*-(6(3-butylthioureido)-6-deoxy)-β-CD **(6c)**

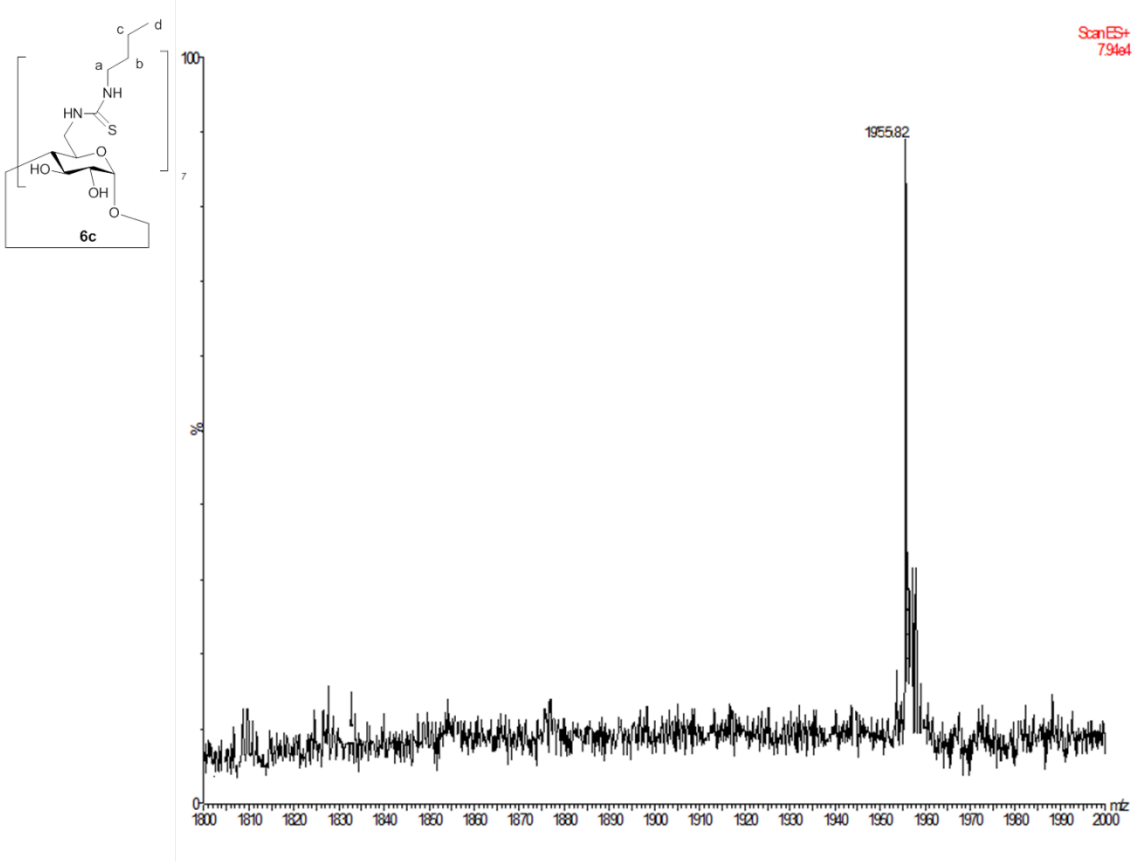

Fig 56. MS (ESI) spectrum of *per*-(6(3-butylthioureido)-6-deoxy)-β-CD **(6c)**

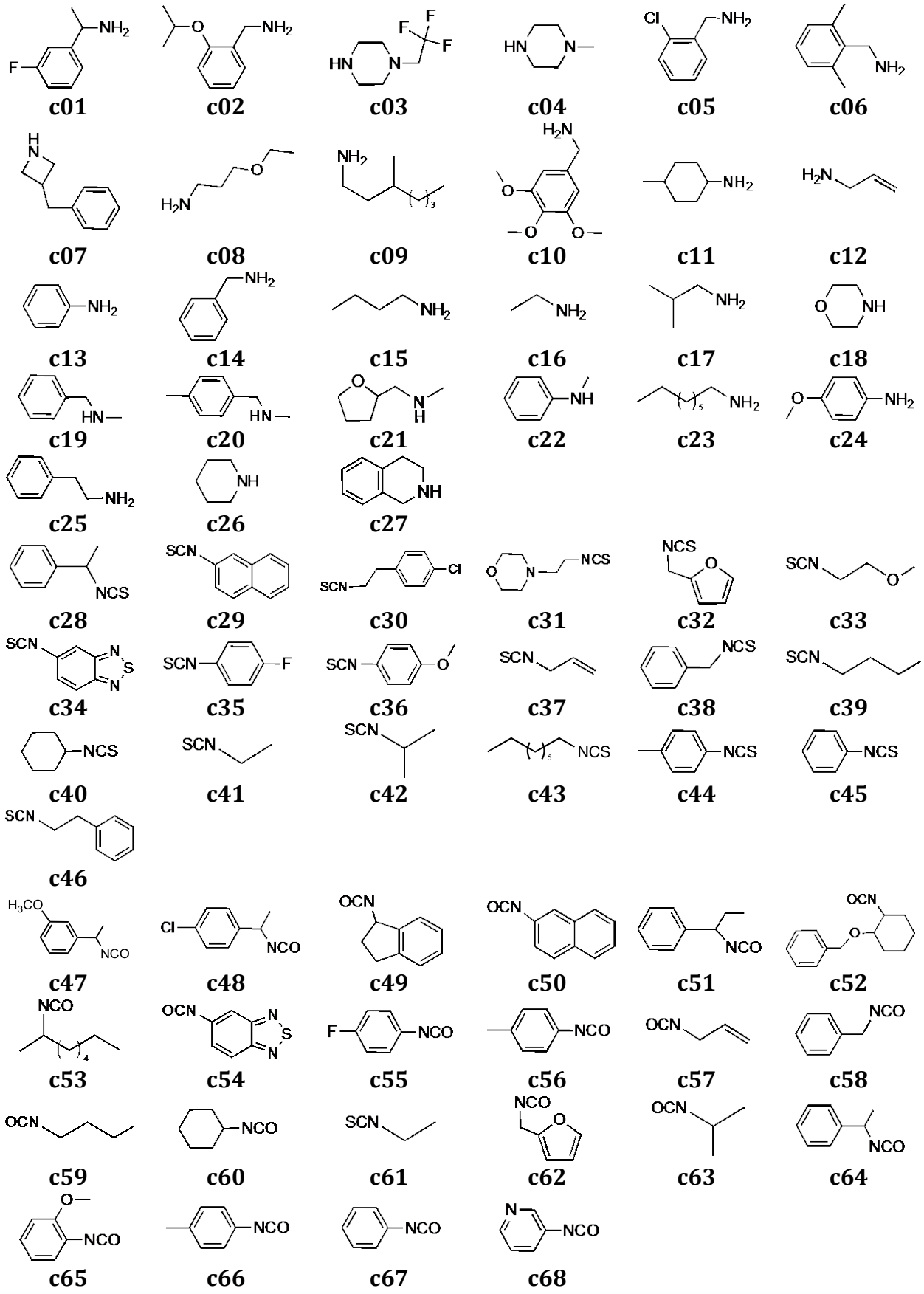

Fig 57. Chemical structure of the substituents

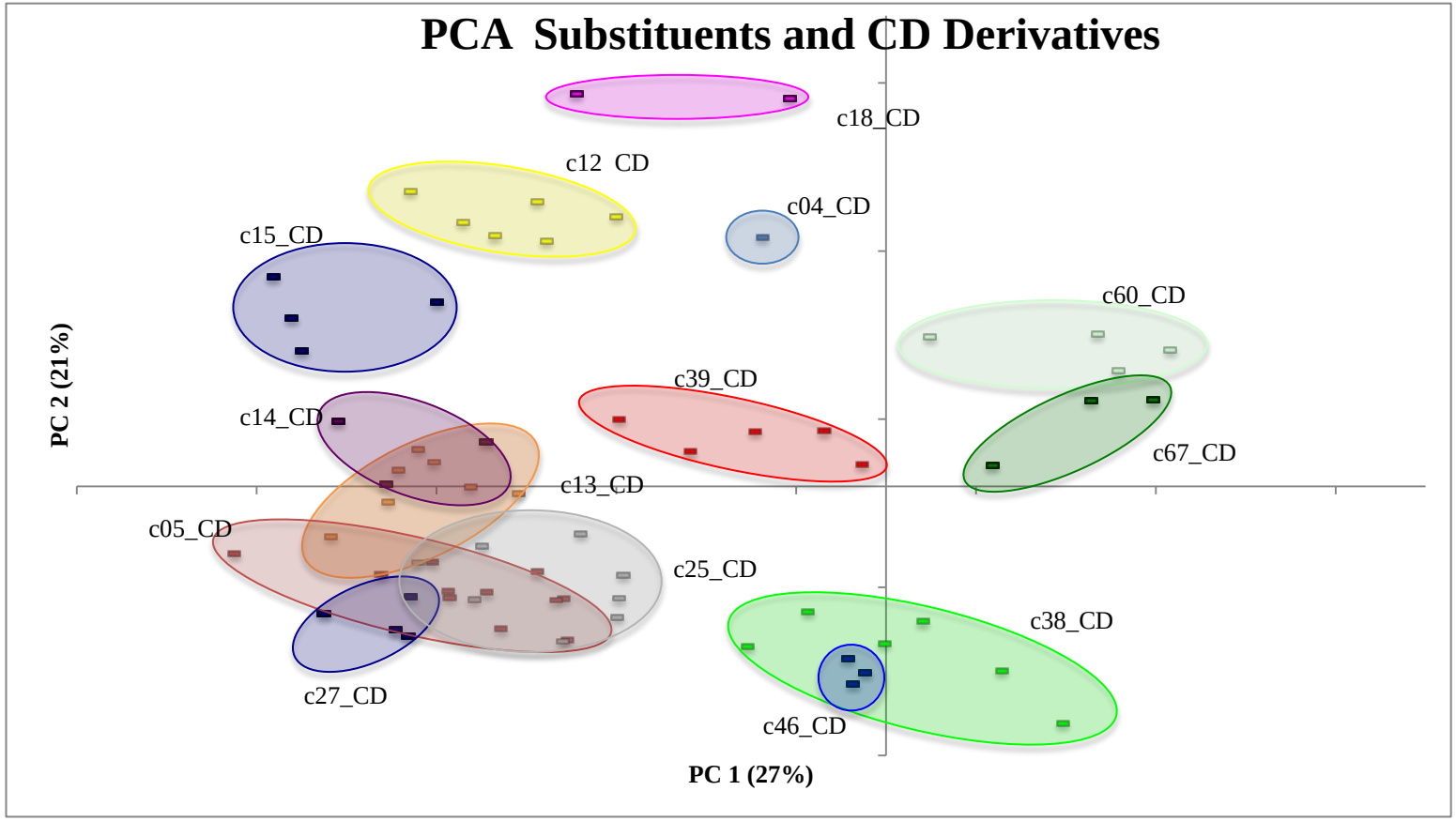

Fig. 58. PCA of the synthetized CD derivatives. VolSurf+ descriptors were calculated for low energy conformations of each CD, obtained as explained in the paper, and submitted to a PCA analysis. The score plot of the first two main PCs (in parenthesis the variance %) is reported. Each CD is shown with a different color and small rectangles with the same color represent the correspondent conformations. Such conformations can be grouped in the highlighted region of the score plot. The plot shows how CD derivatives can be clustered mainly on the basis of substituents properties.