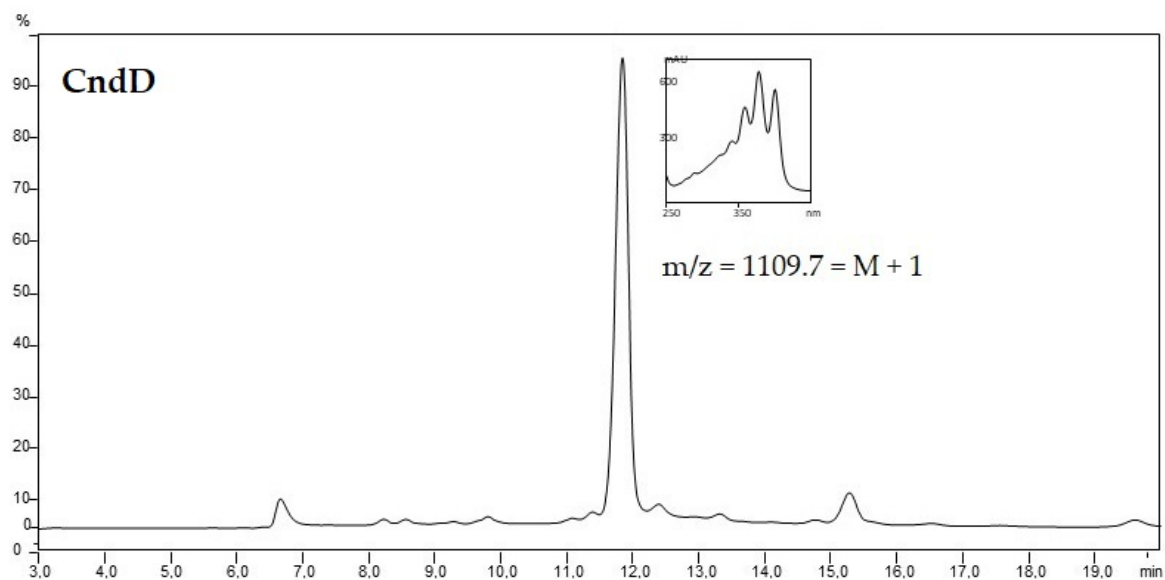


Supplementary materials

Figures S1A-F. HPLC-DAD-ESIMS chromatograms of CndD, ParA, ParB, isoCndD, isoParA and isoParB

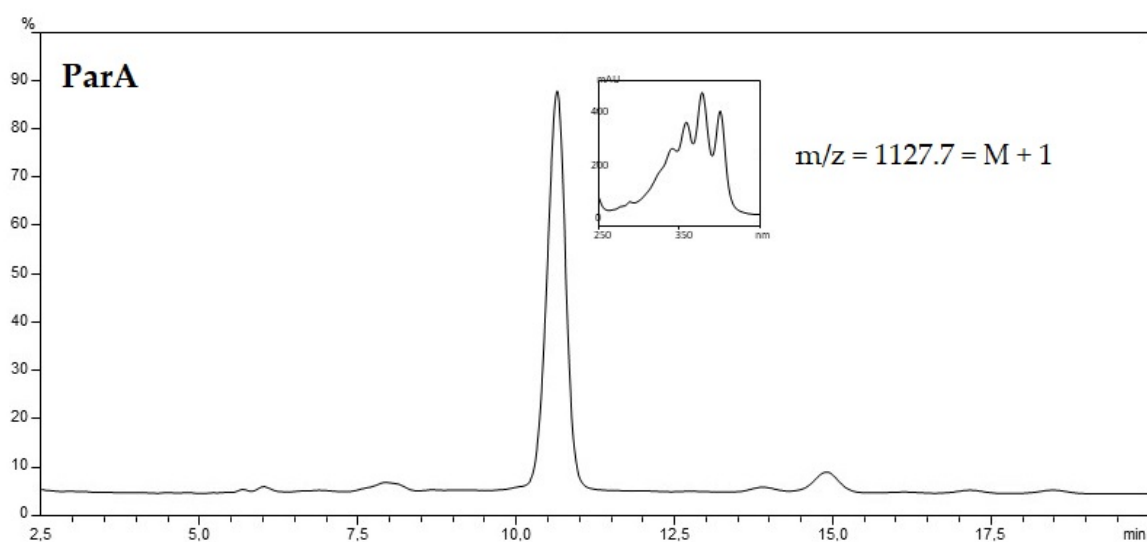
Figure S1A



HPLC-DAD-ESIMS chromatogram of Candidicin D sample.

Chromatographic conditions: column Luna 100 C18(2), (150 mm × 4.6 mm, 5 μm). Mobile phase composition: 38% acetonitrile/ 62% ammonium acetate buffer (5.5 mmol, pH = 4.5), v/v; at a flow rate of 1 mL/min; inj. volume = 10 μL. Detection at 378 nm, room temperature.

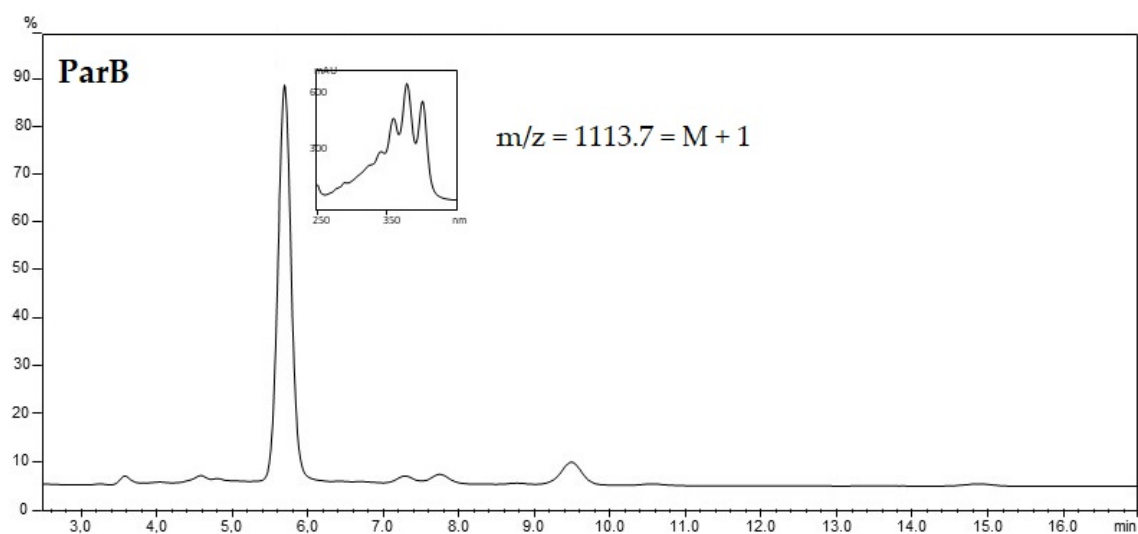
Figure S1B



HPLC-DAD-ESIMS chromatogram of Partricin A sample.

Chromatographic conditions: column Luna 100 C18(2), (150 mm × 4.6 mm, 5 μm). Mobile phase composition: 38% acetonitrile/ 62% ammonium acetate buffer (5.5 mmol, pH = 4.5), v/v; at a flow rate of 1 mL/min; inj. volume = 10 μL. Detection at 378 nm, room temperature.

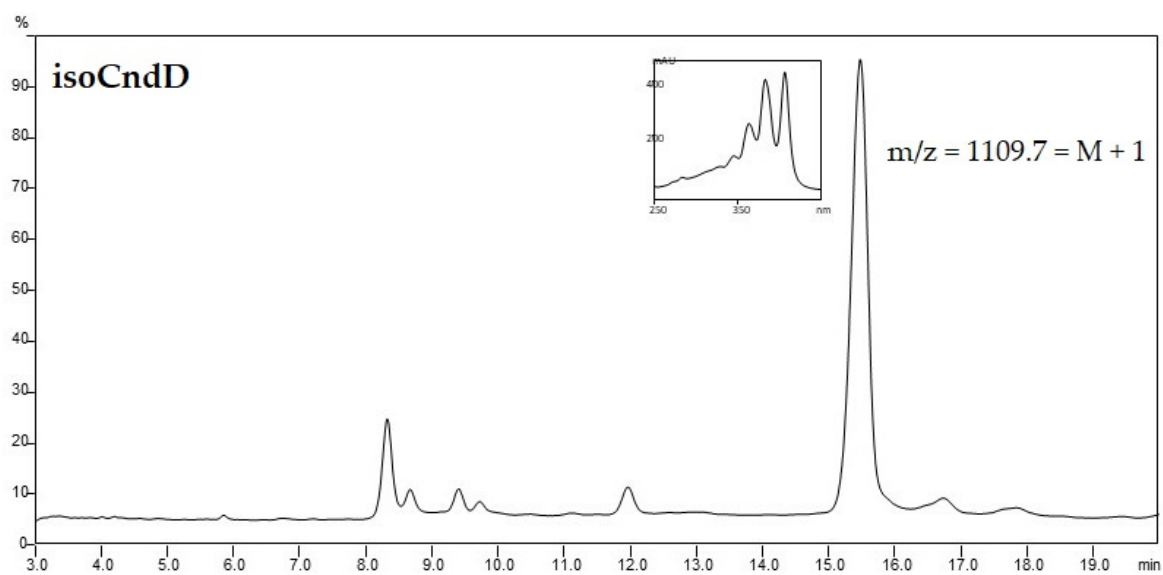
Figure S1C



HPLC-DAD-ESIMS chromatogram of Partricin B sample.

Chromatographic conditions: column Luna 100 C18(2), (150 mm × 4.6 mm, 5 μm). Mobile phase composition: 38% acetonitrile/ 62% ammonium acetate buffer (5.5 mmol, pH = 4.5), v/v; at a flow rate of 1 mL/min; inj. volume = 10 μL. Detection at 378 nm, room temperature.

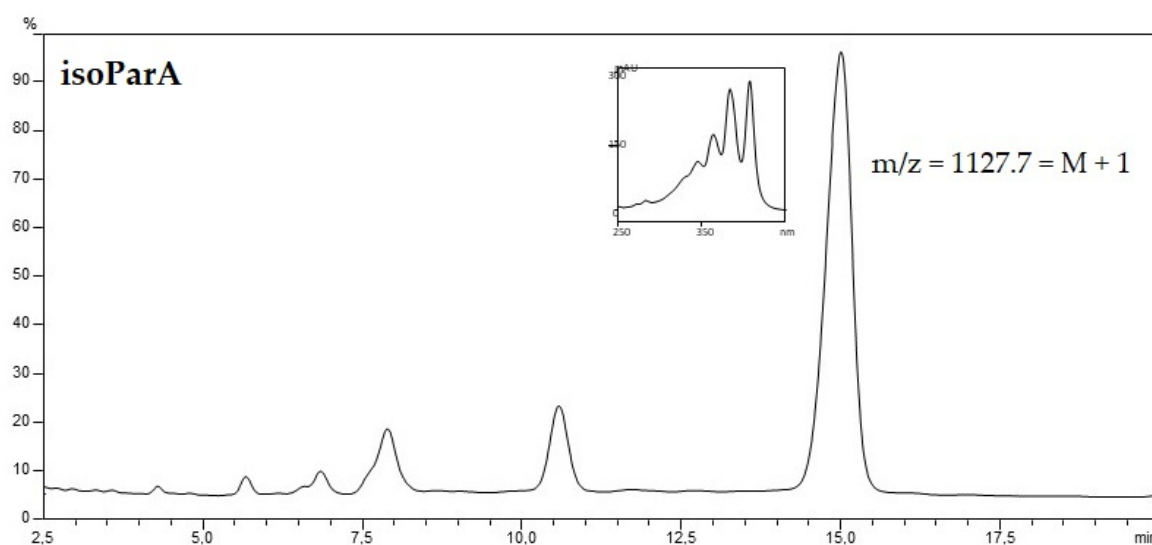
Figure S1D



HPLC-DAD-ESIMS chromatogram of isoCandicidin D sample.

Chromatographic conditions: column Luna 100 C18(2), (150 mm × 4.6 mm, 5 μm). Mobile phase composition: 38% acetonitrile/ 62% ammonium acetate buffer (5.5 mmol, pH = 4.5), v/v; at a flow rate of 1 mL/min; inj. volume = 10 μL. Detection at 378 nm, room temperature.

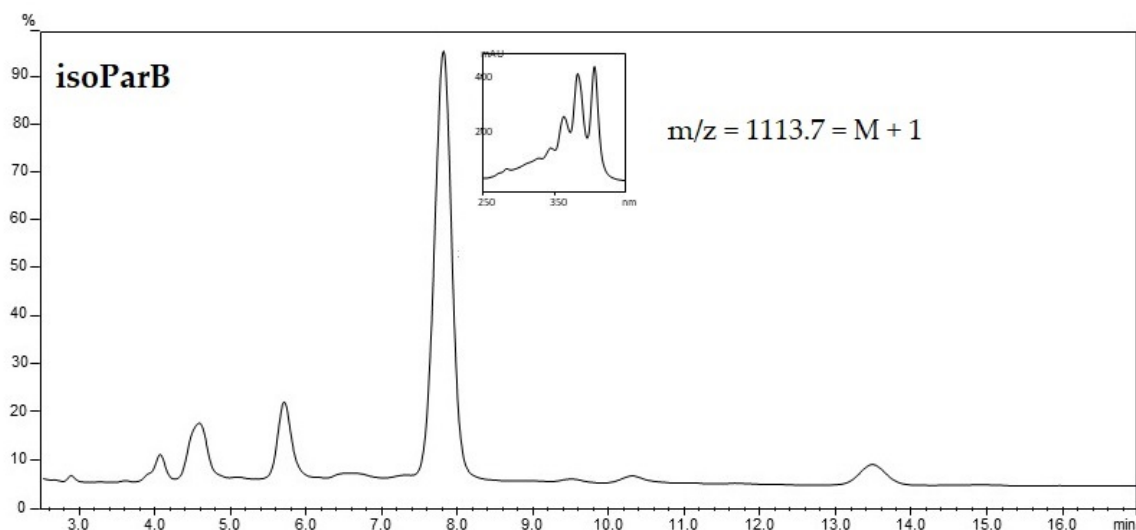
Figure S1E



HPLC-DAD-ESIMS chromatogram of isoPartricin A sample.

Chromatographic conditions: column Luna 100 C18(2), (150 mm × 4.6 mm, 5 μm). Mobile phase composition: 38% acetonitrile/ 62% ammonium acetate buffer (5.5 mmol, pH = 4.5), v/v; at a flow rate of 1 mL/min; inj. volume = 10 μL. Detection at 378 nm, room temperature.

Figure S1F



HPLC-DAD-ESIMS chromatogram of isoPartricin B sample

Chromatographic conditions: column Luna 100 C18(2), (150 mm × 4.6 mm, 5 μm). Mobile phase composition: 38% acetonitrile/ 62% ammonium acetate buffer (5.5 mmol, pH = 4.5), v/v; at a flow rate of 1 mL/min; inj. volume = 10 μL. Detection at 378 nm, room temperature.

Figures S2A-F. ^1H NMR spectra of CndD, ParA, ParB, isoCndD, isoParA and isoParB

Figure S1A

^1H spectrum CndD

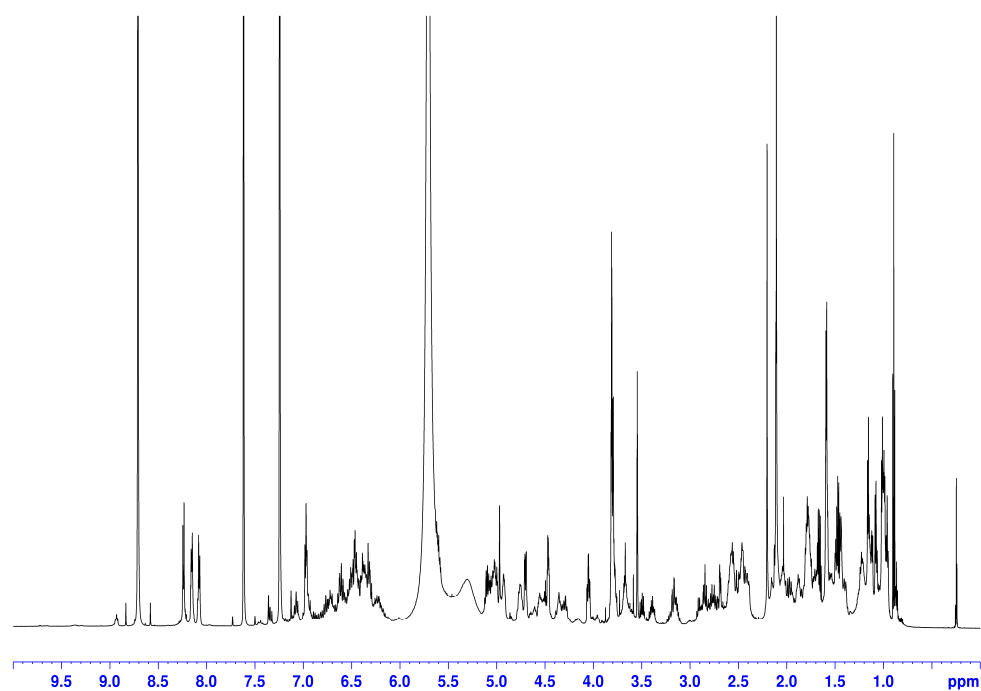


Figure S2B

^1H NMR ParA

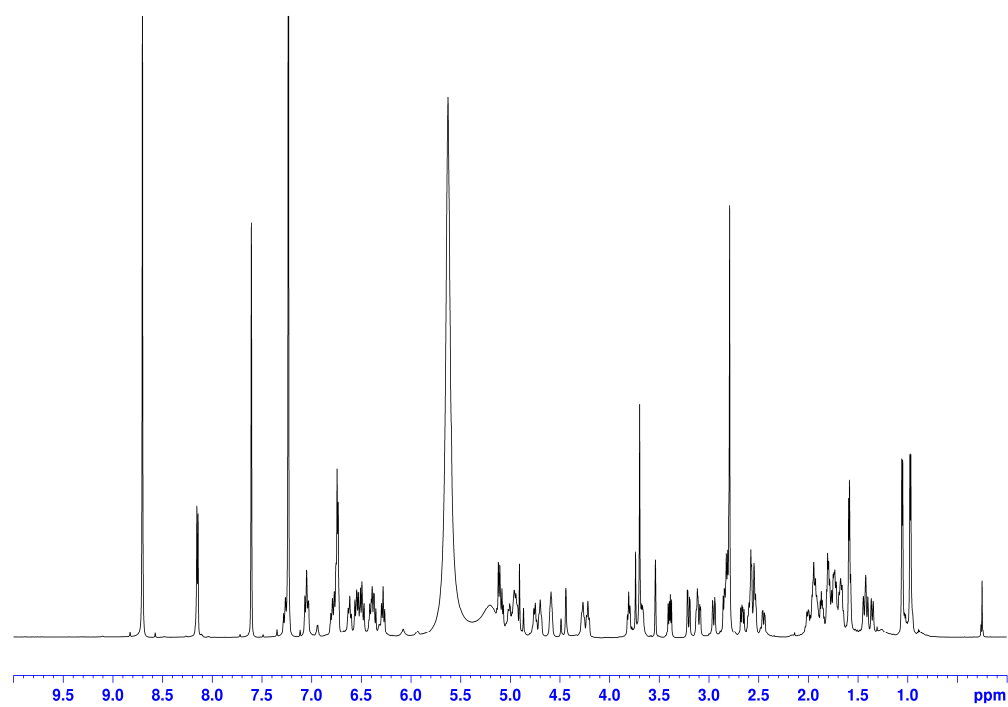


Figure S2C

^1H NMR ParB

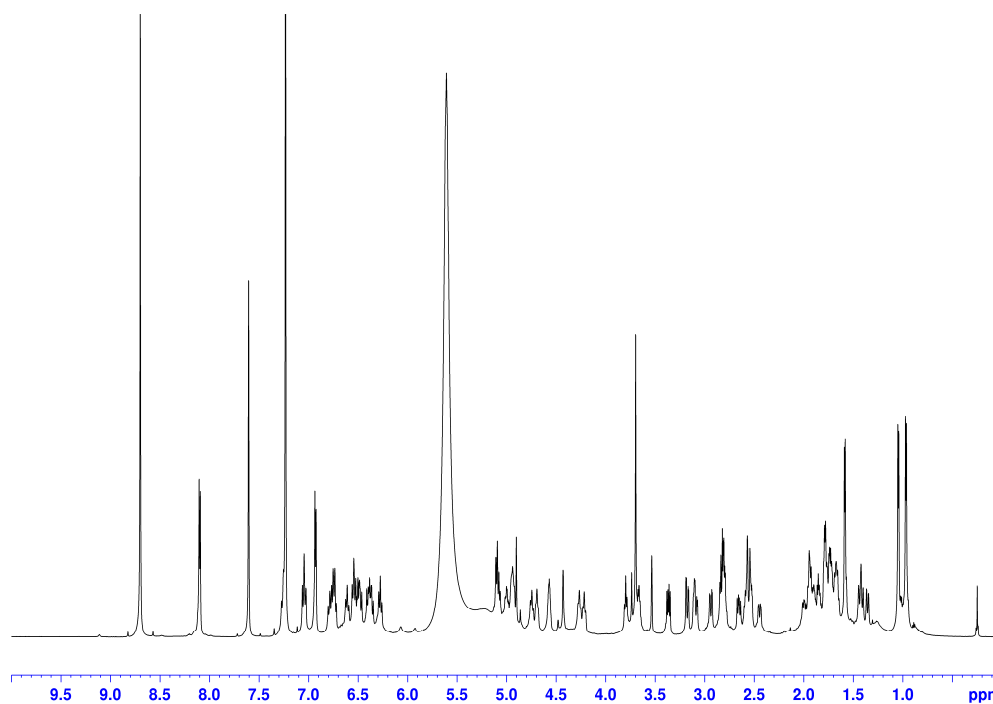


Figure S2D

^1H NMR isoCndD

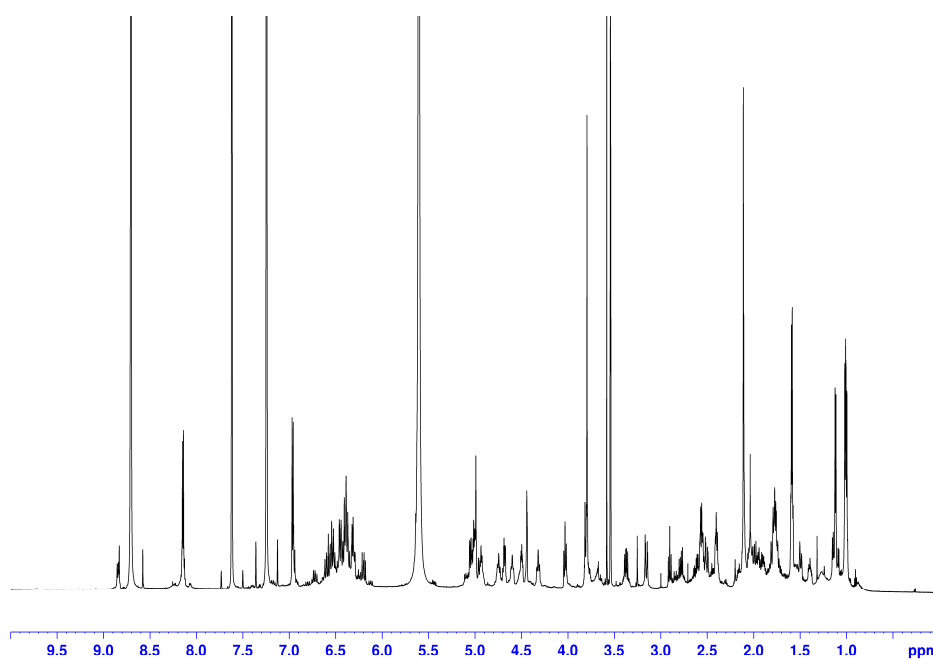


Figure S2E

^1H NMR isoParA

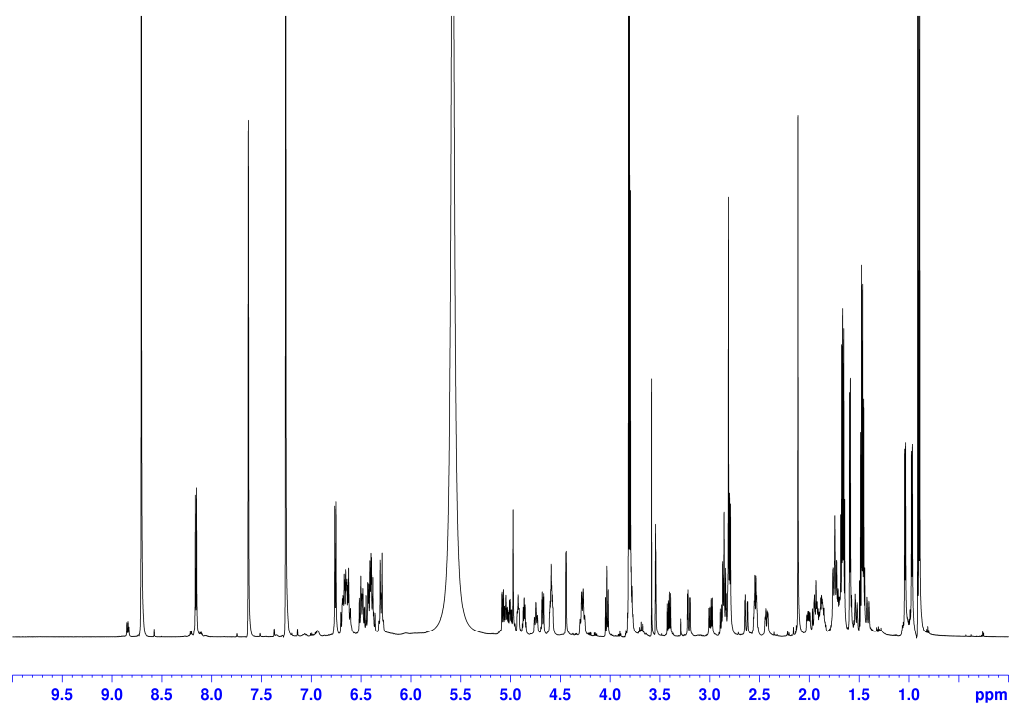
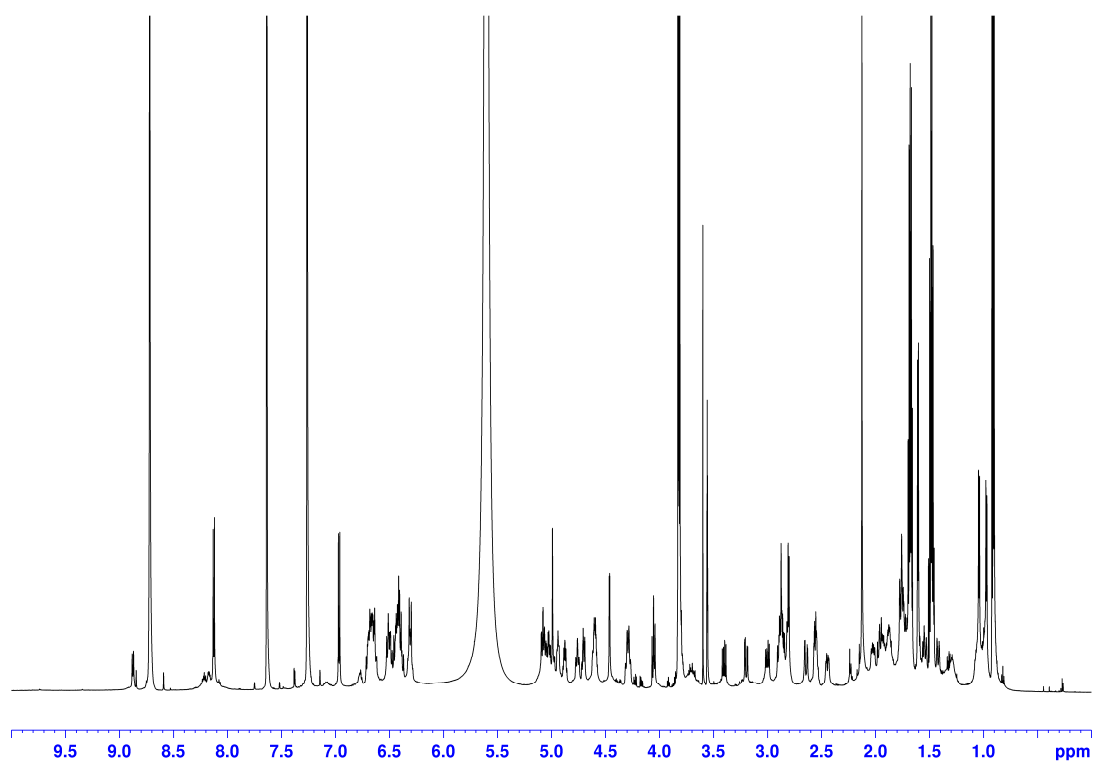


Figure S2F

^1H NMR isoParB



Figures S3A-F. Fragments of 2D DOF-COSY ^1H NMR spectra of CndD, ParA, ParB and their *all-trans* isomers

Figure S3A

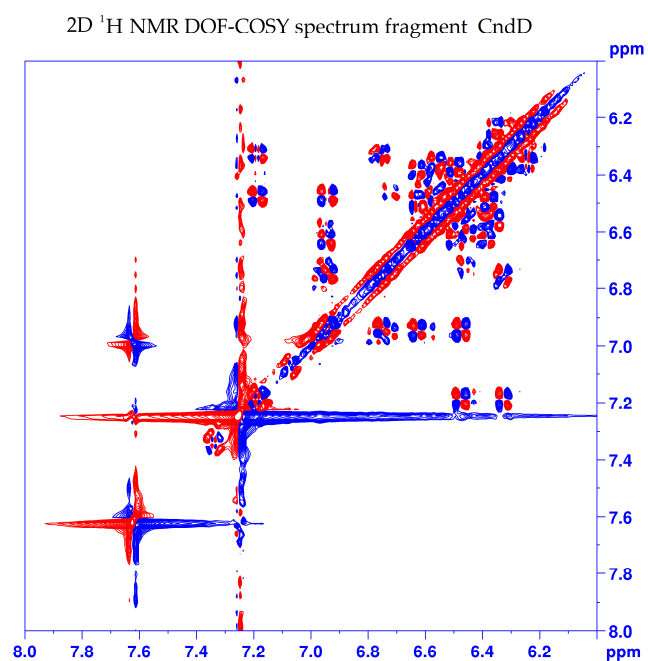


Figure S3B

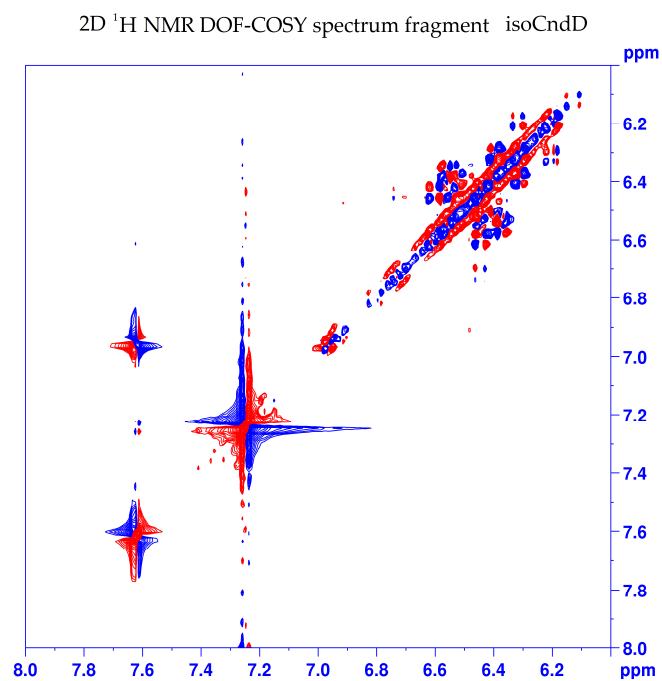


Figure S3C

2D ^1H NMR DOF-COSY spectrum fragment ParA

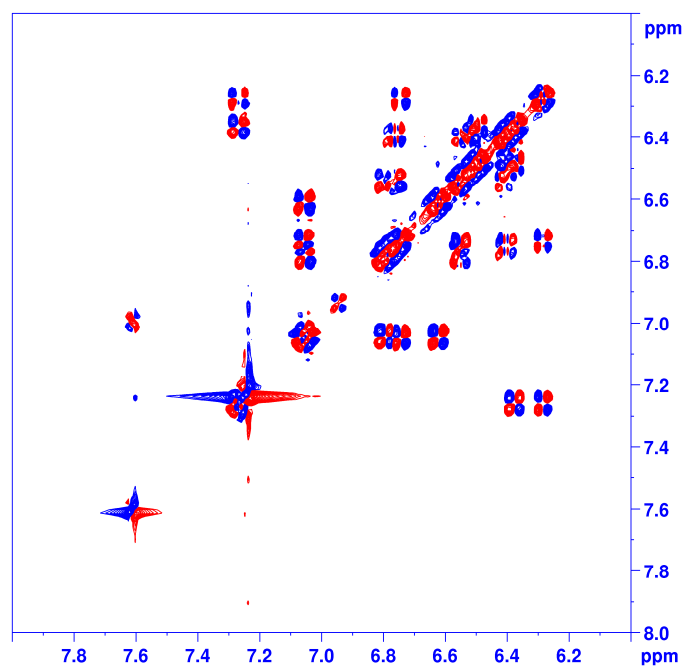


Figure S3D

2D ^1H NMR DOF-COSY spectrum fragment isoParA

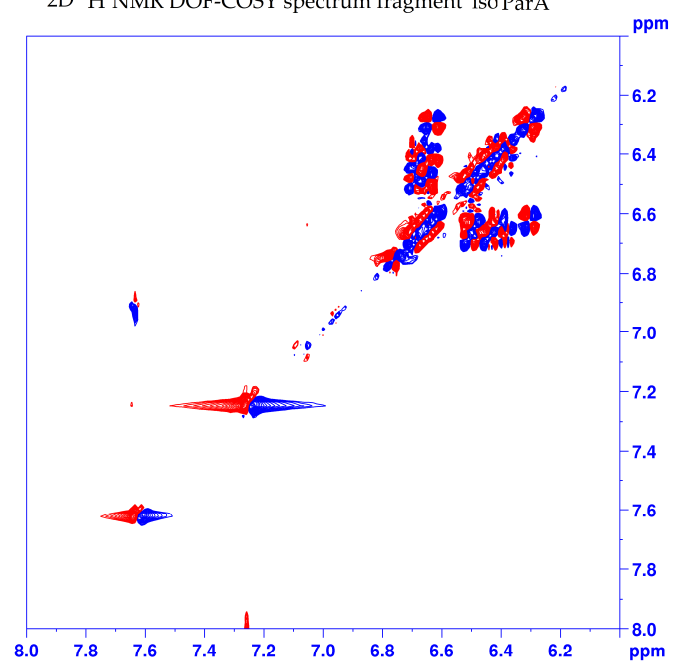


Figure S3E

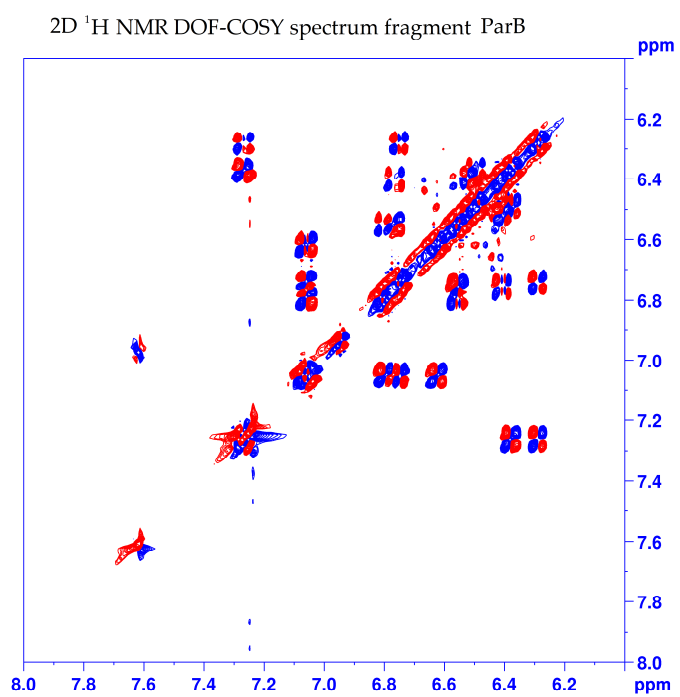


Figure S3F

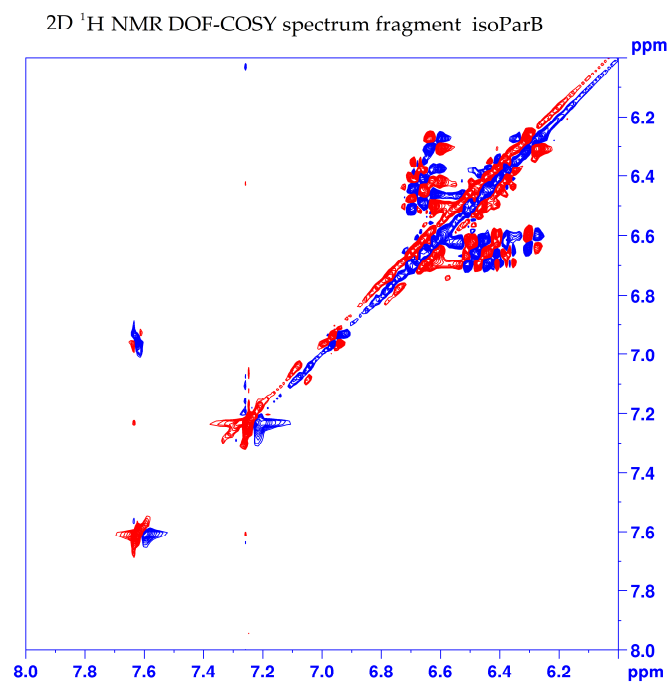

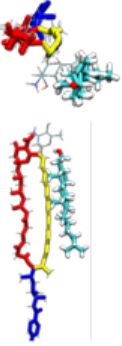

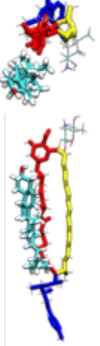
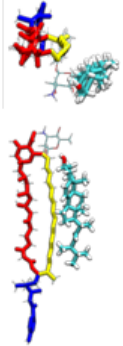

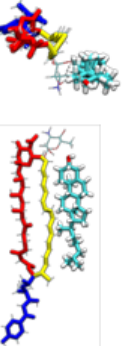

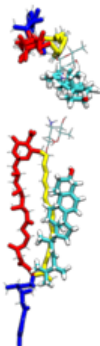
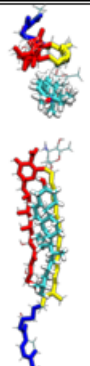
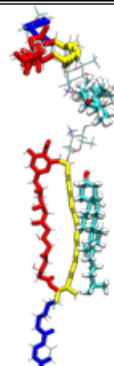
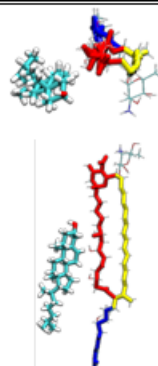
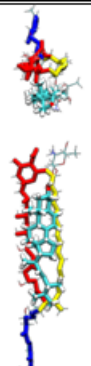
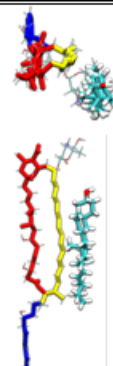
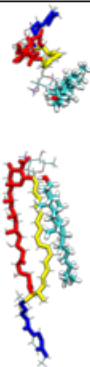
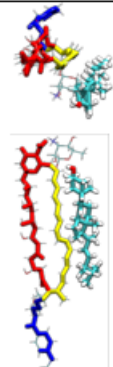

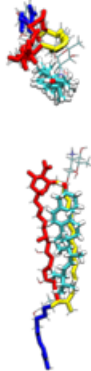
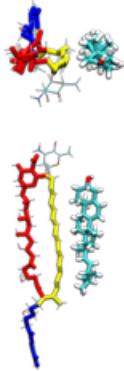
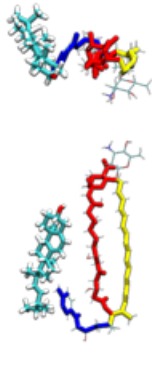


Figure S4. Structures of the AHM/sterol complexes, corresponding to the closer (1: 5-6 Å) and further (2: 7-8 Å) minima of the free energy profiles, obtained by cluster analysis of the resulting US trajectories.

Chol			Erg		
1		2	1	2	
isoCndD					
					

	Chol			Erg	
	1	2		1	2
isoParA					
ParA					

Chol				Erg			
1		2		1	2		
isoParB							
ParB	