

Binaphthalene based cyclic homochiral ureas and their structure-related properties

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Structural characterization of compounds 1-3

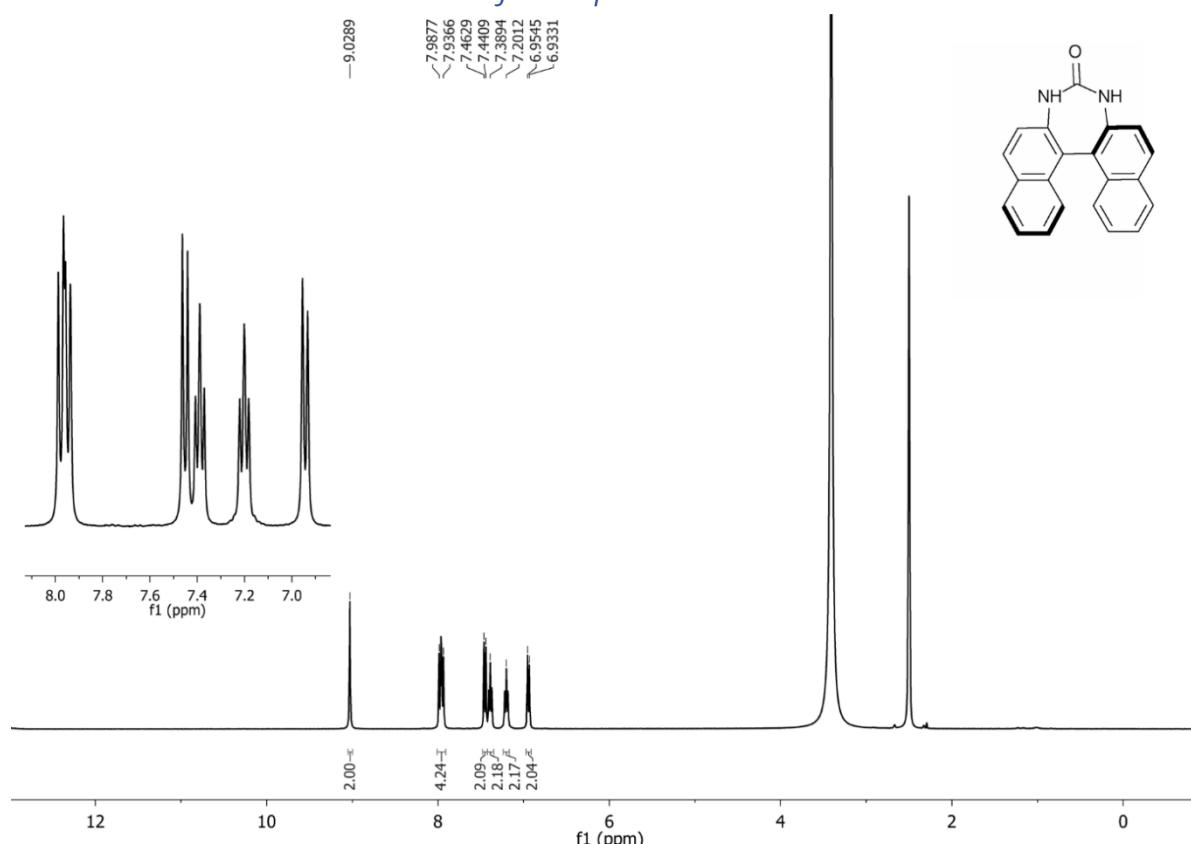


Figure S1, ¹H NMR spectrum of **1**, DMSO-d₆, 25°C, 400MHz.

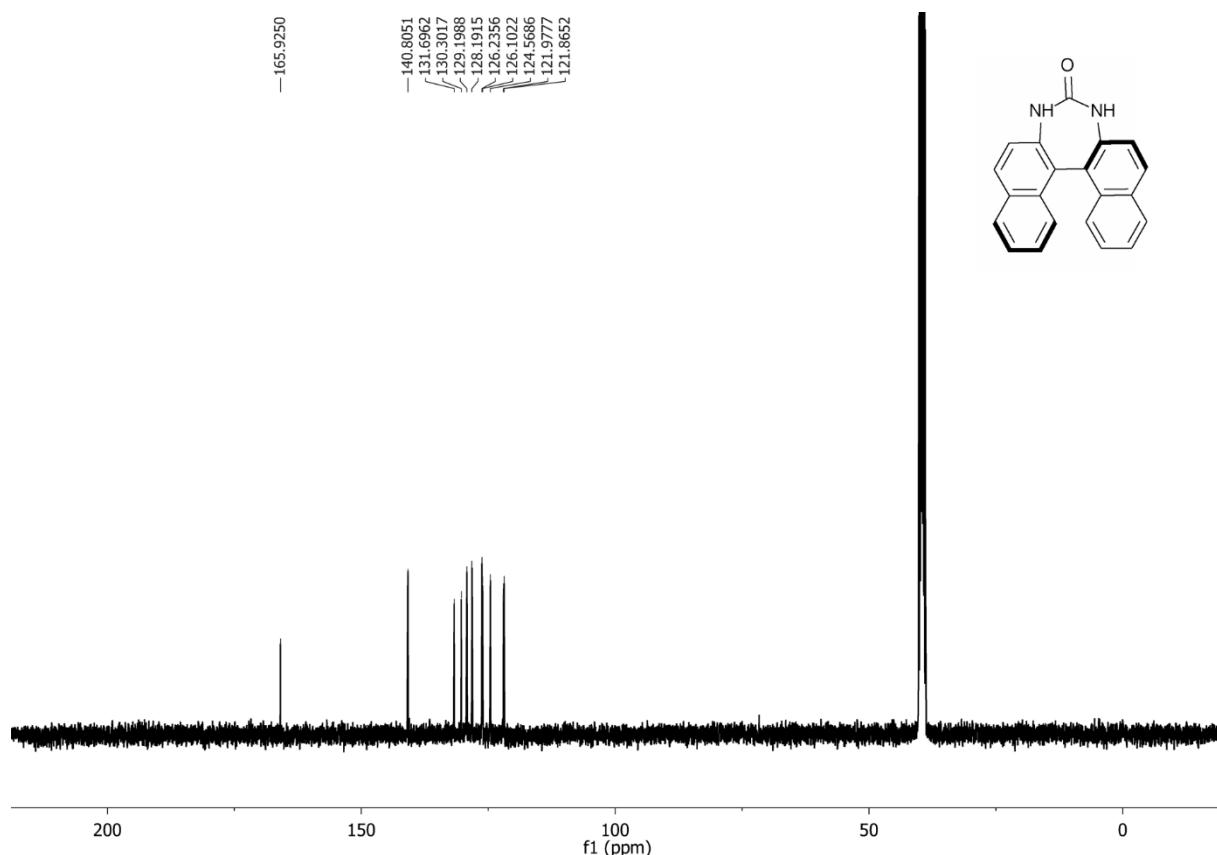


Figure S2, ¹³C NMR spectrum of **1**, DMSO-d₆, 25°C, 400MHz.

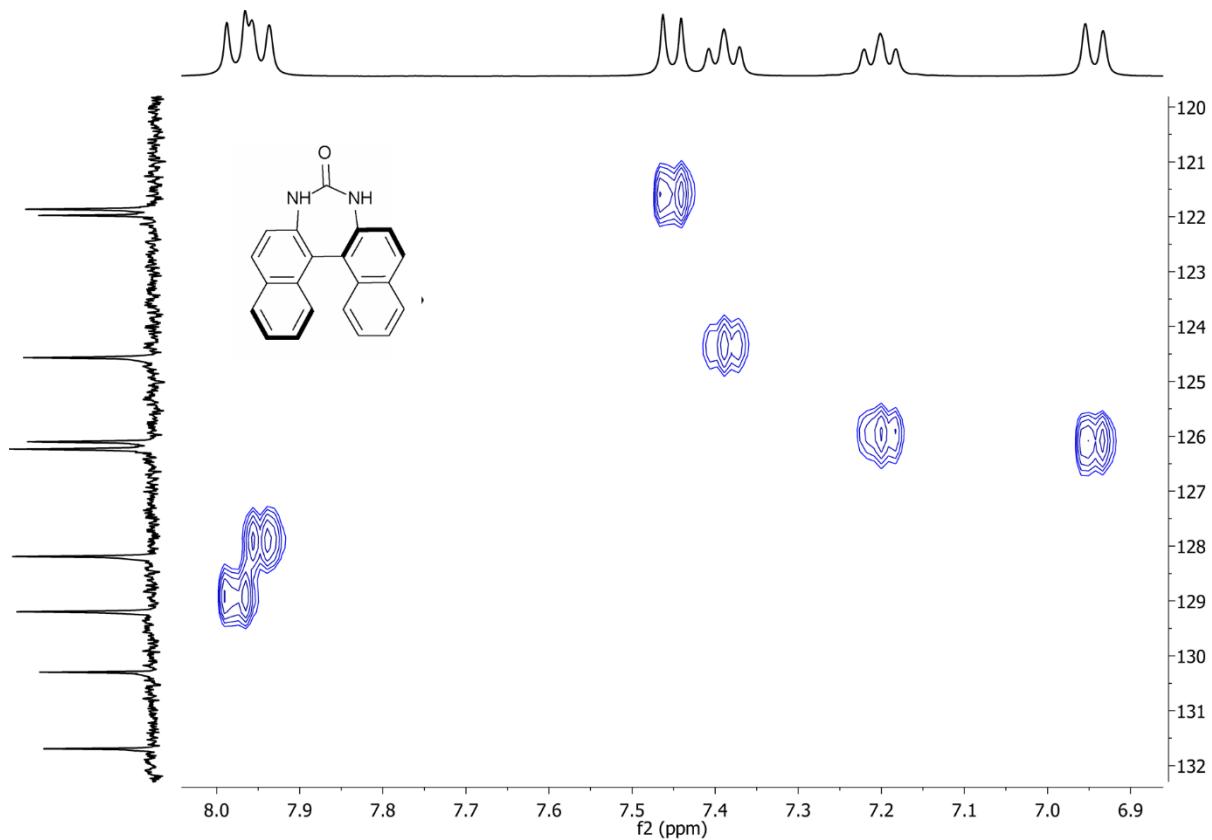


Figure S3, ^1H - ^{13}C HSQC NMR spectrum of **1**, chloroform- d_6 , 25°C, 400/101 MHz.

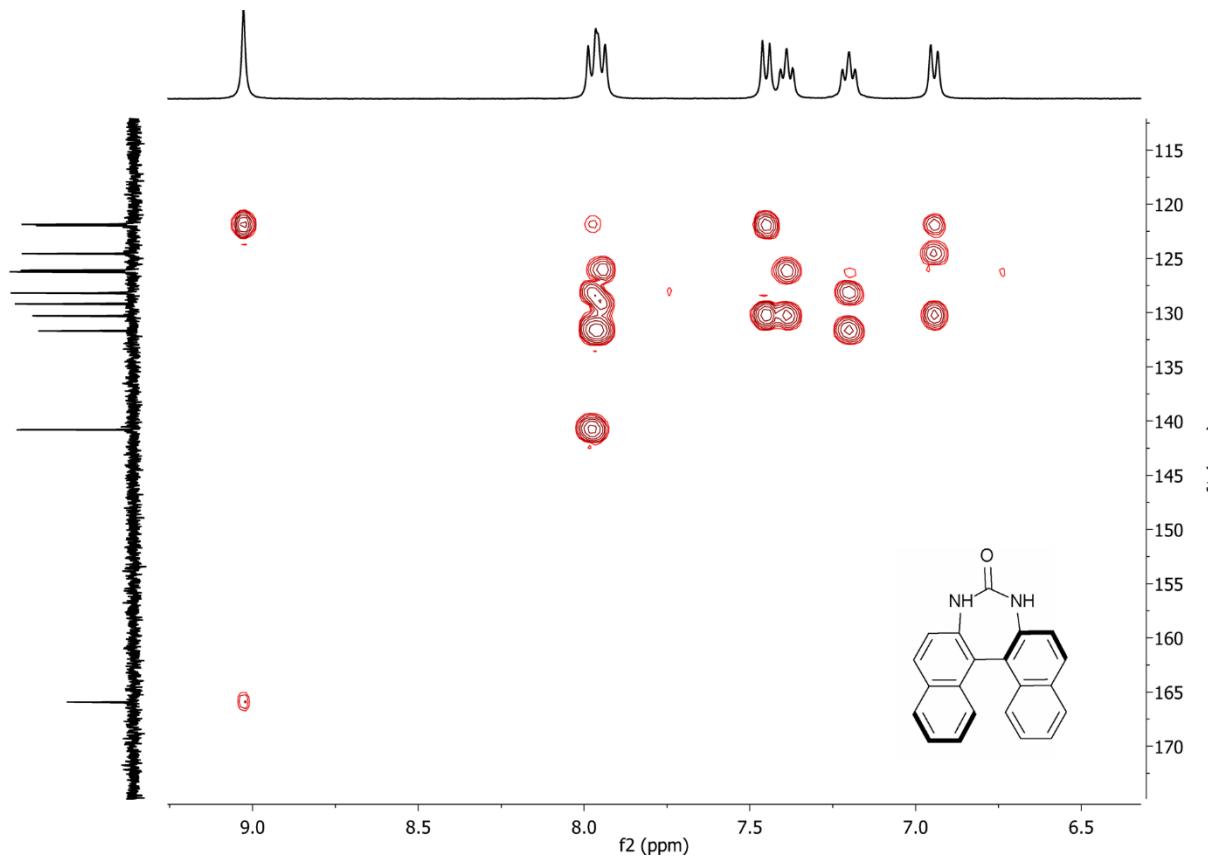


Figure S4, ^1H - ^{13}C HMBC NMR spectrum of **1**, chloroform- d_6 , 25°C, 400/101 MHz.

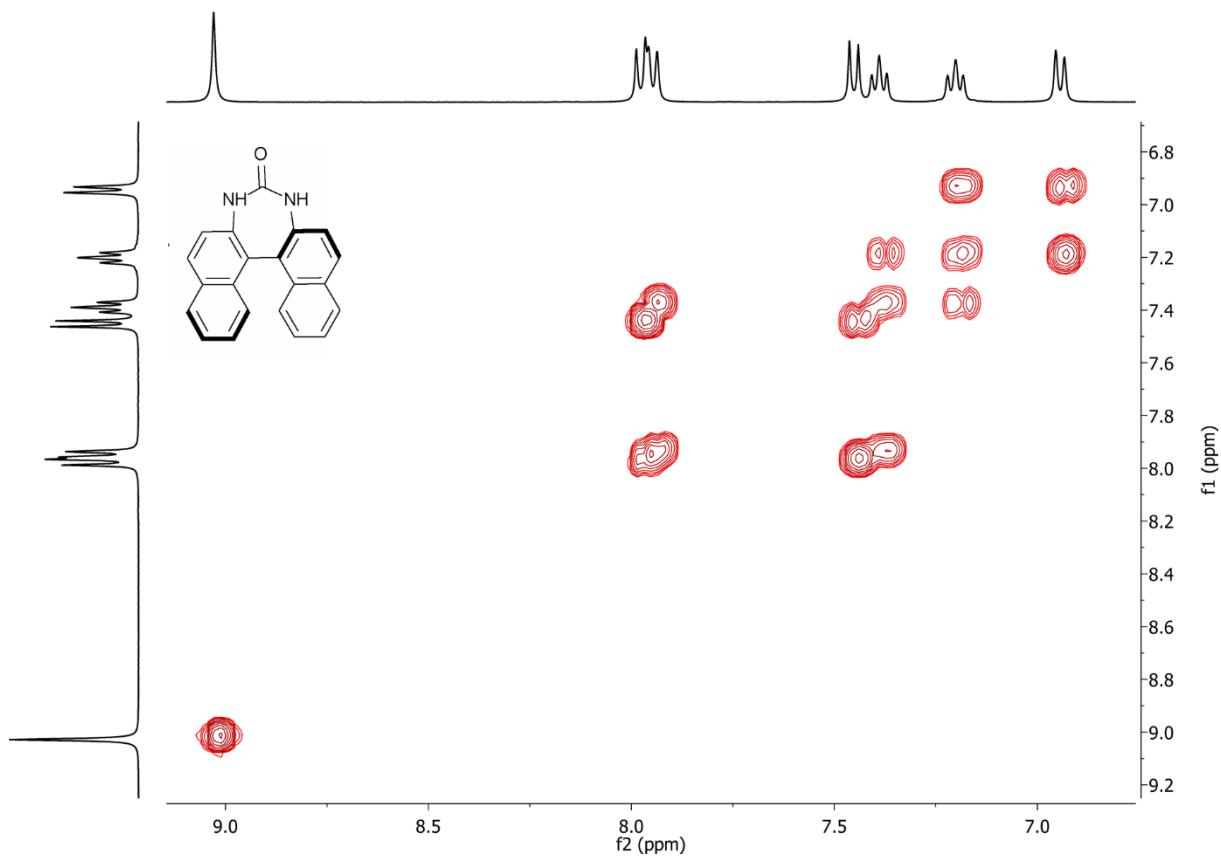


Figure S5, ^1H - ^1H COSY NMR spectrum of **1**, DMSO- d_6 , 25°C, 400/400 MHz.

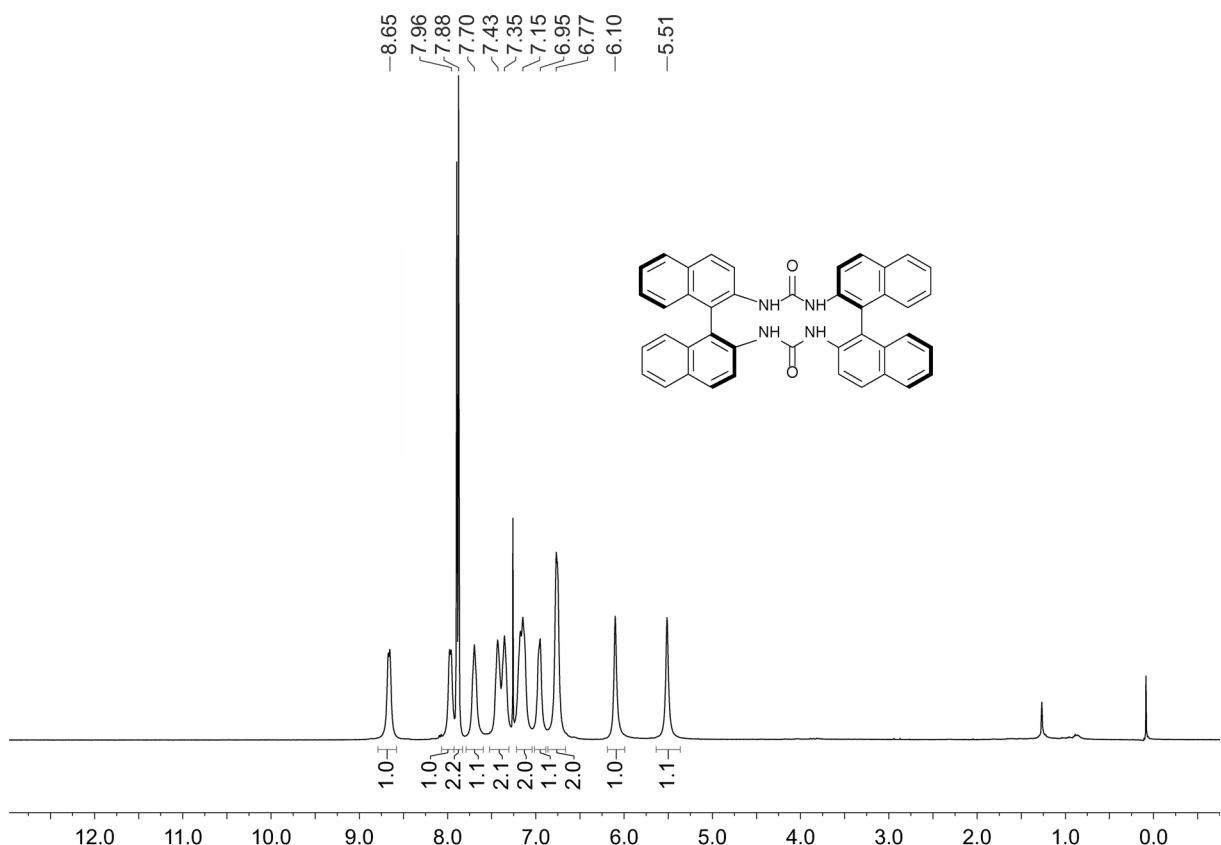


Figure S6, ^1H NMR spectrum of **2**, chloroform- d , 25°C, 400MHz.

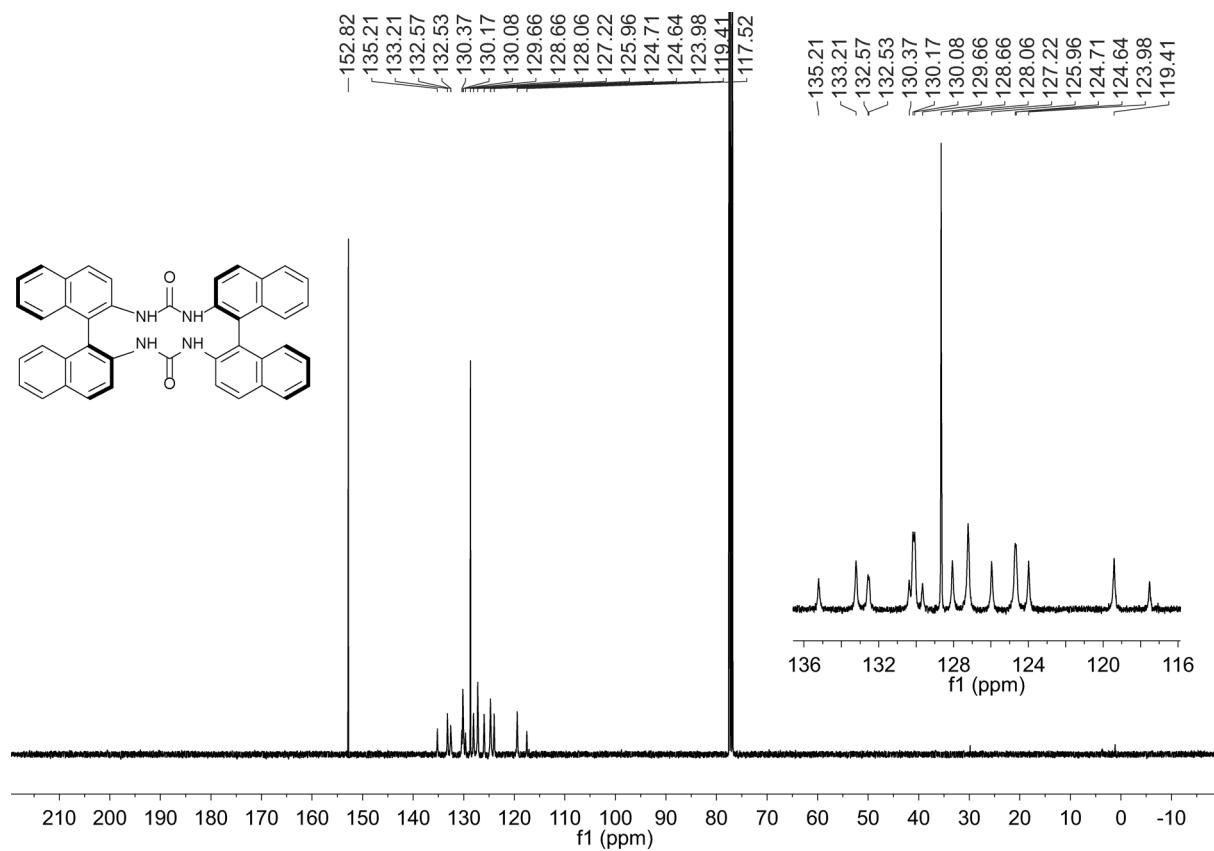


Figure S7, ^{13}C NMR spectrum of **2**, chloroform-*d*, 25°C, 101 MHz.

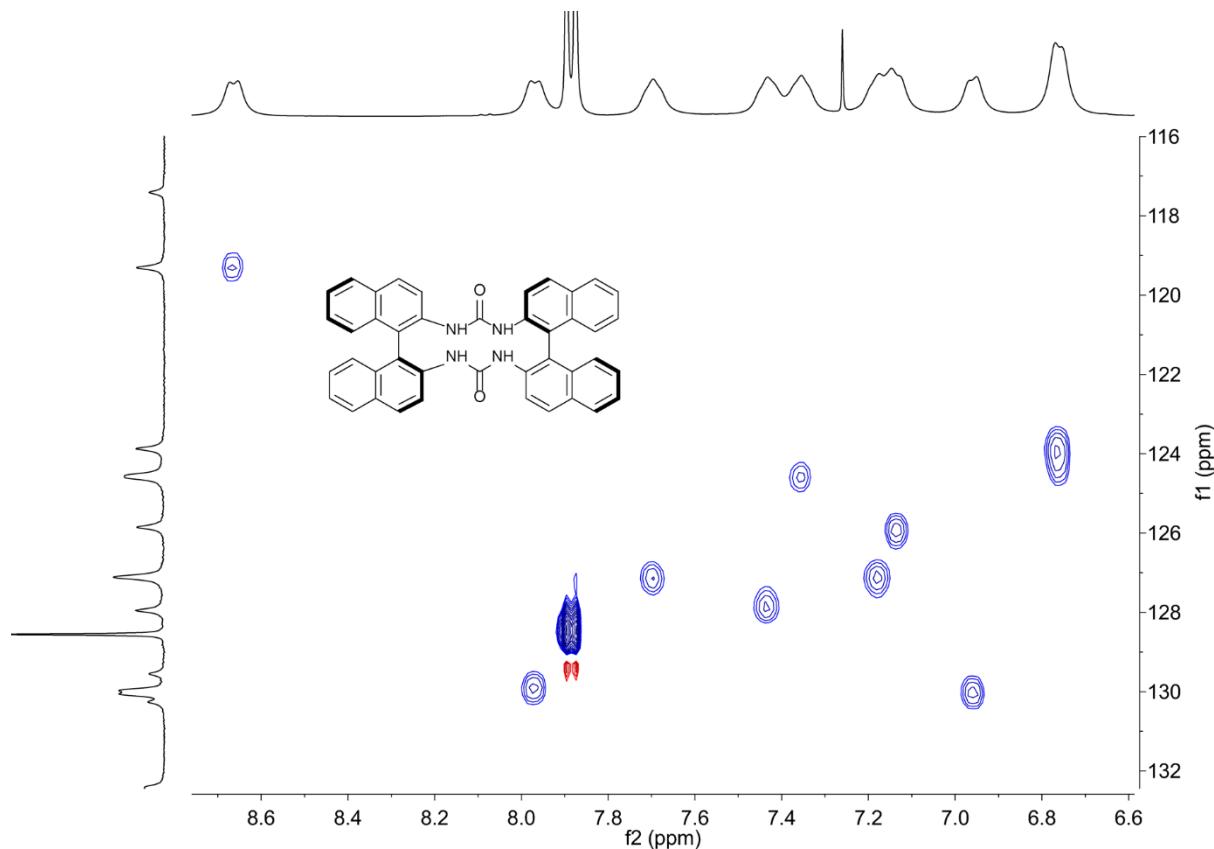


Figure S8, ^1H - ^{13}C HSQC NMR spectrum of **2**, chloroform-*d*, 25°C, 400/101 MHz.

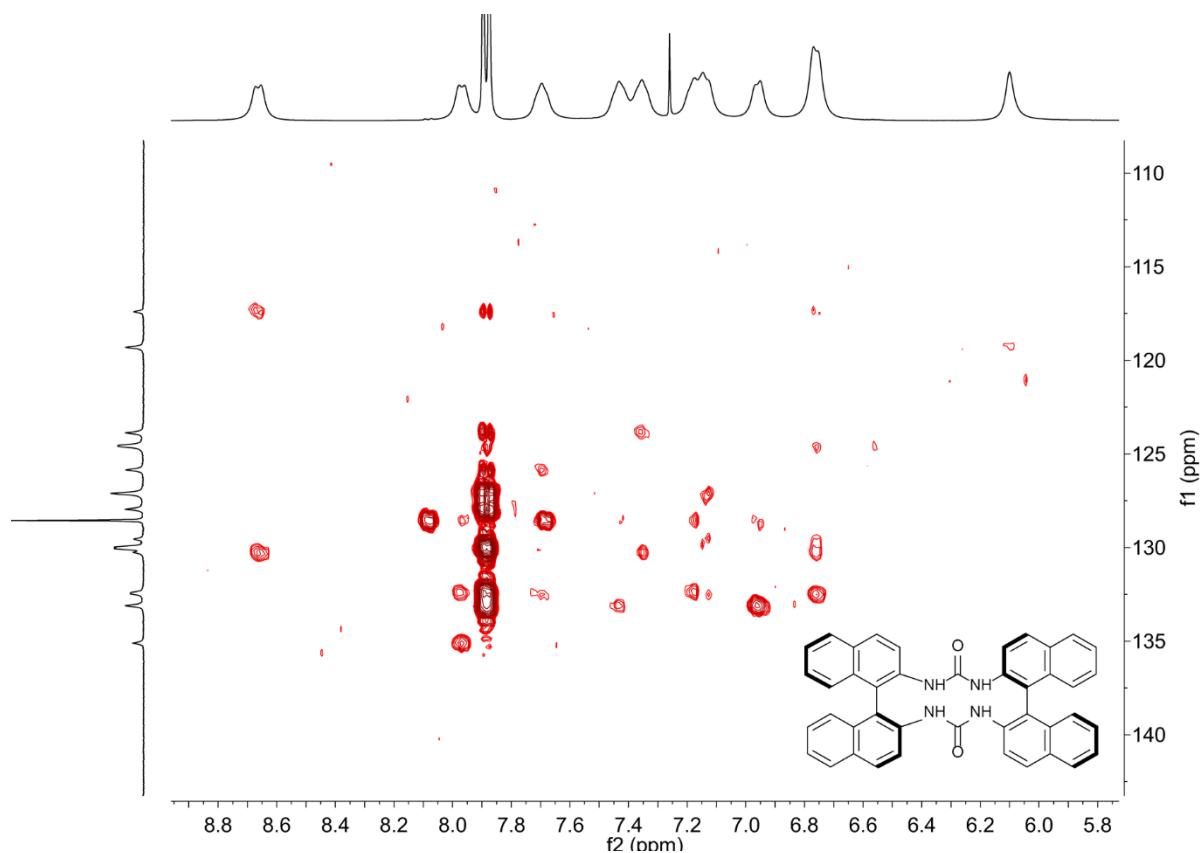


Figure S9, ^1H - ^{13}C HMBC NMR spectrum of **2**, chloroform-*d*, 25°C, 400/101 MHz.

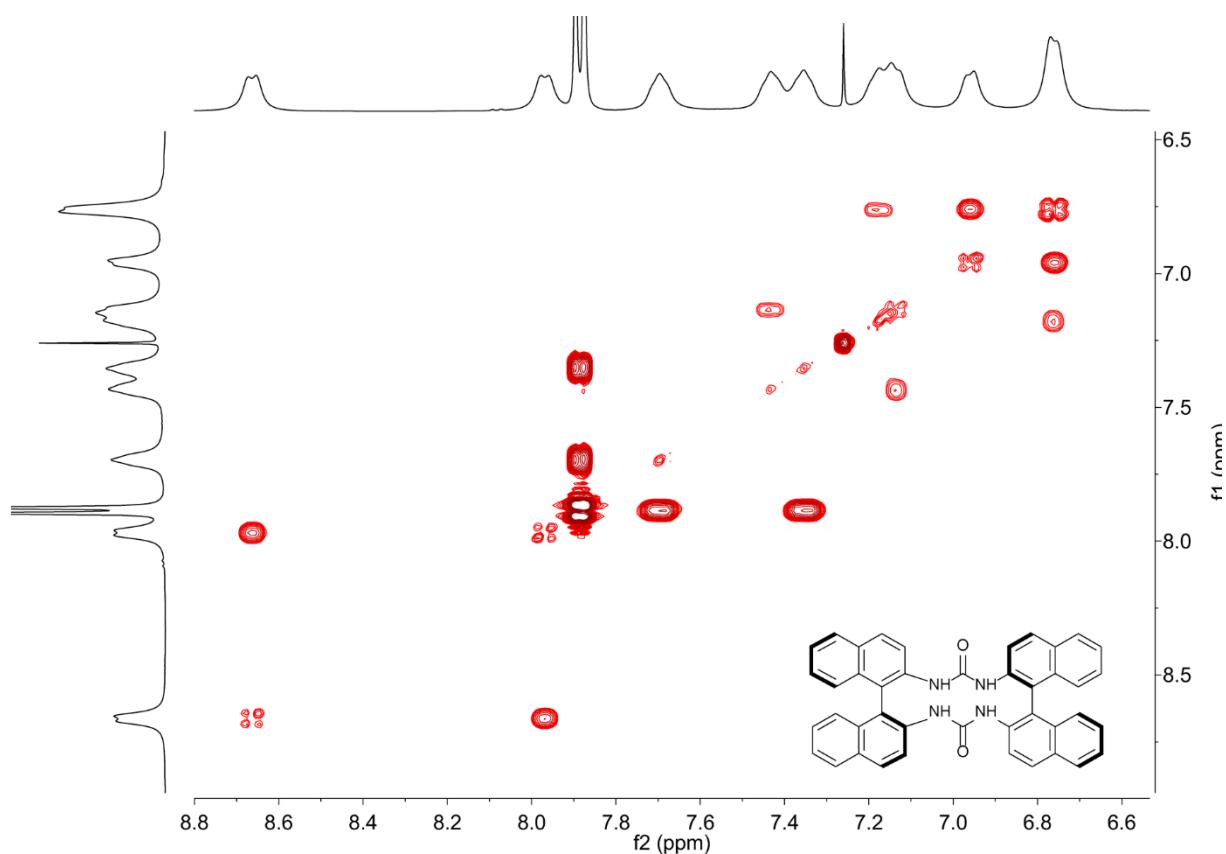


Figure S10, ^1H - ^1H COSY NMR spectrum of **2**, chloroform-*d*, 25°C, 400/400 MHz.

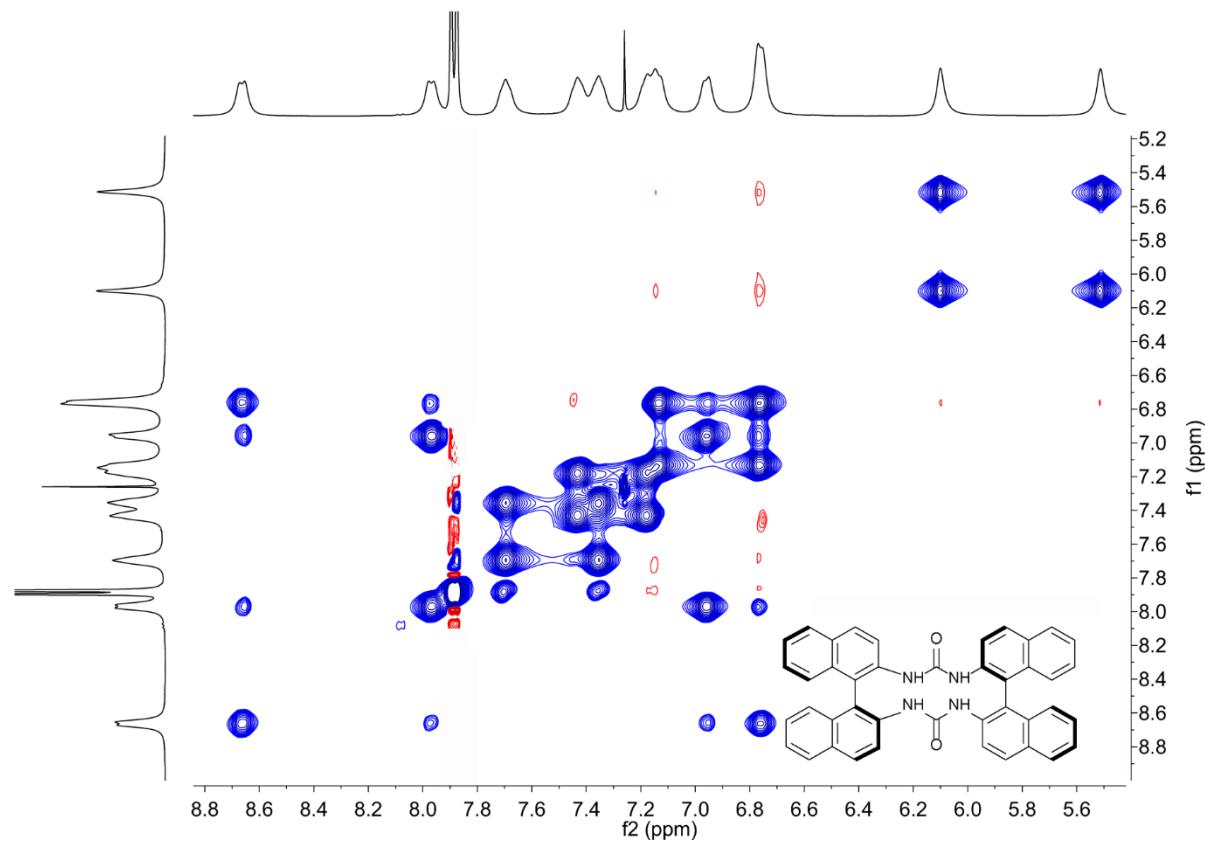


Figure S11, ^1H - ^1H ROESY NMR spectrum of **2**, chloroform-*d*, 25°C, 400/400 MHz, ROESY peaks-red, chemical exchange-blue.

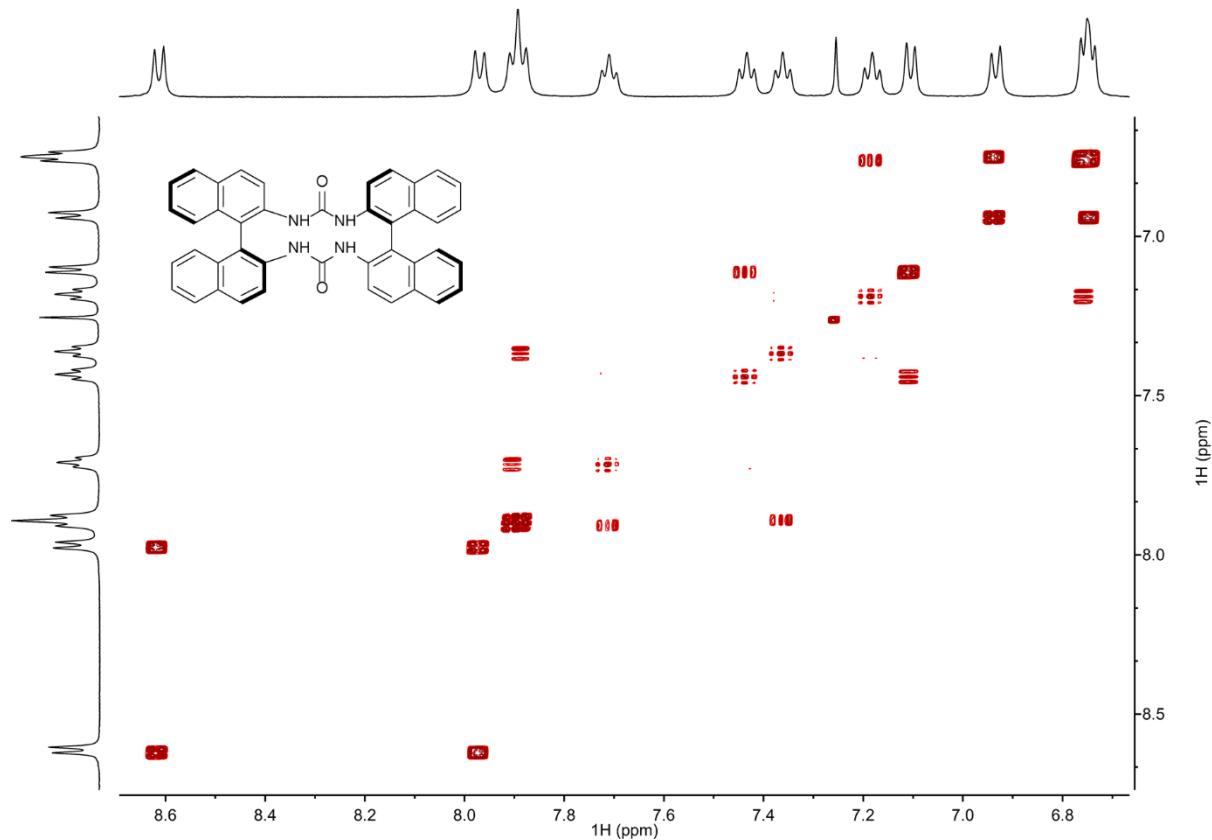


Figure S12, ^1H - ^1H COSY NMR spectrum of **2**, chloroform-*d*, -30°C, 500/500 MHz.

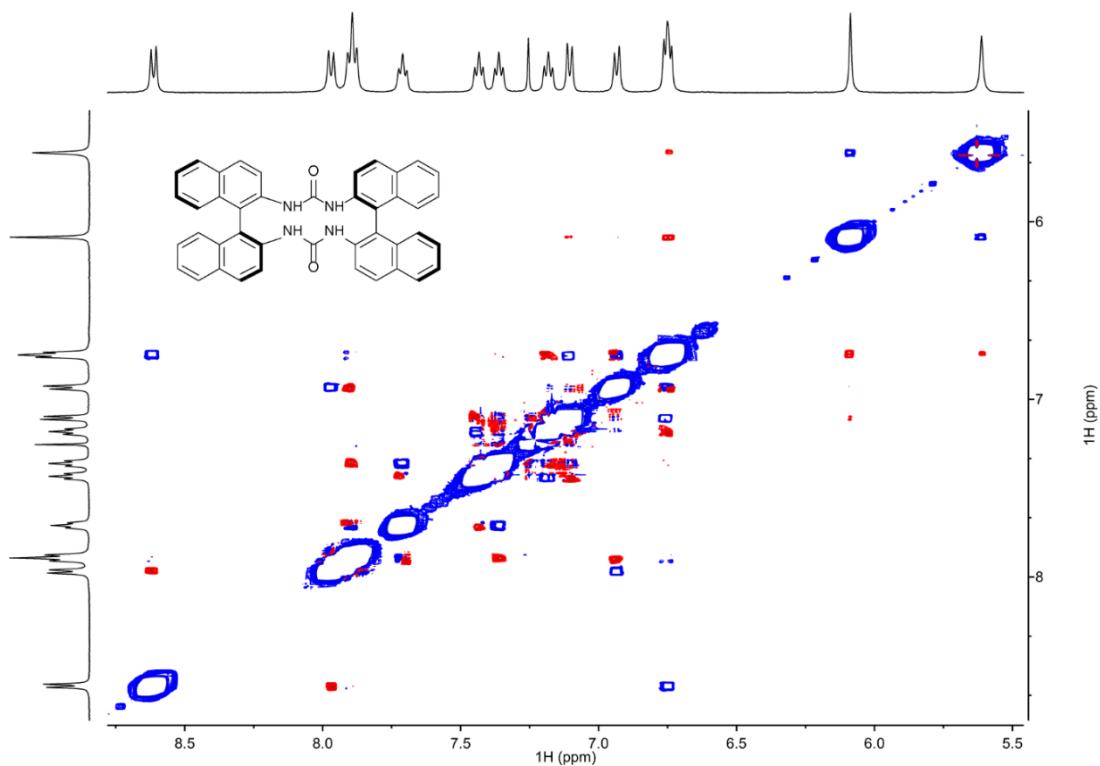


Figure S13, ^1H - ^1H ROESY NMR spectrum of **2**, chloroform-*d*, -30°C, 500/500 MHz, ROESY peaks-red, chemical exchange-blue.

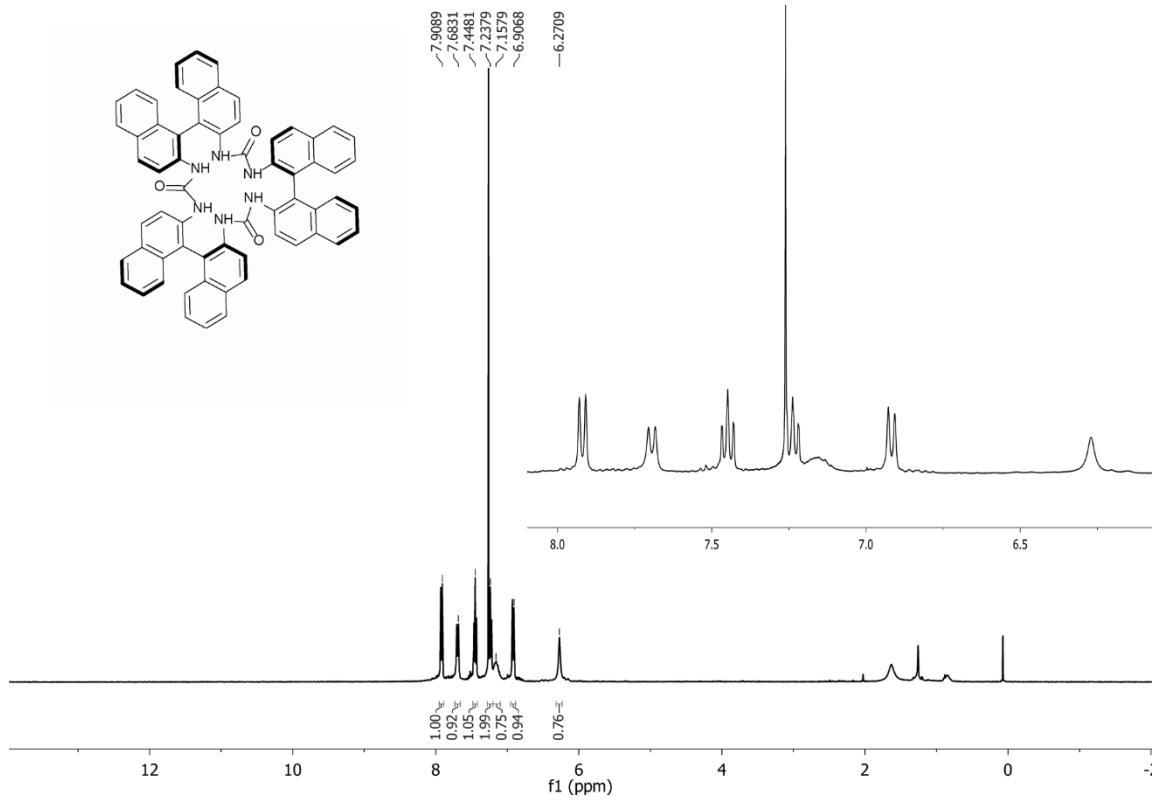


Figure S14, ^1H NMR spectrum of **3**, chloroform-*d*, 25°C, 400MHz.

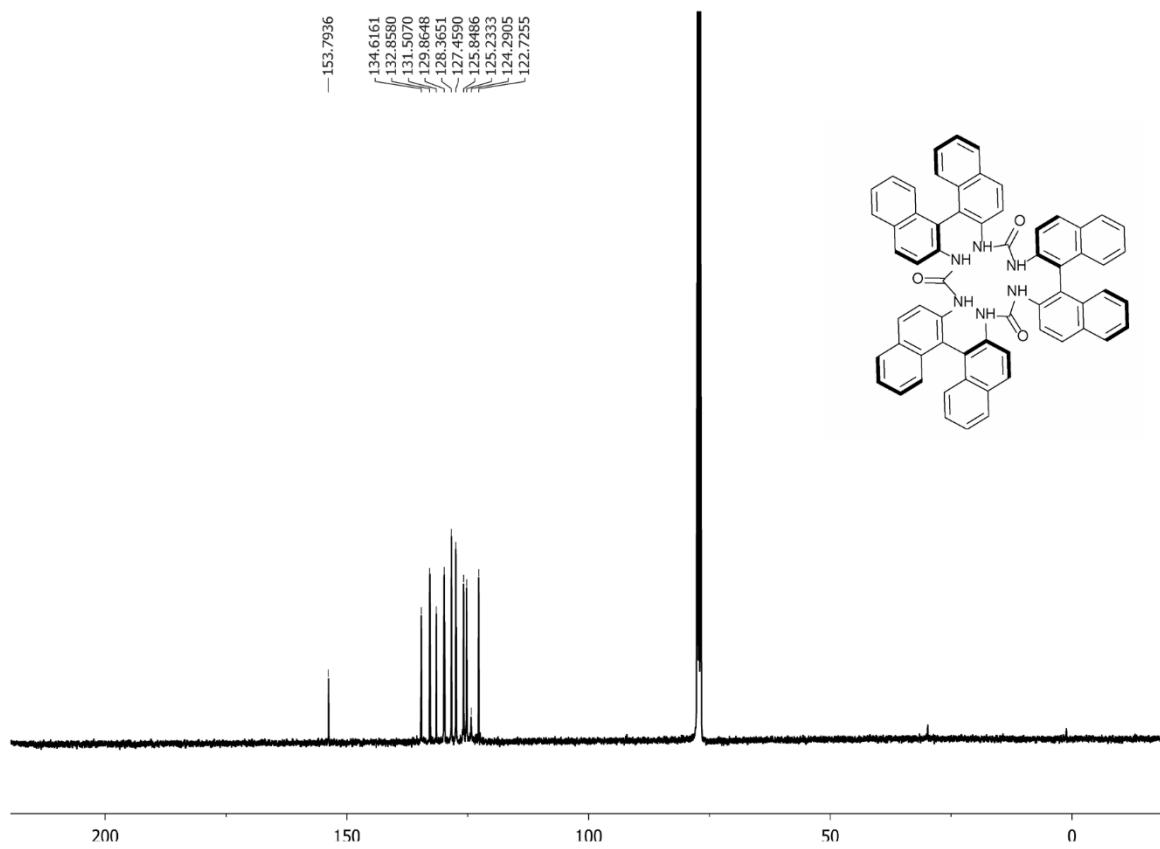


Figure S15, ^{13}C NMR spectrum of **3**, chloroform-*d*, 25°C, 101 MHz.

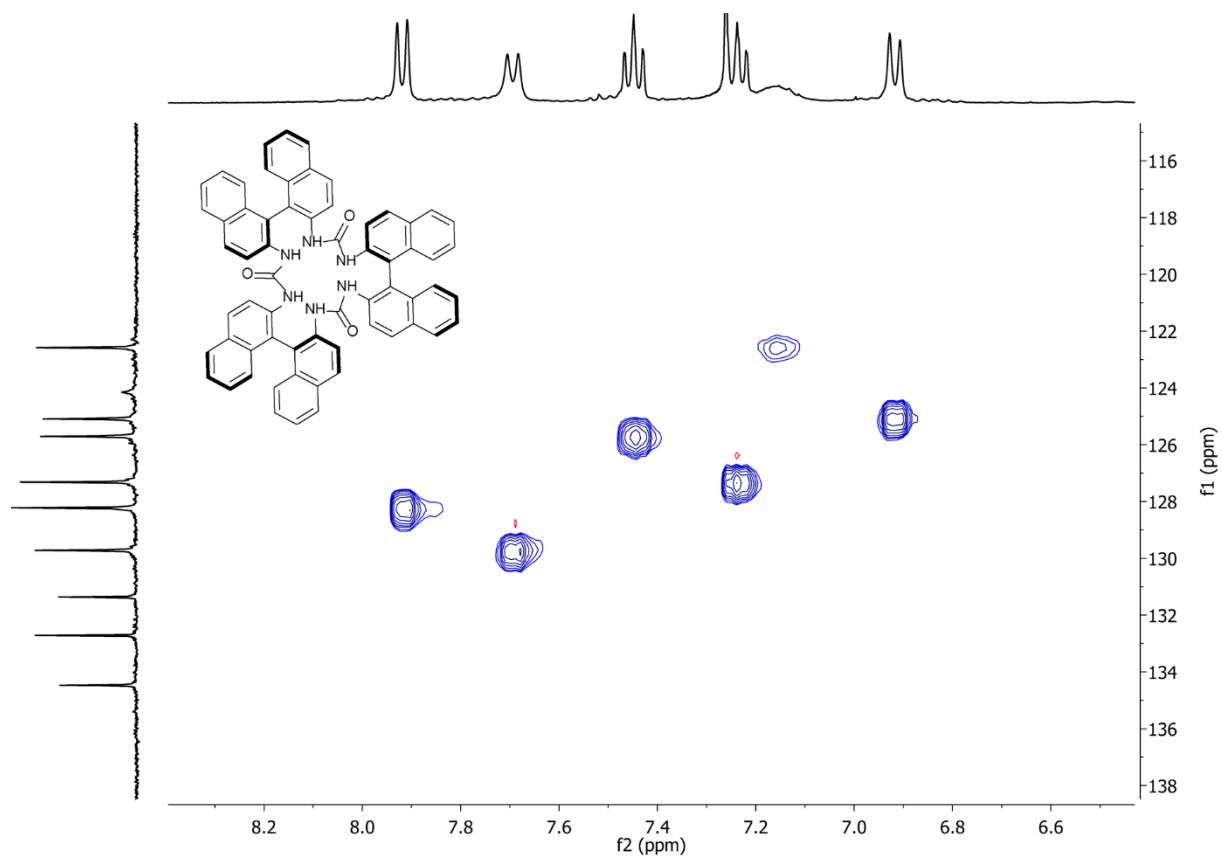


Figure S16, ^1H - ^{13}C HSQC NMR spectrum of **3**, chloroform-*d*, 25°C, 400/101 MHz.

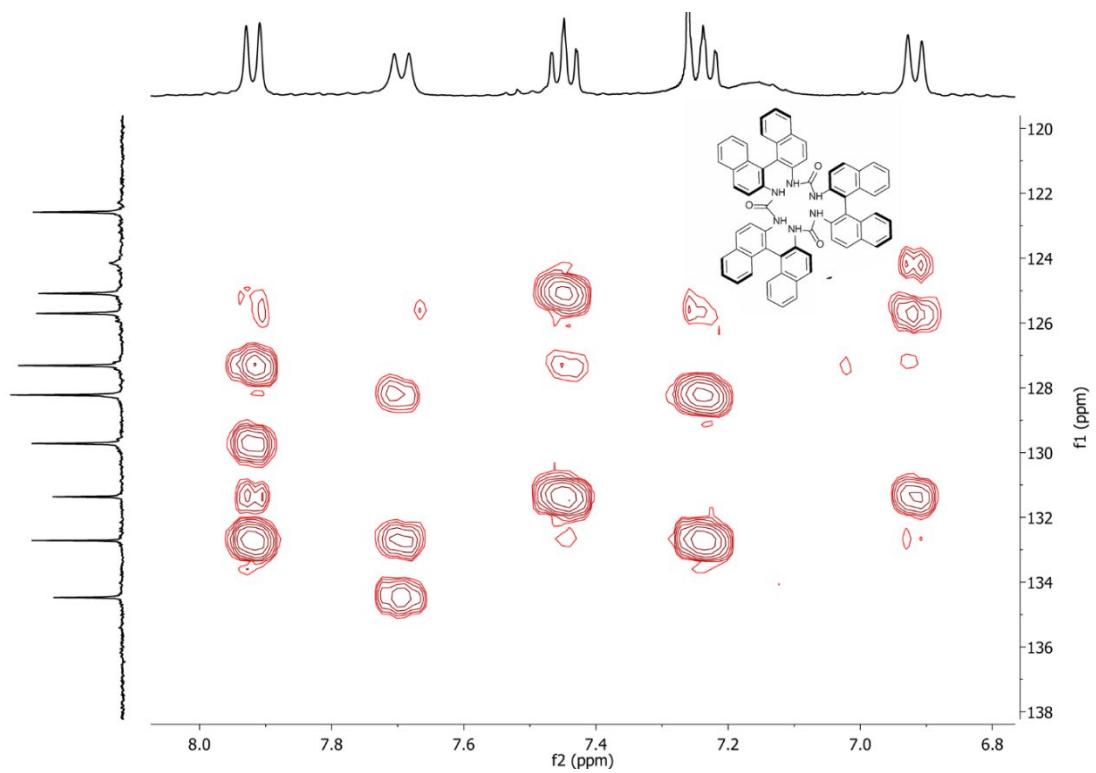


Figure S17, ^1H - ^{13}C HMBC NMR spectrum of **3**, chloroform-*d*, 25°C, 400/101 MHz.

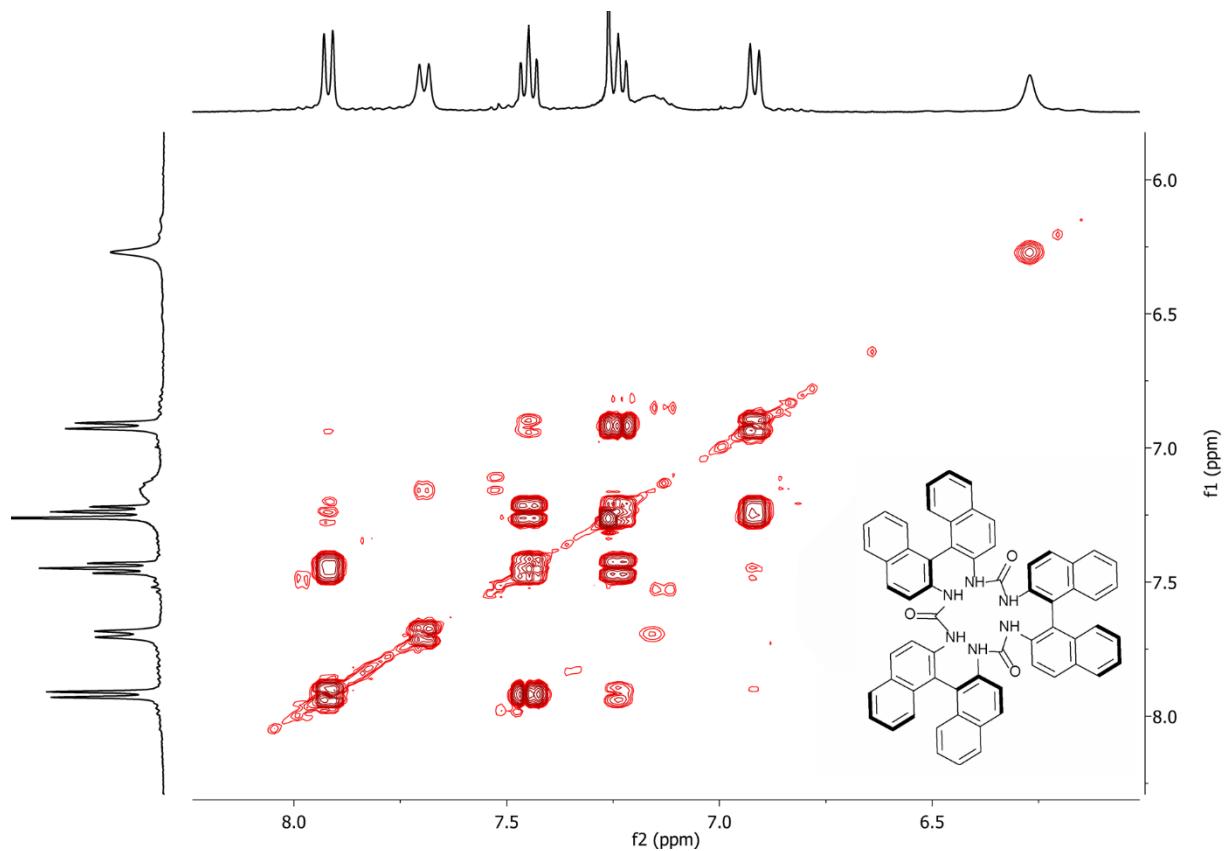


Figure S18, ^1H - ^1H COSY NMR spectrum of **3**, chloroform-*d*, 25°C, 400/101 MHz.

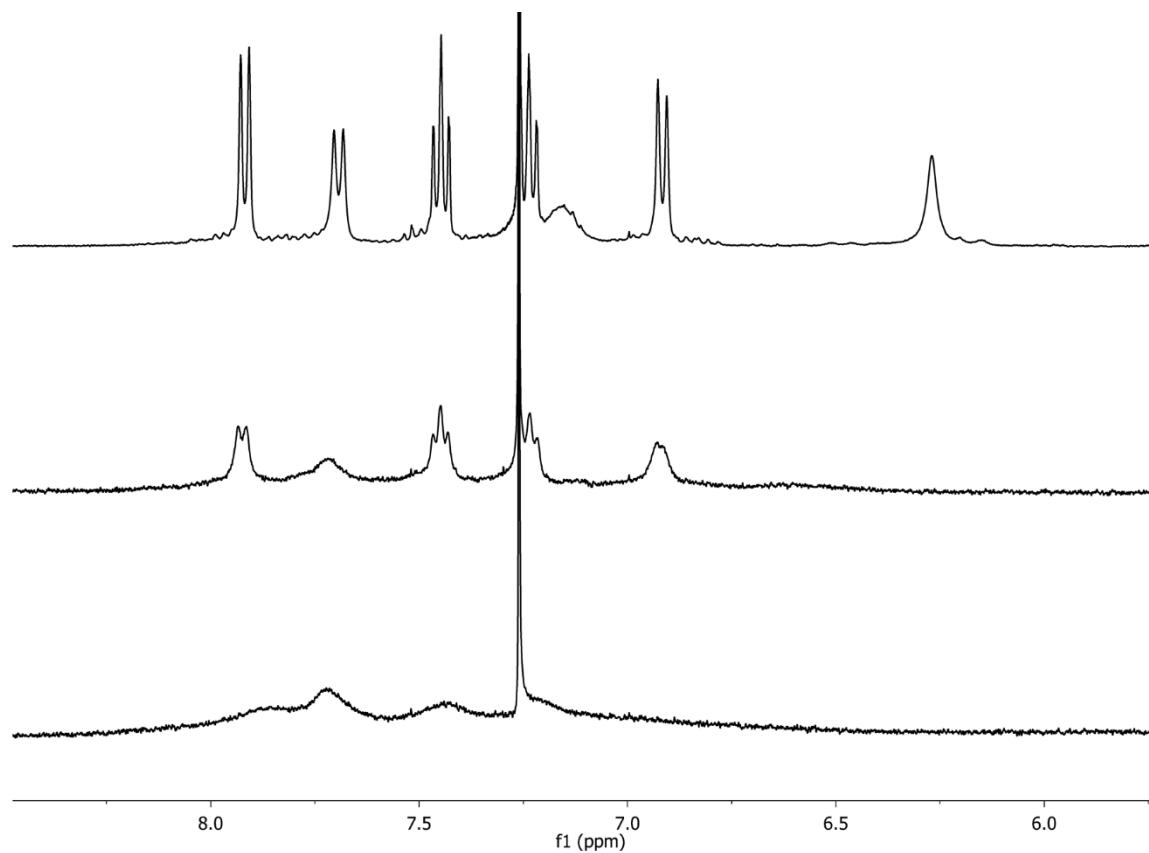
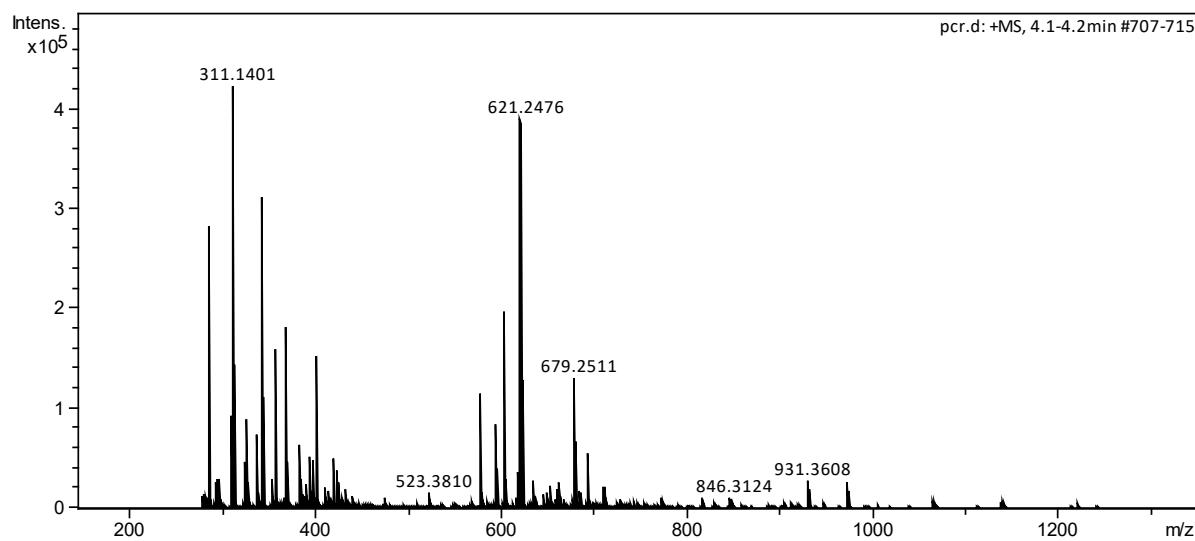


Figure S19, conformational behavior of **3** in chloroform-d₆: bottom to top, 0°C, 15°C, 25°C, ¹H NMR, 400 MHz.



1 [C₂₁H₁₅N₂O]⁺ calc 311.1179 [M+H]⁺

2 [C₄₂H₂₉N₄O₂]⁺ calc 621.2285 [M+H]⁺

3 [C₆₃H₄₃N₆O₃]⁺ calc 931.3391 [M+H]⁺

Figure S20, HRMS spectra of crude products obtained after reaction of phosgene with binaphthyldiamine.

Complexation properties of compound 1

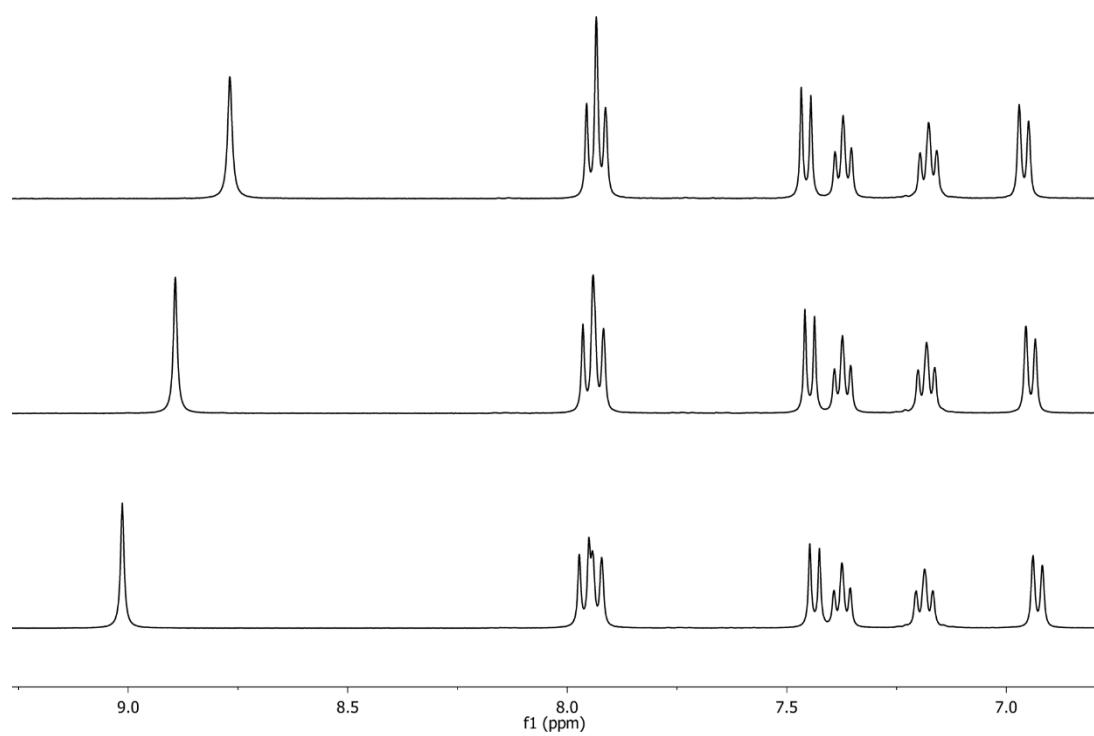


Figure S21, Heating of **1** in DMSO-*d*₆: bottom to top, 25°C, 35°C, 45°C, ¹H NMR, 400 MHz.

Complexation properties of compound 2

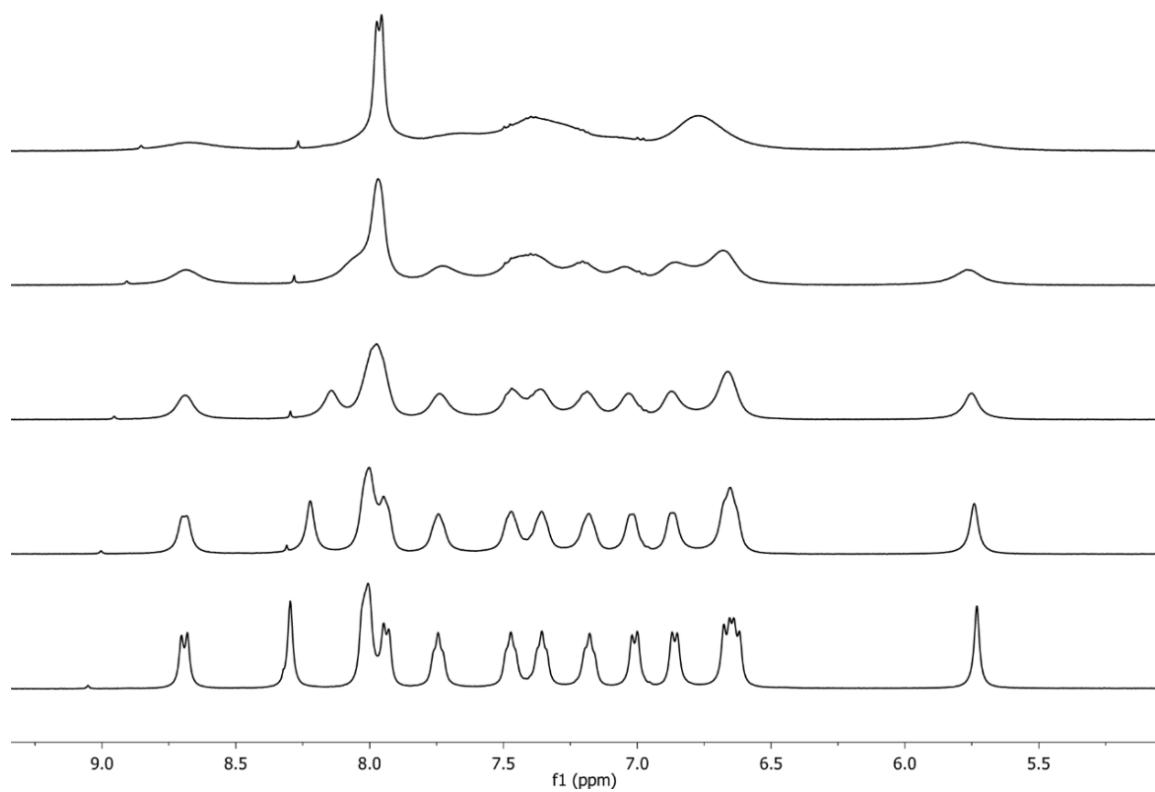


Figure S22, Heating of **2** in DMSO-d₆: bottom to top, 25°C, 35°C, 45°C, 55°C, 60°C, ¹H NMR, 400 MHz.

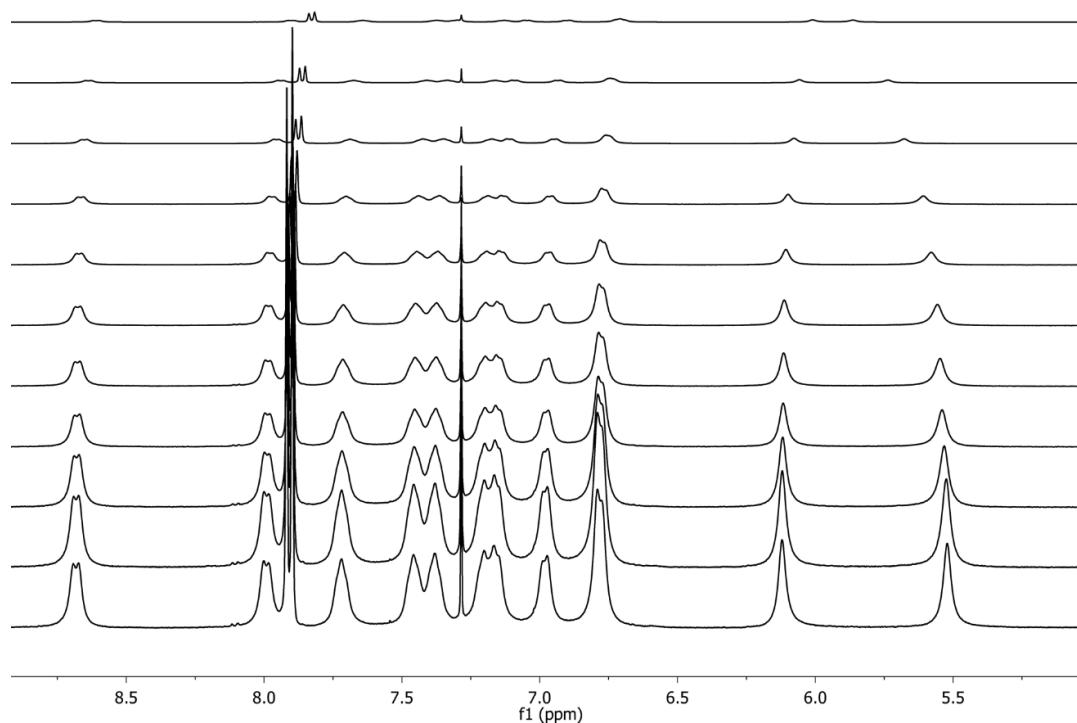


Figure S23, Titration of **2** with DMSO, chloroform-d, ¹H NMR, 400 MHz.

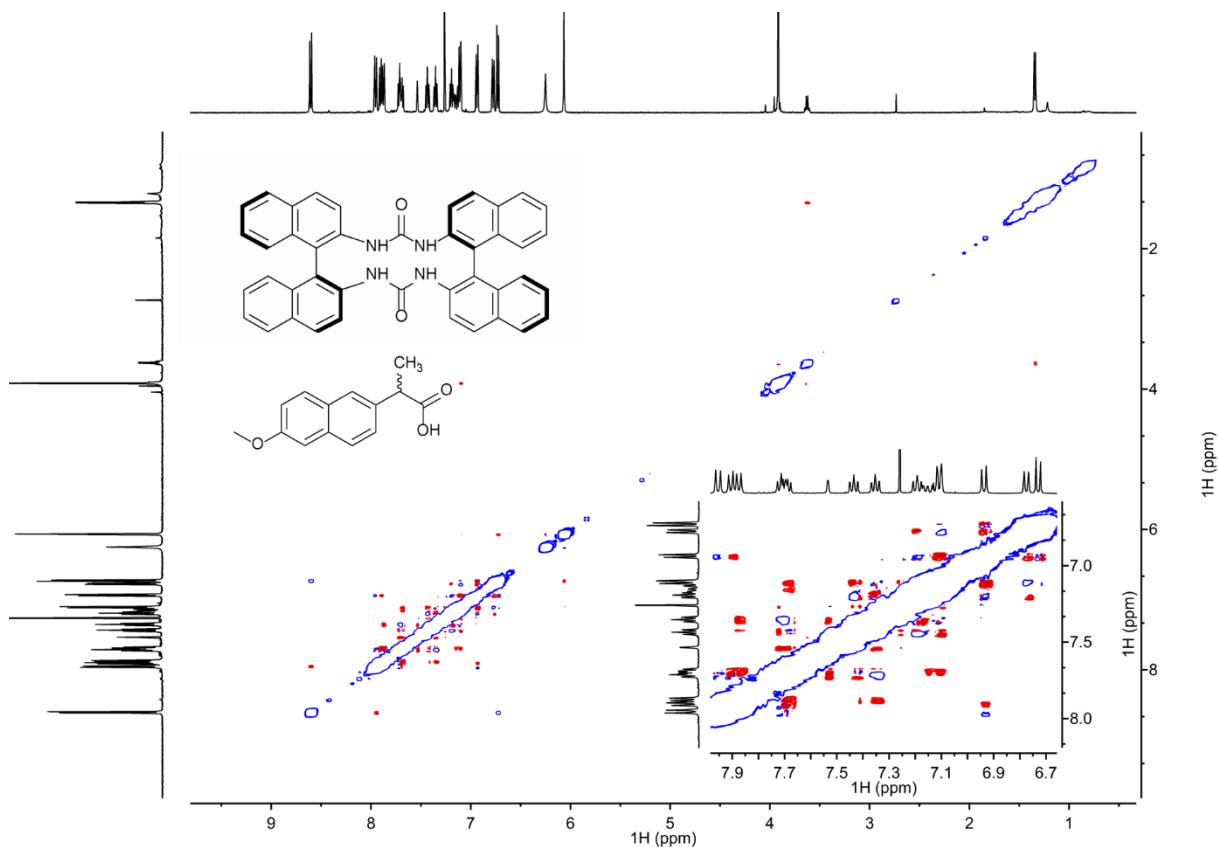


Figure S23, ^1H - ^1H NMR ROESY of the S-naproxen complex with **2**, -30°C , 500/500 MHz, ROESY peaks-red, chemical exchange-blue.

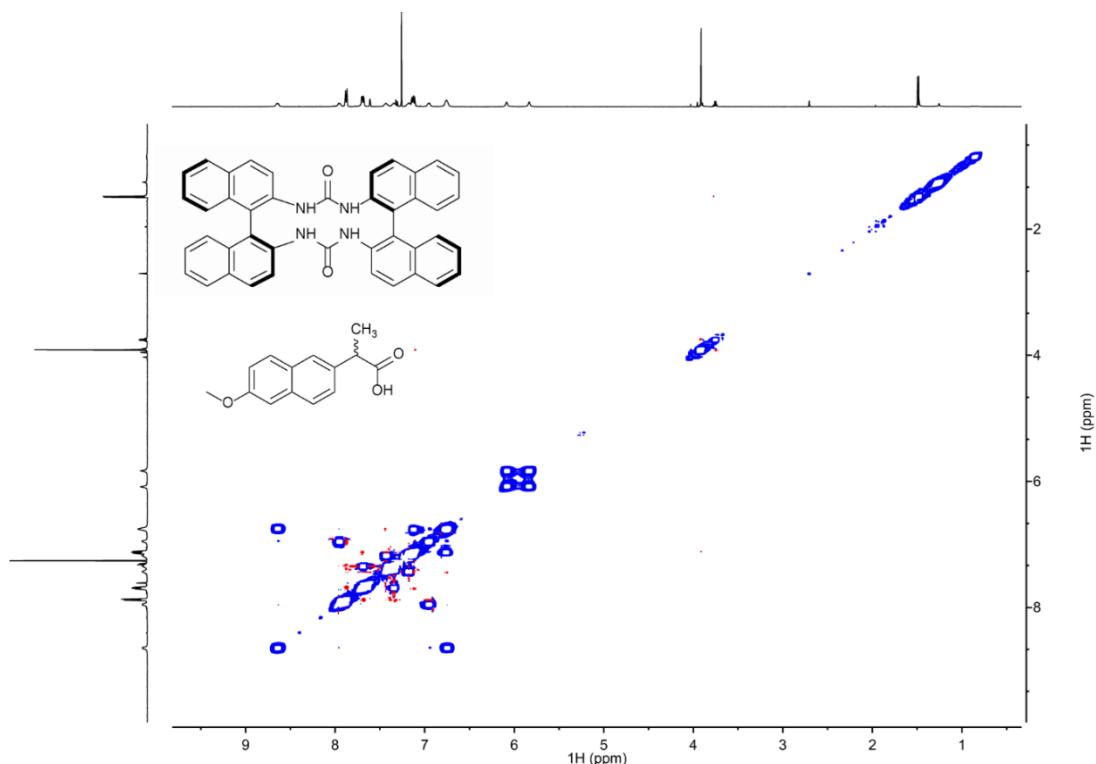


Figure S24, ^1H - ^1H NMR ROESY of the S-naproxen complex with **2**, 25°C , 500/500 MHz; ROESY peaks-red, chemical exchange-blue.

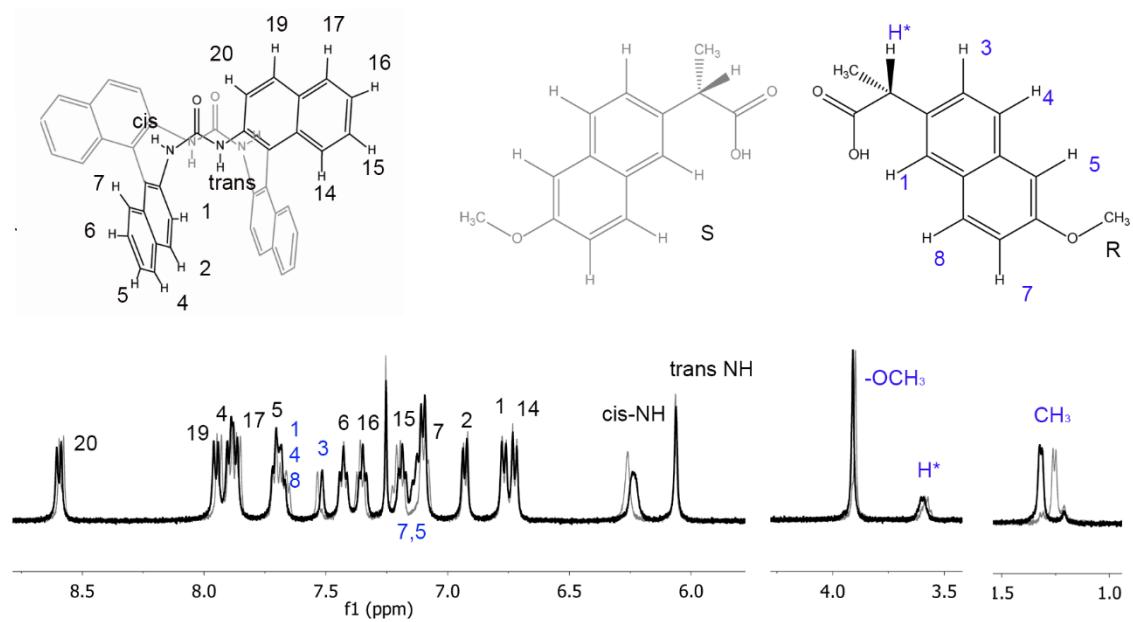


Figure S25, ^1H NMR of the naproxen complex with **2**, 25°C, 400 MHz; R-naproxen- black, S-naproxen- grey.

c 2 [mol/L]	c S-naprox [mol/L]	$\Delta\delta$ [ppm]
0.013	0	0
0.013	0.004163	0.1516
0.013	0.012537	0.3429
0.013	0.019538	0.52715
0.013	0.02514	0.6518
0.013	0.034249	0.7477
0.013	0.047661	0.8823
0.013	0.058001	0.9823
0.013	0.076094	1.0765
0.013	0.099297	1.1591

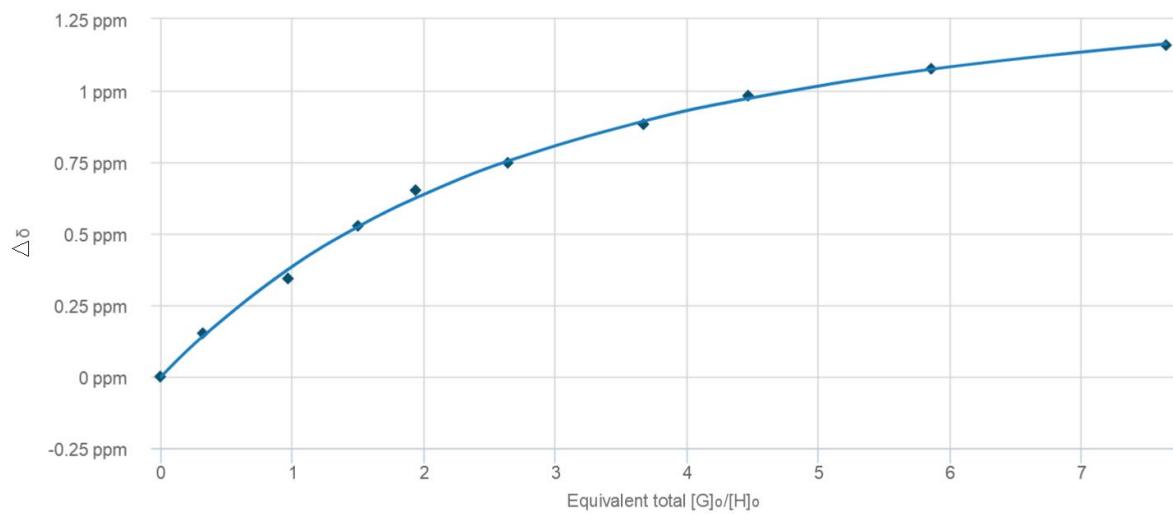


Figure S26, ^1H NMR titration of **2** with S-naproxen, chloroform-d, 400 MHz, 25°C.

c 2 [mol/L]	c R-naprox [mol/L]	$\Delta\delta$ [ppm]
0.013	0	0
0.013	0.003968	0.1663
0.013	0.011454	0.4206
0.013	0.018395	0.6027
0.013	0.02485	0.7089
0.013	0.033725	0.8203
0.013	0.046696	0.9501
0.013	0.057814	1.0549
0.013	0.075881	1.1569
0.013	0.089933	1.2505

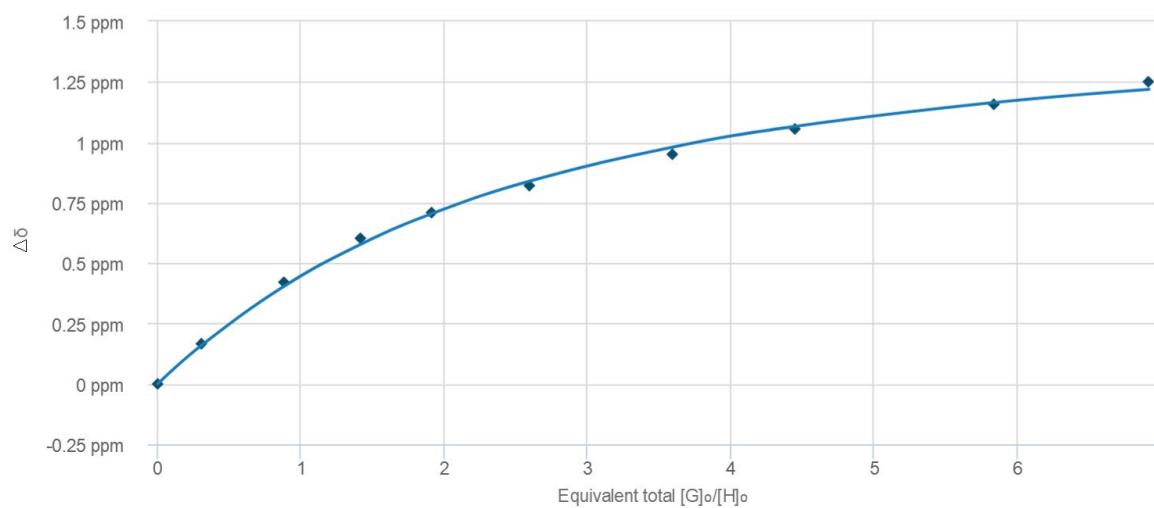


Figure S27, ^1H NMR titration of **2** with R-naproxen, chloroform-*d*, 400 MHz, 25°C.

Complexation of naproxen, -30°C.

c 2 [mol/L]	c S-naprox [mol/L]	$\Delta\delta$ [ppm]
0.013067	0	0
0.013067	0.00209854	0.1998
0.013067	0.00605804	0.4844
0.013067	0.00972958	0.6704
0.013067	0.01314347	0.8144
0.013067	0.01783756	0.9832
0.013067	0.02469817	1.1914
0.013067	0.03057868	1.27
0.013067	0.04013452	1.4184
0.013067	0.04756684	1.5304

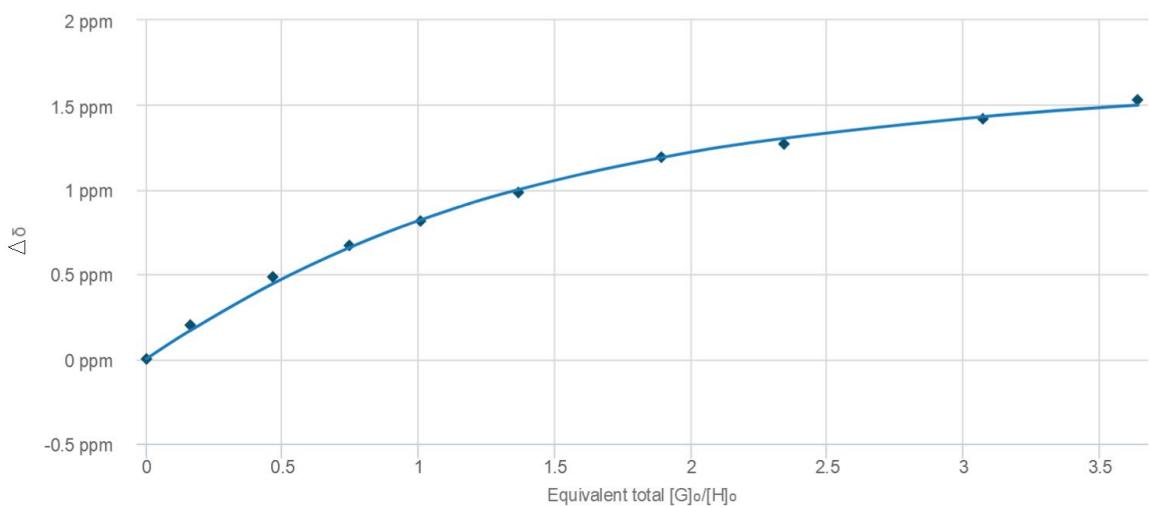


Figure S28, ^1H NMR titration of **2** with S-naproxen, chloroform-*d*, 400 MHz, -30°C.

c 2 [mol/L]	c R-naprox [mol/L]	$\Delta\delta$ [ppm]
0.013067	0	0
0.013067	0.002099	0.1949
0.013067	0.006058	0.4879
0.013067	0.00973	0.6828
0.013067	0.013143	0.8416
0.013067	0.017838	1.0004
0.013067	0.024698	1.1785
0.013067	0.030579	1.3011
0.013067	0.040135	1.4599
0.013067	0.047567	1.5516

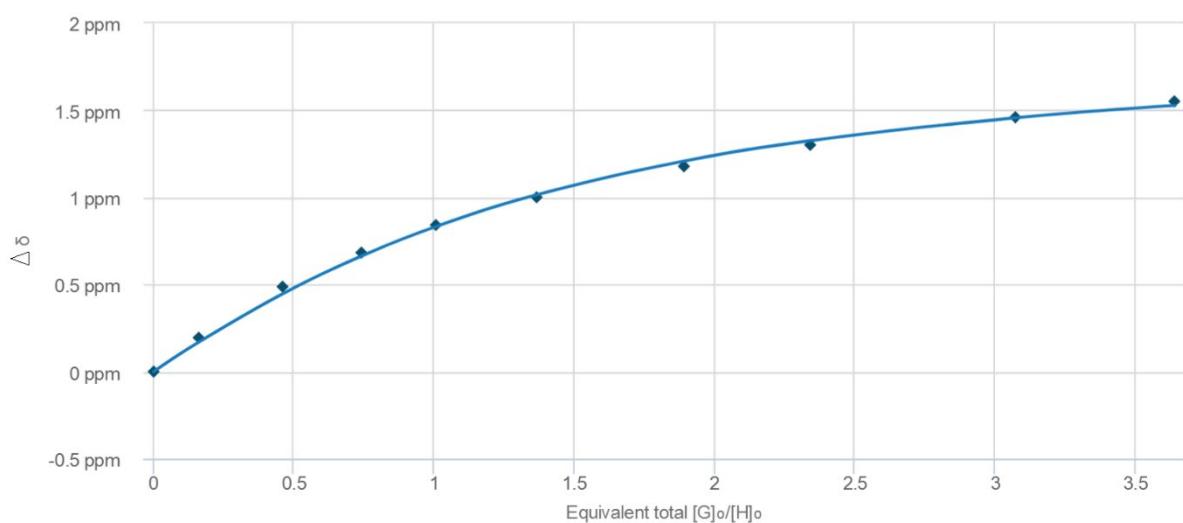


Figure S29, ^1H NMR titration of **2** with R-naproxen, chloroform-*d*, 400 MHz, -30°C.

Complexation properties of compound 3.

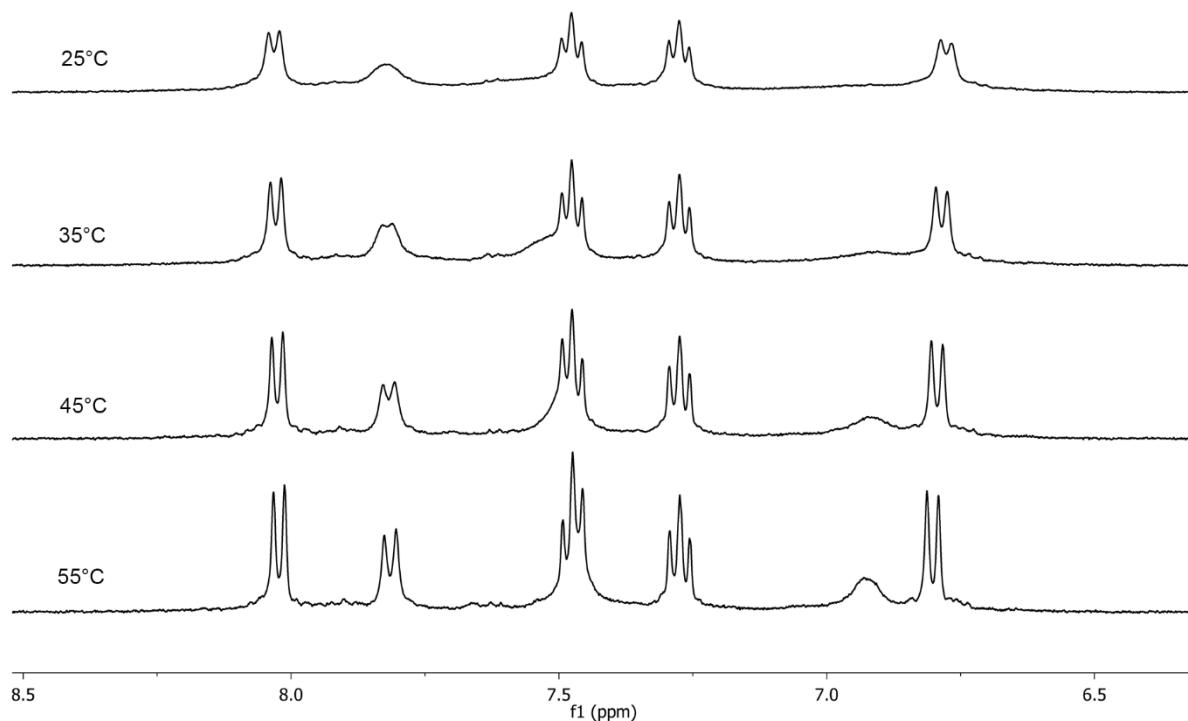


Figure S30, Heating of **3** in DMSO-*d*₆: bottom to top, 25°C, 35°C, 45°C, 55°C, ¹H NMR, 400 MHz.

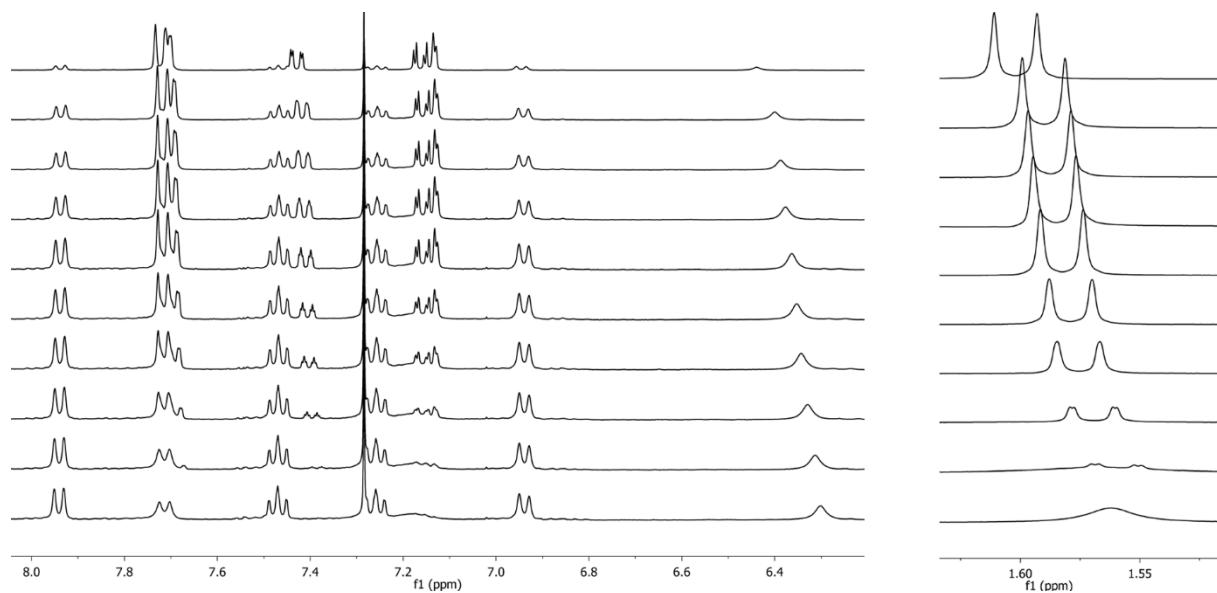


Figure S31, Titration of **3** with racemic naproxen, ¹H NMR 25°C, 400 MHz; right- splitting of naproxen CH₃.

Crystallographic data

Table S1. Crystallographic parameters of measured structures

	1	2
Formula	C ₂₁ H ₁₄ N ₂ O	C ₄₂ H ₂₈ N ₄ O ₂
M _r	310.35	620.71
System	Monoclinic	Monoclinic
Space group	P2 ₁	P2 ₁
T (K)	180	180
a (Å)	9.03801 (13)	9.8861 (6)
b (Å)	6.43800 (9)	15.6415 (10)
c (Å)	13.58790 (18)	10.3461 (7)
β (°)	90.0399 (12)	105.9826 (19)
V (Å ³)	790.64 (2)	1538.01 (17)
Z	2	2
λ (Å)	1.54184	1.54178
μ (mm ⁻¹)	0.64	0.66
Crystal size (mm)	0.22 x 0.12 x 0.08	0.45 x 0.42 x 0.28
T _{min} , T _{max}	0.90, 0.95	0.58, 0.83
Measured refl.	11296	22298
Independent refl.	2832	5623
Observed refl. I > 2σ(I)	2722	5544
θ _{min} , θ _{max} (°)	3.3, 67.6	4.5, 68.3
R _{int}	0.030	0.041
R ₁ [F ² >2σ(F ²)]	0.0280	0.0307
wR ₂ [F ² >2σ(F ²)]	0.0733	0.0849
R ₁ (all)	0.0294	0.0311
wR ₂ (all)	0.0782	0.0854
Δρ _{min} , Δρ _{max} (e Å ⁻³)	-0.13, 0.11	-0.14, 0.16
Flack parameter	0.11 (13)	0.00 (7)
CCDC number	2226943	2226944

DFT calculation obtained coordinates

2

Total energy -1986.89951665
 Number of imaginary frequencies 0
 Zero-point correction= 0.598956 (Hartree/Particle)
 Thermal correction to Energy= 0.634627
 Thermal correction to Enthalpy= 0.635571
 Thermal correction to Gibbs Free Energy= 0.531679
 Sum of electronic and zero-point Energies= -1986.300560
 Sum of electronic and thermal Energies= -1986.264890
 Sum of electronic and thermal Enthalpies= -1986.263946
 Sum of electronic and thermal Free Energies= -1986.367838

O	0.05734300	2.84117200	2.31028300
C	-0.01913300	1.67430200	1.95972400
N	1.05251400	0.90212300	1.53221500

C	2.33890100	1.37429800	1.20360300
C	3.07080600	0.68871200	0.23093800
C	2.46179400	-0.49077900	-0.46713800
C	1.54966700	-0.29395500	-1.50440700
N	1.25007500	1.01150100	-1.96670600
C	0.01891100	1.67410200	-1.96011000
O	-0.05764600	2.84081800	-2.31122300
N	-1.05261000	0.90205000	-1.53222100
C	-2.33901400	1.37422800	-1.20360200
C	-3.07081600	0.68865700	-0.23086400
C	-2.46173300	-0.49081100	0.46720500
C	-1.54972300	-0.29398300	1.50455900
N	-1.25019500	1.01152700	1.96689200
C	-0.94043000	-1.40235800	2.15655200
C	-1.22218500	-2.68614900	1.76177300
C	-2.14571300	-2.94043400	0.71469500
C	-2.78083100	-1.83138700	0.06318200
C	-3.69533100	-2.10581200	-0.99222700
C	-3.97027700	-3.40061200	-1.37287100
C	-3.34843500	-4.49241800	-0.72144200
C	-2.45485200	-4.26288100	0.29963300
C	-4.39056000	1.13254900	0.10585900
C	-5.18346900	0.48975300	1.09898400
C	-6.44396600	0.95099900	1.40921500
C	-6.98463100	2.07755800	0.74566200
C	-6.24386300	2.72307900	-0.21834700
C	-4.94067500	2.27650400	-0.56039000
C	-4.15760100	2.93267700	-1.54493100
C	-2.89624700	2.50114900	-1.86793600
C	0.94029800	-1.40235700	-2.15630200
C	1.22213100	-2.68614000	-1.76156900
C	2.14581800	-2.94040900	-0.71462300
C	2.78098600	-1.83135100	-0.06318700
C	3.69564400	-2.10576500	0.99208900
C	3.97069600	-3.40056100	1.37267100
C	3.34879800	-4.49238000	0.72131600
C	2.45505700	-4.26285300	-0.29962300
C	4.39054700	1.13265000	-0.10573800
C	4.94058000	2.27666500	0.56048300
C	4.15741500	2.93285700	1.54493500
C	2.89606000	2.50129300	1.86788100
C	6.24376500	2.72329100	0.21849900
C	6.98461800	2.07777300	-0.74544700
C	6.44402800	0.95117200	-1.40899200
C	5.18353700	0.48987600	-1.09881300
H	-0.26618200	-1.21067000	2.98546000
H	-0.75068000	-3.52673000	2.26434300
H	-4.67321700	-3.58664500	-2.18032800
H	-3.57866300	-5.50846700	-1.02985100
H	-1.96958700	-5.09321100	0.80727700
H	-4.78365700	-0.37706200	1.61544600
H	-7.02947100	0.44410700	2.17169800

H	-7.98033500	2.42986800	1.00016900
H	-6.64562700	3.59216100	-0.73422300
H	-4.57467900	3.79833500	-2.05375100
H	-2.29907400	3.01506000	-2.60776400
H	0.26596000	-1.21068300	-2.98514300
H	0.75056400	-3.52672700	-2.26407100
H	4.17768800	-1.27536500	1.49658900
H	4.67376600	-3.58657800	2.18001800
H	3.57910300	-5.50842800	1.02967400
H	1.96974300	-5.09319100	-0.80720900
H	4.57441200	3.79856500	2.05373700
H	2.29883800	3.01523700	2.60764700
H	6.64544900	3.59241600	0.73436600
H	7.98032100	2.43011400	-0.99991600
H	7.02958500	0.44428900	-2.17144100
H	4.78379700	-0.37696100	-1.61529000
H	2.01235600	1.67845900	-1.98000900
H	-4.17732600	-1.27541900	-1.49678700
H	-2.01255100	1.67841200	1.97997400
H	0.82349400	0.00412400	1.12531900
H	-0.82351900	0.00418300	-1.12507600

2+naproxen, bridged structure

Total energy	-2755.541748028902
Number of imaginary frequencies	0
Zero-point correction=	0.852748 (Hartree/Particle)
Thermal correction to Energy=	0.905106
Thermal correction to Enthalpy=	0.906050
Thermal correction to Gibbs Free Energy=	0.763061
Sum of electronic and zero-point Energies=	-2753.678486
Sum of electronic and thermal Energies=	-2753.626129
Sum of electronic and thermal Enthalpies=	-2753.625185
Sum of electronic and thermal Free Energies=	-2753.768174

O	1.52468500	0.56033500	-0.68346200
C	0.33232900	0.37301300	-0.88363900
N	-0.17034900	-0.90420700	-1.11140400
C	-1.47848000	-1.26744500	-1.48917200
C	-2.15676800	-2.30923300	-0.84929800
C	-1.52305700	-3.05601600	0.28564600
C	-1.38973100	-2.45307500	1.53167300
N	-1.86633700	-1.13002600	1.71680500
C	-1.12289200	-0.12806000	2.30000500
O	-0.03704600	-0.30512000	2.85597900
N	-1.67174000	1.14667700	2.25521700
C	-2.81497200	1.57373400	1.53365700
C	-2.71696300	2.61873000	0.61377700
C	-1.40539100	3.31070800	0.38748900
C	-0.38678700	2.68355500	-0.33436600
N	-0.61603300	1.39674600	-0.86320000

C	0.85146900	3.34520800	-0.56137100
C	1.06536400	4.59995000	-0.05284500
C	0.07261400	5.27428400	0.70415800
C	-1.18437600	4.62281500	0.92757700
C	-2.15966400	5.30489400	1.70903700
C	-1.90838000	6.55699700	2.22606200
C	-0.67083900	7.20063900	1.99200000
C	0.29702200	6.56650400	1.24675800
C	-3.89466900	3.02585300	-0.10210200
C	-3.86491700	4.05376800	-1.08612500
C	-5.00329400	4.40940800	-1.77496100
C	-6.23555700	3.76278800	-1.51837000
C	-6.29991600	2.76175100	-0.57669400
C	-5.14372000	2.36609200	0.14656200
C	-5.19352700	1.33289600	1.11757000
C	-4.06608200	0.95145900	1.80024200
C	-0.83334000	-3.15090800	2.63380600
C	-0.38460200	-4.43668700	2.47518000
C	-0.46888100	-5.09373600	1.22032800
C	-1.04907700	-4.39860900	0.10920900
C	-1.10819500	-5.07020300	-1.14348400
C	-0.63046300	-6.35437000	-1.28493500
C	-0.07057500	-7.04155200	-0.18262600
C	0.00697400	-6.41951800	1.04260100
C	-3.48658600	-2.64888600	-1.27892400
C	-4.09434800	-1.93022200	-2.36068100
C	-3.35381600	-0.90143700	-2.99757000
C	-2.08579400	-0.58492300	-2.58387800
C	-5.41269700	-2.26045700	-2.77064000
C	-6.12251400	-3.25448300	-2.13678900
C	-5.53418100	-3.95761600	-1.05948200
C	-4.25408300	-3.66589000	-0.64254100
H	1.61949300	2.83210900	-1.12168800
H	2.01696000	5.09574100	-0.22790800
H	-2.66912500	7.05458000	2.82165000
H	-0.48687200	8.18876500	2.40437000
H	1.25654400	7.04497600	1.06474400
H	-2.92661600	4.55666200	-1.29225700
H	-4.95517500	5.19591000	-2.52315800
H	-7.12589200	4.05744900	-2.06678900
H	-7.23938900	2.25388000	-0.37208200
H	-6.14553800	0.85237300	1.32796800
H	-4.11562300	0.18728600	2.56905900
H	-0.76750600	-2.65100700	3.59235000
H	0.04195800	-4.97055500	3.32074500
H	-1.52971700	-4.55468300	-1.99967900
H	-0.68169900	-6.84377500	-2.25382900
H	0.29981500	-8.05528100	-0.30766200
H	0.43913000	-6.93447500	1.89755500
H	-3.79956500	-0.37217500	-3.83607900
H	-1.51346700	0.17810500	-3.10104800
H	-5.85234600	-1.70727700	-3.59736900

H -7.13107100 -3.49937200 -2.45804900
 H -6.09780800 -4.73841400 -0.55584100
 H -3.81783300 -4.21574400 0.18381400
 H -2.58695700 -0.83968400 1.06655200
 H -3.11350500 4.82572000 1.90180600
 H -1.58522900 1.10434800 -0.83954400
 H 0.44945400 -1.61587800 -0.71704000
 H -0.96667400 1.84991800 2.44511000
 C 6.17028700 2.00016700 -1.95778600
 C 7.51355900 1.92034800 -1.50515300
 C 7.88383200 0.94080200 -0.60153700
 C 6.93931500 0.00466300 -0.12116400
 C 5.58375800 0.07573200 -0.57931400
 C 5.23552900 1.09646500 -1.49881700
 C 7.27620200 -1.01539200 0.81225300
 C 6.32747500 -1.90583600 1.25476200
 C 4.98165800 -1.84824700 0.79388800
 C 4.63036200 -0.86726500 -0.11007000
 C 3.99132700 -2.90868300 1.27507500
 C 4.03888100 -4.16756700 0.39127100
 O 8.50395300 2.77543600 -1.91113800
 C 8.18498200 3.78740200 -2.84948500
 C 2.57880200 -2.33881700 1.32375900
 O 1.77639900 -2.46142200 0.41050000
 O 2.33399400 -1.68777100 2.45870400
 H 5.87127400 2.76858400 -2.66181500
 H 8.91620800 0.90074800 -0.26575100
 H 4.20395300 1.15867400 -1.83603500
 H 8.29876900 -1.07697600 1.17761500
 H 6.60491700 -2.67344300 1.97450300
 H 3.60864400 -0.78068400 -0.46960200
 H 4.26161000 -3.17482500 2.30381000
 H 3.36614000 -4.94408500 0.77218500
 H 5.05664300 -4.57013600 0.36243500
 H 3.73075200 -3.92414200 -0.62871800
 H 9.11506700 4.33024400 -3.03055900
 H 7.82431000 3.36635300 -3.79780800
 H 7.43256800 4.48592800 -2.45852900
 H 1.43310100 -1.27469900 2.44283900

2+naproxen, naproxen interacting with only one urea moiety

Total energy	-2755.544446700681
Number of imaginary frequencies	0
Zero-point correction=	0.852411 (Hartree/Particle)
Thermal correction to Energy=	0.904970
Thermal correction to Enthalpy=	0.905914
Thermal correction to Gibbs Free Energy=	0.760507
Sum of electronic and zero-point Energies=	-2753.683401
Sum of electronic and thermal Energies=	-2753.630842
Sum of electronic and thermal Enthalpies=	-2753.629898
Sum of electronic and thermal Free Energies=	-2753.775305

O	0.20438500	-1.83303900	-1.30551900
C	-0.41723600	-1.11924500	-0.50394000
N	0.13012800	0.03078200	0.00082100
C	-0.45727400	0.93917500	0.92329700
C	-0.68771500	2.26668000	0.56272700
C	-0.39681000	2.74454500	-0.82960000
C	-1.30225700	2.48068900	-1.85848900
N	-2.49912800	1.80359000	-1.54542500
C	-3.22004200	0.97174200	-2.38685700
O	-3.01257500	0.83275600	-3.58208100
N	-4.25386200	0.26444600	-1.76082500
C	-4.54623800	0.20136900	-0.37536800
C	-4.44155000	-1.00166800	0.32232700
C	-3.93969900	-2.23234400	-0.37263700
C	-2.56750400	-2.41194500	-0.56792000
N	-1.69266100	-1.42528600	-0.06931100
C	-2.07760900	-3.57784100	-1.21822200
C	-2.95512600	-4.52673900	-1.67813200
C	-4.35741000	-4.38661000	-1.51784800
C	-4.85888300	-3.22149600	-0.85017000
C	-6.26924500	-3.08859000	-0.70304800
C	-7.12708300	-4.05235600	-1.18564500
C	-6.62703300	-5.20310100	-1.83973400
C	-5.26924100	-5.36179100	-1.99985600
C	-4.78971100	-1.03493300	1.71537200
C	-4.69882900	-2.22524500	2.48982500
C	-5.01684500	-2.22469200	3.82993500
C	-5.44466200	-1.03716900	4.46993900
C	-5.54068100	0.13266200	3.75146300
C	-5.21614200	0.16846700	2.36940900
C	-5.30327100	1.36774800	1.61529800
C	-4.99115200	1.38408000	0.27895000
C	-1.04532500	2.92737500	-3.18334300
C	0.10099100	3.62762200	-3.45957800
C	1.04877100	3.93176000	-2.44882200
C	0.79790800	3.48199400	-1.11136600
C	1.76247000	3.78777600	-0.11062600
C	2.89820500	4.50539300	-0.41374800
C	3.13757900	4.95526800	-1.73371700
C	2.22954000	4.66859100	-2.72776700
C	-1.24328100	3.16456700	1.53814200
C	-1.56057700	2.68370700	2.85193200
C	-1.30653600	1.32404500	3.16729600
C	-0.76139100	0.47781800	2.23435000
C	-2.12174700	3.57542400	3.80460200
C	-2.37025200	4.88960100	3.48143400
C	-2.06591600	5.36650700	2.18414500
C	-1.51736700	4.52899500	1.23855800
H	-1.01158900	-3.68861700	-1.35376700
H	-2.57133400	-5.41262600	-2.17822700
H	-8.19966100	-3.92746300	-1.06287700

H	-7.31559000	-5.95521400	-2.21454700
H	-4.87097600	-6.23953300	-2.50356600
H	-4.37367000	-3.14062400	2.00738400
H	-4.94123100	-3.14567300	4.40157800
H	-5.69669700	-1.05310000	5.52668000
H	-5.86803600	1.05159200	4.23211800
H	-5.63851800	2.27672400	2.10803200
H	-5.09588400	2.29189900	-0.30695500
H	-1.76014400	2.69104600	-3.95889200
H	0.29088000	3.96745500	-4.47492600
H	1.59654600	3.44602600	0.90579100
H	3.61920400	4.72720200	0.36865000
H	4.03675300	5.52239300	-1.95824700
H	2.40153100	5.00550400	-3.74758700
H	-1.53777300	0.96090900	4.16538100
H	-0.53559200	-0.55409500	2.48520800
H	-2.35142700	3.19667600	4.79778200
H	-2.79865000	5.56329200	4.21846100
H	-2.26497300	6.40479100	1.93310800
H	-1.28481900	4.90519900	0.24843900
H	-2.67974600	1.70713900	-0.55470400
H	-6.66837400	-2.21221000	-0.20251800
H	-2.14080300	-0.72603100	0.50906800
H	1.03772200	0.27044700	-0.42083600
H	-4.52334500	-0.53570200	-2.32057700
C	7.72193700	-1.55569800	2.73025000
C	8.67429600	-2.42846200	2.14044900
C	8.63419200	-2.67844900	0.78068000
C	7.65346600	-2.07473100	-0.03943600
C	6.68944500	-1.19134600	0.54904800
C	6.75899300	-0.95858800	1.94559600
C	7.57797000	-2.31072100	-1.44010800
C	6.60876200	-1.70799400	-2.20644500
C	5.65268300	-0.82511600	-1.63223200
C	5.70522300	-0.58352000	-0.27402700
C	4.62250400	-0.13861300	-2.52907700
C	4.92937300	1.35711900	-2.72122300
O	9.66163100	-3.06143000	2.84458200
C	9.74568600	-2.84676000	4.24330200
C	3.22488200	-0.33290500	-1.95270300
O	2.73916900	0.42640700	-1.11862900
O	2.61427900	-1.40846600	-2.42642800
H	7.74496900	-1.35394900	3.79512900
H	9.37065400	-3.35049800	0.34960100
H	6.03196700	-0.29110500	2.40224600
H	8.29935600	-2.98273900	-1.89891500
H	6.56624000	-1.90623800	-3.27493600
H	4.97489500	0.07766800	0.18608200
H	4.63505300	-0.64244000	-3.50091900
H	4.21658500	1.81851600	-3.41332100
H	5.93965600	1.48395200	-3.12357600
H	4.86059200	1.88935000	-1.76924900

H	10.59261000	-3.44467300	4.58569600
H	9.93065100	-1.79119800	4.48390200
H	8.83712200	-3.18029800	4.76245800
H	1.71998000	-1.52061400	-1.98574300

3

Total energy -2980.35637086
 Number of imaginary frequencies 0
 Zero-point correction= 0.899890 (Hartree/Particle)
 Thermal correction to Energy= 0.954453
 Thermal correction to Enthalpy= 0.955397
 Thermal correction to Gibbs Free Energy= 0.810045
 Sum of electronic and zero-point Energies= -2979.456480
 Sum of electronic and thermal Energies= -2979.401918
 Sum of electronic and thermal Enthalpies= -2979.400974
 Sum of electronic and thermal Free Energies= -2979.546326

C	0.25411600	5.47413000	-1.06148700
C	0.88242200	6.14129700	-2.16322700
C	1.89382600	5.45448000	-2.88067300
C	2.27899000	4.18052800	-2.54969300
C	1.65811600	3.50754700	-1.45889900
C	0.65566700	4.14005500	-0.71759300
C	-0.00754400	3.44866500	0.43723800
C	-1.20632800	2.75054600	0.24331000
C	-1.88580000	2.17868800	1.35688800
C	-1.35078700	2.25683000	2.61842000
C	-0.12906600	2.93350800	2.86085300
C	0.53941400	3.55840700	1.75716500
N	-1.75215200	2.70885900	-1.04923400
N	2.04363000	2.20622200	-1.08004100
C	2.97116300	1.38250400	-1.69225900
N	3.22506700	0.16668900	-1.05455800
O	3.53979300	1.62818300	-2.74742600
C	-2.68123900	1.88481800	-1.68730600
N	-2.92988800	0.66728900	-1.07954700
O	-3.18063600	2.25895500	-2.73976700
C	-3.86788300	-0.31369100	-1.45820500
C	-3.91493300	-1.50012200	-0.72026800
C	-4.87370000	-2.51110500	-1.06377200
C	-5.76861100	-2.29498200	-2.16198200
C	-5.67834900	-1.07394400	-2.87641000
C	-4.76388500	-0.10694900	-2.54568900
C	-2.98140300	-1.73502700	0.43085200
C	-1.77834500	-2.42372400	0.23029400
C	-0.94359800	-2.73822900	1.34082000
C	-1.27613000	-2.32280100	2.60590800
C	-2.46998500	-1.60028300	2.85469800
C	-3.34633100	-1.32374300	1.75415800
N	-1.46930600	-2.86455600	-1.06588600

C	-0.28976700	-3.24833400	-1.70722500
O	-0.36230700	-3.85620700	-2.76654100
N	0.88800800	-2.86019600	-1.09383000
C	2.81334600	-2.24527700	1.74941700
C	2.99181800	-1.71555900	0.42988300
C	2.98904800	-0.32822500	0.23758600
C	2.83768200	0.54547700	1.35227900
C	2.63899100	0.04212900	2.61358200
C	2.61048100	-1.35447900	2.85439000
C	3.25713200	-2.63476400	-0.72620700
C	4.87489500	-3.83449700	-2.17201300
C	3.77365800	-4.35999600	-2.89354300
C	2.47844400	-4.05223500	-2.56416500
C	2.20744200	-3.18045300	-1.47108600
H	2.37273600	5.95490200	-3.71889700
H	3.04265100	3.66257500	-3.11062600
H	-2.85531800	1.71545000	1.22037100
H	-1.88489300	1.80888900	3.45221600
H	-1.46169000	3.45290600	-1.67277600
H	1.51064500	1.81665700	-0.31269400
H	-2.32461400	0.39767400	-0.31434100
H	-6.35313000	-0.90529300	-3.71225600
H	-4.69607300	0.81447000	-3.10465500
H	-0.06036500	-3.34872000	1.19818400
H	-0.62188200	-2.57035800	3.43755900
H	2.92393200	1.61667700	1.21649400
H	2.52146300	0.72763200	3.44862000
H	3.96657400	-5.02310200	-3.73347200
H	1.64766800	-4.44883800	-3.12858200
H	3.72109000	-0.45738600	-1.68006700
H	0.81736000	-2.20869800	-0.32233300
C	-4.56089200	-0.62987300	2.02412300
C	-2.82803000	-1.17206800	4.16032800
C	-4.00512600	-0.49377600	4.38492400
C	-4.87696100	-0.22344500	3.30226000
H	-5.80980900	0.30373400	3.48326200
C	-4.97862600	-3.73905700	-0.34930700
C	-6.71404900	-3.29675700	-2.50339800
C	-6.78582600	-4.47397500	-1.79411400
H	-7.51244700	-5.23494100	-2.06457900
C	-5.90766100	-4.69145000	-0.70648300
C	4.61261100	-2.95939800	-1.06791400
C	5.72708800	-2.44369600	-0.34590000
C	6.21578000	-4.15180300	-2.51162500
C	7.26979800	-3.63259900	-1.79498600
H	8.29254400	-3.88106600	-2.06416000
C	7.01706700	-2.77149800	-0.70138100
C	2.41472500	-1.88643400	4.15631000
C	2.41573700	-3.24626300	4.37294700
C	2.62104900	-4.13008700	3.28574700
C	2.81894800	-3.64554700	2.01110300
H	2.98679800	-4.33197600	1.18769100

C	1.74686400	4.26707600	2.02041400
C	0.42903400	3.02919400	4.16306500
C	2.26504000	4.33706600	3.29525300
C	1.60411400	3.71309600	4.38115100
C	-0.75608500	6.17697500	-0.34398800
C	0.48236000	7.45942100	-2.50470700
C	-0.50015800	8.10835000	-1.79225700
H	-0.79969400	9.11695000	-2.06282600
C	-1.12150100	7.45624100	-0.70134800
H	-5.24247800	-0.42730900	1.20447300
H	-2.15347000	-1.39736700	4.98323900
H	-4.27263100	-0.17420000	5.38827100
H	-7.38249200	-3.11407000	-3.34158700
H	-4.31682600	-3.91996900	0.49131900
H	-5.96720500	-5.62022700	-0.14535000
H	-0.09642000	2.55470000	4.98875600
H	2.02070900	3.78486400	5.38199600
H	3.18722800	4.88429000	3.47127100
H	2.25588400	4.75925600	1.19818500
H	-1.23912600	5.69394000	0.49907100
H	-1.89544700	7.97065100	-0.13794900
H	0.96994500	7.94745200	-3.34544100
H	2.26992300	-3.64352000	5.37361000
H	2.63057300	-5.20257900	3.46049600
H	2.26963800	-1.19456100	4.98290700
H	5.55132100	-1.78629400	0.49927300
H	7.84999300	-2.36441300	-0.13433200
H	6.39354600	-4.81601700	-3.35422600
H	-2.25814300	-2.97564400	-1.69211300