Electronic Supplementary Material (ESI) for CrystEngComm.

Electronic Supplementary Information for:

Unexpected narcissistic self-sorting at molecular and supramolecular level in racemic chiral calixsalens

Małgorzata Petryk[a,b], Katarzyna Biniek[a], Agnieszka Janiak[a]* and Marcin Kwit[a,b]*

Experimental details

NMR data was collected using a Bruker Ascend™ 600 MHz. Data was manipulated directly using TopSpin (version 2.1) or Mnova (version 6.0.2). Chemical shifts (δ) are reported in ppm relative to $SiMe_4$ and coupling constants (*J*) are given in Hz. Reference values for residual solvents were taken as δ = 7.28 ($CDCl_3$) for ^{1}H NMR; δ = 77.10 ppm ($CDCl_3$) for ^{13}C NMR. Mass spectra were run on a MaldiSYNAPT G2-S HDMS. Mass spectroscopy data was collected on a AB Sciex Triple TOF 5600+ coupled with an electrospray ionization (ESI) source of ion. Infrared data was collected using a Nicolet iS50 FT-IR machine as a thin film unless otherwise stated. A PerkinElmer 341 polarimeter was used for optical rotation ($[\alpha]_D$) measurements (ca. 20 °C). Flash column chromatography was performed on Merck Kieselgel type 60 (250 - 400 mesh). Merck Kieselgel type 60F_{254} analytical plates were employed for TLC. Melting points were measured on Büchi Melting Point B-545 and uncorrected.

All known compounds were identified by spectroscopic comparison with authentic samples.

Aldehydes **4a**-4**d** were prepared according to the literature procedures.[1-3]

General procedure for synthesis of racemic calixsalens 3a-3d:

To (±)-*trans*-1,2-diaminocyclohexane (1 equiv.) dissolved in methylene chloride, a dialdehyde (1 equiv.) was added in one portion. The resulting mixture was stirred at room temperature for 24-48 hours. After evaporation of all volatiles (the temperature of water bath did not exceed 25 °C) the crude product was dried under high vacuum for 5 hours at room temperature and crystallized.

Racemic calixsalens **3a**-**3d** gave all spectra identical as these previously published for enantiomeric ones.[2-4]

Calixsalen 3a

According to above: To (±)-*trans*-1,2-diaminocyclohexane (57 mg, 0.5 mmol) dissolved in 30 mL of methylene chloride 5-bromo-2-hydrooxyisophthaldehyde (114 mg, 0.5 mmol) was added in one portion. The resulting mixture was stirred at room temperature for 24 hours. The solvent was evaporated under vacuum and the yellow solid product was obtained quantitatively. Crystals were obtained by slow evaporation of solvents CH_2Cl_2/MeCN (1:1 *v*/*v*; *c* = 0.008 g mL^{-1}) with 90% yield. HRMS (ESI) calcd. for $C_{42}H_{45}N_6O_3Br_3$ $[M+H]^+$ 919.1176; found 919.1147; m.p. >300 °C (dec.); ^{1}H NMR (600 MHz, $CDCl_3$) δ 14.15 (s, 1H, -O*H*), 8.58 (s, 1H, -N=C*H*-), 8.19 (s, 1H, -N=C*H*-), 7.85 (d, *J* = 1.7 Hz, 1H, *Ar*), 7.21 (s, 1H, *Ar*), 3.36 (dtd, *J* = 14.8, 9.1, 4.9 Hz, 2H, –C*H*N=), 1.91 - 1.80(m, 3H, *Cy*), 1.77 – 1.62 (m, 3H, *Cy*), 1.52 – 1.41 (m, 2H, *Cy*); ^{13}C NMR (151 MHz, $CDCl_3$) δ 162.51 (-N=*C*H-), 160.68 (-N=*C*H-),

154.65 (*C*-OH), 135.70 (*Ar*), 131.68 (*Ar*), 125.56 (*Ar*), 120.48 (*Ar*), 109.99 (*Ar*), 75.14 (-*C*HN=), 73.36 (-*C*HN=), 33.27 (*Cy*), 33.13 (*Cy*), 24.33 (*Cy*), 24.22 (*Cy*); FT-IR (ATR): $\tilde{\nu}$ = 2929, 2857, 1633, 1602, 1579, 1445, 1370, 1295, 1251, 1143, 1097, 1004, 907, 873, 730, 703 cm^{-1}.

Calixsalen 3b

According to above: To (±)-*trans*-1,2-diaminocyclohexane (57 mg, 0.5 mmol) dissolved in 30 mL of methylene chloride 2-hydroxy-5-methylisophthaldehyde (82 mg, 0.5 mmol) was added in one portion. The resulting mixture was stirred at room temperature for 24 hours. The solvent was evaporated under vacuum and the yellow solid product was obtained quantitatively. Crystals were obtained by slow evaporation of solvents mixture CH_2Cl_2/MeCN (1:1 *v*/*v*; *c* = 0.008 g mL^{-1}) with 80% yield. HRMS (ESI) calcd. for $C_{45}H_{54}N_6O_3$ $[M+H]^+$ 727.4330; found 727.4166; m.p. >300 °C (dec.); ^{1}H NMR (600 MHz, $CDCl_3$) δ 13.86 (s, 1H, -O*H*), 8.66 (s, 1H, -N=C*H*-), 8.20 (s, 1H, -N=C*H*-), 7.53 (s, 1H, *Ar*), 6.86 (d, *J* = 21.6 Hz, 1H, *Ar*), 3.51 – 3.18 (m, 2H, –C*H*N=), 2.00 (s, 3H, -CH_3), 1.88 – 1.80 (m, 3H, *Cy*), 1.76 (s, 2H, *Cy*), 1.72 – 1.64 (m, 1H, *Cy*), 1.52 – 1.41 (m, 2H, *Cy*); ^{13}C NMR (151 MHz, $CDCl_3$) δ 163.47 (-N=*C*H-), 159.38 (-N=*C*H-), 156.16 (*C*-OH), 134.25 (*Ar*), 129.60 (*Ar*), 126.88 (*Ar*), 122.94 (*Ar*), 118.76 (*Ar*), 75.43 (-*C*HN=), 73.41 (-*C*HN=), 33.47 (*Cy*), 33.22 (*Cy*), 24.44 (*Cy*), 24.36 (*Cy*), 19.94 (-*C*H_3); FT-IR (ATR): $\tilde{\nu}$ = 2928, 2857, 1634, 1600, 1459, 1448, 1371, 1256, 1142, 1095, 908, 869, 729 cm^{-1}.

Calixsalen 3c

According to above: To (±)-*trans*-1,2-diaminocyclohexane (57 mg, 0.5 mmol) dissolved in 30 mL of methylene chloride 2-hydroxy-5-*tert*-butylisophthaldehyde (103 mg, 0.5 mmol) was added in one portion. The resulting mixture was stirred at room temperature for 24 hours. The solvent was evaporated under vacuum and the yellow solid product was obtained quantitatively. Crystals were obtained by slow evaporation of mixture of solvents CH_2Cl_2/MeCN (1:1 *v*/*v*; *c* = 0.008 g mL^{-1}) with 90% yield. HRMS (ESI) calcd. for $C_{54}H_{72}N_6O_3$ $[M+H]^+$ 853.5739; found 853.5693; m.p. >300 °C (dec.); ^{1}H NMR (600 MHz, $CDCl_3$) δ 13.93 (s, 1H, -O*H*), 8.70 (s, 1H, -N=C*H*-), 8.27 (s, 1H, -N=C*H*-), 7.85 (d, *J* = 2.2 Hz, 1H, *Ar*), 7.12 (s, 1H, *Ar*), 3.52 – 3.26 (m, 2H, –C*H*N=), 1.90 – 1.82 (m, 3H, *Cy*), 1.73 – 1.66 (m, 1H, *Cy*), 1.53 – 1.44 (m, 2H, *Cy*), 1.20 (s, 9H, -C(CH_3)$_3$); ^{13}C NMR (151 MHz, $CDCl_3$) δ 163.84 (-N=*C*H-), 159.36 (-N=*C*H-), 156.09 (*C*-OH), 140.14 (*Ar*), 130.46 (*Ar*), 126.11 (*Ar*), 122.98 (*Ar*), 118.54 (*Ar*), 75.56 (-*C*HN=), 73.16 (-*C*HN=), 33.92 (-*C*(CH_3)$_3$), 33.56 (*Cy*), 33.23 (*Cy*), 31.36 (-C(*C*H_3)$_3$), 24.49 (*Cy*), 24.39 (*Cy*); FT-IR (ATR): $\tilde{\nu}$ = 2930, 2858, 635, 1596, 1461, 1448, 1363, 1284, 1263, 1225, 1144, 1094, 1003, 907, 730 cm^{-1}.

Calixsalen 3d

According to above: To (±)-*trans*-1,2-diaminocyclohexane (57 mg, 0.5 mmol) dissolved in 30 mL of methylene chloride 2-hydroxy-5-methoxyisophthaldehyde (90 mg, 0.5 mmol) was added in one portion. The resulting mixture was stirred at room temperature for 24 hours. The solvent was evaporated under vacuum and the yellow solid product was obtained quantitatively. Crystals were obtained by slow evaporation of mixture of CH_2Cl_2/diethyl ether (1:1 *v*/*v*; *c* = 0.008 g mL^{-1}) with 80% yield. HRMS (ESI) calcd. for $C_{45}H_{54}N_6O_6$ $[M+H]^+$ 775.4178; found 775.4140; m.p. >300 °C (dec.); ^1H NMR (600 MHz, $CDCl_3$) δ 13.54 (s, 1H, -O*H*), 8.67 (s, 1H, -N=C*H*-), 8.21 (s, 1H, -N=C*H*-), 7.39 (d, *J* = 3.1 Hz, 1H, *Ar*), 6.68 (d, *J* = 3.1 Hz, 1H, *Ar*), 3.66 (s, 3H, -OCH_3), 3.38 (dtd, *J* = 14.8, 9.0, 5.0 Hz, 2H, –C*H*N=), 1.90 – 1.81 (m, 3H, *Cy*), 1.79 – 1.69 (m, 3H, *Cy*), 1.54 – 1.44 (m, 2H, *Cy*); ^{13}C NMR (151 MHz, $CDCl_3$) δ 163.18 (s), 155.67 (*C*-OH), 155.61 (-N=*C*H-), 151.35 (*C*-OCH_3), 123.95 (*Ar*), 119.33 (*Ar*), 119.15 (*Ar*), 114.41 (*Ar*), 75.28 (-*C*HN=), 73.54 (-*C*HN=), 55.98 (-O*C*H_3), 33.41 (*Cy*), 33.15 (*Cy*), 24.41 (*Cy*), 24.33 (*Cy*); FT-IR (ATR): $\tilde{\nu}$ = 2929, 2857, 1639, 1598, 1463, 1435, 1375, 1326, 1300, 1254, 1142, 1007 cm^{-1}.

Crystallizations of enantiomerically enriched samples and preparation of standard solutions of 3a and 3c

1A) 10 mg of (*all-R*)-**3a** and 30mg of (*all-S*)-**3a** were dissolved in 5 mL of CH_2Cl_2. After 5 mL of MeCN addition, solution was mixed and left for slow evaporation. Crystals were obtained with 90% (90%) yield, filtered of, dried and grounded. For polarimetric measurements 10 mg of the sample was dissolved in 1 mL of spectroscopic grade chloroform.

1B) 30 mg of (*all-R*)-**3a** and 10 mg of (*all-S*)-**3a** were dissolved in 5 mL of CH_2Cl_2. After 5 mL of MeCN addition, solution was mixed and left for slow evaporation. Crystals were obtained with 90% (90%) yield, filtered of, dried and grounded. 10 mg of sample was dissolved in 1 mL of spectroscopic grade chloroform.

1C) 2.5 mg of (*all-R*)-**3a** and 7.5 mg of (*all-S*)-**3a** were dissolved in 1 mL of spectroscopic grade chloroform.

1D) 7.5 mg of (*all-R*)-**3a** and 2.5mg of (*all-S*)-**3a** were dissolved in 1 mL of spectroscopic grade chloroform.

2A) 10 mg of (*all-R*)-**3c** and 30 mg of (*all-S*)-**3c** were dissolved in 5 mL of CH_2Cl_2. After 5 mL of MeCN addition, solution was mixed and left for slow evaporation. Crystals were obtained with 90% (90%) yield, filtered of, dried and grounded. 10 mg of sample was dissolved in 1 mL of spectroscopic grade chloroform for polarimetry.

2B) 30 mg of (*all-R*)-**3c** and 10 mg of (*all-S*)-**3c** were dissolved in 5 mL of CH_2Cl_2. After 5 mL of MeCN addition, solution was mixed and left for slow evaporation. Crystals were obtained with 90% (90%) yield, filtered of, dried and grounded. 10 mg of sample was dissolved in 1 mL of spectroscopic grade chloroform.

2C) 2.5 mg of (*all-R*)-**3c** and 7.5 mg of (*all-S*)-**3c** were dissolved in 1 mL of spectroscopic grade chloroform.

2D) 7.5 mg of (*all-R*)-**3c** and 2.5 mg of (*all-S*)-**3c** were dissolved in 1 mL of spectroscopic grade chloroform.

Optical rotation measurements of enriched crystals 3a and 3c

Optical rotations were measured with JASCO P-2000 polarimeter at 589 nm. The initial 1 g 100 cm^{-3} solution was made by dissolving of 10mg of enantiomerically enriched crystal samples **1A**-**D** and **2A**-**D** and enantiomerically pure samples (*all-R*)-**3a**, (*all-S*)-**3a**, (*all-R*)-**3c**, (*all-S*)-**3c** in 1 mL of spectroscopic grade chloroform. This procedure was repeated 2 times in chloroform. Measurements of optical rotation at given wavelength were repeated 10 times for each sample. The average OR's values were collected in Table A. Experimental results were compared to optical rotation of standard solutions and enantiomeric excess in samples **3A-B** and **4A-B** were calculated using linear regression (See Table SI_1).

Table SI_1. Measured optical rotations for enantiomerically enriched and enantiomerically pure solutions of **3a** and **3b**.

Sample	Contains X% of (*all-R*)-calixsalen	Contains X% of (*all-S*)-calixsalen	α[˚]
1A	0.27	0.73	78.778
1B	0.71	0.29	-70.911
1C	0.25	0.75	89.077
1D	0.75	0.25	-80.401
(*all-R*)-3a	1.00	-	-170.042
(*all-S*)-3a	-	1.00	166.136
a=	336.7336	-167.1743	=b
Sa=	5.6814371	3.62121983	=Sb
R=	0.999430982	4.491570405	=S
2A	0.23	0.77	91.517
2B	0.78	0.22	-98.823
2C	0.25	0.75	88.572
2D	0.75	0.25	-87.522
(*all-R*)-3c	1.00	-	-175.425
(*all-S*)-3c	-	1.00	168.156
a=	345.302	-174.205625	=b
Sa=	4.445965919	2.833758372	=Sb
R=	0.999668548	3.514844676	=S

a and b are regression coefficients,
Sa and Sb are standard errors of the coefficients,
R is squared correlation coefficient,
S is standard error.

Calculation details

Starting geometry of macrocycle **3a** was obtained from crystallographic data and pre-optimized at the PM6 and then M06L/6-31G(d) level.[5,6] The optimized structure of homochiral, monomeric **3a** was used as the starting point for construction of **3a** diastereomers. The heterochiral **3a** were constructed from homochiral **3a** by replacing one of the diamine units by its enantiomer and pre-optimized the generated structure at the molecular mechanic level then with the use of PM6 and M06L/6-31G(d) method. The heterochiral structures of **3a** were differ in conformation of imine bonds an orientation of respective pairs of C*H and CHN protons. Additionally, for the real minimum energy conformers the single point energies were calculated at the M06L/6-311G(d,p) level.

The initial structures of homochiral dimers of **3a** were based on available crystallographic data.[4] Heterochiral dimers were constructed by replacing one monomer by its enantiomer. The generated structures were optimized at first with the use of PM6 semiempirical method, then at the the M06L/6-31G(d) level. Single-point energies were calculated for optimized structures of homo- and heterochiral dimers employing the same M06L and B3LYP hybrid functional, the latest together with empirical D3 version of Grimme's dispersion with Becke-Johnson damping (D3BJ),[7] using Gaussian09 package.[6] The Boys and Bernardi counterpoise correction has been utilized to precise calculation of interaction energies between monomers involved in dimers.[8]

Table SI_2. Calculated at the M06L/6-311G(d,p) level relative energies (ΔE, kcal mol^{-1}) and some structural parameters that characterize **3a** diastereomers.

Structure	ΔE	Conformation of imine bonds	H-C*-N=C torsion angle [deg]
3a[a]	0.00	*all-s-trans*	-24, 7
3a(1)	3.84	*all-s-trans*	140, 151 / 4, 12 / 5, 4
3a(2)	10.55	*all-s-trans*	159, -7 / -173, 11 / 13, 1
3a(3)	31.52	*s-cis*$_2$, *s-trans*, *s-trans*	169, 124 / -138, 18 / -14, -7

[a] C_3 symmetry

Table SI_3. Calculated at the M06L/6-311G(d,p) level relative energies (ΔE, kcal mol^{-1}) and dimerization energies with and without counterpoise correction (E_{dim}, E_{dim_CP}, in kcal mol^{-1})for **A**-**D** dimers of calixsalen **3a**.

Dimer	ΔE	E_{dim}	E_{dim_CP}
A	0.00	-44.84	-37.73
B	0.11	-39.05	-31.22
C	4.93	-54.72	-43.58
D	7.47	-45.10	-35.43

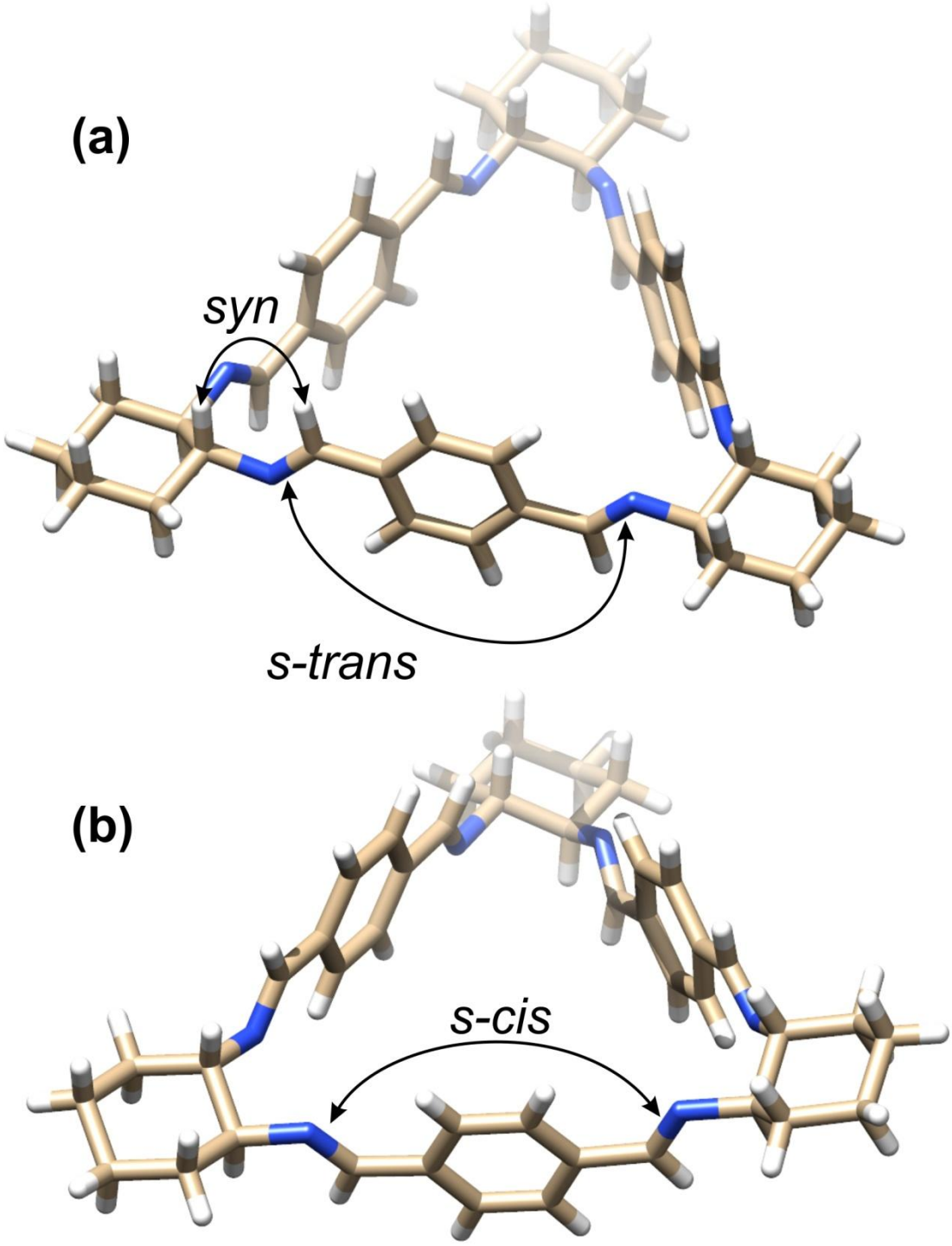


Figure SI_1. Homochiral (a) and heterochiral (b) trianglimine. Drawn on the basis of available crystallographic data.[9]

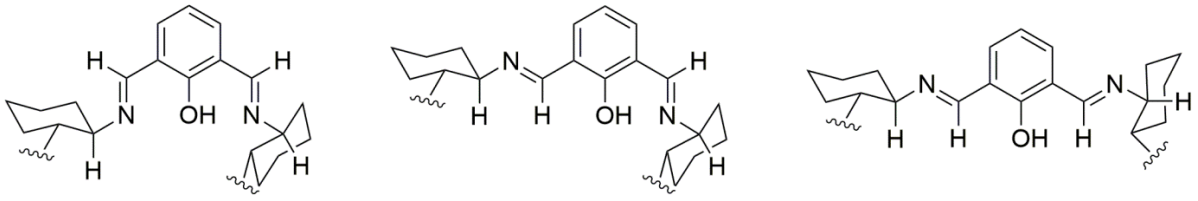


Figure SI_2. Possible conformation of imine bonds in calixsalen (only one third of the whole macrocyclic structure is shown).

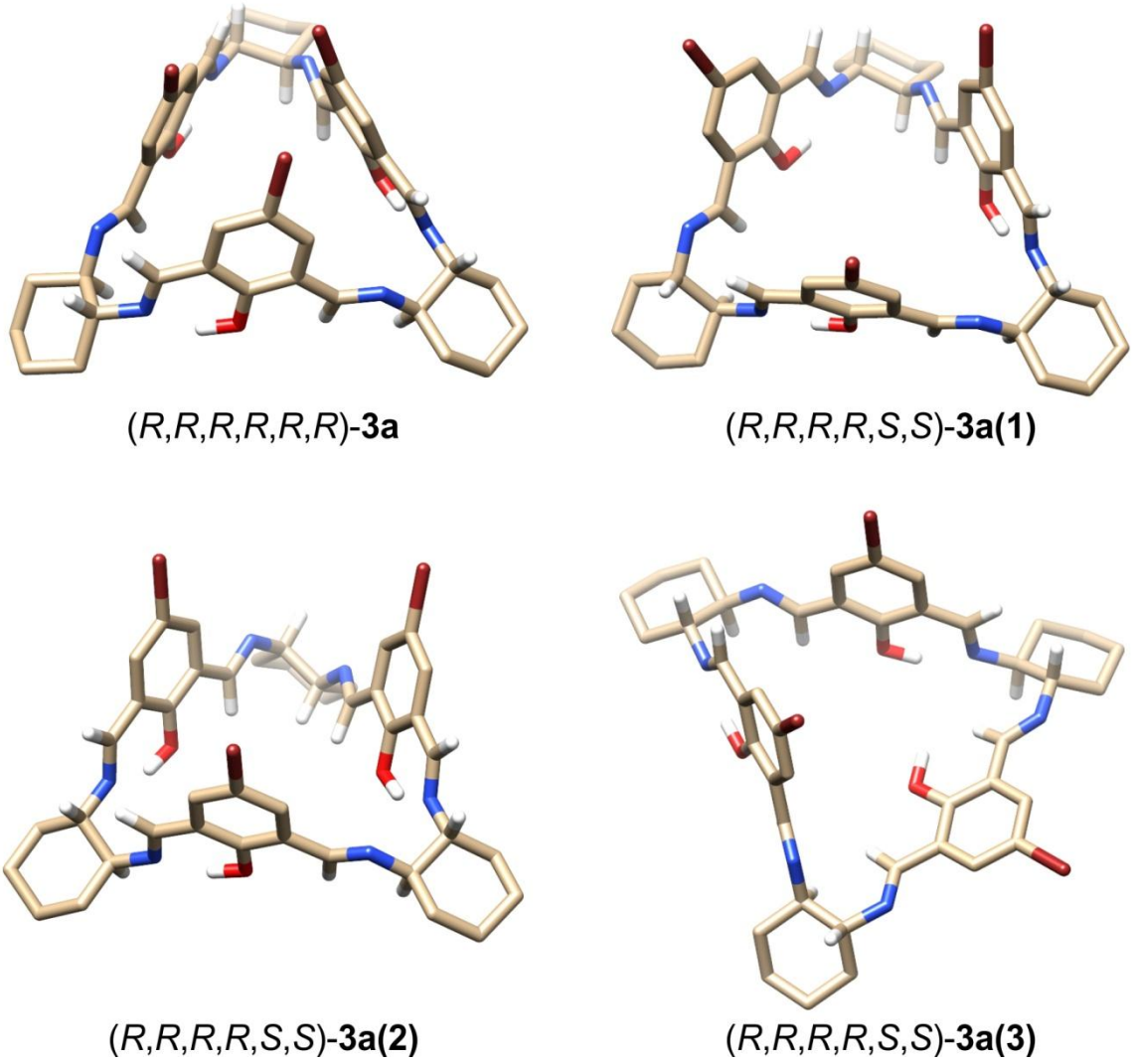


Figure SI_3. Calculated structures of homochiral and heterochiral calixsalene **3a**. Some hydrogen atoms were omitted for clarity.

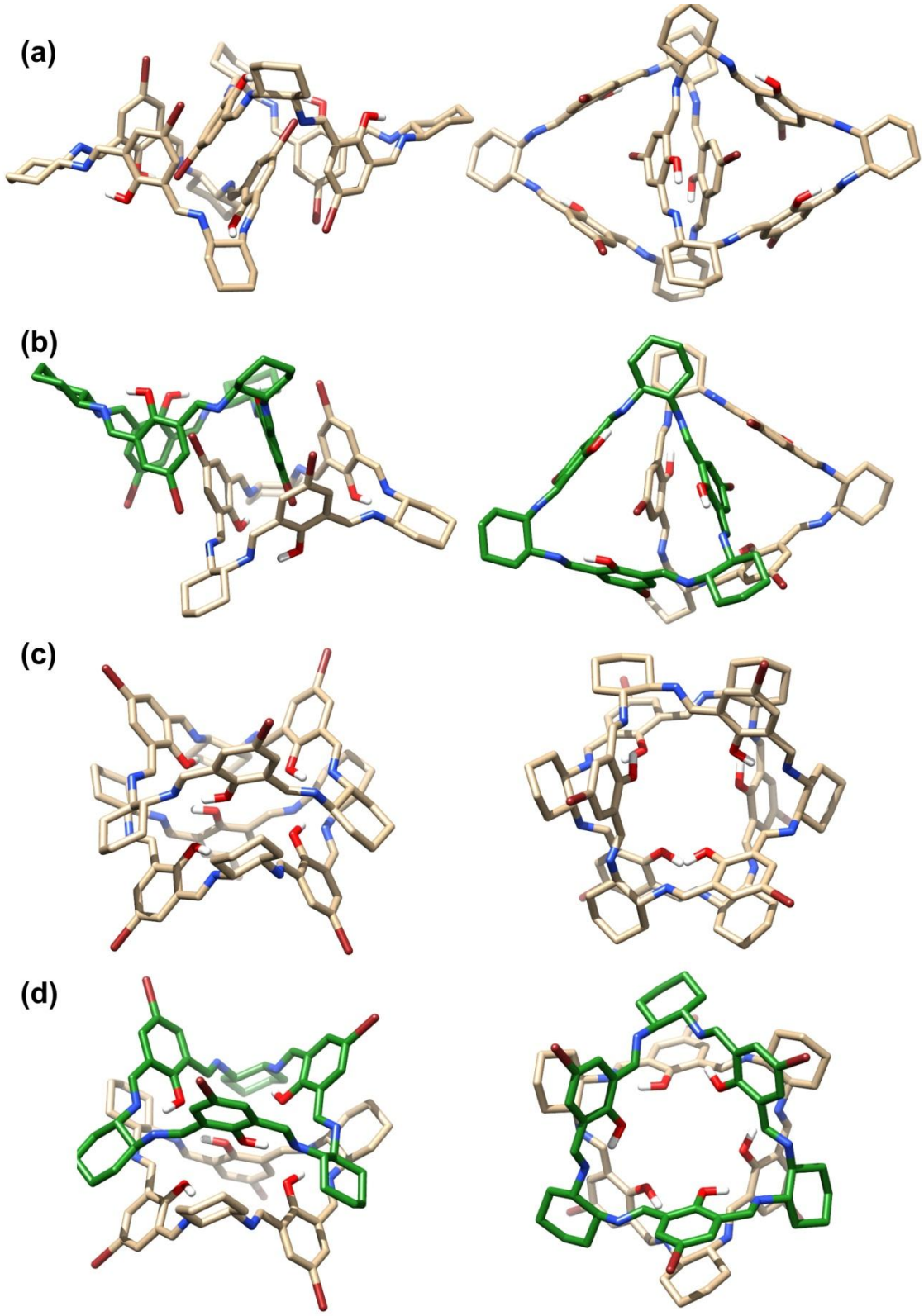


Figure SI_4. Calculated at the M06L/6-31G(d) level structures of homochiral and heterochiral tail-to-tail dimers (a, b) and homochiral and heterochiral capsules (c, d) of calixsalen **3a**. Some hydrogen atoms were omitted for clarity.

Single-Crystal X-ray diffraction

Crystals suitable for single-crystal X-ray diffraction were obtained from the slow evaporation of a mixture of dichloromethane and acetonitrile.

Intensity data collected for **3a** was measured on an Xcalibur diffractometer equipped with a graphite monochromator and MoKα radiation (λ = 0.71073 Å). The data for remaining crystals **3b** and **3c** were collected on a SuperNova diffractometer equipped with Cu microfocus source (λ=1.54178 Å) and 135 mm Atlas CCD detector. Data reduction and analysis for all of the crystals were carried out with the CrysAlisPro program.[10] In all experiments the sample temperature was controlled with an Oxford Instruments Cryosystem cold nitrogen-gas blower. The structures were solved by direct methods using SHELXT[11a] or SIR-2011,[12] and refined by the full-matrix least-squares techniques within SHELXL-2014.[11b] All heavy atoms were refined anisotropically.The hydrogen atoms bound to C atoms were placed at calculated positions and refined using a riding model, and their isotropic displacement parameters were given a value 20% higher than the isotropic equivalent for the atom to which the H atoms were attached (for methyl hydrogen atoms this value has been increased to 50%). The positions of the hydroxyl H atoms were constrained to an ideal geometry [O-H=0.84 Å and U_{iso}(H)=1.2U_{eq}(O)] using the AFIX 147 command integrated in SHELXL.[11b]

Some solvent molecules in **3b** and **3c** were highly disordered and could not be resolved to yield a satisfactory model, therefore their unresolved electron density was treated with Squeeze.[13]

Graphical images were produced in Xseed[14] using Pov-Ray[15] and Mercury[16] programs.

Crystal data for 3a: $C_{42}H_{45}N_6O_3Br_3$*CH_2Cl_2, M_r=1006.49, yellow needle-like crystals, 0.60x0.08x0.08mm^3, monoclinic, space group *C*2/c (No. 15), *a*=31.614(2), *b*=14.2436(4), *c*=24.503(1)Å, *β*=124.645(1)°, *V*=9077.3(10) Å^3, Z=8, D_x=1.473 g/cm^3, *F*000=4080, Xcalibur, Eos, Mo*Kα* radiation, *λ*=0.71073 Å, *T*=100(2)K, $2\vartheta_{max}$=50.1º, 52081 reflections collected, 7995 unique (R_{int}=0.0869). Final GooF=1.019, *R*1=0.045, w*R*2=0.091, *R* indices based on 5899 reflections with *I*>2*σ*(*I*) (refinement on F^2), 544 parameters, 3 restraints. Lp and absorption corrections applied, μ=2.829 mm^{-1}.

In **3a** two dichloromethane molecules located near an inversion centre were found to be disordered over two positions and were refined with fixed site occupancy factors of 0.5.

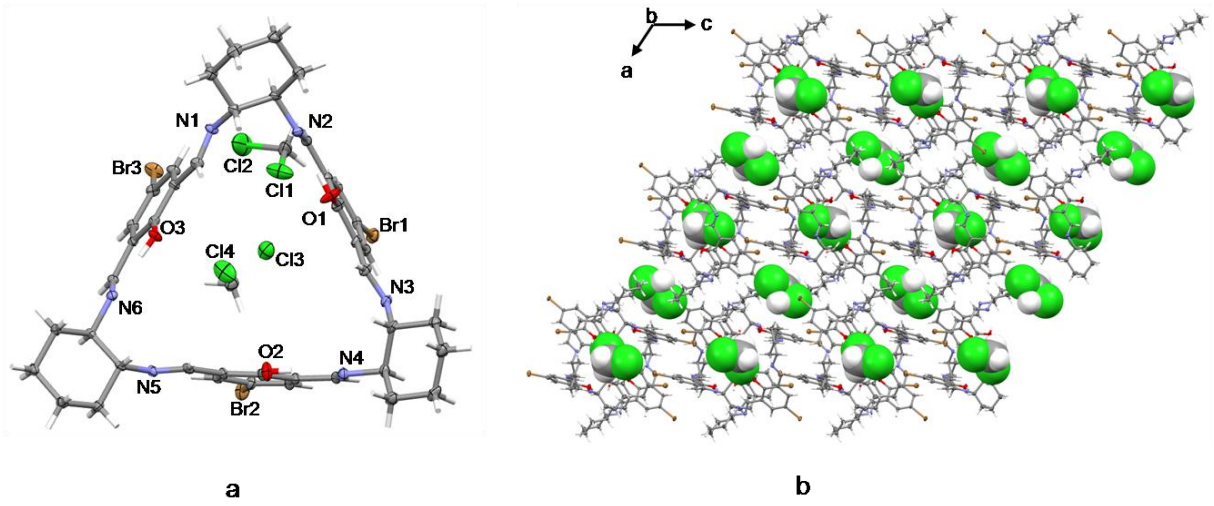


Figure SI_5. a) A perspective view of **3a**. For clarity, only the heteroatoms were labeled. Ellipsoids are drawn at the 40% probability level, hydrogen atoms are represented by spheres of arbitrary radii. (b) A packing diagram of **3a** as viewed along the *b* lattice direction. The host molecules are shown in ellipsoid style whereas the guest molecules are shown in a space-filling model.

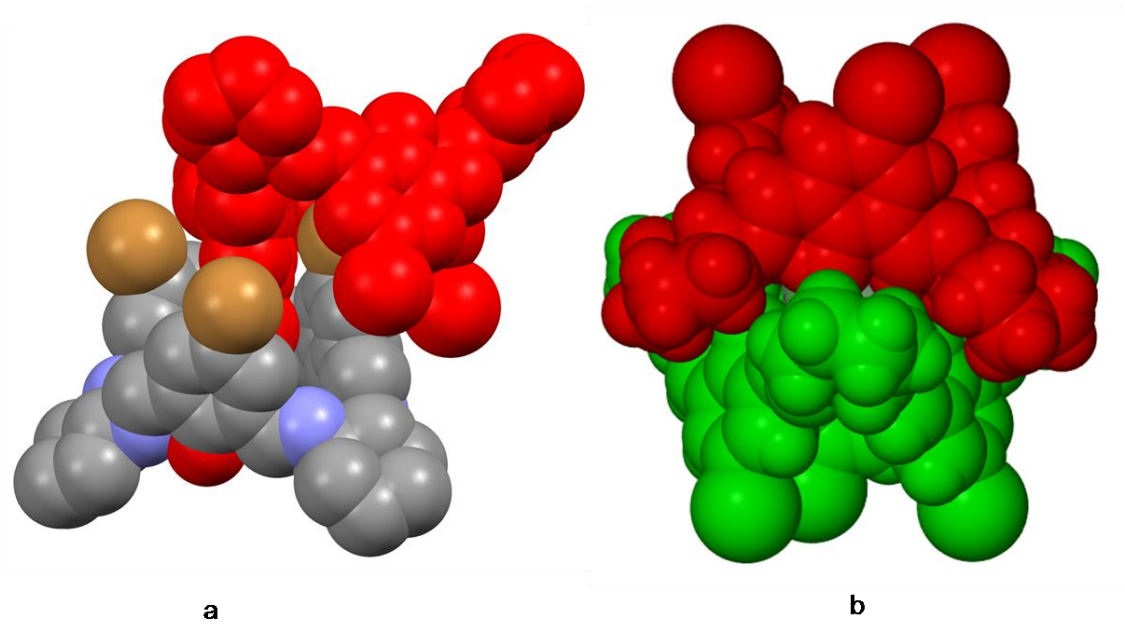


Figure SI_6. Supramolecular arrangemts of calixsalen **3a**, (a) the tail-to-tail dimer formed between two monomers of the same chirality; (b) the head-to-head capsule formed between two monomers of opposite chirality.

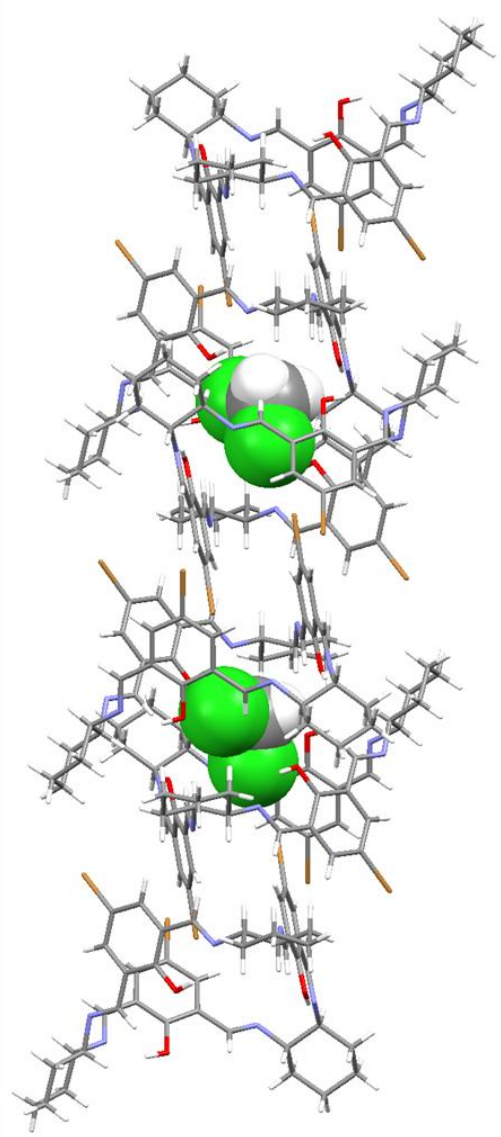


Figure SI_7. Alternate arrangements of two supramolecular dimers and capsules. In each capsules solvent molecule is entrappted.

Crystal data for 3b: $C_{45}H_{54}N_6O_3$*CH_3CN, M_r=767.99, yellow plate crystals, 0.25x0.14x0.05mm^3, monoclinic, space group $P2_1/n$ (No. 14), a=14.1389(2), b=20.7594(2), c=32.7591(4) Å, β=100.665(1)°, V=9449.2(2) Å^3, Z=8, D_x=1.080 g/cm^3, $F000$=3296.0, Cu$K\alpha$ radiation, λ=1.54178 Å, T=130(2)K, $2\vartheta_{max}$=133.2º, 37757 reflections collected, 16672 unique (R_{int}=0.0254). Final GooF=1.037, $R1$=0.0540, w$R2$=0.1562, R indices based on 13552 reflections with $I>2\sigma(I)$ (refinement on F^2), 1013 parameters, 0 restraints. Lp and absorption corrections applied, μ= 0.541 mm^{-1}.

In **3b** there was possible to only determine position for one solvent molecule in the crystal. The remaining solvent molecules were highly disordered and could not be resolved to yield a satisfactory model, therefore their unresolved electron density was treated with SQUEEZE. The estimated electron count is 356/269 in an accessible void volume of 1521 Å^3 and can indicate to squeezed of one molecule of dichloromethane and two molecules of acetonitrile per unit cell. Taking into account the number of the squeezed molecules and solvent molecule that could be modelled, we established the ratio of host to guest (DCM and MeCN, respectively) as 2:1:3.

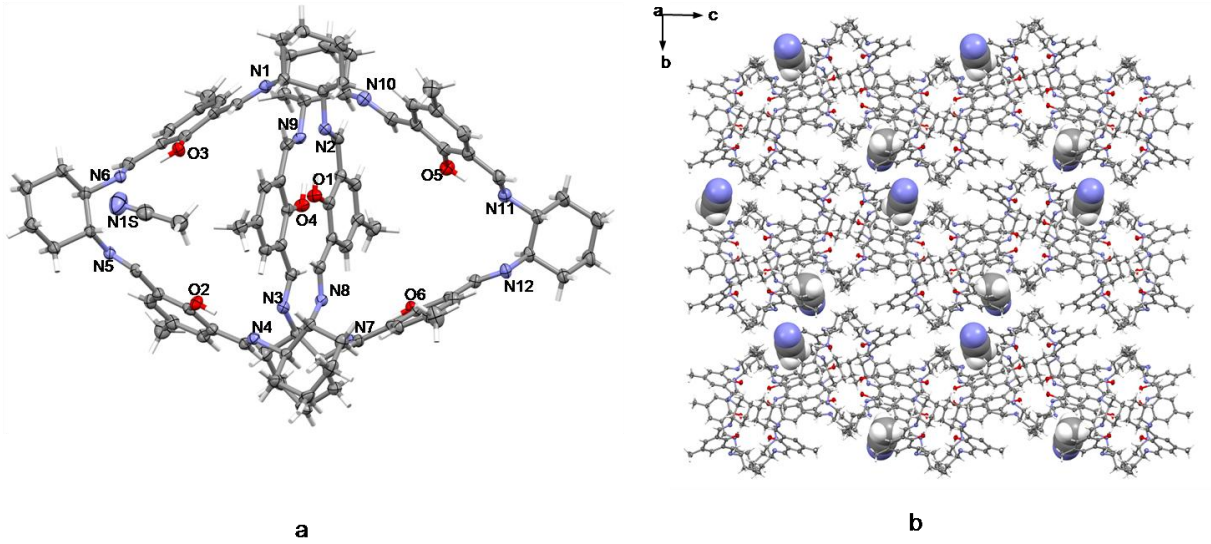


Figure SI_8. a) A perspective view of **3b**. For clarity, only the heteroatoms were labeled. Ellipsoids are drawn at the 40% probability level, hydrogen atoms are represented by spheres of arbitrary radii. (b) A packing diagram of **3b** as viewed along the *a* lattice direction. The host molecules are shown in ellipsoid style whereas the guest molecules are shown in a space-filling model.

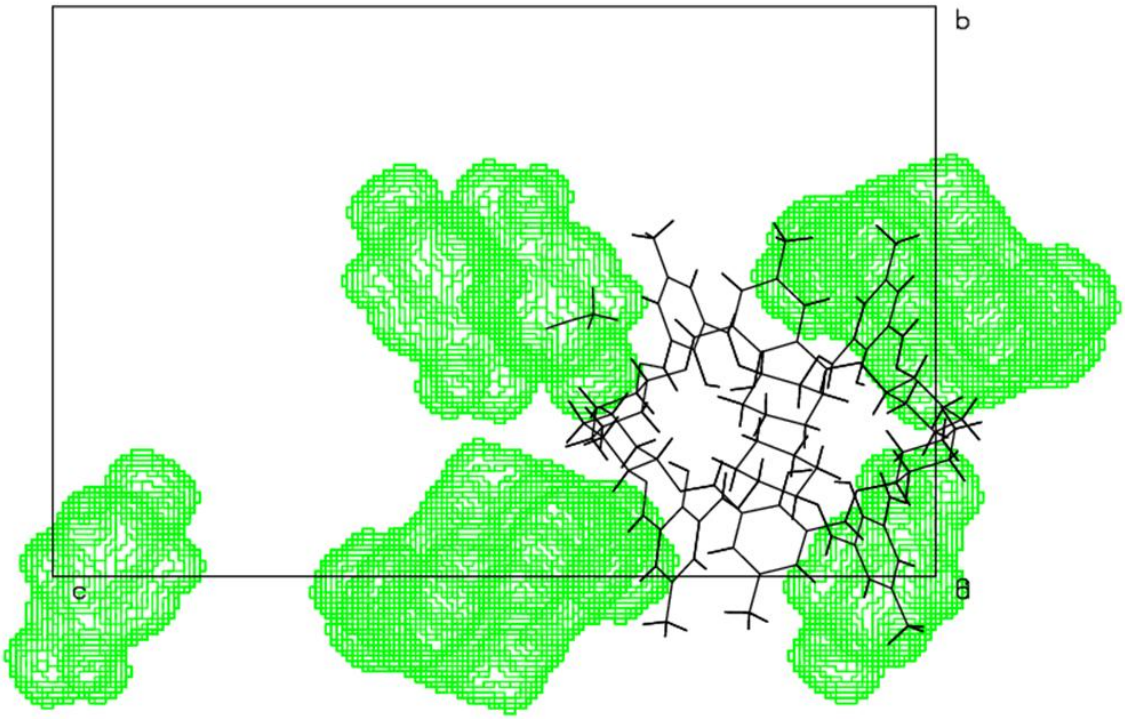


Figure SI_9. The areas in green represents the voids from which the guest molecules were removed as viewed along *a* lattice direction.

Crystal data for 3c: $C_{54}H_{72}N_6O_3$*CH_3CN, M_r= 894.23, yellow prism, 0.30x0.18x0.10 mm^3 monoclinic, space group $P2_1/n$ (No. 14), V= 12244.1(4) $Å^3$, Z=8, D_x=0.970 g/cm^3, $F000$=3872, SuperNova, Cu$K\alpha$ radiation, λ=1.54184 Å, T=150(2)K, $2\vartheta_{max}$=151.3º, 55529 reflections collected, 24826 unique (R_{int}=0.0395). Final GooF=1.002, $R1$=0.0517, w$R2$=0.1392, R indices based on 16678 reflections with $I>2\sigma(I)$ (refinement on F^2), 1215 parameters, 0 restraints. Lp and absorption corrections applied, λ=0.471 mm^{-1}.

In **3c** there was possible to only determine position for two acetonitrile molecules in the crystal. The DCM solvent molecules were highly disordered and could not be resolved to yield a satisfactory model, therefore their unresolved electron density was treated with SQUEEZE. The estimated electron count is 770 in an accessible void volume of 2448 $Å^3$ and can indicate to squeezed of four molecules of dichloromethane and per unit cell. Taking into account the number of the squeezed molecules and solvent molecules that could be modelled, we established the ratio of host to guest (DCM and MeCN, respectively) as 1:2:1.

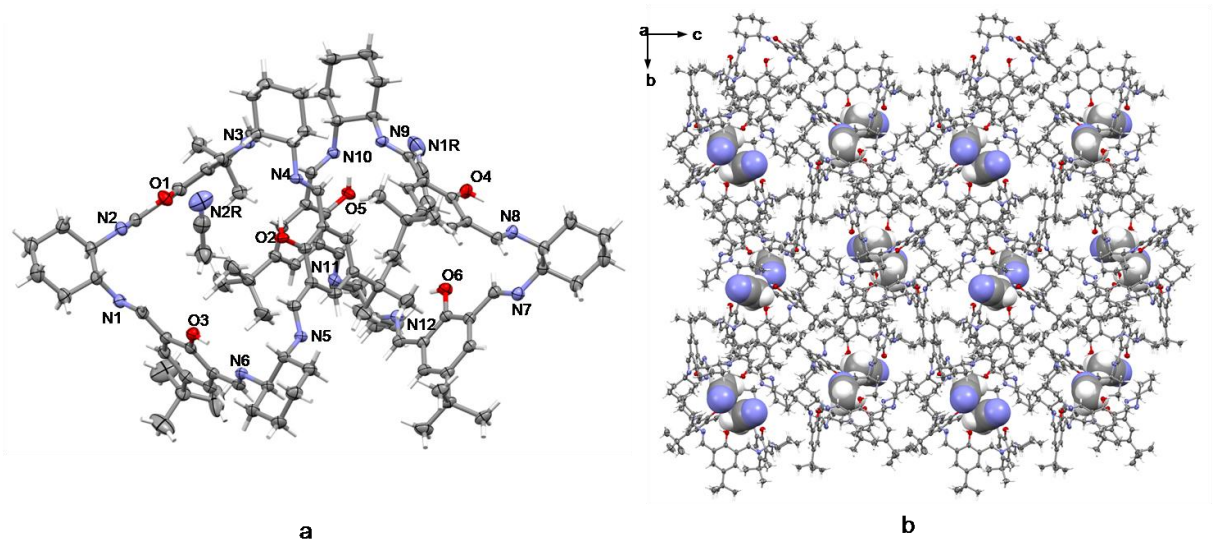


Figure SI_10. a) A perspective view of **3c**. For clarity, only the heteroatoms were labeled. Ellipsoids are drawn at the 40% probability level, hydrogen atoms are represented by spheres of arbitrary radii. b) A packing diagram of **3c**. The two symmetry independent host molecules, which form a dimer, are shown in green and blue in ellipsoid style whereas guest molecules are shown as space-filling model. All H atoms are omitted for clarity.

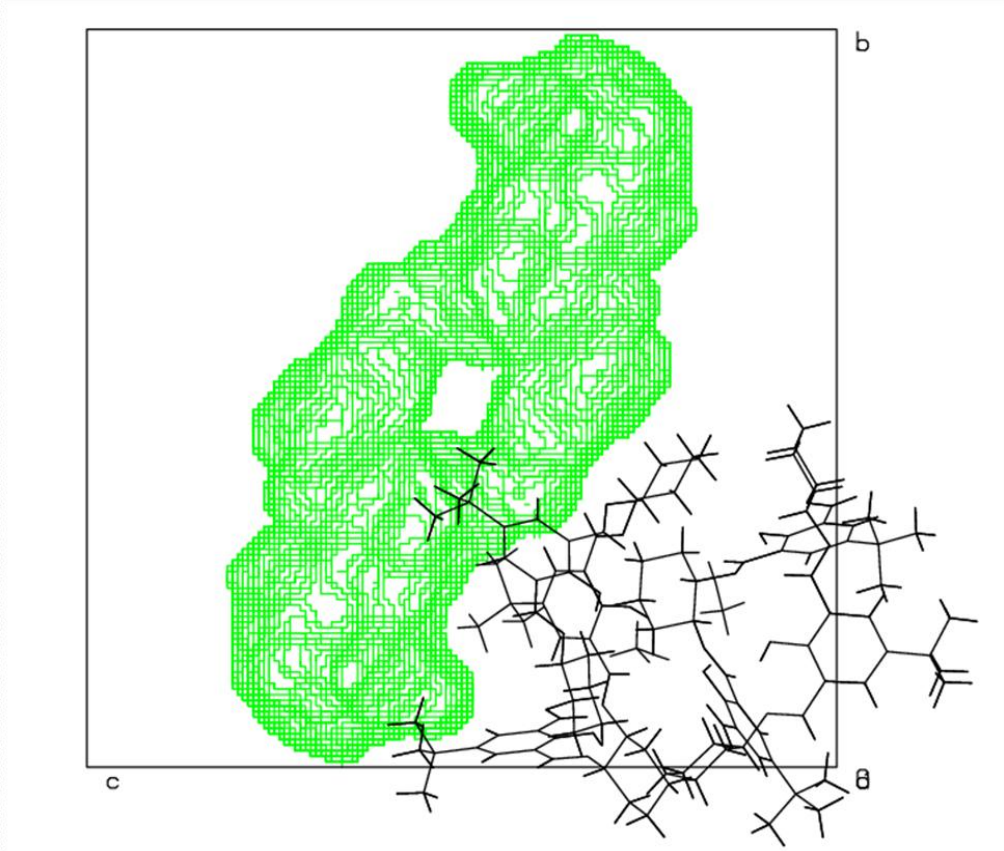


Figure SI_11. The areas in green represents the voids from which the guest molecules were removed as viewed along *a* lattice direction.

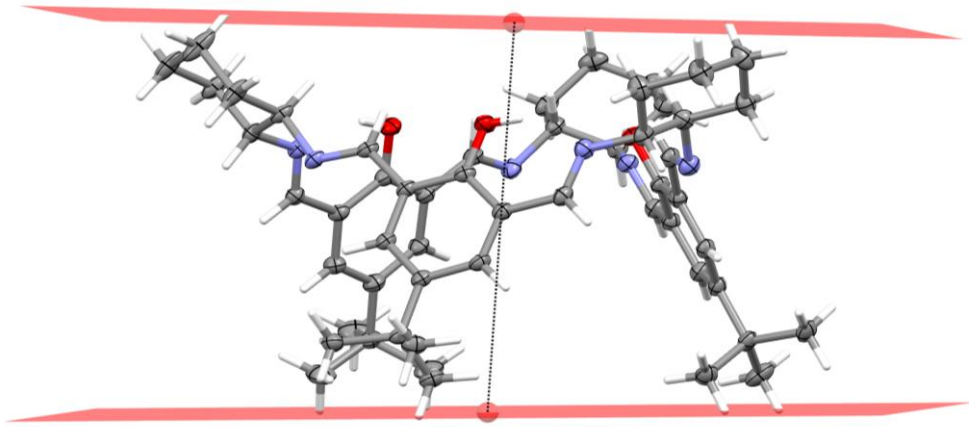


Figure SI_12. Definition of the molecular height calculated.

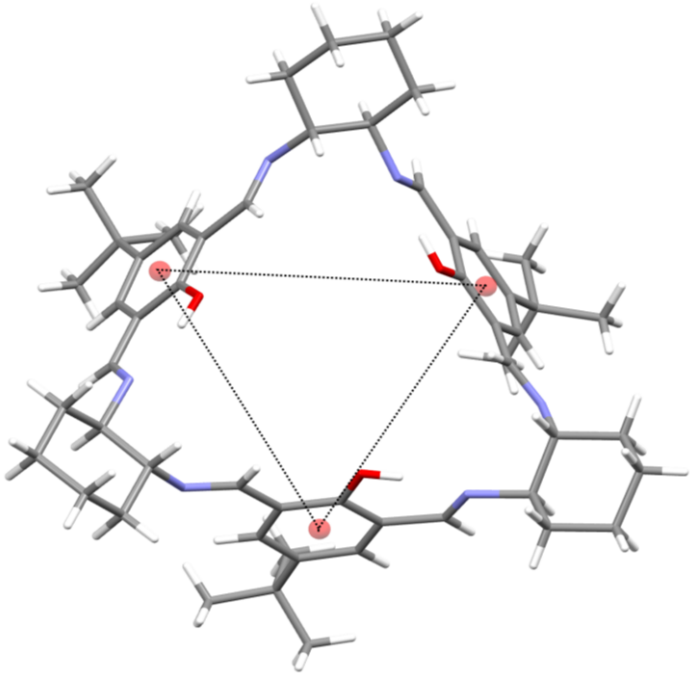


Figure SI_13. Definition of the size of inner cavities calculated.

Table SI_4. The estimated size of the host molecule and its inner cavity in the investigated crystals.

		The height of macrocycle [Å]	Size of the the inner cavity* [Å]			Mean size of the inner cavity [Å]
3a		8.17	6.71	6.25	6.46	6.47
3b	mol1	8.41	6.69	7.27	7.29	7.08
	mol2	8.42	6.82	6.93	7.12	6.96
3c	mol1	9.50	7.41	7.17	7.26	7.28
	mol2	9.57	7.11	7.52	7.28	7.30

Table SI_5. Geometrical parameters of non-covalent interactions and short contacts in the crystals of **3a**, **3b** and **3c**.

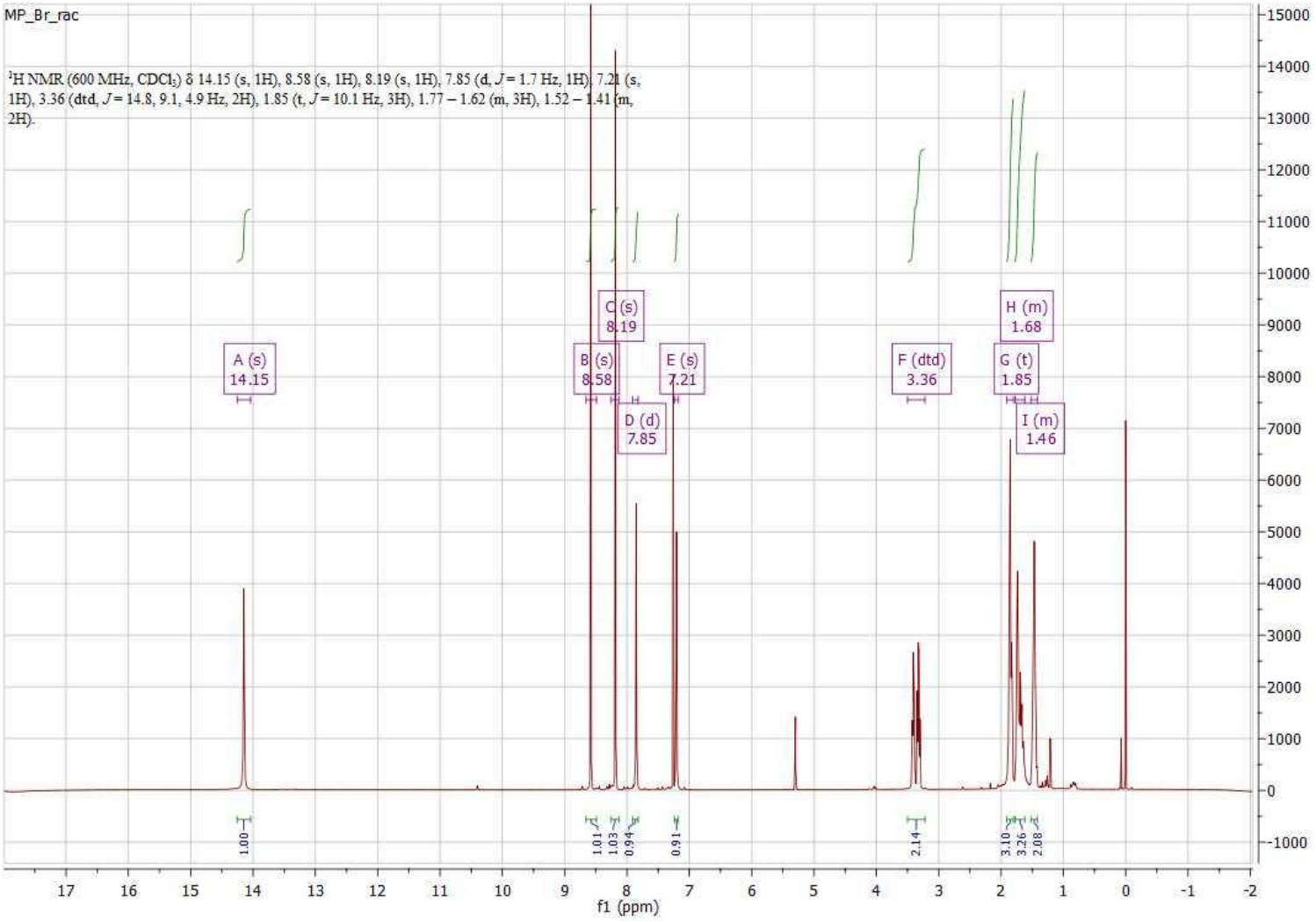
	D-H [Å]	**H…A** [Å]	**D…A** [Å]	**D-H…A** [°]	**Symm**
3a					
C1-H1…O2	1.00	2.50	3.567(4)	150.5	1-x, 1-y, 1-z
C15-H15…O3	1.00	2.57	3.560(5)	172.6	1-x, 1-y, 1-z
C29-H29…O1	1.00	2.66	3.477(4)	164.4	1-x, 1-y, 1-z
C32-H32A…N3	0.99	2.55	3.478(5)	156.7	x, -1+y, z
C41-H41…N5	0.95	2.68	3.495(5)	144.2	1-x, y, 1.5-z
C25-H25…π(C41)	0.95	2.83	3.320(5)	113,2	1-x, y, 1.5-z
C5-H5B…Br3	0.99	2.91	3.596(4)	127.3	x, 1-y, -0.5+z
C32-H32B…Br1	0.99	2.98	3.950(4)	147.5	x, 1-y, -0.5+z
C27-H27…Br1	0.99	3.00	3.944(4)	110.3	1-x, y, 1.5-z
Cl4…Br2			3.157(3)		x, 1-y, -0.5+z
Br2…Cl3			3.846(3)		1-x, y, 1.5-z
Cg_1…Br2			3.934(2)		1-x, y, 1.5-z
Cg_2…Br2			3.666(2)		1-x, y, 1.5-z
3b					
C16-H16…O6	1.00	2.70	3.611(2)	151.2	1.5-x, -0.5+y, 1.5-z

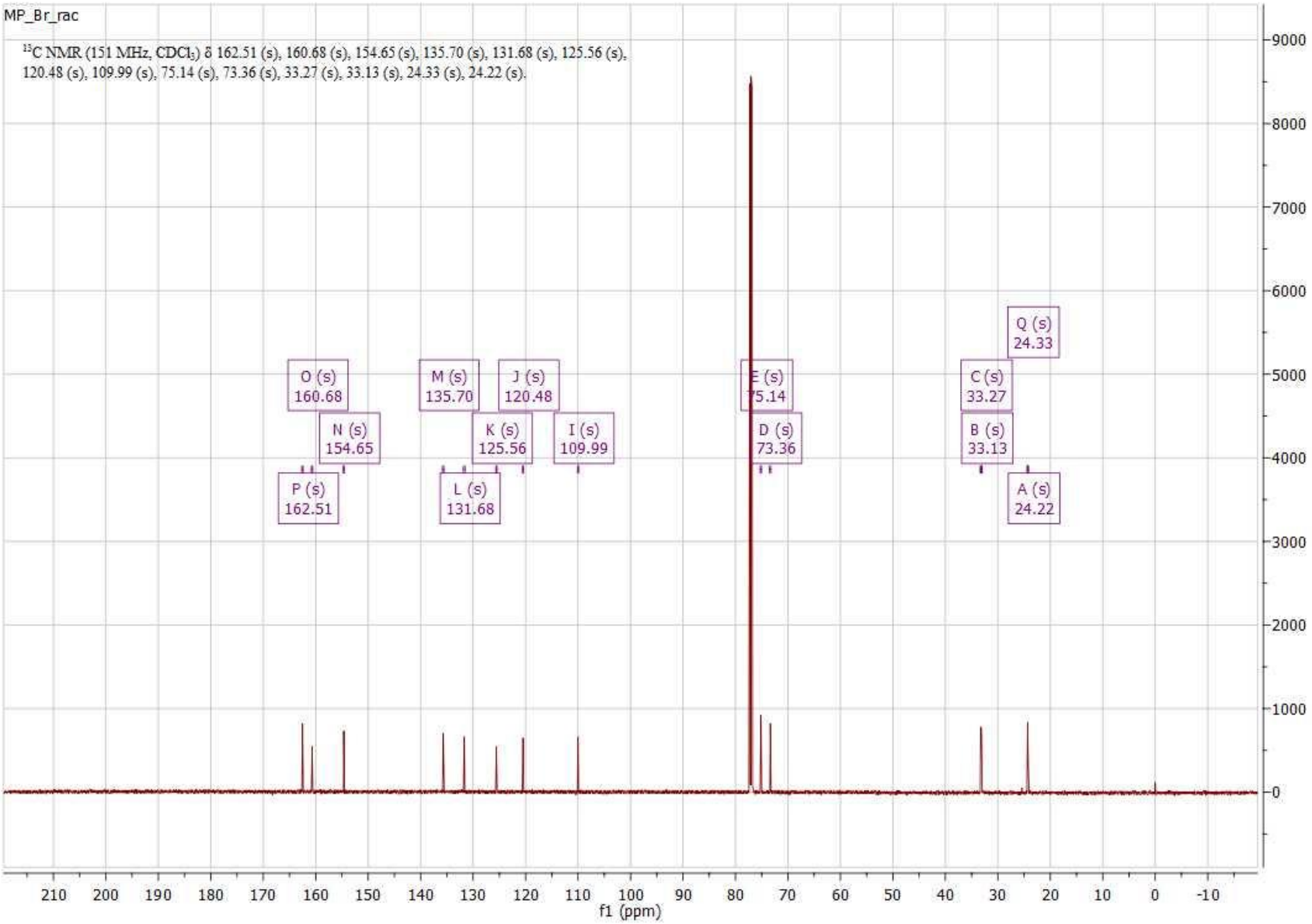
C19-H19A…O5	0.99	2.64	3.512(3)	146.2	1.5-x, -0.5+y, 1.5-z
C20-H20A…O4	0.99	2.69	3.564(3)	148.0	1.5-x, -0.5+y, 1.5-z
C62-H62…O3	1.00	2.50	3.458(2)	160.7	0.5-x, 0.5+y, 1.5-z
C64-H64A…O2	0.99	2.53	3.326(2)	137.5	0.5-x, 0.5+y, 1.5-z
C65-H65A…O1	0.99	2.74	3.519(3)	136.4	0.5-x, 0.5+y, 1.5-z
C11-H11…π(C86)	0.95	2.86	3.611(3)	136.6	
C56-H56…π(C40)	0.95	2.86	3.739(3)	154.6	
C60-H60…π(C41)	0.95	2.89	3.626(3)	135.2	
3c					
C94-H94A..O2	0.99	2.62	3.466(3)	139.0	-0.5+x, 0.5-y, -0.5+z
C109-H109…O3	0.95	2.67	3.440(2)	144.0	0.5+x, 0.5-y, 0.5+z
C39-H39A…π(C101)	0.99	2.71	3.692(3)	173.6	-0.5+x, 0.5-y, -0.5+z
C15-H15A…π (C81)	0.98	2.84	3.775(3)	159.8	
C33-H33c…π (C104)	0.98	2.89	3.811(3)	156.3	
C34-H34A…π (C102)	0.98	2.84	3.814(3)	174.8	
C35-H35A…π (C82)	0.98	2.93	3.910(3)	177.2	
C35-H35B…π (C100)	0.98	2.94	3.893(3)	164.3	
C35-H35C…π (C64)	0.98	2.89	3.843(3)	165.7	
C72-H72C… Cg_3	0.98	2.80	3.782(2)	178.8	
C88-H88B…π (C49)	0.98	2.80	3.748(3)	162.2	
C89-H89C…π (C47)	0.98	3.06	4.020(3)	165.7	
C90-H90A…π (C45)	0.98	2.98	3.946(3)	168.3	
C90-H90B…π (C9)	0.98	2.92	3.860(3)	160.8	

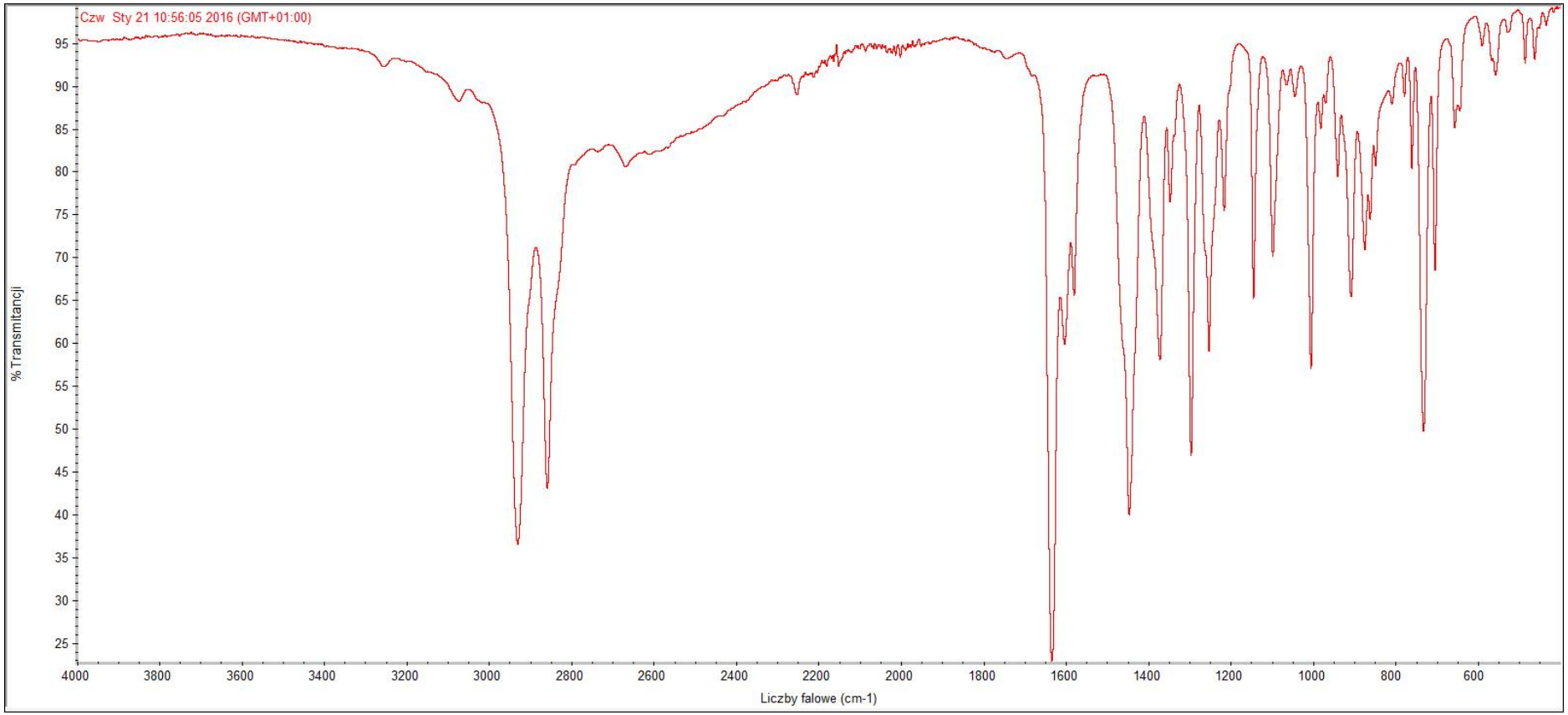
Cg_1 - centroid of the phenyl ring C36-C41; Cg_2 – centroid of the phenyl ring C22-C27; Cg_3 – centroid of the phenyl ring C26-C31.

Copies of ^{1}H NMR, ^{13}C NMR and FT-IR spectra of calixsalens **3a**-**3d**

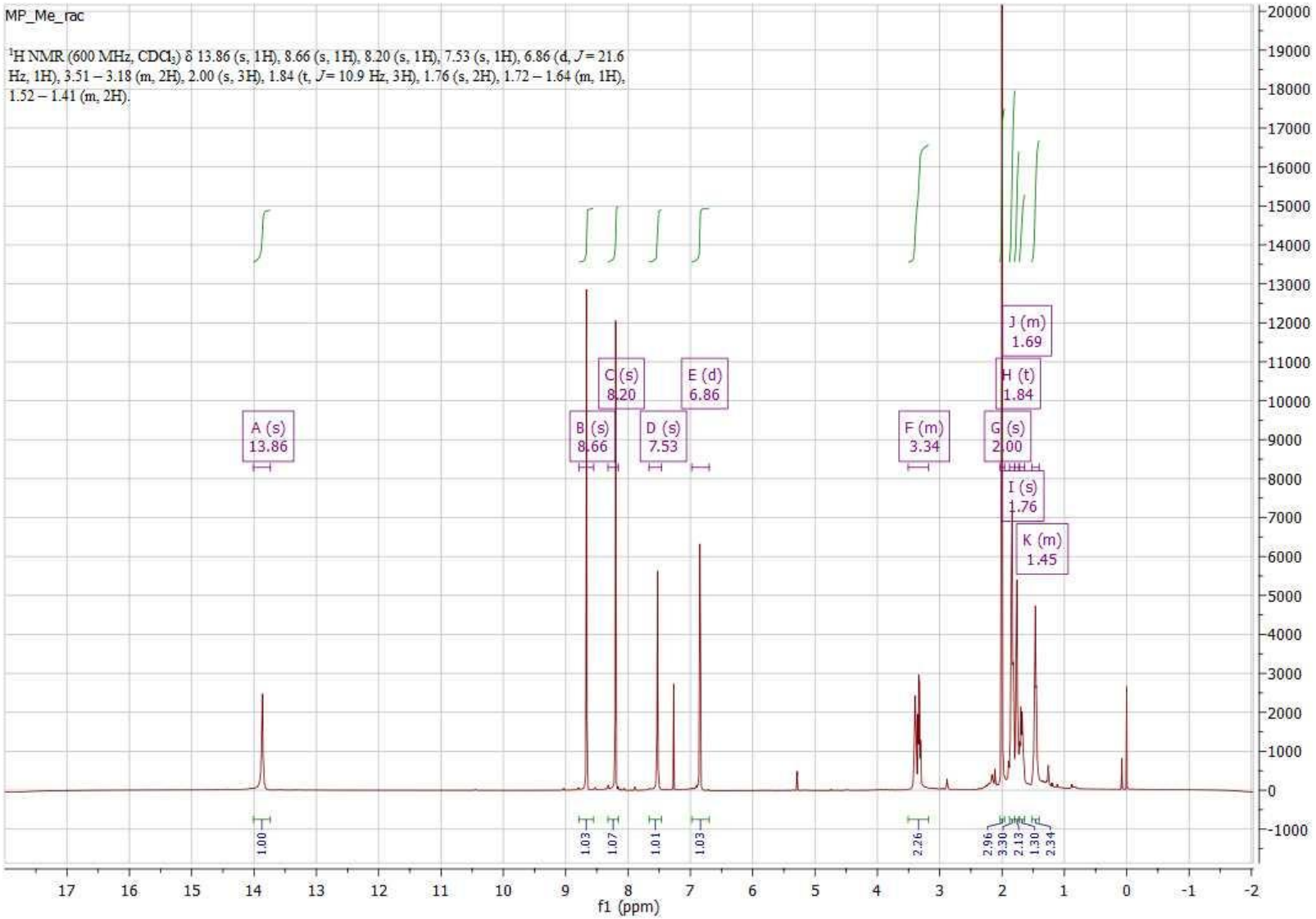
3a

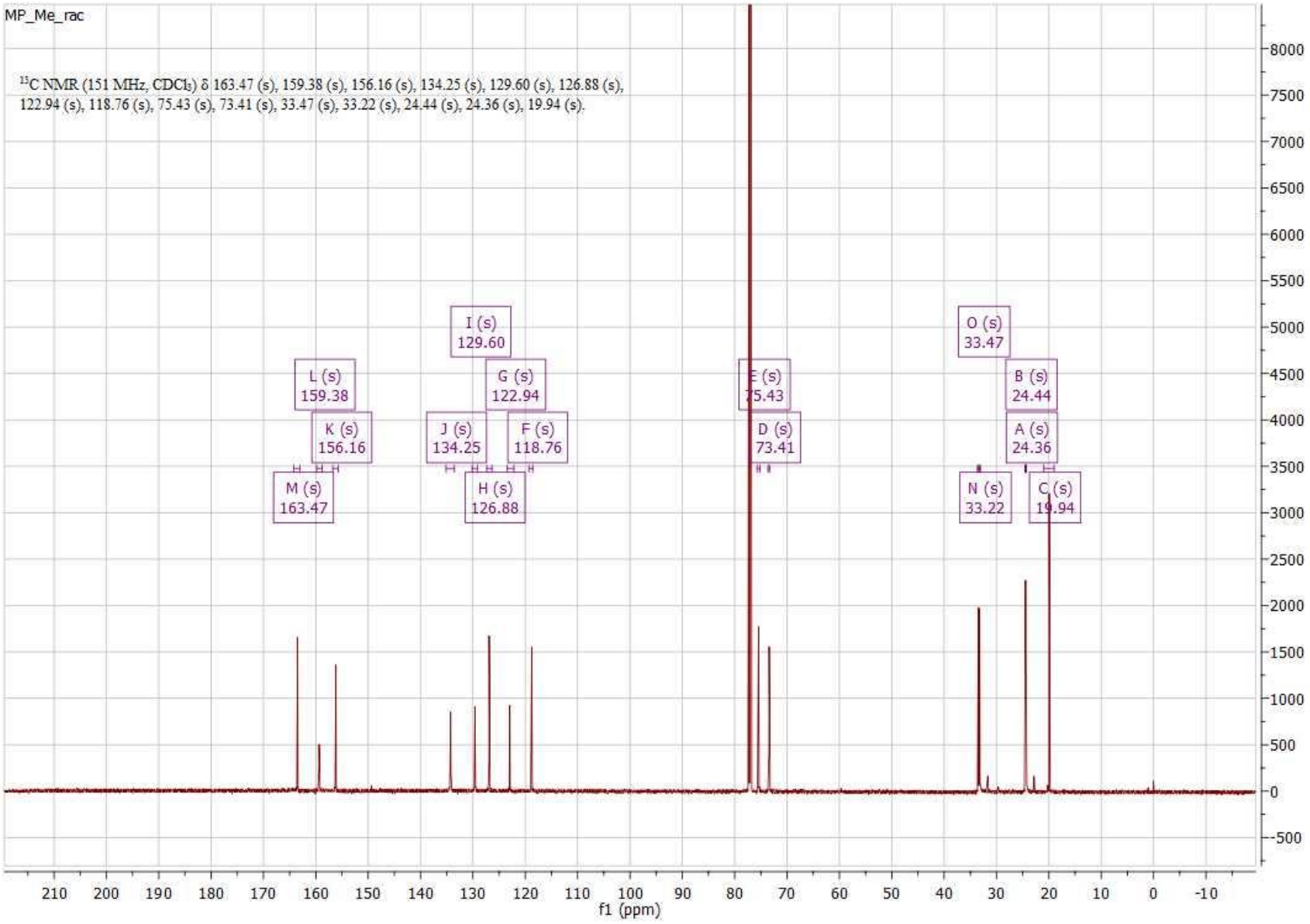


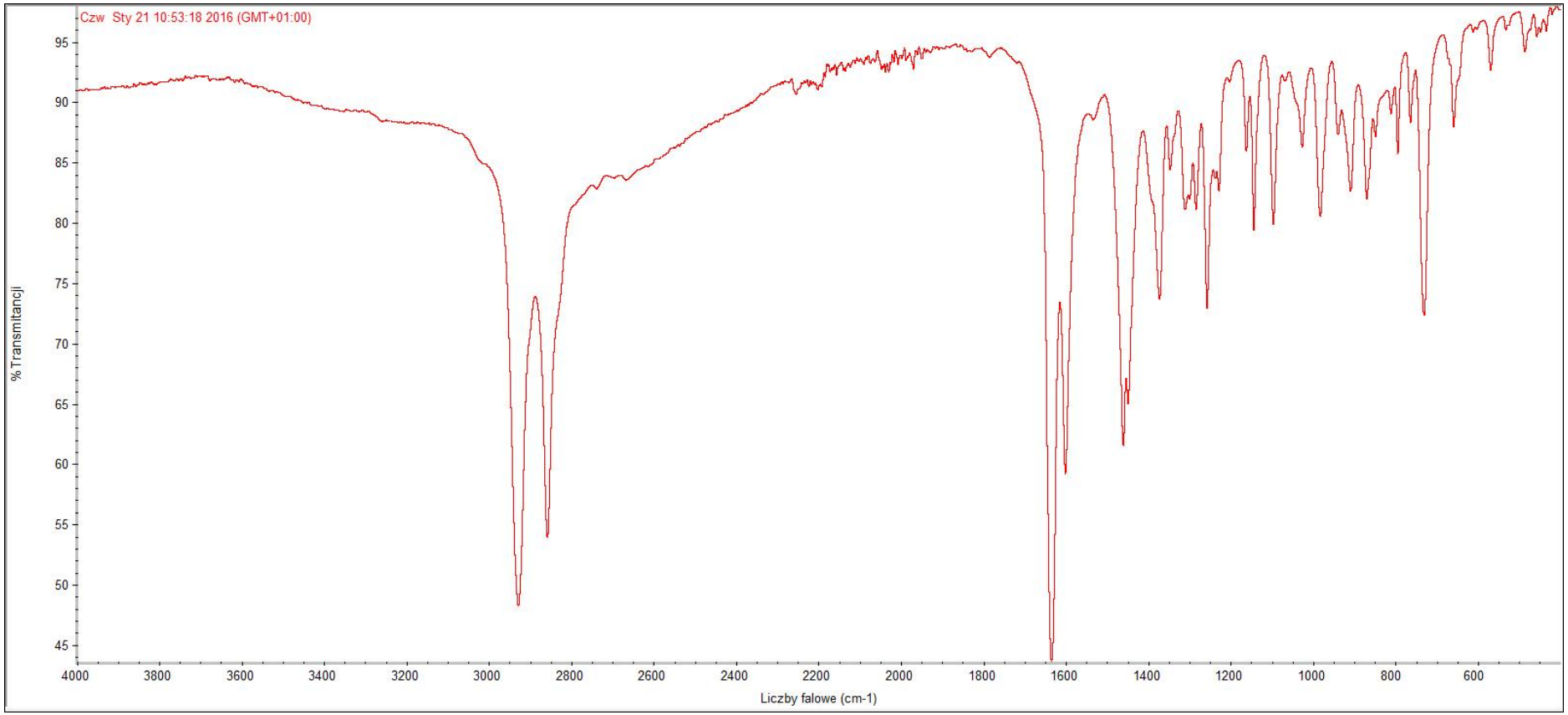

MP_Br_rac
^{13}C NMR (151 MHz, $CDCl_3$) δ 162.51 (s), 160.68 (s), 154.65 (s), 135.70 (s), 131.68 (s), 125.56 (s), 120.48 (s), 109.99 (s), 75.14 (s), 73.36 (s), 33.27 (s), 33.13 (s), 24.33 (s), 24.22 (s).
O (s) 160.68
N (s) 154.65
P (s) 162.51
M (s) 135.70
J (s) 120.48
K (s) 125.56
I (s) 109.99
L (s) 131.68
E (s) 75.14
D (s) 73.36
Q (s) 24.33
C (s) 33.27
B (s) 33.13
A (s) 24.22
f1 (ppm)


Czw Sty 21 10:56:05 2016 (GMT+01:00)
% Transmitancji
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
4000
3800
3600
3400
3200
3000
2800
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
Liczby falowe (cm-1)

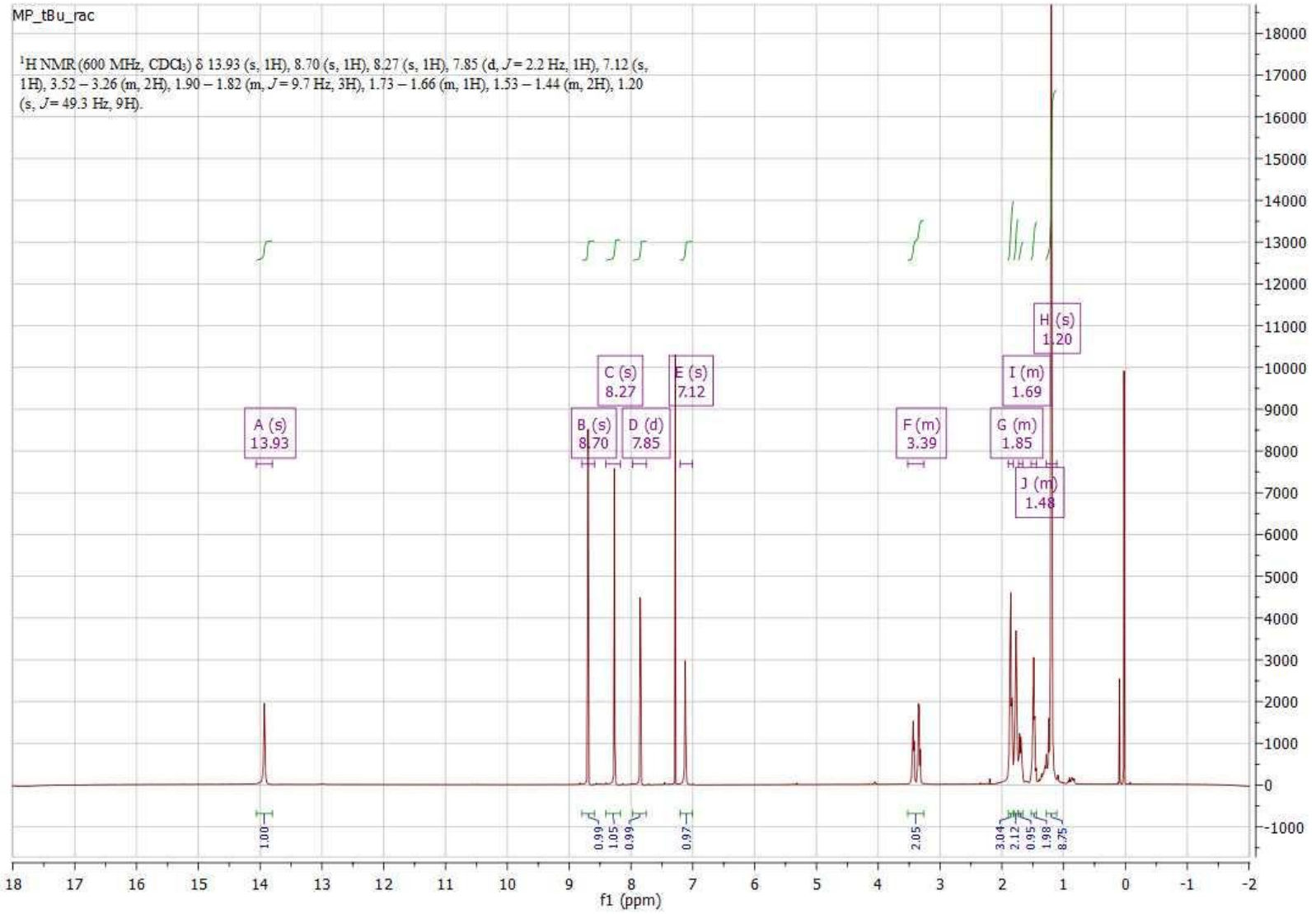
3b

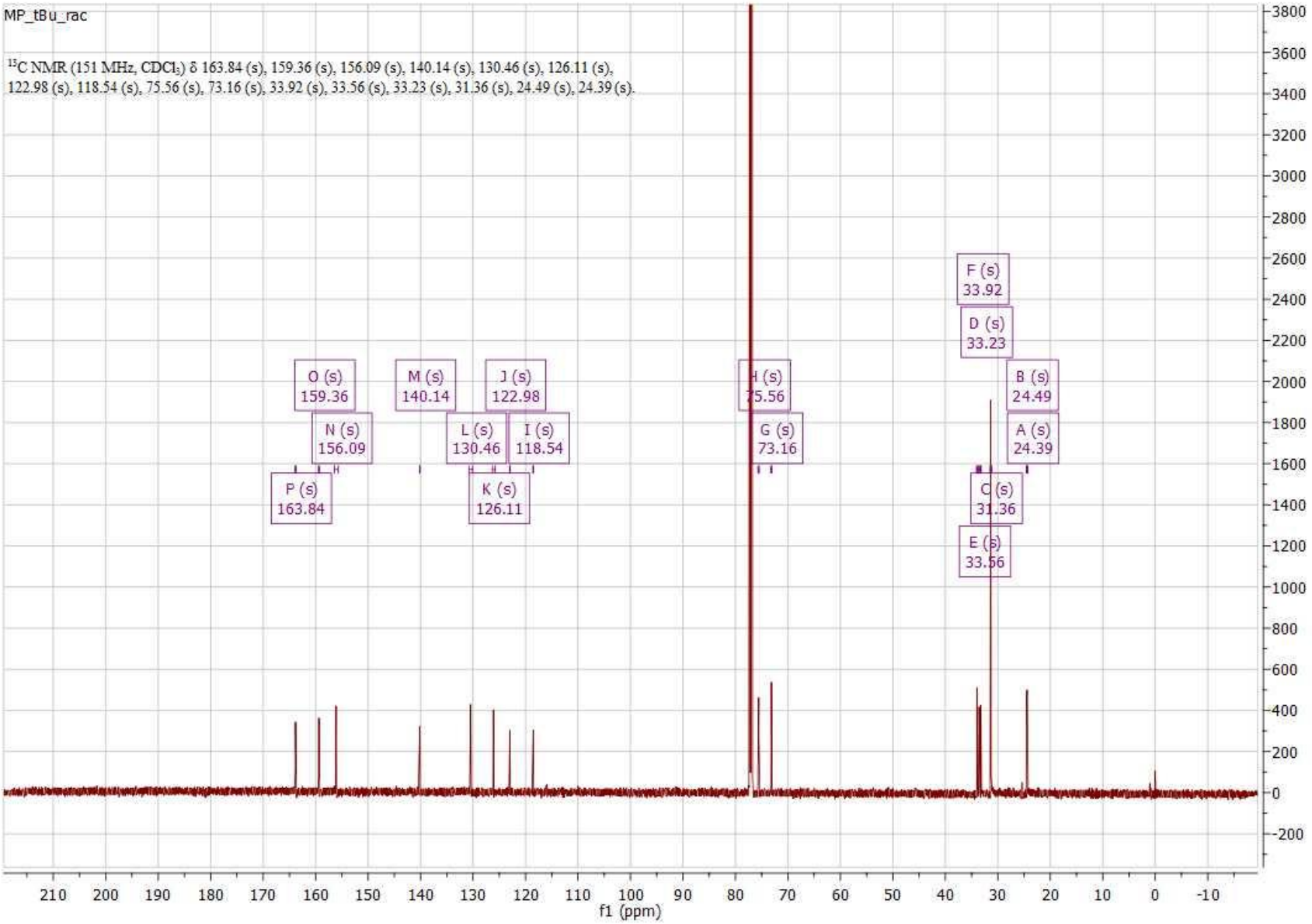

MP_Me_rac
¹H NMR (600 MHz, CDCl₃) δ 13.86 (s, 1H), 8.66 (s, 1H), 8.20 (s, 1H), 7.53 (s, 1H), 6.86 (d, J = 21.6 Hz, 1H), 3.51 – 3.18 (m, 2H), 2.00 (s, 3H), 1.84 (t, J = 10.9 Hz, 3H), 1.76 (s, 2H), 1.72 – 1.64 (m, 1H), 1.52 – 1.41 (m, 2H).
A (s) 13.86
B (s) 8.66
C (s) 8.20
D (s) 7.53
E (d) 6.86
F (m) 3.34
G (s) 2.00
H (t) 1.84
I (s) 1.76
J (m) 1.69
K (m) 1.45
1.00
1.03
1.07
1.01
1.03
2.26
2.96
3.30
2.13
1.30
2.34
f1 (ppm)

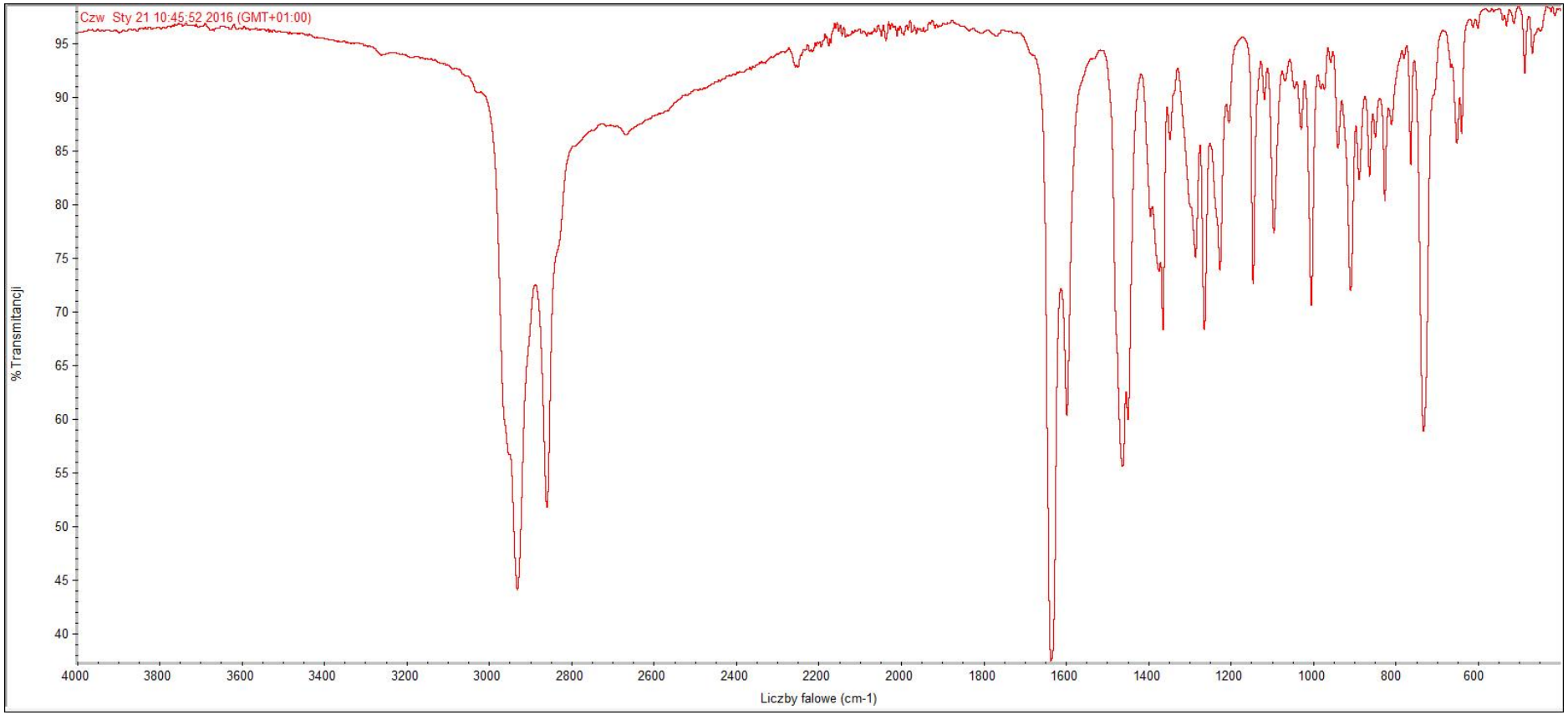

MP_Me_rac
^{13}C NMR (151 MHz, $CDCl_3$) δ 163.47 (s), 159.38 (s), 156.16 (s), 134.25 (s), 129.60 (s), 126.88 (s), 122.94 (s), 118.76 (s), 75.43 (s), 73.41 (s), 33.47 (s), 33.22 (s), 24.44 (s), 24.36 (s), 19.94 (s).
I (s) 129.60
L (s) 159.38
G (s) 122.94
K (s) 156.16
J (s) 134.25
F (s) 118.76
M (s) 163.47
H (s) 126.88
E (s) 75.43
D (s) 73.41
O (s) 33.47
B (s) 24.44
A (s) 24.36
N (s) 33.22
C (s) 19.94
f1 (ppm)


Czw Sty 21 10:53:18 2016 (GMT+01:00)
% Transmitancji
95
90
85
80
75
70
65
60
55
50
45
4000
3800
3600
3400
3200
3000
2800
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
Liczby falowe (cm-1)

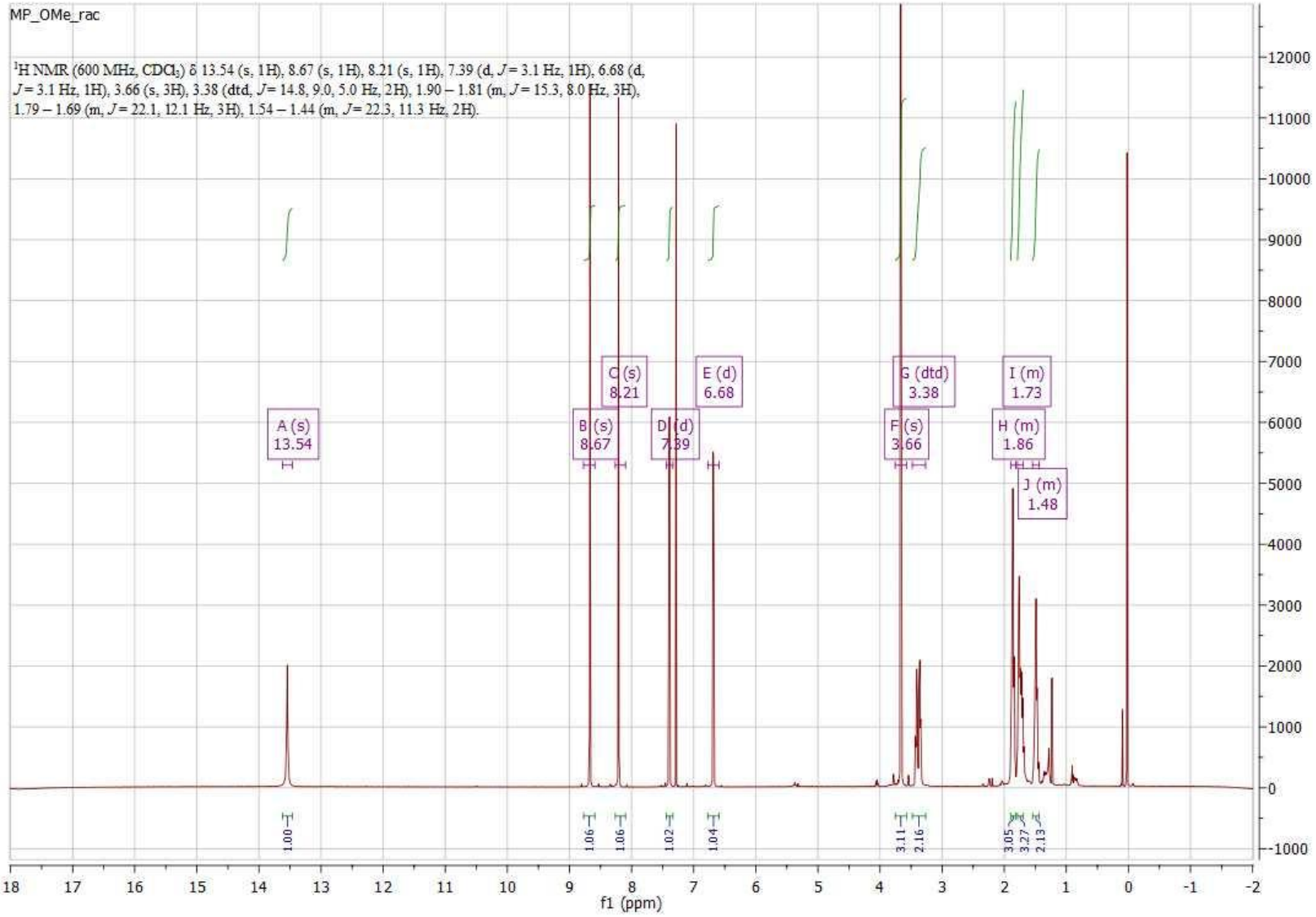
3c

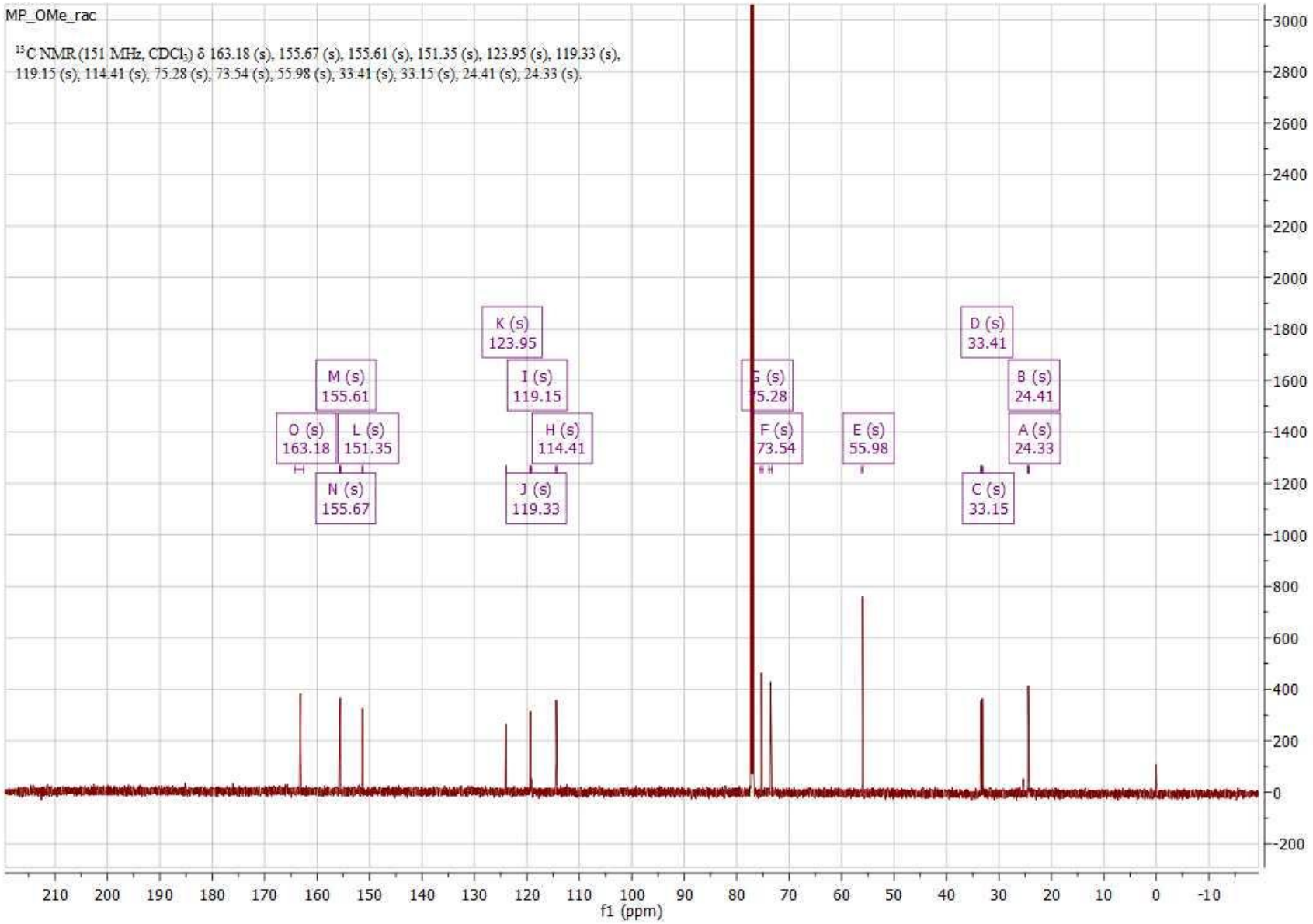

MP_tBu_rac
^{1}H NMR (600 MHz, $CDCl_3$) δ 13.93 (s, 1H), 8.70 (s, 1H), 8.27 (s, 1H), 7.85 (d, J = 2.2 Hz, 1H), 7.12 (s, 1H), 3.52 – 3.26 (m, 2H), 1.90 – 1.82 (m, J = 9.7 Hz, 3H), 1.73 – 1.66 (m, 1H), 1.53 – 1.44 (m, 2H), 1.20 (s, J = 49.3 Hz, 9H).
A (s) 13.93
B (s) 8.70
C (s) 8.27
D (d) 7.85
E (s) 7.12
F (m) 3.39
G (m) 1.85
H (s) 1.20
I (m) 1.69
J (m) 1.48
1.00
0.99
1.05
0.99
0.97
2.05
3.04
2.12
0.95
1.98
8.75
f1 (ppm)

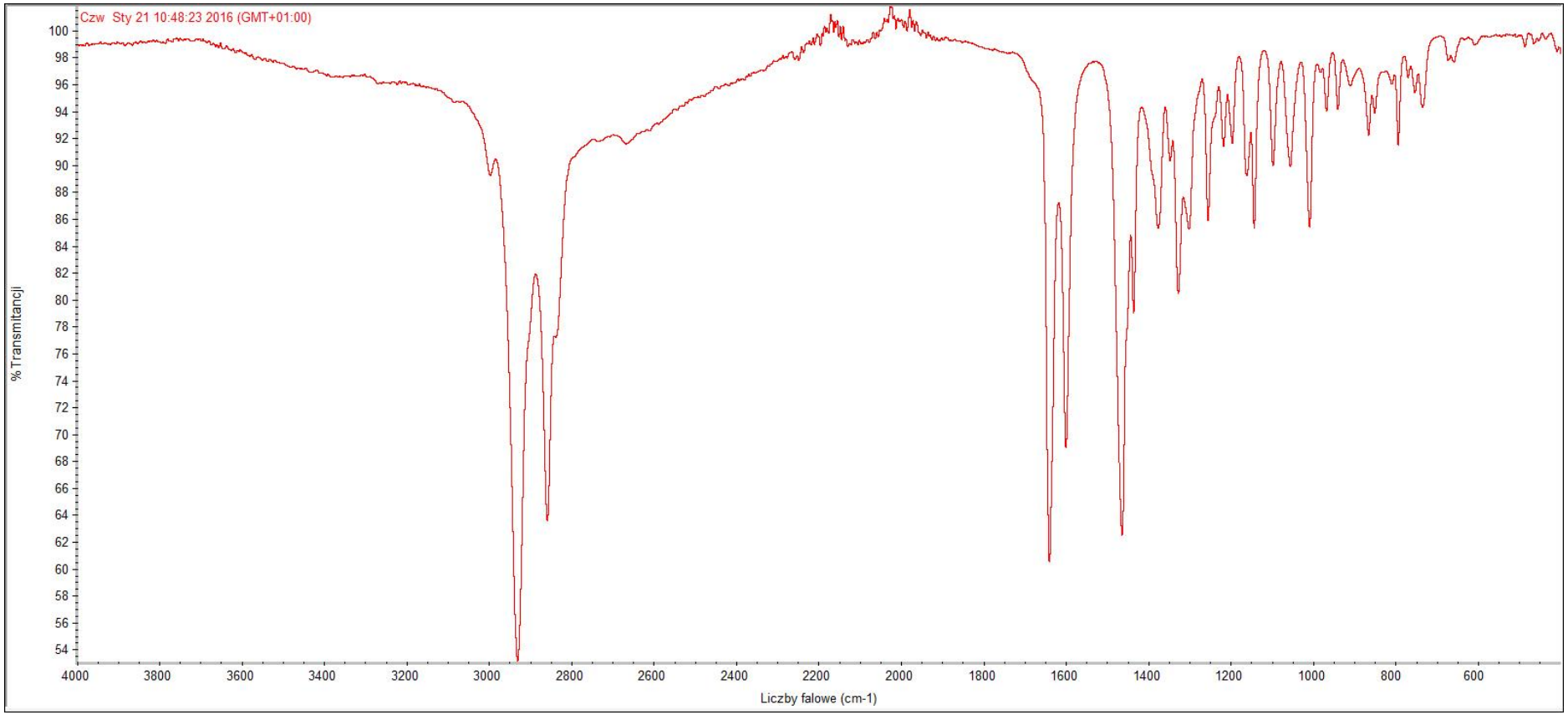

MP_tBu_rac
^{13}C NMR (151 MHz, $CDCl_3$) δ 163.84 (s), 159.36 (s), 156.09 (s), 140.14 (s), 130.46 (s), 126.11 (s), 122.98 (s), 118.54 (s), 75.56 (s), 73.16 (s), 33.92 (s), 33.56 (s), 33.23 (s), 31.36 (s), 24.49 (s), 24.39 (s).
O (s) 159.36
M (s) 140.14
J (s) 122.98
N (s) 156.09
L (s) 130.46
I (s) 118.54
P (s) 163.84
K (s) 126.11
H (s) 75.56
G (s) 73.16
F (s) 33.92
D (s) 33.23
B (s) 24.49
A (s) 24.39
C (s) 31.36
E (s) 33.56
f1 (ppm)


Czw Sty 21 10:45:52 2016 (GMT+01:00)
% Transmitancji
95
90
85
80
75
70
65
60
55
50
45
40
4000
3800
3600
3400
3200
3000
2800
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
Liczby falowe (cm-1)

3d


MP_OMe_rac
¹H NMR (600 MHz, CDCl₃) δ 13.54 (s, 1H), 8.67 (s, 1H), 8.21 (s, 1H), 7.39 (d, J = 3.1 Hz, 1H), 6.68 (d, J = 3.1 Hz, 1H), 3.66 (s, 3H), 3.38 (dtd, J = 14.8, 9.0, 5.0 Hz, 2H), 1.90 – 1.81 (m, J = 15.3, 8.0 Hz, 3H), 1.79 – 1.69 (m, J = 22.1, 12.1 Hz, 3H), 1.54 – 1.44 (m, J = 22.3, 11.3 Hz, 2H).
A (s) 13.54
B (s) 8.67
C (s) 8.21
D (d) 7.39
E (d) 6.68
F (s) 3.66
G (dtd) 3.38
H (m) 1.86
I (m) 1.73
J (m) 1.48
1.00
1.06
1.06
1.02
1.04
3.11
2.16
3.05
3.27
2.13
f1 (ppm)


MP_OMe_rac
^{13}C NMR (151 MHz, CDCl$_3$) δ 163.18 (s), 155.67 (s), 155.61 (s), 151.35 (s), 123.95 (s), 119.33 (s), 119.15 (s), 114.41 (s), 75.28 (s), 73.54 (s), 55.98 (s), 33.41 (s), 33.15 (s), 24.41 (s), 24.33 (s).
K (s) 123.95
M (s) 155.61
I (s) 119.15
O (s) 163.18
L (s) 151.35
H (s) 114.41
N (s) 155.67
J (s) 119.33
F (s) 73.54
E (s) 55.98
D (s) 33.41
B (s) 24.41
A (s) 24.33
C (s) 33.15
f1 (ppm)


Czw Sty 21 10:48:23 2016 (GMT+01:00)
% Transmitancji
100
98
96
94
92
90
88
86
84
82
80
78
76
74
72
70
68
66
64
62
60
58
56
54
4000
3800
3600
3400
3200
3000
2800
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
Liczby falowe (cm-1)

Cartesian coordinates for

3a	C	-4.17421300	6.65709900	-2.90872600
	C	-2.72432300	6.97409700	-3.26660500
	C	-1.76487900	6.47284200	-2.19256900
	C	-1.95237700	4.97915100	-1.94830100
	C	-3.41635500	4.70059500	-1.53771400
	C	-4.37107700	5.17427400	-2.62489900
	H	-4.84830400	6.97302900	-3.71152300
	H	-4.46317900	7.23529900	-2.02174200
	H	-2.58883900	8.04777800	-3.42168300
	H	-2.47814500	6.48934700	-4.21999700
	H	-1.92808100	7.00816000	-1.24837800
	H	-0.72525900	6.65634200	-2.48299700
	H	-1.75708500	4.43718700	-2.89331300
	N	-1.07009100	4.53468200	-0.88813500
	N	-3.54534200	3.28260800	-1.24976900
	H	-3.59032000	5.27984300	-0.61399700
	H	-5.40190800	4.96552600	-2.32143500
	H	-4.18917500	4.58748600	-3.53440800
	C	-0.12773300	3.74906300	-1.23438700
	C	0.76825500	3.10163700	-0.27487800
	C	0.39491400	3.01478900	1.06906000
	C	1.20088600	2.37114200	1.99411400
	C	2.41285100	1.82573900	1.60311800
	C	2.83135000	1.92002300	0.26949800
	C	1.99134400	2.53893200	-0.68766400
	C	4.11883600	1.37251500	-0.10229000

	N	4.55290200	1.35497400	-1.31178400
	C	5.78040000	0.62476000	-1.56119200
	O	2.34597200	2.61967000	-1.97093600
	C	5.42563000	-0.81315200	-2.02733700
	C	6.65479500	1.33332800	-2.58415600
	C	7.93968200	0.54423700	-2.78251000
	C	7.65222000	-0.89357300	-3.19733500
	C	6.72133400	-1.60069800	-2.21374100
	C	-3.37271500	2.88653200	-0.04604500
	C	-3.30830100	1.48147900	0.31497400
	C	-3.01547100	1.12380100	1.63664700
	C	-3.45390700	0.47189600	-0.67319400
	C	-3.34164900	-0.88048500	-0.30992500
	C	-3.08574000	-1.20907500	1.02739900
	C	-2.91596900	-0.21874200	1.98864600
	H	0.02375800	3.47656600	-2.28874300
	H	-0.54079700	3.46883200	1.35861500
	H	3.05881400	1.31438800	2.31463500
	H	4.68884600	0.89505500	0.70658400
	H	6.34445000	0.51292400	-0.61888400
	H	3.21777900	2.14658900	-2.06544300
	H	4.90756500	-0.72853900	-3.00137500
	N	4.57795700	-1.40585600	-1.00490700
	H	6.85605300	2.35601800	-2.25345300
	H	6.10220100	1.41121400	-3.52984700
	H	8.50604300	0.54238700	-1.84201000
	H	8.57654200	1.03510100	-3.52507000

	H	8.58728500	-1.45226600	-3.29163600
	H	7.18992300	-0.89745700	-4.19310200
	H	7.20749300	-1.70020900	-1.23491800
	H	6.48337700	-2.61518300	-2.54880800
	H	-3.23102200	3.60071000	0.77779200
	O	-3.69699700	0.77230300	-1.94798400
	H	-2.95379700	-2.25709500	1.26492600
	C	-3.37914800	-1.93649700	-1.32724000
	N	-3.52282700	-3.16196100	-1.00956700
	C	-3.39797400	-4.13726600	-2.07104800
	C	-2.33852700	-5.18171900	-1.63510700
	C	-4.73231400	-4.84050100	-2.33607800
	C	-4.57044600	-5.94552100	-3.37097600
	C	-3.52382500	-6.96106200	-2.92896000
	C	-2.18501700	-6.29340400	-2.65949600
	H	-2.84465500	1.91576400	2.36464700
	H	-3.73204800	1.77217300	-2.02113500
	H	-3.23624300	-1.61209900	-2.36805600
	H	-3.05719200	-3.66987100	-3.01238700
	N	-1.08719400	-4.49459800	-1.39352300
	H	-2.69667000	-5.59969500	-0.67924600
	H	-5.10177700	-5.25661600	-1.39087500
	H	-5.47111200	-4.10010400	-2.65855800
	H	-5.52698800	-6.44310800	-3.55272100
	H	-4.26600700	-5.50220600	-4.32707300
	H	-3.86831600	-7.45564400	-2.01090800
	H	-3.40801800	-7.75006200	-3.67857600

	H	-1.44968500	-7.02367800	-2.30828900
	H	-1.77470000	-5.86566700	-3.58414900
	C	-0.88490100	-4.08842000	-0.20329500
	C	0.27657300	-3.30632400	0.17522400
	C	0.43142300	-2.92164300	1.51159600
	C	1.26781400	-2.95446600	-0.77844900
	C	2.42103600	-2.25840400	-0.36660100
	C	2.56006000	-1.91882700	0.97926500
	C	1.57899300	-2.23905400	1.90709500
	O	1.14792900	-3.29632700	-2.05890500
	H	-1.58441400	-4.34140200	0.60446500
	H	-0.33243200	-3.21788000	2.22470000
	C	3.41053500	-1.79572800	-1.34395700
	H	3.45868800	-1.38185600	1.25931800
	H	0.28616300	-3.79319800	-2.13887100
	H	3.06827100	-1.76638400	-2.38965800
	Br	0.65434100	2.23513600	3.81134500
	Br	-2.44016200	-0.71621700	3.77514500
	Br	1.84174800	-1.76954300	3.73471700
3a(1)	C	-3.83551500	-4.43100700	-3.40731100
	C	-3.46952400	-5.38561900	-4.53440600
	C	-2.32285600	-4.83084700	-5.37060600
	C	-1.12113500	-4.48974000	-4.50021900
	C	-1.49712500	-3.51678700	-3.38008700
	C	-2.62807800	-4.11403600	-2.52143300
	H	-4.63515000	-4.83970500	-2.78176000
	H	-4.21900200	-3.48816400	-3.82240500

	H	-4.34420700	-5.58506200	-5.16117600
	H	-3.17252400	-6.35275700	-4.10667500
	H	-2.65935300	-3.92402900	-5.89152900
	H	-2.03291000	-5.54189300	-6.15031600
	H	-0.30948400	-4.05810600	-5.09351300
	H	-0.71697400	-5.40267800	-4.04101500
	N	-0.29192300	-3.10732000	-2.67835600
	H	-1.87992200	-2.60170100	-3.86029800
	N	-3.00920000	-3.30263500	-1.37326900
	H	-2.25907800	-5.06909100	-2.11417900
	C	-3.25621500	-2.06404600	-1.55536200
	C	-3.54213400	-1.17857800	-0.42945100
	C	-3.55541100	-1.67826000	0.87467300
	C	-3.75113100	-0.83561700	1.95634000
	C	-3.90909700	0.52809800	1.76104500
	C	-3.90394500	1.06275200	0.46793600
	C	-3.73342500	0.20096400	-0.64482300
	C	-3.98044900	2.49872700	0.29008800
	N	-3.99367900	3.05797000	-0.86452500
	C	-3.84199600	4.49810100	-0.89921700
	O	-3.72399600	0.66667500	-1.89427900
	C	-2.36349600	4.82144400	-1.19659700
	C	-4.74749000	5.15454100	-1.93067400
	C	-4.54091700	6.66478700	-1.93688500
	C	-3.07804800	7.02799600	-2.16825900
	C	-2.16026800	6.33557200	-1.16732100
	C	-0.11115600	-3.34451100	-1.43066800

	C	1.07963900	-2.89145900	-0.73355700
	C	1.21895400	-3.17009100	0.62942100
	C	2.08369700	-2.14335000	-1.39951900
	C	3.20688400	-1.69217400	-0.67807200
	C	3.32665400	-2.01208900	0.67597500
	C	2.34175100	-2.74244900	1.32287900
	H	-3.22439000	-1.57194000	-2.53787100
	H	-3.39912400	-2.74321000	1.00646300
	H	-4.02544300	1.19649200	2.60940800
	H	-3.98056300	3.10239800	1.21088000
	H	-4.05747600	4.91979400	0.09952600
	H	-3.83153300	1.65629700	-1.83778200
	H	-2.13281500	4.45664300	-2.21453700
	N	-1.55156500	4.14949300	-0.20374500
	H	-5.79122200	4.90081700	-1.72019100
	H	-4.52010600	4.73510400	-2.91986200
	H	-4.86799100	7.07651800	-0.97236700
	H	-5.17580600	7.13100500	-2.69661000
	H	-2.94051300	8.11263400	-2.11730500
	H	-2.78860900	6.73146500	-3.18573100
	H	-2.35767900	6.69541200	-0.14903200
	H	-1.10919100	6.55997400	-1.37734200
	H	-0.85244600	-3.86843500	-0.81333400
	O	1.99123700	-1.84697100	-2.69487200
	H	4.20429500	-1.65501900	1.20493100
	C	4.17765300	-0.80848700	-1.31719200
	N	5.26300900	-0.46148500	-0.74377900

	C	6.02862500	0.59331500	-1.36065300
	C	5.97868700	1.82241900	-0.41433700
	C	7.47882300	0.16950400	-1.57376900
	C	8.31898500	1.31310100	-2.12601500
	C	8.25197800	2.53533500	-1.21813000
	C	6.81033300	2.96515500	-0.98065900
	H	0.43230700	-3.71973000	1.13744800
	H	1.12749800	-2.23271900	-3.01494200
	H	3.88214000	-0.40655100	-2.29824900
	H	5.59019500	0.90452200	-2.32885000
	N	4.59473000	2.21747300	-0.23083100
	H	6.40780500	1.48895500	0.54695100
	H	7.88316600	-0.17317100	-0.61251100
	H	7.50284600	-0.69631300	-2.24312800
	H	9.35576200	0.98893600	-2.26011300
	H	7.95173600	1.58429100	-3.12544200
	H	8.72267900	2.29655200	-0.25452700
	H	8.82823800	3.36380500	-1.64145600
	H	6.76003200	3.82159200	-0.30058400
	H	6.35425100	3.29346500	-1.92430400
	C	3.95154100	1.67580000	0.73923100
	C	2.52879500	1.86093200	0.94093000
	C	1.88949100	1.16982400	1.97736000
	C	1.76985800	2.69429600	0.08267200
	C	0.39089100	2.85732200	0.31717700
	C	-0.21245100	2.16436200	1.36743600
	C	0.52542800	1.31265500	2.17734100

	O	2.32787400	3.34689300	-0.93844100
	H	4.45860900	1.01137500	1.45585900
	H	2.47451300	0.51401900	2.61563500
	C	-0.42738800	3.67873300	-0.57441700
	H	-1.27990300	2.29039800	1.51375500
	H	3.29056700	3.09313500	-0.95498600
	H	-0.02984300	3.82667400	-1.59109600
	Br	-3.77556100	-1.55096800	3.71728700
	Br	2.51255400	-3.12052200	3.17779700
	Br	-0.35672000	0.30895400	3.52809400
3a(2)	C	4.05425900	5.66256700	-1.84907100
	C	3.77152800	7.13436800	-2.18188300
	C	2.50855300	7.28228500	-3.04183800
	C	1.30364000	6.59732800	-2.38249100
	C	1.59815300	5.11693100	-2.06581700
	C	2.84956000	4.98326100	-1.16379600
	H	4.92915500	5.57294700	-1.19414300
	H	4.29043900	5.10554200	-2.76598800
	H	4.63740700	7.56927800	-2.69530200
	H	3.64510800	7.70222200	-1.24857800
	H	2.68464200	6.83306800	-4.02959000
	H	2.28553900	8.34176400	-3.21604400
	H	0.41987000	6.65237600	-3.02844000
	H	1.04307900	7.11574200	-1.44822300
	N	0.39532000	4.44531600	-1.56730100
	H	1.84507000	4.61202400	-3.00851000
	N	3.13773600	3.57501500	-0.93514400

	H	2.67104300	5.49809300	-0.20330500
	C	3.42477300	3.17310700	0.25061200
	C	3.72591900	1.78331900	0.56301200
	C	4.07786000	1.43829200	1.87772200
	C	4.35380700	0.11785200	2.20076100
	C	4.26836700	-0.88021000	1.23498700
	C	3.91230300	-0.57368900	-0.08301700
	C	3.64991400	0.76991100	-0.43231600
	C	3.79515800	-1.64495900	-1.09269900
	N	4.10306800	-2.84914900	-0.80661200
	C	3.98355500	-3.89514600	-1.82690800
	O	3.32977200	1.05922300	-1.70319400
	C	2.59768500	-3.98941600	-2.51661700
	C	5.11269400	-3.76830100	-2.87009000
	C	5.09406400	-4.92988700	-3.87249900
	C	3.72195700	-5.05463600	-4.54913400
	C	2.59603300	-5.16921900	-3.51240700
	C	-0.00232000	4.57844900	-0.35320000
	C	-1.20832200	3.91972300	0.13618600
	C	-1.60307300	4.09896900	1.47074700
	C	-1.98349900	3.08427600	-0.71656100
	C	-3.13459400	2.44029200	-0.20634000
	C	-3.49973400	2.64396200	1.12881000
	C	-2.74027600	3.46676000	1.95487700
	H	3.44830900	3.87589200	1.09746600
	H	4.13297600	2.21105200	2.63858600
	H	4.46790800	-1.91798500	1.47728900

	H	3.42425200	-1.32307100	-2.07251200
	H	4.11830300	-4.84521700	-1.29357200
	H	3.17936700	2.04588100	-1.75840000
	H	2.40461600	-3.06153900	-3.08570000
	N	1.57590500	-4.21294900	-1.50628500
	H	6.07405600	-3.71961000	-2.34500400
	H	4.99843700	-2.81427500	-3.40493100
	H	5.32708100	-5.86697400	-3.34668200
	H	5.88121600	-4.78942900	-4.62404900
	H	3.70171700	-5.92527600	-5.21666100
	H	3.54744500	-4.17240100	-5.18242000
	H	2.70057300	-6.10151300	-2.94092700
	H	1.61712100	-5.21206900	-4.00548300
	H	0.54218400	5.18533300	0.38281900
	O	-1.64696400	2.89117200	-1.99738400
	H	-4.38740900	2.14307800	1.49829800
	C	-3.92978800	1.56730300	-1.08543800
	N	-4.98106500	0.96661200	-0.68113100
	C	-5.69865500	0.14575900	-1.64260100
	C	-5.78981300	-1.30727600	-1.12179100
	C	-7.10851600	0.73007100	-1.85830500
	C	-7.95385200	-0.13812000	-2.79974600
	C	-8.03607200	-1.58477000	-2.29451200
	C	-6.63686300	-2.17598100	-2.07370700
	H	-1.01325200	4.73553800	2.12362300
	H	-0.80307400	3.41483600	-2.16262800
	H	-3.55895700	1.46888000	-2.11297400

	H	-5.17352800	0.11470200	-2.61521800
	N	-4.45313100	-1.87691300	-1.00934900
	H	-6.27528400	-1.28051000	-0.13181600
	H	-7.60100800	0.81993300	-0.88063600
	H	-7.00929400	1.74850700	-2.25266600
	H	-8.95880100	0.29011700	-2.89969200
	H	-7.50876600	-0.12980300	-3.80516600
	H	-8.59587300	-1.60820600	-1.34835400
	H	-8.59423700	-2.20890100	-3.00313200
	H	-6.70383900	-3.19029100	-1.66154300
	H	-6.10833500	-2.26207300	-3.03302700
	C	-4.12130800	-2.49478000	0.06530000
	C	-2.81864300	-3.12783100	0.23942100
	C	-2.55755000	-3.84983100	1.41372500
	C	-1.81301800	-3.03037200	-0.76131500
	C	-0.55983000	-3.65041400	-0.55567600
	C	-0.33782200	-4.37409500	0.62175700
	C	-1.32951500	-4.47184000	1.59219200
	O	-2.02780600	-2.36406800	-1.90562800
	H	-4.81975300	-2.57883300	0.91070700
	H	-3.32349100	-3.92057100	2.18017200
	C	0.51115800	-3.51205300	-1.55873700
	H	0.62935200	-4.84469800	0.75708000
	H	-2.96740500	-2.01605300	-1.87594500
	H	0.33868500	-2.75960800	-2.33964300
	Br	4.84239600	-0.33136900	3.99498700
	Br	-3.26196400	3.72981100	3.77677500

	Br	-0.99628200	-5.46146500	3.19600000
3a(3)	C	-3.75401400	-5.59597800	-1.83469500
	C	-3.24943700	-6.96800400	-2.30344200
	C	-2.06323800	-6.79337300	-3.26631800
	C	-0.94481300	-5.99516700	-2.57945300
	C	-1.45884200	-4.61029700	-2.11523600
	C	-2.63401800	-4.79199600	-1.13270800
	H	-4.58925100	-5.68912400	-1.13216100
	H	-4.10372600	-5.00844400	-2.69636100
	H	-4.06267000	-7.52017700	-2.79008500
	H	-2.92297700	-7.55306800	-1.43074400
	H	-2.39895700	-6.25213500	-4.16334700
	H	-1.67808300	-7.76899800	-3.58835300
	H	-0.09061400	-5.84641100	-3.25100200
	H	-0.58639700	-6.53931600	-1.69267100
	N	-0.28557300	-3.85188800	-1.60238500
	H	-1.82088900	-4.06211100	-2.99759300
	N	-3.28421900	-3.56810200	-0.60263600
	H	-2.29818000	-5.37837800	-0.26375100
	C	-2.91390900	-2.40154300	-1.00900000
	C	-3.63423700	-1.18886800	-0.63018000
	C	-4.90940400	-1.29689100	-0.05196300
	C	-5.64348200	-0.15251000	0.23115300
	C	-5.11972800	1.10991100	-0.04338600
	C	-3.84177300	1.23901700	-0.59453700
	C	-3.08670300	0.08604900	-0.88676300
	C	-3.25700700	2.56906600	-0.79973900

	N	-3.92583700	3.62936000	-0.50371900
	C	-3.29743500	4.96525600	-0.64914600
	O	-1.82765500	0.28497400	-1.41652800
	C	-1.82724600	5.01970200	-1.10189400
	C	-4.17643800	5.79735600	-1.60283400
	C	-3.70320100	7.25900600	-1.64088500
	C	-2.22528800	7.33112200	-2.06536500
	C	-1.35542900	6.48826900	-1.11867600
	C	-0.04590400	-3.75363900	-0.32418600
	C	1.15463400	-3.09946200	0.15137000
	C	1.40657900	-2.98179900	1.52946500
	C	2.09019100	-2.58088700	-0.79726200
	C	3.27577600	-1.97561700	-0.31930200
	C	3.51782000	-1.90843700	1.05279900
	C	2.58587100	-2.39115800	1.97059700
	H	-2.06469300	-2.24937300	-1.69547500
	H	-5.29293300	-2.29211500	0.14317200
	H	-5.66186700	2.02342600	0.17646300
	H	-2.23018600	2.55795400	-1.16873600
	H	-3.33690700	5.41533600	0.35453100
	H	-1.26323500	-0.51716500	-1.31259100
	H	-1.72802600	4.60001300	-2.12024100
	N	-1.01501200	4.25035300	-0.11518300
	H	-5.21843900	5.71892000	-1.27258500
	H	-4.10836400	5.35589400	-2.60889500
	H	-3.81084400	7.69875700	-0.63804000
	H	-4.32804800	7.84089500	-2.33069600

	H	-1.87735000	8.37226700	-2.06792800
	H	-2.12565700	6.94195200	-3.09027100
	H	-1.42269700	6.87705800	-0.09225200
	H	-0.30012200	6.51824100	-1.42080500
	H	-0.72867400	-4.14602400	0.43870800
	O	1.86641100	-2.65182500	-2.12194600
	H	4.44450000	-1.44700600	1.37832100
	C	4.18505700	-1.31614600	-1.25172300
	N	5.30839500	-0.82046500	-0.85086900
	C	6.04496900	0.04988900	-1.78653900
	C	6.26636500	1.39844100	-1.04293600
	C	7.41612200	-0.55516600	-2.12481000
	C	8.21721400	0.41093200	-3.01592900
	C	8.39466500	1.77523500	-2.32240500
	C	7.02789300	2.37296000	-1.94440200
	H	0.67685000	-3.35069700	2.24402500
	H	0.93465000	-3.16746700	-2.24016900
	H	3.80440400	-1.21619500	-2.27847100
	H	5.47273000	0.24567900	-2.71258900
	N	4.94436600	1.94472000	-0.65887400
	H	6.85404900	1.16339400	-0.13942400
	H	7.94929800	-0.74033200	-1.18154800
	H	7.27064600	-1.52063900	-2.62555700
	H	9.19598300	-0.02435100	-3.25448800
	H	7.67739900	0.55744600	-3.96385800
	H	8.99363900	1.63921700	-1.40913900
	H	8.93960000	2.46678200	-2.97721700

	H	7.14655900	3.33237100	-1.42579600
	H	6.42969700	2.54930200	-2.85024400
	C	4.41641000	1.49680600	0.44801600
	C	3.06297400	1.82827600	0.82587100
	C	2.48847000	1.26961200	1.97894600
	C	2.29535400	2.68441000	-0.01852300
	C	0.96362500	2.98401100	0.35303400
	C	0.41317800	2.41837700	1.50749300
	C	1.16658300	1.55459600	2.30393700
	O	2.81043400	3.20079800	-1.15007900
	H	4.96984900	0.82636200	1.11640800
	H	3.06171800	0.58825100	2.60190000
	C	0.14461700	3.83431800	-0.50639900
	H	-0.61804200	2.66228000	1.74163400
	H	3.80580100	2.81544000	-1.23677100
	H	0.57482300	4.04054200	-1.49743000
	Br	-7.38186900	-0.31270800	0.99356400
	Br	2.92450900	-2.16983900	3.82730000
	Br	0.37508400	0.71706800	3.82010600
Dimer A	C	-1.95334500	-4.25632700	-3.68037300
	H	-2.42510200	-3.58179200	-4.41992600
	C	-0.43600600	-4.04885100	-3.75790100
	H	0.03166400	-4.73018100	-3.02268500
	C	0.06741000	-4.40036700	-5.15772400
	H	1.14496700	-4.21649400	-5.20988000
	H	-0.39563600	-3.71388200	-5.87916700
	C	-0.26807200	-5.84151400	-5.51546200

	H	0.09855800	-6.07725400	-6.51939400
	H	0.25962200	-6.51790000	-4.82870500
	C	-1.76777300	-6.08879400	-5.41778100
	H	-2.00360200	-7.13609800	-5.63113000
	H	-2.28216700	-5.49555000	-6.18598200
	C	-2.29924000	-5.70276100	-4.04467500
	H	-1.87763800	-6.36111200	-3.27373200
	H	-3.38610000	-5.82689000	-3.99404000
	N	-2.44970900	-3.98728000	-2.34241100
	N	-0.10843700	-2.67553700	-3.43407600
	C	0.59067000	-2.46143000	-2.38263600
	H	0.94046200	-3.29730800	-1.75342600
	C	0.94163100	-1.13395800	-1.92246500
	C	0.45649900	0.02592300	-2.57673900
	C	0.65181100	1.28760500	-1.97656600
	C	1.40149100	1.37308000	-0.80130000
	H	1.49662900	2.34295600	-0.33014800
	C	1.96803400	0.24456300	-0.22864800
	C	1.71205600	-1.00600300	-0.76347800
	H	2.07745300	-1.90323500	-0.27132900
	C	0.02706600	2.47679000	-2.54848900
	H	-0.55630100	2.31533700	-3.46650800
	Br	3.02966800	0.39110400	1.34352400
	O	-0.22508000	-0.05000000	-3.71830500
	H	-0.35023300	-1.01385800	-3.92406800
	C	-0.48372600	4.74825800	-2.70537200
	H	-1.16174200	4.40297900	-3.50904900

	C	-1.31515900	5.57166100	-1.70575000
	H	-0.64119200	5.83436000	-0.86819800
	C	-1.85474500	6.84629100	-2.35372200
	H	-2.58053800	6.55467100	-3.12456600
	H	-2.41777300	7.41403100	-1.60578400
	C	-0.75268900	7.69103000	-2.97452700
	H	-0.08144700	8.05747800	-2.18559200
	H	-1.18167900	8.57987600	-3.44764500
	C	0.04939100	6.87468500	-3.97816100
	H	-0.59889700	6.58827200	-4.81725400
	H	0.86068300	7.47125100	-4.40647800
	C	0.61245400	5.62410900	-3.32071600
	H	1.31104000	5.91367700	-2.52231400
	H	1.19041700	5.02172200	-4.03017400
	N	0.13865400	3.63502900	-2.01867000
	N	-2.43335600	4.78552100	-1.22679700
	C	-2.41637200	4.33276500	-0.02687500
	H	-1.56009200	4.50396000	0.64653100
	C	-3.51012700	3.54365100	0.51034600
	C	-4.65420200	3.24379800	-0.26808600
	C	-5.68285700	2.45601900	0.28539000
	C	-5.53987500	1.94523800	1.57647100
	H	-6.33494700	1.31929600	1.96618800
	C	-4.39959500	2.21175100	2.31890000
	C	-3.40046700	3.02037700	1.80329000
	H	-2.49096900	3.21701600	2.36387000
	C	-6.84407500	2.10164200	-0.52437000

	H	-6.73852000	2.26136500	-1.60835800
	Br	-4.16059100	1.39280300	4.02071400
	O	-4.78537100	3.67916900	-1.52115900
	H	-3.95163900	4.17883700	-1.74039500
	C	-8.93364300	1.17638700	-0.93246500
	H	-8.59739200	1.25226000	-1.98514100
	C	-9.23450700	-0.30686900	-0.64272000
	H	-9.57863600	-0.36094700	0.40604900
	C	-10.33274800	-0.82001000	-1.56582200
	H	-9.96881500	-0.77899200	-2.60109200
	H	-10.52743700	-1.87544200	-1.34974100
	C	-11.60031600	0.01231900	-1.41838100
	H	-12.37261000	-0.35276900	-2.10244500
	H	-12.00321100	-0.11922200	-0.40483100
	C	-11.32335700	1.49156900	-1.66037200
	H	-11.03629700	1.63867900	-2.71056800
	H	-12.23158500	2.08293400	-1.50753000
	C	-10.20669700	2.00158800	-0.75845200
	H	-10.51080500	1.95373000	0.29522200
	H	-9.98140100	3.05251200	-0.96619700
	N	-7.90331600	1.60629100	-0.01628800
	N	-8.01434800	-1.07089400	-0.80305100
	C	-7.41293300	-1.47513800	0.25363700
	H	-7.83752300	-1.29329900	1.25369800
	C	-6.15416700	-2.19368500	0.21219300
	C	-5.47965300	-2.41912200	-1.01343600
	C	-4.27740100	-3.15543500	-1.01920200

	C	-3.78646200	-3.67157700	0.18116700
	H	-2.88311600	-4.27169300	0.13970300
	C	-4.43169900	-3.41768000	1.38144800
	C	-5.60379100	-2.67774600	1.40306100
	H	-6.11373200	-2.47428900	2.33991500
	C	-3.57429400	-3.38672700	-2.27769800
	H	-4.08688900	-3.01841200	-3.17839100
	Br	-3.70515800	-4.09106000	3.00607800
	O	-5.95374800	-1.95161300	-2.16736600
	H	-6.82126500	-1.50581200	-1.96734200
	C	1.99838500	-4.93286800	3.37465700
	H	2.46872100	-4.29049800	4.14396300
	C	0.48152400	-4.69670100	3.43132500
	H	0.02031400	-5.32342100	2.64595700
	C	-0.06830500	-5.10574600	4.79630000
	H	0.37042600	-4.44905100	5.55941800
	H	-1.14761800	-4.92497100	4.81997600
	C	0.25307300	-6.56072900	5.11128800
	H	-0.13927900	-6.82747100	6.09756000
	H	-0.26126900	-7.21139300	4.39090700
	C	1.75287900	-6.81664800	5.03984800
	H	1.97508000	-7.87178100	5.22767600
	H	2.25561900	-6.25074300	5.83583000
	C	2.31460100	-6.39603000	3.68921400
	H	1.89135900	-7.01827800	2.88990100
	H	3.39936000	-6.53967300	3.64966900
	N	2.49364000	-4.61864000	2.05205300

	N	0.21038200	-3.29775800	3.17492600
	C	-0.38416600	-2.98085400	2.08505900
	H	-0.70142200	-3.75260400	1.36406600
	C	-0.67423200	-1.60859400	1.72314400
	C	-0.22780800	-0.52810300	2.52642600
	C	-0.43837400	0.79489500	2.08488500
	C	-1.15241800	1.01199600	0.90546100
	H	-1.27099900	2.03246600	0.56284200
	C	-1.66867800	-0.04614100	0.17435400
	C	-1.39361100	-1.35036800	0.55166400
	H	-1.71545900	-2.18397900	-0.06618200
	C	0.10848300	1.91655000	2.83967400
	H	0.66273800	1.65229100	3.75208800
	Br	-2.74911400	0.30152300	-1.35419800
	O	0.42042800	-0.72982600	3.67150500
	H	0.50408700	-1.71479200	3.79094500
	C	0.46881600	4.16148300	3.35283600
	H	1.16678400	3.74092700	4.10174800
	C	1.22946200	5.21973300	2.53615300
	H	0.53266000	5.59162100	1.76026600
	C	1.66915200	6.38109700	3.42639100
	H	2.40240800	6.00067100	4.14990600
	H	2.19897300	7.11815200	2.81419500
	C	0.49608600	7.01480800	4.15961100
	H	0.84885700	7.82742100	4.80230000
	H	-0.18659200	7.47398200	3.43156700
	C	-0.26137200	5.97171200	4.96994000

	H	-1.12733000	6.41893400	5.46781700
	H	0.38804600	5.58839400	5.76854600
	C	-0.70682100	4.81862100	4.08368900
	H	-1.42144900	5.18127200	3.33084300
	H	-1.23470000	4.05318700	4.66298800
	N	-0.04832800	3.13209700	2.47484600
	N	2.39695600	4.62769900	1.91561700
	C	2.43006800	4.52511800	0.63792000
	H	1.58574700	4.85513800	0.00975200
	C	3.55107400	3.92993100	-0.06568600
	C	4.66267600	3.39659400	0.63046200
	C	5.67747500	2.73496200	-0.08865200
	C	5.58483200	2.63390700	-1.47800500
	H	6.37650200	2.10858600	-2.00047200
	C	4.49959000	3.17040700	-2.15323200
	C	3.48788200	3.81015400	-1.45746000
	H	2.60334100	4.17407900	-1.96939100
	C	6.77845800	2.09778500	0.62708100
	H	6.68696700	2.07550100	1.72348700
	Br	4.35949300	2.98773000	-4.04237800
	O	4.76108500	3.47452400	1.95827900
	H	3.92707000	3.90696000	2.28545300
	C	8.78077800	0.93226000	0.82575900
	H	8.46868400	0.85508200	1.88569000
	C	8.99072500	-0.49496400	0.29418700
	H	9.26229500	-0.40650000	-0.77318400
	C	10.11643800	-1.19555900	1.05216400

	H	10.24905600	-2.20527600	0.65017700
	H	9.80697400	-1.31869200	2.09861000
	C	11.41292500	-0.39983200	0.98029700
	H	12.19898700	-0.91199800	1.54370400
	H	11.75863300	-0.36056000	-0.06166300
	C	11.21348300	1.01860900	1.49813300
	H	12.14015700	1.59461500	1.41293200
	H	10.97237600	0.98230100	2.56917000
	C	10.08905500	1.71941700	0.74898600
	H	10.35451500	1.84380200	-0.30901100
	H	9.91753700	2.72646500	1.14251200
	N	7.77179100	1.57869400	0.01964800
	N	7.75948600	-1.24705500	0.43535800
	C	7.15170300	-1.64914300	-0.61780900
	H	7.54716200	-1.43141700	-1.62256800
	C	5.93012500	-2.43219900	-0.55952700
	C	5.31954200	-2.74279800	0.68329400
	C	4.15874500	-3.54221700	0.70652300
	C	3.64567800	-4.04364500	-0.49174000
	H	2.76827500	-4.68053400	-0.43594000
	C	4.24350100	-3.73203300	-1.70235000
	C	5.37176000	-2.92579700	-1.74237900
	H	5.84121100	-2.68222800	-2.69035500
	C	3.51965500	-3.86518600	1.98052400
	H	3.98919800	-3.43018200	2.87488000
	Br	3.52273900	-4.43211600	-3.32007500
	O	5.82169700	-2.30771500	1.83666900

	H	6.65093500	-1.79937100	1.62040200
Dimer B	C	-0.07866100	-2.35366300	5.38708000
	H	-0.85289400	-1.74858300	5.90730900
	C	-0.73650000	-3.66940000	4.93934000
	H	0.04827600	-4.27173700	4.43887600
	C	-1.24936800	-4.44829900	6.14897900
	H	-2.03536700	-3.85673300	6.64374300
	H	-1.72708900	-5.37619400	5.80793100
	C	-0.11550000	-4.74189300	7.12335700
	H	-0.49964500	-5.28939700	7.99369400
	H	0.61438800	-5.40841100	6.63699800
	C	0.58741600	-3.46145400	7.55849100
	H	1.43262800	-3.69188400	8.21979600
	H	-0.10981600	-2.84831100	8.15130500
	C	1.06390200	-2.65993800	6.35542900
	H	1.53011300	-1.71604900	6.66607600
	H	1.83477700	-3.21490100	5.79683000
	N	0.44852500	-1.67784900	4.23124000
	N	-1.81278500	-3.38819600	4.01447800
	C	-1.72532900	-3.83775400	2.81507200
	H	-0.84191200	-4.40851300	2.47886200
	C	-2.77103300	-3.62687800	1.83007200
	C	-3.87039500	-2.76675000	2.09256400
	C	-4.87725600	-2.60952100	1.11588800
	C	-4.79546400	-3.32958600	-0.07832500
	H	-5.60229900	-3.21341000	-0.79816100
	C	-3.73319700	-4.18879700	-0.31724500

	C	-2.71605100	-4.32790400	0.61843700
	H	-1.87671300	-4.99662600	0.42727400
	C	-6.04326400	-1.76667000	1.37839200
	H	-6.00324800	-1.13853900	2.28442800
	O	-4.00241100	-2.12546800	3.25401700
	H	-3.23485100	-2.40433300	3.83491500
	Br	-3.69231700	-5.20413300	-1.92154400
	C	-8.19830000	-0.97804600	0.94491000
	H	-8.01996400	-0.38122500	1.86455500
	C	-8.45456100	0.01076800	-0.20571600
	H	-8.55632900	-0.58690000	-1.13335000
	C	-9.73510300	0.80843900	0.03493300
	H	-9.58645200	1.43996800	0.92451800
	H	-9.89624300	1.49434900	-0.80706800
	C	-10.93545400	-0.10472400	0.24205900
	H	-11.83612800	0.49456600	0.42680000
	H	-11.12728100	-0.67413900	-0.68128500
	C	-10.68748600	-1.07556000	1.38942100
	H	-11.54242300	-1.75204500	1.51706500
	H	-10.59730100	-0.51063800	2.33079200
	C	-9.41632100	-1.87927300	1.15475300
	H	-9.52824900	-2.51373100	0.26240300
	H	-9.21354600	-2.55901200	1.99246300
	N	-7.05941100	-1.79530600	0.60508100
	N	-7.33003600	0.91283200	-0.30487200
	C	-6.56338600	0.86076200	-1.33376300
	H	-6.75380500	0.14325400	-2.15264600

	C	-5.42817200	1.74743300	-1.49456100
	C	-5.06504500	2.66321600	-0.47062300
	C	-3.95677600	3.51520300	-0.65894600
	C	-3.26719300	3.48503800	-1.87324600
	H	-2.40978200	4.14552600	-1.99077100
	C	-3.62658300	2.58918800	-2.87030800
	C	-4.68384500	1.71255500	-2.68072500
	H	-4.95049900	0.99753200	-3.45793400
	C	-3.50924900	4.37639800	0.43176300
	H	-4.09104100	4.30791300	1.36621800
	O	-5.73810900	2.74119400	0.67789100
	H	-6.49129200	2.08166600	0.62176700
	Br	-2.62380900	2.52267400	-4.47827200
	C	-2.16920700	5.97028800	1.46435000
	H	-2.75641300	5.67656000	2.36015700
	C	-0.67869600	5.81036400	1.80416700
	H	-0.12008600	6.07315200	0.88079400
	C	-0.26451800	6.75853600	2.92645200
	H	-0.79486600	6.46432000	3.84539500
	H	0.80592800	6.62103800	3.13298300
	C	-0.57882200	8.20790500	2.58348400
	H	-0.28883000	8.86552500	3.41305600
	H	0.02635500	8.51803400	1.71617400
	C	-2.05536500	8.37628200	2.24905600
	H	-2.27446700	9.41467300	1.96850200
	H	-2.65785100	8.16515800	3.14675100
	C	-2.47027600	7.43348800	1.12823200

	H	-1.93319500	7.68760400	0.19999200
	H	-3.54006200	7.53208800	0.90123800
	N	-2.49610900	5.14915600	0.31981800
	N	-0.38438800	4.44299900	2.18852700
	C	0.26228200	3.72624500	1.33908300
	H	0.54092600	4.12661800	0.35012900
	C	0.63874500	2.34946300	1.57786400
	C	0.20748000	1.63754200	2.72144700
	C	0.52548100	0.26809800	2.84438000
	C	1.28688200	-0.35841400	1.85002500
	H	1.51114900	-1.41788900	1.96702200
	C	1.72109200	0.35539300	0.74101600
	C	1.39139800	1.69173700	0.59963400
	H	1.67425500	2.23695200	-0.29869500
	C	0.04453800	-0.48989900	3.99435900
	H	-0.68758100	0.02281800	4.64274100
	O	-0.50109300	2.23001500	3.68846100
	H	-0.65325900	3.17544700	3.40587200
	Br	2.69833600	-0.49235900	-0.64688500
	C	8.46444900	-0.42238300	-1.36318500
	H	8.08591200	-0.34096300	-2.40434900
	C	8.46090400	-1.91536800	-0.98430800
	H	8.76978700	-1.97654400	0.07801200
	C	9.43973400	-2.70248300	-1.85166100
	H	9.08045800	-2.67340000	-2.89225500
	H	9.42112000	-3.75761500	-1.54929300
	C	10.84841100	-2.13088600	-1.77349600

	H	11.52543600	-2.70885300	-2.41553500
	H	11.23074800	-2.23742100	-0.74578400
	C	10.85701300	-0.65825000	-2.16291000
	H	11.86771800	-0.23882300	-2.07638300
	H	10.57160100	-0.56068100	-3.22246500
	C	9.88775300	0.13637200	-1.29932700
	H	9.86574600	1.19309800	-1.59569400
	H	10.21357000	0.11821400	-0.24816400
	N	7.63511700	0.30295400	-0.43019000
	N	7.12376400	-2.44144100	-1.15224500
	C	6.40151600	-2.64758000	-0.11066600
	H	6.79481800	-2.45648900	0.90394100
	C	5.04482400	-3.14773400	-0.19650100
	C	4.42708700	-3.39422000	-1.45057900
	C	3.10567700	-3.88333700	-1.49451200
	C	2.41854800	-4.11099700	-0.30073200
	H	1.38993600	-4.46125500	-0.36499600
	C	3.02574800	-3.86177700	0.92188400
	C	4.32429100	-3.38000700	0.97975000
	H	4.79056600	-3.16778800	1.94091700
	C	2.43169400	-4.07217800	-2.77717000
	H	2.89616800	-3.57645300	-3.64698900
	O	5.06167100	-3.17720800	-2.60626400
	H	5.97825900	-2.84220100	-2.37768500
	Br	2.04037700	-4.07639400	2.53076100
	C	0.67887600	-4.75245700	-4.15037100
	H	1.22891800	-4.15749300	-4.91056600

	C	-0.70087200	-4.11238500	-3.94035500
	H	-1.20639800	-4.71262800	-3.16261100
	C	-1.54290500	-4.15876700	-5.21212800
	H	-1.06729900	-3.53125800	-5.98180100
	H	-2.52299400	-3.70889200	-5.00172700
	C	-1.69525900	-5.58769300	-5.71420100
	H	-2.28356400	-5.60478500	-6.64081400
	H	-2.26689800	-6.17098000	-4.97370100
	C	-0.33368900	-6.23935300	-5.92559300
	H	-0.44912300	-7.27980800	-6.25624800
	H	0.19556300	-5.71508700	-6.73729700
	C	0.50589100	-6.18475000	-4.65545100
	H	0.02547100	-6.77222200	-3.85776500
	H	1.49578200	-6.63192500	-4.81490900
	N	1.34956000	-4.74234300	-2.87142000
	N	-0.56683000	-2.73926000	-3.49079300
	C	-1.11961700	-2.43360500	-2.37194100
	H	-1.65036100	-3.19388400	-1.77439600
	C	-1.14073300	-1.09030800	-1.83472200
	C	-0.50017600	-0.01209400	-2.49684300
	C	-0.56822700	1.28079000	-1.93879400
	C	-1.29424200	1.47833500	-0.75890900
	H	-1.34429200	2.48554600	-0.35037700
	C	-1.93173300	0.42314000	-0.12409400
	C	-1.84795200	-0.85591400	-0.65063200
	H	-2.33695000	-1.69190200	-0.15110000
	C	0.09706100	2.40305900	-2.59201000

	H	0.54456200	2.19376200	-3.57824500
	O	0.16652800	-0.18928600	-3.63868000
	H	0.08506300	-1.15634600	-3.88303900
	Br	-2.90489300	0.72216600	1.47483500
	C	0.73232200	4.63763400	-2.82511600
	H	1.25751600	4.25195000	-3.72521000
	C	1.76066500	5.39176700	-1.96993900
	H	1.22449000	5.78404600	-1.08003500
	C	2.34207100	6.57266200	-2.74582100
	H	2.88698500	6.18587800	-3.62090900
	H	3.08344800	7.08672100	-2.11930800
	C	1.23987500	7.52593600	-3.18971900
	H	1.66971700	8.36427500	-3.75286500
	H	0.76131700	7.96371000	-2.29817400
	C	0.18728400	6.79993900	-4.01896300
	H	-0.62466200	7.48392000	-4.29742900
	H	0.64163400	6.45942400	-4.96284600
	C	-0.37357300	5.60016400	-3.26634500
	H	-0.91352200	5.92960600	-2.36228200
	H	-1.09811200	5.04258600	-3.87706100
	N	0.14191400	3.56566100	-2.05687100
	N	2.81213000	4.48658100	-1.55286300
	C	3.12936200	4.45135400	-0.30871200
	H	2.62243100	5.10569600	0.42653000
	C	4.11665600	3.53917200	0.23016600
	C	4.84778000	2.65972700	-0.61021300
	C	5.79690800	1.78473000	-0.04050700

	C	5.94884700	1.75076000	1.34703800
	H	6.67913800	1.06069400	1.76293000
	C	5.19719200	2.58109100	2.16820000
	C	4.30101000	3.48333300	1.61681400
	H	3.71637800	4.14182500	2.25872900
	C	6.64409100	0.95916100	-0.89973200
	H	6.40186900	0.96939200	-1.97603300
	O	4.68076500	2.64972900	-1.93496700
	H	3.95061800	3.29785600	-2.14926900
	Br	5.40202100	2.48897500	4.04921400
Dimer C	O	-1.87113400	2.07643800	-1.34072700
	N	-4.33131500	1.37547900	-1.82259900
	C	-3.13587900	2.90343600	-3.21338500
	C	-0.99536900	4.61051100	-3.79017400
	H	-0.17090900	5.28913000	-3.97817900
	C	-4.30526900	2.11094800	-2.87011800
	H	-5.18082000	2.21139200	-3.52984400
	C	-3.18760900	3.76156400	-4.31648900
	H	-4.07935800	3.77140100	-4.93499600
	C	0.23088300	3.84610000	-1.76664700
	H	0.31756000	3.03338700	-1.03189600
	C	-2.11974900	4.59860700	-4.60195400
	C	-1.96934000	2.87765500	-2.40497600
	C	-0.90480400	3.75919300	-2.68780900
	N	-4.70816200	-1.53051000	-1.78999900
	C	-7.46882500	1.00275800	0.25042700
	H	-7.90494200	1.68439900	0.98797500

	H	-8.23871600	0.84149400	-0.51604200
	C	-5.23517100	-0.62480400	-0.78383500
	H	-4.47794100	-0.41797500	-0.00957700
	C	-5.56791500	0.73451000	-1.41227300
	H	-6.24078600	0.58555000	-2.27391000
	C	-6.24528500	1.64607300	-0.38235200
	H	-6.49599800	2.59739500	-0.86548100
	H	-5.50377600	1.88306300	0.39437600
	C	-6.46044300	-1.25677100	-0.12756500
	H	-6.15806000	-2.19981300	0.34157300
	H	-7.18404000	-1.51626100	-0.91179000
	C	-7.10161000	-0.32664100	0.89244000
	H	-7.98139600	-0.80215100	1.33686100
	H	-6.39880600	-0.14581900	1.71809200
	H	-2.74935200	1.60681500	-1.24429700
	O	2.74144300	0.60359300	-1.32370000
	N	3.37795200	3.08208500	-1.77060000
	C	4.12925600	1.29604500	-3.16287700
	C	4.54501200	-1.40790900	-3.75030700
	H	4.72186900	-2.46074600	-3.94078100
	C	4.01821900	2.70218500	-2.81234600
	H	4.55148000	3.41621300	-3.45874400
	C	4.91928000	0.91816000	-4.25326300
	H	5.38806400	1.68925000	-4.85640900
	C	3.22848000	-2.09727400	-1.75668300
	H	2.47443800	-1.76619900	-1.02874400
	C	5.11368600	-0.42360600	-4.54462500

	C	3.50727800	0.29433800	-2.37323800
	C	3.74245600	-1.06625800	-2.66060600
	N	1.03796800	4.83495500	-1.78045200
	C	4.56461400	5.98935000	0.33483500
	H	5.35177800	6.02962200	1.09472800
	H	4.83316800	6.73127500	-0.42925000
	C	2.06647300	4.85640900	-0.75483200
	H	1.85690700	4.10365700	0.02299900
	C	3.42674100	4.47166000	-1.35102000
	H	3.65306200	5.13315700	-2.20452500
	C	4.52585400	4.60415600	-0.29091600
	H	5.48776900	4.34213400	-0.74609800
	H	4.33636900	3.84757900	0.48474100
	C	2.11123000	6.23941500	-0.11016000
	H	1.13478300	6.44870000	0.33968700
	H	2.26161500	6.98942000	-0.89799400
	C	3.21219500	6.34327700	0.93548500
	H	3.22817700	7.34805200	1.36851600
	H	2.99544600	5.65500500	1.76433800
	H	2.76375700	1.59887500	-1.22658600
	O	-0.86034600	-2.66510600	-1.34698900
	N	0.97540900	-4.44316200	-1.80256800
	C	-0.95822700	-4.21633400	-3.18201200
	C	-3.51562400	-3.23944200	-3.75892600
	H	-4.51808200	-2.87114600	-3.94750700
	C	0.31863200	-4.81782800	-2.83574300
	H	0.66976300	-5.63804600	-3.48086100

	C	-1.68406300	-4.71939900	-4.26639000
	H	-1.25038900	-5.51067700	-4.86961600
	C	-3.45014000	-1.74515900	-1.77197400
	H	-2.78469500	-1.25538200	-1.04717600
	C	-2.94736200	-4.22444600	-4.55225000
	C	-1.51600500	-3.17781800	-2.39179500
	C	-2.81539800	-2.70744400	-2.67470300
	N	3.67321700	-3.29342700	-1.77474500
	C	2.88759400	-6.94728500	0.28305900
	H	2.52101600	-7.66716500	1.02201200
	H	3.41959200	-7.53067500	-0.48050400
	C	3.15724900	-4.19956000	-0.76297500
	H	2.59280800	-3.64527800	0.00519700
	C	2.15621400	-5.17982300	-1.38666300
	H	2.62665200	-5.68727300	-2.24607100
	C	1.71287200	-6.22221100	-0.35383900
	H	1.02068200	-6.92202800	-0.83577800
	H	1.13154400	-5.70057100	0.42051200
	C	4.32164000	-4.93013700	-0.09747700
	H	4.97569200	-4.18853100	0.37429600
	H	4.91792500	-5.42283400	-0.87702600
	C	3.84320400	-5.95199200	0.92368500
	H	4.69889700	-6.46522300	1.37311600
	H	3.32664800	-5.43646500	1.74554000
	H	-0.00560200	-3.17728400	-1.25794100
	O	-2.74047000	0.66745000	1.31902100
	N	-3.30217600	3.16185900	1.76705400

	C	-4.09712000	1.39974800	3.16518900
	C	-4.58694300	-1.29041400	3.75795900
	H	-4.79223700	-2.33768100	3.95042700
	C	-3.94849900	2.80159500	2.81186100
	H	-4.45520600	3.53139900	3.46201300
	C	-4.89330400	1.04601400	4.25899300
	H	-5.33729100	1.83111000	4.86285500
	C	-3.29346600	-2.01886800	1.76240000
	H	-2.53355100	-1.70727200	1.03213000
	C	-5.12557500	-0.28937200	4.55222500
	C	-3.50754700	0.38012500	2.37402500
	C	-3.77875800	-0.97295500	2.66493500
	N	-0.91669900	4.85628100	1.76543100
	C	-4.42200400	6.09451600	-0.33681500
	H	-5.21385900	6.15371800	-1.09061400
	H	-4.66290600	6.84741300	0.42576100
	C	-1.94761500	4.89843300	0.74222000
	H	-1.76080800	4.13563600	-0.03163000
	C	-3.31427400	4.55192800	1.34700000
	H	-3.51742200	5.21987900	2.20138100
	C	-4.41717400	4.71193100	0.29498500
	H	-5.38251300	4.47880900	0.75855200
	H	-4.25523800	3.94714400	-0.47867900
	C	-1.95924400	6.27777800	0.08828300
	H	-0.97977200	6.45580200	-0.36829100
	H	-2.08271600	7.03671600	0.87221400
	C	-3.06472200	6.40582600	-0.95003500

	H	-3.05522100	7.40786900	-1.38964700
	H	-2.87415700	5.70599800	-1.77574400
	H	-2.74110100	1.66241600	1.21703600
	O	0.79785900	-2.66069600	1.34797600
	N	-1.08289800	-4.39857000	1.81425500
	C	0.85509800	-4.20242500	3.19413600
	C	3.43516000	-3.28346300	3.76568600
	H	4.44637100	-2.93810900	3.95061800
	C	-0.43487100	-4.77766500	2.85129200
	H	-0.80194900	-5.58809700	3.49992200
	C	1.56872900	-4.71593300	4.28171900
	H	1.11686300	-5.49427800	4.88833500
	C	3.40635600	-1.80141000	1.76935500
	H	2.75399700	-1.29981800	1.04043400
	C	2.84365000	-4.24992300	4.56502400
	C	1.43752600	-3.18196900	2.39827500
	C	2.74750900	-2.74151800	2.67834900
	N	-3.76190400	-3.20589400	1.78682500
	C	-3.02983900	-6.87723900	-0.26634400
	H	-2.67250300	-7.59873200	-1.00834600
	H	-3.56441100	-7.45761200	0.49776500
	C	-3.26446200	-4.12556100	0.77805600
	H	-2.69594300	-3.58434000	0.00344600
	C	-2.27512300	-5.11803600	1.40174900
	H	-2.75091500	-5.61873500	2.26213700
	C	-1.84629600	-6.16600300	0.36860800
	H	-1.16343000	-6.87485500	0.85030400

	H	-1.25818200	-5.65184000	-0.40560100
	C	-4.44108300	-4.84400600	0.12206800
	H	-5.09048200	-4.09457300	-0.34385200
	H	-5.03665800	-5.33016600	0.90612000
	C	-3.97924500	-5.87178400	-0.90143000
	H	-4.84262600	-6.37676500	-1.34544800
	H	-3.46299900	-5.36143500	-1.72653400
	H	-0.06579100	-3.15638400	1.25525800
	O	1.93461600	2.04043500	1.31615300
	N	4.37430200	1.28746900	1.79141000
	C	3.21127700	2.82620000	3.19653000
	C	1.10691500	4.57425000	3.78288600
	H	0.29555100	5.26739500	3.97558900
	C	4.36307500	2.01047100	2.84784300
	H	5.23632000	2.07650600	3.51484300
	C	3.27800700	3.67161200	4.30875100
	H	4.16768100	3.65554900	4.93028800
	C	-0.13175300	3.84966900	1.75143600
	H	-0.23595400	3.03888300	1.01665400
	C	2.22732000	4.52906400	4.59911100
	C	2.04745900	2.83368000	2.38490800
	C	1.00167300	3.73574500	2.67202300
	N	4.67041700	-1.62433900	1.78274100
	C	7.49508200	0.81392000	-0.28739500
	H	7.94624300	1.47597200	-1.03367600
	H	8.26199500	0.64359900	0.48019000
	C	5.22184900	-0.74461300	0.76705600

	H	4.47115300	-0.52548300	-0.00998400
	C	5.59205000	0.61148200	1.38119000
	H	6.26448500	0.45254600	2.24152800
	C	6.28795400	1.49375300	0.33849000
	H	6.56040400	2.44573300	0.80798100
	H	5.55068700	1.73543600	-0.44088800
	C	6.42958900	-1.41534500	0.11723700
	H	6.10187500	-2.35417400	-0.34279100
	H	7.14653800	-1.68563900	0.90390200
	C	7.09450400	-0.51361600	-0.91322700
	H	7.96170000	-1.01664700	-1.35217000
	H	6.39620500	-0.32450600	-1.74101000
	H	2.80151200	1.54990800	1.22489900
	Br	-3.91814900	-4.92433400	-6.03338100
	Br	-2.20943900	5.75995500	-6.10818800
	Br	3.79952900	-4.96850700	6.04648400
	Br	-6.21836300	-0.74777700	6.04295900
	Br	6.19795000	-0.91538200	-6.03091100
	Br	2.33512700	5.67035400	6.11973000
Dimer D	C	-0.20606400	-5.24779600	-0.79028600
	H	-0.32568600	-4.47403600	-0.01291100
	C	-1.59210400	-5.42343600	-1.43618900
	H	-1.49396200	-6.10842900	-2.30168600
	C	-2.59892800	-6.01439000	-0.43050200
	H	-2.78964200	-5.26363700	0.35275200
	H	-3.55775200	-6.17804600	-0.94934300
	C	-2.09738000	-7.30766200	0.21191200

	H	-2.83877700	-7.66596100	0.94446600
	H	-2.00471000	-8.09507400	-0.55833000
	C	-0.73877300	-7.08843500	0.87961800
	H	-0.36763100	-8.02746800	1.32159900
	H	-0.85283900	-6.37310700	1.71276900
	C	0.27470200	-6.54567500	-0.12799900
	H	1.24153800	-6.34781200	0.35754400
	H	0.46665500	-7.29002300	-0.92050900
	N	0.75612400	-4.83642700	-1.79141600
	N	-2.07099500	-4.12280100	-1.86713100
	C	-2.80258800	-3.99340300	-2.90955300
	H	-3.03935300	-4.85616200	-3.56086400
	C	-3.41568000	-2.71396300	-3.25292600
	C	-3.15541300	-1.56071300	-2.45586200
	C	-3.88981300	-0.37469500	-2.69209000
	C	-4.81298000	-0.33309900	-3.74549000
	H	-5.37460300	0.59079900	-3.88991900
	C	-5.01940200	-1.44812200	-4.55644900
	C	-4.33422300	-2.63604500	-4.31100600
	H	-4.52583200	-3.52013900	-4.92280900
	C	-3.75835600	0.76621800	-1.76793800
	H	-2.95335900	0.69296400	-1.01895100
	O	-2.27903200	-1.60307900	-1.45489200
	Br	-6.27665200	-1.36193300	-5.98881400
	C	-4.44962500	2.79178700	-0.81077300
	H	-3.72401300	2.51128500	-0.02850800
	C	-3.90304400	4.07484900	-1.46160200

	H	-4.54246800	4.32995000	-2.32991500
	C	-3.91115500	5.24732300	-0.46186200
	H	-3.16890200	5.03889800	0.32506400
	H	-3.56882800	6.15579700	-0.98414900
	C	-5.28349800	5.46739000	0.17446300
	H	-5.22294800	6.29194400	0.90317700
	H	-6.00765800	5.77950400	-0.60010700
	C	-5.78029200	4.18618800	0.84625100
	H	-6.78048400	4.33985400	1.28301100
	H	-5.10831200	3.92894900	1.68358500
	C	-5.81638800	3.03244000	-0.15617400
	H	-6.55235400	3.23744500	-0.95330300
	H	-6.13457100	2.09982700	0.33231800
	N	-4.57260200	1.74701000	-1.80627700
	N	-2.53678800	3.83403100	-1.88820100
	C	-2.05693100	4.39860600	-2.93198600
	H	-2.68447400	5.03336600	-3.58614700
	C	-0.64227500	4.28756500	-3.27369800
	C	0.22544700	3.48795900	-2.47343300
	C	1.61993600	3.53015100	-2.70877400
	C	2.11854100	4.30569800	-3.76406000
	H	3.19958300	4.32969100	-3.90774900
	C	1.25690900	5.03966200	-4.57775100
	C	-0.11460600	5.04100200	-4.33345900
	H	-0.78382800	5.64761900	-4.94731100
	C	2.54219500	2.84879900	-1.78229100
	H	2.07694600	2.18827200	-1.03287100

	O	-0.25014500	2.75377000	-1.47006900
	Br	1.96156200	6.08145500	-6.01223200
	C	4.64325700	2.44037600	-0.82410900
	H	4.03879500	1.95100100	-0.04152200
	C	5.48309800	1.32680100	-1.47498600
	H	6.01982200	1.75226400	-2.34610000
	C	6.50694600	0.75268600	-0.47674900
	H	5.95882700	0.21327700	0.31198400
	H	7.12427600	0.00353700	-0.99928900
	C	7.38089100	1.83500600	0.15686900
	H	8.06841500	1.37338100	0.88409200
	H	8.00957900	2.30837800	-0.61938100
	C	6.51683200	2.90221400	0.83046900
	H	7.14765900	3.69402700	1.26617400
	H	5.96143500	2.44662800	1.66871900
	C	5.53174300	3.50667600	-0.17018900
	H	6.07385800	4.04398000	-0.96791000
	H	4.88064600	4.24570900	0.31944200
	N	3.79821000	3.06657600	-1.81971900
	N	4.59247200	0.26080200	-1.89575200
	C	4.83878900	-0.44169300	-2.93712800
	H	5.70010400	-0.21861000	-3.59510900
	C	4.03418700	-1.61297900	-3.27066000
	C	2.90969300	-1.95976600	-2.46553800
	C	2.24727100	-3.18899800	-2.69291900
	C	2.66635800	-4.01459200	-3.74468200
	H	2.14553700	-4.96316400	-3.88177500

	C	3.73099200	-3.64045500	-4.56318700
	C	4.41930300	-2.45249800	-4.32716700
	H	5.27751100	-2.17987100	-4.94509200
	C	1.19772100	-3.64042900	-1.76157200
	H	0.86150300	-2.90274500	-1.01522100
	O	2.51486700	-1.17537300	-1.46515900
	Br	4.27625200	-4.77955000	-5.99325600
	H	-1.97179100	-2.56588100	-1.37317000
	H	-1.23726100	2.96934100	-1.38928200
	H	3.19636400	-0.42849100	-1.39026800
	C	0.20518700	5.24707100	0.79013400
	H	0.32436900	4.47345000	0.01254500
	C	1.59137300	5.42193400	1.43589500
	H	1.49357000	6.10670700	2.30160400
	C	2.59835300	6.01286900	0.43034500
	H	2.78874300	5.26241900	-0.35326900
	H	3.55729200	6.17594200	0.94915500
	C	2.09721700	7.30667000	-0.21134600
	H	2.83864400	7.66506600	-0.94382000
	H	2.00495000	8.09371000	0.55933100
	C	0.73843700	7.08833300	-0.87899000
	H	0.36762600	8.02777600	-1.32038300
	H	0.85212600	6.37347800	-1.71256000
	C	-0.27514100	6.54541200	0.12842800
	H	-1.24211200	6.34813500	-0.35711500
	H	-0.46677600	7.28942800	0.92132500
	N	-0.75697900	4.83583100	1.79130000

	N	2.06984400	4.12098600	1.86651100
	C	2.80299400	3.99161700	2.90783000
	H	3.04122700	4.85451900	3.55842300
	C	3.41620600	2.71211300	3.25073500
	C	3.15430900	1.55859500	2.45460700
	C	3.88914400	0.37264700	2.68986100
	C	4.81431000	0.33140500	3.74153300
	H	5.37630100	-0.59239600	3.88510800
	C	5.02228600	1.44667400	4.55173700
	C	4.33671800	2.63454300	4.30711800
	H	4.52960800	3.51890100	4.91813700
	C	3.75647500	-0.76851700	1.76615100
	H	2.94948600	-0.69633900	1.01920600
	O	2.27621100	1.60075400	1.45512800
	Br	6.28236400	1.36099100	5.98163900
	C	4.44819500	-2.79365200	0.80792900
	H	3.72163500	-2.51380600	0.02634000
	C	3.90231000	-4.07628900	1.46028800
	H	4.54241600	-4.33056000	2.32834400
	C	3.90976700	-5.24958700	0.46152000
	H	3.16687900	-5.04186000	-0.32499200
	H	3.56794400	-6.15764400	0.98485900
	C	5.28159000	-5.47001300	-0.17578900
	H	5.22052100	-6.29527100	-0.90366300
	H	6.00650900	-5.78126900	0.59841500
	C	5.77751700	-4.18934500	-0.84922000
	H	6.77734900	-4.34321400	-1.28672700

	H	5.10475300	-3.93302000	-1.68620500
	C	5.81429400	-3.03466100	0.15208700
	H	6.55113000	-3.23872900	0.94865400
	H	6.13175100	-2.10242500	-0.33759500
	N	4.57220600	-1.74815700	1.80253900
	N	2.53634700	-3.83527300	1.88756900
	C	2.05763900	-4.39717100	2.93332600
	H	2.68598800	-5.02996300	3.58861200
	C	0.64325600	-4.28547900	3.27602900
	C	-0.22522900	-3.48783000	2.47464800
	C	-1.61948800	-3.52929500	2.71148000
	C	-2.11710400	-4.30208500	3.76925200
	H	-3.19799500	-4.32553700	3.91417400
	C	-1.25468400	-5.03400600	4.58396300
	C	0.11658500	-5.03613700	4.33826000
	H	0.78638100	-5.64115000	4.95306900
	C	-2.54246600	-2.84993100	1.78427300
	H	-2.07765000	-2.19145400	1.03277900
	O	0.24944200	-2.75607000	1.46907000
	Br	-1.95791400	-6.07179100	6.02204500
	C	-4.64390000	-2.44247000	0.82691000
	H	-4.03964400	-1.95432900	0.04335600
	C	-5.48404400	-1.32804500	1.47590500
	H	-6.02135200	-1.75239600	2.34720600
	C	-6.50724500	-0.75527300	0.47626200
	H	-5.95859100	-0.21718200	-0.31300900
	H	-7.12469100	-0.00519600	0.99732500

	C	-7.38108100	-1.83842200	-0.15609500
	H	-8.06802500	-1.37786100	-0.88453800
	H	-8.01040300	-2.31024400	0.62058100
	C	-6.51698700	-2.90712700	-0.82730800
	H	-7.14785100	-3.69963100	-1.26170900
	H	-5.96113800	-2.45328300	-1.66624400
	C	-5.53236800	-3.50993100	0.17484600
	H	-6.07485300	-4.04556600	0.97343800
	H	-4.88132700	-4.25004800	-0.31318100
	N	-3.79858400	-3.06682300	1.82345800
	N	-4.59377500	-0.26150500	1.89594600
	C	-4.84042400	0.44149500	2.93690100
	H	-5.70178500	0.21850100	3.59485000
	C	-4.03613700	1.61308600	3.27004200
	C	-2.91156200	1.95972700	2.46497300
	C	-2.24922100	3.18903400	2.69215000
	C	-2.66855500	4.01493000	3.74357700
	H	-2.14772400	4.96351900	3.88053100
	C	-3.73336400	3.64101200	4.56195000
	C	-4.42152700	2.45292000	4.32620000
	H	-5.27982200	2.18042200	4.94405800
	C	-1.19942600	3.64017000	1.76094300
	H	-0.86380100	2.90260600	1.01420800
	O	-2.51645300	1.17504100	1.46493100
	Br	-4.27906900	4.78059800	5.99146300
	H	1.96915600	2.56357500	1.37339400
	H	1.23644500	-2.97210400	1.38776400

	H	-3.19776100	0.42797500	1.39025000

References

1. L. F. Lindoy, G. V. Meehan, N. Svenstrup, *Synthesis*, 1998; **7**, 1029.

2. M. Kwit, J. Gawronski, *Tetrahedron: Asymmetry*, 2003, **14**, 1303.

3. S. R. Korupoju, P. S. Zacharias, *Chem. Commun*. 1998, **12**, 1267.

4. A. Janiak, M. Petryk, L. J. Barbour, M. Kwit, *Org. Biomol. Chem.* 2016, **14**, 669.

5. D. Jacquemin, E. A. Perpète, I. Ciofini, C. Adamo, R. Valero, Y. Zhao, D. G. Truhlar, *J. Chem. Theor.*, 2010, **6**, 2071.

6. Gaussian 09, Revision D.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

7. S. Grimme, S. Ehrlich, L. Goerigk, *J. Comp. Chem.*, 2011, **32**, 1456.

8. S. F. Boys, F. Bernardi, *Mol. Phys.*, 1970, **19**, 553.

9. (a) M. Chadim, M. Buděsĭnský, J. Hodačová, J. Zavada and P. C. Junk, *Tetrahedron: Asymmetry*, 2001, **12**, 127; (b) *Cambridge Structural Database*, version 5.34. F. H. Allen, *Acta Crystallogr., Sect. B: Struct. Sci*. 2002, **58**, 380.

10. (a) CrysAlisPro, version. 1.171.35.4, Agilent Technologies, Ltd, Yarnton, England, 2010; (b) CrysAlisPro 1.171.38.41 (Rigaku OD, 2015)

11. (a) G. M. Sheldrick, Acta Cryst. A, 2015, **71**, 3; (b) G. M. Sheldrick,. Acta Cryst. C, 2015, **71**, 3.

12. M. C. Burla, R. Caliandro, M. Camalli, B. Carrozzini, G. L. Cascarano, C. Giacovazzo, M. Mallamo, A. Mazzone, G. Polidori and R. Spagna, J. Appl. Cryst. 2012, **45**, 351.

13. T. L. Spek, Acta Cryst. A, 1990, **46**, 194.

14. L. J. Barbour, J. Supramol. Chem. 2001, **1**, 189.

15. POV-Ray™ for Windows, version 3.6, Persistence of Vision Raytracer Pty Ltd, Williamstown, Australia, 2004, http://www.povray.org

16. I. J. Bruno, J. C. Cole, P. R. Edgington, M. Kessler, C. F. Macrae, P. McCabe, J. Pearson and R. Taylor, Acta Cryst. B, 2002, **58**, 389.