Electronic Supplementary Information

for

Combined Structural and Theoretical Investigation on Differently Substituted Bispidine Ligands: Predicting the Properties of their Corresponding Coordination Polymers.

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Table of content:

Synthesis of the Bispidine Ligands L1-L7

Procedures for obtaining Ligand **L1,** Ligand **L4** and Piperidone **A** were previously reported by us (ref. 9)

Ligand **L2:** Piperidone **A** (1 g, 2.6 mmol) was suspended in methanol. A second solution consisting of paraformaldehyde (470 mg, 15.7 mmol) and isopropylamine (0.7 mL, 7.8 mmol) in methanol was then added to the piperidone. The reaction was stirred and refluxed overnight. The solution was left to cool, and while the solvent slowly evaporated, crystals were formed. After recrystallization from methanol, 900 mg of product were obtained, affording a 75 % yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.73 (d, *J* = 5.2 Hz, 2H), 8.57 (d, *J* = 5.1 Hz, 2H), 8.16 (d, *J* = 4.9 Hz, 2H), 7.08 (d, *J* = 5.9 Hz, 2H), 4.56 (s, 2H), 3.77 (s, 6H), 3.10 (d, *J* = 13.0 Hz, 2H), 2.84 (d, *J* = 12.9 Hz, 2H), 2.28 (s, 1H), 1.89 (s, 3H), 1.17 (d, *J* = 6.6 Hz, 6H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 203.14, 167.95 (2C), 149.89 (2C), 149.64 (2C), 148.17 (2C), 124.54 (2C), 124.15 (2C), 71.59 (2C), 62.80 (2C), 54.72, 54.05 (2C), 52.74 (2C), 43.56, 18.30 (2C). MS-*ESI calcd* for $C_{25}H_{30}N_4O_5$ 466.22; found: $[M+H]^+$: 467.3.

Ligand L3: Piperidone **A** (1 g, 2.6 mmol) was dissolved in methanol, and a second solution consisting of paraformaldehyde (470 mg, 15.7 mmol) and cyclohexylamine (0.9 mL, 7.8 mmol) in methanol was then added. The reaction was stirred and refluxed overnight. A white solid precipitated, which was then filtrated and washed with cold methanol. The remaining solution was recrystallized from methanol and left to evaporate to afford more product, giving a total of 800 mg (61 % yield). ^{1}H-NMR (400 MHz, Chloroform-*d*) δ 8.74 (d, *J* = 5.1 Hz, 2H), 8.57 (d, *J* = 5.1 Hz, 2H), 8.17 (d, *J* = 5.1 Hz, 2H), 7.08 (d, *J* = 5.1 Hz, 2H), 4.56 (s, 2H), 3.77 (s, 6H), 3.13 (d, *J* = 13.0 Hz, 2H), 2.92 (d, *J* = 12.2 Hz, 2H), 2.39 (d, *J* = 10.1 Hz, 1H), 2.05 – 1.98 (m, 4H), 1.88 (s, 3H), 1.69 (d, *J* = 12.6 Hz, 1H), 1.39 – 1.22 (m, 5H). ^{13}C-NMR (101 MHz, $CDCl_3$) δ 203.17, 167.98 (2C), 149.92 (2C), 149.73 (2C), 148.08 (2C), 124.56 (2C), 124.11 (2C), 71.59, 63.82 (2C), 62.94 (2C), 54.45 (2C), 52.70 (2C), 43.53, 28.77 (2C), 26.17 (2C), 26.06. MS-*ESI calcd* for $C_{28}H_{34}N_4O_5$ 506.25; found: $[M+H]^+$: 507.4

Ligand L5: Piperidone **A** (500 mg, 1.3 mmol) was dissolved in methanol. A second solution consisting of paraformaldehyde (235 mg, 7.8 mmol) and 4-methoxybenzylamine (0.5 mL, 3.9 mmol) in methanol was then added to the piperidone. The reaction was stirred and refluxed for 6 hours. A white solid precipitated, which was then filtrated and washed with cold methanol, while the remaining solution was left to evaporate to afford more product. Yield 64% (450 mg). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.60 (d, *J* = 5.4 Hz, 2H), 8.47 (d, *J* = 5.4 Hz, 2H), 8.08 (d, *J* = 5.4 Hz, 2H), 7.37 – 7.29 (m, 4H), 7.05 (d, *J* = 8.6 Hz, 2H), 4.64 (s, 2H), 3.95 (s, 3H), 3.77 (s, 6H), 3.44 (s, 2H), 3.12 (d, *J* = 13.4 Hz, 2H), 2.80 (d, *J* = 12.5 Hz, 2H), 1.83 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 202.86, 167.62 (2C), 159.72, 149.73 (2C), 147.51 (2C), 147.94 (2C), 131.74 (2C), 128.49, 124.22 (4C), 114.23 (2C), 71.76 (2C), 62.65 (2C), 62.08, 57.83 (2C), 55.60, 52.79 (2C), 43.45. MS-*ESI calcd* for $C_{30}H_{32}N_4O_6$ 544.23; found: $[M+Na]^+$: 567.4

Ligand L6: Piperidone **A** (500 mg, 1.3 mmol) was suspended in methanol. A second solution consisting of paraformaldehyde (235 mg, 7.8 mmol) and 4-(trifluoromethyl)benzylamine (0.56 mL, 3.9 mmol) in methanol was then added to first solution. The reaction was stirred and refluxed for 5 hours. A white solid precipitated, which was then filtrated and washed with cold methanol, while the remaining solution was left to evaporate to afford more product. 350 mg (46 % yield). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.55 (d, 2H), 8.46 (s, 2H), 7.85 (s, 2H), 7.79 (d, *J* = 7.8 Hz, 2H), 7.58 (d, *J* = 7.8 Hz, 2H), 7.10 (d, *J* = 4.7 Hz, 2H), 4.52 (s, 2H), 3.76 (s, 6H), 3.58 (s, 2H), 3.17 (d, *J* = 11.2 Hz, 2H), 2.80 (d, *J* = 12.3 Hz, 2H), 1.83 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 202.36, 167.41 (2C), 149.97 (2C), 149.45 (2C), 147.69 (2C),

140.20, 130.92 (3C), 125.87 (2C), 125.83, 124.26 (2C), 123.82 (2C), 71.71 (2C), 62.58 (2C), 62.28, 57.86 (2C), 52.86 (2C), 43.46. MS-*ESI calcd* for $C_{30}H_{29}F_3N_4O_5$ 582.21; found: $[M+Na]^+$: 605.3

Ligand L7: Piperidone **A** (500 mg, 1.3 mmol) was suspended in methanol. A second solution consisting of paraformaldehyde (235 mg, 7.8 mmol) and 4-(trifluoromethoxy)benzylamine (0.6 mL, 3.9 mmol) in methanol was then added to the suspension. The reaction was stirred and refluxed for 4 hours. A white solid precipitated, which was then filtrated and washed with cold methanol, while the remaining solution was left to evaporate to afford more product. 350 mg of **L7** were obtained (45 % yield). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.54 (d, 2H), 8.46 (d, 2H), 7.91 (d, 2H), 7.46 (d, *J* = 8.1 Hz, 2H), 7.36 (d, *J* = 8.0 Hz, 2H), 7.13 (d, *J* = 4.7 Hz, 2H), 4.53 (s, 2H), 3.74 (s, 6H), 3.50 (s, 2H), 3.14 (d, *J* = 12.5 Hz, 2H), 2.77 (d, *J* = 12.4 Hz, 2H), 1.82 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 202.21, 167.39 (2C), 149.33 (4C), 148.63 (3C), 134.86 (2C), 132.00 (2C), 124.59 (2C), 124.20 (2C), 121.35 (2C), 71.71 (2C), 62.54 (2C), 62.06, 57.83 (2C), 52.96 (2C), 43.56. MS-*ESI calcd* for $C_{30}H_{29}F_3N_4O_6$ 598.20; found: $[M+H]^+$: 599.20

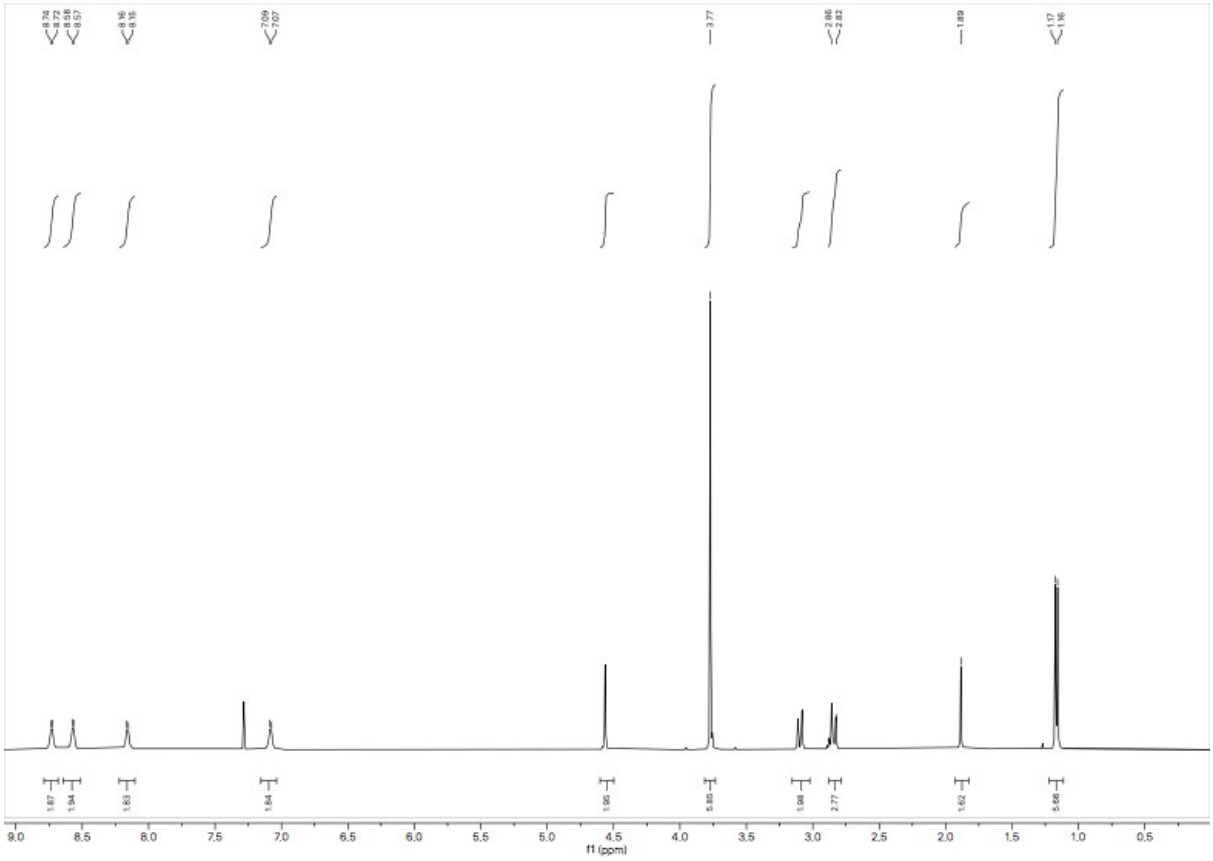

Figure S1. ^{1}H-NMR spectrum of **L2** in $CDCl_3$.

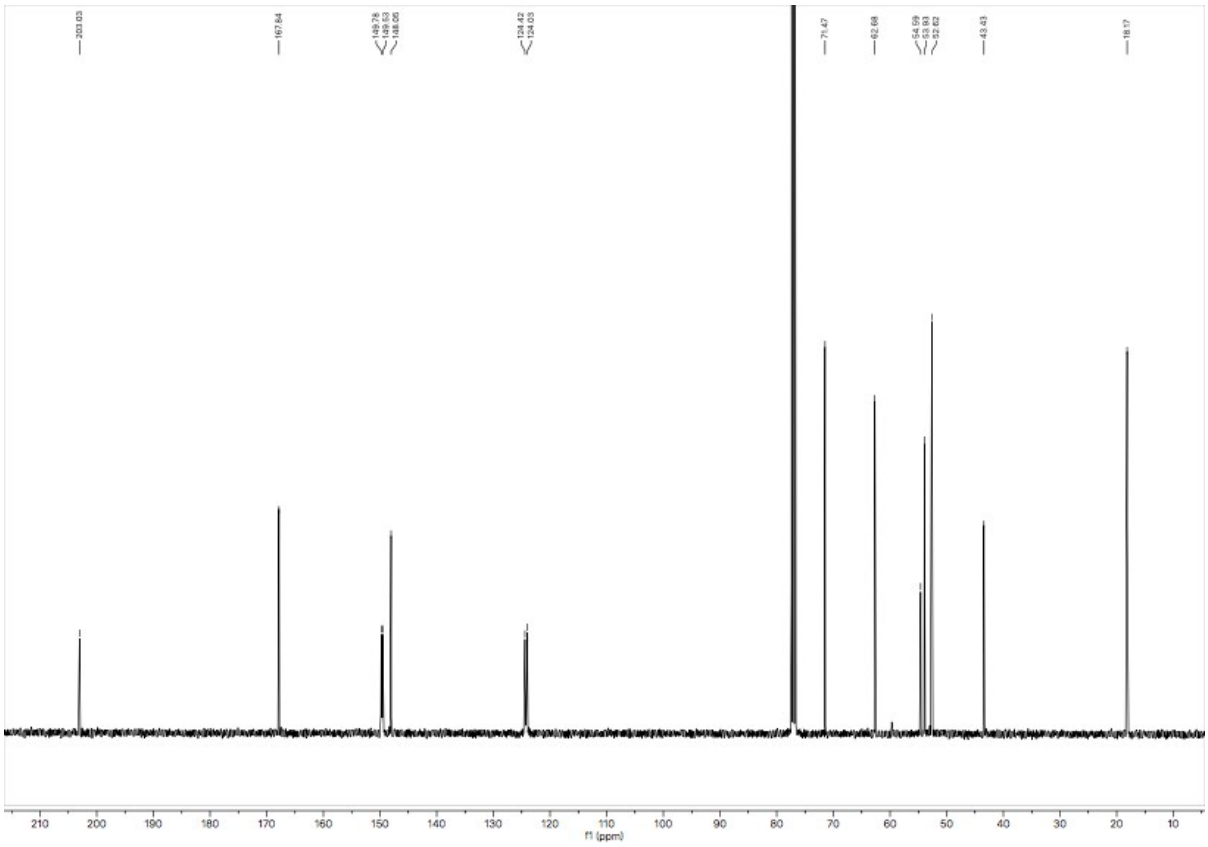

Figure S2. ^{13}C-NMR spectrum of **L2** in $CDCl_3$.

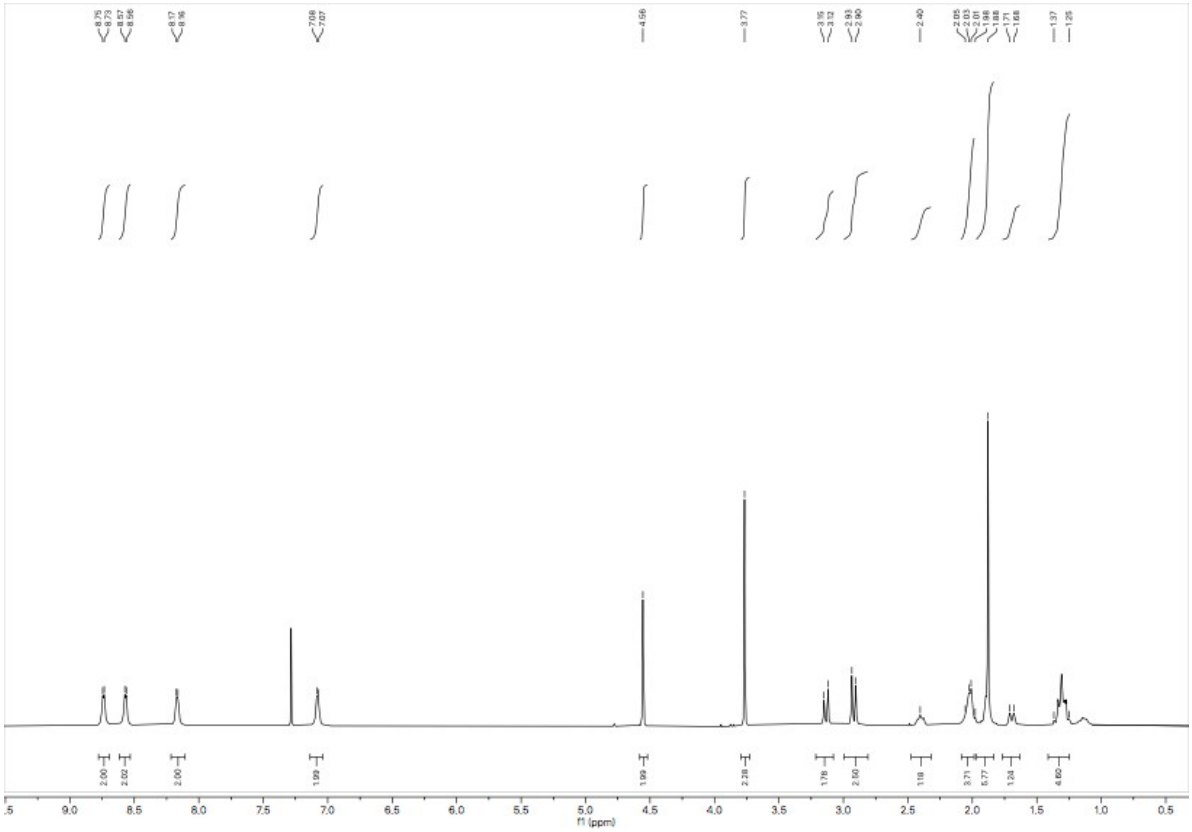

Figure S3. ^{1}H-NMR spectrum of **L3** in $CDCl_3$.

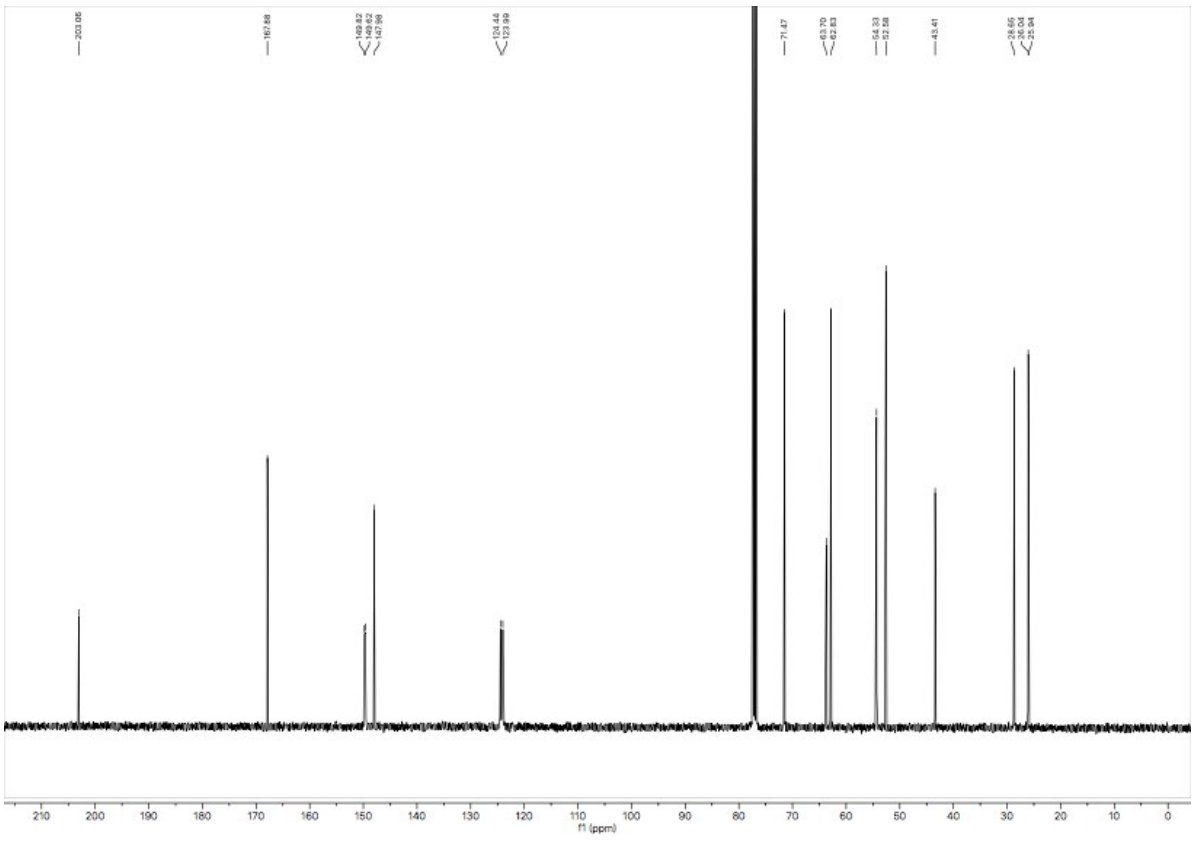

Figure S4. ^{13}C-NMR spectrum of **L3** in $CDCl_3$.

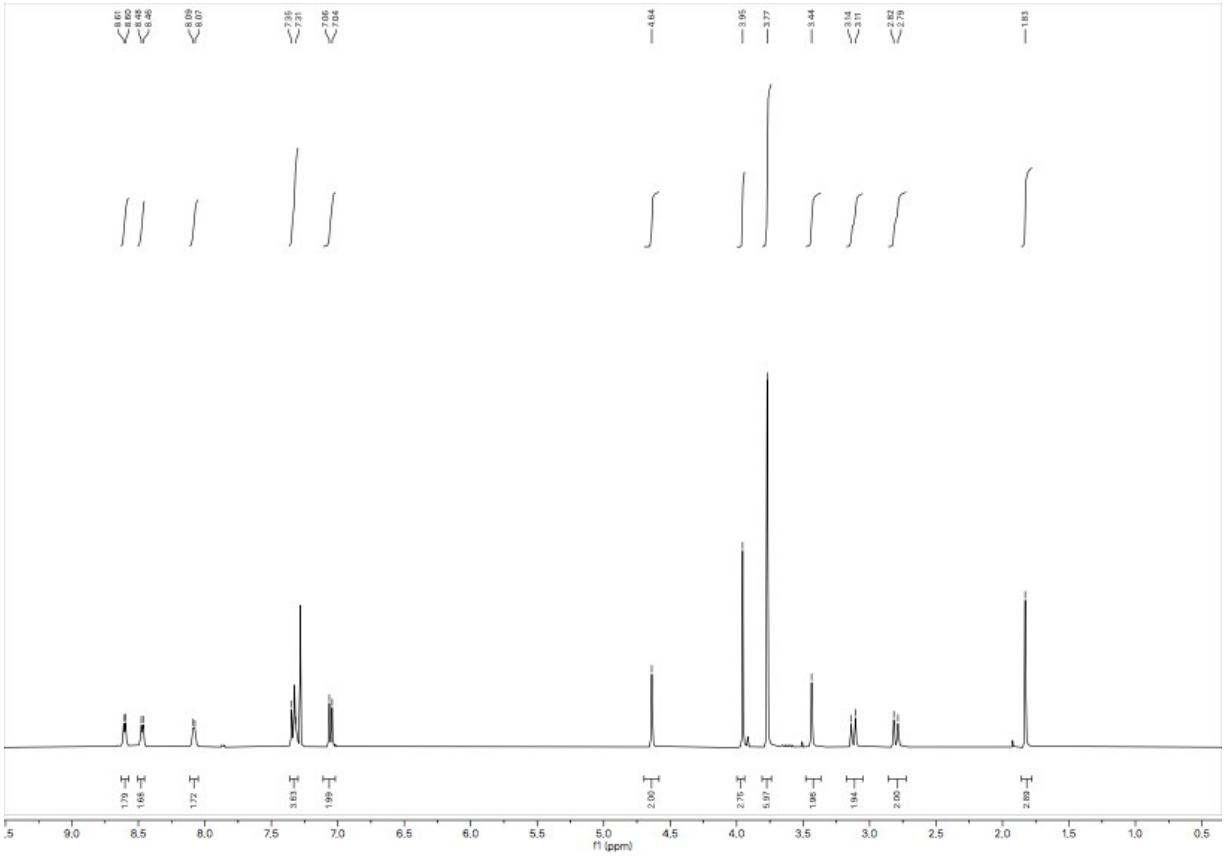

Figure S5. ^{1}H-NMR spectrum of **L5** in $CDCl_3$.

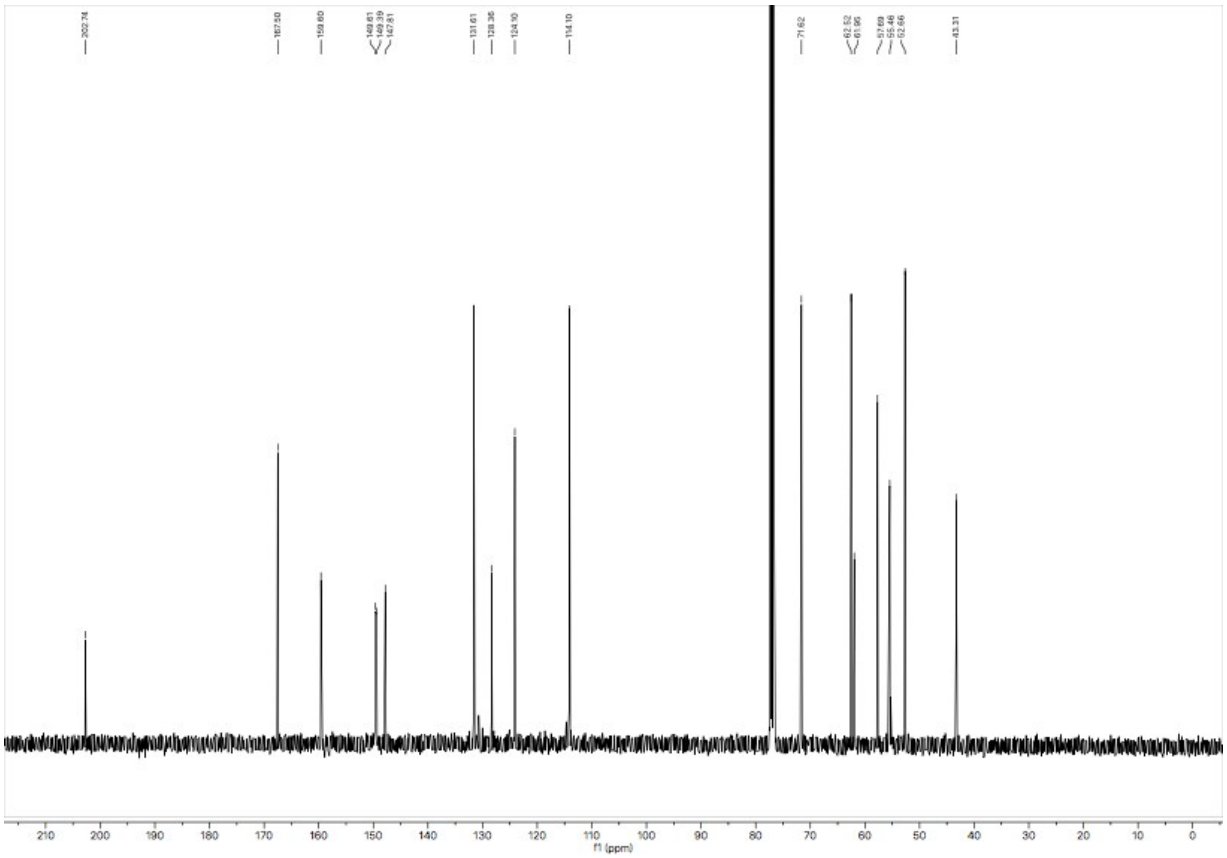

Figure S6. ^{13}C-NMR spectrum of **L5** in $CDCl_3$.

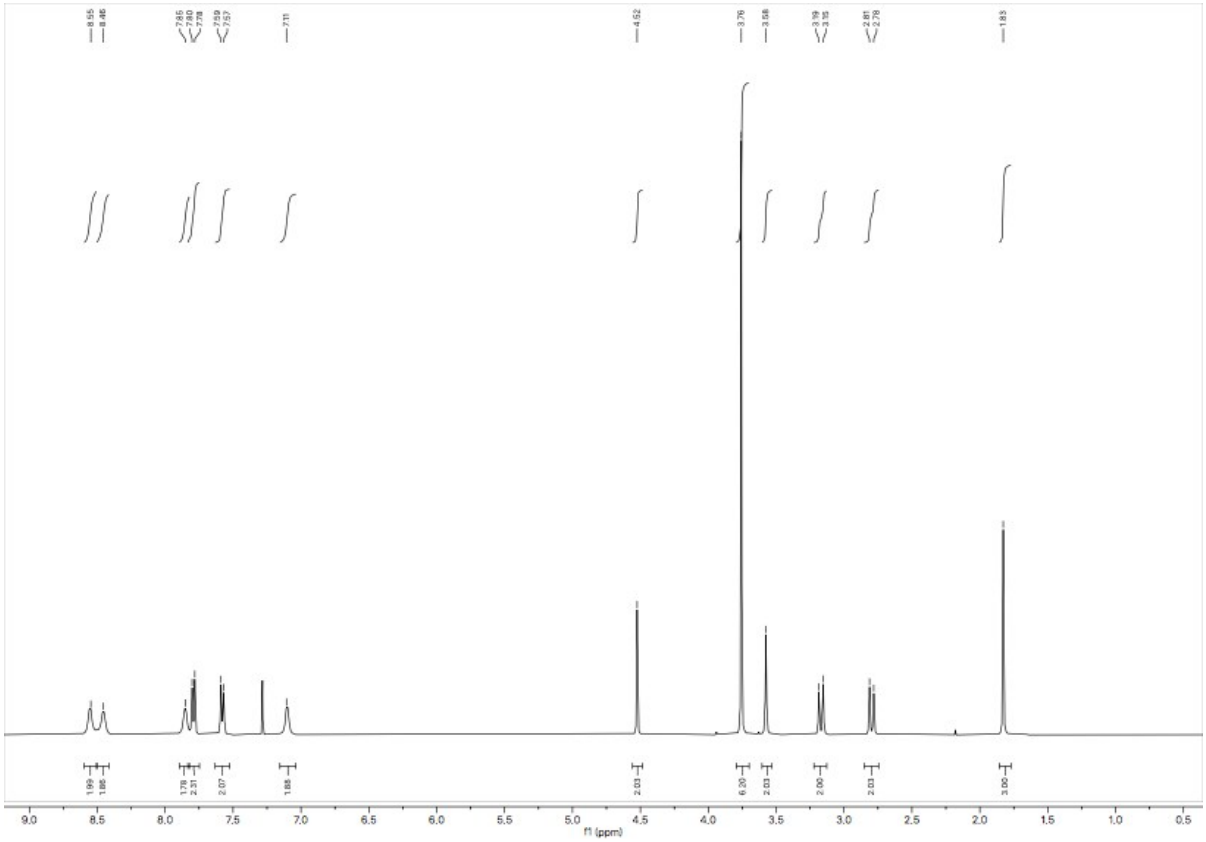

Figure S7. ^{1}H-NMR spectrum of **L6** in $CDCl_3$.

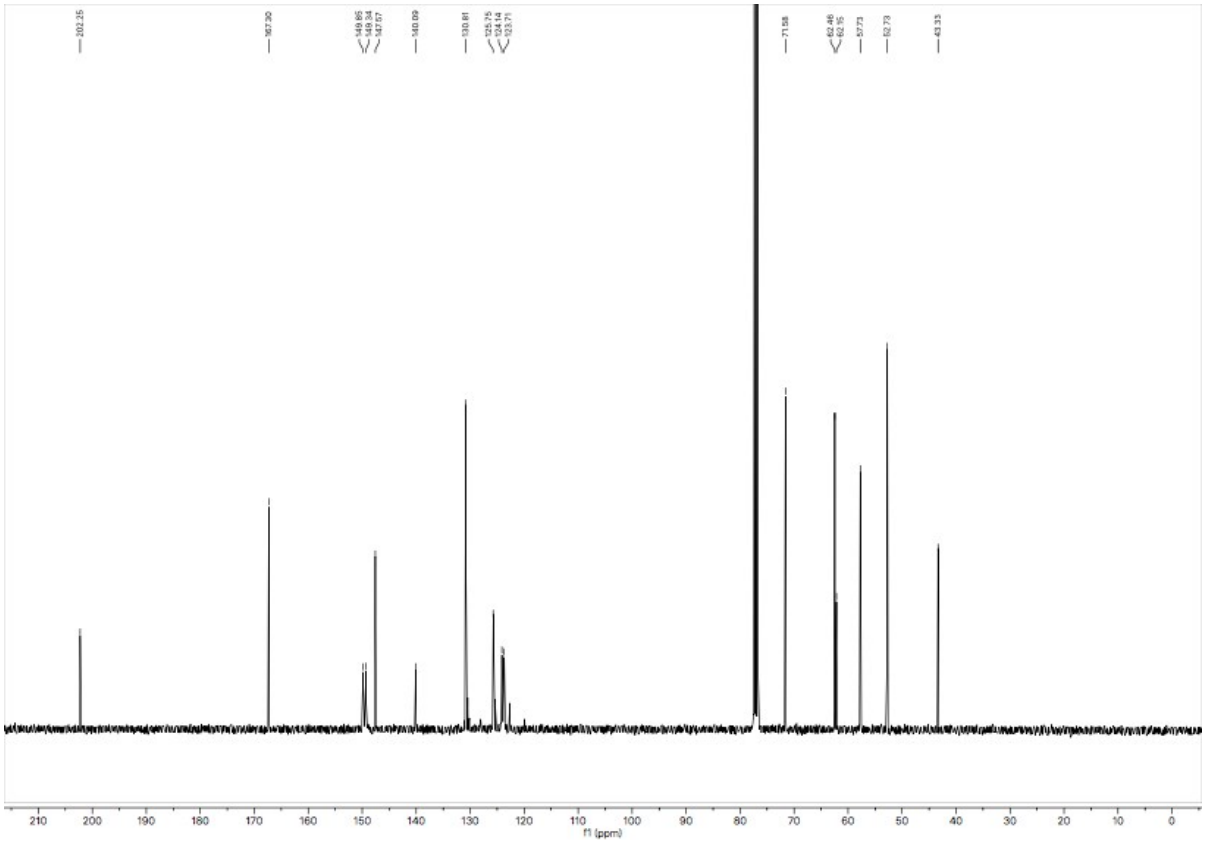

Figure S8. ^{13}C-NMR spectrum of **L6** in $CDCl_3$.

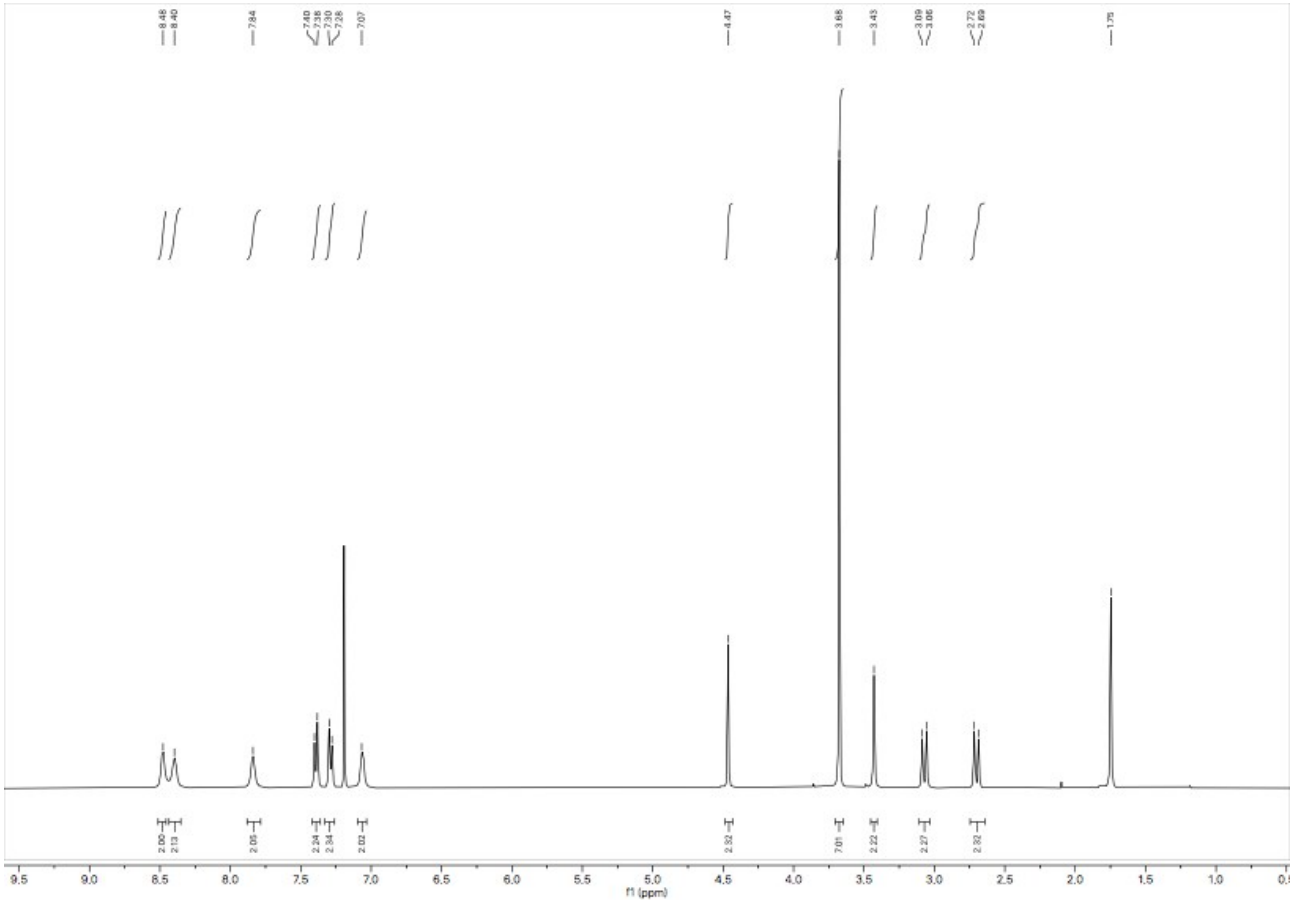

Figure S9. ^{1}H-NMR spectrum of **L7** in $CDCl_3$.

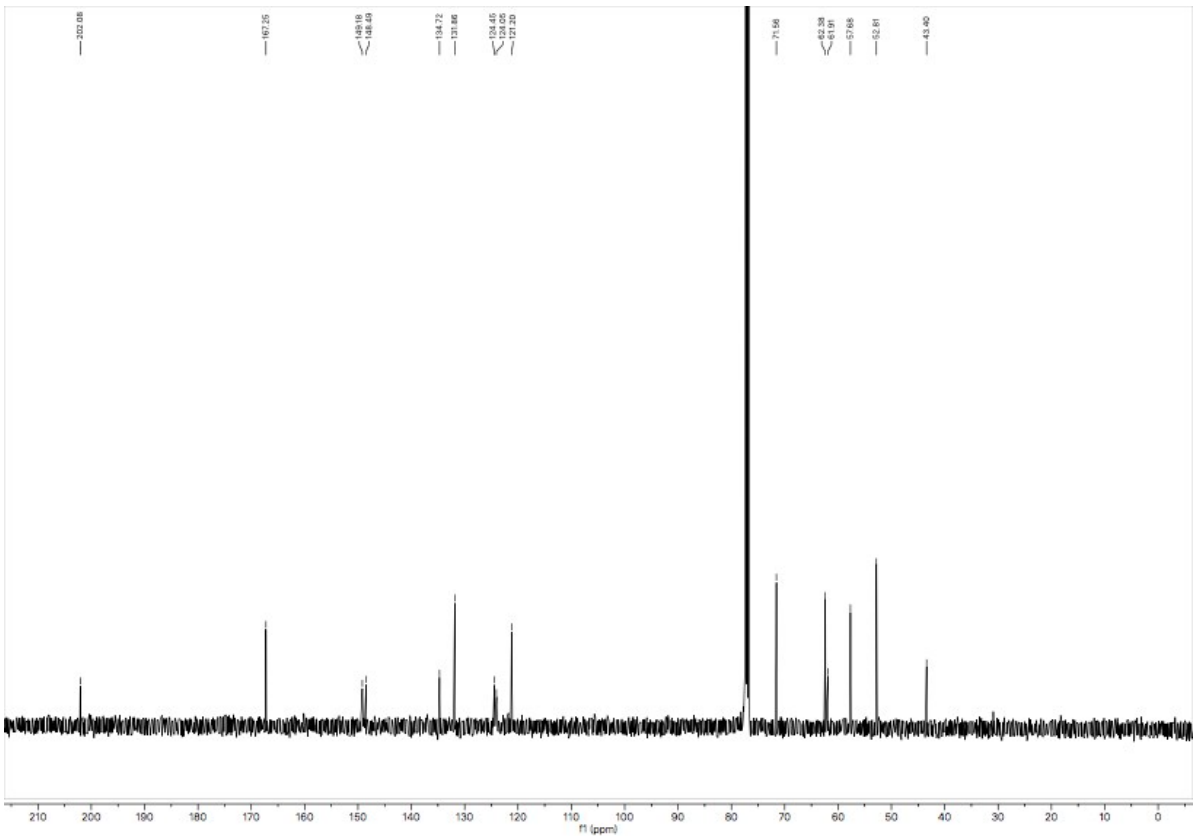

Figure S10. ^{13}C-NMR spectrum of **L7** in CDCl3.

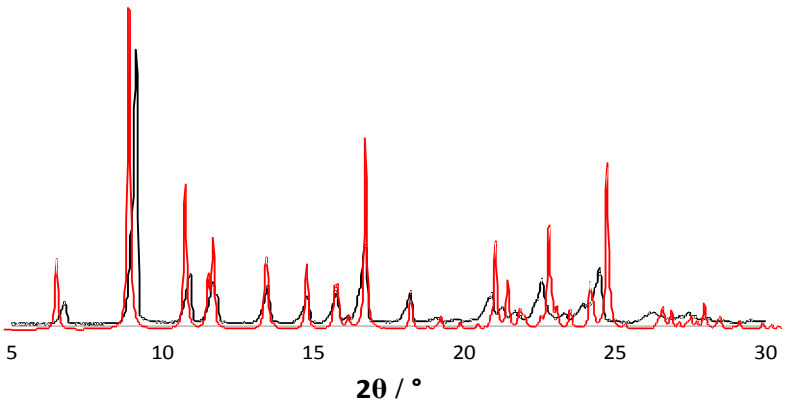

Figure S11. X-ray powder diffraction pattern for **L1** (black line) compared to simulated form SC data (red line).

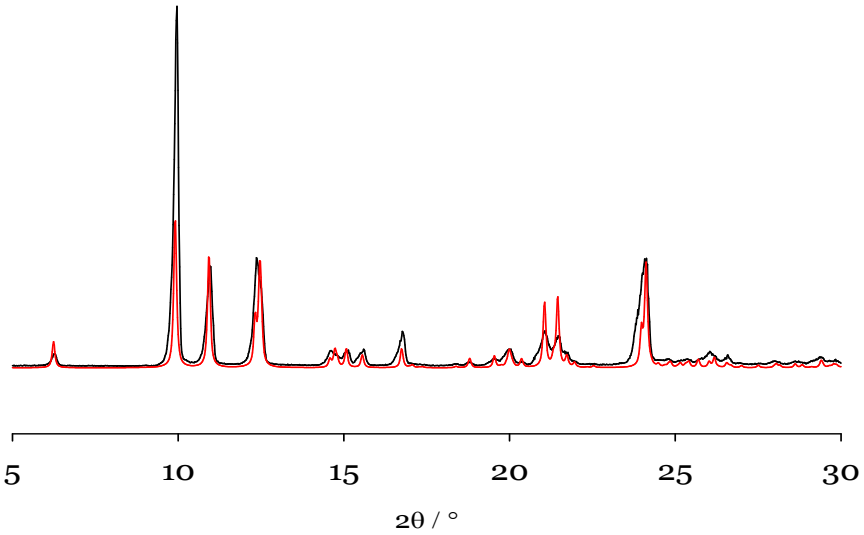

Figure S12. X-ray powder diffraction pattern for **L2** (black line) compared to simulated form SC data (red line).

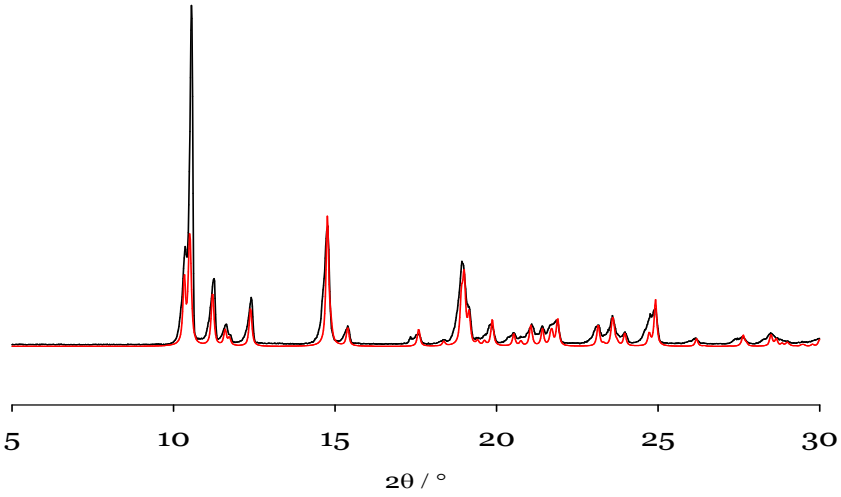

Figure S13. X-ray powder diffraction pattern for **L3** (black line) compared to simulated form SC data (red line).

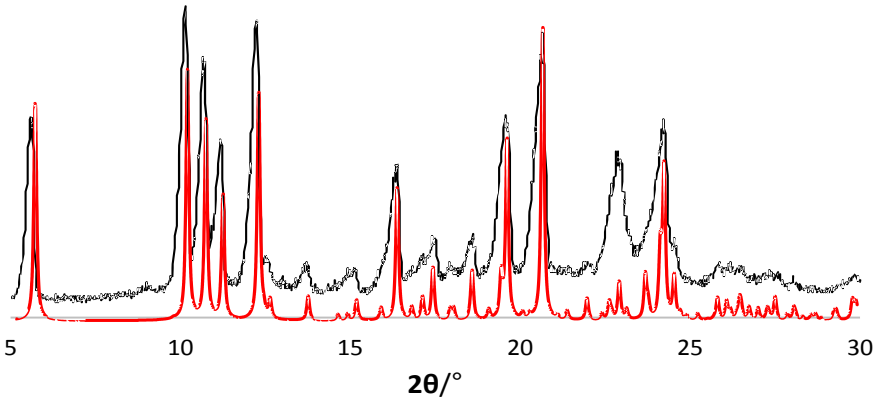

Figure S14. X-ray powder diffraction pattern for **L4** (black line) compared to simulated form SC data (red line).

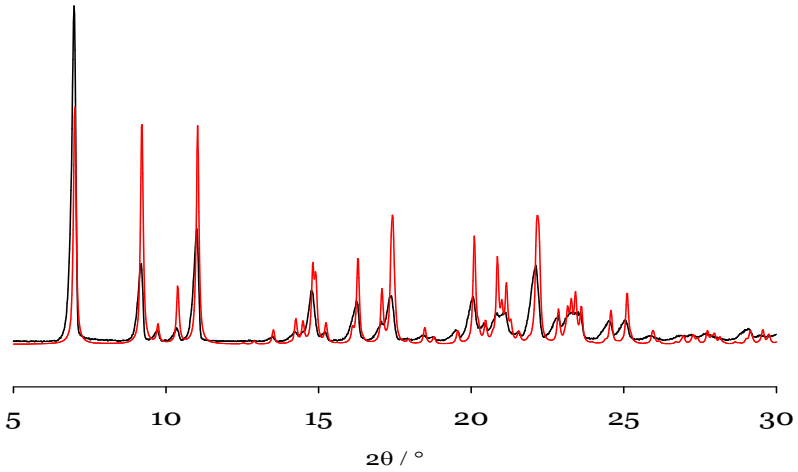

Figure S15. X-ray powder diffraction pattern for **L5** (black line) compared to silmulated form SC data (red line).

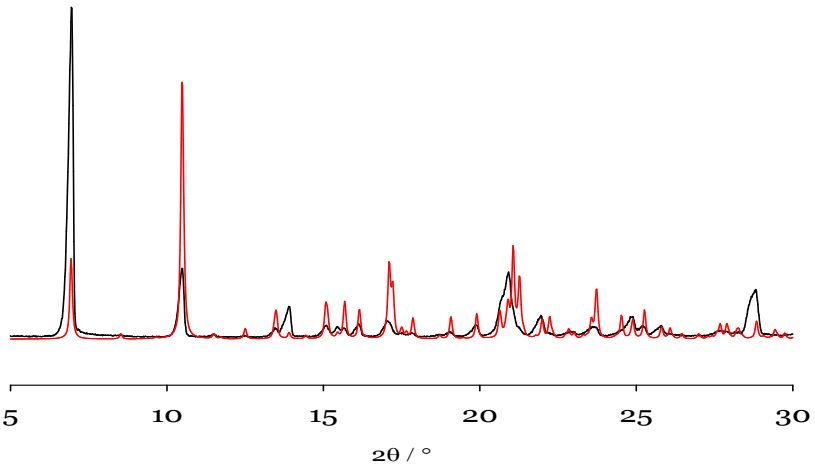

Figure S16 X-ray powder diffraction pattern for **L6** (black line) compared to simulated form SC data (red line).

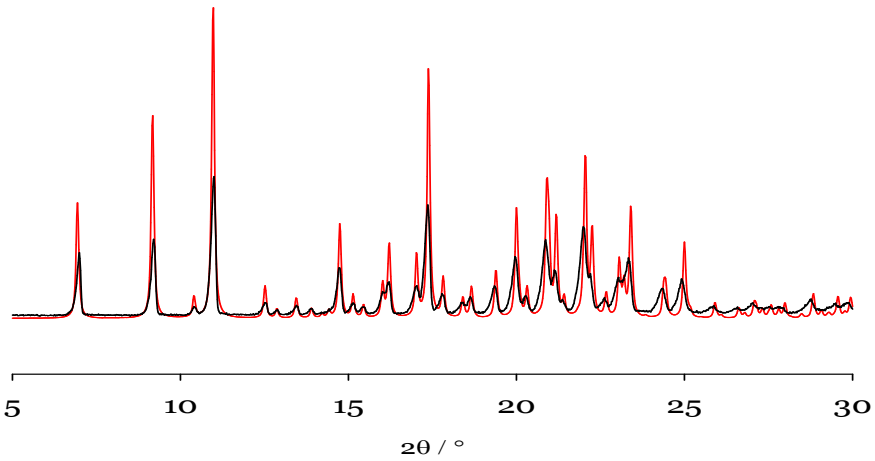

Figure S17. X-ray powder diffraction pattern for **L7** (black line) compared to simulated form SC data (red line).

DFT-CALCULATIONS

Solid-state DFT calculations were performed assuming the GGA PBE functional[1]. A numerical double zeta numerical basis set plus polarisation functions on all atoms (i.e. DNP set, roughly comparable with the usual 6-31G** gaussian contracted basis) centered on atoms has been used. Explicit van der Waals corrections[2] were also included to include important subtle inter and intra-particle interactions.[3] The DMol[3] package[4] was employed for all the solid-state calculations.

In the case of solid-state calculations, fixed experimental X-ray determined unit cells were used while atomic coordinates of all atoms were free to relax maintaining space group symmetry constraints. Lattice energies have been estimated as the difference (normalised by the number of the molecules) between the unit cell (immersed into crystalline architectures) energy and the sum of the energy of the free molecules. Lattice energies were roughly decomposed into van der Waals and dipole components of the interaction by the usage of explicit van der Waals corrections. Geometrical parameters optimised at the PBE/DNP level are listed below in pdb format.

Dipole moments, polarizabilities, volumes and surfaces have been evaluated for isolated molecules assuming the geometrical parameters of solid-state calculations. The corresponding B3LYP/6-31G** calculations have been performed by Gaussian09 suite of programs.[6]

Table S1. Summary of the lattice energy, E_{dimer} values, their break down into van der Waals, E_{vdW} and electrostatic E_{electr} terms(kcal/mol), ($E^* = E_{dimer} / 2$) and Dipole μ (D).

	E_{dimer}	E^*	E_{vdW}	E_{Elettr}	μ	
L1	-125.45	-62.725	-81.31	-44.14	0	
L2	-125.51	-62.755	-83.49	-42.01	0	
L3	-149.42		-93.57	-55.84	6.0765	Dimer 1
	-156.34		-96.30	-60.04	4.0319	Dimer 2
	-150.61		-93.71	-56.90	5.9315	Dimer 3
L4	-166.75		-106.25	-60.49	1.6614	Dimer 1
	-152.76		-106.25	-46.51	3.9757	Dimer 2
	-161.12	-80.56	-105.18	-55.94	0	Dimer 3
L5	-161.31		-102.73	-58.58	4.4619	Dimer 1
	-150.23		-96.86	-53.36	1.9313	Dimer 2
	-156.50		-98.04	-58.47	3.3153	Dimer 3
L6	-136.77	-68.385	-91.50	-45.27	0	
L7	-166.05		-109.22	-56.84	13.4777	Dimer 1
	-160.01		-103.50	-56.50	10.2553	Dimer 2
	-146.05		-98.86	-47.19	5.4034	Dimer 3
	-155.80		-103.03	-52.77	5.5904	Dimer 4

X-ray characterization.

Prism-like colorless single crystals of ligands **L2**, **L3**, **L6** and **L7** and of the **L6** 2:1 complex suitable for SC-XRD are obtained by slow evaporation of a methanol solution at room temperature. A single crystal is glued in a glass fiber and mounted for X-ray diffraction data analysis. The SC-XRD data were recorded at room temperature for **L2** and **L3**, while for **L6** and **L7** at 120 K and 150 K, respectively. The data of the **L6**-complex were also collected at 120K.

Intensity data were collected on a Bruker Apex II CCD diffractometer, using graphite-monochromatized Mo-Kα radiation (λ = 0.71073 Å). Intensity data were corrected for Lorentz-polarization effects and for absorption (*SADABS* [7]). The structures were solved by direct methods (*SIR-97* [8]) and completed by iterative cycles of full-matrix least squares refinement on F_o^2 and ΔF synthesis using the *SHELXL-18* [9] program (*WinGX* suite [10]).

The hydrogen atoms bonded to carbon were included at geometrically calculated positions and refined using a riding model. Uiso(H) were defined as 1·2Ueq of the parent carbon atoms for phenyl and methylene residues and 1·5Ueq of the parent carbon atoms for the methyl group. The hydrogen atoms related to the H_2O molecule in the **L6** dimeric complex were not located. These data can be obtained free of charge *via* www.ccdc.cam.ac.uk/conts/retrieving.html (or from the Cambridge Crystallographic Data Centre, 12, Union Road, Cambridge CB21EZ, UK; fax: ++44 1223 336 033; or deposit@ccdc.cam.ac.uk). CCDC-1921625 (**L2**), CCDC-1921624 (**L3**), CCDC-1921632 (**L6**), CCDC-1921627 (**L7**) and CCDC-1983773 (**L6**, 2:1 Mn-complex) numbers contain the supplementary crystallographic data for this paper. Crystallographic data were summarized in Tables S2-S7.

L5: A block-like colorless single crystal of **L5** was mounted in a nylon loop for single crystal X-ray analysis. Single-crystal XRD data were collected on a Bruker X8 Prospector APEX-II/CCD diffractometer equipped with a microfocusing mirror (Cu-K_α radiation, λ = 1.54178 Å) at room temperature. The structure was determined using direct methods (SHELXTL 97) and refined (based on F2 using all independent data) by full-matrix least-squares methods (SHELX 2014). All non-hydrogen atoms were located from different Fourier maps and refined with anisotropic displacement parameters. Hydrogen atoms were added in riding positions. CCDC-1986612

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Table S2: Crystallographic data of ligand **L2**.

Parameters	**L2**
Empirical formula	C25 H30 N4 O5
Formula weight	466.53
Temperature	294(2) K
Wavelength	0.710738 Å
Crystal system	Monoclinic
Space group	P $2_1/c$
Unit cell dimensions	a = 14.548(7) Å b = 11.382(2) Å β = 103.41(3) ° c = 14.751(3) Å
Volume	2375.8(9) $Å^3$
Z	4
Density (calculated)	1.304 mg/m^3
Absorption coefficient	0.082 mm^{-1}
F (000)	992
Crystal size	N/A
θ range for data collection	1.439 to 31.529°
Index ranges	-21≤h≤21, -16≤k≤16, -21≤l≤21
Reflections collected	24216
Independent reflections	7403 [R(int) = 0.0203]
Completeness to θ = 25.242°	99.9%
Absorption correction	N/A
Refinement method	Full-matrix least-squares on F^2
Data / Restraints / Parameters	7403 / 0 / 427
Goodness-of-fit on F^2	1.036
Final R indices [I>2σ(I)]	R1 = 0.0591, wR2 = 0.1473
R indices (all data)	R1 = 0.0770, wR2 = 0.1638

Largest diff. peak and hole	0.396 and -0.306 e.Å^{-3}

Table S3: Crystallographic data of ligand **L3**.

Parameters	**L3**
Empirical formula	C28 H34 N4 O5
Formula weight	506.59
Temperature	294(2) K
Wavelength	0.071073 Å
Crystal system	Monoclinic
Space group	P 2_1
Unit cell dimensions	*a* = 9.2923(19) Å *b* = 16.814(3) Å β = 114.86(3) ° *c* = 9.4272(12) Å
Volume	1336.4(6) Å^3
Z	2
Density (calculated)	1.259 mg/m^3
Absorption coefficient	0.087 mm^{-1}
F (000)	534
Crystal size	N/A
θ range for data collection	2.381 to 31.674°
Index ranges	-13≤h≤13, -24≤k≤24, -13≤l≤13
Reflections collected	14015
Independent reflections	7970 [R(int) = 0.0164]
Completeness to θ = 25.242°	100.0%
Absorption correction	N/A
Refinement method	Full-matrix least-squares on F^2
Data / Restraints / Parameters	7970 / 0 / 394
Goodness-of-fit on F^2	1.051
Final R indices [I>2σ(I)]	R1 = 0.0485, wR2 = 0.1192
R indices (all data)	R1 = 0.0559, wR2 = 0.1274

Largest diff. peak and hole	0.269 and -0.244 e.Å^{-3}	

Table S4: Crystallographic data of ligand **L5**.

Empirical formula	$C_{30}H_{32}N_4O_6$	
Formula weight	544.59	
Temperature	296(2) K	
Wavelength	1.54178 Å	
Crystal system	Orthorhombic	
Space group	P b c a	
Unit cell dimensions	a = 13.089(11) Å	α= 90°.
	b = 17.019(14) Å	β= 90°.
	c = 25.19(2) Å	γ = 90°.
Volume	5611(8) Å^3	
Z	8	
Density (calculated)	1.289 Mg/m^3	
Absorption coefficient	0.746 mm^{-1}	
F(000)	2304	
Crystal size	0.100 x 0.100 x 0.050 mm^3	
Theta range for data collection	11.426 to 51.052°.	
Index ranges	-12<=h<=10, -14<=k<=17, -25<=l<=22	
Reflections collected	9061	
Independent reflections	2685 [R(int) = 0.2320]	
Completeness to theta = 51.052°	88.8 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2685 / 0 / 365	
Goodness-of-fit on F^2	0.976	
Final R indices [I>2sigma(I)]	R1 = 0.0667, wR2 = 0.1242	
R indices (all data)	R1 = 0.1540, wR2 = 0.1527	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.187 and -0.198 e.Å^{-3}	

Table S5: Crystallographic data of ligand **L6**.

Parameters	**L6**
Empirical formula	C30 H29 F3 N4 O5
Formula weight	582.57
Temperature	120(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P $2_1/c$
Unit cell dimensions	a = 12.767(3) Å b = 13.128(3) Å β = 98.68(3) ° c = 16.753(3) Å
Volume	2779.0(10) $Å^3$
Z	4
Density (calculated)	1.392 mg/m^3
Absorption coefficient	0.109 mm^{-1}
F (000)	1216
Crystal size	N/A
θ range for data collection	1.612 to 31.644°
Index ranges	-18≤h≤17, -19≤k≤19, -23≤l≤24
Reflections collected	31388
Independent reflections	8757 [R(int) = 0.0185]
Completeness to θ = 25.242°	100.0%
Absorption correction	N/A
Refinement method	Full-matrix least-squares on F^2
Data / Restraints / Parameters	8757/ 0 / 379
Goodness-of-fit on F^2	1.058
Final R indices [I>2σ(I)]	R1 = 0.0517, wR2 = 0.1202
R indices (all data)	R1 = 0.0667, wR2 = 0.1299

Largest diff. peak and hole	0.56 and -0.57 e.Å^{-3}

Table S6: Crystallographic data of ligand **L7**.

Parameters	**L7**
Empirical formula	C30 H29 F3 N4 O6
Formula weight	598.20
Temperature	150(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	P b c a
Unit cell dimensions	*a* = 13.1269(3) Å *b* = 16.7438(3) Å *c* = 25.5484(5) Å
Volume	5615.4(2) Å^3
Z	8
Density (calculated)	1.42 mg/m^3
Absorption coefficient	0.113 mm^{-1}
F(000)	2496
Crystal size	N/A
θ range for data collection	1.594 to 21.228°
Index ranges	-13≤h≤13, -17≤k≤16, -25≤l≤25
Reflections collected	22575
Independent reflections	3083 [R(int) = 0.0431]
Completeness to θ = 21.228°	100.0%
Absorption correction	N/A
Refinement method	Full-matrix least-squares on F^2
Data / Restraints / Parameters	2122 / 0 / 388
Goodness-of-fit on F^2	1.015
Final R indices [I>2σ(I)]	R1 = 0.0425, wR2 = 0.0984
R indices (all data)	R1 = 0.0734 wR2 = 0.1079

Largest diff. peak and hole	0.49 and -0.41 e.Å^{-3}

Table S7: Crystallographic data of **L6** dimeric complex.

Parameters	**6·TCM^{SC} H2O MeOH**
Empirical formula	C32 H38 Cl4 F3 Mn0.5 N4 O8
Formula weight	830.92
Temperature	120(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P $2_1/n$
Unit cell dimensions	a = 8.3380(17) Å b = 27.317(6) Å β = 94.12(3) ° c = 16.519(3) Å
Volume	3752.8(13) Å^3
Z	4
Density (calculated)	1.471 mg/m^3
Absorption coefficient	0.544 mm^{-1}
F (000)	1710
Crystal size	0.040 x 0.300 x 0.030 mm^3
Θ range for data collection	1.443 to 26371°
Index ranges	-10≤h≤10, -34≤k≤34, -20≤l≤20
Reflections collected	28376
Independent reflections	7686 [R(int) = 0.0258]
Completeness to θ = 26.371°	100.0%
Refinement method	Full-matrix least-squares on F^2
Data / Restraints / Parameters	7686/ 0 / 477
Goodness-of-fit on F^2	1.065
Final R indices [I>2σ(I)]	R1 = 0.1022, wR2 = 0.2700
R indices (all data)	R1 = 0.1237, wR2 = 0.2892
Largest diff. peak and hole	2.22 and -2.33 e.Å^{-3}

Structure L1 (*pdb file*)

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REMARK  L1 PDB file
CRYST1   8.322   9.858  13.434  85.46  79.77  84.04 P-1
ORIGX1      1.000000  0.000000  0.000000        0.00000
ORIGX2      0.000000  1.000000  0.000000        0.00000
ORIGX3      0.000000  0.000000  1.000000        0.00000
SCALE1      0.120169 -0.012543 -0.020951        0.00000
SCALE2      0.000000  0.101994 -0.006339        0.00000
SCALE3      0.000000  0.000000  0.075786        0.00000
ATOM      1  O5  MOL     2      -0.139  -0.639   8.440  1.00  0.06          O1-
ATOM      2  O2  MOL     2       1.833   4.221  12.358  1.00  0.05           O
ATOM      3  O1  MOL     2       2.252   2.363  13.479  1.00  0.06          O1-
ATOM      4  O3  MOL     2       0.360   1.078  11.482  1.00  0.05          O1-
ATOM      5  O4  MOL     2       0.735  -1.636  10.226  1.00  0.05           O
ATOM      6  C10 MOL     2       3.100  -0.230   9.743  1.00  0.03           C
ATOM      7  H8  MOL     2       3.048  -0.843  10.506  1.00  0.04           H
ATOM      8  N3  MOL     2       4.155   0.757  10.035  1.00  0.03           N
ATOM      9  N4  MOL     2       4.308  -2.595   6.324  1.00  0.06          N1-
ATOM     10  N5  MOL     2       2.433   2.631   8.625  1.00  0.04           N
ATOM     11  C1  MOL     2      -0.193  -2.737  10.057  1.00  0.06           C
ATOM     12  H3  MOL     2      -1.093  -2.411  10.135  1.00  0.09           H
ATOM     13  H1  MOL     2      -0.033  -3.398  10.734  1.00  0.09           H
ATOM     14  H27 MOL     2      -0.069  -3.130   9.190  1.00  0.09           H
ATOM     15  C2  MOL     2       0.653  -0.655   9.331  1.00  0.04           C
ATOM     16  C3  MOL     2       1.695   0.434   9.572  1.00  0.03           C
ATOM     17  C4  MOL     2       3.839   1.643  11.168  1.00  0.03           C
ATOM     18  H22 MOL     2       3.869   1.103  11.985  1.00  0.04           H
ATOM     19  C5  MOL     2       4.915   2.709  11.281  1.00  0.04           C
ATOM     20  C6  MOL     2       5.388   3.397  10.178  1.00  0.05           C
ATOM     21  H23 MOL     2       5.040   3.225   9.333  1.00  0.05           H
ATOM     22  C7  MOL     2       6.382   4.344  10.346  1.00  0.05           C
ATOM     23  H24 MOL     2       6.689   4.795   9.593  1.00  0.06           H
ATOM     24  N1  MOL     2       6.928   4.649  11.527  1.00  0.06          N1-
ATOM     25  C9  MOL     2       3.487  -1.048   8.521  1.00  0.04           C
ATOM     26  C10 MOL     2       3.497  -2.428   8.572  1.00  0.05           C
ATOM     27  H7  MOL     2       3.225  -2.867   9.345  1.00  0.06           H
ATOM     28  C11 MOL     2       3.913  -3.153   7.474  1.00  0.06           C
ATOM     29  H6  MOL     2       3.920  -4.081   7.537  1.00  0.07           H
ATOM     30  C12 MOL     2       4.272  -1.263   6.281  1.00  0.05           C
ATOM     31  H5  MOL     2       4.521  -0.846   5.488  1.00  0.06           H
ATOM     32  C13 MOL     2       3.890  -0.465   7.333  1.00  0.04           C
ATOM     33  H4  MOL     2       3.904   0.461   7.248  1.00  0.05           H
ATOM     34  C14 MOL     2       5.393   0.035  10.359  1.00  0.05           C
ATOM     35  H9  MOL     2       6.095   0.667  10.535  1.00  0.07           H
ATOM     36  H10 MOL     2       5.643  -0.522   9.618  1.00  0.07           H
ATOM     37  H11 MOL     2       5.252  -0.511  11.137  1.00  0.07           H
ATOM     38  C15 MOL     2       2.417   2.293  11.082  1.00  0.03           C
ATOM     39  C16 MOL     2       2.153   2.941  12.440  1.00  0.04           C
ATOM     40  C17 MOL     2       1.548   4.846  13.632  1.00  0.07           C
ATOM     41  H12 MOL     2       0.798   4.408  14.042  1.00  0.10           H
ATOM     42  H14 MOL     2       1.342   5.773  13.495  1.00  0.10           H
ATOM     43  H13 MOL     2       2.315   4.770  14.205  1.00  0.10           H
ATOM     44  C18 MOL     2       2.203   3.277   9.908  1.00  0.04           C
ATOM     45  H21 MOL     2       1.295   3.619   9.936  1.00  0.05           H
ATOM     46  H20 MOL     2       2.808   4.029  10.002  1.00  0.05           H
ATOM     47  C19 MOL     2       1.547   1.486   8.442  1.00  0.04           C
ATOM     48  H15 MOL     2       1.742   1.066   7.590  1.00  0.05           H
ATOM     49  H16 MOL     2       0.628   1.797   8.416  1.00  0.05           H
ATOM     50  C20 MOL     2       2.248   3.584   7.537  1.00  0.06           C
ATOM     51  H18 MOL     2       1.342   3.899   7.537  1.00  0.09           H
ATOM     52  H17 MOL     2       2.438   3.155   6.699  1.00  0.09           H
ATOM     53  H19 MOL     2       2.844   4.327   7.657  1.00  0.09           H
ATOM     54  C21 MOL     2       1.374   1.203  10.846  1.00  0.03           C
ATOM     55  C22 MOL     2       5.486   3.005  12.511  1.00  0.05           C
ATOM     56  H26 MOL     2       5.210   2.561  13.280  1.00  0.06           H
ATOM     57  C23 MOL     2       6.468   3.968  12.573  1.00  0.06           C
ATOM     58  H25 MOL     2       6.835   4.156  13.406  1.00  0.07           H
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CONECT  54  51
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CONECT  56  20  58  57
CONECT  57  56
CONECT  58  25  56   1
END
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Structure L2 (*pdb file*)

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REMARK   L2 PDB file
CRYST1   14.548   11.382   14.751  90.00 103.41  90.00 P21/C
ORIGX1      1.000000  0.000000  0.000000        0.00000
ORIGX2      0.000000  1.000000  0.000000        0.00000
ORIGX3      0.000000  0.000000  1.000000        0.00000
SCALE1      0.068738  0.000000  0.016388        0.00000
SCALE2      0.000000  0.087858  0.000000        0.00000
SCALE3      0.000000  0.000000  0.069692        0.00000
ATOM      1  C1  MOL     2       5.537  -0.436  16.288  1.00  0.03           C
ATOM      2  C2  MOL     2       5.755   1.006  15.859  1.00  0.03           C
ATOM      3  C3  MOL     2       6.750   1.599  16.881  1.00  0.03           C
ATOM      4  C4  MOL     2       7.786  -0.526  17.212  1.00  0.04           C
ATOM      5  C5  MOL     2       6.841  -1.205  16.190  1.00  0.03           C
ATOM      6  C6  MOL     2       7.302  -1.198  14.690  1.00  0.03           C
ATOM      7  C7  MOL     2       6.225   1.006  14.365  1.00  0.03           C
ATOM      8  C8  MOL     2       6.624  -2.648  16.659  1.00  0.04           C
ATOM      9  C9  MOL     2       4.410   1.736  15.887  1.00  0.04           C
ATOM     10  C10 MOL     2       5.720  -4.750  16.129  1.00  0.07           C
ATOM     11  C11 MOL     2       3.142   3.473  16.813  1.00  0.08           C
ATOM     12  C12 MOL     2       8.899   1.486  17.968  1.00  0.05           C
ATOM     13  C13 MOL     2      10.217   0.766  18.092  1.00  0.09           C
ATOM     14  C14 MOL     2       9.161   2.956  17.681  1.00  0.07           C
ATOM     15  C18 MOL     2       7.614   0.054  12.681  1.00  0.04           C
ATOM     16  C19 MOL     2       6.511   2.430  13.920  1.00  0.03           C
ATOM     17  C20 MOL     2       5.578   3.162  13.206  1.00  0.04           C
ATOM     18  C21 MOL     2       5.893   4.461  12.836  1.00  0.06           C
ATOM     19  C22 MOL     2       7.914   4.355  13.822  1.00  0.05           C
ATOM     20  C23 MOL     2       7.719   3.046  14.218  1.00  0.04           C
ATOM     21  C24 MOL     2       8.632  -1.915  14.535  1.00  0.03           C
ATOM     22  C25 MOL     2       8.705  -3.206  14.041  1.00  0.04           C
ATOM     23  C26 MOL     2       9.948  -3.807  13.910  1.00  0.05           C
ATOM     24  C27 MOL     2      11.015  -1.982  14.708  1.00  0.05           C
ATOM     25  C28 MOL     2       9.829  -1.290  14.862  1.00  0.04           C
ATOM     26  N1  MOL     2       8.029   0.884  16.917  1.00  0.03           N
ATOM     27  N2  MOL     2       7.412   0.164  14.136  1.00  0.03           N
ATOM     28  N3  MOL     2       7.028   5.076  13.140  1.00  0.06           N
ATOM     29  N4  MOL     2      11.099  -3.229  14.241  1.00  0.05           N
ATOM     30  O1  MOL     2       4.515  -0.868  16.754  1.00  0.05           O
ATOM     31  O2  MOL     2       3.492   1.457  15.175  1.00  0.06           O
ATOM     32  O3  MOL     2       4.388   2.737  16.761  1.00  0.06           O
ATOM     33  O4  MOL     2       7.027  -3.082  17.689  1.00  0.08           O
ATOM     34  O5  MOL     2       5.936  -3.367  15.779  1.00  0.05           O
ATOM     35  H6  MOL     2       6.624  -1.698  14.197  1.00  0.03           H
ATOM     36  H7  MOL     2       5.451   0.690  13.854  1.00  0.03           H
ATOM     37  H20 MOL     2       4.725   2.777  12.954  1.00  0.05           H
ATOM     38  H21 MOL     2       5.266   4.974  12.308  1.00  0.08           H
ATOM     39  H22 MOL     2       8.771   4.792  14.082  1.00  0.06           H
ATOM     40  H23 MOL     2       8.395   2.577  14.700  1.00  0.04           H
ATOM     41  H25 MOL     2       7.895  -3.654  13.761  1.00  0.05           H
ATOM     42  H26 MOL     2      10.009  -4.667  13.504  1.00  0.07           H
ATOM     43  H27 MOL     2      11.855  -1.548  14.987  1.00  0.07           H
ATOM     44  H28 MOL     2       9.836  -0.388  15.188  1.00  0.04           H
ATOM     45  H31 MOL     2       6.910   2.534  16.630  1.00  0.04           H
ATOM     46  H32 MOL     2       6.296   1.564  17.760  1.00  0.04           H
ATOM     47  H41 MOL     2       8.611  -1.033  17.201  1.00  0.04           H
ATOM     48  H42 MOL     2       7.368  -0.658  18.101  1.00  0.04           H
ATOM     49 1H18 MOL     2       6.824  -0.353  12.248  1.00  0.07           H
ATOM     50 2H18 MOL     2       7.719   0.899  12.273  1.00  0.06           H
ATOM     51 3H18 MOL     2       8.403  -0.478  12.473  1.00  0.06           H
ATOM     52 0H20 MOL     2       8.414   1.410  18.862  1.00  0.06           H
ATOM     53 0H10 MOL     2       5.243  -5.122  15.353  1.00  0.10           H
ATOM     54 1H10 MOL     2       5.194  -4.803  16.960  1.00  0.10           H
ATOM     55 0H11 MOL     2       2.468   2.880  17.046  1.00  0.09           H
ATOM     56 2H11 MOL     2       3.311   4.154  17.477  1.00  0.10           H
ATOM     57 1H11 MOL     2       2.877   3.813  15.942  1.00  0.09           H
ATOM     58 2H10 MOL     2       6.534  -5.145  16.286  1.00  0.11           H
ATOM     59 3H13 MOL     2      10.790   1.275  18.754  1.00  0.10           H
ATOM     60 1H13 MOL     2      10.682   0.740  17.190  1.00  0.11           H
ATOM     61 3H14 MOL     2       9.838   3.301  18.352  1.00  0.09           H
ATOM     62 1H14 MOL     2       9.596   3.073  16.745  1.00  0.13           H
ATOM     63 2H13 MOL     2      10.173  -0.171  18.410  1.00  0.13           H
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ATOM     64 2H14 MOL     2       8.269   3.551  17.793  1.00  0.12          H
TER      65
CONECT    1   15
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CONECT    3    2   10    4    8
CONECT    4    3   27   46   47
CONECT    5   27    6   48   49
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CONECT    8    3   28   17   37
CONECT    9    6   34   35
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CONECT   18   17   19   38
CONECT   19   18   29   39
CONECT   20   29   21   40
CONECT   21   17   20   41
CONECT   22    7   23   26
CONECT   23   22   24   42
CONECT   24   23   30   43
CONECT   25   30   26   44
CONECT   26   22   25   45
CONECT   27    4    5   13
CONECT   28    7    8   16
CONECT   29   19   20
CONECT   30   24   25
CONECT   31    2
CONECT   32   10
CONECT   33   10   12
CONECT   34    9
CONECT   35    9   11
CONECT   36    7
CONECT   37    8
CONECT   38   18
CONECT   39   19
CONECT   40   20
CONECT   41   21
CONECT   42   23
CONECT   43   24
CONECT   44   25
CONECT   45   26
CONECT   46    4
CONECT   47    4
CONECT   48    5
CONECT   49    5
CONECT   50   16
CONECT   51   16
CONECT   52   16
CONECT   53   13
CONECT   54   11
CONECT   55   11
CONECT   56   12
CONECT   57   12
CONECT   58   12
CONECT   59   11
CONECT   60   14
CONECT   61   14
CONECT   62   15
CONECT   63   15
CONECT   64   14
END
```

Structure L3 (*pdb file*)

```
REMARK   L3 PDB file
CRYST1   9.292   16.814    9.427  90.00 114.86  90.00 P21
ORIGX1      1.000000  0.000000  0.000000        0.00000
ORIGX2      0.000000  1.000000  0.000000        0.00000
ORIGX3      0.000000  0.000000  1.000000        0.00000
SCALE1      0.107616  0.000000  0.049862        0.00000
SCALE2      0.000000  0.059474  0.000000        0.00000
SCALE3      0.000000  0.000000  0.116909        0.00000
ATOM      1  N2  MOL     2      -1.861  13.246   1.160  1.00  0.03           N
ATOM      2  O3  MOL     2      -1.430  14.067  -2.875  1.00  0.05           O
ATOM      3  N1  MOL     2      -0.326  15.692   1.528  1.00  0.03           N
ATOM      4  O4  MOL     2       2.911  13.059   1.488  1.00  0.05           O1-
ATOM      5  C2  MOL     2      -0.901  14.727  -0.672  1.00  0.03           C
ATOM      6  O1  MOL     2       1.150  13.778  -1.492  1.00  0.05           O1-
ATOM      7  C4  MOL     2       0.808  14.783   1.668  1.00  0.03           C
ATOM      8  H8A MOL     2       0.919  14.556   2.605  1.00  0.04           H
ATOM      9  H8B MOL     2       1.615  15.233   1.374  1.00  0.04           H
ATOM     10  C1  MOL     2       0.381  13.917  -0.583  1.00  0.03           C
ATOM     11  C5  MOL     2       0.624  13.479   0.847  1.00  0.03           C
ATOM     12  C19 MOL     2      -3.349  14.725  -0.093  1.00  0.03           C
ATOM     13  C12 MOL     2      -0.194  16.935   2.335  1.00  0.04           C
ATOM     14  C6  MOL     2      -0.567  12.560   1.281  1.00  0.03           C
ATOM     15  H13 MOL     2      -0.581  11.781   0.688  1.00  0.03           H
ATOM     16  C24 MOL     2      -0.367  12.066   2.700  1.00  0.03           C
ATOM     17  C7  MOL     2      -2.098  13.866  -0.150  1.00  0.03           C
ATOM     18 5H01 MOL     2      -2.256  13.148  -0.797  1.00  0.04           H
ATOM     19  N3  MOL     2      -5.625  16.368  -0.072  1.00  0.06           N1-
ATOM     20  C28 MOL     2      -0.792  12.784   3.809  1.00  0.04           C
ATOM     21  O2  MOL     2      -1.164  16.236  -2.521  1.00  0.08           O1-
ATOM     22  C25 MOL     2       0.251  10.849   2.941  1.00  0.05           C
ATOM     23 9H01 MOL     2       0.534  10.317   2.233  1.00  0.06           H
ATOM     24  C3  MOL     2      -0.586  16.009   0.141  1.00  0.03           C
ATOM     25 AH02 MOL     2       0.190  16.450  -0.240  1.00  0.04           H
ATOM     26 BH02 MOL     2      -1.336  16.620   0.085  1.00  0.04           H
ATOM     27  C17 MOL     2      -0.423  16.663   3.809  1.00  0.05           C
ATOM     28  C27 MOL     2      -0.578  12.274   5.071  1.00  0.06           C
ATOM     29 2H02 MOL     2      -0.882  12.766   5.800  1.00  0.07           H
ATOM     30  N4  MOL     2       0.042  11.112   5.310  1.00  0.07           N1-
ATOM     31  C9  MOL     2      -1.167  15.125  -2.121  1.00  0.04           C
ATOM     32  C23 MOL     2      -4.248  14.724  -1.147  1.00  0.05           C
ATOM     33 5H02 MOL     2      -4.108  14.179  -1.888  1.00  0.06           H
ATOM     34  C20 MOL     2      -3.629  15.548   0.985  1.00  0.04           C
ATOM     35  C10 MOL     2       3.062  10.762   0.168  1.00  0.05           C
ATOM     36 CH02 MOL     2       3.542  10.875  -0.860  1.00  0.06           H
ATOM     37  C18 MOL     2      -2.933  12.262   1.391  1.00  0.05           C
ATOM     38 DH02 MOL     2      -2.884  11.572   0.725  1.00  0.06           H
ATOM     39 EH02 MOL     2      -3.786  12.699   1.336  1.00  0.06           H
ATOM     40 FH02 MOL     2      -2.829  11.872   2.262  1.00  0.06           H
ATOM     41  C22 MOL     2      -5.361  15.555  -1.078  1.00  0.06           C
ATOM     42  C14 MOL     2       1.099  19.020   2.942  1.00  0.07           C
ATOM     43  C16 MOL     2      -0.419  17.972   4.616  1.00  0.06           C
ATOM     44  C21 MOL     2      -4.758  16.355   0.942  1.00  0.06           C
ATOM     45  C26 MOL     2       0.440  10.436   4.247  1.00  0.07           C
ATOM     46 4H03 MOL     2       0.878   9.628   4.387  1.00  0.08           H
ATOM     47  C15 MOL     2       0.856  18.741   4.411  1.00  0.07           C
ATOM     48  C13 MOL     2       1.099  17.719   2.127  1.00  0.05           C
ATOM     49  C11 MOL     2      -1.652  14.300  -4.276  1.00  0.09           C
ATOM     50 AH03 MOL     2      -2.332  14.970  -4.385  1.00  0.11           H
ATOM     51 BH03 MOL     2      -1.935  13.485  -4.696  1.00  0.11           H
ATOM     52 CH03 MOL     2      -0.837  14.604  -4.683  1.00  0.11           H
ATOM     53  O5  MOL     2       1.854  11.554   0.225  1.00  0.04           O
ATOM     54  C8  MOL     2       1.934  12.691   0.911  1.00  0.03           C
ATOM     55  H1  MOL     2      -1.226  13.603   3.670  1.00  0.04           H
ATOM     56  H10 MOL     2      -3.053  15.568   1.736  1.00  0.04           H
ATOM     57  H11 MOL     2      -4.982  16.949   1.728  1.00  0.06           H
ATOM     58  H12 MOL     2      -5.979  15.536  -1.856  1.00  0.07           H
ATOM     59 AH12 MOL     2      -0.950  17.520   2.070  1.00  0.05           H
ATOM     60 AH17 MOL     2       0.353  16.091   4.191  1.00  0.07           H
ATOM     61 AH16 MOL     2      -1.050  18.529   4.251  1.00  0.05           H
ATOM     62 BH17 MOL     2      -1.351  16.192   3.918  1.00  0.07           H
ATOM     63 BH13 MOL     2       1.216  17.873   1.146  1.00  0.08           H
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ATOM    64 BH14 MOL    2      1.927  19.538   2.720  1.00  0.08        H
ATOM    65 AH13 MOL    2      1.847  17.133   2.472  1.00  0.09        H
ATOM    66 AH14 MOL    2      0.234  19.555   2.643  1.00  0.07        H
ATOM    67 BH16 MOL    2     -0.566  17.772   5.594  1.00  0.08        H
ATOM    68 AH15 MOL    2      1.698  18.159   4.739  1.00  0.09        H
ATOM    69 BH15 MOL    2      0.818  19.588   4.953  1.00  0.09        H
ATOM    70  H   MOL    2     12.100   9.666   0.350  1.00  0.00        H
ATOM    71  H   MOL    2     13.082  11.122   0.968  1.00  0.00        H
TER     72
CONECT   2  18  15  38
CONECT   3  32  50
CONECT   4  25   8  14
CONECT   5  55
CONECT   6  11  32  25  18
CONECT   7  11
CONECT   8   4  12   9  10
CONECT   9   8
CONECT  10   8
CONECT  11   6   7  12
CONECT  12   8  11  55  15
CONECT  13  35  33  18
CONECT  14   4  28  49  60
CONECT  15   2  12  17  16
CONECT  16  15
CONECT  17  15  23  21
CONECT  18   2   6  13  19
CONECT  19  18
CONECT  20  42  45
CONECT  21  17  29  56
CONECT  22  32
CONECT  23  17  46  24
CONECT  24  23
CONECT  25   4   6  26  27
CONECT  26  25
CONECT  27  25
CONECT  28  14  44  61  63
CONECT  29  21  31  30
CONECT  30  29
CONECT  31  29  46
CONECT  32   3   6  22
CONECT  33  13  42  34
CONECT  34  33
CONECT  35  13  45  57
CONECT  36  54  37
CONECT  37  36
CONECT  38   2  39  40  41
CONECT  39  38
CONECT  40  38
CONECT  41  38
CONECT  42  20  33  59
CONECT  43  48  49  65  67
CONECT  44  28  48  62  68
CONECT  45  20  35  58
CONECT  46  23  31  47
CONECT  47  46
CONECT  48  43  44  69  70
CONECT  49  14  43  64  66
CONECT  50   3  51  52  53
CONECT  51  50
CONECT  52  50
CONECT  53  50
CONECT  54  36  55
CONECT  55   5  12  54
CONECT  56  21
CONECT  57  35
CONECT  58  45
CONECT  59  42
CONECT  60  14
CONECT  61  28
CONECT  62  44
CONECT  63  28
CONECT  64  49
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CONECT  65  43
CONECT  66  49
CONECT  67  43
CONECT  68  44
CONECT  69  48
CONECT  70  48
END
```

Structure L4 (*pdb file*)

```
REMARK   L4 PDB file
CRYST1   16.527   11.175   14.691  90.00 106.39  90.00 P21/C
ORIGX1      1.000000  0.000000  0.000000        0.00000
ORIGX2      0.000000  1.000000  0.000000        0.00000
ORIGX3      0.000000  0.000000  1.000000        0.00000
SCALE1      0.060506  0.000000  0.017796        0.00000
SCALE2      0.000000  0.089486  0.000000        0.00000
SCALE3      0.000000  0.000000  0.070952        0.00000
ATOM      1  O1  MOL     2       3.476   6.466  11.702  1.00  0.00           O
ATOM      2  O2  MOL     2       3.691   2.893  11.614  1.00  0.00           O
ATOM      3  O3  MOL     2       4.521   4.138  13.256  1.00  0.00           O
ATOM      4  O4  MOL     2       0.991   8.629  10.707  1.00  0.00           O
ATOM      5  O5  MOL     2       1.999   8.929  12.661  1.00  0.00           O
ATOM      6  N3  MOL     2       0.007   4.662  11.487  1.00  0.00           N
ATOM      7  C20 MOL     2       0.641   6.734  13.697  1.00  0.00           C
ATOM      8  H2  MOL     2       1.260   7.274  14.231  1.00  0.00           H
ATOM      9  N4  MOL     2       0.609   5.380  14.279  1.00  0.00           N
ATOM     10  C1  MOL     2      -2.268   2.381  11.684  1.00  0.00           C
ATOM     11  H29 MOL     2      -2.705   3.078  12.118  1.00  0.00           H
ATOM     12  C2  MOL     2      -1.279   2.661  10.749  1.00  0.00           C
ATOM     13  C3  MOL     2      -0.875   4.082  10.456  1.00  0.00           C
ATOM     14  H26 MOL     2      -0.421   4.109   9.601  1.00  0.00           H
ATOM     15  H27 MOL     2      -1.674   4.628  10.383  1.00  0.00           H
ATOM     16  C4  MOL     2       0.218   6.074  11.177  1.00  0.00           C
ATOM     17  H24 MOL     2      -0.639   6.528  11.157  1.00  0.00           H
ATOM     18  H25 MOL     2       0.617   6.152  10.297  1.00  0.00           H
ATOM     19  C5  MOL     2       1.136   6.762  12.217  1.00  0.00           C
ATOM     20  C6  MOL     2      -0.741   7.352  13.827  1.00  0.00           C
ATOM     21  C7  MOL     2      -1.886   6.639  13.515  1.00  0.00           C
ATOM     22  H20 MOL     2      -1.827   5.760  13.217  1.00  0.00           H
ATOM     23  C8  MOL     2      -3.116   7.250  13.653  1.00  0.00           C
ATOM     24  H19 MOL     2      -3.874   6.760  13.429  1.00  0.00           H
ATOM     25  N1  MOL     2      -3.287   8.499  14.086  1.00  0.00           N
ATOM     26  C10 MOL     2       1.785   4.539  14.035  1.00  0.00           C
ATOM     27  H13 MOL     2       2.518   4.878  14.590  1.00  0.00           H
ATOM     28  C11 MOL     2       1.483   3.118  14.476  1.00  0.00           C
ATOM     29  C12 MOL     2       2.408   2.376  15.184  1.00  0.00           C
ATOM     30  H7  MOL     2       3.245   2.731  15.382  1.00  0.00           H
ATOM     31  C13 MOL     2       2.077   1.106  15.594  1.00  0.00           C
ATOM     32  H6  MOL     2       2.702   0.639  16.098  1.00  0.00           H
ATOM     33  N2  MOL     2       0.938   0.503  15.324  1.00  0.00           N
ATOM     34  C15 MOL     2       0.062   1.215  14.635  1.00  0.00           C
ATOM     35  H4  MOL     2      -0.753   0.815  14.427  1.00  0.00           H
ATOM     36  C16 MOL     2       0.272   2.514  14.205  1.00  0.00           C
ATOM     37  H3  MOL     2      -0.390   2.973  13.740  1.00  0.00           H
ATOM     38  C17 MOL     2       2.262   4.556  12.544  1.00  0.00           C
ATOM     39  C18 MOL     2       2.450   6.005  12.133  1.00  0.00           C
ATOM     40  C19 MOL     2       3.618   3.854  12.520  1.00  0.00           C
ATOM     41  C20 MOL     2       4.965   2.201  11.561  1.00  0.00           C
ATOM     42  H8  MOL     2       5.647   2.812  11.272  1.00  0.00           H
ATOM     43  H10 MOL     2       4.906   1.469  10.943  1.00  0.00           H
ATOM     44  H9  MOL     2       5.183   1.866  12.434  1.00  0.00           H
ATOM     45  C21 MOL     2       1.284   3.947  11.510  1.00  0.00           C
ATOM     46  H11 MOL     2       1.687   3.982  10.628  1.00  0.00           H
ATOM     47  H12 MOL     2       1.125   3.015  11.729  1.00  0.00           H
ATOM     48  C22 MOL     2       0.456   5.514  15.740  1.00  0.00           C
ATOM     49  H15 MOL     2       0.360   4.643  16.133  1.00  0.00           H
ATOM     50  H16 MOL     2      -0.325   6.040  15.933  1.00  0.00           H
ATOM     51  H14 MOL     2       1.231   5.947  16.105  1.00  0.00           H
ATOM     52  C23 MOL     2      -2.184   9.159  14.403  1.00  0.00           C
ATOM     53  H18 MOL     2      -2.275  10.027  14.725  1.00  0.00           H
ATOM     54  C24 MOL     2      -0.906   8.639  14.289  1.00  0.00           C
ATOM     55  H17 MOL     2      -0.166   9.154  14.518  1.00  0.00           H
ATOM     56  C25 MOL     2       1.354   8.197  11.760  1.00  0.00           C
ATOM     57  C26 MOL     2       2.256  10.299  12.301  1.00  0.00           C
ATOM     58  H23 MOL     2       2.818  10.326  11.523  1.00  0.00           H
ATOM     59  H21 MOL     2       2.696  10.745  13.030  1.00  0.00           H
ATOM     60  H22 MOL     2       1.426  10.741  12.111  1.00  0.00           H
ATOM     61  C27 MOL     2      -0.671   1.599  10.103  1.00  0.00           C
ATOM     62  H28 MOL     2      -0.022   1.770   9.460  1.00  0.00           H
ATOM     63  C28 MOL     2      -1.011   0.280  10.396  1.00  0.00           C
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ATOM    64 AH28 MOL    2     -0.591  -0.424   9.956  1.00  0.00         H
ATOM    65  C10 MOL    2     -1.967   0.035  11.334  1.00  0.00         C
ATOM    66 0H10 MOL    2     -2.191  -0.843  11.547  1.00  0.00         H
ATOM    67  C10 MOL    2     -2.603   1.072  11.969  1.00  0.00         C
ATOM    68 1H10 MOL    2     -3.266   0.892  12.597  1.00  0.00         H
TER     69
CONECT   1  68
CONECT   2  40
CONECT   3  41  42
CONECT   4  41
CONECT   5  57
CONECT   6  57  58
CONECT   7  14  17  46
CONECT   8   9  10  20  21
CONECT   9   8
CONECT  10   8  27  49
CONECT  11  12  13  68
CONECT  12  11
CONECT  13  11  14  62
CONECT  14   7  13  15  16
CONECT  15  14
CONECT  16  14
CONECT  17   7  18  19  20
CONECT  18  17
CONECT  19  17
CONECT  20  17   8  40  57
CONECT  21   8  22  55
CONECT  22  21  23  24
CONECT  23  22
CONECT  24  22  25  26
CONECT  25  24
CONECT  26  24  53
CONECT  27  10  28  29  39
CONECT  28  27
CONECT  29  27  30  37
CONECT  30  29  31  32
CONECT  31  30
CONECT  32  30  33  34
CONECT  33  32
CONECT  34  32  35
CONECT  35  34  36  37
CONECT  36  35
CONECT  37  29  35  38
CONECT  38  37
CONECT  39  27  40  41  46
CONECT  40  20  39   2
CONECT  41  39   4   3
CONECT  42   3  43  44  45
CONECT  43  42
CONECT  44  42
CONECT  45  42
CONECT  46   7  39  47  48
CONECT  47  46
CONECT  48  46
CONECT  49  10  50  51  52
CONECT  50  49
CONECT  51  49
CONECT  52  49
CONECT  53  26  54  55
CONECT  54  53
CONECT  55  21  53  56
CONECT  56  55
CONECT  57   6  20   5
CONECT  58   6  59  60  61
CONECT  59  58
CONECT  60  58
CONECT  61  58
CONECT  62  13  63  64
CONECT  63  62
CONECT  64  62  65  66
CONECT  65  64
CONECT  66  64  67  68
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CONECT  67  66
CONECT  68  66  11   1
END
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Structure L5 (*pdb file*)

```
REMARK   L5 PDB file
CRYST1   13.089   17.019   25.190  90.00  90.00  90.00 PBCA
ORIGX1      1.000000  0.000000  0.000000        0.00000
ORIGX2      0.000000  1.000000  0.000000        0.00000
ORIGX3      0.000000  0.000000  1.000000        0.00000
SCALE1      0.076400  0.000000  0.000000        0.00000
SCALE2      0.000000  0.058758  0.000000        0.00000
SCALE3      0.000000  0.000000  0.039698        0.00000
ATOM      1  O1  MOL     2      10.109   0.955   5.497  1.00  0.00           O
ATOM      2  N10 MOL     2      13.501   4.992   5.403  1.00  0.00           N
ATOM      3  C40 MOL     2       8.093   7.752  12.441  1.00  0.00           C
ATOM      4  H40 MOL     2       7.690   8.332  13.047  1.00  0.00           H
ATOM      5  N2  MOL     2       7.317   6.915  11.756  1.00  0.00           N
ATOM      6  O5  MOL     2      14.675   6.082  12.595  1.00  0.00           O
ATOM      7  O6  MOL     2      12.173   7.715  13.900  1.00  0.00           O
ATOM      8  O7  MOL     2      12.276   5.594  14.534  1.00  0.00           O
ATOM      9  O8  MOL     2      15.936   4.148   9.900  1.00  0.00           O
ATOM     10  O9  MOL     2      16.034   6.362  10.054  1.00  0.00           O
ATOM     11  N1  MOL     2      11.847   4.008  10.798  1.00  0.00           N
ATOM     12  C10 MOL     2      13.279   6.438   9.478  1.00  0.00           C
ATOM     13 3H10 MOL     2      13.800   7.266   9.549  1.00  0.00           H
ATOM     14  N3  MOL     2      11.891   6.744   9.817  1.00  0.00           N
ATOM     15  C1  MOL     2       7.936   6.083  10.910  1.00  0.00           C
ATOM     16  H1  MOL     2       7.420   5.475  10.431  1.00  0.00           H
ATOM     17  C2  MOL     2       9.297   6.083  10.718  1.00  0.00           C
ATOM     18  H15 MOL     2       9.682   5.488  10.113  1.00  0.00           H
ATOM     19  C3  MOL     2      10.092   6.961  11.420  1.00  0.00           C
ATOM     20  C4  MOL     2      11.584   6.998  11.245  1.00  0.00           C
ATOM     21  H17 MOL     2      11.896   7.899  11.470  1.00  0.00           H
ATOM     22  C5  MOL     2      12.275   5.977  12.223  1.00  0.00           C
ATOM     23  C6  MOL     2      11.753   4.551  12.154  1.00  0.00           C
ATOM     24  H21 MOL     2      12.265   3.993  12.759  1.00  0.00           H
ATOM     25  H22 MOL     2      10.827   4.535  12.442  1.00  0.00           H
ATOM     26  C7  MOL     2      11.259   2.662  10.751  1.00  0.00           C
ATOM     27  H4  MOL     2      10.439   2.658  11.268  1.00  0.00           H
ATOM     28  H11 MOL     2      11.873   2.036  11.165  1.00  0.00           H
ATOM     29  C8  MOL     2      10.963   2.206   9.381  1.00  0.00           C
ATOM     30  C9  MOL     2       9.840   2.665   8.726  1.00  0.00           C
ATOM     31  H10 MOL     2       9.287   3.259   9.179  1.00  0.00           H
ATOM     32  C10 MOL     2       9.483   2.301   7.439  1.00  0.00           C
ATOM     33  H9  MOL     2       8.713   2.639   7.041  1.00  0.00           H
ATOM     34  C11 MOL     2      10.297   1.431   6.769  1.00  0.00           C
ATOM     35  C12 MOL     2       8.910   1.372   4.847  1.00  0.00           C
ATOM     36  H5  MOL     2       8.151   1.026   5.321  1.00  0.00           H
ATOM     37  H2  MOL     2       8.903   1.038   3.945  1.00  0.00           H
ATOM     38  H6  MOL     2       8.870   2.330   4.833  1.00  0.00           H
ATOM     39  C13 MOL     2      12.497   4.699   6.214  1.00  0.00           C
ATOM     40  H30 MOL     2      11.825   4.149   5.879  1.00  0.00           H
ATOM     41  C14 MOL     2      12.366   5.136   7.505  1.00  0.00           C
ATOM     42  H3  MOL     2      11.632   4.888   8.018  1.00  0.00           H
ATOM     43  C15 MOL     2      13.346   5.957   8.030  1.00  0.00           C
ATOM     44  C16 MOL     2      13.927   5.369  10.415  1.00  0.00           C
ATOM     45  C17 MOL     2      13.230   3.972  10.385  1.00  0.00           C
ATOM     46  H24 MOL     2      13.280   3.616   9.484  1.00  0.00           H
ATOM     47  H23 MOL     2      13.716   3.367  10.968  1.00  0.00           H
ATOM     48  C18 MOL     2      11.411   0.946   7.371  1.00  0.00           C
ATOM     49  H7  MOL     2      11.966   0.358   6.911  1.00  0.00           H
ATOM     50  C19 MOL     2      11.733   1.326   8.680  1.00  0.00           C
ATOM     51  H8  MOL     2      12.491   0.967   9.082  1.00  0.00           H
ATOM     52  C20 MOL     2      11.424   7.900   9.032  1.00  0.00           C
ATOM     53  H14 MOL     2      11.956   8.669   9.246  1.00  0.00           H
ATOM     54  H12 MOL     2      10.504   8.078   9.242  1.00  0.00           H
ATOM     55  H13 MOL     2      11.506   7.705   8.095  1.00  0.00           H
ATOM     56  C21 MOL     2       9.448   7.807  12.300  1.00  0.00           C
ATOM     57  H16 MOL     2       9.941   8.416  12.799  1.00  0.00           H
ATOM     58  C22 MOL     2      13.730   5.890  11.837  1.00  0.00           C
ATOM     59  C23 MOL     2      12.229   6.556  13.626  1.00  0.00           C
ATOM     60  C24 MOL     2      12.220   5.992  15.910  1.00  0.00           C
ATOM     61  H19 MOL     2      13.002   6.504  16.127  1.00  0.00           H
ATOM     62  H18 MOL     2      12.183   5.211  16.468  1.00  0.00           H
ATOM     63  H20 MOL     2      11.436   6.527  16.057  1.00  0.00           H
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ATOM    64  C25 MOL    2     15.401   5.204  10.096  1.00  0.00        C
ATOM    65  C26 MOL    2     17.461   6.275   9.799  1.00  0.00        C
ATOM    66  H25 MOL    2     17.850   5.617  10.381  1.00  0.00        H
ATOM    67  H26 MOL    2     17.868   7.129   9.965  1.00  0.00        H
ATOM    68  H27 MOL    2     17.609   6.022   8.885  1.00  0.00        H
ATOM    69  C27 MOL    2     14.394   6.283   7.207  1.00  0.00        C
ATOM    70  H29 MOL    2     15.077   6.834   7.515  1.00  0.00        H
ATOM    71  C28 MOL    2     14.425   5.788   5.912  1.00  0.00        C
ATOM    72  H28 MOL    2     15.141   6.031   5.367  1.00  0.00        H
TER     73
CONECT   1  72
CONECT   2  35  36
CONECT   3  40  72
CONECT   4   5   6  57
CONECT   5   4
CONECT   6   4  16
CONECT   7  59
CONECT   8  60
CONECT   9  60  61
CONECT  10  65
CONECT  11  65  66
CONECT  12  24  27  46
CONECT  13  14  15  44  45
CONECT  14  13
CONECT  15  13  21  53
CONECT  16   6  17  18
CONECT  17  16
CONECT  18  16  19  20
CONECT  19  18
CONECT  20  18  21  57
CONECT  21  20  15  22  23
CONECT  22  21
CONECT  23  21  24  59  60
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CONECT  25  24
CONECT  26  24
CONECT  27  12  28  29  30
CONECT  28  27
CONECT  29  27
CONECT  30  27  31  51
CONECT  31  30  32  33
CONECT  32  31
CONECT  33  31  34  35
CONECT  34  33
CONECT  35   2  33  49
CONECT  36   2  37  38  39
CONECT  37  36
CONECT  38  36
CONECT  39  36
CONECT  40   3  41  42
CONECT  41  40
CONECT  42  40  43  44
CONECT  43  42
CONECT  44  42  13  70
CONECT  45  13  46  59  65
CONECT  46  45  12  47  48
CONECT  47  46
CONECT  48  46
CONECT  49  35  50  51
CONECT  50  49
CONECT  51  49  30  52
CONECT  52  51
CONECT  53  15  54  55  56
CONECT  54  53
CONECT  55  53
CONECT  56  53
CONECT  57  20   4  58
CONECT  58  57
CONECT  59  23  45   7
CONECT  60   8  23   9
CONECT  61   9  62  63  64
CONECT  62  61
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CONECT  63  61
CONECT  64  61
CONECT  65  10  11  45
CONECT  66  11  67  68  69
CONECT  67  66
CONECT  68  66
CONECT  69  66
CONECT  70  44  71  72
CONECT  71  70
CONECT  72   3  70   1
END
```

Structure L6 (*pdb file*)

```
REMARK   L6 PDB file
CRYST1   12.874   13.172   16.965  90.00  98.68  90.00 P21/C
ORIGX1      1.000000  0.000000  0.000000        0.00000
ORIGX2      0.000000  1.000000  0.000000        0.00000
ORIGX3      0.000000  0.000000  1.000000        0.00000
SCALE1      0.077676  0.000000  0.011858        0.00000
SCALE2      0.000000  0.075919  0.000000        0.00000
SCALE3      0.000000  0.000000  0.059628        0.00000
ATOM      1  C1  UNK C   1      11.302   0.721   5.653  1.00  2.10           C
ATOM      2  C2  UNK C   1      11.679  -0.745   5.789  1.00  2.04           C
ATOM      3  C3  UNK C   1      11.822  -1.288   4.350  1.00  2.24           C
ATOM      4  H3A UNK C   1      12.519  -0.796   3.889  1.00  2.69           H
ATOM      5  H3B UNK C   1      12.087  -2.221   4.384  1.00  2.69           H
ATOM      6  C4  UNK C   1      10.163   0.235   3.525  1.00  2.28           C
ATOM      7  H4A UNK C   1       9.328   0.297   3.036  1.00  2.74           H
ATOM      8  H4B UNK C   1      10.833   0.735   3.034  1.00  2.74           H
ATOM      9  C5  UNK C   1       9.979   0.871   4.924  1.00  2.05           C
ATOM     10  C6  UNK C   1       8.877   0.209   5.812  1.00  2.10           C
ATOM     11  H6  UNK C   1       8.776   0.741   6.628  1.00  2.52           H
ATOM     12  C7  UNK C   1      10.580  -1.444   6.647  1.00  2.15           C
ATOM     13  H7  UNK C   1      10.665  -1.124   7.570  1.00  2.58           H
ATOM     14  C8  UNK C   1       9.700   2.366   4.743  1.00  2.66           C
ATOM     15  C9  UNK C   1      13.022  -0.807   6.533  1.00  2.60           C
ATOM     16  C10 UNK C   1       9.164   4.373   5.866  1.00  4.75           C
ATOM     17 AH10 UNK C   1      10.009   4.813   5.749  1.00  5.71           H
ATOM     18 BH10 UNK C   1       8.769   4.655   6.695  1.00  5.71           H
ATOM     19 CH10 UNK C   1       8.580   4.602   5.140  1.00  5.71           H
ATOM     20  C11 UNK C   1      15.358  -0.755   6.253  1.00  5.40           C
ATOM     21 AH11 UNK C   1      15.540   0.042   6.756  1.00  6.48           H
ATOM     22 BH11 UNK C   1      16.004  -0.842   5.548  1.00  6.48           H
ATOM     23 CH11 UNK C   1      15.411  -1.518   6.832  1.00  6.48           H
ATOM     24  C12 UNK C   1      10.811  -1.708   2.248  1.00  2.84           C
ATOM     25 AH12 UNK C   1      11.294  -2.546   2.322  1.00  3.40           H
ATOM     26 BH12 UNK C   1      11.367  -1.087   1.753  1.00  3.40           H
ATOM     27  C13 UNK C   1       9.538  -1.942   1.484  1.00  2.80           C
ATOM     28  C14 UNK C   1       9.169  -1.136   0.437  1.00  4.28           C
ATOM     29  H14 UNK C   1       9.713  -0.420   0.200  1.00  5.14           H
ATOM     30  C15 UNK C   1       8.003  -1.366  -0.273  1.00  5.34           C
ATOM     31  H15 UNK C   1       7.769  -0.808  -0.979  1.00  6.40           H
ATOM     32  C16 UNK C   1       7.201  -2.412   0.068  1.00  4.69           C
ATOM     33  C17 UNK C   1       7.563  -3.256   1.102  1.00  4.73           C
ATOM     34  H17 UNK C   1       7.023  -3.980   1.324  1.00  5.68           H
ATOM     35  C18 UNK C   1       8.729  -3.021   1.803  1.00  3.90           C
ATOM     36  H18 UNK C   1       8.974  -3.591   2.496  1.00  4.68           H
ATOM     37  C19 UNK C   1       5.957  -2.708  -0.699  1.00  7.28           C
ATOM     38  C20 UNK C   1       8.270  -1.627   7.224  1.00  3.36           C
ATOM     39 AH20 UNK C   1       8.390  -1.107   8.022  1.00  4.03           H
ATOM     40 BH20 UNK C   1       8.436  -2.553   7.418  1.00  4.03           H
ATOM     41 CH20 UNK C   1       7.370  -1.523   6.907  1.00  4.03           H
ATOM     42  C21 UNK C   1      10.772  -2.955   6.653  1.00  2.43           C
ATOM     43  C22 UNK C   1      10.202  -3.750   5.676  1.00  3.22           C
ATOM     44  H22 UNK C   1       9.721  -3.364   4.980  1.00  3.86           H
ATOM     45  C23 UNK C   1      10.354  -5.123   5.742  1.00  3.90           C
ATOM     46  H23 UNK C   1       9.955  -5.639   5.080  1.00  4.68           H
ATOM     47  C24 UNK C   1      11.590  -4.979   7.618  1.00  3.61           C
ATOM     48  H24 UNK C   1      12.082  -5.394   8.289  1.00  4.33           H
ATOM     49  C25 UNK C   1      11.487  -3.594   7.653  1.00  3.04           C
ATOM     50  H25 UNK C   1      11.890  -3.106   8.334  1.00  3.65           H
ATOM     51  C26 UNK C   1       7.548   0.210   5.068  1.00  2.57           C
ATOM     52  C27 UNK C   1       6.663   1.268   5.156  1.00  3.91           C
ATOM     53  H27 UNK C   1       6.857   2.002   5.693  1.00  4.69           H
ATOM     54  C28 UNK C   1       5.479   1.218   4.431  1.00  5.34           C
ATOM     55  H28 UNK C   1       4.904   1.947   4.490  1.00  6.41           H
ATOM     56  C29 UNK C   1       5.977  -0.803   3.587  1.00  4.93           C
ATOM     57  H29 UNK C   1       5.752  -1.529   3.051  1.00  5.91           H
ATOM     58  C30 UNK C   1       7.182  -0.846   4.252  1.00  3.68           C
ATOM     59  H30 UNK C   1       7.746  -1.579   4.152  1.00  4.41           H
ATOM     60  N1  UNK C   1      10.571  -1.169   3.602  1.00  2.18           N
ATOM     61  N2  UNK C   1       9.211  -1.166   6.192  1.00  2.28           N
ATOM     62  N3  UNK C   1      11.035  -5.750   6.694  1.00  3.93           N1-
ATOM     63  N4  UNK C   1       5.113   0.203   3.659  1.00  5.50           N1-
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ATOM    64  O1  UNK C   1      11.995   1.635   6.018  1.00  3.61          O1-
ATOM    65  O2  UNK C   1      13.132  -0.915   7.711  1.00  4.12          O1-
ATOM    66  O3  UNK C   1      14.038  -0.673   5.686  1.00  3.72          O
ATOM    67  O4  UNK C   1       9.798   2.943   3.707  1.00  5.25          O1-
ATOM    68  O5  UNK C   1       9.364   2.945   5.890  1.00  3.55          O
ATOM    69  F1  UNK C   1       5.528  -1.656  -1.425  1.00 14.53          F
ATOM    70  F2  UNK C   1       6.117  -3.523  -1.645  1.00 14.38          F
ATOM    71  F3  UNK C   1       4.970  -3.024  -0.012  1.00 17.08          F
TER     72
CONECT   1   2   9  64
CONECT   2   1  15  12   3
CONECT   3   4   5  60   2
CONECT   4   3
CONECT   5   3
CONECT   6   7   8  60   9
CONECT   7   6
CONECT   8   6
CONECT   9   1  14   6  10
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CONECT  11  10
CONECT  12  13  42  61   2
CONECT  13  12
CONECT  14   9  67  68
CONECT  15   2  65  66
CONECT  16  17  18  19  68
CONECT  17  16
CONECT  18  16
CONECT  19  16
CONECT  20  21  22  23  66
CONECT  21  20
CONECT  22  20
CONECT  23  20
CONECT  24  25  26  27  60
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CONECT  27  24  28  35
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CONECT  38  39  40  41  61
CONECT  39  38
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CONECT  41  38
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CONECT  43  42  44  45
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CONECT  45  43  46  62
CONECT  46  45
CONECT  47  48  49  62
CONECT  48  47
CONECT  49  42  47  50
CONECT  50  49
CONECT  51  10  52  58
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CONECT  53  52
CONECT  54  52  55  63
CONECT  55  54
CONECT  56  57  58  63
CONECT  57  56
CONECT  58  51  56  59
CONECT  59  58
CONECT  60   3   6  24
CONECT  61  10  12  38
CONECT  62  45  47
CONECT  63  54  56
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CONECT  64   1
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CONECT  66  15  20
CONECT  67  14
CONECT  68  14  16
CONECT  69  37
CONECT  70  37
CONECT  71  37
END
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Structure L7 (*pdb file*)

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REMARK   L7 PDB file
CRYST1   13.127   16.744   25.548  90.00  90.00  90.00 PBCA
ORIGX1      1.000000  0.000000  0.000000        0.00000
ORIGX2      0.000000  1.000000  0.000000        0.00000
ORIGX3      0.000000  0.000000  1.000000        0.00000
SCALE1      0.076179  0.000000  0.000000        0.00000
SCALE2      0.000000  0.059723  0.000000        0.00000
SCALE3      0.000000  0.000000  0.039142        0.00000
ATOM      1  O1  UNK C   1       1.603   5.949  25.497  1.00  0.00          O1-
ATOM      2  O2  UNK C   1      -0.935   7.570  24.151  1.00  0.00          O1-
ATOM      3  O3  UNK C   1      -0.752   5.426  23.532  1.00  0.00          O
ATOM      4  O4  UNK C   1       2.953   6.191  28.075  1.00  0.00          O
ATOM      5  O5  UNK C   1       2.812   3.969  28.169  1.00  0.00          O1-
ATOM      6  N1  UNK C   1      -1.265   3.887  27.282  1.00  0.00          N
ATOM      7  N2  UNK C   1      -1.186   6.635  28.246  1.00  0.00          N
ATOM      8  N3  UNK C   1       0.378   4.993  32.725  1.00  0.00          N1-
ATOM      9  N4  UNK C   1      -5.781   6.793  26.354  1.00  0.00          N1-
ATOM     10  F1  UNK C   1      -4.196   0.797  34.459  1.00  0.00          F
ATOM     11  F2  UNK C   1      -4.952   0.266  32.567  1.00  0.00          F
ATOM     12  F3  UNK C   1      -5.001   2.234  33.180  1.00  0.00          F
ATOM     13  C1  UNK C   1       0.676   5.733  26.252  1.00  0.00          C
ATOM     14  C2  UNK C   1       0.826   5.226  27.666  1.00  0.00          C
ATOM     15  C3  UNK C   1       0.204   6.321  28.606  1.00  0.00          C
ATOM     16  H3  UNK C   1       0.737   7.139  28.520  1.00  0.00          H
ATOM     17  C4  UNK C   1      -1.480   6.871  26.820  1.00  0.00          C
ATOM     18  H4  UNK C   1      -1.169   7.772  26.591  1.00  0.00          H
ATOM     19  C5  UNK C   1      -0.776   5.855  25.857  1.00  0.00          C
ATOM     20  C6  UNK C   1      -1.337   4.420  25.924  1.00  0.00          C
ATOM     21 H6A UNK C   1      -2.261   4.421  25.627  1.00  0.00          H
ATOM     22 H6B UNK C   1      -0.831   3.847  25.327  1.00  0.00          H
ATOM     23  C7  UNK C   1       0.127   3.849  27.728  1.00  0.00          C
ATOM     24 H7A UNK C   1       0.617   3.222  27.174  1.00  0.00          H
ATOM     25 H7B UNK C   1       0.156   3.523  28.641  1.00  0.00          H
ATOM     26  C8  UNK C   1      -1.633   7.811  29.007  1.00  0.00          C
ATOM     27 H8A UNK C   1      -1.206   8.598  28.661  1.00  0.00          H
ATOM     28 H8B UNK C   1      -1.400   7.701  29.932  1.00  0.00          H
ATOM     29 H8C UNK C   1      -2.585   7.901  28.926  1.00  0.00          H
ATOM     30  C9  UNK C   1      -2.989   6.837  26.642  1.00  0.00          C
ATOM     31 C10 UNK C   1      -3.627   7.670  25.743  1.00  0.00          C
ATOM     32 H10 UNK C   1      -3.139   8.264  25.220  1.00  0.00          H
ATOM     33 C11 UNK C   1      -5.006   7.606  25.636  1.00  0.00          C
ATOM     34 H11 UNK C   1      -5.420   8.168  25.021  1.00  0.00          H
ATOM     35 C12 UNK C   1      -5.144   5.999  27.216  1.00  0.00          C
ATOM     36 H12 UNK C   1      -5.652   5.418  27.735  1.00  0.00          H
ATOM     37 C13 UNK C   1      -3.782   5.989  27.380  1.00  0.00          C
ATOM     38 H13 UNK C   1      -3.393   5.407  27.993  1.00  0.00          H
ATOM     39 C14 UNK C   1       0.261   5.867  30.045  1.00  0.00          C
ATOM     40 C19 UNK C   1       2.294   5.035  28.005  1.00  0.00          C
ATOM     41 C15 UNK C   1      -0.738   5.080  30.597  1.00  0.00          C
ATOM     42 H15 UNK C   1      -1.472   4.826  30.085  1.00  0.00          H
ATOM     43 C18 UNK C   1       1.309   6.215  30.882  1.00  0.00          C
ATOM     44 H18 UNK C   1       1.998   6.756  30.568  1.00  0.00          H
ATOM     45 C21 UNK C   1      -0.845   6.394  24.441  1.00  0.00          C
ATOM     46 C28 UNK C   1      -1.446   1.286  29.472  1.00  0.00          C
ATOM     47 H28 UNK C   1      -0.690   0.895  29.098  1.00  0.00          H
ATOM     48 C30 UNK C   1      -2.885   1.583  31.332  1.00  0.00          C
ATOM     49 C27 UNK C   1      -2.229   2.136  28.707  1.00  0.00          C
ATOM     50 C31 UNK C   1      -3.708   2.416  30.603  1.00  0.00          C
ATOM     51 H31 UNK C   1      -4.469   2.792  30.984  1.00  0.00          H
ATOM     52 C32 UNK C   1      -3.364   2.673  29.286  1.00  0.00          C
ATOM     53 H32 UNK C   1      -3.913   3.224  28.776  1.00  0.00          H
ATOM     54 C16 UNK C   1      -0.633   4.677  31.914  1.00  0.00          C
ATOM     55 H16 UNK C   1      -1.315   4.147  32.260  1.00  0.00          H
ATOM     56 C25 UNK C   1      -1.856   2.537  27.312  1.00  0.00          C
ATOM     57 AH25 UNK C   1      -1.220   1.899  26.953  1.00  0.00          H
ATOM     58 BH25 UNK C   1      -2.647   2.520  26.750  1.00  0.00          H
ATOM     59 C17 UNK C   1       1.326   5.753  32.190  1.00  0.00          C
ATOM     60 H17 UNK C   1       2.047   5.991  32.726  1.00  0.00          H
ATOM     61 C29 UNK C   1      -1.779   1.013  30.787  1.00  0.00          C
ATOM     62 H29 UNK C   1      -1.249   0.442  31.295  1.00  0.00          H
ATOM     63 C22 UNK C   1      -0.865   5.809  22.145  1.00  0.00          C
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ATOM    64 AH22 UNK C   1     -1.743   6.160  21.980  1.00  0.00         H
ATOM    65 BH22 UNK C   1     -0.718   5.041  21.588  1.00  0.00         H
ATOM    66 CH22 UNK C   1     -0.208   6.480  21.944  1.00  0.00         H
ATOM    67  O6  UNK C   1     -3.078   1.333  32.709  1.00  0.00         O
ATOM    68  C20 UNK C   1      4.371   6.099  28.338  1.00  0.00         C
ATOM    69 AH20 UNK C   1      4.515   5.594  29.141  1.00  0.00         H
ATOM    70 BH20 UNK C   1      4.734   6.981  28.444  1.00  0.00         H
ATOM    71 CH20 UNK C   1      4.805   5.661  27.602  1.00  0.00         H
ATOM    72  C24 UNK C   1     -4.273   1.114  33.187  1.00  0.00         C
TER     73
CONECT   1  13
CONECT   2  45
CONECT   3  45  63
CONECT   4  40  68
CONECT   5  40
CONECT   6  20  23  56
CONECT   7  15  17  26
CONECT   8  54  59
CONECT   9  33  35
CONECT  10  72
CONECT  11  72
CONECT  12  72
CONECT  13   1  14  19
CONECT  14  13  40  23  15
CONECT  15   7  16  39  14
CONECT  16  15
CONECT  17   7  18  30  19
CONECT  18  17
CONECT  19  13  45  17  20
CONECT  20   6  21  22  19
CONECT  21  20
CONECT  22  20
CONECT  23   6  24  25  14
CONECT  24  23
CONECT  25  23
CONECT  26   7  27  28  29
CONECT  27  26
CONECT  28  26
CONECT  29  26
CONECT  30  17  31  37
CONECT  31  30  32  33
CONECT  32  31
CONECT  33   9  31  34
CONECT  34  33
CONECT  35   9  36  37
CONECT  36  35
CONECT  37  30  35  38
CONECT  38  37
CONECT  39  15  41  43
CONECT  40   4   5  14
CONECT  41  39  42  54
CONECT  42  41
CONECT  43  39  44  59
CONECT  44  43
CONECT  45   2   3  19
CONECT  46  47  49  61
CONECT  47  46
CONECT  48  50  61  67
CONECT  49  46  52  56
CONECT  50  48  51  52
CONECT  51  50
CONECT  52  49  50  53
CONECT  53  52
CONECT  54   8  41  55
CONECT  55  54
CONECT  56   6  49  57  58
CONECT  57  56
CONECT  58  56
CONECT  59   8  43  60
CONECT  60  59
CONECT  61  46  48  62
CONECT  62  61
```

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CONECT  63   3  64  65  66
CONECT  64  63
CONECT  65  63
CONECT  66  63
CONECT  67  48  72
CONECT  68   4  69  70  71
CONECT  69  68
CONECT  70  68
CONECT  71  68
CONECT  72  10  11  12  67
END
```