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Supporting Information

for

Structural effects of meso-halogenation on porphyrins

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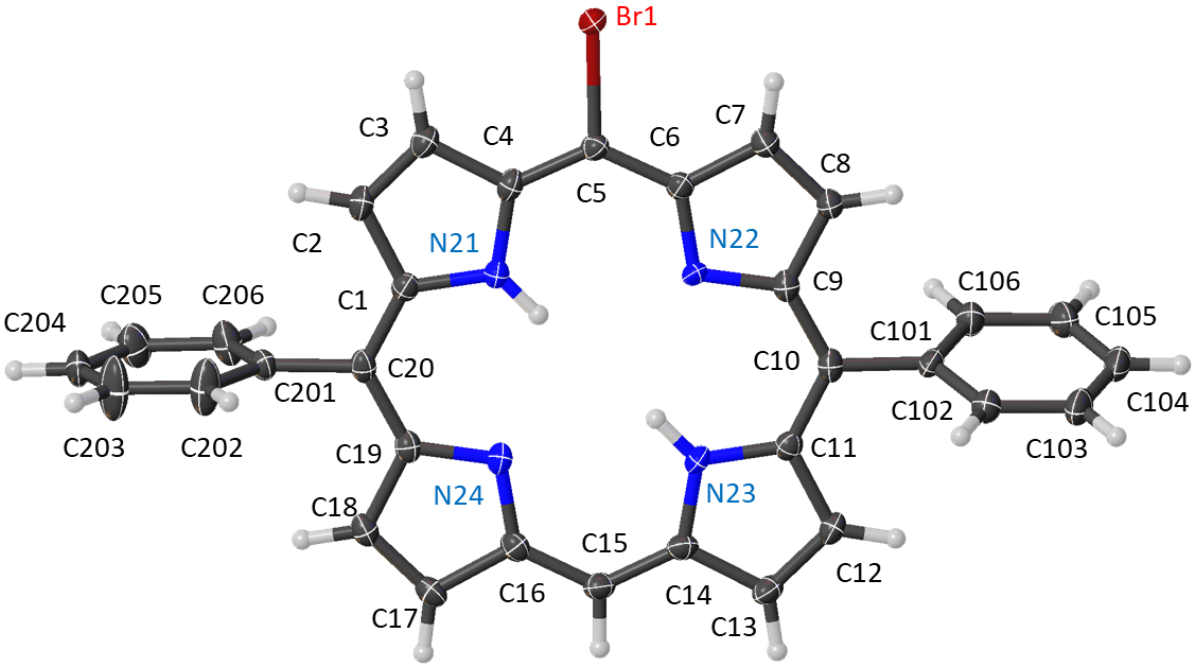


Figure S1: Thermal ellipsoid plot of compound **1** (thermal displacement given as 50% probability). Minor disordered moieties have been omitted.

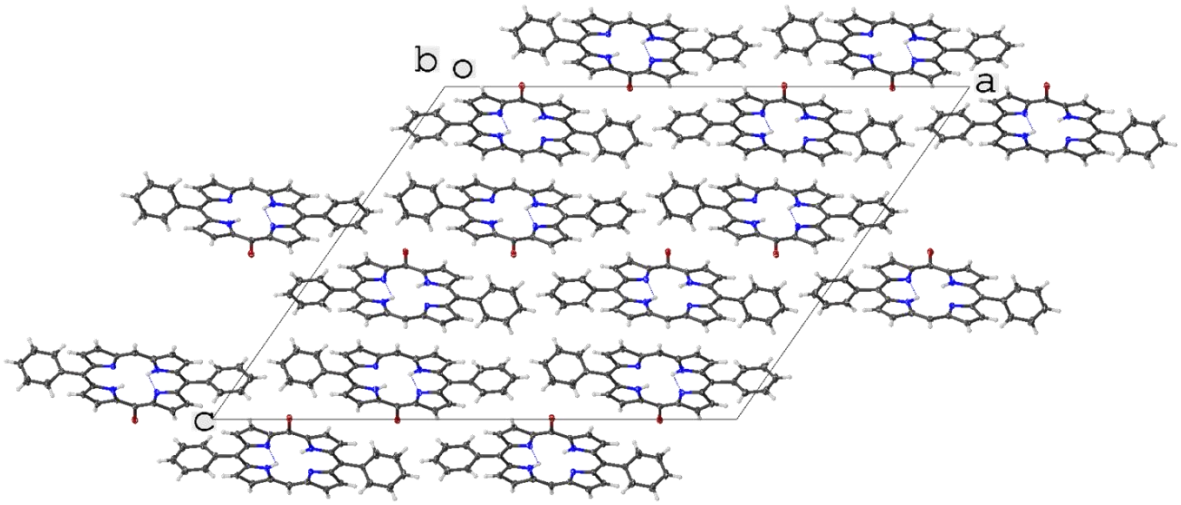


Figure S2: Packing diagram (thermal ellipsoid plot) of compound **1** looking down the *b*-axis (thermal displacement given as 50% probability). Minor disordered moieties have been omitted.

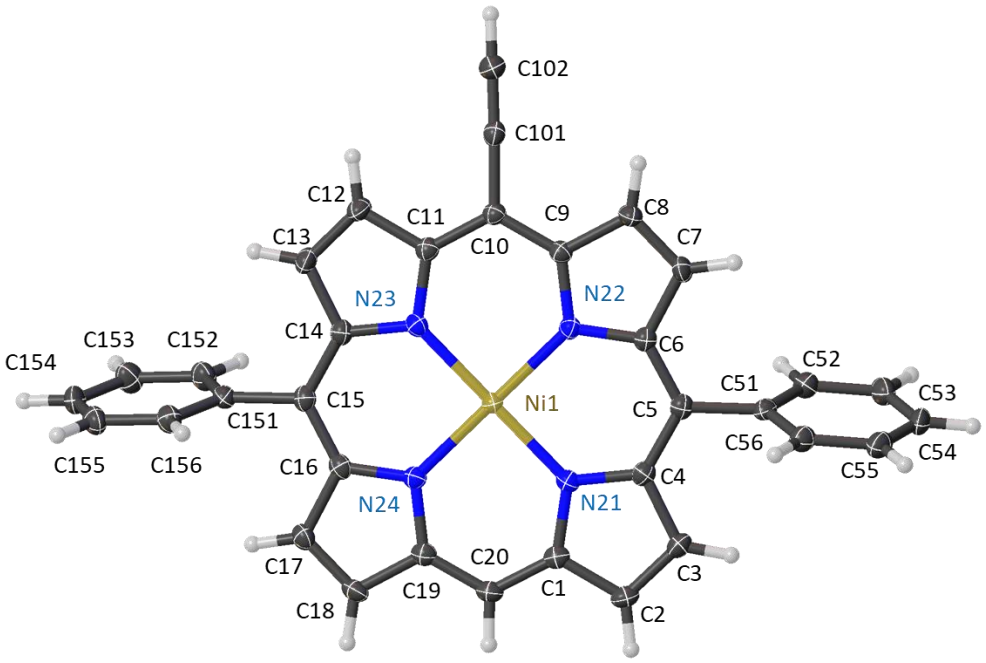


Figure S3: Thermal ellipsoid plot of compound **2A** (thermal displacement given as 50% probability). Minor disordered moieties have been omitted.

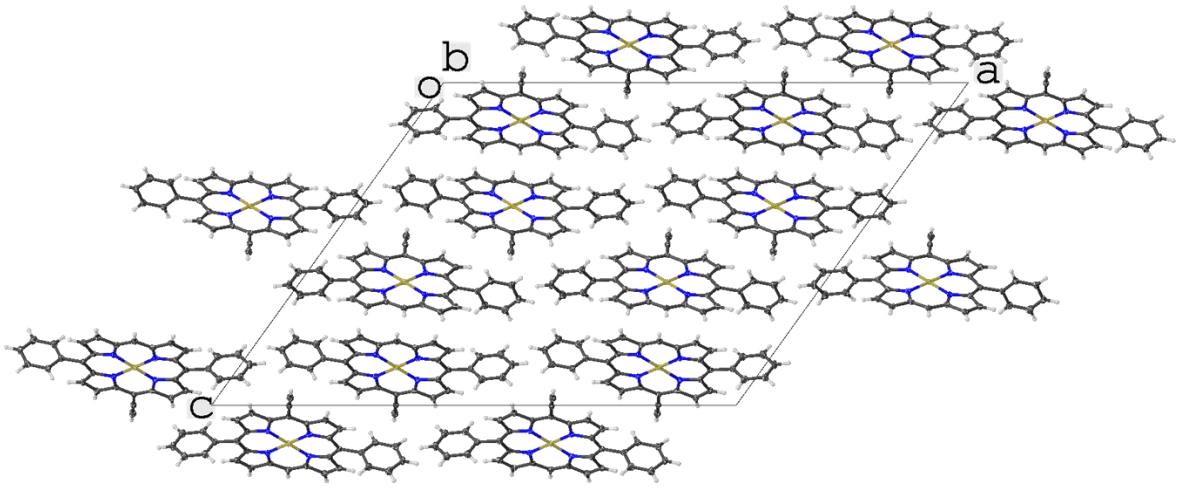


Figure S4: Packing diagram (thermal ellipsoid plot) of compound **2A** looking down the *b*-axis (thermal displacement given as 50% probability). Minor disordered moieties have been omitted.

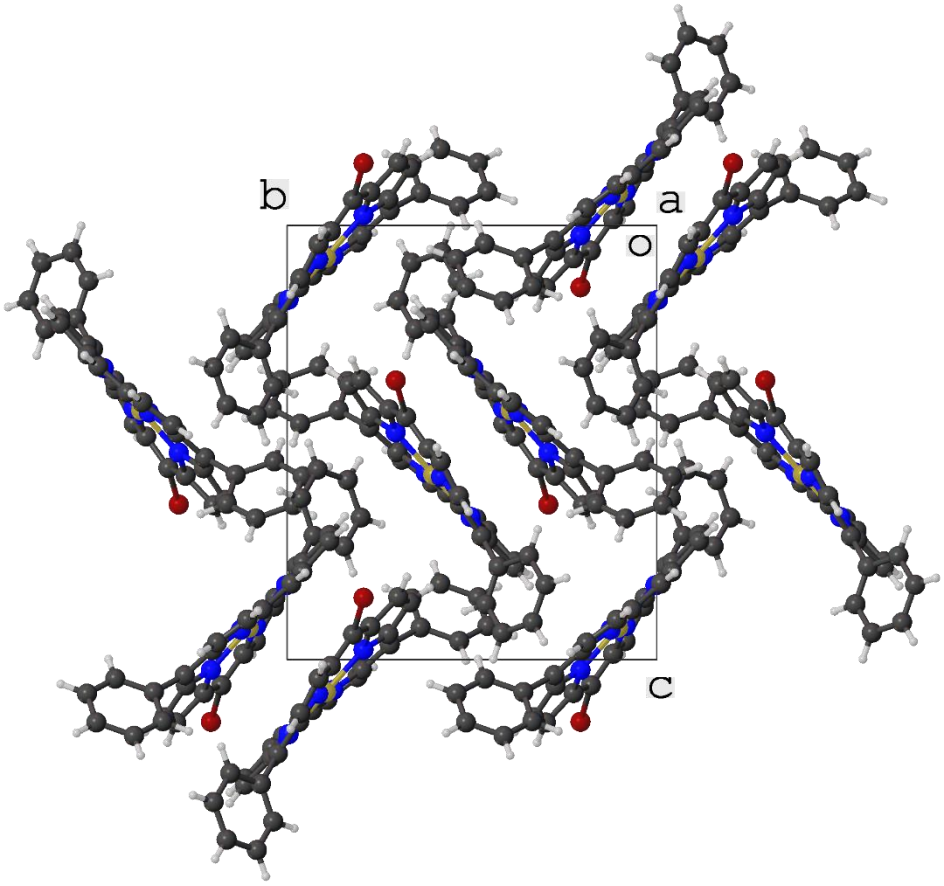


Figure S5: Packing diagram (ball and stick) of compound **2** looking down the *a*-axis.

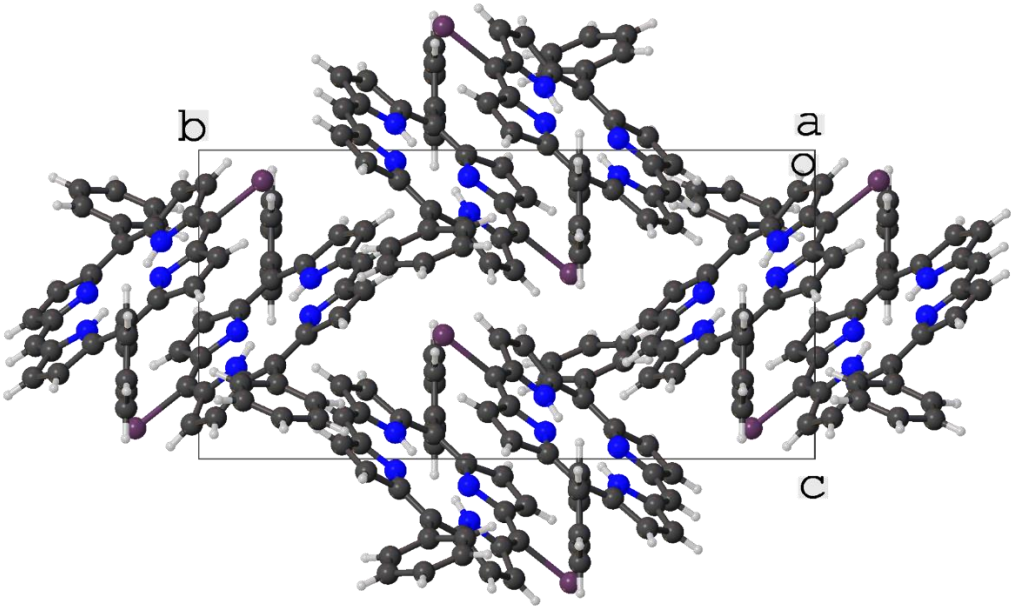


Figure S6: Packing diagram (ball and stick) of compound **3** looking down the *a*-axis.

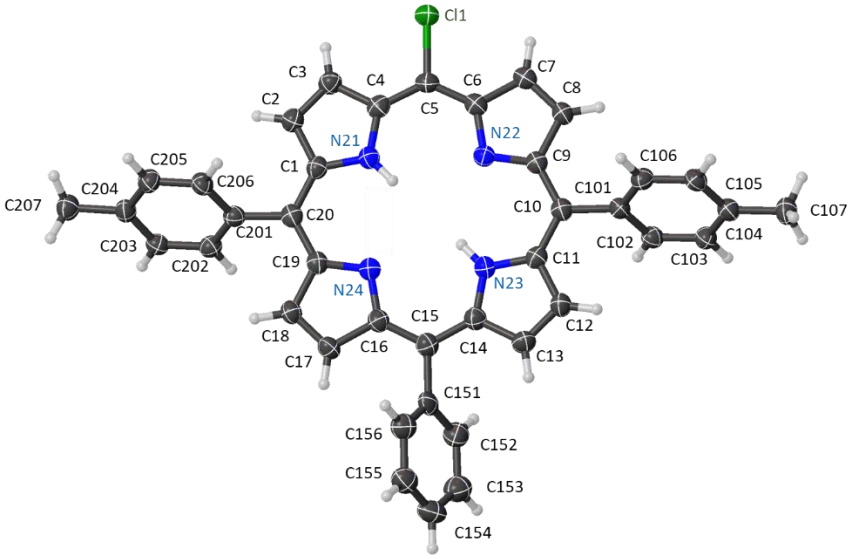
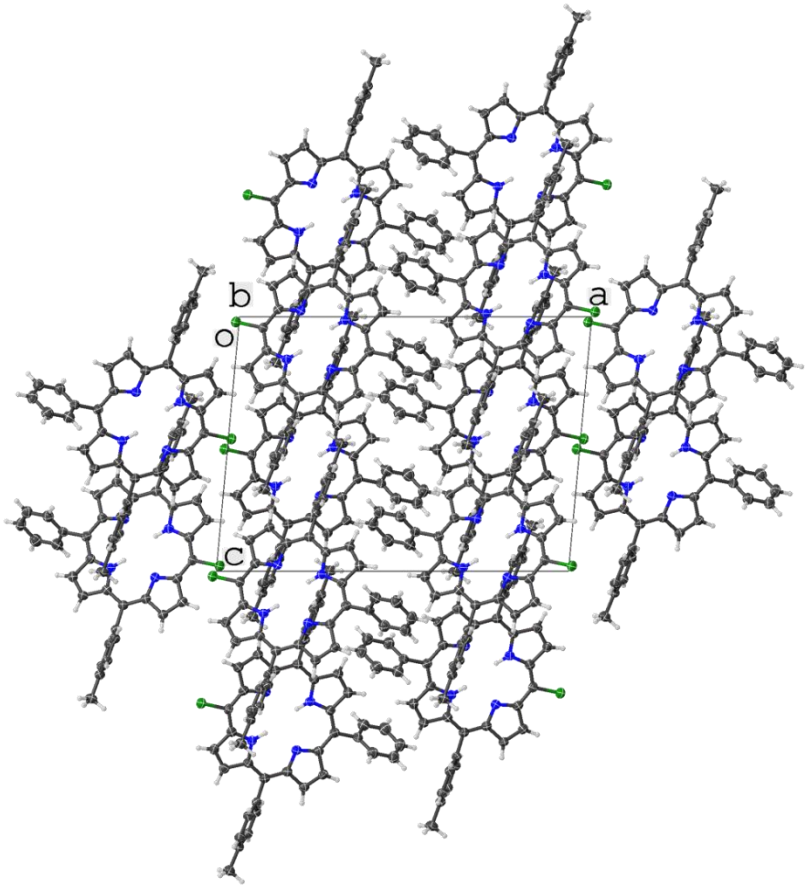


Figure S7: Thermal ellipsoid plot of compound **4** (thermal displacement given as 50% probability). Minor disordered moieties have been omitted.



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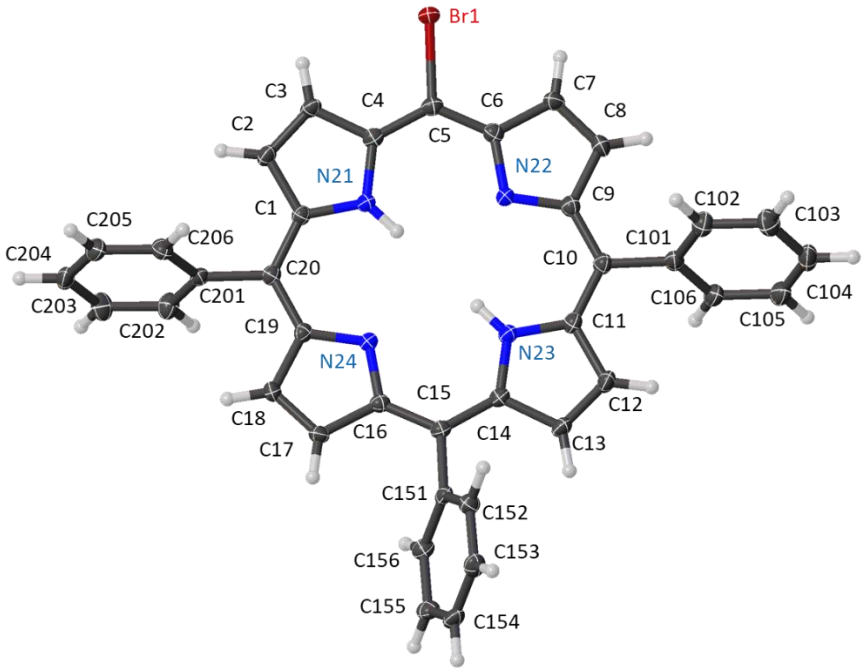

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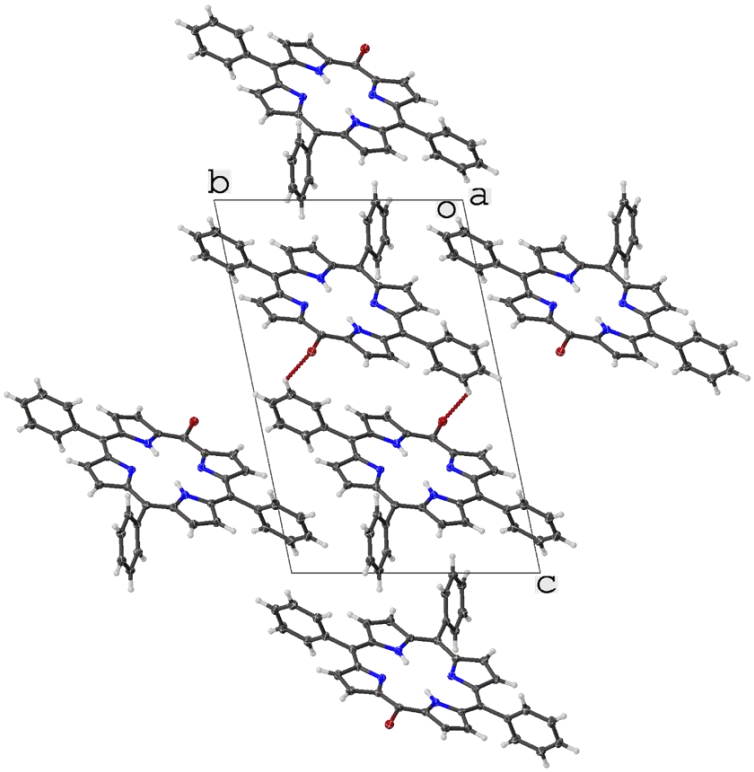

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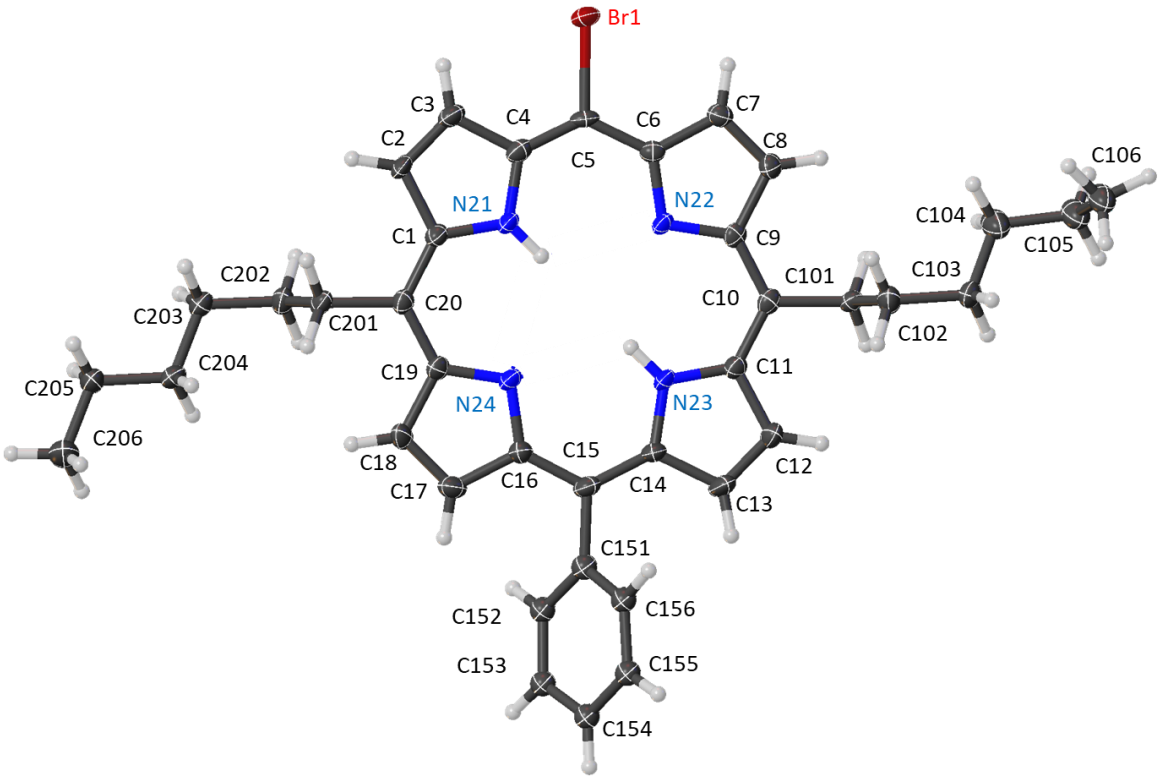

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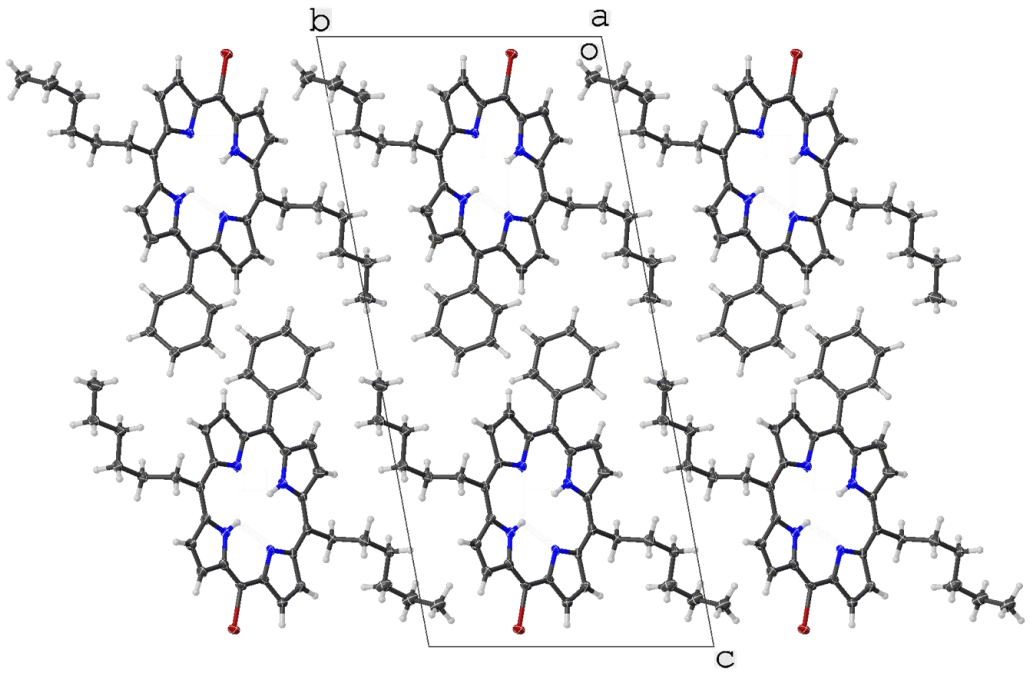


Figure S12: Packing diagram (thermal ellipsoid plot) of compound **6** looking down the *a*-axis (thermal displacement given as 50% probability). Minor disordered moieties have been omitted.

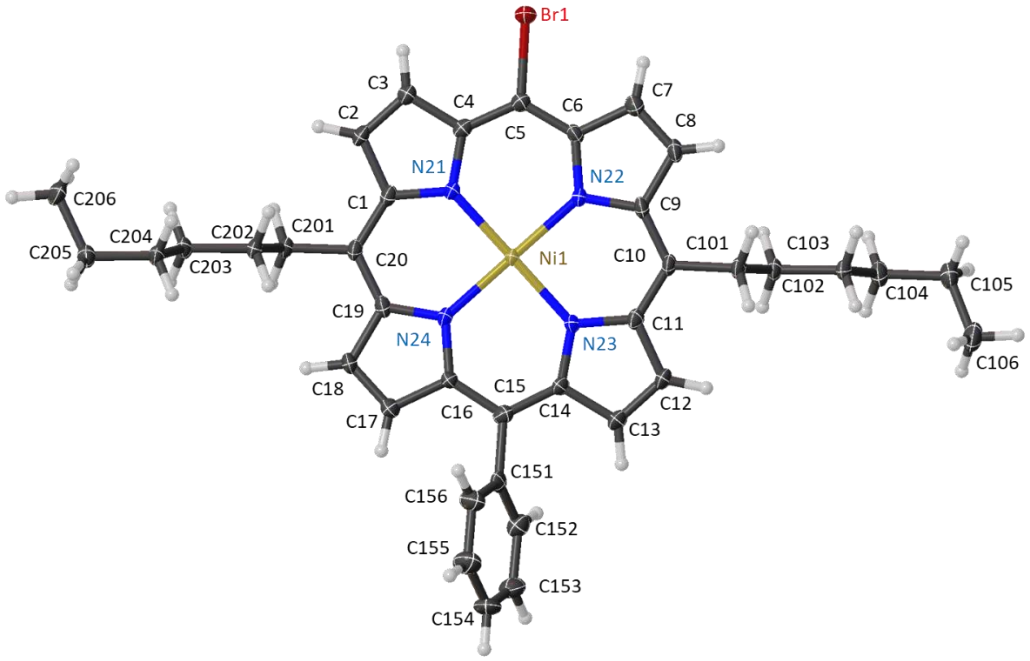
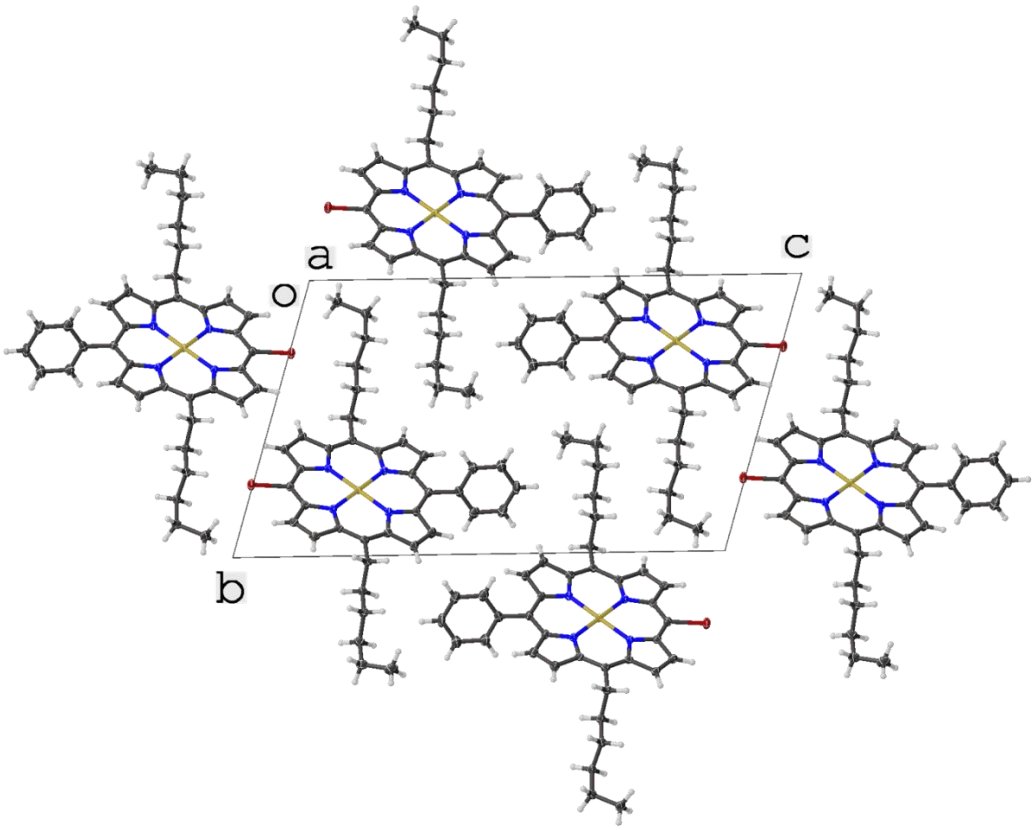


Figure S13: Thermal ellipsoid plot of compound **7** (thermal displacement given as 50% probability). Minor disordered moieties have been omitted.



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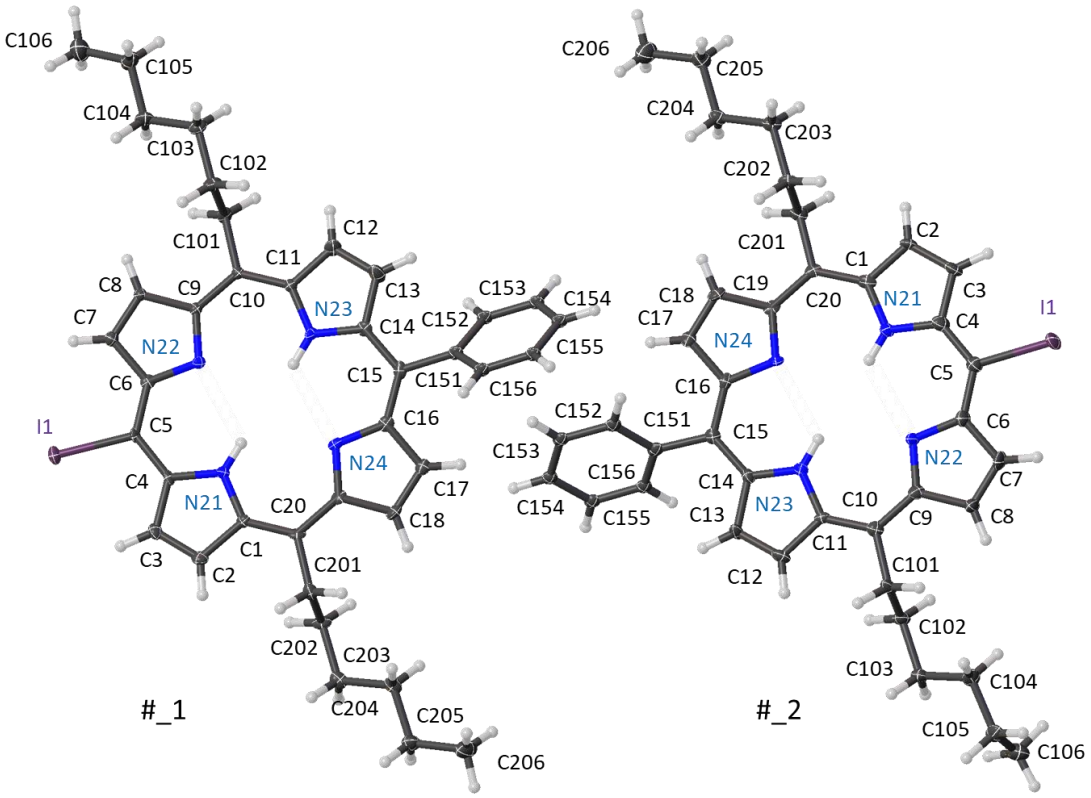

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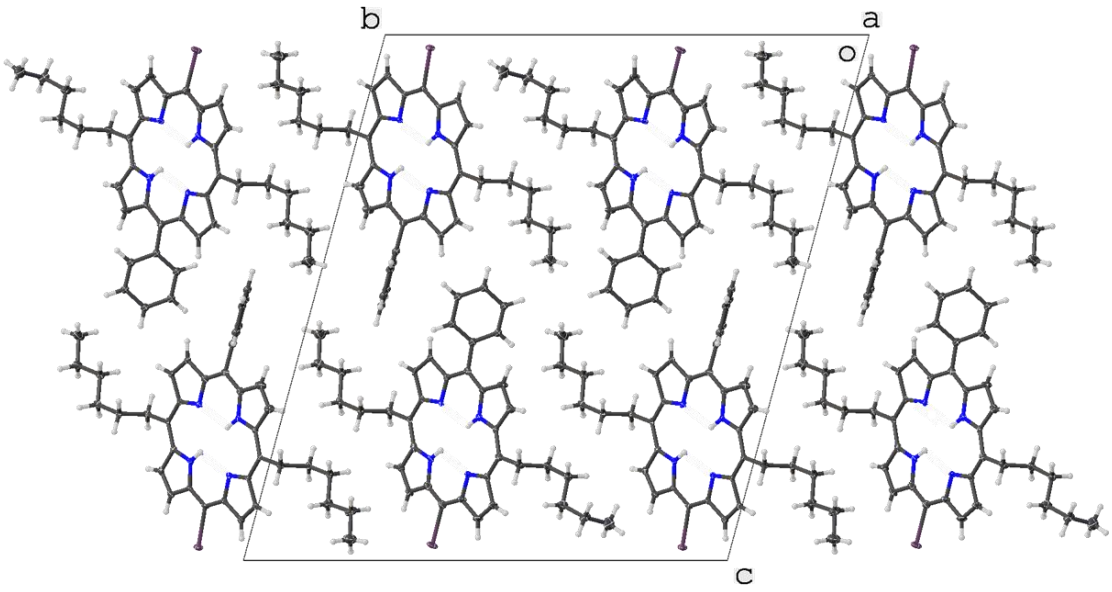

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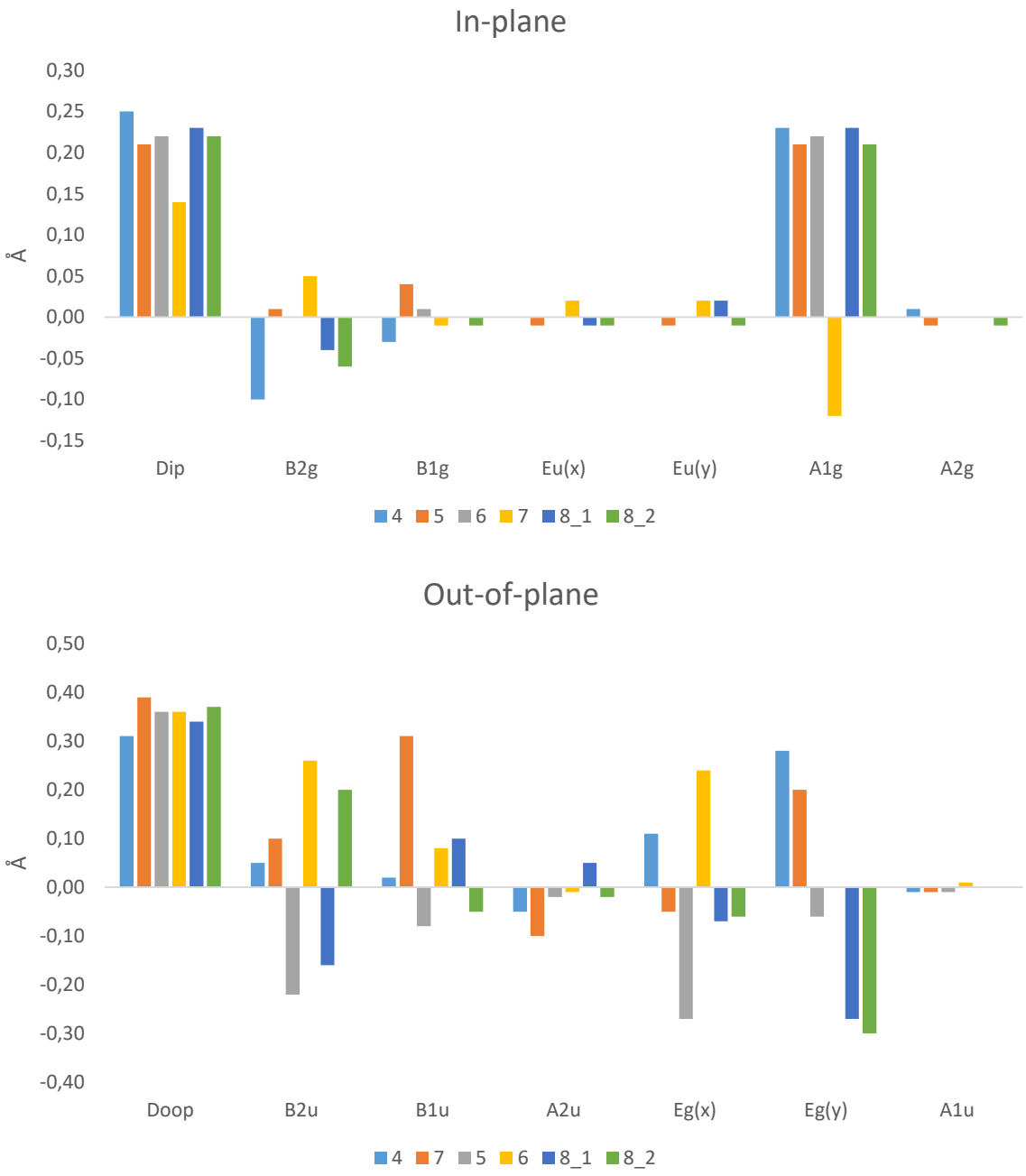

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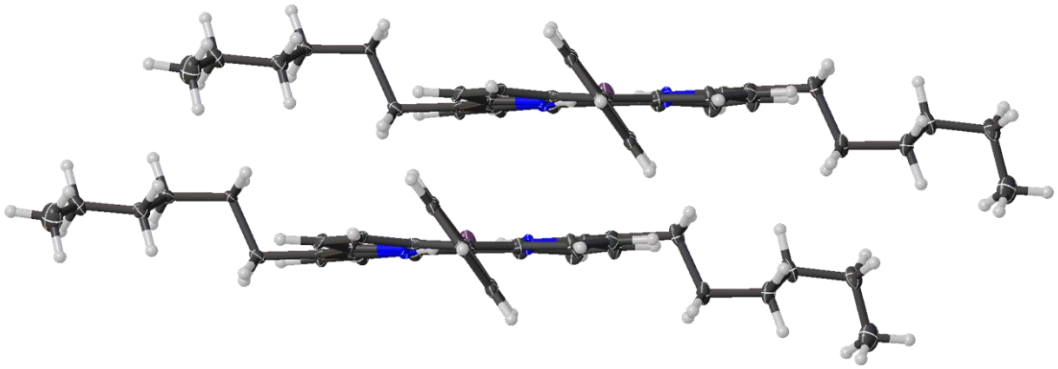

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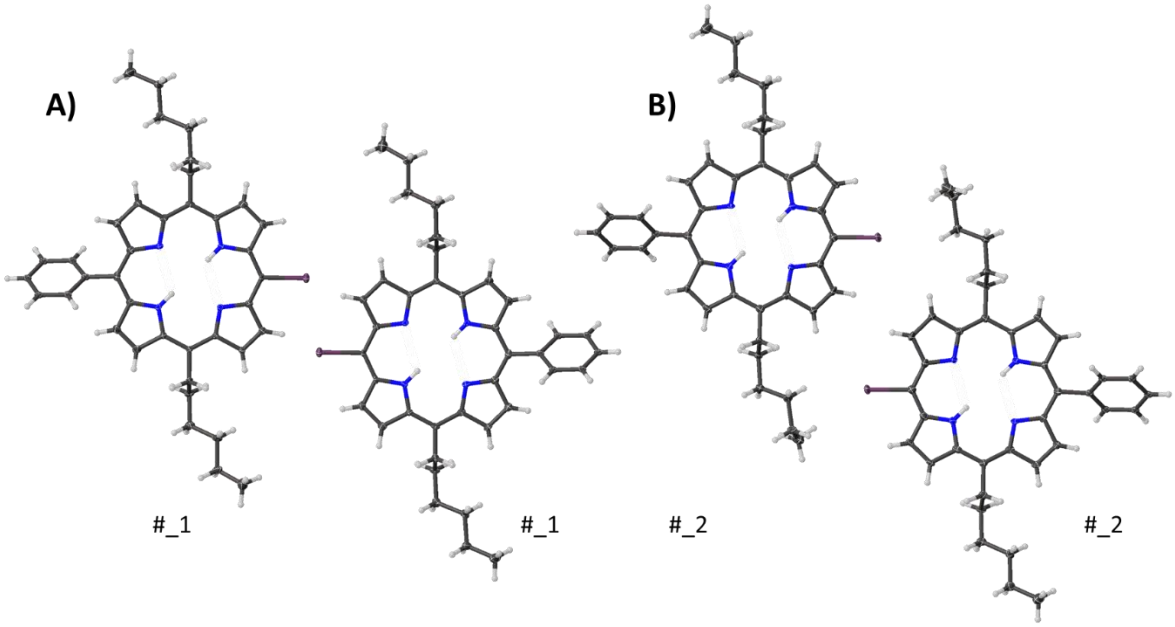

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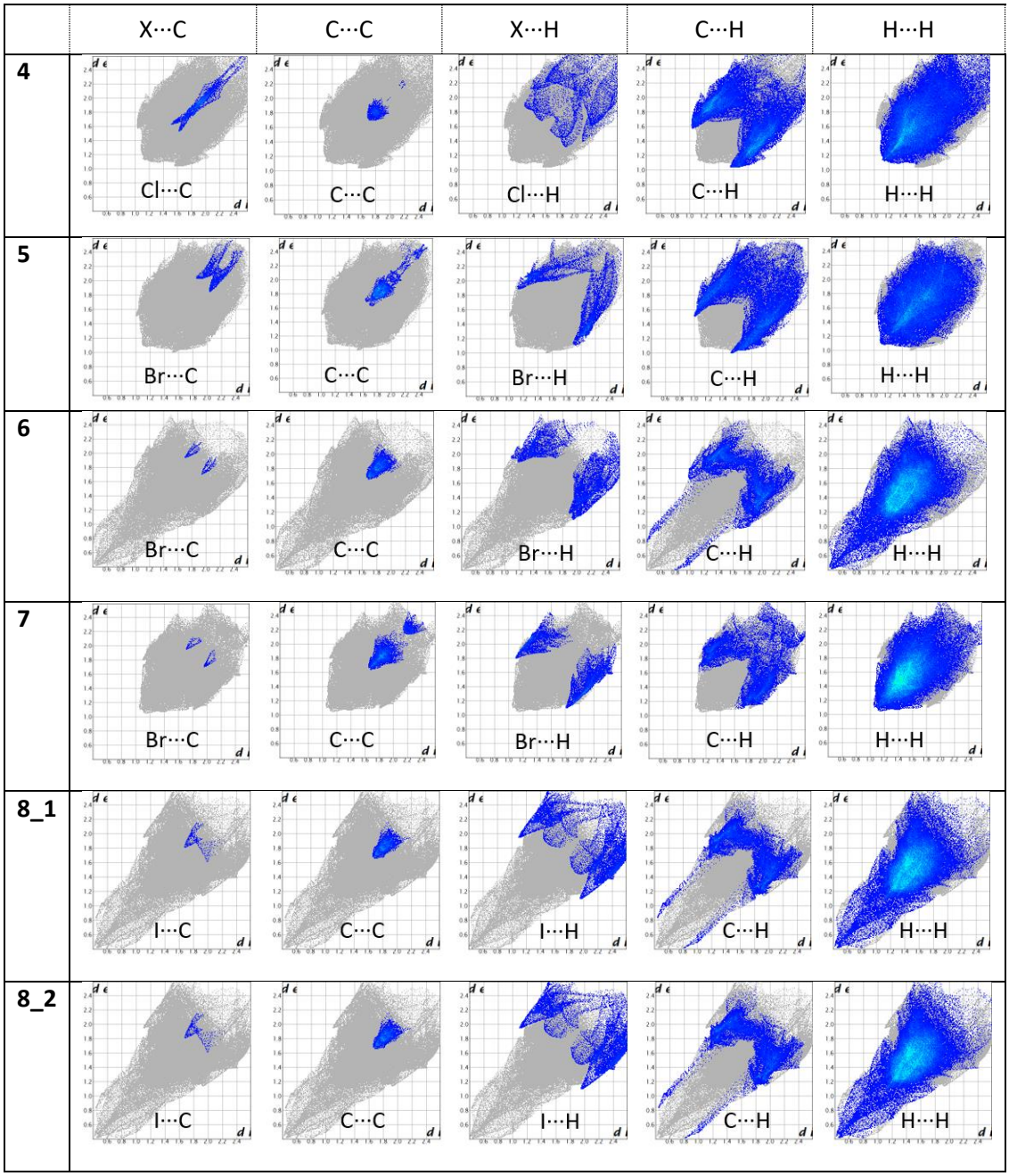

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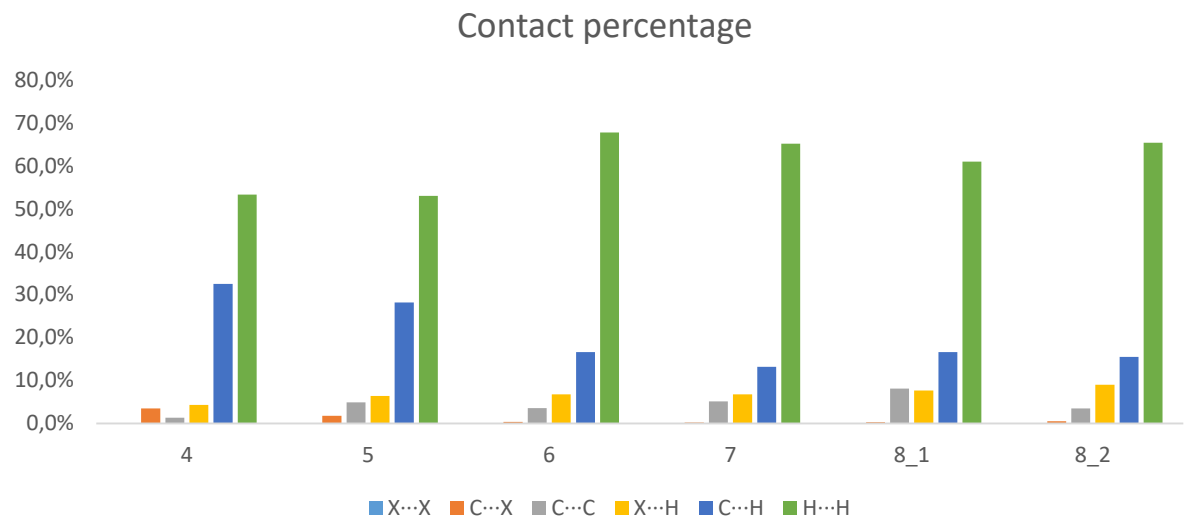

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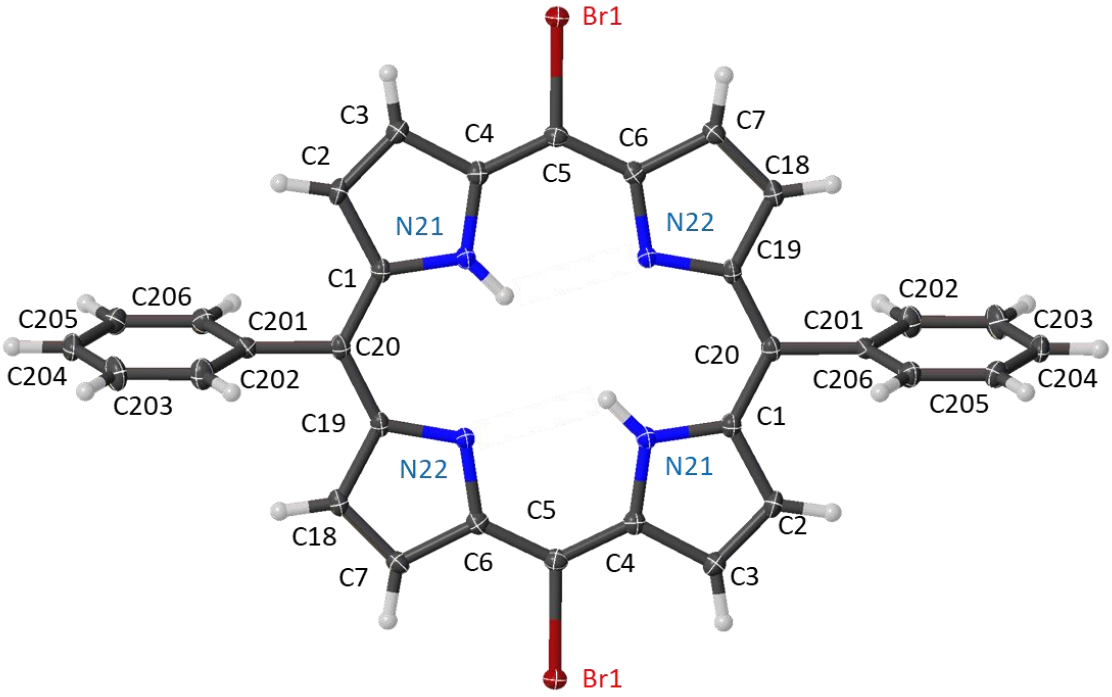
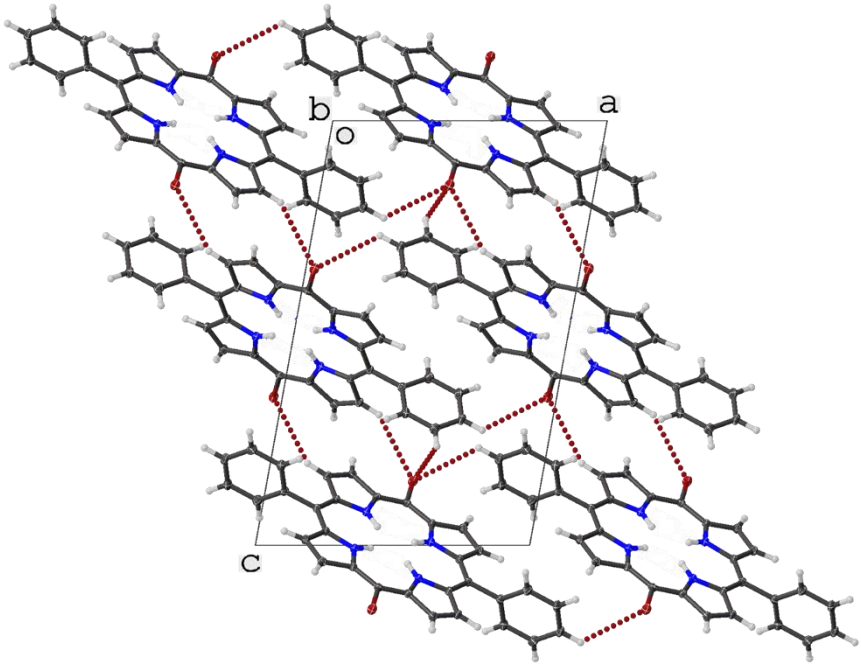


Figure S22: Thermal ellipsoid plot of compound **9** (thermal displacement given as 50% probability). Minor disordered moieties have been omitted.



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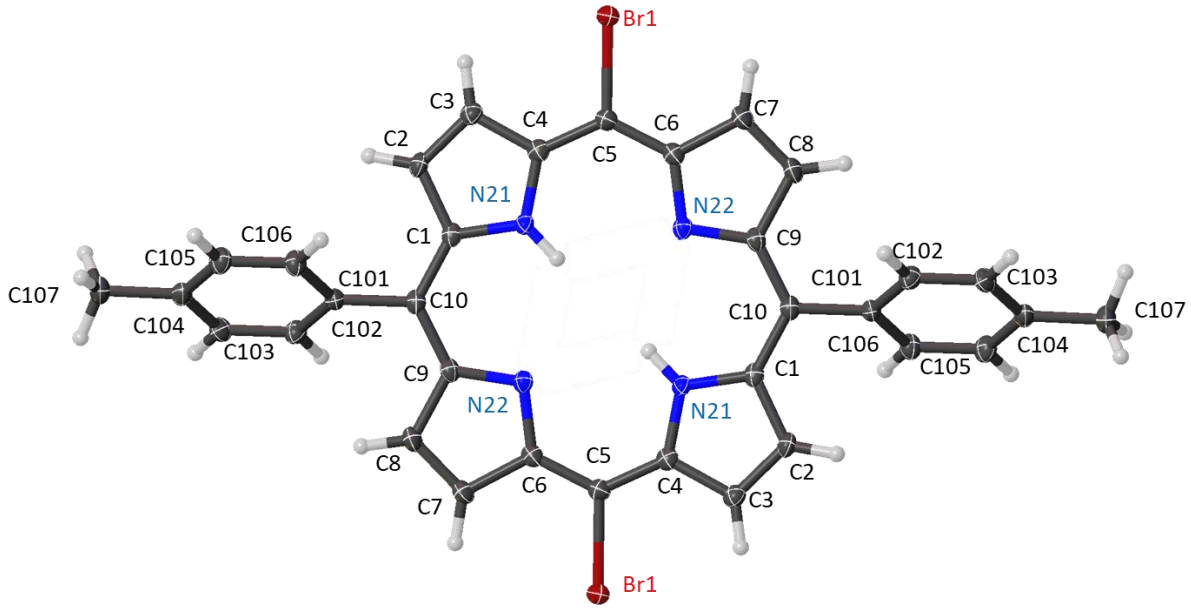

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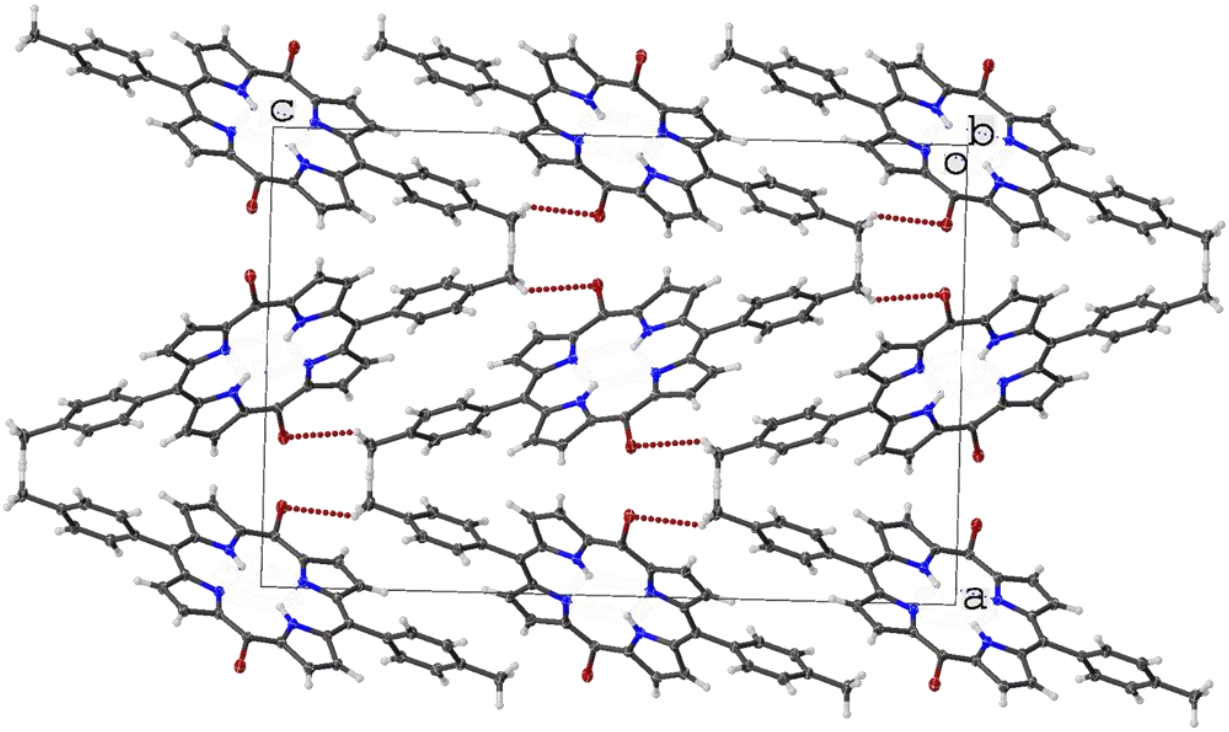

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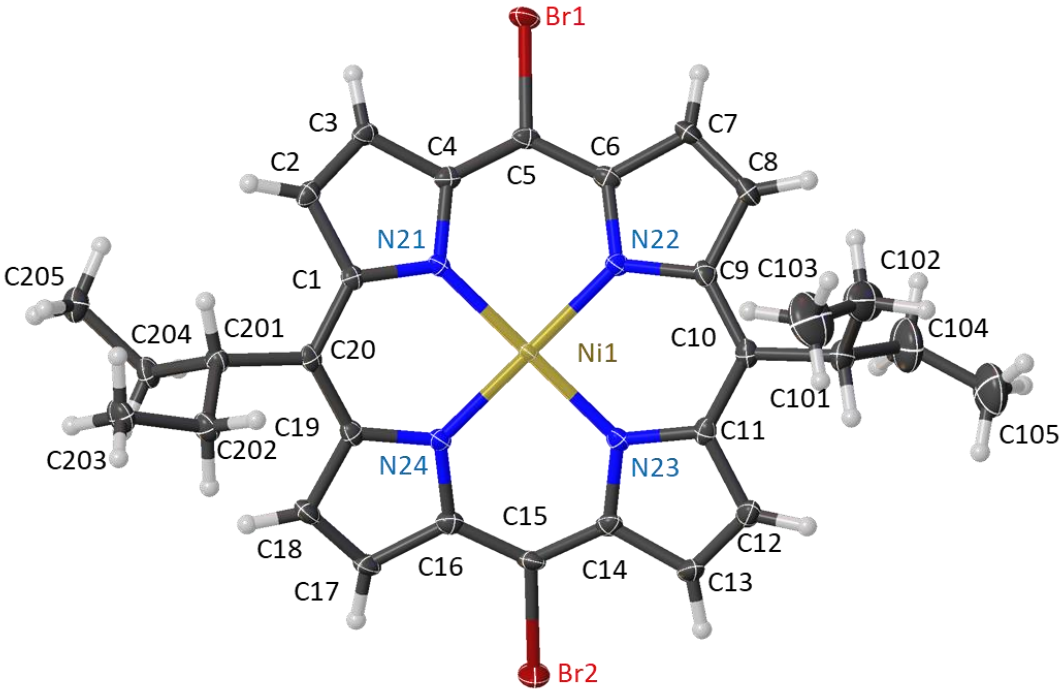


Figure S26: Thermal ellipsoid plot of compound **11** (thermal displacement given as 50% probability). Minor disordered moieties have been omitted.

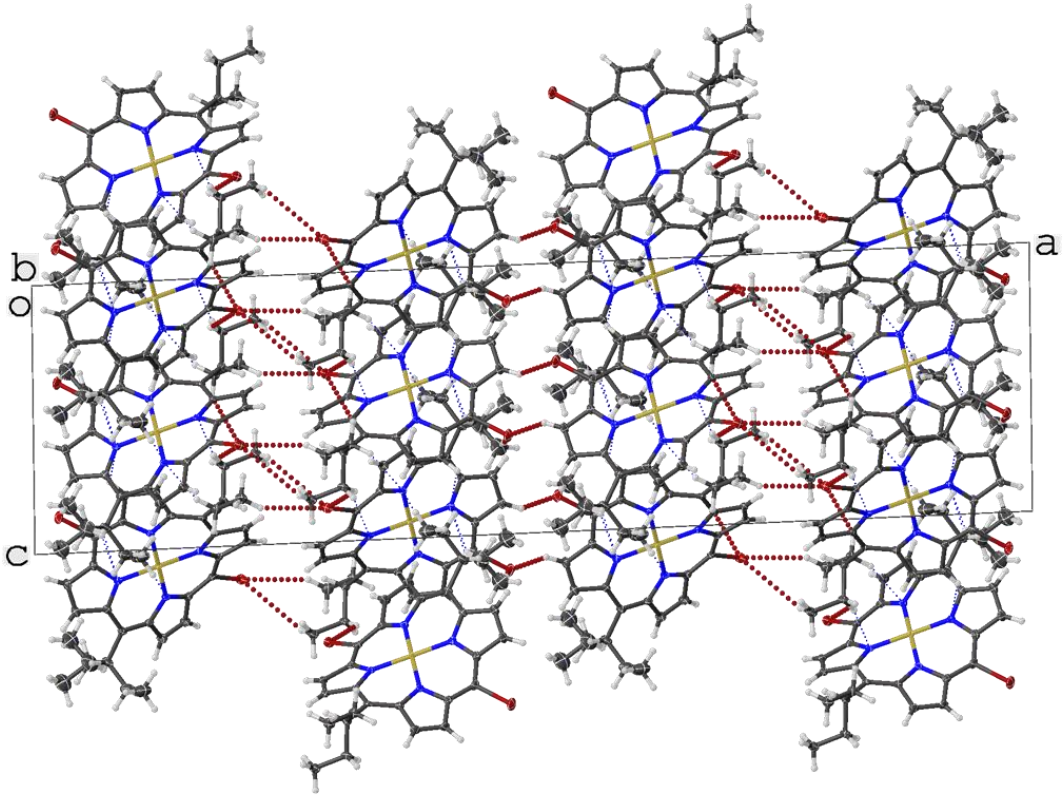


Figure S27: Packing diagram (thermal ellipsoid plot) of compound **11** looking down the *b*-axis (thermal displacement given as 50% probability). Minor disordered moieties have been omitted.

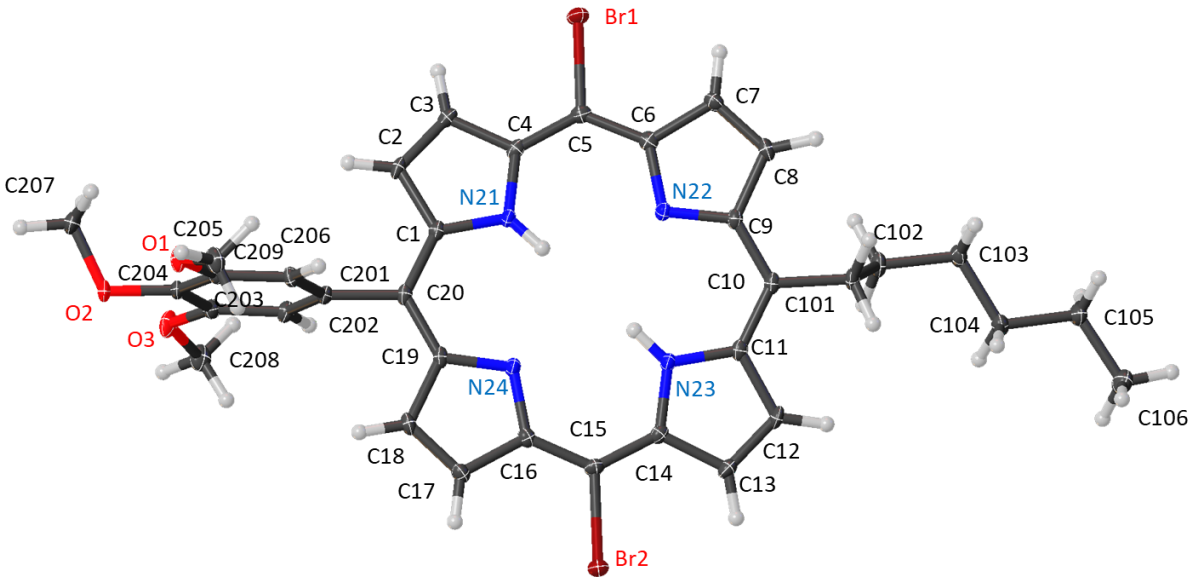


Figure S28: Thermal ellipsoid plot of compound **13** (thermal displacement given as 50% probability). Minor disordered moieties have been omitted.

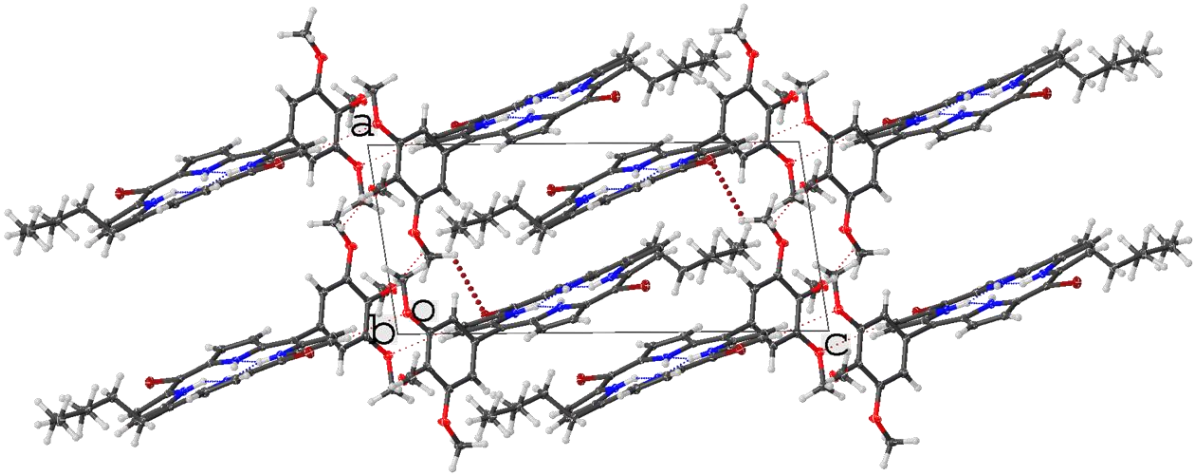
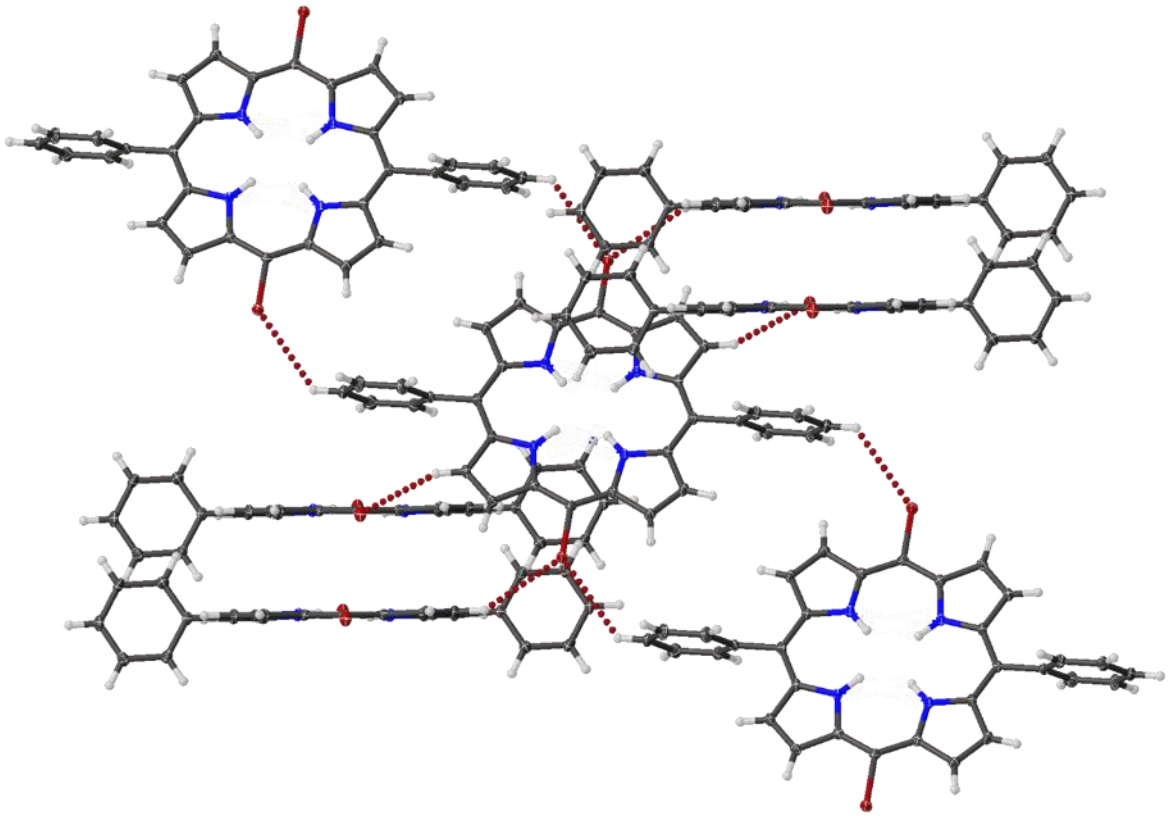


Figure S29: Packing diagram (thermal ellipsoid plot) of compound **13** looking down the *b*-axis (thermal displacement given as 50% probability). Minor disordered moieties have been omitted.



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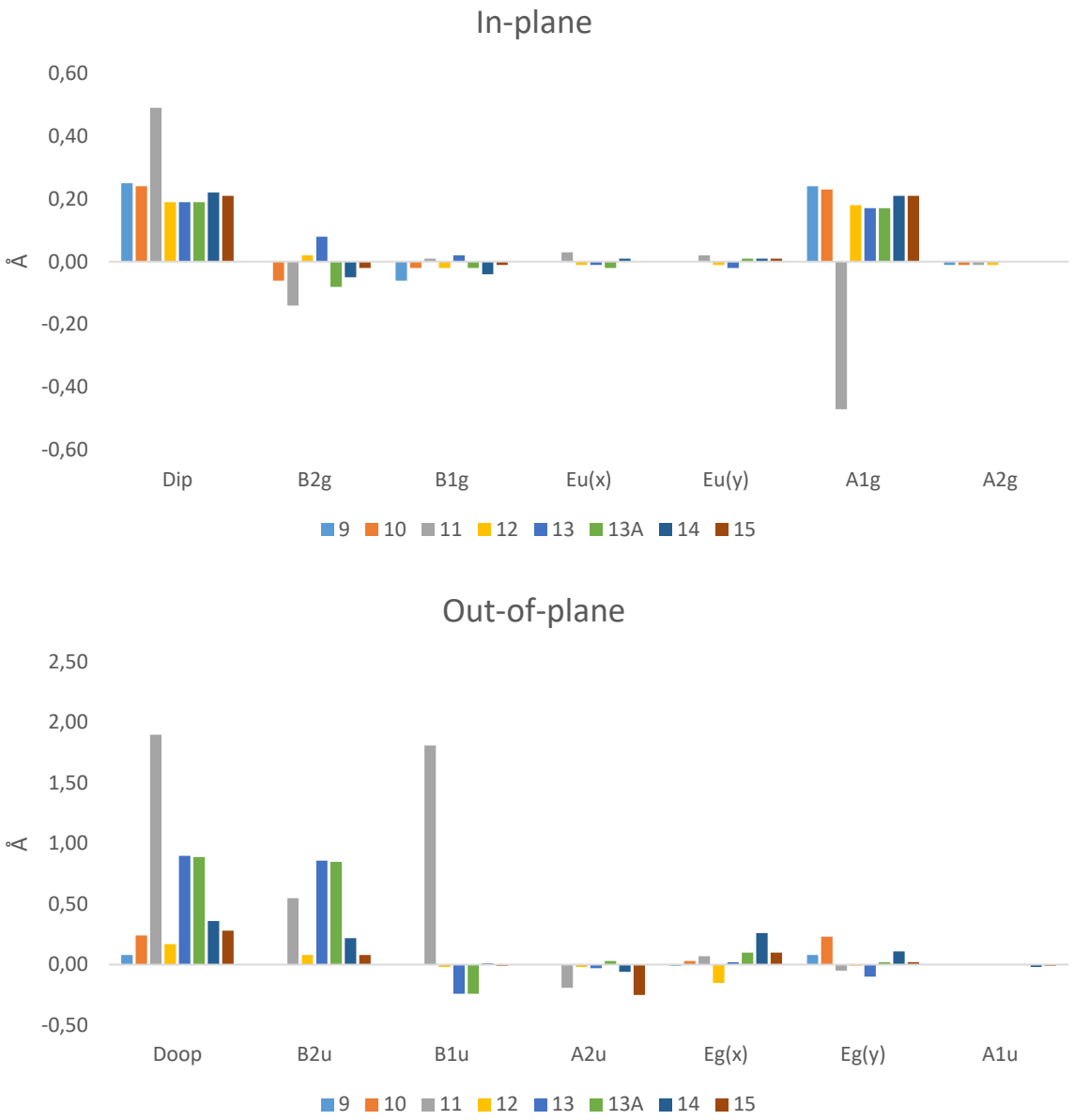


Figure S31: NSD charts for compounds **9**-**15**.

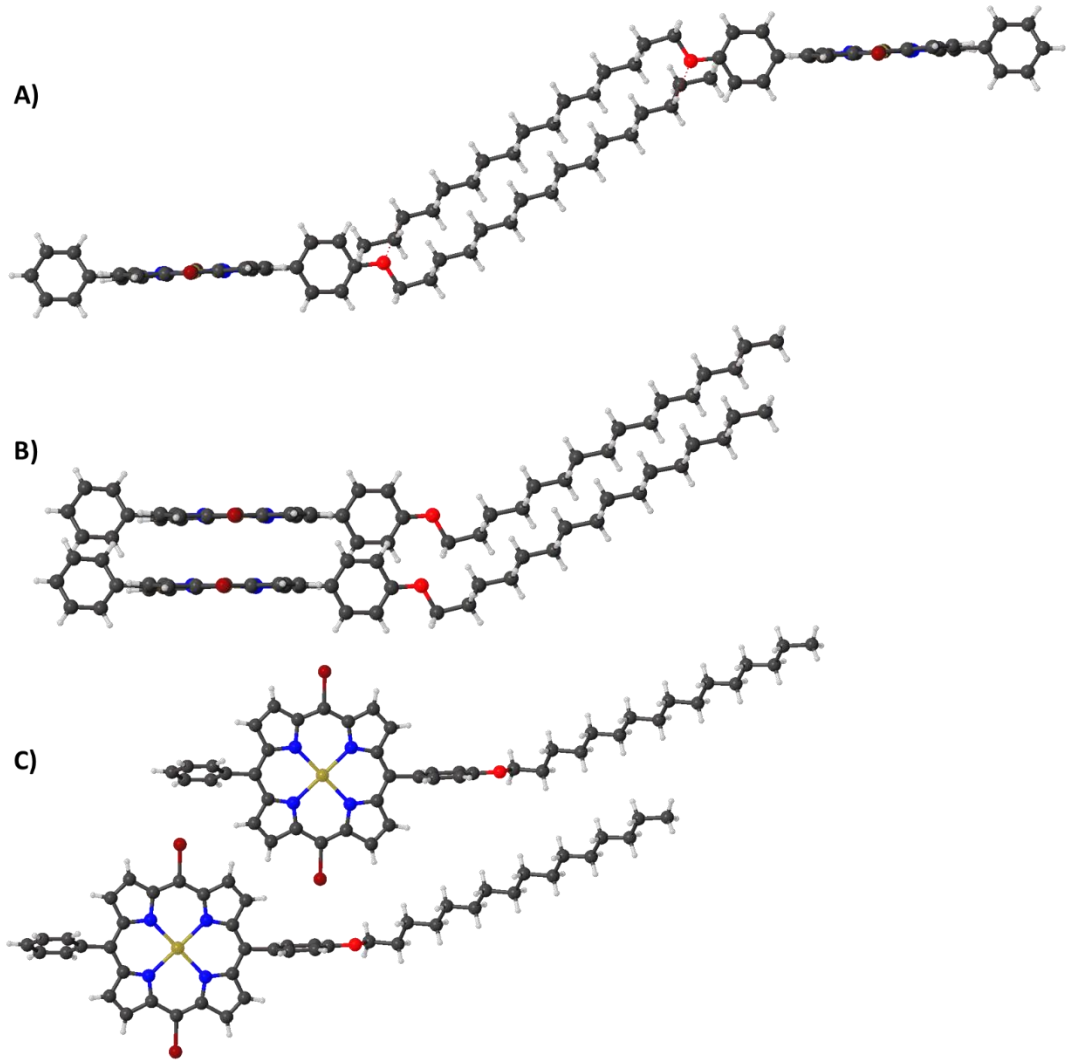


Figure S32: Expanded view (ball and stick) of compound 12 showing the (A) alkyl chain interactions (B) porphyrin stacking (C) close packing side-on alignment.

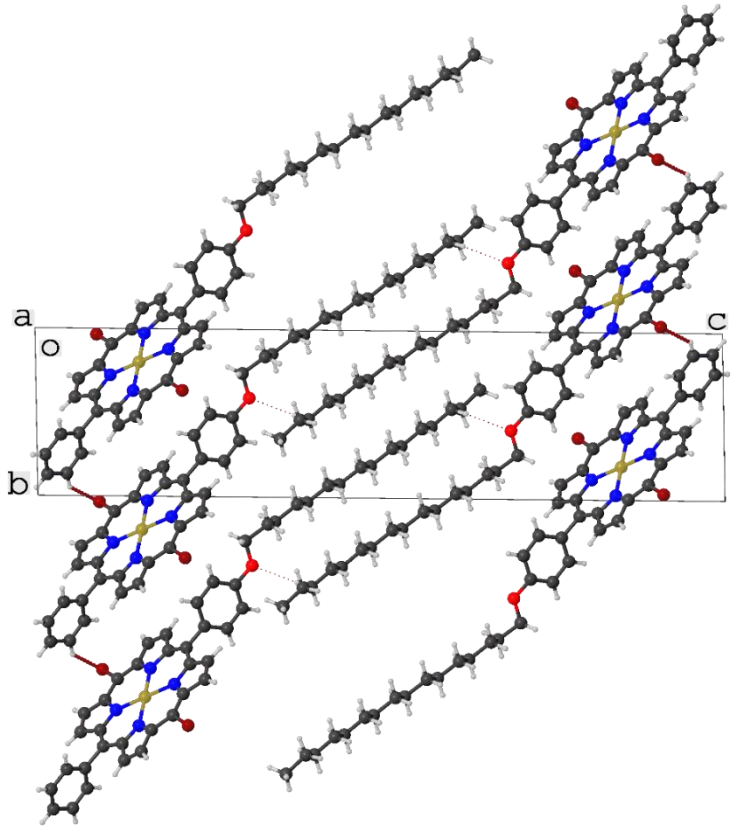


Figure S33: Packing diagram (ball and stick) of compound **12** looking down the *a*-axis.

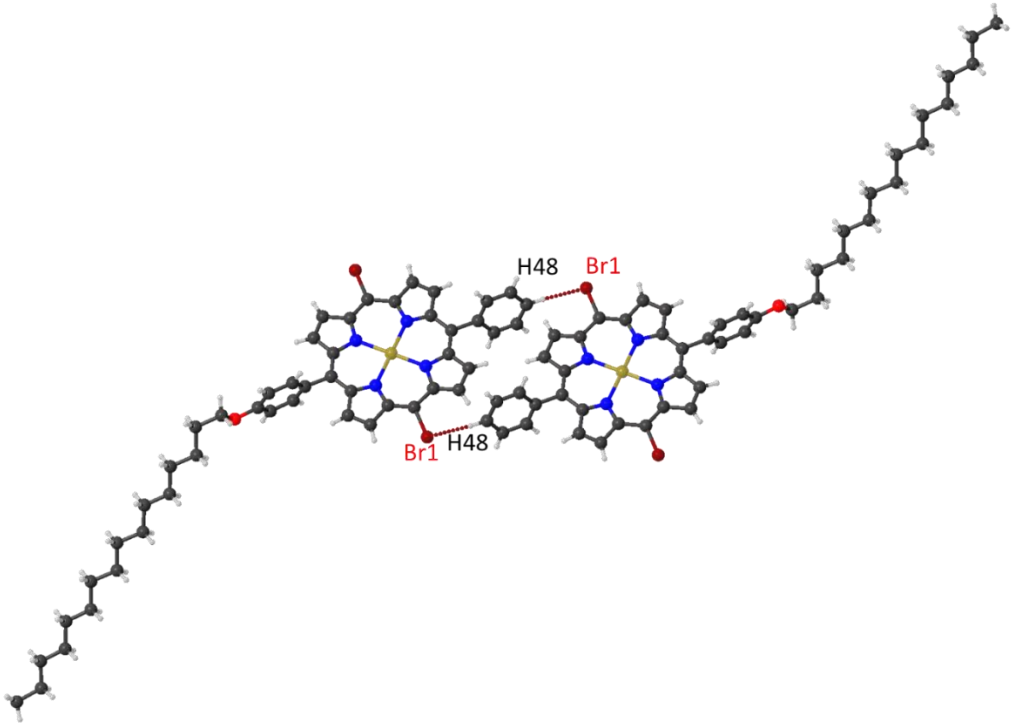
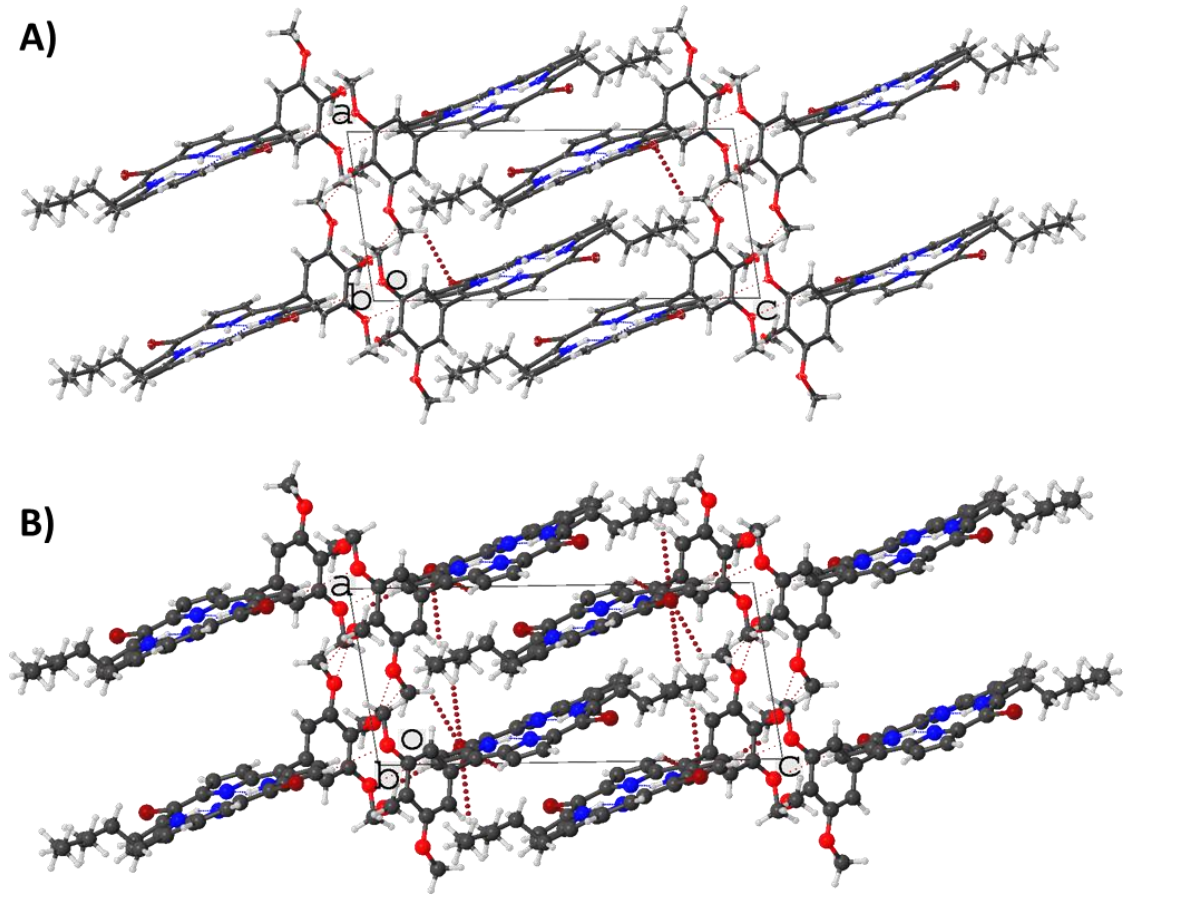


Figure S34: Expanded view (ball and stick) of compound **12** showing the head-to-head Br···H contact.



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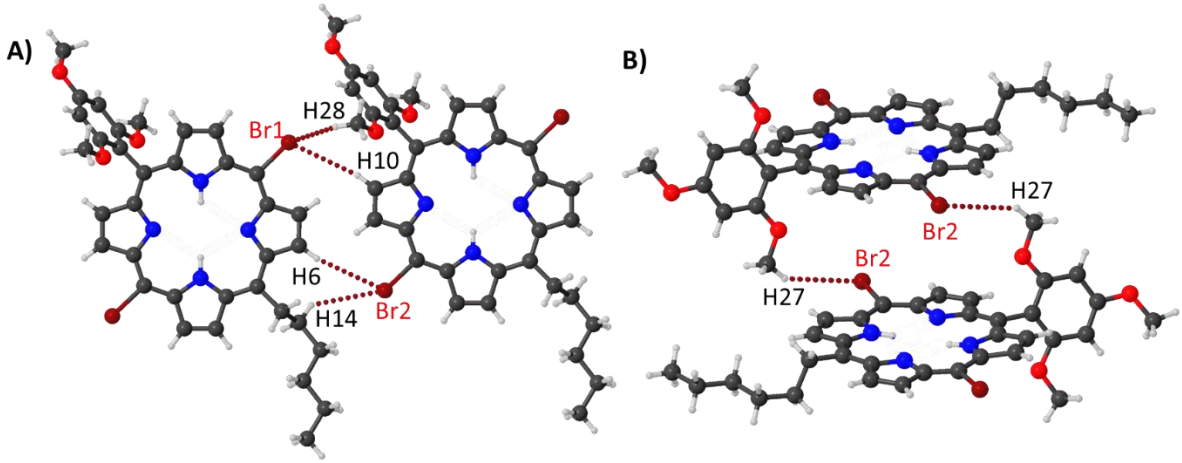

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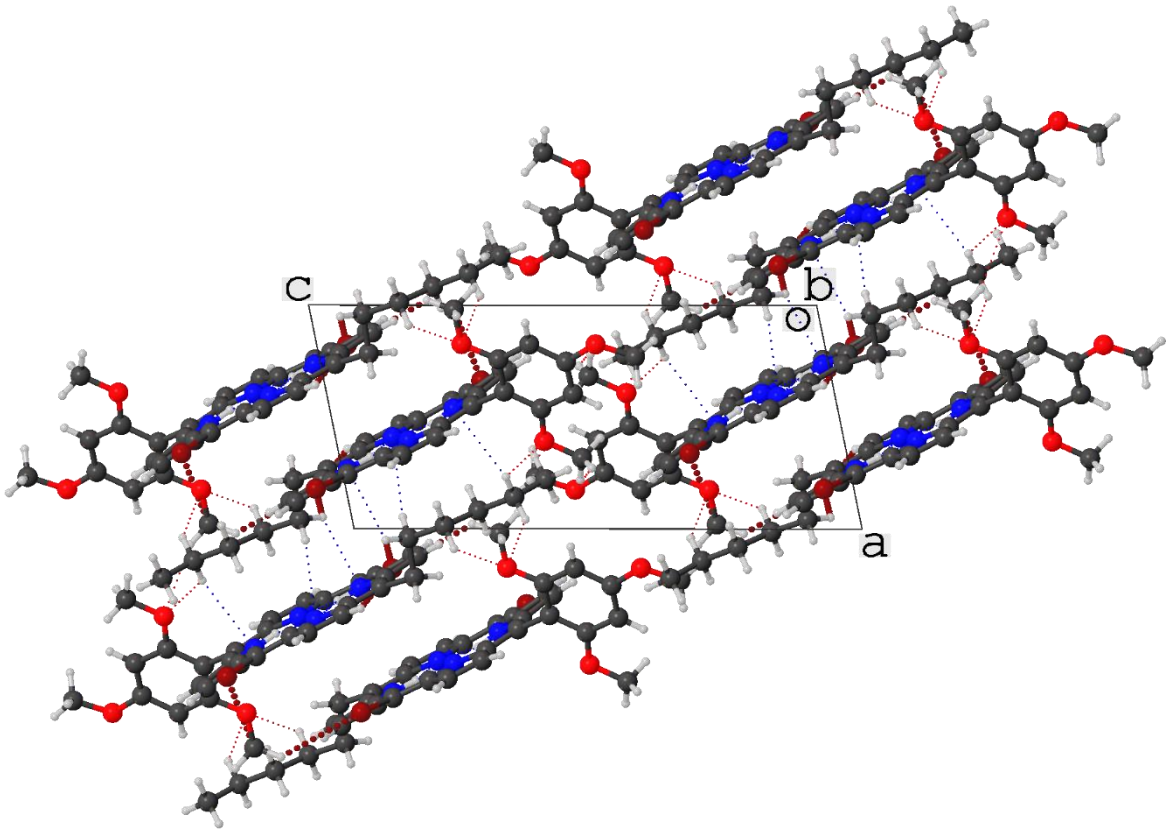

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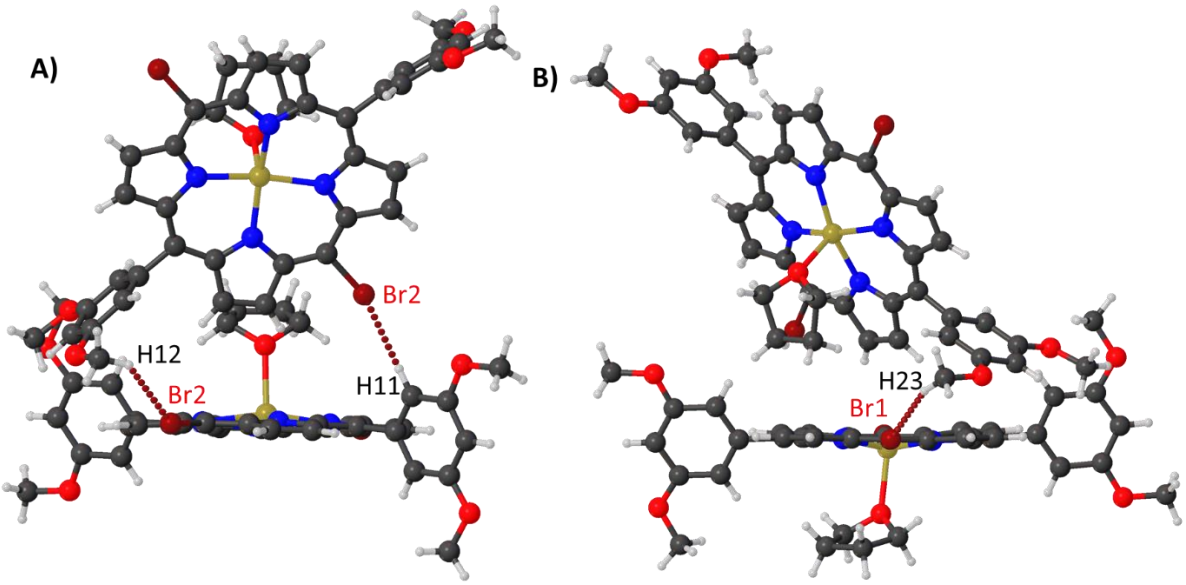

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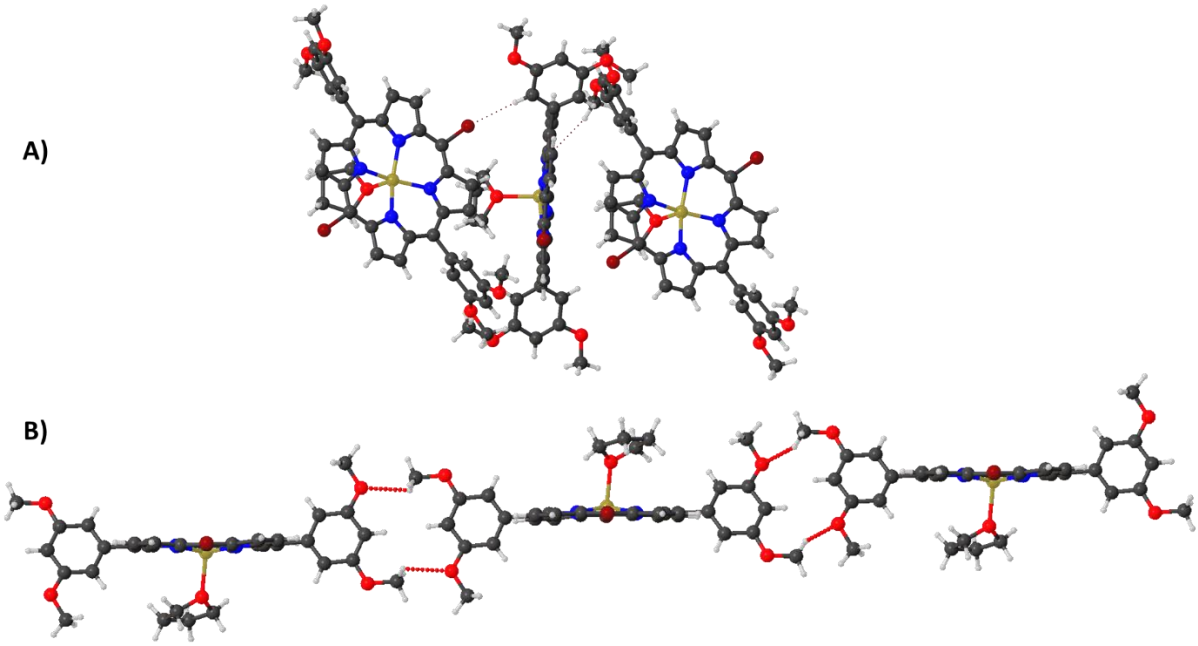

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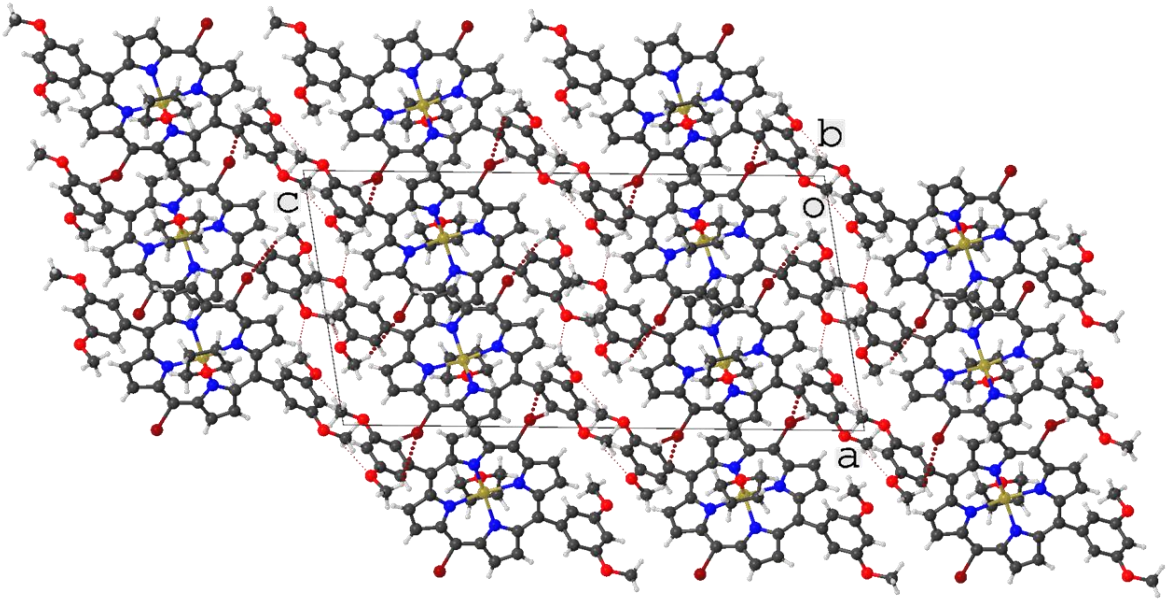

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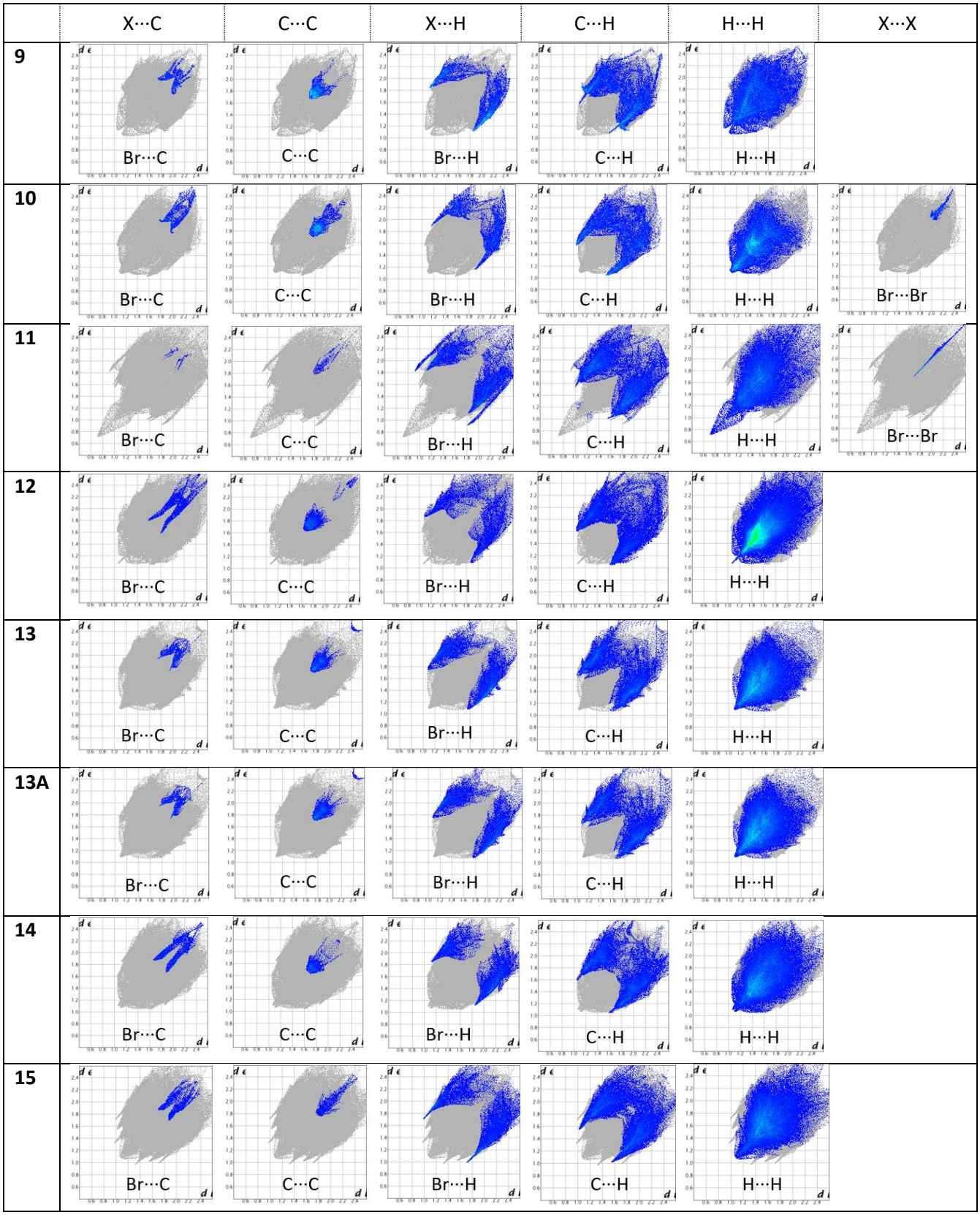

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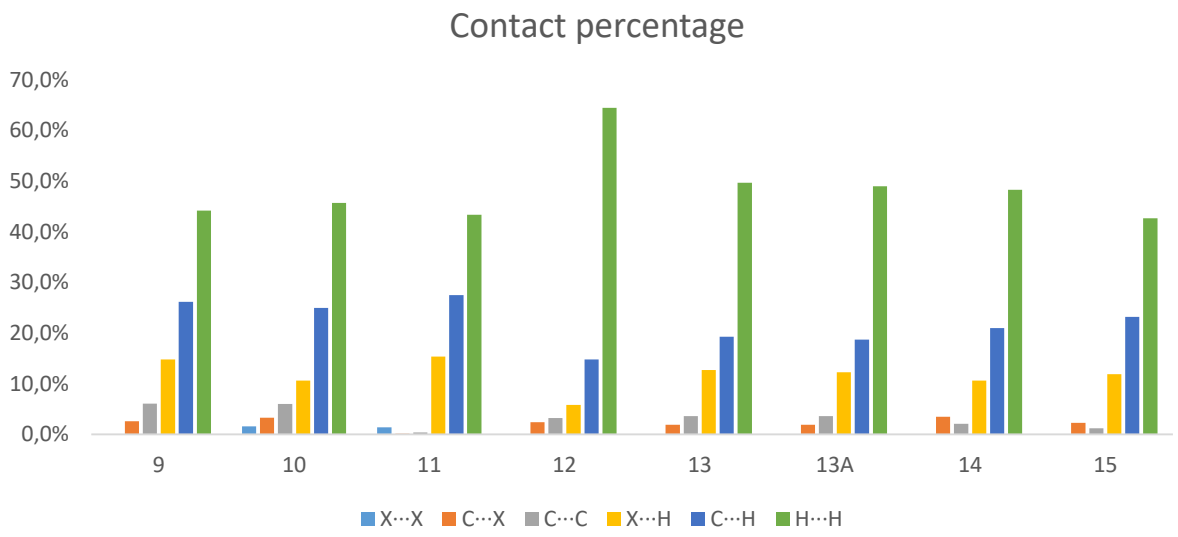


Figure S42: Contact percentages of compounds 9-15.

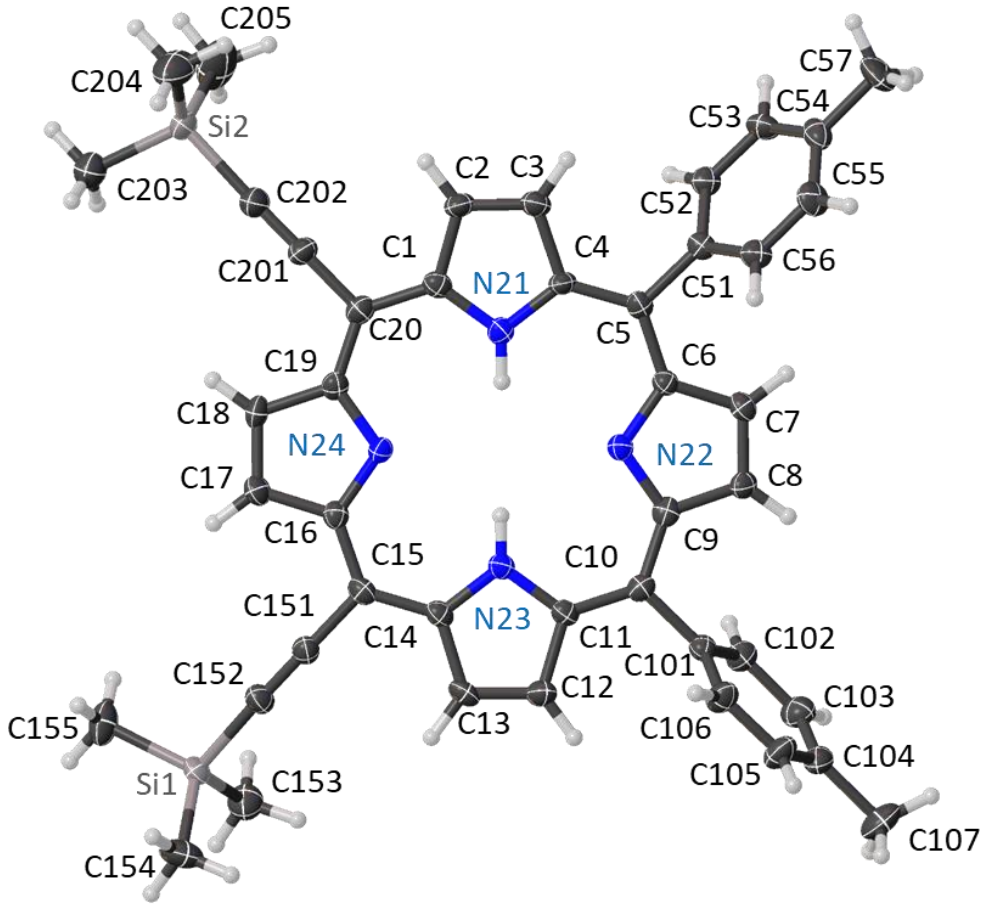


Figure S43: Thermal ellipsoid plot of compound 16A (thermal displacement given as 50% probability). Minor disordered moieties have been omitted.

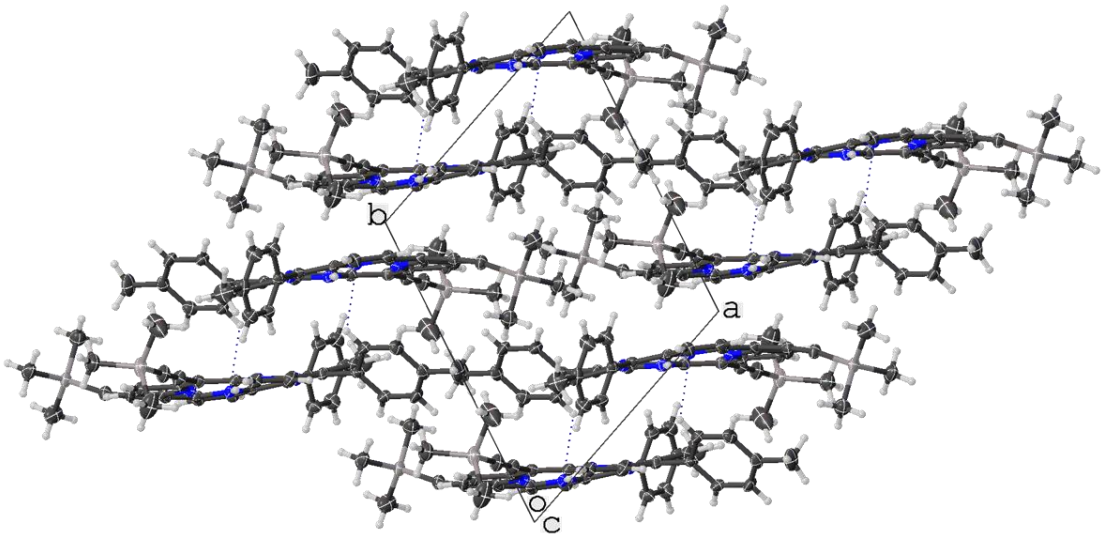
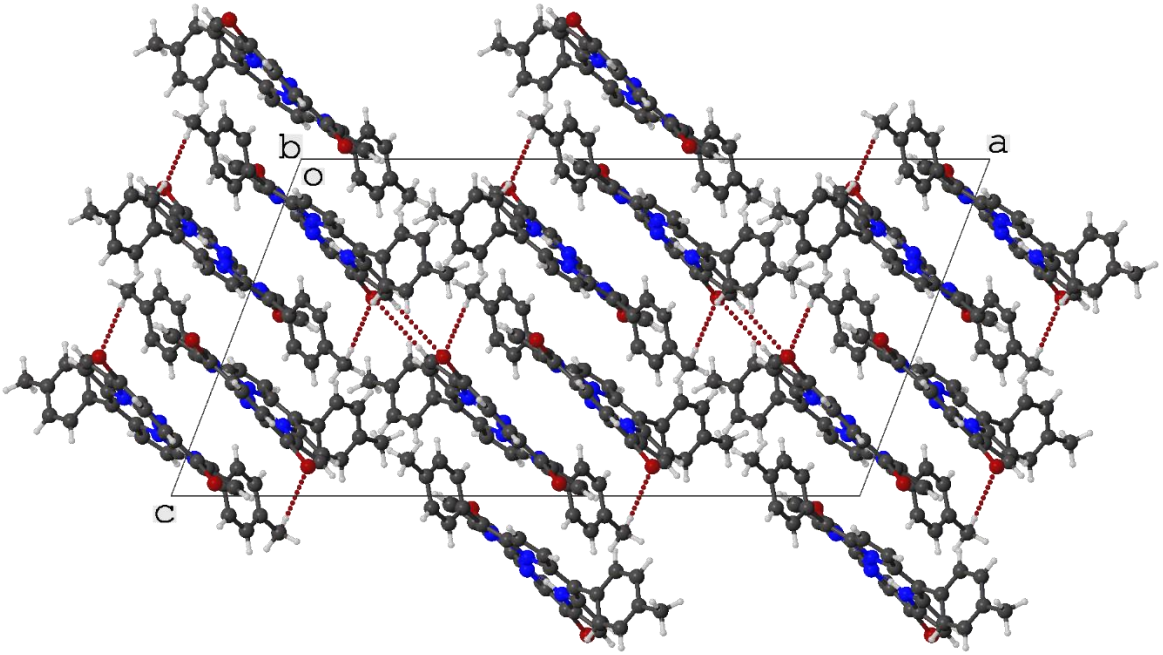


Figure S44: Packing diagram (thermal ellipsoid plot) of compound **16A** looking down the *c*-axis (thermal displacement given as 50% probability). Minor disordered moieties have been omitted.



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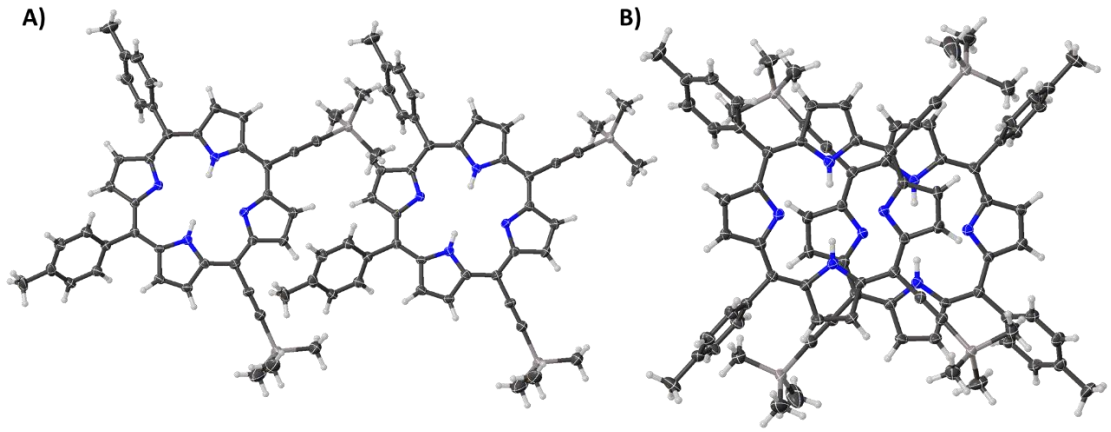
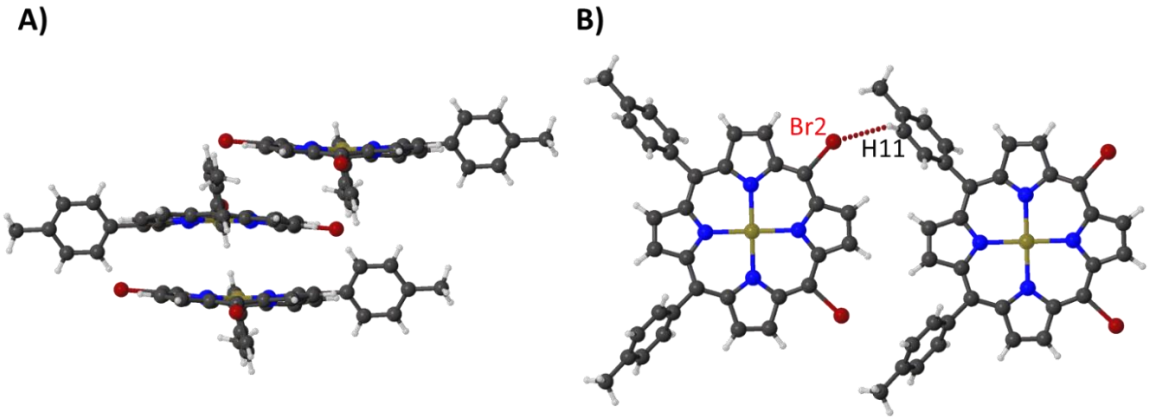


Figure S46: Expanded view (thermal ellipsoid plot) of compound 16A showing (A) linear alignment and (B) stacking.



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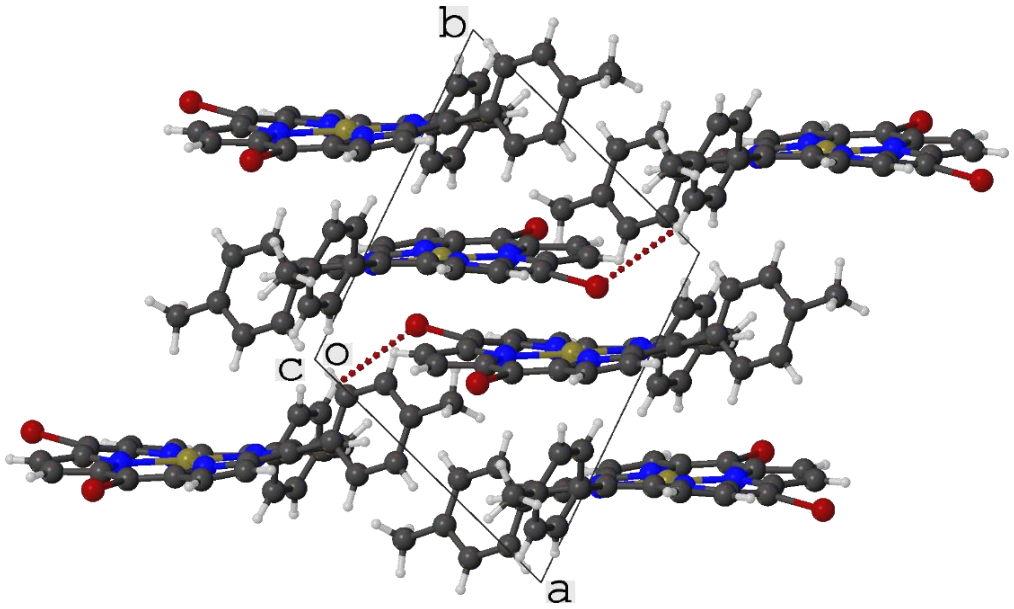


Figure S48: Packing diagram (ball and stick) of compound 17 looking down the *c*-axis.

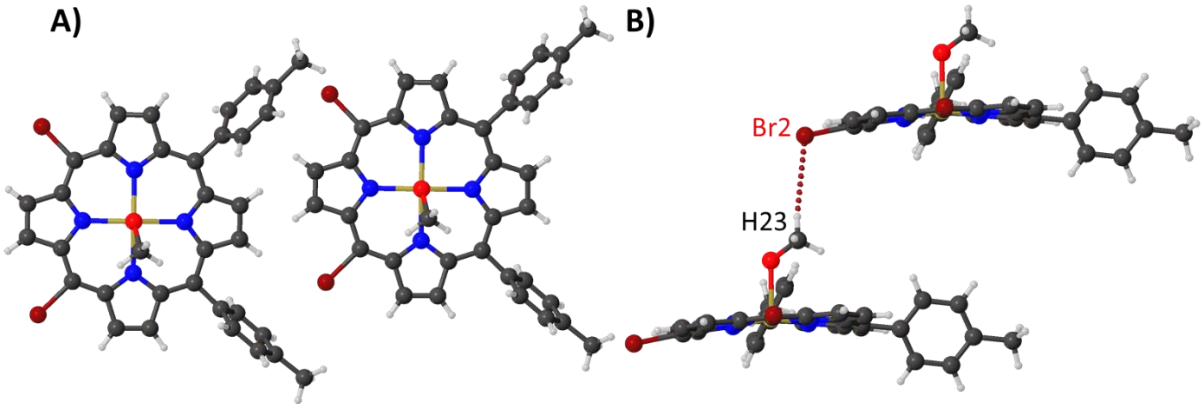


Figure S49: Expanded view (ball and stick) of compound 18 showing the (A) head-to-tail alignment and (B) interaction between the axial ligand and the bromine atoms.

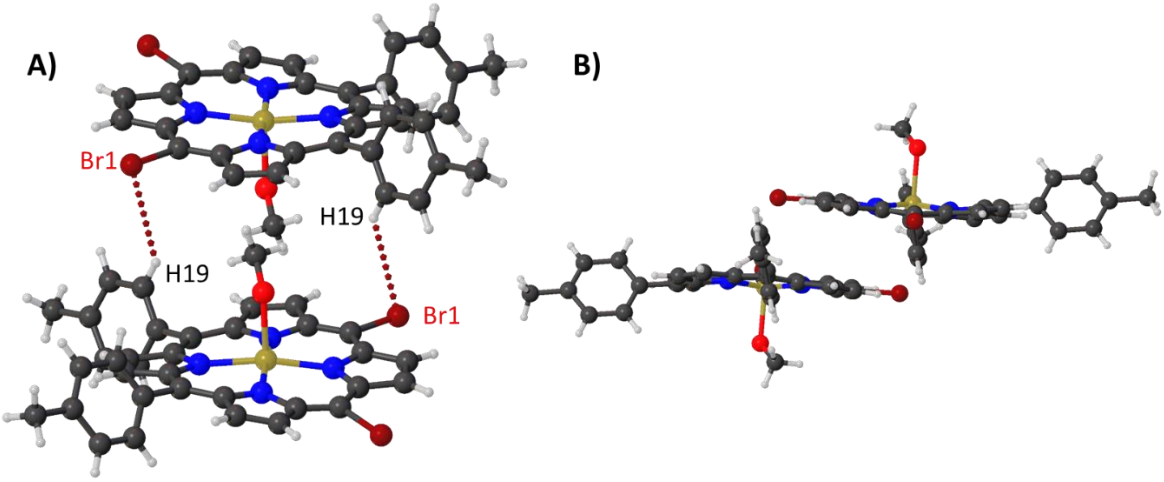


Figure S50: Expanded view (ball and stick) of compound 18 showing the stacking between (A) solvent side of the porphyrin and (B) non-solvent side.

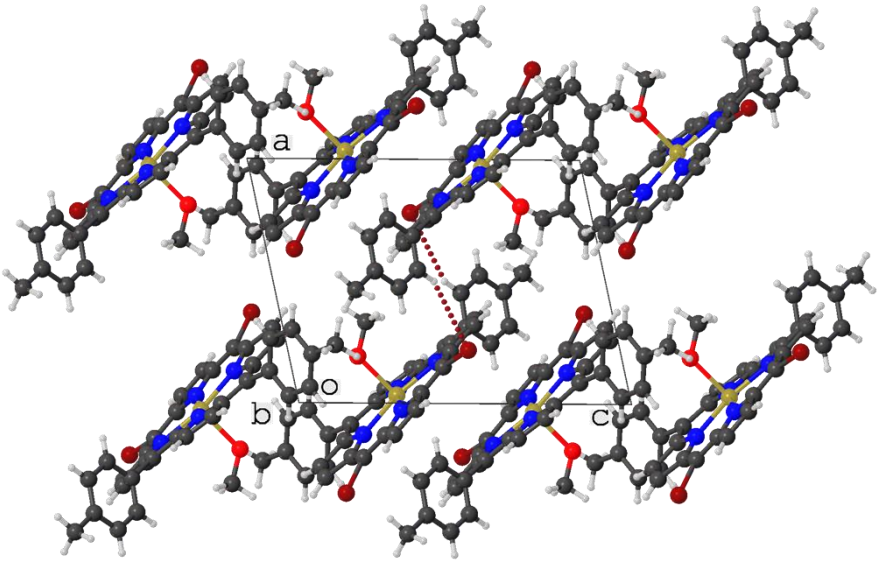


Figure S51: Packing diagram (ball and stick) of compound 18 looking down the *b*-axis.

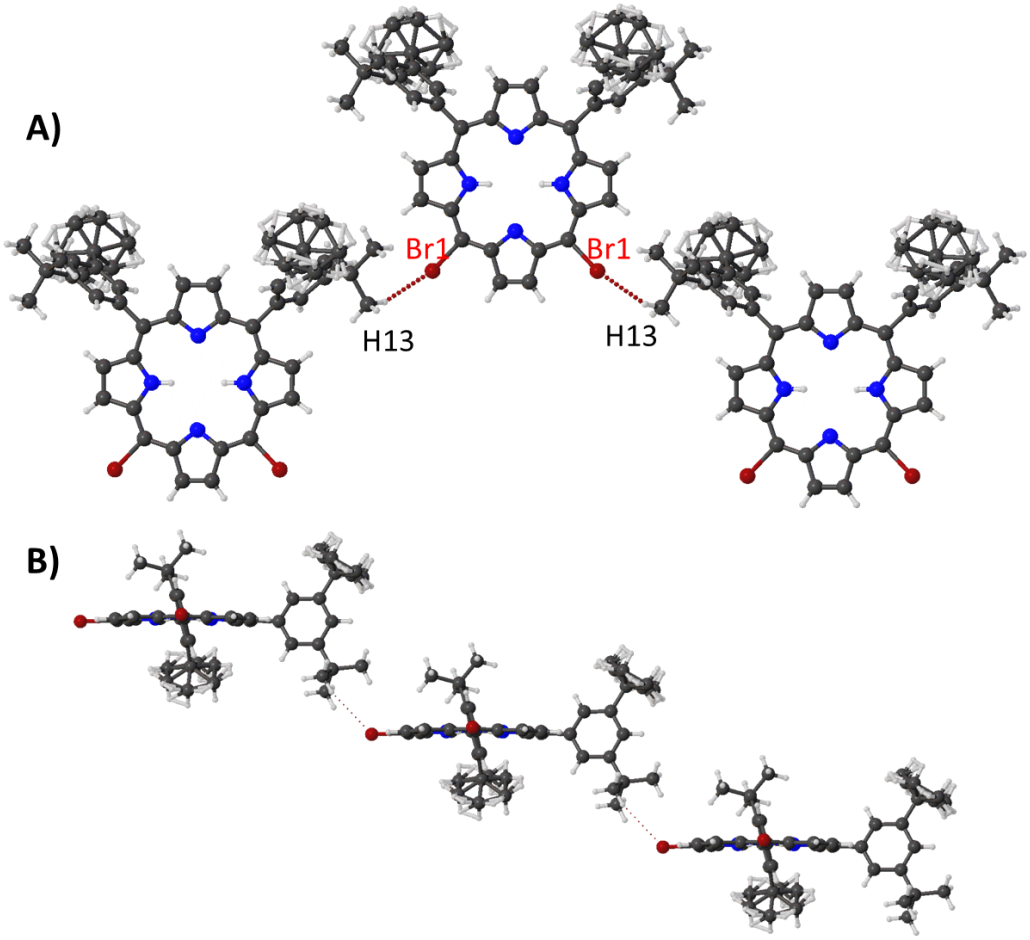


Figure S52: Expanded view (ball and stick) of compound **19** showing the stepwise alignment of porphyrins with Br···H interactions (**A**) top and (**B**) side.

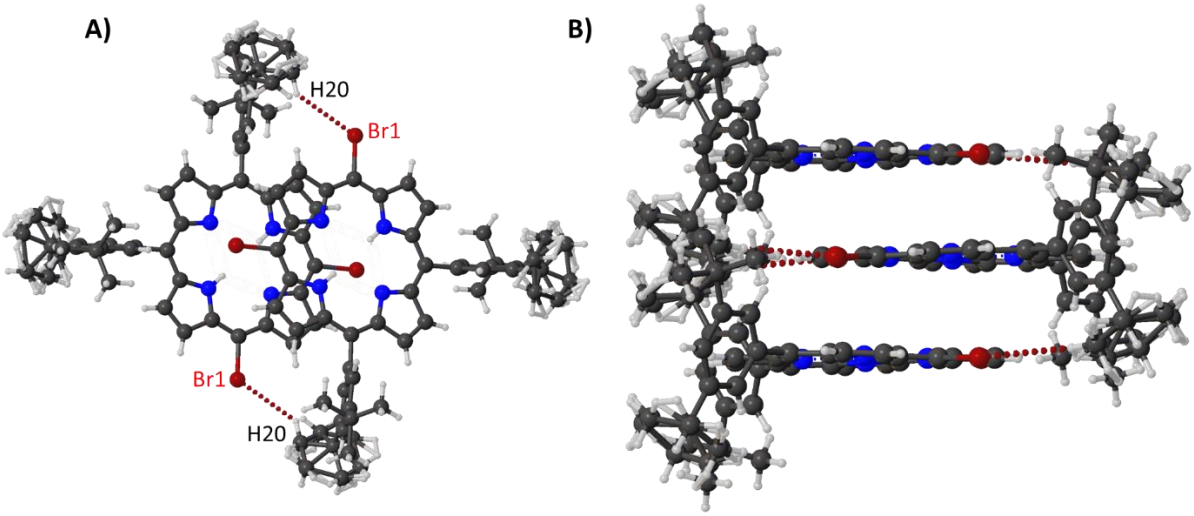


Figure S53: Expanded view (ball and stick) of compound **19** showing the (**A**) top view of stacking and (**B**) edge-on view of stacking.

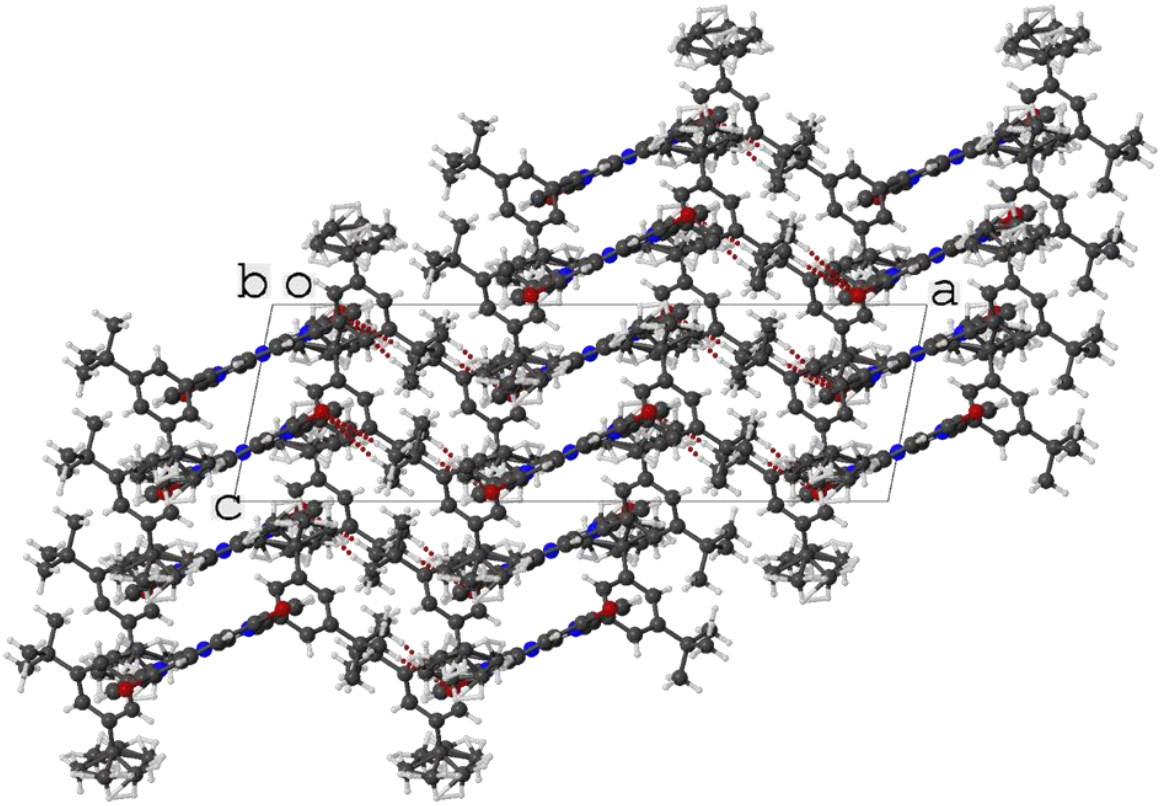
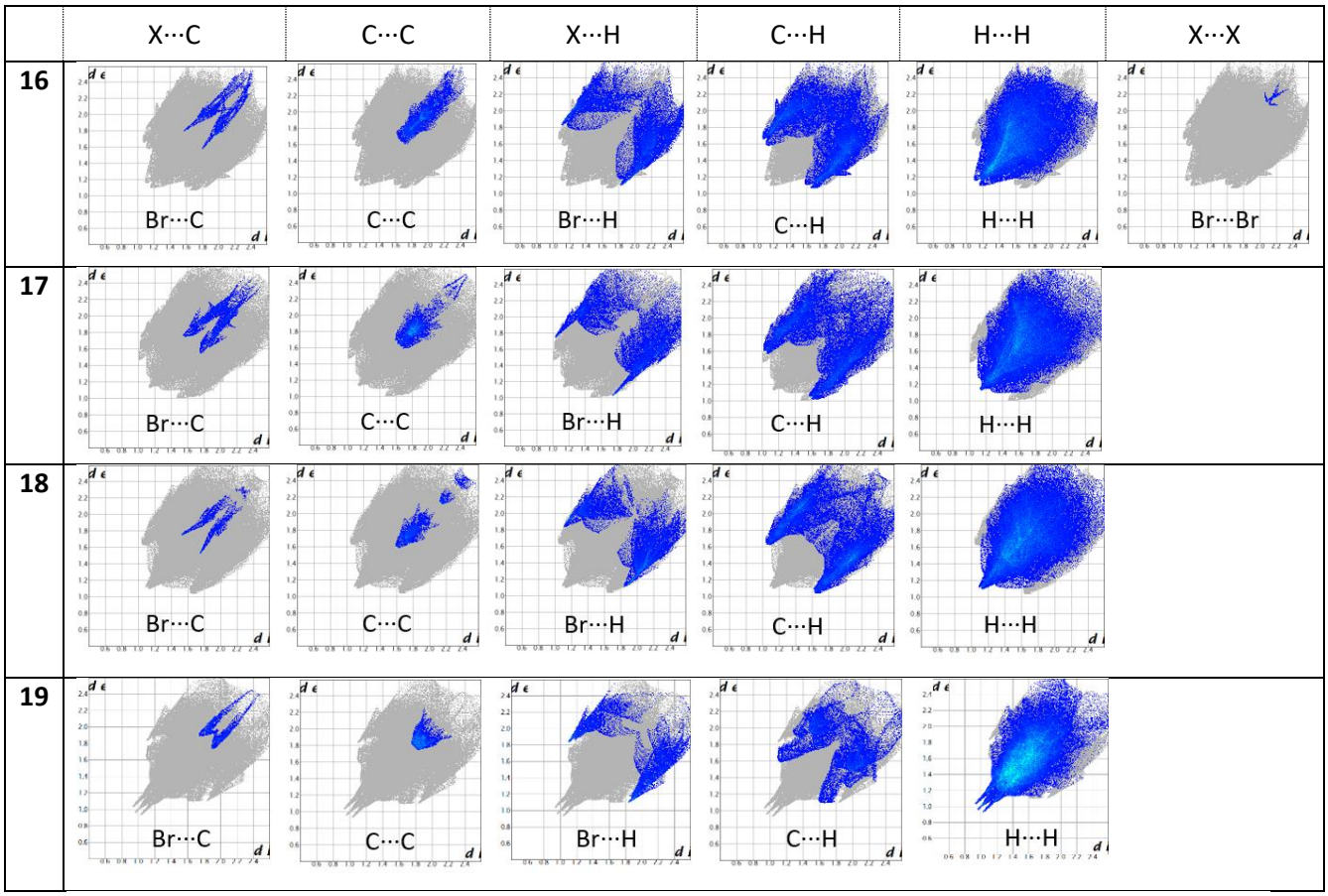


Figure S54: Packing diagram (ball and stick) of compound 19 looking down the *b*-axis.



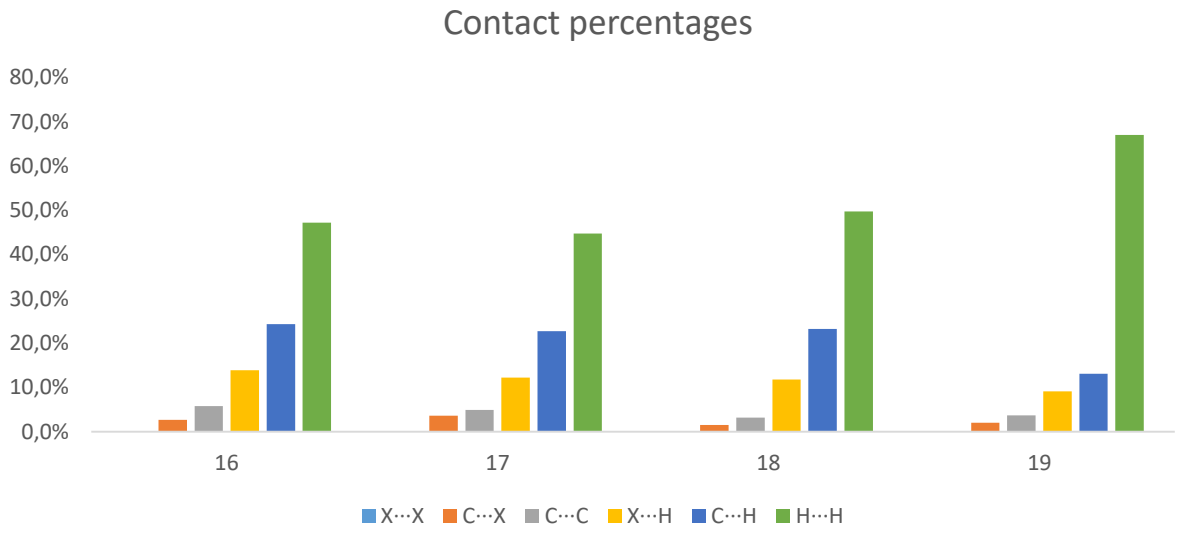


Figure S55: Hirshfeld surfaces and contact percentages of compounds **16**-**19**.

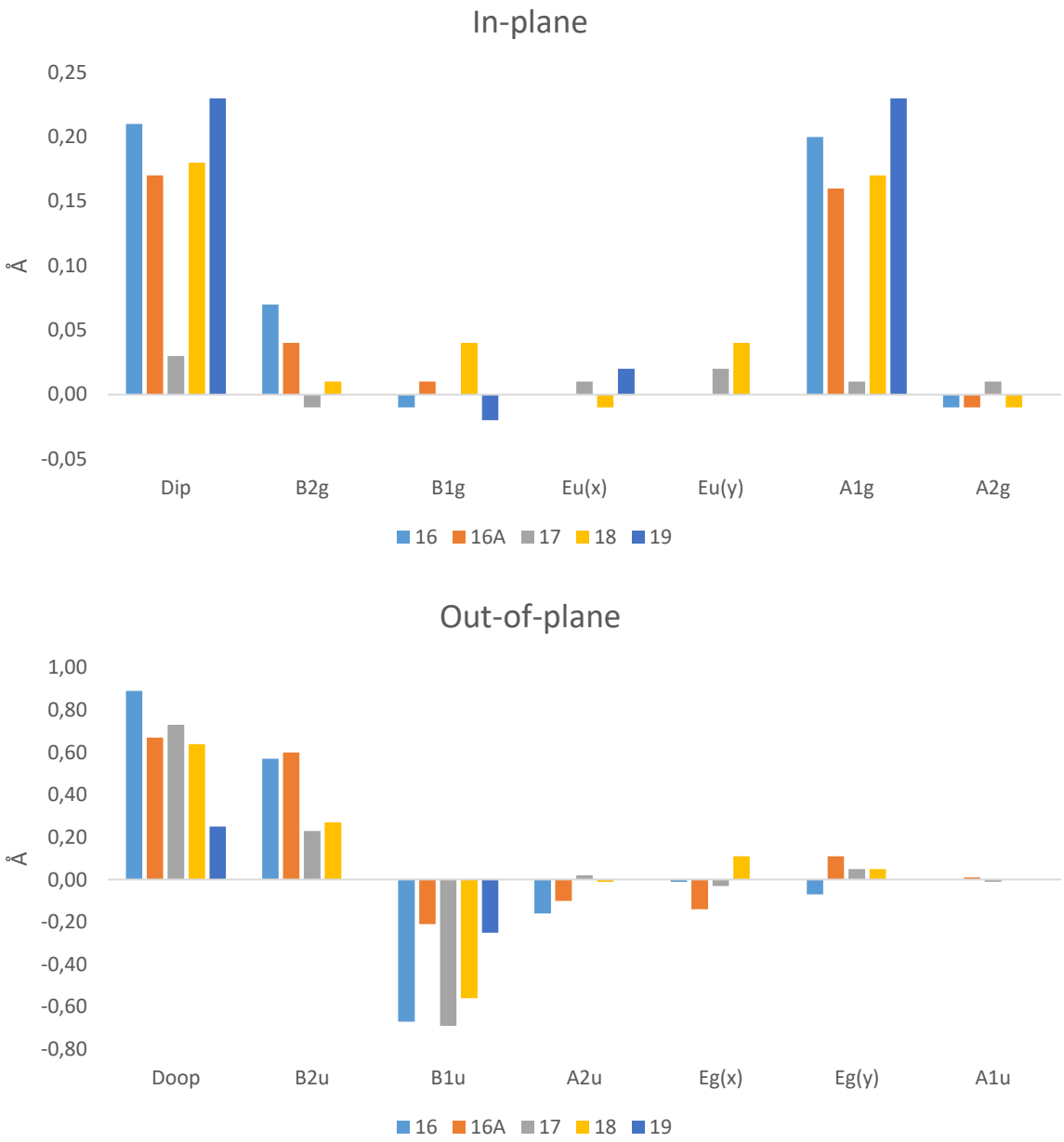


Figure S56: NSD charts for compounds **16**-**19**.

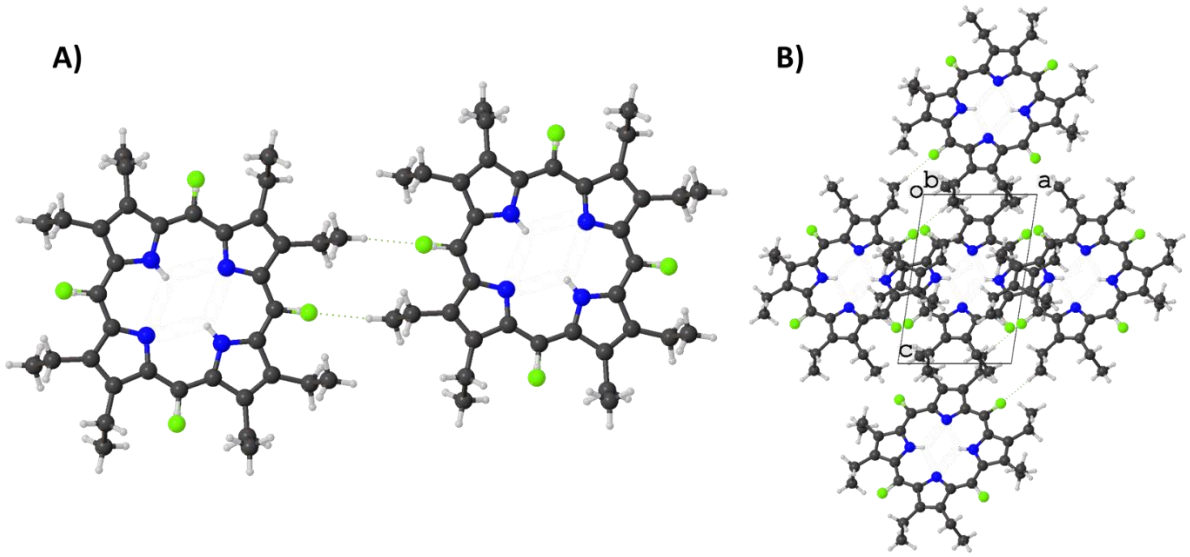


Figure S57: (A) Expanded view (ball and stick) of compound 20 showing the F···H interaction and (B) crystal packing (ball and stick) of compound 20.

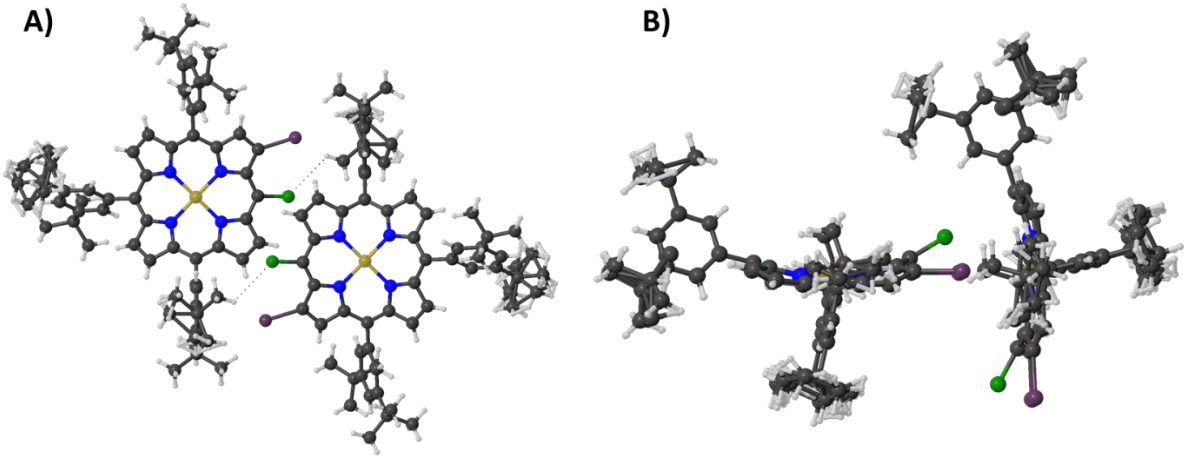


Figure S58: (A) Expanded view (ball and stick) of compound 21 showing the head-to-head interaction (B) Expanded view (ball and stick) of compound 22 showing the face-to-edge interaction.

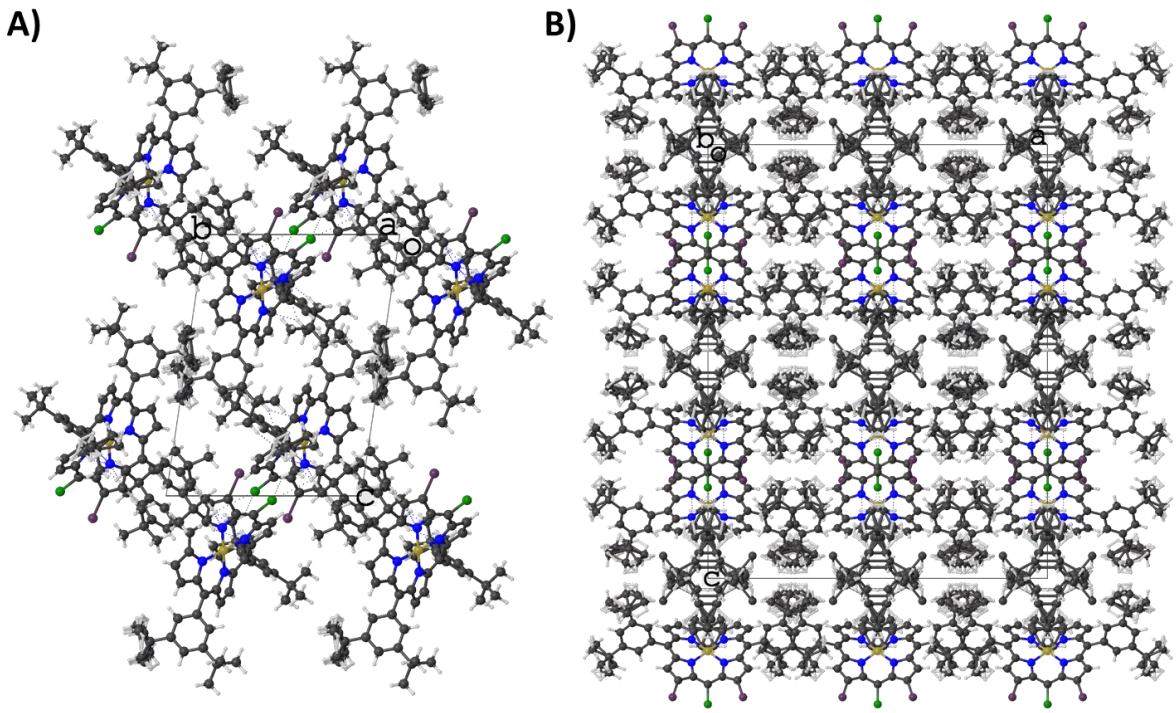


Figure S59: Packing diagram (ball and stick) of compound **21** looking down the *a*-axis (**A**) and **22** looking down the *b*-axis (**B**).

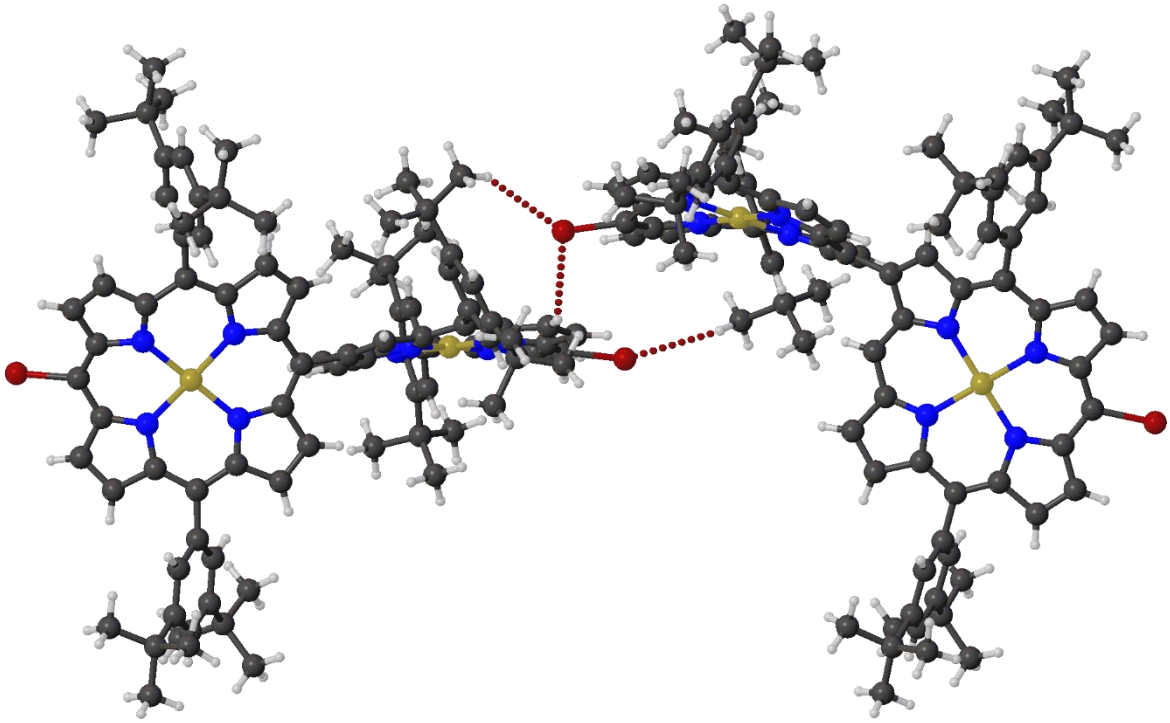


Figure S60: Expanded view (ball and stick) of compound **23** showing the head-to-tail interaction.

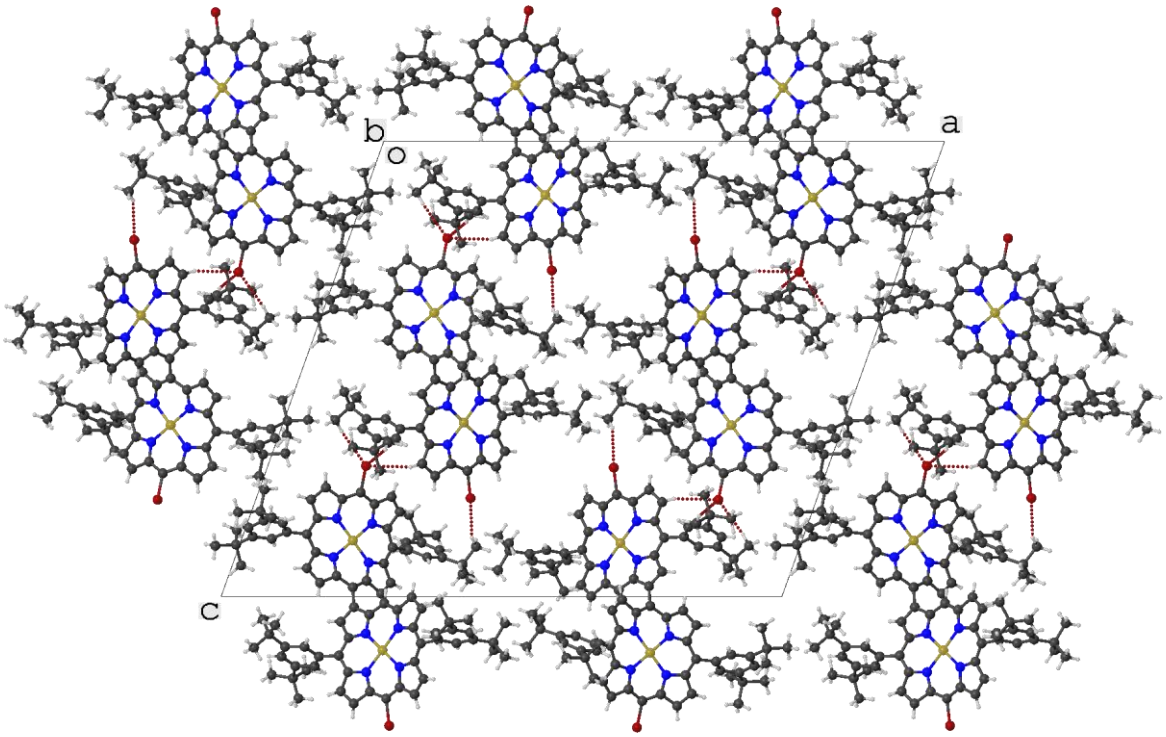


Figure S61: Packing diagram (ball and stick) of compound **23** looking down the *b*-axis.

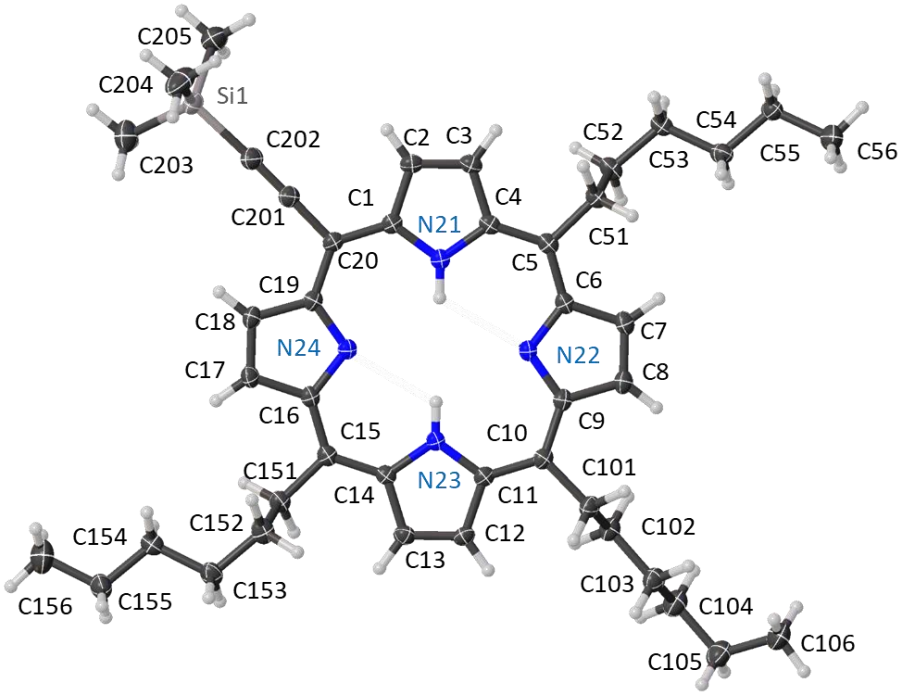


Figure S62: Thermal ellipsoid plot of compound **24** (thermal displacement given as 50% probability). Minor disordered moieties have been omitted.

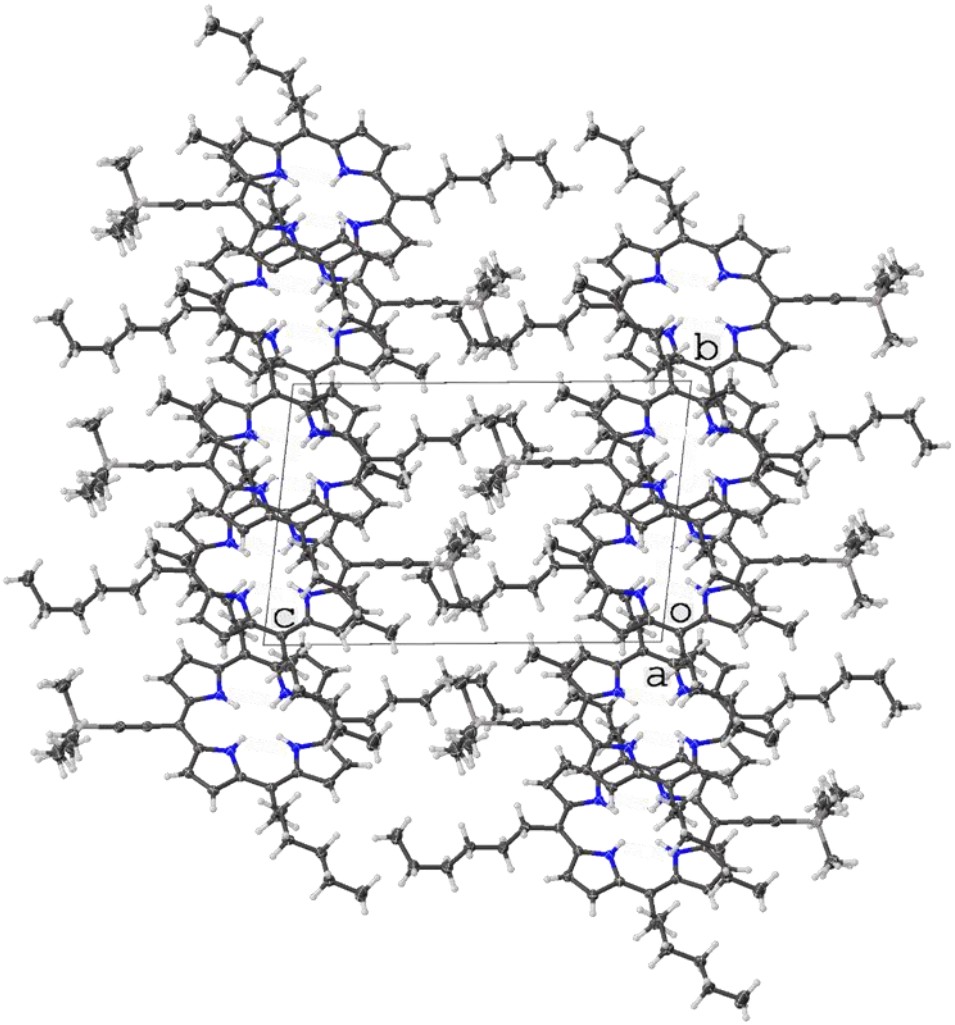


Figure S63: Packing diagram (thermal ellipsoid plot) of compound 24 looking down the *a*-axis (thermal displacement given as 50% probability). Minor disordered moieties have been omitted.

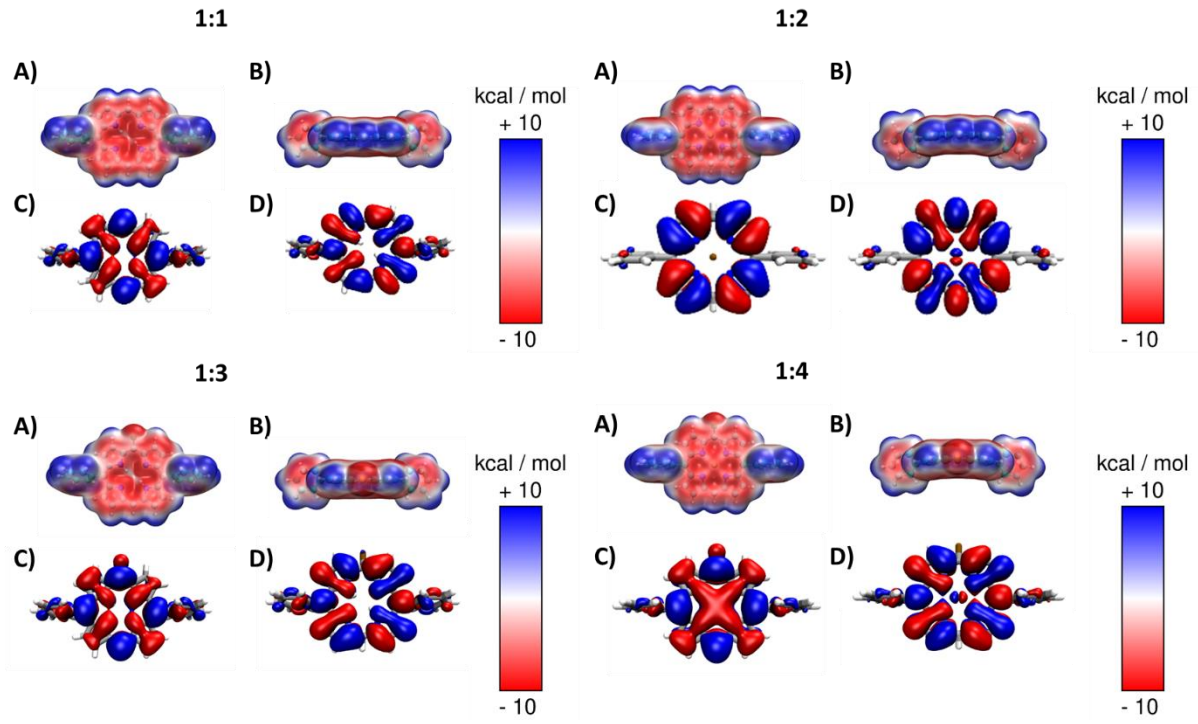


Figure S64: DFT generated images of compounds **1:1-1:4** (**A**) MEP map top view, (**B**) MEP map side view, (**C**) electron density distribution of HOMO, (**D**) electron density distribution of LUMO.

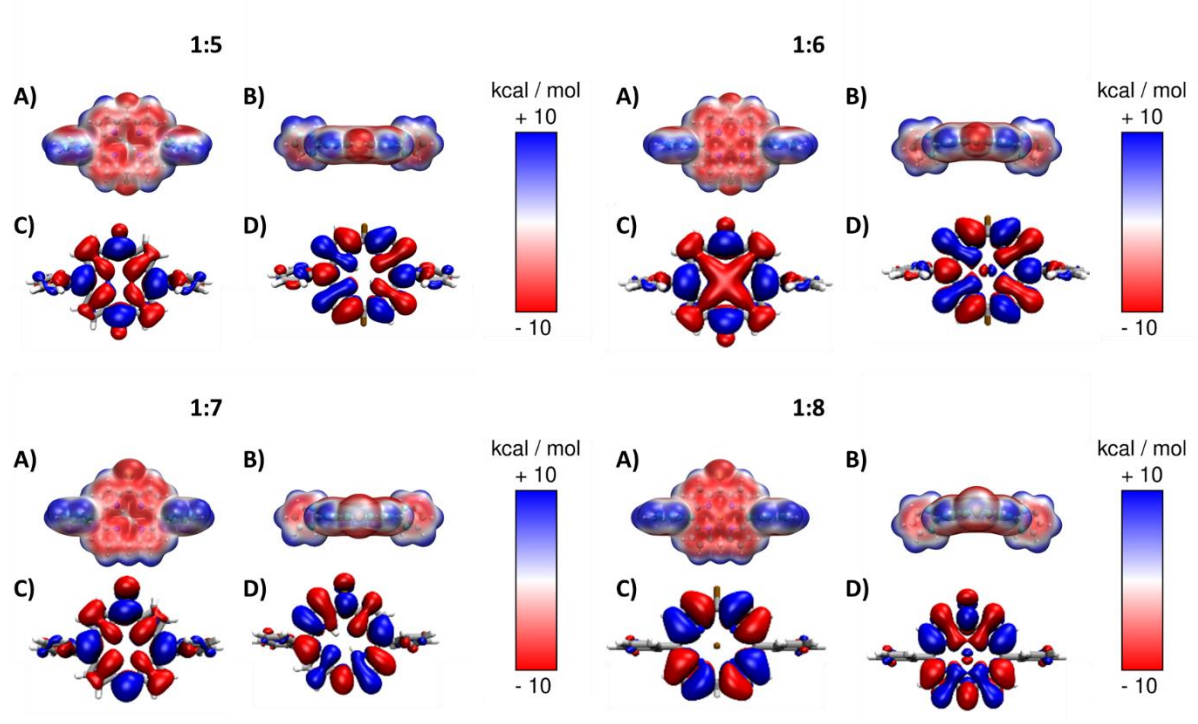


Figure S65: DFT generated images of compounds **1:5-1:8** (**A**) MEP map top view, (**B**) MEP map side view, (**C**) electron density distribution of HOMO, (**D**) electron density distribution of LUMO.

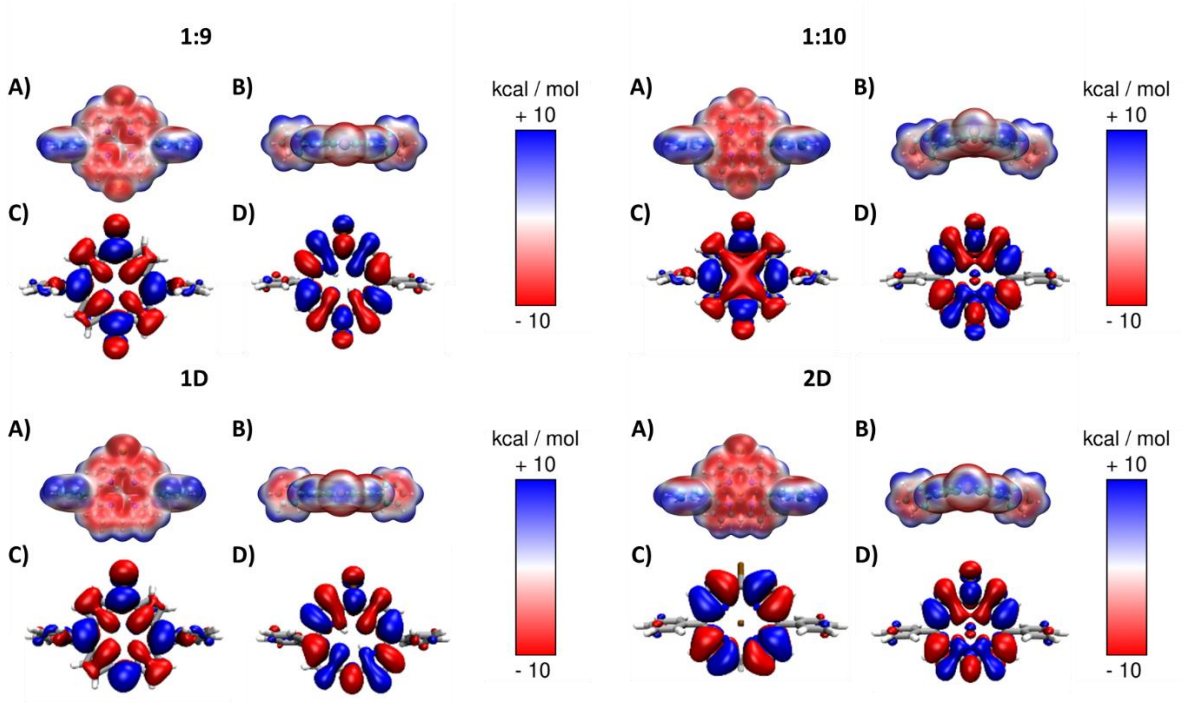


Figure S66: DFT generated images of compounds 1:9, 1:10, 1D, and 2D (A) MEP map top view, (B) MEP map side view, (C) electron density distribution of HOMO, (D) electron density distribution of LUMO.

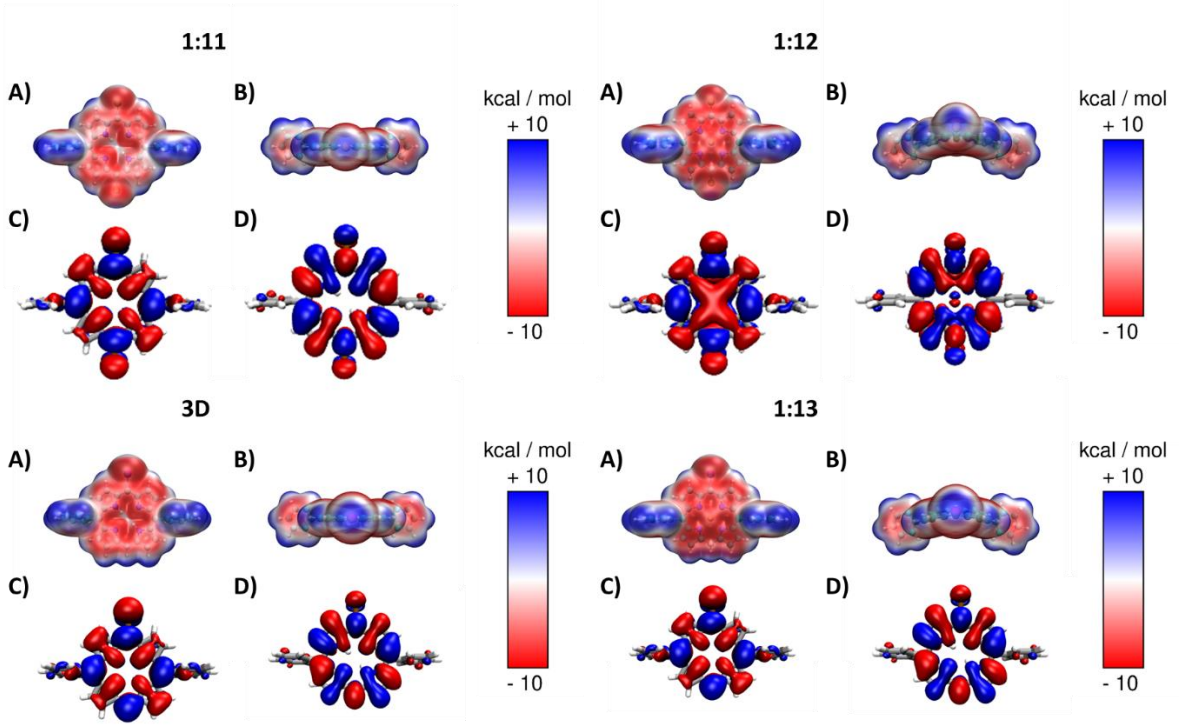


Figure S67: DFT generated images of compounds 1:11-1:13 and 3D (A) MEP map top view, (B) MEP map side view, (C) electron density distribution of HOMO, (D) electron density distribution of LUMO.

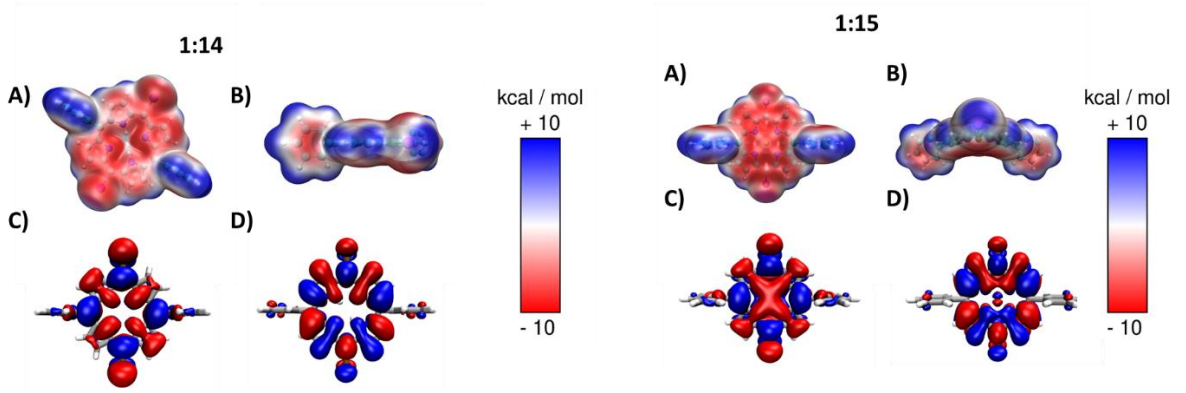


Figure S68: DFT generated images of compounds 1:14 and 1:15 (A) MEP map top view, (B) MEP map side view, (C) electron density distribution of HOMO, (D) electron density distribution of LUMO.

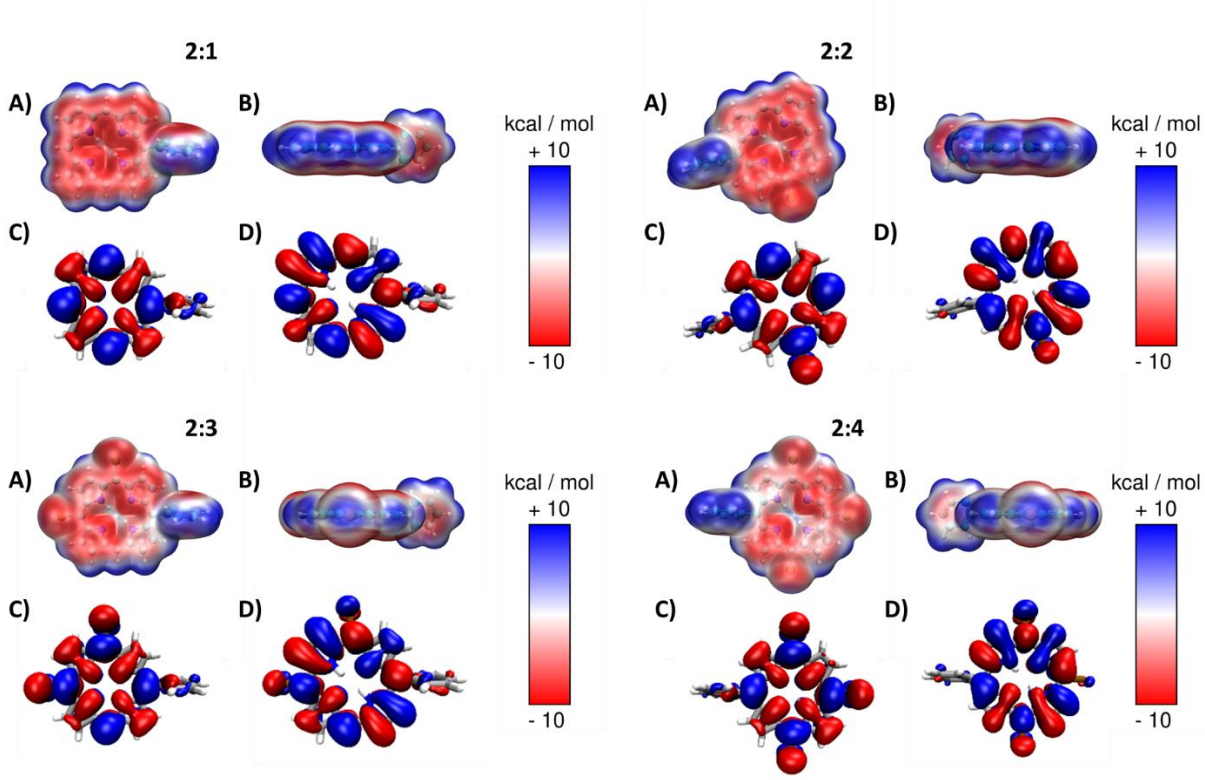


Figure S69: DFT generated images of compounds 2:1-2:4 (A) MEP map top view, (B) MEP map side view, (C) electron density distribution of HOMO, (D) electron density distribution of LUMO.

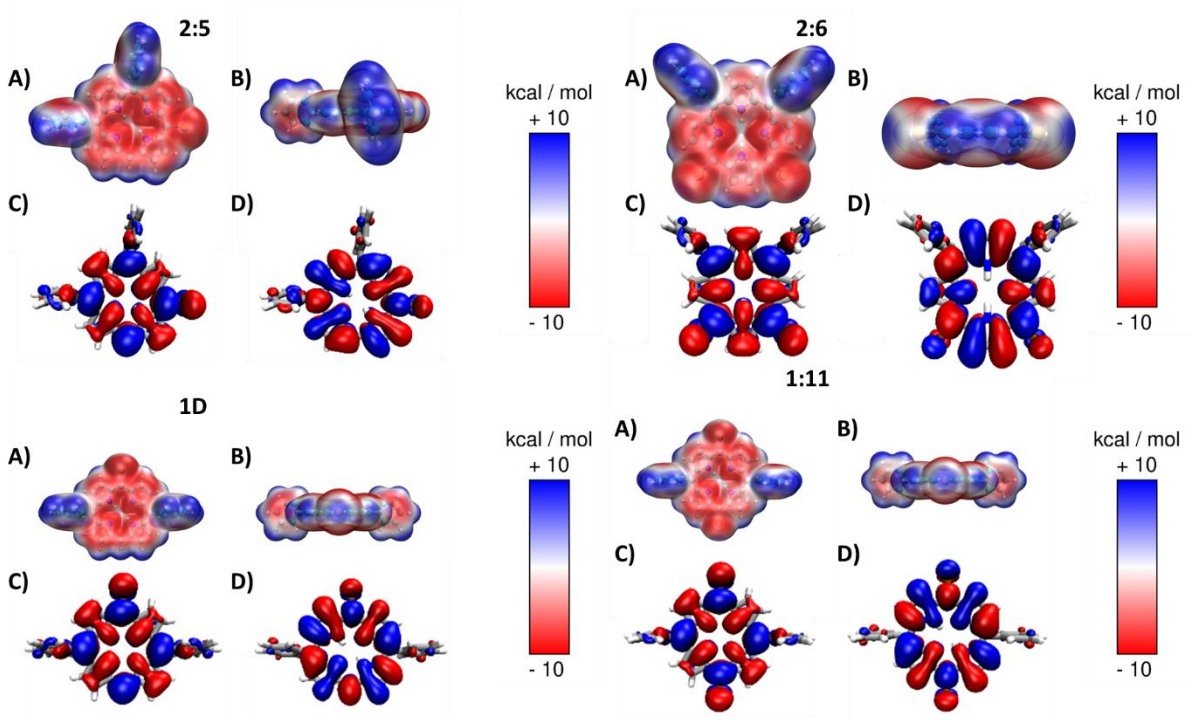


Figure S70: DFT generated images of compounds **2:5**, **2:6**, **1D**, and **1:11** (**A**) MEP map top view, (**B**) MEP map side view, (**C**) electron density distribution of HOMO, (**D**) electron density distribution of LUMO.

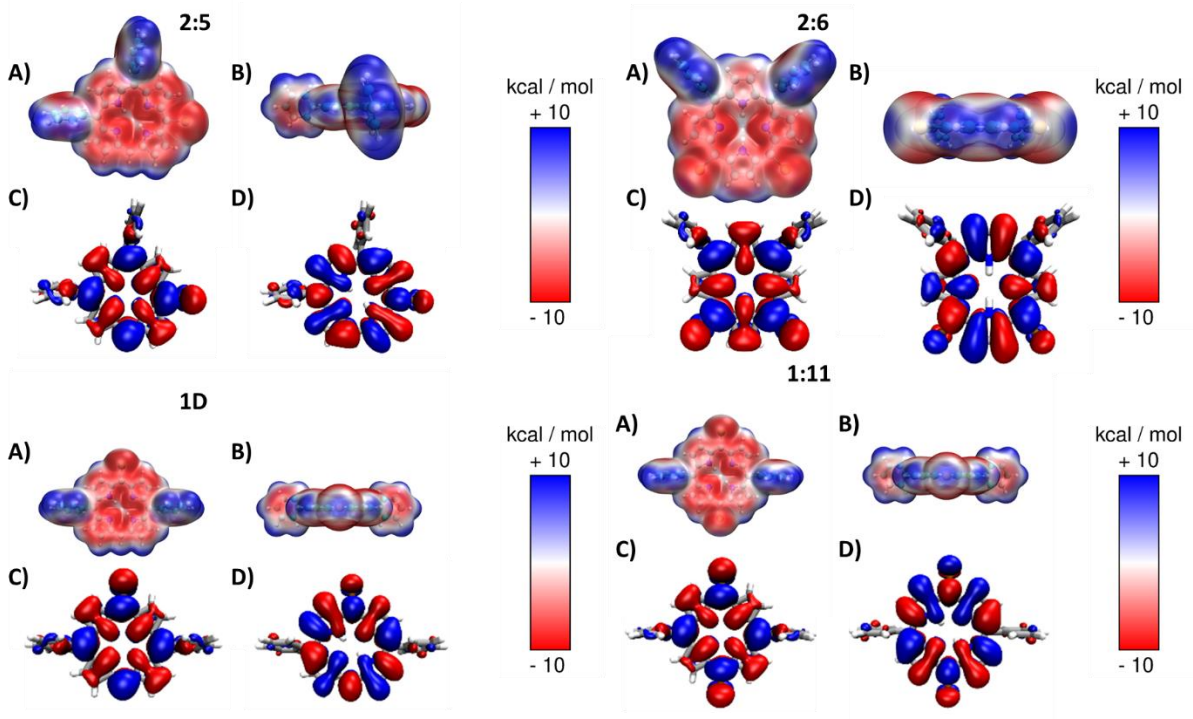


Figure S71: DFT generated images of compounds **3:1-3:3** and **2:6** (**A**) MEP map top view, (**B**) MEP map side view, (**C**) electron density distribution of HOMO, (**D**) electron density distribution of LUMO.

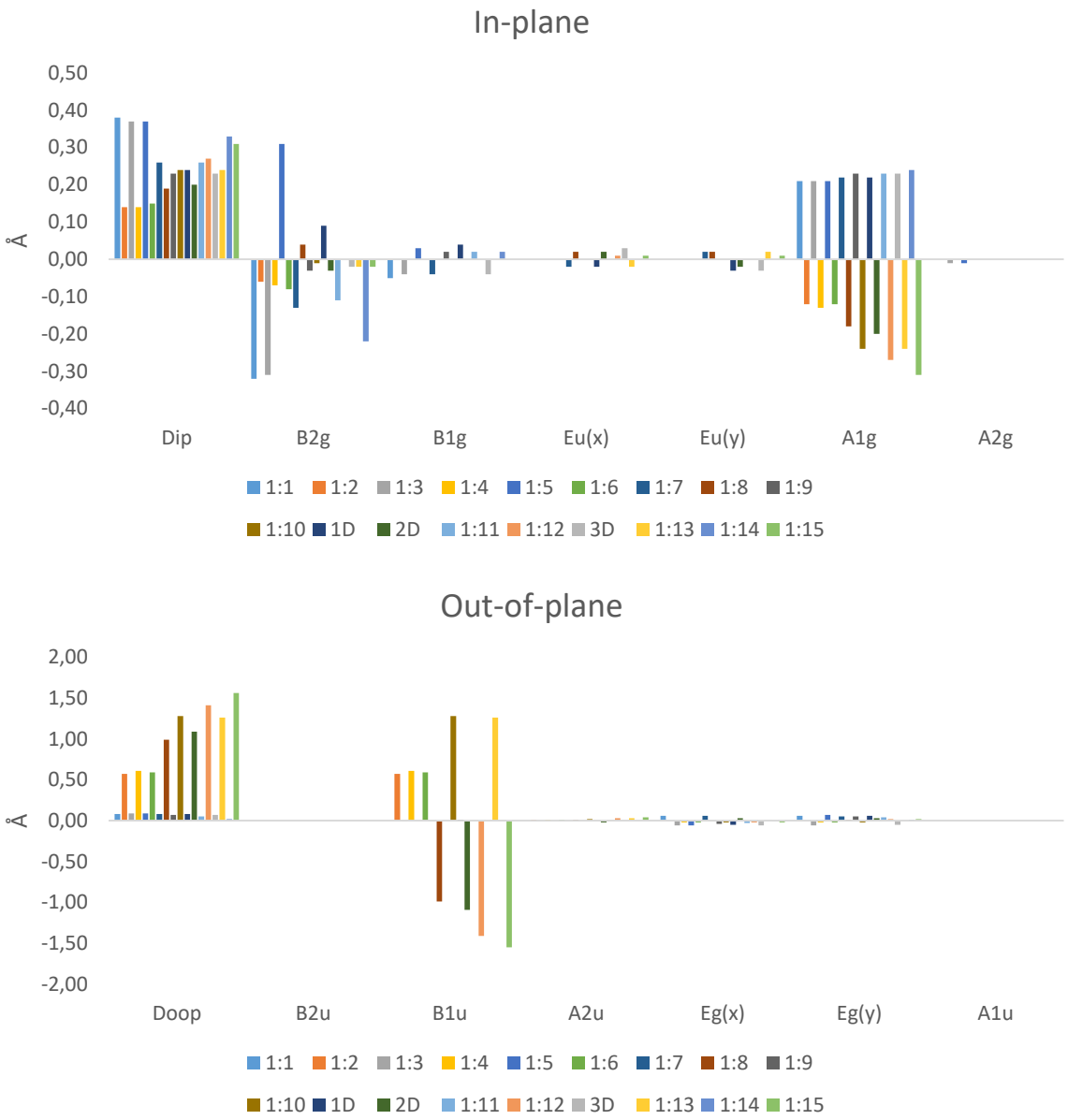


Figure S72: NSD charts for compounds **1:1**-**1:15**.

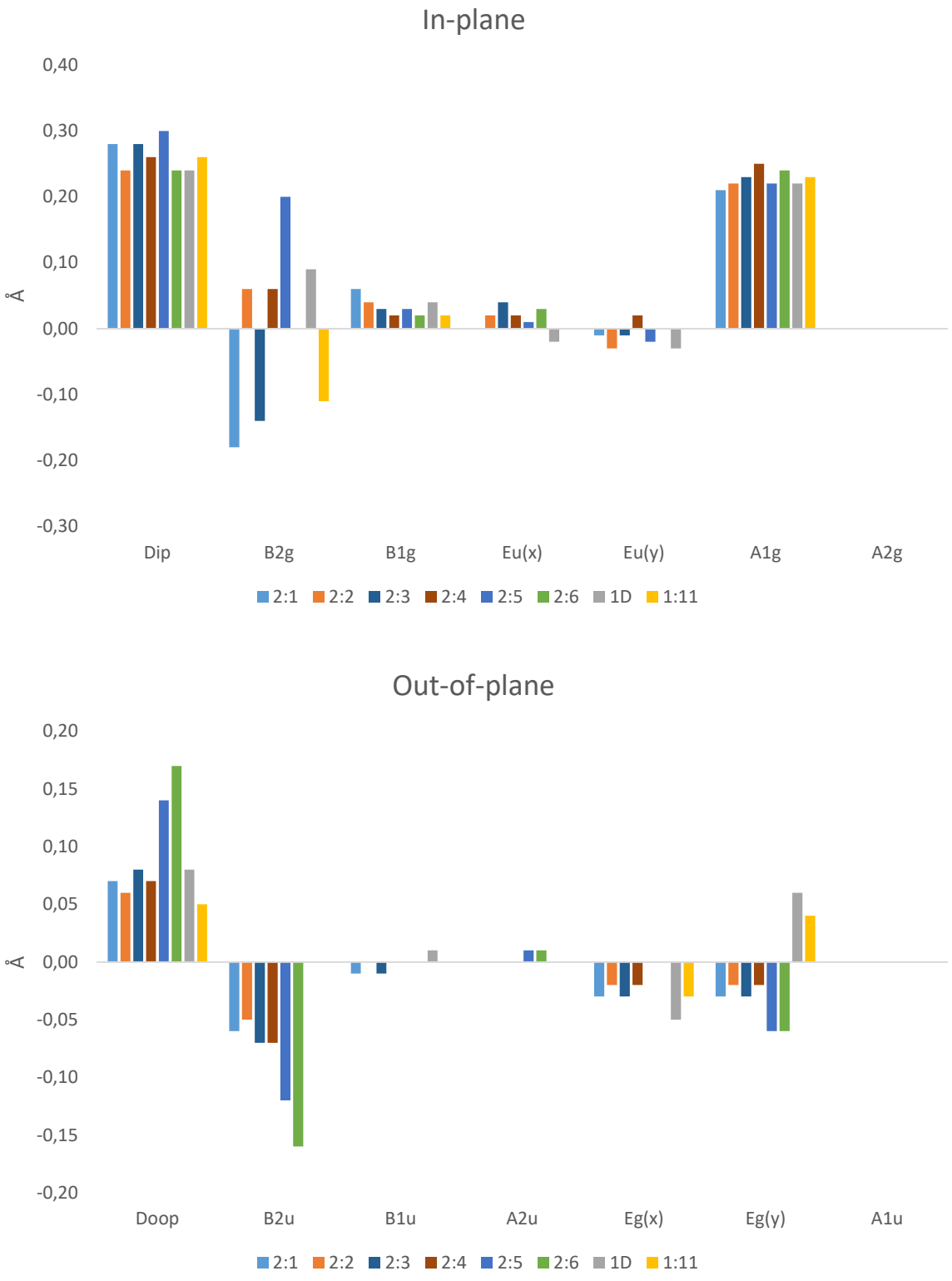


Figure S73: NSD charts for compounds **2:1**-**2:6**, **1D**, and **1:11**.

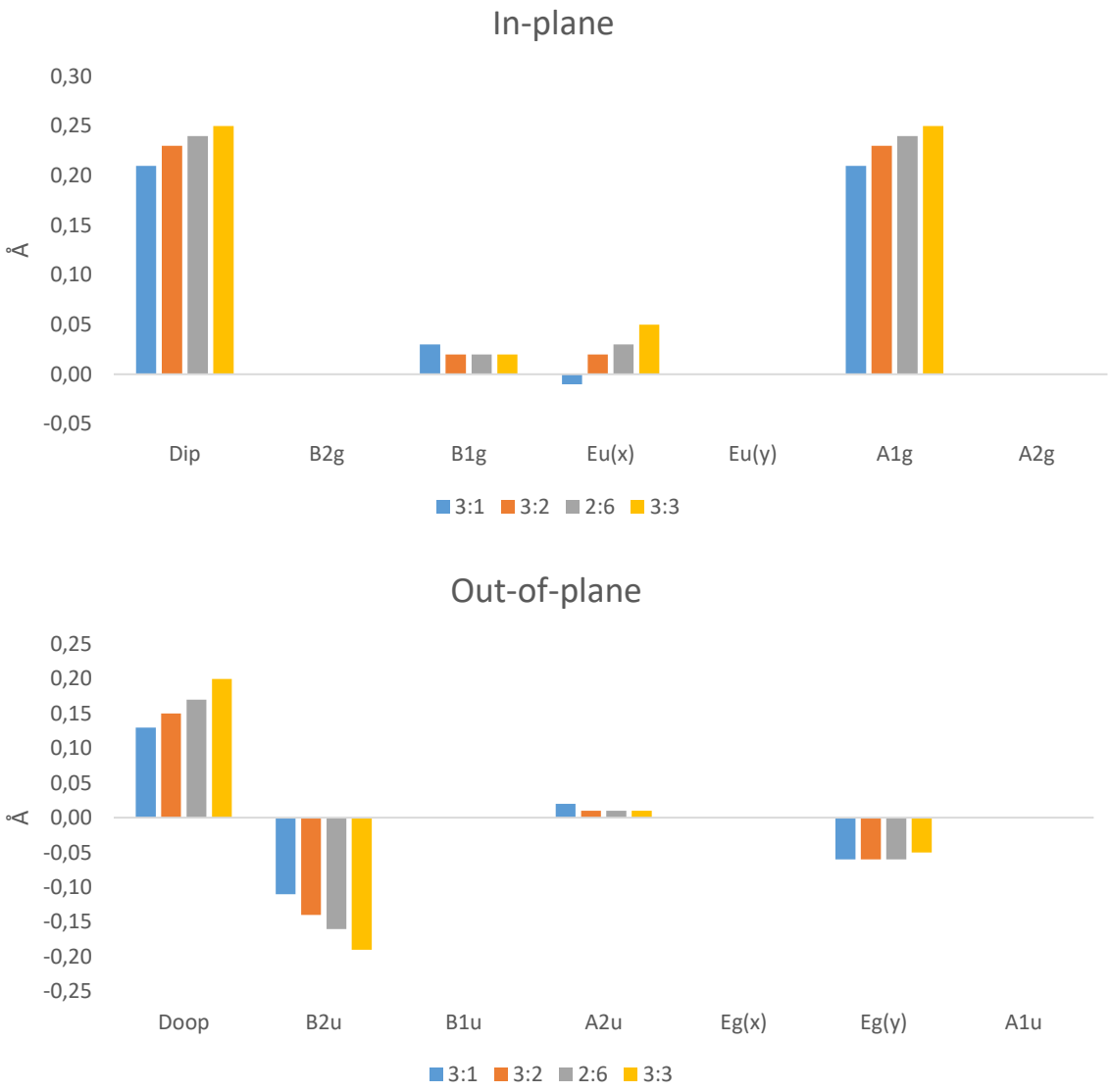


Figure S74: NSD charts for compounds **3:1**-**3:3** and **2:6**.

NSD tables and plots for crystal structures

basis	Δ_{ip}	δ_{ip}	B_{2g}	B_{1g}	$E_u(x)$	$E_u(y)$	A_{1g}	A_{2g}
min.	0.24	0.00	-0.12	0.02	0.03	-0.03	0.20	0.00
ext.	0.24	0.00	-0.12	0.02	0.03	-0.03	0.20	0.00
			0.00	-0.02	-0.01	0.02	0.00	0.00
total	0.25	0.00	-0.12	0.02	0.03	-0.03	0.20	0.00
			0.00	-0.02	-0.01	0.02	0.00	0.00
			-0.02	-0.03	0.00	0.00	0.06	0.00
			0.01	0.00	-0.01	0.01	-0.01	0.00
			0.00	0.00	0.00	0.00	-0.01	0.00
			-0.01	-0.01	0.00	0.00	0.02	
					0.00	0.00		
					-0.01	0.00		
					-0.01	0.00		
					0.00	0.00		
					0.00	0.00		
comp.	0.25	0.00	0.13	0.04	0.03	0.03	0.21	0.00

basis	Δ_{oop}	δ_{oop}	B_{2u}	B_{1u}	A_{2u}	$E_g(x)$	$E_g(y)$	A_{1u}
min.	0.15	0.00	-0.08	0.10	0.05	-0.01	0.06	0.02
ext.	0.17	0.00	-0.07	0.10	0.06	-0.02	0.06	0.02
			0.03	0.01	0.03	-0.02	-0.03	0.01
total	0.17	0.00	-0.07	0.10	0.06	-0.02	0.06	0.02
			0.03	0.01	0.03	-0.02	-0.03	0.01
			0.00	0.01	-0.01	0.00	0.00	
						0.00	0.00	
						-0.01	0.00	
comp.	0.17	0.00	0.08	0.10	0.07	0.03	0.07	0.02

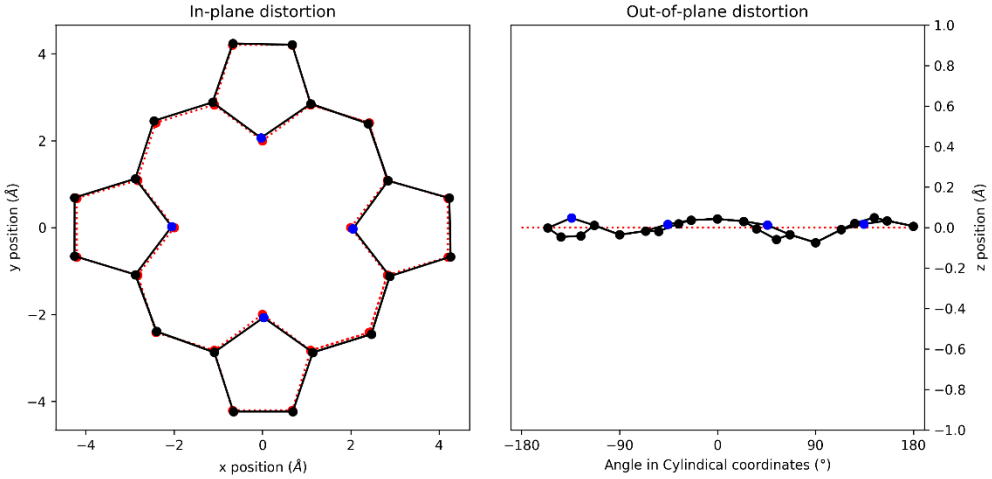


Figure S75: NSD result generated from **1** (in Å) (**A**) in-plane and (**B**) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

basis	Δ_{ip}	δ_{ip}	B_{2g}	B_{1g}	$E_u(x)$	$E_u(y)$	A_{1g}	A_{2g}
min.	0.25	0.00	-0.06	0.02	-0.02	0.01	-0.24	-0.01
ext.	0.25	0.00	-0.06	0.02	-0.02	0.01	-0.24	-0.01
			0.03	0.01	0.02	-0.01	0.02	0.00
total	0.27	0.00	-0.06	0.02	-0.02	0.01	-0.24	-0.01
			0.03	0.01	0.02	-0.01	0.02	0.00
			-0.01	-0.01	0.01	-0.02	-0.01	0.00
			0.02	0.00	0.01	-0.02	-0.06	0.01
			0.00	0.02	-0.01	0.01	-0.03	0.02
			-0.02	0.03	-0.01	0.01	0.04	
					0.00	0.00		
					0.00	-0.01		
					0.01	0.00		
					0.01	0.02		
					0.00	-0.01		
comp.	0.27	0.00	0.07	0.04	0.04	0.04	0.25	0.02

basis	Δ_{oop}	δ_{oop}	B_{2u}	B_{1u}	A_{2u}	$E_g(x)$	$E_g(y)$	A_{1u}
min.	1.01	0.00	0.10	1.00	-0.06	0.03	0.06	0.00
ext.	1.01	0.00	0.10	1.00	-0.06	0.03	0.06	0.00
			-0.03	0.00	0.03	-0.05	-0.05	-0.01
total	1.01	0.00	0.10	1.00	-0.06	0.03	0.06	0.00
			-0.03	0.00	0.03	-0.05	-0.05	-0.01
			0.00	0.01	-0.01	0.01	-0.01	
						0.01	-0.01	
						0.00	0.00	
comp.	1.01	0.00	0.10	1.00	0.06	0.06	0.08	0.01

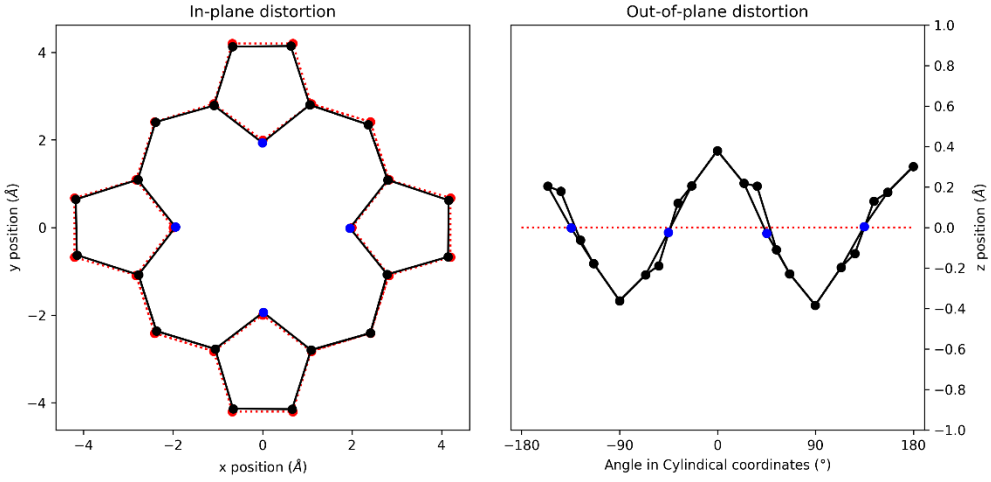


Figure S76: NSD result generated from **2** (in Å) (**A**) in-plane and (**B**) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

basis	Δ_{ip}	δ_{ip}	B_{2g}	B_{1g}	$E_u(x)$	$E_u(y)$	A_{1g}	A_{2g}
min.	0.13	0.00	-0.06	0.02	0.02	-0.02	-0.11	-0.01
ext.	0.14	0.00	-0.06	0.02	0.02	-0.02	-0.12	-0.01
			-0.03	0.00	0.00	0.01	-0.04	0.00
total	0.15	0.00	-0.06	0.02	0.02	-0.02	-0.12	-0.01
			-0.03	0.00	0.00	0.01	-0.04	0.00
			-0.01	0.00	0.00	0.00	-0.03	0.00
			0.00	0.00	0.00	0.00	-0.01	0.00
			0.01	0.00	0.00	0.01	-0.01	0.00
			0.00	0.00	0.00	-0.01	0.00	
					0.00	0.00		
					0.00	0.00		
					0.01	0.00		
					-0.01	0.00		
					0.00	0.00		
comp.	0.15	0.00	0.06	0.02	0.02	0.02	0.13	0.01

basis	Δ_{oop}	δ_{oop}	B_{2u}	B_{1u}	A_{2u}	$E_g(x)$	$E_g(y)$	A_{1u}
min.	0.22	0.00	-0.06	0.20	0.04	0.01	0.07	0.01
ext.	0.23	0.00	-0.06	0.20	0.05	0.01	0.07	0.01
			0.01	0.00	0.03	-0.01	-0.03	0.00
total	0.23	0.00	-0.06	0.20	0.05	0.01	0.07	0.01
			0.01	0.00	0.03	-0.01	-0.03	0.00
			0.00	0.00	-0.01	0.00	0.01	
						-0.01	-0.01	
						0.00	0.00	
comp.	0.23	0.00	0.06	0.20	0.06	0.01	0.08	0.01

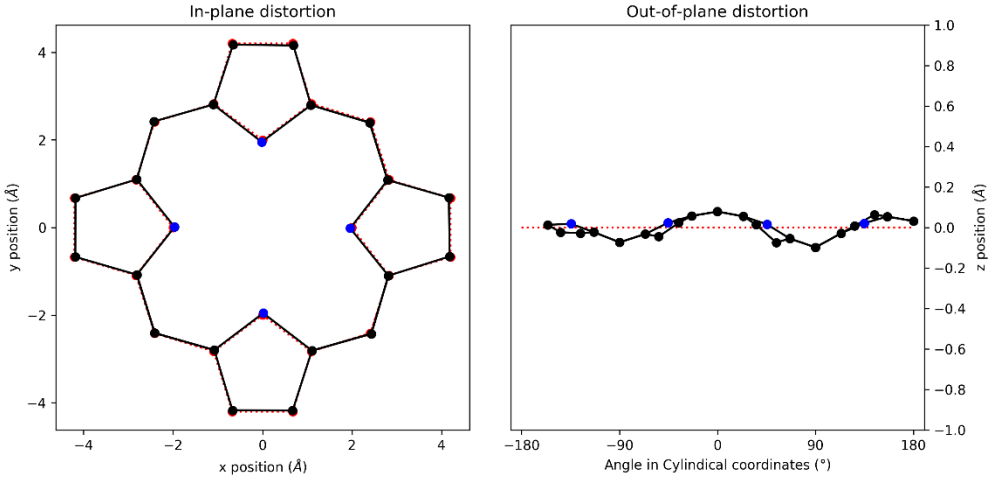


Figure S77: NSD result generated from **2A** (in Å) (**A**) in-plane and (**B**) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

basis	Δ_{ip}	δ_{ip}	B_{2g}	B_{1g}	$E_u(x)$	$E_u(y)$	A_{1g}	A_{2g}
min.	0.29	0.00	-0.20	-0.03	-0.05	0.02	0.20	0.00
ext.	0.30	0.00	-0.20	-0.04	-0.05	0.02	0.20	0.00
			-0.04	-0.07	0.02	-0.04	-0.02	0.01
total	0.32	0.00	-0.20	-0.04	-0.05	0.02	0.20	0.00
			-0.04	-0.07	0.02	-0.04	-0.02	0.01
			-0.01	-0.06	0.00	0.00	0.05	0.00
			0.01	0.00	0.00	0.00	0.00	0.00
			0.00	0.01	0.00	0.01	0.01	0.00
			-0.01	-0.01	0.00	0.00	0.01	
					0.00	0.00		
					0.00	0.00		
					0.00	-0.01		
					0.00	0.00		
					0.00	-0.01		
comp.	0.32	0.00	0.20	0.10	0.05	0.05	0.21	0.01

basis	Δ_{oop}	δ_{oop}	B_{2u}	B_{1u}	A_{2u}	$E_g(x)$	$E_g(y)$	A_{1u}
min.	0.47	0.00	0.42	0.13	-0.06	-0.15	0.09	-0.02
ext.	0.48	0.00	0.41	0.13	-0.06	-0.15	0.09	-0.02
			-0.11	-0.01	0.00	-0.01	0.00	-0.01
total	0.48	0.00	0.41	0.13	-0.06	-0.15	0.09	-0.02
			-0.11	-0.01	0.00	-0.01	0.00	-0.01
			0.00	0.00	0.00	0.00	-0.01	
						0.00	0.00	
						-0.01	0.00	
comp.	0.48	0.00	0.43	0.13	0.06	0.15	0.09	0.02

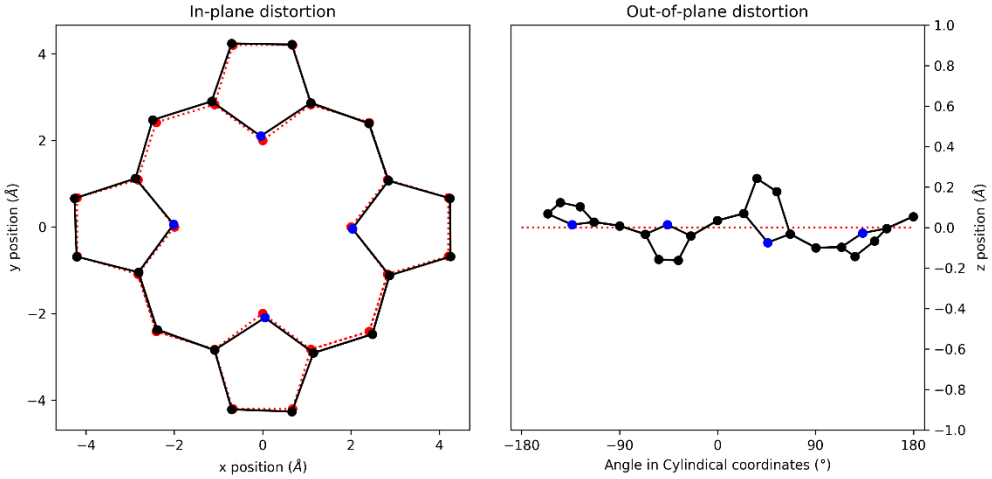


Figure S78: NSD result generated from **3** (in Å) (**A**) in-plane and (**B**) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

basis	Δ_{ip}	δ_{ip}	B_{2g}	B_{1g}	$E_u(x)$	$E_u(y)$	A_{1g}	A_{2g}
min.	0.25	0.00	-0.10	-0.03	0.00	0.00	0.23	0.01
ext.	0.25	0.00	-0.10	-0.03	0.00	0.00	0.23	0.01
			-0.02	0.01	0.01	-0.02	-0.02	0.00
total	0.27	0.00	-0.10	-0.02	0.00	0.00	0.23	0.01
			-0.02	0.01	0.01	-0.01	-0.02	0.00
			-0.01	0.01	0.00	0.01	0.05	0.00
			0.00	0.00	-0.02	0.01	-0.01	0.00
			0.00	0.00	0.00	-0.01	0.02	0.00
			-0.01	0.00	-0.01	0.01	0.01	
					0.00	0.00		
					0.00	0.00		
					-0.01	0.01		
					0.01	-0.01		
					0.00	0.00		
comp.	0.27	0.00	0.10	0.03	0.03	0.03	0.24	0.01

basis	Δ_{oop}	δ_{oop}	B_{2u}	B_{1u}	A_{2u}	$E_g(x)$	$E_g(y)$	A_{1u}
min.	0.31	0.00	0.05	0.02	-0.05	0.11	0.28	-0.01
ext.	0.33	0.00	0.05	0.02	-0.05	0.11	0.28	-0.01
			-0.03	0.00	0.00	0.00	0.10	0.01
total	0.33	0.00	0.05	0.02	-0.05	0.11	0.28	-0.01
			-0.03	0.00	0.00	0.00	0.10	0.01
			0.00	0.00	0.01	-0.01	-0.02	
						-0.01	-0.01	
						0.00	0.01	
comp.	0.33	0.00	0.05	0.02	0.05	0.11	0.30	0.01

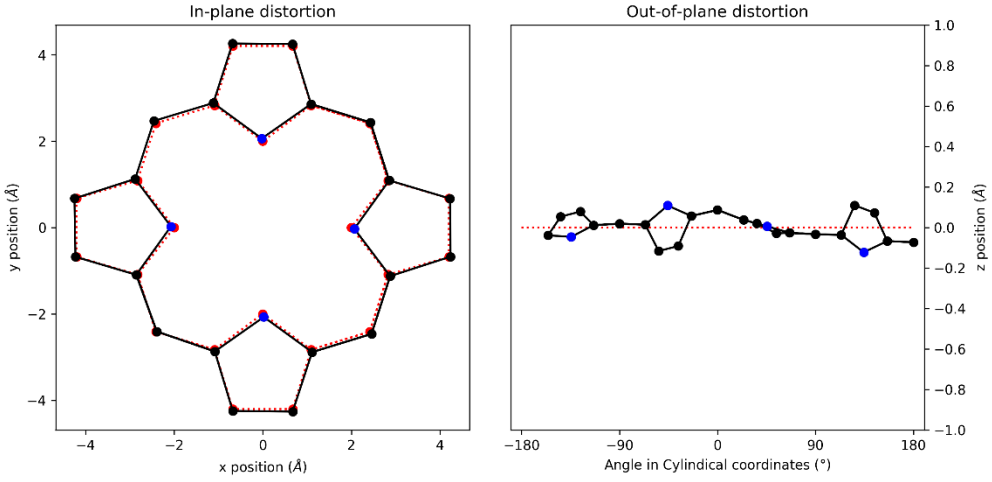


Figure S79: NSD result generated from **4** (in Å) (**A**) in-plane and (**B**) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

basis	Δ_{ip}	δ_{ip}	B_{2g}	B_{1g}	$E_u(x)$	$E_u(y)$	A_{1g}	A_{2g}
min.	0.21	0.00	0.01	0.04	-0.01	-0.01	0.21	-0.01
ext.	0.22	0.00	0.01	0.04	-0.01	-0.01	0.21	-0.01
			0.01	0.03	0.01	0.01	-0.02	0.00
total	0.23	0.00	0.01	0.04	-0.01	-0.01	0.21	-0.01
			0.01	0.03	0.01	0.01	-0.02	0.00
			-0.01	0.02	0.01	0.00	0.05	0.00
			0.01	0.00	0.01	-0.02	-0.01	0.00
			0.00	-0.01	0.00	0.00	0.01	0.00
			-0.01	0.00	0.01	0.00	0.01	
					0.00	0.00		
					0.00	0.00		
					0.00	-0.01		
					0.00	0.00		
					0.00	0.00		
comp.	0.23	0.00	0.03	0.06	0.02	0.02	0.22	0.01

basis	Δ_{oop}	δ_{oop}	B_{2u}	B_{1u}	A_{2u}	$E_g(x)$	$E_g(y)$	A_{1u}
min.	0.39	0.00	0.10	0.31	-0.10	-0.05	0.20	-0.01
ext.	0.41	0.00	0.10	0.31	-0.10	-0.05	0.20	-0.01
			0.03	0.00	-0.04	0.01	0.09	-0.01
total	0.41	0.00	0.10	0.31	-0.10	-0.05	0.20	-0.01
			0.03	0.00	-0.04	0.01	0.09	-0.01
			0.00	0.00	0.01	0.02	0.01	
						0.00	-0.01	
						-0.01	0.01	
comp.	0.41	0.00	0.11	0.31	0.11	0.05	0.22	0.01

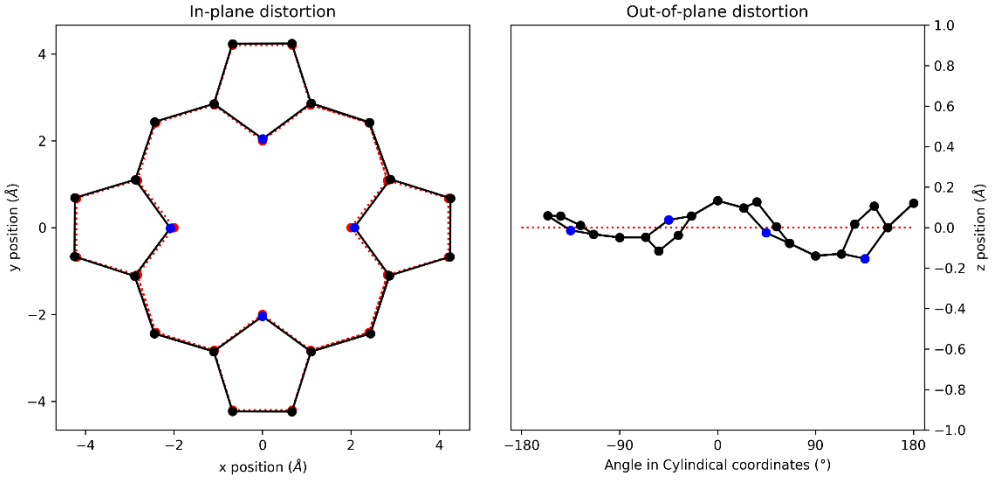


Figure S80: NSD result generated from **5** (in Å) (**A**) in-plane and (**B**) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

basis	Δ_{ip}	δ_{ip}	B_{2g}	B_{1g}	$E_u(x)$	$E_u(y)$	A_{1g}	A_{2g}
min.	0.22	0.00	0.00	0.01	0.00	0.00	0.22	0.00
ext.	0.23	0.00	0.00	0.01	0.01	0.00	0.22	0.00
			-0.01	0.01	0.03	0.02	-0.03	0.00
total	0.25	0.00	0.00	0.01	0.00	0.00	0.23	0.00
			-0.01	0.01	0.03	0.02	-0.03	0.00
			0.01	0.02	-0.01	0.01	0.06	0.00
			-0.01	0.00	-0.01	-0.02	-0.02	-0.01
			-0.01	0.00	0.00	0.00	0.01	0.00
			0.00	0.01	0.00	-0.02	0.03	
					0.00	0.00		
					0.00	-0.01		
					-0.01	0.01		
					0.00	0.00		
					0.01	-0.01		
comp.	0.25	0.00	0.03	0.03	0.03	0.04	0.24	0.01

basis	Δ_{oop}	δ_{oop}	B_{2u}	B_{1u}	A_{2u}	$E_g(x)$	$E_g(y)$	A_{1u}
min.	0.36	0.00	-0.22	-0.08	-0.02	-0.27	-0.06	-0.01
ext.	0.36	0.00	-0.22	-0.08	-0.02	-0.27	-0.06	-0.01
			0.01	0.01	0.00	0.03	0.01	0.00
total	0.36	0.00	-0.22	-0.08	-0.02	-0.27	-0.06	-0.01
			0.02	0.01	0.00	0.03	0.01	0.00
			0.00	0.00	0.00	0.01	0.01	
						0.00	0.00	
						-0.01	0.01	
comp.	0.36	0.00	0.22	0.08	0.02	0.27	0.06	0.01

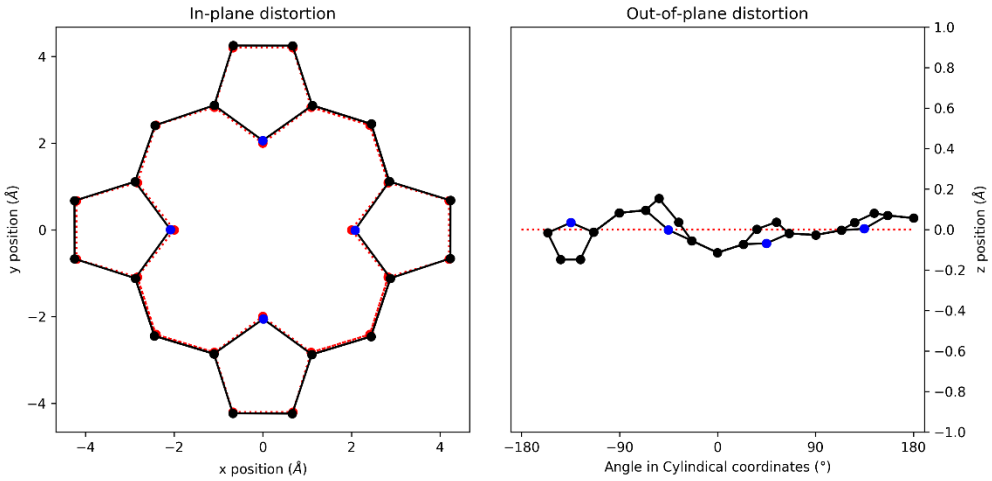


Figure S81: NSD result generated from **6** (in Å) (**A**) in-plane and (**B**) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

basis	Δ_{ip}	δ_{ip}	B_{2g}	B_{1g}	$E_u(x)$	$E_u(y)$	A_{1g}	A_{2g}
min.	0.14	0.00	0.05	-0.01	0.02	0.02	-0.12	0.00
ext.	0.15	0.00	0.05	-0.01	0.02	0.02	-0.12	0.00
			0.00	0.00	0.03	0.01	-0.05	0.00
total	0.16	0.00	0.05	-0.01	0.02	0.02	-0.13	0.00
			0.00	0.00	0.03	0.01	-0.05	0.00
			0.01	0.00	-0.01	-0.01	-0.04	0.00
			-0.01	0.00	-0.02	-0.02	-0.02	0.00
			0.00	0.00	0.00	0.00	-0.01	0.00
			0.00	0.00	-0.01	-0.01	0.01	
					0.00	0.00		
					0.00	0.00		
					-0.01	0.00		
					0.01	0.01		
					0.01	0.00		
comp.	0.16	0.00	0.05	0.01	0.04	0.03	0.14	0.01

basis	Δ_{oop}	δ_{oop}	B_{2u}	B_{1u}	A_{2u}	$E_g(x)$	$E_g(y)$	A_{1u}
min.	0.36	0.00	0.26	0.08	-0.01	0.24	0.00	0.01
ext.	0.37	0.00	0.26	0.08	0.00	0.23	0.00	0.01
			0.00	0.00	0.03	-0.09	-0.02	0.00
total	0.37	0.00	0.26	0.08	0.00	0.23	0.00	0.01
			0.00	0.00	0.03	-0.09	-0.02	0.00
			0.00	0.00	0.00	-0.01	0.00	
						0.00	0.00	
						0.01	0.00	
comp.	0.37	0.00	0.26	0.08	0.03	0.25	0.02	0.01

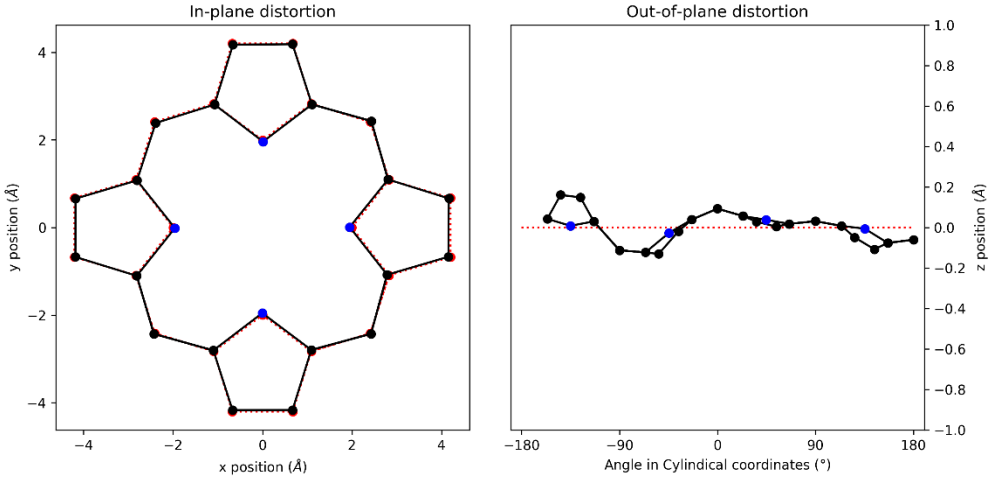


Figure S82: NSD result generated from **7** (in Å) (**A**) in-plane and (**B**) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

basis	Δ_{ip}	δ_{ip}	B_{2g}	B_{1g}	$E_u(x)$	$E_u(y)$	A_{1g}	A_{2g}
min.	0.23	0.00	-0.04	0.00	-0.01	0.02	0.23	0.00
ext.	0.24	0.00	-0.04	0.00	-0.01	0.02	0.23	0.00
			-0.03	-0.03	0.02	0.01	-0.04	-0.01
total	0.26	0.00	-0.04	0.00	-0.01	0.02	0.23	0.00
			-0.03	-0.03	0.02	0.01	-0.04	-0.01
			0.02	-0.02	0.00	0.00	0.06	0.00
			-0.02	0.00	-0.02	-0.01	-0.02	0.00
			-0.01	0.00	0.00	0.00	0.01	0.00
			0.01	0.00	-0.01	-0.01	0.02	
					-0.01	0.01		
					0.00	0.00		
					-0.01	-0.01		
					0.01	0.00		
					0.00	0.00		
comp.	0.26	0.00	0.06	0.04	0.03	0.03	0.24	0.01

basis	Δ_{oop}	δ_{oop}	B_{2u}	B_{1u}	A_{2u}	$E_g(x)$	$E_g(y)$	A_{1u}
min.	0.34	0.00	-0.16	0.10	0.05	-0.07	-0.27	0.00
ext.	0.34	0.00	-0.16	0.10	0.05	-0.07	-0.27	0.00
			0.01	-0.01	0.00	0.01	0.03	0.00
total	0.34	0.00	-0.16	0.10	0.05	-0.07	-0.27	0.00
			0.01	-0.01	0.00	0.01	0.03	0.00
			0.01	0.00	0.00	0.01	0.02	
						0.00	0.00	
						0.01	0.00	
comp.	0.34	0.00	0.16	0.10	0.05	0.07	0.28	0.00

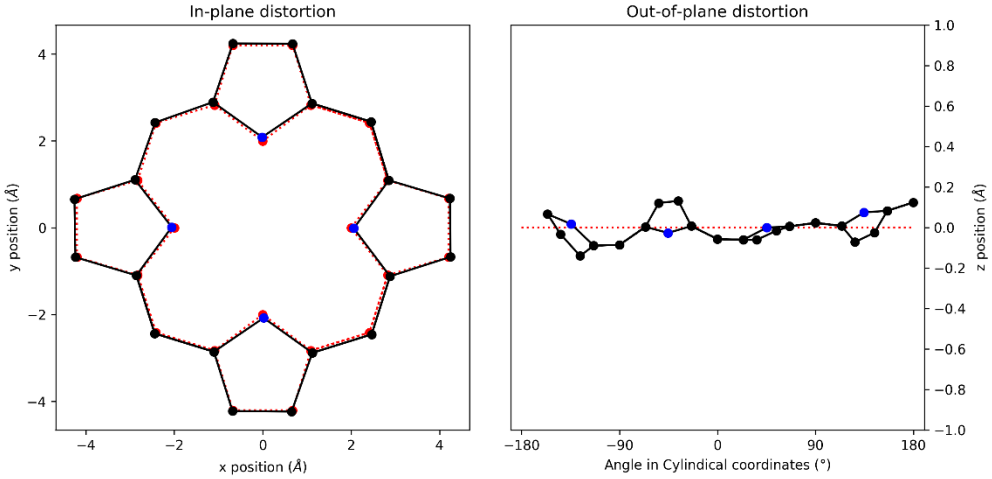


Figure S83: NSD result generated from **8_1** (in Å) (**A**) in-plane and (**B**) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

basis	Δ_{ip}	δ_{ip}	B_{2g}	B_{1g}	$E_u(x)$	$E_u(y)$	A_{1g}	A_{2g}
min.	0.22	0.00	-0.06	-0.01	-0.01	-0.01	0.21	-0.01
ext.	0.23	0.00	-0.06	-0.01	-0.01	-0.01	0.21	-0.01
			-0.03	-0.02	-0.03	-0.02	-0.04	0.00
total	0.25	0.00	-0.06	-0.01	-0.01	-0.01	0.22	-0.01
			-0.03	-0.02	-0.03	-0.02	-0.04	0.00
			0.01	-0.02	0.00	0.01	0.06	0.00
			-0.02	0.00	0.02	0.01	-0.01	-0.01
			0.00	0.01	0.00	0.00	0.00	0.01
			0.01	0.00	0.00	0.00	0.01	
					0.00	0.00		
					0.00	0.00		
					0.01	0.01		
					0.00	0.00		
					0.00	0.01		
comp.	0.25	0.00	0.07	0.03	0.04	0.03	0.23	0.02

basis	Δ_{oop}	δ_{oop}	B_{2u}	B_{1u}	A_{2u}	$E_g(x)$	$E_g(y)$	A_{1u}
min.	0.37	0.00	0.20	-0.05	-0.02	-0.06	-0.30	0.00
ext.	0.37	0.00	0.20	-0.05	-0.02	-0.06	-0.30	0.00
			-0.01	0.00	0.00	0.03	0.04	0.01
total	0.37	0.00	0.20	-0.05	-0.02	-0.06	-0.30	0.00
			-0.01	0.00	0.00	0.03	0.04	0.01
			0.00	-0.01	0.00	-0.01	0.02	
						0.00	0.00	
						0.00	-0.01	
comp.	0.37	0.00	0.20	0.05	0.02	0.06	0.30	0.01

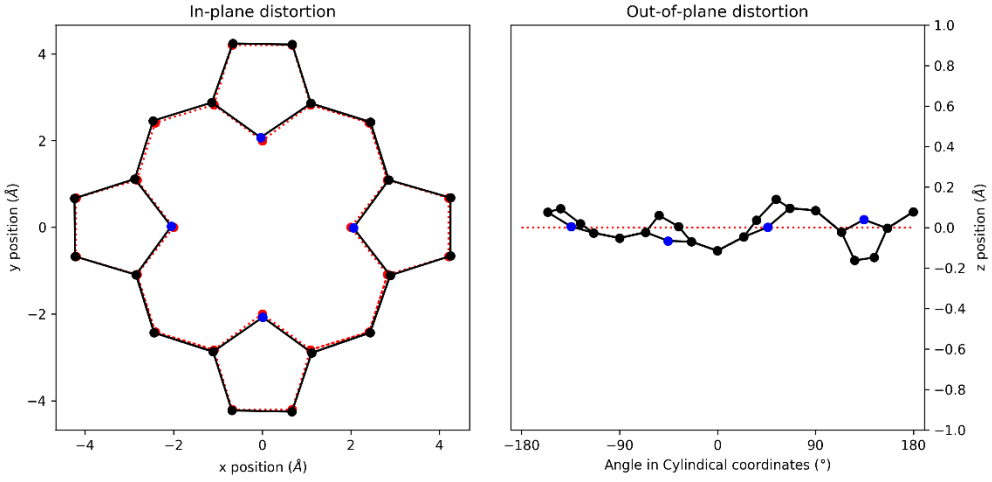


Figure S84: NSD result generated from **8_2** (in Å) (**A**) in-plane and (**B**) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

basis	Δ_{ip}	δ_{ip}	B_{2g}	B_{1g}	$E_u(x)$	$E_u(y)$	A_{1g}	A_{2g}
min.	0.25	0.00	0.00	-0.06	0.00	0.00	0.24	-0.01
ext.	0.25	0.00	0.00	-0.06	0.00	0.00	0.24	-0.01
			-0.02	0.03	0.00	0.00	0.00	0.00
total	0.26	0.00	0.00	-0.06	0.00	0.00	0.24	-0.01
			-0.02	0.03	0.00	0.00	0.00	0.00
			0.03	0.03	0.00	0.00	0.05	0.00
			-0.02	0.00	0.00	0.00	0.00	0.00
			0.00	-0.01	0.00	0.00	-0.01	0.00
			0.01	0.00	0.00	0.00	0.01	
					0.00	0.00		
					0.00	0.00		
					0.00	0.00		
					0.00	0.00		
					0.00	0.00		
comp.	0.26	0.00	0.04	0.08	0.00	0.00	0.25	0.01

basis	Δ_{oop}	δ_{oop}	B_{2u}	B_{1u}	A_{2u}	$E_g(x)$	$E_g(y)$	A_{1u}
min.	0.08	0.00	0.00	0.00	0.00	-0.01	0.08	0.00
ext.	0.11	0.00	0.00	0.00	0.00	-0.01	0.08	0.00
			0.00	0.00	0.00	0.06	0.02	0.00
total	0.11	0.00	0.00	0.00	0.00	-0.01	0.08	0.00
			0.00	0.00	0.00	0.06	0.02	0.00
			0.00	0.00	0.00	0.01	-0.01	
						0.00	0.00	
						0.01	0.00	
comp.	0.11	0.00	0.00	0.00	0.00	0.07	0.08	0.00

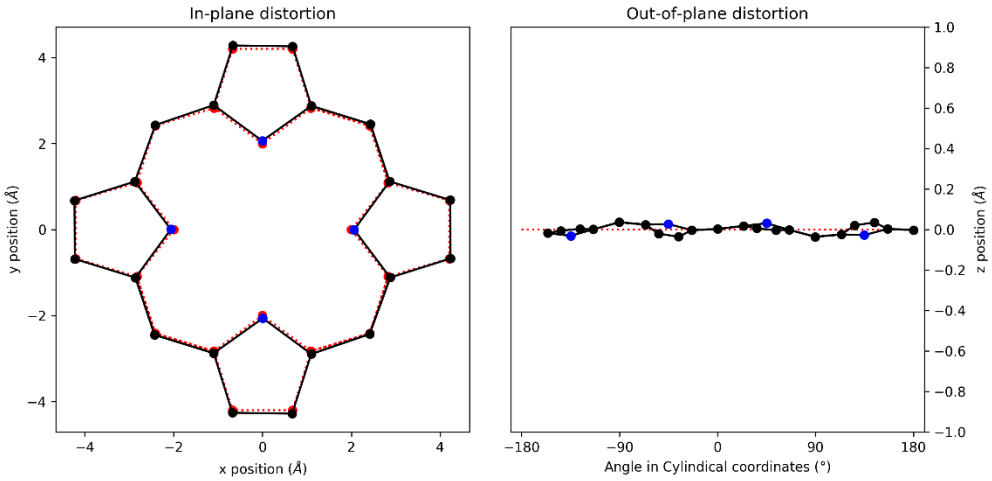


Figure S85: NSD result generated from **9** (in Å) (**A**) in-plane and (**B**) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

basis	Δ_{ip}	δ_{ip}	B_{2g}	B_{1g}	$E_u(x)$	$E_u(y)$	A_{1g}	A_{2g}
min.	0.24	0.00	-0.06	-0.02	0.00	0.00	0.23	-0.01
ext.	0.24	0.00	-0.06	-0.02	0.00	0.00	0.23	-0.01
			-0.01	0.04	0.00	0.00	0.00	-0.01
total	0.26	0.00	-0.06	-0.02	0.00	0.00	0.23	-0.01
			-0.01	0.04	0.00	0.00	0.00	-0.01
			-0.03	0.04	0.00	0.00	0.05	0.00
			0.01	0.00	0.00	0.00	-0.01	0.00
			0.00	-0.01	0.00	0.00	0.00	0.00
			-0.01	0.01	0.00	0.00	0.01	
					0.00	0.00		
					0.00	0.00		
					0.00	0.00		
					0.00	0.00		
					0.00	0.00		
comp.	0.26	0.00	0.07	0.06	0.00	0.00	0.24	0.01

basis	Δ_{oop}	δ_{oop}	B_{2u}	B_{1u}	A_{2u}	$E_g(x)$	$E_g(y)$	A_{1u}
min.	0.24	0.00	0.00	0.00	0.00	0.03	0.23	0.00
ext.	0.24	0.00	0.00	0.00	0.00	0.03	0.23	0.00
			0.00	0.00	0.00	0.04	0.00	0.00
total	0.24	0.00	0.00	0.00	0.00	0.03	0.23	0.00
			0.00	0.00	0.00	0.04	0.00	0.00
			0.00	0.00	0.00	0.02	0.01	
						0.00	-0.02	
						-0.01	0.01	
comp.	0.24	0.00	0.00	0.00	0.00	0.06	0.24	0.00

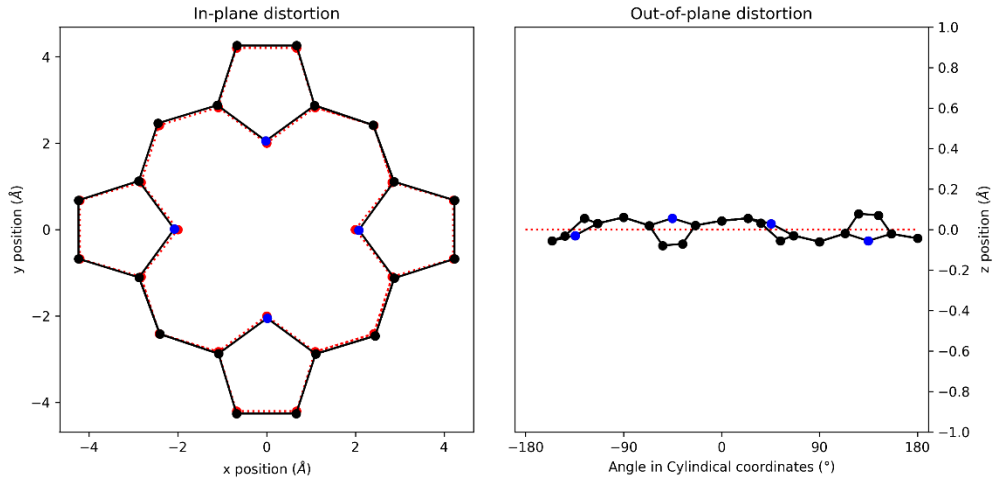


Figure S86: NSD result generated from **10** (in Å) (**A**) in-plane and (**B**) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

basis	Δ_{ip}	δ_{ip}	B_{2g}	B_{1g}	$E_u(x)$	$E_u(y)$	A_{1g}	A_{2g}
min.	0.49	0.01	-0.14	0.01	0.03	0.02	-0.47	-0.01
ext.	0.53	0.01	-0.14	0.01	0.03	0.02	-0.47	-0.01
			0.05	0.01	-0.01	-0.01	0.16	0.07
total	0.54	0.00	-0.14	0.01	0.03	0.02	-0.47	-0.01
			0.05	0.01	-0.01	-0.01	0.16	0.07
			-0.01	-0.01	0.00	0.01	0.02	-0.01
			0.04	0.01	0.02	0.01	-0.11	0.00
			0.00	0.00	0.00	0.00	-0.03	0.02
			0.00	0.01	0.00	0.00	0.07	
					0.01	0.00		
					0.00	0.00		
					-0.02	0.00		
					0.00	-0.01		
					0.00	0.00		
comp.	0.54	0.00	0.15	0.02	0.04	0.03	0.51	0.08

basis	Δ_{oop}	δ_{oop}	B_{2u}	B_{1u}	A_{2u}	$E_g(x)$	$E_g(y)$	A_{1u}
min.	1.90	0.00	0.55	1.81	-0.19	0.07	-0.05	0.00
ext.	1.90	0.00	0.55	1.81	-0.19	0.07	-0.05	0.00
			0.00	0.02	0.06	-0.03	0.00	0.00
total	1.90	0.00	0.54	1.81	-0.19	0.07	-0.05	0.00
			0.00	0.02	0.06	-0.03	0.00	0.00
			-0.01	0.02	-0.01	0.00	0.01	
						0.00	0.00	
						0.00	0.00	
comp.	1.90	0.00	0.55	1.81	0.20	0.07	0.05	0.00

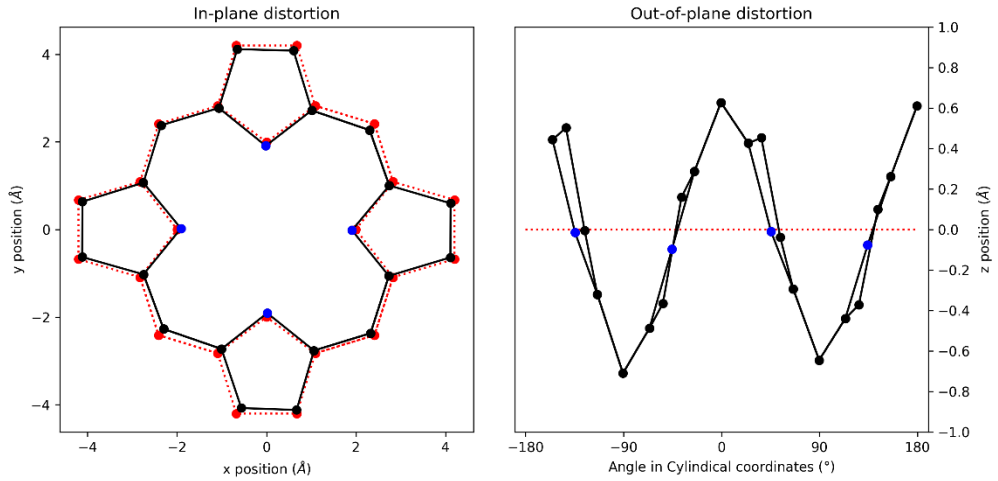


Figure S87: NSD result generated from **11** (in Å) (**A**) in-plane and (**B**) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

basis	Δ_{ip}	δ_{ip}	B_{2g}	B_{1g}	$E_u(x)$	$E_u(y)$	A_{1g}	A_{2g}
min.	0.19	0.01	0.02	-0.02	-0.01	-0.01	0.18	-0.01
ext.	0.21	0.01	0.02	-0.02	-0.01	-0.01	0.18	-0.01
			-0.07	-0.05	-0.01	0.00	0.01	0.01
total	0.26	0.00	0.02	-0.02	-0.01	-0.01	0.18	-0.01
			-0.07	-0.05	-0.01	0.00	0.01	0.01
			0.05	0.03	0.01	-0.01	0.03	0.00
			0.02	0.02	-0.01	-0.01	-0.09	0.00
			0.00	0.05	0.01	-0.01	0.01	-0.01
			-0.02	0.02	-0.01	-0.01	-0.02	
					0.02	-0.01		
					0.02	-0.02		
					-0.05	-0.03		
					0.02	-0.01		
					0.02	-0.01		
comp.	0.26	0.00	0.09	0.08	0.07	0.05	0.21	0.01

basis	Δ_{oop}	δ_{oop}	B_{2u}	B_{1u}	A_{2u}	$E_g(x)$	$E_g(y)$	A_{1u}
min.	0.17	0.00	0.08	-0.02	-0.02	-0.15	-0.01	0.00
ext.	0.19	0.00	0.08	-0.02	-0.02	-0.15	-0.01	0.00
			-0.04	0.02	0.01	0.05	-0.03	0.02
total	0.20	0.00	0.08	-0.02	-0.02	-0.15	-0.01	0.00
			-0.04	0.02	0.01	0.05	-0.03	0.02
			-0.01	0.04	0.00	-0.03	0.00	
						0.02	0.01	
						-0.03	0.00	
comp.	0.20	0.00	0.09	0.04	0.03	0.17	0.04	0.02

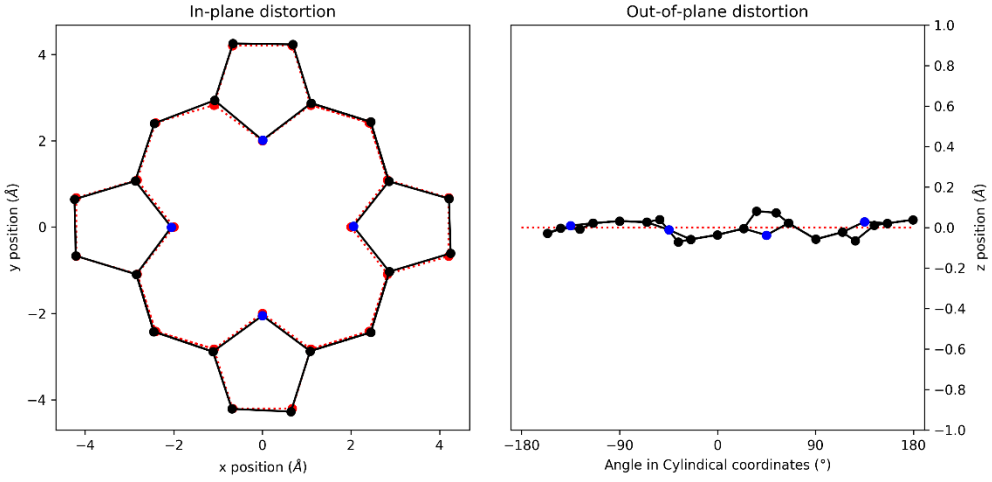


Figure S88: NSD result generated from **12** (in Å) (**A**) in-plane and (**B**) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

basis	Δ_{ip}	δ_{ip}	B_{2g}	B_{1g}	$E_u(x)$	$E_u(y)$	A_{1g}	A_{2g}
min.	0.19	0.00	0.08	0.02	-0.01	-0.02	0.17	0.00
ext.	0.20	0.00	0.08	0.02	-0.01	-0.02	0.17	0.00
			-0.01	0.02	-0.02	0.01	-0.01	-0.02
total	0.21	0.00	0.08	0.02	-0.01	-0.02	0.18	0.00
			-0.01	0.02	-0.02	0.01	-0.01	-0.02
			0.03	0.01	0.00	0.00	0.06	0.00
			-0.02	0.00	0.01	-0.01	-0.01	0.00
			0.00	0.00	0.01	0.00	0.00	0.00
			0.01	0.00	0.00	0.00	0.01	
					0.00	0.00		
					0.00	0.00		
					0.00	0.00		
					0.00	0.00		
					0.00	0.00		
comp.	0.21	0.00	0.09	0.03	0.02	0.02	0.19	0.02

basis	Δ_{oop}	δ_{oop}	B_{2u}	B_{1u}	A_{2u}	$E_g(x)$	$E_g(y)$	A_{1u}
min.	0.90	0.00	0.86	-0.24	-0.03	0.02	-0.10	0.00
ext.	0.90	0.00	0.86	-0.24	-0.03	0.02	-0.10	0.00
			-0.03	0.00	-0.01	0.00	0.01	0.00
total	0.90	0.00	0.86	-0.24	-0.03	0.02	-0.10	0.00
			-0.03	0.00	-0.01	0.00	0.01	0.00
			-0.01	0.00	0.00	0.01	-0.01	
						0.00	0.00	
						0.00	0.00	
comp.	0.90	0.00	0.86	0.24	0.03	0.02	0.10	0.00

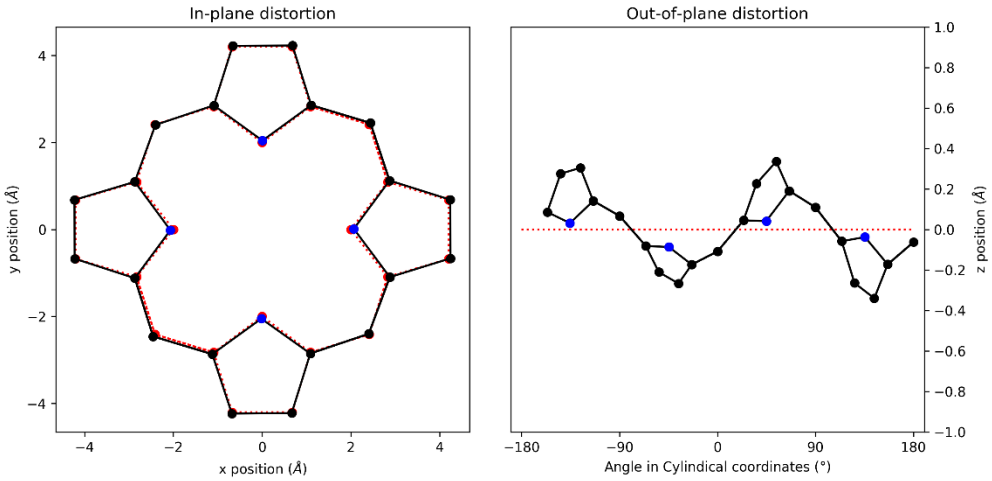


Figure S89: NSD result generated from **13** (in Å) (**A**) in-plane and (**B**) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

basis	Δ_{ip}	δ_{ip}	B_{2g}	B_{1g}	$E_u(x)$	$E_u(y)$	A_{1g}	A_{2g}
min.	0.19	0.00	-0.08	-0.02	-0.02	0.01	0.17	0.00
ext.	0.20	0.00	-0.08	-0.02	-0.02	0.01	0.17	0.00
			0.01	-0.02	0.01	0.02	-0.01	-0.02
total	0.21	0.00	-0.08	-0.02	-0.02	0.01	0.18	0.00
			0.01	-0.02	0.01	0.02	-0.01	-0.02
			-0.03	-0.02	0.00	0.00	0.06	0.00
			0.02	0.00	0.00	-0.01	0.00	0.00
			0.00	0.00	0.00	-0.01	0.00	0.00
			-0.01	0.00	0.00	0.00	0.01	
					0.00	0.00		
					0.00	0.00		
					0.00	0.00		
					0.00	0.00		
					0.00	0.00		
comp.	0.21	0.00	0.09	0.03	0.02	0.02	0.19	0.02

basis	Δ_{oop}	δ_{oop}	B_{2u}	B_{1u}	A_{2u}	$E_g(x)$	$E_g(y)$	A_{1u}
min.	0.89	0.00	0.85	-0.24	0.03	0.10	0.02	0.00
ext.	0.89	0.00	0.85	-0.24	0.03	0.10	0.02	0.00
			-0.03	0.00	0.01	-0.01	0.00	0.00
total	0.89	0.00	0.85	-0.24	0.03	0.10	0.02	0.00
			-0.03	0.00	0.01	-0.01	0.00	0.00
			-0.01	0.00	0.00	0.01	0.01	
						0.00	0.00	
						0.00	0.00	
comp.	0.89	0.00	0.85	0.24	0.03	0.10	0.02	0.00

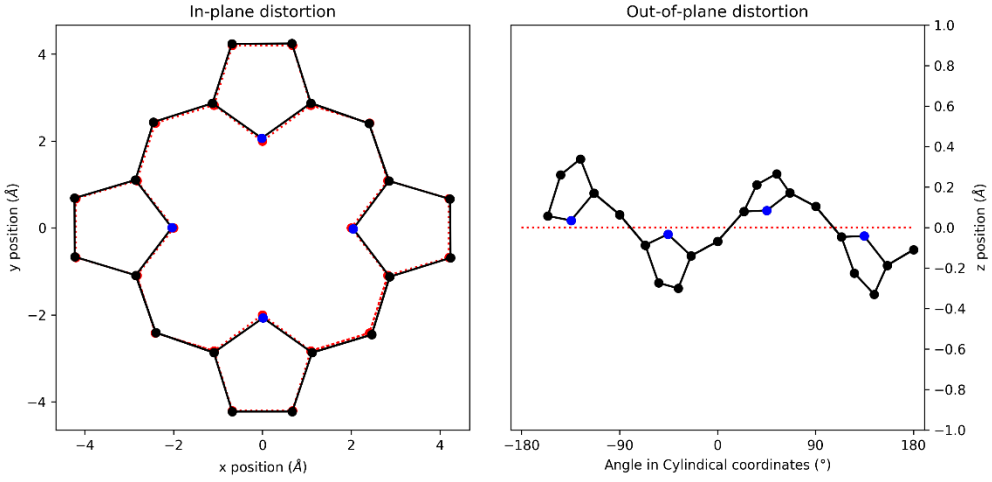


Figure S90: NSD result generated from **13A** (in Å) (**A**) in-plane and (**B**) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

basis	Δ_{ip}	δ_{ip}	B_{2g}	B_{1g}	$E_u(x)$	$E_u(y)$	A_{1g}	A_{2g}
min.	0.22	0.00	-0.05	-0.04	0.01	0.01	0.21	0.00
ext.	0.22	0.00	-0.05	-0.04	0.01	0.01	0.21	0.00
			0.01	-0.02	-0.01	0.00	-0.01	0.00
total	0.23	0.00	-0.05	-0.04	0.01	0.01	0.21	0.00
			0.01	-0.02	-0.01	0.00	-0.01	0.00
			-0.03	-0.02	0.00	0.00	0.06	0.00
			0.02	-0.01	0.00	0.00	-0.01	0.00
			0.01	0.00	0.00	-0.01	0.00	-0.01
			-0.01	0.00	0.00	0.00	0.02	
					0.00	0.00		
					0.00	0.01		
					0.00	0.00		
					0.00	0.00		
					0.00	0.00		
comp.	0.23	0.00	0.06	0.05	0.01	0.02	0.22	0.01

basis	Δ_{oop}	δ_{oop}	B_{2u}	B_{1u}	A_{2u}	$E_g(x)$	$E_g(y)$	A_{1u}
min.	0.36	0.00	0.22	0.01	-0.06	0.26	0.11	-0.02
ext.	0.37	0.00	0.22	0.01	-0.06	0.25	0.11	-0.02
			-0.04	0.00	-0.05	-0.05	0.03	0.00
total	0.37	0.00	0.22	0.01	-0.06	0.25	0.11	-0.02
			-0.04	0.00	-0.05	-0.05	0.03	0.00
			0.00	-0.01	0.00	-0.03	-0.01	
						0.00	0.00	
						0.01	0.00	
comp.	0.37	0.00	0.22	0.01	0.08	0.26	0.11	0.02

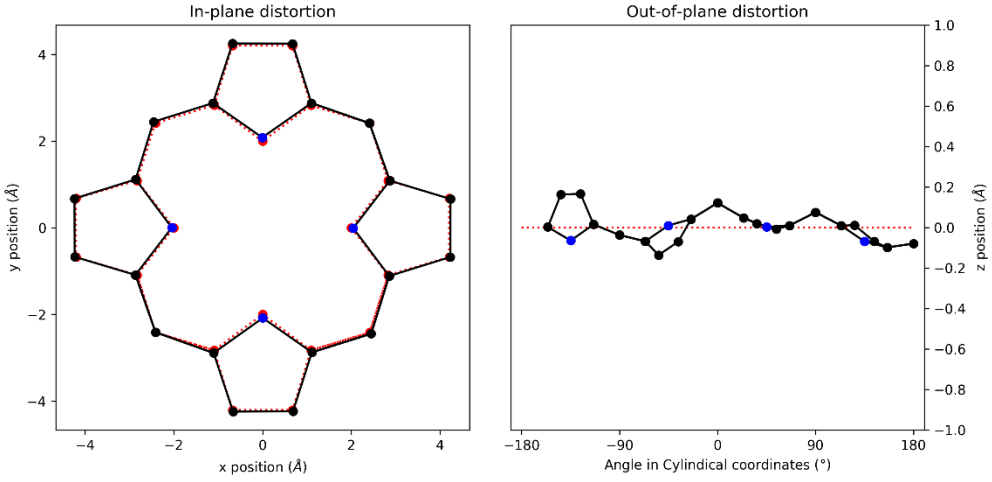


Figure S91: NSD result generated from **14** (in Å) (**A**) in-plane and (**B**) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

basis	Δ_{ip}	δ_{ip}	B_{2g}	B_{1g}	$E_u(x)$	$E_u(y)$	A_{1g}	A_{2g}
min.	0.21	0.00	-0.02	-0.01	0.00	0.01	0.21	0.00
ext.	0.21	0.00	-0.02	-0.01	0.00	0.01	0.21	0.00
			0.02	0.00	0.00	0.01	0.02	0.00
total	0.22	0.00	-0.02	-0.01	0.00	0.01	0.21	0.00
			0.02	0.00	0.00	0.01	0.02	0.00
			-0.03	0.00	0.00	0.00	0.02	0.00
			0.02	0.00	0.00	0.00	-0.01	0.00
			0.01	0.00	0.00	-0.01	-0.01	-0.01
			0.00	-0.01	0.00	0.00	0.01	
					0.00	0.00		
					0.00	0.00		
					0.00	0.00		
					0.00	0.00		
					0.00	0.00		
comp.	0.22	0.00	0.04	0.01	0.01	0.01	0.21	0.01

basis	Δ_{oop}	δ_{oop}	B_{2u}	B_{1u}	A_{2u}	$E_g(x)$	$E_g(y)$	A_{1u}
min.	0.28	0.00	0.08	-0.01	-0.25	0.10	0.02	-0.01
ext.	0.29	0.00	0.08	-0.01	-0.25	0.11	0.02	-0.01
			0.00	0.00	0.03	0.07	0.00	0.00
total	0.29	0.00	0.08	-0.01	-0.25	0.11	0.02	-0.01
			0.00	0.00	0.03	0.07	0.00	0.00
			0.00	0.00	-0.01	0.00	-0.01	
						0.00	-0.01	
						0.00	0.00	
comp.	0.29	0.00	0.08	0.01	0.25	0.13	0.02	0.01

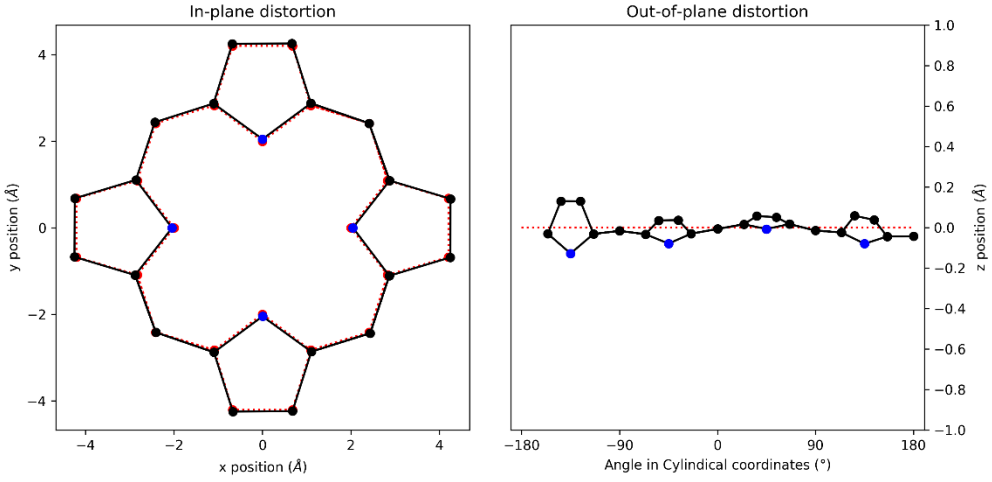


Figure S92: NSD result generated from **15** (in Å) (**A**) in-plane and (**B**) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

basis	Δ_{ip}	δ_{ip}	B_{2g}	B_{1g}	$E_u(x)$	$E_u(y)$	A_{1g}	A_{2g}
min.	0.21	0.00	0.07	-0.01	0.00	0.00	0.20	-0.01
ext.	0.22	0.00	0.07	-0.01	0.00	0.00	0.20	-0.01
			0.00	-0.04	-0.01	0.02	0.00	-0.03
total	0.25	0.00	0.07	-0.01	0.00	0.00	0.20	-0.02
			0.00	-0.04	-0.01	0.02	0.00	-0.03
			-0.01	-0.04	0.00	0.00	0.07	-0.01
			-0.01	0.02	0.00	-0.03	-0.04	0.00
			0.01	0.00	0.02	0.02	0.00	-0.02
			0.01	-0.01	-0.01	0.02	0.02	
					0.00	-0.01		
					0.01	0.00		
					0.00	0.00		
					0.00	0.00		
					0.00	0.00		
comp.	0.25	0.00	0.07	0.07	0.03	0.04	0.22	0.04

basis	Δ_{oop}	δ_{oop}	B_{2u}	B_{1u}	A_{2u}	$E_g(x)$	$E_g(y)$	A_{1u}
min.	0.89	0.00	0.57	-0.67	-0.16	-0.01	-0.07	0.00
ext.	0.90	0.00	0.57	-0.67	-0.16	-0.01	-0.07	0.00
			-0.07	-0.02	-0.01	0.00	-0.05	0.00
total	0.90	0.00	0.57	-0.67	-0.16	-0.01	-0.07	0.00
			-0.07	-0.02	-0.01	0.00	-0.05	0.00
			-0.02	0.01	0.00	0.01	0.00	
						0.00	0.00	
						-0.02	0.00	
comp.	0.90	0.00	0.57	0.67	0.16	0.02	0.08	0.00

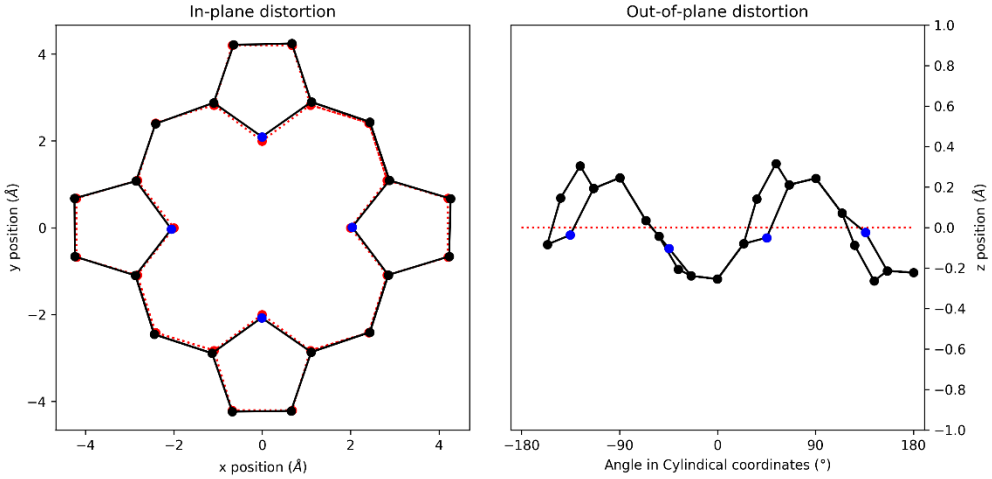


Figure S93: NSD result generated from **16** (in Å) (**A**) in-plane and (**B**) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

basis	Δ_{ip}	δ_{ip}	B_{2g}	B_{1g}	$E_u(x)$	$E_u(y)$	A_{1g}	A_{2g}
min.	0.17	0.00	0.04	0.01	0.00	0.00	0.16	-0.01
ext.	0.19	0.00	0.04	0.00	0.00	0.00	0.16	-0.01
			0.00	-0.06	0.00	-0.04	-0.03	-0.01
total	0.21	0.00	0.04	0.00	0.00	0.00	0.17	-0.01
			0.00	-0.06	0.00	-0.04	-0.03	-0.01
			0.01	-0.05	0.00	0.00	0.07	-0.01
			0.00	0.00	-0.01	0.01	-0.01	0.00
			0.01	0.01	0.00	0.01	0.01	0.01
			0.01	-0.01	0.00	0.00	0.01	
					0.01	0.00		
					0.00	-0.01		
					0.00	0.00		
					0.00	0.00		
					0.00	-0.01		
comp.	0.21	0.00	0.04	0.08	0.02	0.04	0.19	0.02

basis	Δ_{oop}	δ_{oop}	B_{2u}	B_{1u}	A_{2u}	$E_g(x)$	$E_g(y)$	A_{1u}
min.	0.67	0.00	0.60	-0.21	-0.10	-0.14	0.11	0.01
ext.	0.68	0.00	0.60	-0.21	-0.10	-0.14	0.11	0.01
			-0.07	-0.01	-0.02	0.04	0.07	0.01
total	0.68	0.00	0.60	-0.21	-0.10	-0.14	0.11	0.01
			-0.07	-0.01	-0.02	0.04	0.07	0.01
			-0.01	0.00	0.00	0.02	0.01	
						0.01	-0.01	
						-0.02	0.00	
comp.	0.68	0.00	0.61	0.21	0.10	0.15	0.13	0.02

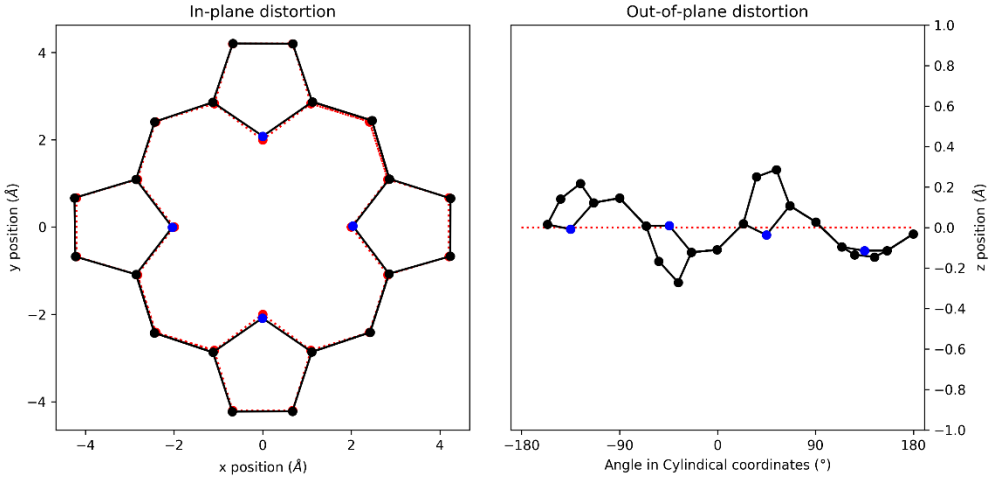


Figure S94: NSD result generated from **16A** (in Å) (**A**) in-plane and (**B**) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

basis	Δ_{ip}	δ_{ip}	B_{2g}	B_{1g}	$E_u(x)$	$E_u(y)$	A_{1g}	A_{2g}
min.	0.03	0.00	-0.01	0.00	0.01	0.02	0.01	0.01
ext.	0.05	0.00	-0.01	0.00	0.01	0.02	0.01	0.01
			-0.02	0.00	0.01	0.00	0.02	-0.01
total	0.09	0.00	-0.01	0.00	0.01	0.02	0.01	0.01
			-0.02	0.00	0.01	0.00	0.02	-0.01
			-0.01	0.01	-0.01	0.00	0.03	0.00
			0.00	0.01	-0.02	0.01	-0.03	0.00
			-0.01	0.00	0.01	0.00	-0.02	-0.01
			-0.01	-0.02	-0.02	-0.01	0.02	
					-0.02	-0.01		
					0.00	0.00		
					-0.03	0.01		
					0.03	0.00		
					0.00	-0.01		
comp.	0.09	0.00	0.03	0.02	0.06	0.03	0.06	0.02

basis	Δ_{oop}	δ_{oop}	B_{2u}	B_{1u}	A_{2u}	$E_g(x)$	$E_g(y)$	A_{1u}
min.	0.73	0.00	0.23	-0.69	0.02	-0.03	0.05	-0.01
ext.	0.74	0.00	0.23	-0.69	0.02	-0.03	0.05	-0.01
			0.04	-0.02	0.06	0.01	0.00	0.01
total	0.74	0.00	0.23	-0.69	0.02	-0.03	0.05	-0.01
			0.04	-0.02	0.06	0.01	0.00	0.01
			-0.01	-0.01	-0.01	0.00	-0.01	
						0.02	0.01	
						0.00	0.00	
comp.	0.74	0.00	0.23	0.69	0.06	0.04	0.05	0.01

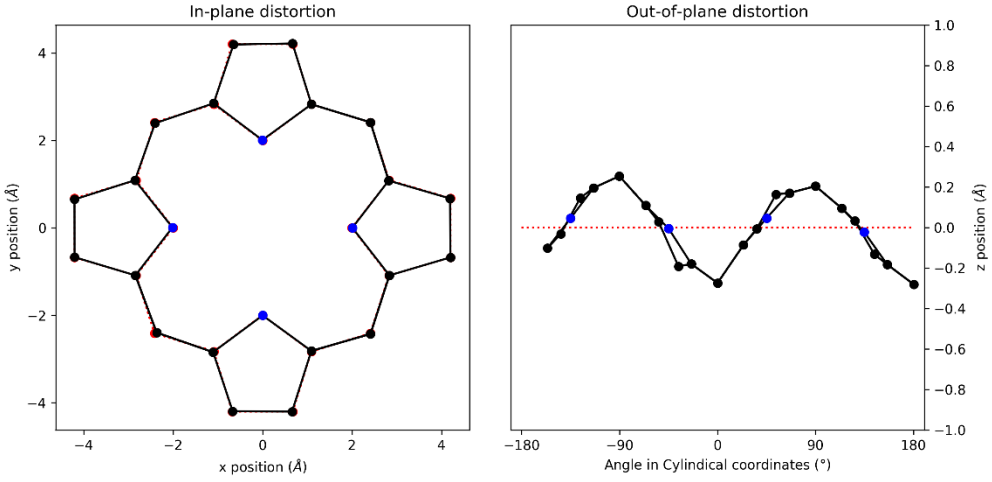


Figure S95: NSD result generated from **17** (in Å) (**A**) in-plane and (**B**) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

basis	Δ_{ip}	δ_{ip}	B_{2g}	B_{1g}	$E_u(x)$	$E_u(y)$	A_{1g}	A_{2g}
min.	0.18	0.00	0.01	0.04	-0.01	0.04	0.17	-0.01
ext.	0.18	0.00	0.01	0.04	-0.01	0.04	0.17	-0.01
			0.01	0.01	-0.01	0.02	0.03	-0.02
total	0.19	0.00	0.01	0.04	-0.01	0.04	0.17	-0.01
			0.01	0.01	-0.01	0.02	0.03	-0.02
			0.00	0.00	-0.01	-0.01	0.03	0.00
			-0.01	0.00	-0.01	-0.02	-0.04	0.00
			0.01	0.01	0.01	0.01	-0.01	0.00
			0.00	0.00	0.00	-0.01	0.01	
					-0.01	0.00		
					-0.01	-0.01		
					0.00	-0.01		
					0.00	0.01		
					0.00	0.00		
comp.	0.19	0.00	0.02	0.04	0.02	0.05	0.18	0.02

basis	Δ_{oop}	δ_{oop}	B_{2u}	B_{1u}	A_{2u}	$E_g(x)$	$E_g(y)$	A_{1u}
min.	0.64	0.00	0.27	-0.56	-0.01	0.11	0.05	0.00
ext.	0.64	0.00	0.27	-0.56	-0.02	0.11	0.05	0.00
			-0.03	-0.01	-0.04	-0.06	-0.05	0.01
total	0.64	0.00	0.27	-0.56	-0.02	0.11	0.05	0.00
			-0.03	-0.01	-0.04	-0.06	-0.05	0.01
			0.00	-0.01	0.01	0.00	0.01	
						0.00	0.00	
						0.00	0.01	
comp.	0.64	0.00	0.27	0.56	0.04	0.12	0.07	0.01

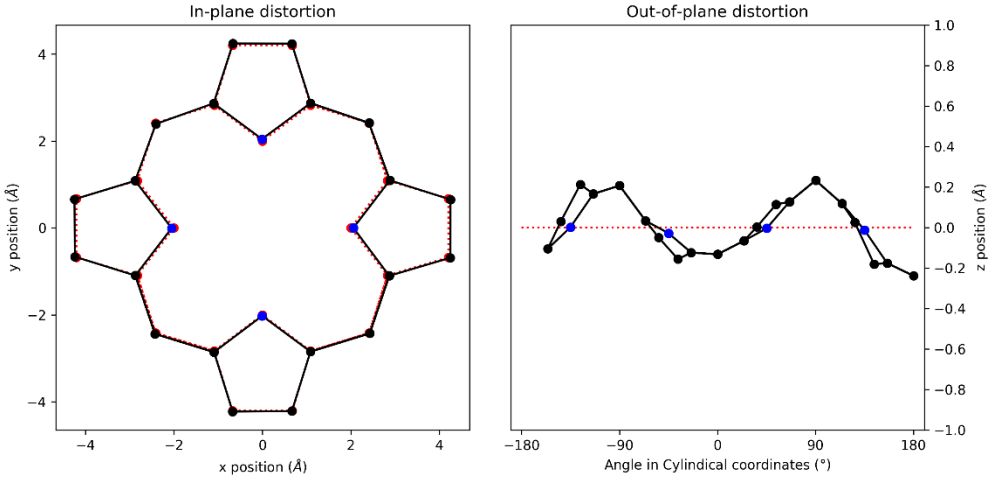


Figure S96: NSD result generated from **18** (in Å) (**A**) in-plane and (**B**) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

basis	Δ_{ip}	δ_{ip}	B_{2g}	B_{1g}	$E_u(x)$	$E_u(y)$	A_{1g}	A_{2g}
min.	0.23	0.00	0.00	-0.02	0.02	0.00	0.23	0.00
ext.	0.23	0.00	0.00	-0.02	0.02	0.00	0.23	0.00
			0.00	-0.04	0.00	0.00	0.01	0.00
total	0.25	0.00	0.00	-0.02	0.02	0.00	0.23	0.00
			0.00	-0.04	0.00	0.00	0.01	0.00
			0.00	-0.03	-0.02	0.00	0.05	0.00
			0.00	0.00	-0.03	0.00	-0.01	0.00
			0.00	0.01	0.01	0.00	0.01	0.00
			0.00	-0.01	0.00	0.00	0.01	
					0.00	0.00		
					0.00	0.00		
					-0.01	0.00		
					0.01	0.00		
					0.00	0.00		
comp.	0.25	0.00	0.00	0.05	0.04	0.00	0.24	0.00

basis	Δ_{oop}	δ_{oop}	B_{2u}	B_{1u}	A_{2u}	$E_g(x)$	$E_g(y)$	A_{1u}
min.	0.25	0.00	0.00	-0.25	0.00	0.00	0.00	0.00
ext.	0.25	0.00	0.00	-0.25	0.00	0.00	0.00	0.00
			0.00	0.00	0.00	-0.02	0.00	0.00
total	0.25	0.00	0.00	-0.25	0.00	0.00	0.00	0.00
			0.00	0.00	0.00	-0.02	0.00	0.00
			0.00	-0.01	0.00	0.01	0.00	
						0.01	0.00	
						0.00	0.00	
comp.	0.25	0.00	0.00	0.25	0.00	0.02	0.00	0.01

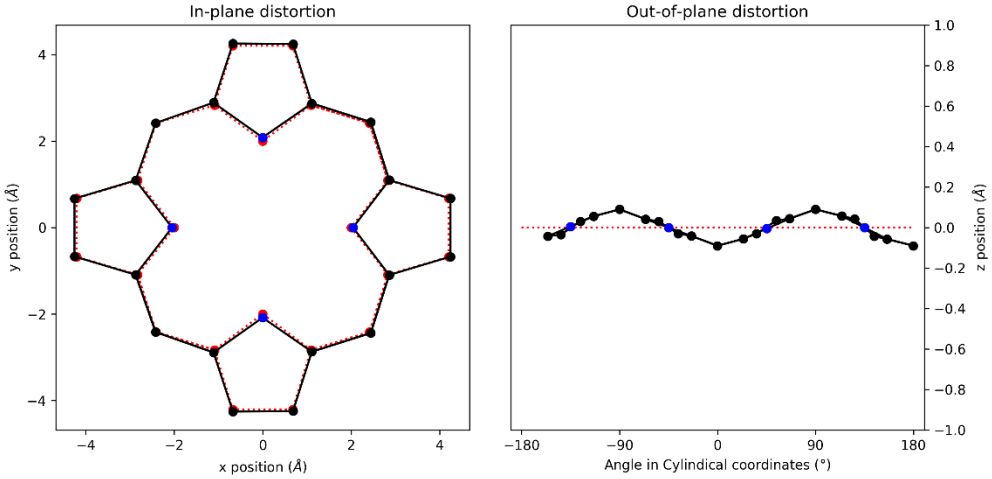


Figure S97: NSD result generated from **19** (in Å) (**A**) in-plane and (**B**) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

basis	Δ_{ip}	δ_{ip}	B_{2g}	B_{1g}	$E_u(x)$	$E_u(y)$	A_{1g}	A_{2g}
min.	0.26	0.00	-0.01	0.06	0.00	0.00	0.26	0.00
ext.	0.28	0.00	-0.01	0.06	0.00	0.00	0.26	0.00
			-0.01	0.06	0.00	0.00	0.06	0.00
total	0.29	0.00	-0.01	0.07	0.00	0.00	0.26	0.00
			-0.01	0.06	0.00	0.00	0.06	0.00
			0.01	0.05	0.00	0.00	0.04	0.00
			0.00	0.00	0.00	0.00	0.02	0.00
			0.00	-0.01	0.00	0.00	0.00	0.00
			0.00	0.01	0.00	0.00	0.01	
					0.00	0.00		
					0.00	0.00		
					0.00	0.00		
					0.00	0.00		
					0.00	0.00		
comp.	0.29	0.00	0.02	0.10	0.00	0.00	0.27	0.00

basis	Δ_{oop}	δ_{oop}	B_{2u}	B_{1u}	A_{2u}	$E_g(x)$	$E_g(y)$	A_{1u}
min.	0.12	0.00	0.00	0.00	0.00	0.08	0.09	0.00
ext.	0.14	0.00	0.00	0.00	0.00	0.09	0.09	0.00
			0.00	0.00	0.00	0.05	-0.02	0.00
total	0.14	0.00	0.00	0.00	0.00	0.09	0.09	0.00
			0.00	0.00	0.00	0.05	-0.02	0.00
			0.00	0.00	0.00	-0.01	0.01	
						0.00	0.00	
						0.00	0.00	
comp.	0.14	0.00	0.00	0.00	0.00	0.10	0.09	0.00

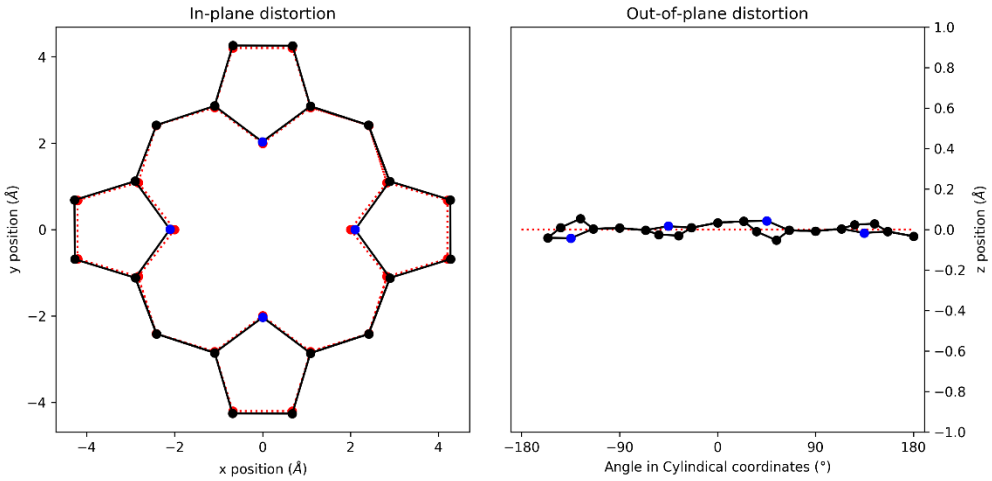


Figure S98: NSD result generated from **20** (in Å) (**A**) in-plane and (**B**) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

basis	Δ_{ip}	δ_{ip}	B_{2g}	B_{1g}	$E_u(x)$	$E_u(y)$	A_{1g}	A_{2g}
min.	0.47	0.01	0.02	-0.01	0.00	-0.03	-0.46	0.04
ext.	0.50	0.01	0.02	-0.01	0.00	-0.03	-0.46	0.04
			0.01	-0.01	-0.02	-0.01	0.17	-0.06
total	0.52	0.00	0.02	-0.01	0.00	-0.03	-0.46	0.03
			0.01	-0.01	-0.02	-0.01	0.17	-0.06
			-0.02	0.00	-0.03	0.00	0.01	0.00
			0.00	0.00	-0.04	0.02	-0.13	-0.01
			0.00	0.00	0.01	-0.01	-0.01	-0.02
			0.00	0.00	0.00	0.00	0.08	
					0.00	-0.01		
					0.00	0.00		
					0.00	0.01		
					0.01	0.00		
					0.00	0.00		
comp.	0.52	0.00	0.03	0.02	0.05	0.04	0.51	0.07

basis	Δ_{oop}	δ_{oop}	B_{2u}	B_{1u}	A_{2u}	$E_g(x)$	$E_g(y)$	A_{1u}
min.	1.89	0.00	0.34	-1.85	-0.09	0.09	0.00	-0.01
ext.	1.89	0.00	0.34	-1.85	-0.09	0.09	0.00	-0.01
			0.00	-0.02	0.01	-0.02	-0.02	0.00
total	1.89	0.00	0.34	-1.85	-0.09	0.09	0.00	-0.01
			0.00	-0.02	0.01	-0.02	-0.02	0.00
			0.00	-0.02	0.00	-0.02	-0.02	
						0.00	0.00	
						0.00	0.01	
comp.	1.89	0.00	0.34	1.85	0.09	0.10	0.03	0.01

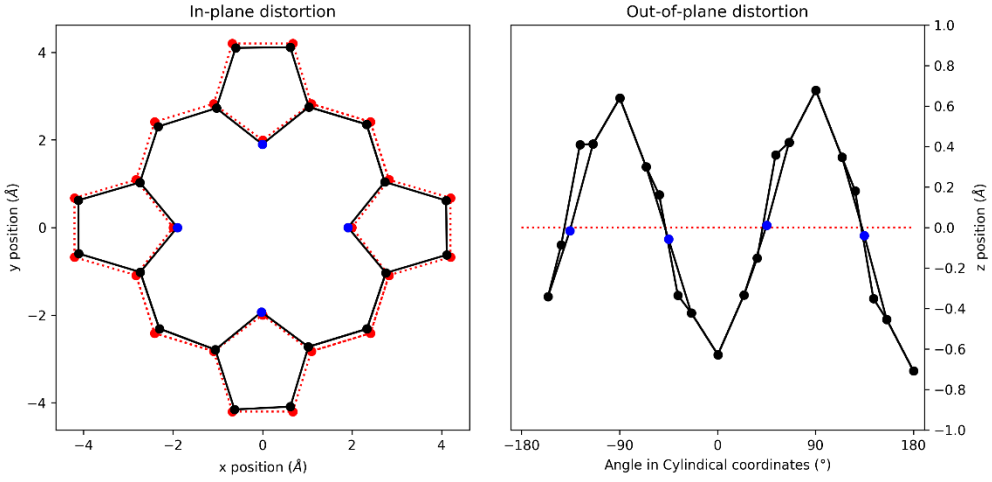


Figure S99: NSD result generated from **21** (in Å) (**A**) in-plane and (**B**) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

basis	Δ_{ip}	δ_{ip}	B_{2g}	B_{1g}	$E_u(x)$	$E_u(y)$	A_{1g}	A_{2g}
min.	0.42	0.01	-0.04	0.00	-0.01	-0.01	-0.41	0.00
ext.	0.44	0.00	-0.04	0.00	-0.01	-0.01	-0.41	0.00
			0.01	0.00	-0.02	-0.02	0.13	0.00
total	0.46	0.00	-0.04	0.00	-0.01	-0.01	-0.41	0.00
			0.01	0.00	-0.02	-0.02	0.13	0.00
			0.03	0.00	0.01	0.01	0.01	0.00
			-0.01	0.00	0.03	0.03	-0.10	0.00
			0.00	0.00	-0.02	-0.02	-0.01	0.00
			0.02	0.00	0.01	0.01	0.06	
					0.00	0.00		
					0.01	0.01		
					0.00	0.00		
					0.00	0.00		
					0.00	0.00		
comp.	0.46	0.00	0.06	0.00	0.05	0.05	0.45	0.00

basis	Δ_{oop}	δ_{oop}	B_{2u}	B_{1u}	A_{2u}	$E_g(x)$	$E_g(y)$	A_{1u}
min.	1.74	0.00	0.00	1.72	-0.09	0.14	-0.14	0.00
ext.	1.74	0.00	0.00	1.72	-0.09	0.14	-0.14	0.00
			0.00	0.02	0.05	-0.01	0.01	0.00
total	1.74	0.00	0.00	1.72	-0.09	0.14	-0.14	0.00
			0.00	0.02	0.05	-0.01	0.01	0.00
			0.00	0.03	0.00	-0.05	0.05	
						-0.01	0.01	
						0.00	0.00	
comp.	1.74	0.00	0.00	1.72	0.10	0.15	0.15	0.00

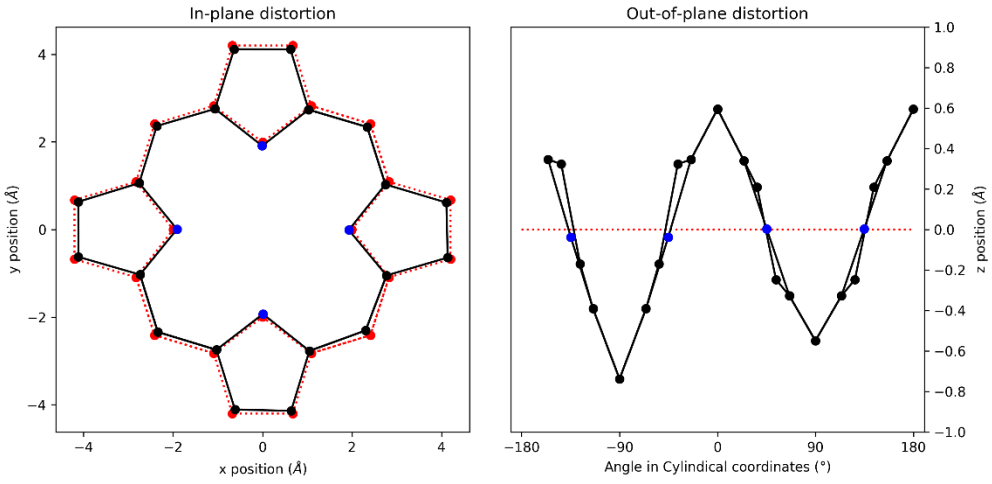


Figure S100: NSD result generated from **22** (in Å) (**A**) in-plane and (**B**) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

basis	Δ_{ip}	δ_{ip}	B_{2g}	B_{1g}	$E_u(x)$	$E_u(y)$	A_{1g}	A_{2g}
min.	0.23	0.00	-0.05	0.01	-0.01	0.02	-0.22	0.00
ext.	0.23	0.00	-0.05	0.01	-0.01	0.02	-0.22	0.00
			0.03	0.01	-0.02	0.00	0.04	-0.01
total	0.26	0.00	-0.05	0.01	-0.01	0.02	-0.22	0.00
			0.03	0.01	-0.02	0.00	0.04	-0.01
			-0.02	-0.01	0.01	0.00	-0.04	0.00
			0.00	0.02	0.00	-0.02	-0.03	-0.03
			0.01	0.01	-0.01	-0.02	-0.03	0.01
			0.00	0.01	0.01	0.01	0.02	
					0.04	0.00		
					0.01	-0.03		
					0.01	-0.01		
					0.00	0.01		
					-0.02	0.00		
comp.	0.26	0.00	0.06	0.03	0.05	0.05	0.24	0.03

basis	Δ_{oop}	δ_{oop}	B_{2u}	B_{1u}	A_{2u}	$E_g(x)$	$E_g(y)$	A_{1u}
min.	0.96	0.00	0.23	0.93	-0.02	0.07	-0.01	-0.02
ext.	0.97	0.00	0.23	0.93	-0.02	0.07	-0.01	-0.02
			0.04	0.02	0.01	-0.04	0.05	0.02
total	0.97	0.00	0.23	0.93	-0.02	0.07	-0.01	-0.02
			0.04	0.02	0.01	-0.04	0.05	0.02
			0.00	0.02	0.01	-0.03	0.02	
						0.01	-0.01	
						0.03	0.00	
comp.	0.97	0.00	0.24	0.93	0.02	0.09	0.05	0.03

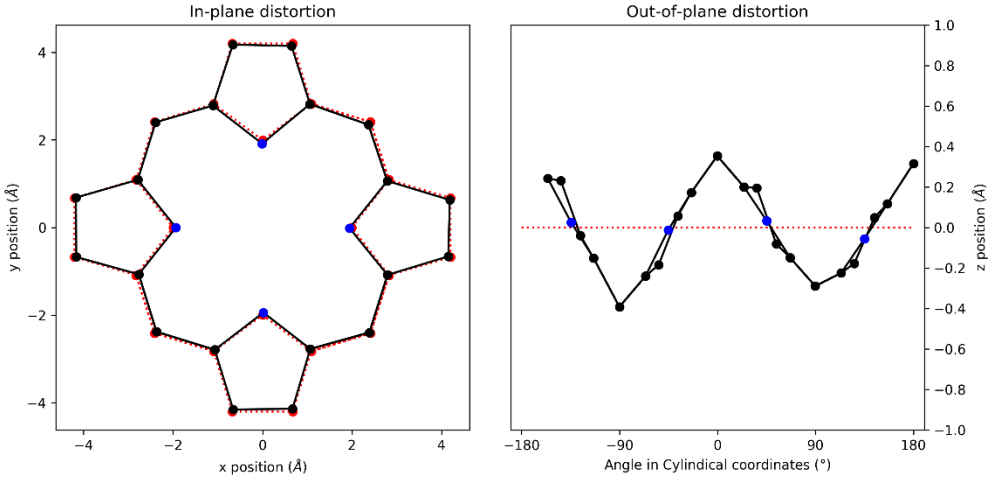


Figure S101: NSD result generated from **23** (in Å) (**A**) in-plane and (**B**) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

basis	Δ_{ip}	δ_{ip}	B_{2g}	B_{1g}	$E_u(x)$	$E_u(y)$	A_{1g}	A_{2g}
min.	0.21	0.00	-0.07	0.01	0.00	0.00	0.20	0.00
ext.	0.22	0.00	-0.07	0.01	0.00	0.00	0.20	0.00
			-0.01	-0.02	-0.02	0.01	-0.04	0.00
total	0.23	0.00	-0.07	0.01	0.00	0.00	0.20	0.00
			-0.01	-0.02	-0.02	0.01	-0.04	0.00
			-0.01	-0.02	0.00	0.00	0.05	0.00
			0.00	0.00	0.00	0.00	-0.01	0.00
			0.00	0.00	0.00	0.00	0.02	0.00
			0.00	0.00	0.00	0.00	0.01	
					0.00	0.00		
					0.00	0.00		
					0.00	0.00		
					0.00	0.00		
					0.00	0.01		
comp.	0.23	0.00	0.07	0.03	0.02	0.02	0.21	0.00

basis	Δ_{oop}	δ_{oop}	B_{2u}	B_{1u}	A_{2u}	$E_g(x)$	$E_g(y)$	A_{1u}
min.	0.29	0.00	-0.10	-0.16	-0.01	0.01	0.21	0.00
ext.	0.30	0.00	-0.10	-0.16	-0.01	0.01	0.21	0.00
			-0.04	-0.01	0.01	0.04	-0.07	0.00
total	0.30	0.00	-0.10	-0.16	-0.01	0.01	0.21	0.00
			-0.04	-0.01	0.01	0.04	-0.07	0.00
			0.00	-0.01	0.00	0.01	-0.02	
						0.00	-0.01	
						0.01	0.01	
comp.	0.30	0.00	0.11	0.16	0.01	0.04	0.22	0.00

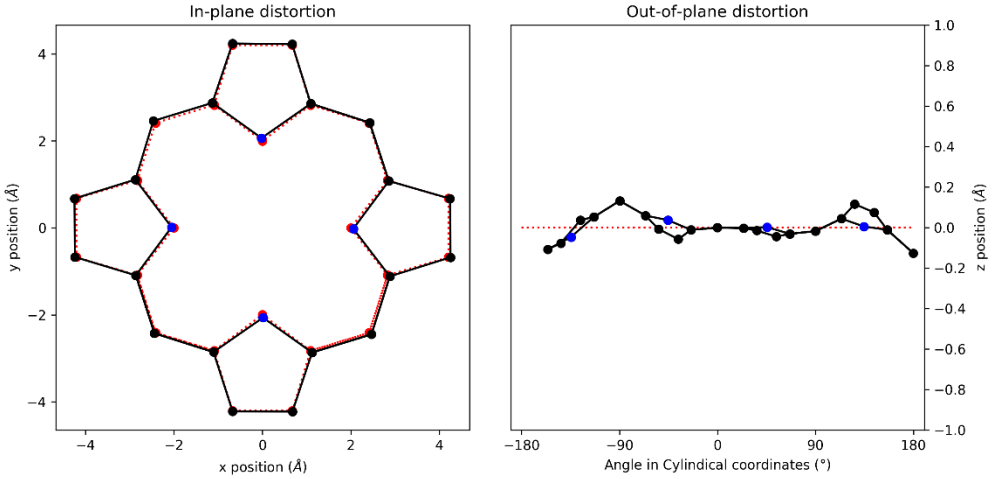


Figure S102: NSD result generated from **24** (in Å) (**A**) in-plane and (**B**) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

NSD tables and plots for DFT structures series 1

basis	Δ_{ip}	δ_{ip}	B_{2g}	B_{1g}	$E_u(x)$	$E_u(y)$	A_{1g}	A_{2g}
min.	0.38	0.00	-0.32	-0.05	0.00	0.00	0.21	0.00
ext.	0.40	0.00	-0.32	-0.05	0.00	0.00	0.21	0.00
			-0.05	-0.09	0.00	0.00	0.00	0.00
total	0.41	0.00	-0.32	-0.05	0.00	0.00	0.21	0.00
			-0.05	-0.09	0.00	0.00	0.00	0.00
			0.00	-0.06	0.00	0.00	0.05	0.00
			0.00	0.00	0.00	0.00	0.01	0.00
			0.00	0.01	0.00	0.00	0.02	0.00
			-0.01	-0.01	0.00	0.00	0.01	
					0.00	0.00		
					0.00	0.00		
					0.00	0.00		
					0.00	0.00		
					0.00	0.00		
comp.	0.41	0.00	0.32	0.12	0.00	0.00	0.22	0.00

basis	Δ_{oop}	δ_{oop}	B_{2u}	B_{1u}	A_{2u}	$E_g(x)$	$E_g(y)$	A_{1u}
min.	0.08	0.00	0.00	0.00	0.00	0.06	0.06	0.00
ext.	0.10	0.00	0.00	0.00	0.00	0.06	0.06	0.00
			0.00	0.00	0.00	0.05	0.03	0.00
total	0.10	0.00	0.00	0.00	0.00	0.06	0.06	0.00
			0.00	0.00	0.00	0.05	0.03	0.00
			0.00	0.00	0.00	0.00	0.00	
						0.00	0.00	
						0.00	0.00	
comp.	0.10	0.00	0.00	0.00	0.00	0.08	0.07	0.00

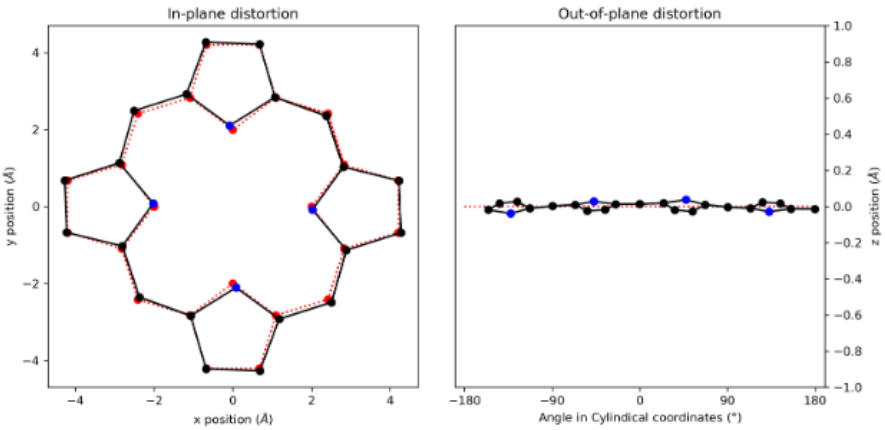


Figure S103: NSD result generated from **1:1** (in Å) (**A**) in-plane and (**B**) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

basis	Δ_{ip}	δ_{ip}	B_{2g}	B_{1g}	$E_u(x)$	$E_u(y)$	A_{1g}	A_{2g}
min.	0.14	0.00	-0.06	0.00	0.00	0.00	-0.12	0.00
ext.	0.14	0.00	-0.07	0.00	0.00	0.00	-0.12	0.00
			-0.02	0.00	0.00	0.00	0.00	0.00
total	0.15	0.00	-0.06	0.00	0.00	0.00	-0.12	0.00
			-0.02	0.00	0.00	0.00	0.00	0.00
			-0.01	0.00	0.00	0.00	-0.03	0.00
			0.01	0.00	0.00	0.00	-0.01	0.00
			0.00	0.00	0.00	0.00	0.00	0.00
			0.00	0.00	0.00	0.00	0.00	
					0.00	0.00		
					0.00	0.00		
					0.00	0.00		
					0.00	0.00		
					0.00	0.00		
comp.	0.15	0.00	0.07	0.00	0.00	0.00	0.13	0.00

basis	Δ_{oop}	δ_{oop}	B_{2u}	B_{1u}	A_{2u}	$E_g(x)$	$E_g(y)$	A_{1u}
min.	0.57	0.00	0.00	0.57	0.01	-0.01	-0.01	0.00
ext.	0.57	0.00	0.00	0.57	0.01	-0.01	-0.01	0.00
			0.00	0.00	0.00	-0.01	-0.01	0.00
total	0.57	0.00	0.00	0.57	0.01	-0.01	-0.01	0.00
			0.00	0.00	0.00	-0.01	-0.01	0.00
			0.00	0.01	0.00	0.00	0.00	
						0.00	0.00	
						0.00	0.00	
comp.	0.57	0.00	0.00	0.57	0.01	0.02	0.02	0.00

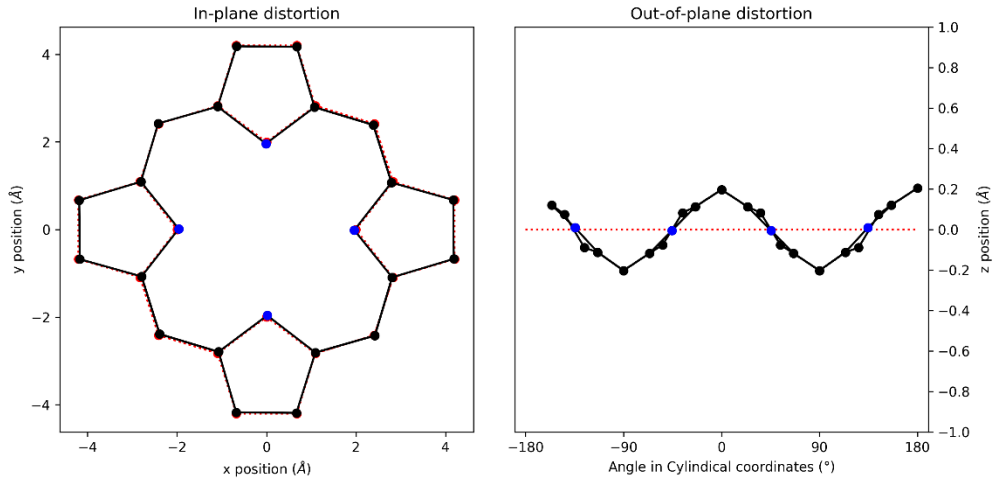


Figure S104: NSD result generated from 1:2 (in Å) (A) in-plane and (B) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

basis	Δ_{ip}	δ_{ip}	B_{2g}	B_{1g}	$E_u(x)$	$E_u(y)$	A_{1g}	A_{2g}
min.	0.37	0.00	-0.31	-0.04	0.00	0.00	0.21	-0.01
ext.	0.39	0.00	-0.31	-0.04	0.00	0.00	0.21	-0.01
			-0.05	-0.09	0.01	0.01	0.01	0.00
total	0.40	0.00	-0.31	-0.04	0.00	0.00	0.21	-0.01
			-0.05	-0.09	0.01	0.01	0.01	0.00
			-0.01	-0.06	0.00	0.00	0.05	0.00
			0.00	0.00	-0.01	0.02	0.01	0.00
			0.00	0.01	0.00	-0.01	0.02	0.00
			-0.01	-0.01	0.00	0.00	0.01	
					0.00	0.00		
					0.00	0.00		
					0.00	0.01		
					0.00	0.00		
					-0.01	0.02		
comp.	0.40	0.00	0.31	0.11	0.02	0.03	0.22	0.01

basis	Δ_{oop}	δ_{oop}	B_{2u}	B_{1u}	A_{2u}	$E_g(x)$	$E_g(y)$	A_{1u}
min.	0.09	0.00	0.00	-0.01	0.00	-0.06	-0.06	0.00
ext.	0.11	0.00	0.00	-0.01	0.00	-0.07	-0.06	0.00
			0.00	0.00	0.00	-0.05	-0.03	0.00
total	0.11	0.00	0.00	-0.01	0.00	-0.07	-0.06	0.00
			0.00	0.00	0.00	-0.05	-0.03	0.00
			0.00	0.00	0.00	0.00	0.00	
						0.00	0.00	
						0.00	0.00	
comp.	0.11	0.00	0.00	0.01	0.00	0.08	0.07	0.00

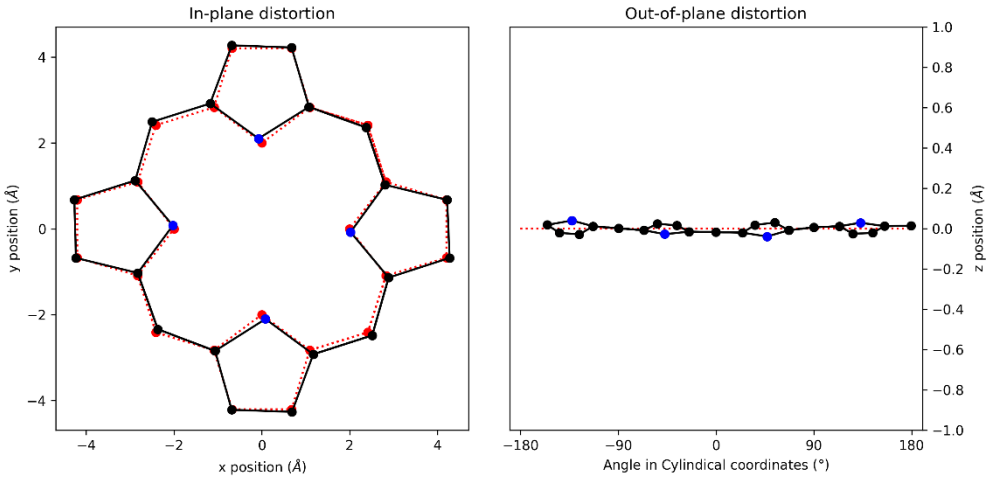


Figure S105: NSD result generated from **1:3** (in Å) (**A**) in-plane and (**B**) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

basis	Δ_{ip}	δ_{ip}	B_{2g}	B_{1g}	$E_u(x)$	$E_u(y)$	A_{1g}	A_{2g}
min.	0.14	0.00	-0.07	0.00	0.00	0.00	-0.13	0.00
ext.	0.15	0.00	-0.07	0.00	0.00	0.00	-0.13	0.00
			-0.02	0.00	0.00	0.00	0.01	0.00
total	0.15	0.00	-0.07	0.00	0.00	0.00	-0.13	0.00
			-0.02	0.00	0.00	0.00	0.01	0.00
			-0.02	0.00	0.00	0.00	-0.03	0.00
			0.01	0.00	0.01	-0.01	-0.01	0.00
			0.00	0.00	0.00	0.00	0.00	0.00
			-0.01	0.00	0.00	0.00	0.00	
					0.00	0.00		
					0.00	0.00		
					0.01	0.00		
					0.00	0.00		
					0.01	-0.01		
comp.	0.15	0.00	0.08	0.00	0.02	0.02	0.13	0.00

basis	Δ_{oop}	δ_{oop}	B_{2u}	B_{1u}	A_{2u}	$E_g(x)$	$E_g(y)$	A_{1u}
min.	0.61	0.00	0.00	0.61	0.01	-0.02	-0.02	0.00
ext.	0.61	0.00	0.00	0.61	0.01	-0.02	-0.02	0.00
			0.00	0.00	0.00	-0.01	-0.01	0.00
total	0.61	0.00	0.00	0.61	0.01	-0.02	-0.02	0.00
			0.00	0.00	0.00	-0.01	-0.01	0.00
			0.00	0.01	0.00	0.00	0.00	
						0.00	0.00	
						0.00	0.00	
comp.	0.61	0.00	0.00	0.61	0.01	0.02	0.02	0.00

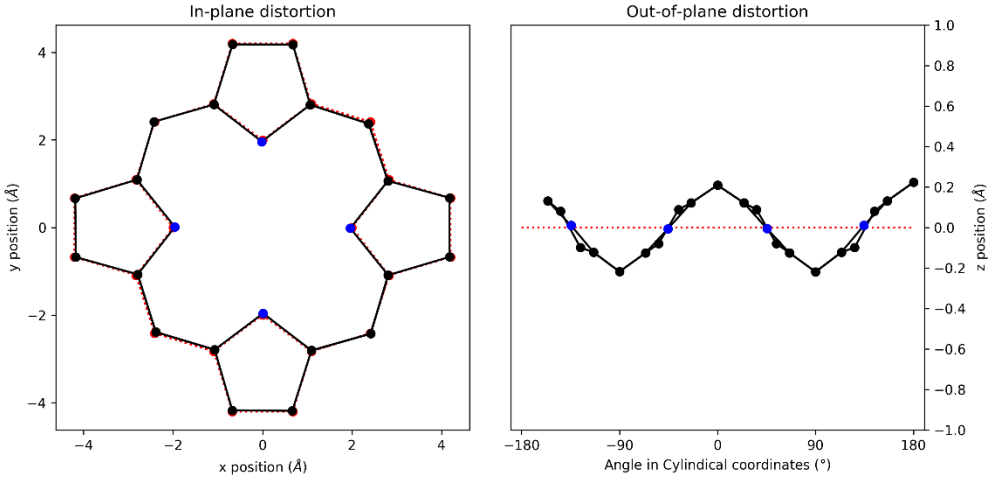


Figure S106: NSD result generated from **1:4** (in Å) (**A**) in-plane and (**B**) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

basis	Δ_{ip}	δ_{ip}	B_{2g}	B_{1g}	$E_u(x)$	$E_u(y)$	A_{1g}	A_{2g}
min.	0.37	0.00	0.31	0.03	0.00	0.00	0.21	-0.01
ext.	0.39	0.00	0.31	0.03	0.00	0.00	0.21	-0.01
			0.05	0.08	0.00	0.00	0.02	0.01
total	0.40	0.00	0.31	0.03	0.00	0.00	0.21	-0.01
			0.05	0.09	0.00	0.00	0.02	0.01
			0.03	0.06	0.00	0.00	0.05	0.00
			-0.01	0.00	0.00	0.00	0.00	0.00
			0.00	-0.01	0.00	0.00	0.02	0.00
			0.01	0.01	0.00	0.00	0.00	
					0.00	0.00		
					0.00	0.00		
					0.00	0.00		
					0.00	0.00		
					0.00	0.00		
comp.	0.40	0.00	0.32	0.11	0.00	0.00	0.22	0.01

basis	Δ_{oop}	δ_{oop}	B_{2u}	B_{1u}	A_{2u}	$E_g(x)$	$E_g(y)$	A_{1u}
min.	0.09	0.00	0.00	0.00	0.00	-0.06	0.07	0.00
ext.	0.11	0.00	0.00	0.00	0.00	-0.06	0.07	0.00
			0.00	0.00	0.00	-0.03	0.05	0.00
total	0.11	0.00	0.00	0.00	0.00	-0.06	0.07	0.00
			0.00	0.00	0.00	-0.03	0.05	0.00
			0.00	0.00	0.00	0.00	0.00	
						0.00	0.00	
						0.00	0.00	
comp.	0.11	0.00	0.00	0.00	0.00	0.07	0.09	0.00

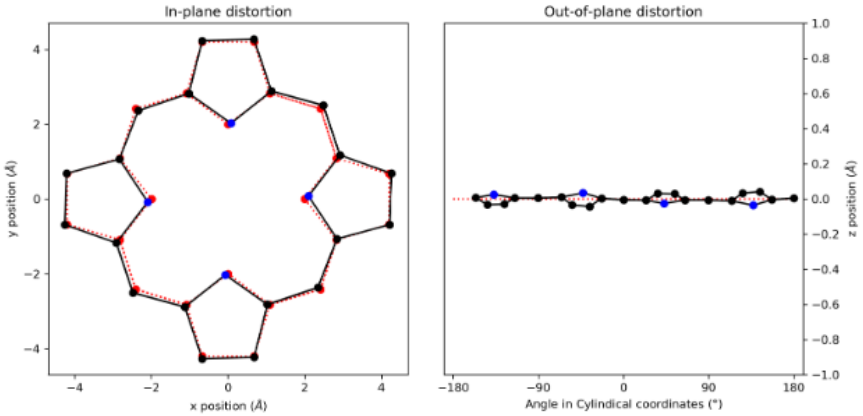


Figure S107: NSD result generated from 1:5 (in Å) (A) in-plane and (B) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

basis	Δ_{ip}	δ_{ip}	B_{2g}	B_{1g}	$E_u(x)$	$E_u(y)$	A_{1g}	A_{2g}
min.	0.15	0.00	-0.08	0.00	0.00	0.00	-0.12	0.00
ext.	0.15	0.00	-0.08	0.00	0.00	0.00	-0.12	0.00
			-0.02	0.00	0.00	0.00	0.02	0.00
total	0.16	0.00	-0.08	0.00	0.00	0.00	-0.13	0.00
			-0.02	0.00	0.00	0.00	0.02	0.00
			-0.03	0.00	0.00	0.00	-0.03	0.00
			0.02	0.00	0.00	0.00	-0.01	0.00
			0.01	0.00	0.00	0.00	-0.01	0.00
			-0.01	0.00	0.00	0.00	0.00	
					0.00	0.00		
					0.00	0.00		
					0.00	0.00		
					0.00	0.00		
					0.00	0.00		
comp.	0.16	0.00	0.09	0.00	0.00	0.00	0.13	0.00

basis	Δ_{oop}	δ_{oop}	B_{2u}	B_{1u}	A_{2u}	$E_g(x)$	$E_g(y)$	A_{1u}
min.	0.59	0.00	0.00	0.59	0.01	-0.02	-0.02	0.00
ext.	0.59	0.00	0.00	0.59	0.01	-0.02	-0.02	0.00
			0.00	0.00	0.00	-0.01	-0.01	0.00
total	0.59	0.00	0.00	0.59	0.01	-0.02	-0.02	0.00
			0.00	0.00	0.00	-0.01	-0.01	0.00
			0.00	0.01	0.00	0.00	0.00	
						0.00	0.00	
						0.00	0.00	
comp.	0.59	0.00	0.00	0.59	0.01	0.02	0.02	0.00

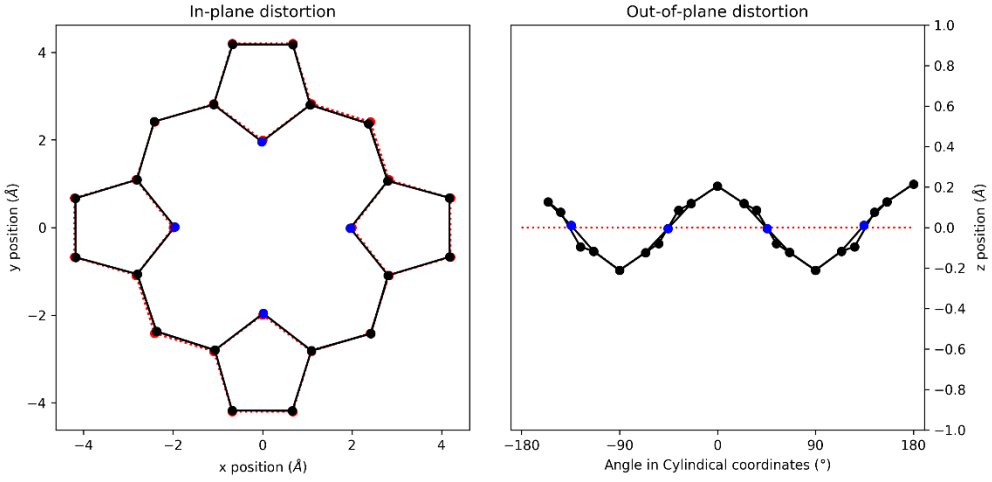


Figure S108: NSD result generated from **1:6** (in Å) (**A**) in-plane and (**B**) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

basis	Δ_{ip}	δ_{ip}	B_{2g}	B_{1g}	$E_u(x)$	$E_u(y)$	A_{1g}	A_{2g}
min.	0.26	0.00	-0.13	-0.04	-0.02	0.02	0.22	0.00
ext.	0.28	0.00	-0.13	-0.04	-0.02	0.02	0.22	0.00
			-0.01	-0.09	0.01	-0.02	0.00	0.00
total	0.29	0.00	-0.13	-0.04	-0.02	0.02	0.22	0.00
			-0.01	-0.09	0.01	-0.02	0.00	0.00
			-0.01	-0.06	0.00	0.00	0.04	0.00
			0.01	0.00	0.01	-0.01	0.00	0.00
			0.00	0.01	0.00	0.00	0.02	0.00
			-0.01	-0.01	0.00	0.00	0.01	
					0.00	0.00		
					0.00	0.00		
					0.00	0.00		
					0.00	0.00		
					0.00	0.00		
comp.	0.29	0.00	0.14	0.12	0.02	0.03	0.23	0.00

basis	Δ_{oop}	δ_{oop}	B_{2u}	B_{1u}	A_{2u}	$E_g(x)$	$E_g(y)$	A_{1u}
min.	0.08	0.00	0.00	-0.01	0.00	0.06	0.05	0.00
ext.	0.10	0.00	0.00	-0.01	0.00	0.06	0.06	0.00
			0.00	0.00	0.00	0.04	0.02	0.00
total	0.10	0.00	0.00	-0.01	0.00	0.06	0.06	0.00
			0.00	0.00	0.00	0.04	0.02	0.00
			0.00	0.00	0.00	0.00	0.00	
						0.00	0.00	
						0.00	0.00	
comp.	0.10	0.00	0.00	0.01	0.00	0.08	0.06	0.00

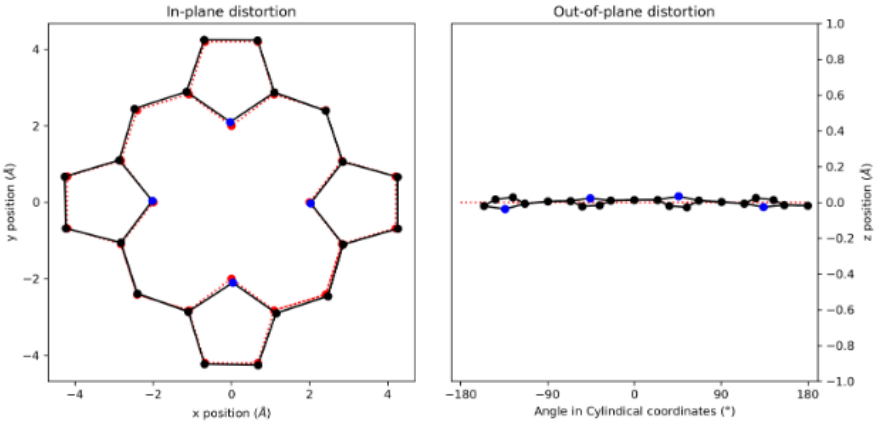


Figure S109: NSD result generated from 1:7 (in Å) (A) in-plane and (B) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

basis	Δ_{ip}	δ_{ip}	B_{2g}	B_{1g}	$E_u(x)$	$E_u(y)$	A_{1g}	A_{2g}
min.	0.19	0.00	0.04	0.00	0.02	0.02	-0.18	0.00
ext.	0.19	0.00	0.04	0.00	0.02	0.02	-0.18	0.00
			0.00	0.00	-0.01	-0.01	0.04	0.00
total	0.20	0.00	0.04	0.00	0.02	0.02	-0.18	0.00
			0.00	0.00	-0.01	-0.01	0.04	0.00
			0.01	0.00	-0.01	0.00	-0.02	0.00
			-0.01	0.00	-0.01	-0.01	-0.03	0.00
			0.00	0.00	0.00	0.00	0.00	0.00
			0.00	0.00	0.00	0.00	0.01	
					0.00	0.00		
					0.00	0.00		
					0.00	0.00		
					0.00	0.00		
					0.00	0.00		
comp.	0.20	0.00	0.04	0.00	0.03	0.03	0.19	0.00

basis	Δ_{oop}	δ_{oop}	B_{2u}	B_{1u}	A_{2u}	$E_g(x)$	$E_g(y)$	A_{1u}
min.	0.99	0.00	0.00	-0.99	0.01	-0.01	0.01	0.00
ext.	0.99	0.00	0.00	-0.99	0.01	-0.01	0.01	0.00
			0.00	0.00	0.00	-0.02	0.02	0.00
total	0.99	0.00	0.00	-0.99	0.01	-0.01	0.01	0.00
			0.00	0.00	0.00	-0.02	0.02	0.00
			0.00	-0.02	0.00	0.00	0.00	
						0.00	0.00	
						0.00	0.00	
comp.	0.99	0.00	0.00	0.99	0.01	0.02	0.02	0.00

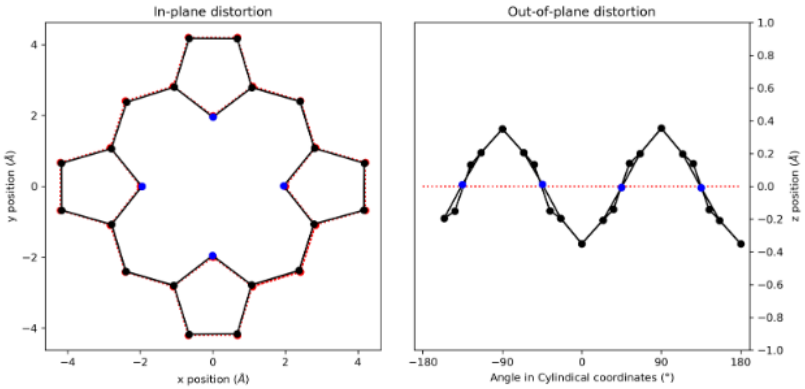


Figure S110: NSD result generated from 1:8 (in Å) (A) in-plane and (B) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

basis	Δ_{ip}	δ_{ip}	B_{2g}	B_{1g}	$E_u(x)$	$E_u(y)$	A_{1g}	A_{2g}
min.	0.23	0.00	-0.03	0.02	0.00	0.00	0.23	0.00
ext.	0.25	0.00	-0.03	0.02	0.00	0.00	0.23	0.00
			-0.02	0.09	0.00	0.00	0.01	0.00
total	0.26	0.00	-0.04	0.03	0.00	0.00	0.23	0.00
			-0.02	0.09	0.00	0.00	0.01	0.00
			0.02	0.06	0.00	0.00	0.04	0.00
			-0.01	0.00	0.00	0.00	0.00	0.00
			0.00	-0.01	0.00	0.00	0.02	0.00
			0.00	0.01	0.00	0.00	0.01	
					0.00	0.00		
					0.00	0.00		
					0.00	0.00		
					0.00	0.00		
					0.00	0.00		
comp.	0.26	0.00	0.05	0.11	0.00	0.00	0.24	0.00

basis	Δ_{oop}	δ_{oop}	B_{2u}	B_{1u}	A_{2u}	$E_g(x)$	$E_g(y)$	A_{1u}
min.	0.07	0.00	0.00	0.00	0.00	-0.04	0.05	0.00
ext.	0.08	0.00	0.00	0.00	0.00	-0.04	0.05	0.00
			0.00	0.00	0.00	-0.02	0.03	0.00
total	0.08	0.00	0.00	0.00	0.00	-0.04	0.05	0.00
			0.00	0.00	0.00	-0.02	0.03	0.00
			0.00	0.00	0.00	0.00	0.00	
						0.00	0.00	
						0.00	0.00	
comp.	0.08	0.00	0.00	0.00	0.00	0.05	0.06	0.00

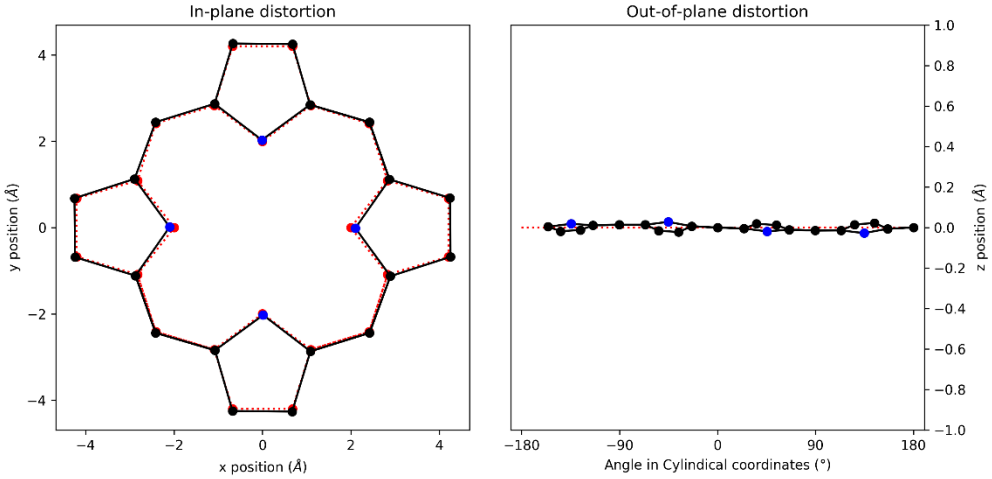


Figure S111: NSD result generated from **1:9** (in Å) (**A**) in-plane and (**B**) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

basis	Δ_{ip}	δ_{ip}	B_{2g}	B_{1g}	$E_u(x)$	$E_u(y)$	A_{1g}	A_{2g}
min.	0.24	0.00	-0.01	0.00	0.00	0.00	-0.24	0.00
ext.	0.26	0.00	-0.01	0.00	0.00	0.00	-0.24	0.00
			0.01	0.00	0.00	0.00	0.09	0.00
total	0.27	0.00	-0.01	0.00	0.00	0.00	-0.24	0.00
			0.01	0.00	0.00	0.00	0.09	0.00
			-0.02	0.00	0.00	0.00	-0.02	0.00
			0.01	0.00	0.00	0.00	-0.05	0.00
			0.00	0.00	0.00	0.00	0.00	0.00
			0.00	0.00	0.00	0.00	0.02	
					0.00	0.00		
					0.00	0.00		
					0.00	0.00		
					0.00	0.00		
					0.00	0.00		
comp.	0.27	0.00	0.03	0.00	0.01	0.01	0.26	0.00

basis	Δ_{oop}	δ_{oop}	B_{2u}	B_{1u}	A_{2u}	$E_g(x)$	$E_g(y)$	A_{1u}
min.	1.28	0.00	0.00	1.28	0.02	-0.02	-0.02	0.00
ext.	1.28	0.00	0.00	1.28	0.02	-0.02	-0.02	0.00
			0.00	0.00	-0.01	-0.01	-0.01	0.00
total	1.28	0.00	0.00	1.28	0.02	-0.02	-0.02	0.00
			0.00	0.00	-0.01	-0.01	-0.01	0.00
			0.00	0.02	0.00	0.00	0.00	
						0.00	0.00	
						0.00	0.00	
comp.	1.28	0.00	0.00	1.28	0.03	0.02	0.02	0.00

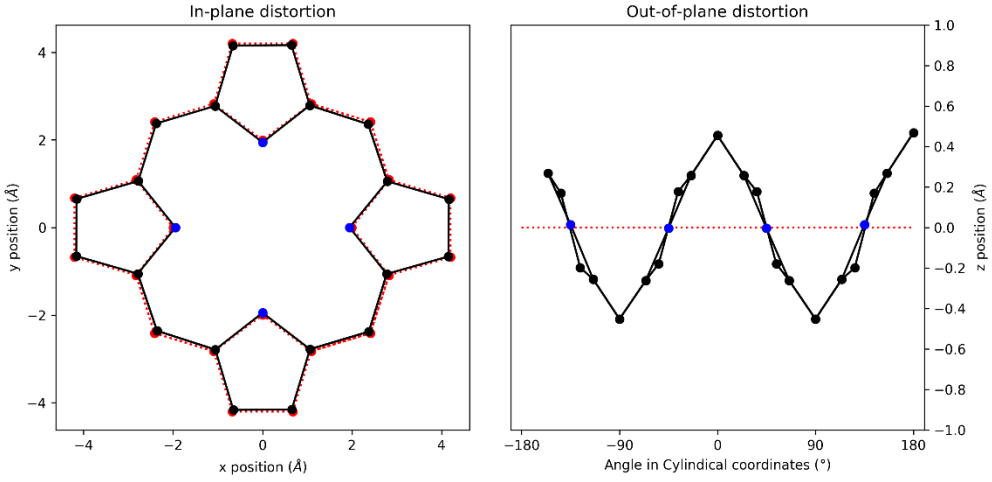


Figure S112: NSD result generated from **1:10** (in Å) (**A**) in-plane and (**B**) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

basis	Δ_{ip}	δ_{ip}	B_{2g}	B_{1g}	$E_u(x)$	$E_u(y)$	A_{1g}	A_{2g}
min.	0.24	0.00	0.09	0.04	-0.02	-0.03	0.22	0.00
ext.	0.26	0.00	0.09	0.04	-0.02	-0.03	0.22	0.00
			0.00	0.09	0.03	0.01	0.00	0.00
total	0.28	0.00	0.09	0.04	-0.02	-0.03	0.23	0.00
			0.00	0.09	0.03	0.01	0.00	0.00
			0.01	0.06	0.01	0.00	0.04	0.00
			-0.01	0.00	0.01	0.01	0.00	0.00
			0.00	-0.01	0.00	0.00	0.02	0.00
			0.01	0.01	0.00	0.00	0.01	
					0.00	0.00		
					0.00	0.00		
					0.00	0.00		
					0.00	0.00		
					0.00	0.00		
comp.	0.28	0.00	0.09	0.11	0.04	0.03	0.23	0.00

basis	Δ_{oop}	δ_{oop}	B_{2u}	B_{1u}	A_{2u}	$E_g(x)$	$E_g(y)$	A_{1u}
min.	0.08	0.00	0.00	0.01	0.00	-0.05	0.06	0.00
ext.	0.09	0.00	0.00	0.01	0.00	-0.05	0.06	0.00
			0.00	0.00	0.00	-0.02	0.04	0.00
total	0.09	0.00	0.00	0.01	0.00	-0.05	0.06	0.00
			0.00	0.00	0.00	-0.02	0.04	0.00
			0.00	0.00	0.00	0.00	0.00	
						0.00	0.00	
						0.00	0.00	
comp.	0.09	0.00	0.00	0.01	0.00	0.06	0.07	0.00

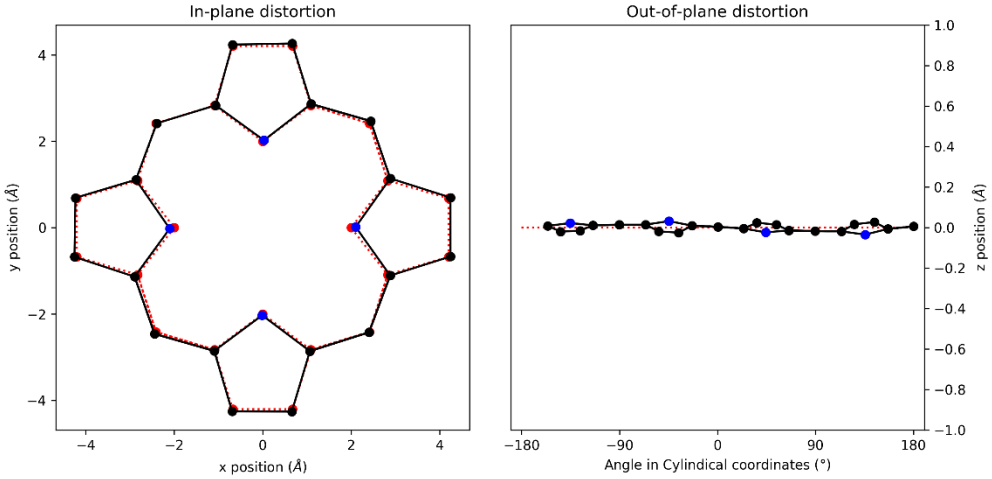


Figure S113: NSD result generated from **1D** (in Å) (**A**) in-plane and (**B**) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

basis	Δ_{ip}	δ_{ip}	B_{2g}	B_{1g}	$E_u(x)$	$E_u(y)$	A_{1g}	A_{2g}
min.	0.20	0.00	-0.03	0.00	0.02	-0.02	-0.20	0.00
ext.	0.21	0.00	-0.03	0.00	0.02	-0.02	-0.20	0.00
			0.00	0.00	-0.01	0.01	0.06	0.00
total	0.22	0.00	-0.03	0.00	0.02	-0.02	-0.20	0.00
			0.00	0.00	-0.01	0.01	0.06	0.00
			-0.02	0.00	0.00	0.00	-0.02	0.00
			0.01	0.00	-0.01	0.01	-0.04	0.00
			0.00	0.00	0.00	0.00	0.00	0.00
			-0.01	0.00	0.00	0.00	0.02	
					0.00	0.00		
					0.00	0.00		
					0.00	0.00		
					0.00	0.00		
					0.00	0.00		
comp.	0.22	0.00	0.03	0.00	0.02	0.02	0.21	0.00

basis	Δ_{oop}	δ_{oop}	B_{2u}	B_{1u}	A_{2u}	$E_g(x)$	$E_g(y)$	A_{1u}
min.	1.09	0.00	0.00	-1.09	-0.02	0.03	0.03	0.00
ext.	1.09	0.00	0.00	-1.09	-0.02	0.03	0.03	0.00
			0.00	0.00	0.01	0.00	0.00	0.00
total	1.09	0.00	0.00	-1.09	-0.02	0.03	0.03	0.00
			0.00	0.00	0.01	0.00	0.00	0.00
			0.00	-0.02	0.00	0.00	0.00	
						0.00	0.00	
						0.00	0.00	
comp.	1.09	0.00	0.00	1.09	0.02	0.03	0.03	0.00

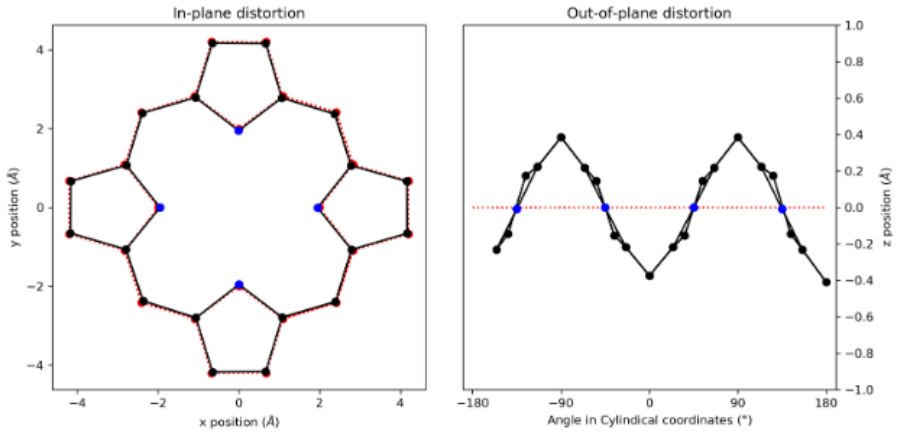


Figure S114: NSD result generated from 2D (in Å) (A) in-plane and (B) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

basis	Δ_{ip}	δ_{ip}	B_{2g}	B_{1g}	$E_u(x)$	$E_u(y)$	A_{1g}	A_{2g}
min.	0.26	0.00	-0.11	0.02	0.00	0.00	0.23	0.00
ext.	0.28	0.00	-0.11	0.02	0.00	0.00	0.23	0.00
			-0.04	0.08	0.00	0.00	0.01	0.00
total	0.29	0.00	-0.11	0.03	0.00	0.00	0.24	0.00
			-0.04	0.09	0.00	0.00	0.01	0.00
			0.02	0.06	0.00	0.00	0.04	0.00
			-0.02	0.00	0.00	0.00	0.00	0.00
			-0.01	-0.01	0.00	0.00	0.02	0.00
			0.00	0.01	0.00	0.00	0.01	
					0.00	0.00		
					0.00	0.00		
					0.00	0.00		
					0.00	0.00		
					0.00	0.00		
comp.	0.29	0.00	0.13	0.11	0.00	0.00	0.24	0.00

basis	Δ_{oop}	δ_{oop}	B_{2u}	B_{1u}	A_{2u}	$E_g(x)$	$E_g(y)$	A_{1u}
min.	0.05	0.00	0.00	0.00	0.00	-0.03	0.04	0.00
ext.	0.06	0.00	0.00	0.00	0.00	-0.03	0.04	0.00
			0.00	0.00	0.00	-0.01	0.02	0.00
total	0.06	0.00	0.00	0.00	0.00	-0.03	0.04	0.00
			0.00	0.00	0.00	-0.01	0.02	0.00
			0.00	0.00	0.00	0.00	0.00	
						0.00	0.00	
						0.00	0.00	
comp.	0.06	0.00	0.00	0.00	0.00	0.04	0.04	0.00

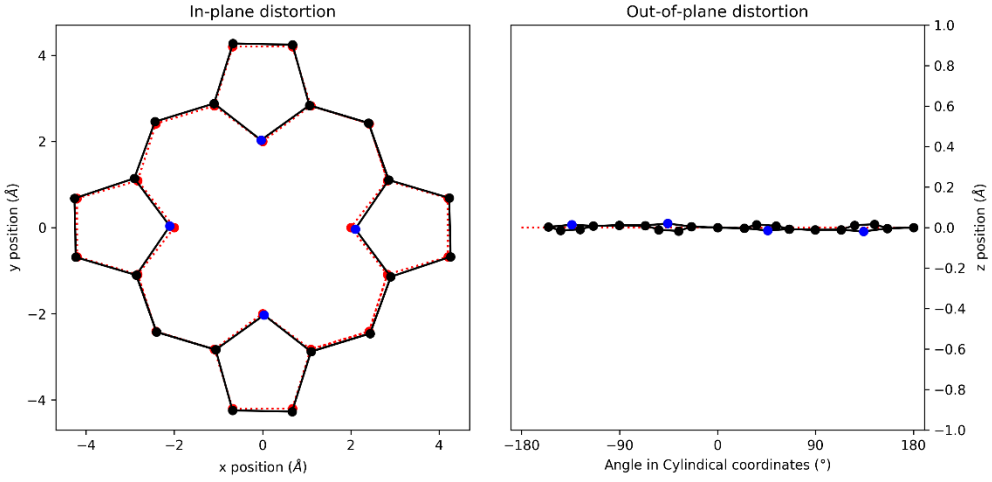


Figure S115: NSD result generated from **1:11** (in Å) (**A**) in-plane and (**B**) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

basis	Δ_{ip}	δ_{ip}	B_{2g}	B_{1g}	$E_u(x)$	$E_u(y)$	A_{1g}	A_{2g}
min.	0.27	0.00	0.00	0.00	0.01	0.00	-0.27	0.00
ext.	0.29	0.00	0.00	0.00	0.01	0.00	-0.27	0.00
			-0.02	0.00	-0.01	-0.01	0.11	0.00
total	0.30	0.00	0.00	0.00	0.01	0.00	-0.27	0.00
			-0.02	0.00	-0.01	-0.01	0.11	0.00
			0.02	0.00	0.00	0.00	-0.01	0.00
			-0.01	0.00	0.00	0.00	-0.07	0.00
			0.00	0.00	0.00	0.00	0.00	0.00
			0.01	0.00	0.00	0.00	0.03	
					0.00	0.00		
					0.00	0.00		
					0.00	0.00		
					0.00	0.00		
					0.00	0.00		
comp.	0.30	0.00	0.04	0.00	0.01	0.01	0.30	0.00

basis	Δ_{oop}	δ_{oop}	B_{2u}	B_{1u}	A_{2u}	$E_g(x)$	$E_g(y)$	A_{1u}
min.	1.41	0.00	0.00	-1.41	0.03	-0.02	0.02	0.00
ext.	1.41	0.00	0.00	-1.41	0.03	-0.02	0.02	0.00
			0.00	0.00	-0.02	-0.01	0.01	0.00
total	1.41	0.00	0.00	-1.41	0.03	-0.02	0.02	0.00
			0.00	0.00	-0.02	-0.01	0.01	0.00
			0.00	-0.02	0.00	0.00	0.00	
						0.00	0.00	
						0.00	0.00	
comp.	1.41	0.00	0.00	1.41	0.03	0.02	0.02	0.00

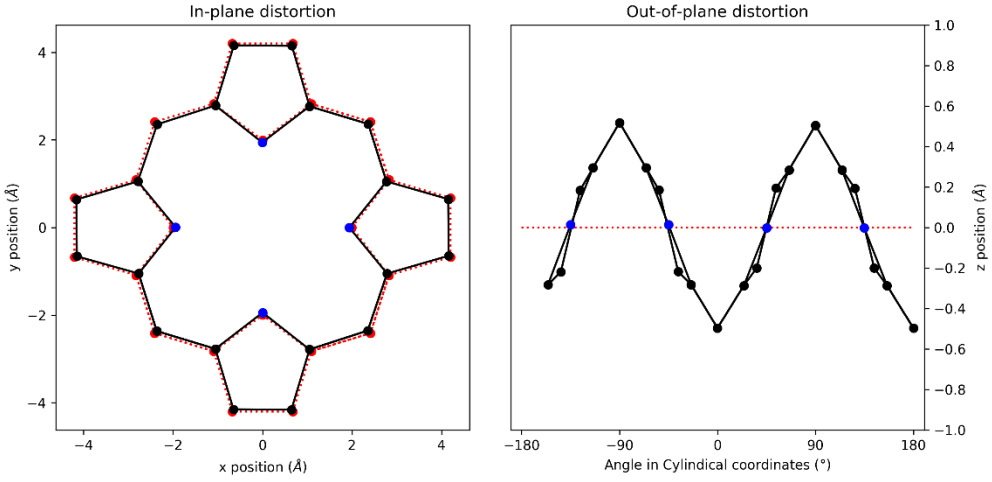


Figure S116: NSD result generated from **1:12** (in Å) (**A**) in-plane and (**B**) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

basis	Δ_{ip}	δ_{ip}	B_{2g}	B_{1g}	$E_u(x)$	$E_u(y)$	A_{1g}	A_{2g}
min.	0.23	0.00	-0.02	-0.04	0.03	-0.03	0.23	0.00
ext.	0.25	0.00	-0.02	-0.04	0.03	-0.03	0.23	0.00
			0.01	-0.09	-0.02	0.03	0.00	0.00
total	0.27	0.00	-0.02	-0.04	0.03	-0.03	0.23	0.00
			0.01	-0.09	-0.02	0.03	0.00	0.00
			-0.01	-0.06	0.00	0.01	0.04	0.00
			0.01	0.00	0.00	0.00	0.00	0.00
			0.00	0.01	0.00	0.00	0.02	0.00
			-0.01	-0.01	0.00	0.00	0.01	
					0.00	0.00		
					0.00	0.00		
					0.00	0.00		
					0.00	0.00		
					0.00	0.00		
comp.	0.27	0.00	0.03	0.12	0.04	0.04	0.23	0.00

basis	Δ_{oop}	δ_{oop}	B_{2u}	B_{1u}	A_{2u}	$E_g(x)$	$E_g(y)$	A_{1u}
min.	0.07	0.00	0.00	-0.01	0.00	-0.06	-0.05	0.00
ext.	0.09	0.00	0.00	-0.01	0.00	-0.06	-0.05	0.00
			0.00	0.00	0.00	-0.04	-0.02	0.00
total	0.09	0.00	0.00	-0.01	0.00	-0.06	-0.05	0.00
			0.00	0.00	0.00	-0.04	-0.02	0.00
			0.00	0.00	0.00	0.00	0.00	
						0.00	0.00	
						0.00	0.00	
comp.	0.09	0.00	0.00	0.01	0.00	0.07	0.05	0.00

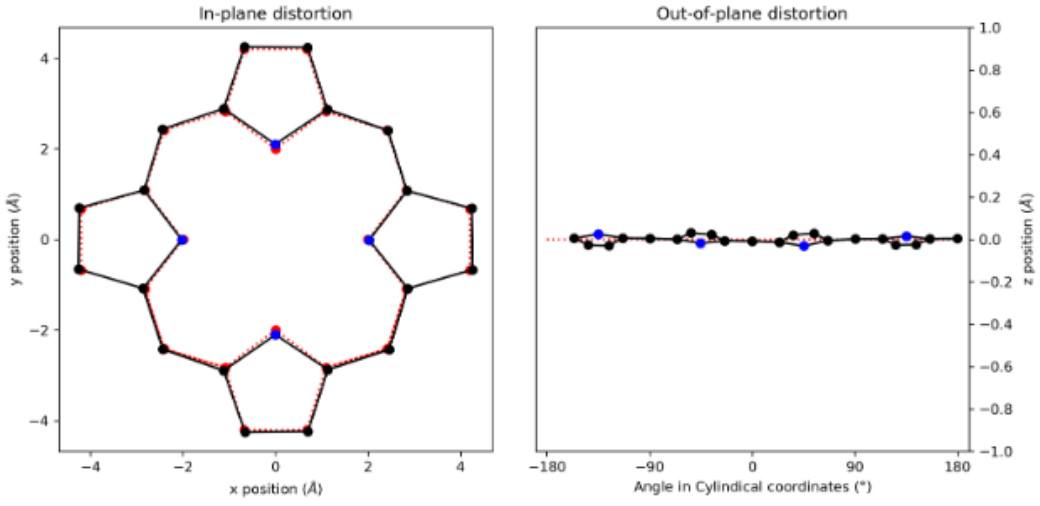


Figure S117: NSD result generated from 3D (in Å) (A) in-plane and (B) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

basis	Δ_{ip}	δ_{ip}	B_{2g}	B_{1g}	$E_u(x)$	$E_u(y)$	A_{1g}	A_{2g}
min.	0.24	0.00	-0.02	0.00	-0.02	0.02	-0.24	0.00
ext.	0.26	0.00	-0.02	0.00	-0.02	0.02	-0.24	0.00
			0.01	0.00	0.02	-0.02	0.08	0.00
total	0.26	0.00	-0.02	0.00	-0.02	0.02	-0.24	0.00
			0.01	0.00	0.02	-0.02	0.08	0.00
			-0.01	0.00	0.01	-0.01	-0.02	0.00
			0.01	0.00	0.01	-0.01	-0.05	0.00
			0.00	0.00	0.00	0.00	0.00	0.00
			-0.01	0.00	0.00	0.00	0.02	
					0.00	0.00		
					0.00	0.00		
					0.00	0.00		
					0.00	0.00		
					0.00	0.00		
comp.	0.26	0.00	0.02	0.00	0.04	0.03	0.26	0.00

basis	Δ_{oop}	δ_{oop}	B_{2u}	B_{1u}	A_{2u}	$E_g(x)$	$E_g(y)$	A_{1u}
min.	1.26	0.00	0.00	1.26	0.03	0.00	0.00	0.00
ext.	1.27	0.00	0.00	1.26	0.03	0.00	0.00	0.00
			0.00	0.00	-0.01	-0.03	-0.03	0.00
total	1.27	0.00	0.00	1.26	0.03	0.00	0.00	0.00
			0.00	0.00	-0.01	-0.03	-0.03	0.00
			0.00	0.02	0.00	0.00	-0.01	
						0.00	0.00	
						0.00	0.00	
comp.	1.27	0.00	0.00	1.26	0.03	0.03	0.03	0.00

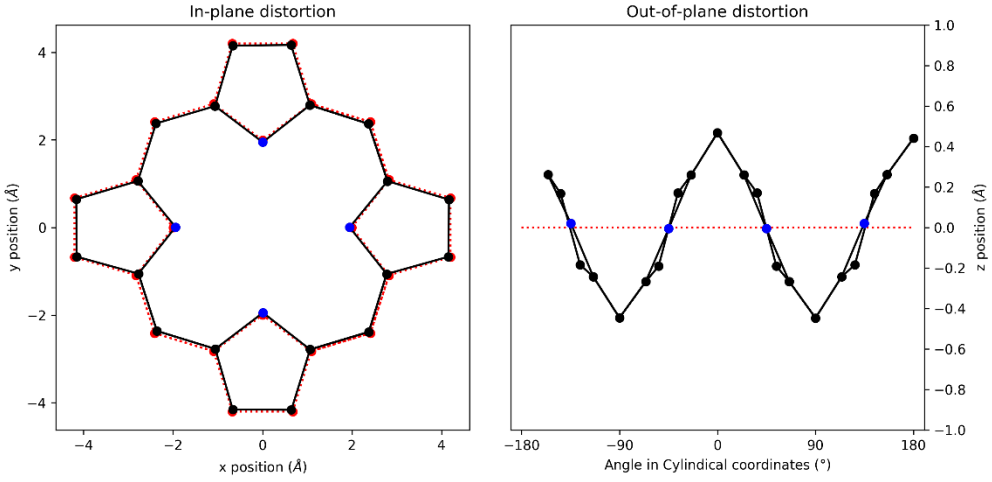


Figure S118: NSD result generated from **1:13** (in Å) (**A**) in-plane and (**B**) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

basis	Δ_{ip}	δ_{ip}	B_{2g}	B_{1g}	$E_u(x)$	$E_u(y)$	A_{1g}	A_{2g}
min.	0.33	0.00	-0.22	0.02	0.00	0.00	0.24	0.00
ext.	0.35	0.00	-0.22	0.02	0.00	0.00	0.24	0.00
			-0.07	0.08	0.00	0.00	0.00	0.00
total	0.36	0.00	-0.22	0.02	0.00	0.00	0.25	0.00
			-0.07	0.09	0.00	0.00	0.00	0.00
			0.02	0.06	0.00	0.00	0.04	0.00
			-0.02	0.00	0.00	0.00	0.00	0.00
			-0.01	-0.01	0.00	0.00	0.02	0.00
			0.00	0.01	0.00	0.00	0.01	
					0.00	0.00		
					0.00	0.00		
					0.00	0.00		
					0.00	0.00		
					0.00	0.00		
comp.	0.36	0.00	0.24	0.11	0.00	0.00	0.25	0.01

basis	Δ_{oop}	δ_{oop}	B_{2u}	B_{1u}	A_{2u}	$E_g(x)$	$E_g(y)$	A_{1u}
min.	0.02	0.00	0.00	0.00	0.00	-0.01	0.01	0.00
ext.	0.02	0.00	0.00	0.00	0.00	-0.01	0.01	0.00
			0.00	0.00	0.00	0.00	0.01	0.00
total	0.02	0.00	0.00	0.00	0.00	-0.01	0.01	0.00
			0.00	0.00	0.00	0.00	0.01	0.00
			0.00	0.00	0.00	0.00	0.00	
						0.00	0.00	
						0.00	0.00	
comp.	0.02	0.00	0.00	0.00	0.00	0.01	0.01	0.00

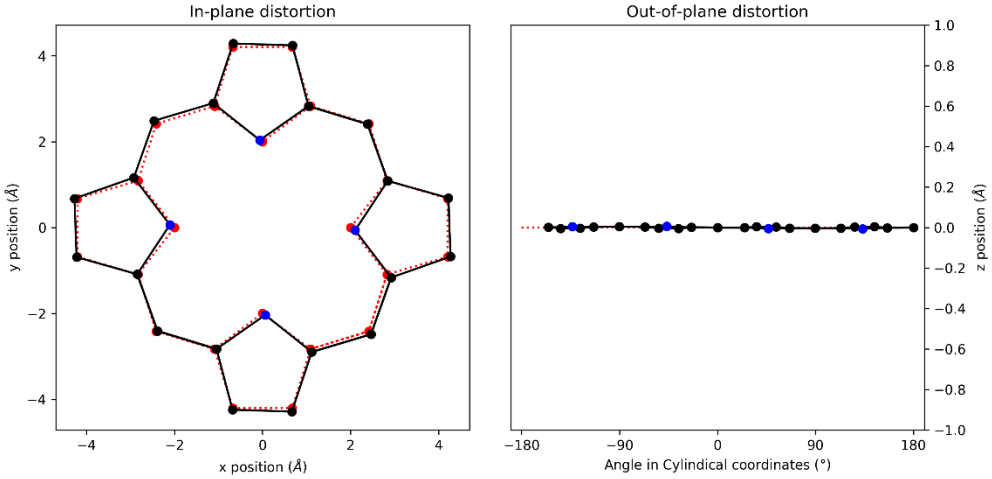


Figure S119: NSD result generated from **1:14** (in Å) (**A**) in-plane and (**B**) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

basis	Δ_{ip}	δ_{ip}	B_{2g}	B_{1g}	$E_u(x)$	$E_u(y)$	A_{1g}	A_{2g}
min.	0.31	0.01	-0.02	0.00	0.01	0.01	-0.31	0.00
ext.	0.34	0.00	-0.02	0.00	0.01	0.01	-0.31	0.00
			-0.03	0.00	-0.01	-0.01	0.13	0.00
total	0.35	0.00	-0.02	0.00	0.01	0.01	-0.31	0.00
			-0.03	0.00	-0.01	-0.01	0.13	0.00
			0.02	0.00	0.00	0.00	-0.01	0.00
			-0.01	0.00	0.00	0.00	-0.08	0.00
			0.00	0.00	0.00	0.00	0.00	0.00
			0.01	0.00	0.00	0.00	0.04	
					0.00	0.00		
					0.00	0.00		
					0.00	0.00		
					0.00	0.00		
					0.00	0.00		
comp.	0.35	0.00	0.05	0.00	0.01	0.01	0.35	0.00

basis	Δ_{oop}	δ_{oop}	B_{2u}	B_{1u}	A_{2u}	$E_g(x)$	$E_g(y)$	A_{1u}
min.	1.56	0.00	0.00	-1.55	0.04	-0.02	0.02	0.00
ext.	1.56	0.00	0.00	-1.55	0.04	-0.02	0.02	0.00
			0.00	0.00	-0.03	-0.01	0.01	0.00
total	1.56	0.00	0.00	-1.55	0.04	-0.02	0.02	0.00
			0.00	0.00	-0.03	-0.01	0.01	0.00
			0.00	-0.03	0.00	0.00	0.00	
						0.00	0.00	
						0.00	0.00	
comp.	1.56	0.00	0.00	1.56	0.05	0.02	0.02	0.00

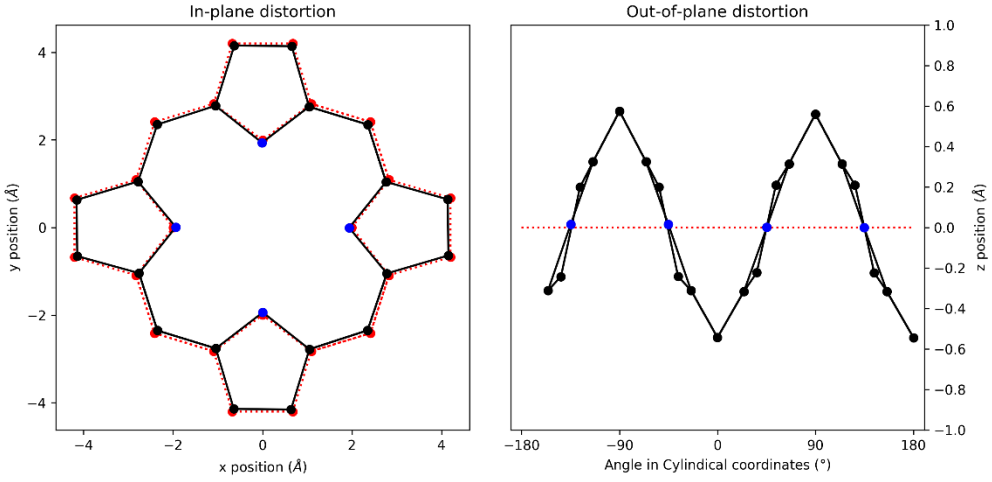


Figure S120: NSD result generated from **1:15** (in Å) (**A**) in-plane and (**B**) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

NSD tables and plots for DFT structures series 2

basis	Δ_{ip}	δ_{ip}	B_{2g}	B_{1g}	$E_u(x)$	$E_u(y)$	A_{1g}	A_{2g}
min.	0.28	0.00	-0.18	0.06	0.00	-0.01	0.21	0.00
ext.	0.30	0.00	-0.18	0.06	0.00	-0.01	0.21	0.00
			-0.03	0.09	0.02	0.01	0.01	0.00
total	0.31	0.00	-0.18	0.06	0.00	-0.01	0.21	0.00
			-0.03	0.09	0.02	0.01	0.01	0.00
			0.00	0.06	0.00	0.00	0.05	0.00
			0.00	0.00	0.00	0.00	0.01	0.00
			0.00	-0.01	0.00	0.00	0.02	0.00
			0.00	0.01	0.00	0.00	0.01	
					0.00	0.00		
					0.00	0.00		
					0.00	0.00		
					0.00	0.00		
					0.00	0.00		
comp.	0.31	0.00	0.18	0.13	0.02	0.02	0.22	0.00

basis	Δ_{oop}	δ_{oop}	B_{2u}	B_{1u}	A_{2u}	$E_g(x)$	$E_g(y)$	A_{1u}
min.	0.07	0.00	-0.06	-0.01	0.00	-0.03	-0.03	0.00
ext.	0.08	0.00	-0.05	-0.01	0.00	-0.03	-0.03	0.00
			0.02	0.00	0.00	-0.01	-0.02	0.00
total	0.08	0.00	-0.05	-0.01	0.00	-0.03	-0.03	0.00
			0.02	0.00	0.00	-0.01	-0.02	0.00
			0.00	0.00	0.00	0.00	0.00	
						0.00	0.00	
						0.00	0.00	
comp.	0.08	0.00	0.06	0.01	0.00	0.03	0.04	0.00

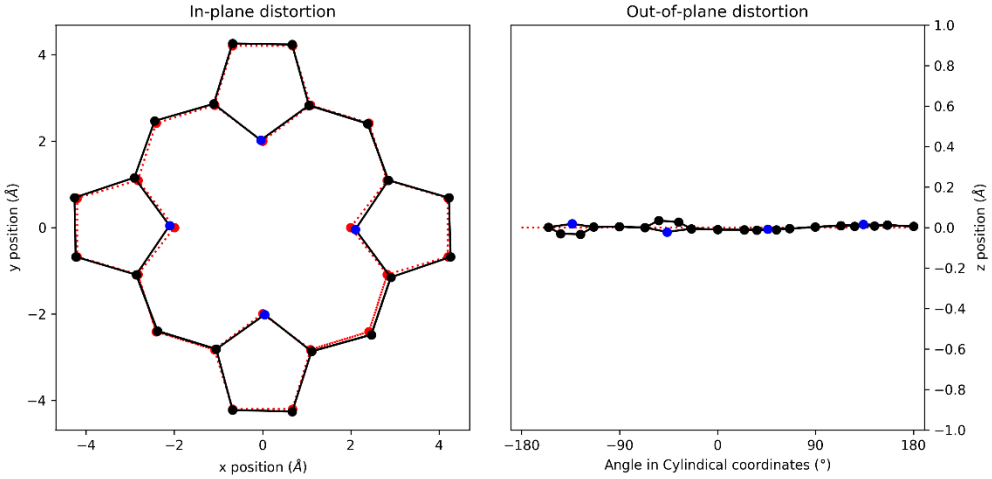


Figure S121: NSD result generated from **2:1** (in Å) (**A**) in-plane and (**B**) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

basis	Δ_{ip}	δ_{ip}	B_{2g}	B_{1g}	$E_u(x)$	$E_u(y)$	A_{1g}	A_{2g}
min.	0.24	0.00	0.06	0.04	0.02	-0.03	0.22	0.00
ext.	0.25	0.00	0.07	0.04	0.02	-0.03	0.22	0.00
			0.02	0.09	0.00	0.03	0.01	0.00
total	0.27	0.00	0.07	0.05	0.01	-0.03	0.22	0.00
			0.02	0.09	0.00	0.03	0.01	0.00
			-0.01	0.06	-0.01	0.00	0.05	0.00
			0.01	0.00	-0.01	0.00	0.01	0.00
			0.00	-0.01	0.00	0.00	0.02	0.00
			0.00	0.01	0.00	0.00	0.01	
					0.00	0.00		
					0.00	0.00		
					0.00	0.00		
					0.00	0.00		
					0.00	0.00		
comp.	0.27	0.00	0.07	0.12	0.02	0.04	0.23	0.00

basis	Δ_{oop}	δ_{oop}	B_{2u}	B_{1u}	A_{2u}	$E_g(x)$	$E_g(y)$	A_{1u}
min.	0.06	0.00	-0.05	0.00	0.00	-0.02	-0.02	0.00
ext.	0.07	0.00	-0.05	0.00	0.00	-0.03	-0.02	0.00
			0.02	0.00	0.00	-0.01	-0.02	0.00
total	0.07	0.00	-0.05	0.00	0.00	-0.03	-0.02	0.00
			0.02	0.00	0.00	-0.01	-0.02	0.00
			0.00	0.00	0.00	0.00	0.00	
						0.00	0.00	
						0.00	0.00	
comp.	0.07	0.00	0.06	0.00	0.00	0.03	0.03	0.00

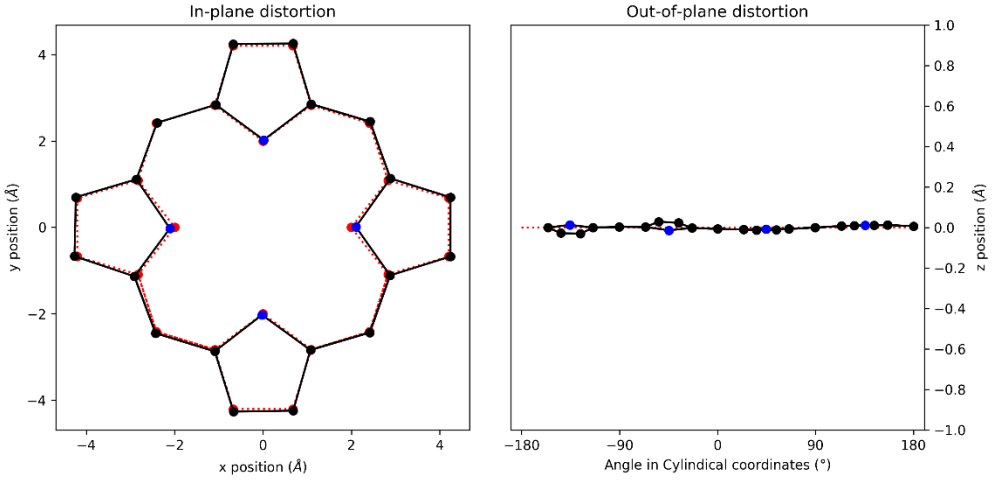


Figure S122: NSD result generated from **2:2** (in Å) (**A**) in-plane and (**B**) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

basis	Δ_{ip}	δ_{ip}	B_{2g}	B_{1g}	$E_u(x)$	$E_u(y)$	A_{1g}	A_{2g}
min.	0.28	0.00	-0.14	0.03	0.04	-0.01	0.23	0.00
ext.	0.29	0.00	-0.14	0.03	0.04	-0.01	0.23	0.00
			-0.02	0.09	-0.03	0.02	0.02	0.00
total	0.31	0.00	-0.14	0.04	0.04	-0.01	0.24	0.00
			-0.02	0.09	-0.03	0.02	0.02	0.00
			0.00	0.06	-0.01	0.00	0.05	0.00
			0.00	0.00	-0.02	0.00	0.00	0.00
			0.00	-0.01	0.00	0.00	0.02	0.00
			0.00	0.01	0.00	0.00	0.01	
					0.00	0.00		
					0.00	0.00		
					0.00	0.00		
					0.00	0.00		
					0.00	0.00		
comp.	0.31	0.00	0.14	0.11	0.05	0.02	0.24	0.00

basis	Δ_{oop}	δ_{oop}	B_{2u}	B_{1u}	A_{2u}	$E_g(x)$	$E_g(y)$	A_{1u}
min.	0.08	0.00	-0.07	-0.01	0.00	-0.03	-0.03	0.00
ext.	0.09	0.00	-0.07	-0.01	0.00	-0.03	-0.03	0.00
			0.02	0.00	0.00	-0.01	-0.02	0.00
total	0.09	0.00	-0.07	-0.01	0.00	-0.03	-0.03	0.00
			0.02	0.00	0.00	-0.01	-0.02	0.00
			0.00	0.00	0.00	0.00	0.00	
						0.00	0.00	
						0.00	0.00	
comp.	0.09	0.00	0.08	0.01	0.00	0.03	0.03	0.00

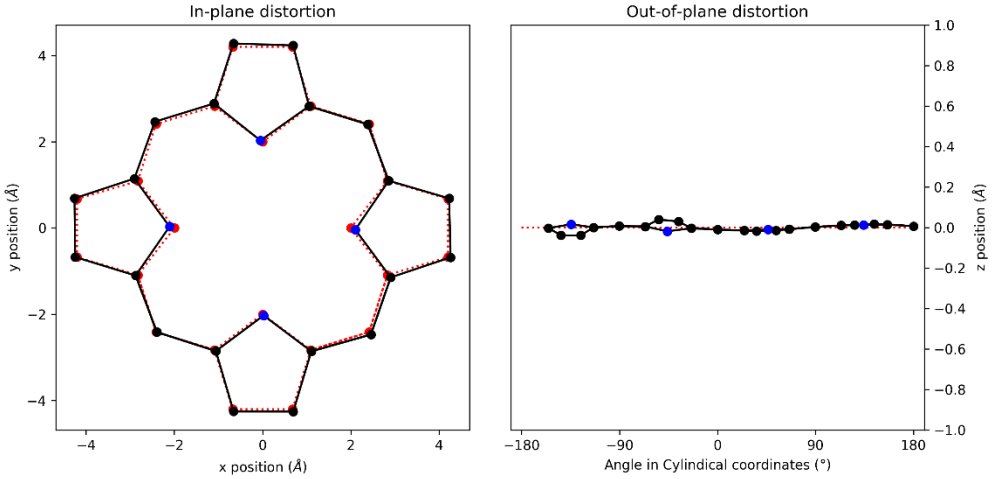


Figure S123: NSD result generated from **2:3** (in Å) (**A**) in-plane and (**B**) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

basis	Δ_{ip}	δ_{ip}	B_{2g}	B_{1g}	$E_u(x)$	$E_u(y)$	A_{1g}	A_{2g}
min.	0.26	0.00	0.06	0.02	0.02	0.02	0.25	0.00
ext.	0.27	0.00	0.06	0.02	0.02	0.02	0.25	0.00
			0.02	0.09	0.00	0.00	0.02	0.00
total	0.29	0.00	0.06	0.02	0.02	0.02	0.25	0.00
			0.02	0.09	-0.01	0.00	0.02	0.00
			-0.01	0.06	-0.01	0.00	0.05	0.00
			0.01	0.00	-0.01	-0.01	0.00	0.00
			0.00	-0.01	0.00	0.00	0.01	0.00
			0.00	0.01	0.00	0.00	0.01	
					0.00	0.00		
					0.00	0.00		
					0.00	0.00		
					0.00	0.00		
					0.00	0.00		
comp.	0.29	0.00	0.07	0.11	0.02	0.02	0.26	0.00

basis	Δ_{oop}	δ_{oop}	B_{2u}	B_{1u}	A_{2u}	$E_g(x)$	$E_g(y)$	A_{1u}
min.	0.07	0.00	-0.07	0.00	0.00	-0.02	-0.02	0.00
ext.	0.07	0.00	-0.06	0.00	0.00	-0.02	-0.02	0.00
			0.01	0.00	0.00	-0.01	-0.01	0.00
total	0.07	0.00	-0.06	0.00	0.00	-0.02	-0.02	0.00
			0.01	0.00	0.00	-0.01	-0.01	0.00
			0.00	0.00	0.00	0.00	0.00	
						0.00	0.00	
						0.00	0.00	
comp.	0.07	0.00	0.07	0.00	0.00	0.02	0.03	0.00

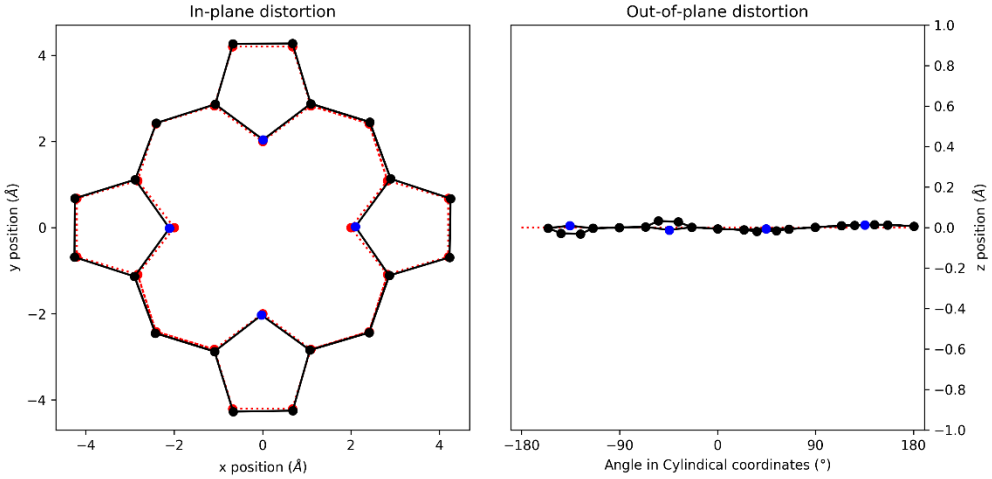


Figure S124: NSD result generated from **2:4** (in Å) (**A**) in-plane and (**B**) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

basis	Δ_{ip}	δ_{ip}	B_{2g}	B_{1g}	$E_u(x)$	$E_u(y)$	A_{1g}	A_{2g}
min.	0.30	0.00	0.20	0.03	0.01	-0.02	0.22	0.00
ext.	0.32	0.00	0.20	0.03	0.01	-0.02	0.22	0.00
			0.04	0.09	0.02	0.01	0.00	0.00
total	0.33	0.00	0.21	0.04	0.01	-0.02	0.22	0.00
			0.04	0.09	0.02	0.01	0.00	0.00
			-0.01	0.06	-0.01	0.00	0.04	0.00
			0.01	0.00	-0.01	0.01	0.00	0.00
			0.00	-0.01	0.00	0.00	0.02	0.00
			0.00	0.01	-0.01	0.00	0.01	
					0.00	0.00		
					0.00	0.00		
					0.00	0.00		
					0.00	0.00		
					0.00	0.00		
comp.	0.33	0.00	0.21	0.11	0.03	0.03	0.23	0.00

basis	Δ_{oop}	δ_{oop}	B_{2u}	B_{1u}	A_{2u}	$E_g(x)$	$E_g(y)$	A_{1u}
min.	0.14	0.00	-0.12	0.00	0.01	0.00	-0.06	0.00
ext.	0.15	0.00	-0.12	0.00	0.01	0.00	-0.06	0.00
			0.04	0.00	0.00	0.00	-0.04	0.00
total	0.15	0.00	-0.12	0.00	0.01	0.00	-0.06	0.00
			0.04	0.00	0.00	0.00	-0.04	0.00
			0.00	0.00	0.00	0.00	0.00	
						0.00	0.00	
						0.00	0.00	
comp.	0.15	0.00	0.13	0.00	0.01	0.01	0.07	0.00

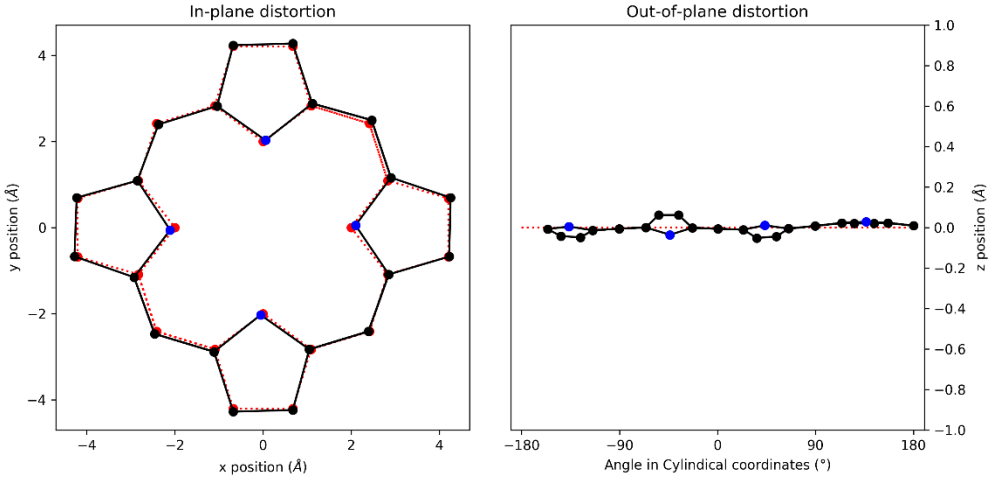


Figure S125: NSD result generated from **2:5** (in Å) (**A**) in-plane and (**B**) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

basis	Δ_{ip}	δ_{ip}	B_{2g}	B_{1g}	$E_u(x)$	$E_u(y)$	A_{1g}	A_{2g}
min.	0.24	0.00	0.00	0.02	0.03	0.00	0.24	0.00
ext.	0.25	0.00	0.00	0.02	0.03	0.00	0.24	0.00
			0.00	0.08	-0.01	0.00	0.01	0.00
total	0.27	0.00	0.00	0.02	0.03	0.00	0.24	0.00
			0.00	0.09	-0.01	0.00	0.01	0.00
			0.00	0.06	-0.01	0.00	0.04	0.00
			0.00	0.00	-0.02	0.00	0.00	0.00
			0.00	-0.01	0.00	0.00	0.02	0.00
			0.00	0.01	-0.01	0.00	0.01	
					0.00	0.00		
					-0.01	0.00		
					-0.01	0.00		
					0.00	0.00		
					0.01	0.00		
comp.	0.27	0.00	0.00	0.11	0.04	0.00	0.24	0.00

basis	Δ_{oop}	δ_{oop}	B_{2u}	B_{1u}	A_{2u}	$E_g(x)$	$E_g(y)$	A_{1u}
min.	0.17	0.00	-0.16	0.00	0.01	0.00	-0.06	0.00
ext.	0.18	0.00	-0.16	0.00	0.01	0.00	-0.06	0.00
			0.04	0.00	-0.01	0.00	-0.03	0.00
total	0.18	0.00	-0.16	0.00	0.01	0.00	-0.06	0.00
			0.04	0.00	-0.01	0.00	-0.03	0.00
			0.00	0.00	0.00	0.00	0.00	
						0.00	0.00	
						0.00	0.00	
comp.	0.18	0.00	0.17	0.00	0.01	0.00	0.07	0.00

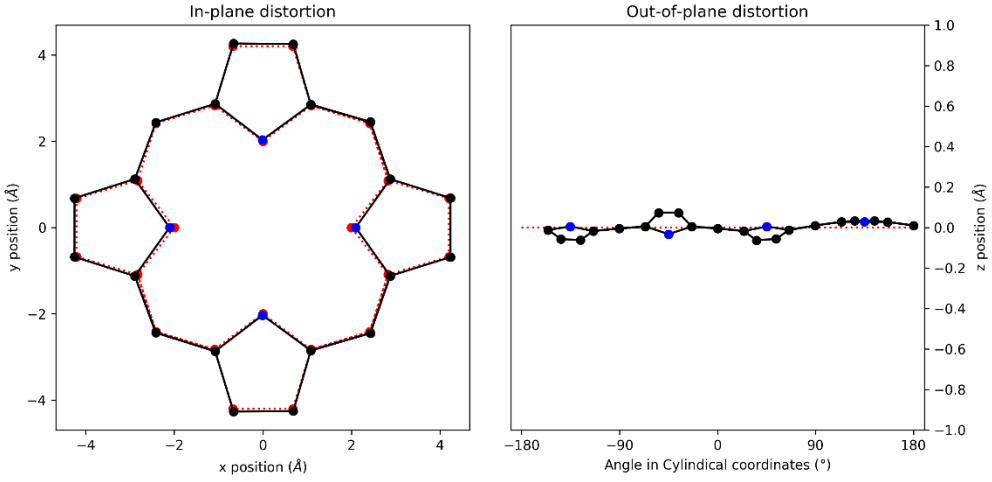


Figure S126: NSD result generated from **2:6** (in Å) (**A**) in-plane and (**B**) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

NSD tables and plots for DFT structures series 3

basis	Δ_{ip}	δ_{ip}	B_{2g}	B_{1g}	$E_u(x)$	$E_u(y)$	A_{1g}	A_{2g}
min.	0.21	0.00	0.00	0.03	-0.01	0.00	0.21	0.00
ext.	0.23	0.00	0.00	0.04	-0.01	0.00	0.21	0.00
			0.00	0.09	0.03	0.00	0.02	0.00
total	0.26	0.00	0.00	0.04	-0.01	0.00	0.21	0.00
			0.00	0.09	0.03	0.00	0.02	0.00
			0.00	0.06	0.00	0.00	0.04	0.00
			0.00	0.00	-0.04	0.00	0.01	0.00
			0.00	-0.01	0.02	0.00	0.02	0.00
			0.00	0.01	-0.01	0.00	0.00	
					0.00	0.00		
					0.00	0.00		
					-0.02	0.00		
					0.01	0.00		
					-0.03	0.00		
comp.	0.26	0.00	0.00	0.11	0.06	0.00	0.22	0.00

basis	Δ_{oop}	δ_{oop}	B_{2u}	B_{1u}	A_{2u}	$E_g(x)$	$E_g(y)$	A_{1u}
min.	0.13	0.00	-0.11	0.00	0.02	0.00	-0.06	0.00
ext.	0.14	0.00	-0.11	0.00	0.02	0.00	-0.06	0.00
			0.04	0.00	-0.01	0.00	-0.04	0.00
total	0.14	0.00	-0.11	0.00	0.02	0.00	-0.06	0.00
			0.04	0.00	-0.01	0.00	-0.04	0.00
			0.00	0.00	0.00	0.00	0.00	
						0.00	0.00	
						0.00	0.00	
comp.	0.14	0.00	0.11	0.00	0.02	0.00	0.07	0.00

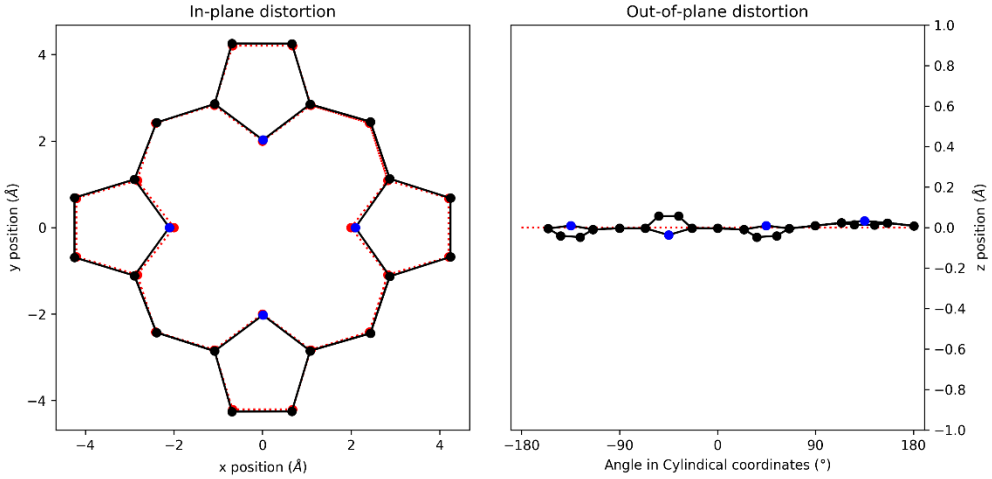


Figure S127: NSD result generated from **3:1** (in Å) (**A**) in-plane and (**B**) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

basis	Δ_{ip}	δ_{ip}	B_{2g}	B_{1g}	$E_u(x)$	$E_u(y)$	A_{1g}	A_{2g}
min.	0.23	0.00	0.00	0.02	0.02	0.00	0.23	0.00
ext.	0.25	0.00	0.00	0.02	0.02	0.00	0.23	0.00
			0.00	0.09	0.00	0.00	0.01	0.00
total	0.26	0.00	0.00	0.03	0.02	0.00	0.23	0.00
			0.00	0.09	0.00	0.00	0.01	0.00
			0.00	0.06	-0.01	0.00	0.04	0.00
			0.00	0.00	-0.02	0.00	0.00	0.00
			0.00	-0.01	0.01	0.00	0.02	0.00
			0.00	0.01	-0.01	0.00	0.01	
					0.00	0.00		
					0.00	0.00		
					-0.01	0.00		
					0.00	0.00		
					0.00	0.00		
comp.	0.26	0.00	0.00	0.11	0.03	0.00	0.24	0.00

basis	Δ_{oop}	δ_{oop}	B_{2u}	B_{1u}	A_{2u}	$E_g(x)$	$E_g(y)$	A_{1u}
min.	0.15	0.00	-0.14	0.00	0.01	0.00	-0.06	0.00
ext.	0.16	0.00	-0.14	0.00	0.01	0.00	-0.06	0.00
			0.04	0.00	-0.01	0.00	-0.04	0.00
total	0.16	0.00	-0.14	0.00	0.01	0.00	-0.06	0.00
			0.04	0.00	-0.01	0.00	-0.04	0.00
			0.00	0.00	0.00	0.00	0.00	
						0.00	0.00	
						0.00	0.00	
comp.	0.16	0.00	0.15	0.00	0.01	0.00	0.07	0.00

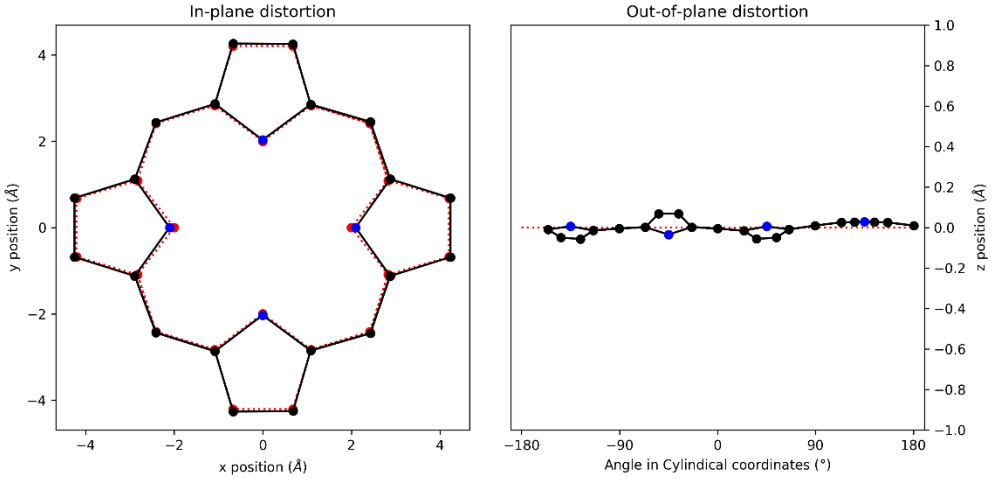


Figure S128: NSD result generated from **3:2** (in Å) (**A**) in-plane and (**B**) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

basis	Δ_{ip}	δ_{ip}	B_{2g}	B_{1g}	$E_u(x)$	$E_u(y)$	A_{1g}	A_{2g}
min.	0.25	0.00	0.00	0.02	0.05	0.00	0.25	0.00
ext.	0.27	0.00	0.00	0.02	0.05	0.00	0.25	0.00
			0.00	0.09	-0.02	0.00	0.00	0.00
total	0.28	0.00	0.00	0.02	0.05	0.00	0.25	0.00
			0.00	0.09	-0.02	0.00	0.00	0.00
			0.00	0.06	-0.02	0.00	0.04	0.00
			0.00	0.00	-0.01	0.00	0.00	0.00
			0.00	-0.01	0.00	0.00	0.02	0.00
			0.00	0.01	0.00	0.00	0.01	
					0.00	0.00		
					-0.01	0.00		
					0.00	0.00		
					0.00	0.00		
					0.01	0.00		
comp.	0.28	0.00	0.00	0.11	0.06	0.00	0.25	0.00

basis	Δ_{oop}	δ_{oop}	B_{2u}	B_{1u}	A_{2u}	$E_g(x)$	$E_g(y)$	A_{1u}
min.	0.20	0.00	-0.19	0.00	0.01	0.00	-0.05	0.00
ext.	0.20	0.00	-0.19	0.00	0.01	0.00	-0.05	0.00
			0.04	0.00	-0.01	0.00	-0.03	0.00
total	0.20	0.00	-0.19	0.00	0.01	0.00	-0.05	0.00
			0.04	0.00	-0.01	0.00	-0.03	0.00
			0.00	0.00	0.00	0.00	0.00	
						0.00	0.00	
						0.00	0.00	
comp.	0.20	0.00	0.19	0.00	0.01	0.00	0.06	0.00

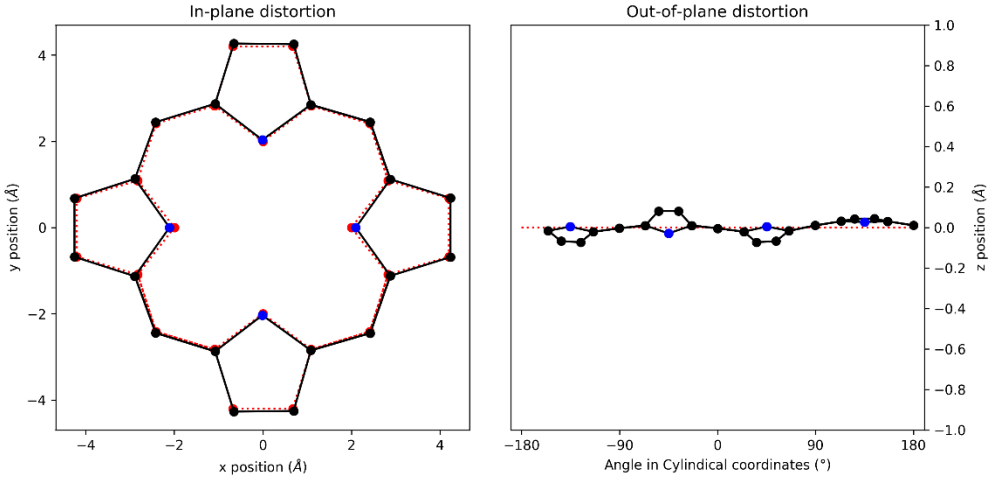


Figure S129: NSD result generated from **3:3** (in Å) (**A**) in-plane and (**B**) out-of-plane skeletal plots of the porphyrin core. Porphyrin is represented in black (C) and blue (N), with the reference structure (CuTPP) in red dotted lines.

NMR and UV spectrum.

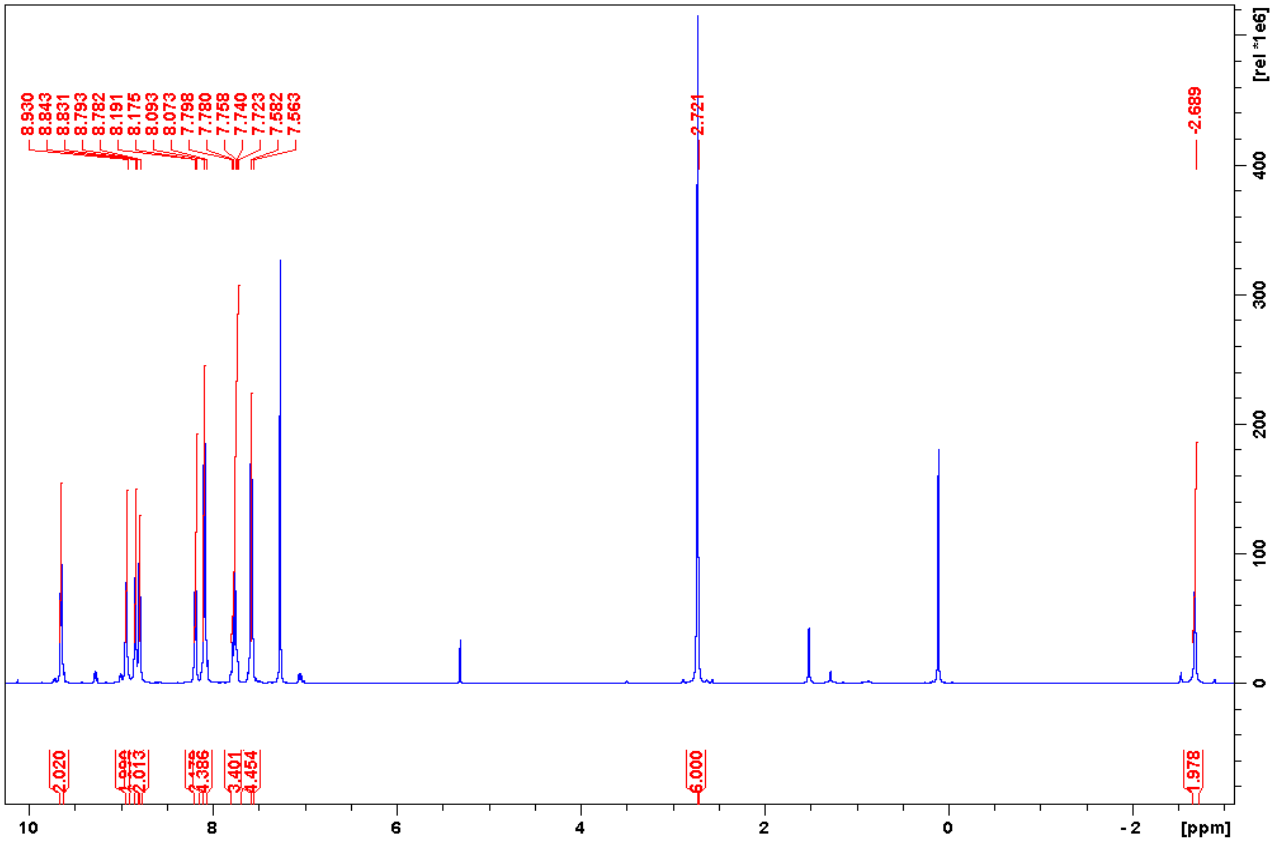


Figure S130: ^{1}H NMR spectrum of compound **4** in $CDCl_3$.

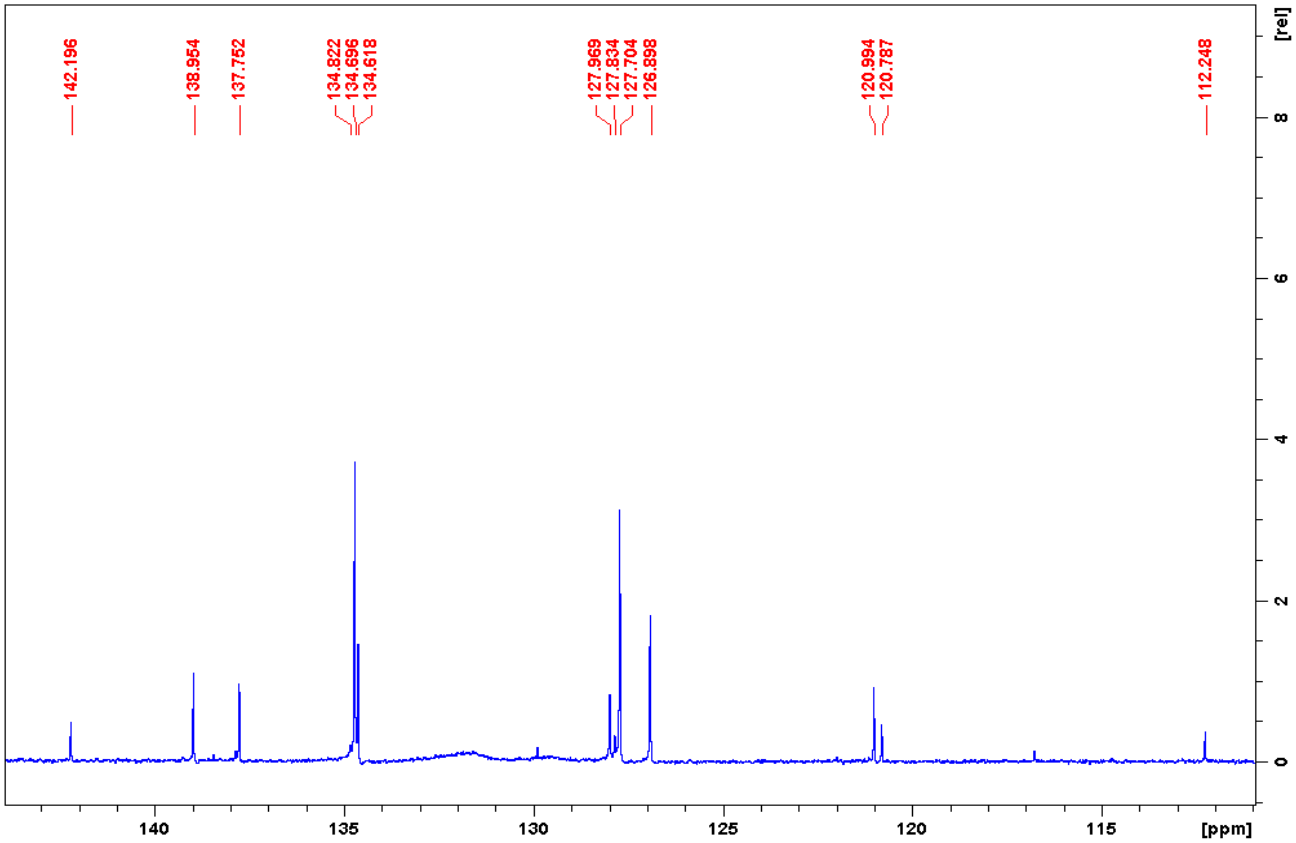


Figure S131: ^{13}C NMR spectrum of compound **4** in $CDCl_3$.

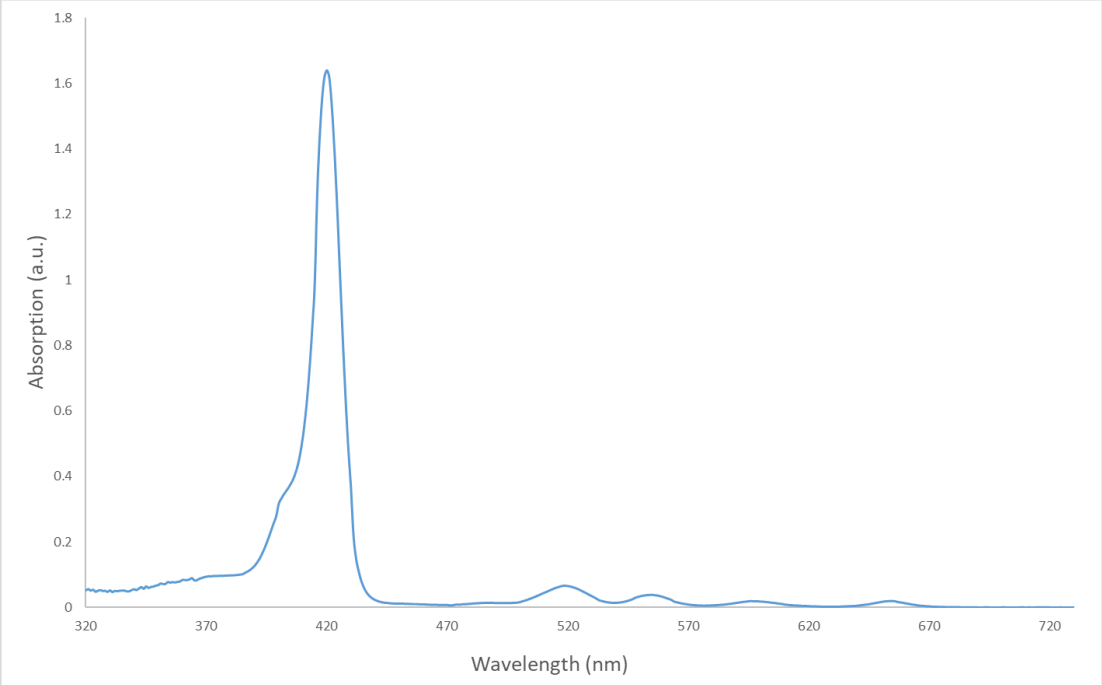


Figure S132: UV-visible spectrum of compound **4** in dichloromethane.