Supporting Information for

Structure Determination of Difficult-to-Crystallize Organic Molecules by Co-Crystallization of Phosphorylated Macrocycle

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1. Supplementary Methods

All reactions were performed in an air atmosphere unless otherwise stated. Deuterium solvents were purchased from Aldrich. All other reagents were obtained from commercial sources and were used without further purification unless indicated otherwise. All yields were given as isolated yields. ^{1}H **NMR** and ^{13}C **NMR** spectra were recorded on a **BRUKER AVANCE III** 400 **MHz**, and the chemical shifts (δ) for **^{1}H NMR** spectra, given in ppm, are referenced to the residual proton signal of the deuterated solvent. Diffraction data were collected on an **X-ray** single crystal diffractometer at **Bruker AXS GmbH**, Germany, at 193 K using **Cu Kα** (λ = 1.54178 Å). Cell refinement and data reduction were performed with the **SAIN**T program package. Absorption correction was performed with **SADBAS**. Structures were solved by direct methods using **OLEX 2** [1]. After obtaining the initial structure for refinement using the standard **SHELXT** program by using the **OLEX 2** software, the refinement of the main frame should be performed first. After anisotropic refinement of all non-H atoms in the framework, the positions of the **H** atoms were calculated geometrically with riding models. If there is a disorder in the molecule, the **PART** command is used to change the part number/occupancy for the given/selected atom; The **DELU** command restrains the **ADPs** of the atoms in the direction of the bond between them to be equal within the given standard uncertainty; The **SIMU** constraint command was used to make the atomic displacement parameters of selected bonds or atom pairs within the given atoms similar with the given estimated standard deviation. Some crystal structures have completely disordered dichloromethane solvent molecules and the **SQUEEZE** method was used to further refine the data. The crystallographic data reported have been deposited with the **Cambridge Crystallographic Data Centre** (**CCDC**). The graphics of crystal structures were generated with the programs **Mercury 2020.1 and VMD 1.9.3**. The **B3LYP** [2] density functional

method with the **D3**(**BJ**) [3] dispersion correction was employed in this work to carry out all the computations. The **6-31G(d**) [2] basis set was used for the atoms in geometry optimizations using the **PCM** model with dichloroethane as the solvent. Vibrational frequency analyses at the same level of theory were performed to characterize stationary points as local minima without any imaginary frequencies. All **DFT** theoretical calculations have been carried out using the Gaussian program package.

2. General Protocol for Co-Crystallization Experiment

(1). General Protocol for Co-Crystallization Experiment:

The detailed synthetic procedure for **F[3]A1-[P(O)Ph]$_3$** is described in previous work. [4,5] The following is the general procedure for co-crystallization experiments of the host macrocyclic **F[3]A1-[P(O)Ph]$_3$** and a guest molecule by solvent volatilization, where the guest molecule is exemplified by 4-fluoroaniline (**G9**). A solid **F[3]A1-[P(O)Ph]$_3$** samples (2 mg, 0.002 mmol) was placed in a 3 mL heat-resistant glass vial, and the liquid guest molecule 4-fluoroaniline (35 μL, 0.36 mmol) was added to a solution of 25 μL dichloromethane and 25 μL dichloroethane and sonicated to dissolve the sample until a completely clear solution was formed. The solvent was slowly evaporated and co-crystals were obtained after 48 hours. Suitable crystals were selected, collected, and analyzed by X-ray diffraction. Details of the co-crystallization of all guest molecules with the host macrocyclic **F[3]A1-[P(O)Ph]$_3$** are given in **Table S1**.

(2). General Protocol for Thermal Co-Crystallization [5]

The following is the general protocol of the thermal co-crystallization experiment, where the guest molecule is exemplified by 4-chlorophenol (**G17**). A solid **F[3]A1-[P(O)Ph]$_3$** samples (2 mg, 0.002 mmol) was placed in a 3 mL heat-resistant glass vial and 50 μL of liquid analyte 4-chlorophenol (65 mg, 0.510 mmol) was added. The resulting suspension was briefly heated on a heated stirrer or hot plate until a clear solution was formed. The temperature of the hot plate is adjusted to the boiling point of the analyte or up to 80°C. The temperature of the hot plate is then adjusted and cooled to room temperature at a rate of 1 °C /h. [6] Suitable crystals are selected, collected, and analyzed by X-ray diffraction. Details of the crystallization run of the analytes are given in **Table S1**.

3. Supplementary Tables

Table S1. Typical amounts of **F[3]A1-[P(O)Ph]$_3$**, liquid guest and solvent, as used for the crystallization experiments of **Figure 2**.

Chaperone	[mg]	Entry No.	Analyte [3]	[µL]	solvent	[µL]
F[3]A1-[P(O)Ph]$_3$	2 mg	**G1**	Acetonitrile	50	—	—
F[3]A1-[P(O)Ph]$_3$	2 mg	**G2**	3-Buten-1-ol	50	DCM/EDC=1:1	50
F[3]A1-[P(O)Ph]$_3$	2 mg	**G3**	Dichloroethane	55	—	—
F[3]A1-[P(O)Ph]$_3$	2 mg	**G4**	Phenylacetylene	45	DCM/EDC=1:1	50
F[3]A1-[P(O)Ph]$_3$	2 mg	**G5**	Ethylbenzene	50	DCM/EDC=1:1	50
F[3]A1-[P(O)Ph]$_3$	2 mg	**G6**	4-Pyridinecarboxaldehyde	50	DCM/EDC=1:1	50
F[3]A1-[P(O)Ph]$_3$	2 mg	**G7**	N-Methylaniline	50	DCM/EDC=1:1	50
F[3]A1-[P(O)Ph]$_3$	2 mg	**G8**	2-Chloropropionic acid	45	DCM/EDC=1:1	50
F[3]A1-[P(O)Ph]$_3$	2 mg	**G9**	4-Fluoroaniline	35	DCM/EDC=1:1	50
F[3]A1-[P(O)Ph]$_3$	2 mg	**G10**	4-Fluorophenylacetylene	40	DCM/EDC=1:1	50
F[3]A1-[P(O)Ph]$_3$	2 mg	**G11**	3-Methylbenzylamine	40	DCM/EDC=1:1	50
F[3]A1-[P(O)Ph]$_3$	2 mg	**G12**	3-methylbenzyl alcohol	40	DCM/EDC=1:1	50
F[3]A1-[P(O)Ph]$_3$	2 mg	**G13**	Phenethyl alcohol	45	DCM/EDC=1:1	50
F[3]A1-[P(O)Ph]$_3$	2 mg	**G14**	3-Methoxyaniline	40	DCM/EDC=1:1	50
F[3]A1-[P(O)Ph]$_3$	2 mg	**G15**	3-Fluorobenzoic acid	45	DCM/EDC=1:1	50
F[3]A1-[P(O)Ph]$_3$	2 mg	**G16**	*p*-Cresol	50	DCM/EDC=1:1	50
F[3]A1-[P(O)Ph]$_3$	2 mg	**G17**	4-Chlorophenol	50	—	—
F[3]A1-[P(O)Ph]$_3$	2 mg	**G18**	3-Phenylprop-2-enal	45	DCM/EDC=1:1	50
F[3]A1-[P(O)Ph]$_3$	2 mg	**G19**	4-(prop-2-ynyl)phenol	35	DCM/EDC=1:1	50

F[3]A1-[P(O)Ph]$_3$	2 mg	**G20**	2-(p-Methylphenyl)propene	35	DCM/EDC=1:1	50
F[3]A1-[P(O)Ph]$_3$	2 mg	**G21**	4-Fluoroacetophenone	45	DCM/EDC=1:1	50
F[3]A1-[P(O)Ph]$_3$	2 mg	**G22**	Bromoacetic acid	40	DCM/EDC=1:1	50
F[3]A1-[P(O)Ph]$_3$	2 mg	**G23**	4-Fluorophenethyl alcohol	50	DCM/EDC=1:1	50
F[3]A1-[P(O)Ph]$_3$	2 mg	**G24**	1-Methylnaphthalene	50	DCM/EDC=1:1	50
F[3]A1-[P(O)Ph]$_3$	2 mg	**G25**	4'-Methylpropiophenone	45	DCM/EDC=1:1	50
F[3]A1-[P(O)Ph]$_3$	2 mg	**G26**	2-Chloro-4-methylbenzaldehyde	40	DCM/EDC=1:1	50
F[3]A1-[P(O)Ph]$_3$	2 mg	**G27**	3-Chlorophenethyl alcohol	60	—	—
F[3]A1-[P(O)Ph]$_3$	2 mg	**G28**	3-Chloroacetophenone	50	—	—
F[3]A1-[P(O)Ph]$_3$	2 mg	**G29**	4-Chloro-3-fluorobenzylamine	50	—	—
F[3]A1-[P(O)Ph]$_3$	2 mg	**G30**	4-Chloro-3-fluoroanisole	40	—	—
F[3]A1-[P(O)Ph]$_3$	2 mg	**G31**	4-(Trifluoromethyl)phenylacetylene	55	DCM/EDC=1:1	50
F[3]A1-[P(O)Ph]$_3$	2 mg	**G32**	4-(Trifluoromethyl)benzyl alcohol	45	DCM/EDC=1:1	50
F[3]A1-[P(O)Ph]$_3$	2 mg	**G33**	4-Bromobenzaldehyde	50	—	—
F[3]A1-[P(O)Ph]$_3$	2 mg	**G34**	4-Bromoethylbenzene	45	—	—
F[3]A1-[P(O)Ph]$_3$	2 mg	**G35**	Ethylferrocene	50	DCM/EDC=1:1	50
F[3]A1-[P(O)Ph]$_3$	2 mg	**G36**	18-Crown-6	35	Chlorobenzene	50
F[3]A1-[P(O)Ph]$_3$	2 mg	**G37**	Dithianon	4 mg	Chlorobenzene	60
F[3]A1-[P(O)Ph]$_3$	2 mg	**G38**	muscone	50	DCM/EDC=1:1	50
F[3]A1-[P(O)Ph]$_3$	2 mg	**G39**	farnesol	55	DCM/EDC=1:1	50
F[3]A1-[P(O)Ph]$_3$	2 mg	**G40**	a-humulene	60	DCM/EDC=1:1	50
F[3]A1-[P(O)Ph]$_3$	2 mg	**G41**	geranyl acetate	60	DCM/EDC=1:1	50
F[3]A1-[P(O)Ph]$_3$	2 mg	**G42**	L-erythrulose	45	DCM/EDC=1:1	50
F[3]A1-[P(O)Ph]$_3$	2 mg	**G43**	all-trans-retinol	65	DCM/EDC=1:1	50
F[3]A1-[P(O)Ph]$_3$	2 mg	**G44**	phytol	70	DCM/EDC=1:1	50

Table S2. Data details of relative molecular mass and **Log P** of guest molecules in co-crystallisation experiments and **CCDC** numbers.

Entry No.	Analyte	Molecular weight [g/mol]	Log P	CCDC entry numbers[a]
G1	Acetonitrile	41.05	-0.34	2330011
G2	3-Buten-1-ol	72.11	0.03	2356284
G3	Dichloroethane	98.96	1.45	2330015
G4	Phenylacetylene	102.13	2.34	2330006
G5	Ethylbenzene	106.17	3.03	2330014
G6	4-Pyridinecarboxaldehyde	107.11	0.435	2330017
G7	N-Methylaniline	107.15	1.7	2330018
G8	2-Chloropropionic acid	108.52	0.82	2330020
G9	4-Fluoroaniline	111.12	1.15	2330007
G10	4-Fluorophenylacetylene	120.12	2.72	2356642
G11	3-Methylbenzylamine	121.18	1.52	2330012
G12	3-methylbenzyl alcohol	122.16	1.6	2330010
G13	Phenethyl alcohol	122.16	1.36	2330019
G14	3-Methoxyaniline	123.15	0.93	2330016
G15	3-Fluorobenzoic acid	124.11	1.42	2330009
G16	*p*-Cresol	124.14	1.41	2330077
G17	4-Chlorophenol	128.56	2.39	2330080
G18	3-Phenylprop-2-enal	132.16	1.9	2330073
G19	4-(2-Propyn-1-yl)phenol	132.16	2.7	2356657
G20	2-(p-Methylphenyl)propene	136.17	1.17	2330066
G21	4-Fluoroacetophenone	138.14	1.64	2330078
G22	Bromoacetic acid	138.95	1.53	2356658
G23	4-Fluorophenethyl alcohol	140.15	1.49	2356643
G24	1-Methylnaphthalene	142.2	3.87	2330068
G25	4'-Methylpropiophenone	148.2	2.51	2330060
G26	2-Chloro-4-methylbenzaldehyde	154.59	2.625	2330075
G27	3-Chlorophenethyl alcohol	154.59	1.55	2356645
G28	3-Chloroacetophenone	154.59	1.68	2330076
G29	4-Chloro-3-fluorobenzylamine	159.59	1.82	2359297
G30	4-Chloro-3-fluoroanisole	160.57	2.79	2356646
G31	4-(Trifluoromethyl)phenylacetylene	170.13	2.59	2330072
G32	4-(Trifluoromethyl)benzyl alcohol	176.14	1.97	2330059
G33	4-Bromobenzaldehyde	185.02	2.46	2356659
G34	4-Bromoethylbenzene	185.06	3.82	2356654
G35	Ethylferrocene	214.08	3.71	2330061
G36	18-Crown-6	264.32	-0.831	2330062
G37	Dithianon	296.32	2.23	2356656
G38	muscone	238.4	6.06	—
G39	farnesol	222.37	4.8	—
G40	a-humulene	204	6.3	—

G41	geranyl acetate	196.29	4.17	—
G42	L-erythrulose	286.45	5.68	—
G43	all-trans-retinol	296.53	9.83	—
G44	phytol	238.4	6.06	—

a) **CCDC** entry numbers are given for runs that were successful and led to a high-resolution structure.

4. Crystallographic data

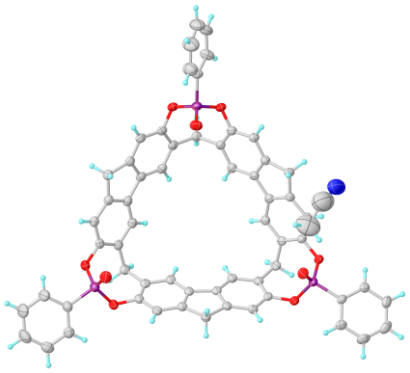


Figure S1. X-ray crystal structure of **F[3]A1-[P(O)Ph]$_3$** with (**G1**) acetonitrile. Thermal ellipsoids were shown at 50% probability level.

CCDC number	2330011
Empirical formula	$C_{61}H_{44.5}N_{0.50}O_{11}P_3$
Formula weight	1053.38
Temperature [K]	193.00
Crystal system	monoclinic
Space group (number)	$P2_1/c$
a [Å]	17.1058(3)
b [Å]	13.2609(3)
c [Å]	21.8092(4)
α [°]	90
β [°]	92.3200(10)
γ [°]	90
Volume [Å^3]	4943.11(17)
Z	4
ρ_{calc} [gcm^{-3}]	1.415
μ [mm^{-1}]	1.666
F(000)	2188
Crystal size [mm^3]	0.15×0.14×0.13
Radiation	CuK_α (λ=1.54178 Å)
2θ range [°]	8.11 to 136.58 (0.83 Å)
Index ranges	−20 ≤ h ≤ 20, −15 ≤ k ≤ 15, −26 ≤ l ≤ 26
Reflections collected	69137
Independent reflections	9032, R_{int} = 0.0759, R_{sigma} = 0.0359
Completeness to θ = 67.679°	99.9 %
Data / Restraints / Parameters	9032/12/701
Goodness-of-fit on F^2	1.075
Final *R* indexes [$I \geq 2\sigma(I)$]	R_1 = 0.0453, wR_2 = 0.1352
Final *R* indexes [all data]	R_1 = 0.0549, wR_2 = 0. 1411,
Largest peak/hole [eÅ^{-3}]	0.90/-0.59

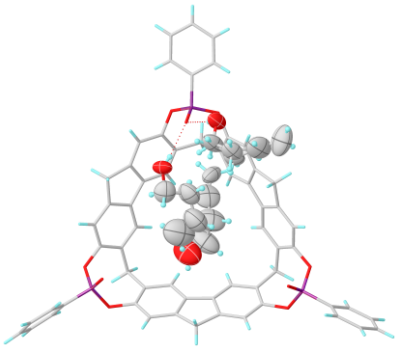


Figure S2. X-ray crystal structure of **F[3]A1-[P(O)Ph]$_3$** with (**G2**) **3-Buten-1-ol** Thermal ellipsoids were shown at 50% probability level.

CCDC number	2356284
Empirical formula	$C_{72}H_{63}O_{12}P_3$
Formula weight	1212.13
Temperature [K]	193.0
Crystal system	triclinic
Space group (number)	P-1
a [Å]	14.186(4)
b [Å]	14.529(4)
c [Å]	17.292(5)
α [°]	73.882(8)
β [°]	70.645(6)
γ [°]	79.586(7)
Volume [Å^3]	3215.0(16)
Z	4
ρ_{calc} [gcm^{-3}]	1.253
μ [mm^{-1}]	0.155
F(000)	1272
Radiation	CuK_α (λ=1.54178 Å)
2θ range [°]	6.09 to 138.86 (0.82 Å)
Index ranges	−14 ≤ h ≤ 14, −21 ≤ k ≤ 25, −24 ≤ l ≤ 24
Reflections collected	36200
Independent reflections	14276, R_{int} = 0.1288, R_{sigma} = 0.1707
Completeness to θ = 67.679°	97 %
Data / Restraints / Parameters	14276/80/796
Goodness-of-fit on F^2	1.038
Final *R* indexes [$I \geq 2\sigma(I)$]	R_1 = 0.0861, wR_2 = 0.1972
Final *R* indexes [all data]	R_1 = 0.1818, wR_2 = 0.2492
Largest peak/hole [eÅ^{-3}]	0.85/−0.64

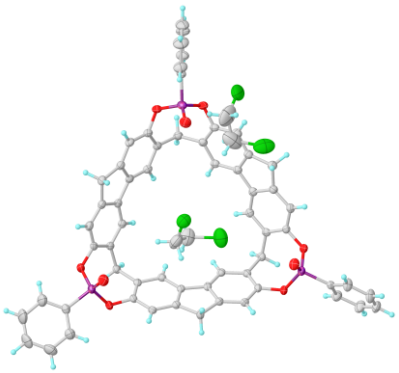


Figure S3. X-ray crystal structure of **F[3]A1-[P(O)Ph]$_3$** with (**G3**) **dichloroethane** Thermal ellipsoids were shown at 50% probability level.

CCDC number	2330015
Empirical formula	$C_{64}H_{49}Cl_4O_9P_3$
Formula weight	1212.72
Temperature [K]	193.00
Crystal system	triclinic
Space group (number)	$P\bar{1}$ (2)
a [Å]	10.9167(10)
b [Å]	18.5273(12)
c [Å]	18.9059(13)
α [°]	114.169(2)
β [°]	99.202(3)
γ [°]	104.391(3)
Volume [Å^3]	3227.6(4)
Z	2
ρ_{calc} [gcm^{-3}]	1.248
μ [mm^{-1}]	0.312
F(000)	1252
Radiation	MoK_α (λ=0.71073 Å)
2θ range [°]	4.03 to 55.03 (0.77 Å)
Index ranges	−14 ≤ h ≤ 14, −24 ≤ k ≤ 24, −24 ≤ l ≤ 24
Reflections collected	78665
Independent reflections	14646, R_{int} = 0.0934, R_{sigma} = 0.0610
Completeness to θ = 25.242°	98.5 %
Data / Restraints / Parameters	14646/12/749
Goodness-of-fit on F^2	1.037
Final *R* indexes [$I \geq 2\sigma(I)$]	R_1 = 0.0673, wR_2 = 0.1918
Final *R* indexes [all data]	R_1 = 0.0879, wR_2 = 0.2088
Largest peak/hole [eÅ^{-3}]	0.86/-0.98

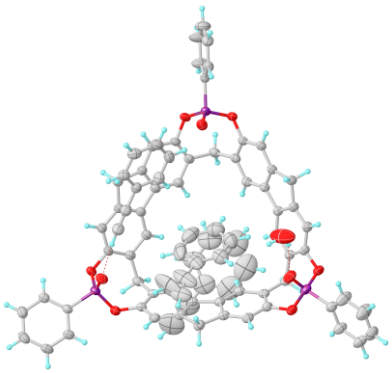


Figure S4. X-ray crystal structure of **F[3]A1-[P(O)Ph]$_3$** with (**G4**) **phenylacetylene**
Thermal ellipsoids were shown at 50% probability level.

CCDC number	2330006
Empirical formula	$C_{84}H_{59}O_{10}P_3$
Formula weight	1321.22
Temperature [K]	193.0
Crystal system	triclinic
Space group (number)	$P\bar{1}$ (2)
a [Å]	11.8512(5)
b [Å]	15.6819(8)
c [Å]	18.9279(6)
α [°]	83.373(2)
β [°]	73.483(2)
γ [°]	85.472(2)
Volume [Å^3]	3346.1(2)
Z	2
ρ_{calc} [gcm^{-3}]	1.311
μ [mm^{-1}]	0.861
F(000)	1376
Radiation	GaK_α (λ=1.34139 Å)
2θ range [°]	4.94 to 107.94 (0.83 Å)
Index ranges	−14 ≤ h ≤ 14, −18 ≤ k ≤ 18, −22 ≤ l ≤ 22
Reflections collected	34538
Independent reflections	12054, R_{int} = 0.0338, R_{sigma} = 0.0331
Completeness to θ = 53.594°	98.2 %
Data / Restraints / Parameters	12054/12/875
Goodness-of-fit on F^2	1.028
Final *R* indexes [$I \geq 2\sigma(I)$]	R_1 = 0.0500, wR_2 = 0.1453
Final *R* indexes [all data]	R_1 = 0.0534, wR_2 = 0.1487
Largest peak/hole [eÅ^{-3}]	0.99/−0.42

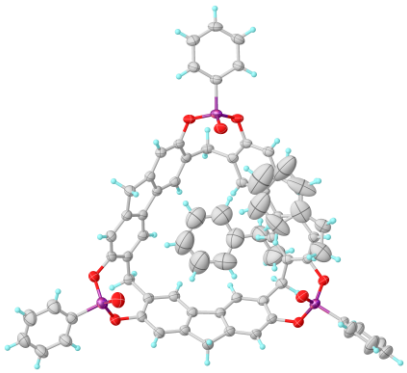


Figure S5. X-ray crystal structure of **F[3]A1-[P(O)Ph]$_3$** with (**G5**) **ethylbenzene** Thermal ellipsoids were shown at 50% probability level.

CCDC number	2330014
Empirical formula	$C_{76}H_{59}O_9P_3$
Formula weight	1209.14
Temperature [K]	193.00
Crystal system	monoclinic
Space group (number)	$P2_1/n$ (14)
a [Å]	15.5508(5)
b [Å]	20.5957(6)
c [Å]	19.1864(6)
α [°]	90
β [°]	102.901(2)
γ [°]	90
Volume [Å^3]	5989.9(3)
Z	4
ρ_{calc} [gcm^{-3}]	1.341
μ [mm^{-1}]	1.419
F(000)	2528
Radiation	CuK_α (λ=1.54184 Å)
2θ range [°]	6.38 to 136.70 (0.83 Å)
Index ranges	−18 ≤ h ≤ 18, −24 ≤ k ≤ 24, −23 ≤ l ≤ 23
Reflections collected	83760
Independent reflections	10967, R_{int} = 0.0658, R_{sigma} = 0.0308
Completeness to θ = 67.684°	100.0 %
Data / Restraints / Parameters	10967/9/794
Goodness-of-fit on F^2	1.062
Final *R* indexes [$I \geq 2\sigma(I)$]	R_1 = 0.0594, wR_2 = 0.1777
Final *R* indexes [all data]	R_1 = 0.0704, wR_2 = 0.1879
Largest peak/hole [eÅ^{-3}]	0.84/−0.70

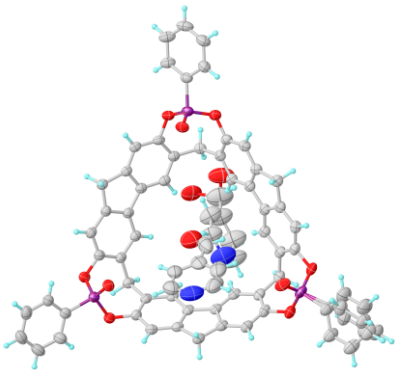


Figure S6. X-ray crystal structure of **F[3]A1-[P(O)Ph]$_3$** with (**G6**) **4-pyridinecarboxaldehyde**

Thermal ellipsoids were shown at 50% probability level.

CCDC number	2330017
Empirical formula	$C_{72}H_{49}N_2O_{11}P_3$
Formula weight	1211.04
Temperature [K]	193.00
Crystal system	triclinic
Space group (number)	$P\bar{1}$ (2)
a [Å]	13.3547(10)
b [Å]	14.8169(9)
c [Å]	18.9025(13)
α [°]	70.696(2)
β [°]	71.926(3)
γ [°]	76.581(2)
Volume [Å^3]	3320.7(4)
Z	2
ρ_{calc} [gcm^{-3}]	1.211
μ [mm^{-1}]	0.150
F(000)	1256
Radiation	MoK_α (λ=0.71073 Å)
2θ range [°]	4.05 to 55.29 (0.77 Å)
Index ranges	−17 ≤ h ≤ 17, −19 ≤ k ≤ 16, −24 ≤ l ≤ 24
Reflections collected	85737
Independent reflections	15307, R_{int} = 0.1093, R_{sigma} = 0.0680
Completeness to θ = 25.242°	99.9 %
Data / Restraints / Parameters	15307/13/833
Goodness-of-fit on F^2	1.015
Final *R* indexes [$I \geq 2\sigma(I)$]	R_1 = 0.0670, wR_2 = 0.1839
Final *R* indexes [all data]	R_1 = 0.1026, wR_2 = 0.2185
Largest peak/hole [eÅ^{-3}]	1.12/-0.66

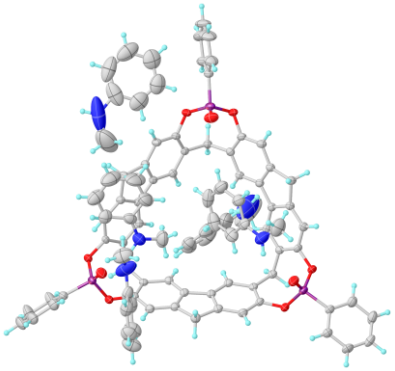


Figure S7. X-ray crystal structure of **F[3]A1-[P(O)Ph]$_3$** with (**G7**) **N-methylaniline** Thermal ellipsoids were shown at 50% probability level.

CCDC number	2330018
Empirical formula	$C_{95}H_{84}N_5O_9P_3$
Formula weight	1532.58
Temperature [K]	193.00
Crystal system	triclinic
Space group (number)	$P\bar{1}$ (2)
a [Å]	12.8799(6)
b [Å]	19.0892(9)
c [Å]	19.3225(10)
α [°]	111.977(2)
β [°]	99.799(2)
γ [°]	103.358(2)
Volume [Å^3]	4109.3(4)
Z	2
ρ_{calc} [gcm^{-3}]	1.239
μ [mm^{-1}]	0.135
F(000)	1612
Radiation	MoK_α (λ=0.71073 Å)
2θ range [°]	4.06 to 55.11 (0.77 Å)
Index ranges	−16 ≤ h ≤ 16, −24 ≤ k ≤ 24, −25 ≤ l ≤ 25
Reflections collected	90603
Independent reflections	18708, R_{int} = 0.1115, R_{sigma} = 0.0779
Completeness to θ = 25.242°	99.2 %
Data / Restraints / Parameters	18708/4/990
Goodness-of-fit on F^2	1.101
Final *R* indexes [$I \geq 2\sigma(I)$]	R_1 = 0.0692, wR_2 = 0.1706
Final *R* indexes [all data]	R_1 = 0.1078, wR_2 = 0.1973
Largest peak/hole [eÅ^{-3}]	1.06/−0.86

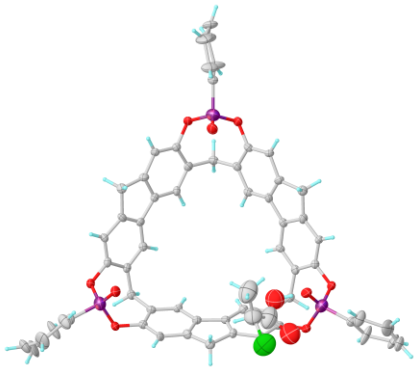


Figure S8. X-ray crystal structure of **F[3]A1-[P(O)Ph]$_3$** with (**G8**) **2-chloropropionic-acid**

Thermal ellipsoids were shown at 50% probability level.

CCDC number	2330020
Empirical formula	$C_{43}H_{30}ClO_8P_2$
Formula weight	772.06
Temperature [K]	193.0
Crystal system	trigonal
Space group (number)	$R3$ *
a [Å]	18.9846(4)
b [Å]	18.9846(4)
c [Å]	40.8214(17)
α [°]	90
β [°]	90
γ [°]	120
Volume [Å^3]	12741.5(8)
Z	1
ρ_{calc} [gcm^{-3}]	0.906
μ [mm^{-1}]	1.435
F(000)	3591
Radiation	CuK_α (λ=1.54178 Å)
2θ range [°]	5.79 to 136.89 (0.83 Å)
Index ranges	−22 ≤ h ≤ 22, −22 ≤ k ≤ 22, −49 ≤ l ≤ 49
Reflections collected	181503
Independent reflections	10372, R_{int} = 0.0608, R_{sigma} = 0.0212
Completeness to θ = 67.679°	100.0 %
Data / Restraints / Parameters	10372/12/546
Goodness-of-fit on F^2	1.113
Final *R* indexes [$I \geq 2\sigma(I)$]	R_1 = 0.0457, wR_2 = 0.1381
Final *R* indexes [all data]	R_1 = 0.0492, wR_2 = 0.1420
Largest peak/hole [eÅ^{-3}]	0.20/−0.30

*: **G8** and **F[3]A1-[P(O)Ph]$_3$** form a racemic mixture.

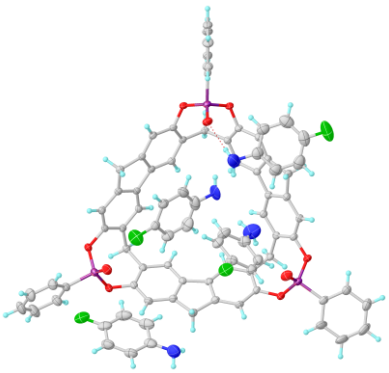


Figure S9. X-ray crystal structure of **F[3]A1-[P(O)Ph]$_3$** with (**G9**) **4-fluoroaniline** Thermal ellipsoids were shown at 50% probability level.

CCDC number	2330007
Empirical formula	$C_{84}H_{63}F_4N_4O_9P_3$
Formula weight	1441.29
Temperature [K]	193.00
Crystal system	triclinic
Space group (number)	$P\bar{1}$ (2)
a [Å]	11.1731(8)
b [Å]	17.0700(12)
c [Å]	20.0546(13)
α [°]	103.439(3)
β [°]	97.936(4)
γ [°]	106.945(4)
Volume [Å^3]	3470.5(4)
Z	2
ρ_{calc} [gcm^{-3}]	1.379
μ [mm^{-1}]	1.421
F(000)	1496
Radiation	CuK_α (λ=1.54178 Å)
2θ range [°]	4.65 to 136.49 (0.83 Å)
Index ranges	−13 ≤ h ≤ 13, −20 ≤ k ≤ 20, −24 ≤ l ≤ 22
Reflections collected	37028
Independent reflections	12549, R_{int} = 0.0750, R_{sigma} = 0.0803
Completeness to θ = 67.679°	98.8 %
Data / Restraints / Parameters	12549/0/941
Goodness-of-fit on F^2	1.074
Final *R* indexes [$I \geq 2\sigma(I)$]	R_1 = 0.0498, wR_2 = 0.1410
Final *R* indexes [all data]	R_1 = 0.0750, wR_2 = 0.1490
Largest peak/hole [eÅ^{-3}]	0.56/−0.74

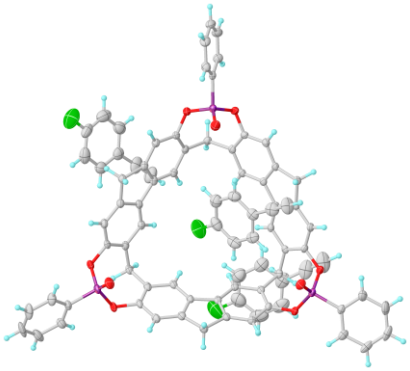


Figure S10. X-ray crystal structure of **F[3]A1-[P(O)Ph]$_3$** with (**G10**) **4-fluorophenylacetylene**

Thermal ellipsoids were shown at 50% probability level.

CCDC number	2356642
Empirical formula	$C_{84}H_{61}Cl_5F_3O_9P_3$
Formula weight	1601.53
Temperature [K]	193.00
Crystal system	triclinic
Space group (number)	$P\bar{1}$ (2)
a [Å]	11.1544(6)
b [Å]	17.3791(9)
c [Å]	19.6218(10)
α [°]	82.448(2)
β [°]	87.009(2)
γ [°]	83.127(2)
Volume [Å^3]	3741.1(3)
Z	2
ρ_{calc} [gcm^{-3}]	1.422
μ [mm^{-1}]	2.946
F(000)	1648
Radiation	CuK_α (λ=1.54178 Å)
2θ range [°]	4.55 to 140.14 (0.82 Å)
Index ranges	−13 ≤ h ≤ 13, −21 ≤ k ≤ 21, −23 ≤ l ≤ 23
Reflections collected	62252
Independent reflections	13980, R_{int} = 0.0427, R_{sigma} = 0.0364
Completeness to θ = 67.679°	98.8 %
Data / Restraints / Parameters	13980/28/892
Goodness-of-fit on F^2	1.056
Final *R* indexes [$I \geq 2\sigma(I)$]	R_1 = 0.0587, wR_2 = 0.1596
Final *R* indexes [all data]	R_1 = 0.0632, wR_2 = 0.1624
Largest peak/hole [eÅ^{-3}]	0.99/−1.04

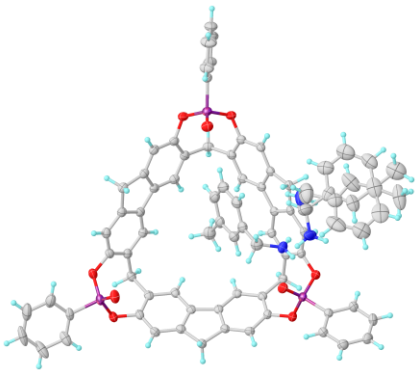


Figure S11. X-ray crystal structure of **F[3]A1-[P(O)Ph]$_3$** with (**G11**) **3-methylbenzylamine**

Thermal ellipsoids were shown at 50% probability level.

CCDC number	2330012
Empirical formula	$C_{76}H_{60}N_2O_9P_3$
Formula weight	1238.17
Temperature [K]	193(2)
Crystal system	triclinic
Space group (number)	$P\bar{1}$ (2)
a [Å]	13.680(3)
b [Å]	14.519(2)
c [Å]	16.454(3)
α [°]	73.660(7)
β [°]	80.822(6)
γ [°]	74.493(8)
Volume [Å^3]	3009.3(10)
Z	2
ρ_{calc} [gcm^{-3}]	1.366
μ [mm^{-1}]	0.164
F(000)	1294
Radiation	MoK_α (λ=0.71073 Å)
2θ range [°]	5.14 to 55.06 (0.77 Å)
Index ranges	−17 ≤ h ≤ 17, −18 ≤ k ≤ 18, −21 ≤ l ≤ 21
Reflections collected	65778
Independent reflections	13701, R_{int} = 0.0881, R_{sigma} = 0.0617
Completeness to θ = 25.242°	98.8 %
Data / Restraints / Parameters	13701/8/886
Goodness-of-fit on F^2	1.030
Final *R* indexes [$I \geq 2\sigma(I)$]	R_1 = 0.0548, wR_2 = 0.1348
Final *R* indexes [all data]	R_1 = 0.0807, wR_2 = 0.1544
Largest peak/hole [eÅ^{-3}]	0.56/−0.62

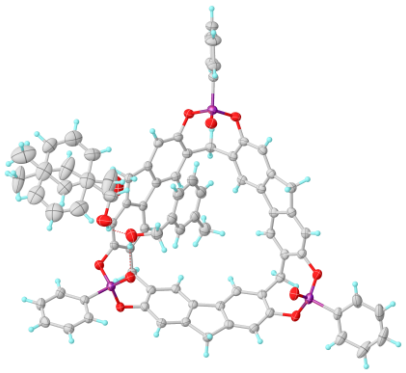


Figure S12. X-ray crystal structure of **F[3]A1-[P(O)Ph]$_3$** with (**G12**) **3-methylbenzyl alcohol**

Thermal ellipsoids were shown at 50% probability level.

CCDC number	2330010
Empirical formula	$C_{76}H_{58}O_{11}P_3$
Formula weight	1240.13
Temperature [K]	193.00
Crystal system	triclinic
Space group (number)	$P\bar{1}$ (2)
a [Å]	13.683(2)
b [Å]	14.523(2)
c [Å]	16.463(3)
α [°]	73.664(5)
β [°]	80.764(6)
γ [°]	74.490(4)
Volume [Å^3]	3012.3(8)
Z	2
ρ_{calc} [gcm^{-3}]	1.367
μ [mm^{-1}]	0.166
F(000)	1294
Radiation	MoK_α (λ=0.71073 Å)
2θ range [°]	3.85 to 55.08 (0.77 Å)
Index ranges	−17 ≤ h ≤ 17, −18 ≤ k ≤ 17, −21 ≤ l ≤ 21
Reflections collected	79405
Independent reflections	13827, R_{int} = 0.1185, R_{sigma} = 0.0753
Completeness to θ = 25.242°	99.9 %
Data / Restraints / Parameters	13827/0/880
Goodness-of-fit on F^2	1.035
Final *R* indexes [$I \geq 2\sigma(I)$]	R_1 = 0.0547, wR_2 = 0.1220
Final *R* indexes [all data]	R_1 = 0.0898, wR_2 = 0.1514
Largest peak/hole [eÅ^{-3}]	0.57/−0.45

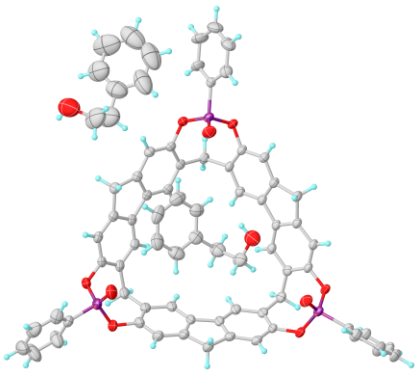


Figure S13. X-ray crystal structure of **F[3]A1-[P(O)Ph]$_3$** with (**G13**) **phenethyl alcohol**

Thermal ellipsoids were shown at 50% probability level.

CCDC number	2330019
Empirical formula	$C_{144}H_{108}O_{21}P_6$
Formula weight	2360.12
Temperature [K]	193.15
Crystal system	triclinic
Space group (number)	$P\bar{1}$ (2)
a [Å]	13.325(6)
b [Å]	16.308(5)
c [Å]	31.821(8)
α [°]	102.082(14)
β [°]	93.45(2)
γ [°]	99.70(2)
Volume [Å^3]	6632(4)
Z	2
ρ_{calc} [gcm^{-3}]	1.182
μ [mm^{-1}]	1.287
F(000)	2460
Radiation	CuK_α (λ=1.54178 Å)
2θ range [°]	5.64 to 137.87 (0.83 Å)
Index ranges	−16 ≤ h ≤ 16, −19 ≤ k ≤ 19, −38 ≤ l ≤ 38
Reflections collected	105094
Independent reflections	24358, R_{int} = 0.0600, R_{sigma} = 0.0470
Completeness to θ = 67.679°	99.7 %
Data / Restraints / Parameters	24358/6/1488
Goodness-of-fit on F^2	1.052
Final *R* indexes [$I \geq 2\sigma(I)$]	R_1 = 0.0894, wR_2 = 0.2684
Final *R* indexes [all data]	R_1 = 0.1060, wR_2 = 0.2892
Largest peak/hole [eÅ^{-3}]	1.46/−0.77

IUCr's Checkcif provided one level B errors:

PLAT420_ALERT_2_B D-H Bond Without Acceptor O03C –H2.
PLAT420_ALERT_2_B D-H Bond Without Acceptor O00R --H00R.
PLAT420_ALERT_2_B D-H Bond Without Acceptor O046 --H046.

RESPONSE:

The structure of the co-crystals shows that (**G13**) phenethyl alcohol is present on the outside of the cavity of the macrocyclic **F[3]A1-[P(O)Ph]$_3$** and that there are no weak hydrogen-bonding interactions between the oxygen atoms **O03C**, **O00R** and **O046** and any adjacent **F[3]A1-[P(O)Ph]$_3$**, resulting in no receptor for the oxygen atom on the hydroxyl group.

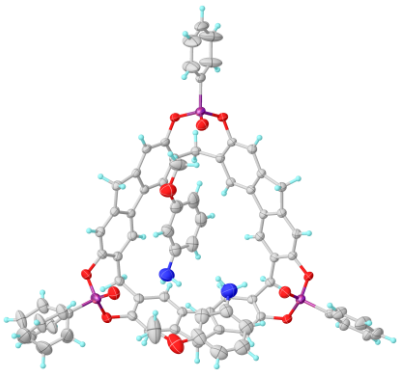


Figure S14. X-ray crystal structure of **F[3]A1-[P(O)Ph]$_3$** with (**G14**) **3-methoxyaniline**

Thermal ellipsoids were shown at 50% probability level.

CCDC number	2330016
Empirical formula	$C_{74}H_{57}N_2O_{11}P_3$
Formula weight	1243.12
Temperature [K]	193.00
Crystal system	triclinic
Space group (number)	$P\bar{1}$ (2)
a [Å]	11.8580(12)
b [Å]	15.8015(16)
c [Å]	18.275(2)
α [°]	106.903(3)
β [°]	106.952(3)
γ [°]	98.989(5)
Volume [Å^3]	3023.4(6)
Z	2
ρ_{calc} [gcm^{-3}]	1.366
μ [mm^{-1}]	0.166
F(000)	1296
Radiation	MoK_α (λ=0.71073 Å)
2θ range [°]	4.02 to 55.05 (0.77 Å)
Index ranges	−15 ≤ h ≤ 15, −20 ≤ k ≤ 20, −23 ≤ l ≤ 23
Reflections collected	85189
Independent reflections	13875, R_{int} = 0.0965, R_{sigma} = 0.0601
Completeness to θ = 25.242°	99.9 %
Data / Restraints / Parameters	13875/6/839
Goodness-of-fit on F^2	1.039
Final *R* indexes [$I \geq 2\sigma(I)$]	R_1 = 0.0625, wR_2 = 0.1635
Final *R* indexes [all data]	R_1 = 0.0886, wR_2 = 0.1898
Largest peak/hole [eÅ^{-3}]	0.99/−0.85

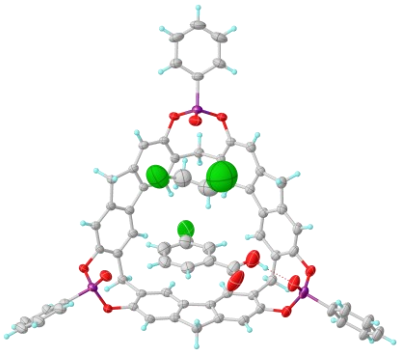


Figure S15. X-ray crystal structure of **F[3]A1-[P(O)Ph]$_3$** with (**G15**) **3-fluorobenzoic acid**

Thermal ellipsoids were shown at 50% probability level.

CCDC number	2330009
Empirical formula	$C_{71}H_{52}FCl_4O_{11}P_3$
Formula weight	1334.83
Temperature [K]	193.00
Crystal system	triclinic
Space group (number)	$P\bar{1}$ (2)
a [Å]	11.6380(3)
b [Å]	17.0699(4)
c [Å]	18.9097(4)
α [°]	91.8030(10)
β [°]	91.359(2)
γ [°]	97.2050(10)
Volume [Å^3]	3723.63(15)
Z	2
ρ_{calc} [gcm^{-3}]	1.091
μ [mm^{-1}]	2.517
F(000)	1376
Radiation	CuK_α (λ=1.54178 Å)
2θ range [°]	4.68 to 136.81 (0.83 Å)
Index ranges	−13 ≤ h ≤ 14, −20 ≤ k ≤ 19, −22 ≤ l ≤ 22
Reflections collected	48340
Independent reflections	13419, R_{int} = 0.0879, R_{sigma} = 0.0747
Completeness to θ = 67.679°	98.6 %
Data / Restraints / Parameters	13419/70/753
Goodness-of-fit on F^2	1.021
Final *R* indexes [I≥2σ(I)]	R_1 = 0.0922, wR_2 = 0.2504
Final *R* indexes [all data]	R_1 = 0.1266, wR_2 = 0.2710
Largest peak/hole [eÅ^{-3}]	0.83/−0.87

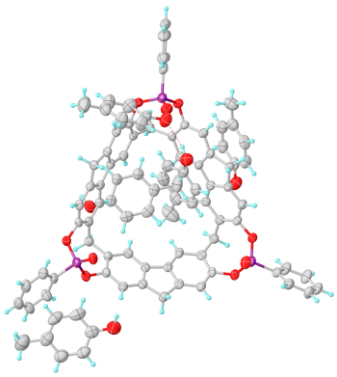


Figure S16. X-ray crystal structure of **F[3]A1-[P(O)Ph]$_3$** with (**G16**) **p-Cresol**
Thermal ellipsoids were shown at 50% probability level.

CCDC number	2330077
Empirical formula	$C_{95}H_{79}O_{14}P_3$
Formula weight	1537.49
Temperature [K]	193.00
Crystal system	triclinic
Space group (number)	$P\bar{1}$ (2)
a [Å]	9.8466(19)
b [Å]	19.666(4)
c [Å]	21.194(4)
α [°]	69.437(5)
β [°]	85.502(6)
γ [°]	87.697(5)
Volume [Å^3]	3830.3(12)
Z	2
ρ_{calc} [gcm^{-3}]	1.333
μ [mm^{-1}]	0.148
F(000)	1612
Radiation	MoK_α (λ=0.71073 Å)
2θ range [°]	4.11 to 52.39 (0.81 Å)
Index ranges	−12 ≤ h ≤ 12, −24 ≤ k ≤ 24, −26 ≤ l ≤ 26
Reflections collected	74454
Independent reflections	15361, R_{int} = 0.1773, R_{sigma} = 0.1535
Completeness to θ = 25.242°	99.9 %
Data / Restraints / Parameters	15361/0/1018
Goodness-of-fit on F^2	1.032
Final *R* indexes [$I \geq 2\sigma(I)$]	R_1 = 0.0781, wR_2 = 0.1824
Final *R* indexes [all data]	R_1 = 0.1675, wR_2 = 0.2492
Largest peak/hole [eÅ^{-3}]	0.50/−0.54

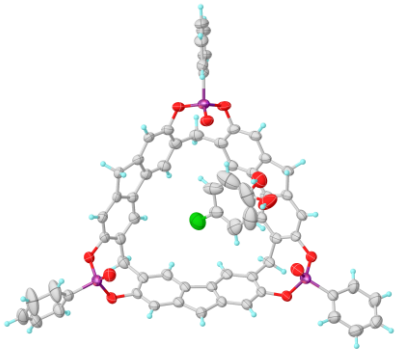


Figure S17. X-ray crystal structure of **F[3]A1-[P(O)Ph]$_3$** with (**G17**) **4-chlorophenol**

Thermal ellipsoids were shown at 50% probability level.

CCDC number	2330080
Empirical formula	$C_{72}H_{50}Cl_2O_{12}P_3$
Formula weight	1261.86
Temperature [K]	193.0
Crystal system	triclinic
Space group (number)	$P\bar{1}$ (2)
a [Å]	12.6751(13)
b [Å]	16.3436(14)
c [Å]	18.4284(18)
α [°]	65.171(3)
β [°]	70.641(3)
γ [°]	84.331(3)
Volume [Å^3]	3265.2(5)
Z	2
ρ_{calc} [gcm^{-3}]	1.283
μ [mm^{-1}]	0.232
F(000)	1305
Radiation	MoK_α (λ=0.71073 Å)
2θ range [°]	4.28 to 55.30 (0.77 Å)
Index ranges	−16 ≤ h ≤ 16, −21 ≤ k ≤ 19, −23 ≤ l ≤ 23
Reflections collected	79447
Independent reflections	15095, R_{int} = 0.1418, R_{sigma} = 0.0986
Completeness to θ = 25.242°	99.9 %
Data / Restraints / Parameters	15095/29/707
Goodness-of-fit on F^2	1.016
Final *R* indexes [$I \geq 2\sigma(I)$]	R_1 = 0.0710, wR_2 = 0.1886
Final *R* indexes [all data]	R_1 = 0.1467, wR_2 = 0.2468
Largest peak/hole [eÅ^{-3}]	1.11/−0.49

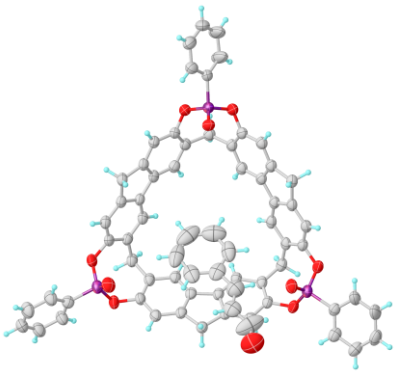


Figure S18. X-ray crystal structure of **F[3]A1-[P(O)Ph]$_3$** with (**G18**) **3-phenylprop-2-enal**

Thermal ellipsoids were shown at 50% probability level.

CCDC number	2330073
Empirical formula	$C_{69}H_{47}O_{10}P_3$
Formula weight	1128.97
Temperature [K]	193.00
Crystal system	triclinic
Space group (number)	$P\bar{1}$ (2)
a [Å]	12.664(3)
b [Å]	15.602(4)
c [Å]	16.023(4)
α [°]	79.818(6)
β [°]	87.132(6)
γ [°]	81.471(6)
Volume [Å^3]	3080.6(12)
Z	2
ρ_{calc} [gcm^{-3}]	1.217
μ [mm^{-1}]	0.154
F(000)	1172
Radiation	MoK_α (λ=0.71073 Å)
2θ range [°]	3.91 to 55.14 (0.77 Å)
Index ranges	−16 ≤ h ≤ 16, −20 ≤ k ≤ 20, −20 ≤ l ≤ 20
Reflections collected	120046
Independent reflections	14162, R_{int} = 0.1561, R_{sigma} = 0.0825
Completeness to θ = 25.242°	99.9 %
Data / Restraints / Parameters	14162/21/727
Goodness-of-fit on F^2	1.033
Final *R* indexes [$I \geq 2\sigma(I)$]	R_1 = 0.0671, wR_2 = 0.1757
Final *R* indexes [all data]	R_1 = 0.1327, wR_2 = 0.2188
Largest peak/hole [eÅ^{-3}]	1.03/−0.55

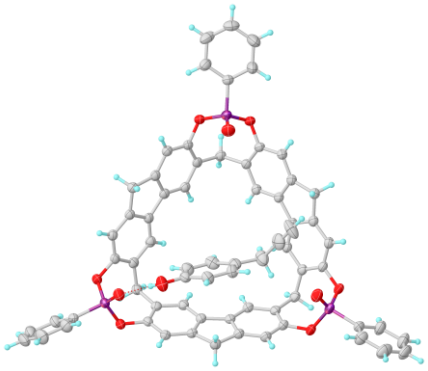


Figure S19. X-ray crystal structure of **F[3]A1-[P(O)Ph]$_3$** with (**G19**) **4-(prop-2-ynyl)phenol**

Thermal ellipsoids were shown at 50% probability level.

CCDC number	2356657
Empirical formula	$C_{74}H_{57}Cl_5O_{10}P_3$
Formula weight	1376.35
Temperature [K]	193.0
Crystal system	triclinic
Space group (number)	$P\bar{1}$ (2)
a [Å]	9.1046(6)
b [Å]	19.4136(11)
c [Å]	19.7970(11)
α [°]	104.993(2)
β [°]	96.273(3)
γ [°]	101.231(2)
Volume [Å^3]	3267.9(3)
Z	2
ρ_{calc} [gcm^{-3}]	1.399
μ [mm^{-1}]	3.217
F(000)	1422
Radiation	CuK_α (λ=1.54178 Å)
2θ range [°]	4.69 to 136.49 (0.83 Å)
Index ranges	−10 ≤ h ≤ 10, −23 ≤ k ≤ 23, −23 ≤ l ≤ 23
Reflections collected	54935
Independent reflections	11902, R_{int} = 0.0505, R_{sigma} = 0.0376
Completeness to θ = 67.679°	99.8 %
Data / Restraints / Parameters	11902/33/740
Goodness-of-fit on F^2	1.067
Final *R* indexes [$I \geq 2\sigma(I)$]	R_1 = 0.0656, wR_2 = 0.1895
Final *R* indexes [all data]	R_1 = 0.0777, wR_2 = 0.1964
Largest peak/hole [eÅ^{-3}]	1.35/−0.84

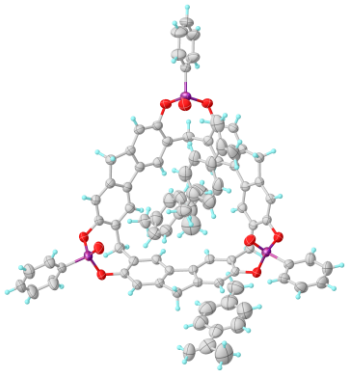


Figure S20. X-ray crystal structure of **F[3]A1-[P(O)Ph]$_3$** with (**G20**) **2-(p-Methylphenyl)propene**

Thermal ellipsoids were shown at 50% probability level.

CCDC number	2330066
Empirical formula	$C_{95}H_{81.5}O_9P_3$
Formula weight	1460
Temperature [K]	193.00
Crystal system	triclinic
Space group (number)	$P\bar{1}$ (2)
a [Å]	14.110(3)
b [Å]	15.998(3)
c [Å]	18.215(4)
α [°]	69.252(9)
β [°]	71.053(9)
γ [°]	75.876(9)
Volume [Å^3]	3597.9(13)
Z	2
ρ_{calc} [gcm^{-3}]	1.348
μ [mm^{-1}]	1.277
F(000)	1537
Radiation	CuK_α (λ=1.54178 Å)
2θ range [°]	5.38 to 133.19 (0.84 Å)
Index ranges	−16 ≤ h ≤ 16, −19 ≤ k ≤ 18, −21 ≤ l ≤ 21
Reflections collected	55260
Independent reflections	12542, R_{int} = 0.0424, R_{sigma} = 0.0365
Completeness to θ = 66.595°	98.7 %
Data / Restraints / Parameters	12542/24/830
Goodness-of-fit on F^2	1.052
Final *R* indexes [$I \geq 2\sigma(I)$]	R_1 = 0.0688, wR_2 = 0.2115
Final *R* indexes [all data]	R_1 = 0.0784, wR_2 = 0.2194
Largest peak/hole [eÅ^{-3}]	1.26/−0.64

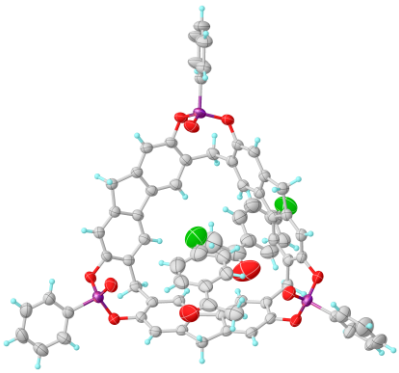


Figure S21. X-ray crystal structure of **F[3]A1-[P(O)Ph]$_3$** with (**G21**) **4-fluoroacetophenone**

Thermal ellipsoids were shown at 50% probability level.

CCDC number	2330078
Empirical formula	$C_{88}H_{63.5}F_{3.5}O_{12.5}P_3$
Formula weight	1480.29
Temperature [K]	193.00
Crystal system	triclinic
Space group (number)	$P\bar{1}$ (2)
a [Å]	14.106(3)
b [Å]	16.000(3)
c [Å]	18.220(4)
α [°]	69.246(9)
β [°]	71.087(10)
γ [°]	75.904(10)
Volume [Å^3]	3599.1(13)
Z	2
ρ_{calc} [gcm^{-3}]	1.366
μ [mm^{-1}]	1.397
F(000)	1536
Radiation	CuK_α (λ=1.54178 Å)
2θ range [°]	5.37 to 137.52 (0.83 Å)
Index ranges	−17 ≤ h ≤ 16, −19 ≤ k ≤ 19, −21 ≤ l ≤ 21
Reflections collected	57018
Independent reflections	13124, R_{int} = 0.0422, R_{sigma} = 0.0369
Completeness to θ = 67.679°	99.4 %
Data / Restraints / Parameters	13124/34/831
Goodness-of-fit on F^2	1.034
Final *R* indexes [$I \geq 2\sigma(I)$]	R_1 = 0.0451, wR_2 = 0.1256
Final *R* indexes [all data]	R_1 = 0.0519, wR_2 = 0.1290
Largest peak/hole [eÅ^{-3}]	0.38/−0.35

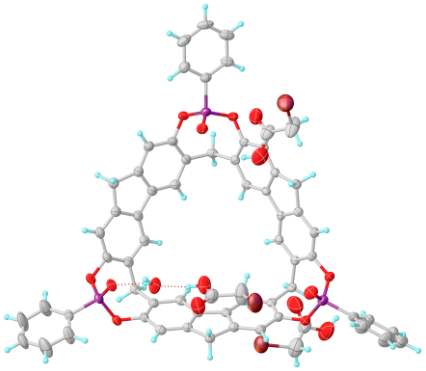


Figure S22. X-ray crystal structure of **F[3]A1-[P(O)Ph]$_3$** with (**G22**) **bromoacetic acid**

Thermal ellipsoids were shown at 50% probability level.

CCDC number	2356658
Empirical formula	$C_{70}H_{59.84}Br_5O_{22}P_3$
Formula weight	1745.48
Temperature [K]	193.0
Crystal system	triclinic
Space group (number)	$P\bar{1}$ (2)
a [Å]	14.5256(5)
b [Å]	16.3572(5)
c [Å]	17.4590(6)
α [°]	67.275(2)
β [°]	72.659(2)
γ [°]	67.045(2)
Volume [Å^3]	3469.7(2)
Z	2
ρ_{calc} [gcm^{-3}]	1.671
μ [mm^{-1}]	4.822
F(000)	1752
Radiation	CuK_α (λ=1.54178 Å)
2θ range [°]	5.57 to 136.48 (0.83 Å)
Index ranges	−17 ≤ h ≤ 17, −19 ≤ k ≤ 19, −20 ≤ l ≤ 21
Reflections collected	50871
Independent reflections	12621, R_{int} = 0.0489, R_{sigma} = 0.0411
Completeness to θ = 67.679°	99.6 %
Data / Restraints / Parameters	12621/2/797
Goodness-of-fit on F^2	1.053
Final *R* indexes [$I \geq 2\sigma(I)$]	R_1 = 0.0716, wR_2 = 0.2121
Final *R* indexes [all data]	R_1 = 0.0832, wR_2 = 0.2196
Largest peak/hole [eÅ^{-3}]	1.34/−1.91

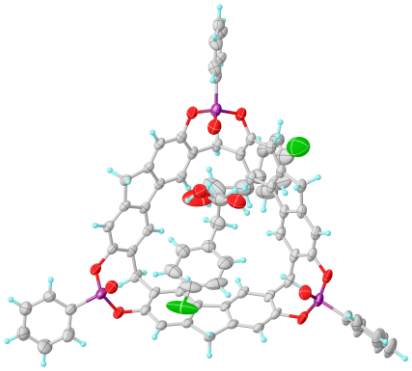


Figure S23. X-ray crystal structure of **F[3]A1-[P(O)Ph]$_3$** with (**G23**) **4-fluorophenethyl alcohol**

Thermal ellipsoids were shown at 50% probability level.

CCDC number	2356643
Empirical formula	$C_{84}H_{67}F_3O_{13}P_3$
Formula weight	1433.11
Temperature [K]	193.0
Crystal system	triclinic
Space group (number)	$P\bar{1}$ (2)
a [Å]	14.2667(4)
b [Å]	16.6495(5)
c [Å]	16.6960(5)
α [°]	67.7370(10)
β [°]	74.097(2)
γ [°]	74.823(2)
Volume [Å^3]	3473.70(18)
Z	2
ρ_{calc} [gcm^{-3}]	1.371
μ [mm^{-1}]	1.421
F(000)	1493
Radiation	CuK_α (λ=1.54178 Å)
2θ range [°]	5.83 to 136.49 (0.83 Å)
Index ranges	−17 ≤ h ≤ 17, −20 ≤ k ≤ 20, −19 ≤ l ≤ 20
Reflections collected	52085
Independent reflections	12690, R_{int} = 0.0575, R_{sigma} = 0.0584
Completeness to θ = 67.679°	99.9 %
Data / Restraints / Parameters	12690/23/840
Goodness-of-fit on F^2	1.059
Final *R* indexes [$I \geq 2\sigma(I)$]	R_1 = 0.0658, wR_2 = 0.1783
Final *R* indexes [all data]	R_1 = 0.0957, wR_2 = 0.1903
Largest peak/hole [eÅ^{-3}]	1.15/−0.67

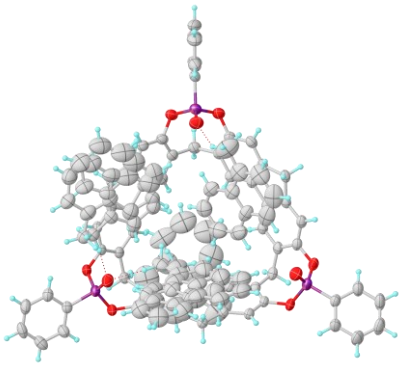


Figure S24. X-ray crystal structure of **F[3]A1-[P(O)Ph]$_3$** with (**G24**) **1-methylnaphthalene**

Thermal ellipsoids were shown at 50% probability level.

CCDC number	2330068
Empirical formula	$C_{105}H_{75}N_{4.5}O_9P_3$
Formula weight	1636.12
Temperature [K]	193.0
Crystal system	triclinic
Space group (number)	$P\bar{1}$ (2)
a [Å]	14.9533(8)
b [Å]	17.3114(10)
c [Å]	19.1689(11)
α [°]	66.900(2)
β [°]	69.827(2)
γ [°]	73.481(2)
Volume [Å^3]	4220.0(4)
Z	2
ρ_{calc} [gcm^{-3}]	1.288
μ [mm^{-1}]	0.136
F(000)	1706
Radiation	MoK_α (λ=0.71073 Å)
2θ range [°]	4.07 to 55.00 (0.77 Å)
Index ranges	−19 ≤ h ≤ 19, −22 ≤ k ≤ 22, −24 ≤ l ≤ 24
Reflections collected	103080
Independent reflections	19288, R_{int} = 0.1202, R_{sigma} = 0.0755
Completeness to θ = 25.242°	99.9 %
Data / Restraints / Parameters	19288/37/724
Goodness-of-fit on F^2	1.032
Final *R* indexes [I≥2σ(I)]	R_1 = 0.0772, wR_2 = 0.2117
Final *R* indexes [all data]	R_1 = 0.1279, wR_2 = 0.2606
Largest peak/hole [eÅ^{-3}]	1.27/−0.66

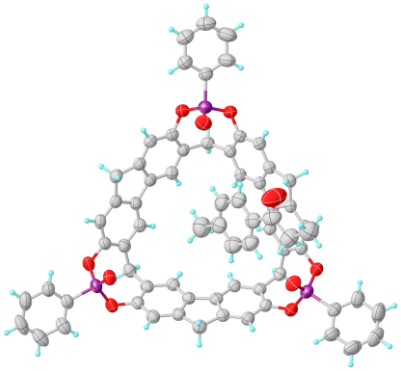


Figure S25. X-ray crystal structure of **F[3]A1-[P(O)Ph]$_3$** with (**G25**) **4-methylpropiophenone**

Thermal ellipsoids were shown at 50% probability level.

CCDC number	2330060
Empirical formula	$C_{70}H_{53}O_{11}P_3$
Formula weight	1163.02
Temperature [K]	193.00
Crystal system	triclinic
Space group (number)	$P\bar{1}$ (2)
a [Å]	11.7390(5)
b [Å]	16.0204(6)
c [Å]	17.1979(7)
α [°]	80.920(2)
β [°]	84.697(3)
γ [°]	76.830(2)
Volume [Å^3]	3104.4(2)
Z	2
ρ_{calc} [gcm^{-3}]	1.244
μ [mm^{-1}]	1.373
F(000)	1212
Radiation	CuK_α (λ=1.54178 Å)
2θ range [°]	5.21 to 136.91 (0.83 Å)
Index ranges	−14 ≤ h ≤ 14, −19 ≤ k ≤ 16, −18 ≤ l ≤ 20
Reflections collected	33673
Independent reflections	10964, R_{int} = 0.0854, R_{sigma} = 0.0964
Completeness to θ = 67.679°	96.8 %
Data / Restraints / Parameters	10964/0/750
Goodness-of-fit on F^2	1.088
Final *R* indexes [I≥2σ(I)]	R_1 = 0.0697, wR_2 = 0.1992
Final *R* indexes [all data]	R_1 = 0.1206, wR_2 = 0.2239
Largest peak/hole [eÅ^{-3}]	0.28/−0.49

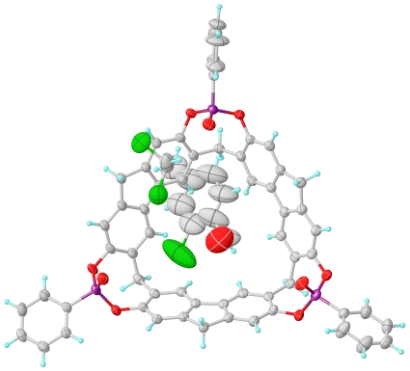


Figure S26. X-ray crystal structure of **F[3]A1-[P(O)Ph]$_3$** with (**G26**) **2-chloro-4-methylbenzaldehyde**

Thermal ellipsoids were shown at 50% probability level.

CCDC number	2330075
Empirical formula	$C_{69}H_{48}Cl_3O_{10}P_3$
Formula weight	1236.33
Temperature [K]	193.0
Crystal system	monoclinic
Space group (number)	$P2_1/n$ (14)
a [Å]	15.5402(3)
b [Å]	20.7308(4)
c [Å]	18.9595(4)
α [°]	90
β [°]	102.5440(10)
γ [°]	90
Volume [Å^3]	5962.2(2)
Z	4
ρ_{calc} [gcm^{-3}]	1.377
μ [mm^{-1}]	2.659
F(000)	2552
Radiation	CuK_α (λ=1.54178 Å)
2θ range [°]	6.68 to 136.70 (0.83 Å)
Index ranges	−18 ≤ h ≤ 18, −24 ≤ k ≤ 24, −22 ≤ l ≤ 22
Reflections collected	86354
Independent reflections	10907, R_{int} = 0.0620, R_{sigma} = 0.0312
Completeness to θ = 67.679°	99.9 %
Data / Restraints / Parameters	10907/41/755
Goodness-of-fit on F^2	1.079
Final *R* indexes [$I \geq 2\sigma(I)$]	R_1 = 0.0725, wR_2 = 0.2162
Final *R* indexes [all data]	R_1 = 0.0855, wR_2 = 0.2299
Largest peak/hole [eÅ^{-3}]	1.18/−0.94

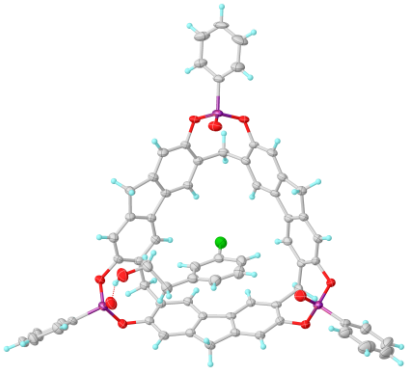


Figure S27. X-ray crystal structure of **F[3]A1-[P(O)Ph]$_3$** with (**G27**) **3-chlorophenethyl alcohol**

Thermal ellipsoids were shown at 50% probability level.

CCDC number	2356645
Empirical formula	$C_{146}H_{116}Cl_{12}O_{20}P_6$
Formula weight	2801.84
Temperature [K]	193.00
Crystal system	triclinic
Space group (number)	$P\bar{1}$ (2)
a [Å]	18.9066(5)
b [Å]	19.4901(5)
c [Å]	21.9910(6)
α [°]	71.010(2)
β [°]	89.114(2)
γ [°]	86.945(2)
Volume [Å^3]	7651.6(4)
Z	2
ρ_{calc} [gcm^{-3}]	1.216
μ [mm^{-1}]	3.070
F(000)	2892
Radiation	CuK_α (λ=1.54178 Å)
2θ range [°]	4.25 to 136.88 (0.83 Å)
Index ranges	−21 ≤ h ≤ 22, −23 ≤ k ≤ 23, −26 ≤ l ≤ 26
Reflections collected	106068
Independent reflections	27971, R_{int} = 0.0778, R_{sigma} = 0.0658
Completeness to θ = 67.679°	99.8 %
Data / Restraints / Parameters	27971/17/1479
Goodness-of-fit on F^2	1.075
Final *R* indexes [$I \geq 2\sigma(I)$]	R_1 = 0.0775, wR_2 = 0.2207
Final *R* indexes [all data]	R_1 = 0.1113, wR_2 = 0.2475
Largest peak/hole [eÅ^{-3}]	1.58/−1.04

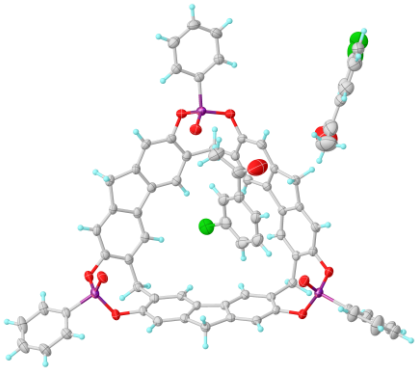


Figure S28. X-ray crystal structure of **F[3]A1-[P(O)Ph]$_3$** with (**G28**) **3-chloroacetophenone**

Thermal ellipsoids were shown at 50% probability level.

CCDC number	2330076
Empirical formula	$C_{76}H_{53}Cl_2O_{11}P_3$
Formula weight	1305.99
Temperature [K]	200.00
Crystal system	triclinic
Space group (number)	$P\bar{1}$ (2)
a [Å]	13.5554(7)
b [Å]	14.7207(9)
c [Å]	16.5017(7)
α [°]	74.173(2)
β [°]	82.141(2)
γ [°]	74.909(2)
Volume [Å^3]	3051.1(3)
Z	2
ρ_{calc} [gcm^{-3}]	1.422
μ [mm^{-1}]	0.252
F(000)	1352
Radiation	MoK_α (λ=0.71073 Å)
2θ range [°]	3.90 to 54.99 (0.77 Å)
Index ranges	−17 ≤ h ≤ 17, −19 ≤ k ≤ 19, −20 ≤ l ≤ 21
Reflections collected	108099
Independent reflections	13990, R_{int} = 0.1743, R_{sigma} = 0.0808
Completeness to θ = 25.242°	99.9 %
Data / Restraints / Parameters	13990/7/841
Goodness-of-fit on F^2	1.039
Final *R* indexes [$I \geq 2\sigma(I)$]	R_1 = 0.0556, wR_2 = 0.1378
Final *R* indexes [all data]	R_1 = 0.1044, wR_2 = 0.1636
Largest peak/hole [eÅ^{-3}]	0.55/−0.43

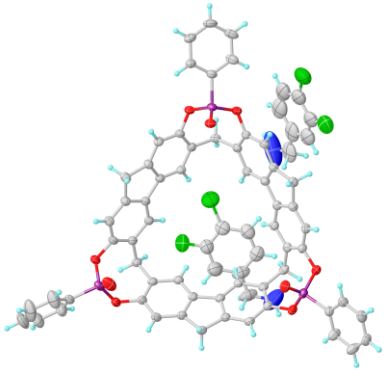


Figure S29. X-ray crystal structure of **F[3]A1-[P(O)Ph]$_3$** with (**G29**) **4-chloro-3-fluorobenzylamine**

Thermal ellipsoids were shown at 50% probability level.

CCDC number	2359297
Empirical formula	$C_{81}H_{61}Cl_3F_3N_3O_{10}P_3$
Formula weight	1493
Temperature [K]	193.0
Crystal system	triclinic
Space group (number)	$P\bar{1}$ (2)
a [Å]	13.5682(3)
b [Å]	14.6203(3)
c [Å]	18.9481(4)
α [°]	74.0480(10)
β [°]	73.7440(10)
γ [°]	80.8830(10)
Volume [Å^3]	3455.97(13)
Z	2
ρ_{calc} [gcm^{-3}]	1.431
μ [mm^{-1}]	2.473
F(000)	1536
Radiation	CuK_α (λ=1.54178 Å)
2θ range [°]	5.01 to 136.43 (0.83 Å)
Index ranges	−16 ≤ h ≤ 16, −17 ≤ k ≤ 17, −22 ≤ l ≤ 22
Reflections collected	41610
Independent reflections	12546, R_{int} = 0.0363, R_{sigma} = 0.0328
Completeness to θ = 67.679°	99.3 %
Data / Restraints / Parameters	12546/34/829
Goodness-of-fit on F^2	1.045
Final *R* indexes [I≥2σ(I)]	R_1 = 0.0713, wR_2 = 0.2160
Final *R* indexes [all data]	R_1 = 0.0818, wR_2 = 0.2250
Largest peak/hole [eÅ^{-3}]	1.54/−1.25

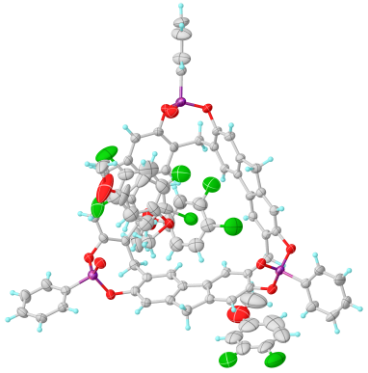


Figure S30. X-ray crystal structure of **F[3]A1-[P(O)Ph]$_3$** with (**G30**) **4-chloro-3-fluoroanisole**

Thermal ellipsoids were shown at 50% probability level.

CCDC number	2356646
Empirical formula	$C_{81}H_{59}Cl_3F_3O_{13}P_3$
Formula weight	1496.52
Temperature [K]	193.0
Crystal system	triclinic
Space group (number)	$P\bar{1}$ (2)
a [Å]	13.5831(11)
b [Å]	14.6115(10)
c [Å]	18.9586(15)
α [°]	74.170(3)
β [°]	73.795(3)
γ [°]	80.974(3)
Volume [Å^3]	3462.9(5)
Z	2
ρ_{calc} [gcm^{-3}]	1.435
μ [mm^{-1}]	0.278
F(000)	1544
Radiation	MoK_α (λ=0.71073 Å)
2θ range [°]	2.31 to 55.19 (0.77 Å)
Index ranges	−17 ≤ h ≤ 17, −17 ≤ k ≤ 19, −24 ≤ l ≤ 24
Reflections collected	136387
Independent reflections	15886, R_{int} = 0.1713, R_{sigma} = 0.0931
Completeness to θ = 25.242°	99.9 %
Data / Restraints / Parameters	15886/27/982
Goodness-of-fit on F^2	1.024
Final *R* indexes [$I \geq 2\sigma(I)$]	R_1 = 0.1002, wR_2 = 0.2308
Final *R* indexes [all data]	R_1 = 0.1831, wR_2 = 0.3069
Largest peak/hole [eÅ^{-3}]	1.37/−0.80

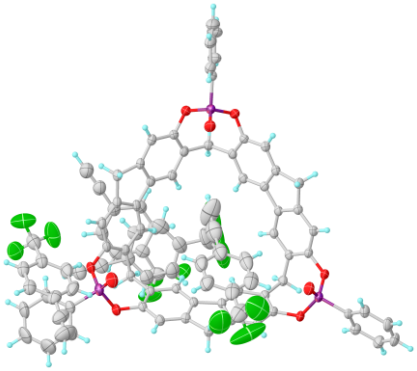


Figure S31. X-ray crystal structure of **F[3]A1-[P(O)Ph]$_3$** with (**G31**) **4-(trifluoromethyl)phenylacetylene**

Thermal ellipsoids were shown at 50% probability level.

CCDC number	2330072
Empirical formula	$C_{156}H_{100}F_{12}O_{19}P_6$
Formula weight	2692.16
Temperature [K]	193.15
Crystal system	triclinic
Space group (number)	$P\bar{1}$ (2)
a [Å]	15.313(7)
b [Å]	19.519(10)
c [Å]	22.918(15)
α [°]	85.77(2)
β [°]	71.15(3)
γ [°]	89.82(2)
Volume [Å^3]	6463(6)
Z	2
ρ_{calc} [gcm^{-3}]	1.383
μ [mm^{-1}]	1.520
F(000)	2772
Radiation	CuK_α (λ=1.54178 Å)
2θ range [°]	4.09 to 136.95 (0.83 Å)
Index ranges	−18 ≤ h ≤ 18, −23 ≤ k ≤ 23, −27 ≤ l ≤ 27
Reflections collected	111673
Independent reflections	23379, R_{int} = 0.1061, R_{sigma} = 0.0949
Completeness to θ = 67.679°	98.7 %
Data / Restraints / Parameters	23379/26/1741
Goodness-of-fit on F^2	1.043
Final *R* indexes [I≥2σ(I)]	R_1 = 0.0512, wR_2 = 0.1368
Final *R* indexes [all data]	R_1 = 0.0979, wR_2 = 0.1525
Largest peak/hole [eÅ^{-3}]	1.34/−0.44

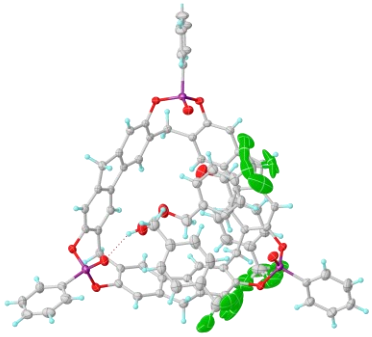


Figure S32. X-ray crystal structure of **F[3]A1-[P(O)Ph]$_3$** with (**G32**) **4-(trifluoromethyl)benzyl alcohol**

Thermal ellipsoids were shown at 50% probability level.

CCDC number	2330059
Empirical formula	$C_{84}H_{60}F_9O_{12}P_3$
Formula weight	1525.23
Temperature [K]	193.0
Crystal system	triclinic
Space group (number)	$P\bar{1}$ (2)
a [Å]	10.9487(5)
b [Å]	18.1314(9)
c [Å]	19.7308(9)
α [°]	68.2040(10)
β [°]	78.033(2)
γ [°]	79.738(2)
Volume [Å^3]	3535.7(3)
Z	2
ρ_{calc} [gcm^{-3}]	1.433
μ [mm^{-1}]	0.998
F(000)	1572
Radiation	GaK_α (λ=1.34139 Å)
2θ range [°]	4.25 to 108.00 (0.83 Å)
Index ranges	−13 ≤ h ≤ 13, −21 ≤ k ≤ 21, −22 ≤ l ≤ 23
Reflections collected	41743
Independent reflections	12772, R_{int} = 0.0427, R_{sigma} = 0.0381
Completeness to θ = 53.594°	98.2 %
Data / Restraints / Parameters	12772/12/1056
Goodness-of-fit on F^2	1.023
Final *R* indexes [$I \geq 2\sigma(I)$]	R_1 = 0.0387, wR_2 = 0.1018
Final *R* indexes [all data]	R_1 = 0.0408, wR_2 = 0.1034
Largest peak/hole [eÅ^{-3}]	0.25/−0.37

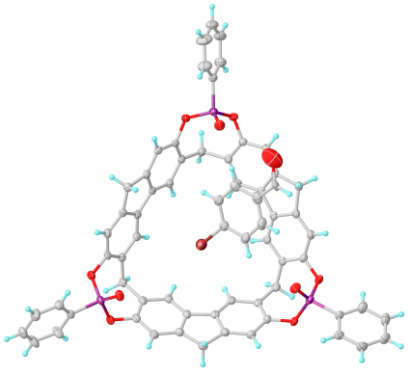


Figure S33. X-ray crystal structure of **F[3]A1-[P(O)Ph]$_3$** with (**G33**) **4-bromobenzaldehyde**

Thermal ellipsoids were shown at 50% probability level.

CCDC number	2356659
Empirical formula	$C_{74}H_{49}Br_2O_{11}P_3$
Formula weight	1366.84
Temperature [K]	193.15
Crystal system	triclinic
Space group (number)	$P\bar{1}$ (2)
a [Å]	13.6016(9)
b [Å]	15.1897(10)
c [Å]	15.7610(8)
α [°]	75.719(2)
β [°]	83.088(2)
γ [°]	77.816(2)
Volume [Å^3]	3076.6(3)
Z	2
ρ_{calc} [gcm^{-3}]	1.475
μ [mm^{-1}]	1.461
F(000)	1392
Radiation	MoK_α (λ=0.71073 Å)
2θ range [°]	3.92 to 54.92 (0.77 Å)
Index ranges	−17 ≤ h ≤ 17, −19 ≤ k ≤ 19, −20 ≤ l ≤ 18
Reflections collected	107180
Independent reflections	14073, R_{int} = 0.0860, R_{sigma} = 0.0492
Completeness to θ = 25.242°	99.8 %
Data / Restraints / Parameters	14073/2/730
Goodness-of-fit on F^2	1.053
Final *R* indexes [$I \geq 2\sigma(I)$]	R_1 = 0.0636, wR_2 = 0.1926
Final *R* indexes [all data]	R_1 = 0.0755, wR_2 = 0.2034
Largest peak/hole [eÅ^{-3}]	2.23/−2.18

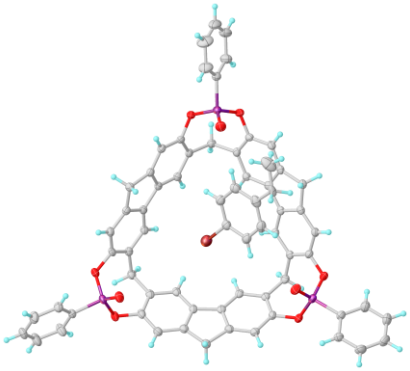


Figure S34. X-ray crystal structure of **F[3]A1-[P(O)Ph]$_3$** with (**G34**) **4-bromoethylbenzene**

Thermal ellipsoids were shown at 50% probability level.

CCDC number	2356654
Empirical formula	$C_{76}H_{57}Br_2O_9P_3$
Formula weight	1366.88
Temperature [K]	193.00
Crystal system	triclinic
Space group (number)	$P\bar{1}$ (2)
a [Å]	13.6026(9)
b [Å]	15.1921(9)
c [Å]	15.7610(8)
α [°]	75.719(2)
β [°]	83.091(2)
γ [°]	77.819(2)
Volume [Å^3]	3077.3(3)
Z	2
ρ_{calc} [gcm^{-3}]	1.2475
μ [mm^{-1}]	1.458
F(000)	1400
Radiation	MoK_α (λ=0.71073 Å)
2θ range [°]	3.92 to 54.94 (0.77 Å)
Index ranges	−17 ≤ h ≤ 17, −19 ≤ k ≤ 19, −20 ≤ l ≤ 18
Reflections collected	148601
Independent reflections	14061, R_{int} = 0.0747, R_{sigma} = 0.0468
Completeness to θ = 25.242°	99.7 %
Data / Restraints / Parameters	14061/29/730
Goodness-of-fit on F^2	1.020
Final *R* indexes [$I \geq 2\sigma(I)$]	R_1 = 0.0632, wR_2 = 0.1837
Final *R* indexes [all data]	R_1 = 0.0719, wR_2 = 0.1913
Largest peak/hole [eÅ^{-3}]	1.65/−2.22

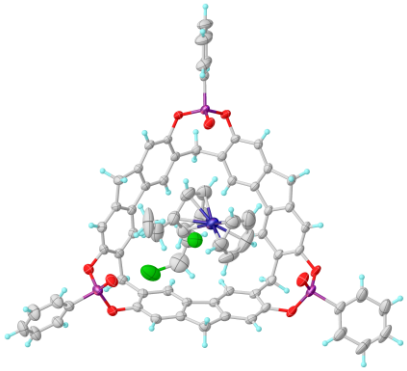


Figure S35. X-ray crystal structure of **F[3]A1-[P(O)Ph]$_3$** with (**G35**) **ethylferrocene**

Thermal ellipsoids were shown at 50% probability level.

CCDC number	2330061
Empirical formula	$C_{74}H_{57}Cl_2FeO_9P_3$
Formula weight	1309.85
Temperature [K]	193.0
Crystal system	triclinic
Space group (number)	$P\bar{1}$ (2)
a [Å]	11.3186(6)
b [Å]	17.3978(9)
c [Å]	19.4271(10)
α [°]	84.705(2)
β [°]	86.771(2)
γ [°]	81.802(2)
Volume [Å^3]	3766.7(3)
Z	2
ρ_{calc} [gcm^{-3}]	1.155
μ [mm^{-1}]	2.160
F(000)	1356
Radiation	GaK_α (λ=1.34139 Å)
2θ range [°]	3.98 to 108.09 (0.83 Å)
Index ranges	−13 ≤ h ≤ 13, −20 ≤ k ≤ 20, −23 ≤ l ≤ 23
Reflections collected	35833
Independent reflections	13631, R_{int} = 0.0384, R_{sigma} = 0.0434
Completeness to θ = 53.594°	98.7 %
Data / Restraints / Parameters	13631/25/802
Goodness-of-fit on F^2	1.109
Final *R* indexes [$I \geq 2\sigma(I)$]	R_1 = 0.0678, wR_2 = 0.2102
Final *R* indexes [all data]	R_1 = 0.0742, wR_2 = 0.2180
Largest peak/hole [eÅ^{-3}]	1.97/−1.27

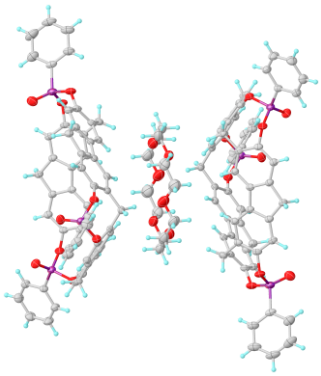


Figure S36. X-ray crystal structure of **F[3]A1-[P(O)Ph]$_3$** with (**G36**) **18-crown-6** Thermal ellipsoids were shown at 50% probability level.

CCDC number	2330062
Empirical formula	$C_{75}H_{63}Cl_{1.5}O_{14}P_3$
Formula weight	1334.30
Temperature [K]	193.00
Crystal system	triclinic
Space group (number)	$P\bar{1}$ (2)
a [Å]	13.726(19)
b [Å]	14.832(12)
c [Å]	15.35(2)
α [°]	91.27(6)
β [°]	94.06(15)
γ [°]	91.93(5)
Volume [Å^3]	3115(7)
Z	2
ρ_{calc} [gcm^{-3}]	1.423
μ [mm^{-1}]	2.057
F(000)	1391
Radiation	CuK_α (λ=1.54178 Å)
2θ range [°]	5.77 to 136.48 (0.83 Å)
Index ranges	−16 ≤ h ≤ 16, −17 ≤ k ≤ 17, −18 ≤ l ≤ 18
Reflections collected	45076
Independent reflections	11296, R_{int} = 0.0418, R_{sigma} = 0.0389
Completeness to θ = 67.679°	99.3 %
Data / Restraints / Parameters	11296/29/749
Goodness-of-fit on F^2	1.032
Final *R* indexes [$I \geq 2\sigma(I)$]	R_1 = 0.0473, wR_2 = 0.1303
Final *R* indexes [all data]	R_1 = 0.0507, wR_2 = 0.1322
Largest peak/hole [eÅ^{-3}]	0.47/−0.53

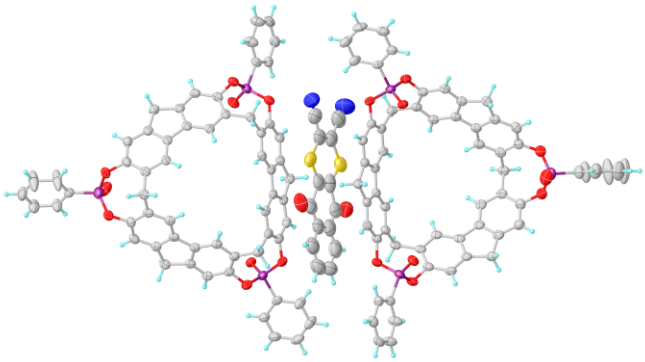


Figure S37. X-ray crystal structure of **F[3]A1-[P(O)Ph]$_3$** with (**G37**) **dithianon** Thermal ellipsoids were shown at 50% probability level.

CCDC number	2356656
Empirical formula	$C_{75}H_{62.5}Cl_{1.5}O_{14}P_3$
Formula weight	1333.56
Temperature [K]	193.15
Crystal system	triclinic
Space group (number)	$P\bar{1}$ (2)
a [Å]	14.9110(3)
b [Å]	19.8365(4)
c [Å]	25.6177(5)
α [°]	104.3670(10)
β [°]	104.5610(10)
γ [°]	99.0420(10)
Volume [Å^3]	6907.0(2)
Z	2
ρ_{calc} [gcm^{-3}]	1.422
μ [mm^{-1}]	2.057
F(000)	1389
Radiation	CuK_α (λ=1.54178 Å)
2θ range [°]	3.74 to 136.76 (0.83 Å)
Index ranges	−17 ≤ h ≤ 17, −23 ≤ k ≤ 23, −27 ≤ l ≤ 30
Reflections collected	99441
Independent reflections	25217, R_{int} = 0.0652, R_{sigma} = 0.0470
Completeness to θ = 67.679°	99.9 %
Data / Restraints / Parameters	25217/58/1587
Goodness-of-fit on F^2	1.022
Final *R* indexes [$I \geq 2\sigma(I)$]	R_1 = 0.0471, wR_2 = 0.1288
Final *R* indexes [all data]	R_1 = 0.0505, wR_2 = 0.1307
Largest peak/hole [eÅ^{-3}]	0.27/−0.54

5. Co-crystal analysis of F[3]A1-[P(O)Ph]$_3$ and G36-G37

5.1 Co-crystal of 18-crown-6 (G36) and F[3]A1-[P(O)Ph]$_3$

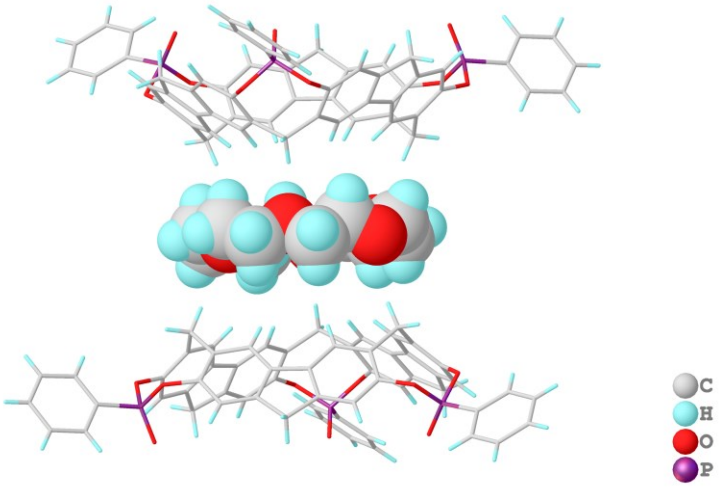
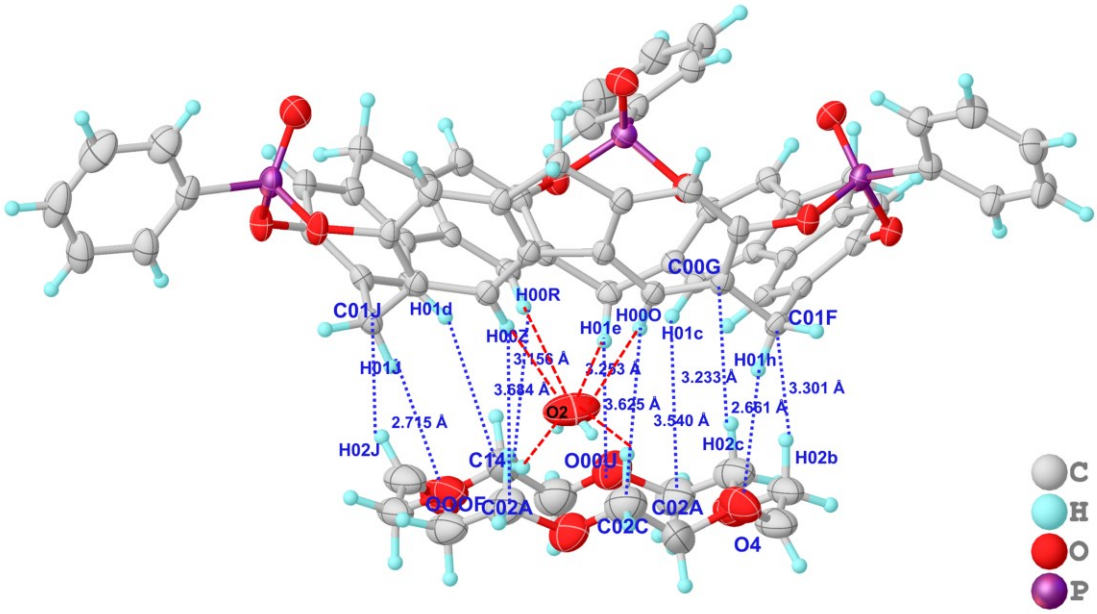


Figure S38. Sandwich construction of 18-crown-6 and **F[3]A1-[P(O)Ph]$_3$** cocrystals. Solvent molecules are omitted to clarify.



H02b-CO1F: 3.301 Å
H01h-O4: 2.661 Å
H02c-COOG: 3.233Å
H01c-C02A:3.540 Å
H00O-C02C: 3.645 Å
H01e-O00U: 3.253 Å
H00Z-C02A: 3.684 Å
H00R-C14: 3.156 Å
H01J-O00F 2.715 Å
H01d-C14: 3.429 Å
H02J-C01J : 3.578 Å
O2-H00Z: 2.605 Å
O2-H01D: 2.935 Å
O2-H00O: 2.613 Å
O2-H00G: 2.782 Å
O2-H00R: 3.521 Å
O2-H01C: 3.434 Å
H2B-O00Y: 2.228 Å
H2B-O00F: 2.959 Å
H2B-O00U: 2.951 Å

Figure S39. Donor-acceptor interactions between (**G36**) 18-crown-6 and **F[3]A1-[P(O)Ph]$_3$**. Solvent molecules are omitted to clarify. Thermal ellipsoids were shown at 50% probability level.

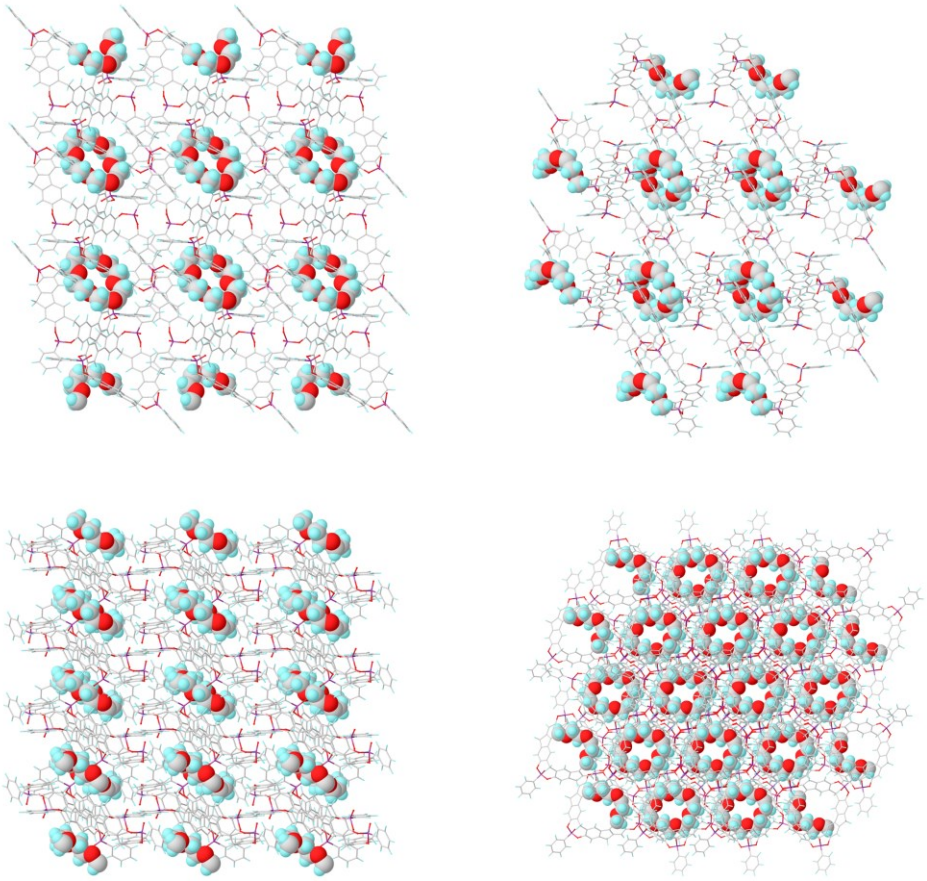


Figure S40. Packing mode of 18-crown-6 and **F[3]A1-[P(O)Ph]$_3$** cocrystals. Thermal ellipsoids were shown at 50% probability level.

5.2 Co-crystal of dithianon (G37) and F[3]A1-[P(O)Ph]$_3$

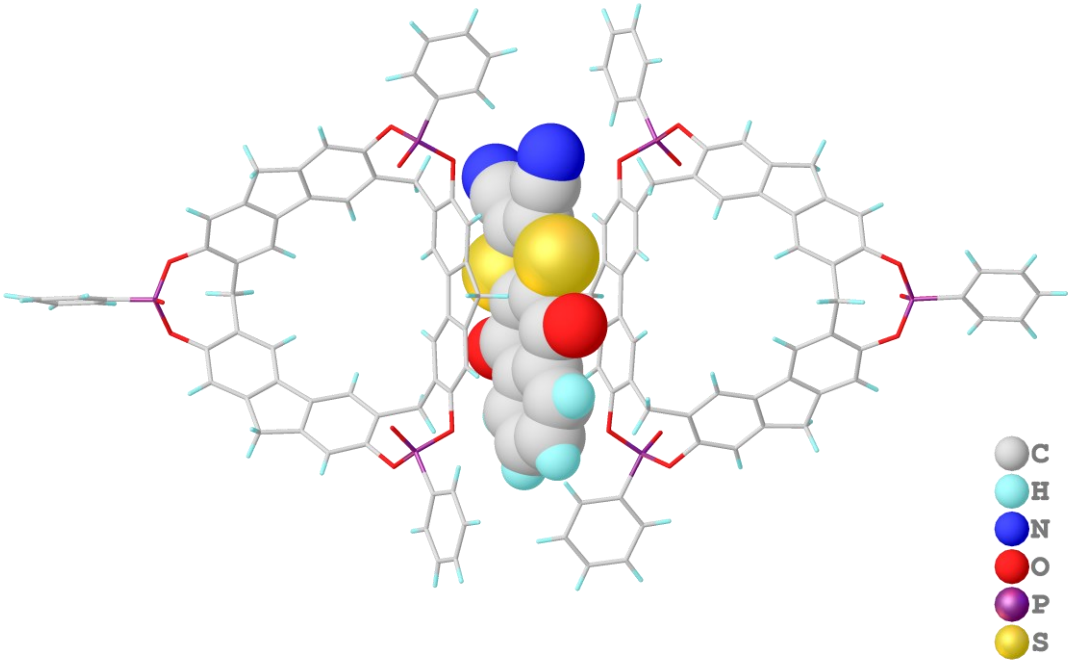


Figure S41. The structure of dithianon and **F[3]A1-[P(O)Ph]$_3$** cocrystals. Solvent molecules are omitted to clarify.

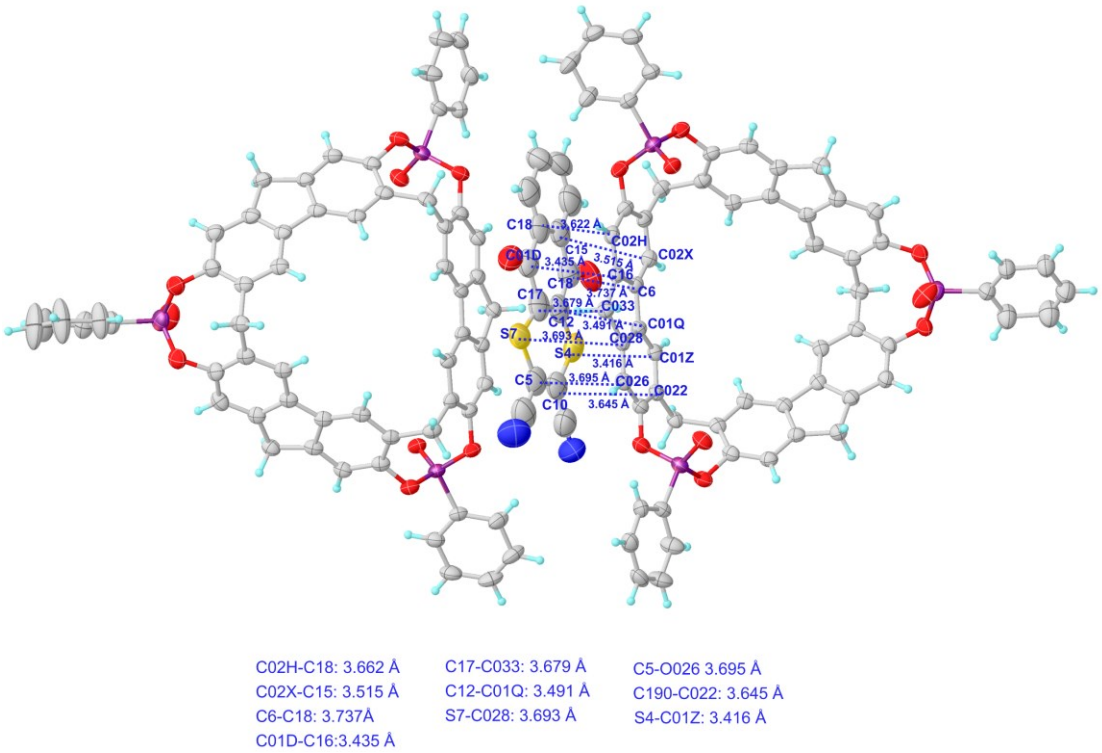


Figure S42. Donor-acceptor interactions between (**G37**) dithianon and **F[3]A1-[P(O)Ph]$_3$**. Solvent molecules are omitted to clarify. Thermal ellipsoids were shown at 50% probability level.

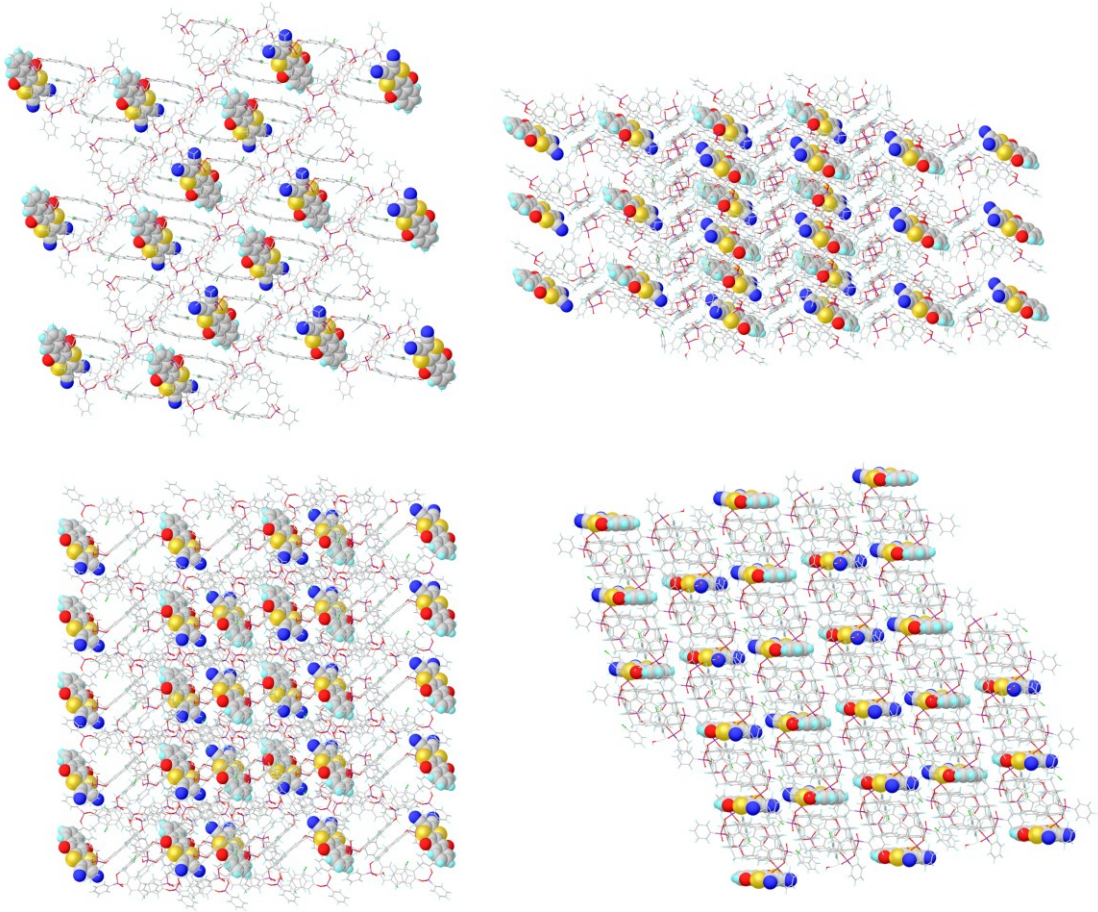


Figure S43. Packing mode of dithianon and **F[3]A1-[P(O)Ph]$_3$** cocrystals. Thermal ellipsoids were shown at 50% probability level.

6. The 2D Hirshfeld fingerprint plots

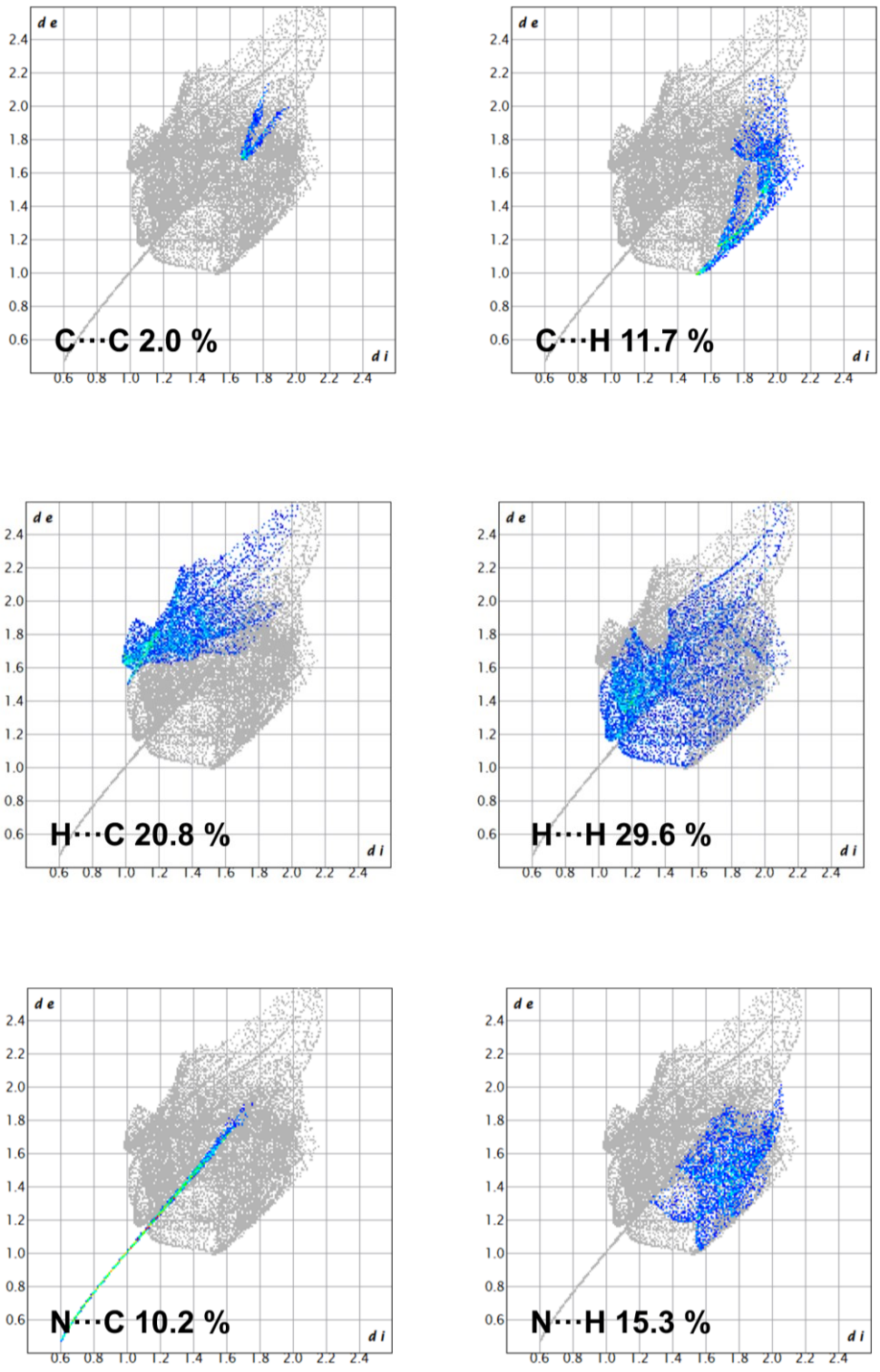


Figure S44. The **2D** Hirshfeld fingerprints of (**G1**)

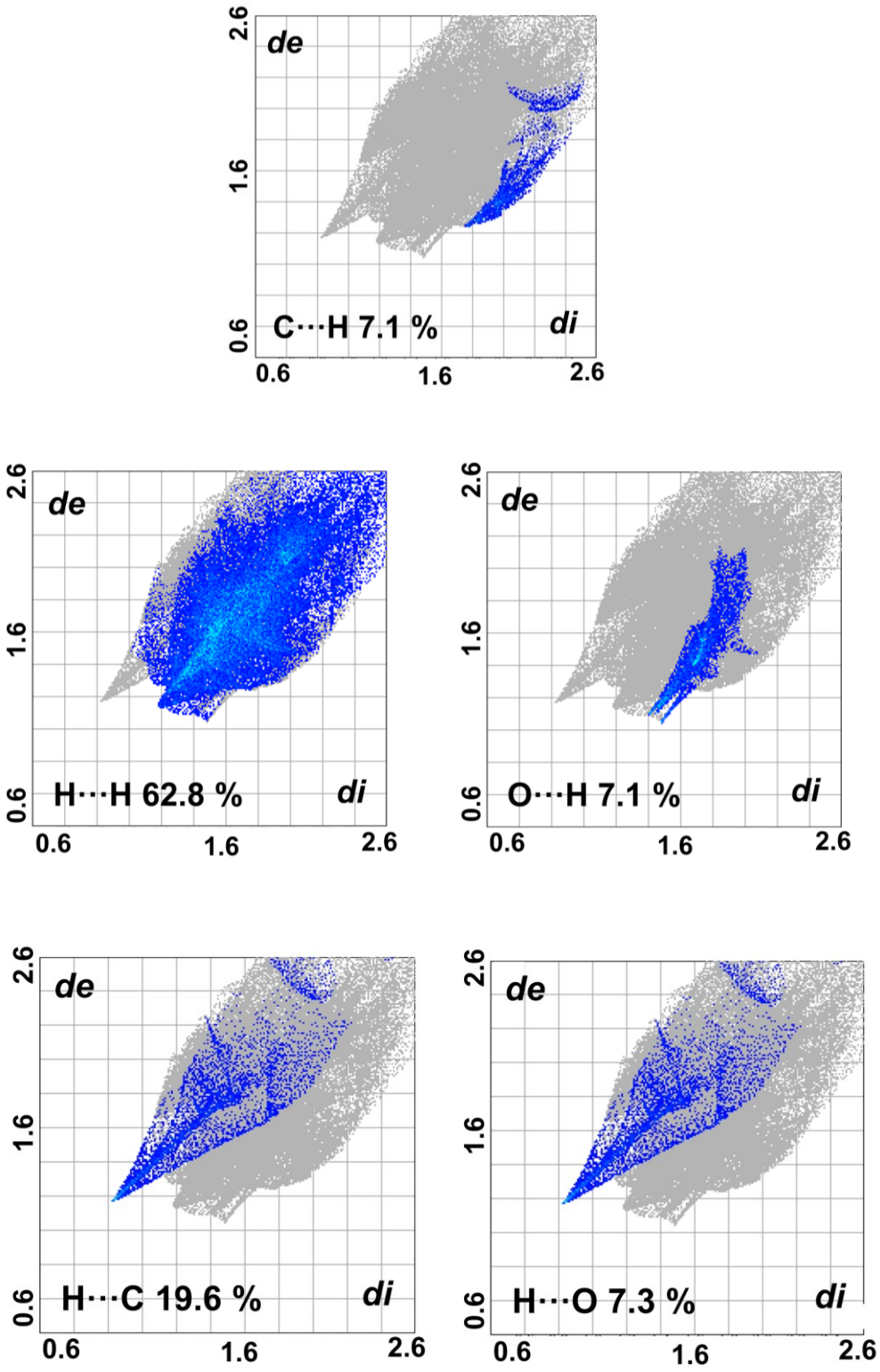


Figure S45. The **2D** Hirshfeld fingerprints of (**G2**)

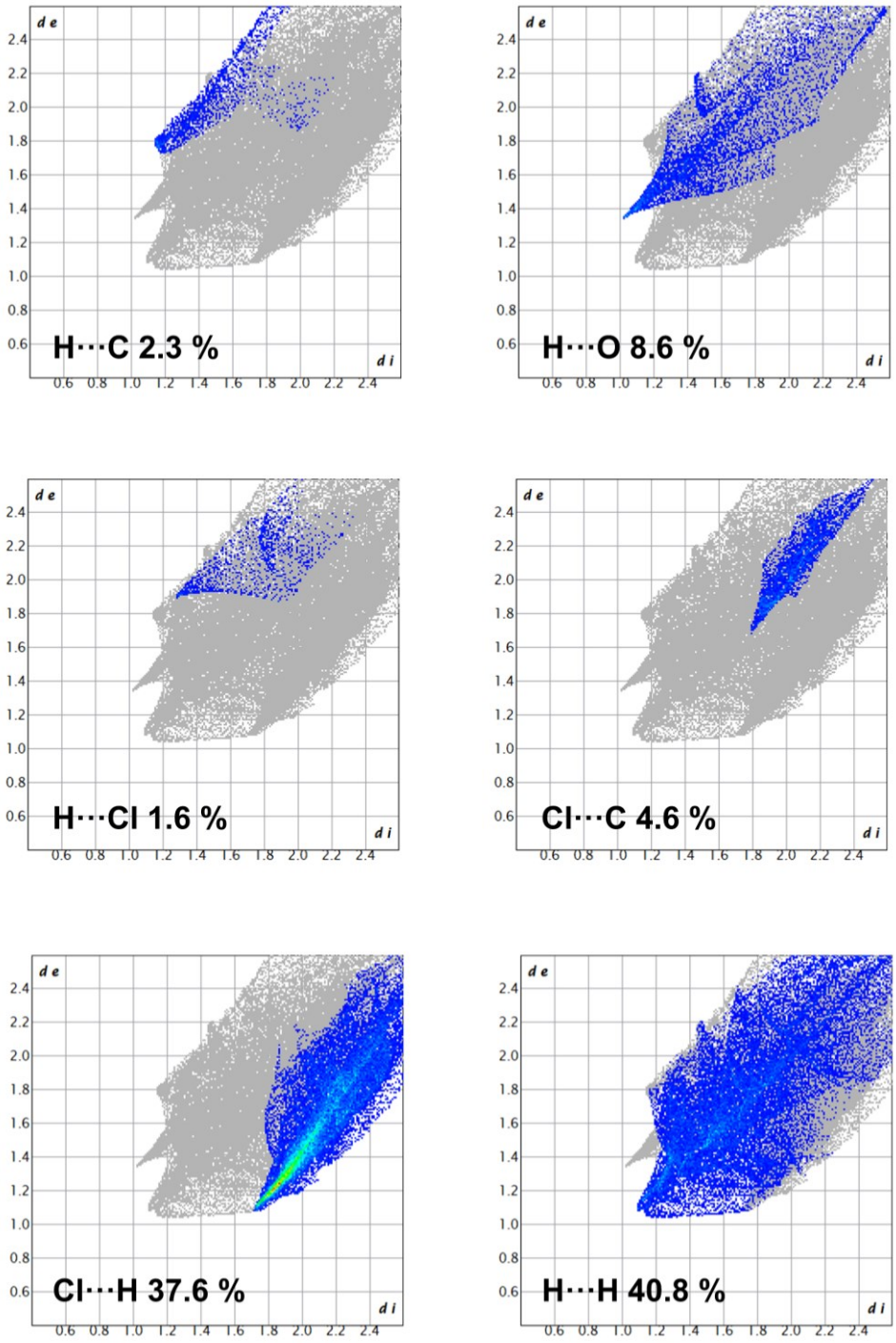


Figure S46. The **2D** Hirshfeld fingerprints of (**G3**)

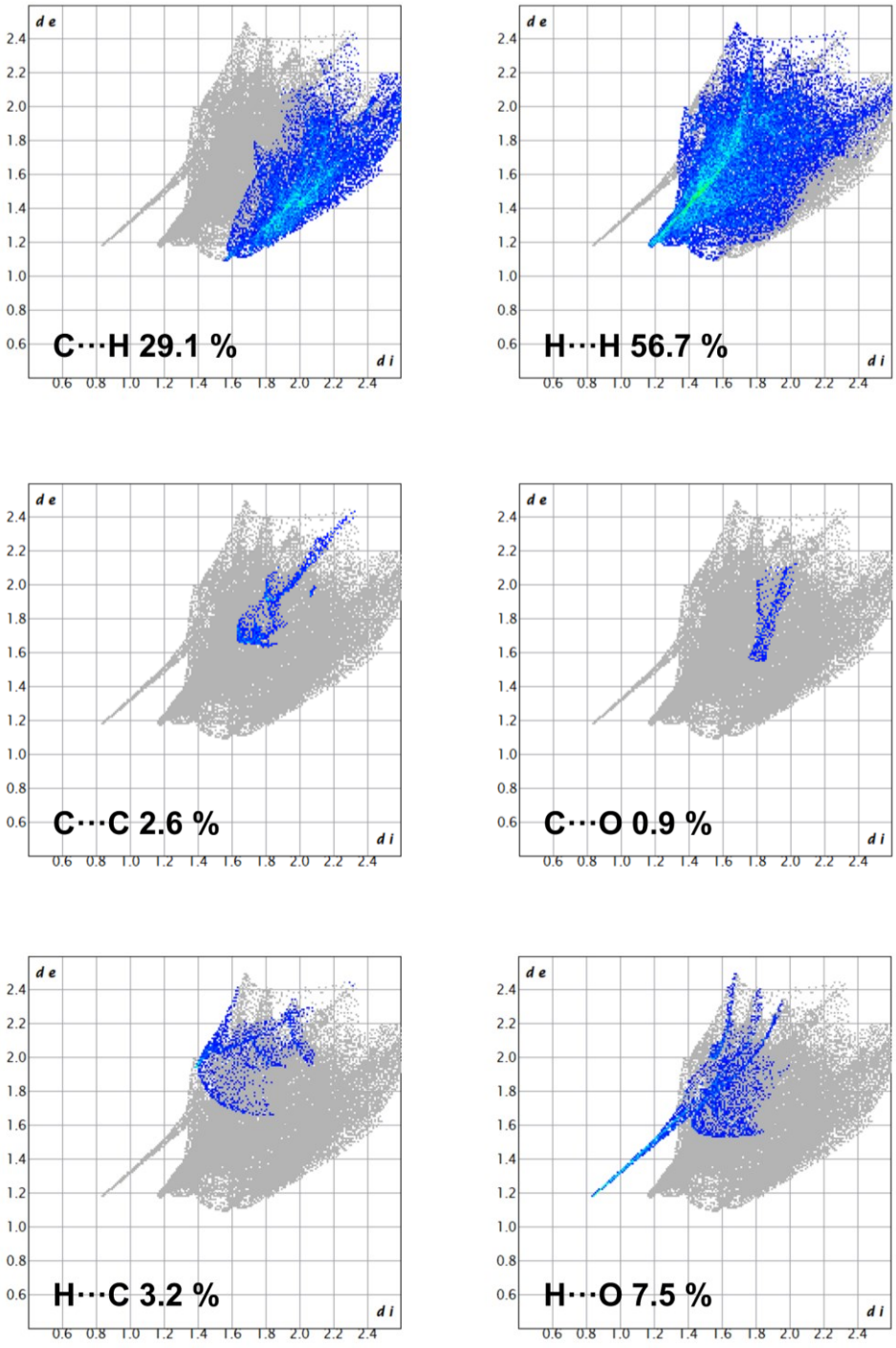


Figure S47. The **2D** Hirshfeld fingerprints of (**G4**)

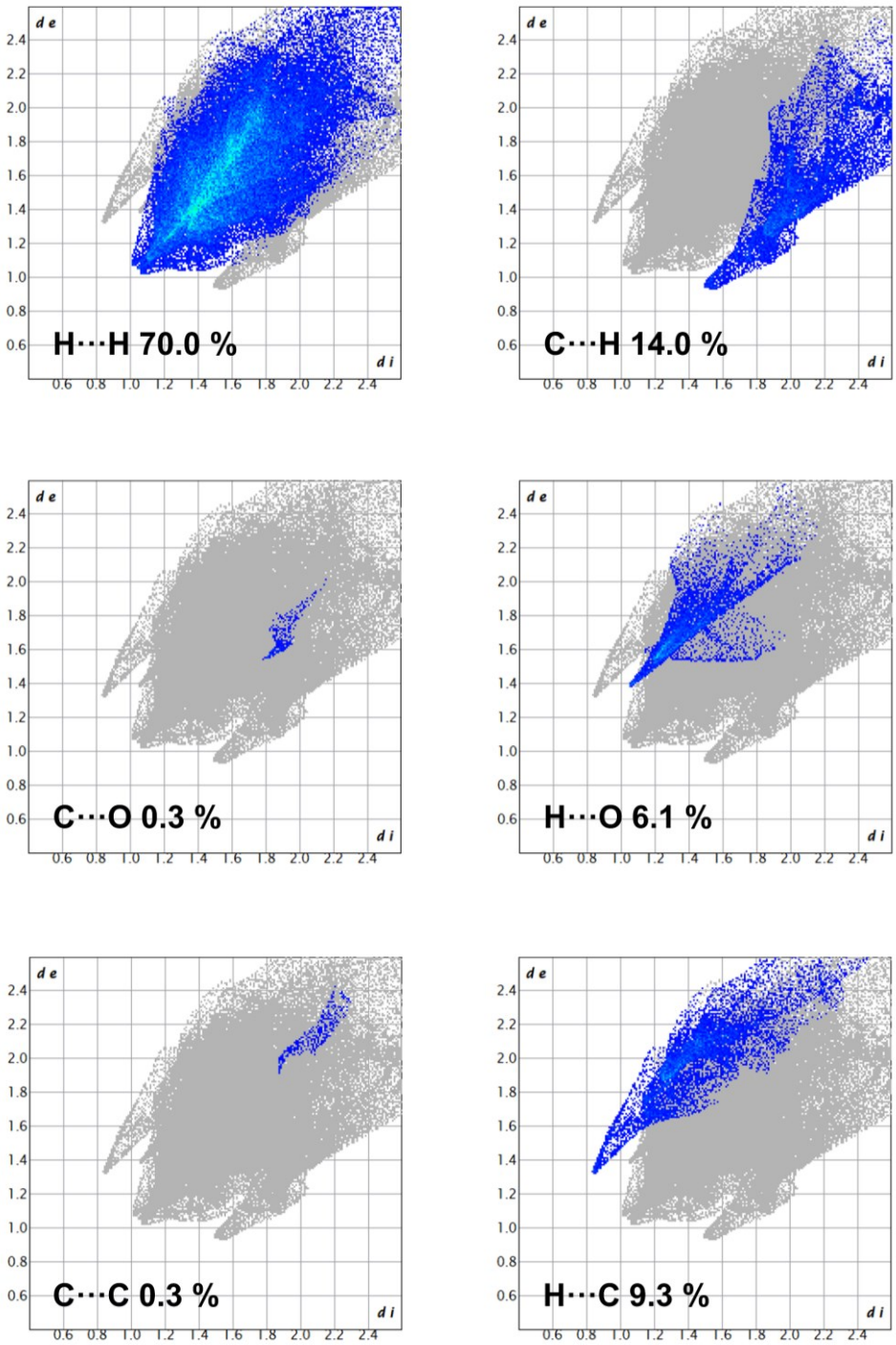


Figure S48. The **2D** Hirshfeld fingerprints of (**G5**)

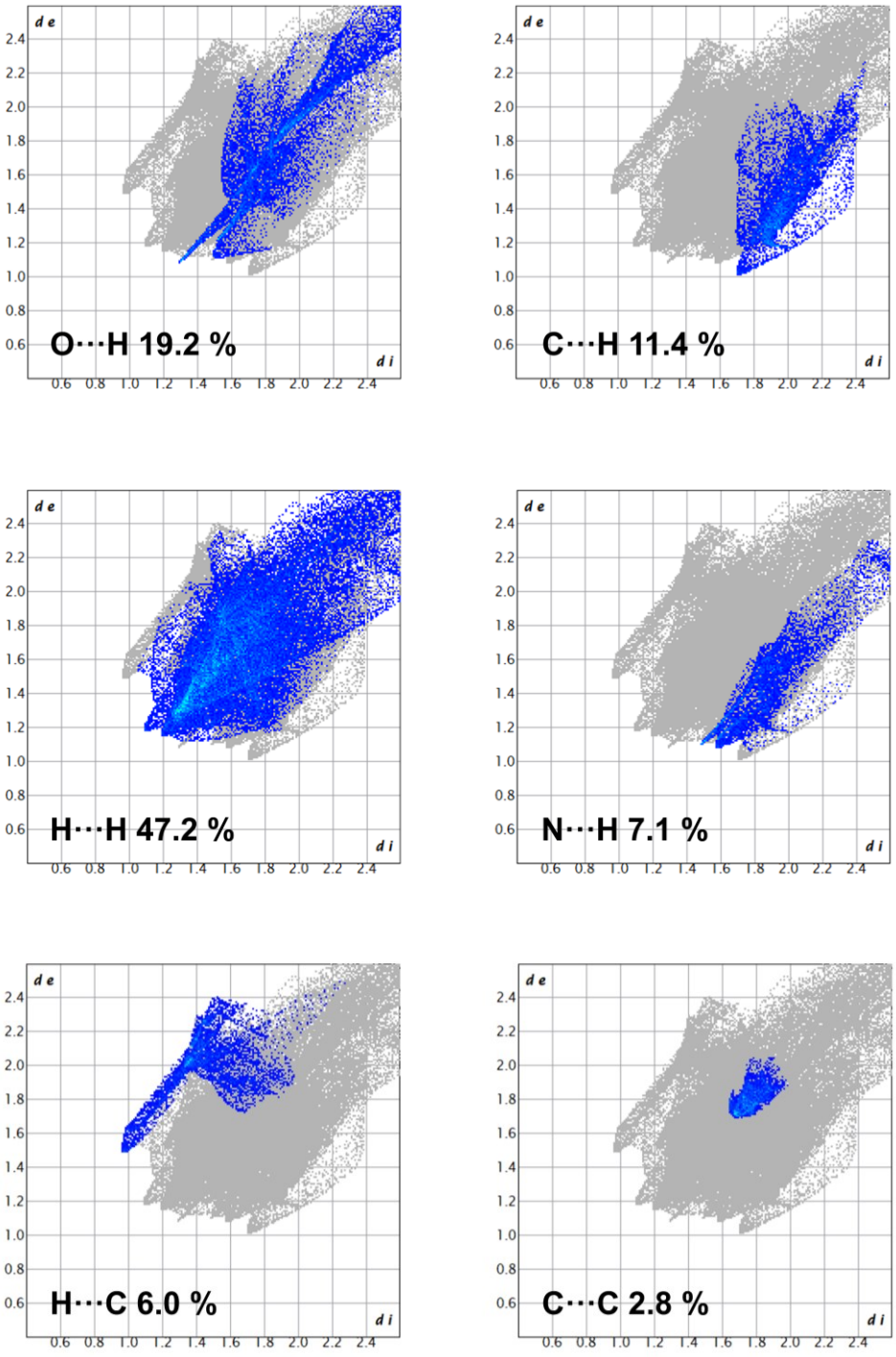


Figure S49. The **2D** Hirshfeld fingerprints of (**G6**)

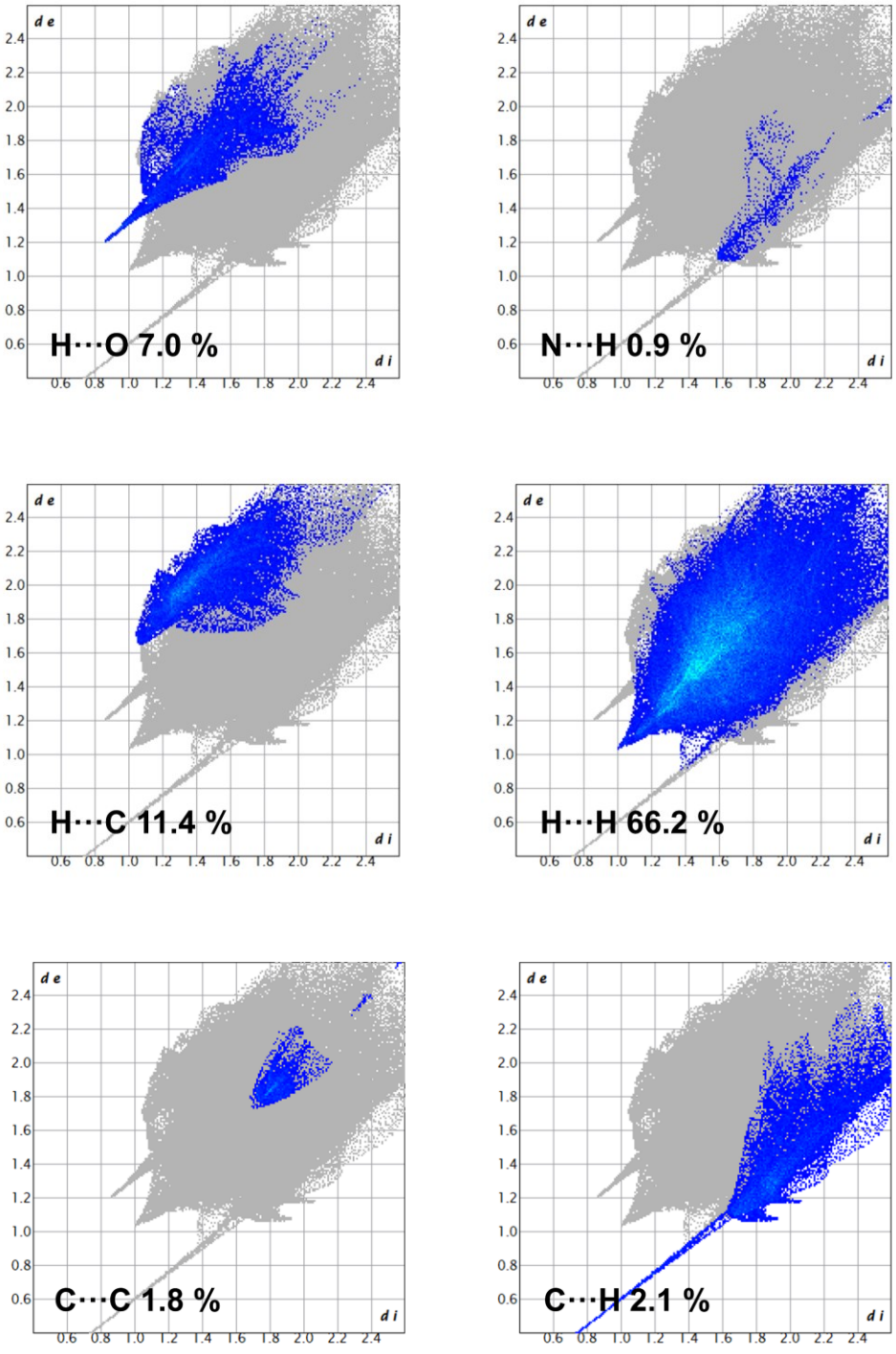


Figure S50. The **2D** Hirshfeld fingerprints of (**G7**)

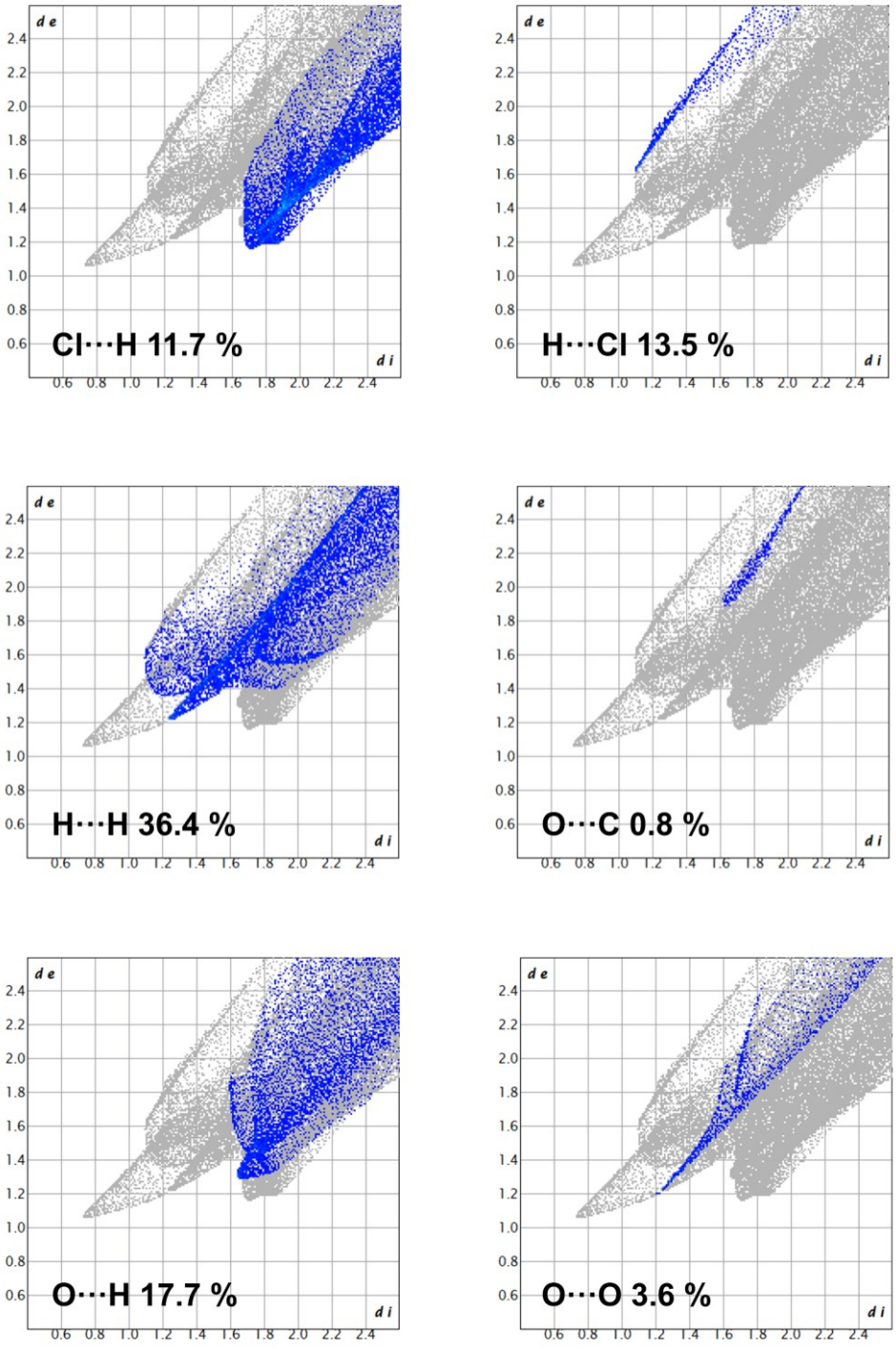


Figure S51. The **2D** Hirshfeld fingerprints of (**G8**)

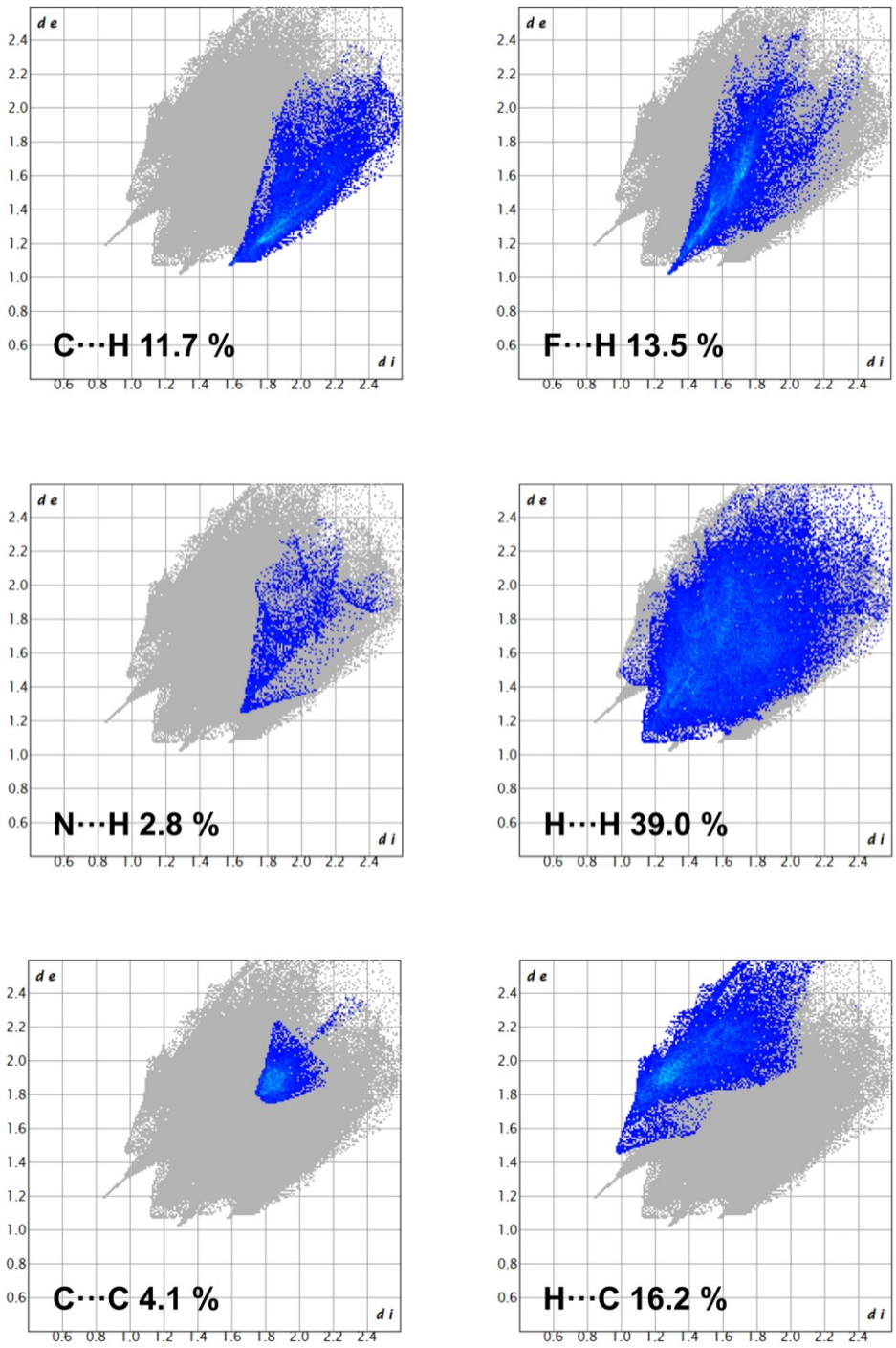


Figure S52. The **2D** Hirshfeld fingerprints of (**G9**)

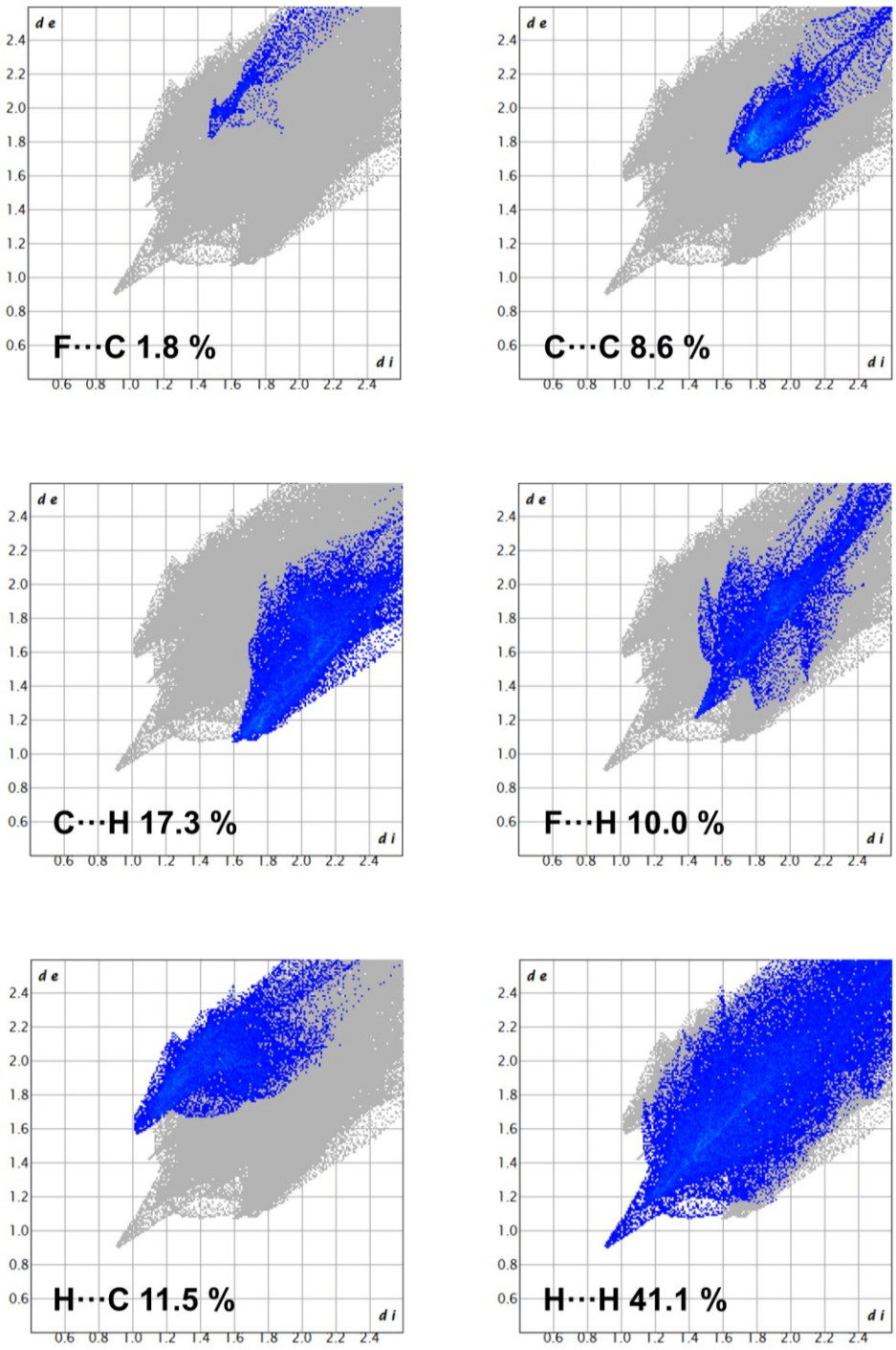


Figure S53. The **2D** Hirshfeld fingerprints of (**G10**)

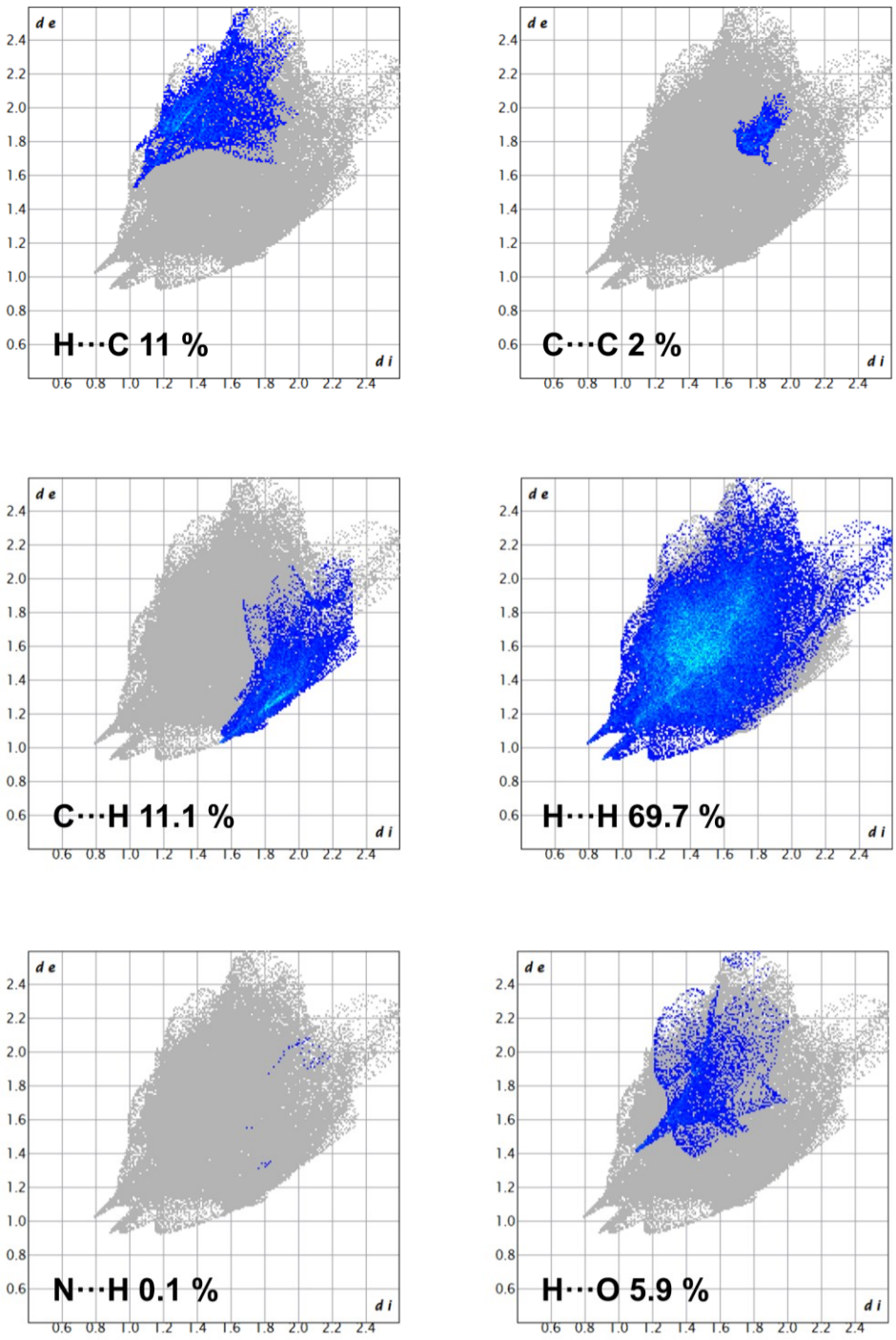


Figure S54. The **2D** Hirshfeld fingerprints of (**G11**)

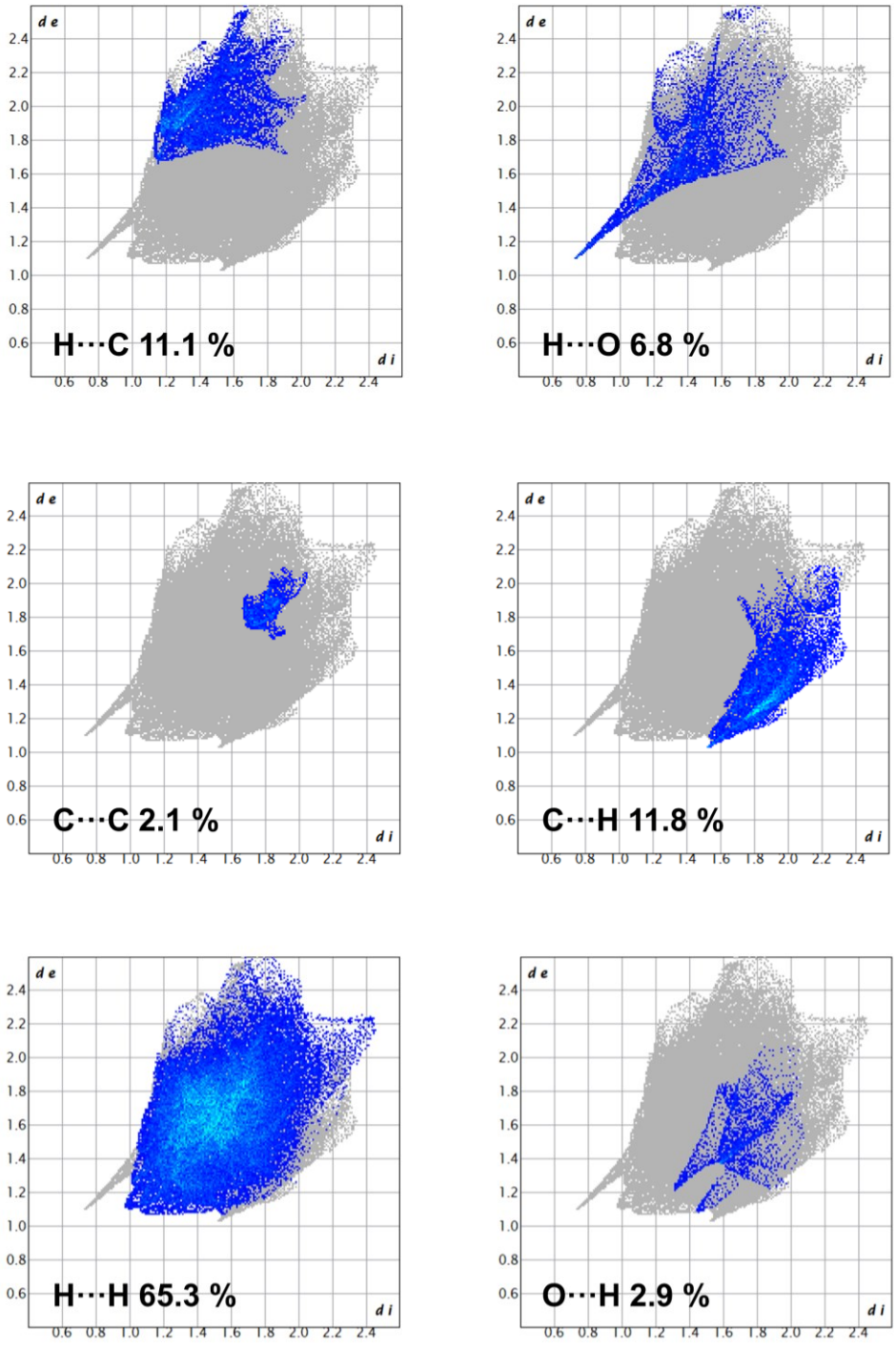


Figure S55. The **2D** Hirshfeld fingerprints of (**G12**)

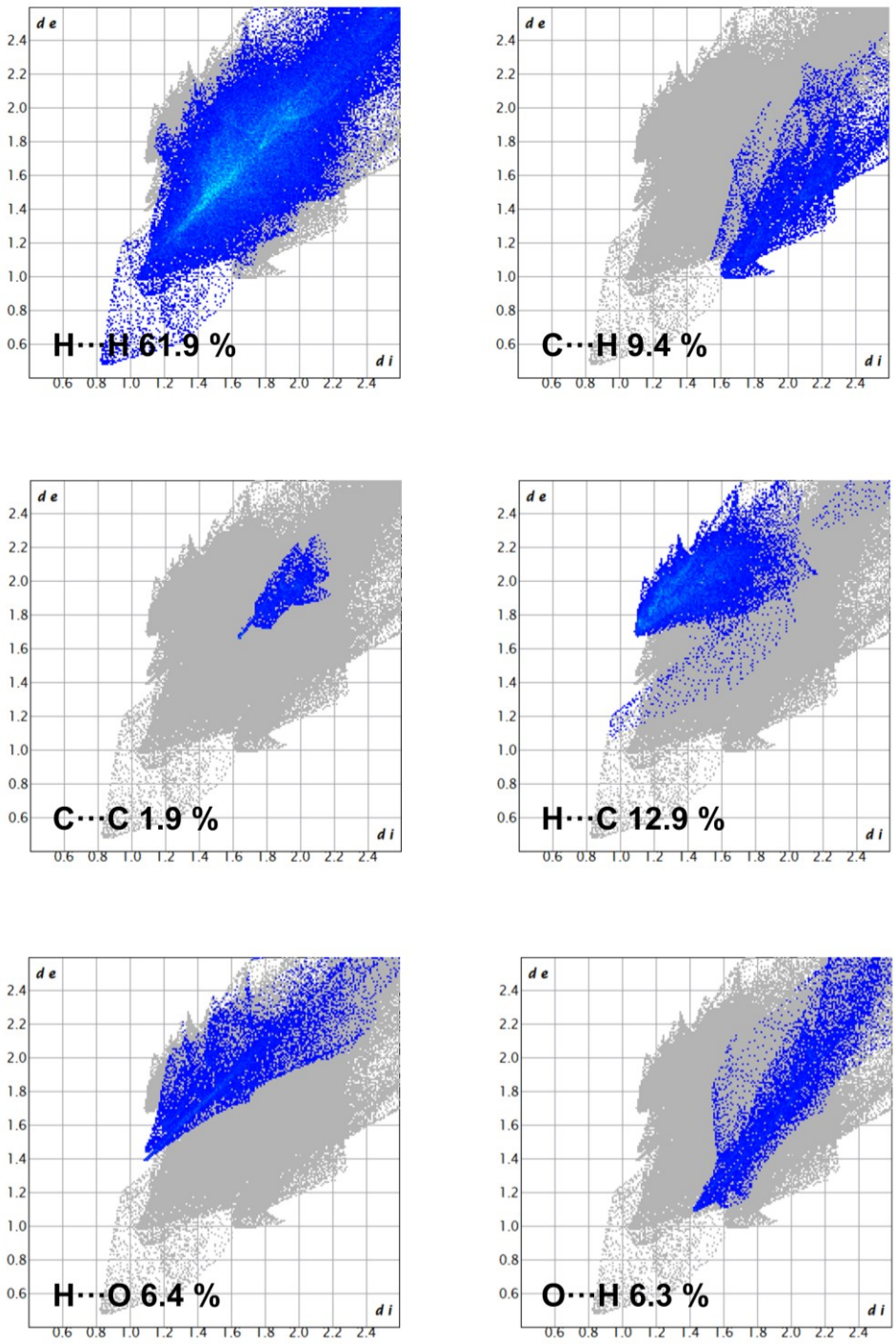


Figure S56. The **2D** Hirshfeld fingerprints of (**G13**)

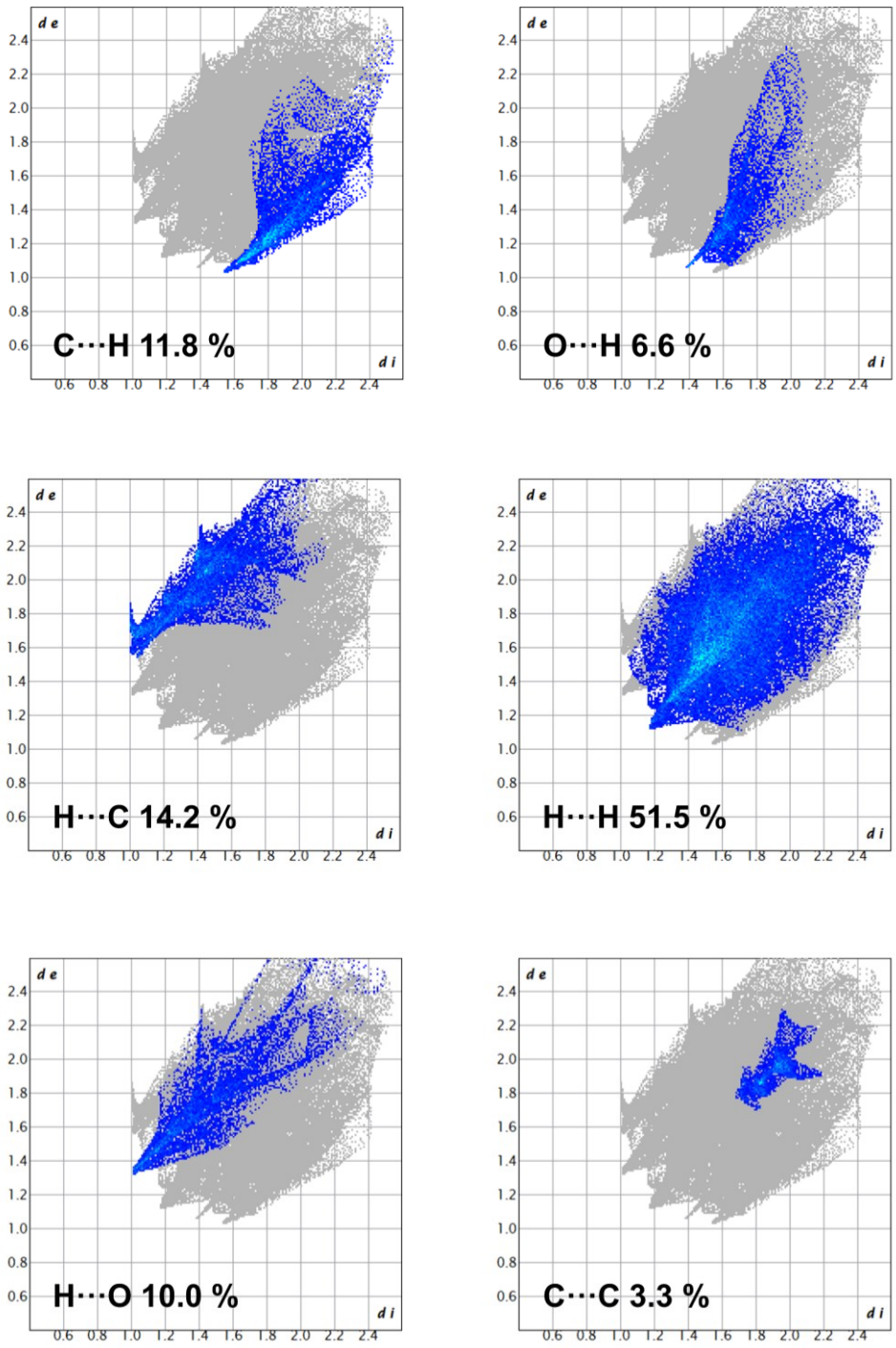


Figure S57. The **2D** Hirshfeld fingerprints of (**G14**)

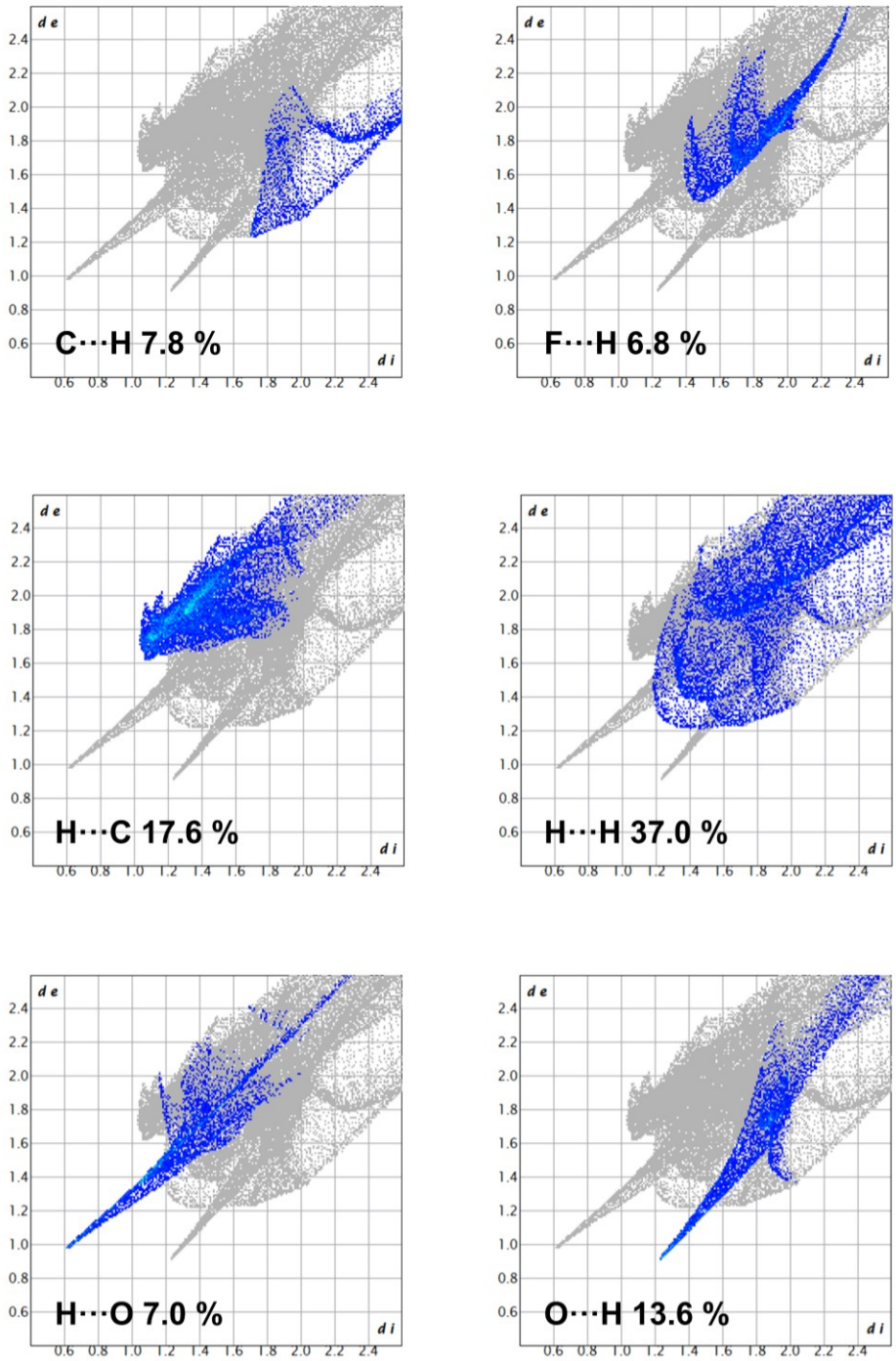


Figure S58. The **2D** Hirshfeld fingerprints of (**G15**)

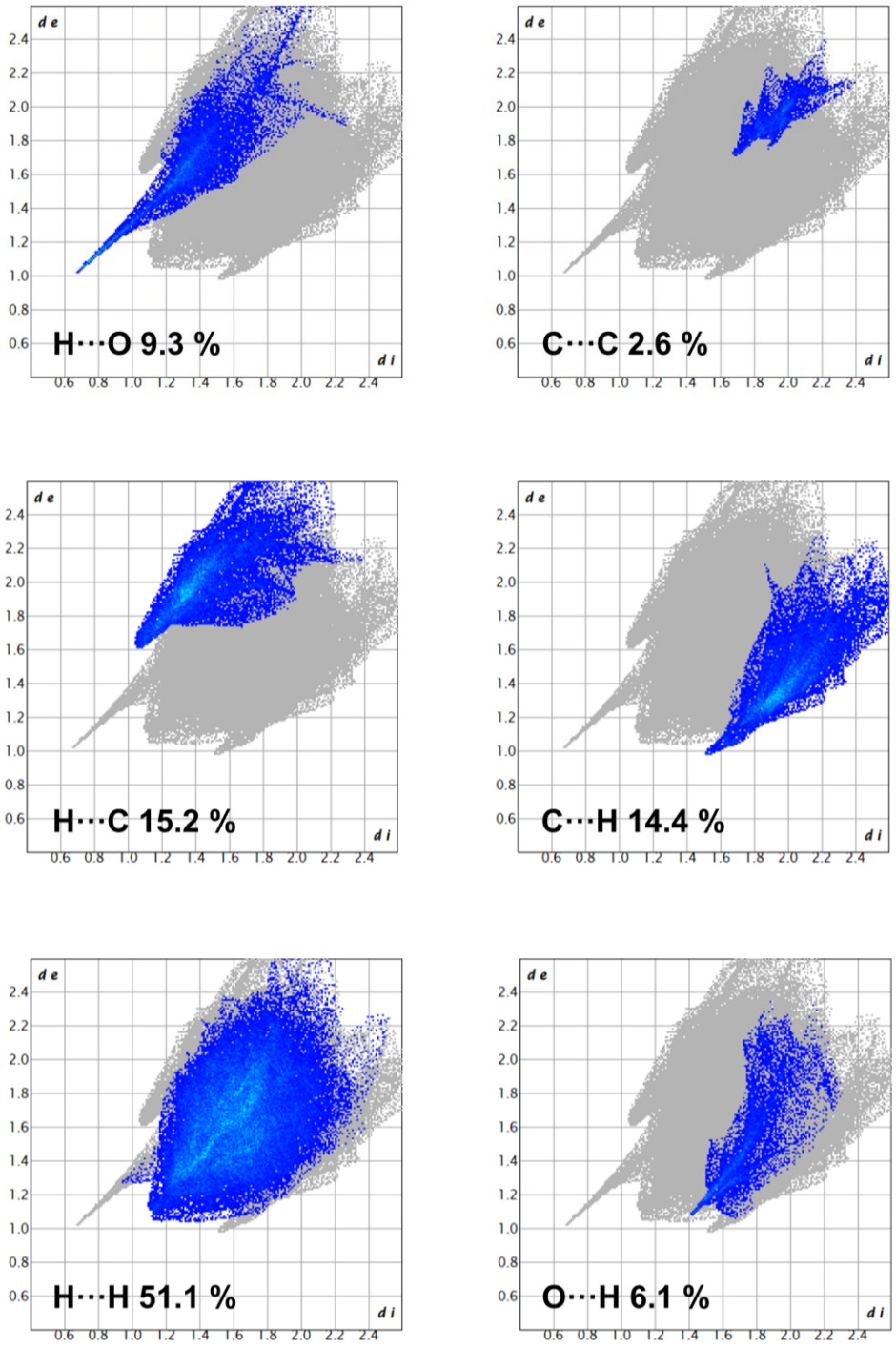


Figure S59. The **2D** Hirshfeld fingerprints of (**G16**)

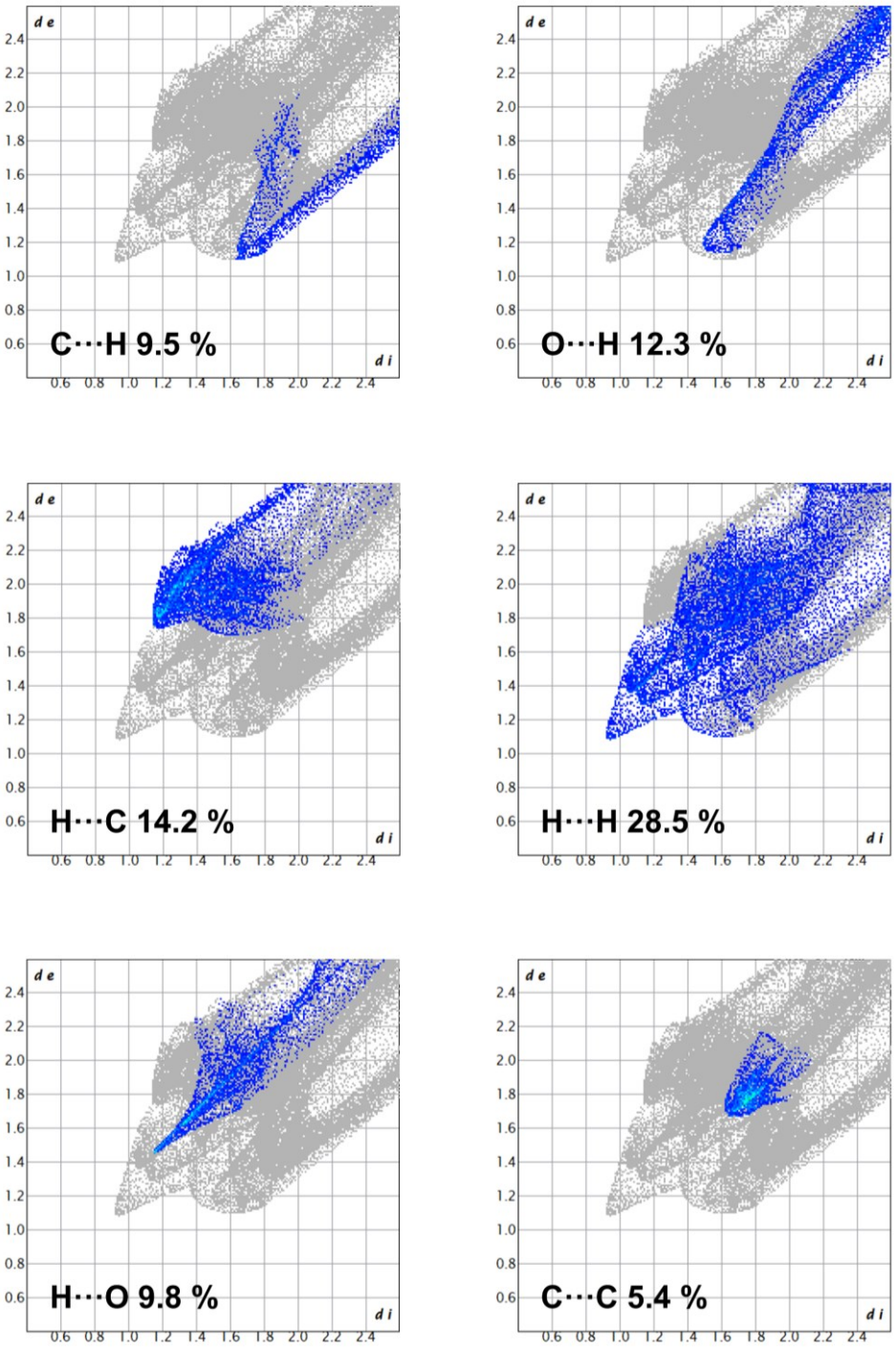


Figure S60. The **2D** Hirshfeld fingerprints of (**G17**)

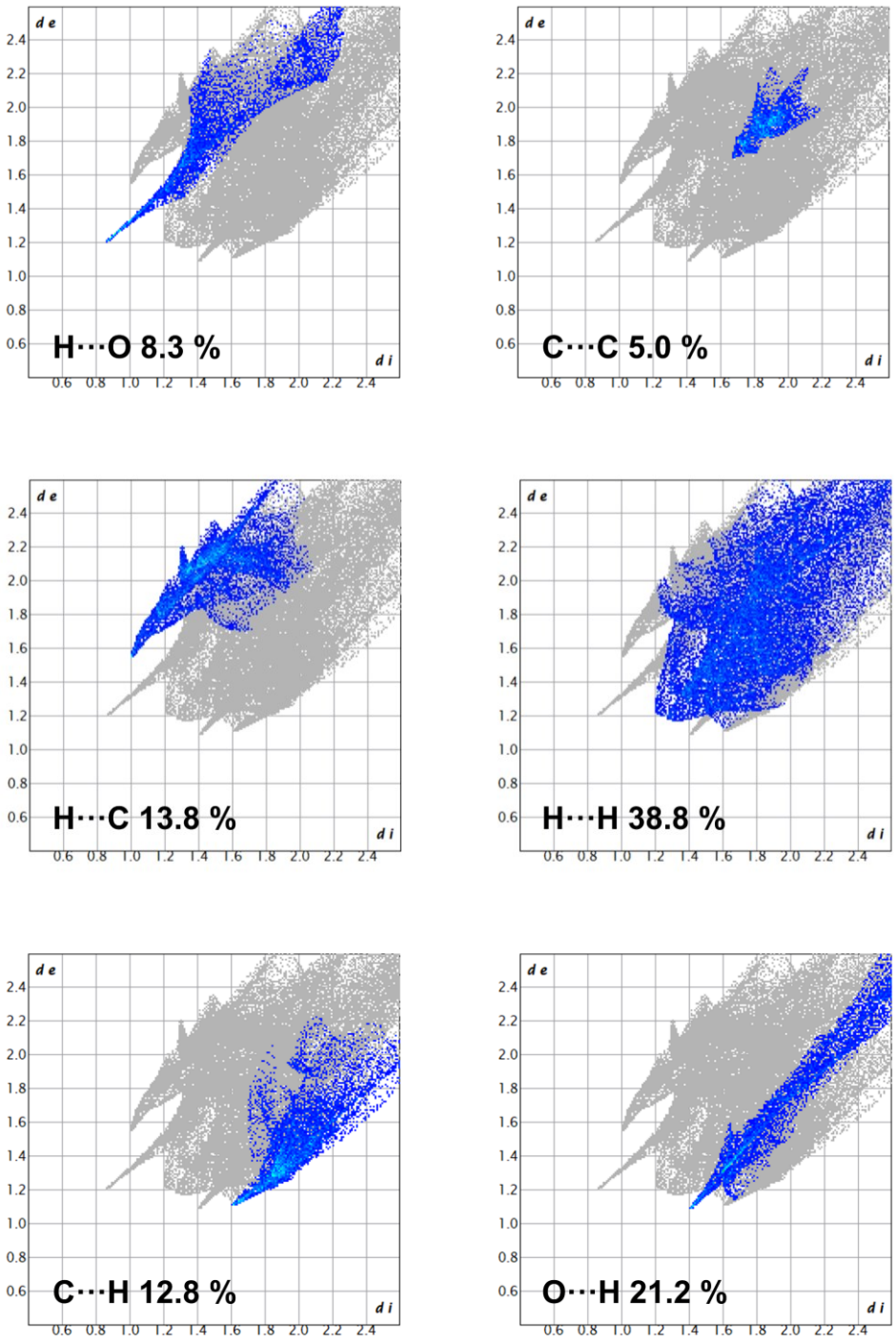


Figure S61. The **2D** Hirshfeld fingerprints of (**G18**)

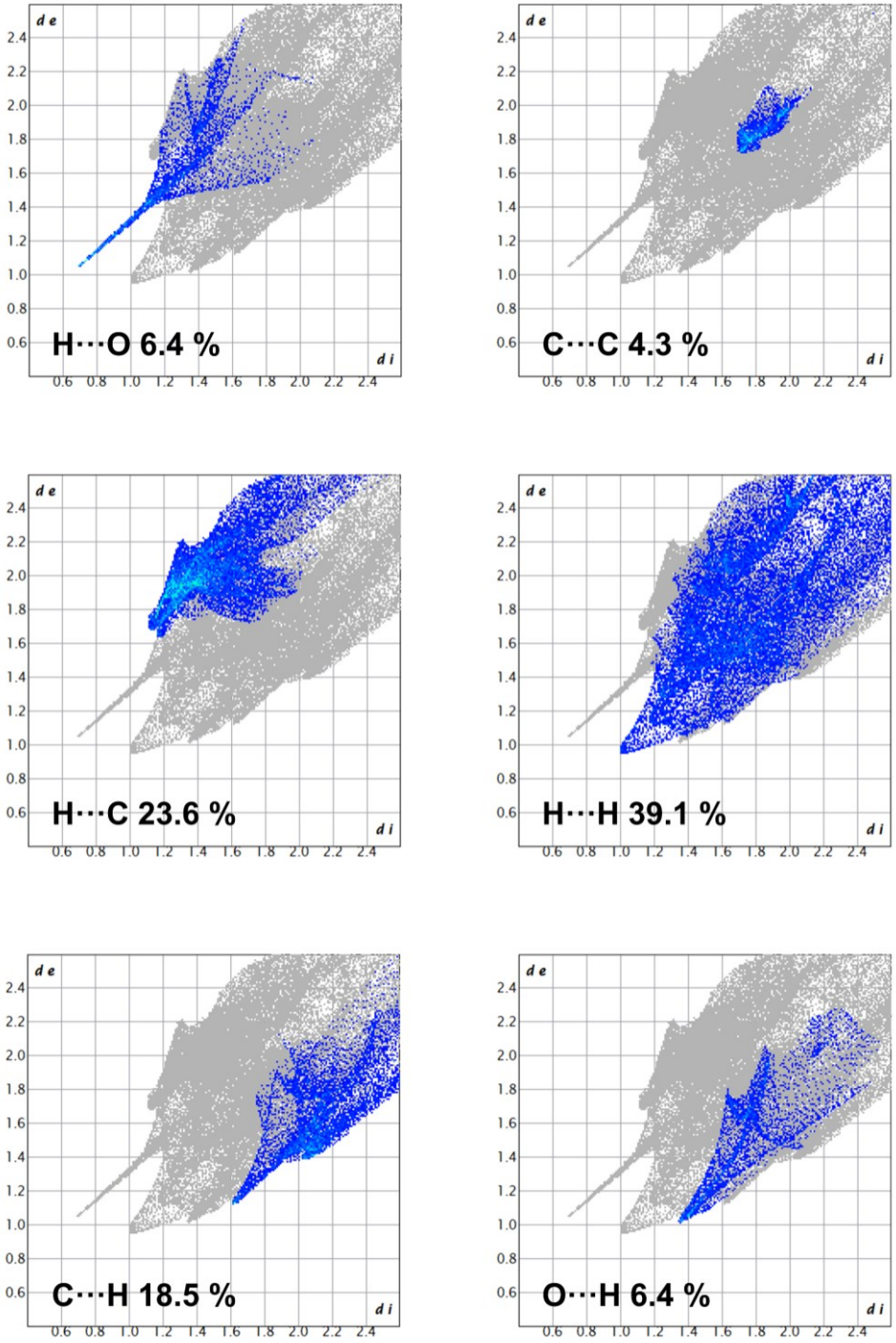


Figure S62. The **2D** Hirshfeld fingerprints of (**G19**)

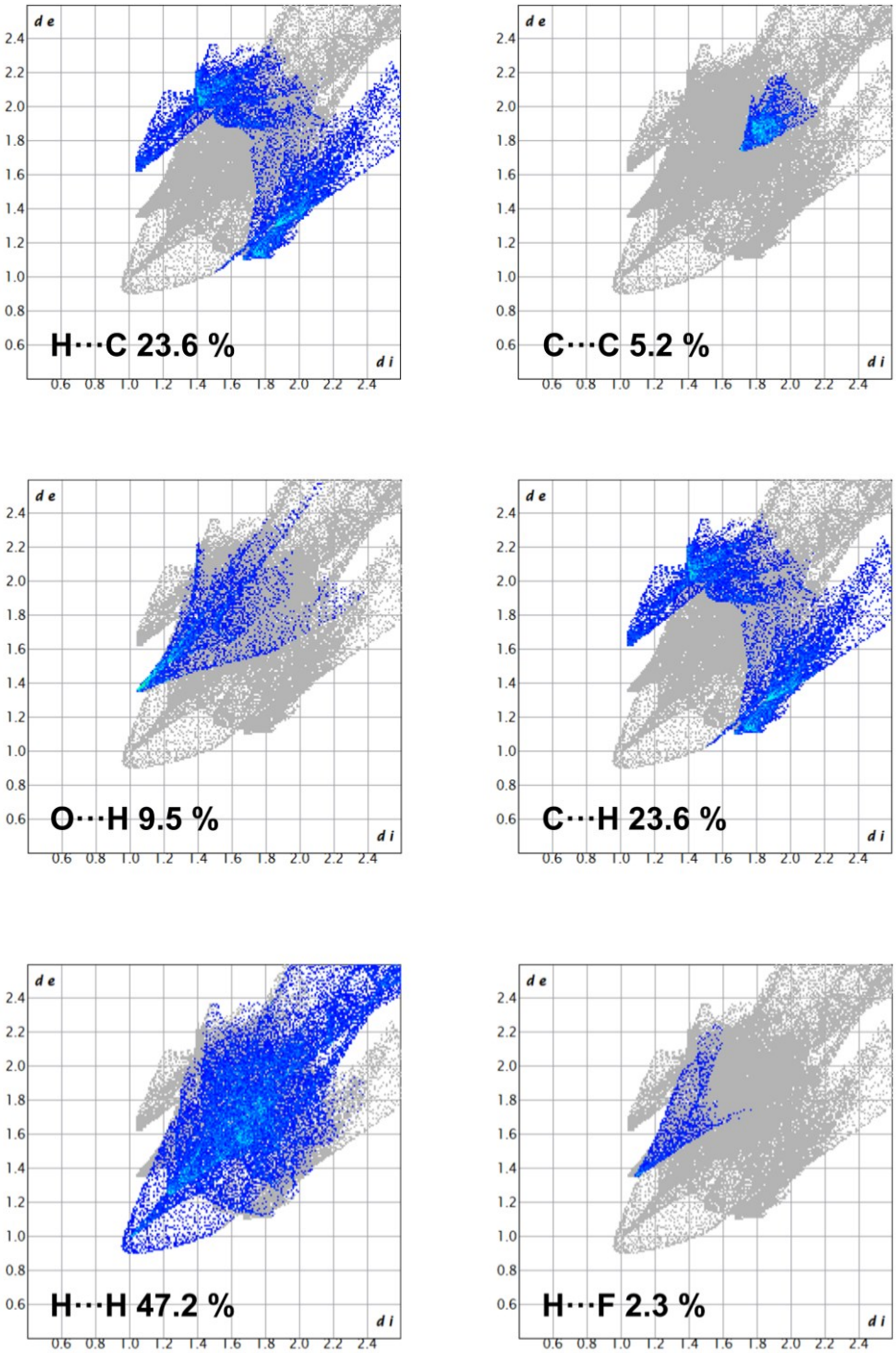


Figure S63. The **2D** Hirshfeld fingerprints of (**G20**)

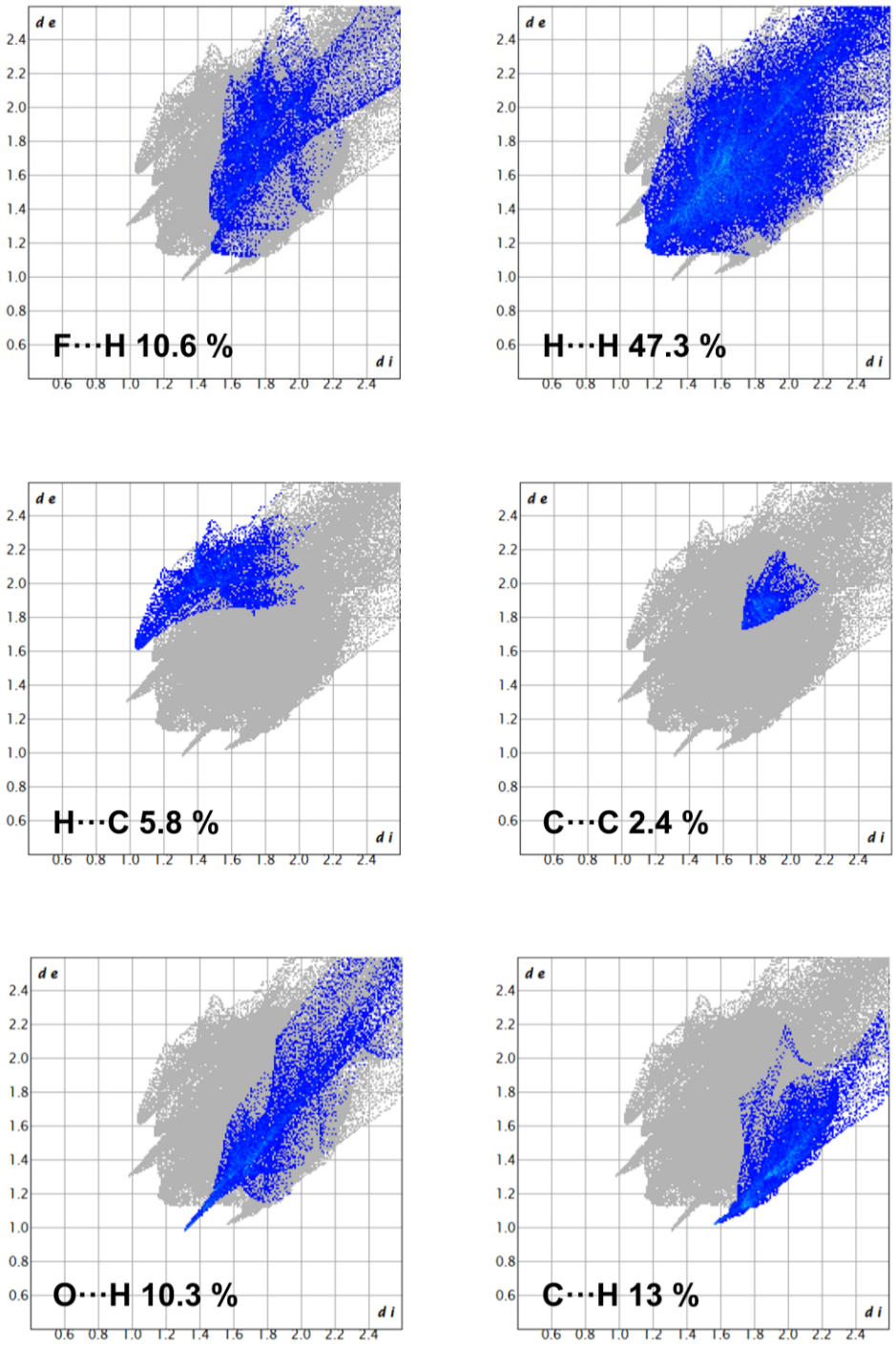


Figure S64. The **2D** Hirshfeld fingerprints of (**G21**)

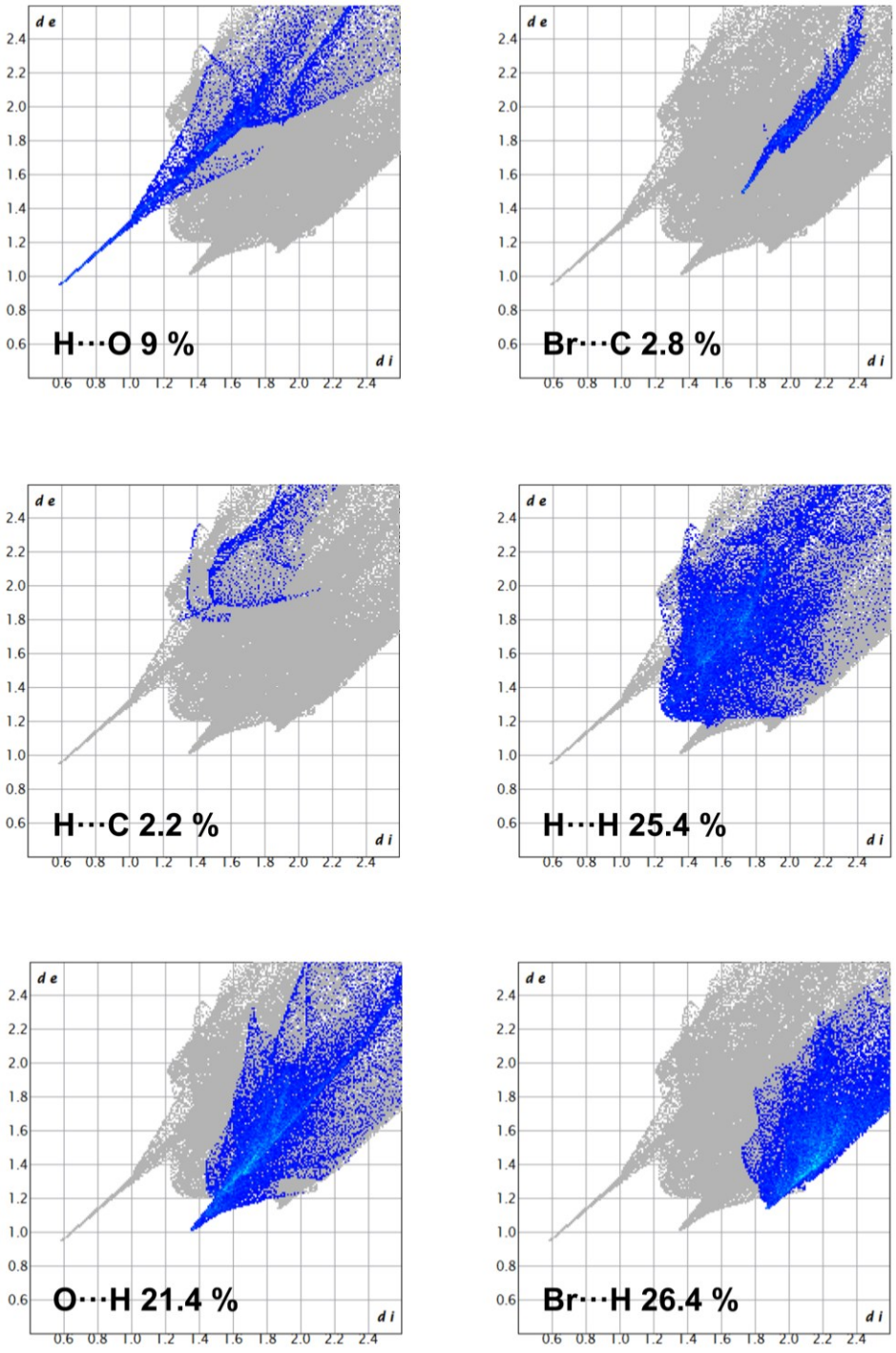


Figure S65. The **2D** Hirshfeld fingerprints of (**G22**)

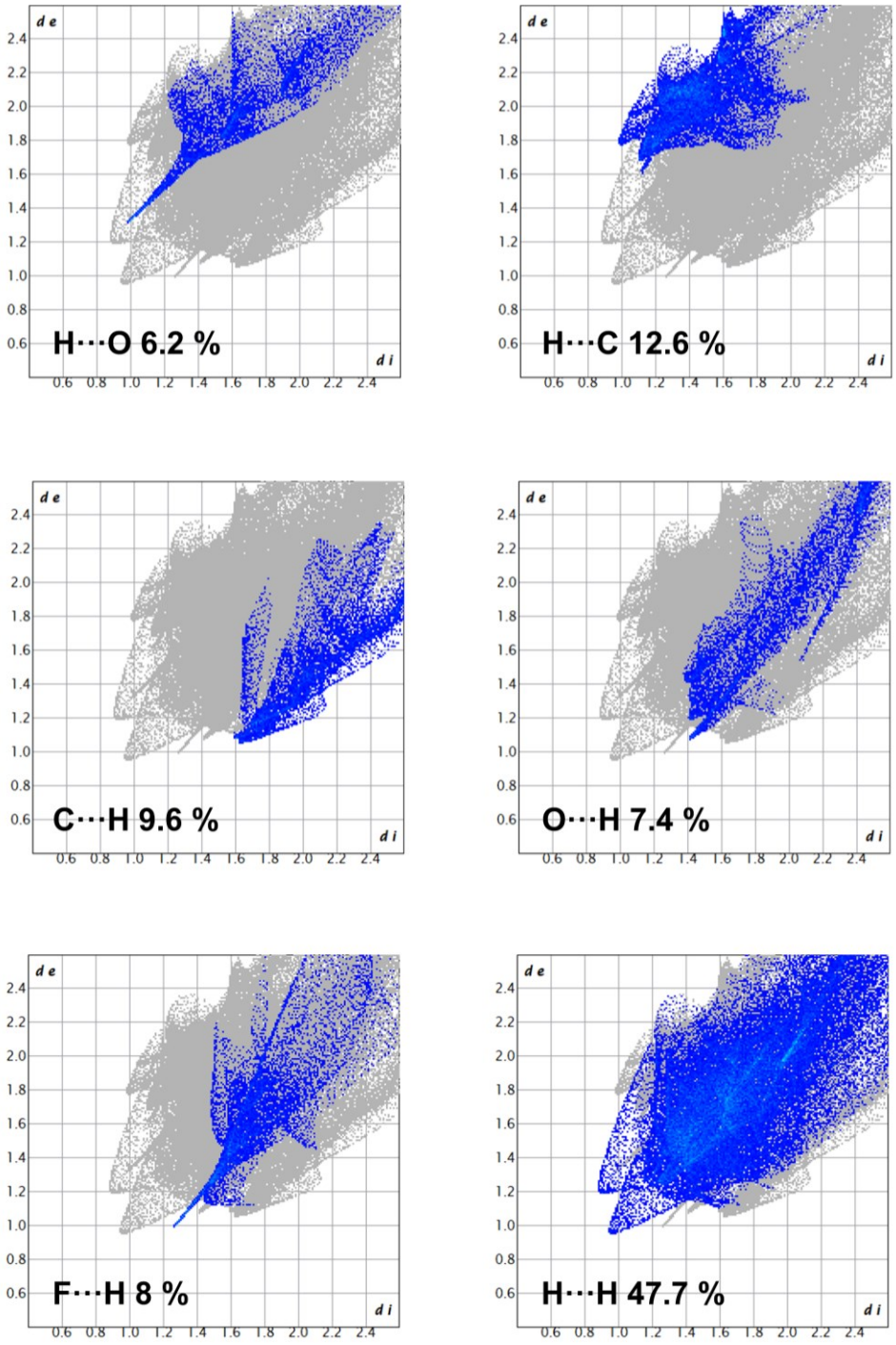


Figure S66. The **2D** Hirshfeld fingerprints of (**G23**)

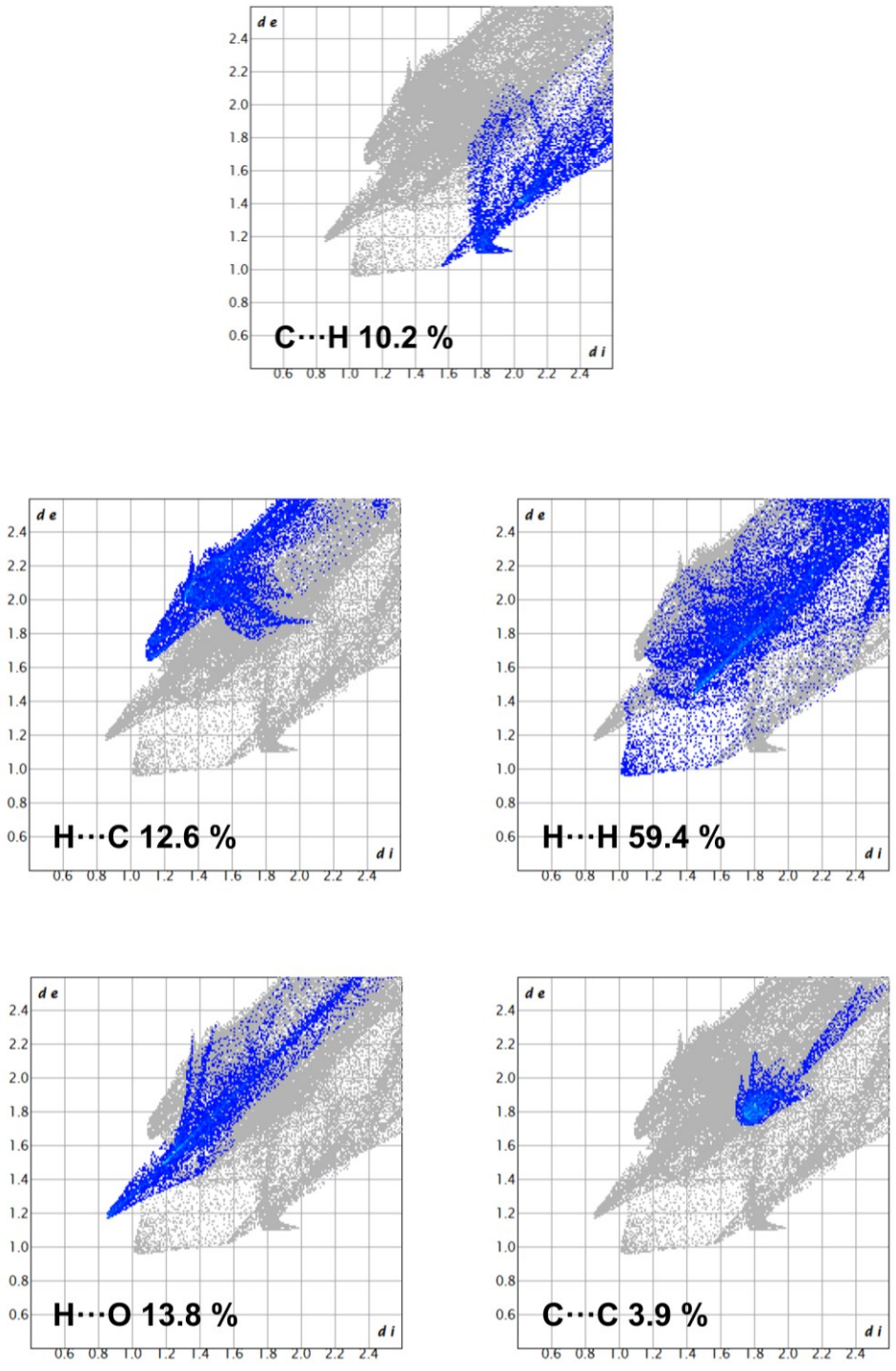


Figure S67. The **2D** Hirshfeld fingerprints of (**G24**)

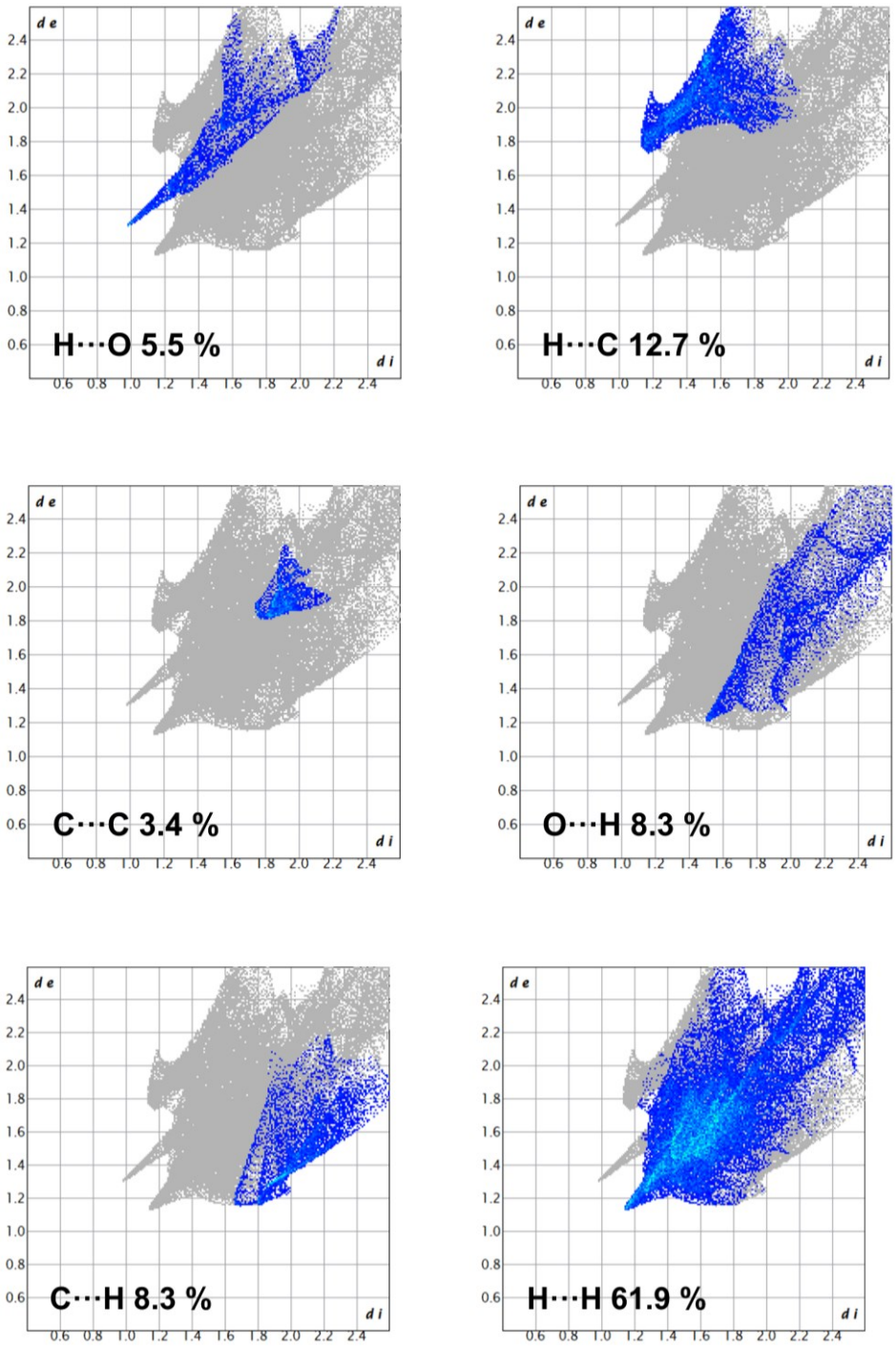


Figure S68. The **2D** Hirshfeld fingerprints of (**G25**)

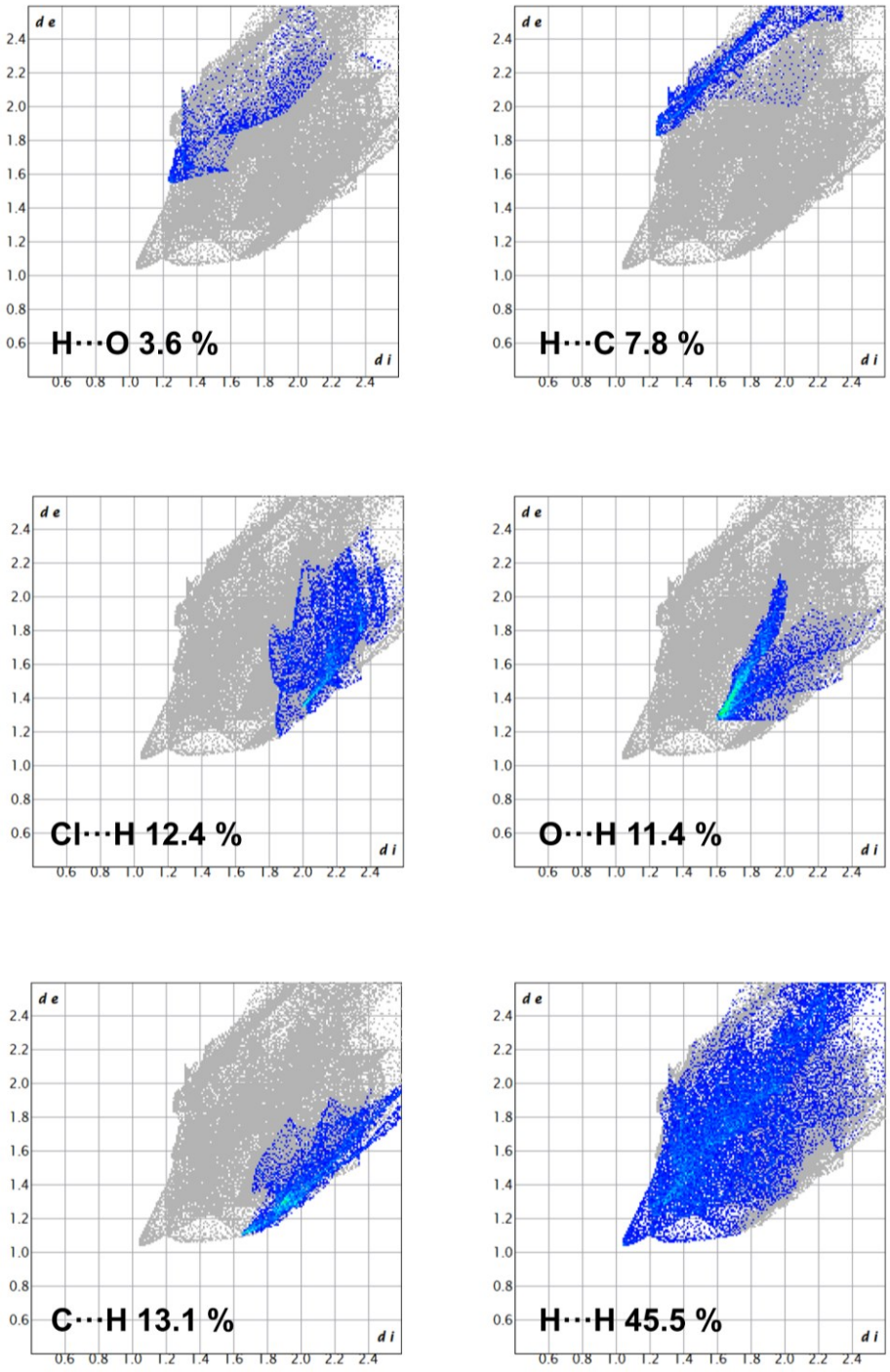


Figure S69. The **2D** Hirshfeld fingerprints of (**G26**)

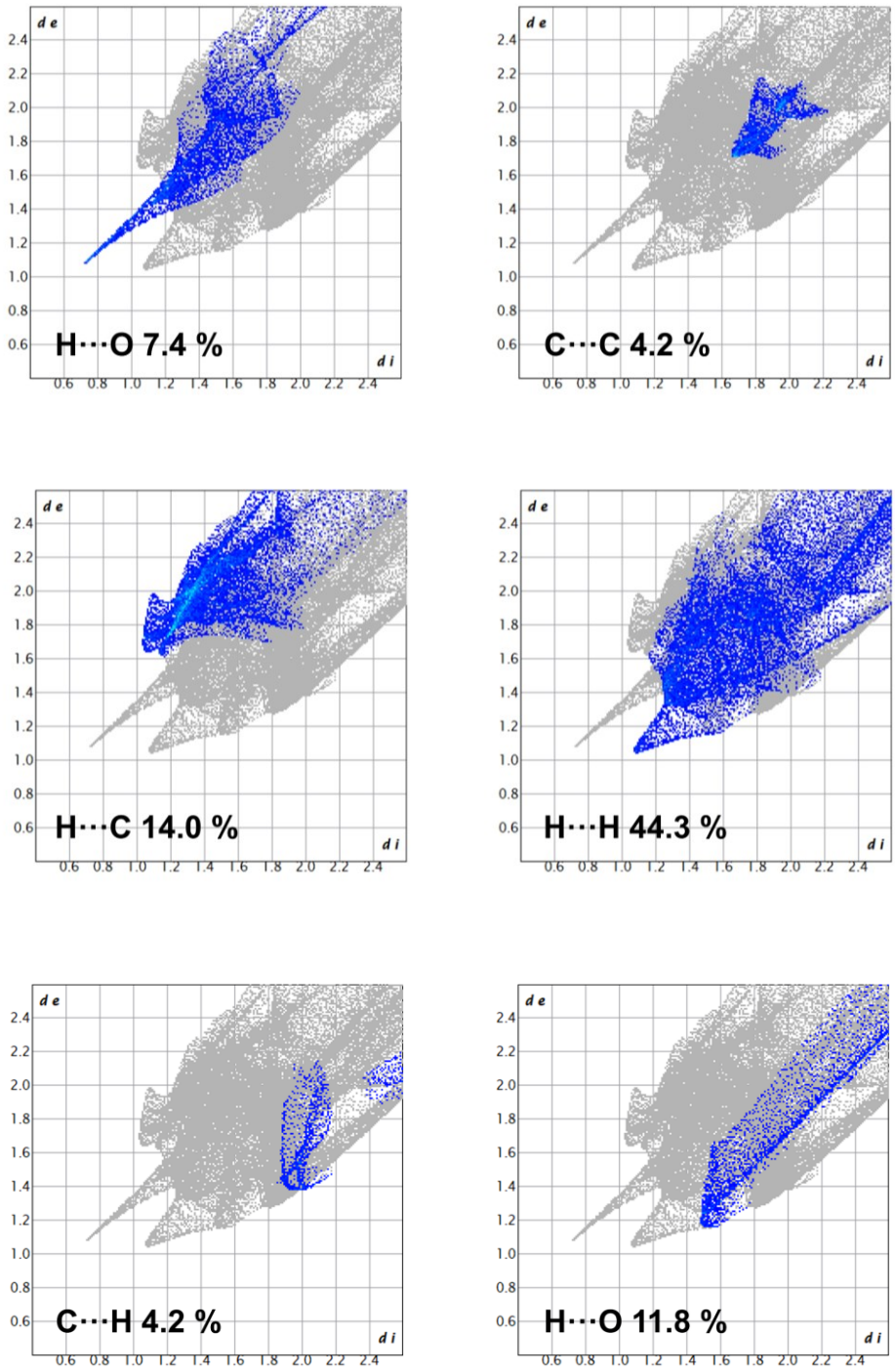


Figure S70. The **2D** Hirshfeld fingerprints of (**G27**)

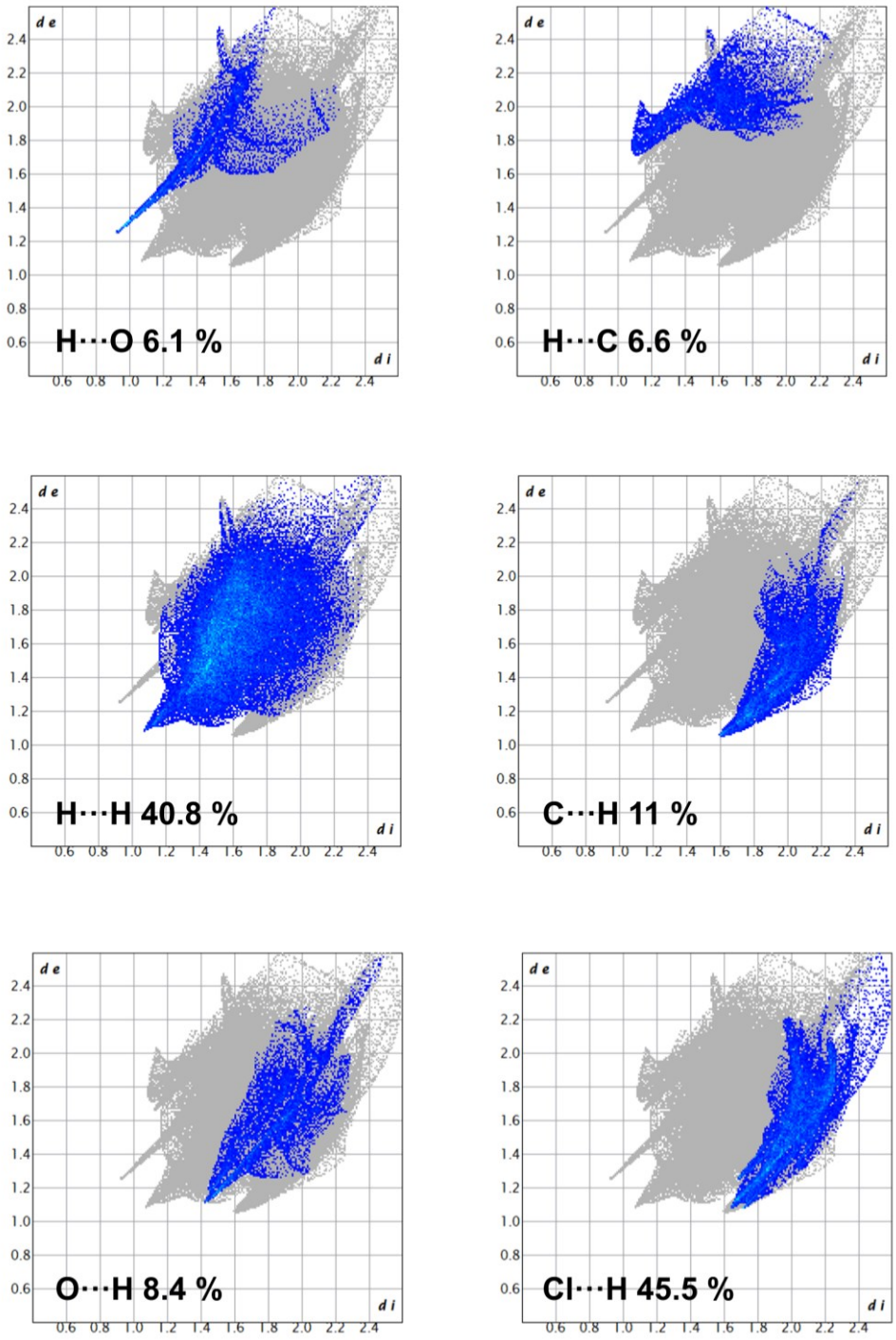


Figure S71. The **2D** Hirshfeld fingerprints of (**G28**)

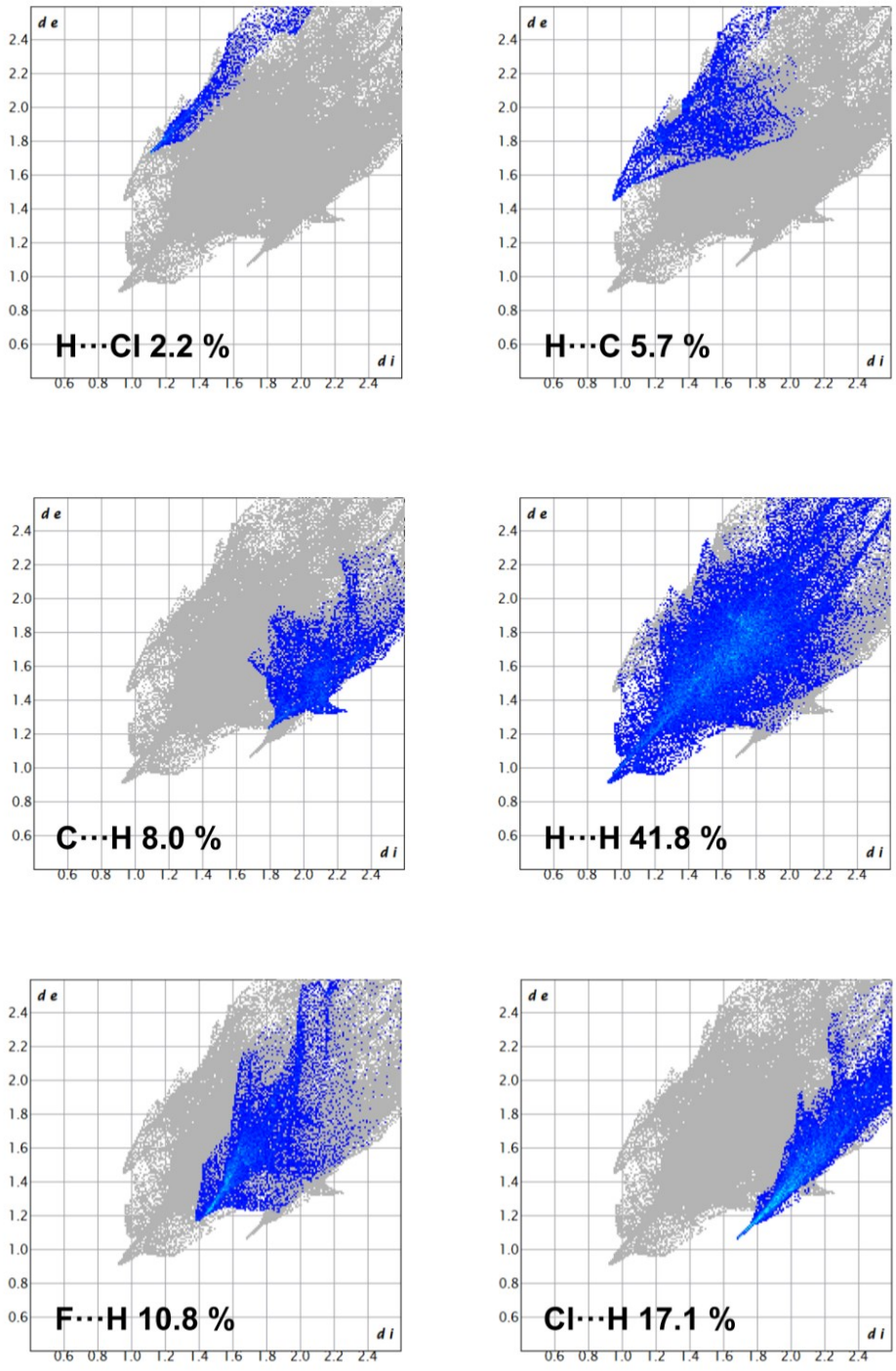


Figure S72. The **2D** Hirshfeld fingerprints of (**G29**)

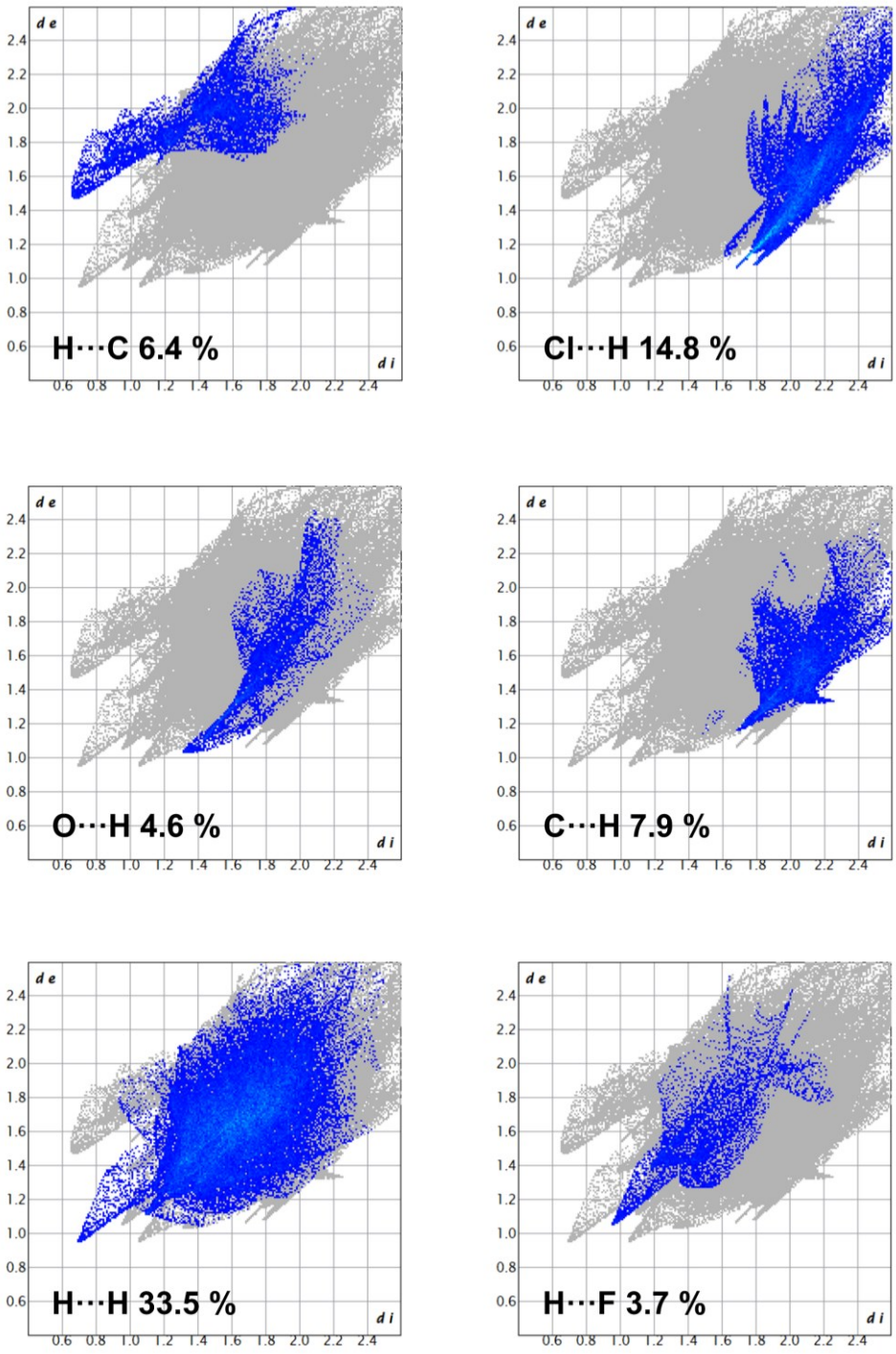


Figure S73. The **2D** Hirshfeld fingerprints of (**G30**)

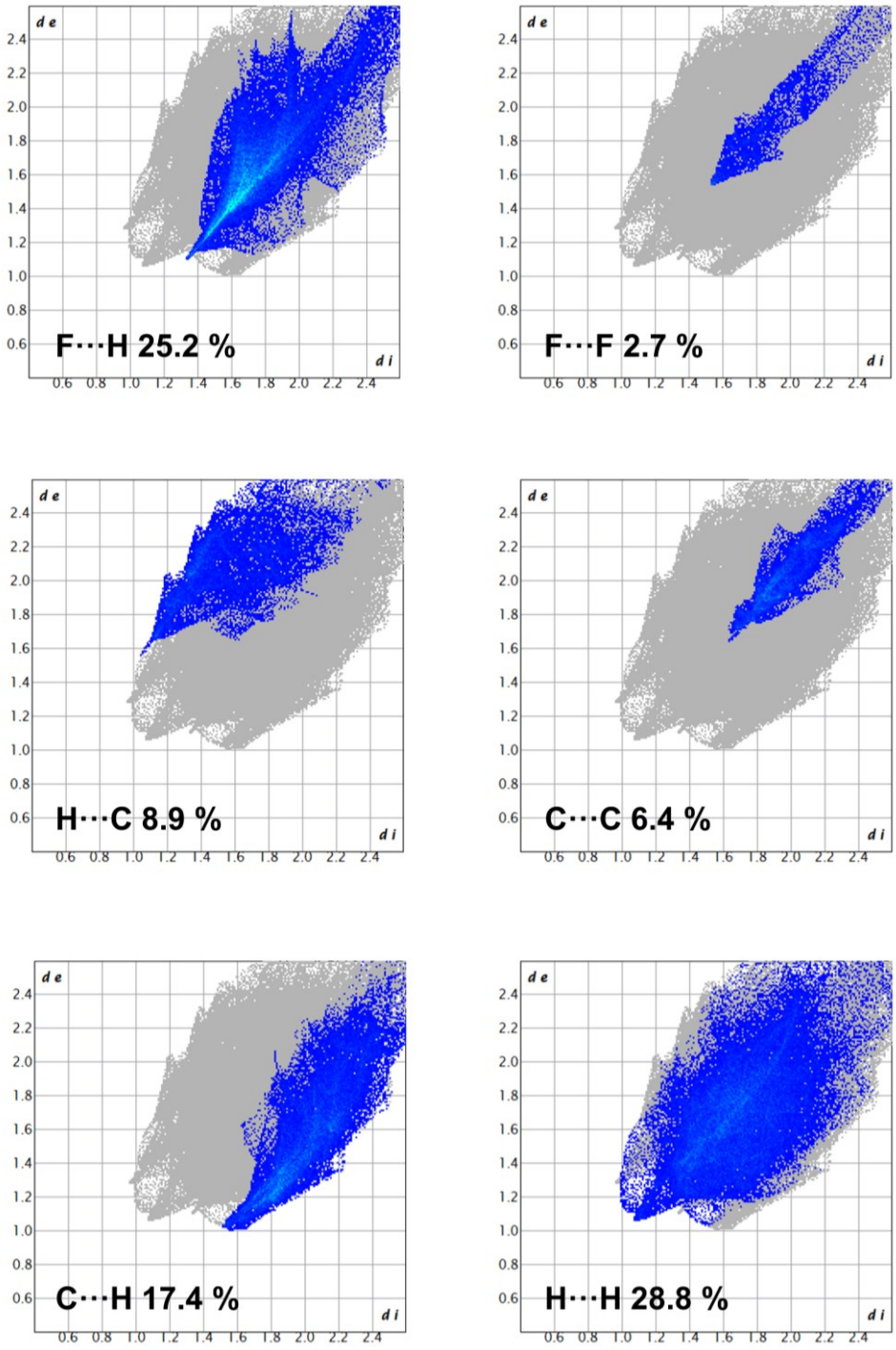


Figure S74. The **2D** Hirshfeld fingerprints of (**G31**)

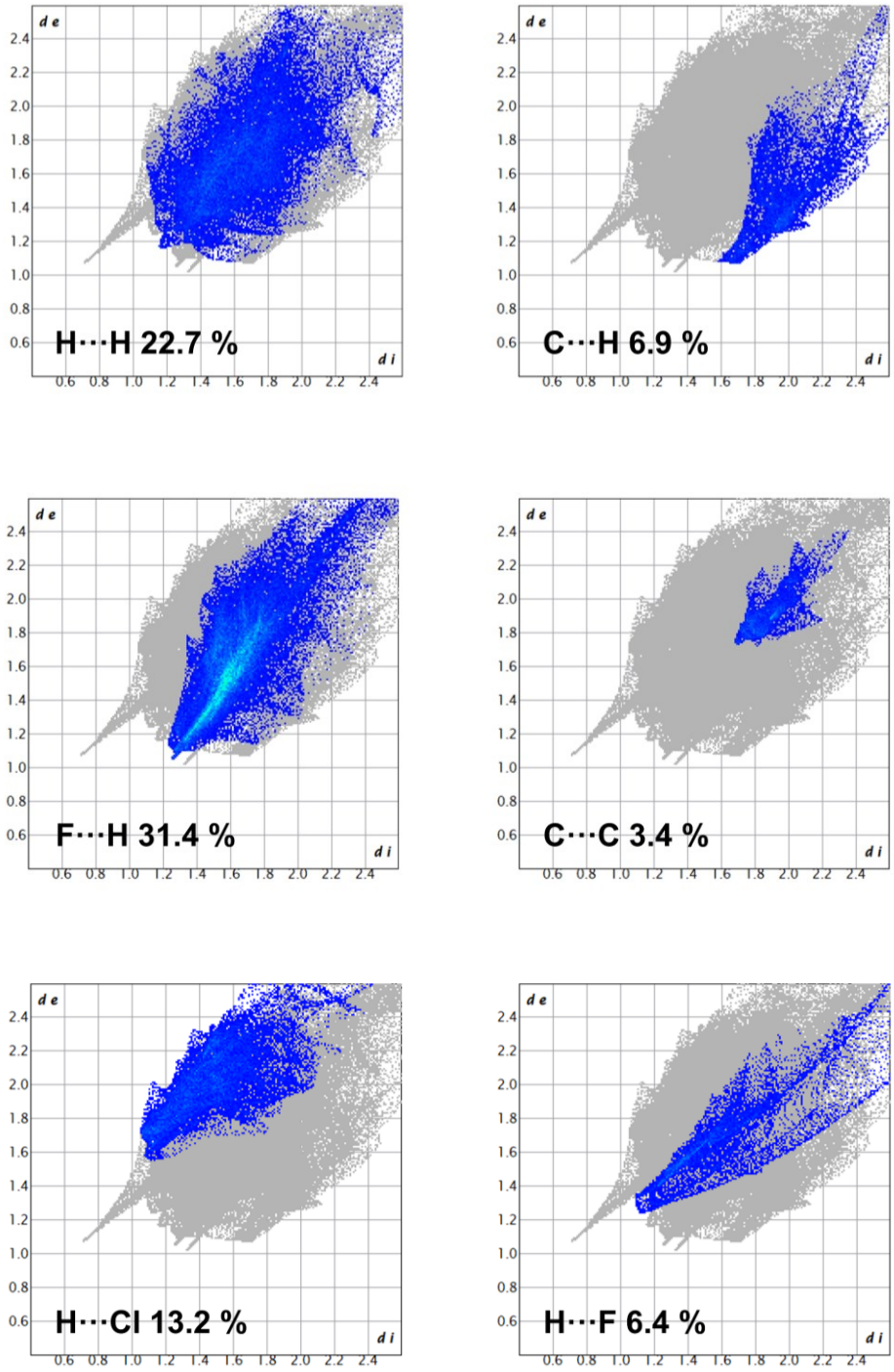


Figure S75. The **2D** Hirshfeld fingerprints of (**G32**)

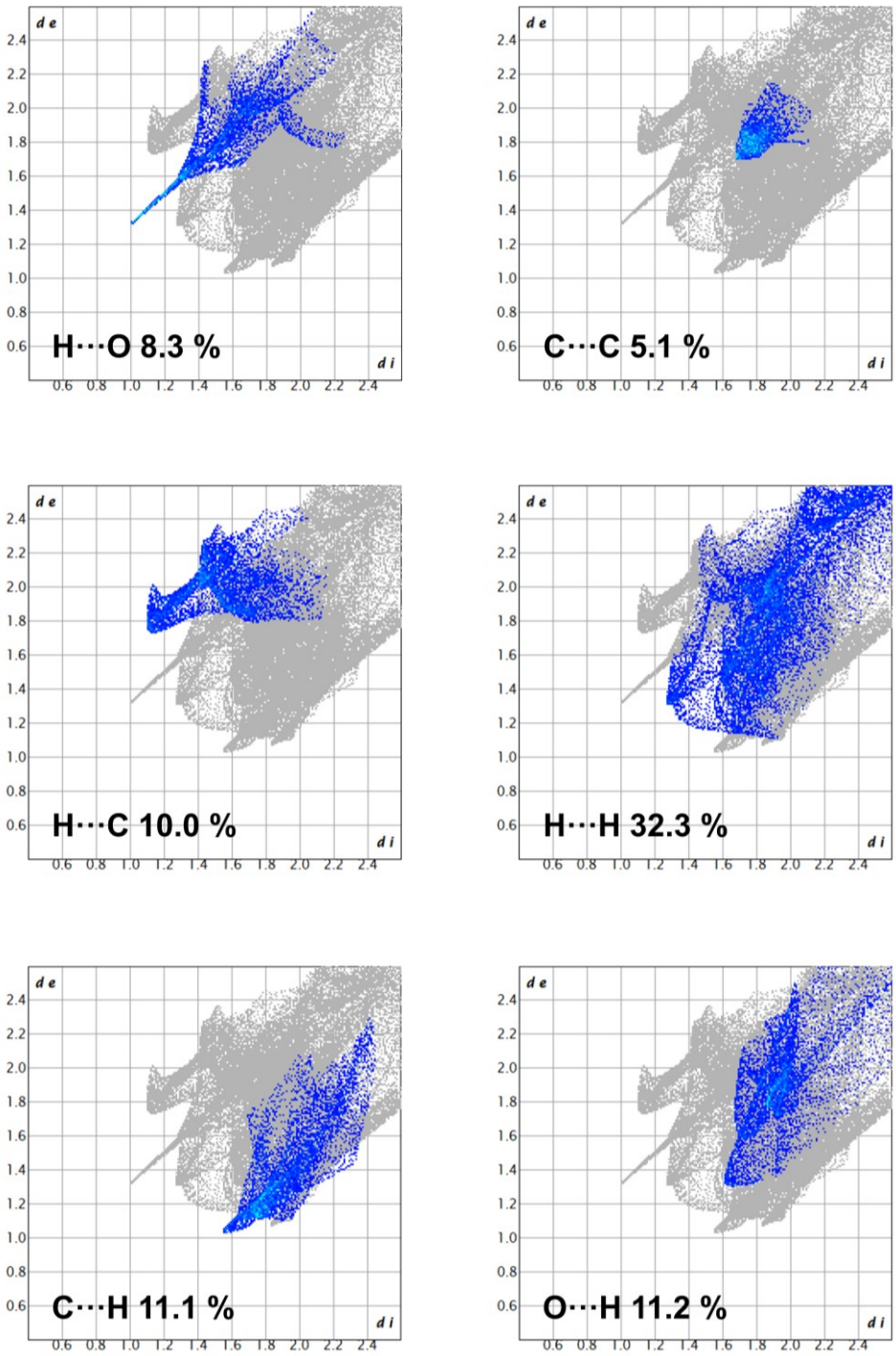


Figure S76. The **2D** Hirshfeld fingerprints of (**G33**)

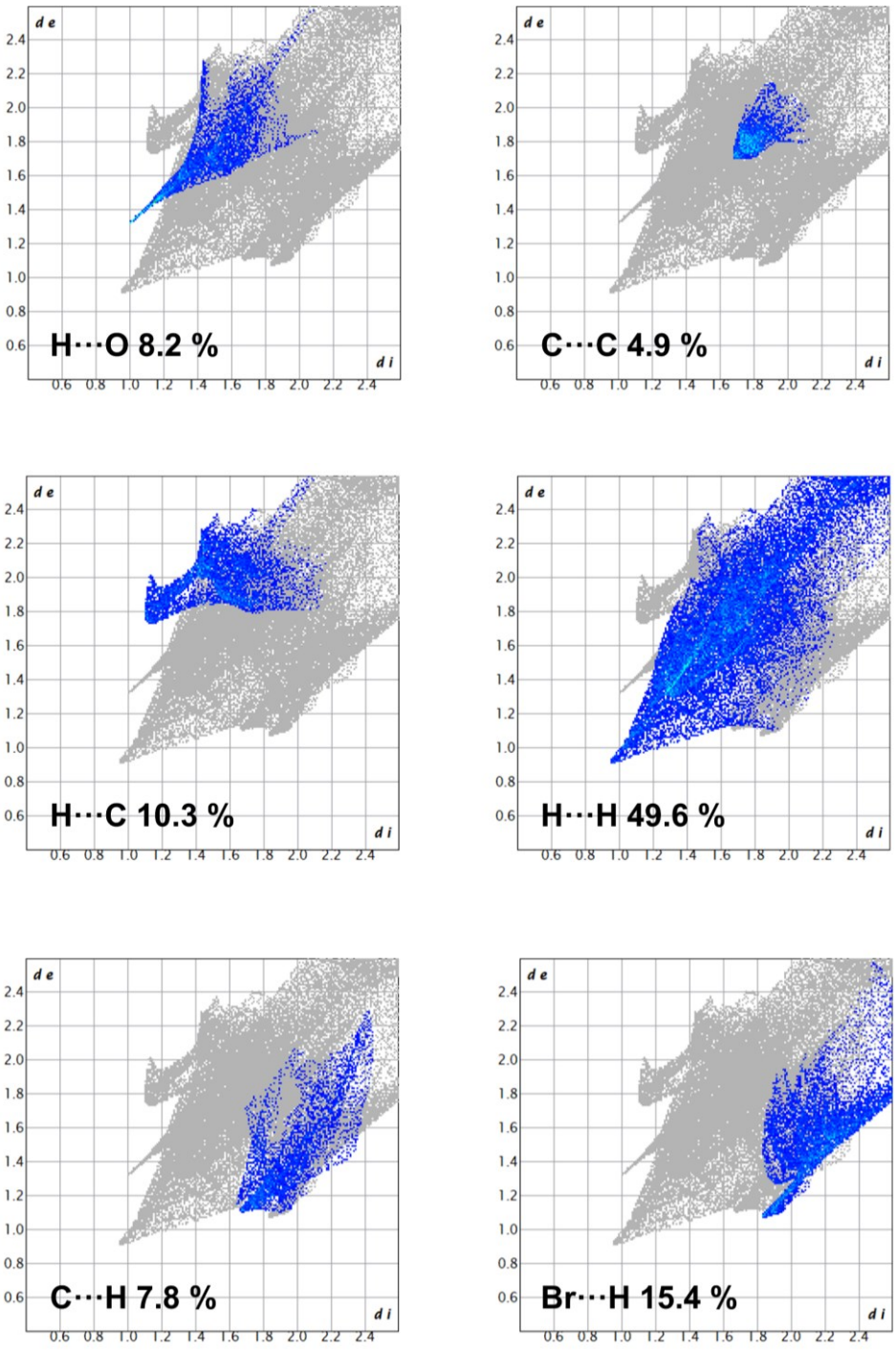


Figure S77. The **2D** Hirshfeld fingerprints of (**G34**)

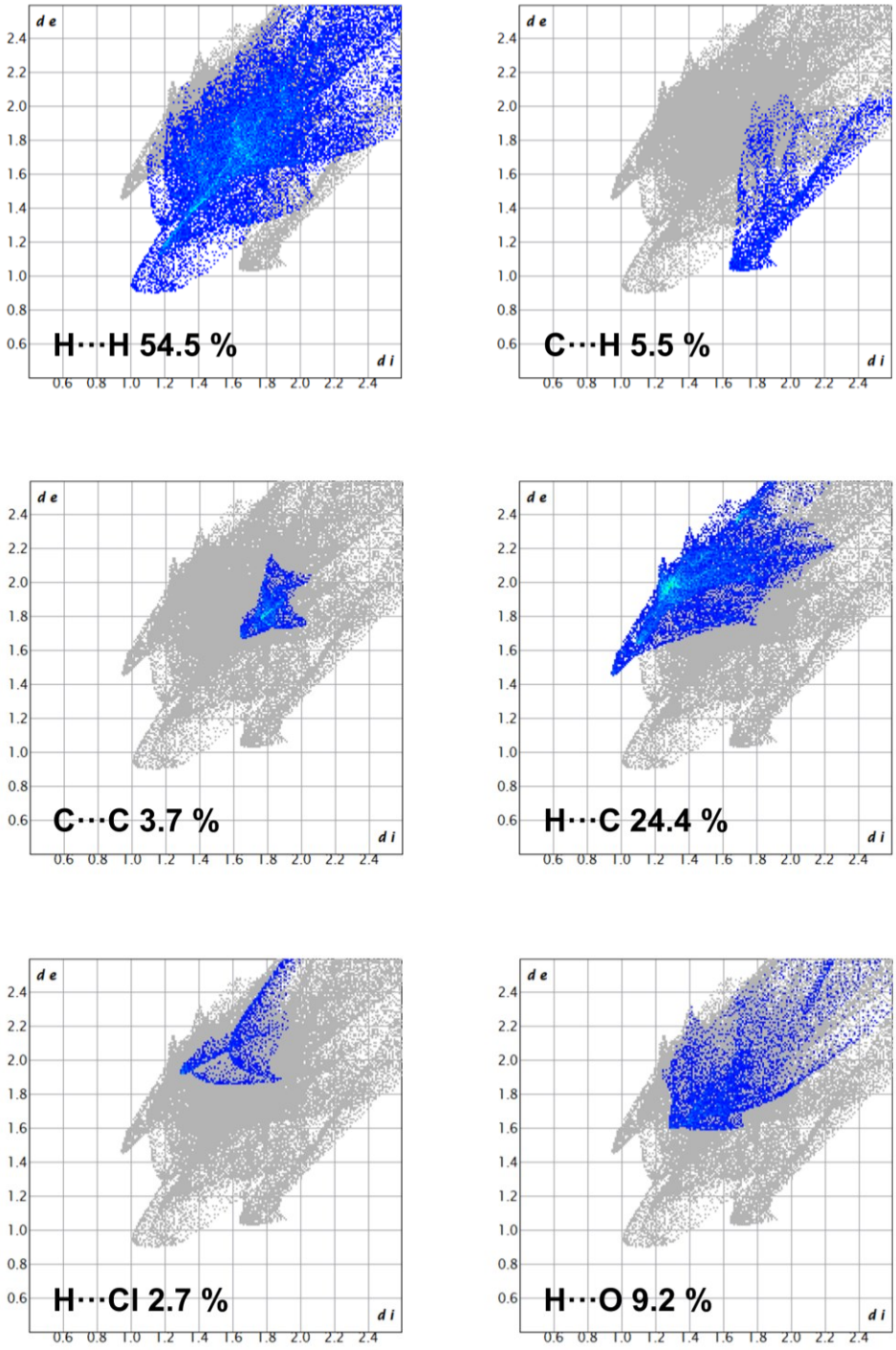


Figure S78. The **2D** Hirshfeld fingerprints of (**G35**)

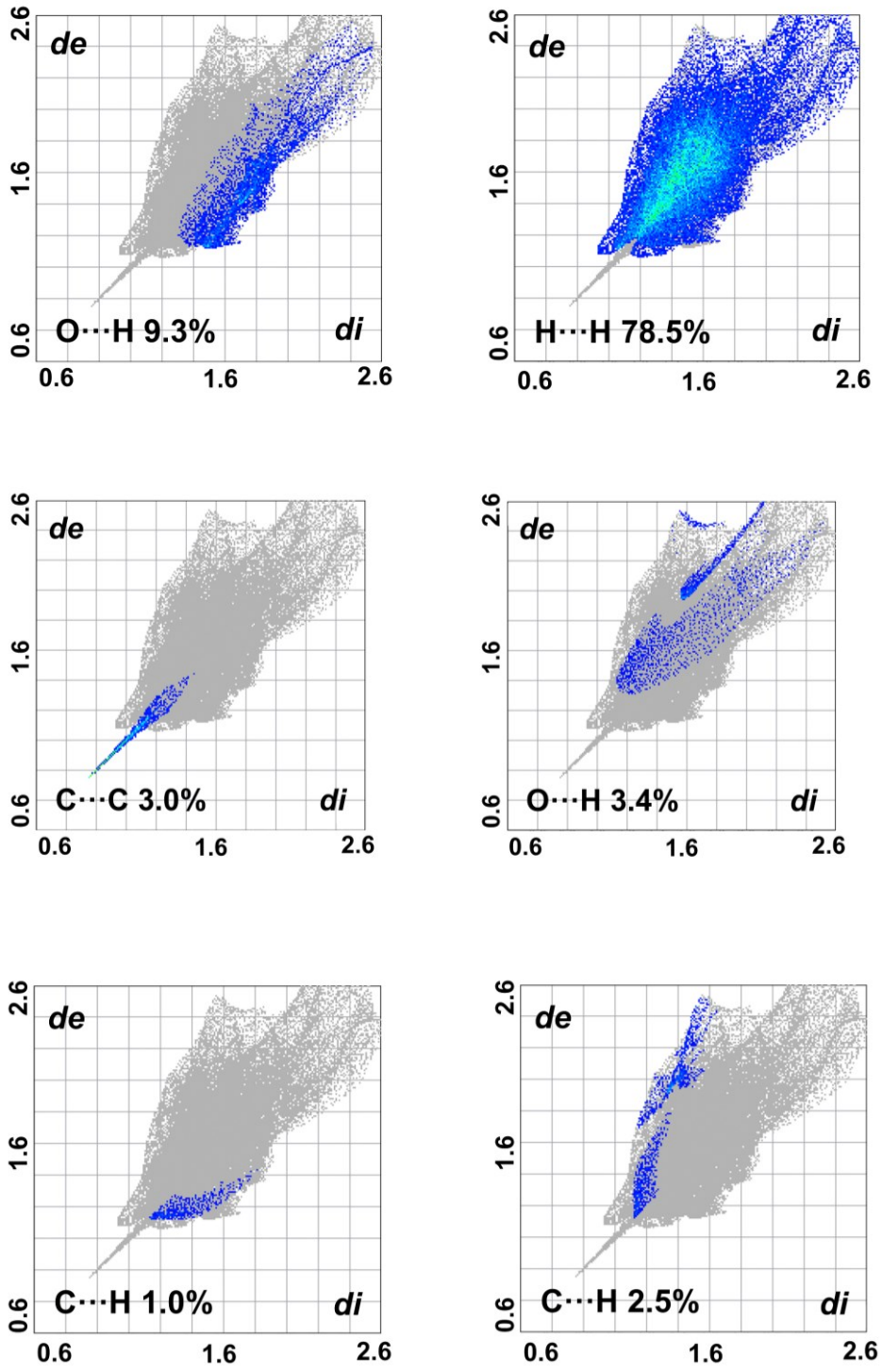


Figure S79. The **2D** Hirshfeld fingerprints of (**G36**)

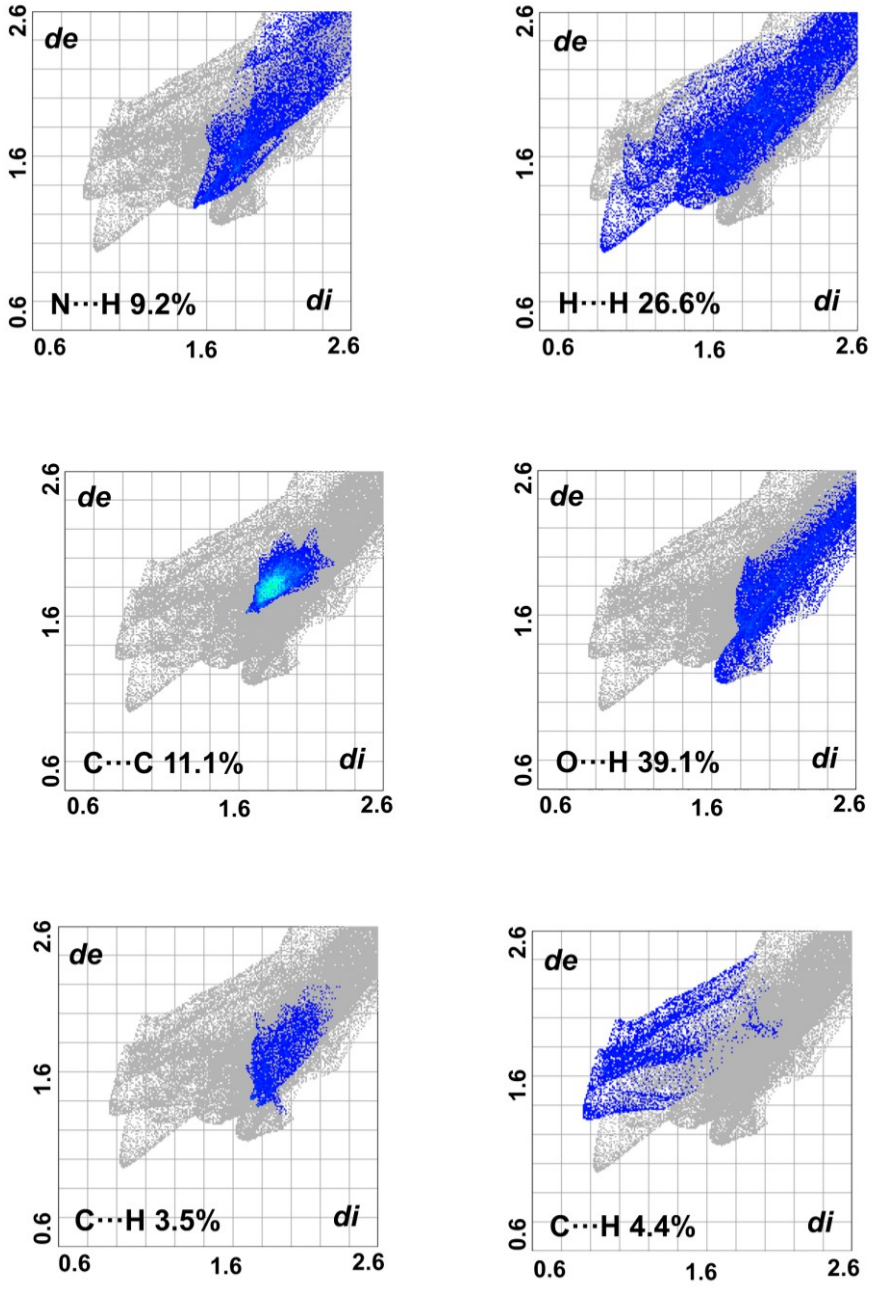


Figure S80. The **2D** Hirshfeld fingerprints of (**G37**)

7. DFT-calculated ESP surfaces of all guests

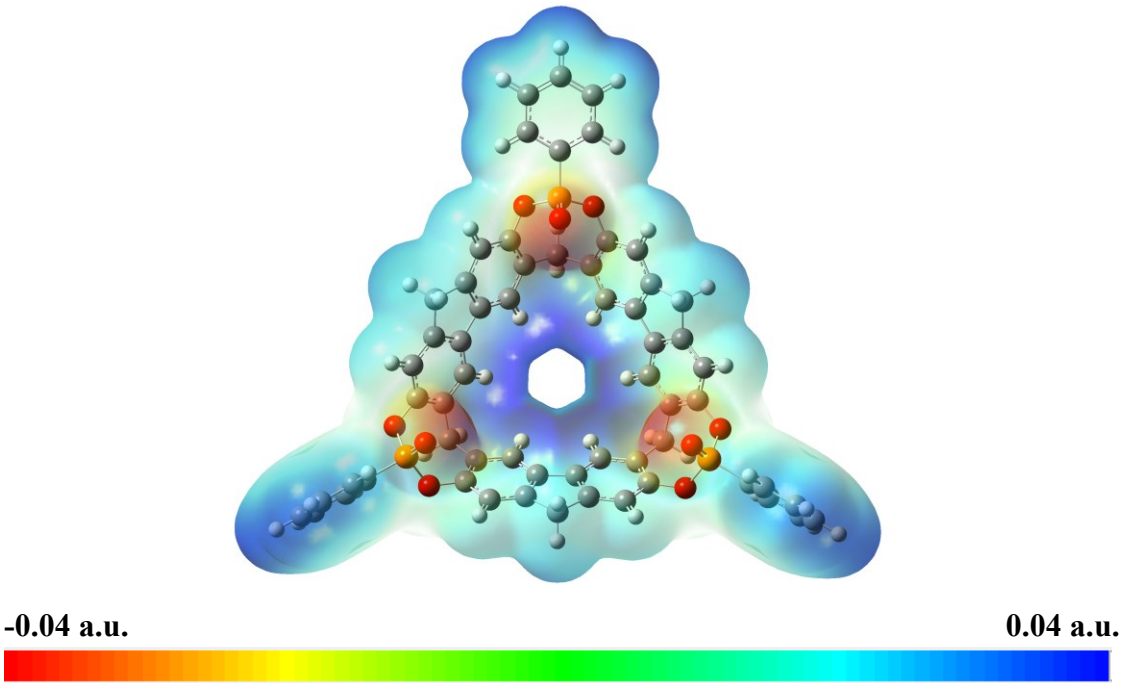


Figure S81. DFT-calculated **ESP** surfaces of **F[3]A1-[P(O)Ph]$_3$**

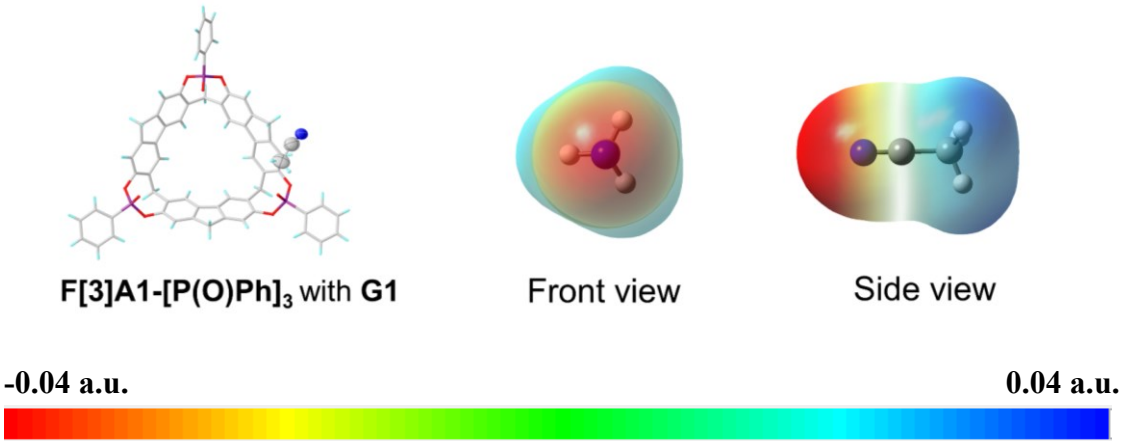


Figure S82. DFT-calculated **ESP** surfaces of **G1**

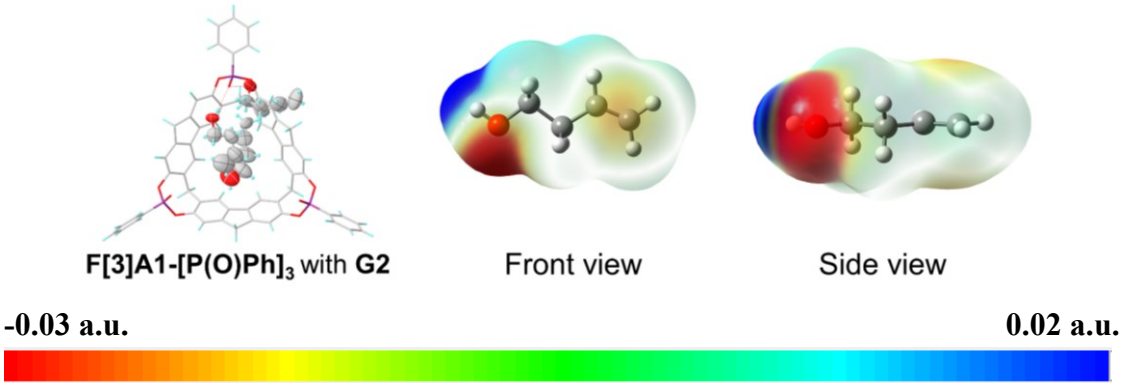


Figure S83. DFT-calculated **ESP** surfaces of **G2**

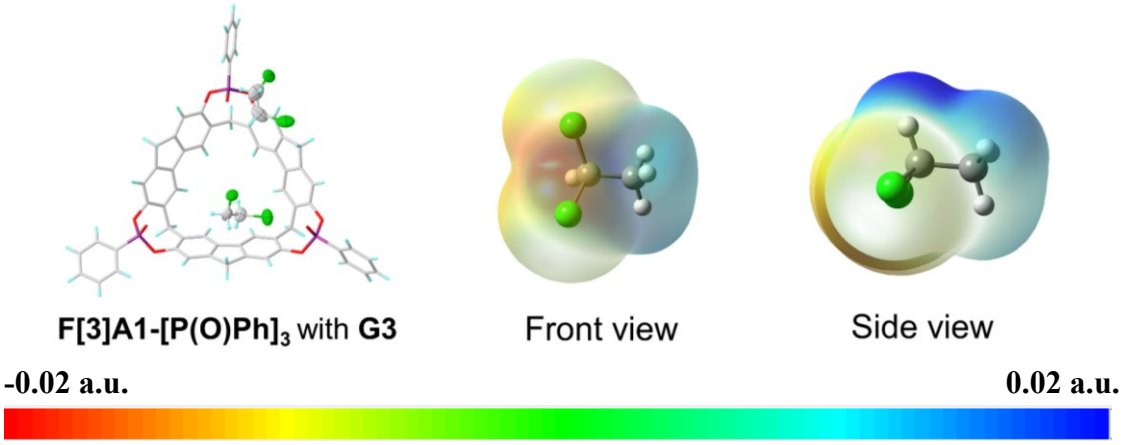


Figure S84. DFT-calculated **ESP** surfaces of **G3**

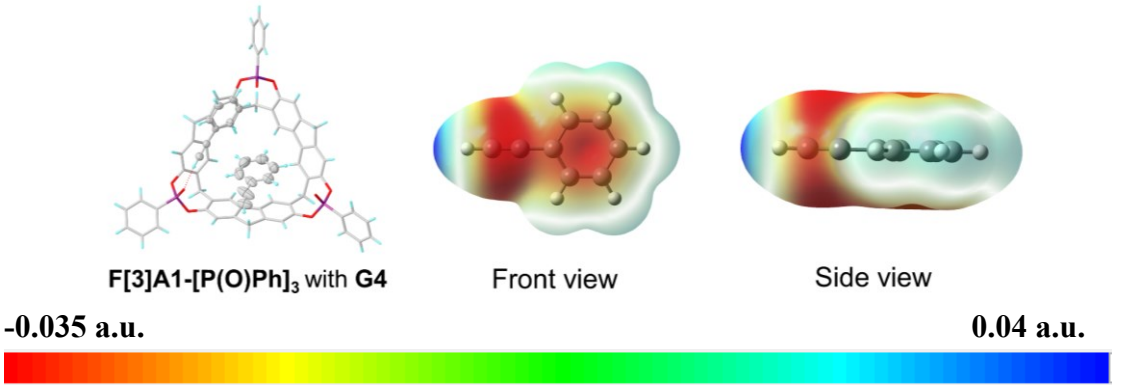


Figure S85. DFT-calculated **ESP** surfaces of **G4**

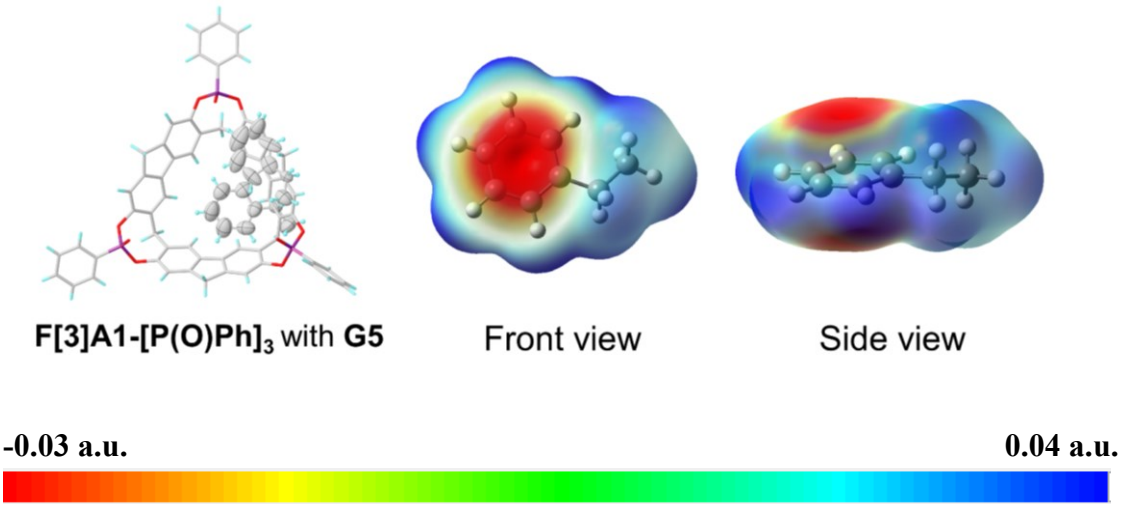


Figure S86. DFT-calculated **ESP** surfaces of **G5**

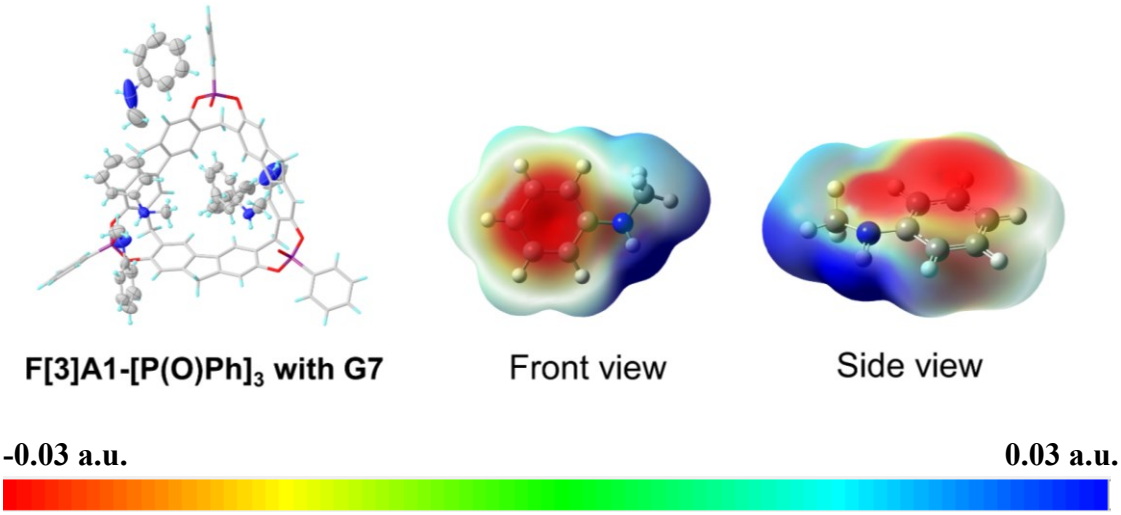


Figure S87. DFT-calculated **ESP** surfaces of **G7**

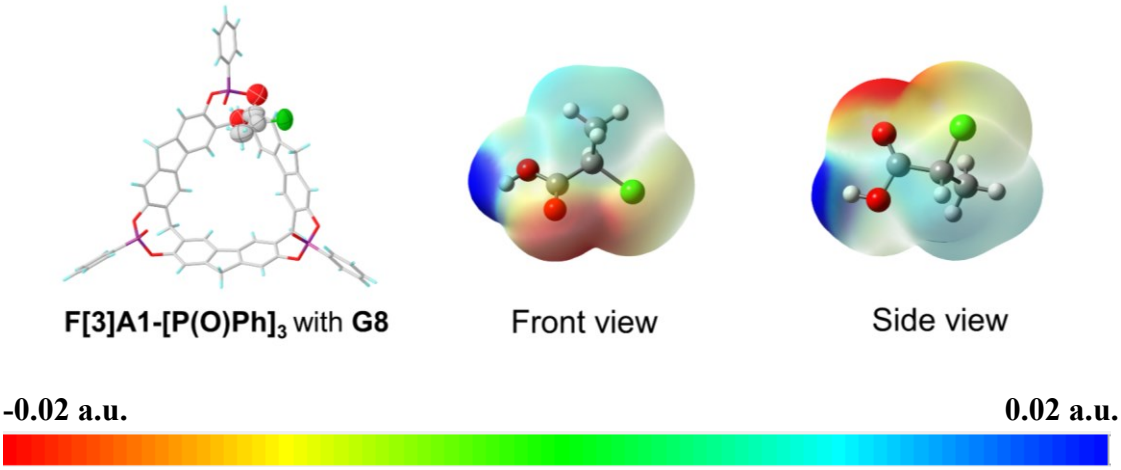


Figure S88. DFT-calculated **ESP** surfaces of **G8**

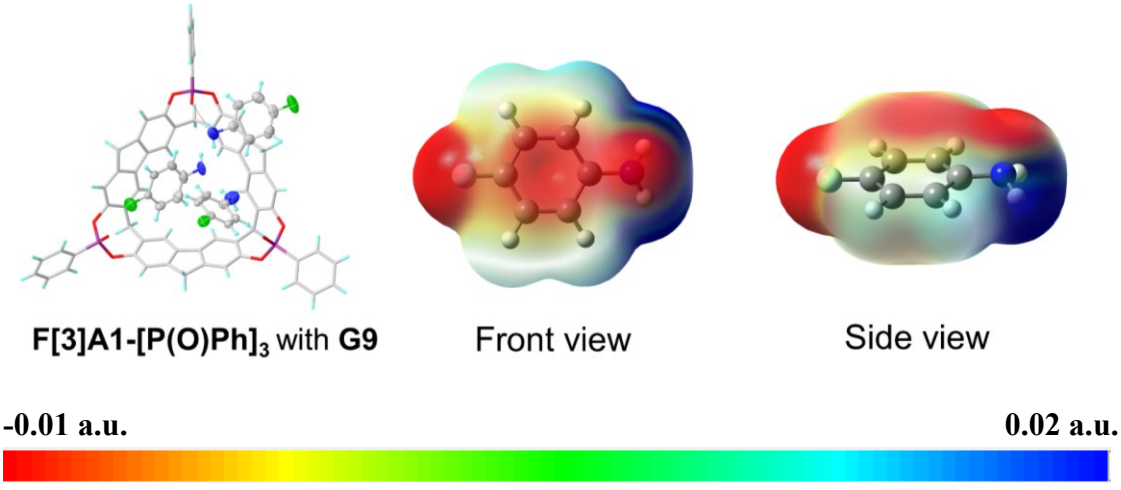


Figure S89. DFT-calculated **ESP** surfaces of **G9**

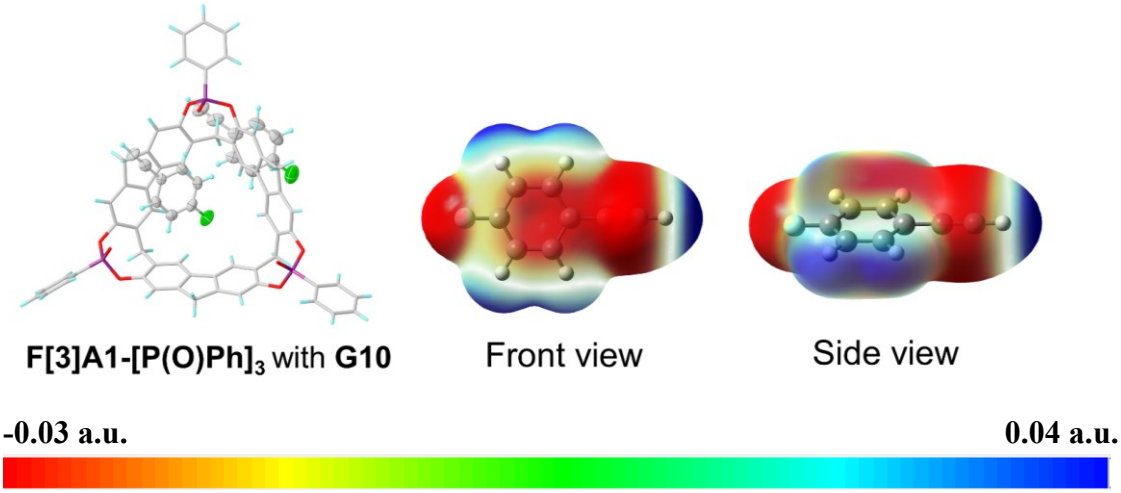


Figure S90. DFT-calculated **ESP** surfaces of **G10**

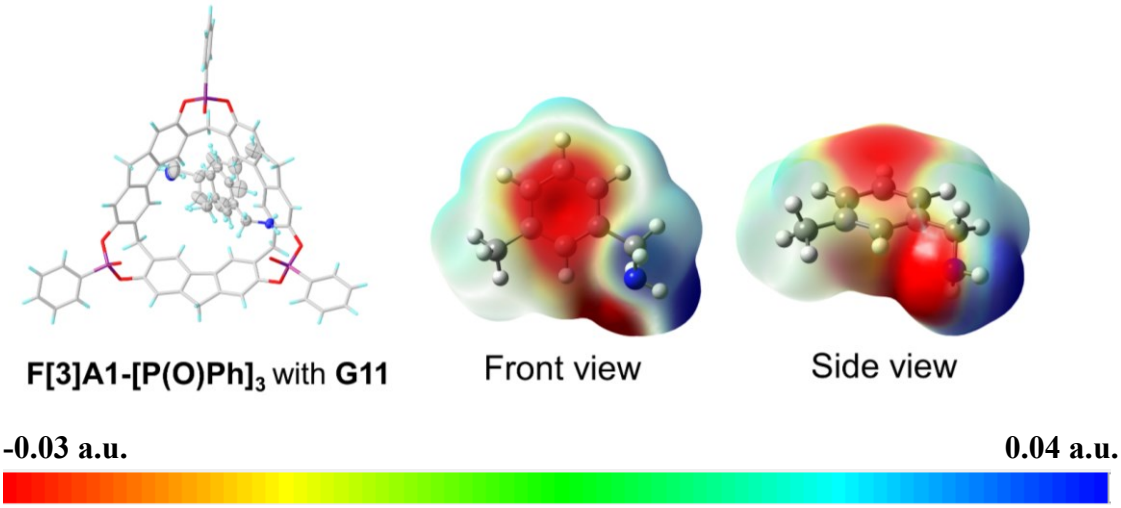


Figure S91. DFT-calculated **ESP** surfaces of **G11**

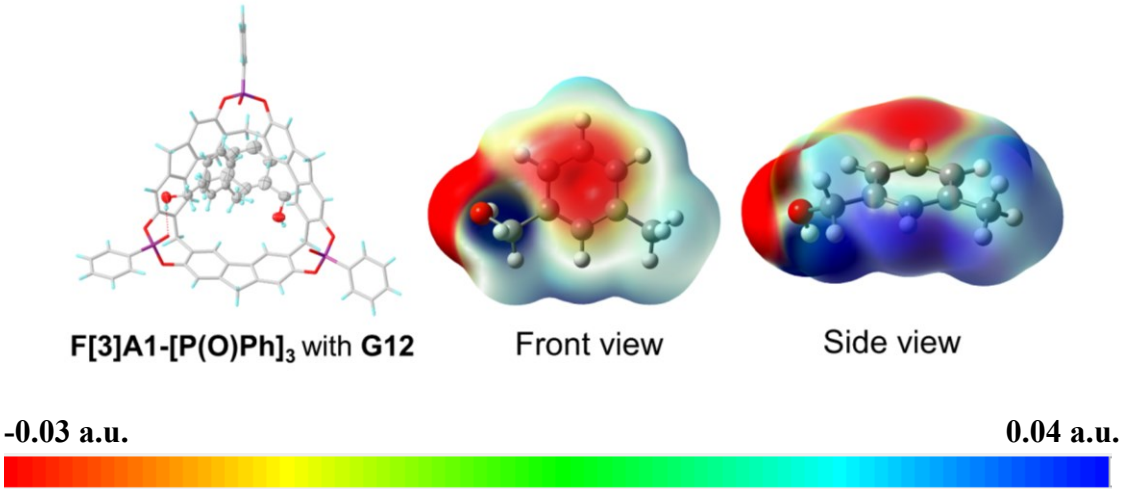


Figure S92. DFT-calculated **ESP** surfaces of **G12**

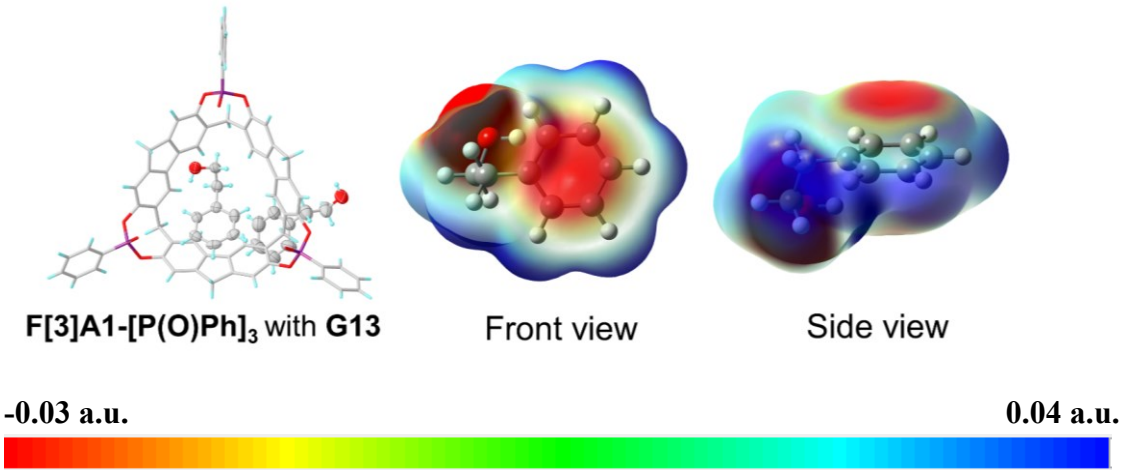


Figure S93. DFT-calculated **ESP** surfaces of **G13**

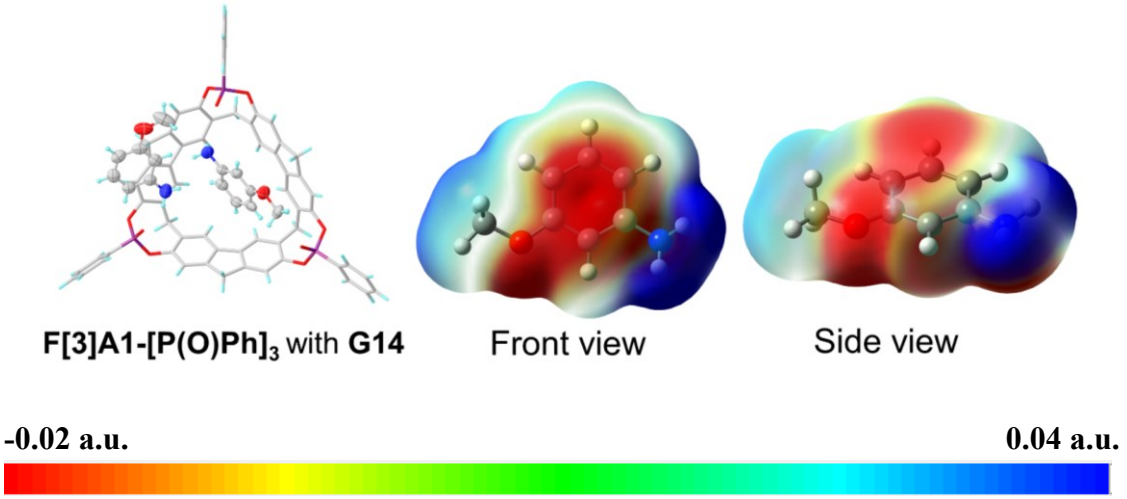


Figure S94. DFT-calculated **ESP** surfaces of **G14**

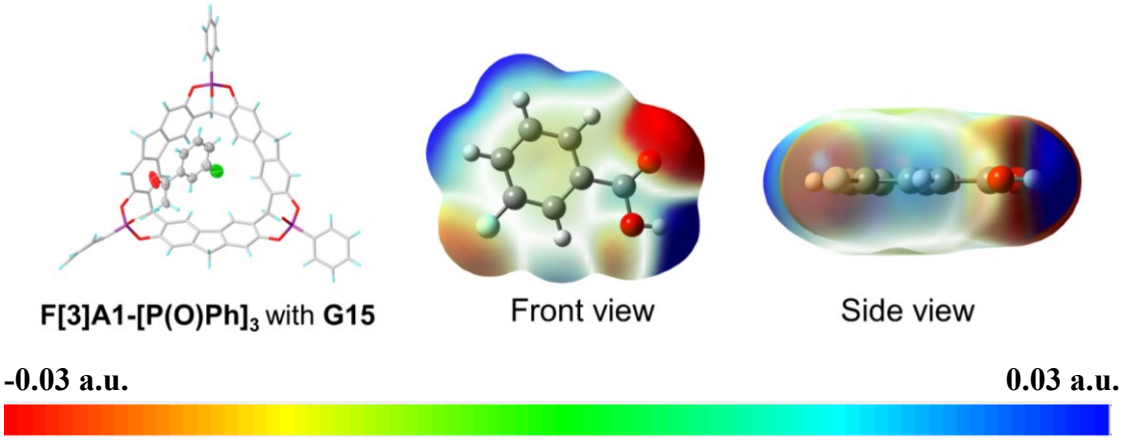


Figure S95. DFT-calculated **ESP** surfaces of **G15**

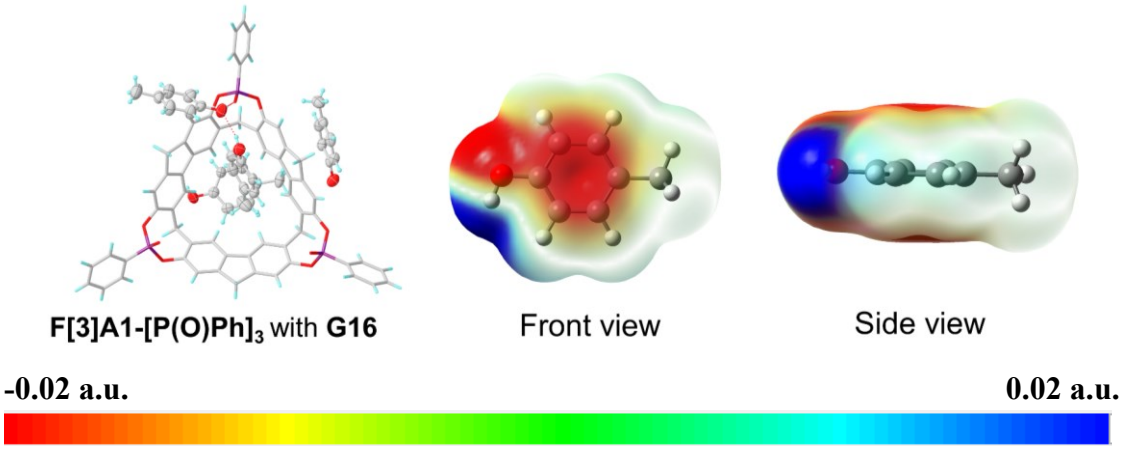


Figure S96. DFT-calculated **ESP** surfaces of **G16**

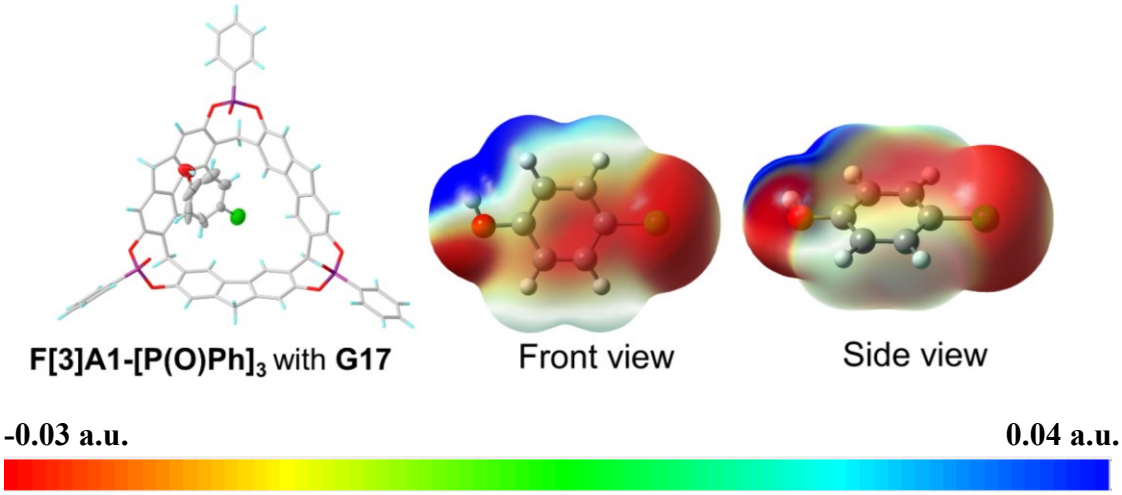


Figure S97. DFT-calculated **ESP** surfaces of **G17**

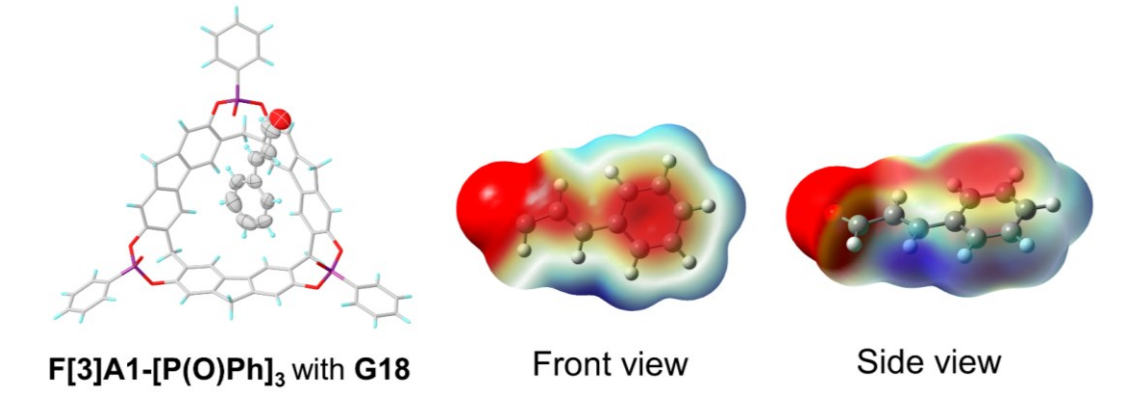


Figure S98. DFT-calculated **ESP** surfaces of **G18**

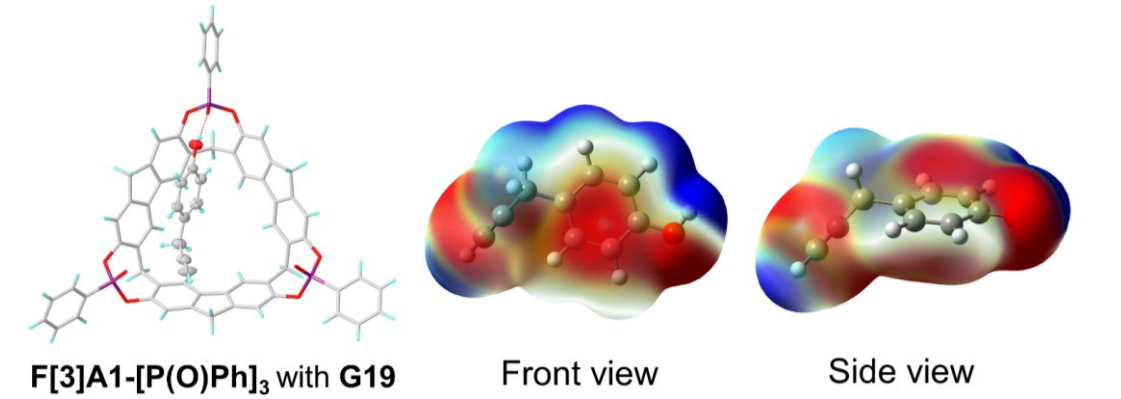


Figure S99. DFT-calculated **ESP** surfaces of **G19**

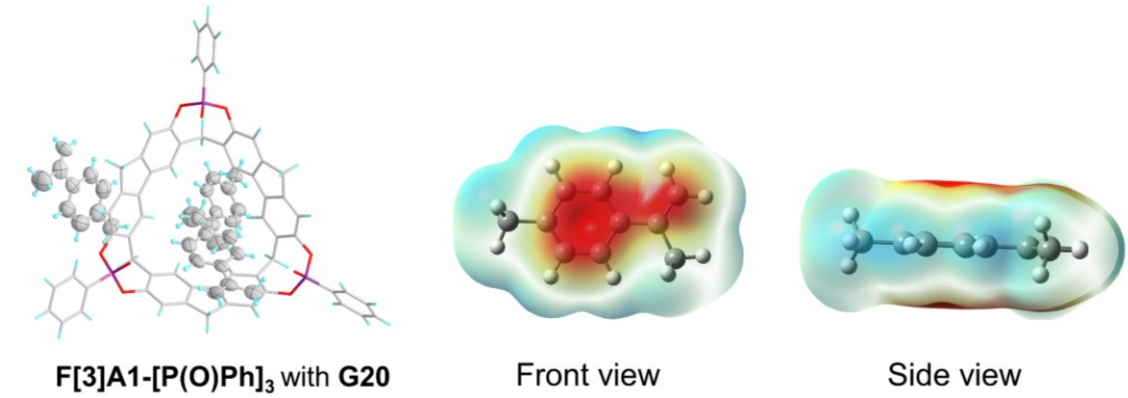


Figure S100. DFT-calculated **ESP** surfaces of **G20**

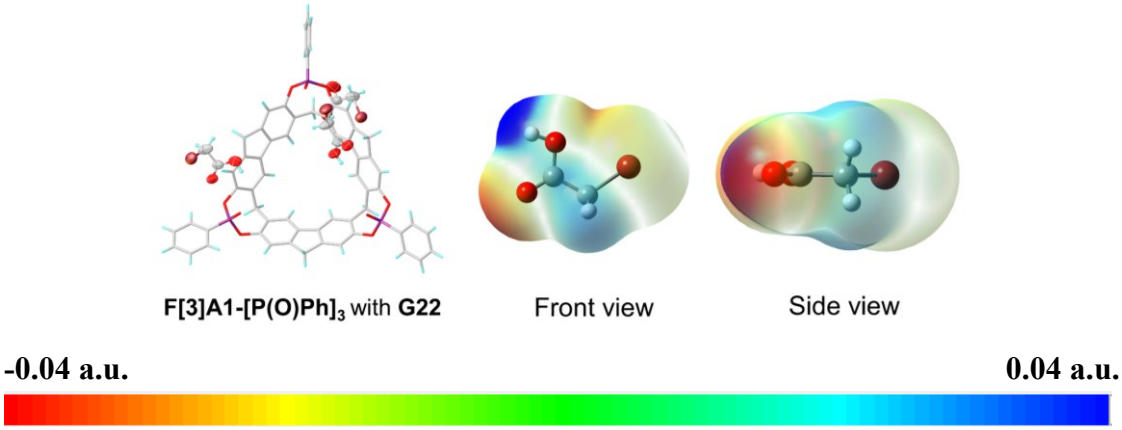


Figure S101. DFT-calculated **ESP** surfaces of **G22**

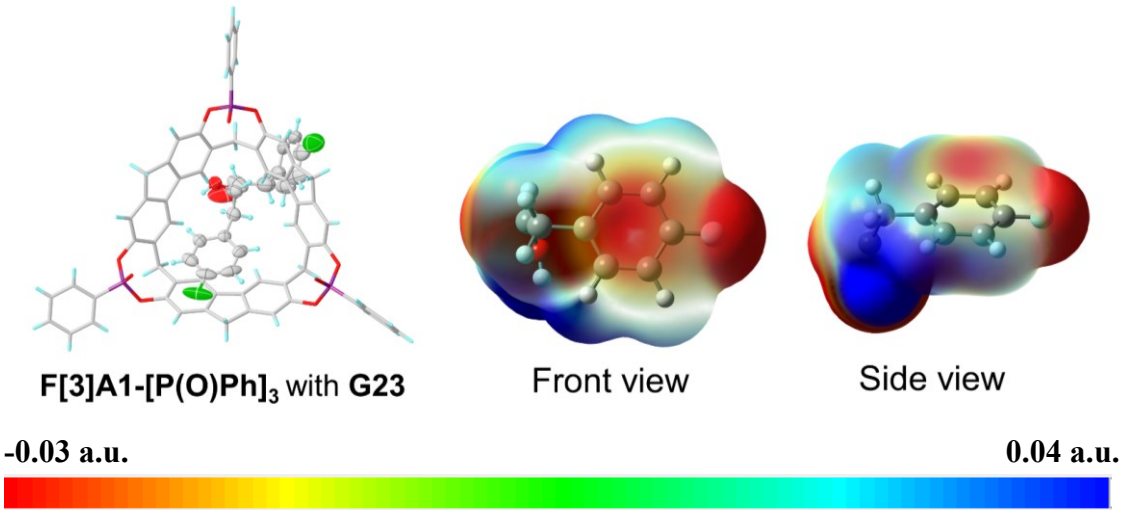


Figure S102. DFT-calculated **ESP** surfaces of **G23**

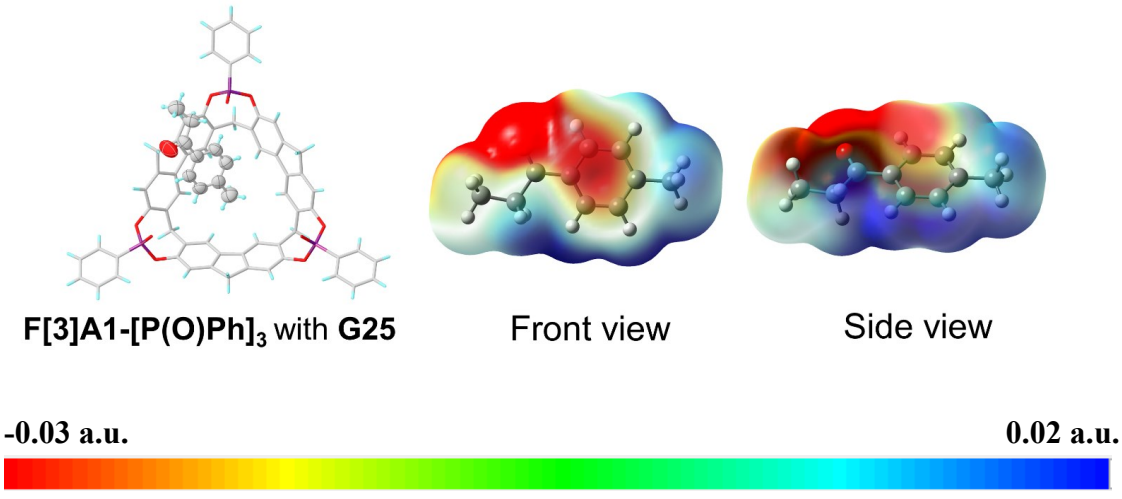


Figure S103. DFT-calculated **ESP** surfaces of **G25**

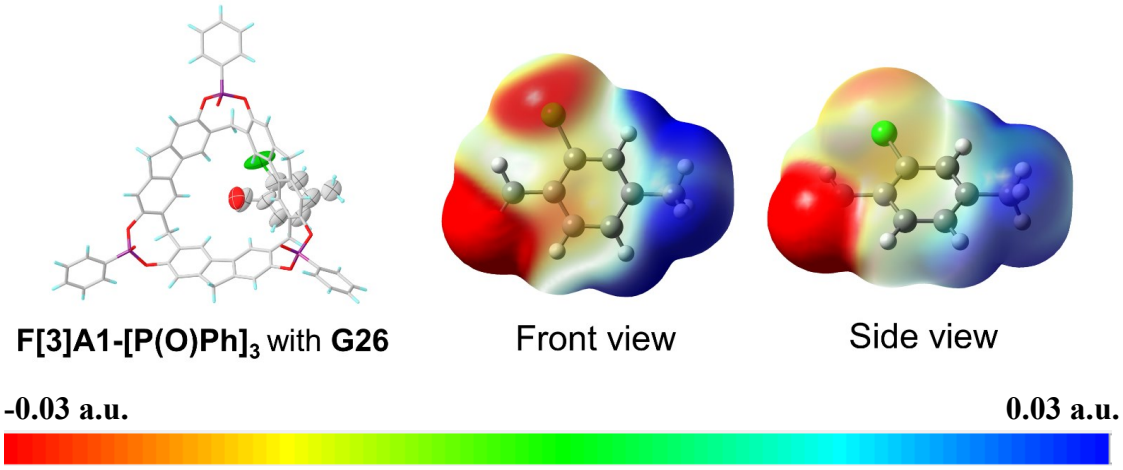


Figure S104. DFT-calculated **ESP** surfaces of **G26**

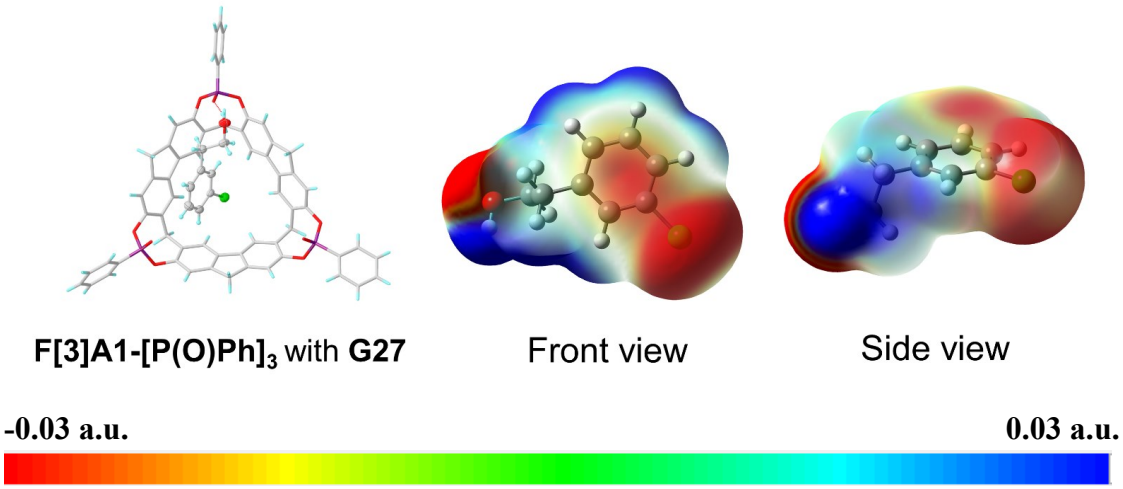


Figure S105. DFT-calculated **ESP** surfaces of **G27**

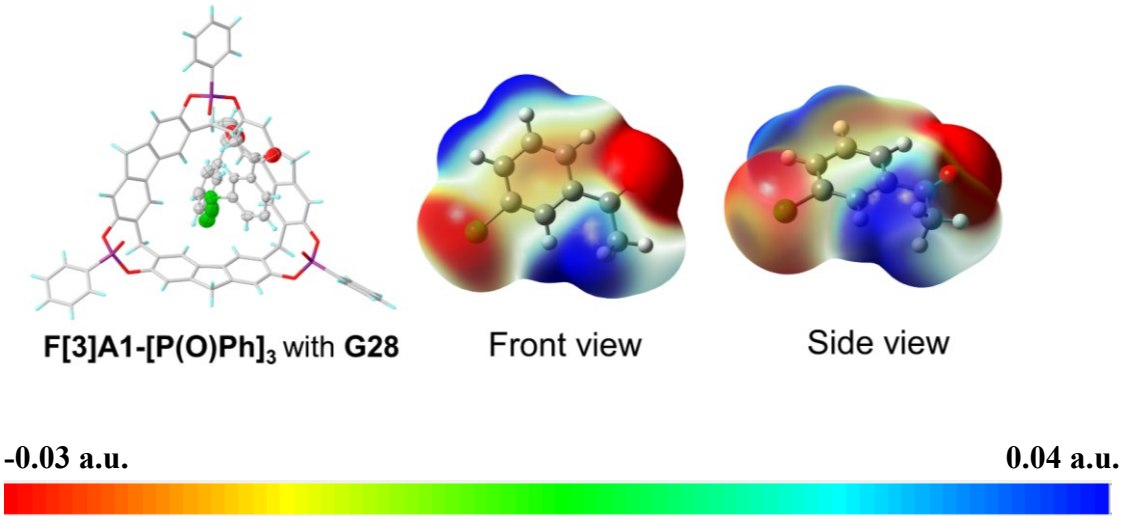


Figure S106. DFT-calculated **ESP** surfaces of **G28**

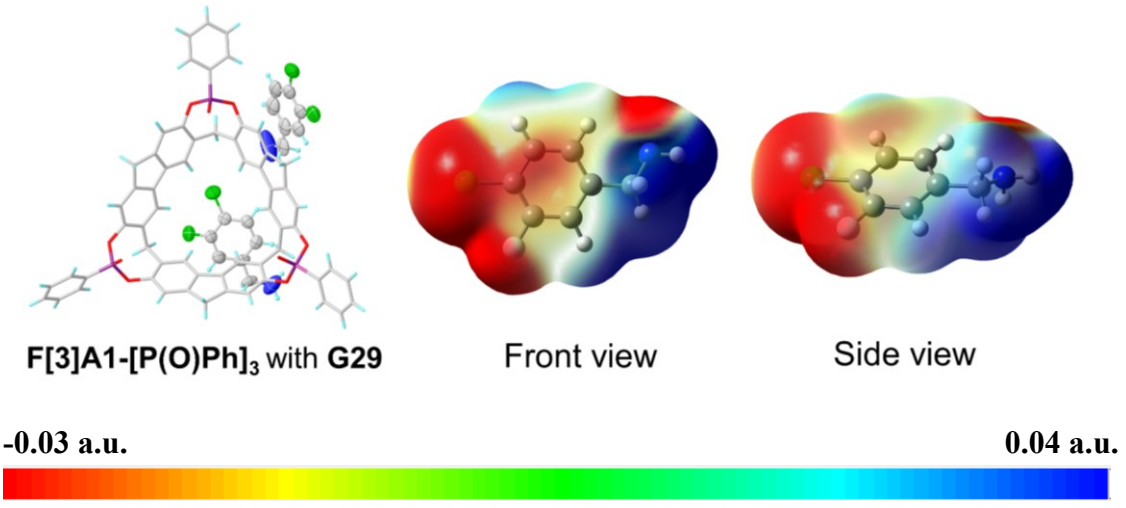


Figure S107. DFT-calculated **ESP** surfaces of **G29**

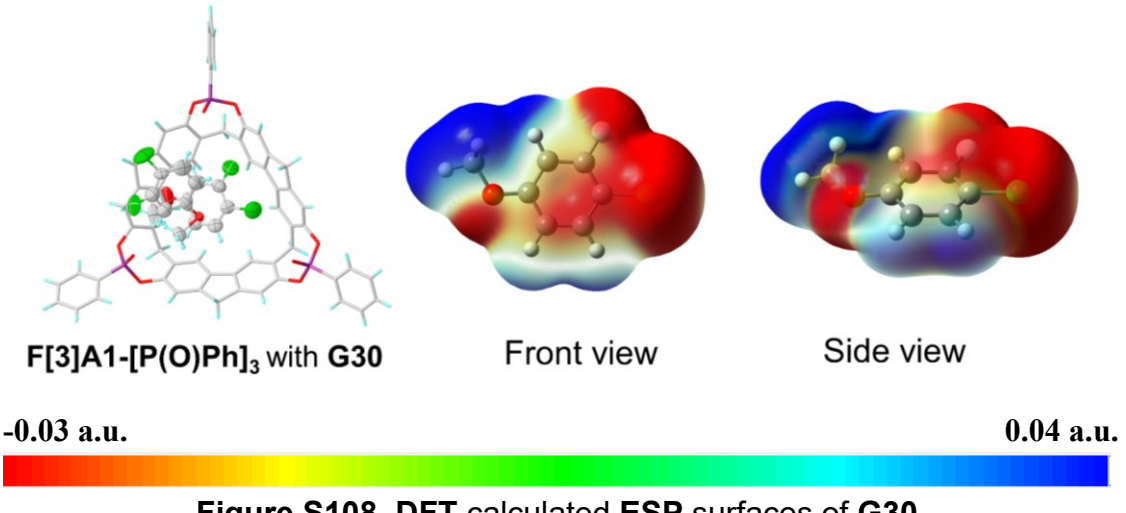


Figure S108. DFT-calculated **ESP** surfaces of **G30**

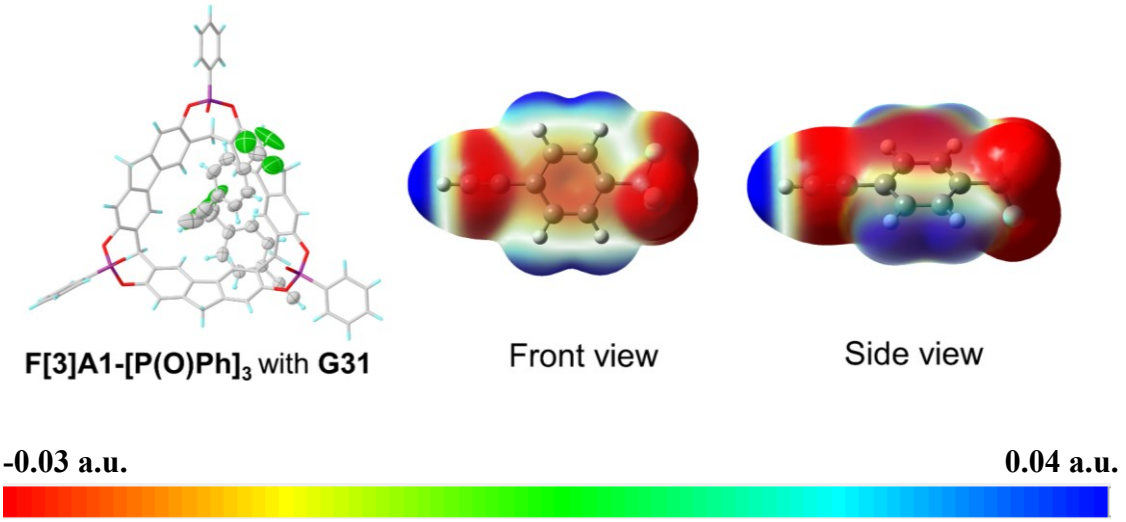


Figure S109. DFT-calculated **ESP** surfaces of **G31**

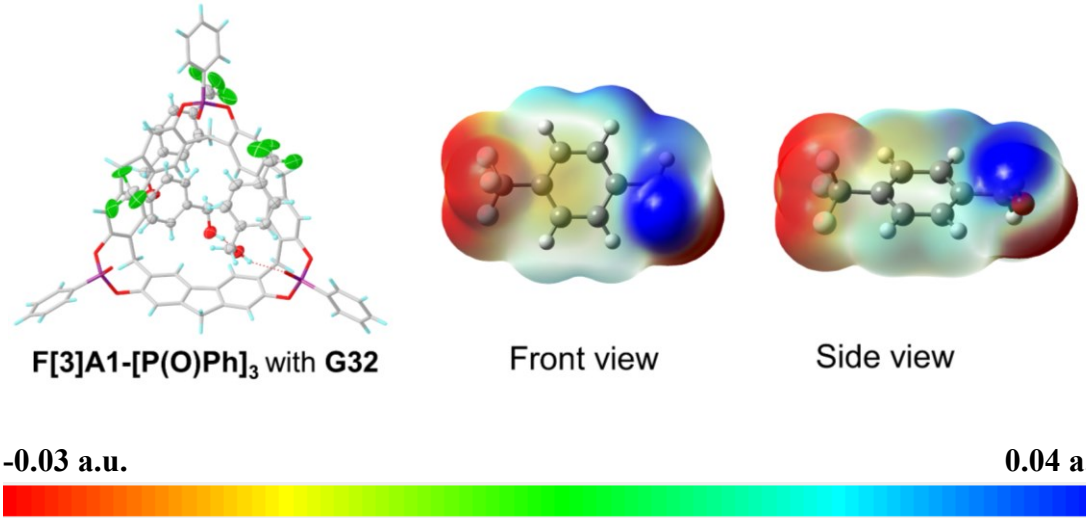


Figure S110. DFT-calculated **ESP** surfaces of **G32**

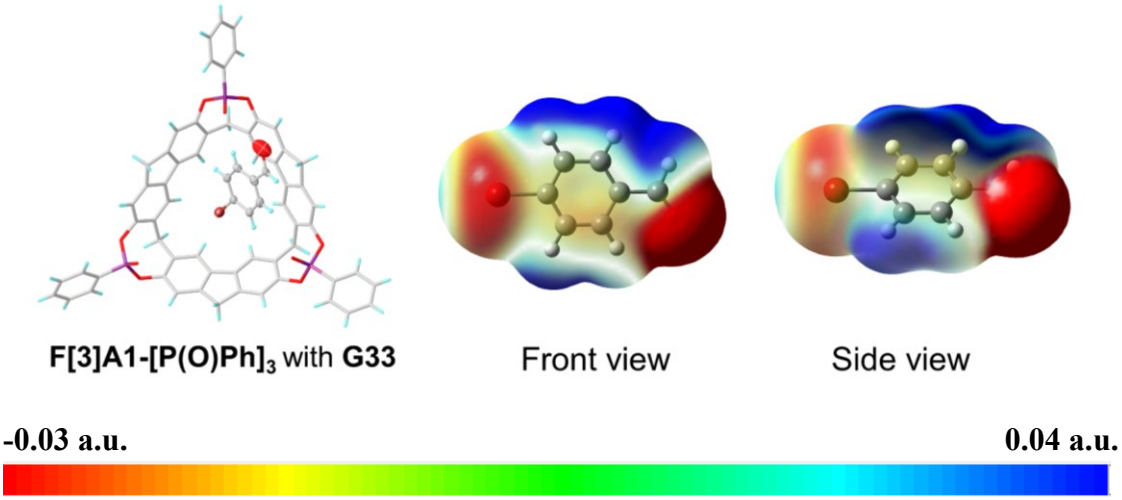


Figure S111. DFT-calculated **ESP** surfaces of **G33**

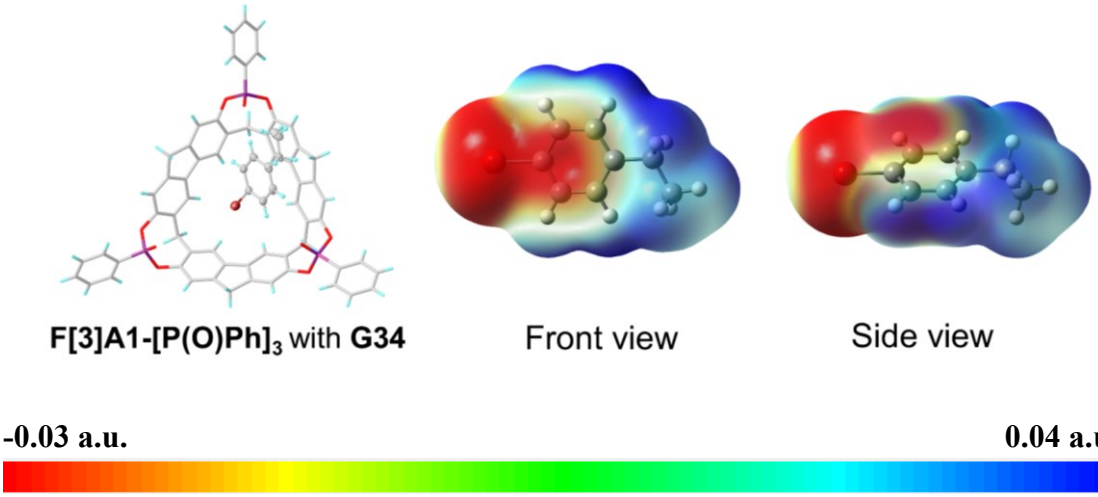


Figure S112. DFT-calculated **ESP** surfaces of **G34**

8. Structural breadth of the chaperone effect

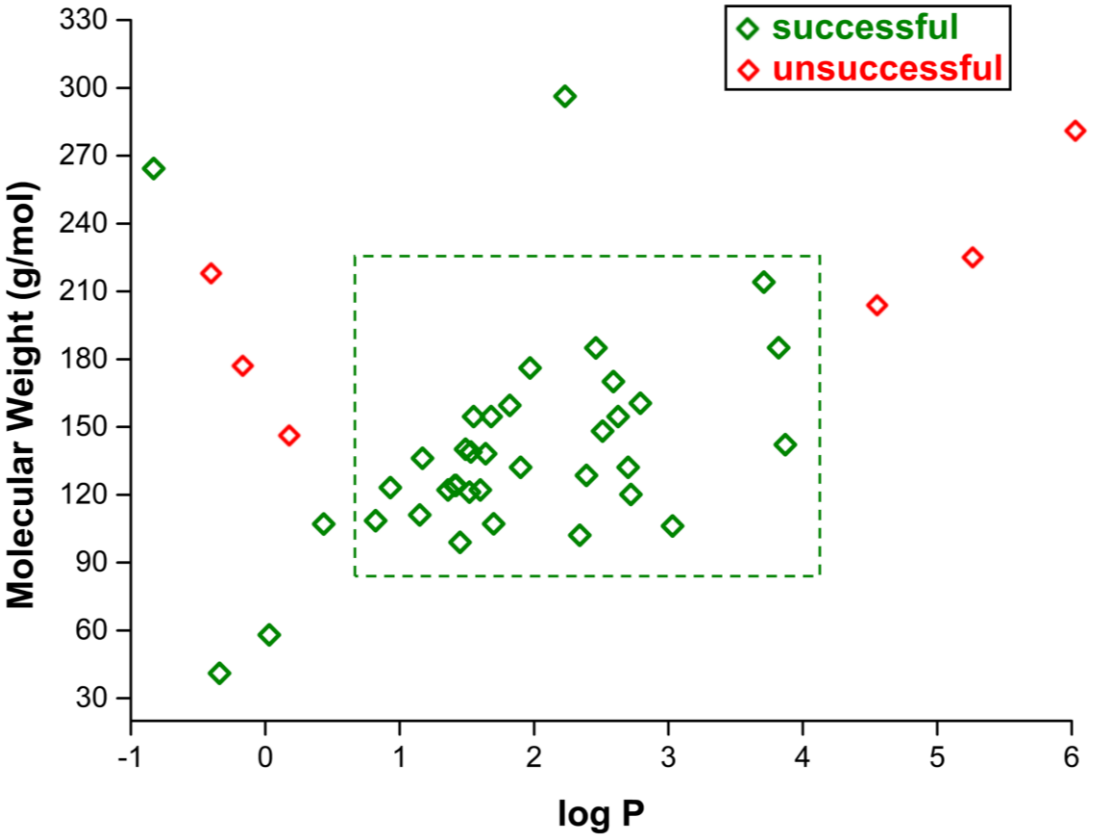


Figure S113. Diversity of analytes co-crystallized with **F[3]A1-[P(O)Ph]$_3$** visualized as a plot of calculated lipophilicities (**log P** values) of analytes vs their molecular weight.

9. Details of DFT calculations

Coordinates of the fully optimized structure of F[3]A1-[P(O)Ph]$_3$

P -1.56312623 1.63326651 0.00000000
P 3.59987377 11.53626651 2.81800000
P -0.11812623 4.56126651 10.69700000
O 3.95787377 10.55926651 1.61400000
O -0.31212623 2.29726651 -0.73000000
O 4.54387377 11.14026651 4.03000000
O -0.94012623 0.61826651 1.05400000
O 0.19687377 3.07326651 10.23700000
O 1.31187377 5.25326651 10.87500000
O 2.17387377 11.56126651 3.14700000
O -2.52712623 2.56626651 0.56700000
O -1.02112623 5.30626651 9.82700000
C 2.24287377 4.10126651 1.20000000
H 2.94887377 3.92426651 1.81000000
C 2.63587377 6.65926651 1.14000000
C 1.99187377 5.39826651 0.78300000
C 4.40387377 7.76226651 5.47000000
H 4.69787377 6.87926651 5.28200000
C 1.45287377 3.05426651 0.72000000
C 1.68487377 2.57426651 6.91000000
H 2.51187377 2.68526651 6.45600000
C 3.69387377 6.91326651 2.00500000
H 4.10987377 6.19226651 2.46400000
C 3.23587377 7.12226651 7.70900000
C 0.43387377 3.35126651 -0.16500000
C 3.47987377 9.23926651 1.50300000
C 4.14687377 8.21026651 2.20400000
C 3.72287377 8.03326651 6.65400000
C 1.99887377 7.70426651 0.46700000
C 1.56687377 2.94326651 8.24800000
C -2.14012623 0.50526651 -1.24400000
C 0.94687377 5.67026651 -0.12700000
C 3.32587377 5.76026651 7.82700000
H 3.82487377 5.26026651 7.19100000
C 2.41787377 9.01126651 0.64600000
H 1.98887377 9.73026651 0.19400000
C -0.91512623 1.22526651 4.65700000
C 0.40287377 1.66626651 4.83500000
C 1.27987377 1.74026651 3.75400000

H 2.18287377 2.00526651 3.88600000
C 1.69687377 1.65126651 1.25600000
H 1.48287377 0.98326651 0.55800000
H 2.65087377 1.54626651 1.50400000
C 0.58687377 2.04326651 6.23900000
C 3.56287377 10.37226651 6.08700000
H 3.30087377 11.26226651 6.29100000
C 0.33287377 2.74126651 8.87300000
C 4.65287377 8.79626651 4.55600000
C 1.85287377 7.25826651 9.68200000
H 1.35487377 7.75726651 10.32000000
C -0.49312623 0.99526651 2.33700000
C 2.67987377 5.09526651 8.89000000
C 2.71787377 3.58826651 8.97700000
H 3.56987377 3.26326651 8.59000000
H 2.69287377 3.31726651 9.92800000
C 3.29287377 9.33526651 6.94900000
C -1.36512623 0.86426651 3.40200000
H -2.24712623 0.53526651 3.27500000
C 4.23487377 10.07426651 4.90600000
C 0.81887377 1.42326651 2.47700000
C 5.24687377 8.49726651 3.19500000
H 5.77887377 9.27226651 2.88600000
H 5.84887377 7.71526651 3.25800000
C 0.16287377 4.64626651 -0.61200000
H -0.53912623 4.81526651 -1.22900000
C 1.95787377 5.87926651 9.78100000
C 2.49087377 7.88626651 8.63300000
C -0.76212623 2.18026651 8.24000000
H -1.57612623 2.03326651 8.70800000
C 0.88487377 7.15726651 -0.41700000
H 0.00487377 7.53726651 -0.16700000
H 1.05887377 7.34526651 -1.37400000
C -1.67212623 1.28726651 5.95700000
H -1.97312623 0.38526651 6.24200000
H -2.45812623 1.88326651 5.88800000
C -0.65912623 4.31126651 12.36700000
C 4.34687377 13.04326651 2.25300000
C 2.50087377 9.34126651 8.23200000
H 1.58287377 9.67826651 8.08200000
H 2.94287377 9.89926651 8.92100000
C -0.63912623 1.84526651 6.91100000
C -1.21512623 -0.26173349 -1.99600000
H -0.28112623 -0.18073349 -1.83700000

C -3.48912623 0.34526651 -1.46000000
H -4.11012623 0.83526651 -0.93500000
C -3.94912623 -0.52173349 -2.43700000
H -4.88312623 -0.61273349 -2.58700000
C -0.02212623 3.43126651 13.20400000
H 0.74787377 2.96726651 12.90000000
C -3.06012623 -1.24973349 -3.18700000
H -3.37812623 -1.83573349 -3.86400000
C -1.69012623 -1.13373349 -2.95900000
H -1.08112623 -1.65473349 -3.46800000
C -1.80612623 4.96726651 12.80400000
H -2.25512623 5.57126651 12.22700000
C -0.48812623 3.21026651 14.49300000
H -0.03112623 2.62126651 15.08100000
C -1.64412623 3.87426651 14.90100000
H -1.98812623 3.71926651 15.77300000
C 4.98487377 13.90826651 3.10400000
H 5.04887377 13.70026651 4.02800000
C 4.25987377 13.37626651 0.90400000
H 3.84387377 12.77726651 0.29600000
C -2.28812623 4.74126651 14.06800000
H -3.07012623 5.18826651 14.36400000
C 4.77687377 14.57726651 0.43800000
H 4.66787377 14.82126651 -0.47300000
C 5.44087377 15.40126651 1.29300000
H 5.83787377 16.20026651 0.96800000
C 5.53787377 15.08126651 2.61900000
H 5.98687377 15.67126651 3.21400000

Coordinates of the fully optimized structure of F[3]A1-[P(O)Ph]$_3$ with (**G6**) 4-Pyridinecarboxaldehyde

P	-0.56506848	1.90924663	0.00000000
P	-3.81406848	8.70824663	-7.94600000
P	-8.51906848	9.71324663	1.92100000
O	-1.83206848	1.64324663	0.91800000
O	-3.59806848	7.18824663	-8.38400000
O	-5.39006848	8.94124663	-7.98100000
O	-0.88706848	1.21924663	-1.40400000
O	-3.19806848	9.04224663	-6.66300000
O	-0.19506848	3.31624663	-0.11200000
O	-9.47506848	9.72224663	0.64300000
O	-8.63306848	8.24424663	2.53200000

O	-7.15506848	10.13424663	1.65100000
C	-2.12906848	4.74924663	-6.09000000
C	-6.16906848	5.18424663	1.20500000
C	-8.16806848	8.57224663	-3.12600000
C	-3.49906848	6.19224663	-7.38300000
C	-3.27906848	4.30024663	-5.42400000
C	-7.54006848	8.45324663	-4.45400000
C	-4.67706848	5.72324663	-6.78200000
C	-4.54306848	4.77124663	-5.77900000
H	-5.31406848	4.44024663	-5.33500000
C	-1.55806848	1.95024663	-2.41400000
C	-3.59806848	2.76924663	-3.35000000
H	-4.54406848	2.85224663	-3.33800000
C	-7.19406848	7.33424663	-5.19100000
H	-7.44906848	6.46924663	-4.89000000
C	-5.12506848	4.18324663	0.95400000
C	-2.94706848	2.53124663	0.90900000
C	-0.80406848	2.53824663	-3.40800000
H	0.14093152	2.44524663	-3.42300000
C	-6.12906848	8.75824663	-6.77800000
C	-2.95006848	2.01824663	-2.36300000
C	-4.99806848	3.24524663	-0.06800000
H	-5.65906848	3.18924663	-0.74700000
C	-2.85906848	3.39224663	-4.34900000
C	-8.20506848	9.93424663	-2.78400000
C	-6.47106848	7.47624663	-6.37600000
C	-2.23506848	5.72424663	-7.07800000
H	-1.46706848	6.05624663	-7.52600000
C	-4.16506848	4.26624663	1.96600000
C	-7.31606848	5.48724663	0.47900000
H	-7.53406848	4.98924663	-0.30000000
C	-7.19806848	9.74224663	-4.90000000
C	0.62393152	0.78724663	0.70100000
C	-1.46206848	3.26824663	-4.38100000
C	-7.63806848	10.77624663	-3.88800000
H	-6.87006848	11.31524663	-3.57000000
H	-8.32406848	11.38024663	-4.26700000
C	-3.90306848	2.39324663	-0.09400000
C	-9.01006848	7.96424663	-0.95000000
C	-9.02006848	9.32624663	-0.64300000
C	-8.14606848	6.53024663	0.90300000
C	-8.65006848	10.31024663	-1.53000000
H	-8.69806848	11.22624663	-1.28700000
C	-3.73606848	1.40524663	-1.22600000

H	-4.62806848	1.12524663	-1.55500000
H	-3.26506848	0.59924663	-0.89500000
C	-3.06306848	3.43324663	1.95200000
H	-2.40506848	3.47824663	2.63600000
C	-8.58306848	7.59924663	-2.22700000
H	-8.57606848	6.68324663	-2.48100000
C	-6.04006848	6.25724663	-7.17900000
H	-6.71206848	5.54024663	-7.05800000
H	-6.02306848	6.49624663	-8.14000000
C	-5.84806848	5.87724663	2.37000000
C	-4.58106848	5.31724663	2.97900000
H	-4.75606848	4.91124663	3.86500000
H	-3.88706848	6.01824663	3.07300000
C	-3.25906848	9.59124663	-9.38000000
C	-0.89606848	4.09024663	-5.53200000
H	-0.24506848	4.76224663	-5.20900000
H	-0.46006848	3.51224663	-6.20800000
C	-6.48406848	9.90024663	-6.07700000
H	-6.24606848	10.76424663	-6.39400000
C	-7.77706848	7.21624663	2.05200000
C	-9.36206848	6.91824663	0.07600000
H	-9.71706848	6.11424663	-0.38100000
H	-10.06906848	7.26724663	0.67300000
C	-1.87906848	9.68024663	-9.58000000
H	-1.28206848	9.22824663	-8.99400000
C	-6.65606848	6.91324663	2.80600000
H	-6.44806848	7.40124663	3.59500000
C	-1.38306848	10.42724663	-10.62800000
H	-0.44406848	10.48924663	-10.75700000
C	-2.23506848	11.08424663	-11.49400000
H	-1.88406848	11.60324663	-12.20800000
C	0.98893152	0.97024663	2.03100000
H	0.57193152	1.64724663	2.55000000
C	1.24293152	-0.20875337	-0.05200000
H	0.99793152	-0.34175337	-0.95900000
C	-4.12006848	10.25024663	-10.26200000
H	-5.06106848	10.19424663	-10.14300000
C	2.21893152	-1.00375337	0.53000000
H	2.64793152	-1.67775337	0.01500000
C	-3.59306848	10.98224663	-11.31500000
H	-4.18006848	11.42224663	-11.91800000
C	2.56793152	-0.81875337	1.84800000
H	3.23393152	-1.37075337	2.24100000
C	1.96393152	0.15724663	2.60000000

H	2.20993152	0.27824663	3.50900000
C	-9.52306848	11.68924663	5.22400000
H	-9.22906848	11.68924663	6.12600000
C	-8.94506848	10.82124663	4.30500000
H	-8.25606848	10.22924663	4.57700000
C	-9.37806848	10.82124663	2.98300000
C	-10.38906848	11.68824663	2.58300000
H	-10.68406848	11.68724663	1.67900000
C	-10.96706848	12.55424663	3.50200000
H	-11.65906848	13.14524663	3.22800000
C	-10.53506848	12.55524663	4.82400000
H	-10.93006848	13.14624663	5.45200000
O	-5.18306848	6.11124663	-2.74800000
C	-4.37006848	8.86924663	-3.27600000
H	-4.16206848	8.30124663	-4.01100000
C	-4.93106848	8.35324663	-2.13100000
C	-5.27806848	6.90524663	-1.92200000
H	-5.58906848	6.63324663	-1.06600000
C	-5.20106848	9.19324663	-1.13400000
H	-5.60206848	8.83924663	-0.34900000
C	-4.11906848	10.22124663	-3.33800000
H	-3.74306848	10.62624663	-4.11100000
N	-4.43306848	10.92924663	-2.26000000
C	-4.93306848	10.54324663	-1.17500000
H	-5.11106848	11.12924663	-0.44900000
N	-5.51606848	18.47324663	-3.10900000
C	-4.38406848	17.84524663	-3.11800000
H	-3.58606848	18.36124663	-3.14200000
C	-4.27006848	16.50624663	-3.09200000
H	-3.40906848	16.10924663	-3.03800000
O	-4.33306848	13.83824663	-2.40900000
C	-5.39006848	15.69824663	-3.14400000
C	-6.62306848	17.73724663	-3.20900000
H	-7.45506848	18.18624663	-3.30700000
C	-6.62006848	16.35024663	-3.17600000
H	-7.43306848	15.85924663	-3.17600000
C	-5.39406848	14.18324663	-3.18100000
H	-5.99706848	13.60824663	-3.64000000

Coordinates of the fully optimized structure of F[3]A1-[P(O)Ph]$_3$ with (G21) 4-Fluoroacetophenone

P	-2.46575339	1.36130141	0.00000000

P	-7.81075339	2.04230141	9.61800000
P	0.09624661	-5.97469859	7.69900000
O	-2.28375339	-0.15269859	-0.47800000
O	-0.19975339	-6.60269859	6.25700000
O	-4.02875339	1.62530141	-0.05500000
O	-7.90675339	0.53130141	10.11400000
O	-1.25375339	-6.16969859	8.52900000
O	-8.68075339	2.09730141	8.28700000
O	-1.85275339	1.64630141	1.29500000
O	0.59824661	-4.60569859	7.66000000
O	-6.45475339	2.55330141	9.46700000
C	-6.05575339	-0.06069859	2.51100000
H	-6.35775339	-0.91069859	2.73800000
C	-5.99175339	2.32430141	2.94000000
C	-6.40675339	1.03230141	3.28900000
C	-1.04675339	-2.76369859	1.73900000
C	-5.25275339	0.11530141	1.38700000
C	-1.92475339	-4.19969859	3.34900000
C	-4.83475339	1.41130141	1.08500000
C	-3.50175339	-1.65369859	0.97700000
C	-3.45675339	-2.67269859	1.93300000
H	-4.24475339	-2.99069859	2.31000000
C	-0.79875339	-5.79569859	5.26100000
C	-7.15075339	2.44330141	4.98400000
C	-2.24675339	-3.20469859	2.31900000
C	-5.46875339	-2.51569859	8.73300000
C	-7.12875339	1.10330141	4.57100000
C	-2.73775339	-4.85769859	4.26500000
H	-3.66075339	-4.75269859	4.22200000
C	-6.59775339	-2.18269859	8.01100000
H	-6.81175339	-2.65769859	7.24100000
C	-7.67775339	2.77030141	6.22200000
H	-7.71575339	3.65530141	6.50600000
C	-4.44575339	-3.53969859	8.49200000
C	-0.53875339	-4.37169859	3.37300000
C	-8.15375339	0.40330141	6.63900000
C	-5.20175339	2.52330141	1.82400000
H	-4.92675339	3.37630141	1.57700000
C	-3.24575339	-5.35069859	7.45800000
C	-3.05275339	-6.30969859	6.30400000
H	-2.63575339	-7.12569859	6.62300000
H	-3.91375339	-6.53869859	5.92200000
C	-4.32175339	-4.47669859	7.47500000
H	-4.96275339	-4.51769859	6.80200000

C	-7.64175339	0.10030141	5.37600000
H	-7.64475339	-0.77869859	5.07400000
C	-2.17875339	-5.67369859	5.24400000
C	-2.31375339	-5.25069859	8.49000000
C	0.11124661	-3.52969859	2.30500000
H	0.77524661	-2.93369859	2.68300000
H	0.52924661	-4.08369859	1.62800000
C	-6.47675339	3.32630141	3.96100000
H	-5.73775339	3.81730141	4.35200000
H	-7.10375339	3.95430141	3.57000000
C	-8.14475339	1.74630141	7.02500000
C	-7.41275339	-1.14169859	8.43200000
C	-3.86375339	-2.37169859	10.48700000
H	-4.01675339	-2.72969859	11.37600000
H	-3.17175339	-1.69369859	10.53100000
C	-2.28175339	-1.19769859	0.47200000
C	-1.06175339	-1.73769859	0.81300000
H	-0.27375339	-1.42269859	0.43300000
C	-8.85475339	2.89130141	10.76300000
C	-7.05075339	-0.47769859	9.61000000
C	0.03224661	-5.18269859	4.33800000
H	0.95324661	-5.31269859	4.36700000
C	-4.82275339	-1.07069859	0.54600000
H	-5.50375339	-1.75869859	0.60000000
H	-4.75775339	-0.79269859	-0.38100000
C	-3.49575339	-3.46469859	9.51400000
C	-1.87175339	2.25930141	-1.41400000
C	-5.13075339	-1.81669859	9.90000000
C	-2.42175339	-4.33469859	9.52300000
H	-1.78975339	-4.30669859	10.20500000
C	1.15224661	-7.20469859	8.41800000
C	-8.58475339	-0.70169859	7.58900000
H	-9.29675339	-0.37969859	8.16300000
H	-8.92275339	-1.45569859	7.08200000
C	-5.93875339	-0.78669859	10.35100000
H	-5.73475339	-0.31969859	11.12900000
C	-0.51075339	2.25730141	-1.65900000
H	0.05724661	1.75530141	-1.12100000
C	2.10824661	-6.78369859	9.31600000
H	2.17124661	-5.88269859	9.54100000
C	-2.71375339	3.00730141	-2.22200000
H	-3.63075339	3.01630141	-2.06300000
C	-10.23275339	2.76730141	10.72000000
H	-10.63275339	2.20630141	10.09700000

C	0.00624661	3.00430141	-2.70800000
H	0.92224661	3.00630141	-2.86900000
C	-0.83175339	3.73930141	-3.50700000
H	-0.48375339	4.23630141	-4.21200000
C	-8.27975339	3.71130141	11.72300000
H	-7.35475339	3.78930141	11.77400000
C	2.97424661	-7.69969859	9.88400000
H	3.62224661	-7.41469859	10.48700000
C	-11.00875339	3.48230141	11.60900000
H	-11.93475339	3.40130141	11.57300000
C	2.87724661	-9.02069859	9.56100000
H	3.46424661	-9.63369859	9.94100000
C	1.05124661	-8.54969859	8.10500000
H	0.40024661	-8.84569859	7.50900000
C	-2.18175339	3.74130141	-3.26700000
H	-2.74575339	4.23930141	-3.81300000
C	-10.44375339	4.30430141	12.53700000
H	-10.98075339	4.78730141	13.12200000
C	1.92424661	-9.44769859	8.68400000
H	1.86124661	-10.35269859	8.47600000
C	-9.08275339	4.41430141	12.60100000
H	-8.69275339	4.96630141	13.24200000
F	-10.54175339	-9.16069859	5.41300000
C	-8.03575339	-6.76469859	4.44400000
H	-7.15275339	-6.75169859	4.15300000
C	-8.73175339	-5.58269859	4.59100000
C	-8.65375339	-7.97569859	4.73100000
H	-8.18475339	-8.77369859	4.65000000
C	-10.04275339	-5.63369859	5.01600000
H	-10.51875339	-4.84269859	5.12500000
C	-10.66175339	-6.84469859	5.28100000
H	-11.54975339	-6.87369859	5.55600000
C	-9.95475339	-7.97669859	5.13400000
O	-8.63875339	-3.24969859	4.71700000
C	-8.07375339	-4.25669859	4.37400000
C	-6.71675339	-4.17169859	3.81500000
H	-6.27175339	-3.40069859	4.17000000
H	-6.76975339	-4.10069859	2.85800000
H	-6.22375339	-4.96269859	4.04800000
F	-3.70175339	-1.36769859	5.16700000
C	-4.23475339	1.69130141	6.96300000
H	-4.61675339	1.98030141	7.76100000
O	-3.10775339	4.86030141	5.66300000
C	-3.68975339	2.62230141	6.09600000

C	-4.22375339	0.35130141	6.66900000
H	-4.57775339	-0.26969859	7.26400000
C	-3.12775339	0.84430141	4.57700000
H	-2.76575339	0.54930141	3.77200000
C	-3.72475339	4.09930141	6.38600000
C	-4.51575339	4.62130141	7.51600000
H	-4.65775339	5.56330141	7.39700000
H	-4.04075339	4.47030141	8.33600000
H	-5.36275339	4.17130141	7.54900000
C	-3.13175339	2.17330141	4.90700000
H	-2.75375339	2.78730141	4.32100000
C	-3.67975339	-0.04669859	5.47900000

Coordinates of the fully optimized structure of F[3]A1-[P(O)Ph]$_3$ with (G24) 1-Methylnaphthalene

P	-1.02739724	0.77910961	0.00000000
P	4.09260276	-8.95889039	-3.04500000
P	2.97960276	-0.59889039	-10.41800000
O	-1.87239724	1.18210961	-1.29300000
O	-1.52039724	-0.66489039	0.42900000
O	3.57160276	-9.28389039	-4.50900000
O	2.80460276	-8.86089039	-2.12000000
O	1.53660276	0.04510961	-10.18300000
O	2.70360276	-2.11289039	-10.84100000
O	0.42060276	0.87110961	-0.20800000
O	3.89560276	-0.42589039	-9.28700000
O	4.95660276	-7.78389039	-2.96600000
C	0.50260276	-5.44089039	-1.69000000
C	2.35660276	-6.31689039	-7.15100000
C	-0.15739724	-4.18389039	-1.30600000
C	2.21460276	-5.22489039	-8.13500000
C	3.17160276	-8.24789039	-5.38700000
C	0.41860276	-3.73389039	-0.11000000
C	1.45060276	-6.82789039	-6.22700000
H	0.55460276	-6.51389039	-6.22000000
C	3.67760276	-6.77489039	-7.19200000
C	0.28860276	-6.26389039	-2.79400000
H	-0.39139724	-6.04889039	-3.42200000
C	2.26960276	-6.88289039	-0.89500000
H	2.93660276	-7.11089039	-0.25800000
C	1.49060276	-5.73489039	-0.73700000

C	1.27960276	-3.33989039	-9.31500000
C	-0.79839724	1.67310961	-3.38300000
H	-0.53439724	2.52210961	-3.04800000
C	-0.47639724	1.27510961	-4.67200000
C	2.04460276	-7.67789039	-2.00200000
C	-0.46839724	-1.23189039	-7.38300000
H	-0.98139724	-1.99489039	-7.14100000
C	-1.16439724	-3.46889039	-1.93800000
H	-1.54539724	-3.79089039	-2.74600000
C	-0.35739724	-0.15889039	-6.50700000
C	1.85060276	-7.79289039	-5.31800000
C	1.07160276	-7.40589039	-2.97800000
C	0.17760276	-1.18489039	-8.62500000
C	1.51060276	-4.67689039	0.34400000
H	1.30560276	-5.06389039	1.23100000
H	2.38860276	-4.21889039	0.38300000
C	3.45160276	-5.02489039	-8.74600000
C	-0.89139724	0.02210961	-5.15000000
C	0.91460276	-0.03889039	-8.91700000
C	-1.02639724	-1.84589039	-0.17600000
C	4.09060276	-7.76589039	-6.30700000
H	4.97860276	-8.10389039	-6.33200000
C	0.35260276	1.98710961	-5.71500000
H	1.26460276	2.18010961	-5.38000000
H	-0.07639724	2.83210961	-6.00000000
C	1.13860276	-4.40089039	-8.41900000
H	0.29960276	-4.55789039	-8.00200000
C	0.92060276	-8.26289039	-4.21200000
H	-0.01639724	-8.22189039	-4.52900000
H	1.12660276	-9.20389039	-3.98500000
C	4.47660276	-6.01189039	-8.21400000
H	4.80960276	-6.60789039	-8.93000000
H	5.24360276	-5.54489039	-7.79600000
C	-0.03139724	-2.55289039	0.47400000
H	0.33460276	-2.24189039	1.29400000
C	-1.52039724	0.78210961	-2.59800000
C	-1.61239724	-2.27589039	-1.37800000
C	2.53760276	-3.15089039	-9.89500000
C	0.38260276	0.97510961	-6.84200000
C	-1.63139724	-0.83889039	-4.35600000
H	-1.91939724	-1.67689039	-4.69800000
C	3.61660276	-3.98089039	-9.65400000
H	4.44660276	-3.84289039	-10.09500000
C	-1.94939724	-0.46489039	-3.04400000

C	-2.64439724	-1.44189039	-2.10700000
H	-3.19339724	-0.94389039	-1.45200000
H	-3.24439724	-2.03389039	-2.62700000
C	3.44360276	0.12010961	-11.97500000
C	4.75560276	-10.52889039	-2.53000000
C	1.03760276	1.03610961	-8.05700000
H	1.55760276	1.79610961	-8.29400000
C	0.12560276	-2.37989039	-9.56100000
H	0.15860276	-2.06289039	-10.49900000
H	-0.73039724	-2.85889039	-9.43300000
C	-1.77139724	1.82710961	1.21300000
C	-2.09739724	4.06810961	2.00500000
H	-1.94439724	5.00110961	1.92400000
C	-2.86539724	3.58710961	3.03600000
H	-3.24139724	4.19010961	3.66600000
C	-1.55239724	3.20310961	1.09600000
H	-1.02539724	3.54010961	0.38100000
C	5.32560276	-11.40089039	-3.43800000
H	5.32260276	-11.19389039	-4.36400000
C	4.62660276	0.82810961	-12.05000000
H	5.16860276	0.93710961	-11.27800000
C	-2.53739724	1.35110961	2.25000000
H	-2.68639724	0.41810961	2.34500000
C	2.64460276	-0.04089039	-13.09700000
H	1.82760276	-0.51889039	-13.04100000
C	4.77160276	-10.85989039	-1.17300000
H	4.38260276	-10.26989039	-0.53900000
C	-3.09339724	2.24410961	3.16000000
H	-3.63339724	1.92010961	3.87000000
C	4.22660276	1.21110961	-14.37600000
H	4.50060276	1.59010961	-15.20400000
C	3.05960276	0.51210961	-14.30500000
H	2.52660276	0.40010961	-15.08400000
C	5.90960276	-12.88889039	-1.65400000
H	6.30760276	-13.69889039	-1.35600000
C	5.89960276	-12.57689039	-2.99400000
H	6.29060276	-13.17489039	-3.62000000
C	5.01360276	1.37210961	-13.25600000
H	5.82660276	1.85910961	-13.31500000
C	5.34860276	-12.03489039	-0.75100000
H	5.35560276	-12.25289039	0.17200000
C	5.84760276	-2.71889039	-6.76500000
C	7.03760276	-3.41489039	-6.58700000
H	7.81260276	-3.16289039	-7.07300000

C	7.09160276	-4.48289039	-5.69800000
H	7.90460276	-4.95789039	-5.57700000
C	5.95560276	-4.85389039	-4.98800000
H	5.99360276	-5.58289039	-4.38000000
C	4.76660276	-4.15789039	-5.16600000
C	4.71160276	-3.09089039	-6.05400000
C	3.52160276	-2.39489039	-6.23200000
H	3.48460276	-1.66489039	-6.84000000
C	2.38660276	-2.76589039	-5.52200000
H	1.57360276	-2.28889039	-5.64300000
C	2.44060276	-3.83289039	-4.63300000
H	1.66460276	-4.08689039	-4.14900000
C	3.63060276	-4.52889039	-4.45500000
H	3.66860276	-5.25989039	-3.84800000
C	5.91160276	-1.60889039	-7.61000000
H	5.02760276	-1.19089039	-7.66800000
H	6.55460276	-0.96289039	-7.25300000
H	6.19760276	-1.89489039	-8.50300000

Coordinates of the fully optimized structure of F[3]A1-[P(O)Ph]$_3$ with (**G35**) Ethylferrocene

Fe	0.18835616	2.26883568	0.00000000
C	-1.64564384	2.64383568	0.79000000
H	-2.01064384	2.25283568	1.63600000
C	1.17435616	0.94383568	1.23800000
C	0.00835616	-0.42516432	2.74700000
H	-0.15964384	-0.48316432	3.71200000
H	-0.84364384	-0.32016432	2.27400000
H	0.45535616	-1.24116432	2.44200000
C	2.21535616	2.48583568	-0.26500000
H	2.66435616	3.25283568	-0.59800000
C	1.69635616	1.35183568	-1.03700000
H	1.76335616	1.24383568	-1.97800000
C	1.09535616	0.46683568	-0.15700000
H	0.68335616	-0.34916432	-0.41800000
C	1.91535616	2.19983568	1.03900000
H	2.16535616	2.76783568	1.76000000
C	-0.90764384	3.82783568	0.68700000
H	-0.67564384	4.40583568	1.40400000
C	-1.78864384	2.11383568	-0.46800000
H	-2.25464384	1.31883568	-0.69800000

C	0.79135616	0.63383568	2.49600000
H	1.61735616	0.51583568	3.02800000
H	0.32835616	1.42883568	2.86100000
C	-1.10464384	2.98283568	-1.36100000
H	-1.03364384	2.86083568	-2.30000000
C	-0.56964384	4.01583568	-0.66000000
H	-0.05964384	4.73283568	-1.01700000
P	3.42035616	-1.31216432	-4.29100000
P	-1.02264384	8.54183568	-1.63800000
P	2.49935616	1.49283568	6.60300000
O	3.91035616	-0.04116432	-5.12700000
O	4.58435616	-1.60416432	-3.23900000
O	0.07835616	8.41383568	-2.78000000
O	-0.26764384	8.97883568	-0.31000000
O	2.10035616	-1.16916432	-3.69600000
O	2.75135616	3.06983568	6.61900000
O	3.80635616	0.85683568	5.97800000
O	-1.84264384	7.34283568	-1.48900000
O	1.25235616	1.08083568	5.96700000
C	2.78135616	5.95683568	-2.40500000
H	3.58235616	5.82683568	-1.90800000
C	2.38935616	5.02883568	-3.34900000
C	1.68935616	6.36283568	2.22700000
C	3.60935616	1.24783568	-4.64000000
C	4.75135616	0.12383568	0.51600000
C	2.18535616	3.14383568	-4.70600000
C	5.23935616	0.83783568	-0.57100000
H	5.61435616	1.70083568	-0.44300000
C	2.15035616	5.45783568	3.28400000
C	3.36435616	4.78483568	3.42200000
H	4.04435616	4.88383568	2.76500000
C	3.57335616	3.96383568	4.53300000
C	4.43435616	1.82283568	-3.67700000
C	5.17635616	0.28383568	-1.84600000
C	2.98335616	3.73883568	-3.72100000
C	0.38935616	8.06883568	0.53000000
C	2.50235616	1.88583568	-5.18000000
H	1.97935616	1.47183568	-5.85600000
C	1.98735616	7.09583568	-2.18900000
C	4.95335616	1.68083568	2.58300000
H	5.37435616	2.38783568	2.10800000
C	2.32535616	6.78983568	1.07200000
H	3.20535616	6.48983568	0.87900000
C	1.01435616	4.03983568	-5.04000000

H	1.03735616	4.32483568	-5.98800000
H	0.15135616	3.58783568	-4.85700000
C	4.63435616	0.50083568	1.93600000
C	4.10935616	3.10183568	-3.22000000
H	4.65435616	3.53183568	-2.57300000
C	1.68335616	7.65183568	0.19800000
C	4.61635616	-0.99516432	-1.97100000
C	1.22835616	5.20883568	-4.11200000
C	4.65435616	1.82183568	3.94100000
C	0.85035616	7.24783568	-2.95600000
C	2.34835616	8.06583568	-1.08700000
H	3.33035616	8.08083568	-0.96500000
H	2.05435616	8.97783568	-1.33600000
C	4.01735616	-0.55316432	2.63200000
C	4.05435616	0.75183568	4.59200000
C	2.70435616	1.08383568	8.31500000
C	-0.04664384	6.18083568	3.84700000
H	-0.22964384	6.87683568	4.52700000
H	-0.85664384	5.62583568	3.72500000
C	4.75235616	-2.68116432	-6.27500000
H	5.42135616	-2.00816432	-6.21800000
C	1.14235616	5.33583568	4.23700000
C	2.54235616	3.84983568	5.45900000
C	0.40135616	6.79583568	2.53800000
C	3.64935616	-2.62716432	-5.45200000
C	-0.26564384	7.66083568	1.68800000
H	-1.14164384	7.96583568	1.88900000
C	5.59935616	1.07183568	-3.06900000
H	6.30735616	1.71683568	-2.81500000
H	5.97835616	0.45283568	-3.74200000
C	1.33335616	4.52283568	5.35700000
H	0.66135616	4.43483568	6.02300000
C	4.21335616	-1.16016432	0.35300000
C	0.44935616	6.34283568	-3.92400000
H	-0.33164384	6.49383568	-4.44400000
C	4.85635616	3.15383568	4.64500000
H	5.60535616	3.64683568	4.22600000
H	5.07835616	3.00183568	5.59800000
C	4.15235616	-1.73316432	-0.90200000
H	3.80135616	-2.60716432	-1.02500000
C	3.63635616	1.73283568	9.11800000
H	4.16735616	2.43283568	8.75600000
C	3.71135616	-0.42216432	4.01100000
H	3.28835616	-1.11816432	4.50000000

C	2.65635616	-3.60416432	-5.55100000
H	1.89035616	-3.56616432	-4.98900000
C	3.72735616	-1.70216432	1.69400000
H	2.76035616	-1.91016432	1.66900000
H	4.22835616	-2.51416432	1.95700000
C	4.88335616	-3.71416432	-7.18300000
H	5.65535616	-3.76716432	-7.73500000
C	-1.78864384	10.07583568	-2.12200000
C	1.95435616	0.04883568	8.84500000
H	1.32435616	-0.40416432	8.29800000
C	3.79335616	1.36683568	10.42400000
H	4.42235616	1.81983568	10.97000000
C	3.03435616	0.33383568	10.95300000
H	3.14735616	0.08483568	11.86300000
C	2.11435616	-0.33616432	10.16600000
H	1.59935616	-1.04716432	10.52800000
C	-2.06664384	11.06383568	-1.19900000
H	-1.83164384	10.94383568	-0.28700000
C	-2.12164384	10.27783568	-3.42500000
H	-1.91764384	9.60683568	-4.06700000
C	3.90435616	-4.66516432	-7.28500000
H	3.98835616	-5.36016432	-7.92600000
C	2.79235616	-4.61916432	-6.46100000
H	2.12335616	-5.29116432	-6.52900000
C	-3.03264384	12.41683568	-2.87800000
H	-3.47264384	13.21983568	-3.13900000
C	-2.74864384	11.43783568	-3.83500000
H	-2.98364384	11.56883568	-4.74500000
C	-2.69164384	12.23083568	-1.61200000
H	-2.87864384	12.91083568	-0.97700000

Coordinates of the fully optimized structure of F[3]A1-[P(O)Ph]$_3$ with (**G36**) **18-crown-6**

P	3.39900000	-0.43600000	16.27900000
P	-1.71900000	2.15700000	7.08800000
P	6.27100000	9.24100000	10.70900000
O	1.80100000	-0.47700000	16.43100000
O	3.85900000	0.93500000	16.92200000
O	-2.63300000	1.69700000	8.31300000
O	-1.91500000	3.73300000	6.94900000
O	6.10300000	9.02700000	12.26500000

O	4.85200000	9.69600000	10.16200000
O	3.88700000	-0.64900000	14.92500000
O	-0.31800000	1.73600000	7.19300000
O	6.86100000	8.09800000	10.03000000
C	0.02600000	2.03100000	14.41200000
H	-0.14800000	2.96500000	14.39600000
C	-0.45900000	1.22100000	13.40900000
C	4.04800000	4.56500000	14.93900000
C	0.76700000	6.12500000	7.64200000
C	-1.29200000	0.37200000	11.42000000
C	-1.14200000	1.55300000	12.15600000
C	0.50400000	-0.72500000	14.45500000
H	0.66100000	-1.66100000	14.48500000
C	0.53800000	6.34800000	9.00000000
C	2.81400000	4.11500000	15.40500000
H	2.03300000	4.64000000	15.27600000
C	1.00700000	0.11100000	15.42600000
C	5.15700000	2.59500000	15.78400000
H	5.94100000	2.07800000	15.92800000
C	-0.50500000	5.72100000	9.67200000
H	-0.64100000	5.89100000	10.59600000
C	2.73400000	2.88900000	16.06100000
C	0.77200000	1.47700000	15.44800000
C	4.38400000	5.78300000	14.20200000
C	-0.23300000	-0.16100000	13.44000000
C	-2.06700000	2.83700000	10.34100000
C	3.57000000	6.80700000	13.74800000
H	2.63400000	6.78000000	13.91200000
C	1.57300000	7.25500000	9.48900000
C	3.91500000	2.15600000	16.22200000
C	-1.76200000	0.41800000	10.12900000
H	-1.83300000	-0.37000000	9.60500000
C	-0.81600000	-0.81400000	12.22600000
H	-1.56800000	-1.41100000	12.46600000
H	-0.13200000	-1.33300000	11.73400000
C	-2.12900000	1.65200000	9.61900000
C	-0.05100000	5.24400000	6.96500000
H	0.08700000	5.06900000	6.04100000
C	5.76900000	5.78900000	13.95400000
C	4.12700000	7.87800000	13.05000000
C	-1.35100000	4.84500000	8.99700000
C	2.91700000	8.52200000	11.01100000
C	-1.54600000	2.77300000	11.62400000
H	-1.46400000	3.56600000	12.14100000

C	1.81400000	7.70700000	10.76900000
H	1.23200000	7.46500000	11.48000000
C	5.21300000	3.81500000	15.13100000
C	-2.49100000	4.15700000	9.72900000
H	-2.82500000	4.75400000	10.44500000
H	-3.23500000	3.99700000	9.09500000
C	-1.07900000	4.61700000	7.65800000
C	1.38300000	2.35400000	16.51000000
H	1.49600000	1.83300000	17.34400000
H	0.77600000	3.11200000	16.70100000
C	3.91700000	-1.59600000	17.51600000
C	5.51400000	7.88600000	12.85700000
C	6.34600000	6.86300000	13.28100000
H	7.28100000	6.89300000	13.11800000
C	3.24900000	8.93500000	12.42400000
H	2.41600000	9.03500000	12.95000000
H	3.72000000	9.80500000	12.41900000
C	6.40600000	4.53700000	14.51600000
H	7.08600000	4.75700000	15.20100000
H	6.82600000	3.99500000	13.80300000
C	1.97400000	6.91400000	7.17600000
H	2.68000000	6.31600000	6.82300000
H	1.72600000	7.57100000	6.47800000
C	5.29500000	-1.79800000	17.65700000
H	5.90500000	-1.33200000	17.09900000
C	3.75200000	8.83800000	9.94200000
C	2.42100000	7.59800000	8.43000000
C	3.01700000	-2.28500000	18.33200000
H	2.08100000	-2.15800000	18.23000000
C	-2.66600000	1.54000000	5.72600000
C	3.53500000	8.40500000	8.65300000
H	4.12000000	8.64700000	7.94500000
C	-2.71300000	0.16200000	5.55900000
H	-2.28700000	-0.41100000	6.18500000
C	7.17100000	10.78000000	10.61600000
C	-3.30700000	2.37700000	4.81700000
H	-3.28400000	3.32000000	4.93500000
C	3.50300000	-3.15100000	19.28800000
H	2.90000000	-3.61800000	19.85300000
C	-4.00700000	0.46300000	3.56800000
H	-4.46000000	0.09500000	2.81800000
C	-3.38500000	-0.37100000	4.47100000
H	-3.41800000	-1.31200000	4.34800000
C	5.76300000	-2.67800000	18.61100000

H	6.69600000	-2.82600000	18.70700000
C	-3.97500000	1.82300000	3.74400000
H	-4.41700000	2.38900000	3.12200000
C	6.51400000	11.99800000	10.62100000
H	5.56900000	12.02600000	10.70900000
C	4.86700000	-3.34200000	19.42800000
H	5.19100000	-3.93800000	20.09300000
C	7.23100000	13.17700000	10.49800000
H	6.77700000	14.01200000	10.49600000
C	8.55200000	10.74400000	10.50200000
H	9.01300000	9.91400000	10.50500000
C	9.26100000	11.94900000	10.38200000
H	10.20800000	11.93500000	10.30100000
C	8.59400000	13.14000000	10.38100000
H	9.08100000	13.95100000	10.29800000
O	0.34600000	9.35300000	14.68000000
O	-1.87000000	8.90200000	13.17800000
C	-0.19400000	10.36500000	13.85300000
H	0.52200000	10.98900000	13.57700000
H	-0.87600000	10.87800000	14.35500000
C	0.78600000	9.87700000	15.89800000
H	0.03500000	10.32000000	16.36700000
H	1.49600000	10.54800000	15.74100000
C	-3.99200000	5.32200000	13.88300000
H	-4.50600000	4.95400000	13.12100000
H	-4.60600000	5.87300000	14.42900000
C	-0.80300000	9.76000000	12.67600000
H	-0.13600000	9.22800000	12.17300000
H	-1.16900000	10.45700000	12.07600000
C	-3.47000000	7.28000000	12.69900000
H	-4.02900000	7.79800000	13.32900000
H	-4.05900000	6.95900000	11.97000000
C	-2.44900000	8.18700000	12.11500000
H	-1.75700000	7.66200000	11.63900000
H	-2.87000000	8.80900000	11.47200000
O	-2.93400000	6.13700000	13.39100000
O	-3.01900000	4.71600000	15.93400000
O	-0.80300000	5.16700000	17.43500000
C	-2.47900000	3.70500000	16.76100000
H	-3.19600000	3.08100000	17.03700000
H	-1.79800000	3.19100000	16.25900000
C	-3.45900000	4.19300000	14.71600000
H	-2.70800000	3.75000000	14.24700000
H	-4.16900000	3.52200000	14.87200000

C	1.31900000	8.74700000	16.73000000
H	1.83300000	9.11600000	17.49200000
H	1.93300000	8.19600000	16.18400000
C	-1.87000000	4.30900000	17.93800000
H	-2.53700000	4.84200000	18.44100000
H	-1.50400000	3.61200000	18.53800000
C	0.79700000	6.79000000	17.91500000
H	1.35600000	6.27200000	17.28500000
H	1.38600000	7.11100000	18.64400000
C	-0.22400000	5.88300000	18.49800000
H	-0.91600000	6.40700000	18.97500000
H	0.19700000	5.26100000	19.14200000
O	0.26100000	7.93300000	17.22300000

Coordinates of the fully optimized structure of F[3]A1-[P(O)Ph]$_3$ with (**G37**) **dithianon**

P	-0.32534246	2.45719185	0.00000000
P	-6.47734246	-2.57680815	7.76700000
P	-6.25734246	8.49219185	7.65500000
O	-1.77934246	2.35919185	-0.11200000
O	0.32665754	1.24719185	0.81400000
O	-6.30134246	-1.85680815	9.17700000
O	-4.80534246	8.86919185	7.13700000
O	-5.04234246	-3.17180815	7.40900000
O	-6.06234246	7.72419185	9.03000000
O	0.19365754	3.78819185	0.70100000
O	-7.03834246	-1.71980815	6.72100000
O	-7.04834246	7.74819185	6.68500000
C	-5.33434246	2.18119185	9.31400000
C	-2.39734246	6.26119185	4.99100000
C	-5.29934246	3.65019185	9.28000000
C	-1.63334246	5.48819185	4.00900000
C	-6.66534246	1.77319185	9.47000000
C	-1.53834246	-0.22480815	4.21300000
C	-2.45834246	6.15619185	6.36800000
H	-1.94034246	5.49319185	6.81100000
C	-1.77134246	-0.84480815	2.97100000
C	-5.96434246	-0.47680815	9.22500000
C	-4.48034246	5.89919185	8.96500000
C	-6.60934246	4.12819185	9.43000000
C	-4.32334246	1.24319185	9.14100000

H	-3.42134246	1.53019185	9.06000000
C	-0.75934246	4.43119185	4.18700000
H	-0.57834246	4.11019185	5.06200000
C	-2.34734246	-0.91480815	5.22400000
C	-6.98734246	0.42719185	9.43200000
H	-7.88434246	0.13519185	9.54500000
C	-0.45234246	4.34819185	1.83400000
C	-2.48034246	-0.67780815	6.58400000
H	-1.96134246	-0.00080815	7.00100000
C	-4.24334246	4.52419185	9.06700000
H	-3.35834246	4.18819185	8.99200000
C	-3.37234246	-1.42880815	7.34000000
C	-3.14134246	7.24019185	4.31300000
C	-4.12334246	-2.40080815	6.67700000
C	-3.99834246	-2.66880815	5.32000000
H	-4.52134246	-3.34280815	4.90300000
C	-4.62634246	-0.11580815	9.08600000
C	-3.08734246	-1.92080815	4.59800000
C	-1.30634246	5.41819185	1.62200000
H	-1.47834246	5.74419185	0.74600000
C	-0.14434246	3.83619185	3.09100000
C	0.63365754	2.45019185	-1.49600000
C	-1.15034246	-0.34780815	1.82500000
H	-1.29434246	-0.74780815	0.97600000
C	-3.37434246	6.85919185	8.60600000
H	-3.55934246	7.74319185	9.01300000
H	-2.51634246	6.52619185	8.97000000
C	-1.89834246	5.99419185	2.72900000
C	-3.96934246	8.09619185	5.02900000
H	-4.48734246	8.75919185	4.58900000
C	-6.86234246	5.48119185	9.34000000
H	-7.74434246	5.81719185	9.44300000
C	-4.01234246	7.95019185	6.40500000
C	-3.55134246	-1.15180815	8.82300000
H	-3.79134246	-1.99480815	9.28500000
H	-2.69234246	-0.83380815	9.20000000
C	-2.85834246	7.16319185	2.83200000
H	-2.44034246	7.99819185	2.50600000
H	-3.68734246	6.99119185	2.31900000
C	-3.26534246	7.00319185	7.11300000
C	-0.69234246	0.86619185	4.31500000
H	-0.53834246	1.26519185	5.16300000
C	0.76165754	2.64719185	3.26600000
H	1.21565754	2.69719185	4.14400000

H	1.45265754	2.64419185	2.55800000
C	-0.31534246	0.75019185	1.96600000
C	-5.80134246	6.33519185	9.09900000
C	-2.74934246	-1.98380815	3.12600000
H	-2.33134246	-2.84980815	2.88900000
H	-3.55334246	-1.84480815	2.56500000
C	-7.39734246	-4.03580815	8.20600000
C	-7.76234246	-4.90580815	7.17700000
H	-7.45734246	-4.75280815	6.29100000
C	-0.06634246	1.38019185	3.18500000
C	0.37665754	3.45419185	-2.43100000
H	-0.25834246	4.13319185	-2.23800000
C	-7.57034246	2.97019185	9.58300000
H	-8.02534246	2.99419185	10.46200000
H	-8.25134246	2.97319185	8.86400000
C	-8.57434246	-5.99480815	7.45600000
H	-8.83034246	-6.58380815	6.75700000
C	-9.00934246	-6.22580815	8.74200000
H	-9.55834246	-6.97880815	8.92500000
C	-7.83534246	-4.27680815	9.49400000
H	-7.57834246	-3.69380815	10.20000000
C	1.98165754	2.48219185	-3.91000000
H	2.45065754	2.49719185	-4.73700000
C	1.04765754	3.46219185	-3.63800000
H	0.86565754	4.13819185	-4.27800000
C	1.56865754	1.45719185	-1.78000000
H	1.74165754	0.77019185	-1.14800000
C	-8.65434246	-5.37480815	9.75900000
H	-8.96434246	-5.53380815	10.64200000
C	2.24365754	1.47819185	-2.99200000
H	2.88365754	0.80619185	-3.19100000
C	-6.64734246	10.16519185	8.28400000
C	-5.87834246	10.80519185	9.24900000
H	-5.09234246	10.39019185	9.58300000
C	-6.26234246	12.05419185	9.72600000
H	-5.73634246	12.49119185	10.38700000
C	-7.41234246	12.66119185	9.23700000
H	-7.67434246	13.51519185	9.56400000
C	-8.18134246	12.02019185	8.27300000
H	-8.96734246	12.43719185	7.93900000
C	-7.79934246	10.77219185	7.79600000
H	-8.32334246	10.33319185	7.13800000
C	2.36065754	-0.85280815	4.05200000
C	2.02165754	-1.64080815	2.95900000

C	2.56465754	-1.36680815	1.70900000
C	3.24365754	0.20919185	3.89600000
C	0.82865754	-2.33880815	5.57700000
C	0.50065754	-3.10980815	4.53100000
C	-1.78734246	-5.74580815	6.29900000
H	-2.01034246	-6.29080815	5.55400000
C	-0.97534246	-4.63080815	6.12600000
C	-0.64934246	-3.83280815	7.21600000
C	-1.13434246	-4.14980815	8.47900000
H	-0.91134246	-3.60380815	9.22600000
C	-1.94634246	-5.26480815	8.65300000
H	-2.27834246	-5.47980815	9.51700000
C	-2.27334246	-6.06280815	7.56300000
H	-2.82834246	-6.82480815	7.68200000
O	-0.78734246	-5.08180815	3.83900000
S	1.75265754	-1.03780815	5.76200000
C	0.28565754	-2.63380815	6.77400000
S	0.85565754	-3.06280815	3.02800000
N	3.99865754	1.02819185	3.94600000
O	0.53665754	-1.98080815	8.04300000
C	-0.51634246	-4.30980815	4.98800000
N	2.98665754	-1.19480815	0.67300000
P	1.93165754	-8.07980815	10.26000000
P	7.62465754	-2.82980815	2.44700000
P	7.51665754	-13.94780815	2.26400000
O	3.38965754	-7.96480815	10.20100000
O	1.16865754	-6.87780815	9.53800000
O	1.35865754	-9.41180815	9.60500000
O	6.19765754	-2.23880815	2.83400000
O	8.18965754	-3.70380815	3.47100000
O	7.41965754	-3.52380815	1.02600000
O	6.08565754	-14.31980815	2.83100000
O	7.27165754	-13.10680815	0.93300000
O	8.37665754	-13.29180815	3.23900000
C	3.04565754	-11.03680815	6.18000000
C	2.15965754	-9.97580815	6.06300000
H	1.94765754	-9.62880815	5.20600000
C	7.80665754	-7.13780815	0.61100000
C	1.57965754	-9.42180815	7.19400000
C	3.03965754	-4.65580815	7.31900000
C	3.77865754	-11.76780815	5.15600000
C	5.43365754	-9.92180815	1.04700000
H	4.54865754	-9.59780815	1.17200000
C	6.48865754	-7.56480815	0.80800000

C	1.94565754	-9.96080815	8.43400000
C	3.66765754	-4.77680815	3.69000000
H	3.14665754	-5.45480815	3.27600000
C	1.70865754	-6.32280815	8.35500000
C	2.79165754	-5.26680815	6.08100000
C	3.55865754	-4.55180815	5.05400000
C	1.16465754	-8.09980815	11.86700000
C	4.54365754	-4.00780815	2.92300000
C	3.78365754	-11.62180815	3.77700000
H	3.25265754	-10.94480815	3.37300000
C	2.81465754	-11.02480815	8.58000000
H	3.02965754	-11.36680815	9.44100000
C	3.36465754	-11.57780815	7.43900000
C	5.18665754	-2.76680815	4.93800000
H	5.70365754	-2.08380815	5.34800000
C	4.55065754	-12.76680815	5.77000000
C	2.49565754	-5.18680815	8.46900000
H	2.65465754	-4.78580815	9.31600000
C	8.11165754	-5.78880815	0.67300000
H	8.99865754	-5.48280815	0.52900000
C	6.46865754	-9.02980815	0.80300000
C	7.77065754	-9.49380815	0.59100000
C	4.55865754	-12.45380815	2.98200000
C	5.46965754	-6.63980815	1.04000000
H	4.57465754	-6.93980815	1.14100000
C	5.29665754	-3.03380815	3.58400000
C	4.68665754	-4.25880815	1.43800000
H	4.90765754	-3.40680815	0.98500000
H	3.81965754	-4.57680815	1.08000000
C	5.76065754	-5.28280815	1.12200000
C	3.97365754	-3.48480815	7.15000000
H	4.79065754	-3.59380815	7.69800000
H	3.53065754	-2.63380815	7.39300000
C	1.98465754	-6.39280815	5.98700000
H	1.80865754	-6.78480815	5.14000000
C	4.59365754	-12.27180815	1.48600000
H	3.71865754	-11.93280815	1.17200000
H	4.76265754	-13.14380815	1.04900000
C	4.29465754	-3.53080815	5.67700000
C	1.59365754	-9.05980815	12.76500000
H	2.24265754	-9.70080815	12.50100000
C	5.68865754	-11.28880815	1.10900000
C	0.64665754	-8.23780815	7.08100000
H	-0.01234246	-8.26180815	7.82100000

H	0.15165754	-8.28480815	6.22500000
C	4.32165754	-12.73380815	7.26800000
H	3.91965754	-13.58080815	7.58700000
H	5.16765754	-12.57180815	7.75500000
C	8.96365754	-0.54080815	3.05400000
H	8.64965754	-0.69380815	3.93900000
C	7.09165754	-4.90180815	0.95200000
C	1.43365754	-6.94480815	7.14400000
C	8.56265754	-1.37980815	2.02500000
C	5.34065754	-13.41880815	3.63100000
C	8.72065754	-8.32480815	0.41800000
H	9.43865754	-8.34080815	1.10100000
H	9.12865754	-8.32280815	-0.48300000
C	5.35765754	-13.59380815	5.00100000
H	5.90365754	-14.25780815	5.40500000
C	9.82365754	0.52419185	2.79700000
H	10.09565754	1.09619185	3.50600000
C	6.99265754	-11.71580815	0.91100000
C	0.22665754	-7.14480815	12.25400000
H	-0.05934246	-6.47580815	11.64200000
C	1.07465754	-9.08380815	14.04800000
H	1.36165754	-9.74580815	14.66700000
C	8.04665754	-10.84880815	0.64000000
H	8.92565754	-11.17580815	0.49300000
C	8.99965754	-1.12580815	0.73800000
H	8.71065754	-1.67680815	0.02000000
C	10.27965754	0.74719185	1.52000000
H	10.88265754	1.46219185	1.34700000
C	0.14065754	-8.14180815	14.42400000
H	-0.21234246	-8.15780815	15.30700000
C	8.07665754	-15.49580815	1.60300000
C	-0.28534246	-7.18080815	13.54100000
H	-0.93134246	-6.53980815	13.81300000
C	9.86365754	-0.06280815	0.49400000
H	10.16765754	0.10319185	-0.39100000
C	9.19265754	-16.08180815	2.15900000
H	9.61265754	-15.68780815	2.91500000
C	7.42165754	-16.10980815	0.53500000
H	6.63465754	-15.72180815	0.17200000
C	9.70965754	-17.27380815	1.60100000
H	10.49965754	-17.66680815	1.95500000
C	7.92565754	-17.28680815	0.00800000
H	7.48965754	-17.70480815	-0.72400000
C	9.05965754	-17.85080815	0.55000000

H 9.39765754 -18.65780815 0.18400000

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