

Intermolecular interactions in the solid state structures of isoflavones: the relationship between torsions angle, supramolecular structure, melting point and solubility

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Supporting Information (SI)

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1. Calculation of the Lattice Energies

Table S 1: GK-13

	N	Symop	R	Electron Density	E_ele	E_pol	E_dis	E_rep	E_tot
	2.00	-x+1/2, y+1/2, z+1/2	14,97	B3LYP/6-31G(d,p)	0.10	0.00	-0.20	0.00	-0.10
	2.00	x+1/2, -y+1/2, z	16.91	B3LYP/6-31G(d,p)	0.00	0.00	-0.20	0.00	-0.20
	2.00	x+1/2, -y+1/2, z	15.53	B3LYP/6-31G(d,p)	0.20	-0.10	-0.60	0.00	-0.40
	2.00	-x+1/2, y+1/2, z+1/2	11,60	B3LYP/6-31G(d,p)	0.10	-0.10	-2.10	0.00	-1.80
	2.00	x, y, z	23.11	B3LYP/6-31G(d,p)	-0.10	0.00	-0.10	0.00	-0.20
	2.00	x+1/2, -y+1/2, z	16.91	B3LYP/6-31G(d,p)	-0.50	0.00	-0.30	0.00	-0.80
	2.00	-x+1/2, y+1/2, z+1/2	11,60	B3LYP/6-31G(d,p)	-2.80	-0.90	-12.40	4.40	-11.80
	2.00	-x+1/2, y+1/2, z+1/2	23,68	B3LYP/6-31G(d,p)	0.10	0.00	0.00	0.00	0.00
	2.00	-x+1/2, y+1/2, z+1/2	14,97	B3LYP/6-31G(d,p)	-1.20	-0.10	-0.40	0.00	-1.70
	2.00	x+1/2, -y+1/2, z	11.34	B3LYP/6-31G(d,p)	-1.50	-0.20	-10.70	7.60	-6.30
	2.00	x+1/2, -y+1/2, z	9.16	B3LYP/6-31G(d,p)	-7.20	-2.00	-36.40	24.00	-25.90
	2.00	-x, -y, z+1/2	18,45	B3LYP/6-31G(d,p)	-0.10	0.00	-0.10	0.00	-0.10
	2.00	x+1/2, -y+1/2, z	11.34	B3LYP/6-31G(d,p)	1.40	-0.30	-3.80	1.50	-1.00
	2.00	x, y, z	13.38	B3LYP/6-31G(d,p)	0.20	0.00	-0.30	0.00	-0.10
	2.00	x, y, z	6.69	B3LYP/6-31G(d,p)	-15.00	-4.00	-33.60	25.60	-32.30
	2.00	-x, -y, z+1/2	11,40	B3LYP/6-31G(d,p)	-0.40	-0.10	-0.80	0.00	-1.20
	2.00	x, y, z	16.06	B3LYP/6-31G(d,p)	0.10	0.00	-0.30	0.00	-0.20
	2.00	-x, -y, z+1/2	6,37	B3LYP/6-31G(d,p)	-18.20	-4.50	-66.20	42.20	-54.20
	2.00	-x+1/2, y+1/2, z+1/2	15,65	B3LYP/6-31G(d,p)	0.40	0.00	-0.20	0.00	0.20
	2.00	x, y, z	14.60	B3LYP/6-31G(d,p)	0.10	-0.10	-1.50	0.00	-1.30
	2.00	-x+1/2, y+1/2, z+1/2	12,47	B3LYP/6-31G(d,p)	1.70	-0.10	-1.90	0.00	0.10
	2.00	-x, -y, z+1/2	20,27	B3LYP/6-31G(d,p)	0.10	0.00	-0.10	0.00	0.10
	2.00	x, y, z	16.06	B3LYP/6-31G(d,p)	-0.10	0.00	-0.50	0.00	-0.50
	2.00	-x+1/2, y+1/2, z+1/2	12,47	B3LYP/6-31G(d,p)	0.70	-0.10	-2.40	0.00	-1.40
	2.00	x+1/2, -y+1/2, z	16.22	B3LYP/6-31G(d,p)	0.10	0.00	-0.10	0.00	0.00
	2.00	-x, -y, z+1/2	13,64	B3LYP/6-31G(d,p)	-0.10	-0.10	-0.60	0.00	-0.70
	2.00	-x, -y, z+1/2	9,82	B3LYP/6-31G(d,p)	-11.90	-3.50	-38.00	23.90	-33.50
	2.00	-x+1/2, y+1/2, z+1/2	15,65	B3LYP/6-31G(d,p)	0.00	0.00	-0.20	0.00	-0.20
	2.00	x+1/2, -y+1/2, z	19.94	B3LYP/6-31G(d,p)	-0.10	0.00	-0.10	0.00	-0.20
	2.00	x+1/2, -y+1/2, z	16.22	B3LYP/6-31G(d,p)	0.10	0.00	-0.10	0.00	0.00
	2.00	x+1/2, -y+1/2, z	18.79	B3LYP/6-31G(d,p)	0.00	0.00	-0.20	0.00	-0.10
	2.00	x+1/2, -y+1/2, z	19.94	B3LYP/6-31G(d,p)	0.10	0.00	-0.10	0.00	0.00
	2.00	-x, -y, z+1/2	20,93	B3LYP/6-31G(d,p)	0.10	0.00	-0.10	0.00	0.10

Table S 2: GK-13B

	N	Symop	R	Electron Density	E_ele	E_pol	E_dis	E_rep	E_tot
	1.00	-x, -y, -z	13,21	B3LYP/6-31G(d,p)	1.20	0.00	-0.20	0.00	1.10
	2.00	x, y, z	10.48	B3LYP/6-31G(d,p)	-0.60	-0.10	-1.10	0.00	-1.60
	2.00	x, y, z	16.62	B3LYP/6-31G(d,p)	-0.50	0.00	-0.10	0.00	-0.60
	1.00	-x, -y, -z	10,51	B3LYP/6-31G(d,p)	1.00	-0.20	-0.80	0.00	0.20
	2.00	x, y, z	13.85	B3LYP/6-31G(d,p)	0.30	0.00	-0.20	0.00	0.20
	2.00	x, y, z	16.04	B3LYP/6-31G(d,p)	-0.50	0.00	-0.20	0.00	-0.80
	2.00	x, y, z	8.02	B3LYP/6-31G(d,p)	-65.80	-16.30	-39.50	82.00	-65.40
	1.00	-x, -y, -z	12,02	B3LYP/6-31G(d,p)	0.60	-0.20	-9.40	0.00	-7.70
	1.00	-x, -y, -z	20,50	B3LYP/6-31G(d,p)	-0.30	0.00	-0.10	0.00	-0.40
	2.00	x, y, z	14.78	B3LYP/6-31G(d,p)	0.10	0.00	-0.40	0.00	-0.30
	2.00	x, y, z	20.61	B3LYP/6-31G(d,p)	-0.10	0.00	0.00	0.00	-0.20
	2.00	x, y, z	19.55	B3LYP/6-31G(d,p)	0.40	0.00	-0.10	0.00	0.40
	1.00	-x, -y, -z	13,80	B3LYP/6-31G(d,p)	-1.80	-0.10	-0.60	0.00	-2.40
	2.00	x, y, z	12.76	B3LYP/6-31G(d,p)	-5.20	-1.00	-14.20	0.00	-18.70
	1.00	-x, -y, -z	13,25	B3LYP/6-31G(d,p)	-9.40	-0.90	-15.00	0.00	-23.80
	1.00	-x, -y, -z	18,72	B3LYP/6-31G(d,p)	-0.30	0.00	-0.30	0.00	-0.60
	2.00	x, y, z	18.20	B3LYP/6-31G(d,p)	-0.10	0.00	-0.10	0.00	-0.20
	1.00	-x, -y, -z	11,17	B3LYP/6-31G(d,p)	-1.10	-0.30	-2.10	0.00	-3.20
	2.00	x, y, z	13.73	B3LYP/6-31G(d,p)	0.10	0.00	-0.10	0.00	0.00
	2.00	x, y, z	12.81	B3LYP/6-31G(d,p)	0.50	0.00	-0.60	0.00	0.00

	N	Symp	R	Electron Density	E_ele	E_pol	E_dis	E_rep	E_tot
	1.00	-x, -y, -z	13,93	B3LYP/6-31G(d,p)	0.10	0.00	-0.20	0.00	0.00
	2.00	x, y, z	8.48	B3LYP/6-31G(d,p)	-5.80	-1.90	-20.10	8.40	-19.90
	2.00	x, y, z	16.97	B3LYP/6-31G(d,p)	-0.10	0.00	-0.10	0.00	-0.20
	1.00	-x, -y, -z	16,04	B3LYP/6-31G(d,p)	0.30	0.00	-0.10	0.00	0.30
	2.00	x, y, z	17.68	B3LYP/6-31G(d,p)	0.00	0.00	-0.10	0.00	-0.10
	1.00	-x, -y, -z	5,85	B3LYP/6-31G(d,p)	0.30	-4.30	-30.70	10.50	-23.10
	2.00	x, y, z	11.87	B3LYP/6-31G(d,p)	0.60	0.00	-0.60	0.00	0.10
	1.00	-x, -y, -z	7,40	B3LYP/6-31G(d,p)	-3.00	-0.70	-29.80	14.70	-20.60
	2.00	x, y, z	16.17	B3LYP/6-31G(d,p)	0.10	0.00	-0.10	0.00	0.10
	1.00	-x, -y, -z	9,36	B3LYP/6-31G(d,p)	-1.50	-0.20	-3.30	0.00	-4.60
	1.00	-x, -y, -z	20,35	B3LYP/6-31G(d,p)	0.00	0.00	0.00	0.00	-0.10
	1.00	-x, -y, -z	7,70	B3LYP/6-31G(d,p)	-11.70	-1.70	-55.70	35.50	-40.20
	2.00	x, y, z	16.38	B3LYP/6-31G(d,p)	0.00	0.00	-0.50	0.00	-0.40
	2.00	x, y, z	20.13	B3LYP/6-31G(d,p)	0.00	0.00	-0.10	0.00	-0.10
	1.00	-x, -y, -z	16,88	B3LYP/6-31G(d,p)	0.00	0.00	-0.10	0.00	-0.10
	1.00	-x, -y, -z	14,42	B3LYP/6-31G(d,p)	-0.20	0.00	-0.70	0.00	-0.90
	2.00	x, y, z	21.49	B3LYP/6-31G(d,p)	0.00	0.00	0.00	0.00	0.00
	1.00	-x, -y, -z	14,27	B3LYP/6-31G(d,p)	-7.40	-0.80	-8.90	0.00	-16.20
	1.00	-x, -y, -z	16,11	B3LYP/6-31G(d,p)	-0.30	0.00	-0.10	0.00	-0.40
	1.00	-x, -y, -z	9,30	B3LYP/6-31G(d,p)	-13.70	-1.90	-48.70	30.60	-39.40
	1.00	-x, -y, -z	9,68	B3LYP/6-31G(d,p)	-1.10	-0.20	-2.00	0.00	-3.10
	1.00	-x, -y, -z	18,89	B3LYP/6-31G(d,p)	-0.10	0.00	0.00	0.00	-0.10
	1.00	-x, -y, -z	10,65	B3LYP/6-31G(d,p)	0.50	-0.10	-1.00	0.00	-0.30
	1.00	-x, -y, -z	8,47	B3LYP/6-31G(d,p)	-0.60	-0.10	-2.20	0.00	-2.60
	1.00	-x, -y, -z	17,68	B3LYP/6-31G(d,p)	-0.20	0.00	-0.10	0.00	-0.20
	1.00	-x, -y, -z	13,92	B3LYP/6-31G(d,p)	0.20	0.00	-0.20	0.00	0.10
	1.00	-x, -y, -z	20,27	B3LYP/6-31G(d,p)	-0.60	0.00	-0.10	0.00	-0.70
	1.00	-x, -y, -z	16,35	B3LYP/6-31G(d,p)	1.30	-0.20	-0.50	0.00	0.80
	1.00	-x, -y, -z	16,16	B3LYP/6-31G(d,p)	0.00	0.00	-0.10	0.00	-0.20
	1.00	-x, -y, -z	16,36	B3LYP/6-31G(d,p)	0.30	0.00	-0.10	0.00	0.30
	1.00	-x, -y, -z	14,58	B3LYP/6-31G(d,p)	0.10	0.00	-0.10	0.00	0.00

	N	Symp	R	Electron Density	E_ele	E_pol	E_dis	E_rep	E_tot
	2	x+1/2, -y+1/2, z+1/2	9.32	B3LYP/6-31G(d,p)	-7.9	-2.2	-25.3	11.3	-25.1
	1	-x, -y, -z	13.23	B3LYP/6-31G(d,p)	-1.2	-0.2	-6.8	1	-6.8
	2	x+1/2, -y+1/2, z+1/2	14.96	B3LYP/6-31G(d,p)	-0.4	-0.1	-3.4	1.5	-2.6
	2	x+1/2, -y+1/2, z+1/2	9.13	B3LYP/6-31G(d,p)	-0.7	-0.7	-15.8	9.4	-9.2
	2	x, y, z	8.17	B3LYP/6-31G(d,p)	-65.3	-15.7	-49	85.7	-70.4
	2	-x+1/2, y+1/2, -z+1/2	7.93	B3LYP/6-31G(d,p)	-5.2	-1	-41.4	20.6	-29.5
	1	-x, -y, -z	13.95	B3LYP/6-31G(d,p)	-1.2	0	-11.7	7.3	-6.9
	1	-x, -y, -z	5.97	B3LYP/6-31G(d,p)	0.9	-3.9	-30.5	8.1	-23.5
	1	-x, -y, -z	9.95	B3LYP/6-31G(d,p)	-13	-1.8	-45.1	27.4	-37.4
	2	-x+1/2, y+1/2, -z+1/2	10.92	B3LYP/6-31G(d,p)	-2.7	-1	-9.6	6.1	-8.3
	2	x, y, z	31.8	B3LYP/6-31G(d,p)	0	0	0	0	0
	2	-x+1/2, y+1/2, -z+1/2	26.78	B3LYP/6-31G(d,p)	0	0	0	0	0
	2	x+1/2, -y+1/2, z+1/2	23.86	B3LYP/6-31G(d,p)	-0.1	0	0	0	-0.1
	1	-x, -y, -z	30.1	B3LYP/6-31G(d,p)	0	0	0	0	0
	1	-x, -y, -z	29.79	B3LYP/6-31G(d,p)	0	0	0	0	0
	2	x+1/2, -y+1/2, z+1/2	28.97	B3LYP/6-31G(d,p)	0	0	0	0	0
	2	-x+1/2, y+1/2, -z+1/2	21.22	B3LYP/6-31G(d,p)	0.1	0	0	0	0
	2	x+1/2, -y+1/2, z+1/2	25.17	B3LYP/6-31G(d,p)	-0.1	0	0	0	-0.1
	1	-x, -y, -z	26.5	B3LYP/6-31G(d,p)	0	0	0	0	0
	2	x+1/2, -y+1/2, z+1/2	27.76	B3LYP/6-31G(d,p)	-0.1	0	0	0	-0.1
	2	x, y, z	28.48	B3LYP/6-31G(d,p)	0	0	0	0	0
	2	x+1/2, -y+1/2, z+1/2	20.79	B3LYP/6-31G(d,p)	-0.1	0	0	0	-0.1
	1	-x, -y, -z	26.15	B3LYP/6-31G(d,p)	0	0	0	0	-0.1
	2	-x+1/2, y+1/2, -z+1/2	17.8	B3LYP/6-31G(d,p)	0.1	0	-0.1	0	0
	2	-x+1/2, y+1/2, -z+1/2	21.12	B3LYP/6-31G(d,p)	0	0	0	0	0
	2	x+1/2, -y+1/2, z+1/2	25.1	B3LYP/6-31G(d,p)	-0.1	0	0	0	-0.1
	1	-x, -y, -z	25.14	B3LYP/6-31G(d,p)	0	0	0	0	0
	2	x, y, z	27.28	B3LYP/6-31G(d,p)	0	0	0	0	0
	2	x+1/2, -y+1/2, z+1/2	20.7	B3LYP/6-31G(d,p)	-0.1	0	0	0	-0.1
	1	-x, -y, -z	24.77	B3LYP/6-31G(d,p)	0	0	0	0	0
	2	x+1/2, -y+1/2, z+1/2	23.64	B3LYP/6-31G(d,p)	-0.1	0	0	0	-0.1
	1	-x, -y, -z	26.37	B3LYP/6-31G(d,p)	0	0	0	0	0
	2	x, y, z	29.56	B3LYP/6-31G(d,p)	0.1	0	0	0	0.1

	N	Symp	R	Electron Density	E_ele	E_pol	E_dis	E_rep	E_tot
	1	-x, -y, -z	19.46	B3LYP/6-31G(d,p)	-0.2	0	-0.1	0	-0.3
	2	x+1/2, -y+1/2, z+1/2	22.23	B3LYP/6-31G(d,p)	0.1	0	0	0	0
	1	-x, -y, -z	26.76	B3LYP/6-31G(d,p)	-0.1	0	0	0	-0.1
	2	x, y, z	23.25	B3LYP/6-31G(d,p)	0.1	0	0	0	0.1
	2	x+1/2, -y+1/2, z+1/2	29.97	B3LYP/6-31G(d,p)	0	0	0	0	0
	1	-x, -y, -z	30.38	B3LYP/6-31G(d,p)	0	0	0	0	0
	2	-x+1/2, y+1/2, -z+1/2	30.38	B3LYP/6-31G(d,p)	0	0	0	0	0
	2	-x+1/2, y+1/2, -z+1/2	22.86	B3LYP/6-31G(d,p)	0	0	0	0	0
	2	x, y, z	28.65	B3LYP/6-31G(d,p)	0	0	0	0	0
	2	-x+1/2, y+1/2, -z+1/2	29.39	B3LYP/6-31G(d,p)	-0.1	0	0	0	-0.1
	2	x+1/2, -y+1/2, z+1/2	24.26	B3LYP/6-31G(d,p)	0.1	0	0	0	0.1
	2	-x+1/2, y+1/2, -z+1/2	21.52	B3LYP/6-31G(d,p)	-0.1	0	0	0	-0.2
	1	-x, -y, -z	19.55	B3LYP/6-31G(d,p)	0	0	-0.1	0	-0.1
	1	-x, -y, -z	24.21	B3LYP/6-31G(d,p)	-0.1	0	0	0	-0.1
	2	-x+1/2, y+1/2, -z+1/2	28.38	B3LYP/6-31G(d,p)	0	0	0	0	0
	2	x+1/2, -y+1/2, z+1/2	29.74	B3LYP/6-31G(d,p)	0	0	0	0	0
	2	x, y, z	18.44	B3LYP/6-31G(d,p)	0	0	-0.1	0	-0.1
	2	x, y, z	22.06	B3LYP/6-31G(d,p)	0.1	0	0	0	0
	2	-x+1/2, y+1/2, -z+1/2	15.99	B3LYP/6-31G(d,p)	0.1	0	-0.3	0	-0.1
	2	x, y, z	16.93	B3LYP/6-31G(d,p)	0.1	0	-0.2	0	-0.1
	1	-x, -y, -z	21.27	B3LYP/6-31G(d,p)	0	0	0	0	-0.1
	2	x+1/2, -y+1/2, z+1/2	17.84	B3LYP/6-31G(d,p)	0.2	0	-0.1	0	0.1
	1	-x, -y, -z	25.61	B3LYP/6-31G(d,p)	0	0	0	0	0
	2	-x+1/2, y+1/2, -z+1/2	24.08	B3LYP/6-31G(d,p)	0	0	0	0	0
	2	-x+1/2, y+1/2, -z+1/2	14.01	B3LYP/6-31G(d,p)	-0.6	-0.1	-0.8	0	-1.3
	2	-x+1/2, y+1/2, -z+1/2	24.93	B3LYP/6-31G(d,p)	0	0	0	0	0
	1	-x, -y, -z	17.66	B3LYP/6-31G(d,p)	0	0	-0.1	0	0
	2	x+1/2, -y+1/2, z+1/2	21.84	B3LYP/6-31G(d,p)	0	0	0	0	0
	2	-x+1/2, y+1/2, -z+1/2	25.92	B3LYP/6-31G(d,p)	0	0	0	0	0
	2	x+1/2, -y+1/2, z+1/2	24.78	B3LYP/6-31G(d,p)	0	0	0	0	0
	2	x, y, z	16.53	B3LYP/6-31G(d,p)	-0.2	0	-0.1	0	-0.3
	1	-x, -y, -z	10.24	B3LYP/6-31G(d,p)	-0.3	0	-2.1	0	-2.2
	2	-x+1/2, y+1/2, -z+1/2	11.05	B3LYP/6-31G(d,p)	-1	-0.1	-1.5	0	-2.4
	2	x, y, z	14.83	B3LYP/6-31G(d,p)	0.2	0	-0.2	0	0
	2	x+1/2, -y+1/2, z+1/2	26.74	B3LYP/6-31G(d,p)	0	0	0	0	0
	1	-x, -y, -z	19.55	B3LYP/6-31G(d,p)	-0.1	0	0	0	-0.1
	2	x+1/2, -y+1/2, z+1/2	13.46	B3LYP/6-31G(d,p)	0.4	0	-0.5	0	0
	2	x, y, z	26.79	B3LYP/6-31G(d,p)	0	0	0	0	0
	2	-x+1/2, y+1/2, -z+1/2	22.09	B3LYP/6-31G(d,p)	0	0	0	0	0
	2	x, y, z	30.3	B3LYP/6-31G(d,p)	0	0	0	0	0
	1	-x, -y, -z	19.37	B3LYP/6-31G(d,p)	0.1	0	0	0	0.1
	2	x+1/2, -y+1/2, z+1/2	21.76	B3LYP/6-31G(d,p)	0	0	0	0	0
	2	x, y, z	28.49	B3LYP/6-31G(d,p)	0	0	0	0	0
	2	x, y, z	18.44	B3LYP/6-31G(d,p)	-0.2	0	-0.1	0	-0.2
	1	-x, -y, -z	12.97	B3LYP/6-31G(d,p)	0	0	-0.3	0	-0.3
	2	x, y, z	16.93	B3LYP/6-31G(d,p)	-0.1	0	-0.1	0	-0.1
	2	x+1/2, -y+1/2, z+1/2	26.68	B3LYP/6-31G(d,p)	0	0	0	0	0
	1	-x, -y, -z	21.11	B3LYP/6-31G(d,p)	-0.1	0	0	0	-0.1
	2	x+1/2, -y+1/2, z+1/2	13.33	B3LYP/6-31G(d,p)	-0.2	0	-0.5	0	-0.6
	2	x, y, z	25.51	B3LYP/6-31G(d,p)	0.1	0	0	0	0
	2	x+1/2, -y+1/2, z+1/2	27.57	B3LYP/6-31G(d,p)	0	0	0	0	0
	1	-x, -y, -z	23.92	B3LYP/6-31G(d,p)	0.1	0	0	0	0.1
	1	-x, -y, -z	19.1	B3LYP/6-31G(d,p)	0.1	0	0	0	0.1
	2	x+1/2, -y+1/2, z+1/2	14.61	B3LYP/6-31G(d,p)	0.1	0	-0.6	0	-0.5
	2	x, y, z	23.25	B3LYP/6-31G(d,p)	-0.1	0	0	0	-0.1
	2	x, y, z	22.06	B3LYP/6-31G(d,p)	-0.1	0	0	0	-0.2
	2	x+1/2, -y+1/2, z+1/2	17.54	B3LYP/6-31G(d,p)	-0.2	0	-0.1	0	-0.3
	2	x+1/2, -y+1/2, z+1/2	24.57	B3LYP/6-31G(d,p)	0	0	0	0	0
	2	x+1/2, -y+1/2, z+1/2	28.67	B3LYP/6-31G(d,p)	0	0	0	0	0
	1	-x, -y, -z	26.37	B3LYP/6-31G(d,p)	0.1	0	0	0	0.1
	2	x+1/2, -y+1/2, z+1/2	21.84	B3LYP/6-31G(d,p)	0.2	0	0	0	0.1
	2	x+1/2, -y+1/2, z+1/2	23.9	B3LYP/6-31G(d,p)	0	0	0	0	0
	2	x+1/2, -y+1/2, z+1/2	29.56	B3LYP/6-31G(d,p)	0.1	0	0	0	0.1
	1	-x, -y, -z	17.6	B3LYP/6-31G(d,p)	-0.1	0	-0.1	0	-0.1
	2	x, y, z	24.51	B3LYP/6-31G(d,p)	-0.1	0	0	0	-0.1
	1	-x, -y, -z	25.43	B3LYP/6-31G(d,p)	0	0	0	0	0
	2	x, y, z	22.57	B3LYP/6-31G(d,p)	0	0	0	0	0

	N	Symp	R	Electron Density	E_ele	E_pol	E_dis	E_rep	E_tot
	2	x, y, z	16.34	B3LYP/6-31G(d,p)	-0.6	-0.1	-0.3	0	-0.9
	1	-x, -y, -z	19.96	B3LYP/6-31G(d,p)	0.1	0	-0.1	0	0
	2	-x+1/2, y+1/2, -z+1/2	30.33	B3LYP/6-31G(d,p)	-0.1	0	0	0	-0.1
	1	-x, -y, -z	27.12	B3LYP/6-31G(d,p)	0	0	0	0	0
	2	x, y, z	22.57	B3LYP/6-31G(d,p)	0	0	0	0	-0.1
	2	-x+1/2, y+1/2, -z+1/2	22.8	B3LYP/6-31G(d,p)	-0.2	0	0	0	-0.2
	2	x, y, z	29.03	B3LYP/6-31G(d,p)	0	0	0	0	0
	1	-x, -y, -z	22.4	B3LYP/6-31G(d,p)	-0.1	0	0	0	-0.1
	2	x, y, z	17.58	B3LYP/6-31G(d,p)	0.1	0	-0.1	0	0.1
	2	-x+1/2, y+1/2, -z+1/2	27.71	B3LYP/6-31G(d,p)	-0.1	0	0	0	-0.1
	1	-x, -y, -z	10.29	B3LYP/6-31G(d,p)	0.8	-0.2	-1.2	0	-0.4
	2	-x+1/2, y+1/2, -z+1/2	22.38	B3LYP/6-31G(d,p)	-0.1	0	0	0	-0.1
	2	-x+1/2, y+1/2, -z+1/2	15.9	B3LYP/6-31G(d,p)	-0.4	0	-0.4	0	-0.8
	2	x, y, z	17.58	B3LYP/6-31G(d,p)	0	0	-0.1	0	-0.1
	2	-x+1/2, y+1/2, -z+1/2	27.5	B3LYP/6-31G(d,p)	0	0	0	0	0
	1	-x, -y, -z	31.17	B3LYP/6-31G(d,p)	0	0	0	0	0
	2	-x+1/2, y+1/2, -z+1/2	22.12	B3LYP/6-31G(d,p)	0	0	0	0	0
	1	-x, -y, -z	20.78	B3LYP/6-31G(d,p)	-0.1	0	0	0	-0.2
	2	x, y, z	15.57	B3LYP/6-31G(d,p)	0.2	0	-0.2	0	0
	1	-x, -y, -z	26.56	B3LYP/6-31G(d,p)	-0.1	0	0	0	-0.1
	2	-x+1/2, y+1/2, -z+1/2	19.16	B3LYP/6-31G(d,p)	0.1	0	0	0	0.1
	1	-x, -y, -z	11.15	B3LYP/6-31G(d,p)	0	-0.1	-2	0	-1.7
	1	-x, -y, -z	27.71	B3LYP/6-31G(d,p)	0	0	0	0	0
	2	-x+1/2, y+1/2, -z+1/2	18.86	B3LYP/6-31G(d,p)	0.1	0	-0.1	0	0.1
	1	-x, -y, -z	22.25	B3LYP/6-31G(d,p)	-0.1	0	0	0	-0.1
	2	-x+1/2, y+1/2, -z+1/2	25.81	B3LYP/6-31G(d,p)	0	0	0	0	0
	1	-x, -y, -z	13.7	B3LYP/6-31G(d,p)	-0.4	0	-0.3	0	-0.7
	1	-x, -y, -z	26.41	B3LYP/6-31G(d,p)	0	0	0	0	0
	1	-x, -y, -z	26.3	B3LYP/6-31G(d,p)	-0.1	0	0	0	-0.1
	1	-x, -y, -z	17.2	B3LYP/6-31G(d,p)	1.5	-0.1	-0.5	0	1.1
	1	-x, -y, -z	19.61	B3LYP/6-31G(d,p)	-0.2	0	0	0	-0.2
	1	-x, -y, -z	25.02	B3LYP/6-31G(d,p)	0.2	0	0	0	0.2
	1	-x, -y, -z	26.73	B3LYP/6-31G(d,p)	0	0	0	0	0
	2	x+1/2, -y+1/2, z+1/2	31.12	B3LYP/6-31G(d,p)	0	0	0	0	0
	1	-x, -y, -z	21.83	B3LYP/6-31G(d,p)	0.2	0	0	0	0.2
	1	-x, -y, -z	24.08	B3LYP/6-31G(d,p)	0.1	0	0	0	0.1
	1	-x, -y, -z	19.4	B3LYP/6-31G(d,p)	0.2	0	0	0	0.2
	1	-x, -y, -z	20.16	B3LYP/6-31G(d,p)	0.1	0	0	0	0.1
	2	-x+1/2, y+1/2, -z+1/2	27.36	B3LYP/6-31G(d,p)	0	0	0	0	0
	1	-x, -y, -z	17.5	B3LYP/6-31G(d,p)	0.1	0	-0.1	0	0.1
	2	-x+1/2, y+1/2, -z+1/2	24.8	B3LYP/6-31G(d,p)	0.1	0	0	0	0.1
	2	-x+1/2, y+1/2, -z+1/2	28.22	B3LYP/6-31G(d,p)	0	0	0	0	0
	1	-x, -y, -z	27.58	B3LYP/6-31G(d,p)	0	0	0	0	0
	1	-x, -y, -z	21.67	B3LYP/6-31G(d,p)	-0.1	0	0	0	-0.2
	1	-x, -y, -z	19.22	B3LYP/6-31G(d,p)	-0.1	0	-0.1	0	-0.2
	1	-x, -y, -z	26.28	B3LYP/6-31G(d,p)	0	0	0	0	0
	2	-x+1/2, y+1/2, -z+1/2	25.75	B3LYP/6-31G(d,p)	0.1	0	0	0	0.1
	1	-x, -y, -z	25.81	B3LYP/6-31G(d,p)	-0.1	0	0	0	-0.2
	1	-x, -y, -z	23.79	B3LYP/6-31G(d,p)	-0.2	0	0	0	-0.2
	1	-x, -y, -z	31.57	B3LYP/6-31G(d,p)	-0.1	0	0	0	-0.1
	1	-x, -y, -z	29.94	B3LYP/6-31G(d,p)	-0.1	0	0	0	-0.1

2. Mogul Geometry Check Results

Type	Fragment	Classification	No. of hits	Query value	Mean	Std. dev.	z-score	x - mean	Minimum	Maximum	Median
torsion	C16 O1 C1 C2	Not unusual (enough hits)	326	-12.116							
torsion	C16 O1 C1 C6	Not unusual (enough hits)	326	167.221							
torsion	C1 O1 C16 O2	Not unusual (enough hits)	514	73.105							
torsion	C17 O2 C16 O1	Not unusual (enough hits)	844	72.034							
torsion	C21 O5 C13 C14	Not unusual (enough hits)	7561	2.922							
torsion	C21 O5 C13 C12	Not unusual (enough hits)	8397	-179.496							
torsion	C13 C12 C18 C19	Not unusual (enough hits)	111	86.434							
torsion	C11 C12 C18 C19	Not unusual (enough hits)	176	-96.557							
torsion	C15 C10 C8 C9	Not unusual (enough hits)	640	48.973							
torsion	C15 C10 C8 C7	Not unusual (enough hits)	380	-133.630							
torsion	C11 C10 C8 C9	Not unusual (enough hits)	640	-128.460							
torsion	C11 C10 C8 C7	Not unusual (enough hits)	380	48.937							
torsion	C20 C19 C18 C12	Not unusual (enough hits)	291	8.886							
bond	O1 C1	Not unusual (enough hits)	5844	1.360	1.372	0.020	0.600	0.012	1.028	1.613	1.371
bond	O1 C16	Not unusual (enough hits)	519	1.437	1.421	0.020	0.791	0.016	1.299	1.606	1.421
bond	C2 C1	Not unusual (enough hits)	5895	1.386	1.385	0.016	0.074	0.001	0.998	1.603	1.386
bond	C6 C1	Not unusual (enough hits)	7563	1.407	1.383	0.017	1.412	0.024	0.921	1.552	1.385
bond	O2 C17	Not unusual (enough hits)	4828	1.427	1.415	0.042	0.275	0.012	1.067	1.770	1.418
bond	O2 C16	Not unusual (enough hits)	845	1.385	1.387	0.035	0.047	0.002	0.848	1.671	1.391
bond	C2 C3	Not unusual (enough hits)	8559	1.396	1.383	0.016	0.865	0.013	1.148	1.585	1.384
bond	O3 C3	Not unusual (enough hits)	482	1.369	1.375	0.011	0.569	0.006	1.313	1.474	1.374
bond	C4 C3	Not unusual (enough hits)	5308	1.388	1.396	0.015	0.582	0.009	1.241	1.613	1.396
bond	O3 C7	Not unusual (enough hits)	511	1.354	1.351	0.014	0.219	0.003	1.313	1.496	1.351
bond	C5 C4	Not unusual (enough hits)	8111	1.407	1.394	0.013	0.950	0.012	1.287	1.541	1.395
bond	C6 C5	Not unusual (enough hits)	12044	1.378	1.383	0.014	0.365	0.005	1.259	1.538	1.383
bond	O5 C13	Not unusual (enough hits)	7636	1.373	1.368	0.013	0.353	0.005	1.002	1.513	1.367
bond	O5 C21	Not unusual (enough hits)	8424	1.428	1.424	0.024	0.183	0.004	0.925	1.683	1.426
bond	C4 C9	Not unusual (enough hits)	4438	1.468	1.476	0.018	0.441	0.008	1.359	1.775	1.477
bond	O4 C9	Not unusual (enough hits)	9195	1.232	1.228	0.020	0.178	0.004	1.060	1.712	1.224
bond	C14 C15	Not unusual (enough hits)	12044	1.395	1.383	0.014	0.883	0.012	1.259	1.538	1.383
bond	C15 C10	Not unusual (enough hits)	11213	1.388	1.391	0.014	0.204	0.003	0.898	1.626	1.391
bond	C14 C13	Not unusual (enough hits)	5398	1.390	1.386	0.017	0.275	0.005	1.108	1.608	1.385

Type	Fragment	Classification	No. of hits	Query value	Mean	Std. dev.	z-score	x - mean	Minimum	Maximum	Median
bond	C13 C12	Not unusual (enough hits)	7316	1.401	1.393	0.015	0.569	0.008	1.241	1.640	1.394
bond	C11 C12	Not unusual (enough hits)	6370	1.388	1.390	0.015	0.157	0.002	1.213	1.535	1.391
bond	C18 C12	Not unusual (enough hits)	182	1.508	1.516	0.014	0.551	0.007	1.484	1.620	1.514
bond	C11 C10	Not unusual (enough hits)	4841	1.400	1.392	0.013	0.594	0.008	1.285	1.505	1.391
bond	C10 C8	Not unusual (enough hits)	3265	1.485	1.482	0.014	0.249	0.004	1.357	1.571	1.483
bond	C8 C9	Not unusual (enough hits)	223	1.465	1.463	0.013	0.191	0.003	1.414	1.513	1.461
bond	C7 C8	Not unusual (enough hits)	217	1.352	1.343	0.010	0.851	0.009	1.299	1.382	1.343
bond	C18 C19	Not unusual (enough hits)	291	1.493	1.476	0.048	0.350	0.017	1.297	1.622	1.489
bond	C20 C19	Not unusual (enough hits)	4843	1.302	1.286	0.062	0.266	0.017	0.849	1.849	1.301
angle	C16 O1 C1	Not unusual (enough hits)	163	117.713	118.495	1.852	0.422	0.782	111.549	125.181	118.462
angle	O1 C1 C2	Not unusual (enough hits)	5068	123.896	119.573	4.859	0.890	4.323	96.322	146.635	118.662
angle	O1 C1 C6	Not unusual (enough hits)	6288	115.337	120.070	4.806	0.985	4.733	99.723	140.989	119.937
angle	C6 C1 C2	Not unusual (enough hits)	6454	120.764	120.607	1.271	0.124	0.157	106.816	141.830	120.425
angle	C17 O2 C16	Not unusual (enough hits)	845	113.954	112.867	2.314	0.470	1.088	88.836	134.884	112.919
angle	C3 C2 C1	Not unusual (enough hits)	3971	118.030	118.966	1.446	0.647	0.936	103.617	133.270	119.069
angle	O3 C3 C2	Not unusual (enough hits)	206	115.511	115.804	1.181	0.248	0.292	108.589	119.547	115.942
angle	C2 C3 C4	Not unusual (enough hits)	1848	122.766	121.744	1.548	0.660	1.021	112.017	129.309	121.845
angle	O3 C3 C4	Not unusual (enough hits)	344	121.707	121.590	0.544	0.215	0.117	119.153	123.423	121.638
angle	C3 O3 C7	Not unusual (enough hits)	453	118.305	118.239	1.050	0.062	0.065	102.729	120.642	118.334
angle	C6 C5 C4	Not unusual (enough hits)	6889	120.971	120.803	1.613	0.104	0.167	103.521	132.161	121.140
angle	C21 O5 C13	Not unusual (enough hits)	7566	117.559	117.508	1.189	0.043	0.051	102.613	135.555	117.460
angle	C5 C4 C3	Not unusual (enough hits)	4906	117.760	117.913	1.172	0.131	0.154	106.398	129.706	118.027
angle	C3 C4 C9	Not unusual (enough hits)	851	120.685	120.193	0.823	0.599	0.493	116.359	123.290	120.159
angle	C5 C4 C9	Not unusual (enough hits)	3496	121.549	120.044	1.424	1.057	1.506	103.343	126.543	119.915
angle	O2 C16 O1	Not unusual (enough hits)	307	113.048	112.138	2.222	0.410	0.910	96.120	120.290	112.602
angle	C14 C15 C10	Not unusual (enough hits)	8494	120.941	120.858	1.000	0.084	0.084	89.761	133.847	120.840
angle	C15 C14 C13	Not unusual (enough hits)	5710	119.590	119.442	1.702	0.087	0.147	100.709	133.580	119.875
angle	O5 C13 C14	Not unusual (enough hits)	5490	123.979	124.291	1.532	0.203	0.312	102.228	133.747	124.477
angle	O5 C13 C12	Not unusual (enough hits)	3277	115.078	115.933	1.188	0.720	0.855	99.693	126.856	115.908
angle	C14 C13 C12	Not unusual (enough hits)	1708	120.898	121.034	1.334	0.102	0.136	109.206	138.718	120.925
angle	C11 C12 C13	Not unusual (enough hits)	6362	117.916	118.153	0.894	0.265	0.237	109.963	129.343	118.194
angle	C18 C12 C13	Not unusual (enough hits)	21	121.149	120.475	1.534	0.439	0.673	117.269	123.505	120.438
angle	C18 C12 C11	Not unusual (enough hits)	91	120.870	121.063	1.883	0.102	0.193	114.471	124.449	121.293
angle	C10 C11 C12	Not unusual (enough hits)	1228	122.397	121.503	1.376	0.650	0.895	113.619	154.930	121.510

Type	Fragment	Classification	No. of hits	Query value	Mean	Std. dev.	z-score	x - mean	Minimum	Maximum	Median
angle	C15 C10 C11	Not unusual (enough hits)	5467	118.158	119.263	1.172	0.943	1.105	99.773	129.034	119.329
angle	C15 C10 C8	Not unusual (enough hits)	6168	122.039	120.972	1.374	0.777	1.068	108.331	133.239	120.935
angle	C11 C10 C8	Not unusual (enough hits)	324	119.755	120.556	1.304	0.614	0.801	114.431	124.283	120.580
angle	O4 C9 C4	Not unusual (enough hits)	4438	122.239	121.613	1.497	0.418	0.626	102.913	129.947	121.704
angle	C4 C9 C8	Not unusual (enough hits)	112	114.564	115.386	1.218	0.675	0.822	112.905	120.358	115.053
angle	O4 C9 C8	Not unusual (enough hits)	223	123.190	122.463	0.996	0.730	0.727	119.451	124.903	122.622
angle	C10 C8 C9	Not unusual (enough hits)	192	120.750	121.581	1.106	0.751	0.831	117.447	125.199	121.693
angle	C10 C8 C7	Not unusual (enough hits)	190	119.954	119.766	1.063	0.176	0.188	115.774	123.295	119.731
angle	C7 C8 C9	Not unusual (enough hits)	200	119.246	118.621	0.908	0.689	0.625	116.170	124.393	118.605
angle	O3 C7 C8	Not unusual (enough hits)	202	125.441	125.748	0.881	0.349	0.307	120.737	127.504	125.828
angle	C5 C6 C1	Not unusual (enough hits)	7557	119.695	119.761	1.028	0.064	0.065	89.677	128.045	119.787
angle	C18 C19 C20	Not unusual (enough hits)	291	127.504	127.683	8.292	0.022	0.179	88.843	169.593	126.320
angle	C12 C18 C19	Not unusual (enough hits)	87	116.329	114.447	2.442	0.771	1.882	106.892	120.482	114.601

Table S 3: compound 3

Type	Fragment	Classification	No. of hits	Query value	Mean	Std. dev.	z-score	x - mean	Minimum	Maximum	Median
torsion	C16 O4 C13 C12	Not unusual (enough hits)	7561	3.817							
torsion	C16 O4 C13 C14	Not unusual (enough hits)	8397	-176.036							
torsion	C11 C10 C8 C7	Not unusual (enough hits)	380	65.483							
torsion	C13 C14 C17 C18	Not unusual (enough hits)	111	152.785							
torsion	C15 C14 C17 C18	Not unusual (enough hits)	176	-28.135							
torsion	C19 C18 C17 C14	Not unusual (enough hits)	291	118.046							
torsion	C15 C10 C8 C7	Unusual (enough hits)	380	-111.682							
torsion	C11 C10 C8 C9	Unusual (enough hits)	640	-114.693							
torsion	C15 C10 C8 C9	Unusual (enough hits)	640	68.143							
bond	O1 C2	Not unusual (enough hits)	7525	1.354	1.366	0.018	0.675	0.012	1.119	1.720	1.366
bond	O2 C4	Not unusual (enough hits)	482	1.368	1.375	0.011	0.634	0.007	1.313	1.474	1.374
bond	O2 C7	Not unusual (enough hits)	511	1.346	1.351	0.014	0.362	0.005	1.313	1.496	1.351
bond	O3 C9	Not unusual (enough hits)	9195	1.239	1.228	0.020	0.569	0.011	1.060	1.712	1.224
bond	O4 C13	Not unusual (enough hits)	7636	1.367	1.368	0.013	0.068	0.001	1.002	1.513	1.367
bond	O4 C16	Not unusual (enough hits)	8424	1.421	1.424	0.024	0.108	0.003	0.925	1.683	1.426
bond	C1 C2	Not unusual (enough hits)	7716	1.411	1.386	0.016	1.526	0.025	1.204	1.700	1.386
bond	C6 C1	Not unusual (enough hits)	12044	1.368	1.383	0.014	1.074	0.015	1.259	1.538	1.383
bond	C3 C2	Not unusual (enough hits)	7179	1.380	1.386	0.013	0.457	0.006	1.248	1.556	1.387

Type	Fragment	Classification	No. of hits	Query value	Mean	Std. dev.	z-score	x - mean	Minimum	Maximum	Median
bond	C3 C4	Not unusual (enough hits)	8559	1.385	1.383	0.016	0.174	0.003	1.148	1.585	1.384
bond	C5 C4	Not unusual (enough hits)	5308	1.398	1.396	0.015	0.149	0.002	1.241	1.613	1.396
bond	C6 C5	Not unusual (enough hits)	8111	1.404	1.394	0.013	0.757	0.010	1.287	1.541	1.395
bond	C5 C9	Not unusual (enough hits)	4438	1.451	1.476	0.018	1.426	0.025	1.359	1.775	1.477
bond	C7 C8	Not unusual (enough hits)	217	1.344	1.343	0.010	0.070	0.001	1.299	1.382	1.343
bond	C8 C9	Not unusual (enough hits)	223	1.456	1.463	0.013	0.494	0.007	1.414	1.513	1.461
bond	C10 C8	Not unusual (enough hits)	3265	1.481	1.482	0.014	0.039	0.001	1.357	1.571	1.483
bond	C11 C10	Not unusual (enough hits)	11213	1.391	1.391	0.014	0.012	0.000	0.898	1.626	1.391
bond	C15 C10	Not unusual (enough hits)	4841	1.398	1.392	0.013	0.490	0.007	1.285	1.505	1.391
bond	C12 C11	Not unusual (enough hits)	12044	1.387	1.383	0.014	0.324	0.004	1.259	1.538	1.383
bond	C12 C13	Not unusual (enough hits)	5398	1.392	1.386	0.017	0.396	0.007	1.108	1.608	1.385
bond	C13 C14	Not unusual (enough hits)	7316	1.403	1.393	0.015	0.689	0.010	1.241	1.640	1.394
bond	C15 C14	Not unusual (enough hits)	6370	1.382	1.390	0.015	0.563	0.008	1.213	1.535	1.391
bond	C17 C14	Not unusual (enough hits)	182	1.514	1.516	0.014	0.093	0.001	1.484	1.620	1.514
bond	C17 C18	Not unusual (enough hits)	291	1.493	1.476	0.048	0.362	0.018	1.297	1.622	1.489
bond	C19 C18	Not unusual (enough hits)	4843	1.307	1.286	0.062	0.349	0.022	0.849	1.849	1.301
angle	C4 O2 C7	Not unusual (enough hits)	453	118.194	118.239	1.050	0.043	0.046	102.729	120.642	118.334
angle	C16 O4 C13	Not unusual (enough hits)	7566	117.377	117.508	1.189	0.110	0.131	102.613	135.555	117.460
angle	C6 C1 C2	Not unusual (enough hits)	7794	119.942	119.896	0.965	0.047	0.046	102.986	129.406	119.936
angle	O1 C2 C1	Not unusual (enough hits)	7710	117.196	119.991	2.675	1.045	2.795	96.605	147.073	119.451
angle	O1 C2 C3	Not unusual (enough hits)	7201	122.216	119.808	2.541	0.948	2.408	87.775	133.131	120.218
angle	C1 C2 C3	Not unusual (enough hits)	2847	120.588	120.202	0.957	0.403	0.386	113.839	132.500	120.112
angle	C4 C3 C2	Not unusual (enough hits)	760	118.084	118.455	1.250	0.297	0.371	108.760	123.835	118.561
angle	O2 C4 C3	Not unusual (enough hits)	206	115.588	115.804	1.181	0.183	0.216	108.589	119.547	115.942
angle	O2 C4 C5	Not unusual (enough hits)	344	121.312	121.590	0.544	0.511	0.278	119.153	123.423	121.638
angle	C3 C4 C5	Not unusual (enough hits)	1848	123.100	121.744	1.548	0.876	1.356	112.017	129.309	121.845
angle	C6 C5 C4	Not unusual (enough hits)	4906	117.094	117.913	1.172	0.699	0.820	106.398	129.706	118.027
angle	C4 C5 C9	Not unusual (enough hits)	851	120.462	120.193	0.823	0.328	0.270	116.359	123.290	120.159
angle	C6 C5 C9	Not unusual (enough hits)	3496	122.444	120.044	1.424	1.685	2.400	103.343	126.543	119.915
angle	C1 C6 C5	Not unusual (enough hits)	6889	121.178	120.803	1.613	0.232	0.375	103.521	132.161	121.140
angle	O2 C7 C8	Not unusual (enough hits)	202	125.696	125.748	0.881	0.060	0.053	120.737	127.504	125.828
angle	C7 C8 C9	Not unusual (enough hits)	200	119.250	118.621	0.908	0.693	0.629	116.170	124.393	118.605
angle	C10 C8 C7	Not unusual (enough hits)	190	119.015	119.766	1.063	0.706	0.751	115.774	123.295	119.731
angle	C10 C8 C9	Not unusual (enough hits)	192	121.734	121.581	1.106	0.139	0.154	117.447	125.199	121.693

Type	Fragment	Classification	No. of hits	Query value	Mean	Std. dev.	z-score	x - mean	Minimum	Maximum	Median
angle	O3 C9 C5	Not unusual (enough hits)	4438	122.873	121.613	1.497	0.842	1.260	102.913	129.947	121.704
angle	O3 C9 C8	Not unusual (enough hits)	223	122.081	122.463	0.996	0.384	0.383	119.451	124.903	122.622
angle	C5 C9 C8	Not unusual (enough hits)	112	115.045	115.386	1.218	0.280	0.341	112.905	120.358	115.053
angle	C11 C10 C8	Not unusual (enough hits)	6168	120.864	120.972	1.374	0.078	0.107	108.331	133.239	120.935
angle	C15 C10 C8	Not unusual (enough hits)	324	120.528	120.556	1.304	0.022	0.029	114.431	124.283	120.580
angle	C11 C10 C15	Not unusual (enough hits)	5467	118.549	119.263	1.172	0.609	0.714	99.773	129.034	119.329
angle	C12 C11 C10	Not unusual (enough hits)	8494	120.830	120.858	1.000	0.028	0.028	89.761	133.847	120.840
angle	C11 C12 C13	Not unusual (enough hits)	5710	119.634	119.442	1.702	0.113	0.192	100.709	133.580	119.875
angle	O4 C13 C12	Not unusual (enough hits)	5490	123.906	124.291	1.532	0.251	0.385	102.228	133.747	124.477
angle	O4 C13 C14	Not unusual (enough hits)	3277	115.412	115.933	1.188	0.439	0.521	99.693	126.856	115.908
angle	C12 C13 C14	Not unusual (enough hits)	1708	120.681	121.034	1.334	0.264	0.353	109.206	138.718	120.925
angle	C15 C14 C13	Not unusual (enough hits)	6362	118.371	118.153	0.894	0.244	0.218	109.963	129.343	118.194
angle	C17 C14 C13	Not unusual (enough hits)	21	120.303	120.475	1.534	0.113	0.173	117.269	123.505	120.438
angle	C17 C14 C15	Not unusual (enough hits)	91	121.320	121.063	1.883	0.137	0.257	114.471	124.449	121.293
angle	C10 C15 C14	Not unusual (enough hits)	1228	121.927	121.503	1.376	0.308	0.424	113.619	154.930	121.510
angle	C14 C17 C18	Not unusual (enough hits)	87	113.599	114.447	2.442	0.347	0.848	106.892	120.482	114.601
angle	C17 C18 C19	Not unusual (enough hits)	291	125.830	127.683	8.292	0.223	1.852	88.843	169.593	126.320

Table S 4: GK-15

Type	Fragment	Classification	No. of hits	Query value	Mean	Std. dev.	z-score	x - mean	Minimum	Maximum	Median
torsion	C11 C10 C8 C7	Not unusual (enough hits)	380	54.256							
torsion	C15 C10 C8 C7	Not unusual (enough hits)	380	-122.736							
torsion	C11 C10 C8 C9	Not unusual (enough hits)	640	-123.539							
torsion	C15 C10 C8 C9	Not unusual (enough hits)	640	59.469							
torsion	C21 O4 C13 C12	Not unusual (enough hits)	7561	0.914							
torsion	C21 O4 C13 C14	Not unusual (enough hits)	8397	-179.118							
torsion	C13 C14 C16 C17	Not unusual (enough hits)	111	-171.541							
torsion	C15 C14 C16 C17	Not unusual (enough hits)	176	9.954							
torsion	C18 C17 C16 C14	Not unusual (enough hits)	325	-118.609							
torsion	C16 C17 C18 C19	Not unusual (enough hits)	2440	-174.891							
torsion	C16 C17 C18 C20	Not unusual (enough hits)	2440	2.612							
bond	C1 C2	Not unusual (enough hits)	7716	1.405	1.386	0.016	1.210	0.020	1.204	1.700	1.386
bond	C6 C1	Not unusual (enough hits)	12044	1.362	1.383	0.014	1.502	0.021	1.259	1.538	1.383
bond	C3 C2	Not unusual (enough hits)	7179	1.378	1.386	0.013	0.610	0.008	1.248	1.556	1.387

Type	Fragment	Classification	No. of hits	Query value	Mean	Std. dev.	z-score	x - mean	Minimum	Maximum	Median
bond	O1 C2	Not unusual (enough hits)	7525	1.350	1.366	0.018	0.865	0.016	1.119	1.720	1.366
bond	C3 C4	Not unusual (enough hits)	8559	1.383	1.383	0.016	0.010	0.000	1.148	1.585	1.384
bond	C5 C4	Not unusual (enough hits)	5308	1.393	1.396	0.015	0.222	0.003	1.241	1.613	1.396
bond	O2 C4	Not unusual (enough hits)	482	1.369	1.375	0.011	0.589	0.006	1.313	1.474	1.374
bond	C6 C5	Not unusual (enough hits)	8111	1.404	1.394	0.013	0.730	0.009	1.287	1.541	1.395
bond	C5 C9	Not unusual (enough hits)	4438	1.453	1.476	0.018	1.310	0.023	1.359	1.775	1.477
bond	C7 C8	Not unusual (enough hits)	217	1.343	1.343	0.010	0.022	0.000	1.299	1.382	1.343
bond	O2 C7	Not unusual (enough hits)	511	1.347	1.351	0.014	0.321	0.004	1.313	1.496	1.351
bond	C8 C9	Not unusual (enough hits)	223	1.457	1.463	0.013	0.454	0.006	1.414	1.513	1.461
bond	C10 C8	Not unusual (enough hits)	3265	1.482	1.482	0.014	0.053	0.001	1.357	1.571	1.483
bond	O3 C9	Not unusual (enough hits)	9195	1.237	1.228	0.020	0.454	0.009	1.060	1.712	1.224
bond	C11 C10	Not unusual (enough hits)	11213	1.380	1.391	0.014	0.786	0.011	0.898	1.626	1.391
bond	C15 C10	Not unusual (enough hits)	4841	1.398	1.392	0.013	0.432	0.006	1.285	1.505	1.391
bond	C12 C11	Not unusual (enough hits)	12044	1.387	1.383	0.014	0.265	0.004	1.259	1.538	1.383
bond	C12 C13	Not unusual (enough hits)	5398	1.378	1.386	0.017	0.469	0.008	1.108	1.608	1.385
bond	C13 C14	Not unusual (enough hits)	7316	1.403	1.393	0.015	0.699	0.010	1.241	1.640	1.394
bond	O4 C13	Not unusual (enough hits)	7636	1.369	1.368	0.013	0.056	0.001	1.002	1.513	1.367
bond	C15 C14	Not unusual (enough hits)	6370	1.382	1.390	0.015	0.596	0.009	1.213	1.535	1.391
bond	C16 C14	Not unusual (enough hits)	182	1.513	1.516	0.014	0.185	0.003	1.484	1.620	1.514
bond	C16 C17	Not unusual (enough hits)	341	1.497	1.501	0.022	0.181	0.004	1.321	1.575	1.503
bond	C17 C18	Not unusual (enough hits)	1355	1.326	1.320	0.029	0.177	0.005	0.902	1.512	1.324
bond	C19 C18	Not unusual (enough hits)	3580	1.502	1.499	0.025	0.089	0.002	1.192	1.836	1.501
bond	C20 C18	Not unusual (enough hits)	3580	1.498	1.499	0.025	0.064	0.002	1.192	1.836	1.501
bond	O4 C21	Not unusual (enough hits)	8424	1.419	1.424	0.024	0.212	0.005	0.925	1.683	1.426
angle	C6 C1 C2	Not unusual (enough hits)	7794	120.070	119.896	0.965	0.179	0.173	102.986	129.406	119.936
angle	C1 C2 C3	Not unusual (enough hits)	2847	120.301	120.202	0.957	0.104	0.099	113.839	132.500	120.112
angle	O1 C2 C1	Not unusual (enough hits)	7710	116.898	119.991	2.675	1.156	3.093	96.605	147.073	119.451
angle	O1 C2 C3	Not unusual (enough hits)	7201	122.799	119.808	2.541	1.177	2.990	87.775	133.131	120.218
angle	C4 C3 C2	Not unusual (enough hits)	760	118.188	118.455	1.250	0.214	0.267	108.760	123.835	118.561
angle	C3 C4 C5	Not unusual (enough hits)	1848	123.306	121.744	1.548	1.009	1.562	112.017	129.309	121.845
angle	O2 C4 C3	Not unusual (enough hits)	206	115.638	115.804	1.181	0.140	0.165	108.589	119.547	115.942
angle	O2 C4 C5	Not unusual (enough hits)	344	121.055	121.590	0.544	0.983	0.535	119.153	123.423	121.638
angle	C6 C5 C4	Not unusual (enough hits)	4906	116.640	117.913	1.172	1.087	1.273	106.398	129.706	118.027
angle	C4 C5 C9	Not unusual (enough hits)	851	120.705	120.193	0.823	0.623	0.513	116.359	123.290	120.159

Type	Fragment	Classification	No. of hits	Query value	Mean	Std. dev.	z-score	x - mean	Minimum	Maximum	Median
angle	C6 C5 C9	Not unusual (enough hits)	3496	122.654	120.044	1.424	1.833	2.611	103.343	126.543	119.15
angle	C1 C6 C5	Not unusual (enough hits)	6889	121.456	120.803	1.613	0.405	0.653	103.521	132.161	121.40
angle	O2 C7 C8	Not unusual (enough hits)	202	125.988	125.748	0.881	0.272	0.239	120.737	127.504	125.828
angle	C7 C8 C9	Not unusual (enough hits)	200	118.810	118.621	0.908	0.208	0.189	116.170	124.393	118.605
angle	C10 C8 C7	Not unusual (enough hits)	190	118.753	119.766	1.063	0.952	1.013	115.774	123.295	119.731
angle	C10 C8 C9	Not unusual (enough hits)	192	122.400	121.581	1.106	0.741	0.820	117.447	125.199	121.693
angle	C5 C9 C8	Not unusual (enough hits)	112	115.144	115.386	1.218	0.199	0.242	112.905	120.358	115.053
angle	O3 C9 C5	Not unusual (enough hits)	4438	122.497	121.613	1.497	0.591	0.885	102.913	129.947	121.704
angle	O3 C9 C8	Not unusual (enough hits)	223	122.359	122.463	0.996	0.105	0.105	119.451	124.903	122.622
angle	C11 C10 C8	Not unusual (enough hits)	6168	120.250	120.972	1.374	0.525	0.721	108.331	133.239	120.935
angle	C15 C10 C8	Not unusual (enough hits)	324	121.403	120.556	1.304	0.649	0.847	114.431	124.283	120.580
angle	C11 C10 C15	Not unusual (enough hits)	5467	118.280	119.263	1.172	0.838	0.983	99.773	129.034	119.329
angle	C12 C11 C10	Not unusual (enough hits)	8494	121.129	120.858	1.000	0.272	0.272	89.761	133.847	120.840
angle	C11 C12 C13	Not unusual (enough hits)	5710	119.711	119.442	1.702	0.158	0.269	100.709	133.580	119.875
angle	C12 C13 C14	Not unusual (enough hits)	1708	120.809	121.034	1.334	0.168	0.225	109.206	138.718	120.925
angle	O4 C13 C12	Not unusual (enough hits)	5490	124.013	124.291	1.532	0.182	0.279	102.228	133.747	124.477
angle	O4 C13 C14	Not unusual (enough hits)	3277	115.178	115.933	1.188	0.636	0.755	99.693	126.856	115.908
angle	C15 C14 C13	Not unusual (enough hits)	6362	118.057	118.153	0.894	0.108	0.097	109.963	129.343	118.194
angle	C16 C14 C13	Not unusual (enough hits)	21	119.044	120.475	1.534	0.933	1.431	117.269	123.505	120.438
angle	C16 C14 C15	Not unusual (enough hits)	91	122.883	121.063	1.883	0.967	1.820	114.471	124.449	121.293
angle	C10 C15 C14	Not unusual (enough hits)	1228	122.002	121.503	1.376	0.363	0.500	113.619	154.930	121.510
angle	C14 C16 C17	Not unusual (enough hits)	67	115.615	112.614	2.087	1.438	3.001	107.009	118.113	112.513
angle	C16 C17 C18	Not unusual (enough hits)	220	127.970	127.625	1.353	0.255	0.345	124.405	135.843	127.607
angle	C19 C18 C17	Not unusual (enough hits)	2710	120.717	122.663	2.864	0.679	1.946	92.847	157.283	122.606
angle	C20 C18 C17	Not unusual (enough hits)	2710	124.776	122.663	2.864	0.738	2.113	92.847	157.283	122.606
angle	C20 C18 C19	Not unusual (enough hits)	1790	114.465	114.574	2.086	0.052	0.109	100.007	139.344	114.591
angle	C4 O2 C7	Not unusual (enough hits)	453	118.230	118.239	1.050	0.009	0.010	102.729	120.642	118.334
angle	C21 O4 C13	Not unusual (enough hits)	7566	117.943	117.508	1.189	0.366	0.435	102.613	135.555	117.460

3. Hirshfeld Analysis

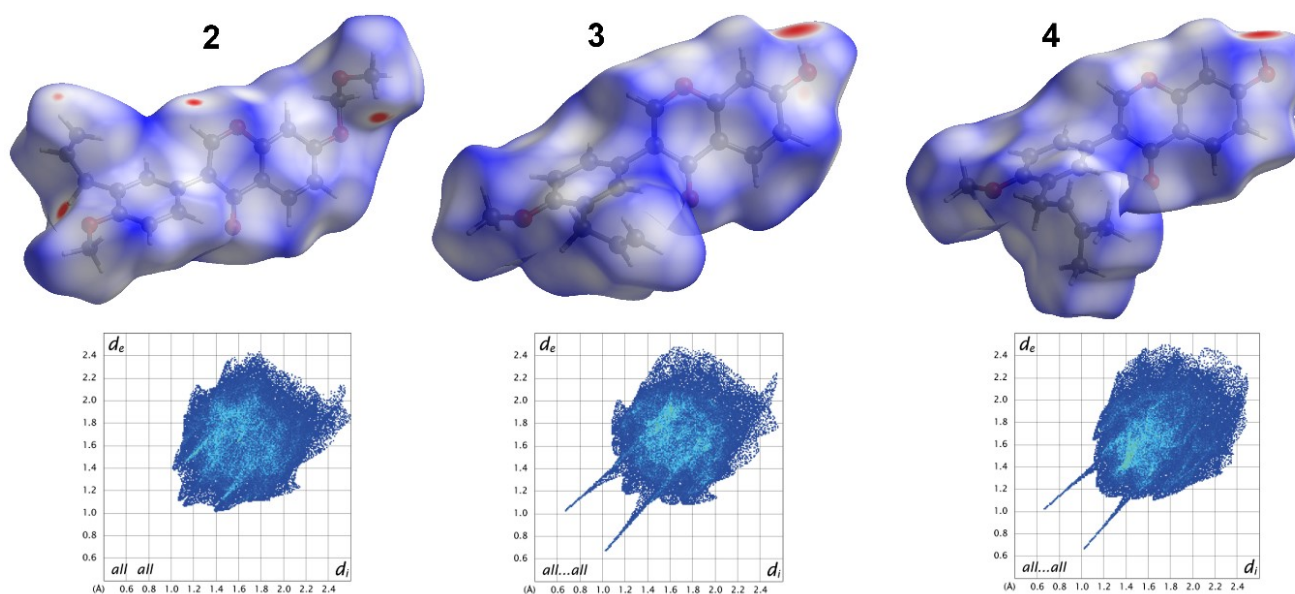


Figure S 1: Illustration of d_{norm} of Hirshfeld surfaces from **2-4** (top) and 2D fingerprint plot of all intermolecular contacts.

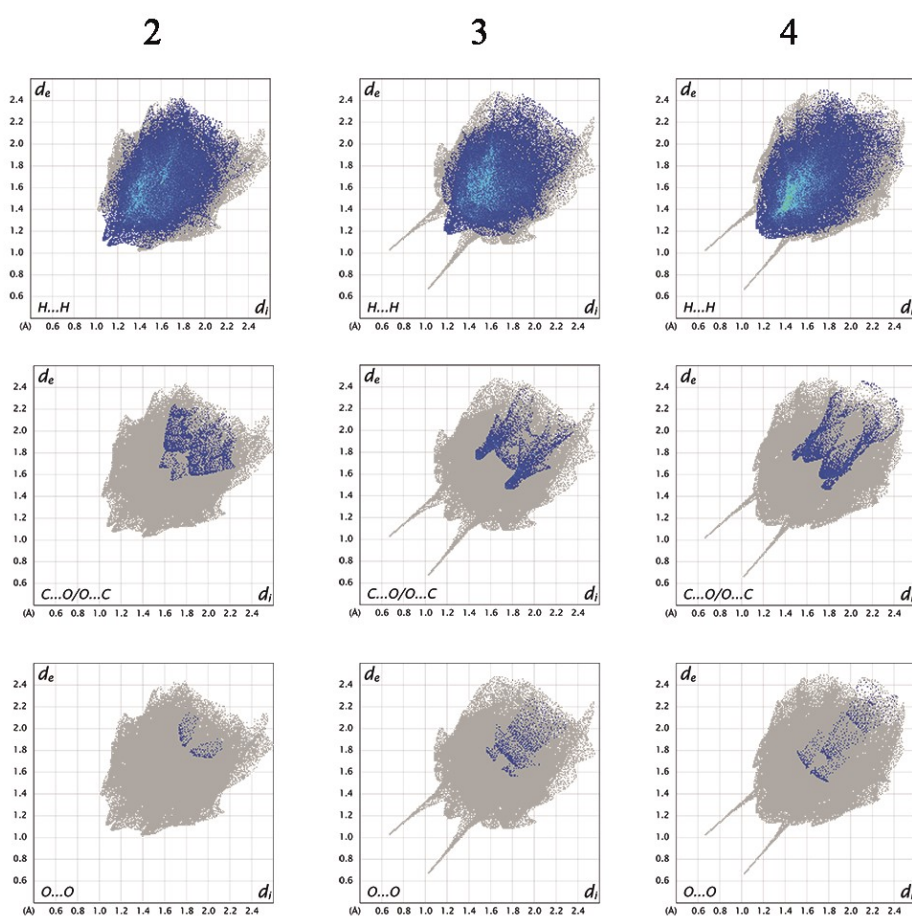


Figure S 2: Representation of the 2D fingerprint plots of the $H...H$ contacts (top), of the $C...O/O...C$ contacts (center) and of the $O...O$ contacts (bottom) of the compound **2** (left), **3** (middle), and **4** (right).

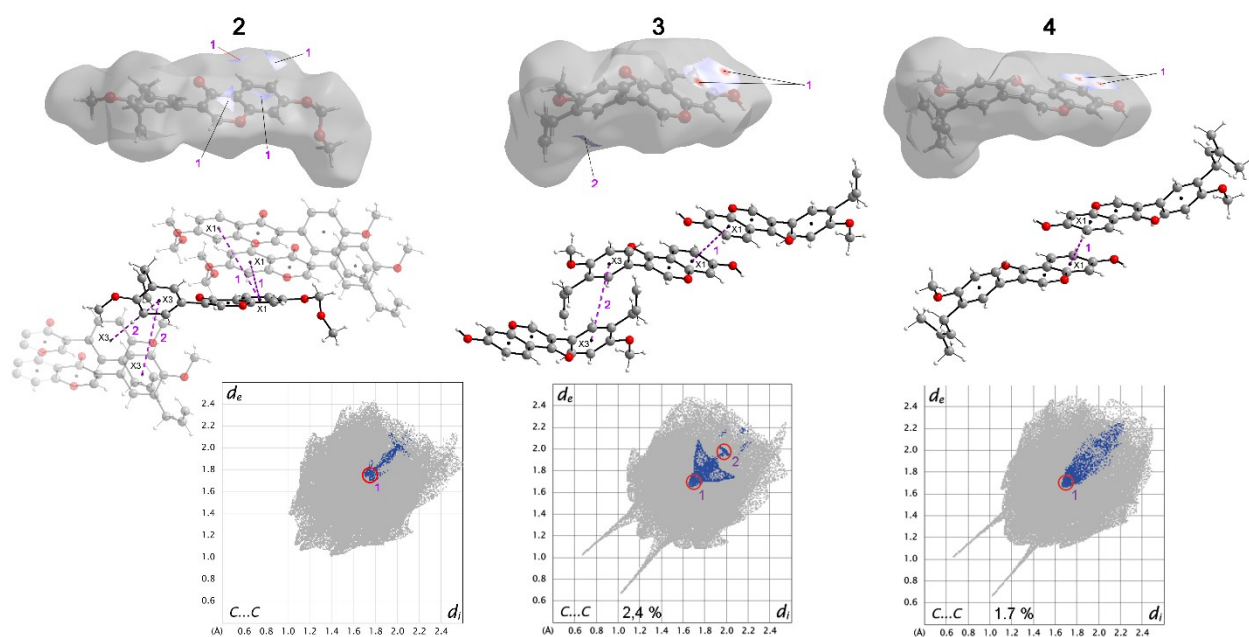


Figure S 3: Representation of the Hirshfeld surface of the C...C contacts (top), the molecular view with labels (center) and the 2D fingerprint plot of the C...C contacts (bottom) of compound **2** (left), **3** (middle), and **4** (right).

4. Aromatic Analyser Results

Table 1: Stacking interactions in compound **2** (symmetry equivalent interactions excluded)

Centroid1	Centroid2	Distance (Ang.)	Relative Orientation (Degrees)	Score
2	12	5.22	62.62	7.8
1	7	5.2	22.07	6.7
1	8	6.39	70.4	3.7
1	3	6.69	0	3.4
1	22	6.03	67.46	3.3
1	10	6.87	70.4	2
2	4	6.69	0	0.9
1	20	8.65	67.46	0.7
1	4	9.03	48.51	0.6
1	12	9.43	70.4	0.5
1	15	9.44	56.66	0.5
1	16	9.14	86.77	0.5
1	6	9.7	48.51	0.4
1	14	9.76	70.4	0.4
2	22	9.84	37.5	0.4
1	24	9.35	67.46	0.3

Table 2: Stacking interactions in compound **3** (symmetry equivalent interactions excluded)

Centroid1	Centroid2	Distance (Ang.)	Relative Orientation (Degrees)	Score
1	27	3.7	0	8.4
1	14	5.32	68.37	7.4
2	24	4.66	0	7.4
1	20	5.09	68.37	4.3
1	8	6.1	68.37	3.9
1	25	6.65	0	3.3
1	12	7.01	68.37	2.1
1	28	7.58	68.37	1.7
1	19	7.81	0	1.2
1	3	8.02	0	1
2	4	8.02	0	1
2	8	8.48	0	0.9
1	7	8.48	0	0.8
1	22	8.5	68.37	0.7
2	18	8.93	0	0.6
2	20	8.75	0	0.6
2	22	9.27	0	0.6
1	24	9.25	68.37	0.5
2	16	10.84	0	0.1

Table 3: Stacking interactions in compound **4** (symmetry equivalent interactions excluded)

Centroid1	Centroid2	Distance (Ang.)	Relative Orientation (Degrees)	Score
1	19	4	0	8.9
1	6	5.26	58.46	7.5
1	32	5.61	62.54	5.8
1	18	4.98	58.46	4.1
1	11	6.77	6.82	3.5
1	20	7.39	58.46	1.9
1	17	8.26	0	1
1	3	8.17	0	0.9
1	30	8.26	62.54	0.9
2	4	8.17	0	0.9
2	8	8.47	62.78	0.8
2	18	8.21	0	0.8
2	24	8.37	62.78	0.8
1	25	8.86	6.82	0.7
1	10	8.41	62.54	0.5
1	14	9.61	62.54	0.4
2	26	10.74	62.78	0.1

5. Packing of compound 2

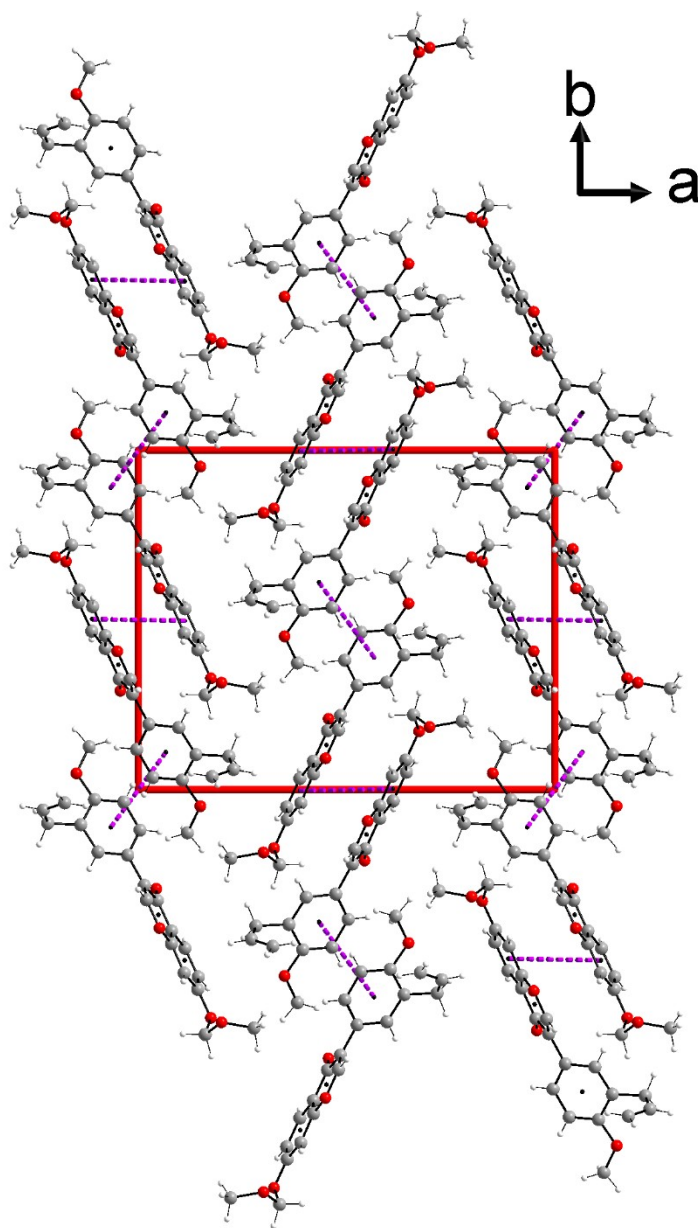


Figure S 4: Cell view of compound **2** with viewing direction along the crystallographic *c*-axis. Stacking interactions are shown as purple lines.

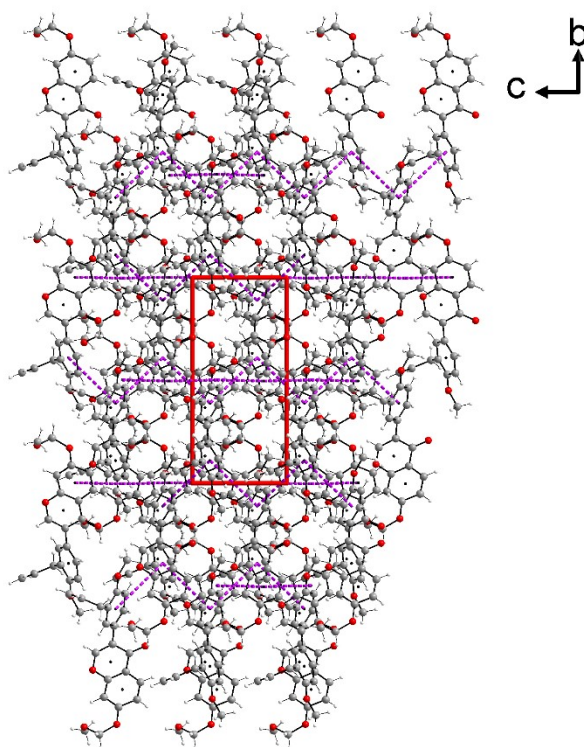


Figure S 5: Cell view of compound **2** with viewing direction along the crystallographic *a*-axis. Stacking interactions are shown as purple lines.

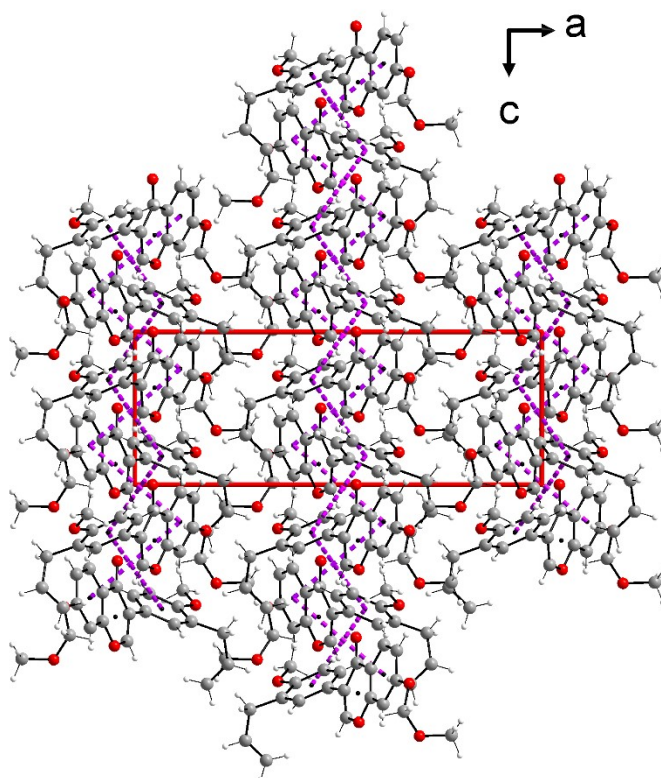


Figure S 6: Cell view of compound **2** with viewing direction along the crystallographic *b*-axis. Stacking interactions are shown as purple lines.