Electronic Supplementary Material (ESI) for New Journal of Chemistry.

gem-Dibromovinyl phthalonitriles: Synthesis, structure elucidation, Hirshfeld surface analysis and energy framework calculations

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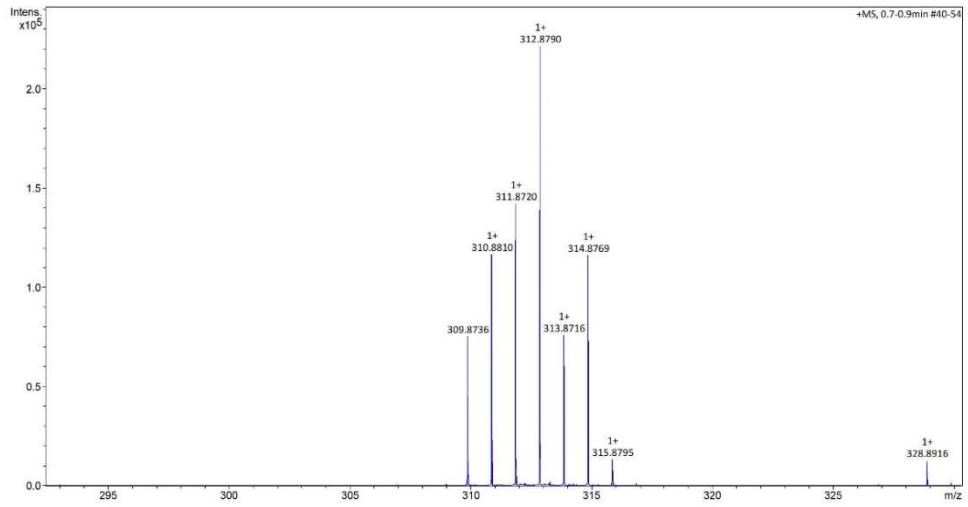

Fig. S1. APCI+-MS spectrum of **2**.

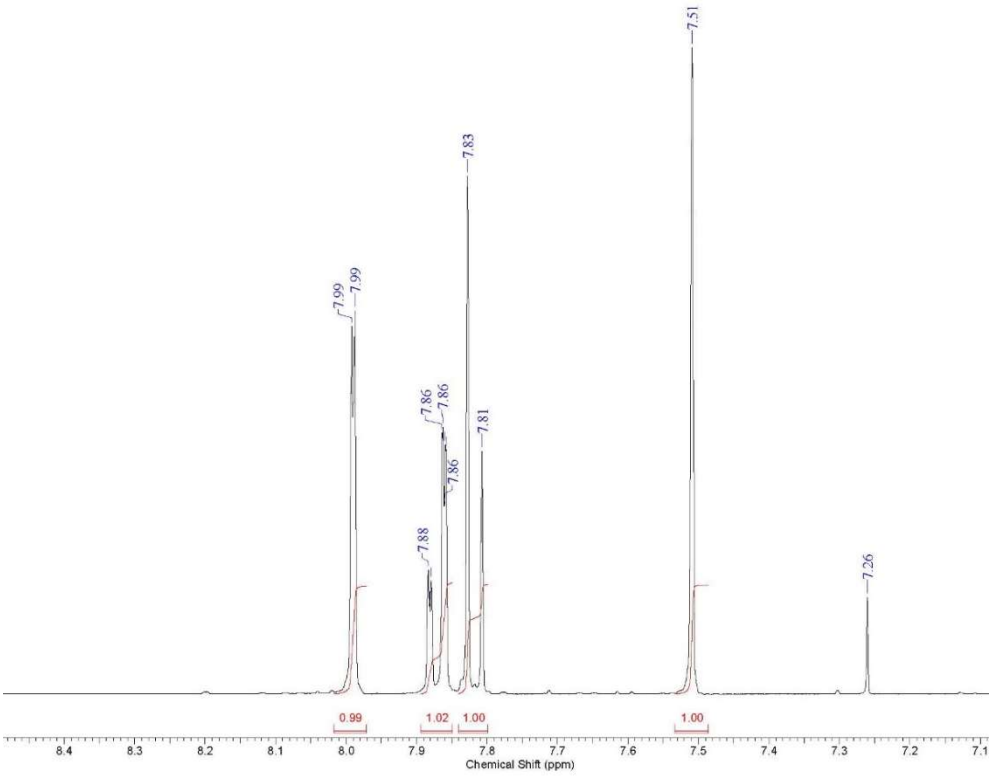

Fig. S2. ^{1}H NMR of spectrum **2** in $CDCl_3$.

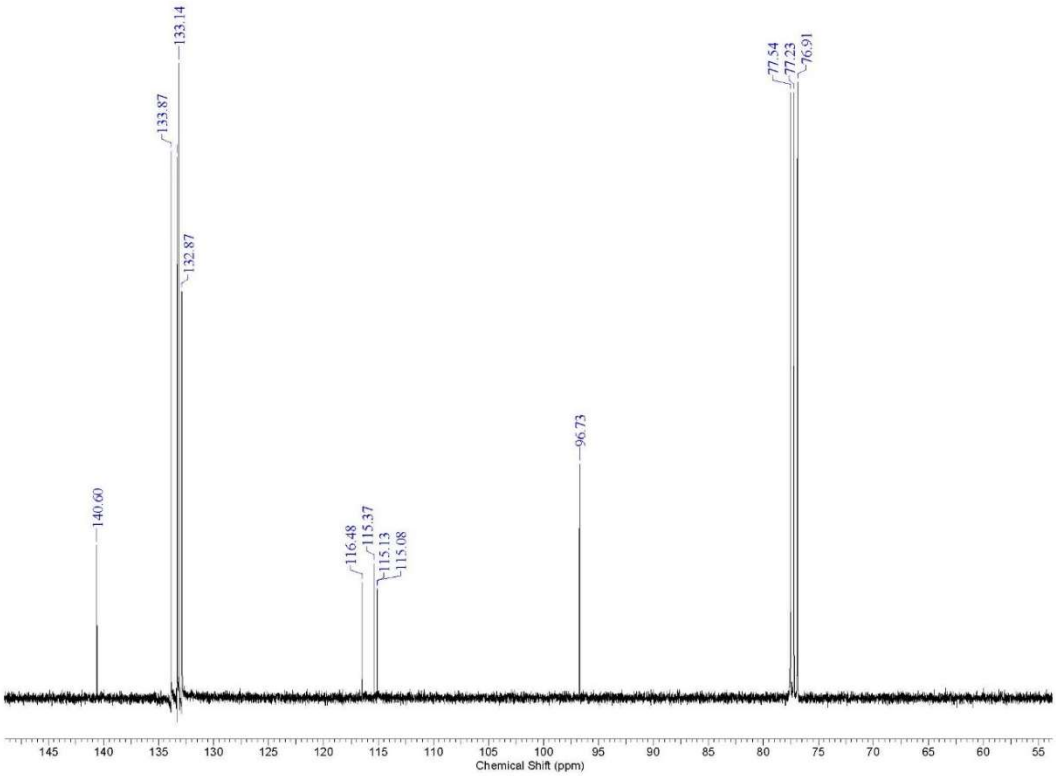

Fig. S3. ^{13}C NMR of spectrum **2** in $CDCl_3$.

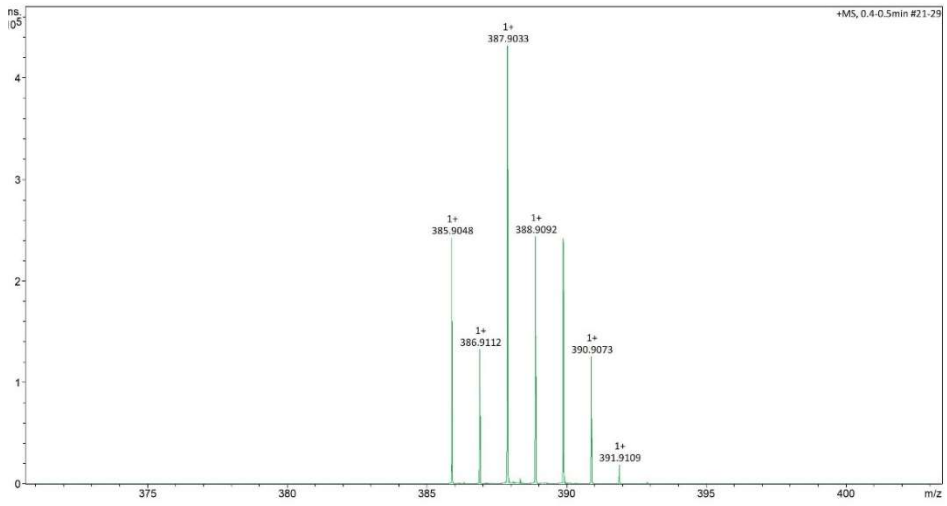

Fig. S4. APCI+-MS spectrum of **4**.

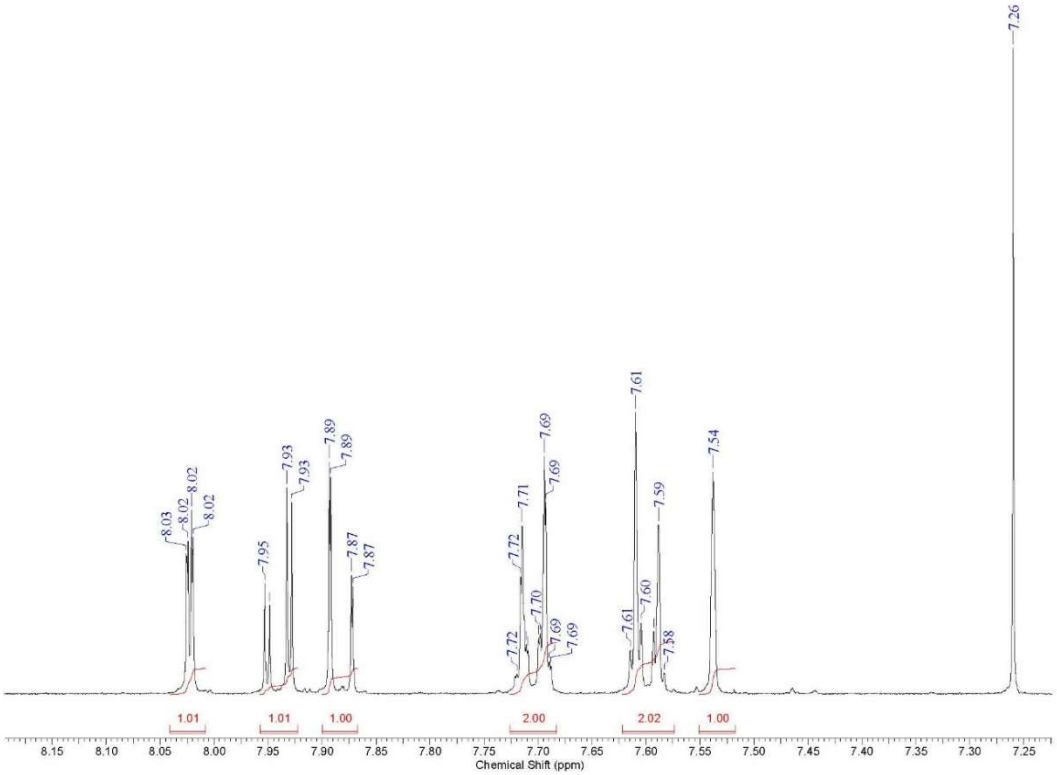

Fig. S5. ^{1}H NMR of spectrum **4** in $CDCl_3$.

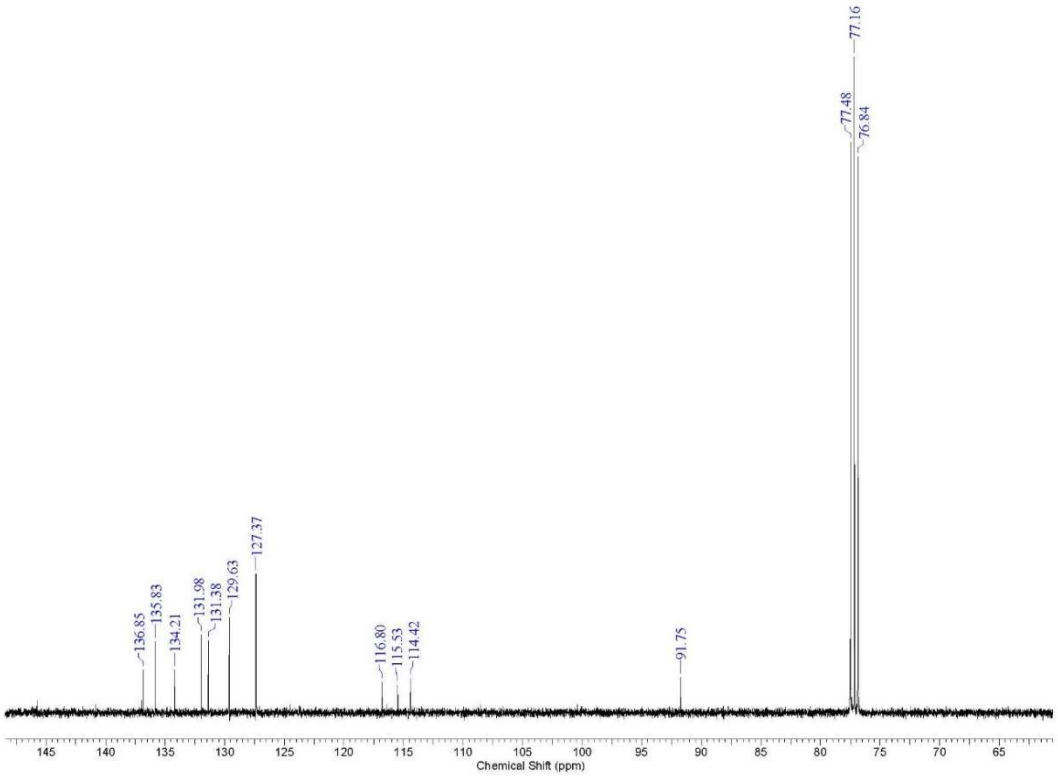

Fig. S6. ^{13}C NMR of spectrum **4** in $CDCl_3$.

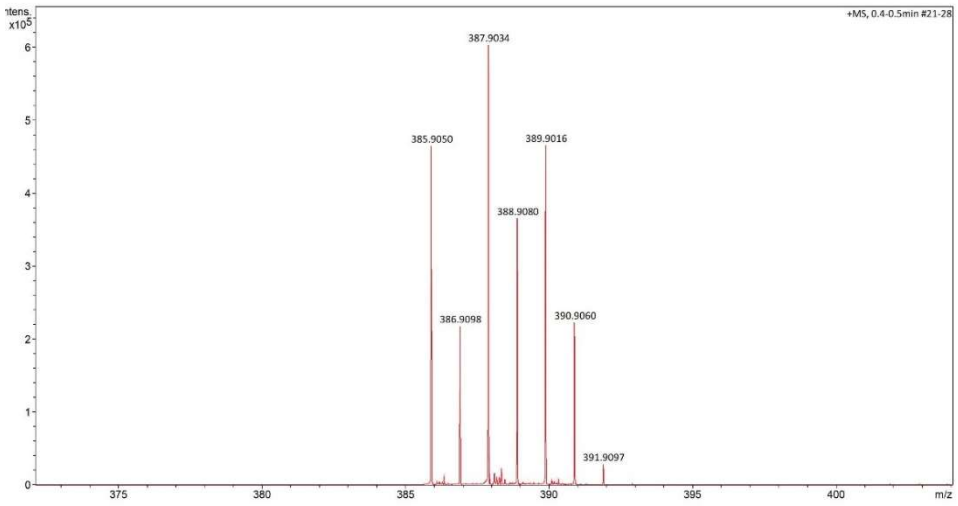

Fig. S7. APCI+-MS spectrum of **7**.

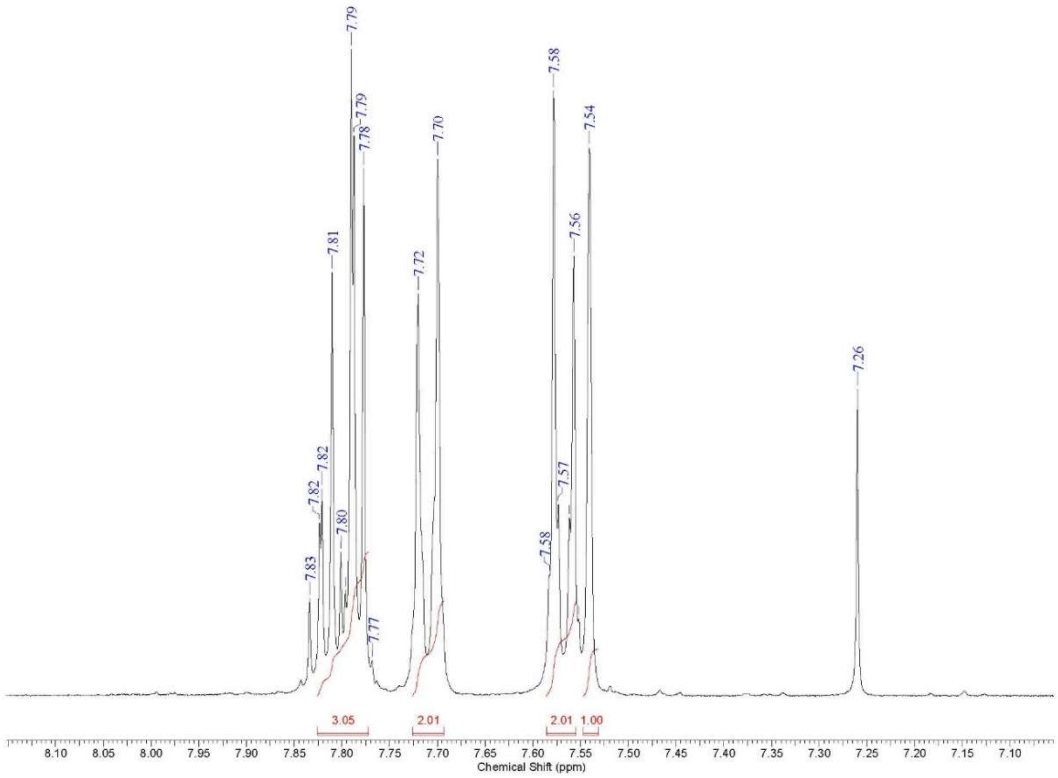

Fig. S8. ^{1}H NMR of spectrum **7** in $CDCl_3$.

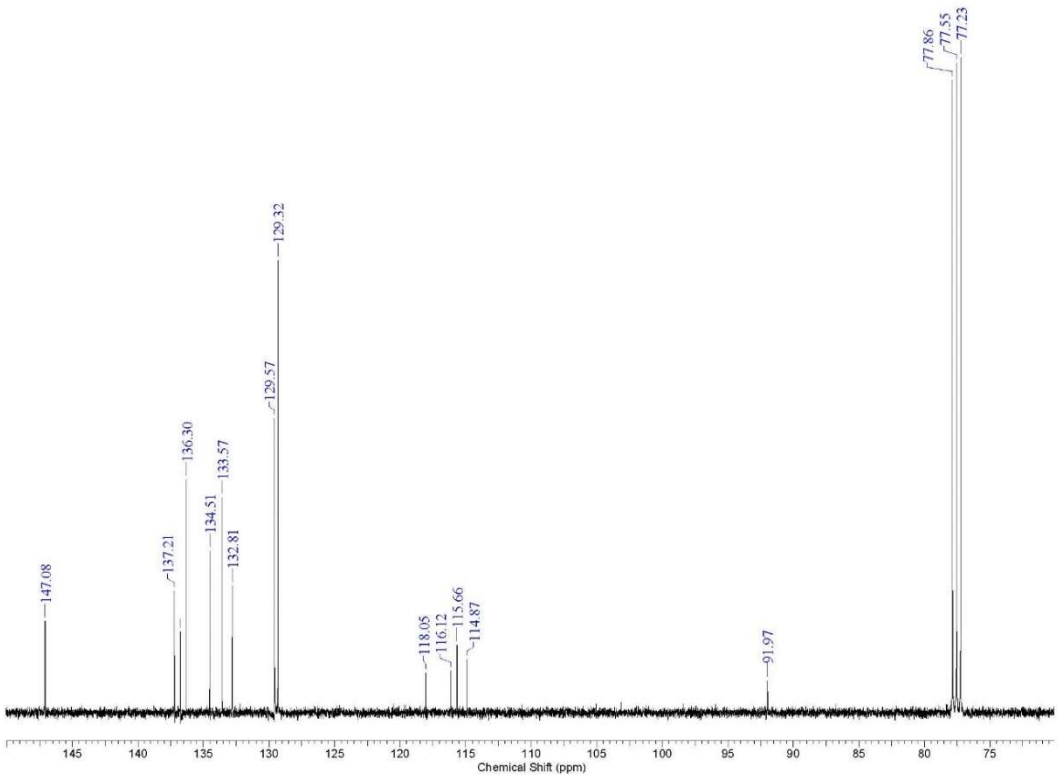

Fig. S9. ^{13}C NMR of spectrum **7** in $CDCl_3$.

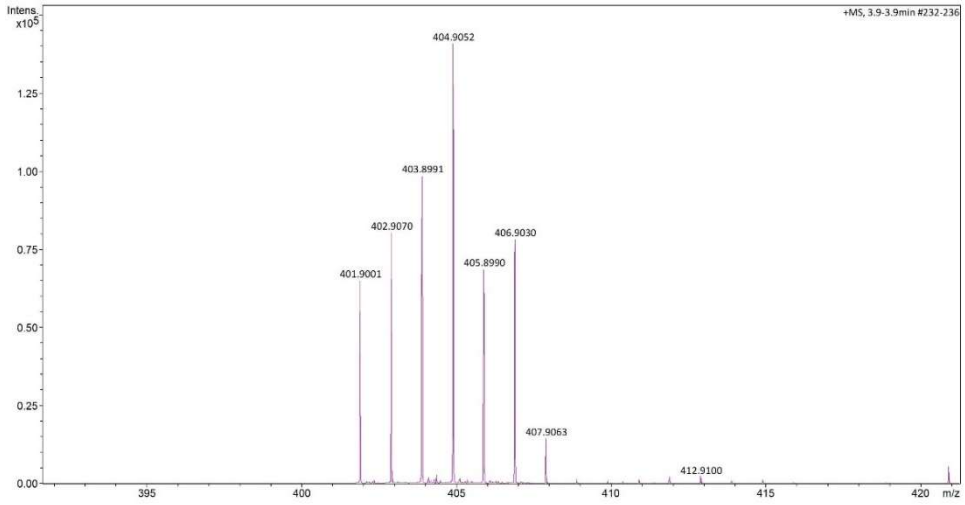

Fig. S10. APCI+-MS spectrum of **9**.

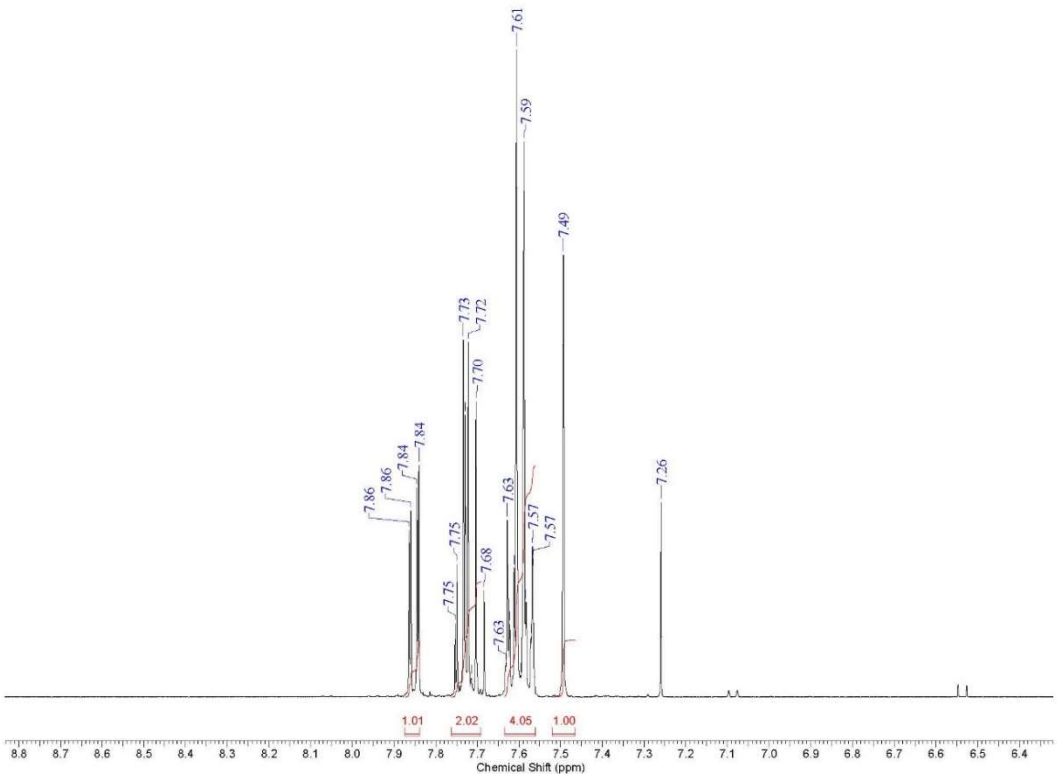

Fig. S11. ^{1}H NMR of spectrum **9** in $CDCl_3$.

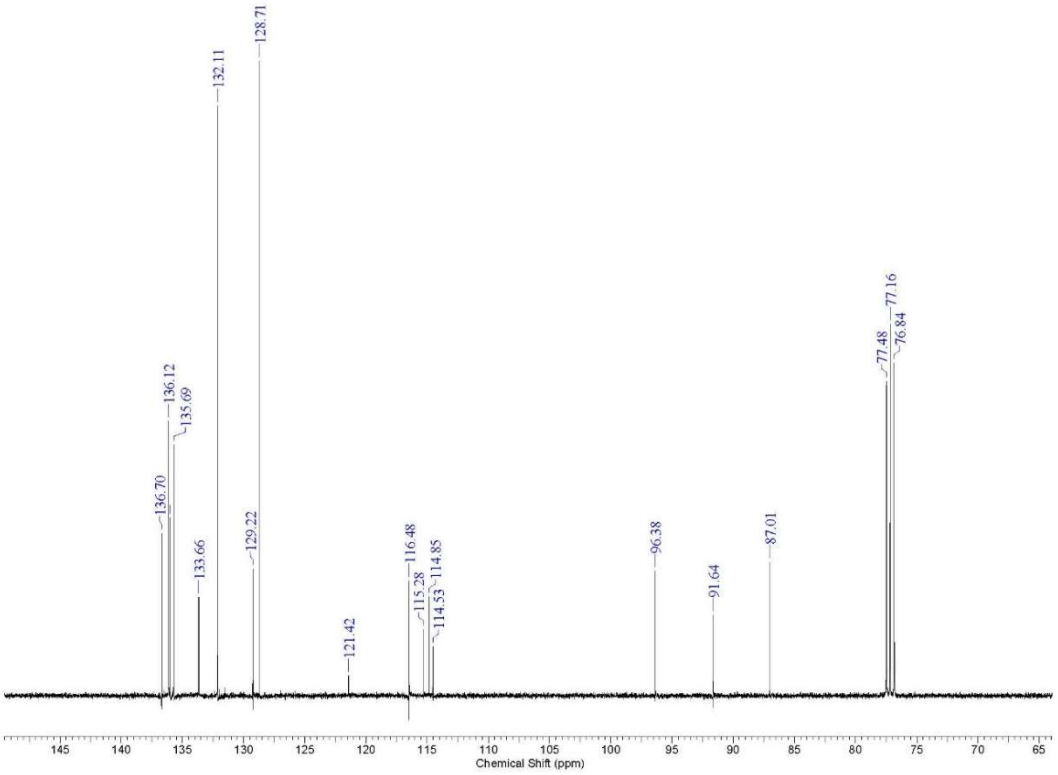

Fig. S12. ^{13}C NMR of spectrum **9** in $CDCl_3$.

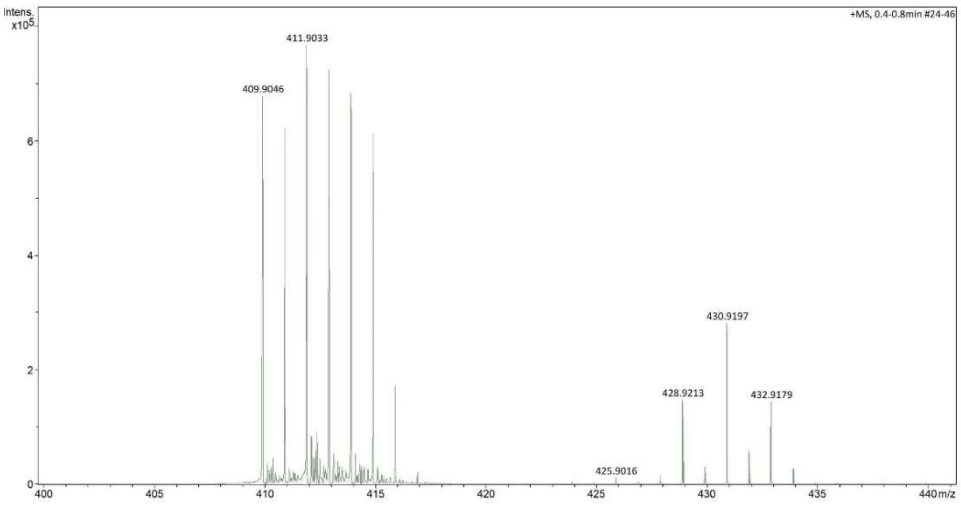

Fig. S13. APCI+-MS spectrum of **11**.

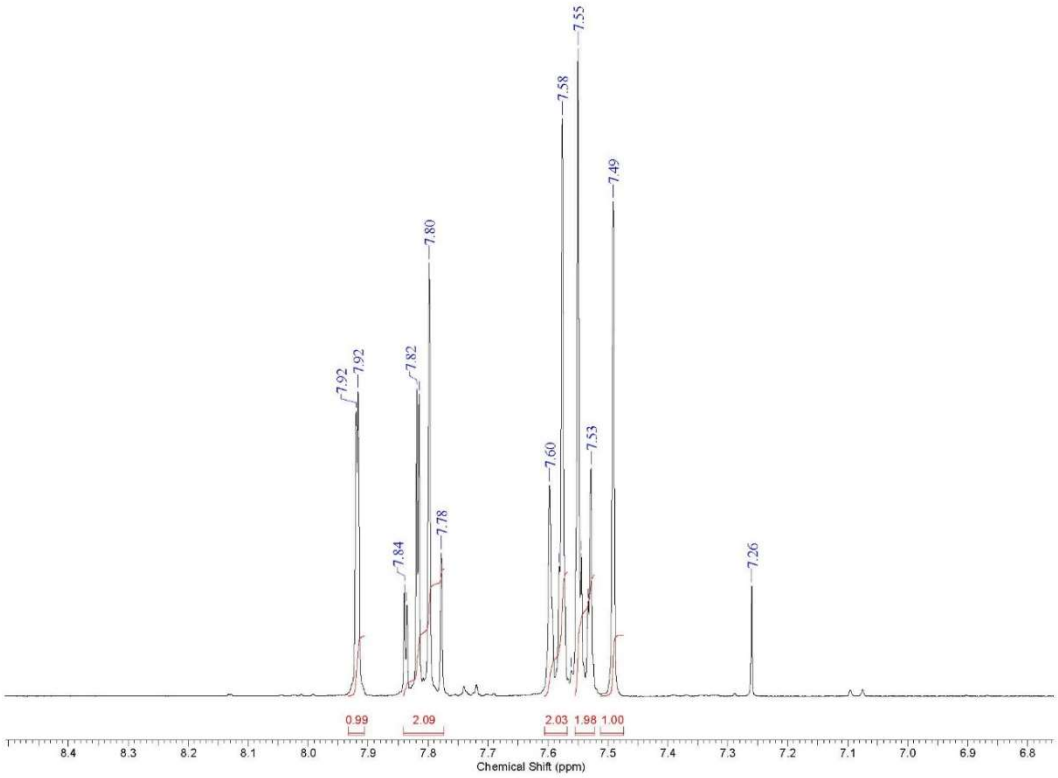

Fig. S14. ^{1}H NMR of spectrum **11** in $CDCl_3$.

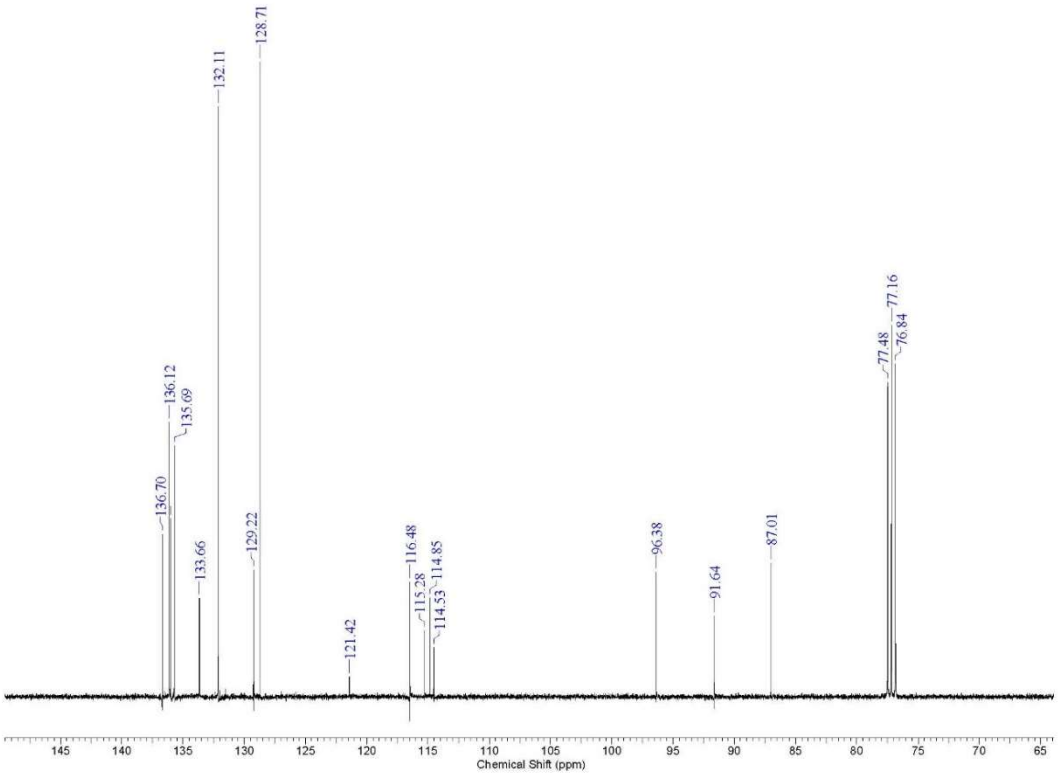

Fig. S15. ^{13}C NMR of spectrum **11** in $CDCl_3$.

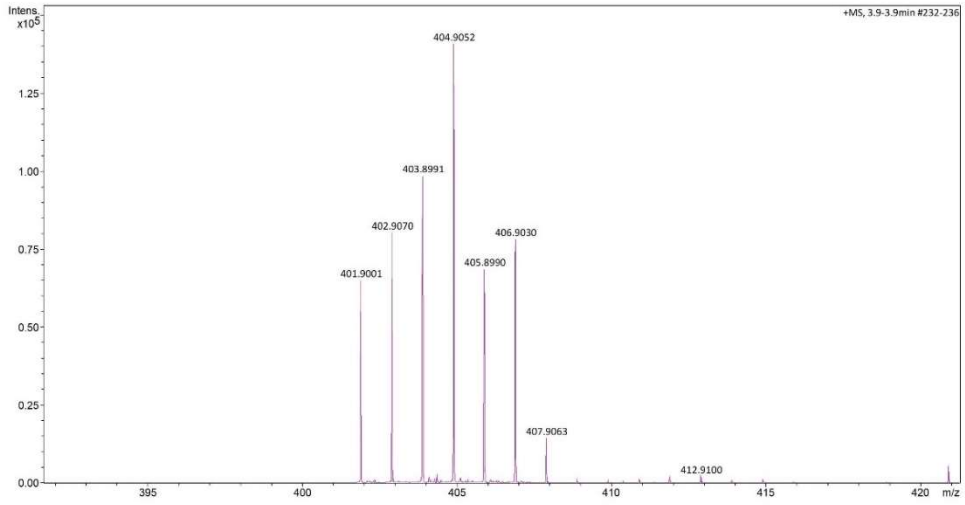

Fig. S16. APCI+-MS spectrum of **13**.

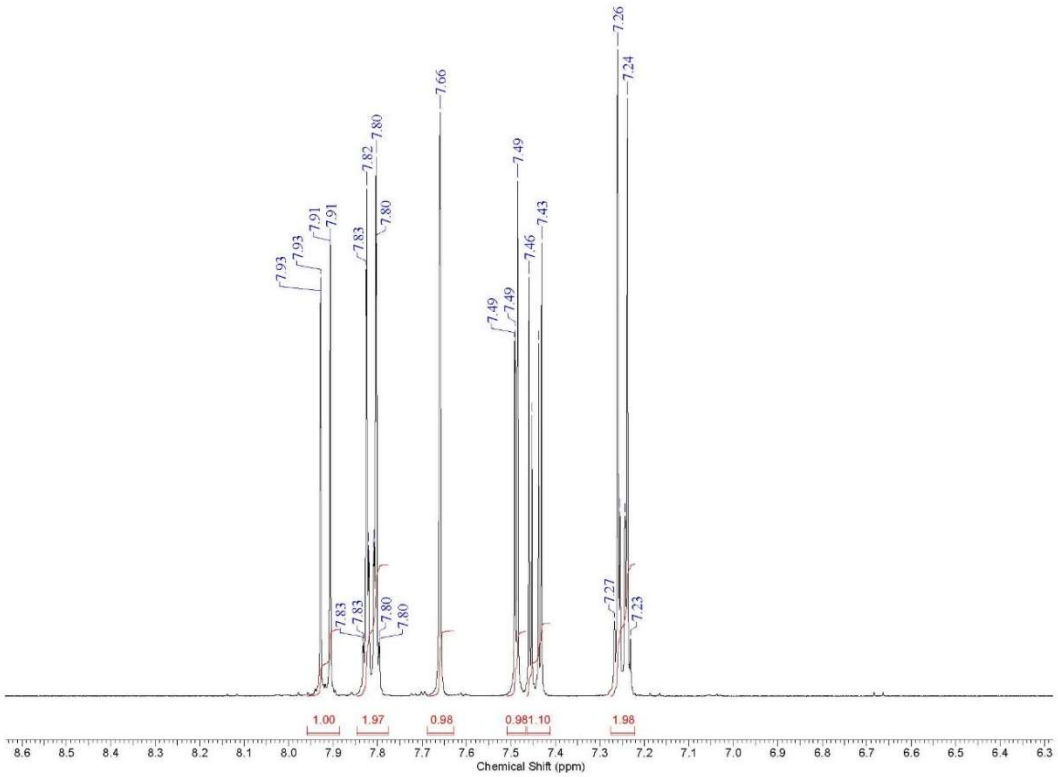

Fig. S17. ^{1}H NMR of spectrum **13** in $CDCl_3$.

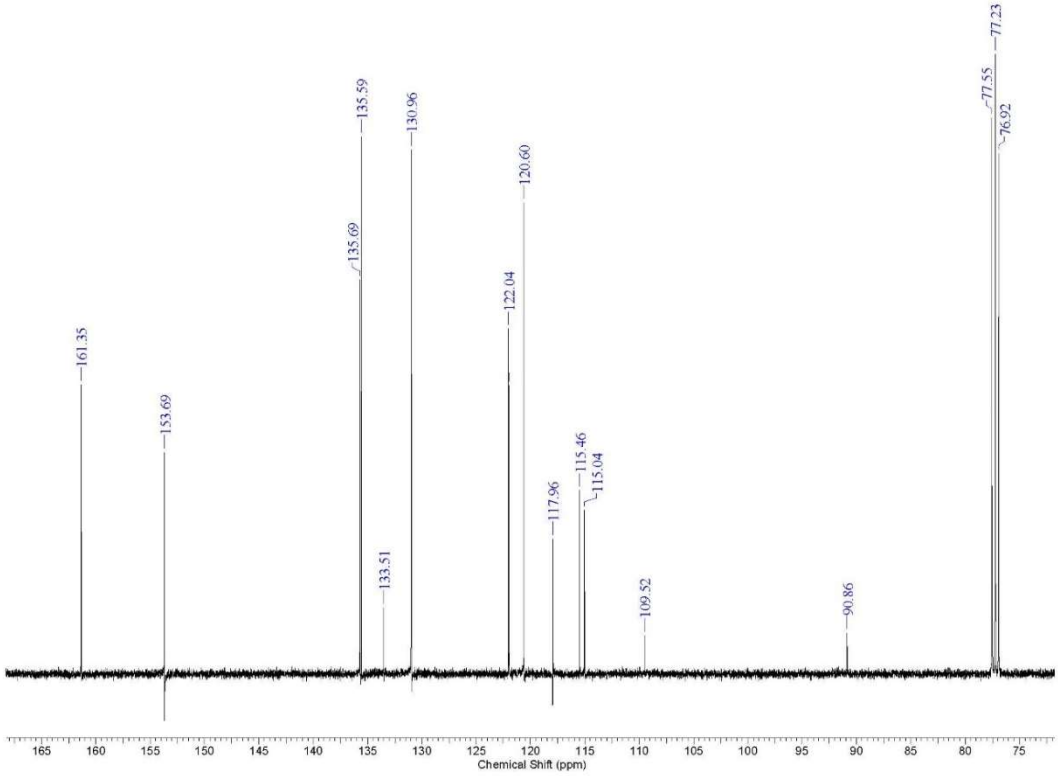

Fig. S18. ^{13}C NMR of spectrum **13** in $CDCl_3$.

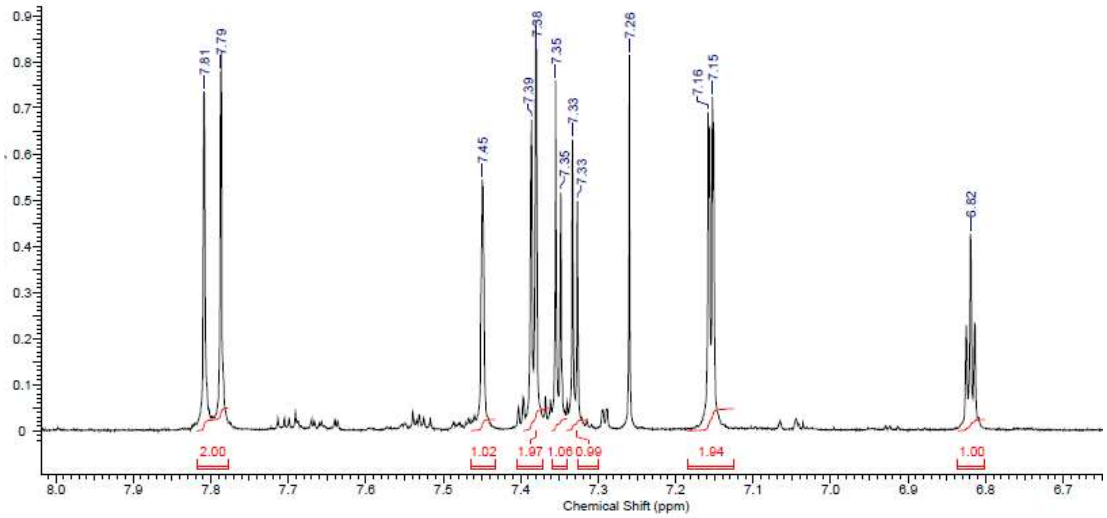

Fig. S19. ^{1}H NMR of spectrum **16** in $CDCl_3$.

Table S1: Comparison of some selected bond lengths [Å] and bond angles [°] obtained from X-ray crystal structures.

Compound	—C≡N1	—C≡N2	N1C-C	N2C-C
2A	1.138(10)	1.137(9)	1.449(10)	1.447(9)
2B	1.139(10)	1.1445(9)	1.456(10)	1.439(10)
4	1.134(7)	1.136(7)	1.465(7)	1.447(8)
7	1.136(8)	1.139(9)	1.442(9)	1.437(9)
9	1.146(7)	1.137(7)	1.439(7)	1.443(7)
11	1.140(4)	1.439(4)	1.443(4)	1.439(4)
13	1.137(5)	1.137(4)	1.438(5)	1.445(4)
16	1.152(14) 1.124(12)	1.153(13) 1.140(11)	1.436(15) 1.438(14)	1.441(13) 1.477(12)

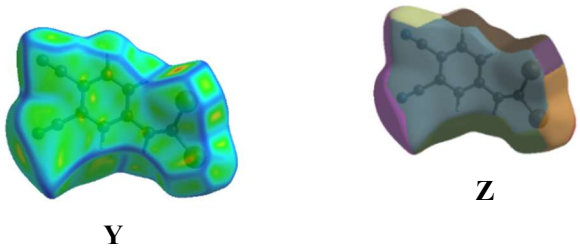

Fig. S20. Perspective view of Hirshfeld surfaces of **2A** (Y) curvedness, (Z) Fragment Patch.

Fig. S21. Perspective view of Hirshfeld surfaces of **2B** (Y) curvedness, (Z) Fragment Patch.

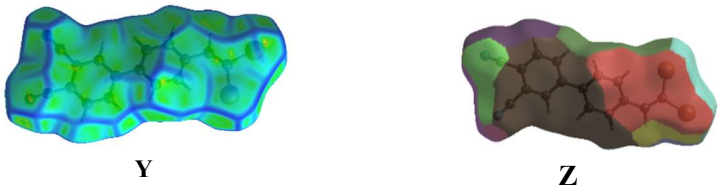

Fig. S22. Perspective view of Hirshfeld surfaces of **4** (Y) curvedness, (Z) Fragment Patch.

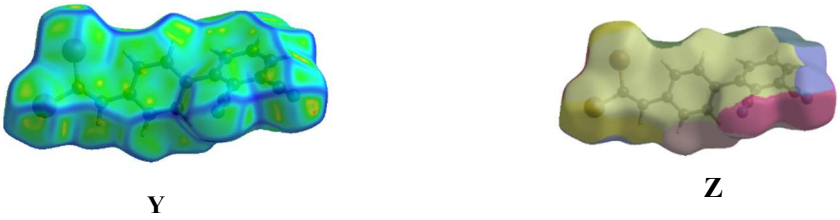

Fig. S23. Perspective view of Hirshfeld surfaces of **7** (Y) curvedness, (Z) Fragment Patch.

Fig. S24. Perspective view of Hirshfeld surfaces of **9** (Y) curvedness, (Z) Fragment Patch.

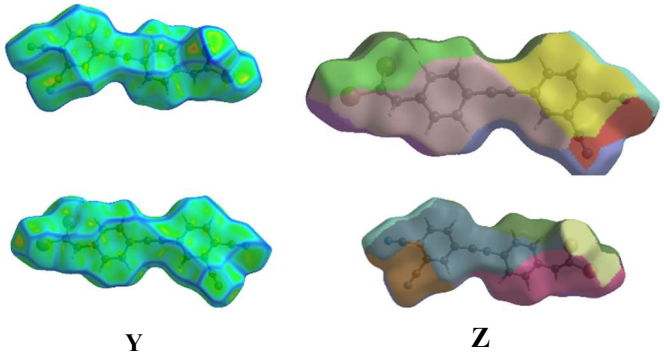

Fig. S25. Perspective view of Hirshfeld surfaces of **11** (Y) curvedness, (Z) Fragment Patch.

Fig. S26. Perspective view of Hirshfeld surfaces of **13** (Y) curvedness, (Z) Fragment Patch.

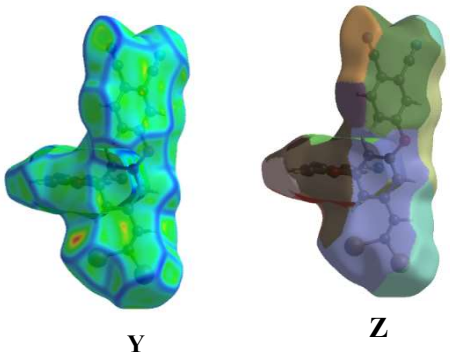

Fig. S27. Perspective view of Hirshfeld surfaces of **16** (Y) curvedness, (Z) Fragment Patch.

Total energies, only reported for two benchmarked energy models, are the sum of the four energy components, scaled appropriately (scale factor table below)

Interaction energies. N refers to the number of molecules, R is the distance between molecular centroids (mean atomic position) in Å. Energies in kJ mol^{-1}.
Scale factors for benchmarked energy models
See Mackenzie et al. IUCrJ (2017)

Energy Model	k_ele	k_pol	k_disp	k_rep
CE-HF ... HF/3-21G electron densities	1.019	0.651	0.901	0.811
CE-B3LYP ... B3LYP/6-31G(d,p) electron densities	1.057	0.740	0.871	0.618

Fig. S28. Interaction energies of **2A**.

	N	Symop	R	Electron Density	E_ele	E_pol	E_dis	E_rep	E_tot
	1	-x, -y, -z	13.40	B3LYP/6-31G(d,p)	-5.5	-1.2	-3.4	0.0	-9.7
	2	x, y, z	3.89	B3LYP/6-31G(d,p)	0.2	-3.2	-59.2	44.2	-26.4
	1	-	10.04	B3LYP/6-31G(d,p)	-19.9	-0.1	-9.4	21.3	-16.1
	1	-x, -y, -z	12.12	B3LYP/6-31G(d,p)	-18.0	0.0	-11.7	0.0	-29.3
	1	-	7.70	B3LYP/6-31G(d,p)	-4.4	-5.5	-15.3	16.5	-11.9
	1	-	7.96	B3LYP/6-31G(d,p)	-0.0	-1.0	-9.8	6.5	-5.3
	1	-	9.33	B3LYP/6-31G(d,p)	-9.5	-5.1	-12.3	10.1	-18.4
	1	-	9.48	B3LYP/6-31G(d,p)	-10.9	-3.2	-13.3	12.6	-17.6
	1	-x, -y, -z	8.51	B3LYP/6-31G(d,p)	-3.3	-0.2	-6.4	8.9	-3.6
	1	-	7.43	B3LYP/6-31G(d,p)	-2.9	-0.8	-12.7	10.9	-8.1
	1	-	9.02	B3LYP/6-31G(d,p)	2.0	-0.2	-5.8	2.8	-1.4
	1	-	10.41	B3LYP/6-31G(d,p)	-17.2	-2.3	-9.7	16.3	-18.2

Fig. S29. Interaction energies of **2B**.

	N	Symop	R	Electron Density	E_ele	E_pol	E_dis	E_rep	E_tot
	2	x, y, z	3.89	B3LYP/6-31G(d,p)	0.2	-3.8	-58.9	44.0	-26.7
	1	-	7.70	B3LYP/6-31G(d,p)	-19.9	-3.8	-9.4	21.3	-18.9
	1	-	9.48	B3LYP/6-31G(d,p)	1.0	-0.0	-0.0	0.0	1.1
	1	-	9.33	B3LYP/6-31G(d,p)	0.0	-4.2	0.0	0.0	-3.1
	1	-	9.02	B3LYP/6-31G(d,p)	-0.5	-1.0	-0.0	0.0	-1.2
	1	-x, -y, -z	8.77	B3LYP/6-31G(d,p)	-23.2	-0.3	-18.0	17.4	-29.7
	1	-	7.43	B3LYP/6-31G(d,p)	-1.7	-0.3	-0.8	0.0	-2.6
	1	-	10.41	B3LYP/6-31G(d,p)	0.8	-0.0	-0.0	0.0	0.9
	1	-	10.04	B3LYP/6-31G(d,p)	-4.4	-2.6	-15.3	16.5	-9.7
	1	-	7.96	B3LYP/6-31G(d,p)	-0.6	-0.0	-0.0	0.0	-0.6
	1	-x, -y, -z	9.63	B3LYP/6-31G(d,p)	-26.8	-3.2	-13.1	21.3	-29.0

Fig. S30. Interaction energies of **4**.

	N	Symop	R	Electron Density	E_ele	E_pol	E_dis	E_rep	E_tot
	1	-	9.43	B3LYP/6-31G(d,p)	-8.8	-2.8	-16.8	18.5	-14.6
	2	x, y, z	13.37	B3LYP/6-31G(d,p)	-0.4	-1.0	-4.6	0.0	-5.2
	1	-	4.97	B3LYP/6-31G(d,p)	-7.6	-2.8	-61.0	35.3	-41.4
	1	-	12.23	B3LYP/6-31G(d,p)	-29.9	-4.7	-12.3	0.0	-45.8
	1	-	15.15	B3LYP/6-31G(d,p)	6.0	-2.2	-8.4	0.0	-2.6
	1	-	10.40	B3LYP/6-31G(d,p)	-2.3	-2.1	-11.6	9.4	-8.3
	2	x, y, z	9.14	B3LYP/6-31G(d,p)	-10.4	-2.1	-43.3	28.5	-32.6
	2	x, y, z	12.01	B3LYP/6-31G(d,p)	-8.0	-2.2	-11.7	0.0	-20.2
	1	-	4.97	B3LYP/6-31G(d,p)	-7.7	-2.5	-61.1	35.7	-41.0
	1	-	15.15	B3LYP/6-31G(d,p)	2.1	-2.2	-8.4	0.0	-6.6
	1	-	12.23	B3LYP/6-31G(d,p)	-16.7	-4.7	-12.3	0.0	-31.9
	1	-	10.40	B3LYP/6-31G(d,p)	-2.3	-0.3	-11.5	9.3	-7.0
	1	-	9.43	B3LYP/6-31G(d,p)	-8.8	-0.3	-16.8	18.6	-12.6

Fig. S31. Interaction energies of **7**.

	N	Symop	R	Electron Density	E_ele	E_pol	E_dis	E_rep	E_tot
	2	x, y, z	8.15	B3LYP/6-31G(d,p)	-16.6	-4.5	-13.1	11.1	-25.4
	1	-x, -y, -z	16.55	B3LYP/6-31G(d,p)	-8.6	-2.8	-9.1	0.0	-19.1
	2	x, y, z	3.94	B3LYP/6-31G(d,p)	-4.1	-3.8	-91.5	62.6	-48.2
	1	-x, -y, -z	9.37	B3LYP/6-31G(d,p)	-4.6	-0.4	-14.3	11.1	-10.7
	2	x, y, z	9.17	B3LYP/6-31G(d,p)	2.7	-0.5	-5.6	0.6	-2.0
	2	x, y, z	7.73	B3LYP/6-31G(d,p)	-9.2	-4.1	-23.9	18.3	-22.3
	1	-x, -y, -z	17.24	B3LYP/6-31G(d,p)	-18.7	-3.4	-9.9	0.0	-31.0
	1	-x, -y, -z	8.93	B3LYP/6-31G(d,p)	-5.2	-0.9	-16.4	16.4	-10.2
	1	-x, -y, -z	14.40	B3LYP/6-31G(d,p)	4.2	-1.8	-11.4	0.0	-6.8
	1	-x, -y, -z	15.90	B3LYP/6-31G(d,p)	5.2	-1.0	-3.4	0.0	1.8

Fig. S32. Interaction energies of **9**.

	N	Symop	R	Electron Density	E_ele	E_pol	E_dis	E_rep	E_tot
	2	x, y, z	13.76	B3LYP/6-31G(d,p)	-7.0	-3.1	-8.5	0.0	-17.2
	1	-x, -y, -z	6.59	B3LYP/6-31G(d,p)	-19.0	-4.7	-60.2	37.3	-52.9
	2	x, -y+1/2, z+1/2	10.60	B3LYP/6-31G(d,p)	-3.4	-2.1	-25.7	13.4	-19.3
	1	-x, -y, -z	11.80	B3LYP/6-31G(d,p)	-22.1	-6.8	-25.9	25.4	-35.3
	2	-x, y+1/2, -z+1/2	11.54	B3LYP/6-31G(d,p)	-17.6	-5.6	-22.1	21.7	-28.5
	2	x, -y+1/2, z+1/2	7.88	B3LYP/6-31G(d,p)	-3.6	-0.5	-17.9	17.0	-9.3
	1	-x, -y, -z	4.75	B3LYP/6-31G(d,p)	-9.9	-0.8	-59.7	35.5	-41.1
	2	-x, y+1/2, -z+1/2	9.73	B3LYP/6-31G(d,p)	-4.4	-0.6	-20.7	21.2	-10.1
	1	-x, -y, -z	9.10	B3LYP/6-31G(d,p)	-3.8	-1.4	-19.3	11.4	-14.8

Fig. S33. Interaction energies of **11**.

	N	Symop	R	Electron Density	E_ele	E_pol	E_dis	E_rep	E_tot
	1	-x, -y, -z	17.39	B3LYP/6-31G(d,p)	-18.3	-4.1	-19.4	0.0	-39.2
	2	x, y, z	16.11	B3LYP/6-31G(d,p)	-10.6	-1.2	-10.9	0.0	-21.7
	2	x, y, z	6.79	B3LYP/6-31G(d,p)	-8.4	-2.7	-59.2	42.1	-36.5
	1	-x, -y, -z	14.41	B3LYP/6-31G(d,p)	10.4	-3.1	-37.7	0.0	-24.1
	1	-x, -y, -z	5.68	B3LYP/6-31G(d,p)	-13.0	-1.6	-37.5	35.5	-25.7
	1	-x, -y, -z	13.11	B3LYP/6-31G(d,p)	-31.4	-6.9	-19.9	0.0	-55.6
	1	-x, -y, -z	5.96	B3LYP/6-31G(d,p)	-9.5	-1.5	-44.7	28.3	-32.6
	1	-x, -y, -z	8.39	B3LYP/6-31G(d,p)	-4.3	-0.8	-27.7	16.8	-19.0

Fig. S34. Interaction energies of **13**.

	N	Symop	R	Electron Density	E_ele	E_pol	E_dis	E_rep	E_tot
	1	-x, -y, -z	17.79	B3LYP/6-31G(d,p)	-24.2	-3.7	-9.7	0.0	-36.8
	2	x, y, z	10.56	B3LYP/6-31G(d,p)	0.6	-0.9	-18.5	12.9	-8.2
	2	x, -y+1/2, z+1/2	13.78	B3LYP/6-31G(d,p)	-14.2	-3.0	-11.2	0.0	-27.0
	2	-x, y+1/2, -z+1/2	7.67	B3LYP/6-31G(d,p)	-6.3	-3.6	-55.4	32.7	-37.3
	2	x, -y+1/2, z+1/2	9.87	B3LYP/6-31G(d,p)	-9.4	-2.0	-4.5	3.5	-13.3
	1	-x, -y, -z	14.31	B3LYP/6-31G(d,p)	1.5	-1.0	-1.9	0.0	-0.8
	1	-x, -y, -z	9.65	B3LYP/6-31G(d,p)	-23.7	-7.0	-42.4	29.9	-48.7
	2	-x, y+1/2, -z+1/2	6.26	B3LYP/6-31G(d,p)	-13.0	-2.0	-34.1	39.4	-20.6
	2	x, -y+1/2, z+1/2	12.61	B3LYP/6-31G(d,p)	4.1	-0.7	-12.2	0.0	-6.8
	1	-x, -y, -z	8.31	B3LYP/6-31G(d,p)	-8.2	-1.3	-20.3	23.4	-12.8

Fig. S35. Interaction energies of **16**.

	N	Symop	R	Electron Density	E_ele	E_pol	E_dis	E_rep	E_tot
	2	-x+1/2, -y, z+1/2	14.93	B3LYP/6-31G(d,p)	-13.0	-2.8	-6.6	0.0	-21.6
	2	x+1/2, -y+1/2, -z	15.63	B3LYP/6-31G(d,p)	-15.2	-3.1	-9.0	0.0	-26.1
	2	x, y, z	6.13	B3LYP/6-31G(d,p)	7.2	-7.0	-54.0	33.6	-23.8
	2	-x+1/2, -y, z+1/2	11.89	B3LYP/6-31G(d,p)	-12.3	-4.4	-38.5	23.9	-35.0
	2	-x, y+1/2, -z+1/2	10.23	B3LYP/6-31G(d,p)	-8.7	-2.8	-8.2	7.1	-13.9
	2	x+1/2, -y+1/2, -z	14.79	B3LYP/6-31G(d,p)	-19.3	-3.5	-11.9	0.0	-33.4
	2	-x, y+1/2, -z+1/2	7.78	B3LYP/6-31G(d,p)	-26.0	-6.6	-64.6	60.3	-51.4
	2	-x, y+1/2, -z+1/2	9.57	B3LYP/6-31G(d,p)	-18.8	-4.4	-27.4	29.6	-28.7
	2	-x+1/2, -y, z+1/2	11.61	B3LYP/6-31G(d,p)	-3.7	-1.6	-9.8	5.6	-10.2