Supporting Information:

Synthesis, Crystal Structure, Hirshfeld Surface Analysis, Energy Framework calculations, and halogen Bonding Investigation of Benzene-1,3,5-triyltris((4-chlorophenyl)methanone)

Hawazen M. Hassanain *, Samah AlSharif, Huda A. AlGhamdi, Layla M. Nahari, Ahlam I. Al-Sulami, Sameera M. Mousally and Khadijah M. Al-Zaydi *

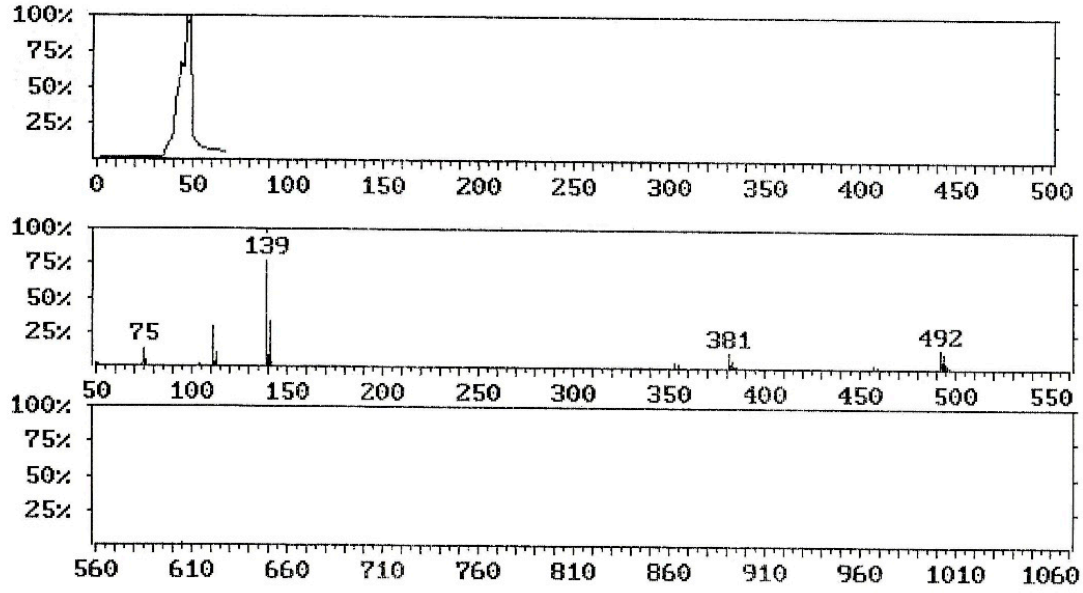

Figure S1 MS. of Benzene-1,3,5-triyltris((4-chlorophenyl)methanone).

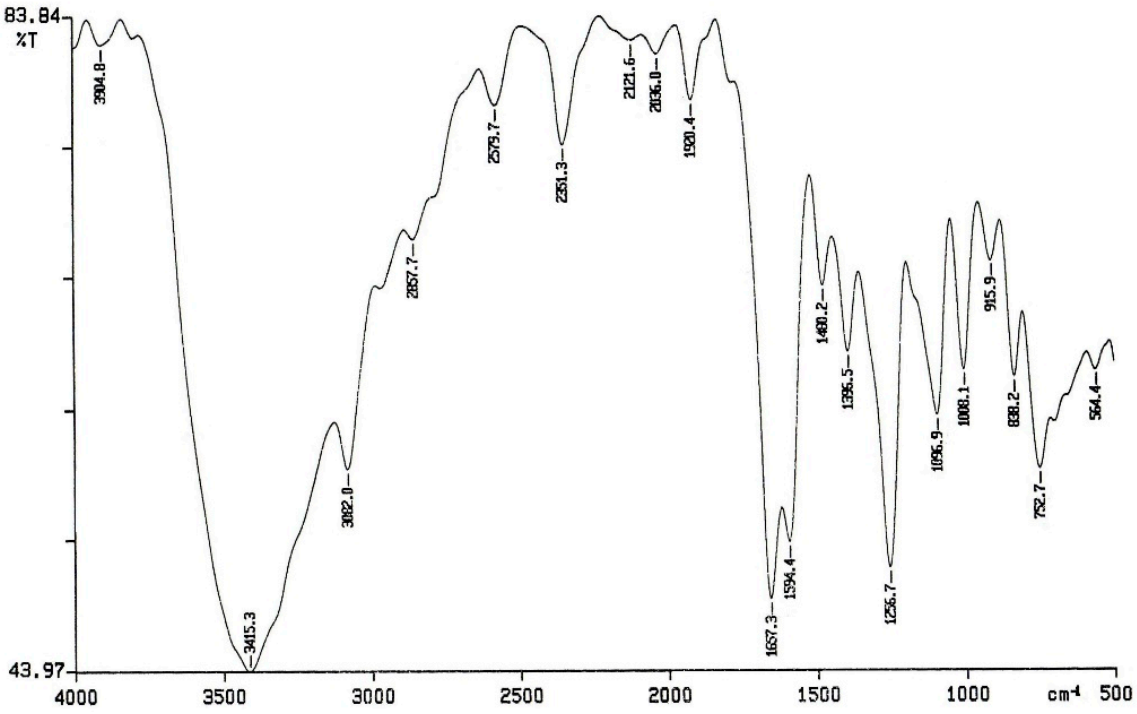

Figure S2 IR. of Benzene-1,3,5-triyltris((4-chlorophenyl)methanone).

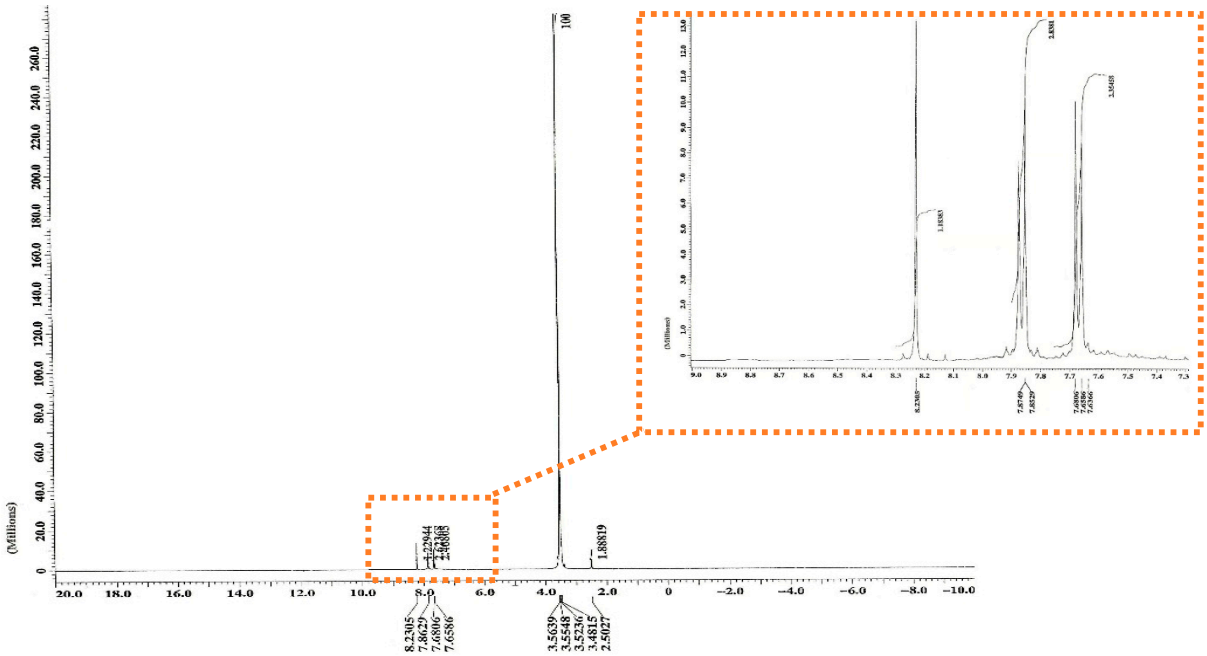

Figure S3 [1]H-NMR. of Benzene-1,3,5-triyltris((4-chlorophenyl)methanone).

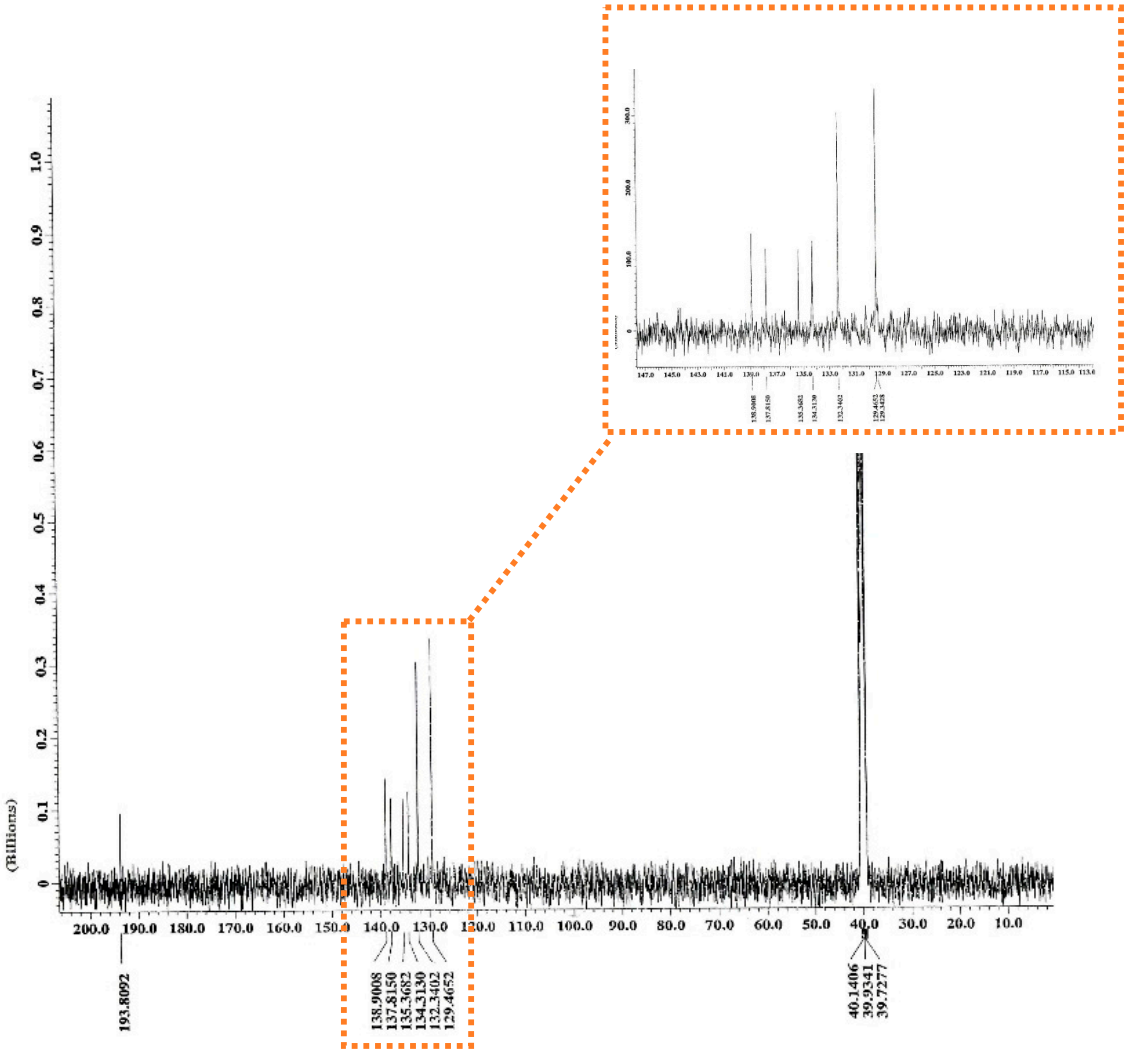

Figure S4 ^{13}C-NMR. of Benzene-1,3,5-triyltris((4-chlorophenyl)methanone).

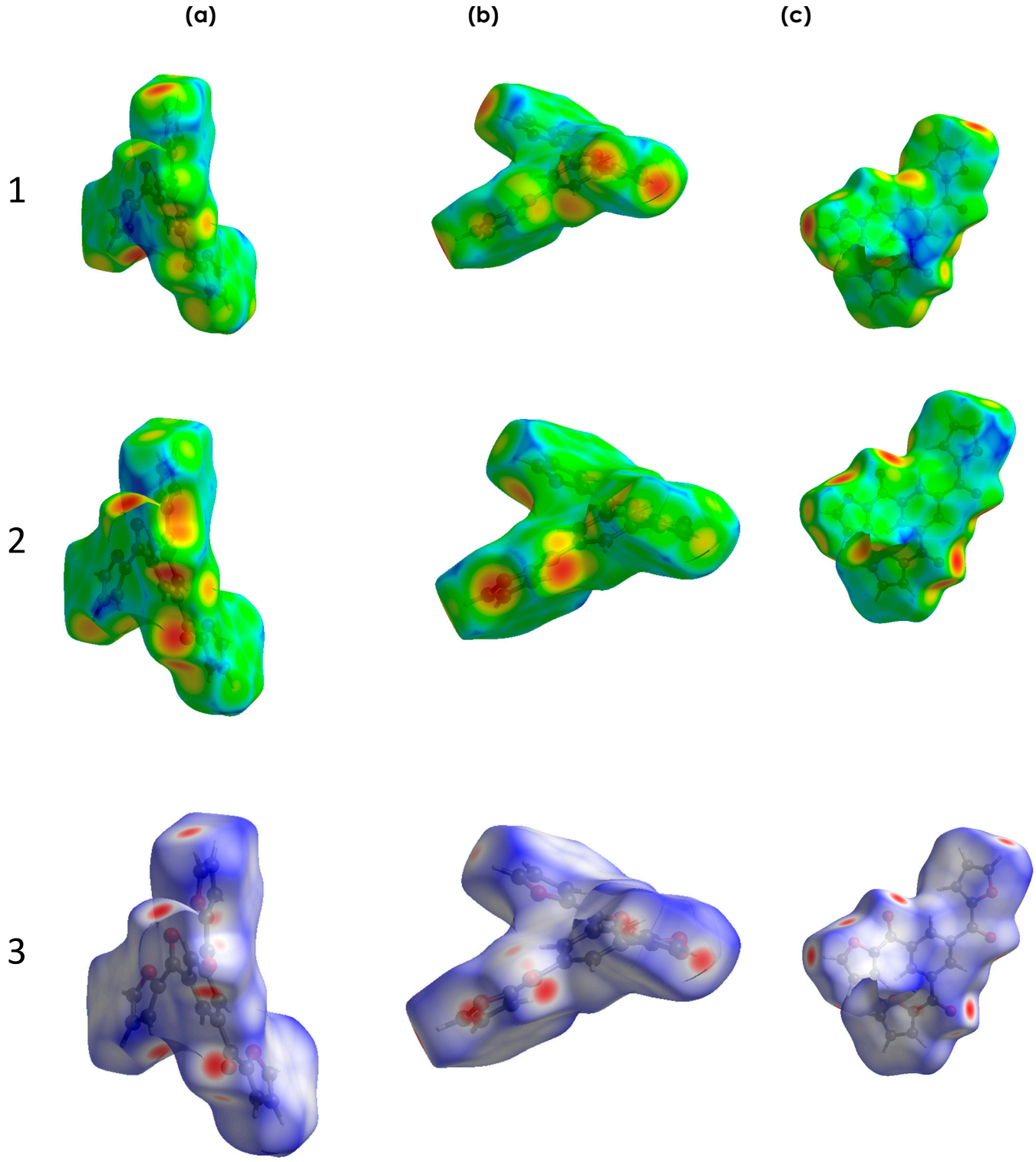
(a)
(b)
(c)
1
2
3

Figure S5 Hirshfeld surfaces mapped of compound **A** with (1) d_i, (2) d_e , and (3)d_{norm} red spots corresponding to close contact.

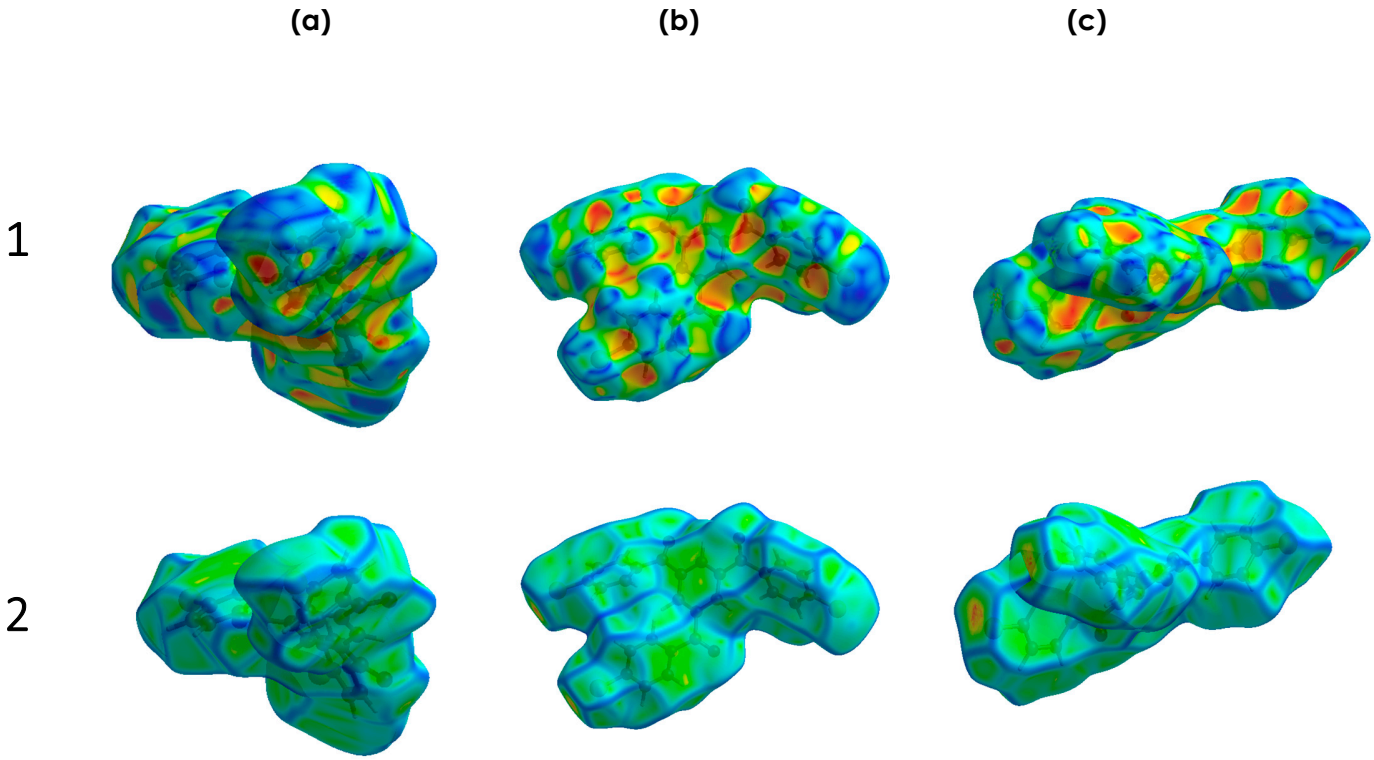

Figure S6 Hirshfeld surfaces of compound **A** mapped with (1)shape index surfaces for compounds **2P** along a, b, and c axis . Shape index surfaces (top, color code: hollow—red; bumps—blue). (2) Hirshfeld surfaces mapped with curvedness surfaces for compounds 2P along a, b, and c axis. Curvedness surfaces (bottom, color code: edges—blue; flat regions—green)

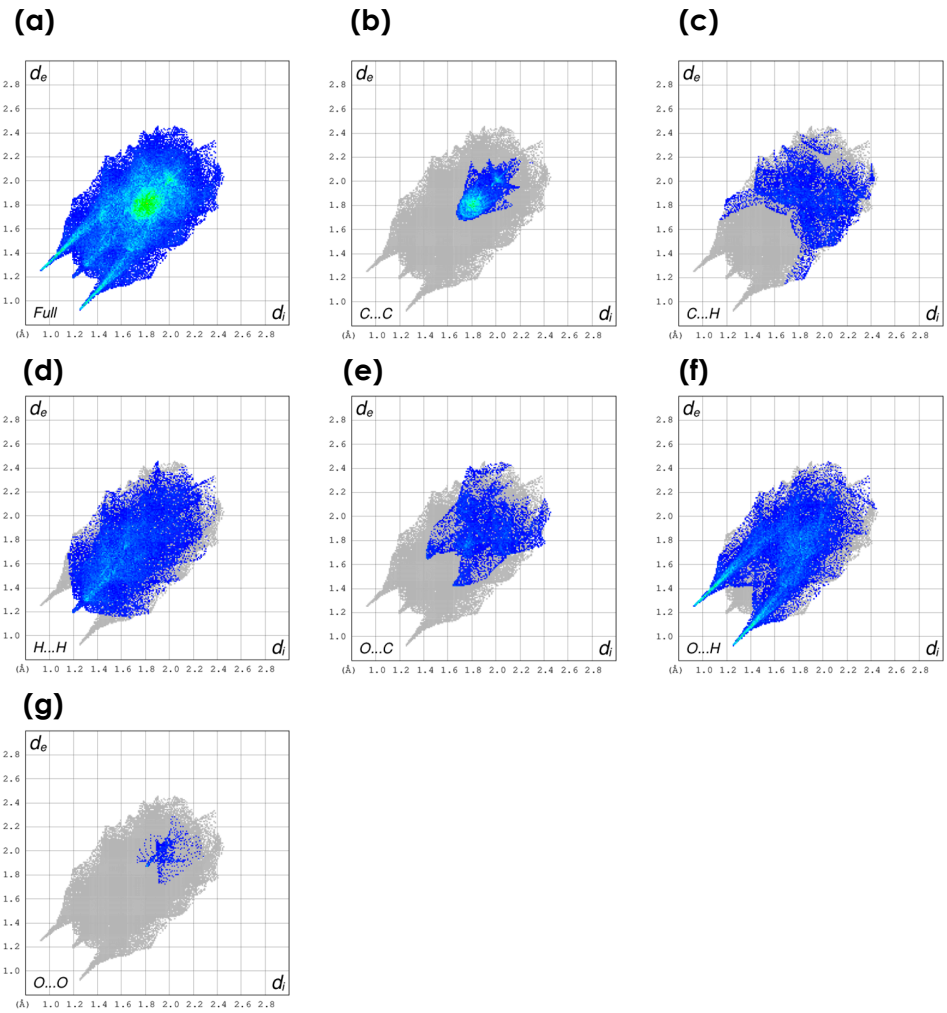

Figure S7 2D fingerprint plots of compound **A** highlighting (a)all interaction, (b) C···C, (c) C···H, (d) H···H, (e)O···C, (f) O···H, (g) O···O

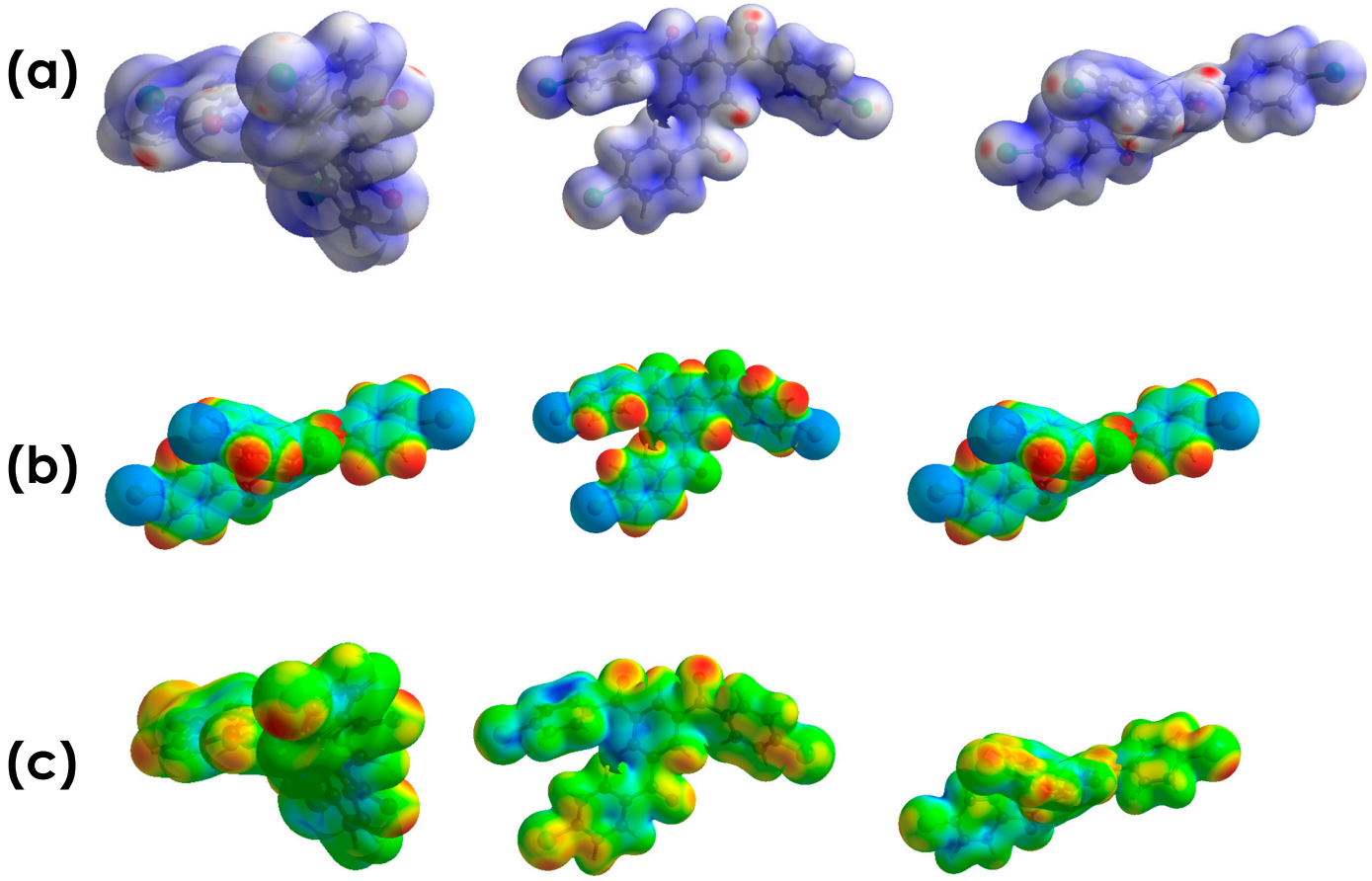

Figure S8 Electrostatic Potential (PE) mapped on Hirshfeld surface of the molecule of **A**: (a) dnorm, (b) de, (c) di.

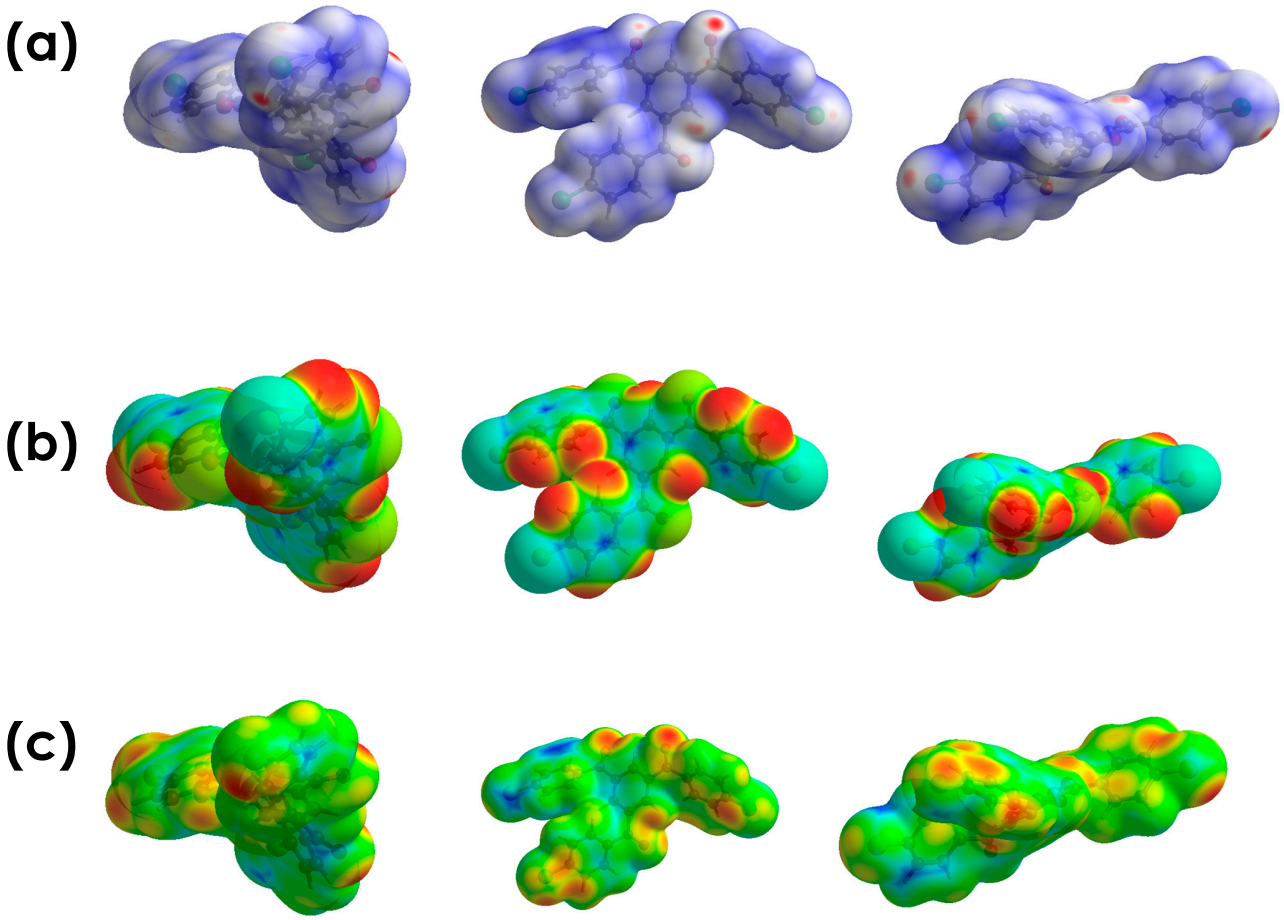

Figure S9 Promolecule Density mapped on Hirshfeld surface of the molecule of **A**: (a) dnorm, (b) de, (c) di.