crystals

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Role of Halogen Substituents on Halogen Bonding in 4,5-Di-Bromohexahydro-3a,6-Epoxyisoindol-1(4H) -ones

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Supplementary Materials

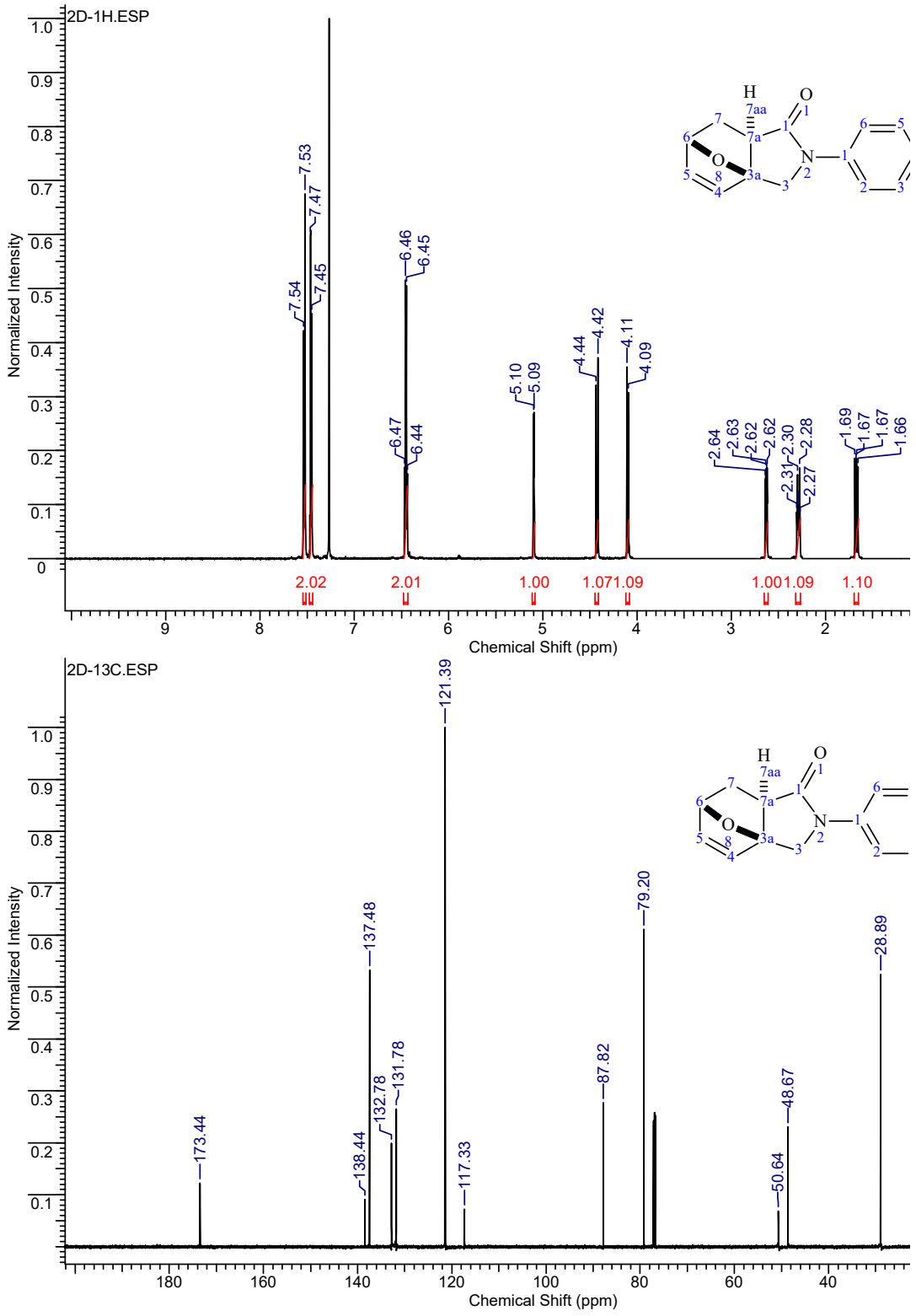

Figure S1. ^{1}H and ^{13}C NMR spectra (in $CDCl_3$) of **2d.**

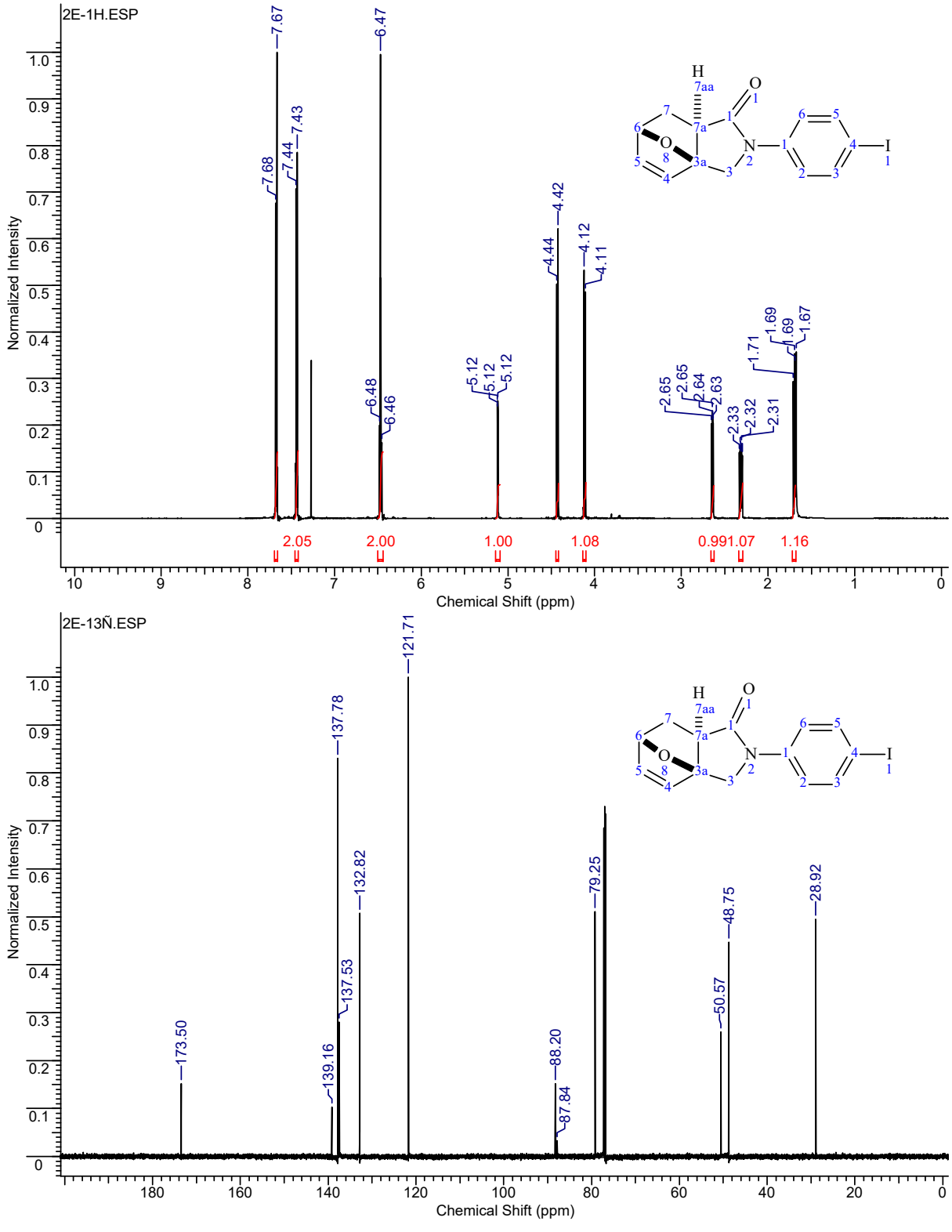

Figure S2. ^{1}H and ^{13}C NMR spectra (in $CDCl_3$) of **2e.**

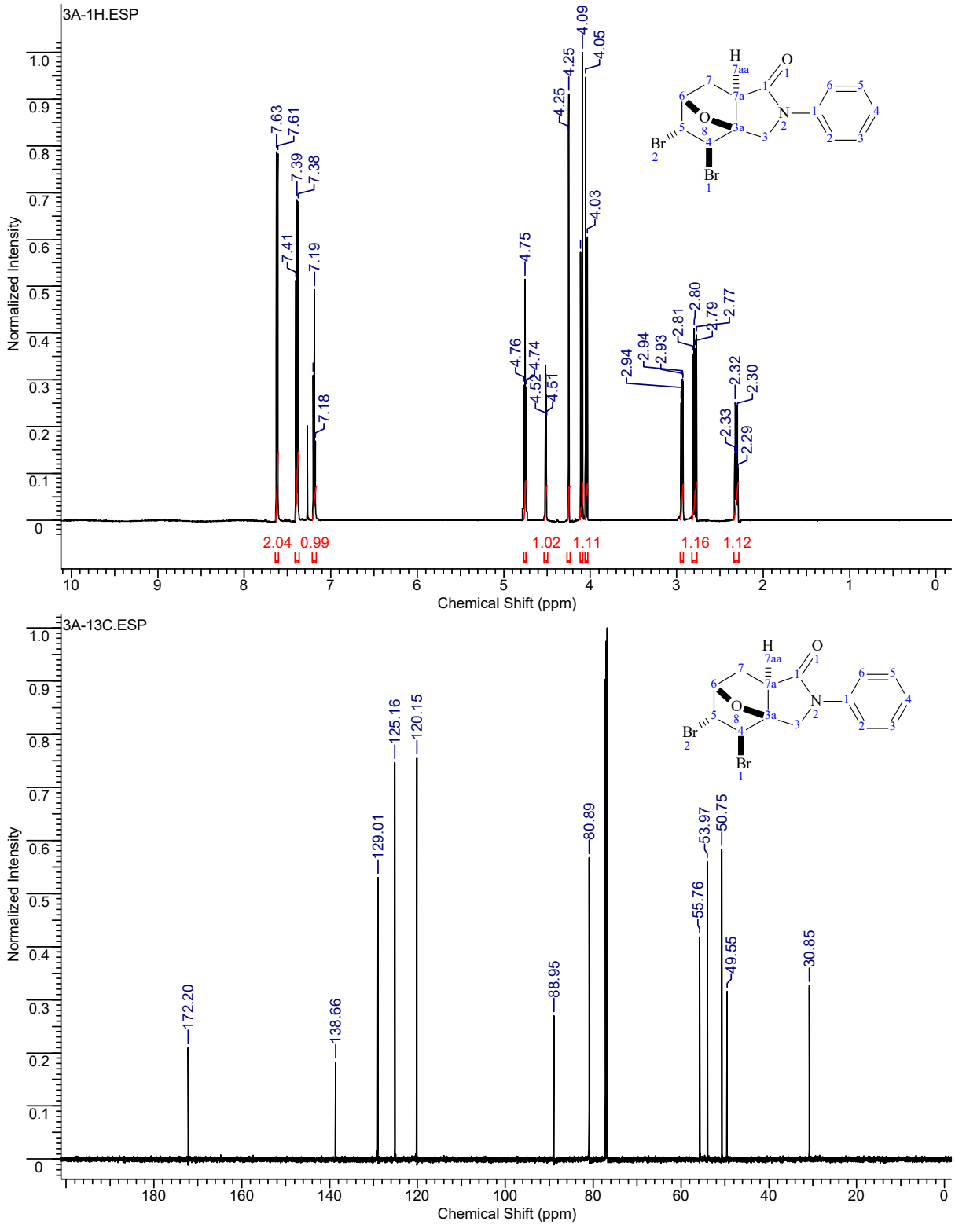

Figure S3. ^{1}H and ^{13}C NMR spectra (in $CDCl_3$) of **3a.**

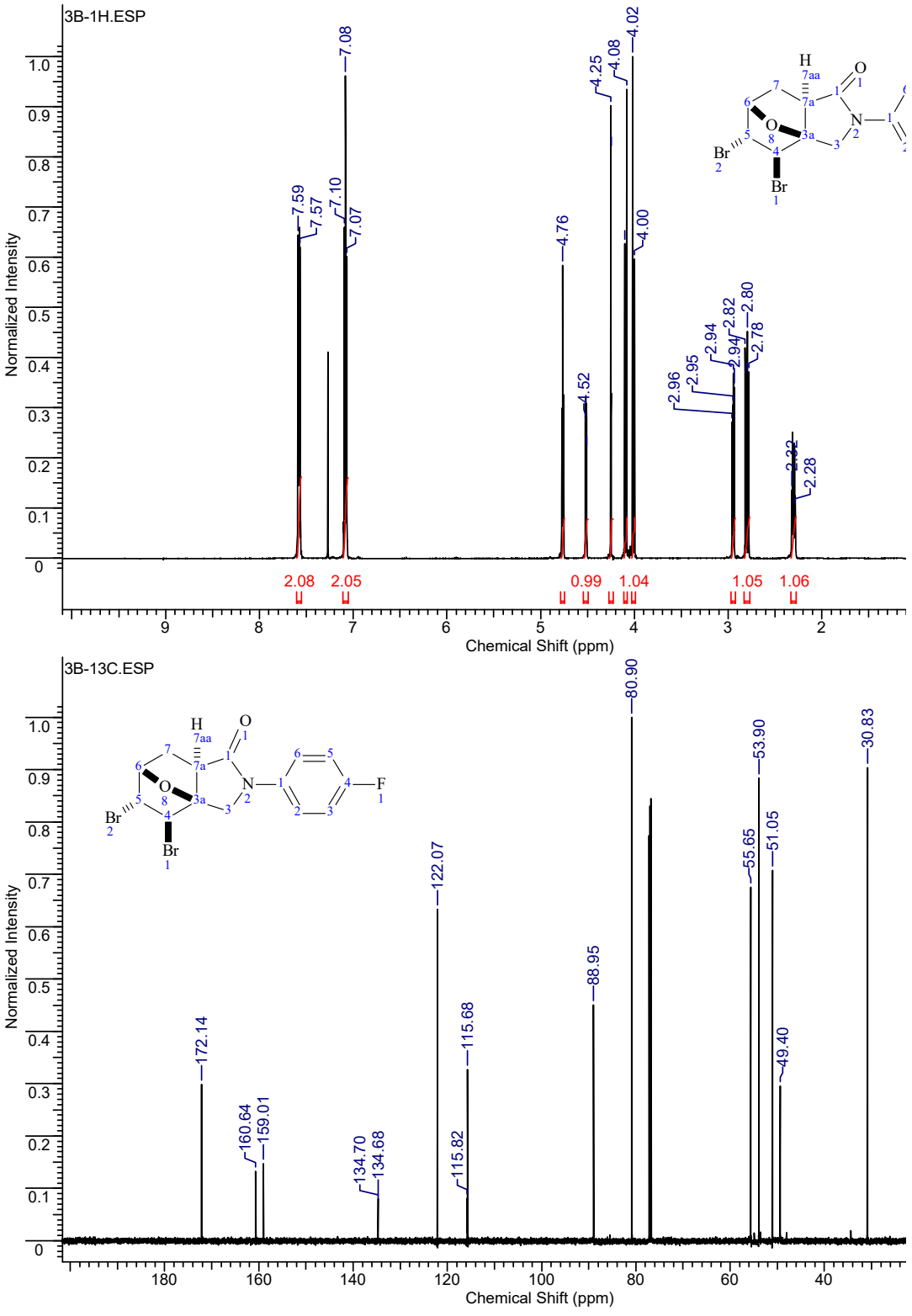

Figure S4. ^{1}H and ^{13}C NMR spectra (in $CDCl_3$) of **3b.**

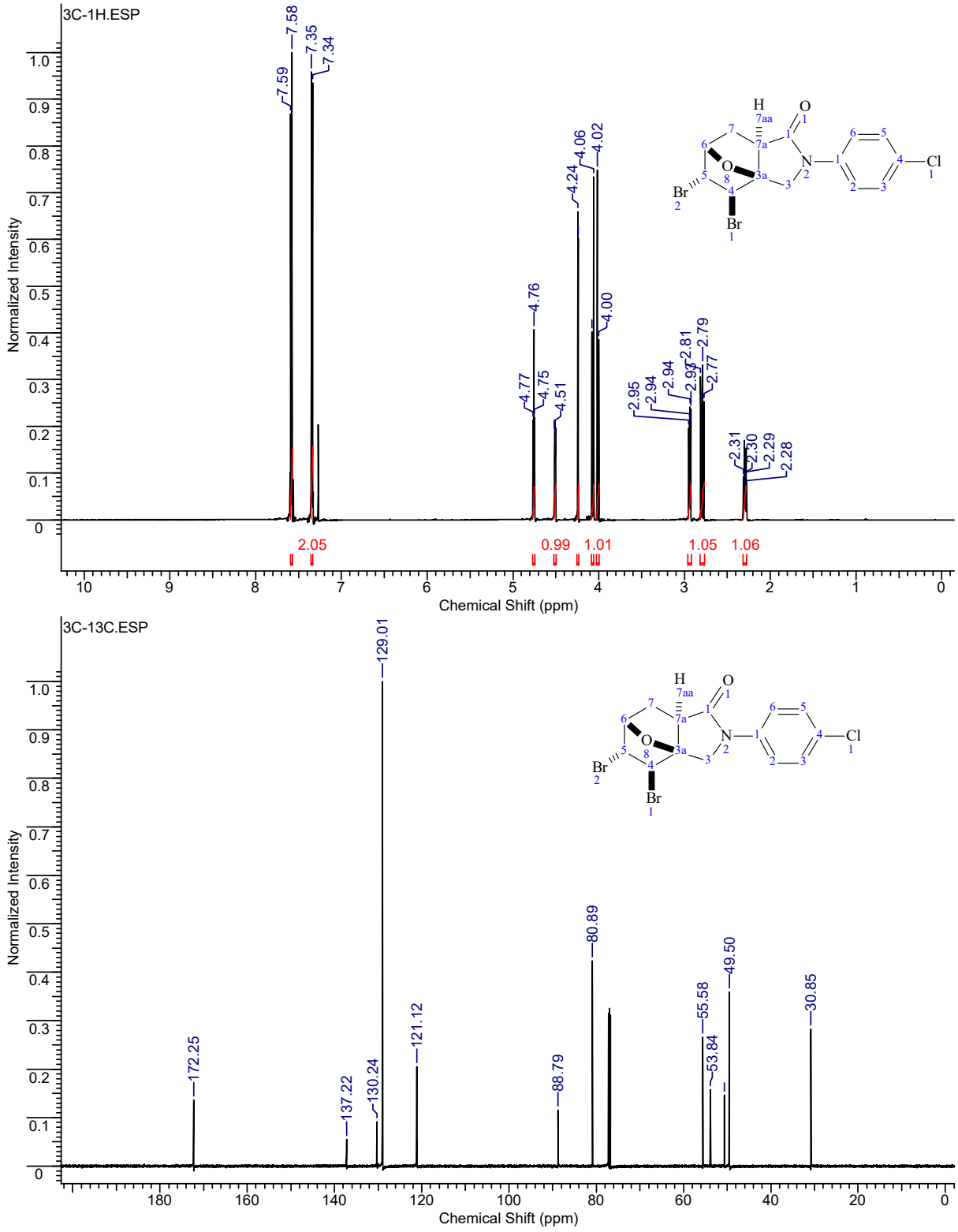

Figure S5. ^{1}H and ^{13}C NMR spectra (in $CDCl_3$) of **3c.**

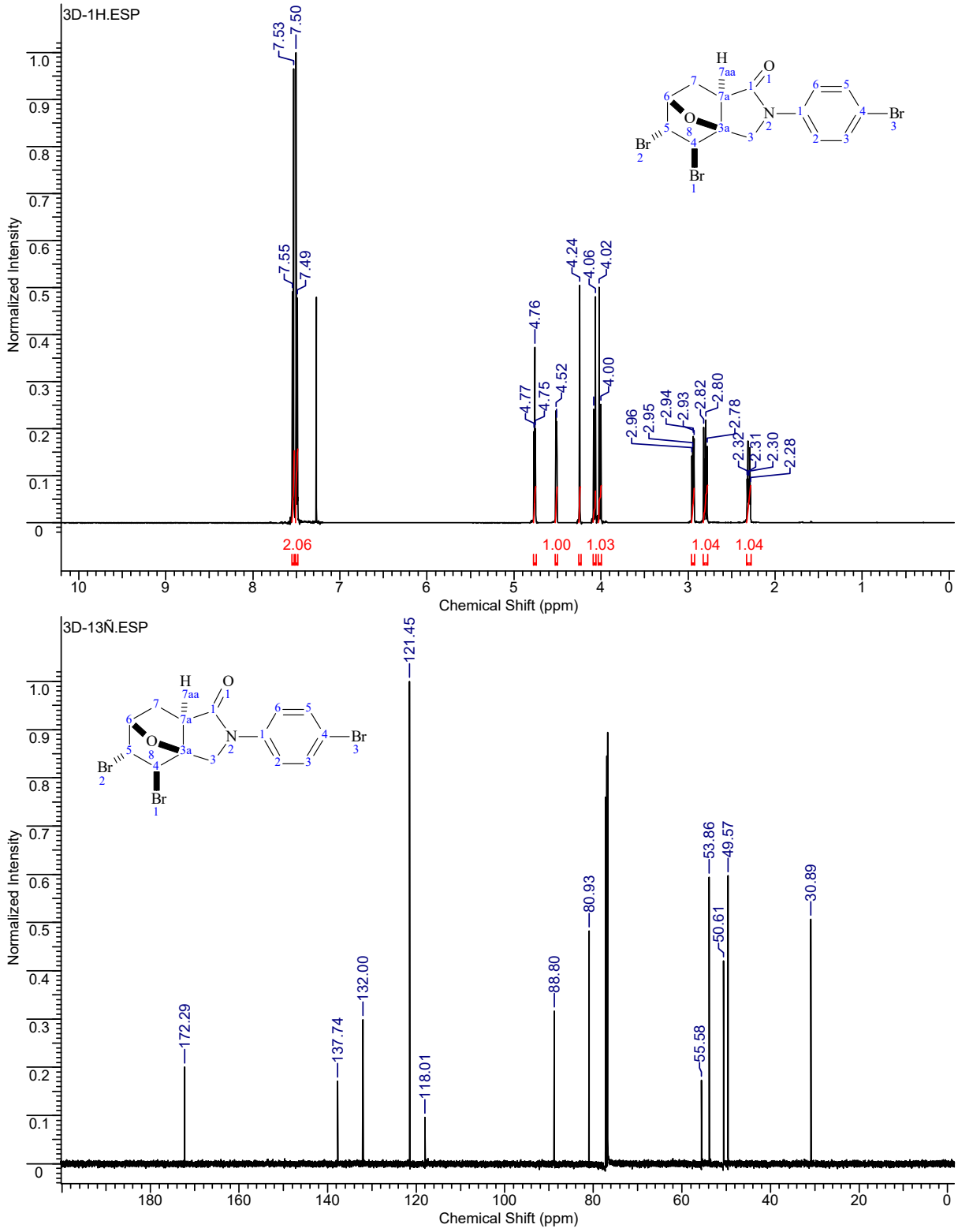

Figure S6. ^{1}H and ^{13}C NMR spectra (in $CDCl_3$) of **3d.**

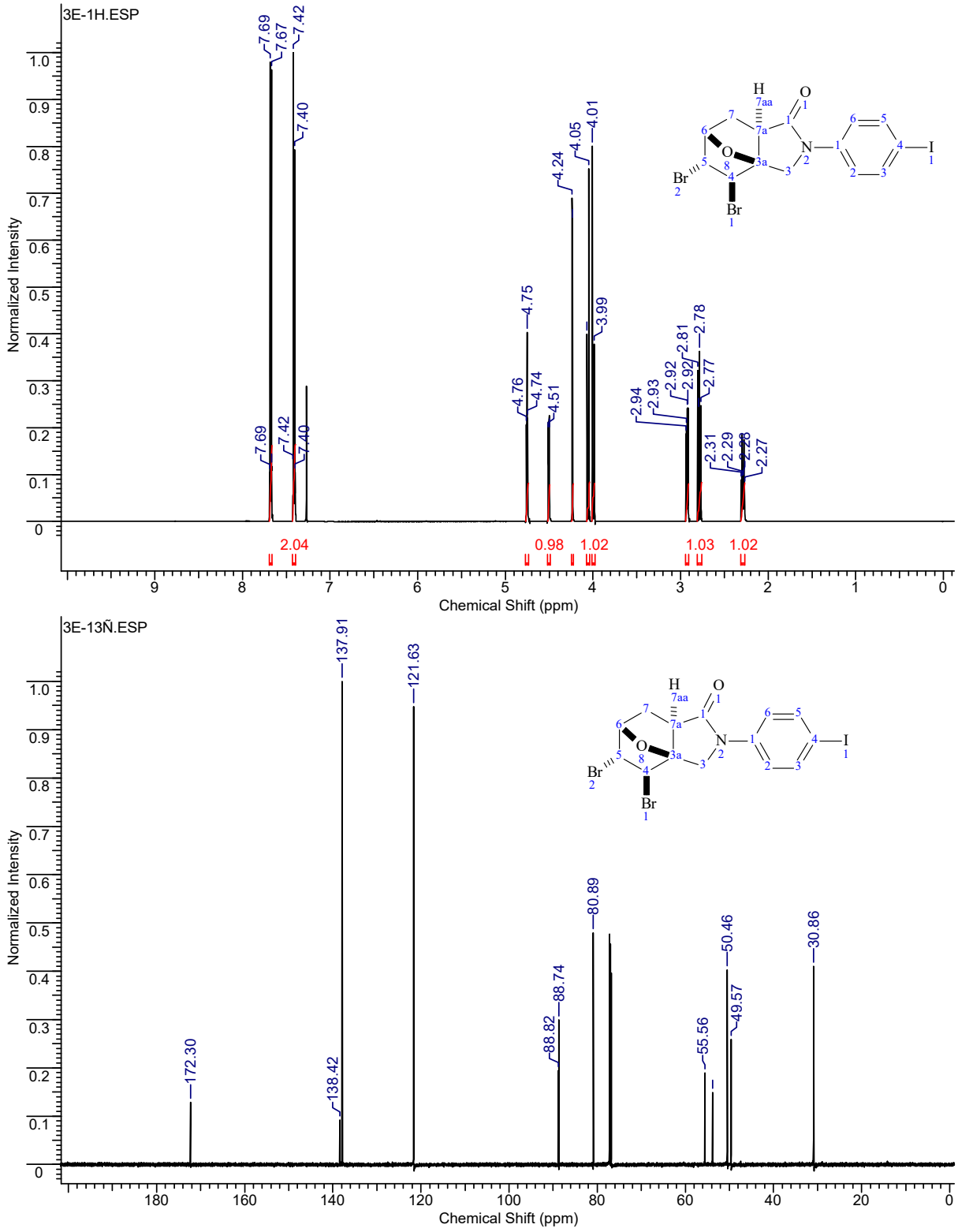

Figure S7. ^{1}H and ^{13}C NMR spectra (in $CDCl_3$) of **3e.**

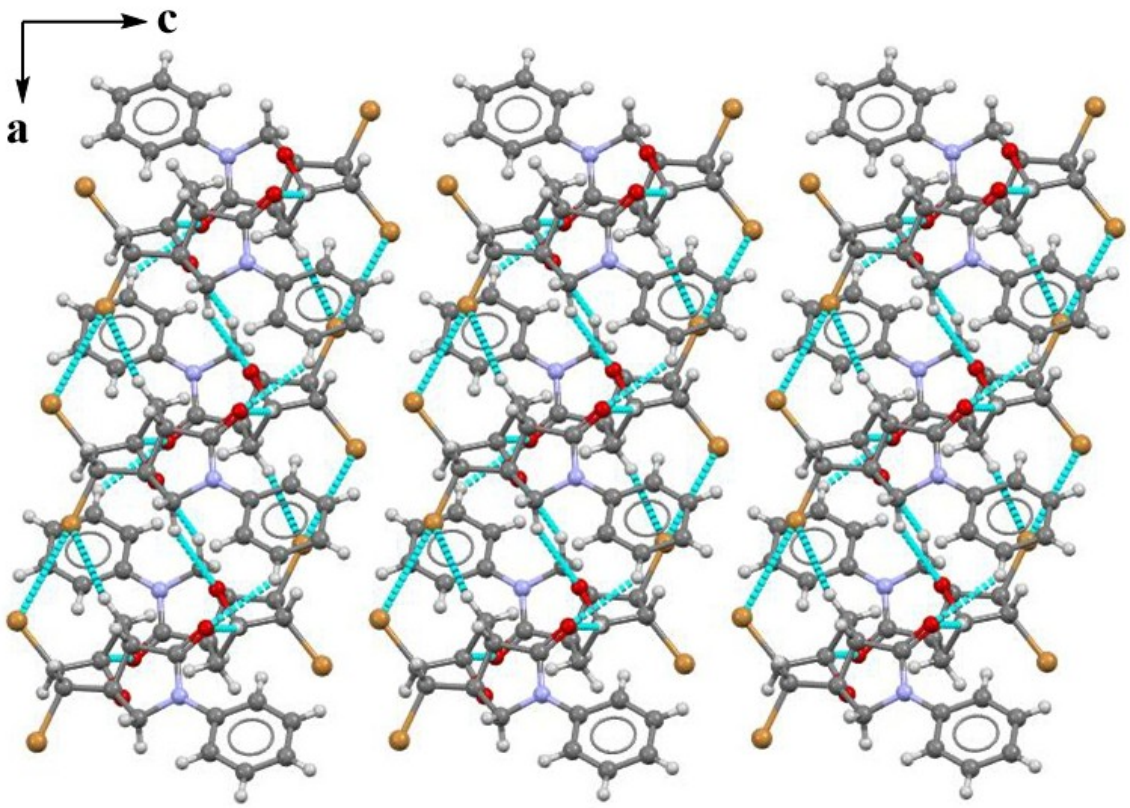

Figure S8. Packing diagram of **3a.** x,y,z; -x,-y,-z.

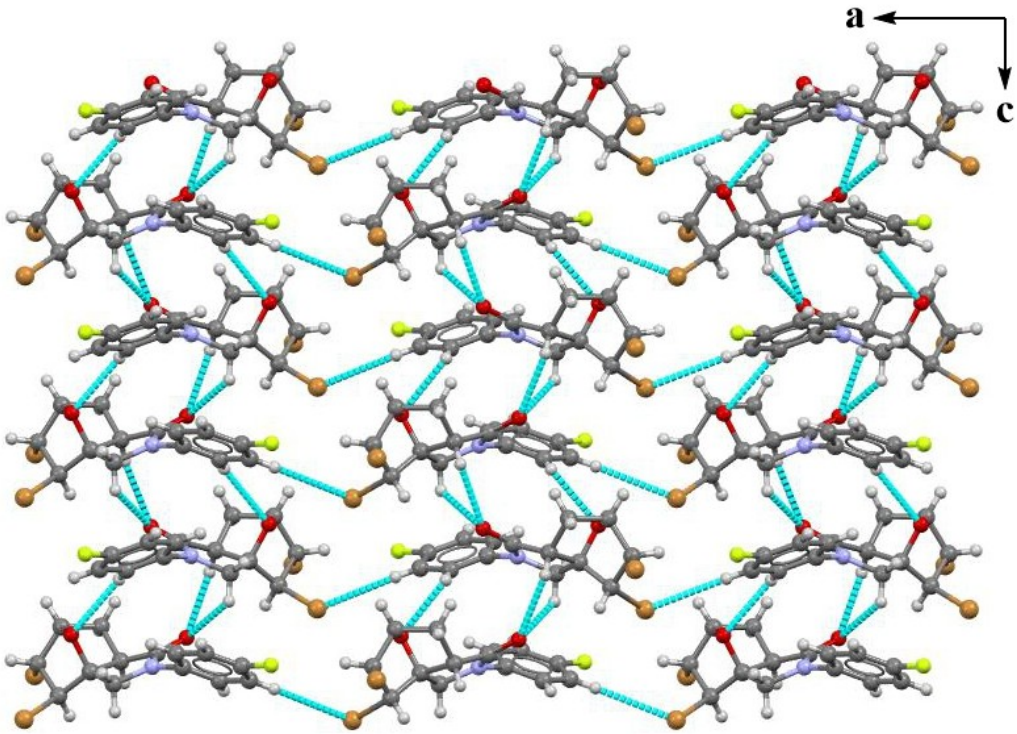

Figure S9. Packing diagram of **3b.** x,y,z; -x,-y,1/2+z; 1/2+x,-y,z; 1/2-x,y,1/2+z.

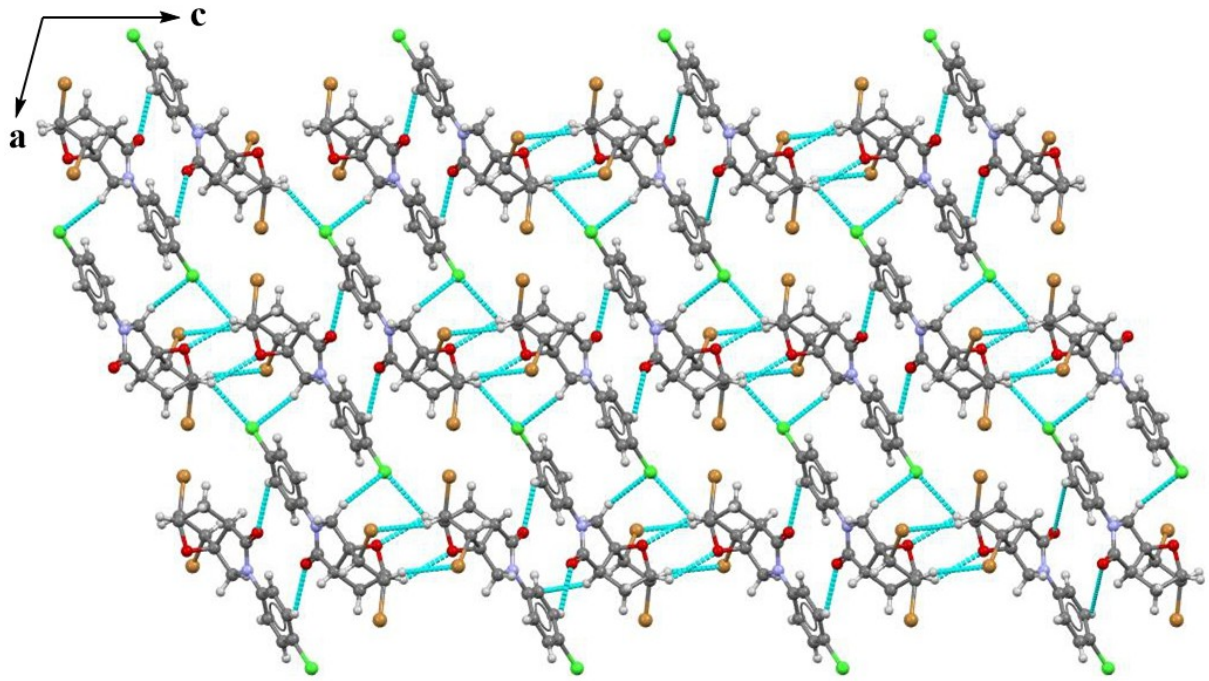

Figure S10. Packing diagram of **3c.** x, y, z; −x, y, 1/2 − z; 1/2 + x, 1/2 + y, z; 1/2 − x, 1/2 + y, 1/2 − z; −x, −y, −z; x, −y, 1/2 + z; 1/2 − x, 1/2 − y, −z; 1/2 + x, 1/2 − y, 1/2 + z.

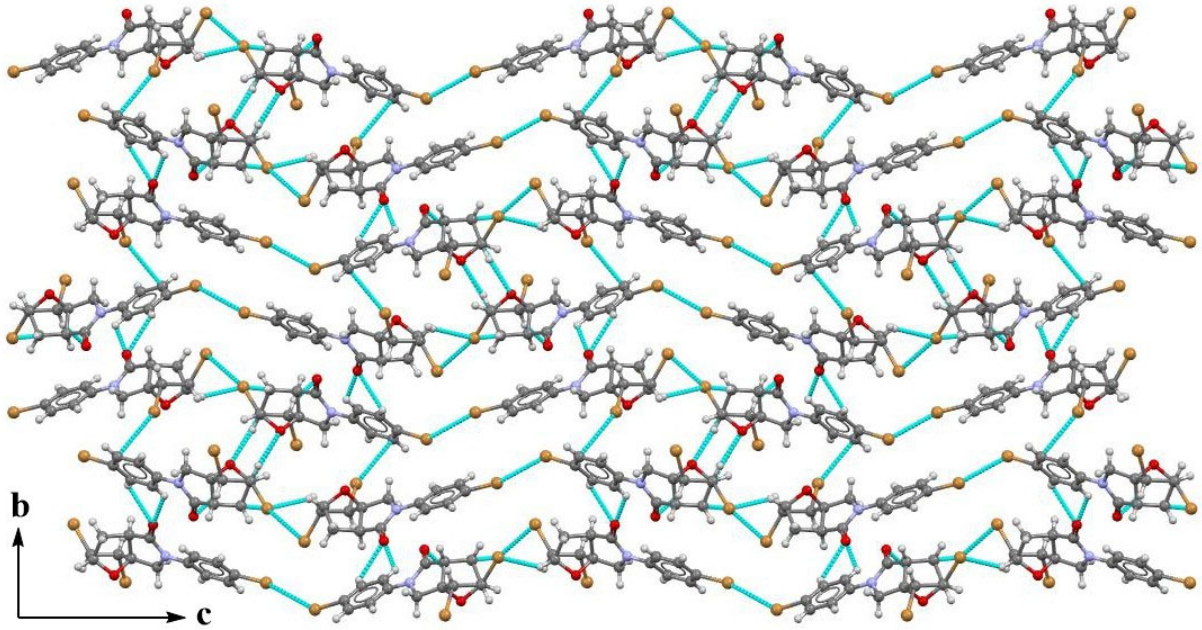

Figure S11. Packing diagram of **3d.** x, y, z; −x, 1/2 + y, 1/2 − z; −-x, −y, −z; x, 1/2 − y, 1/2 + z.

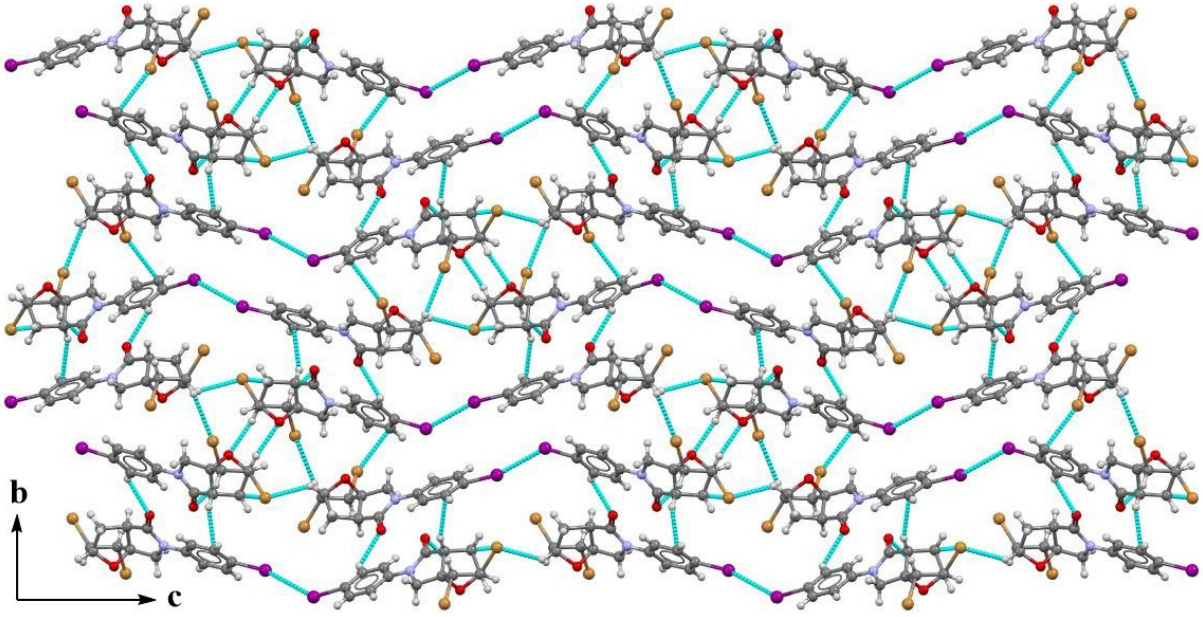

Figure S12. Packing diagram of **3e.** x, y, z; −x, 1/2 + y, 1/2 − z; −x, −y, −z; x, 1/2 − y, 1/2 + z.

Supplementary Materials: The following are available online at www.mdpi.com/xxx/s1: $^{1}H/^{13}C$ NMR spectra of 2d,e and 3a–e (Figures S1–S7), packing diagrams of 3a–e (Figures S8–S12).

Author Contributions: Conceptualization, F.I.Z. and A.V.G.; methodology, H.H.T.; investigation, D.F.M., M.A.N. and E.V.N.; resources, M.S.G.; data curation, V.P.Z.; writing-original draft preparation, F.I.Z., A.V.G. and K.T.M.; writing-review and editing, V.P.Z. and M.S.G.; visualization, H.H.T.; supervision, A.J.L.P. All authors have read and agreed to the published version of the manuscript.#

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