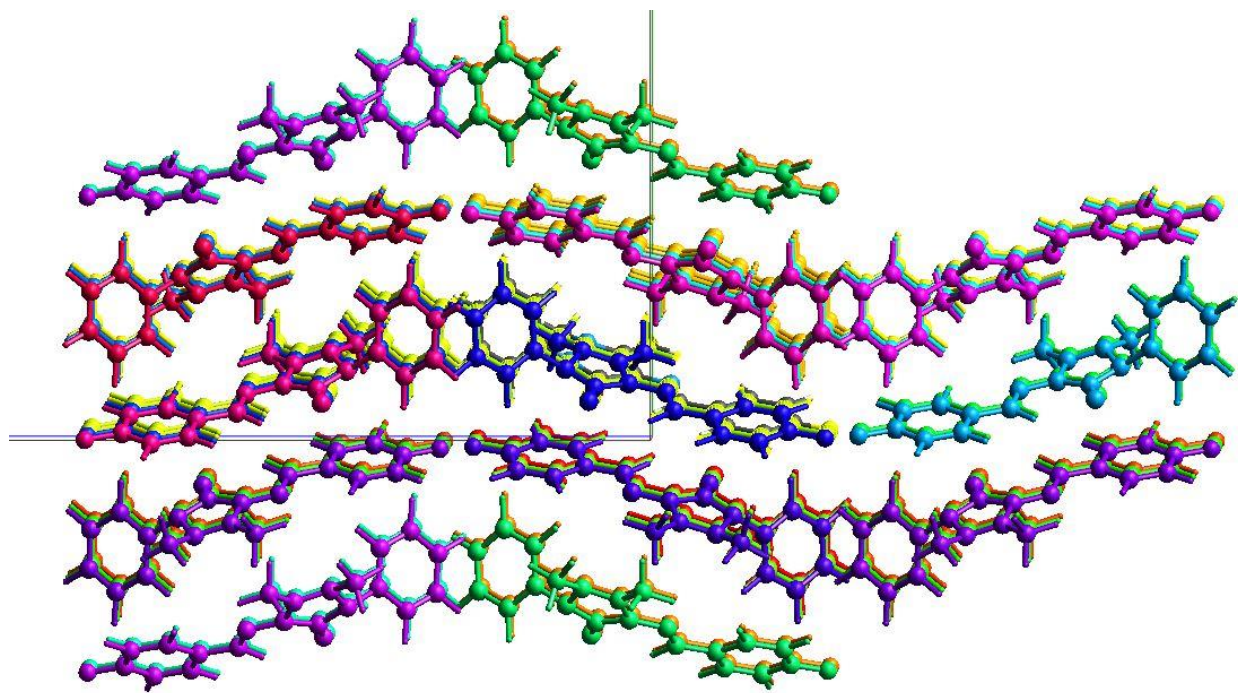


| | N | Symop | R | Electron Density | E_ele | E_pol | E_dis | E_rep | E_tot |
|--|---|-----------------------|-------|------------------|-------|-------|-------|-------|-------|
| | 2 | x+1/2, y+1/2, z | 9.28 | HF/3-21G | -8.2 | -6.4 | -34.6 | 18.4 | -28.8 |
| | 2 | -x+1/2, y+1/2, -z+1/2 | 15.85 | HF/3-21G | -8.3 | -1.5 | -18.9 | 0.0 | -26.5 |
| | 2 | x, y, z | 7.09 | HF/3-21G | -17.6 | -7.9 | -40.7 | 24.3 | -40.1 |
| | 2 | -x, y, -z+1/2 | 11.45 | HF/3-21G | -3.6 | -1.0 | -8.8 | 3.1 | -9.7 |
| | 2 | x+1/2, y+1/2, z | 13.67 | HF/3-21G | 1.1 | -0.1 | -0.6 | 0.0 | 0.5 |
| | 2 | -x+1/2, y+1/2, -z+1/2 | 18.75 | HF/3-21G | 0.4 | -0.0 | -0.3 | 0.0 | 0.1 |
| | 1 | -x, y, -z+1/2 | 8.99 | HF/3-21G | -7.2 | -3.3 | -65.5 | 38.0 | -37.6 |
| | 2 | x, y, z | 17.16 | HF/3-21G | -0.5 | -0.0 | -0.9 | 0.0 | -1.3 |
| | 2 | -x+1/2, y+1/2, -z+1/2 | 9.10 | HF/3-21G | 1.0 | -0.2 | -2.2 | 0.0 | -1.1 |
| | 1 | -x, -y, -z | 9.28 | HF/3-21G | 3.5 | -0.4 | -2.8 | 0.0 | 0.7 |
| | 2 | x+1/2, y+1/2, z | 9.28 | HF/3-21G | -12.0 | -5.0 | -49.4 | 21.4 | -42.6 |
| | 1 | -x, -y, -z | 8.82 | HF/3-21G | 1.6 | -0.3 | -2.3 | 0.0 | -0.7 |
| | 1 | -x+1/2, -y+1/2, -z | 10.85 | HF/3-21G | -8.8 | -4.9 | -45.4 | 18.2 | -38.3 |
| | 2 | x+1/2, y+1/2, z | 13.67 | HF/3-21G | 0.6 | -0.1 | -1.3 | 0.0 | -0.6 |
| | 1 | -x, -y, -z | 18.17 | HF/3-21G | 19.3 | -0.6 | -22.9 | 0.0 | -1.4 |
| | 1 | -x+1/2, -y+1/2, -z | 13.28 | HF/3-21G | -3.1 | -0.8 | -16.2 | 0.0 | -18.3 |
| | 1 | -x, -y, -z | 20.95 | HF/3-21G | -0.1 | -0.0 | -0.5 | 0.0 | -0.6 |
| | 1 | -x, -y, -z | 17.94 | HF/3-21G | 1.6 | -0.2 | -6.7 | 0.0 | -4.6 |
| | 1 | -x+1/2, -y+1/2, -z | 12.64 | HF/3-21G | -0.1 | -0.1 | -1.7 | 0.0 | -1.8 |

Fig. S1 The colour-coded interaction mapping within a radius of 6 Å of a central reference molecule and the various contributions to the total energy (E_{tot}) for compound **I**.



| | N | Symp | R | Electron Density | E_ele | E_pol | E_dis | E_rep | E_tot |
|--|---|-------------------|-------|------------------|-------|-------|-------|-------|-------|
| | 1 | -x, -y, -z | 4.63 | HF/3-21G | -7.7 | -6.1 | -88.6 | 54.5 | -47.5 |
| | 1 | -x+1/2, -y, z+1/2 | 14.33 | HF/3-21G | -1.6 | -0.7 | -5.8 | 0.0 | -7.4 |
| | 1 | -x+1/2, y+1/2, z | 8.60 | HF/3-21G | -0.4 | -0.4 | -2.6 | 0.0 | -3.0 |
| | 1 | x+1/2, -y+1/2, -z | 5.36 | HF/3-21G | -9.4 | -5.2 | -54.5 | 31.0 | -36.9 |
| | 0 | x, -y+1/2, z+1/2 | 14.05 | HF/3-21G | -1.2 | -0.4 | -6.3 | 0.0 | -7.2 |
| | 1 | x+1/2, y, -z+1/2 | 12.74 | HF/3-21G | 15.0 | -1.9 | -20.4 | 0.0 | -4.4 |
| | 1 | x, y, z | 6.79 | HF/3-21G | -19.3 | -6.7 | -30.3 | 13.0 | -40.7 |
| | 0 | -x, -y, -z | 7.22 | HF/3-21G | -21.5 | -12.8 | -29.2 | 17.9 | -42.1 |
| | 0 | -x+1/2, -y, z+1/2 | 16.80 | HF/3-21G | 0.8 | -0.0 | -0.3 | 0.0 | 0.5 |
| | 1 | x+1/2, y, -z+1/2 | 15.06 | HF/3-21G | -3.3 | -1.1 | -5.6 | 0.0 | -9.1 |
| | 0 | -x+1/2, y+1/2, z | 12.28 | HF/3-21G | -0.1 | -0.0 | -0.3 | 0.0 | -0.4 |
| | 0 | -x, y+1/2, -z+1/2 | 15.86 | HF/3-21G | -0.7 | -0.0 | -0.3 | 0.0 | -1.0 |
| | 1 | x+1/2, -y+1/2, -z | 11.00 | HF/3-21G | -2.7 | -0.2 | -1.0 | 0.0 | -3.8 |
| | 0 | x, -y+1/2, z+1/2 | 15.61 | HF/3-21G | -0.9 | -0.1 | -0.6 | 0.0 | -1.5 |
| | 1 | x+1/2, y, -z+1/2 | 17.86 | HF/3-21G | -0.2 | -0.0 | -0.1 | 0.0 | -0.3 |
| | 1 | x, -y+1/2, z+1/2 | 15.61 | HF/3-21G | 1.0 | -0.0 | -0.4 | 0.0 | 0.6 |
| | 1 | x+1/2, y, -z+1/2 | 15.95 | HF/3-21G | 0.8 | -0.1 | -0.3 | 0.0 | 0.5 |
| | 1 | x, y, z | 13.58 | HF/3-21G | -1.4 | -0.1 | -0.2 | 0.0 | -1.7 |
| | 0 | -x, -y, -z | 13.23 | HF/3-21G | -0.3 | -0.0 | -0.3 | 0.0 | -0.5 |
| | 0 | -x+1/2, -y, z+1/2 | 21.24 | HF/3-21G | 0.2 | -0.0 | -0.0 | 0.0 | 0.2 |
| | 0 | -x, y+1/2, -z+1/2 | 19.35 | HF/3-21G | -0.3 | -0.0 | -0.0 | 0.0 | -0.3 |
| | 0 | x, -y+1/2, z+1/2 | 19.54 | HF/3-21G | -0.7 | -0.0 | -0.1 | 0.0 | -0.8 |
| | 0 | x+1/2, -y+1/2, -z | 17.47 | HF/3-21G | -0.8 | -0.0 | -0.0 | 0.0 | -0.9 |
| | 1 | x+1/2, y, -z+1/2 | 20.95 | HF/3-21G | -0.0 | -0.0 | -0.0 | 0.0 | -0.1 |
| | 1 | x, -y+1/2, z+1/2 | 19.54 | HF/3-21G | 0.4 | -0.0 | -0.0 | 0.0 | 0.4 |

Fig. S2 The colour-coded interaction mapping within a radius of 6 Å of a central reference molecule and the various contributions to the total energy (E_{tot}) for compound **II**.

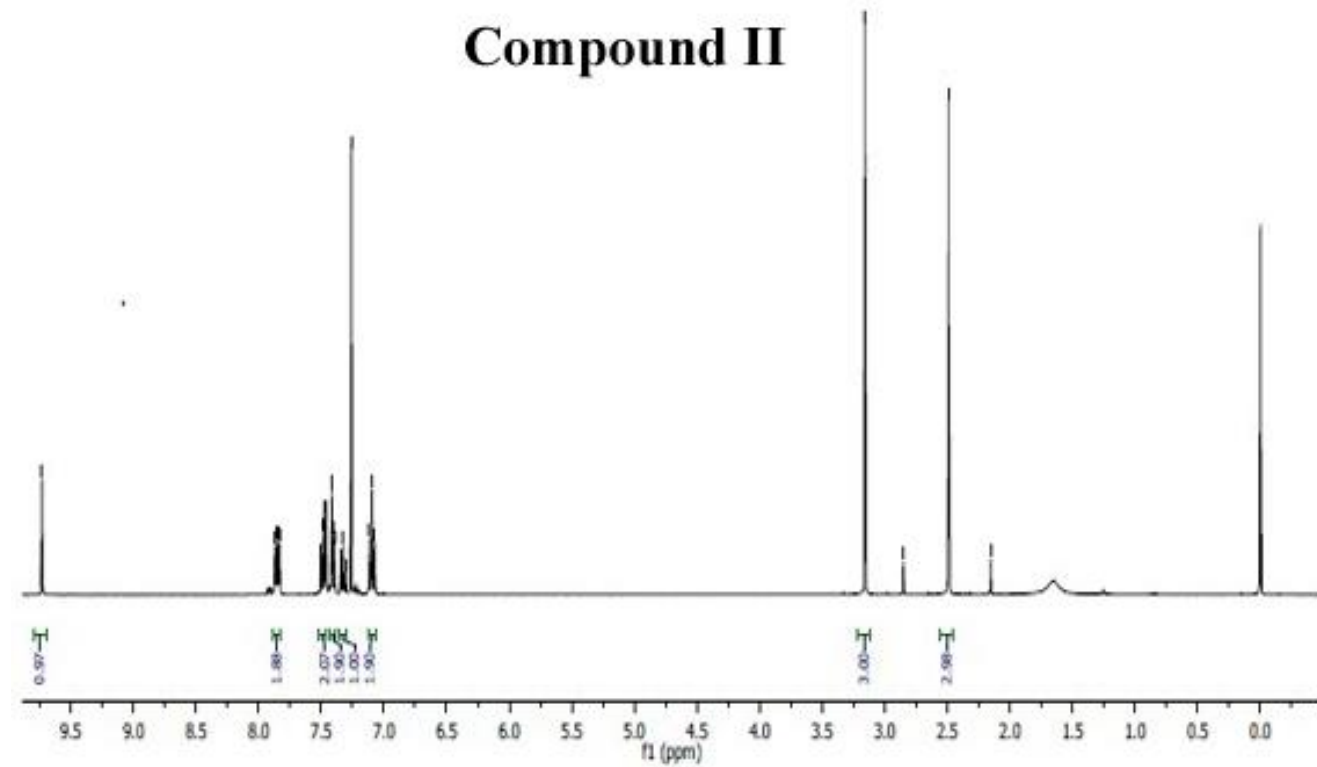
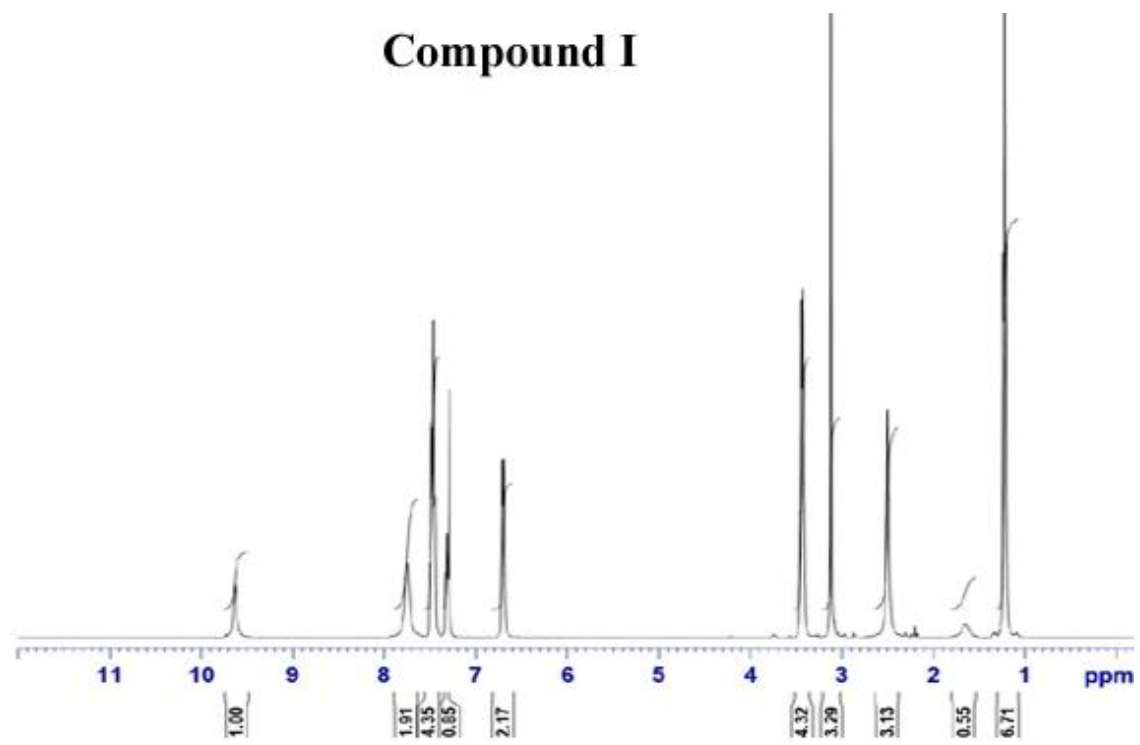


Fig. S3 ^1H NMR Spectra

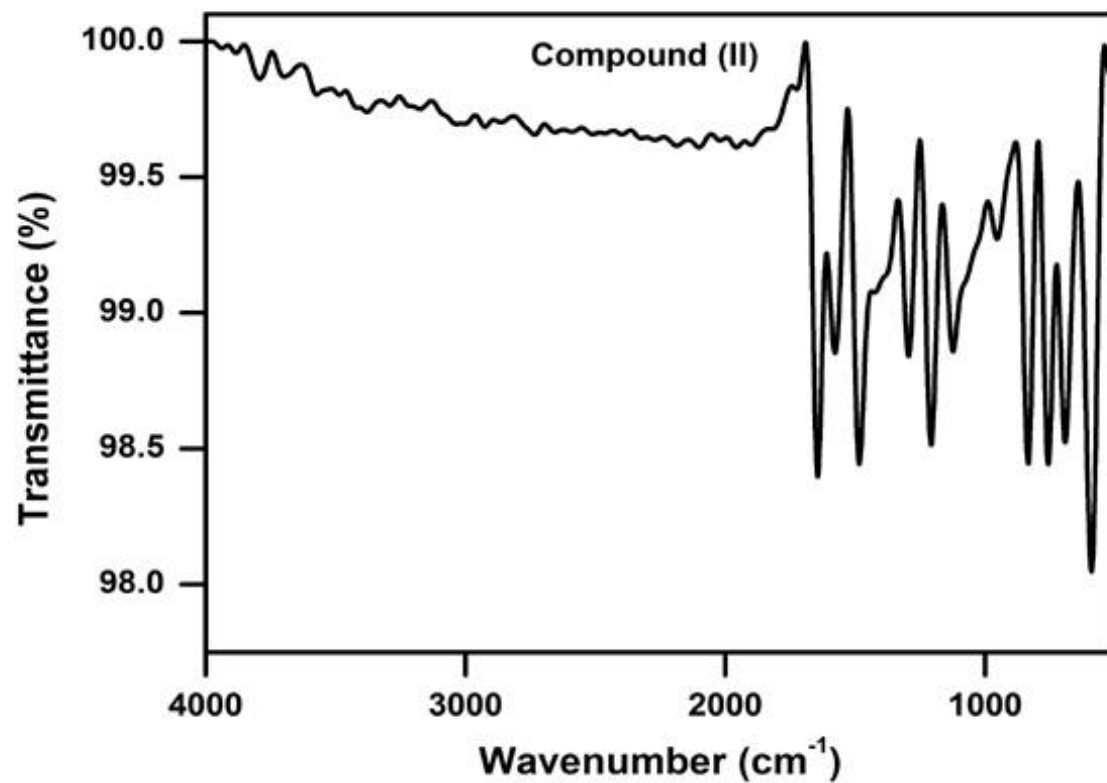
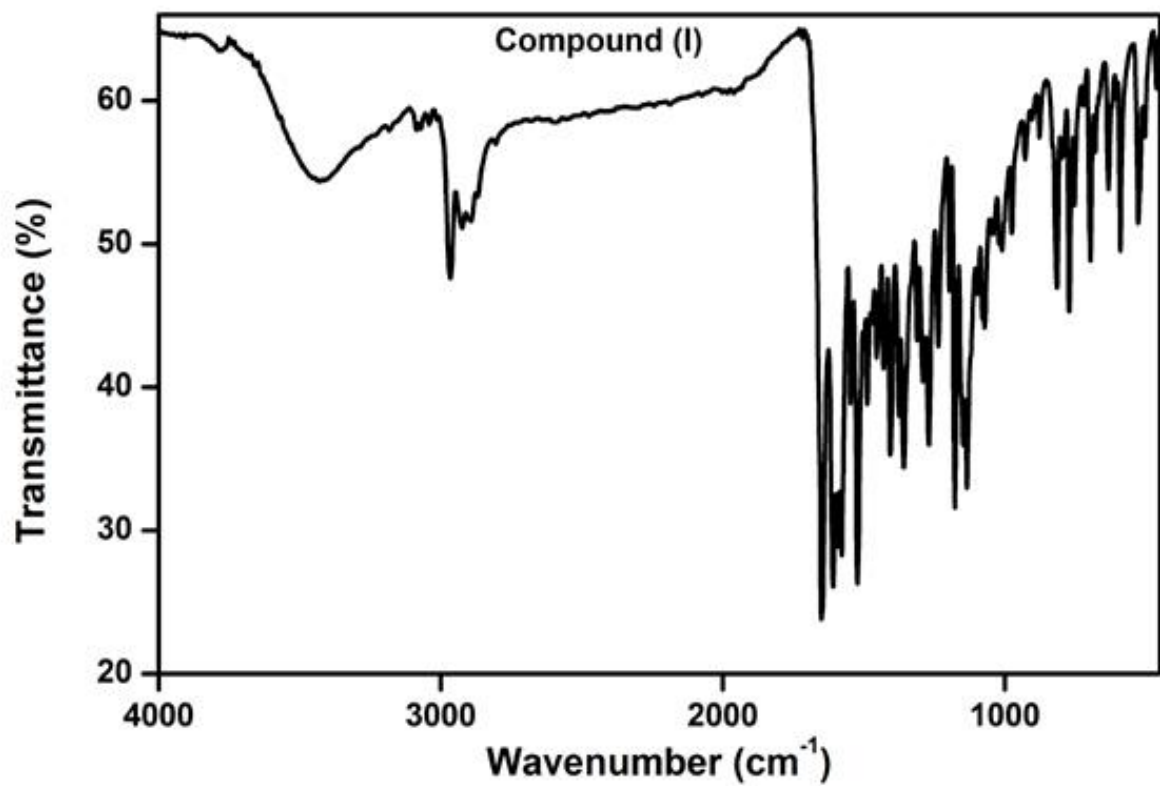


Fig. S4 FT-IR Spectra