## Supporting information for 4-(tris(4-methyl-1*H*-pyrazol-yl)methyl)aniline

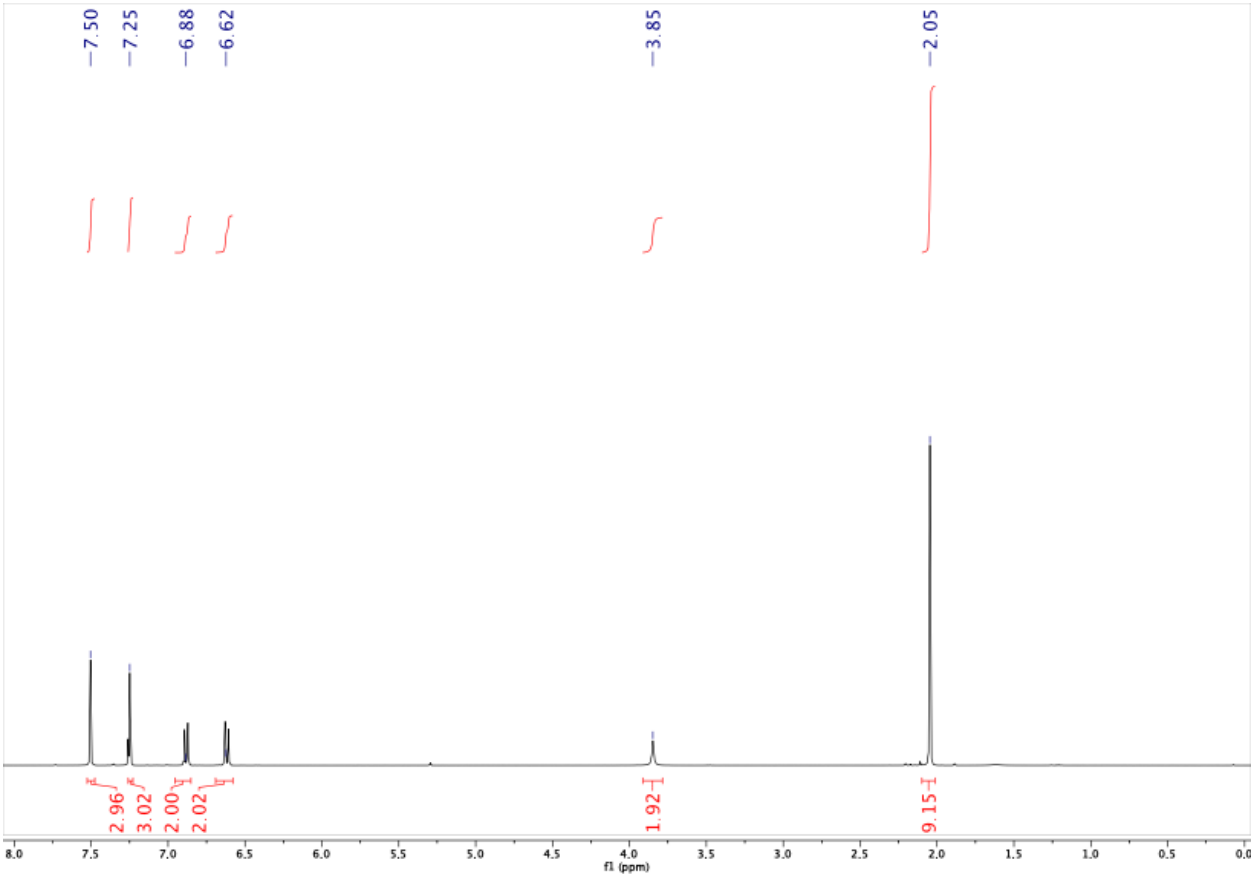



**Figure S1.** $^{1}$H-NMR of title compound in $CDCl_3$

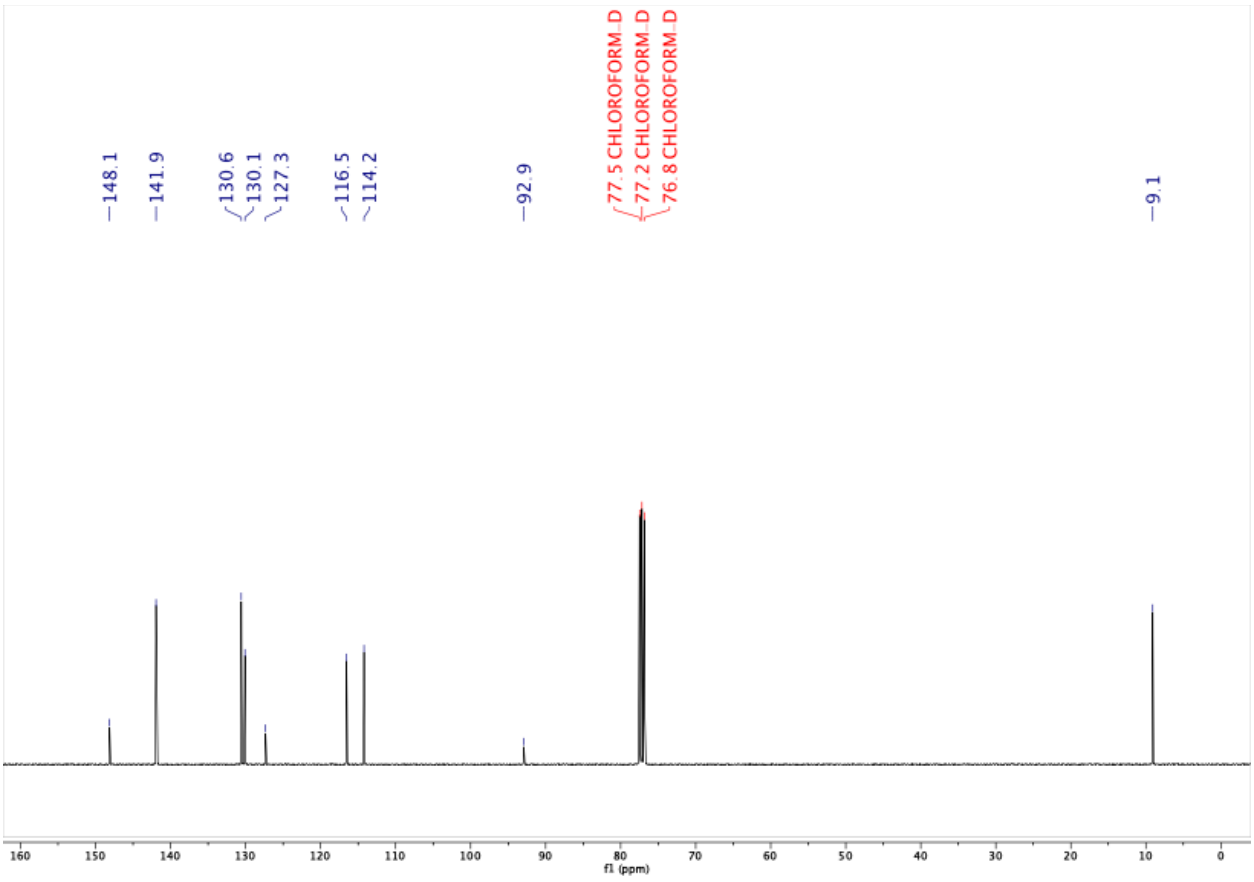



**Figure S2.** $^{13}$C-NMR of title compound in $CDCl_3$

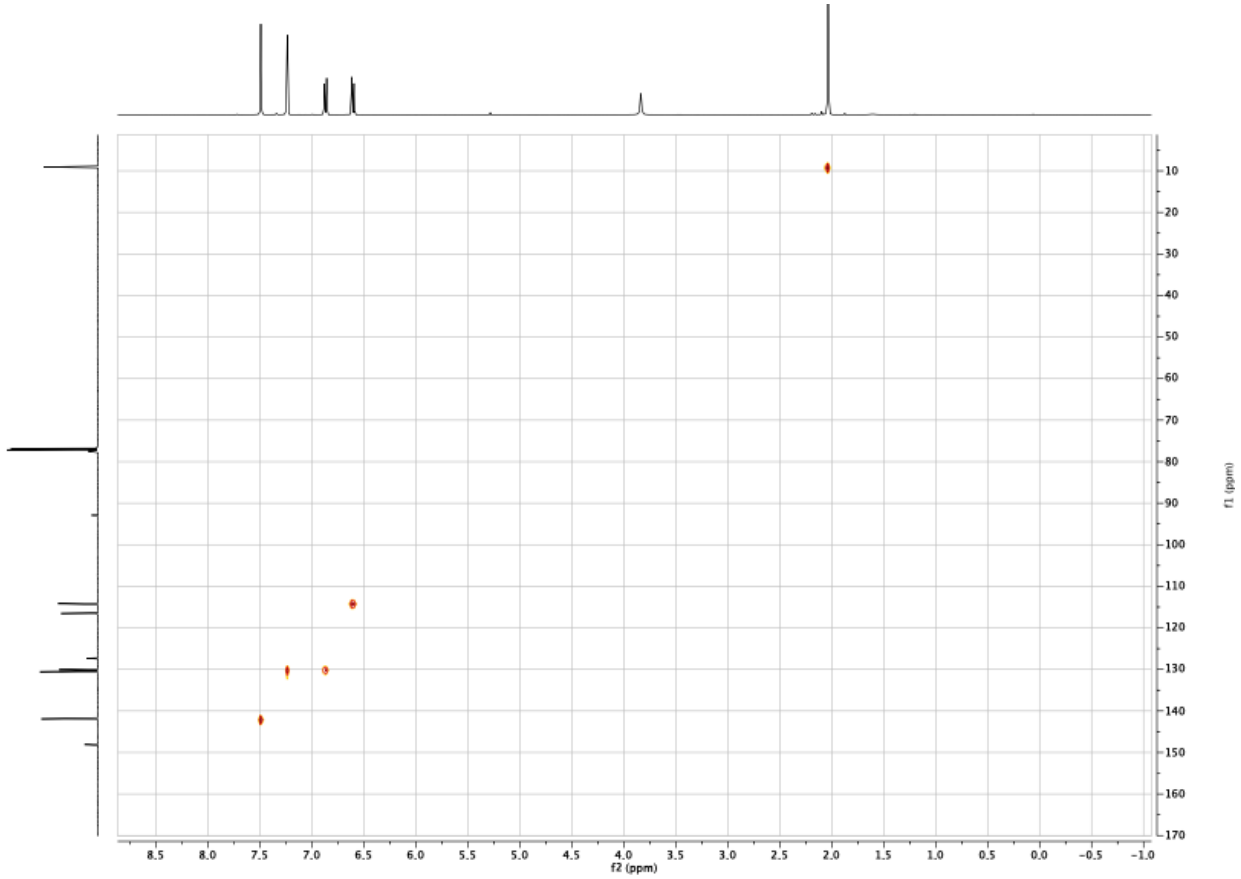
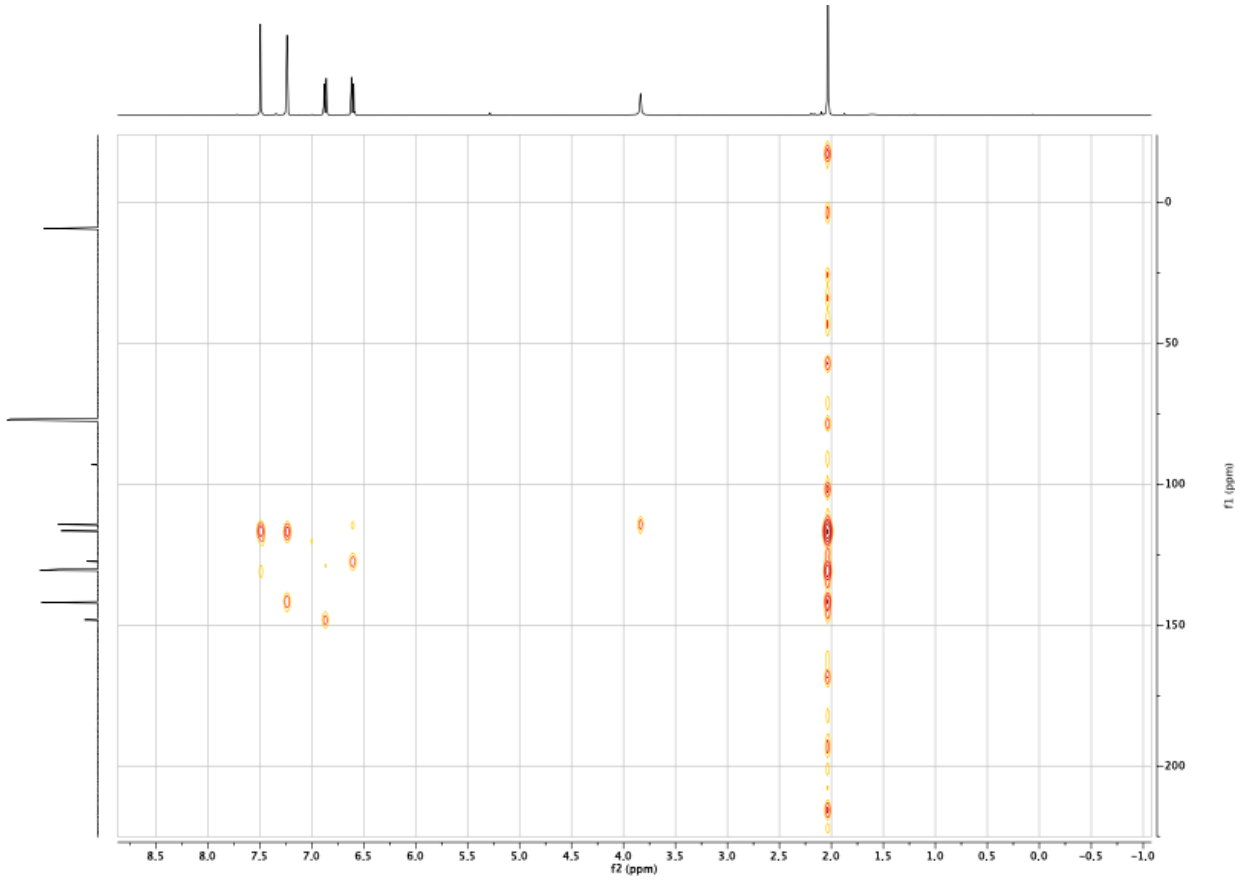
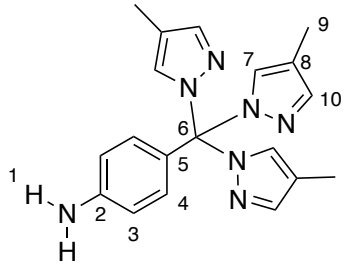



**Figure S3.** HSQC of title compound in $CDCl_3$




$^{1}$H-NMR ($CDCl_3$): 7.50 (H7 or H10), 7.25 (H7 or H10), 6.88 (H3), 6.62 (H4), 3.85 (H1), 2.05 (H9).
$^{13}$C-NMR ($CDCl_3$, 101 MHz), $\delta$ (ppm): 148.1 (C2), 141.9 (C7 or C10), 130.6 (C7 or C10), 130.1 (C3), 127.3 (C5), 116.5 (C8), 114.2 (C4), 92.9 (C6), 9.1 (C9).

**Figure S4.** HMBC of title compound in $CDCl_3$ and NMR assignments based on 2D-data

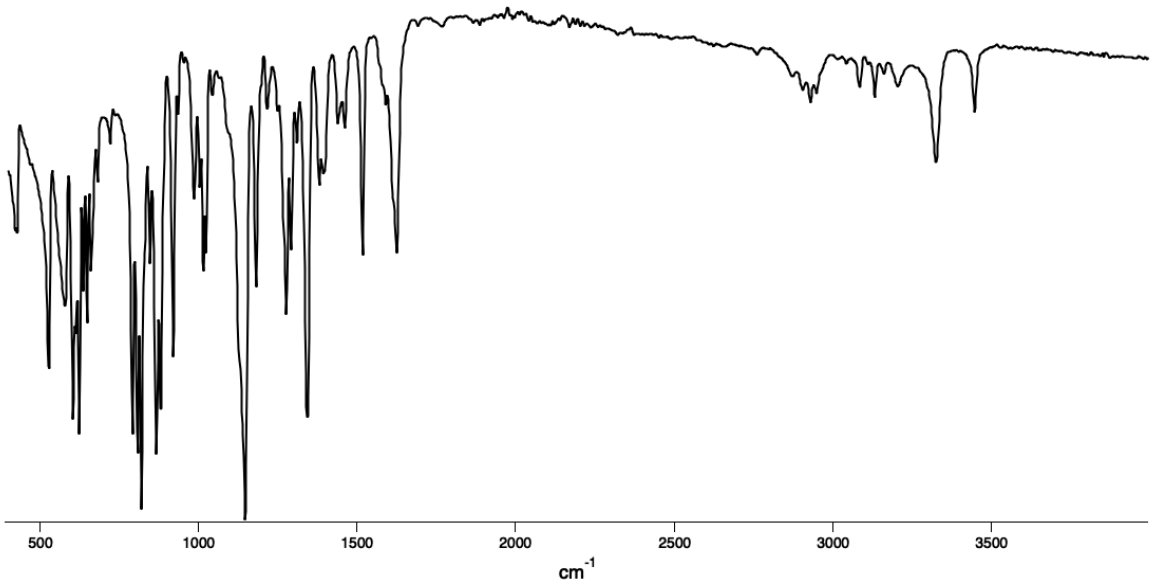



**Figure S5.** IR of title compound

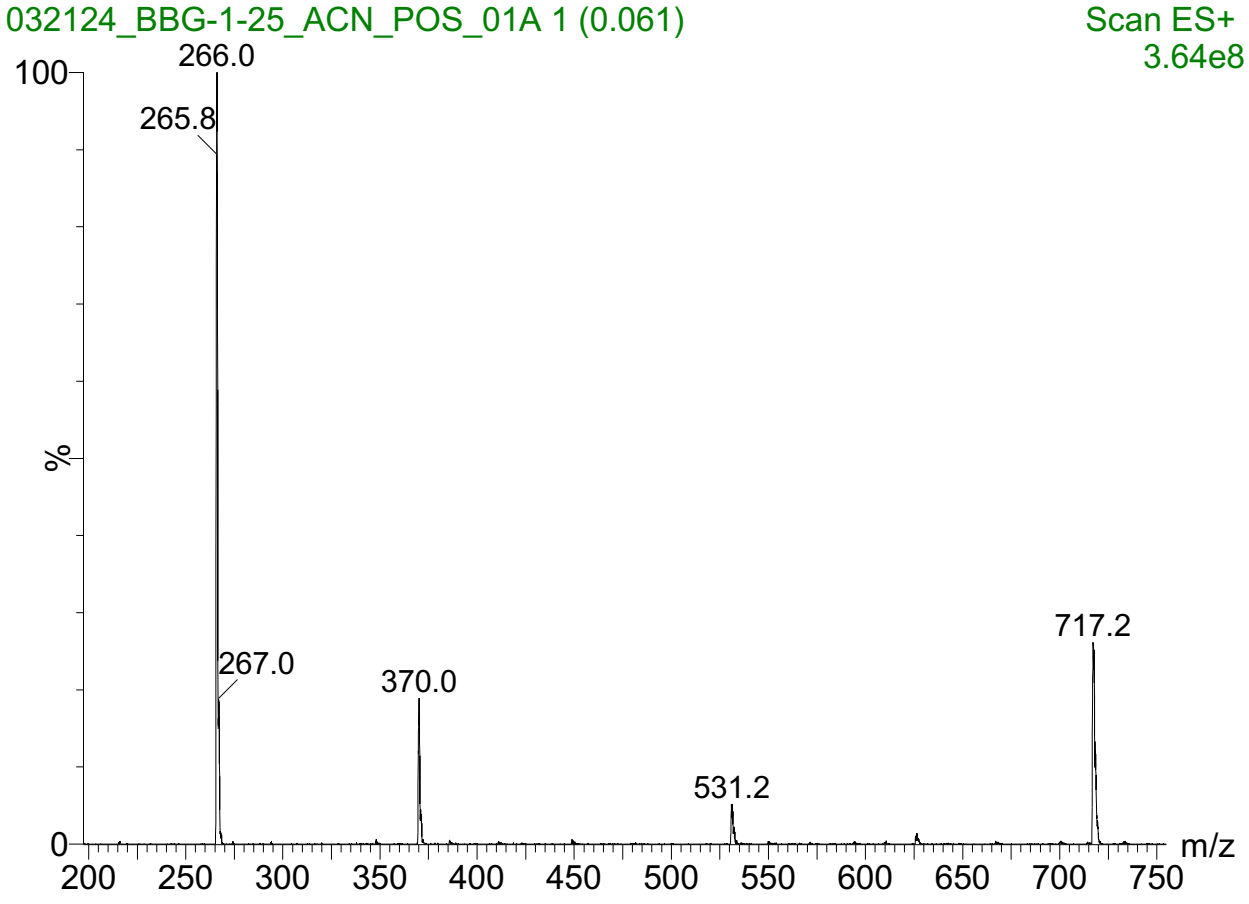



**Figure S6.** MS of title compound

**Table S1.** Crystallographic data for polymorphs of the title compound

| | **Polymorph I** | **Polymorph II** |
|---|---|---|
| empirical formula | $C_{19}H_{21}N_7$ | $C_{19}H_{21}N_7$ |
| formula wt. (g/mol) | 347.43 | 347.43 |
| crystal system | monoclinic | monoclinic |
| space group, *Z* | $P2_1/n$, 4 | $C2/c$, 8 |
| temperature (K) | 100(2) | 100(2) |
| *a* (Å) | 8.2901(5) | 16.9046(11) |
| *b* (Å) | 14.0159(7) | 6.7132(4) |
| *c* (Å) | 15.1240(8) | 30.5690(17) |
| *β* (°) | 92.4818(19) | 94.325(5) |
| volume (Å$^3$) | 1755.66(17) | 3459.2(4) |
| $D_{calc}$ (g/cm$^3$) | 1.314 | 1.334 |
| crystal size | 0.17 x 0.14 x 0.11 | 0.26 x 0.06 x 0.02 |
| diffractometer | Bruker D8 Quest | Bruker D8 Quest |
| detector | Photon 3 | Photon 3 |
| wavelength (Å) | 0.71073 | 0.71073 |
| abs. coeff. (mm$^{-1}$) | 0.084 | 0.085 |
| F(000) | 736 | 1472 |
| Tmax, Tmin | 1.000, 0.972 | 1.000, 0.896 |
| Θ range for data | 3.20-27.15 | 3.32-25.82 |
| reflections coll. | 64870 | 47225 |
| data/restr./param. | 3867/0/246 | 3312/0/246 |
| R(int) | 0.0784 | 0.0981 |
| final R [$I > 2\sigma(I)$] R1, wR2 | 0.0455, 0.1079 | 0.0560, 0.1265 |
| final R (all data) R1, wR2 | 0.0551, 0.1168 | 0.0908, 0.1439 |
| goodness-of-fit on $F^2$ | 1.048 | 1.039 |
| larg. diff. peak, hole (eÅ$^{-3}$) | 0.297, -0.233 | 0.359, -0.240 |
| CCDC Deposition No. | 2344377 | 2344378 |

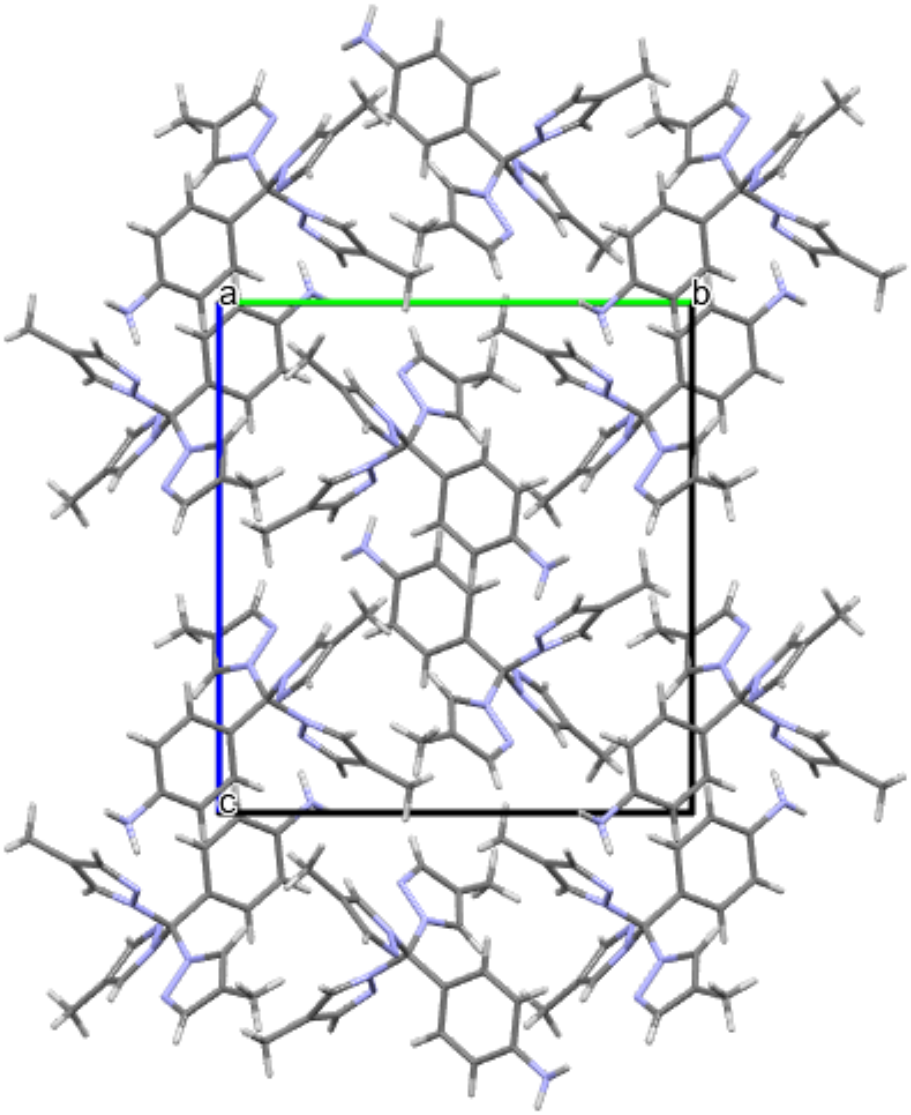



**Figure S7.** Packing diagram of polymorph I, viewed along the *a*-axis

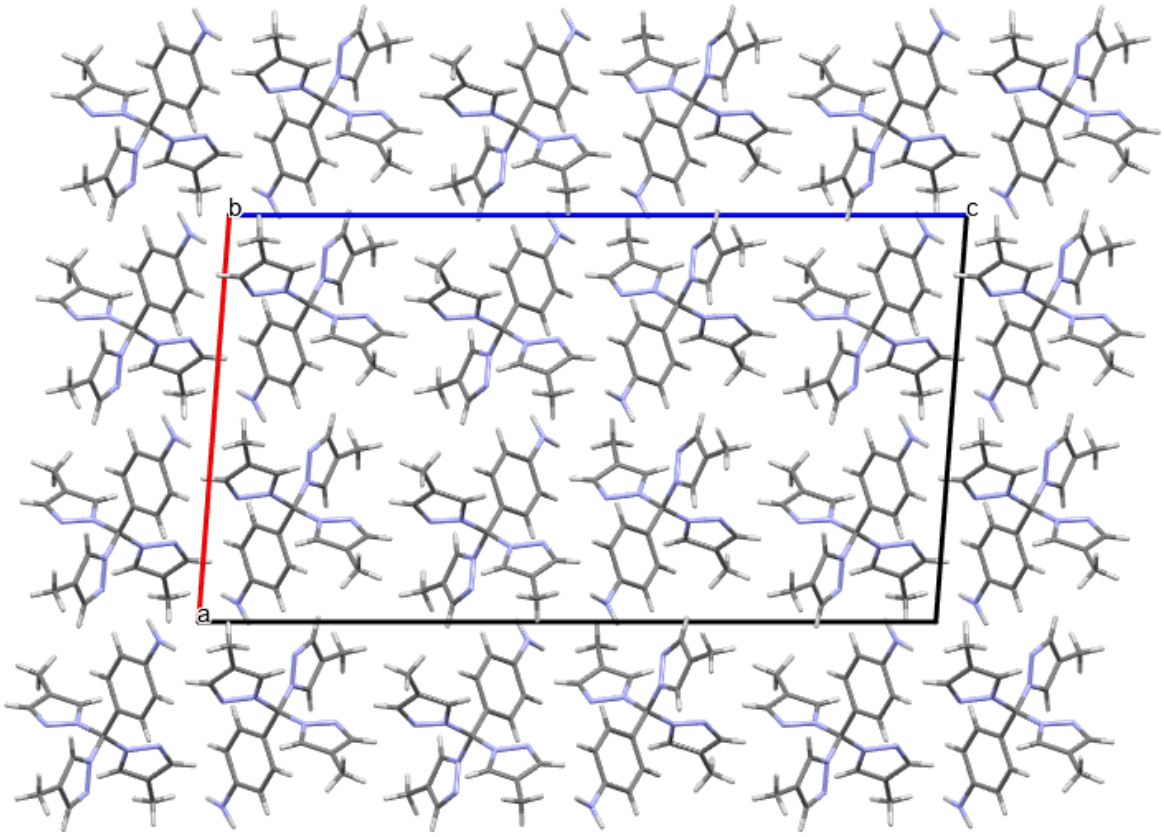



**Figure S8.** Packing diagram of polymorph II, viewed along the *b*-axis

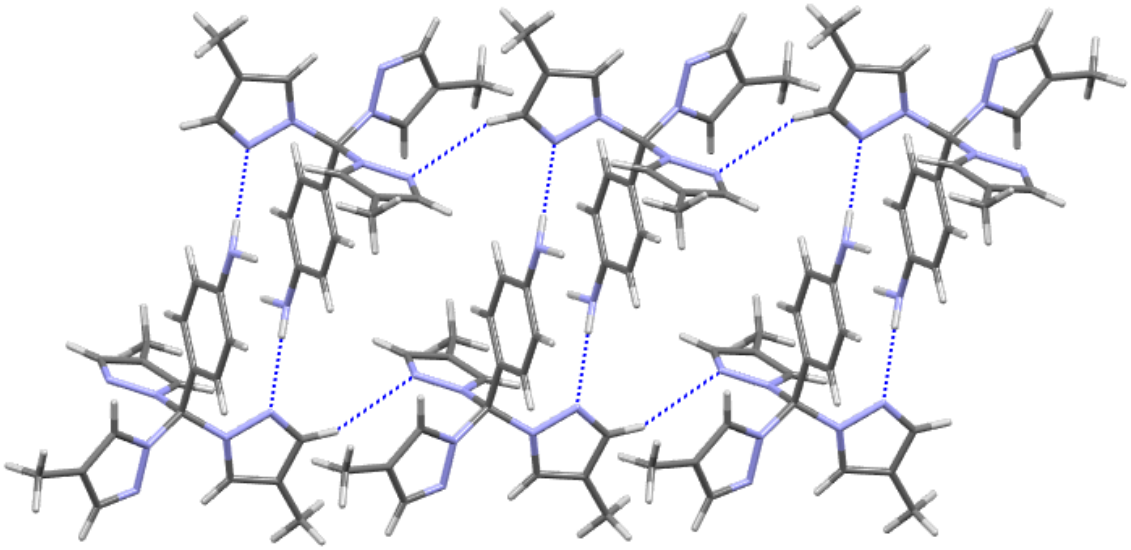


**Figure S9.** N-H···N dimers connected into chains via C-H···N interactions in polymorph I. Chains propagate along the *a*-axis