Support information

Regiosselective Cyclocondensations with Thiobarbituric Acid: Spirocyclic and Azocine Products, X-ray Characterization, and Antioxidant Evaluation

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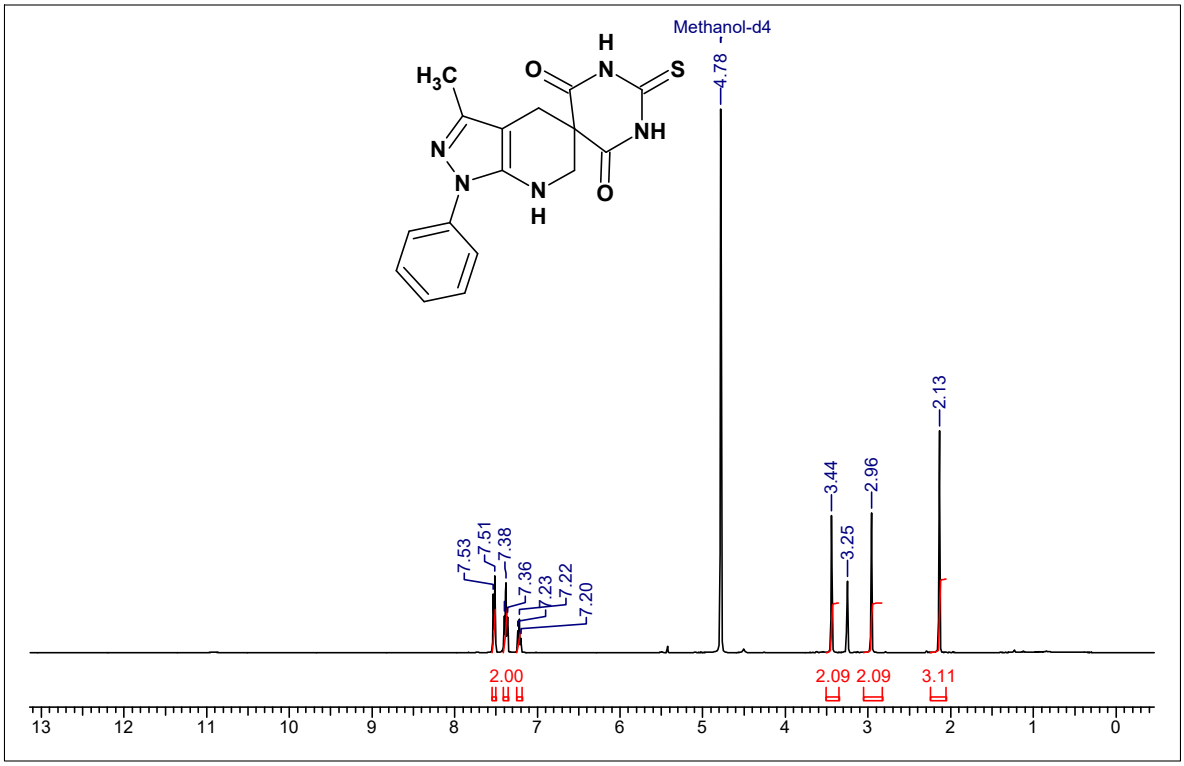


Figure SI-1. ^{1}H-NMR spectrum of compound 4a

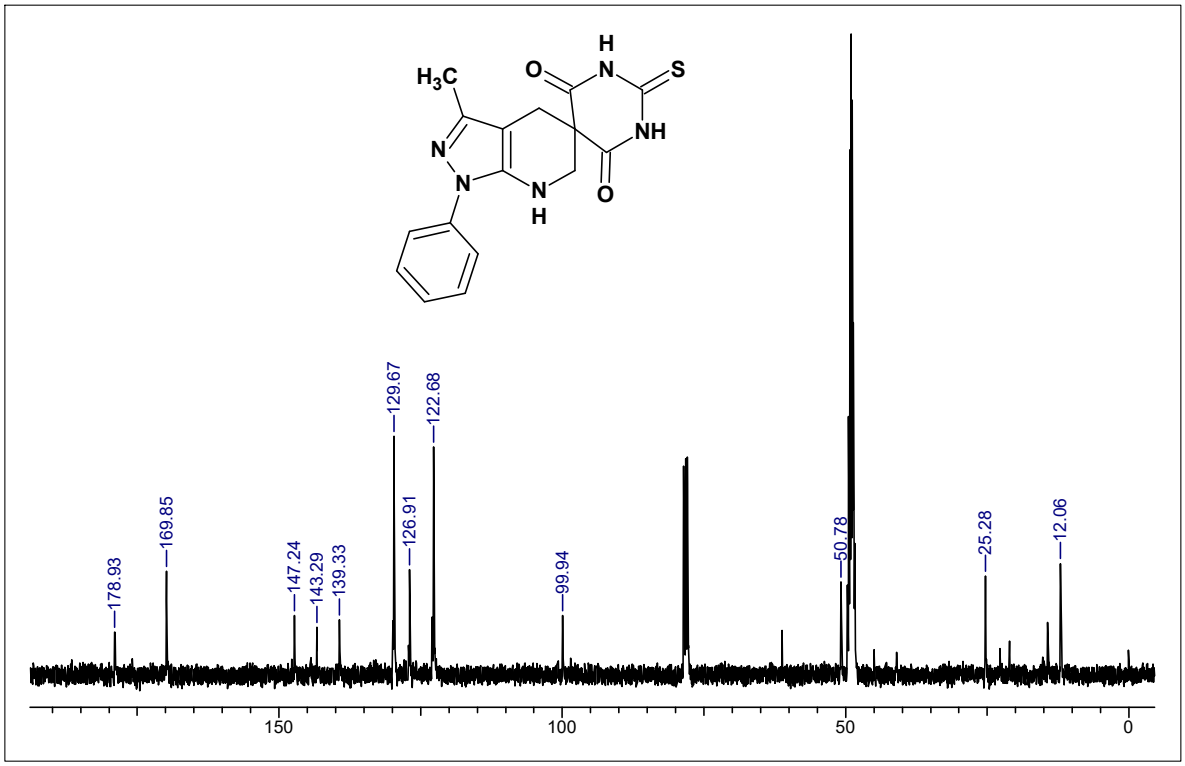


Figure SI-2. ^{13}C-NMR spectrum of compound 4a

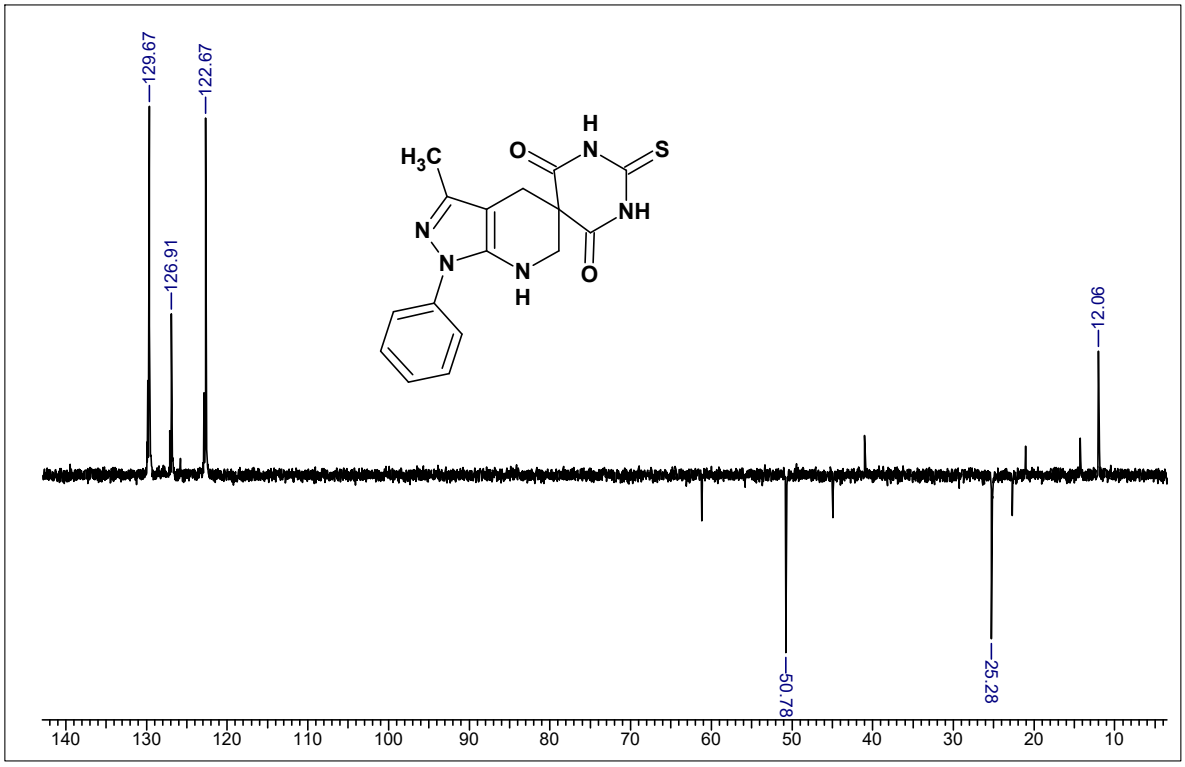


Figure SI-2. Dept-135 spectrum of compound 4a

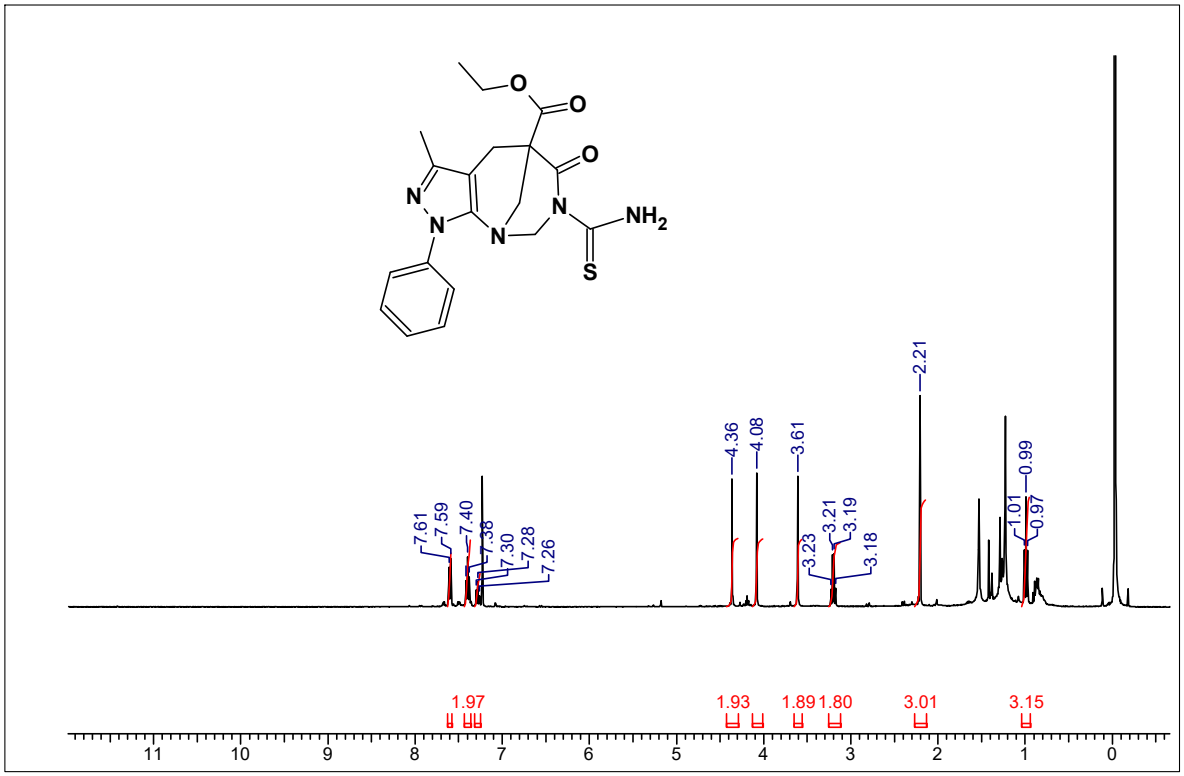


Figure SI-3. ^{1}H-NMR spectrum of compound 4b

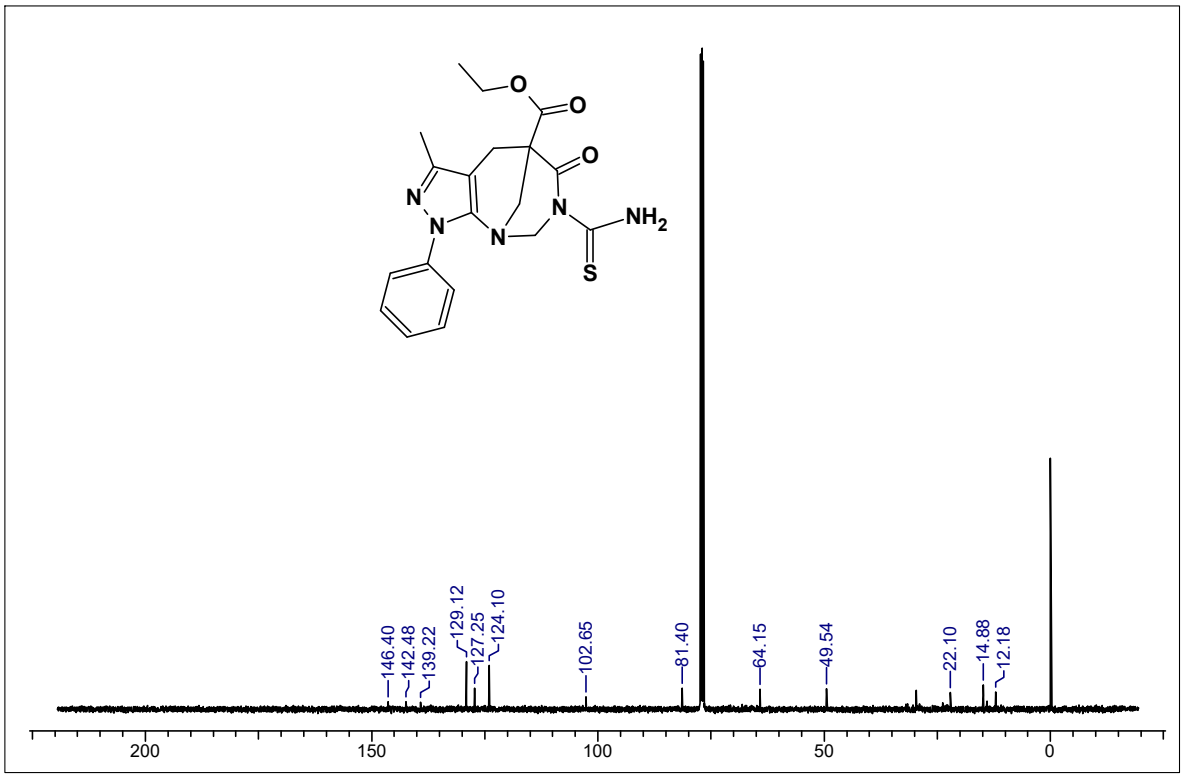


Figure SI-4. ^{13}C-NMR spectrum of compound 4b

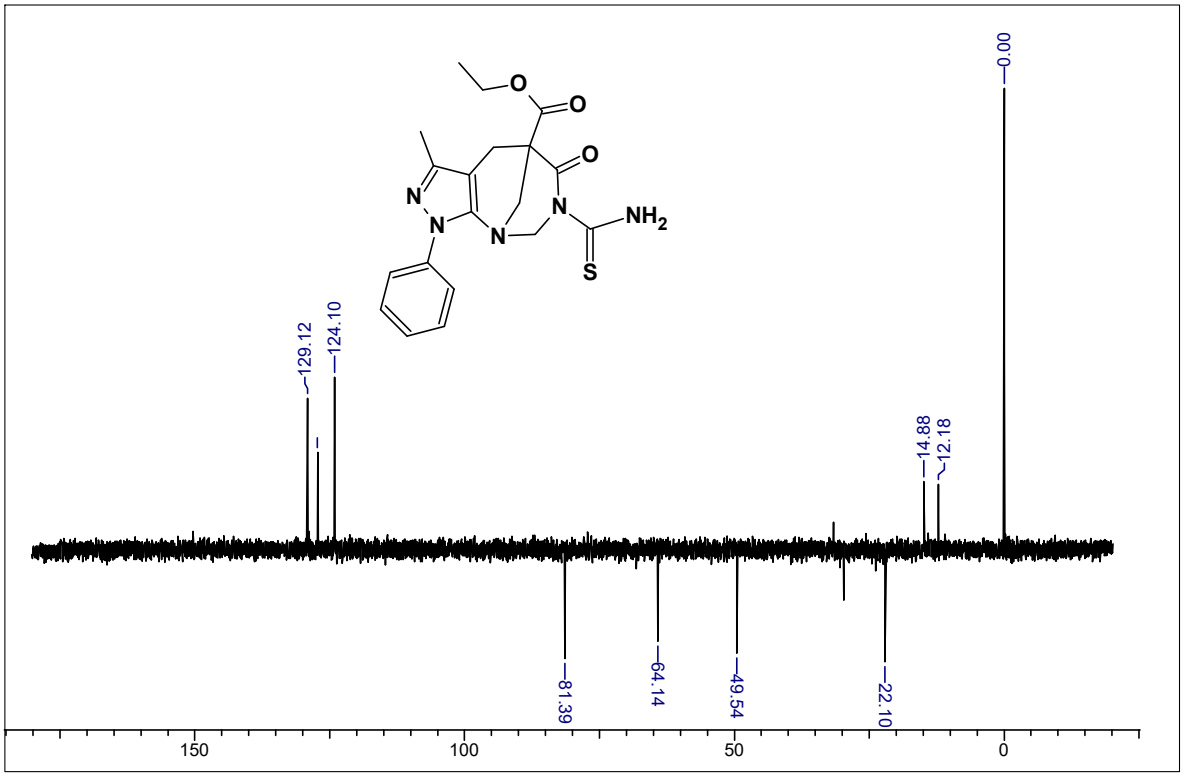
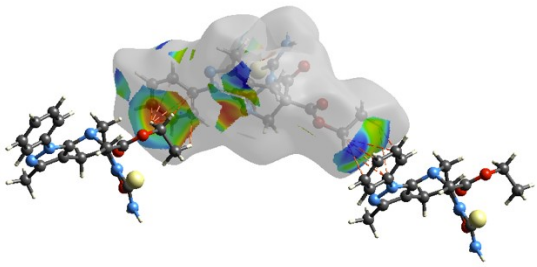


Figure SI-4. Dept-135 spectrum of compound 4b



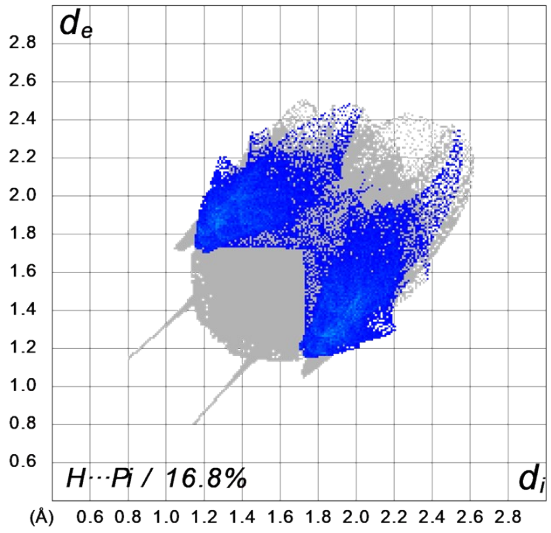


Figure SI-5. H···π interaction in the compound 4b.

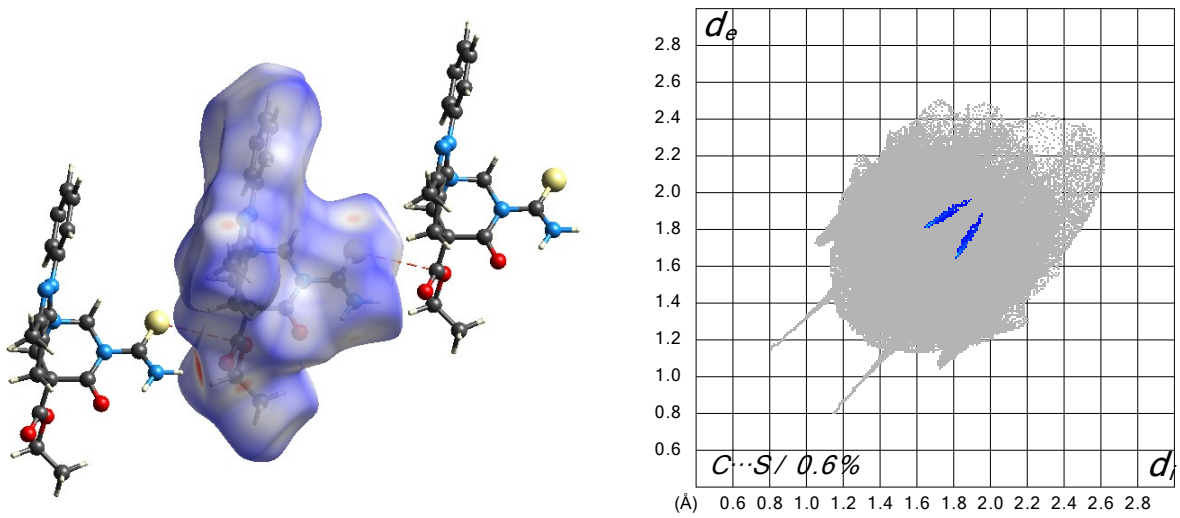
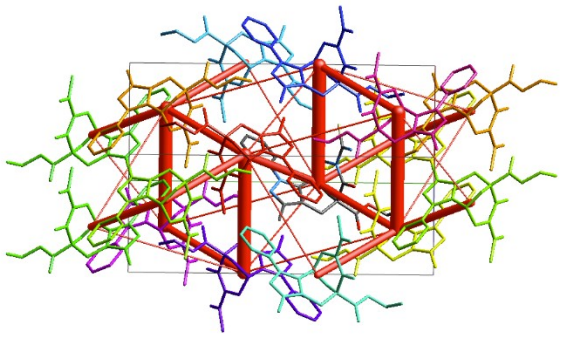


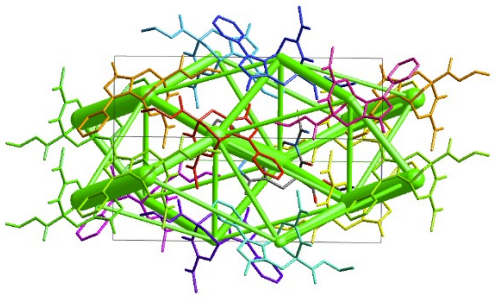
Figure SI-6. dnorm surface for the title compound(left) and its fingerprint plot (right), showing Chalcogen bond interactions.

-111.6 Kj·mol-1



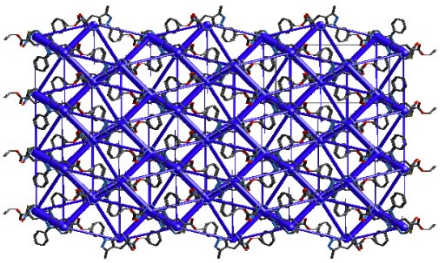
E_ele

-279.9 Kj·mol-1



E_dis

251.1 Kj·mol-1



E_tot

Figure SI-7. Energy framework of the compound 4b.

N	Symop	R	E_ele	E_pol	E_dis	E_rep	E_tot
1	-x, -y, -z	6.35	-26.0	-3.9	-95.3	66.8	-72.0
2	-x, y+1/2, -z+1/2	11.22	-3.2	-1.0	-22.3	11.3	-16.5
2	x, -y+1/2, z+1/2	7.60	-24.0	-5.5	-47.6	40.4	-46.0
2	-x, y+1/2, -z+1/2	13.28	-0.2	-0.0	-0.9	0.0	-1.0
2	x, -y+1/2, z+1/2	16.18	0.5	-0.0	-0.7	0.0	-0.1
1	x, y, z	10.77	-0.8	-0.1	-4.8	1.8	-4.0
1	-x, -y, -z	10.30	-5.3	-2.4	-24.0	13.8	-19.8
1	x, y, z	8.62	-43.1	-8.3	-23.2	50.2	-40.8
1	-x, -y, -z	8.30	-5.3	-1.7	-36.6	15.5	-29.2
1	-x, y+1/2, -z+1/2	11.61	-5.9	-1.5	-19.6	8.9	-18.9
1	x, -y+1/2, z+1/2	10.60	1.7	-0.6	-4.9	0.2	-2.8

Table SI-1. Total energy force diagrams and the details of interaction with symmetry operation (Symop) and distances between molecular centroids (R) in Å for compounds.