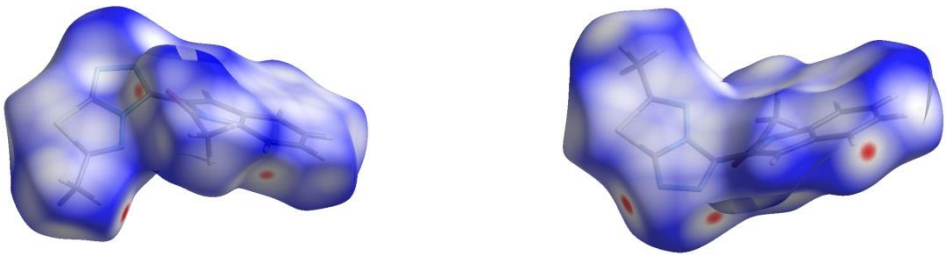
Supplementary Data

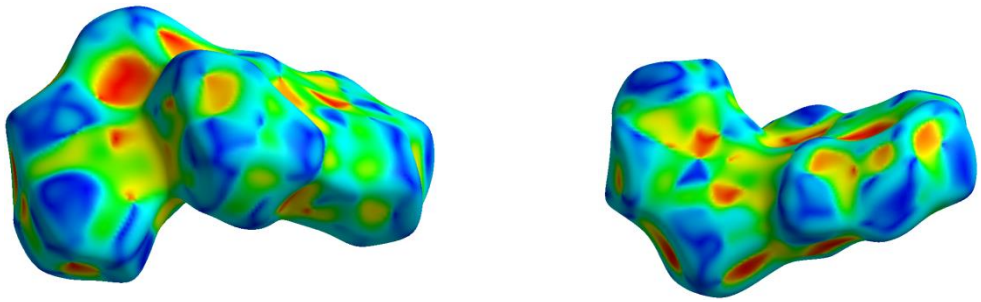
N-Acetyl Indole Linked to a Fused Triazolo/Thiadiazole Scaffold: Synthesis, Single Crystal X-Ray Structure, and Molecular Insight

Ahmed T. A. Boraei [1,*], Saied M. Soliman [2], Sammer Yousuf [3], Memoona Bibi [3], Assem Barakat [4,*]

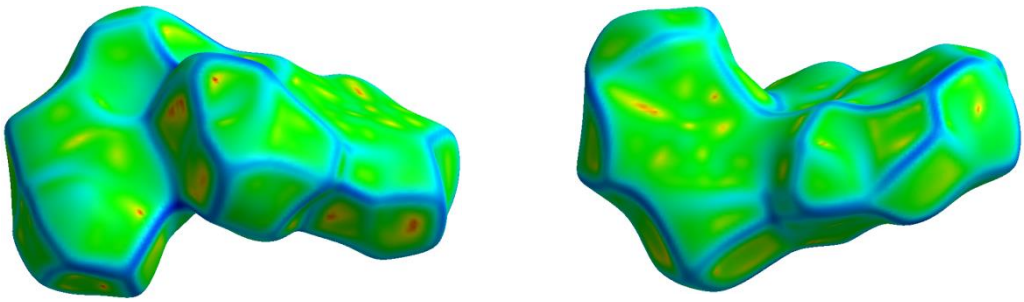
[1] Chemistry Department, Faculty of Science, Suez Canal University, Ismailia 41522, Egypt
[2] Department of Chemistry, Faculty of Science, Alexandria University, P.O. Box 426, Ibrahimia, Alexandria 21321, Egypt; saied1soliman@yahoo.com
[3] H.E.J. Research Institute of Chemistry, International Center for Chemical and Biological Sciences, University of Karachi, Karachi 75270, Pakistan; dr.sammer.yousuf@gmail.com (S.Y.); momauok702@gmail.com (M.B.)
[4] Department of Chemistry, College of Science, King Saud University, P. O. Box 2455, Riyadh 11451, Saudi Arabia
* Correspondence: ahmed_tawfeek83@yahoo.com (A.T.A.B.); ambarakat@ksu.edu.sa (A.B.); Tel.: +966-11467-5901 (A.B.); Fax: +966-11467-5992 (A.B.)



d_{norm}



Shape index



Curvedness

Figure S1. Hirshfeld surfaces of the studied compound.

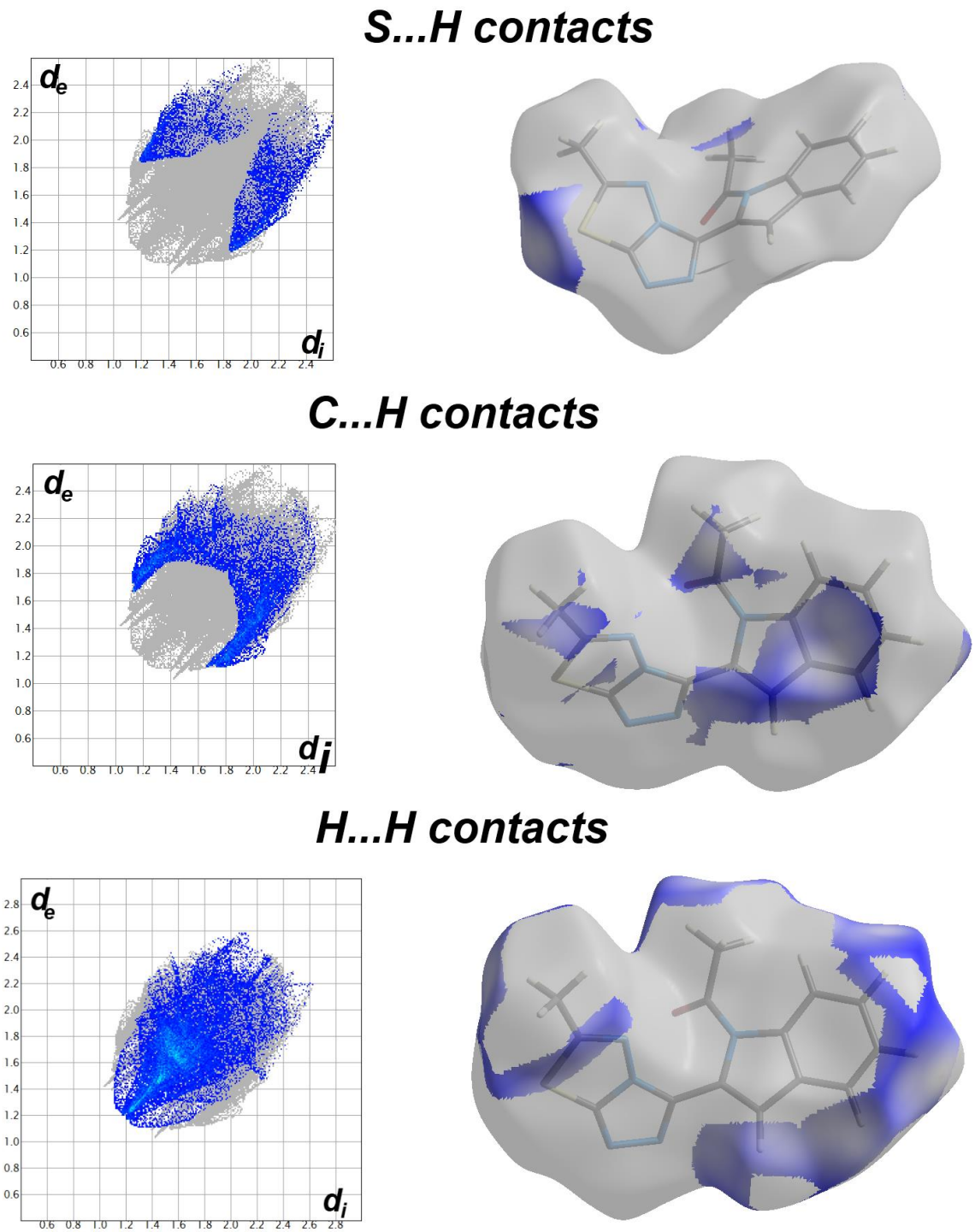


Figure S2. The fingerprint (left) and d_{norm} (right) of the weak intermolecular contacts in the target compound.

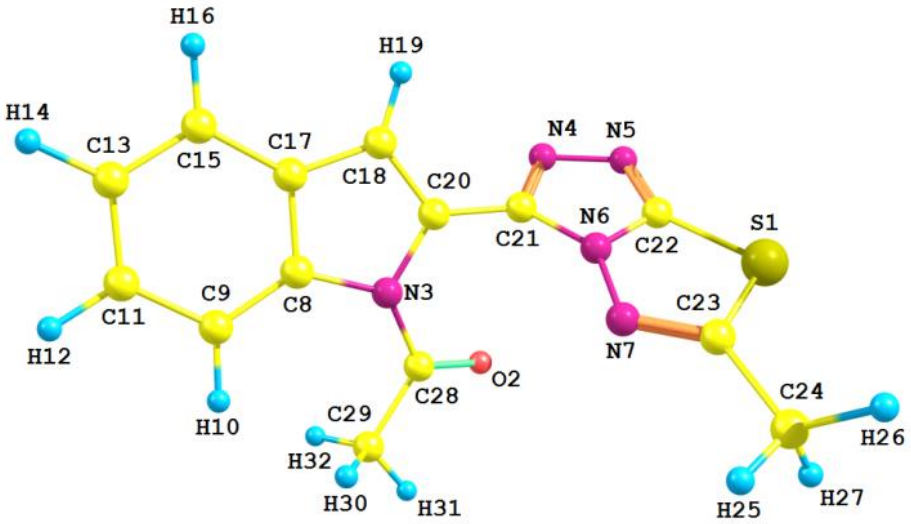


Figure S3. Atom numbering of the optimized structure (**See Table S1** and **S2**).

Table S1. The calculated geometric parameters of the studied compound.

Bond distances			Bond angles		
Bond	**Calc.**	**Exp.**	**Bond**	**Calc.**	**Exp.**
R(1-22)	1.752	1.732	A(22-1-23)	87.397	88.035
R(1-23)	1.793	1.757	A(1-22-5)	139.647	139.986
R(2-28)	1.215	1.202	A(1-22-6)	108.568	108.371
R(3-8)	1.418	1.419	A(1-23-7)	116.163	116.902
R(3-20)	1.422	1.413	A(1-23-24)	120.948	120.36
R(3-28)	1.414	1.411	A(2-28-3)	120.334	119.656
R(4-5)	1.388	1.402	A(2-28-29)	121.229	122.646
R(4-21)	1.324	1.313	A(8-3-20)	107.236	107.212
R(5-22)	1.308	1.314	A(8-3-28)	129.129	127.669
R(6-7)	1.365	1.377	A(3-8-9)	132.28	131.433
R(6-21)	1.376	1.375	A(3-8-17)	107.446	107.169
R(6-22)	1.372	1.352	A(20-3-28)	122.2	122.67
R(7-23)	1.294	1.293	A(3-20-18)	109.603	109.865
R(8-9)	1.4	1.386	A(3-20-21)	126.016	123.351
R(8-17)	1.42	1.408	A(3-28-29)	118.434	117.689
R(9-11)	1.394	1.382	A(5-4-21)	109.595	109.229
R(11-13)	1.403	1.387	A(4-5-22)	105.418	105.027
R(13-15)	1.388	1.377	A(4-21-6)	108.184	108.264
R(15-17)	1.401	1.403	A(4-21-20)	124.134	125.866
R(17-18)	1.433	1.432	A(5-22-6)	111.784	111.642
R(18-20)	1.362	1.355	A(7-6-21)	135.981	134.829
R(20-21)	1.456	1.444	A(7-6-22)	119.015	119.323
R(23-24)	1.493	1.49	A(6-7-23)	108.855	107.329
R(28-29)	1.512	1.491	A(21-6-22)	105.002	105.833
			A(6-21-20)	127.131	125.661
			A(7-23-24)	122.889	122.737
			A(9-8-17)	120.273	121.397
			A(8-9-11)	118.185	117.313
			A(8-17-15)	120.52	119.849
			A(8-17-18)	107.473	107.801
			A(9-11-13)	121.8	122.258
			A(11-13-15)	120.24	120.761
			A(13-15-17)	118.979	118.362
			A(15-17-18)	131.997	132.35
			A(17-18-20)	108.224	107.888
			A(18-20-21)	124.348	126.437

Table S2. The calculated and experimental chemical shifts (ppm) for the studied compound.

Atom	Calc.	Exp.	Atom	Calc.	Exp.
C 8	124.847	136.366	H 10	8.139	8.105
C 9	102.768	115.157	H 12	7.891	7.484
C 11	114.254	126.405	H 14	7.782	7.362
C 13	111.963	123.714	H 16	8.090	7.776
C 15	110.617	121.995	H 19	7.416	7.345
C 17	118.325	128.225	H 25	2.813	
C 18	106.459	114.937	H 26	2.945	2.729
C 20	115.616	123.274	H 27	2.978	
C 21	133.244	140.474	H 30	3.236	
C 22	148.534	154.764	H 31	2.578	2.516
C 23	160.683	167.377	H 32	3.198	
C 24	11.514	17.954			
C 28	157.386	170.030			
C 29	18.770	26.351			