Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Preferential intermolecular interactions in a racemic mixture of amino acid Schiff base, conformational structures in solid state and DFT studies.

Jesús A. Lara-Cerón,[a,*] Víctor M. Jiménez-Pérez,[a] Areli A. Molina-Paredes,[a] Mario Sánchez,[b] H. V. Rasika Dias,[c] Pedro I. Ramirez-Montes,[d] Blanca M. Muñoz-Flores.[a,*]

a. Universidad Autónoma de Nuevo León, Facultad de Ciencias Químicas, Ciudad Universitaria, Av. Universidad s/n. C. P. 66451, Nuevo León, México.

b. Centro de Investigación en Materiales Avanzados, S.C., Alianza Norte 202, PIIT, Carretera Monterrey-Aeropuerto Km. 10, C. P. 66628, Apodaca, Nuevo León, México.

c. Department of Chemistry and Biochemistry, The University of Texas at Arlington, Arlington, Texas 76019-0065, USA.

d. Universidad Nacional Autónoma de México, Facultad de Estudios Superiores Cuautitlán, Departamento de Matemáticas, Carr. Cuautitlán-Teoloyucan Km. 2.5, San Sebastián Xhala, 54714 Cuautitlán Izcalli, México.

* Corresponding author: Tel +52(81)83294000, ext. 3401; Fax: 52 (81)83760570.

E-mail: jesus.laracrn@uanl.edu.mx (J. A. Lara-Cerón) and blanca.munozfl@uanl.edu.mx (B. M. Muñoz-Flores).

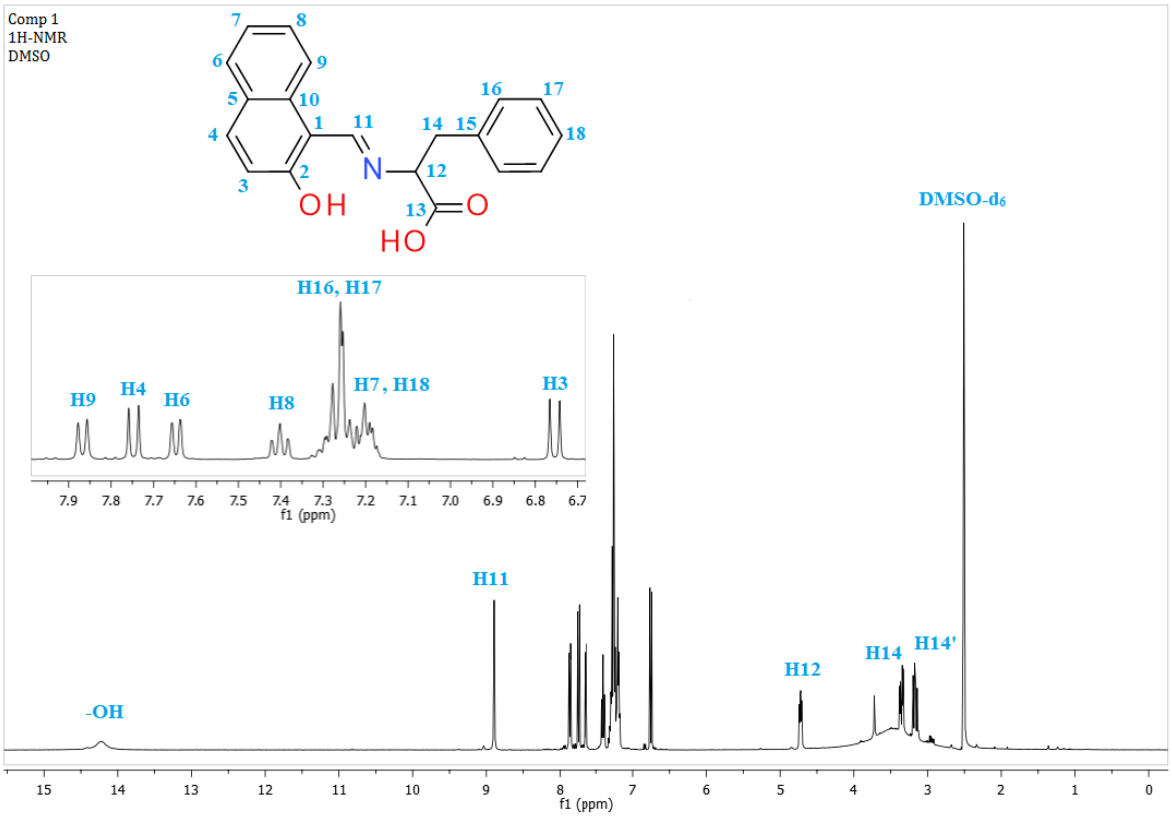

Fig S 1. ^{11}H NMR spectrum of compound **1** in DMSO at 400MHz.

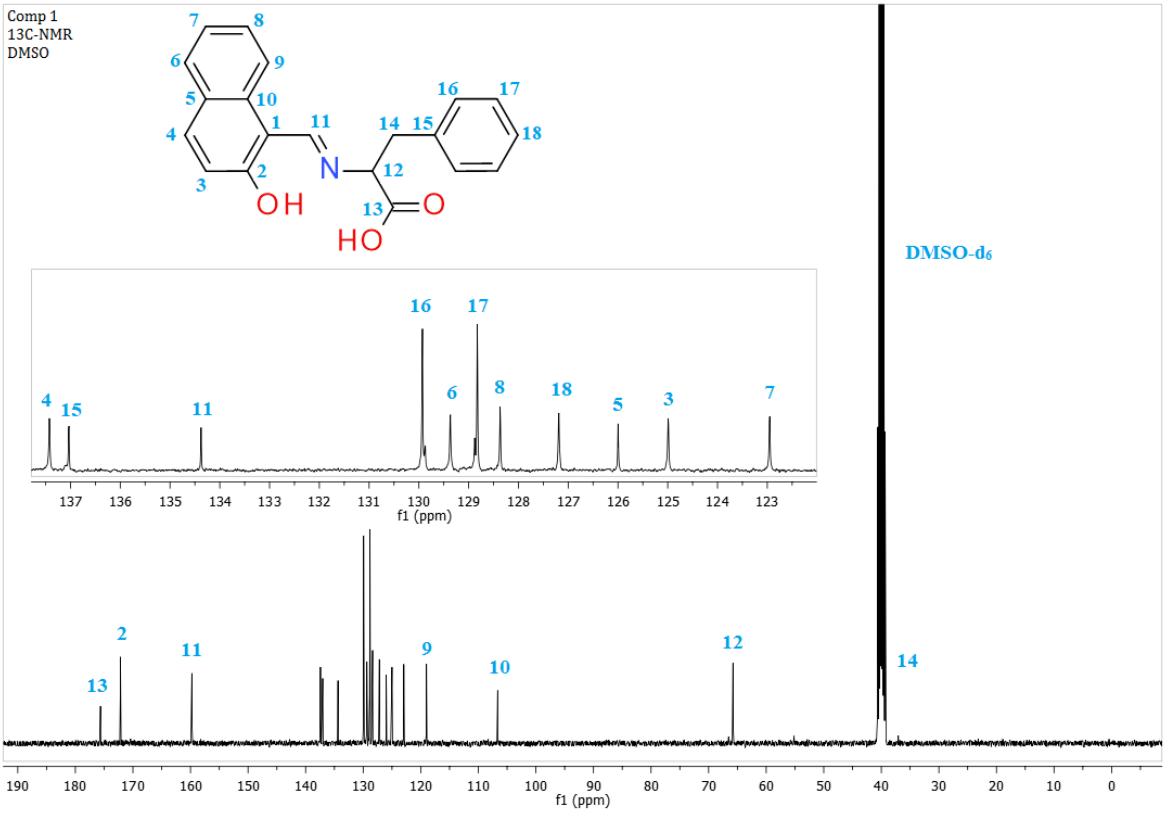

Fig S 2. ^{13}C NMR spectrum of compound **1** in DMSO at 100MHz.

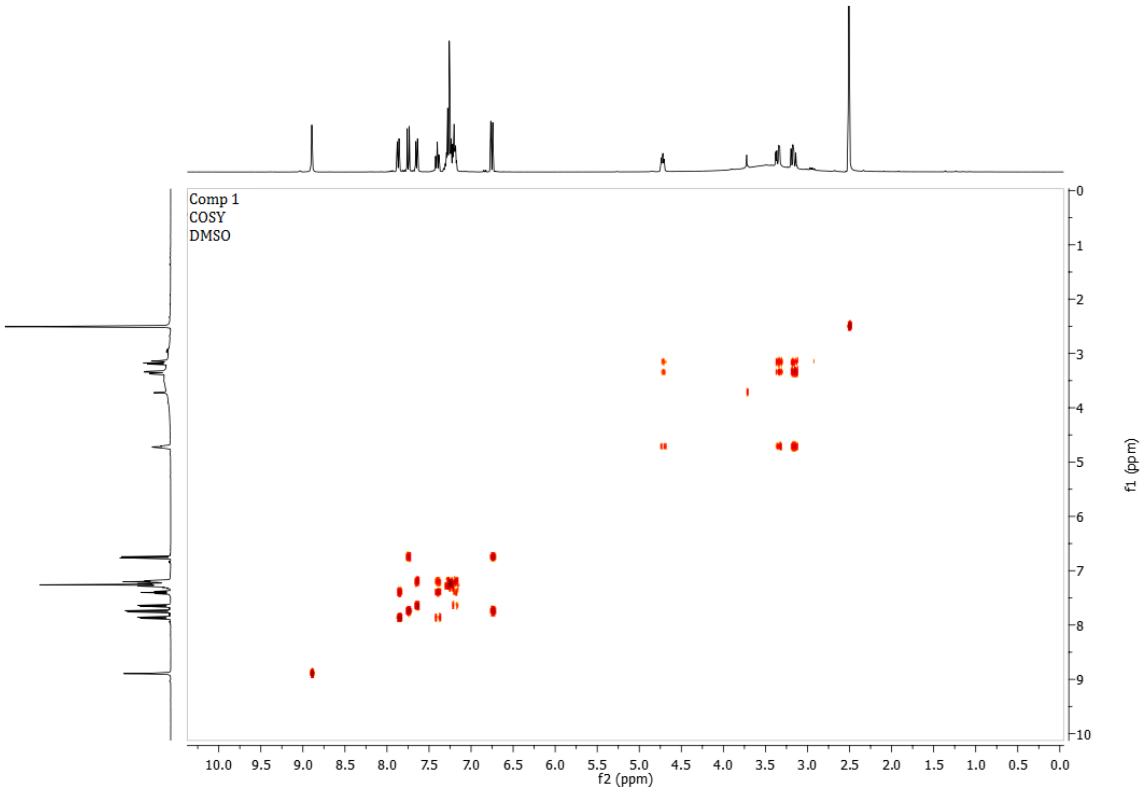

Fig S 3. COSY spectrum of compound **1** in DMSO.

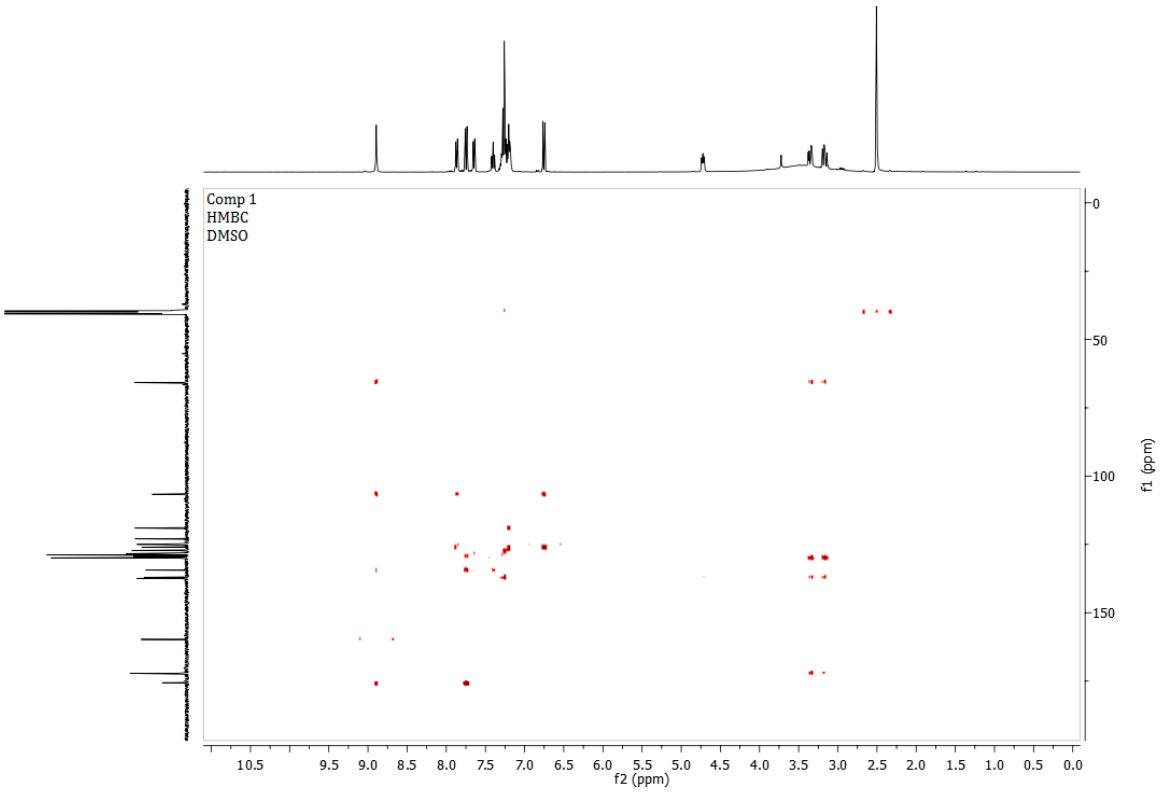

Fig S 4. HMBC spectrum of compound **1** in DMSO.

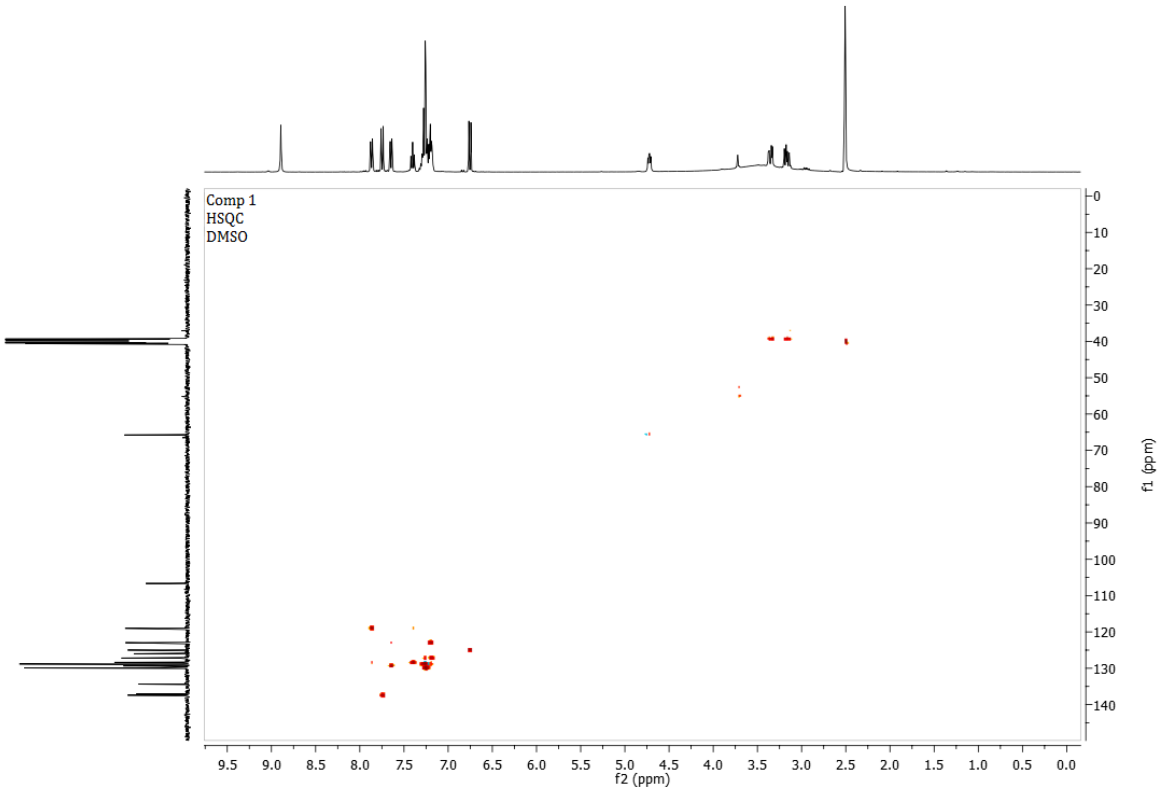

Fig S 5. HSQC spectrum of compound **1** in DMSO.

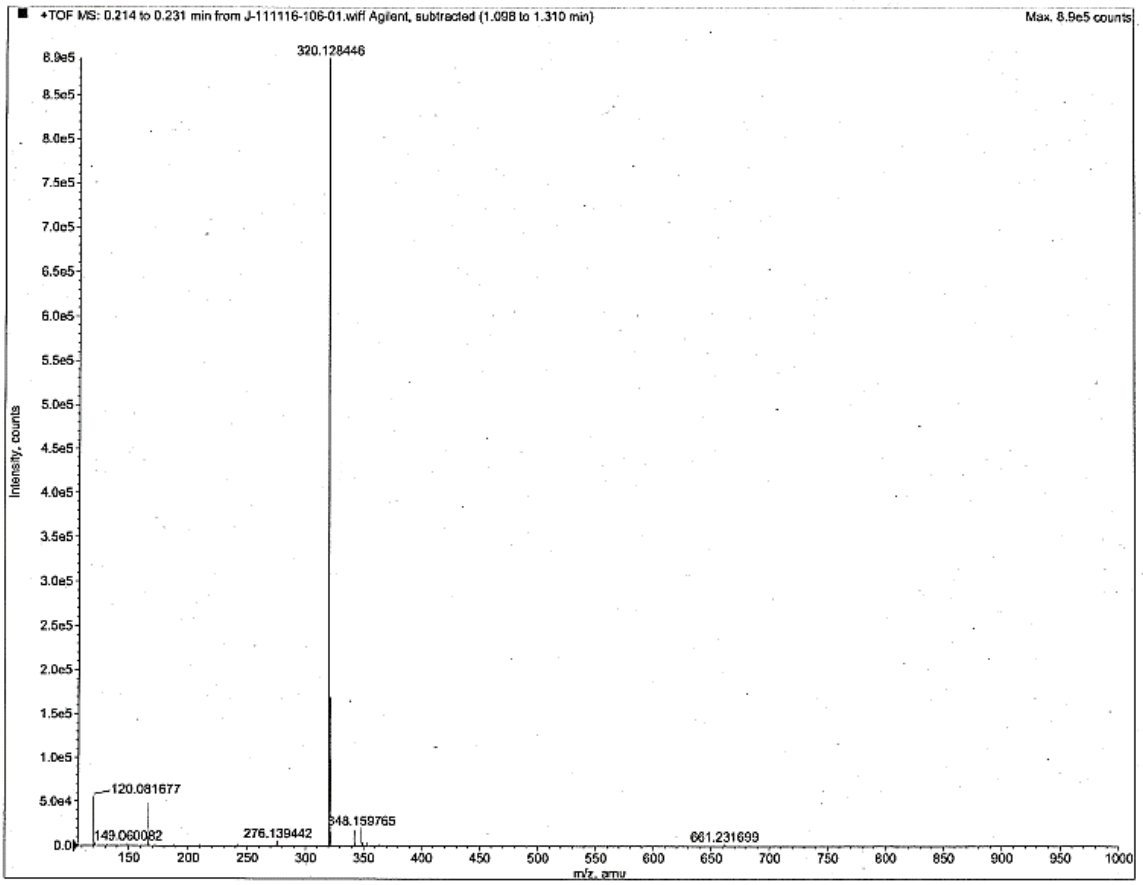

Fig S 6. Mass spectroscopy of compound **1**.

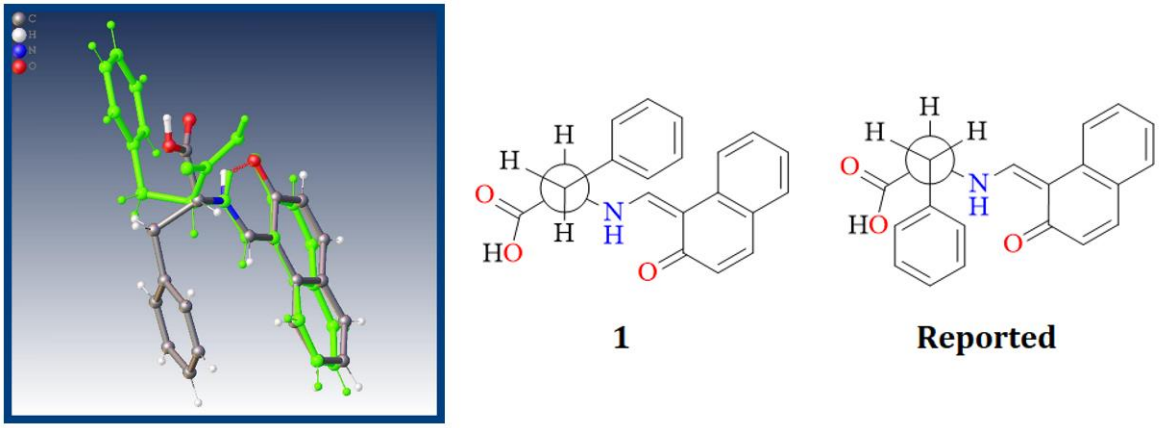

Fig S 7. Overlay visualization of conformers **1** and the reported (green) and their Newman projections.

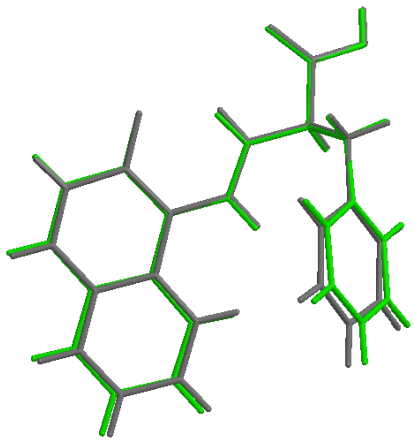

Fig S 8. Overlay visualization of the two crystallographically independent molecules in the asymmetric unit of **1**.

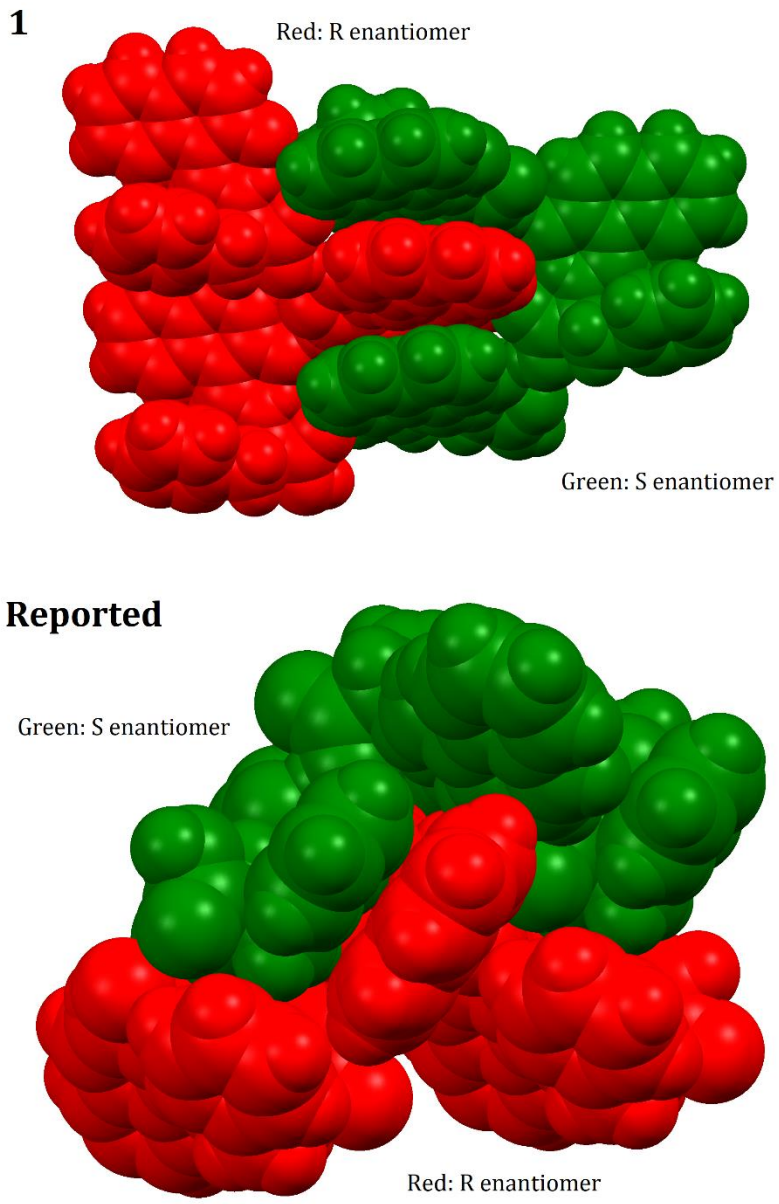

Fig S 9. Spacefill view of enantiomeric mixture in X-ray structures of **1** and previously reported.

Table 1. Statistical Data from the CSD for the tautomers phenol-imine and keto-amine, and values in angstroms (Å) for the X-ray structures of 1 and previously reported.

Tautomer	**O1-C2**	**C2-C1**	**C1-C11**	**C11-N**

Phenol-imine[Error! Bookmark not defined.]	1.343	1.406	1.450	1.286
Keto-amine[Error! Bookmark not defined.]	1.291	1.431	1.414	1.303
1	1.286	1.425	1.411	1.307
Reported[18]	1.300	1.420	1.411	1.303

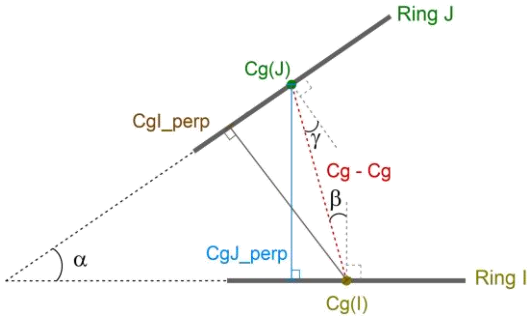

Fig S 10. Sketch of the geometrical parameters in *edge-to-face* or *face-to-face* interactions as calculated in PLATON, where Cg(I) = geometrical center of the I ring, Cg(J) = geometrical center of the J ring. Cg-Cg = distance between Cg(I) and Cg(J), α = angle between the ring planes, β = angle between the Cg-Cg vector and the normal to the ring plane I. γ= angle between Cg-Cg vector and the normal to the ring plane J. CgJ_perp = perpendicular distance between Cg(J) and ring I. CgI_perp = perpendicular distance between Cg(I) and ring J.

Table 2. Geometrical parameters for the ·π ···π interactions observed on the crystal packing of compound **1**.

	Interaction	**Cg ···Cg (Å)**	**α (°)**	**β (°)**	**γ(°)**	**CgI_Perp (Å)**	**CgJ_Perp(Å)**
Form I	Ph - Naph[i]	3.5306(9)	3.28(6)	2.1	2.8	3.5262(7)	3.5282(5)*
Form II	Naph mol 1 – Naph mol 2[ii]	4.9110(18)	62.52(11)	8.5	69.7	1.7017(12)	4.8576(12)
	Naph mol 2 – Naph mol 1[iii]	4.9214(17)	60.76(11)	9.0	67.0	1.9241(12)	4.8615(12)
	Ph mol 2 – Ph mol 1[iv]	4.767(3)	42.3(2)	21.9	62.0	2.2409(17)	4.423(2)

* Slippage of 0.130 Å
i = 1 -x, -y, 1 -z; ii = -1/2 + x, 1/2 - y, -1/2 + z; iii = 1/2 + x, -1/2 + y, 1 + z; iv =-1/2 + x, 1/2 -y, 1/2 + z;

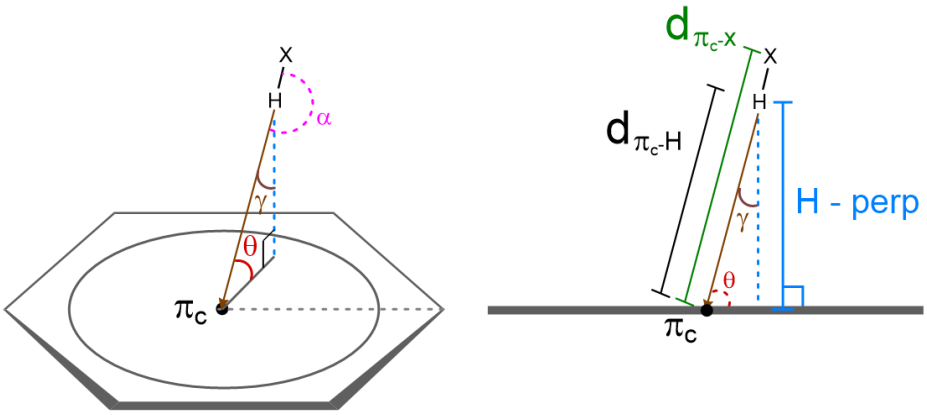

Fig S 11. Geometrical parameters in C-H···π interactions where π_c = carbon atoms centroid, $d_{\pi c\text{-}H}$ = distance between π_c and the hydrogen atom, $d_{\pi c\text{-}X}$ = distance between π_c and the X (Carbon) atom, H - perp = perpendicular distance between hydrogen atom and π_c, θ = angle of the C-H bond with ring plane, γ = angle between π_c and the H atom vector with plane normal , α = angle X-H ···π_c.

Table 3. Geometrical parameters for the C-H···π interactions observed on the crystal packing of compound **1** (Form II).

Interaction	$d_{\pi c\text{-}H}$ (Å)	H-Perp(Å)	γ(°)	α(°)	$d_{\pi c\text{-}x}$ (Å)	θ (°)
C2-H2··· Naph mol 1[i]	2.73	2.68	10.15	151	3.613(4)	57
C7-H7··· Naph mol 2[ii]	2.83	2.73	15.40	138	3.573(4)	60
C22-H22··· Naph mol 2[iii]	2.90	-2.74	19.28	157	3.817(4)	59

* Slippage of 0.130 Å
i = x, 1 -y, 1/2 + z ; ii = -1/2 + x,1/2 + y,-1 + z; iii = x, -y, 1/2 + z

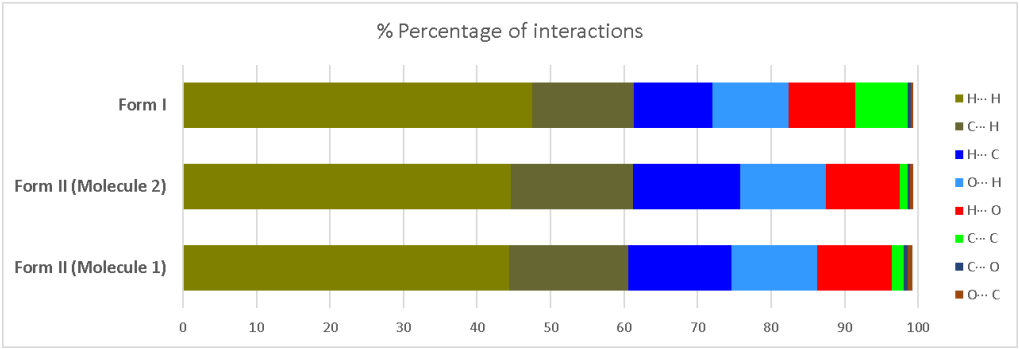

Fig S 12. Percentage of contribution to total observed atom promolecule interactions broken down by element type. For Form I and II of compound **1**.

Table 4. Percentage of contribution of each pair of elements to the fingerprint plot.

		Form II		Form I
		Molecule 1	Molecule 2	
	Inside-Outside	% Contribution		% Contribution
1	C··· C	1.6	1.1	7.1
2	C··· N	0.3	0.2	0.0
3	N··· C	0.3	0.2	0.0
4	C··· H	16.2	16.6	13.8
5	H··· C	14.0	14.6	10.7
6	C··· O	0.6	0.3	0.4
7	O··· C	0.6	0.4	0.3
8	N··· N	0.0	0.0	0.0
9	N··· H	0.1	0.2	0.2
10	H··· N	0.1	0.2	0.2
11	N··· O	0.0	0.0	0.1
12	O··· N	0.0	0.0	0.1
13	O··· H	11.7	11.7	10.4
14	H··· O	10.1	10.0	9.1
15	H··· H	44.4	44.6	47.5

Table 5. Optimized structure coordinates of compound **1**.

Atomic number	***x***	***y***	***z***
8	-4.03973	-2.32775	-1.62156
1	-4.46905	-3.20044	-1.60719
8	-2.78247	-3.35496	-0.05123
8	0.322517	-1.6345	2.114211
7	-1.03549	-1.19345	-0.01016
6	-3.04111	-2.37606	-0.7087
6	-2.34418	-1.02112	-0.59309
1	-2.23521	-0.60083	-1.59845
6	0.091755	-0.7064	-0.52461
1	0.001669	-0.25708	-1.51082
6	1.320322	-0.72976	0.13465
6	1.344166	-1.18827	1.524252
6	2.608629	-1.08219	2.235862
1	2.607797	-1.4115	3.26976
6	3.723629	-0.60245	1.633023

1	4.656554	-0.53741	2.189396
6	3.737882	-0.17252	0.257063
6	4.92693	0.303946	-0.33092
1	5.825973	0.34808	0.278889
6	4.960746	0.706102	-1.65475
1	5.882123	1.071122	-2.09758
6	3.787826	0.6247	-2.42075
1	3.801011	0.92411	-3.46494
6	2.608392	0.155742	-1.86231
1	1.731984	0.088293	-2.49863
6	2.538207	-0.24347	-0.50905
6	-3.24123	-0.06357	0.254318
1	-4.23738	-0.05589	-0.19902
1	-3.3407	-0.50208	1.253632
6	-2.69403	1.342592	0.344305
6	-1.7272	1.677702	1.302949
1	-1.36922	0.917535	1.991989
6	-1.21213	2.972484	1.367649
1	-0.46314	3.215814	2.115341
6	-1.65711	3.951292	0.477419
1	-1.25816	4.959923	0.531453
6	-2.61954	3.628503	-0.48037
1	-2.97509	4.385514	-1.17345
6	-3.13245	2.332655	-0.54512
1	-3.88835	2.088378	-1.28809
1	-0.90194	-1.60113	0.936387

Table 6. Optimized structure coordinates of conformer of **1** previously reported.

Atomic number	***x***	***y***	***z***
8	0.187365	1.738117	0.638063
8	-1.79427	-1.6549	1.983189
1	-2.33536	-2.06847	2.677905
8	-3.06909	-3.02562	0.72631
7	-0.4544	-0.63918	-0.07592
1	-0.67159	0.306008	0.296456
6	1.834974	0.105688	0.050536
6	1.40042	1.437756	0.474003
6	2.435608	2.436253	0.69266
1	2.097882	3.420685	0.999544
6	3.747949	2.145286	0.521716

1	4.50111	2.911758	0.693013
6	5.584975	0.584933	-0.03697
1	6.286147	1.394867	0.148295
6	6.04534	-0.66408	-0.41546
1	7.108493	-0.84894	-0.53239
6	5.116369	-1.69113	-0.64082
1	5.461124	-2.67928	-0.932
6	3.756885	-1.46207	-0.49128
1	3.078837	-2.29119	-0.66552
6	3.255976	-0.19578	-0.1151
6	4.207501	0.83921	0.119292
6	0.853678	-0.84655	-0.21932
1	1.130106	-1.83263	-0.58616
6	-1.47091	-1.61282	-0.40444
1	-0.97443	-2.47469	-0.86759
6	-2.20545	-2.18099	0.816839
6	-2.50762	-1.07041	-1.43027
1	-1.94621	-0.76139	-2.31779
1	-3.1403	-1.91559	-1.7139
6	-3.36602	0.069466	-0.92129
6	-4.63809	-0.18688	-0.38841
1	-5.00351	-1.20924	-0.35
6	-5.43281	0.854522	0.090865
1	-6.41798	0.638352	0.494213
6	-4.96613	2.169233	0.047992
1	-5.58471	2.980713	0.420025
6	-3.70146	2.435718	-0.4776
1	-3.32704	3.454279	-0.51187
6	-2.9094	1.394639	-0.96272
1	-1.92447	1.616248	-1.36264

Table 7. Fractional atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for the crystal structure of **1**. Ueq is defined as 1/3 of the trace of the orthogonalized U_{IJ} tensor.

Atom	***x***	***y***	***z***	**U(eq)**
O1	4334.0(18)	1780.4(13)	8988(2)	58.7(7)
O2	5830(2)	2121.7(15)	5623(2)	65.5(8)
O3	5385(2)	2524.3(14)	7060(3)	71.8(8)
N1	5010.8(17)	1170.8(16)	7589(2)	39.1(6)
C1	4232.3(18)	492.9(18)	8602(2)	36.2(7)
C2	4068(2)	1139.5(19)	9171(3)	43.5(8)
C3	3603(2)	1052(2)	9962(3)	50.3(9)

C4	3331(2)	385(2)	10163(3)	49.3(9)
C5	3492.7(19)	-274.8(19)	9628(3)	40.6(7)
C6	3204(2)	-968(2)	9863(3)	52.3(9)
C7	3359(3)	-1601(2)	9346(4)	61.5(10)
C8	3817(3)	-1561(2)	8584(4)	57.1(9)
C9	4107(2)	-892.8(19)	8336(3)	45.9(8)
C10	3951.5(19)	-227.9(17)	8838(3)	35.7(7)
C11	4675.6(19)	557.5(18)	7800(3)	35.8(6)
C12	5483(2)	1222.1(17)	6776(3)	38.9(7)
C13	5552(2)	2032.9(19)	6500(3)	47.0(8)
C14	6378(2)	879(2)	7331(3)	49.4(8)
C15	6345(2)	55(2)	7540(3)	43.8(8)
C16	6571(2)	-224(2)	8694(3)	52.1(9)
C17	6490(3)	-969(3)	8881(4)	65.0(11)
C18	6177(3)	-1447(3)	7932(4)	67.5(11)
C19	5957(3)	-1177(2)	6778(4)	65.6(11)
C20	6043(2)	-433(2)	6586(3)	54.7(9)
O1A	681(2)	-1629.4(14)	4656(2)	62.7(7)
O2A	-829(2)	-1976.4(15)	-183(2)	62.6(7)
O3A	-337(2)	-2376.4(14)	1719(2)	69.0(8)
N1A	-20.3(17)	-1011.2(16)	2597(2)	39.5(6)
C1A	764(2)	-336.7(18)	4399(3)	36.7(7)
C2A	943(2)	-991(2)	5119(3)	45.4(8)
C3A	1414(2)	-918(2)	6382(3)	53.9(9)
C4A	1683(2)	-254(2)	6876(3)	51.6(9)
C5A	1516(2)	414(2)	6195(3)	43.0(8)
C6A	1796(2)	1102(2)	6753(3)	54.7(10)
C7A	1623(3)	1743(2)	6102(4)	61.9(10)
C8A	1171(3)	1715(2)	4874(4)	58.9(10)
C9A	889(2)	1050.5(19)	4303(3)	46.9(8)
C10A	1052.8(19)	380.5(18)	4939(3)	37.3(7)
C11A	301.6(19)	-394.0(18)	3154(3)	36.2(7)
C12A	-494(2)	-1073.2(18)	1310(3)	39.0(7)
C13A	-533(2)	-1886.1(19)	980(3)	45.8(8)
C14A	-1396(2)	-762(2)	944(3)	51.3(9)
C15A	-1430(2)	57(2)	1122(3)	46.6(8)
C16A	-1707(2)	350(2)	1991(4)	58.4(10)
C17A	-1714(3)	1107(3)	2162(5)	77.4(14)
C18A	-1436(3)	1577(3)	1484(5)	88.0(16)
C19A	-1163(4)	1300(3)	631(5)	82.3(14)
C20A	-1164(3)	545(2)	440(4)	62.4(10)

Table 8. Anisotropic displacement parameters (Å2×103) for the crystal structure of **1**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$

Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**

O1	83.0(19)	49.2(15)	55.7(15)	-12.1(12)	39.3(14)	-8.7(13)
O2	109(2)	45.3(16)	62.2(17)	8.0(13)	54.6(17)	-2.0(15)
O3	118(3)	44.8(15)	71.5(18)	-2.3(14)	56.8(19)	-1.5(16)
N1	44.2(15)	42.1(16)	34.0(13)	-2.3(12)	17.6(12)	-3.8(12)
C1	34.3(16)	47.3(18)	27.2(14)	-0.4(12)	11.2(13)	-1.5(13)
C2	46.2(18)	51(2)	34.5(16)	-7.1(14)	16.1(14)	-3.9(15)
C3	56(2)	61(2)	41.3(18)	-12.2(16)	26.3(17)	1.0(17)
C4	41.9(18)	76(3)	37.5(17)	-2.5(17)	22.8(15)	-2.9(17)
C5	32.4(15)	57(2)	30.9(15)	3.2(14)	9.7(13)	-1.3(14)
C6	44.4(19)	70(3)	46(2)	12.8(18)	21.5(16)	-2.8(17)
C7	65(2)	55(2)	69(3)	12(2)	30(2)	-9.0(19)
C8	64(2)	48(2)	63(2)	1.6(17)	28(2)	-2.4(18)
C9	48.2(19)	50(2)	44.5(18)	0.0(15)	22.3(16)	-1.8(15)
C10	31.1(15)	47.6(18)	26.7(14)	4.0(12)	8.6(12)	-1.5(13)
C11	34.1(15)	44.4(17)	28.2(14)	-0.4(12)	10.5(12)	-0.9(13)
C12	44.9(18)	41.2(17)	33.0(16)	1.7(13)	17.1(14)	-4.2(14)
C13	56(2)	48(2)	38.6(18)	3.9(15)	18.5(16)	-4.6(16)
C14	44.4(19)	54(2)	53(2)	6.9(16)	21.0(17)	-3.5(16)
C15	33.9(16)	54(2)	45.2(18)	7.3(16)	16.7(14)	1.3(15)
C16	41.3(18)	70(2)	42.6(18)	6.2(17)	11.8(15)	-3.3(17)
C17	51(2)	80(3)	60(2)	28(2)	14.6(19)	1(2)
C18	53(2)	57(2)	86(3)	17(2)	16(2)	3.5(19)
C19	62(3)	62(3)	69(3)	-11(2)	19(2)	1(2)
C20	55(2)	66(2)	44.2(19)	3.2(17)	19.4(17)	8.7(18)
O1A	90(2)	49.4(16)	46.2(14)	9.0(12)	22.1(14)	-10.4(14)
O2A	88(2)	49.9(16)	45.1(14)	-10.5(12)	18.0(14)	3.8(15)
O3A	103(2)	47.9(15)	53.3(16)	4.5(13)	24.6(16)	0.8(15)
N1A	44.7(15)	43.8(16)	31.2(13)	2.4(12)	15.2(11)	-2.7(12)
C1A	36.0(15)	44.6(18)	32.7(15)	5.3(13)	16.1(13)	-0.6(13)
C2A	49.1(19)	54(2)	36.6(17)	8.1(15)	19.8(15)	-1.4(16)
C3A	55(2)	68(2)	35.4(17)	17.1(17)	12.4(16)	-0.9(18)
C4A	39.7(18)	82(3)	29.1(15)	4.3(17)	7.9(14)	-0.4(17)
C5A	32.1(15)	62(2)	38.0(16)	-4.7(15)	16.5(13)	-1.3(15)
C6A	42.7(19)	77(3)	43.0(19)	-14.0(19)	13.6(16)	-1.5(18)
C7A	59(2)	62(3)	64(2)	-22(2)	22(2)	-2.6(19)
C8A	61(2)	52(2)	64(2)	-3.8(19)	23(2)	7.0(18)
C9A	51(2)	48(2)	41.2(18)	-3.6(15)	15.6(16)	5.5(15)
C10A	29.3(14)	53(2)	32.0(15)	-1.7(14)	14.5(12)	2.2(13)
C11A	34.4(15)	43.8(17)	33.5(15)	4.6(13)	16.0(13)	1.2(13)
C12A	40.7(17)	44.8(18)	33.4(16)	-2.3(13)	15.5(14)	-3.7(14)
C13A	46.5(19)	51(2)	43.3(19)	-5.5(16)	20.7(16)	-1.4(16)
C14A	41.3(19)	53(2)	57(2)	-9.9(17)	14.2(16)	-3.7(16)
C15A	35.8(17)	55(2)	42.7(18)	-3.0(16)	6.5(14)	5.7(15)
C16A	48(2)	74(3)	54(2)	-9.4(19)	20.1(18)	3.5(18)
C17A	69(3)	90(4)	75(3)	-29(3)	29(2)	8(3)
C18A	83(4)	65(3)	116(4)	-21(3)	36(3)	5(3)
C19A	93(4)	62(3)	100(4)	10(3)	44(3)	4(3)
C20A	67(3)	67(3)	57(2)	-0.8(19)	28(2)	10(2)

Table 9. Bond lengths for the crystal structure of **1**.

Atom	Atom	Length/Å
O1	C2	1.286(4)
O2	C13	1.297(4)
O3	C13	1.200(4)
N1	C11	1.307(4)
N1	C12	1.459(4)
C1	C2	1.424(4)
C1	C10	1.445(4)
C1	C11	1.411(4)
C2	C3	1.432(5)
C3	C4	1.340(5)
C4	C5	1.420(5)
C5	C6	1.406(5)
C5	C10	1.418(4)
C6	C7	1.365(6)
C7	C8	1.386(5)
C8	C9	1.371(5)
C9	C10	1.405(5)
C12	C13	1.512(5)
C12	C14	1.543(5)
C14	C15	1.511(5)
C15	C16	1.381(5)
C15	C20	1.380(5)
C16	C17	1.375(6)
C17	C18	1.366(6)
C18	C19	1.376(6)
C19	C20	1.379(6)
O1A	C2A	1.285(4)
O2A	C13A	1.300(4)
O3A	C13A	1.206(4)
N1A	C11A	1.309(4)
N1A	C12A	1.454(4)
C1A	C2A	1.424(4)
C1A	C10A	1.448(4)
C1A	C11A	1.408(4)
C2A	C3A	1.431(5)
C3A	C4A	1.340(5)
C4A	C5A	1.422(5)
C5A	C6A	1.407(5)
C5A	C10A	1.416(4)
C6A	C7A	1.363(6)
C7A	C8A	1.384(6)
C8A	C9A	1.375(5)
C9A	C10A	1.399(5)
C12A	C13A	1.513(5)
C12A	C14A	1.530(5)
C14A	C15A	1.496(5)
C15A	C16A	1.382(5)
C15A	C20A	1.376(5)

C16A	C17A	1.380(6)
C17A	C18A	1.364(7)
C18A	C19A	1.351(7)
C19A	C20A	1.381(6)

Table 10. Bond angles for the crystal structure of **1**.

Atom	Atom	Atom	Angle/°
C11	N1	C12	123.9(3)
C2	C1	C10	120.8(3)
C11	C1	C2	119.5(3)
C11	C1	C10	119.6(3)
O1	C2	C1	121.2(3)
O1	C2	C3	121.0(3)
C1	C2	C3	117.8(3)
C4	C3	C2	121.2(3)
C3	C4	C5	122.7(3)
C6	C5	C4	121.4(3)
C6	C5	C10	119.7(3)
C10	C5	C4	119.0(3)
C7	C6	C5	121.2(3)
C6	C7	C8	119.4(4)
C9	C8	C7	120.8(4)
C8	C9	C10	121.6(3)
C5	C10	C1	118.5(3)
C9	C10	C1	124.2(3)
C9	C10	C5	117.3(3)
N1	C11	C1	124.7(3)
N1	C12	C13	107.9(3)
N1	C12	C14	112.0(3)
C13	C12	C14	110.0(3)
O2	C13	C12	111.8(3)
O3	C13	O2	125.3(3)
O3	C13	C12	122.8(3)
C15	C14	C12	112.1(3)
C16	C15	C14	120.6(3)
C20	C15	C14	121.1(3)
C20	C15	C16	118.2(3)
C17	C16	C15	120.6(4)
C18	C17	C16	121.0(4)
C17	C18	C19	119.1(4)
C18	C19	C20	120.2(4)
C19	C20	C15	121.0(4)
C11A	N1A	C12A	124.7(3)
C2A	C1A	C10A	120.6(3)
C11A	C1A	C2A	119.3(3)
C11A	C1A	C10A	120.2(3)
O1A	C2A	C1A	121.3(3)
O1A	C2A	C3A	120.5(3)
C1A	C2A	C3A	118.2(3)

C4A	C3A	C2A	121.0(3)
C3A	C4A	C5A	122.8(3)
C6A	C5A	C4A	121.0(3)
C6A	C5A	C10A	120.0(3)
C10A	C5A	C4A	119.1(3)
C7A	C6A	C5A	120.9(3)
C6A	C7A	C8A	119.5(4)
C9A	C8A	C7A	120.9(4)
C8A	C9A	C10A	121.3(3)
C5A	C10A	C1A	118.4(3)
C9A	C10A	C1A	124.2(3)
C9A	C10A	C5A	117.4(3)
N1A	C11A	C1A	124.5(3)
N1A	C12A	C13A	107.7(3)
N1A	C12A	C14A	112.7(3)
C13A	C12A	C14A	109.6(3)
O2A	C13A	C12A	111.2(3)
O3A	C13A	O2A	125.6(3)
O3A	C13A	C12A	123.1(3)
C15A	C14A	C12A	114.0(3)
C16A	C15A	C14A	121.6(3)
C20A	C15A	C14A	120.7(3)
C20A	C15A	C16A	117.7(4)
C17A	C16A	C15A	120.8(4)
C18A	C17A	C16A	120.3(4)
C19A	C18A	C17A	119.7(5)
C18A	C19A	C20A	120.5(5)
C15A	C20A	C19A	121.0(4)

Table 11. Torsion angles for the crystal structure of **1**.

A	B	C	D	Angle/°
O1	C2	C3	C4	-179.4(3)
N1	C12	C13	O2	-168.7(3)
N1	C12	C13	O3	13.0(5)
N1	C12	C14	C15	64.2(4)
C1	C2	C3	C4	0.0(5)
C2	C1	C10	C5	1.3(4)
C2	C1	C10	C9	-178.4(3)
C2	C1	C11	N1	5.1(4)
C2	C3	C4	C5	0.9(6)
C3	C4	C5	C6	179.5(3)
C3	C4	C5	C10	-0.8(5)
C4	C5	C6	C7	179.9(3)
C4	C5	C10	C1	-0.4(4)
C4	C5	C10	C9	179.3(3)
C5	C6	C7	C8	0.6(6)
C6	C5	C10	C1	179.3(3)
C6	C5	C10	C9	-1.0(4)
C6	C7	C8	C9	-0.6(6)

C7	C8	C9	C10	-0.1(6)
C8	C9	C10	C1	-179.4(3)
C8	C9	C10	C5	0.9(5)
C10	C1	C2	O1	178.3(3)
C10	C1	C2	C3	-1.2(4)
C10	C1	C11	N1	-174.8(3)
C10	C5	C6	C7	0.2(5)
C11	N1	C12	C13	164.4(3)
C11	N1	C12	C14	-74.5(4)
C11	C1	C2	O1	-1.6(5)
C11	C1	C2	C3	178.9(3)
C11	C1	C10	C5	-178.7(3)
C11	C1	C10	C9	1.6(4)
C12	N1	C11	C1	178.6(3)
C12	C14	C15	C16	-108.9(4)
C12	C14	C15	C20	67.4(4)
C13	C12	C14	C15	-175.8(3)
C14	C12	C13	O2	68.9(4)
C14	C12	C13	O3	-109.4(4)
C14	C15	C16	C17	176.0(3)
C14	C15	C20	C19	-175.4(3)
C15	C16	C17	C18	-0.6(6)
C16	C15	C20	C19	1.0(5)
C16	C17	C18	C19	1.2(6)
C17	C18	C19	C20	-0.6(6)
C18	C19	C20	C15	-0.5(6)
C20	C15	C16	C17	-0.5(5)
O1A	C2A	C3A	C4A	-179.3(4)
N1A	C12A	C13A	O2A	-169.9(3)
N1A	C12A	C13A	O3A	12.3(5)
N1A	C12A	C14A	C15A	65.7(4)
C1A	C2A	C3A	C4A	-0.2(5)
C2A	C1A	C10A	C5A	0.0(4)
C2A	C1A	C10A	C9A	-178.5(3)
C2A	C1A	C11A	N1A	3.4(5)
C2A	C3A	C4A	C5A	0.5(6)
C3A	C4A	C5A	C6A	178.8(3)
C3A	C4A	C5A	C10A	-0.6(5)
C4A	C5A	C6A	C7A	-178.9(3)
C4A	C5A	C10A	C1A	0.3(4)
C4A	C5A	C10A	C9A	179.0(3)
C5A	C6A	C7A	C8A	-0.5(6)
C6A	C5A	C10A	C1A	-179.1(3)
C6A	C5A	C10A	C9A	-0.4(4)
C6A	C7A	C8A	C9A	0.4(6)
C7A	C8A	C9A	C10A	-0.4(6)
C8A	C9A	C10A	C1A	179.0(3)
C8A	C9A	C10A	C5A	0.4(5)
C10A	C1A	C2A	O1A	179.0(3)
C10A	C1A	C2A	C3A	-0.1(5)
C10A	C1A	C11A	N1A	-176.5(3)

C10A	C5A	C6A	C7A	0.5(5)
C11A	N1A	C12A	C13A	164.2(3)
C11A	N1A	C12A	C14A	-74.9(4)
C11A	C1A	C2A	O1A	-0.9(5)
C11A	C1A	C2A	C3A	180.0(3)
C11A	C1A	C10A	C5A	180.0(3)
C11A	C1A	C10A	C9A	1.4(4)
C12A	N1A	C11A	C1A	-179.6(3)
C12A	C14A	C15A	C16A	-111.3(4)
C12A	C14A	C15A	C20A	67.0(4)
C13A	C12A	C14A	C15A	-174.4(3)
C14A	C12A	C13A	O2A	67.2(4)
C14A	C12A	C13A	O3A	-110.6(4)
C14A	C15A	C16A	C17A	178.4(4)
C14A	C15A	C20A	C19A	-177.5(4)
C15A	C16A	C17A	C18A	-0.9(7)
C16A	C15A	C20A	C19A	0.8(6)
C16A	C17A	C18A	C19A	0.8(8)
C17A	C18A	C19A	C20A	0.1(8)
C18A	C19A	C20A	C15A	-0.9(8)
C20A	C15A	C16A	C17A	0.1(6)

Table 12. Hydrogen atom coordinates ($Å \times 10^4$) and isotropic displacement parameters ($Å^2 \times 10^3$) for the crystal structure of **1**.

Atom	***x***	***y***	***z***	**U(eq)**
H1	4930(30)	1620(20)	7960(30)	56(11)
H3	3488.22	1466.68	10342.87	60
H4	3024.2	351.89	10672.93	59
H6	2901.44	-996.57	10380.11	63
H7	3159.67	-2055.4	9504.04	74
H8	3928.21	-1991.41	8237.17	69
H9	4413.31	-879.78	7823.58	55
H11	4733.15	132.92	7392.21	43
H12	5167.03	961.29	6025.51	47
H14A	6688.04	966.4	6795.39	59
H14B	6684.32	1121.5	8091.96	59
H16	6779.38	93.33	9351.27	63
H17	6650.32	-1148.82	9664.3	78
H18	6114.72	-1948.06	8065.62	81
H19	5748.38	-1497.83	6124.58	79
H20	5896.1	-256.29	5801.92	66
H1A	100(30)	-1430(20)	3090(40)	57(11)
H3A	1536.06	-1338.5	6867.42	65
H4A	1991.48	-228.12	7699.48	62
H6A	2103.42	1120.14	7576.94	66
H7A	1807.38	2195.51	6480.19	74
H8A	1055.58	2151.96	4428.55	71
H9A	583.38	1046.29	3477.56	56
H11A	218.99	36.36	2694.68	43

H12A	-189.08	-804.34	873.16	47
H14C	-1701.92	-875.81	101.27	62
H14D	-1685.88	-1010.01	1411	62
H16A	-1889.67	34.19	2466.88	70
H17A	-1909.31	1296.73	2742.97	93
H18A	-1435.32	2086.63	1607.86	106
H19A	-972.97	1620.32	168.35	99
H20A	-981.39	362.87	-158.43	75
H2A	-790(30)	-2430(16)	-410(40)	84(15)
H2	5800(30)	2573(15)	5370(40)	74(14)