Supplementary Information

Structural, theoretical investigations, Hirshfeld surface analyses and cytotoxicity of a naphthalene based chiral compound

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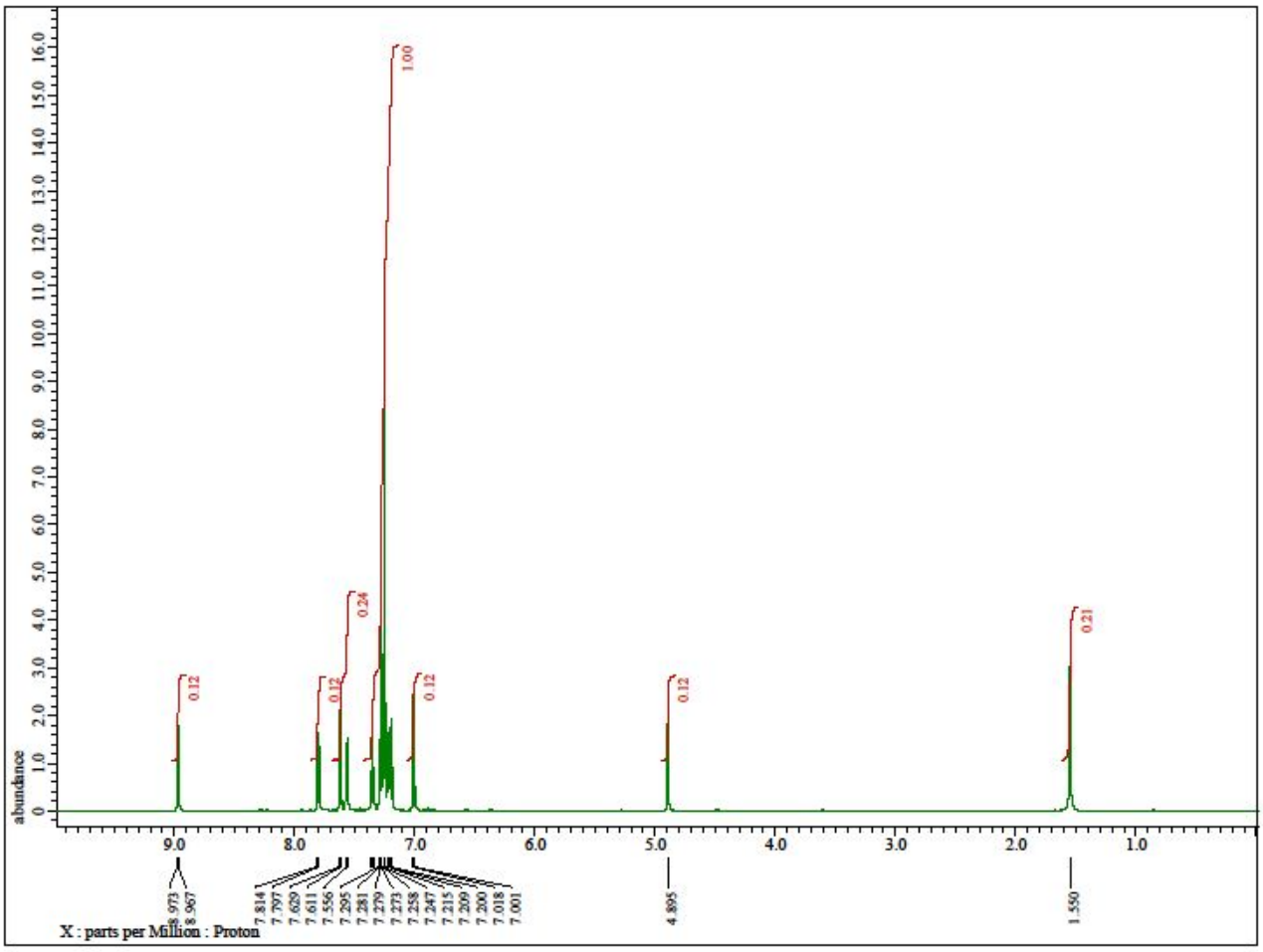
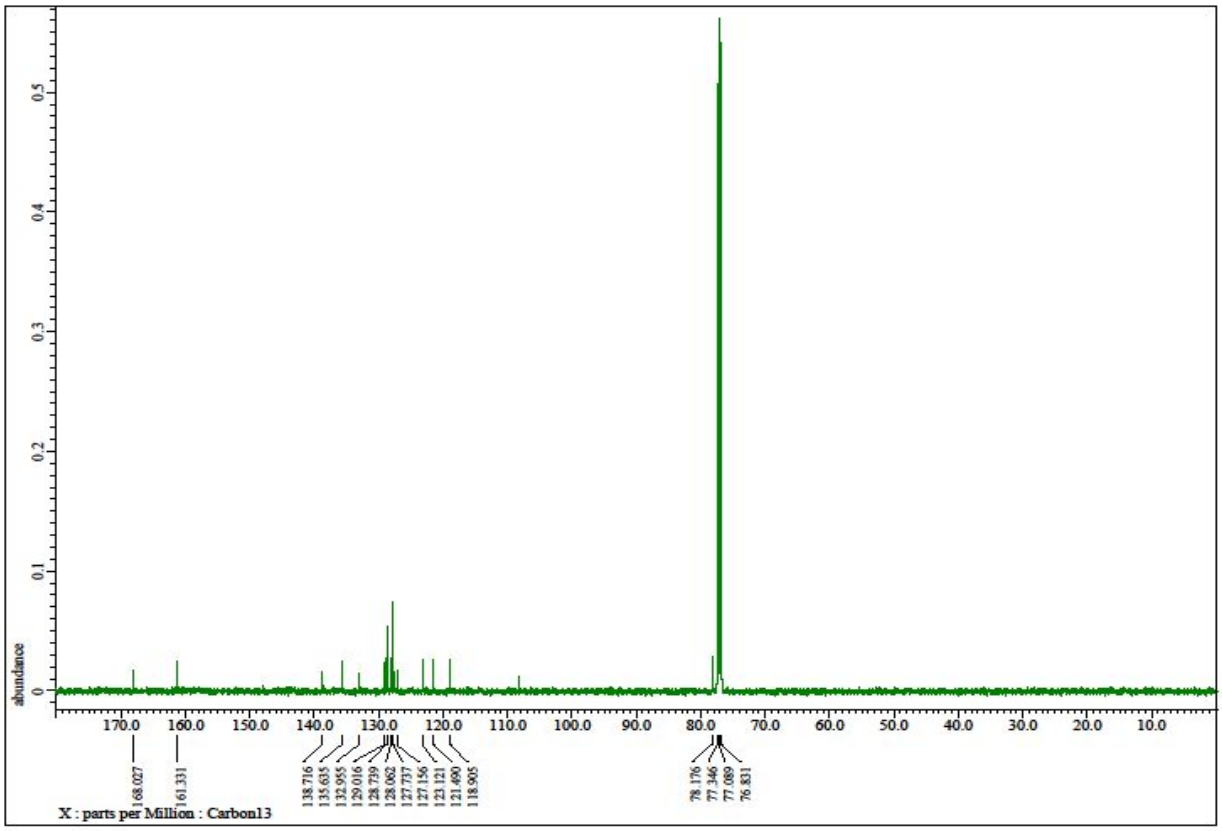
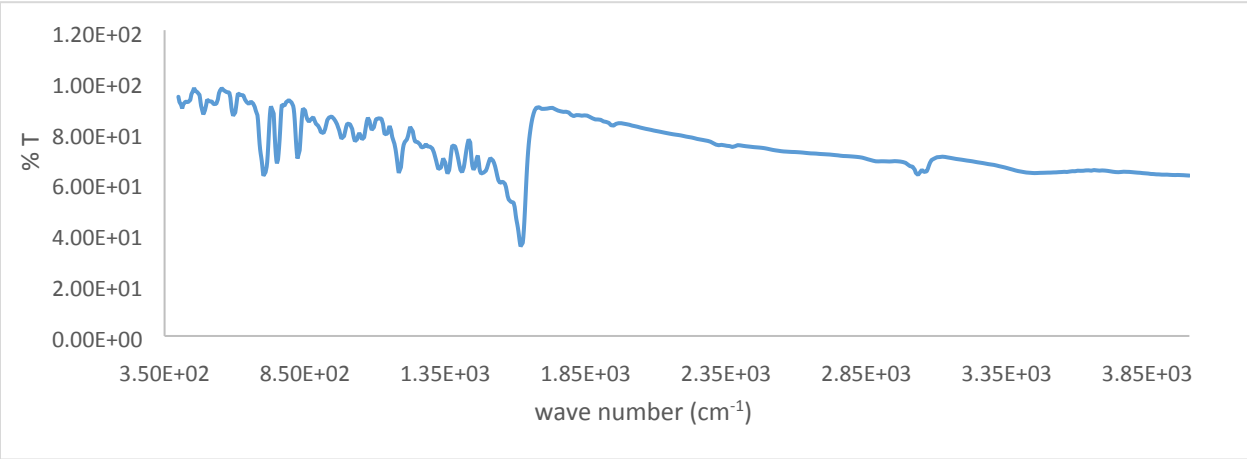


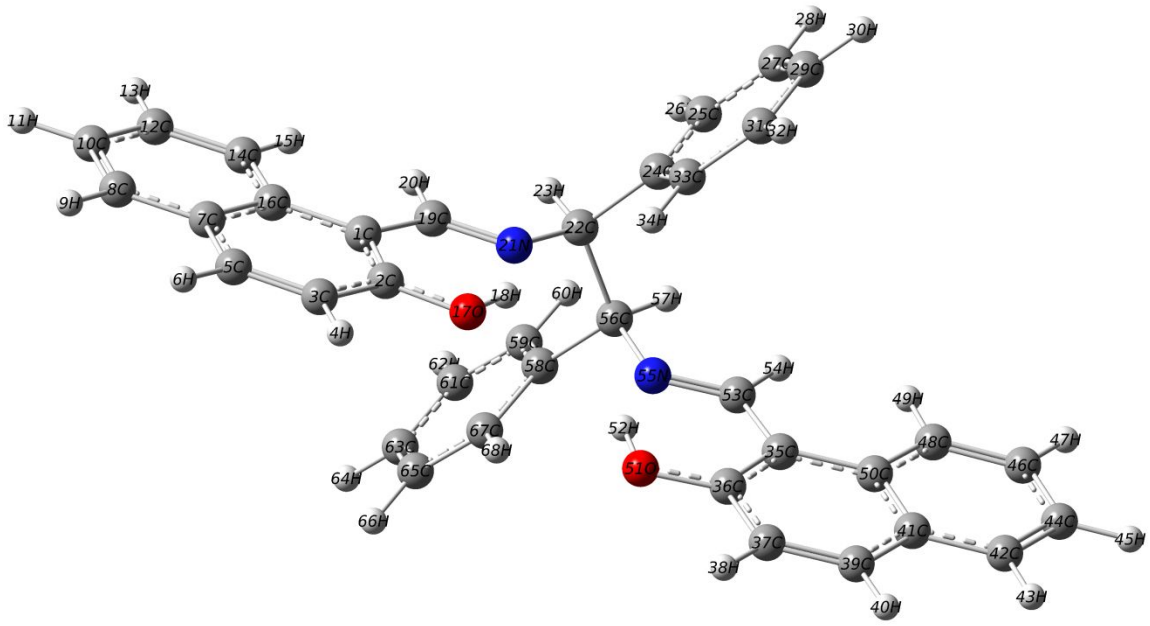
Supplementary Information Figure S1. ^{1}H NMR Spectrum of Schiff base compound



Supplementary Information Figure S2. ^{13}C NMR Spectrum of Schiff base compound



Supplementary Information Figure S3. IR Spectrum of Schiff base compound



Supplementary Information Figure S4. Atom numbering of the optimized structure (See Table S1, S2 and S3).

Table S1 The calculated geometric parameters of the studied compound[a].

Parameter	Calc	Exp
R(1-2)	1.411	1.412
R(1-16)	1.445	1.447
R(1-19)	1.450	1.440
R(2-3)	1.421	1.424
R(2-17)	1.334	1.318
R(3-5)	1.367	1.355
R(5-7)	1.425	1.426
R(7-8)	1.417	1.420
R(7-16)	1.433	1.423
R(8-10)	1.377	1.365
R(10-12)	1.410	1.404
R(12-14)	1.380	1.379
R(14-16)	1.421	1.415
R(19-21)	1.291	1.296
R(21-22)	1.449	1.457
R(22-24)	1.523	1.522
R(22-56)	1.580	1.570
R(24-25)	1.401	1.390
R(24-33)	1.400	1.392
R(25-27)	1.395	1.393
R(27-29)	1.396	1.385
R(29-31)	1.395	1.385
R(31-33)	1.396	1.394
R(35-36)	1.411	1.412
R(35-50)	1.445	1.447
R(35-53)	1.450	1.440
R(36-37)	1.421	1.424
R(36-51)	1.334	1.318
R(37-39)	1.367	1.355
R(39-41)	1.425	1.426
R(41-42)	1.417	1.420
R(41-50)	1.433	1.423

R(42-44)	1.377	1.365
R(44-46)	1.410	1.404
R(46-48)	1.380	1.379
R(48-50)	1.421	1.415
R(53-55)	1.291	1.296
R(55-56)	1.449	1.457
R(56-58)	1.523	1.522
R(58-59)	1.401	1.390
R(58-67)	1.400	1.392
R(59-61)	1.395	1.393
R(61-63)	1.396	1.385
R(63-65)	1.395	1.385
R(65-67)	1.396	1.394
A(2-1-16)	119.264	119.842
A(2-1-19)	118.805	118.868
A(1-2-3)	120.658	119.383
A(1-2-17)	122.516	122.344
A(16-1-19)	121.930	121.127
A(1-16-7)	119.020	118.987
A(1-16-14)	123.747	123.272
A(1-19-20)	118.120	119.073
A(1-19-21)	122.445	121.875
A(3-2-17)	116.825	118.262
A(2-3-5)	120.222	120.885
A(2-17-18)	106.795	102.547
A(3-5-7)	121.643	121.901
A(5-7-8)	120.784	121.294
A(5-7-16)	119.191	118.907
A(8-7-16)	120.024	119.770
A(7-8-10)	121.140	120.811
A(7-16-14)	117.233	117.739
A(8-10-12)	119.213	119.836
A(10-12-14)	120.926	120.703
A(13-12-14)	119.384	119.653

A(12-14-16)	121.464	121.051
A(19-21-22)	119.388	119.827
A(21-22-24)	111.770	111.492
A(21-22-56)	110.383	108.679
A(24-22-56)	111.035	110.887
A(22-24-25)	119.039	118.543
A(22-24-33)	122.236	122.177
A(22-56-55)	110.383	108.679
A(22-56-57)	105.160	108.598
A(22-56-58)	111.035	110.887
A(25-24-33)	118.708	119.268
A(24-25-27)	120.901	120.362
A(24-33-31)	120.452	120.192
A(24-33-34)	119.619	119.905
A(25-27-29)	119.976	120.167
A(27-29-31)	119.547	119.772
A(29-31-33)	120.414	120.227
A(36-35-50)	119.264	119.842
A(36-35-53)	118.805	118.868
A(35-36-37)	120.658	119.383
A(35-36-51)	122.516	122.344
A(50-35-53)	121.930	121.127
A(35-50-41)	119.020	118.987
A(35-50-48)	123.747	123.272
A(35-53-54)	118.120	119.073
A(35-53-55)	122.445	121.875
A(37-36-51)	116.825	118.262
A(36-37-39)	120.222	120.885
A(36-51-52)	106.795	102.547
A(37-39-41)	121.643	121.901
A(39-41-42)	120.784	121.294
A(39-41-50)	119.191	118.907
A(42-41-50)	120.024	119.770
A(41-42-44)	121.140	120.811

A(41-50-48)	117.233	117.739
A(42-44-46)	119.213	119.836
A(44-46-48)	120.926	120.703
A(46-48-50)	121.464	121.051
A(51-52-55)	148.983	157.601
A(53-55-56)	119.388	119.827
A(53-55-52)	100.402	96.040
A(55-56-58)	111.770	111.492
A(56-55-52)	140.183	143.048
A(56-58-59)	119.039	118.543
A(56-58-67)	122.236	122.177
A(59-58-67)	118.708	119.268
A(58-59-61)	120.901	120.362
A(58-67-65)	120.452	120.192
A(58-67-68)	119.619	119.905
A(59-61-63)	119.976	120.167
A(61-63-65)	119.547	119.772
A(63-65-67)	120.414	120.227

[a]Atom numbering refer to Supplementary Information Figure S1

Supplementary Information Table S2. The calculated natural charges of the studied compound

Atom	Charge	Atom	Charge
C1	-0.1931	C35	-0.1931
C2	0.4032	C36	0.4032
C3	-0.2791	C37	-0.2791
H4	0.2556	H38	0.2556
C5	-0.1754	C39	-0.1754
H6	0.2409	H40	0.2409
C7	-0.0807	C41	-0.0807
C8	-0.2012	C42	-0.2012
H9	0.2369	H43	0.2369
C10	-0.2517	C44	-0.2517
H11	0.2410	H45	0.2410
C12	-0.2231	C46	-0.2231
H13	0.2401	H47	0.2401
C14	-0.2306	C48	-0.2306
H15	0.2304	H49	0.2304
C16	-0.0119	C50	-0.0119
O17	-0.6872	O51	-0.6872
H18	0.5170	H52	0.5170
C19	0.1358	C53	0.1358
H20	0.1970	H54	0.1970
N21	-0.5373	N55	-0.5373
C22	-0.0581	C56	-0.0581
H23	0.2327	H57	0.2327
C24	-0.0480	C58	-0.0480
C25	-0.2377	C59	-0.2377
H26	0.2331	H60	0.2331
C27	-0.2331	C61	-0.2331
H28	0.2397	H62	0.2397
C29	-0.2391	C63	-0.2391
H30	0.2401	H64	0.2401
C31	-0.2277	C65	-0.2277

H32	0.2428	H66	0.2428
C33	-0.2223	C67	-0.2223
H34	0.2510	H68	0.2510

[a]Atom numbering refer to Supplementary Information Figure S1

Supplementary Table S3. The $E^{(2)}$ (kcal/mol) values for the charge transfer interactions in the studied compound

Donor NBO	**Acceptor NBO**	**$E^{(2)}$**	**Donor NBO**	**Acceptor NBO**	**$E^{(2)}$**
π→π*			**n→π***		
BD(2)C1-C2	BD*(2)C3-C5	12.09	LP(2)O17	BD*(2)C1-C2	42.84
BD(2)C1-C2	BD*(2)C7-C16	20.19	LP(2)O51	BD*(2)C35-C36	42.84
BD(2)C1-C2	BD*(2)C19-N21	24.62			
BD(2)C3-C5	BD*(2)C1-C2	20.13	**n→σ***		
BD(2)C3-C5	BD*(2)C7-C16	13.38	LP(1)O51	BD*(1)C35-C36	8.17
BD(2)C7-C16	BD*(2)C1-C2	13.99	LP(3)O51	BD*(1)C36-C37	5.16
BD(2)C7-C16	BD*(2)C3-C5	17.67	LP(3)O17	BD*(1)C2-C3	5.16
BD(2)C7-C16	BD*(2)C8-C10	18.29	LP(1)N21	BD*(1)C19-H20	10.12
BD(2)C7-C16	BD*(2)C12-C14	16.28	LP(1)N21	BD*(1)C22-H23	5.51
BD(2)C8-C10	BD*(2)C7-C16	15.88	LP(1)N55	BD*(1)C53-H54	10.12
BD(2)C8-C10	BD*(2)C12-C14	19.19	LP(1)N55	BD*(1)C56-H57	5.51
BD(2)C12-C14	BD*(2)C7-C16	17.33			
BD(2)C12-C14	BD*(2)C8-C10	16.67			
BD(2)C24-C25	BD*(2)C27-C29	20.86			
BD(2)C24-C25	BD*(2)C31-C33	19.23			
BD(2)C27-C29	BD*(2)C24-C25	20.05			
BD(2)C27-C29	BD*(2)C31-C33	20.05			
BD(2)C31-C33	BD*(2)C24-C25	21.37			
BD(2)C31-C33	BD*(2)C27-C29	20.57			
BD(2)C35-C36	BD*(2)C37-C39	12.09			
BD(2)C35-C36	BD*(2)C41-C50	20.19			
BD(2)C35-C36	BD*(2)C53-N55	24.62			
BD(2)C37-C39	BD*(2)C35-C36	20.13			
BD(2)C37-C39	BD*(2)C41-C50	13.38			
BD(2)C41-C50	BD*(2)C35-C36	13.99			
BD(2)C41-C50	BD*(2)C37-C39	17.67			
BD(2)C41-C50	BD*(2)C42-C44	18.29			
BD(2)C41-C50	BD*(2)C46-C48	16.28			
BD(2)C42-C44	BD*(2)C41-C50	15.88			
BD(2)C42-C44	BD*(2)C46-C48	19.19			

BD(2)C46-C48	BD*(2)C41-C50	17.33
BD(2)C46-C48	BD*(2)C42-C44	16.67
BD(2)C53-N55	BD*(2)C35-C36	6.06
BD(2)C58-C59	BD*(2)C61-C63	20.86
BD(2)C58-C59	BD*(2)C65-C67	19.23
BD(2)C61-C63	BD*(2)C58-C59	20.05
BD(2)C61-C63	BD*(2)C65-C67	20.05
BD(2)C61-C63	BD*(2)C58-C59	21.37
BD(2)C61-C63	BD*(2)C61-C63	20.57

[a]Atom numbering refer to **Fig. S1**

Crystal structure determination

The yellow prism crystal of the Schiff base compound. (1S,2S)-1,2-diphenyl-N,N'-bis[(E)-2-hydroxynaphthalen-1-ylmethylidene]ethane-1,2-diamine was mounted on a Rigaku Synergy Dualflex automatic diffractometer equipped with Pilatus 300K detector, and used for data collection. X-ray intensity data were collected with mirror monochromated CuK_α (λ = 1.54178 Å, micro-focus sealed PhotonJet X-ray tube) radiation at temperature of 100.0(1) K, with ω scan mode. The shuterless mode was used, and reflections inside Ewald sphere were collected up to θ = 70°. The unit cell parameters were determined from 1094 strongest reflections. Details concerning crystal data and refinement are given in Table 1. Examination of the same reference reflections, measured before and after measurement, showed no loss of the intensity during measurement. Lorentz, polarization and empirical absorption (using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm) corrections were applied during the data reduction. The structure was solved by partial structure expansion procedure. All the non-hydrogen atoms were refined anisotropically using full-matrix, least-squares technique on F^2. All the hydrogen atoms were found from difference Fourier synthesis after four cycles of anisotropic

refinement, and refined as “riding” on the adjacent atom with geometric idealisation after each cycle of refinement and individual isotropic displacement factors equal 1.2 times the value of equivalent displacement factors of the parent carbon atoms, and 1.5 times of parent oxygen atoms. The SHELXS[17], SHELXL[18] and SHELXTL[19] programs were used for all the calculations. Atomic scattering factors were taken from International Tables for Crystallography[20]. The Flack parameter was determined in the Parsons-Flack-Wagner extension[21] using 1043 quotients[22]. Selected interatomic bond distances and dihedral angles are listed in Table 2 and intermolecular interactions are listed in Table 3.