Supplementary materials of New organic-inorganic salt based on fluconazole drug: TD-DFT Benchmark and computational insights into halogen substitution

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Table S1

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Sn1	1.18781 (3)	0.14677 (2)	0.47919 (2)	0.03890 (8)
Cl6	1.25999 (11)	0.08587 (3)	0.63572 (9)	0.05174 (19)
Cl1	1.01125 (11)	0.18582 (3)	0.60870 (9)	0.0543 (2)
Cl4	1.35721 (11)	0.10812 (3)	0.33621 (8)	0.0534 (2)
Cl2	1.43827 (10)	0.18700 (3)	0.58938 (9)	0.05293 (19)
Cl5	0.94373 (11)	0.10427 (3)	0.37042 (9)	0.0559 (2)
Cl3	1.13177 (14)	0.20755 (3)	0.31815 (9)	0.0637 (2)
F2	0.5046 (2)	0.46091 (7)	0.5909 (2)	0.0590 (5)
O1	0.2655 (3)	0.35109 (7)	0.3613 (2)	0.0472 (5)
N1	0.3370 (3)	0.42854 (8)	0.2208 (3)	0.0403 (5)
F1	−0.0055 (4)	0.49542 (9)	0.7217 (3)	0.0903 (9)
N4	0.5973 (3)	0.32775 (9)	0.4857 (3)	0.0452 (6)
O2	0.1788 (3)	0.29241 (8)	0.5450 (3)	0.0635 (7)
O3	0.6540 (3)	0.18062 (8)	0.3026 (3)	0.0667 (7)
N2	0.3685 (4)	0.47119 (9)	0.1776 (3)	0.0535 (7)
N6	0.6745 (4)	0.26532 (11)	0.4142 (3)	0.0560 (7)
N3	0.1518 (4)	0.44026 (11)	0.0493 (3)	0.0546 (7)
C6	0.2626 (4)	0.41760 (10)	0.5007 (3)	0.0407 (6)
N5	0.7466 (4)	0.33679 (12)	0.4459 (3)	0.0595 (7)
C5	0.3360 (4)	0.45267 (10)	0.5814 (3)	0.0448 (7)
C12	0.5553 (5)	0.28516 (12)	0.4662 (4)	0.0559 (8)
C7	0.3672 (4)	0.38537 (10)	0.4320 (3)	0.0402 (6)
C11	0.5036 (4)	0.36322 (10)	0.5391 (3)	0.0450 (7)
C8	0.4543 (4)	0.40911 (11)	0.3319 (3)	0.0436 (7)
C4	0.2512 (5)	0.47946 (11)	0.6561 (4)	0.0533 (8)
C1	0.0900 (4)	0.41137 (11)	0.4926 (4)	0.0484 (7)
C3	0.0815 (5)	0.47052 (12)	0.6457 (4)	0.0594 (9)
C9	0.2087 (4)	0.41008 (12)	0.1430 (4)	0.0514 (7)
H9	0.164965	0.381162	0.151257	0.062*

C13	0.7876 (4)	0.29782 (14)	0.4028 (4)	0.0617 (9)
H13	0.884670	0.292939	0.367820	0.074*
C10	0.2530 (5)	0.47684 (13)	0.0732 (4)	0.0592 (9)
H10	0.241459	0.502925	0.021367	0.071*
C2	−0.0018 (5)	0.43763 (12)	0.5654 (4)	0.0588 (9)

Atomic displacement parameters (Å^2)

	U11	*U22*	*U33*	*U12*	*U13*	*U23*
Sn1	0.04669 (13)	0.03443 (12)	0.03599 (12)	−0.00020 (8)	0.00889 (8)	0.00013 (7)
Cl6	0.0634 (5)	0.0432 (4)	0.0522 (5)	0.0073 (3)	0.0200 (4)	0.0117 (3)
Cl1	0.0611 (5)	0.0537 (4)	0.0501 (5)	0.0112 (4)	0.0154 (4)	−0.0059 (3)
Cl4	0.0574 (4)	0.0621 (5)	0.0435 (4)	0.0033 (4)	0.0166 (4)	−0.0077 (3)
Cl2	0.0552 (4)	0.0473 (4)	0.0537 (5)	−0.0094 (3)	0.0035 (4)	−0.0009 (3)
Cl5	0.0534 (4)	0.0558 (5)	0.0573 (5)	−0.0103 (4)	0.0077 (4)	−0.0102 (4)
Cl3	0.1003 (7)	0.0460 (4)	0.0413 (4)	0.0004 (4)	0.0041 (4)	0.0080 (3)
F2	0.0517 (10)	0.0549 (11)	0.0704 (14)	−0.0165 (9)	0.0111 (9)	−0.0154 (10)
O1	0.0577 (13)	0.0413 (12)	0.0417 (12)	−0.0112 (9)	0.0073 (10)	−0.0032 (9)
N1	0.0432 (12)	0.0411 (13)	0.0376 (13)	−0.0027 (10)	0.0099 (10)	0.0000 (10)
F1	0.1039 (18)	0.0678 (15)	0.118 (2)	0.0022 (13)	0.0691 (18)	−0.0207 (15)
N4	0.0491 (14)	0.0453 (14)	0.0416 (14)	0.0022 (11)	0.0097 (11)	0.0041 (11)
O2	0.0801 (17)	0.0470 (13)	0.0672 (17)	−0.0070 (12)	0.0238 (14)	0.0006 (12)
O3	0.0649 (15)	0.0568 (15)	0.083 (2)	0.0041 (12)	0.0257 (14)	0.0036 (13)
N2	0.0603 (16)	0.0411 (14)	0.0581 (18)	−0.0023 (12)	0.0089 (14)	0.0068 (12)
N6	0.0636 (18)	0.0497 (16)	0.0545 (18)	0.0105 (14)	0.0110 (14)	0.0005 (13)
N3	0.0513 (16)	0.0654 (19)	0.0448 (16)	0.0036 (14)	0.0031 (13)	0.0060 (14)
C6	0.0474 (15)	0.0373 (14)	0.0383 (15)	−0.0037 (12)	0.0102 (12)	0.0011 (12)
N5	0.0432 (14)	0.0671 (18)	0.068 (2)	−0.0047 (14)	0.0099 (14)	−0.0050 (16)
C5	0.0501 (16)	0.0391 (15)	0.0455 (17)	−0.0058 (12)	0.0101 (13)	0.0042 (12)
C12	0.064 (2)	0.0450 (18)	0.062 (2)	0.0035 (15)	0.0200 (17)	0.0076 (15)
C7	0.0453 (15)	0.0376 (14)	0.0374 (15)	−0.0050 (11)	0.0074 (12)	−0.0018 (11)
C11	0.0559 (17)	0.0419 (15)	0.0371 (16)	0.0025 (13)	0.0086 (14)	−0.0018 (12)
C8	0.0424 (15)	0.0494 (17)	0.0384 (16)	−0.0042 (12)	0.0066 (12)	0.0023 (12)
C4	0.072 (2)	0.0367 (16)	0.054 (2)	−0.0064 (15)	0.0190 (17)	−0.0054 (14)
C1	0.0500 (17)	0.0439 (16)	0.0523 (19)	−0.0067 (13)	0.0120 (14)	0.0014 (14)
C3	0.074 (2)	0.0447 (18)	0.069 (2)	0.0047 (16)	0.037 (2)	0.0013 (16)
C9	0.0547 (18)	0.0519 (18)	0.0465 (18)	−0.0080 (14)	0.0067 (15)	0.0003 (14)
C13	0.0476 (18)	0.074 (2)	0.063 (2)	0.0078 (17)	0.0090 (17)	−0.0067 (19)
C10	0.064 (2)	0.0536 (19)	0.059 (2)	0.0090 (16)	0.0084 (18)	0.0109 (16)
C2	0.0530 (18)	0.055 (2)	0.074 (2)	−0.0018 (16)	0.0246 (18)	0.0069 (18)

Table S2
Selected Bond Lengths (Å) and Bond Angles (°) for (H2Fluconazole)$SnCl_6.2H_2O$.

Selected Bond lengths			
Sn1-Cl6	**2.4090 (8)**	**N3-C9**	**1.329 (5)**
Sn1-Cl5	2.4156 (8)	**N3-C10**	1.343 (5)
Sn1-Cl1	2.4161 (8)	**C6-C1**	1.386 (4)
Sn1-Cl2	2.4242 (8)	**C6-C5**	1.386 (4)
Sn1-Cl3	2.4251 (9)	**C6-C7**	1.527 (4)
Sn1-Cl4	2.4669 (8)	**N5-C13**	1.295 (5)
F2-C5	1.360 (4)	**C5-C4**	1.371 (5)
O1-C7	1.411 (4)	**C7-C8**	1.523 (4)
O1-H1	0.8200	**C7-C11**	1.546 (4)
N1-C9	1.300 (4)	**N2-C10**	1.294 (5)
N1-N2	1.371 (4)	**N6-C12**	1.320 (5)
N1-C8	1.457 (4)	**N6-C13**	1.339 (5)
F1-C3	1.360 (4)	**C4-C3**	1.372 (5)
N4-C12	1.302 (4)	**C1-C2**	1.384 (5)
N4-N5	1.366 (4)	**C3-C2**	1.364 (6)
N4-C11	1.455 (4)		

Selected Bond Angles			
Cl6-Sn1-Cl5	**89.94 (3)**	**O1-C7-C8**	**105.7 (2)**
Cl6-Sn1-Cl1	94.21 (3)	**O1-C7-C6**	111.6 (2)
Cl5-Sn1-Cl1	89.64 (3)	**C8-C7-C6**	113.2 (2)
Cl6-Sn1-Cl2	88.53 (3)	**O1-C7-C11**	109.4 (2)
Cl5-Sn1-Cl2	178.03 (3)	**C8-C7-C11**	109.0 (2)
Cl1-Sn1-Cl2	91.72 (3)	**C6-C7-C11**	107.8 (2)
Cl6-Sn1-Cl3	176.56 (3)	**N4-C11-C7**	112.2 (3)
Cl5-Sn1-Cl3	91.89 (3)	**N1-C8-C7**	113.8 (2)
Cl1-Sn1-Cl3	88.72 (3)	**C5-C4-C3**	116.0 (3)
Cl2-Sn1-Cl3	89.58 (3)	**C2-C1-C6**	121.6 (3)
Cl6-Sn1-Cl4	88.26 (3)	**F1-C3-C2**	119.1 (3)
Cl5-Sn1-Cl4	88.52 (3)	**F1-C3-C4**	117.6 (4)
Cl1-Sn1-Cl4	176.92 (3)	**C2-C3-C4**	123.3 (3)
Cl2-Sn1-Cl4	90.18 (3)	**N1-C9-N3**	107.2 (3)
Cl3-Sn1-Cl4	88.87 (3)	**C1-C6-C7**	121.5 (3)
C9-N1-N2	110.7 (3)	**C5-C6-C7**	122.2 (3)
C9-N1-C8	130.0 (3)	**C13-N5-N4**	103.1 (3)
N2-N1-C8	118.9 (2)	**F2-C5-C4**	116.8 (3)
C12-N4-N5	110.9 (3)	**F2-C5-C6**	118.7 (3)
C12-N4-C11	127.6 (3)	**C4-C5-C6**	124.5 (3)
N5-N4-C11	121.5 (3)	**N4-C12-N6**	107.5 (3)
C10-N2-N1	104.0 (3)	**N5-C13-N6**	112.3 (3)
C12-N6-C13	106.1 (3)	**N2-C10-N3**	111.4 (3)
C9-N3-C10	106.7 (3)	**C3-C2-C1**	118.4 (3)
C1-C6-C5	116.2 (3)		

Table S3: Calculated UV-Vis spectrum, oscillator strength and the major contribution calculated using HSE1PBE functional.

λ_{cal} (nm)	Excitation energy (eV)	Oscillator strength	Major contributions
347.71	3.5657	0.0012	H -->L (0.705150
238.23	5.2043	0.0265	H-3 -->L+2 (0.60696)
219.39	5.6512	0.0126	H-10 -->L+2 (0.30488) H-8 -->L+2 (0.45574)

Table S4: Theoretical and experimental equilibrium geometry of the (H2Fluconazole).$SnCl_6.2H_2O$

	HSE1PBE	Exp	Error %
Sn-Cl4	2.5692	2.4669	3.98%
Sn-Cl2	2.3656	2.4090	1.83%
O1-H1	0.9803	0.8200	16.3%
N1-N2	1.3563	1.371	1.08%
F1-C3	1.3384	1.360	1.61%
C5-F2	1.3557	1.360	0.31%
C5-C4	1.3872	1.371	1.16%

xyz coordinates of the optimized geometries using HSEH1PBE functional

Sn	1.960313	5.381978	5.153225
Cl	1.518408	3.356576	6.588149
Cl	1.418836	6.745826	7.171278
Cl	2.742911	3.779412	3.386555
Cl	4.371846	5.362417	6.039703
Cl	-0.261855	5.381152	4.341681
Cl	2.683917	7.333745	3.907815
F	6.523035	1.558048	10.584922
O	3.260131	3.808861	9.039252
H	2.830469	3.504626	8.212299
N	4.571382	1.997279	7.157952
F	3.486012	-1.094141	12.944765
N	5.365865	5.517215	9.438756
N	3.788255	0.944088	7.500221
N	5.029543	7.335366	8.370605
N	3.677026	1.344376	5.349575

C	4.211995	2.011113	10.331782
N	6.597805	5.976631	9.109105
C	5.237250	1.261030	10.895264
C	4.417727	6.324632	8.979023
H	3.351790	6.165965	9.042587
C	4.457623	3.182265	9.376129
C	5.221103	4.267636	10.174629
H	6.226799	3.954803	10.450099
H	4.645342	4.463290	11.080544
C	5.308746	2.773944	8.148170
H	6.178231	2.201969	8.472032
H	5.636192	3.670281	7.618926
C	5.028221	0.213048	11.769851
H	5.858473	-0.346315	12.181472
C	2.913260	1.675902	10.710749
H	2.096753	2.254120	10.295837
C	3.718047	-0.083125	12.098904
C	4.510130	2.248472	5.860587
H	5.043332	3.005731	5.284428
C	6.359518	7.076802	8.451467
H	7.124055	7.705888	8.024705
C	3.231404	0.580690	6.384009
H	2.511583	-0.215383	6.286428
C	2.651446	0.633264	11.587499
H	1.639578	0.374515	11.873845
H	4.528645	8.025196	7.708979
H	3.284515	1.438681	4.416198
O	3.687633	8.843074	6.697002
H	2.780032	8.524134	6.853829
H	3.824752	8.588690	5.771231
O	5.955920	3.855161	3.700695
H	6.025414	4.725151	4.106941
H	5.123334	3.922262	3.211736

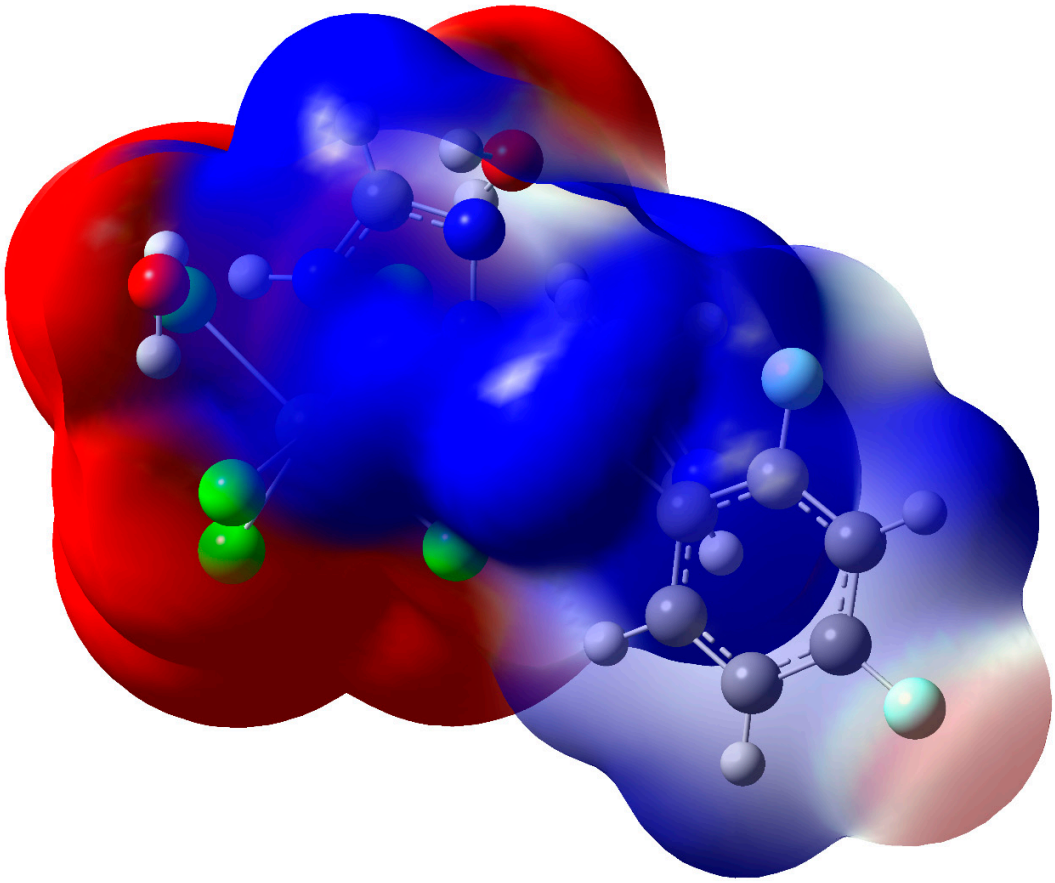

Figure S1: The electrostatic potential map of the (H2Fluconazole).$SnCl_6.2H_2O$

2.3.2. $SnCl_6$ internal modes

The Raman spectrum (Figure 6b) shows a weak band at 314 cm^{-1} is assigned to the (Sn-Cl) asymmetric stretching (ν_1(Sn-Cl)). The symmetric stretching (ν_2(Sn-Cl)) vibration and the bending vibration in the ν_5(Cl-Sn-Cl) plane are overlapped with other vibrations. The weak bands located at 171, 155 and 128 cm^{-1} in the Raman spectrum are attributed to the bending vibrations of (Cl-Sn-Cl) planes.

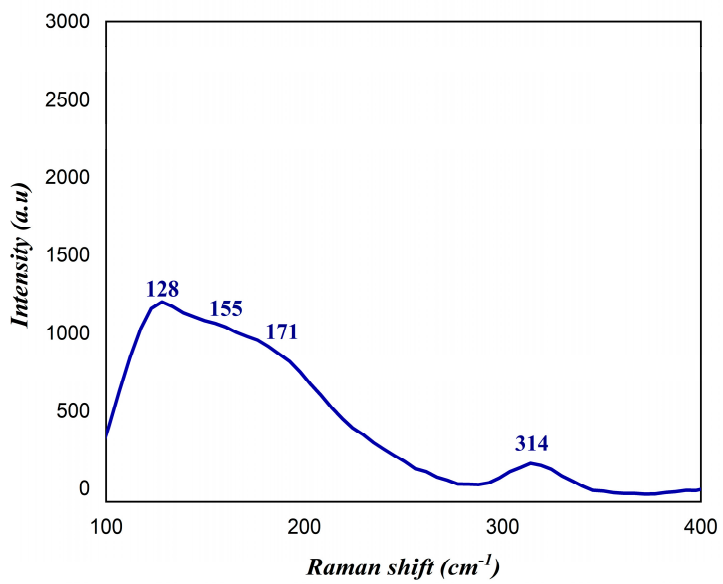

Figure S2. Raman spectrum of (H2Fluconazole).$SnCl_6.2H_2O$ at room temperature.