

Supplementary Table (1). Selected geometric atomic charges of hydrazones ligand.

	Atomic charges		Atomic charges		Atomic charges
C1	-0.1748	C24	0.26058	H47	0.190235
C2	-0.17453	S25	0.050765	H48	0.203301
C3	-0.23287	N26	-0.58603	H49	0.19898
C4	0.050591	N27	-0.31454	H50	0.191296
C5	0.122532	C28	0.213842	H51	0.190665
C6	-0.21005	C29	0.682837	H52	0.191116
C7	0.327617	C30	0.042186	H53	0.203444
C8	-0.3657	O31	-0.46788	H54	0.361302
C9	-0.33616	N32	-0.84768	H55	0.393287
C10	0.06115	C33	0.378159	H56	0.329713
C11	0.085568	C34	-0.18623	H57	0.189629
N12	-0.42832	C35	-0.17936	H58	0.196182
C13	-0.20419	C36	-0.18304	H59	0.189818
C14	-0.18171	C37	-0.25022	H60	0.196074
C15	-0.18535	H38	0.202477		
C16	-0.18349	H39	0.205071		
C17	-0.18973	H40	0.204927		
C18	-0.18898	H41	0.204987		
C19	-0.18537	H42	0.220502		
C20	-0.18554	H43	0.24965		
C21	-0.1842	H44	0.199844		
C22	-0.20628	H45	0.194255		
N23	-0.54139	H46	0.191039		

Supplementary Table (2).Selected geometric bond length of hydrazones ligand.

	Bond length		Bond length		Bond length
R(C1,C2)	1.3993	R(N12,N23)	1.4149	R(N26,N27)	1.3732
R(C1,C6)	1.399	R(C13,C14)	1.3973	R(N26,H55)	1.0211
R(C1,H38)	1.0836	R(C13,H44)	1.0823	R(N27,C28)	1.2964
R(C2,C3)	1.3956	R(C14,C15)	1.395	R(C28,C29)	1.5207
R(C2,H39)	1.0832	R(C14,H45)	1.0839	R(C28,C30)	1.4687
R(C3,C4)	1.4023	R(C15,C16)	1.3968	R(C29,O31)	1.226
R(C3,H40)	1.0825	R(C15,H46)	1.0836	R(C29,N32)	1.4059
R(C4,C5)	1.4102	R(C16,C17)	1.3948	R(C30,C33)	1.4232
R(C4,C7)	1.4745	R(C16,H47)	1.084	R(C30,C37)	1.3968
R(C5,C6)	1.3905	R(C17,H49)	1.0831	R(N32,C33)	1.3917
R(C5,C9)	1.5415	R(C18,C19)	1.395	R(N32,H56)	1.0122
R(C6,H41)	1.0829	R(C18,H48)	1.0833	R(C33,C34)	1.388
R(C7,C8)	1.5241	R(C19,C20)	1.3971	R(C34,C35)	1.399
R(C7,N12)	1.2916	R(C19,H50)	1.084	R(C34,H57)	1.0829
R(C8,C9)	1.5732	R(C20,C21)	1.3953	R(C35,C36)	1.3967
R(C8,H42)	1.0905	R(C20,H51)	1.0837	R(C35,H58)	1.0836
R(C8,H43)	1.0963	R(C21,C22)	1.3973	R(C36,C37)	1.3999
R(C9,C10)	1.5353	R(C21,H52)	1.084	R(C36,H59)	1.0829
R(C9,C11)	1.5444	R(C22,H53)	1.0828	R(C37,H60)	1.0833
R(C10,C18)	1.4041	R(N23,C24)	1.3784		
R(C10,C22)	1.4017	R(N23,H54)	1.018		
R(C11,C13)	1.4014	R(C24,S25)	1.7034		
R(C11,C17)	1.4036	R(C24,N26)	1.3672		

Supplementary Table (3). Selected geometric bond angles (°) of hydrazones ligand.

	Bond Angles (°)		Bond Angles (°)		Bond Angles (°)
A(C2,C1,C6)	120.6281	A(C7,C8,H43)	108.779	A(C14,C15,C16)	119.4069
A(C2,C1,H38)	119.694	A(C9,C8,H42)	113.1094	A(C14,C15,H46)	120.2873
A(C6,C1,H38)	119.6755	A(C9,C8,H43)	107.5534	A(C16,C15,H46)	120.3058
A(C1,C2,C3)	120.4696	A(H42,C8,H43)	109.0338	A(C15,C16,C17)	120.2141
A(C1,C2,H39)	119.8918	A(C5,C9,C8)	101.1922	A(C15,C16,H47)	120.1142
A(C3,C2,H39)	119.638	A(C5,C9,C10)	114.7443	A(C17,C16,H47)	119.6715
A(C2,C3,C4)	119.0392	A(C5,C9,C11)	106.2797	A(C11,C17,C16)	120.8748
A(C2,C3,H40)	119.3885	A(C8,C9,C10)	108.6241	A(C11,C17,H49)	119.3833
A(C4,C3,H40)	121.4889	A(C8,C9,C11)	112.7522	A(C16,C17,H49)	119.7328
A(C3,C4,C5)	120.2559	A(C10,C9,C11)	112.7644	A(C10,C18,C19)	120.7793
A(C3,C4,C7)	130.6373	A(C9,C10,C18)	119.6543	A(C10,C18,H48)	119.3387
A(C5,C4,C7)	109.0762	A(C9,C10,C22)	121.5514	A(C19,C18,H48)	119.8778
A(C4,C5,C6)	120.3424	A(C18,C10,C22)	118.5155	A(C18,C19,C20)	120.2323
A(C4,C5,C9)	111.4253	A(C9,C11,C13)	121.6873	A(C18,C19,H50)	119.6757
A(C6,C5,C9)	128.1849	A(C9,C11,C17)	119.7823	A(C20,C19,H50)	120.092
A(C1,C6,C5)	119.2159	A(C13,C11,C17)	118.4301	A(C19,C20,C21)	119.4634
A(C1,C6,H41)	120.375	A(C7,N12,N23)	119.0724	A(C19,C20,H51)	120.2596
A(C5,C6,H41)	120.4074	A(C11,C13,C14)	120.7247	A(C21,C20,H51)	120.277
A(C4,C7,C8)	106.8028	A(C11,C13,H44)	120.2597	A(C20,C21,C22)	120.2939
A(C4,C7,N12)	132.8387	A(C14,C13,H44)	119.0075	A(C20,C21,H52)	120.1048
A(C8,C7,N12)	120.3362	A(C13,C14,C15)	120.3469	A(C22,C21,H52)	119.6012
A(C7,C8,C9)	104.9021	A(C13,C14,H45)	119.5201	A(C10,C22,C21)	120.7098
A(C7,C8,H42)	113.213	A(C15,C14,H45)	120.133	A(C10,C22,H53)	119.5808

Supplementary Table (3). Selected geometric bond angles (°) of hydrazones ligand.

	Bond Angles (°)		Bond Angles (°)		Bond Angles (°)
A(C21,C22,H53)	119.7094	A(C28,C29,O31)	129.8023	A(C33,C34,H57)	120.886
A(N12,N23,C24)	119.1589	A(C28,C29,N32)	104.3726	A(C35,C34,H57)	120.6227
A(N12,N23,H54)	122.0163	A(O31,C29,N32)	125.8249	A(C34,C35,C36)	120.9371
A(C24,N23,H54)	117.3721	A(C28,C30,C33)	106.4267	A(C34,C35,H58)	119.2887
A(N23,C24,S25)	120.3537	A(C28,C30,C37)	134.4695	A(C36,C35,H58)	119.7741
A(N23,C24,N26)	111.6041	A(C33,C30,C37)	119.103	A(C35,C36,C37)	120.5084
A(S25,C24,N26)	128.0419	A(C29,N32,C33)	112.1817	A(C35,C36,H59)	119.9045
A(C24,N26,N27)	121.9947	A(C29,N32,H56)	122.3727	A(C37,C36,H59)	119.5871
A(C24,N26,H55)	114.9109	A(C33,N32,H56)	125.4454	A(C30,C37,C36)	119.5319
A(N27,N26,H55)	123.0921	A(C30,C33,N32)	109.8434	A(C30,C37,H60)	122.4634
A(N26,N27,C28)	117.5483	A(C30,C33,C34)	121.4276	A(C36,C37,H60)	118.0041
A(N27,C28,C29)	117.4965	A(C29,C28,C30)	107.1748	A(N27,C28,C30)	135.3286

Supplementary Table (4).Selected geometric Dihedral Bond angles (°) of hydrazones ligand.

	Dihedral Bond angles (°)		Dihedral Bond angles (°)		Dihedral Bond angles (°)
D(C6,C1,C2,C3)	1.283	D(C5,C4,C7,N12)	163.3081	D(H42,C8,C9,C5)	-148.107
D(C6,C1,C2,H39)	-178.434	D(C4,C5,C6,C1)	-1.695	D(H42,C8,C9,C10)	90.7656
D(H38,C1,C2,C3)	-179.27	D(C4,C5,C6,H41)	178.7784	D(H42,C8,C9,C11)	-34.9746
D(H38,C1,C2,H39)	1.0137	D(C9,C5,C6,C1)	-178.965	D(H43,C8,C9,C5)	91.4369
D(C2,C1,C6,C5)	-0.2319	D(C9,C5,C6,H41)	1.5089	D(H43,C8,C9,C10)	-29.6906
D(C2,C1,C6,H41)	179.2948	D(C4,C5,C9,C8)	16.3812	D(H43,C8,C9,C11)	-155.431
D(H38,C1,C6,C5)	-179.679	D(C4,C5,C9,C10)	133.1027	D(C5,C9,C10,C18)	164.1145
D(H38,C1,C6,H41)	-0.1525	D(C4,C5,C9,C11)	-101.556	D(C5,C9,C10,C22)	-22.0412
D(C1,C2,C3,C4)	-0.3813	D(C6,C5,C9,C8)	-166.15	D(C8,C9,C10,C18)	-83.4988
D(C1,C2,C3,H40)	-177.111	D(C6,C5,C9,C10)	-49.4286	D(C8,C9,C10,C22)	90.3455
D(H39,C2,C3,C4)	179.3359	D(C6,C5,C9,C11)	75.9132	D(C11,C9,C10,C18)	42.2343
D(H39,C2,C3,H40)	2.6063	D(C4,C7,C8,C9)	24.7853	D(C11,C9,C10,C22)	-143.921
D(C2,C3,C4,C5)	-1.5399	D(C4,C7,C8,H42)	148.5686	D(C5,C9,C11,C13)	89.0998
D(C2,C3,C4,C7)	-179.292	D(C4,C7,C8,H43)	-90.057	D(C5,C9,C11,C17)	-87.2007
D(H40,C3,C4,C5)	175.1184	D(N12,C7,C8,C9)	-153.709	D(C8,C9,C11,C13)	-20.8835
D(H40,C3,C4,C7)	-2.6332	D(N12,C7,C8,H42)	-29.926	D(C8,C9,C11,C17)	162.816
D(C3,C4,C5,C6)	2.6038	D(N12,C7,C8,H43)	91.4484	D(C10,C9,C11,C13)	-144.357
D(C3,C4,C5,C9)	-179.702	D(C4,C7,N12,N23)	-2.4056	D(C10,C9,C11,C17)	39.343
D(C7,C4,C5,C6)	-179.201	D(C8,C7,N12,N23)	175.6289	D(C9,C10,C18,C19)	174.7557
D(C7,C4,C5,C9)	-1.5067	D(C7,C8,C9,C5)	-24.2574	D(C9,C10,C18,H48)	-5.9867
D(C3,C4,C7,C8)	163.0251	D(C7,C8,C9,C10)	-145.385	D(C22,C10,C18,C19)	0.7249
D(C3,C4,C7,N12)	-18.7468	D(C7,C8,C9,C11)	88.8748	D(C22,C10,C18,H48)	179.9825
D(C5,C4,C7,C8)	-14.9199	D(C9,C10,C22,C21)	-174.797	D(C9,C10,C22,H53)	5.2102

Dihedral Bond angles (°)

	Dihedral Bond angles (°)		Dihedral Bond angles (°)		Dihedral Bond angles (°)
D(C18,C10,C22,C21)	-0.8852	D(H46,C15,C16,H47)	0.0132	D(N12,N23,C24,N26)	-5.5546
D(C18,C10,C22,H53)	179.1224	D(C15,C16,C17,C11)	-0.1068	D(H54,N23,C24,S25)	8.1157
D(C9,C11,C13,C14)	-176.908	D(C15,C16,C17,H49)	-178.999	D(H54,N23,C24,N26)	-172.087
D(C9,C11,C13,H44)	2.0471	D(H47,C16,C17,C11)	179.7133	D(N23,C24,N26,N27)	-177.953
D(C17,C11,C13,C14)	-0.5591	D(H47,C16,C17,H49)	0.821	D(N23,C24,N26,H55)	2.5786
D(C17,C11,C13,H44)	178.396	D(C10,C18,C19,C20)	-0.1272	D(S25,C24,N26,N27)	1.825
D(C9,C11,C17,C16)	176.927	D(C10,C18,C19,H50)	179.8122	D(S25,C24,N26,H55)	-177.643
D(C9,C11,C17,H49)	-4.1768	D(H48,C18,C19,C20)	-179.381	D(C24,N26,N27,C28)	-178.155
D(C13,C11,C17,C16)	0.5066	D(H48,C18,C19,H50)	0.5585	D(H55,N26,N27,C28)	1.27
D(C13,C11,C17,H49)	179.4028	D(C18,C19,C20,C21)	-0.3233	D(N26,N27,C28,C29)	-179.099
D(C7,N12,N23,C24)	176.0237	D(C18,C19,C20,H51)	179.7699	D(N26,N27,C28,C30)	0.738
D(C7,N12,N23,H54)	-18.0945	D(H50,C19,C20,C21)	179.7375	D(N27,C28,C29,O31)	-0.2526
D(C11,C13,C14,C15)	0.2136	D(H50,C19,C20,H51)	-0.1693	D(N27,C28,C29,N32)	179.5917
D(C11,C13,C14,H45)	-179.909	D(C19,C20,C21,C22)	0.1634	D(C30,C28,C29,O31)	179.8674
D(H44,C13,C14,C15)	-178.754	D(C19,C20,C21,H52)	-179.721	D(C30,C28,C29,N32)	-0.2883
D(H44,C13,C14,H45)	1.1233	D(H51,C20,C21,C22)	-179.93	D(N27,C28,C30,C33)	-179.602
D(C13,C14,C15,C16)	0.1967	D(H51,C20,C21,H52)	0.1863	D(N27,C28,C30,C37)	0.7204
D(C13,C14,C15,H46)	-179.885	D(C20,C21,C22,C10)	0.4504	D(C29,C28,C30,C33)	0.2468
D(H45,C14,C15,C16)	-179.68	D(C20,C21,C22,H53)	-179.557	D(C29,C28,C30,C37)	-179.431
D(H45,C14,C15,H46)	0.2378	D(H52,C21,C22,C10)	-179.665	D(C28,C29,N32,C33)	0.2287
D(C14,C15,C16,C17)	-0.2494	D(H52,C21,C22,H53)	0.3273	D(C28,C29,N32,H56)	-179.931
D(C14,C15,C16,H47)	179.9313	D(N12,N23,C24,S25)	174.648	D(O31,C29,N32,C33)	-179.919