Supplementary Information

Novel sulfone 2-aminobenzimidazole derivatives and their coordination compounds. Contribution of the ethyl and phenyl substituents on non-covalent molecular interactions. Biological antiproliferative activity.

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Table S1. Representative vibrations and intensities for the ligands sfabz and seabz and their coordination compounds

Compound	$\nu_{as}(NH_2)$ cm^{-1} **intensity**	$\nu_{s}(NH_2)$ cm^{-1} **intensity**	$\nu(C=C)+\delta_{sc}(NH_2)$ $+\nu(C\text{-}N)$ cm^{-1} **intensity**	$\nu(C=N)+\rho(NH_2)$ $+\nu(C\text{-}N)$ cm^{-1} **intensity**	$\nu_{as}(SO_2)$ cm^{-1} **intensity**	$\nu_{s}(SO_2)$ cm^{-1} **intensity**
sfabz	3434 **very strong**	3341 **weak**	1664 **very strong**	1552 **very strong**	1286 **strong**	1140 **strong**
seabz	3460 **very strong**	3373 **very strong**	1639 **very strong**	1549 **very strong**	1281 **strong**	1132 **strong**
$[Ni(sfabz)_2Cl_2]$ **1**	3387 **strong**	3305 **strong**	1645 **very strong**	1552 **very strong**	1292 **strong**	1141 **strong**
$[Ni(sfabz)_2Br_2]$ **2**	3418 **strong**	3307 **strong**	1643 **strong**	1549 **very strong**	1290 **very strong**	1146 **very strong**
$[Ni(seabz)_2Cl_2]$ **3**	3407 **medium**	3321 **strong**	1646 **very strong**	1559 **strong**	1295 **strong**	1128 **strong**
$[Ni(seabz)_2Br_2]$ **4**	3387 **very strong**	3311 **very strong**	1645 **very strong**	1550 **very strong**	1294 **very strong**	1126 **strong**
$[Cu(sfabz)_2Cl_2]$ **5**	3440 **medium**	3372 **medium**	1638 **strong**	1546 **medium**	1289 **strong**	1138 **strong**
$[Cu(sfabz)_2Br_2]$ **6**	3525 **medium**	3318 **strong**	1643 **strong**	1557 **medium**	1294 **strong**	1141 **very strong**
$[Cu(seabz)_2Cl_2]$ **7**	3397 **medium**	3308 **medium**	1645 **very strong**	1558 **strong**	1294 **strong**	1125 **strong**
$[Cu(seabz)_2Br_2]$ **8**	3388 **medium**	3321 **medium**	1639 **very strong**	1549 **strong**	1289 **strong**	1123 **strong**
$[Zn(sfabz)_2Cl_2]$ **9**	3390 **medium**	3315 **medium**	1646 **very strong**	1556 **very strong**	1293 **strong**	1142 **strong**
$[Zn(sfabz)_2Br_2]$ **10**	3415 **medium**	3312 **medium**	1627 **strong**	1152 **very strong**	1290 **very strong**	1136 **very strong**
$[Zn(seabz)_2Cl_2]$ **11**	3411 **medium**	3328 **medium**	1650 **very strong**	1562 **strong**	1295 **strong**	1128 **strong**
$[Zn(seabz)_2Br_2]$ **12**	3400 **strong**	3330 **medium**	1640 **very strong**	1550 **very strong**	1290 **very strong**	1124 **very strong**
$[Cd(sfabz)_2Cl_2]$ **13**	3419 **medium**	3356 **strong**	1655 **very strong**	1568 **strong**	1289 **strong**	1144 **very strong**
$[Cd(seabz)_2Cl_2]$ **14**	3400 **medium**	3332 **strong**	1648 **very strong**	1558 **very strong**	1295 **very strong**	1127 **strong**
$[Hg(sfabz)_2Cl_2]$ **15**	3387 **medium**	3311 **strong**	1645 **very strong**	1552 **strong**	1292 **very strong**	1141 **very strong**
$[Hg(seabz)_2Cl_2]$ **16**	3403 **medium**	3331 **medium**	1647 **very strong**	1559 **strong**	1295 **strong**	1125 **strong**

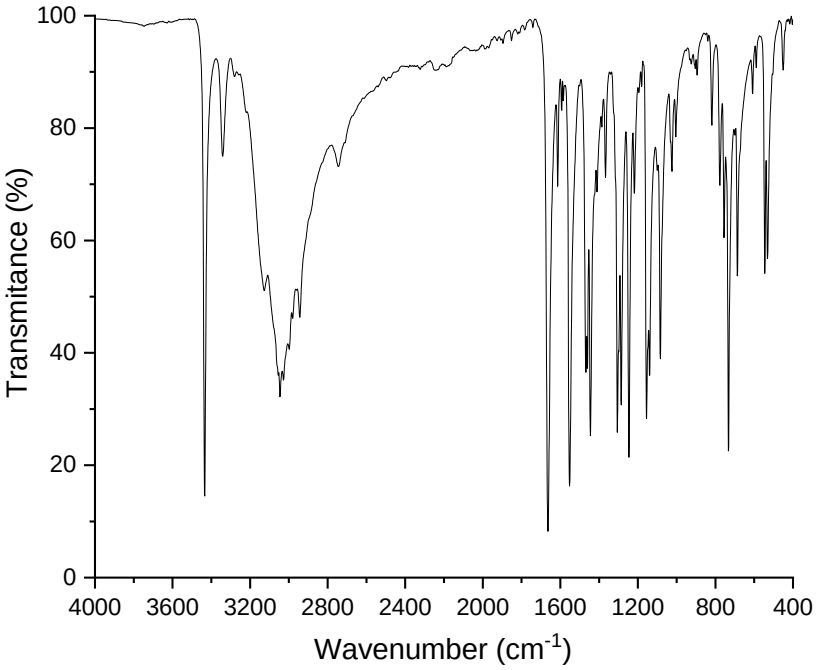

Figure S1. IR spectrum of sfabz.

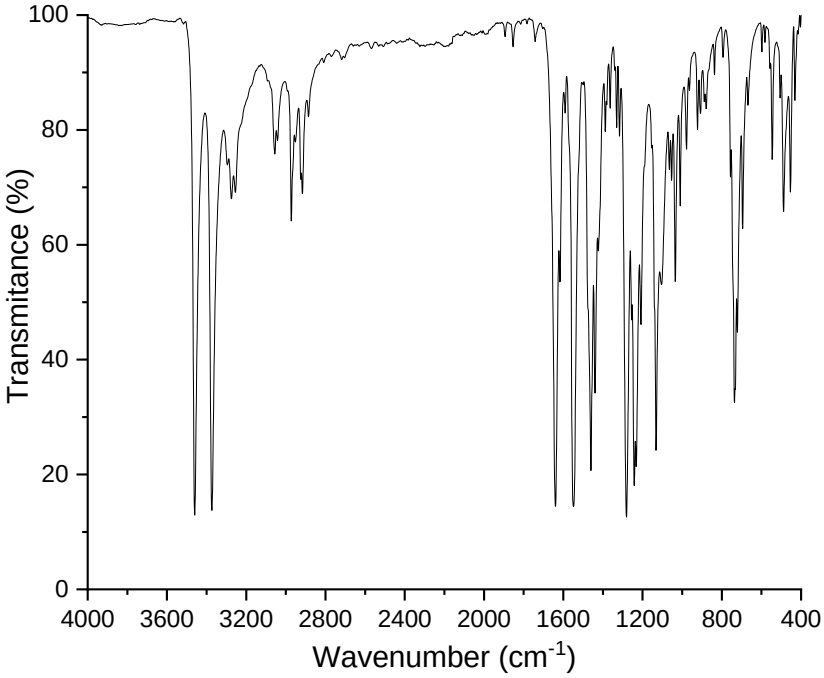

Figure S2. IR spectrum of seabz.

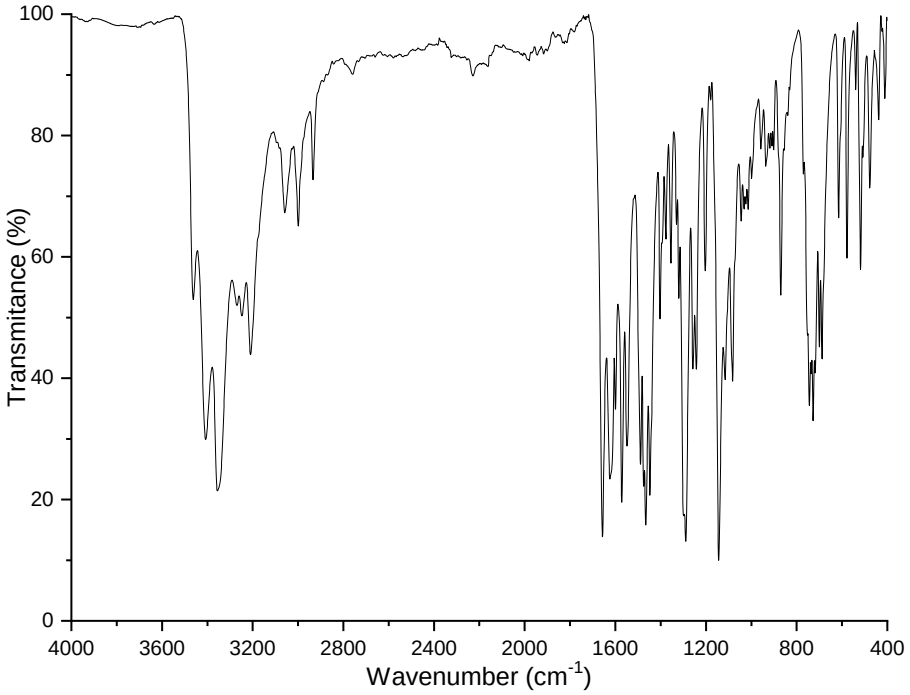

Figure S3. IR spectrum of $[Hg(sfabz)_2Cl_2]$.

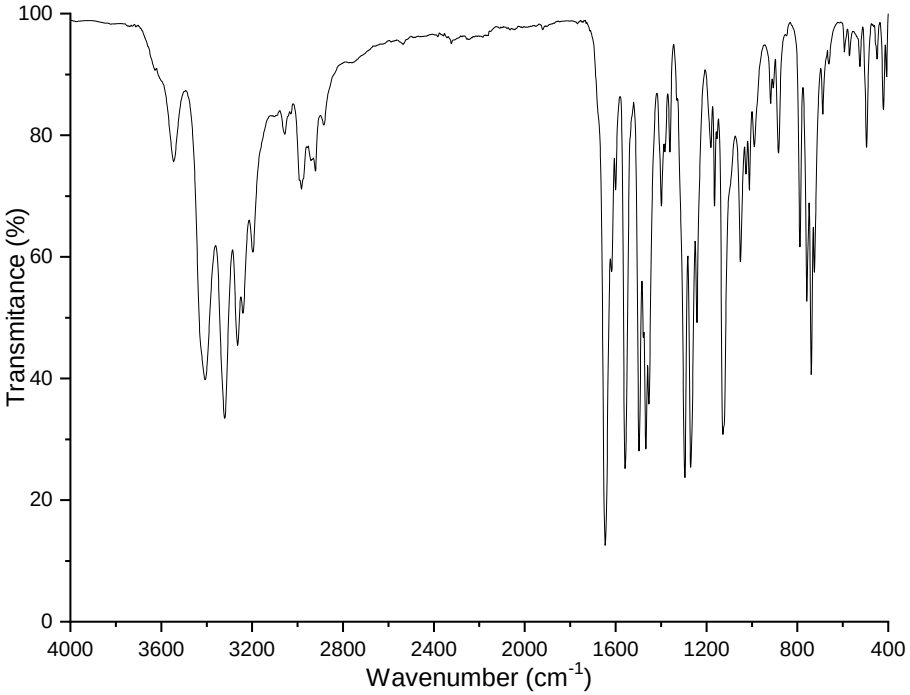

Figure S4. IR spectrum of $[Ni(seabz)_2Cl_2]$.

Table S2. Crystallographic data of sfabz, seabz and compound 1.

Compounds	*sfabz*	*seabz*	*1*
Chemical formula	$C_{15}H_{15}N_3O_2S$	$C_{11}H_{15}N_3O_2S$	$NiC_{30}H_{30}N_6O_4S_2Cl_2$
Formula weight (g mol^{-1})	301.36	253.32	732.33
Crystal size (mm)	0.5x0.09x0.01	0.48x0.21x0.19	0.39x0.18x0.07
Crystal color	Colourless	Colourless	Blue
Crystal system	Monoclinic	Monoclinic	Triclinic
Space group	P 21/n	P 21/n	P-1
a (Å)	9.9313(12)	5.6408(8)	9.5656(13)
b (Å)	5.4217(5)	18.453(3)	9.9837(9)
c (Å)	26.904(3)	11.1532(15)	17.3370(19)
α (°)	90	90	83.852(9)
β (°)	99.497(12)	97.747(13)	87.640(10)
γ (°)	90	90	78.220(10)
V (Å^3)	1428.8(3)	1150.3(3)	1611.2(3)
Z	4	4	2
D_{calc} (mg cm^{-3})	1.401	1.463	1.51
μ (mm^{-1})	0.235	0.275	0.944
F(000)	632	536	756
Temp. (K)	130(2)	130(2)	130(2)
θ range (°) data collection	3.836-29.631	3.687-29.73	3.417-29.598
Index range			
h	-13-13	-6-7	-12-13
k	-7-7	-25-25	-13-13
l	-35-35	-15-14	-22-23
Measured reflections	18416	6496	21425
Independent reflections	3697	2754	7779
Reflections observed [I>2σ(I)]	2836	1922	5740
R_{int}	0.0494	0.0629	0.0627
Parameters	196	155	406
R [F^2 > 2σ(F^2)]	0.0445	0.0527	0.0549
wR_2 (F^2)	0.102	0.1255	0.1495
S	1.068	1.078	1.072
$(Δ/σ)_{max}$	0.001	0	0.001
$Δρ_{max}$ (eÅ^{-3})	0.403	0.424	1.024
$Δρ_{min}$ (eÅ^{-3})	-0.454	-0.593	-0.514

Table S3. Crystallographic data of 2, 3 and 5.

Compounds	*2*	*3*	*5*
Chemical formula	$Ni_2C_{63}H_{64}N_{12}O_9S_4Br_4$	$NiC_{22}H_{30}N_6O_4S_2Cl_2$	$CuC_{30}H_{30}N_6O_4S_2Cl_2$
Formula weight (g mol^{-1})	1698.56	636.25	737.16
Crystal size (mm)	0.42x0.38x0.23	0.49x0.21x0.13	0.242x0.192x0.089
Crystal color	Dark green	Blue	Green
Crystal system	Triclinic	Monoclinic	Triclinic
Space group	P-1	P 21/c	P-1
a (Å)	10.6925(6)	16.9816(12)	10.365(2)
b (Å)	11.1876(6)	15.3376(8)	11.384(2)
c (Å)	14.4961(9)	10.2625(7)	13.918(3)
α (°)	76.685(5)	90	100.833(4)
β (°)	89.622(5)	100.987(7)	94.543(4)
γ (°)	89.579(4)	90	97.599(4)
V (Å^3)	1687.39(17)	2623.9(3)	1589.8(5)
Z	1	4	2
D_{calc} (mg cm^{-3})	1.672	1.611	1.540
μ (mm^{-1})	3.115	1.145	1.033
F(000)	858	1320	758
Temp. (K)	130(2)	130(2)	298(2)
θ range (°) data collection	3.452-30.163	3.61-29.496	1.498-26.022
Index range			
h	-14-14	-16-23	-12-12
k	-15-14	-21-19	-14-14
l	-19-20	-13-10	-17-17
Measured reflections	24487	13678	39236
Independent reflections	8685	6288	6231
Reflections observed [I>2σ(I)]	7059	4365	3167
R_{int}	0.032	0.0518	0.1178
Parameters	433	336	620
R [$F^2 > 2\sigma(F^2)$]	0.0334	0.0486	0.0682
wR_2 (F^2)	0.0781	0.1035	0.1744
S	1.034	1.048	0.96
$(\Delta/\sigma)_{max}$	0.002	0.001	0
$\Delta\rho_{max}$ (eÅ^{-3})	0.567	0.592	0.501
$\Delta\rho_{min}$ (eÅ^{-3})	-0.593	-0.501	-0.0435

Table S4. Crystallographic data of 9 and 10.

Compounds	*9*	*10*
Chemical formula	$ZnC_{30}H_{30}N_6O_4S_2Cl_2$	$ZnC_{32}H_{32}N_6O_5S_2Br_2$
Formula weight (g mol^{-1})	738.99	869.94
Crystal size (mm)	0.433x0.248x0.070	0.28x0.25x0.19
Crystal color	colourless	Colourless
Crystal system	Triclinic	Triclinic
Space group	P-1	P-1
a (Å)	10.367(11)	10.6872(5)
b (Å)	10.928(12)	11.2000(5)
c (Å)	14.556(15)	14.5708(7)
α (°)	78.18(2)	76.451(4)
β (°)	89.19(2)	89.503(4)
γ (°)	85.37(2)	89.511(4)
V (Å^3)	1609(3)	1695.44(14)
Z	2	2
D_{calc} (mg cm^{-3})	1.526	1.704
μ (mm^{-1})	1.105	5.342
F(000)	760	876
Temp. (K)	150(2)	130(2)
θ range (°) data collection	2.432-26.414	4.060-73.656
Index range		
h	-12-12	-13-13
k	-13-13	-13-13
l	-18-18	-18-18
Measured reflections	33661	36795
Independent reflections	6549	6720
Reflections observed [I>2σ(I)]	3903	5824
R_{int}	0.1339	0.0435
Parameters	418	433
R [$F^2 > 2\sigma(F^2)$]	0.0586	0.0394
wR_2 (F^2)	0.1087	0.1106
S	1.022	1.081
$(\Delta/\sigma)_{max}$	0	0.001
$\Delta\rho_{max}$ (eÅ^{-3})	0.449	0.637
$\Delta\rho_{min}$ (eÅ^{-3})	-0.619	-1.329

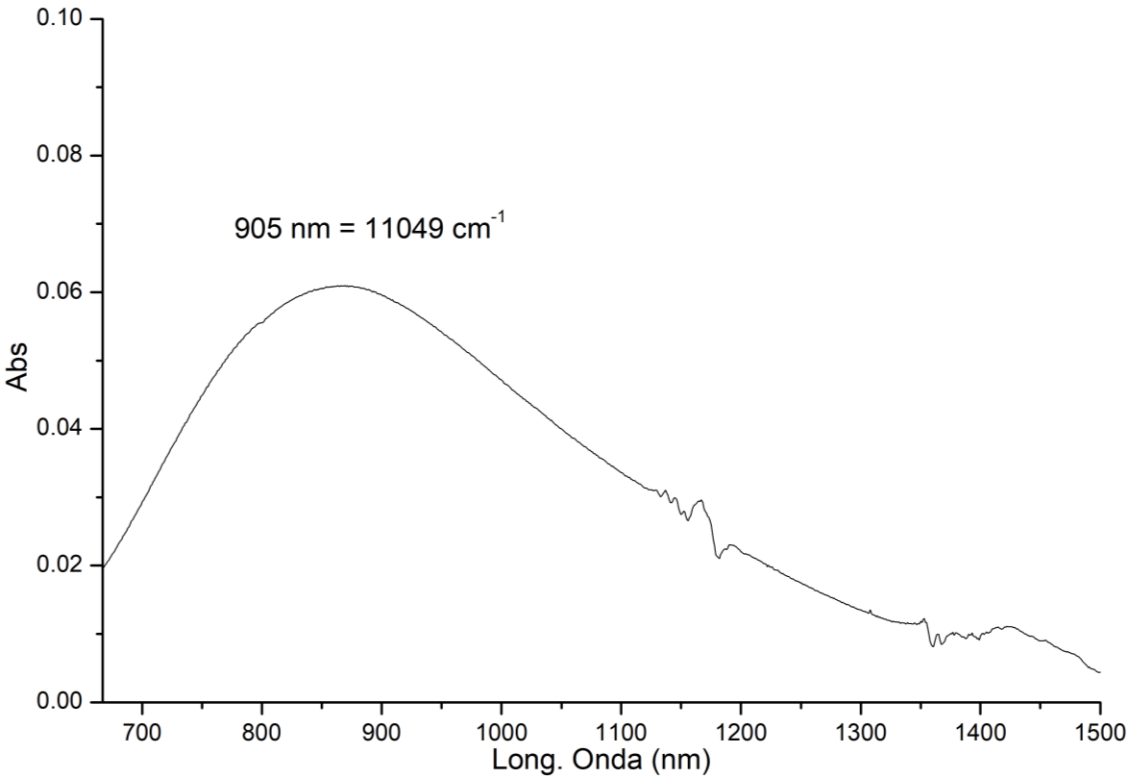

Figure S5. Solution spectrum of $[Cu(sfabz)_2Cl_2]$ in DMSO, $1x10^{-3}$ M.

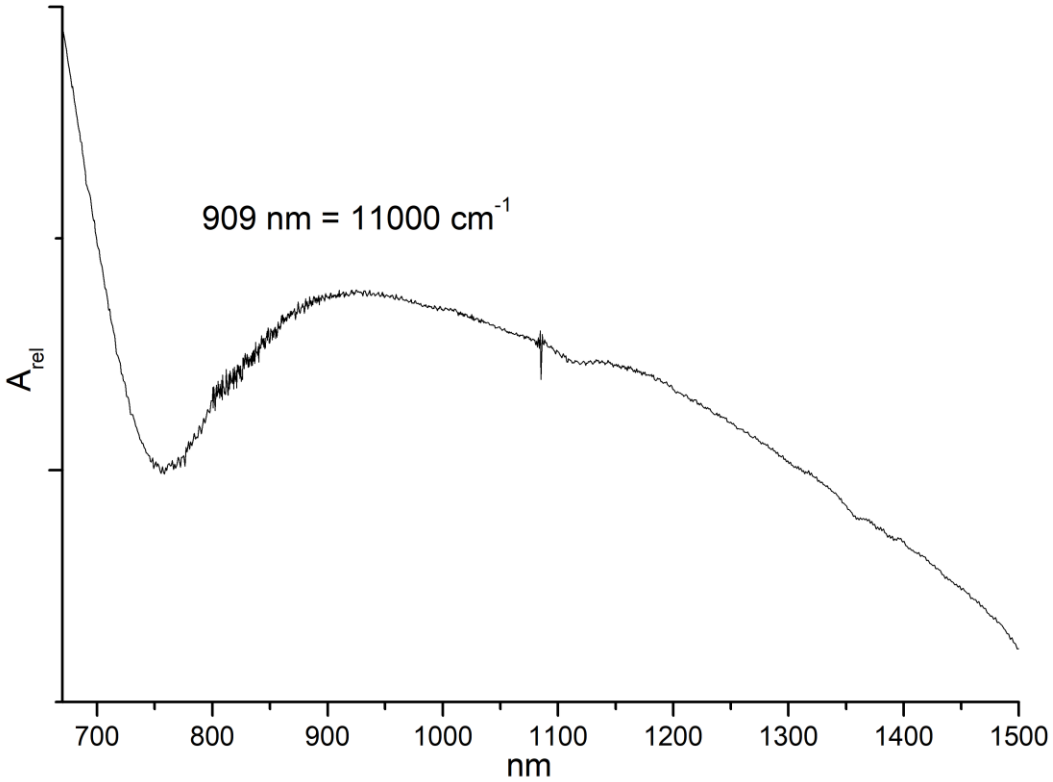

Figure S6. Diffuse reflectance spectrum of $[Cu(sfabz)_2Cl_2]$.

Table S5. ^{1}H-NMR for sfabz and its coordination compounds (DMSO d^{6}).

Signal	*sfabz*	*[Zn(sfabz)$_2$Cl$_2$] (9)*	*[Zn(sfabz)$_2$Br$_2$] (10)*	*[Cd(sfabz)$_2$Cl$_2$] (13)*	*[Hg(sfabz)$_2$Cl$_2$] (15)*
4	7.05 ppm (d)	7.21 ppm (s, broad)	7.23 ppm (d)	7.22 ppm (d)	7.22 ppm (d)
5	6.89 ppm (t)	6.94 ppm (m)	6.94 ppm (t)	6.92 ppm (t)	6.98 ppm (m)
6	6.79 ppm (t)	6.92 ppm (m)	6.92 ppm (m)	6.85 ppm (t)	6.94 ppm (m)
7	6.74 ppm (d)	6.92 ppm (m)	6.92 ppm (m)	6.82 ppm (d)	6.94 ppm (m)
10 (2H)	6.43 ppm (s, broad)	7.21 ppm (s, broad)	7.10 ppm (s, broad)	6.75 ppm (s, broad)	7.12 ppm (s, broad)
11 (2H)	4.28 ppm (t)	4.40 ppm (t)	4.40 ppm (t)	4.32 ppm (t)	4.39 ppm (t)
12 (2H)	3.72 ppm (t)	3.81 ppm (t)	3.81 ppm (t)	3.74 ppm (t)	3.81 ppm (t)
17 (2H)	7.86 ppm (d)	7.84 ppm (m)	7.84 ppm (d)	7.85 ppm (d)	7.85 ppm (d)
18 (2H)	7.58 ppm (t)	7.55 ppm (m)	7.56 ppm (t)	7.58 ppm (t)	7.52 ppm (t)
19	7.71 ppm (t)	7.67 ppm (m)	7.68 ppm (t)	7.69 ppm (t)	7.63 ppm (t)

Table S6. ^{13}C-NMR for sfabz and its coordination compounds (DMSO d^{6}).

Signal	*sfabz*	*[Zn(sfabz)$_2$Cl$_2$] (9)*	*[Zn(sfabz)$_2$Br$_2$] (10)*	*[Cd(sfabz)$_2$Cl$_2$] (13)*	*[Hg(sfabz)$_2$Cl$_2$] (15)*
2	154.82 ppm	154.92 ppm	154.76 ppm	154.97 ppm	155.06 ppm
4	115.27 ppm	114.62 ppm	114.81 ppm	115.43 ppm	114.36 ppm
5	121.10 ppm	122.24 ppm	122.16 ppm	121.54 ppm	122.21 ppm
6	118.66 ppm	120.62 ppm	120.55 ppm	119.62 ppm	120.57 ppm
7	107.73 ppm	108.98 ppm	108.90 ppm	108.25 ppm	109.08 ppm
8	133.91 ppm	132.33 ppm	132.43 ppm	133.09 ppm	132.49 ppm
9	142.92 ppm	139.08 ppm	139.10 ppm	140.91 ppm	139.29 ppm
11	36.08 ppm	36.37 ppm	36.36 ppm	36.21 ppm	36.58 ppm
12	53.18 ppm	52.54 ppm	52.59 ppm	52.86 ppm	52.52 ppm
16	136.17 ppm	138.70 ppm	138.87 ppm	139.10 ppm	139.05 ppm
17 (2C)	127.96 ppm	127.80 ppm	127.83 ppm	127.91 ppm	127.73 ppm
18 (2C)	129.84 ppm	129.83 ppm	129.86 ppm	129.88 ppm	129.78 ppm
19	134.44 ppm	134.49 ppm	134.51 ppm	134.50 ppm	134.43 ppm

Table S7. ^{1}H-NMR for seabz and its coordination compounds (d^{6} DMSO).

Signal	*seabz*	*[Zn(seabz)$_2$Cl$_2$] (11)*	*[Zn(seabz)$_2$Br$_2$] (12)*	*[Cd(seabz)$_2$Cl$_2$] (14)*	*[Hg(seabz)$_2$Cl$_2$] (16)*
4	7.13 ppm (dd, overlapped)	7.28 ppm (m, overlapped)	7.28 ppm (dd, overlapped)	7.33 ppm (dd)	7.29 ppm (m, overlapped)
5	6.88 ppm (td)	7.01 ppm (m, overlapped)	6.99 ppm (m, overlapped)	6.98 ppm (m, overlapped)	7.02 ppm (m, overlapped)
6	6.94 ppm (td)	6.99 ppm (m, overlapped)	7.02 ppm (m, overlapped)	6.97 ppm (m, overlapped)	7.02 ppm (m, overlapped)
7	7.15 ppm (dd, overlapped)	7.26 ppm (m, overlapped)	7.29 ppm (dd, overlapped)	7.22 ppm (dd)	7.28 ppm (m, overlapped)
10 (2H)	6.48 ppm (s, broad)	7.32 ppm (s, broad)	7.18 ppm (s, broad)	6.86 ppm (s, broad)	7.13 ppm (s, broad)
11 (2H)	4.39 ppm (t)	4.49 ppm (t)	4.49 ppm (t)	4.42 ppm (t)	4.46 ppm (t)
12 (2H)	3.46 ppm (t)	3.55 ppm (t)	3.55 ppm (t)	3.48 ppm (t)	3.52 ppm (t)
16 (2H)	3.08 ppm (q)	3.14 ppm (q)	3.14 ppm (q)	3.12 ppm (q)	3.13 ppm (q)
17 (3H)	1.15 ppm (t)	1.17 ppm (t)	1.17 ppm (t)	1.16 ppm (t)	1.16 ppm (t)

Table S8. ^{13}C-NMR for seabz and its coordination compounds (d^{6} DMSO).

Signal	*seabz*	*[Zn(seabz)$_2$Cl$_2$] (11)*	*[Zn(seabz)$_2$Br$_2$] (12)*	*[Cd(seabz)$_2$Cl$_2$] (14)*	*[Hg(seabz)$_2$Cl$_2$] (16)*
2	155.05 ppm	155.10 ppm	154.92 ppm	155.12 ppm	155.25 ppm
4	115.40 ppm	114.65 ppm	114.84 ppm	115.59 ppm	114.57 ppm
5	121.17 ppm	122.37 ppm	122.29 ppm	121.70 ppm	122.20 ppm
6	118.78 ppm	120.81 ppm	120.74 ppm	119.92 ppm	120.55 ppm
7	108.12 ppm	109.36 ppm	109.29 ppm	108.70 ppm	109.26 ppm
8	134.05 ppm	132.45 ppm	132.55 ppm	133.11 ppm	132.78 ppm
9	143.19 ppm	138.81 ppm	138.99 ppm	140.74 ppm	139.78 ppm
11	35.60 ppm	35.78 ppm	35.78 ppm	35.70 ppm	35.91 ppm
12	49.62 ppm	49.04 ppm	49.07 ppm	49.30 ppm	49.16 ppm
16	47.29 ppm	47.34 ppm	47.35 ppm	47.31 ppm	47.32 ppm
17	6.34 ppm	6.28 ppm	6.30 ppm	6.32 ppm	6.30 ppm