Supporting Information

Synthesis and Characterization of Novel Rhenium Tricarbonyl Complexes with Dipicolylamine Sulfonamide Ligands: Potential Serine/Threonine Kinase Inhibitors for Cancer Therapy

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^{1}H NMR spectroscopy data

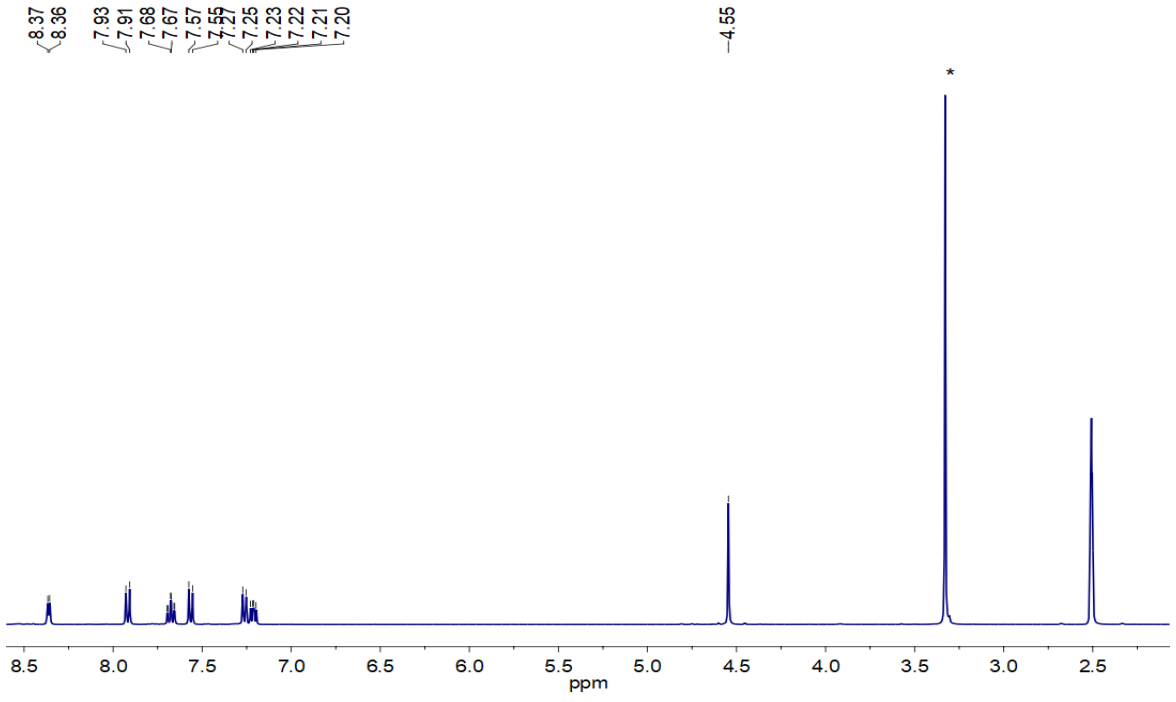

Fig. S.1: ^{1}H NMR spectrum of L1 in DMSO-d_6

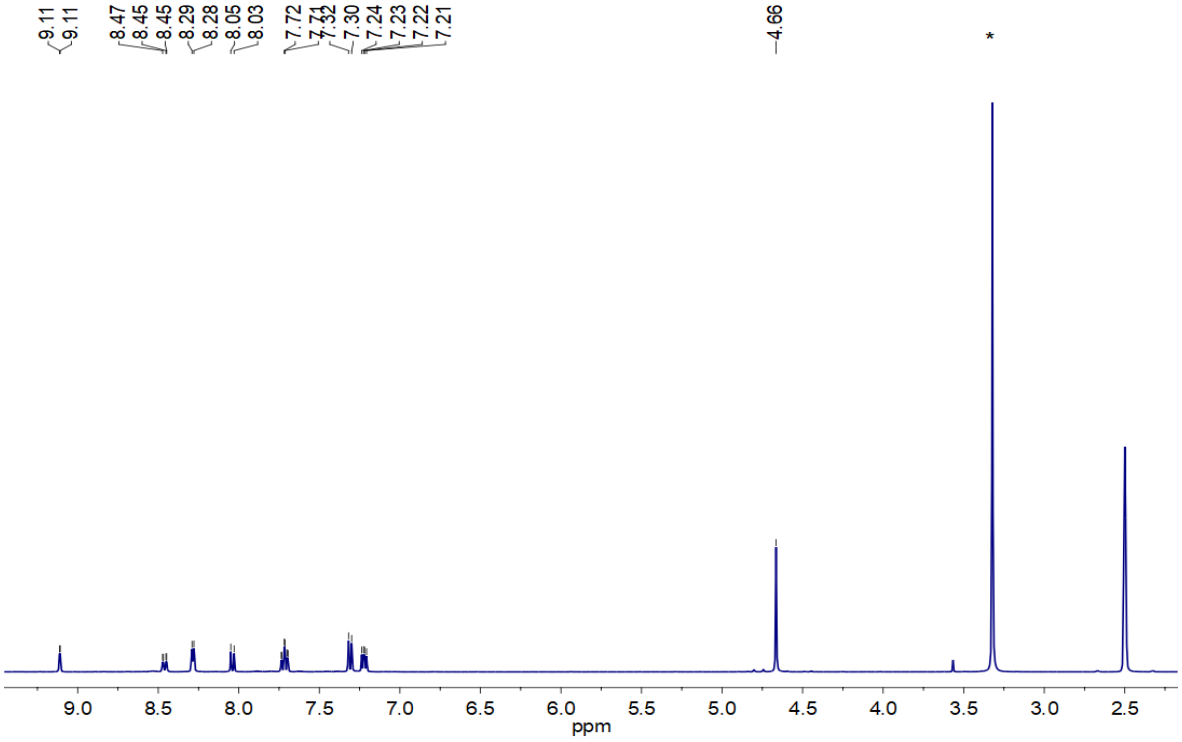

Fig. S.2: ^{1}H NMR spectrum of L2 in DMSO-d_6

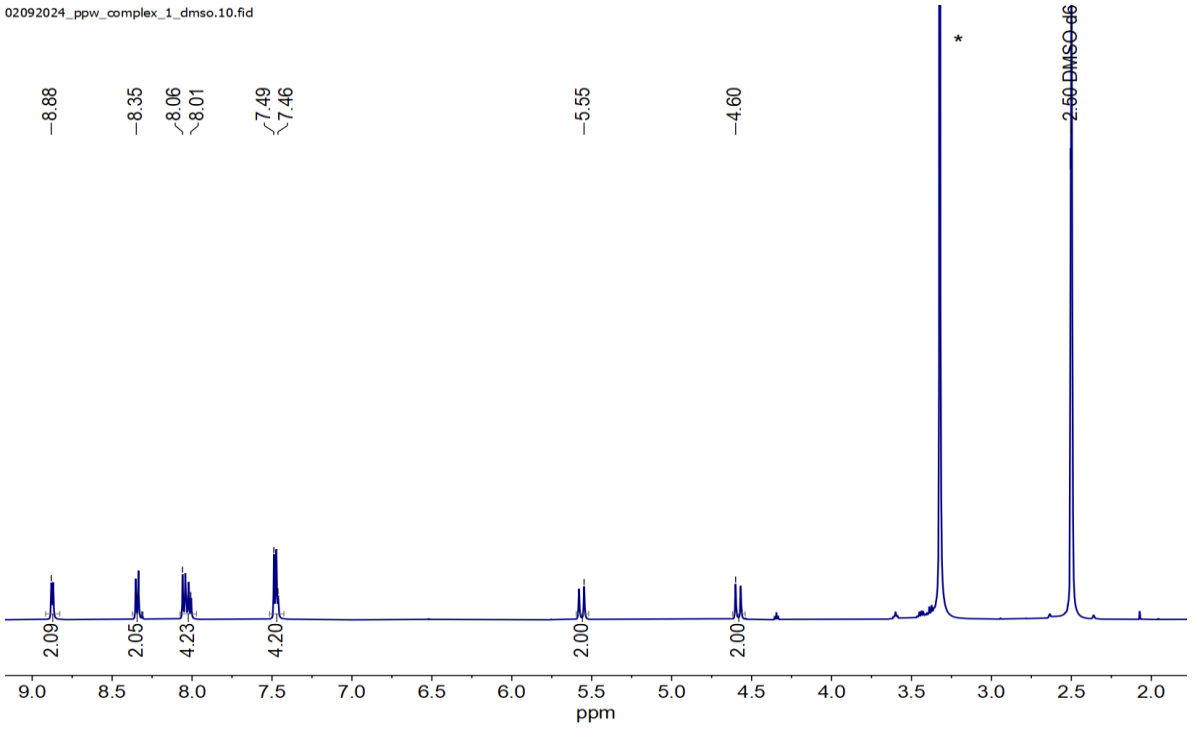

Fig. S.3: ^{1}H NMR spectrum of C1 in DMSO-d_6

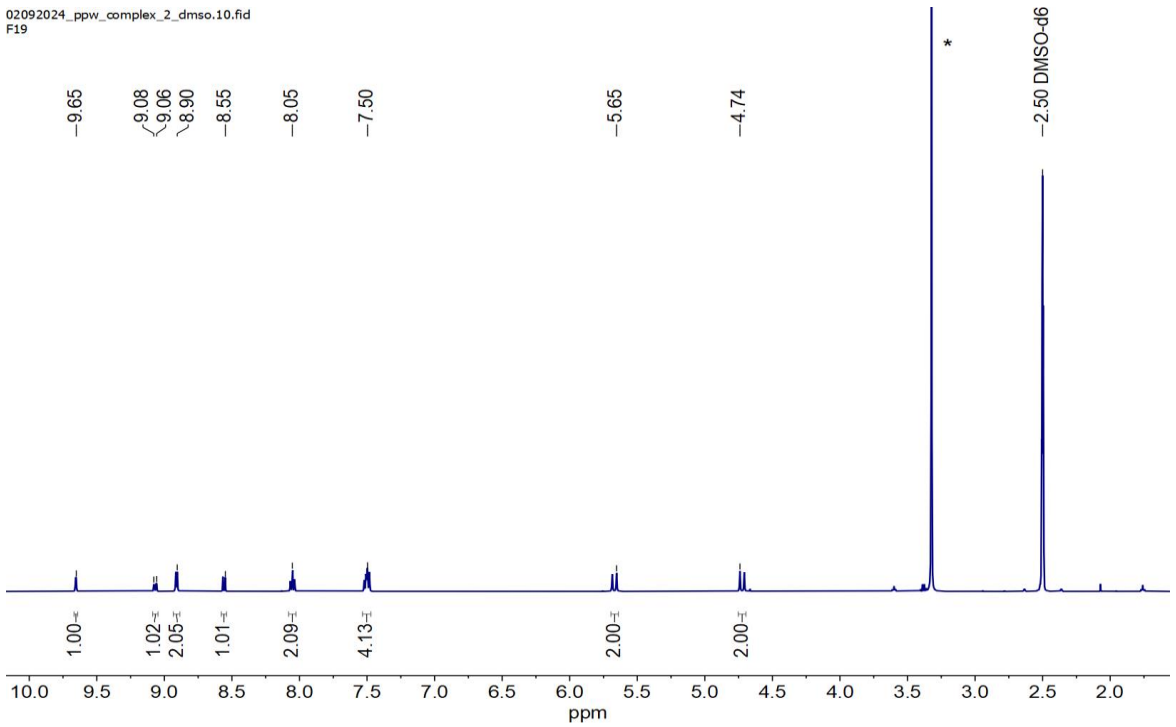

Fig. S.4: ^{1}H NMR spectrum of C2 in DMSO-d_6

s

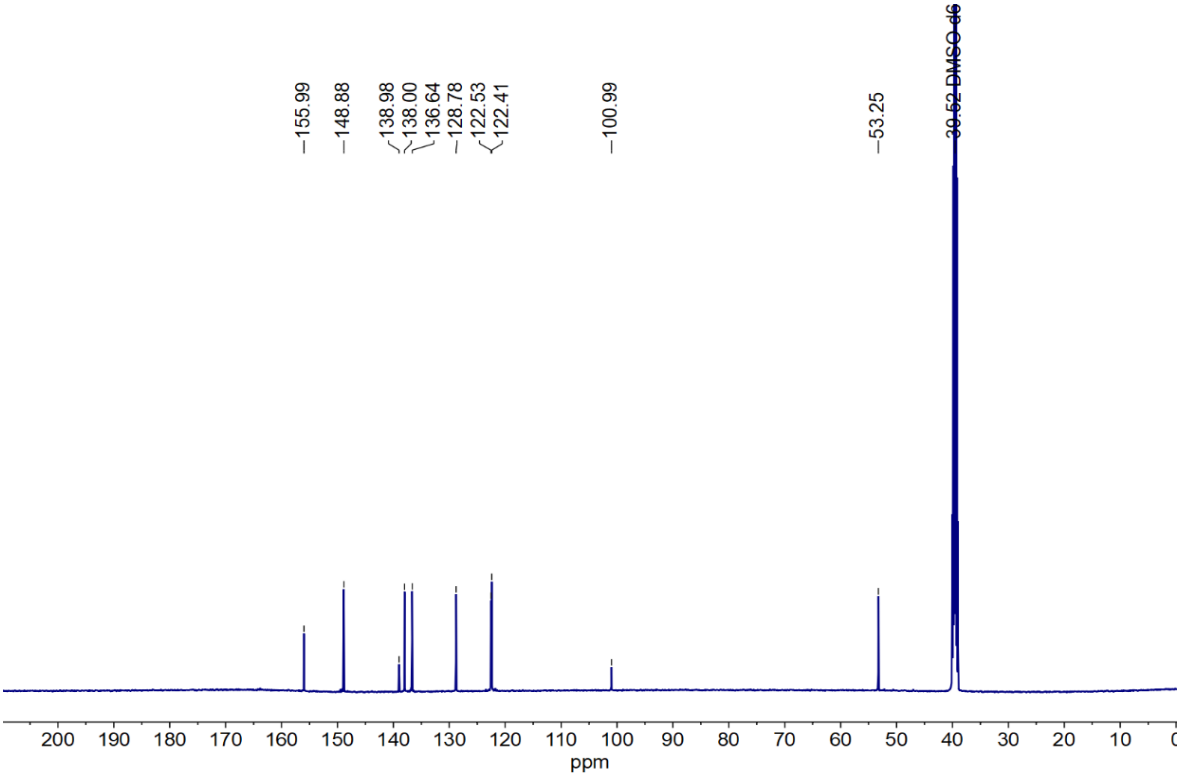

Fig. S.5: ^{13}C NMR spectrum of L1 in DMSO-d_6

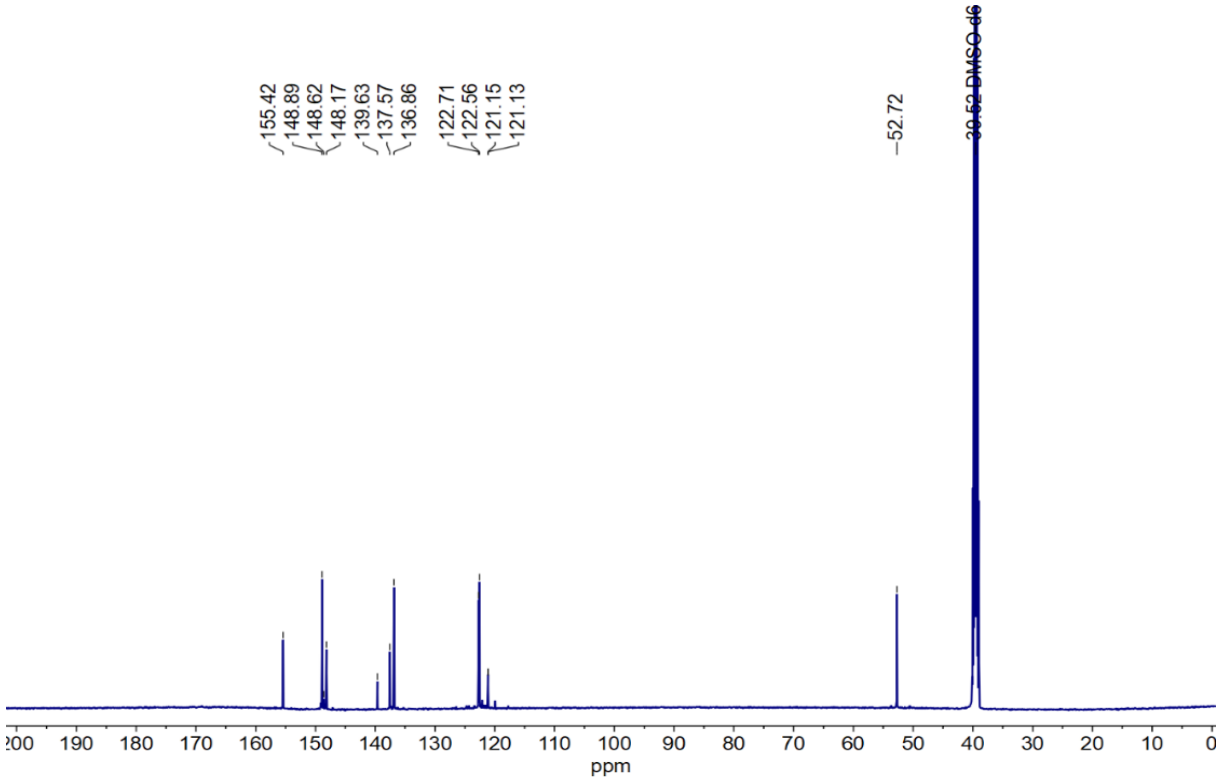

Fig. S.6: ^{13}C NMR spectrum of L2 in DMSO-d_6

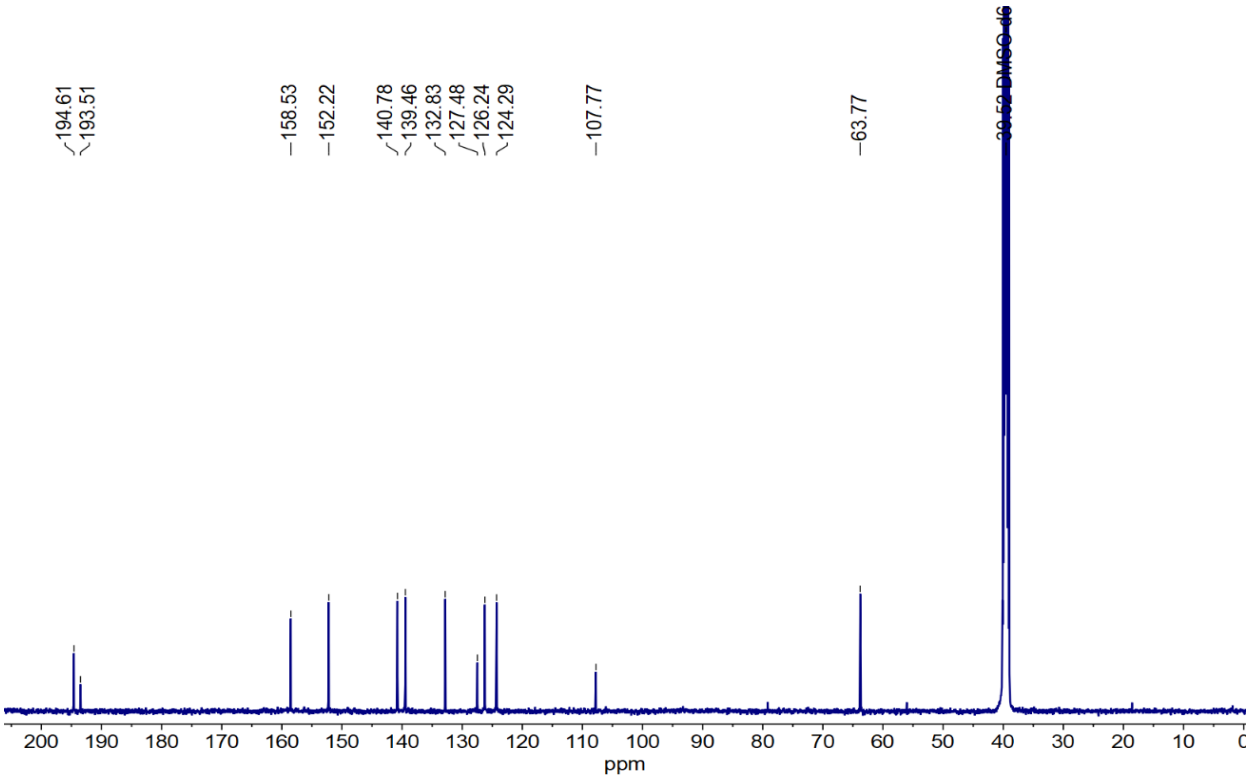

Fig. S.7: ^{13}C NMR spectrum of C1 in DMSO-d_6

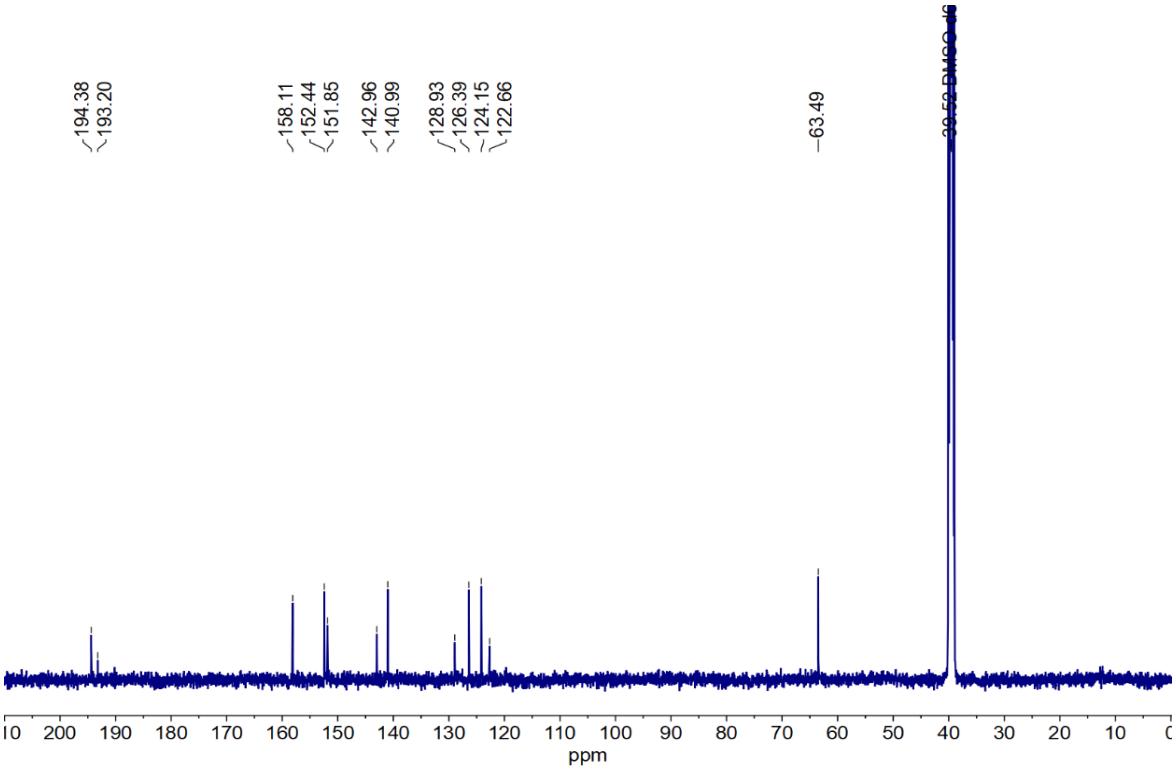

Fig. S.8: ^{13}C NMR spectrum of C2 in DMSO-d_6

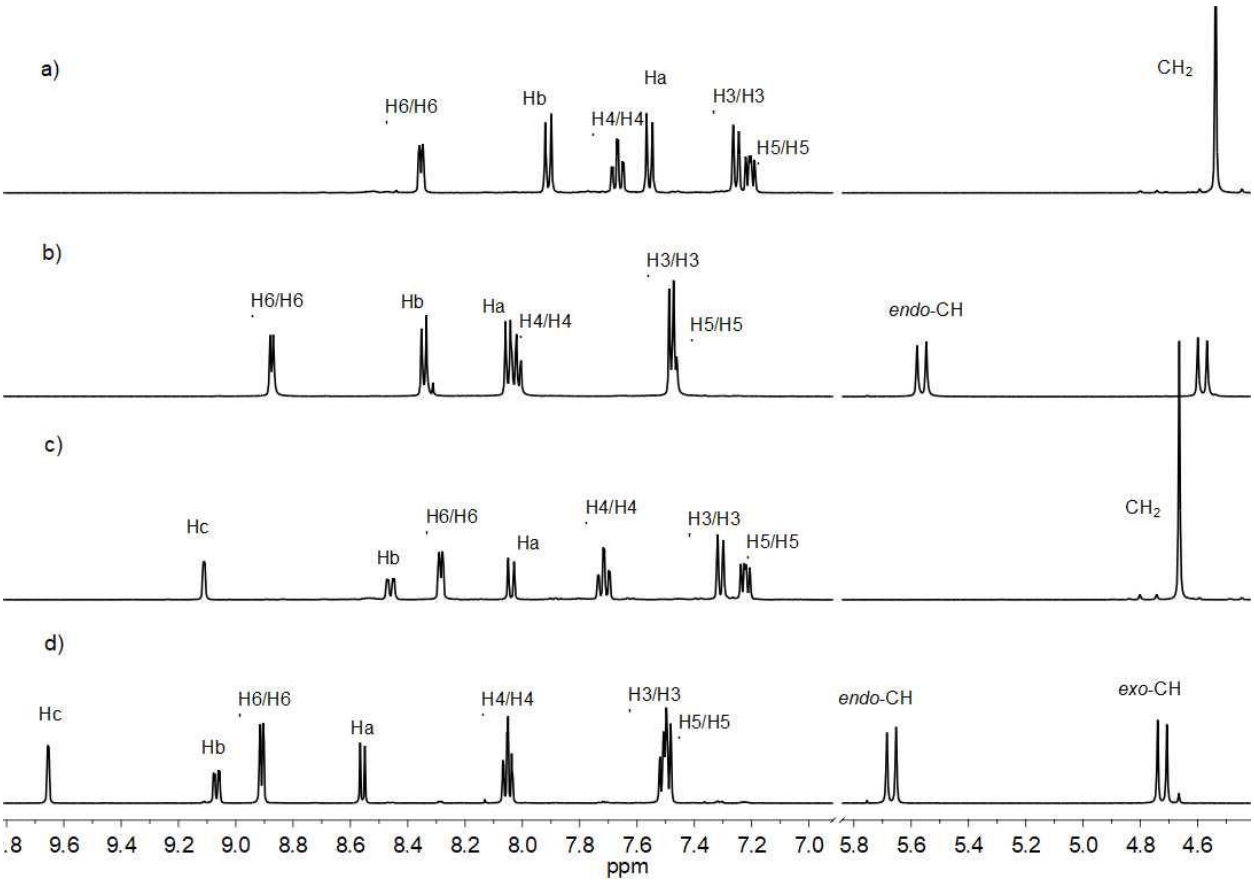

Fig. S.9: Expanded ^{1}H NMR spectra of a) *N*(SO_2(Iodobenz))dpa (L1), b) [Re$(CO)_3$L1]$^+$ (C1), c) *N*(SO_2(tfm)py)dpa (L2) and d) [Re$(CO)_3$L2]$^+$ (C2) in DMSO-d_6

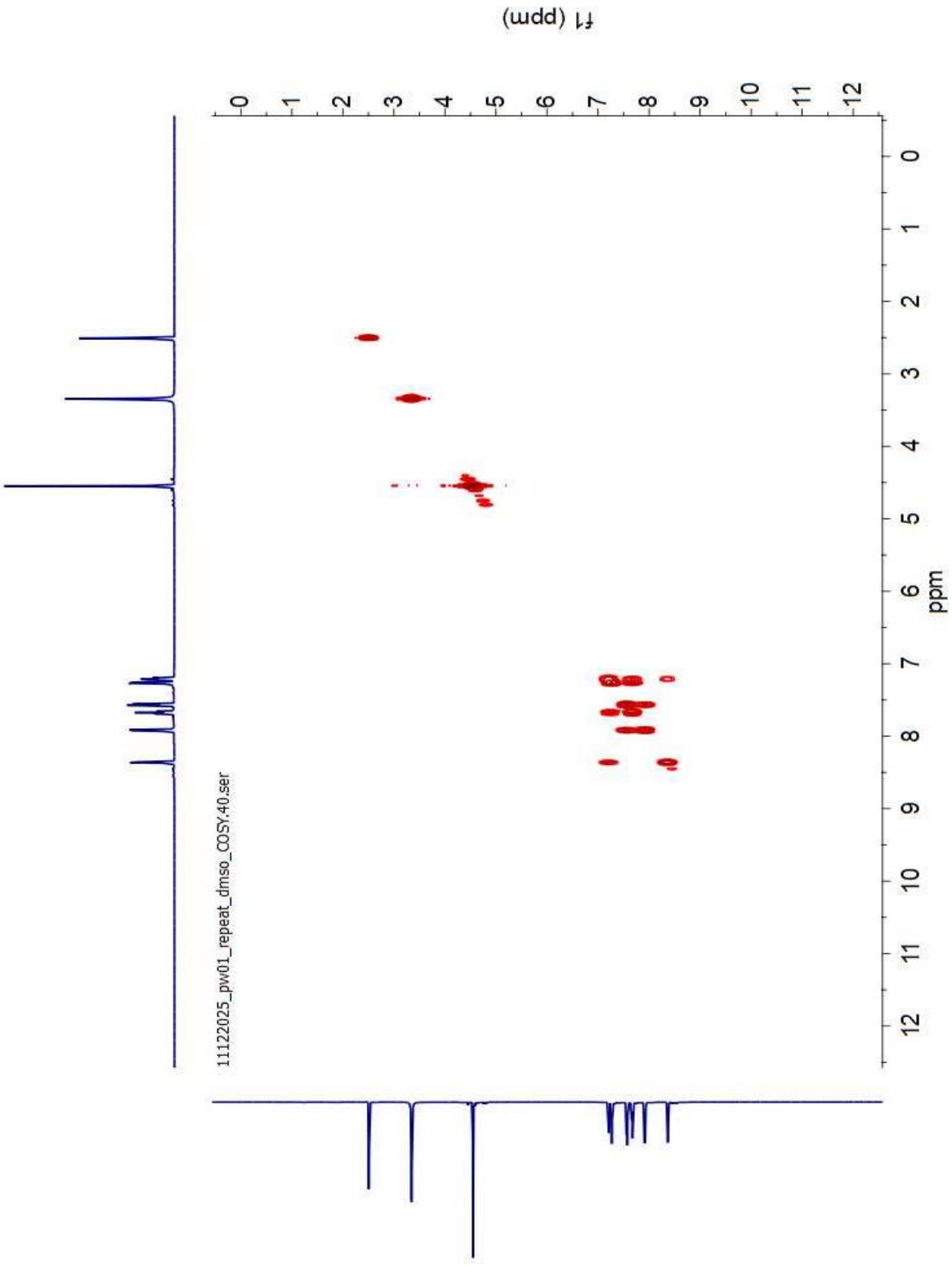

Fig. **S.10:** COSY spectrum of L1 in DMSO-d_6

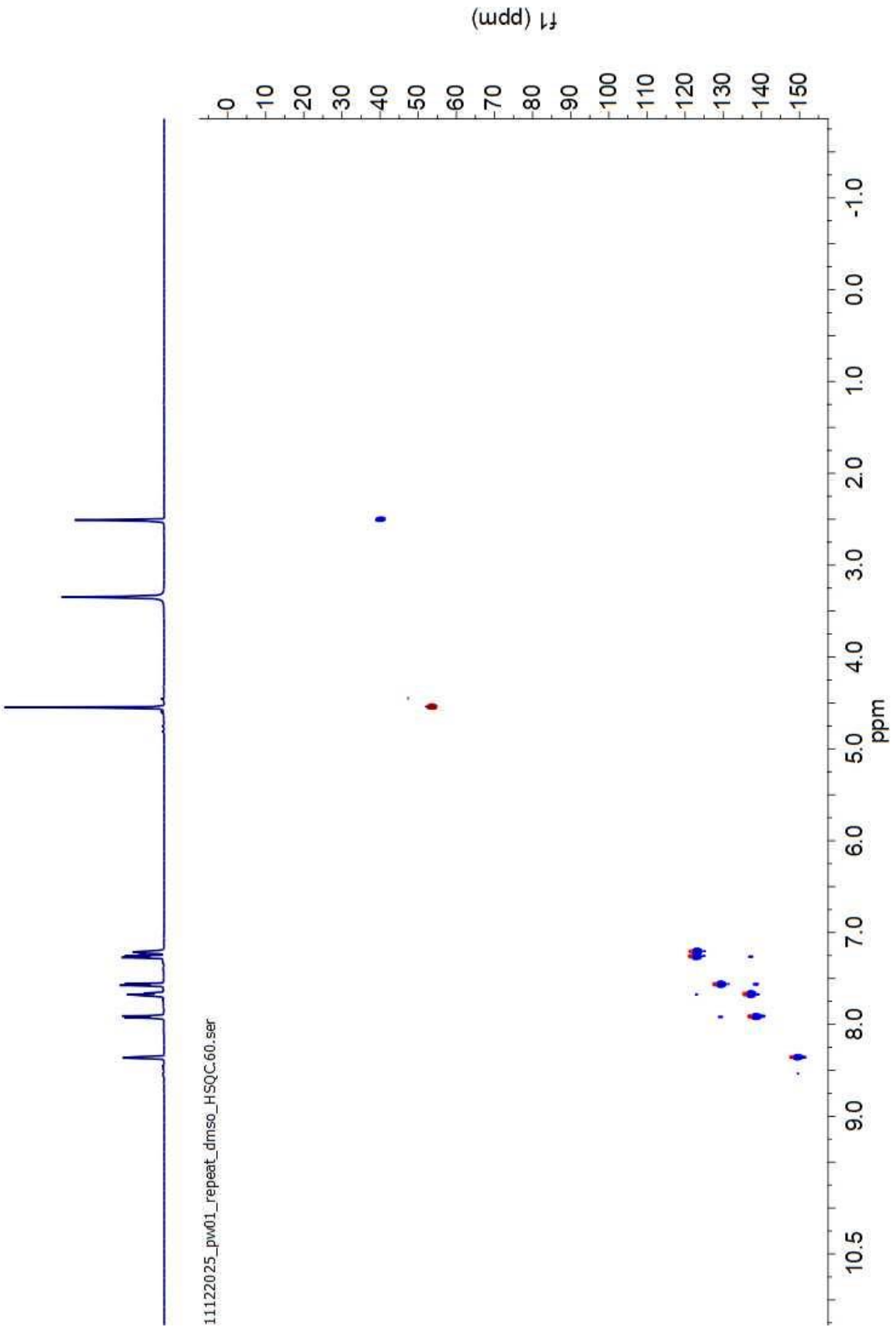

Fig. **S.11:** HSQC spectrum of L1 in DMSO-d_6

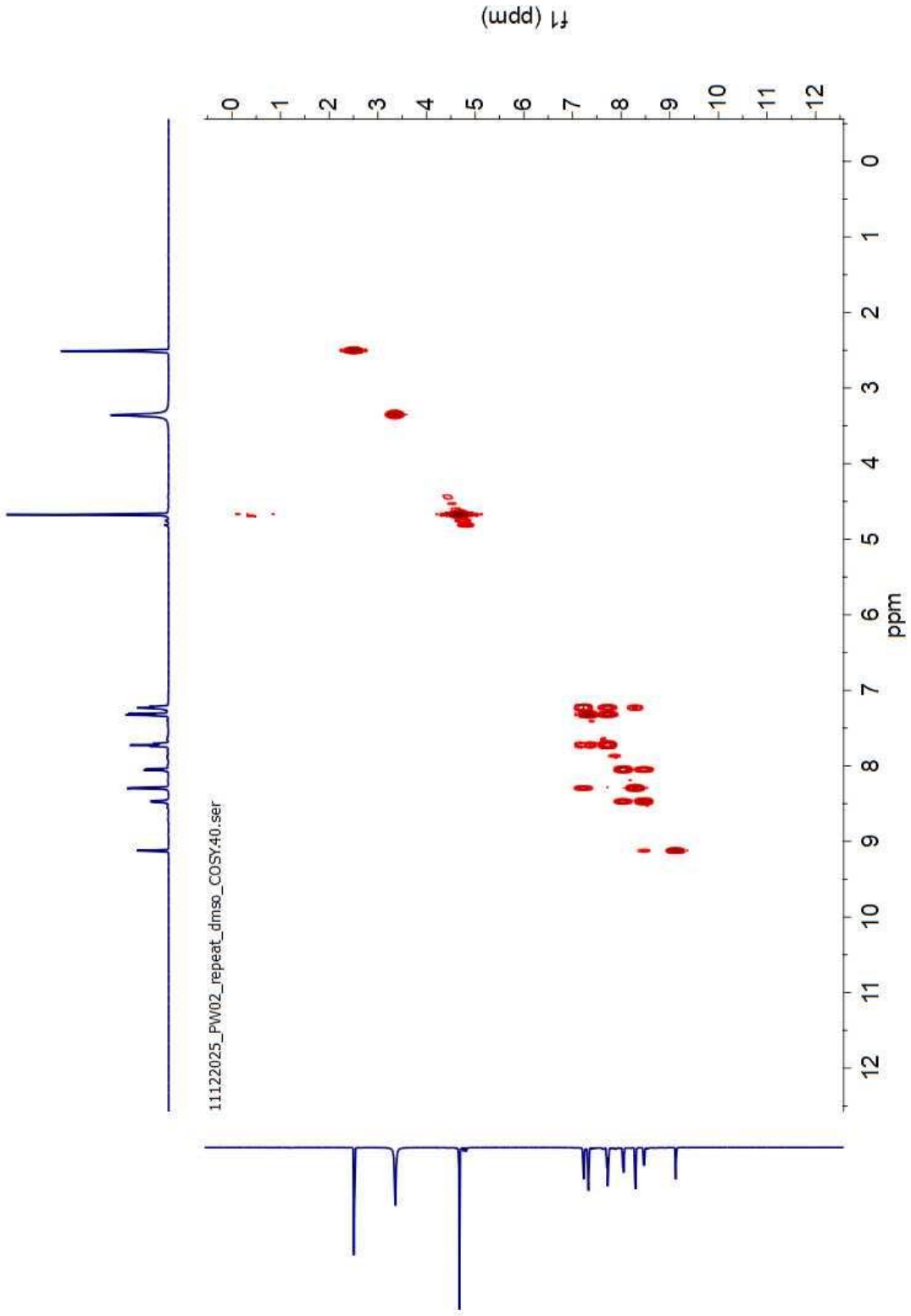

Fig. **S.12:** COSY spectrum of L2 in DMSO-d_6

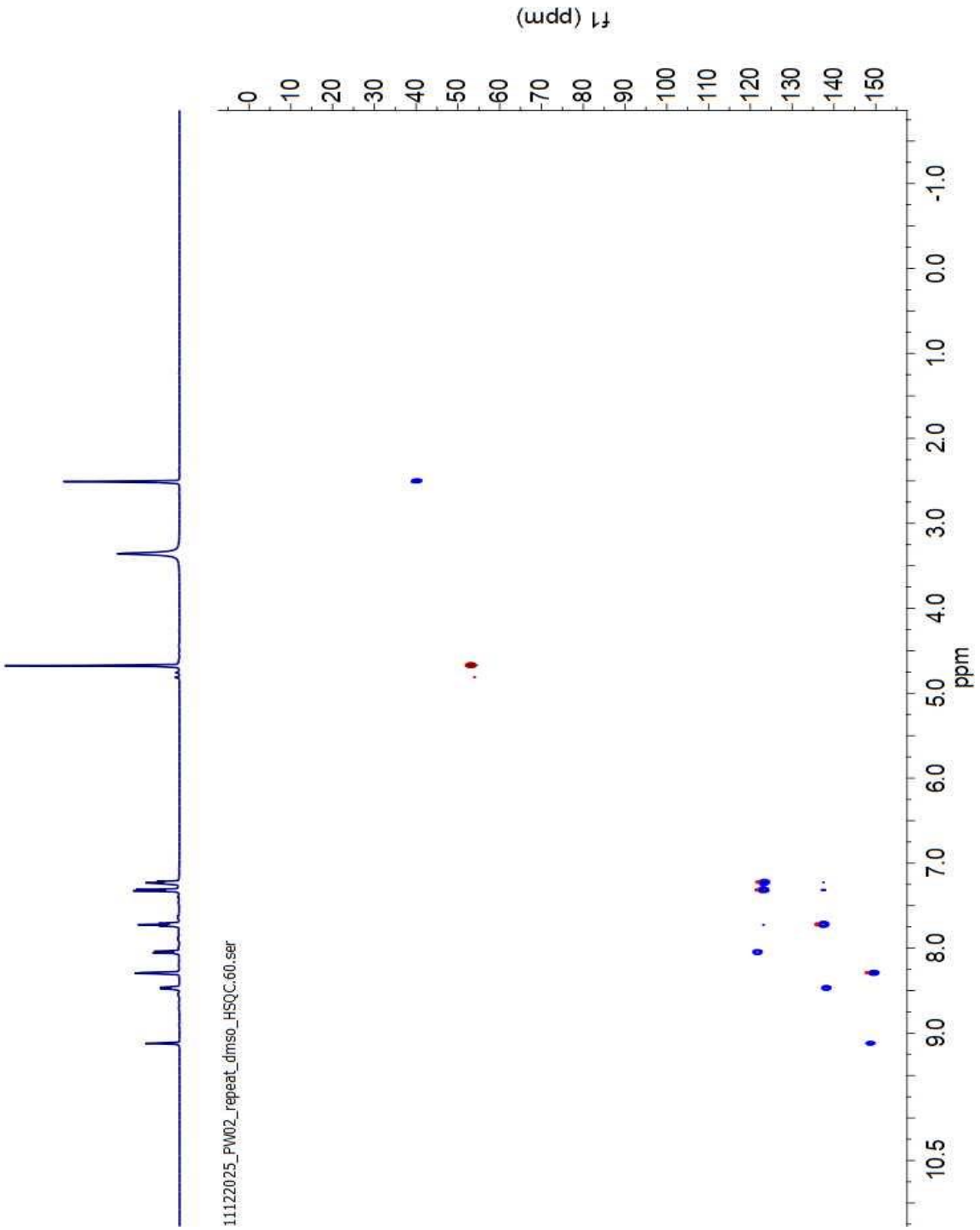

Fig. **S.13:** HSQC spectrum of L2 in DMSO-d_6

UV-Visible spectroscopy data

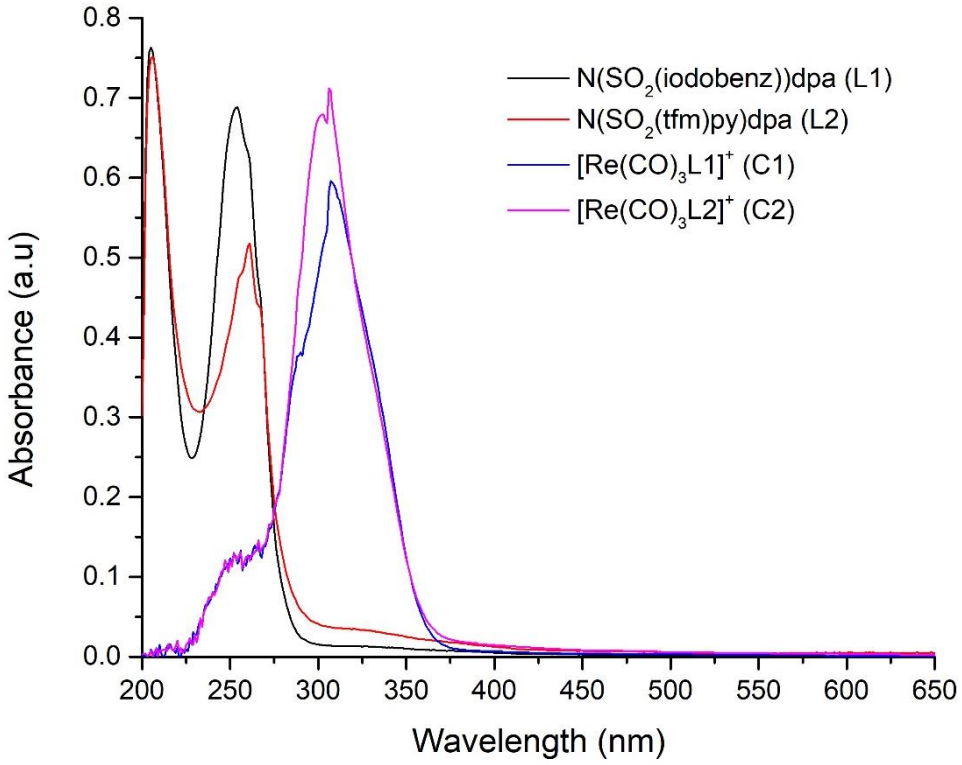

Fig. S.14: UV-Vis spectra of ligands and complexes in MeOH

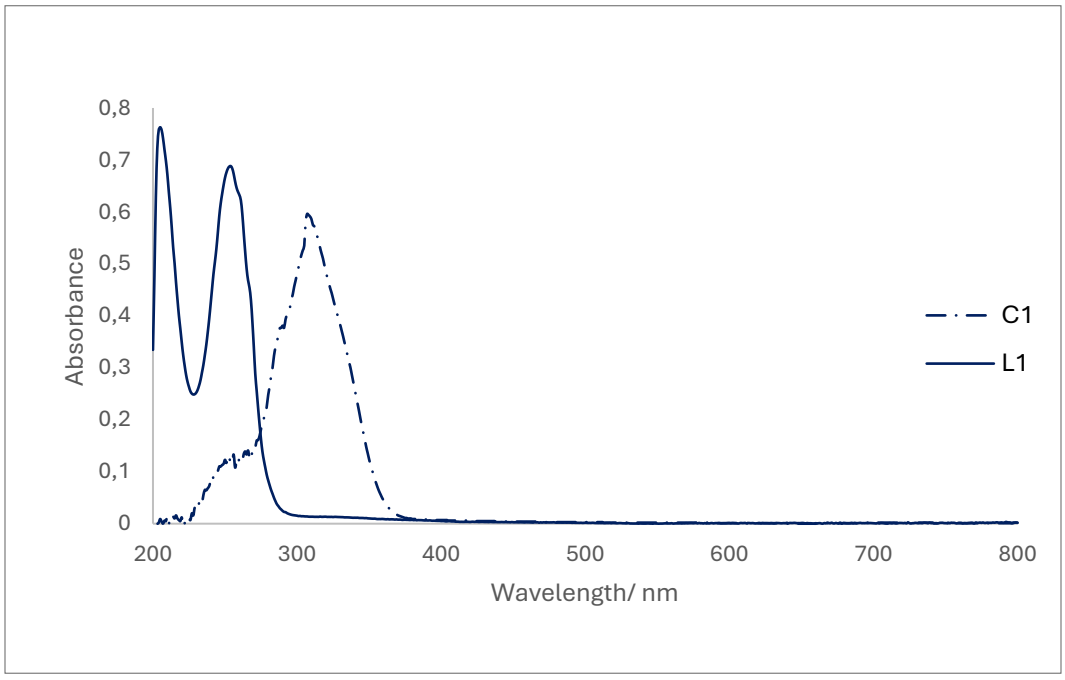

Fig. S.15: UV-Vis spectra comparison of L1 and C1 in MeOH

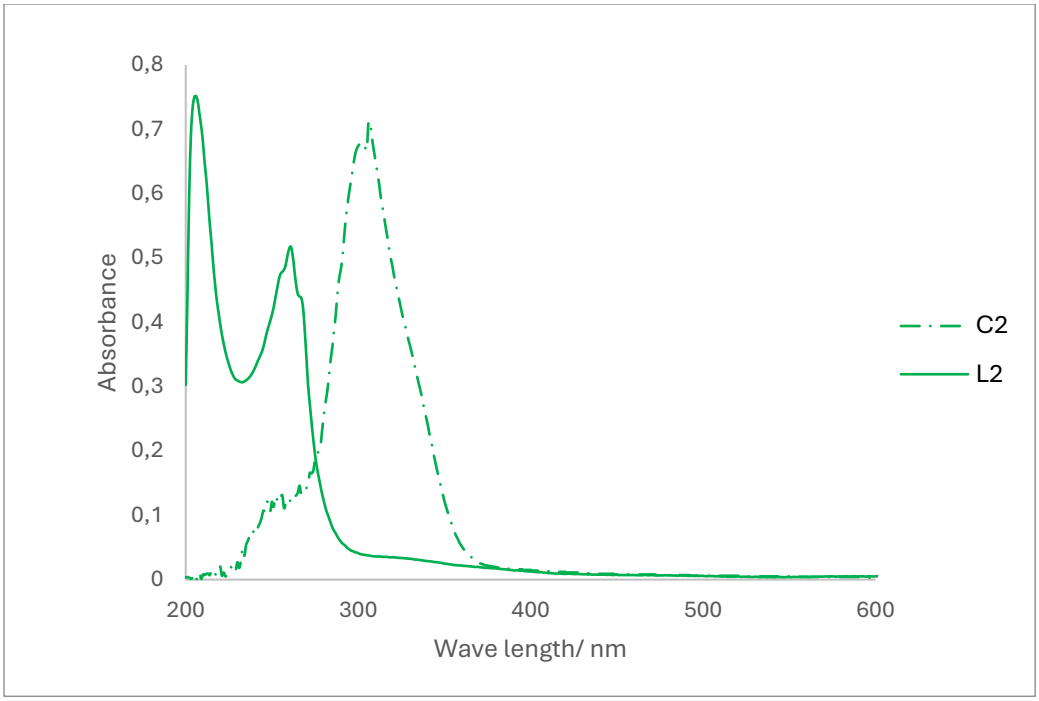

Fig. S.16: UV-Vis spectra comparison of L2 and C2 in MeOH

Single crystal X-ray data

Table **S.1**. Crystal data and structure refinement for L1, L2, C1 and C2

Crystal data	**L1**	**L2**	**C1**	**C2**
Molecular formula	$C_{18}H_{16}IN_3O_2S$	$C_{18}H_{15}F_3N_4O_2S$	$C_{21}H_{16}IN_3O_5ReS{\cdot}0.826(BF_4)\cdot0.174(I)$	$C_{21}H_{15}F_3N_4O_5SRe.PF_6$
Mr	465.30	408.40	829.45	823.60
Crystal description	Lath fragment, colourless	Needle, colourless	Prism, colourless	Lath, colorless
Crystal system	Triclinic	Monoclinic	Orthorhombic	Triclinic
Space group	*P* ī	*I2/a*	$P2_12_12_1$	P ī

Crystal size (mm)	0.29 x 0.20 x 0.09	0.18 x 0.06 x 0.03	0.18 × 0.14 × 0.07	0.25 x 0.10 x 0.03
Temperature (K)	100	90	100	90
a (Å)	7.9629 (4)	23.3099 (13)	10.8624 (3)	12.8219 (4)
b (Å)	12.8004 (6)	6.1488 (4)	12.7681 (4)	15.3365 (5)
c (Å)	18.5913 (8)	26..524 (2)	18.1816 (5)	16.0045 (5)
α (deg)	95.211 (2)	-		103.6599 (18)
β (deg)	99.482 (2)	114.639 (3)		100.6477 (18)
γ (deg)	102.267 (2)	-		114.0384 (16)
V (Å^3)	1810.78 (15)	3455.5 (4)	2521.65 (13)	2649.25 (15)
Z	4	8	4	4
T_{min}	0.762	0.732	0.672	0.699
T_{max}	0.848	0.938	0.795	0.869
Index range	h= -13 – 13 k= -21 – 22 l= -31 – 32	h= -28 – 19 k= -7 – 7 l= -32 – 30	*h* = -17 - 18 *k* = -21 - 21 *l* = -29 - 30	h= -20 – 20 k= -24 – 24 l= -25 – 25
Radiation type	Mo *Kα*	Cu *Kα*	Ag *Kα*	Mo *Kα*
Radiation wavelength/ λ (Å)	0.71073	1.54184	0.56086	0.71073
abs coeff / μ (mm^{-1})	1.90	2.17	3.44	4.83
$2\theta_{max}$ (deg)	75.6°	69.4	55.8	68.8
D_x (Mgm^{-3})	1.707	1.570	2.185	2.065
R[F^2> $2\sigma(F^2)$]	0.037	0.033	0.031	0.022
wR(F^2)	0.083	0.086	0.060	0.046

(Δ/σ)max	0.002	0.001	0.001	0.003
res. dens (e Å^{-3})	-4.31 – 3.41	-0.45 – 0.48	-1.87 – 1.78	-0.94 – 1.15

$w = 1/[\sigma^2(F_o^2) + (0.0303P)^2 + 1.7184P]$ where $P = (F_o^2 + 2F_c^2)/3$ for **L1**

$w = 1/[\sigma^2(F_o^2) + (0.0424P)^2 + 4.6548P]$ where $P = (F_o^2 + 2F_c^2)/3$ for **L2**

$w = 1/[s^2(F_o^2) + (0.0118P)^2 + 5.5332P]$ where $P = (F_o^2 + 2F_c^2)/3$ for **C1**

$w = 1/[\sigma^2(F_o^2) + (0.0183P)^2 + 1.1147P]$ where $P = (F_o^2 + 2F_c^2)/3$ for **C2**

Table **S.1.** Bond distances for L1

	Bond length (Å)		**Bond length (Å)**
I1—C16	2.0879 (14)	I2—C34	2.0970 (17)
S1—O2	1.4349 (13)	S2—O3	1.4349 (12)
S1—O1	1.4363 (13)	S2—O4	1.4350 (13)
S1—N2	1.6366 (15)	S2—N5	1.6332(14)
S1—C13	1.7578 (15)	S2—C31	1.7688 (16)
N1—C5	1.336 (2)	N4—C19	1.339 (3)
N1—C1	1.344 (3)	N4—C23	1.339 (2)
N2—C7	1.474 (2)	N5—C24	1.470 (2)
N2—C6	1.477 (2)	N5—C25	1.482 (2)
N3—C8	1.342 (2)	N6—C26	1.358 (3)
N3—C12	1.342 (2)	N6—C30	1.365 (3)
C1—C2	1.379 (4)	C19—C20	1.381 (3)
C1—H1	0.9500	C19—H19	0.9500
C2—C3	1.384 (4)	C20—C21	1.381 (3)
C2—H2	0.9500	C20—H20	0.9500
C3—C4	1.382 (3)	C21—C22	1.390 (3)
C3—H3	0.9500	C21—H21	0.9500
C4—C5	1.393 (2)	C22—C23	1.388 (2)
C4—H4	0.9500	C22—H22	0.9500
C5—C6	1.509 (2)	C23—C24	1.513 (2)
C6—H6A	0.9900	C23—H24A	0.9900
C6—H6B	0.9900	C24—H24B	0.9900
C7—C8	1.512 (2)	C25—C26	1.511(2)
C7—H7A	0.9900	C25—H25A	0.9900
C7—H7B	0.9900	C25—H25B	0.9900
C8—C9	1.391 (2)	C26—C27	1.363 (2)
C9—C10	1.385 (2)	C27—C28	1.373 (3)
C9—H9	0.9500	C27—H27	0.9500

C10—C11	1.385 (2)	C28—C29	1.376 (4)
C10—H10	0.9500	C28—H28	0.9500
C11—C12	1.385 (3)	C29—C30	1.375 (4)
C11—H11	0.9500	C29—H29	0.9500
C12—H12	0.9500	C12—H12	0.9500
C13—C14	1.394 (2)	C31—C32	1.391 (2)
C13—C18	1.389 (2)	C31—C36	1.391 (2)
C14—C15	1.388 (2)	C32—C33	1.397 (3)
C14—H14	0.9500	C32—H32	0.9500
C15—C16	1.388 (2)	C33—C34	1.385 (3)
C15—H15	0.9500	C33—H33	0.9500
C16—C17	1.392 (2)	C34—C35	1.389 (3)
C17—C18	1.394 (2)	C35—C36	1.395 (2)
C17—H17	0.9500	C35—H35	0.9500
C18—H18	0.9500	C36—H36	0.9500

Table **S.2.** Bond angles (deg) for L1

	Bond angle (°)		**Bond angle (°)**
O2—S1—O1	119.53 (8)	O3—S2—O4	119.92 (8)
O2—S1—N2	107.07 (8)	O3—S2—N5	106.42 (7)
O1—S1—N2	106.47 (8)	O4—S2—N5	107.12 (7)
O2—S1—C13	108.53 (8)	O3—S2—C31	108.44 (8)
O1—S1—C13	107.83 (7)	O4—S2—C31	107.60 (8)
N2—S1—C13	106.77 (7)	N5—S2—C31	106.64 (7)
C5—N1—C1	117.15 (18)	C19—N4—C23	117.25 (18)
C7—N2—C6	114.93 (15)	C24—N5—C25	115.17 (14)
C7—N2—S1	117.39 (12)	C24—N5—S2	117.59 (11)
C6—N2—S1	116.09 (12)	C25—N5—S2	117.07 (11)
C8—N3—C12	116.90 (15)	C26—N6—C30	117.70 (2)
N1—C1—C2	123.4 (2)	N4—C19—C20	123.85 (19)
N1—C1—H1	118.3	N4—C19—H19	118.1
C2—C1—H1	118.3	C20—C19—H19	118.1
C1—C2—C3	118.90 (19)	C21—C20—C19	118.28 (18)
C1—C2—H2	120.6	C21—C20—H20	120.9
C3—C2—H2	120.6	C19—C20—H20	120.9
C4—C3—C2	118.6 (2)	C20—C21—C22	119.03 (19)
C4—C3—H3	120.7	C20—C21—H21	120.5
C2—C3—H3	120.7	C22—C21—H21	120.5
C3—C4—C5	118.71 (19)	C23—C22—C21	118.49 (17)
C3—C4—H4	120.6	C23—C22—H22	120.8
C5—C4—H4	120.6	C21—C22—H22	120.8
N1—C5—C4	123.19 (17)	N4—C23—C22	123.07 (16)
N1—C5—C6	116.04 (16)	N4—C23—C24	114.48 (15)
C4—C5—C6	120.75 (16)	C22—C23—C24	122.42 (15)

N2—C6—C5	112.39 (13)	N5—C24—C23	112.74 (14)
N2—C6—H6A	109.1	N5—C24—H24A	109.0
C5—C6—H6A	109.1	C23—C24—H24A	109.0
N2—C6—H6B	109.1	N5—C24—H24B	109.0
C5—C6—H6B	109.1	C23—C24—H24B	109.0
H6A—C6—H6B	107.9	H24A—C24—H24B	107.8
N2—C7—C8	111.70 (14)	N5—C25—C26	110.29 (13)
N2—C7—H7A	109.3	N5—C25—H25A	109.6
C8—C7—H7A	109.3	C26—C25—H25A	109.6
N2—C7—H7B	109.3	N5—C25—H25B	109.6
C8—C7—H7B	109.3	C26—C25—H25B	109.6
H7A—C7—H7B	107.9	H25A—C25—H25B	108.1
N3—C8—C9	123.25 (16)	N6—C26—C27	123.01 (17)
N3—C8—C7	115.99 (14)	N6—C26—C25	117.59 (16)
C9—C8—C7	120.73 (15)	C27—C26—C25	119.34 (17)
C10—C9—C8	118.56 (16)	C26—C27—C28	117.98 (19)
C10—C9—H9	120.7	C26—C27—H27	121.0
C8—C9—H9	120.7	C28—C27—H27	121.0
C11—C10—C9	119.08 (16)	C27—C28—C29	121.1 (2)
C11—C10—H10	120.5	C27—C28—H28	119.4
C9—C10—H11	120.5	C29—C28—H28	119.4
C12—C11—C10	118.18 (16)	C30—C29—C28	118.15 (19)
C12—C11—H11	120.9	C30—C29—H29	120.9
C10—C11—C11	120.9	C28—C29—C29	120.9
N3—C12—C11	124.00 (17)	N6—C30—C29	122.00 (2)
N3—C12—H12	118.0	N6—C30—H30	119.0
C11—C12—H12	118.0	C29—C30—H30	119.0
C18—C13—C14	121.73 (14)	C32—C31—C36	120.90 (15)
C18—C13—S1	120.12 (11)	C32—C31—S2	119.18 (13)
C14—C13—S1	118.09 (12)	C36—C31—S2	119.87 (12)
C15—C14—C13	119.02 (15)	C31—C32—C33	119.24 (18)
C15—C14—H14	120.5	C31—C32—H32	120.4
C13—C14—H14	120.5	C33—C32—H32	120.4
C14—C15—C16	119.36 (14)	C34—C33—C32	119.51 (17)
C14—C15—H15	120.3	C34—C33—H33	120.2
C16—C15—H15	120.3	C32—C33—H33	120.2
C15—C16—C17	121.79 (14)	C33—C34—C35	121.56 (16)
C15—C16—I1	118.31 (11)	C33—C34—I2	119.03 (14)
C17—C16—I1	119.89 (11)	C35—C34—I2	119.89 (11)
C16—C17—C18	118.93 (14)	C34—C35—C36	118.89 (18)
C16—C17—H17	120.5	C34—C35—H35	120.6
C18—C17—H17	120.5	C36—C35—H35	120.6
C13—C18—C17	119.17 (14)	C31—C36—C35	119.88 (16)
C13—C18—H18	120.4	C31—C36—H36	120.1
C17—C18—H18	120.4	C35—C36—H36	120.1

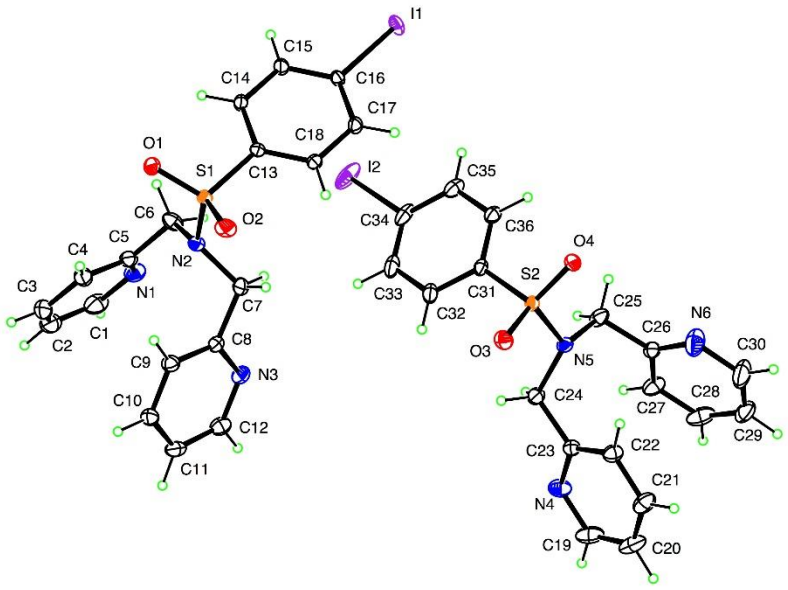

Fig. S.17: ORTEP plot of the *N*(SO_2(iodo-benz)dpa. Thermal ellipsoids are drawn with 50% probability.

Table **S.4**. Bond distances for L2

	Bond length (Å)		**Bond length (Å)**
S1—O1	1.4264 (13)	C5—C6	1.515 (2)
S1—O2	1.4332 (12)	C6—H6A	0.9900
S1—N2	1.6205 (14)	C6—H6B	0.9900
S1—C13	1.7751 (16)	C7—C8	1.511(2)
F1—C18	1.335 (2)	C7—H7A	0.9900
F2—C18	1.344 (2)	C7—H7B	0.9900
F3—C18	1.335 (2)	C8—C9	1.386 (2)
N1—C5	1.347 (2)	C9—C10	1.385 (2)
N1—C1	1.336 (2)	C9—H9	0.9500
N2—C7	1.473 (2)	C10—C11	1.385 (3)
N2—C6	1.476 (2)	C10—H10	0.9500
N3—C12	1.335 (2)	C11—C12	1.385 (3)
N3—C8	1.339 (2)	C11—H11	0.9500
N4—C14	1.336 (2)	C12—H12	0.9500
N4—C15	1.339 (2)	C13—C17	1.388 (2)
C1—C2	1.384 (3)	C13—C14	1.394 (2)
C1—H1	0.9500	C14—H14	0.9500
C2—C3	1.380 (3)	C15—C16	1.383 (2)
C2—H2	0.9500	C15—C18	1.508 (2)
C3—C4	1.391 (3)	C16—C17	1.387 (2)

C3—H3	0.9500	C16—H16	0.9500
C4—C5	1.387 (2)	C17—H17	0.9500
C4—H4	0.9500		

Table **S.5.** Bond angles (deg) for L2

	Bond angle (°)		**Bond angle (°)**
O2—S1—O1	120.66 (7)	H7A—C7—H7B	107.8
O2—S1—N2	107.22 (7)	N3—C8—C9	123.21 (15)
O1—S1—N2	106.90 (7)	N3—C8—C7	113.36 (14)
O2—S1—C13	107.24 (7)	C9—C8—C7	123.43 (15)
O1—S1—C13	106.96 (7)	C10—C9—C8	118.53 (16)
N2—S1—C13	107.20 (7)	C10—C9—H9	120.7
C5—N1—C1	117.21 (15)	C8—C9—H9	120.7
C7—N2—C6	117.39 (13)	C11—C10—C9	119.15 (16)
C7—N2—S1	119.27 (11)	C11—C10—H10	120.4
C6—N2—S1	118.75 (11)	C9—C10—H11	120.4
C8—N3—C12	117.09 (15)	C12—C11—C10	117.90 (16)
N1—C1—C2	124.07 (16)	C12—C11—H11	121.0
N1—C1—H1	118.0	C10—C11—C11	121.0
C2—C1—H1	118.0	N3—C12—C11	124.12 (16)
C1—C2—C3	118.21 (16)	N3—C12—H12	117.9
C1—C2—H2	120.9	C11—C12—H12	117.9
C1—C2—H2	120.9	C17—C13—C14	119.98 (15)
C4—C3—C2	118.99 (16)	C17—C13—S1	120.59 (13)
C2—C3—H3	120.5	C14—C13—S1	119.29 (12)
C4—C3—H3	120.5	N4—C14—C13	122.45 (15)
C3—C4—C5	118.74 (16)	N4—C14—H14	118.8
C3—C4—H4	120.6	C13—C14—H14	118.8
C5—C4—H4	120.6	N4—C15—C16	124.82 (16)
N1—C5—C4	122.77 (15)	N4—C15—C18	114 76 (15)
N1—C5—C6	115.82 (15)	C16—C15—C18	120.34 (15)
C4—C5—C6	121.40 (15)	C15—C16—C17	118.18 (16)
N2—C6—C5	113.98 (13)	C15—C16—H16	120.9
N2—C6—H6A	108.8	C17—C16—H16	120.9
C5—C6—H6A	108.8	C16—C17—C13	117.74 (16)
N2—C6—H6B	108.8	C16—C17—H17	121.1
C5—C6—H6B	108.8	C13—C17—H17	121.1
H6A—C6—H6B	107.7	F2—C18—F1	107.15 (14)
N2—C7—C8	112.88 (14)	F2—C18—F3	106.81 (14)
N2—C7—H7A	109.0	F1—C18—F3	106.50 (14)
C8—C7—H7A	109.0	F2—C18—C15	113.04 (14)
N2—C7—H7B	109.0	F1—C18—C15	111.98 (14)
C8—C7—H7B	109.0	F3—C18—C15	110.98 (14)

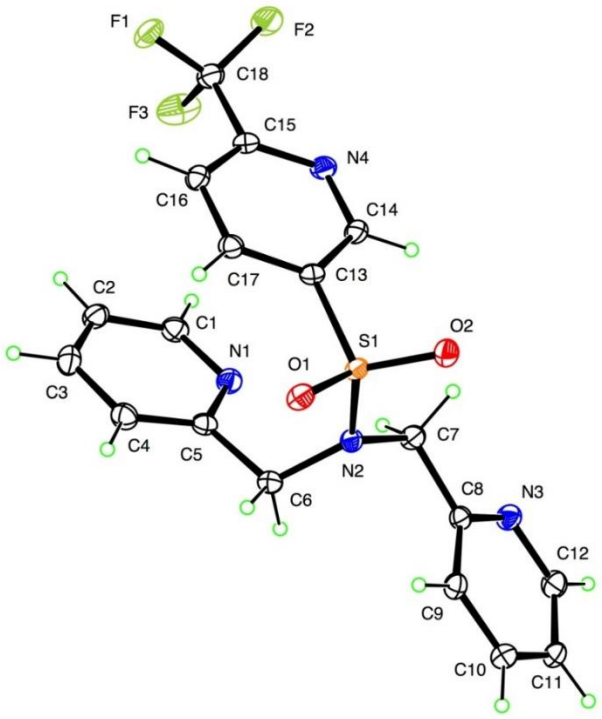

Fig. S.18: ORTEP plot of the *N*(SO_2(tfm)dpa. Thermal ellipsoids are drawn with 50% probability.

Table **S.6** Bond distances for C2

	Bond length (Å)		**Bond length (Å)**
Re1—C20	1.9048 (19)	S2—O2	1.4231 (14)
Re1—C19	1.927 (2)	S2—O7	1.4283 (14)
Re1—C21	1.943 (2)	S2—N6	1.7447 (15)
Re1—N3	2.1611 (15)	S2—C34	1.7575 (18)
Re1—N1	2.1775 (16)	F4—C39	1.333 (2)
Re1—N2	2.2888 (14)	F5—C39	1.331 (2)
S1—O1	1.4243 (14)	F6—C39	1.338 (2)
S1—O2	1.4285 (14)	O8—C40	1.148 (2)
S1—N2	1.7593 (15)	O9—C41	1.152 (2)
S1—C13	1.7595 (18)	O10—C42	1.149 (2)
F1—C18	1.343 (2)	N5—C22	1.351 (2)
F2—C18	1.336 (2)	N5—C26	1.356 (2)
F3—C18	1.326 (2)	N6—C28	1.512 (2)
O3—C19	1.153 (2)	N6—C33	1.512 (2)
O4—C20	1.149 (2)	N7—C33	1.346 (2)
O5—C21	1.144 (2)	N7—C29	1.355 (3)
N1—C5	1.351 (2)	N8—C35	1.333 (2)
N1—C1	1.349 (2)	N8—C36	1.337 (2)
N2—C7	1.509 (2)	C22—C23	1.380 (3)
N2—C6	1.515 (2)	C22—H22	0.9500

N3—C12	1.358 (2)	C23—C24	1.391 (3)
N3—C8	1.343 (2)	C23—H23	0.9500
N4—C14	1.333 (2)	C24—C25	1.381 (3)
N4—C15	1.335 (2)	C24—H24	0.9500
C1—C2	1.379 (3)	C25—C26	1.389 (3)
C1—H1	0.9500	C25—H25	0.9500
C2—C3	1.386 (3)	C26—C27	1.494 (2)
C2—H2	0.9500	C27—H27A	0.9900
C3—C4	1.383 (3)	C27—H27B	0.9900
C3—H3	0.9500	C28—C29	1.494 (2)
C4—C5	1.386 (2)	C28—H28A	0.9900
C4—H4	0.9500	C28—H28B	0.9900
C5—C6	1.498 (2)	C29—C30	1.382 (2)
C6—H6A	0.9900	C30—C31	1.386 (3)
C6—H6B	0.9900	C30—H30	0.9500
C7—C8	1.508 (2)	C31—C32	1.387 (3)
C7—H7A	0.9900	C31—H31	0.9500
C7—H7B	0.9900	C32—C33	1.381 (3)
C8—C9	1.394 (2)	C32—H32	0.9500
C9—C10	1.382 (2)	C33—H33	0.9500
C9—H9	0.9500	C34—C38	1.392 (3)
C10—C11	1.390 (3)	C34—C35	1.394 (2)
C10—H10	0.9500	C35—H35	0.9500
C11—C12	1.374 (3)	C36—C37	1.383 (3)
C11—H11	0.9500	C36—C39	1.508 (3)
C12—H12	0.9500	C37—C38	1.387 (3)
C13—C17	1.389 (3)	C37—H37	0.9500
C13—C14	1.394 (2)	C38—H38	0.9500
C14—H14	0.9500	P1—F11	1.5871 (14)
C15—C16	1.384 (3)	P1—F10	1.5952 (15)
C15—C18	1.514 (3)	P1—F9	1.5986 (14)
C16—C17	1.383 (3)	P1—F8	1.6003 (15)
C16—H16	0.9500	P1—F7	1.6038 (15)
C17—H17	0.9500	P1—F12	1.6093 (13)
Re2—C41	1.9087 (19)	P2—F14	1.5909 (14)
Re2—C42	1.9184 (19)	P2—F16	1.5943 (13)
Re2—C40	1.9329 (19)	P2—F15	1.6058 (14)
Re2—N5	2.1858 (15)	P2—F18	1.6067 (13)
Re2—N6	2.1899 (15)	P2—F17	1.6102 (14)
Re2—N7	2.2648 (15)	P2—F13	1.6134 (13)

Table **S.7.** Bond angles (deg) for C2

	Bond angle (°)		**Bond angle (°)**
C20—Re1—C19	87.75 (8)	O6—S2—O7	121.61 (9)
C20—Re1—C21	86.90 (9)	O6—S2—N6	106.52 (8)
C19—Re1—C21	91.03 (8)	O7—S2—N6	105.98 (8)
C20—Re1—N3	96.75 (7)	O6—S2—C34	108.98 (9)
C19—Re1—N3	91.56 (7)	O7—S2—C34	109.01 (8)
C21—Re1—N3	175.60 (7)	N6—S2—C34	103.14 (8)
C20—Re1—N1	95.42 (8)	C22—N5—C26	118.24 (16)
C19—Re1—N1	173.67 (7)	C22—N5—Re2	123.45 (13)
C21—Re1—N1	94.60 (7)	C26—N5—Re2	115.49 (11)
N3—Re1—N1	82.64 (6)	C28—N6—C27	111.21 (14)
C20—Re1—N2	170.17 (7)	C28—N6—S2	109.06 (11)
C19—Re1—N2	100.41 (7)	C27—N6—S2	110.18 (11)
C21—Re1—N2	98.32 (7)	C28—N6—Re2	107.42 (10)
N3—Re1—N2	77.71 (5)	C27—N6—Re2	107.20 (10)
N1—Re1—N2	75.95 (5)	S2—N6—Re2	111.75 (7)
O2—S1—O1	121.47 (9)	C33—N7—C29	118.22 (16)
O2—S1—N2	105.01 (8)	C33—N7—Re2	124.63 (12)
O1—S1—N2	105.38 (8)	C29—N7—Re2	115.42 (12)
O2—S1—C13	109.56 (8)	C35—N8—C36	116.86 (17)
O1—S1—C13	108.10 (8)	N5—C22—C23	122.62 (18)
N2—S1—C13	106.5 (8)	N5—C22—H22	118.7
C5—N1—C1	118.02 (16)	C23—C22—H22	118.7
C1—N1—Re1	124.52 (13)	C22—C23—C24	118.73 (18)
C5—N1—Re1	117.39 (12)	C22—C23—H23	120.6
C7—N2—C6	111.59 (13)	C24—C23—H23	120.6
C7—N2—S1	110.35 (11)	C25—C24—C23	119.26 (18)
C6—N2—S1	108.59 (11)	C25—C24—H24	120.4
C7—N2—Re1	109.55 (10)	C23—C24—H24	120.4
C6—N2—Re1	106.49 (10)	C24—C25—C26	119.11 (18)
S1—N2—Re1	110.21 (7)	C24—C25—H25	120.4
C8—N3—C12	118.74 (16)	C26—C25—H25	120.4
C8—N3—Re1	118.07 (12)	N5—C26—C25	121.95 (17)
C12—N3—Re1	123.19 (12)	N5—C26—C27	115.54 (15)
C14—N4—C15	117.27 (16)	C25—C26—C27	122.49 (17)
N1—C1—C2	122.12 (18)	N6—C27—C26	110.25 (14)
N1—C1—H1	118.9	N6—C27—H27A	109.6
C2—C1—H1	118.9	C26—C27—H27A	109.6
C1—C2—C3	119.53 (18)	N6—C27—H27B	109.6
C1—C2—H2	120.2	C26—C27—H27B	109.6
C3—C2—H2	120.2	H27A—C27—H27B	108.1
C4—C3—C2	118.82 (18)	N6—C28—C29	111.62 (14)
C2—C3—H3	120.6	N6—C28—H28A	109.3

C4—C3—H3	120.6	C29—C28—H28A	109.3
C3—C4—C5	118.71 (18)	N6—C28—H28B	109.3
C3—C4—H4	120.6	C29—C28—H28B	109.3
C5—C4—H4	120.6	H28A—C28—H28B	108.1
N1—C5—C4	122.72 (17)	N7—C29—C30	122.45 (17)
N1—C5—C6	116.10 (16)	N7—C29—C28	116.33 (15)
C4—C5—C6	120.85 (16)	C30—C29—C28	121.11 (16)
N2—C6—C5	110.75 (14)	C29—C30—C31	118.68 (17)
N2—C6—H6A	109.5	C29—C30—H30	120.7
C5—C6—H6A	109.5	C31—C30—H30	120.7
N2—C6—H6B	109.5	C30—C31—C32	119.31 (17)
C5—C6—H68	109.5	C30—C31—H31	120.3
H6A—C6—H6B	108.1	C32—C31—H31	120.3
N2—C7—C8	114.36 (14)	C33—C32—C31	118.91 (18)
N2—C7—H7A	108.7	C33—C32—H32	120.5
C8—C7—H7A	108.7	C31—C32—H32	120.5
N2—C7—H7B	108.7	N7—C33—C32	122.42 (17)
C8—C7—H7B	108.7	N7—C33—H33	118.8
H7A—C7—H7B	107.6	C32—C33—H33	118.8
N3—C8—C9	121.47 (16)	C38—C34—C35	120.73 (17)
N3—C8—C7	118.43 (15)	C38—C34—S2	120.83 (14)
C9—C8—C7	119.95 (15)	C35—C34—S2	118.40 (14)
C10—C9—C8	119.59 (17)	N8—C35—C34	121.79 (17)
C10—C9—H9	120.2	N8—C35—H35	119.1
C8—C9—H9	120.2	C34—C35—H35	119.1
C11—C10—C9	118.74 (18)	N8—C36—C37	125.46 (18)
C11—C10—H10	120.6	N8—C36—C39	112.66 (17)
C9—C10—H11	120.6	C37—C36—C39	121.89 (18)
C12—C11—C10	119.14 (18)	C36—C37—C38	117.77 (18)
C12—C11—H11	120.4	C36—C37—H37	121.1
C10—C11—H11	120.4	C38—C37—H37	121.1
N3—C12—H11	122.31 (18)	C37—C38—C34	117.37 (18)
N3—C12—H12	118.8	C37—C38—H38	121.3
C11—C12—H12	118.8	C34—C38—H38	121.3
C17—C13—C14	120.60 (16)	F5—C39—F4	107.15 (17)
C17—C13—S1	120.61 (14)	F5—C39—F6	107.69 (17)
C14—C13—S1	118.62 (13)	F4—C39—F6	106.01 (17)
N4—C14—C13	121.60 (14)	F5—C39—C36	112.52 (17)
N4—C14—H14	119.2	F4—C39—C36	111.79 (16)
C13—C14—H14	119.2	F6—C39—C36	111.34 (17)
N4—C15—C16	125.02 (17)	O8—C40—Re2	177.82 (16)
N4—C15—C18	114.46 (16)	O9—C41—Re2	177.43 (17)
C16—C15—C18	120.46 (16)	O10—C42—Re2	176.18 (17)
C15—C16—C17	117.89 (17)	F11—P1—F10	89.96 (9)
C15—C16—H16	121.1	F11—P1—F9	90.72 (8)

C17—C16—H16	121.1	F10—P1—F9	90.55 (8)
C16—C17—C13	117.62 (17)	F11—P1—F8	179.22 (9)
C16—C17—H18	121.2	F10—P1—F8	89.96 (10)
C13—C17—H18	121.2	F9—P1—F8	90.05 (8)
F2—C18—F1	106.62 (16)	F11—P1—F7	89.95 (9)
F2—C18—F3	107.69 (17)	F10—P1—F7	179.78 (9)
F1—C18—F3	107.05 (17)	F9—P1—F7	89.65 (8)
F2—C18—C15	111.90 (16)	F8—P1—F7	90.13 (10)
F1—C18—C15	110.65 (17)	F11—P1—F12	90.28 (8)
F3—C18—C15	112.61 (16)	F10—P1—F12	89.79 (8)
O3—C19—Re1	177.68 (17)	F9—P1—F12	178.94 (8)
O4—C20—Re1	178.4 (2)	F8—P1—F12	88.95 (8)
O5—C21—Re1	177.90 (19)	F7—P1—F12	90.01 (8)
C41—Re2—C42	86.83 (8)	F14—P2—F16	90.83 (7)
C41—Re2—C40	89.44 (8)	F14—P2—F15	90.45 (8)
C42—Re2—C40	87.01 (8)	F16—P2—F15	90.98 (7)
C41—Re2—N5	95.05 (7)	F14—P2—F18	90.30 (8)
C42—Re2—N5	99.25 (7)	F16—P2—F18	89.97 (7)
C40—Re2—N5	172.47(7)	F15—P2—F18	178.79 (8)
C41—Re2—N7	96.93 (7)	F14—P2—F17	178.97 (8)
C42—Re2—N7	174.82 (7)	F16—P2—F17	90.07 (7)
C40—Re2—N7	96.55 (7)	F15—P2—F17	90.03 (8)
N5—Re2—N7	76.93 (6)	F18—P2—F17	89.21 (7)
C41—Re2—N6	171.13 (7)	F14—P2—F13	89.44 (7)
C42—Re2—N6	98.32 (7)	F16—P2—F13	179.36 (8)
C40—Re2—N6	98.00 (6)	F15—P2—F13	89.60 (7)
N5—Re2—N6	77.05 (5)	F18—P2—F13	89.45 (7)
N7—Re2—N6	77.51 (6)	F17—P2—F13	89.65 (7)

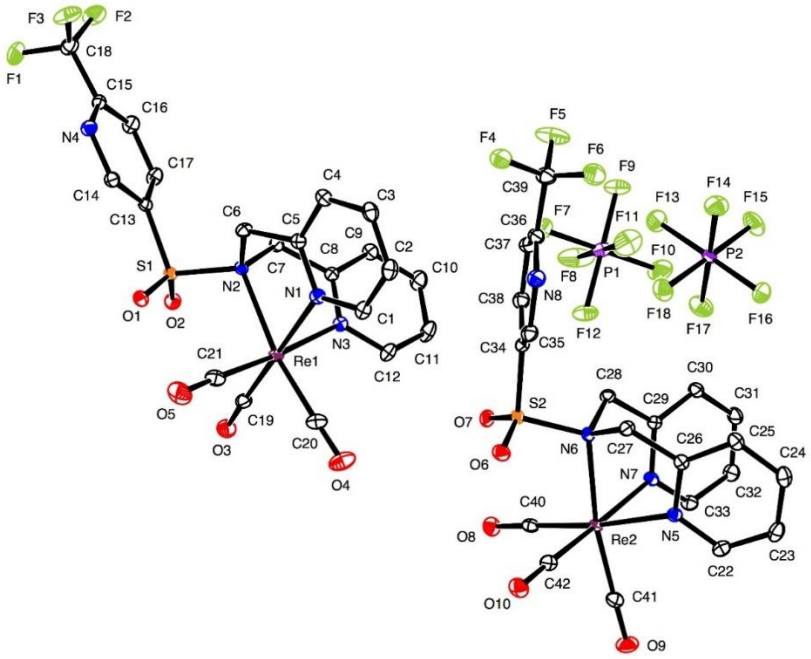

Fig. S.19. ORTEP plot of the **C2**. Thermal ellipsoids are drawn with 50% probability.

Table **S.8.** Bond distances for C1

	Bond length (Å)		**Bond length (Å)**
Re1—C20	1.902 (5)	C8—C9	1.377 (7)
Re1—C21	1.926 (5)	C9—C10	1.391 (7)
Re1—C19	1.928 (5)	C9—H9	0.9500
Re1—N1	2.174 (4)	C10—C11	1.385 (8)
Re1—N3	2.178 (4)	C10—H10	0.9500
Re1—N2	2.259 (3)	C11—C12	1.374 (7)
I1—C16	2.093 (4)	C11—H11	0.9500
S1—O1	1.426 (4)	C12—H12	0.9500
S1—O2	1.426 (3)	C13—C18	1.385 (6)
S1—C13	1.742 (4)	C13—C14	1.392 (7)
S1—N2	1.757 (4)	C14—C15	1.382 (6)
O3—C19	1.150 (6)	C14—H14	0.9500
O4—C20	1.153 (6)	C15—C16	1.391 (7)

O5—C21	1.147 (6)	C15—H15	0.9500
N1—C5	1.345 (6)	C16—C17	1.378 (7)
N1—C1	1.361 (6)	C17—C18	1.393 (6)
N2—C6	1.502 (6)	C17—H17	0.9500
N2—C7	1.503 (6)	C18—H18	0.9500
N3—C12	1.350 (6)	I2—F3	1.272 (9)
N3—C8	1.357 (6)	I2—F2	1.288 (6)
C1—C2	1.373 (7)	I2—F2A	1.291 (16)
C1—H1	0.9500	I2—F4A	1.371 (16)
C2—C3	1.383 (8)	I2—F3A	1.418 (13)
C2—H2	0.9500	I2—F4	1.459 (8)
C3—C4	1.389 (8)	I2—F1A	1.500 (12)
C3—H3	0.9500	I2—F1	1.579 (8)
C4—C5	1.384 (6)	B1—F3	1.331 (14)
C4—H4	0.9500	B1—F4A	1.345 (15)
C5—C6	1.499 (6)	B1—F1A	1.350 (14)
C6—H6A	0.9900	B1—F2	1.398 (13)
C6—H6B	0.9900	B1—F4	1.400 (14)
C7—C8	1.496 (6)	B1—F2A	1.421 (15)
C7—H7A	0.9900	B1—F1	1.431 (13)
C7—H7B	0.9900	B1—F3A	1.463 (14)

Table **S.9.** Bond angles (deg) for C1

	Bond angle (°)		**Bond angle (°)**
C20—Re1—C21	90.0 (2)	C8—C9—H9	120.5
C20—Re1—C19	90.9 (2)	C10—C9—H9	120.5
C21—Re1—C19	88.5 (2)	C11—C10—C9	118.8 (4)
C20—Re1—N1	93.97 (19)	C11—C10—H10	120.6
C21—Re1—N1	90.47 (19)	C9—C10—H10	120.6
C19—Re1—N1	175.02 (18)	C12—C11—C10	119.3 (5)
C20—Re1—N3	95.72 (18)	C12—C11—H11	120.4
C21—Re1—N3	174.05 (16)	C10—C11—H11	120.4

C19—Re1—N3	89.8 (2)	N3—C12—C11	122.4 (4)
N1—Re1—N3	90.75 (14)	N3—C12—H12	118.8
C20—Re1—N2	166.46 (17)	C11—C12—H12	118.8
C21—Re1—N2	100.00 (16)	C18—C13—C14	121.5 (4)
C19—Re1—N2	98.40 (18)	C18—C13—S1	118.6 (4)
N1—Re1—N2	76.99 (13)	C14—C13—S1	119.8 (4)
N3—Re1—N2	74.62 (13)	C15—C14—C13	119.2 (4)
O1—S1—O2	121.3 (2)	C15—C14—H14	120.4
O1—S1—C13	110.9 (2)	C13—C14—H14	120.4
O2—S1—C13	109.0 (2)	C14—C15—C16	119.3 (4)
O1—S1—N2	104.1 (2)	C14—C15—H15	120.3
O2—S1—N2	105.75 (19)	C16—C15—H15	120.3
C13—S1—N2	104.23 (19)	C17—C16—C15	121.4 (4)
C5—N1—C1	118.0 (4)	C17—C16—I1	119.5 (4)
C5—N1—Re1	117.7 (3)	C15—C16—I1	119.1 (4)
C1—N1—Re1	123.6 (3)	C16—C17—C18	119.6 (5)
C6—N2—C7	108.6 (3)	C16—C17—H17	120.2
C6—N2—S1	111.0 (3)	C18—C17—H17	120.2
C7—N2—S1	112.0 (3)	C13—C18—C17	118.9 (4)
C6—N2—Re1	109.9 (2)	C13—C18—H18	120.6
C7—N2—Re1	104.9 (3)	C17—C18—H18	120.6
S1—N2—Re1	110.29 (16)	O3—C19—Re1	179.4 (6)
C12—N3—C8	118.2 (4)	O4—C20—Re1	175.0 (4)
C12—N3—Re1	125.7 (3)	O5—C21—Re1	178.7 (5)
C8—N3—Re1	116.0 (3)	F3—I2—F2	123.0 (6)
N1—C1—C2	122.7 (5)	F2A—I2—F4A	119.8 (13)
N1—C1—H1	118.7	F2A—I2—F3A	110.0 (12)
C2—C1—H1	118.7	F4A—I2—F3A	108.1 (12)
C1—C2—C3	118.8 (5)	F3—I2—F4	112.5 (7)
C1—C2—H2	120.6	F2—I2—F4	109.6 (6)
C3—C2—H2	120.6	F2A—I2—F1A	109.3 (11)
C2—C3—C4	119.3 (5)	F4A—I2—F1A	105.4 (10)
C2—C3—H3	120.3	F3A—I2—F1A	102.9 (7)

C4—C3—H3	120.3	F3—I2—F1	107.1 (6)
C5—C4—C3	118.9 (5)	F2—I2—F1	105.2 (5)
C5—C4—H4	120.6	F4—I2—F1	95.4 (4)
C3—C4—H4	120.6	F4A—B1—F1A	116.0 (13)
N1—C5—C4	122.3 (4)	F3—B1—F2	111.1 (10)
N1—C5—C6	116.7 (4)	F3—B1—F4	112.7 (11)
C4—C5—C6	120.9 (4)	F2—B1—F4	106.9 (10)
C5—C6—N2	113.0 (3)	F4A—B1—F2A	112.7 (14)
C5—C6—H6A	109.0	F1A—B1—F2A	110.7 (13)
N2—C6—H6A	109.0	F3—B1—F1	112.8 (11)
C5—C6—H6B	109.0	F2—B1—F1	107.8 (9)
N2—C6—H6B	109.0	F4—B1—F1	105.3 (9)
H6A—C6—H6B	107.8	F4A—B1—F3A	107.0 (13)
C8—C7—N2	108.8 (4)	F1A—B1—F3A	108.5 (11)
C8—C7—H7A	109.9	F2A—B1—F3A	100.7 (11)
N2—C7—H7A	109.9	B1—F1—I2	3.7 (7)
C8—C7—H7B	109.9	I2—F2—B1	5.9 (7)
N2—C7—H7B	109.9	I2—F3—B1	7.3 (7)
H7A—C7—H7B	108.3	B1—F4—I2	6.7 (6)
N3—C8—C9	122.1 (4)	B1—F1A—I2	3.7 (7)
N3—C8—C7	115.5 (4)	I2—F2A—B1	5.1 (7)
C9—C8—C7	122.4 (4)	I2—F3A—B1	6.8 (6)
C8—C9—C10	119.1 (5)	B1—F4A—I2	7.4 (6)
O1—S1—N2—C6	45.6 (3)	I1—C16—C17—C18	-179.6 (3)
O2—S1—N2—C6	174.5 (3)	C14—C13—C18—C17	-2.8 (7)
C13—S1—N2—C6	-70.7 (3)	S1—C13—C18—C17	177.0 (4)
O1—S1—N2—C7	167.1 (3)	C16—C17—C18—C13	1.3 (7)
O2—S1—N2—C7	-64.0 (3)	F3—B1—F1—I2	-82 (10)
C13—S1—N2—C7	50.8 (3)	F2—B1—F1—I2	41 (10)
O1—S1—N2—Re1	-76.5 (2)	F4—B1—F1—I2	155 (11)
O2—S1—N2—Re1	52.4 (2)	F3—I2—F1—B1	92 (10)
C13—S1—N2—Re1	167.2 (2)	F2—I2—F1—B1	-135 (10)

C5—N1—C1—C2	1.3 (7)	F4—I2—F1—B1	-23 (10)
Re1—N1—C1—C2	171.9 (4)	F3—I2—F2—B1	149 (7)
N1—C1—C2—C3	-2.0 (7)	F4—I2—F2—B1	-75 (7)
C1—C2—C3—C4	0.6 (8)	F1—I2—F2—B1	26 (7)
C2—C3—C4—C5	1.3 (7)	F3—B1—F2—I2	-26 (6)
C1—N1—C5—C4	0.8 (6)	F4—B1—F2—I2	97 (7)
Re1—N1—C5—C4	-170.5 (3)	F1—B1—F2—I2	-150 (8)
C1—N1—C5—C6	-174.4 (4)	F2—I2—F3—B1	-154 (6)
Re1—N1—C5—C6	14.4 (5)	F4—I2—F3—B1	71 (6)
C3—C4—C5—N1	-2.0 (7)	F1—I2—F3—B1	-32 (6)
C3—C4—C5—C6	172.9 (4)	F2—B1—F3—I2	21 (5)
N1—C5—C6—N2	-26.4 (5)	F4—B1—F3—I2	-99 (6)
C4—C5—C6—N2	158.4 (4)	F1—B1—F3—I2	142 (7)
C7—N2—C6—C5	138.6 (4)	F3—B1—F4—I2	71 (6)
S1—N2—C6—C5	-97.9 (4)	F2—B1—F4—I2	-51 (5)
Re1—N2—C6—C5	24.4 (4)	F1—B1—F4—I2	-165 (6)
C6—N2—C7—C8	-70.0 (4)	F3—I2—F4—B1	-98 (6)
S1—N2—C7—C8	167.1 (3)	F2—I2—F4—B1	121 (6)
Re1—N2—C7—C8	47.5 (4)	F1—I2—F4—B1	13 (6)
C12—N3—C8—C9	3.5 (7)	F4A—B1—F1A—I2	155 (12)
Re1—N3—C8—C9	-179.9 (4)	F2A—B1—F1A—I2	25 (10)
C12—N3—C8—C7	-174.4 (4)	F3A—B1—F1A—I2	-85 (11)
Re1—N3—C8—C7	2.2 (5)	F2A—I2—F1A—B1	-153 (11)
N2—C7—C8—N3	-34.8 (6)	F4A—I2—F1A—B1	-23 (11)
N2—C7—C8—C9	147.3 (4)	F3A—I2—F1A—B1	90 (11)
N3—C8—C9—C10	-1.9 (8)	F4A—I2—F2A—B1	-103 (8)
C7—C8—C9—C10	175.9 (5)	F3A—I2—F2A—B1	131 (8)
C8—C9—C10—C11	-1.6 (8)	F1A—I2—F2A—B1	19 (8)
C9—C10—C11—C12	3.4 (8)	F4A—B1—F2A—I2	69 (8)
C8—N3—C12—C11	-1.6 (7)	F1A—B1—F2A—I2	-159 (9)
Re1—N3—C12—C11	-177.9 (4)	F3A—B1—F2A—I2	-44 (8)
C10—C11—C12—N3	-1.8 (7)	F2A—I2—F3A—B1	-147 (6)
O1—S1—C13—C18	162.7 (4)	F4A—I2—F3A—B1	81 (6)

O2—S1—C13—C18	26.7 (4)	F1A—I2—F3A—B1	-30 (5)
N2—S1—C13—C18	-85.9 (4)	F4A—B1—F3A—I2	-90 (6)
O1—S1—C13—C14	-17.6 (4)	F1A—B1—F3A—I2	145 (6)
O2—S1—C13—C14	-153.6 (4)	F2A—B1—F3A—I2	28 (5)
N2—S1—C13—C14	93.9 (4)	F1A—B1—F4A—I2	-166 (6)
C18—C13—C14—C15	1.5 (7)	F2A—B1—F4A—I2	-37 (5)
S1—C13—C14—C15	-178.2 (4)	F3A—B1—F4A—I2	72 (5)
C13—C14—C15—C16	1.2 (7)	F2A—I2—F4A—B1	135 (6)
C14—C15—C16—C17	-2.7 (7)	F3A—I2—F4A—B1	-98 (6)
C14—C15—C16—I1	178.4 (3)	F1A—I2—F4A—B1	11 (5)
C15—C16—C17—C18	1.4 (7)		

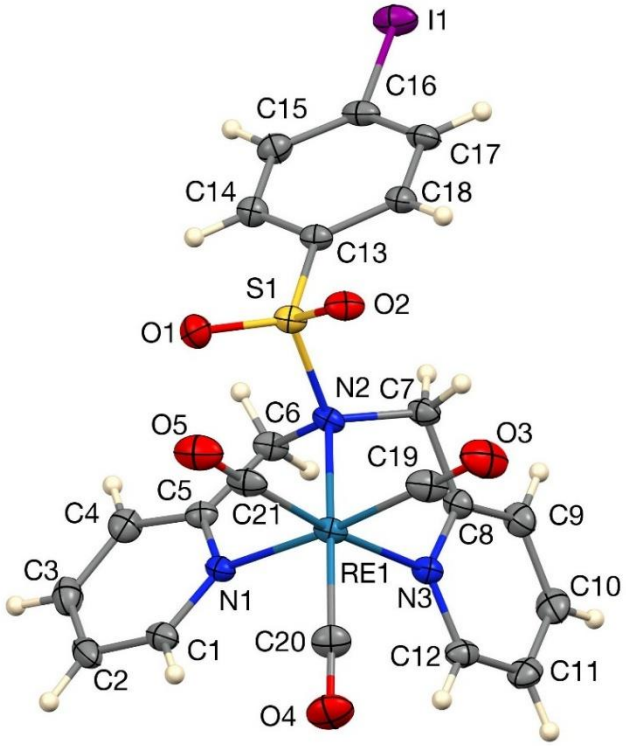

Fig. S.20. ORTEP plot of the **C1**. Thermal ellipsoids are drawn with 50% probability.

Fluorescence spectroscopic data

Table S.10 Fluoresence data of **L1** and **L2** in methanol

Compound	Excited wavelength/ nm	Emission wavelength/ nm

L1	300	403
L2	308	392

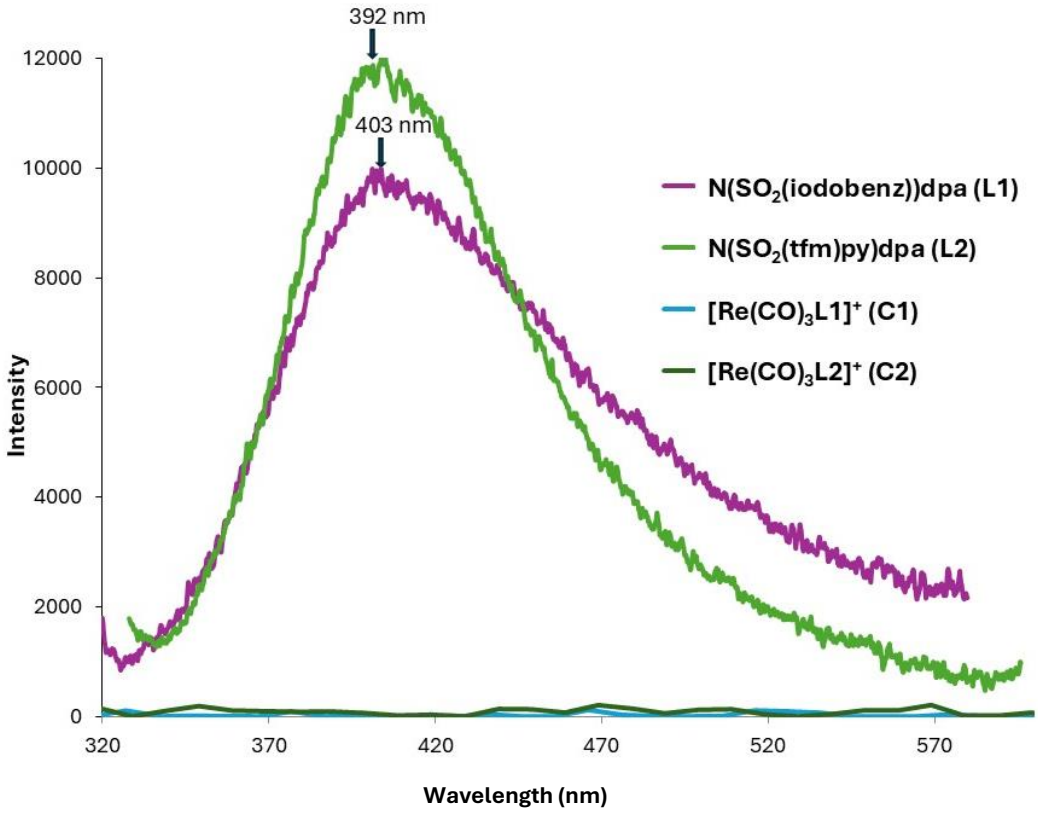

Fig. S.21. Fluorescence spectra of ligands and complexes in methanol at room temperature