Supplementary information

Photophysical characteristic of imaging agents.

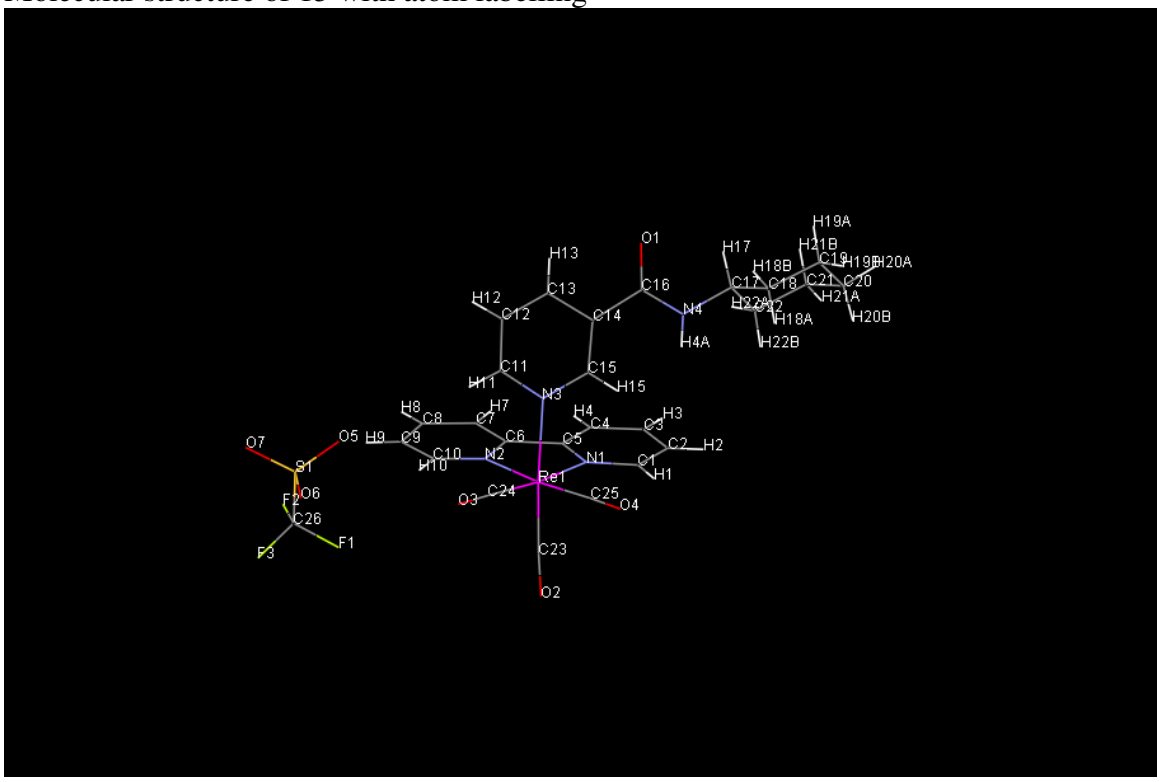
Complex	λ max_{abs}(nm) (assignment)	λ max_{em}(assignment) (nm)
2	318 (IL) 365 (^{1}MLCT)	556 (^{3}MLCT)
8	318 (IL) 360 (^{1}MLCT)	554 (^{3}MLCT)
9	316 (IL) 355 (^{1}MLCT)	554 (^{3}MLCT)
10	319 (IL) 358 (^{1}MLCT)	552 (^{3}MLCT)
14	313 (IL) 389 (^{1}MLCT)	553 (^{3}MLCT)
15	313 (IL) 376 (^{1}MLCT)	539 (^{3}MLCT)
22	285 (IL) 375(^{1}MLCT)	566 (^{3}MLCT)
23	282 (IL) 378(^{1}MLCT)	563 (^{3}MLCT)
28	336 (IL) 393 (^{1}MLCT)	558 (^{3}MLCT)
29	314 (IL) 358 (^{1}MLCT)	551 (^{3}MLCT)

X ray crystallography.

Crystal data for **15**:

$C_{26}H_{24}F_3N_4O_7ReS$, M = 779.75, 0.20 × 0.20 × 0.20 mm^3, monoclinic, space group $P2_1/c$ (No. 14), a = 12.1380(3), b = 12.1560(3), c = 19.4130(5) Å, β = 105.8630(10)°, V = 2755.30(12) Å^3, Z = 4, D_c = 1.880 g/cm^3, F_{000} = 1528, MoKα radiation, λ = 0.71073 Å, T = 293(2)K, $2\theta_{max}$ = 61.0º, 11446 reflections collected, 7278 unique (R_{int} = 0.0300). Final *GooF* = 1.071, *R1* = 0.0373, *wR2* = 0.0698, *R* indices based on 6007 reflections with I >2sigma(I) (refinement on F^2), 379 parameters, 0 restraints. Lp and absorption corrections applied, μ = 4.559 mm^{-1}.

Molecular structure of 15 with atom labelling

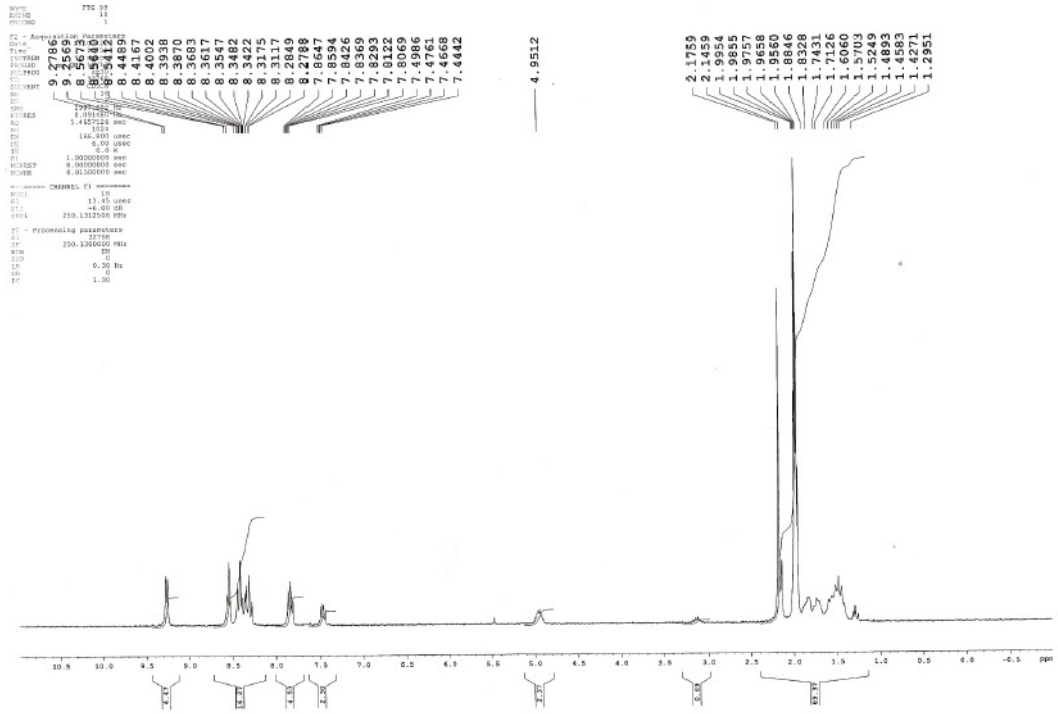


Selected bond lengths and angles for **15**

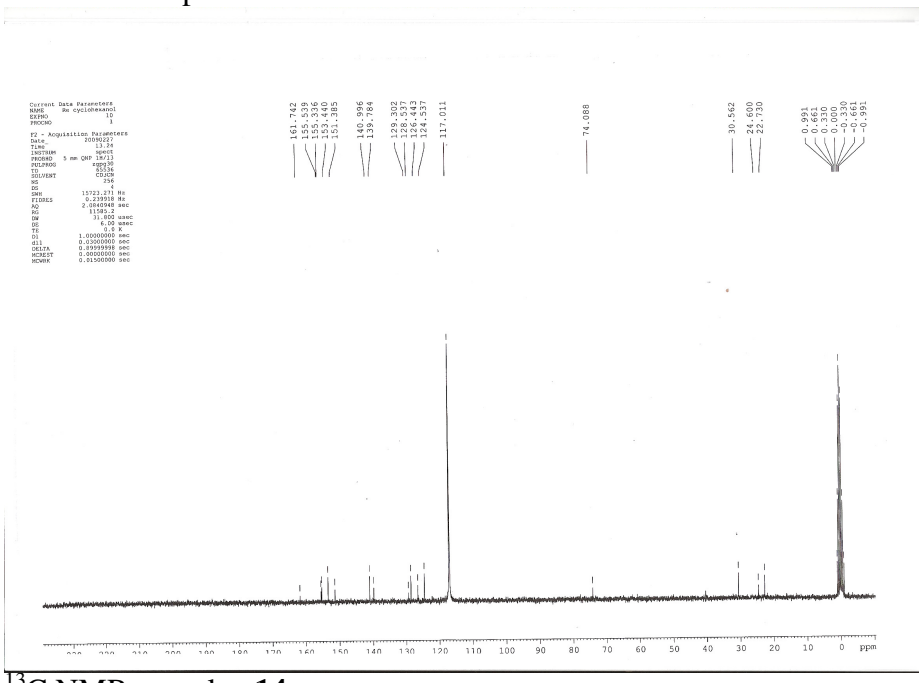
Bond	Bond length (Å)	Bond angle (°)
Re1-C23	1.915(4)	
Re1-C24	1.930(4)	

Re1-C25	1.928(4)	
Re1-N1	2.161(3)	
Re1-N2	2.172(3)	
Re1-N3	2.220(3)	
N1-Re1-N2		74.83(12)
N1-Re1-N3		83.21(12)
N2-Re1-N3		84.21(12)
C23-Re1-N2		96.04(14)
C23-Re1-C24		89.79(16)
C25-Re1-N3		92.55(14)

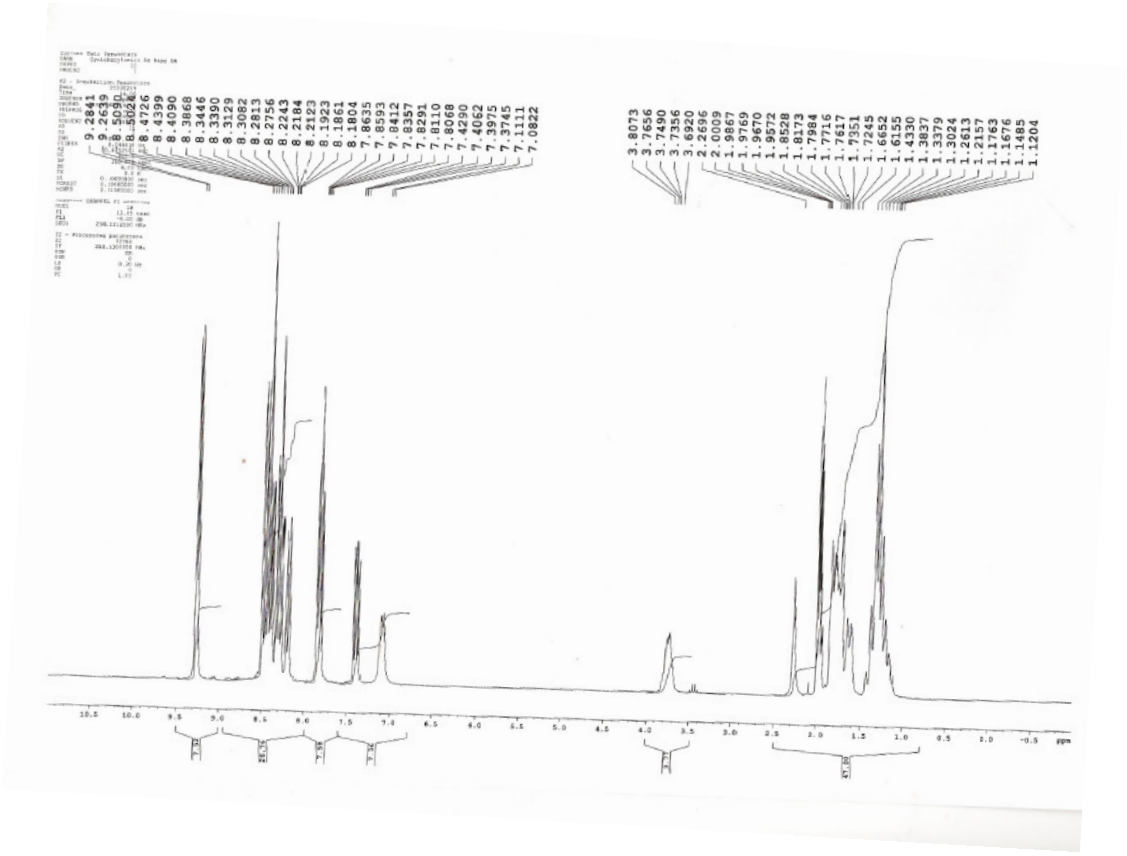
NMR spectra of complexes **14**, **15.**



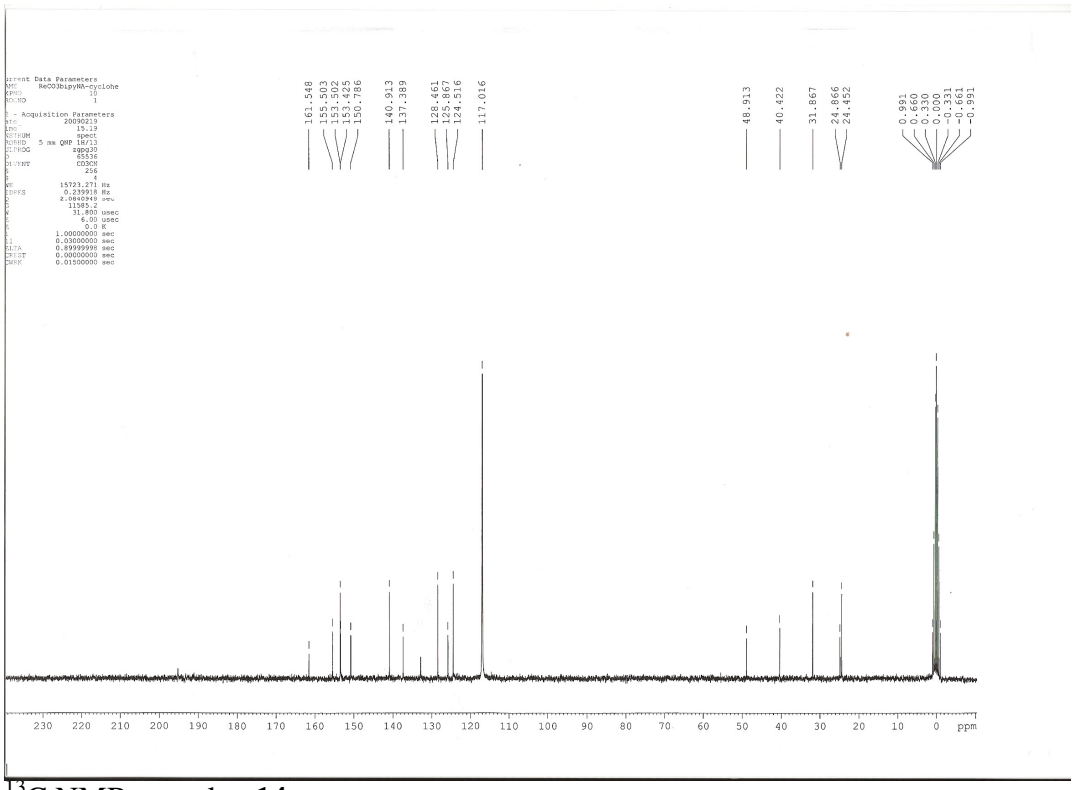
^{1}H NMR complex **14**



^{13}C NMR complex **14**



^{1}H NMR complex **15**



^{13}C NMR complex **14**