Supplementary Information

Phosphorescent Rhenium-Dipyrrinates: Efficient Photosensitizers for Singlet Oxygen Generation

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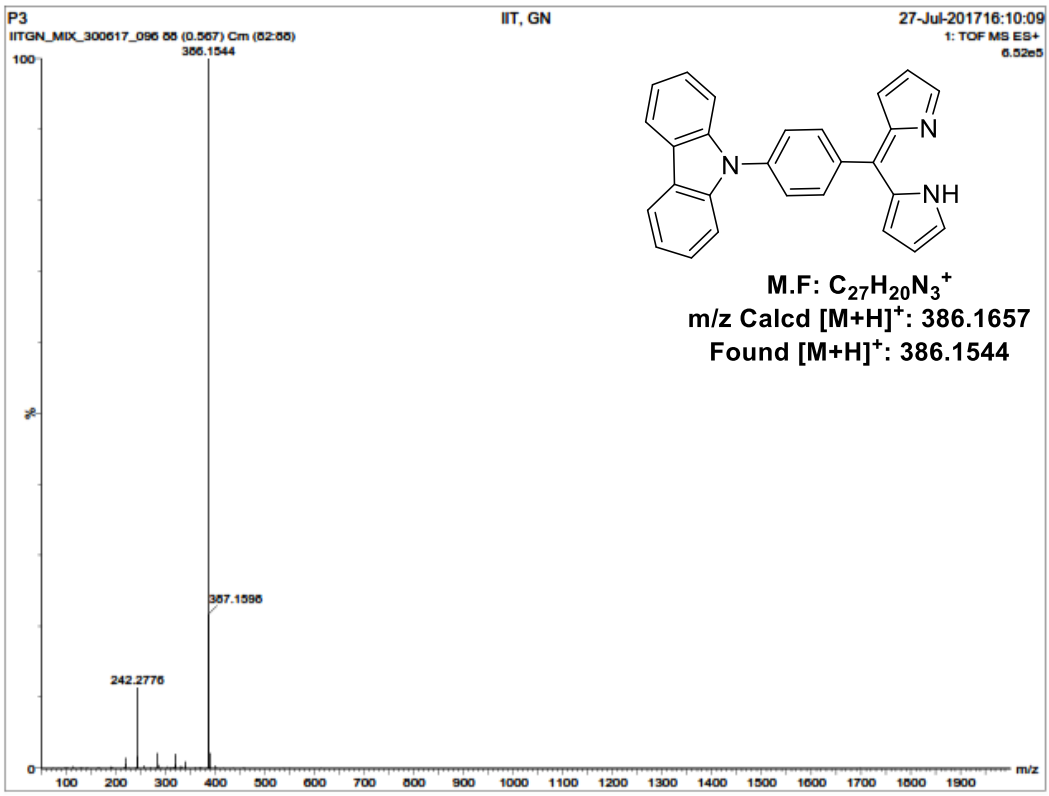


Figure 1. ESI-MS of compound **1**

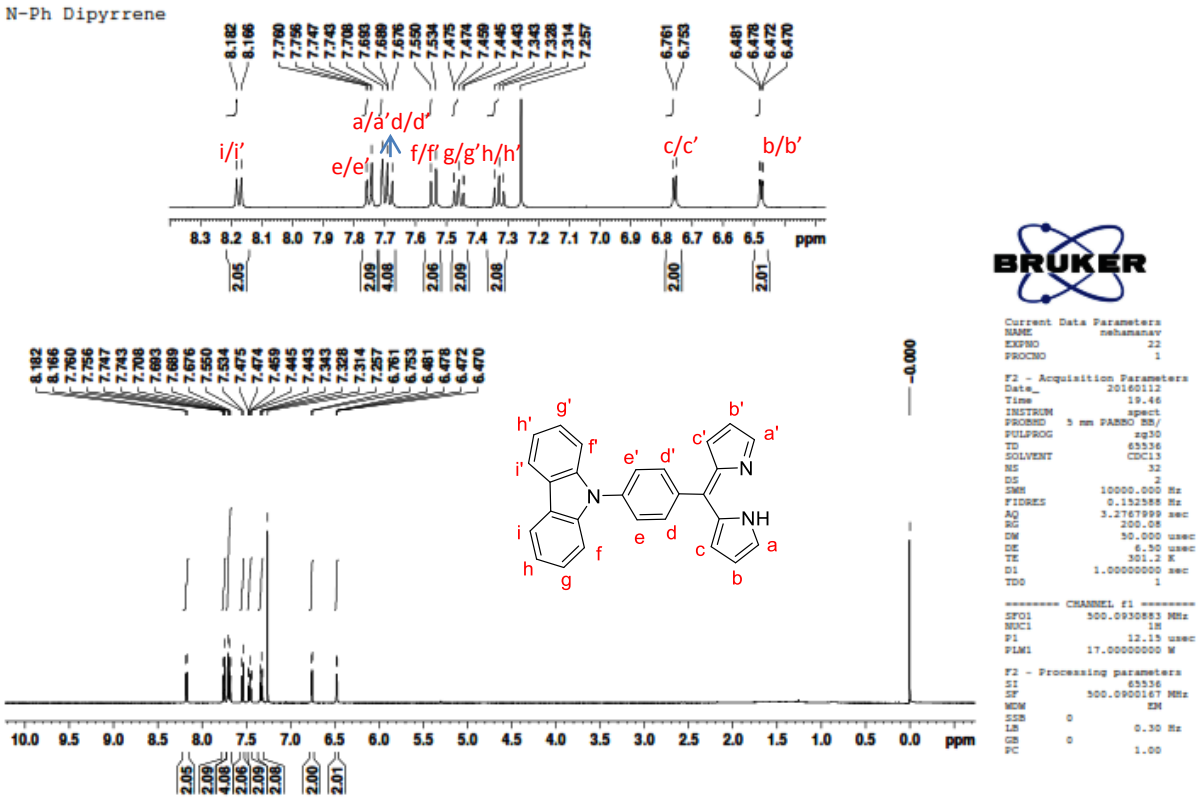


Figure 2. ^{1}H-NMR of compound **1** in $CDCl_3$

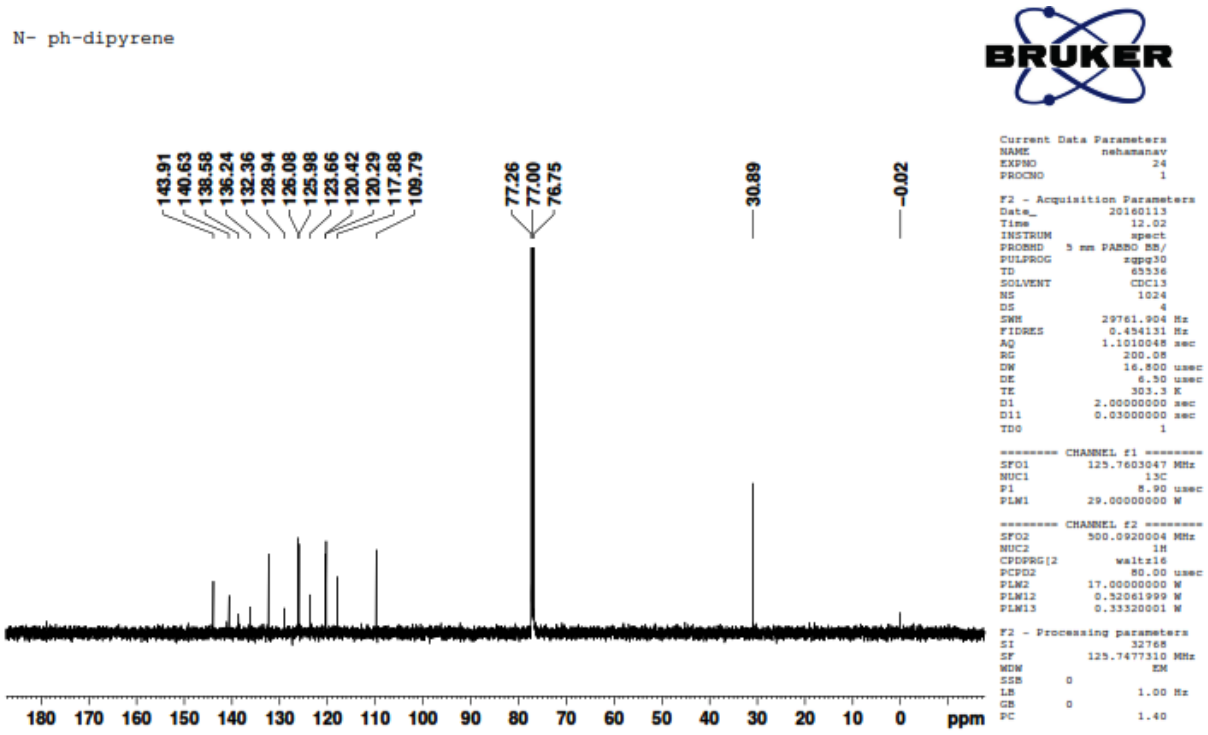


Figure 3. ^{13}C-NMR of compound **1** in $CDCl_3$

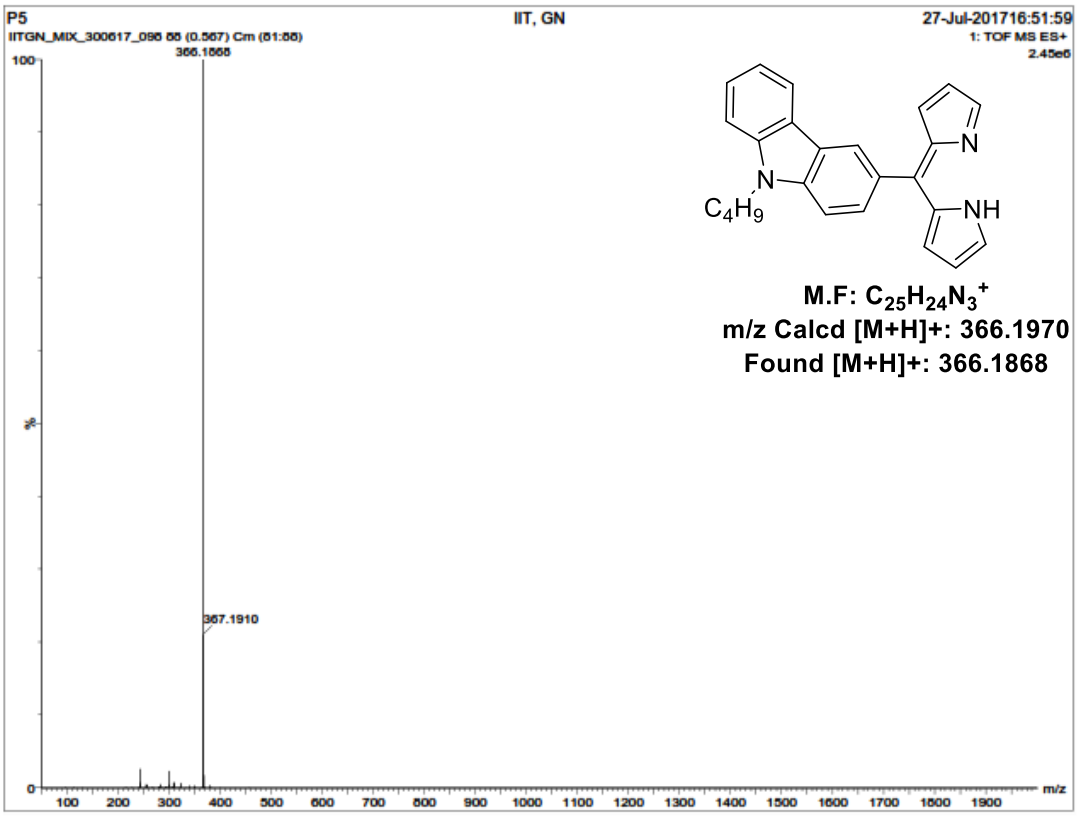


Figure 4. ESI-MS of compound **2**

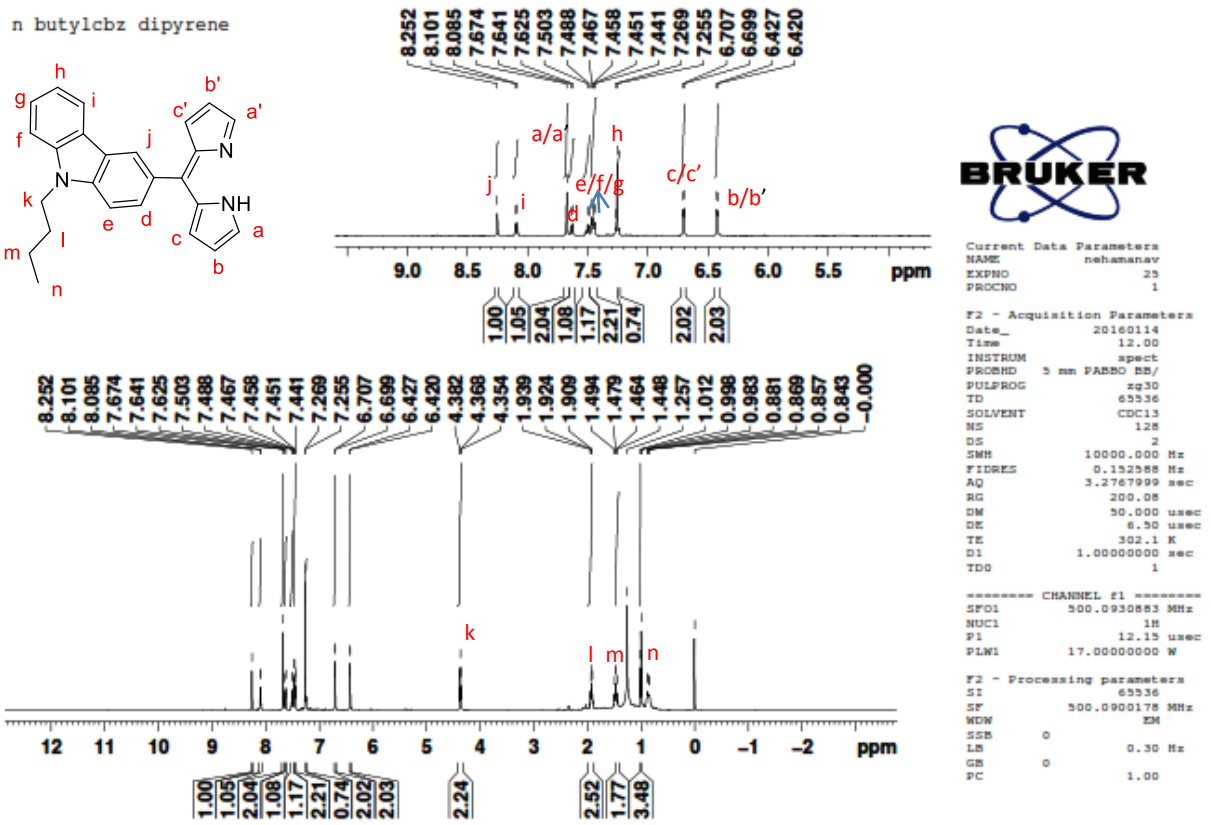


Figure 5. ^{1}H-NMR of compound **2** in $CDCl_3$

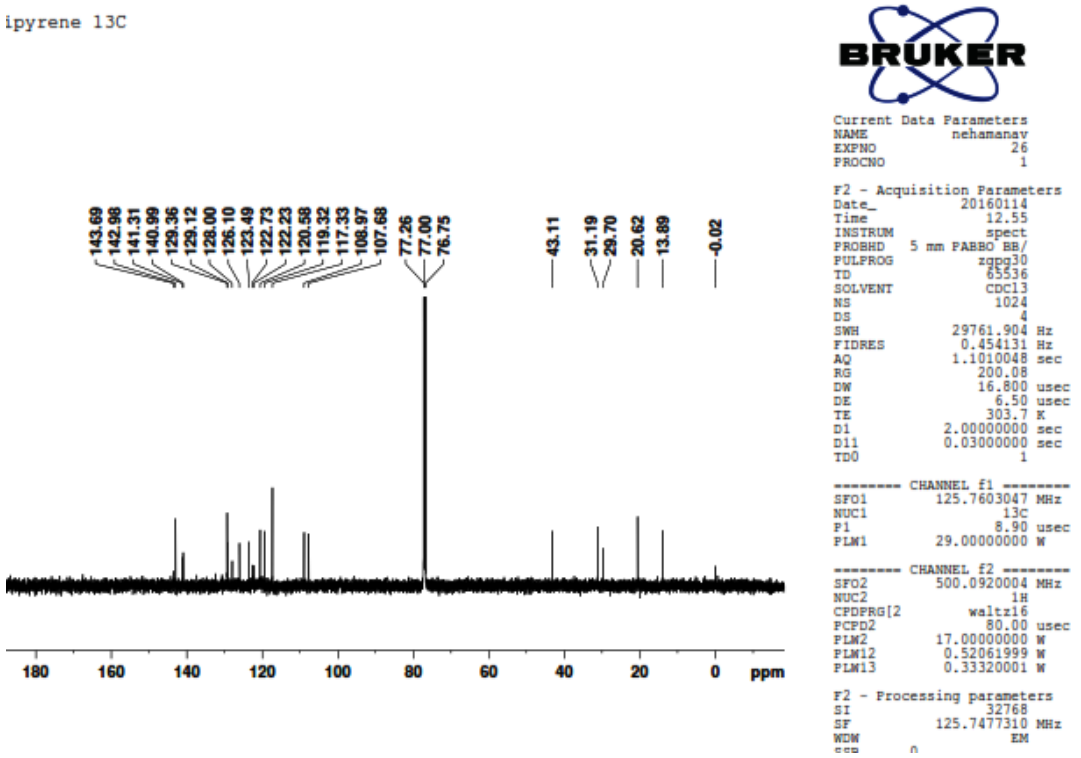


Figure 6. ^{13}C-NMR of compound **2** in $CDCl_3$

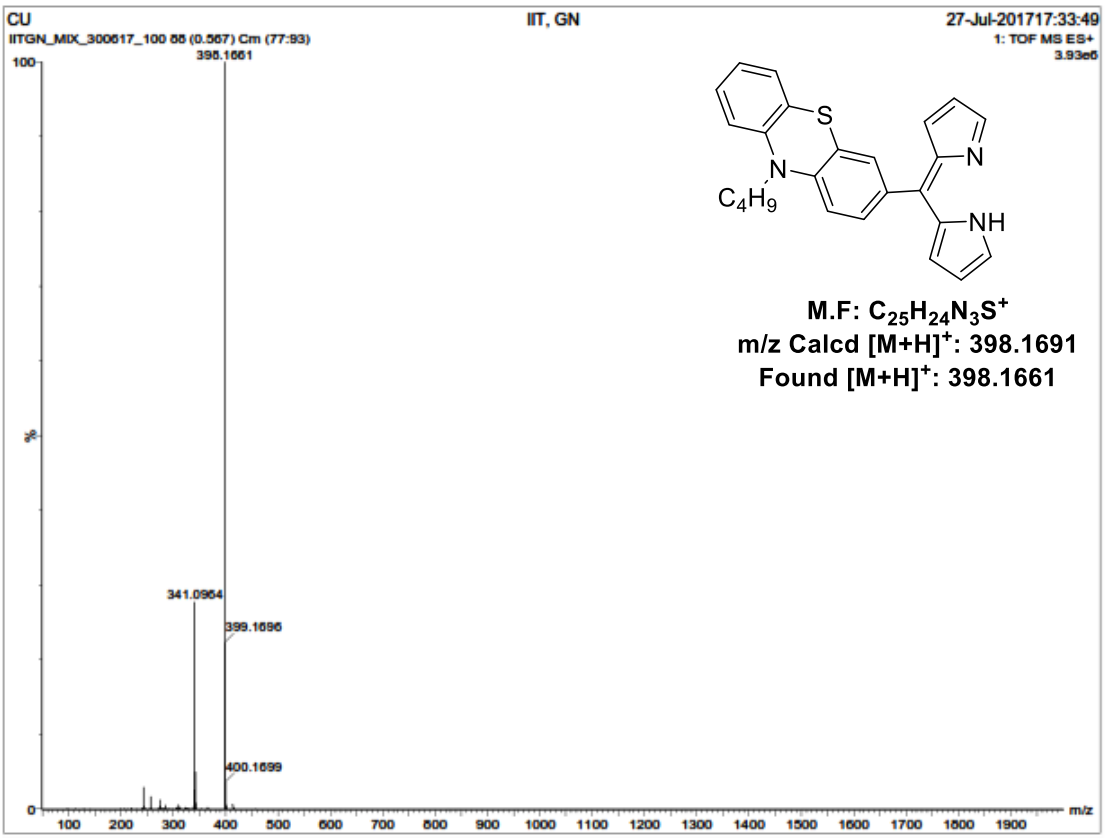


Figure 7. ESI-MS of compound **3**

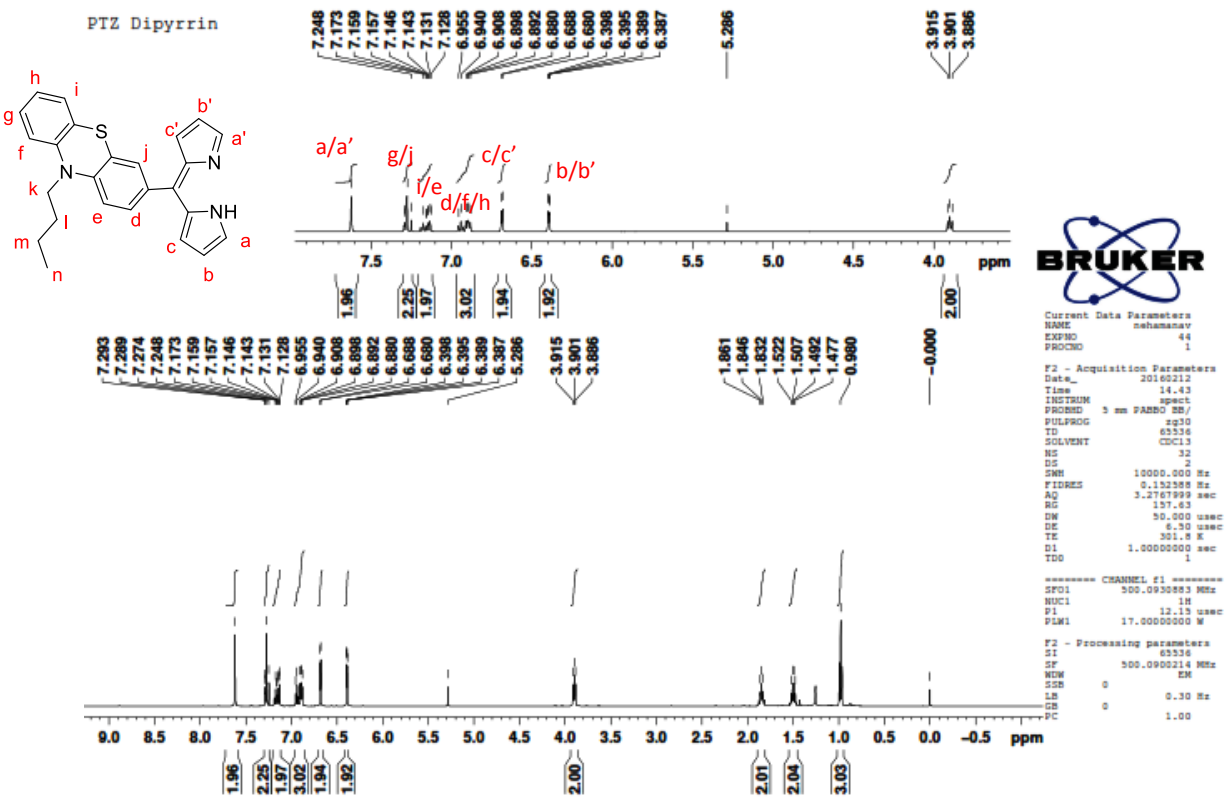


Figure 8. ^{1}H-NMR of compound **3** in $CDCl_3$

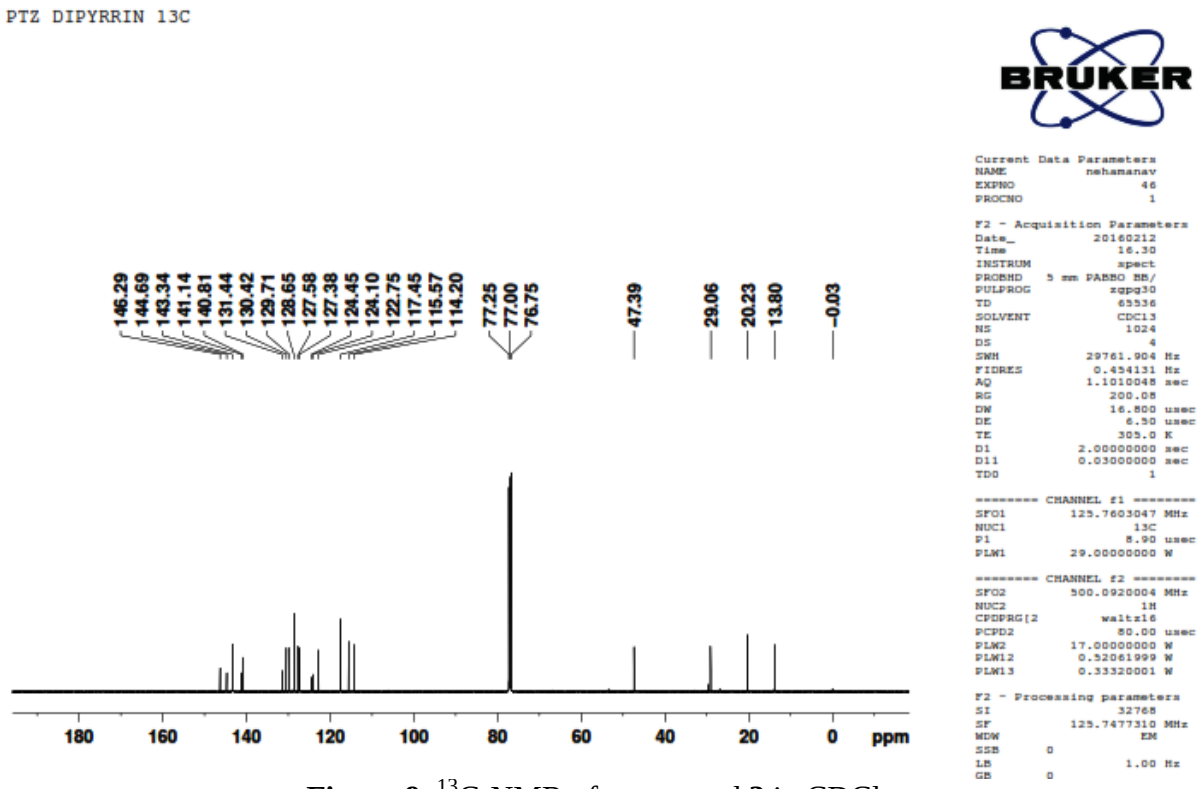


Figure 9. ^{13}C-NMR of compound **3** in $CDCl_3$

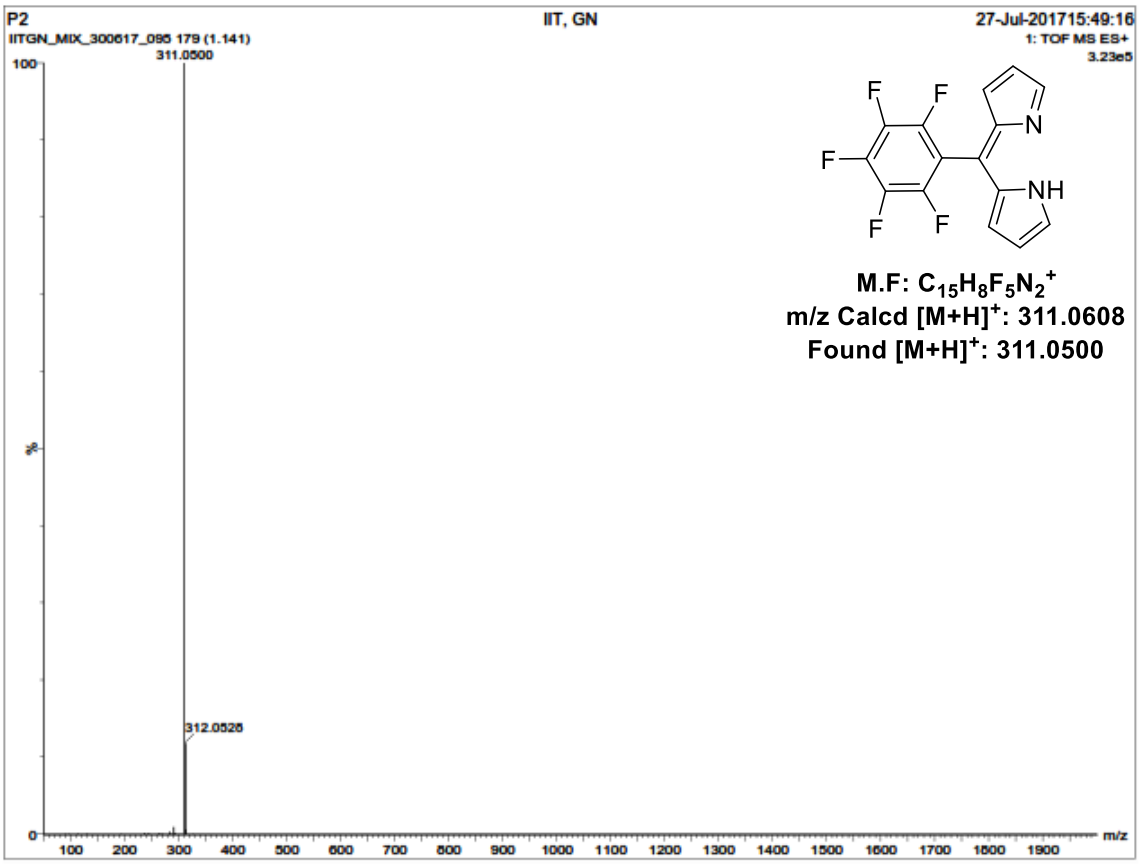


Figure 10. ESI-MS of compound **4**

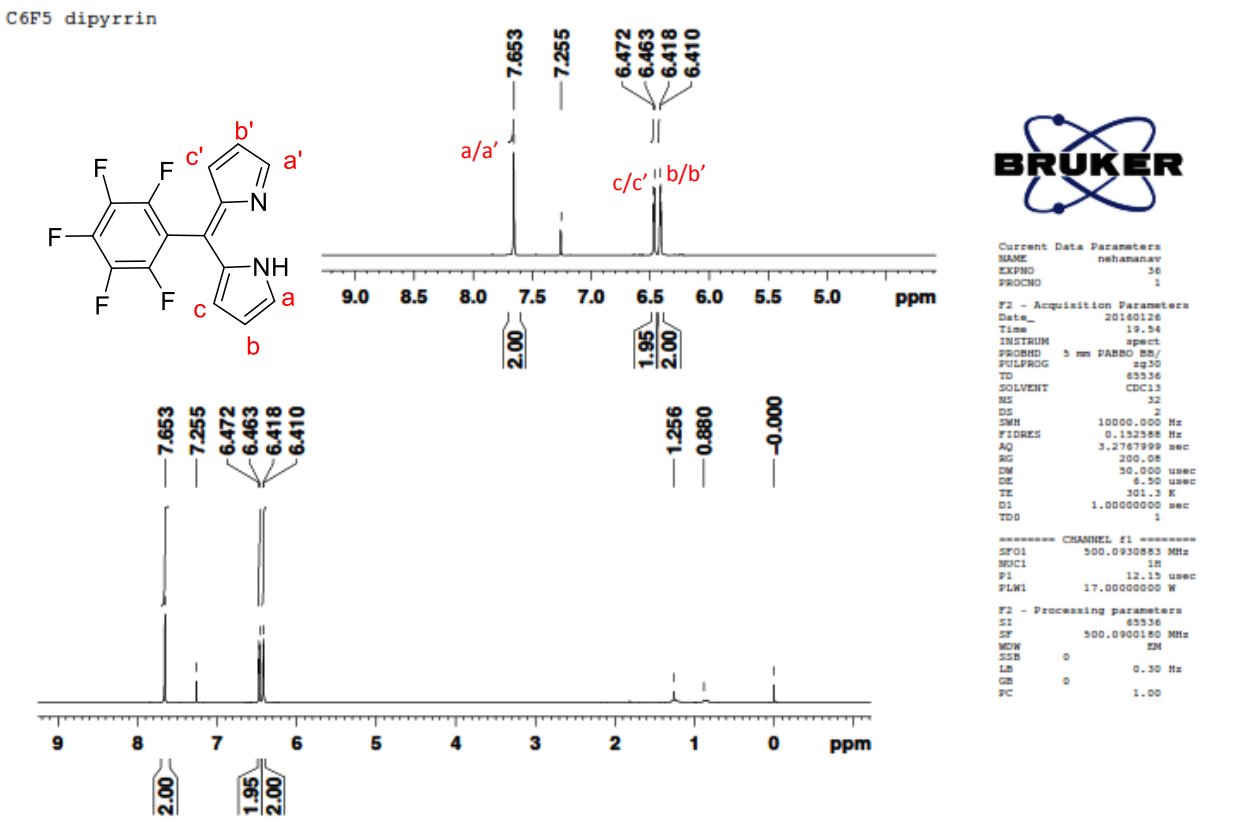


Figure 11. ^{1}H-NMR of compound **4** in $CDCl_3$

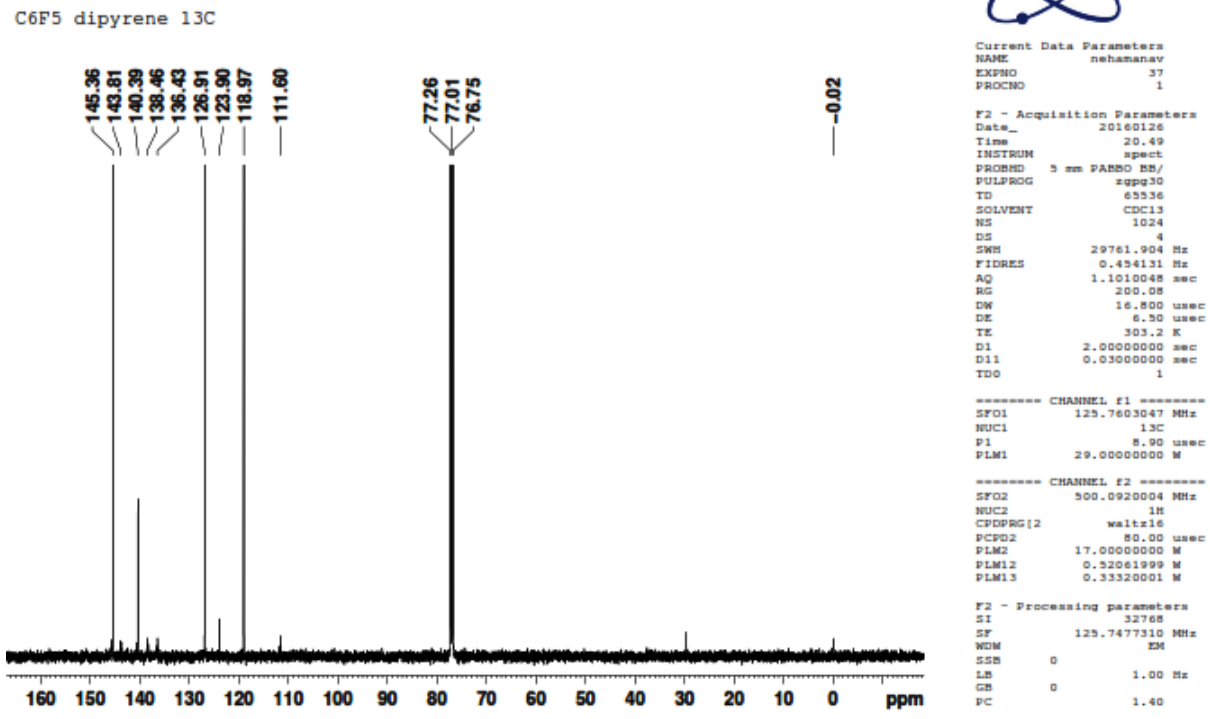


Figure 12. ^{13}C-NMR of compound **4** in $CDCl_3$

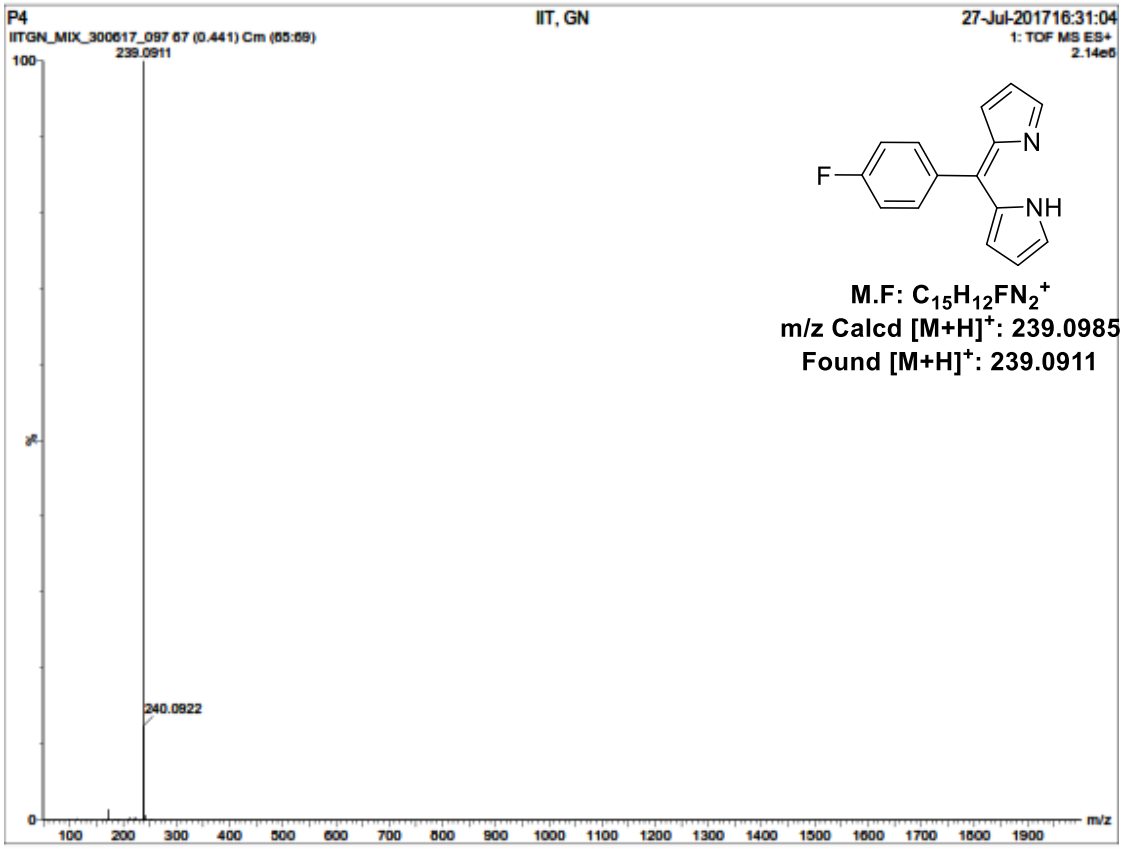


Figure 13. ESI-MS of compound **5**

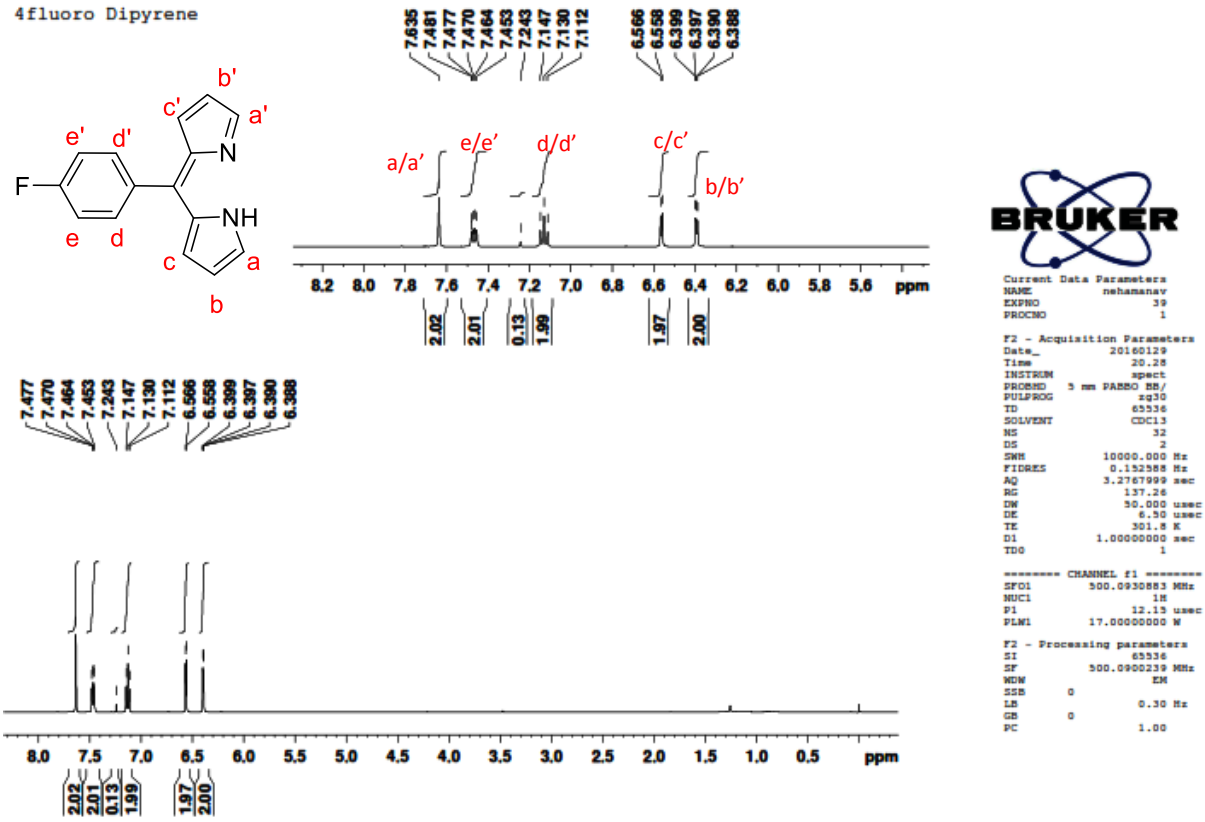


Figure 14. ^{1}H-NMR of compound **5** in $CDCl_3$

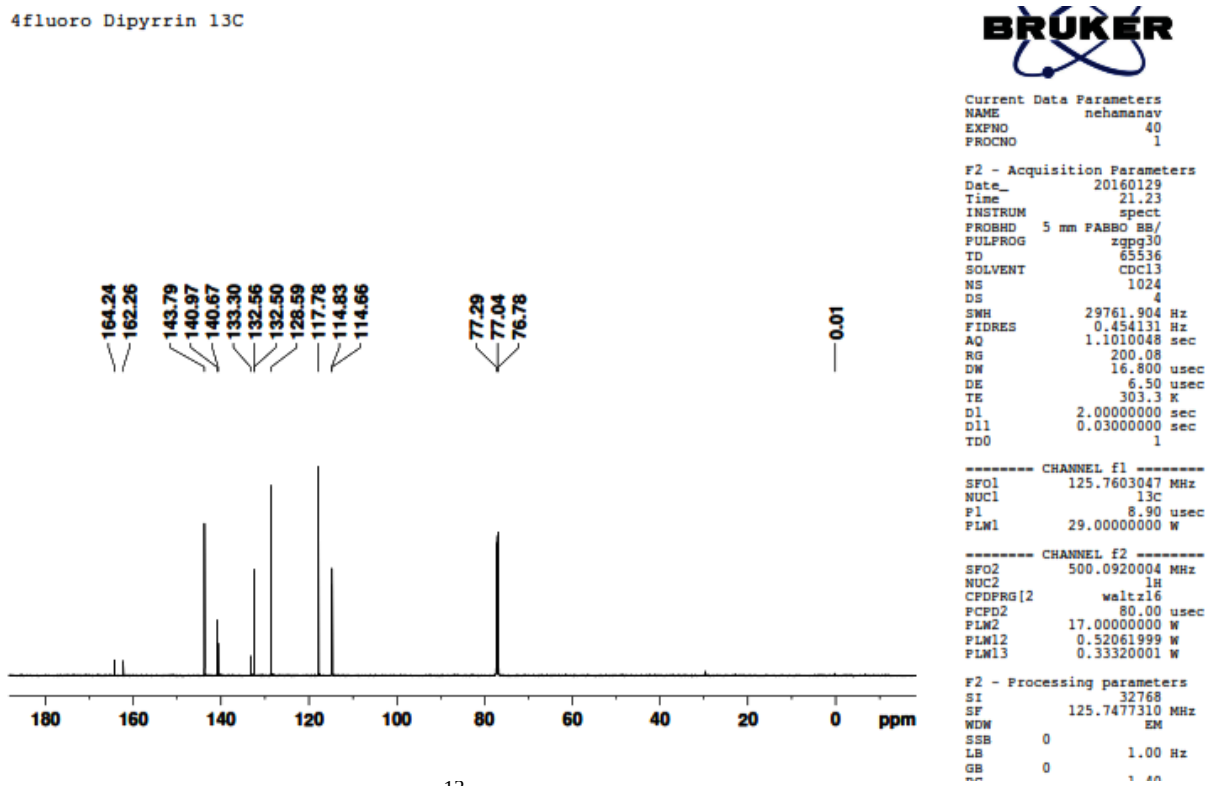


Figure 15. ^{13}C-NMR of compound **5** in $CDCl_3$

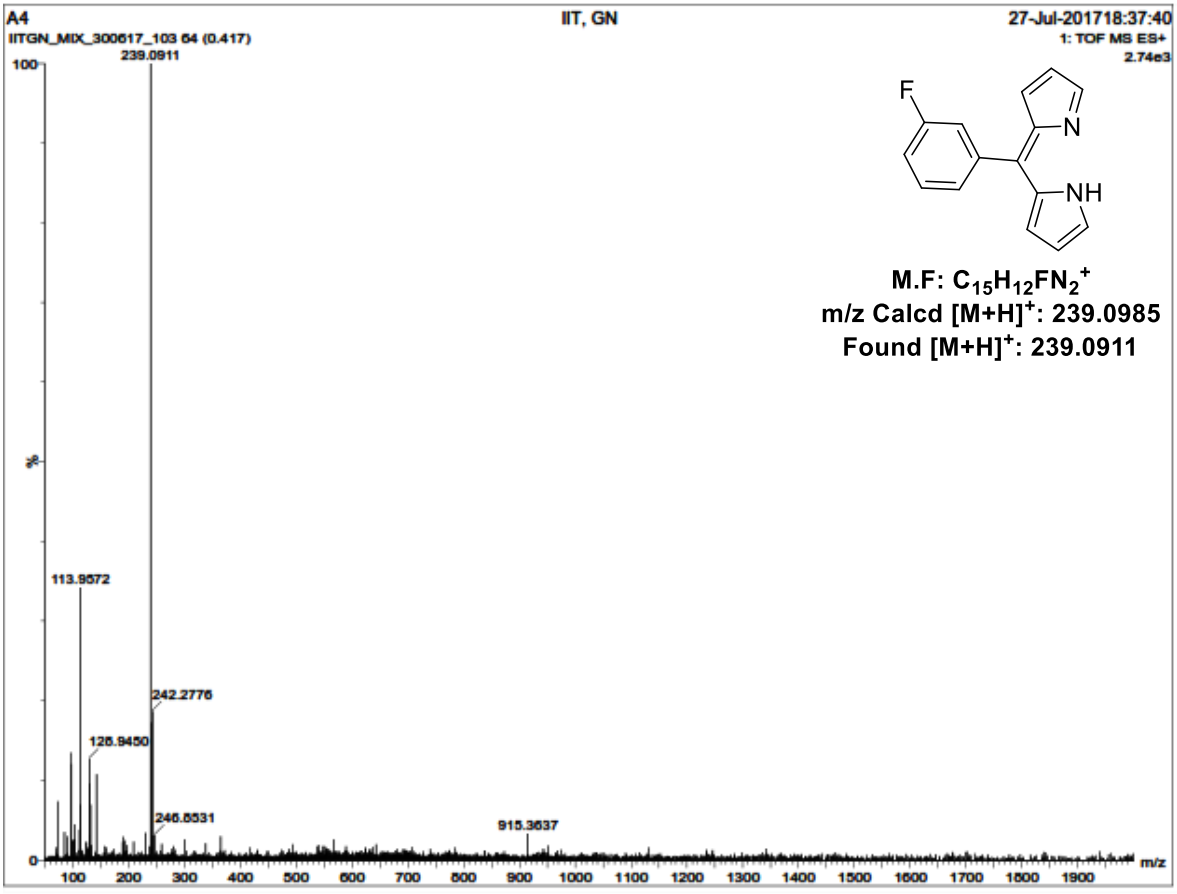


Figure 16. ESI-MS of compound **6**

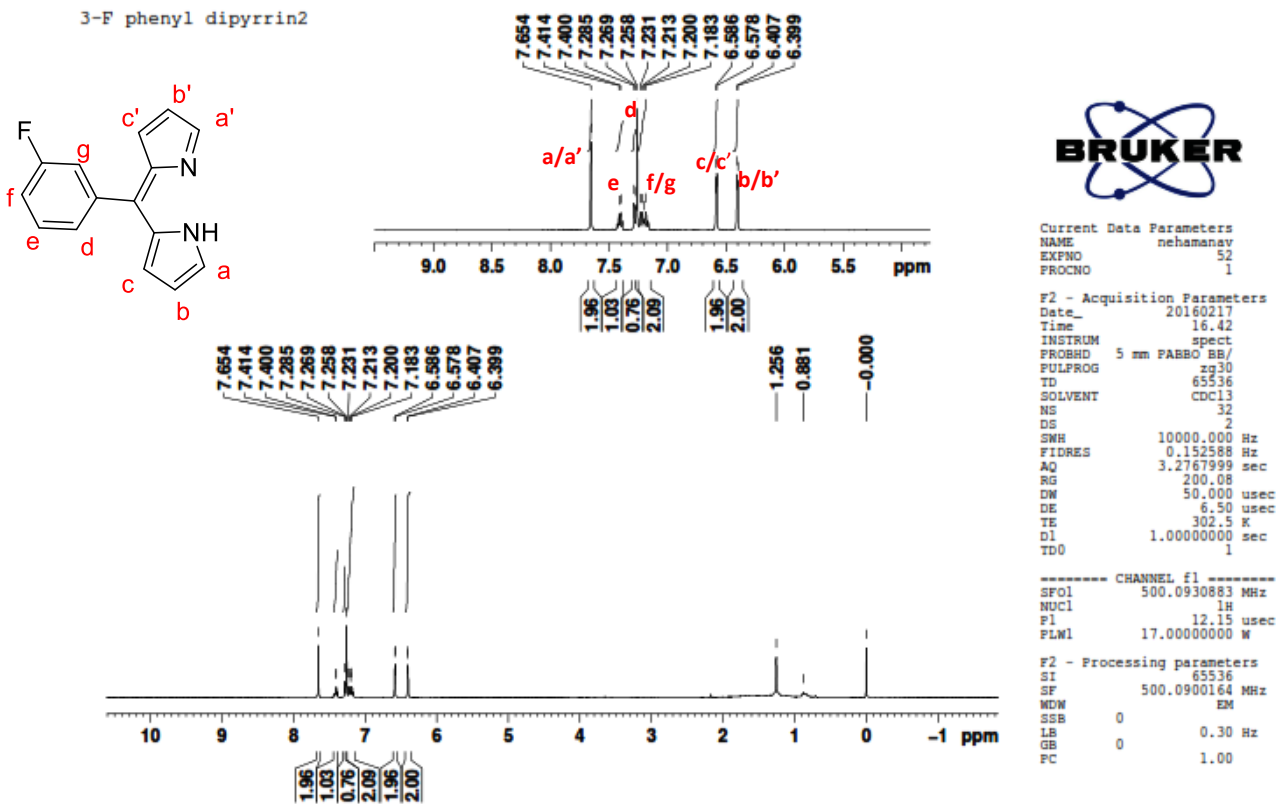


Figure 17. ^{1}H-NMR of compound **6** in $CDCl_3$

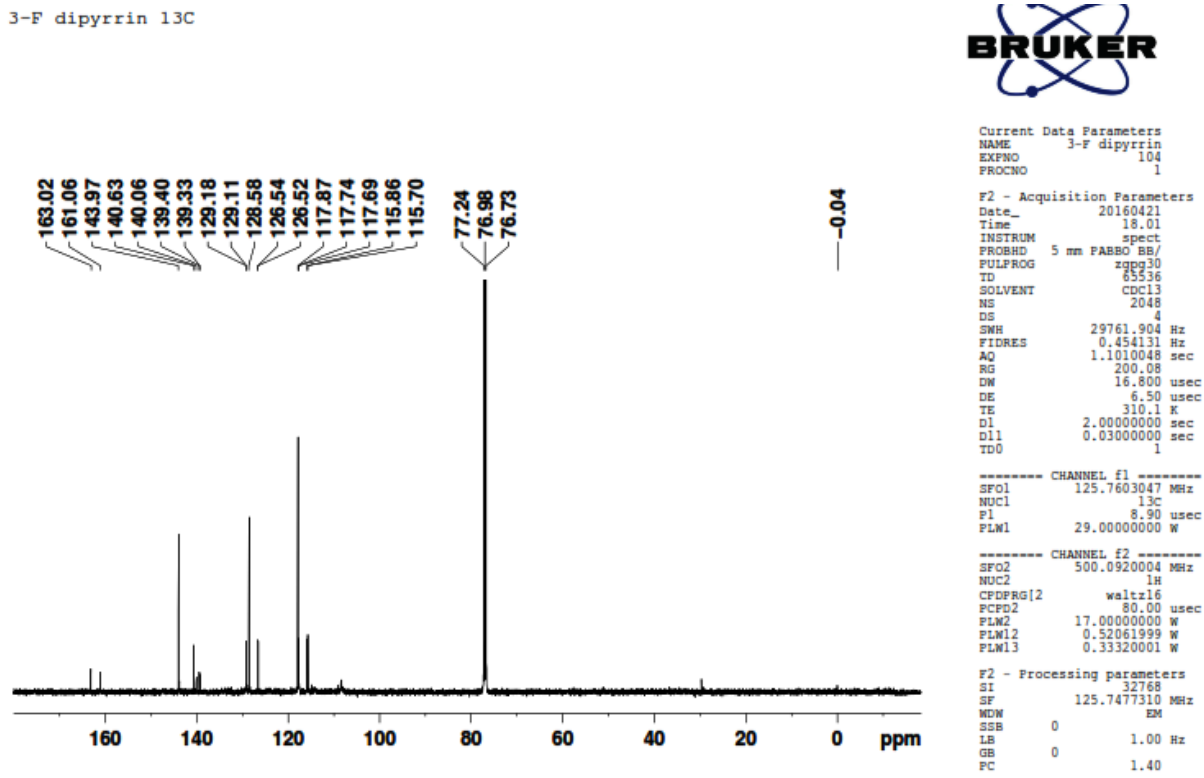


Figure 18. ^{13}C-NMR of compound **6** in $CDCl_3$

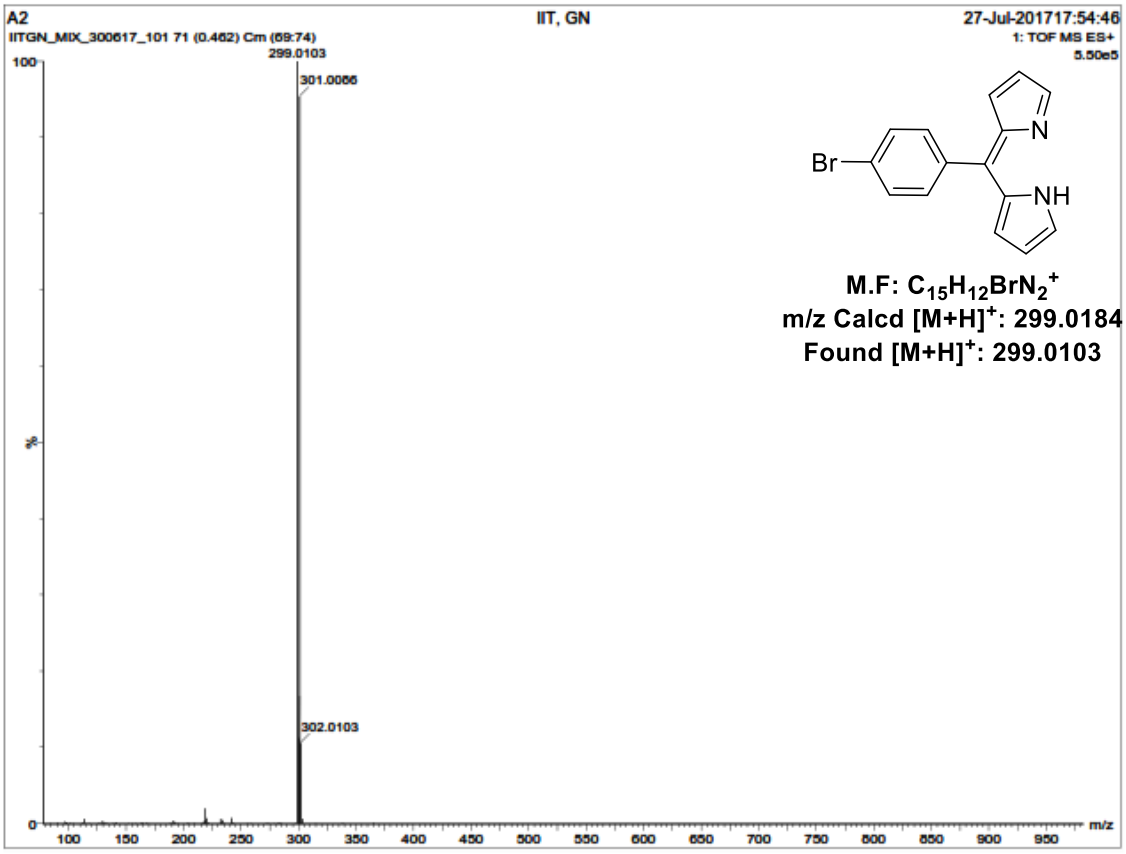


Figure 19. ESI-MS of compound **7**

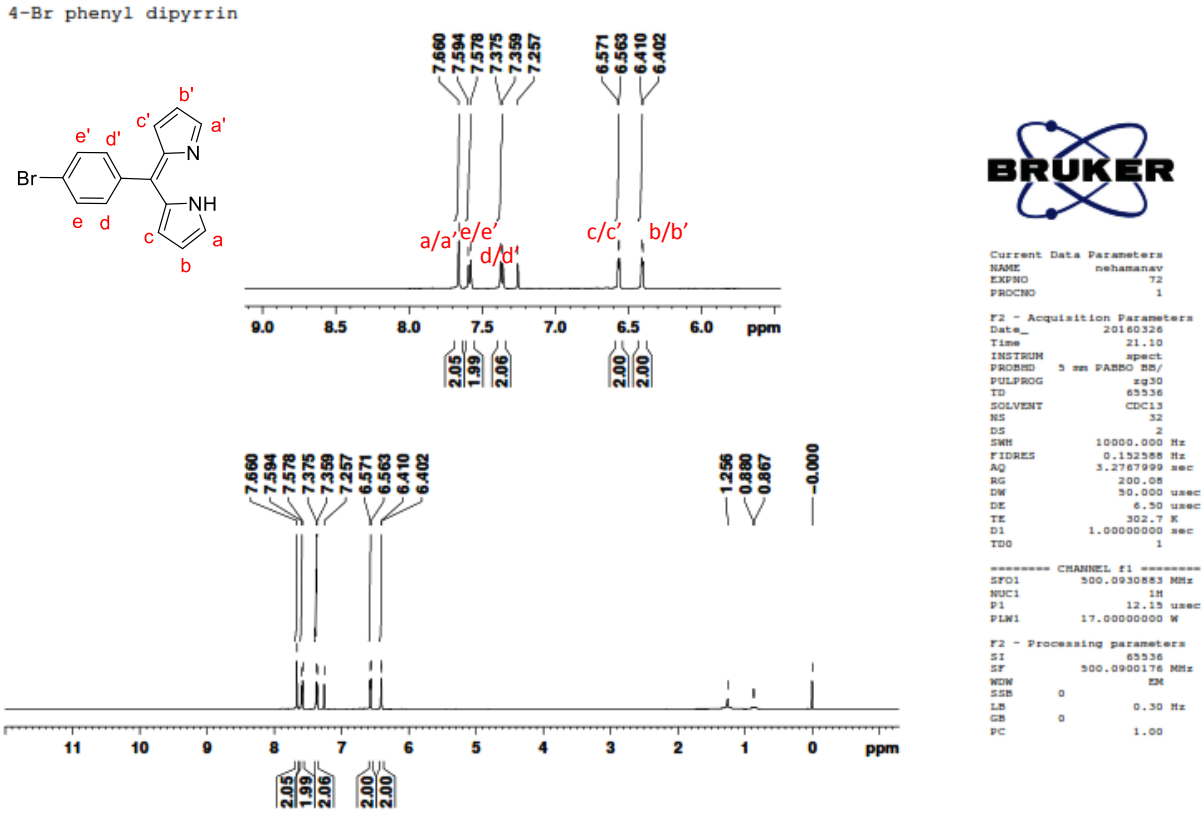


Figure 20. ^{1}H-NMR of compound **7** in $CDCl_3$

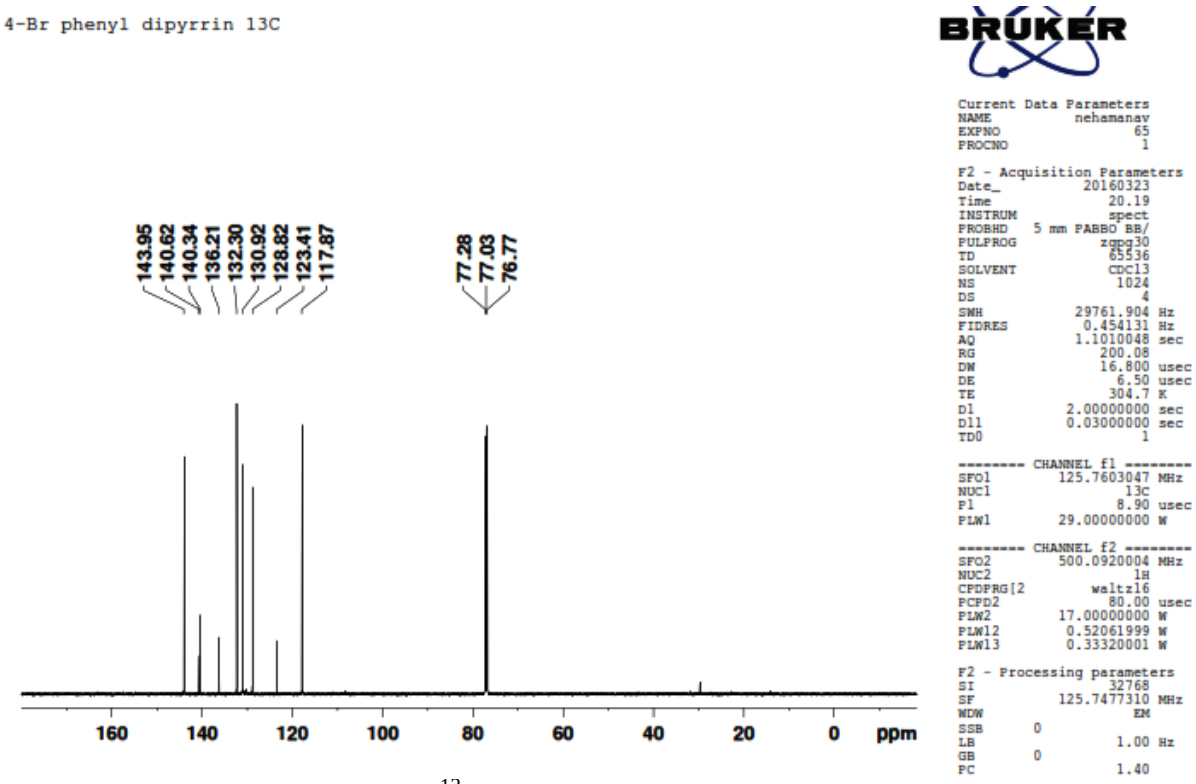


Figure 21. ^{13}C-NMR of compound **7** in $CDCl_3$

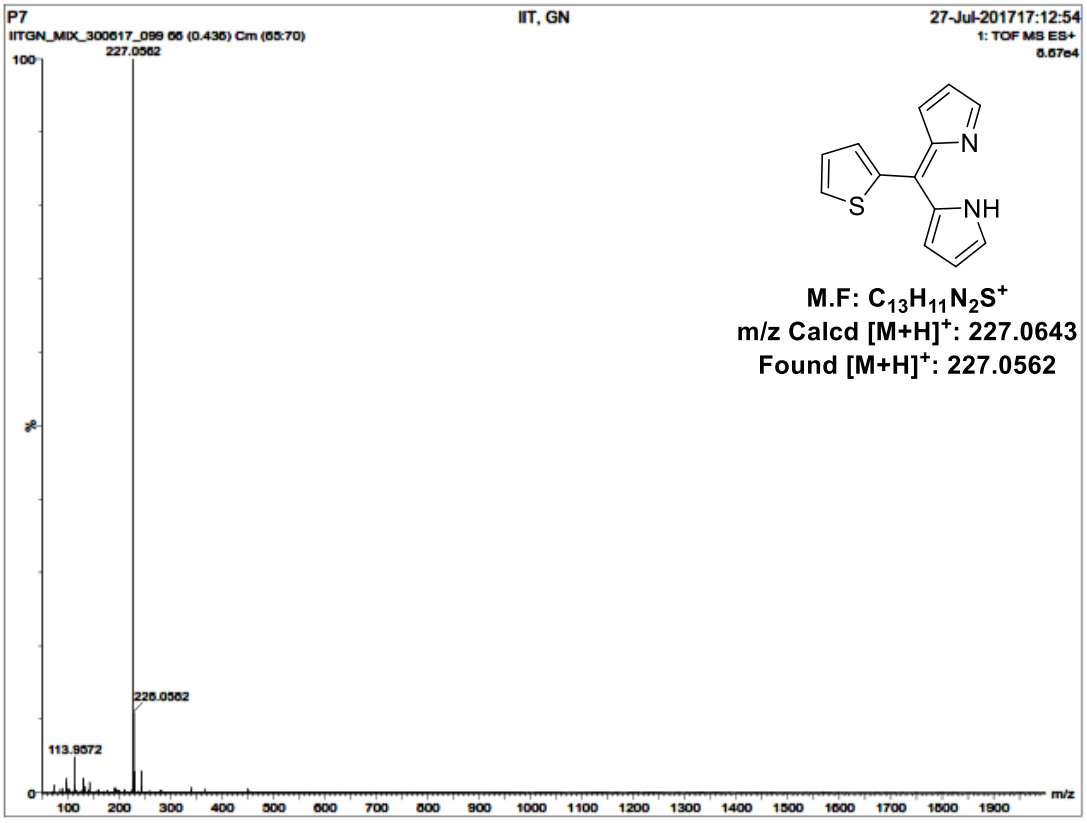


Figure 22. ESI-MS of compound **8**

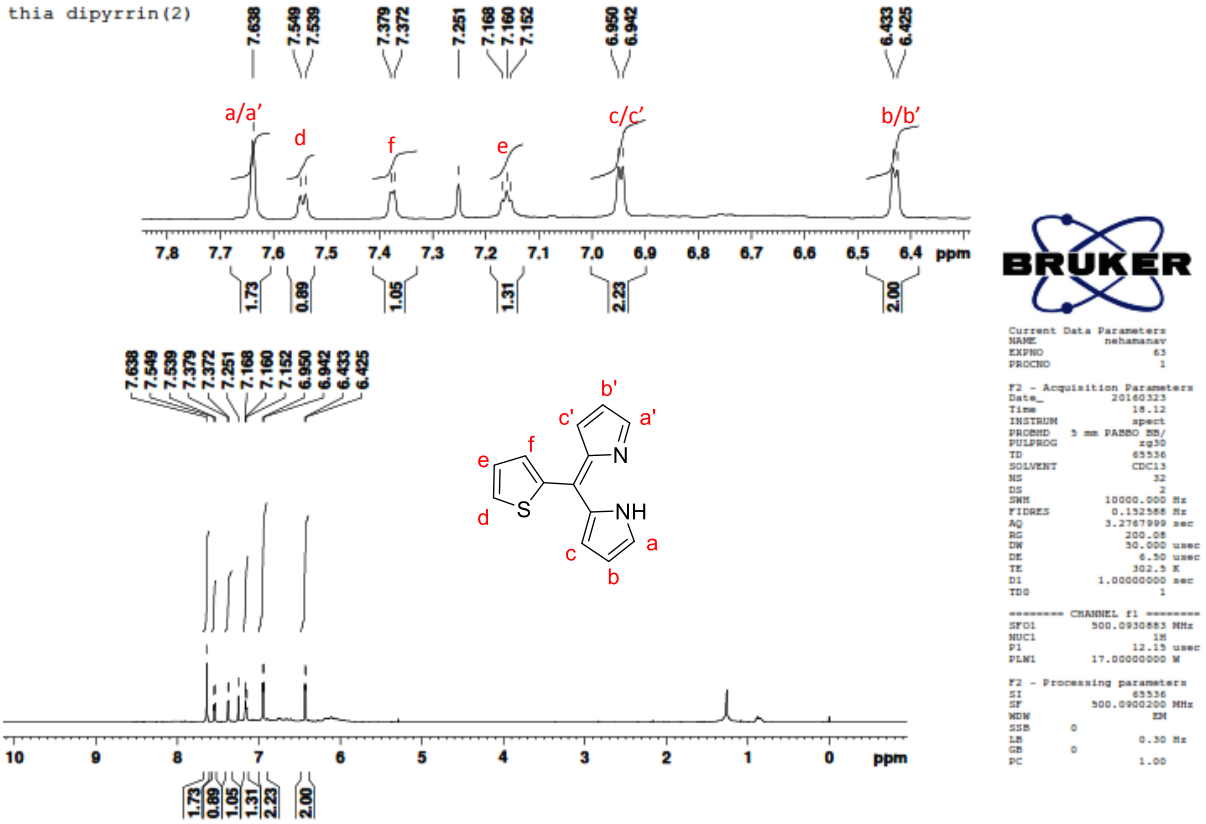


Figure 23. ^{1}H-NMR of compound **8** in $CDCl_3$

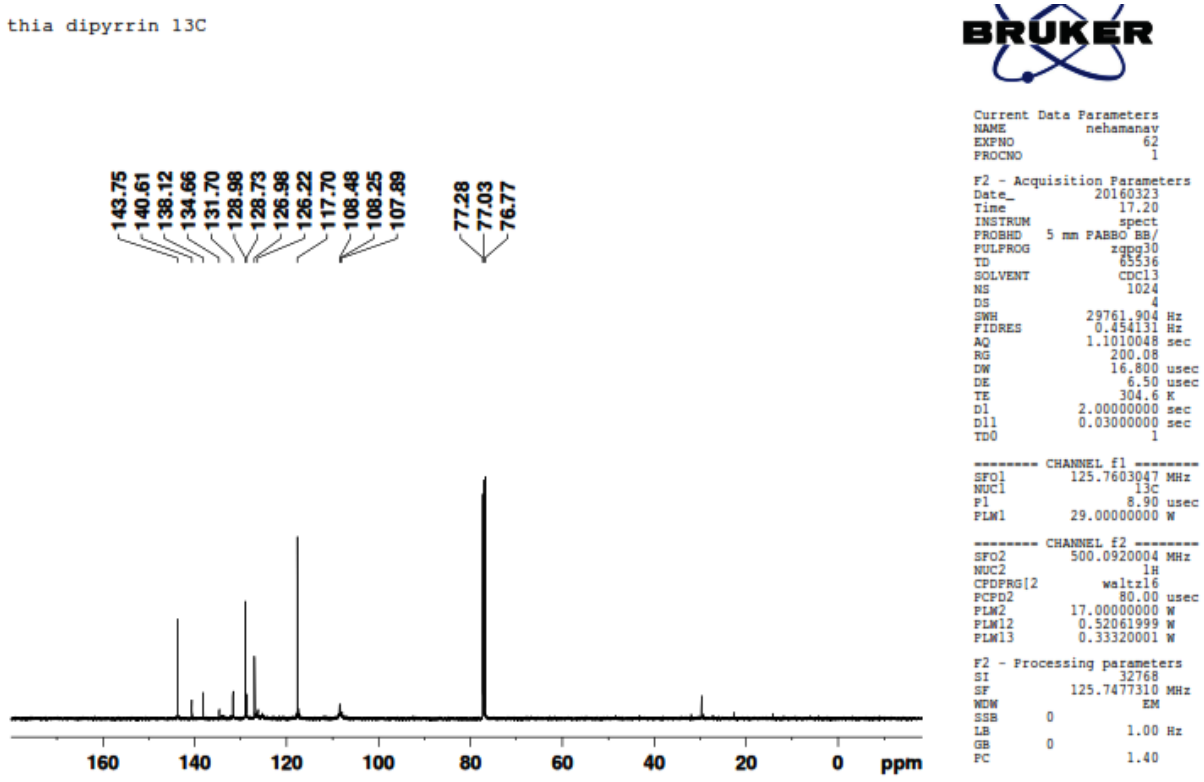


Figure 24. ^{13}C-NMR of compound **8** in $CDCl_3$

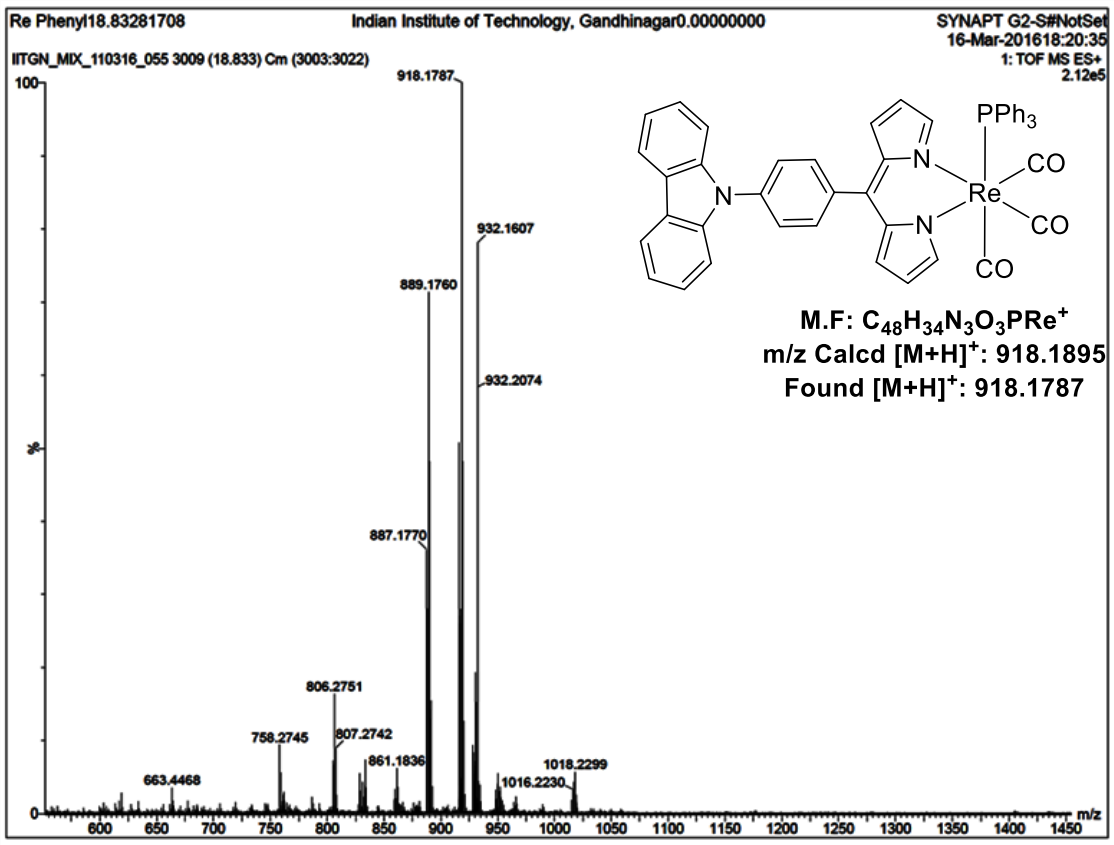


Figure 25. ESI-MS of compound **Re1**

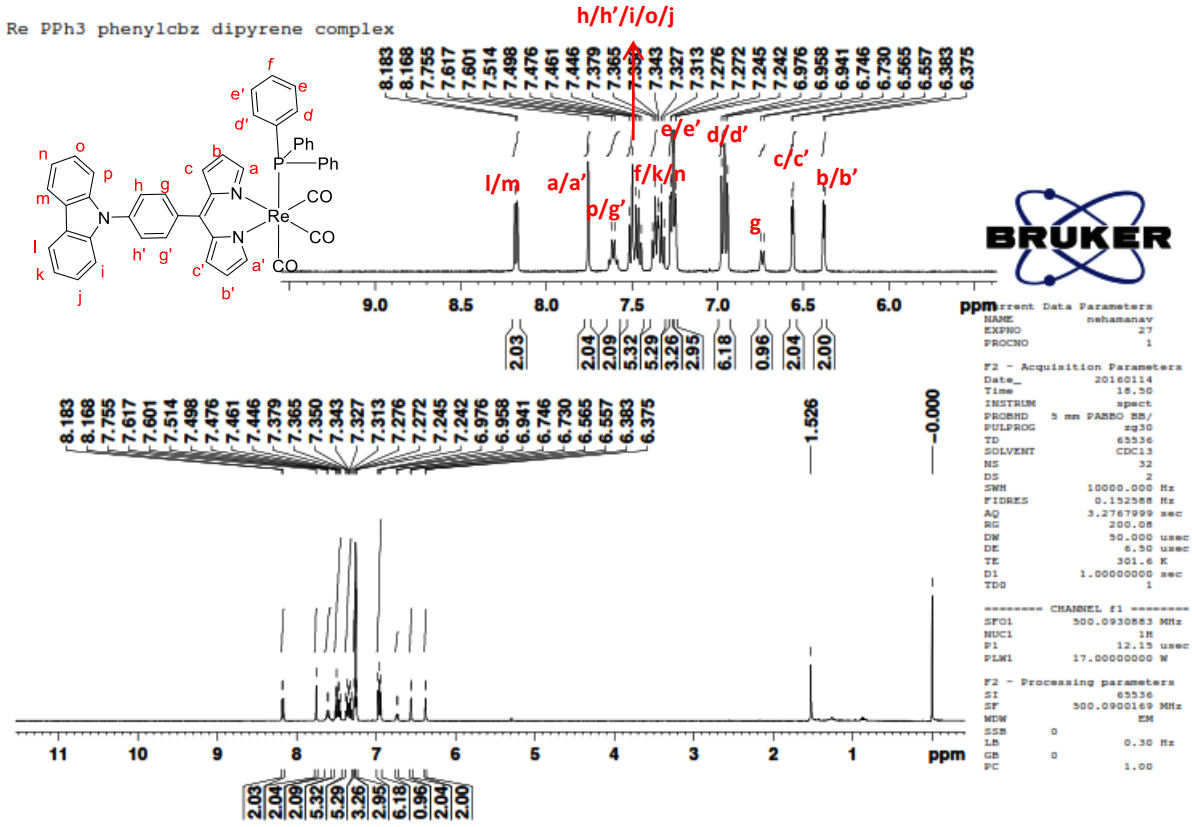


Figure 26. ^{1}H-NMR of compound **Re1** in $CDCl_3$

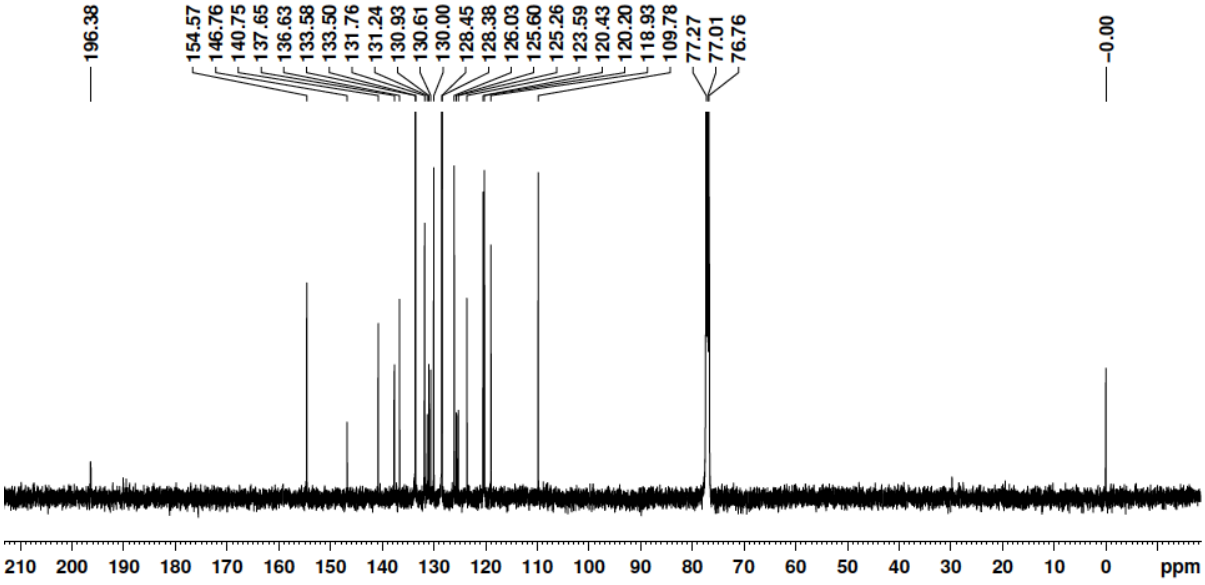


Figure 27. ^{13}C-NMR of compound **Re1** in $CDCl_3$

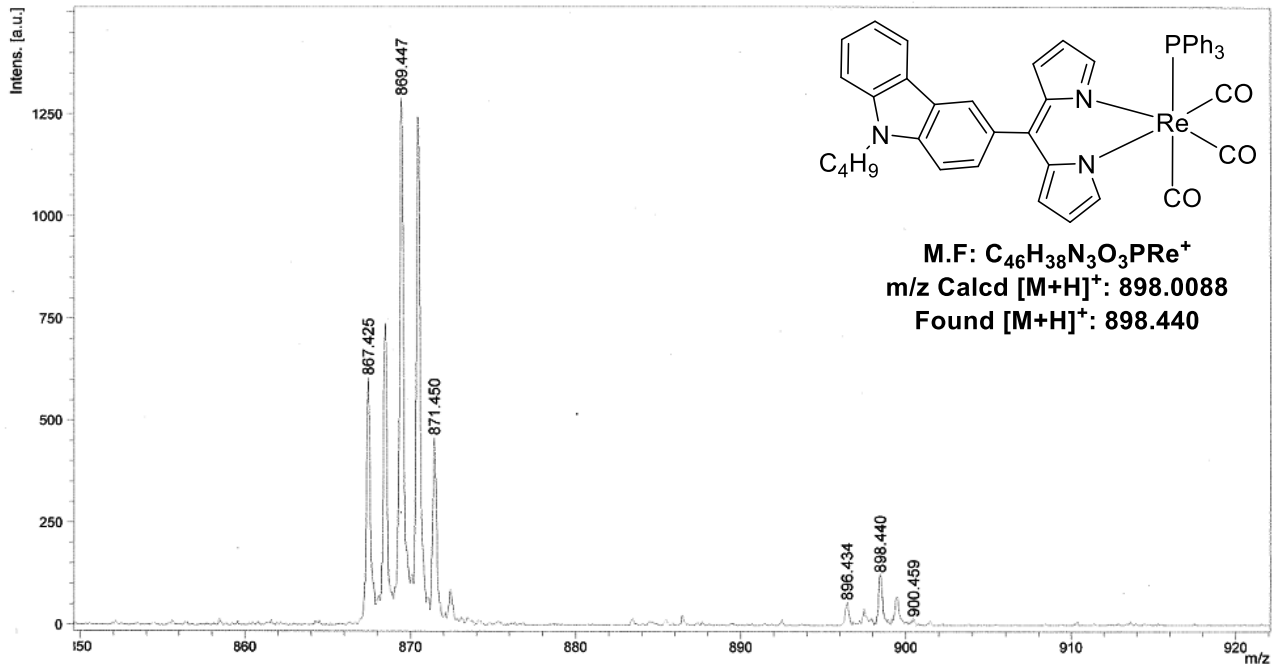


Figure 28. MALDI-MS of compound **Re2**

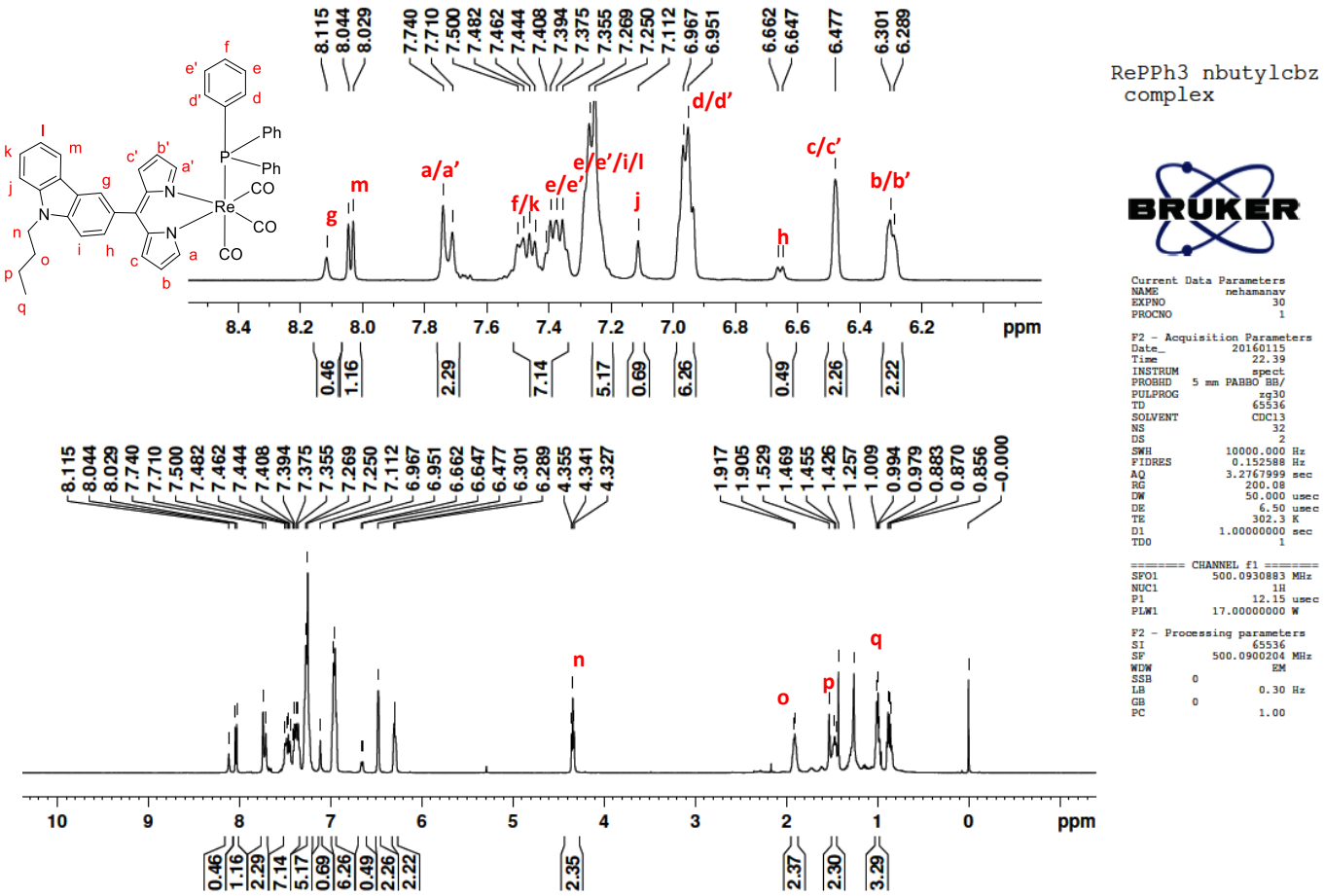


Figure 29. ^{1}H-NMR of compound **Re2** in $CDCl_3$

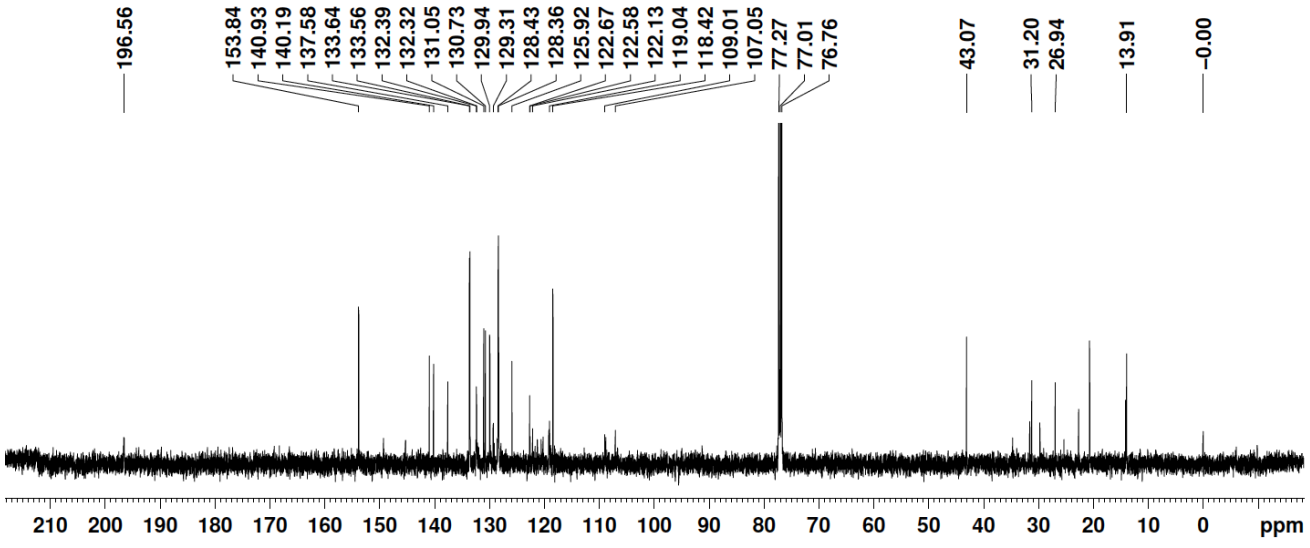


Figure 30. ^{13}C-NMR of compound **Re2** in $CDCl_3$

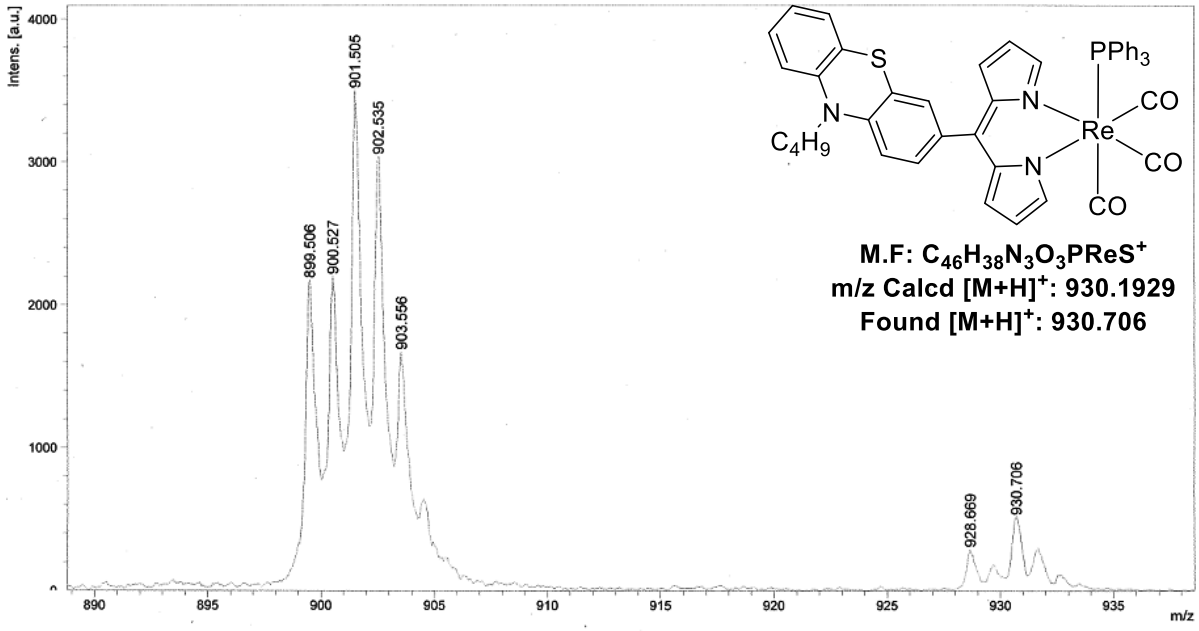


Figure 31. MALDI-MS of compound **Re3**

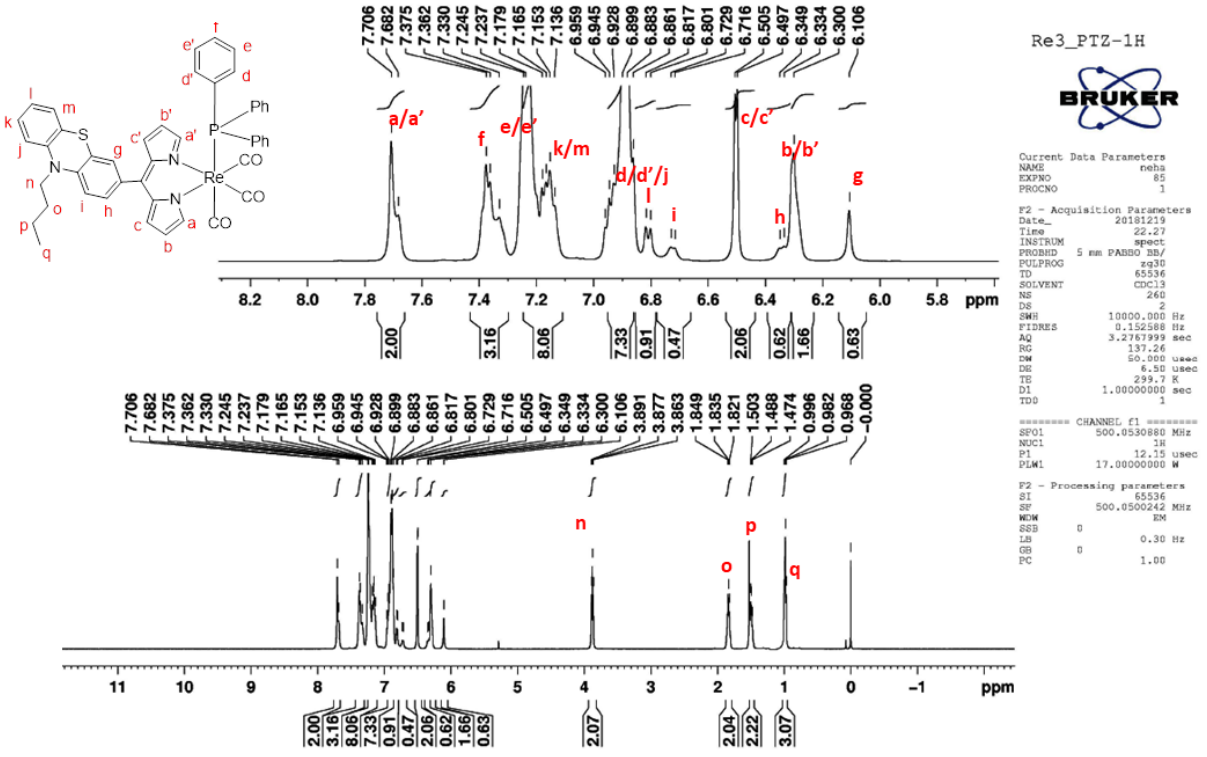


Figure 32. ^{1}H-NMR of compound **Re3** in $CDCl_3$

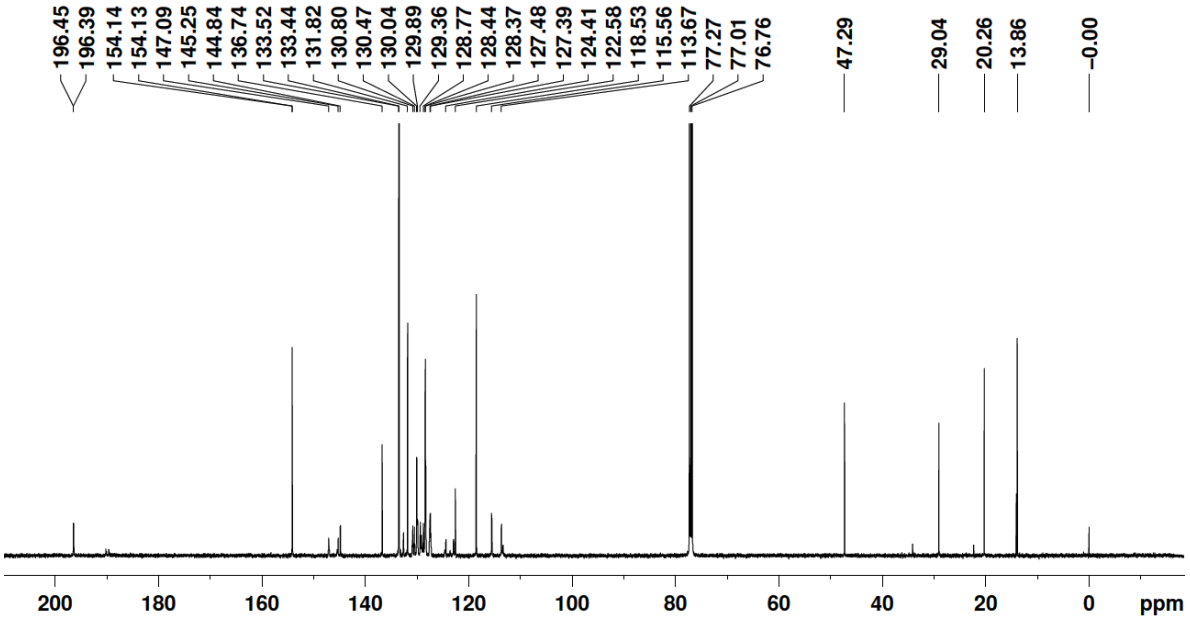


Figure 33. ^{13}C-NMR of compound **Re3** in $CDCl_3$

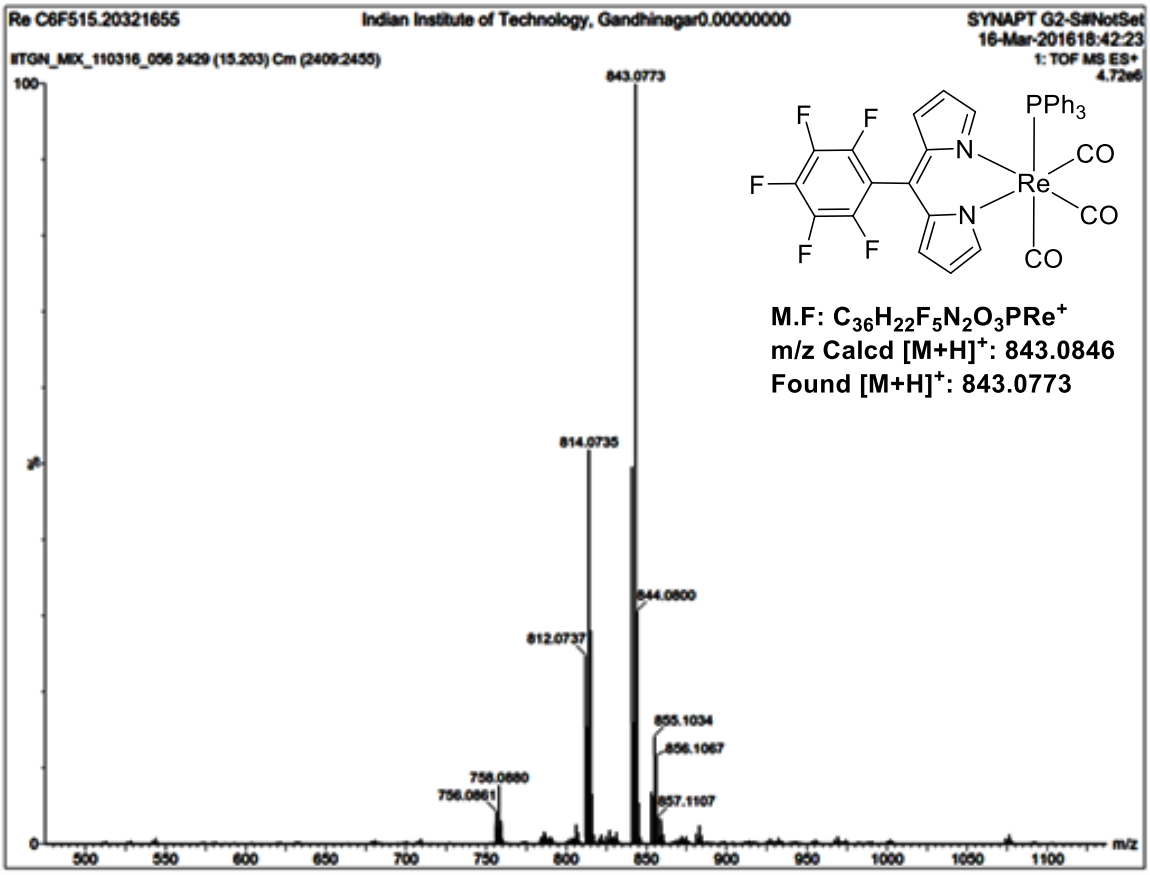


Figure 34. ESI-MS of compound **Re4**

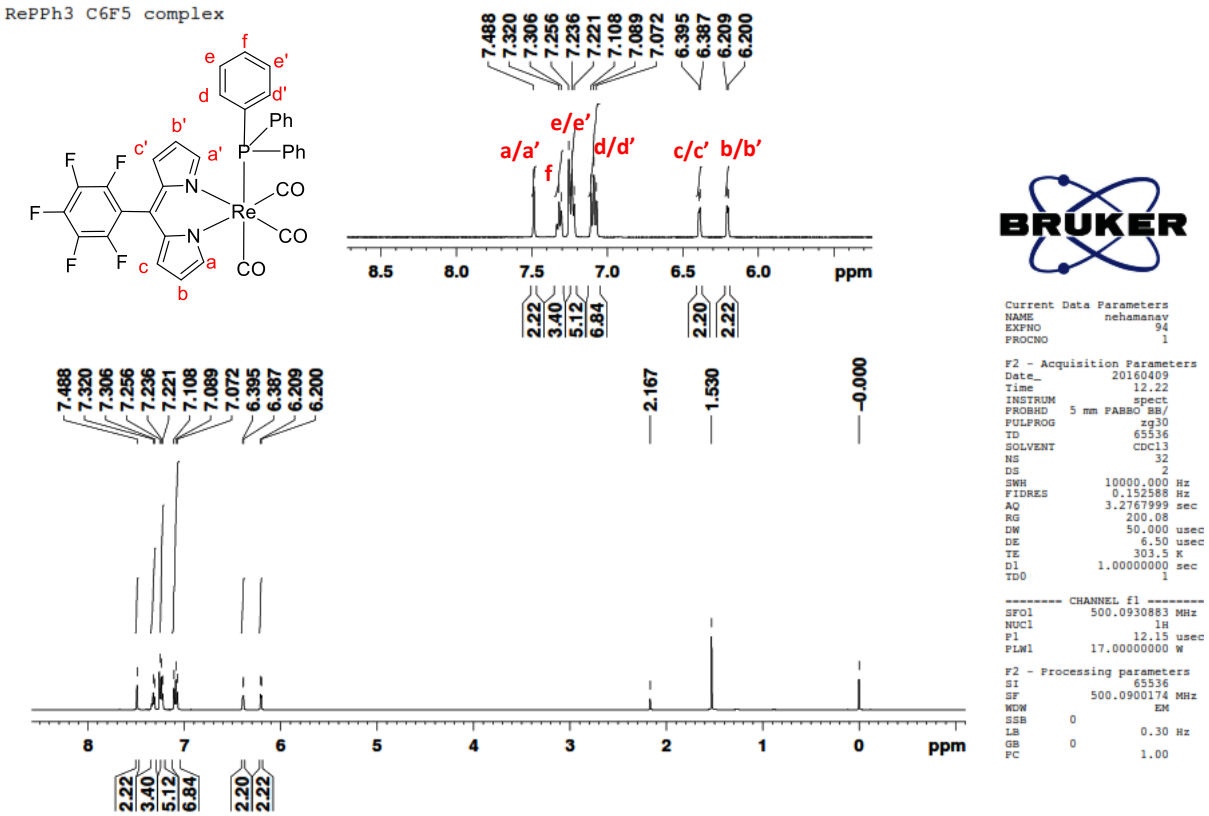


Figure 35. ^{1}H-NMR of compound **Re4** in $CDCl_3$

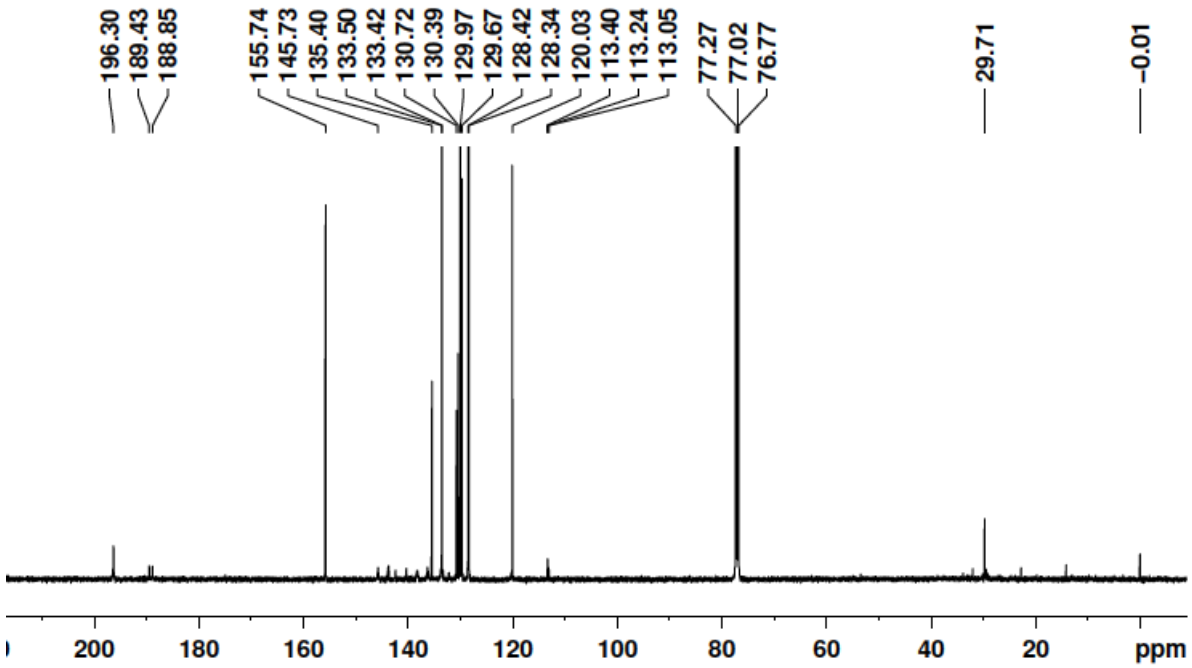


Figure 36. ^{13}C-NMR of compound **Re4** in $CDCl_3$

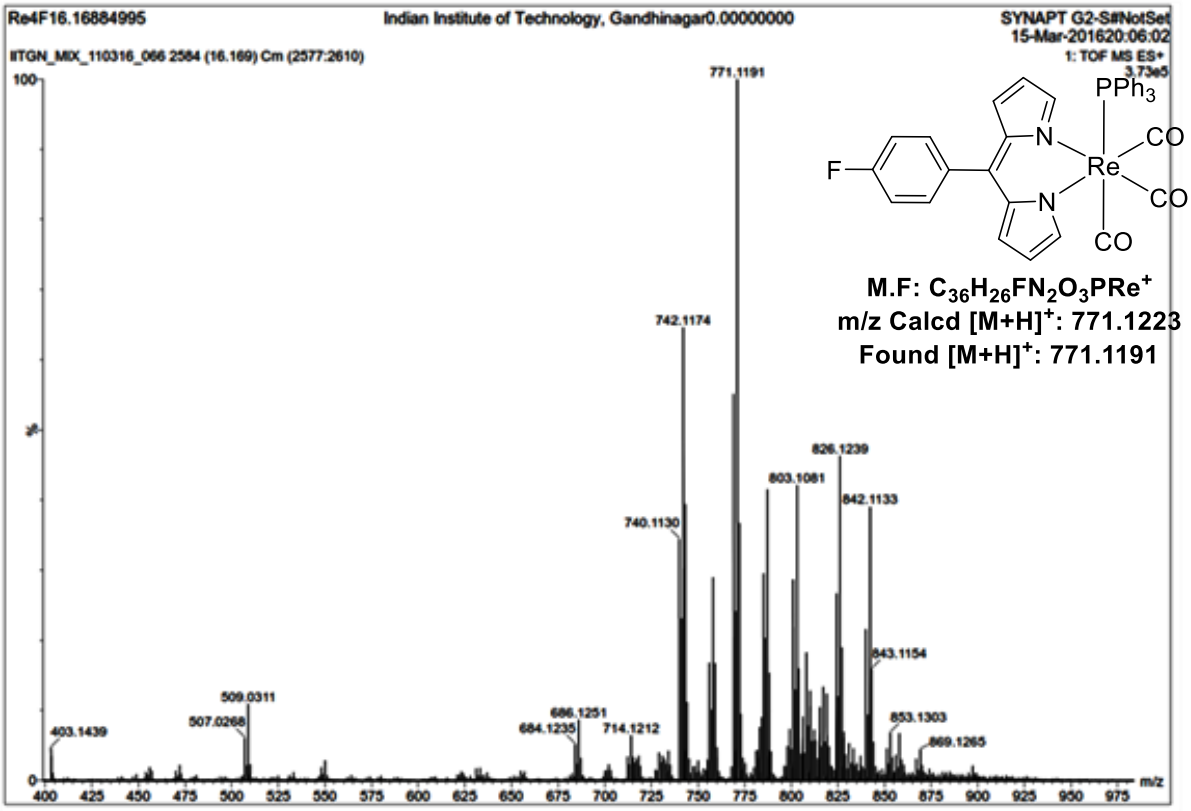


Figure 37. ESI-MS of compound **Re5**

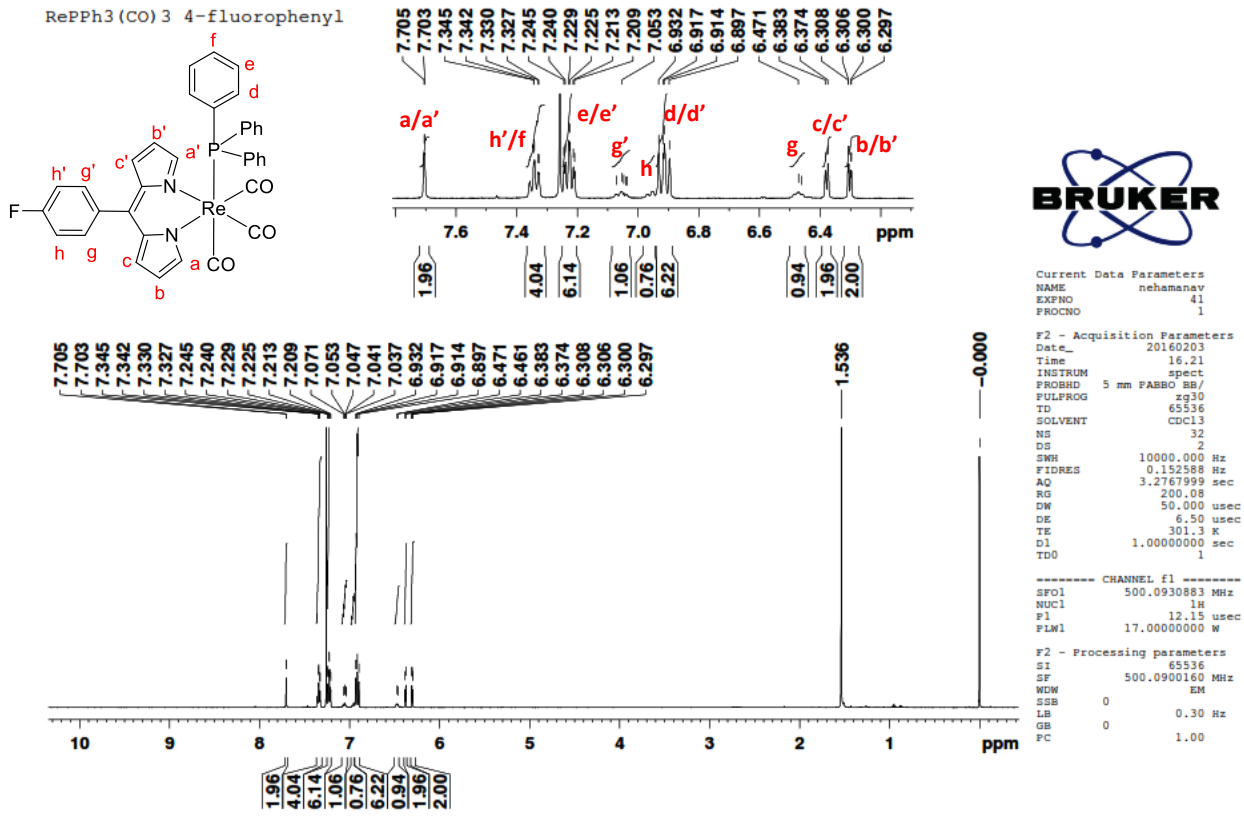


Figure 38. ^{1}H-NMR of compound **Re5** in $CDCl_3$

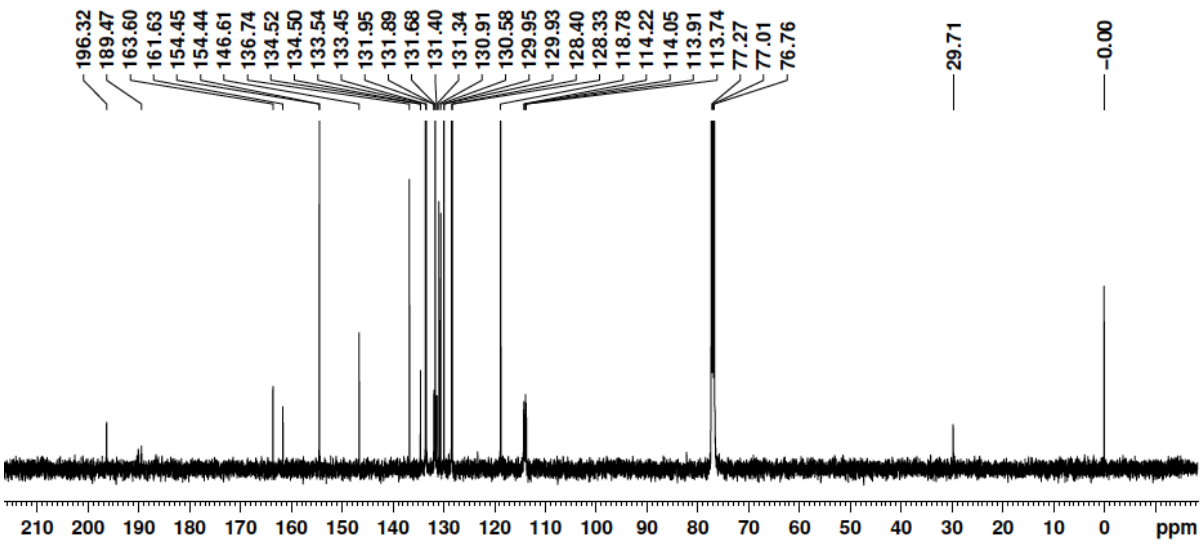


Figure 39. ^{13}C-NMR of compound **Re5** in $CDCl_3$

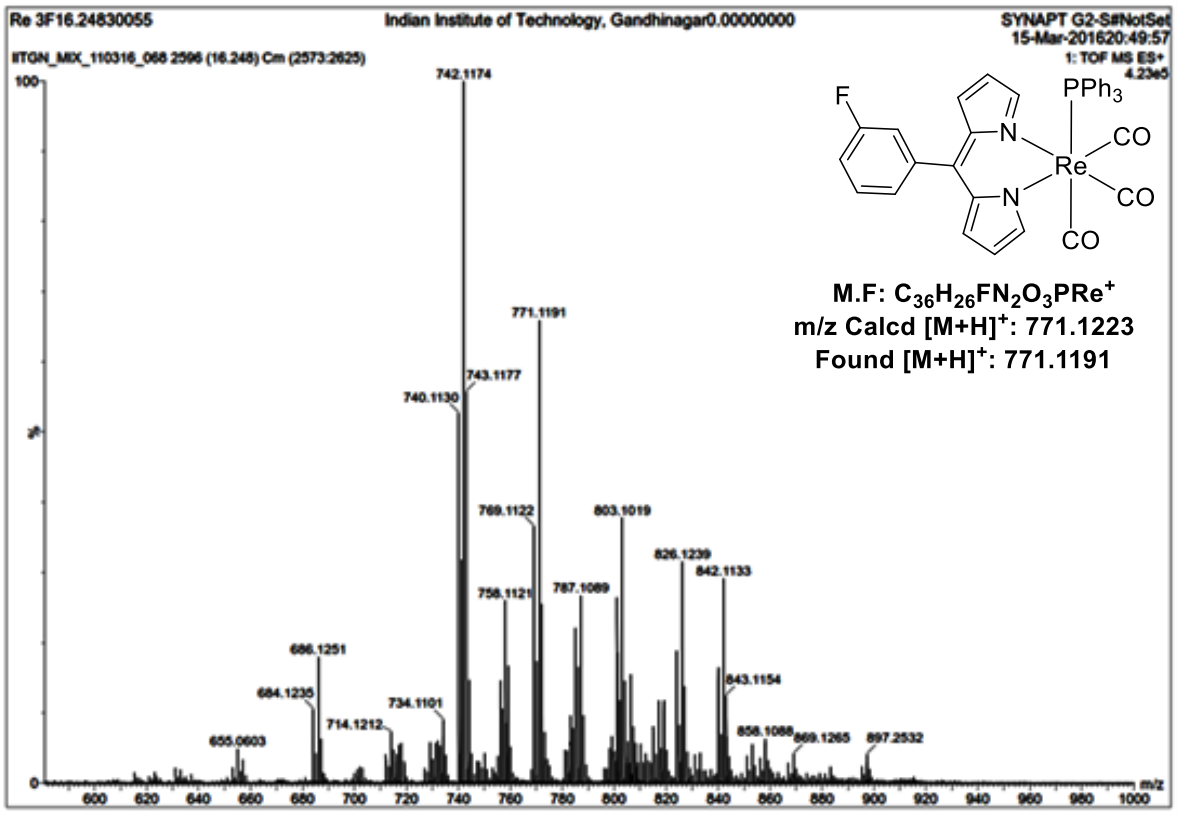


Figure 40. ESI-MS of compound **Re6**

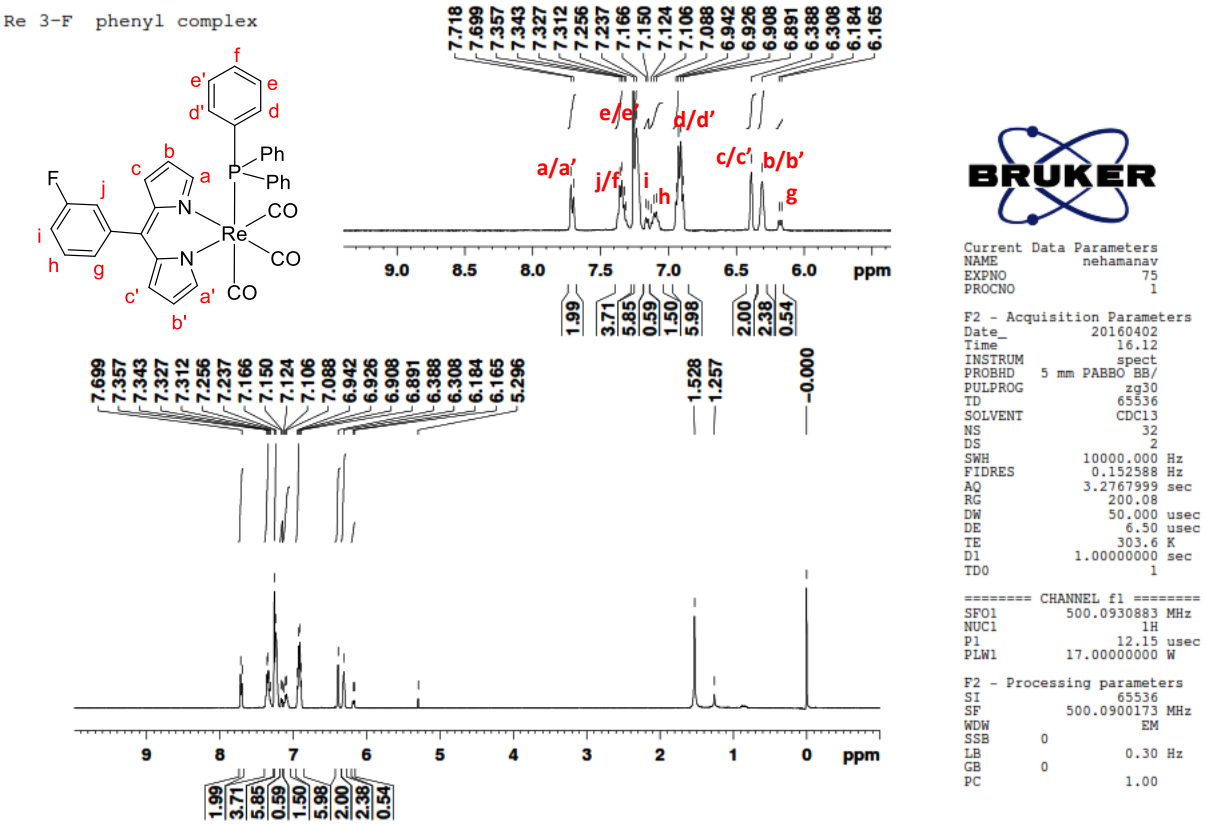


Figure 41. ^{1}H-NMR of compound **Re6** in $CDCl_3$

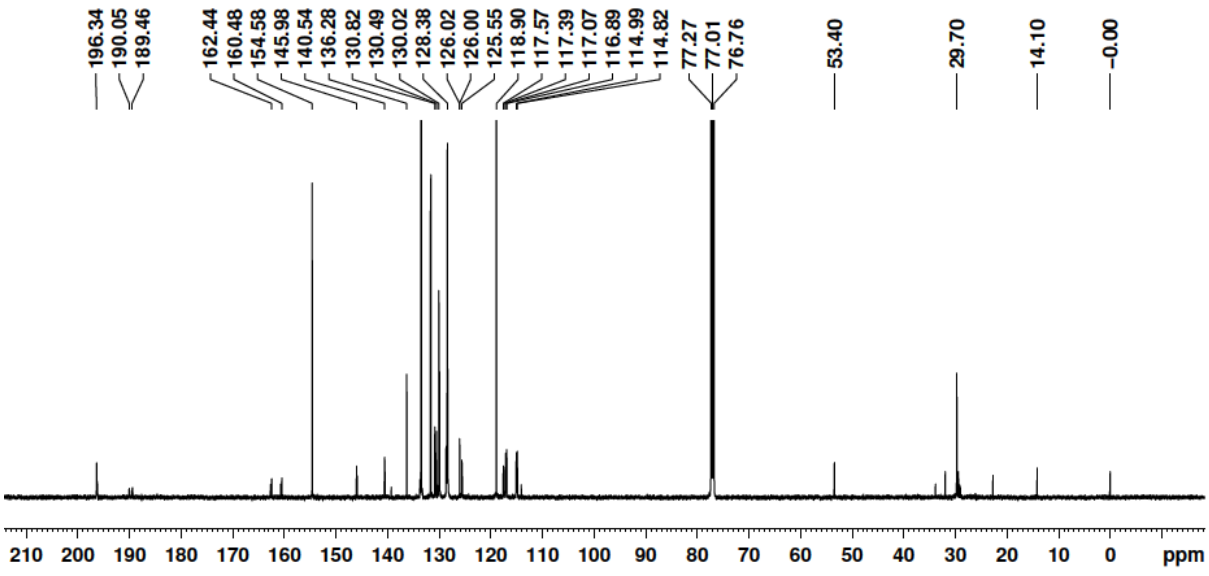


Figure 42. ^{13}C-NMR of compound **Re6** in $CDCl_3$

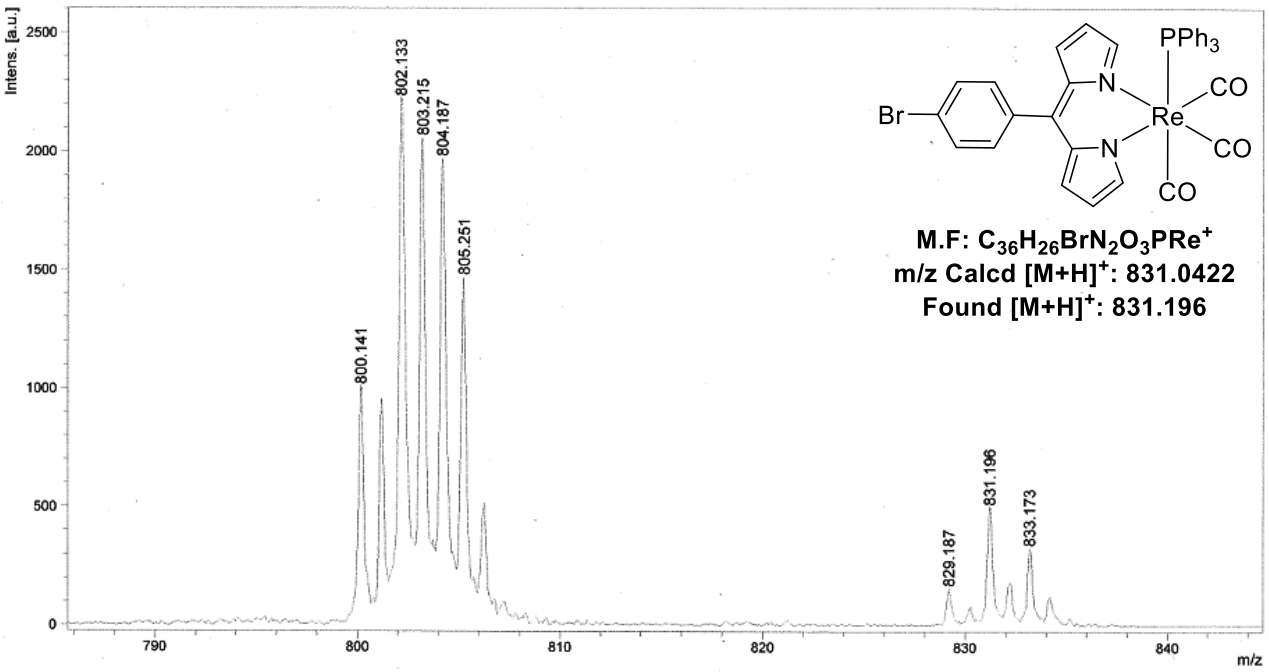


Figure 43. MALDI-MS of compound **Re7**

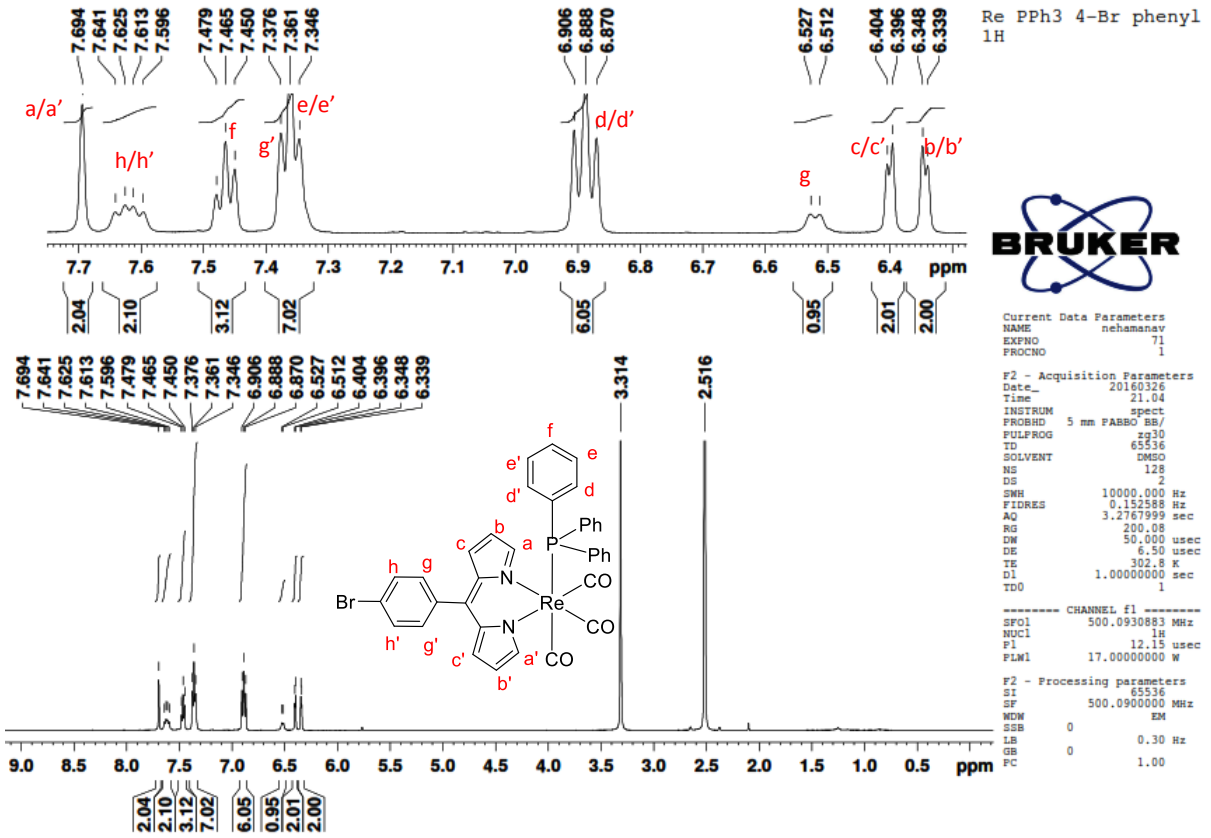


Figure 44. ^{1}H-NMR of compound **Re7** in DMSO

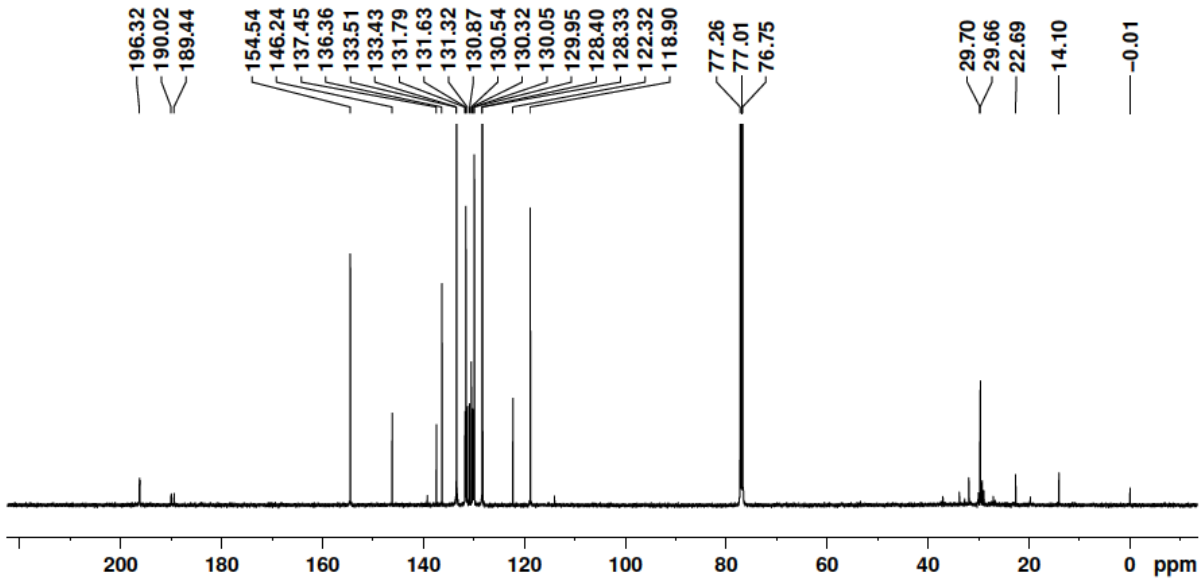


Figure 45. ^{13}C-NMR of compound **Re7** in $CDCl_3$

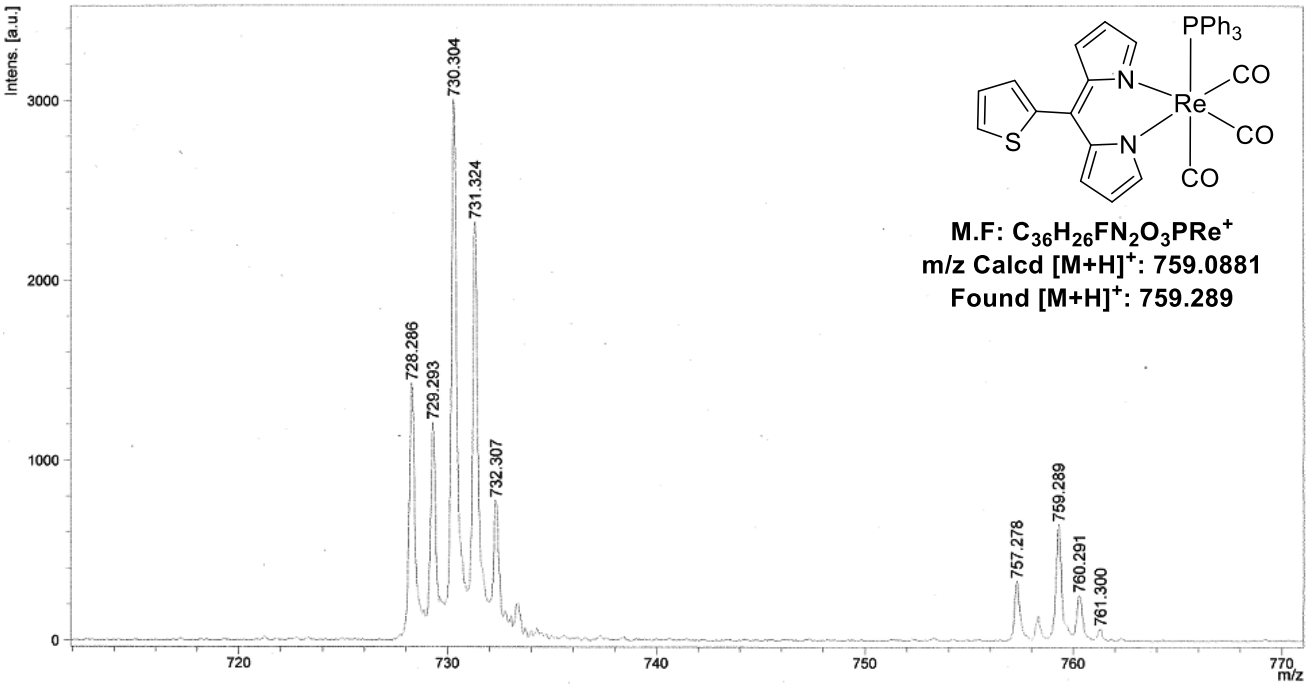


Figure 46. MALDI-MS of compound Re**8**

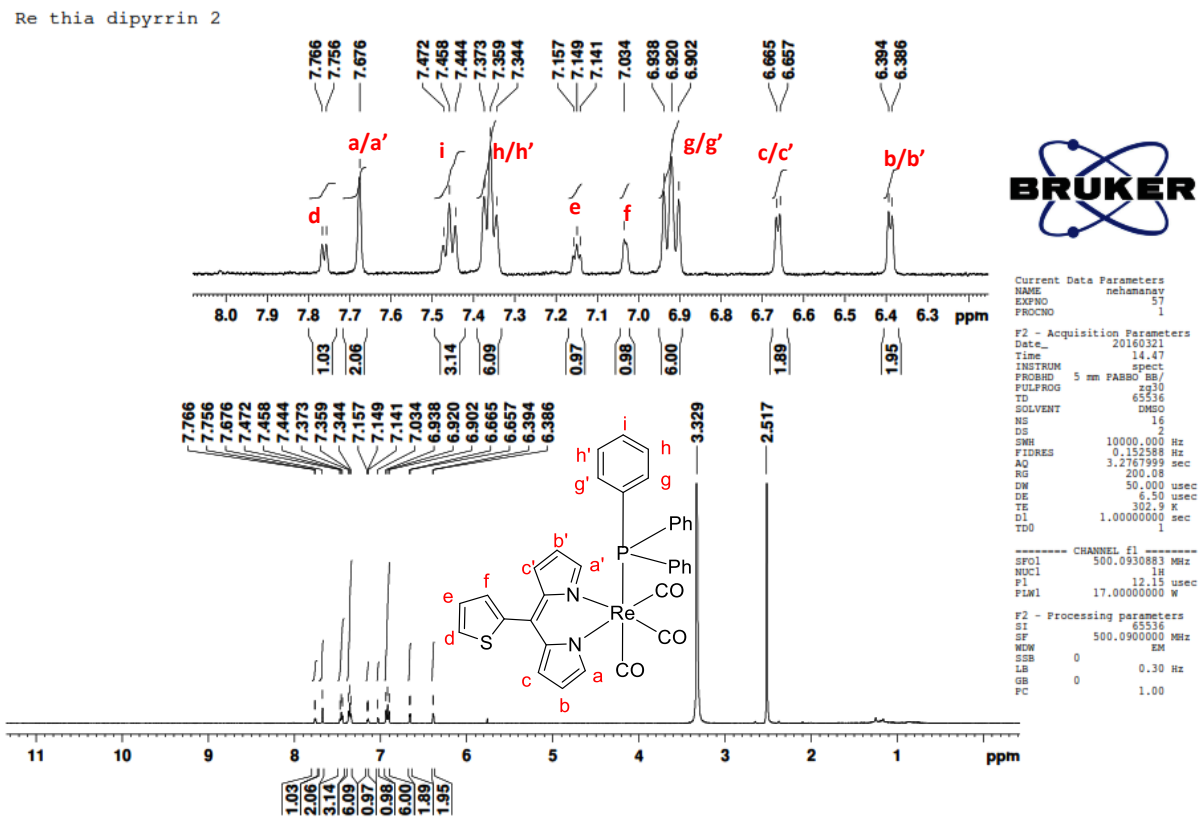


Figure 47. ^{1}H-NMR of compound **Re8** in DMSO

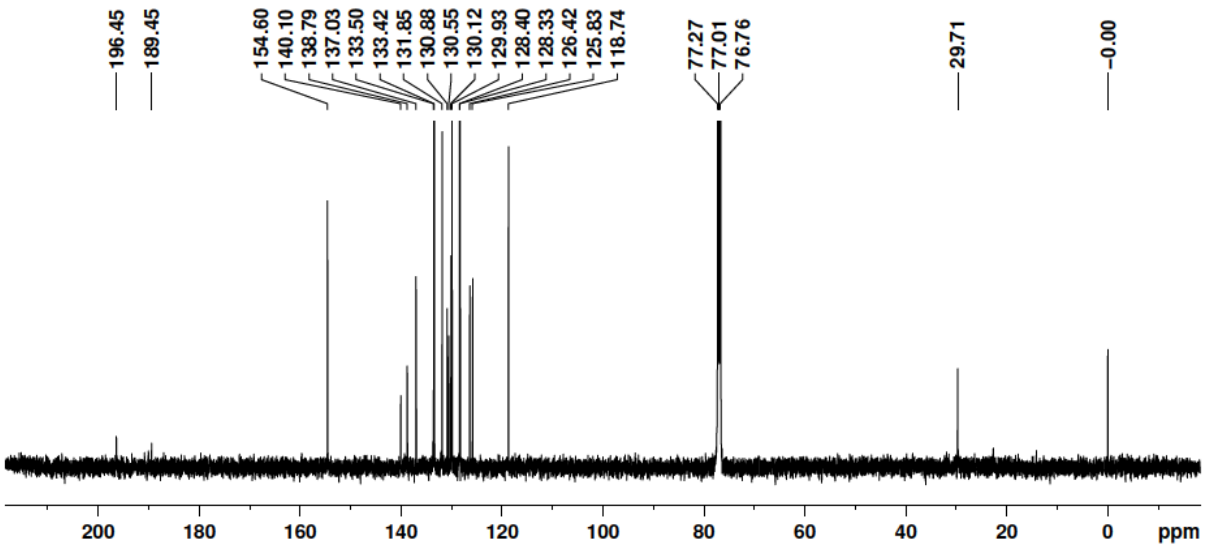


Figure 48. ^{13}C-NMR of compound **Re8** in $CDCl_3$

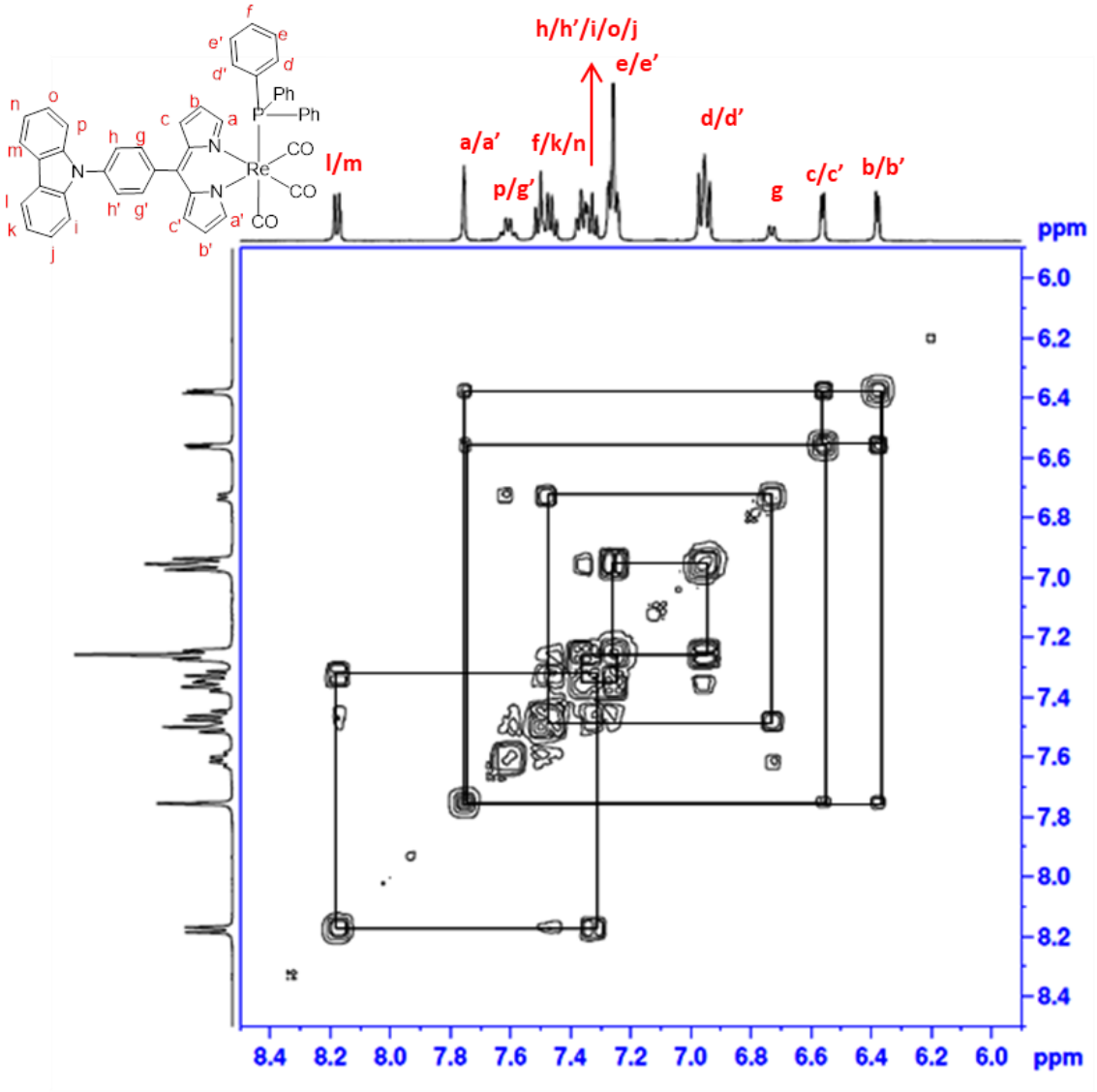


Figure 49. ^{1}H-^{1}H COSY spectra of compound **Re1** in $CDCl_3$

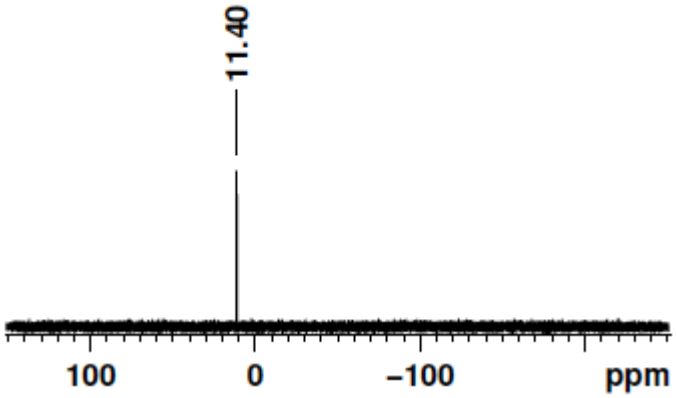


Figure 50. ^{31}P- NMR of compound Re**1** in $CDCl_3$

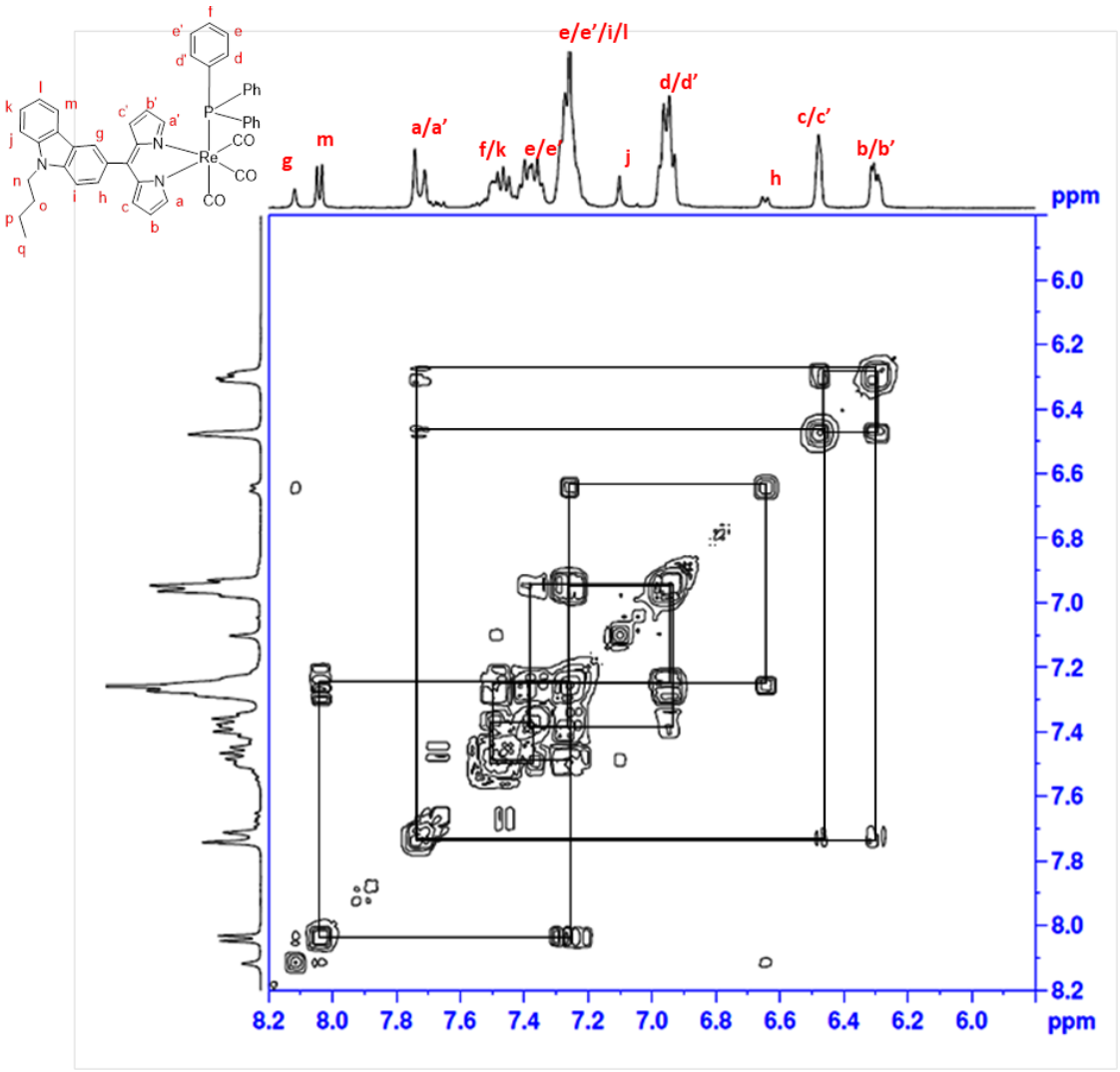


Figure 51. ^{1}H-^{1}H COSY spectra of compound **Re2** in $CDCl_3$

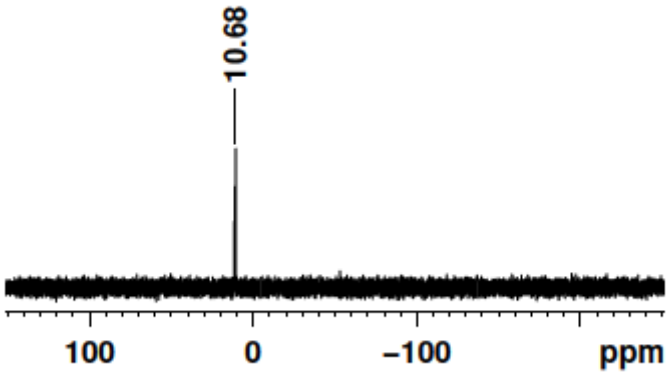


Figure 52. ^{31}P-NMR of compound Re**2** in $CDCl_3$

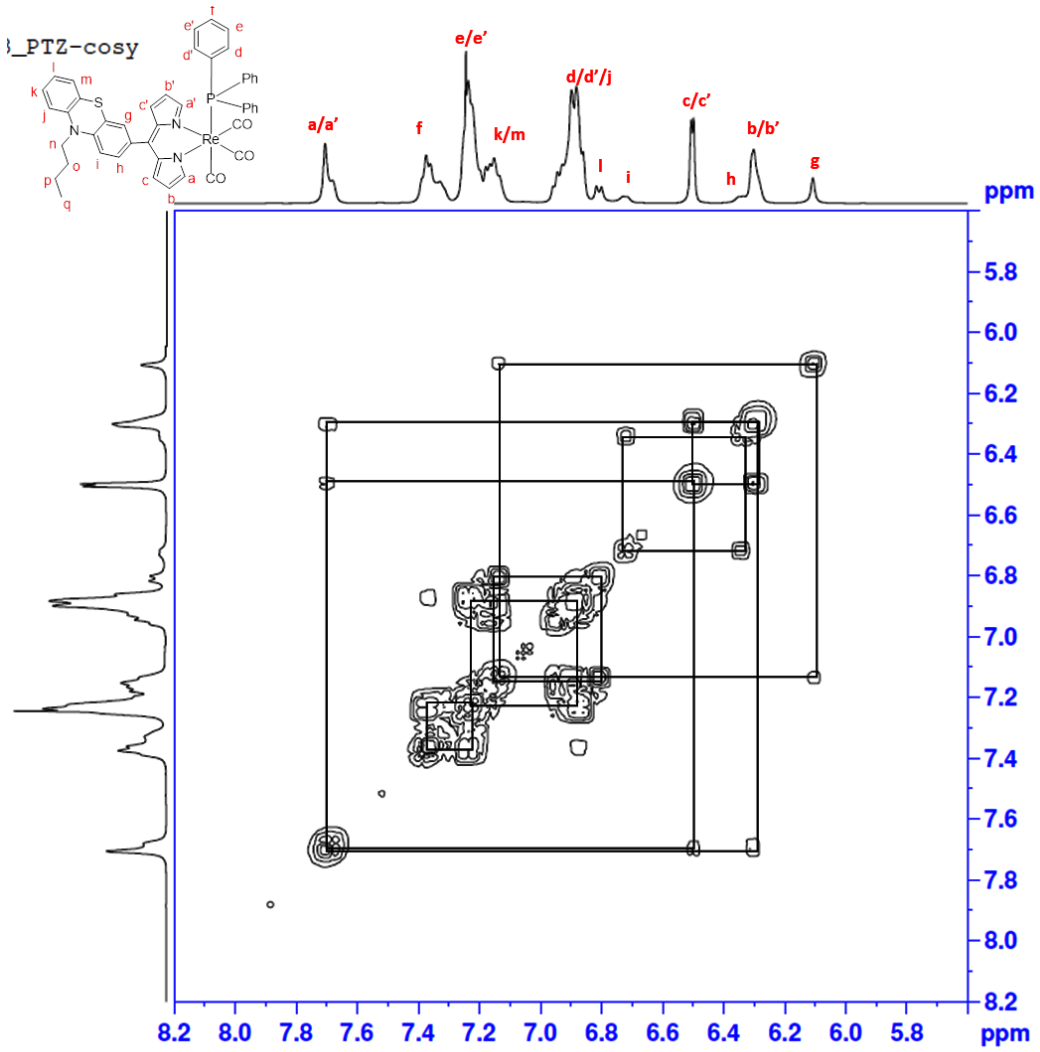


Figure 53. ^{1}H-^{1}H COSY spectra of compound **Re3** in $CDCl_3$

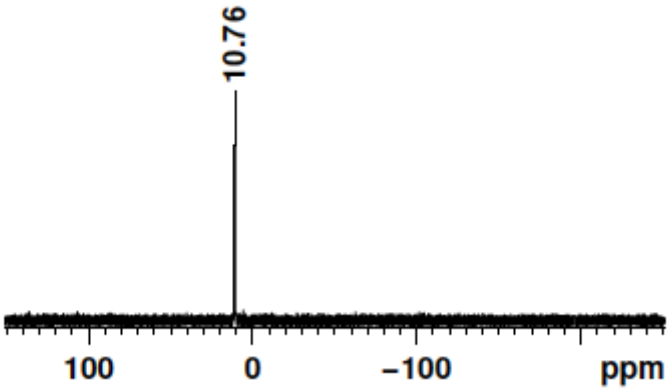


Figure 54. ^{31}P-NMR of compound Re**3** in $CDCl_3$

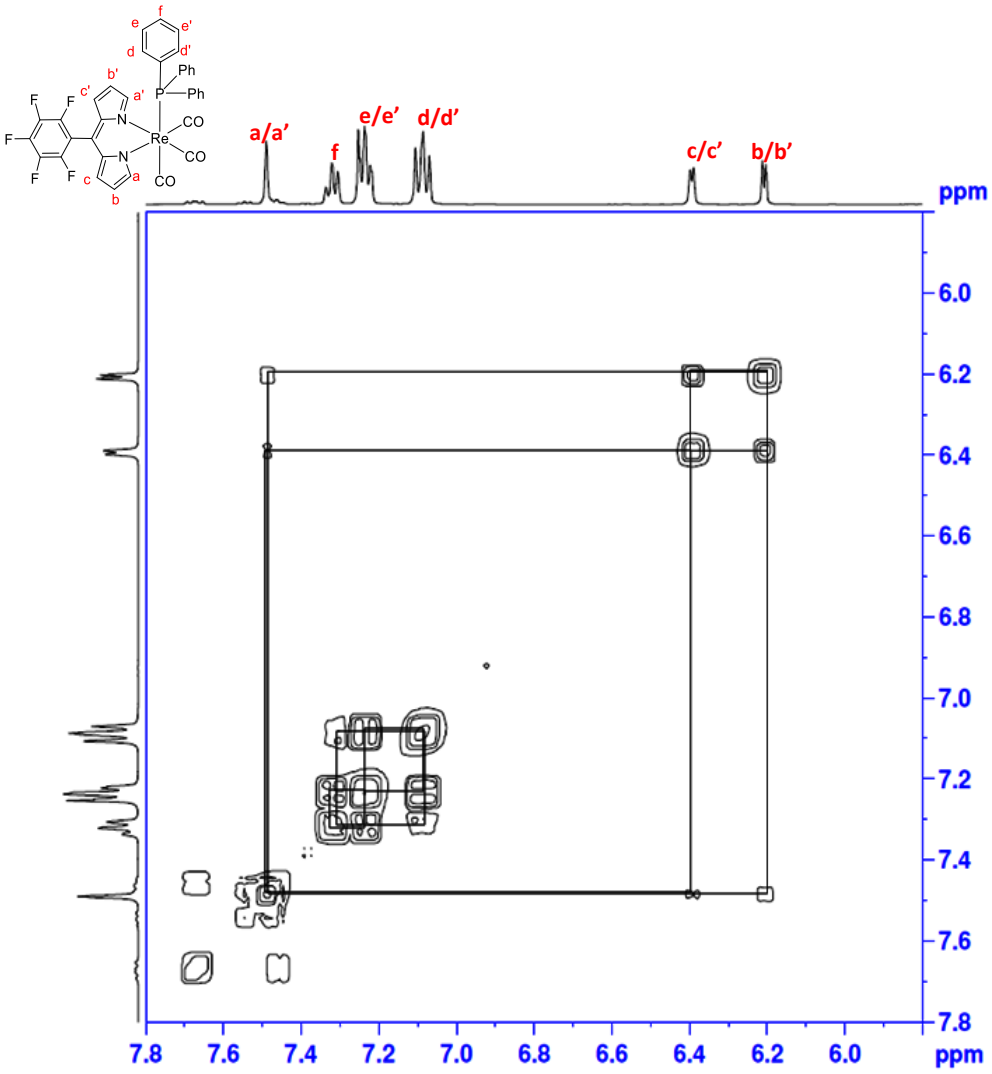


Figure 55. ^{1}H-^{1}H COSY spectra of compound **Re4** in $CDCl_3$

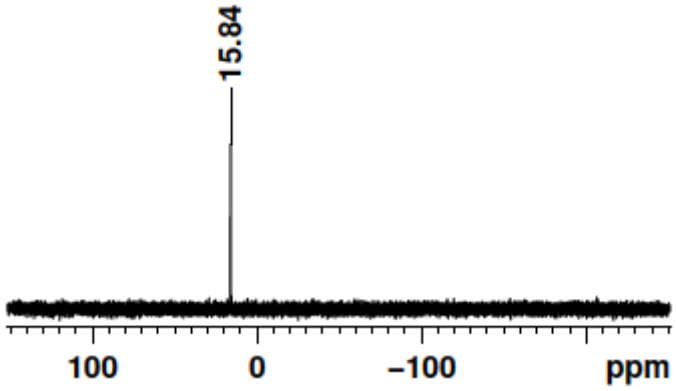


Figure 56. ^{31}P-NMR of compound Re**4** in $CDCl_3$

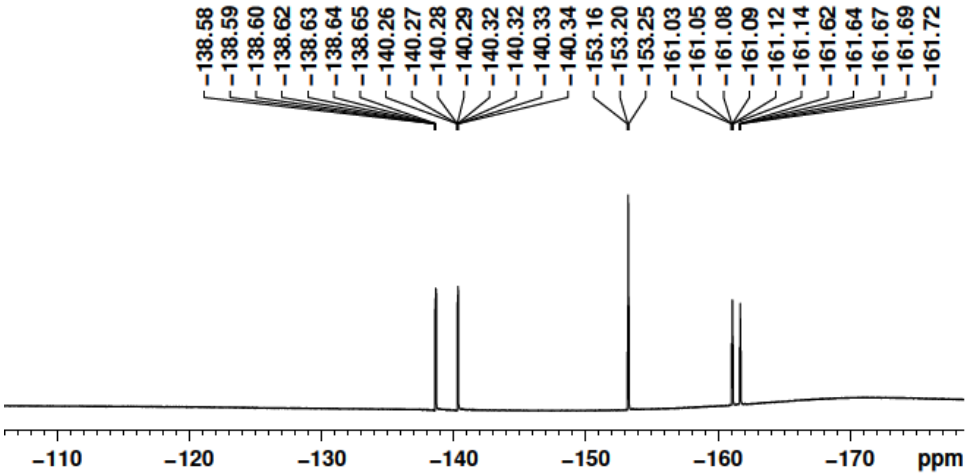


Figure 57. ^{19}F-NMR of compound Re**4** in $CDCl_3$

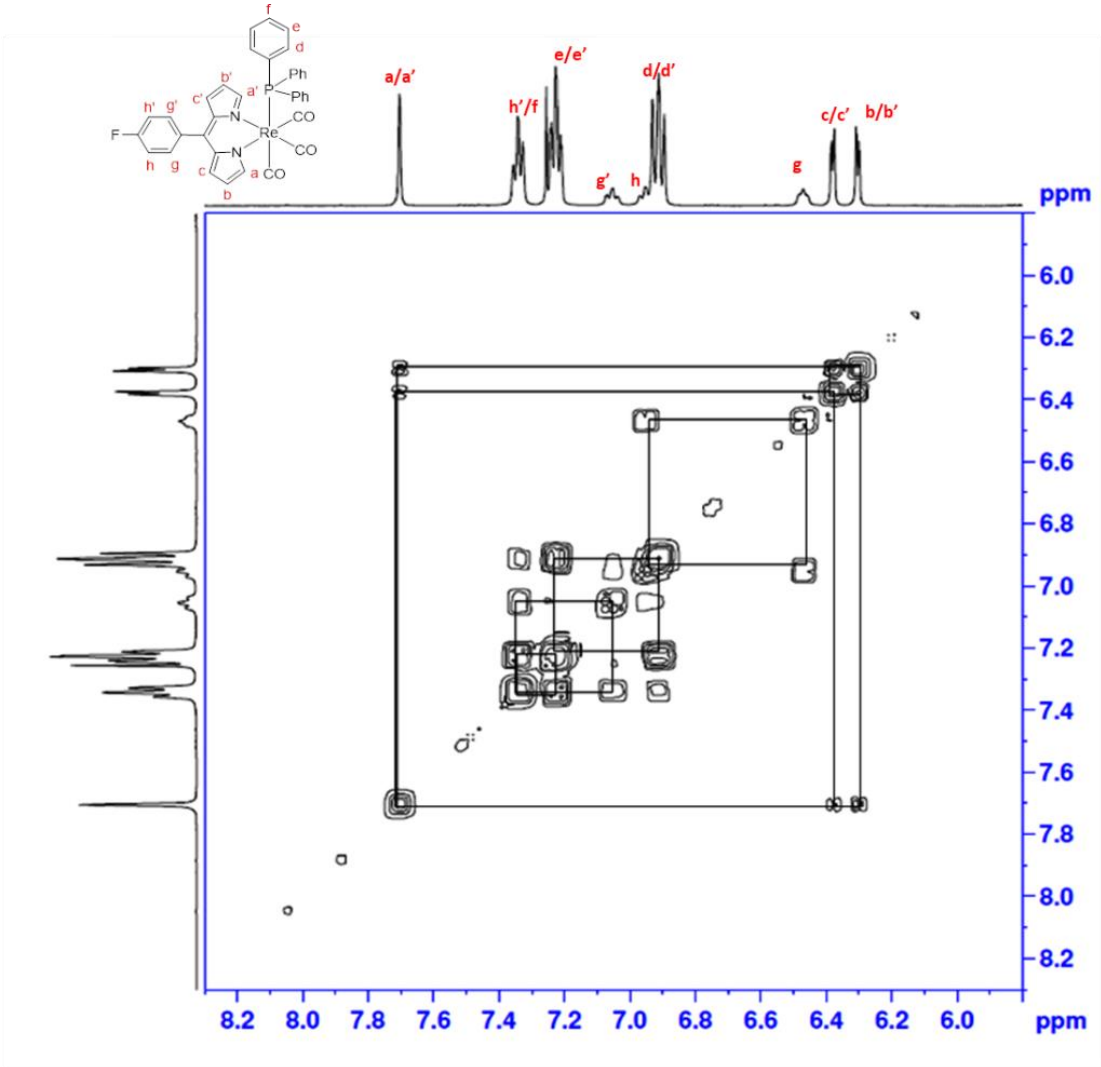


Figure 58. ^{1}H-^{1}H COSY spectra of compound **Re5** in $CDCl_3$

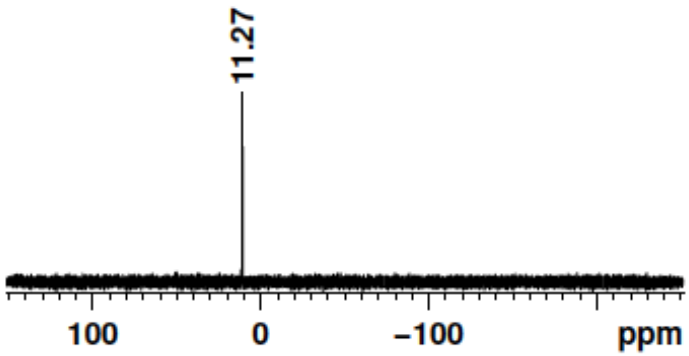


Figure 59. ^{31}P-NMR of compound Re**5** in $CDCl_3$

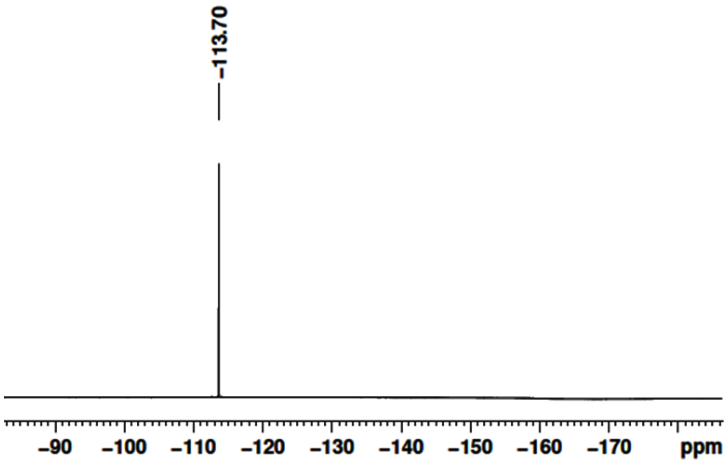


Figure 60. ^{19}F-NMR of compound Re**5** in $CDCl_3$

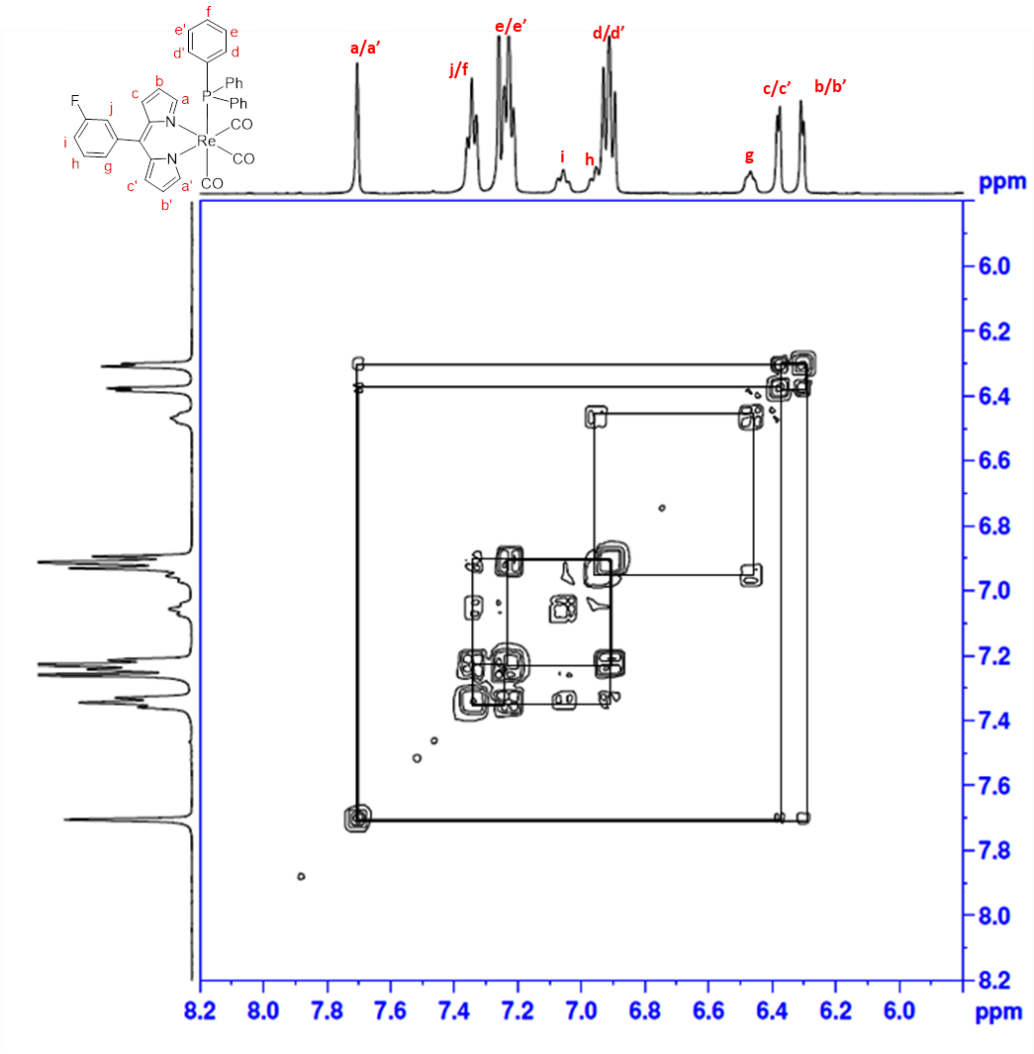


Figure 61. ^{1}H-^{1}H COSY spectra of compound **Re6** in $CDCl_3$

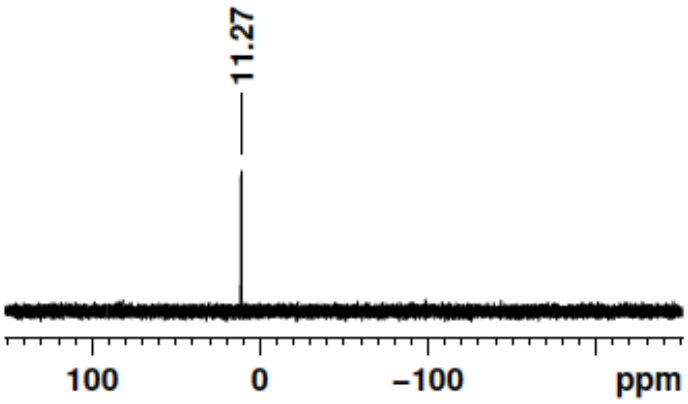


Figure 62. ^{31}P-NMR of compound Re**6** in $CDCl_3$

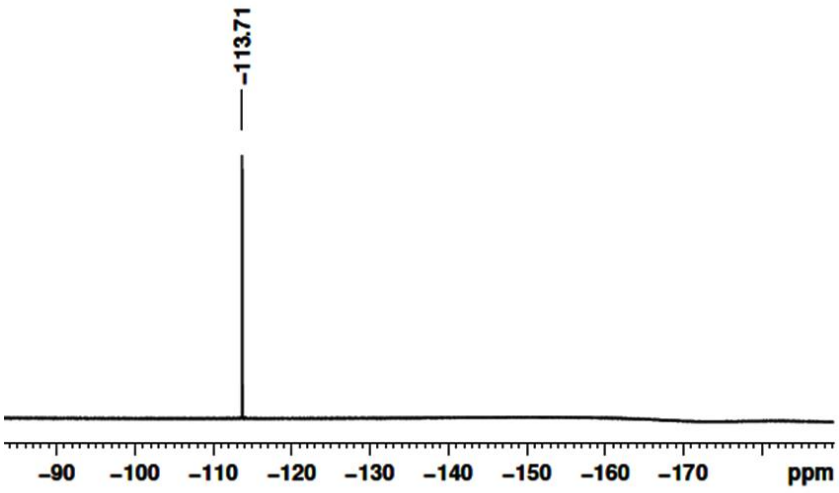


Figure 63. ^{19}F-NMR of compound Re**6** in $CDCl_3$

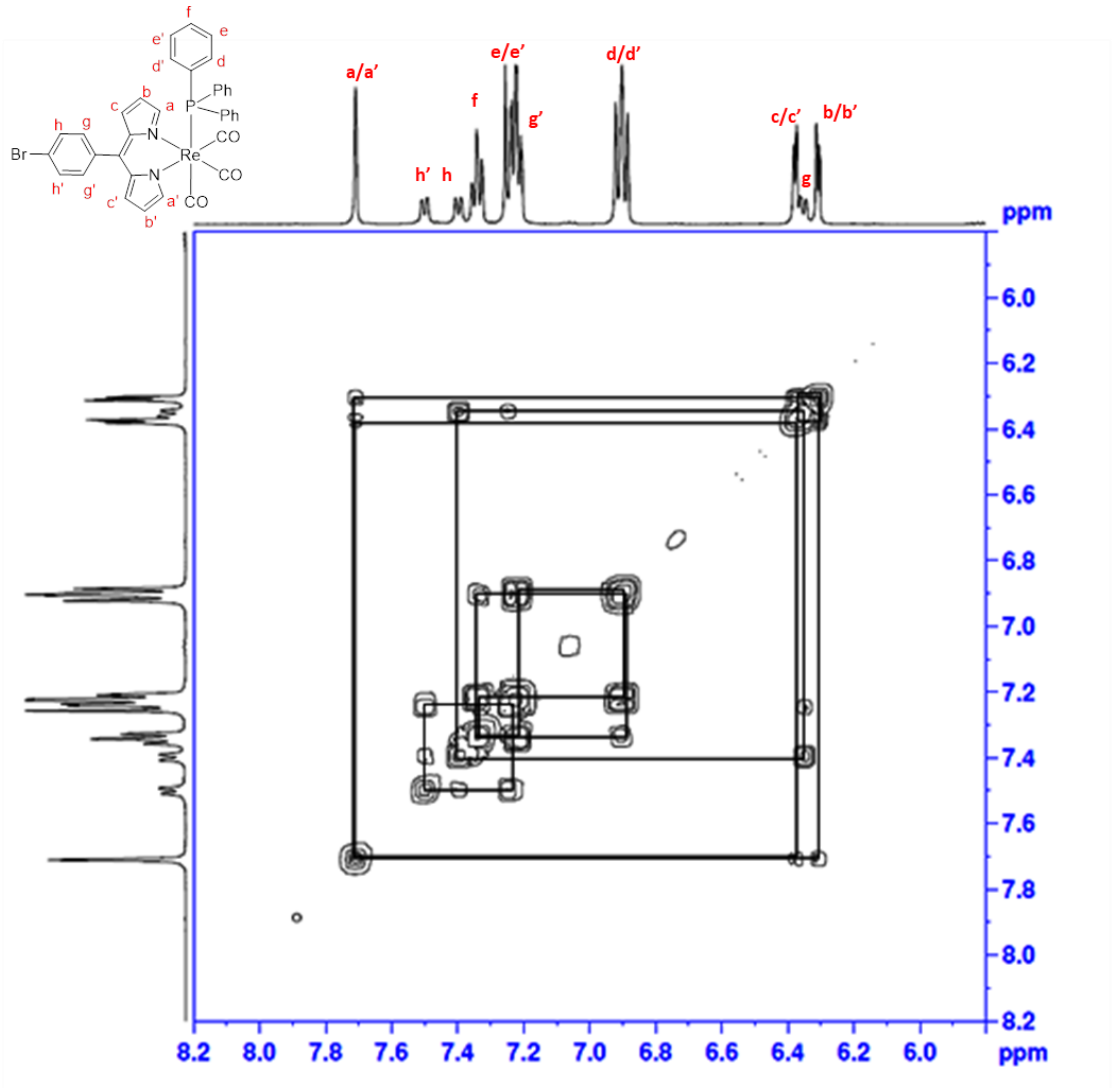


Figure 64. ^{1}H-^{1}H COSY spectra of compound **Re7** in $CDCl_3$

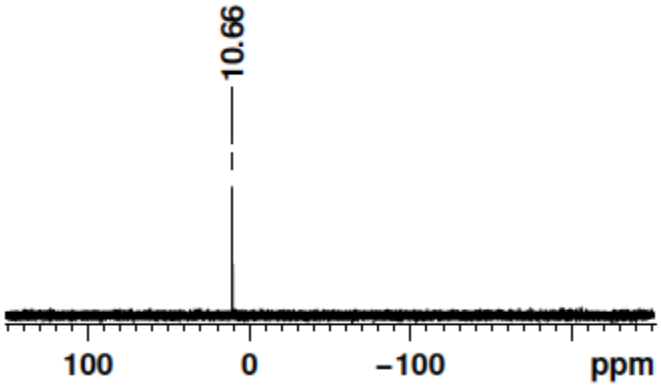


Figure 65. ^{31}P NMR of compound Re**7** in $CDCl_3$

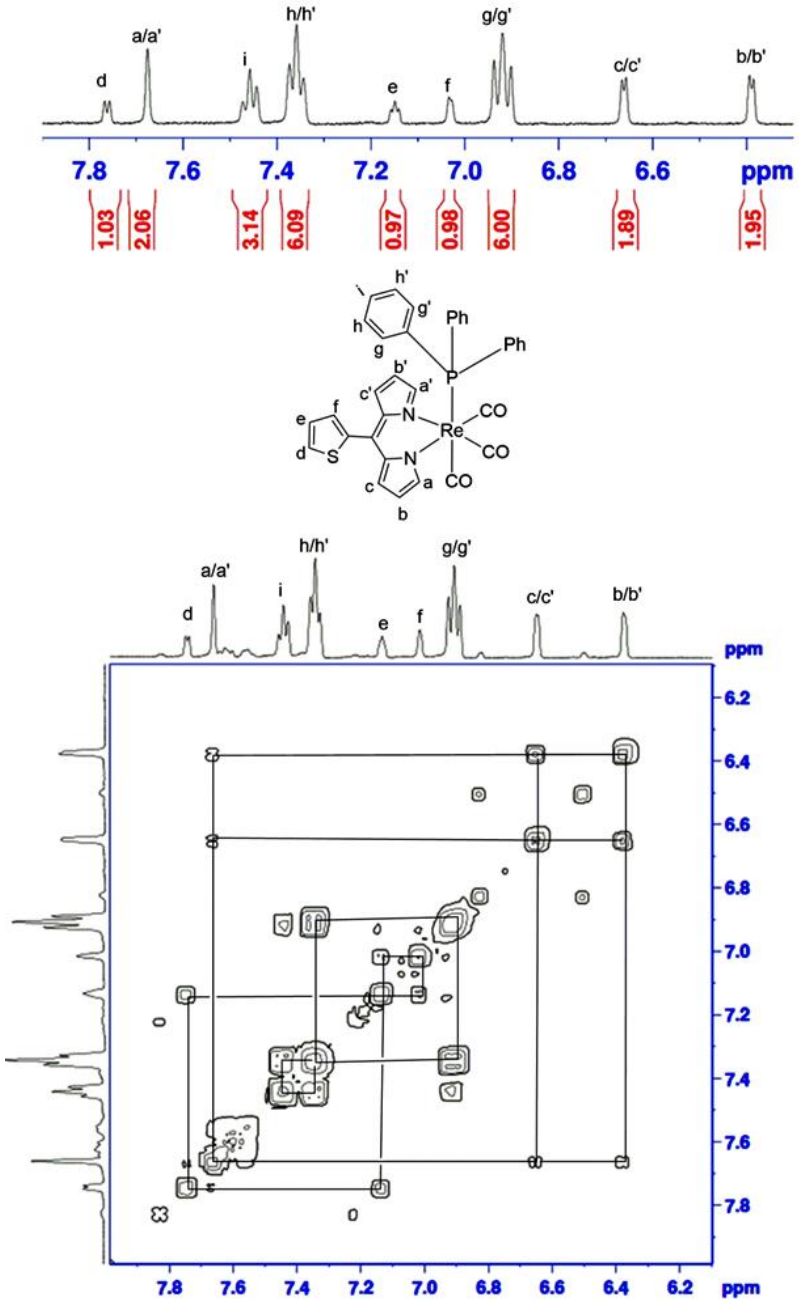


Figure 66. ^{1}H NMR and ^{1}H-^{1}H COSY spectra of compound **Re8** in DMSO

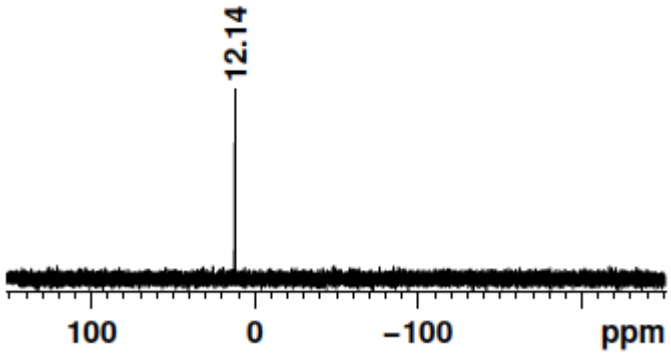


Figure 67. ^{31}P NMR of compound Re**8** in $CDCl_3$

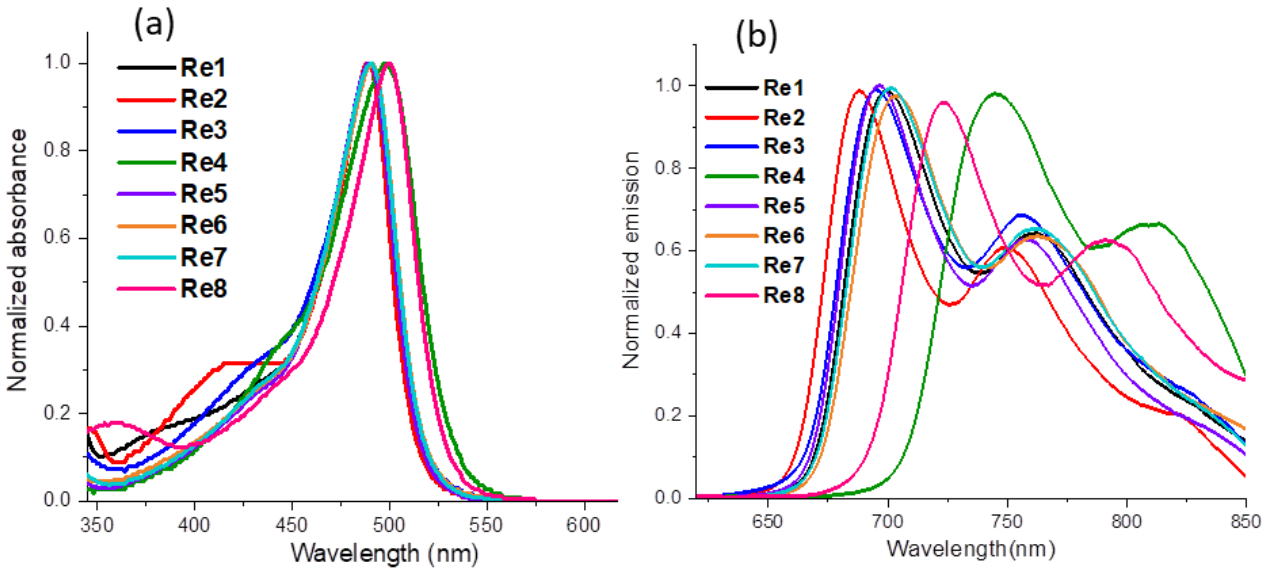


Figure 68. (a) Absorption (b) emission of compound **Re1-Re8** in deoxygenated DCM

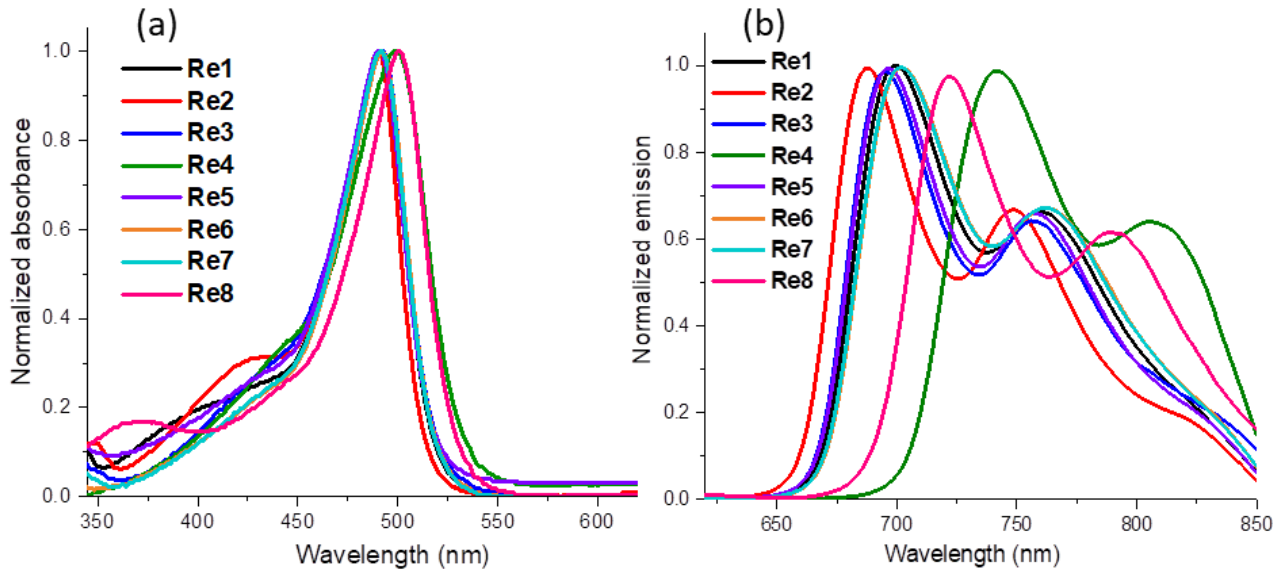


Figure 69. (a) Absorption (b) emission of compound **Re1-Re8** in deoxygenated DMSO

Table S1. Absorption data and phosphorescence data of rhenium dipyrrinates in deoxygenated DCM and DMSO

Complex	λ_{ab} (nm) DCM	λ_{em} (nm) DCM	Stokes shift (cm^{-1}) DCM	ϕ_{em} $\lambda_{ex} = 485nm$ DCM	λ_{ab} (nm) DMSO	λ_{em} (nm) DMSO	Stokes shift (cm^{-1}) DMSO	ϕ_{em} $\lambda_{ex} = 485nm$ DMSO
Re1	491	701, 760	6101	0.001	492	699, 757	6019	0.003
Re2	489	685, 749	5851	0.002	491	687, 747	5810	0.009
Re3	490	694, 760	5998	0.002	493	695, 755	5895	0.001
Re4	498	745, 814	6657	0.001	499	743, 808	6581	0.001
Re5	490	699, 756	6102	0.001	492	696, 757	5957	0.004
Re6	491	705, 760	6182	0.001	492	703, 761	6100	0.003
Re7	491	702, 761	6121	0.002	492	700, 764	6039	0.003
Re8	499	724, 790	6227	0.001	500	723, 790	6168	0.001

Triphenylamine substituted corresponding rhenium dipyrrinate was used as standard [Φ_{PL}=0.5% in DCM][29]

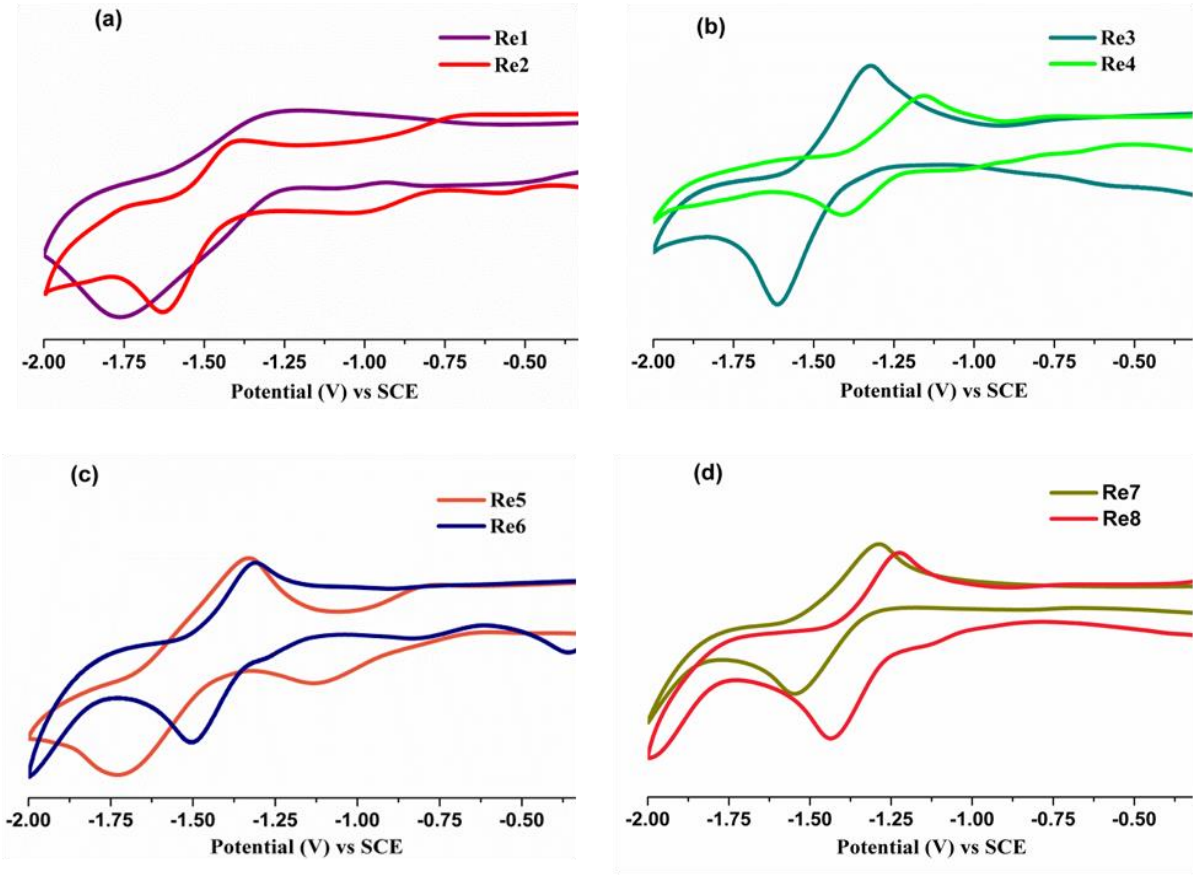


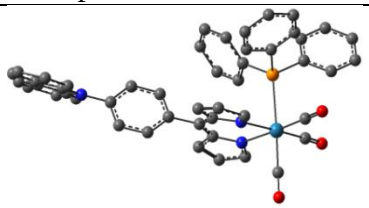
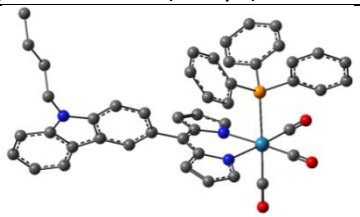
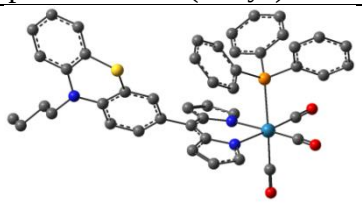
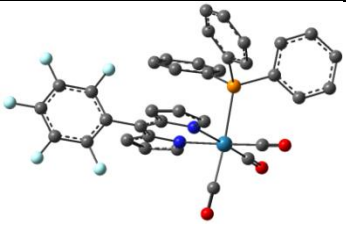
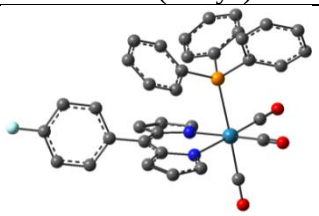
Figure 70. Comparison of the reduction waves of **Re1**–**Re8** in DCM containing 0.1 M TBAP as a supporting electrolyte, recorded at a 50 mV/s scan speed (V *vs.* SCE).

Table S2: Crystallographic parameters of the rhenium dipyrrinates.

Complex	**Re1**	**Re3**	**Re4**
Empirical Formula	$C_{55}H_{49}N_3O_3PRe$	$C_{46}H_{37}N_3O_3PReS$	$C_{36}H_{21}F_5N_2O_3PRe$
Crystal System	Monoclinic	Monoclinic	Monoclinic
Space Group	$P2_1/n$ (#14)	$P2_1/c$ (#14)	$P2_1/n$ (#14)
R_1 ($I > 2.00\sigma(I)$)	0.0568	0.0353	0.0167
${}_wR_2$ (All reflections)	0.1123	0.0694	0.0389
GOF	1.189	1.054	1.054
Lattice Parameters	a = 17.9756(4) Å b = 12.9438(2) Å c = 19.8103(4) Å β = 98.620(2)° V = 4557.25(16) Å^3	a = 23.5467(4) Å b = 12.5757(2) Å c = 12.8889(2) Å β = 90.8795(17)° V = 3816.16(11) Å^3	a = 13.62250(16) Å b = 16.54880(19) Å c = 13.64270(15) Å β = 100.6110(11)° V = 3022.96(6) Å^3
Z	4	4	4
T	-173.0°C	-173.0°C	-173.0°C
D_{calc}	1.482 g/cm^3	1.617 g/cm^3	1.617 g/cm^3
F_{000}	2056.00	1856.00	1640.00
$2\theta_{max}$	56.0°	56.0°	56.0°
No. of Reflections Measured	Total: 76496 Unique: 10991 (R_{int} = 0.0834)	Total: 63430 Unique: 9220 (R_{int} = 0.0754)	Total: 50333 Unique: 7270 (R_{int} = 0.0344)
CCDC number	1475522	1494889	1475523
Complex	**Re5**	**Re6**	**Re7**
Empirical Formula	$C_{36}H_{25}FN_2O_3PRe$	$C_{36}H_{25}FN_2O_3PRe$	$C_{36}H_{25}BrN_2O_3PRe$
Crystal System	Monoclinic	Monoclinic	Monoclinic
Space Group	*Ia* (#9)	*Ia* (#9)	$P2_1/c$ (#14)
R_1 (I>2.00σ(I))	0.0279	0.0294	0.0393
${}_wR_2$ (All reflections)	0.0638	0.0600	0.0737
GOF	1.023	1.018	1.042
Lattice Parameters	a = 17.5172(3) Å b = 8.35500(14) Å c = 19.9929(3) Å β = 94.9322(16)° V = 2915.25(8) Å^3	a = 17.6737(4) Å b = 8.37774(19) Å c = 19.8176(4) Å β = 95.5269(19)° V = 2920.66(11) Å^3	a = 19.1355(3) Å b = 35.4097(5) Å c = 9.05694(14) Å β = 90.2575(14)° V = 6136.76(16) Å^3
Z	4	4	8
T	-173.0°C	-173.0°C	-173.0°C
D_{calc}	1.751 g/cm^3	1.754 g/cm^3	1.798 g/cm^3
F_{000}	1512.00	1512.00	3232.00
$2\theta_{max}$	56.0°	56.0°	56.0°
No. of Reflections Measured	Total: 23602 Unique: 7038 (R_{int} = 0.0471)	Total: 23313 Unique: 7038 (R_{int} = 0.0406)	Total: 87154 Unique: 14722 (R_{int} = 0.0745)

CCDC number	1501525	1501521	1474972

Table S3. DFT-D3 based Geometry optimized structure of **Re1-Re8.**

Compound	Optimized Structure
Re1	 Energy (a.u.): -2658.8635 Dipole Moment (Debye): 6.1262
Re2	 Energy (a.u.): -2585.0719 Dipole Moment (Debye): 9.3462
Re3	 Energy (a.u.): -2983.2369 Dipole Moment (Debye): 7.7314
Re4	 Energy (a.u.): -2638.7058 Dipole Moment (Debye): 6.2425
Re5	 Energy (a.u.): -2241.8104 Dipole Moment (Debye): 6.1295

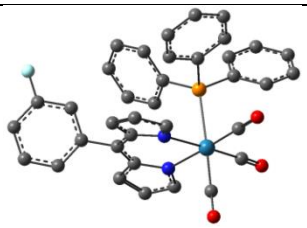
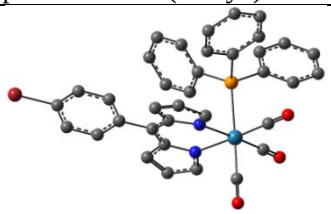
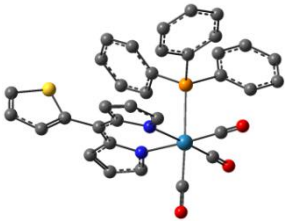
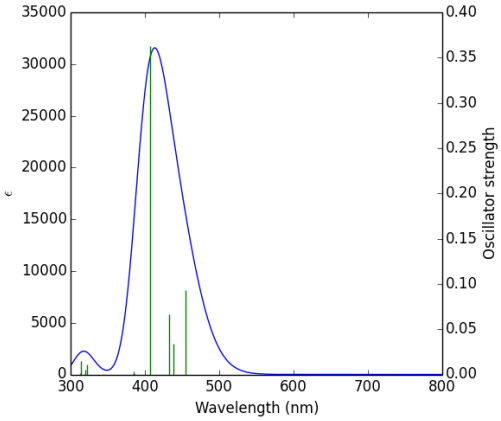
Re6	 Energy (a.u.): -2241.8106 Dipole Moment (Debye): 5.7657
Re7	 Energy (a.u.): -4713.3836 Dipole Moment (Debye): 5.9239
Re8	 Energy (a.u.): -2463.3272 Dipole Moment (Debye): 6.8015

Table S4. Calculated Electronic Excitation Energies and Corresponding Oscillator Strengths of the Low-Lying Singlet Excited States of **Re1-Re8.**

Re1

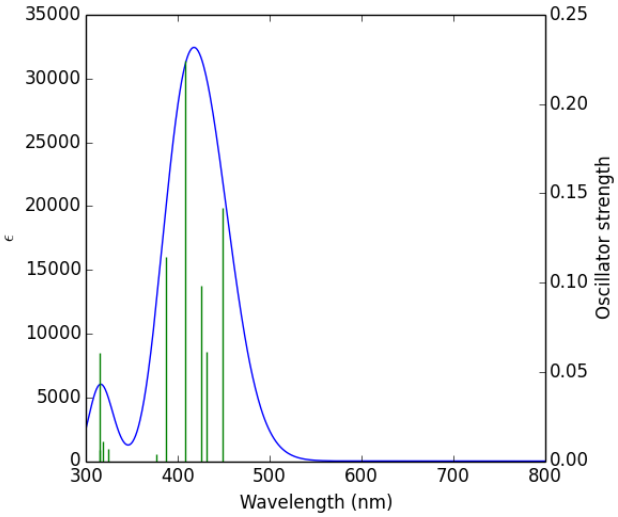
No.	Wavelength (nm)	Osc. Strength	Symmetry	Major contributions
2	438	0.0338	Singlet-A	H-4->LUMO (60%), H-2->LUMO (27%), H-1->LUMO (12%)
3	432	0.0663	Singlet-A	H-4->LUMO (17%), H-2->LUMO (70%), H-1->LUMO (12%)
4	407	0.3623	Singlet-A	H-4->LUMO (23%), H-1->LUMO (71%)
5	386	0.0002	Singlet-A	H-3->LUMO (99%)
6	385	0.0033	Singlet-A	H-5->LUMO (98%)
7	322	0.0106	Singlet-A	H-6->LUMO (97%)
8	319	0.0051	Singlet-A	H-1->L+1 (82%)
9	314	0.0152	Singlet-A	H-2->L+1 (16%), H-1->L+2 (59%)
10	312	0.0017	Singlet-A	H-2->L+1 (39%), H-1->L+2 (30%)



Re2

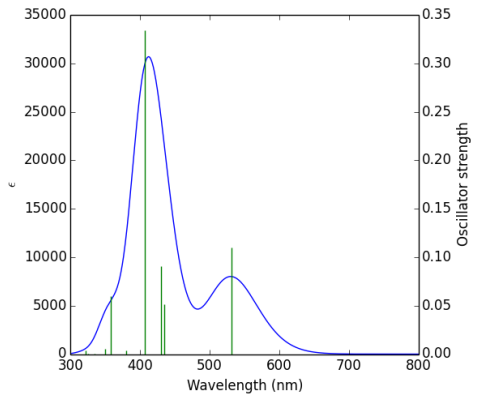
No.	Wavelength (nm)	Osc. Strength	Symmetry	Major contributions
1	448	0.1416	Singlet-A	H-1->LUMO (98%)
2	430	0.0615	Singlet-A	H-3->LUMO (50%), H-2->LUMO (25%), HOMO->LUMO (20%)
3	425	0.0983	Singlet-A	H-2->LUMO (71%), HOMO->LUMO (18%)
4	408	0.2242	Singlet-A	H-3->LUMO (40%), HOMO->LUMO (51%)
5	386	0.1144	Singlet-A	H-4->LUMO (88%)

6	376	0.0037	Singlet-A	H-5->LUMO (99%)
7	324	0.0066	Singlet-A	HOMO->L+1 (93%)
8	318	0.0111	Singlet-A	HOMO->L+2 (29%), HOMO->L+3 (63%)
9	315	0.0608	Singlet-A	H-1->L+2 (72%), H-1->L+3 (10%)
10	314	0.0064	Singlet-A	H-6->LUMO (25%), H-2->L+1 (37%)



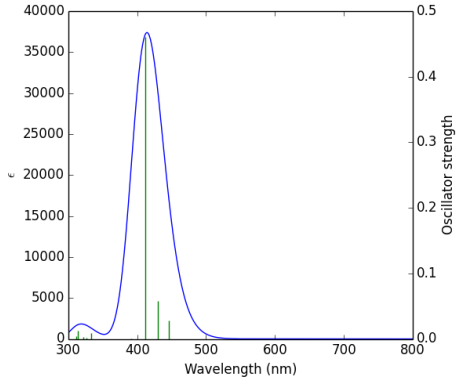
Re3

No.	Wavelength (nm)	Osc. Strength	Symmetry	Major contributions
1	530	0.11	Singlet-A	HOMO->LUMO (99%)
2	434	0.0515	Singlet-A	H-3->LUMO (65%), H-2->LUMO (16%), H-1->LUMO (18%)
3	430	0.091	Singlet-A	H-2->LUMO (81%), H-1->LUMO (12%)
4	407	0.3343	Singlet-A	H-3->LUMO (28%), H-1->LUMO (68%)
5	380	0.0035	Singlet-A	H-4->LUMO (93%)
6	357	0.0595	Singlet-A	H-5->LUMO (88%)
7	349	0.0053	Singlet-A	HOMO->L+4 (94%)
8	334	0.0004	Singlet-A	HOMO->L+1 (64%), HOMO->L+2 (33%)
9	325	0.0006	Singlet-A	HOMO->L+1 (33%), HOMO->L+2 (63%)
10	321	0.0034	Singlet-A	H-1->L+1 (90%)



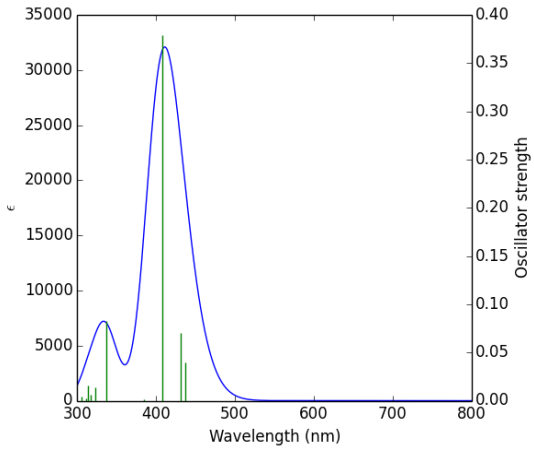
Re4

No.	Wavelength (nm)	Osc. Strength	Symmetry	Major contributions
1	446	0.0277	Singlet-A	H-1->LUMO (89%), HOMO->LUMO (10%)
2	429	0.0581	Singlet-A	H-2->LUMO (98%)
3	412	0.4606	Singlet-A	HOMO->LUMO (89%)
4	391	0.0002	Singlet-A	H-3->LUMO (100%)
5	333	0.009	Singlet-A	H-5->LUMO (19%), H-4->LUMO (79%)
6	326	0.0013	Singlet-A	H-5->LUMO (75%), H-4->LUMO (19%)
7	321	0.0035	Singlet-A	HOMO->L+1 (90%)
8	313	0.0129	Singlet-A	H-6->LUMO (89%)
9	312	0.0007	Singlet-A	H-7->LUMO (72%), HOMO->L+2 (16%)
10	312	0.0036	Singlet-A	H-7->LUMO (15%), HOMO->L+2 (77%)



Re5

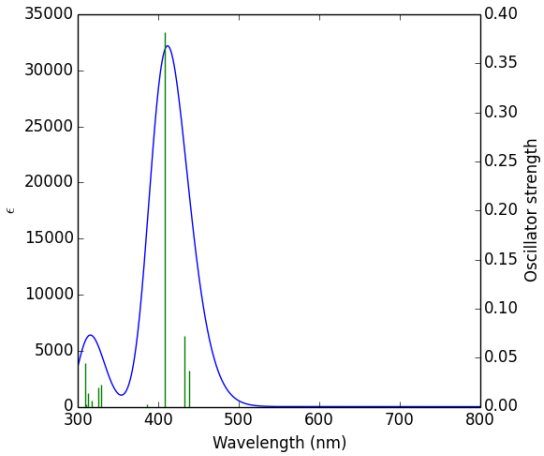
No.	Wavelength (nm)	Osc. Strength	Symmetry	Major contributions
1	437	0.0393	Singlet-A	H-2->LUMO (71%), H-1->LUMO (15%), HOMO->LUMO (14%)
2	431	0.0706	Singlet-A	H-1->LUMO (83%)
3	407	0.3794	Singlet-A	H-2->LUMO (21%), HOMO->LUMO (75%)
4	384	0.0019	Singlet-A	H-3->LUMO (100%)
5	337	0.0823	Singlet-A	H-4->LUMO (88%)
6	323	0.0142	Singlet-A	H-5->LUMO (88%)
7	317	0.0066	Singlet-A	HOMO->L+1 (90%)
8	313	0.0155	Singlet-A	HOMO->L+2 (82%)
9	311	0.0021	Singlet-A	H-1->L+1 (50%), H-1->L+2 (10%), HOMO->L+2 (15%)
10	305	0.004	Singlet-A	H-8->LUMO (50%), H-7->LUMO (30%)



Re6

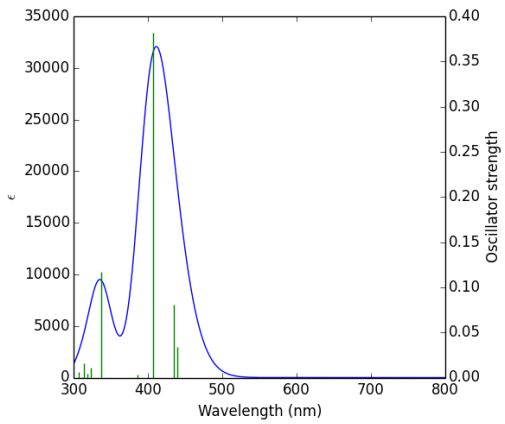
No.	Wavelength (nm)	Osc. Strength	Symmetry	Major contributions
1	438	0.0368	Singlet-A	H-2->LUMO (68%), H-1->LUMO (18%), HOMO->LUMO (14%)
2	432	0.0721	Singlet-A	H-2->LUMO (11%), H-1->LUMO (80%)
3	407	0.3821	Singlet-A	H-2->LUMO (21%), HOMO->LUMO (76%)
4	385	0.0021	Singlet-A	H-3->LUMO (100%)
5	328	0.022	Singlet-A	H-5->LUMO (93%)
6	324	0.0198	Singlet-A	H-4->LUMO (93%)
7	316	0.0065	Singlet-A	HOMO->L+1 (90%)
8	312	0.0134	Singlet-A	HOMO->L+2 (82%)
9	310	0.002	Singlet-A	H-1->L+1 (48%), H-1->L+2 (13%), HOMO->L+2

				(15%)
10	308	0.0445	Singlet-A	H-10->LUMO (12%), H-9->LUMO (28%), H-6->LUMO (51%)



Re7

No.	Wavelength (nm)	Osc. Strength	Symmetry	Major contributions
1	439	0.0344	Singlet-A	H-2->LUMO (64%), H-1->LUMO (23%), HOMO->LUMO (13%)
2	434	0.081	Singlet-A	H-2->LUMO (14%), H-1->LUMO (75%), HOMO->LUMO (11%)
3	407	0.3821	Singlet-A	H-2->LUMO (22%), HOMO->LUMO (75%)
4	386	0.0037	Singlet-A	H-3->LUMO (99%)
5	337	0.1175	Singlet-A	H-4->LUMO (98%)
6	323	0.011	Singlet-A	H-5->LUMO (98%)
7	318	0.0046	Singlet-A	HOMO->L+1 (91%)
8	313	0.0156	Singlet-A	H-1->L+1 (23%), H-1->L+2 (10%), HOMO->L+2 (51%)
9	311	0.0004	Singlet-A	H-1->L+1 (32%), HOMO->L+2 (46%)
10	306	0.006	Singlet-A	H-8->LUMO (36%), H-7->LUMO (16%), H-6->LUMO (31%)



Re8

No.	Wavelength (nm)	Osc. Strength	Symmetry	Major contributions
1	447	0.0253	Singlet-A	H-2->LUMO (65%), H-1->LUMO (25%)
2	440	0.0722	Singlet-A	H-2->LUMO (18%), H-1->LUMO (74%)
3	415	0.3933	Singlet-A	H-2->LUMO (16%), HOMO->LUMO (81%)
4	390	0.0065	Singlet-A	H-3->LUMO (99%)
5	373	0.1037	Singlet-A	H-4->LUMO (98%)
6	330	0.0084	Singlet-A	H-5->LUMO (97%)
7	321	0.0013	Singlet-A	H-9->LUMO (15%), H-6->LUMO (74%)
8	320	0.0035	Singlet-A	HOMO->L+1 (88%)
9	313	0.0086	Singlet-A	H-2->L+1 (11%), H-1->L+1 (58%)
10	313	0.0052	Singlet-A	H-7->LUMO (89%)

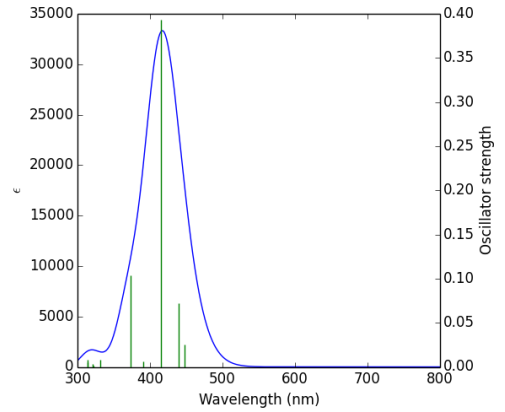


Table S5. Triplet state energies (E_T) of **Re1-Re8.**

Compound	E_T (Ev) calculated	E_T (Ev) Experimental
Re1	1.77	1.79
Re2	1.81	1.82
Re3	1.78	1.80
Re4	1.64	1.68
Re5	1.78	1.79
Re6	1.77	1.77
Re7	1.77	1.78
Re8	1.70	1.72

Table S6. B3LYP/6-31G//B3LYP/SDD gas phase optimized coordinates of complexes **Re1-Re8.**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	75	0	3.032447	-0.647518	-1.305160
2	15	0	2.769744	0.530599	0.959032
3	8	0	5.238455	-2.414239	-0.011721
4	8	0	3.260823	-2.194124	-4.001239
5	8	0	5.092534	1.457226	-2.295852
6	7	0	1.422981	-2.014934	-0.670773
7	7	0	1.366309	0.515568	-2.144733
8	7	0	-6.182838	-0.030100	-0.057886
9	6	0	1.619640	-3.234297	-0.144908
10	1	0	2.614369	-3.653347	-0.079185
11	6	0	0.407402	-3.808673	0.307577
12	1	0	0.298593	-4.779074	0.771718
13	6	0	-0.579934	-2.875100	0.053934
14	1	0	-1.633716	-2.959574	0.272881
15	6	0	0.048450	-1.756964	-0.585225
16	6	0	-0.593632	-0.621500	-1.108706
17	6	0	0.000513	0.399757	-1.869749
18	6	0	-0.694291	1.426953	-2.582854
19	1	0	-1.764133	1.574137	-2.576382
20	6	0	0.252075	2.143467	-3.292678
21	1	0	0.089462	2.981842	-3.956025
22	6	0	1.501107	1.548830	-2.994199
23	1	0	2.477299	1.842155	-3.356374
24	6	0	-2.058359	-0.485240	-0.854066
25	6	0	-2.518534	0.578562	-0.063975
26	1	0	-1.805062	1.283052	0.346964
27	6	0	-3.874782	0.720992	0.214024

28	1	0	-4.221585	1.524770	0.854641
29	6	0	-4.799688	-0.181402	-0.326907
30	6	0	-4.350893	-1.232325	-1.137328
31	1	0	-5.071550	-1.913453	-1.576777
32	6	0	-2.989179	-1.389029	-1.385191
33	1	0	-2.644272	-2.204817	-2.012088
34	6	0	-7.032688	-1.024138	0.441525
35	6	0	-6.739774	-2.339930	0.811825
36	1	0	-5.736075	-2.739549	0.720069
37	6	0	-7.783257	-3.119184	1.309412
38	1	0	-7.582134	-4.145452	1.602485
39	6	0	-9.085940	-2.604596	1.441584
40	1	0	-9.875762	-3.240043	1.830396
41	6	0	-9.368022	-1.288331	1.083976
42	1	0	-10.370713	-0.885693	1.195625
43	6	0	-8.337268	-0.484641	0.582714
44	6	0	-8.271203	0.894352	0.147641
45	6	0	-9.220322	1.918027	0.043883
46	1	0	-10.250976	1.740106	0.337207
47	6	0	-8.823877	3.160783	-0.444443
48	1	0	-9.548784	3.964640	-0.528772
49	6	0	-7.491250	3.384189	-0.836111
50	1	0	-7.204381	4.357573	-1.223206
51	6	0	-6.527012	2.381614	-0.742251
52	1	0	-5.503693	2.557141	-1.054616
53	6	0	-6.928261	1.141025	-0.237846
54	6	0	1.313781	1.628504	1.210017
55	6	0	0.499978	1.591817	2.351919
56	1	0	0.677001	0.856853	3.128489
57	6	0	-0.541005	2.511419	2.505164
58	1	0	-1.164837	2.470069	3.393042
59	6	0	-0.776480	3.478886	1.526096
60	1	0	-1.588051	4.190328	1.646791
61	6	0	0.034366	3.524255	0.388559
62	1	0	-0.144603	4.264855	-0.384519
63	6	0	1.072615	2.607769	0.233034
64	1	0	1.693156	2.652540	-0.653956
65	6	0	4.180384	1.636698	1.394907
66	6	0	3.987724	2.820918	2.123310
67	1	0	2.989245	3.123130	2.419520
68	6	0	5.077153	3.621435	2.470201
69	1	0	4.911896	4.538554	3.027901
70	6	0	6.371502	3.246019	2.104974
71	1	0	7.217368	3.871331	2.374784
72	6	0	6.573921	2.063158	1.391106
73	1	0	7.576537	1.761194	1.103757
74	6	0	5.486070	1.265837	1.034090
75	1	0	5.658792	0.350832	0.480096
76	6	0	2.720312	-0.675689	2.348864
77	6	0	3.821543	-0.867196	3.197120

78	1	0	4.707745	-0.251128	3.094147
79	6	0	3.787078	-1.853448	4.185084
80	1	0	4.647279	-1.990204	4.833755
81	6	0	2.654400	-2.654128	4.342764
82	1	0	2.630087	-3.419574	5.112806
83	6	0	1.553507	-2.466201	3.504324
84	1	0	0.668759	-3.086573	3.609882
85	6	0	1.587504	-1.489991	2.509539
86	1	0	0.726538	-1.364524	1.863225
87	6	0	4.417601	-1.746409	-0.502515
88	6	0	3.175813	-1.616545	-2.999403
89	6	0	4.335687	0.661045	-1.906233

Re2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.355085	-0.709333	-0.419009
2	6	0	2.697596	0.571655	-0.909768
3	6	0	4.020180	0.993529	-0.996825
4	6	0	5.019919	0.098191	-0.601290
5	6	0	4.698316	-1.196598	-0.107612
6	6	0	3.362415	-1.593498	-0.017946
7	1	0	1.902453	1.241250	-1.215618
8	1	0	4.256304	1.989005	-1.358164
9	1	0	3.102806	-2.581054	0.350287
10	6	0	6.977969	-0.903502	-0.097242
11	6	0	8.328313	-1.198944	0.115057
12	6	0	8.641975	-2.455388	0.632073
13	6	0	7.640704	-3.396126	0.936335
14	6	0	6.296225	-3.094200	0.730495
15	6	0	5.954377	-1.839516	0.213494
16	1	0	9.108558	-0.478601	-0.107769
17	1	0	9.683397	-2.710231	0.805900
18	1	0	7.921336	-4.365034	1.337774
19	1	0	5.522290	-3.818384	0.968584
20	7	0	6.397446	0.252699	-0.609507
21	6	0	7.107476	1.471668	-0.962782
22	1	0	8.084111	1.190187	-1.369795
23	1	0	6.561828	1.959147	-1.777642
24	6	0	7.275625	2.433691	0.220111
25	1	0	6.283076	2.685947	0.614916
26	1	0	7.810073	1.914377	1.025756
27	6	0	8.025517	3.711374	-0.169560
28	1	0	7.488313	4.212270	-0.986535
29	1	0	9.012410	3.444304	-0.571396
30	6	0	8.193387	4.679863	1.005297

31	1	0	8.730853	5.584645	0.703825
32	1	0	7.219832	4.985582	1.404906
33	1	0	8.754724	4.212959	1.822465
34	6	0	0.912957	-1.084329	-0.345333
35	6	0	0.372695	-1.353332	0.926525
36	6	0	0.225797	-1.158827	-1.571723
37	6	0	-1.368905	-1.513016	-3.046509
38	1	0	-2.365712	-1.703158	-3.421185
39	6	0	0.824734	-1.115419	-2.869182
40	1	0	1.876310	-0.964718	-3.062344
41	6	0	-0.180173	-1.342054	-3.793234
42	1	0	-0.091763	-1.396644	-4.869683
43	6	0	1.093781	-1.431275	2.161800
44	1	0	2.146486	-1.226552	2.284229
45	6	0	-1.057739	-1.948031	2.492587
46	1	0	-2.010001	-2.197952	2.939955
47	6	0	0.196398	-1.828763	3.136314
48	1	0	0.390612	-1.999157	4.186227
49	75	0	-2.697502	-1.490332	-0.175607
50	6	0	-4.111235	-1.304746	-1.493609
51	6	0	-3.981175	-1.554033	1.280260
52	8	0	-4.934984	-1.208690	-2.313010
53	8	0	-4.741608	-1.587906	2.164561
54	6	0	-2.734843	-3.438285	-0.361217
55	8	0	-2.758061	-4.592817	-0.467425
56	15	0	-2.570244	1.047182	0.159163
57	6	0	-2.413553	1.497941	1.937563
58	6	0	-3.491465	2.027478	2.663087
59	6	0	-1.211097	1.221970	2.608171
60	6	0	-3.366461	2.273371	4.032049
61	1	0	-4.429730	2.250791	2.167968
62	6	0	-1.087673	1.478385	3.973000
63	1	0	-0.365959	0.810788	2.068474
64	6	0	-2.166003	2.000649	4.690494
65	1	0	-4.209699	2.682496	4.580737
66	1	0	-0.150488	1.253507	4.472863
67	1	0	-2.071733	2.192861	5.755256
68	6	0	-4.089972	1.946385	-0.378121
69	6	0	-4.024727	3.235098	-0.930284
70	6	0	-5.348464	1.353961	-0.183096
71	6	0	-5.192693	3.908875	-1.290903
72	1	0	-3.064207	3.715356	-1.080786
73	6	0	-6.514524	2.034091	-0.535412
74	1	0	-5.423715	0.363726	0.250310
75	6	0	-6.439285	3.310963	-1.095519
76	1	0	-5.126055	4.903017	-1.723057
77	1	0	-7.479022	1.560913	-0.377698
78	1	0	-7.346616	3.836693	-1.377870
79	6	0	-1.234018	1.979481	-0.697855
80	6	0	-0.437229	2.945117	-0.065635

81	6	0	-1.074595	1.759682	-2.075612
82	6	0	0.506347	3.669681	-0.798274
83	1	0	-0.552469	3.142042	0.993834
84	6	0	-0.134425	2.485798	-2.804496
85	1	0	-1.680443	1.016648	-2.580569
86	6	0	0.659344	3.443752	-2.167563
87	1	0	1.118831	4.412191	-0.295419
88	1	0	-0.016147	2.291938	-3.865917
89	1	0	1.395061	4.006870	-2.734237
90	7	0	-1.142349	-1.400605	-1.725383
91	7	0	-0.969906	-1.662971	1.183017

Re3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	75	0	-3.039755	-1.410731	-0.442791
2	16	0	4.335604	2.218204	-1.255952
3	15	0	-2.664144	0.975048	0.417309
4	8	0	-5.087676	-1.814144	1.859983
5	8	0	-5.228776	-0.449749	-2.427086
6	8	0	-3.410869	-4.354677	-1.397194
7	7	0	-1.473109	-1.149231	-1.963468
8	7	0	-1.345450	-2.049140	0.817116
9	7	0	6.211014	-0.105672	-0.549635
10	6	0	-1.698716	-0.956728	-3.275132
11	1	0	-2.706168	-0.966486	-3.669070
12	6	0	-0.493412	-0.740660	-3.983476
13	1	0	-0.402451	-0.572656	-5.047854
14	6	0	0.520865	-0.805252	-3.044921
15	1	0	1.583162	-0.712419	-3.215540
16	6	0	-0.089815	-1.070785	-1.779130
17	6	0	0.590661	-1.328460	-0.575067
18	6	0	0.022159	-1.823897	0.613216
19	6	0	0.725726	-2.238090	1.789964
20	1	0	1.792881	-2.169077	1.936870
21	6	0	-0.212220	-2.746615	2.669993
22	1	0	-0.041889	-3.158649	3.655025
23	6	0	-1.468508	-2.599765	2.035960
24	1	0	-2.443448	-2.845404	2.434119
25	6	0	2.054982	-1.053644	-0.574325
26	6	0	2.499699	0.260511	-0.775554
27	1	0	1.773496	1.046696	-0.943362
28	6	0	3.856598	0.568892	-0.790531
29	6	0	4.836944	-0.423651	-0.561532
30	6	0	4.375736	-1.741370	-0.375959
31	1	0	5.074215	-2.551786	-0.223230

32	6	0	3.016525	-2.050114	-0.390144
33	1	0	2.705526	-3.080845	-0.255295
34	6	0	5.872230	2.328251	-0.366542
35	6	0	6.671630	1.179821	-0.173747
36	6	0	7.947617	1.372466	0.387954
37	1	0	8.608688	0.532383	0.548321
38	6	0	8.399487	2.642995	0.748896
39	1	0	9.394936	2.745788	1.170204
40	6	0	7.583282	3.759391	0.589157
41	1	0	7.924135	4.747026	0.882241
42	6	0	6.313072	3.589610	0.037189
43	1	0	5.660451	4.445546	-0.108844
44	6	0	7.182368	-1.206173	-0.601166
45	1	0	8.102994	-0.808616	-1.038866
46	1	0	6.806692	-1.942388	-1.318455
47	6	0	7.497675	-1.898062	0.738110
48	1	0	6.579303	-2.301110	1.178043
49	1	0	7.872133	-1.165561	1.460958
50	6	0	8.524029	-3.022980	0.562128
51	1	0	8.140783	-3.753724	-0.163089
52	1	0	9.442692	-2.610495	0.122967
53	6	0	8.855417	-3.730077	1.879727
54	1	0	7.958184	-4.178046	2.321565
55	1	0	9.268045	-3.025500	2.610691
56	1	0	9.590024	-4.528049	1.731683
57	6	0	-1.257674	1.934492	-0.282446
58	6	0	-1.158320	2.000767	-1.681517
59	1	0	-1.859016	1.453730	-2.301261
60	6	0	-0.156654	2.758993	-2.285140
61	1	0	-0.084822	2.784418	-3.367891
62	6	0	0.757502	3.466093	-1.499314
63	1	0	1.546582	4.046640	-1.966807
64	6	0	0.662050	3.410693	-0.107321
65	1	0	1.373459	3.952068	0.508663
66	6	0	-0.341367	2.652241	0.500651
67	1	0	-0.407707	2.627968	1.582178
68	6	0	-2.435007	1.029850	2.243074
69	6	0	-1.260638	0.499951	2.801393
70	1	0	-0.474132	0.118550	2.160640
71	6	0	-1.089557	0.463428	4.184553
72	1	0	-0.174901	0.047559	4.595889
73	6	0	-2.093404	0.940986	5.029998
74	1	0	-1.962442	0.905516	6.107555
75	6	0	-3.266832	1.463140	4.482861
76	1	0	-4.052189	1.839080	5.132000
77	6	0	-3.437975	1.511692	3.097802
78	1	0	-4.352845	1.926735	2.690251
79	6	0	-4.095744	2.104896	0.131759
80	6	0	-3.907720	3.470011	-0.135525
81	1	0	-2.905530	3.877946	-0.207963

82	6	0	-5.005740	4.313324	-0.311938
83	1	0	-4.844006	5.365874	-0.525170
84	6	0	-6.303926	3.808681	-0.213595
85	1	0	-7.156890	4.466221	-0.353021
86	6	0	-6.500784	2.454707	0.064884
87	1	0	-7.506118	2.052431	0.145612
88	6	0	-5.405191	1.607152	0.232415
89	1	0	-5.576326	0.559411	0.448412
90	6	0	-4.326804	-1.661971	0.988632
91	6	0	-4.422071	-0.803435	-1.663518
92	6	0	-3.271841	-3.258986	-1.043939

Re4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	75	0	1.243432	-1.617591	-0.249701
2	15	0	2.046092	0.767858	0.091067
3	9	0	-3.034121	2.258650	-0.225546
4	9	0	-5.626427	3.021791	-0.102869
5	9	0	-7.589804	1.151983	0.226808
6	9	0	-6.941686	-1.490238	0.429302
7	9	0	-4.346465	-2.263864	0.299373
8	8	0	3.307015	-2.688343	1.809946
9	8	0	0.042528	-4.472562	-0.653416
10	8	0	3.194959	-2.042038	-2.630604
11	7	0	-0.268969	-1.258549	1.315513
12	7	0	-0.299518	-0.831835	-1.618897
13	6	0	-0.100520	-1.497311	2.624034
14	1	0	0.831300	-1.895985	2.998393
15	6	0	-1.257088	-1.164012	3.373276
16	1	0	-1.367367	-1.256001	4.444755
17	6	0	-2.185640	-0.706215	2.460667
18	1	0	-3.190534	-0.361709	2.659408
19	6	0	-1.573793	-0.772600	1.167553
20	6	0	-2.187777	-0.460817	-0.050876
21	6	0	-1.628487	-0.500974	-1.332799
22	6	0	-2.286389	-0.151357	-2.554444
23	1	0	-3.320246	0.150440	-2.643150
24	6	0	-1.352046	-0.264563	-3.564470
25	1	0	-1.487746	-0.072115	-4.619563
26	6	0	-0.148873	-0.684046	-2.943714
27	1	0	0.802991	-0.878285	-3.418268
28	6	0	-3.618093	-0.027680	0.027677
29	6	0	-3.980586	1.315100	-0.071948
30	6	0	-5.308963	1.725499	-0.007090
31	6	0	-6.310956	0.772359	0.162636

32	6	0	-5.978430	-0.576738	0.267257
33	6	0	-4.641483	-0.960850	0.199324
34	6	0	1.649277	1.488412	1.740594
35	6	0	2.100209	0.770431	2.860931
36	1	0	2.638203	-0.162507	2.726922
37	6	0	1.874514	1.250991	4.149066
38	1	0	2.228114	0.682689	5.004204
39	6	0	1.189023	2.454084	4.337348
40	1	0	1.005655	2.825820	5.341077
41	6	0	0.749299	3.179616	3.229862
42	1	0	0.228094	4.122574	3.366731
43	6	0	0.982555	2.704741	1.936093
44	1	0	0.650555	3.292781	1.088625
45	6	0	1.351658	1.908378	-1.165994
46	6	0	-0.012893	2.234223	-1.118400
47	1	0	-0.629299	1.891492	-0.297175
48	6	0	-0.596228	2.987216	-2.135024
49	1	0	-1.654625	3.218213	-2.080286
50	6	0	0.174618	3.418366	-3.217283
51	1	0	-0.280279	4.001943	-4.012269
52	6	0	1.529778	3.088623	-3.278583
53	1	0	2.134094	3.416241	-4.119448
54	6	0	2.117959	2.334122	-2.260713
55	1	0	3.171240	2.081502	-2.322009
56	6	0	3.861527	1.070359	0.019911
57	6	0	4.344186	2.372342	0.244778
58	1	0	3.646756	3.180035	0.446940
59	6	0	5.711593	2.633472	0.212591
60	1	0	6.071980	3.643237	0.385203
61	6	0	6.617217	1.596425	-0.036167
62	1	0	7.683785	1.799808	-0.057718
63	6	0	6.147525	0.301422	-0.251571
64	1	0	6.844404	-0.509587	-0.440321
65	6	0	4.774824	0.038090	-0.224268
66	1	0	4.425588	-0.972634	-0.388303
67	6	0	2.539469	-2.288958	1.026517
68	6	0	0.489357	-3.414399	-0.506645
69	6	0	2.478398	-1.881282	-1.725040

Re5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	75	0	-1.134922	-1.590363	0.037146
2	15	0	-1.281585	0.970989	-0.099492
3	9	0	7.610734	1.324452	0.033936
4	8	0	-3.393381	-1.487668	2.169035
5	8	0	-3.161790	-1.986146	-2.284732

6	8	0	-0.869048	-4.674757	0.389259
7	7	0	0.559901	-1.646964	-1.375177
8	7	0	0.449829	-1.275539	1.529083
9	6	0	0.463602	-1.995062	-2.669970
10	1	0	-0.468459	-2.365588	-3.074936
11	6	0	1.682216	-1.780859	-3.358006
12	1	0	1.864991	-1.981728	-4.404718
13	6	0	2.566019	-1.268158	-2.425682
14	1	0	3.592698	-0.974663	-2.585070
15	6	0	1.872078	-1.204349	-1.176859
16	6	0	2.407197	-0.801193	0.056553
17	6	0	1.772521	-0.872929	1.308244
18	6	0	2.406298	-0.690475	2.579856
19	1	0	3.436154	-0.397723	2.722947
20	6	0	1.472551	-1.003736	3.550413
21	1	0	1.601623	-0.992264	4.623846
22	6	0	0.286212	-1.351257	2.859096
23	1	0	-0.669966	-1.628051	3.281778
24	6	0	3.798872	-0.257083	0.049916
25	6	0	4.003034	1.105570	0.314269
26	1	0	3.148769	1.745454	0.507140
27	6	0	5.287423	1.647461	0.304333
28	1	0	5.462366	2.700556	0.494886
29	6	0	6.363008	0.806694	0.039933
30	6	0	6.196612	-0.549276	-0.219119
31	1	0	7.064331	-1.169296	-0.414991
32	6	0	4.905047	-1.076231	-0.216366
33	1	0	4.752261	-2.131591	-0.417283
34	6	0	0.101582	1.901647	-0.879375
35	6	0	0.564658	1.458038	-2.127409
36	1	0	0.133403	0.575804	-2.585336
37	6	0	1.591008	2.135749	-2.783995
38	1	0	1.948294	1.763760	-3.738973
39	6	0	2.166410	3.268650	-2.205443
40	1	0	2.973986	3.789427	-2.711308
41	6	0	1.696988	3.731070	-0.974180
42	1	0	2.130257	4.618765	-0.522673
43	6	0	0.667278	3.056025	-0.314907
44	1	0	0.309142	3.432765	0.635992
45	6	0	-1.451321	1.705189	1.581659
46	6	0	-0.342264	1.696610	2.443959
47	1	0	0.616062	1.327811	2.097850
48	6	0	-0.457499	2.172951	3.749015
49	1	0	0.411472	2.155557	4.399829
50	6	0	-1.683115	2.653056	4.216336
51	1	0	-1.773816	3.018390	5.235038
52	6	0	-2.790748	2.661475	3.366812
53	1	0	-3.746843	3.036720	3.719670
54	6	0	-2.677774	2.192849	2.056097
55	1	0	-3.547686	2.212386	1.409342

56	6	0	-2.762186	1.586955	-1.008600
57	6	0	-3.990938	0.924411	-0.850726
58	1	0	-4.060653	0.049503	-0.214453
59	6	0	-5.134488	1.387901	-1.501354
60	1	0	-6.076471	0.864796	-1.367233
61	6	0	-5.063821	2.511555	-2.327805
62	1	0	-5.952033	2.866344	-2.842109
63	6	0	-3.846866	3.176036	-2.490562
64	1	0	-3.784518	4.051663	-3.130005
65	6	0	-2.703023	2.721842	-1.831684
66	1	0	-1.766123	3.251960	-1.962660
67	6	0	-2.551045	-1.524928	1.363055
68	6	0	-2.418833	-1.829210	-1.400584
69	6	0	-0.967913	-3.527377	0.252843

Re6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	75	0	1.155231	-1.580132	0.045664
2	15	0	1.183494	0.985690	-0.109066
3	8	0	3.205605	-1.897273	-2.267412
4	8	0	3.398594	-1.347625	2.183493
5	8	0	1.042486	-4.670908	0.421093
6	7	0	-0.446591	-1.333494	1.534259
7	7	0	-0.529292	-1.728033	-1.371080
8	6	0	-0.285183	-1.384547	2.865254
9	1	0	0.679564	-1.618023	3.294677
10	6	0	-1.486623	-1.071362	3.548449
11	1	0	-1.619222	-1.049327	4.621270
12	6	0	-2.427263	-0.804084	2.571243
13	1	0	-3.467254	-0.544399	2.705820
14	6	0	-1.782556	-0.982942	1.304769
15	6	0	-2.413511	-0.955553	0.051688
16	6	0	-1.862212	-1.351811	-1.175761
17	6	0	-2.554427	-1.464390	-2.421768
18	1	0	-3.597251	-1.232031	-2.578279
19	6	0	-1.645580	-1.937048	-3.351121
20	1	0	-1.819010	-2.158399	-4.395286
21	6	0	-0.416027	-2.080568	-2.663244
22	1	0	0.533622	-2.405249	-3.066646
23	6	0	-3.823553	-0.456726	0.027829
24	6	0	-4.047237	0.917004	0.184679
25	1	0	-3.224728	1.609754	0.316023
26	6	0	-5.351491	1.390739	0.137608
27	9	0	-5.560445	2.719955	0.271722
28	6	0	-6.445220	0.551362	-0.042800

29	1	0	-7.445446	0.969343	-0.068207
30	6	0	-6.210588	-0.817490	-0.188438
31	1	0	-7.049178	-1.492776	-0.326902
32	6	0	-4.909108	-1.323107	-0.158390
33	1	0	-4.729403	-2.386374	-0.277202
34	6	0	-0.239989	1.863784	-0.878498
35	6	0	-0.816866	3.018039	-0.323942
36	1	0	-0.447813	3.417967	0.613210
37	6	0	-1.871553	3.662182	-0.974365
38	1	0	-2.315337	4.547478	-0.528854
39	6	0	-2.356732	3.167720	-2.187132
40	1	0	-3.185392	3.662857	-2.684418
41	6	0	-1.772053	2.034746	-2.755856
42	1	0	-2.141358	1.638311	-3.696367
43	6	0	-0.719175	1.388593	-2.108684
44	1	0	-0.277578	0.508991	-2.561282
45	6	0	2.634347	1.657011	-1.027756
46	6	0	2.523723	2.776741	-1.866217
47	1	0	1.564356	3.263460	-2.002641
48	6	0	3.645343	3.272141	-2.533759
49	1	0	3.543037	4.135435	-3.184707
50	6	0	4.890794	2.664534	-2.365034
51	1	0	5.761565	3.051409	-2.885973
52	6	0	5.012362	1.555959	-1.524232
53	1	0	5.976670	1.076481	-1.385727
54	6	0	3.891611	1.050996	-0.865016
55	1	0	4.001612	0.187215	-0.219089
56	6	0	1.332461	1.726778	1.571197
57	6	0	2.544202	2.248744	2.046602
58	1	0	3.412969	2.295999	1.399748
59	6	0	2.643797	2.716625	3.358676
60	1	0	3.588556	3.118878	3.712320
61	6	0	1.537252	2.672964	4.208526
62	1	0	1.617575	3.037707	5.228303
63	6	0	0.325931	2.158975	3.739924
64	1	0	-0.542098	2.114887	4.390708
65	6	0	0.224197	1.683462	2.433444
66	1	0	-0.723731	1.288978	2.086426
67	6	0	2.453474	-1.767453	-1.386713
68	6	0	2.561866	-1.433765	1.375587
69	6	0	1.084298	-3.521003	0.276435

Re7

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	75	0	1.797728	-1.525617	-0.193340

2	35	0	-7.737081	0.702748	0.080226
3	15	0	1.745989	1.026160	0.064344
4	8	0	4.040005	-1.578848	1.958323
5	8	0	1.788323	-4.637547	-0.368796
6	8	0	3.836227	-1.360988	-2.532163
7	7	0	0.198517	-1.614872	1.320956
8	7	0	0.109841	-1.472241	-1.604086
9	6	0	0.393526	-1.858814	2.626227
10	1	0	1.376886	-2.109289	2.999764
11	6	0	-0.801214	-1.703225	3.370131
12	1	0	-0.907209	-1.839984	4.437341
13	6	0	-1.774109	-1.327699	2.463072
14	1	0	-2.812503	-1.112635	2.666246
15	6	0	-1.157425	-1.295871	1.169778
16	6	0	-1.799394	-1.063415	-0.058117
17	6	0	-1.233426	-1.191237	-1.337531
18	6	0	-1.946891	-1.168855	-2.577328
19	1	0	-3.007307	-0.993285	-2.682355
20	6	0	-1.035268	-1.451379	-3.578167
21	1	0	-1.220965	-1.535463	-4.640130
22	6	0	0.212847	-1.630695	-2.934885
23	1	0	1.167326	-1.855417	-3.391696
24	6	0	-3.237140	-0.659568	-0.012629
25	6	0	-3.599796	0.624034	-0.444676
26	1	0	-2.835217	1.302244	-0.805804
27	6	0	-4.930853	1.036950	-0.412562
28	1	0	-5.204775	2.033338	-0.740278
29	6	0	-5.904707	0.149351	0.044054
30	6	0	-5.570540	-1.135632	0.470450
31	1	0	-6.340247	-1.816463	0.815243
32	6	0	-4.233600	-1.532933	0.442873
33	1	0	-3.962944	-2.531416	0.770569
34	6	0	0.347594	1.959710	-0.685164
35	6	0	-0.352022	2.973981	-0.014394
36	1	0	-0.116330	3.212638	1.016179
37	6	0	-1.353342	3.692727	-0.672358
38	1	0	-1.889185	4.473347	-0.140610
39	6	0	-1.661432	3.412677	-2.005403
40	1	0	-2.442143	3.971200	-2.513268
41	6	0	-0.963864	2.407604	-2.681187
42	1	0	-1.201924	2.172347	-3.713704
43	6	0	0.033994	1.687606	-2.026490
44	1	0	0.564849	0.908701	-2.560670
45	6	0	1.764961	1.523342	1.836794
46	6	0	2.920892	2.032798	2.447069
47	1	0	3.815751	2.212938	1.862096
48	6	0	2.929860	2.314449	3.814777
49	1	0	3.832121	2.708012	4.273539
50	6	0	1.786969	2.097484	4.586625
51	1	0	1.796762	2.317925	5.649998

52	6	0	0.631480	1.594883	3.984314
53	1	0	-0.262531	1.414049	4.573223
54	6	0	0.621054	1.303052	2.621100
55	1	0	-0.282734	0.907529	2.171832
56	6	0	3.221945	1.878102	-0.643370
57	6	0	3.121750	3.145813	-1.237414
58	1	0	2.158225	3.637354	-1.313640
59	6	0	4.258591	3.784019	-1.735903
60	1	0	4.164329	4.761718	-2.199214
61	6	0	5.509567	3.171761	-1.637640
62	1	0	6.392690	3.669819	-2.026645
63	6	0	5.620694	1.916156	-1.036784
64	1	0	6.589253	1.432453	-0.953588
65	6	0	4.484888	1.270571	-0.547269
66	1	0	4.588810	0.296524	-0.083991
67	6	0	3.204912	-1.560437	1.144151
68	6	0	1.790799	-3.479769	-0.306291
69	6	0	3.089118	-1.413647	-1.639189

Re8

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.037886	0.043585	0.140330
2	6	0	-5.169379	-0.547760	0.648421
3	6	0	-6.318946	0.295760	0.602757
4	6	0	-6.047626	1.527549	0.070931
5	16	0	-4.385238	1.674418	-0.398466
6	1	0	-5.170496	-1.561667	1.030759
7	1	0	-7.301105	-0.003288	0.950166
8	1	0	-6.724491	2.359139	-0.072352
9	6	0	-2.673651	-0.528006	0.041993
10	6	0	-2.048181	-0.872576	1.256561
11	6	0	-2.624106	-0.792591	2.565908
12	6	0	-1.702815	-1.320347	3.451044
13	6	0	-0.574274	-1.681365	2.677376
14	6	0	-2.154022	-0.721654	-1.250939
15	6	0	-2.882176	-0.590572	-2.476167
16	6	0	-2.044746	-1.001808	-3.495830
17	6	0	-0.825302	-1.368245	-2.878931
18	7	0	-0.762205	-1.416112	1.374187
19	7	0	-0.874085	-1.202489	-1.546261
20	75	0	0.792781	-1.633123	-0.174909
21	15	0	1.256331	0.869546	0.063769
22	6	0	2.882968	1.405400	-0.620059
23	6	0	3.048400	2.680535	-1.183361
24	6	0	3.995193	0.554058	-0.525688

25	6	0	4.296363	3.086613	-1.657301
26	1	0	2.203287	3.356655	-1.255864
27	6	0	5.243956	0.966215	-0.992902
28	1	0	3.893607	-0.429598	-0.082986
29	6	0	5.396057	2.230595	-1.565289
30	1	0	4.408006	4.073207	-2.097322
31	1	0	6.093648	0.294749	-0.914300
32	1	0	6.366102	2.547407	-1.936797
33	6	0	0.071149	1.983215	-0.793114
34	6	0	-0.627428	3.022461	-0.164685
35	6	0	-0.109723	1.771814	-2.169941
36	6	0	-1.508142	3.820694	-0.899308
37	1	0	-0.486713	3.219341	0.891531
38	6	0	-0.990102	2.567349	-2.898481
39	1	0	0.432686	0.978131	-2.670487
40	6	0	-1.696102	3.592427	-2.262870
41	1	0	-2.047925	4.619872	-0.400264
42	1	0	-1.131009	2.378888	-3.958124
43	1	0	-2.388085	4.209449	-2.828289
44	6	0	1.322904	1.442485	1.811014
45	6	0	2.530832	1.832821	2.409998
46	6	0	0.154514	1.417333	2.590240
47	6	0	2.565627	2.190866	3.759193
48	1	0	3.446503	1.860551	1.830250
49	6	0	0.192220	1.786404	3.934276
50	1	0	-0.790086	1.116183	2.153147
51	6	0	1.398146	2.170491	4.524395
52	1	0	3.508069	2.489851	4.208541
53	1	0	-0.722480	1.757910	4.518434
54	1	0	1.428178	2.450725	5.573244
55	6	0	0.368998	-3.541253	-0.308574
56	6	0	2.056307	-1.774206	-1.642251
57	6	0	2.187284	-1.980775	1.130158
58	8	0	2.785481	-1.867323	-2.547134
59	8	0	0.120177	-4.671045	-0.384205
60	8	0	3.016360	-2.182799	1.925791
61	1	0	-3.602468	-0.397900	2.792953
62	1	0	-1.798908	-1.427073	4.522643
63	1	0	0.362681	-2.092161	3.027375
64	1	0	-3.909374	-0.269148	-2.559069
65	1	0	-2.262786	-1.052190	-4.553728
66	1	0	0.073483	-1.734217	-3.356877
