Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Contents

Supplementary material 1: ^{1}H NMR & ^{13}C NMR spectra
Figure S1: NMR
5'-(*1H*-Imidazol-1-yl)-3'-methyl-1',2-diphenyl-5-(pyridin-2-yl)-3,4-dihydro-*1'H,2H*-3,4'-bipyrazole (bpy-N) [4a]

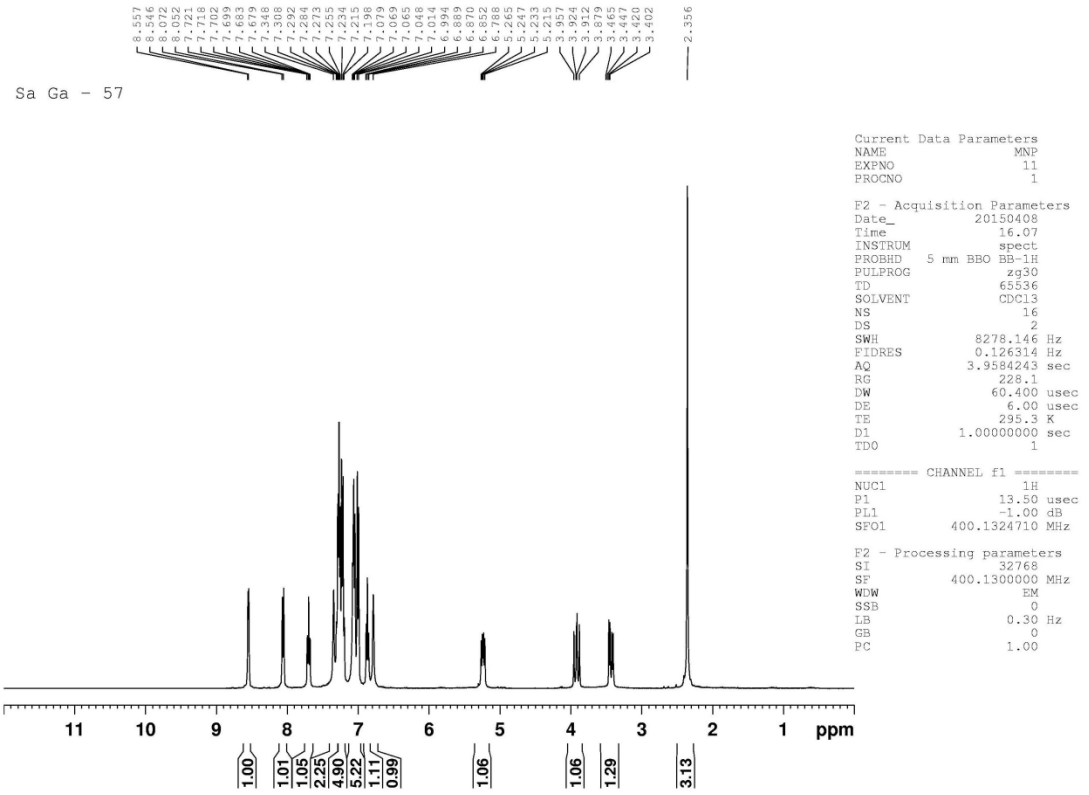
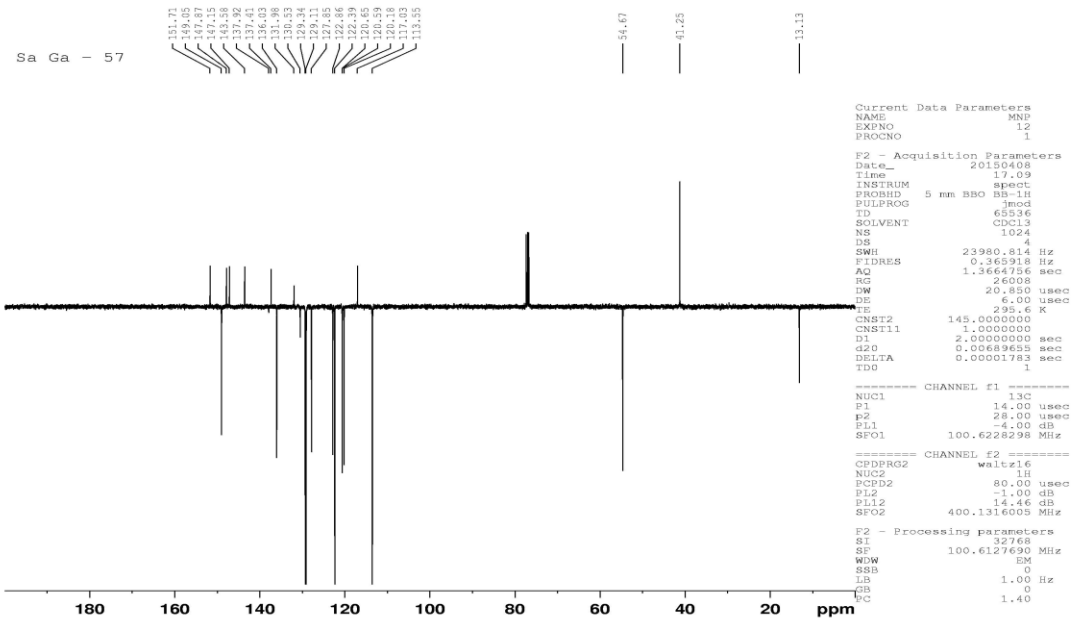


Figure S2: APT



3'-Methyl-5'-phenoxy-1',2-diphenyl-5-(pyridin-2-yl)-3,4-dihydro-*1'H,2H*-3,4'-bipyrazole (bpy-O) [4b]

Figure S3: ^{1}H NMR

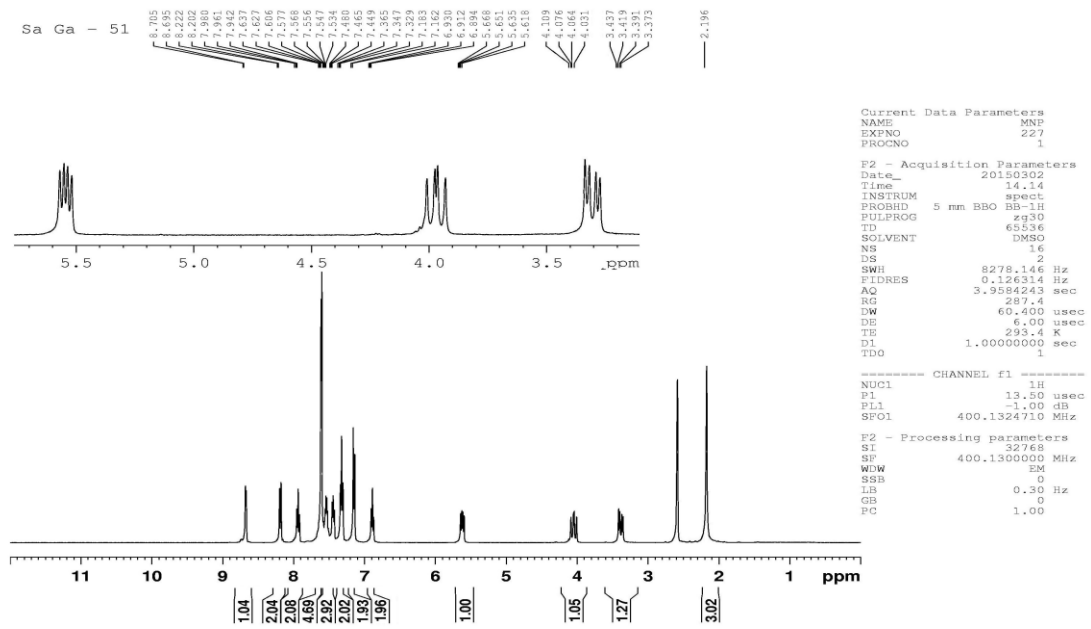
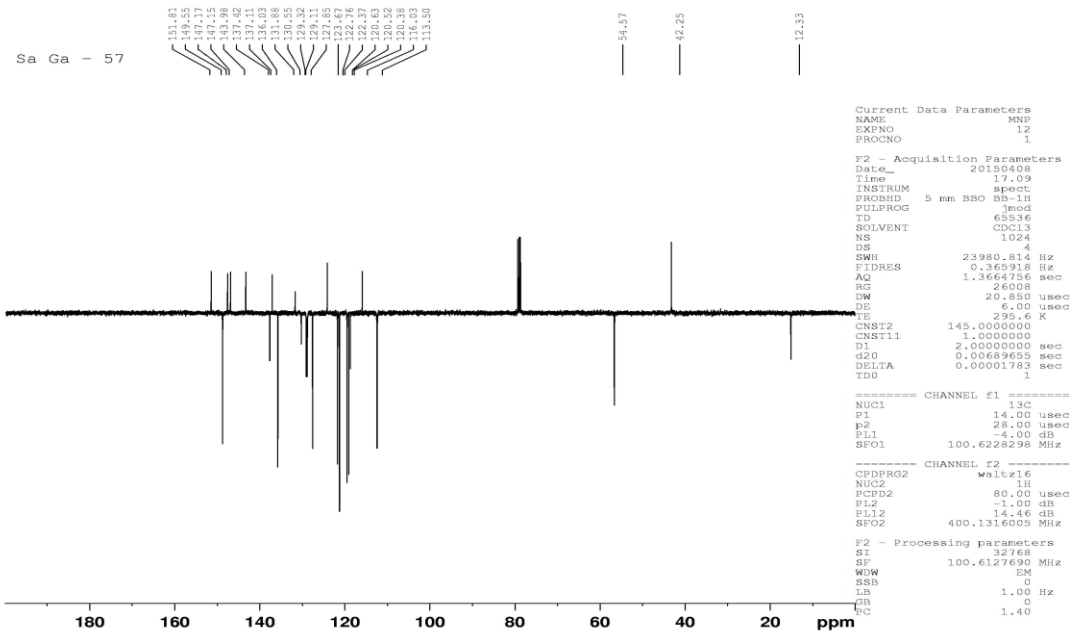


Figure S4: APT



4-(5-(*1H*-Imidazol-1-yl)-3-methyl-1-phenyl-*1H*-pyrazol-4-yl)-6-(pyridin-2-yl)pyrimidin-2-amine (pma-N) [5a]

Figure S5: ^{1}H NMR

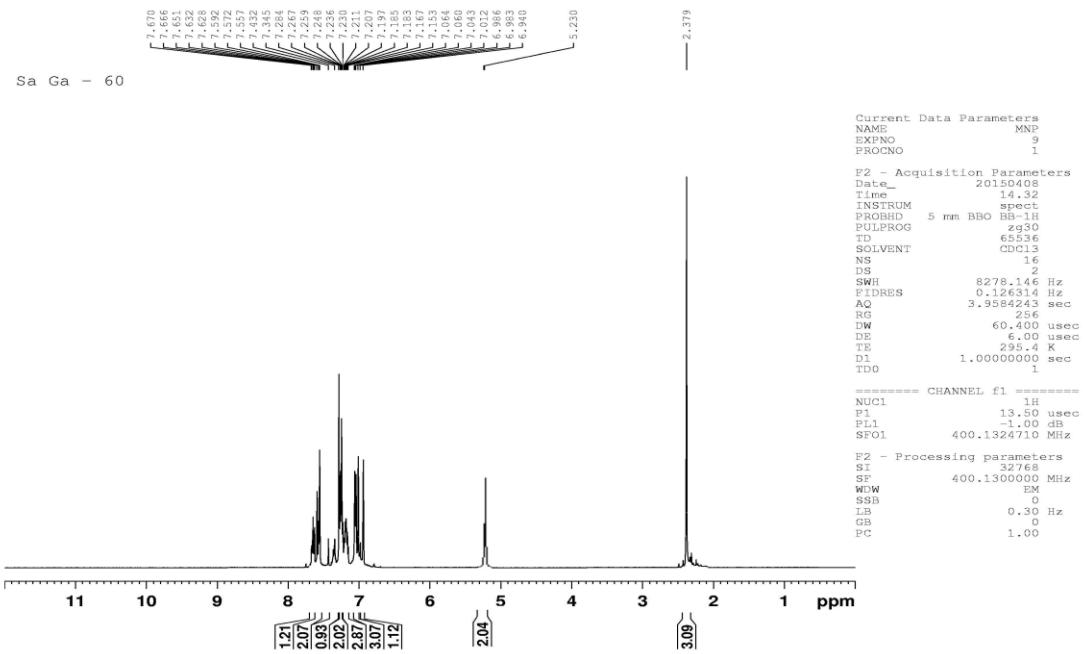
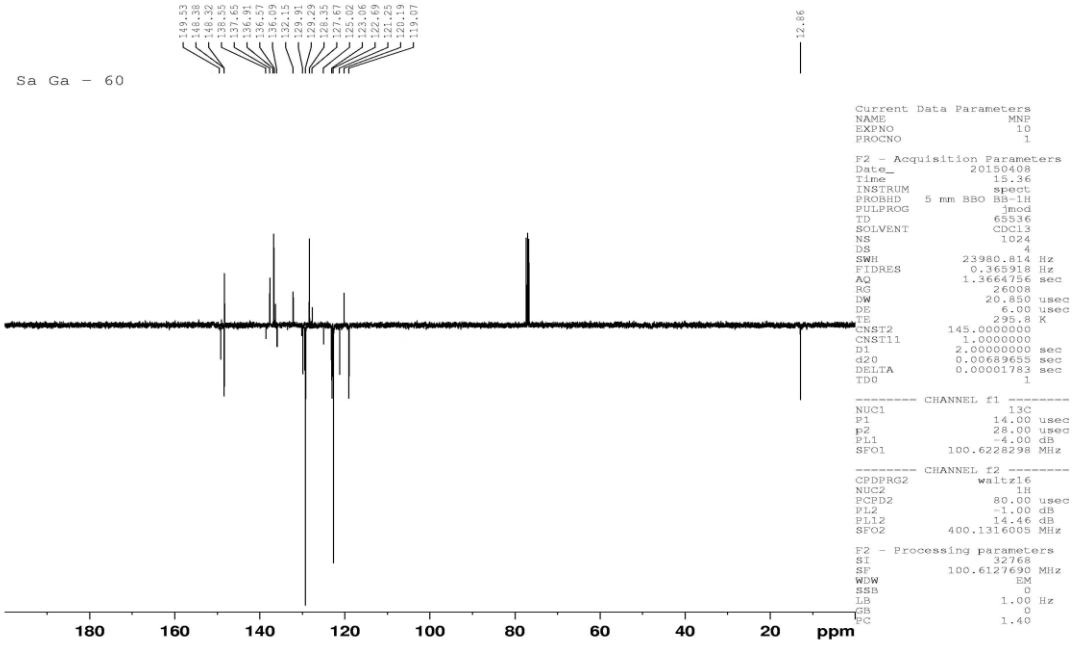


Figure S6: APT



4-(3-Methyl-5-phenoxy-1-phenyl-*1H*-pyrazol-4-yl)-6-(pyridin-2-yl)pyrimidin-2-amine (pma-O) [5b]

Figure S7: ^{1}H NMR

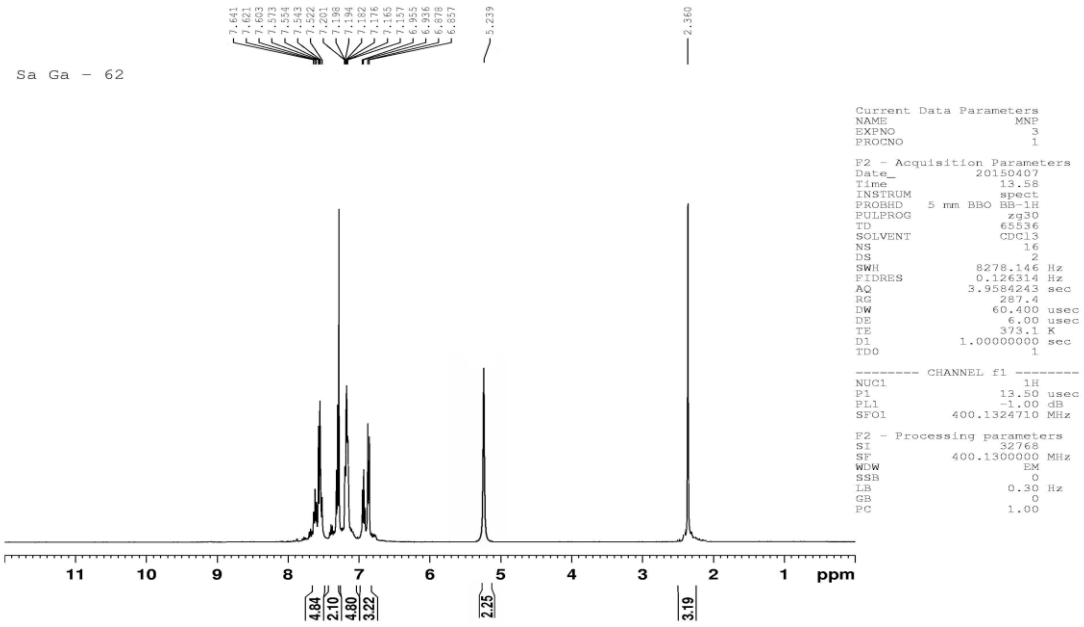
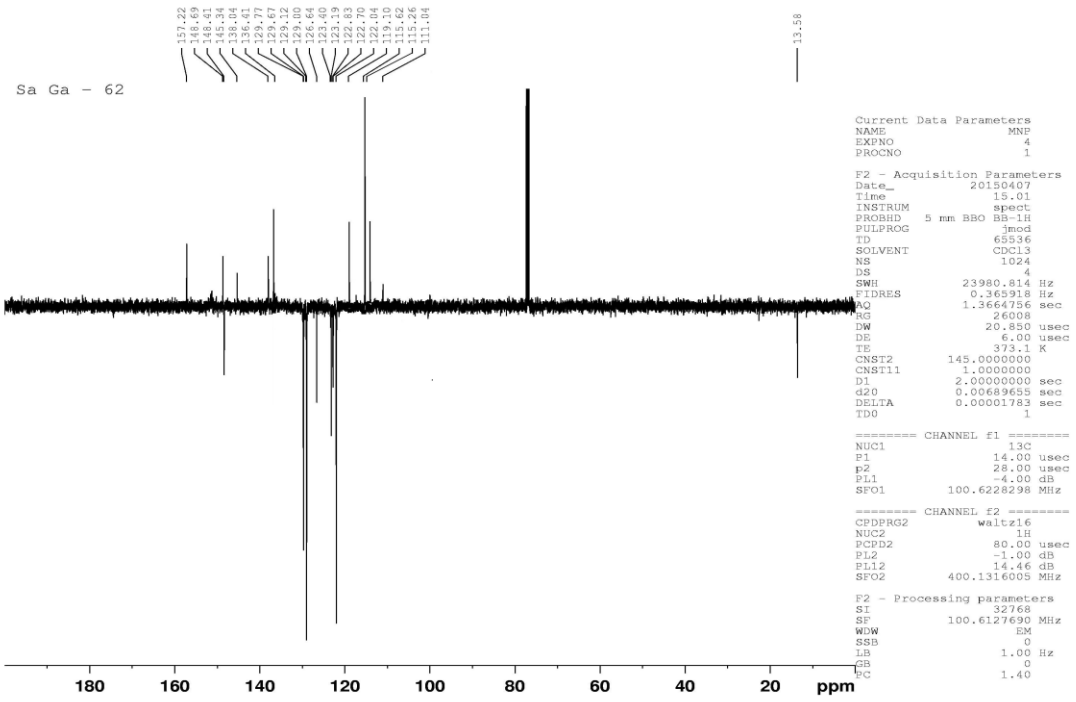


Figure S8: APT



7-(5-(*1H*-Imidazol-1-yl)-3-methyl-1-phenyl-*1H*-pyrazol-4-yl)-5-(pyridin-2-yl)-[1,2,4]triazolo[1,5-a]pyrimidine (tpm-N) [6a]

Figure S9:[1]H NMR

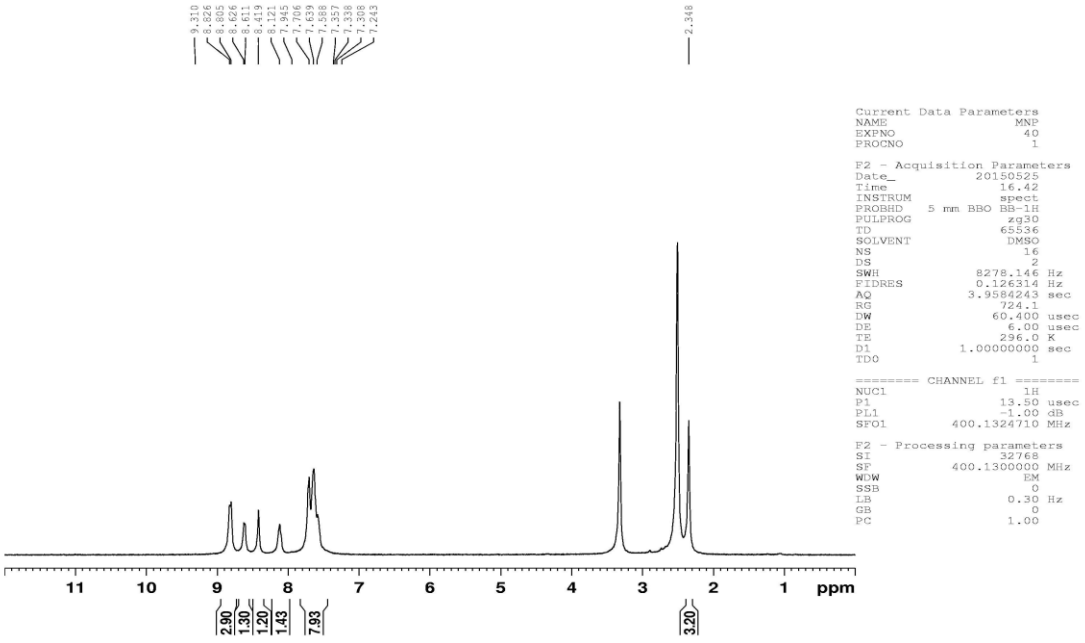
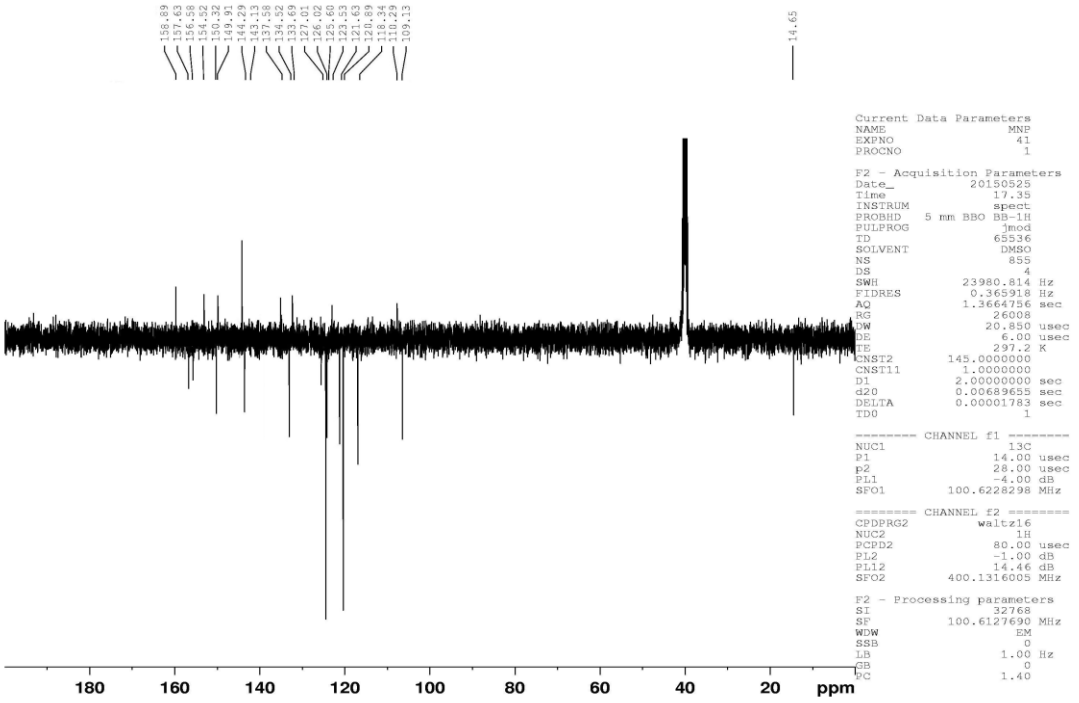


Figure S10: APT



7-(3-Methyl-5-phenoxy-1-phenyl-*1H*-pyrazol-4-yl)-5-(pyridin-2-yl)-[1,2,4]triazolo[1,5-a]pyrimidine (tpm-O) [6b]

Figure S11:^{1}H NMR

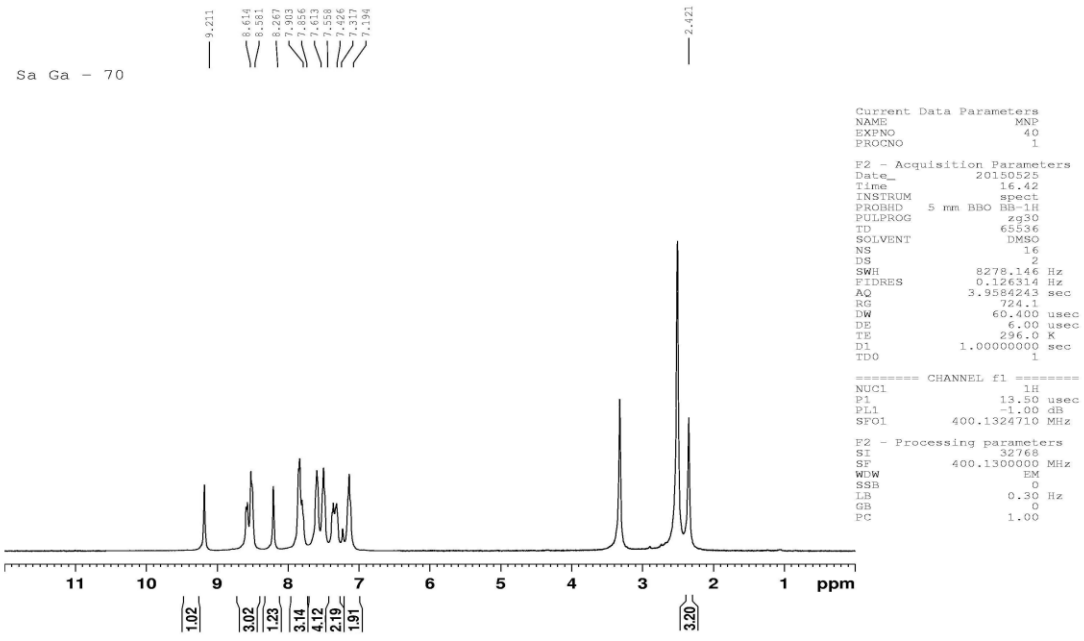
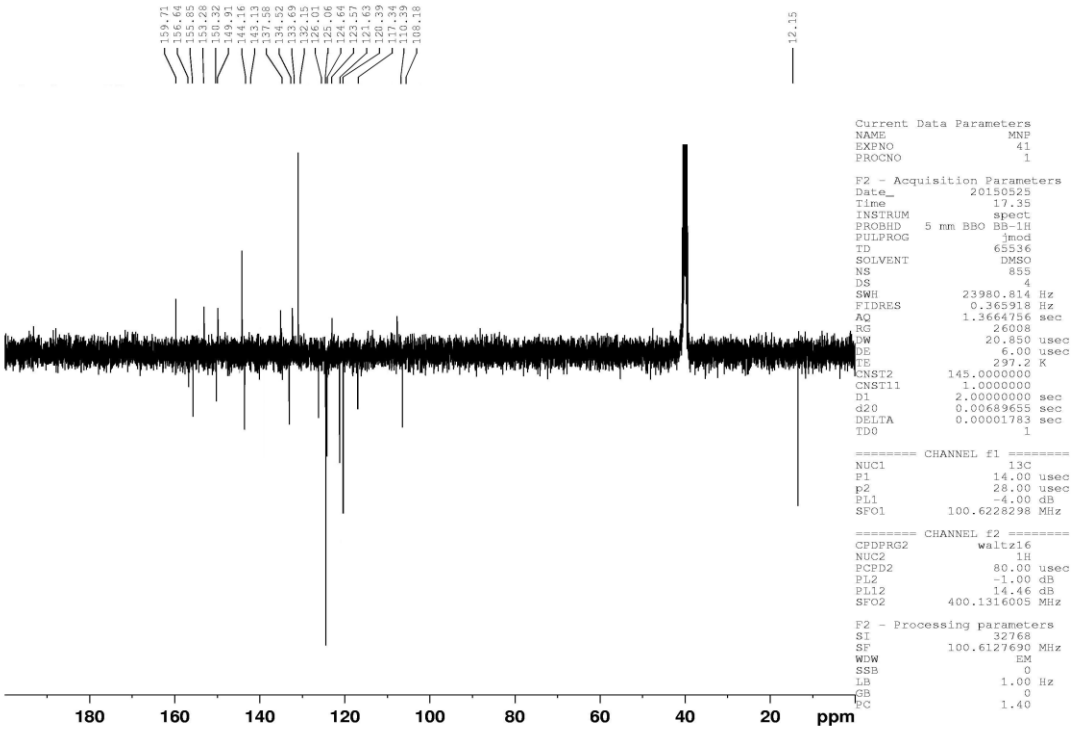


Figure S12: APT



[(η^5-C_5Me_5)Ir(bpy-N)Cl]Cl [7a]

Figure S13: ^{1}H NMR

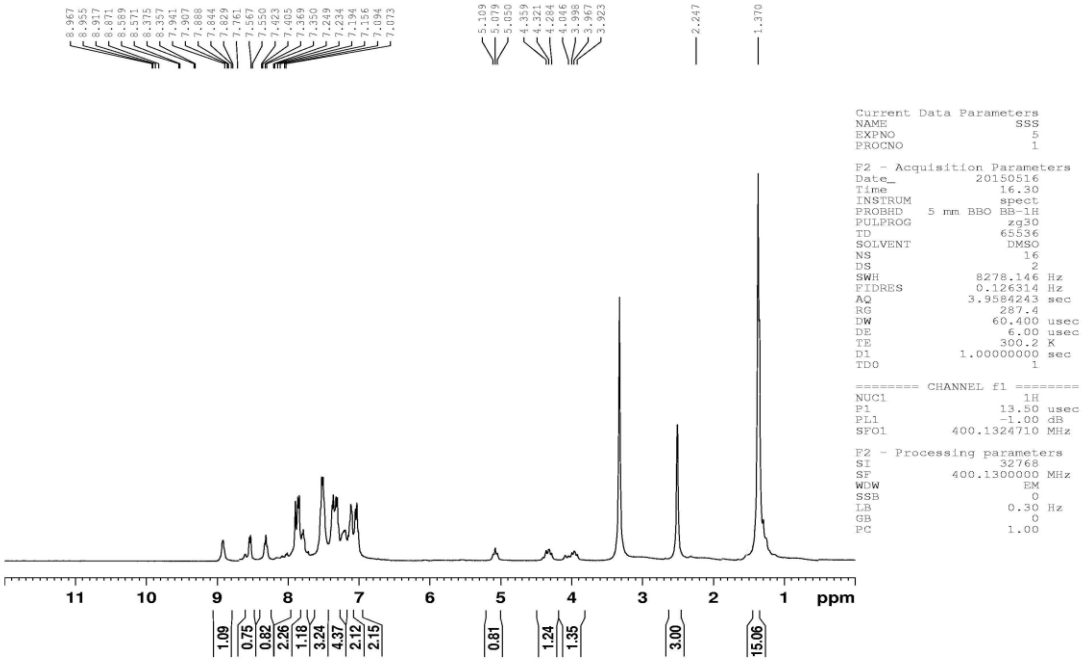
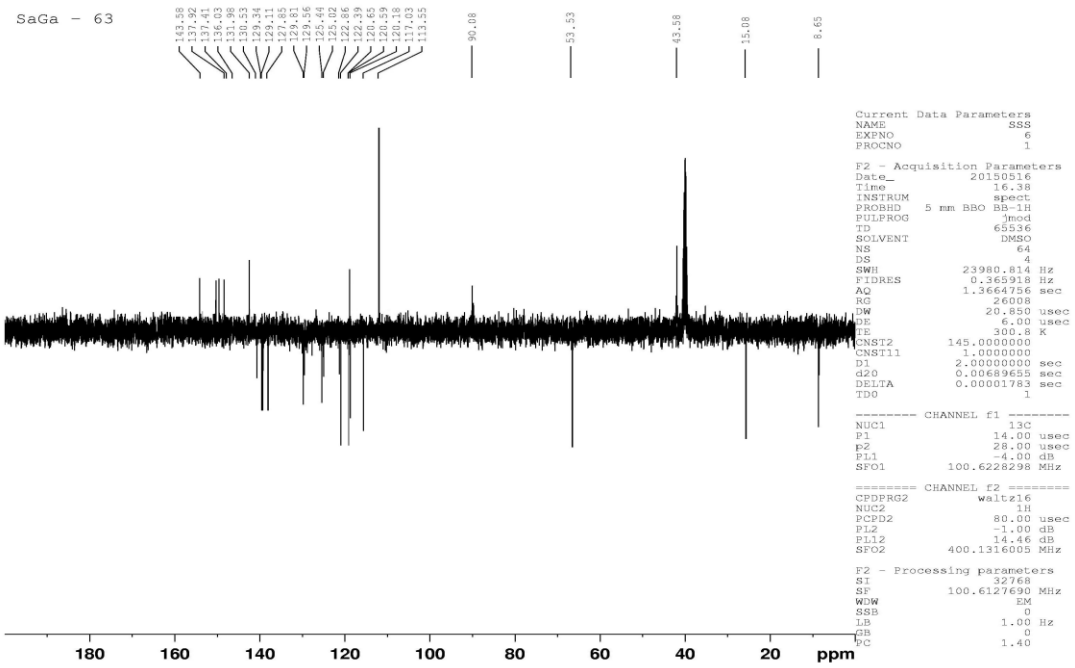


Figure S14: APT



[(η^5-C_5Me_5)Ir(bpy-O)Cl]Cl [7b]

Figure S15: ^{1}H NMR

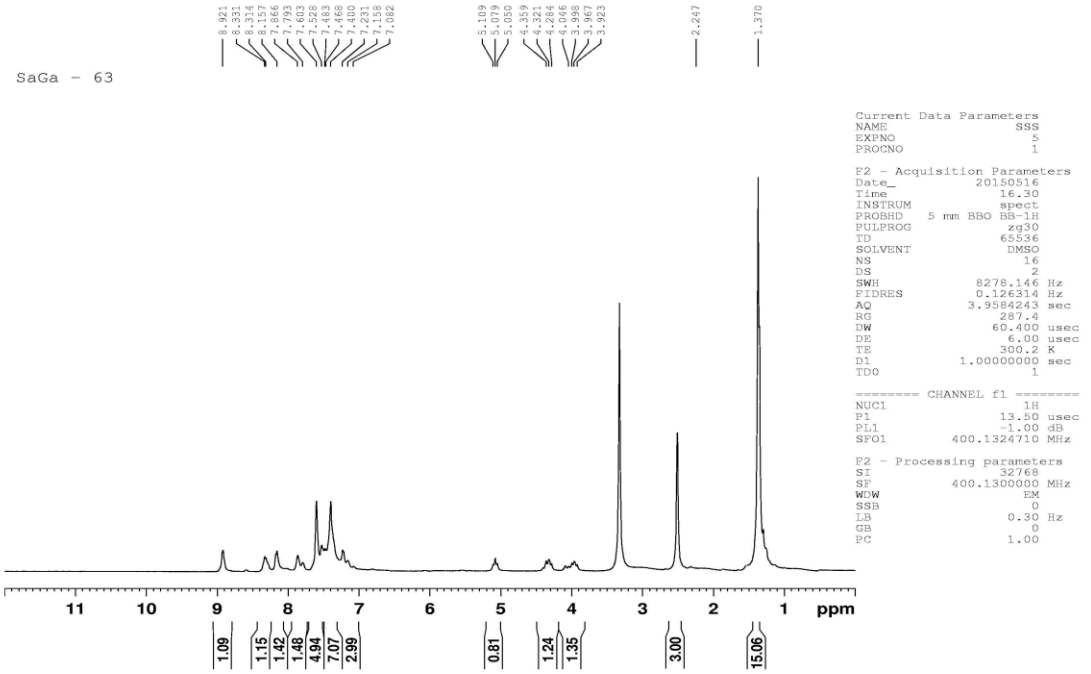
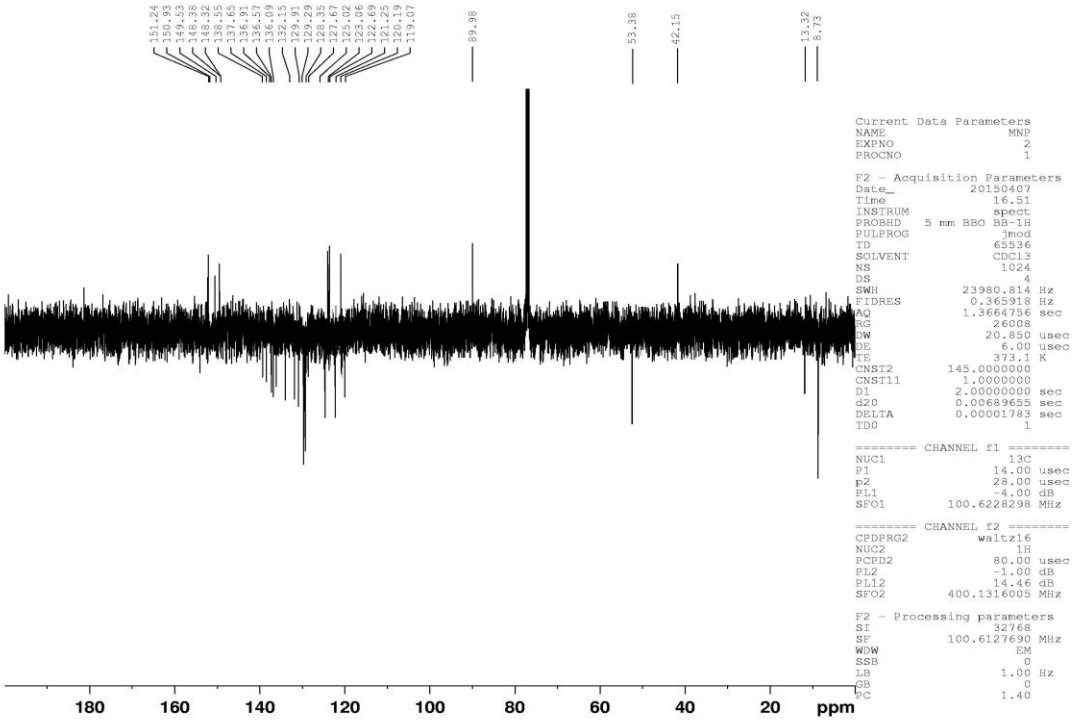


Figure S16: APT



[(η^5-C_5Me_5)Ir(pma-N)Cl]Cl [8a]

Figure S17: ^{1}H NMR

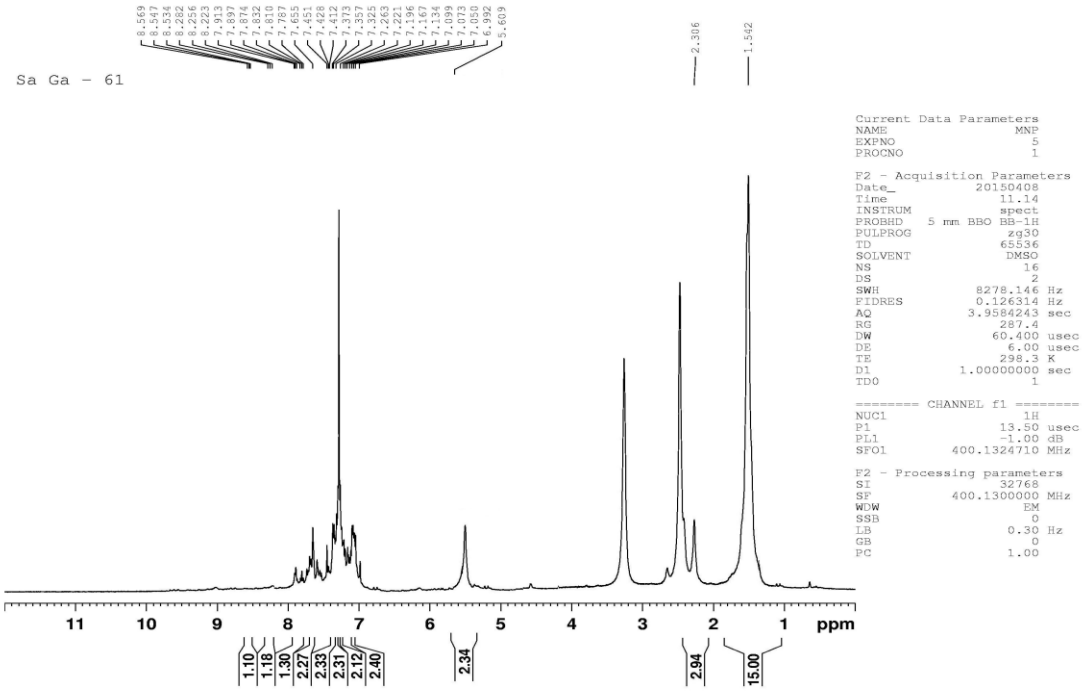
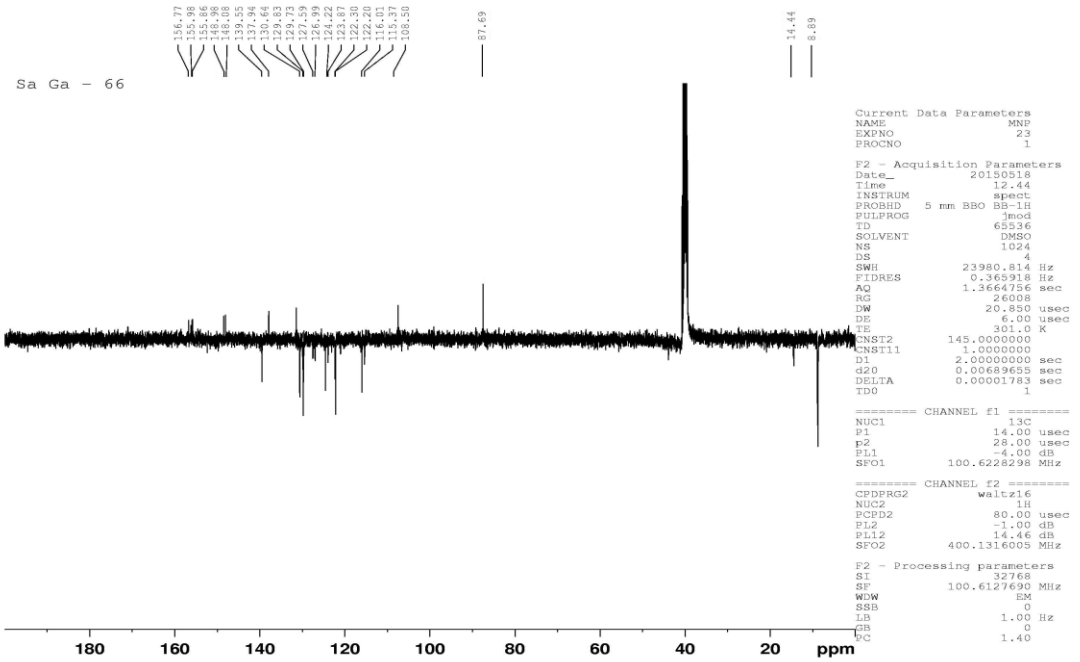


Figure S18: APT



[(η^5-C$_5$Me$_5$)Ir(pma-O)Cl]Cl [8b]

Figure S19: ^{1}H NMR

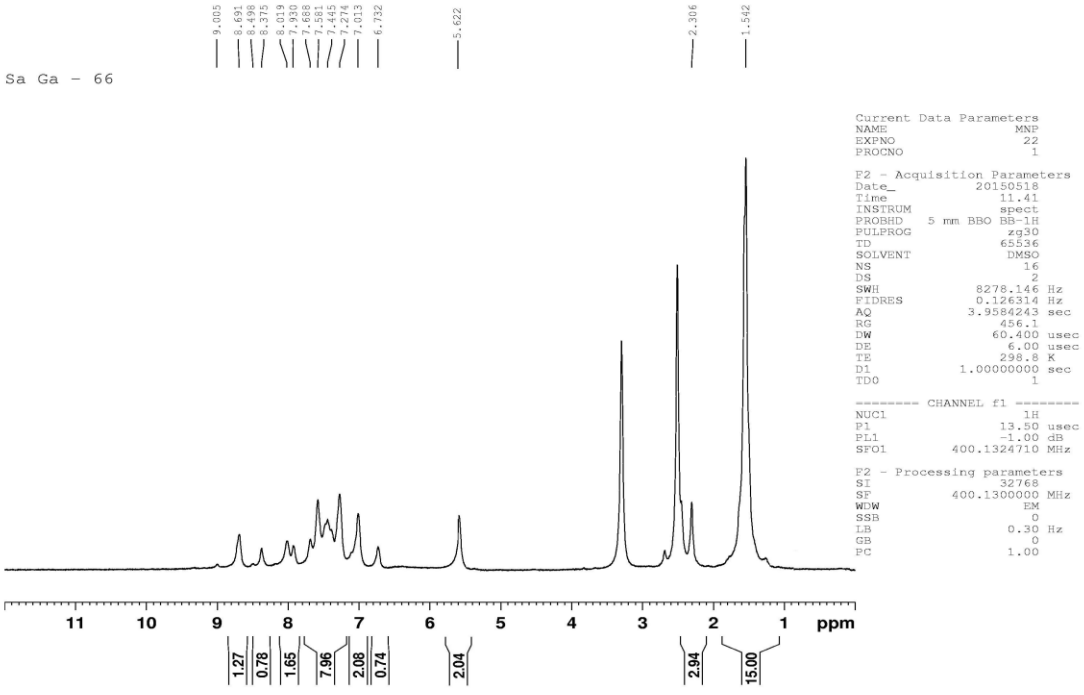
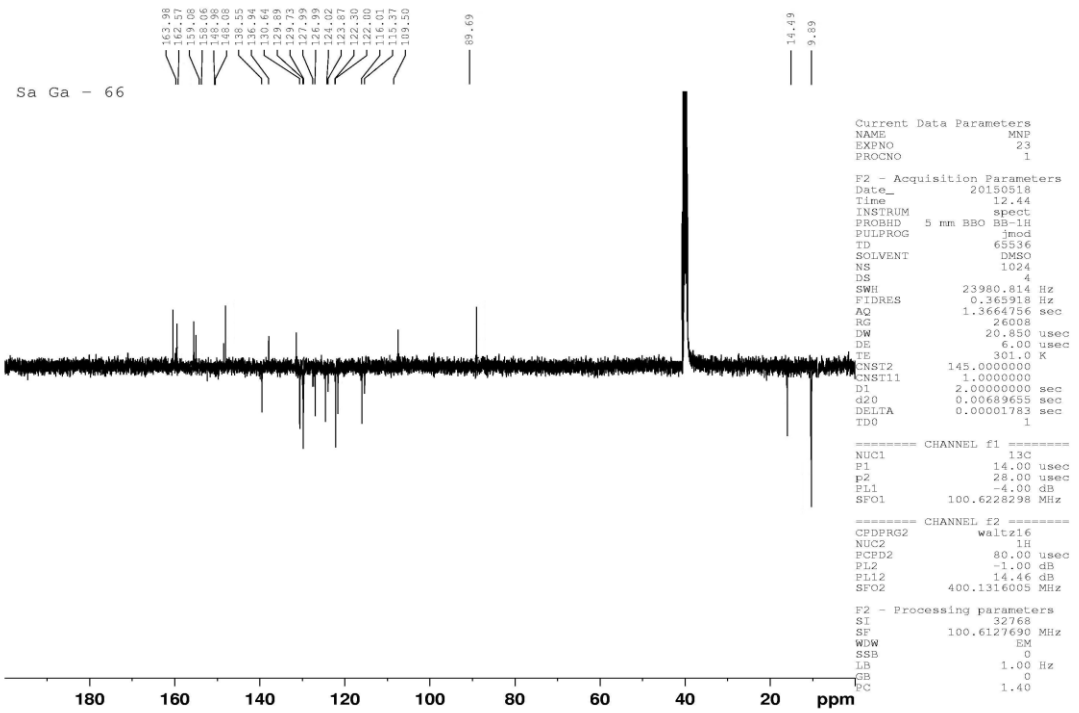


Figure S20: APT



[(η^5-C_5Me_5)Ir(tpm-N)Cl]Cl [9a]

Figure S21: ^{1}H NMR

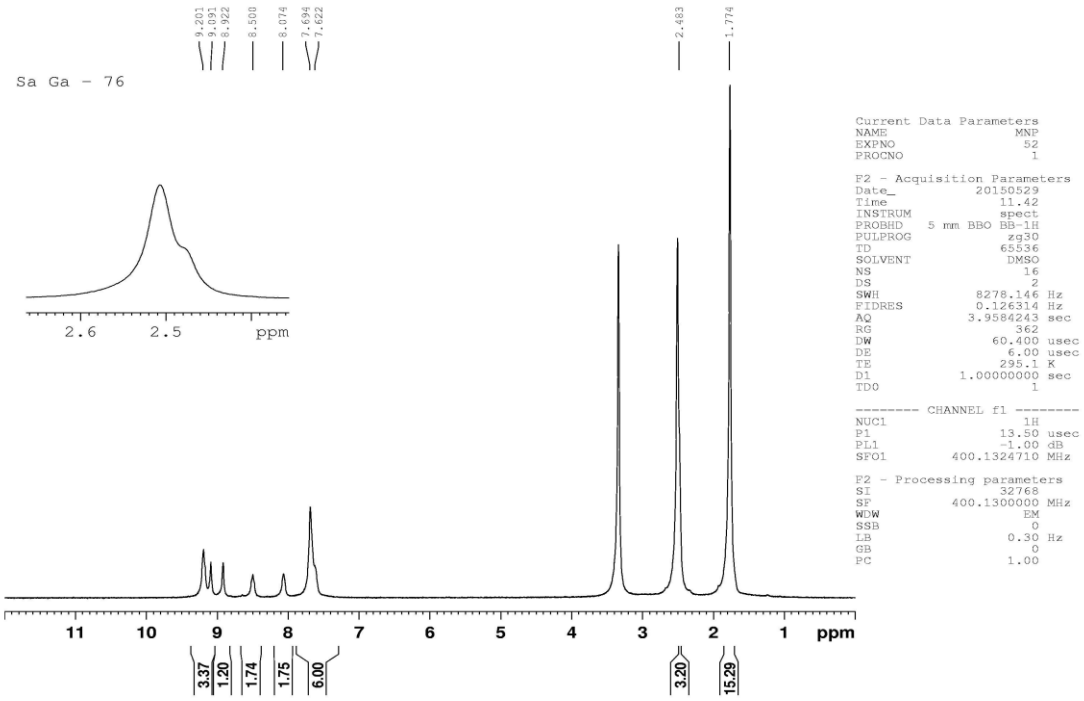
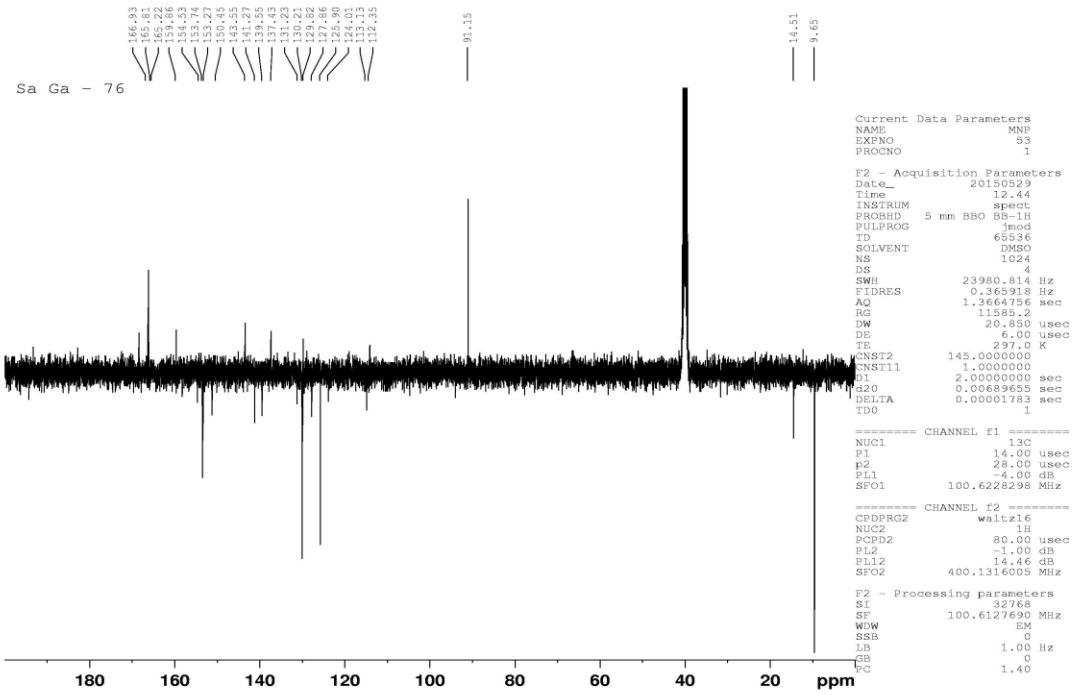


Figure S22: APT



[(η^5-C_5Me_5)Ir(tpm-O)Cl]Cl [9b]

Figure S23: ^{1}H NMR

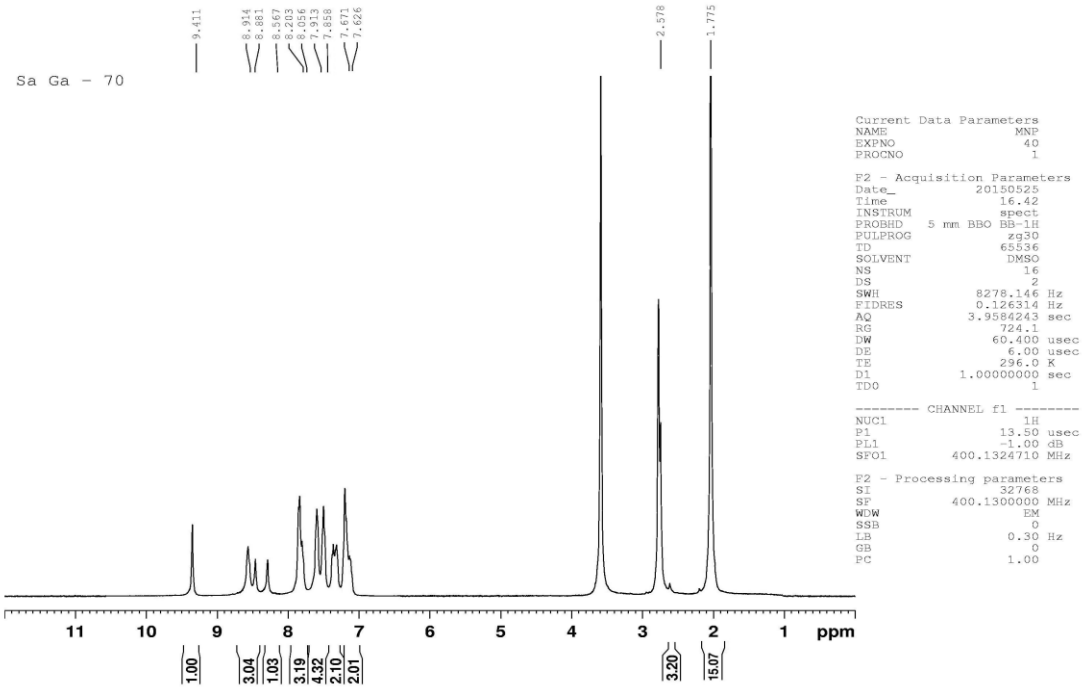
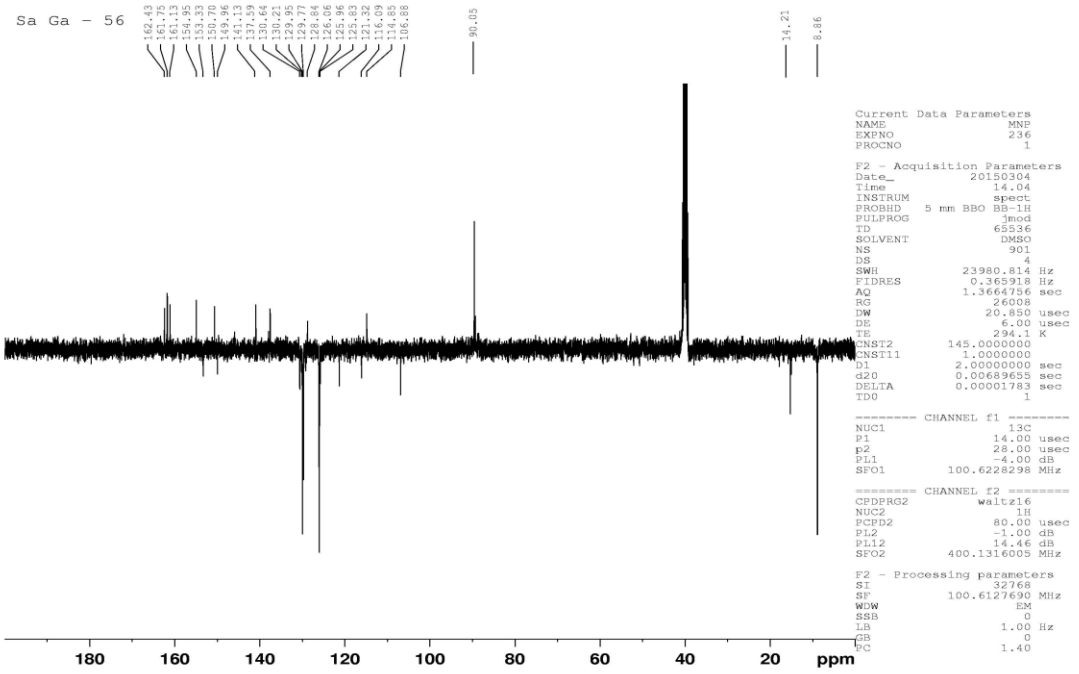
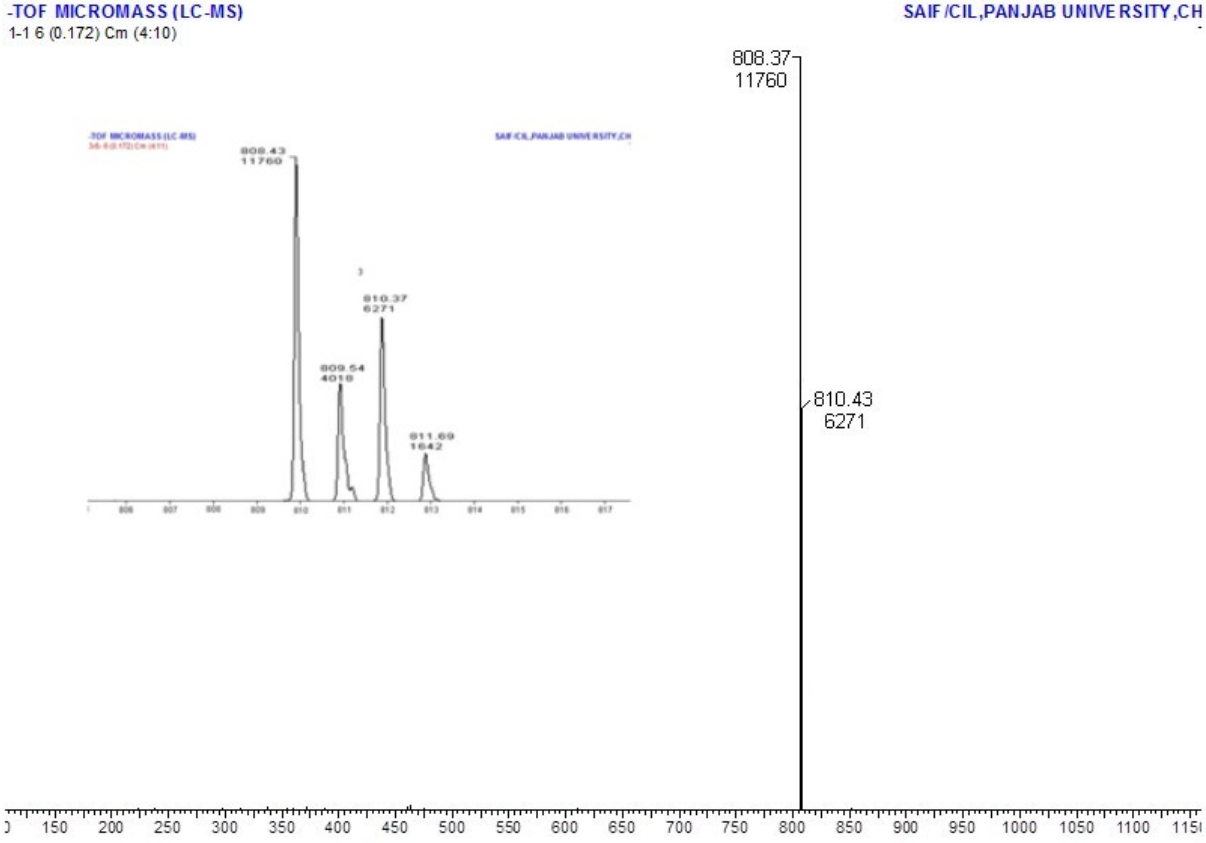


Figure S24: APT



Supplementary material 2: ESI-MS
Figure S25: Complex 7a



Supplementary material 3: Molecular docking

Figure S26: 4a

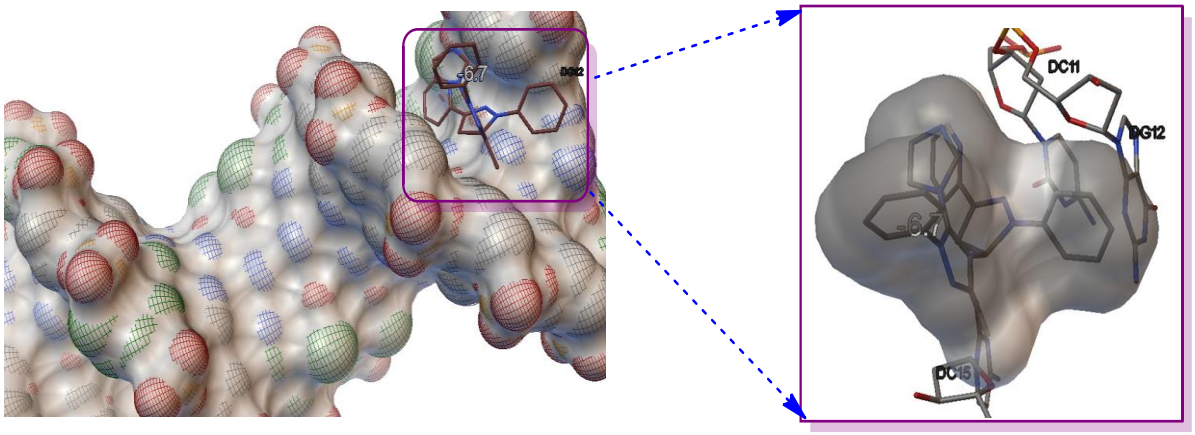


Figure S27: 4b

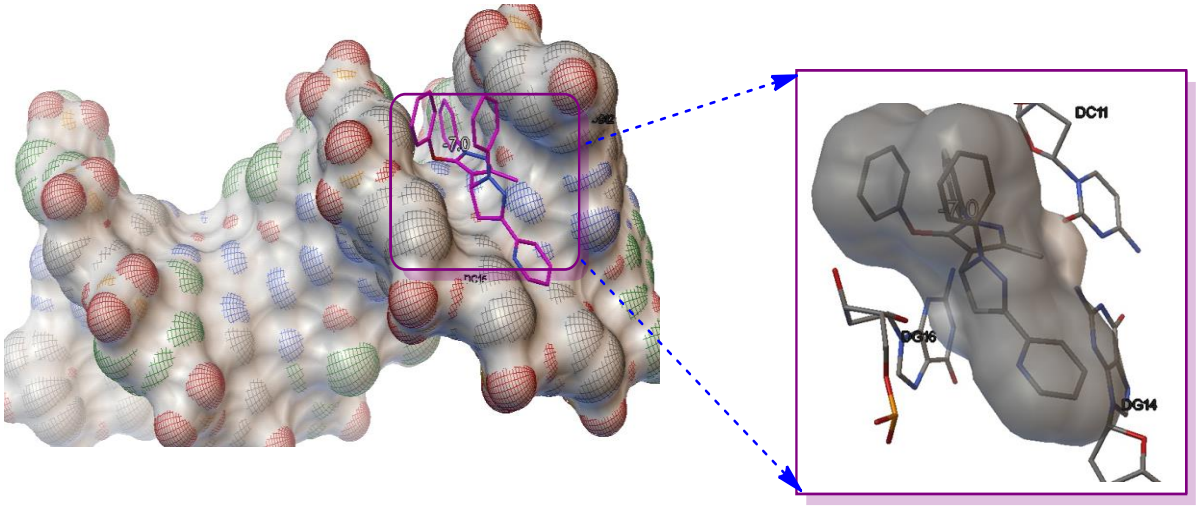


Figure S28: 5a

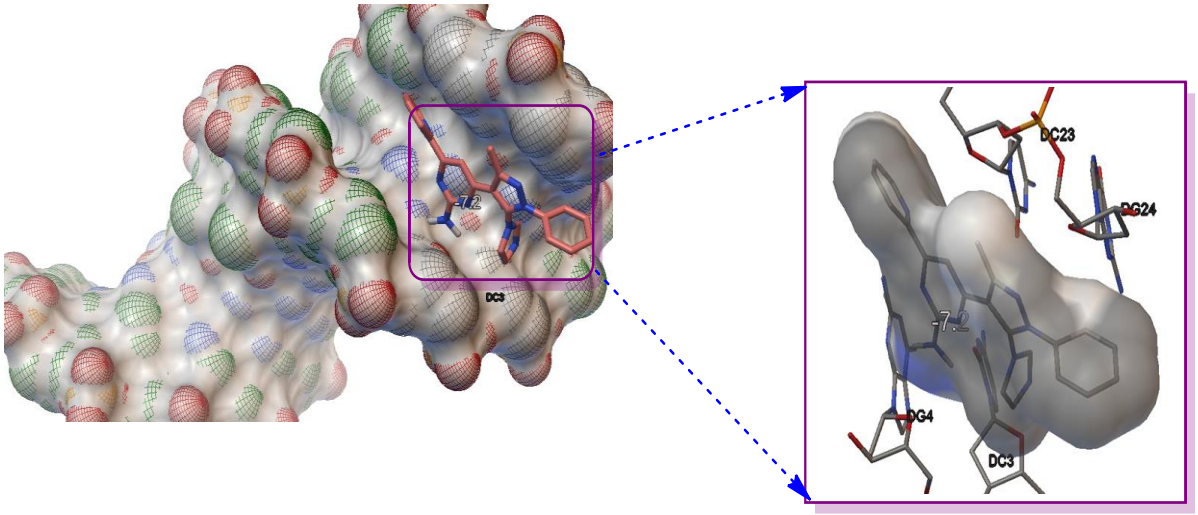


Figure S29: 5b

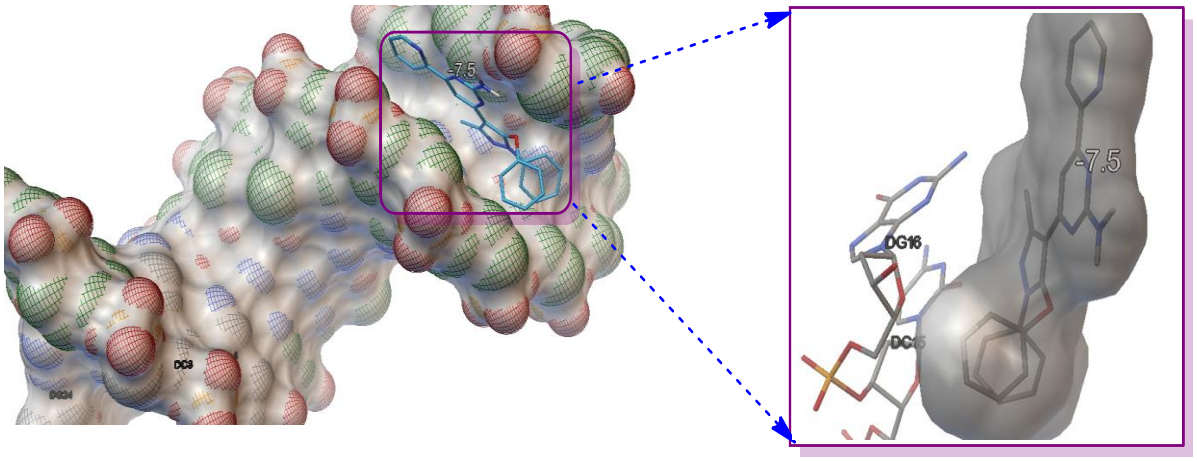


Figure S30: 6b

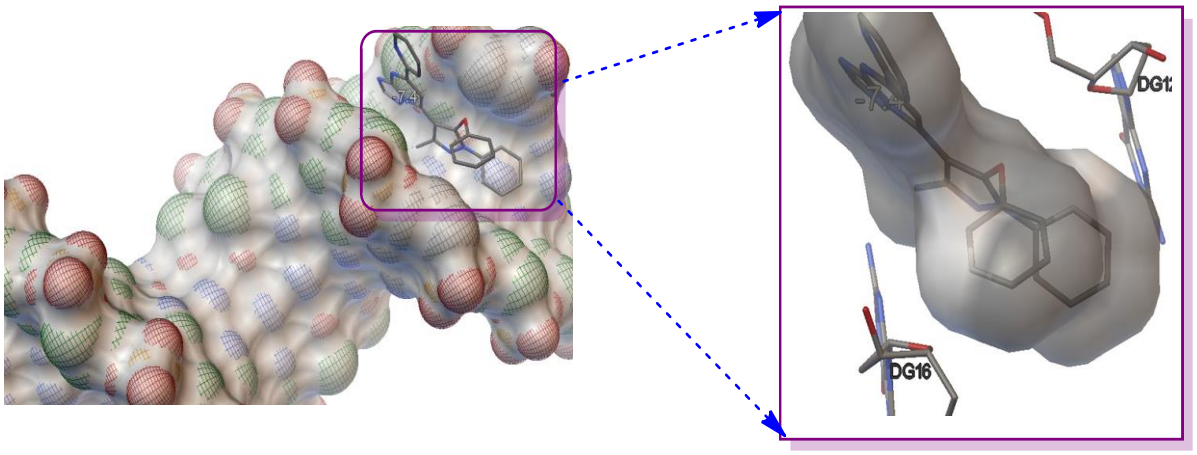


Figure S31: 7a

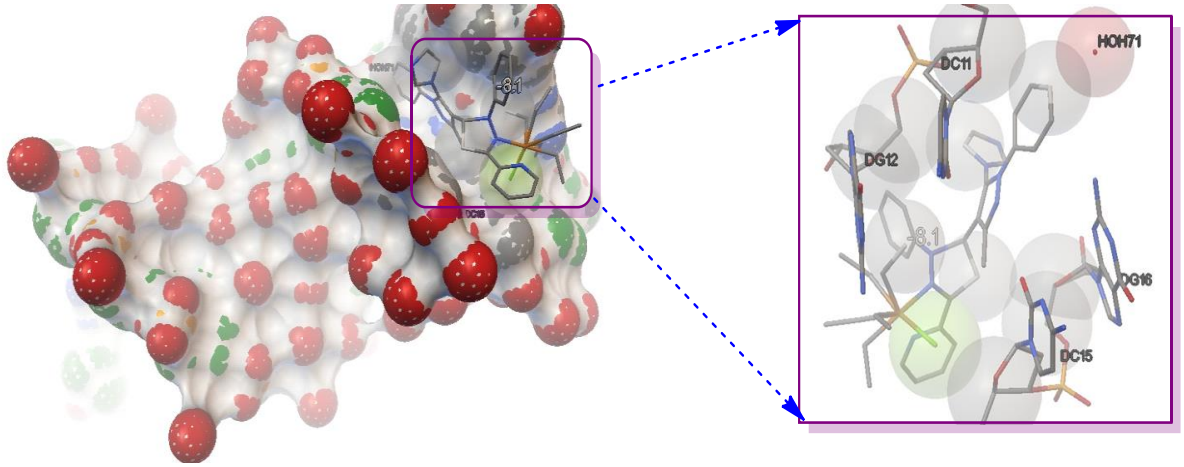


Figure S32: 7b

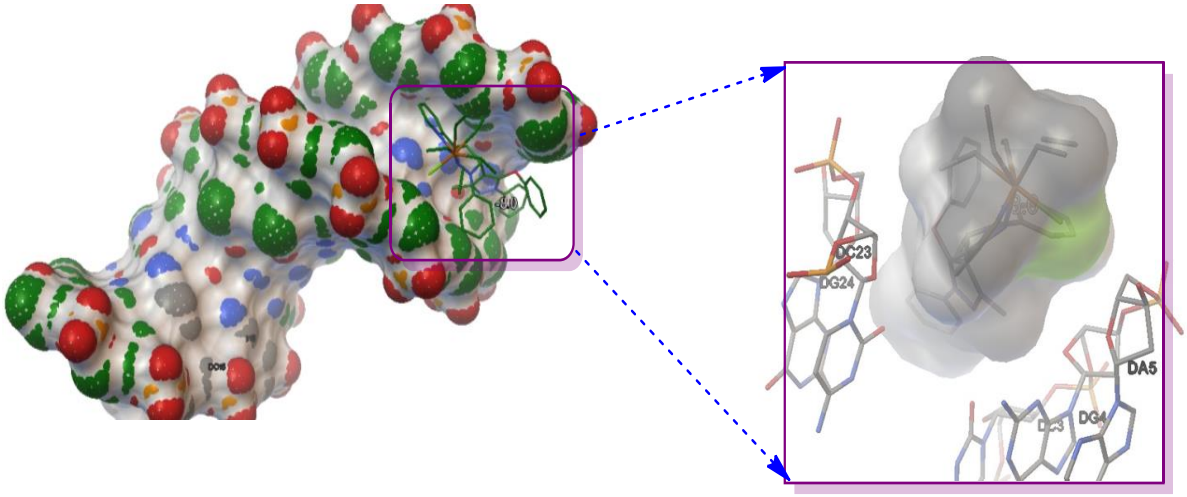
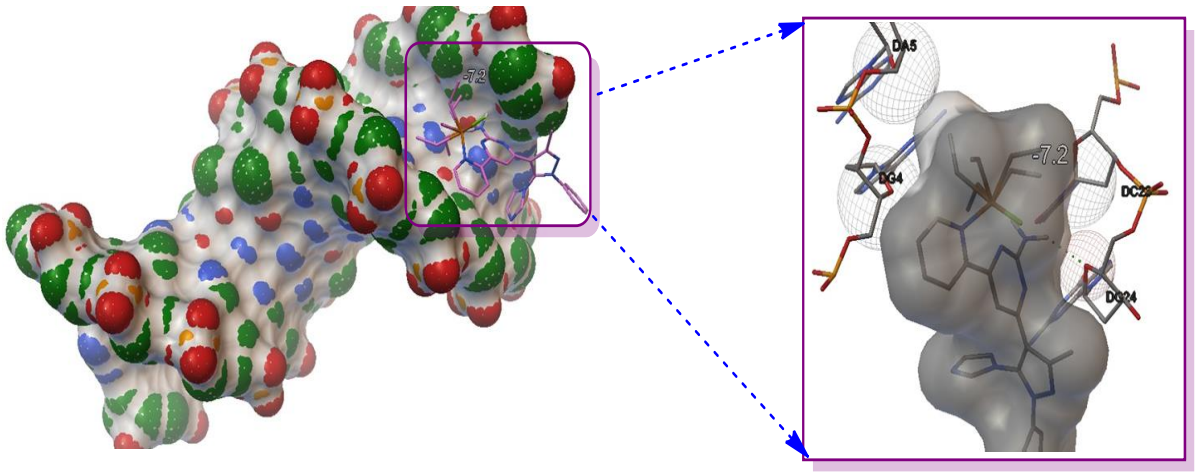


Figure S33: 8a



Supplementary material 4: DNA cleavage activity data presented with standard deviation for three independent experiments.

Table S34:

Compounds	SC	L	NC
DNA control	81 ± 1.5	19 ± 1.7	-
Salt	66 ± 1.7	14 ± 1.5	20 ± 1.1
4a	14 ± 2.0	47 ± 1.0	39 ± 1.0
4b	21 ± 1.5	49 ± 2.0	30 ± 1.5
5a	23 ± 1.1	43 ± 1.1	34 ± 1.1
5b	25 ± 2.0	40 ± 1.2	35 ± 2.0
6a	30 ± 1.0	35 ± 1.7	35 ± 2.0
6b	23 ± 1.5	41 ± 1.5	36 ± 1.5
7a	10 ± 1.5	32 ± 2.2	58 ± 1.5
7b	19 ± 2.0	29 ± 1.2	52 ± 1.0
8a	20 ± 2.0	39 ± 0.9	41 ± 2.0
8b	20 ± 1.1	25 ± 1.1	55 ± 1.1
9a	21 ± 1.5	28 ± 1.6	51 ± 1.5
9b	30 ± 1.0	31 ± 2.1	38 ± 1.7

Supplementary material 5: Anticancer activity on A549 (lung) cancer cell line, IC_{50}data presented with standard deviation for three independent experiments.

Table S35:

Compounds	IC_{50} (µM)
4a	387 ± 1.20
4b	220 ± 0.82
5a	197 ± 2.12
5b	88 ± 0.98
6a	290 ± 3.20
6b	170 ± 1.65
7a	245 ± 4.23
7b	89 ± 0.79
8a	96 ± 1.72
8b	74 ± 2.78
9a	163 ± 0.43
9b	116 ± 3.49

Supplementary material 6: MIC values of ligands and complexes in µM presented with standard deviation for three independent experiments.

Table S36:

Compounds	Gram positive (in µM)		Gram negative (in µM)		
	S.aureus	*B.subtilis*	*S.marcescens*	*P.aeruginosa*	*E.coli*
Salt	566 ± 12	572 ± 6	544 ± 8	530 ± 14	504 ± 7
4a	303 ± 5	301 ± 5	272 ± 7	273 ± 7	297 ± 17
4b	316 ± 6	317 ± 6	295 ± 5	294 ± 6	303 ± 7
5a	341 ± 12	337 ± 12	296 ± 6	300 ± 12	318 ± 17
5b	353 ± 4	353 ± 4	312 ± 8	317 ± 7	338 ± 14
6a	283 ± 5	280 ± 8	253 ± 4	254 ± 2	264 ± 8
6b	297 ± 8	292 ± 11	263 ± 5	266 ± 4	277 ± 14
7a	103 ± 4	105 ± 6	71 ± 7	73 ± 7	104 ± 6
7b	114 ± 5	117 ± 8	84 ± 5	86 ± 3	115 ± 8
8a	109 ± 9	111 ± 9	79 ± 3	80 ± 2	110 ± 7
8b	117 ± 4	120 ± 6	81± 8	83 ± 4	117 ± 4
9a	93 ± 5	95 ± 5	67 ± 2	67 ± 1	91 ± 3
9b	97 ± 2	99 ± 4	75 ± 5	76 ± 2	99 ± 4

Supplementary material 7: Brine shrimp lethality bioassay data presented with standard deviation for three independent experiments.

Table S37:

Compounds	LC_{50} (µg/mL)
4a	7.05 ± 0.074
4b	7.53 ± 0.071
5a	7.80 ± 0.067
5b	8.49 ± 0.065
6a	5.00 ± 0.032
6b	5.34 ± 0.059
7a	6.33 ± 0.099
7b	6.63 ± 0.066
8a	6.12 ± 0.096
8b	7.77 ± 0.101
9a	2.91 ± 0.044
9b	4.83 ± 0.053