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Structural characterization of aluminium (III) and iron (III) complexes of coumarinic acid in aqueous solution from combined experimental and theoretical investigations

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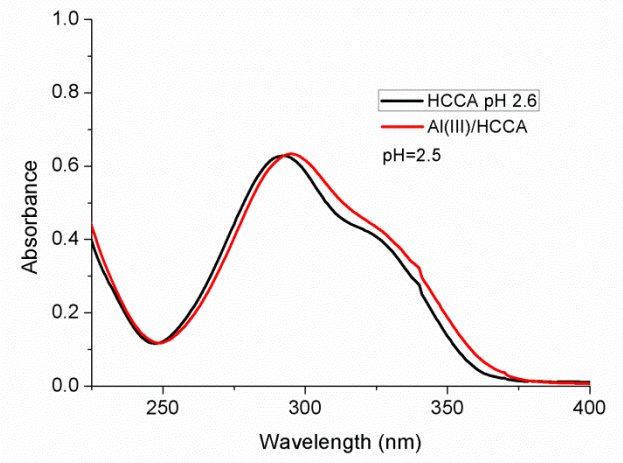

Figure S1. UV-Vis spectra of the free ligand 0.1 mM (black line) and of the complexes formed between ligand and $AlCl_3$ 0.1 mM (red line) at pH 2.5

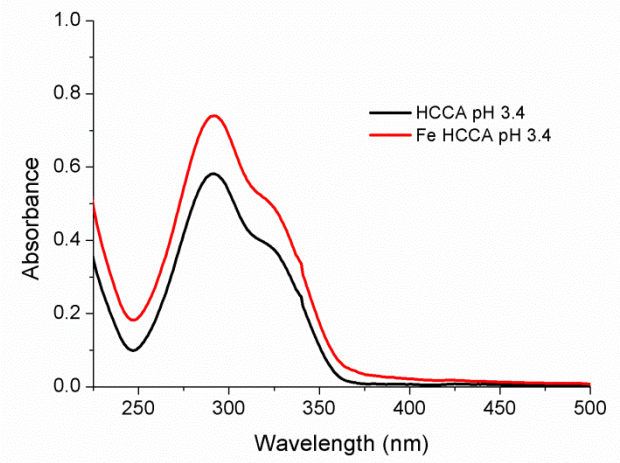

Figure S2. UV-Vis spectra of the free ligand 0.1 mM (black line) and of the complexes formed between ligand and $FeCl_3$ 0.1 mM (red line) at pH 3.4

Table S1. NBO charge values (|e|) for some atoms of the lowest energy complexes of alluminium in typology (1,-4,1) in comparison with the free ligand.

	Free ligand	Al-octa (a)	Al-tetra (c)
C2	0.797	0.857	0.802
C3	-0.198	-0.236	-0.236
C4	-0.175	-0.110	-0.118
C5	-0.213	-0.199	-0.197
C6	-0.282	-0.275	-0.280
C7	-0.250	-0.230	-0.231
C8	-0.286	-0.280	-0.287
C11	0.767	0.819	0.811
O_a	-0.796	-0.712	**-0.878**
O_b	-0.749	**-0.805**	-0.637
O	-0.574	**-0.628**	-0.562
Al	-	2.029	2.063