Electronic Supplementary Informations

Synthesis of a tube-like tetra-bipyridyl, tetra-ethylacetato-calix[4]arene in 1,3-alternate conformation and the unexpected crystal structure of its [bpy($CoCl_2$)]$_3$-[bpy($CoCl_2$)(H_2O)] complex†

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† Supplementary Information available: Crystallographic data CCDC 2357976

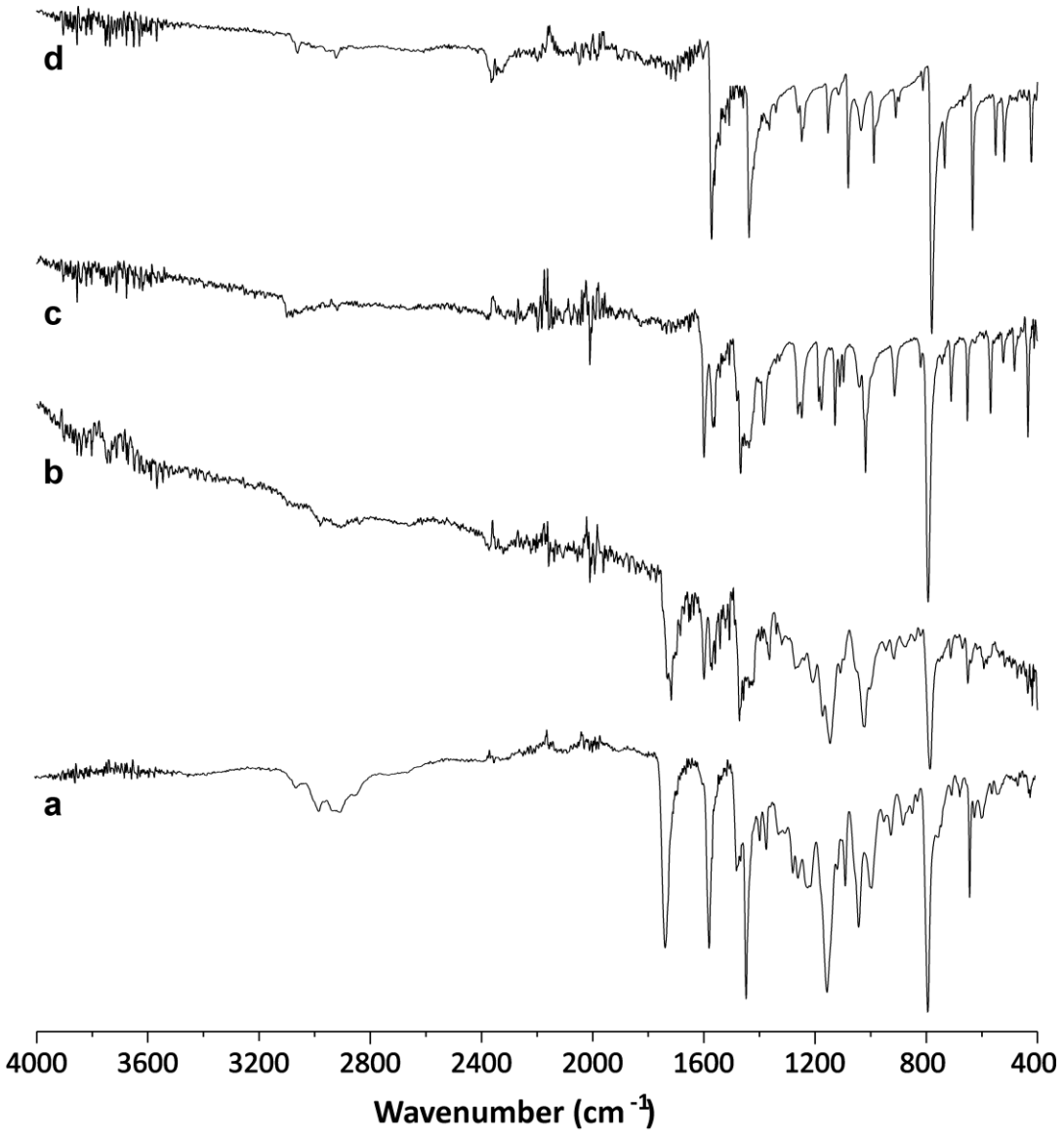

Figure ESI 1: 4000-400 cm^{-1} FTIR (ATR mode) spectra of (**a**) ligand **2**, (**b**) crystals of tetranuclear complex **3**, (**c**) microcrystalline dmbp($CoCl_2$) complex **4** and (**d**) 6,6'-dimethyl-2,2'-bipyridine (dmbp).

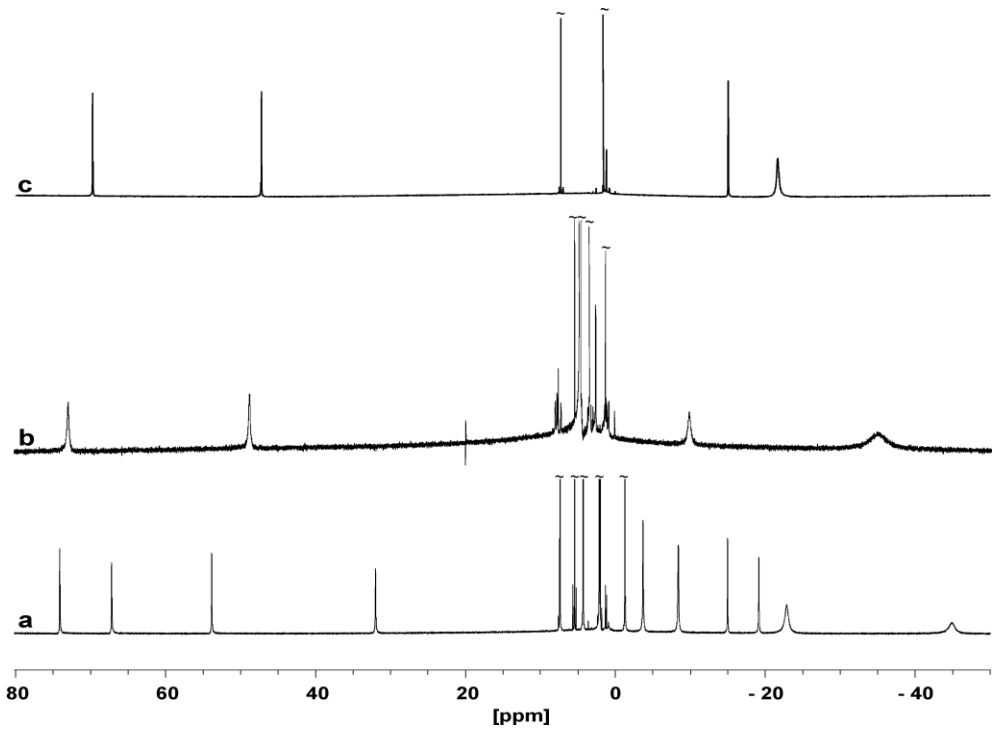

Figure ESI 2: ^{1}H-NMR Spectra of **a**) complex **3** in CD_3CN + CD_2Cl_2, **b**) complex **4** in CD_3OD + $CDCl_3$, **c**) complex **4** in $CDCl_3$. (400 MHz, rt)

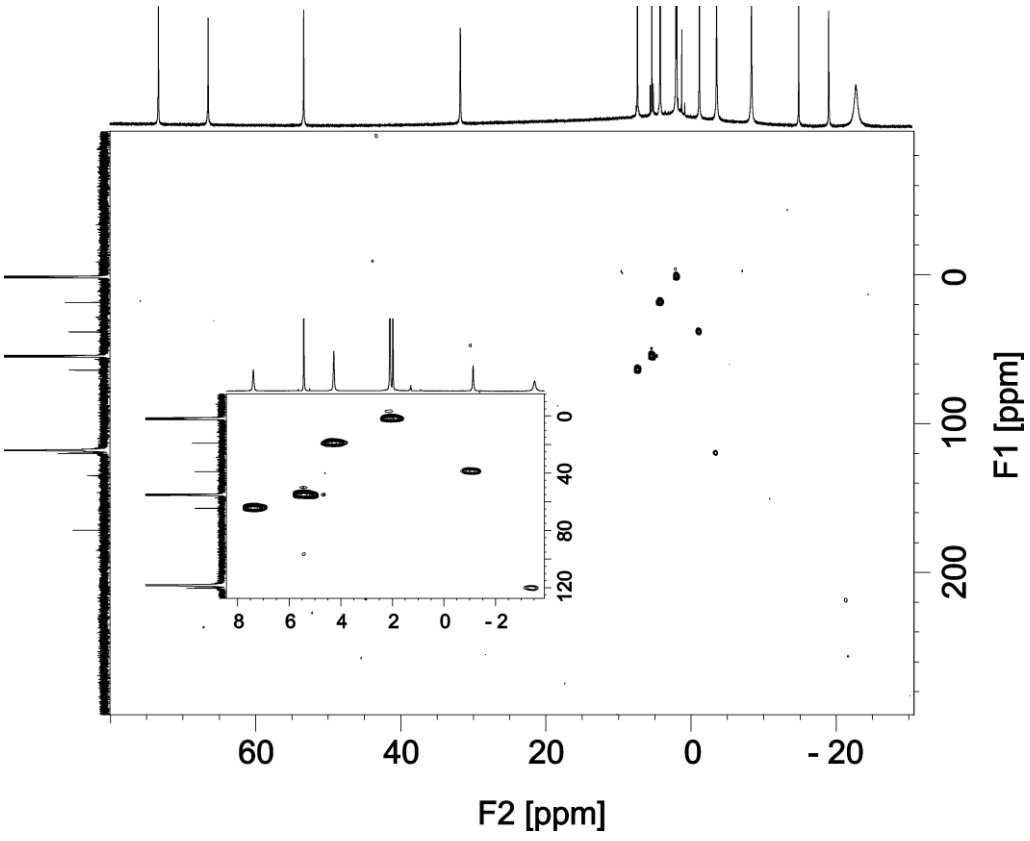

Figure ESI 3: ^{1}H,^{13}C-HSQC NMR Spectrum of complex **3** in CD_3CN + CD_2Cl_2.

Table ESI 1. Selected geometric parameters within calixarene platform in complex **3**.

Ar-CH_2-AR angles [°]		**Ar-CH_2-AR torsion angles [°]**	
C610-C619-C616	88.9(1)	C610-C619-C616-C622	-1.1(1)
C619-C616-C622	90.8(1)	C619-C616-C622-C610	1.1(1)
C616-C622-C610	88.4(1)	C616-C622-C610-C619	-1.1(1)
C622-C610-C619	91.9(1)	C622-C610-C619-C616	1.1(1)

Ar-CH_2-AR distances [Å]		**Phenyl rings parallelity: C_{ortho}-C_{meta} distances [Å]**			
C610-C619	5.055(9)	**Phenyl Co1-Co3**		**Phenyl Co2-Co4**	
C619-C616	5.066(8)	C518-C623	5.337(8)	C620-C611	5.40(1)
C616-C622	5.121(9)	C612-C630	5.304(8)	C624-C617	5.33(1)
C622-C610	5.043(8)	C621-C626	5.515(8)	C517-C627	5.68(1)
C619-C622	7.25(1)	C515-C629	5.446(8)	C613-C615	5.55(1)
C610-C616	7.087(7)				

Table ESI 2: Selected geometric parameters around the cobalt(II) atoms in complex **3**.

Inter-cobalt distances [Å]

Co1-Co2	10.793(2)	Co2-Co3	10.379(2)
Co1-Co3	13.545(2)	Co2-Co4	13.558(2)
Co1-Co4	11.777(2)	Co4-Co3	11.067(2)

Angles in the cobalt quadrangle [°]

Co1-Co4-Co3	72.65(1)	Co2-Co1-Co4	73.70(1)
Co1-Co2-Co3	79.52(1)	Co2-Co3-Co4	78.35(1)

Interplane angle [°]

Along Co2/Co4 axis:	(Co2-Co1-Co4)/(Co2-Co3-Co4)	104.5[a]
Along Co1-Co3 axis:	(Co1-Co4-Co3)/(Co1-Co2-Co3)	102.5[a]

a: esd not available

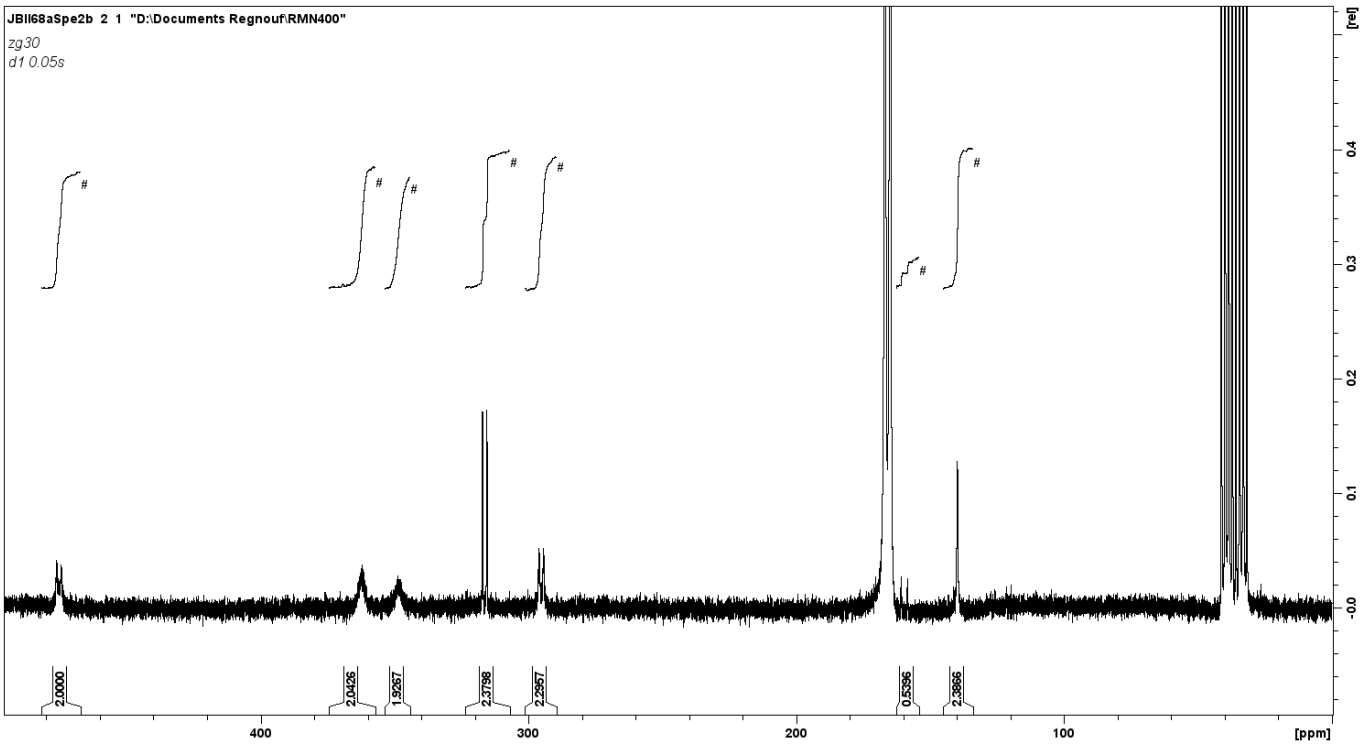

Figure ESI 4: ^{13}C-NMR Spectrum of complex **4** in (*H*)DMF (500-0 ppm; 100 Mhz, rt).

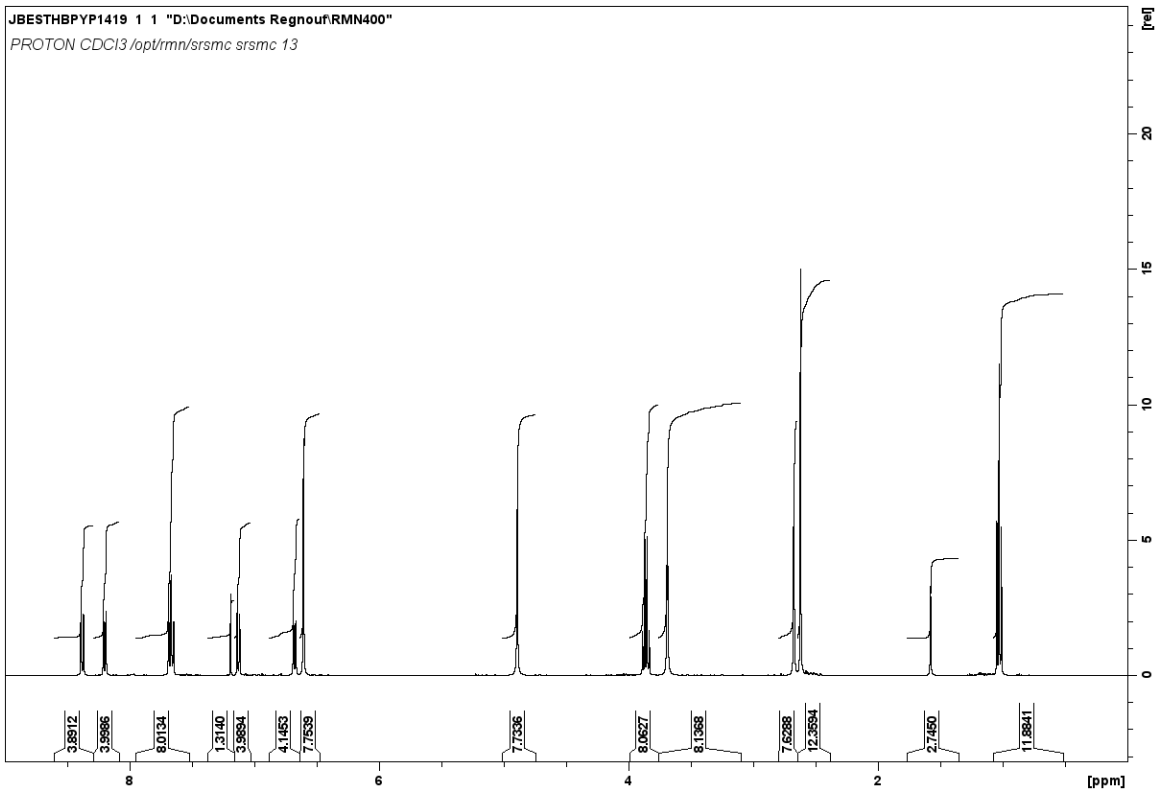

Figure ESI 5: ^{1}H-NMR Spectrum of ligand **2** in $CDCl_3$ (400 Mhz, rt).

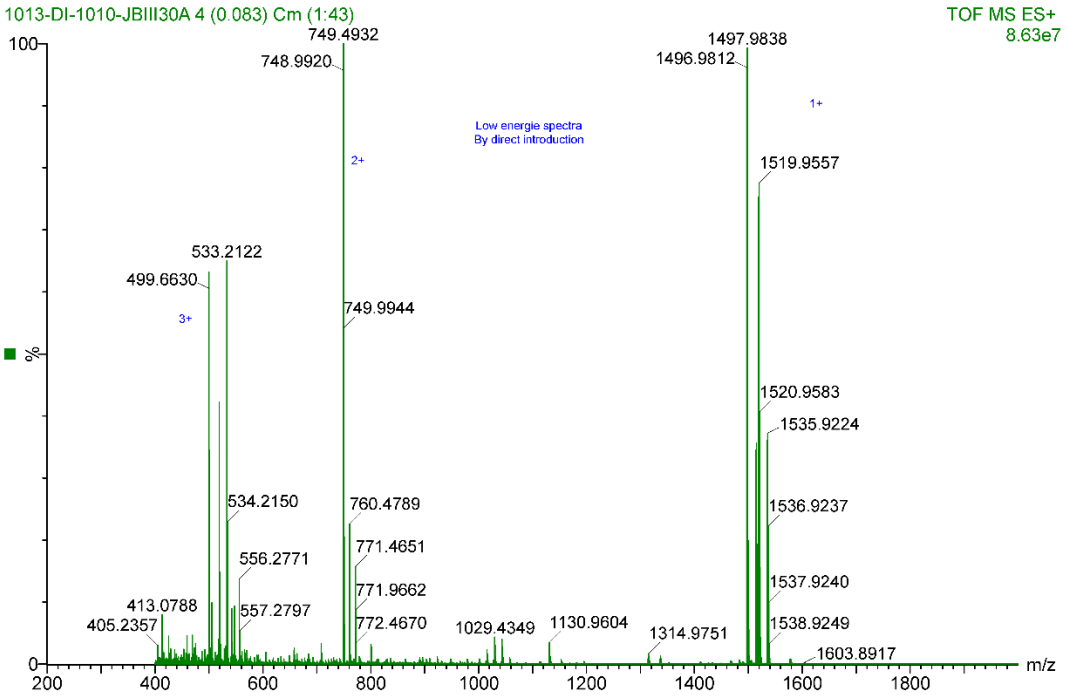

Figure ESI 6: ES-MS positive mode Mass spectrum of complex **3**; direct introduction.

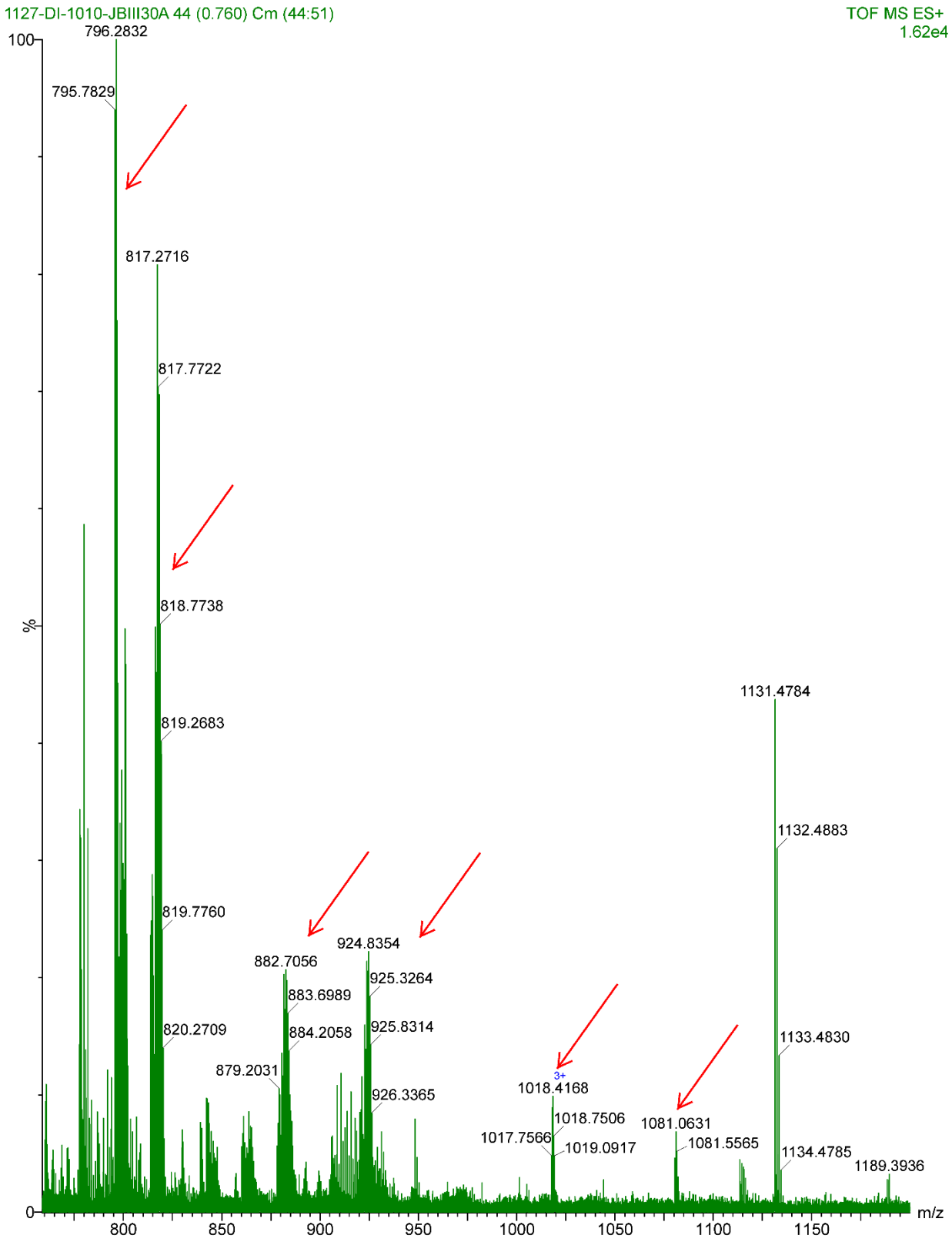

Figure ESI 7: ES-MS positive mode Mass spectrum of complex **3**; direct introduction.