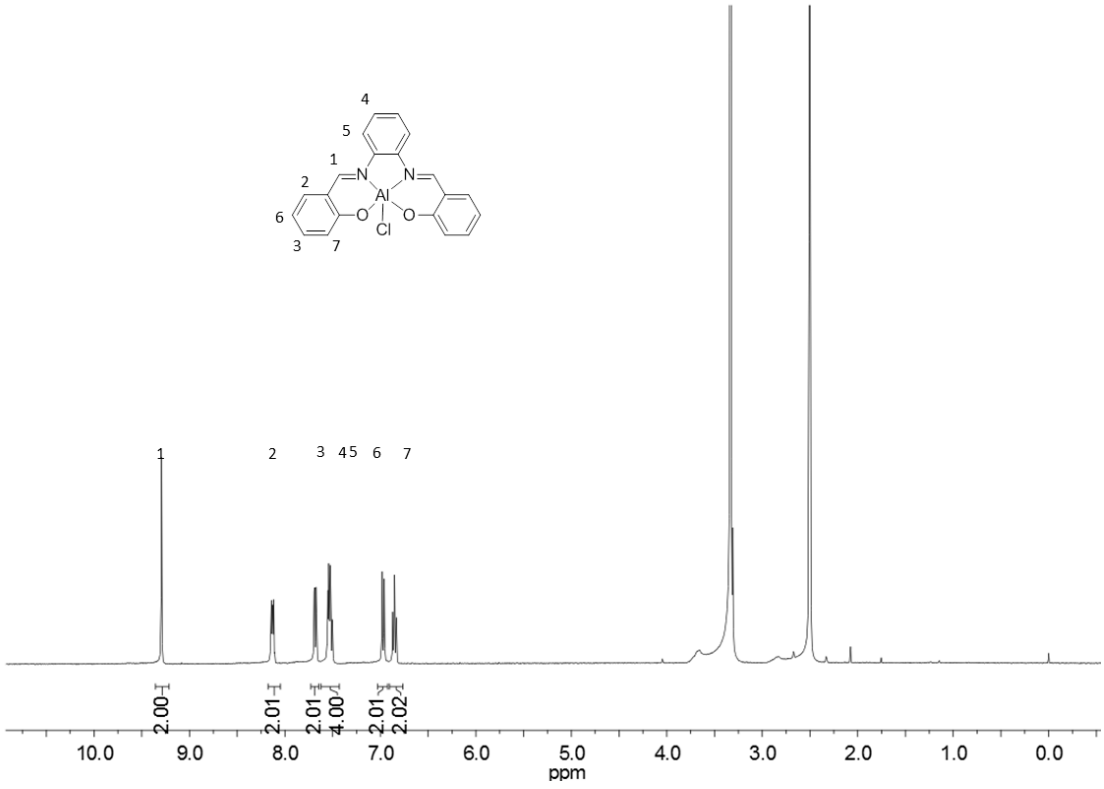
A cryptand-type aluminum tris(salophen) complex: Synthesis, characterization, and cell imaging application

1. ^{1}H-NMR Spectra and HR-ESI MS spectra

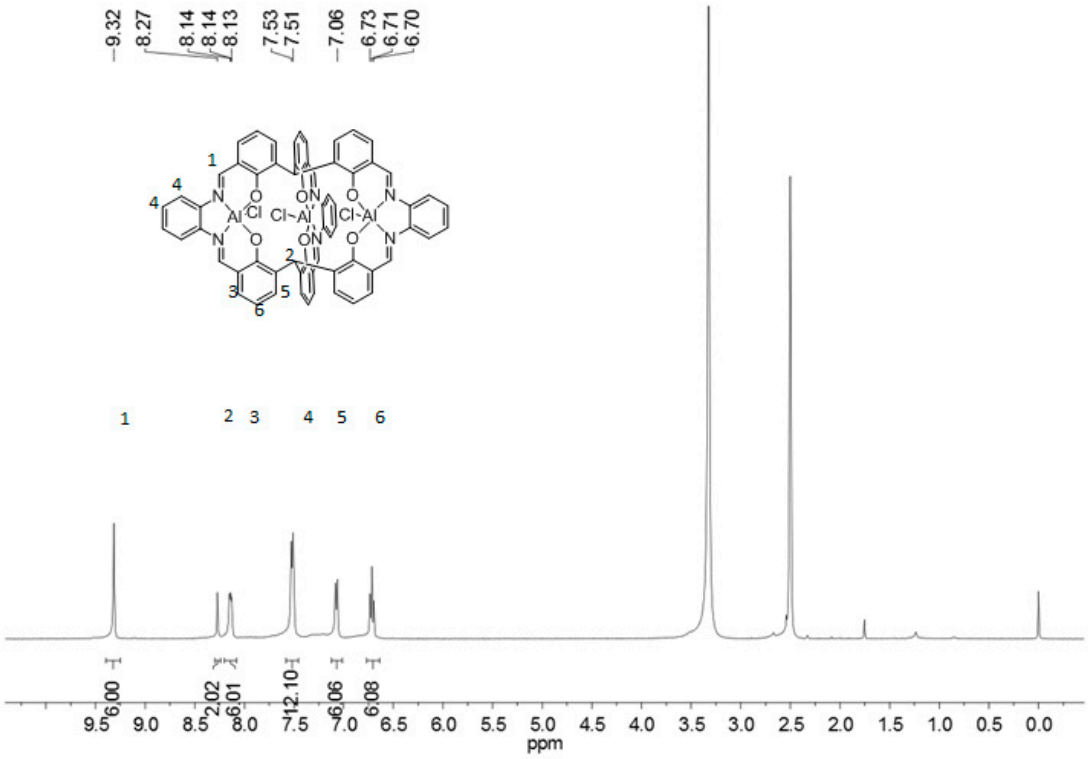
1.1 ^{1}H-NMR Spectra

Unless specially mentioned, the ^{1}H NMR spectra were recorded in DMSO-d6 and the peaks for residue solvent (DMSO, δ= 2.50 ppm), water (δ= 3.33 ppm) and TMS (δ= 0 ppm) were omitted for clarity.

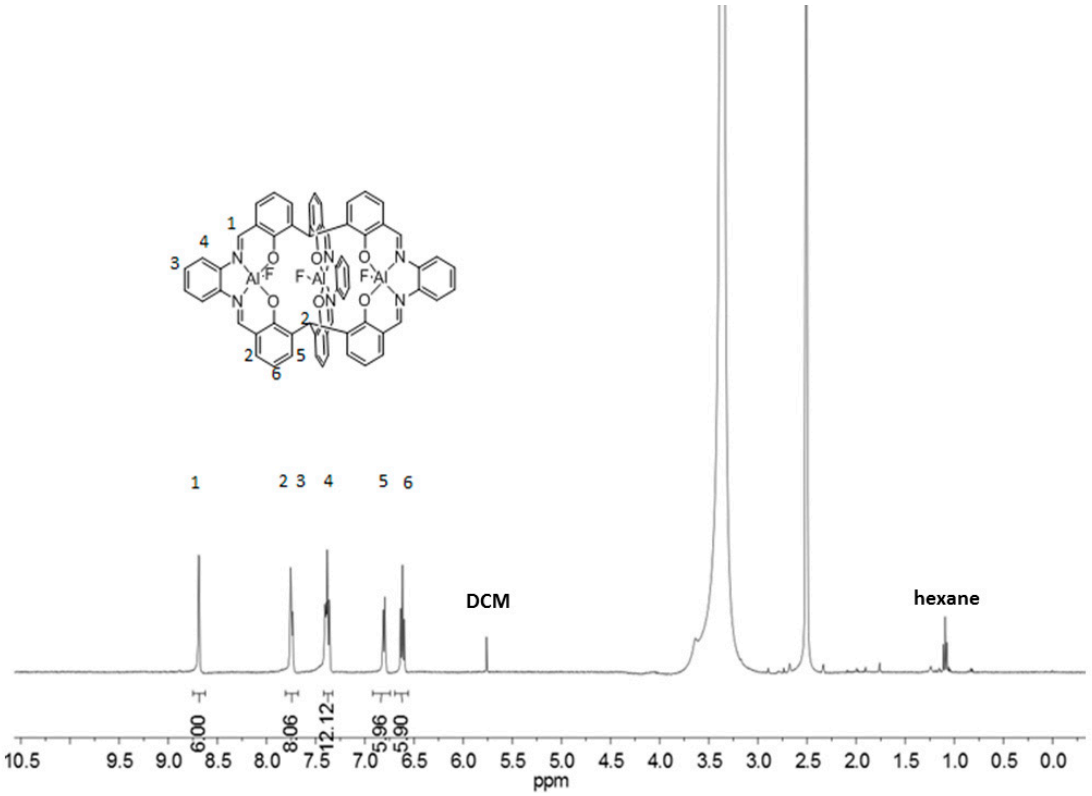
LAl



LAl$_3$

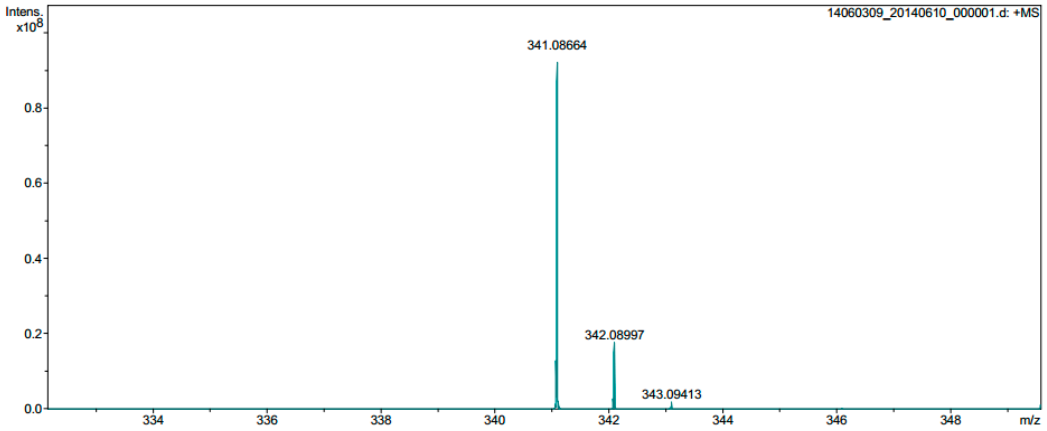

9.32
8.27
8.14
8.14
8.13
7.53
7.51
7.06
6.73
6.71
6.70
Cl-Al
Cl-Al
Cl-Al
1 2 3 4 5 6
6.00
2.02
6.01
12.10
6.06
6.08
ppm

LAl_3-F


F-Al
F-Al
F-Al
1 2 3 4 5 6
DCM
hexane
6.00
8.06
12.12
5.96
5.90
ppm

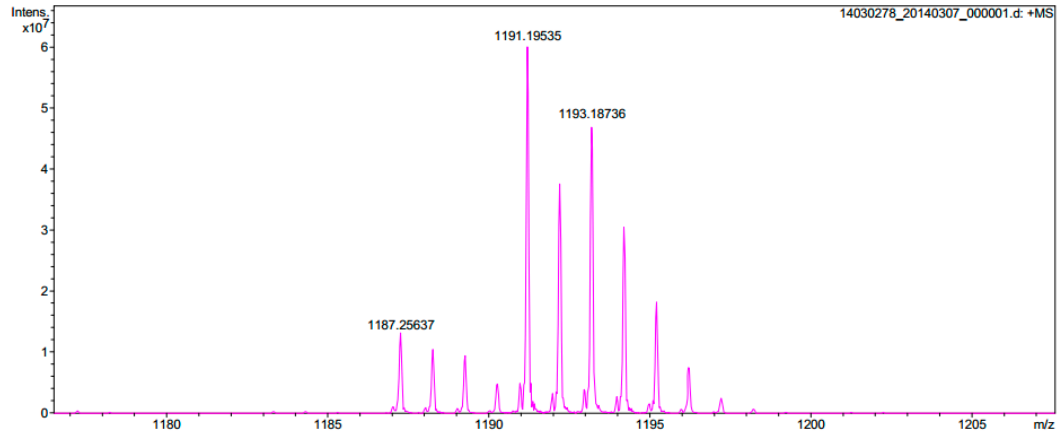
1.2 HR-ESI MS Spectra

LAl



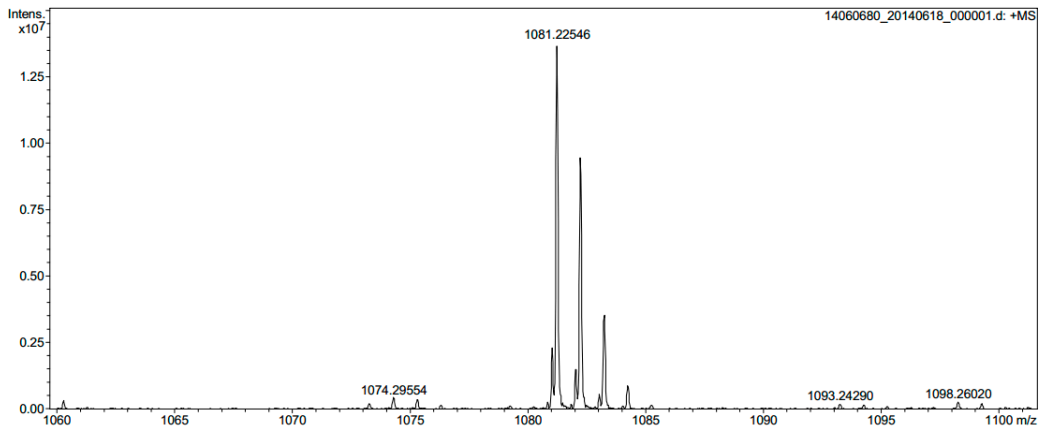
Meas. m/z	I	Formula	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
341.08664	94630888	C 20 H 14 Al N 2 O 2	341.08652	-0.13	-0.37	21.3	15.5	even	ok

LAl_3



Meas. m/z	I	Formula	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
1191.19535	60639056	C 64 H 44 Al 3 Cl 2 N 6 O 7 S	1191.18099	-14.36	-12.05	75.4	46.5	even	ok

LAl_3-F



Meas. m/z	I	Formula	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
1081.22546	13817777	C 62 H 38 Al 3 F 2 N 6 O 6	1081.22616	0.70	0.65	7.0	47.5	even	ok

1.3 Table S1. Crystal data and structure refinement parameters

complex	**LAl_3-F**
molecular formula	C65 H47 Al3 F3 N6 O9
formula wt. (g mol^{-1})	1194.02
temperature (K)	296(2)
radiation (λ, Å)	0.71073
crystal system	Triclinic
space group	*P -1*
a (Å)	13.060(6)
b (Å)	19.920(10)
c (Å)	21.490(11)
α (°)	65.028(6)
β (°)	87.853(7)
γ (°)	89.408(7)
volume ($Å^3$)	5064(4)
Z	2
ρ_{calcd} (mg m^{-3})	0.783
μ (mm^{-1})	0.080
F(000)	1234
crystal size (mm^3)	0.42×0.4× 0.2
theta range (°)	1.834 ~ 24.858
reflections collected	26408
completeness to theta = 24.86°	97.9%
independent reflections	17212 [R(int) = 0.0424]
goodness-of-fit on F^2	1.014
final R indices[R > 2σ (I)]	R_1 = 0.0556, wR_2 = 0.1471
R indices (all data)	R_1 = 0.0991, wR_2 = 0.1635
largest diff. peak and hole (e $Å^{-3}$)	0.460 and -0.292