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

Supporting information

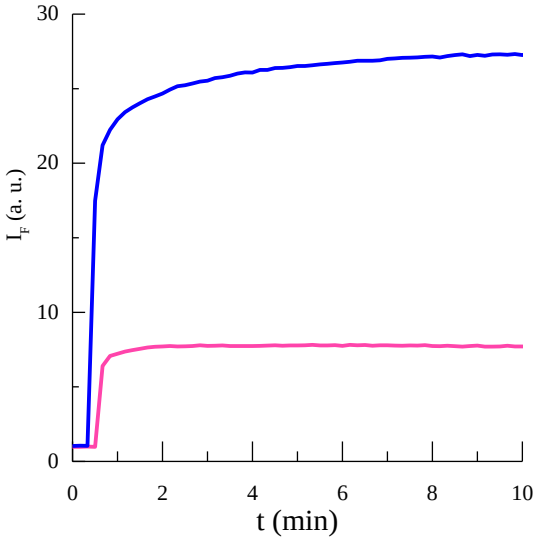


Figure S1: Kinetics study of the complex: [PSSA] = 5 µM with [Al(III)] = 30 µM (pink curve) and [Al(III)] = 150 µM (blue curve) in HEPES (pH 7, 10 mM); λexc. = 390 nm; λobs. = 511 nm

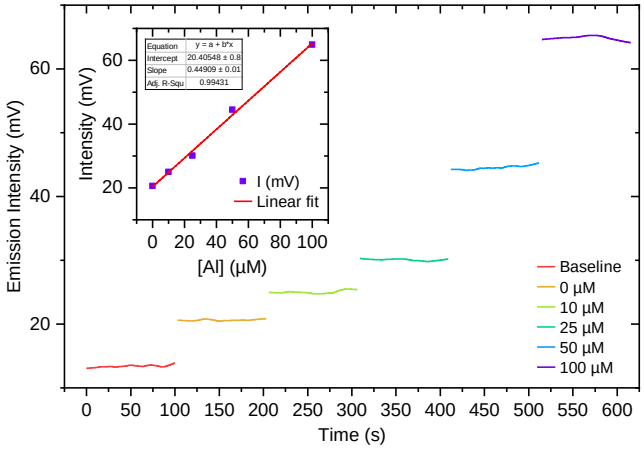
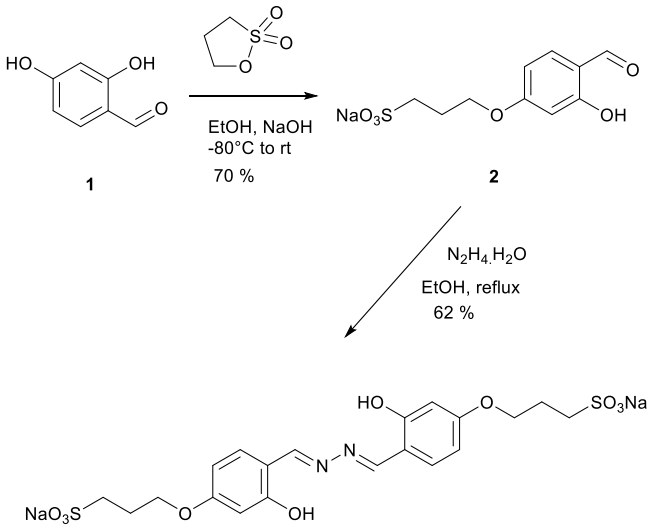


Figure S2 ; Aluminum titration experiments in aqueous HEPES buffer (pH = 7, 10 mM) in function of time for several Al(III) concentration in microfluidic setup functioning in droplet (water-in-oil) regime(λ_{exc} = 365 nm, λ_{em} > 416 nm) [PSSA]= 5 µM

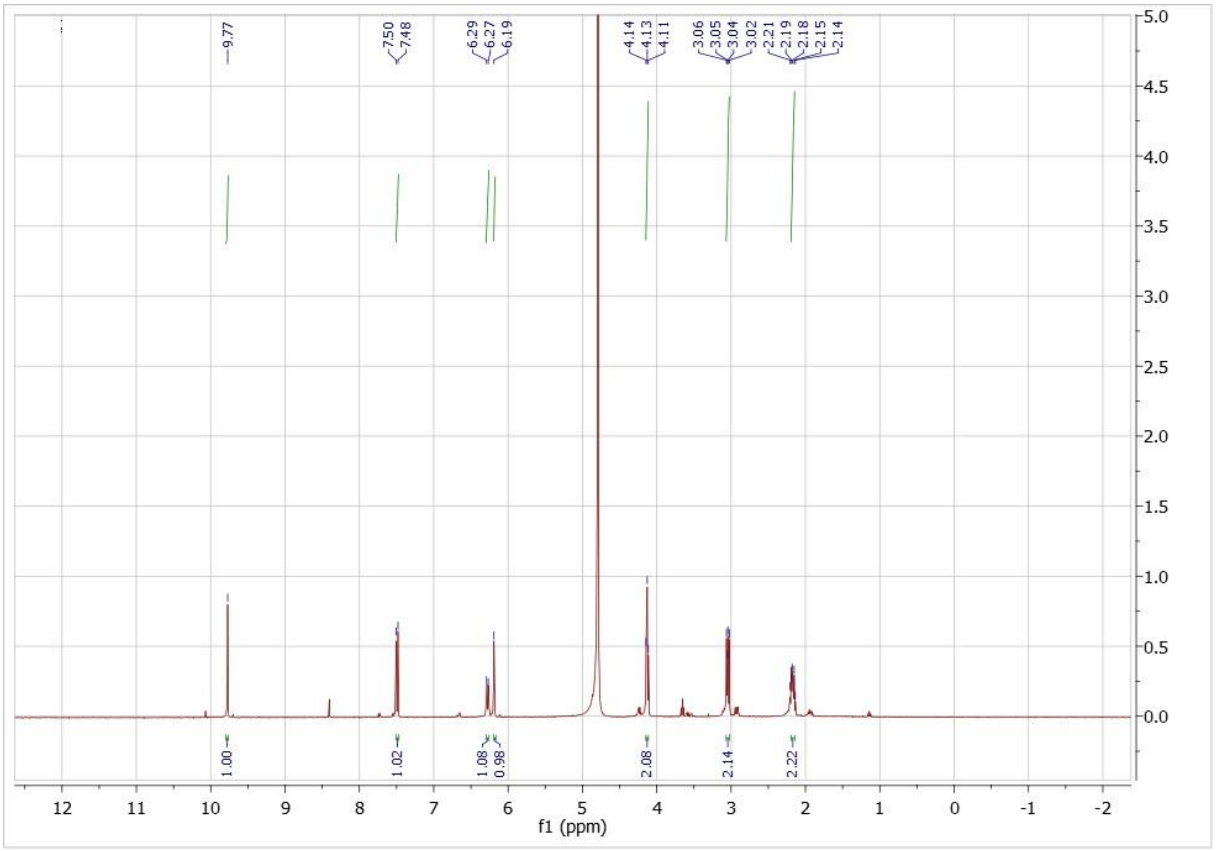


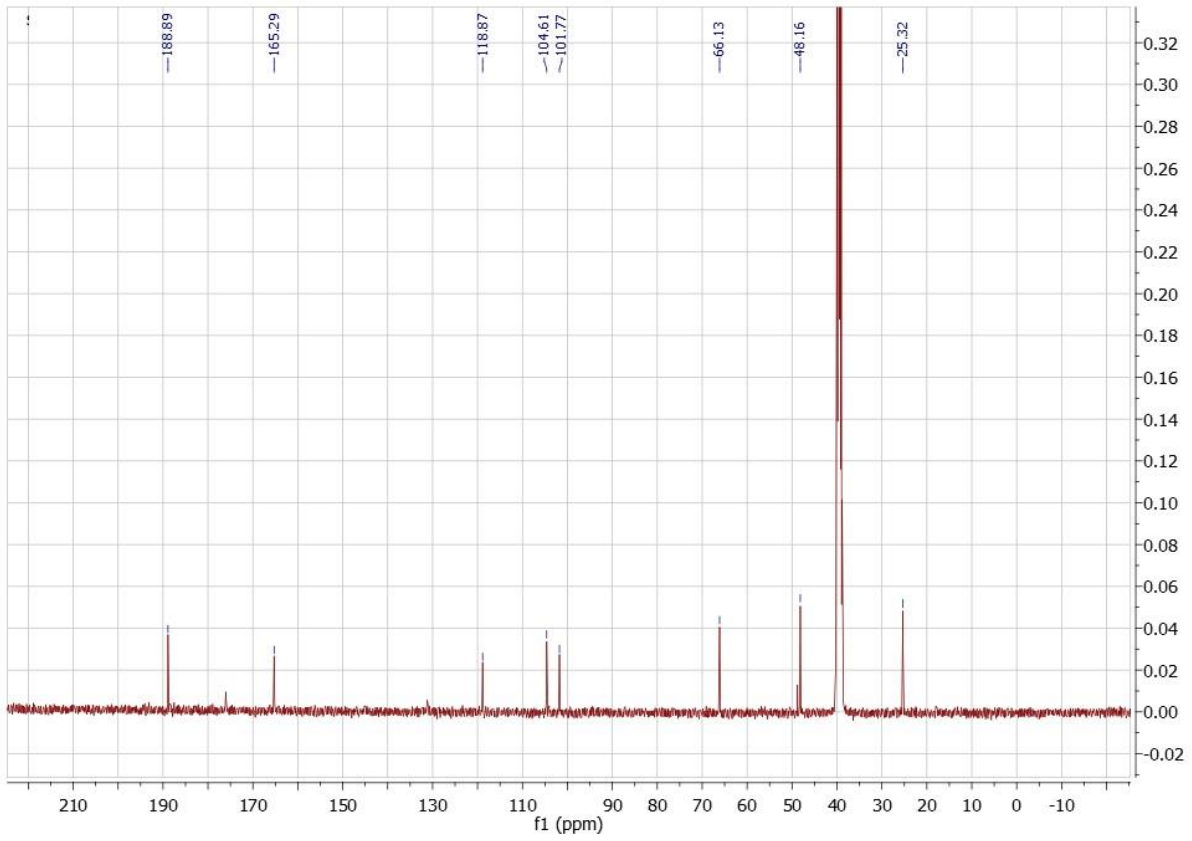
PSSA

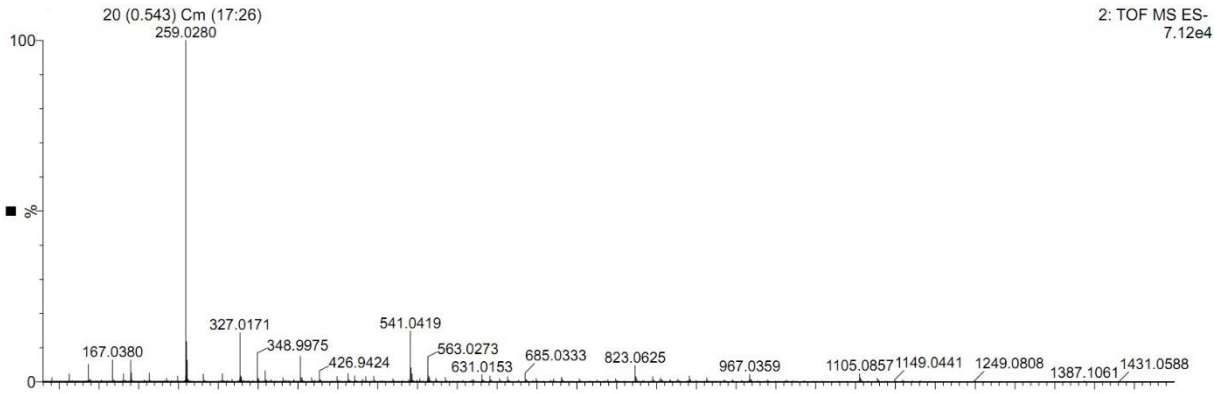
Scheme 1 Synthesis of PSSA ligand:

Compound 2:

^{1}H NMR (D_2O, 400 MHz): δ = 9.77 (s, 1 H, CHO), 7.49 (d, *J* = 8.8 Hz, 2 H, Ar-H), 6.27 (d, *J* = 11.2 Hz, 2 H, Ar-H), 6.18 (s, 1 H, Ar-H), 4.12 (t, *J* = 6 Hz, 2 H, CH_2), 3.02 – 3.06 (m, 2 H, CH_2), 2.16 – 2.20 (m, 2 H, CH_2) ppm. **^{13}C NMR (DMSO-*d*$_6$, 100 MHz):** δ = 188.9, 165.3, 118.9, 104.6, 101.8, 66.1, 48.2, 25.3 ppm. **HRMS (TOF MS ESI):** Calc. for $C_{10}H_{11}O_6S^-$ (m/z): $[M\text{-}Na]^-$ = 259.0276; Found: $[M\text{-}Na]^-$ = 259.0280

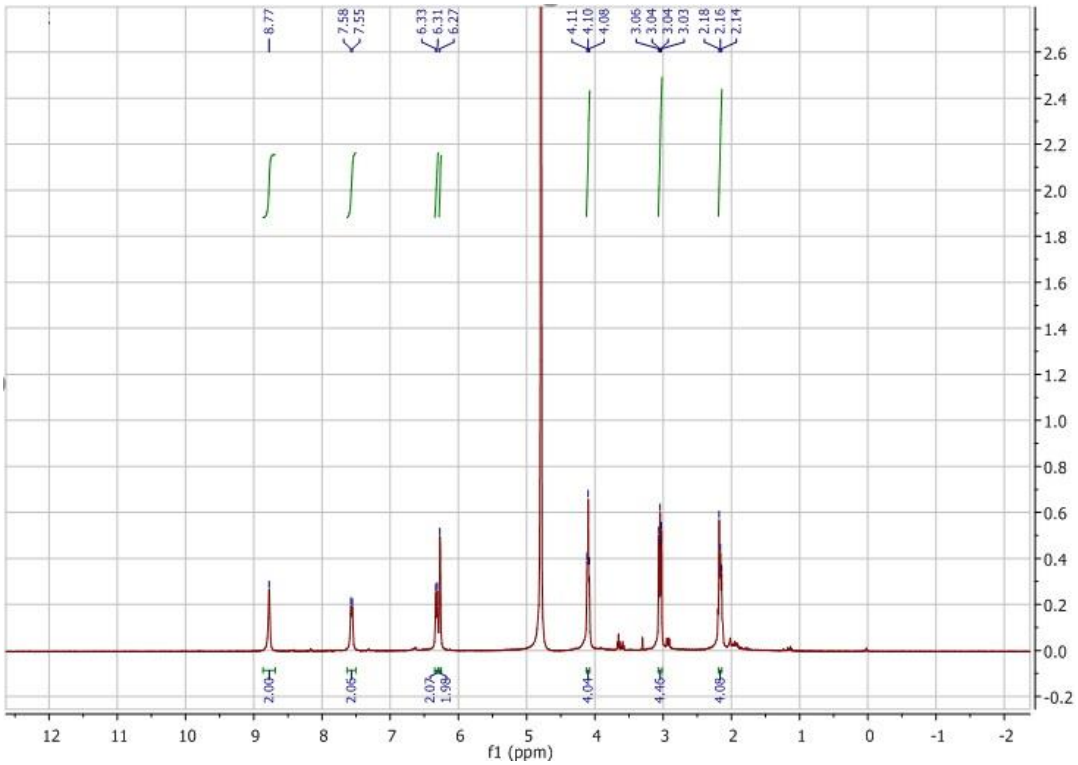






PSSA:

^{1}H NMR (D_2O, 400 MHz): δ = 8.77 (s, 2 H, CHN), 7.56 (d, *J* = 8 Hz, 2 H, Ar-H), 6.31 (d, *J* = 4.4 Hz, 2 H, Ar-H), 6.27 (s, 2 H, Ar-H), 4.09 (t, *J* = 6 Hz, 4 H, CH_2), 3.02 – 3.06 (m, 4 H, CH_2), 2.14 – 2.18 (m, 4 H, CH_2) ppm. **^{13}C NMR (D_2O, 100 MHz):** δ = 163.1, 159.5, 114.4, 104.2, 66.1, 47.8, 24.2 ppm. **HRMS (TOF MS ESI):** Calc. for $C_{20}H_{22}N_2O_{10}NaS_2^-$ (m/z): $[M\text{-}Na]^-$ = 537.0614; Found: $[M\text{-}Na]^-$ = 537.0608


8.77
7.58
7.55
6.33
6.31
6.27
4.11
4.10
4.08
3.06
3.04
3.04
3.03
2.18
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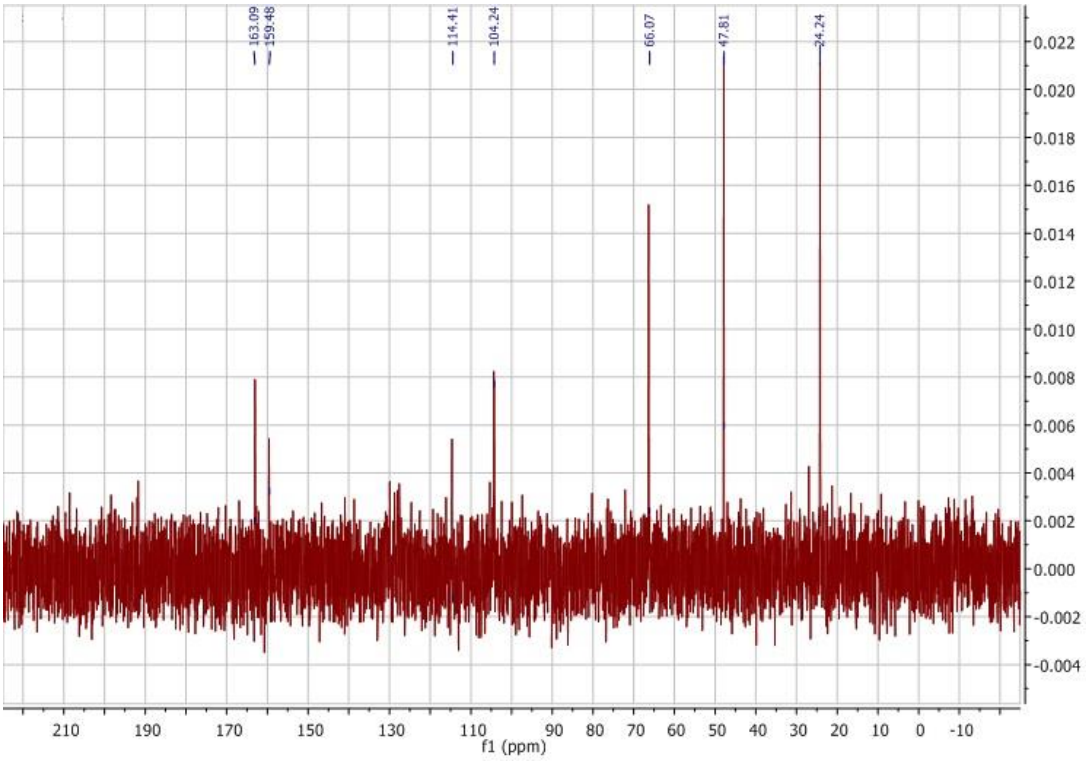
2.14
2.00
2.06
2.07
1.99
4.04
4.46
4.08
f1 (ppm)


163.09
159.48
114.41
104.24
66.07
47.81
24.24
f1 (ppm)

Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 9

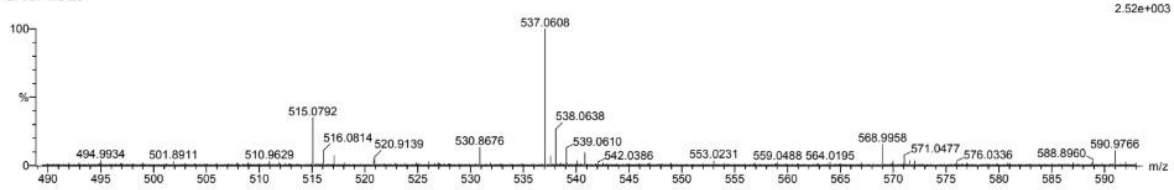
Monoisotopic Mass, Even Electron Ions
336 formula(e) evaluated with 2 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-100 H: 0-110 N: 0-5 O: 0-10 Na: 1-1 S: 2-2

24-Feb-2016 11:45:55
2: TOF MS ES-

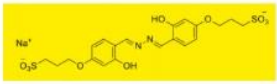
LCT Premier XE KE483

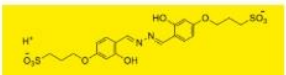
20 (0.543) Cm (17:26)

2.52e+003



Minimum:				-1.5				
Maximum:		6.3	5.0	100.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula	
537.0608	537.0614	-0.6	-1.1	10.5	819.5	0.0	C20 H22 N2 O10 Na S2	
	537.0595	1.3	2.4	23.5	824.1	4.6	C32 H18 O3 Na S2	





Chemical Formula: $C_{20}H_{23}N_2O_{10}S_2^-$
Exact Mass: 515.0800
Molecular Weight: 515.5346
m/z: 515.0799 (100.0%),