

Supplementary Information

Table S1: Formula, m/z and isotope distribution of main metal(III) containing ions detected by ESI-MS.

Ion composition	m/z (isotopic distribution, %)
[La(Mon)₃(H₂O)₃], 1	
[La(C₃₆H₆₀O₁₁)₃]⁺ (C₃₆H₆₀LaO₁₁)⁺ Exact Mass: 807.32	807.32 (100.0%) , 808.32 (39.3%), 809.33 (7.8%), 809.32 (2.3%), 810.33 (1.9%)
[La(C₃₆H₆₁O₁₁)₂]⁺ (C₇₂H₁₂₂LaO₂₂)⁺ Exact Mass: 1477.75	1477.75 (100.0%) , 1478.75 (78.7%), 1479.76 (31.6%), 1480.76 (11.8%), 1479.75 (4.5%), 1481.76 (3.0%), 1478.76 (1.4%)
[La(C₃₆H₆₁O₁₁)(C₃₆H₆₀O₁₁Na)]⁺ (C₇₂H₁₂₁LaNaO₂₂)⁺ Exact Mass: 1499.73	1499.73 (100.0%) , 1500.73 (77.9%), 1501.74 (36.2%), 1502.74 (11.8%), 1503.74 (2.9%), 1500.74 (2.3%)
[La(C₃₆H₆₁O₁₁)₃Na]⁺ (C₁₀₈H₁₈₃LaNaO₃₃)⁺ Exact Mass: 2170.16	2171.16 (100.0%) , 2170.16 (84.8%), 2172.17 (60.6%), 2173.17 (30.7%), 2174.17 (10.8%), 2172.16 (5.7%), 2171.17 (1.8%), 2175.17 (1.7%), 2175.18 (1.7%)
[La(C₃₆H₆₁O₁₁Na)(C₃₆H₆₀O₁₁)₂]⁺ (C₁₀₈H₁₈₂LaNa₂O₃₃)⁺ Exact Mass: 2192.14	2193.15 (100.0%) , 2192.14 (83.2%), 2194.15 (65.2%), 2195.15 (29.0%), 2196.16 (6.9%), 2196.15 (4.1%), 2197.16 (3.1%), 2195.16 (1.2%)
[Nd(Mon)₃(H₂O)₃], 2	
[Nd(C₃₆H₆₀O₁₁)₃]⁺ (C₃₆H₆₀NdO₁₁)⁺ Exact Mass: 810.32	810.32 (100.0%) , 812.32 (87.5%), 814.33 (85.3%), 811.32 (83.8%), 813.33 (72.0%), 815.33 (30.0%), 812.33 (28.0%), 816.33 (27.6%), 818.33 (21.1%), 817.33 (8.8%), 819.34 (8.6%), 820.34 (2.1%), 818.34 (1.8%), 811.33 (1.1%)
[Nd(C₃₆H₆₁O₁₁)₂]⁺ (C₇₂H₁₂₂NdO₂₂)⁺ Exact Mass: 1480.75	1483.76 (100.0%) , 1484.76 (99.0%), 1481.75 (96.0%), 1480.75 (77.7%), 1482.75 (71.5%), 1485.76 (56.5%), 1482.76 (52.5%), 1486.76 (35.4%), 1488.76 (16.8%), 1489.77 (15.1%), 1487.76 (14.6%), 1488.77 (6.8%), 1490.77 (6.3%), 1487.77 (5.4%), 1486.77 (3.9%), 1491.77 (1.9%), 1481.76 (1.1%), 1485.77 (1.0%)
[Nd(C₃₆H₆₁O₁₁Na)(C₃₆H₆₀O₁₁)₂]⁺ (C₁₀₈H₁₈₂Na₂NdO₃₃)⁺ Exact Mass: 2195.14	2197.15 (100.0%) , 2198.15 (93.1%), 2199.15 (79.5%), 2196.15 (75.1%), 2195.14 (45.5%), 2200.15 (38.1%), 2201.16 (31.9%), 2200.16 (26.2%), 2202.16 (25.4%), 2203.16 (21.0%), 2204.16 (15.2%), 2201.15 (11.6%), 2199.16 (10.5%), 2205.16 (7.6%), 2206.17 (3.0%), 2207.17 (1.3%), 2205.17 (1.2%), 2198.16 (1.1%)
[Nd₂(C₃₆H₆₀O₁₁)₂(C₃₆H₆₁O₁₁)₂]⁺ (C₁₀₈H₁₈₁Nd₂O₃₃)⁺ Exact Mass: 2290.06	2294.07 (100.0%) , 2293.07 (85.7%), 2297.08 (73.2%), 2295.07 (73.1%), 2292.07 (68.5%), 2298.08 (62.0%), 2296.07 (54.8%), 2299.08 (52.6%), 2296.08 (44.8%), 2300.08 (38.2%), 2291.07 (37.7%), 2295.08 (31.4%), 2301.08 (21.2%), 2290.06 (18.0%), 2302.09 (15.9%), 2303.09 (13.8%), 2301.09 (9.0%), 2304.09 (8.1%), 2298.07 (7.2%), 2294.08 (7.1%), 2297.07 (6.9%), 2302.08 (6.2%), 2300.09 (4.8%), 2305.09 (4.0%), 2306.09 (2.1%), 2299.09 (1.3%), 2307.09 (1.0%)

Table S2: Statistical analysis of experimental results using MDB-MB-231 cell line, MTT test (ns – not significant; * p < 0.05; ** p < 0.01; *** p < 0.001).

Dunnett's Multiple Comparison Test	Mean Diff.	q	Significant? p < 0.05?	Summary
24 h				
Control vs [La(Mon) ₃ (H ₂ O) ₃], 1	24.74	1.748	No	ns
Control vs [Nd(Mon) ₃ (H ₂ O) ₃], 2	26.55	1.876	No	ns
48 h				
Control vs Monensic acid	25.10	1.511	No	ns
Control vs [La(Mon) ₃ (H ₂ O) ₃], 1	71.19	4.286	Yes	**
Control vs [Nd(Mon) ₃ (H ₂ O) ₃], 2	71.95	4.332	Yes	**
72 h				
Control vs DMSO	28.03	2.862	Yes	*
Control vs Monensic acid	90.10	9.198	Yes	***
Control vs [La(Mon) ₃ (H ₂ O) ₃], 1	85.93	8.773	Yes	***
Control vs [Nd(Mon) ₃ (H ₂ O) ₃], 2	87.55	8.938	Yes	***

Table S3: Statistical analysis of experimental results using LSF-SR-SR cell line, MTT test (ns – not significant; * p < 0.05; ** p < 0.01; *** p < 0.001).

Dunnett's Multiple Comparison Test	Mean Diff.	q	Significant? p < 0.05?	Summary
24 h				
Control vs [La(Mon) ₃ (H ₂ O) ₃], 1	13.42	0.7587	No	ns
Control vs [Nd(Mon) ₃ (H ₂ O) ₃], 2	20.71	1.171	No	ns
48 h				
Control vs [La(Mon) ₃ (H ₂ O) ₃], 1	77.93	5.834	Yes	***
Control vs [Nd(Mon) ₃ (H ₂ O) ₃], 2	73.42	5.496	Yes	***
72 h				
Control vs DMSO	28.03	2.862	Yes	*
Control vs Monensic acid	90.10	9.198	Yes	***
Control vs [La(Mon) ₃ (H ₂ O) ₃], 1	85.93	8.773	Yes	***
Control vs [Nd(Mon) ₃ (H ₂ O) ₃], 2	87.55	8.938	Yes	***