

Supplementary Information

Structural speciation of Ti(IV)-(α -hydroxycarboxylic acid) complexes in metabolism-related (patho)physiology. *In vitro* approaches to (pre)adipocyte differentiation and mineralization.

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Figure Captions

Figure S1: ESI-MS spectrum of compound **1** in water (positive mode). Full scan spectrum, and simulated spectrum: $M_1 = [\text{Ti}(\text{L}_1)_3]$, ($m/z = 357.0683$, $z = 1$, $[\text{M}_1\text{H}_3]^+$).

Figure S2: ESI-MS spectrum of compound **2** in water (positive mode). Full scan spectrum, and simulated spectrum: $M_2 = [\text{Ti}(\text{L}_1)_3((\text{CH}_6\text{N}_3)_2)]$, ($m/z = 475.1627$, $z = 1$, $[\text{M}_2\text{H}]^+$).

Figure S3: ESI-MS spectrum of compound **3** in water (positive mode). Full scan spectrum, and simulated spectrum: $M_{3_1} = [\text{Ti}(\text{L}_2)_3]$, ($m/z = 621.1262$, $z = 1$, $[\text{M}_{3_1}\text{H}_3]^+$) and $M_{3_2} = [\text{Ti}(\text{L}_2)_2]$, ($m/z = 429.0590$, $z = 1$, $[\text{M}_{3_2}\text{H}]^+$).

Figure S4: ESI-MS spectrum of compound **4** in water (positive mode). Full scan spectrum, and simulated spectrum: $M_4 = [\text{Ti}(\text{L}_3\text{H})_2(\text{L}_3)]$, ($m/z = 479.1509$, $z = 1$, $[\text{M}_4\text{K}]^+$).

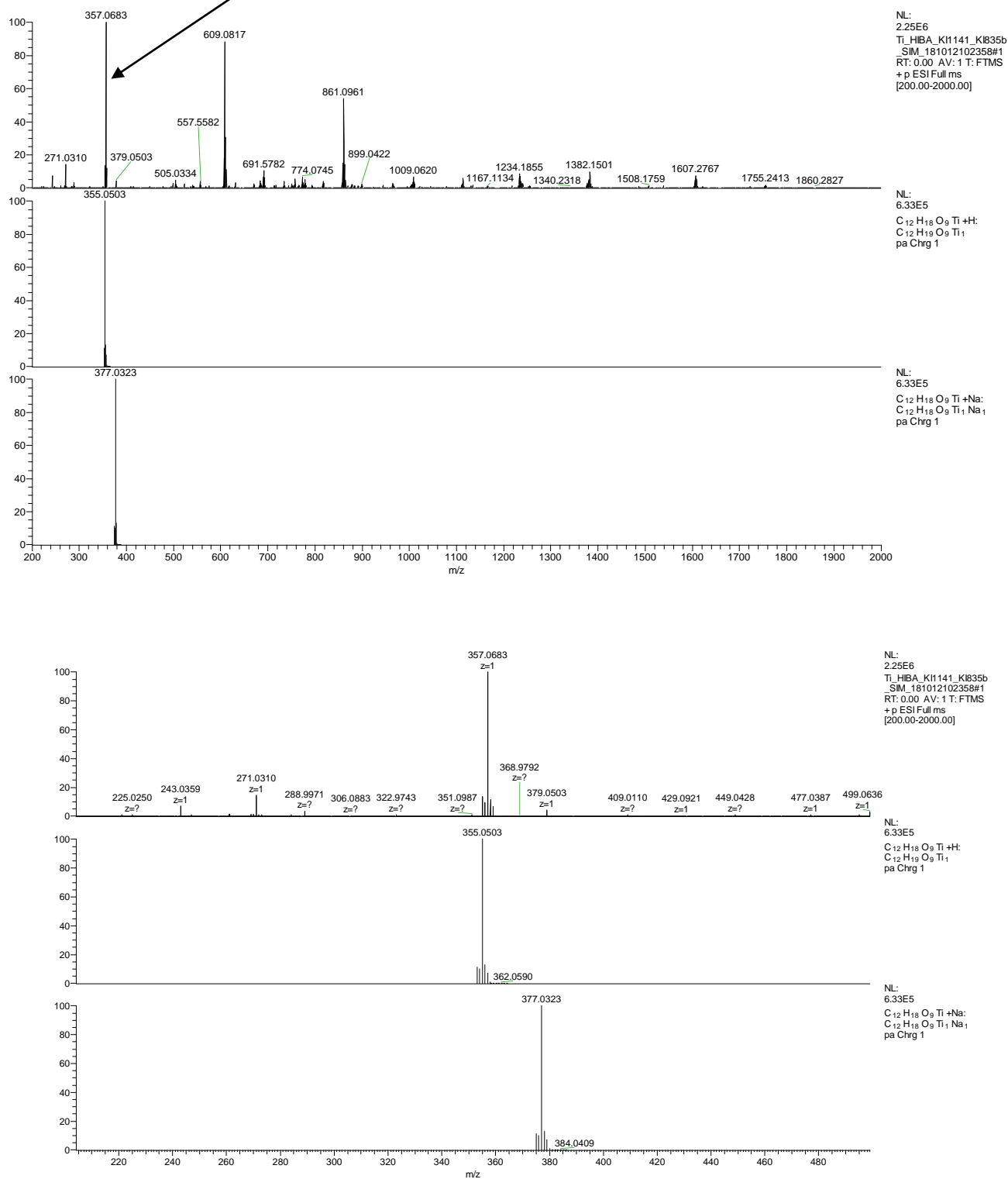
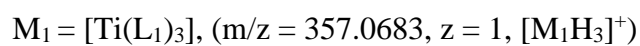


Figure S1

$M_2 = [Ti(L_1)_3((CH_6N_3)_2)]$, ($m/z = 475.1627$, $z = 1$, $[M_2H]^+$)

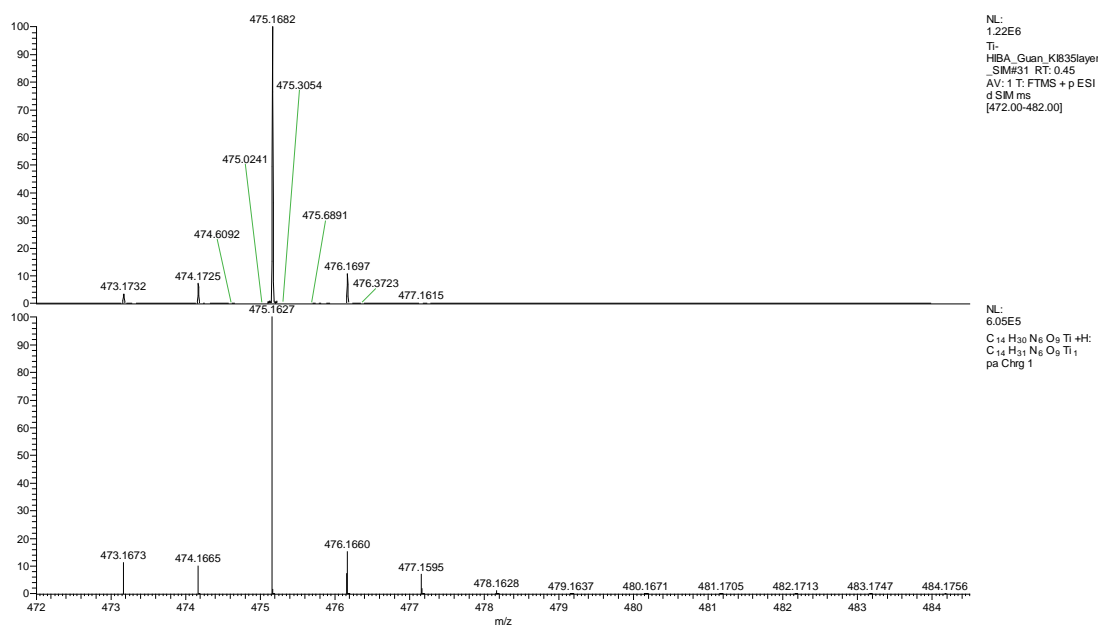
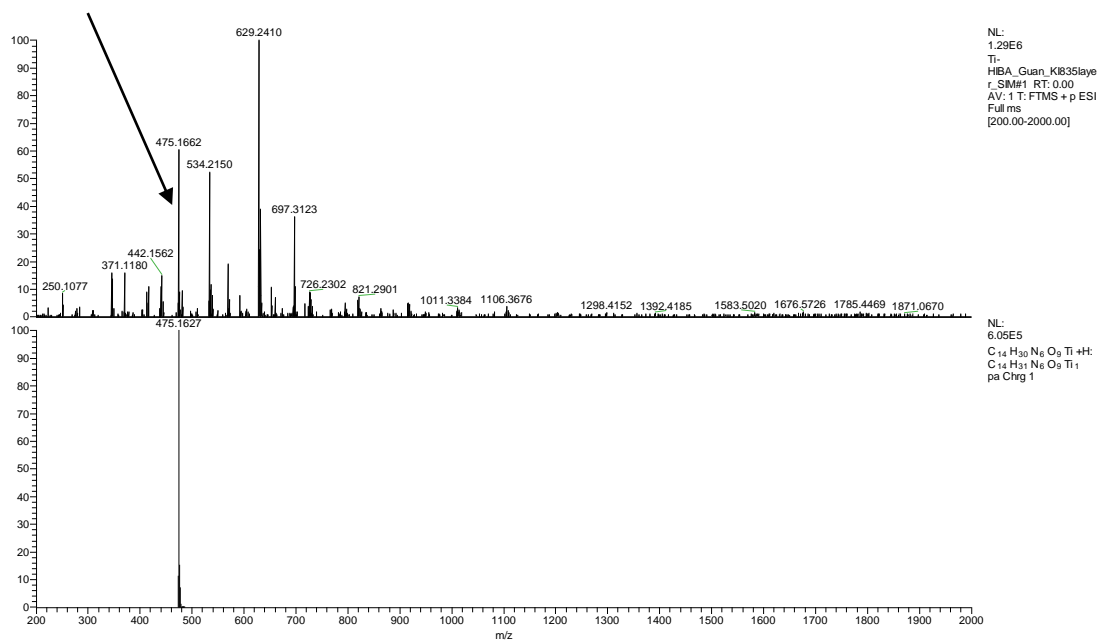


Figure S2

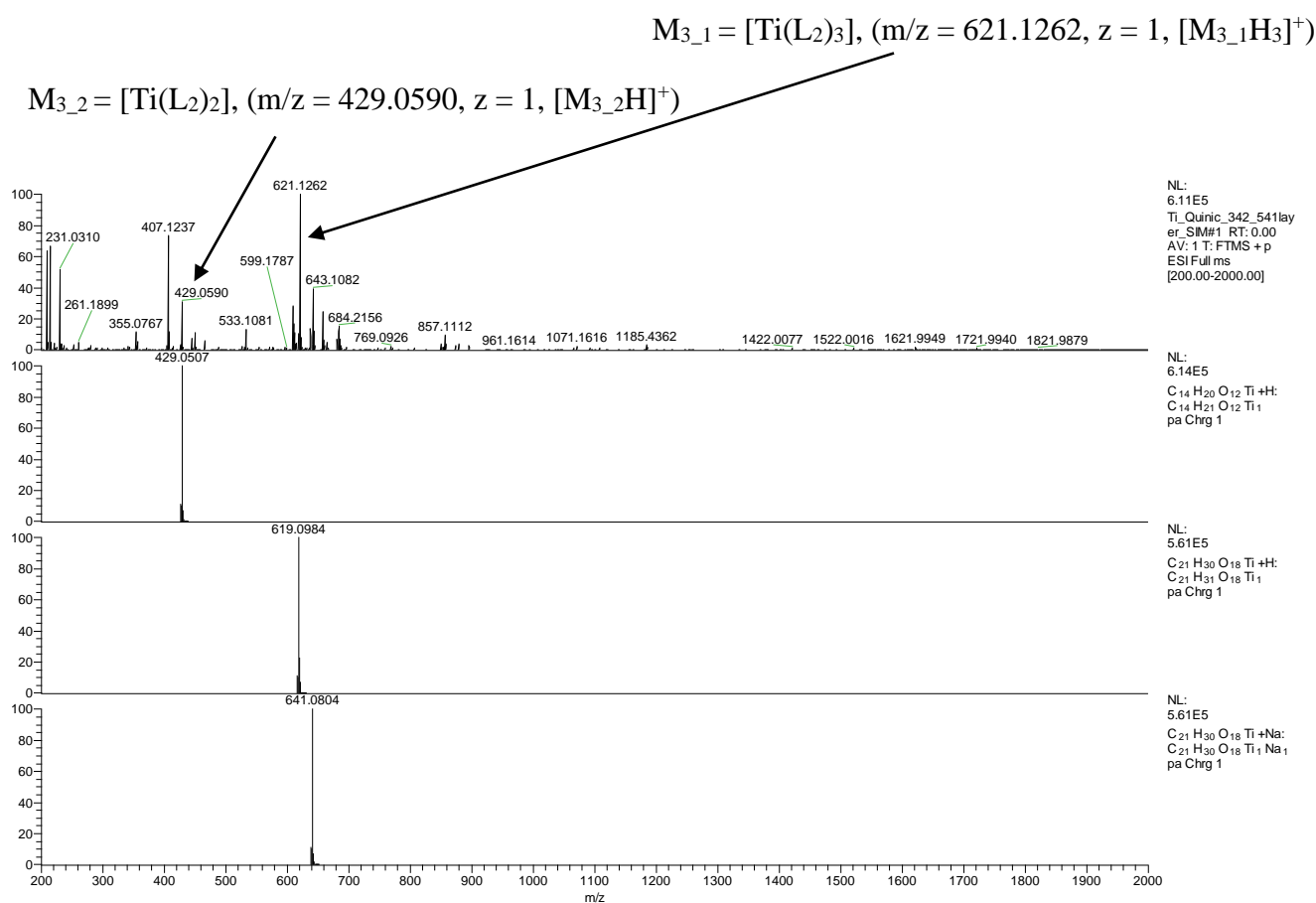


Figure S3

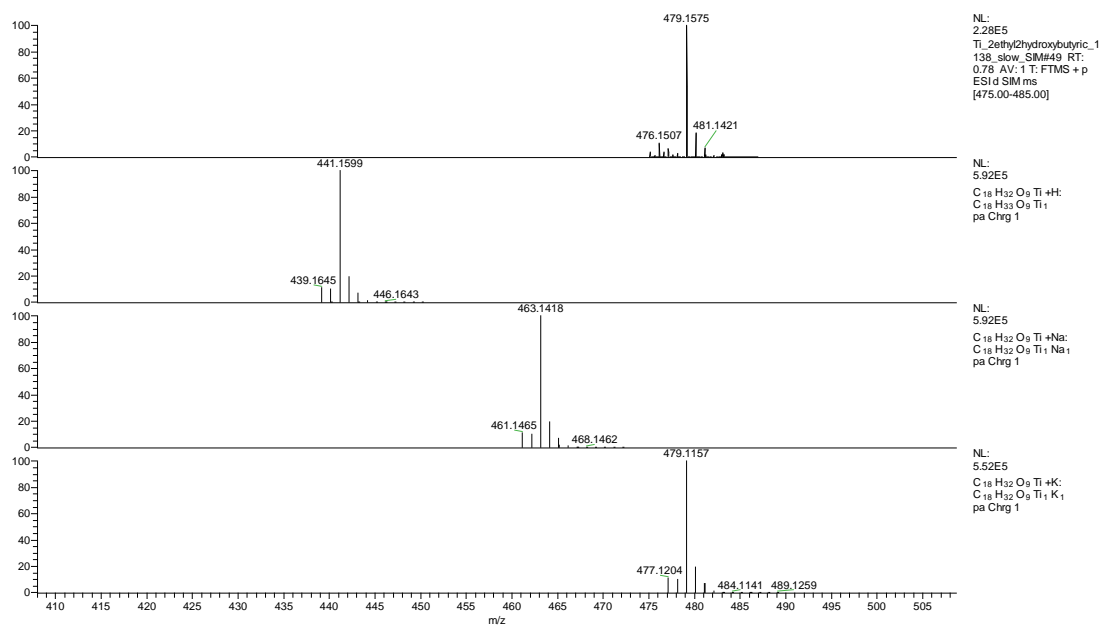
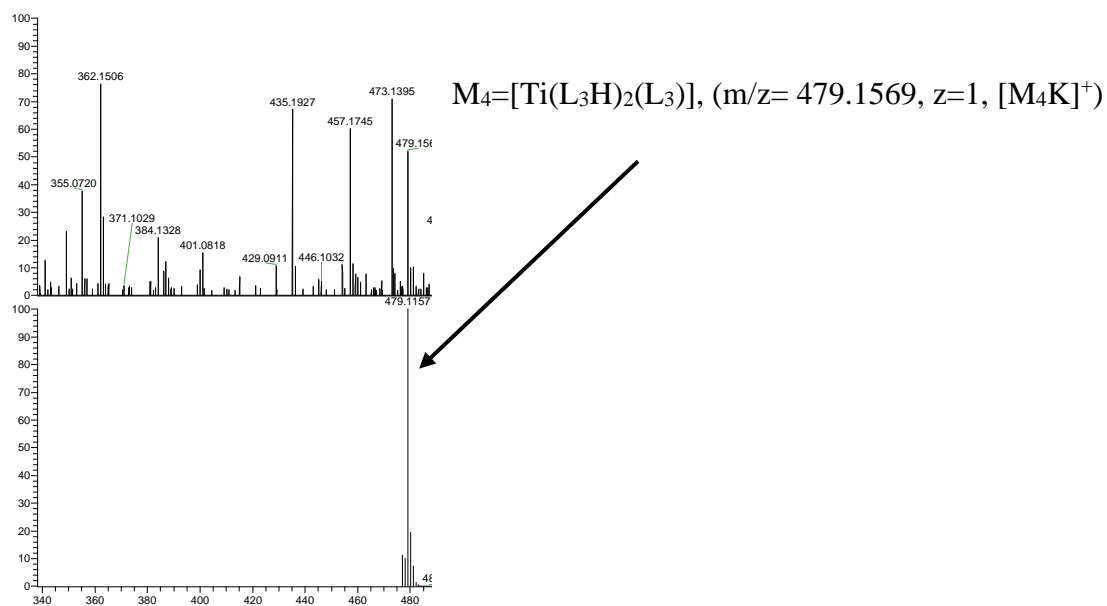


Figure S4