## **Supplementing Material**





(b) Peaks for species  $[Zn_2LaL(L-CH_2)(OH)(OCN)(CH_3CN)(H_2O)]^+$ Theoretical isotope:  $C_{38}H_{40}O_{11}N_6Zn_2La = 1027.0364$  (Error: 3.6025 ppm)



(c) Peaks for species  $[Zn_2La(L-CH_2)_2(OCN)_2(CH_3CN)(H_2O)]^+$ Theoretical isotope:  $C_{36}H_{33}O_{11}N_7Zn_2La = 1009.9846$  (Error: 4.3565 ppm)









(b) Peaks for species  $[Zn_2Nd(L-CH_2)_2(OCN)_2(OH)(CH_3CN)(H_2O)]^+$ Theoretical isotope:  $C_{37}H_{38}O_{11}N_6Zn_2Nd = 1016.0259$  (Error: -3.3463 ppm)



(c) Peaks for species  $[Zn_2Nd(L-CH_2)L(OCN)(OH)(CH_3CN)(H_2O)]^+$ Theoretical isotope:  $C_{38}H_{40}O_{11}N_6Zn_2Nd = 1030.0416$  (Error: -5.4366 ppm)



(d) Peaks for species  $[Zn_2NdL_2(OCN)(OH)(CH_3CN)(H_2O)]^+$ Theoretical isotope:  $C_{39}H_{42}O_{11}N_6Zn_2Nd = 1044.0573$  (Error: -2.2029 ppm)





(b) Peaks for species  $[M - NO_3]^+$ Theoretical isotope:  $C_{38}H_{36}O_8N_6S_2Zn_2La = 1038.9643$  (Error: 4.0424 ppm)



## Figure 4. ESI HR-MS spectrum of the complex 3b:

(b) Peaks for species  $[M - NO_3]^+$ Theoretical isotope:  $C_{38}H_{36}O_8N_6S_2Zn_2Nd = 1041.9696$  (Error: 1.5355 ppm)