Electronic Supplementary Information.

Selective union of ATP vs ADP to an amino/amide macrocycle and its Cu^{2+} complexes: potentiometric, spectrophotometric and theoretical approximations.

Armando Ferrer Serrano and Yennys Hernández Molina

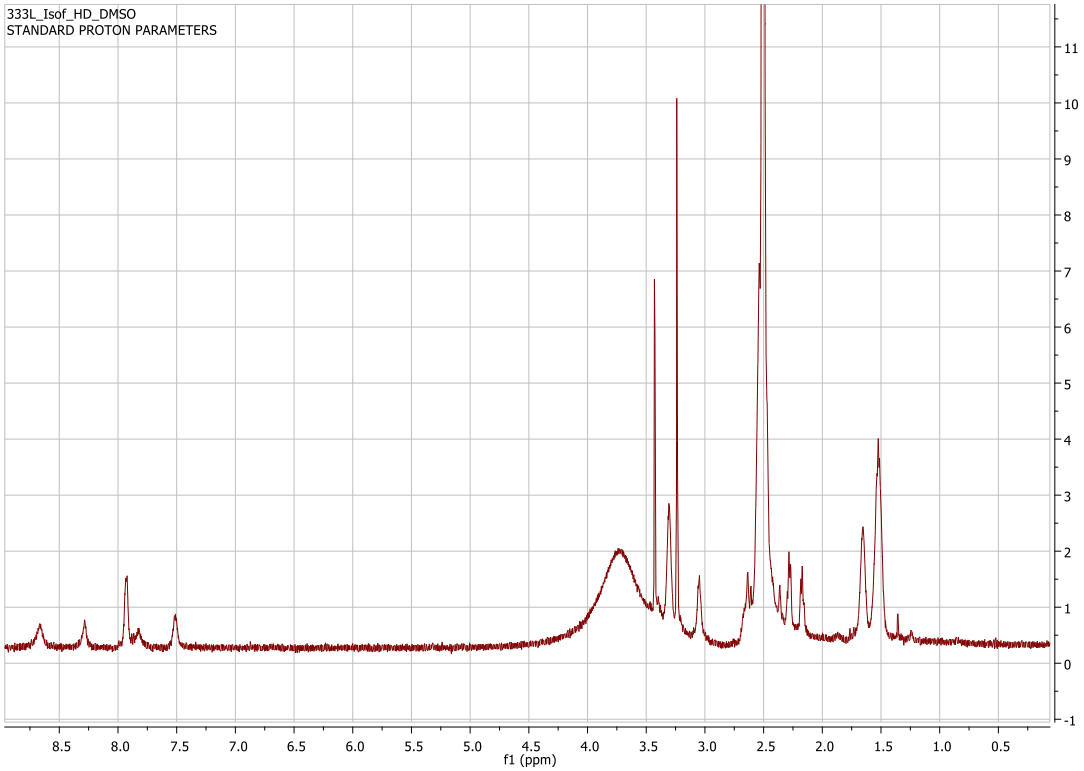
[a] *Chemistry Department, Faculty of Natural and Exact Sciences, Universidad de Oriente, Avenida Patricio Lumumba S/N, 90500, Santiago de Cuba, Cuba. Email: yhmolina@uo.edu.cu, aferrer@uo.edu.cu*

S1. Spectroscopic characterization of L.

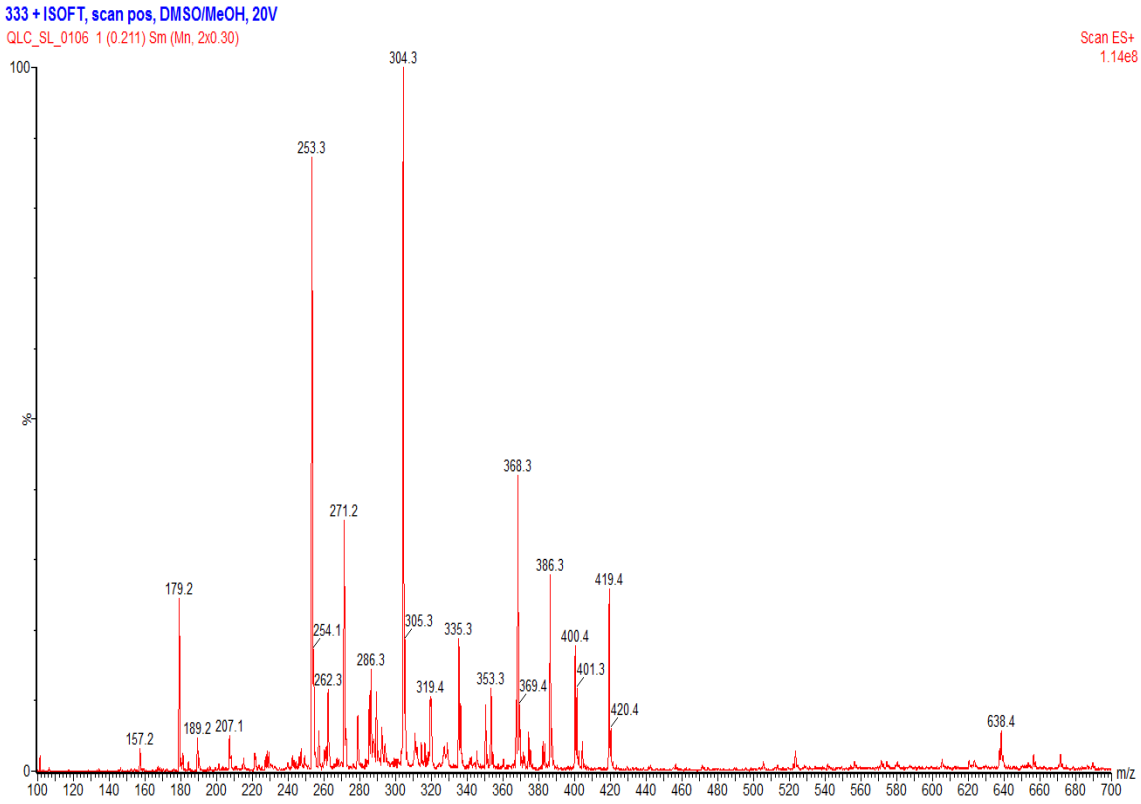
L: 2,16,22,36-tetraoxo-3,7,11,15,23,27,31,35-octazatricyiclo[37.3.1.117,21]dotetraconta - 1(41),17(42),18,20,37,39-hexaene.

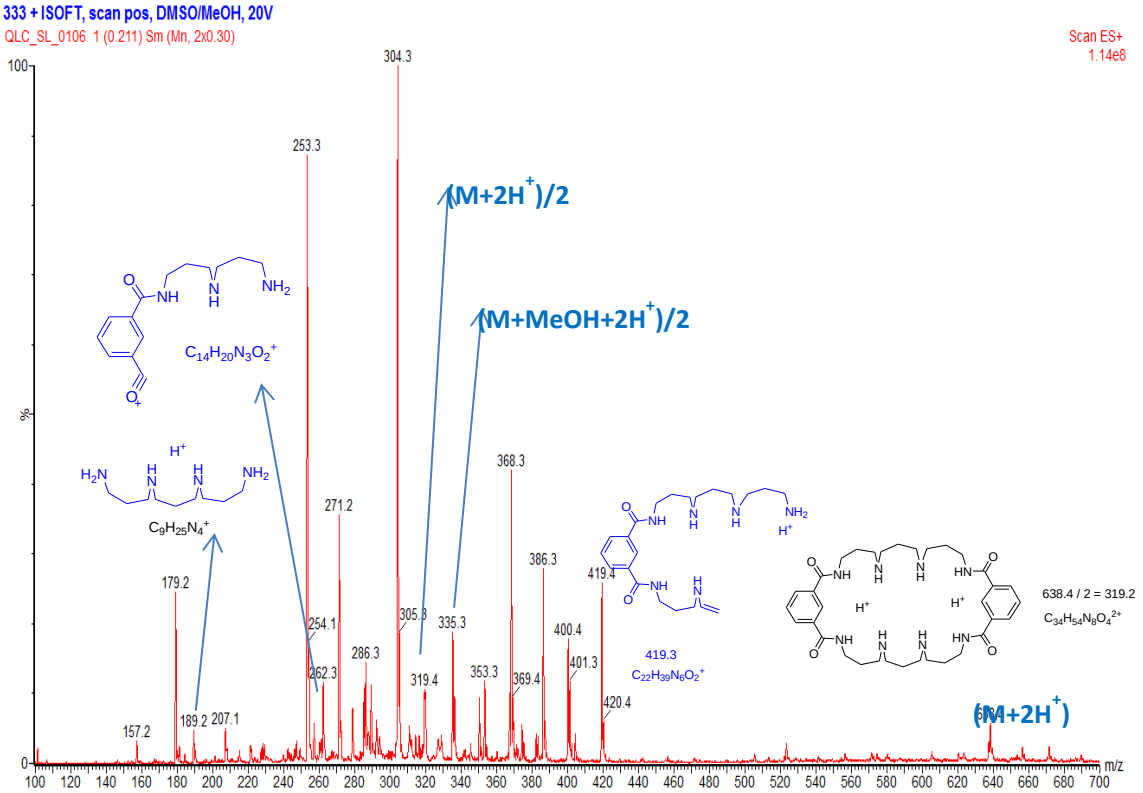
Yield: 72 %; T.f. 131-132 ºC; white solid.

^{1}HNMR (500 MHz, DMSO-d_6): δ(ppm): 8,67 (2H, s, Ar-H); 8,28 (4H, d, Ar-H); 7,93 (4H,s, amide); 7,51 (2H, s, Ar-H), 3.31 (8H, t, -CH_2- amide); 2,18-2,28 (4H, m, -NH-); 1,65 (8H, m, -CH_2-); 1,52 (4H, m, -CH_2-).



ESI-MSMS (m/z,%): 638,4 ([M + 2H]$^+$, 6); 419,4 (MW-218,2 +1, 26); 368,3 ($C_{17}H_{30}N_5O_2$+ + MeOH, 42), 335,3 ((M+ MeOH + 2H+)/2, 19); 319,4 ((M + 2H+)/2, 11); 304,3 (MW-333,2 + 1, 100); 253,3 ((MW-132,02 + 3)/2, 88).
(Weissberg, A.; Dagan, S., Interpretation of ESI(+)-MS-MS spectra—Towards the identification of "unknowns". *Int. J. Mass Spectrom.* **2011,** 299, (2-3), 158-168)





Elemental Analysis: Exp: C(63,23); N(18,34), H(8,56); Theo: C(64,12); N(17,60); H(8,23).