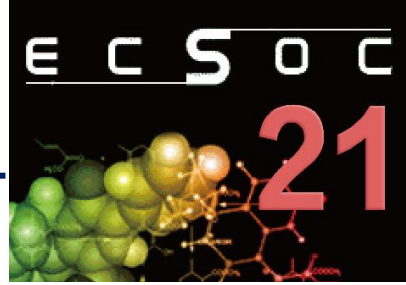
The 21th International Electronic Conference on Synthetic Organic Chemist



Synthesis and structural characterization of a novel amine-bis(phenolate)ligand

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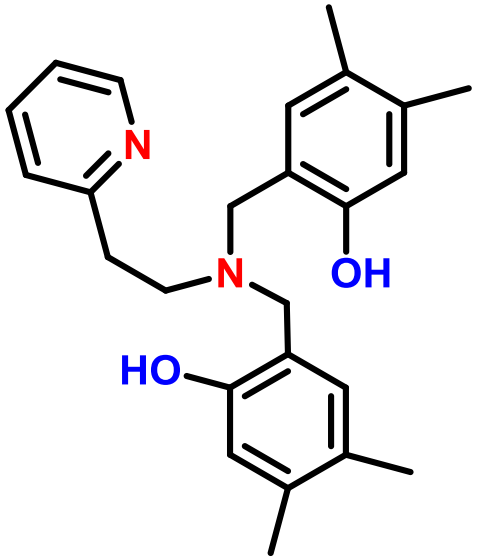
The interest of this ligand …

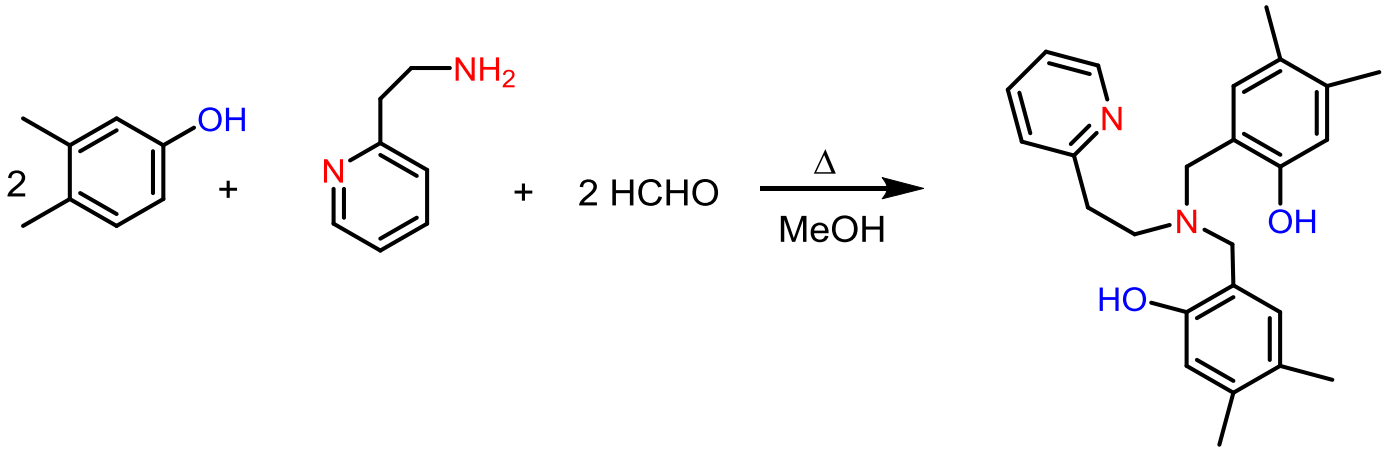
This ligand has recently played an increasingly important role in transition-metal catalyst design and modelling of metalloenzyme active-sites



amine-bis(phenol) ligand H_2L

The behaviour exhibited by these ligands, mainly due to the potential reduction capacity showed by the chemical group which leads to a great variety of coordination patterns

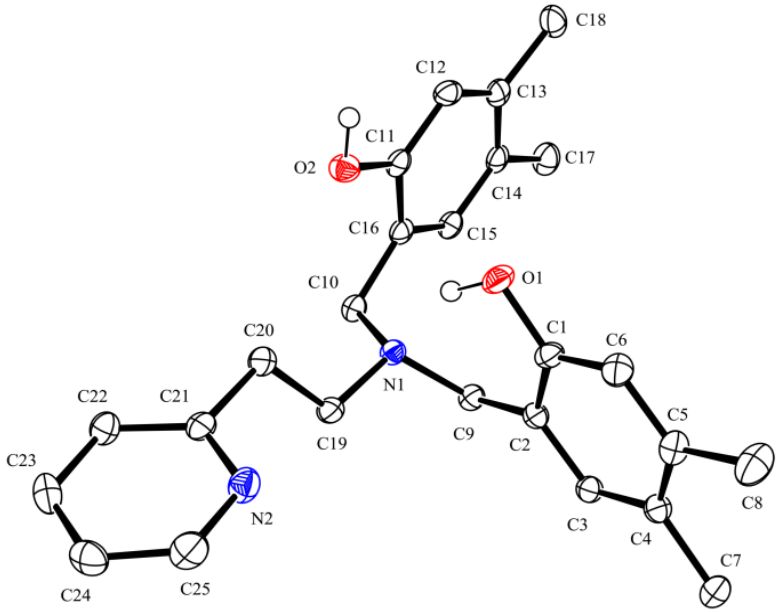
Designing and Synthesis …



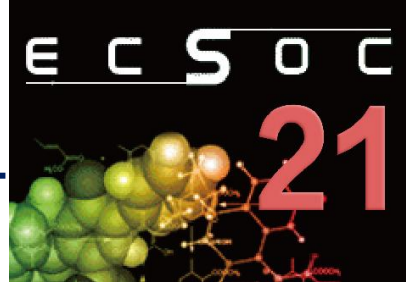
Characterization (EA, MS , IR, 1H NMR, X-ray diffraction)

Ligand H_2L: Anal Calc. for $C_{25}H_{30}N_2O_2$: C, 76.8; H, 7.7; N, 7.1. Found: C, 76.9; H, 7.7; N, 7.1%. MS ES (m/z): 391.2 ; IR (KBr, cm^{-1}): E(O-H) 3266.6, E(C-O) 1284,5, ^1H NMR ($CDCl_3$, ppm): 8,9 (s br, 2H, OH), 8.6, 7.6, 7.2 and 7,1 (4H pyridine), 6.8 (s, 2H, phenyl), 6.6 (s, 2H, phenyl), 3.7 (s, 2H, CH_2), 3.1 (t, 2H, N-CH_2), 2.9 (t, 2H, C-CH_2), 2.1), (s, 6H, CH_3), 2.0(s, 6H, CH_3). ^{13}C NMR ($CDCl_3$, ppm): 160.4 (pyridine), 155.1(C-OH), 149.5-117.3 (phenyl, pyridine), 54.2 and 52.9 (N-CH_2), 34.5 (CH_2), 19.9 and 10.0 (CH_3).

Designing and Synthesis …



- Aminic nitrogen atom adopts a distorted pyramidal geometry.
- Intra and intermolecular hydrogen bond interactions are observed



Our conclusions…

- The tetradentate tripodal ligand H_2L has been synthesized and characterized by different techniques, including X-ray diffraction studies.

- This organic compound is capable of coordinating different metal centres, leading different topologies, for instance, leaving two *cis* positions in octahedral geometries or imposing C_3 symmetry in four- and five-coordinate metal centres.