

Supporting information

Make Pyrophosphate Visible: The First Precipitable and Real-time Fluorescent Sensor for Pyrophosphate in HEPES buffer

Medium

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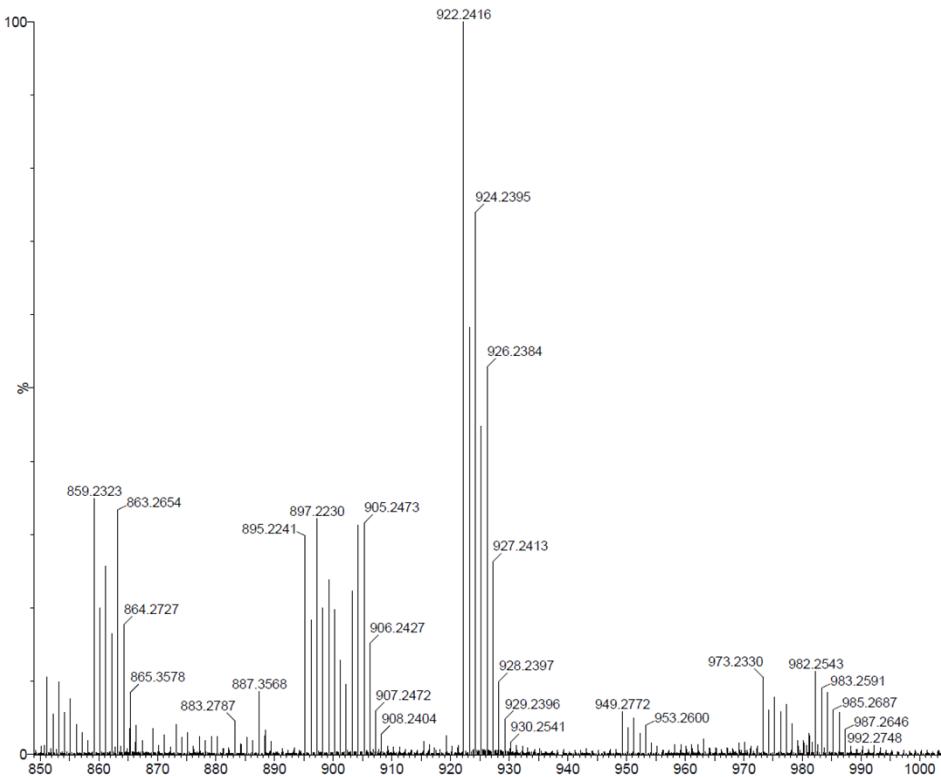


Fig. S1 HRMS for **R1-Zn(II)** complex.

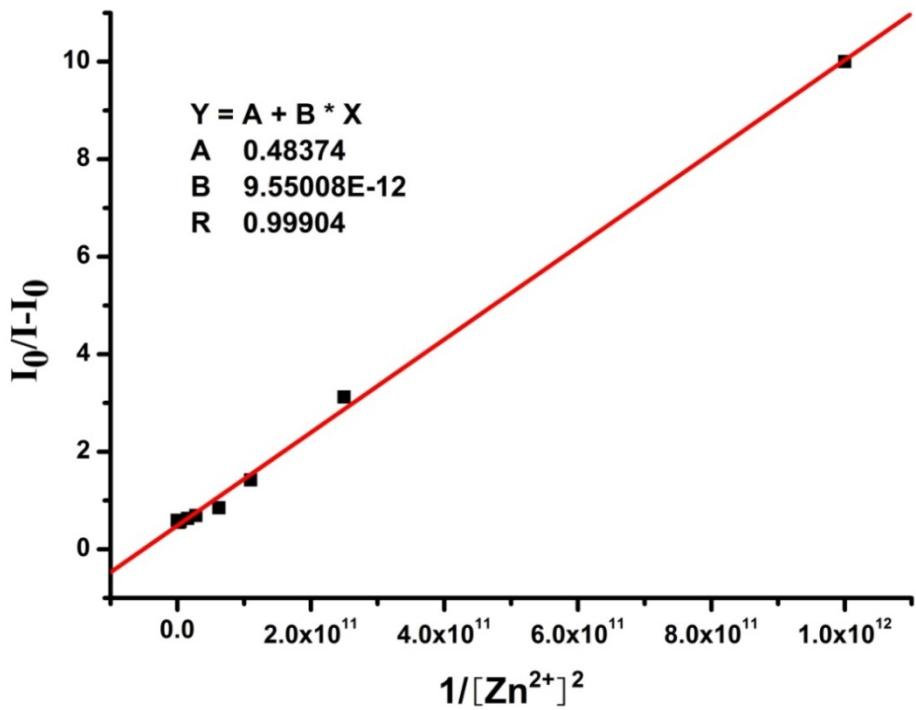


Fig. S2 The binding constant of **R1** with Zn^{2+} by using the linear Benesi-Hildebrand expression (The binding constant of **R1-Zn(II)** with PPi by using the linear Benesi-Hildebrand equation $I_0/I - I_0 = b/a - b \cdot \{1/K[M]^2 + 1\}$ $K = A/B = 5.06 \times 10^{10} M^{-2}$)

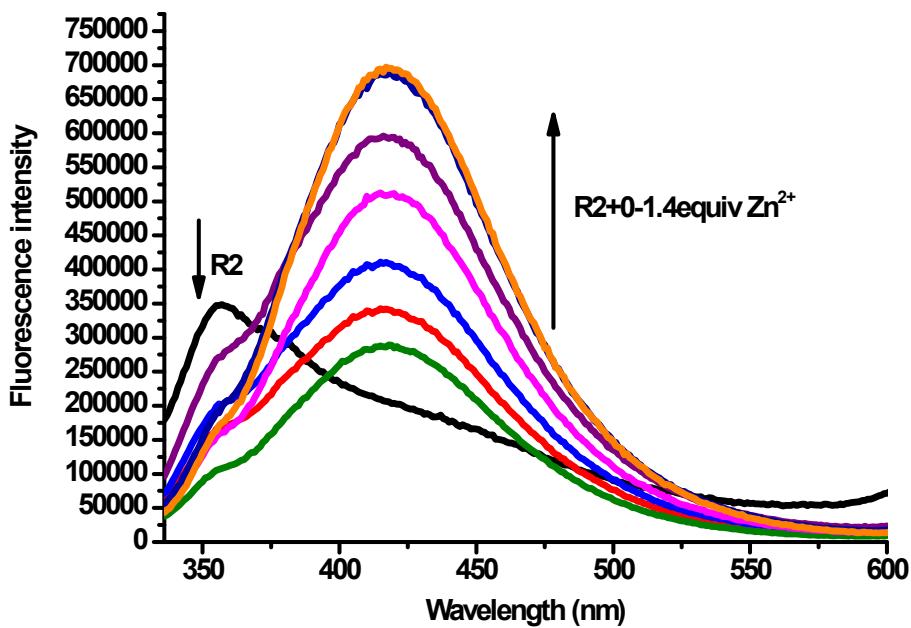


Fig.S3 The fluorescence response of R2 towards Zn^{2+}

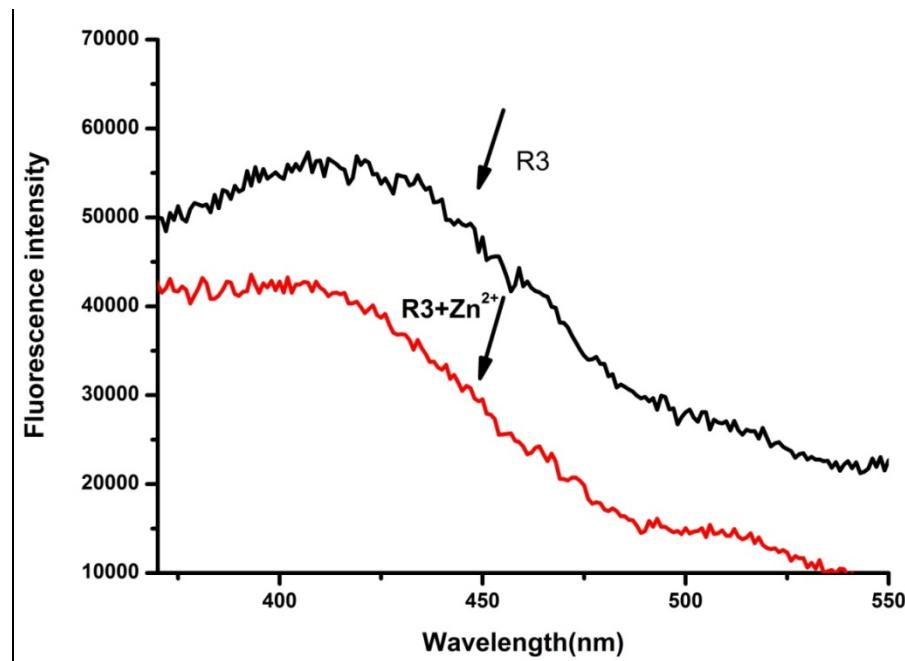


Fig.S4 The fluorescence response of R3 towards Zn^{2+}

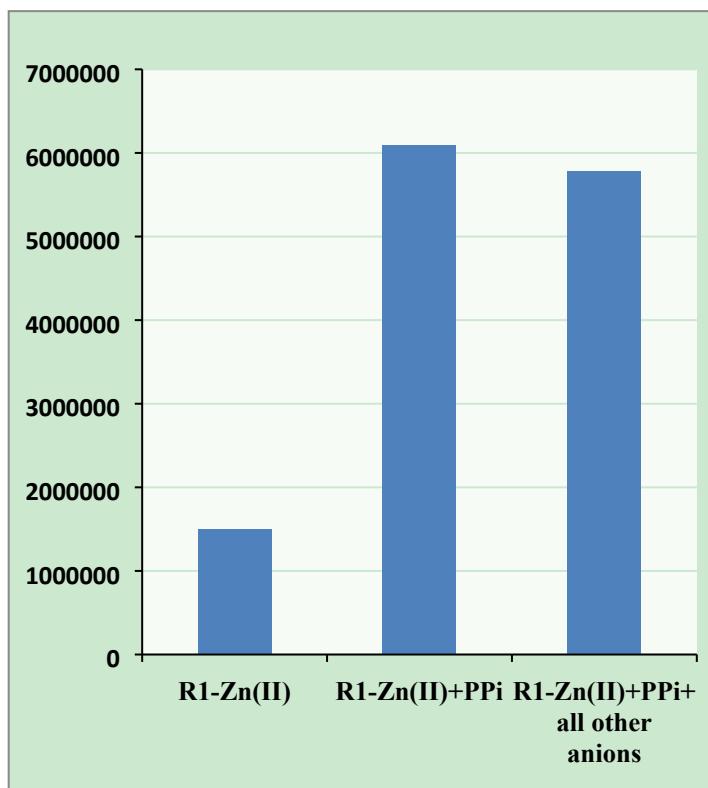


Fig.S5 The fluorescence intensity of mixing (**R1-Zn²⁺**) + PPi + (tested anions all together). Test anions: F⁻, SCN⁻, H₂PO₄⁻, HCO₃⁻, Br⁻, PO₄³⁻, NO₃⁻, AcO⁻, Citrate, I⁻, N₃⁻, SO₄²⁻ (50 μM).

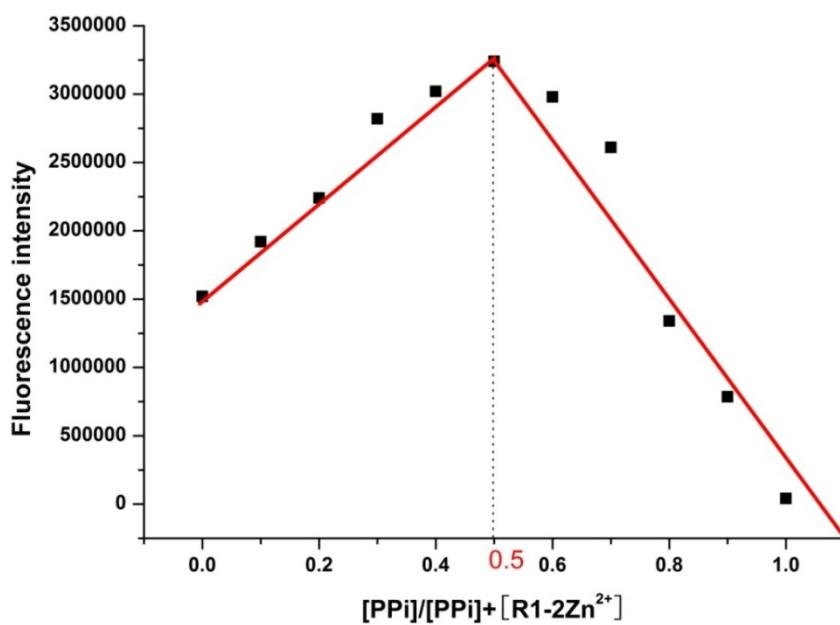
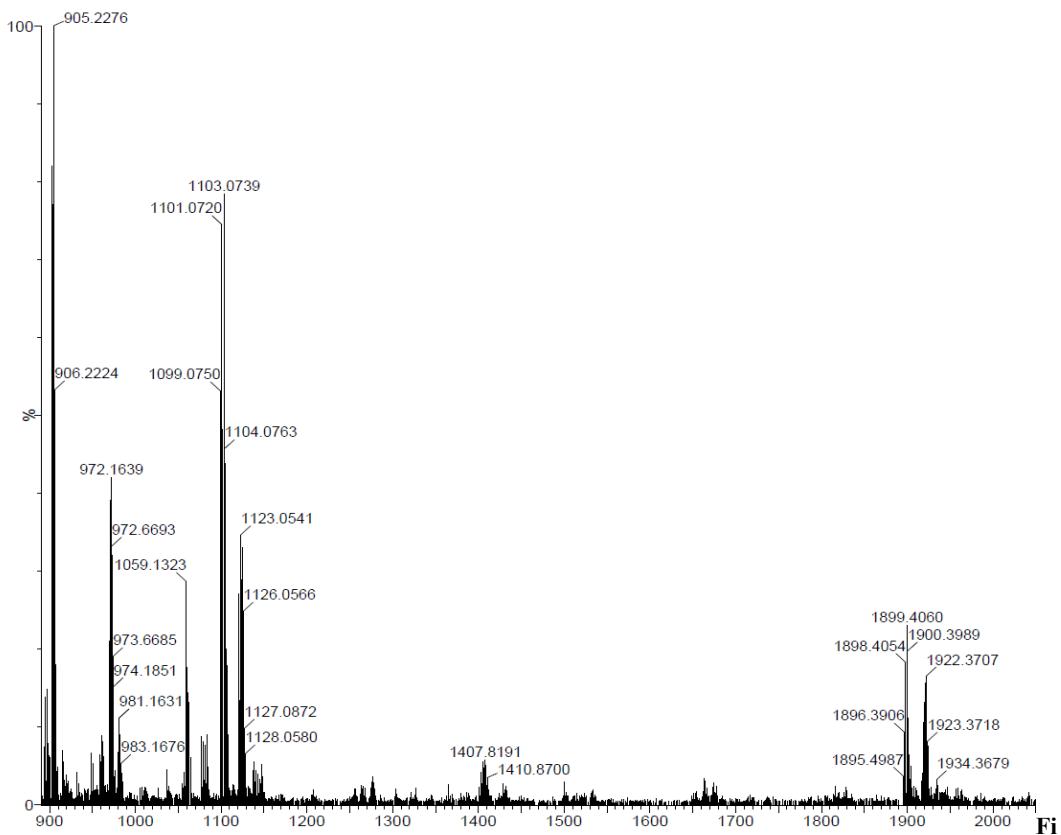


Fig.S6 Job's plot obtained from the fluorescent titration of R1-Zn(II) with PPi in HEPES, the total concentration is 10 μM.



g.S7 The HRMS of R1-Zn(II) and PPi (the precipitate).

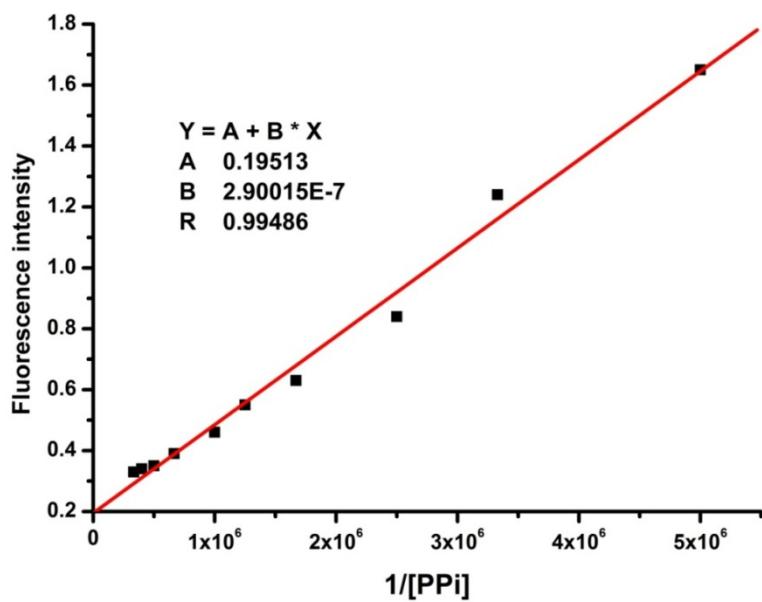


Fig.S8 The binding constant of R1-Zn(II) with PPi by using the linear Benesi-Hildebrand expression (The binding constant of R1-2Zn²⁺ with PPi by using the linear Benesi-Hildebrand expression: $I_0/I - I_0 = b/a - b \cdot \{1/K[M] + 1\}$, $K = A/B = 6.7 \times 10^5 M^{-1}$).

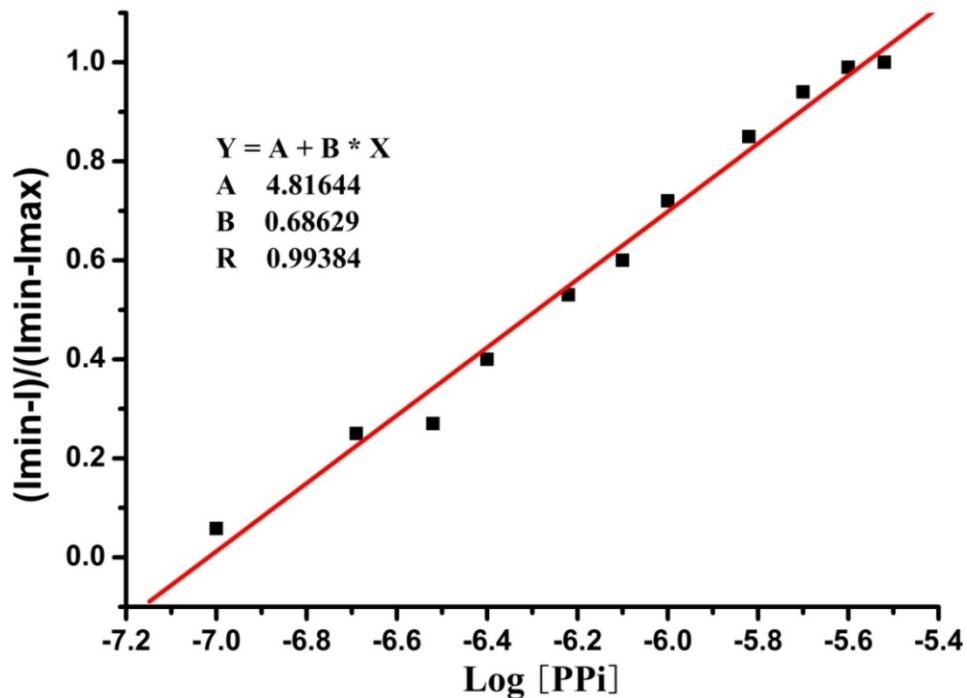


Fig.S9 The determination R1-Zn(II) of the detection limit (LOD) for PPi in HEPES buffer (10 mM, pH =7.4)

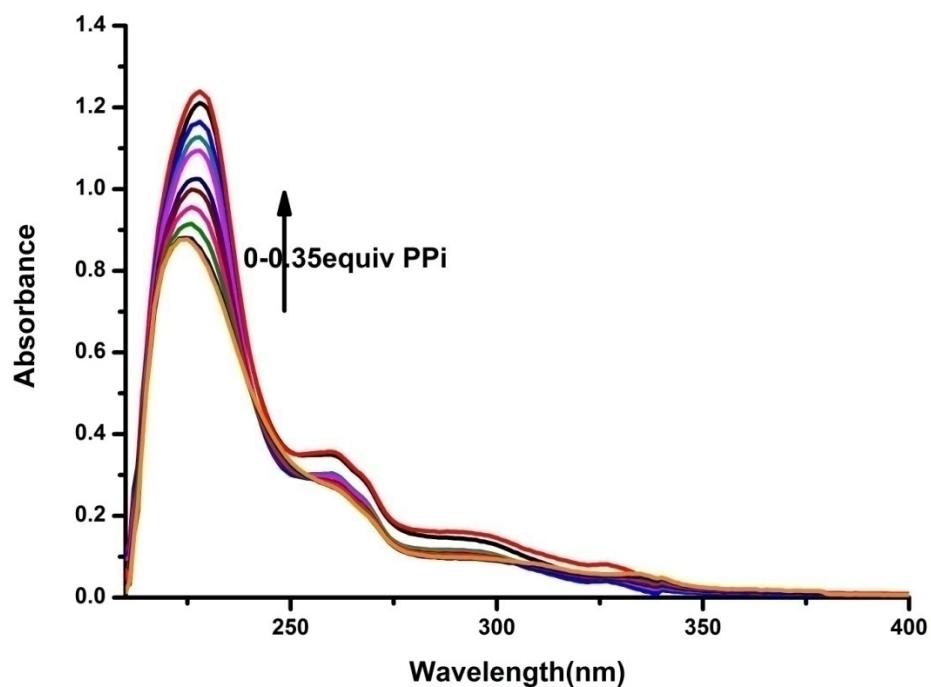
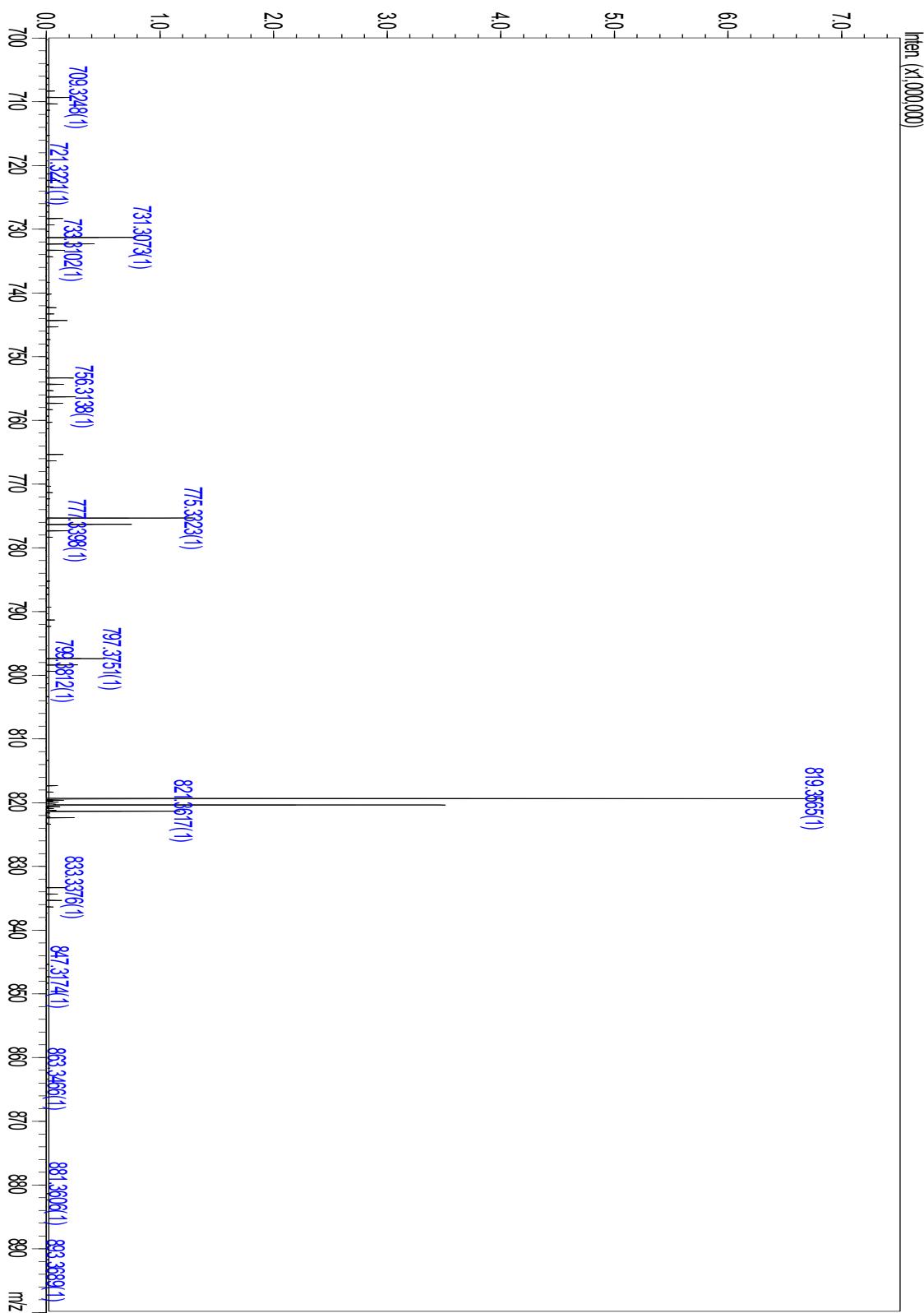


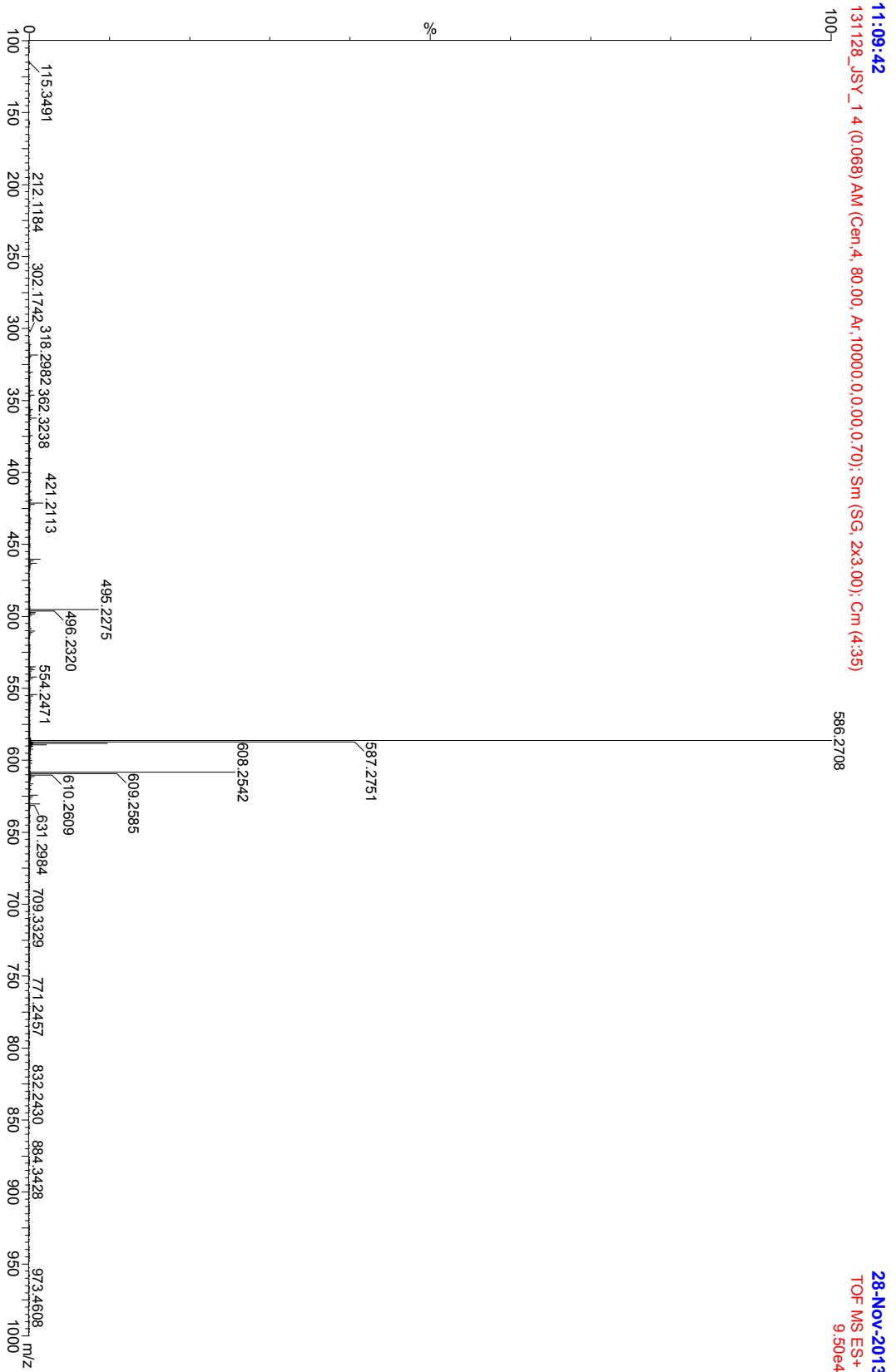
Fig.S10 Absorption spectra of during the titration R1-Zn(II) with PPi (0-0.35 equiv) in HEPES (10 mM, pH = 7.4)

1. ^1H -NMR, ^{13}C -NMR and HRMS spectra of R1/R2/R3 and intermediates.

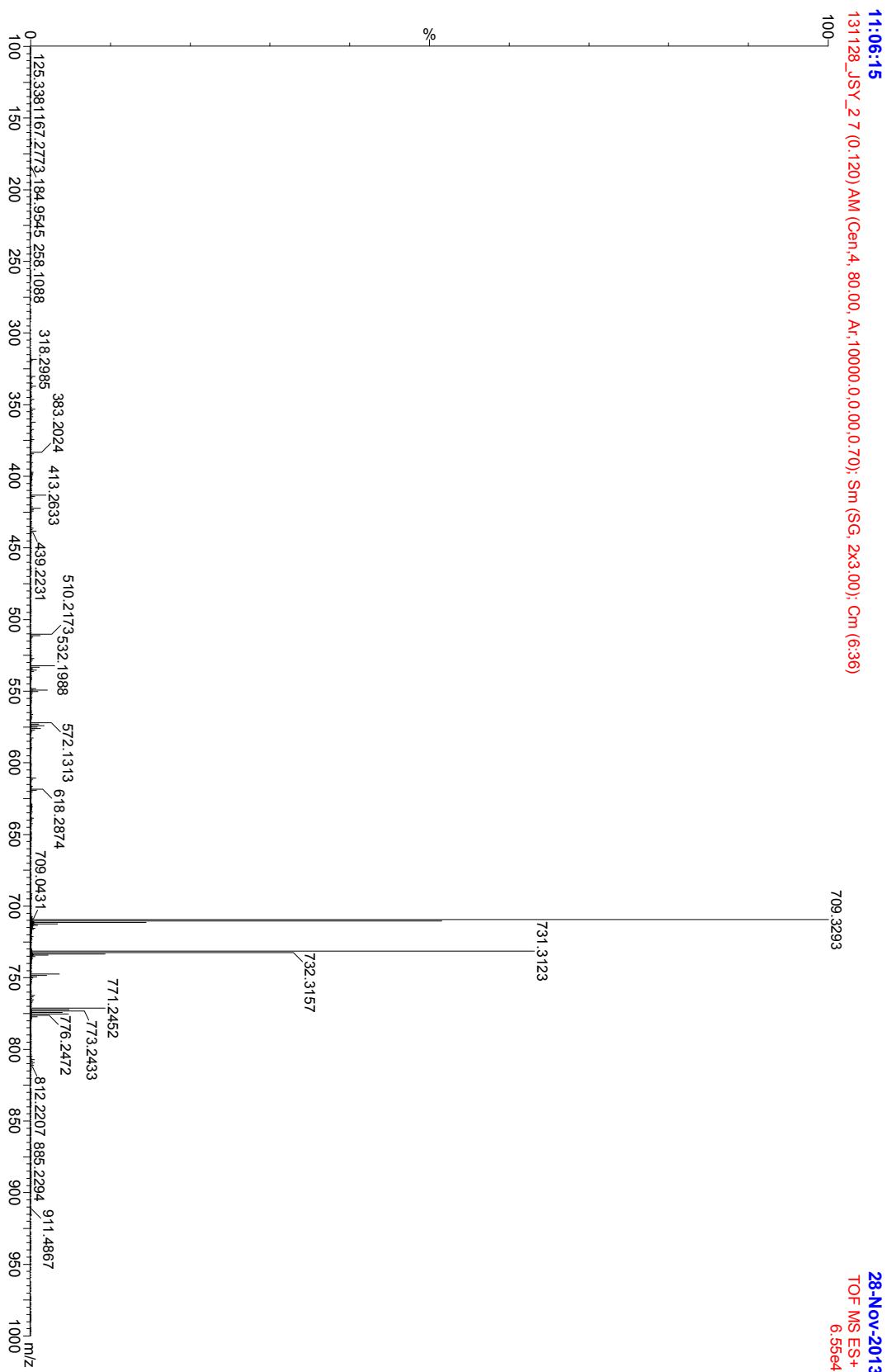
1.1 The HRMS of R1



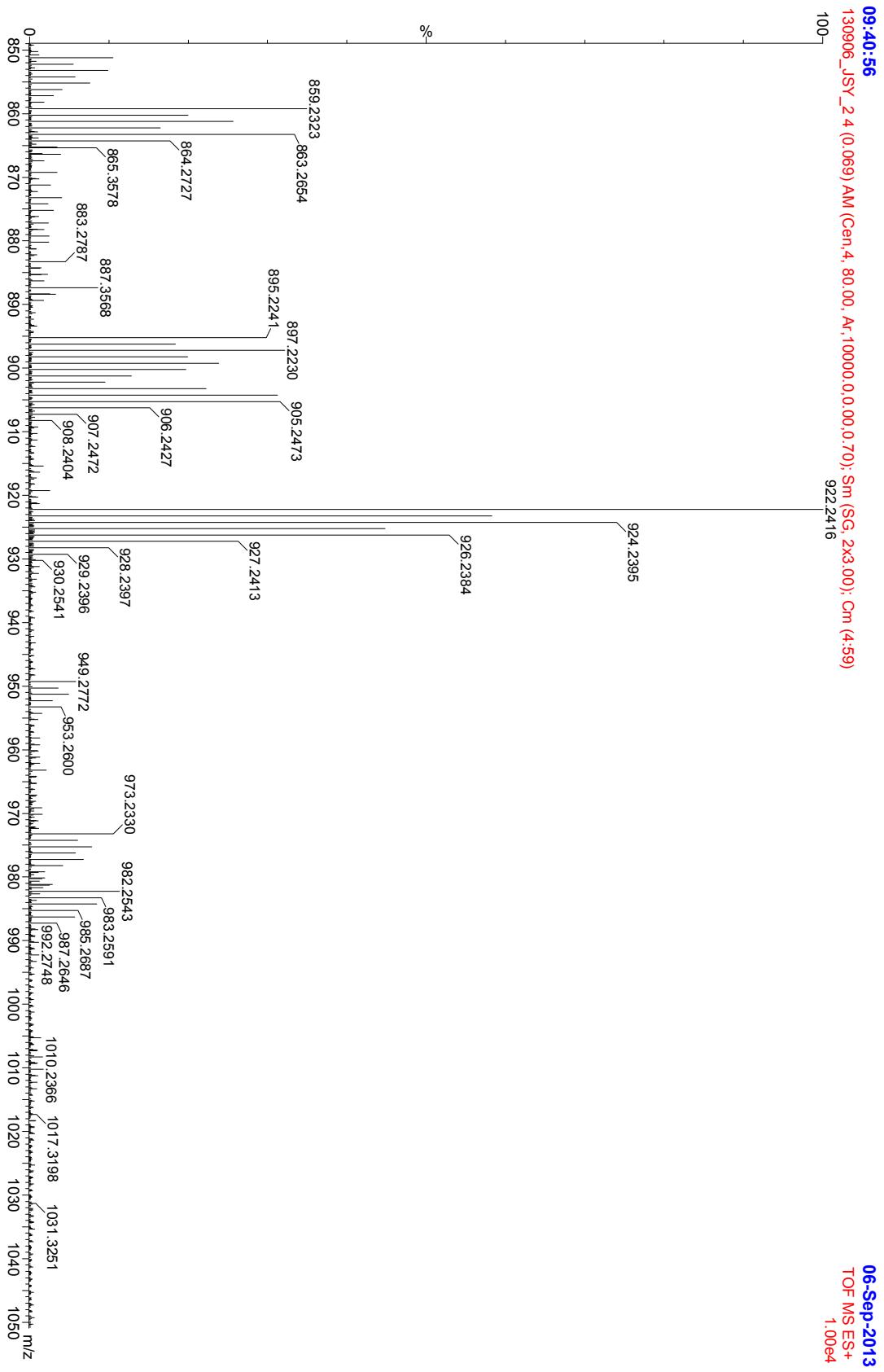
2.2 The HRMS of R2



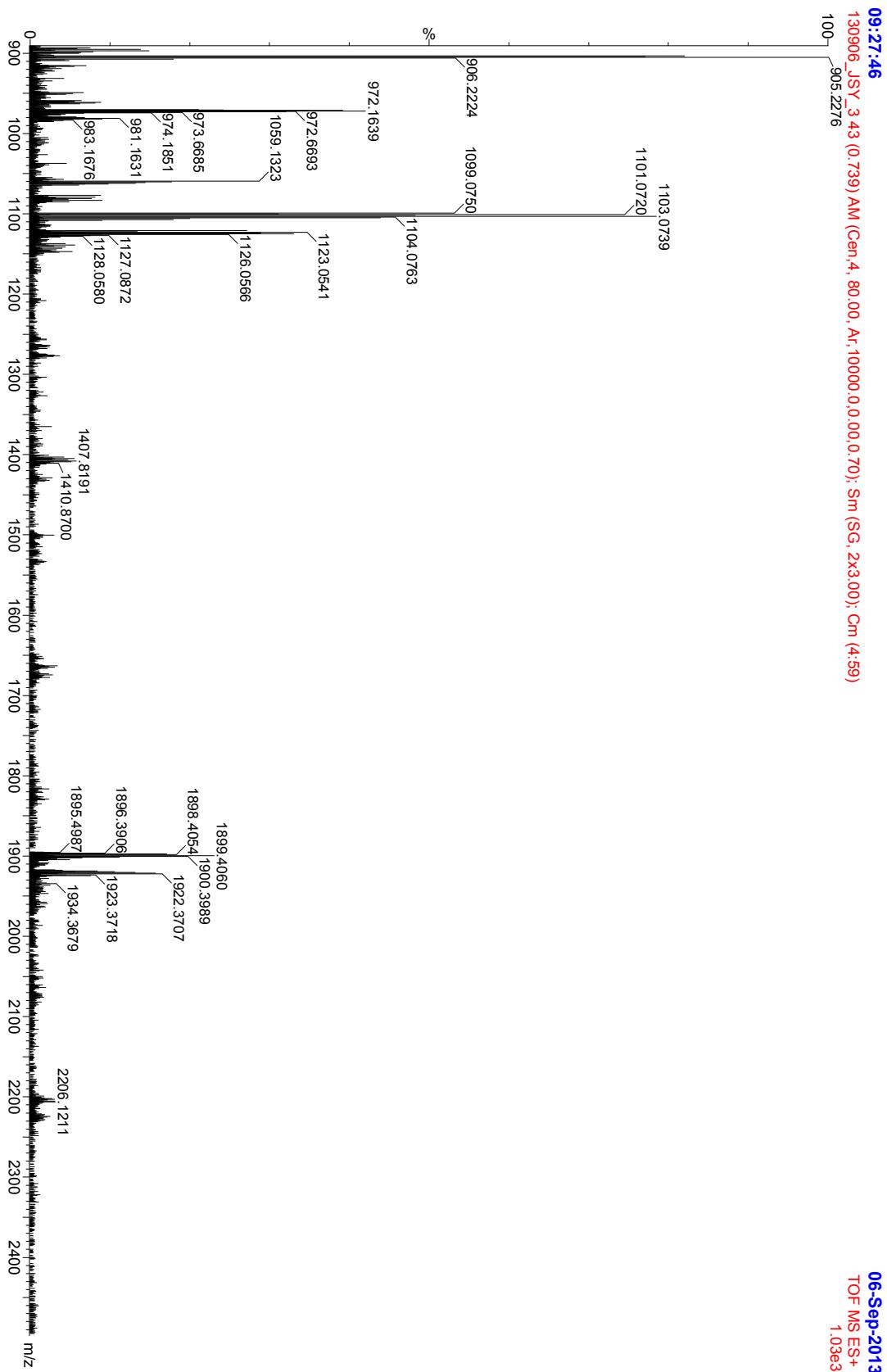
2.3 The HRMS of R3+H⁺



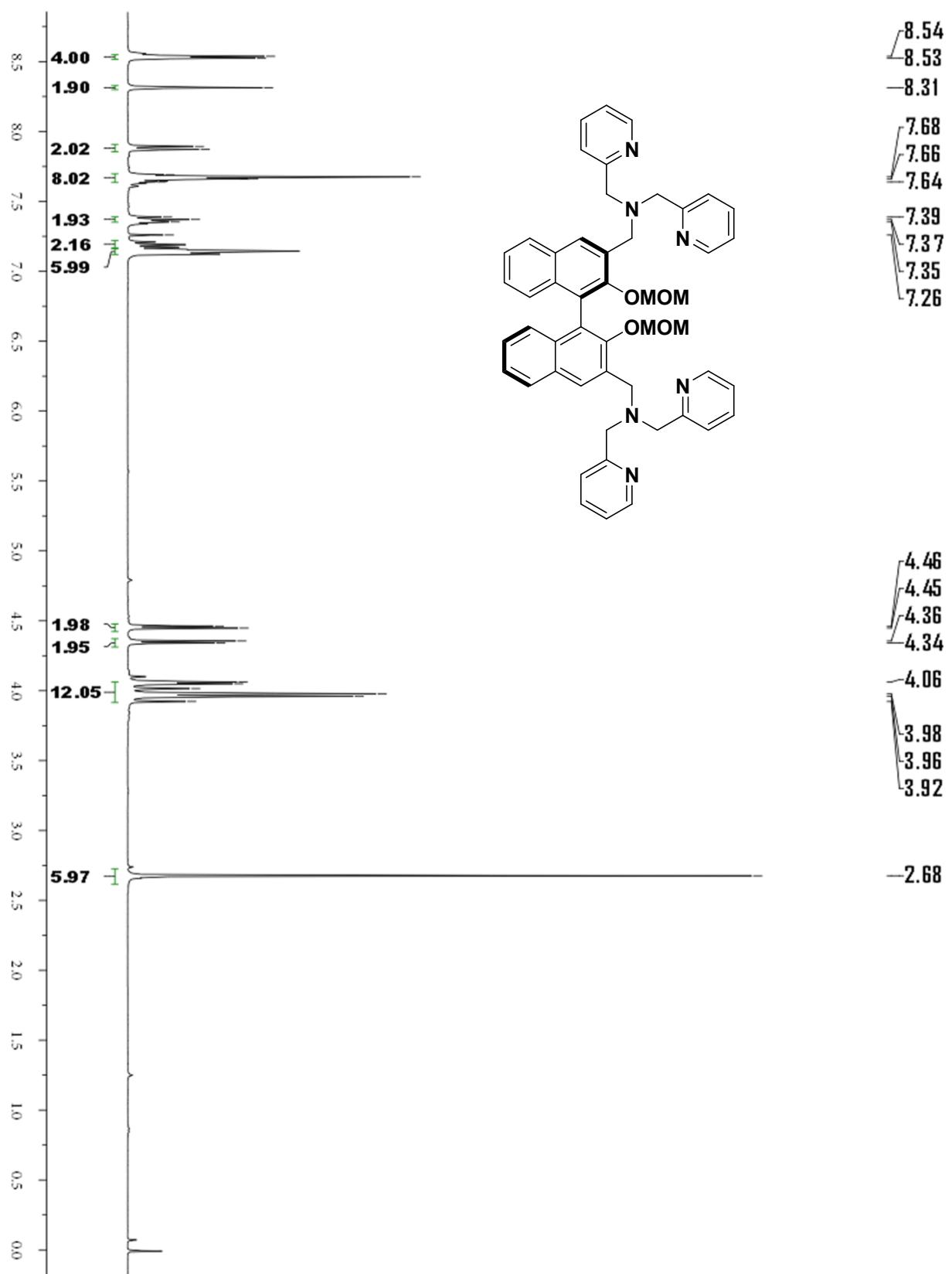
2.4 The HRMS of R1-Zn(II)



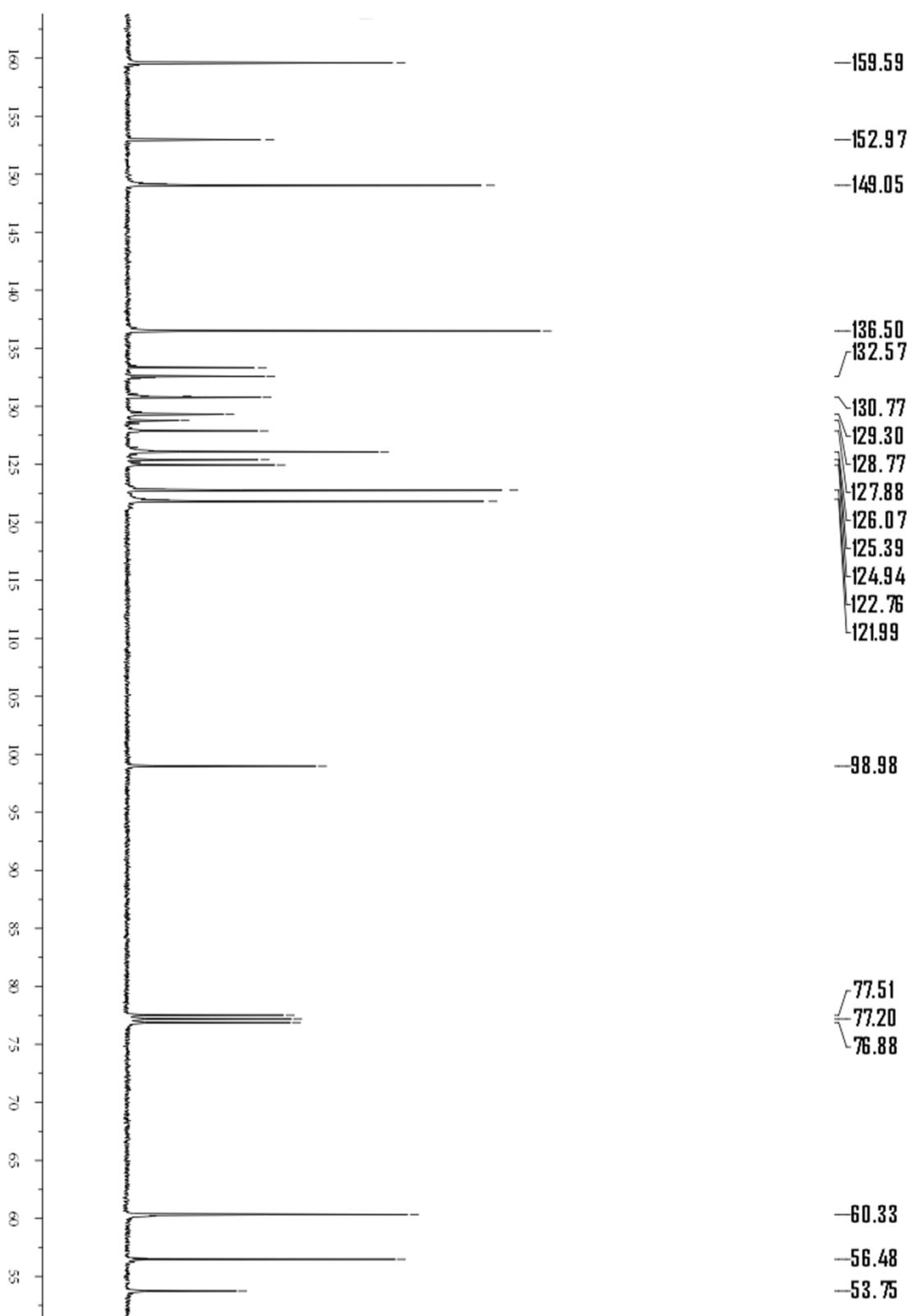
2.5 The HRMS of R1-Zn(II)-P₂O₇⁴⁻+Na⁺-2H⁺



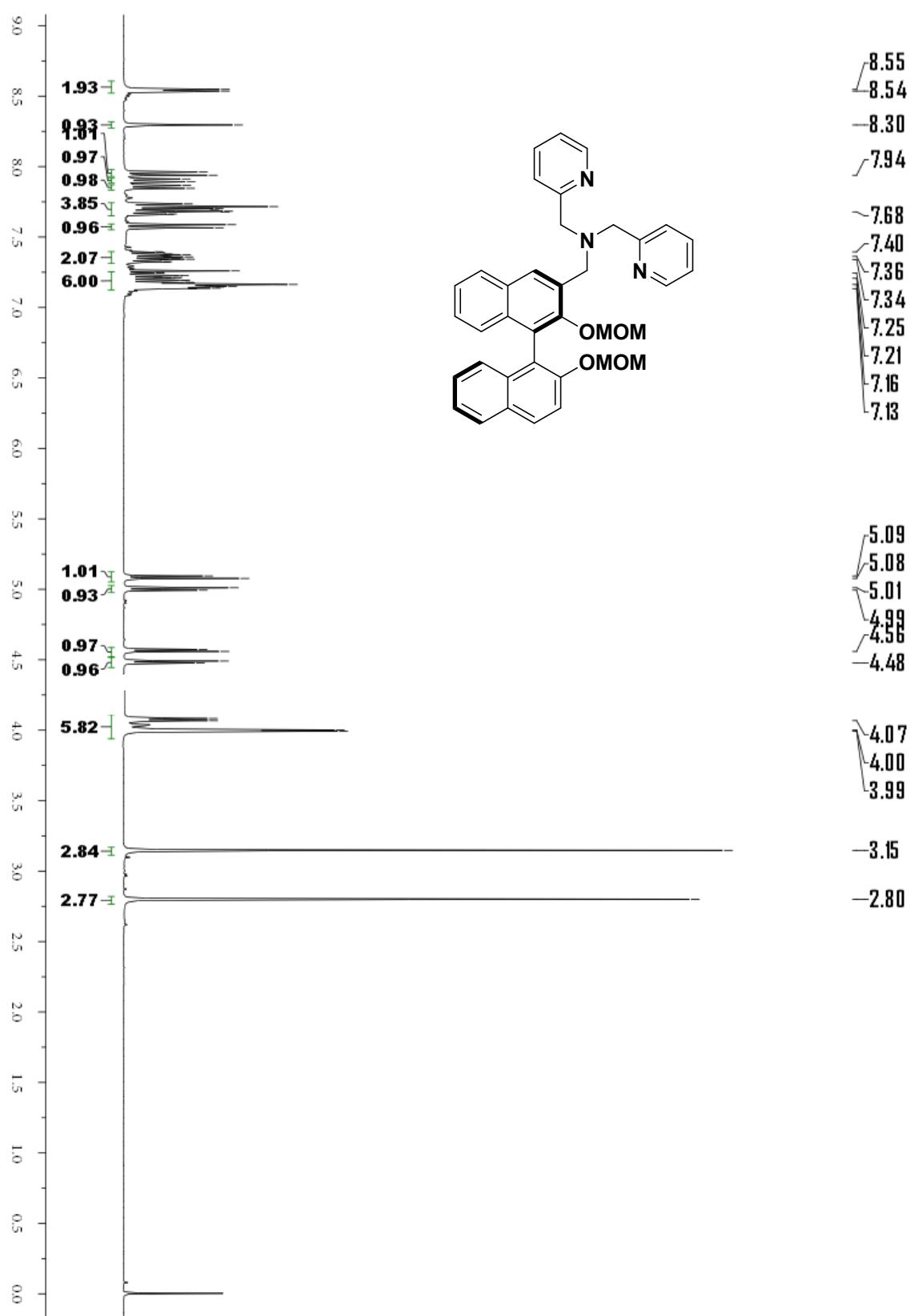
2.6 $^1\text{H-NMR}$ of R1



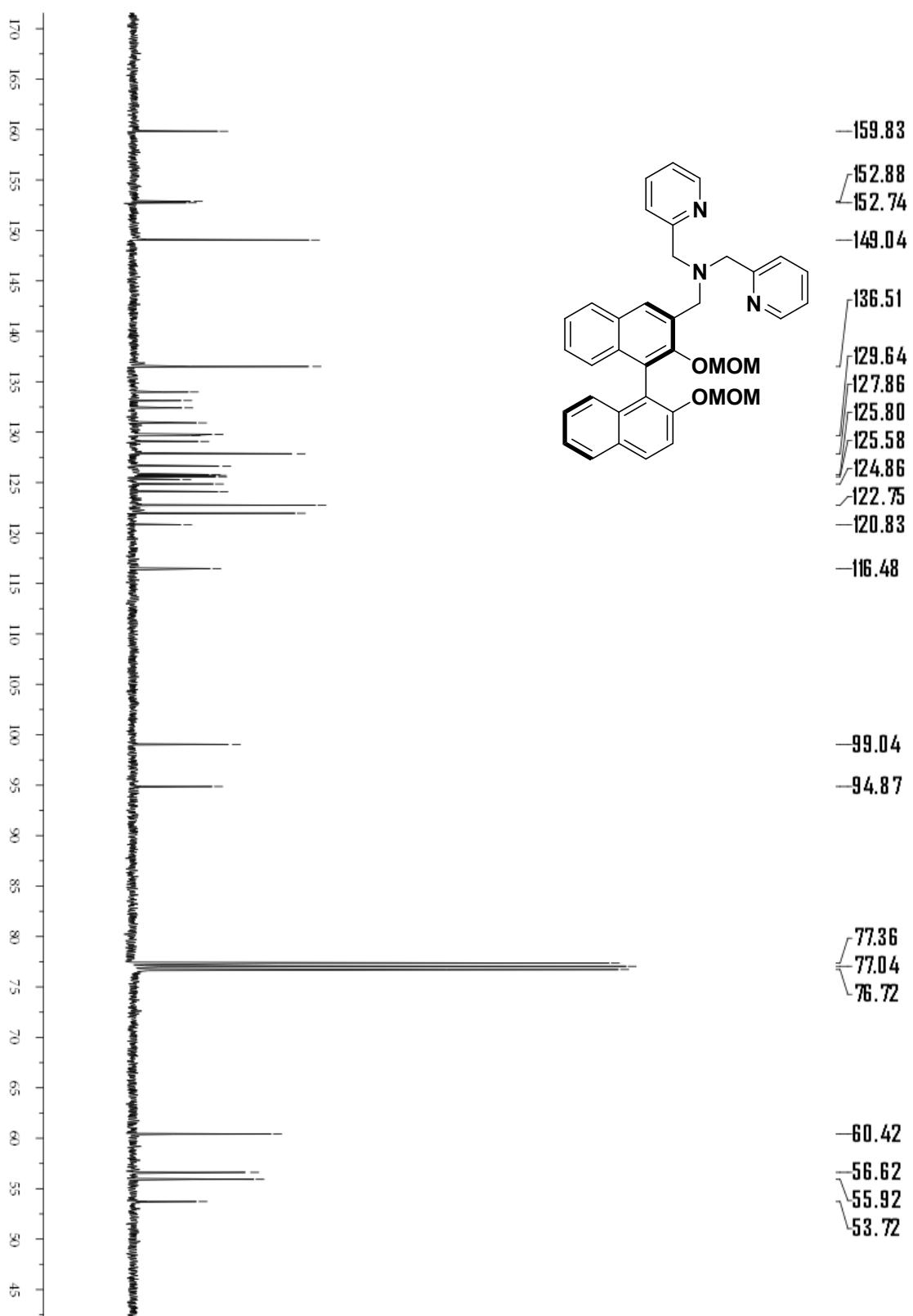
2.7 ^{13}C -NMR of R1



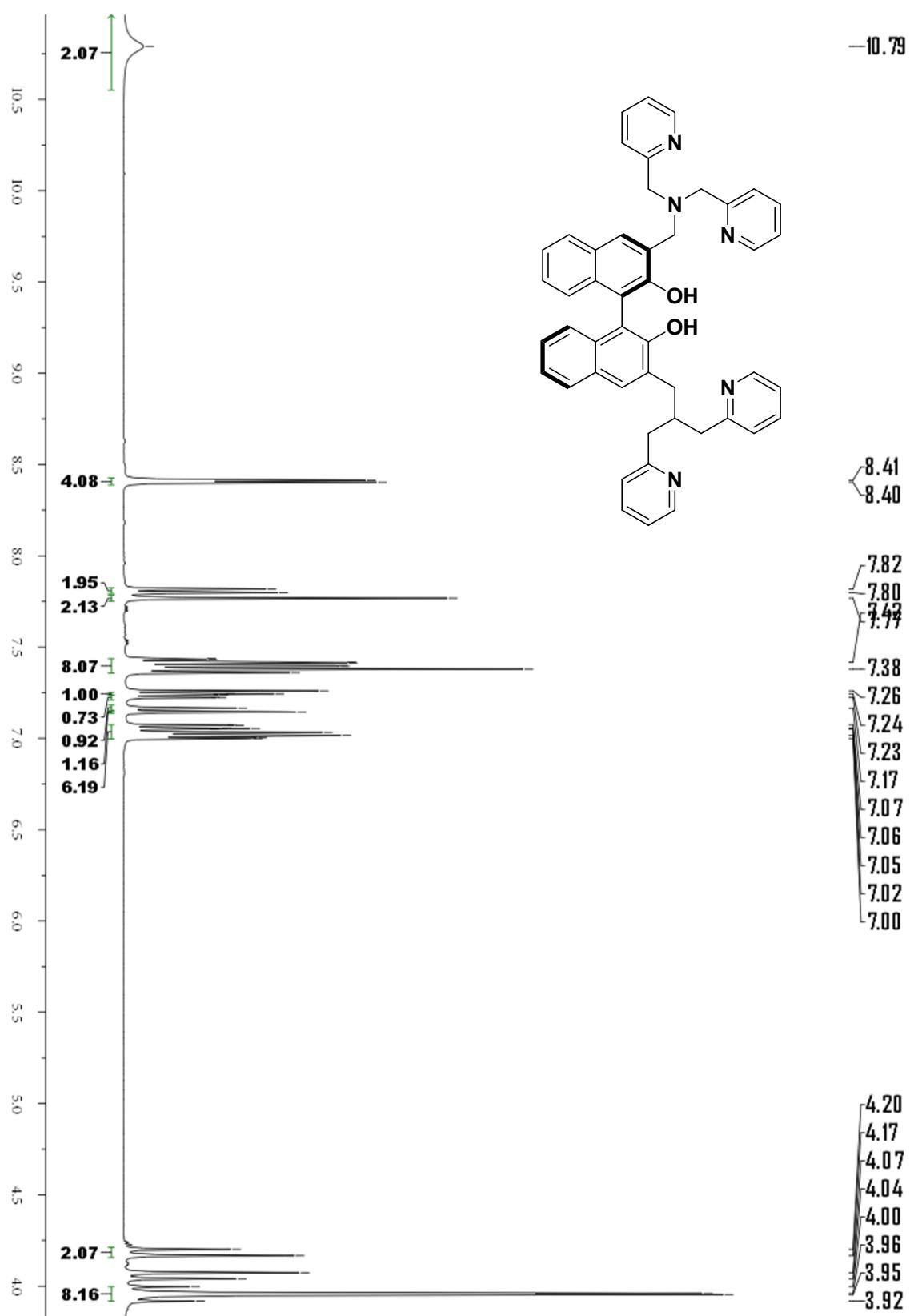
2.8 $^1\text{H-NMR}$ of R2



2.9 ^{13}C -NMR of R2



2.10 $^1\text{H-NMR}$ of R3



2.11 ^{13}C -NMR of R3

