Electronic supplementary information for publication

Synthesis and evaluation of oxovanadium(IV) complexes of Schiff-base condensates from 5-substituted-2-hydroxybenzaldehyde and 2-substituted-benzenamine as selective inhibitors of protein tyrosine phosphatase1B

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S1 Bond valence sum calculations

S2 The experimental and simulation isotopic distribution patterns of ESI-MS spectra of complexes *1-5* at the their molecular ion peaks

Legends to supplemental figures

Fig. S1. The experimental (black) and peaks assigned to major species (blue) of complex *1*, the species with m/z 420.86 observed at the peak may be assigned to [*1*-H]$^-$ (m/z = 420.92). Insert for isotopic distribution patterns at the molecular ion peaks.

Fig. S2. The experimental (black) and peaks assigned to major species (blue) of complex *2*, the species with m/z 385.94 observed at the peak may be assigned to [*2*-H]$^-$ (m/z = 386.00). Insert for isotopic distribution patterns at the molecular ion peaks.

Fig. S3. The experimental (black) and peaks assigned to major species (blue) of complex *3*, the species with m/z 528.04 observed at the peak may be assigned to [*3*+H]$^+$ (m/z = 528.02). Insert for isotopic distribution patterns at the molecular ion peaks.

Fig. S4. The experimental (black) and peaks assigned to major species (blue) of complex *3*, the species with m/z 616.92 observed at the peak may be assigned to [*4*]$^+$ (m/z = 617.18). Insert for isotopic distribution patterns at the molecular ion peaks.

Fig. S5. The experimental (black) and peaks assigned to major species (blue) of complex *3*, the species with m/z 549.07 observed at the peak may be assigned to [*5*]$^+$ (m/z = 549.06). Insert for isotopic distribution patterns at the molecular ion peaks.

S1 Bond valence sum calculations

To assign the oxidation state of the vanadium center in **1**, we have taken recourse to the calculation on the basis of bond valence sum (BVS) model[S1]. In this method, the valence S of a bond between two atoms i and j is related by an empirical expression (1) where R_{ij} is the length of the bond (expressed in Å), R_0 is a parameter characteristic of the bond and b is 0.37[S2] for V-O and V-N.

$$S_{ij} = \exp\left[(R_0 - R_{ij}) \middle/ b \right] \qquad (1)$$

This R_0, known as bond valence parameter is, however, geometry and coordination number specific. The oxidation number N_i of the atom i is simply the algebraic sum (2) of these S values of all the bonds (n) around the atom, i.

$$N_i = \sum_{i=1}^{n} s_i \qquad (2)$$

Taking these R_0 values, when we apply this BVS method (Table S1) to our vanadium complex **1** following equation (1)[S2], the BVS values for vanadium atom in **1** come out to be 4.14 and 4.35 for V(IV) and V(V), respectively. The oxidation state of the vanadium atom can be taken as the value of 4+. The presence of water molecules is confirmed by Bond Valence Sum calculations (0.3038 v.u. for O6 (H_2O) and 0.5047 v.u. for O5 (H_2O)).

Table S1 Bond valence values for vanadium in **1**

Bond type	Bond distance (Å)	V^{IV}-O R_0=1.784Å b=0.37 V^{IV}-N R_0=1.86Å b=0.37	V^{V}-O R_0=1.803Å b=0.37 V^{V}-N R_0=1.86Å b=0.37	V^{IV}	V^{V}
V1—N1	2.078(2)	0.4518	0.4756		
V1—O1	1.585(2)	1.7123	1.8025	4.1362	4.3542
V1—O2	1.957(2)	0.6265	0.6595		
V1—O3	1.985(2)	0.5809	0.6115		
V1—O5	2.056(2)	0.4794	0.5047		
V1—O6	2.248(2)	0.2853	0.3038		

S2 The experimental and simulation isotopic distribution patterns of ESI-MS spectra of complexes *1*-*5*.

Electrospray ionization mass spectra (ESI-MS) were recorded with a micrOTOF-Q instrument (Bruker) in methanol solution. The assignment of the major species in each spectrum corresponds relative complexes.
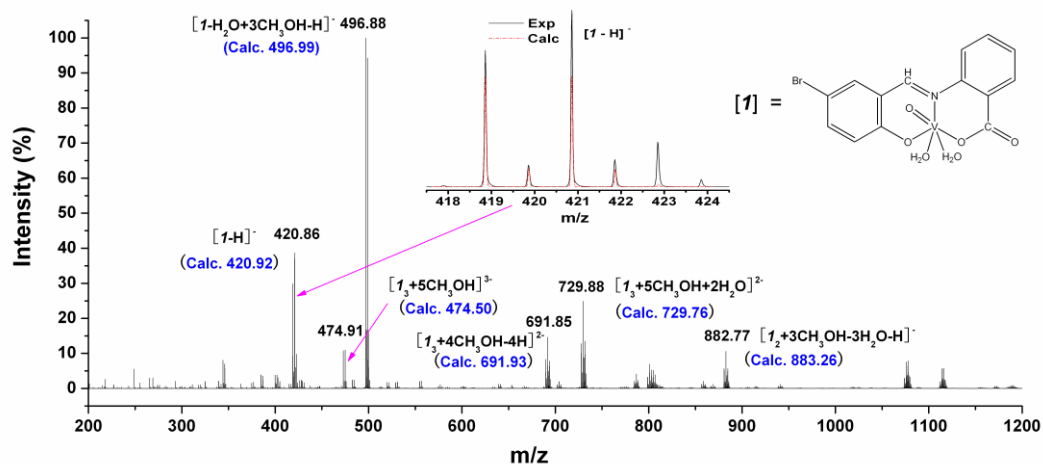

Fig. S1. The experimental (black) and peaks assigned to major species (blue) of complex *1*, the species with m/z 420.86 observed at the peak may be assigned to [*1*-H]⁻ (m/z = 420.92). Insert for isotopic distribution patterns at the molecular ion peaks.
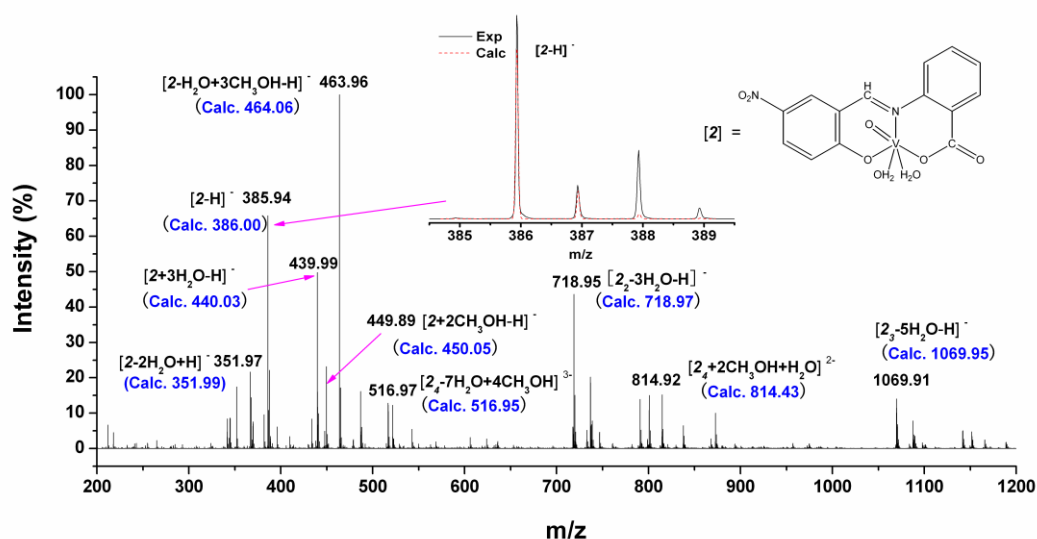

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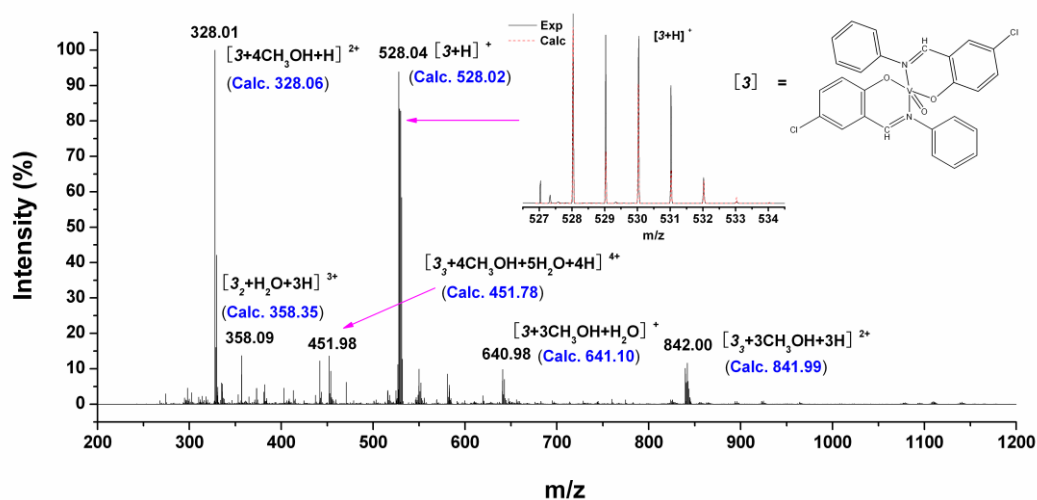
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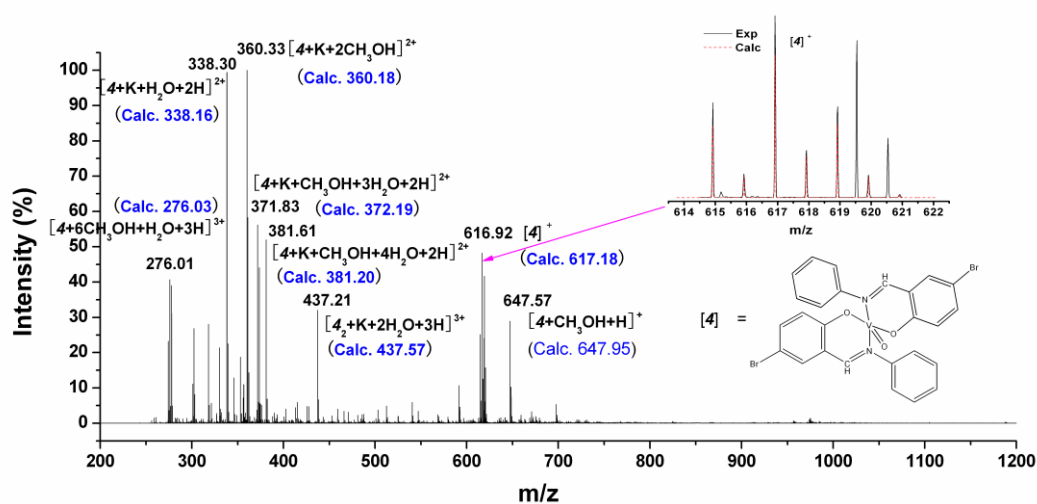

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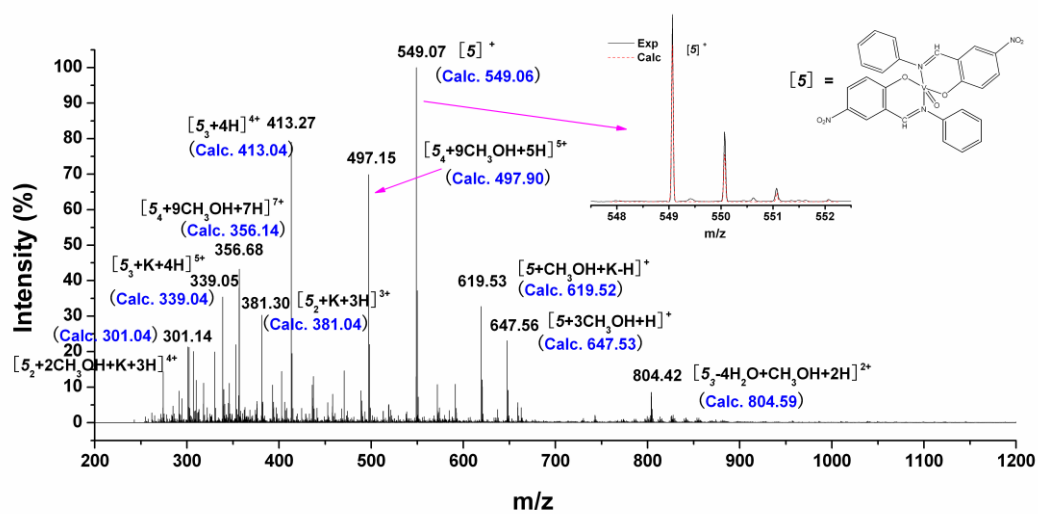
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Reference

S1 I. D. Brown, *Chem Rev*, 2009, **109**, 6858.

S2 N. E. Brese and M. O'Keeffe, *Acta Cryst,* 1991, **B47**, 192.