***Supplementary Information***

# Syntheses, spectral characterization and antidiabetic activities of oxidovanadium(V) complexes with bi-and tridentate ligands

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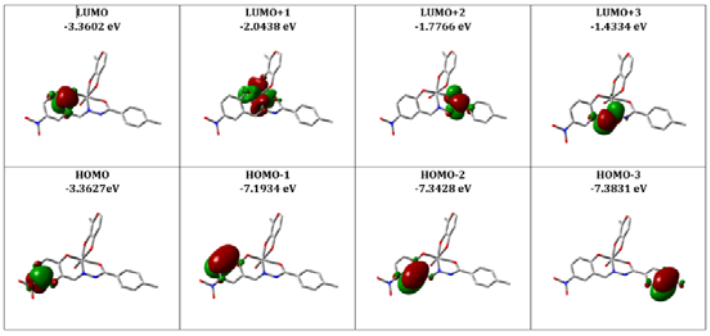


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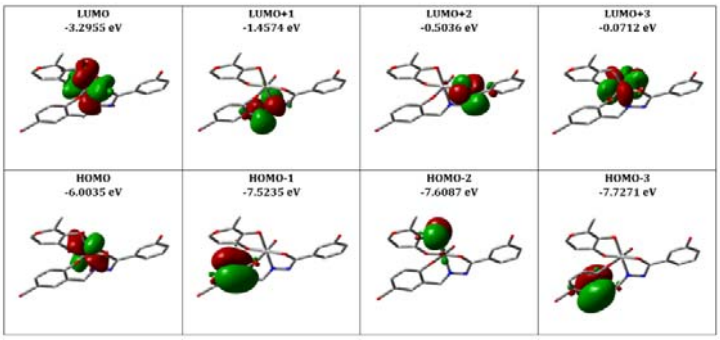


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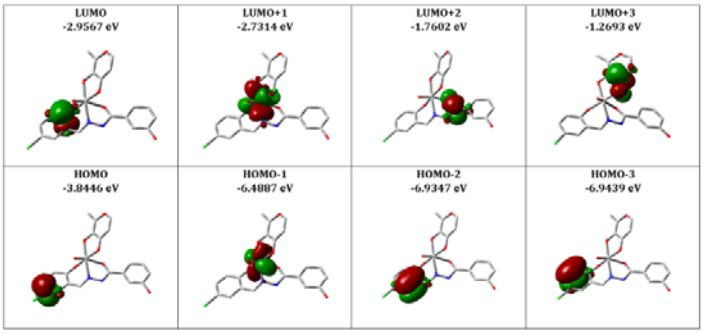


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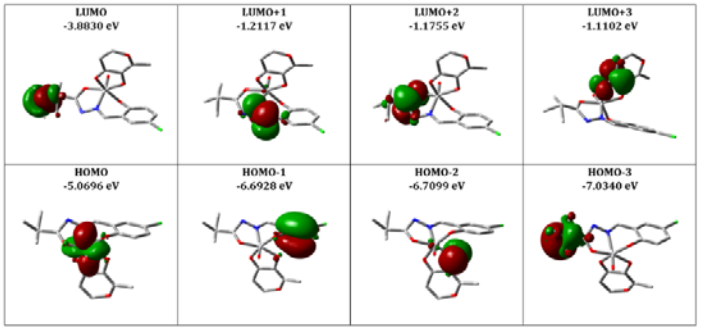
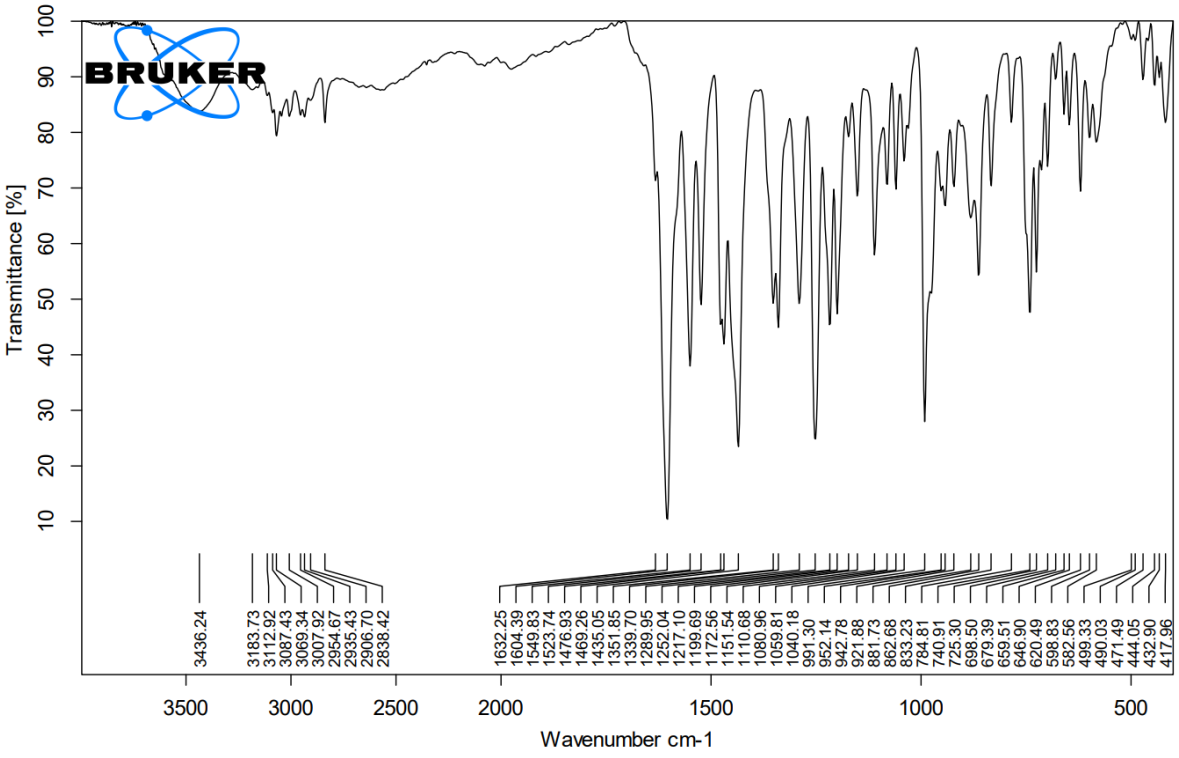
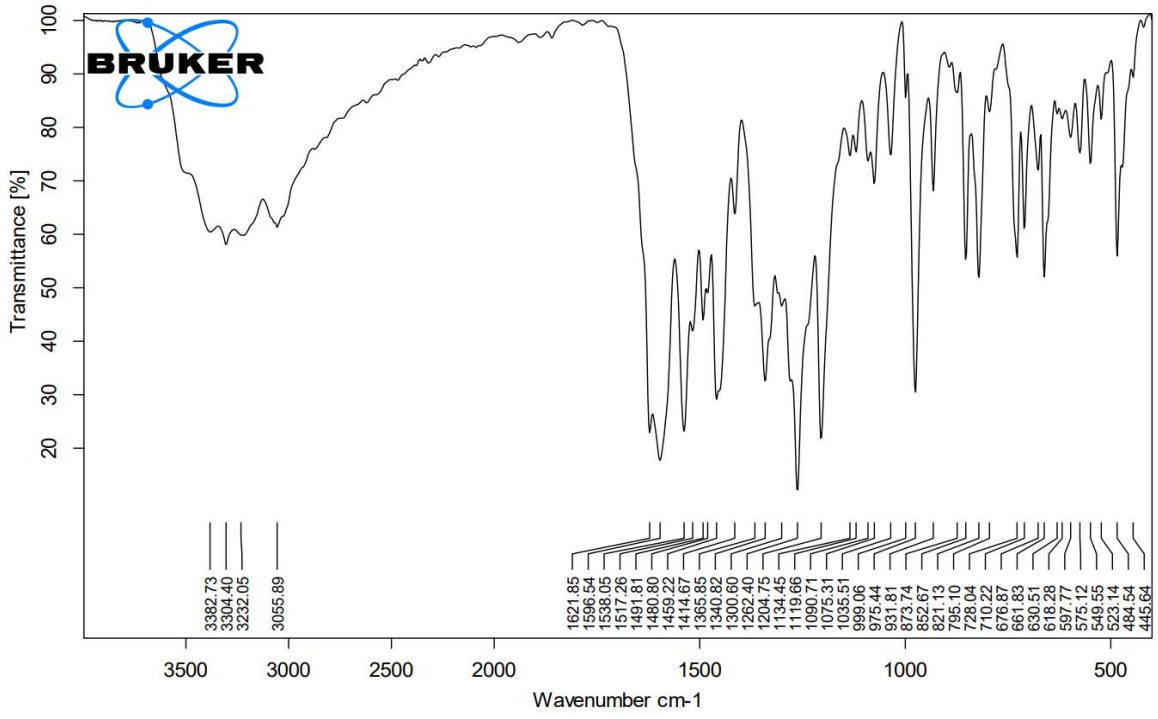



**4**

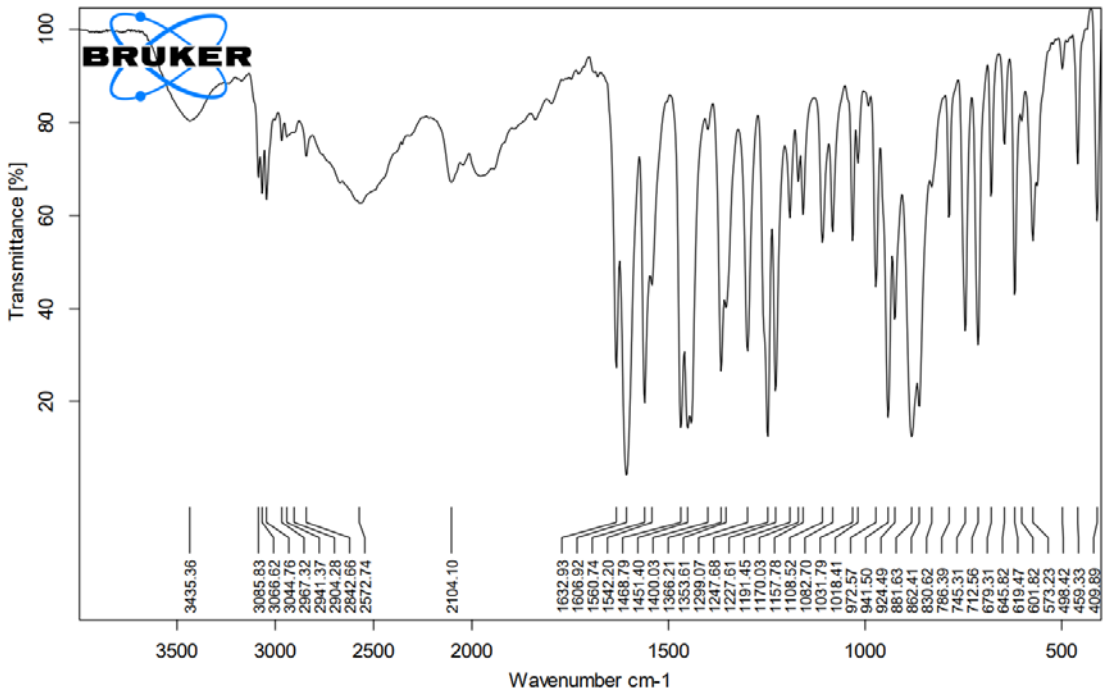
**Fig. S1 —** HOMO-LUMO of complexes **1-4**


BRUKER
Transmittance [%]
Wavenumber cm-1
3436.24
3183.73
3112.92
3087.43
3069.34
3007.92
2954.67
2935.43
2906.70
2838.42
1632.25
1604.39
1549.83
1523.74
1476.93
1469.26
1435.05
1351.85
1339.70
1289.95
1252.04
1217.10
1199.69
1172.56
1151.54
1110.68
1080.96
1059.81
1040.18
991.30
952.14
942.78
921.88
881.73
862.68
833.23
784.81
740.91
725.30
698.50
679.39
659.51
646.90
620.49
598.83
582.56
499.33
490.03
471.49
444.05
432.90
417.96

**1**


BRUKER
Transmittance [%]
Wavenumber cm-1
3382.73
3304.40
3232.05
3055.89
1621.85
1596.54
1538.05
1517.26
1491.81
1480.80
1459.22
1414.67
1365.85
1340.82
1300.60
1262.40
1204.75
1134.45
1119.66
1090.71
1075.31
1035.51
999.06
975.44
931.81
873.74
852.67
821.13
795.10
728.04
710.22
676.87
661.83
630.51
618.28
597.77
575.12
549.55
523.14
484.54
445.64

**2**

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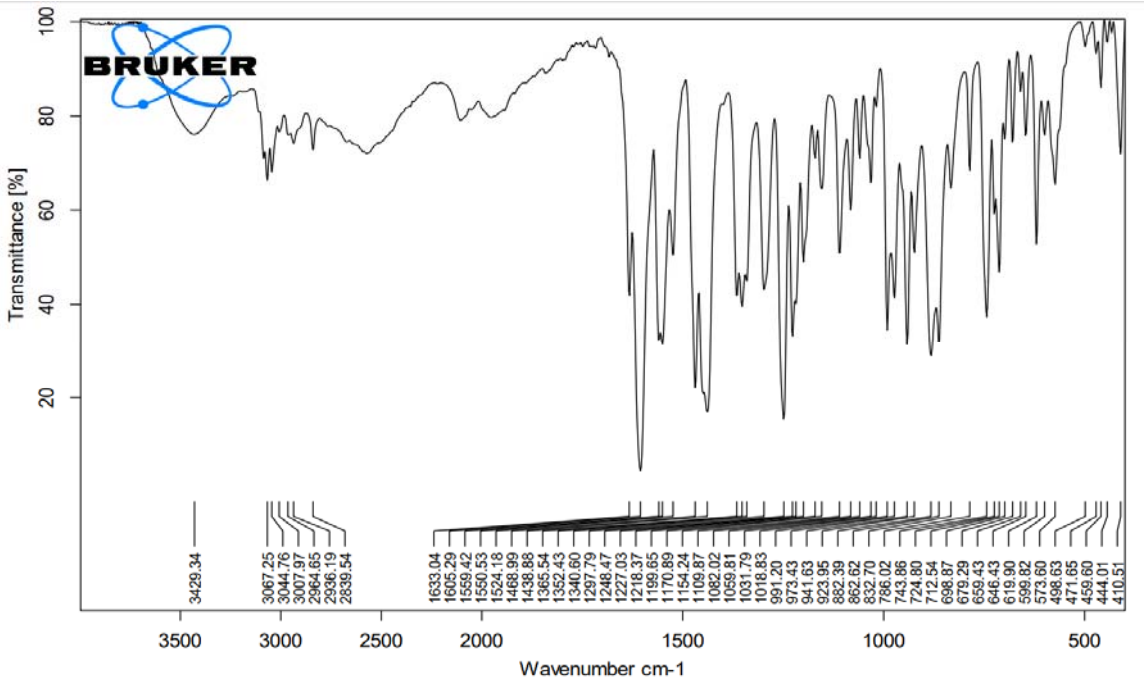
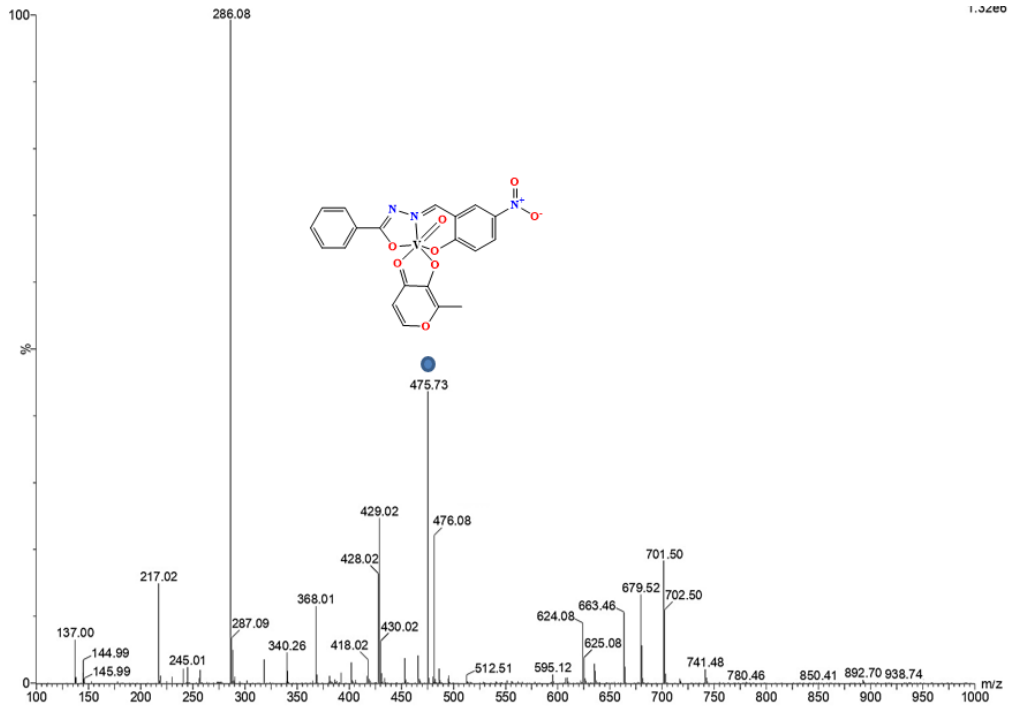
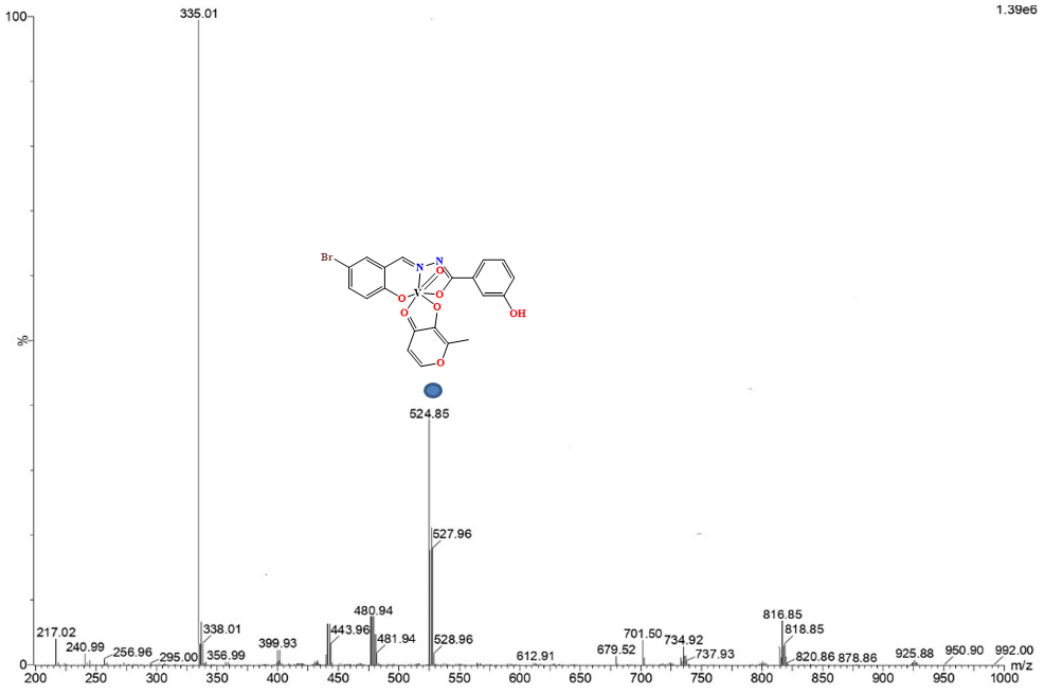



**4**

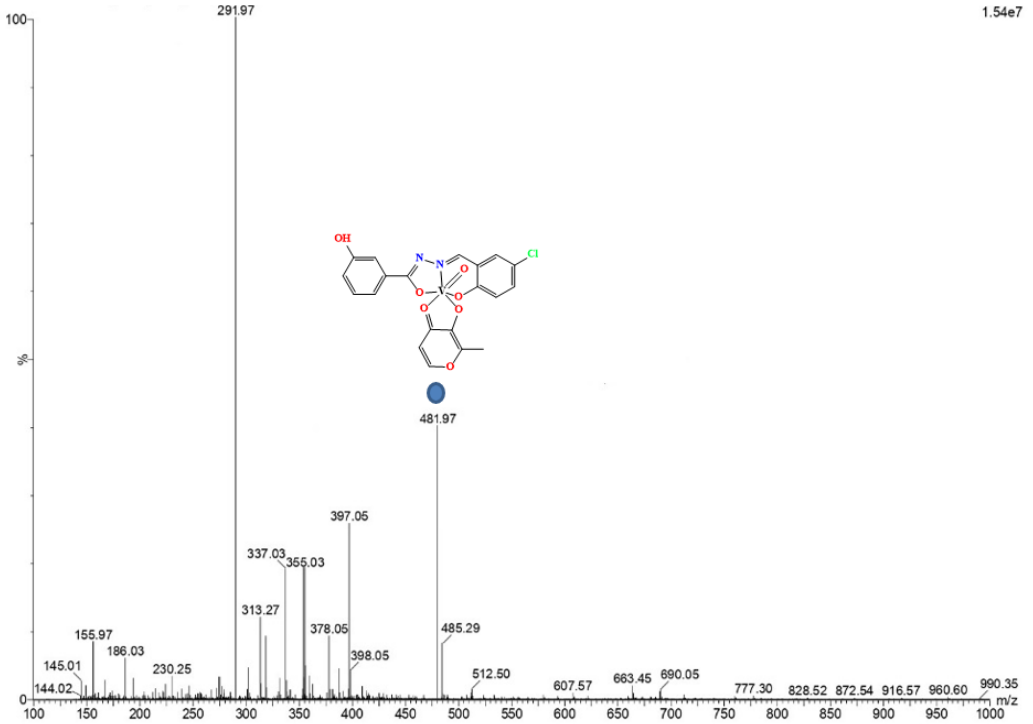
**Fig. S2 —** FTIR spectra of complexes **1-4**


100
%
0
286.08
475.73
429.02
476.08
428.02
217.02
701.50
679.52
702.50
368.01
663.46
624.08
287.09
430.02
137.00
144.99
145.99
340.26
418.02
625.08
245.01
512.51
595.12
741.48
780.46
850.41
892.70
938.74
m/z
100 150 200 250 300 350 400 450 500 550 600 650 700 750 800 850 900 950 1000

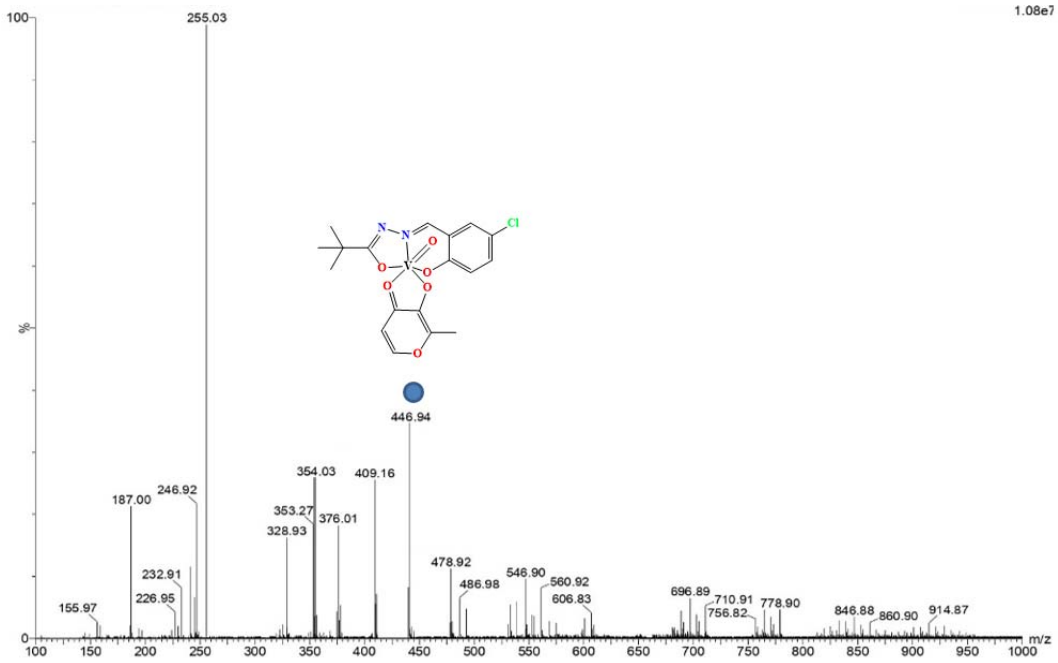
**1**


100
%
0
1.39e6
335.01
524.85
527.96
480.94
443.96
481.94
338.01
528.96
217.02
240.99
256.96
295.00
356.99
399.93
612.91
679.52
701.50
734.92
737.93
816.85
818.85
820.86
878.86
925.88
950.90
992.00
m/z
200 250 300 350 400 450 500 550 600 650 700 750 800 850 900 950 1000

**2**




**3**




**4**

**Fig. S3 —** ESI Mass spectra of complexes**1-4**

| **Table S1 —** Theoretical Bond lengths [Å] and angles [°] for complexes **1-4** | | | |
|---|---|---|---|
| **1** | | | |
| **Bond lengths** | | | |
| V(22)-O(4) | 1.863 | V(22)-O(29) | 1.868 |
| V(22)-O(20) | 1.865 | V(22)-O(33) | 1.636 |
| V(22)-O(27) | 1.866 | V(22)-N(9) | 1.887 |
| **Bond angles** | | | |
| O(4)-V(22)-N(9) | 95.593 | N(9)-V(22)-O(33) | 89.664 |
| O(4)-V(22)-O(27) | 89.094 | O(20)-V(22)-O(27) | 86.246 |
| O(4)-V(22)-O(29) | 88.541 | O(20)-V(22)-O(29) | 96.998 |
| O(4)-V(22)-O(33) | 89.487 | O(20)-V(22)-O(33) | 95.727 |
| N(9)-V(22)-O(20) | 79.260 | O(27)-V(22)-O(29) | 87.951 |
| **N(9)-V(22)-O(27)** | 96.330 | O(29)-V(22)-O(33) | 86.131 |
| **2** | | | |
| **Bond lengths** | | | |
| V(21)-O(4) | 1.872 | V(21)-O(27) | 1.871 |
| V(21)-O(18) | 1.826 | V(21)-O(29) | 1.862 |
| V(21)-O(22) | 1.614 | V(21)-N(9) | 1.827 |
| **Bond angles** | | | |
| O(4)-V(21)-N(9) | 93.905 | N(9)-V(21)-O(27) | 94.893 |
| O(4)-V(21)-O(18) | 88.448 | O(18)-V(21)-O(22) | 91.362 |
| O(4)-V(21)-O(27) | 90.910 | O(18)-V(21)-O(29) | 98.379 |
| O(4)-V(21)-O(29) | 86.156 | O(22)-V(21)-O(27) | 89.281 |
| N(9)-V(21)-O(18) | 81.612 | O(22)-V(21)-O(29) | 93.814 |
| N(9)-V(21)-O(22) | 86.123 | O(27)-V(21)-O(29) | 85.116 |
| **3** | | | |
| **Bond lengths** | | | |
| V(21)-O(4) | 1.848 | V(21)-O(27) | 1.880 |
| V(21)-O(18) | 1.864 | V(21)-O(29) | 1.881 |
| V(21)-O(22) | 1.635 | V(21)-N(9) | 1.869 |
| **Bond angles** | | | |
| O(4)-V(21)-N(9) | 92.229 | N(9)-V(21)-O(27) | 96.818 |
| O(4)-V(21)-O(18) | 93.620 | O(18)-V(21)-O(27) | 79.266 |
| O(4)-V(21)-O(22) | 94.544 | O(18)-V(21)-O(29) | 105.617 |
| O(4)-V(21)-O(29) | 83.708 | O(22)-V(21)-O(27) | 94.697 |
| N(9)-V(21)-O(18) | 80.266 | O(22)-V(21)-O(29) | 87.232 |
| N(9)-V(21)-O(22) | 87.413 | O(27)-V(21)-O(29) | 88.109 |

| **4** | | | |
|---|---|---|---|
| **Bond lengths** | | | |
| V(18)-O(4) | 1.859 | V(18)-O(24) | 1.885 |
| V(18)-O(16) | 1.870 | V(18)-O(26) | 1.892 |
| V(18)-O(19) | 1.636 | V(18)-N(9) | 1.911 |
| **Bond angles** | | | |
| O(4)-V(18)-N(9) | 85.096 | N(9)-V(18)-O(26) | 112.532 |
| O(4)-V(18)-O(16) | 119.342 | O(16)-V(18)-O(19) | 79.671 |
| O(4)-V(18)-O(19) | 88.530 | O(16)-V(18)-O(24) | 83.750 |
| O(4)-V(18)-O(24) | 155.044 | O(16)-V(18)-O(26) | 162.891 |
| O(4)-V(18)-O(26) | 73.791 | O(19)-V(18)-O(24) | 106.063 |
| N(9)-V(18)-O(16) | 80.960 | O(19)-V(18)-O(26) | 90.342 |
| N(9)-V(18)-O(19) | 153.289 | O(24)-V(18)-O(26) | 85.752 |
| N(9)-V(18)-O(24) | 89.856 | | |

**Table S2 —** The spin densities of metal and donor atoms for complexes **1-4**

| **Complexes** | **Metal and Donor atom** | **Spin population** | **Mulliken population** | **Natural population** |
|---|---|---|---|---|
| **1** | V(22) | +0.383 | +0.576 | +0.696 |
| | N(9) | -0.257 | -0.182 | -0.265 |
| | O(4) | -0.522 | -0.432 | -0.545 |
| | O(20) | -0.518 | -0.327 | -0.573 |
| | O(27) | -0.533 | -0.352 | -0.619 |
| | O(29) | -0.545 | -0.380 | -0.583 |
| | O(33) | -0.214 | -0.318 | -0.294 |
| **2** | V(21) | +0.375 | +0.514 | -0.284 |
| | N(9) | -0.240 | -0.171 | -0.092 |
| | O(4) | -0.612 | -0.440 | -0.301 |
| | O(18) | -0.442 | -0.259 | -0.220 |
| | O(22) | -0.346 | -0.410 | -0.087 |
| | O(27) | -0.495 | -0.283 | -0.246 |
| | O(29) | -0.581 | -0.434 | -0.301 |
| **3** | V(21) | +0.430 | +0.568 | -0.262 |
| | N(9) | -0.263 | -0.161 | -0.101 |
| | O(4) | -0.582 | -0.453 | -0.342 |
| | O(18) | -0.507 | -0.333 | -0.251 |
| | O(22) | -0.320 | -0.387 | -0.056 |
| | O(27) | -0.540 | -0.357 | -0.274 |

| | | | | |
|---|---|---|---|---|
| | O(29) | -0.581 | -0.405 | -0.294 |
| **4** | V(18) | +0.482 | +0.581 | -0.171 |
| | N(9) | -0.267 | -0.191 | -0.104 |
| | O(4) | -0.567 | -0.420 | -0.320 |
| | O(16) | -0.522 | -0.306 | -0.242 |
| | O(19) | -0.282 | -0.358 | -0.053 |
| | O(24) | -0.518 | -0.350 | -0.260 |
| | O(26) | -0.607 | -0.436 | -0.309 |