Electronic Supplementary Material (ESI) for Dalton Transactions

Supporting online material for

Modelling the Site of Bromide Binding in Vanadate-Dependent Bromoperoxidases†

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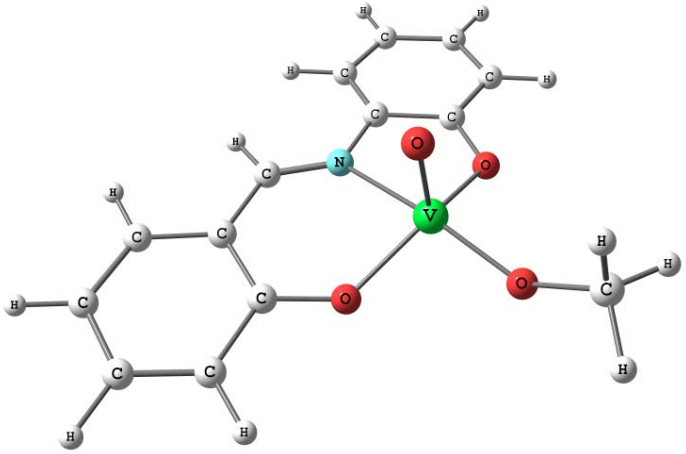
Computational results

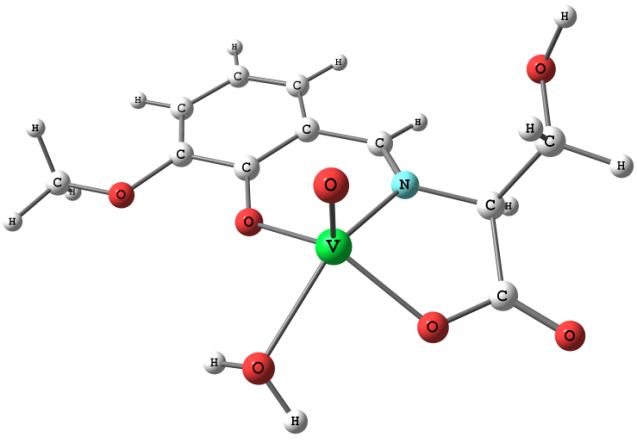
Table S1
Total energy in [H] and cartesian coordinates of the optimized geometry (DFT/ B3LYP) for **[V^{V}O(Amp-sal)OMe(MeOH)] (1)** in [Å] (xmol xyz format).
Basis set: 6-311++g(d,p) for all atoms.
Energy = -1840.7850408



C	0.005459000	-0.030417000	-0.022124000
C	0.012563000	-0.047759000	1.376767000
C	1.233369000	-0.071574000	2.079414000
C	2.445078000	-0.057771000	1.379595000
C	2.424547000	-0.032022000	-0.009276000
C	1.211983000	-0.017682000	-0.711206000
N	-1.084623000	-0.065432000	2.254480000
C	-2.316178000	-0.138782000	1.861293000
C	-3.442712000	-0.256939000	2.742767000
C	-4.749834000	-0.225353000	2.211165000
C	-5.855517000	-0.391350000	3.022230000
C	-5.671155000	-0.612548000	4.396139000
C	-4.400872000	-0.659265000	4.946558000
C	-3.268260000	-0.475651000	4.134905000
O	1.171007000	-0.139651000	3.409889000

O	-2.063598000	-0.552264000	4.679918000
V	-0.414134000	0.246455000	4.353111000
O	0.318336000	-0.096760000	5.914912000
C	0.900732000	0.645732000	6.962196000
H	-0.926180000	-0.014001000	-0.575711000
H	3.374189000	-0.074329000	1.935650000
H	3.360485000	-0.023015000	-0.556439000
H	1.212520000	0.008072000	-1.794237000
H	-2.541835000	-0.135652000	0.793622000
H	-4.874682000	-0.064234000	1.145054000
H	-6.853583000	-0.356235000	2.603343000
H	-4.248132000	-0.836177000	6.003982000
H	0.551949000	0.242240000	7.917765000
H	-6.533785000	-0.750477000	5.038688000
H	0.628861000	1.704042000	6.887715000
H	1.989997000	0.545215000	6.912792000
O	-0.630432000	1.802442000	4.299039000

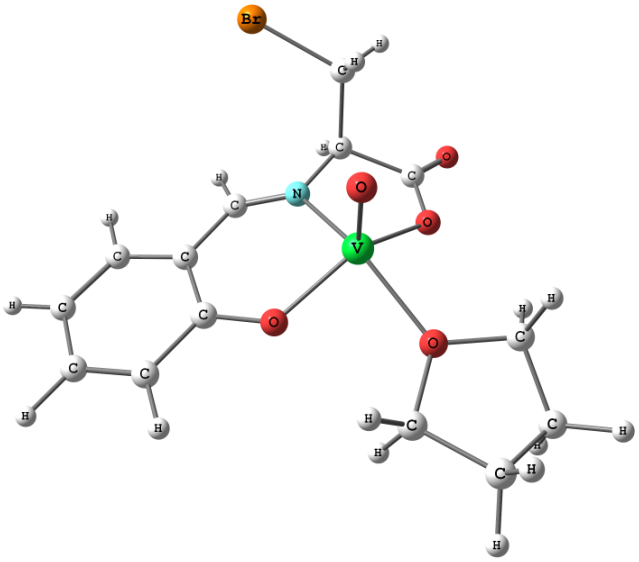
Table S2
Total energy in [H] and cartesian coordinates of the optimized geometry (DFT/ B3LYP) for **[VO(Ser-van)(H_2O)] (2)** in [Å] (xmol xyz format).
Basis set: Basis set: 6-311++g(d,p) for all atoms.
Energy = -1852.8040884



N	-0.375673000	-0.045796000	-0.070541000
V	0.542578000	0.159108000	1.740678000
O	2.069854000	0.409218000	1.420831000
O	-0.492151000	1.765918000	1.974609000
O	0.259587000	0.034877000	3.833562000
C	-1.002905000	0.872378000	-0.729479000
C	-0.986485000	2.590259000	1.077735000
C	-1.233089000	2.217504000	-0.270598000
C	-1.801529000	3.146440000	-1.175500000
C	-2.103091000	4.424001000	-0.765889000
C	-1.873129000	4.805114000	0.569120000
C	-1.338235000	3.912167000	1.484897000

C	-0.317832000	-1.426686000	-0.559097000
C	-0.233063000	-2.359464000	0.675495000
O	0.052915000	-1.726836000	1.796298000
O	-0.409982000	-3.550314000	0.564783000
H	-1.421784000	0.611342000	-1.702198000
H	-1.987185000	2.835935000	-2.197738000
H	-2.125467000	5.811228000	0.877243000
H	-1.223145000	-1.678703000	-1.119602000
C	0.885836000	-1.653210000	-1.477133000
H	0.946894000	-2.724066000	-1.694763000
H	1.802948000	-1.330770000	-0.972612000
O	0.661342000	-0.895770000	-2.667689000
H	1.493458000	-0.800287000	-3.139944000
H	-2.525477000	5.140845000	-1.459084000
O	-1.104057000	4.186887000	2.796968000
C	-1.398644000	5.492737000	3.273491000
H	-2.464526000	5.725674000	3.172166000
H	-1.128580000	5.491501000	4.328186000
H	-0.807513000	6.251899000	2.749795000
H	-0.089984000	-0.821683000	4.113549000
H	-0.321695000	0.741159000	4.147685000

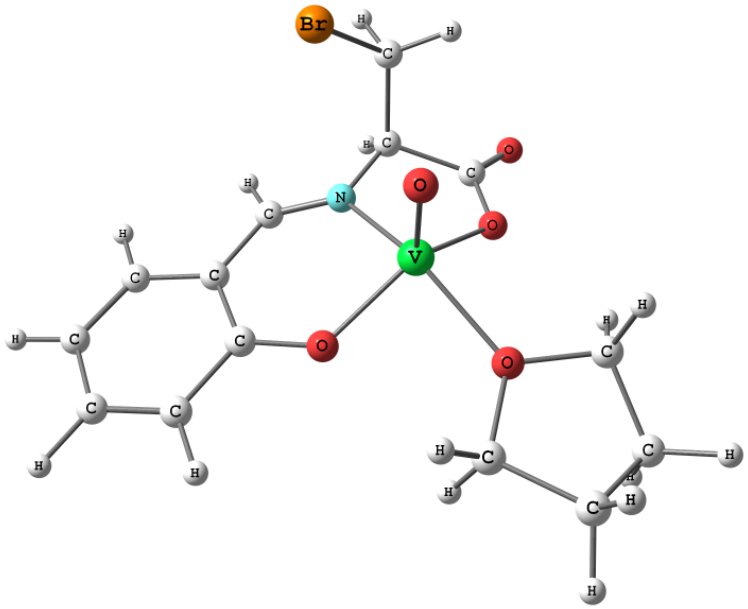
Table S3
Total energy in [H] and cartesian coordinates of the optimized geometry (DFT/ B3LYP) for **[VO(sal-BrAla)THF] (4, equilibrium state)** in [Å] (xmol xyz format).
Basis set: Basis set: 6-311++g(d,p) for all atoms.
Energy = -4492.62047886



V	0.000000000	0.000000000	0.000000000
O	0.000000000	0.000000000	1.582243000
O	2.017585000	0.000000000	-0.528632000
C	2.860526000	1.197294000	-0.451146000
C	2.843106000	-1.201094000	-0.690488000

C	4.186406000	0.755707000	-1.051321000
H	2.339532000	1.986816000	-0.986469000
H	2.954912000	1.471335000	0.603462000
C	4.285210000	-0.707654000	-0.591519000
H	2.558891000	-1.910973000	0.084411000
H	2.603545000	-1.624223000	-1.666699000
H	5.017066000	1.370191000	-0.700761000
H	4.151017000	0.818450000	-2.142524000
H	4.636847000	-0.757027000	0.442546000
H	4.959022000	-1.306178000	-1.206618000
N	-1.992422000	0.180551000	-0.515011000
O	-0.075060000	-1.774822000	-0.745957000
O	-0.053146000	1.815450000	-0.726843000
C	-1.083419000	-2.587982000	-0.979897000
C	-0.827312000	-3.960221000	-1.187071000
C	-2.433996000	-2.137217000	-1.078591000
C	-1.854450000	-4.842211000	-1.470064000
H	0.198774000	-4.299752000	-1.114241000
C	-3.457378000	-3.060743000	-1.388641000
C	-3.183793000	-4.400254000	-1.574362000
H	-1.626169000	-5.892591000	-1.616597000
H	-4.476779000	-2.696704000	-1.468686000
H	-3.979220000	-5.099565000	-1.799434000
C	-2.787023000	-0.753507000	-0.925679000
H	-3.808828000	-0.481965000	-1.196579000
C	-1.192519000	2.455162000	-0.836494000
C	-2.432250000	1.576574000	-0.488780000
H	-3.203007000	1.767801000	-1.239732000
O	-1.332160000	3.614575000	-1.151949000
C	-2.936795000	2.010981000	0.885810000
H	-3.104235000	3.084307000	0.894526000
H	-2.255780000	1.714315000	1.680187000
Br	-4.684104000	1.196431000	1.353408000

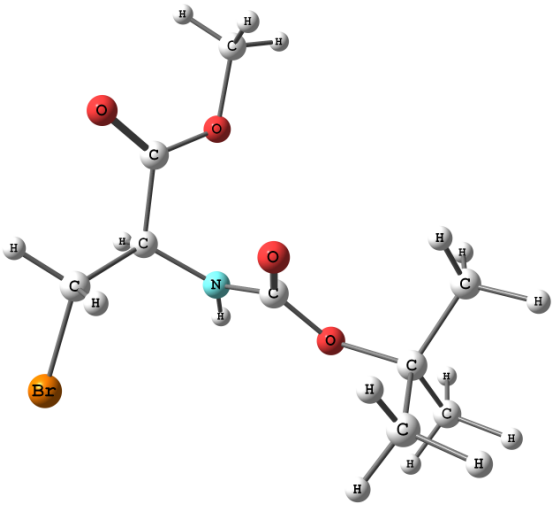
Table S4
Total energy in [H] and cartesian coordinates of the optimized geometry (DFT/ B3LYP) for **[VO(sal-BrAla)THF], 4 (dihedral angle Br-C13/C12-N = -2°)** in [Å] (xmol xyz format).
Basis set: Basis set: 6-311++g(d,p) for all atoms.
Energy = -4492.59856912



V	0.000000000	0.000000000	0.000000000
O	0.000000000	0.000000000	1.582243000
O	2.017585000	0.000000000	-0.528632000
C	2.860526000	1.197294000	-0.451146000
C	2.843106000	-1.201094000	-0.690488000
C	4.186406000	0.755707000	-1.051321000
H	2.339532000	1.986816000	-0.986469000
H	2.954912000	1.471335000	0.603462000
C	4.285210000	-0.707654000	-0.591519000
H	2.558891000	-1.910973000	0.084411000
H	2.603545000	-1.624223000	-1.666699000
H	5.017066000	1.370191000	-0.700761000
H	4.151017000	0.818450000	-2.142524000
H	4.636847000	-0.757027000	0.442546000
H	4.959022000	-1.306178000	-1.206618000
N	-1.992422000	0.180551000	-0.515011000
O	-0.075060000	-1.774822000	-0.745957000
O	-0.053146000	1.815450000	-0.726843000
C	-1.083419000	-2.587982000	-0.979897000
C	-0.827312000	-3.960221000	-1.187071000
C	-2.433996000	-2.137217000	-1.078591000
C	-1.854450000	-4.842211000	-1.470064000
H	0.198774000	-4.299752000	-1.114241000
C	-3.457378000	-3.060743000	-1.388641000
C	-3.183793000	-4.400254000	-1.574362000
H	-1.626169000	-5.892591000	-1.616597000
H	-4.476779000	-2.696704000	-1.468686000
H	-3.979220000	-5.099565000	-1.799434000
C	-2.787023000	-0.753507000	-0.925679000
H	-3.808828000	-0.481965000	-1.196579000
C	-1.192519000	2.455162000	-0.836494000
C	-2.432250000	1.576574000	-0.488780000
H	-3.203007000	1.767801000	-1.239732000
O	-1.332160000	3.614575000	-1.151949000

C	-2.936795000	2.010981000	0.885810000
H	-3.976215000	2.319065000	0.816301000
H	-2.322068000	2.800082000	1.312724000
Br	-2.906534000	0.537820000	2.214007000

Table S5
Total energy in [H] and cartesian coordinates of the optimized geometry (DFT/B3LYP) for **Boc-BrAlaMe** in [Å] (xmol xyz format).
Basis set: 6-311++g(3d,3p) for all atoms.
Energy = -3282.67461860

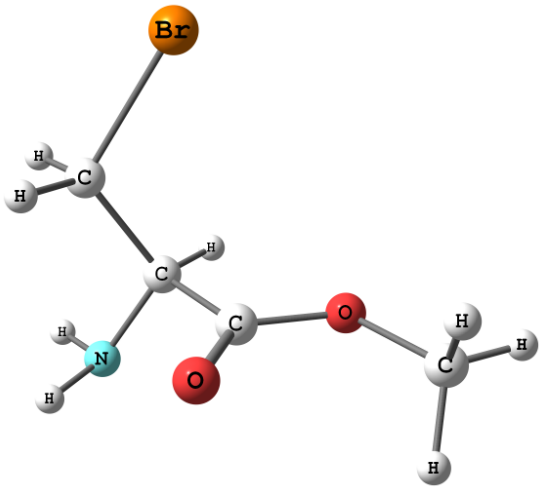


C	0.030148000	-0.139456000	0.168149000
C	-0.011018000	0.269916000	1.653753000
O	1.193354000	0.636435000	2.101638000
O	-1.026498000	0.331335000	2.297292000
C	1.244504000	1.050699000	3.480166000
N	1.228698000	-0.868075000	-0.182912000
C	1.575121000	-2.020401000	0.464157000
O	2.644897000	-2.576722000	-0.132884000
O	0.986435000	-2.438551000	1.441181000
C	3.236895000	-3.835291000	0.364004000
C	4.387186000	-4.066925000	-0.614434000
C	2.212658000	-4.967129000	0.274026000
C	3.764795000	-3.638520000	1.785534000
H	2.280977000	1.313940000	3.664255000
H	0.934968000	0.232382000	4.126589000
H	0.593779000	1.907155000	3.643751000
H	1.686220000	-0.662541000	-1.053497000
H	4.917746000	-4.982559000	-0.353370000
H	5.092914000	-3.237058000	-0.582357000
H	4.012426000	-4.162905000	-1.633247000
H	2.698305000	-5.912630000	0.519113000
H	1.818166000	-5.042309000	-0.739800000

H	1.388214000	-4.810551000	0.963930000
H	4.310381000	-4.531340000	2.094023000
H	2.953603000	-3.466291000	2.487350000
H	4.451719000	-2.792323000	1.821344000
C	-1.270868000	-0.859792000	-0.186366000
H	-1.297567000	-1.859602000	0.229091000
H	-2.135190000	-0.293580000	0.134136000
H	0.067754000	0.801607000	-0.384686000
Br	-1.447250000	-1.066900000	-2.146492000

Table S6

Total energy in [H] and cartesian coordinates of the optimized geometry (DFT/B3LYP) for **BrAlaMe** in [Å] (xmol xyz format).
Basis set: 6-311++g(3d,3p) for all atoms.
Energy = -2936.7246676



C	0.013736000	0.090263000	0.013451000
C	0.024413000	0.172638000	1.538976000
O	1.236918000	-0.044895000	2.054385000
O	-0.967370000	0.393385000	2.188833000
C	1.329162000	0.013046000	3.491753000
C	-0.448420000	1.418771000	-0.588370000
N	-0.887873000	-1.008980000	-0.337890000
Br	0.830135000	2.901423000	-0.257245000
H	1.014700000	-0.150278000	-0.338386000
H	2.371327000	-0.181078000	3.722294000
H	0.687287000	-0.742023000	3.940273000
H	1.032717000	0.997695000	3.846407000
H	-1.391078000	1.739771000	-0.156875000
H	-0.526196000	1.345966000	-1.668255000
H	-0.967825000	-1.109965000	-1.342263000
H	-1.812805000	-0.842259000	0.043000000