New Journal of Chemistry

Electronic Supplementary Information (ESI)

Syntheses, crystal structure, DFT calculations, protein interaction, anticancer potential and bromoperoxidase mimicking activity of oxidoalkoxidovanadium(V) complexes

Debanjana Biswal[a], Nikhil Ranjan Pramanik[*b], Michael G.B Drew[c], Nancy Jangra[d], Mannar R. Maurya[d], Mousumi Kundu[e], Parames C. Sil[e], Syamal Chakrabarti[*a]

[a]*Department of Chemistry, University College of Science, 92, Acharya Prafulla Chandra Road, Kolkata:700009, West Bengal, India.*
[b]*Department of Chemistry, Bidhannagar College, EB-2, Salt Lake, Kolkata: 700064, India.*
[c]*Department of Chemistry, The University of Reading, Whiteknights, Reading RG6 6AD, UK.*
[d]*Department of Chemistry, Indian Institute of Technology Roorkee, Roorkee-247667, India.*
[e]*Division of Molecular Medicine, Bose Institute, P-1/12, CIT Scheme VII M, Kolkata 700054, India.*

Table of Contents:

Fig. S8 The frontier orbitals in complex [VOL(OPr)(H_2O)] (**2**).

Fig. S9 CD spectra of BSA (1×10^{-5} M) in the UV-region in the absence and presence of the complexes **1**-**3** (2×10^{-5} M) at 25°C and pH 7.

Table S1 CD secondary structure estimation of BSA in the absence and presence of complexes **1**-**3** using CDNN Software

Table S2 Results of molecular docking: Adjacent residues and hydrogen bonding interactions

Fig. S1 Single crystals of [VOL(OPr)(H_2O)] (**2**) isolated by solvent evaporation at low temperature.

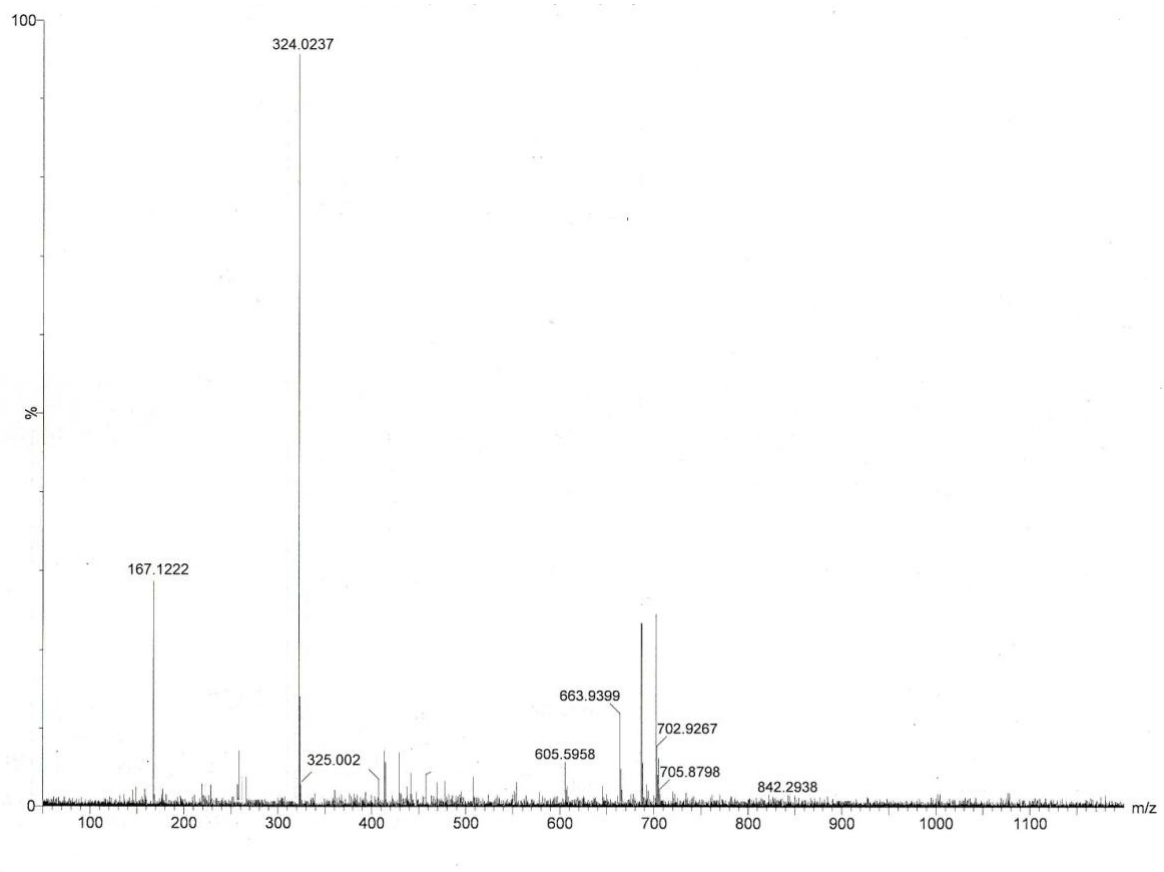
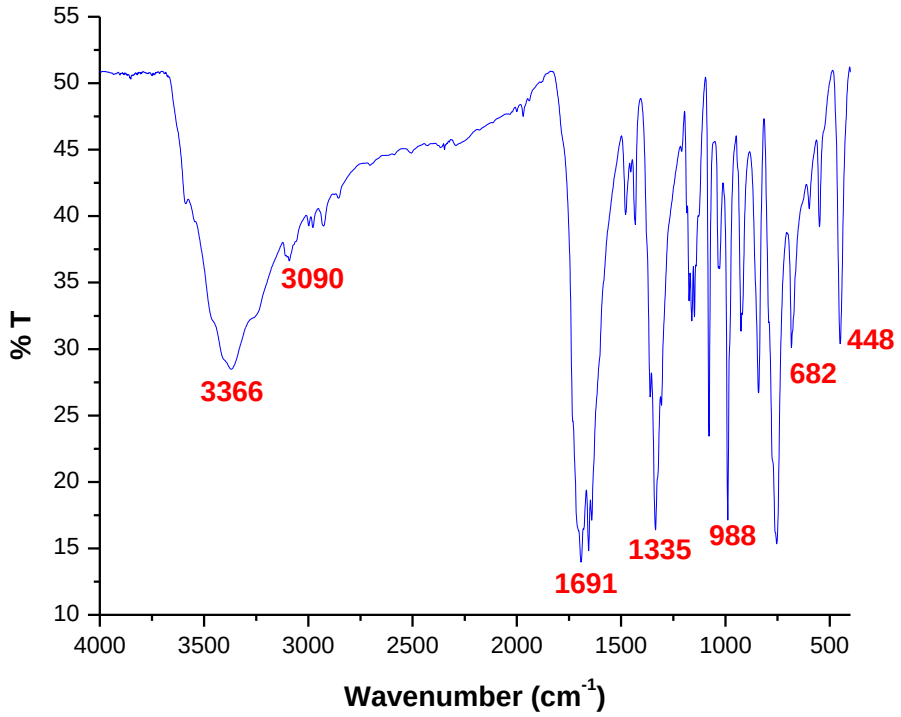
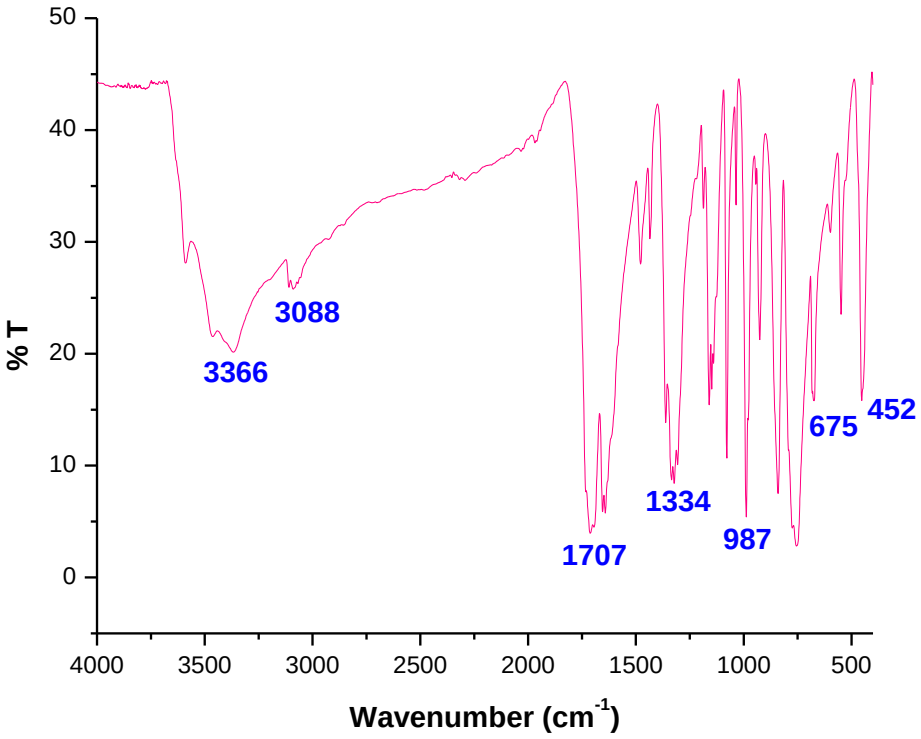


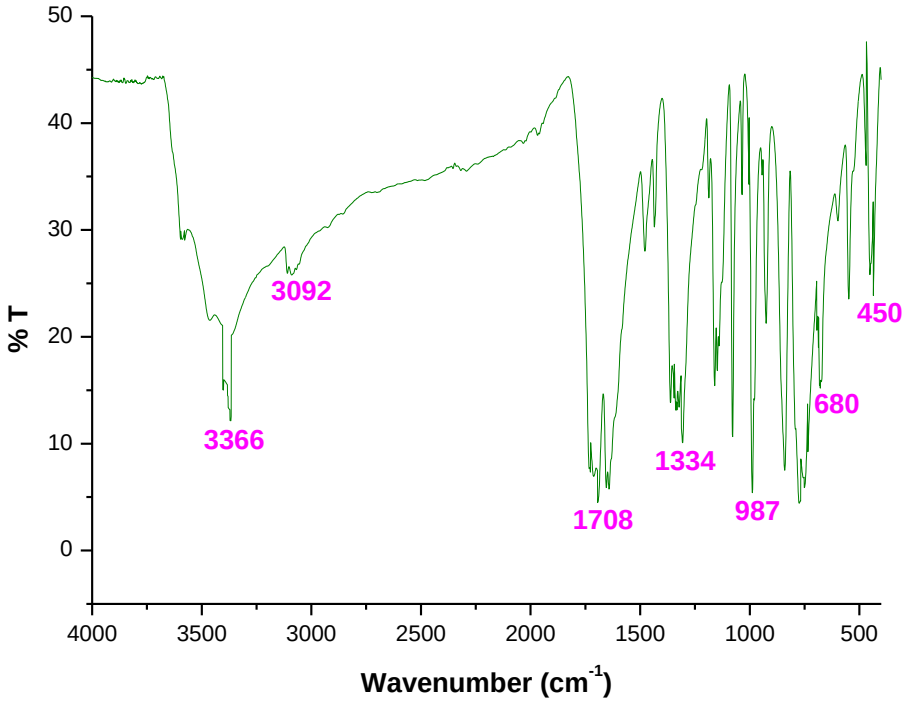
Fig. S2 ESI-MS of [VOL(OBu)(H_2O)] (**3**).



(a)

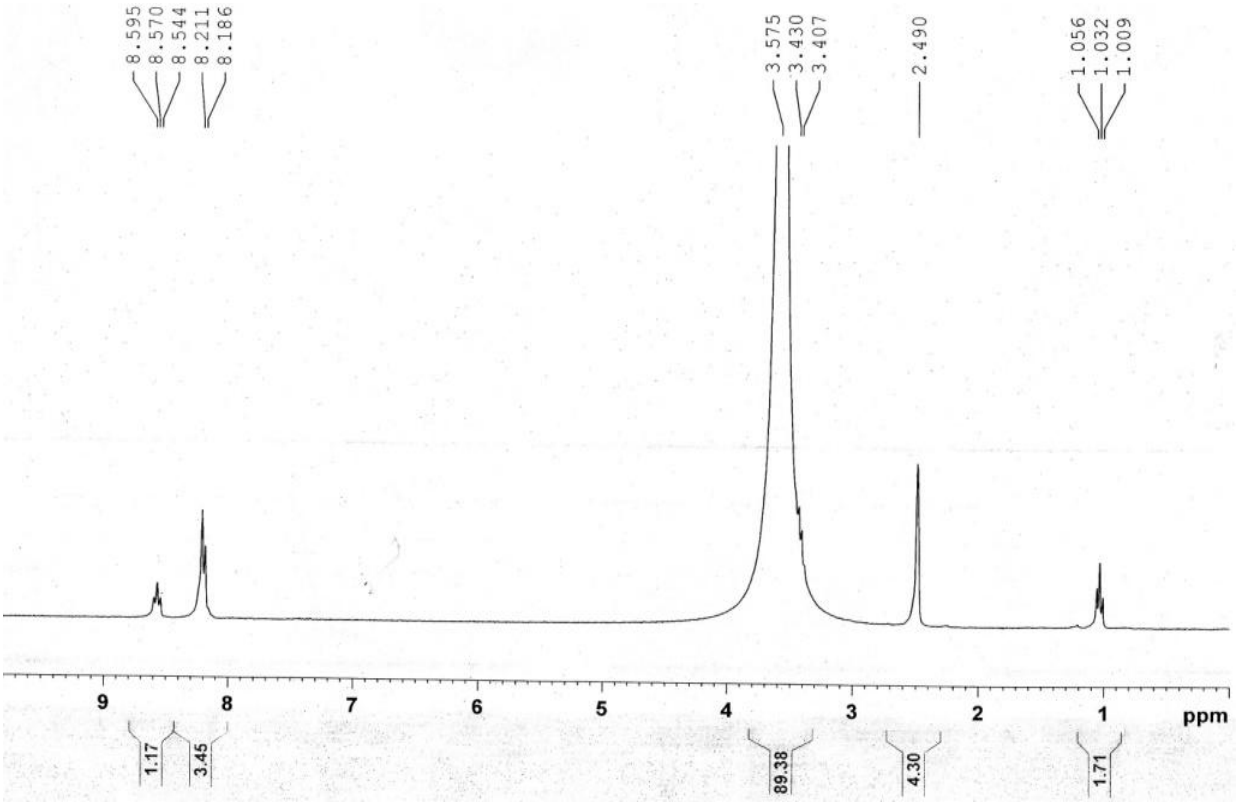


(b)

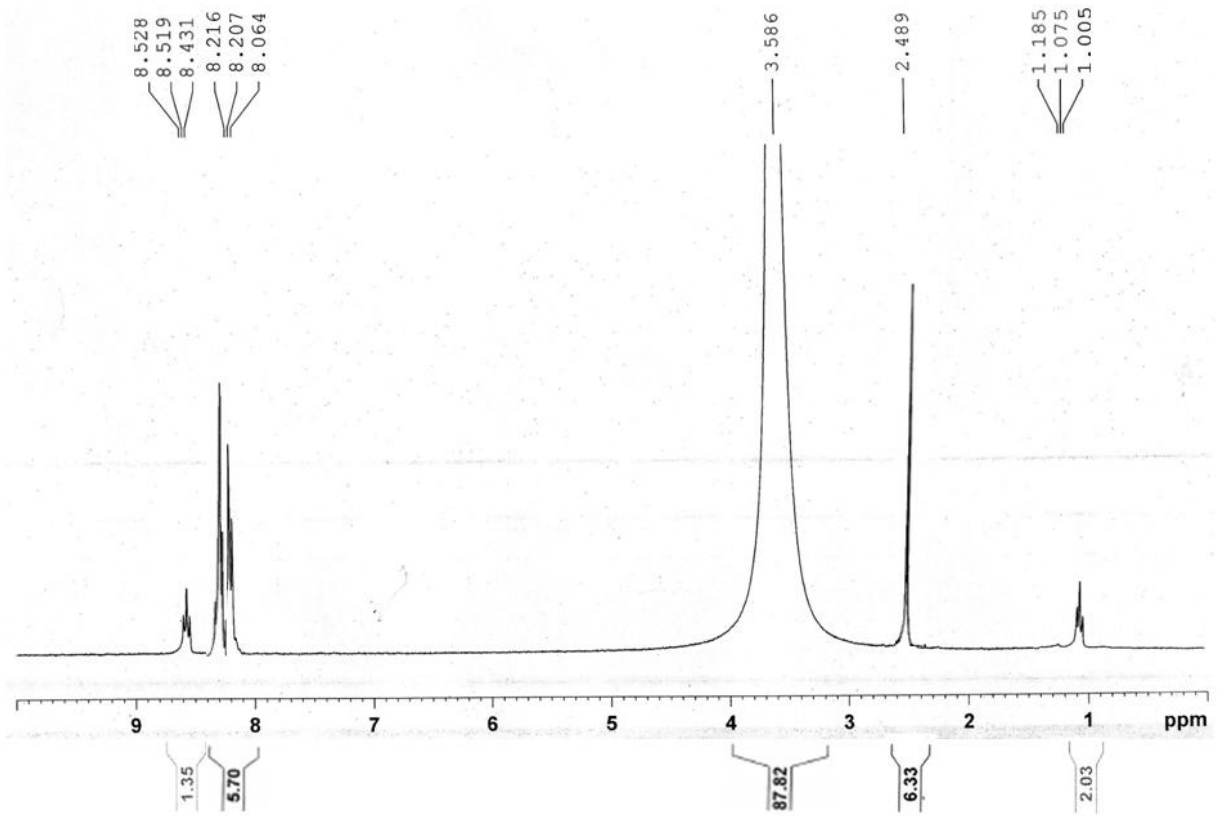


(c)

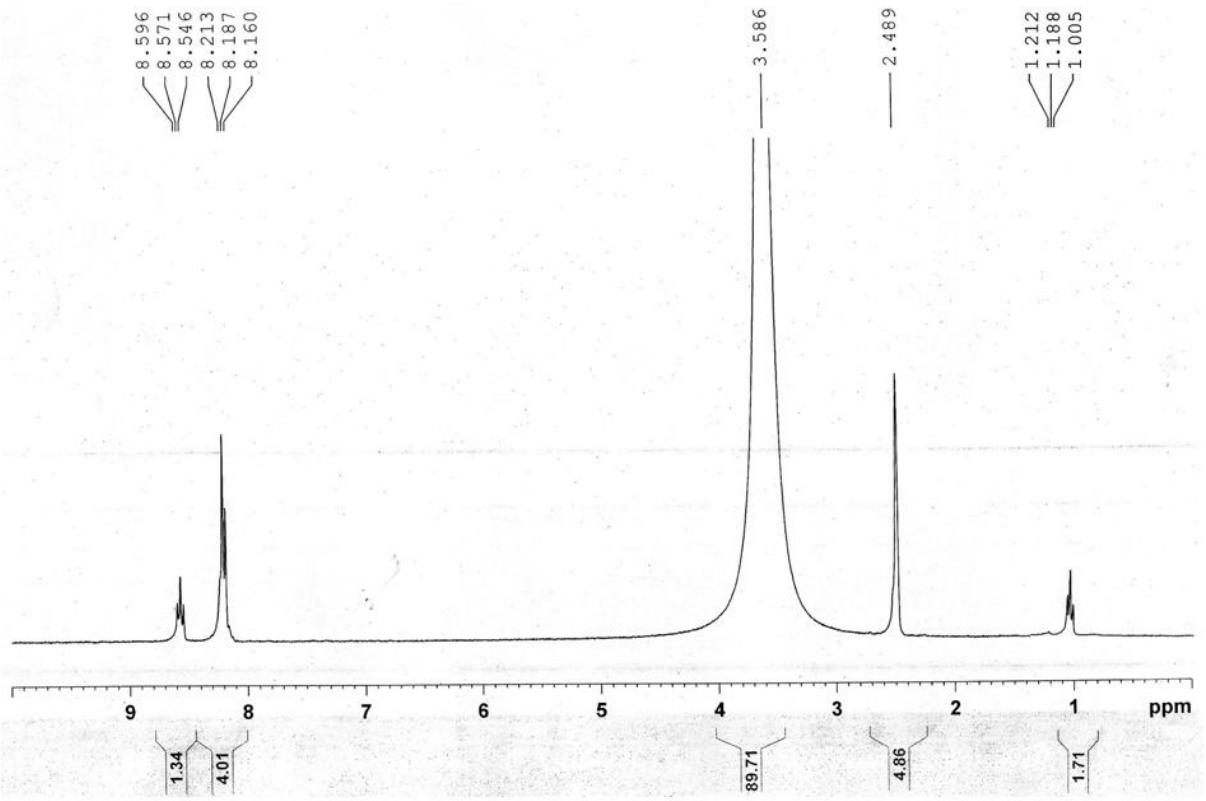
Fig. S3 IR spectra of complexes **(a)** [VOL(OEt)(H_2O)] (**1**), **(b)** [VOL(OPr)(H_2O)] (**2**) and **(c)** [VOL(OBu)(H_2O)] (**3**) in KBr pellets.


8.595
8.570
8.544
8.211
8.186
3.575
3.430
3.407
2.490
1.056
1.032
1.009
9
8
7
6
5
4
3
2
1
ppm
1.17
3.45
89.38
4.30
1.71

(a)

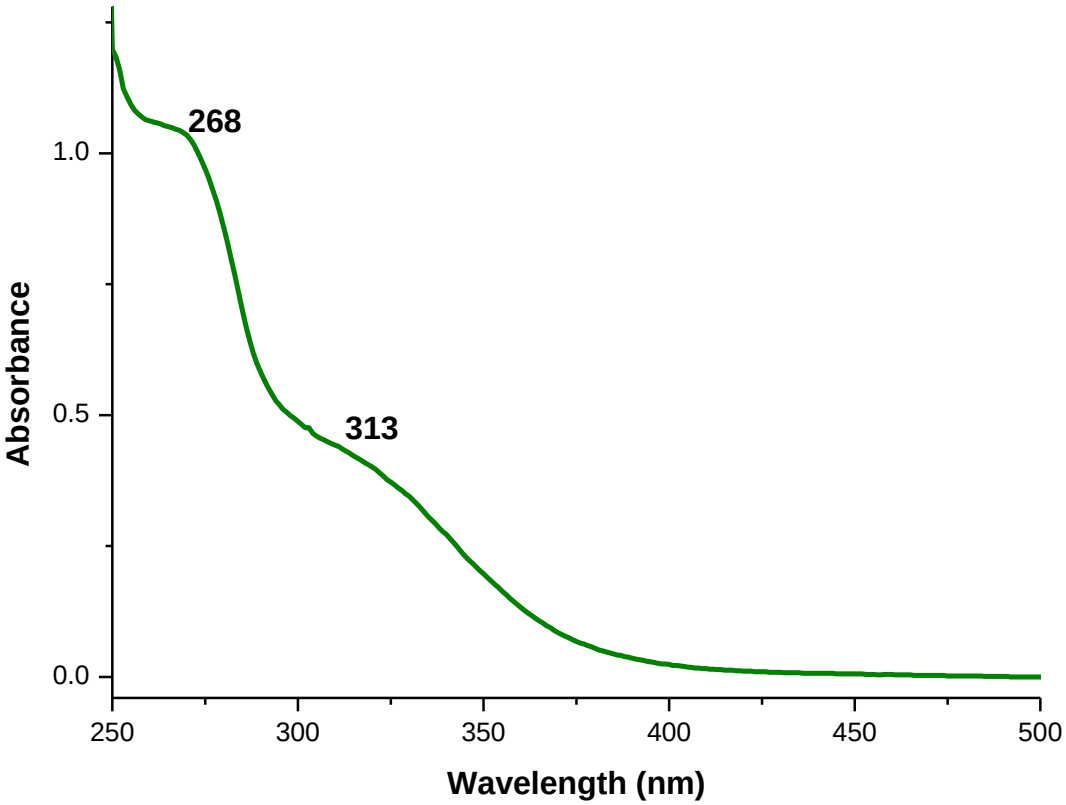

8.528
8.519
8.431
8.216
8.207
8.064
3.586
2.489
1.185
1.075
1.005
9
8
7
6
5
4
3
2
1
ppm
1.35
5.70
87.82
6.33
2.03

(b)

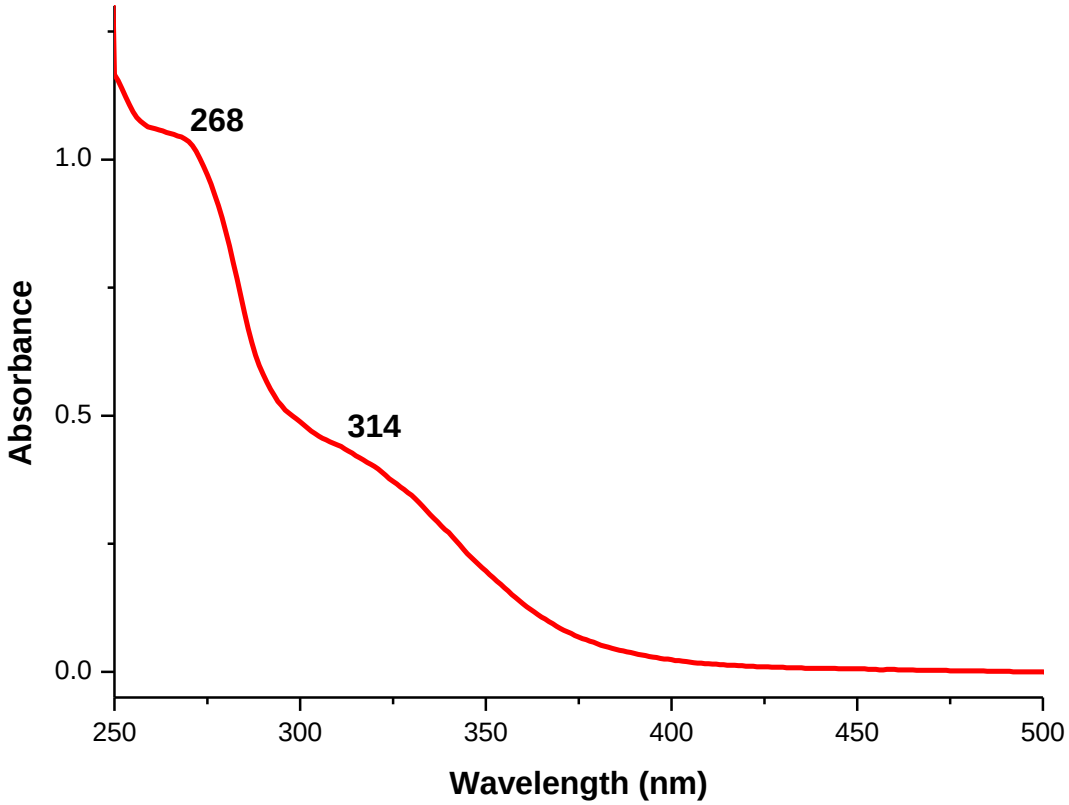


(c)

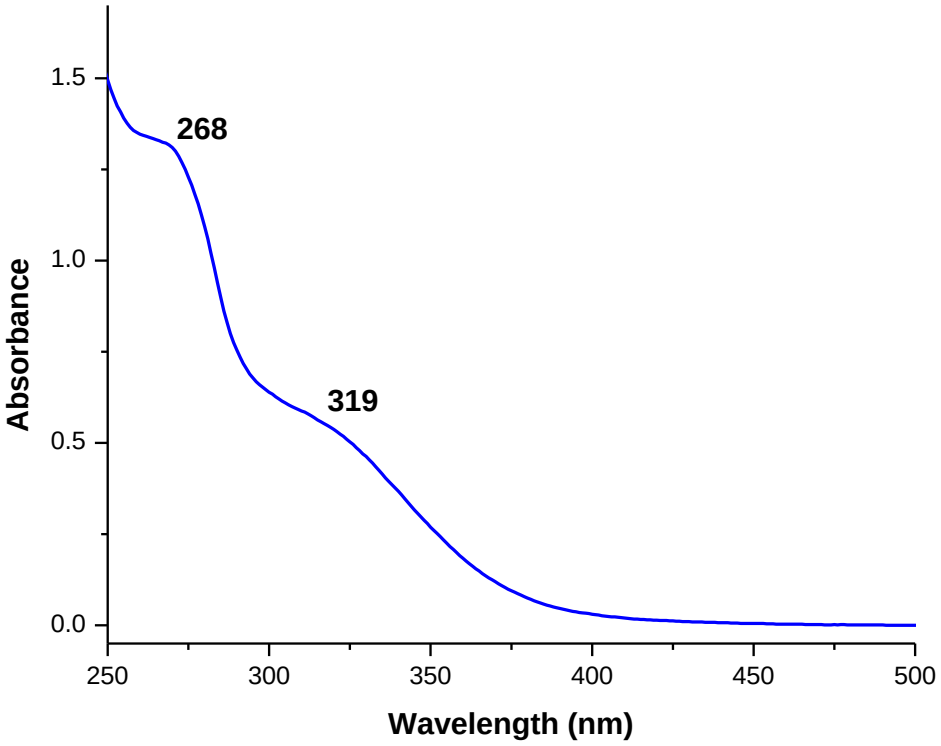
Fig. S4 ^{1}H NMR spectrum of complexes **(a)** [VOL(OEt)(H_2O)] (**1**), **(b)** [VOL(OPr)(H_2O)] (**2**) and **(c)** [VOL(OBu)(H_2O)] (**3**) in DMSO-d_6.


268
313
1.0
0.5
0.0
Absorbance
250
300
350
400
450
500
Wavelength (nm)

(a)


268
314
1.0
0.5
0.0
Absorbance
250
300
350
400
450
500
Wavelength (nm)

(b)



(c)

Fig. S5 Electronic spectrum of complexes **(a)** [VOL(OEt)(H_2O)] (**1**), **(b)** [VOL(OPr)(H_2O)] (**2**) and **(c)** [VOL(OBu)(H_2O)] (**3**) in water at room temperature.

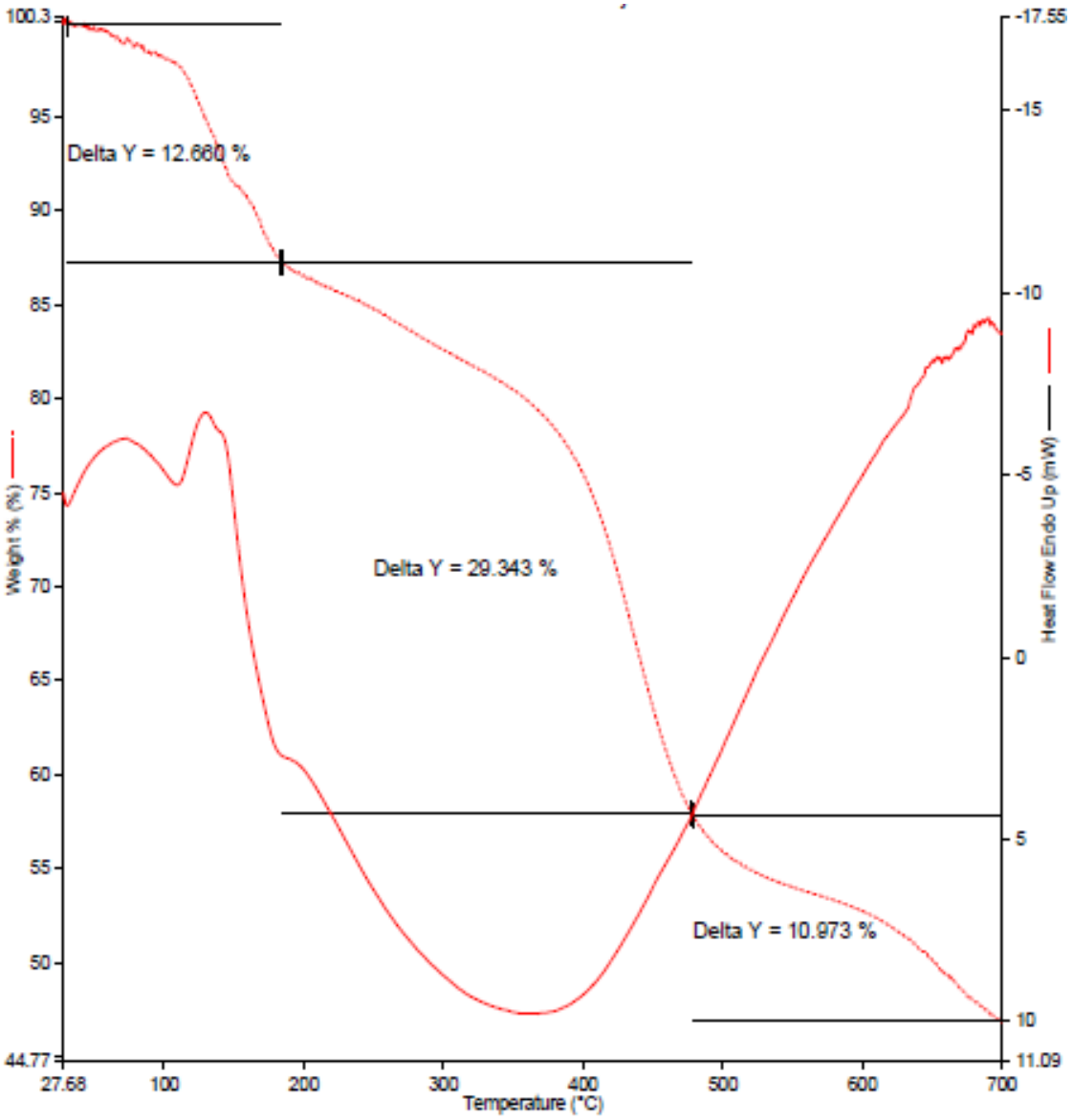


Fig. S6 TG-DTA curve of complex [VOL(OEt)(H_2O)] (**1**) under N_2 atmosphere.

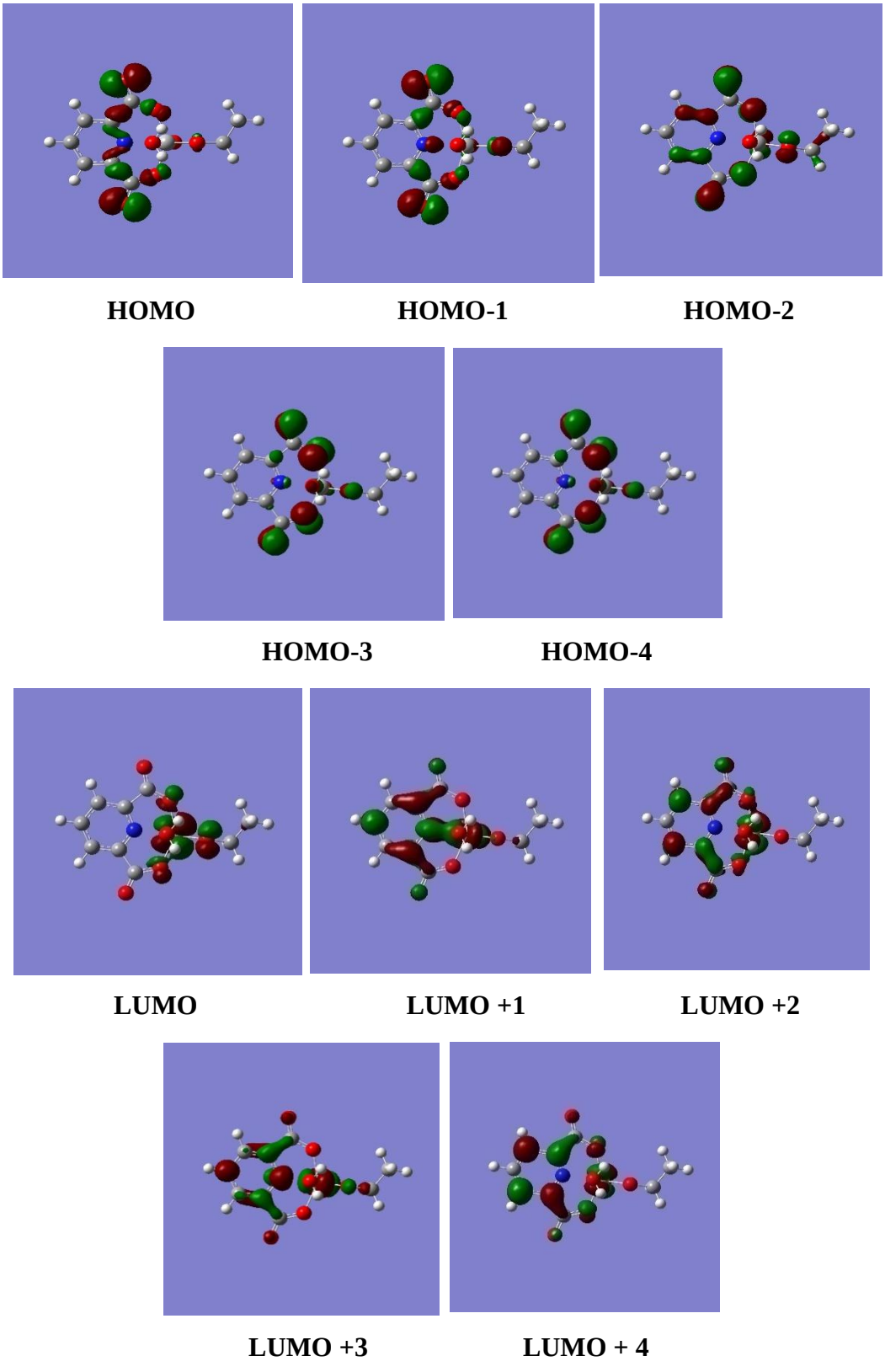


Fig. S7 The frontier orbitals in complex [VOL(OEt)(H_2O)] (**1**).

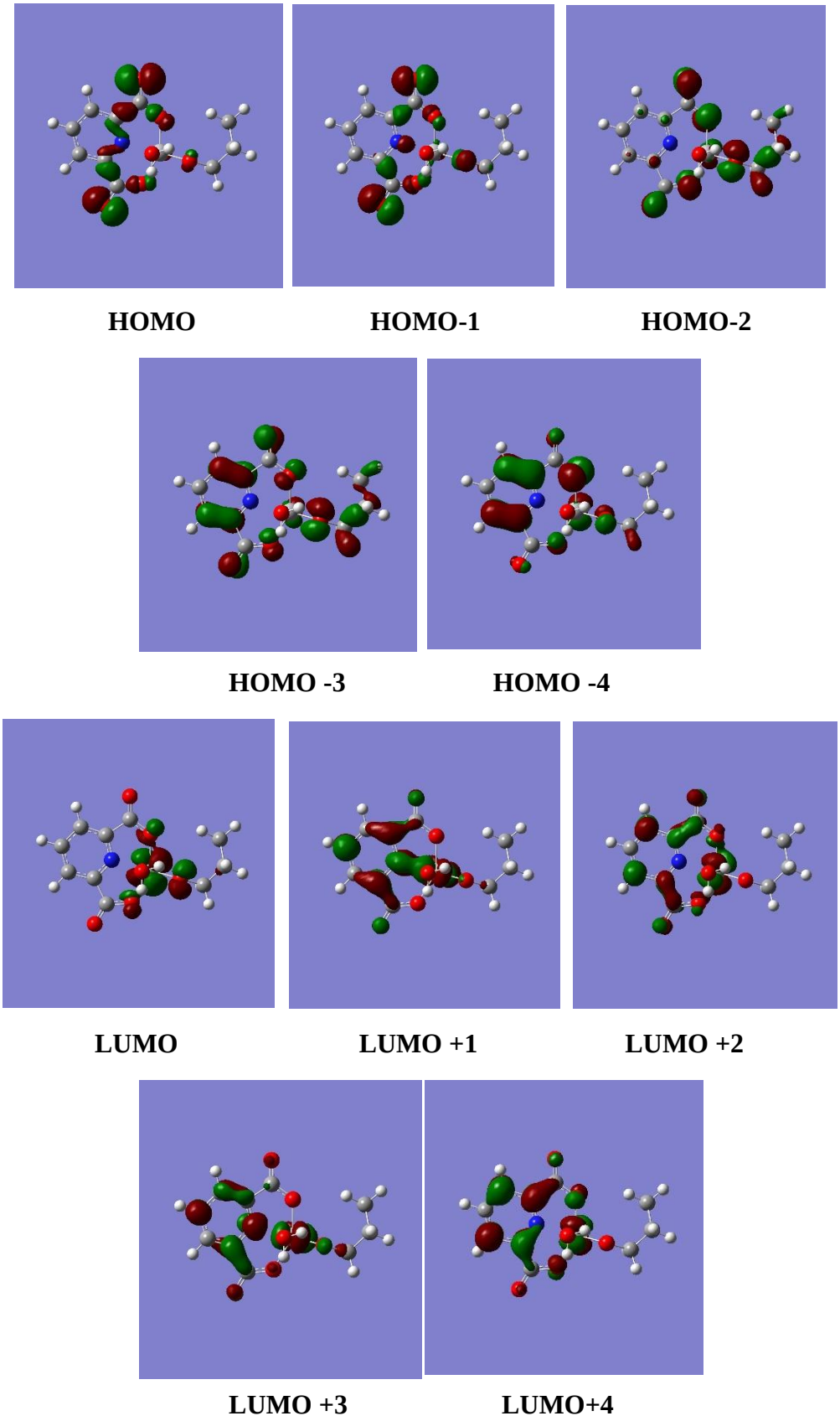


Fig. S8 The frontier orbitals in complex [VOL(OPr)(H_2O)] (**2**).

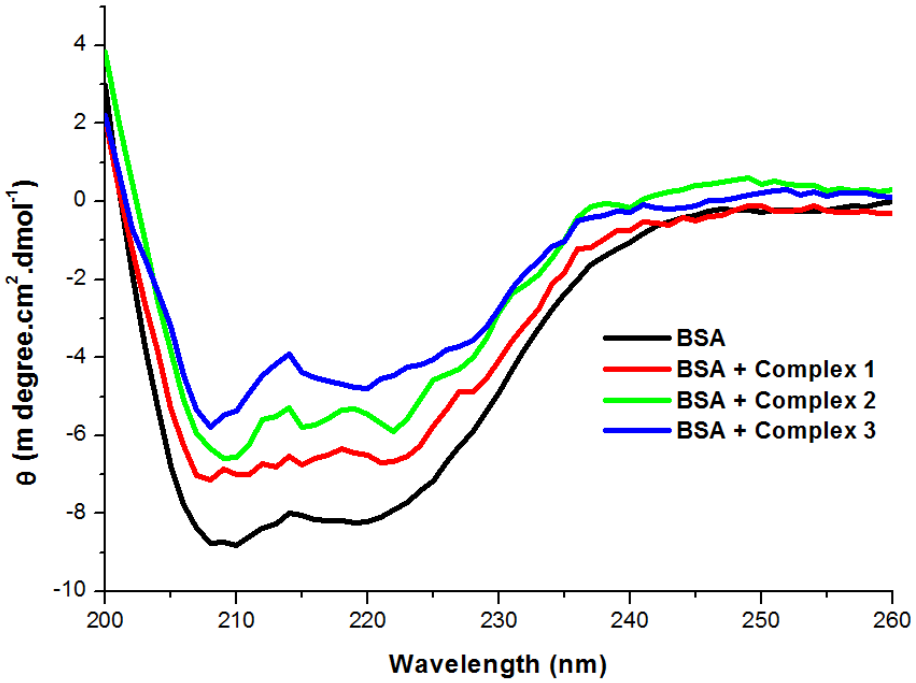


Fig. S9 CD spectra of BSA (1×10^{-5} M) in the UV-region in the absence and presence of the complexes **1-3** (2×10^{-5} M) at 25°C and pH 7.

Table S1

CD secondary structure estimation of BSA in the absence and presence of complexes **1-3** using CDNN Software

Components conformation	**Free BSA (1×10^{-5} M)**	**BSA + Complex 1 (2×10^{-5} M)**	**BSA + Complex 2 (2×10^{-5} M)**	**BSA + Complex 3 (2×10^{-5} M)**
α-Helix (%)	85.0	72.2	66.3	52.0
β-sheet (Antiparallel) (%)	1.3	2.4	3.0	4.8
β-sheet (Parallel) (%)	1.5	2.6	3.4	5.1
β-Turn (%)	9.3	11.3	12.1	14.1
Random Coil (%)	7.0	12.0	15.2	21.0

Table S2

Results of molecular docking: Adjacent residues and hydrogen bonding interactions

Complexes	**Hydrogen bonding interactions**	**Adjacent amino acids**
BSA···Complex **1**	(Arg-198)-NH-H···O=V = 1.6 Å (Arg-198)-N-H···O=V = 2.7 Å (Arg-217)-NH-H···O=C = 2.7 Å	Tyr-149, Tyr-155, Tyr-156, Arg-194, Arg-198, Arg-217, Arg-256, Ala-290, Glu-291
BSA···Complex **2**	(Arg-198)-NH-**H**···O=V = 1.5 Å (Arg-198)-N**H**-H···O=V = 2.7 Å (Arg-198)-N-H···O=V = 2.8 Å (Arg-217)-NH-H···O=C = 2.4 Å (Arg-217)-NH-H···O-C = 2.7 Å	Tyr-149, Tyr-155, Tyr-156, Ser-191, Arg-194, Arg-198, Arg-217, Ile-263, Ala-290