Supporting Material for

Enzyme graphene oxide interaction: the case system of β-lactamases

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1 Graphene oxide edge-to-surface atom ratio

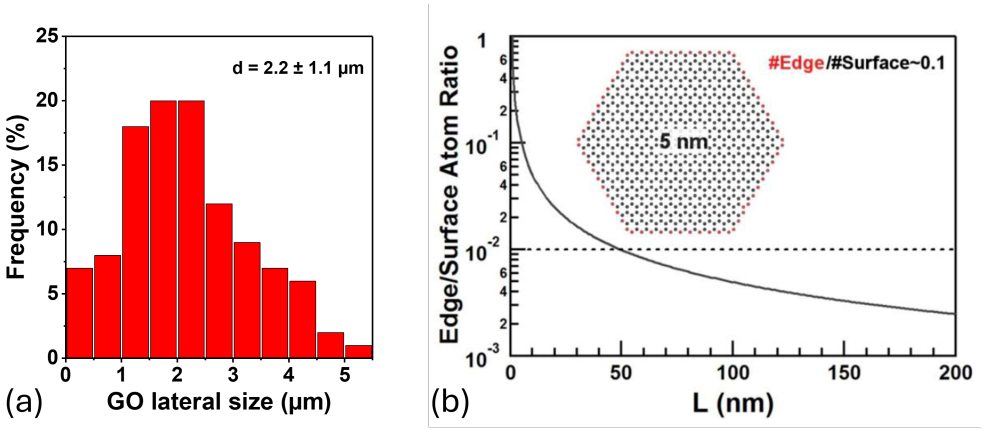

Figure S 1 (a) Graphene oxide lateral size distribution, estimated by the SEM images analysis. (b) Graphene oxide edge-to-surface atom ratio as a function of the flake size.

2 DFT interaction configuration of Nitrocefin with graphene oxide

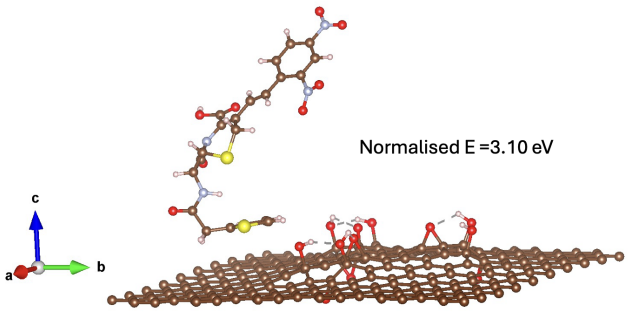

Figure S 2 Vertical configuration 1: molecule attached to only C atoms.

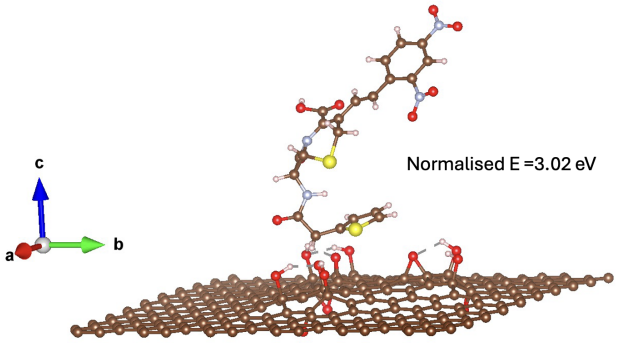

Figure S 3 Vertical configuration 2: molecule attached to graphene oxide ligands.

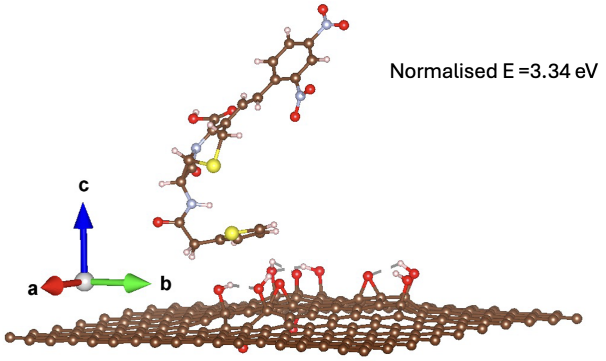

Figure S 4 Vertical configuration 3: molecule attached to graphene oxide ligands

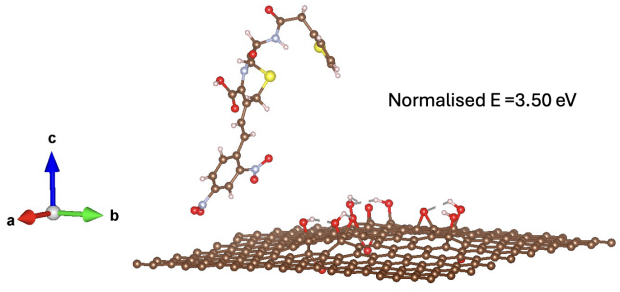

Figure S 5 Vertical configuration 4: flipped molecule attached to only C atoms.

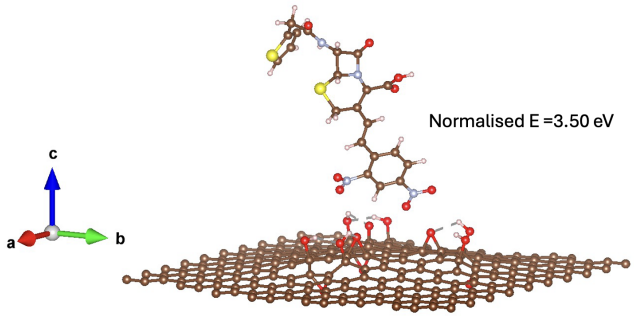

Figure S 6 Vertical configuration 5: flipped molecule attached to graphene oxide ligands

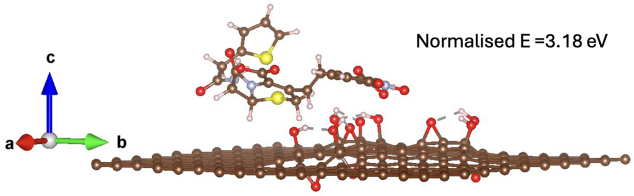

Figure S 7 Horizontal configuration 1.

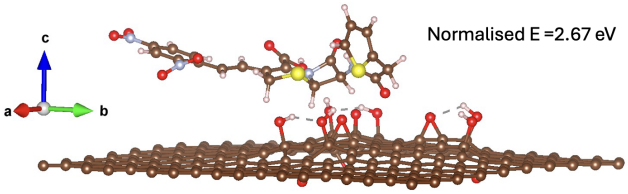

Figure S 8 Horizontal configuration 2.

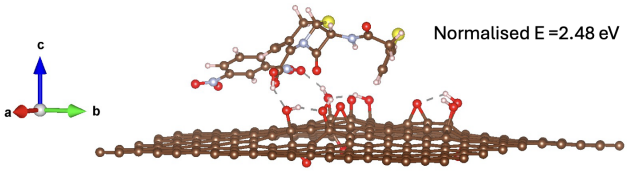

Figure S 9 Horizontal configuration 3.

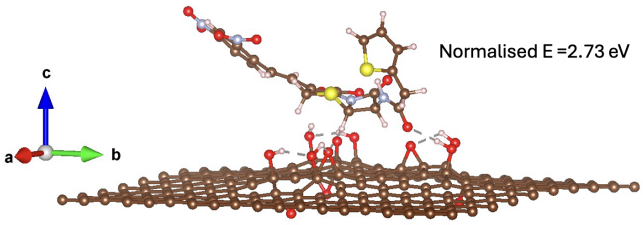

Figure S 10 Horizontal configuration 4.

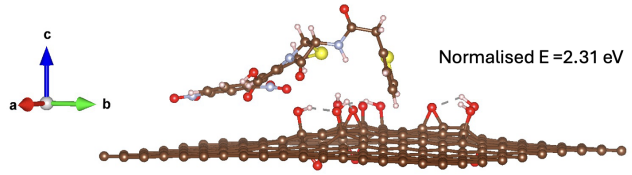

Figure S 11 Horizontal configuration 5.

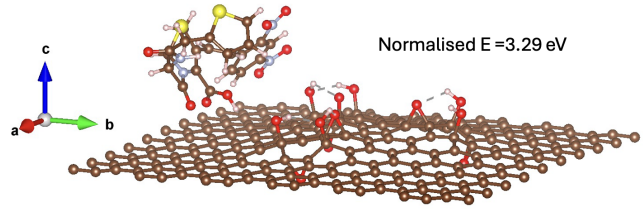

Figure S 12 Horizontal configuration 6.

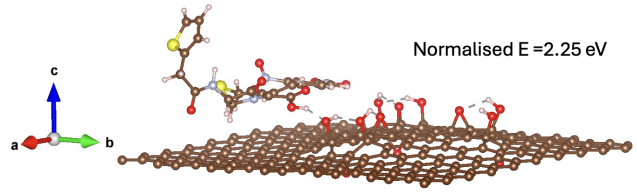

Figure S 13 Horizontal configuration 7.

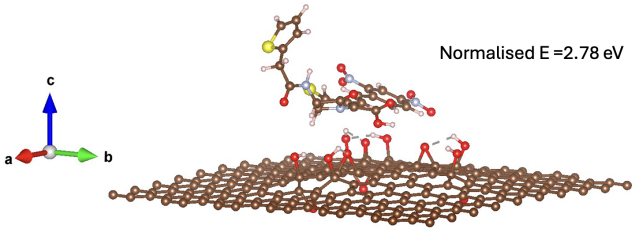

Figure S 14 Horizontal configuration 8.

3 C 1s XPS of Nitrocefin and graphene oxide

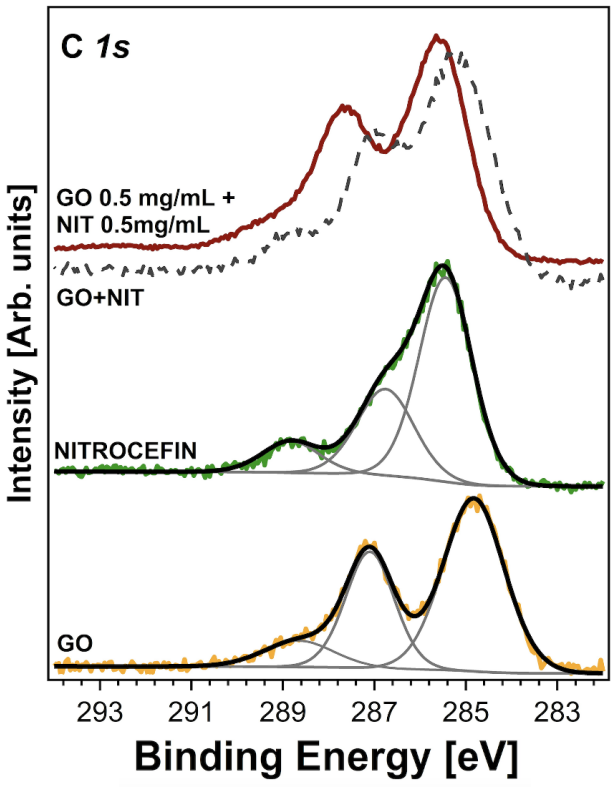

Figure S 15 (b) C 1s XPS core level spectral analysis for (from bottom to top): pure GO 0.5 mg/ml (yellow), pure Nitrocefin 0.5 mg/ml (green), and GO 0.5 mg/ml mixed with Nitrocefin 0.5 mg/ml (red).

4 Modeled Gaussian surfaces of the SBL and MBL

All the class A SBL show similar features in their tridimensional structure. They have a pear-shaped structure once the active serine site is visible. As expected the surface exposing the active site is concave in shape, while (images on the bottom left in each figure) a convex shape is observed on their opposite surface. The distribution and number of positive lysine and arginine residues on each enzyme is very enzyme specific, however, all the SBL considered are characterised in each figure (bottom left frame) by a "Y" shaped local structure of four Arginine residues (for example in GES-1 they are the ARG residue nr 148, 156, 173, an 59). This Y-shaped arrangement of Arginine residue can be identified in all the convex-shaped surfaces (opposed to the active site) of all the SBL.

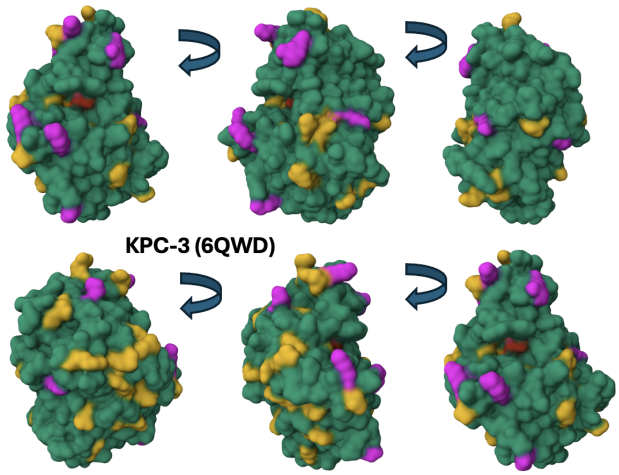

Figure S 16 KPC-3 SBL enzyme structure (Gaussian Surface) as generated from https://www.rcsb.org/ , (ID: 6QWD). Lysine (Arginine) residues are coloured in purple (mustard). The active catalytic pocket is indicated in red. To have a complete view of the enzyme surface, from top left to bottom right the 3D generated model is left handed turned 72^o around the vertical axis in the figure.

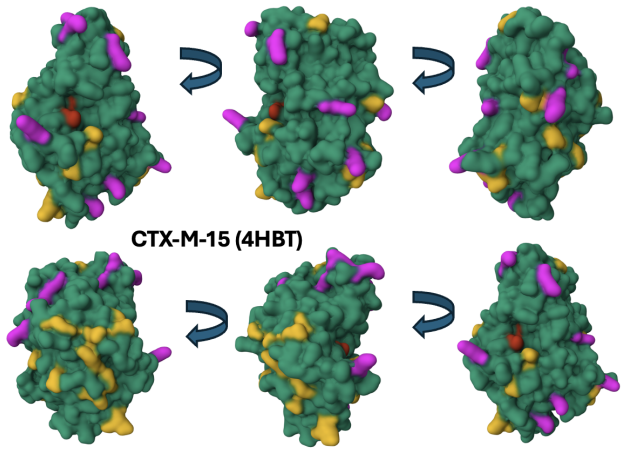

Figure S 17 CTX-M-15 SBL enzyme structure (Gaussian Surface) as generated from https://www.rcsb.org/ , (ID ID: 4HBT). Lysine (Arginine) residues are coloured in purple (mustard). The active catalytic pocket is indicated in red. To have a complete view of the enzyme surface, from top left to bottom right the 3D generated model is left handed turned 72^o around the vertical axis in the figure.

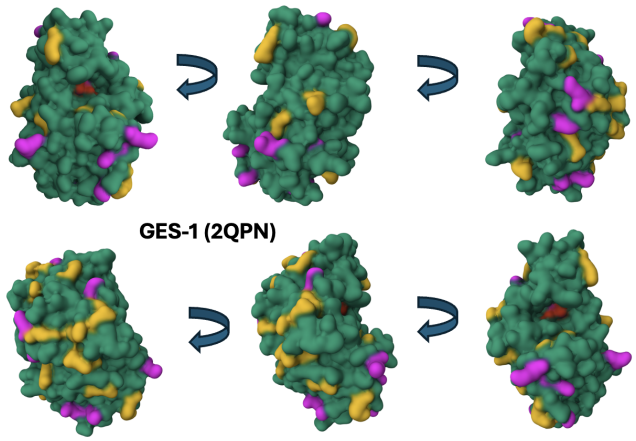

Figure S 18 GES-1 SBL enzyme structure (Gaussian Surface) as generated from https://www.rcsb.org/ , (ID: 2QPN). Lysine (Arginine) residues are coloured in purple (mustard). The active catalytic pocket is indicated in red. To have a complete view of the enzyme surface, from top left to bottom right the 3D generated model is left handed turned 72^o around the vertical axis in the figure.

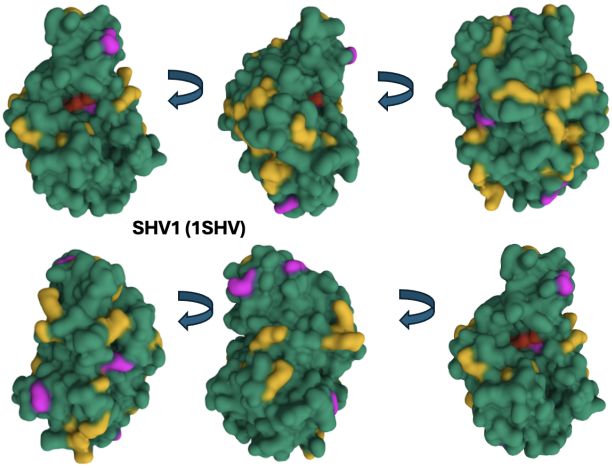

Figure S 19 SHV1 SBL enzyme structure (Gaussian Surface) as generated from https://www.rcsb.org/ , (ID: 1SHV). Lysine (Arginine) residues are coloured in purple (mustard). The active catalytic pocket is indicated in red. To have a complete view of the enzyme surface, from top left to bottom right the 3D generated model is left handed turned 72^o around the vertical axis in the figure.

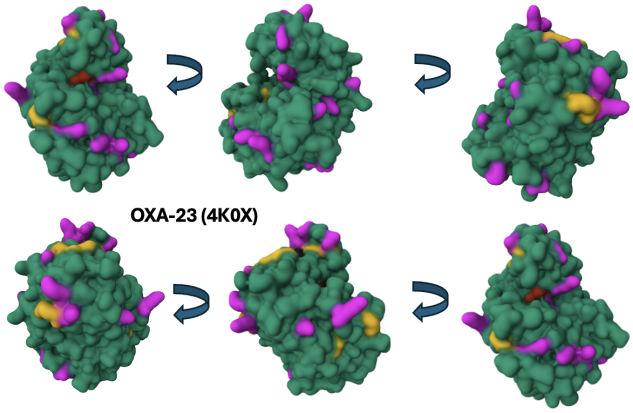

Figure S 20 OXA-23 SBL enzyme structure (Gaussian Surface) as generated from https://www.rcsb.org/ , (ID: 4K0X). Lysine (Arginine) residues are coloured in purple (mustard). The active catalytic pocket is indicated in red. To have a complete view of the enzyme surface, from top left to bottom right the 3D generated model is left handed turned 72^o around the vertical axis in the figure.

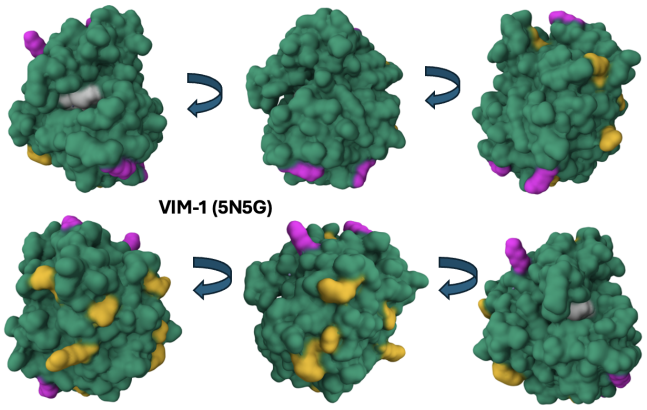

Figure S 21 VIM-1 MBL enzyme structure (Gaussian Surface) as generated from https://www.rcsb.org/ , (ID: 5N5G). Lysine (Arginine) residues are coloured in purple (mustard). The active catalytic pocket is indicated in grey. To have a complete view of the enzyme surface, from top left to bottom right the 3D generated model is lefthanded turned 72^o around the vertical axis in the figure.

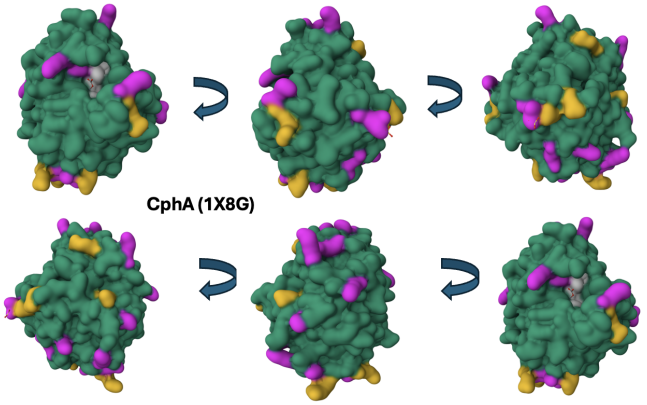

Figure S 22 CphA MBL enzyme structure (Gaussian Surface) as generated from https://www.rcsb.org/ , (ID: 1X8G). Lysine (Arginine) residues are coloured in purple (mustard). The active catalytic pocket is indicated in grey. To have a complete view of the enzyme surface, from top left to bottom right the 3D generated model is left handed turned 72^o around the vertical axis in the figure.

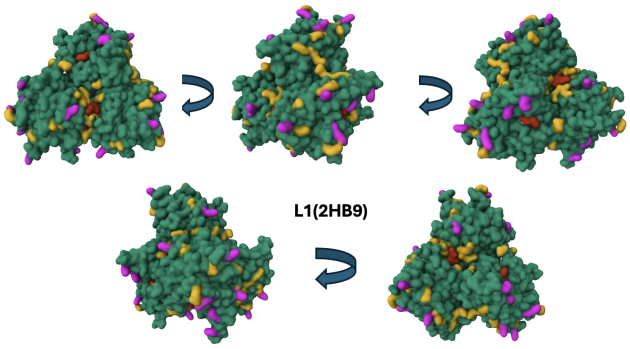

Figure S 23 L1 MBL enzyme structure (Gaussian Surface) as generated from https://www.rcsb.org/ , (ID: 2HB9). Lysine (Arginine) residues are coloured in purple (mustard). The active catalytic pocket is indicated in red. To have a complete view of the enzyme surface, from top left to bottom right, the 3D generated model is left handed turned 72^o around the vertical axis in the figure.