Detailed below are the lists of residues that comprise the detected binding sites that are within 6Å distance from the docked ligand.

Residues participating in the NS-C_{60} pocket of type 1 on HSA are: Ala191, Ser192, Lys195, Gln196, Leu198, Lys199, Trp214, Arg218, Arg222, Ala291, Glu292, Val293, Val343, Lys436, Cys437, Pro447, Cys448, Ala449, Asp451, Tyr452, Leu453 and Val455.

Residues participating in the CF pocket of type 1 HSA are: Glu153, Glu188, Ala191, Ser192, Ala194, Lys195, Gln196, Leu198, Lys199, Trp214, Arg218, Gln221, Arg222, His288, Cys289, Ile290, Ala291, Glu292, Val293, Glu294, Asn295, Pro339, Val343, Lys436, Cys437, His440, Lys444, Pro447, Cys448, Ala449, Asp451, Tyr452 and Val455.

Residues participating in the NS-C_{60} pocket of type 2 on HSA are: Asp108, Asn109, Pro110, Asn111, Leu112, Pro113, Arg114, Leu115, Glu141, Arg145, His146, Arg186, Lys190, Pro421, Glu425, Gln459 and Leu463.

Residues participating in the CF pocket of type 2 on HSA are: Asp108, Asn109, Pro110, Asn111, Leu112, Pro113, Arg114, Leu115, Val116, Glu141, Ile142, Arg145, His146, Pro147, Arg186, Lys190, Ser193, Ala194, Pro421, Thr422, Val424, Glu425, Val426, Arg428, Asn429, Lys432, Gln459, Leu463, Lys519, Glu520 and Ile523.

Residues participating in the HIV binding site for NS-C_{60} (Chain A:) Leu23, Asp25, Gly27, Ala28, Asp29, Asp30, Val32, Ile47, Gly48, Gly49, Ile50, Thr80, Pro81, Val82, Ile84, (Chain B:) Arg8, Leu23, Asp25, Gly27, Ala28, Gly48, Gly49, Ile50, Thr80, Pro81, Val82 and Ile84.

Residues participating in the HIV binding site for CF (chain A:) Arg8, Leu23, Asp25, Gly27, Ala28, Asp29, Asp30, Val32, Ile47, Gly48, Gly49, Ile50, Ile54, Pro79, Thr80, Pro81, Val82, Asn83, Ile84.

(Chain B:) Leu23, Asp25, Thr26, Gly27, Ala28, Asp29, Ile47, Gly48, Gly49, Ile50, Gly51, Gly52, Phe53, Ile54, Pro81, Val82 and Ile84.

Residues participating in the fullerene specific antibody binding site for NS-C_{60} (chain L) Tyr32, Asn34, Tyr49, Tyr50, Tyr91, And Phe96; (chain H)Ser32, Trp33, Arg50, Thr98, Ser99, Ser100 and Ala104.

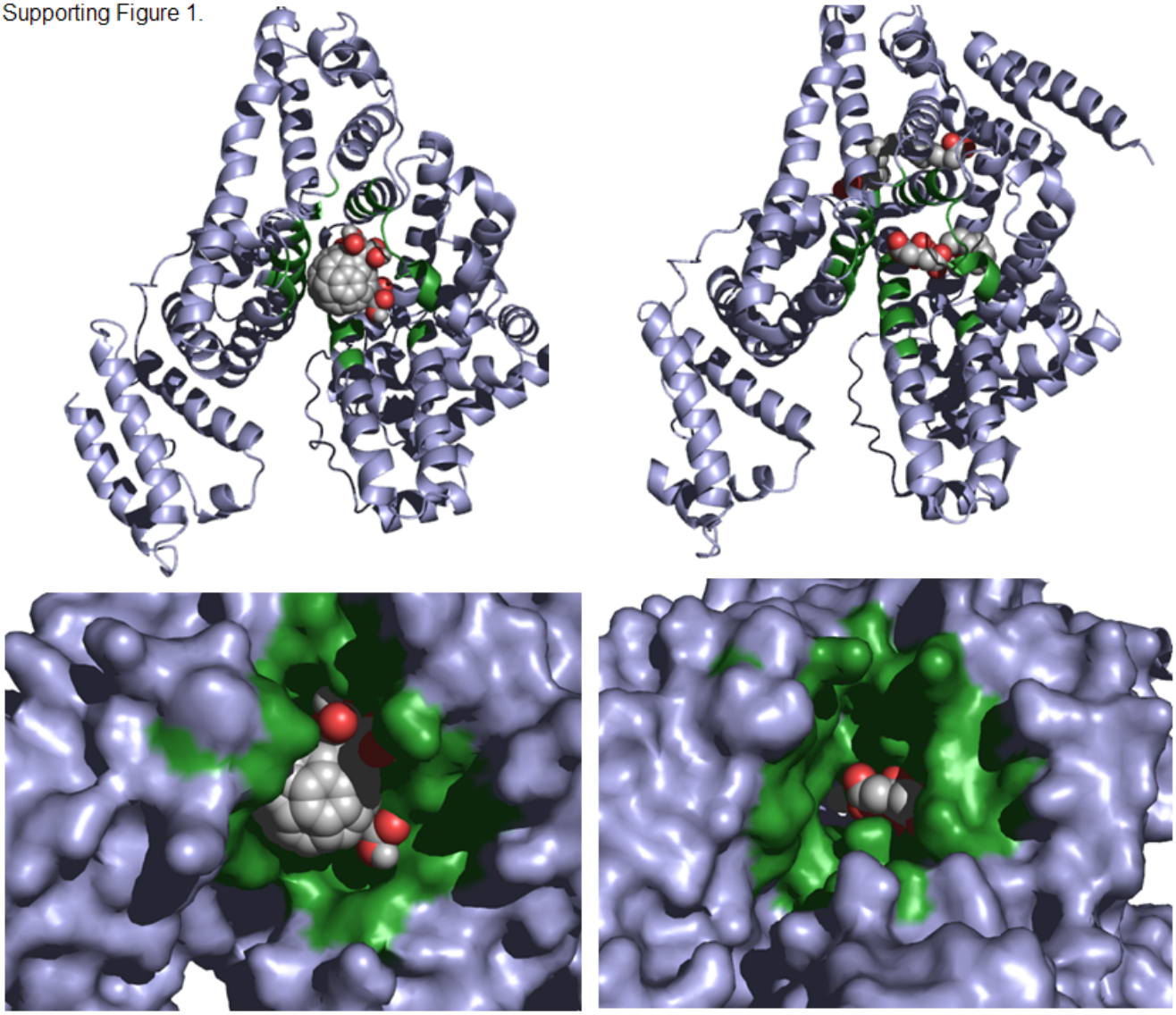
Residues participating in the fullerene specific antibody binding site for CF (chain L) Ser30, Asn31, Tyr32, Leu33, Asn34, Tyr36, Leu46, Tyr49, Tyr50, Ser53, Arg55, Gln89, Tyr91, Ser92, Arg93, Leu94 and Phe96; (chain H) Ser31, Ser32, Trp33, Asn35, Arg50, Thr98, Ser99, Ser100 and Ala104.

FIGURE CAPTIONS FOR SUPPORTING INFORMATION

Supplementary Figure 1. Predicted binding site for carboxy-fullererene on HSA occupying the known binding site for cytric acid. In all the four sub-figures, predicted binding site residues are colored green. Left: NS-C_{60} in its predicted binding site on free HSA (PDB: 1ao6). Right: the crystal structure of HSA complexed with cytric acid and decanoic acid (PDB: 1tf0). The lower figures provide a closer look on the surface of the binding sites.

Supplementary Figure 2. Similarity relationships between the four binding sites of HSA-type 1, HSA-type 2, HIVP and a fullerene-specific antibody. The dendrogram was constructed according to the score of MultiBind plotted using the statistical toolbox of Matlab. The similarity relationships are the same for both non-substituted fullerene and carboxyfullerene binding sites.

Supporting Figure 1.



Supporting Figure 2.