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Supporting information for article:

**Crystal structures of serum albumins from domesticated ruminants
and their complexes with 3,5-diiodosalicylic acid**

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Table S1 Distances due to polar contacts between DIS and residues in the binding pockets, and halogen bonds between iodine atoms (marked violet) in OSA-DIS and CSA-DIS complexes.

| | | OSA-DIS1 | | | OSA-DIS2 | | |
|------|---------|-----------------|---------------------|--------------------------------------|-----------------------|-----------------------------|--|
| | Residue | Atom | Distance (Å) | Residue | Atom | Distance (Å) | |
| COOH | Tyr149 | OH | 2.68 | Arg198 | NH2; NE; NE | 2.55; 3.34; 3.02 | |
| | His241 | NE2 | 3.24 | | | | |
| | Arg256 | NH2; NE | 2.91; 2.93 | | | | |
| OH | Arg217 | NH1; NH2 | 3.28; 2.81 | - | - | - | |
| 3'I | Arg217 | NH1; NH2 | 4.52; 4.58 | Trp213 Asp450 | NE1 O; OD1 | 4.39 3.50; 4.09 | |
| | Lys221 | NZ | 4.33 | | | | |
| | Ile289 | O | 4.53 | | | | |
| 5'I | Arg256 | O | 3.87 | Leu197 Ser201 Trp213 | O OG NE1 | 4.40 3.01 4.35 | |
| | Ala260 | N | 3.47 | | | | |
| | Ser286 | OG; O | 4.43; 4.61 | | | | |
| | | CSA-DIS1 | | | CSA-DIS2 | | |
| | Residue | Atom | Distance (Å) | Residue | Atom | Distance (Å) | |
| COOH | Tyr149 | OH | 2.63 | Arg198 | NH1; NH1; NE NE | 2.98; 3.30; 2.87 3.46 | |
| | His241 | NE2 | 3.37 | | | | |
| | Arg256 | NH2; NE | 3.08; 3.10 | Arg217 | | | |
| OH | Arg217 | NH1; NH2 | 3.10; 3.16 | | | | |
| 3'I | Arg217 | NH1 | 4.54 | Ser453 Asp450 | OG O; OD1 | 4.53 3.31; 4.28 | |
| | Lys221 | NZ | 2.84 | | | | |
| | Ile289 | O | 4.38 | | | | |
| 5'I | Arg256 | O | 3.85 | Leu197 Ser201 JE4 | O OG N1 | 4.54 3.91 4.34 | |
| | Ala260 | N | 3.78 | | | | |
| | Ser286 | OG | 4.48 | | | | |
| | | CSA-DIS3 | | | CSA-DIS4 | | |
| | Residue | Atom | Distance (Å) | Residue | Atom | Distance (Å) | |
| COOH | Arg409 | NH2 | 2.66 | His145 | NE2 | 3.26 | |
| | Ser488 | OG | 2.84 | | NE2 | 3.31 | |
| OH | Asn390 | OD1; ND2 | 3.28; 3.46 | - | - | - | |
| 3'I | Ile387 | O | 4.51 | Tyr137 Ile181 Met184 Arg185 | OH | 3.80 | |
| | Cys391 | N; SG | 4.51; 4.13 | | O | 4.20 | |
| | Cys437 | SG | 4.52 | | SD | 3.16 | |
| 5'I | Pro383 | O | 4.29 | Tyr160 Pro117 | OH N | 3.45 4.52 | |
| | Thr448 | OG1 | 4.23 | | | | |
| | Glu449 | OE1; OE2 | 3.81; 4.27 | | | | |
| | Arg484 | NH1; NH2; NE | 4.37; 3.82; 3.56 | | | | |
| | | | | | | | |
| | | CSA-DIS5 | | | CSA-DIS6 | | |
| | Residue | Atom | Distance (Å) | Residue | Atom | Distance (Å) | |
| COOH | His397 | ND1 | 3.07 | Lys132 | NZ; NZ | 2.75; 3.07 | |
| 3'I | Leu543 | O | 4.23 | Gln20 | O | 4.47 | |
| | Lys544 | N | 4.19 | Gly21 | N | 4.58 | |
| 5'I | Asp540 | OD1; OD2 | 4.19; 3.61 | Gln20 | OE1; NE2 | 4.16; 4.23 | |