| Name   | Structure of Structure | Pose | S score   |
|--------|------------------------|------|-----------|
| Atosiban |                        | C Pose 1 | -9.9765187 |
| Atosiban |                        | C Pose 2 | -8.3580637 |
| Atosiban |                        | C Pose 3 | -8.0395444 |
| Atosiban |                        | C Pose 4 | -7.7653613 |
| Atosiban |                        | C Pose 5 | -7.6741771 |
| RV2     |                        | C Pose 1 | -10.5528772 |
| RV2     |                        | C Pose 2 | -9.9645477 |
| RV2     |                        | C Pose 3 | -9.7060776 |
| RV2     |                        | C Pose 4 | -9.6723614 |
| Name     | Structure of Structure | Pose | S score |
|----------|------------------------|------|---------|
| RV2      | [Image of structure]   | 5    | -9.6440516 |
| Rifampicin | [Image of structure]  | 1    | -9.7330208 |
| Rifampicin | [Image of structure]  | 2    | -9.5062268 |
| Rifampicin | [Image of structure]  | 3    | -9.4370085 |
| Rifampicin | [Image of structure]  | 4    | -9.2959588 |
| Rifampicin | [Image of structure]  | 5    | -9.2261534 |
| FXPT00686 | [Image of structure]  | 1    | -7.6593571 |
| FXPT00686 | [Image of structure]  | 2    | -7.5369987 |
| FXPT00686 | [Image of structure]  | 3    | -7.4847758 |
| Name       | Structure of Structure | Poses | S score  |
|------------|------------------------|-------|----------|
| EXPT00886  |                        | F Pose 4 | -7.3919034 |
| EXPT00886  |                        | F Pose 5 | -7.3577949 |
| EXPT00779  |                        | C Pose 1 | -10.334968 |
| EXPT00779  |                        | C Pose 2 | -9.976676  |
| EXPT00779  |                        | C Pose 3 | -9.7267321 |
| EXPT00779  |                        | C Pose 4 | -9.578848  |
| EXPT00779  |                        | C Pose 5 | -9.3824735 |
| Felypressin|                        | C Pose 1 | -8.3267183 |
| Felypressin|                        | C Pose 2 | -8.2110882 |
| Name                        | Structure of Structure | Poses | S score   |
|-----------------------------|------------------------|-------|-----------|
| Felypressin                 |                        | C Pose 3 | -7.958099 |
| Felypressin                 |                        | C Pose 4 | -7.759357 |
| Felypressin                 |                        | C Pose 5 | -7.358969 |
| Glycinamide Ribonucleotide  |                        | F Pose 1 | -5.581888 |
| Glycinamide Ribonucleotide  |                        | F Pose 2 | -5.354827 |
| Glycinamide Ribonucleotide  |                        | F Pose 3 | -5.200637 |
| Glycinamide Ribonucleotide  |                        | F Pose 4 | -5.193592 |
| Glycinamide Ribonucleotide  |                        | F Pose 5 | -5.130796 |
| Gonadorelin                 |                        | C Pose 1 | -9.808157 |
| Name          | Structure of Structure | Poses | S score  |
|---------------|------------------------|-------|----------|
| Gonadorelin   |                        | C Pose 2 | -9.7502749 |
| Gonadorelin   |                        | C Pose 3 | -9.4418246  |
| Gonadorelin   |                        | C Pose 4 | -9.4041004  |
| Gonadorelin   |                        | C Pose 5 | -9.3112503  |
| Icatibant     |                        | C Pose 1 | -9.6560271  |
| Icatibant     |                        | C Pose 2 | -9.6064632  |
| Icatibant     |                        | C Pose 3 | -9.5558416  |
| Icatibant     |                        | C Pose 4 | -9.4601755  |
| Icatibant     |                        | C Pose 5 | -9.1451349  |
| Name                                                                 | Structure of Structure | Poses | S score   |
|----------------------------------------------------------------------|------------------------|-------|-----------|
| Mixed Carbamic Phosphoric Acid Anhydride of 7,8-Diaminooctanoic Acid | F-Pose 1               |       | -5.7088005 |
| Mixed Carbamic Phosphoric Acid Anhydride of 7,8-Diaminooctanoic Acid | F-Pose 2               |       | -5.7007484 |
| Mixed Carbamic Phosphoric Acid Anhydride of 7,8-Diaminooctanoic Acid | F-Pose 3               |       | -5.5531179 |
| Mixed Carbamic Phosphoric Acid Anhydride of 7,8-Diaminooctanoic Acid | F-Pose 4               |       | -5.4036317 |
| Mixed Carbamic Phosphoric Acid Anhydride of 7,8-Diaminooctanoic Acid | F-Pose 5               |       | -5.4000859 |
| Nafarelin                                                           | C-Pose 1               |       | -9.7578158 |
| Nafarelin                                                           | C-Pose 2               |       | -9.5953712 |
| Nafarelin                                                           | C-Pose 3               |       | -9.5231056 |
| Nafarelin                                                           | C-Pose 4               |       | -9.3675677 |
| Name                                      | Structure of Structure | Poses | S score  |
|-------------------------------------------|------------------------|-------|----------|
| Nafarelin                                 |                        | FPose | -9.1661434 |
| P1-(adenosine-5'-P5-uridine-5')pentaphosphate |                        | FPose | -9.0627352 |
| P1-(adenosine-5'-P5-uridine-5')pentaphosphate |                        | FPose | -8.5044509 |
| P1-(adenosine-5'-P5-uridine-5')pentaphosphate |                        | FPose | -8.4444618 |
| P1-(adenosine-5'-P5-uridine-5')pentaphosphate |                        | FPose | -8.3571162 |
| P1-(adenosine-5'-P5-uridine-5')pentaphosphate |                        | FPose | -8.232872  |
| Sar9 Met (O2)11-Substance P               |                        | SPose | -10.627831 |
| Sar9 Met (O2)11-Substance P               |                        | SPose | -10.590092 |
| Sar9 Met (O2)11-Substance P               |                        | SPose | -10.522081 |
| Name                              | Structure of Structure | Poses | S score  |
|----------------------------------|------------------------|-------|----------|
| Sar9 Met (O2)11-Substance P       |                        | S Pose 4 | -10.442977 |
| Serine-3’-aminoadenosine         |                        | C Pose 1 | -5.8694892  |
| Serine-3’-aminoadenosine         |                        | C Pose 2 | -5.810942F  |
| Serine-3’-aminoadenosine         |                        | C Pose 3 | -5.701160F  |
| Serine-3’-aminoadenosine         |                        | C Pose 4 | -5.686870F  |
| Serine-3’-aminoadenosine         |                        | C Pose 5 | -5.6719384F |
| Thymopentin                       |                        | C Pose 1 | -7.547617  |
| Thymopentin                       |                        | C Pose 2 | -7.3551712 |

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| Name                                      | Structure of Structure | Poses | S score  |
|-------------------------------------------|------------------------|-------|----------|
| Thymopentin                               |                        | C Pose 3 | -7.2386456 |
| Thymopentin                               |                        | C Pose 4 | -8.8311429 |
| Thymopentin                               |                        | C Pose 5 | -8.7853174 |
| p1-(5'-arachnoyl)\(\text{pS}\)-(5'-thymirlyl)pentaphosphate |                        | F Pose 1 | -8.6776606 |
| p1-(5'-arachnoyl)\(\text{pS}\)-(5'-thymirlyl)pentaphosphate |                        | F Pose 2 | -8.5978627 |
| p1-(5'-arachnoyl)\(\text{pS}\)-(5'-thymirlyl)pentaphosphate |                        | F Pose 3 | -8.2307749 |
| p1-(5'-arachnoyl)\(\text{pS}\)-(5'-thymirlyl)pentaphosphate |                        | F Pose 4 | -8.2097178 |
| p1-(5'-arachnoyl)\(\text{pS}\)-(5'-thymirlyl)pentaphosphate |                        | F Pose 5 | -8.1676407 |