**Supplementary table. 1**

*In silico* docking of 71 different chemical compounds using Auto Dock and Hex 6.3 with binding energy

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Sl.No** | **Name of the compound** | **PUB CHEM ID** | **SUMO1** |  | **UBC9** |  |
|  |  |  | **Autodock Kcal/mol** | **Hex**  **K cal /mol** | **Autodock Kcal/mol** | **Hex**  **K cal/mol** |
| 1 | **1,2,3-Trichloropropane (TCP)** | CID (16217550) | -2.9 | -231 | -3 | -264.9 |
| 2 | **3,3'- Dichlorobisphenol A** | CID(66238) | -5.8 | -1246.2 | -5.9 | -548.12 |
| 3 | **4-vinylcyclohexene** | (CID 7499) | -3.4 | -345 | -3.5 | -321 |
| 4 | **Aldrin** | (CID 12310947) | -4.5 | -465.5 | -5.6 | -455 |
| 5 | **Arsenic** | (CID 5359596) | -5.5 | -543.7 | -5.2 | -499 |
| 6 | **astemizole** | (CID 2247) | -8.45 | -1198.1 | -8.67 | -843.97 |
| 7 | **Attapulgite** | (CID 56842194) | -2.1 | -345 | -3 | -323.9 |
| 8 | **Bentonite** | CID 517273) | -3.3 | -324.6 | -3.1 | -330 |
| 9 | **Benzidine** | (CID 7111) | -4.8 | -980 | -4.7 | -897 |
| 10 | **Bisphenol A** | (CID 6623) | -5.4 | -1318.1 | -6.2 | -695.1 |
| 11 | **Bisphenol B** | (CID66166) | -5.3 | -1454.5 | -6.1 | -736.13 |
| 12 | **Bisphenol S** | (CID6626) | -6 | -1021.7 | -6 | -463.12 |
| 13 | **Boron** | (CID 5462311) | -5.1 | -897 | -5.2 | -876.5 |
| 14 | **Cadmium** | (CID 23973) | -4.3 | -625 | -4.1 | ND |
| 15 | **Caffeine (PHARMACEUTICALS)** | (CID 2519) | -4.5 | -567.9 | -4.2 | -679 |
| 16 | **carbendazim** | (CID25429) | -2.3 | -256.9 | -2.1 | -199 |
| 17 | **Carbon disulphide** | (CID6348) | -1.4 | -211.8 | -1.1 | -189 |
| 18 | **Carbon monoxide** | (CID 281) | -3.9 | -389 | 4.2 | -412 |
| 19 | **carbon tetrachloride** | (CID 5943) |  |  |  |  |
| 20 | **Chlordan** | (CID12303038) | -5.5 | -290.75 | -5.6 | NA |
| 21 | **Chlordene** | (CID19519) | -5.3 | -321.05 | -6.0 | -379.84 |
| 22 | **Chloropyrifos - methyl** | (CID21803) | -3.6 | -333 | -3.2 | NA |
| 23 | **chlorpyrifos** | (CID2730) | -3.3 | -342 | -3.1 |  |
| 24 | **Cypermethrin** | (CID2912) | -2 | ND | -1.5 |  |
| 25 | **DDT/DDE** | (CID 3035) | -5.4 | -848.45 | -5.2 | -678.9 |
| 26 | **Deltamethrin** | (CID40585) | -3.1 | -321 | -2.8 |  |
| 27 | **Diazinon** | (CID3017) | -2.9 | NA | -2.7 |  |
| 28 | **dibromochloropropane** | (CID 7280 | -1.2 | NS | NA | NA |
| 29 | **Dichlorvas** | (CID3039) | -1.6 | NA | -1.3 |  |
| 30 | **Dieldrin(Organ chlorine)** | (CID 60963) | -5.5 | -373.57 | -6.2 | -390.57 |
| 31 | **Endosulfan (Organ chlorine)** | (CID 3224) | -5.9 | -344.35 | -5.4 | -395.42 |
| 32 | **Endosulphun sulphate** | (CID13940) | -6.1 | -306.2 | -5.9 | -439.54 |
| 32 | **Ethylene dibromide** | (CID7839) | -1.9 |  | -1.9 |  |
| 33 | **Ethylene Glycol** | (CID 174) | -2.8 | -247 | -2.7 | -240 |
| 34 | **Flubendiamide** | (CID11193251) | -2.4 | -237 | -2.2 | -231 |
| 35 | **formaldehyde** | (CID 712) | -1.5 | -123.56 | -1.3 | -129 |
| 36 | **HEOM** | (CID6454255) | -6 | -381.4 | -6.1 | -383.28 |
| 37 | **Heptachlor** | (CID3589) | -5.5 | -253.45 | -5.8 | -364.51 |
| 38 | **Heptachlor Epoxide (Organ chlorine)** | (CID 13930) | -5.3 | -280.9 | -5.5 | -289 |
| 39 | **Hexa bromo cyclo dodecan** | (CID 23459299) | -2.7 | -189 | -2.3 | -239.8 |
| 40 | **Illite (Not Exact)** | CID 164282) | -4.4 | -2905 | -4 |  |
| 41 | **kaolinite** | (CID 9942228) | -0.9 |  | NA |  |
| 42 | **Lead** | (CID 5352425) | -4.9 | -444 | -4.8 | -431 |
| 43 | **Malathion** | (CID4004) | -2.3 | -234 | -2.1 | -239 |
| 44 | **metalloid selenium** | (CID 6326970) | -2.1 | -200 | -2 | -156.9 |
| 45 | **Methyl mercury** | (CID 6860) | -3.2 | -278 | -3 | -289.9 |
| 46 | **methyl parathion** | (CID 4130) | -2 | NA | -1.9 | -123.9 |
| 47 | **Methylenebis(chloroaniline)** | (CID7543) | -1.8 | NA | -1.8 | -190.9 |
| 48 | **metolachlor (Organ chlorine)** | (CID 4169) | -4.1 | -1421 | -4 | -1321 |
| 49 | **Mirex** | (CID 16945) | -2.1 | -123.56 | -2.2 | -123.42 |
| 50 | **Monocrotophos** | (CID5371562) | -0.8 | NA | -0.8 |  |
| 51 | **M-ontmorillonite** | (CID 16211228) | -0.9 | NA | -1 |  |
| 52 | **nicotine** | (CID 89594) | -4.1 | -290.75 | -4 | -265.78 |
| 53 | **nitric oxide** | (CID 145068) | -5 | -430.89 | -4.9 | -498.9 |
| 54 | **Nitrite ion** | (CID 946) | -2.8 | -212.89 | -2.9 | -234.8 |
| 55 | **Nitrogen dioxide** | (CID 3032552) | -3.3 | -233 | -3 | -243 |
| 56 | **Oxydemeton methyl** | (CID4618) | -3.6 | -243 | -3.3 | -213 |
| 57 | **Parathion** | (CID991) | -3.2 | -199 | -3.4 | -209.9 |
| 58 | **Parathion- methyl** | (CID 4130) | -3 | -202 | -3.5 | -204.8 |
| 59 | **pentachlorophenol** | (CID 992) | -3.9 | -303 | -3.3 | -300.8 |
| 60 | **Per fluoro octanoic acid (PFOA)** | (CID 9554) | -3.13 | -922.47 | -3.69 | -988.69 |
| 61 | **perchloroethylene phosphate** | (CID 31373 | -3.9 | -765 | -3.8 | -697.4 |
| 62 | **polybrominated biphenyls** | (CID 158629) | -4.9 | -1198 | -4.7 | -1150 |
| 63 | **polychlorinated biphenyl (PCB) 3,3',4,4'-Tetrachlorobiphenyl; PCB 77; 3,4,3',4'-TETRACHLOROBIPHENYL ...** | (CID 36187) | -2.6 | -345 | -2.5 | -367 |
| 64 | **Quinalphos** | (CID26124) | -2 | NA | -2 |  |
| 65 | **tetrabromobisphenol A** | (CID 6618) | -5.8 | -956.34 | -5.8 | -548.12 |
| 66 | **Toxaphene** | (CID 5284469) | -4 | -432.98 | -4.1 | -453.9 |
| 67 | **Tri phenyl phosphate** | CID (8289) | -3.8 | -342.67 | -3.3 | -326.9 |
| 68 | **Trichloroethylene** | (CID 6575) | -3.7 | -287.98 | -3.8 | -303.4 |
| 69 | **triclosan** | (CID 5564) | -5 | -673 | -4.9 | -675.9 |
| 70 | **Triortho cresyl phosphate** | (CID6275) | -2.5 | -123.56 | -2.6 | -100.9 |
| 71 | **Tris (chloropropyl ) PHOSPHATE** | (CID 22522) | -3.6 | -278.65 | -3.5 | -267.9 |

NMR structure of human SUMO and X-ray crystallographic structure of human UBC9 from the PDB (Protein Data Bank) were docked with chemical structures of the compounds retrieved from PubChem using Autodock 4.2 and Hex6.3. Lowest binding energies obtained were tabulated.