**Table 1.** Pharmacokinetic, drug likeness and toxicity parameters of synthesized benzo[d]thiazol-2 amine derivatives and reference standard drug.

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| CCa | GIAb | BBBc | Log Kp | CARd | MUTe | REf | SIg | BSh | ABS (%)i | Lipinski |
| G-1 | High | No | -4.38 | Non-toxic | Non-toxic | Non-toxic | Non-toxic | 0.55 | 97.28 | Yes |
| G-2 | High | No | -5.39 | Non-toxic | Non-toxic | Non-toxic | Non-toxic | 0.55 | 97.28 | Yes |
| G-3 | Low | No | -4.78 | Non-toxic | Non-toxic | Non-toxic | Non-toxic | 0.55 | 78.64 | Yes |
| G-4 | High | No | -4.96 | Non-toxic | Non-toxic | Non-toxic | Non-toxic | 0.55 | 87.77 | Yes |
| G-5 | High | No | -4.69 | Non-toxic | Non-toxic | Non-toxic | Non-toxic | 0.55 | 97.28 | Yes |
| G-6 | High | No | -4.46 | Non-toxic | Non-toxic | Non-toxic | Non-toxic | 0.55 | 97.28 | Yes |
| G-7 | High | No | -4.90 | Non-toxic | Non-toxic | Non-toxic | Non-toxic | 0.55 | 93.71 | Yes |
| G-8 | High | No | -4.73 | Non-toxic | Non-toxic | Non-toxic | Non-toxic | 0.55 | 96.12 | Yes |
| G-9 | Low | No | -4.78 | Non-toxic | Non-toxic | Non-toxic | Non-toxic | 0.55 | 78.64 | Yes |
| G-10 | High | No | -5.27 | Non-toxic | Non-toxic | Non-toxic | Non-toxic | 0.55 | 87.77 | Yes |
| G-11 | High | No | -3.99 | Non-toxic | Non-toxic | Non-toxic | Non-toxic | 0.55 | 97.28 | Yes |
| G-12 | High | No | -4.46 | Non-toxic | Non-toxic | Non-toxic | Non-toxic | 0.55 | 97.28 | Yes |
| G-13 | High | No | -5.39 | Non-toxic | Non-toxic | Non-toxic | Non-toxic | 0.55 | 97.28 | Yes |
| Ind. | High | Yes | -5.45 | Non-toxic | Non-toxic | Non-toxic | Non-toxic | 0.85 | 85.94 | Yes |

a Compound Code

b GI absorption

c Blood brain barrier permeation

d Carcinogenicity.

e Mutagenicity.

f Reproductive effects.

g Skin irritation.

h Bioavailability score.

iAbsorption

**Table 2.** Structures of newly synthesized benzo[d]thiazol-2-amine derivatives.

|  |  |
| --- | --- |
| G1 | G2 |
| G3 | G4 |
| G5 | G6 |
| G7 | G8 |
| G9 | G10 |
| G11 | G12 |
| G13 |  |

|  |  |
| --- | --- |
| **G-1** | **G-2** |
| **G-3** | **G-4** |
| **G-5** | **G-6** |
| **G-7** | **G-8** |
| **G-9** | **G-10** |
| **G-11** | **G-12** |
| **G-13** |  |

**Figure 1.** The hydrophobic interactions surfaces for molecule G-1, G-2, G-3, G-4, G-5, G-6, G-7, G-8, G-9, G-10, G-11 and G-12 with COX-1.

|  |  |
| --- | --- |
| **G-1** | **G-2** |
| **G-3** | **G-4** |
| **G-5** | **G-6** |
| **G-7** | **G-8** |
| **G-9** | **G-10** |
| **G-11** | **G-12** |
| **G-13** |  |

**Figure 2.** The hydrogen bond surfaces for molecule G-1, G-2, G-3, G-4, G-5, G-6, G-7, G-8, G-9, G-10, G-11 and G-12 with COX-1.

|  |  |
| --- | --- |
| G-1 | G-2 |
| G-3 | G-4 |
| G-5 | G-6 |
| G-7 | G-8 |
| G-9 | G-10 |
| G-11 | G-12 |
| G-13 | COX1_AK26  Diclofenac Sodium |

**Figure 3:** COX-1 complex with G-1, G-2, G-3, G-4, G-5, G-6, G-7, G-8, G-9, G-10, G-11, G-12 and G-13.

|  |  |
| --- | --- |
| **G-1** | **G-2** |
| **G-3** | **G-4** |
| **G-5** | **G-6** |
| **G-7** | **G-8** |
| **G-9** | **G-10** |
| **G-11** | **G-12** |
| **G-13** |  |

**Figure 4.** Hydrophobic interactions surfaces for molecule G-1, G-2, G-3, G-4, G-5, G-6, G-7, G-8, G-9, G-10, G-11, G-12 and G-13 with COX-2.

|  |  |
| --- | --- |
| **G-1** | **G-2** |
| **G-3** | **G-4** |
| **G-5** | **G-6** |
| **G-7** | **G-8** |
| **G-9** | **G-10** |
| **G-11** | **G-12** |
| **G-13** |  |

**Figure 5.** The hydrogen bond surfaces for molecule G-1, G-2, G-3, G-4, G-5, G-6, G-7, G-8, G-9, G-10, G-11, G-12 and G-13 with COX-2

|  |  |
| --- | --- |
| G-1 | G-2 |
| G-3 | G-4 |
| G-5 | G-6 |
| G-7 | G-8 |
| G-9 | G-10 |
| G-11 | G-12 |
| G-13 | C:\Users\omprakash\Desktop\Deepika\Docking_Process\Complex_Indomethacin.png  Indomethacin |

**Figure 6.** COX-2 complex with G-1, G-2, G-3, G-4, G-5, G-6, G-7, G-8, G-9, G-10, G-11, G-12, G-13 and Indomethacin.

|  |  |
| --- | --- |
| http://www.swissadme.ch/results/1531962002/molecule1/radar.png  G-1 | http://www.swissadme.ch/results/1471630664/molecule1/radar.png  G-2 |
| http://www.swissadme.ch/results/500382702/molecule2/radar.png  G-3 | http://www.swissadme.ch/results/1752127536/molecule3/radar.png  G-4 |
| http://www.swissadme.ch/results/1900481423/molecule4/radar.png  G-5 | http://www.swissadme.ch/results/1624076381/molecule1/radar.png  G-6 |
| http://www.swissadme.ch/results/1322556445/molecule1/radar.png  G-7 | http://www.swissadme.ch/results/1157970038/molecule1/radar.png  G-8 |
| http://www.swissadme.ch/results/820941616/molecule1/radar.png  G-9 | http://www.swissadme.ch/results/2117196826/molecule3/radar.png  G-10 |
| http://www.swissadme.ch/results/1235752055/molecule1/radar.png  G-11 | http://www.swissadme.ch/results/660511002/molecule2/radar.png  G-12 |
| http://www.swissadme.ch/results/1471630664/molecule1/radar.png  G-13 |  |

**Figure 7.** Bioavailability radar graph of benzo(d)thiazol-2-amine derivatives G-1-G-13 (pink area reflects the allowed values of drug likeness properties of the molecule).