| Ligand | BP | qed | mol | logp | rot | acc | don | area | AMES | Max. TDH | hERG I | hERG II | LD50 | LOAEL | Hepat | S. Sensib | T. Pyr | M.Txc |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **compound 1** | GTP-BP | **0.592084605862** | **479.002** | **3.3746** | **10** | **7** | **2** | **195.905** | **No** | **-0.97** | **No** | **Yes** | **2.978** | **1.111** | **Yes** | **No** | **0.**  **695** | **0.**  **484** |
| **compound 2** | SAH-BP | **0.455640403929** | **455.599** | **3.3292** | **8** | **6** | **0** | **196.59** | **No** | **-0.21** | **No** | **Yes** | **2.766** | **1.32** | **Yes** | **No** | **0.**  **883** | **0.**  **761** |
| **compound 3** | GTP-BP | **0.455640403929** | **455.599** | **3.3292** | **8** | **6** | **0** | **196.59** | **No** | **-0.21** | **No** | **Yes** | **2.766** | **1.32** | **Yes** | **No** | **0.**  **883** | **0.**  **761** |
| **compound 4** | SAH-BP | **0.565938640397** | **444.967** | **2.4372** | **7** | **7** | **1** | **185.613** | **No** | **-0.**  **115** | **No** | **Yes** | **2.881** | **1.454** | **Yes** | **No** | **0.**  **861** | **1.013** |
| **compound 5** | GTP-BP | **0.565938640397** | **444.967** | **2.4372** | **7** | **7** | **1** | **185.613** | **No** | **-0.**  **115** | **No** | **Yes** | **2.881** | **1.454** | **Yes** | **No** | **0.**  **861** | **1.013** |
| **compound 6** | GTP-BP | **0.379453028029** | **471.557** | **4.86484** | **9** | **6** | **1** | **203.866** | **No** | **-0.**  **289** | **No** | **Yes** | **2.912** | **0.**  **934** | **Yes** | **No** | **0.**  **772** | **0.**  **471** |
| **compound 7** | SAH-BP | **0.379453028029** | **471.557** | **4.86484** | **9** | **6** | **1** | **203.866** | **No** | **-0.**  **289** | **No** | **Yes** | **2.912** | **0.**  **934** | **Yes** | **No** | **0.**  **772** | **0.**  **471** |
| **compound 8** | GTP-BP | **0.465223006333** | **386.521** | **3.45242** | **8** | **6** | **1** | **162.189** | **No** | **0.**  **292** | **No** | **Yes** | **2.87** | **1.204** | **Yes** | **No** | **1.556** | **0.72** |
| **compound 9** | SAH-BP | **0.465223006333** | **386.521** | **3.45242** | **8** | **6** | **1** | **162.189** | **No** | **0.**  **292** | **No** | **Yes** | **2.87** | **1.204** | **Yes** | **No** | **1.556** | **0.72** |
| **compound 10** | SAH-BP | **0.621567230689** | **332.404** | **2.60982** | **7** | **7** | **0** | **139.077** | **No** | **0.**  **464** | **No** | **Yes** | **2.824** | **1.424** | **Yes** | **No** | **1.602** | **1.172** |

| Ligand | BP | qed | mol | logp | rot | acc | don | area | AMES | Max. TDH | hERG I | hERG II | LD50 | LOAEL | Hepat | S. Sensib | T. Pyr | M.Txc |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **compound 11** | GTP-BP | **0.621567230689** | **332.404** | **2.60982** | **7** | **7** | **0** | **139.077** | **No** | **0.**  **464** | **No** | **Yes** | **2.824** | **1.424** | **Yes** | **No** | **1.602** | **1.172** |
| **compound 12** | SAH-BP | **0.551112766738** | **466.542** | **1.4212** | **8** | **9** | **0** | **196.835** | **No** | **-0.17** | **No** | **Yes** | **2.695** | **1.525** | **Yes** | **No** | **0.**  **652** | **1.423** |
| **compound 13** | SAH-BP | **0.339528803626** | **492.572** | **5.0017** | **9** | **4** | **1** | **203.694** | **No** | **-0.**  **278** | **No** | **Yes** | **3.037** | **0.86** | **Yes** | **No** | **0.**  **743** | **0.**  **442** |
| **compound 14** | GTP-BP | **0.551112766738** | **466.542** | **1.4212** | **8** | **9** | **0** | **196.835** | **No** | **-0.17** | **No** | **Yes** | **2.695** | **1.525** | **Yes** | **No** | **0.**  **652** | **1.423** |
| **compound 15** | GTP-BP | **0.339528803626** | **492.572** | **5.0017** | **9** | **4** | **1** | **203.694** | **No** | **-0.**  **278** | **No** | **Yes** | **3.037** | **0.86** | **Yes** | **No** | **0.**  **743** | **0.**  **442** |
| compound 16 | GTP-BP | **0.552513163691** | **456.564** | **3.2088** | **8** | **6** | **1** | **188.495** | **No** | **-0.**  **152** | **No** | **Yes** | **2.884** | **1.431** | **Yes** | **No** | **0.**  **876** | **0.**  **868** |
| compound 17 | SAH-BP | **0.551112766738** | **466.542** | **1.4212** | **8** | **9** | **0** | **196.835** | **No** | **-0.17** | **No** | **Yes** | **2.695** | **1.525** | **Yes** | **No** | **0.**  **652** | **1.423** |
| compound 18 | SAH-BP | **0.552513163691** | **456.564** | **3.2088** | **8** | **6** | **1** | **188.495** | **No** | **-0.**  **152** | **No** | **Yes** | **2.884** | **1.431** | **Yes** | **No** | **0.**  **876** | **0.**  **868** |
| compound 19 | GTP-BP | **0.684683825999** | **434.533** | **4.112** | **8** | **4** | **1** | **176.643** | **No** | **0.**  **142** | **No** | **Yes** | **3.027** | **1.051** | **Yes** | **No** | **1.354** | **0.**  **651** |
| compound 20 | SAH-BP | **0.454877844322** | **444.543** | **3.74502** | **8** | **8** | **1** | **191.348** | **No** | **-0.**  **492** | **No** | **Yes** | **3.108** | **1.024** | **Yes** | **No** | **0.**  **401** | **0.**  **831** |

| Ligand | BP | qed | mol | logp | rot | acc | don | area | AMES | Max. TDH | hERG I | hERG II | LD50 | LOAEL | Hepat | S. Sensib | T. Pyr | M.Txc |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **compound 21** | GTP-BP | **0.454877844322** | **444.543** | **3.74502** | **8** | **8** | **1** | **191.348** | **No** | **-0.**  **492** | **No** | **Yes** | **3.108** | **1.024** | **Yes** | **No** | **0.**  **401** | **0.**  **831** |
| **compound 22** | GTP-BP | **0.667567440215** | **369.425** | **2.0865** | **7** | **7** | **0** | **156.868** | **Yes** | **0.**  **98** | **No** | **Yes** | **2.854** | **1.449** | **Yes** | **No** | **1.03** | **1.288** |
| compound 23 | SAH-BP | **0.601356197371** | **402.498** | **4.89902** | **5** | **5** | **1** | **175.886** | **No** | **-0.**  **145** | **No** | **Yes** | **2.971** | **0.**  **928** | **Yes** | **No** | **1.119** | **0.**  **624** |
| compound 24 | GTP-BP | **0.603404611513** | **396.922** | **4.1619** | **6** | **4** | **0** | **170.072** | **No** | **0.**  **22** | **No** | **Yes** | **2.968** | **1.119** | **Yes** | **No** | **1.296** | **0.**  **569** |
| compound 25 | SAH-BP | **0.667567440215** | **369.425** | **2.0865** | **7** | **7** | **0** | **156.868** | **Yes** | **0.**  **98** | **No** | **Yes** | **2.854** | **1.449** | **Yes** | **No** | **1.03** | **1.288** |
| compound 26 | SAH-BP | **0.603404611513** | **396.922** | **4.1619** | **6** | **4** | **0** | **170.072** | **No** | **0.**  **22** | **No** | **Yes** | **2.968** | **1.119** | **Yes** | **No** | **1.296** | **0.**  **569** |
| compound 27 | SAH-BP | **0.861457172737** | **296.436** | **3.2388** | **8** | **3** | **1** | **124.665** | **No** | **0.**  **941** | **No** | **Yes** | **2.679** | **1.458** | **Yes** | **No** | **2.346** | **0.**  **676** |
| compound 28 | GTP-BP | **0.861457172737** | **296.436** | **3.2388** | **8** | **3** | **1** | **124.665** | **No** | **0.**  **941** | **No** | **Yes** | **2.679** | **1.458** | **Yes** | **No** | **2.346** | **0.**  **676** |
| **compound 29** | GTP-BP | **0.606419832232** | **449.342** | **2.2383** | **5** | **7** | **1** | **182.496** | **No** | **-0.**  **107** | **No** | **Yes** | **2.953** | **1.44** | **Yes** | **No** | **0.**  **863** | **1.07** |
| **compound 30** | SAH-BP | **0.339020686477** | **476.577** | **5.25414** | **9** | **6** | **1** | **201.733** | **No** | **-0.**  **226** | **No** | **Yes** | **3.127** | **0.**  **799** | **Yes** | **No** | **0.**  **806** | **0.**  **252** |

| Ligand | BP | qed | mol | logp | rot | acc | don | area | AMES | Max. TDH | hERG I | hERG II | LD50 | LOAEL | Hepat | S. Sensib | T. Pyr | M.Txc |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **compound 29** | SAH-BP | **0.339020686477** | **476.577** | **5.25414** | **9** | **6** | **1** | **201.733** | **No** | **-0.**  **226** | **No** | **Yes** | **3.127** | **0.**  **799** | **Yes** | **No** | **0.**  **806** | **0.**  **252** |
| compound 30 | GTP-BP | **0.606419832232** | **449.342** | **2.2383** | **5** | **7** | **1** | **182.496** | **No** | **-0.**  **107** | **No** | **Yes** | **2.953** | **1.44** | **Yes** | **No** | **0.**  **863** | **1.07** |
| compound 31 | SAH-BP | **0.529992760887** | **485.968** | **4.0572** | **8** | **7** | **0** | **203.603** | **No** | **-0.**  **253** | **No** | **Yes** | **3.015** | **1.06** | **Yes** | **No** | **0.**  **754** | **0.**  **537** |
| compound 32 | GTP-BP | **0.666169325921** | **386.477** | **2.88014** | **6** | **7** | **0** | **161.069** | **No** | **0.**  **59** | **No** | **Yes** | **2.993** | **1.401** | **Yes** | **No** | **1.112** | **0.**  **997** |
| compound 33 | SAH-BP | **0.41668780986** | **430.761** | **4.60182** | **7** | **5** | **1** | **157.103** | **No** | **0.**  **524** | **No** | **Yes** | **3.62** | **0.**  **738** | **Yes** | **No** | **1.3** | **0.65** |
| **compound 34** | SAH-BP | **0.666169325921** | **386.477** | **2.88014** | **6** | **7** | **0** | **161.069** | **No** | **0.**  **59** | **No** | **Yes** | **2.993** | **1.401** | **Yes** | **No** | **1.112** | **0.**  **997** |
| compound 35 | GTP-BP | **0.41668780986** | **430.761** | **4.60182** | **7** | **5** | **1** | **157.103** | **No** | **0.**  **524** | **No** | **Yes** | **3.62** | **0.**  **738** | **Yes** | **No** | **1.3** | **0.65** |
| compound 36 | GTP-BP | **0.51626943326** | **407.492** | **2.8479** | **9** | **5** | **3** | **165.328** | **No** | **0.**  **333** | **No** | **Yes** | **3.002** | **1.365** | **Yes** | **No** | **1.353** | **0.**  **719** |
| compound 37 | SAH-BP | **0.51626943326** | **407.492** | **2.8479** | **9** | **5** | **3** | **165.328** | **No** | **0.**  **333** | **No** | **Yes** | **3.002** | **1.365** | **Yes** | **No** | **1.353** | **0.**  **719** |
| compound 38 | GTP-BP | **0.461609607999** | **447.451** | **1.6574** | **8** | **9** | **1** | **187.612** | **No** | **-0.**  **136** | **No** | **Yes** | **2.688** | **1.434** | **Yes** | **No** | **0.**  **632** | **1.479** |

| Ligand | BP | qed | mol | logp | rot | acc | don | area | AMES | Max. TDH | hERG I | hERG II | LD50 | LOAEL | Hepat | S. Sensib | T. Pyr | M.Txc |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **compound 39** | SAH-BP | 0.529992760887 | **485.968** | **4.0572** | **8** | **7** | **0** | **203.603** | **No** | **-0.**  **253** | **No** | **Yes** | **3.015** | **1.06** | **Yes** | **No** | **0.**  **754** | **0.**  **537** |
| compound 40 | SAH-BP | 0.399537942918 | **469.563** | **4.88114** | **6** | **6** | **0** | **189.158** | **No** | **-0.21** | **No** | **Yes** | **3.246** | **0.**  **849** | **Yes** | **No** | **0.**  **897** | **0.**  **523** |
| compound 41 | GTP-BP | 0.399537942918 | **469.563** | **4.88114** | **6** | **6** | **0** | **189.158** | **No** | **-0.21** | **No** | **Yes** | **3.246** | **0.**  **849** | **Yes** | **No** | **0.**  **897** | **0.**  **523** |
| compound 42 | GTP-BP | 0.562202896891 | **456.587** | **4.0241** | **8** | **6** | **1** | **190.632** | **No** | **-0.**  **155** | **No** | **Yes** | **3.028** | **1.089** | **Yes** | **No** | **0.**  **912** | **0.**  **593** |
| compound 43 | GTP-BP | 0.377018473775 | **472.431** | **4.81484** | **5** | **5** | **1** | **185.571** | **No** | **-0.**  **422** | **No** | **Yes** | **2.736** | **0.86** | **No** | **No** | **0.**  **371** | **0.**  **322** |
| compound 44 | SAH-BP | 0.562202896891 | **456.587** | **4.0241** | **8** | **6** | **1** | **190.632** | **No** | **-0.**  **155** | **No** | **Yes** | **3.028** | **1.089** | **Yes** | **No** | **0.**  **912** | **0.**  **593** |
| compound 45 | SAH-BP | 0.532372542228 | **344.422** | **3.0076** | **6** | **6** | **0** | **151.681** | **No** | **0.**  **132** | **No** | **Yes** | **2.821** | **1.471** | **Yes** | **No** | **1.277** | **1.085** |
| **compound 46** | GTP-BP | 0.367500536579 | **455.345** | **5.267** | **8** | **5** | **0** | **189.528** | **No** | **-0.**  **123** | **No** | **Yes** | **3.228** | **0.**  **757** | **Yes** | **No** | **0.**  **958** | **0.**  **125** |
| compound 47 | GTP-BP | 0.461609607999 | **447.451** | **1.6574** | **8** | **9** | **1** | **187.612** | **No** | **-0.**  **136** | **No** | **Yes** | **2.688** | **1.434** | **Yes** | **No** | **0.**  **632** | **1.479** |
| compound 48 | SAH-BP | 0.377018473775 | **472.431** | **4.81484** | **5** | **5** | **1** | **185.571** | **No** | **-0.**  **422** | **No** | **Yes** | **2.736** | **0.86** | **No** | **No** | **0.**  **371** | **0.**  **322** |