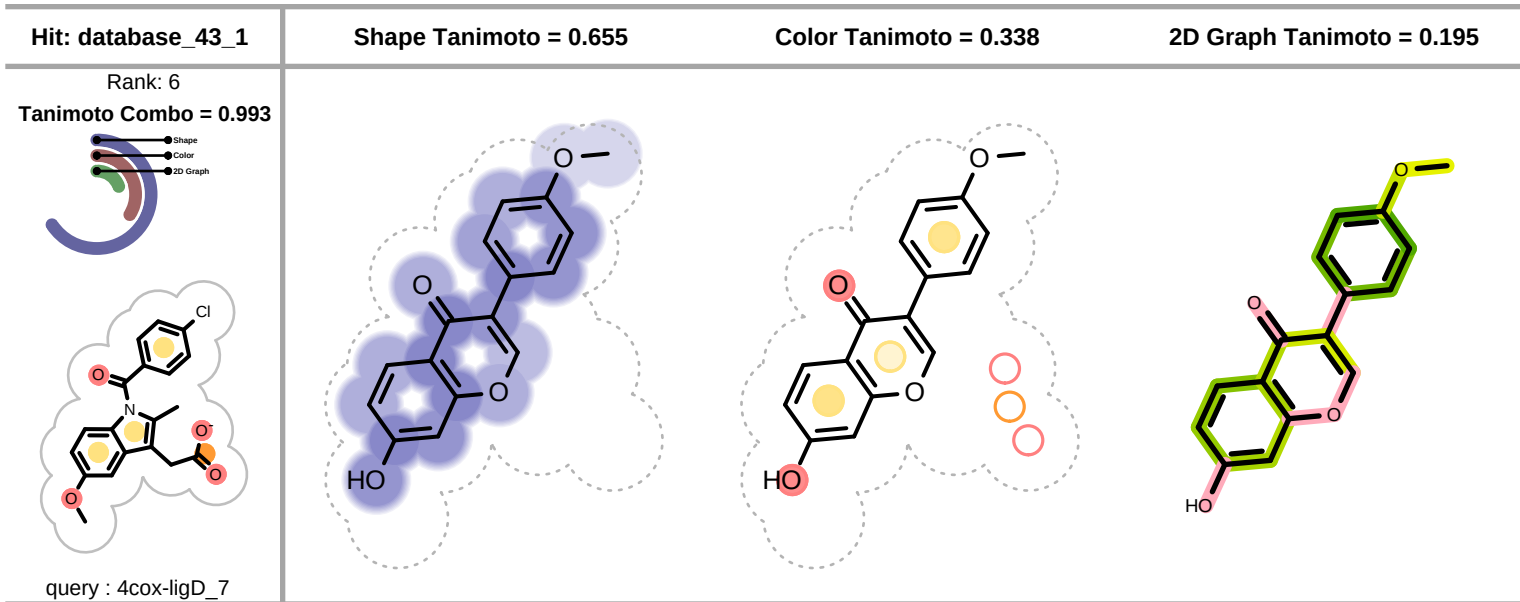
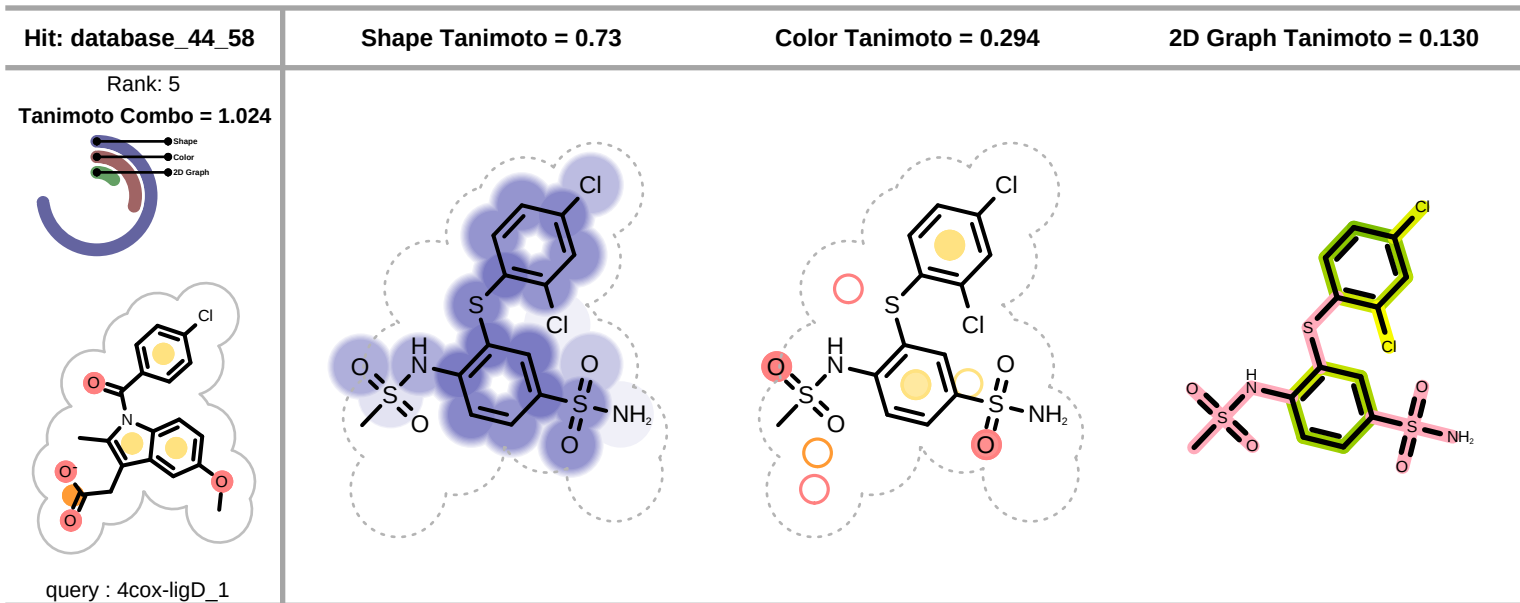
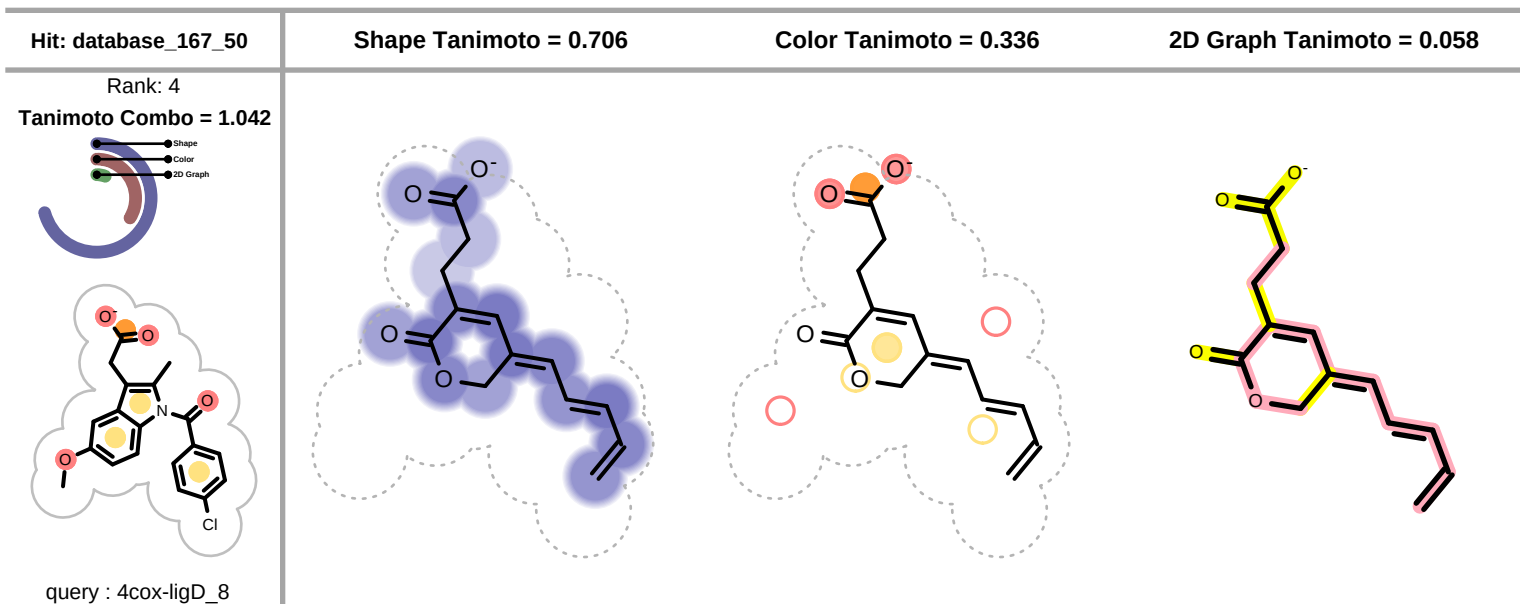
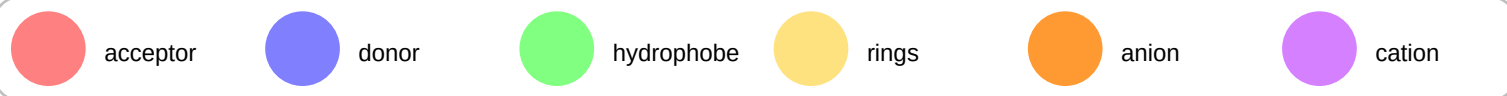
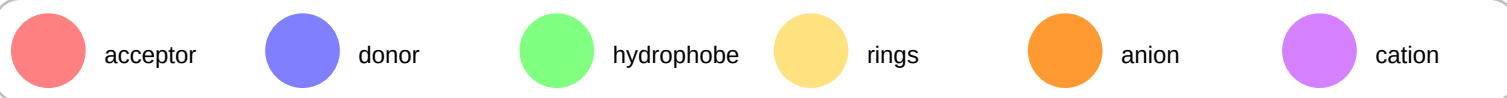
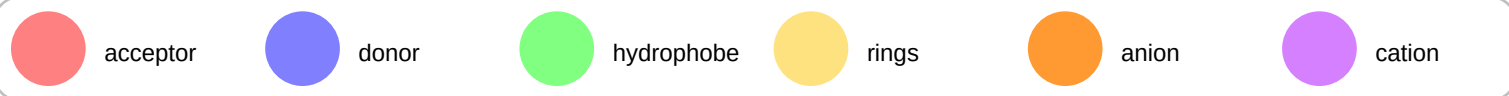


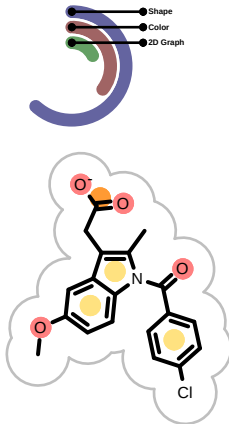
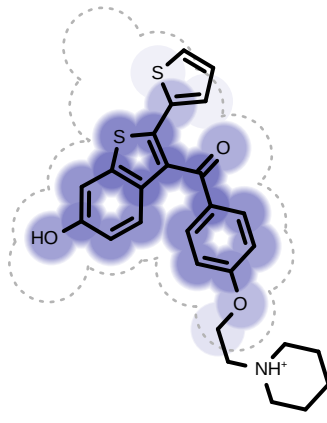
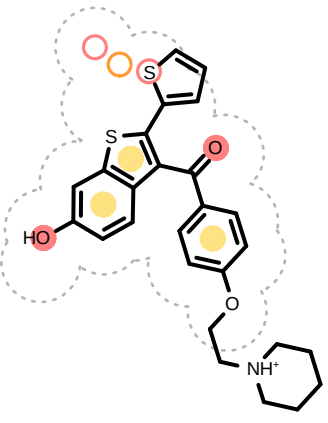
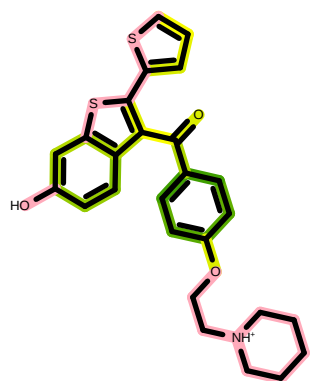
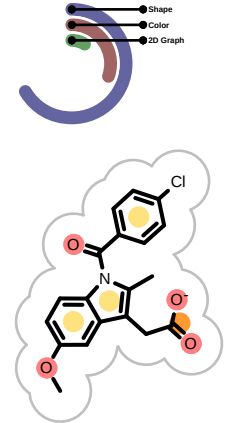
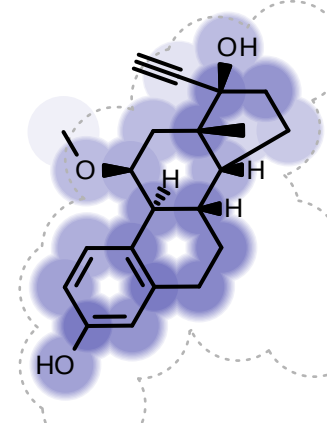
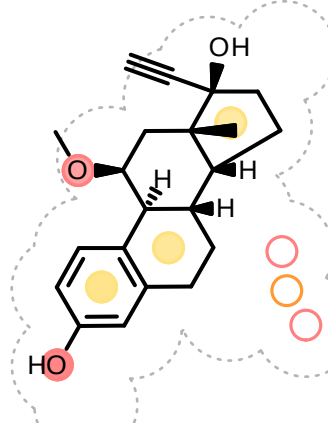
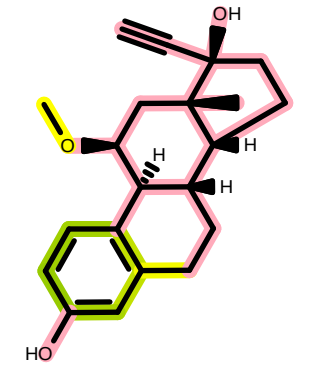
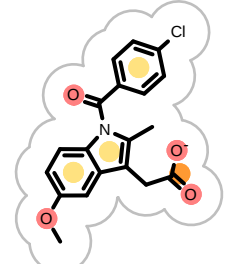
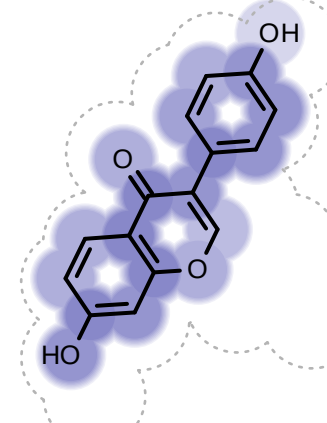
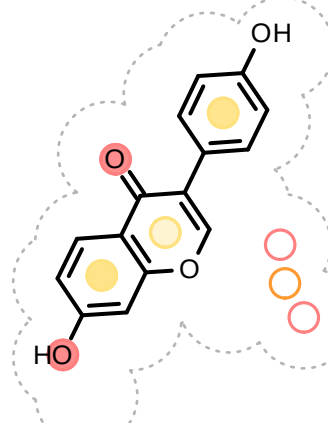
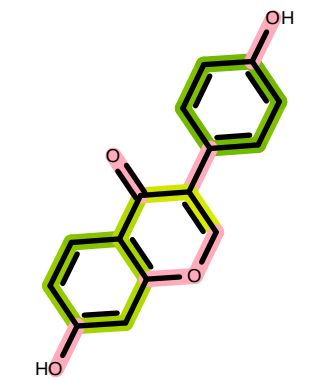
|                                                                                                      |                               |                               |                                  |
|------------------------------------------------------------------------------------------------------|-------------------------------|-------------------------------|----------------------------------|
| <p>Hit: database_130_144</p> <p>Rank: 1</p> <p>Tanimoto Combo = 1.086</p> <p>query : 4cox-ligD_2</p> | <p>Shape Tanimoto = 0.734</p> | <p>Color Tanimoto = 0.352</p> | <p>2D Graph Tanimoto = 0.181</p> |
| <p>Hit: database_168_47</p> <p>Rank: 2</p> <p>Tanimoto Combo = 1.072</p> <p>query : 4cox-ligD_8</p>  | <p>Shape Tanimoto = 0.78</p>  | <p>Color Tanimoto = 0.292</p> | <p>2D Graph Tanimoto = 0.123</p> |
| <p>Hit: database_41_8</p> <p>Rank: 3</p> <p>Tanimoto Combo = 1.068</p> <p>query : 4cox-ligD_5</p>    | <p>Shape Tanimoto = 0.652</p> | <p>Color Tanimoto = 0.416</p> | <p>2D Graph Tanimoto = 0.196</p> |

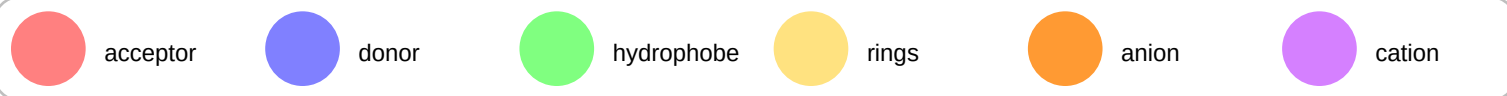




|                                                                                                      |                               |                               |                                  |
|------------------------------------------------------------------------------------------------------|-------------------------------|-------------------------------|----------------------------------|
| <p>Hit: database_142_197</p> <p>Rank: 7</p> <p>Tanimoto Combo = 0.99</p> <p>query : 4cox-ligD_8</p>  | <p>Shape Tanimoto = 0.723</p> | <p>Color Tanimoto = 0.267</p> | <p>2D Graph Tanimoto = 0.100</p> |
| <p>Hit: database_126_2</p> <p>Rank: 8</p> <p>Tanimoto Combo = 0.989</p> <p>query : 4cox-ligD_1</p>   | <p>Shape Tanimoto = 0.673</p> | <p>Color Tanimoto = 0.316</p> | <p>2D Graph Tanimoto = 0.117</p> |
| <p>Hit: database_105_168</p> <p>Rank: 9</p> <p>Tanimoto Combo = 0.977</p> <p>query : 4cox-ligD_9</p> | <p>Shape Tanimoto = 0.654</p> | <p>Color Tanimoto = 0.323</p> | <p>2D Graph Tanimoto = 0.147</p> |



|                                                                                                                                                                                     |                                                                                                                   |                                                                                                                    |                                                                                                                        |
|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------|
| <p>Hit: database_189_87</p> <p>Rank: 10<br/>Tanimoto Combo = 0.969</p>  <p>query : 4cox-ligD_8</p>  | <p>Shape Tanimoto = 0.616</p>    | <p>Color Tanimoto = 0.353</p>    | <p>2D Graph Tanimoto = 0.177</p>    |
| <p>Hit: database_20</p> <p>Rank: 11<br/>Tanimoto Combo = 0.967</p>  <p>query : 4cox-ligD_7</p>     | <p>Shape Tanimoto = 0.664</p>   | <p>Color Tanimoto = 0.303</p>   | <p>2D Graph Tanimoto = 0.092</p>   |
| <p>Hit: database_171_0</p> <p>Rank: 12<br/>Tanimoto Combo = 0.963</p>  <p>query : 4cox-ligD_7</p> | <p>Shape Tanimoto = 0.651</p>  | <p>Color Tanimoto = 0.312</p>  | <p>2D Graph Tanimoto = 0.143</p>  |



|                                                                                                      |                               |                               |                                  |
|------------------------------------------------------------------------------------------------------|-------------------------------|-------------------------------|----------------------------------|
| <p>Hit: database_11_173</p> <p>Rank: 13</p> <p>Tanimoto Combo = 0.959</p> <p>query : 4cox-ligD_7</p> | <p>Shape Tanimoto = 0.652</p> | <p>Color Tanimoto = 0.307</p> | <p>2D Graph Tanimoto = 0.129</p> |
| <p>Hit: database_51_7</p> <p>Rank: 14</p> <p>Tanimoto Combo = 0.955</p> <p>query : 4cox-ligD_9</p>   | <p>Shape Tanimoto = 0.633</p> | <p>Color Tanimoto = 0.322</p> | <p>2D Graph Tanimoto = 0.184</p> |
| <p>Hit: database_161_12</p> <p>Rank: 15</p> <p>Tanimoto Combo = 0.949</p> <p>query : 4cox-ligD_9</p> | <p>Shape Tanimoto = 0.763</p> | <p>Color Tanimoto = 0.186</p> | <p>2D Graph Tanimoto = 0.093</p> |



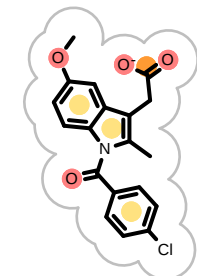
Hit: database\_159\_116

Shape Tanimoto = 0.695

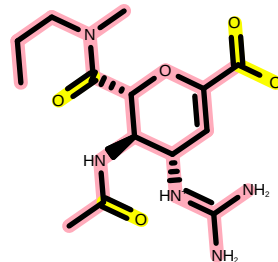
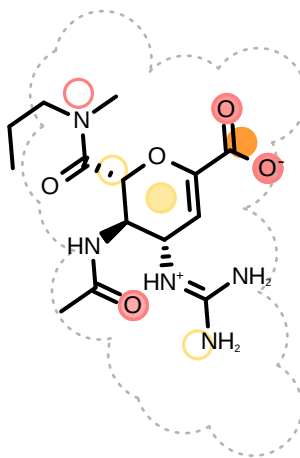
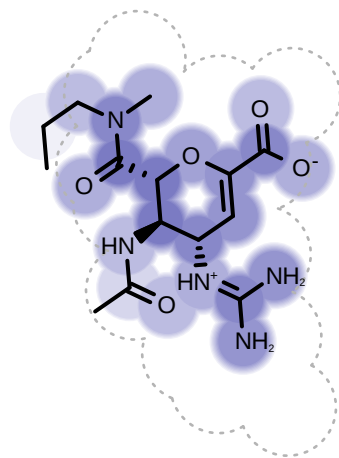
Color Tanimoto = 0.251

2D Graph Tanimoto = 0.053

Rank: 16  
Tanimoto Combo = 0.946



query : 4cox-ligD\_5



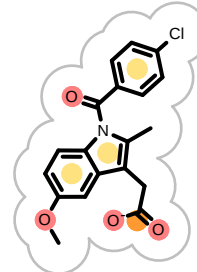
Hit: database\_90\_4

Shape Tanimoto = 0.644

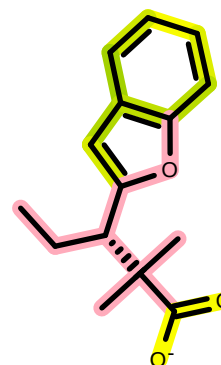
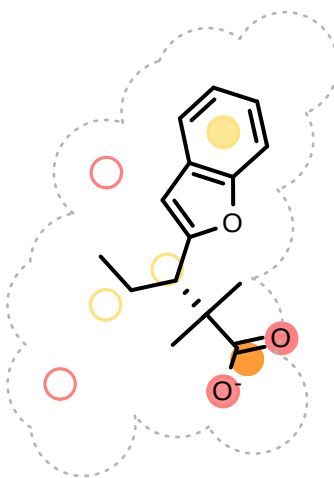
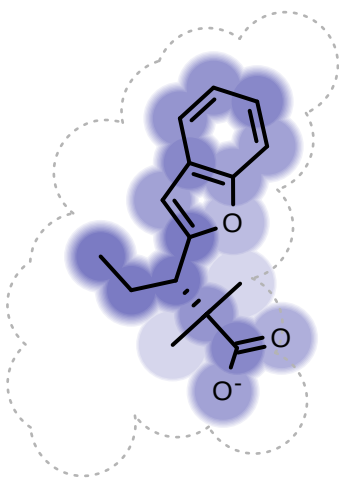
Color Tanimoto = 0.302

2D Graph Tanimoto = 0.103

Rank: 17  
Tanimoto Combo = 0.946



query : 4cox-ligD\_9



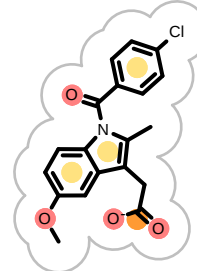
Hit: database\_21\_5

Shape Tanimoto = 0.742

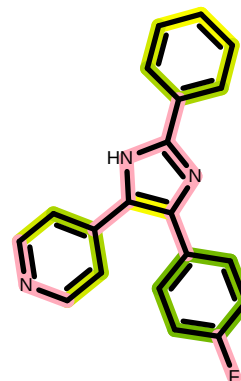
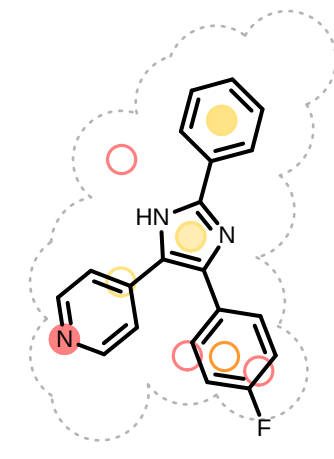
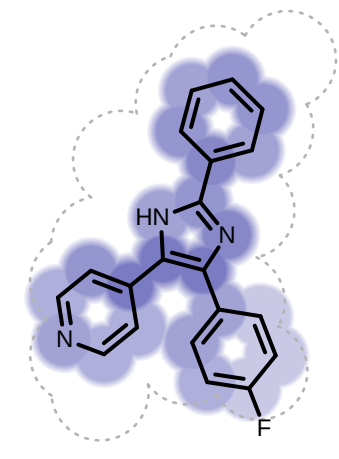
Color Tanimoto = 0.201

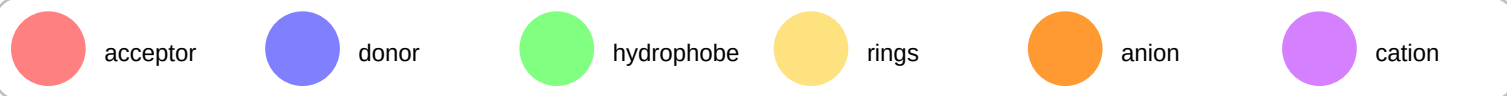
2D Graph Tanimoto = 0.069

Rank: 18  
Tanimoto Combo = 0.943



query : 4cox-ligD\_9





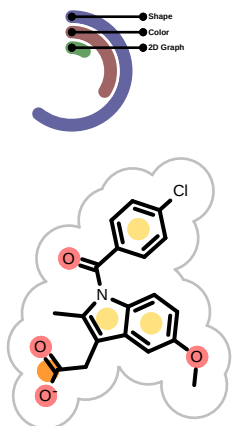
Hit: database\_114\_7

Shape Tanimoto = 0.605

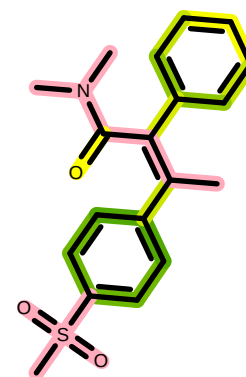
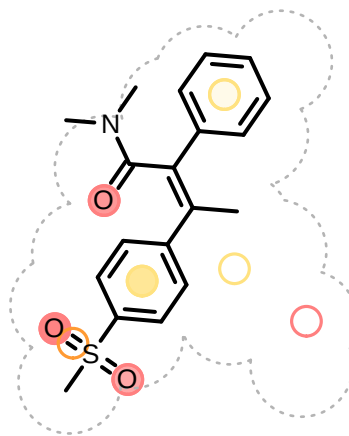
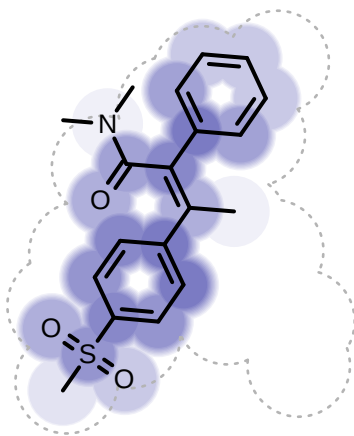
Color Tanimoto = 0.339

2D Graph Tanimoto = 0.091

Rank: 19  
Tanimoto Combo = 0.943



query : 4cox-ligD\_4



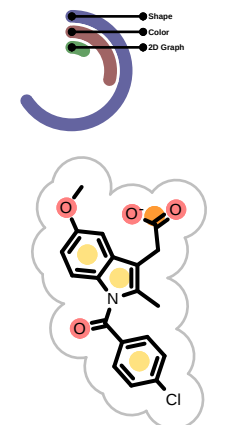
Hit: database\_132\_0

Shape Tanimoto = 0.656

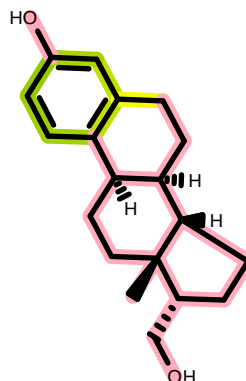
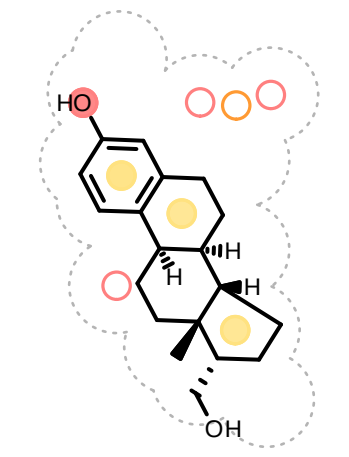
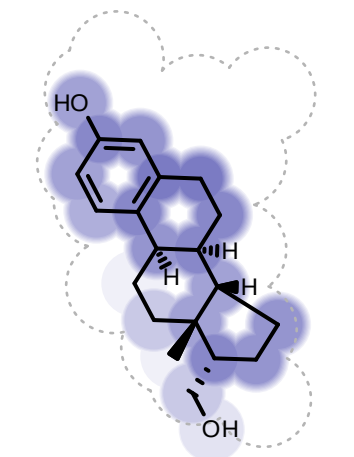
Color Tanimoto = 0.287

2D Graph Tanimoto = 0.085

Rank: 20  
Tanimoto Combo = 0.943



query : 4cox-ligD\_5



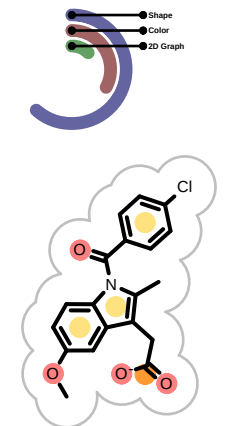
Hit: database\_170\_0

Shape Tanimoto = 0.614

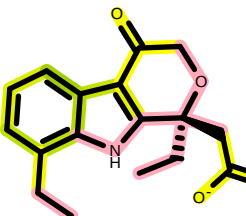
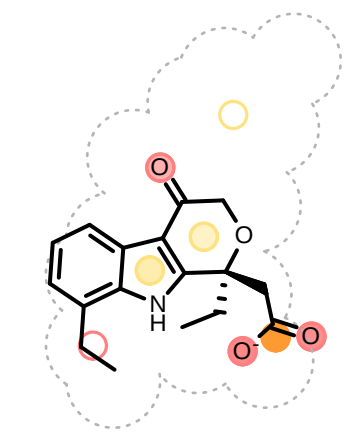
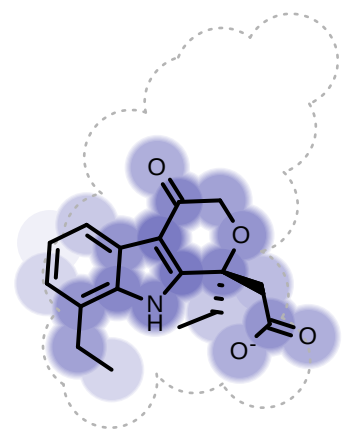
Color Tanimoto = 0.327

2D Graph Tanimoto = 0.124

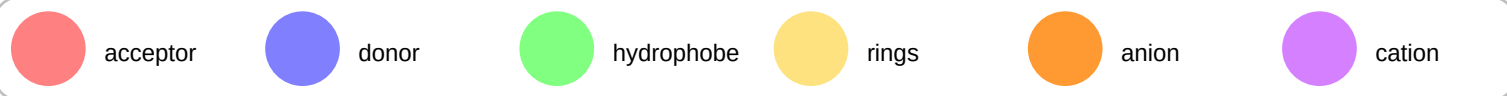
Rank: 21  
Tanimoto Combo = 0.94

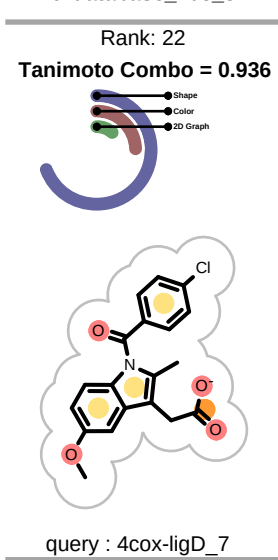
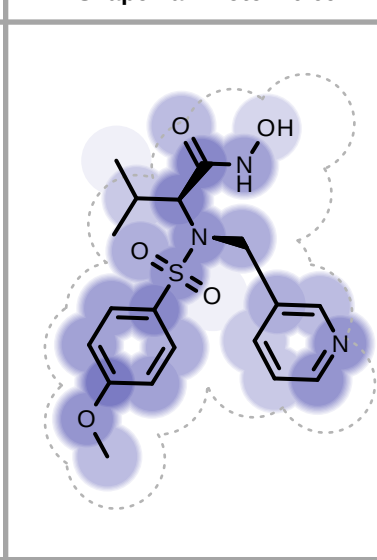
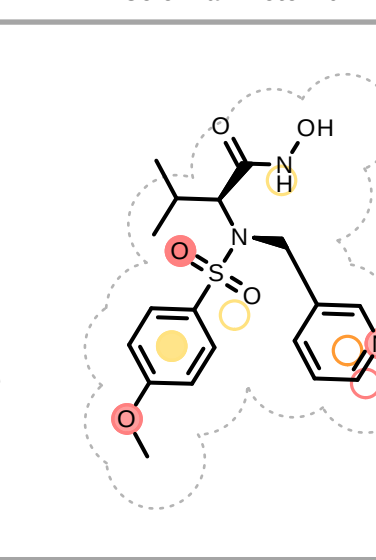
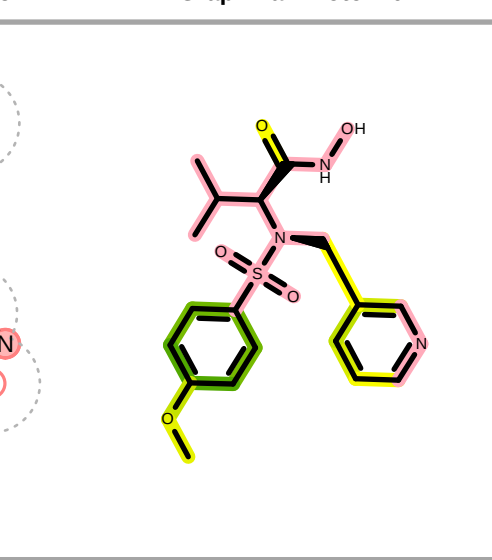
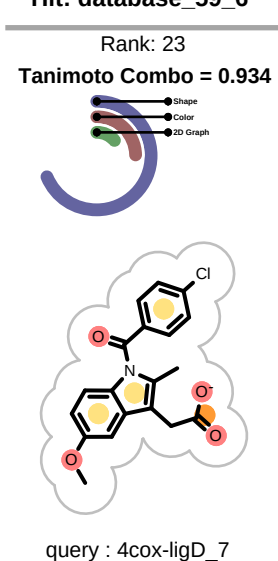
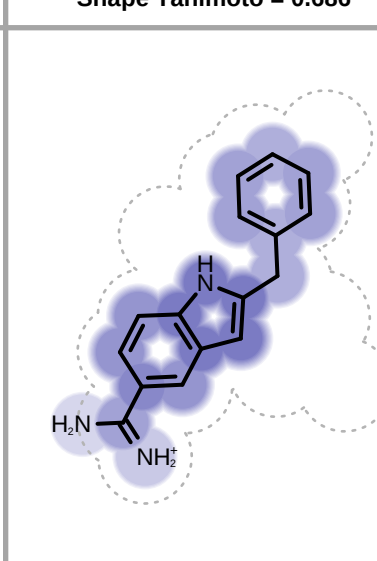
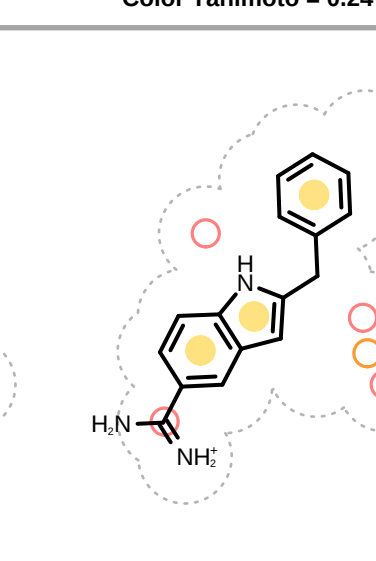
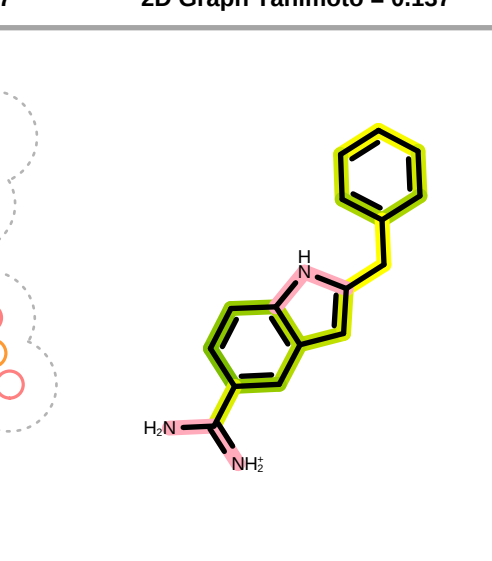
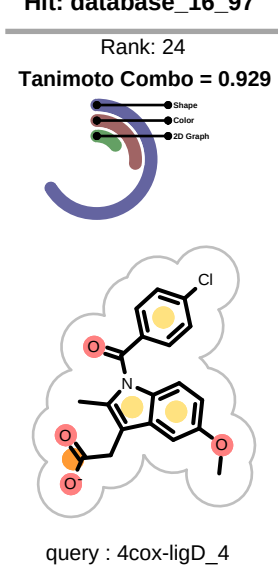
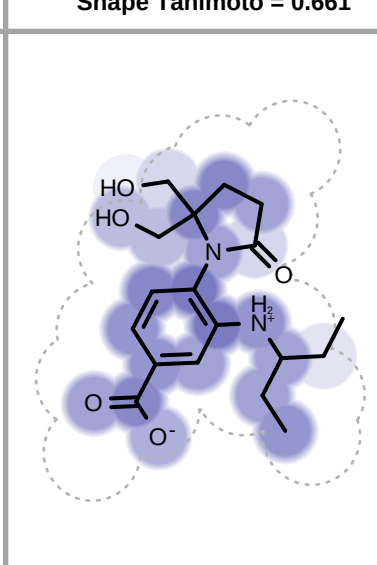
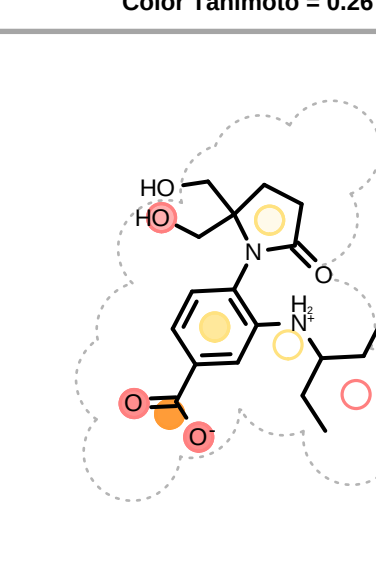
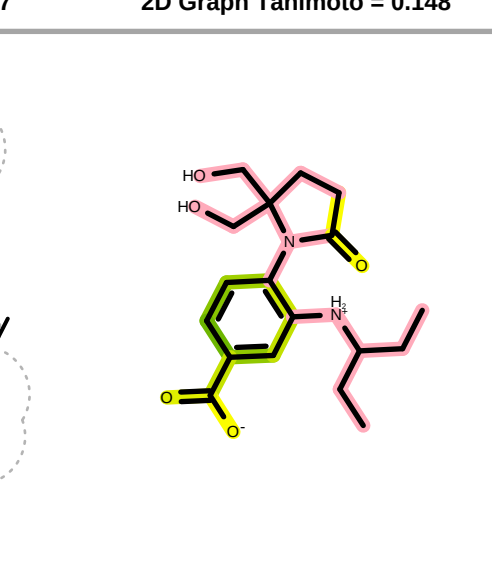


query : 4cox-ligD\_9

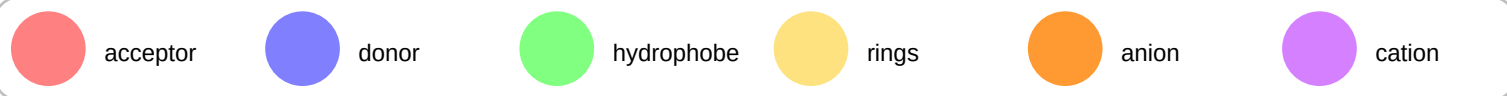


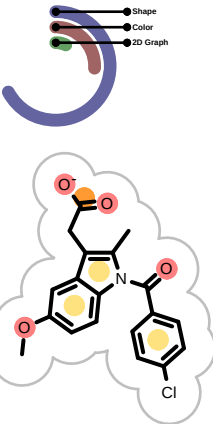
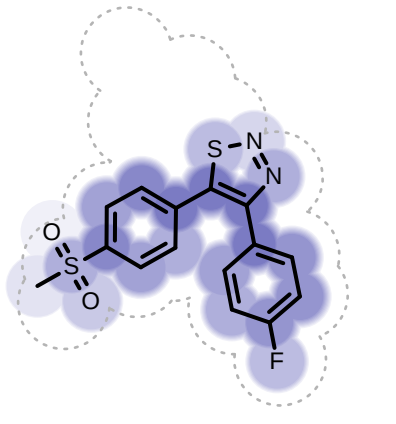
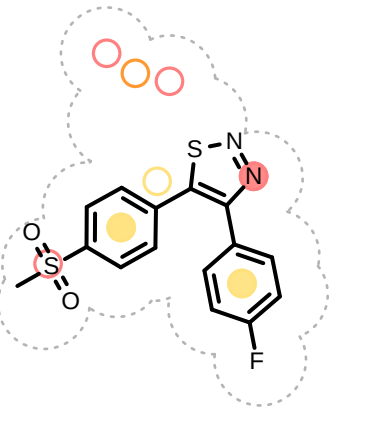
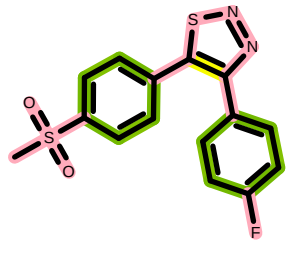
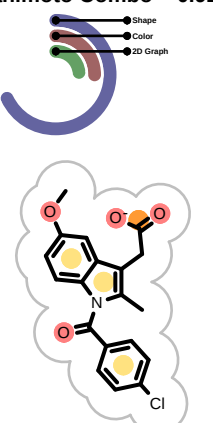
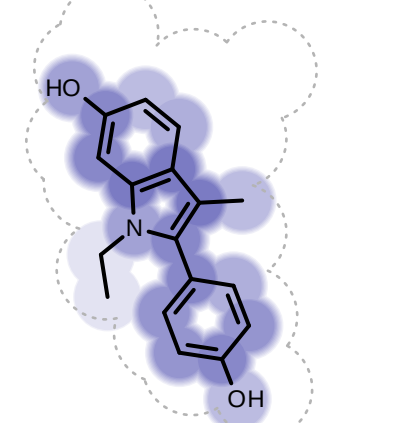
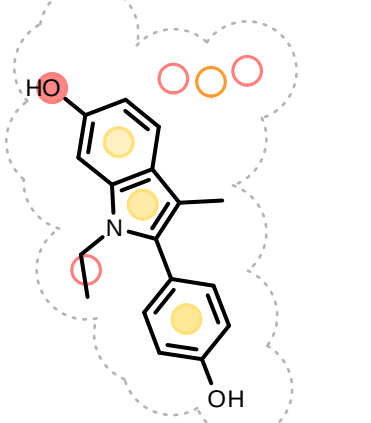
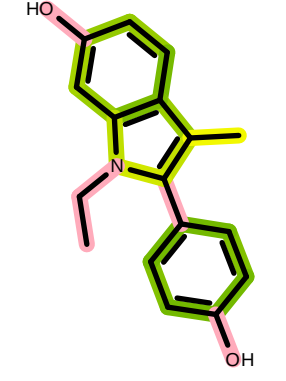
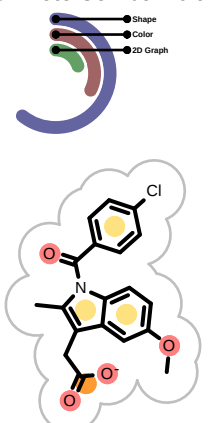
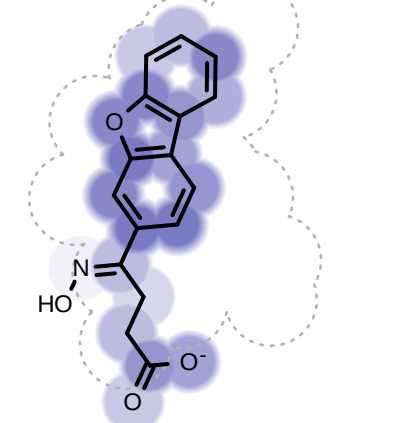
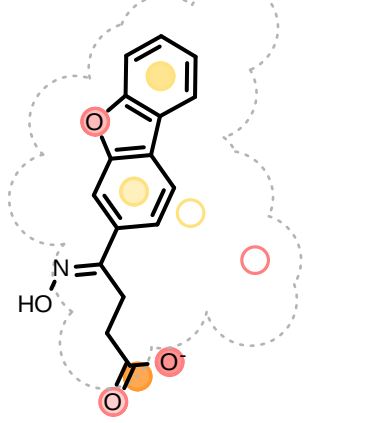
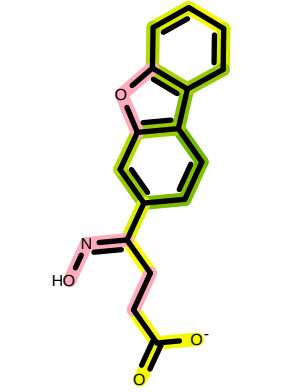


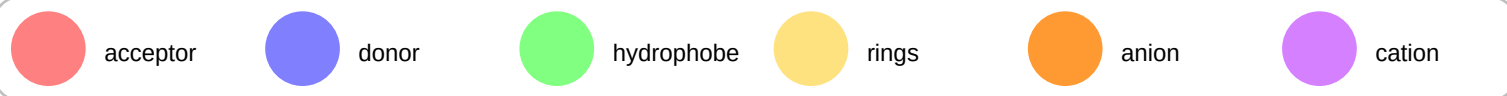


|                                                                                                                                                                                        |                                                                                                                   |                                                                                                                    |                                                                                                                        |
|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------|
| <p>Hit: database_108_34</p> <p>Rank: 22</p> <p>Tanimoto Combo = 0.936</p>  <p>query : 4cox-ligD_7</p>  | <p>Shape Tanimoto = 0.691</p>    | <p>Color Tanimoto = 0.245</p>    | <p>2D Graph Tanimoto = 0.114</p>    |
| <p>Hit: database_59_6</p> <p>Rank: 23</p> <p>Tanimoto Combo = 0.934</p>  <p>query : 4cox-ligD_7</p>   | <p>Shape Tanimoto = 0.686</p>   | <p>Color Tanimoto = 0.247</p>   | <p>2D Graph Tanimoto = 0.137</p>   |
| <p>Hit: database_16_97</p> <p>Rank: 24</p> <p>Tanimoto Combo = 0.929</p>  <p>query : 4cox-ligD_4</p> | <p>Shape Tanimoto = 0.661</p>  | <p>Color Tanimoto = 0.267</p>  | <p>2D Graph Tanimoto = 0.148</p>  |





|                                                                                                                                                                                                      |                                                                                                                          |                                                                                                                           |                                                                                                                               |
|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------|
| <p><b>Hit: database_19_2</b></p> <p>Rank: 25</p> <p><b>Tanimoto Combo = 0.929</b></p>  <p>query : 4cox-ligD_2</p>    | <p><b>Shape Tanimoto = 0.67</b></p>     | <p><b>Color Tanimoto = 0.259</b></p>    | <p><b>2D Graph Tanimoto = 0.070</b></p>    |
| <p><b>Hit: database_141_1</b></p> <p>Rank: 26</p> <p><b>Tanimoto Combo = 0.928</b></p>  <p>query : 4cox-ligD_5</p>  | <p><b>Shape Tanimoto = 0.678</b></p>   | <p><b>Color Tanimoto = 0.251</b></p>   | <p><b>2D Graph Tanimoto = 0.235</b></p>   |
| <p><b>Hit: database_25_17</b></p> <p>Rank: 27</p> <p><b>Tanimoto Combo = 0.927</b></p>  <p>query : 4cox-ligD_0</p> | <p><b>Shape Tanimoto = 0.606</b></p>  | <p><b>Color Tanimoto = 0.322</b></p>  | <p><b>2D Graph Tanimoto = 0.200</b></p>  |



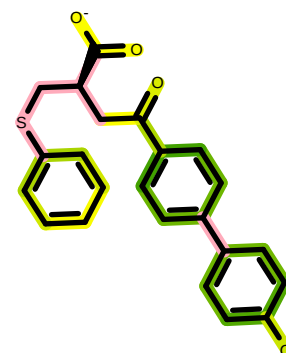
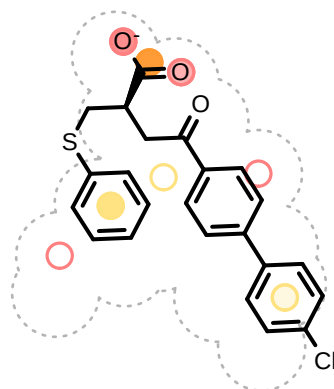
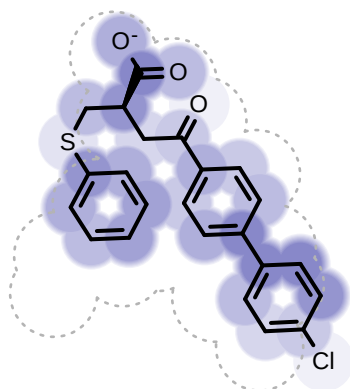
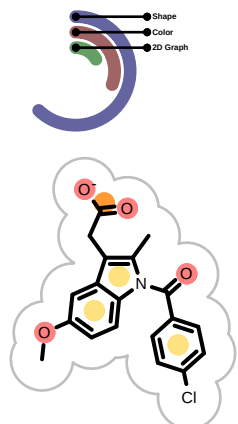
Hit: database\_38\_20

Shape Tanimoto = 0.62

Color Tanimoto = 0.307

2D Graph Tanimoto = 0.166

Rank: 28  
Tanimoto Combo = 0.927



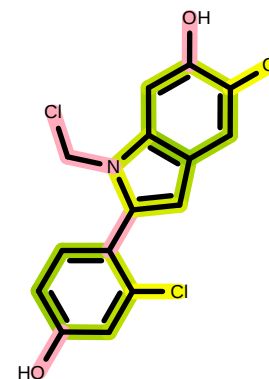
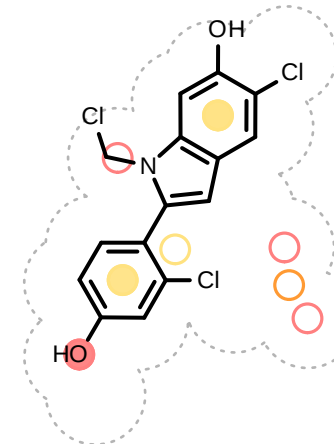
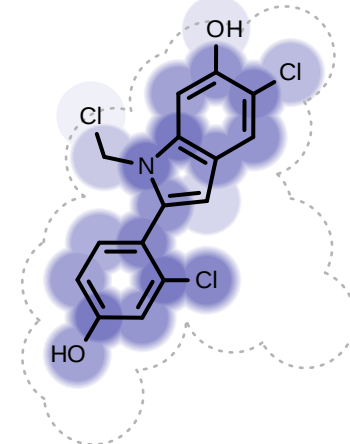
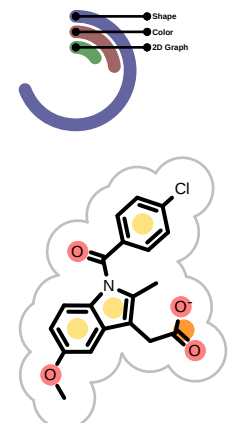
Hit: database\_128\_1

Shape Tanimoto = 0.693

Color Tanimoto = 0.233

2D Graph Tanimoto = 0.158

Rank: 29  
Tanimoto Combo = 0.927



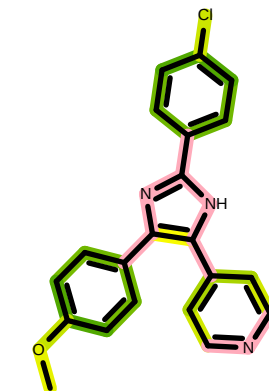
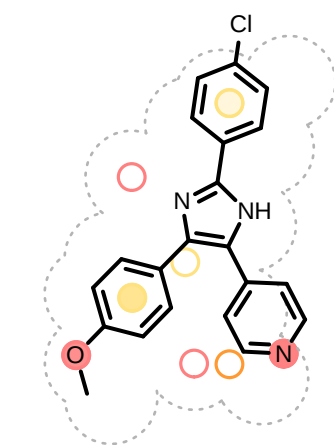
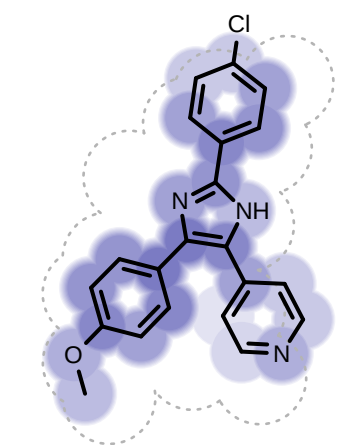
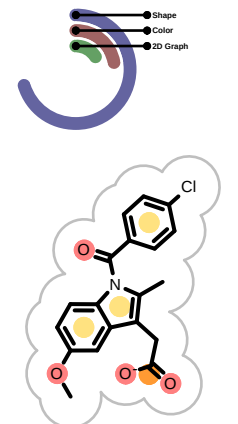
Hit: database\_89\_16

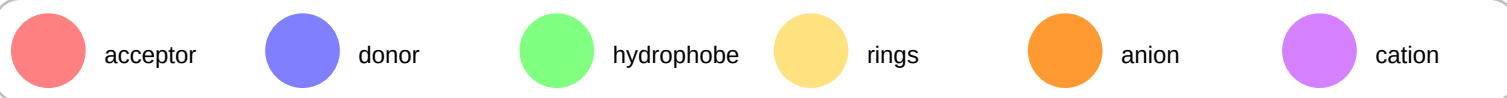
Shape Tanimoto = 0.702

Color Tanimoto = 0.222

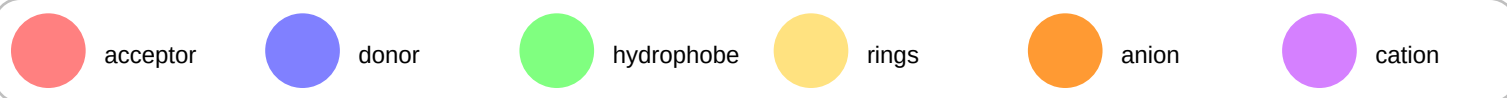
2D Graph Tanimoto = 0.160

Rank: 30  
Tanimoto Combo = 0.924





|                                                                                                      |                               |                               |                                  |
|------------------------------------------------------------------------------------------------------|-------------------------------|-------------------------------|----------------------------------|
| <p>Hit: database_57_13</p> <p>Rank: 31</p> <p>Tanimoto Combo = 0.92</p> <p>query : 4cox-ligD_3</p>   | <p>Shape Tanimoto = 0.741</p> | <p>Color Tanimoto = 0.179</p> | <p>2D Graph Tanimoto = 0.112</p> |
| <p>Hit: database_49_0</p> <p>Rank: 32</p> <p>Tanimoto Combo = 0.918</p> <p>query : 4cox-ligD_8</p>   | <p>Shape Tanimoto = 0.575</p> | <p>Color Tanimoto = 0.343</p> | <p>2D Graph Tanimoto = 0.185</p> |
| <p>Hit: database_92_171</p> <p>Rank: 33</p> <p>Tanimoto Combo = 0.917</p> <p>query : 4cox-ligD_2</p> | <p>Shape Tanimoto = 0.624</p> | <p>Color Tanimoto = 0.293</p> | <p>2D Graph Tanimoto = 0.102</p> |



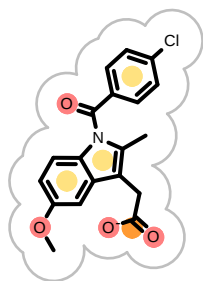
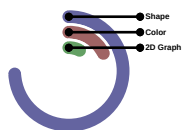
Hit: database\_209\_8

Shape Tanimoto = 0.741

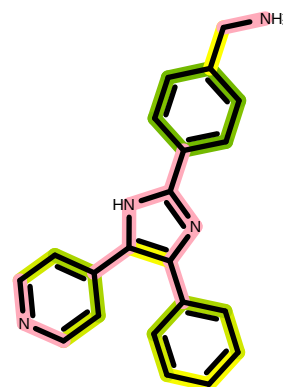
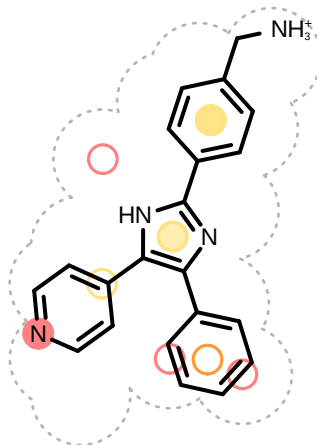
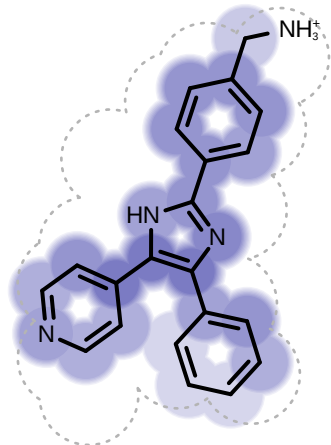
Color Tanimoto = 0.175

2D Graph Tanimoto = 0.076

Rank: 34  
Tanimoto Combo = 0.917



query : 4cox-ligD\_9



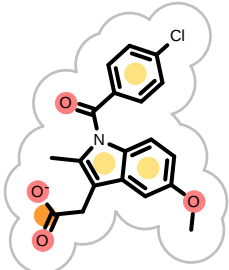
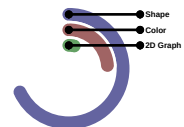
Hit: database\_188\_14

Shape Tanimoto = 0.679

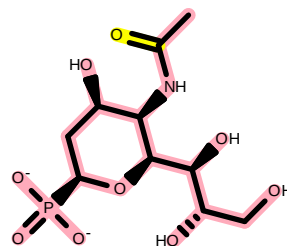
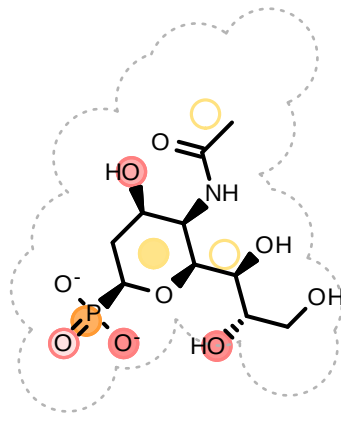
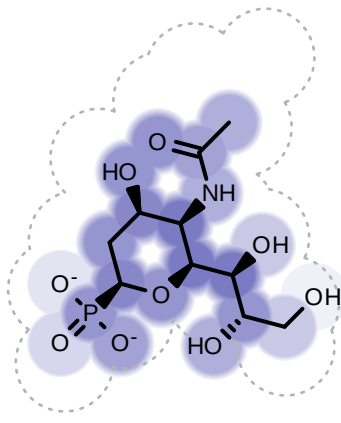
Color Tanimoto = 0.237

2D Graph Tanimoto = 0.037

Rank: 35  
Tanimoto Combo = 0.916



query : 4cox-ligD\_6



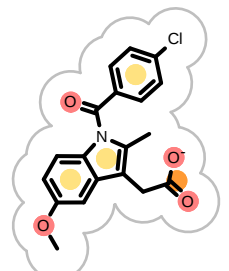
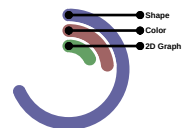
Hit: database\_133\_1

Shape Tanimoto = 0.683

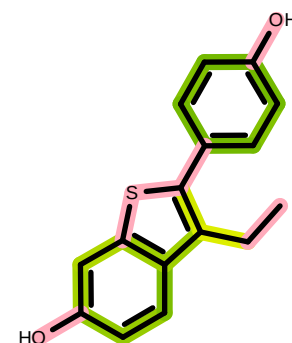
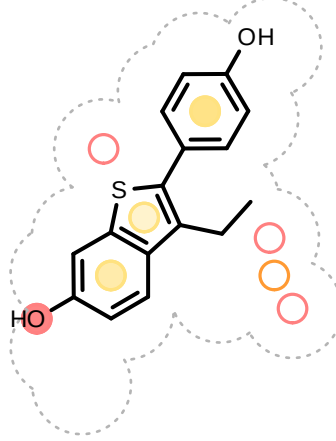
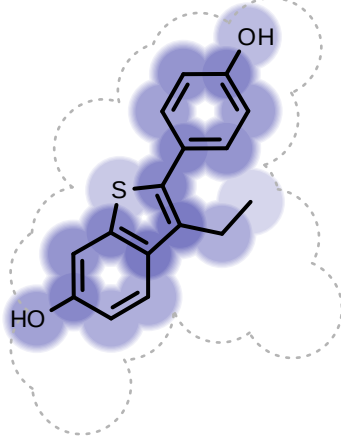
Color Tanimoto = 0.233

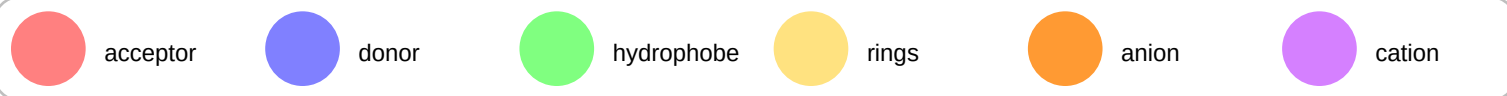
2D Graph Tanimoto = 0.177

Rank: 36  
Tanimoto Combo = 0.916

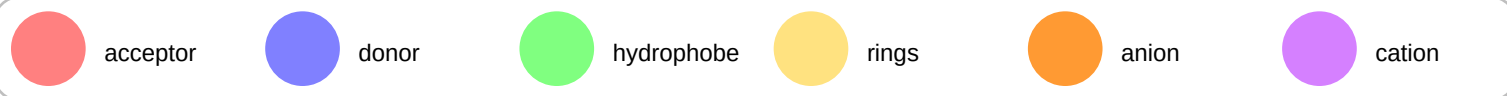


query : 4cox-ligD\_7

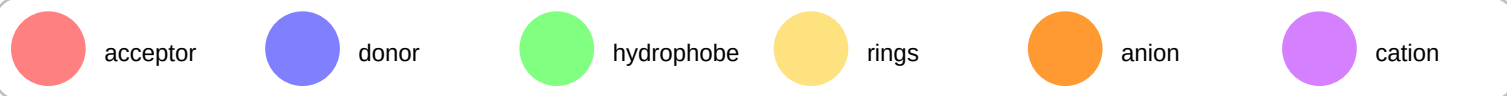




|                                                                                                      |                               |                               |                                  |
|------------------------------------------------------------------------------------------------------|-------------------------------|-------------------------------|----------------------------------|
| <p>Hit: database_119_14</p> <p>Rank: 37</p> <p>Tanimoto Combo = 0.915</p> <p>query : 4cox-ligD_5</p> | <p>Shape Tanimoto = 0.732</p> | <p>Color Tanimoto = 0.183</p> | <p>2D Graph Tanimoto = 0.088</p> |
| <p>Hit: database_163_52</p> <p>Rank: 38</p> <p>Tanimoto Combo = 0.915</p> <p>query : 4cox-ligD_5</p> | <p>Shape Tanimoto = 0.699</p> | <p>Color Tanimoto = 0.216</p> | <p>2D Graph Tanimoto = 0.069</p> |
| <p>Hit: database_99_9</p> <p>Rank: 39</p> <p>Tanimoto Combo = 0.914</p> <p>query : 4cox-ligD_4</p>   | <p>Shape Tanimoto = 0.687</p> | <p>Color Tanimoto = 0.227</p> | <p>2D Graph Tanimoto = 0.171</p> |

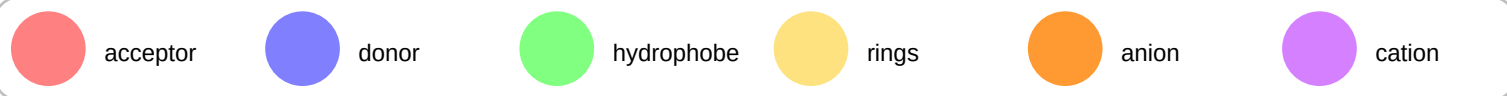


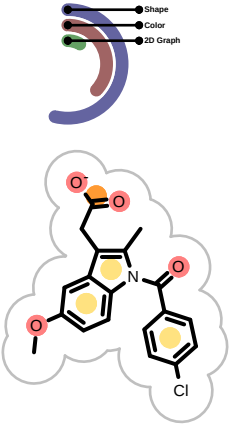
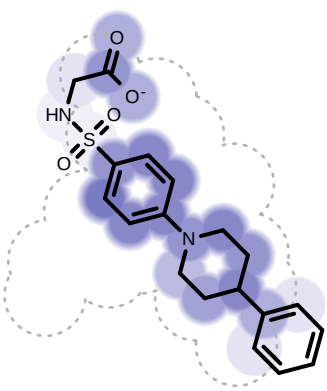
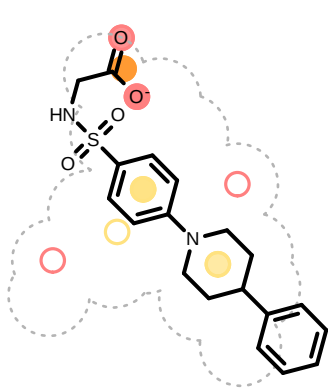
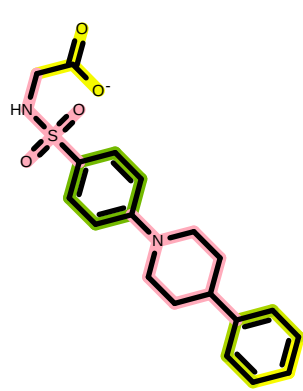
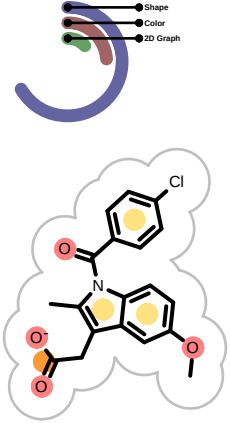
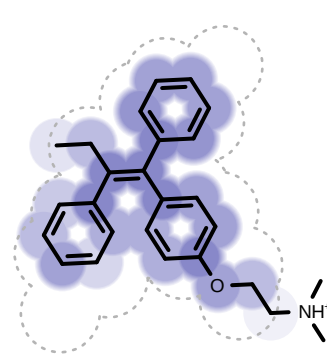
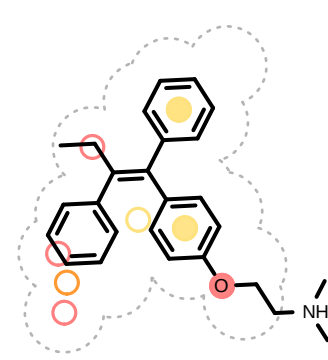
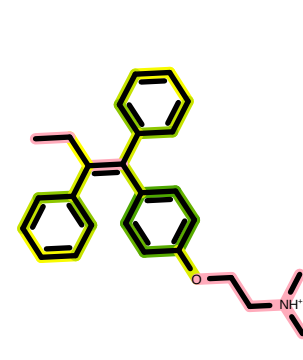
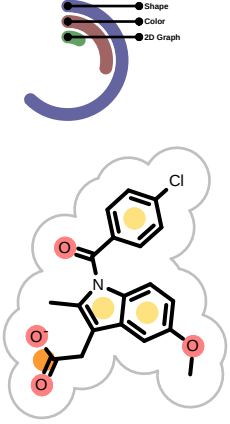
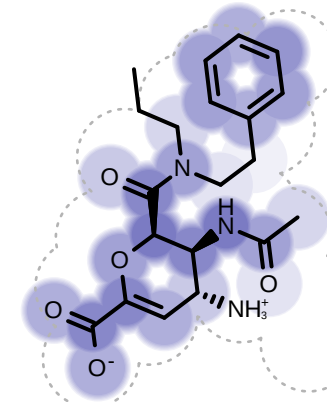
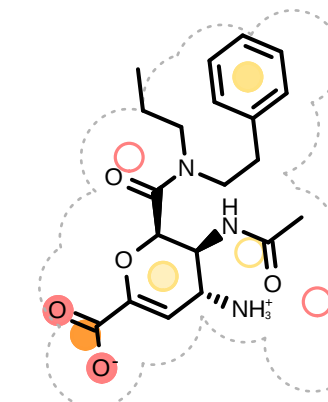
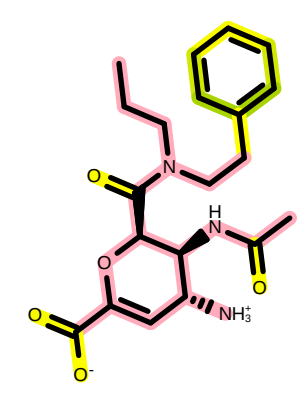
|                                                                                                       |                               |                               |                                  |
|-------------------------------------------------------------------------------------------------------|-------------------------------|-------------------------------|----------------------------------|
| <p>Hit: database_145_66</p> <p>Rank: 40</p> <p>Tanimoto Combo = 0.914</p> <p>query : 4cox-ligD_1</p>  | <p>Shape Tanimoto = 0.654</p> | <p>Color Tanimoto = 0.261</p> | <p>2D Graph Tanimoto = 0.127</p> |
| <p>Hit: database_146_139</p> <p>Rank: 41</p> <p>Tanimoto Combo = 0.914</p> <p>query : 4cox-ligD_5</p> | <p>Shape Tanimoto = 0.693</p> | <p>Color Tanimoto = 0.221</p> | <p>2D Graph Tanimoto = 0.045</p> |
| <p>Hit: database_101_20</p> <p>Rank: 42</p> <p>Tanimoto Combo = 0.914</p> <p>query : 4cox-ligD_6</p>  | <p>Shape Tanimoto = 0.679</p> | <p>Color Tanimoto = 0.235</p> | <p>2D Graph Tanimoto = 0.052</p> |

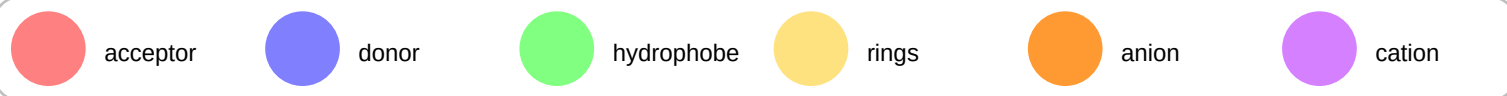


|                                                                                                        |                                      |                                      |                                         |
|--------------------------------------------------------------------------------------------------------|--------------------------------------|--------------------------------------|-----------------------------------------|
| <p><b>Hit: database_71_1</b></p> <p>Rank: 43<br/>Tanimoto Combo = 0.914</p> <p>query : 4cox-ligD_9</p> | <p><b>Shape Tanimoto = 0.678</b></p> | <p><b>Color Tanimoto = 0.235</b></p> | <p><b>2D Graph Tanimoto = 0.063</b></p> |
| <p><b>Hit: database_18_2</b></p> <p>Rank: 44<br/>Tanimoto Combo = 0.911</p> <p>query : 4cox-ligD_1</p> | <p><b>Shape Tanimoto = 0.594</b></p> | <p><b>Color Tanimoto = 0.317</b></p> | <p><b>2D Graph Tanimoto = 0.123</b></p> |
| <p><b>Hit: database_91_1</b></p> <p>Rank: 45<br/>Tanimoto Combo = 0.91</p> <p>query : 4cox-ligD_1</p>  | <p><b>Shape Tanimoto = 0.646</b></p> | <p><b>Color Tanimoto = 0.264</b></p> | <p><b>2D Graph Tanimoto = 0.185</b></p> |





|                                                                                                                                                                                         |                                                                                                                   |                                                                                                                    |                                                                                                                        |
|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------|
| <p>Hit: database_162_163</p> <p>Rank: 46</p> <p>Tanimoto Combo = 0.906</p>  <p>query : 4cox-ligD_8</p>  | <p>Shape Tanimoto = 0.538</p>    | <p>Color Tanimoto = 0.368</p>    | <p>2D Graph Tanimoto = 0.086</p>    |
| <p>Hit: database_154_17</p> <p>Rank: 47</p> <p>Tanimoto Combo = 0.904</p>  <p>query : 4cox-ligD_1</p>  | <p>Shape Tanimoto = 0.665</p>   | <p>Color Tanimoto = 0.239</p>   | <p>2D Graph Tanimoto = 0.130</p>   |
| <p>Hit: database_174_73</p> <p>Rank: 48</p> <p>Tanimoto Combo = 0.903</p>  <p>query : 4cox-ligD_1</p> | <p>Shape Tanimoto = 0.621</p>  | <p>Color Tanimoto = 0.282</p>  | <p>2D Graph Tanimoto = 0.082</p>  |



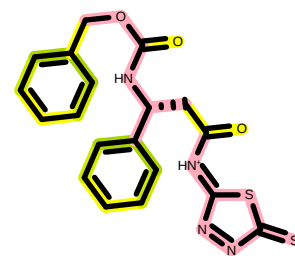
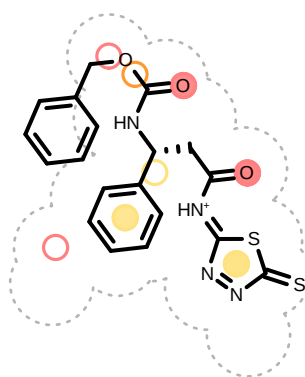
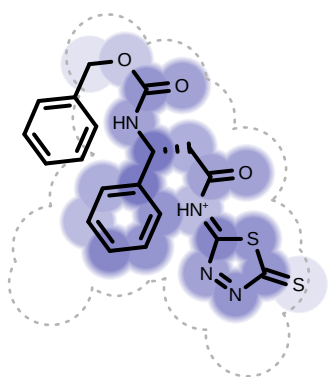
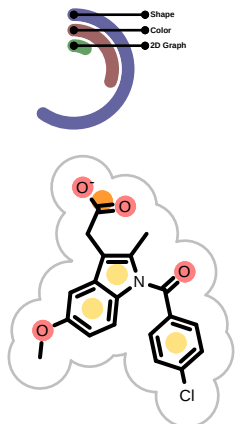
Hit: database\_149\_148

Shape Tanimoto = 0.596

Color Tanimoto = 0.302

2D Graph Tanimoto = 0.082

Rank: 49  
Tanimoto Combo = 0.898



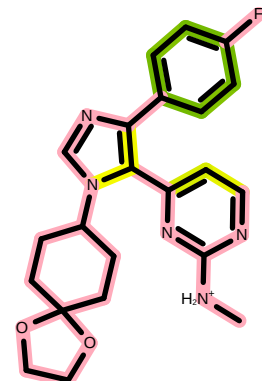
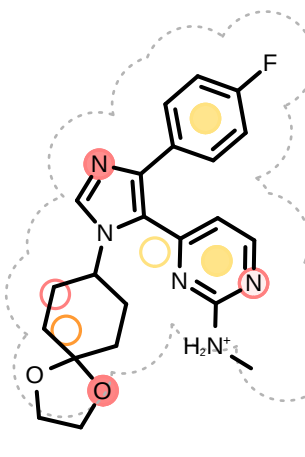
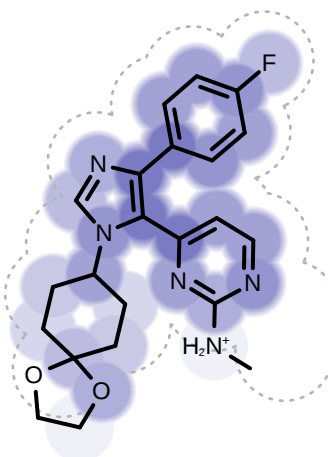
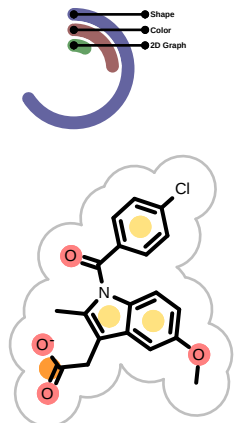
Hit: database\_70\_49

Shape Tanimoto = 0.657

Color Tanimoto = 0.24

2D Graph Tanimoto = 0.080

Rank: 50  
Tanimoto Combo = 0.898



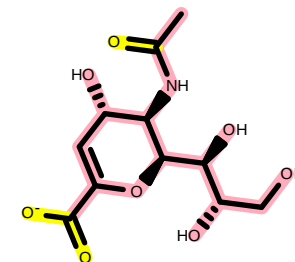
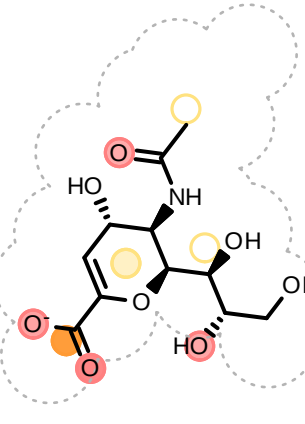
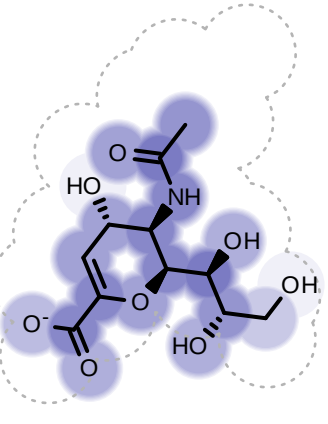
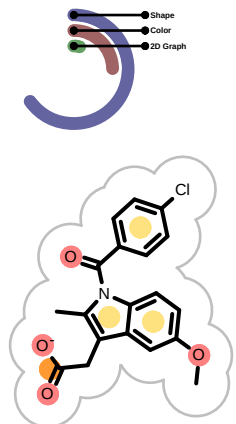
Hit: database\_82\_53

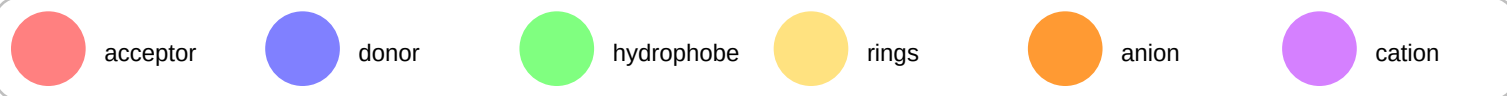
Shape Tanimoto = 0.649

Color Tanimoto = 0.247

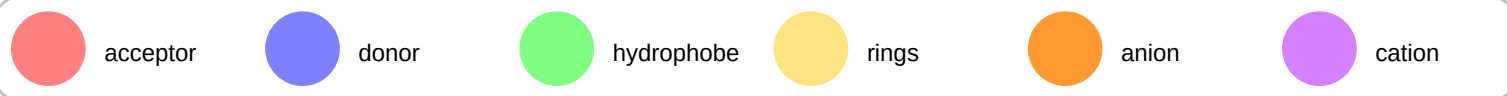
2D Graph Tanimoto = 0.040

Rank: 51  
Tanimoto Combo = 0.896

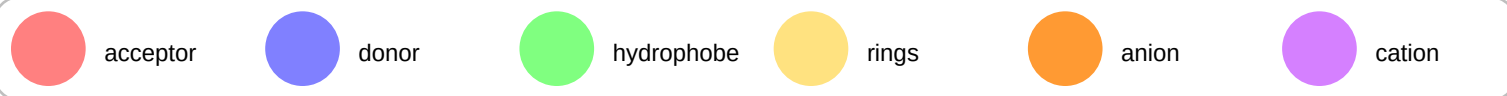




|                                                                                                   |                               |                               |                                  |
|---------------------------------------------------------------------------------------------------|-------------------------------|-------------------------------|----------------------------------|
| <p>Hit: database_175_6</p> <p>Rank: 52<br/>Tanimoto Combo = 0.895</p> <p>query : 4cox-ligD_5</p>  | <p>Shape Tanimoto = 0.717</p> | <p>Color Tanimoto = 0.178</p> | <p>2D Graph Tanimoto = 0.074</p> |
| <p>Hit: database_208_27</p> <p>Rank: 53<br/>Tanimoto Combo = 0.891</p> <p>query : 4cox-ligD_9</p> | <p>Shape Tanimoto = 0.704</p> | <p>Color Tanimoto = 0.188</p> | <p>2D Graph Tanimoto = 0.076</p> |
| <p>Hit: database_193_36</p> <p>Rank: 54<br/>Tanimoto Combo = 0.89</p> <p>query : 4cox-ligD_9</p>  | <p>Shape Tanimoto = 0.741</p> | <p>Color Tanimoto = 0.149</p> | <p>2D Graph Tanimoto = 0.125</p> |



|                                                                                                      |                               |                               |                                  |
|------------------------------------------------------------------------------------------------------|-------------------------------|-------------------------------|----------------------------------|
| <p>Hit: database_166_48</p> <p>Rank: 55</p> <p>Tanimoto Combo = 0.889</p> <p>query : 4cox-ligD_8</p> | <p>Shape Tanimoto = 0.58</p>  | <p>Color Tanimoto = 0.309</p> | <p>2D Graph Tanimoto = 0.189</p> |
| <p>Hit: database_14_97</p> <p>Rank: 56</p> <p>Tanimoto Combo = 0.889</p> <p>query : 4cox-ligD_8</p>  | <p>Shape Tanimoto = 0.58</p>  | <p>Color Tanimoto = 0.309</p> | <p>2D Graph Tanimoto = 0.182</p> |
| <p>Hit: database_73_178</p> <p>Rank: 57</p> <p>Tanimoto Combo = 0.888</p> <p>query : 4cox-ligD_1</p> | <p>Shape Tanimoto = 0.628</p> | <p>Color Tanimoto = 0.26</p>  | <p>2D Graph Tanimoto = 0.126</p> |



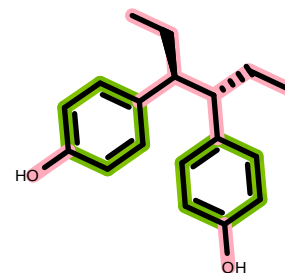
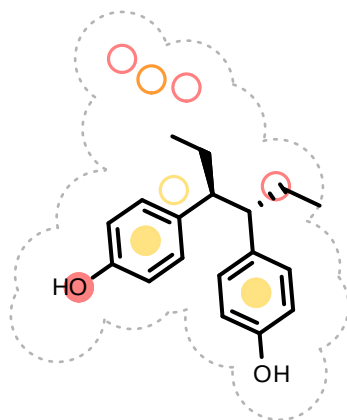
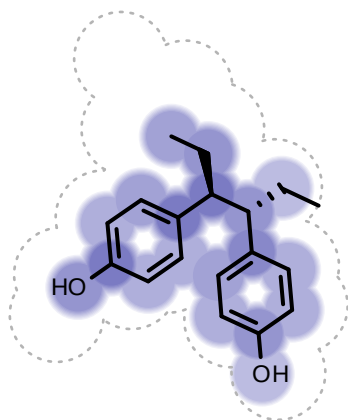
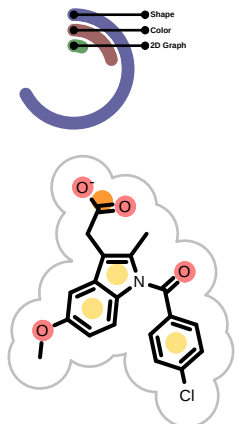
Hit: database\_137\_1

Shape Tanimoto = 0.673

Color Tanimoto = 0.211

2D Graph Tanimoto = 0.056

Rank: 58  
Tanimoto Combo = 0.884



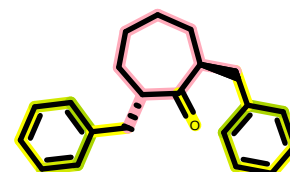
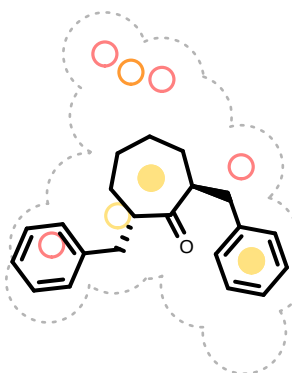
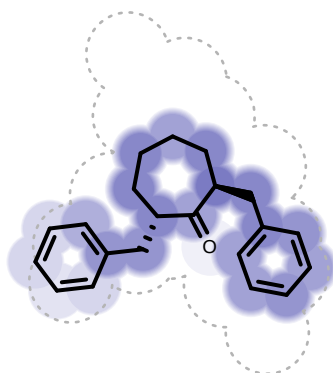
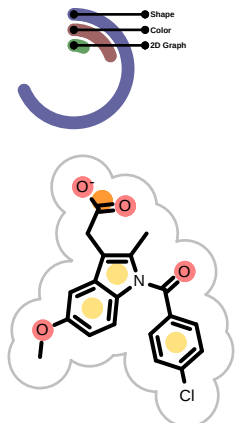
Hit: database\_4\_9

Shape Tanimoto = 0.685

Color Tanimoto = 0.197

2D Graph Tanimoto = 0.068

Rank: 59  
Tanimoto Combo = 0.882



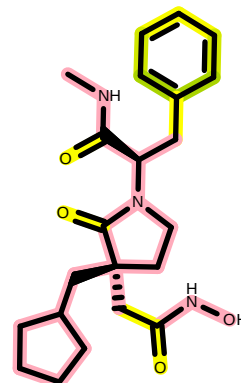
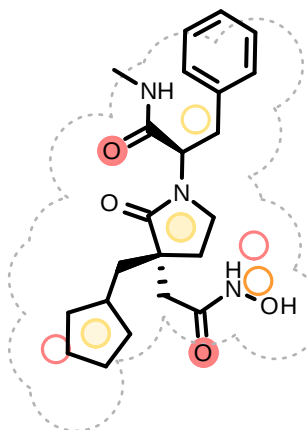
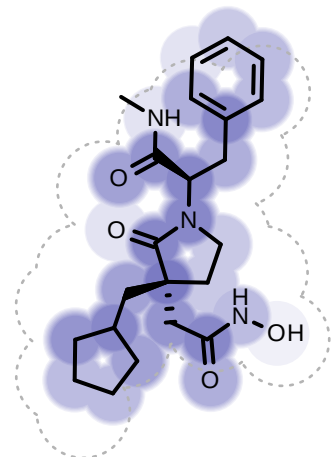
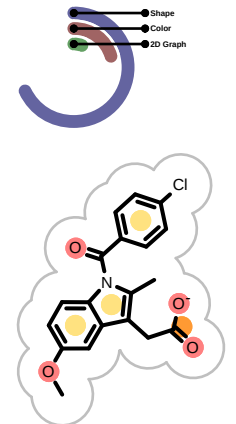
Hit: database\_63\_52

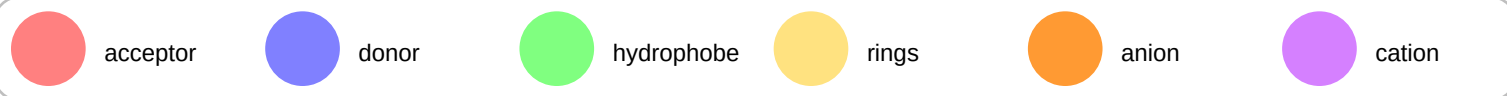
Shape Tanimoto = 0.678

Color Tanimoto = 0.204

2D Graph Tanimoto = 0.056

Rank: 60  
Tanimoto Combo = 0.882





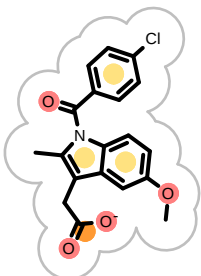
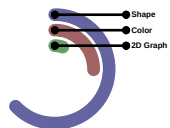
Hit: database\_135\_9

Shape Tanimoto = 0.629

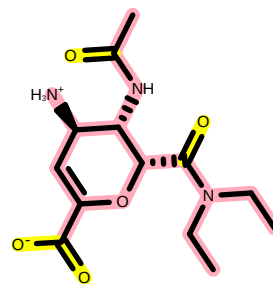
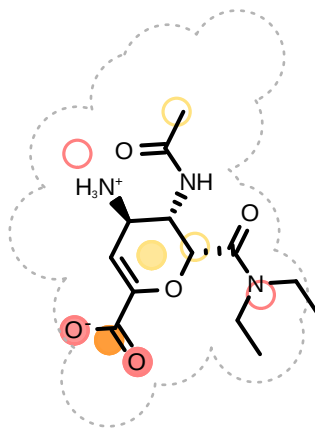
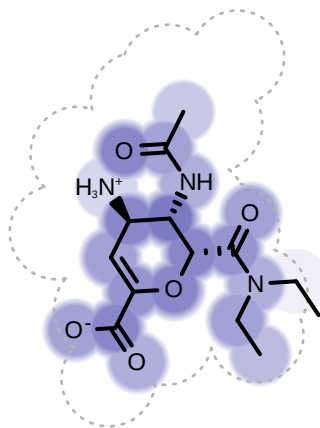
Color Tanimoto = 0.253

2D Graph Tanimoto = 0.055

Rank: 61  
Tanimoto Combo = 0.881



query : 4cox-ligD\_0



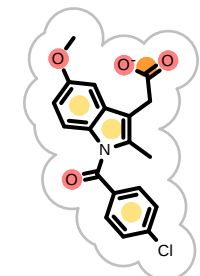
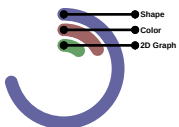
Hit: database\_54\_23

Shape Tanimoto = 0.71

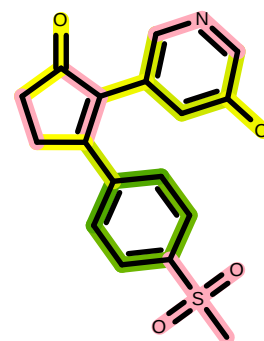
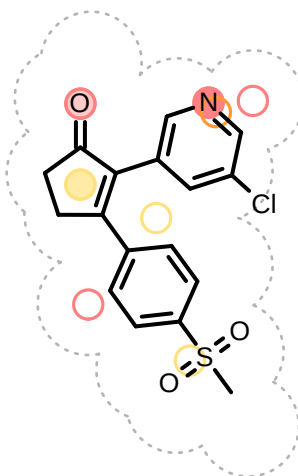
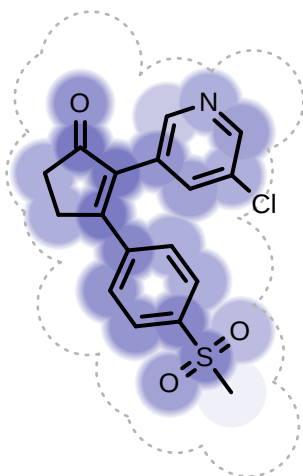
Color Tanimoto = 0.168

2D Graph Tanimoto = 0.110

Rank: 62  
Tanimoto Combo = 0.878



query : 4cox-ligD\_5



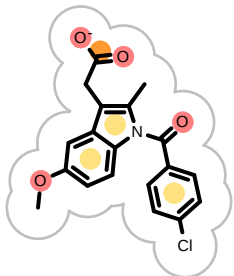
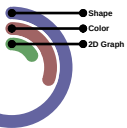
Hit: database\_36\_171

Shape Tanimoto = 0.576

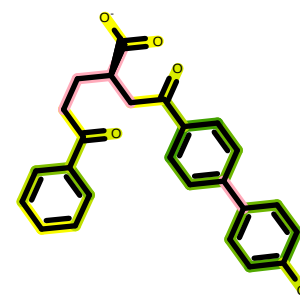
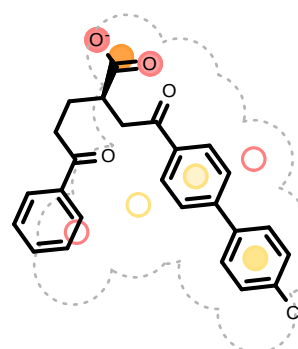
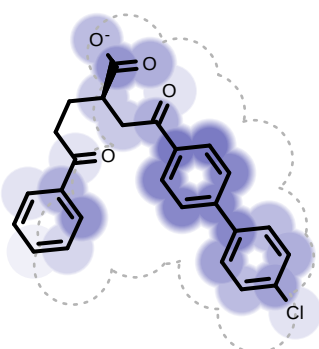
Color Tanimoto = 0.301

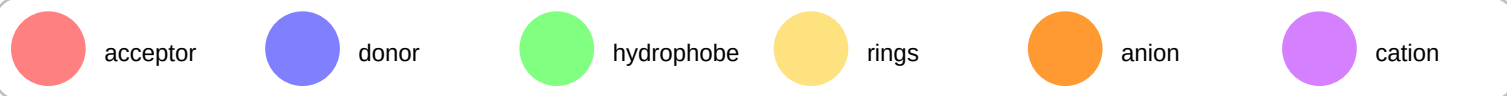
2D Graph Tanimoto = 0.165

Rank: 63  
Tanimoto Combo = 0.877



query : 4cox-ligD\_3





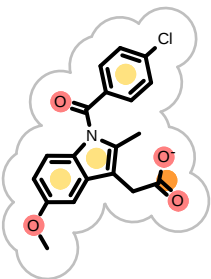
Hit: database\_181\_1

Shape Tanimoto = 0.653

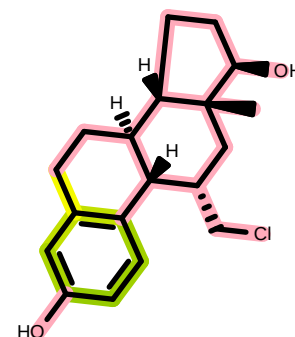
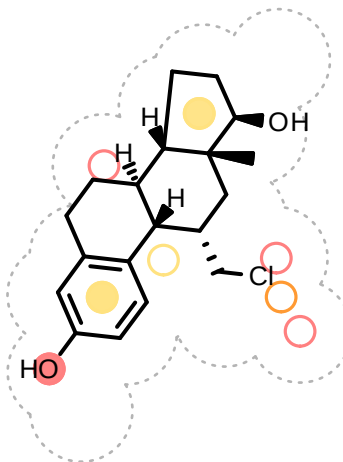
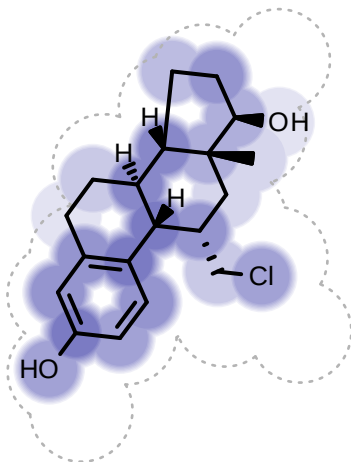
Color Tanimoto = 0.221

2D Graph Tanimoto = 0.089

Rank: 64  
Tanimoto Combo = 0.875



query : 4cox-ligD\_7



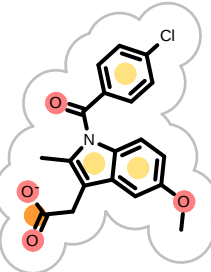
Hit: database\_55\_14

Shape Tanimoto = 0.667

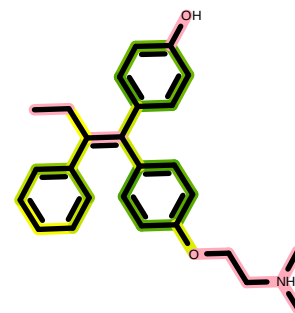
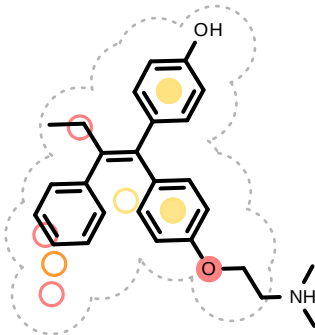
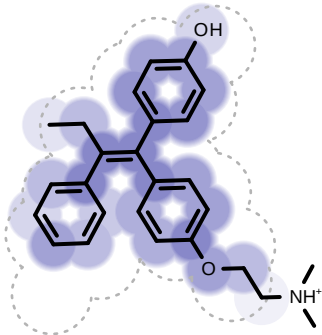
Color Tanimoto = 0.205

2D Graph Tanimoto = 0.126

Rank: 65  
Tanimoto Combo = 0.872



query : 4cox-ligD\_1



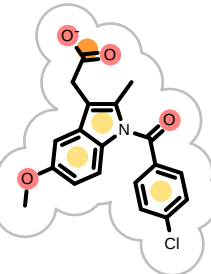
Hit: database\_81\_50

Shape Tanimoto = 0.61

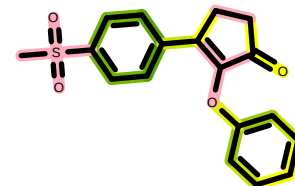
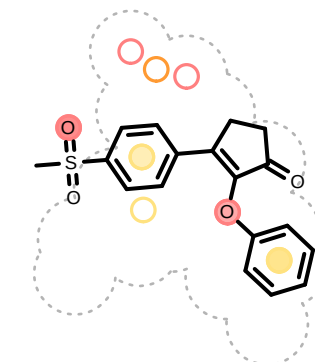
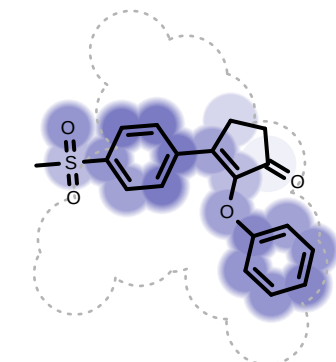
Color Tanimoto = 0.262

2D Graph Tanimoto = 0.123

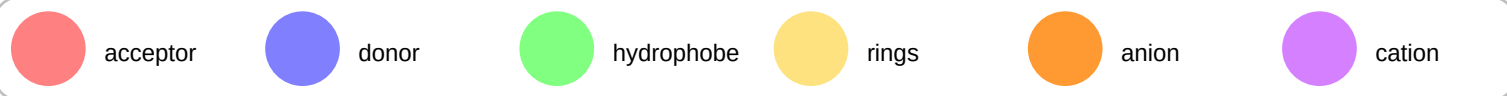
Rank: 66  
Tanimoto Combo = 0.872



query : 4cox-ligD\_8







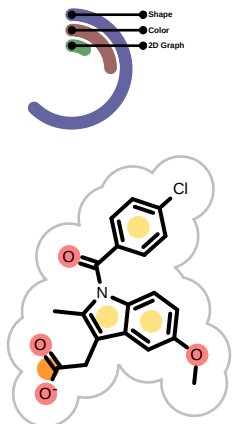
Hit: database\_76\_30

Shape Tanimoto = 0.622

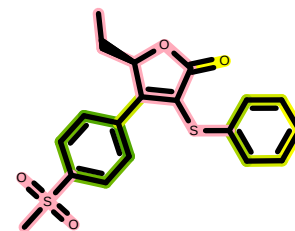
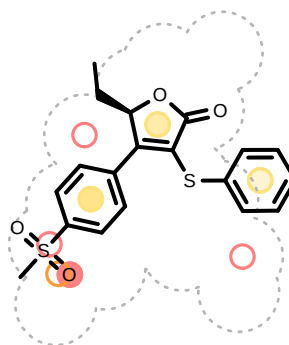
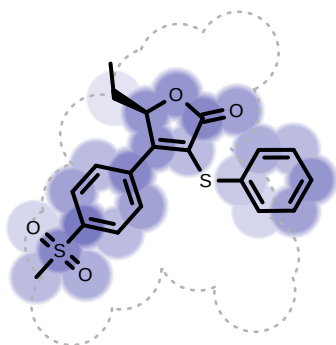
Color Tanimoto = 0.245

2D Graph Tanimoto = 0.093

Rank: 67  
Tanimoto Combo = 0.868



query : 4cox-ligD\_4



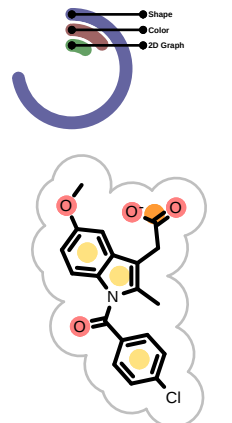
Hit: database\_203\_0

Shape Tanimoto = 0.722

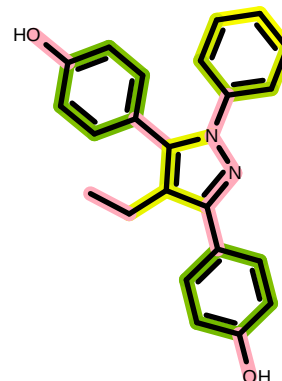
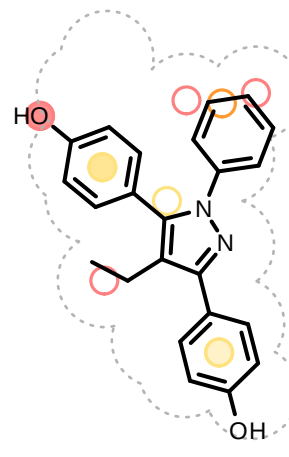
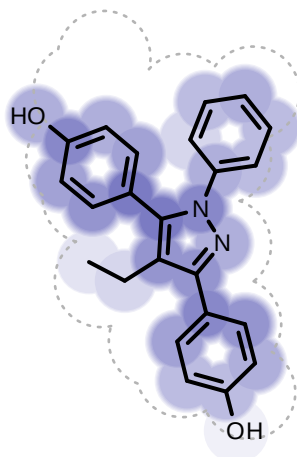
Color Tanimoto = 0.142

2D Graph Tanimoto = 0.099

Rank: 68  
Tanimoto Combo = 0.865



query : 4cox-ligD\_5



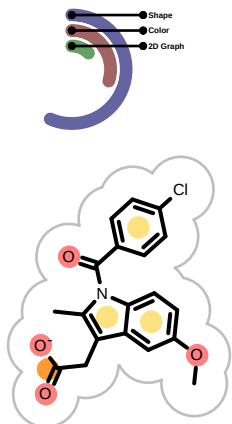
Hit: database\_143\_57

Shape Tanimoto = 0.565

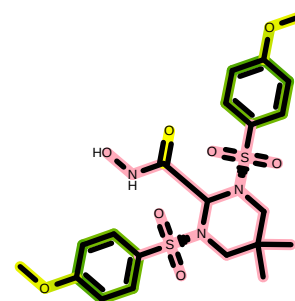
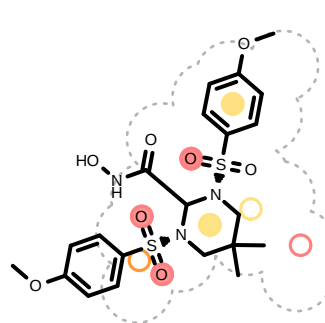
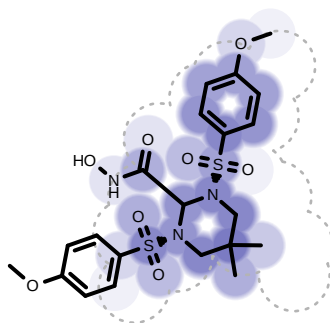
Color Tanimoto = 0.299

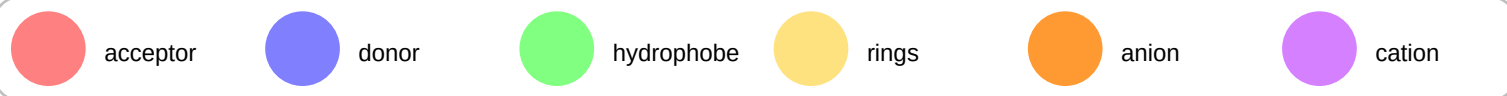
2D Graph Tanimoto = 0.126

Rank: 69  
Tanimoto Combo = 0.864

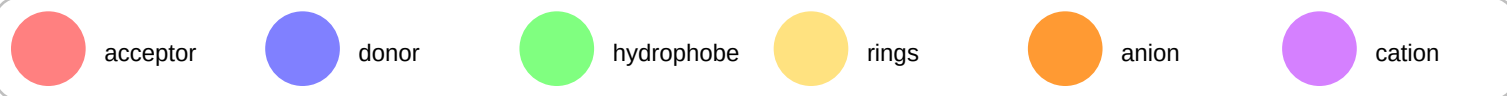


query : 4cox-ligD\_6





|                                                                                                      |                               |                               |                                  |
|------------------------------------------------------------------------------------------------------|-------------------------------|-------------------------------|----------------------------------|
| <p>Hit: database_24_114</p> <p>Rank: 70</p> <p>Tanimoto Combo = 0.861</p> <p>query : 4cox-ligD_9</p> | <p>Shape Tanimoto = 0.53</p>  | <p>Color Tanimoto = 0.331</p> | <p>2D Graph Tanimoto = 0.179</p> |
| <p>Hit: database_195_18</p> <p>Rank: 71</p> <p>Tanimoto Combo = 0.861</p> <p>query : 4cox-ligD_8</p> | <p>Shape Tanimoto = 0.552</p> | <p>Color Tanimoto = 0.309</p> | <p>2D Graph Tanimoto = 0.198</p> |
| <p>Hit: database_109_9</p> <p>Rank: 72</p> <p>Tanimoto Combo = 0.858</p> <p>query : 4cox-ligD_3</p>  | <p>Shape Tanimoto = 0.646</p> | <p>Color Tanimoto = 0.212</p> | <p>2D Graph Tanimoto = 0.118</p> |



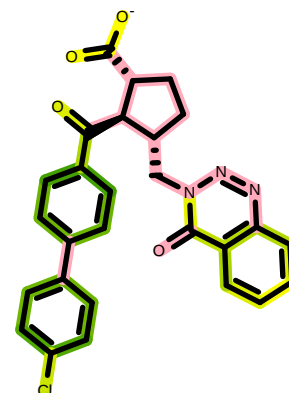
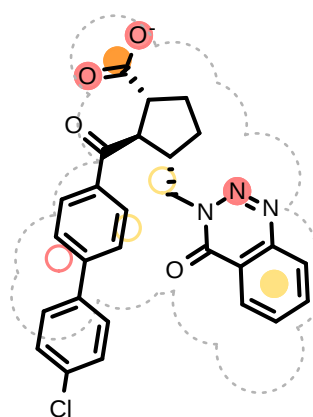
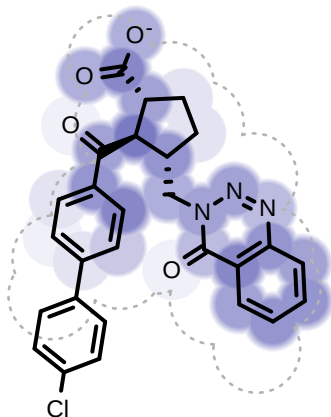
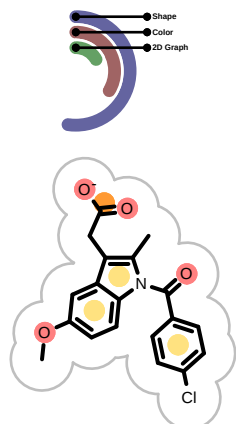
Hit: database\_28\_20

Shape Tanimoto = 0.523

Color Tanimoto = 0.335

2D Graph Tanimoto = 0.168

Rank: 73  
Tanimoto Combo = 0.858



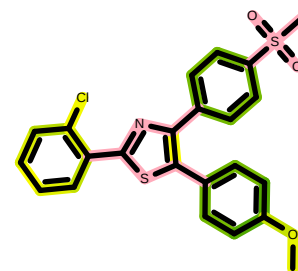
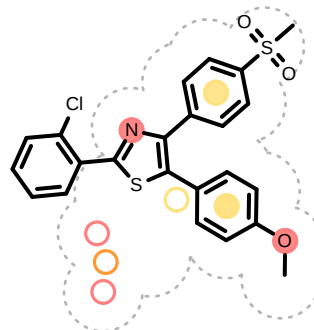
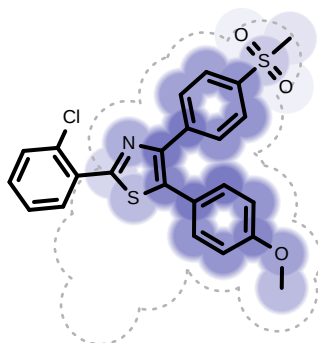
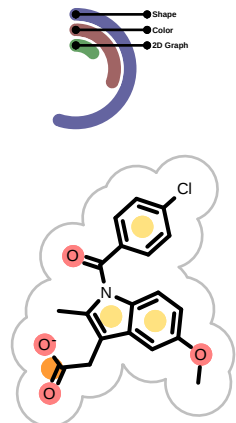
Hit: database\_152\_40

Shape Tanimoto = 0.55

Color Tanimoto = 0.306

2D Graph Tanimoto = 0.132

Rank: 74  
Tanimoto Combo = 0.856



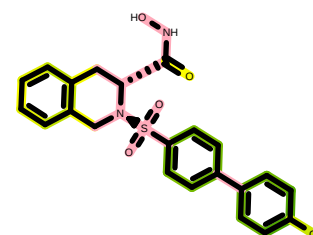
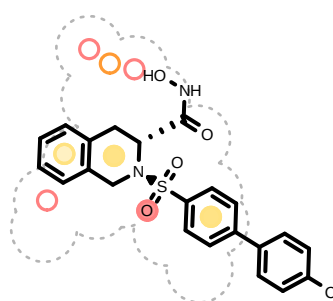
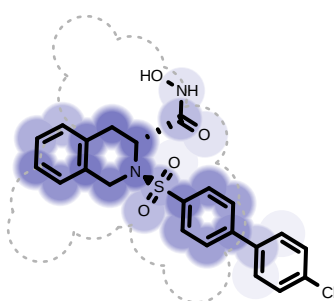
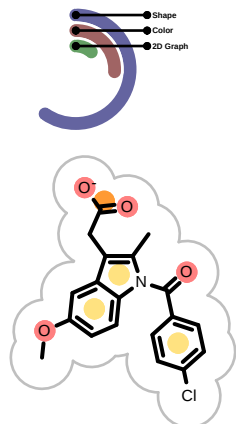
Hit: database\_17\_7

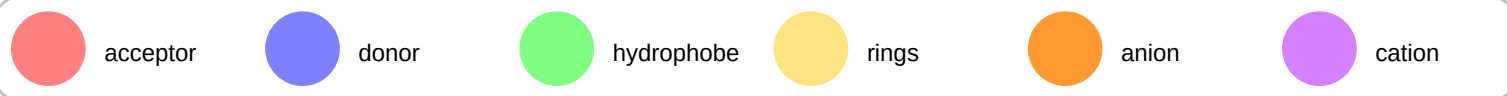
Shape Tanimoto = 0.596

Color Tanimoto = 0.26

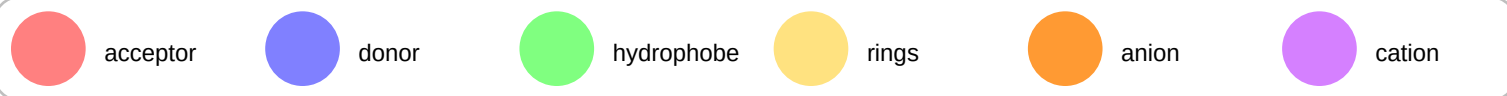
2D Graph Tanimoto = 0.116

Rank: 75  
Tanimoto Combo = 0.856





|                                                                                                      |                               |                               |                                  |
|------------------------------------------------------------------------------------------------------|-------------------------------|-------------------------------|----------------------------------|
| <p>Hit: database_35_147</p> <p>Rank: 76</p> <p>Tanimoto Combo = 0.856</p> <p>query : 4cox-ligD_0</p> | <p>Shape Tanimoto = 0.582</p> | <p>Color Tanimoto = 0.274</p> | <p>2D Graph Tanimoto = 0.201</p> |
| <p>Hit: database_122</p> <p>Rank: 77</p> <p>Tanimoto Combo = 0.851</p> <p>query : 4cox-ligD_1</p>    | <p>Shape Tanimoto = 0.551</p> | <p>Color Tanimoto = 0.301</p> | <p>2D Graph Tanimoto = 0.176</p> |
| <p>Hit: database_111_1</p> <p>Rank: 78</p> <p>Tanimoto Combo = 0.85</p> <p>query : 4cox-ligD_7</p>   | <p>Shape Tanimoto = 0.622</p> | <p>Color Tanimoto = 0.229</p> | <p>2D Graph Tanimoto = 0.102</p> |



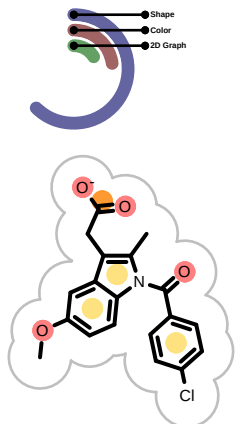
Hit: database\_10\_58

Shape Tanimoto = 0.622

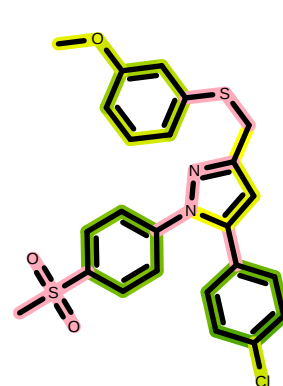
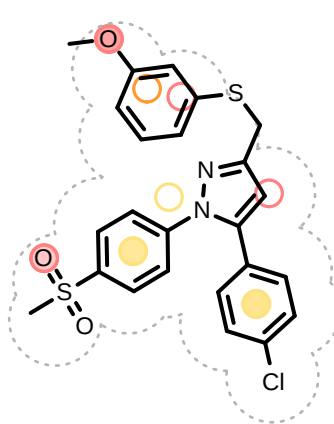
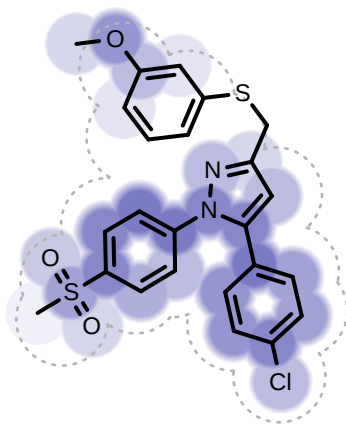
Color Tanimoto = 0.227

2D Graph Tanimoto = 0.162

Rank: 79  
Tanimoto Combo = 0.849



query : 4cox-ligD\_3



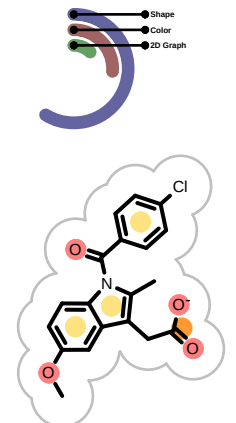
Hit: database\_5\_73

Shape Tanimoto = 0.587

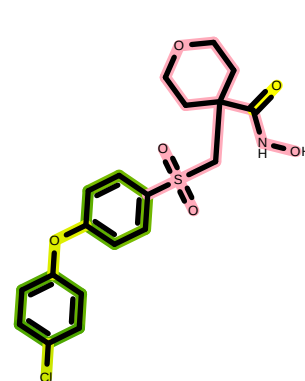
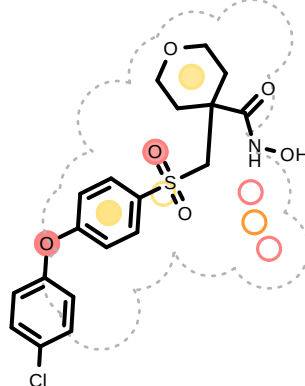
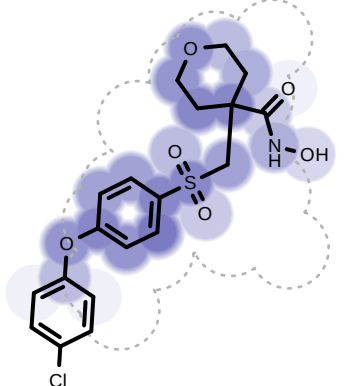
Color Tanimoto = 0.261

2D Graph Tanimoto = 0.124

Rank: 80  
Tanimoto Combo = 0.847



query : 4cox-ligD\_7



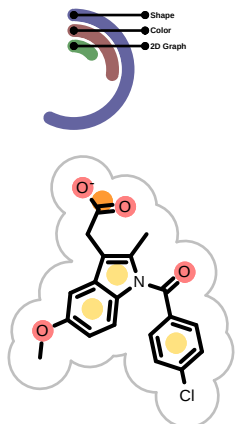
Hit: database\_94\_42

Shape Tanimoto = 0.573

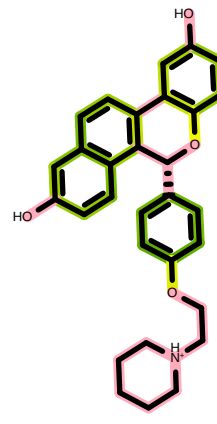
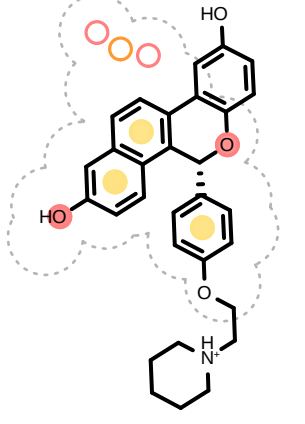
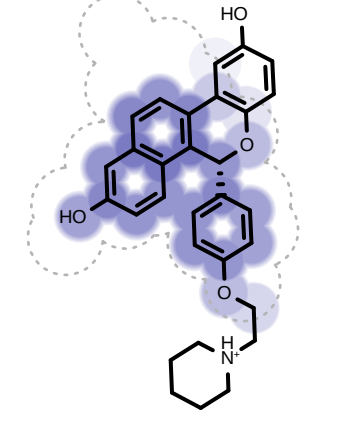
Color Tanimoto = 0.272

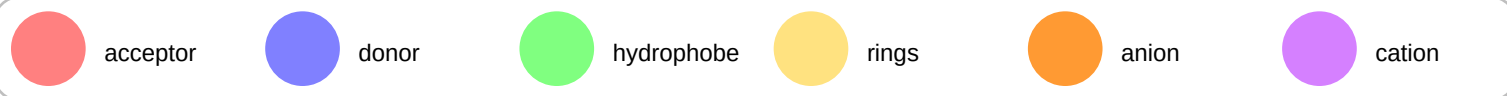
2D Graph Tanimoto = 0.139

Rank: 81  
Tanimoto Combo = 0.844



query : 4cox-ligD\_8





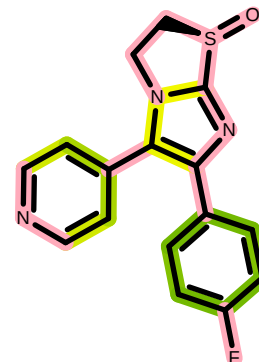
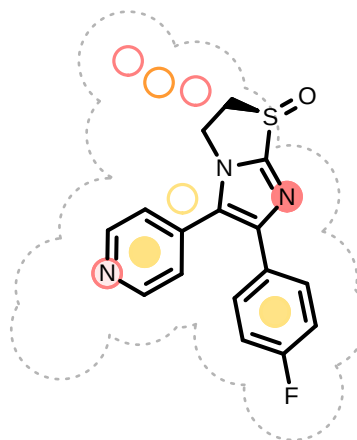
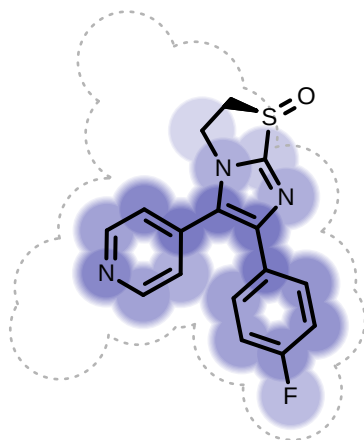
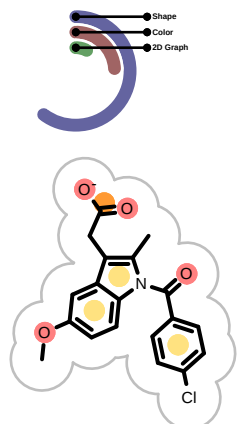
Hit: database\_112\_1

Shape Tanimoto = 0.601

Color Tanimoto = 0.24

2D Graph Tanimoto = 0.077

Rank: 82  
Tanimoto Combo = 0.841



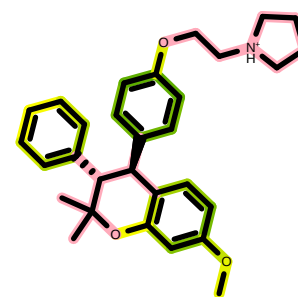
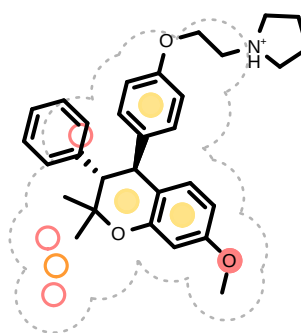
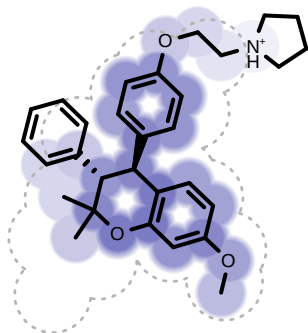
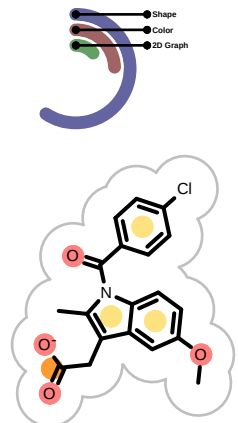
Hit: database\_12\_52

Shape Tanimoto = 0.593

Color Tanimoto = 0.244

2D Graph Tanimoto = 0.134

Rank: 83  
Tanimoto Combo = 0.837



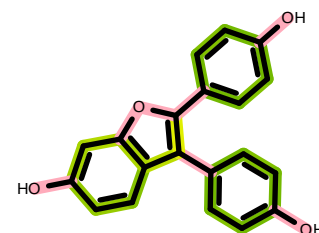
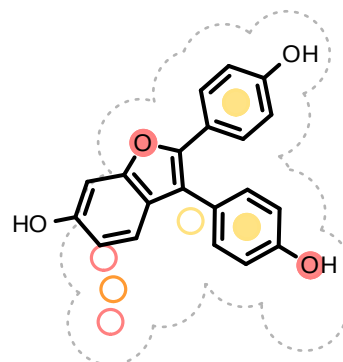
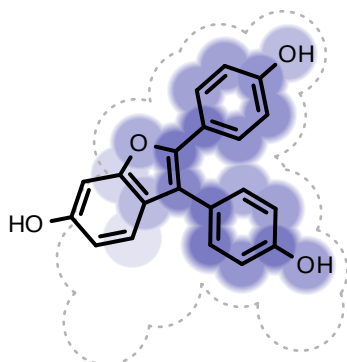
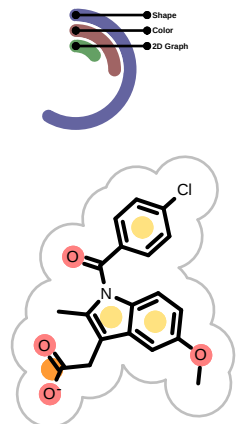
Hit: database\_157\_0

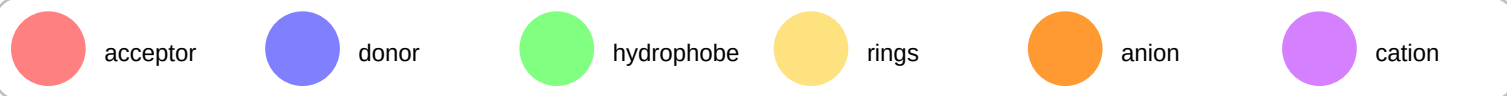
Shape Tanimoto = 0.584

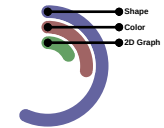
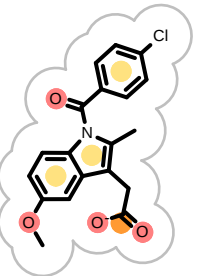
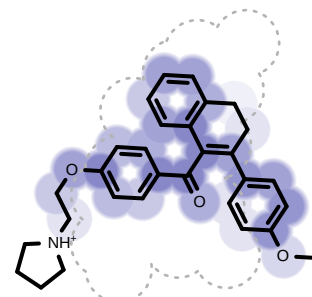
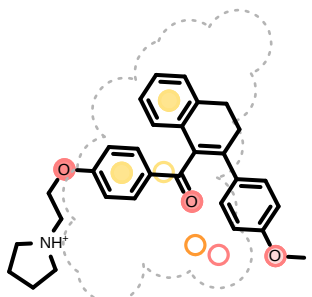
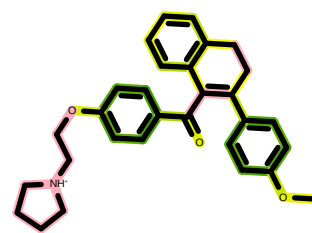
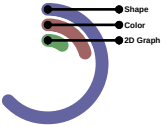
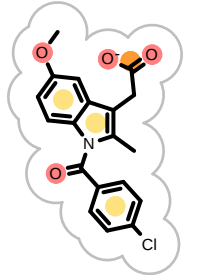
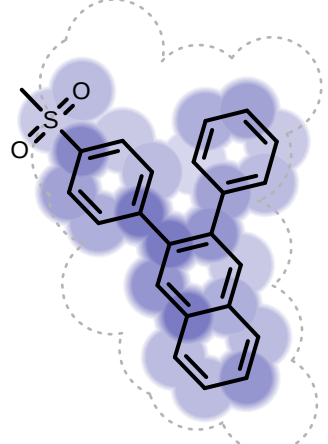
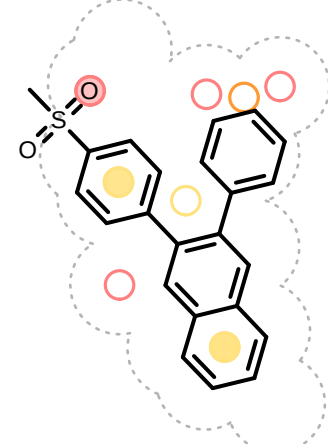
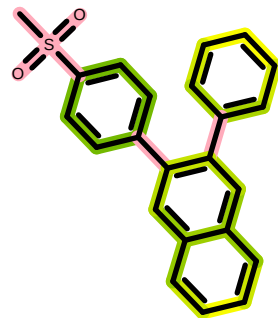
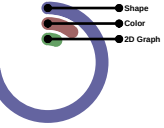
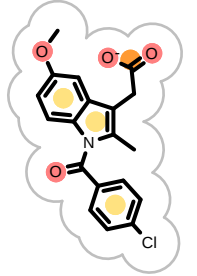
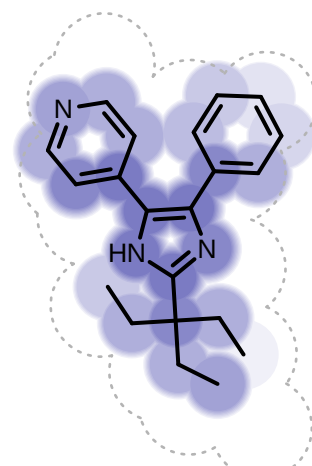
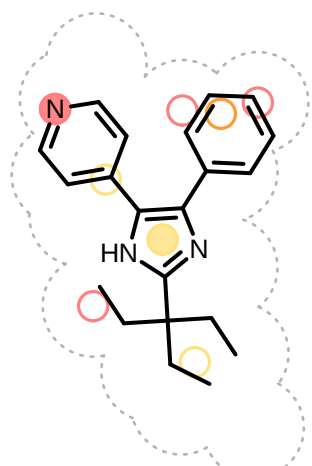
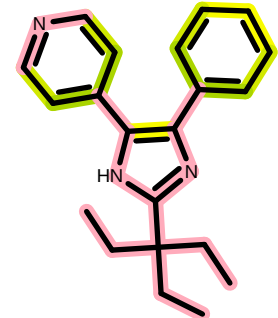
Color Tanimoto = 0.253

2D Graph Tanimoto = 0.148

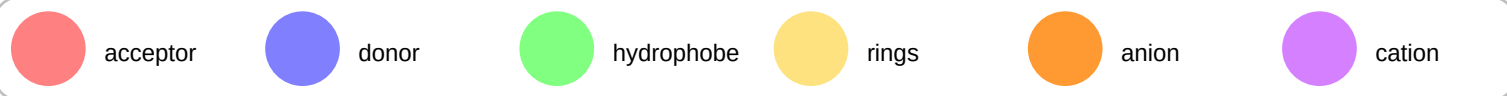
Rank: 84  
Tanimoto Combo = 0.837





|                                                                                                                                                                                                                                                                            |                                                                                                                   |                                                                                                                    |                                                                                                                        |
|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------|
| <p>Hit: database_69_125</p> <p>Rank: 85</p> <p>Tanimoto Combo = 0.837</p>   <p>query : 4cox-ligD_9</p>     | <p>Shape Tanimoto = 0.567</p>    | <p>Color Tanimoto = 0.27</p>     | <p>2D Graph Tanimoto = 0.175</p>    |
| <p>Hit: database_210_1</p> <p>Rank: 86</p> <p>Tanimoto Combo = 0.836</p>   <p>query : 4cox-ligD_5</p>   | <p>Shape Tanimoto = 0.63</p>    | <p>Color Tanimoto = 0.206</p>   | <p>2D Graph Tanimoto = 0.106</p>   |
| <p>Hit: database_150_17</p> <p>Rank: 87</p> <p>Tanimoto Combo = 0.833</p>   <p>query : 4cox-ligD_5</p> | <p>Shape Tanimoto = 0.726</p>  | <p>Color Tanimoto = 0.107</p>  | <p>2D Graph Tanimoto = 0.057</p>  |





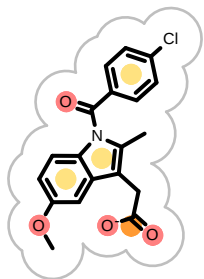
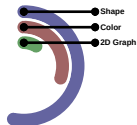
Hit: database\_100\_4

Shape Tanimoto = 0.531

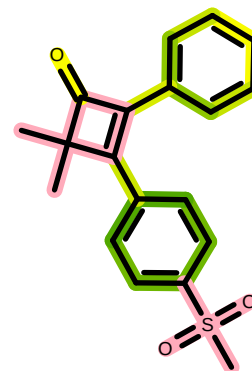
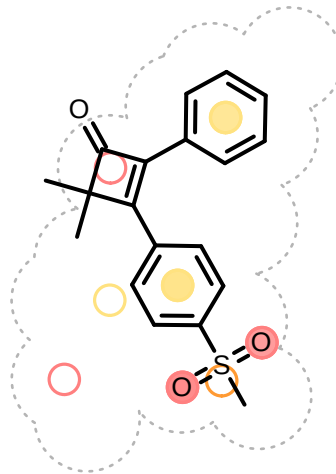
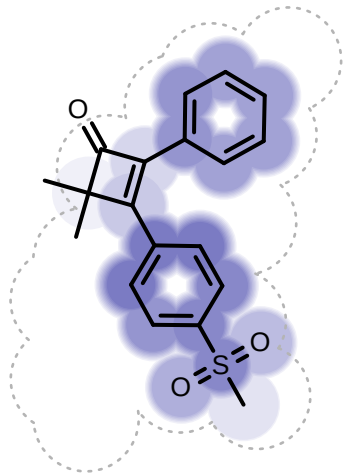
Color Tanimoto = 0.301

2D Graph Tanimoto = 0.088

Rank: 88  
Tanimoto Combo = 0.832



query : 4cox-ligD\_9



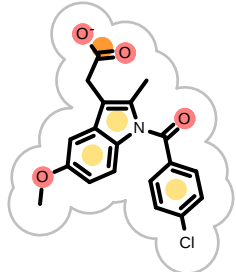
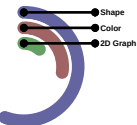
Hit: database\_34\_163

Shape Tanimoto = 0.557

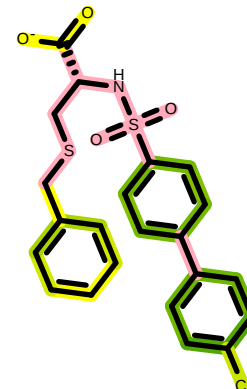
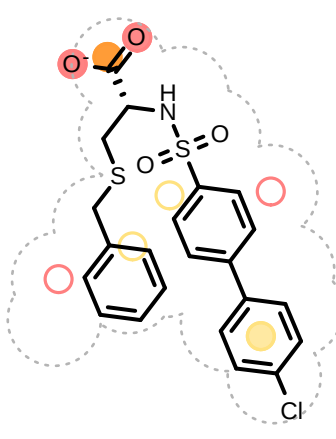
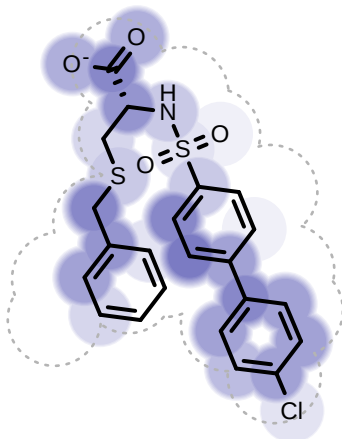
Color Tanimoto = 0.274

2D Graph Tanimoto = 0.117

Rank: 89  
Tanimoto Combo = 0.83



query : 4cox-ligD\_2



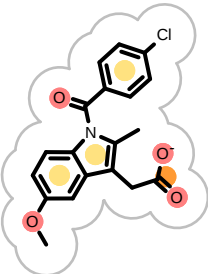
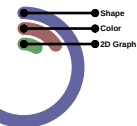
Hit: database\_47\_3

Shape Tanimoto = 0.675

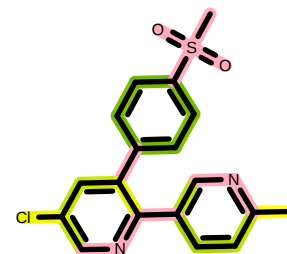
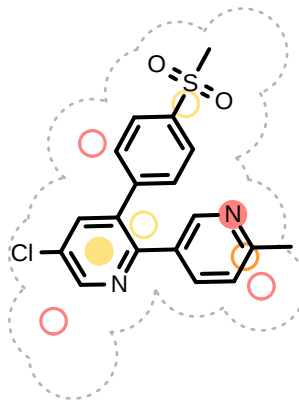
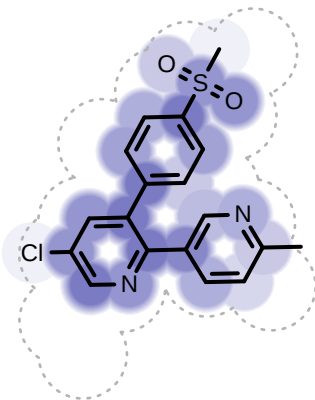
Color Tanimoto = 0.154

2D Graph Tanimoto = 0.090

Rank: 90  
Tanimoto Combo = 0.83

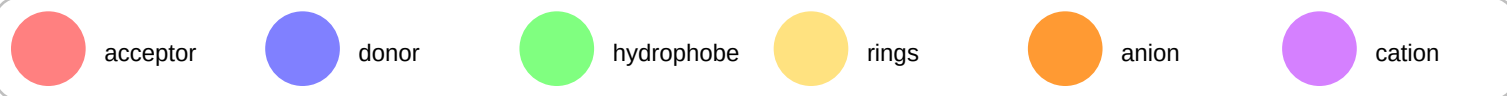


query : 4cox-ligD\_7





|                                                                                                       |                               |                               |                                  |
|-------------------------------------------------------------------------------------------------------|-------------------------------|-------------------------------|----------------------------------|
| <p>Hit: database_201_11</p> <p>Rank: 91</p> <p>Tanimoto Combo = 0.828</p> <p>query : 4cox-ligD_5</p>  | <p>Shape Tanimoto = 0.718</p> | <p>Color Tanimoto = 0.11</p>  | <p>2D Graph Tanimoto = 0.075</p> |
| <p>Hit: database_125_116</p> <p>Rank: 92</p> <p>Tanimoto Combo = 0.828</p> <p>query : 4cox-ligD_5</p> | <p>Shape Tanimoto = 0.607</p> | <p>Color Tanimoto = 0.221</p> | <p>2D Graph Tanimoto = 0.037</p> |
| <p>Hit: database_23_2</p> <p>Rank: 93</p> <p>Tanimoto Combo = 0.827</p> <p>query : 4cox-ligD_0</p>    | <p>Shape Tanimoto = 0.594</p> | <p>Color Tanimoto = 0.233</p> | <p>2D Graph Tanimoto = 0.067</p> |



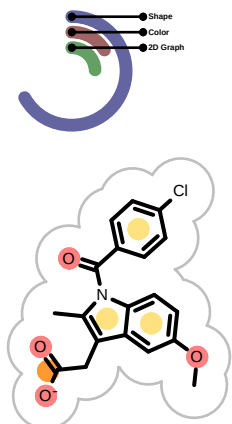
Hit: database\_30\_90

Shape Tanimoto = 0.668

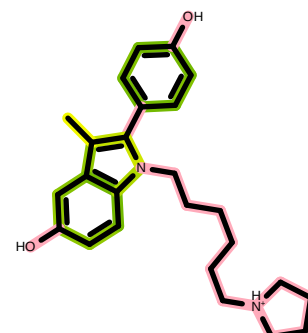
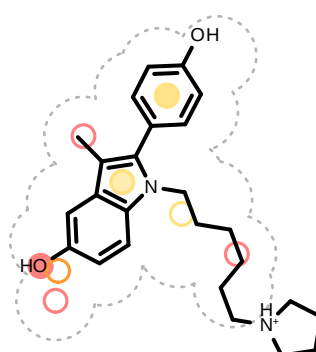
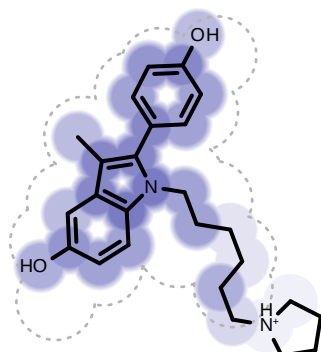
Color Tanimoto = 0.159

2D Graph Tanimoto = 0.242

Rank: 94  
Tanimoto Combo = 0.826



query : 4cox-ligD\_4



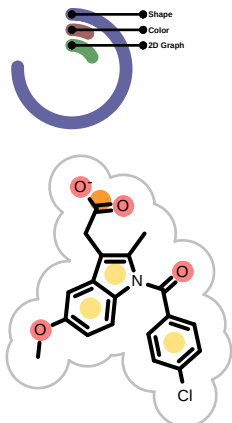
Hit: database\_83\_16

Shape Tanimoto = 0.755

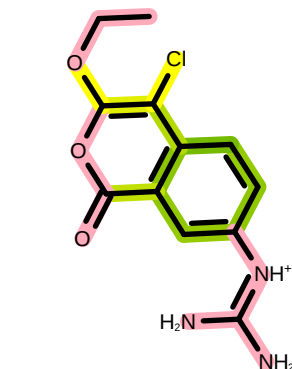
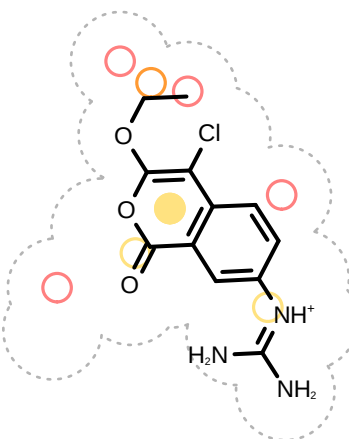
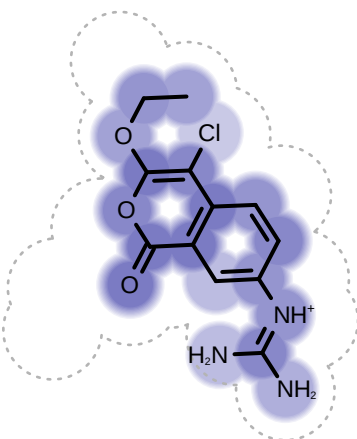
Color Tanimoto = 0.068

2D Graph Tanimoto = 0.169

Rank: 95  
Tanimoto Combo = 0.823



query : 4cox-ligD\_3



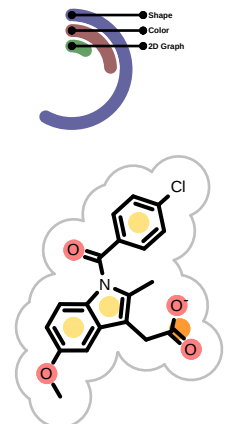
Hit: database\_75\_69

Shape Tanimoto = 0.58

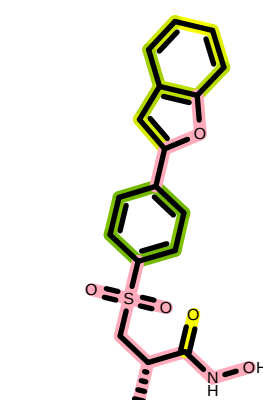
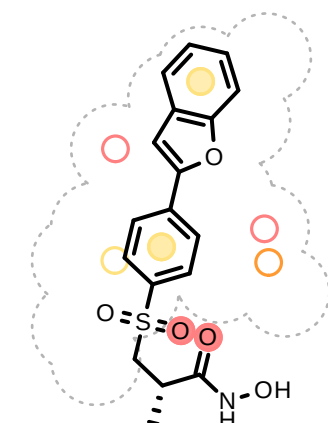
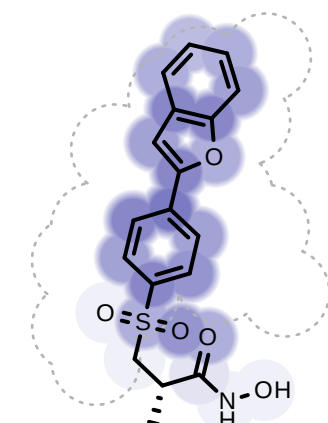
Color Tanimoto = 0.242

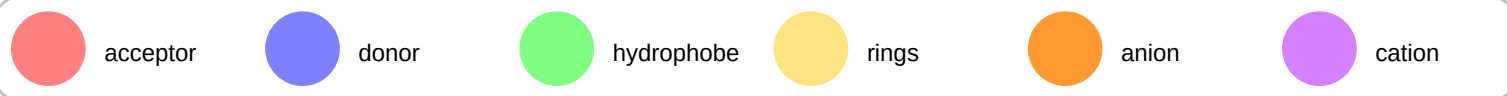
2D Graph Tanimoto = 0.100

Rank: 96  
Tanimoto Combo = 0.822

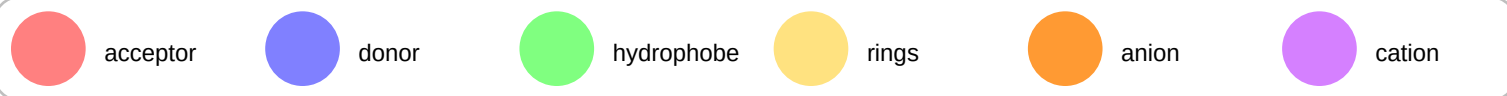


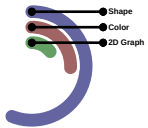
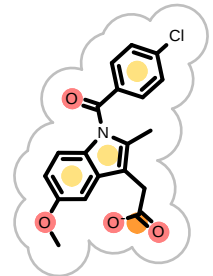
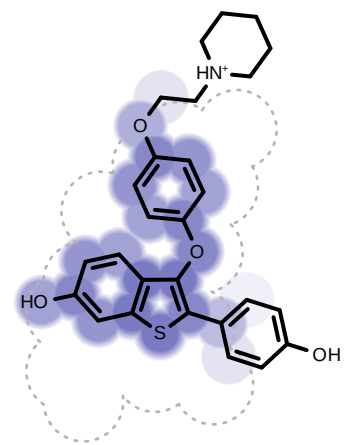
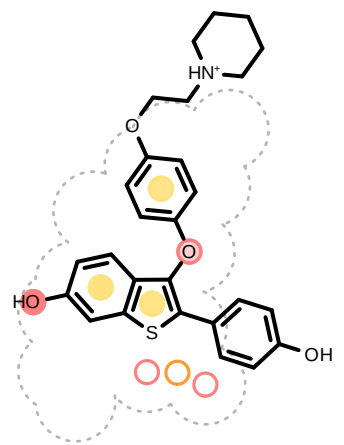
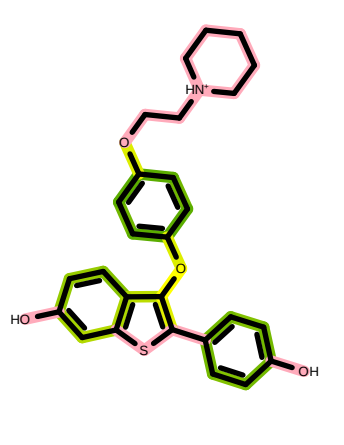
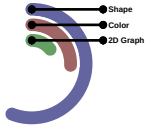
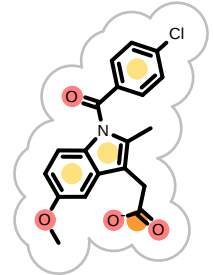
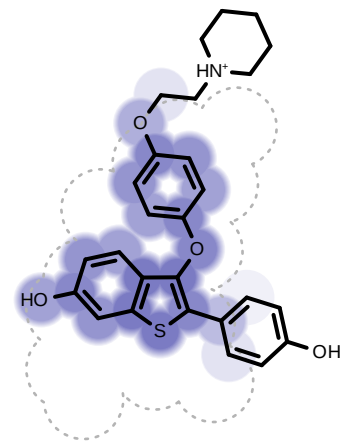
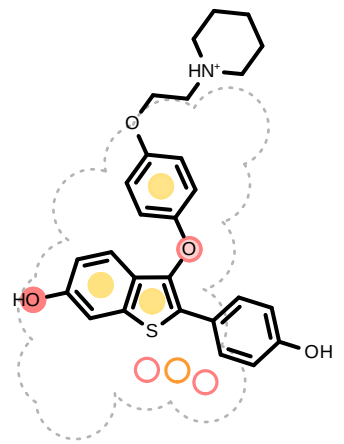
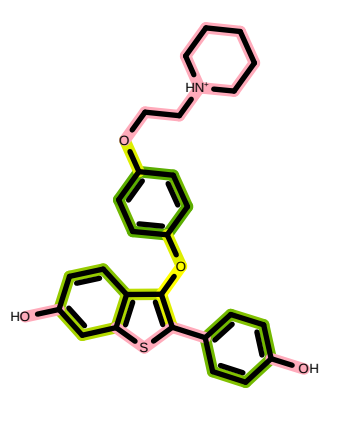
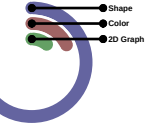
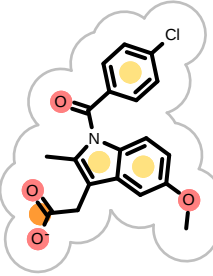
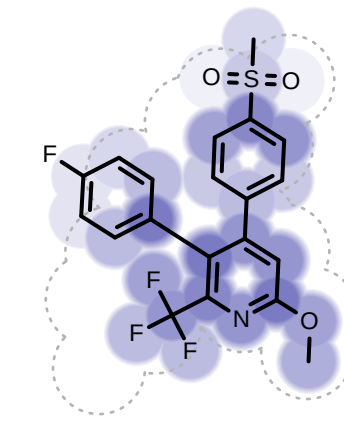
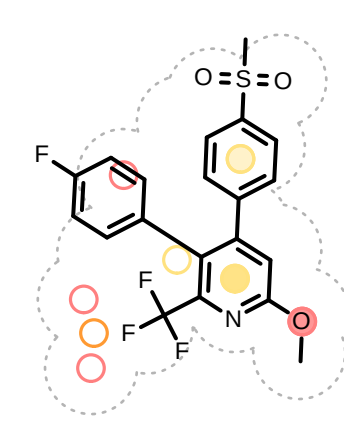
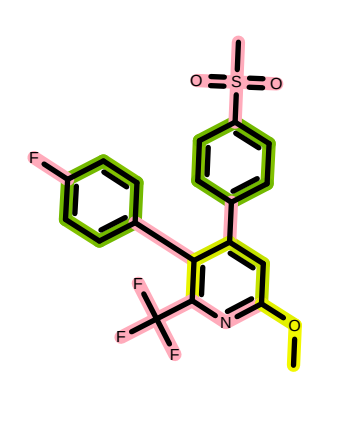
query : 4cox-ligD\_7

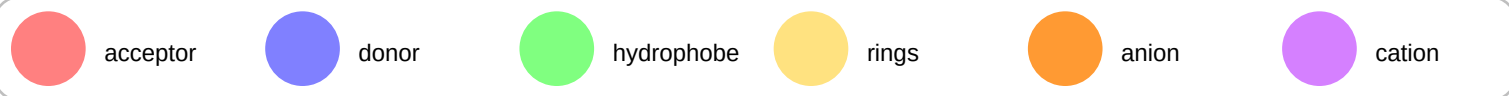


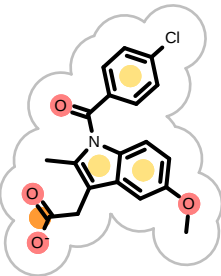
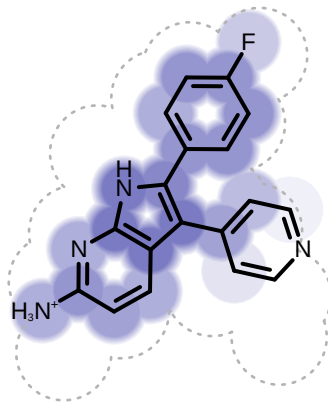
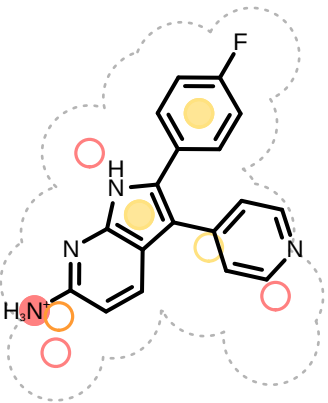
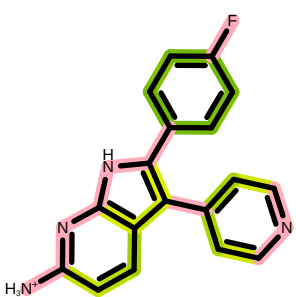
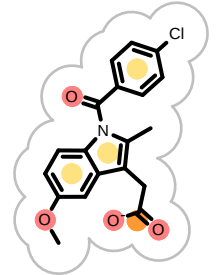
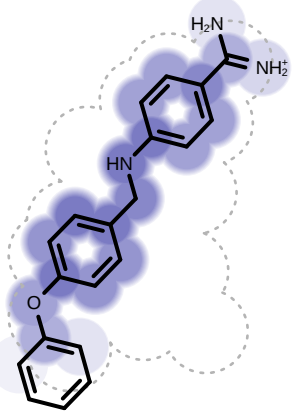
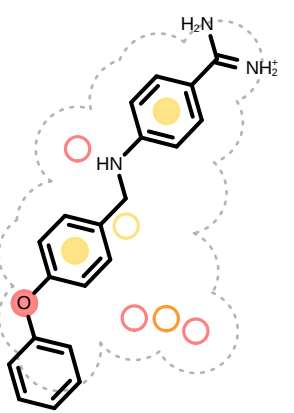
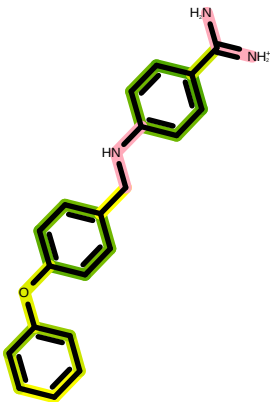
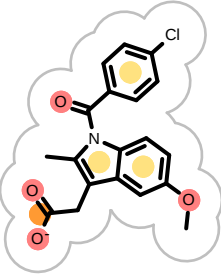
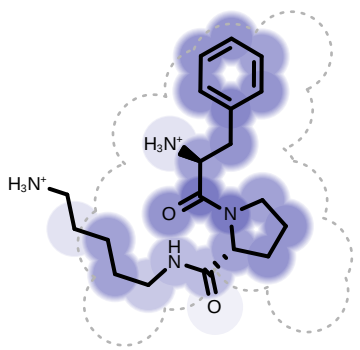
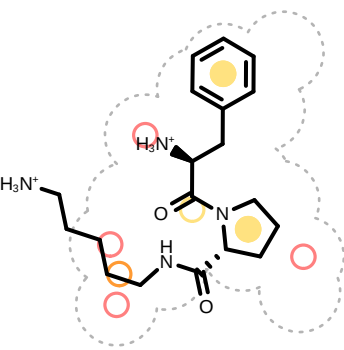
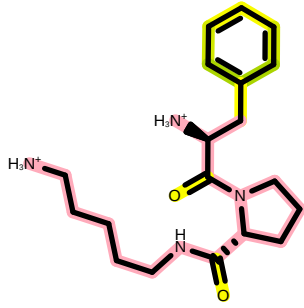


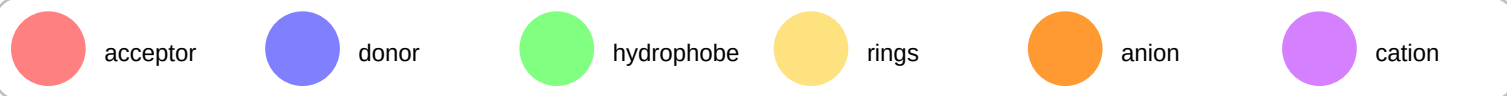
|                                                                                                     |                               |                               |                                  |
|-----------------------------------------------------------------------------------------------------|-------------------------------|-------------------------------|----------------------------------|
| <p>Hit: database_164_78</p> <p>Rank: 97</p> <p>Tanimoto Combo = 0.82</p> <p>query : 4cox-ligD_8</p> | <p>Shape Tanimoto = 0.56</p>  | <p>Color Tanimoto = 0.261</p> | <p>2D Graph Tanimoto = 0.131</p> |
| <p>Hit: database_46_2</p> <p>Rank: 98</p> <p>Tanimoto Combo = 0.819</p> <p>query : 4cox-ligD_3</p>  | <p>Shape Tanimoto = 0.66</p>  | <p>Color Tanimoto = 0.159</p> | <p>2D Graph Tanimoto = 0.084</p> |
| <p>Hit: database_67_58</p> <p>Rank: 99</p> <p>Tanimoto Combo = 0.818</p> <p>query : 4cox-ligD_9</p> | <p>Shape Tanimoto = 0.647</p> | <p>Color Tanimoto = 0.171</p> | <p>2D Graph Tanimoto = 0.055</p> |



|                                                                                                                                                                                                                                                                              |                                                                                                                  |                                                                                                                    |                                                                                                                        |
|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------|
| <p>Hit: database_136_115</p> <p>Rank: 100</p> <p>Tanimoto Combo = 0.817</p>   <p>query : 4cox-ligD_9</p>    | <p>Shape Tanimoto = 0.56</p>    | <p>Color Tanimoto = 0.257</p>    | <p>2D Graph Tanimoto = 0.144</p>    |
| <p>Hit: database_194_115</p> <p>Rank: 101</p> <p>Tanimoto Combo = 0.817</p>   <p>query : 4cox-ligD_9</p> | <p>Shape Tanimoto = 0.56</p>   | <p>Color Tanimoto = 0.257</p>   | <p>2D Graph Tanimoto = 0.144</p>   |
| <p>Hit: database_131_1</p> <p>Rank: 102</p> <p>Tanimoto Combo = 0.816</p>   <p>query : 4cox-ligD_4</p>  | <p>Shape Tanimoto = 0.64</p>  | <p>Color Tanimoto = 0.176</p>  | <p>2D Graph Tanimoto = 0.110</p>  |

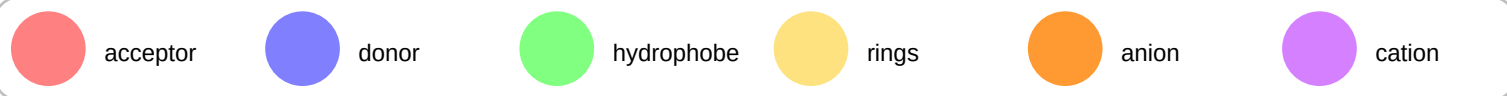


|                                                                                                                                                                                                                                                                                   |                                                                                                                          |                                                                                                                           |                                                                                                                               |
|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------|
| <p><b>Hit: database_104_1</b></p> <p>Rank: 103<br/>Tanimoto Combo = 0.816</p>   <p>query : 4cox-ligD_4</p>       | <p><b>Shape Tanimoto = 0.625</b></p>    | <p><b>Color Tanimoto = 0.191</b></p>    | <p><b>2D Graph Tanimoto = 0.102</b></p>    |
| <p><b>Hit: database_113_127</b></p> <p>Rank: 104<br/>Tanimoto Combo = 0.813</p>   <p>query : 4cox-ligD_9</p>   | <p><b>Shape Tanimoto = 0.6</b></p>     | <p><b>Color Tanimoto = 0.213</b></p>   | <p><b>2D Graph Tanimoto = 0.126</b></p>   |
| <p><b>Hit: database_176_163</b></p> <p>Rank: 105<br/>Tanimoto Combo = 0.812</p>   <p>query : 4cox-ligD_4</p> | <p><b>Shape Tanimoto = 0.678</b></p>  | <p><b>Color Tanimoto = 0.134</b></p>  | <p><b>2D Graph Tanimoto = 0.071</b></p>  |



|                                                                                                        |                               |                               |                                  |
|--------------------------------------------------------------------------------------------------------|-------------------------------|-------------------------------|----------------------------------|
| <p>Hit: database_156_166</p> <p>Rank: 106</p> <p>Tanimoto Combo = 0.811</p> <p>query : 4cox-ligD_7</p> | <p>Shape Tanimoto = 0.627</p> | <p>Color Tanimoto = 0.185</p> | <p>2D Graph Tanimoto = 0.078</p> |
| <p>Hit: database_96_132</p> <p>Rank: 107</p> <p>Tanimoto Combo = 0.811</p> <p>query : 4cox-ligD_6</p>  | <p>Shape Tanimoto = 0.563</p> | <p>Color Tanimoto = 0.248</p> | <p>2D Graph Tanimoto = 0.178</p> |
| <p>Hit: database_117_58</p> <p>Rank: 108</p> <p>Tanimoto Combo = 0.807</p> <p>query : 4cox-ligD_9</p>  | <p>Shape Tanimoto = 0.557</p> | <p>Color Tanimoto = 0.25</p>  | <p>2D Graph Tanimoto = 0.094</p> |





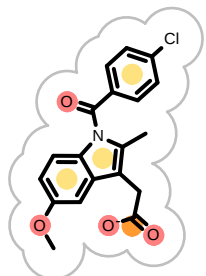
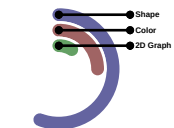
Hit: database\_33\_58

Shape Tanimoto = 0.557

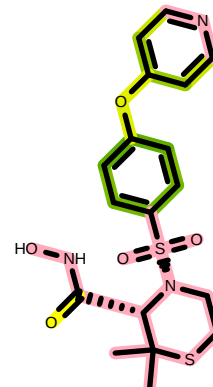
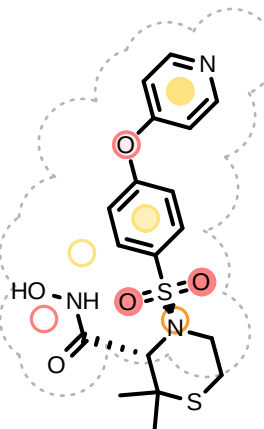
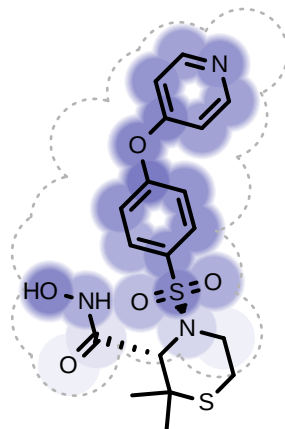
Color Tanimoto = 0.25

2D Graph Tanimoto = 0.094

Rank: 109  
Tanimoto Combo = 0.807



query : 4cox-ligD\_9



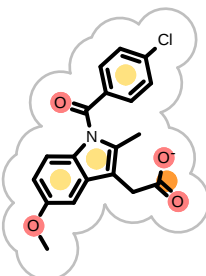
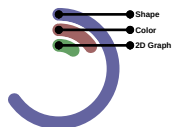
Hit: database\_22\_50

Shape Tanimoto = 0.653

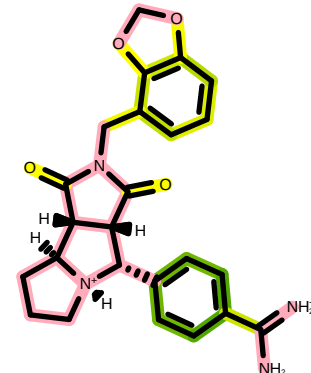
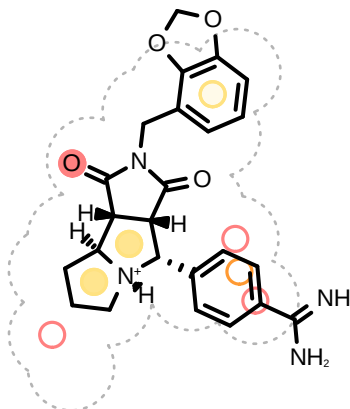
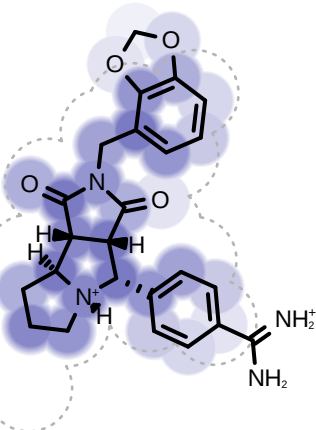
Color Tanimoto = 0.154

2D Graph Tanimoto = 0.106

Rank: 110  
Tanimoto Combo = 0.807



query : 4cox-ligD\_7



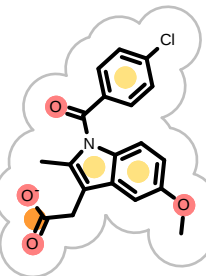
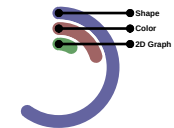
Hit: database\_13\_197

Shape Tanimoto = 0.599

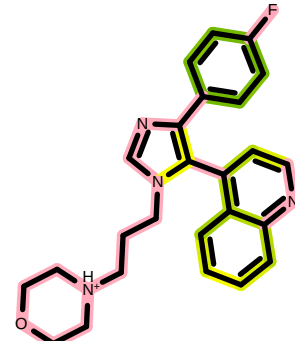
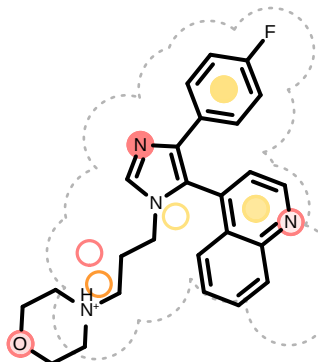
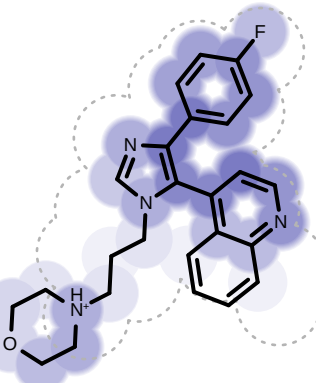
Color Tanimoto = 0.205

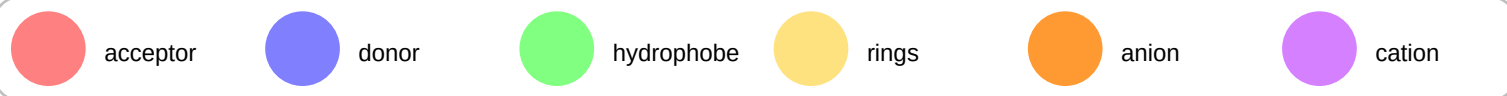
2D Graph Tanimoto = 0.089

Rank: 111  
Tanimoto Combo = 0.803

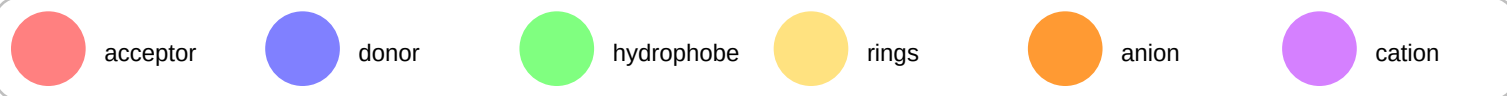


query : 4cox-ligD\_6





|                                                                                                       |                               |                               |                                  |
|-------------------------------------------------------------------------------------------------------|-------------------------------|-------------------------------|----------------------------------|
| <p>Hit: database_85_197</p> <p>Rank: 112</p> <p>Tanimoto Combo = 0.803</p> <p>query : 4cox-ligD_6</p> | <p>Shape Tanimoto = 0.599</p> | <p>Color Tanimoto = 0.205</p> | <p>2D Graph Tanimoto = 0.089</p> |
| <p>Hit: database_165_51</p> <p>Rank: 113</p> <p>Tanimoto Combo = 0.801</p> <p>query : 4cox-ligD_8</p> | <p>Shape Tanimoto = 0.668</p> | <p>Color Tanimoto = 0.134</p> | <p>2D Graph Tanimoto = 0.116</p> |
| <p>Hit: database_53_194</p> <p>Rank: 114</p> <p>Tanimoto Combo = 0.798</p> <p>query : 4cox-ligD_3</p> | <p>Shape Tanimoto = 0.739</p> | <p>Color Tanimoto = 0.059</p> | <p>2D Graph Tanimoto = 0.035</p> |



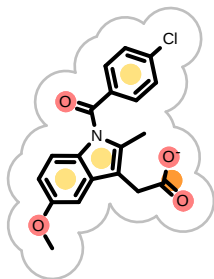
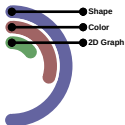
Hit: database\_88\_31

Shape Tanimoto = 0.501

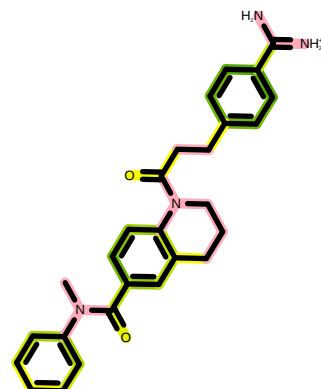
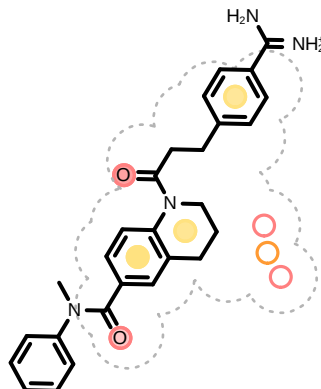
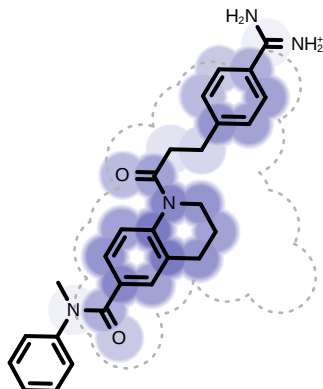
Color Tanimoto = 0.297

2D Graph Tanimoto = 0.148

Rank: 115  
Tanimoto Combo = 0.798



query : 4cox-ligD\_7



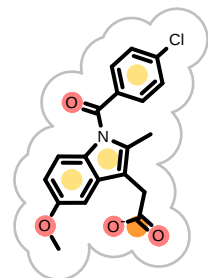
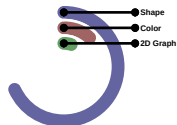
Hit: database\_29\_58

Shape Tanimoto = 0.681

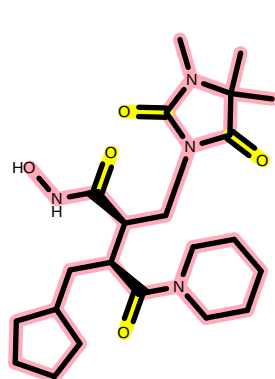
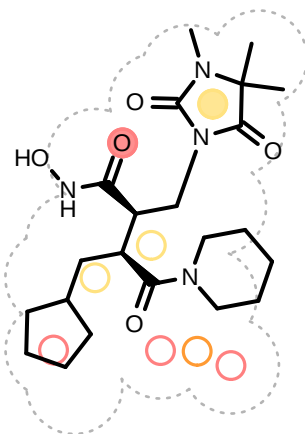
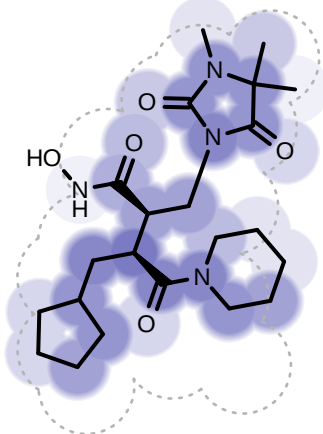
Color Tanimoto = 0.116

2D Graph Tanimoto = 0.051

Rank: 116  
Tanimoto Combo = 0.797



query : 4cox-ligD\_9



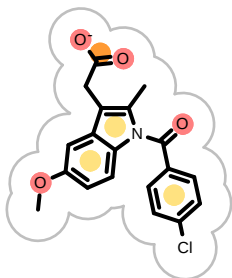
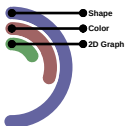
Hit: database\_185\_27

Shape Tanimoto = 0.503

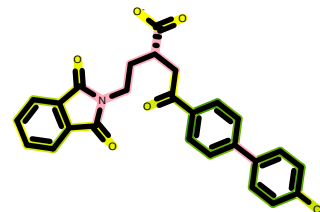
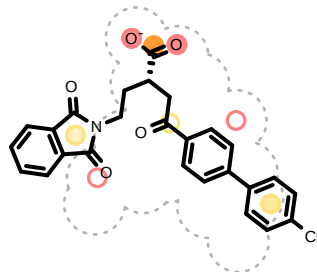
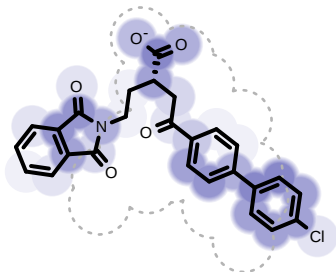
Color Tanimoto = 0.294

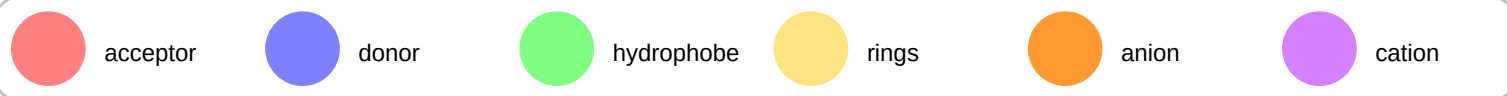
2D Graph Tanimoto = 0.168

Rank: 117  
Tanimoto Combo = 0.797

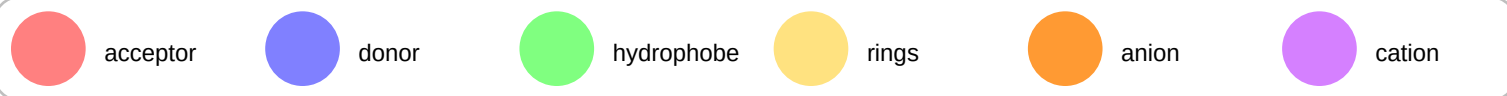


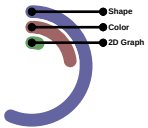
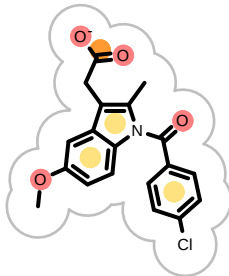
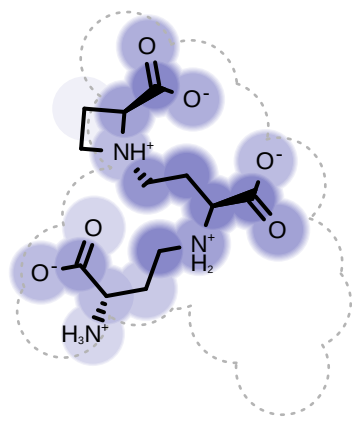
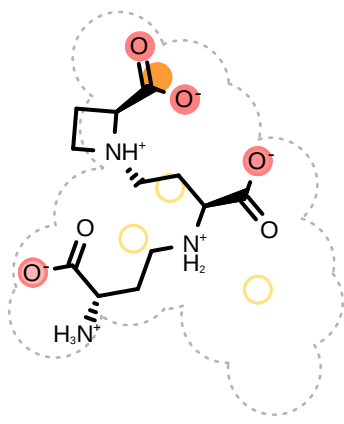
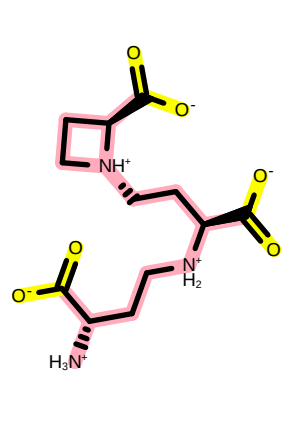
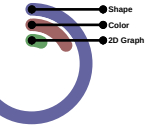
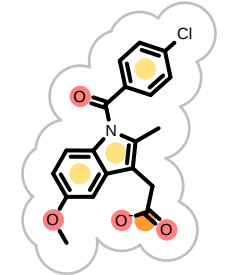
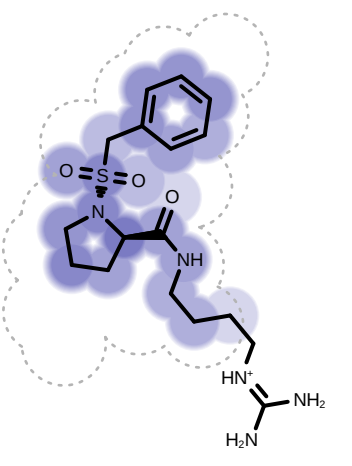
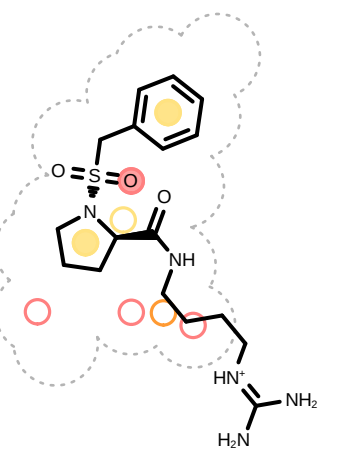
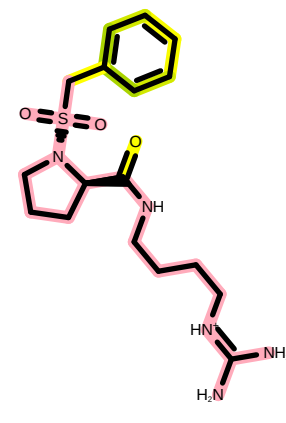
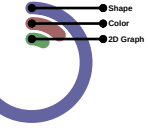
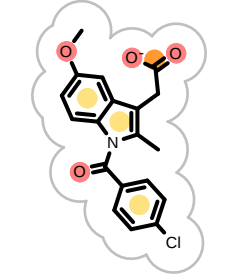
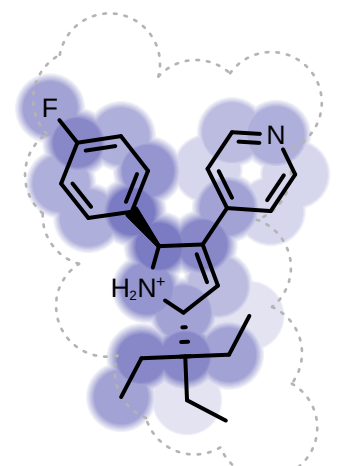
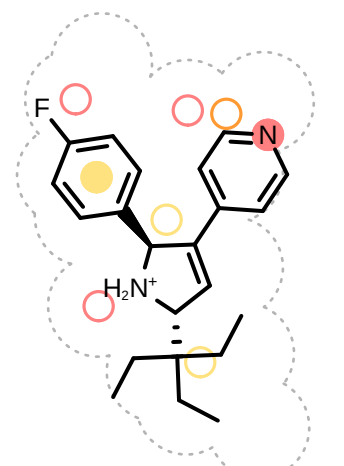
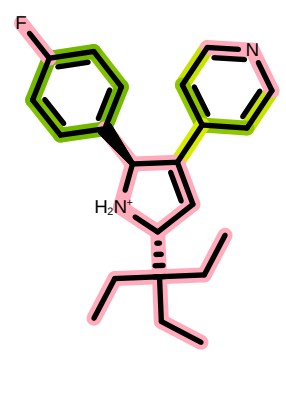
query : 4cox-ligD\_2

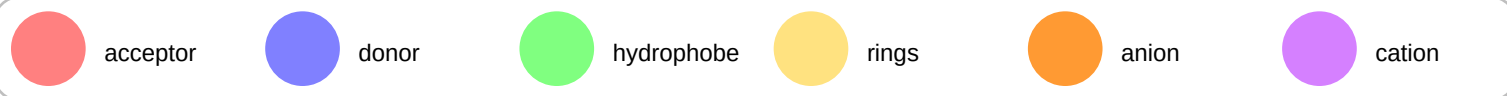




|                                                                                                        |                               |                               |                                  |
|--------------------------------------------------------------------------------------------------------|-------------------------------|-------------------------------|----------------------------------|
| <p>Hit: database_68_123</p> <p>Rank: 118</p> <p>Tanimoto Combo = 0.796</p> <p>query : 4cox-ligD_9</p>  | <p>Shape Tanimoto = 0.57</p>  | <p>Color Tanimoto = 0.227</p> | <p>2D Graph Tanimoto = 0.101</p> |
| <p>Hit: database_50_9</p> <p>Rank: 119</p> <p>Tanimoto Combo = 0.796</p> <p>query : 4cox-ligD_5</p>    | <p>Shape Tanimoto = 0.689</p> | <p>Color Tanimoto = 0.106</p> | <p>2D Graph Tanimoto = 0.065</p> |
| <p>Hit: database_138_145</p> <p>Rank: 120</p> <p>Tanimoto Combo = 0.794</p> <p>query : 4cox-ligD_4</p> | <p>Shape Tanimoto = 0.631</p> | <p>Color Tanimoto = 0.163</p> | <p>2D Graph Tanimoto = 0.072</p> |



|                                                                                                                                                                                                                                                                              |                                                                                                                   |                                                                                                                    |                                                                                                                        |
|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------|
| <p>Hit: database_196_73</p> <p>Rank: 121</p> <p>Tanimoto Combo = 0.793</p>   <p>query : 4cox-ligD_8</p>     | <p>Shape Tanimoto = 0.564</p>    | <p>Color Tanimoto = 0.229</p>    | <p>2D Graph Tanimoto = 0.042</p>    |
| <p>Hit: database_206_150</p> <p>Rank: 122</p> <p>Tanimoto Combo = 0.792</p>   <p>query : 4cox-ligD_9</p> | <p>Shape Tanimoto = 0.619</p>   | <p>Color Tanimoto = 0.172</p>   | <p>2D Graph Tanimoto = 0.065</p>   |
| <p>Hit: database_153_3</p> <p>Rank: 123</p> <p>Tanimoto Combo = 0.788</p>   <p>query : 4cox-ligD_5</p>  | <p>Shape Tanimoto = 0.662</p>  | <p>Color Tanimoto = 0.126</p>  | <p>2D Graph Tanimoto = 0.081</p>  |



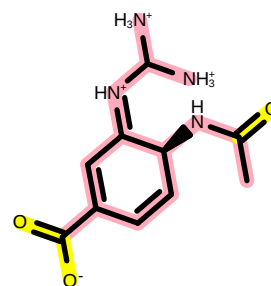
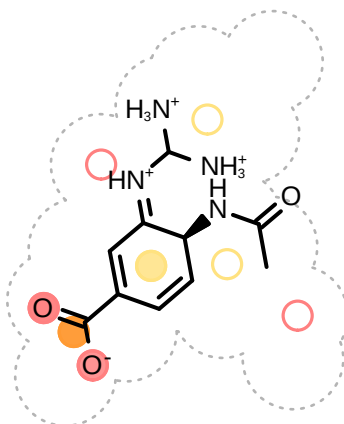
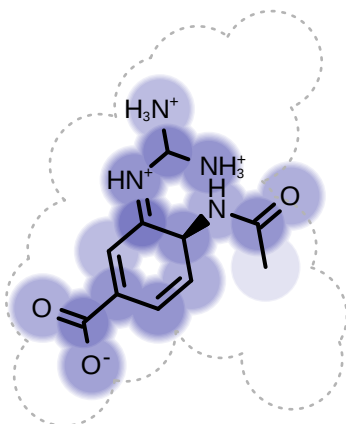
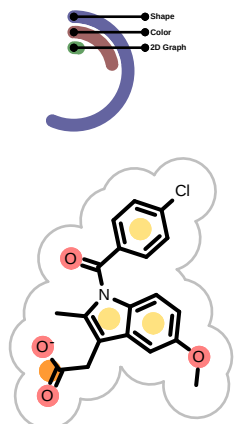
Hit: database\_116\_3

Shape Tanimoto = 0.565

Color Tanimoto = 0.223

2D Graph Tanimoto = 0.032

Rank: 124  
Tanimoto Combo = 0.788



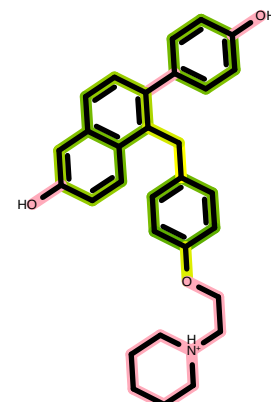
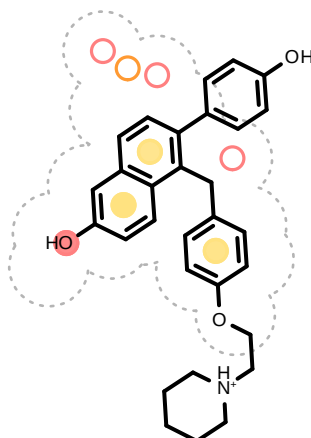
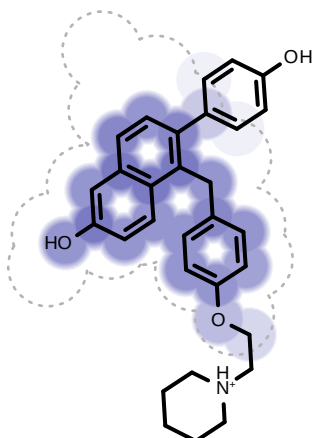
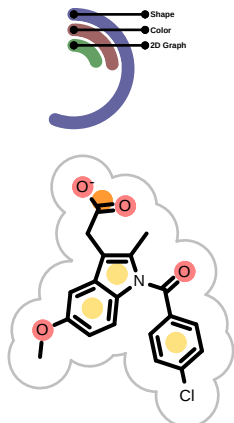
Hit: database\_180\_152

Shape Tanimoto = 0.556

Color Tanimoto = 0.231

2D Graph Tanimoto = 0.200

Rank: 125  
Tanimoto Combo = 0.787



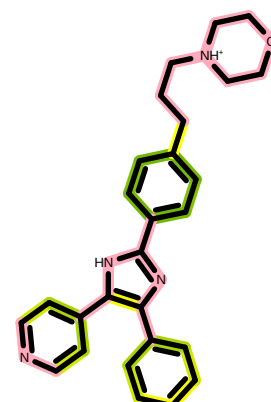
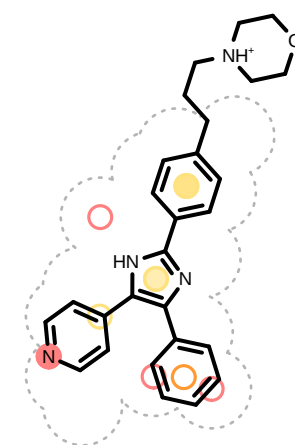
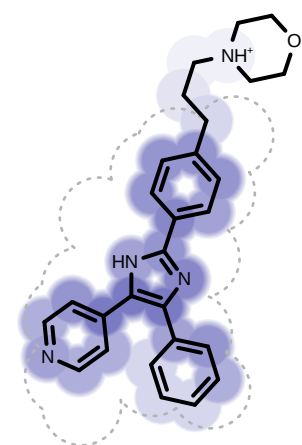
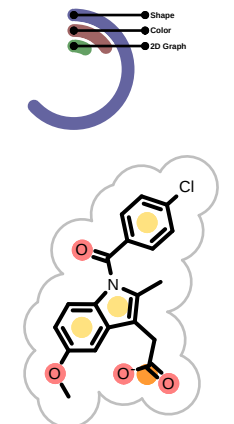
Hit: database\_72\_91

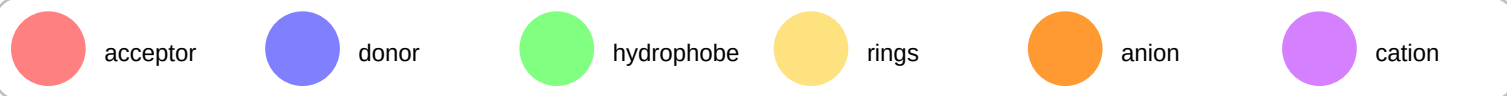
Shape Tanimoto = 0.631

Color Tanimoto = 0.155

2D Graph Tanimoto = 0.082

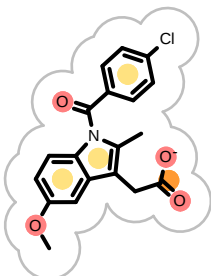
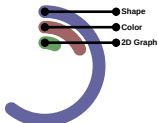
Rank: 126  
Tanimoto Combo = 0.786



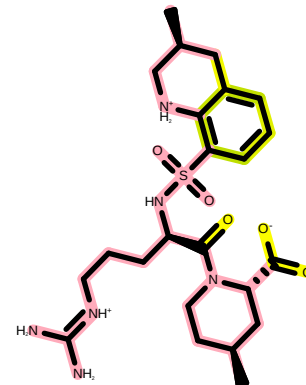
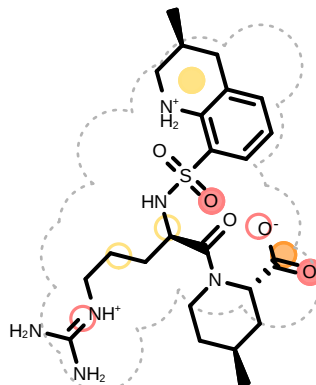
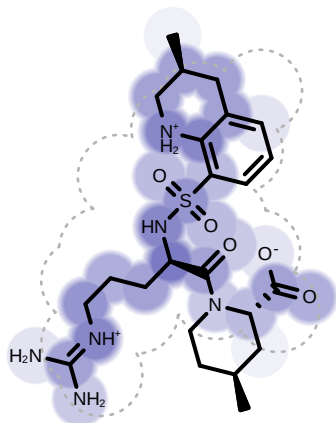


Hit: database\_129\_191      Shape Tanimoto = 0.606      Color Tanimoto = 0.179      2D Graph Tanimoto = 0.070

Rank: 127  
Tanimoto Combo = 0.785



query : 4cox-ligD\_7



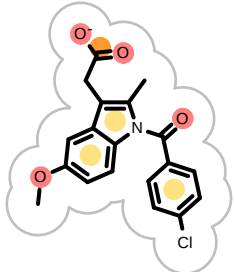
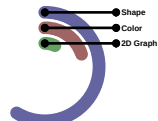
Hit: database\_103\_2

Shape Tanimoto = 0.587

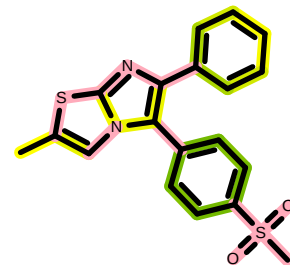
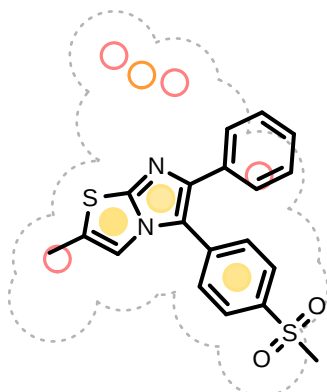
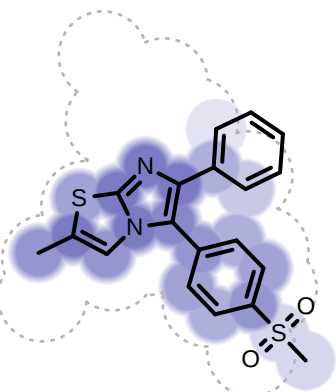
Color Tanimoto = 0.198

2D Graph Tanimoto = 0.071

Rank: 128  
Tanimoto Combo = 0.784



query : 4cox-ligD\_2



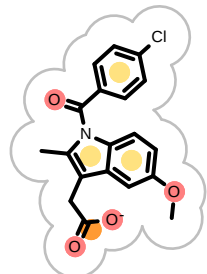
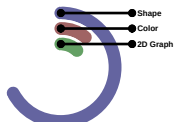
Hit: database\_184\_199

Shape Tanimoto = 0.671

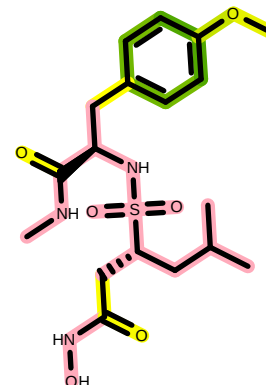
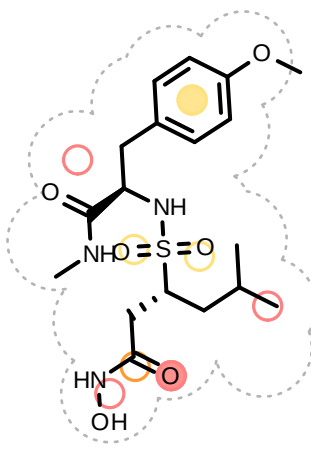
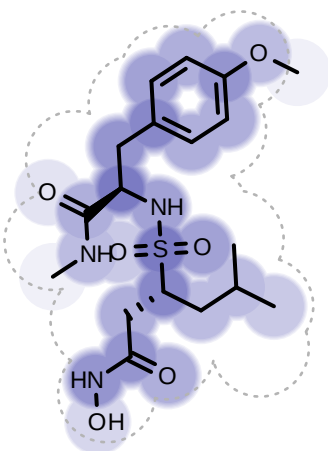
Color Tanimoto = 0.109

2D Graph Tanimoto = 0.122

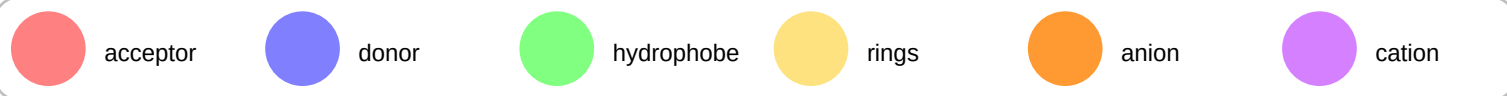
Rank: 129  
Tanimoto Combo = 0.78



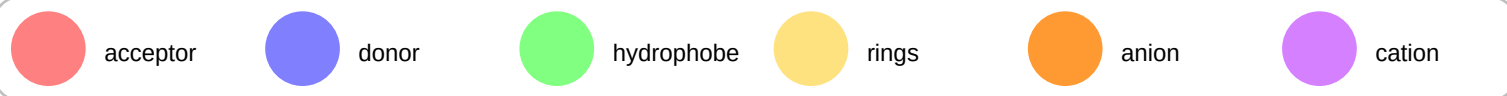
query : 4cox-ligD\_0







|                                                                                                        |                               |                               |                                  |
|--------------------------------------------------------------------------------------------------------|-------------------------------|-------------------------------|----------------------------------|
| <p>Hit: database_56_189</p> <p>Rank: 130</p> <p>Tanimoto Combo = 0.779</p> <p>query : 4cox-ligD_5</p>  | <p>Shape Tanimoto = 0.654</p> | <p>Color Tanimoto = 0.125</p> | <p>2D Graph Tanimoto = 0.077</p> |
| <p>Hit: database_186_40</p> <p>Rank: 131</p> <p>Tanimoto Combo = 0.779</p> <p>query : 4cox-ligD_6</p>  | <p>Shape Tanimoto = 0.663</p> | <p>Color Tanimoto = 0.115</p> | <p>2D Graph Tanimoto = 0.099</p> |
| <p>Hit: database_192_197</p> <p>Rank: 132</p> <p>Tanimoto Combo = 0.778</p> <p>query : 4cox-ligD_7</p> | <p>Shape Tanimoto = 0.587</p> | <p>Color Tanimoto = 0.191</p> | <p>2D Graph Tanimoto = 0.082</p> |



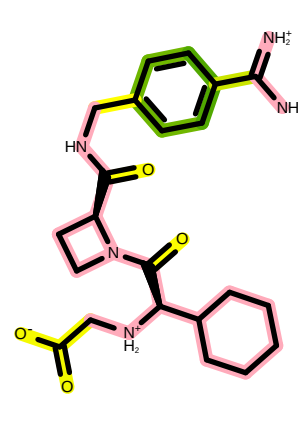
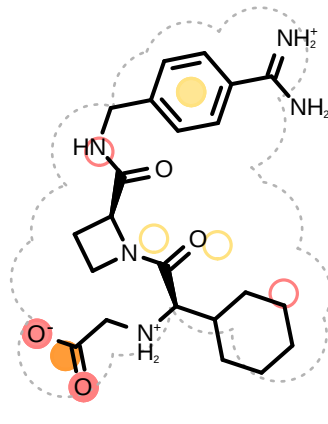
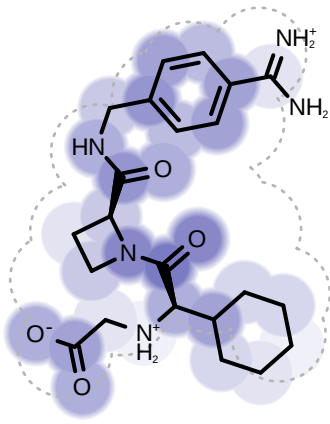
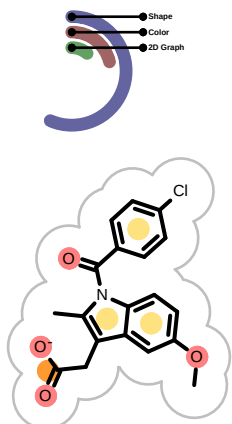
Hit: database\_120\_137

Shape Tanimoto = 0.565

Color Tanimoto = 0.212

2D Graph Tanimoto = 0.113

Rank: 133  
Tanimoto Combo = 0.777



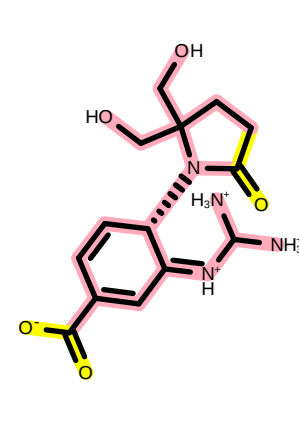
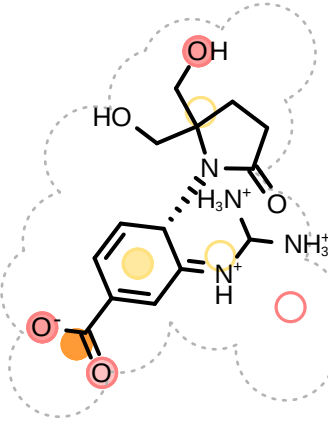
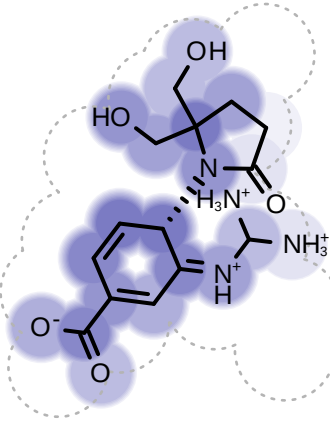
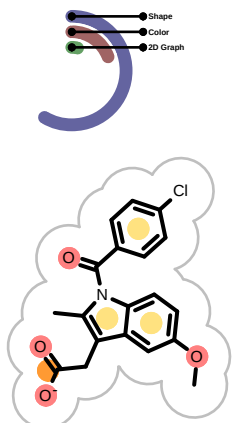
Hit: database\_191\_3

Shape Tanimoto = 0.584

Color Tanimoto = 0.192

2D Graph Tanimoto = 0.039

Rank: 134  
Tanimoto Combo = 0.776



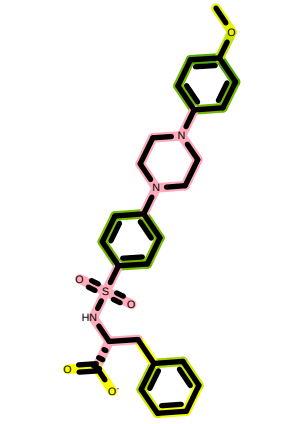
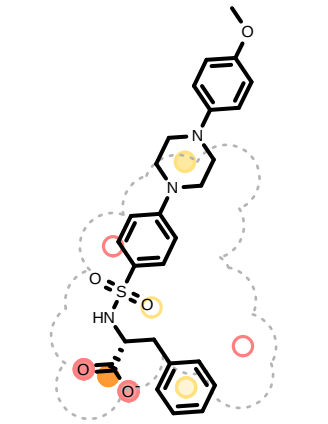
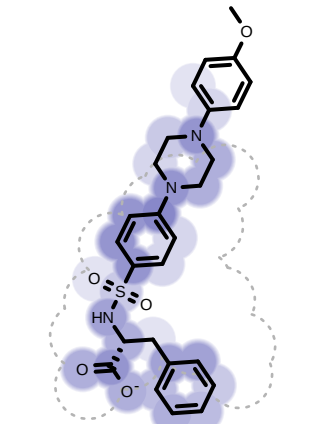
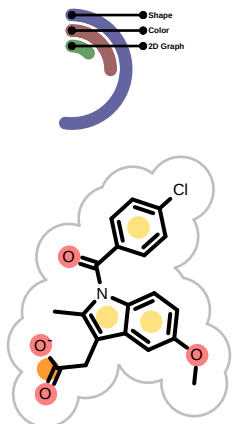
Hit: database\_58\_184

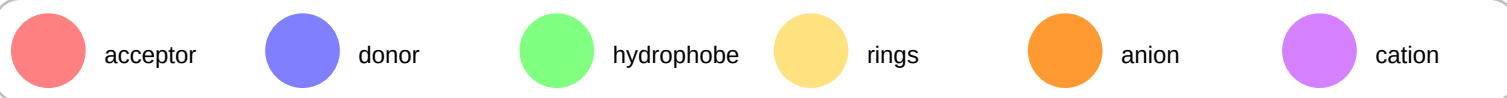
Shape Tanimoto = 0.519

Color Tanimoto = 0.252

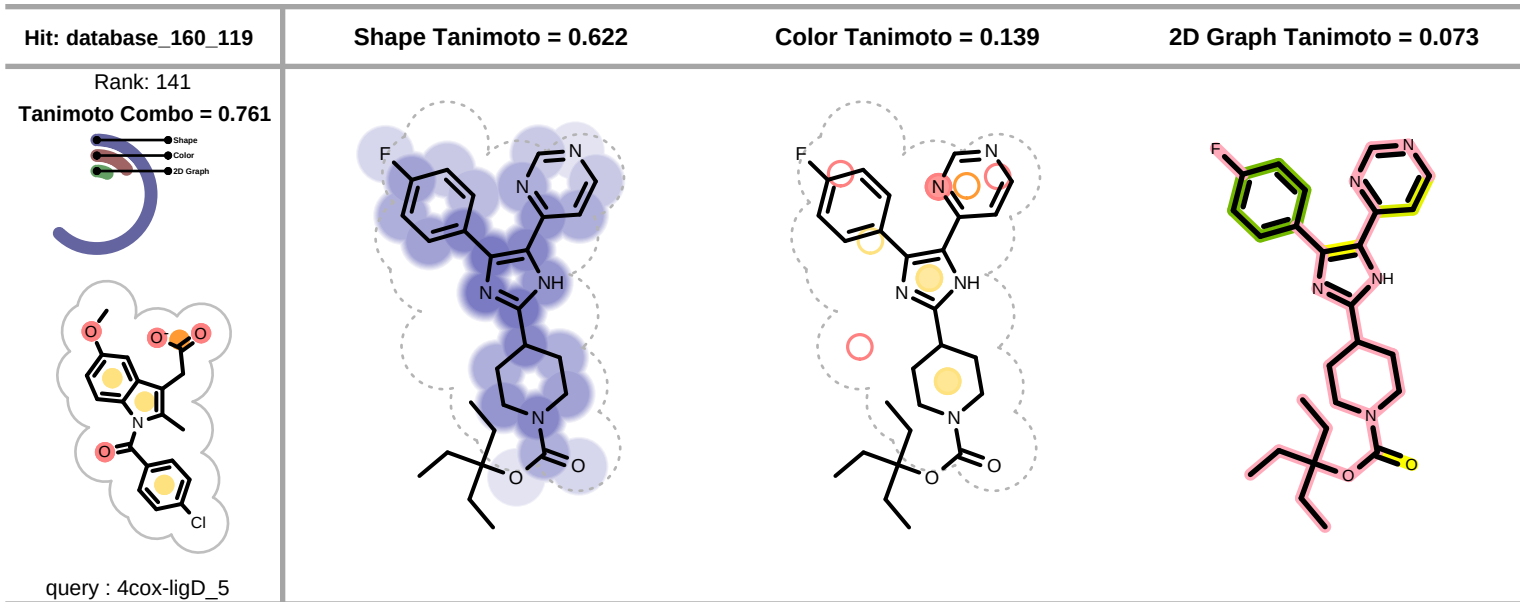
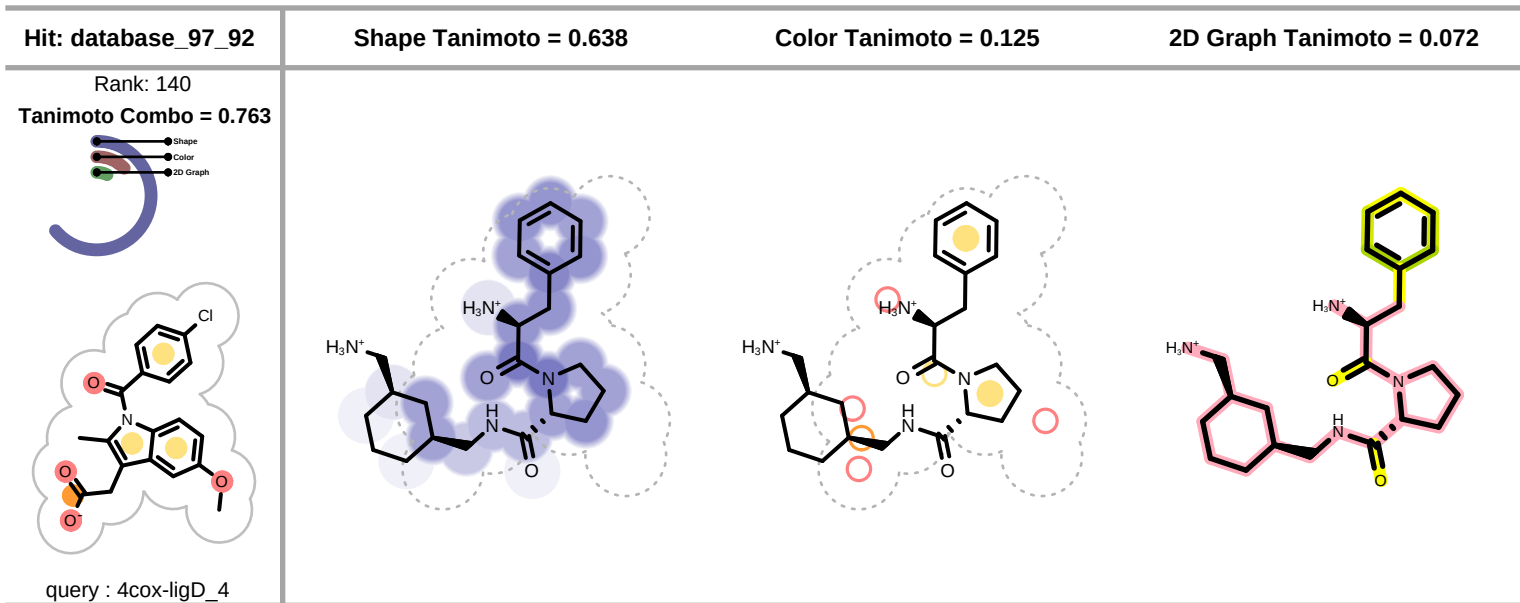
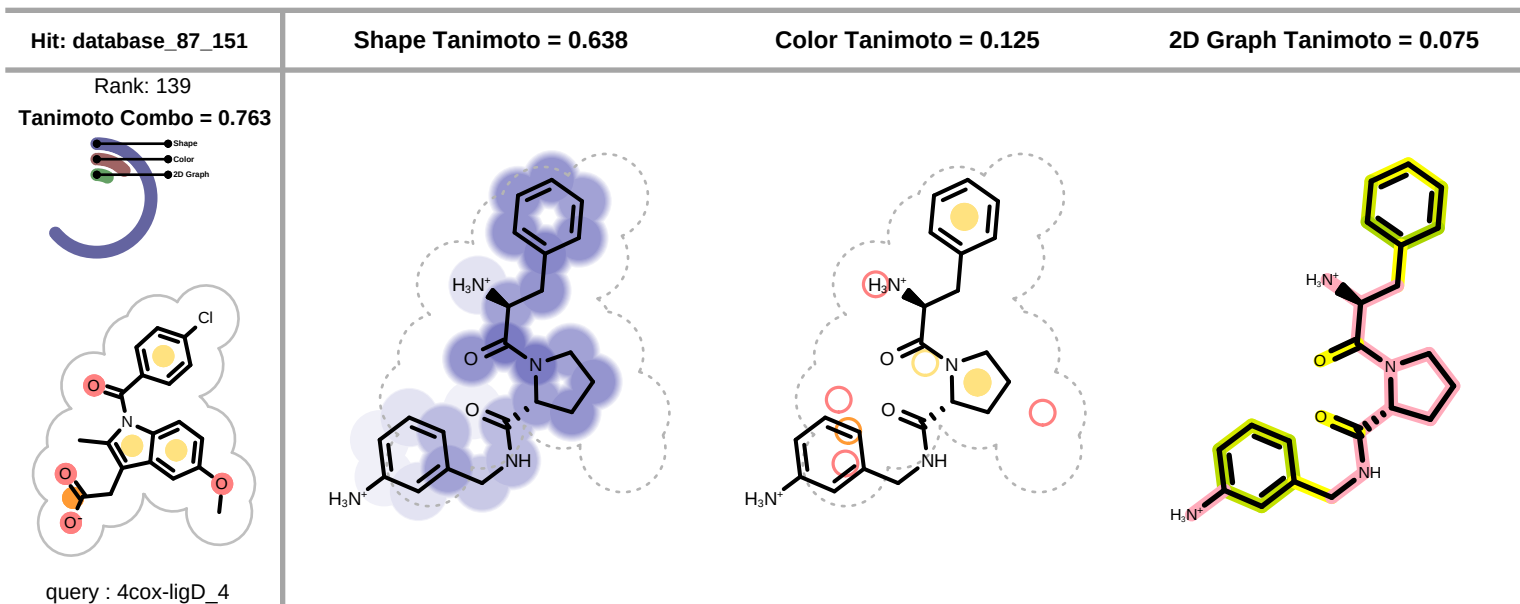
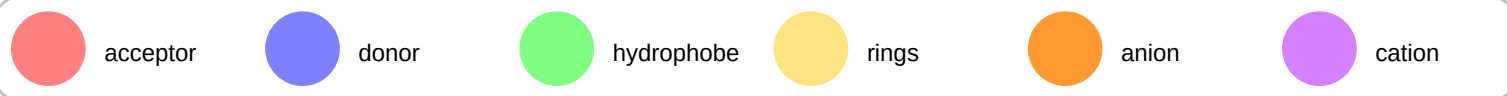
2D Graph Tanimoto = 0.128

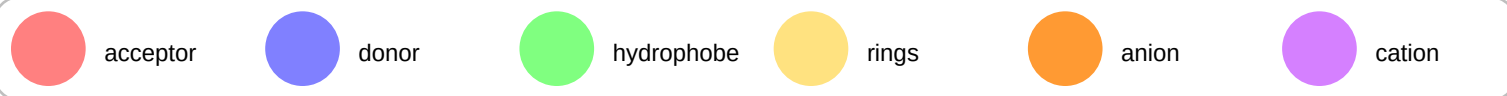
Rank: 135  
Tanimoto Combo = 0.771

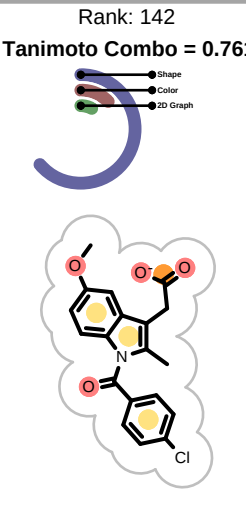
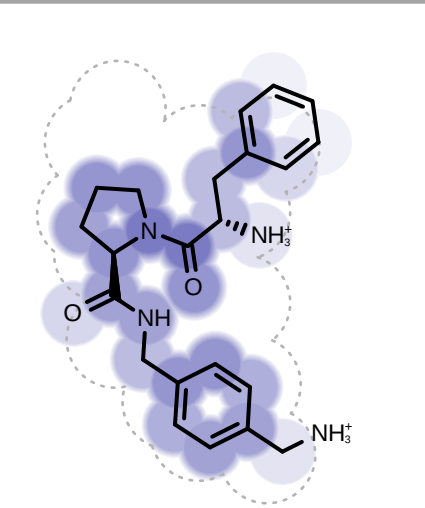
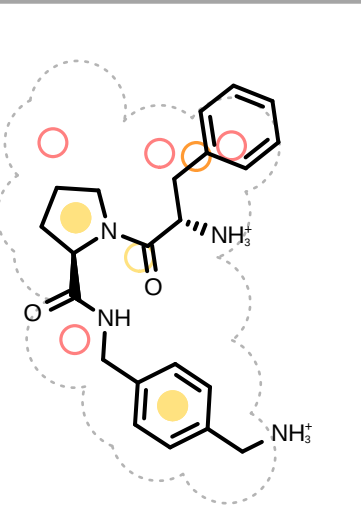
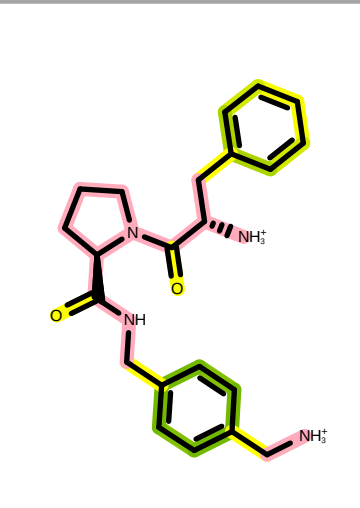
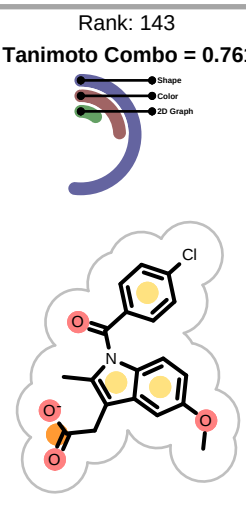
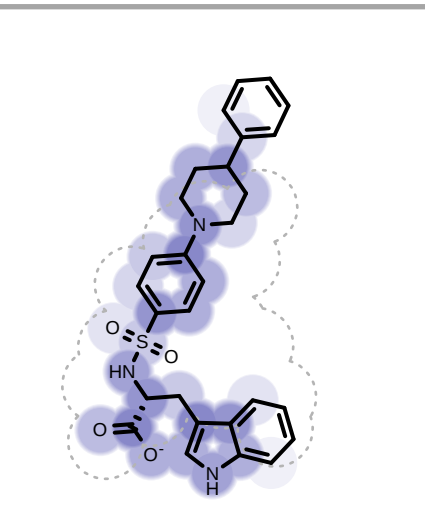
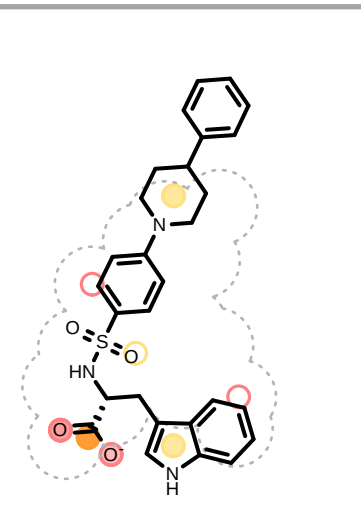
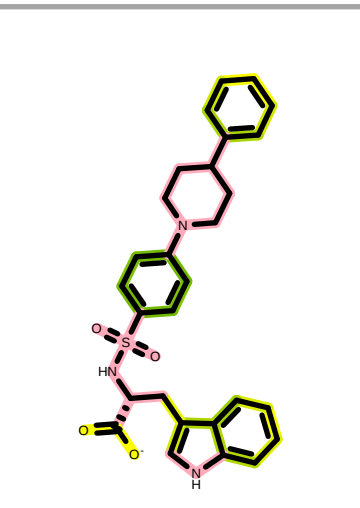
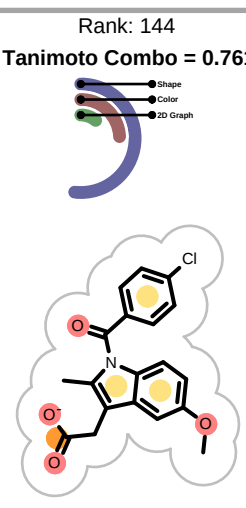
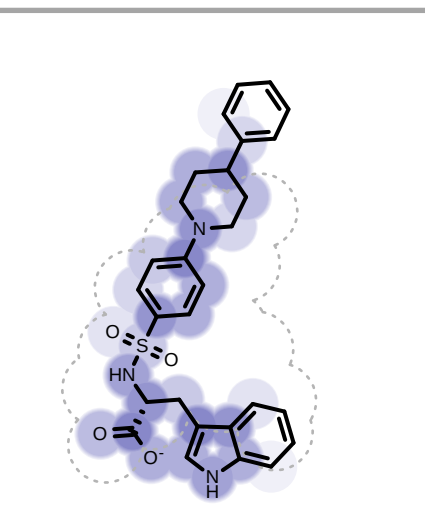
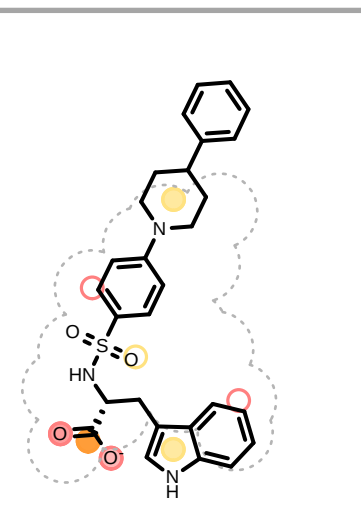
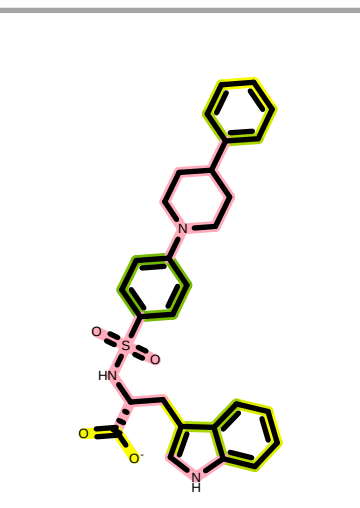


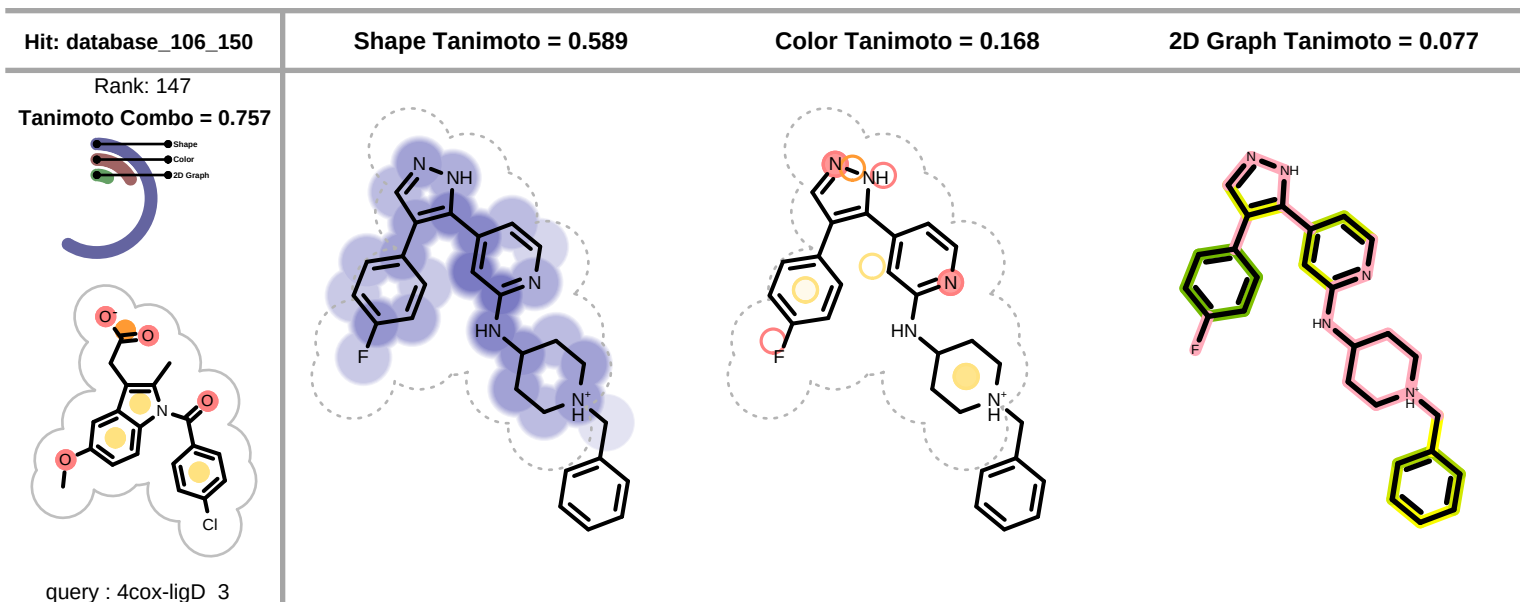
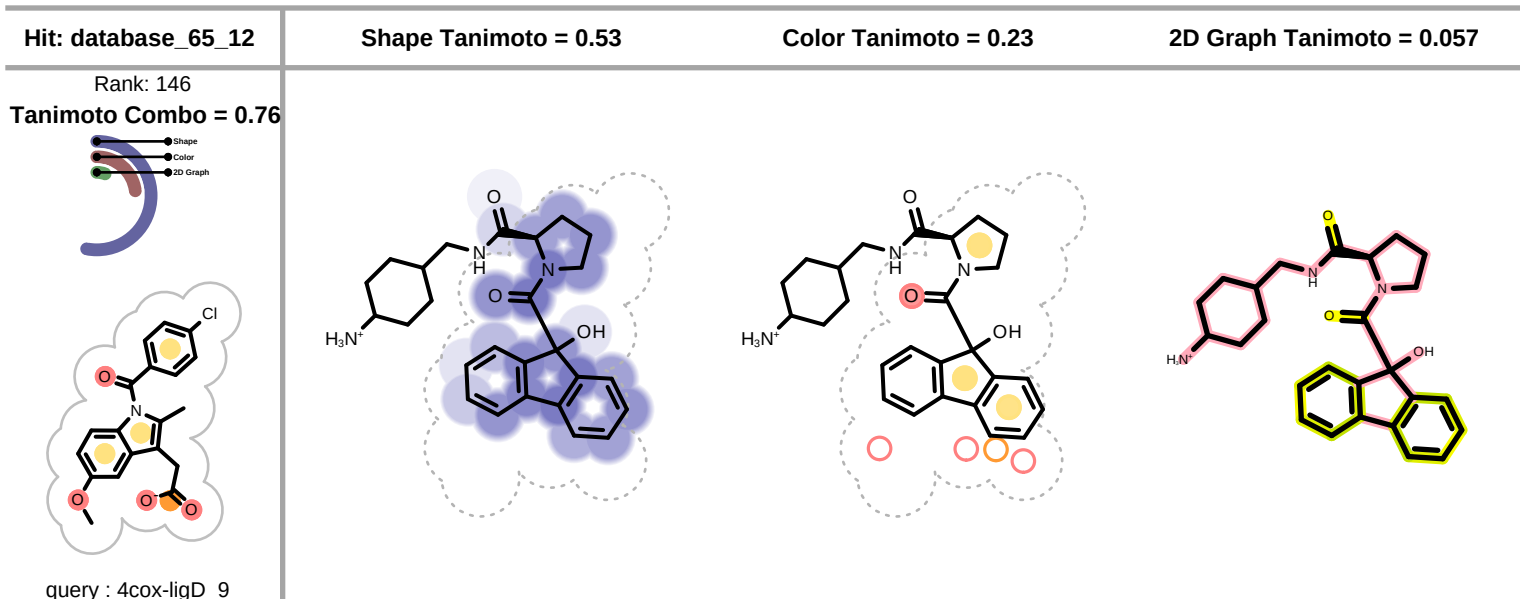
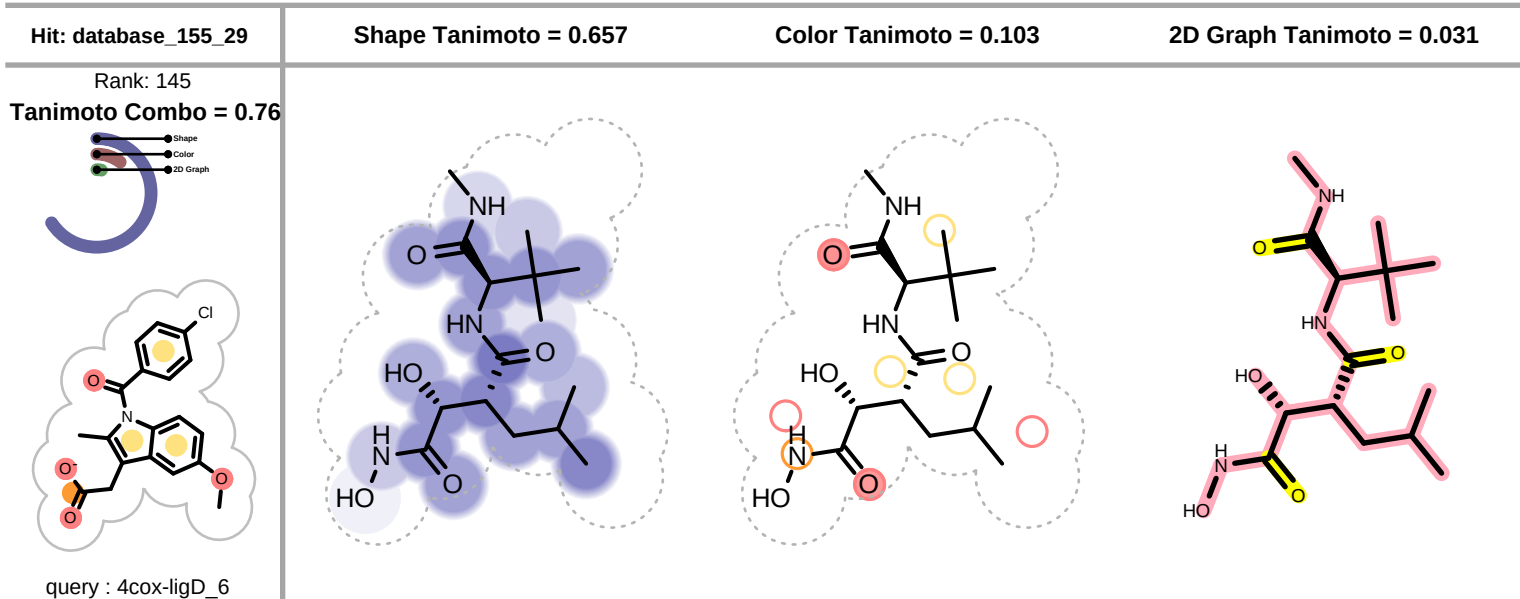
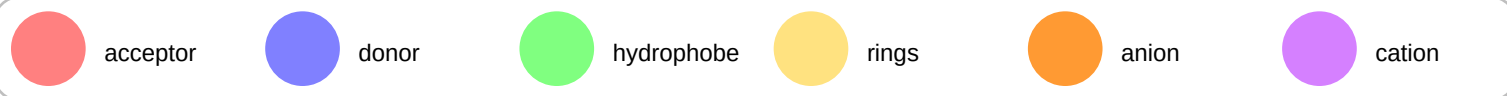


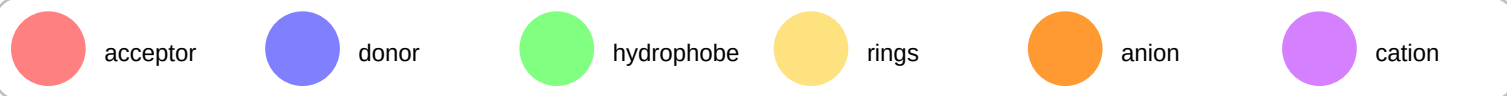
|                                                                                                        |                               |                               |                                  |
|--------------------------------------------------------------------------------------------------------|-------------------------------|-------------------------------|----------------------------------|
| <p>Hit: database_200_141</p> <p>Rank: 136</p> <p>Tanimoto Combo = 0.771</p> <p>query : 4cox-ligD_6</p> | <p>Shape Tanimoto = 0.532</p> | <p>Color Tanimoto = 0.239</p> | <p>2D Graph Tanimoto = 0.137</p> |
| <p>Hit: database_31_0</p> <p>Rank: 137</p> <p>Tanimoto Combo = 0.768</p> <p>query : 4cox-ligD_9</p>    | <p>Shape Tanimoto = 0.621</p> | <p>Color Tanimoto = 0.147</p> | <p>2D Graph Tanimoto = 0.054</p> |
| <p>Hit: database_26_8</p> <p>Rank: 138</p> <p>Tanimoto Combo = 0.765</p> <p>query : 4cox-ligD_7</p>    | <p>Shape Tanimoto = 0.577</p> | <p>Color Tanimoto = 0.187</p> | <p>2D Graph Tanimoto = 0.069</p> |

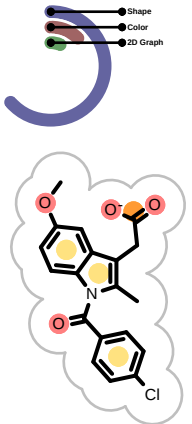
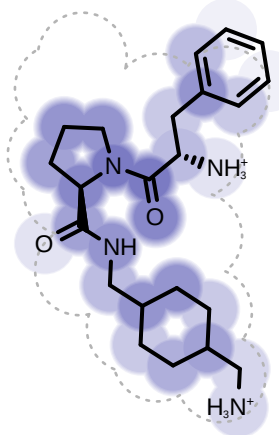
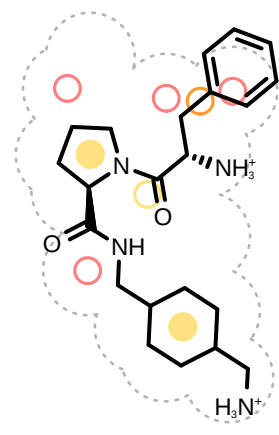
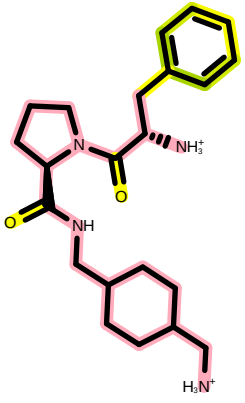
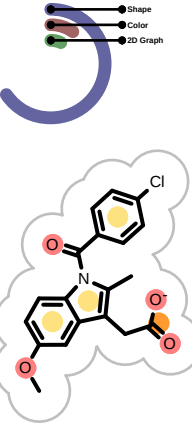
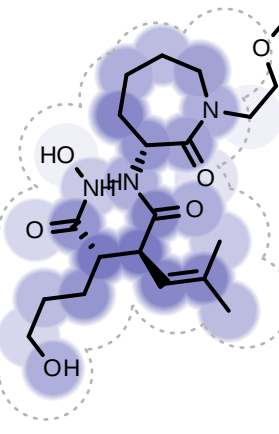
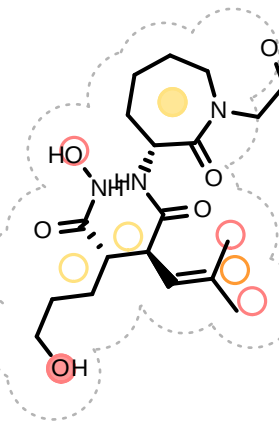
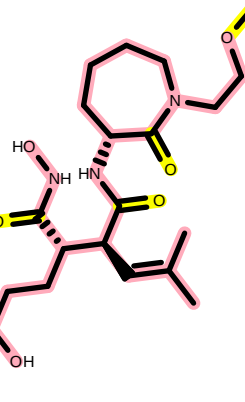
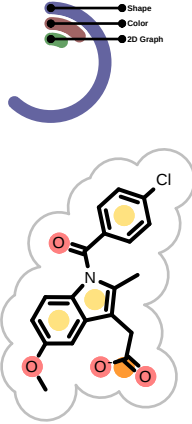
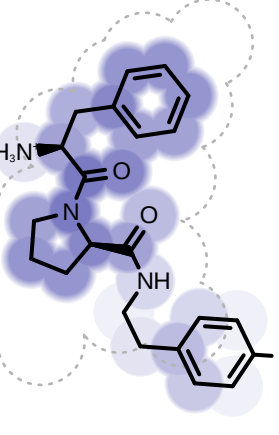
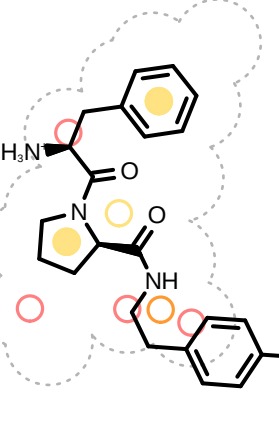
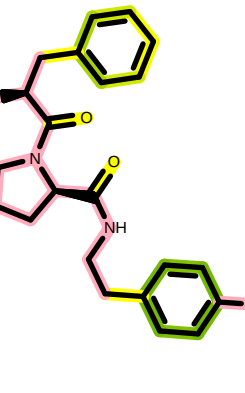




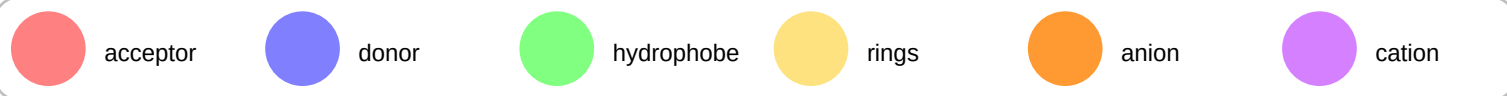
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|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------|
| <p>Hit: database_86_168</p> <p>Rank: 142</p> <p>Tanimoto Combo = 0.761</p>  <p>query : 4cox-ligD_5</p>  | <p>Shape Tanimoto = 0.636</p>    | <p>Color Tanimoto = 0.125</p>    | <p>2D Graph Tanimoto = 0.077</p>    |
| <p>Hit: database_127_68</p> <p>Rank: 143</p> <p>Tanimoto Combo = 0.761</p>  <p>query : 4cox-ligD_6</p> | <p>Shape Tanimoto = 0.518</p>   | <p>Color Tanimoto = 0.243</p>   | <p>2D Graph Tanimoto = 0.110</p>   |
| <p>Hit: database_42_68</p> <p>Rank: 144</p> <p>Tanimoto Combo = 0.761</p>  <p>query : 4cox-ligD_6</p> | <p>Shape Tanimoto = 0.518</p>  | <p>Color Tanimoto = 0.243</p>  | <p>2D Graph Tanimoto = 0.110</p>  |

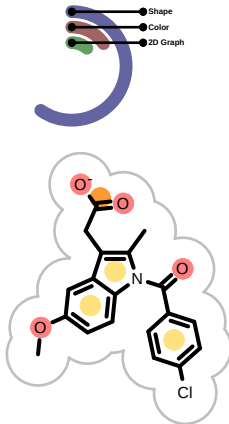
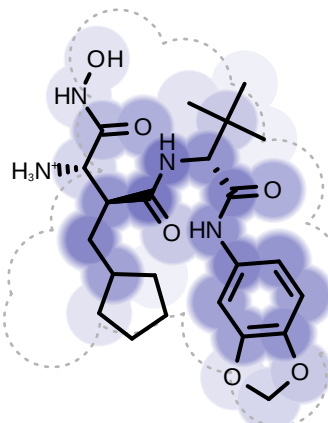
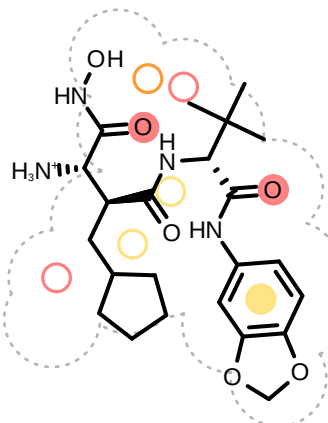
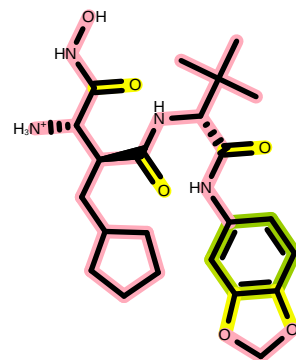
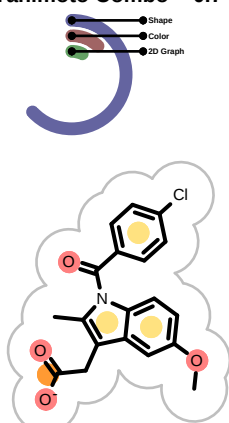
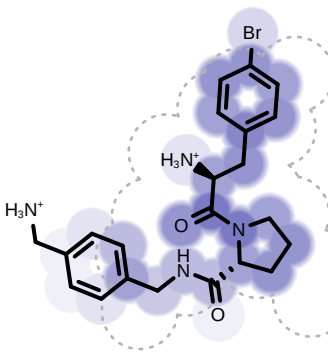
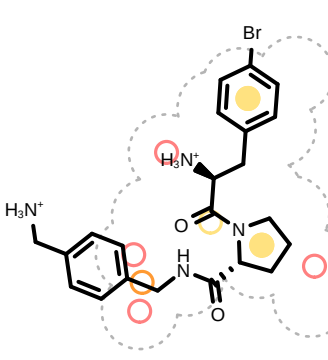
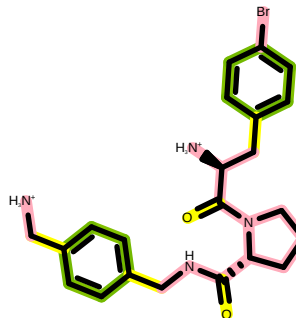
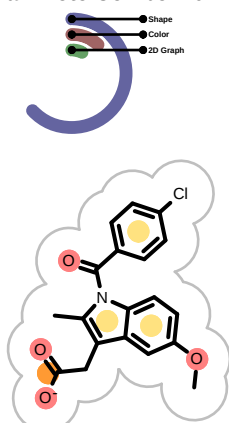
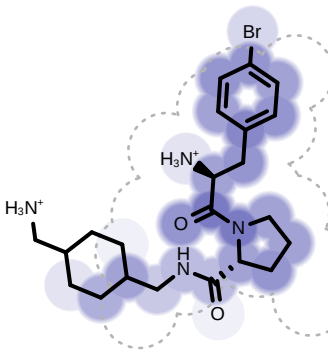
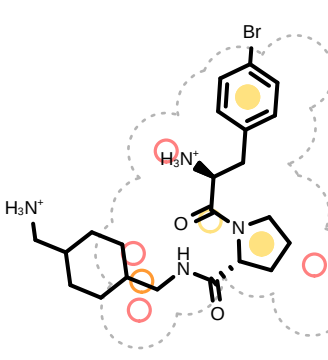
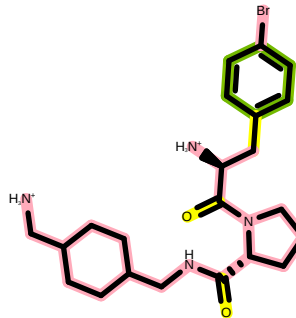


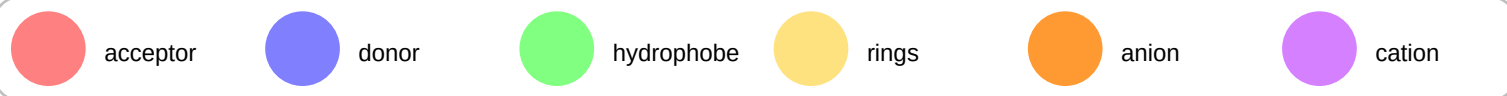


|                                                                                                                                                                                           |                                                                                                                   |                                                                                                                    |                                                                                                                        |
|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------|
| <p>Hit: database_179_162</p> <p>Rank: 148</p> <p>Tanimoto Combo = 0.756</p>  <p>query : 4cox-ligD_5</p>   | <p>Shape Tanimoto = 0.633</p>    | <p>Color Tanimoto = 0.123</p>    | <p>2D Graph Tanimoto = 0.065</p>    |
| <p>Hit: database_177_189</p> <p>Rank: 149</p> <p>Tanimoto Combo = 0.749</p>  <p>query : 4cox-ligD_7</p>  | <p>Shape Tanimoto = 0.653</p>   | <p>Color Tanimoto = 0.096</p>   | <p>2D Graph Tanimoto = 0.070</p>   |
| <p>Hit: database_123_191</p> <p>Rank: 150</p> <p>Tanimoto Combo = 0.749</p>  <p>query : 4cox-ligD_9</p> | <p>Shape Tanimoto = 0.617</p>  | <p>Color Tanimoto = 0.132</p>  | <p>2D Graph Tanimoto = 0.076</p>  |

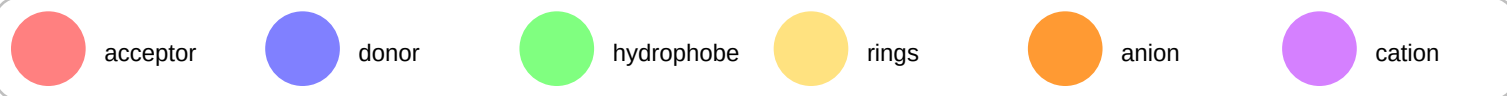


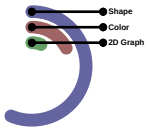
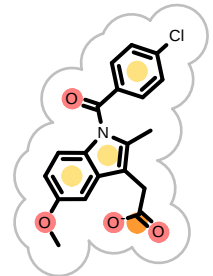
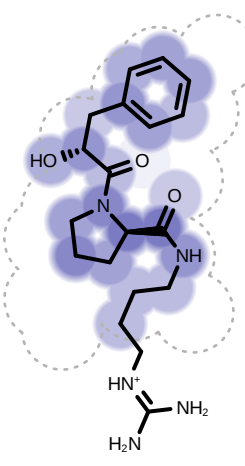
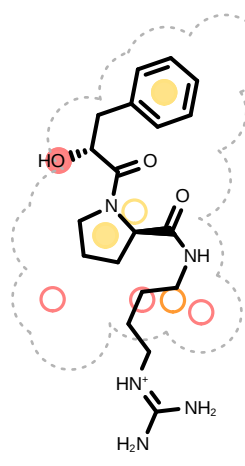
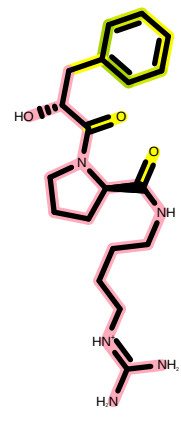
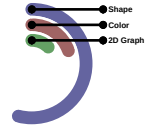
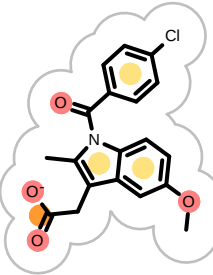
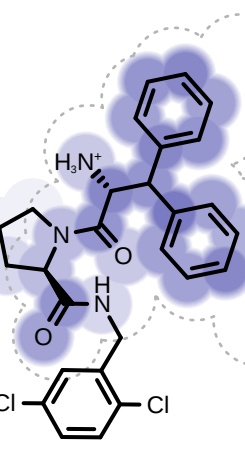
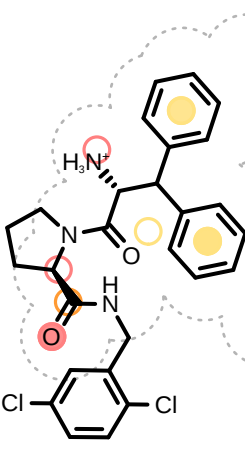
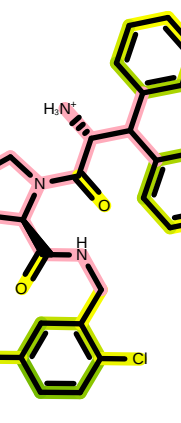
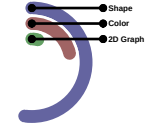
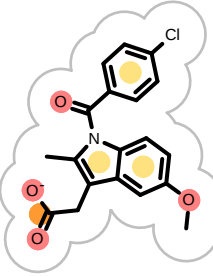
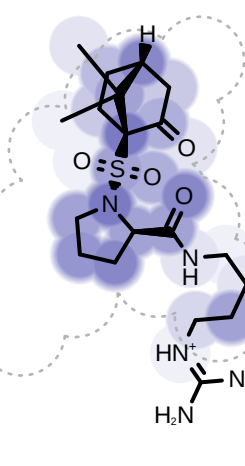
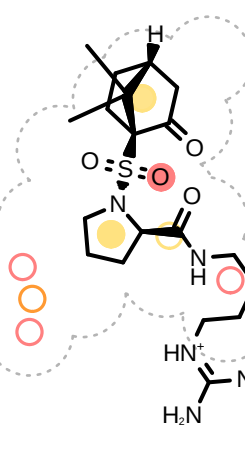
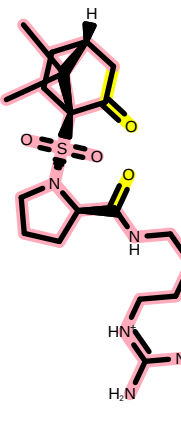


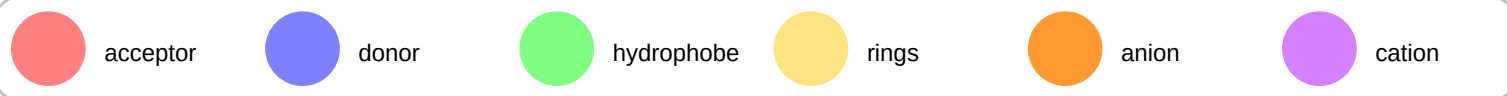
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|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------|
| <p>Hit: database_205_181</p> <p>Rank: 151</p> <p>Tanimoto Combo = 0.749</p>  <p>query : 4cox-ligD_8</p>  | <p>Shape Tanimoto = 0.597</p>    | <p>Color Tanimoto = 0.152</p>    | <p>2D Graph Tanimoto = 0.112</p>    |
| <p>Hit: database_118_130</p> <p>Rank: 152</p> <p>Tanimoto Combo = 0.747</p>  <p>query : 4cox-ligD_4</p> | <p>Shape Tanimoto = 0.629</p>   | <p>Color Tanimoto = 0.118</p>   | <p>2D Graph Tanimoto = 0.074</p>   |
| <p>Hit: database_80_147</p> <p>Rank: 153</p> <p>Tanimoto Combo = 0.747</p>  <p>query : 4cox-ligD_4</p> | <p>Shape Tanimoto = 0.629</p>  | <p>Color Tanimoto = 0.118</p>  | <p>2D Graph Tanimoto = 0.072</p>  |



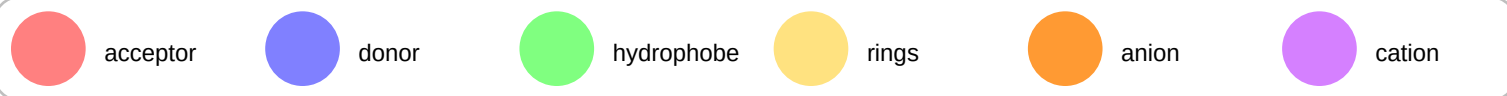
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|----------------------------------------------------------------------------------------------------------------------|--------------------------------------|--------------------------------------|-----------------------------------------|
| <p><b>Hit: database_61_52</b></p> <p>Rank: 154</p> <p><b>Tanimoto Combo = 0.739</b></p> <p>query : 4cox-ligD_4</p>   | <p><b>Shape Tanimoto = 0.522</b></p> | <p><b>Color Tanimoto = 0.217</b></p> | <p><b>2D Graph Tanimoto = 0.144</b></p> |
| <p><b>Hit: database_95_23</b></p> <p>Rank: 155</p> <p><b>Tanimoto Combo = 0.739</b></p> <p>query : 4cox-ligD_2</p>   | <p><b>Shape Tanimoto = 0.514</b></p> | <p><b>Color Tanimoto = 0.225</b></p> | <p><b>2D Graph Tanimoto = 0.060</b></p> |
| <p><b>Hit: database_204_134</b></p> <p>Rank: 156</p> <p><b>Tanimoto Combo = 0.738</b></p> <p>query : 4cox-ligD_5</p> | <p><b>Shape Tanimoto = 0.613</b></p> | <p><b>Color Tanimoto = 0.125</b></p> | <p><b>2D Graph Tanimoto = 0.075</b></p> |



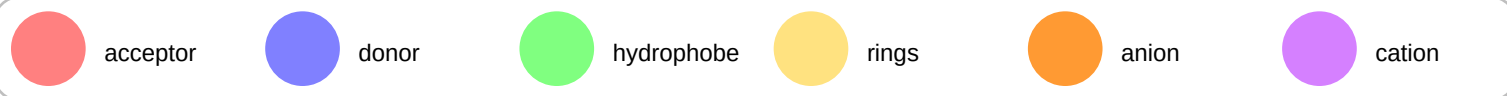
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|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------|
| <p>Hit: database_62_169</p> <p>Rank: 157</p> <p>Tanimoto Combo = 0.737</p>   <p>query : 4cox-ligD_9</p>     | <p>Shape Tanimoto = 0.563</p>    | <p>Color Tanimoto = 0.174</p>    | <p>2D Graph Tanimoto = 0.064</p>    |
| <p>Hit: database_52_170</p> <p>Rank: 158</p> <p>Tanimoto Combo = 0.736</p>   <p>query : 4cox-ligD_1</p>  | <p>Shape Tanimoto = 0.54</p>    | <p>Color Tanimoto = 0.196</p>   | <p>2D Graph Tanimoto = 0.124</p>   |
| <p>Hit: database_98_163</p> <p>Rank: 159</p> <p>Tanimoto Combo = 0.734</p>   <p>query : 4cox-ligD_6</p> | <p>Shape Tanimoto = 0.521</p>  | <p>Color Tanimoto = 0.213</p>  | <p>2D Graph Tanimoto = 0.041</p>  |



|                                                                                                        |                               |                               |                                  |
|--------------------------------------------------------------------------------------------------------|-------------------------------|-------------------------------|----------------------------------|
| <p>Hit: database_197_142</p> <p>Rank: 160</p> <p>Tanimoto Combo = 0.733</p> <p>query : 4cox-ligD_4</p> | <p>Shape Tanimoto = 0.596</p> | <p>Color Tanimoto = 0.137</p> | <p>2D Graph Tanimoto = 0.073</p> |
| <p>Hit: database_140_192</p> <p>Rank: 161</p> <p>Tanimoto Combo = 0.732</p> <p>query : 4cox-ligD_9</p> | <p>Shape Tanimoto = 0.552</p> | <p>Color Tanimoto = 0.18</p>  | <p>2D Graph Tanimoto = 0.134</p> |
| <p>Hit: database_178_61</p> <p>Rank: 162</p> <p>Tanimoto Combo = 0.731</p> <p>query : 4cox-ligD_8</p>  | <p>Shape Tanimoto = 0.542</p> | <p>Color Tanimoto = 0.189</p> | <p>2D Graph Tanimoto = 0.154</p> |



|                                                                                                        |                               |                               |                                  |
|--------------------------------------------------------------------------------------------------------|-------------------------------|-------------------------------|----------------------------------|
| <p>Hit: database_151_181</p> <p>Rank: 163</p> <p>Tanimoto Combo = 0.729</p> <p>query : 4cox-ligD_8</p> | <p>Shape Tanimoto = 0.524</p> | <p>Color Tanimoto = 0.204</p> | <p>2D Graph Tanimoto = 0.101</p> |
| <p>Hit: database_40_31</p> <p>Rank: 164</p> <p>Tanimoto Combo = 0.728</p> <p>query : 4cox-ligD_9</p>   | <p>Shape Tanimoto = 0.546</p> | <p>Color Tanimoto = 0.182</p> | <p>2D Graph Tanimoto = 0.082</p> |
| <p>Hit: database_15_36</p> <p>Rank: 165</p> <p>Tanimoto Combo = 0.727</p> <p>query : 4cox-ligD_1</p>   | <p>Shape Tanimoto = 0.511</p> | <p>Color Tanimoto = 0.216</p> | <p>2D Graph Tanimoto = 0.067</p> |



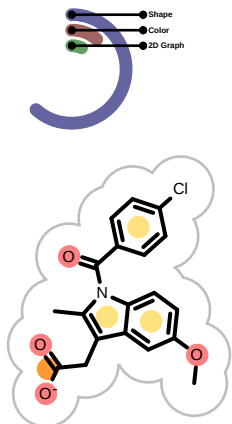
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Shape Tanimoto = 0.615

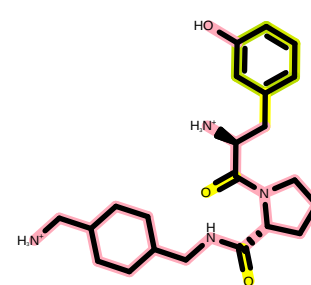
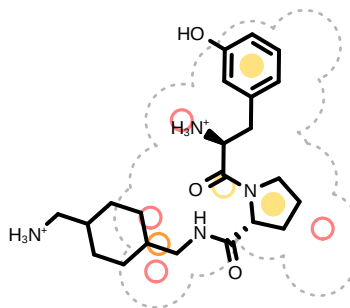
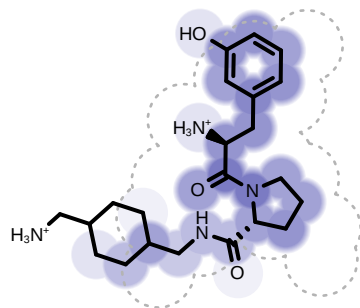
Color Tanimoto = 0.111

2D Graph Tanimoto = 0.069

Rank: 166  
Tanimoto Combo = 0.726



query : 4cox-ligD\_4



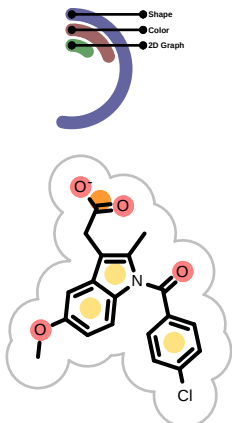
Hit: database\_134\_176

Shape Tanimoto = 0.527

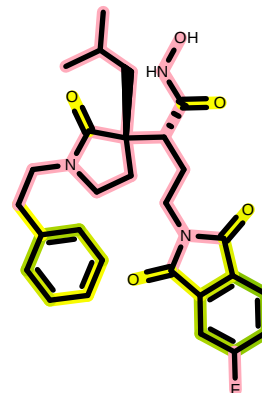
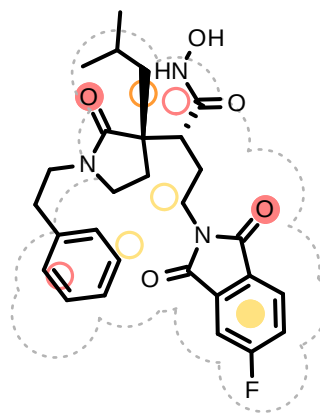
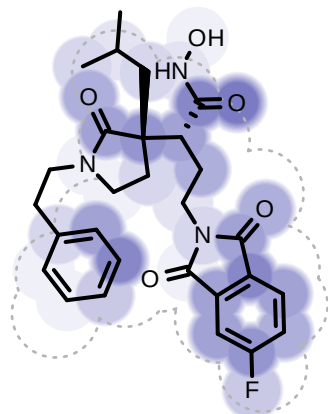
Color Tanimoto = 0.199

2D Graph Tanimoto = 0.117

Rank: 167  
Tanimoto Combo = 0.726



query : 4cox-ligD\_8



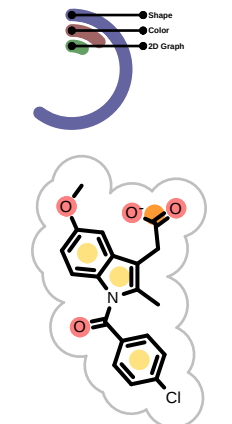
Hit: database\_3\_113

Shape Tanimoto = 0.601

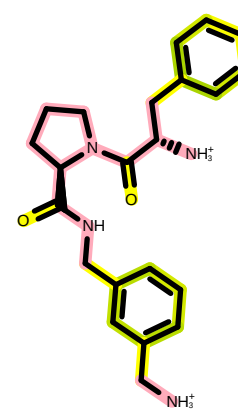
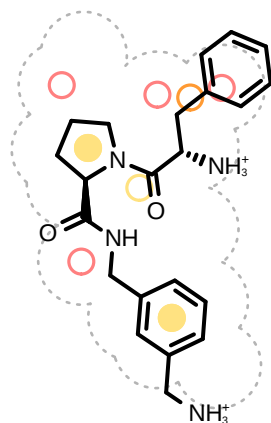
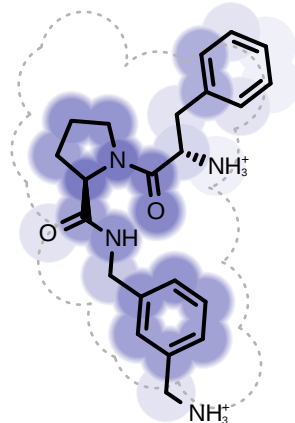
Color Tanimoto = 0.125

2D Graph Tanimoto = 0.075

Rank: 168  
Tanimoto Combo = 0.725

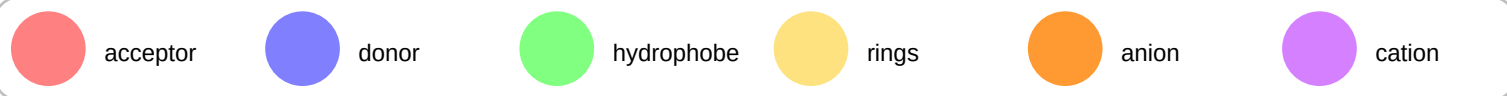


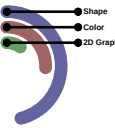
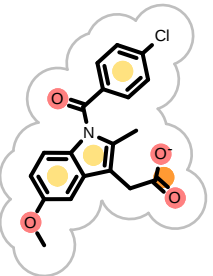
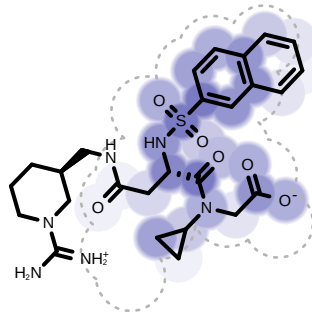
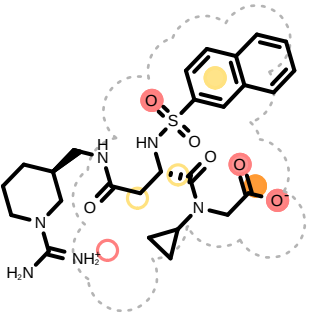
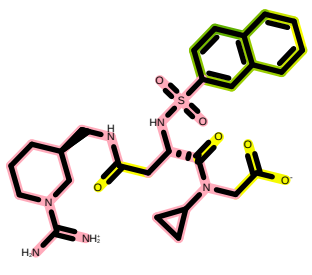
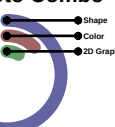
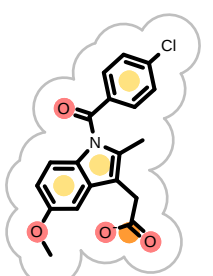
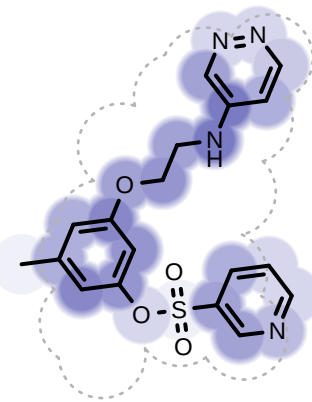
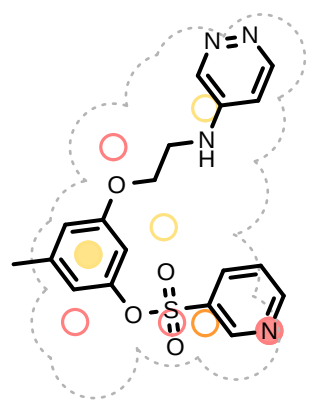
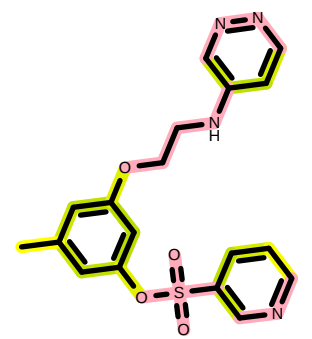
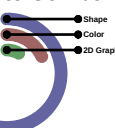
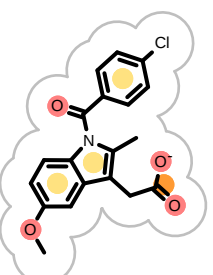
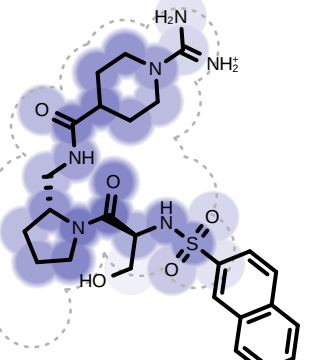
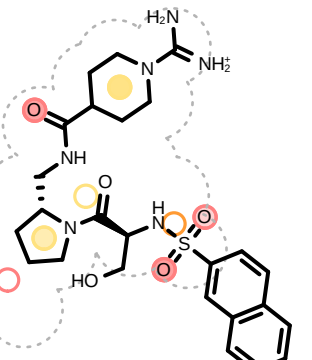
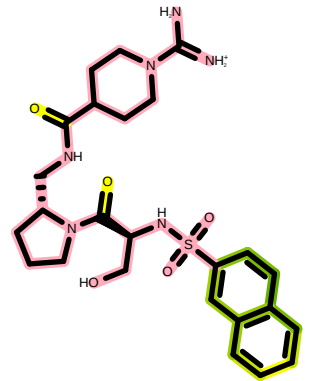
query : 4cox-ligD\_5

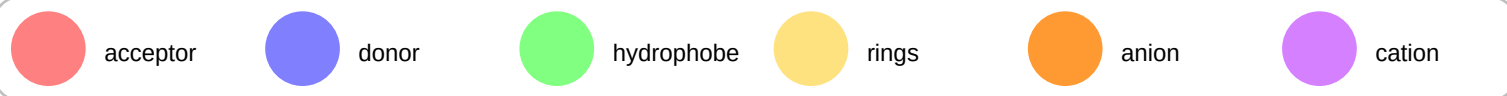


|                                                                                                                      |                                      |                                      |                                         |
|----------------------------------------------------------------------------------------------------------------------|--------------------------------------|--------------------------------------|-----------------------------------------|
| <p><b>Hit: database_8_121</b></p> <p>Rank: 169</p> <p><b>Tanimoto Combo = 0.721</b></p> <p>query : 4cox-ligD_0</p>   | <p><b>Shape Tanimoto = 0.668</b></p> | <p><b>Color Tanimoto = 0.053</b></p> | <p><b>2D Graph Tanimoto = 0.072</b></p> |
| <p><b>Hit: database_169_149</b></p> <p>Rank: 170</p> <p><b>Tanimoto Combo = 0.718</b></p> <p>query : 4cox-ligD_4</p> | <p><b>Shape Tanimoto = 0.6</b></p>   | <p><b>Color Tanimoto = 0.118</b></p> | <p><b>2D Graph Tanimoto = 0.104</b></p> |
| <p><b>Hit: database_39_191</b></p> <p>Rank: 171</p> <p><b>Tanimoto Combo = 0.717</b></p> <p>query : 4cox-ligD_9</p>  | <p><b>Shape Tanimoto = 0.537</b></p> | <p><b>Color Tanimoto = 0.18</b></p>  | <p><b>2D Graph Tanimoto = 0.139</b></p> |

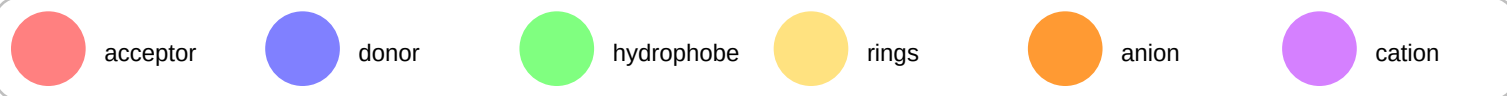




|                                                                                                                                                                                                                                                                             |                                                                                                                   |                                                                                                                    |                                                                                                                        |
|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------|
| <p>Hit: database_198_196</p> <p>Rank: 172</p> <p>Tanimoto Combo = 0.715</p>   <p>query : 4cox-ligD_7</p>   | <p>Shape Tanimoto = 0.458</p>    | <p>Color Tanimoto = 0.257</p>    | <p>2D Graph Tanimoto = 0.098</p>    |
| <p>Hit: database_78_140</p> <p>Rank: 173</p> <p>Tanimoto Combo = 0.715</p>   <p>query : 4cox-ligD_9</p> | <p>Shape Tanimoto = 0.589</p>   | <p>Color Tanimoto = 0.126</p>   | <p>2D Graph Tanimoto = 0.083</p>   |
| <p>Hit: database_1_102</p> <p>Rank: 174</p> <p>Tanimoto Combo = 0.715</p>   <p>query : 4cox-ligD_7</p> | <p>Shape Tanimoto = 0.535</p>  | <p>Color Tanimoto = 0.179</p>  | <p>2D Graph Tanimoto = 0.085</p>  |



|                                                                                                       |                               |                               |                                  |
|-------------------------------------------------------------------------------------------------------|-------------------------------|-------------------------------|----------------------------------|
| <p>Hit: database_32_165</p> <p>Rank: 175</p> <p>Tanimoto Combo = 0.714</p> <p>query : 4cox-ligD_4</p> | <p>Shape Tanimoto = 0.587</p> | <p>Color Tanimoto = 0.127</p> | <p>2D Graph Tanimoto = 0.102</p> |
| <p>Hit: database_37_96</p> <p>Rank: 176</p> <p>Tanimoto Combo = 0.705</p> <p>query : 4cox-ligD_6</p>  | <p>Shape Tanimoto = 0.579</p> | <p>Color Tanimoto = 0.126</p> | <p>2D Graph Tanimoto = 0.091</p> |
| <p>Hit: database_79_125</p> <p>Rank: 177</p> <p>Tanimoto Combo = 0.705</p> <p>query : 4cox-ligD_7</p> | <p>Shape Tanimoto = 0.545</p> | <p>Color Tanimoto = 0.159</p> | <p>2D Graph Tanimoto = 0.062</p> |



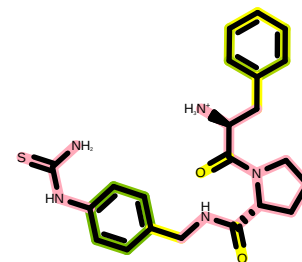
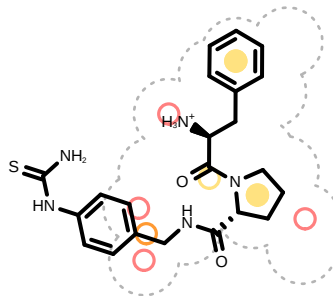
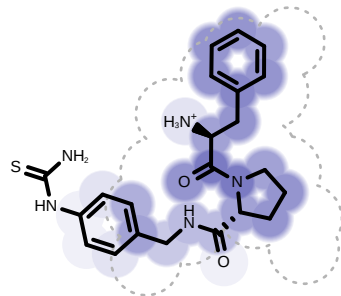
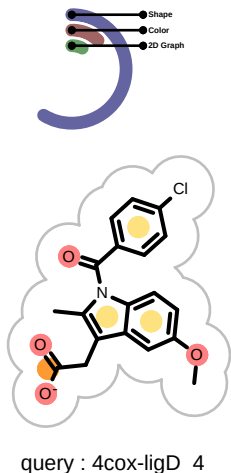
Hit: database\_172\_166

Shape Tanimoto = 0.587

Color Tanimoto = 0.118

2D Graph Tanimoto = 0.073

Rank: 178  
Tanimoto Combo = 0.705



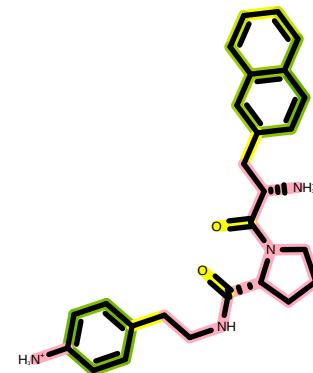
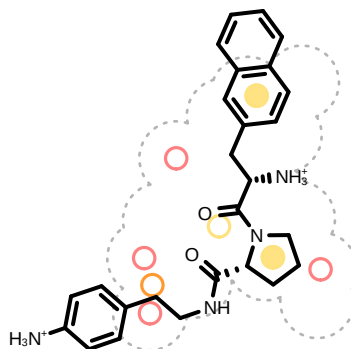
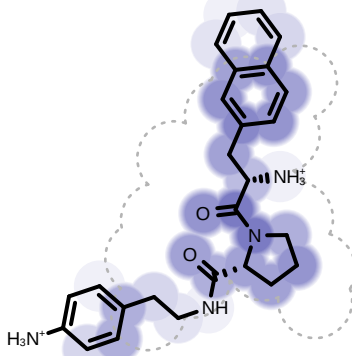
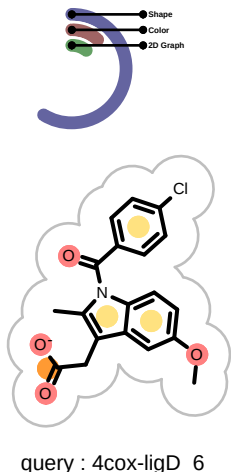
Hit: database\_107\_113

Shape Tanimoto = 0.587

Color Tanimoto = 0.116

2D Graph Tanimoto = 0.106

Rank: 179  
Tanimoto Combo = 0.703



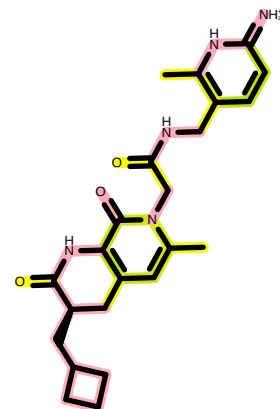
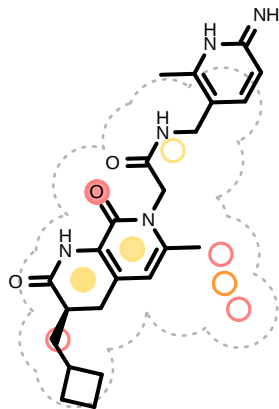
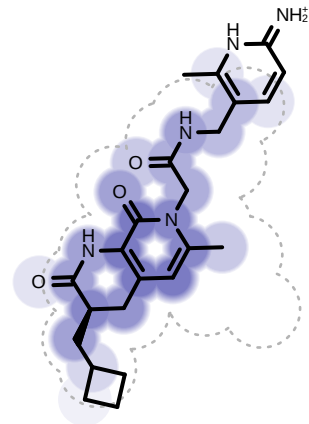
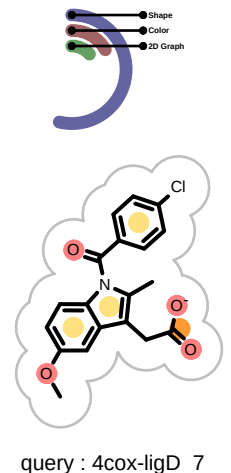
Hit: database\_202\_197

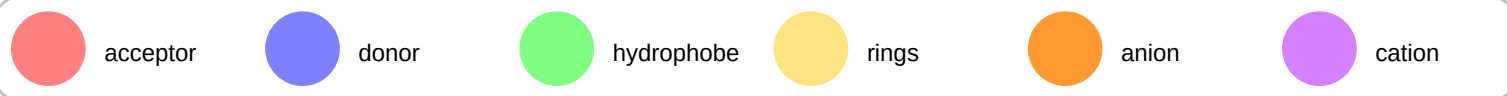
Shape Tanimoto = 0.537

Color Tanimoto = 0.166

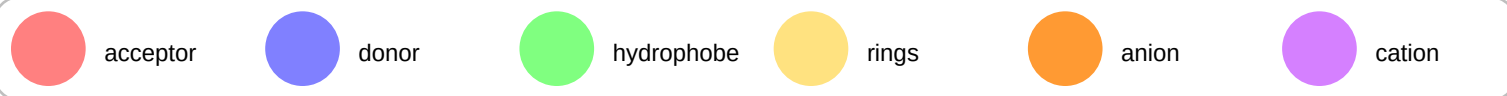
2D Graph Tanimoto = 0.136

Rank: 180  
Tanimoto Combo = 0.703

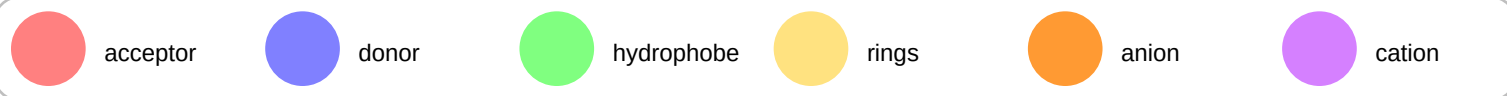


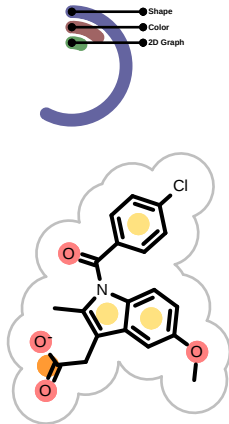
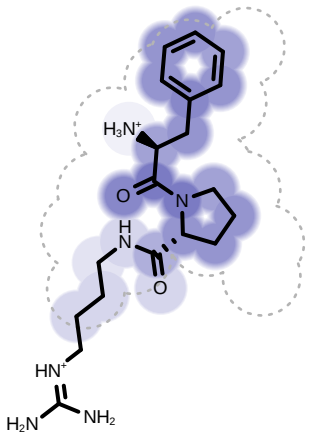
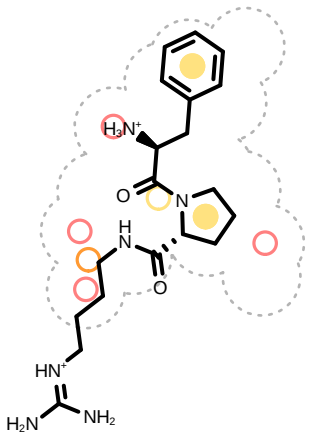
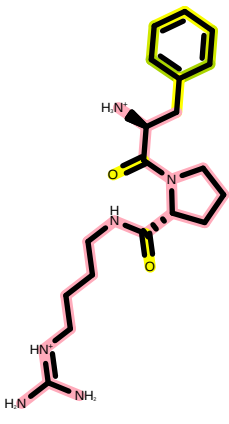
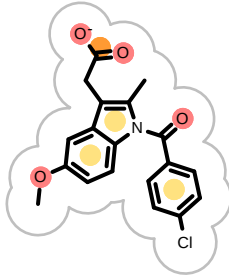
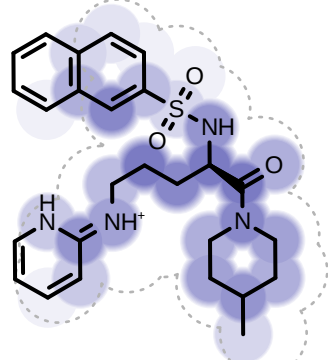
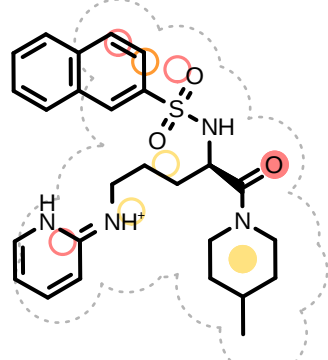
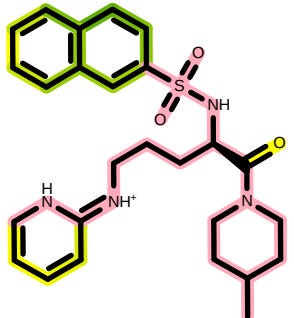
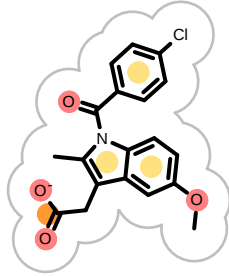
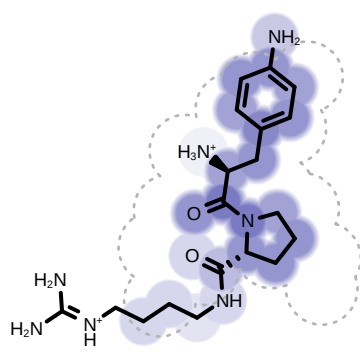
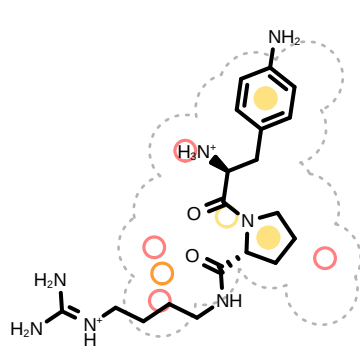
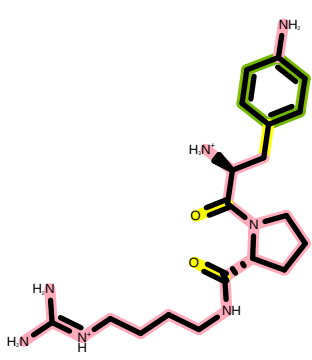


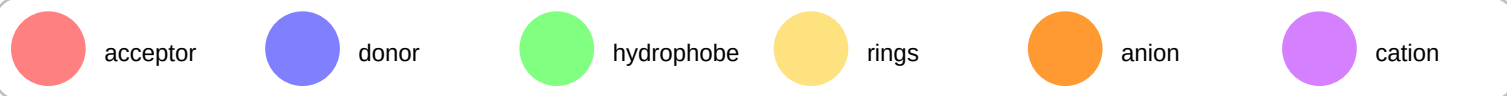
|                                                                                                        |                               |                               |                                  |
|--------------------------------------------------------------------------------------------------------|-------------------------------|-------------------------------|----------------------------------|
| <p>Hit: database_183_21</p> <p>Rank: 181</p> <p>Tanimoto Combo = 0.703</p> <p>query : 4cox-ligD_8</p>  | <p>Shape Tanimoto = 0.567</p> | <p>Color Tanimoto = 0.135</p> | <p>2D Graph Tanimoto = 0.071</p> |
| <p>Hit: database_66_15</p> <p>Rank: 182</p> <p>Tanimoto Combo = 0.703</p> <p>query : 4cox-ligD_6</p>   | <p>Shape Tanimoto = 0.591</p> | <p>Color Tanimoto = 0.111</p> | <p>2D Graph Tanimoto = 0.083</p> |
| <p>Hit: database_147_186</p> <p>Rank: 183</p> <p>Tanimoto Combo = 0.702</p> <p>query : 4cox-ligD_6</p> | <p>Shape Tanimoto = 0.526</p> | <p>Color Tanimoto = 0.176</p> | <p>2D Graph Tanimoto = 0.073</p> |



|                                                                                                        |                               |                               |                                  |
|--------------------------------------------------------------------------------------------------------|-------------------------------|-------------------------------|----------------------------------|
| <p>Hit: database_182_33</p> <p>Rank: 184</p> <p>Tanimoto Combo = 0.7</p> <p>query : 4cox-ligD_5</p>    | <p>Shape Tanimoto = 0.497</p> | <p>Color Tanimoto = 0.202</p> | <p>2D Graph Tanimoto = 0.138</p> |
| <p>Hit: database_139_102</p> <p>Rank: 185</p> <p>Tanimoto Combo = 0.699</p> <p>query : 4cox-ligD_5</p> | <p>Shape Tanimoto = 0.588</p> | <p>Color Tanimoto = 0.111</p> | <p>2D Graph Tanimoto = 0.084</p> |
| <p>Hit: database_64_136</p> <p>Rank: 186</p> <p>Tanimoto Combo = 0.698</p> <p>query : 4cox-ligD_6</p>  | <p>Shape Tanimoto = 0.586</p> | <p>Color Tanimoto = 0.111</p> | <p>2D Graph Tanimoto = 0.071</p> |



|                                                                                                                                                                                           |                                                                                                                   |                                                                                                                    |                                                                                                                        |
|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------|
| <p>Hit: database_74_150</p> <p>Rank: 187</p> <p>Tanimoto Combo = 0.696</p>  <p>query : 4cox-ligD_6</p>    | <p>Shape Tanimoto = 0.578</p>    | <p>Color Tanimoto = 0.118</p>    | <p>2D Graph Tanimoto = 0.065</p>    |
| <p>Hit: database_190_123</p> <p>Rank: 188</p> <p>Tanimoto Combo = 0.694</p>  <p>query : 4cox-ligD_8</p> | <p>Shape Tanimoto = 0.57</p>    | <p>Color Tanimoto = 0.124</p>   | <p>2D Graph Tanimoto = 0.099</p>   |
| <p>Hit: database_27_141</p> <p>Rank: 189</p> <p>Tanimoto Combo = 0.693</p>  <p>query : 4cox-ligD_6</p>  | <p>Shape Tanimoto = 0.588</p>  | <p>Color Tanimoto = 0.106</p>  | <p>2D Graph Tanimoto = 0.071</p>  |



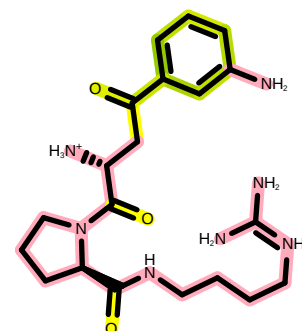
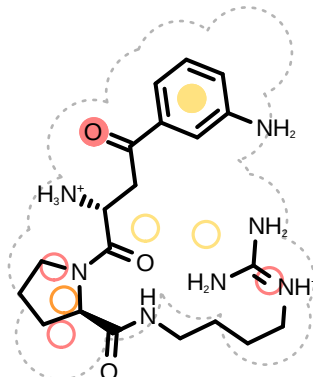
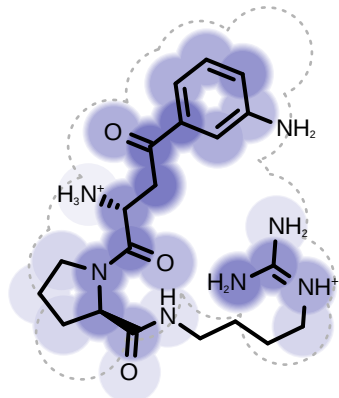
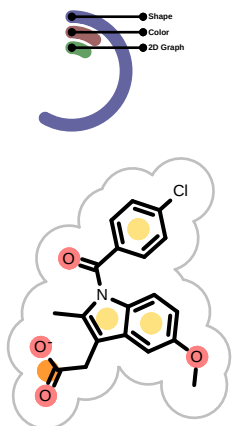
Hit: database\_60\_51

Shape Tanimoto = 0.582

Color Tanimoto = 0.101

2D Graph Tanimoto = 0.097

Rank: 190  
Tanimoto Combo = 0.683



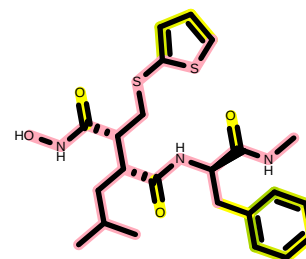
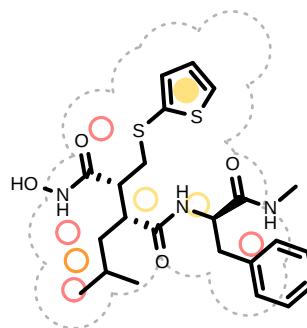
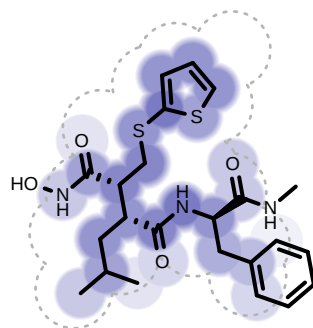
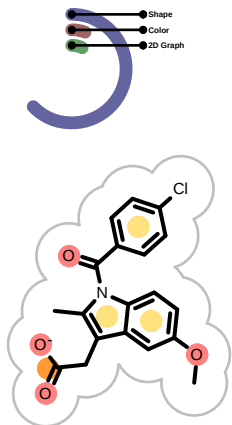
Hit: database\_148\_146

Shape Tanimoto = 0.626

Color Tanimoto = 0.055

2D Graph Tanimoto = 0.073

Rank: 191  
Tanimoto Combo = 0.681



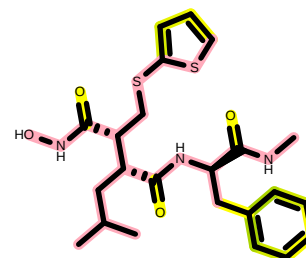
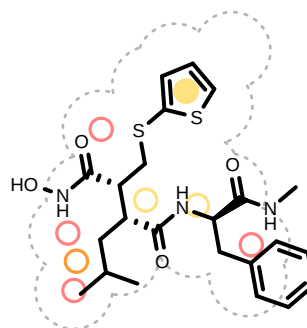
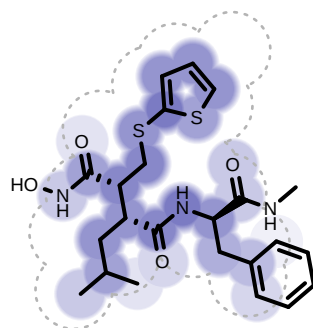
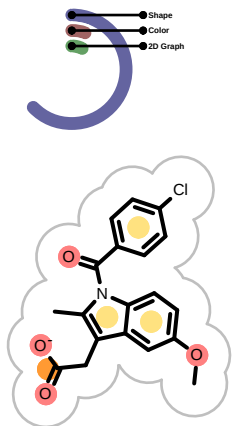
Hit: database\_207\_146

Shape Tanimoto = 0.626

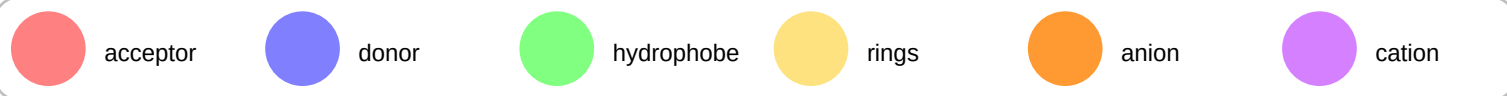
Color Tanimoto = 0.055

2D Graph Tanimoto = 0.073

Rank: 192  
Tanimoto Combo = 0.681







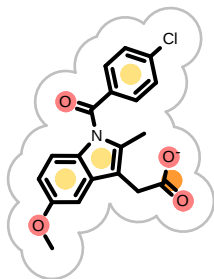
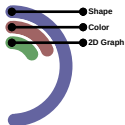
Hit: database\_48\_25

Shape Tanimoto = 0.493

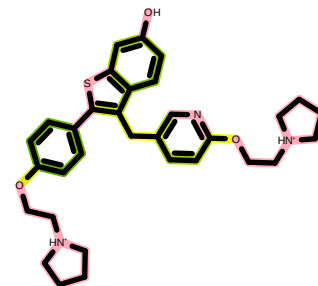
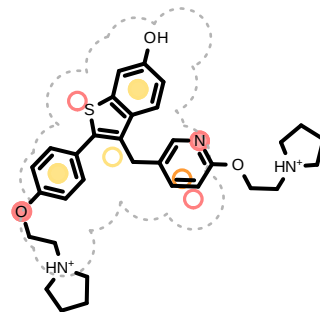
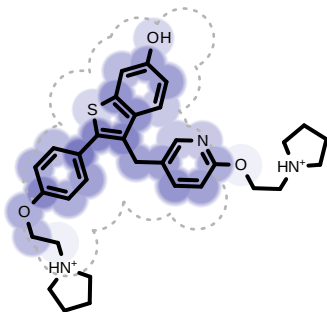
Color Tanimoto = 0.183

2D Graph Tanimoto = 0.165

Rank: 193  
Tanimoto Combo = 0.677



query : 4cox-ligD\_7



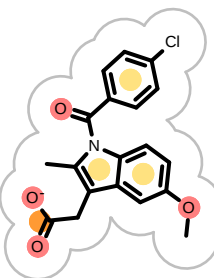
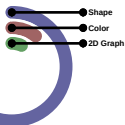
Hit: database\_77\_166

Shape Tanimoto = 0.571

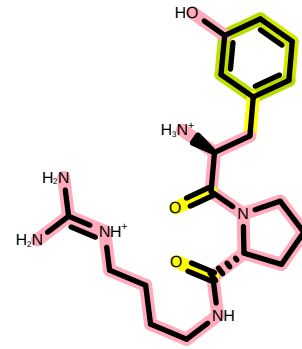
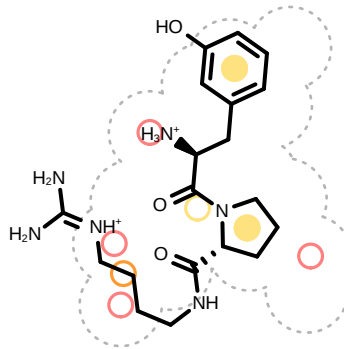
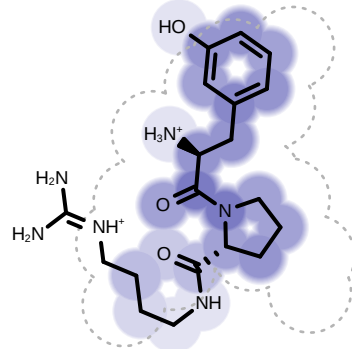
Color Tanimoto = 0.105

2D Graph Tanimoto = 0.068

Rank: 194  
Tanimoto Combo = 0.677



query : 4cox-ligD\_6



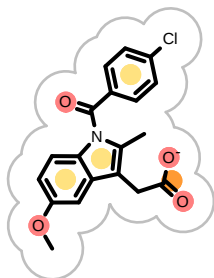
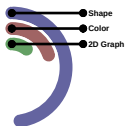
Hit: database\_121\_61

Shape Tanimoto = 0.476

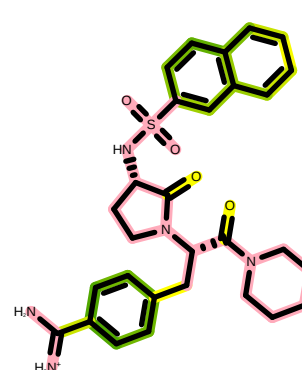
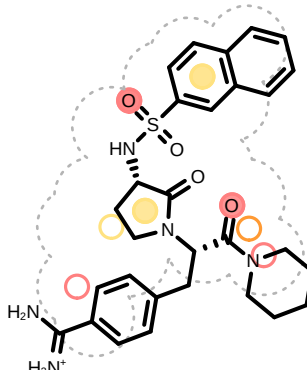
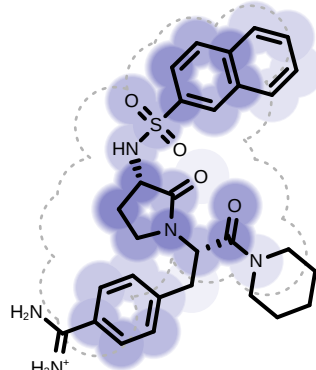
Color Tanimoto = 0.199

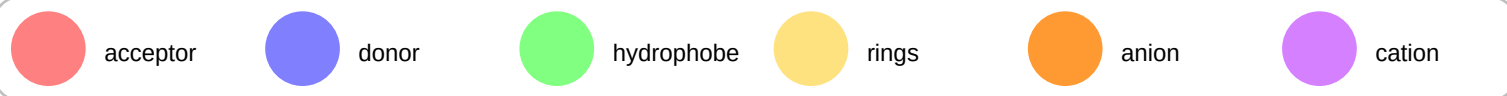
2D Graph Tanimoto = 0.108

Rank: 195  
Tanimoto Combo = 0.675



query : 4cox-ligD\_7





Hit: database\_144\_169

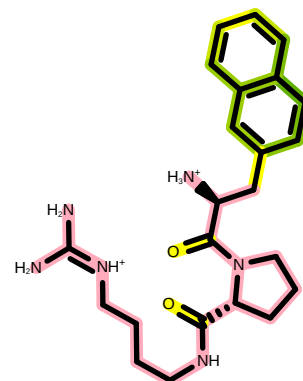
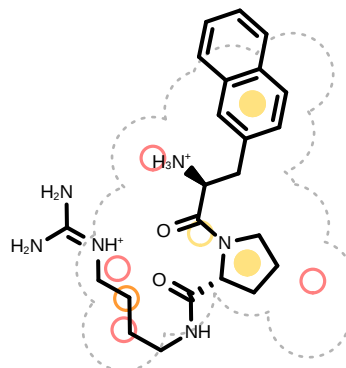
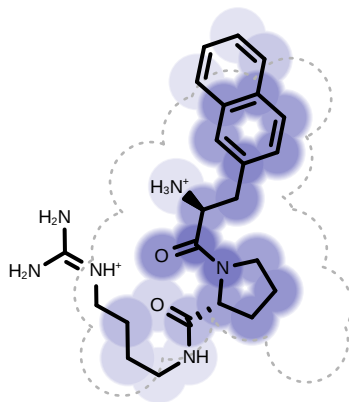
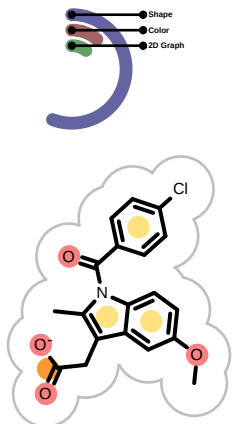
Shape Tanimoto = 0.558

Color Tanimoto = 0.112

2D Graph Tanimoto = 0.103

Rank: 196

Tanimoto Combo = 0.669



Hit: database\_7\_123

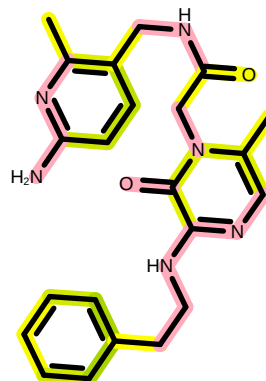
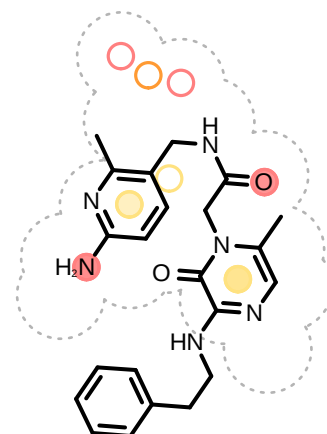
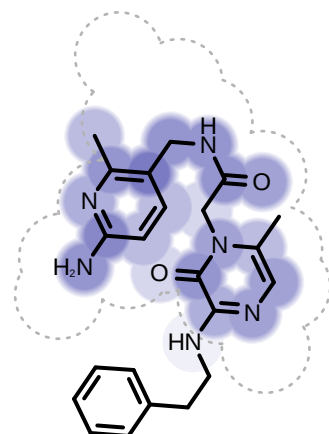
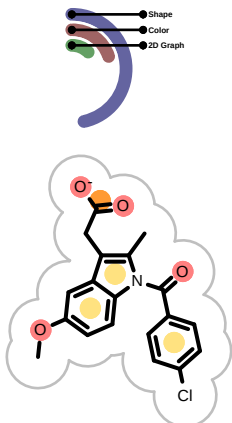
Shape Tanimoto = 0.464

Color Tanimoto = 0.199

2D Graph Tanimoto = 0.124

Rank: 197

Tanimoto Combo = 0.663



Hit: database\_124\_107

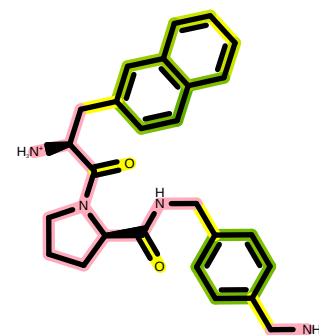
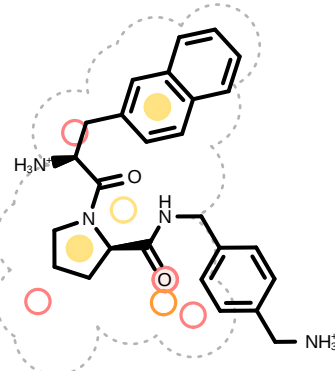
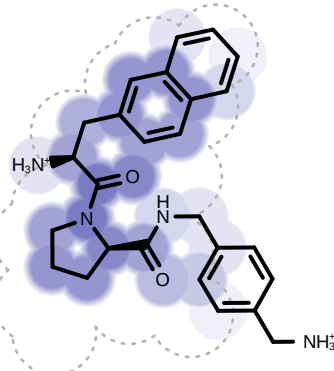
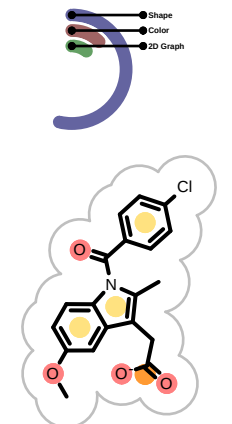
Shape Tanimoto = 0.537

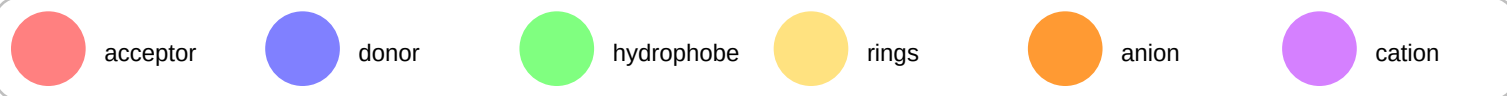
Color Tanimoto = 0.124

2D Graph Tanimoto = 0.107

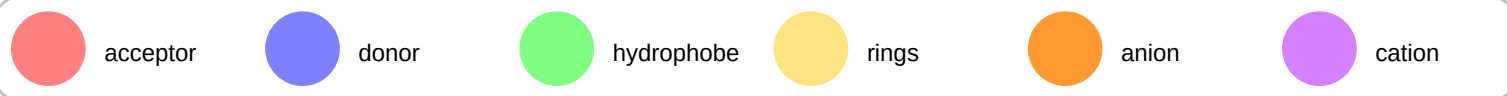
Rank: 198

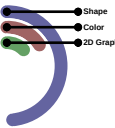
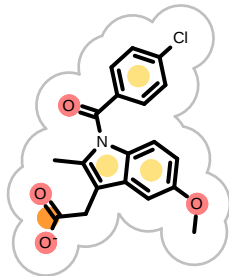
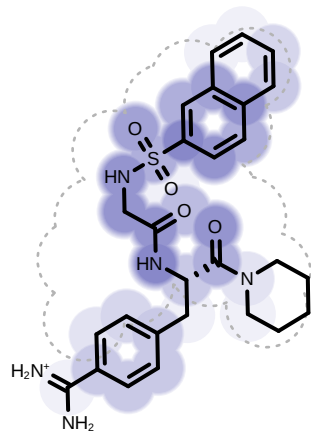
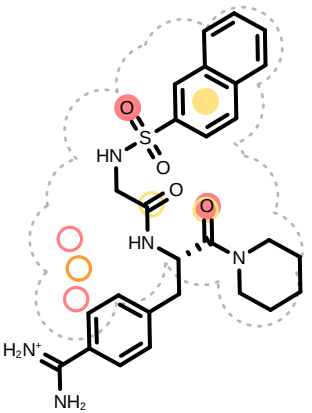
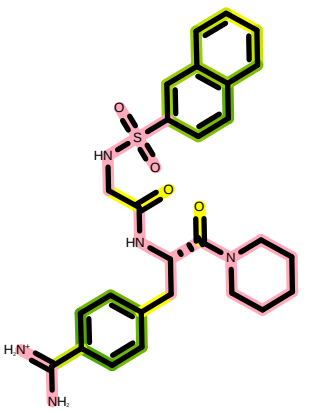
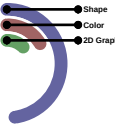
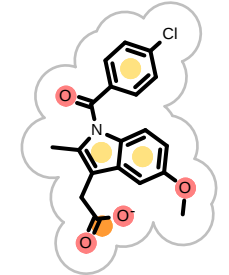
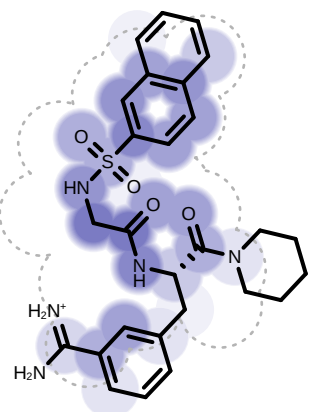
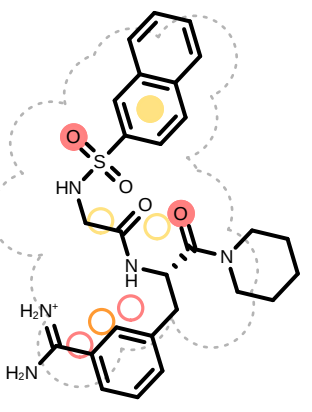
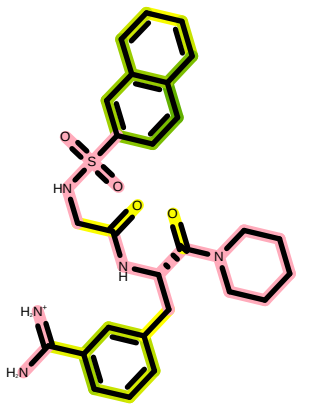
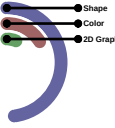
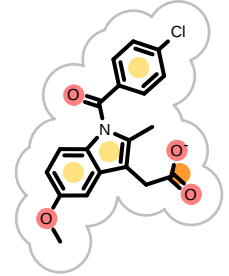
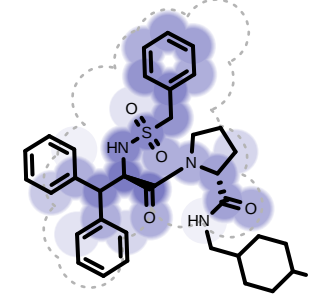
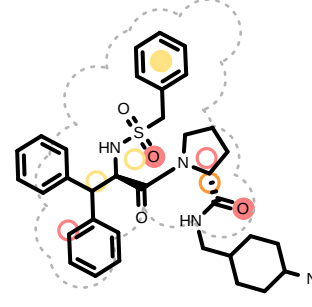
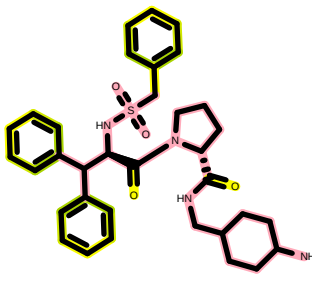
Tanimoto Combo = 0.661

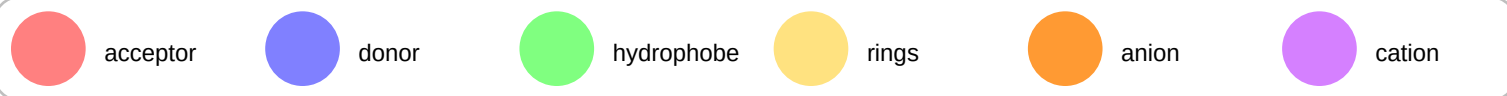




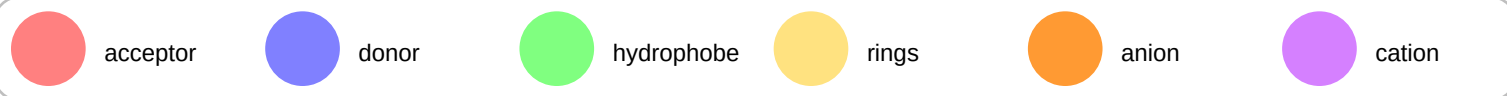
|                                                                                                        |                               |                               |                                  |
|--------------------------------------------------------------------------------------------------------|-------------------------------|-------------------------------|----------------------------------|
| <p>Hit: database_158_153</p> <p>Rank: 199</p> <p>Tanimoto Combo = 0.656</p> <p>query : 4cox-ligD_6</p> | <p>Shape Tanimoto = 0.553</p> | <p>Color Tanimoto = 0.103</p> | <p>2D Graph Tanimoto = 0.084</p> |
| <p>Hit: database_6_55</p> <p>Rank: 200</p> <p>Tanimoto Combo = 0.648</p> <p>query : 4cox-ligD_9</p>    | <p>Shape Tanimoto = 0.47</p>  | <p>Color Tanimoto = 0.178</p> | <p>2D Graph Tanimoto = 0.094</p> |
| <p>Hit: database_84_0</p> <p>Rank: 201</p> <p>Tanimoto Combo = 0.645</p> <p>query : 4cox-ligD_5</p>    | <p>Shape Tanimoto = 0.494</p> | <p>Color Tanimoto = 0.152</p> | <p>2D Graph Tanimoto = 0.087</p> |



|                                                                                                                                                                                                                                                                                           |                                                                                                                          |                                                                                                                           |                                                                                                                               |
|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------|
| <p><b>Hit: database_9_89</b></p> <p>Rank: 202</p> <p><b>Tanimoto Combo = 0.643</b></p>   <p>query : 4cox-ligD_4</p>      | <p><b>Shape Tanimoto = 0.483</b></p>    | <p><b>Color Tanimoto = 0.159</b></p>    | <p><b>2D Graph Tanimoto = 0.128</b></p>    |
| <p><b>Hit: database_102_48</b></p> <p>Rank: 203</p> <p><b>Tanimoto Combo = 0.64</b></p>   <p>query : 4cox-ligD_0</p>  | <p><b>Shape Tanimoto = 0.476</b></p>   | <p><b>Color Tanimoto = 0.164</b></p>   | <p><b>2D Graph Tanimoto = 0.124</b></p>   |
| <p><b>Hit: database_2_180</b></p> <p>Rank: 204</p> <p><b>Tanimoto Combo = 0.639</b></p>   <p>query : 4cox-ligD_7</p> | <p><b>Shape Tanimoto = 0.478</b></p>  | <p><b>Color Tanimoto = 0.161</b></p>  | <p><b>2D Graph Tanimoto = 0.064</b></p>  |



|                                                                                                        |                               |                               |                                  |
|--------------------------------------------------------------------------------------------------------|-------------------------------|-------------------------------|----------------------------------|
| <p>Hit: database_45_166</p> <p>Rank: 205</p> <p>Tanimoto Combo = 0.638</p> <p>query : 4cox-ligD_3</p>  | <p>Shape Tanimoto = 0.493</p> | <p>Color Tanimoto = 0.145</p> | <p>2D Graph Tanimoto = 0.101</p> |
| <p>Hit: database_115_158</p> <p>Rank: 206</p> <p>Tanimoto Combo = 0.636</p> <p>query : 4cox-ligD_3</p> | <p>Shape Tanimoto = 0.446</p> | <p>Color Tanimoto = 0.19</p>  | <p>2D Graph Tanimoto = 0.122</p> |
| <p>Hit: database_93_167</p> <p>Rank: 207</p> <p>Tanimoto Combo = 0.629</p> <p>query : 4cox-ligD_8</p>  | <p>Shape Tanimoto = 0.499</p> | <p>Color Tanimoto = 0.13</p>  | <p>2D Graph Tanimoto = 0.056</p> |



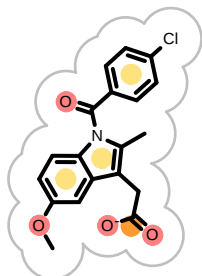
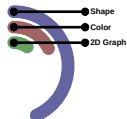
Hit: database\_187\_7

Shape Tanimoto = 0.432

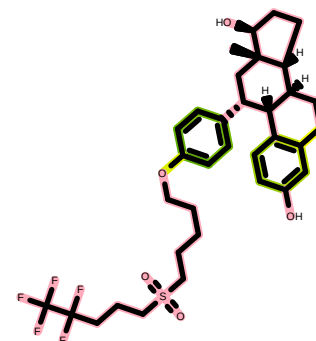
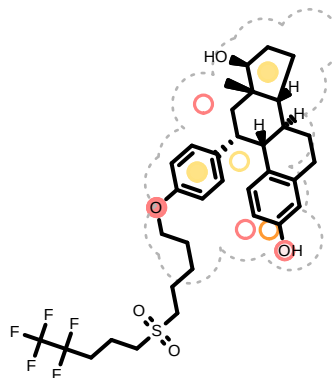
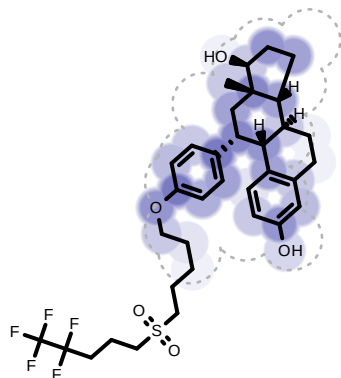
Color Tanimoto = 0.176

2D Graph Tanimoto = 0.098

Rank: 208  
Tanimoto Combo = 0.609



query : 4cox-ligD\_9



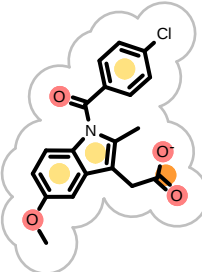
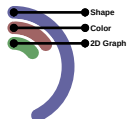
Hit: database\_110\_1

Shape Tanimoto = 0.428

Color Tanimoto = 0.154

2D Graph Tanimoto = 0.148

Rank: 209  
Tanimoto Combo = 0.582



query : 4cox-ligD\_7

