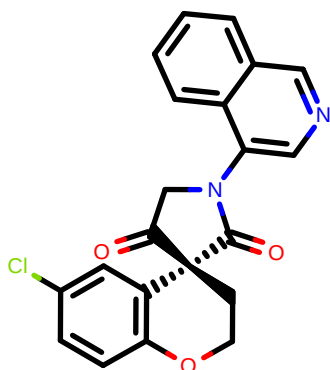
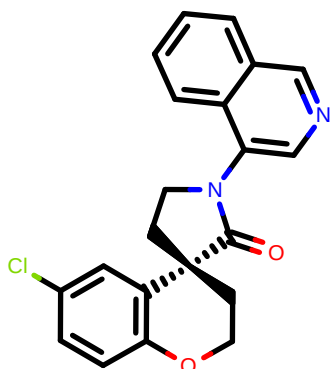


DAR-DIA-0f7b7cd9-9\_1



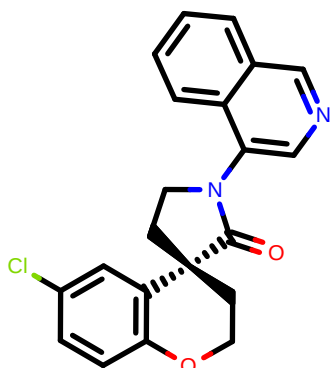
|                  |                                                                   |
|------------------|-------------------------------------------------------------------|
| CID:             | DAR-DIA-0f7b7cd9-9_1                                              |
| SMILES:          | <chem>c1ccc2c(c1)cncc2N3CC(=O)[C@@]4(C3=O)CCOc5c4cc(cc5)Cl</chem> |
| RUN:             | RUN1047                                                           |
| DDG (kcal/mol):  | -2.29                                                             |
| dDDG (kcal/mol): | 0.12                                                              |

ALP-POS-477dc5b7-4\_1



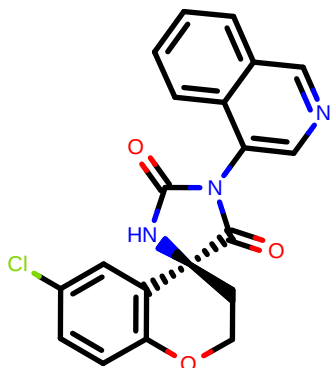
|                  |                                                               |
|------------------|---------------------------------------------------------------|
| CID:             | ALP-POS-477dc5b7-4_1                                          |
| SMILES:          | <chem>c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CCOc5c4cc(cc5)Cl</chem> |
| RUN:             | RUN1035                                                       |
| DDG (kcal/mol):  | -1.87                                                         |
| dDDG (kcal/mol): | 0.09                                                          |

EDJ-MED-159244ea-1\_1



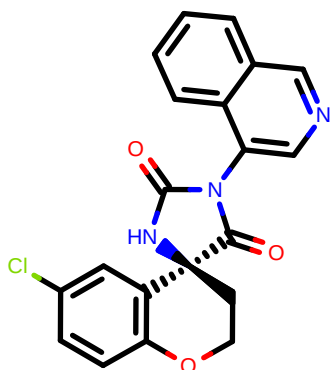
|                  |                                                               |
|------------------|---------------------------------------------------------------|
| CID:             | EDJ-MED-159244ea-1_1                                          |
| SMILES:          | <chem>c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CCOc5c4cc(cc5)Cl</chem> |
| RUN:             | RUN1022                                                       |
| DDG (kcal/mol):  | -1.75                                                         |
| dDDG (kcal/mol): | 0.08                                                          |

VLA-UNK-cf7facf1-1\_1



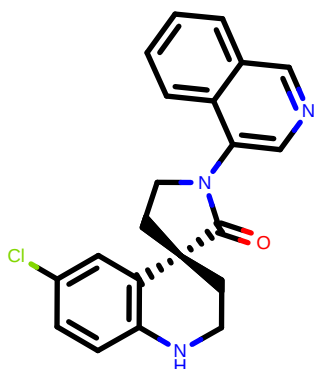
|                  |                                                                   |
|------------------|-------------------------------------------------------------------|
| CID:             | VLA-UNK-cf7facf1-1_1                                              |
| SMILES:          | <chem>c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)NC3=O</chem> |
| RUN:             | RUN1039                                                           |
| DDG (kcal/mol):  | -1.59                                                             |
| dDDG (kcal/mol): | 0.08                                                              |

## VLA-UCB-34f3ed0c-11\_1



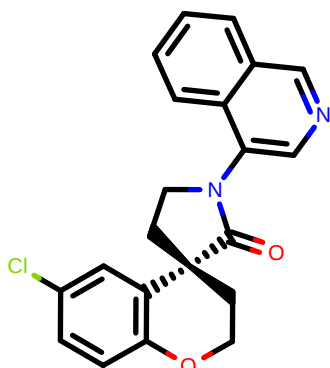
|                  |                                                                   |
|------------------|-------------------------------------------------------------------|
| CID:             | VLA-UCB-34f3ed0c-11_1                                             |
| SMILES:          | <chem>c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)NC3=O</chem> |
| RUN:             | RUN1029                                                           |
| DDG (kcal/mol):  | -1.46                                                             |
| dDDG (kcal/mol): | 0.08                                                              |

## DAR-DIA-6be260fc-5\_1



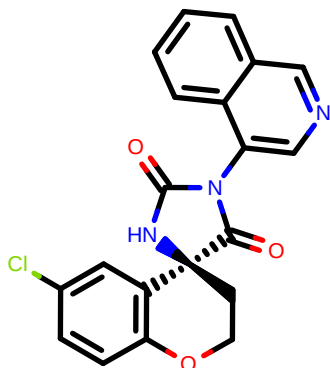
|                  |                                                               |
|------------------|---------------------------------------------------------------|
| CID:             | DAR-DIA-6be260fc-5_1                                          |
| SMILES:          | <chem>c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CCNc5c4cc(cc5)Cl</chem> |
| RUN:             | RUN1032                                                       |
| DDG (kcal/mol):  | -1.44                                                         |
| dDDG (kcal/mol): | 0.15                                                          |

## MAT-POS-983b399a-1\_1



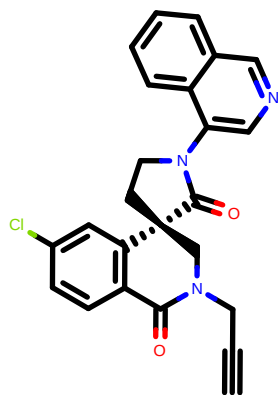
|                  |                                                               |
|------------------|---------------------------------------------------------------|
| CID:             | MAT-POS-983b399a-1_1                                          |
| SMILES:          | <chem>c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CCOc5c4cc(cc5)Cl</chem> |
| RUN:             | RUN1031                                                       |
| DDG (kcal/mol):  | -1.36                                                         |
| dDDG (kcal/mol): | 0.10                                                          |

## VLA-UCB-29506327-1\_1



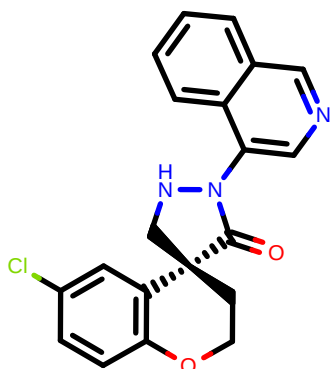
|                  |                                                                   |
|------------------|-------------------------------------------------------------------|
| CID:             | VLA-UCB-29506327-1_1                                              |
| SMILES:          | <chem>c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)NC3=O</chem> |
| RUN:             | RUN1037                                                           |
| DDG (kcal/mol):  | -1.36                                                             |
| dDDG (kcal/mol): | 0.09                                                              |

## PET-UNK-aa57768f-9\_1



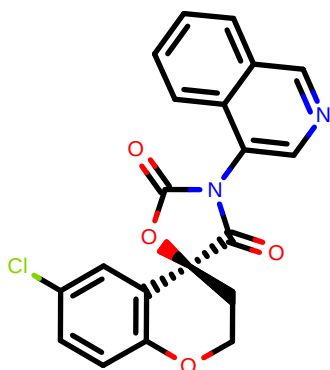
|                  |                                                                    |
|------------------|--------------------------------------------------------------------|
| CID:             | PET-UNK-aa57768f-9_1                                               |
| SMILES:          | <chem>C#CCN1C[C@]2(CCN(C2=O)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl</chem> |
| RUN:             | RUN1052                                                            |
| DDG (kcal/mol):  | -1.27                                                              |
| dDDG (kcal/mol): | 0.16                                                               |

## BEN-BAS-c2bc0d80-3\_1



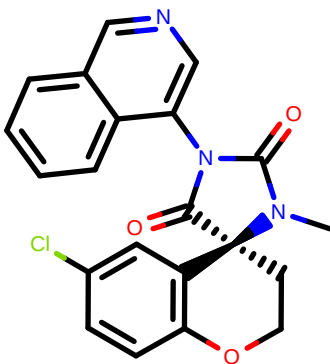
|                  |                                                                 |
|------------------|-----------------------------------------------------------------|
| CID:             | BEN-BAS-c2bc0d80-3_1                                            |
| SMILES:          | <chem>c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)CN3</chem> |
| RUN:             | RUN1034                                                         |
| DDG (kcal/mol):  | -1.01                                                           |
| dDDG (kcal/mol): | 0.09                                                            |

## MAT-POS-90505e2b-1\_1



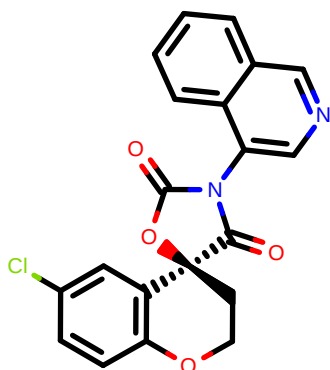
|                  |                                                                   |
|------------------|-------------------------------------------------------------------|
| CID:             | MAT-POS-90505e2b-1_1                                              |
| SMILES:          | <chem>c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)OC3=O</chem> |
| RUN:             | RUN1030                                                           |
| DDG (kcal/mol):  | -0.55                                                             |
| dDDG (kcal/mol): | 0.06                                                              |

## BEN-BAS-c2bc0d80-7\_1



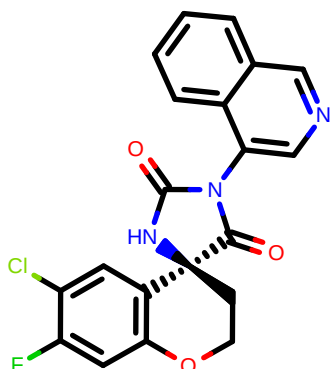
|                  |                                                                    |
|------------------|--------------------------------------------------------------------|
| CID:             | BEN-BAS-c2bc0d80-7_1                                               |
| SMILES:          | <chem>CN1C(=O)N(C(=O)[C@@]12CCOC3c2cc(cc3)Cl)c4cncc5c4cccc5</chem> |
| RUN:             | RUN1049                                                            |
| DDG (kcal/mol):  | -0.53                                                              |
| dDDG (kcal/mol): | 0.10                                                               |

MAT-POS-ec6d90b7-2\_1



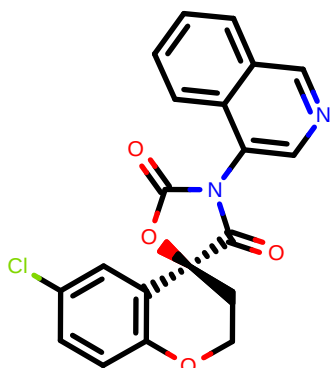
|                  |                                                                   |
|------------------|-------------------------------------------------------------------|
| CID:             | MAT-POS-ec6d90b7-2_1                                              |
| SMILES:          | <chem>c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)OC3=O</chem> |
| RUN:             | RUN1050                                                           |
| DDG (kcal/mol):  | -0.47                                                             |
| dDDG (kcal/mol): | 0.08                                                              |

VLA-UNK-3a43cd95-1\_1



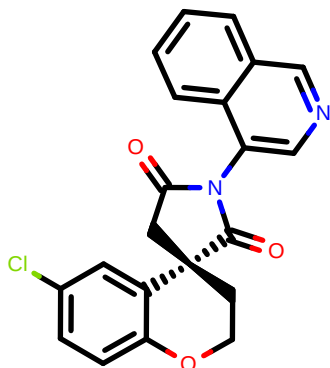
|                  |                                                                      |
|------------------|----------------------------------------------------------------------|
| CID:             | VLA-UNK-3a43cd95-1_1                                                 |
| SMILES:          | <chem>c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(c(c5)F)Cl)NC3=O</chem> |
| RUN:             | RUN1046                                                              |
| DDG (kcal/mol):  | -0.31                                                                |
| dDDG (kcal/mol): | 0.08                                                                 |

MAT-POS-ec6d90b7-1\_1



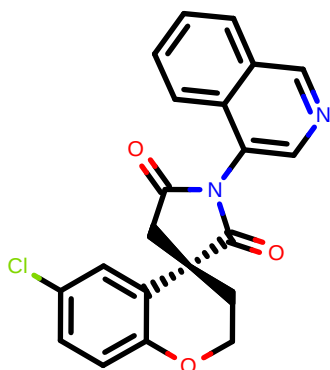
|                  |                                                                   |
|------------------|-------------------------------------------------------------------|
| CID:             | MAT-POS-ec6d90b7-1_1                                              |
| SMILES:          | <chem>c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)OC3=O</chem> |
| RUN:             | RUN1038                                                           |
| DDG (kcal/mol):  | -0.02                                                             |
| dDDG (kcal/mol): | 0.06                                                              |

VLA-UCB-50c39ae8-2\_1



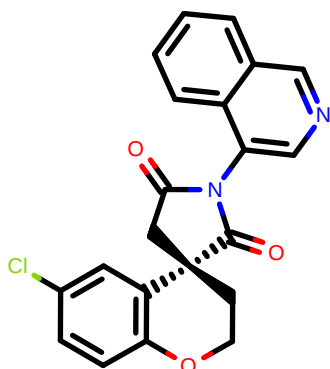
|                  |                                                                   |
|------------------|-------------------------------------------------------------------|
| CID:             | VLA-UCB-50c39ae8-2_1                                              |
| SMILES:          | <chem>c1ccc2c(c1)cncc2N3C(=O)C[C@@]4(C3=O)CCOc5c4cc(cc5)Cl</chem> |
| RUN:             | RUN1033                                                           |
| DDG (kcal/mol):  | -0.01                                                             |
| dDDG (kcal/mol): | 0.03                                                              |

BEN-BAS-c2bc0d80-6\_1



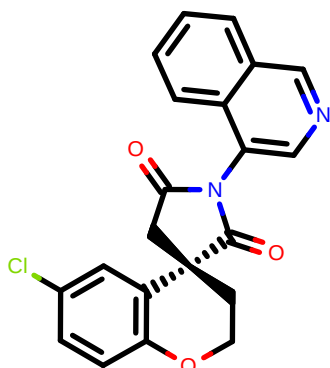
|                  |                                                                   |
|------------------|-------------------------------------------------------------------|
| CID:             | BEN-BAS-c2bc0d80-6_1                                              |
| SMILES:          | <chem>c1ccc2c(c1)cncc2N3C(=O)C[C@@]4(C3=O)CCOc5c4cc(cc5)Cl</chem> |
| RUN:             | RUN1036                                                           |
| DDG (kcal/mol):  | 0.00                                                              |
| dDDG (kcal/mol): | 0.00                                                              |

VLA-UCB-05e51b3f-5\_1



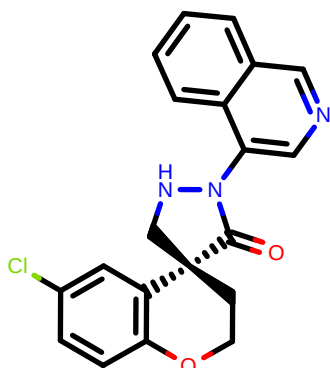
|                  |                                                                   |
|------------------|-------------------------------------------------------------------|
| CID:             | VLA-UCB-05e51b3f-5_1                                              |
| SMILES:          | <chem>c1ccc2c(c1)cncc2N3C(=O)C[C@@]4(C3=O)CCOc5c4cc(cc5)Cl</chem> |
| RUN:             | RUN1043                                                           |
| DDG (kcal/mol):  | -0.00                                                             |
| dDDG (kcal/mol): | 0.00                                                              |

MAT-POS-94643566-1\_1



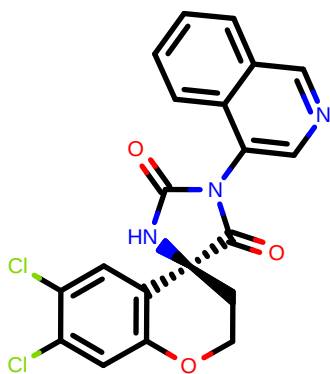
|                  |                                                                   |
|------------------|-------------------------------------------------------------------|
| CID:             | MAT-POS-94643566-1_1                                              |
| SMILES:          | <chem>c1ccc2c(c1)cncc2N3C(=O)C[C@@]4(C3=O)CCOc5c4cc(cc5)Cl</chem> |
| RUN:             | RUN1041                                                           |
| DDG (kcal/mol):  | 0.03                                                              |
| dDDG (kcal/mol): | 0.04                                                              |

BRU-THA-73c97d88-1\_1



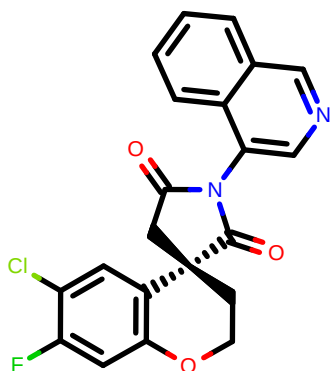
|                  |                                                                  |
|------------------|------------------------------------------------------------------|
| CID:             | BRU-THA-73c97d88-1_1                                             |
| SMILES:          | <chem>c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)C=N3</chem> |
| RUN:             | RUN1024                                                          |
| DDG (kcal/mol):  | 0.42                                                             |
| dDDG (kcal/mol): | 0.07                                                             |

VLA-UNK-56836b69-2\_1



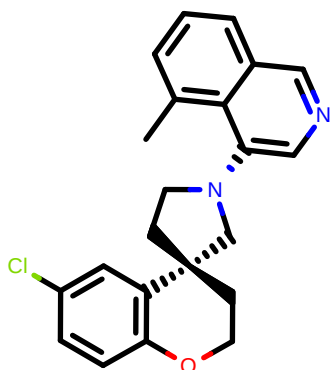
|                  |                                                                      |
|------------------|----------------------------------------------------------------------|
| CID:             | VLA-UNK-56836b69-2_1                                                 |
| SMILES:          | <chem>c1ccc2c(c1)cnc2N3C(=O)[C@@]4(CCOC5c4cc(c(c5)Cl)Cl)NC3=O</chem> |
| RUN:             | RUN1048                                                              |
| DDG (kcal/mol):  | 0.65                                                                 |
| dDDG (kcal/mol): | 0.11                                                                 |

VLA-UNK-3a43cd95-3\_1



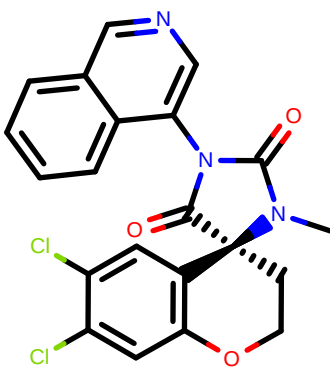
|                  |                                                                     |
|------------------|---------------------------------------------------------------------|
| CID:             | VLA-UNK-3a43cd95-3_1                                                |
| SMILES:          | <chem>c1ccc2c(c1)cnc2N3C(=O)C[C@@]4(C3=O)CCOC5c4cc(c(c5)F)Cl</chem> |
| RUN:             | RUN1042                                                             |
| DDG (kcal/mol):  | 0.69                                                                |
| dDDG (kcal/mol): | 0.15                                                                |

EDJ-MED-a6bab6fb-1\_1



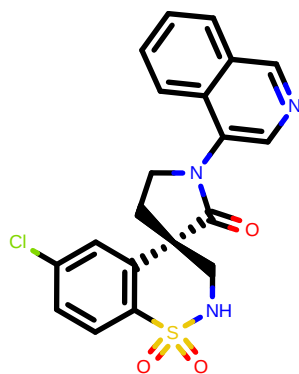
|                  |                                                              |
|------------------|--------------------------------------------------------------|
| CID:             | EDJ-MED-a6bab6fb-1_1                                         |
| SMILES:          | <chem>Cc1cccc2c1c(cnc2)N3CC[C@@]4(C3)CCOC5c4cc(cc5)Cl</chem> |
| RUN:             | RUN1025                                                      |
| DDG (kcal/mol):  | 0.93                                                         |
| dDDG (kcal/mol): | 0.13                                                         |

VLA-UNK-56836b69-3\_1



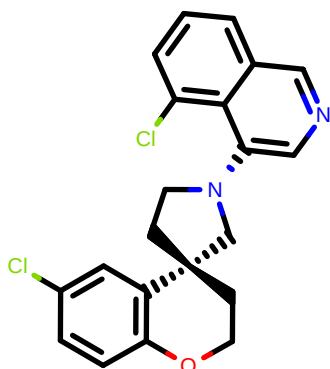
|                  |                                                                       |
|------------------|-----------------------------------------------------------------------|
| CID:             | VLA-UNK-56836b69-3_1                                                  |
| SMILES:          | <chem>CN1C(=O)N(C(=O)[C@@]12CCOC3c2cc(c(c3)Cl)Cl)c4cnc5c4cccc5</chem> |
| RUN:             | RUN1044                                                               |
| DDG (kcal/mol):  | 0.97                                                                  |
| dDDG (kcal/mol): | 0.14                                                                  |

## ALP-POS-4483ae88-1\_1



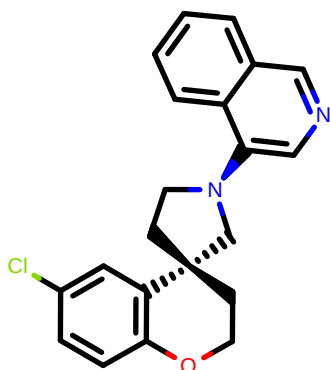
|                  |                                                                      |
|------------------|----------------------------------------------------------------------|
| CID:             | ALP-POS-4483ae88-1_1                                                 |
| SMILES:          | <chem>c1ccc2c(c1)cncc2N3CC[C@]4(C3=O)CNS(=O)(=O)c5c4cc(cc5)Cl</chem> |
| RUN:             | RUN1053                                                              |
| DDG (kcal/mol):  | 1.02                                                                 |
| dDDG (kcal/mol): | 0.19                                                                 |

## EDJ-MED-e78d5f1a-1\_1



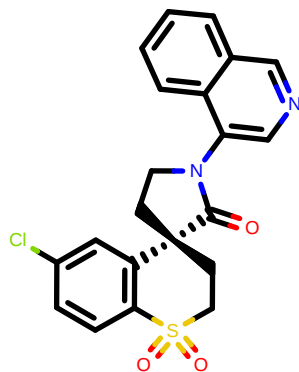
|                  |                                                                |
|------------------|----------------------------------------------------------------|
| CID:             | EDJ-MED-e78d5f1a-1_1                                           |
| SMILES:          | <chem>c1cc2cncc(c2c(c1)Cl)N3CC[C@]4(C3)CCOc5c4cc(cc5)Cl</chem> |
| RUN:             | RUN1027                                                        |
| DDG (kcal/mol):  | 1.12                                                           |
| dDDG (kcal/mol): | 0.12                                                           |

## EDJ-MED-159244ea-2\_1



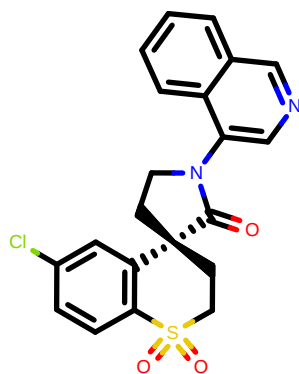
|                  |                                                            |
|------------------|------------------------------------------------------------|
| CID:             | EDJ-MED-159244ea-2_1                                       |
| SMILES:          | <chem>c1ccc2c(c1)cncc2N3CC[C@]4(C3)CCOc5c4cc(cc5)Cl</chem> |
| RUN:             | RUN1023                                                    |
| DDG (kcal/mol):  | 1.42                                                       |
| dDDG (kcal/mol): | 0.12                                                       |

## ALP-POS-41e2080f-1\_1



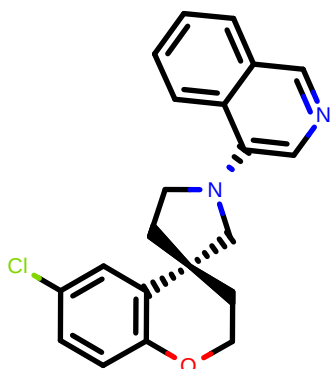
|                  |                                                                      |
|------------------|----------------------------------------------------------------------|
| CID:             | ALP-POS-41e2080f-1_1                                                 |
| SMILES:          | <chem>c1ccc2c(c1)cncc2N3CC[C@]4(C3=O)CCS(=O)(=O)c5c4cc(cc5)Cl</chem> |
| RUN:             | RUN1045                                                              |
| DDG (kcal/mol):  | 1.42                                                                 |
| dDDG (kcal/mol): | 0.16                                                                 |

EDJ-MED-d4864bdc-3\_1



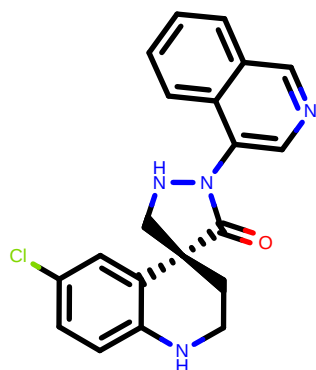
|                  |                                                                      |
|------------------|----------------------------------------------------------------------|
| CID:             | EDJ-MED-d4864bdc-3_1                                                 |
| SMILES:          | <chem>c1ccc2c(c1)cncc2N3CC[C@]4(C3=O)CCS(=O)(=O)c5c4cc(cc5)Cl</chem> |
| RUN:             | RUN1051                                                              |
| DDG (kcal/mol):  | 1.66                                                                 |
| dDDG (kcal/mol): | 0.20                                                                 |

MAT-POS-983b399a-2\_1



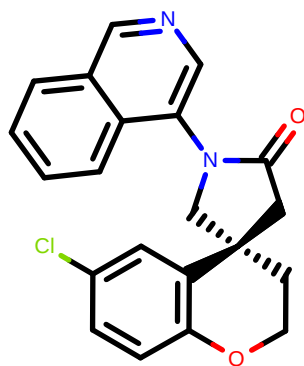
|                  |                                                            |
|------------------|------------------------------------------------------------|
| CID:             | MAT-POS-983b399a-2_1                                       |
| SMILES:          | <chem>c1ccc2c(c1)cncc2N3CC[C@]4(C3)CCOc5c4cc(cc5)Cl</chem> |
| RUN:             | RUN1020                                                    |
| DDG (kcal/mol):  | 2.06                                                       |
| dDDG (kcal/mol): | 0.16                                                       |

BRU-THA-55eab31a-1\_1



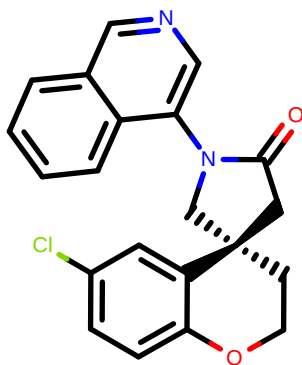
|                  |                                                                  |
|------------------|------------------------------------------------------------------|
| CID:             | BRU-THA-55eab31a-1_1                                             |
| SMILES:          | <chem>c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCNc5c4cc(cc5)Cl)C=N3</chem> |
| RUN:             | RUN1028                                                          |
| DDG (kcal/mol):  | 2.68                                                             |
| dDDG (kcal/mol): | 0.19                                                             |

EDJ-MED-159244ea-3\_1



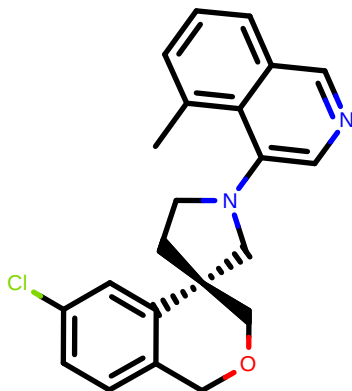
|                  |                                                              |
|------------------|--------------------------------------------------------------|
| CID:             | EDJ-MED-159244ea-3_1                                         |
| SMILES:          | <chem>c1ccc2c(c1)cncc2N3C[C@]4(CCOc5c4cc(cc5)Cl)CC3=O</chem> |
| RUN:             | RUN1021                                                      |
| DDG (kcal/mol):  | 2.98                                                         |
| dDDG (kcal/mol): | 0.10                                                         |

MAT-POS-983b399a-3\_1



|                  |                                                              |
|------------------|--------------------------------------------------------------|
| CID:             | MAT-POS-983b399a-3_1                                         |
| SMILES:          | <chem>c1ccc2c(c1)cnc2N3C[C@@]4(CCOc5c4cc(cc5)Cl)CC3=O</chem> |
| RUN:             | RUN1026                                                      |
| DDG (kcal/mol):  | 3.56                                                         |
| dDDG (kcal/mol): | 0.11                                                         |

EDJ-MED-f3cfbbb5-1\_1



|                  |                                                              |
|------------------|--------------------------------------------------------------|
| CID:             | EDJ-MED-f3cfbbb5-1_1                                         |
| SMILES:          | <chem>Cc1cccc2c1c(cnc2)N3CC[C@@]4(C3)COCc5c4cc(cc5)Cl</chem> |
| RUN:             | RUN1040                                                      |
| DDG (kcal/mol):  | 3.92                                                         |
| dDDG (kcal/mol): | 0.17                                                         |