

REINVENT4 Runs Comparison Report

Generated: 2025-10-18 11:18:14
Total Runs: 12

SUMMARY OF ALL RUNS

archive:
 Gold candidates: 0
 High candidates: 0
 Good candidates: 0
 Promising: 0

run12_t1200:
 Gold candidates: 59
 High candidates: 114803
 Good candidates: 247898
 Promising: 61
 Total molecules: 511792

run13b:
 Gold candidates: 89
 High candidates: 177539
 Good candidates: 380718
 Promising: 97
 Total molecules: 835852

run13c:
 Gold candidates: 316
 High candidates: 93676
 Good candidates: 177781
 Promising: 747
 Total molecules: 1021353

run14a:
 Gold candidates: 113
 High candidates: 303121
 Good candidates: 674225
 Promising: 123
 Total molecules: 943233

run15:
 Gold candidates: 112
 High candidates: 148661
 Good candidates: 366052
 Promising: 125
 Total molecules: 903297

run3:
 Gold candidates: 0
 High candidates: 0
 Good candidates: 0
 Promising: 2233
 Total molecules: 122551

run4:
 Gold candidates: 0
 High candidates: 0
 Good candidates: 0
 Promising: 440
 Total molecules: 125965

run5_labinvent:
 Gold candidates: 6
 High candidates: 28230
 Good candidates: 47662
 Promising: 6
 Total molecules: 95998

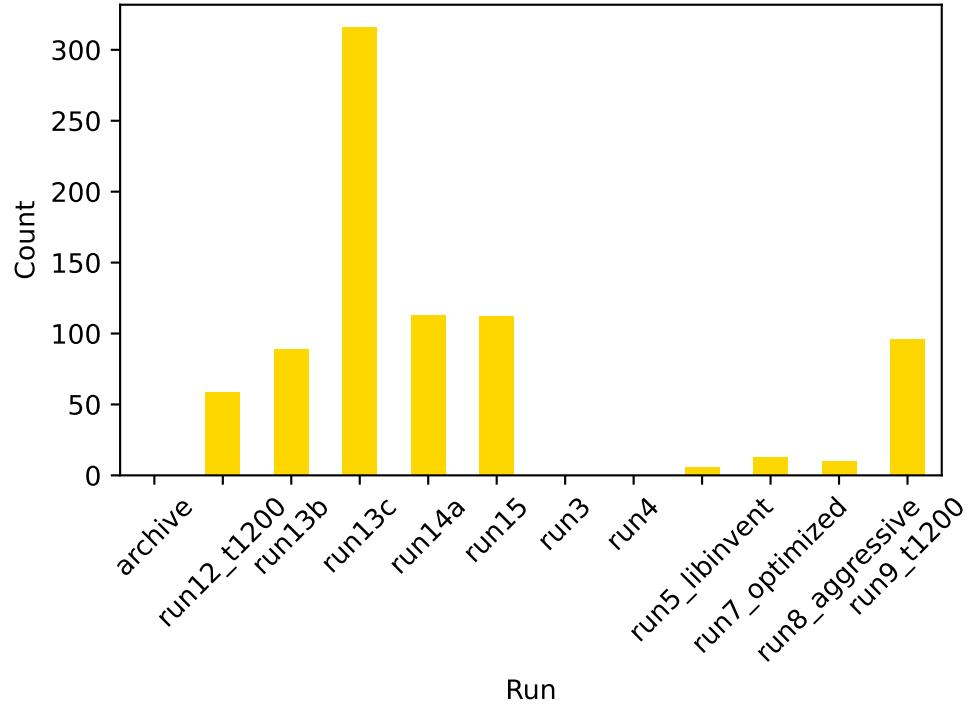
run7_optimized:
 Gold candidates: 13
 High candidates: 43866
 Good candidates: 63356
 Promising: 15
 Total molecules: 95997

run8_aggressive:
 Gold candidates: 10
 High candidates: 11831
 Good candidates: 17227
 Promising: 10
 Total molecules: 27776

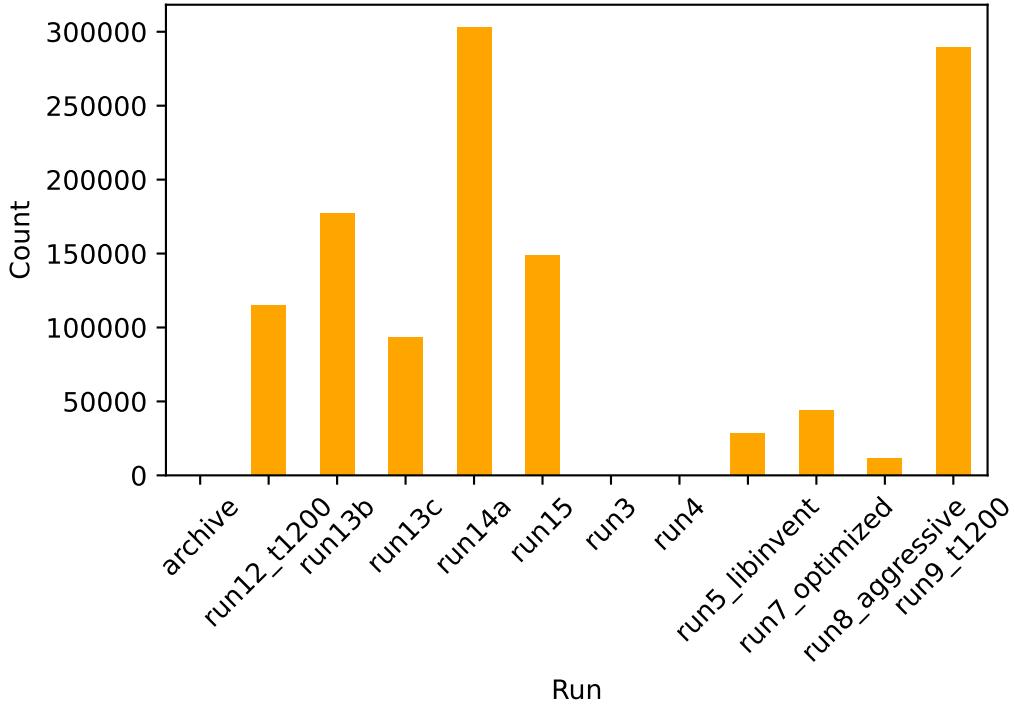
run9_t1200:
 Gold candidates: 96
 High candidates: 289397
 Good candidates: 607640
 Promising: 103
 Total molecules: 1136114

Candidates Comparison Across Runs

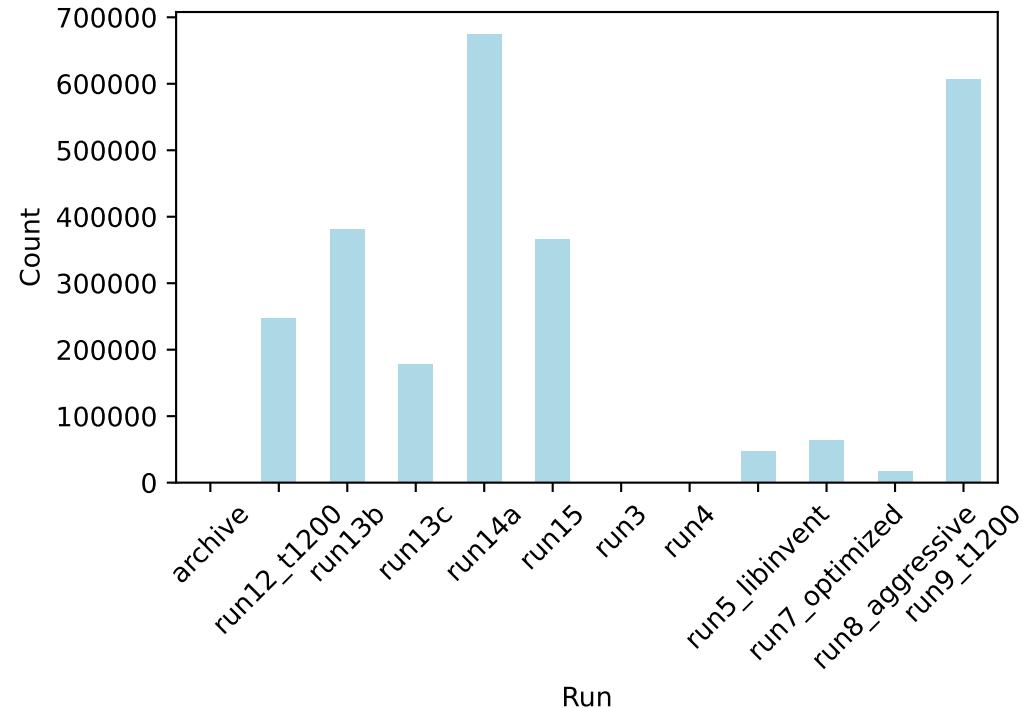
Gold Candidates



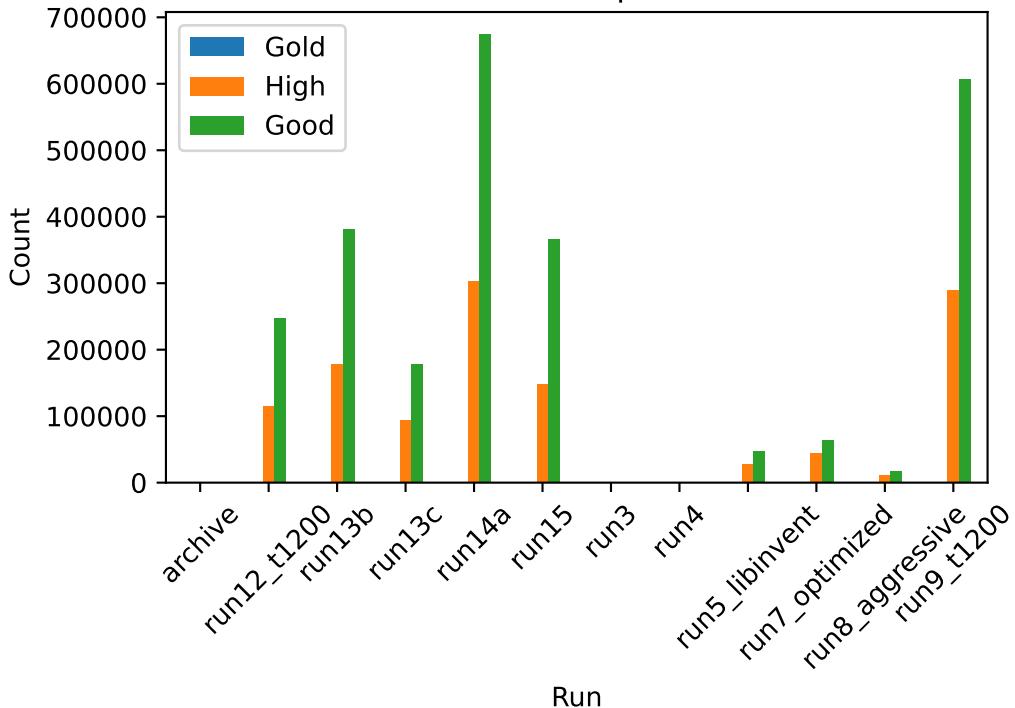
High Quality Candidates



Good Candidates



Overall Comparison



Detailed Results: archive

Run: archive
Directory: experiments/runs/archive

STATISTICS

gold_count: 0
high_count: 0
good_count: 0
promising_count: 0

Detailed Results: run12_t1200

Run: run12_t1200
Directory: experiments/runs/run12_t1200

STATISTICS

total_molecules: 511792
gold_count: 59
high_count: 114803
good_count: 247898
promising_count: 61

TOP GOLD CANDIDATES

- #1
SMILES: CN1C(c2ccccc2)CC(C(=O)NCC2CCNC2)C1c1cccc1
Score: 0.7208
- #2
SMILES: Cc1ccc(C2C(C(=O)NCC3CCNCC3)CC(c3ccccc3)N2C)cc1
Score: 0.7132
- #3
SMILES: O=C(NCC1CC1)C1CC(c2ccccc2)N(C(=O)N2CCCNCC2)C1c1cccc1
Score: 0.7128
- #4
SMILES: CC(=O)NC(=O)C1CC(c2cccc(C)c2)N(CC2CCNCC2)C1c1cccc1
Score: 0.7085
- #5
SMILES: O=C(NC1CC1)C1CC(c2ccccc2)N(C(=O)CC2CCNCC2)C1c1cccc1
Score: 0.7079
- #6
SMILES: CN1C(c2ccccc2)CC(C(=O)NCC2CCNC2)C1c1ccncc1
Score: 0.7075
- #7
SMILES: CN1C(c2ccccc2)CC(C(=O)NCC2CCNCC2)C1c1cccn1
Score: 0.7046
- #8
SMILES: O=C(NCC1CC1)C1CC(c2ccccc2)N(C(=O)C2CCNC2)C1c1cccc1
Score: 0.7010
- #9
SMILES: CNC(=O)C1CC(c2ccccc2)N(CCC2CCNCC2)C1c1cccnc1
Score: 0.7008
- #10
SMILES: O=C(NCC1CC1)C1CC(c2ccccc2)N(C(=O)C2CCNCC2)C1c1cccc1
Score: 0.7001

Detailed Results: run13b

Run: run13b
Directory: experiments/runs/run13b

STATISTICS

total_molecules: 835852
gold_count: 89
high_count: 177539
good_count: 380718
promising_count: 97

TOP GOLD CANDIDATES

#1
SMILES: CCNC(=O)C1CC(c2ccccc2)N(C2CCNCC2)C1c1cccc1
Score: 0.7247

#2
SMILES: CN1C(c2ccccc2)CC(C(=O)NCC2CCNC2)C1c1cccc1
Score: 0.7208

#3
SMILES: CCNC(=O)C1CC(c2cccc(C)c2)N(C2CCNCC2)C1c1cccc1
Score: 0.7204

#4
SMILES: Cc1cccc(C2CC(C(=O)NCC3CCNC3)C(c3ccccc3)N2C)c1
Score: 0.7172

#5
SMILES: CN1C(c2ccccc2)CC(C(=O)NCC2CCNCC2)C1c1cccc1
Score: 0.7165

#6
SMILES: CNC(=O)C1CC(c2cccn2)N(CC2CCNCC2)C1c1cccc1
Score: 0.7104

#7
SMILES: CNC(=O)C1CC(c2ccccc2)N(CC2CCNCC2)C1c1ccncl
Score: 0.7098

#8
SMILES: CC(=O)NC(=O)C1CC(c2cccc(C)c2)N(CC2CCNCC2)C1c1cccc1
Score: 0.7085

#9
SMILES: CC(=O)NC(=O)C1CC(c2ccccc2)N(C(=O)CC2CCNCC2)C1c1ccc(C)cc1
Score: 0.7083

#10
SMILES: CN1C(c2ccccc2)CC(C(=O)NCC2CCNC2)C1c1ccncl
Score: 0.7075

Detailed Results: run13c

Run: run13c
Directory: experiments/runs/run13c

STATISTICS

total_molecules: 1021353
gold_count: 316
high_count: 93676
good_count: 177781
promising_count: 747

TOP GOLD CANDIDATES

#1
SMILES: CN1C(c2ccccc2)CC(C(=O)NCC2CCNCC2)C1c1cccc1
Score: 0.7578

#2
SMILES: Cc1ccc(C2C(C(=O)NCC3CCNCC3)CC(c3ccccc3)N2C)cc1
Score: 0.7546

#3
SMILES: CC(=O)N1C(c2ccccc2)CC(C(=O)NCC2CCNCC2)C1c1cccc1
Score: 0.7532

#4
SMILES: Cc1cccc(C2CC(C(=O)NCC3CCNCC3)C(c3ccccc3)N2C)c1
Score: 0.7512

#5
SMILES: CC(=O)N1C(c2ccccc2)CC(C(=O)NCC2CCNCC2)C1c1ccc(C)cc1
Score: 0.7498

#6
SMILES: CN1C(c2ccccc2)CC(C(=O)NCC2CCNCC2)C1c1cccc1
Score: 0.7473

#7
SMILES: CC(=O)N1C(c2cccc(C)c2)CC(C(=O)NCC2CCNCC2)C1c1cccc1
Score: 0.7469

#8
SMILES: COC(=O)N1C(c2ccccc2)CC(C(=O)NCC2CCNCC2)C1c1cccc1
Score: 0.7439

#9
SMILES: CN(C)C(=O)N1C(c2ccccc2)CC(C(=O)NCC2CCNCC2)C1c1cccc1
Score: 0.7436

#10
SMILES: CC(=O)N1C(c2ccccc2)CC(C(=O)NCC2CCNCC2)C1c1cccc1
Score: 0.7434

Detailed Results: run14a

Run: run14a
Directory: experiments/runs/run14a

STATISTICS

total_molecules: 943233
gold_count: 113
high_count: 303121
good_count: 674225
promising_count: 123

TOP GOLD CANDIDATES

- #1
SMILES: CNC(=O)C1CC(c2cccn2)N(CC2CCNCC2)C1c1cccc1
Score: 0.7155
- #2
SMILES: CN1C(c2cccc2)CC(C(=O)NCC2CC2)C1c1ccc(N2CCNCC2)cc1
Score: 0.7126
- #3
SMILES: CN1C(c2cccc2)CC(C(=O)NC(=O)N2CCCC3CNCCC32)C1c1cccc1
Score: 0.7117
- #4
SMILES: O=C(NCC1CCNC1)C1CC(c2cccc2)N(C(=O)N2CCCC2)C1c1cccc1
Score: 0.7114
- #5
SMILES: CN1C(c2cccc2)CC(C(=O)NCC2CCNC2)C1c1ccncl
Score: 0.7111
- #6
SMILES: CC(=O)N1C(c2cccc2)CC(C(=O)NCC2CCNCC2)C1c1cccc1
Score: 0.7103
- #7
SMILES: CN1C(c2cccc2)CC(C(=O)NCC2CCNCC2)C1c1ccco1
Score: 0.7096
- #8
SMILES: CN1C(c2cccc2)CC(C(=O)NCCC2CCNCC2)C1c1ccncl
Score: 0.7079
- #9
SMILES: O=C(NCC1CCNC1)C1CC(c2cccc2)N(C2CC2)C1c1cccc1
Score: 0.7068
- #10
SMILES: O=C(NCC1CCNCC1)C1CC(c2cccc2)N(C(=O)N2CC2)C1c1cccc1
Score: 0.7068

Detailed Results: run15

Run: run15
Directory: experiments/runs/run15

STATISTICS

total_molecules: 903297
gold_count: 112
high_count: 148661
good_count: 366052
promising_count: 125

TOP GOLD CANDIDATES

#1
SMILES: CN1C(c2ccccc2)CC(C(=O)NCC2CCNC2)C1c1cccc1
Score: 0.7263

#2
SMILES: CN1C(c2ccccc2)CC(C(=O)NCC2CCNCC2)C1c1cccc1
Score: 0.7220

#3
SMILES: CN1C(c2ccccc2)CC(C(=O)NCC2CCNC2)C1c1ccncc1
Score: 0.7123

#4
SMILES: CN1C(c2cccn2)CC(C(=O)NCC2CCNC2)C1c1cccc1
Score: 0.7117

#5
SMILES: CN1C(c2ccccc2)CC(C(=O)NCC2CCNCC2)C1c1cccc1
Score: 0.7114

#6
SMILES: O=C(NCC1CCNC1)C1CC(c2ccccc2)N(C(=O)N2CCCC2)C1c1cccc1
Score: 0.7114

#7
SMILES: CN1C(c2ccccc2)CC(C(=O)NCC2CCNC2)C1c1ccncc1
Score: 0.7111

#8
SMILES: CCNC(=O)C1CC(c2ccn2)N(C2CCNCC2)C1c1cccc1
Score: 0.7088

#9
SMILES: CN1C(c2cccs2)CC(C(=O)NCC2CCNC2)C1c1cccc1
Score: 0.7087

#10
SMILES: CN(C)C(=O)N1C(c2ccn2)CC(C(=O)NCC2CCNC2)C1c1cccc1
Score: 0.7084

Detailed Results: run3

Run: run3
Directory: experiments/runs/run3

STATISTICS

total_molecules: 122551
gold_count: 0
high_count: 0
good_count: 0
promising_count: 2233

Detailed Results: run4

Run: run4
Directory: experiments/runs/run4

STATISTICS

total_molecules: 125965
gold_count: 0
high_count: 0
good_count: 0
promising_count: 440

Detailed Results: run5_libinvent

Run: run5_libinvent
Directory: experiments/runs/run5_libinvent

STATISTICS

total_molecules: 95998
gold_count: 6
high_count: 28230
good_count: 47662
promising_count: 6

TOP GOLD CANDIDATES

#1
SMILES: Cc1ccc(C2NC(CC3CCNCC3)C(C)C2C(=O)Nc2ccncc2)cc1
Score: 0.8723

#2
SMILES: Cc1ccc(C2NC(C)C(CC3CCNCC3)C2C(=O)Nc2cccnc2)cc1
Score: 0.8721

#3
SMILES: Cc1ccc(C2NC(C)C(Cc3cccc3)C2C(=O)NCC2CCNCC2)cc1
Score: 0.8707

#4
SMILES: CC1NC(c2ccc(C3CCC3)cc2)C(C(=O)NCC2CCNCC2)C1C
Score: 0.8581

#5
SMILES: Cc1ccc(C2NC(C)C(N3CCC3)C2C(=O)NCC2CCNCC2)cc1
Score: 0.8530

#6
SMILES: Cc1ccc(C2NC(C)C(CC3CCC3)C2C(=O)NCC2CCNCC2)cc1
Score: 0.8461

Detailed Results: run7_optimized

Run: run7_optimized
Directory: experiments/runs/run7_optimized

STATISTICS

total_molecules: 95997
gold_count: 13
high_count: 43866
good_count: 63356
promising_count: 15

TOP GOLD CANDIDATES

#1
SMILES: Cc1ccc(C2NC(C)C(C)C2C(=O)NCC2CCNCC2)cc1
Score: 0.5980

#2
SMILES: CC(=O)NC(=O)C1C(c2ccc(C)cc2)NC(CC2CCNCC2)C1C
Score: 0.5978

#3
SMILES: CCCC1C(CC2CCNCC2)NC(c2ccc(C)cc2)C1C(=O)NC(C)=O
Score: 0.5799

#4
SMILES: CCCC1NC(c2ccc(C)cc2)C(C(=O)NC(C)=O)C1CC1CCNCC1
Score: 0.5798

#5
SMILES: Cc1ccc(C2NC(C)C(C3CCNCC3)C2C(=O)NCC2CCC2)cc1
Score: 0.5720

#6
SMILES: Cc1ccc(C2NC(C3CCC3)C(C)C2C(=O)NCC2CCNCC2)cc1
Score: 0.5702

#7
SMILES: Cc1ccc(C2NC(C3CC3)C(C)C2C(=O)NCC2CCNCC2)cc1
Score: 0.5698

#8
SMILES: Cc1ccc(C2NC(C)C(C3CC3)C2C(=O)NCC2CCNCC2)cc1
Score: 0.5696

#9
SMILES: CCNC(=O)C1C(c2ccc(C)cc2)NC(C2CC2)C1CC1CCNCC1
Score: 0.5692

#10
SMILES: Cc1ccc(C2NC(C)C(N3CCCC3)C2C(=O)NCC2CCNCC2)cc1
Score: 0.5614

Detailed Results: run8_aggressive

Run: run8_aggressive
Directory: experiments/runs/run8_aggressive

STATISTICS

total_molecules: 27776
gold_count: 10
high_count: 11831
good_count: 17227
promising_count: 10

TOP GOLD CANDIDATES

#1
SMILES: Cc1ccc(C2NC(C)C(C)C2C(=O)NCC2CCNC2)cc1
Score: 0.7168

#2
SMILES: CCc1ccc(C2NC(CC)C(C)C2C(=O)NCC2CCNC2)cc1
Score: 0.6981

#3
SMILES: CCc1ccc(C2NC(C)C(CC)C2C(=O)NCC2CCNC2)cc1
Score: 0.6922

#4
SMILES: Cc1ccc(C2NC(C)C(C3CCNC3)C2C(=O)NCC2CC2)cc1
Score: 0.6785

#5
SMILES: Cc1ccc(C2NC(C3CCC3)C(C)C2C(=O)NCC2CCNC2)cc1
Score: 0.6718

#6
SMILES: Cc1ccc(C2NC(C3CCCC3)C(C)C2C(=O)NCC2CCNC2)cc1
Score: 0.6705

#7
SMILES: CC1NC(c2ccc(-c3cccc3)cc2)C(C(=O)NCC2CCNC2)C1C
Score: 0.6698

#8
SMILES: Cc1ccc(C2NC(C)C(C3CCCC3)C2C(=O)NCC2CCNC2)cc1
Score: 0.6691

#9
SMILES: CCC1NC(c2ccc(C)cc2)C(C(=O)NCC2CCNC2)C1C1CCC1
Score: 0.6626

#10
SMILES: Cc1ccc(C2NC(N3CC0CC3)C(C)C2C(=O)NCC2CCNC2)cc1
Score: 0.6468

Detailed Results: run9_t1200

Run: run9_t1200
Directory: experiments/runs/run9_t1200

STATISTICS

total_molecules: 1136114
gold_count: 96
high_count: 289397
good_count: 607640
promising_count: 103

TOP GOLD CANDIDATES

- #1
SMILES: CN1C(c2ccccc2)CC(C(=O)NCC2CCNC2)C1c1cccc1
Score: 0.7208
- #2
SMILES: CCNC(=O)C1CC(c2ccccc2)N(C2CCNCC2)C1c1ccc(C)cc1
Score: 0.7206
- #3
SMILES: CC(=O)NC(=O)C1CC(c2ccccc2)N(CC2CCNCC2)C1c1cccc1
Score: 0.7119
- #4
SMILES: Cc1ccc(C2C(C(=O)NC(=O)CC3CCNCC3)CC(c3ccccc3)N2C)cc1
Score: 0.7119
- #5
SMILES: CC(=O)NC(=O)C1CC(c2ccccc2)N(C(=O)CC2CCNCC2)C1c1cccc1
Score: 0.7115
- #6
SMILES: CNC(=O)C1CC(c2cccn2)N(CC2CCNCC2)C1c1cccc1
Score: 0.7104
- #7
SMILES: CC(=O)NC(=O)C1CC(c2ccccc2)N(CC2CCNCC2)C1c1ccc(C)cc1
Score: 0.7102
- #8
SMILES: CN1C(c2ccccc2)CC(C(=O)NCC2CCNC2)C1c1ccnc1
Score: 0.7063
- #9
SMILES: CN1C(c2cccs2)CC(C(=O)NCC2CCNC2)C1c1cccc1
Score: 0.7040
- #10
SMILES: CC(=O)N1C(c2ccccc2)CC(C(=O)NCC2CCNCC2)C1c1ccco1
Score: 0.7027