

# REINVENT4 Runs Comparison Report

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

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## SUMMARY OF ALL RUNS

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

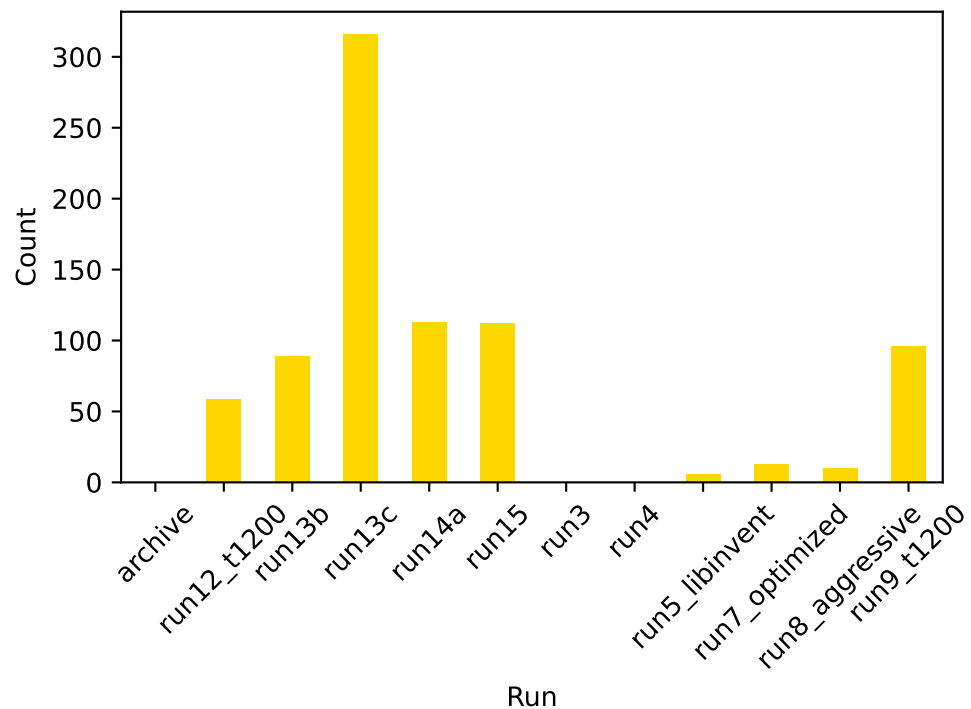
run7\_optimized:  
Gold candidates: 13  
High candidates: 43866  
Good candidates: 63356  
Promising: 15  
Total molecules: 95997

run8\_aggressive:  
Gold candidates: 10  
High candidates: 11831  
Good candidates: 17227  
Promising: 10  
Total molecules: 27776

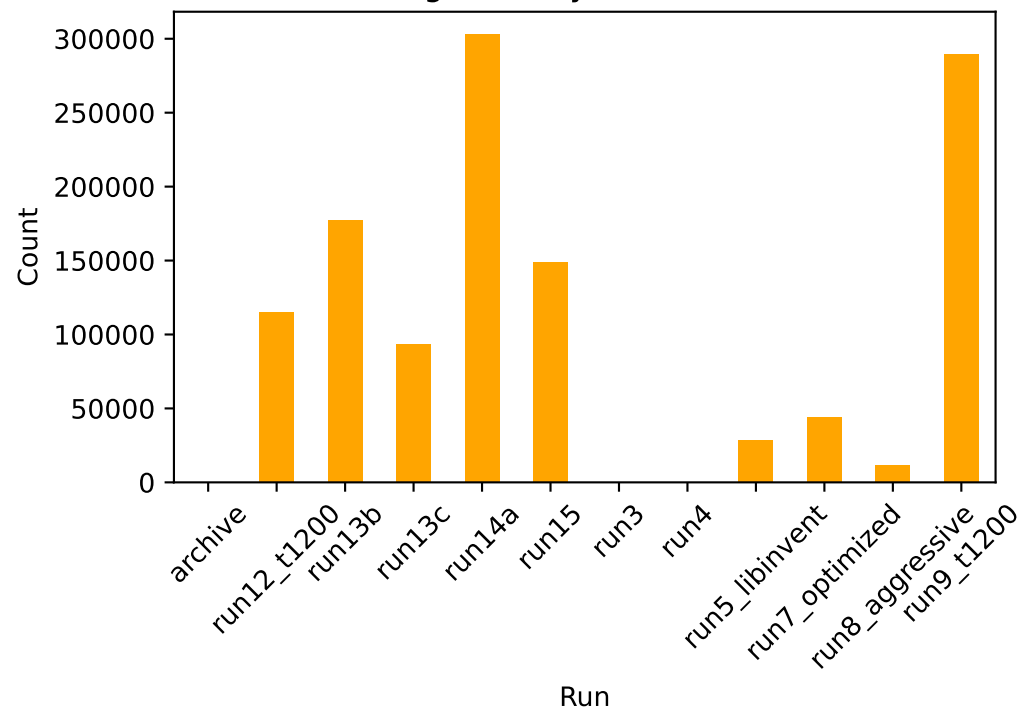
run9\_t1200:  
Gold candidates: 96  
High candidates: 289397  
Good candidates: 607640  
Promising: 103  
Total molecules: 1136114

# Candidates Comparison Across Runs

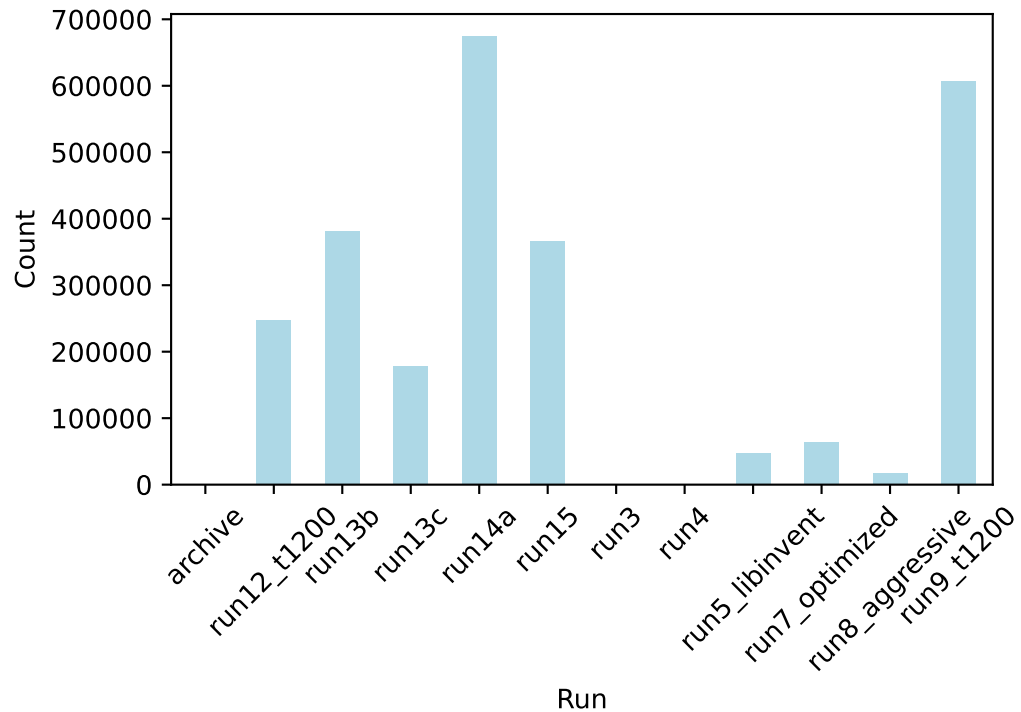
## Gold Candidates



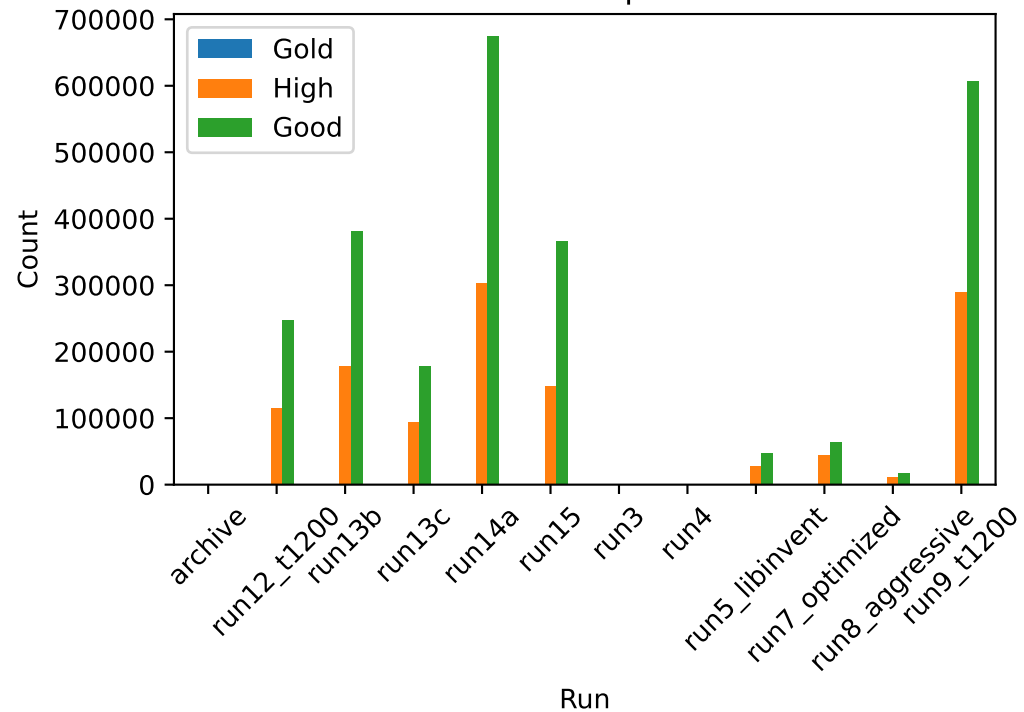
## High Quality Candidates



## Good Candidates



## Overall Comparison



# Detailed Results: archive

Run: archive  
Directory: experiments/runs/archive

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## STATISTICS

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gold\_count: 0  
high\_count: 0  
good\_count: 0  
promising\_count: 0

# Detailed Results: run12\_t1200

Run: run12\_t1200  
Directory: experiments/runs/run12\_t1200

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## STATISTICS

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total\_molecules: 511792  
gold\_count: 59  
high\_count: 114803  
good\_count: 247898  
promising\_count: 61

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## TOP GOLD CANDIDATES

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#1

SMILES: CN1C(c2cccc2)CC(C(=O)NCC2CCNC2)C1c1cccc1  
Score: 0.7208

#2

SMILES: Cc1ccc(C2C(C(=O)NCC3CCNCC3)CC(c3cccc3)N2C)cc1  
Score: 0.7132

#3

SMILES: O=C(NCC1CC1)C1CC(c2cccc2)N(C(=O)N2CCNCC2)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(c2cccc2)N(C(=O)CC2CCNCC2)C1c1cccc1  
Score: 0.7079

#6

SMILES: CN1C(c2cccc2)CC(C(=O)NCC2CCNC2)C1c1ccncc1  
Score: 0.7075

#7

SMILES: CN1C(c2cccc2)CC(C(=O)NCC2CCNCC2)C1c1cccn1  
Score: 0.7046

#8

SMILES: O=C(NCC1CCC1)C1CC(c2cccc2)N(C(=O)C2CCNC2)C1c1cccc1  
Score: 0.7010

#9

SMILES: CNC(=O)C1CC(c2cccc2)N(CCC2CCNCC2)C1c1ccnc1  
Score: 0.7008

#10

SMILES: O=C(NCC1CC1)C1CC(c2cccc2)N(C(=O)C2CCNCC2)C1c1cccc1  
Score: 0.7001

# Detailed Results: run13b

Run: run13b  
Directory: experiments/runs/run13b

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## STATISTICS

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total\_molecules: 835852  
gold\_count: 89  
high\_count: 177539  
good\_count: 380718  
promising\_count: 97

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## TOP GOLD CANDIDATES

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#1

SMILES: CCNC(=O)C1CC(c2cccc2)N(C2CCNCC2)C1c1cccc1  
Score: 0.7247

#2

SMILES: CN1C(c2cccc2)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(c3cccc3)N2C)c1  
Score: 0.7172

#5

SMILES: CN1C(c2cccc2)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(c2cccc2)N(CC2CCNCC2)C1c1cccn1  
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(c2cccc2)N(C(=O)CC2CCNCC2)C1c1ccc(C)cc1  
Score: 0.7083

#10

SMILES: CN1C(c2cccc2)CC(C(=O)NCC2CCNC2)C1c1ccncc1  
Score: 0.7075

# Detailed Results: run13c

Run: run13c  
Directory: experiments/runs/run13c

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## STATISTICS

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total\_molecules: 1021353  
gold\_count: 316  
high\_count: 93676  
good\_count: 177781  
promising\_count: 747

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## TOP GOLD CANDIDATES

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#1

SMILES: CN1C(c2ccccc2)CC(C(=O)NCC2CCNCC2)C1c1ccccc1  
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)C1c1ccccc1  
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)NCC2CCNC2)C1c1ccccc1  
Score: 0.7473

#7

SMILES: CC(=O)N1C(c2cccc(C)c2)CC(C(=O)NCC2CCNCC2)C1c1ccccc1  
Score: 0.7469

#8

SMILES: COC(=O)N1C(c2ccccc2)CC(C(=O)NCC2CCNCC2)C1c1ccccc1  
Score: 0.7439

#9

SMILES: CN(C)C(=O)N1C(c2ccccc2)CC(C(=O)NCC2CCNCC2)C1c1ccccc1  
Score: 0.7436

#10

SMILES: CC(=O)N1C(c2ccccc2)CC(C(=O)NCC2CCNCC2)C1c1ccccc1  
Score: 0.7434

# Detailed Results: run14a

Run: run14a  
Directory: experiments/runs/run14a

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## STATISTICS

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total\_molecules: 943233  
gold\_count: 113  
high\_count: 303121  
good\_count: 674225  
promising\_count: 123

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## TOP GOLD CANDIDATES

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#1

SMILES: CNC(=O)C1CC(c2ccnc2)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)C1c1ccnc1  
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)C1c1ccc1  
Score: 0.7096

#8

SMILES: CN1C(c2cccc2)CC(C(=O)NCCC2CCNCC2)C1c1ccnc1  
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

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## STATISTICS

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total\_molecules: 903297  
gold\_count: 112  
high\_count: 148661  
good\_count: 366052  
promising\_count: 125

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## TOP GOLD CANDIDATES

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#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(c2ccncc2)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)C1c1cccncc1  
Score: 0.7111

#8

SMILES: CCNC(=O)C1CC(c2ccncc2)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(c2ccncc2)CC(C(=O)NCC2CCNC2)C1c1cccc1  
Score: 0.7084



# Detailed Results: run3

Run: run3

Directory: experiments/runs/run3

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## STATISTICS

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total\_molecules: 122551

gold\_count: 0

high\_count: 0

good\_count: 0

promising\_count: 2233

# Detailed Results: run4

Run: run4

Directory: experiments/runs/run4

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## STATISTICS

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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

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## STATISTICS

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total\_molecules: 95998  
gold\_count: 6  
high\_count: 28230  
good\_count: 47662  
promising\_count: 6

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## TOP GOLD CANDIDATES

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#1  
SMILES: Cc1ccc(C2NC(CC3CCNCC3)C(C)C2C(=O)Nc2ccnc2)cc1  
Score: 0.8723

#2  
SMILES: Cc1ccc(C2NC(C)C(CC3CCNCC3)C2C(=O)Nc2ccnc2)cc1  
Score: 0.8721

#3  
SMILES: Cc1ccc(C2NC(C)C(Cc3ccccc3)C2C(=O)NCC2CCNC2)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

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## STATISTICS

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total\_molecules: 95997  
gold\_count: 13  
high\_count: 43866  
good\_count: 63356  
promising\_count: 15

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## TOP GOLD CANDIDATES

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#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

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## STATISTICS

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total\_molecules: 27776  
gold\_count: 10  
high\_count: 11831  
good\_count: 17227  
promising\_count: 10

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## TOP GOLD CANDIDATES

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#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)NCC2CCNCC2)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)NCC2CCNCC2)cc1  
Score: 0.6718

#6

SMILES: Cc1ccc(C2NC(C3CCCC3)C(C)C2C(=O)NCC2CCNCC2)cc1  
Score: 0.6705

#7

SMILES: CC1NC(c2ccc(-c3ccccc3)cc2)C(C(=O)NCC2CCNC2)C1C  
Score: 0.6698

#8

SMILES: Cc1ccc(C2NC(C)C(C3CCCC3)C2C(=O)NCC2CCNCC2)cc1  
Score: 0.6691

#9

SMILES: CCC1NC(c2ccc(C)cc2)C(C(=O)NCC2CCNCC2)C1C1CCC1  
Score: 0.6626

#10

SMILES: Cc1ccc(C2NC(N3CCOCC3)C(C)C2C(=O)NCC2CCNCC2)cc1  
Score: 0.6468

# Detailed Results: run9\_t1200

Run: run9\_t1200  
Directory: experiments/runs/run9\_t1200

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## STATISTICS

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total\_molecules: 1136114  
gold\_count: 96  
high\_count: 289397  
good\_count: 607640  
promising\_count: 103

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## TOP GOLD CANDIDATES

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#1

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

#2

SMILES: CCNC(=O)C1CC(c2ccccc2)N(CC2CCNCC2)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)C1c1cccn1  
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