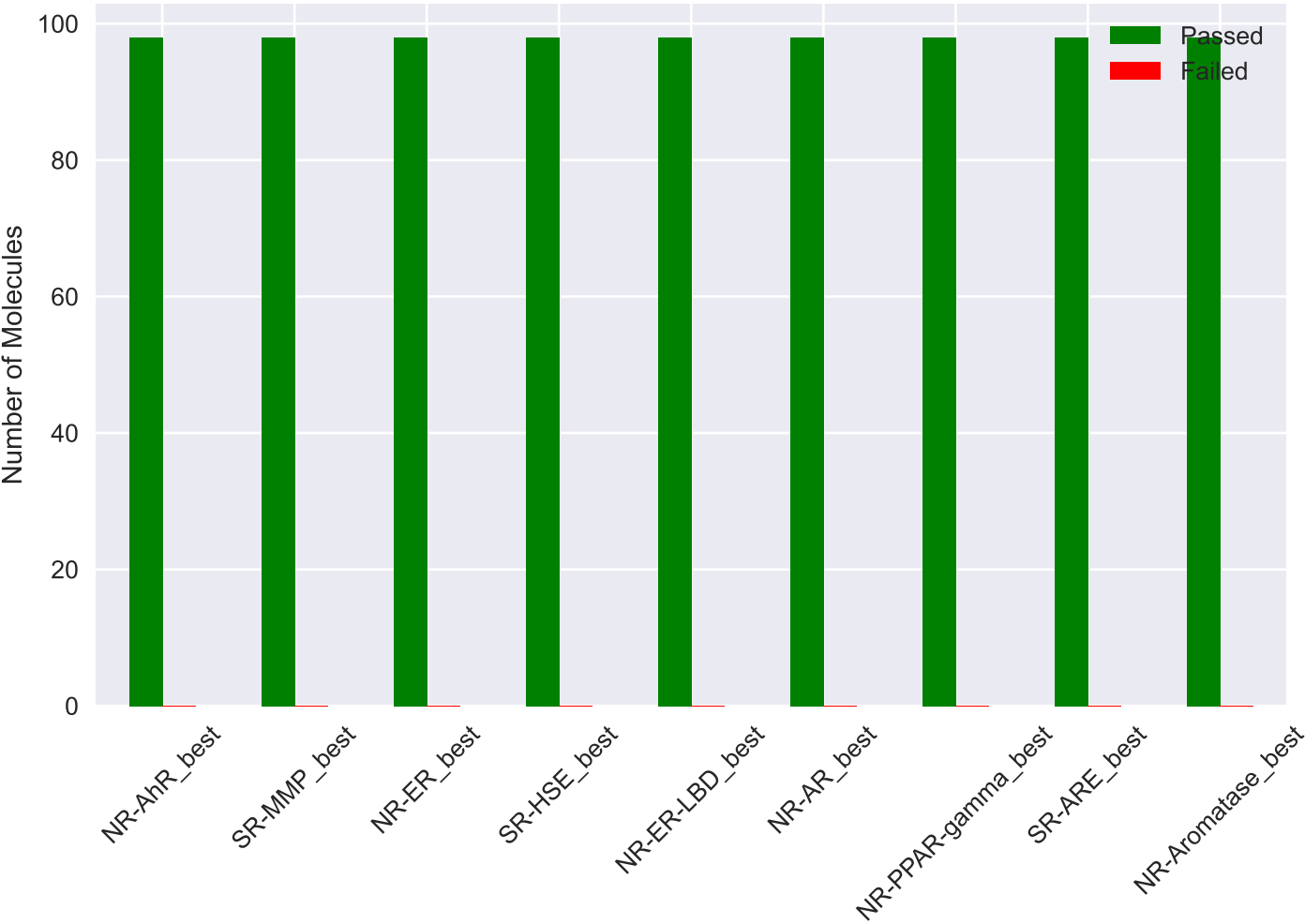
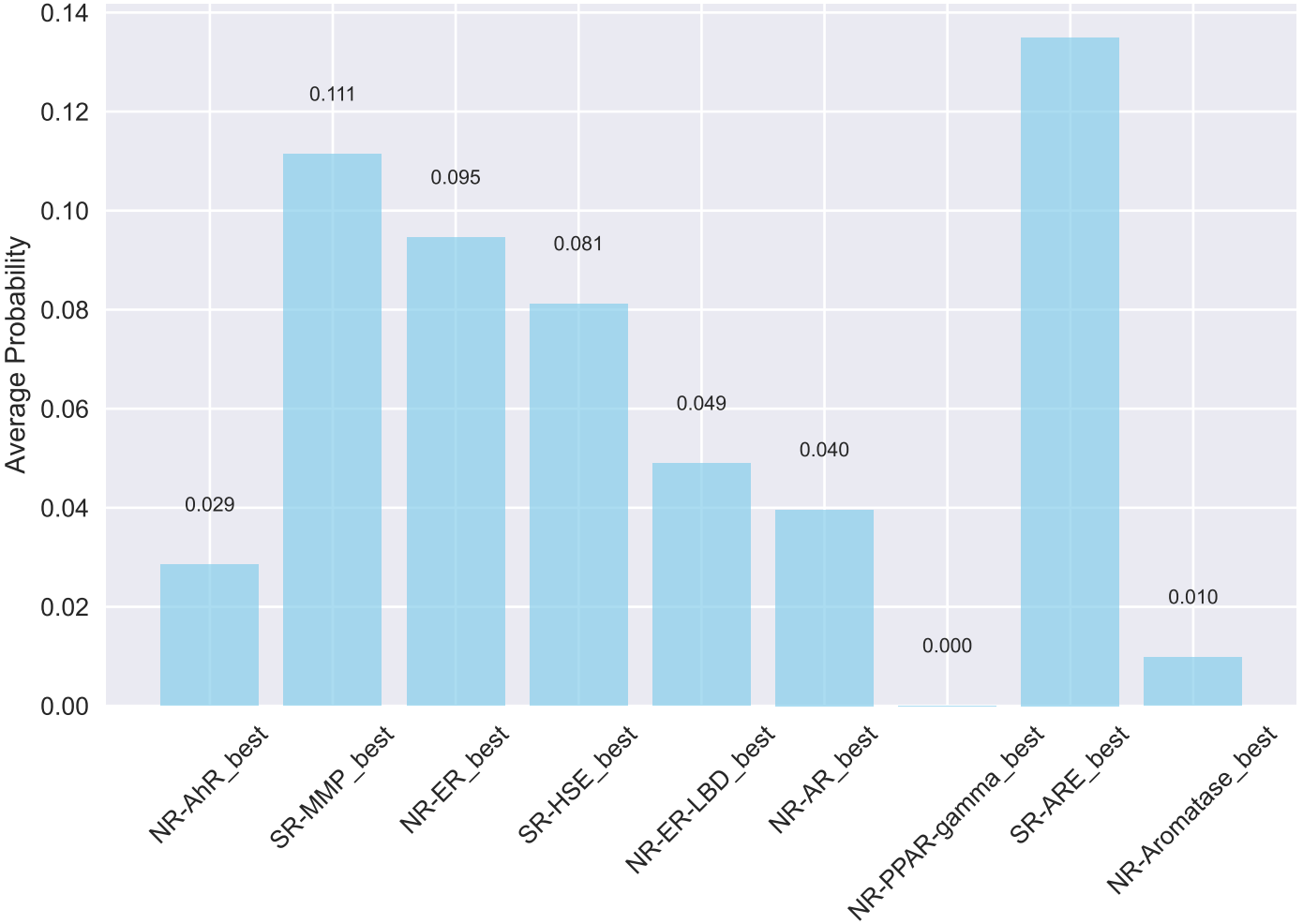


Tox21 Toxicity Prediction Summary

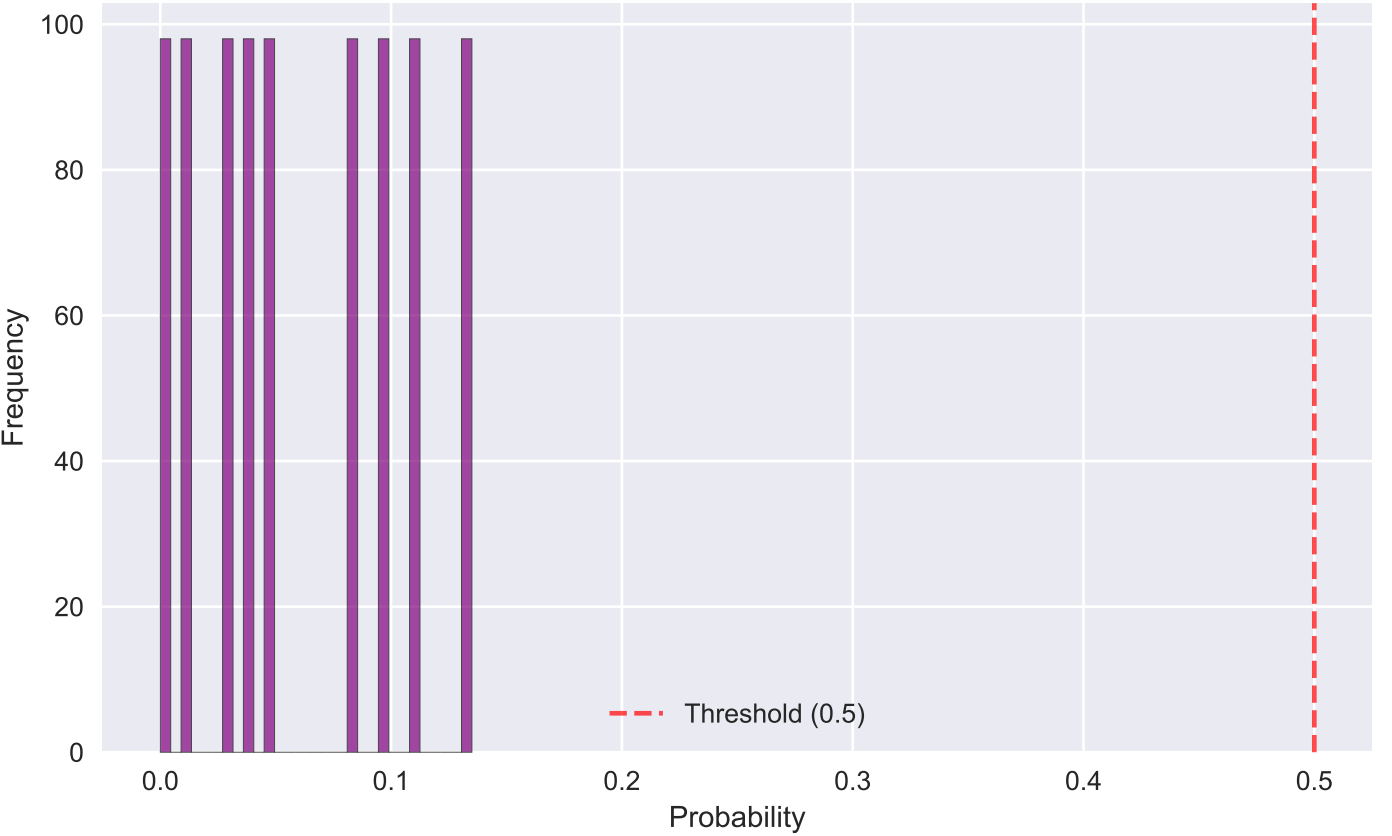
Molecules Passed vs Failed by Target



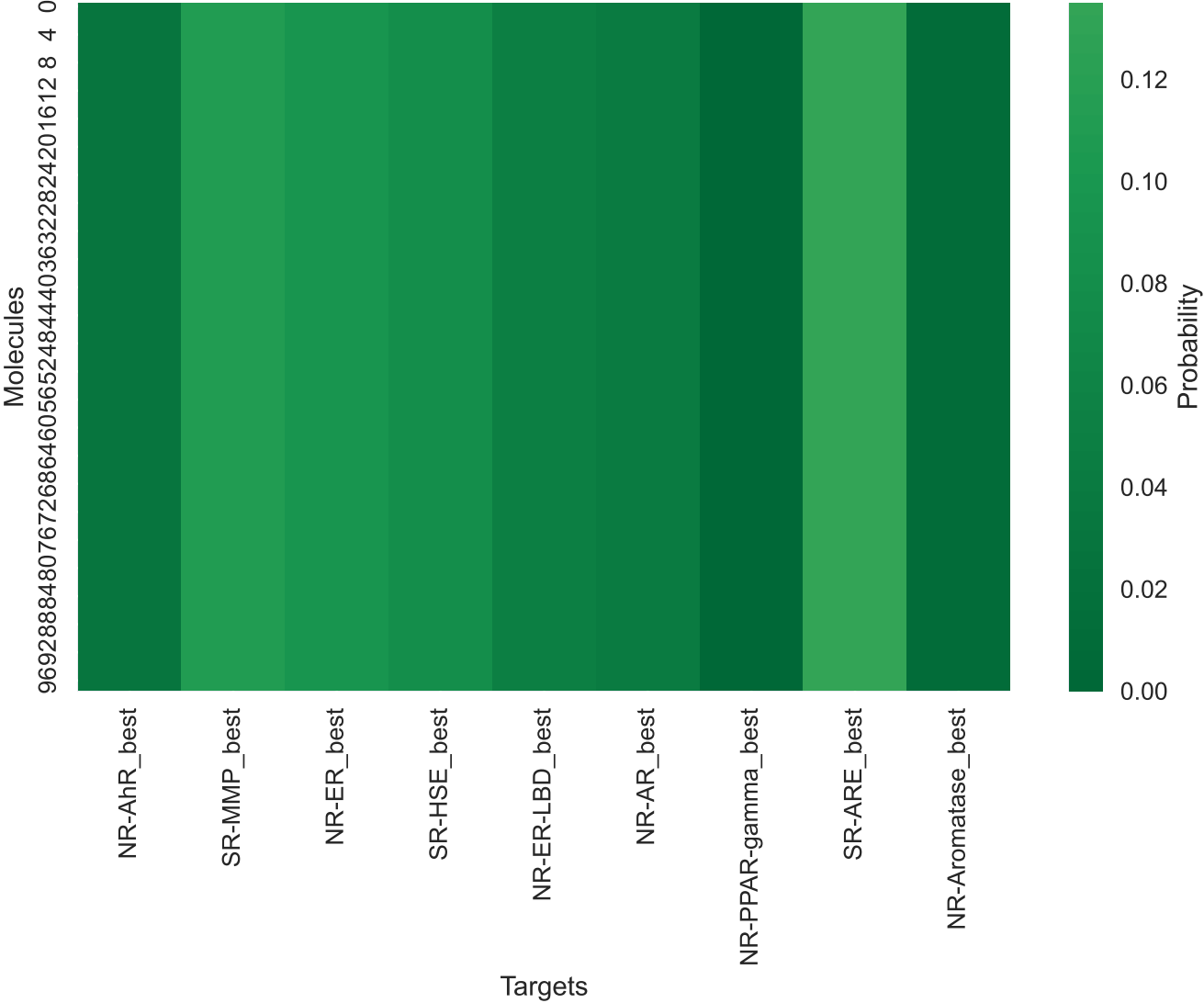
Average Toxicity Probability by Target



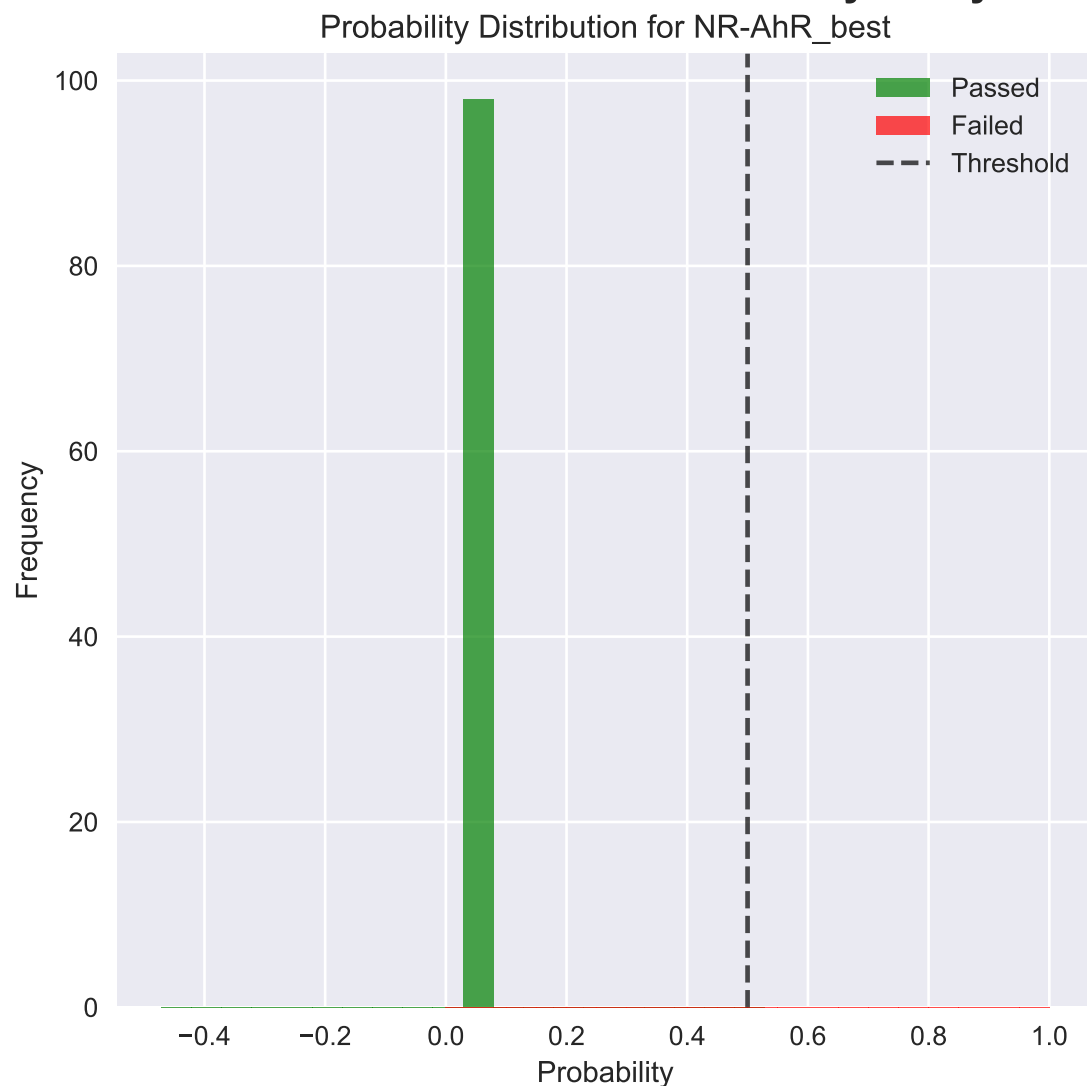
Distribution of All Toxicity Probabilities



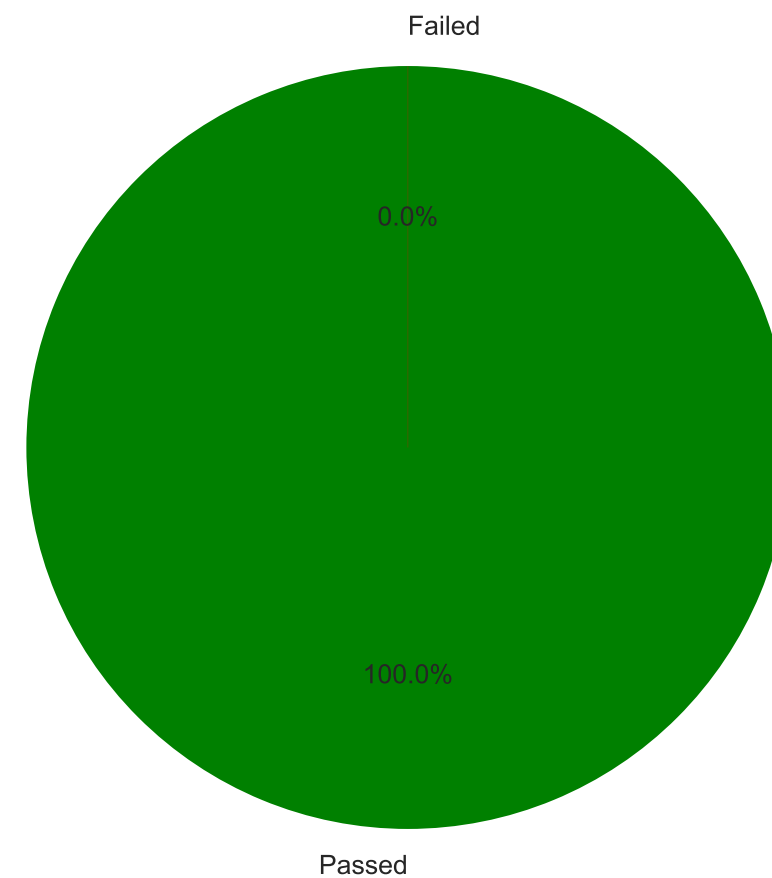
Toxicity Probability Heatmap



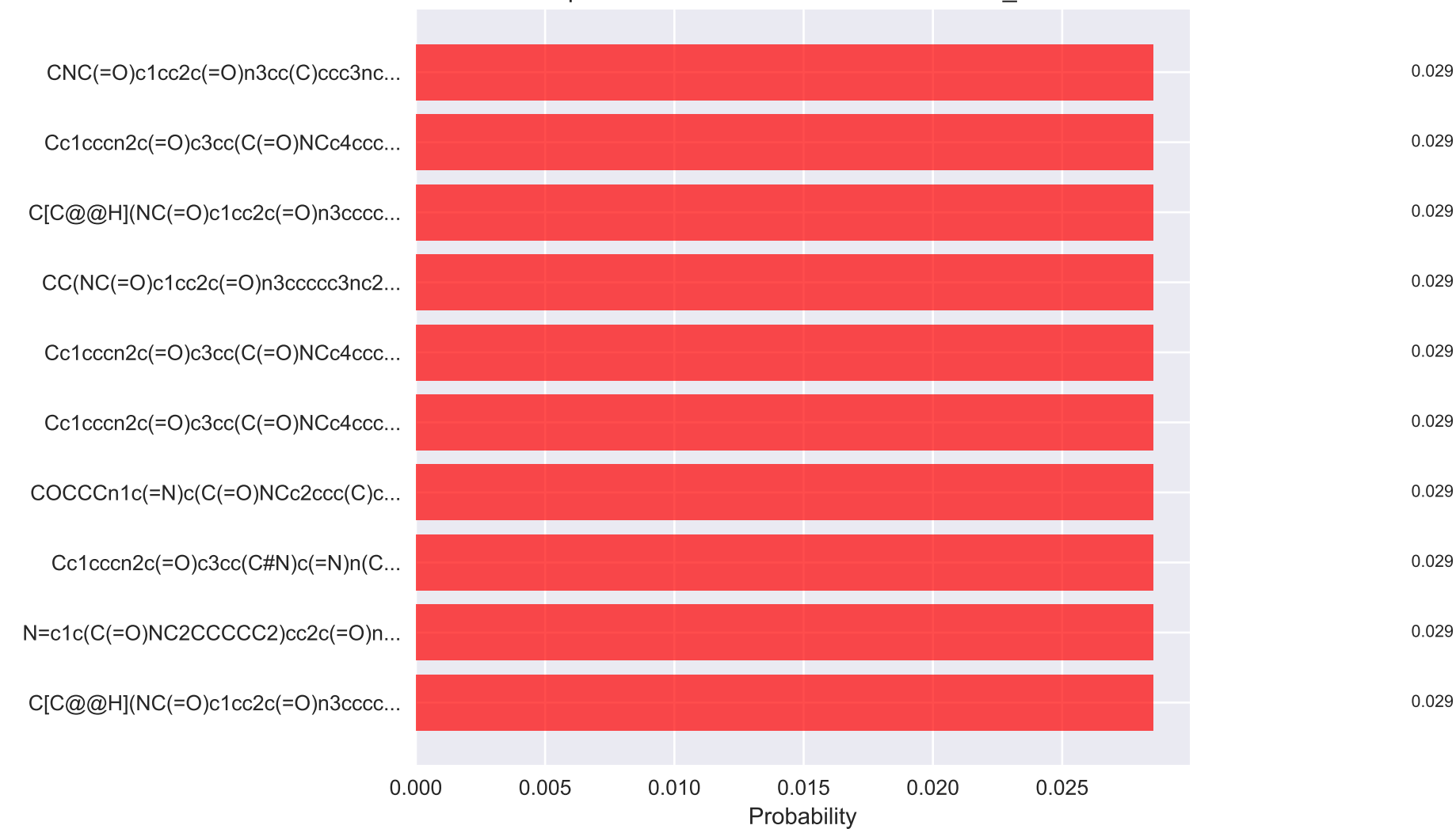
# Toxicity Analysis: NR-AhR\_best



Pass/Fail Distribution for NR-AhR\_best



Top 10 Most Toxic Molecules for NR-AhR\_best



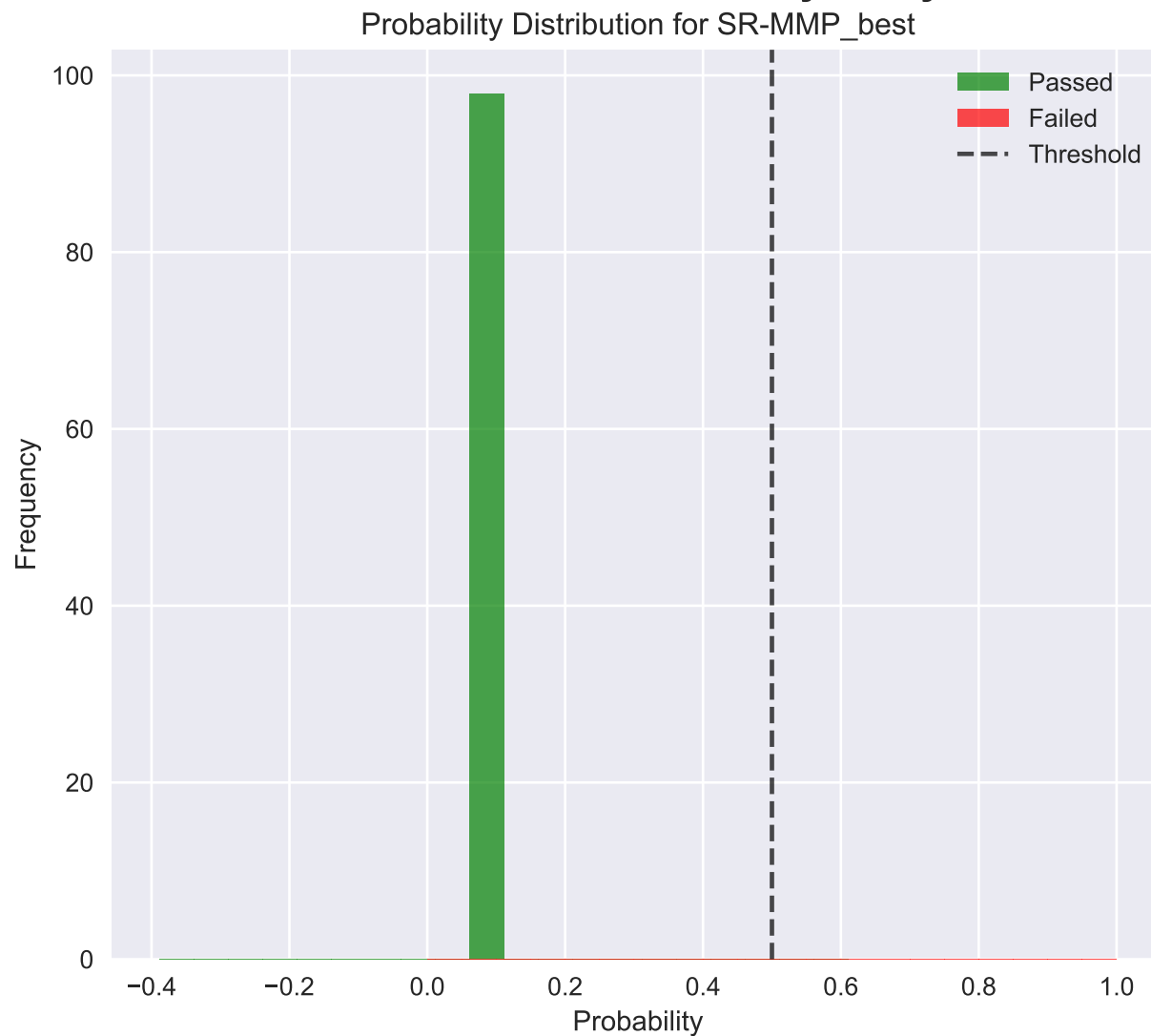
Target: NR-AhR\_best

Total Molecules: 98  
Passed: 98 (100.0%)  
Failed: 0 (0.0%)

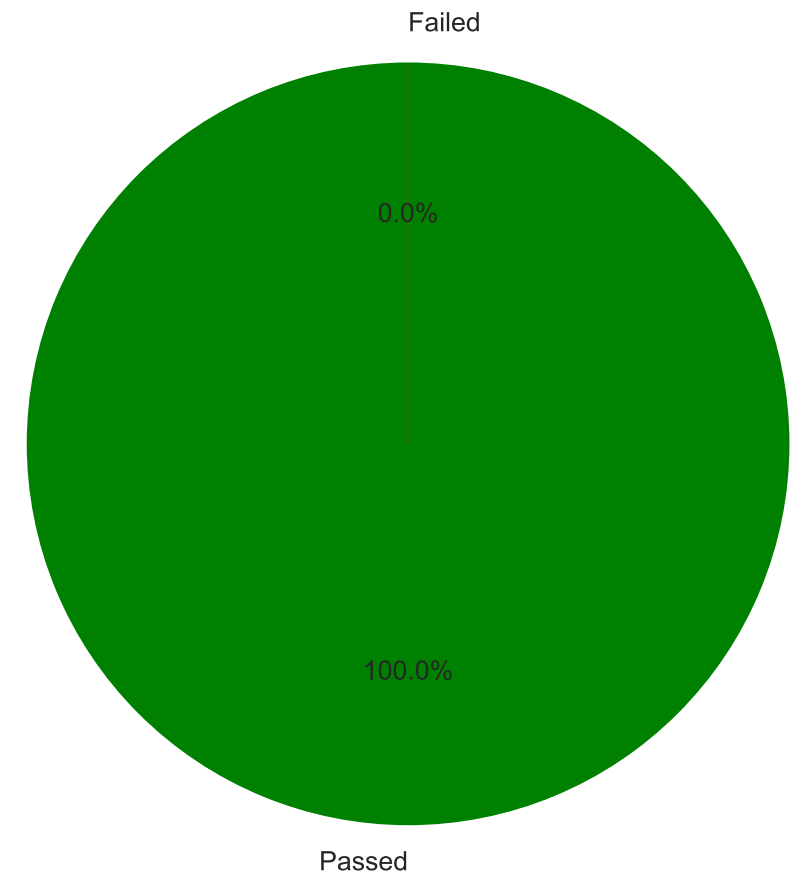
Probability Statistics:  
Mean: 0.029  
Median: 0.029  
Std: 0.000  
Min: 0.029  
Max: 0.029

Threshold: 0.5

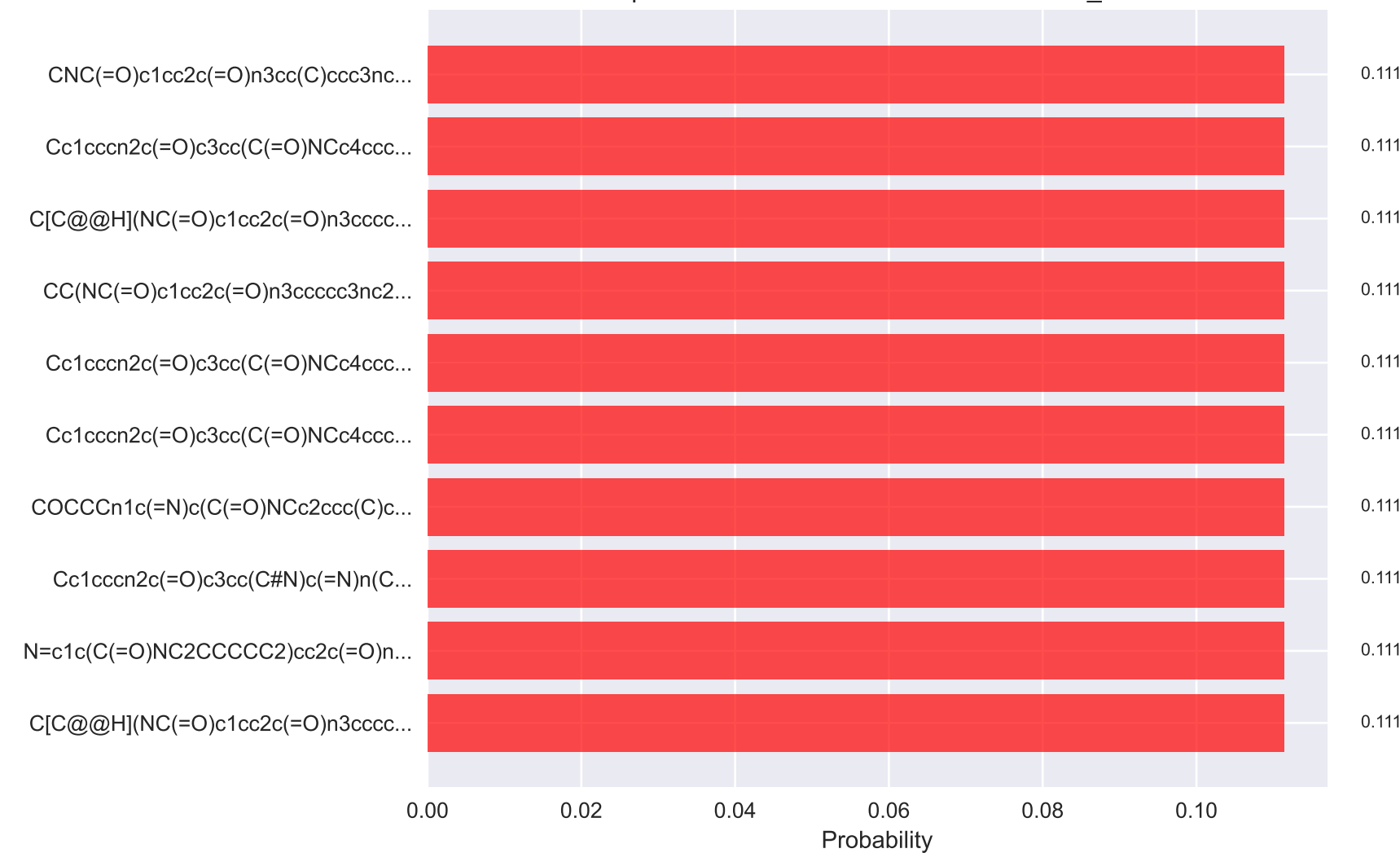
# Toxicity Analysis: SR-MMP\_best



Pass/Fail Distribution for SR-MMP\_best



Top 10 Most Toxic Molecules for SR-MMP\_best



Target: SR-MMP\_best

Total Molecules: 98

Passed: 98 (100.0%)

Failed: 0 (0.0%)

Probability Statistics:

Mean: 0.111

Median: 0.111

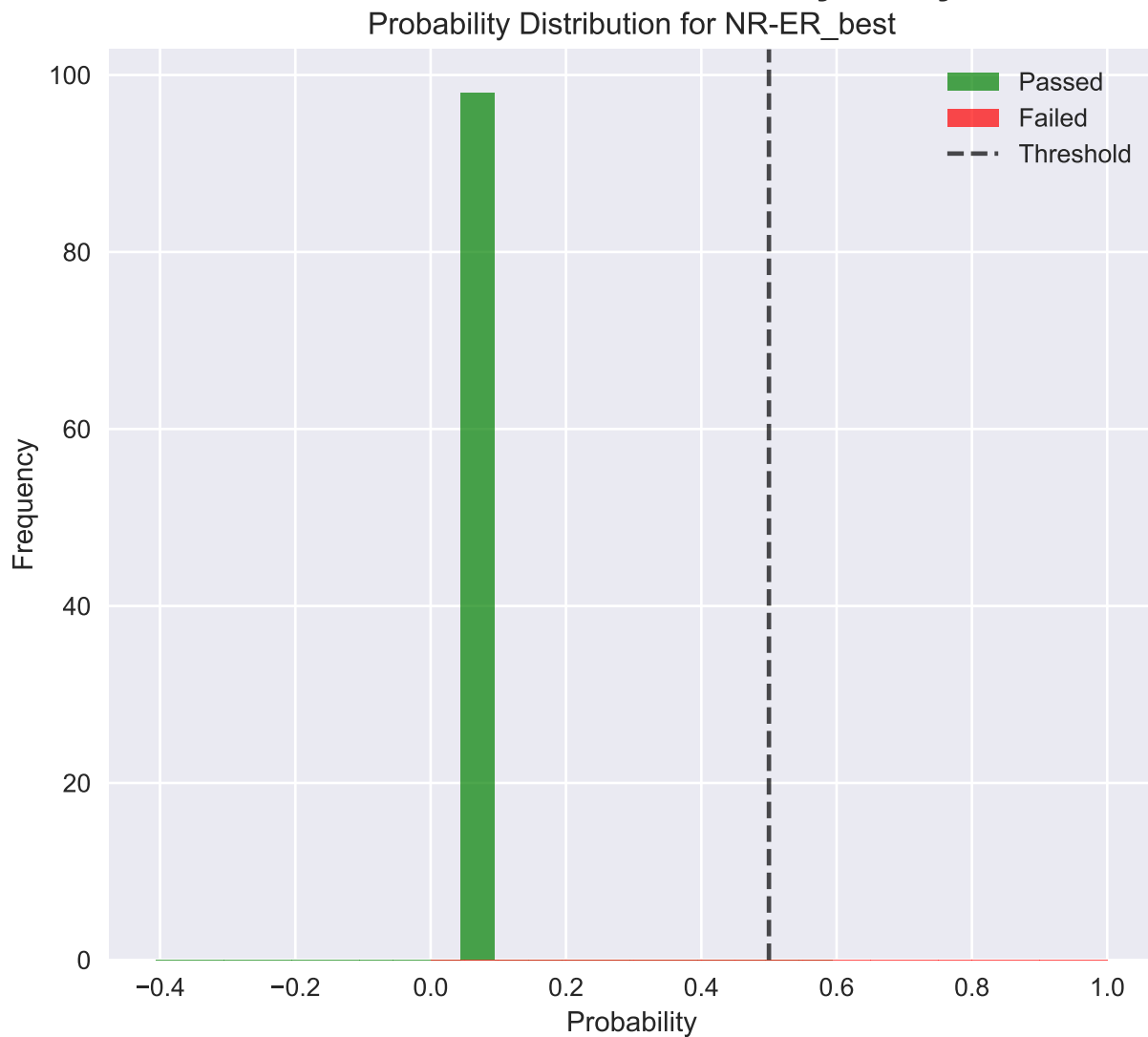
Std: 0.000

Min: 0.111

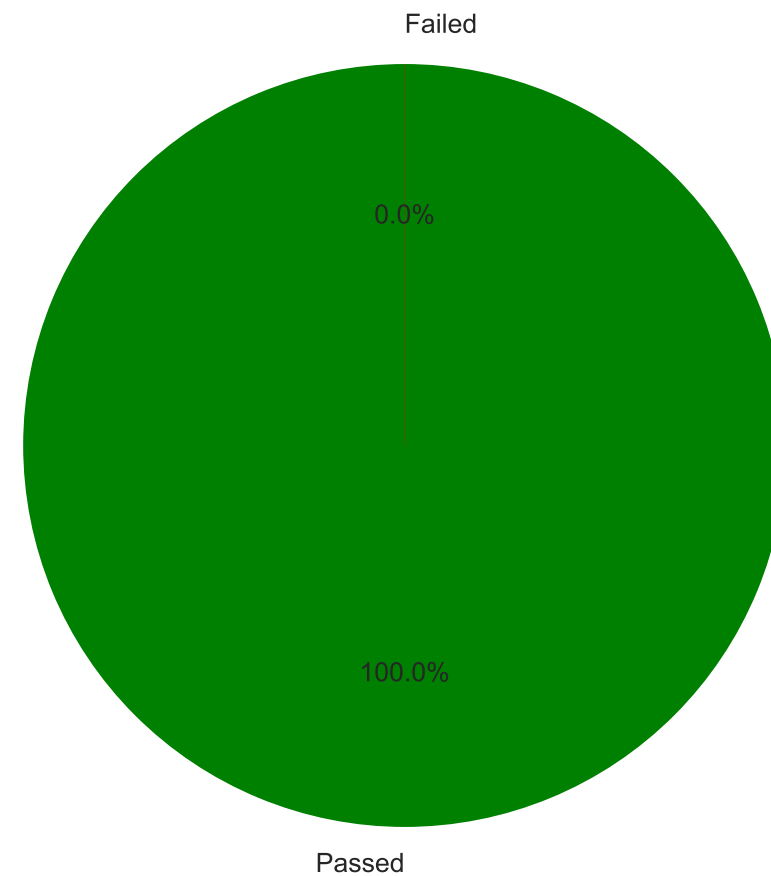
Max: 0.111

Threshold: 0.5

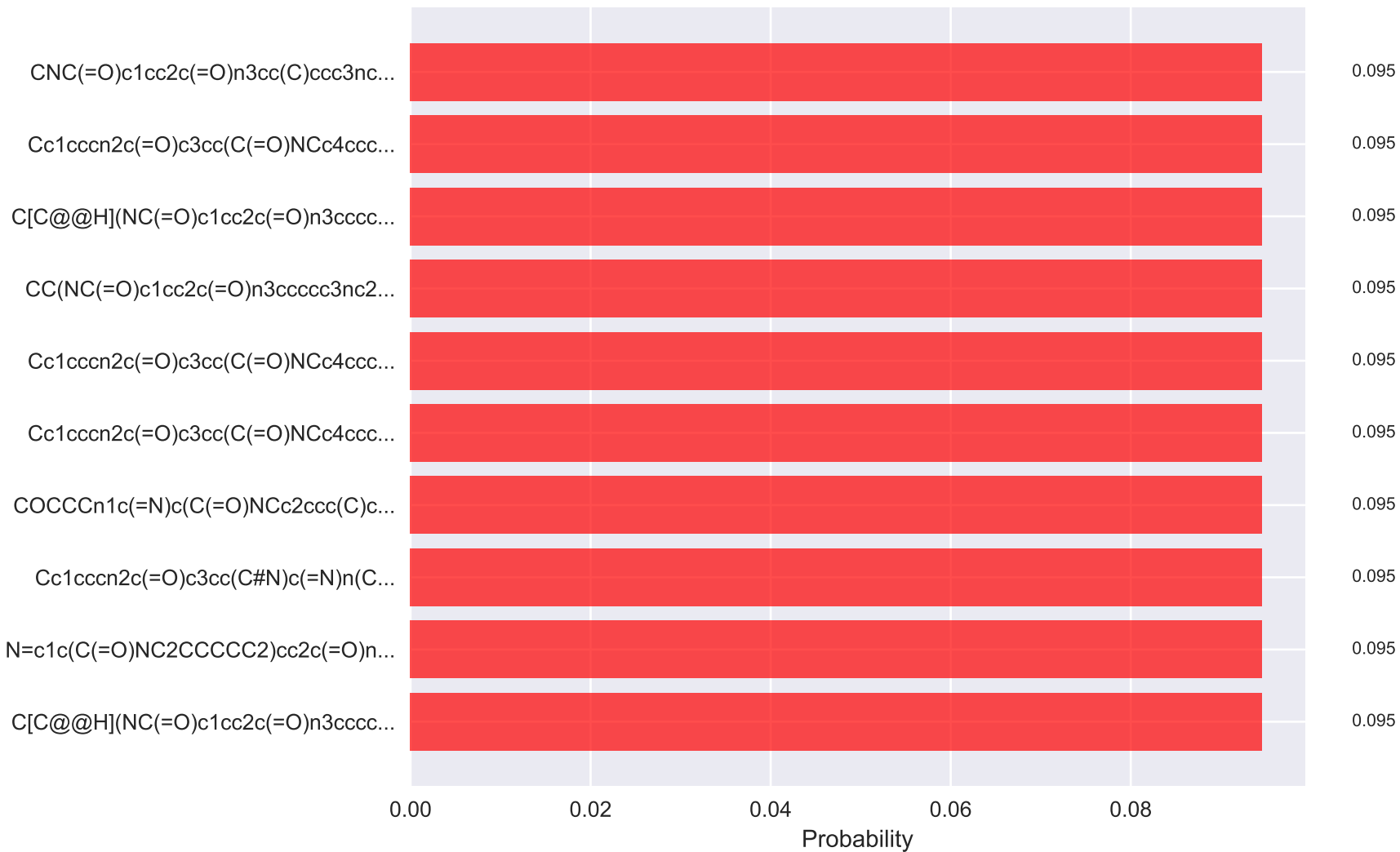
# Toxicity Analysis: NR-ER\_best



Pass/Fail Distribution for NR-ER\_best



Top 10 Most Toxic Molecules for NR-ER\_best



Target: NR-ER\_best

Total Molecules: 98

Passed: 98 (100.0%)

Failed: 0 (0.0%)

Probability Statistics:

Mean: 0.095

Median: 0.095

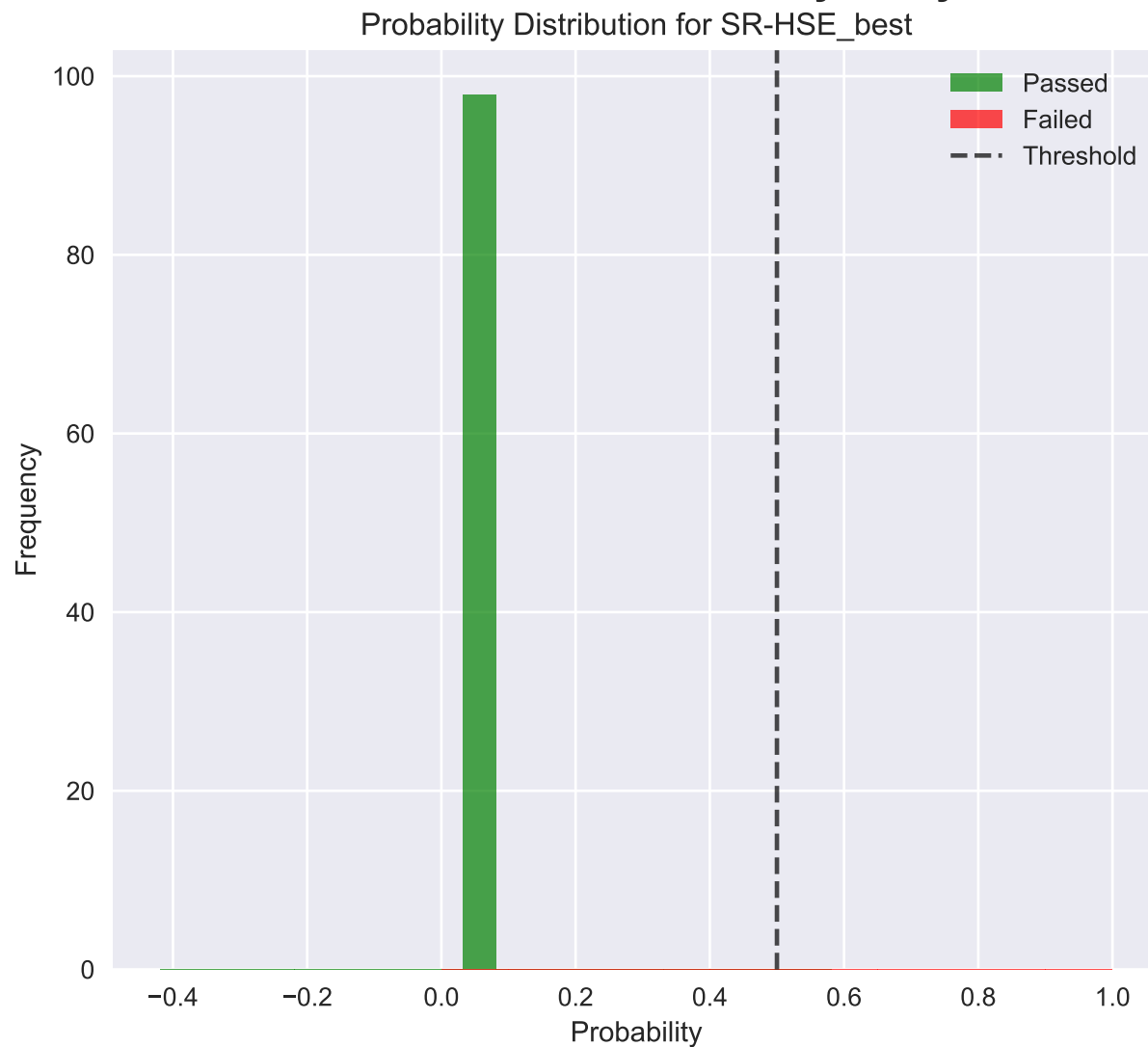
Std: 0.000

Min: 0.095

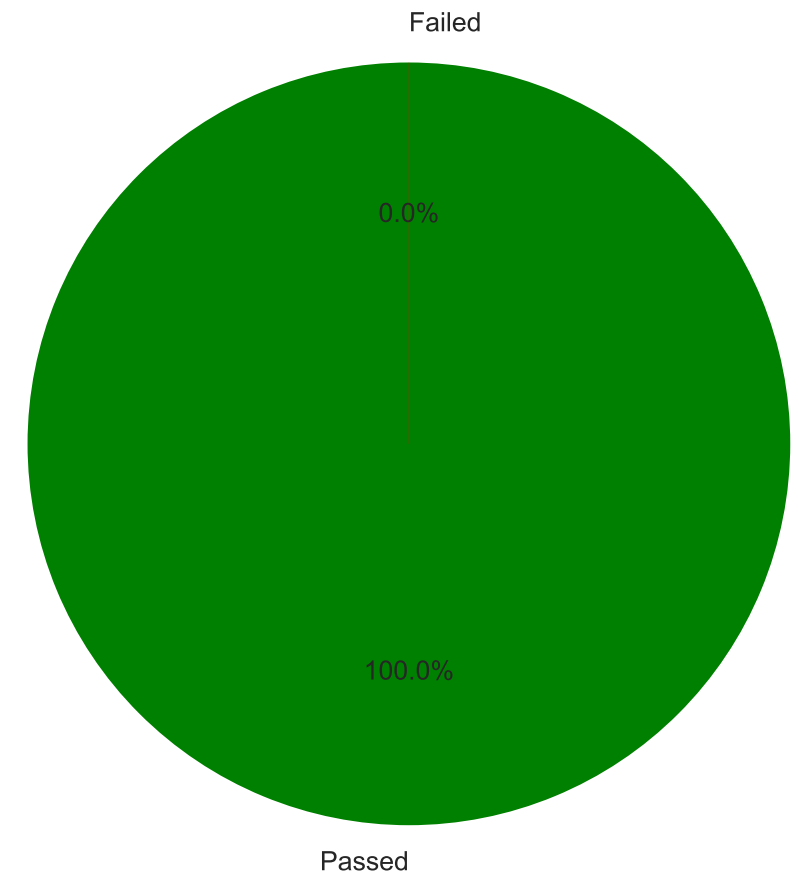
Max: 0.095

Threshold: 0.5

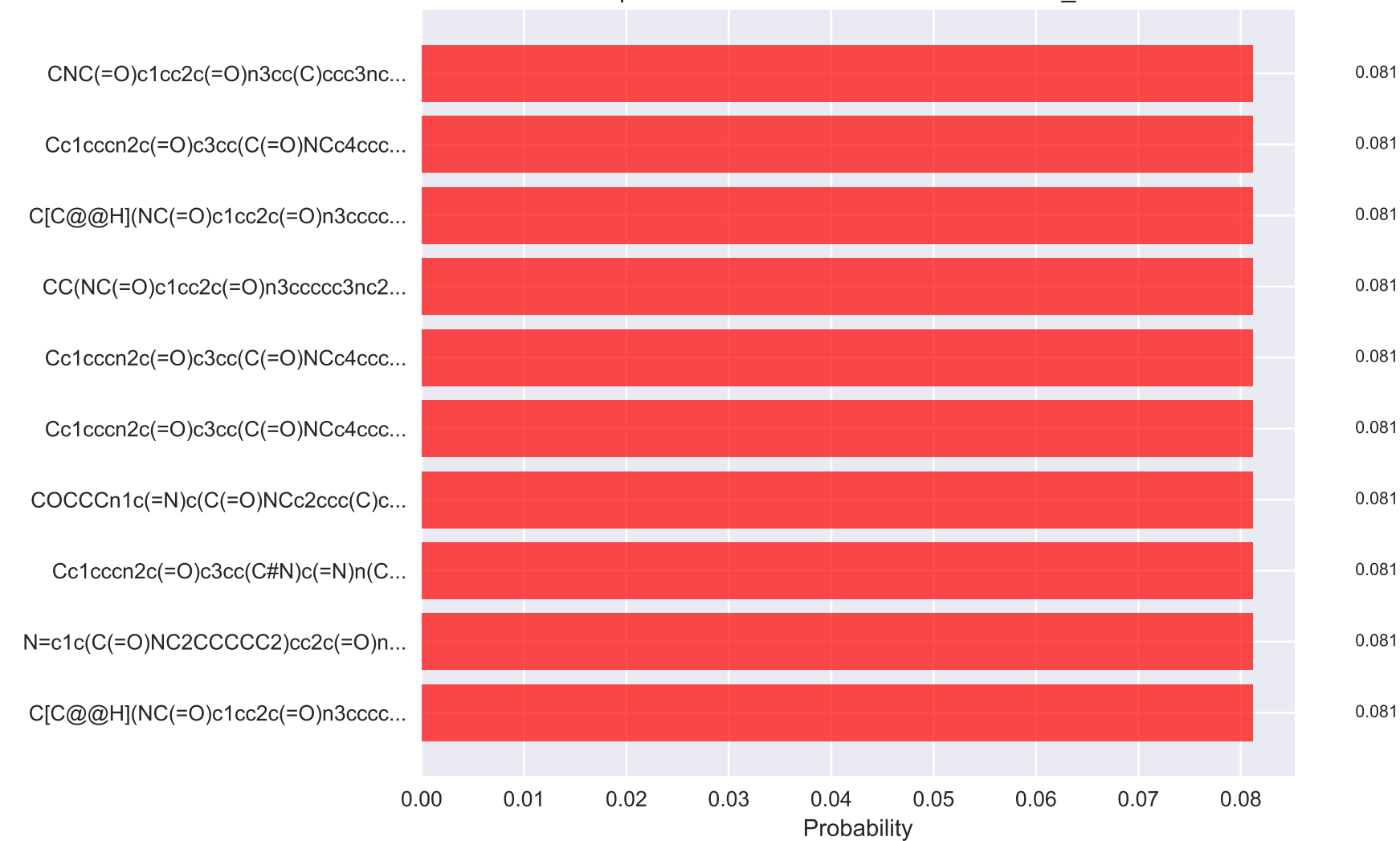
# Toxicity Analysis: SR-HSE\_best



Pass/Fail Distribution for SR-HSE\_best



Top 10 Most Toxic Molecules for SR-HSE\_best



Target: SR-HSE\_best

Total Molecules: 98

Passed: 98 (100.0%)

Failed: 0 (0.0%)

Probability Statistics:

Mean: 0.081

Median: 0.081

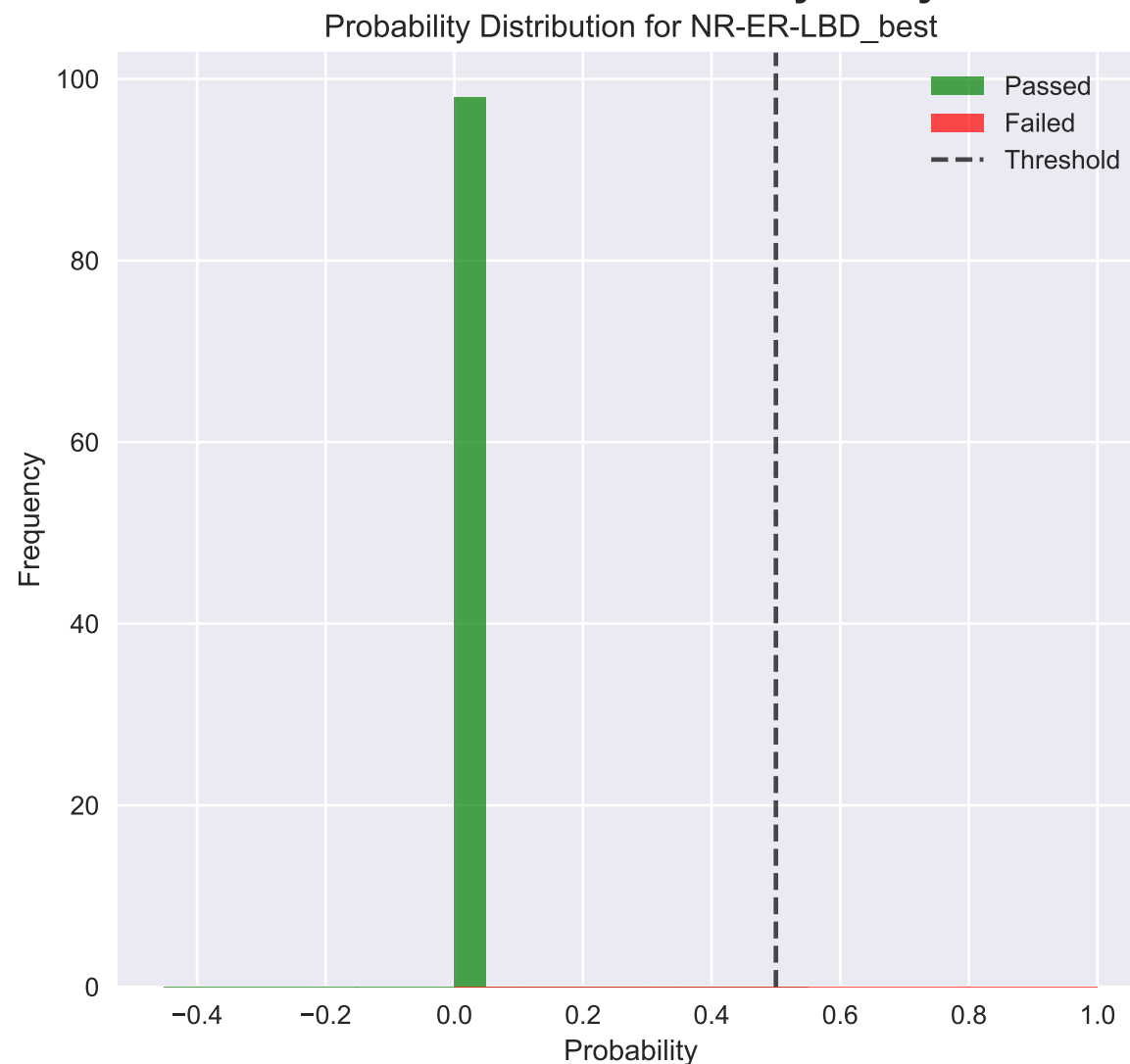
Std: 0.000

Min: 0.081

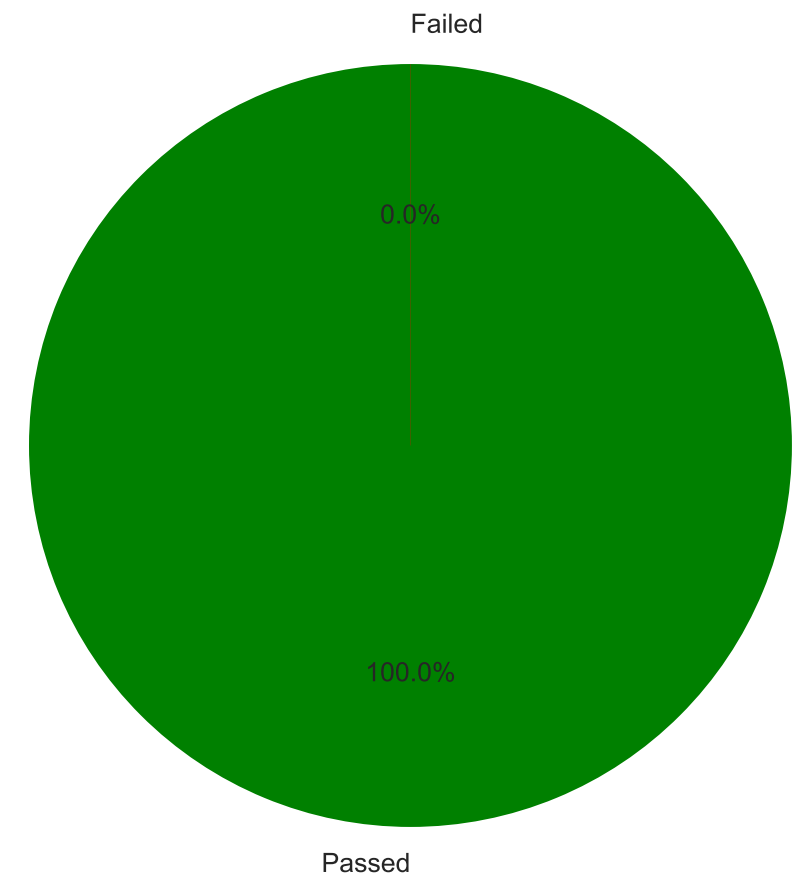
Max: 0.081

Threshold: 0.5

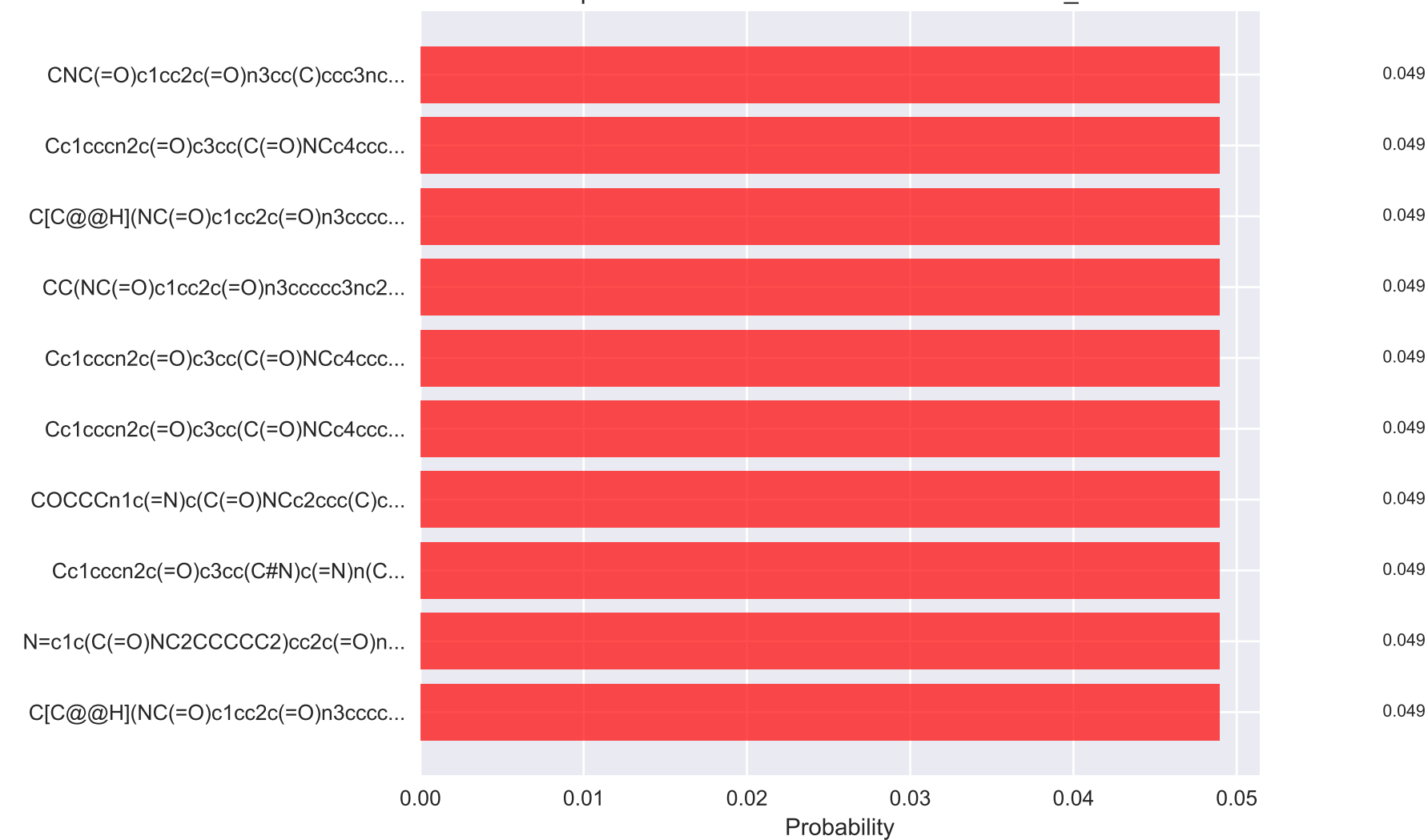
# Toxicity Analysis: NR-ER-LBD\_best



Pass/Fail Distribution for NR-ER-LBD\_best



Top 10 Most Toxic Molecules for NR-ER-LBD\_best



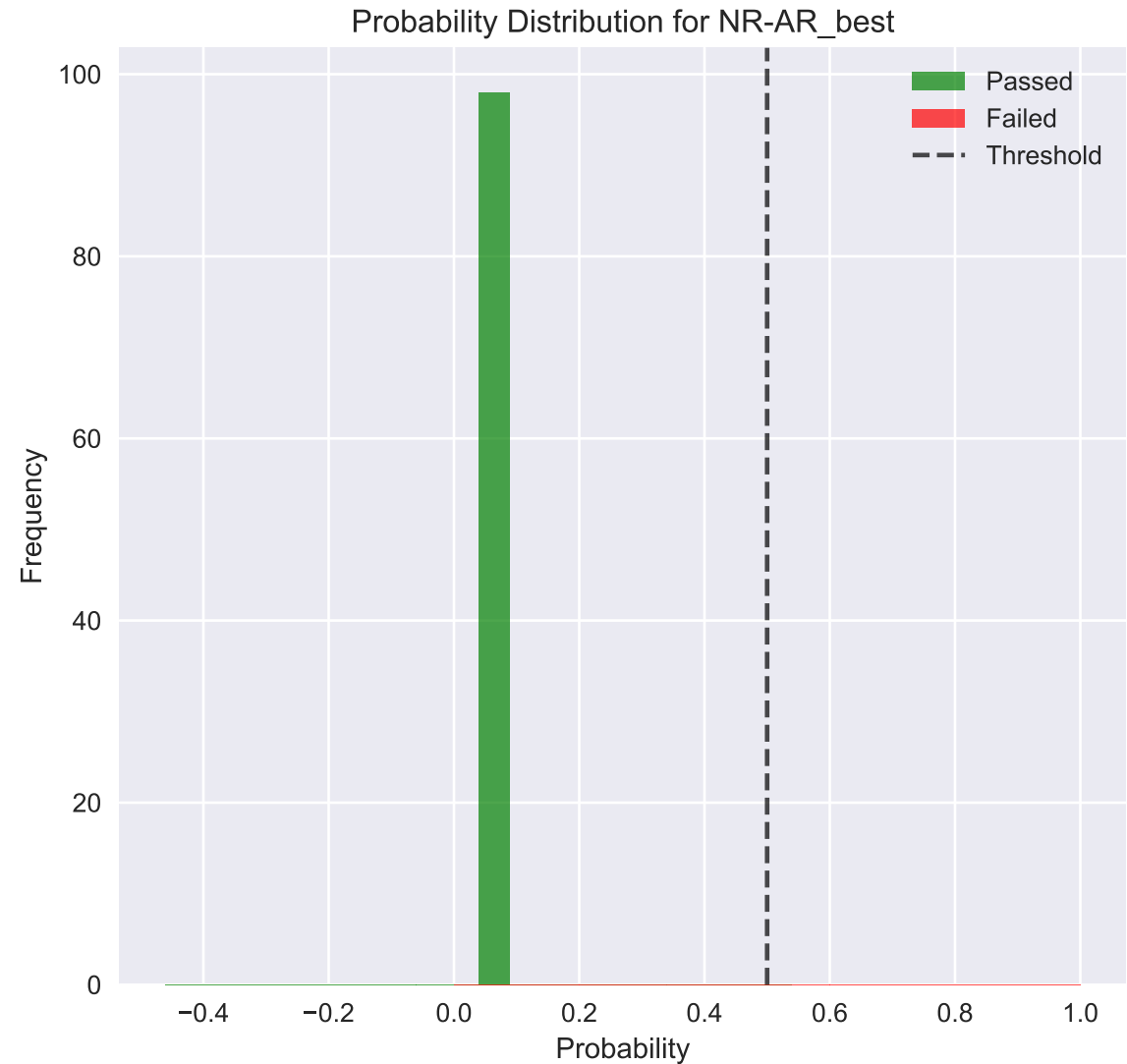
Target: NR-ER-LBD\_best

Total Molecules: 98  
Passed: 98 (100.0%)  
Failed: 0 (0.0%)

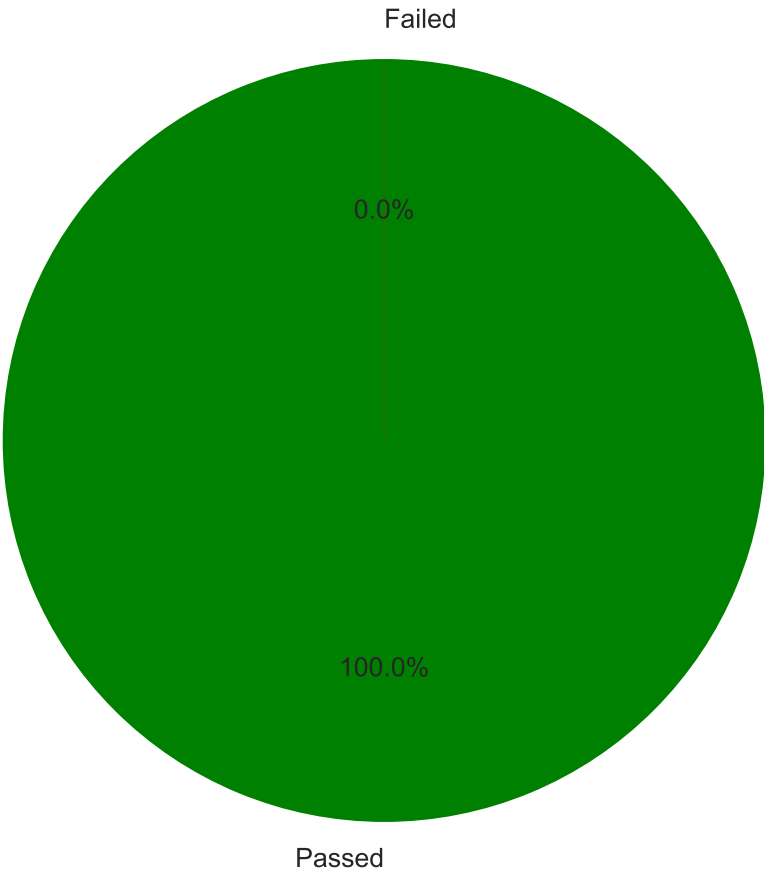
Probability Statistics:  
Mean: 0.049  
Median: 0.049  
Std: 0.000  
Min: 0.049  
Max: 0.049

Threshold: 0.5

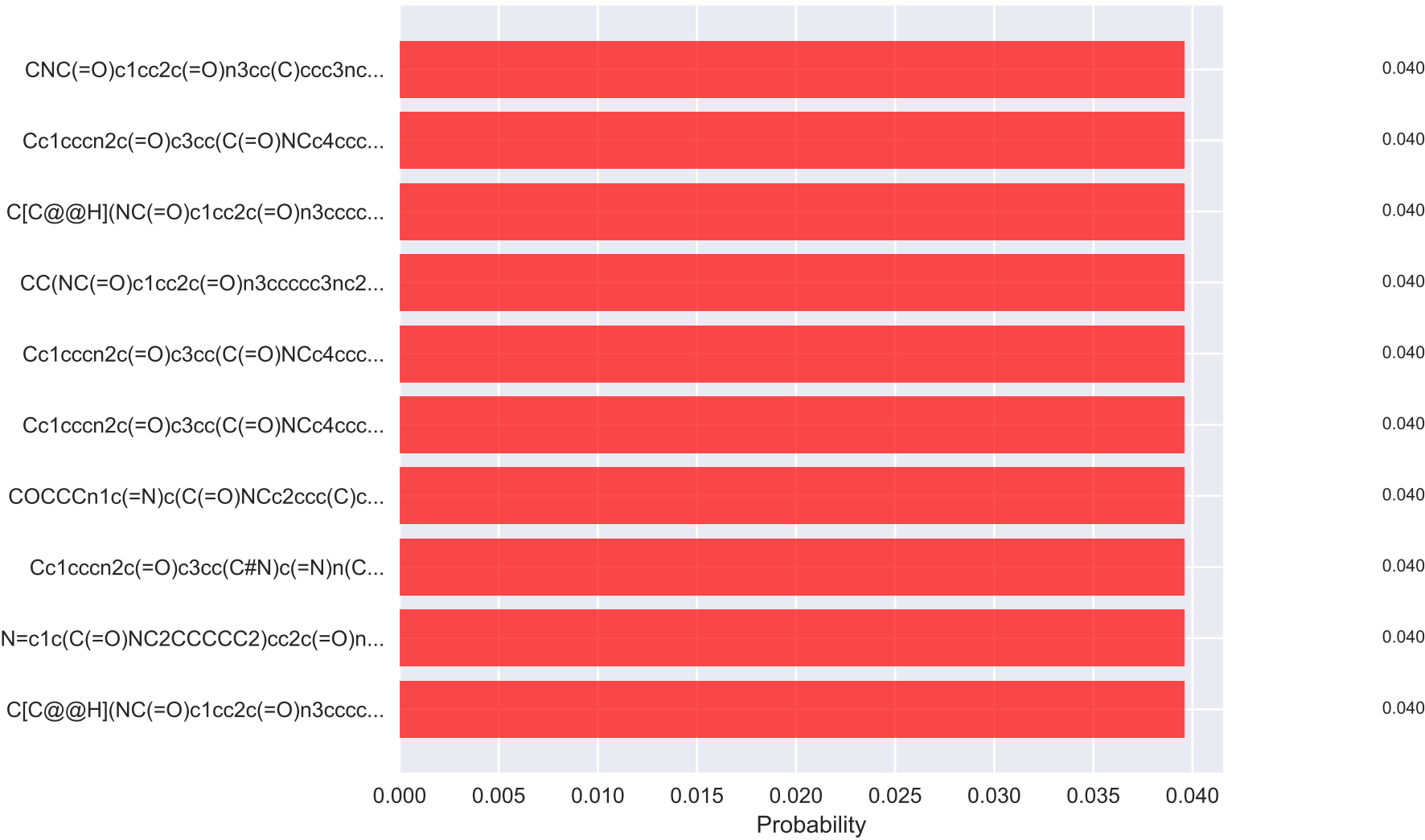
Toxicity Analysis: NR-AR\_best



Pass/Fail Distribution for NR-AR\_best



Top 10 Most Toxic Molecules for NR-AR\_best



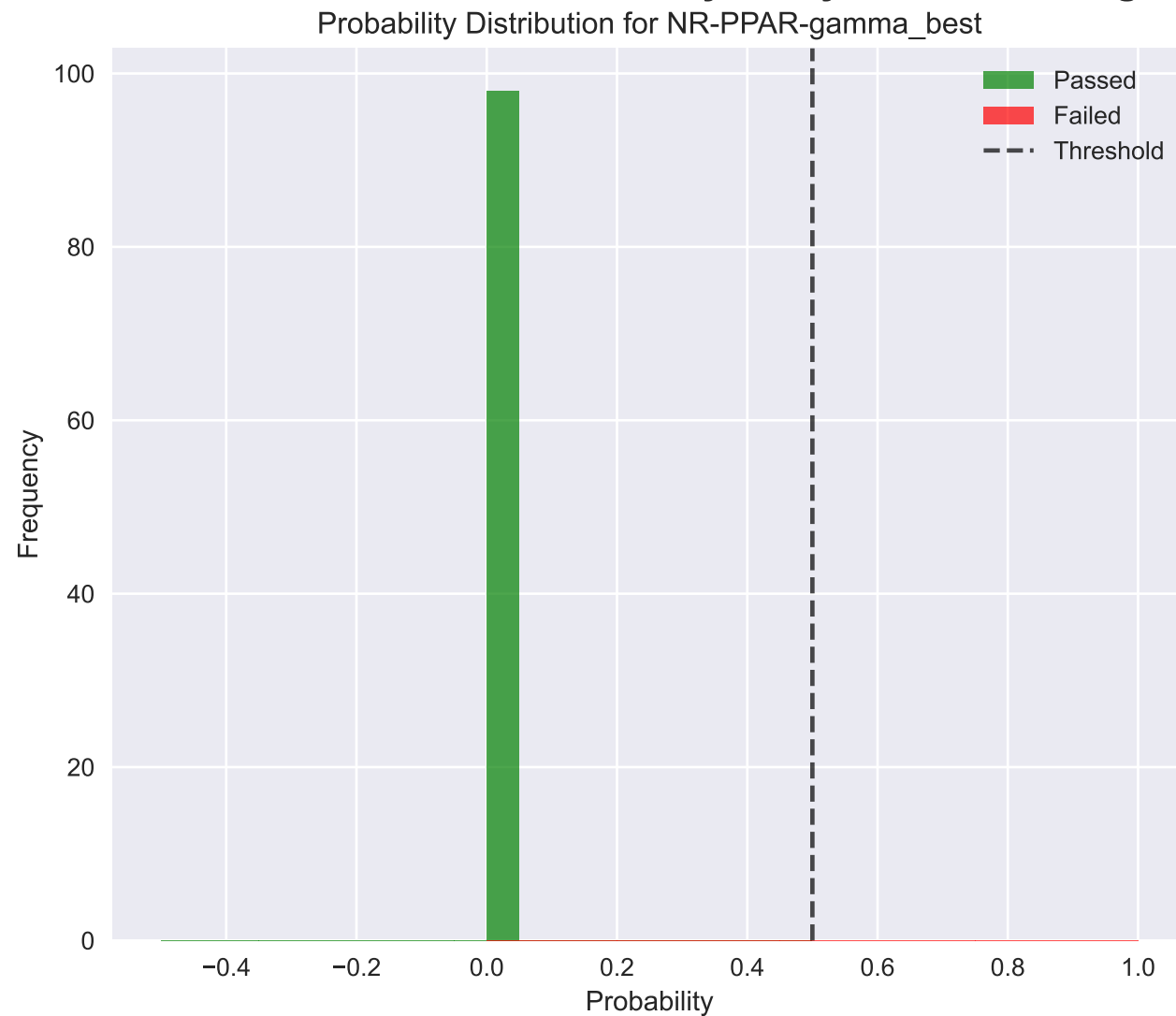
Target: NR-AR\_best

Total Molecules: 98  
Passed: 98 (100.0%)  
Failed: 0 (0.0%)

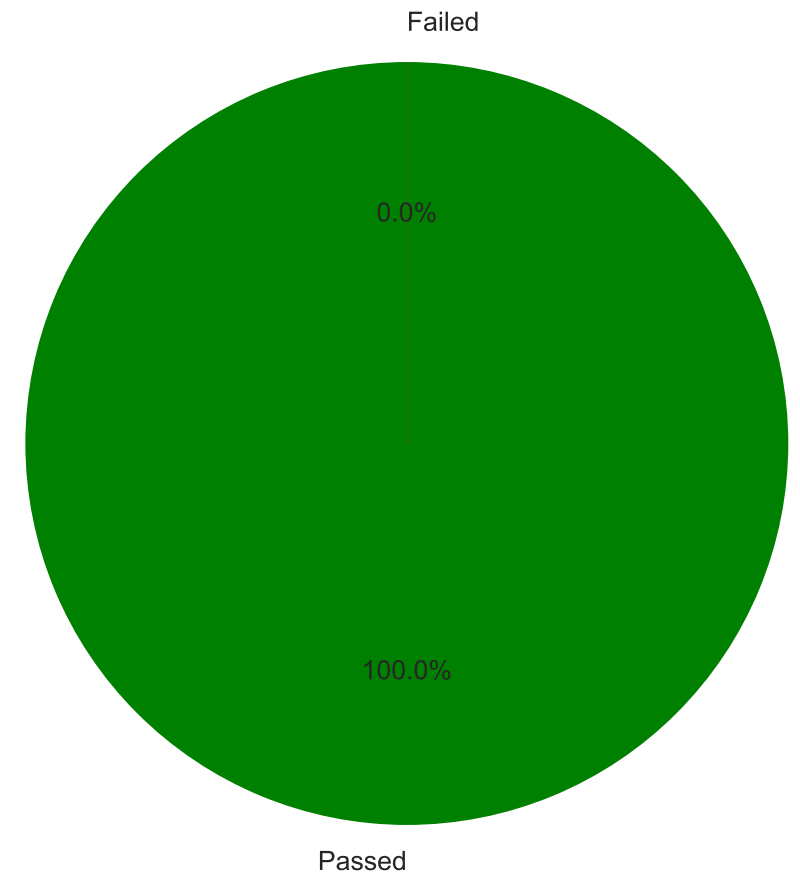
Probability Statistics:  
Mean: 0.040  
Median: 0.040  
Std: 0.000  
Min: 0.040  
Max: 0.040

Threshold: 0.5

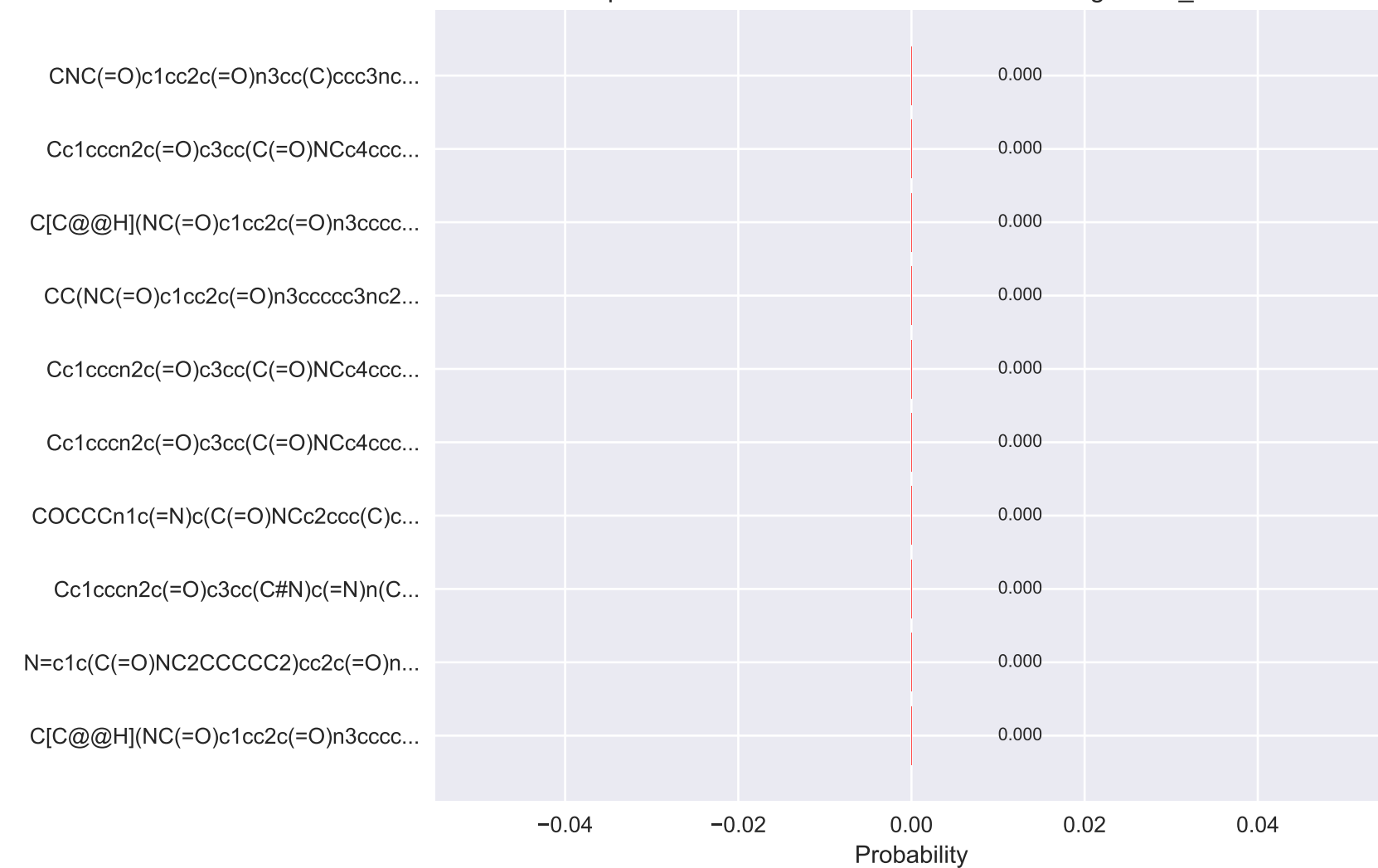
# Toxicity Analysis: NR-PPAR-gamma\_best



Pass/Fail Distribution for NR-PPAR-gamma\_best



Top 10 Most Toxic Molecules for NR-PPAR-gamma\_best



Target: NR-PPAR-gamma\_best

Total Molecules: 98

Passed: 98 (100.0%)

Failed: 0 (0.0%)

Probability Statistics:

Mean: 0.000

Median: 0.000

Std: 0.000

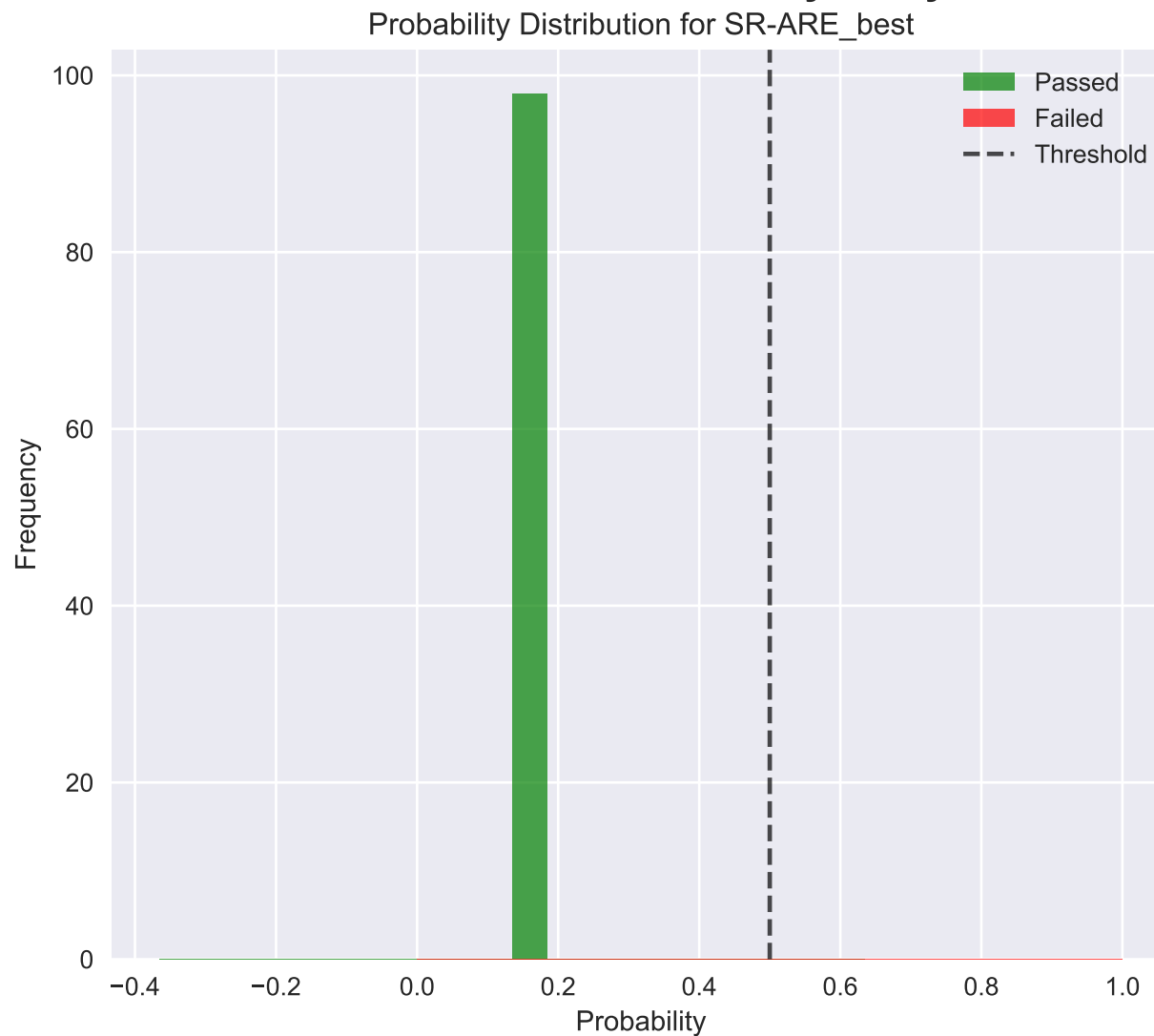
Min: 0.000

Max: 0.000

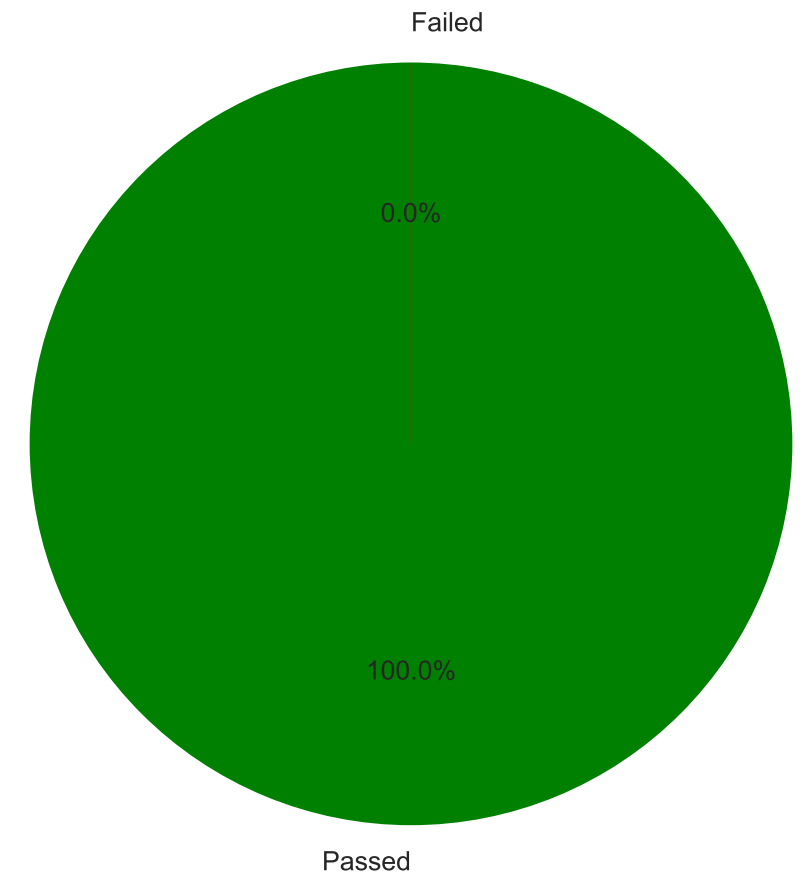
Threshold: 0.5



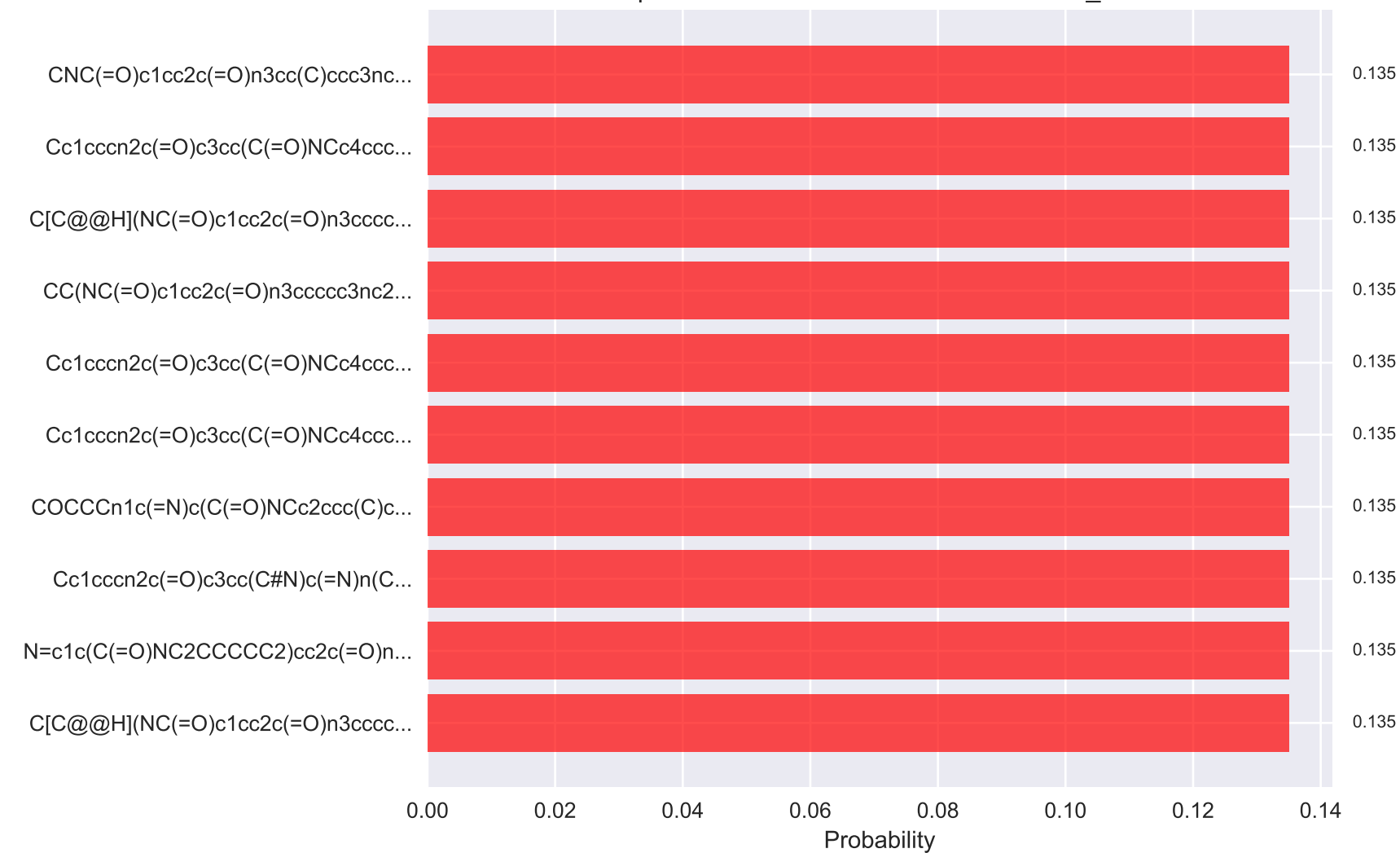
# Toxicity Analysis: SR-ARE\_best



Pass/Fail Distribution for SR-ARE\_best



Top 10 Most Toxic Molecules for SR-ARE\_best



Target: SR-ARE\_best

Total Molecules: 98

Passed: 98 (100.0%)

Failed: 0 (0.0%)

Probability Statistics:

Mean: 0.135

Median: 0.135

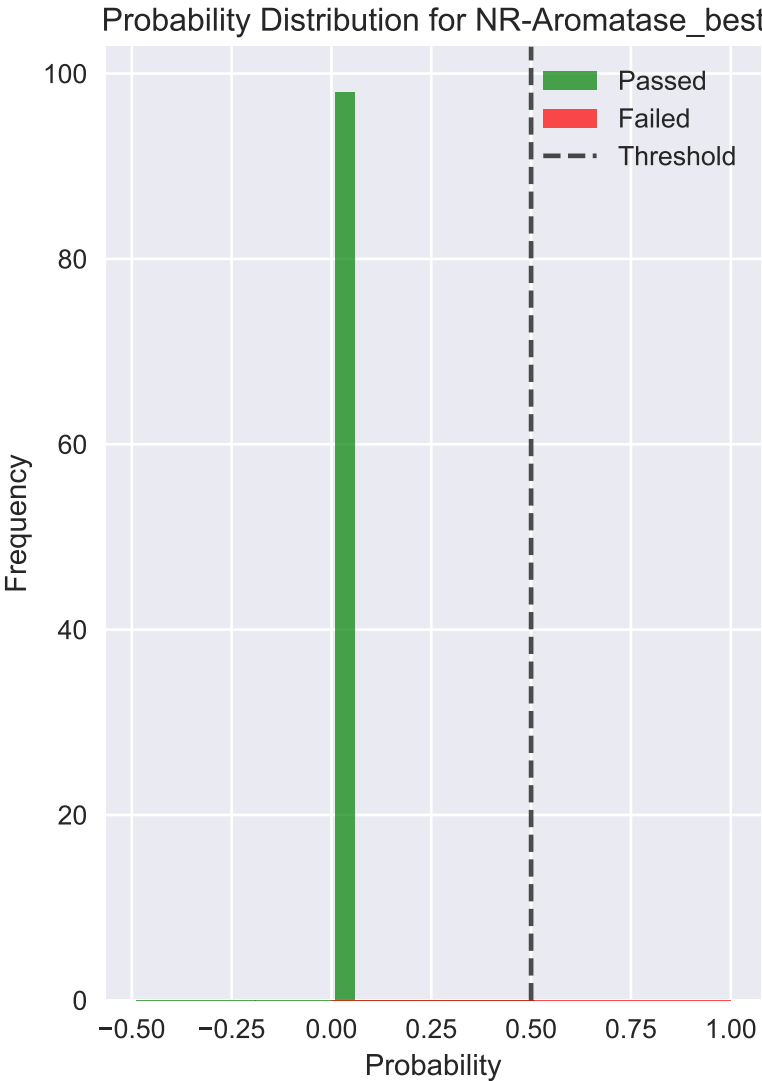
Std: 0.000

Min: 0.135

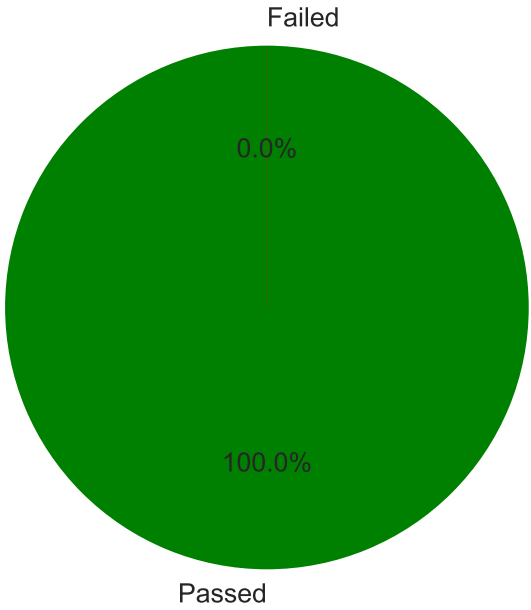
Max: 0.135

Threshold: 0.5

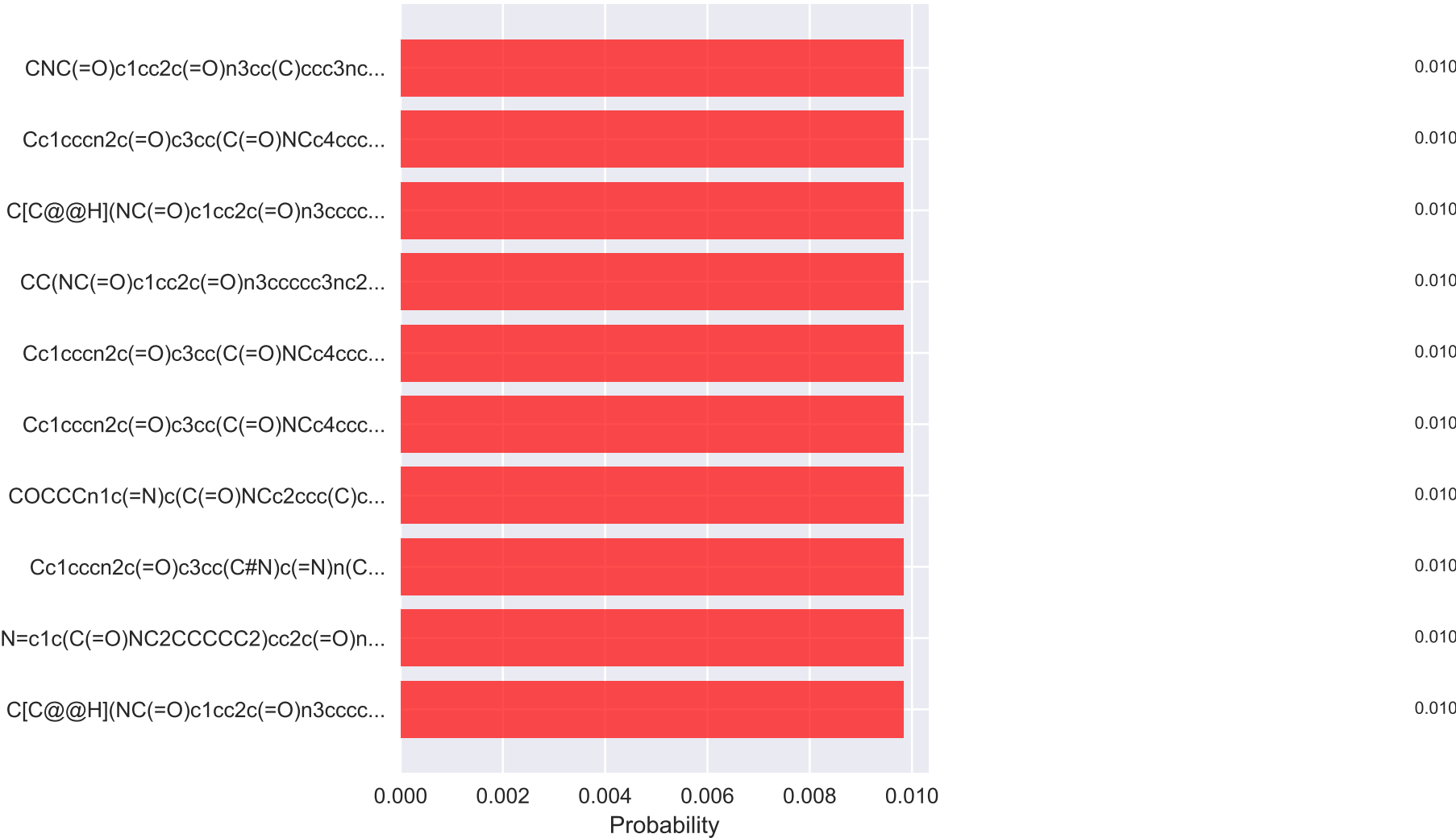
Toxicity Analysis: NR-Aromatase\_best



Pass/Fail Distribution for NR-Aromatase\_best



Top 10 Most Toxic Molecules for NR-Aromatase\_best



Target: NR-Aromatase

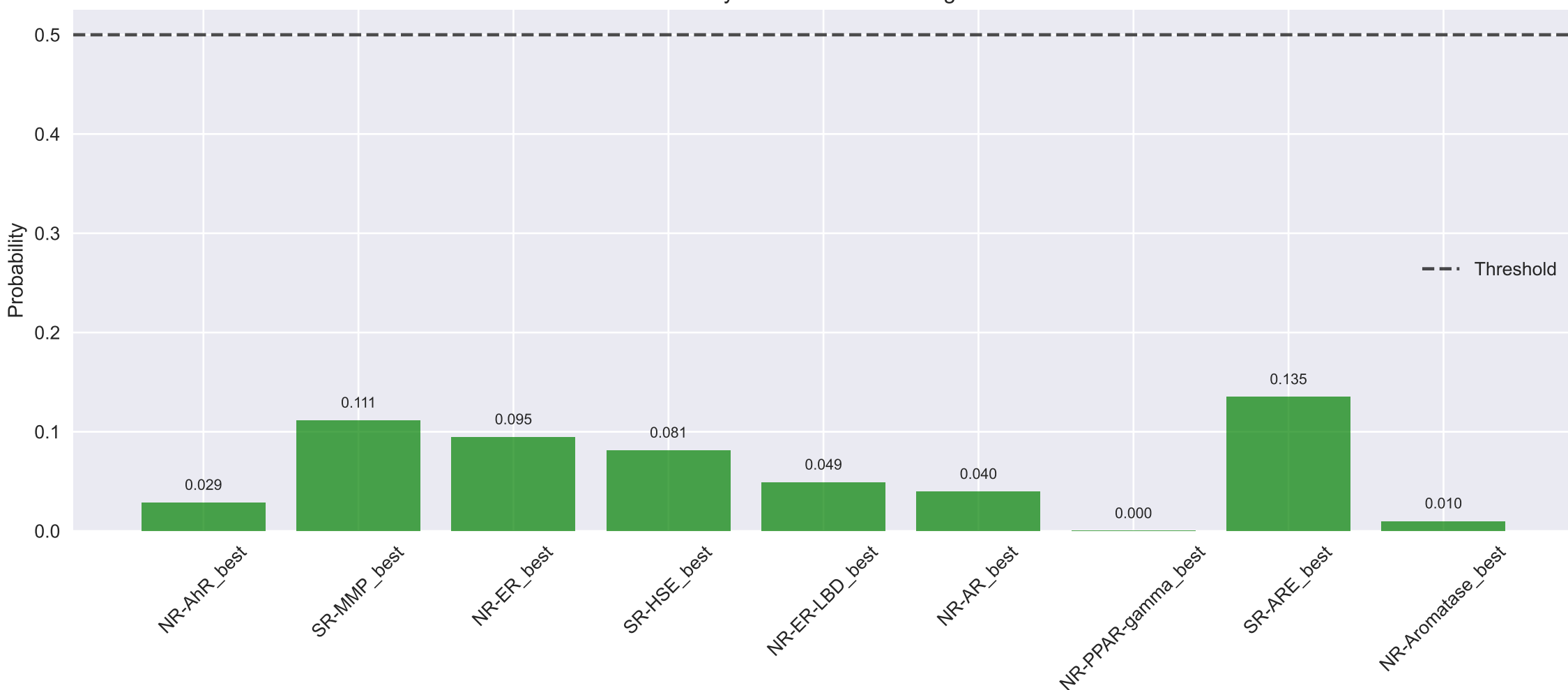
Total Molecules: 98  
Passed: 98 (100.0%)  
Failed: 0 (0.0%)

Probability Statistics:  
Mean: 0.010  
Median: 0.010  
Std: 0.000  
Min: 0.010  
Max: 0.010

Threshold: 0.5

# Molecule 1: C[C@@H](NC(=O)c1cc2c(=O)n3ccccc3nc2n(C[C@H]2CCCO2)c1=N)c1ccccc1

Toxicity Profile Across All Targets



## Molecule Summary:

SMILES: C[C@@H](NC(=O)c1cc2c(=O)n3ccccc3nc2n(C[C@H]2CCCO2)c1=N)c1ccccc1  
Average Toxicity: 0.061

Targets Passed: 9/9

Targets Failed: 0/9

## Highest Risk Targets:

1. SR-ARE\_best: 0.135
2. SR-MMP\_best: 0.111
3. NR-ER\_best: 0.095

## Molecule 2: N=c1c(C(=O)NC2CCCCC2)cc2c(=O)n3ccccc3nc2n1Cc1cccnc...

Toxicity Profile Across All Targets



### Molecule Summary:

SMILES: N=c1c(C(=O)NC2CCCCC2)cc2c(=O)n3ccccc3nc2n1Cc1cccnc1

Average Toxicity: 0.061

Targets Passed: 9/9

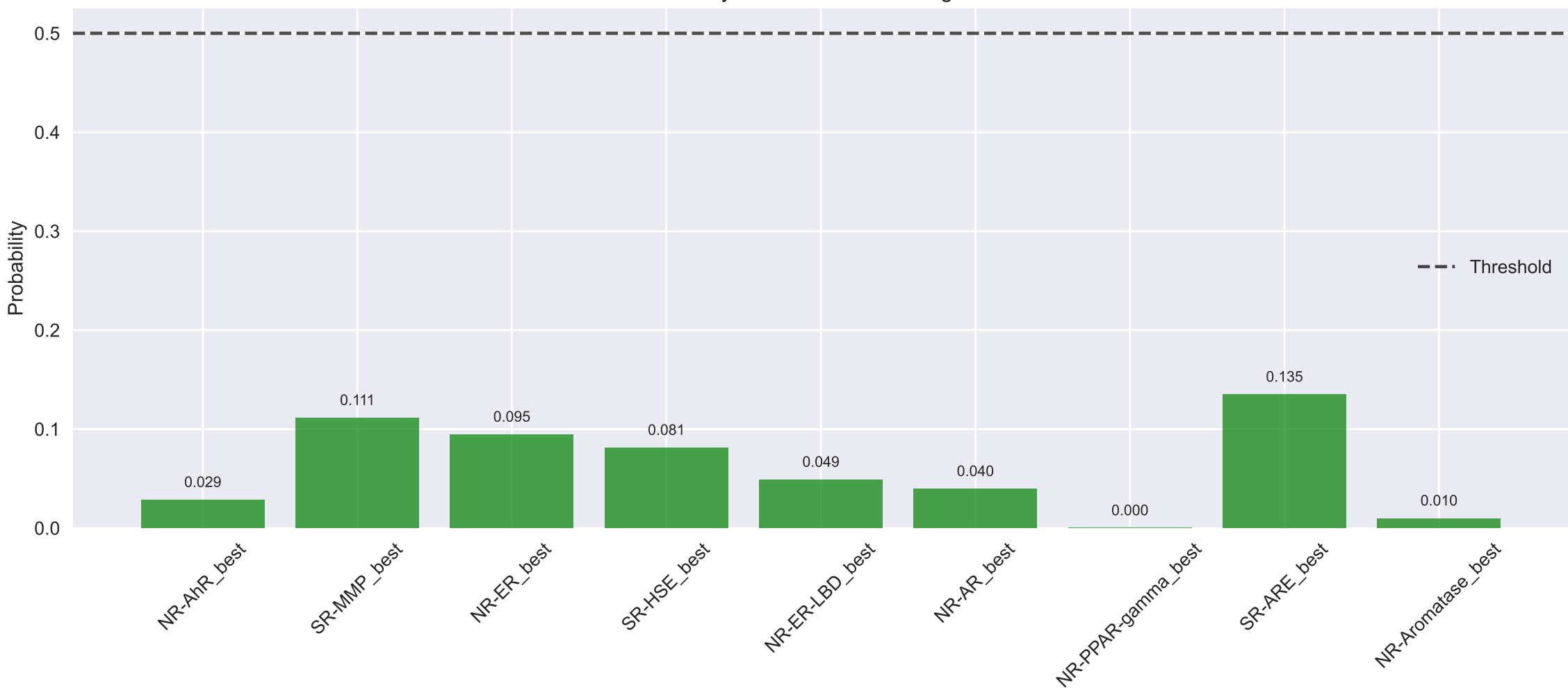
Targets Failed: 0/9

### Highest Risk Targets:

1. SR-ARE\_best: 0.135
2. SR-MMP\_best: 0.111
3. NR-ER\_best: 0.095

# Molecule 3: Cc1cccn2c(=O)c3cc(C#N)c(=N)n(Cc4ccccc4)c3nc12...

Toxicity Profile Across All Targets



## Molecule Summary:

SMILES: Cc1cccn2c(=O)c3cc(C#N)c(=N)n(Cc4ccccc4)c3nc12

Average Toxicity: 0.061

Targets Passed: 9/9

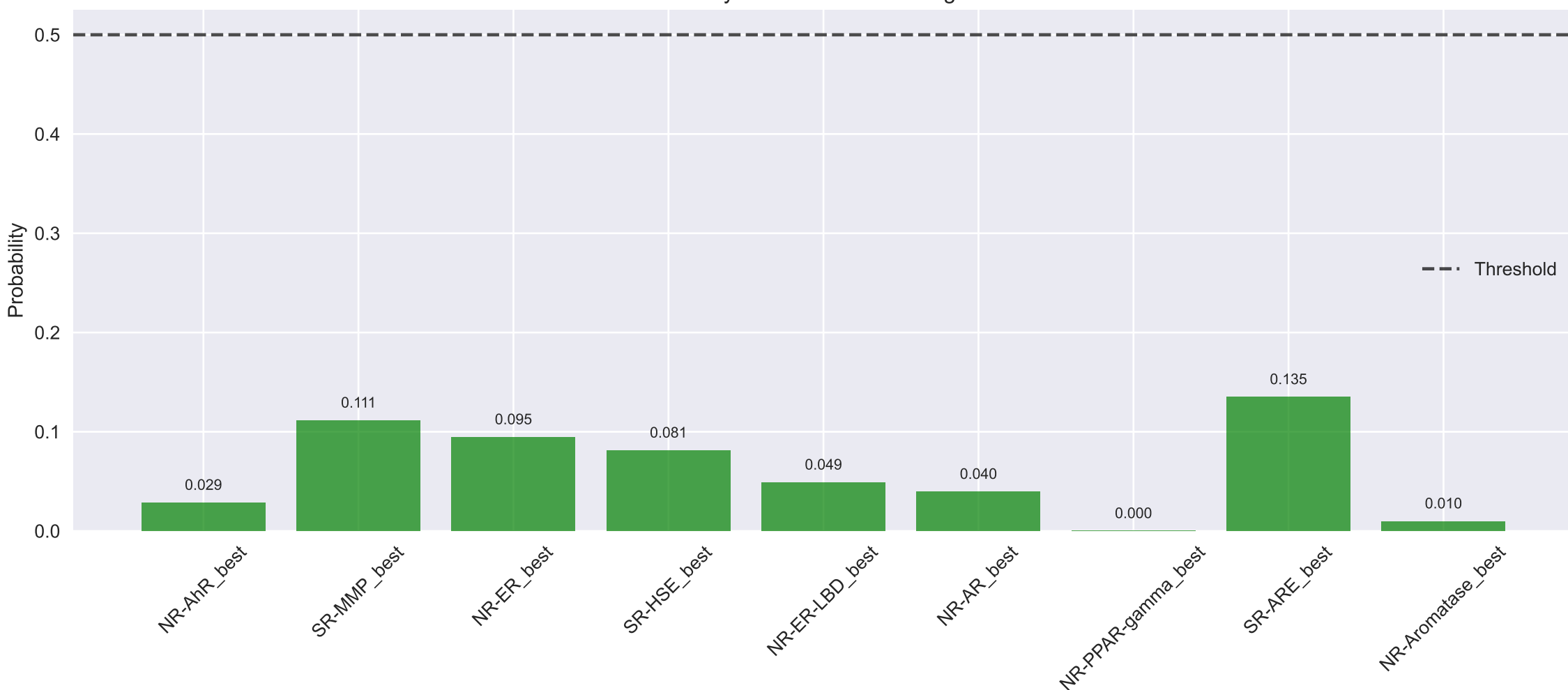
Targets Failed: 0/9

## Highest Risk Targets:

1. SR-ARE\_best: 0.135
2. SR-MMP\_best: 0.111
3. NR-ER\_best: 0.095

# Molecule 4: COCCCN1c(=N)c(C(=O)NCc2ccc(C)cc2)cc2c(=O)n3ccccc3n...

Toxicity Profile Across All Targets



## Molecule Summary:

SMILES: COCCCN1c(=N)c(C(=O)NCc2ccc(C)cc2)cc2c(=O)n3ccccc3nc21  
Average Toxicity: 0.061

Targets Passed: 9/9

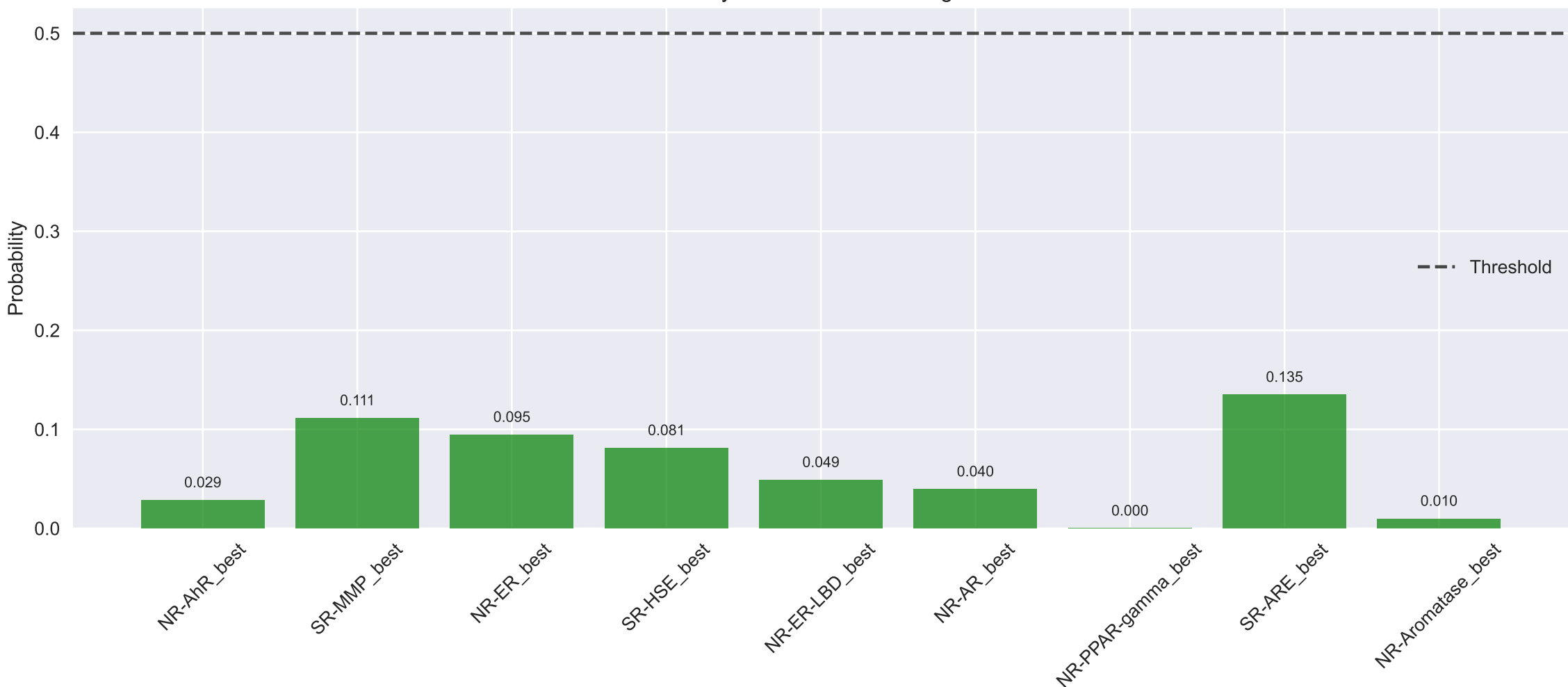
Targets Failed: 0/9

## Highest Risk Targets:

1. SR-ARE\_best: 0.135
2. SR-MMP\_best: 0.111
3. NR-ER\_best: 0.095

# Molecule 5: Cc1cccn2c(=O)c3cc(C(=O)NCc4cccnc4)c(=N)n(Cc4ccc(F)cc4)c3nc12

Toxicity Profile Across All Targets



## Molecule Summary:

SMILES: Cc1cccn2c(=O)c3cc(C(=O)NCc4cccnc4)c(=N)n(Cc4ccc(F)cc4)c3nc12  
Average Toxicity: 0.061

Targets Passed: 9/9

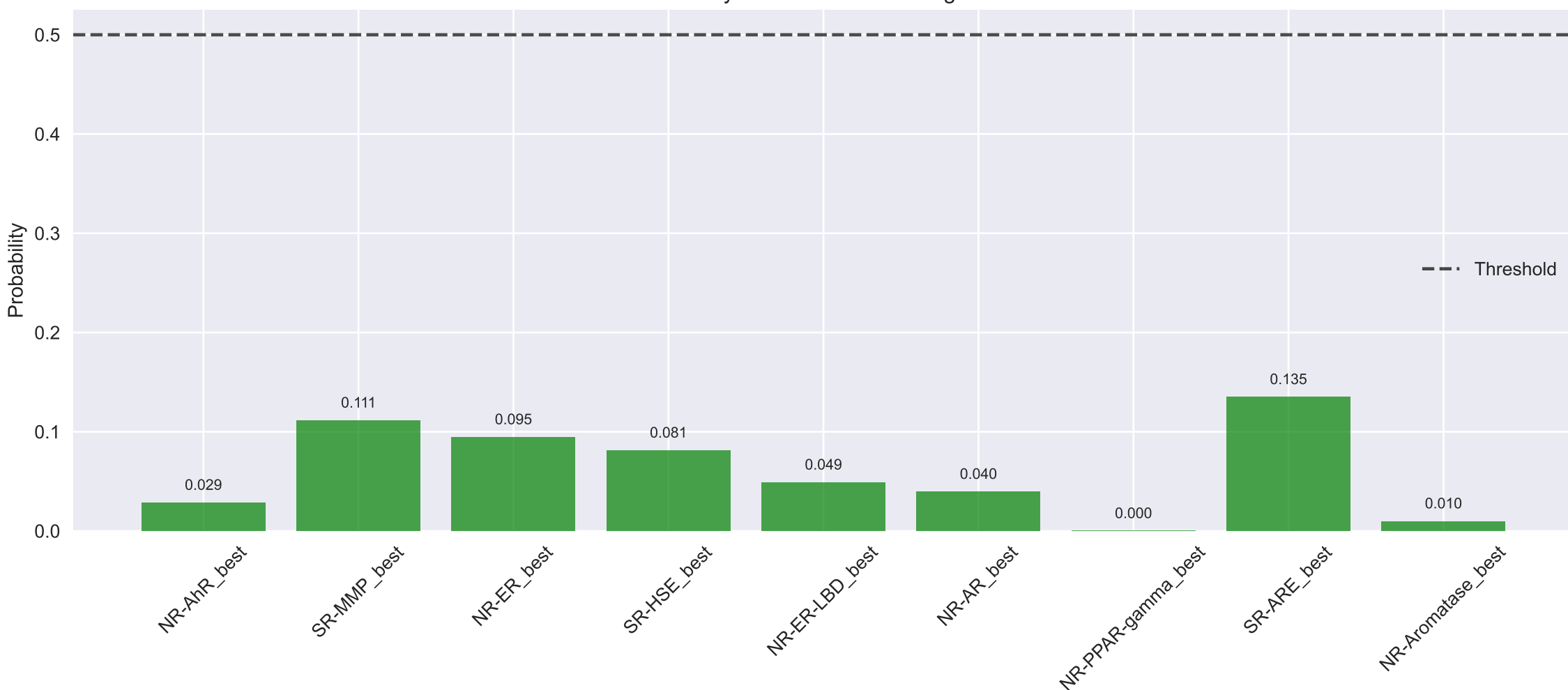
Targets Failed: 0/9

## Highest Risk Targets:

1. SR-ARE\_best: 0.135
2. SR-MMP\_best: 0.111
3. NR-ER\_best: 0.095

# Molecule 6: Cc1cccn2c(=O)c3cc(C(=O)NCc4cccnc4)c(=N)n(CC4CCCO4)...

Toxicity Profile Across All Targets



## Molecule Summary:

SMILES: Cc1cccn2c(=O)c3cc(C(=O)NCc4cccnc4)c(=N)n(CC4CCCO4)c3nc12  
Average Toxicity: 0.061

Targets Passed: 9/9

Targets Failed: 0/9

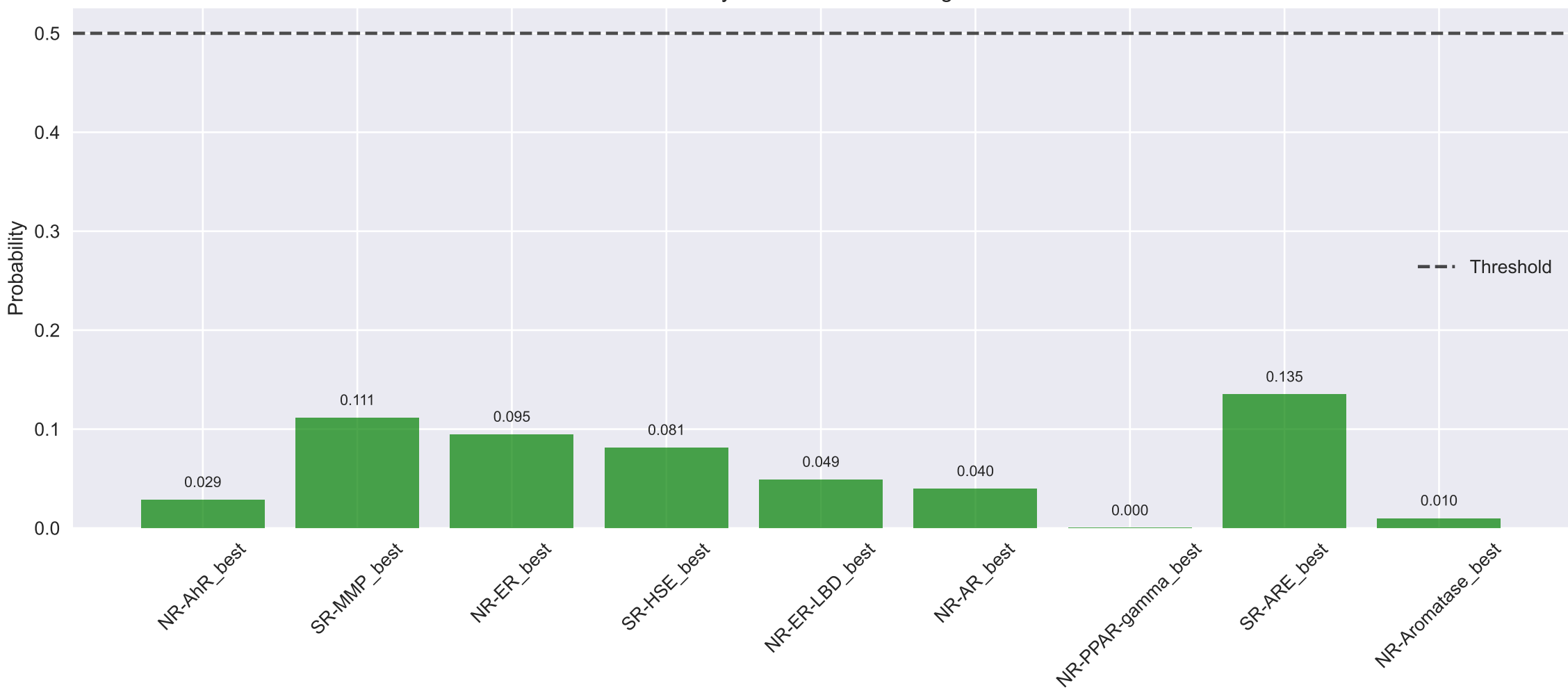
## Highest Risk Targets:

1. SR-ARE\_best: 0.135
2. SR-MMP\_best: 0.111
3. NR-ER\_best: 0.095



# Molecule 7: CC(NC(=O)c1cc2c(=O)n3ccccc3nc2n(Cc2ccccc2)c1=N)c1c...

Toxicity Profile Across All Targets



## Molecule Summary:

SMILES: CC(NC(=O)c1cc2c(=O)n3ccccc3nc2n(Cc2ccccc2)c1=N)c1ccccc1  
Average Toxicity: 0.061

Targets Passed: 9/9

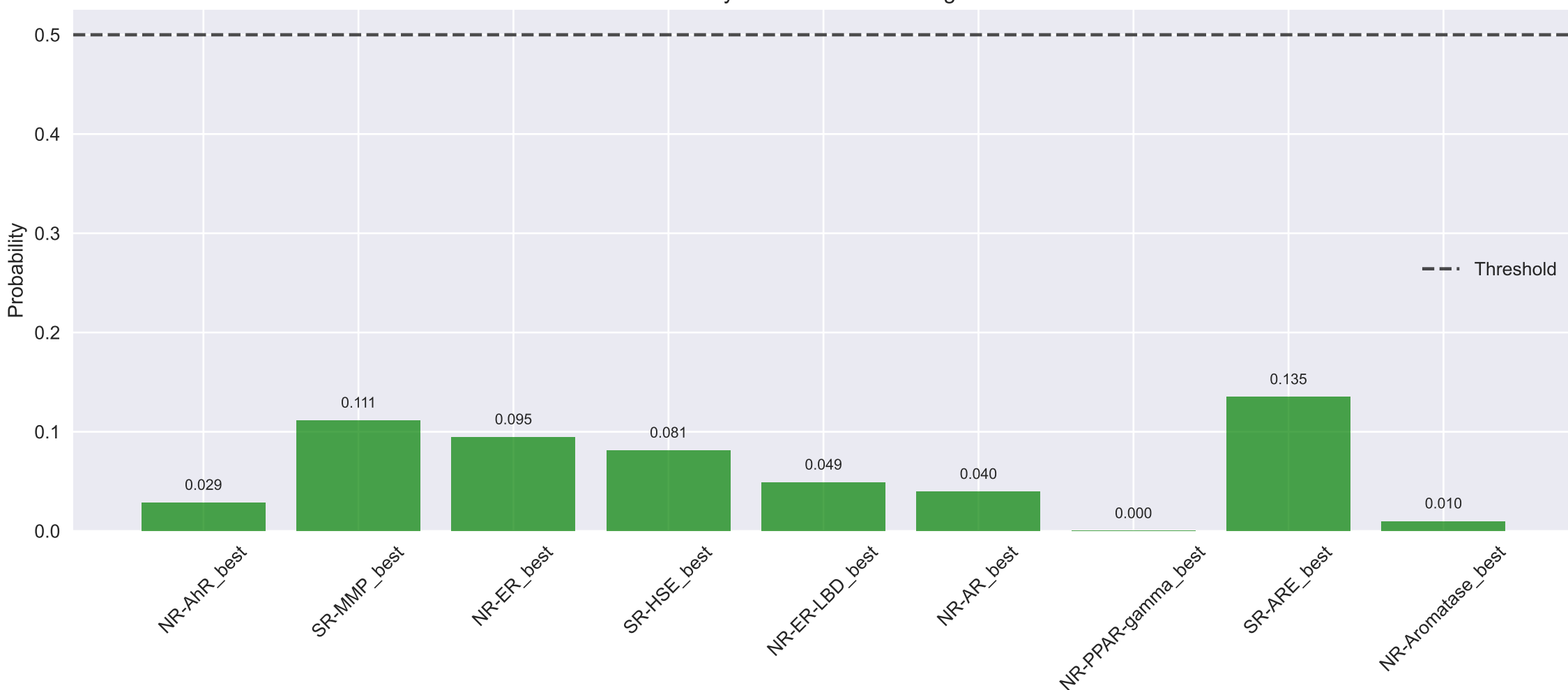
Targets Failed: 0/9

## Highest Risk Targets:

1. SR-ARE\_best: 0.135
2. SR-MMP\_best: 0.111
3. NR-ER\_best: 0.095

# Molecule 8: C[C@@H](NC(=O)c1cc2c(=O)n3ccccc3nc2n(C[C@H]2CCCO2)c1=N)c1ccccc1

Toxicity Profile Across All Targets



## Molecule Summary:

SMILES: C[C@@H](NC(=O)c1cc2c(=O)n3ccccc3nc2n(C[C@H]2CCCO2)c1=N)c1ccccc1  
Average Toxicity: 0.061

Targets Passed: 9/9

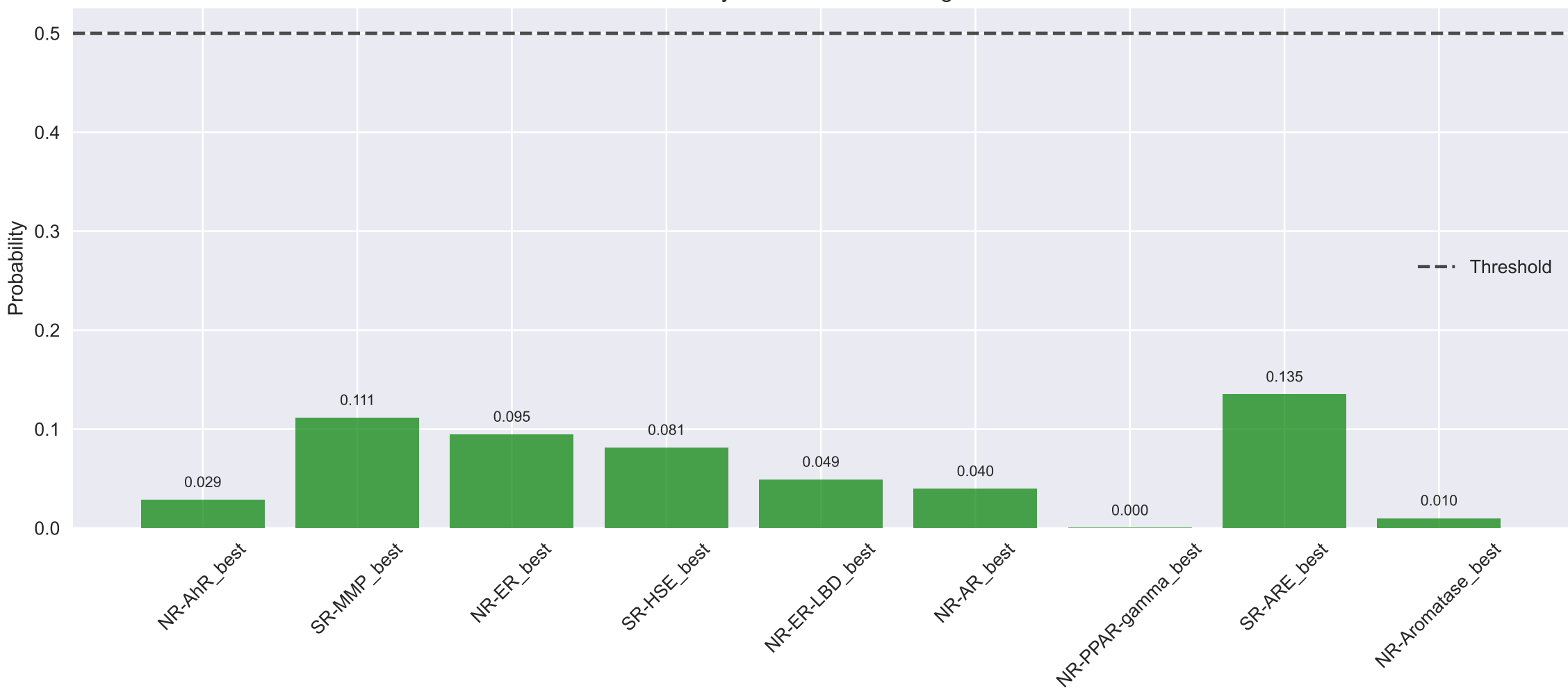
Targets Failed: 0/9

## Highest Risk Targets:

1. SR-ARE\_best: 0.135
2. SR-MMP\_best: 0.111
3. NR-ER\_best: 0.095

# Molecule 9: Cc1cccn2c(=O)c3cc(C(=O)NCc4cccnc4)c(=N)n(Cc4ccc(F)cc4)c3nc12

Toxicity Profile Across All Targets



## Molecule Summary:

SMILES: Cc1cccn2c(=O)c3cc(C(=O)NCc4cccnc4)c(=N)n(Cc4ccc(F)cc4)c3nc12  
Average Toxicity: 0.061

Targets Passed: 9/9

Targets Failed: 0/9

## Highest Risk Targets:

1. SR-ARE\_best: 0.135
2. SR-MMP\_best: 0.111
3. NR-ER\_best: 0.095

# Molecule 10: CNC(=O)c1cc2c(=O)n3cc(C)ccc3nc2n(Cc2cccnc2)c1=N...

Toxicity Profile Across All Targets



## Molecule Summary:

SMILES: CNC(=O)c1cc2c(=O)n3cc(C)ccc3nc2n(Cc2cccnc2)c1=N...  
Average Toxicity: 0.061

Targets Passed: 9/9

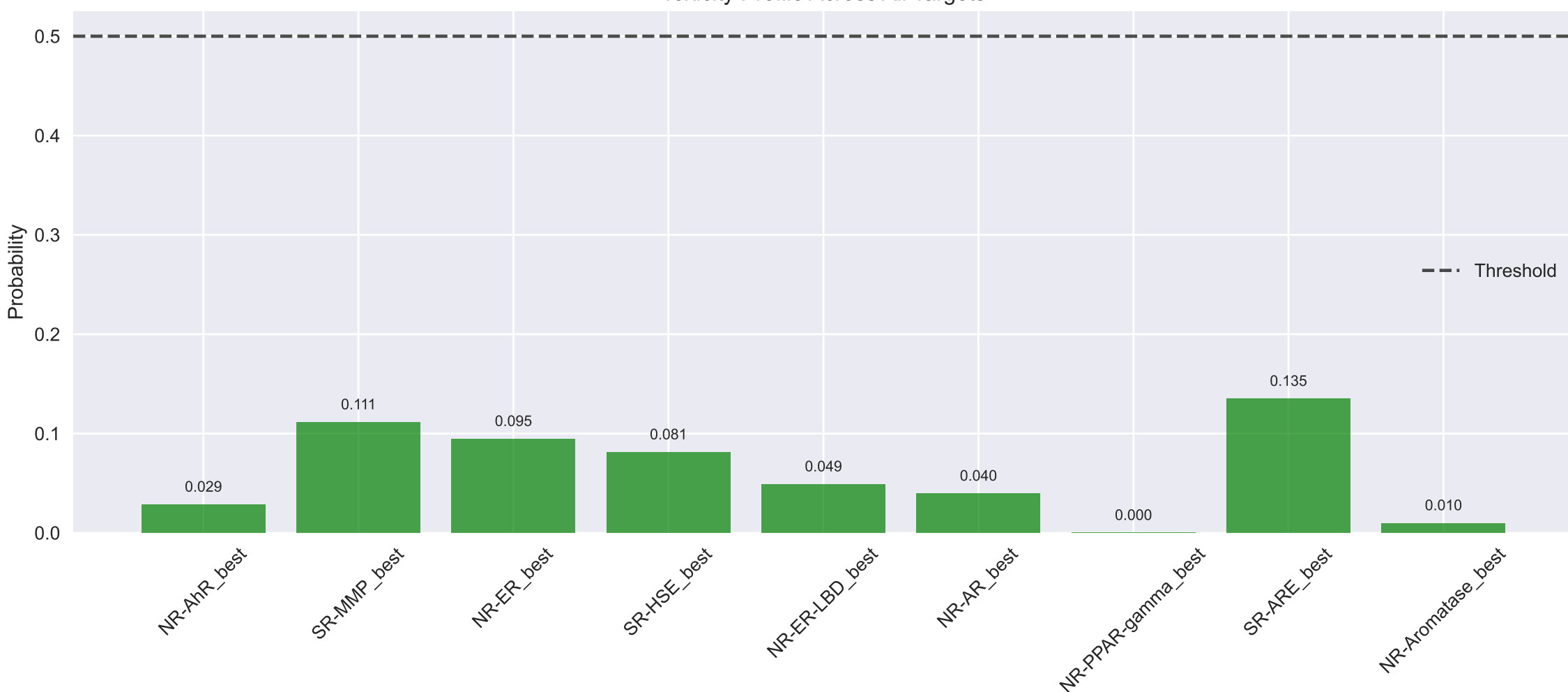
Targets Failed: 0/9

## Highest Risk Targets:

1. SR-ARE\_best: 0.135
2. SR-MMP\_best: 0.111
3. NR-ER\_best: 0.095

# Molecule 11: COCCCN1c(=N)c(C(=O)NCc2ccc(F)cc2)cc2c(=O)n3ccccc3n...

Toxicity Profile Across All Targets



## Molecule Summary:

SMILES: COCCCN1c(=N)c(C(=O)NCc2ccc(F)cc2)cc2c(=O)n3ccccc3nc21  
Average Toxicity: 0.061

Targets Passed: 9/9

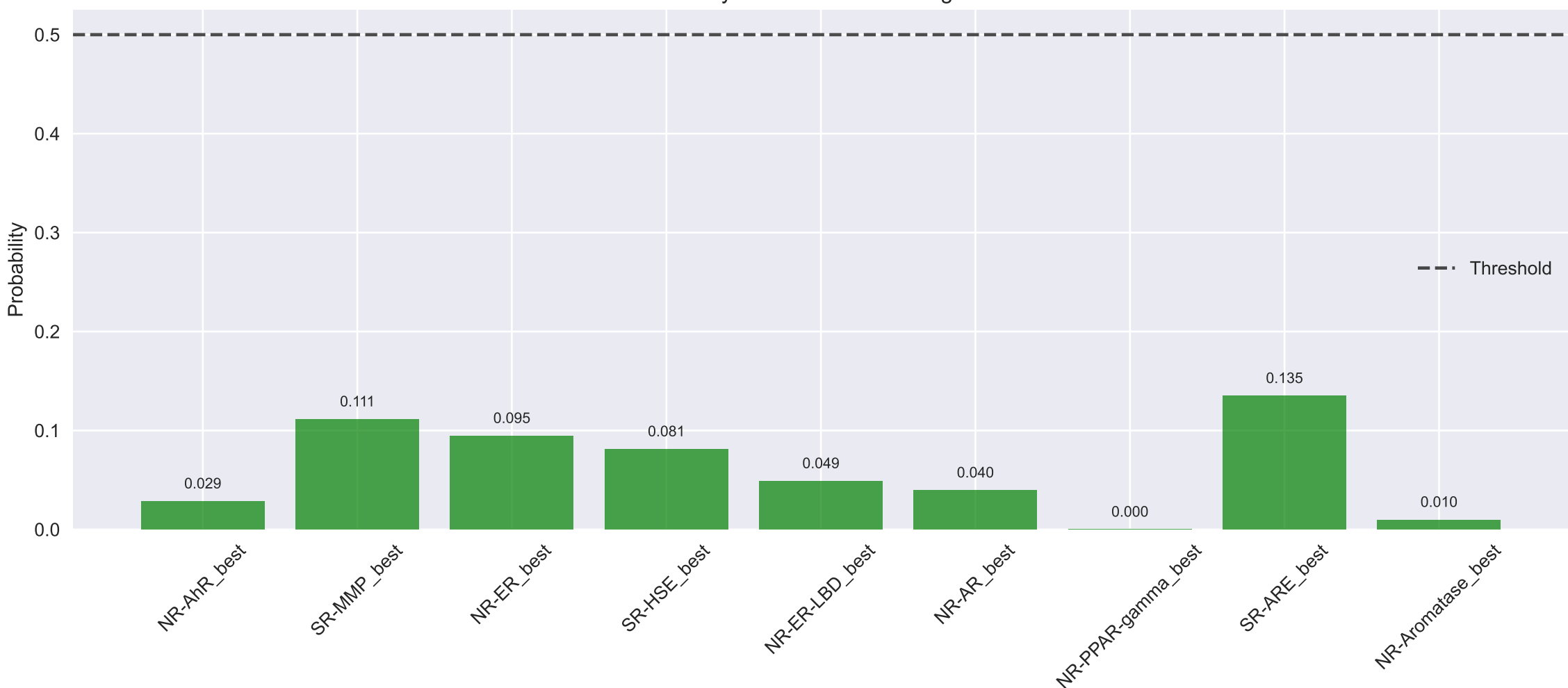
Targets Failed: 0/9

## Highest Risk Targets:

1. SR-ARE\_best: 0.135
2. SR-MMP\_best: 0.111
3. NR-ER\_best: 0.095

# Molecule 12: Cc1cccn2c(=O)c3cc(C#N)c(=N)n(Cc4cccnc4)c3nc12...

Toxicity Profile Across All Targets



## Molecule Summary:

SMILES: Cc1cccn2c(=O)c3cc(C#N)c(=N)n(Cc4cccnc4)c3nc12  
Average Toxicity: 0.061

Targets Passed: 9/9

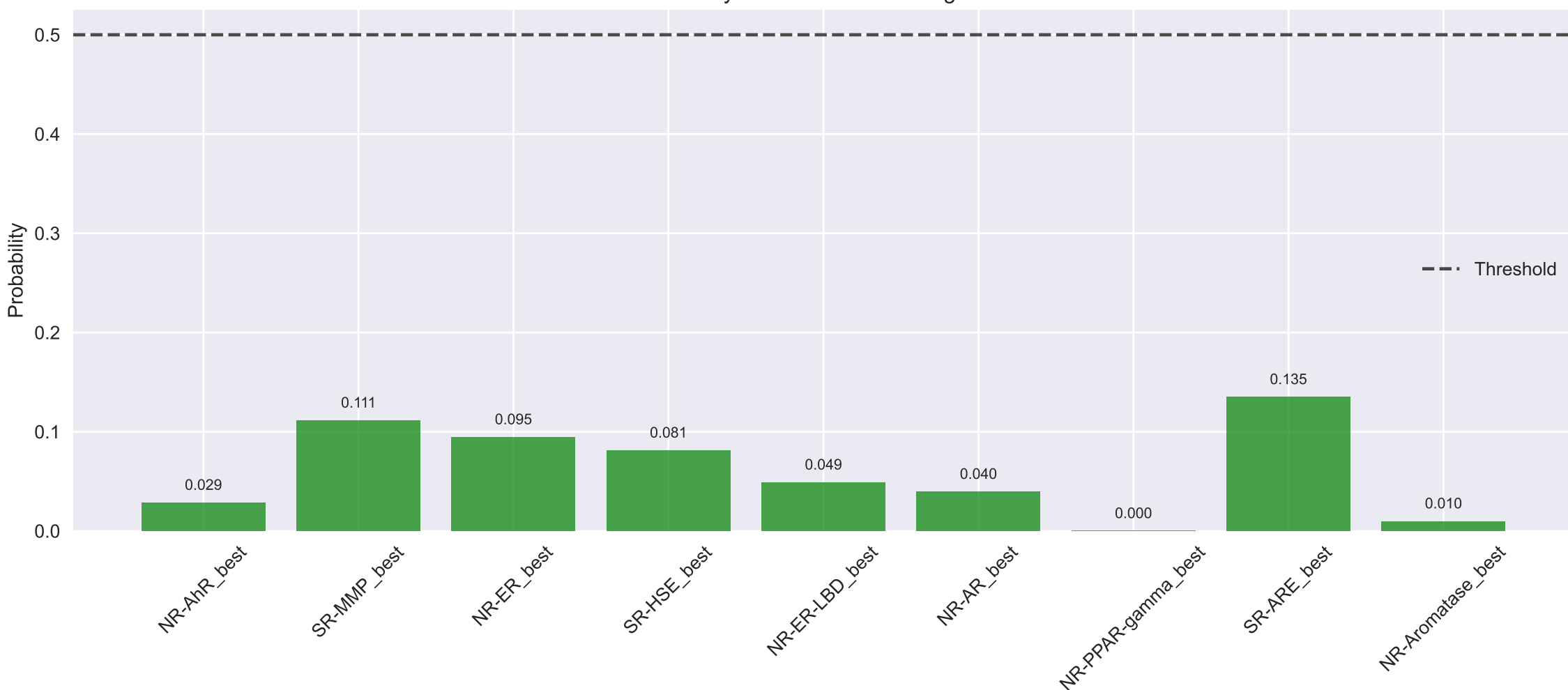
Targets Failed: 0/9

## Highest Risk Targets:

1. SR-ARE\_best: 0.135
2. SR-MMP\_best: 0.111
3. NR-ER\_best: 0.095

# Molecule 13: Cc1cccn2c(=O)c3cc(C(=O)NCc4cccnc4)c(=N)n(Cc4ccco4)...

Toxicity Profile Across All Targets



## Molecule Summary:

SMILES: Cc1cccn2c(=O)c3cc(C(=O)NCc4cccnc4)c(=N)n(Cc4ccco4)c3nc12  
Average Toxicity: 0.061

Targets Passed: 9/9

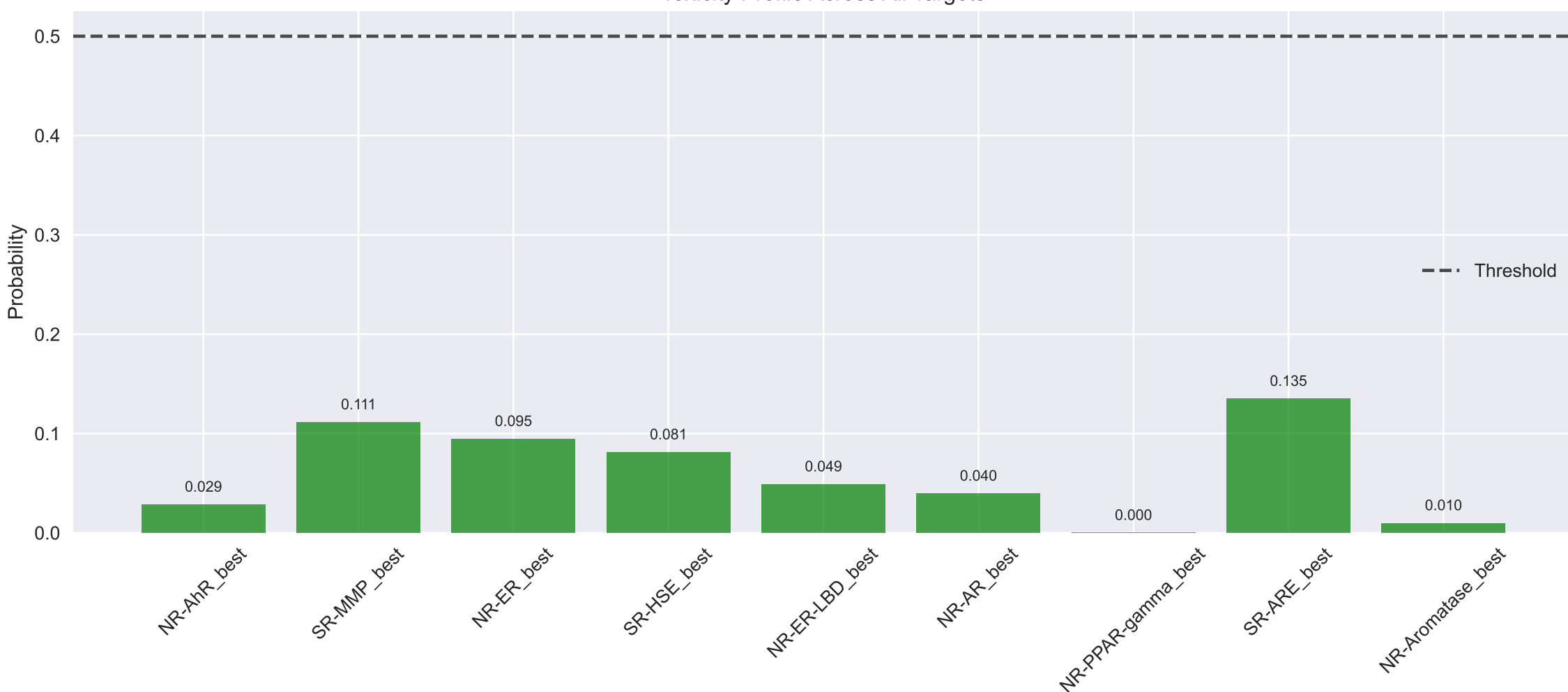
Targets Failed: 0/9

## Highest Risk Targets:

1. SR-ARE\_best: 0.135
2. SR-MMP\_best: 0.111
3. NR-ER\_best: 0.095

# Molecule 14: COCCCN1c(=N)c(C(=O)NCc2ccc(OC)cc2)cc2c(=O)n3ccccc3...

Toxicity Profile Across All Targets



## Molecule Summary:

SMILES: COCCCN1c(=N)c(C(=O)NCc2ccc(OC)cc2)cc2c(=O)n3ccccc3nc21  
Average Toxicity: 0.061

Targets Passed: 9/9

Targets Failed: 0/9

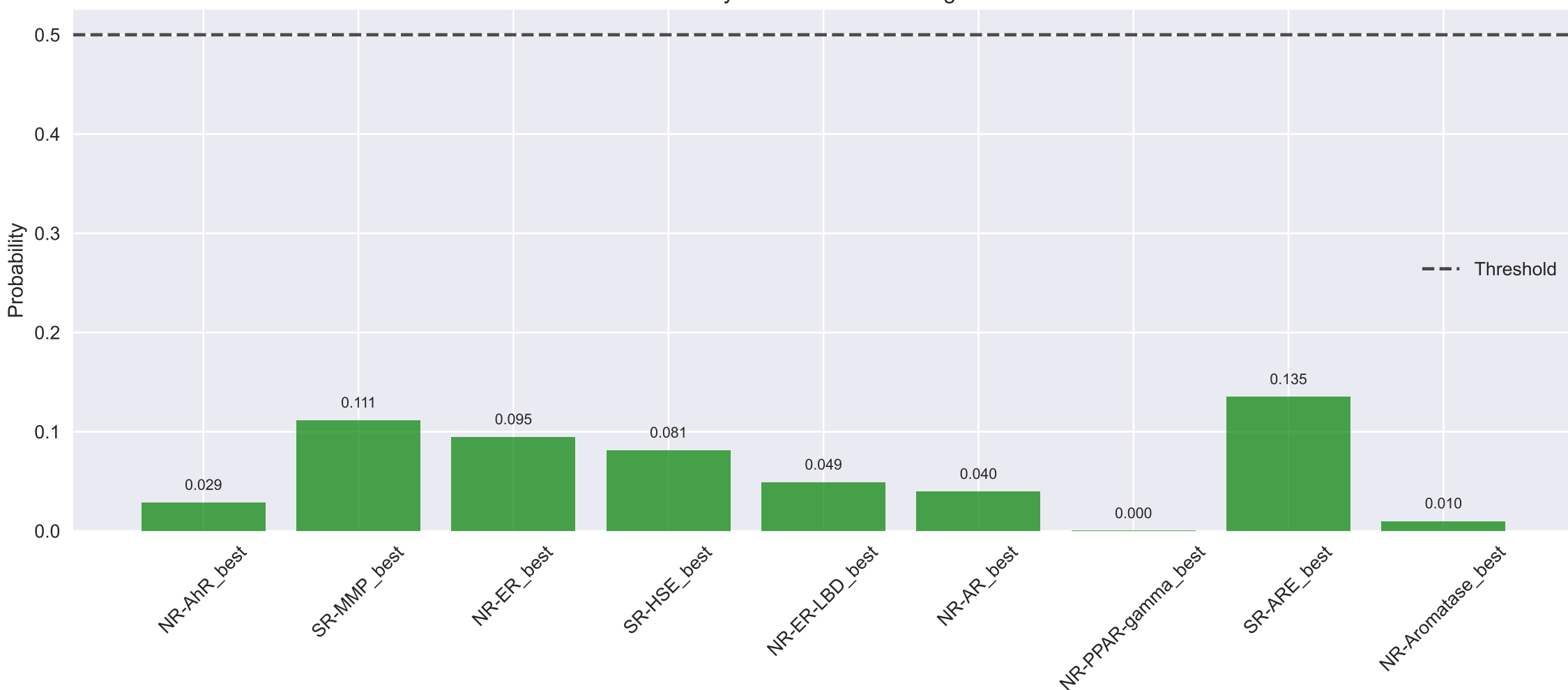
## Highest Risk Targets:

1. SR-ARE\_best: 0.135
2. SR-MMP\_best: 0.111
3. NR-ER\_best: 0.095



# Molecule 15: Cc1cccn2c(=O)c3cc(C(=O)NCc4cccnc4)c(=N)n(CC4CCCO4)...

Toxicity Profile Across All Targets



## Molecule Summary:

SMILES: Cc1cccn2c(=O)c3cc(C(=O)NCc4cccnc4)c(=N)n(CC4CCCO4)c3nc12  
Average Toxicity: 0.061

Targets Passed: 9/9

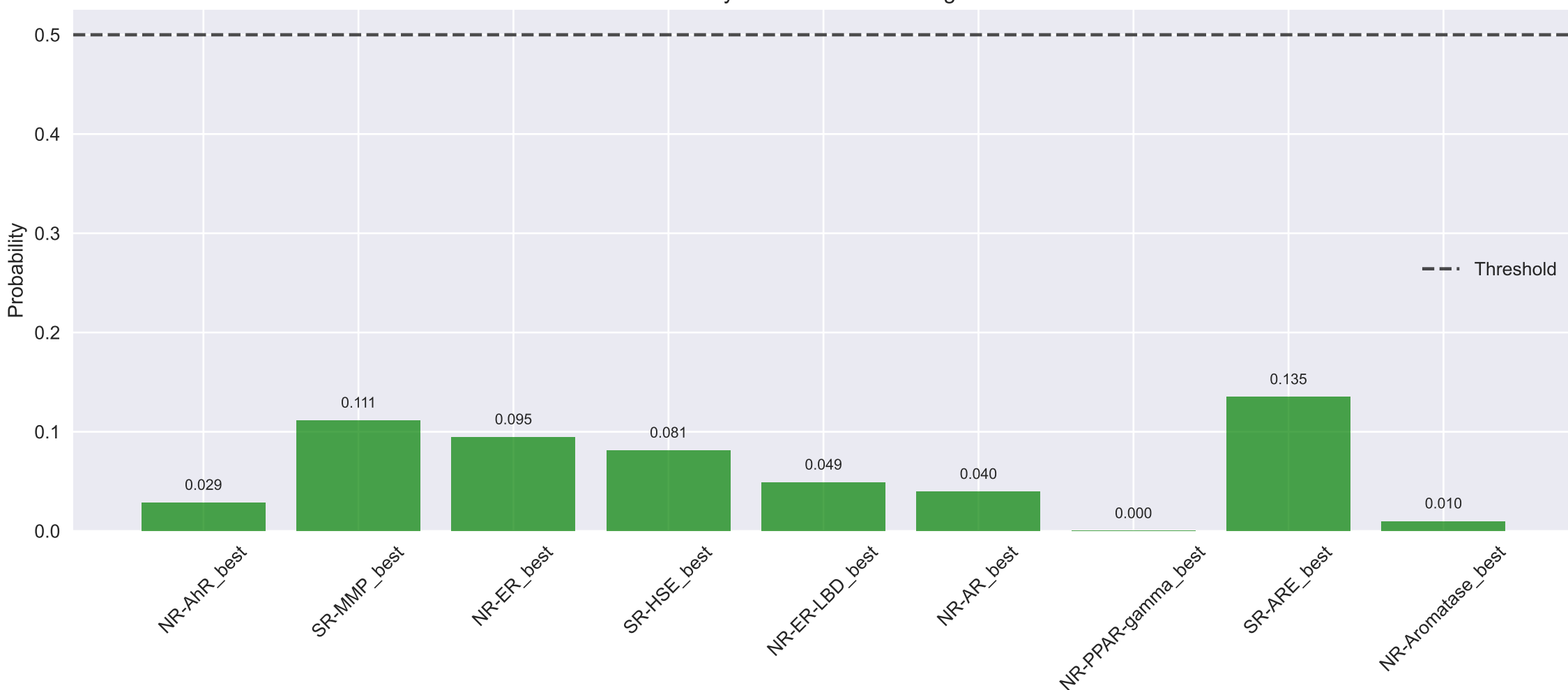
Targets Failed: 0/9

## Highest Risk Targets:

1. SR-ARE\_best: 0.135
2. SR-MMP\_best: 0.111
3. NR-ER\_best: 0.095

# Molecule 16: CC(NC(=O)c1cc2c(=O)n3ccccc3nc2n(Cc2ccccc2)c1=N)c1c...

Toxicity Profile Across All Targets



## Molecule Summary:

SMILES: CC(NC(=O)c1cc2c(=O)n3ccccc3nc2n(Cc2ccccc2)c1=N)c1ccccc1  
Average Toxicity: 0.061

Targets Passed: 9/9

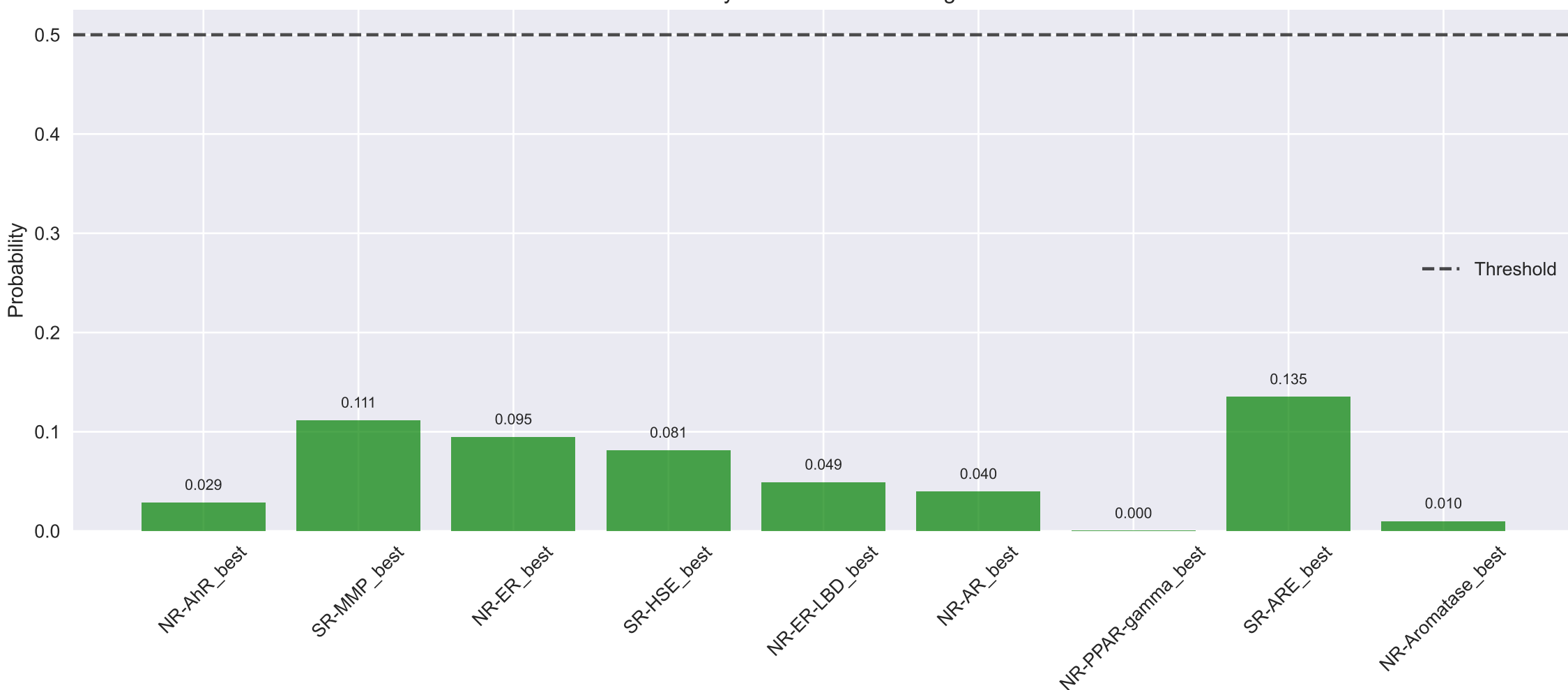
Targets Failed: 0/9

## Highest Risk Targets:

1. SR-ARE\_best: 0.135
2. SR-MMP\_best: 0.111
3. NR-ER\_best: 0.095

# Molecule 17: CC(NC(=O)c1cc2c(=O)n3ccccc3nc2n(Cc2ccccc2)c1=N)c1c...

Toxicity Profile Across All Targets



## Molecule Summary:

SMILES: CC(NC(=O)c1cc2c(=O)n3ccccc3nc2n(Cc2ccccc2)c1=N)c1ccccc1  
Average Toxicity: 0.061

Targets Passed: 9/9

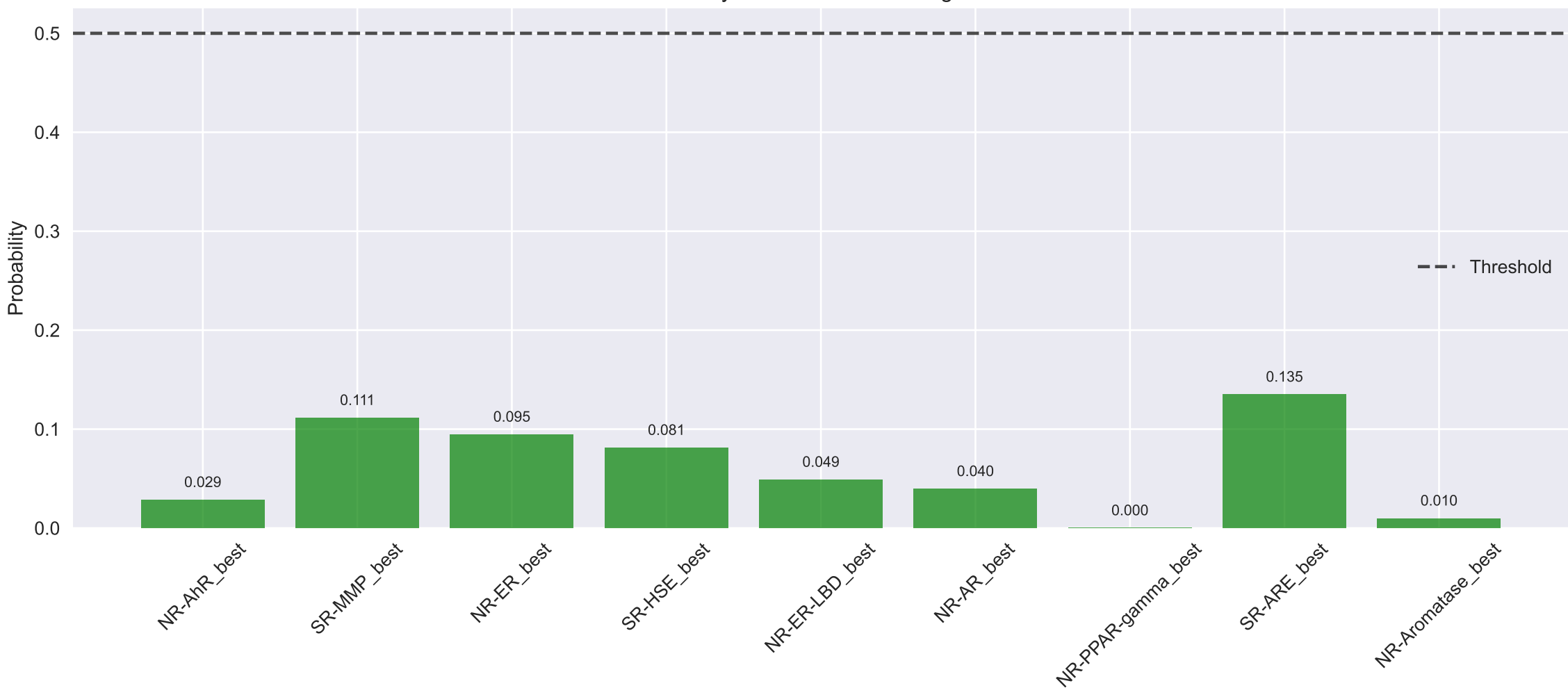
Targets Failed: 0/9

## Highest Risk Targets:

1. SR-ARE\_best: 0.135
2. SR-MMP\_best: 0.111
3. NR-ER\_best: 0.095

# Molecule 18: N=c1c(C(=O)NCc2cccnc2)cc2c(=O)n3ccccc3nc2n1Cc1cccc...

Toxicity Profile Across All Targets



## Molecule Summary:

SMILES: N=c1c(C(=O)NCc2cccnc2)cc2c(=O)n3ccccc3nc2n1Cc1cccc1

Average Toxicity: 0.061

Targets Passed: 9/9

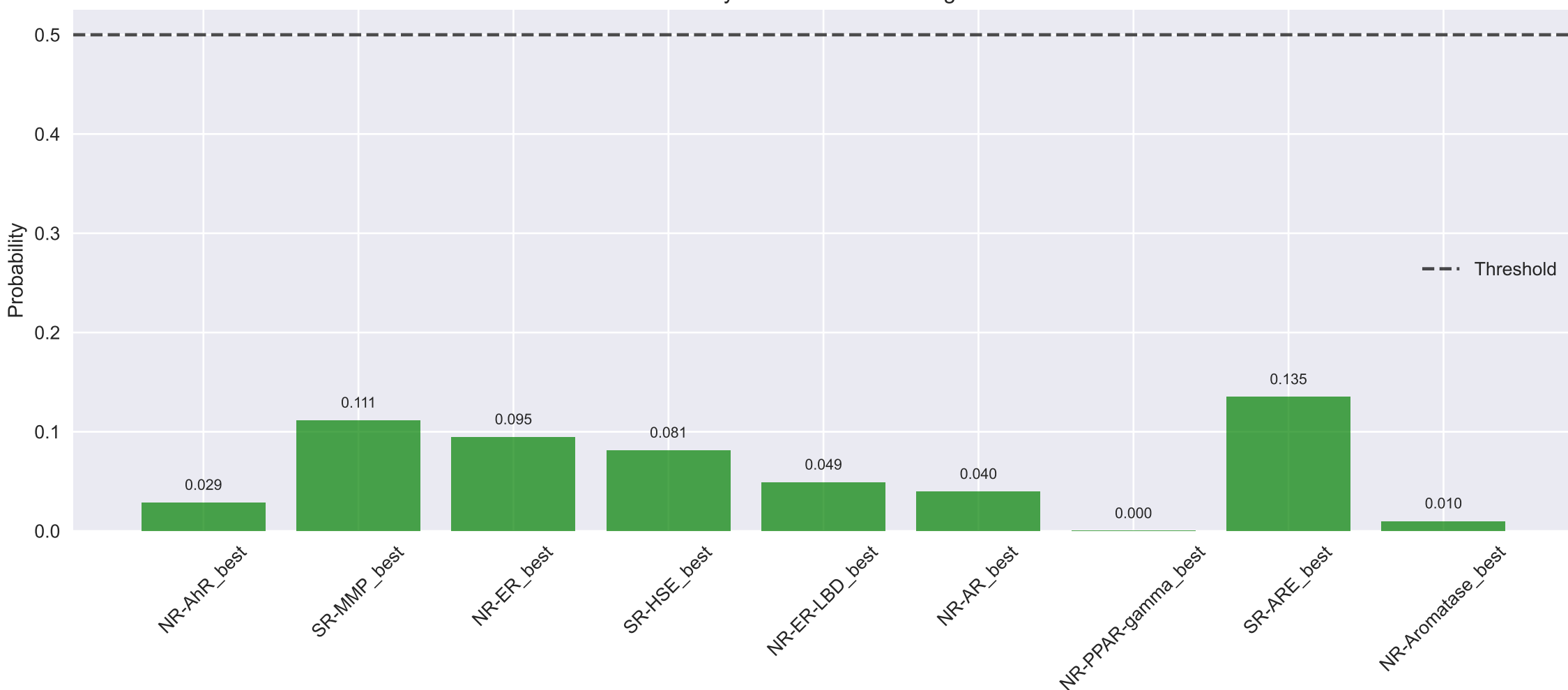
Targets Failed: 0/9

## Highest Risk Targets:

1. SR-ARE\_best: 0.135
2. SR-MMP\_best: 0.111
3. NR-ER\_best: 0.095

# Molecule 19: Cc1ccc2nc3c(cc(C(=O)NCc4cccn4)c(=N)n3C[C@H]3CCCO3)c(=O)n2c1

Toxicity Profile Across All Targets



## Molecule Summary:

SMILES: Cc1ccc2nc3c(cc(C(=O)NCc4cccn4)c(=N)n3C[C@H]3CCCO3)c(=O)n2c1  
Average Toxicity: 0.061

Targets Passed: 9/9

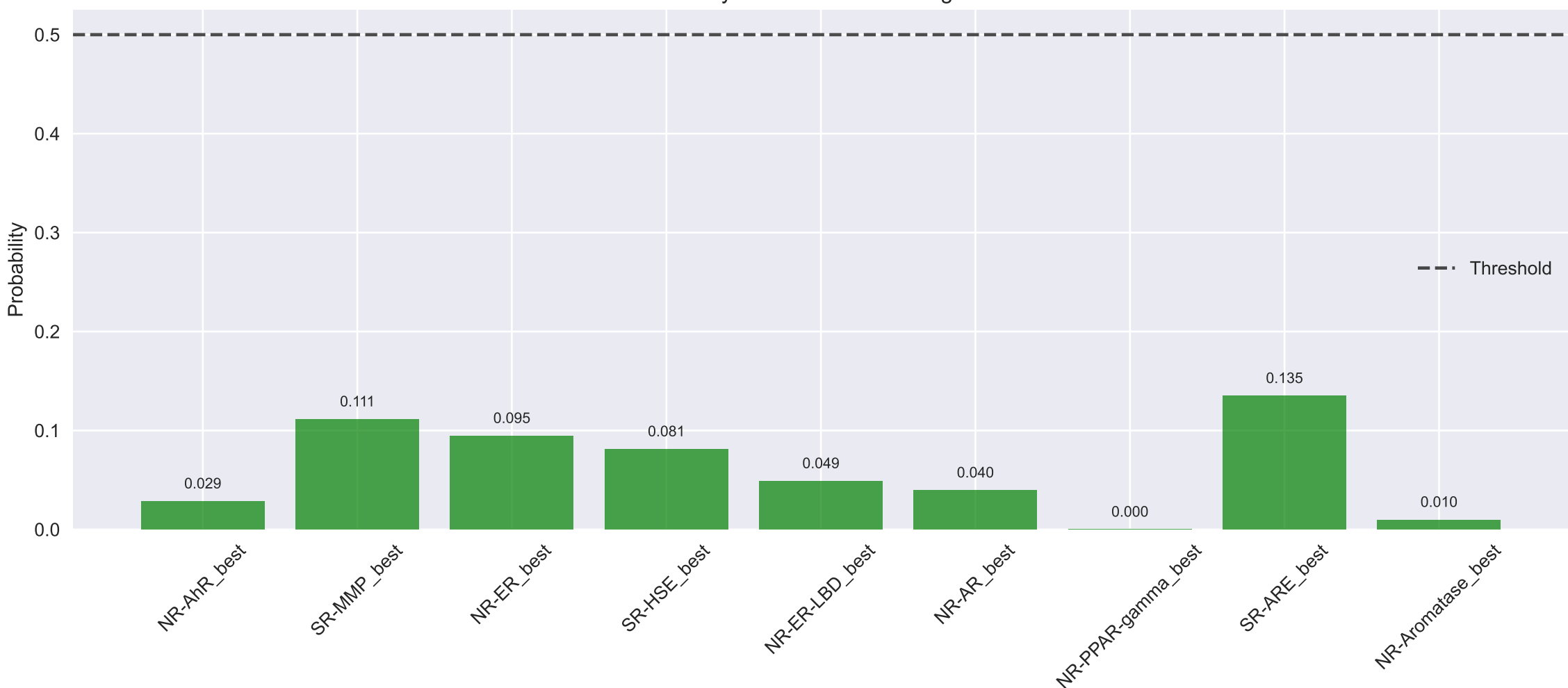
Targets Failed: 0/9

## Highest Risk Targets:

1. SR-ARE\_best: 0.135
2. SR-MMP\_best: 0.111
3. NR-ER\_best: 0.095

# Molecule 20: Cc1cccn2c(=O)c3cc(C#N)c(=N)n(Cc4cccnc4)c3nc12...

Toxicity Profile Across All Targets



## Molecule Summary:

SMILES: Cc1cccn2c(=O)c3cc(C#N)c(=N)n(Cc4cccnc4)c3nc12  
Average Toxicity: 0.061

Targets Passed: 9/9

Targets Failed: 0/9

## Highest Risk Targets:

1. SR-ARE\_best: 0.135
2. SR-MMP\_best: 0.111
3. NR-ER\_best: 0.095