

Molecule Toxicity Summary

	Molecule 1
	Molecule 5
	Molecule 9
	Molecule 13
	Molecule 17
	Molecule 21
	Molecule 25
	Molecule 29
	Molecule 33
	Molecule 37
	Molecule 41
	Molecule 45
	Molecule 49
	Molecule 53
	Molecule 57
	Molecule 61
	Molecule 65
	Molecule 69
	Molecule 73
	Molecule 77
	Molecule 81
	Molecule 85
	Molecule 89
	Molecule 93
	Molecule 97
	ALL PASS
	Avg: 0.061

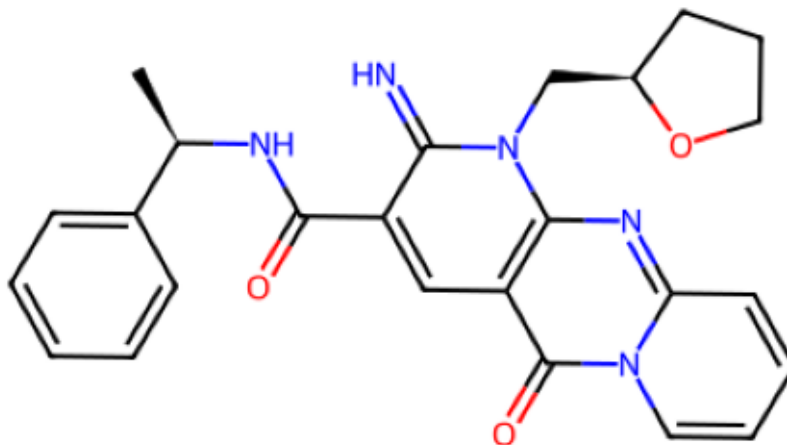
	Molecule 2
	Molecule 6
	Molecule 10
	Molecule 14
	Molecule 18
	Molecule 22
	Molecule 26
	Molecule 30
	Molecule 34
	Molecule 38
	Molecule 42
	Molecule 46
	Molecule 50
	Molecule 54
	Molecule 58
	Molecule 62
	Molecule 66
	Molecule 70
	Molecule 74
	Molecule 78
	Molecule 82
	Molecule 86
	Molecule 90
	Molecule 94
	Molecule 98
	ALL PASS
	Avg: 0.061

	Molecule 3
	Molecule 7
	Molecule 11
	Molecule 15
	Molecule 19
	Molecule 23
	Molecule 27
	Molecule 31
	Molecule 35
	Molecule 39
	Molecule 43
	Molecule 47
	Molecule 51
	Molecule 55
	Molecule 59
	Molecule 63
	Molecule 67
	Molecule 71
	Molecule 75
	Molecule 79
	Molecule 83
	Molecule 87
	Molecule 91
	Molecule 95
	ALL PASS
	Avg: 0.061

	Molecule 4
	Molecule 8
	Molecule 12
	Molecule 16
	Molecule 20
	Molecule 24
	Molecule 28
	Molecule 32
	Molecule 36
	Molecule 40
	Molecule 44
	Molecule 48
	Molecule 52
	Molecule 56
	Molecule 60
	Molecule 64
	Molecule 68
	Molecule 72
	Molecule 76
	Molecule 80
	Molecule 84
	Molecule 88
	Molecule 92
	Molecule 96
	ALL PASS
	Avg: 0.061

# Molecule 1

Molecular Structure



## Toxicity Predictions

NR-AhR\_best  
PASS  
0.029

SR-HSE\_best  
PASS  
0.081

NR-PPAR-gamma\_best  
PASS  
0.000

SR-MMP\_best  
PASS  
0.111

NR-ER-LBD\_best  
PASS  
0.049

SR-ARE\_best  
PASS  
0.135

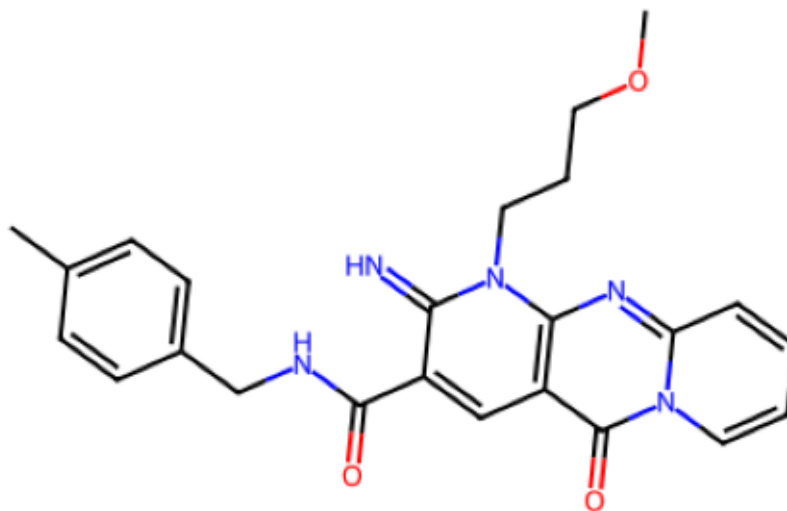
NR-ER\_best  
PASS  
0.095

NR-AR\_best  
PASS  
0.040

NR-Aromatase\_best  
PASS  
0.010

## Molecule 2

Molecular Structure



## Toxicity Predictions

NR-AhR\_best  
PASS  
0.029

SR-HSE\_best  
PASS  
0.081

NR-PPAR-gamma\_best  
PASS  
0.000

SR-MMP\_best  
PASS  
0.111

NR-ER-LBD\_best  
PASS  
0.049

SR-ARE\_best  
PASS  
0.135

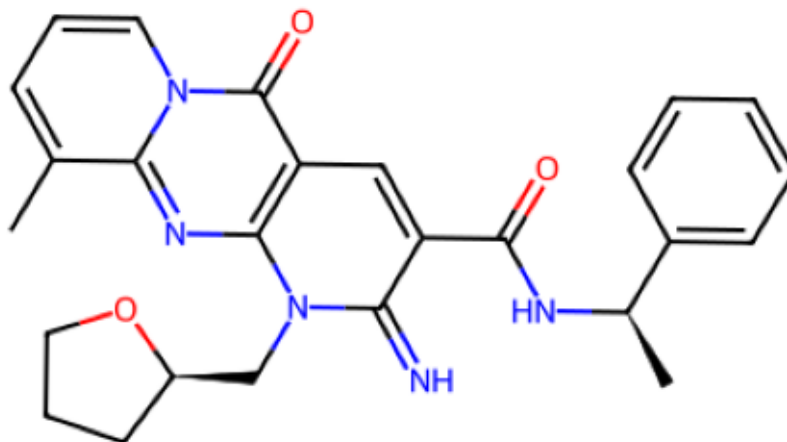
NR-ER\_best  
PASS  
0.095

NR-AR\_best  
PASS  
0.040

NR-Aromatase\_best  
PASS  
0.010

# Molecule 3

Molecular Structure



Toxicity Predictions

NR-AhR\_best  
PASS  
0.029

SR-HSE\_best  
PASS  
0.081

NR-PPAR-gamma\_best  
PASS  
0.000

SR-MMP\_best  
PASS  
0.111

NR-ER-LBD\_best  
PASS  
0.049

SR-ARE\_best  
PASS  
0.135

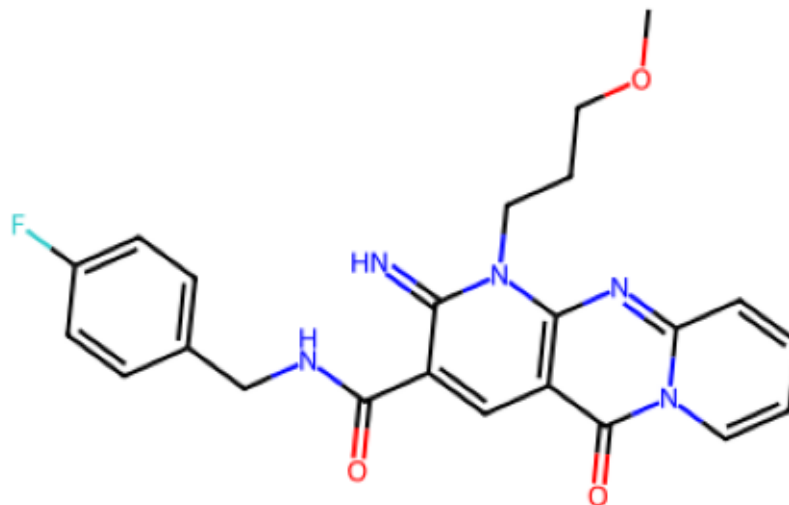
NR-ER\_best  
PASS  
0.095

NR-AR\_best  
PASS  
0.040

NR-Aromatase\_best  
PASS  
0.010

## Molecule 4

Molecular Structure



Toxicity Predictions

NR-AhR\_best  
PASS  
0.029

SR-HSE\_best  
PASS  
0.081

NR-PPAR-gamma\_best  
PASS  
0.000

SR-MMP\_best  
PASS  
0.111

NR-ER-LBD\_best  
PASS  
0.049

SR-ARE\_best  
PASS  
0.135

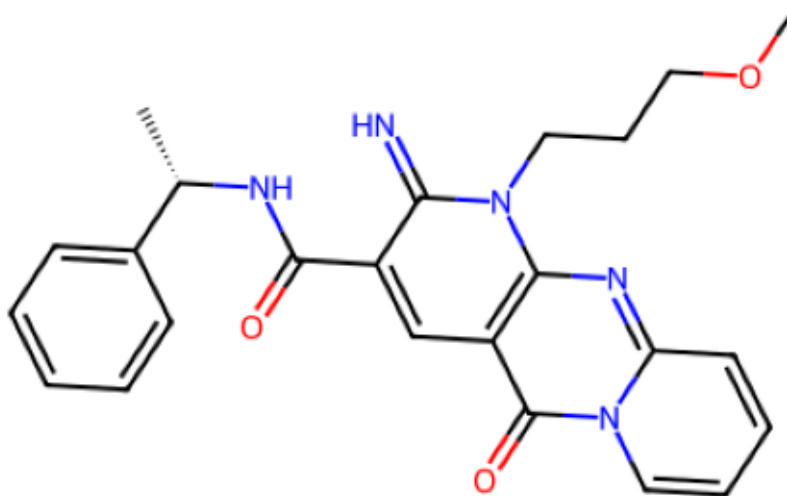
NR-ER\_best  
PASS  
0.095

NR-AR\_best  
PASS  
0.040

NR-Aromatase\_best  
PASS  
0.010

## Molecule 5

Molecular Structure



## Toxicity Predictions

NR-AhR\_best  
PASS  
0.029

SR-HSE\_best  
PASS  
0.081

NR-PPAR-gamma\_best  
PASS  
0.000

SR-MMP\_best  
PASS  
0.111

NR-ER-LBD\_best  
PASS  
0.049

SR-ARE\_best  
PASS  
0.135

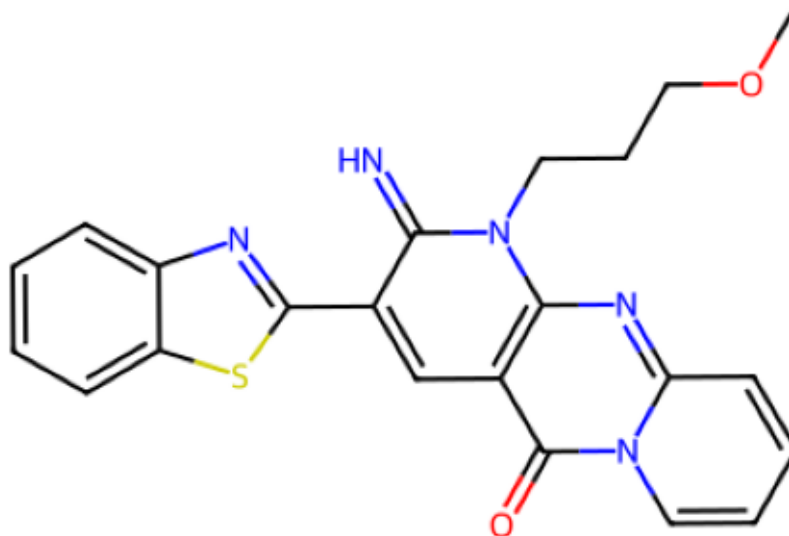
NR-ER\_best  
PASS  
0.095

NR-AR\_best  
PASS  
0.040

NR-Aromatase\_best  
PASS  
0.010

## Molecule 6

Molecular Structure



## Toxicity Predictions

NR-AhR\_best  
PASS  
0.029

SR-HSE\_best  
PASS  
0.081

NR-PPAR-gamma\_best  
PASS  
0.000

SR-MMP\_best  
PASS  
0.111

NR-ER-LBD\_best  
PASS  
0.049

SR-ARE\_best  
PASS  
0.135

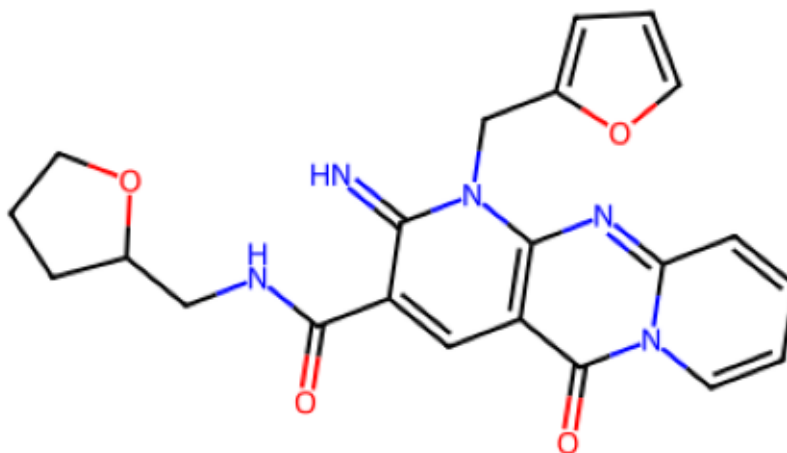
NR-ER\_best  
PASS  
0.095

NR-AR\_best  
PASS  
0.040

NR-Aromatase\_best  
PASS  
0.010

## Molecule 7

Molecular Structure



## Toxicity Predictions

NR-AhR\_best  
PASS  
0.029

SR-HSE\_best  
PASS  
0.081

NR-PPAR-gamma\_best  
PASS  
0.000

SR-MMP\_best  
PASS  
0.111

NR-ER-LBD\_best  
PASS  
0.049

SR-ARE\_best  
PASS  
0.135

NR-ER\_best  
PASS  
0.095

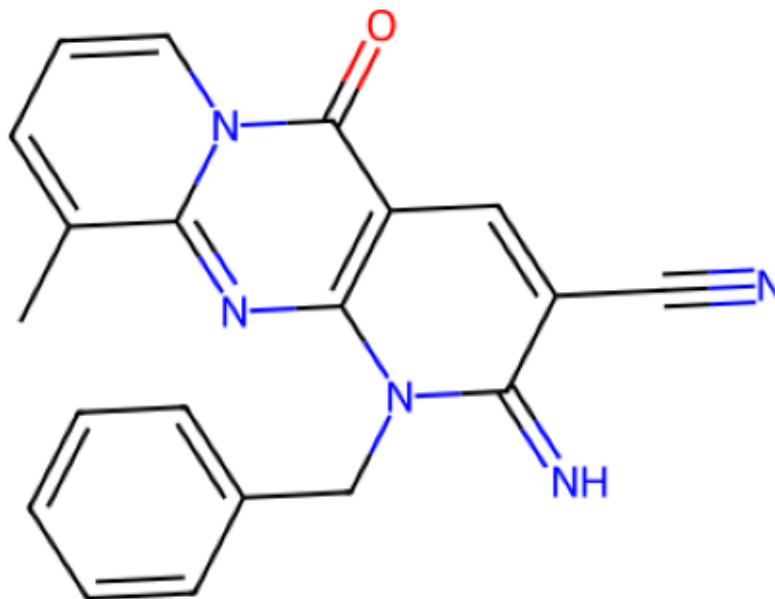
NR-AR\_best  
PASS  
0.040

NR-Aromatase\_best  
PASS  
0.010



## Molecule 8

Molecular Structure



Toxicity Predictions

NR-AhR\_best  
PASS  
0.029

SR-HSE\_best  
PASS  
0.081

NR-PPAR-gamma\_best  
PASS  
0.000

SR-MMP\_best  
PASS  
0.111

NR-ER-LBD\_best  
PASS  
0.049

SR-ARE\_best  
PASS  
0.135

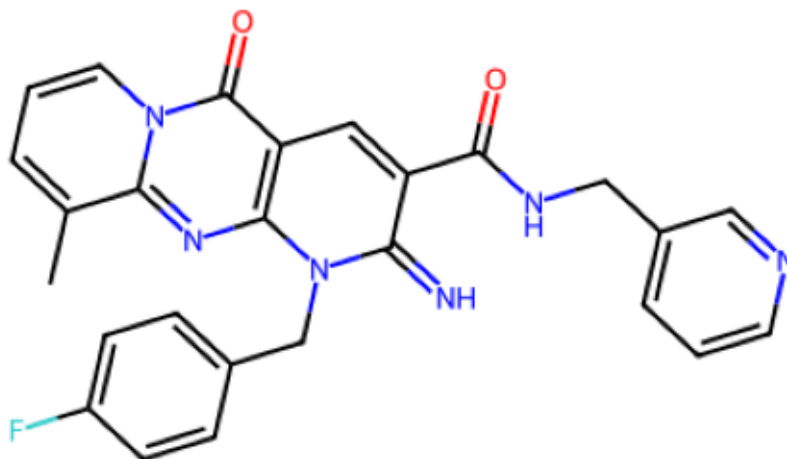
NR-ER\_best  
PASS  
0.095

NR-AR\_best  
PASS  
0.040

NR-Aromatase\_best  
PASS  
0.010

## Molecule 9

Molecular Structure



## Toxicity Predictions

NR-AhR\_best  
PASS  
0.029

SR-HSE\_best  
PASS  
0.081

NR-PPAR-gamma\_best  
PASS  
0.000

SR-MMP\_best  
PASS  
0.111

NR-ER-LBD\_best  
PASS  
0.049

SR-ARE\_best  
PASS  
0.135

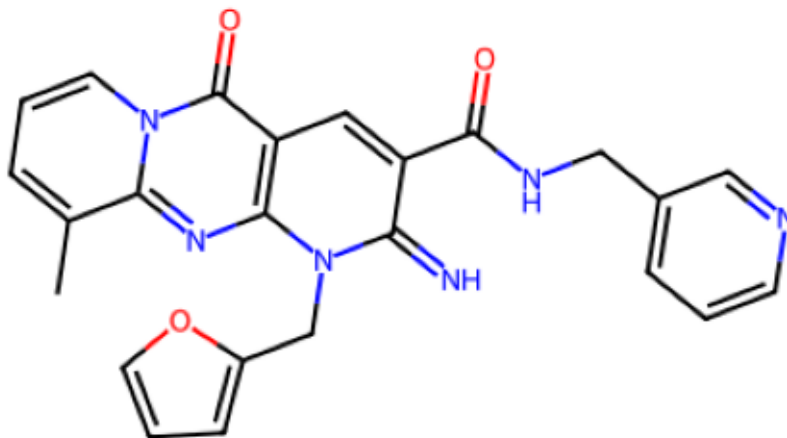
NR-ER\_best  
PASS  
0.095

NR-AR\_best  
PASS  
0.040

NR-Aromatase\_best  
PASS  
0.010

## Molecule 10

Molecular Structure



## Toxicity Predictions

NR-AhR\_best  
PASS  
0.029

SR-HSE\_best  
PASS  
0.081

NR-PPAR-gamma\_best  
PASS  
0.000

SR-MMP\_best  
PASS  
0.111

NR-ER-LBD\_best  
PASS  
0.049

SR-ARE\_best  
PASS  
0.135

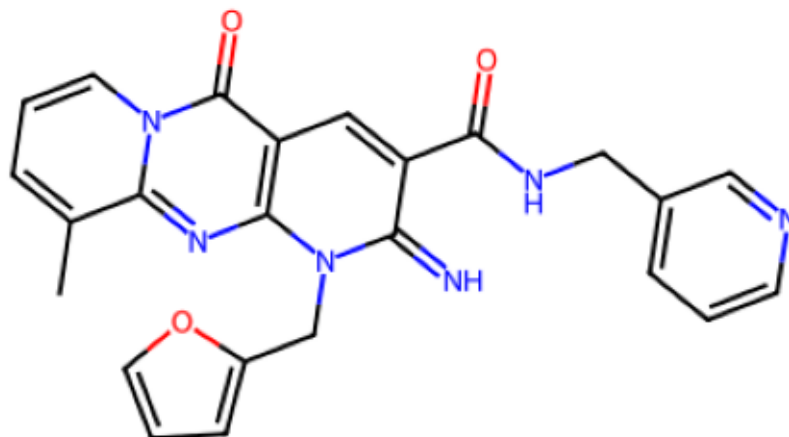
NR-ER\_best  
PASS  
0.095

NR-AR\_best  
PASS  
0.040

NR-Aromatase\_best  
PASS  
0.010

## Molecule 11

Molecular Structure



## Toxicity Predictions

NR-AhR\_best  
PASS  
0.029

SR-HSE\_best  
PASS  
0.081

NR-PPAR-gamma\_best  
PASS  
0.000

SR-MMP\_best  
PASS  
0.111

NR-ER-LBD\_best  
PASS  
0.049

SR-ARE\_best  
PASS  
0.135

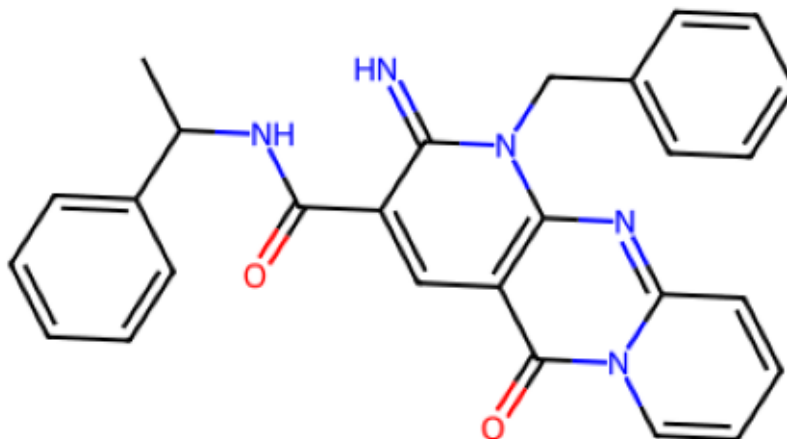
NR-ER\_best  
PASS  
0.095

NR-AR\_best  
PASS  
0.040

NR-Aromatase\_best  
PASS  
0.010

## Molecule 12

Molecular Structure



## Toxicity Predictions

NR-AhR\_best  
PASS  
0.029

SR-HSE\_best  
PASS  
0.081

NR-PPAR-gamma\_best  
PASS  
0.000

SR-MMP\_best  
PASS  
0.111

NR-ER-LBD\_best  
PASS  
0.049

SR-ARE\_best  
PASS  
0.135

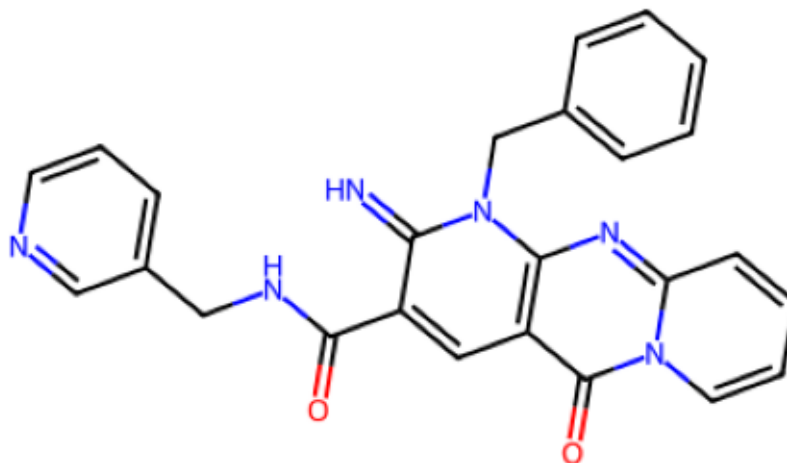
NR-ER\_best  
PASS  
0.095

NR-AR\_best  
PASS  
0.040

NR-Aromatase\_best  
PASS  
0.010

## Molecule 13

Molecular Structure



### Toxicity Predictions

NR-AhR\_best  
PASS  
0.029

SR-HSE\_best  
PASS  
0.081

NR-PPAR-gamma\_best  
PASS  
0.000

SR-MMP\_best  
PASS  
0.111

NR-ER-LBD\_best  
PASS  
0.049

SR-ARE\_best  
PASS  
0.135

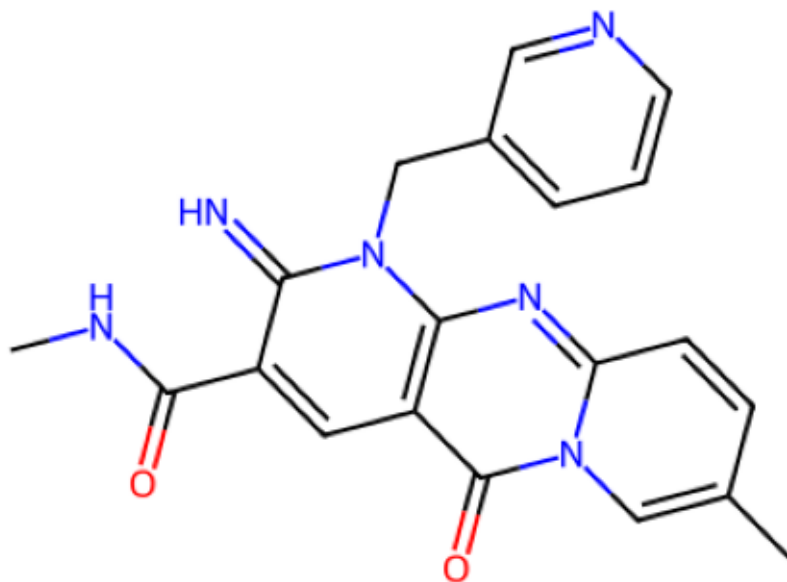
NR-ER\_best  
PASS  
0.095

NR-AR\_best  
PASS  
0.040

NR-Aromatase\_best  
PASS  
0.010

## Molecule 14

Molecular Structure



Toxicity Predictions

NR-AhR\_best  
PASS  
0.029

SR-HSE\_best  
PASS  
0.081

NR-PPAR-gamma\_best  
PASS  
0.000

SR-MMP\_best  
PASS  
0.111

NR-ER-LBD\_best  
PASS  
0.049

SR-ARE\_best  
PASS  
0.135

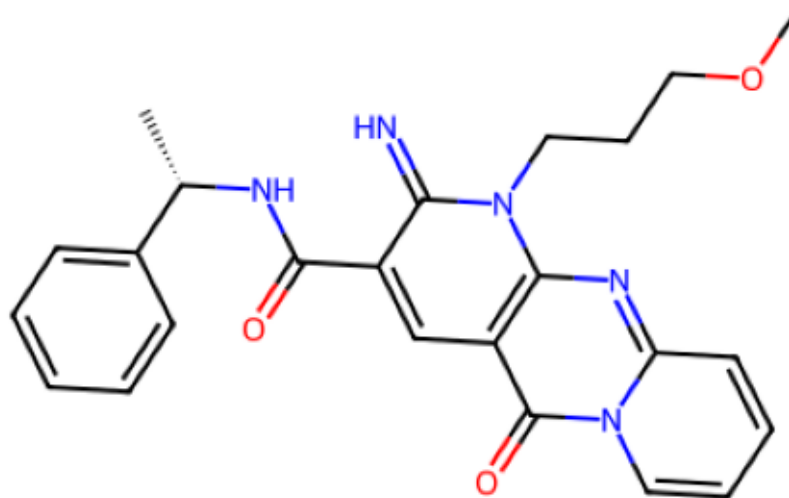
NR-ER\_best  
PASS  
0.095

NR-AR\_best  
PASS  
0.040

NR-Aromatase\_best  
PASS  
0.010

## Molecule 15

Molecular Structure



## Toxicity Predictions

NR-AhR\_best  
PASS  
0.029

SR-HSE\_best  
PASS  
0.081

NR-PPAR-gamma\_best  
PASS  
0.000

SR-MMP\_best  
PASS  
0.111

NR-ER-LBD\_best  
PASS  
0.049

SR-ARE\_best  
PASS  
0.135

NR-ER\_best  
PASS  
0.095

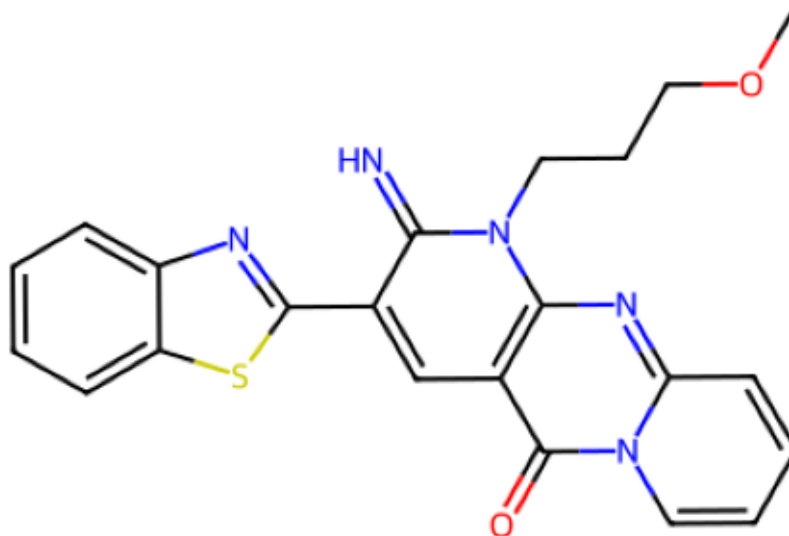
NR-AR\_best  
PASS  
0.040

NR-Aromatase\_best  
PASS  
0.010



## Molecule 16

Molecular Structure



Toxicity Predictions

NR-AhR\_best  
PASS  
0.029

SR-HSE\_best  
PASS  
0.081

NR-PPAR-gamma\_best  
PASS  
0.000

SR-MMP\_best  
PASS  
0.111

NR-ER-LBD\_best  
PASS  
0.049

SR-ARE\_best  
PASS  
0.135

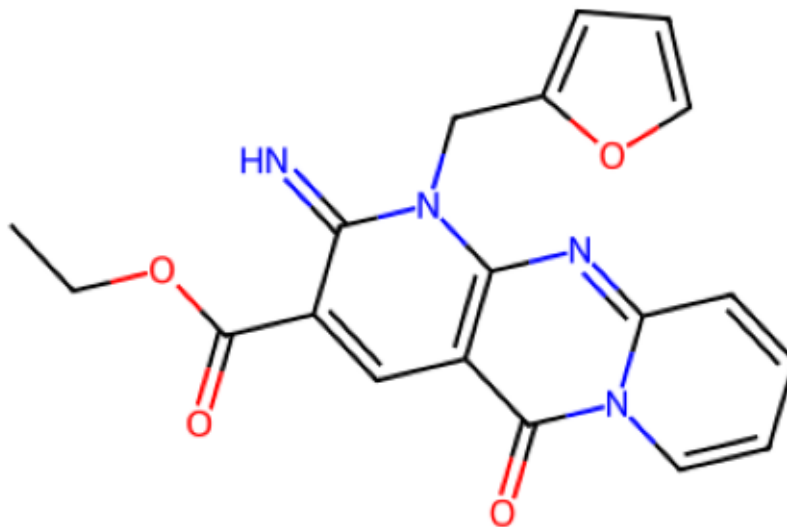
NR-ER\_best  
PASS  
0.095

NR-AR\_best  
PASS  
0.040

NR-Aromatase\_best  
PASS  
0.010

## Molecule 17

Molecular Structure



Toxicity Predictions

NR-AhR\_best  
PASS  
0.029

SR-HSE\_best  
PASS  
0.081

NR-PPAR-gamma\_best  
PASS  
0.000

SR-MMP\_best  
PASS  
0.111

NR-ER-LBD\_best  
PASS  
0.049

SR-ARE\_best  
PASS  
0.135

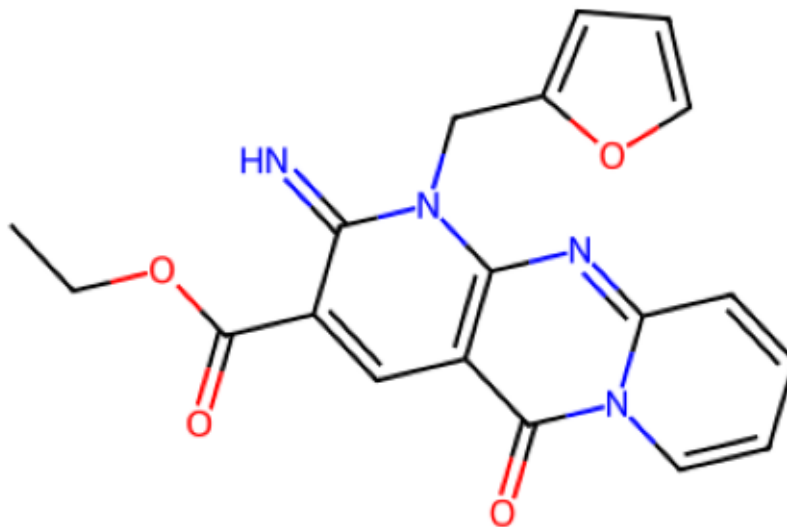
NR-ER\_best  
PASS  
0.095

NR-AR\_best  
PASS  
0.040

NR-Aromatase\_best  
PASS  
0.010

## Molecule 18

Molecular Structure



Toxicity Predictions

NR-AhR\_best  
PASS  
0.029

SR-HSE\_best  
PASS  
0.081

NR-PPAR-gamma\_best  
PASS  
0.000

SR-MMP\_best  
PASS  
0.111

NR-ER-LBD\_best  
PASS  
0.049

SR-ARE\_best  
PASS  
0.135

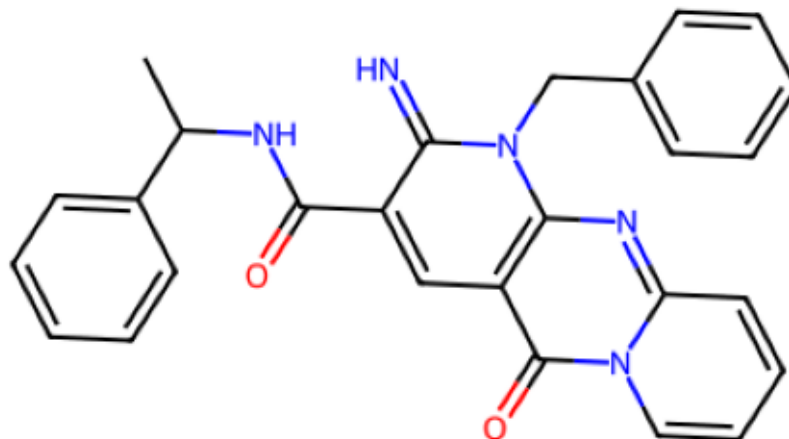
NR-ER\_best  
PASS  
0.095

NR-AR\_best  
PASS  
0.040

NR-Aromatase\_best  
PASS  
0.010

## Molecule 19

Molecular Structure



## Toxicity Predictions

NR-AhR\_best  
PASS  
0.029

SR-HSE\_best  
PASS  
0.081

NR-PPAR-gamma\_best  
PASS  
0.000

SR-MMP\_best  
PASS  
0.111

NR-ER-LBD\_best  
PASS  
0.049

SR-ARE\_best  
PASS  
0.135

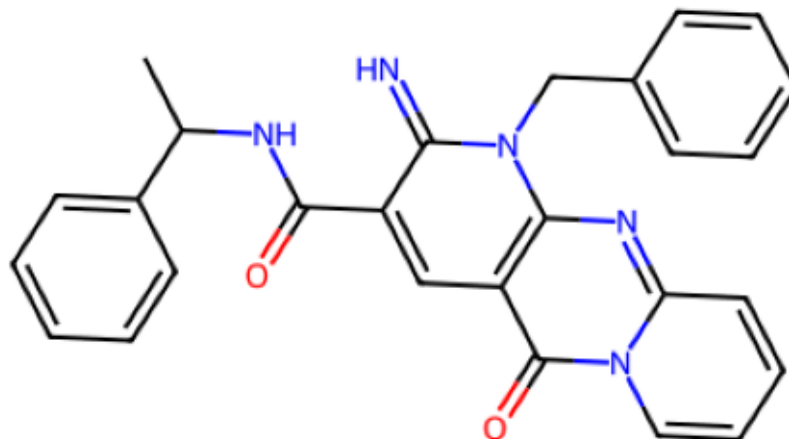
NR-ER\_best  
PASS  
0.095

NR-AR\_best  
PASS  
0.040

NR-Aromatase\_best  
PASS  
0.010

## Molecule 20

Molecular Structure



## Toxicity Predictions

NR-AhR\_best  
PASS  
0.029

SR-HSE\_best  
PASS  
0.081

NR-PPAR-gamma\_best  
PASS  
0.000

SR-MMP\_best  
PASS  
0.111

NR-ER-LBD\_best  
PASS  
0.049

SR-ARE\_best  
PASS  
0.135

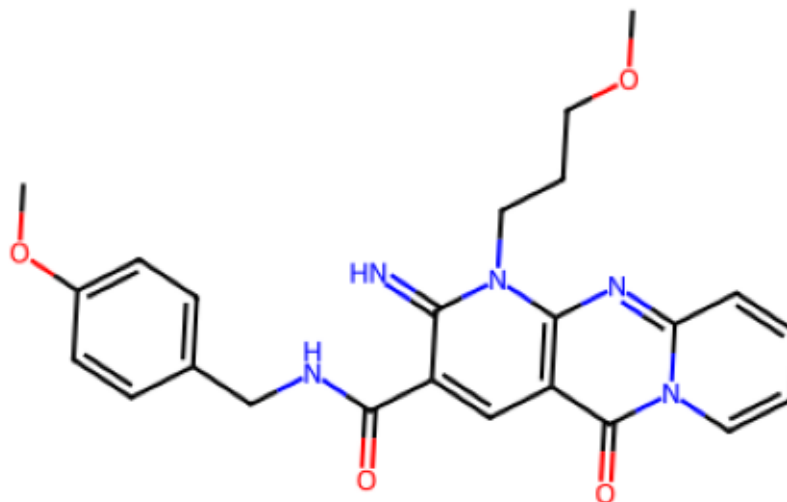
NR-ER\_best  
PASS  
0.095

NR-AR\_best  
PASS  
0.040

NR-Aromatase\_best  
PASS  
0.010

## Molecule 21

Molecular Structure



### Toxicity Predictions

NR-AhR\_best  
PASS  
0.029

SR-HSE\_best  
PASS  
0.081

NR-PPAR-gamma\_best  
PASS  
0.000

SR-MMP\_best  
PASS  
0.111

NR-ER-LBD\_best  
PASS  
0.049

SR-ARE\_best  
PASS  
0.135

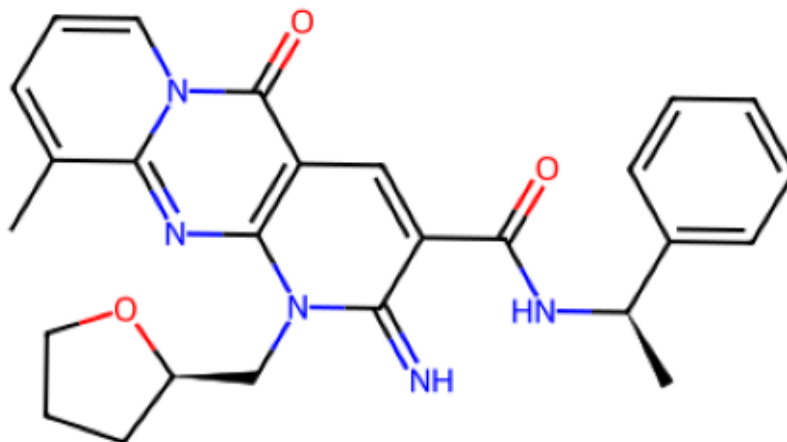
NR-ER\_best  
PASS  
0.095

NR-AR\_best  
PASS  
0.040

NR-Aromatase\_best  
PASS  
0.010

## Molecule 22

Molecular Structure



## Toxicity Predictions

NR-AhR\_best  
PASS  
0.029

SR-HSE\_best  
PASS  
0.081

NR-PPAR-gamma\_best  
PASS  
0.000

SR-MMP\_best  
PASS  
0.111

NR-ER-LBD\_best  
PASS  
0.049

SR-ARE\_best  
PASS  
0.135

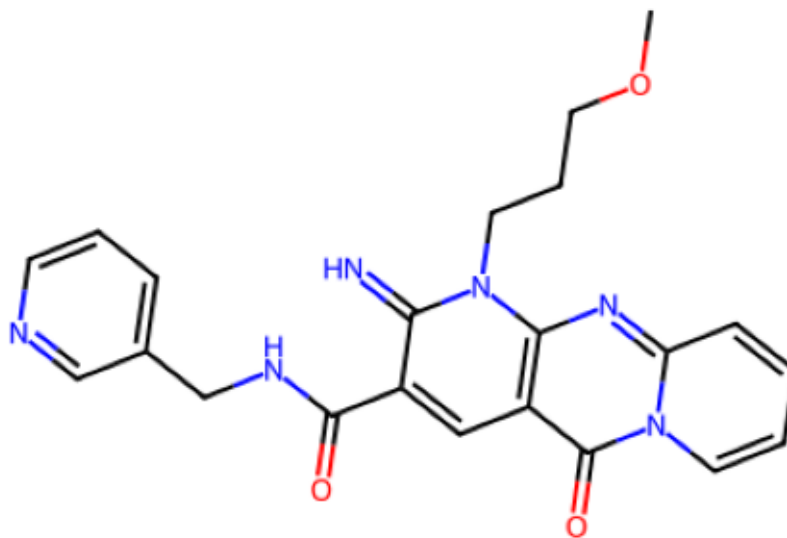
NR-ER\_best  
PASS  
0.095

NR-AR\_best  
PASS  
0.040

NR-Aromatase\_best  
PASS  
0.010

## Molecule 23

Molecular Structure



Toxicity Predictions

NR-AhR\_best  
PASS  
0.029

SR-HSE\_best  
PASS  
0.081

NR-PPAR-gamma\_best  
PASS  
0.000

SR-MMP\_best  
PASS  
0.111

NR-ER-LBD\_best  
PASS  
0.049

SR-ARE\_best  
PASS  
0.135

NR-ER\_best  
PASS  
0.095

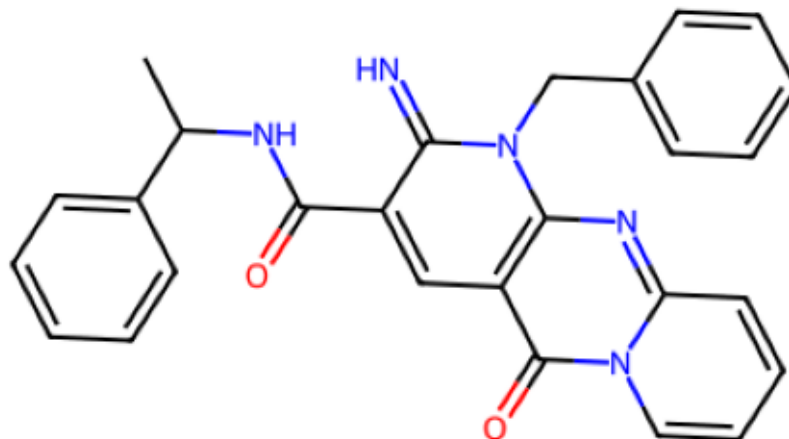
NR-AR\_best  
PASS  
0.040

NR-Aromatase\_best  
PASS  
0.010



## Molecule 24

Molecular Structure



## Toxicity Predictions

NR-AhR\_best  
PASS  
0.029

SR-HSE\_best  
PASS  
0.081

NR-PPAR-gamma\_best  
PASS  
0.000

SR-MMP\_best  
PASS  
0.111

NR-ER-LBD\_best  
PASS  
0.049

SR-ARE\_best  
PASS  
0.135

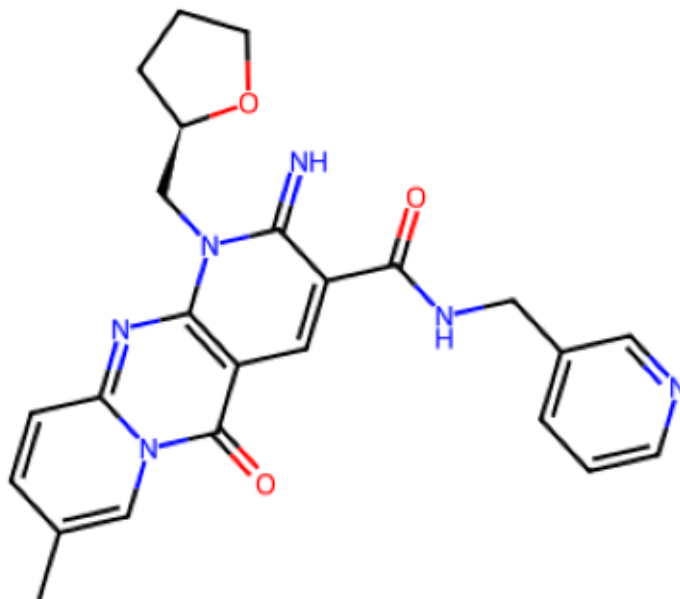
NR-ER\_best  
PASS  
0.095

NR-AR\_best  
PASS  
0.040

NR-Aromatase\_best  
PASS  
0.010

## Molecule 25

Molecular Structure



Toxicity Predictions

NR-AhR\_best  
PASS  
0.029

SR-HSE\_best  
PASS  
0.081

NR-PPAR-gamma\_best  
PASS  
0.000

SR-MMP\_best  
PASS  
0.111

NR-ER-LBD\_best  
PASS  
0.049

SR-ARE\_best  
PASS  
0.135

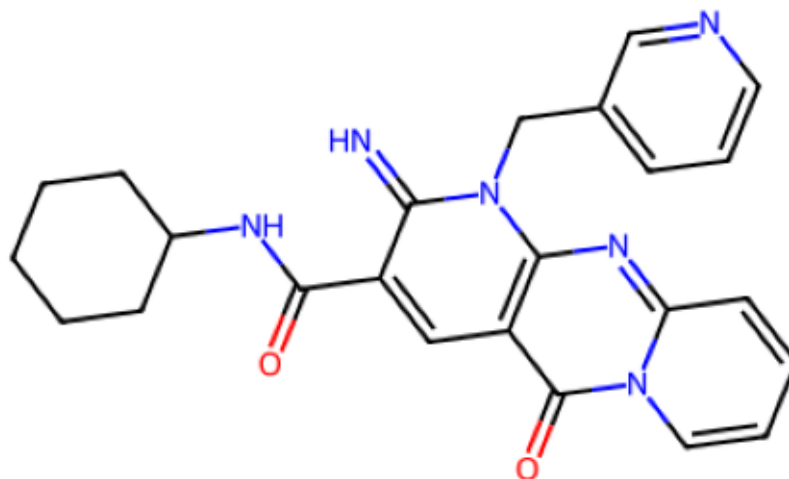
NR-ER\_best  
PASS  
0.095

NR-AR\_best  
PASS  
0.040

NR-Aromatase\_best  
PASS  
0.010

## Molecule 26

Molecular Structure



## Toxicity Predictions

NR-AhR\_best  
PASS  
0.029

SR-HSE\_best  
PASS  
0.081

NR-PPAR-gamma\_best  
PASS  
0.000

SR-MMP\_best  
PASS  
0.111

NR-ER-LBD\_best  
PASS  
0.049

SR-ARE\_best  
PASS  
0.135

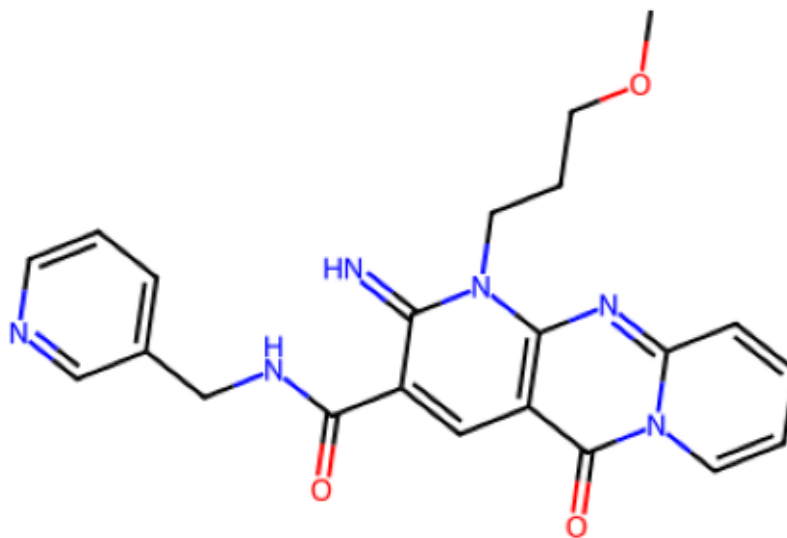
NR-ER\_best  
PASS  
0.095

NR-AR\_best  
PASS  
0.040

NR-Aromatase\_best  
PASS  
0.010

## Molecule 27

Molecular Structure



Toxicity Predictions

NR-AhR\_best  
PASS  
0.029

SR-HSE\_best  
PASS  
0.081

NR-PPAR-gamma\_best  
PASS  
0.000

SR-MMP\_best  
PASS  
0.111

NR-ER-LBD\_best  
PASS  
0.049

SR-ARE\_best  
PASS  
0.135

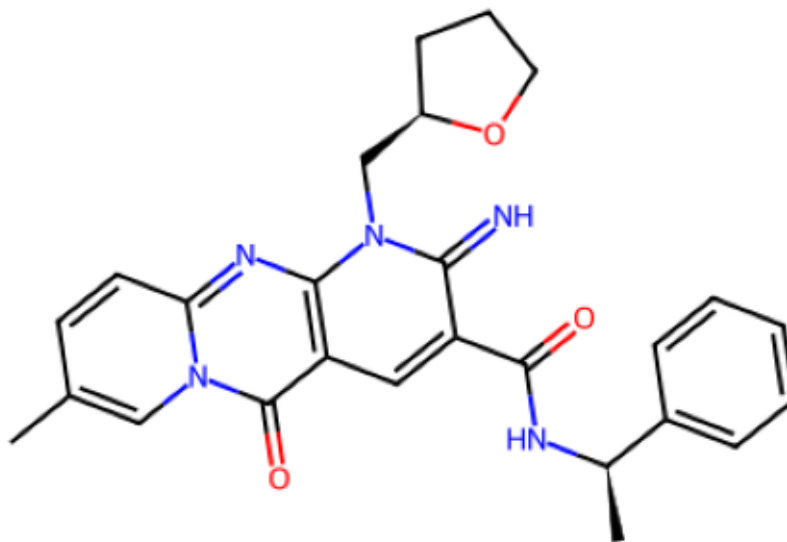
NR-ER\_best  
PASS  
0.095

NR-AR\_best  
PASS  
0.040

NR-Aromatase\_best  
PASS  
0.010

## Molecule 28

Molecular Structure



Toxicity Predictions

NR-AhR\_best  
PASS  
0.029

SR-HSE\_best  
PASS  
0.081

NR-PPAR-gamma\_best  
PASS  
0.000

SR-MMP\_best  
PASS  
0.111

NR-ER-LBD\_best  
PASS  
0.049

SR-ARE\_best  
PASS  
0.135

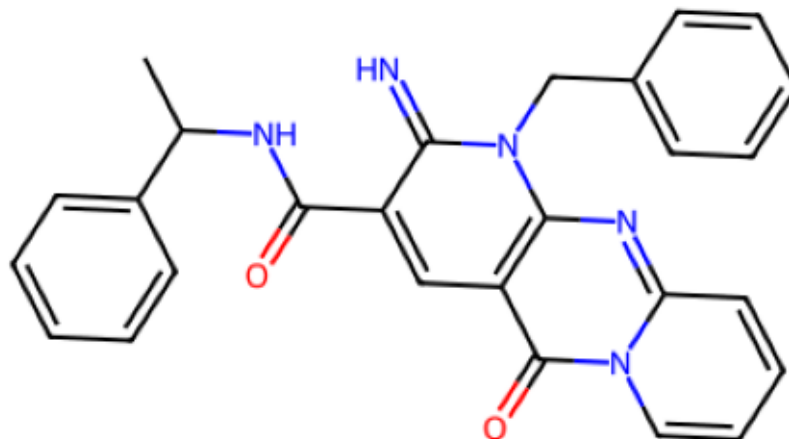
NR-ER\_best  
PASS  
0.095

NR-AR\_best  
PASS  
0.040

NR-Aromatase\_best  
PASS  
0.010

## Molecule 29

Molecular Structure



## Toxicity Predictions

NR-AhR\_best  
PASS  
0.029

SR-HSE\_best  
PASS  
0.081

NR-PPAR-gamma\_best  
PASS  
0.000

SR-MMP\_best  
PASS  
0.111

NR-ER-LBD\_best  
PASS  
0.049

SR-ARE\_best  
PASS  
0.135

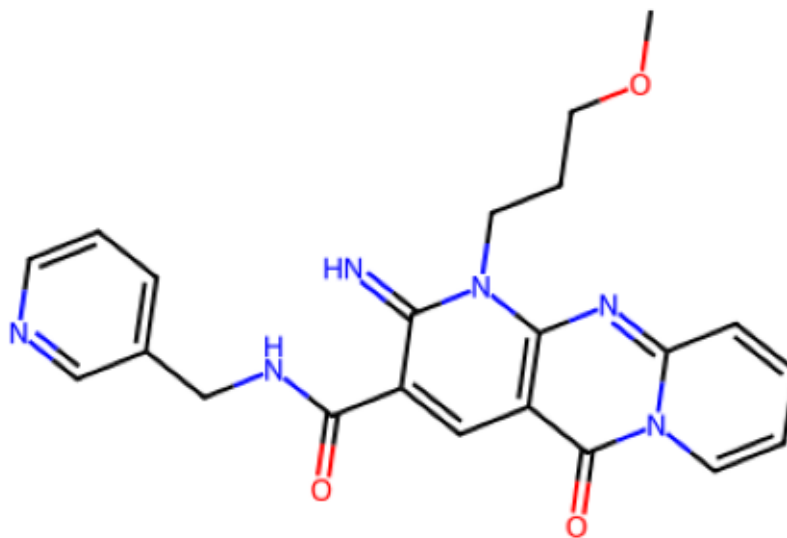
NR-ER\_best  
PASS  
0.095

NR-AR\_best  
PASS  
0.040

NR-Aromatase\_best  
PASS  
0.010

## Molecule 30

Molecular Structure



Toxicity Predictions

NR-AhR\_best  
PASS  
0.029

SR-HSE\_best  
PASS  
0.081

NR-PPAR-gamma\_best  
PASS  
0.000

SR-MMP\_best  
PASS  
0.111

NR-ER-LBD\_best  
PASS  
0.049

SR-ARE\_best  
PASS  
0.135

NR-ER\_best  
PASS  
0.095

NR-AR\_best  
PASS  
0.040

NR-Aromatase\_best  
PASS  
0.010