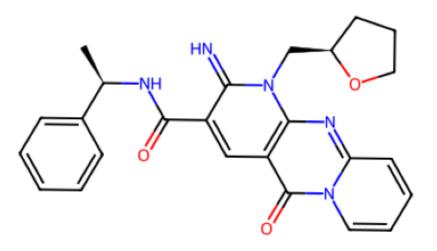
Molecule Toxicity Summary

Molecule 5Molecule 6Molecule 7Molecule 8Molecule 9Molecule 10Molecule 11Molecule 12Molecule 13Molecule 14Molecule 15Molecule 16Molecule 17Molecule 18Molecule 19Molecule 20Molecule 21Molecule 22Molecule 23Molecule 24Molecule 25Molecule 26Molecule 27Molecule 28Molecule 29Molecule 30Molecule 31Molecule 32Molecule 33Molecule 34Molecule 35Molecule 36				
Molecule 10 Molecule 11 Molecule 12 Molecule 13 Molecule 14 Molecule 15 Molecule 16 Molecule 17 Molecule 18 Molecule 19 Molecule 19 Molecule 20 Molecule 21 Molecule 22 Molecule 23 Molecule 23 Molecule 25 Molecule 26 Molecule 27 Molecule 28 Molecule 28 Molecule 29 Molecule 30 Molecule 31 Molecule 32 Molecule 32 Molecule 33 Molecule 34 Molecule 35 Molecule 36 Molecule 37 Molecule 38 Molecule 39 Molecule 40 Molecule 40 Molecule 40 Molecule 41 Molecule 42 Molecule 43 Molecule 44 Molecule 45 Molecule 46 Molecule 47 Molecule 48 Molecule 49 Molecule 49 Molecule 50 Molecule 51 Molecule 52 Molecule 53 Molecule 54 Molecule 55 Molecule 56 Molecule 57 Molecule 58 Molecule 59 Molecule 50 Molecule 60 Molecule 70 Molecule 80 Molecule 90 Molecule 90 Molecule 90 Molecule 90 Molecule 91 Molecule 90 Molecule 91 Molecule 90 Molecule 91 Molecule 90 Molecule 91	Molecule 1	Molecule 2	Molecule 3	Molecule 4
Molecule 13 Molecule 14 Molecule 15 Molecule 16 Molecule 17 Molecule 18 Molecule 19 Molecule 20 Molecule 21 Molecule 22 Molecule 23 Molecule 24 Molecule 25 Molecule 26 Molecule 27 Molecule 28 Molecule 28 Molecule 29 Molecule 30 Molecule 31 Molecule 30 Molecule 33 Molecule 34 Molecule 35 Molecule 36 Molecule 37 Molecule 38 Molecule 39 Molecule 39 Molecule 30 Molecule 39 Molecule 40 Molecule 40 Molecule 41 Molecule 42 Molecule 43 Molecule 44 Molecule 45 Molecule 46 Molecule 47 Molecule 48 Molecule 49 Molecule 50 Molecule 51 Molecule 51 Molecule 52 Molecule 53 Molecule 54 Molecule 55 Molecule 56 Molecule 57 Molecule 58 Molecule 59 Molecule 66 Molecule 66 Molecule 67 Molecule 68 Molecule 69 Molecule 69 Molecule 60 Molecule 60 Molecule 61 Molecule 66 Molecule 67 Molecule 68 Molecule 69 Molecule 69 Molecule 69 Molecule 60 Molecule 60 Molecule 61 Molecule 62 Molecule 67 Molecule 68 Molecule 69 Molecule 69 Molecule 70 Molecule 71 Molecule 71 Molecule 72 Molecule 73 Molecule 74 Molecule 75 Molecule 75 Molecule 76 Molecule 77 Molecule 78 Molecule 79 Molecule 79 Molecule 80 Molecule 90	Molecule 5	Molecule 6	Molecule 7	Molecule 8
Molecule 17 Molecule 28 Molecule 29 Molecule 29 Molecule 24 Molecule 25 Molecule 26 Molecule 26 Molecule 27 Molecule 28 Molecule 28 Molecule 29 Molecule 30 Molecule 31 Molecule 32 Molecule 33 Molecule 34 Molecule 35 Molecule 36 Molecule 37 Molecule 38 Molecule 39 Molecule 39 Molecule 30 Molecule 39 Molecule 30 Molecule 30 Molecule 35 Molecule 36 Molecule 36 Molecule 37 Molecule 38 Molecule 39 Molecule 30 Molecule 30 Molecule 30 Molecule 40 Molecule 41 Molecule 42 Molecule 43 Molecule 44 Molecule 45 Molecule 46 Molecule 47 Molecule 48 Molecule 49 Molecule 50 Molecule 51 Molecule 50 Molecule 51 Molecule 50 Molecule 51 Molecule 50 Molecule 51 Molecule 50 Molecule 60	Molecule 9	Molecule 10	Molecule 11	Molecule 12
Molecule 21 Molecule 22 Molecule 23 Molecule 24 Molecule 25 Molecule 26 Molecule 27 Molecule 27 Molecule 28 Molecule 30 Molecule 31 Molecule 31 Molecule 32 Molecule 32 Molecule 33 Molecule 34 Molecule 35 Molecule 35 Molecule 36 Molecule 37 Molecule 38 Molecule 39 Molecule 30 Molecule 30 Molecule 30 Molecule 30 Molecule 30 Molecule 41 Molecule 42 Molecule 43 Molecule 43 Molecule 44 Molecule 45 Molecule 46 Molecule 47 Molecule 48 Molecule 49 Molecule 50 Molecule 51 Molecule 55 Molecule 55 Molecule 55 Molecule 56 Molecule 57 Molecule 58 Molecule 59 Molecule 60 Molecule 61 Molecule 62 Molecule 63 Molecule 64 Molecule 65 Molecule 65 Molecule 66 Molecule 67 Molecule 67 Molecule 68 Molecule 69 Molecule 60 Molecule 60 Molecule 67 Molecule 67 Molecule 68 Molecule 70 Molecule 71 Molecule 72 Molecule 72 Molecule 73 Molecule 74 Molecule 75 Molecule 76 Molecule 77 Molecule 78 Molecule 79 Molecule 79 Molecule 80 Molecule 81 Molecule 81 Molecule 82 Molecule 83 Molecule 84 Molecule 85 Molecule 86 Molecule 87 Molecule 88 Molecule 89 Molecule 90 Molecule 90 Molecule 91 Molecule 91 Molecule 92 Molecule 93 Molecule 94 Molecule 95 Molecule 97 ALL PASS	Molecule 13	Molecule 14	Molecule 15	Molecule 16
Molecule 25 Molecule 26 Molecule 27 Molecule 28 Molecule 28 Molecule 30 Molecule 31 Molecule 32 Molecule 32 Molecule 35 Molecule 36 Molecule 35 Molecule 36 Molecule 38 Molecule 39 Molecule 40 Molecule 41 Molecule 42 Molecule 43 Molecule 44 Molecule 45 Molecule 46 Molecule 47 Molecule 48 Molecule 48 Molecule 49 Molecule 50 Molecule 51 Molecule 52 Molecule 53 Molecule 54 Molecule 55 Molecule 56 Molecule 56 Molecule 57 Molecule 58 Molecule 59 Molecule 60 Molecule 61 Molecule 62 Molecule 63 Molecule 64 Molecule 65 Molecule 66 Molecule 67 Molecule 68 Molecule 69 Molecule 66 Molecule 70 Molecule 71 Molecule 72 Molecule 73 Molecule 74 Molecule 75 Molecule 75 Molecule 76 Molecule 76 Molecule 77 Molecule 78 Molecule 79 Molecule 79 Molecule 79 Molecule 80 Molecule 81 Molecule 82 Molecule 83 Molecule 84 Molecule 85 Molecule 86 Molecule 87 Molecule 88 Molecule 89 Molecule 80 Molecule 87 Molecule 88 Molecule 89 Molecule 80 Molecule 90 Molecule 91 Molecule 96 Molecule 97 Molecule 98 Molecule 99 Molecule 99 Molecule 90 Molecule 91 Molecule 95 Molecule 96 Molecule 97 ALL PASS ALL PA	Molecule 17	Molecule 18	Molecule 19	Molecule 20
Molecule 30 Molecule 31 Molecule 32 Molecule 33 Molecule 34 Molecule 35 Molecule 36 Molecule 36 Molecule 36 Molecule 38 Molecule 39 Molecule 40 Molecule 41 Molecule 42 Molecule 43 Molecule 44 Molecule 45 Molecule 46 Molecule 47 Molecule 48 Molecule 49 Molecule 50 Molecule 51 Molecule 51 Molecule 54 Molecule 53 Molecule 54 Molecule 55 Molecule 56 Molecule 57 Molecule 58 Molecule 59 Molecule 50 Molecule 60 Molecule 61 Molecule 62 Molecule 63 Molecule 64 Molecule 65 Molecule 66 Molecule 67 Molecule 67 Molecule 67 Molecule 67 Molecule 69 Molecule 70 Molecule 80 Molecule 90	Molecule 21	Molecule 22	Molecule 23	Molecule 24
Molecule 33 Molecule 34 Molecule 35 Molecule 36 Molecule 37 Molecule 38 Molecule 39 Molecule 40 Molecule 41 Molecule 42 Molecule 43 Molecule 44 Molecule 45 Molecule 46 Molecule 47 Molecule 48 Molecule 48 Molecule 49 Molecule 50 Molecule 51 Molecule 52 Molecule 53 Molecule 54 Molecule 55 Molecule 55 Molecule 56 Molecule 57 Molecule 58 Molecule 59 Molecule 60 Molecule 61 Molecule 62 Molecule 63 Molecule 64 Molecule 65 Molecule 65 Molecule 66 Molecule 67 Molecule 67 Molecule 68 Molecule 67 Molecule 67 Molecule 68 Molecule 70 Molecule 73 Molecule 74 Molecule 75 Molecule 75 Molecule 76 Molecule 76 Molecule 77 Molecule 78 Molecule 79 Molecule 80 Molecule 81 Molecule 82 Molecule 83 Molecule 84 Molecule 85 Molecule 85 Molecule 86 Molecule 87 Molecule 88 Molecule 89 Molecule 89 Molecule 90 Molecule 91 Molecule 91 Molecule 92 Molecule 93 Molecule 94 Molecule 95 Molecule 95 Molecule 96 Molecule 97 Molecule 98 Molecule 99	Molecule 25	Molecule 26	Molecule 27	Molecule 28
Molecule 37 Molecule 38 Molecule 39 Molecule 40 Molecule 41 Molecule 42 Molecule 43 Molecule 44 Molecule 45 Molecule 50 Molecule 51 Molecule 52 Molecule 53 Molecule 54 Molecule 55 Molecule 55 Molecule 57 Molecule 58 Molecule 59 Molecule 60 Molecule 61 Molecule 62 Molecule 63 Molecule 67 Molecule 65 Molecule 66 Molecule 67 Molecule 70 Molecule 73 Molecule 70 Molecule 71 Molecule 72 Molecule 75 Molecule 75 Molecule 76 Molecule 76 Molecule 70 Molecule 75 Molecule 76 Molecule 76 Molecule 70 Molecule 75 Molecule 70 Molecule 75 Molecule 81 Molecule 82 Molecule 83 Molecule 80 Molecule 85 Molecule 86 Molecule 87 Molecule 88 Molecule 89 Molecule 80 Molecule 81 Molecule 81 Molecule 90 Molecule 91 Molecule 92 Molecule 93 <t< td=""><td>Molecule 29</td><td>Molecule 30</td><td>Molecule 31</td><td>Molecule 32</td></t<>	Molecule 29	Molecule 30	Molecule 31	Molecule 32
Molecule 41 Molecule 45 Molecule 45 Molecule 46 Molecule 47 Molecule 48 Molecule 49 Molecule 50 Molecule 51 Molecule 53 Molecule 57 Molecule 58 Molecule 50 Molecule 50 Molecule 50 Molecule 50 Molecule 51 Molecule 55 Molecule 59 Molecule 50 Molecule 50 Molecule 50 Molecule 50 Molecule 50 Molecule 50 Molecule 61 Molecule 62 Molecule 63 Molecule 63 Molecule 65 Molecule 69 Molecule 69 Molecule 70 Molecule 71 Molecule 71 Molecule 72 Molecule 73 Molecule 74 Molecule 75 Molecule 75 Molecule 81 Molecule 81 Molecule 82 Molecule 83 Molecule 85 Molecule 85 Molecule 80 Molecule 90 Molecule 91 Molecule 93 Molecule 97 ALL PASS ALL PASS ALL PASS ALL PASS AVg: 0.061	Molecule 33	Molecule 34	Molecule 35	Molecule 36
Molecule 45 Molecule 49 Molecule 50 Molecule 51 Molecule 53 Molecule 57 Molecule 58 Molecule 59 Molecule 61 Molecule 62 Molecule 65 Molecule 65 Molecule 65 Molecule 65 Molecule 66 Molecule 69 Molecule 69 Molecule 70 Molecule 71 Molecule 72 Molecule 73 Molecule 74 Molecule 75 Molecule 75 Molecule 81 Molecule 82 Molecule 83 Molecule 83 Molecule 84 Molecule 85 Molecule 85 Molecule 85 Molecule 87 Molecule 88 Molecule 89 Molecule 89 Molecule 90 Molecule 91 Molecule 97 Molecule 97 Molecule 97 Molecule 98 Molecule 97 Molecule 98 Molecule 97 Molecule 97 Molecule 98 Molecule 97 Molecule 97 Molecule 98 Molecule 98 Molecule 99 Molecule 97 Molecule 98 ALL PASS Avg: 0.061	Molecule 37	Molecule 38	Molecule 39	Molecule 40
Molecule 49 Molecule 50 Molecule 53 Molecule 54 Molecule 55 Molecule 57 Molecule 57 Molecule 61 Molecule 65 Molecule 65 Molecule 65 Molecule 65 Molecule 69 Molecule 73 Molecule 73 Molecule 74 Molecule 75 Molecule 75 Molecule 78 Molecule 79 Molecule 81 Molecule 82 Molecule 85 Molecule 85 Molecule 85 Molecule 85 Molecule 85 Molecule 85 Molecule 95 Molecule 95 Molecule 95 Molecule 97 Molecule 98 Molecule 99 Molecule 97 Molecule 97 Molecule 98 Molecule 97 Molecule 98 Molecule 97 Molecule 97 Molecule 98 Molecule 97 ALL PASS Avg: 0.061	Molecule 41	Molecule 42	Molecule 43	Molecule 44
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Molecule 57 Molecule 61 Molecule 62 Molecule 63 Molecule 65 Molecule 65 Molecule 69 Molecule 69 Molecule 70 Molecule 71 Molecule 73 Molecule 74 Molecule 75 Molecule 75 Molecule 78 Molecule 78 Molecule 81 Molecule 82 Molecule 83 Molecule 85 Molecule 85 Molecule 80 Molecu	Molecule 49	Molecule 50	Molecule 51	Molecule 52
Molecule 61Molecule 62Molecule 63Molecule 64Molecule 65Molecule 66Molecule 67Molecule 68Molecule 69Molecule 70Molecule 71Molecule 72Molecule 73Molecule 74Molecule 75Molecule 75Molecule 87Molecule 89Molecule 82Molecule 83Molecule 84Molecule 89Molecule 80Molecule 87Molecule 88Molecule 89Molecule 90Molecule 91Molecule 92Molecule 93Molecule 94Molecule 95Molecule 96Molecule 97ALL PASSALL PASSALL PASSALL PASSAVg: 0.061Avg: 0.061	Molecule 53	Molecule 54	Molecule 55	Molecule 56
Molecule 65 Molecule 66 Molecule 67 Molecule 67 Molecule 68 Molecule 73 Molecule 74 Molecule 75 Molecule 75 Molecule 76 Molecule 87 Molecule 89 Molecule 80 Molecule 83 Molecule 83 Molecule 89 Molecule 90 Molecule 91 Molecule 92 Molecule 97 Molecule 98 Molecule 95 Molecule 96 Molecule 97 Molecule 98 ALL PASS ALL PASS ALL PASS Avg: 0.061 Avg: 0.061	Molecule 57	Molecule 58	Molecule 59	Molecule 60
Molecule 69Molecule 70Molecule 71Molecule 71Molecule 72Molecule 73Molecule 74Molecule 75Molecule 75Molecule 77Molecule 78Molecule 79Molecule 80Molecule 81Molecule 82Molecule 83Molecule 84Molecule 85Molecule 86Molecule 87Molecule 88Molecule 89Molecule 90Molecule 91Molecule 92Molecule 93Molecule 94Molecule 95Molecule 95Molecule 97Molecule 98ALL PASSAVg: 0.061	Molecule 61	Molecule 62	Molecule 63	Molecule 64
Molecule 73Molecule 74Molecule 75Molecule 75Molecule 76Molecule 87Molecule 80Molecule 80Molecule 81Molecule 82Molecule 83Molecule 84Molecule 85Molecule 86Molecule 87Molecule 88Molecule 89Molecule 90Molecule 91Molecule 92Molecule 93Molecule 94Molecule 95Molecule 95Molecule 97Molecule 98ALL PASSALL PASSALL PASSAvg: 0.061Avg: 0.061	Molecule 65	Molecule 66	Molecule 67	Molecule 68
Molecule 77 Molecule 81 Molecule 82 Molecule 85 Molecule 89 Molecule 90 Molecule 93 Molecule 97 ALL PASS Molecule 97 ALL PASS Molecule 97 ALL PASS Molecule 98 Molecule 98 ALL PASS Molecule 98 Molecule 98 ALL PASS Molecule 98 ALL PASS Avg: 0.061	Molecule 69	Molecule 70	Molecule 71	Molecule 72
Molecule 81 Molecule 85 Molecule 85 Molecule 89 Molecule 90 Molecule 93 Molecule 97 ALL PASS Molecule 97 ALL PASS Molecule 98 ALL PASS Molecule 98 ALL PASS Molecule 98 ALL PASS Avg: 0.061	Molecule 73	Molecule 74	Molecule 75	Molecule 76
Molecule 85Molecule 86Molecule 87Molecule 88Molecule 89Molecule 90Molecule 91Molecule 92Molecule 93Molecule 94Molecule 95Molecule 95Molecule 97Molecule 98ALL PASSALL PASSALL PASSAvg: 0.061Avg: 0.061	Molecule 77	Molecule 78	Molecule 79	Molecule 80
Molecule 89 Molecule 90 Molecule 93 Molecule 94 Molecule 97 ALL PASS ALL PASS ALL PASS Molecule 98 ALL PASS AVg: 0.061 Molecule 91 Molecule 95 ALL PASS Avg: 0.061	Molecule 81	Molecule 82	Molecule 83	Molecule 84
Molecule 93 Molecule 94 Molecule 97 ALL PASS ALL PASS ALL PASS Avg: 0.061 Molecule 95 ALL PASS Avg: 0.061	Molecule 85	Molecule 86	Molecule 87	Molecule 88
Molecule 97 ALL PASS ALL PASS ALL PASS ALL PASS AVg: 0.061	Molecule 89	Molecule 90	Molecule 91	Molecule 92
ALL PASS Avg: 0.061 Avg: 0.061	Molecule 93	Molecule 94	Molecule 95	Molecule 96
	Molecule 97	Molecule 98		
[Avg: 0.061]			Avg: 0.061	Avg: 0.061
	Avg: 0.061	Avg: 0.061		

Molecular Structure



Toxicity Predictions

NR-AhR_best
PASS
0.029
SR-HSE_best
PASS
0.081

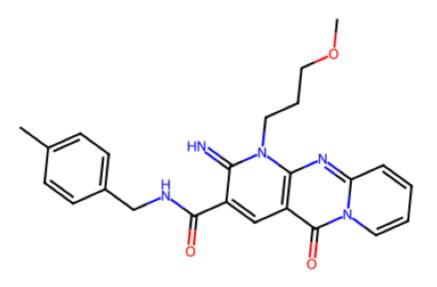
NR-PPAR-gamma_best
PASS
0.000

SR-MMP_best
PASS
0.111

NR-ER-LBD_best
PASS
0.049

SR-ARE_best
PASS
0.135

Molecular Structure



Toxicity Predictions

NR-AhR_best
PASS
0.029
SR-HSE_best
PASS
0.081

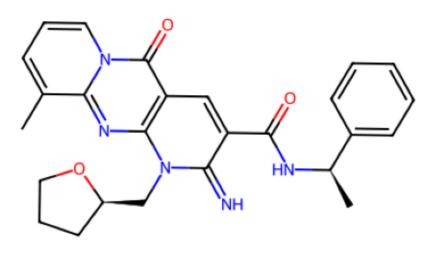
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PASS
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PASS
0.111

NR-ER-LBD_best
PASS
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SR-ARE_best
PASS
0.135

Molecular Structure



Toxicity Predictions

NR-AhR_best
PASS
0.029
SR-HSE_best
PASS
0.081

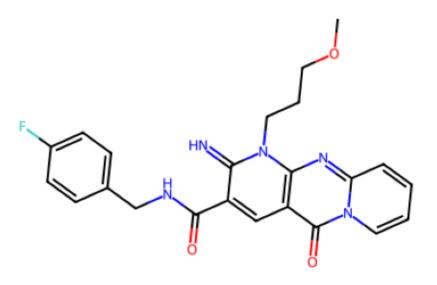
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PASS
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NR-ER-LBD_best
PASS
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SR-ARE_best
PASS
0.135

Molecular Structure



Toxicity Predictions

NR-AhR_best
PASS
0.029
SR-HSE_best
PASS
0.081

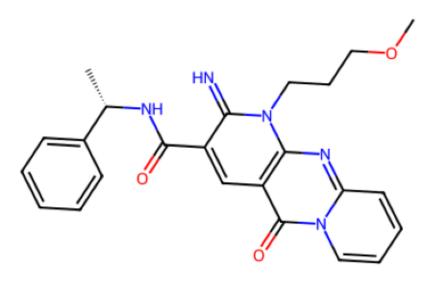
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PASS
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NR-ER-LBD_best
PASS
0.049

SR-ARE_best
PASS
0.135

Molecular Structure



Toxicity Predictions

NR-AhR_best
PASS
0.029
SR-HSE_best
PASS
0.081

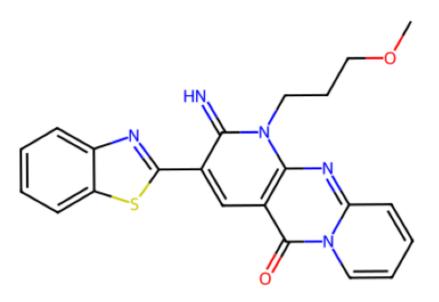
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PASS
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NR-ER-LBD_best
PASS
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SR-ARE_best
PASS
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Molecular Structure



Toxicity Predictions

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PASS
0.029
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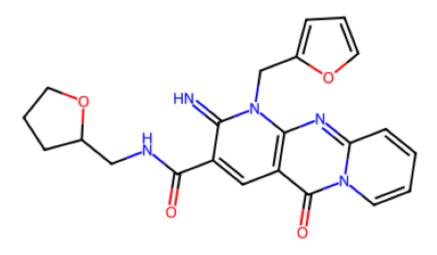
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PASS
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NR-ER-LBD_best
PASS
0.049

SR-ARE_best
PASS
0.135

Molecular Structure



Toxicity Predictions

NR-AhR_best
PASS
0.029
SR-HSE_best
PASS
0.081

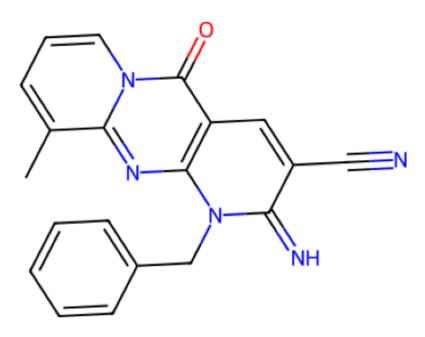
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PASS
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NR-ER-LBD_best
PASS
0.049

SR-ARE_best
PASS
0.135

Molecular Structure

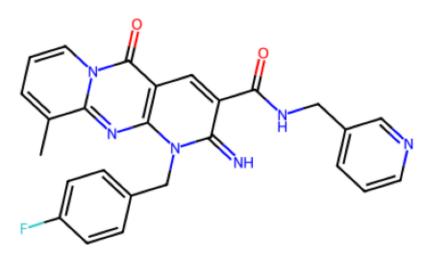


Toxicity Predictions

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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

Molecular Structure



Toxicity Predictions

NR-AhR_best
PASS
0.029
SR-HSE_best
PASS
0.081

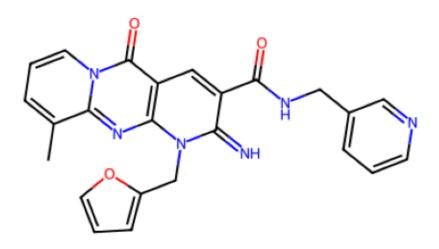
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PASS
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NR-ER-LBD_best
PASS
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PASS
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Molecular Structure



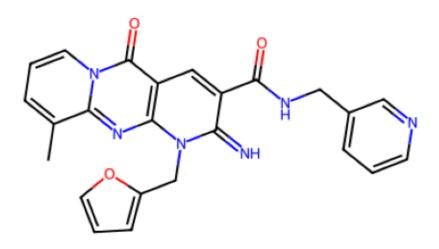
Toxicity Predictions

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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

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
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SR-ARE_best
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Molecular Structure

Toxicity Predictions

NR-AhR_best
PASS
0.029
SR-HSE_best
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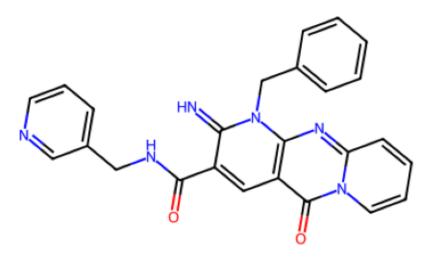
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NR-ER-LBD_best
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Molecular Structure



Toxicity Predictions

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PASS
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SR-HSE_best
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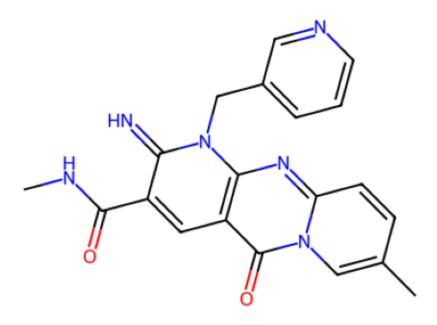
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NR-ER-LBD_best
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Molecular Structure



Toxicity Predictions

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SR-HSE_best
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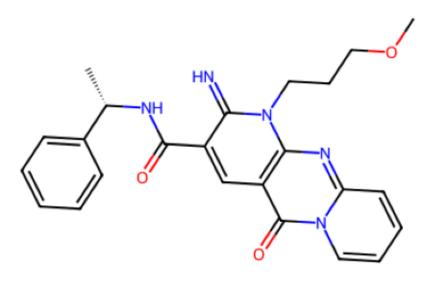
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Molecular Structure



Toxicity Predictions

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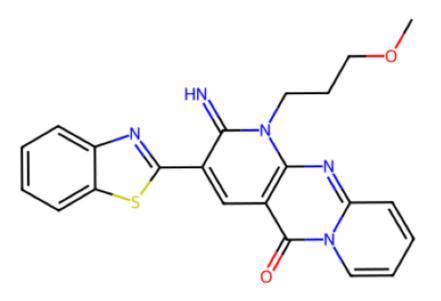
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Molecular Structure



Toxicity Predictions

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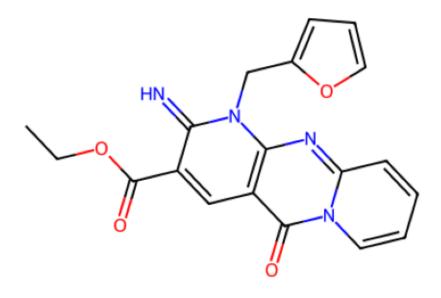
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Molecular Structure



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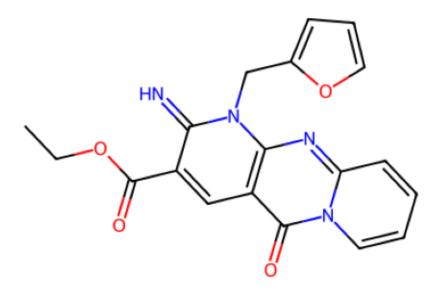
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Molecular Structure



Toxicity Predictions

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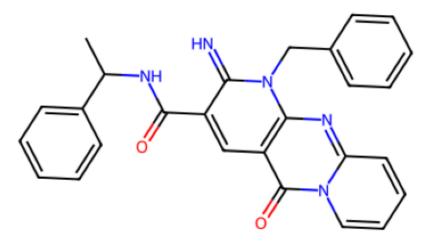
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Molecular Structure



Toxicity Predictions

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Molecular Structure

Toxicity Predictions

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Molecular Structure

Toxicity Predictions

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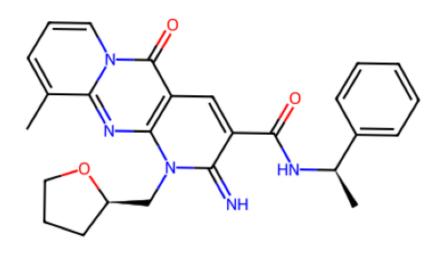
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Molecular Structure



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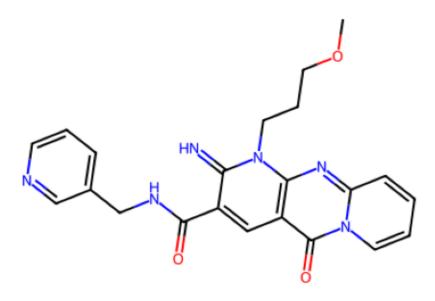
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Molecular Structure



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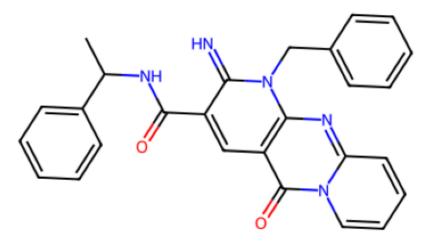
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Molecular Structure



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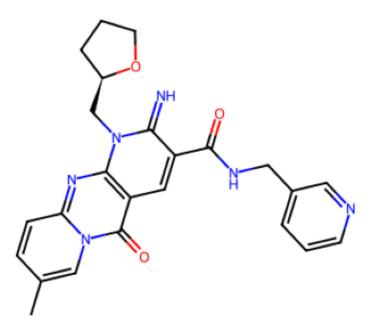
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Molecular Structure



Toxicity Predictions

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PASS
0.135

Molecular Structure

Toxicity Predictions

NR-AhR_best
PASS
0.029
SR-HSE_best
PASS
0.081

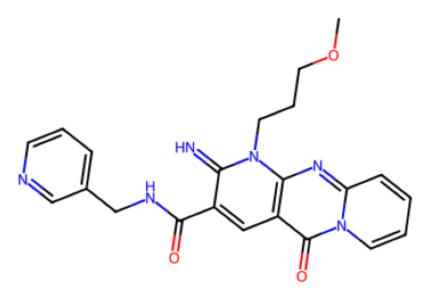
NR-PPAR-gamma_best
PASS
0.000

SR-MMP_best
PASS
0.111

NR-ER-LBD_best
PASS
0.049

SR-ARE_best
PASS
0.135

Molecular Structure



Toxicity Predictions

NR-AhR_best
PASS
0.029
SR-HSE_best
PASS
0.081

NR-PPAR-gamma_best
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Molecular Structure

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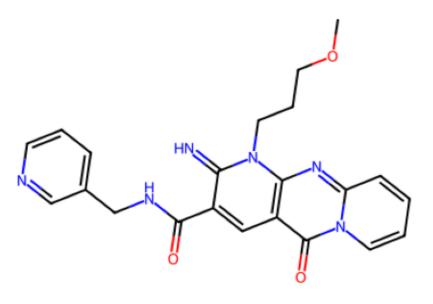
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