Supporting Information

Docking Covalent Inhibitors: a Parameter Free Approach to Pose Prediction and Scoring

Kai Zhu,[‡] Kenneth W. Borrelli,[‡] Jeremy R. Greenwood, Tyler Day, Robert Abel, Ramy S. Farid, Edward Harder[*]

Schrodinger Inc., 120 W 45th Street, New York, NY 10036
*Email: ed.harder@schrodinger.com

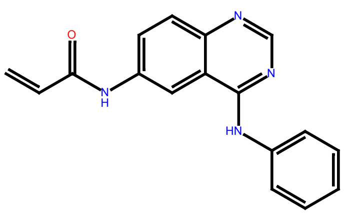
Table S1. The list of PDB IDs and our pose prediction results of the 76 complexes used in CovalentDock. Top1 means the lowest Prime energy pose, and top10 means the best RMSD pose in the 10 lowest Prime energy poses.

PDBID	Reaction Type	Chain	Attachment Residue Number	Top1		Top10	
				RMSD	PrimeEnergy	RMSD	PrimeEnergy
2awz	Michael	A	366	2.94	-23656.00	2.84	-23652.40
2ax0	Michael	A	366	2.14	-23465.34	1.81	-23453.63
2ax1	Michael	A	366	6.19	-23529.08	2.73	-23527.29
2e14	Michael	A	166	1.07	-12859.88	1.00	-12832.97
2hwo	Michael	A	345	4.95	-10513.41	4.87	-10510.41
2hwp	Michael	A	345	2.74	-10287.16	2.06	-10278.61
2jiv	Michael	A	797	0.94	-9674.42	0.94	-9674.42
2qlq	Michael	B	345	1.96	-10512.50	1.24	-10499.02
3c9w	Michael	A	164	0.52	-14067.29	0.16	-14063.47
3ika	Michael	A	797	0.89	-24610.54	0.89	-24610.54
3lok	Michael	B	345	1.22	-10061.80	0.39	-10054.78
3oyp	Michael	A	159	0.46	-7436.06	0.41	-7434.29
3t9t	Michael	A	442	0.69	-11325.48	0.69	-11325.48
1b12	Beta-Lactam	A	90	1.30	-10075.99	1.34	-10075.99
1bt5	Beta-Lactam	A	70	3.28	-12231.63	1.72	-12221.92
1cef	Beta-Lactam	A	62	3.04	-15700.98	1.09	-15695.54
1ceg	Beta-Lactam	A	62	1.54	-15772.80	1.68	-15772.31
1fcm	Beta-Lactam	A	61	0.85	-15034.98	0.47	-15030.31
1fcn	Beta-Lactam	A	61	1.16	-15041.74	0.97	-15041.74
1fco	Beta-Lactam	A	61	3.24	-15251.98	2.78	-15250.64
1fr6	Beta-Lactam	A	64	0.82	-15409.82	0.71	-15409.82
1ghm	Beta-Lactam	A	70	0.70	-11835.09	0.45	-11827.20
1ghp	Beta-Lactam	A	70	2.42	-11682.90	1.60	-11676.70
1i5q	Beta-Lactam	A	64	2.17	-15434.94	1.35	-15423.30
1iyp	Beta-Lactam	A	70	1.10	-11865.01	0.57	-11864.10
1iyq	Beta-Lactam	A	70	0.30	-11881.96	0.19	-11881.96
1kvm	Beta-Lactam	B	64	1.92	-15761.79	1.89	-15761.79
1ll5	Beta-Lactam	A	64	7.37	-15238.18	6.01	-15233.76
1ll9	Beta-Lactam	B	64	2.05	-15669.87	1.95	-15608.44
1llb	Beta-Lactam	B	64	0.61	-15681.56	0.17	-15681.54
1pw8	Beta-Lactam	A	62	1.24	-15787.62	1.11	-15787.38
1pwd	Beta-Lactam	A	62	2.77	-15719.49	2.77	-15719.49
1pwg	Beta-Lactam	A	62	0.56	-15760.51	0.16	-15759.68

1qmf	Beta-Lactam	A	337	0.58	-24533.78	0.28	-24528.84
1w8y	Beta-Lactam	A	49	2.39	55700.71	2.42	55700.73
1ymx	Beta-Lactam	A	70	0.75	-11839.32	0.74	-11839.31
2c5w	Beta-Lactam	B	370	0.71	57307.22	0.66	57307.41
2ex6	Beta-Lactam	A	62	3.64	-19693.99	3.44	-19692.62
2ex8	Beta-Lactam	A	62	1.29	-20077.05	0.68	-20077.02
2ex9	Beta-Lactam	A	62	1.40	-19272.51	1.34	-19272.35
2exa	Beta-Lactam	A	62	2.89	-19252.47	2.44	-19251.23
2exb	Beta-Lactam	A	62	3.18	-19492.61	2.60	-19479.36
2j8y	Beta-Lactam	A	61	1.12	-12084.07	0.60	-12073.90
2jbf	Beta-Lactam	A	61	0.93	-12091.53	0.31	-12085.60
2vgj	Beta-Lactam	A	49	0.99	-19918.63	0.86	-19918.62
2wkh	Beta-Lactam	A	67	2.41	-11010.05	2.34	-11010.05
2xd1	Beta-Lactam	A	460	3.50	2139.64	0.97	2144.04
2z2m	Beta-Lactam	B	337	0.83	-16048.39	0.81	-16048.16
2zc3	Beta-Lactam	B	337	2.09	-16173.79	1.44	-16171.31
2zc4	Beta-Lactam	B	337	2.77	-16160.53	1.43	-16150.56
2zc5	Beta-Lactam	B	370	1.91	-17483.05	1.91	-17483.05
2zc6	Beta-Lactam	B	370	3.27	-17692.12	3.20	-17683.36
2zd8	Beta-Lactam	A	70	1.82	-12282.62	1.72	-12282.62
2zq9	Beta-Lactam	A	70	0.96	-11933.22	0.35	-11931.94
2zqa	Beta-Lactam	A	70	1.21	-12030.65	0.50	-12020.91
2zqc	Beta-Lactam	A	70	1.47	-12045.92	1.34	-12036.98
2zqd	Beta-Lactam	A	70	0.61	-12057.61	0.48	-12057.60
3a3e	Beta-Lactam	A	69	1.56	-19176.47	1.59	-19176.39
3a3f	Beta-Lactam	A	69	0.79	-20145.69	0.67	-20145.68
3a3i	Beta-Lactam	A	69	1.22	-20149.35	0.23	-20149.31
3beb	Beta-Lactam	A	44	1.22	-15834.78	1.23	-15834.78
3bec	Beta-Lactam	A	44	1.09	-15970.62	0.68	-15969.90
3dwz	Beta-Lactam	A	84	2.33	-11857.97	2.17	-11852.03
3iqa	Beta-Lactam	A	84	2.72	-11873.71	2.65	-11872.47
3ita	Beta-Lactam	A	40	3.10	-15214.66	2.40	-15207.36
3kgo	Beta-Lactam	A	70	1.18	-3263.64	1.00	-3263.63
3ly4	Beta-Lactam	A	70	1.04	-11712.33	0.74	-11710.67
3m6b	Beta-Lactam	A	84	1.14	-11928.68	0.98	-11928.68
3m6h	Beta-Lactam	A	84	2.63	-11869.53	0.64	-11868.94
3mzd	Beta-Lactam	A	44	2.29	-15880.82	2.35	-15880.77
3mze	Beta-Lactam	A	44	2.54	-15774.39	1.73	-15766.74
3mzf	Beta-Lactam	A	44	0.66	-16023.34	0.70	-16023.06
3n8s	Beta-Lactam	A	84	1.58	-11839.32	1.58	-11839.29
3ocl	Beta-Lactam	A	294	1.00	-21418.48	0.85	-21418.41

3ocn	Beta-Lactam	A	294	0.94	-21505.76	0.65	-21505.48
3pbo	Beta-Lactam	A	294	0.92	-20397.16	0.68	-20391.99
	% of <=2.0			68.6%		77.6%	
	Mean			1.81		1.39	

Table S2. The chemical structures of 10 active compounds and 100 decoy compounds used in the virtual screening study.



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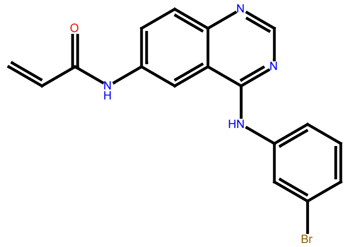

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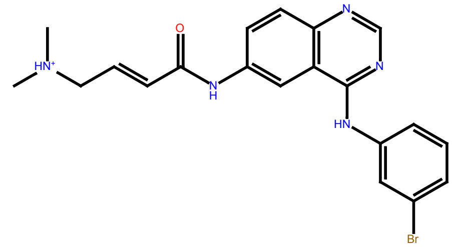

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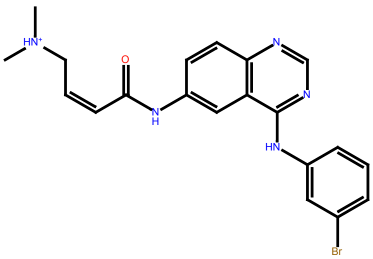

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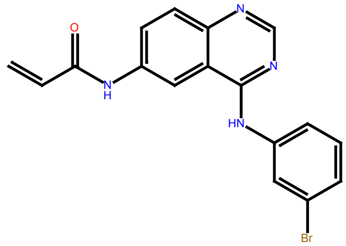

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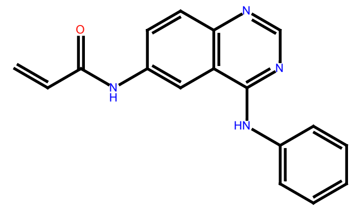

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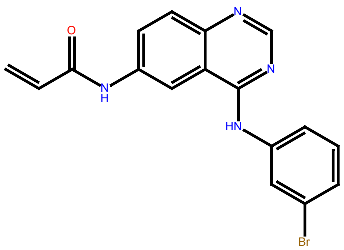

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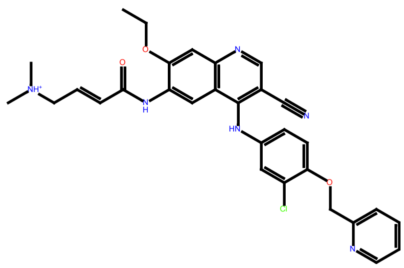

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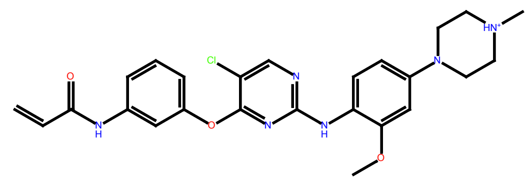

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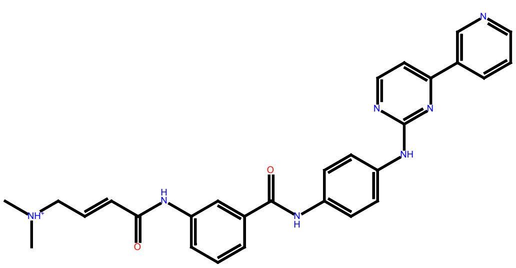

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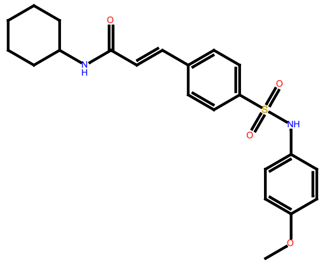

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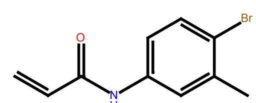

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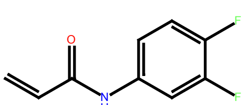

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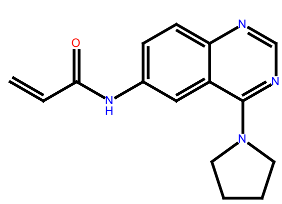

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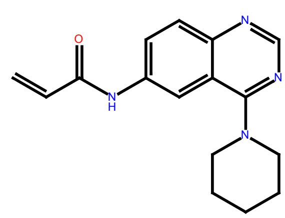

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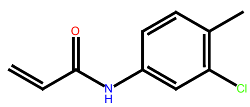

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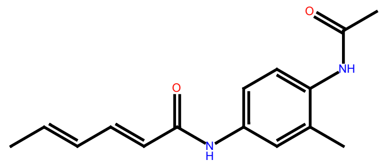

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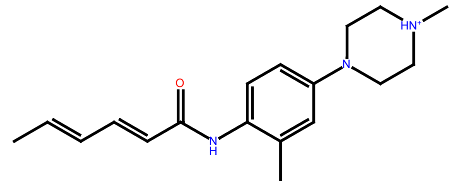

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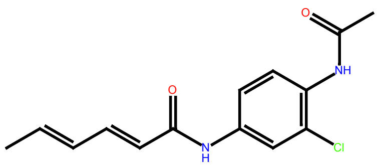

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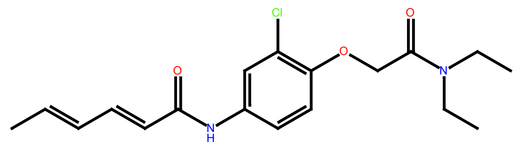

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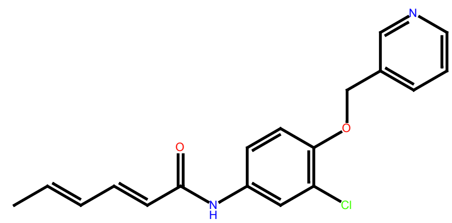

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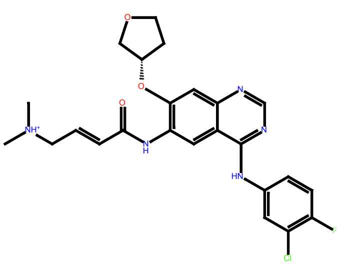

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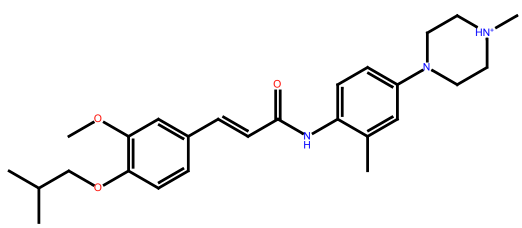

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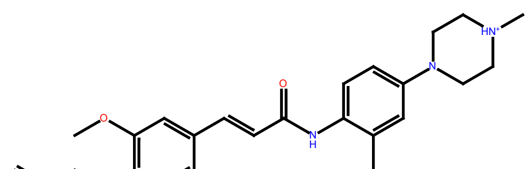

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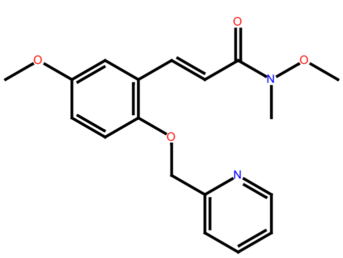

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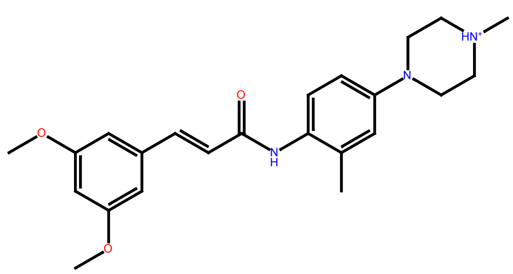

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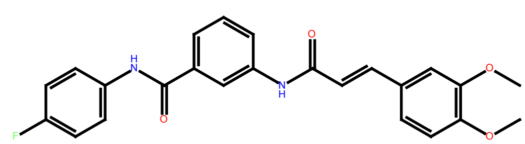

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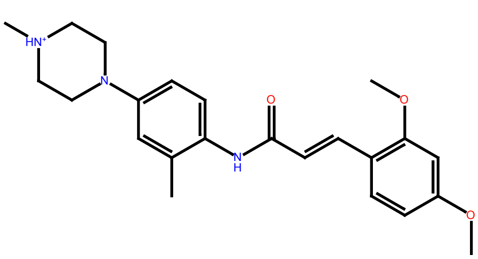

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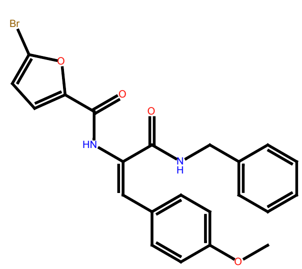

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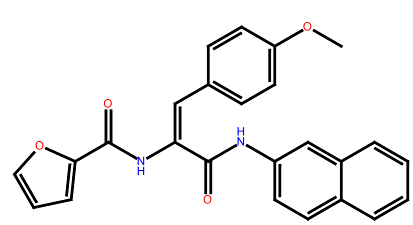

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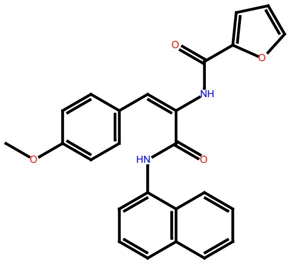

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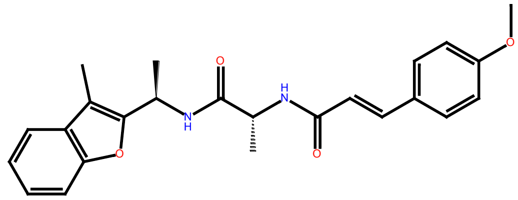

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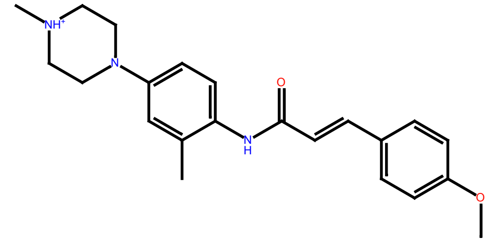

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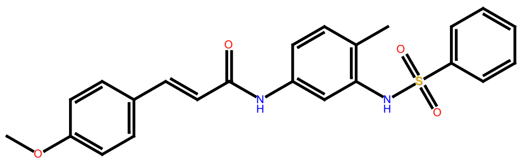

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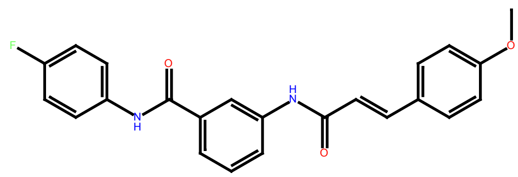

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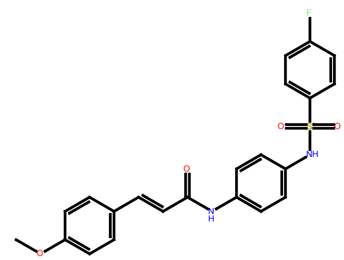

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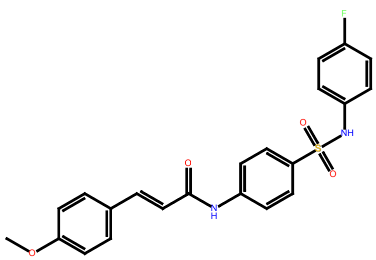

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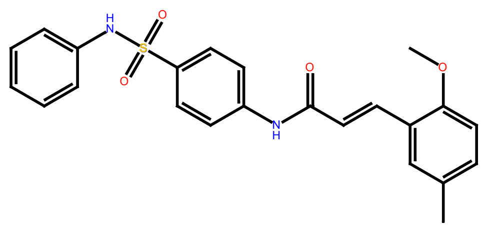

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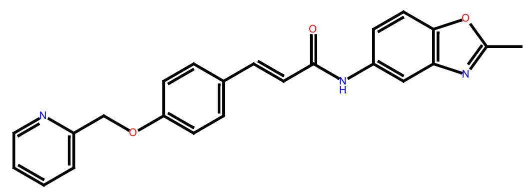

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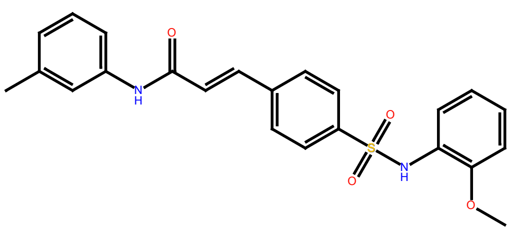

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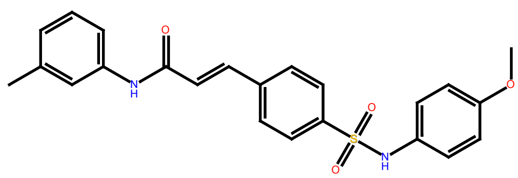

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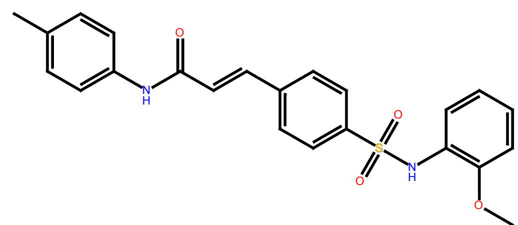

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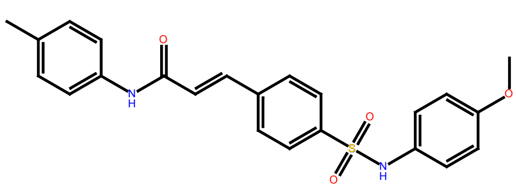

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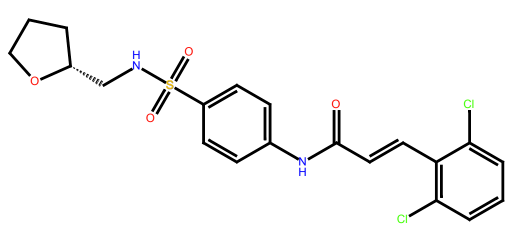

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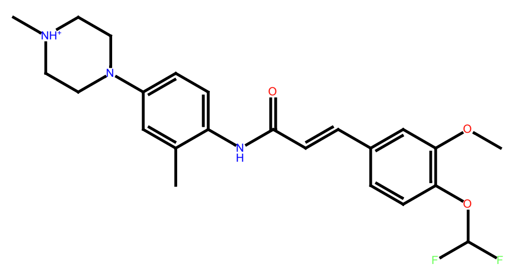

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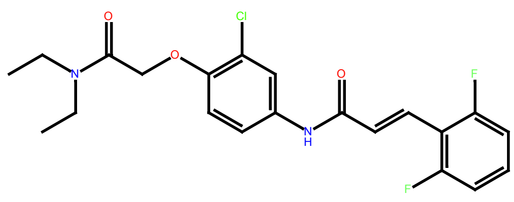

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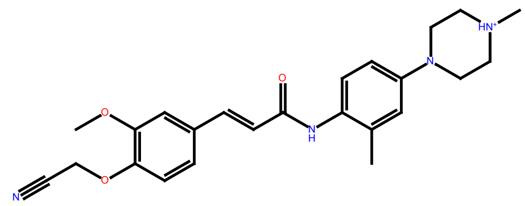

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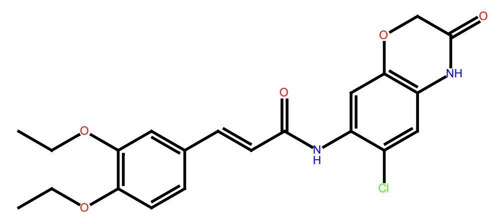

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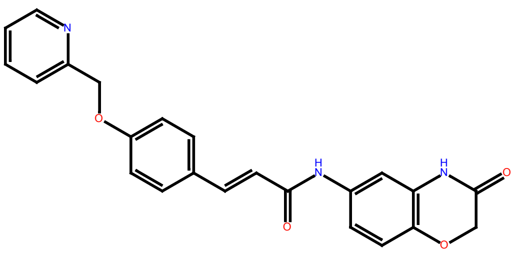

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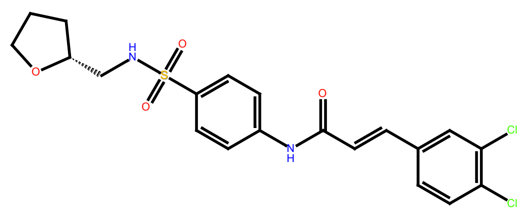

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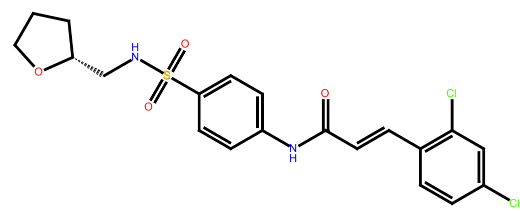

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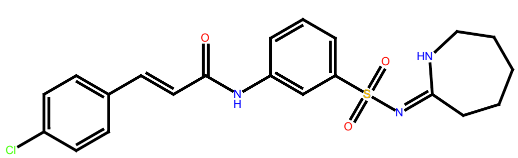

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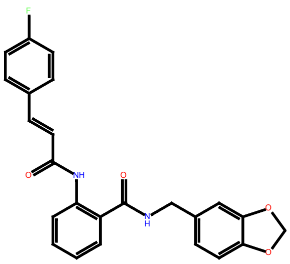

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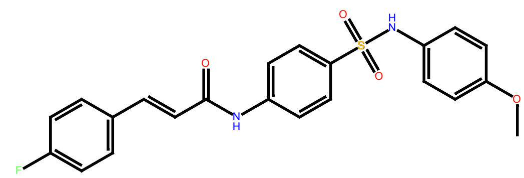

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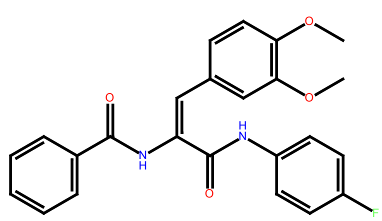

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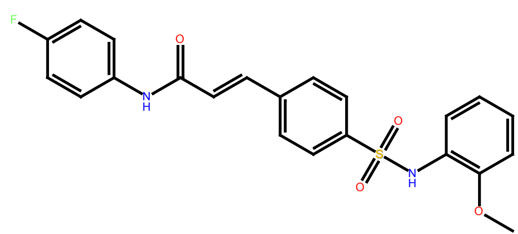

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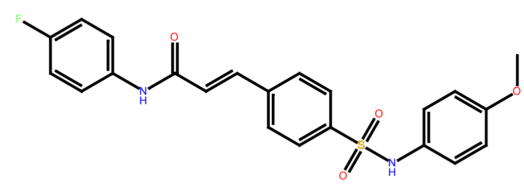

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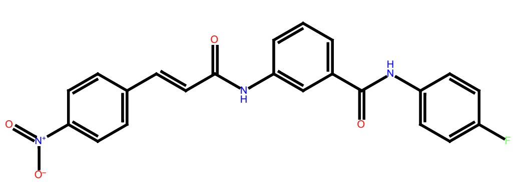

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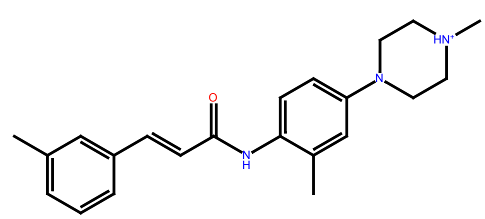

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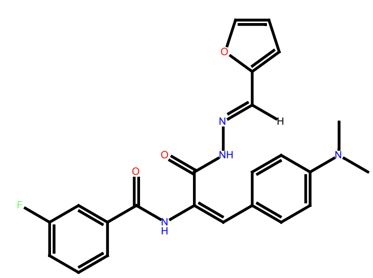

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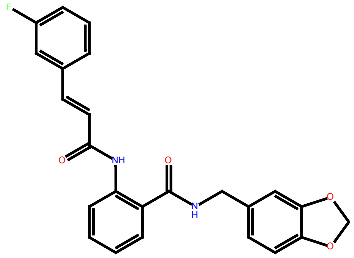

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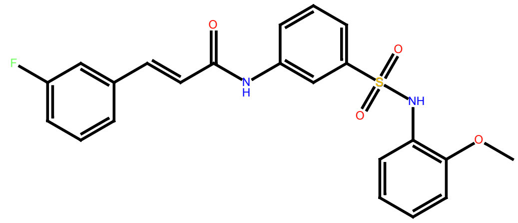

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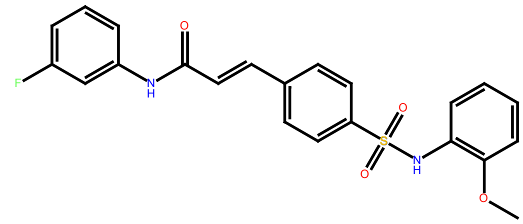

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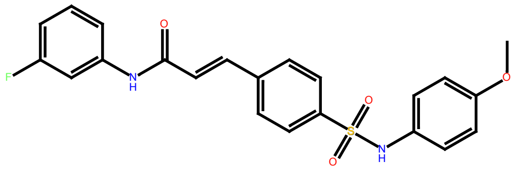

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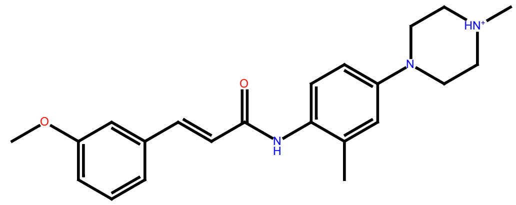

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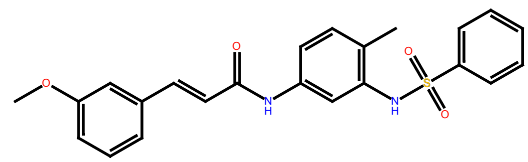

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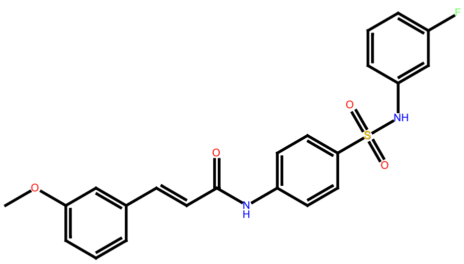

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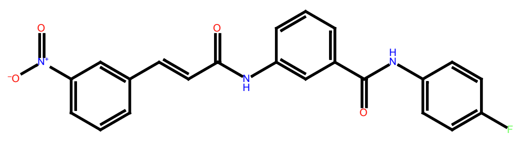

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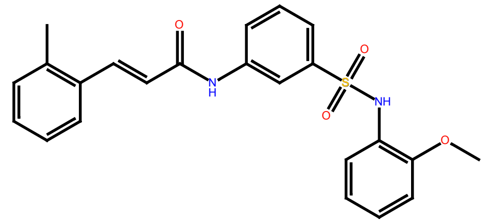

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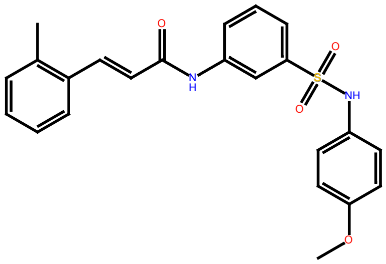

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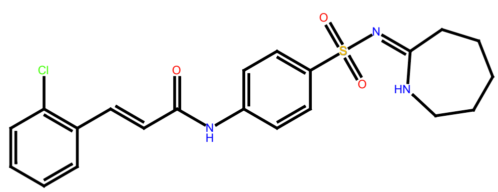

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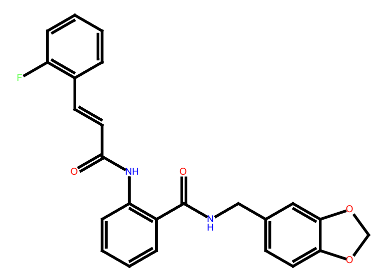

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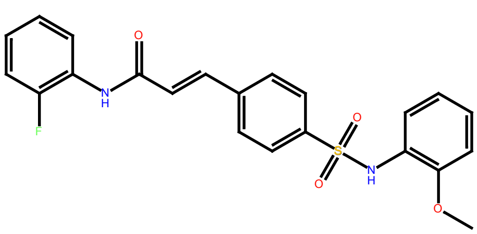

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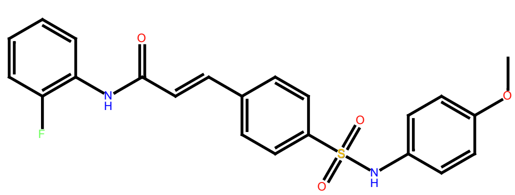

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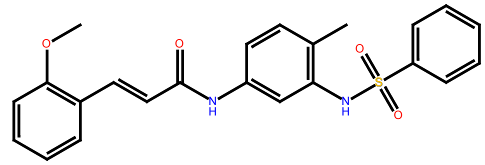

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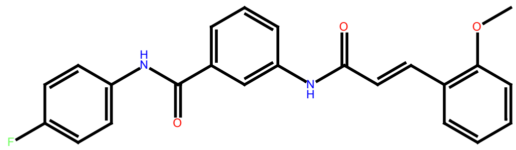

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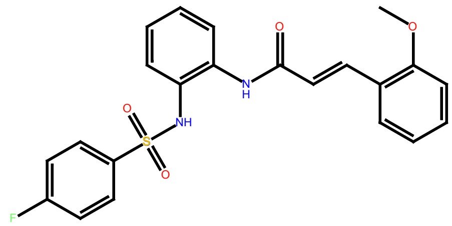

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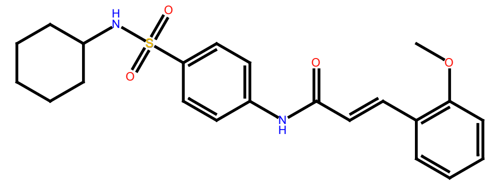

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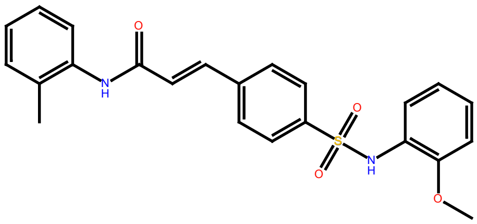

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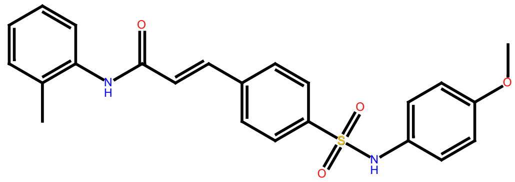

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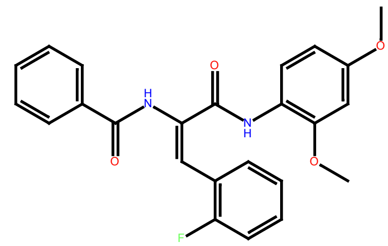

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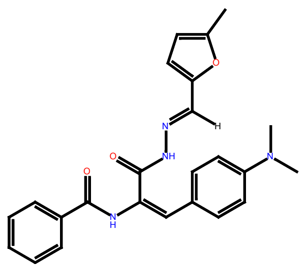

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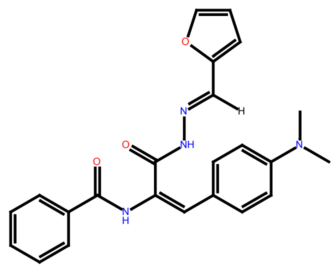

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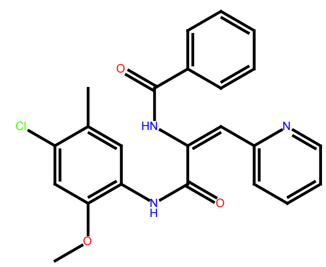

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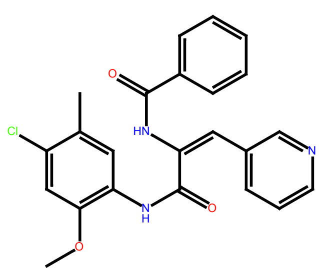

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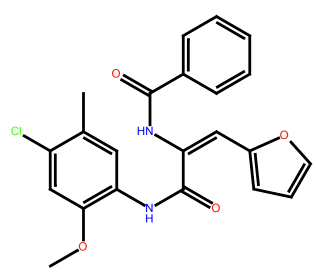

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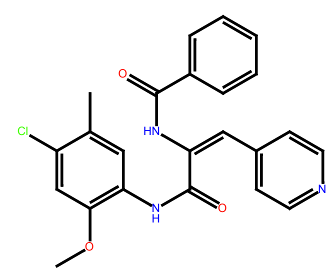

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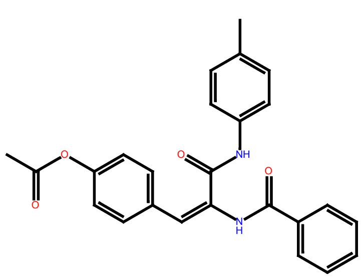

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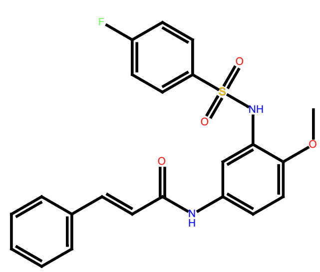

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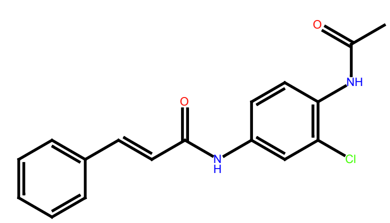

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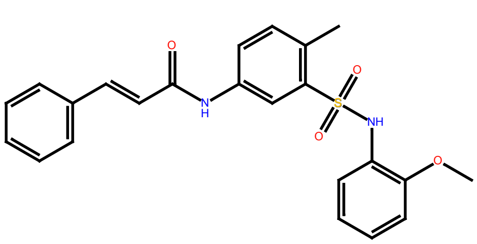

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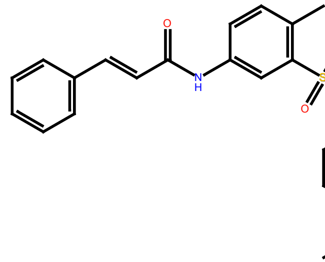

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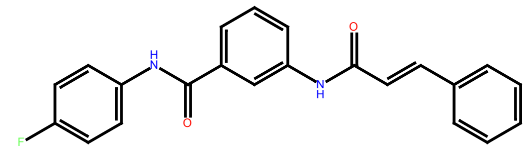

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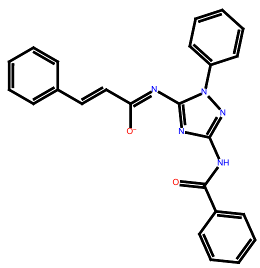

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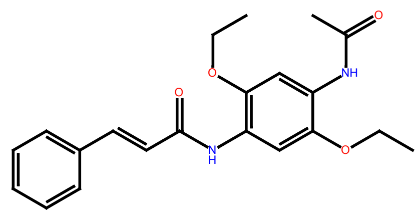

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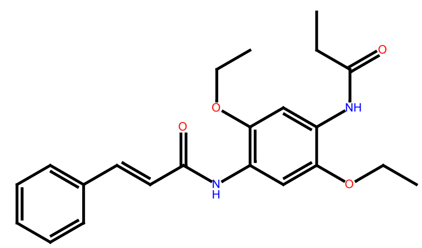

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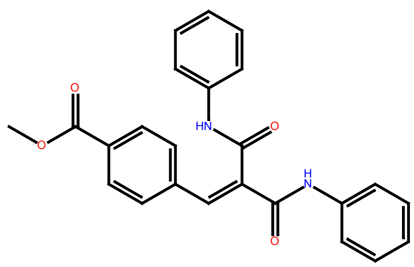

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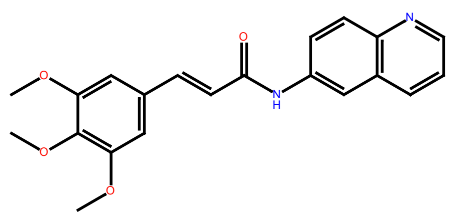

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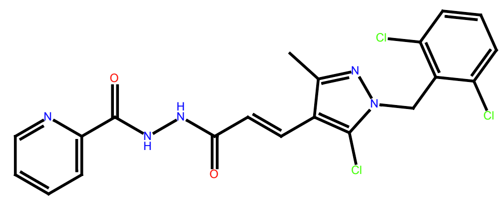

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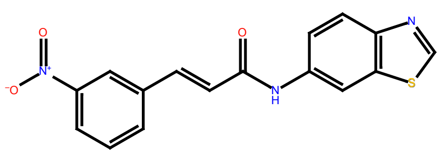

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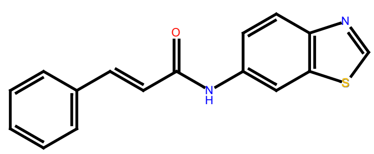

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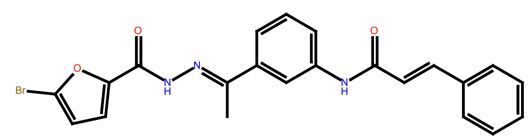

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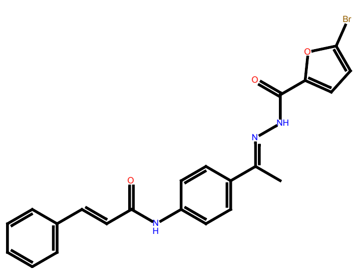

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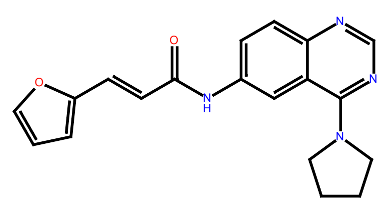

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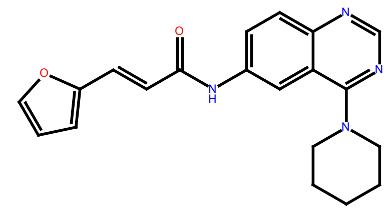

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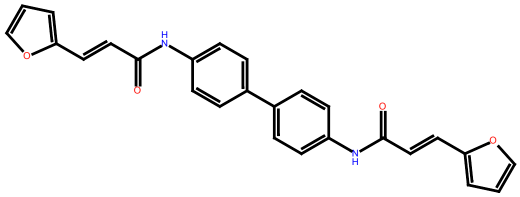

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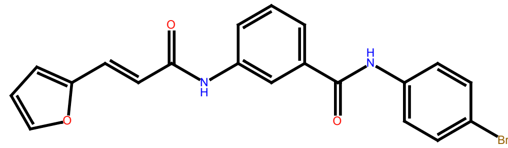

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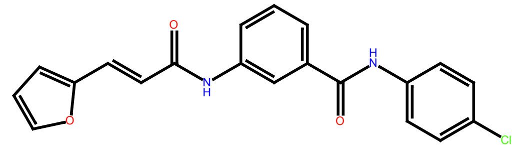

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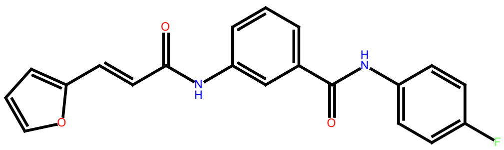

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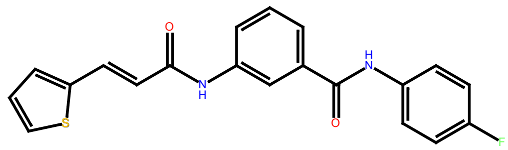

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