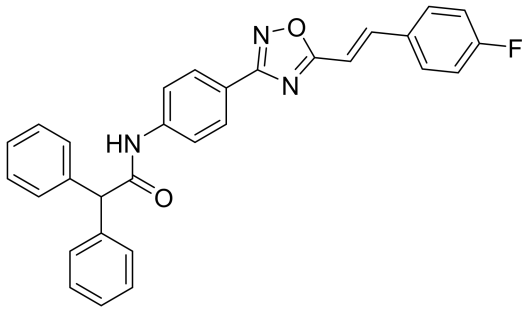
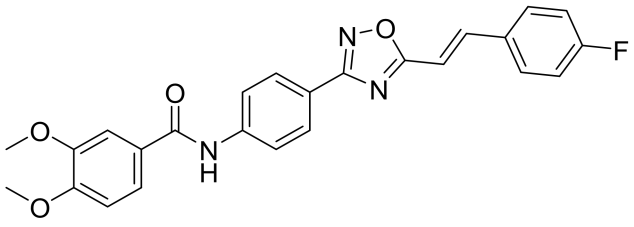
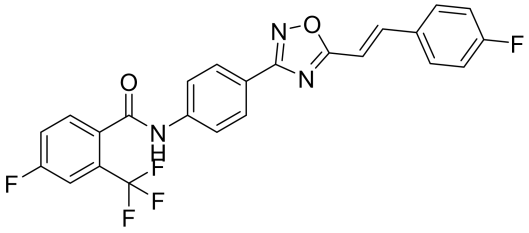


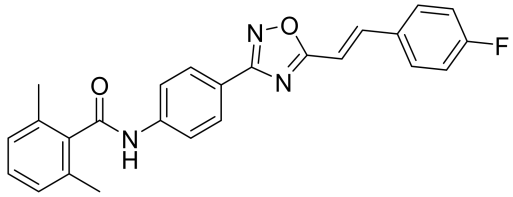
PS-001



PS-002



PS-003



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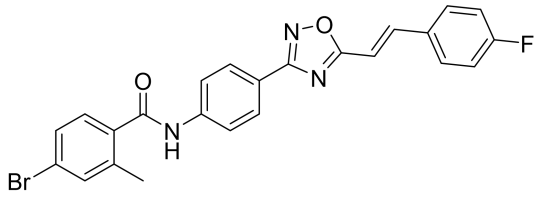
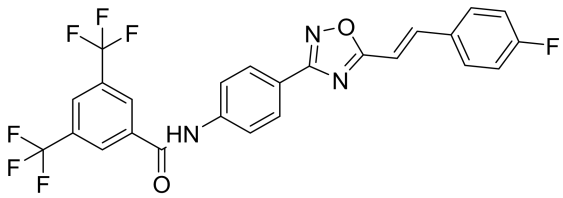


PS-005



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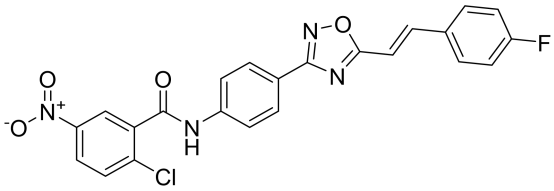

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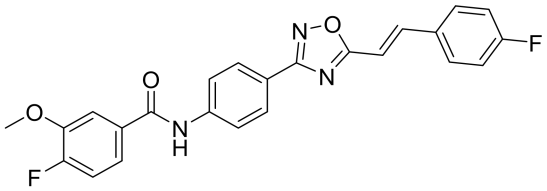
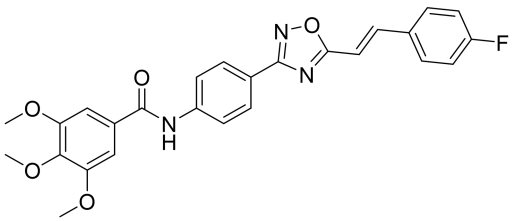


PS-008



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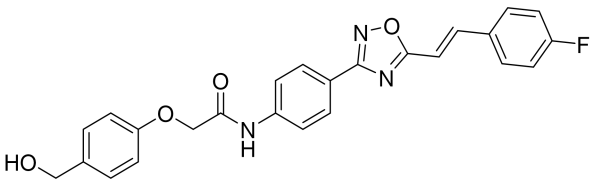

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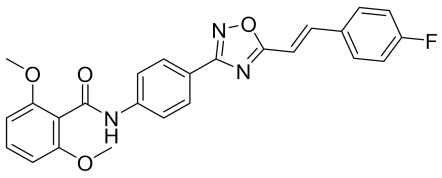
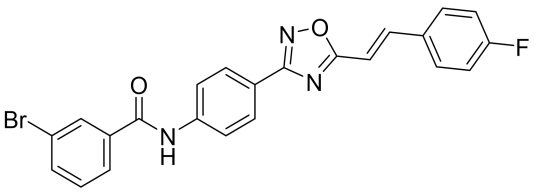
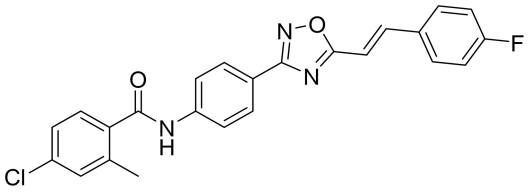


PS-011



PS-012



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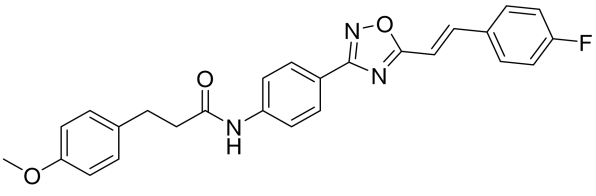

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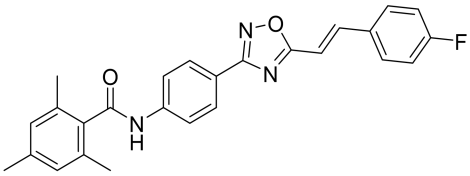

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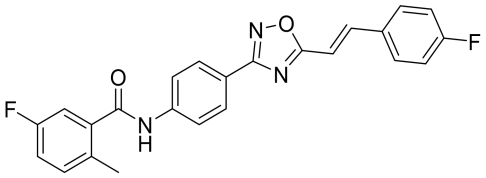

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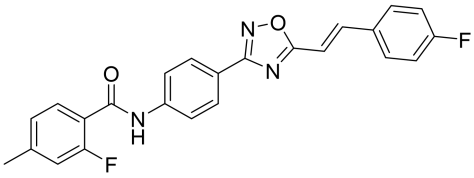

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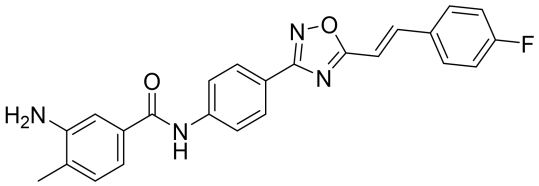

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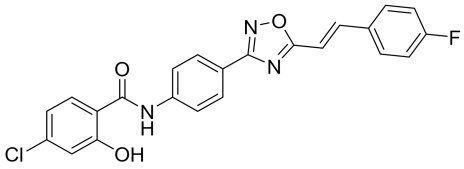

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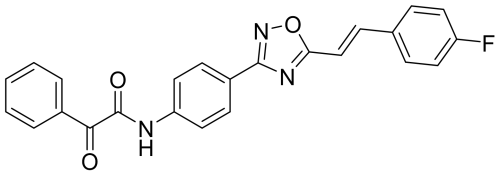

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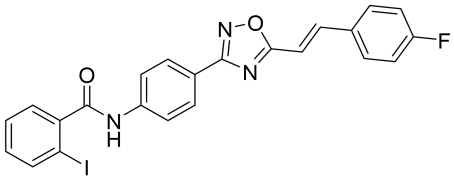
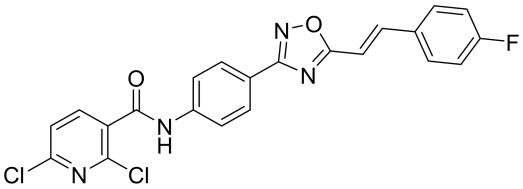


PS-021



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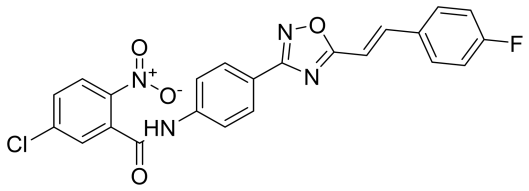

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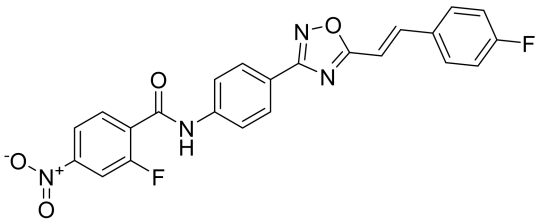

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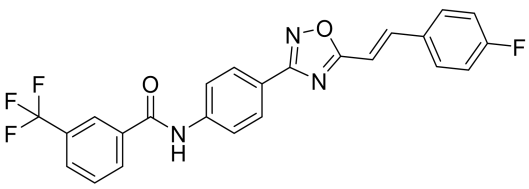

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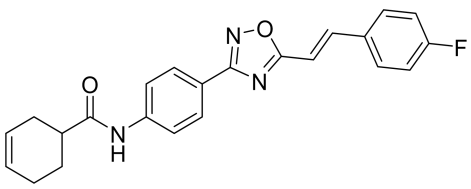

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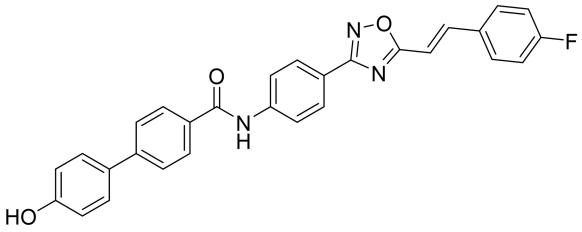

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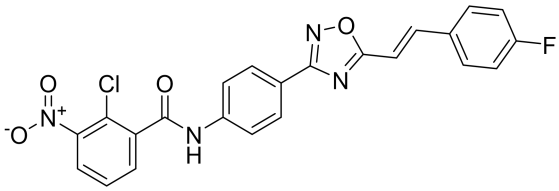

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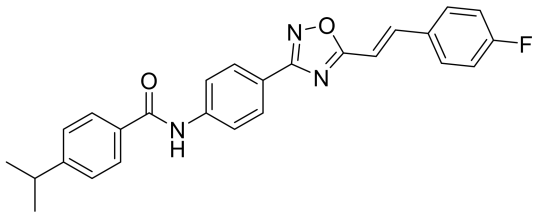

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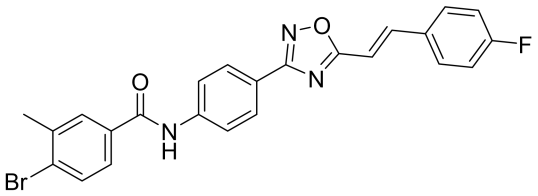

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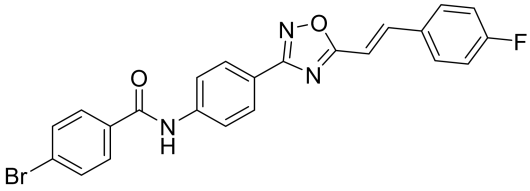

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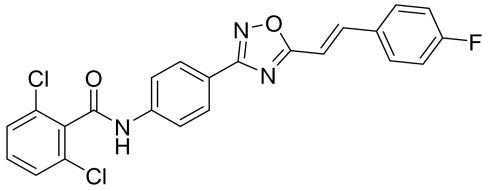
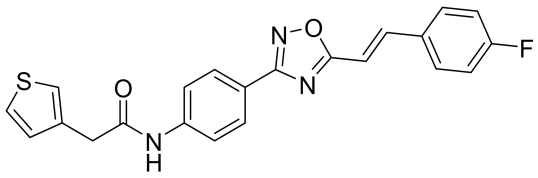


PS-032



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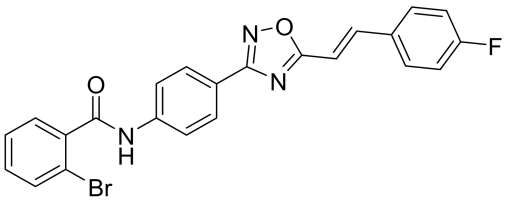

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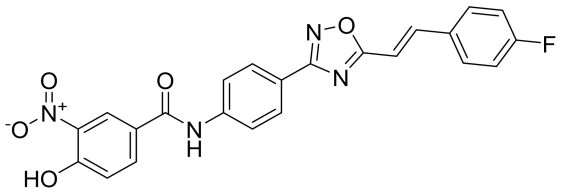
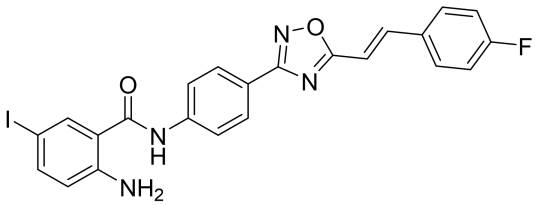
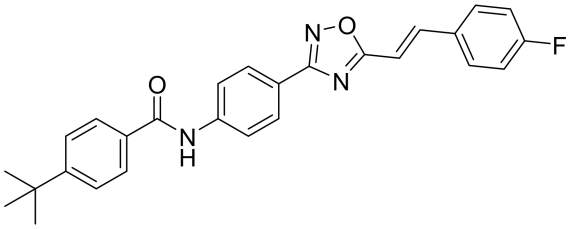


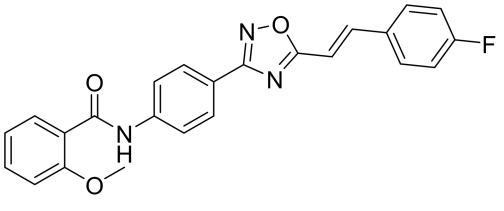
PS-035



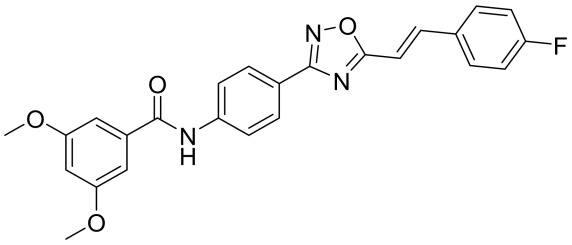
PS-036



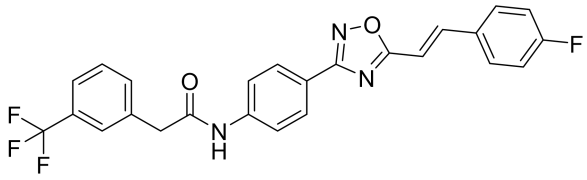
PS-037



PS-038



PS-039



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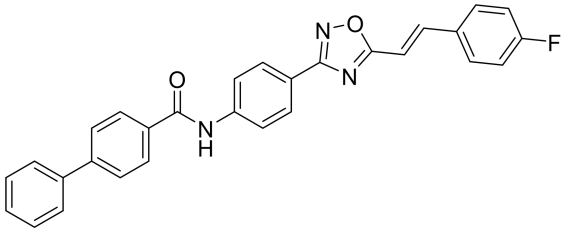
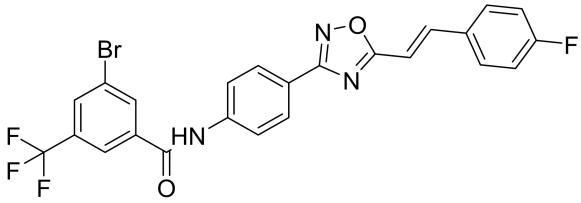
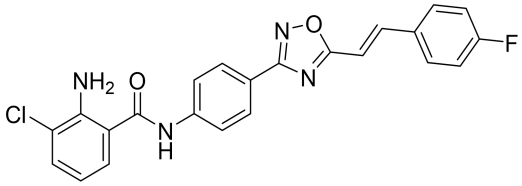


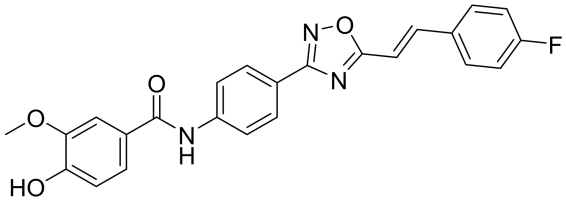
PS-041



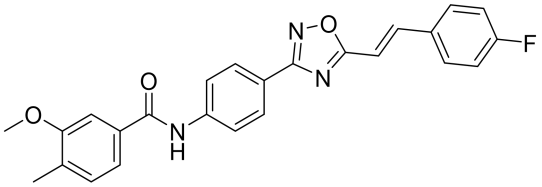
PS-042



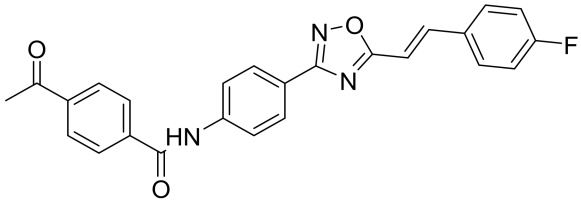
PS-043



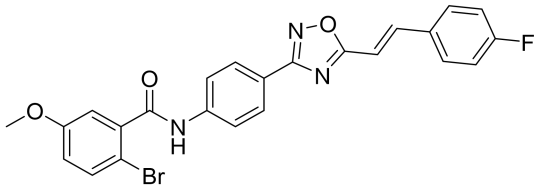
PS-044



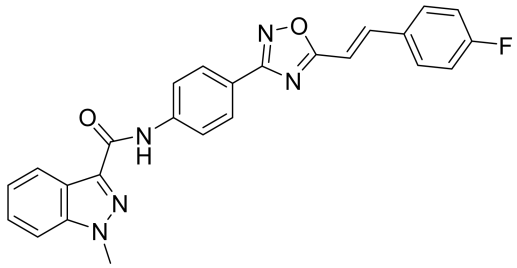
PS-045



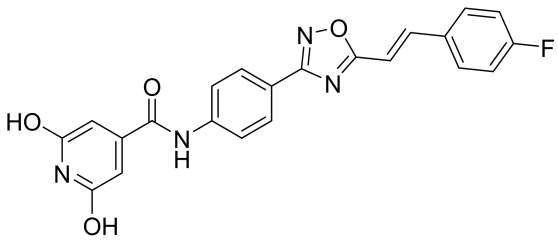
PS-046



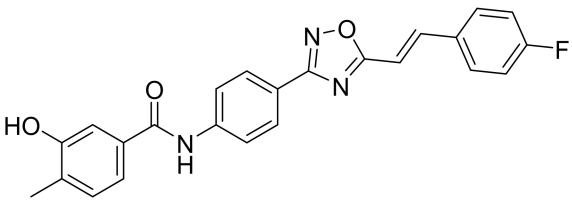
PS-047



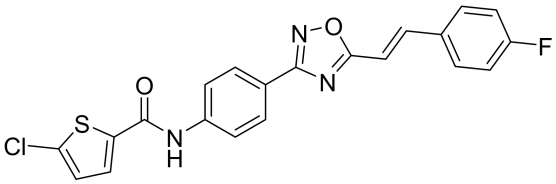
PS-048



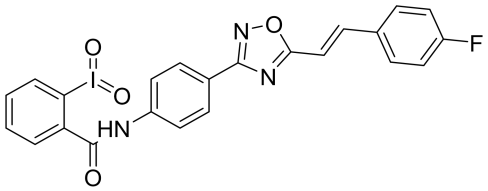
PS-049



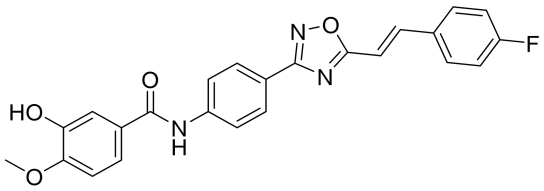
PS-050



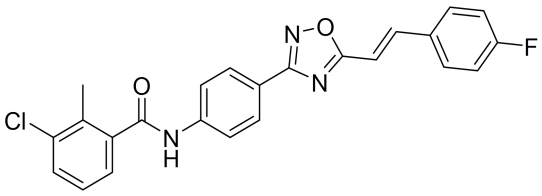
PS-051



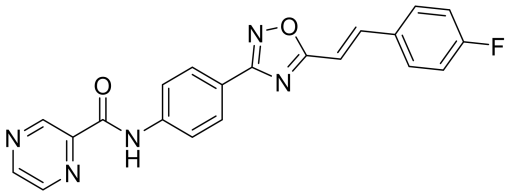
PS-052



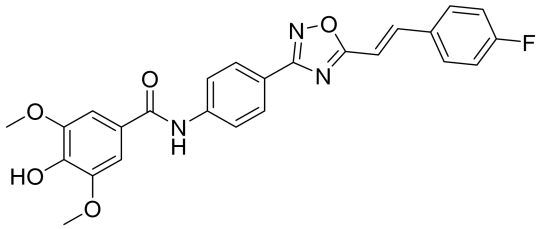
PS-053



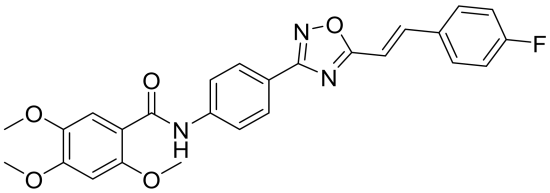
PS-054



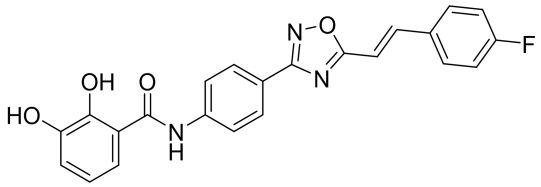
PS-055



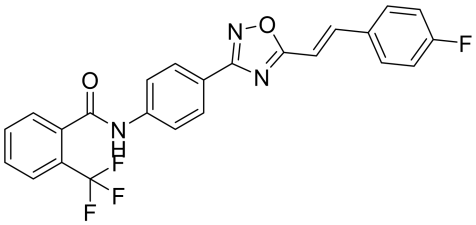
PS-056



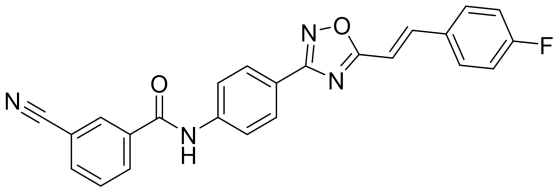
PS-057



PS-058



PS-059



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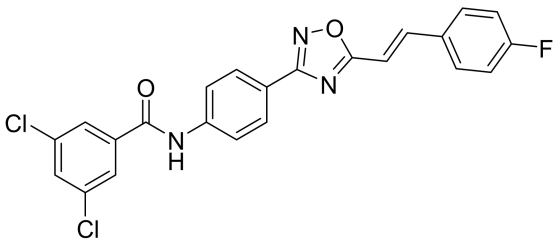

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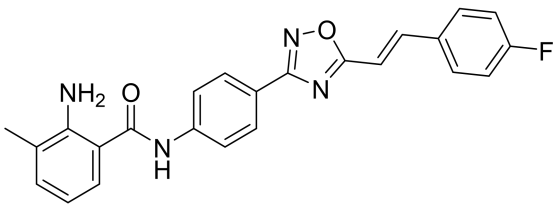

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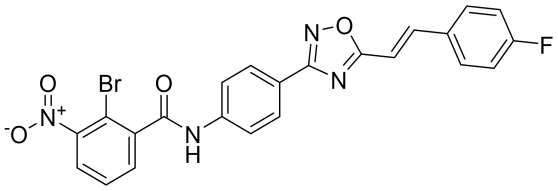

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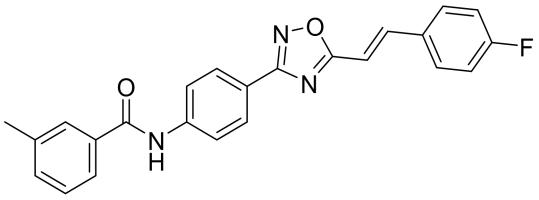

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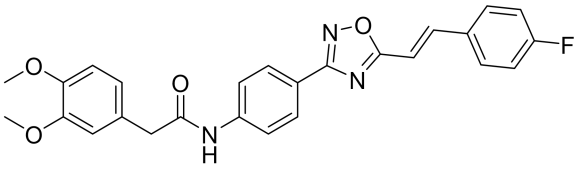

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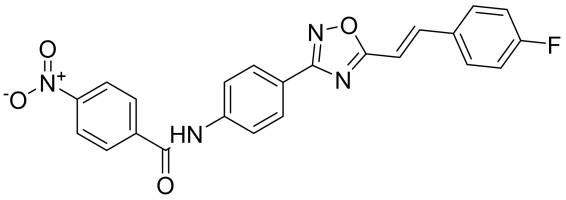

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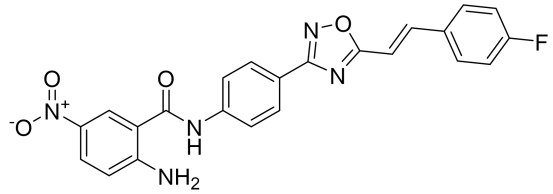

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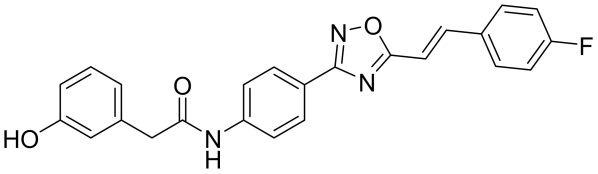

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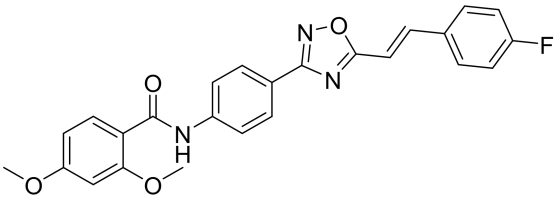

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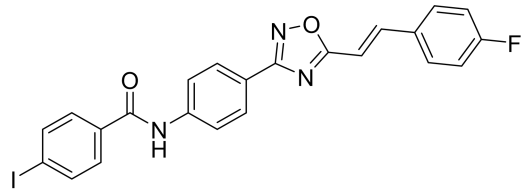

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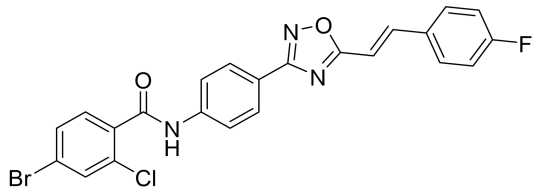

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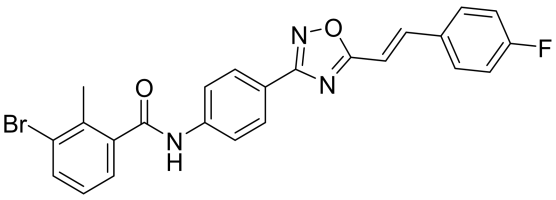

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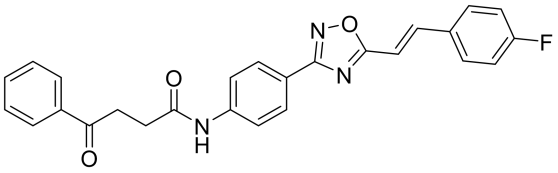

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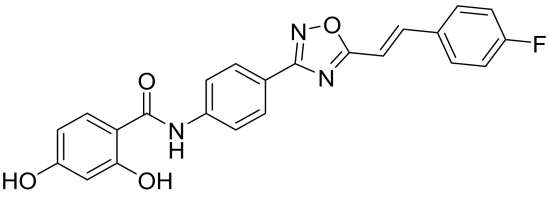

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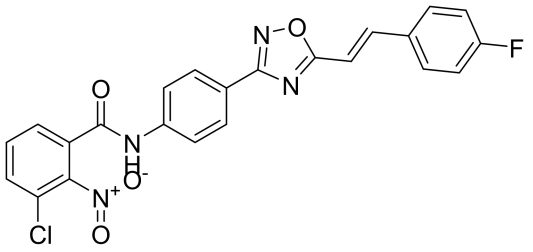

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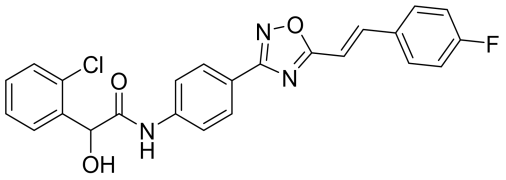

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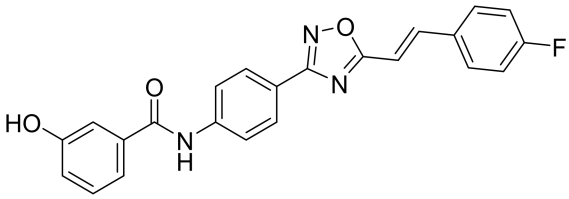

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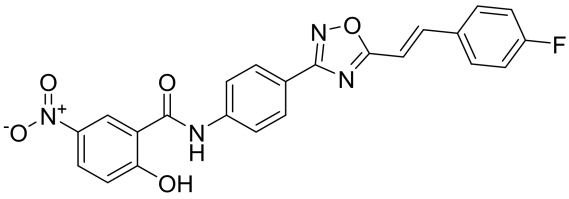

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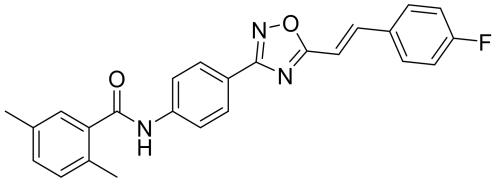

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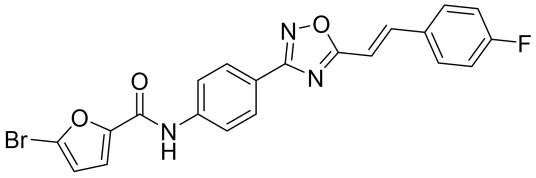

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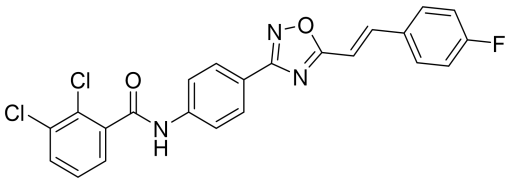

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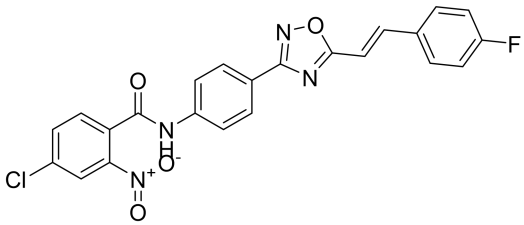

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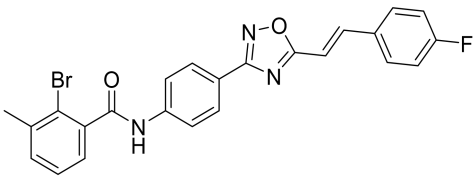

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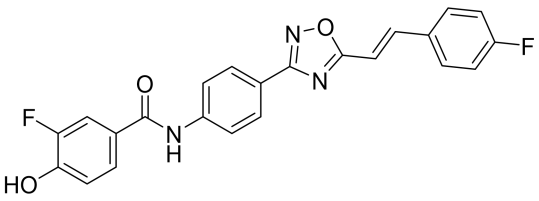

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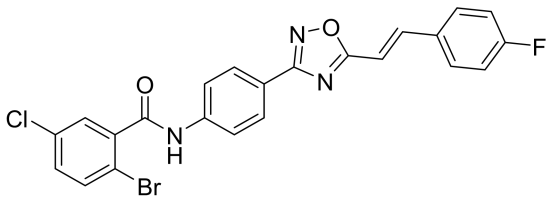

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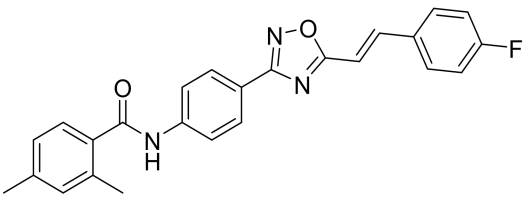

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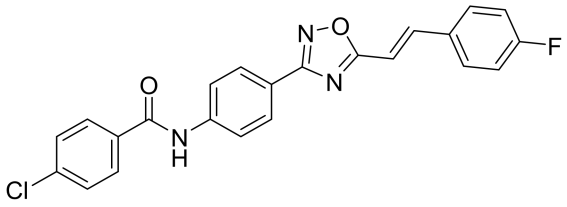

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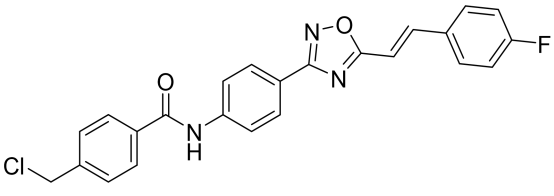

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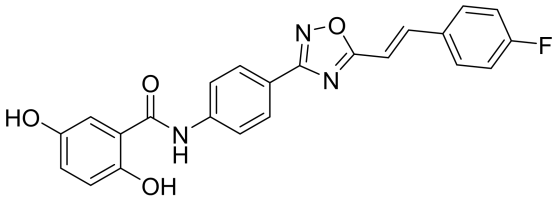

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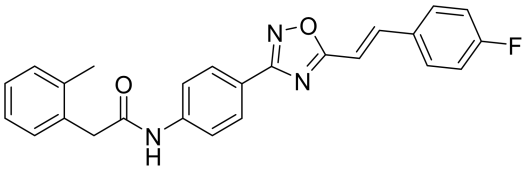

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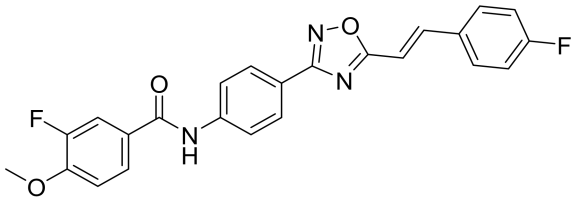

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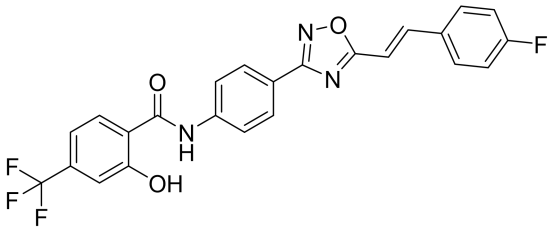

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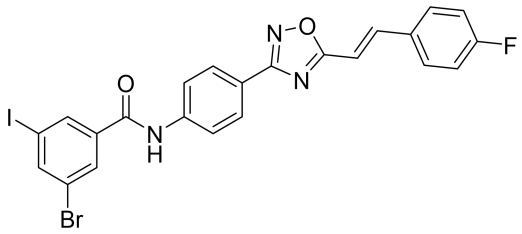

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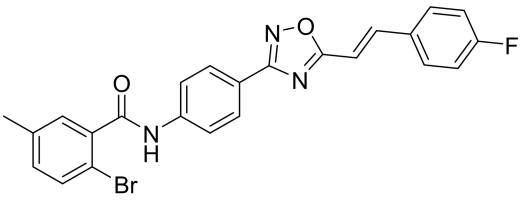

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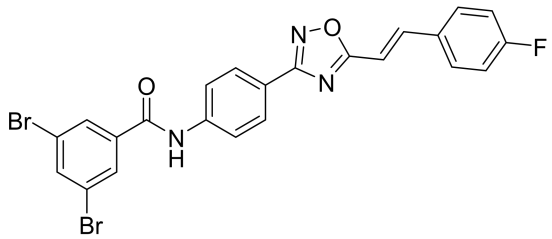

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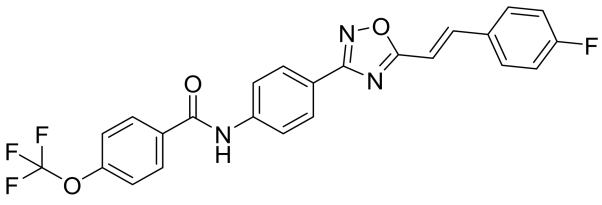

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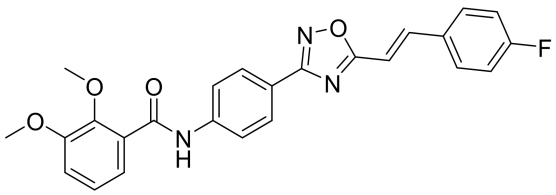

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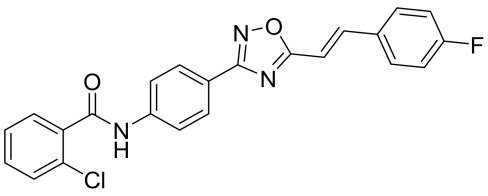

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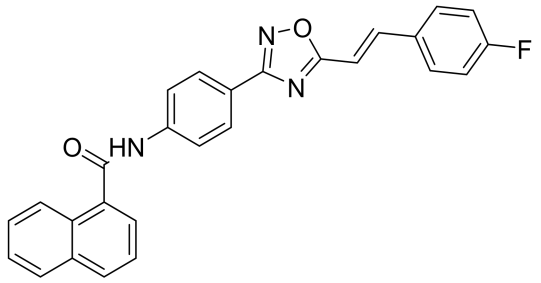

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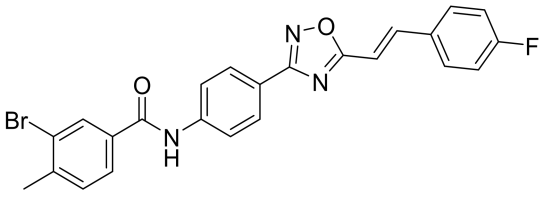

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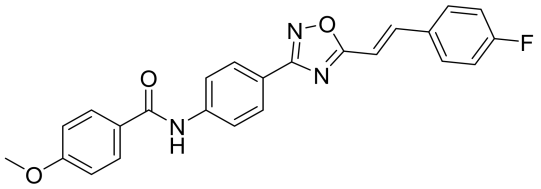

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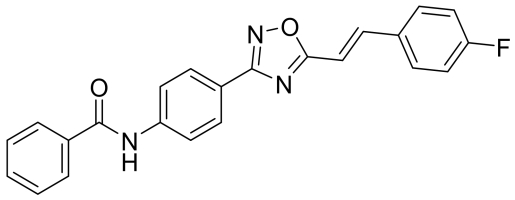

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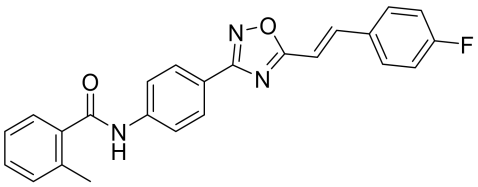

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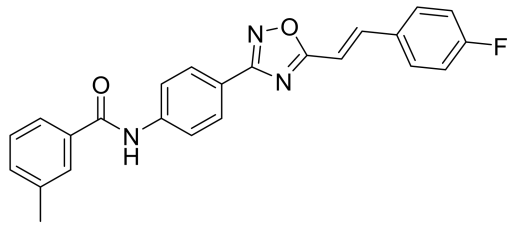

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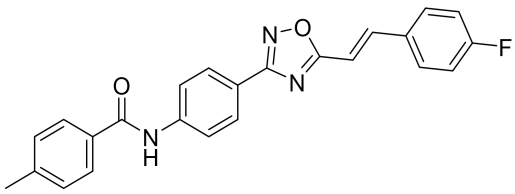

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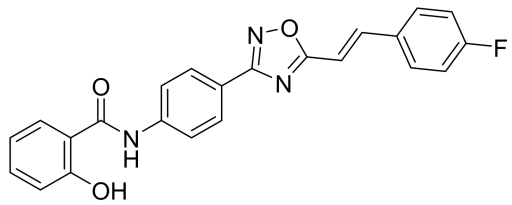

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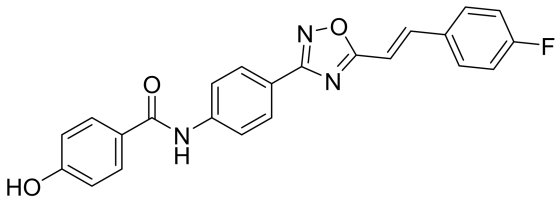

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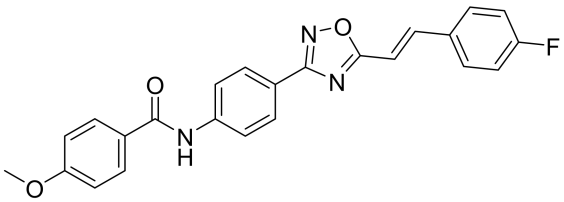

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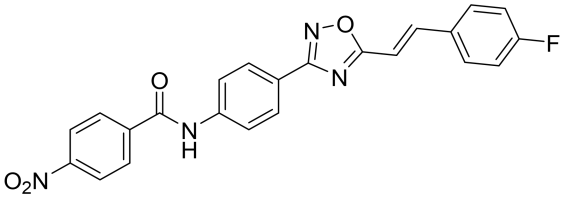

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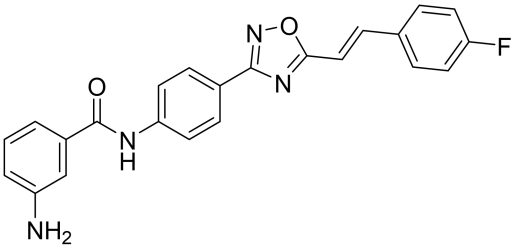

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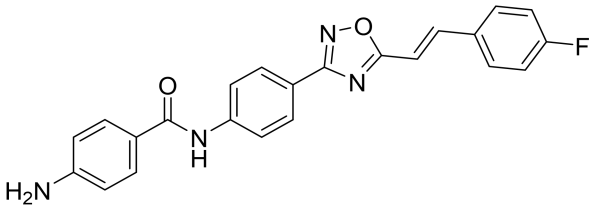

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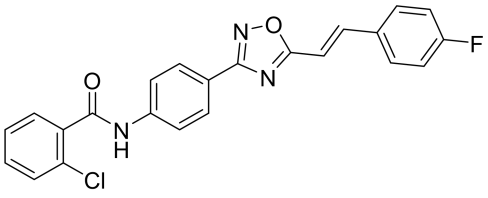

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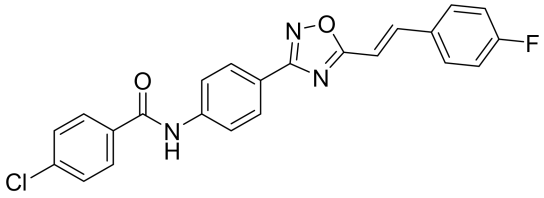

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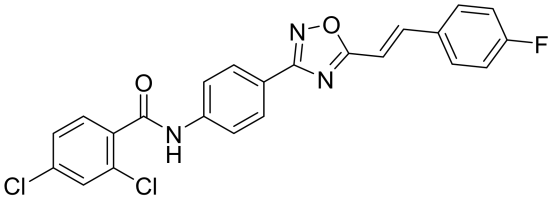

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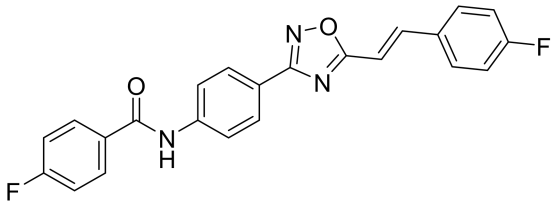

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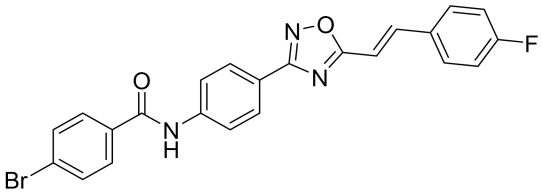

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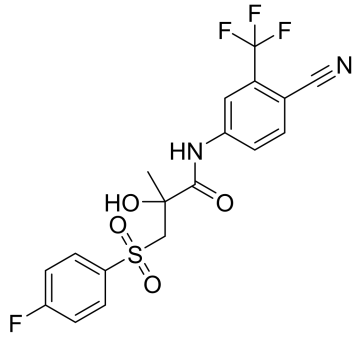


Bicalutamide

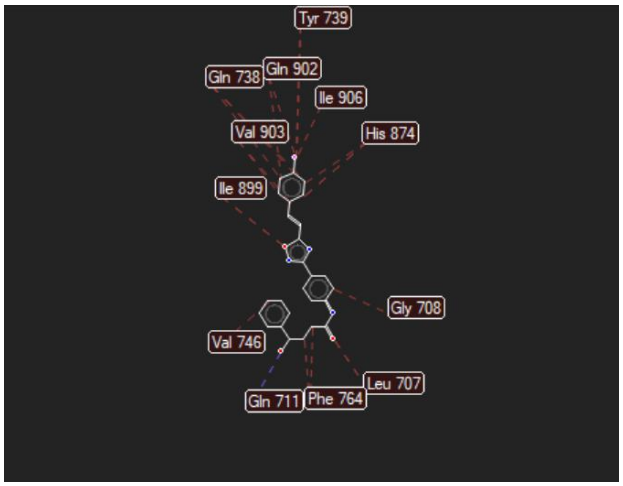
Figure S1. Properly rendered 2D chemical structures of the designed PS analogue series (PS-001 to PS-116) developed through structural modification of the 1,2,4-oxadiazole scaffold for androgen receptor inhibition.

Table S1. Molecular, drug likeness properties, MolDock docking scores of designed PS analogs and bicalutamide in androgen receptor binding site

Comp Code	MW	MolDock Score	log P	RB	HBA	HBD	Interactions
Bicalutamide	430.37	-131.19	2.88	5	5	2	Hydrogen bonds: Asn 705; Steric interactions: Phe 764
PS-002	445.44	-125.89	5.32	7	6	1	Hydrogen Bonds: Leu 704 Steric Interactions: Val 903, Gln 738, Val 746, Met 787, Met 745, Leu 707, Leu 704, Met 749
PS-004	413.44	-126.35	5.92	5	1	4	Steric Interactions: Gln 738, Ile 906, Tyr 739, Val 903, Met 745, Leu 704, Leu 707, Phe 764
PS-008	433.41	-142.80	5.45	6	5	1	Steric Interactions: Ile 898, Gln 738, Val 903, Leu 704, Met 787, Val 746, Gly 708, Met 745, Leu 707, Phe 764
PS-014	443.47	-143.92	5.63	8	5	1	Steric interactions: Val 903, Ile 898, Gln 738, Met 745, Leu 704, Met 742, Met 749, Phe 764, Arg 752
PS-016	417.41	-128.48	5.75	5	4	1	Hydrogen bonds: Leu 704 Steric interactions: Gln 738, Val 903, Met 745, Leu 704, Phe 764, Leu 873, Leu 707
PS-025	453.39	-128.37	6.32	5	4	1	Hydrogen bonds: Thr 877, Leu 704 Steric interactions: Gln 738, Val 903, Met 745, Leu 707, Thr 877, Leu 704
PS-031	464.29	-125.58	6.06	5	4	1	Steric interactions: Gln 738, Val 903, Leu 704, Val 746, Met 787, Met 745, Leu 707, Gly 708, Phe 764
PS-035	446.39	-129.28	4.91	6	7	2	Steric interactions: Val 903, Gln 738, Leu 704, Val 746, Met 787, Met 745, Gln 711, Phe 764
PS-036	526.30	-140.04	5.49	5	5	2	Hydrogen bonds: Met 745 Steric interactions: Val 903, Met 745, Gly 708, Leu 707, Phe 764, Gly 738
PS-042	532.28	-145.66	7.08	5	4	1	Steric interactions: Val 903, Gln 711, Met 742, Arg 752, Met 745, Val 746, Gly 708, Leu 704, Leu 707, Gln 738
PS-044	431.42	-128.58	5.01	6	6	2	Steric interactions: Leu 704, Val 746, Met 745, Phe 764, Gln 738, Val 903, Gln 711
PS-045	429.44	-125.37	5.62	6	5	1	Steric interactions: Gln 738, Val 903, Leu 704, Val 746, Met 787, Met 745, Gln 711, Phe 764
PS-047	494.31	-133.49	6.07	6	5	1	Steric interactions: Val 903, Ile 898, Met 745, Leu 704, Leu 873, Leu 707, Gln 738
PS-048	439.44	-135.24	5.19	5	6	1	Steric interactions: Gln 738, Val 903, Ile 898, Met 895, Val 746, Phe 764, Leu 704, Thr 877
PS-049	418.38	-142.71	4.10	5	7	3	Hydrogen bonds: Met 745, Gln 711, Arg 752 Steric interactions: Val 903, Met 745, Leu 707, Leu 704, Gly 708, Gln 738,
PS-050	415.42	-134.35	5.31	5	5	2	Steric interactions: Val 903, Leu 704, Met 745, Val 746, Met 787, Gly 708, Leu 707, Phe 764, Gln 738
PS-051	425.86	-126.24	6.01	5	5	1	Steric interactions: Gln 738, Val 903, Leu 707, Met 745
PS-052	425.86	-126.24	5.67	6	6	1	Hydrogen bonds: Leu 704 Steric interactions: Gln 738, Val 903, Leu 704, Leu 707, Val 746, Met 787, Met 745, His 874
PS-055	387.37	-127.80	4.09	5	6	1	Steric interactions: Val 903, Ile 898, Gln 738, Met 745, Gly 708, Leu 707, Phe 764
PS-057	475.47	-132.74	5.32	8	7	1	Hydrogen bonds: Leu 704 Steric interactions: Val 903, Ile 899, Gln 738, Met 745, Gln 711, Val 746, Met 787, Leu 704, Leu 707
PS-060	410.40	-140.03	5.17	5	5	1	Steric interactions: Val 903, Ile 898, Met 749, Met 742, Met 745, Gly 708, Leu 707, Phe 764
PS-064	399.42	-140.93	5.61	5	4	1	Steric interactions: Val 903, Ile 898, Met 742, Met 749, Met 745, Gly 708, Leu 707, Phe 764
PS-067	445.40	-137.98	4.79	6	7	2	Hydrogen bonds: Met 745 Steric interactions: Gln 738, Val 903, Leu 704, Met 745, Leu 707
PS-073	441.45	-155.84	5.65	8	5	1	Hydrogen bonds: Gln 711 Steric interactions: Tyr 739, Gln 738, Ile 906, Gln 902, Val 903, His 874, Ile 899, Val 746, Phe 764, Leu 707, Gly 708

Continued.

PS-077	401.39	-142.39	5.00	5	5	2	Hydrogen bonds: Met 742 Steric interactions: Gln 738, Val 903, Met 742, Met 745, Gly 708, Leu 707, Phe 764
PS-079	413.44	-128.02	5.92	5	4	1	Hydrogen bonds: Leu 704 Steric interactions: Val 903, Gln 738, Met 745, Tyr 739, Leu 707, Gln 711, Leu 704
PS-085	498.73	-129.70	6.71	5	4	1	Steric interactions: Val 903, Ile 898, Met 745, Gly 738, Leu 707, Leu704, Ile 906
PS-087	419.84	-127.31	5.95	5	4	1	Steric interactions: Gln 738, Val 903, Leu 704, Leu 707, Val 746, Met 787, Met 745, Gly 708, Phe 764
PS-088	433.86	-125.33	6.04	6	4	1	Steric interactions: Gln 738, Val 903, Val 746, Met 787, Met 749, Gly 708, Met 745, Leu 704, Leu 707
PS-089	417.39	-126.21	4.71	5	6	3	Hydrogen bonds: Met 745, Gln 711, Arg 752 Steric interactions: His 874, Gln 738, Val 903, Leu 707, Met 745, Gln 711
PS-095	543.18	-127.47	6.82	5	4	1	Steric interactions: Gln 738, Val 903, Gln 711, Met 745, Gly 708, Leu 707, Leu 704
PS-098	419.84	-127.91	5.95	5	4	1	Hydrogen bonds: Leu 704 Steric interactions: Gln 738, Gln 902, Val 903, Ile 898, Tyr 739, His 874, Met 745, Leu 707, Leu 704
PS-100	478.31	-134.21	6.37	5	4	1	Steric interactions: Gln 738, Val 903, Leu 704, Met 787, Met 745, Val 746, Gly 708, Leu 707, Phe 764
PS-104	399.42	-140.39	5.61	5	4	1	Steric interactions: Val 903, Ile 898, Met 749, Met 742, Met 745, Gly 708, Leu 707, Phe 764
PS-105	399.42	-128.56	5.61	5	4	1	Steric interactions: Leu 704, Val 746, Met 745, Phe 764, Gln 738, Val 903, Gln 711, Leu 707
PS-110	400.41	-142.31	4.88	5	5	2	Hydrogen bonds: Met 742 Steric interactions: Gln 738, Ile 898, Val 903, Val 746, Met 745, Gly 708, Leu 707, Phe 764
PS-113	419.84	-127.16	5.95	5	4	1	Steric interactions: Gln 738, Val 903, Leu 704, Leu 707, Val 746, Met 787, Met 745, Gly708, Phe 764
PS-116	464.29	-125.46	6.06	5	4	1	Steric interactions: Gln 738, Val 903, Leu 704, Leu 707, Val 746, Met 787, Met 745, Gln 708, Phe 764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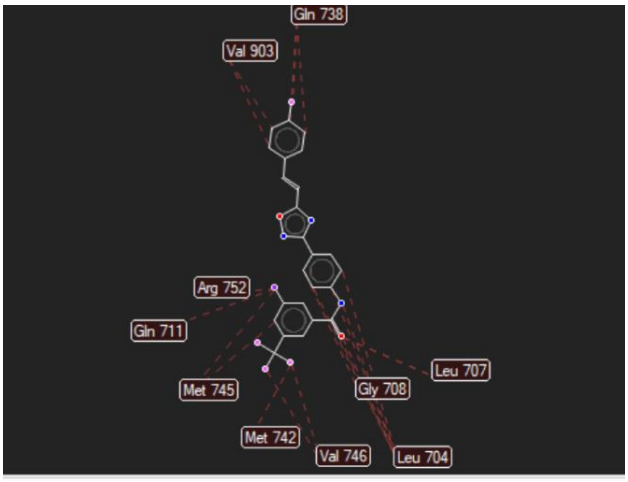
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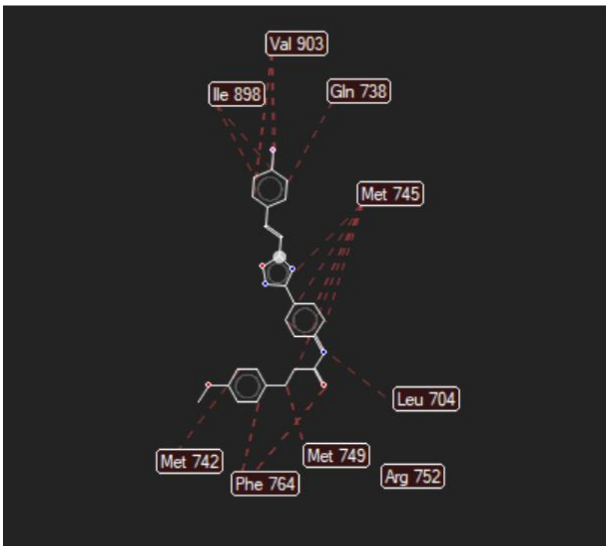
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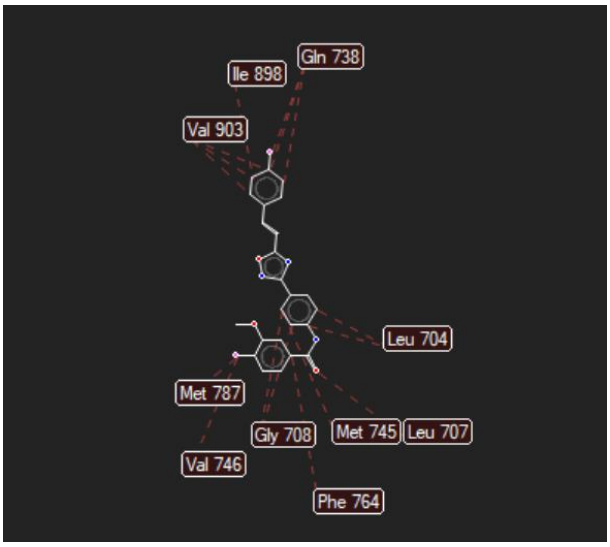
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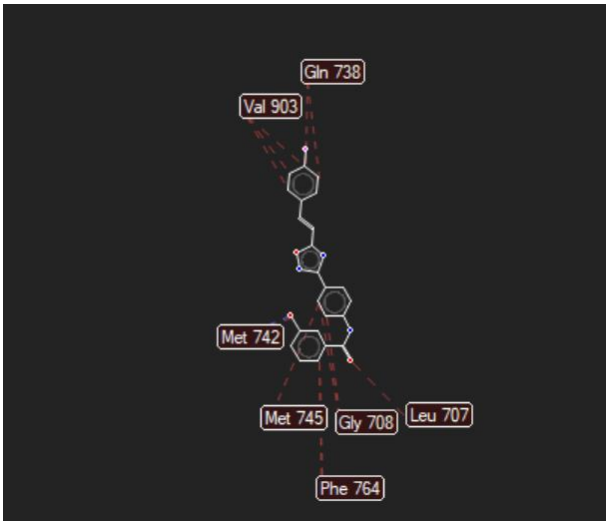
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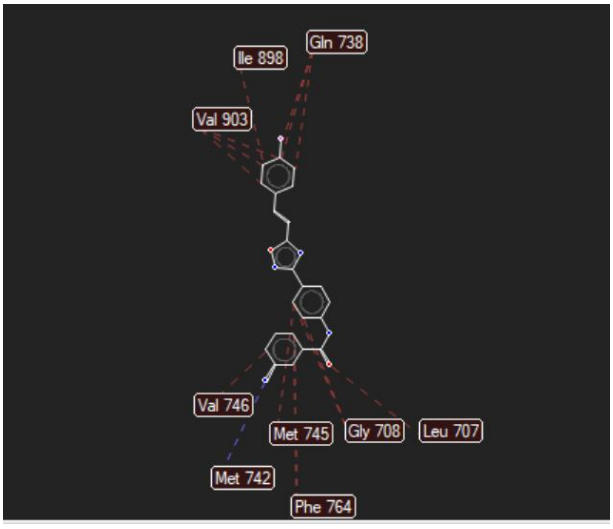
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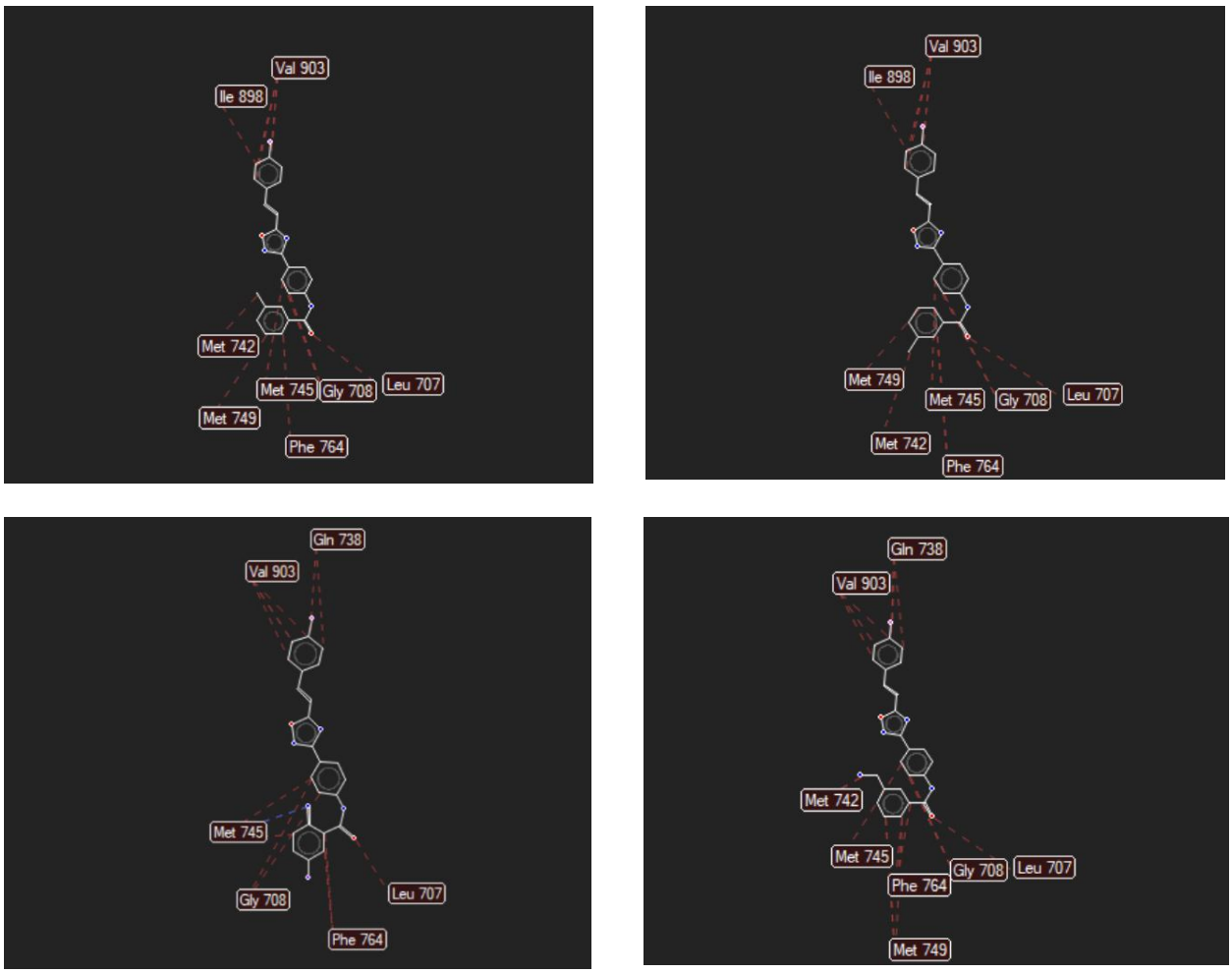

Figure S2. 2D interaction diagrams of representative PS analogues within the androgen receptor ligand-binding pocket highlighting hydrogen bonding, hydrophobic interactions, van der Waals contacts, and key interacting residues including Met745, Gln738, Leu704, Val903, and Gln711.