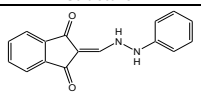
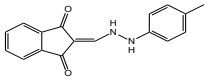
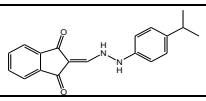
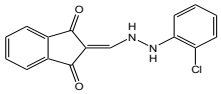
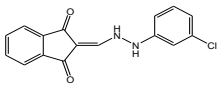
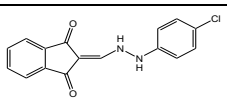
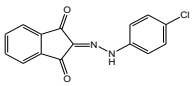
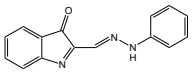
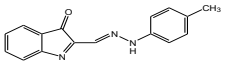
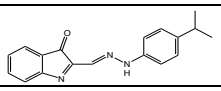
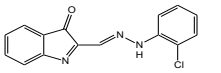
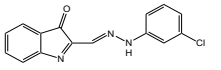
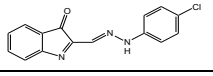
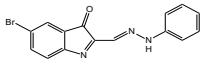
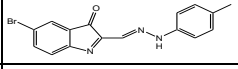
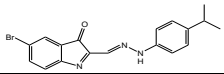
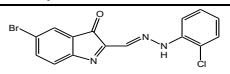
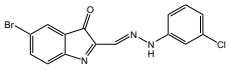
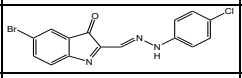
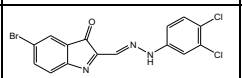
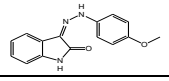
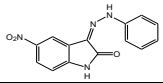
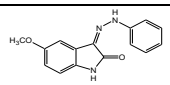
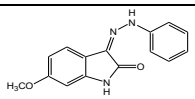
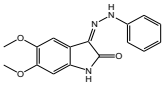
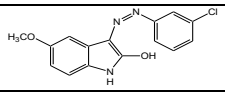
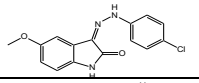
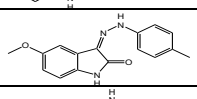
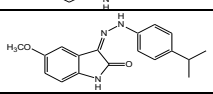
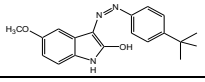
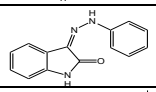
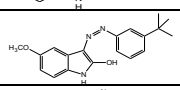
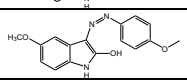
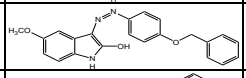
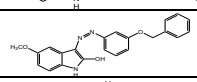
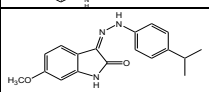
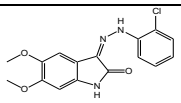
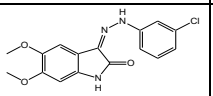
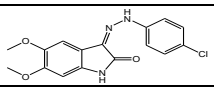
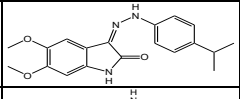
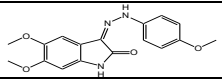
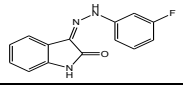
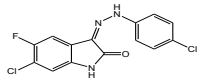
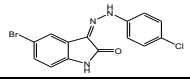
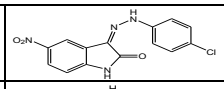
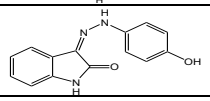
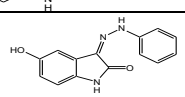
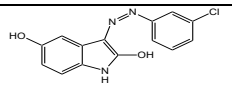
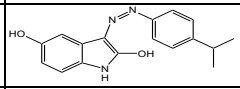
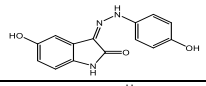
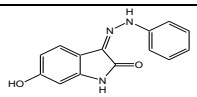
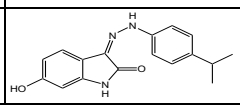
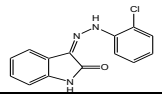
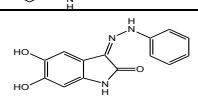
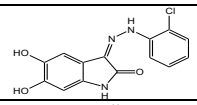
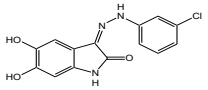
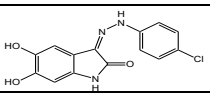
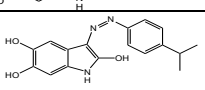
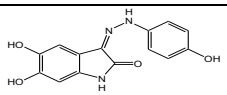
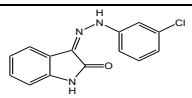
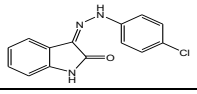
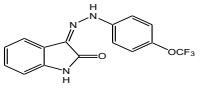
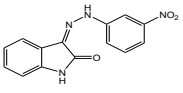
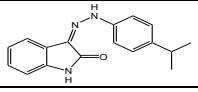
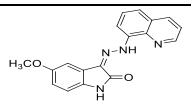
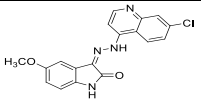
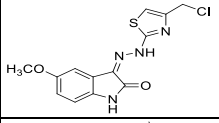
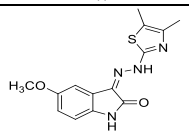
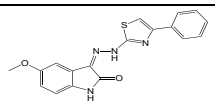
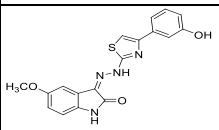
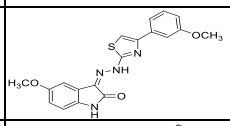
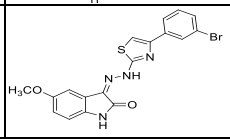
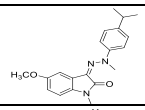
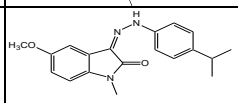
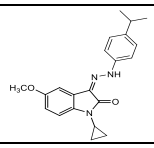
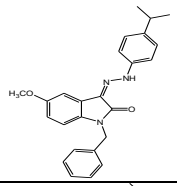
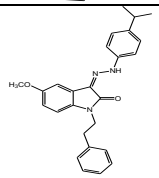
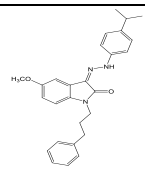
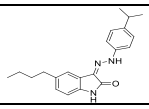
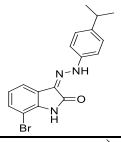
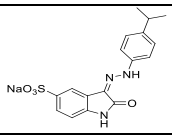
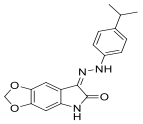
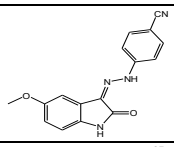
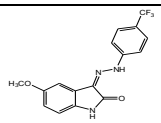
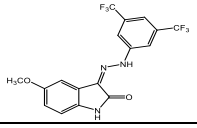
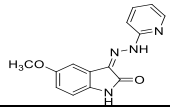
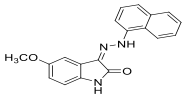
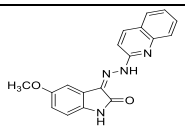
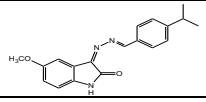
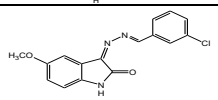
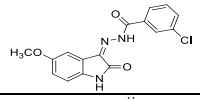
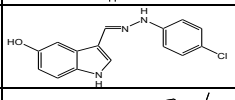
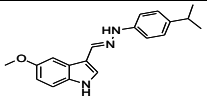
Code	Structure	SMILES	% inhib. @ 100 μM	IC_{50} (μM)	ref.	core structure
S1		O=C(C1=CC=CC=C1C/2=O)C2=C/NNC3=CC=CC=C3	49±2.0		15	Indandione
S2		O=C(C1=CC=CC=C1C/2=O)C2=C/NNC3=CC=C(C)C=C3	44±4.0		15	
S3		O=C(C1=CC=CC=C1C/2=O)C2=C/NNC3=CC=C(C(C)C)C=C3		**18**	15	
S4		O=C(C1=CC=CC=C1C/2=O)C2=C/NNC3=CC=CC=C3Cl		**32**	15	
S5		O=C(C1=CC=CC=C1C/2=O)C2=C/NNC3=CC=CC(Cl)=C3		**18**	15	
S6		O=C(C1=CC=CC=C1C/2=O)C2=C/NNC3=CC=C(Cl)C=C3		**23**	15	
S7		O=C(C1=CC=CC=C1C/2=O)C2=N\NC3=CC=C(Cl)C=C3	38±5.3		15	
S8		O=C1C(/C=N/NC2=CC=CC=C2)=NC3=CC=CC=C31		**8,8**	15	3-indolinone
S9		O=C1C(/C=N/NC2=CC=C(C)C=C2)=NC3=CC=CC=C31		**3,6**	15	
S10		O=C1C(/C=N/NC2=CC=C(C(C)C)C=C2)=NC3=CC=CC=C31		**1,4**	15	
S11		O=C1C(/C=N/NC2=CC=CC=C2Cl)=NC3=CC=CC=C31		**13**	15	
S12		O=C1C(/C=N/NC2=CC=CC(Cl)=C2)=NC3=CC=CC=C31		**2,5**	15	
S13		O=C1C(/C=N/NC2=CC=C(Cl)C=C2)=NC3=CC=CC=C31	33±1.0		15	
S14		O=C1C(/C=N/NC2=CC=CC=C2)=NC3=CC=C(Br)C=C31		**35**	15	
S15		O=C1C(/C=N/NC2=CC=C(C)C=C2)=NC3=CC=C(Br)C=C31		**51**	15	
S16		O=C1C(/C=N/NC2=CC=C(C(C)C)C=C2)=NC3=CC=C(Br)C=C31		**23**	15	
S17		O=C1C(/C=N/NC2=CC=CC=C2Cl)=NC3=CC=C(Br)C=C31		**7,8**	15	
S18		O=C1C(/C=N/NC2=CC=CC(Cl)=C2)=NC3=CC=C(Br)C=C31		**4,4**	15	
S19		O=C1C(/C=N/NC2=CC=C(Cl)C=C2)=NC3=CC=C(Br)C=C31	46±7.0		15	
S20		O=C1C(/C=N/NC2=CC=C(Cl)C(Cl)=C2)=NC3=CC=C(Br)C=C31	23±2.3		15	
S21		O=C1NC2=CC=CC=C2/C1=N/NC3=CC=C(OC)C=C3		**13**	16	
S22		O=C1NC2=CC=C([N+]([O-])=O)C=C2/C1=N/NC3=CC=CC=C3	-2±7		16	

S23		O=C1NC2=CC=C(OC)C=C2/C1=N/NC3=CC=CC=C3	52±8		16
S24		O=C1NC2=CC(OC)=CC=C2/C1=N/NC3=CC=CC=C3		**5,8**	16
S25		O=C1NC2=CC(OC)=C(OC)C=C2/C1=N/NC3=CC=CC=C3		**63**	16
S26		O=C1NC2=CC=C(OC)C=C2/C1=N/NC3=CC(Cl)=CC=C3	*72±1*		16
S27		O=C1NC2=CC=C(OC)C=C2/C1=N/NC3=CC=C(Cl)C=C3	43±2		16
S28		O=C1NC2=CC=C(OC)C=C2/C1=N/NC3=CC=C(C)C=C3	29±4		16
S29		O=C1NC2=CC=C(OC)C=C2/C1=N/NC3=CC=C(C(C)C)C=C3		**0,43**	16
S30		O=C1NC2=CC=C(OC)C=C2/C1=N/NC3=CC=C(C(C)(C)C)C=C3	*66±4*	**15**	16
S31		O=C1NC2=CC=CC=C2/C1=N/NC3=CC=CC=C3	(I) 36±2.2 (II) 61±0.7		16
S32		O=C1NC2=CC=C(OC)C=C2/C1=N/NC3=CC(C(C)(C)C)=CC=C3	56±2		16
S33		O=C1NC2=CC=C(OC)C=C2/C1=N/NC3=CC=C(OC)C=C3		**3,7**	16
S34		O=C1NC2=CC=C(OC)C=C2/C1=N/NC3=CC=C(OCC4=CC=CC=C4)C=C3	20±1		16
S35		O=C1NC2=CC=C(OC)C=C2/C1=N/NC3=CC=CC(OCC4=CC=CC=C4)=C3	44±4 (I)		16
S36		O=C1NC2=CC(OC)=CC=C2/C1=N/NC3=CC=C(C(C)C)C=C3		**7,1**	16
S37		O=C1NC2=CC(OC)=C(OC)C=C2/C1=N/NC3=C(Cl)C=CC=C3	*70±3*		16
S38		O=C1NC2=CC(OC)=C(OC)C=C2/C1=N/NC3=CC(Cl)=CC=C3		**17**	16
S39		O=C1NC2=CC(OC)=C(OC)C=C2/C1=N/NC3=CC=C(Cl)C=C3		**33**	16
S40		O=C1NC2=CC(OC)=C(OC)C=C2/C1=N/NC3=CC=C(C(C)C)C=C3		**4,4**	16
S41		O=C1NC2=CC(OC)=C(OC)C=C2/C1=N/NC3=CC=C(OC)C=C3		**22**	16
S42		O=C1NC2=CC=CC=C2/C1=N/NC3=CC(F)=CC=C3	52±0.9		16
S43		O=C1NC2=CC(Cl)=C(F)C=C2/C1=N/NC3=CC=C(Cl)C=C3	28±3.7		16
S44		O=C1NC2=CC=C(Br)C=C2/C1=N/NC3=CC=C(Cl)C=C3	63±4		16

S45		O=C1NC2=CC=C([N+]([O-])=O)C=C2/C1=N/NC3=CC=C(Cl)C=C3	12±2		16	
S46		O=C1NC2=CC=CC=C2/C1=N/NC3=CC=C(O)C=C3		**9,3**	16	
S47		O=C1NC2=CC=C(O)C=C2/C1=N/NC3=CC=CC=C3	62±3		16	
S48		O=C1NC2=CC=C(O)C=C2/C1=N/NC3=CC(Cl)=CC=C3		**18**	16	
S49		O=C1NC2=CC=C(O)C=C2/C1=N/NC3=CC=C(C(C)C)C=C3		**21**	16	
S50		O=C1NC2=CC=C(O)C=C2/C1=N/NC3=CC=C(O)C=C3	61±2		16	
S51		O=C1NC2=CC(O)=CC=C2/C1=N/NC3=CC=CC=C3		**22**	16	
S52		O=C1NC2=CC(O)=CC=C2/C1=N/NC3=CC=C(C(C)C)C=C3		**6**	16	
S53		O=C1NC2=CC=CC=C2/C1=N/NC3=C(Cl)C=CC=C3	44±5		16	
S54		O=C1NC2=CC(O)=C(O)C=C2/C1=N/NC3=CC=CC=C3		**4,3**	16	
S55		O=C1NC2=CC(O)=C(O)C=C2/C1=N/NC3=C(Cl)C=CC=C3		**11**	16	
S56		O=C1NC2=CC(O)=C(O)C=C2/C1=N/NC3=CC(Cl)=CC=C3		**1,1**	16,18	
S57		O=C1NC2=CC(O)=C(O)C=C2/C1=N/NC3=CC=C(Cl)C=C3		**17**	16	
S58		O=C1NC2=CC(O)=C(O)C=C2/C1=N/NC3=CC=C(C(C)C)C=C3		**1,6**	16	
S59		O=C1NC2=CC(O)=C(O)C=C2/C1=N/NC3=CC=C(O)C=C3		**24**	16	
S60		O=C1NC2=CC=CC=C2/C1=N/NC3=CC(Cl)=CC=C3	39±5		16	Isatin 3-hydrazones
S61		O=C1NC2=CC=CC=C2/C1=N/NC3=CC=C(Cl)C=C3	24±4.9		16	
S62		O=C1NC2=CC=CC=C2/C1=N/NC3=CC=C(OC(F)(F)F)C=C3	57±3		16	
S63		O=C1NC2=CC=CC=C2/C1=N/NC3=CC([N+]([O-])=O)=CC=C3	29±1.2		16	
S64		O=C1NC2=CC=CC=C2/C1=N/NC3=CC=C(C(C)C)C=C3	64±4		16	

S65		O=C1NC2=CC=C(OC)C=C2/C1=N/NC3=C(N=CC=C4)C4=CC=C3	*58 ± 4 (SD)*		19
S66		O=C1NC2=CC=C(OC)C=C2/C1=N/NC3=C(C=CC(Cl)=C4)C4=NC=C3	*14 ± 12,5 (SD)*		19
S67		O=C1NC2=CC=C(OC)C=C2/C1=N/NC3=NC(CCl)=CS3		**13**	19
S68		O=C1NC2=CC=C(OC)C=C2/C1=N/NC3=NC(C)=C(C)S3	*43 ± 1.0 (SD)*		19
S69		O=C1NC2=CC=C(OC)C=C2/C1=N/NC3=NC(C4=CC=CC=C4)=CS3		**1,21**	19
S70		O=C1NC2=CC=C(OC)C=C2/C1=N/NC3=NC(C4=CC(O)=CC=C4)=CS3		**16**	19
S71		O=C1NC2=CC=C(OC)C=C2/C1=N/NC3=NC(C4=CC(OC)=CC=C4)=CS3		**34**	19
S72		O=C1NC2=CC=C(OC)C=C2/C1=N/NC3=NC(C4=CC(Br)=CC=C4)=CS3		**40**	19
S73		O=C1N(C)C2=CC=C(OC)C=C2/C1=N/N(C)C3=CC=C(C(C)C)C=C3		**11**	19
S74		O=C1N(C)C2=CC=C(OC)C=C2/C1=N/NC3=CC=C(C(C)C)C=C3		**0,81**	19
S75		O=C1N(C2CC2)C3=CC=C(OC)C=C3/C1=N/NC4=CC=C(C(C)C)C=C4		**0,8**	19
S76		O=C1N(CC2=CC=CC=C2)C3=CC=C(OC)C=C3/C1=N/NC4=CC=C(C(C)C)C=C4		**0,53**	19
S77		O=C1N(CCC2=CC=CC=C2)C3=CC=C(OC)C=C3/C1=N/NC4=CC=C(C(C)C)C=C4		**0,61**	19
S78		O=C1N(CCCC2=CC=CC=C2)C3=CC=C(OC)C=C3/C1=N/NC4=CC=C(C(C)C)C=C4		**0,83**	19

S79		O=C1NC2=CC=C(CCCC)C=C2/C1=N/NC3=CC=C(C(C)C)C=C3	*55±0.9 (SD)*		19	
S80		O=C1NC2=C(Br)C=CC=C2/C1=N/NC3=CC=C(C(C)C)C=C3	*1±9.3 (SD)*		19	
S81		O=C1NC2=CC=C(S([O-])(=O)=O)C=C2/C1=N/NC3=CC=C(C(C)C)C=C3	*35±4.1 (SD)*		19	
S82		O=C1NC2=CC3=C(OCO3)C=C2/C1=N/NC4=CC=C(C(C)C)C=C4	*70±2.9 (SD)*		19	
S83		O=C1NC2=CC=C(OC)C=C2/C1=N/NC3=CC=C(C#N)C=C3	*16±3.0 (SD)*		19	
S84		O=C1NC2=CC=C(OC)C=C2/C1=N/NC3=CC=C(C(F)(F)F)C=C3	*57±9.0 (SD)*		19	
S85		O=C1NC2=CC=C(OC)C=C2/C1=N/NC3=CC(C(F)(F)F)=CC(C(F)(F)F)=C3		**9,9**	19	
S86		O=C1NC2=CC=C(OC)C=C2/C1=N/NC3=NC=CC=C3		**90**	19	
S87		O=C1NC2=CC=C(OC)C=C2/C1=N/NC3=C(C=CC=C4)C4=CC=C3		**28**	19	
S88		O=C1NC2=CC=C(OC)C=C2/C1=N/NC3=NC(C=CC=C4)=C4C=C3	*67% ± 3,8 (SD)*		19	
S89		O=C1NC2=CC=C(OC)C=C2/C1=N/N=C/C3=CC=C(C(C)C)C=C3		**6,7**	19	
S90		O=C1NC2=CC=C(OC)C=C2/C1=N/N=C/C3=CC(Cl)=CC=C3		**11**	19	
S91		O=C1NC2=CC=C(OC)C=C2/C1=N/NC(C3=CC(Cl)=CC=C3)=O	*31±2.9 (SD)*		19	Other
S92		OC1=CC=C(NC=C2/C=N/NC3=CC=C(Cl)C=C3)C2=C1		**21**	15	
S93		COC1=CC=C(NC=C2/C=N/NC3=CC=C(C(C)C)C=C3)C2=C1		**41**	19	