

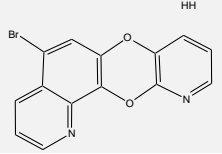
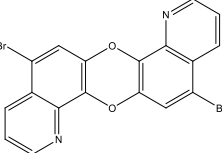
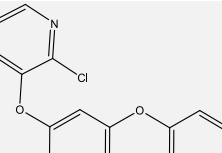
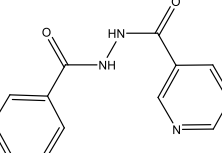
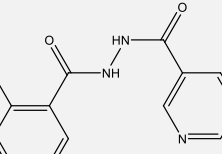
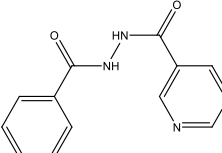
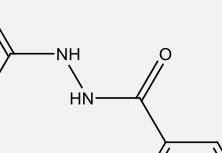
Supplementary Materials for

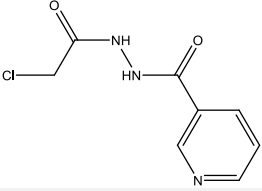
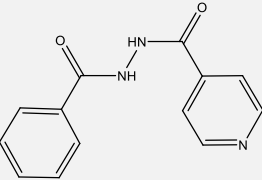
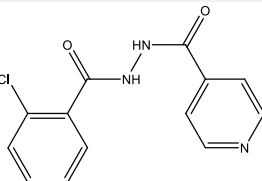
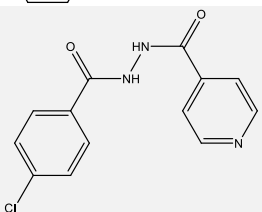
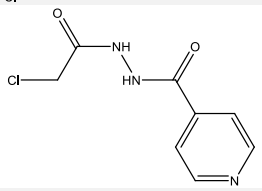
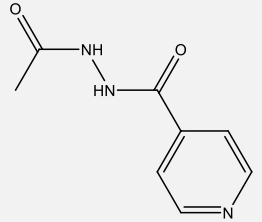
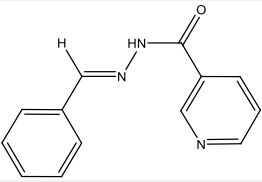
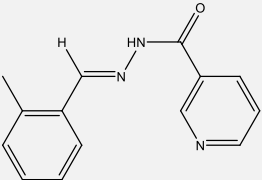
Identification of 2, 4 -Diaminoquinazoline Derivative as a Potential Small-Molecule Inhibitor against Chikungunya and Ross River Viruses

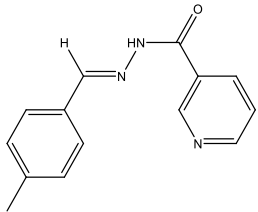
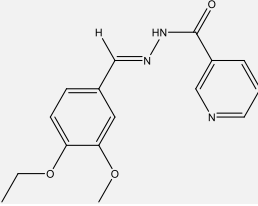
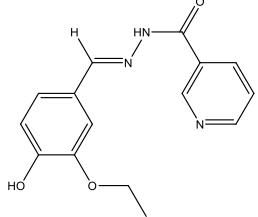
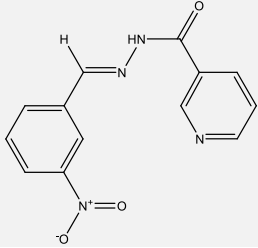
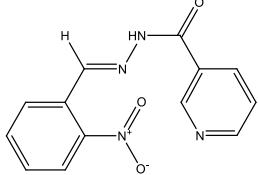
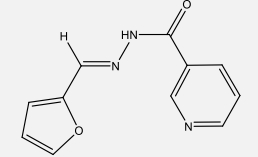
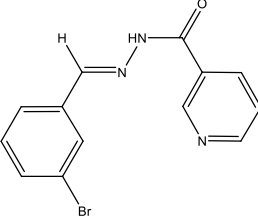
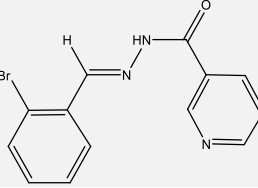
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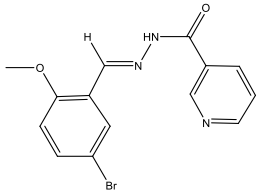
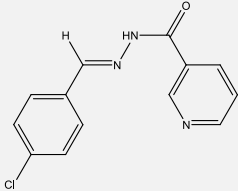
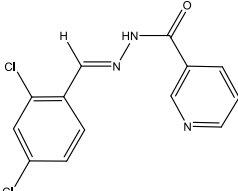
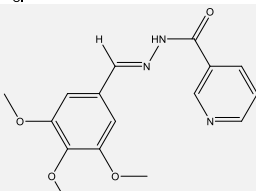
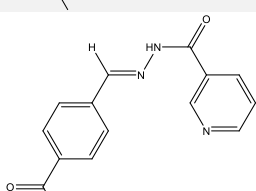
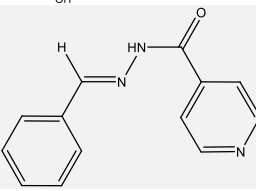
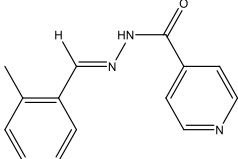
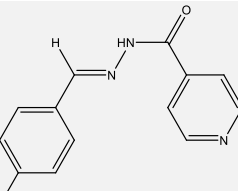
Table S1

Table S1: List of in-house small molecules screened for CHIKV

DCR code	Structure	IUPAC name	Mol Formula	Mol Wt (Da)	MNTD* (μM)	CPE**	% Cell viability***	Reference
DCR1		5-Bromo-7,12-dioxo-1,11-diaza-benzo[a]anthracene	C ₁₄ H ₇ BrN ₂ O ₂	315.12	50	++	72	BN Acharya et al, Med Chem Res, 2008, 17, 487-494
DCR2		10,21-dibromo-2,13-dioxo-5,16-diazapentacyclo[12.8.0.0 ^{3,12} .0 ^{4,9} .0 ^{15,20}]docosa-1(14),3(12),4,6,8,10,15(20),16,18,21-decaene	C ₁₈ H ₈ Br ₂ N ₂ O ₂	444.07	50	++	63	BN Acharya et al, Med Chem Res, 2008, 17, 487-494
DCR3		7-[(2-chloropyridin-3-yl)oxy]-5,12-dioxo-1,11-diazatetraphene	C ₁₉ H ₁₀ ClN ₃ O ₃	363.754	50	++	69.9	BN Acharya et al, Med Chem Res, 2008, 17, 487-494
DCR4		N'-(benzoyl)nicotinohydrazide	C ₁₃ H ₁₁ N ₃ O ₂	241.24	31.25	++++	15	
DCR5		N'-(2-chlorobenzoyl)nicotinohydrazide	C ₁₃ H ₁₀ ClN ₃ O ₂	275.69	31.25	++++	13.49	
DCR6		N'-(4-chlorobenzoyl)nicotinohydrazide	C ₁₃ H ₁₀ ClN ₃ O ₂	275.69	31.25	++++	16.98	
DCR7		N'-(acetyl)nicotinohydrazide	C ₈ H ₉ N ₃ O ₂	179.17	62.5	++++	20.31	

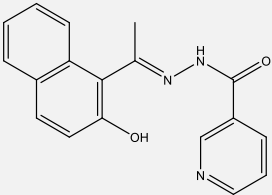
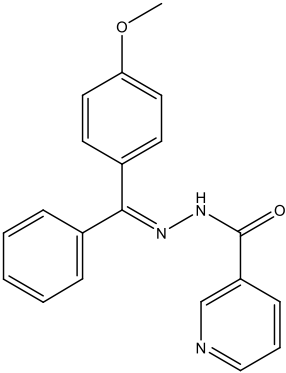
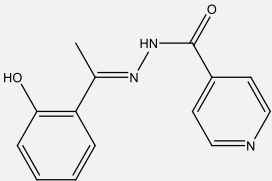
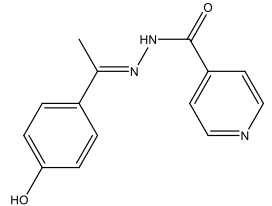
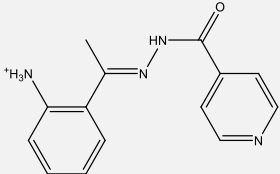
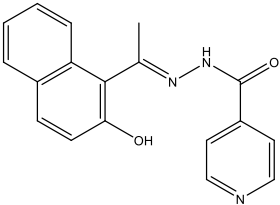
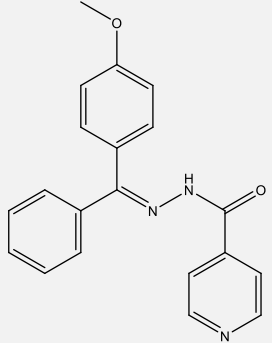
DCR8		N'-(2-chloroacetyl)nicotinohydrazide	C ₈ H ₈ ClN ₃ O ₂	213.62	31.25	++++	13.8
DCR9		N'-benzoylisonicotinohydrazide	C ₁₃ H ₁₁ N ₃ O ₂	241.24	31.25	++++	9.92
DCR10		N'-(2-chlorobenzoyl)isonicotinohydrazide	C ₁₃ H ₁₀ ClN ₃ O ₂	275.69	31.25	++++	21.19
DCR11		N'-(4-chlorobenzoyl)isonicotinohydrazide	C ₁₃ H ₁₀ ClN ₃ O ₂	275.69	31.25	++++	22.85
DCR12		N'-(2-chloroacetyl)isonicotinohydrazide	C ₈ H ₈ ClN ₃ O ₂	213.62	31.25	++++	16.34
DCR13		N'-acetylisonicotinohydrazide	C ₈ H ₉ N ₃ O ₂	179.17	62.5	++++	15.07
DCR14		(E)-N'-benzylidenenicotinohydrazide	C ₁₃ H ₁₁ N ₃ O	225.24	31.25	++++	22.93
DCR15		(E)-N'-(2-methylbenzylidene)nicotinohydrazide	C ₁₄ H ₁₃ N ₃ O	239.27	31.25	++++	14.76

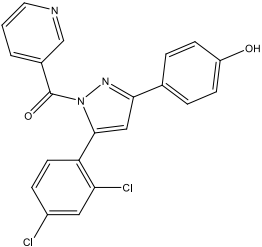
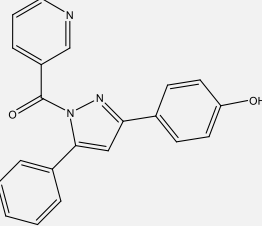
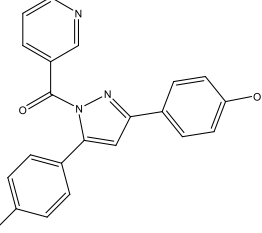
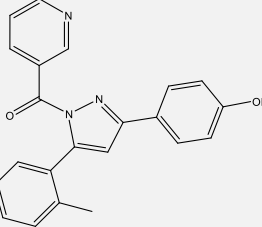
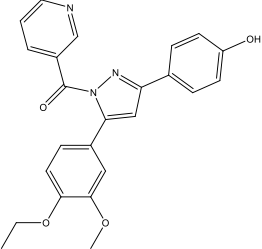
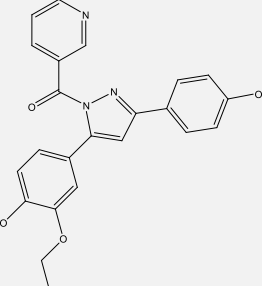
DCR16		(E)-N'-(4-methylbenzylidene)nicotinohydrazide	C ₁₄ H ₁₃ N ₃ O	239.27	31.25	++++	18.49
DCR17		(E)-N'-(4-ethoxy-3-methoxybenzylidene)nicotinohydrazide	C ₁₆ H ₁₇ N ₃ O ₃	299.32	31.25	++++	0.1
DCR18		(E)-N'-(3-ethoxy-4-hydroxybenzylidene)nicotinohydrazide	C ₁₅ H ₁₅ N ₃ O ₃	285.29	31.25	++++	15.39
DCR19		(E)-N'-(3-nitrobenzylidene)nicotinohydrazide	C ₁₃ H ₁₀ N ₄ O ₃	270.24	62.5	++++	20.39
DCR20		(E)-N'-(2-nitrobenzylidene)nicotinohydrazide	C ₁₃ H ₁₀ N ₄ O ₃	270.24	31.25	++++	22.69
DCR21		(E)-N'-(furan-2-ylmethylene)nicotinohydrazide	C ₁₁ H ₉ N ₃ O ₂	215.20	62.5	++++	0
DCR22		(E)-N'-(3-bromobenzylidene)nicotinohydrazide	C ₁₃ H ₁₀ BrN ₃ O	304.14	15.6	++++	19.28
DCR23		(E)-N'-(2-bromobenzylidene)nicotinohydrazide	C ₁₃ H ₁₀ BrN ₃ O	304.14	15.6	++++	28.01

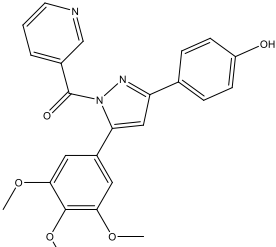
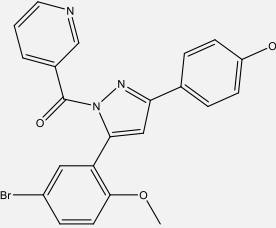
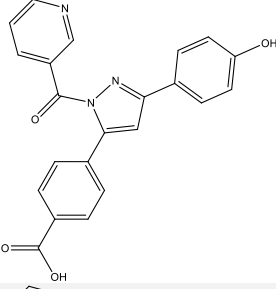
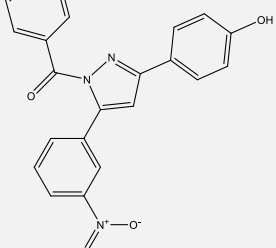
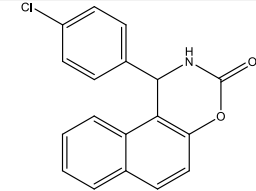
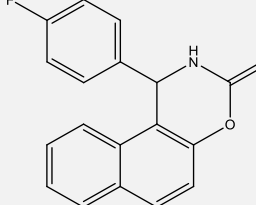
DCR24		(E)-N'-(5-bromo-2-methoxybenzylidene)nicotinohydrazide	C ₁₄ H ₁₂ BrN ₃ O ₂	334.16	15.6	++++	25.23
DCR25		(E)-N'-(4-chlorobenzylidene)nicotinohydrazide	C ₁₃ H ₁₀ ClN ₃ O	259.69	62.5	++++	30.15
DCR26		(E)-N'-(2,4-dichlorobenzylidene)nicotinohydrazide	C ₁₃ H ₉ Cl ₂ N ₃ O	294.13	31.25	++++	26.11
DCR27		(E)-N'-(3,4,5-trimethoxybenzylidene)nicotinohydrazide	C ₁₆ H ₁₇ N ₃ O ₄	315.32	31.25	++++	21.26
DCR28		(E)-4-((2-nicotinoylhydrazono)methyl)benzoic acid	C ₁₄ H ₁₁ N ₃ O ₃	269.25	62.5	++++	15.63
DCR29			C ₁₃ H ₁₁ N ₃ O	225.24	62.5	++++	20.79
DCR30		(E)-N'-(2-methylbenzylidene)isoquinolinohydrazide	C ₁₄ H ₁₃ N ₃ O	239.27	62.5	++++	23.8
DCR31		(E)-N'-(4-methylbenzylidene)isoquinolinohydrazide	C ₁₄ H ₁₃ N ₃ O	239.27	62.5	++++	1.03

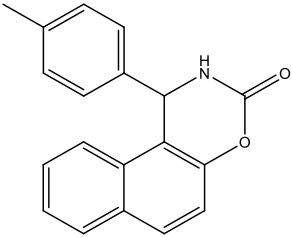
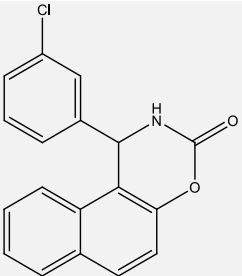
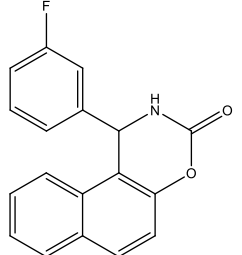
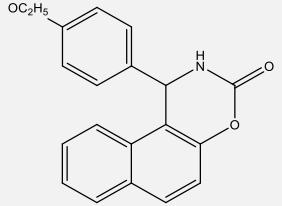
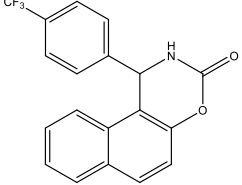
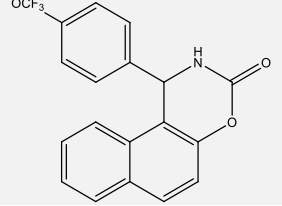
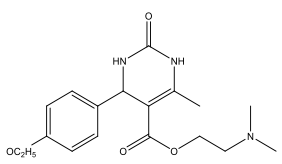
DCR32		(E)-N'-(4-ethoxy-3-methoxybenzylidene)isonicotinohydrazide	C ₁₆ H ₁₇ N ₃ O ₃	299.32	31.25	++++	6.03
DCR33		(E)-N'-(3-ethoxy-4-hydroxybenzylidene)isonicotinohydrazide	C ₁₅ H ₁₅ N ₃ O ₃	285.29	62.5	++++	0
DCR34		(E)-N'-(3-nitrobenzylidene)isonicotinohydrazide	C ₁₃ H ₁₀ N ₄ O ₃	270.24	62.5	++++	6.42
DCR35		(E)-N'-(2-nitrobenzylidene)isonicotinohydrazide	C ₁₃ H ₁₀ N ₄ O ₃	270.24	62.5	++++	9.84
DCR36		(E)-N'-(furan-2-ylmethylene)isonicotinohydrazide	C ₁₁ H ₉ N ₃ O ₂	215.20	62.5	++++	5
DCR37		(E)-N'-(3-bromobenzylidene)isonicotinohydrazide	C ₁₃ H ₁₀ BrN ₃ O	304.14	31.25	++++	14.36
DCR38		(E)-N'-(2-bromobenzylidene)isonicotinohydrazide	C ₁₃ H ₁₀ BrN ₃ O	304.14	31.25	++++	25.1

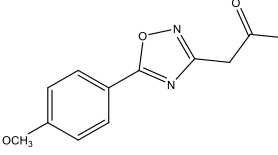
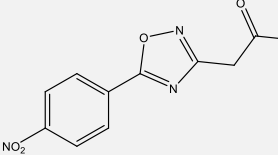
DCR39		(E)-N'-(5-bromo-2-methoxybenzylidene)isonicotinohydrazide	C ₁₄ H ₁₂ BrN ₃ O ₂	334.16	31.25	++++	3.81
DCR40		(E)-N'-(4-chlorobenzylidene)isonicotinohydrazide	C ₁₃ H ₁₀ ClN ₃ O	259.69	31.25	++++	5.23
DCR41		(E)-N'-(2,4-dichlorobenzylidene)isonicotinohydrazide	C ₁₃ H ₉ Cl ₂ N ₃ O	294.13	31.25	++++	35.79
DCR42		(E)-N'-(3,4,5-trimethoxybenzylidene)isonicotinohydrazide	C ₁₆ H ₁₇ N ₃ O ₄	315.32	31.25	++++	12.22
DCR43		(E)-4-((2-isonicotinoylhydrazono)methyl)benzoic acid	C ₁₄ H ₁₁ N ₃ O ₃	269.25	31.25	++++	16.82
DCR44		(E)-N'-(1-(2-hydroxyphenyl)ethylidene)isonicotinohydrazide	C ₁₄ H ₁₃ N ₃ O ₂	255.27	31.25	++++	18.88
DCR45		(E)-N'-(1-(4-hydroxyphenyl)ethylidene)nicotinohydrazide	C ₁₄ H ₁₃ N ₃ O ₂	255.27	31.25	++++	15.55
DCR46		(E)-2-(1-(2-nicotinoylhydrazono)ethyl)benzenaminium	C ₁₄ H ₁₅ N ₄ O	255.29	31.25	++++	27.31

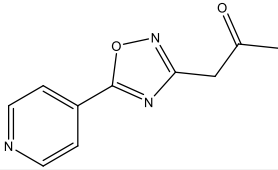
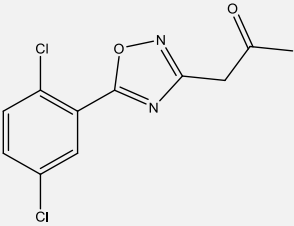
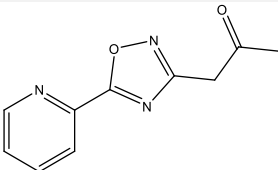
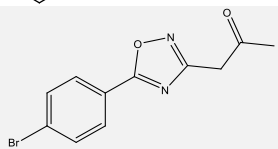
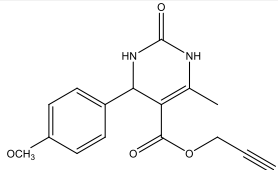
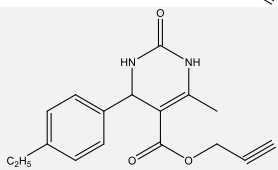
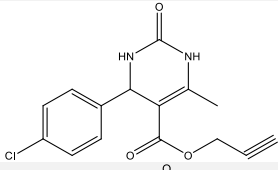
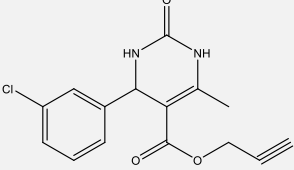
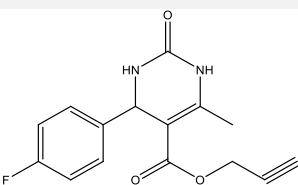
DCR47		(E)-N'-(1-(2-hydroxynaphthalen-1-yl)ethylidene)nicotino hydrazide	C ₁₈ H ₁₅ N ₃ O ₂	305.33	31.25	++++	6.42
DCR48		(Z)-N'-((4-methoxyphenyl)(phenyl)methylidene)nicotino hydrazide	C ₂₀ H ₁₇ N ₃ O ₂	331.36	31.25	++++	20.87
DCR49		(E)-N'-(1-(2-hydroxyphenyl)ethylidene)isonicotino hydrazide	C ₁₄ H ₁₃ N ₃ O ₂	255.27	62.5	+++	48.9
DCR50		(E)-N'-(1-(4-hydroxyphenyl)ethylidene)isonicotino hydrazide	C ₁₄ H ₁₃ N ₃ O ₂	255.27	62.5	++++	18.01
DCR51		(E)-2-(1-(2-isonicotinoethylhydrazono)ethyl)benzenaminium	C ₁₄ H ₁₅ N ₄ O	255.29	62.5	++++	-2.93
DCR52		N'-[(1E)-1-(2-hydroxynaphthalen-1-yl)ethylidene]pyridine-4-carbohydrazide	C ₁₈ H ₁₅ N ₃ O ₂	305.33	31.25	++++	30.87
DCR53		N'-[(1Z)-(4-methoxyphenyl)(phenyl)methylidene]pyridine-4-carbohydrazide	C ₂₀ H ₁₇ N ₃ O ₂	331.36	31.25	++++	11.42

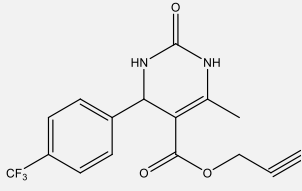
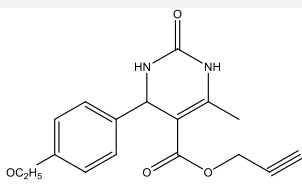
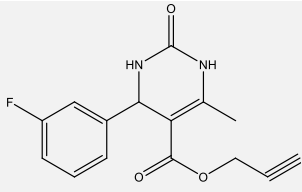
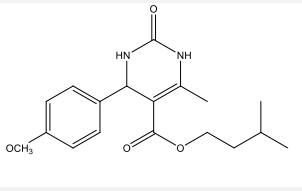
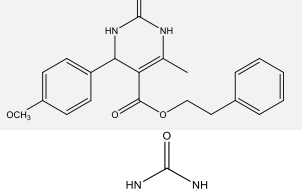
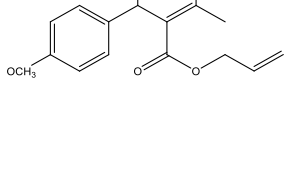
DCR54		4-[5-(2,4-dichlorophenyl)-1-(pyridine-3-carbonyl)-1H-pyrazol-3-yl]phenol	C ₂₁ H ₁₃ Cl ₂ N ₃ O ₂	410.25	15.62	++++	8.73	BN Acharya et al, Eu. J. Med.Chem, 2010, 45, 430-438
DCR55		4-[5-phenyl-1-(pyridine-3-carbonyl)-1H-pyrazol-3-yl]phenol	C ₂₁ H ₁₅ N ₃ O ₂	341.36	31.25	++++	17.69	BN Acharya et al, Eu. J. Med.Chem, 2010, 45, 430-438
DCR56		4-[5-(4-methylphenyl)-1-(pyridine-3-carbonyl)-1H-pyrazol-3-yl]phenol	C ₂₂ H ₁₇ N ₃ O ₂	355.38	31.25	++++	24.2	BN Acharya et al, Eu. J. Med.Chem, 2010, 45, 430-438
DCR57		4-[5-(4-methylphenyl)-1-(pyridine-3-carbonyl)-1H-pyrazol-3-yl]phenol	C ₂₂ H ₁₇ N ₃ O ₂	355.38	31.25	++++	24.84	BN Acharya et al, Eu. J. Med.Chem, 2010, 45, 430-438
DCR58		4-[5-(4-ethoxy-3-methoxyphenyl)-1-(pyridine-3-carbonyl)-1H-pyrazol-3-yl]phenol	C ₂₄ H ₂₁ N ₃ O ₄	415.44	15.62	++++	8.17	BN Acharya et al, Eu. J. Med.Chem, 2010, 45, 430-438
DCR59		2-ethoxy-4-[3-(4-hydroxyphenyl)-1-(pyridine-3-carbonyl)-1H-pyrazol-5-yl]phenol	C ₂₃ H ₁₉ N ₃ O ₄	401.41	15.62	+++	49.1	BN Acharya et al, Eu. J. Med.Chem, 2010, 45, 430-438

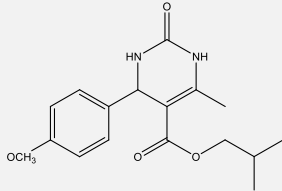
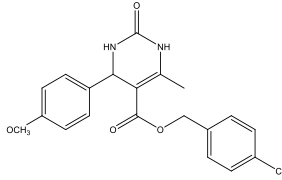
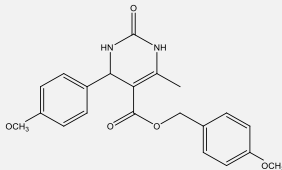
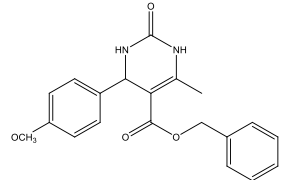
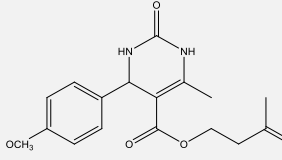
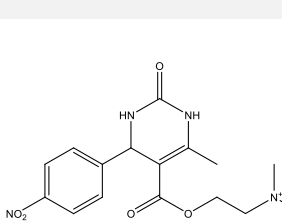
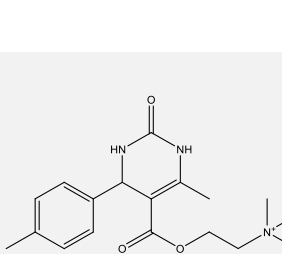
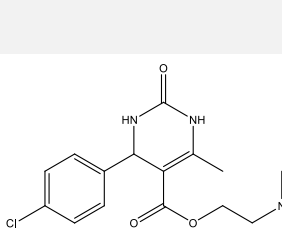
DCR60		4-[1-(pyridine-3-carbonyl)-5-(3,4,5-trimethoxyphenyl)-1H-pyrazol-3-yl]phenol	$C_{24}H_{21}N_3O_5$	431.44	31.25	++++	-3.41	BN Acharya et al, Eu. J. Med.Chem, 2010, 45, 430-438
DCR61		4-[5-(5-bromo-2-methoxyphenyl)-1-(pyridine-3-carbonyl)-1H-pyrazol-3-yl]phenol	$C_{22}H_{16}BrN_3O_3$	450.28	31.25	++++	12.22	BN Acharya et al, Eu. J. Med.Chem, 2010, 45, 430-438
DCR62		4-[3-(4-hydroxyphenyl)-1-(pyridine-3-carbonyl)-1H-pyrazol-5-yl]benzoic acid	$C_{22}H_{15}N_3O_4$	385.37	31.25	++++	-27.93	BN Acharya et al, Eu. J. Med.Chem, 2010, 45, 430-438
DCR63		4-[5-(3-nitrophenyl)-1-(pyridine-3-carbonyl)-1H-pyrazol-3-yl]phenol	$C_{21}H_{14}N_4O_4$	386.36	31.25	++++	-4.2	BN Acharya et al, Eu. J. Med.Chem, 2010, 45, 430-438
DCR64		1-(4-chlorophenyl)-1H,2H,3H-naphtho[1,2-e][1,3]oxazin-3-one	$C_{18}H_{12}ClNO_2$	309.74	31.25	++++	-3.8	GBD Rao et al, Tetrahedron Lett. 2012, 53, 2741-2744
DCR65		1-(4-fluorophenyl)-1H,2H,3H-naphtho[1,2-e][1,3]oxazin-3-one	$C_{18}H_{12}FNO_2$	293.29	53.27	++++	12.63	GBD Rao et al, Tetrahedron Lett. 2012, 53, 2741-2744

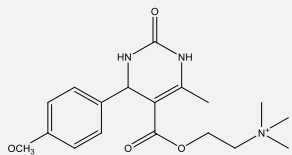
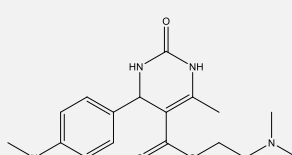
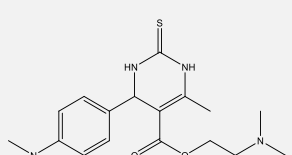
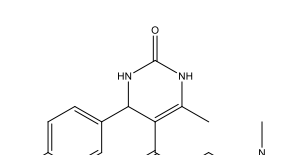
DCR66		1-(4-methylphenyl)-1H,2H,3H-naphtho[1,2-e][1,3]oxazin-3-one	C ₁₉ H ₁₅ NO ₂	289.32	54	++++	12.24	GBD Rao et al, Tetrahedron Lett. 2012, 53, 2741-2744
DCR67		1-(3-chlorophenyl)-1H,2H,3H-naphtho[1,2-e][1,3]oxazin-3-one	C ₁₈ H ₁₂ ClNO ₂	309.74	50.44	++++	10.94	GBD Rao et al, Tetrahedron Lett. 2012, 53, 2741-2744
DCR68		1-(3-fluorophenyl)-1H,2H,3H-naphtho[1,2-e][1,3]oxazin-3-one	C ₁₈ H ₁₂ FNO ₂	293.29	53.27	++++	10.84	GBD Rao et al, Tetrahedron Lett. 2012, 53, 2741-2744
DCR69		1-(4-ethoxyphenyl)-1H,2H,3H-naphtho[1,2-e][1,3]oxazin-3-one	C ₂₀ H ₁₇ NO ₃	319.35	195.71	++++	7.61	GBD Rao et al, Tetrahedron Lett. 2012, 53, 2741-2744
DCR70		1-[4-(trifluoromethyl)phenyl]-1H,2H,3H-naphtho[1,2-e][1,3]oxazin-3-one	C ₁₉ H ₁₂ F ₃ NO ₂	343.29	45.44	++++	10.59	GBD Rao et al, Tetrahedron Lett. 2012, 53, 2741-2744
DCR71		1-[4-(trifluoromethoxy)phenyl]-1H,2H,3H-naphtho[1,2-e][1,3]oxazin-3-one	C ₁₉ H ₁₂ F ₃ NO ₃	359.29	43.42	++++	7.44	GBD Rao et al, Tetrahedron Lett. 2012, 53, 2741-2744
DCR72		2-(dimethylamino)ethyl 4-(4-ethoxyphenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate	C ₁₈ H ₂₅ N ₃ O ₄	347.40	31.25	++++	25.42	BN Acharya et al, Med Chem Res, 2015, 24, 1763-1775

DCR73		2-(dimethylamino)ethyl 6-methyl-4-(4-nitrophenyl)-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate	$C_{16}H_{20}N_4O_5$	348.35	31.25	++++	24.54	BN Acharya et al, Med Chem Res, 2015, 24, 1763-1775
DCR74		2-(dimethylamino)ethyl 6-methyl-4-(4-methylphenyl)-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate	$C_{17}H_{23}N_3O_3$	317.38	31.25	++++	12.75	BN Acharya et al, Med Chem Res, 2015, 24, 1763-1775
DCR75		{2-[4-(4-ethoxyphenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carbonyloxy]ethyl} tri methylazanium	$C_{19}H_{28}N_3O_4$	362.44	31.25	++++	10.21	BN Acharya et al, Med Chem Res, 2015, 24, 1763-1775
DCR76		1-[5-(4-methoxyphenyl)-1,2,4-oxadiazol-3-yl]propan-2-one	$C_{12}H_{12}N_2O_3$	232.23	125	++++	19.42	
DCR77		1-[5-(4-nitrophenyl)-1,2,4-oxadiazol-3-yl]propan-2-one	$C_{11}H_9N_3O_4$	247.20	125	++++	10.43	
DCR78		1-(5-phenyl-1,2,4-oxadiazol-3-yl)propan-2-one	$C_{11}H_{10}N_2O_2$	202.20	125	++++	17.32	
DCR79		1-[5-(diphenylmethyl)-1,2,4-oxadiazol-3-yl]propan-2-one	$C_{18}H_{16}N_2O_2$	292.33	125	++++	16.42	
DCR80		1-(5-cyclohexyl-1,2,4-oxadiazol-3-yl)propan-2-one	$C_{11}H_{16}N_2O_2$	208.25	125	++++	29.64	
DCR81		1-[5-(3-nitrophenyl)-1,2,4-oxadiazol-3-yl]propan-2-one	$C_{11}H_9N_3O_4$	247.20	125	++++	0	

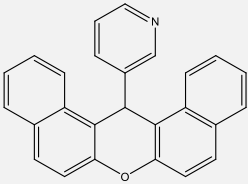
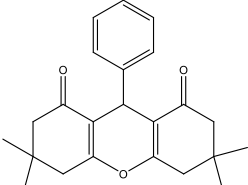
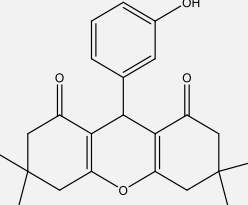
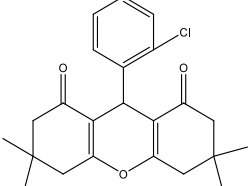
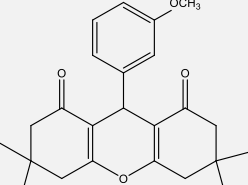
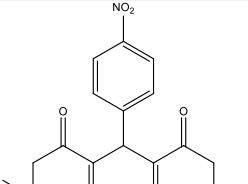
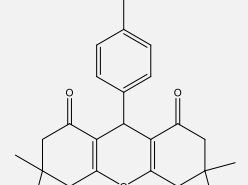
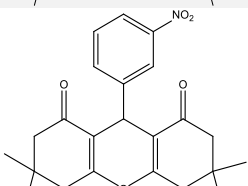
DCR82		1-[5-(pyridin-4-yl)-1,2,4-oxadiazol-3-yl]propan-2-one	C ₁₀ H ₉ N ₃ O ₂	203.19	125	++++	14.42	
DCR83		1-[5-(2,5-dichlorophenyl)-1,2,4-oxadiazol-3-yl]propan-2-one	C ₁₁ H ₈ Cl ₂ N ₂ O ₂	271.09	230.55	++++	10.49	
DCR84		1-[5-(pyridin-2-yl)-1,2,4-oxadiazol-3-yl]propan-2-one	C ₁₀ H ₉ N ₃ O ₂	203.19	125	++++	2.86	
DCR85		1-[5-(4-bromophenyl)-1,2,4-oxadiazol-3-yl]propan-2-one	C ₁₁ H ₉ BrN ₂ O ₂	281.10	222.34	++++	10.38	
DCR86		prop-2-yn-1-yl 4-(4-methoxyphenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate	C ₁₆ H ₁₆ N ₂ O ₄	300.30	208.12	++++	10.59	GBD Rao et al, RSC Adv, 2014, 4, 43321-43325
DCR87		prop-2-yn-1-yl 4-(4-ethylphenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate	C ₁₇ H ₁₈ N ₂ O ₃	298.33	104.58	++++	11.61	GBD Rao et al, RSC Adv, 2014, 4, 43321-43325
DCR88		prop-2-yn-1-yl 4-(4-chlorophenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate	C ₁₅ H ₁₃ ClN ₂ O ₃	304.72	205.1	++++	11.05	GBD Rao et al, RSC Adv, 2014, 4, 43321-43325
DCR89		prop-2-yn-1-yl 4-(3-chlorophenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate	C ₁₅ H ₁₃ ClN ₂ O ₃	304.72	205.1	++++	10.94	GBD Rao et al, RSC Adv, 2014, 4, 43321-43325
DCR90		prop-2-yn-1-yl 4-(4-fluorophenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate	C ₁₅ H ₁₃ FN ₂ O ₃	288.27	433.62	++++	12.59	GBD Rao et al, RSC Adv, 2014, 4, 43321-43325

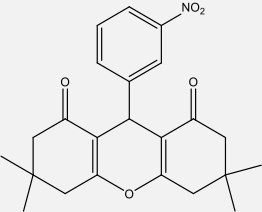
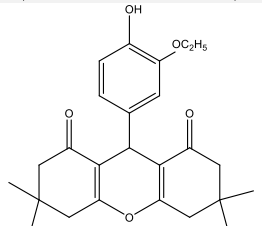
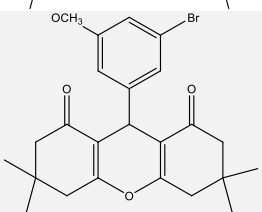
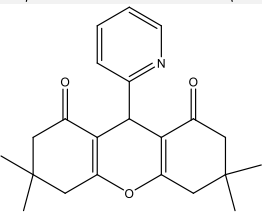
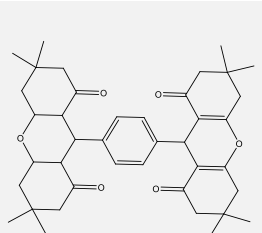
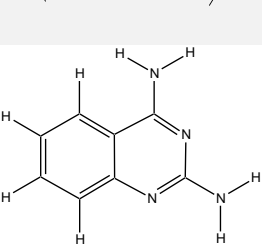
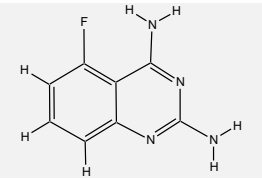
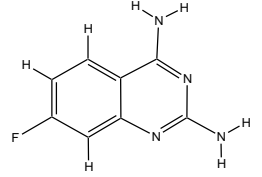
DCR91		prop-2-yn-1-yl 6-methyl-2-oxo-4-[4-(trifluoromethyl)phenyl]-1,2,3,4-tetrahydropyrimidine-5-carboxylate	C ₁₆ H ₁₃ F ₃ N ₂ O ₃	338.28	369.52	++++	13.12	GBD Rao et al, RSC Adv, 2014, 4, 43321-43325
DCR92		prop-2-yn-1-yl 6-methyl-2-oxo-4-phenyl-1,2,3,4-tetrahydropyrimidine-5-carboxylate	C ₁₅ H ₁₄ N ₂ O ₃	270.28	462.48	++++	12.8	GBD Rao et al, RSC Adv, 2014, 4, 43321-43325
DCR93		prop-2-yn-1-yl 6-methyl-4-(4-nitrophenyl)-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate	C ₁₅ H ₁₃ N ₃ O ₅	315.28	315.28	++++	12.17	GBD Rao et al, RSC Adv, 2014, 4, 43321-43325
DCR94		prop-2-yn-1-yl 4-(4-ethoxyphenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate	C ₁₇ H ₁₈ N ₂ O ₄	314.33	198.83	++++	19.5	GBD Rao et al, RSC Adv, 2014, 4, 43321-43325
DCR95		prop-2-yn-1-yl 4-(3-fluorophenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate	C ₁₅ H ₁₃ FN ₂ O ₃	288.27	433.62	++++	11.54	GBD Rao et al, RSC Adv, 2014, 4, 43321-43325
DCR96		3-methylbutyl 4-(4-methoxyphenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate	C ₁₈ H ₂₄ N ₂ O ₄	332.39	376.06	++++	11.71	GBD Rao et al, RSC Adv, 2014, 4, 43321-43325
DCR97		2-phenylethyl 4-(4-methoxyphenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate	C ₂₁ H ₂₂ N ₂ O ₄	366.41	170.57	++++	11.19	GBD Rao et al, RSC Adv, 2014, 4, 43321-43325
DCR98		prop-2-en-1-yl 4-(4-methoxyphenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate	C ₁₆ H ₁₈ N ₂ O ₄	302.32	413.46	++++	12.66	GBD Rao et al, RSC Adv, 2014, 4, 43321-43325

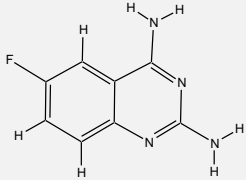
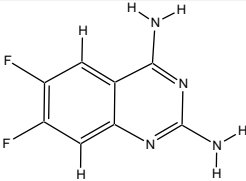
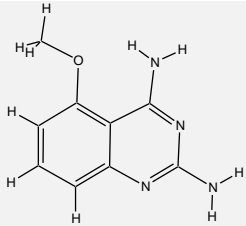
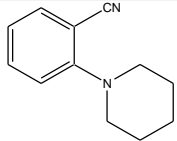
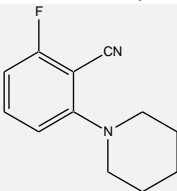
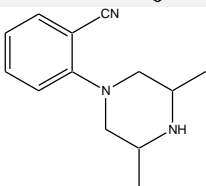
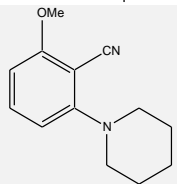
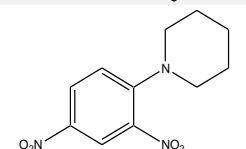
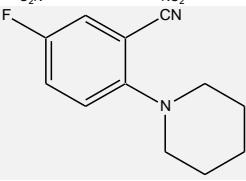
DCR99		2-methylpropyl 4-(4-methoxyphenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate	$C_{17}H_{22}N_2O_4$	318.36	392.64	++++	11.29	GBD Rao et al, RSC Adv, 2014, 4, 43321-43325
DCR100		(4-chlorophenyl)methyl 4-(4-methoxyphenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate	$C_{20}H_{19}ClN_2O_4$	386.82	323.15	++++	12.84	GBD Rao et al, RSC Adv, 2014, 4, 43321-43325
DCR101		4-methoxybenzyl 4-(4-methoxyphenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate	$C_{21}H_{22}N_2O_5$	382.40	250	++++	7.02	GBD Rao et al, RSC Adv, 2014, 4, 43321-43325
DCR102		benzyl 4-(4-methoxyphenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate	$C_{20}H_{20}N_2O_4$	352.38	250	++++	8.11	GBD Rao et al, RSC Adv, 2014, 4, 43321-43325
DCR103		3-methylbut-3-en-1-yl 4-(4-methoxyphenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate	$C_{18}H_{22}N_2O_4$	330.37	250	++++	21.11	GBD Rao et al, RSC Adv, 2014, 4, 43321-43325
DCR104		<i>N,N,N</i> -trimethyl-2-((6-methyl-4-(4-nitrophenyl)-2-oxo-1,2,3,4-tetrahydropyrimidin-5-yl)carbonyl)oxy)ethanaminium	$C_{17}H_{23}N_4O_5$	363.38	125	++++	9.09	BN Acharya et al, Med Chem Res, 2015, 24, 1763-1775
DCR105		<i>N,N,N</i> -trimethyl-2-((6-methyl-4-(4-methylphenyl)-2-oxo-1,2,3,4-tetrahydropyrimidin-5-yl)carbonyl)oxy)ethanaminium	$C_{18}H_{26}N_3O_3$	332.41	125	++++	2.45	BN Acharya et al, Med Chem Res, 2015, 24, 1763-1775
DCR106		2-((4-(4-chlorophenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidin-5-yl)carbonyl)oxy)- <i>N,N,N</i> -	$C_{17}H_{23}ClN_3O_3$	352.83	62.5	++++	3.33	BN Acharya et al, Med Chem Res, 2015, 24, 1763-1775

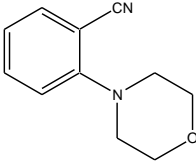
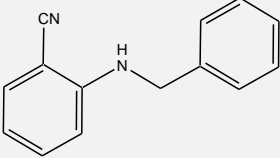
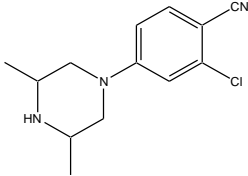
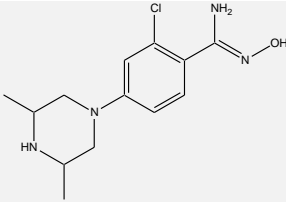
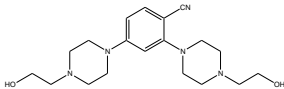
		trimethylethanaminium							
DCR107		{2-[4-(4-methoxyphenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carbonyloxy]ethyl} trimethylazanium	C ₁₈ H ₂₆ N ₃ O ₄	348.41	62.5	++++	13.22	BN Acharya et al, Med Chem Res, 2015, 24, 1763-1775	
DCR108		2-(dimethylamino)ethyl 4-(4-chlorophenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate	C ₁₆ H ₂₀ ClN ₃ O ₃	337.80	62.5	++++	13.99	BN Acharya et al, Med Chem Res, 2015, 24, 1763-1775	
DCR109		2-(dimethylamino)ethyl 4-[4-(dimethylamino)phenyl]-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate	C ₁₈ H ₂₆ N ₄ O ₃	346.42	62.5	++++	15.11	BN Acharya et al, Med Chem Res, 2015, 24, 1763-1775	
DCR110		2-(dimethylamino)ethyl 4-(4-hydroxyphenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate	C ₁₆ H ₂₁ N ₃ O ₄	319.35	62.5	++++	12.01	BN Acharya et al, Med Chem Res, 2015, 24, 1763-1775	
DCR111		2-(dimethylamino)ethyl 4-[4-(dimethylamino)phenyl]-6-methyl-2-sulfanylidene-1,2,3,4-tetrahydropyrimidine-5-carboxylate	C ₁₈ H ₂₆ N ₄ O ₂ S	362.48	62.5	++++	10.08	BN Acharya et al, Med Chem Res, 2015, 24, 1763-1775	
DCR112		2-(dimethylamino)ethyl 4-(4-methoxyphenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate	C ₁₇ H ₂₃ N ₃ O ₄	333.38	62.5	++++	2.09	BN Acharya et al, Med Chem Res, 2015, 24, 1763-1775	

DCR113		2-(4-methoxyphenyl)-13-oxapentacyclo[12.8.0.0 ^{3,12} .0 ^{4,9} .0 ^{17,22}]docosa-1(14),3,5,7,9,11,15,17(22),18,20-decaene	C ₂₈ H ₂₀ O ₂	388.45	31.25	++++	5.04	GBD Rao et al, Tetrahedron Lett. 2012, 53, 2741-2744
DCR114		2-(4-ethoxyphenyl)-13-oxapentacyclo[12.8.0.0 ^{3,12} .0 ^{4,9} .0 ^{17,22}]docosa-1(14),3,5,7,9,11,15,17(22),18,20-decaene	C ₂₉ H ₂₂ O ₂	402.48	31.25	++++	4.05	GBD Rao et al, Tetrahedron Lett. 2012, 53, 2741-2744
DCR115		2-(4-chlorophenyl)-13-oxapentacyclo[12.8.0.0 ^{3,12} .0 ^{4,9} .0 ^{17,22}]docosa-1(14),3,5,7,9,11,15,17(22),18,20-decaene	C ₂₇ H ₁₇ ClO	392.87	125	++++	17.1	GBD Rao et al, Tetrahedron Lett. 2012, 53, 2741-2744
DCR116		2-(3-chlorophenyl)-13-oxapentacyclo[12.8.0.0 ^{3,12} .0 ^{4,9} .0 ^{17,22}]docosa-1(14),3,5,7,9,11,15,17(22),18,20-decaene	C ₂₇ H ₁₇ ClO	392.87	31.25	++++	10.84	GBD Rao et al, Tetrahedron Lett. 2012, 53, 2741-2744
DCR117		2-(4-fluorophenyl)-13-oxapentacyclo[12.8.0.0 ^{3,12} .0 ^{4,9} .0 ^{17,22}]docosa-1(14),3,5,7,9,11,15,17(22),18,20-decaene	C ₂₇ H ₁₇ FO	376.42	125	++++	14.01	GBD Rao et al, Tetrahedron Lett. 2012, 53, 2741-2744
DCR118		2-(4-ethylphenyl)-13-oxapentacyclo[12.8.0.0 ^{3,12} .0 ^{4,9} .0 ^{17,22}]docosa-1(14),3,5,7,9,11,15,17(22),18,20-decaene	C ₂₉ H ₂₂ O	386.48	31.25	++++	14.23	GBD Rao et al, Tetrahedron Lett. 2012, 53, 2741-2744
DCR119		2-(3-fluorophenyl)-13-oxapentacyclo[12.8.0.0 ^{3,12} .0 ^{4,9} .0 ^{17,22}]docosa-1(14),3,5,7,9,11,15,17(22),18,20-decaene	C ₂₇ H ₁₇ FO	376.42	31.25	++++	18.74	GBD Rao et al, Tetrahedron Lett. 2012, 53, 2741-2744
DCR120		2-(propan-2-yl)-13-oxapentacyclo[12.8.0.0 ^{3,12} .0 ^{4,9} .0 ^{17,22}]docosa-1(14),3,5,7,9,11,15,17(22),18,20-decaene	C ₂₄ H ₂₀ O	324.41	31.25	++++	19.24	GBD Rao et al, Tetrahedron Lett. 2012, 53, 2741-2744

DCR121		3-{13-oxapentacyclo[12.8.0.0 ³ ,12.0 ⁴ ,9.0 ¹⁷ ,22]docosa-1(14),3,5,7,9,11,15,17(22),18,20-decaen-2-yl}pyridine	C ₂₆ H ₁₇ NO	359.41	31.25	++++	8.03	GBD Rao et al, Tetrahedron Lett. 2012, 53, 2741-2744
DCR122		9-(4-chlorophenyl)-3,3,6,6-tetramethyl-2,3,4,5,6,7,8,9-octahydro-1H-xanthene-1,8-dione	C ₂₃ H ₂₅ ClO ₃	384.89	31.25	++++	11.09	GBD Rao et al, Heterocyclic Lett., 2012, 2, 411-418.
DCR123		9-(3-hydroxyphenyl)-3,3,6,6-tetramethyl-2,3,4,5,6,7,8,9-octahydro-1H-xanthene-1,8-dione	C ₂₃ H ₂₆ O ₄	366.45	125	++++	12.01	GBD Rao et al, Heterocyclic Lett., 2012, 2, 411-418.
DCR124		9-(2-chlorophenyl)-3,3,6,6-tetramethyl-2,3,4,5,6,7,8,9-octahydro-1H-xanthene-1,8-dione	C ₂₃ H ₂₅ ClO ₃	384.89	125	++++	11.05	GBD Rao et al, Heterocyclic Lett., 2012, 2, 411-418.
DCR125		9-(3-methoxyphenyl)-3,3,6,6-tetramethyl-2,3,4,5,6,7,8,9-octahydro-1H-xanthene-1,8-dione	C ₂₄ H ₂₈ O ₄	380.47	125	++++	11.19	GBD Rao et al, Heterocyclic Lett., 2012, 2, 411-418.
DCR126		3,3,6,6-tetramethyl-9-(4-nitrophenyl)-2,3,4,5,6,7,8,9-octahydro-1H-xanthene-1,8-dione	C ₂₃ H ₂₅ NO ₅	395.44	15.6	++++	17.99	GBD Rao et al, Heterocyclic Lett., 2012, 2, 411-418.
DCR127		3,3,6,6-tetramethyl-9-(4-methylphenyl)-2,3,4,5,6,7,8,9-octahydro-1H-xanthene-1,8-dione	C ₂₄ H ₂₈ O ₃	364.47	125	++++	10.21	GBD Rao et al, Heterocyclic Lett., 2012, 2, 411-418.
DCR128		9-(4-methoxyphenyl)-3,3,6,6-tetramethyl-2,3,4,5,6,7,8,9-octahydro-1H-xanthene-1,8-dione	C ₂₄ H ₂₈ O ₄	380.47	125	++++	11.01	GBD Rao et al, Heterocyclic Lett., 2012, 2, 411-418.

DCR129		3,3,6,6-tetramethyl-9-(3-nitrophenyl)-2,3,4,5,6,7,8,9-octahydro-1H-xanthene-1,8-dione	C ₂₃ H ₂₅ NO ₅	395.44	31.25	++++	16.85	GBD Rao et al, Heterocyclic Lett., 2012, 2, 411-418.
DCR130		9-(3-ethoxy-4-hydroxyphenyl)-3,3,6,6-tetramethyl-2,3,4,5,6,7,8,9-octahydro-1H-xanthene-1,8-dione	C ₂₅ H ₃₀ O ₅	410.50	15.6	++++	17.21	GBD Rao et al, Heterocyclic Lett., 2012, 2, 411-418.
DCR131		9-(3-bromo-5-methoxyphenyl)-3,3,6,6-tetramethyl-2,3,4,5,6,7,8,9-octahydro-1H-xanthene-1,8-dione	C ₂₄ H ₂₇ BrO ₄	459.37	125	++++	8.01	GBD Rao et al, Heterocyclic Lett., 2012, 2, 411-418.
DCR132		3,3,6,6-tetramethyl-9-(pyridin-2-yl)-2,3,4,5,6,7,8,9-octahydro-1H-xanthene-1,8-dione	C ₂₂ H ₂₅ NO ₃	351.43	125	++++	9.06	GBD Rao et al, Heterocyclic Lett., 2012, 2, 411-418.
DCR133		3,3,6,6-tetramethyl-9-[4-(3,3,6,6-tetramethyl-1,8-dioxo-dodecahydro-1H-xanthene-9-yl)phenyl]-2,3,4,5,6,7,8,9-octahydro-1H-xanthene-1,8-dione	C ₄₀ H ₅₀ O ₆	626.82	125	++++	11.14	GBD Rao et al, Heterocyclic Lett., 2012, 2, 411-418.
DCR134		Quinazoline-2,4-diamine	C ₈ H ₈ N ₄	160.18	150	+	75.9	N Shelke et al, RSC Adv. 2015, 5, 31226-31230
DCR135		5-Fluoro-quinazoline-2,4-diamine	C ₈ H ₇ FN ₄	178.17	250	++	61	N Shelke et al, RSC Adv. 2015, 5, 31226-31230
DCR136		7-Fluoro-quinazoline-2,4-diamine	C ₈ H ₇ FN ₄	178.17	250	++	54	N Shelke et al, RSC Adv. 2015, 5, 31226-31230

DCR137		6-Fluoro-quinazoline-2,4-diamine	C ₈ H ₇ N ₄	178.17	300	+	90.3	N Shelke et al, RSC Adv. 2015, 5, 31226-31230
DCR138		6,7-Difluoro-quinazoline-2,4-diamine	C ₈ H ₆ F ₂ N ₄	196.16	250	++	51	N Shelke et al, RSC Adv. 2015, 5, 31226-31230
DCR139		5-Methoxy-quinazoline-2,4-diamine	C ₉ H ₁₀ N ₄ O	190.20	250	++	57	N Shelke et al, RSC Adv. 2015, 5, 31226-31230
DCR140		2-Piperidin-1-yl-benzonitrile	C ₁₂ H ₁₄ N ₂	186.25	250	++++	14.97	N Shelke et al, RSC Adv. 2015, 5, 31226-31230
DCR141		2-Fluoro-6-piperidin-1-yl-benzonitrile	C ₁₂ H ₁₃ FN ₂	204.24	125	++++	19.24	N Shelke et al, RSC Adv. 2015, 5, 31226-31230
DCR142		2-(3,5-Dimethyl-piperazin-1-yl)-benzonitrile	C ₁₃ H ₁₇ N ₃	215.29	125	++++	13.08	N Shelke et al, RSC Adv. 2015, 5, 31226-31230
DCR143		2-Methoxy-6-piperidin-1-yl-benzonitrile	C ₁₃ H ₁₆ N ₂ O	216.28	125	++++	17.42	N Shelke et al, RSC Adv. 2015, 5, 31226-31230
DCR144		1-(2,4-Dinitro-phenyl)-piperidine	C ₁₁ H ₁₃ N ₃ O ₄	251.24	125	++++	25.21	N Shelke et al, RSC Adv. 2015, 5, 31226-31230
DCR145		5-Fluoro-2-piperidin-1-yl-benzonitrile	C ₁₂ H ₁₃ FN ₂	204.24	125	++++	0	N Shelke et al, RSC Adv. 2015, 5, 31226-31230

DCR146		2-Morpholin-4-yl-benzonitrile	C11H12N2O	188.23	250	++++	-3.98	N Shelke et al, RSC Adv. 2015, 5, 31226-31230
DCR147		2-Benzylamino-benzonitrile	C14H12N2	208.26	125	++++	17.97	N Shelke et al, RSC Adv. 2015, 5, 31226-31230
DCR148		2-Chloro-4-(3,5-dimethyl-piperazin-1-yl)-benzonitrile	C13H16ClN3	249.74	125	++++	14.42	
DCR149		2-Chloro-4-(3,5-dimethyl-piperazin-1-yl)-N-hydroxy-benzamidine	C13H19ClN4O	282.77	125	++++	-21.8	
DCR150		2,4-Bis-[4-(2-hydroxy-ethyl)-piperazin-1-yl]-benzonitrile	C19H29N5O2	359.47	62.5	++++	18.09	

*Maximum nontoxic dose (MNTD) of all the compounds were calculated on Vero cells.

**Arbitrary score given on the basis of visualization of the cytopathic effect (CPE) at >48 hpi: >60% (++++), 60-50% (+++), 50-30% (++) , and <30% (+).

***Cell viability at 72 hpi as assessed by MTT assay.