

# Supporting Information

## Structural elucidation of Rift Valley Fever Virus L protein towards the discovery of its potential inhibitors

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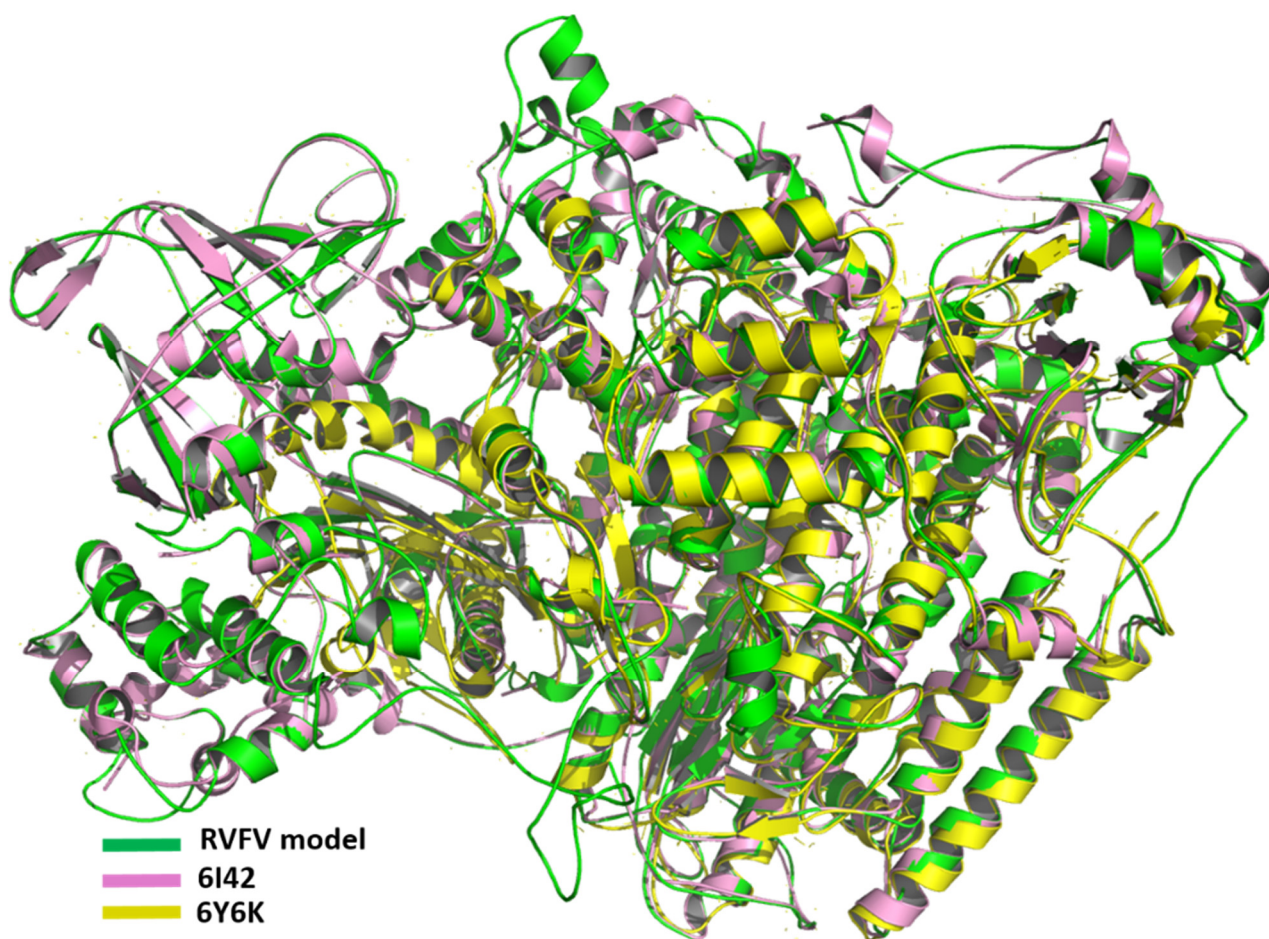
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RVFV_L	sequencequery----	MDSILSK--QLVDKTGFVRVPIKHFDCTMLTLALPTFDVSKMV	54	
6L42_0_0	--structureL-FIRSTX-----	-----GLPDLDDVTVD	27	
6Y6K_1_0	--structureYKFIRSTX-----	-----GLPDLDDVTVD	28	
	. . * *	** .** :*: .		
RVFV_L	DRITIDFNLDIQQGASEIGSTLLPSM-SIDVEDMANFVHDFTFGHLADKTDRLLMREFPM		113	
6L42_0_0	TGVTVDIGAVP-DSAS-----	SEAYKINHDTFSGLSKTTDRRLSEVFP	71	
6Y6K_1_0	TGVTVDIGAVP-DSASQLGSSINAGLITIQ	SEAYKINHDTFSGLSKTTDRRLSEVFP	87	
	:*:*. . :.**	.: : : ***** . *:..** * . **:		
RVFV_L	MNDGFDHLSPDMI IKTTSGVYNIVEFTNFRGDERGAFQAAM- IKLAKYEVPCENRS---	Q	169	
6L42_0_0	THDGS DGMTPDVIHTRLDGTIVVVEFTTTRSHNIGGLEAAYRTKIEKYRDPISRRVDIME		131	
6Y6K_1_0	THDGS DGMTPDVIHTRLDGTIVVVEFTTTRSHNIGGLEAAYRTKIEKYRDPISRRVDIME		147	
	:** * :*:*. . .*. :****. *:..* :*:** *: ** . * ..* :			
RVFV_L	GRTVVLYVVSAYRAWCMVYLELERTLKQREM VYRYRLALSVMDELRTLFP--	ELSSTDEE	227	
6L42_0_0	NPRVFFGVIVVSSGGVLSNMPLTQD-EAEELMYRFCIANEIYTKARSMADIELQKSEEE		190	
6Y6K_1_0	NPRVFFGVIVVSSGGVLSNMPLTQD-EAEELMYRFCIANEIYTKARSMADIELQKSEEE		206	
	. *: . * : . . : : * : : .*:***: * .: : * : : **..:***			
RVFV_L	LGKTERELPAMVSSIQINWSVTESVFPF SREMFD RFRSSPPDSEYITRIVSRCLINSQE		287	
6L42_0_0	LEAISRAL-SFFSLFEPNIERVEGTFPNSEIEMLEQFLSTPADVDFITKTLKAKEVEAYA		249	
6Y6K_1_0	LEAISRAL-SFFSLFEPNIERVEGTFPNSEIEMLEQFLSTPADVDFITKTLKAKEVEAYA		265	
	* . * * :*: . : * . .*.** . :*:** * : * * :*: : . : :			
RVFV_L	KLINSSFFAEGNDKALRF SKNAEECSLAVERALNQYRAEDNLRDLNDHKSTIQ	LPPWLSY	347	
6L42_0_0	DLCDSHYLKPEKTIQERLEINRCEAIDKTQDLLAGLHARSN-KQTS	LNRGTVKLPWLPK	308	
6Y6K_1_0	DLCDSHYLKPEKTIQERLEINRCEAIDKTQDLLAGLHARSN-KQTS	LNRGTVKLPWLPK	324	
	. * : * : : : * : . * . .: * : * : . : . : : : : *****			
RVFV_L	HDVDGKDLCPQLQGLDVRGDH-PMC NLWREVVTSANLEEIERMHDDAAAELEFAFGS---	K	403	
6L42_0_0	PSSSIDIKTDSGFGSLMDHGAYGELWAKCLLDVSLGNVEGVVSDP--	ELDIA-----	359	
6Y6K_1_0	PSS-----	GAYGELWAKCLL-----	339	
	. : ** : :	***		
RVFV_L	GQARE-RNRYHRVHLNMGSDVLVYIAALGVNGKKHK---	ADTLVQQMRDRSKQPFSP---	456	
6L42_0_0	DTPKEAKITYRRFK---	PALSSSARQEFSLQG-----	LSPFLD	394
6Y6K_1_0	-----	SHETLSP---	FLD	349
		***		
RVFV_L	DHDVITYLNF-S-LHALVTCGQOMRTCT--	ALSLVIRDSVGSPEDSSAILVRKGFHEIIT	512	
6L42_0_0	VEDIGDFLT-FNNLLADSRYGDE-SVQR--	AVSILL-----	EKASAMQDTELTHALND	443
6Y6K_1_0	VEDIGDFLT-FNNLLTDSRYGDESIQ---	RAVSILL-----	EKASAMQDTELTHALND	398
	.*: :*. . * : :*: * *:***: * :*: : : * :			
RVFV_L	EHYKFMGSRIGHGCMVSLIGAEL SASVKQHVKPNYFVIKRLLGSGIFLLIKPTSSKSHI		572	
6L42_0_0	SFKRNLSSNVVQWSLWVSLAQELASALKQHCRAGEFIIKKLKF	WPIYVVIKPTKSSSHI	503	
6Y6K_1_0	SFKRNLSSNVVQWSLWVSLAQELASALKQHCRAGEFIIKKLKF	WPIYVVIKPTKSSSHI	458	
	.. : :*. : : . ** : . *****: * . *:***. * :*:*****.***			
RVFV_L	FVSFALSALAGPLISPLPG-FSSPTKMLGILLVTD	FVSYKLSKLTNLCKCVSLMESSFSF	631	
6L42_0_0	F--YSLGIRKADVTRRLTGRVFS	ETIDAGEWELTEFKSLKTKCLTNLVNLPCTMLNSIAF	561	
6Y6K_1_0	F--YSLGIRKADVTRRLTGRVFS	ETIDAGEWELTEFKSLKTKCLTNLVNLPCTMLNSIAF	516	
	* :*: . . : * * . * * * :*: * * .*****: . * .*:*			
RVFV_L	WAEAFGIQAGTLVGDFVPRSSDSAAMDASYMGKLSLLTLEDKAATEELQTIARYIIMEG		691	
6L42_0_0	WREKLGV-----	APWLVRKPCSELREQVGLTFLISLEDKSKTEEIIITLTRYTQMEG	612	
6Y6K_1_0	WREKLGV-----	APWLVRKPCSELREQVGLTFLISLEDKSKTEEIIITLTRYTQMEG	567	
	* * :*: . * . . : :*: * *****: * :*:** *			
RVFV_L	FVSPPEIPKPHKMTSKFPKVLRS	ELQVYLLNCLCRTIQRIAGEPFILKKKDGSI	SWGGMF	751
6L42_0_0	FVSPMPLPKPQKMLGKLDGPLR	TKLQVYLLRKHLDCMVRIASQPFSLIPREGRVEWGGTF	672	
6Y6K_1_0	FVSPMPLPKPQKMLGKLDGPLR	TKLQVYLLRKHLDCMVRIASQPFSLIPREGRVEWGGTF	627	
	***** :*:** .*: :*:*****. : **:** * :*: .*** *			
RVFV_L	NPFSGRPLLDMP	LISCCYNGYFKNKEEETEPSSLSGMYKKIIELEHLRPQSDAFLGYKD	811	
6L42_0_0	HAISGRST-NLENMVNSWYIGYK	NKEESTELNALGEMYKKIVEMEEDKPSSPEFLGWGD	731	
6Y6K_1_0	HAISGRST-NLENMVNSWYIGYK	NKEESTELNALGEMYKKIVEMEEDKPSSPEFLGWGD	686	
	: :*** :*: :*. * *****.* :*. *****:*. . * . * :*			
RVFV_L	PELPRMHEFSVSYLKEACNHAKLV	LRSLYQNFMEQIDNQIIRLSGLTLERLATLKATS	871	

6L42_0_0	TDSPKKHEFSRSFLRAACSSLEREIAQRHGRQWKQNLEERVLRIGTKNILDLASMKATS	791
6Y6K_1_0	TDSPKKHEFSRSFLRAACSSLEREIAQRHGRQWKQNLEERVLRIGTKNILDASMKATS : *: **** *:*: **: : : . :*::: ::::::::::*:.. .: **::****	746
RVFV_L	NFNENWYVYKDVADKNYTRDKLLVKMSKYASEGKS LAIQKFEDCMRQIESQGCMHICLFK	931
6L42_0_0	NFSKDWELYSEVQTKEYHRSKLLEKMATLIEKGVMWYIDAVGQAWKA VLDDGCMRICLFK	851
6Y6K_1_0	NFSKDWELYSEVQTKEYHRSKLLEKMATLIEKGVMWYIDAVGQAWKA VLDDGCMRICLFK **.:*: :.*: *:* *.*** **: . .* * : . : : : :.****:*****	806
RVFV_L	KQQHGGLREIYVMGAEE RIVQS SVETIARSIGKFFASDTLCNP PNKV KIPETHGIRARKQ	991
6L42_0_0	KNQHGG LREIY VMDANARLV QFGVETMARCVC ELSPHETVANPRLKNS I IENHGLKSARS	911
6Y6K_1_0	KNQHGG LREIY VMDANARLV QFGVETMARCVC ELSPHETVANPRLKNS I IENHGLKSARS *:*****. *: **: ***:*.:: : : :*:.* * .* *.*::: ..	866
RVFV_L	CKGPVWTCATSD DARKWNQGH FVTKFALMLCEFTS PKWWPLI IRGCSMF TTKRMMMNLY	1051
6L42_0_0	LGPSIN INSNDAKKWNQ GHYT TKLALVL CWFMPAKFH RFIWAA ISMFRKKMMVDLRF	971
6Y6K_1_0	LGPSIN INSNDAKKWNQ GHYT TKLALVL CWFMPAKFH RFIWAA ISMFRKKMMVDLRF . :*:**:*****:.**:**:* * *: :* . *** :*:***:*.:	926
RVFV_L	LKILDG HRELDIRDD FVMDL FKAYHGEAEVP WAFK GKTYLET TTGM MQGILHYTSSL LHT	1111
6L42_0_0	LAHLS-----DPFREAM TD AFHGNREVSW MDKGR TYIKT ETGMMQ GILHFTSSL LHS	1023
6Y6K_1_0	LAHLSS-----DPFREAM TD AFHGNRDVS WMDKGR TYIKT ETGMMQ GILHFTSSL LHS * *. :*:***: * * **:***:~* *****:*****:	979
RVFV_L	IHQEYIRSLSFKIFNLKV APEMSKSLVCDMMQSGDSSMLISFPADDEKVLTRCKVA AA I	1171
6L42_0_0	CVQSFYKSYFVSKLKEGY MGE-SISGVVDV IEGSDDS AIMISIRPKSDMDEVSRFFVAN	1082
6Y6K_1_0	CVQSFYKSYFVSKLKEGY MGE-SISGVVDV IEGSDDS AIMISIRPKSDMDEVSRFFVAN *.: ~* .. :~* * * * *:~*:*****:~*: ..: .*.~* .*	1038
RVFV_L	CFRMKKELGVYLAIYPSEKSTANTDFVMEYNSEFYFHTQHVRPTIRWIAACC SLPEVETL	1231
6L42_0_0	LLHSV KF LNPLFGIYSSEKSTVNTVYC VEYNSEFHFHRHLVRPTLRWIAASHQISETEAL	1142
6Y6K_1_0	LLHSV KF LNPLFGIYSSEKSTVNTVYC VEYNSEFHFHRHLVRPTLRWIAASHQISETEAL ::~ * *. :.** *****.* : :*****:* : *****:*****. :~*.*:*	1098
RVFV_L	VARQEASNLMTSVTEGGGSFLA AI IQQAQCT LH YMLMG MVSEL FLEYK KAVLK WNDP	1291
6L42_0_0	ASRQEDYSNLLTQCLEGGASFSLTYLIQCAQLLHHYMLLG LCLHPLFGTFMGMLISDPDP	1202
6Y6K_1_0	ASRQEDYSNLLTQCLEGGASFSLTYLIQCAQLLHHYMLLG LCLHPLFGTFMGMLISDPDP .:***: ***:~* . ***.***: :** ** *****: : ~* : :~* . **	1158
RVFV_L	GLGFFLLDNPYACGLGGFRNFLKAITRTDLQKLYAFFMKVKVGSAA RDWADEDVTIPET	1351
6L42_0_0	ALGFFLMDNPAFAGGAGFRNFLWRACKTTDLGRKYAYYFNEI-----YRALDA	1250
6Y6K_1_0	ALGFFLMDNPAFAGGAGFRNFLWRACKTTDLGRKYAY----- .****:*** ~* .*****:~* . *** : **:	1195
RVFV_L	CSVSPGGALILSSSLKWGSRKKFQKLDRDLNIPENWIELINENPEVLYRAPRTGPEILLR	1411
6L42_0_0	TS---GGTLSHSVMVYWGDRKKYQALLNRMG LPEDWVEQ IDENPGVLYRRANKKELLK	1307
6Y6K_1_0	----- -----	1195
RVFV_L	IAEKVHSPGVVSSLS SGNVCKVMASAVYFLSATIFEDT---GRPEFNFLDSKYSLLO	1467
6L42_0_0	LAEKVHSPGVTSSLSKGHVPRVVAAGVYLLSRHCF-FSSSIH--G----STQKASLIK	1359
6Y6K_1_0	-----HVVPRVVAAGVYLL----- :~* :*:~*.*:*	1209
RVFV_L	--KMAAYS GFHGFNDMEPEDILFLFPNIEELESLSIVYNKGEIDIIPRVNIRDATQTRV	1525
6L42_0_0	LLMMSSISAMKHGGS LNPNQERMLFPQAQ EYDRVCTLLEEVEH-----VRERNIVRSRI	1413
6Y6K_1_0	-----GGS LNPNQERMLFPQAQ EYDRVCTLLEEVEHLTGFVVRERNIVRSRI ...*:~: *****:~* : : :~: : . *.*. :*:~:	1257
RVFV_L	TIFNEQKNLRTSPEKLVSDKWFGTQKSRIGKTTF LAEW EK LK KIV KWLED APEATLAHTP	1585
6L42_0_0	DLFQEPVDLRCKAEDLVSEVWFG LRKTK LGPRL LKEEWD KL RASFAWLSTD PSETLRDGP	1473
6Y6K_1_0	DL----- :	1259
RVFV_L	LNNHIQVRNFFARMESKP-RTVRITGAPVKKRSGVSKIAMVIRDHF SRMGHLRGVEDLAG	1644
6L42_0_0	FLSHVQFRNFI-----SLDN	1488
6Y6K_1_0	-----RSVRLL-----GAP--- *	1268
RVFV_L	FTRSVAEILKHFLFCILQGPYESYKLQLIYRVLSSVS NVEIKESDGK-----	1693
6L42_0_0	QERLESISILKHVLFMVLNGPYTEEYKLEMIEAFSTL-----	1529

6Y6K_1_0	-----TIS---QVVRM-----NFFPGFSLE----- : . :.: : :.:*****	1285
RVFV_L	-----TKTNLIGILQRFLD--GDHVVPPIEEMGAGTVGGFIKRQQSK	1733
6L42_0_0	-----RTMTLCLLSN-----SILDQIERAQSGTLGGFSKPQ-KT	1559
6Y6K_1_0	----- ***** **	1285
RVFV_L	V--VQNKVYYYGVGIWRGFMDGY-QVHLEIENDIGQPPRLRNVTTNCQSSPWDLSIPIRQ	1790
6L42_0_0	FIRPGGGVGYKKGVTGVME-DTHVQILIDGD-GTSNWLEEIRLSSDARLYDVIESIRR	1617
6Y6K_1_0	-----	1285
RVFV_L	WAEDMGVTNNQDYSSKSSRGARYWMHSFRMQG-PSKPFGCPVYIIKGDMSDVIRLRK---	1846
6L42_0_0	LCDDLGINNRVASAYRGHCMVR--LSGFKIKPASRTD-GCPVRI---MERGFRIRELQN	1670
6Y6K_1_0	-----	1285
RVFV_L	-EEVEMKVRGSTLNLYTKHSHQDLHILSYTASDNDLSPGIFKSIISDEGVAQALQLFERE	1905
6L42_0_0	PDEVKMRVRGDILNLSVTIQEGRVMNILSYRPRDTDISESAAAYLWSN--RDLFSFGKKE	1728
6Y6K_1_0	-----	1285
RVFV_L	PSNCWVRCESVAPKFISAILEICEGKRQIKGINRTLSEIVRICSESSLRSKVGSMFSFV	1965
6L42_0_0	PSCSWICLKT-----ASVLLANDRKTQGIDNRAMGNIFRDCLEGLSLR-KQGLMRSKL	1779
6Y6K_1_0	-----	1285
RVFV_L	ANVEEAHDVDYDA--LMDLMIEDAKNNAFHVDC-IELDVSGPYEMES-FHGRSTLTCT	2021
6L42_0_0	TEMVEKNVPLTTQELVDILEEDID---FSDVI-AV-ELS-EGSLDIESIFDGAPIL---	1830
6Y6K_1_0	-----	1285
RVFV_L	PSTILIRTYTFYLTTHQTMSVQAFQVILDEGVLLIALVNNYLRGSKANCWVRCESVAPK	2081
6L42_0_0	-----	1830
6Y6K_1_0	-----	1285
RVFV_L	FISAILEICEGK-RQIK-GINRT-RLSEI-VEFVLNLPKIKSRIYVLICRQCHGANFPPI	2137
6L42_0_0	-----	1830
6Y6K_1_0	----- * * * *	1285
RVFV_L	SVRRLMLEDIASVARRLIIVASFGS*	2162
6L42_0_0	-----*-	1830
6Y6K_1_0	-----*-	1285

**Figure S1.** Sequence alignment of RVFV L protein with the templates (Structure of the alpha-Synuclein (PDB ID: 6I42 and severe fever with thrombocytopenia syndrome virus L protein (PDB ID: 6Y6K)).



**Figure S2. Structural superposition of the RVFV L protein model with the templates.** The RMSD values between the model and 6I42 and 6Y6K are 0.179 and 1.165 Å, respectively.

**Table S1.** Reverse template comparison of RVFV L protein model with the representative structures in PDB using ProFunc reverse template search program.

Hit no. <sup>a</sup>	Matched PDB entry	E-value	RMSD (Å) <sup>b</sup>	Similarity score	Seq id (%)	Structural attributes	
						Longest fitted segment <sup>c</sup>	Structural similarity (%)
1	6l42	0	0.26	702.3	32.78%	1756/1756	99.9

**Note:** <sup>a</sup> Hit number corresponds to the best ranked hit from PDB (against a representative subset of structures in the PDB).

<sup>b</sup> Root-mean-square-deviation between Cα between templates (in PDB) and RVFV L protein model.

<sup>c</sup> Represents structural significant superimposition between query and template structures, which starts from a sliding window of seven residues lengthwise is slide along the alignment and the C-alpha atoms of the equivalenced residues in both structures through superimposition. The fit gives an rmsd below the cut-off of 3.0Å along the length of the window size, which extends until that cut-off.

**Table S2.** Virtual Screening result of Selleckchem Nucleoside Analogue Library (compounds with binding affinity > -1.5 kcal/mol) against model of RVFV-L RdRp core.

No.	Ligand	Binding Energy (kcal/mol)
1	VER155008	-9.6
2	S9012 Khasianine	-9.1
3	A-317491	-8.7
4	S9430 Tomatidine	-8.7
5	LLY-283	-8.5
6	Cilostazol	-8.4
7	S5461 Cimicifugoside	-8.4
8	etravirine	-8.4
9	Guanosine.	-8.3
10	NADIDE	-8.3
11	S5402 Dasabuvir(ABT-333)	-8.3
12	Fludarabine	-8.1
13	S4994 Methylcobalamin	-8.1
14	SGC_0946	-8.1
15	S5109 Ademetionine	-8
16	S5246 Entecavir.cdx uff E=616.44	-8
17	CGS-21680 hydrochloride	-7.9
18	Dapivirine	-7.9
19	S5358 Regadenoson	-7.9
20	S9007 2-Deoxyguanosine monohydrate	-7.9
21	6688	-7.8
22	Dibutyryl-cAMP	-7.8
23	S3641 Osalmid	-7.8
24	S3757 2'-Deoxyinosine	-7.8
25	S5215 Abacavir	-7.8
26	8-Bromo-cAMP	-7.7
27	Clevudine	-7.7
28	Capecitabine (Xeloda)	-7.6

29	N6-methyladenosine	-7.6
30	Blasticidin S hydrochloride	-7.5
31	Puromycin dihydrochloride	-7.5
32	Sofosbuvir(PSI-7977)	-7.5
33	CELLCEPT (mycophenolate mofetil)	-7.4
34	EPZ004777	-7.4
35	Fludara (Fludarabine Phosphate)	-7.4
36	Ribothymidine Thymine riboside	-7.4
37	Rilpivirine	-7.4
38	S3610 Cordycepin	-7.4
39	S9366 5-Adenylic acid.	-7.4
40	DIDANOSINE (didanosine)	-7.3
41	Doxifluridine.cdx uff E=510.10	-7.3
42	S5259Nicotinamide Mononucleotide	-7.3
43	S5374 5'-Cytidylic acid	-7.3
44	S9368 ADP	-7.3
45	Spongouridine 1-beta-D-Arabinofuranosyluracil	-7.3
46	TRIFLURIDINE (trifluridine)	-7.3
47	VIDAZA (azacitidine)	-7.3
48	valganciclovir hydrochloride	-7.3
49	6-Thio-dG	-7.2
50	Arranon (Nelarabine)	-7.2
51	DEPOCYT (cytarabine)	-7.2
52	Inosine	-7.2
53	S4984 2-Cyclouridine	-7.2
54	S5009 Brivudine	-7.2
55	S5582 Cytarabine hydrochloride	-7.2
56	S5678 trans-Zeatin-riboside	-7.2
57	S9369 Xanthosine Dihydrate	-7.2
58	untitled	-7.2
59	Floxuridine	-7.1
60	Gemcitabine hydrochloride	-7.1
61	Ribavirin	-7.1
62	S3737 Cangrelor Tetrasodium	-7.1
63	TYZEKA (telbivudine)	-7.1
64	Clofarabine	-7
65	Cyclocytidine hydrochloride	-7
66	Penciclovir	-7
67	S9275 Isoguanosine	-7
68	Stavudine	-7
69	VIRA-A (vidarabine)	-7
70	S5505 2-deoxyuridine	-6.9
71	Uridylic acid	-6.9
72	aicar	-6.9
73	decitabine (2-deoxy-5-azacytidine)	-6.9
74	Acyclovir	-6.8
75	Adenosine	-6.8

76	Cladribine	-6.8
77	5-Iodotubercidin	-6.7
78	S4685 Efavirenz	-6.7
79	TAS-102	-6.7
80	Tubercidin	-6.7
81	Ganciclovir	-6.6
82	HIVID (zalcitabine)	-6.6
83	NEVIRAPINE (nevirapine)	-6.6
84	NSC23766	-6.6
85	6853	-6.5
86	Azaguanine-8	-6.5
87	Emtricitabine	-6.5
88	Ftorafur	-6.5
89	GEMCITABINE (gemcitabine)	-6.5
90	5-Methyldeoxycytidine	-6.4
91	5110	-6.4
92	Mizoribine	-6.4
93	S5362 Citicholine	-6.4
94	Zidovudine	-6.4
95	Bromodeoxyuridine	-6.3
96	S4803 Thymidine	-6.3
97	Uridine	-6.3
98	Cytidine	-6.2
99	EPIVIR (lamivudine)	-6.2
100	Idoxuridine	-6.2
101	S5307 2-deoxy-2-fluoro-2-C-methyluridine	-6.2
102	SQ22536	-6.2
103	Zebularine	-6.1
104	vistonuridine	-6.1
105	LM-3264 Triapine	-6
106	5143 uff E=60.88	-5.6
107	Adrucil (Fluorouracil)	-5.5
108	Hypoxanthine	-5.5
109	S4785 Nicotinamide N-oxide	-5.3
110	S3651 4-Amino-5-imidazolecarboxamide	-5.1
111	Hydroxyurea	-4.1
112	S5016 Isoprinosine	-3.8
113	s4515 Ademetionine Ademetionine disulfate tosylate	-3.7
114	2416	-3.6
115	5383	-3.6
116	Entecavir hydrate	-1.8
117	S9351 2-Deoxyadenosine monohydrate	-1.8
118	S5284 Adenosine 5-monophosphate monohydrate	-1.7
119	S5297 Vidarabine monohydrate	-1.7