Supporting information

Lead Identification for the K-Ras Protein: Virtual screening and combinatorial fragment-based approaches

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Figures and Tables

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Figure S2: Ligands interactions with GDP bound conformation of K-Ras protein: **a).** interactions with GDP; **b).** interactions with M1; **c).** interactions with M2; **d).** interactions with M3; **e).** interactions with M4; **f).** interactions with M5; **g).** interactions with M6; **h).** interactions with M7; **i).** interactions with M8; **j).** interactions with M9; **k).** interactions with M10; **l).** interactions with M11; **m).** interactions with M12; **n).** interactions with M13. * Colour code label: H-bonding residues in brown, pi-pi and pi-cation interacting residues in green, active site residues in black, hydrophobic residues in grey.

Figure S3: Ligands interactions with GTP bound conformation of K-Ras protein: **a).** interactions with GTP; **b).** interactions with M12; **c).** interactions with M13; **d).** interactions with M14; **e).** interactions with M15; **f).** interactions with M16; **g).** interactions with M17; **h).** interactions with M18; **i).** interactions with M19; **j).** interactions with M20; **k).** interactions with M5; **l).** interactions with M21; **m).** interactions with M22; **n).** interactions with M23; **o).** interactions with M24; **p).** interactions with M25; **q).** interactions with M26; **r)**. interactions with M27; **s).** interactions with M28. * Colour code label: H-bonding residues in brown, pi-pi and pi-cation interacting residues in green, active site residues in black, hydrophobic residues in grey.

Figure S4: Contribution of H-Bond interaction of active site residues of the top 13 designed molecules for GDP bound conformation of K-Ras protein on glide docking

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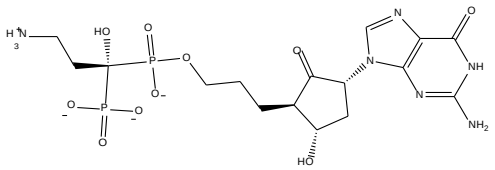
Figure S9: Contribution of Coulomb interaction of active site residues of the top 18 designed molecules for GTP bound conformation of K-Ras protein on glide docking

Figure S10: Comparison of docking methods (rigid and flexible docking) a). Top 13 designed molecules for GDP bound conformation of K-Ras protein. b). Top 18 designed molecules for GTP bound conformation of K-Ras protein.



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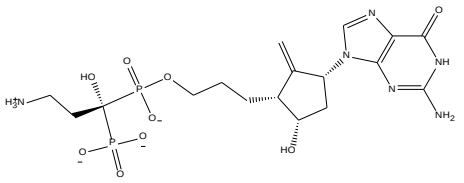

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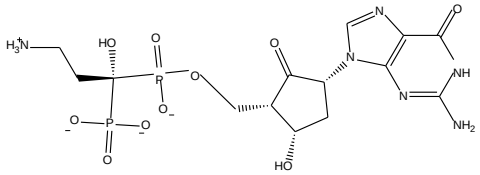

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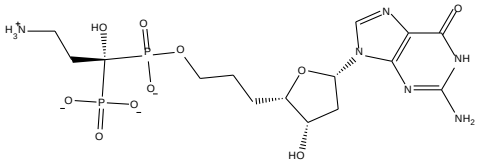

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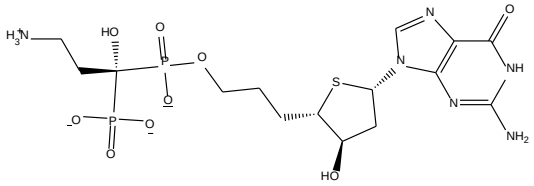

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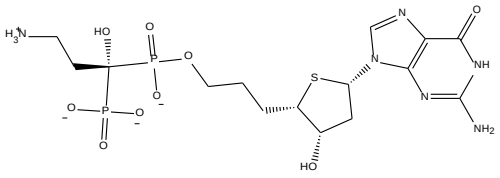

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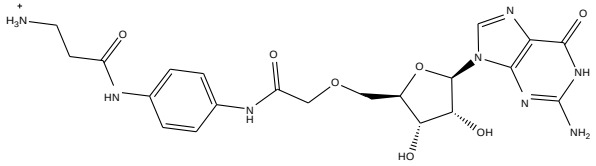

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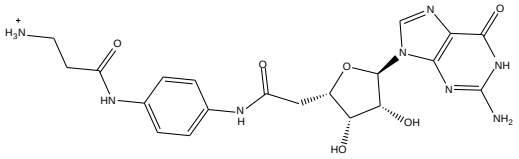

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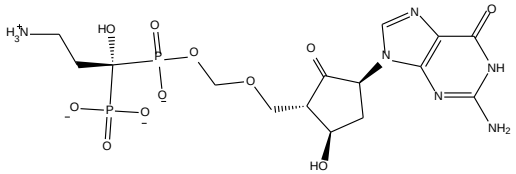

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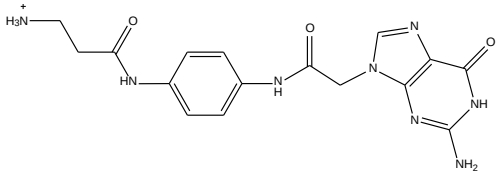

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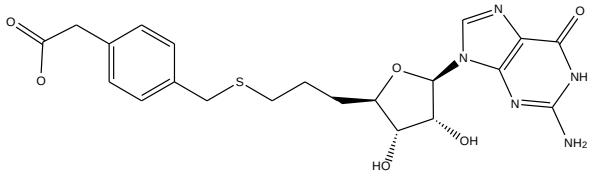

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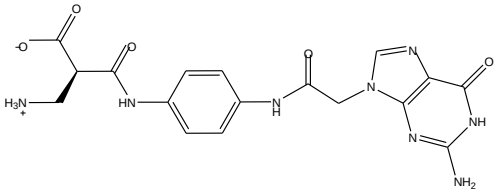

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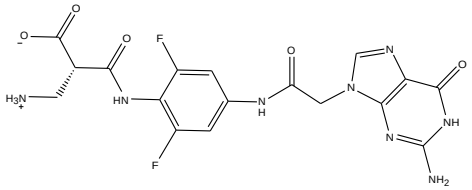

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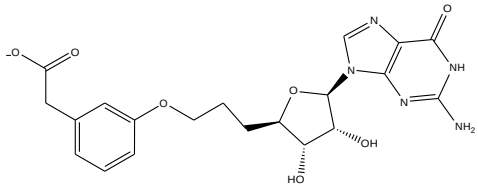

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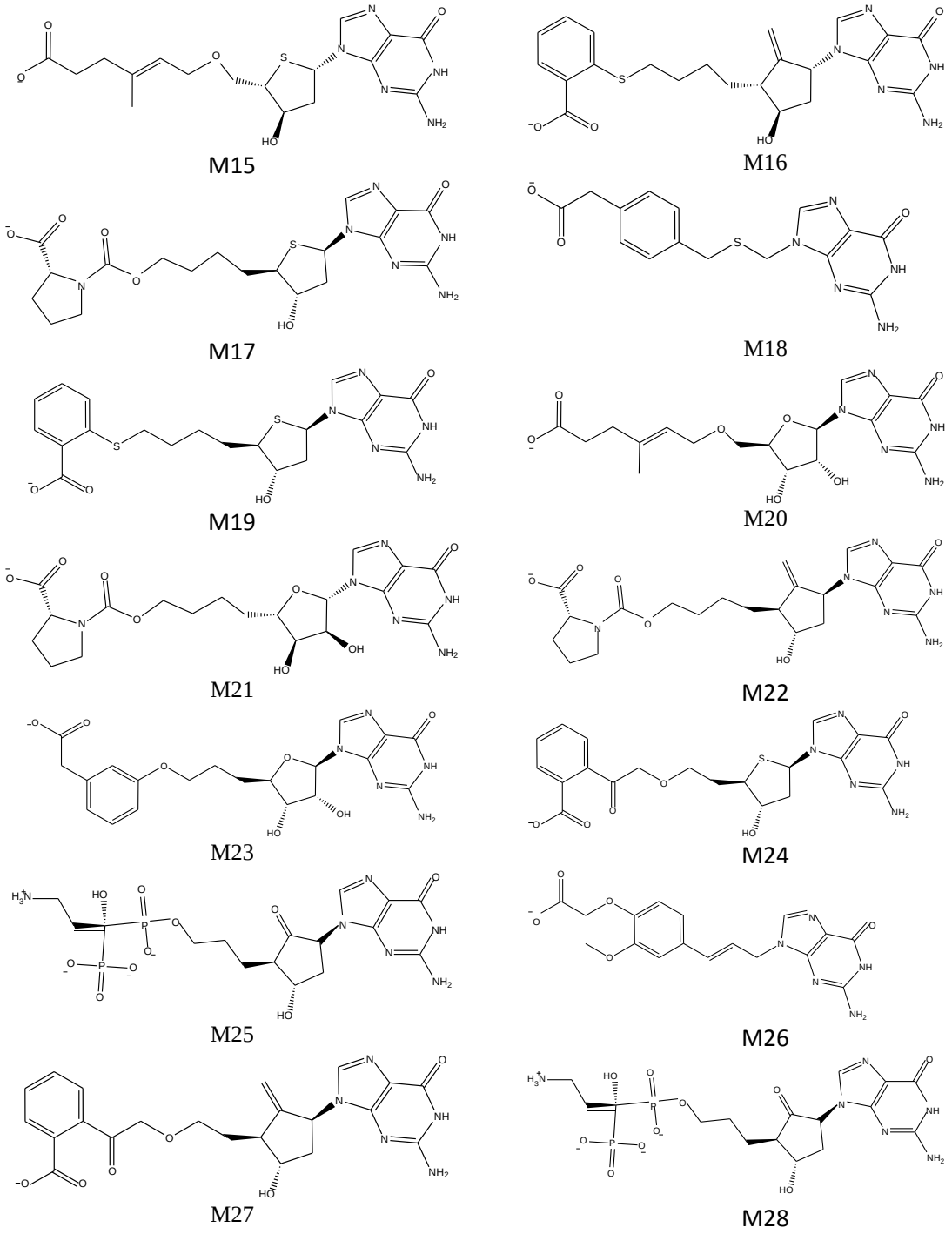
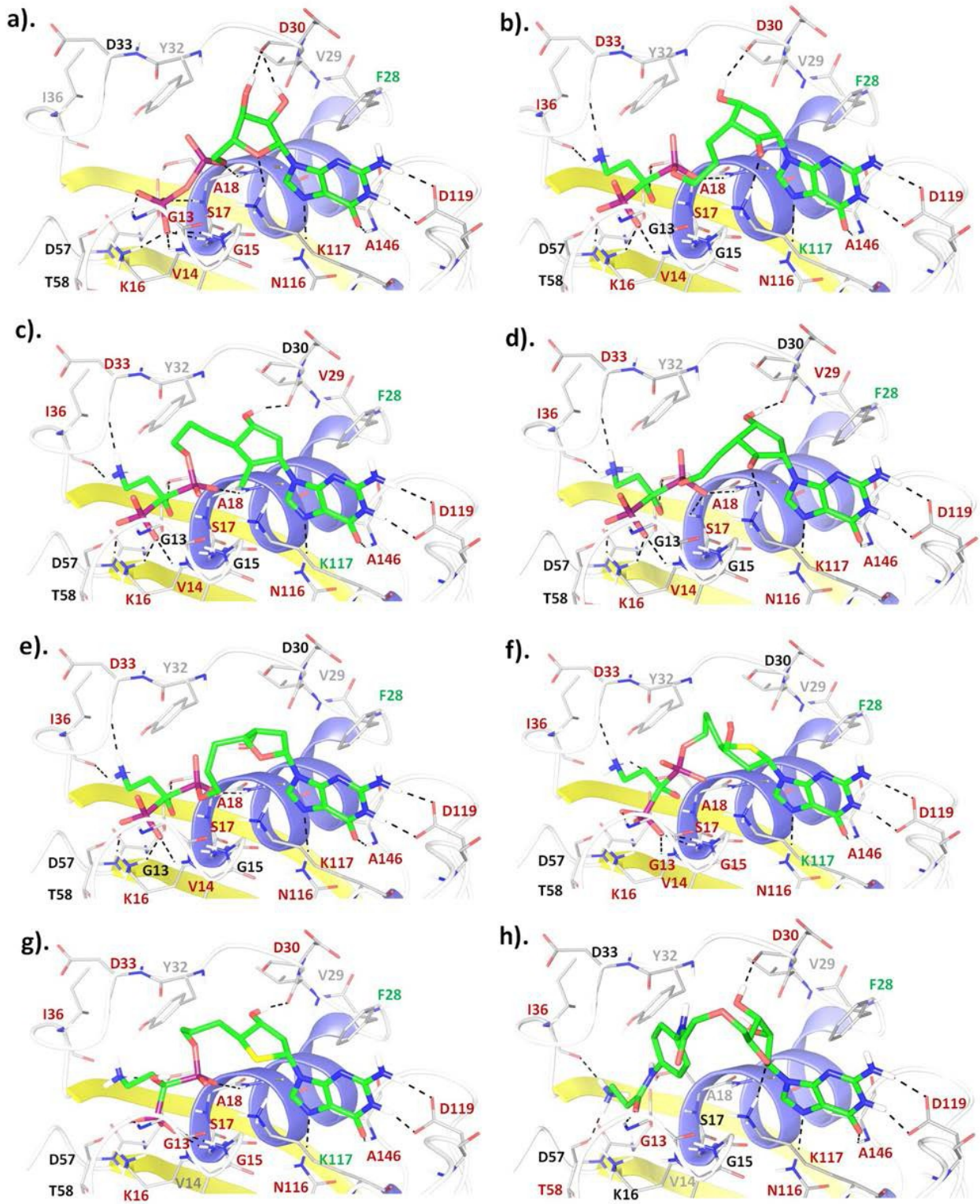


Figure S1: structure of top docking scored designed molecules for K-Ras protein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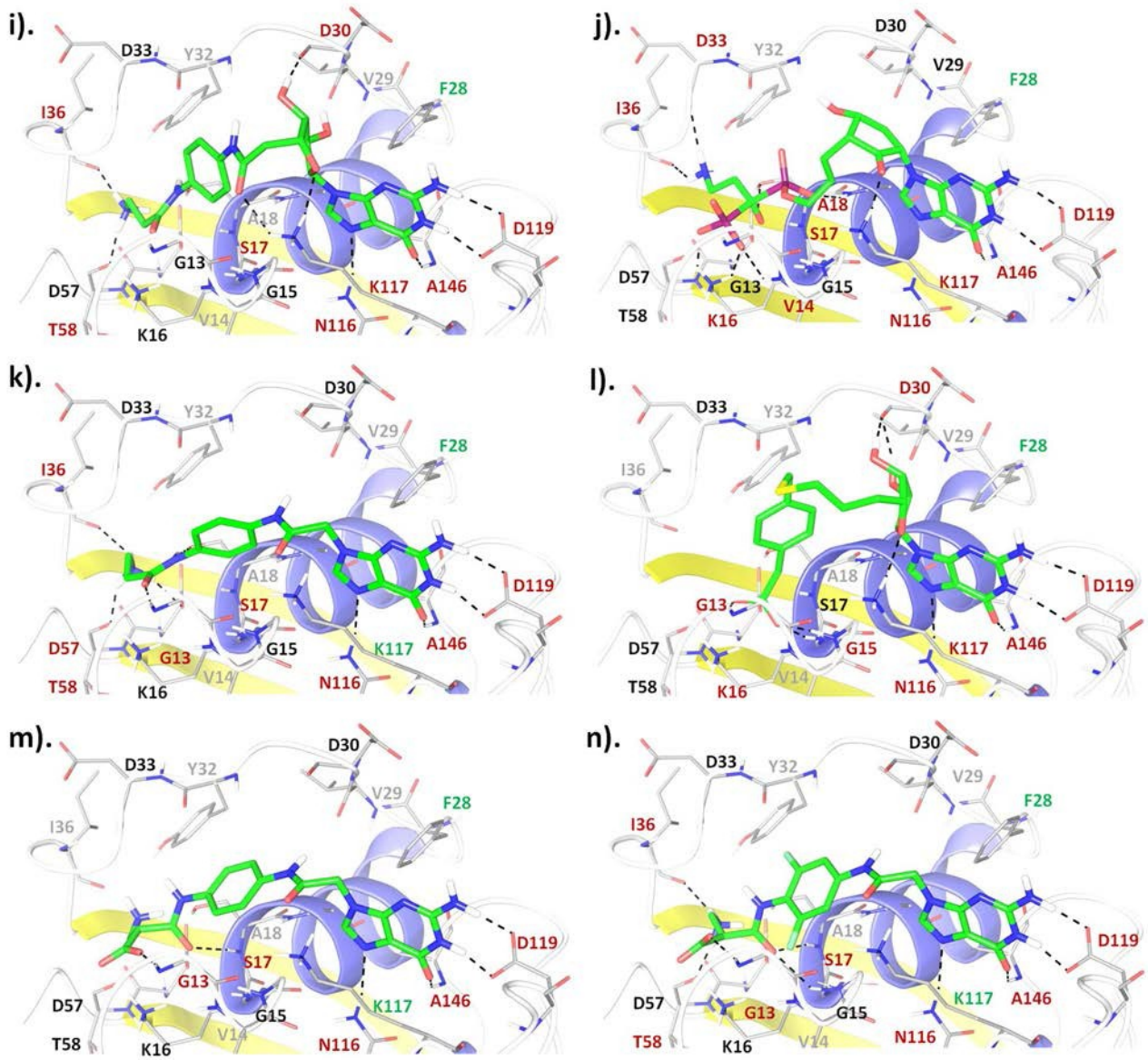
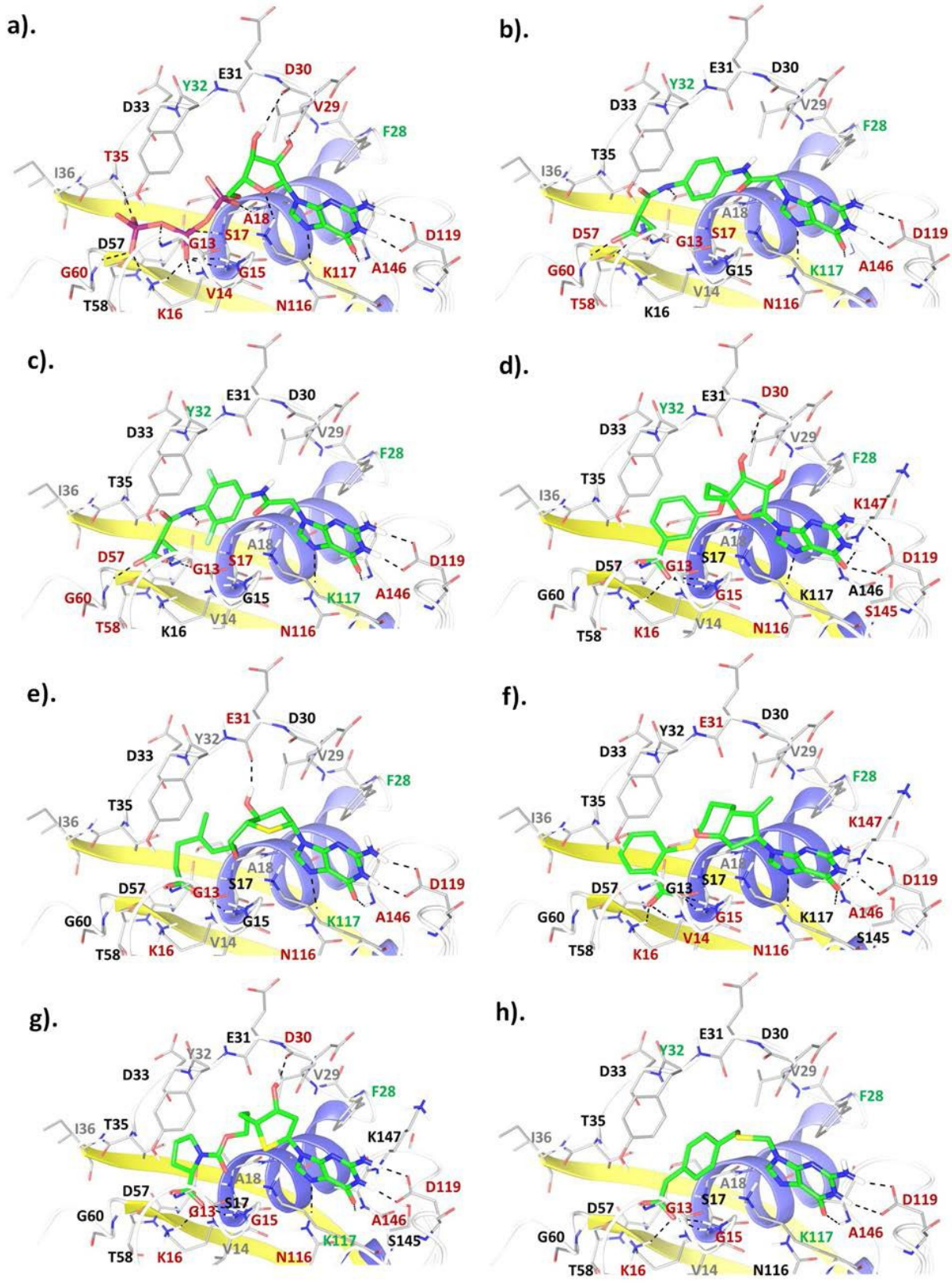


Figure S2: Ligands interactions with GDP bound conformation of K-Ras protein: **a).** interactions with GDP; **b).** interactions with M1; **c).** interactions with M2; **d).** interactions with M3; **e).** interactions with M4; **f).** interactions with M5; **g).** interactions with M6; **h).** interactions with M7; **i).** interactions with M8; **j).** interactions with M9; **k).** interactions with M10; **l).** interactions with M11; **m).** interactions with M12; **n).** interactions with M13. * Colour code label: H-bonding residues in brown, pi-pi and pi-cation interacting residues in green, active site residues in black, hydrophobic residues in grey.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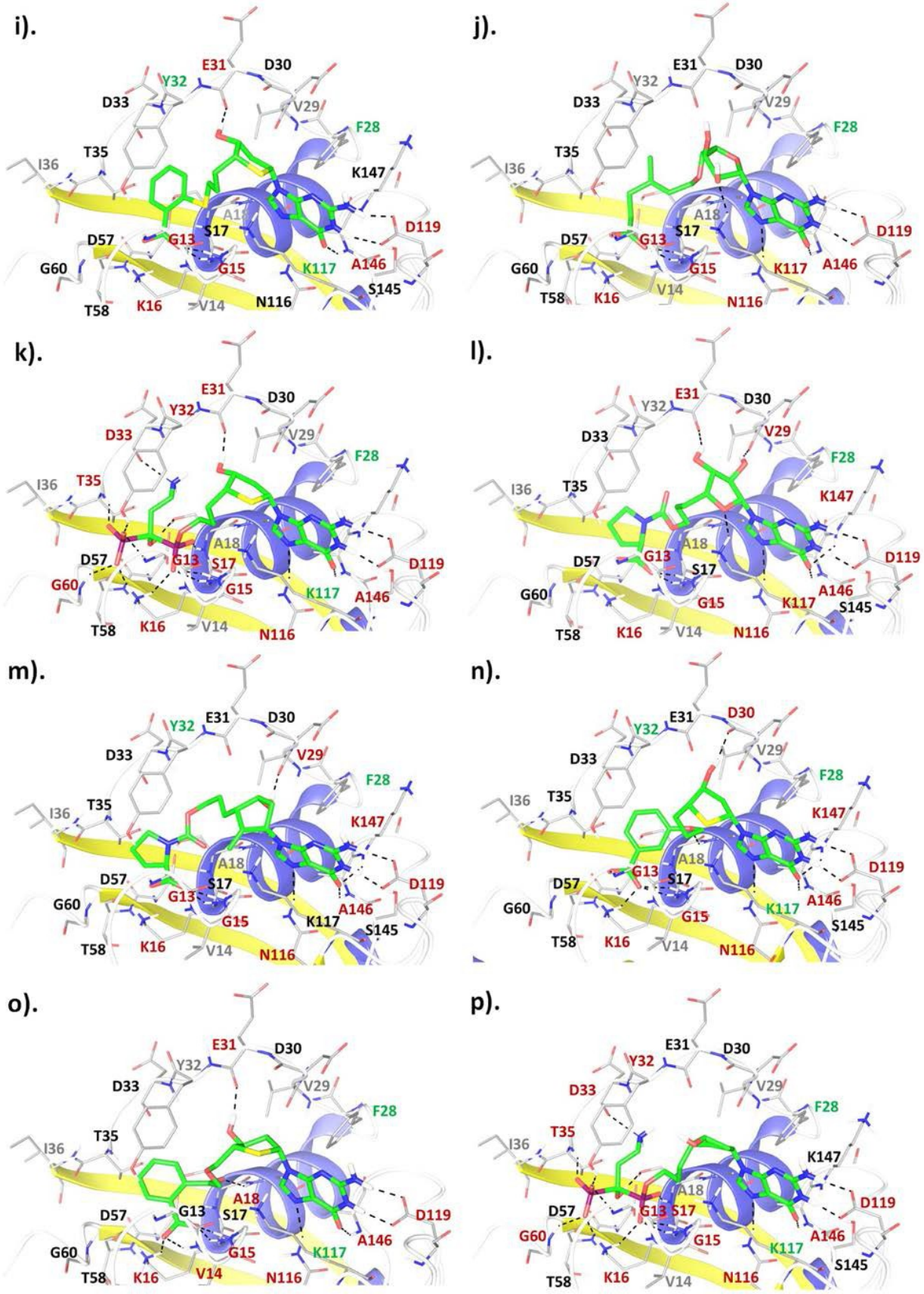
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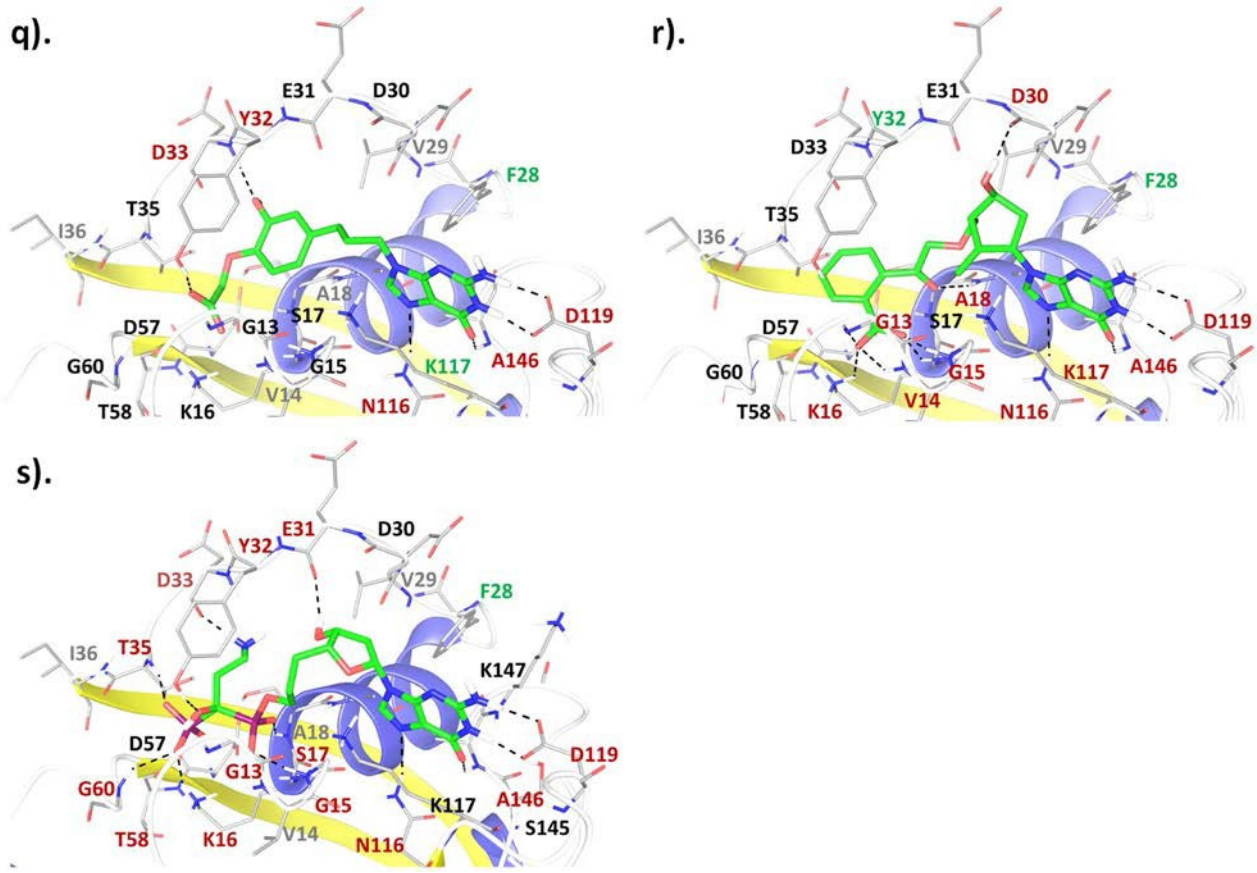

Figure S3: Ligands interactions with GTP bound conformation of K-Ras protein: **a).** interactions with GTP; **b).** interactions with M12; **c).** interactions with M13; **d).** interactions with M14; **e).** interactions with M15; **f).** interactions with M16; **g).** interactions with M17; **h).** interactions with M18; **i).** interactions with M19; **j).** interactions with M20; **k).** interactions with M5; **l).** interactions with M21; **m).** interactions with M22; **n).** interactions with M23; **o).** interactions with M24; **p).** interactions with M25; **q).** interactions with M26; **r)**. interactions with M27; **s).** interactions with M28. * Colour code label: H-bonding residues in brown, pi-pi and pi-cation interacting residues in green, active site residues in black, hydrophobic residues in grey.

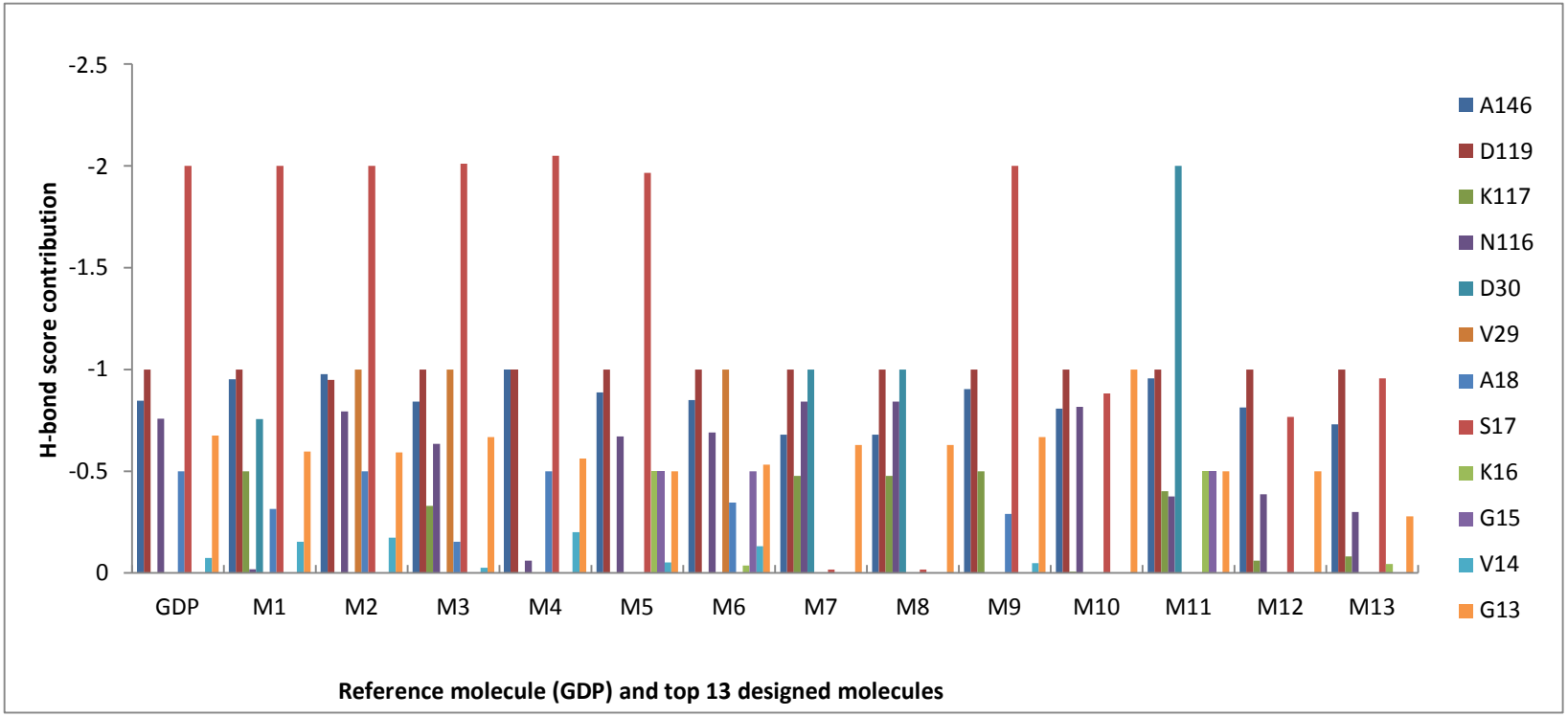

Figure S4: Contribution of H-Bond interaction of active site residues of the top 13 designed molecules for GDP bound conformation of K-Ras protein on glide docking

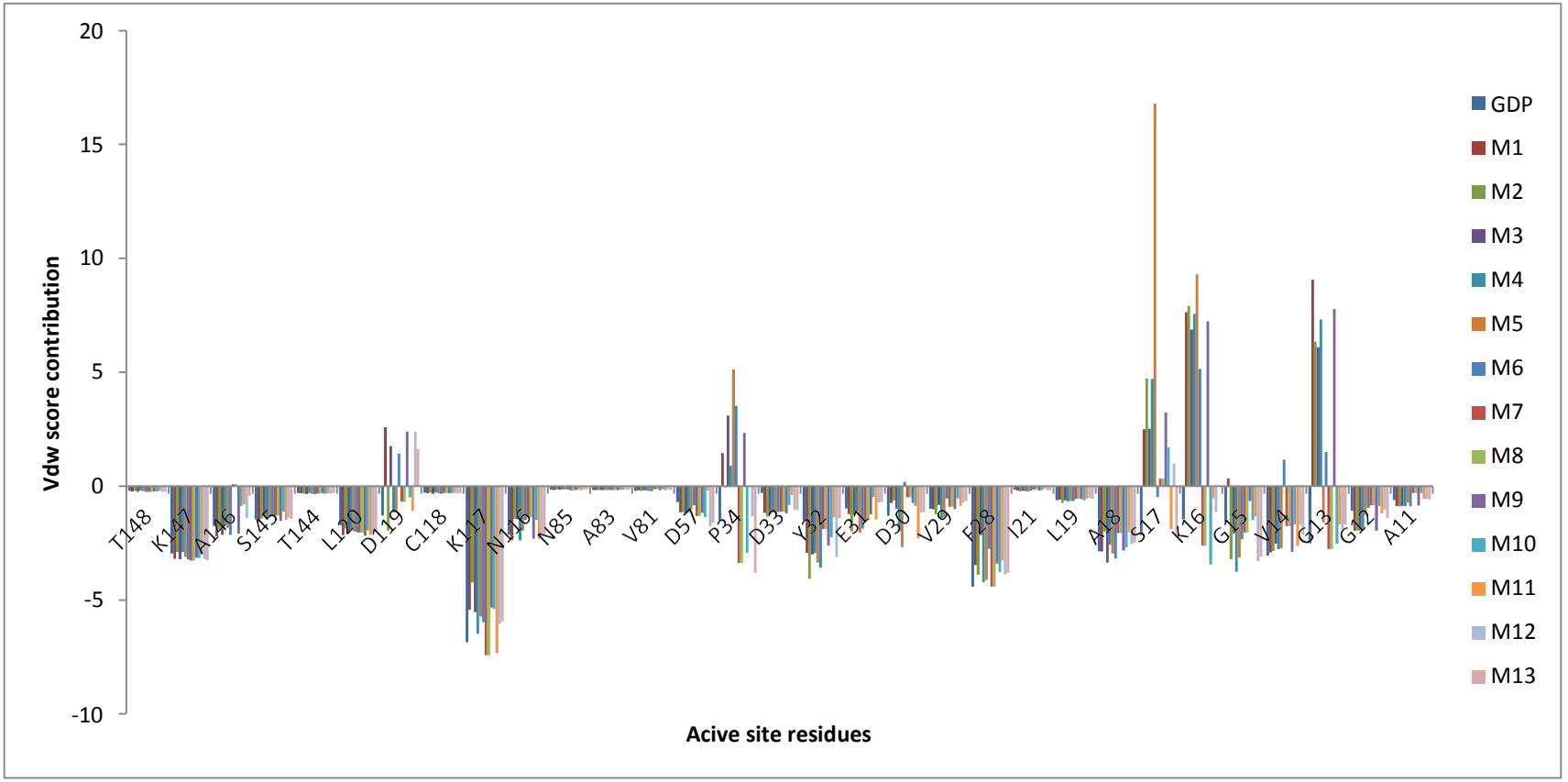

Figure S5: Contribution of Van der walls interaction of active site residues of the top 13 designed molecules for GDP bound conformation of K-Ras protein on glide docking.

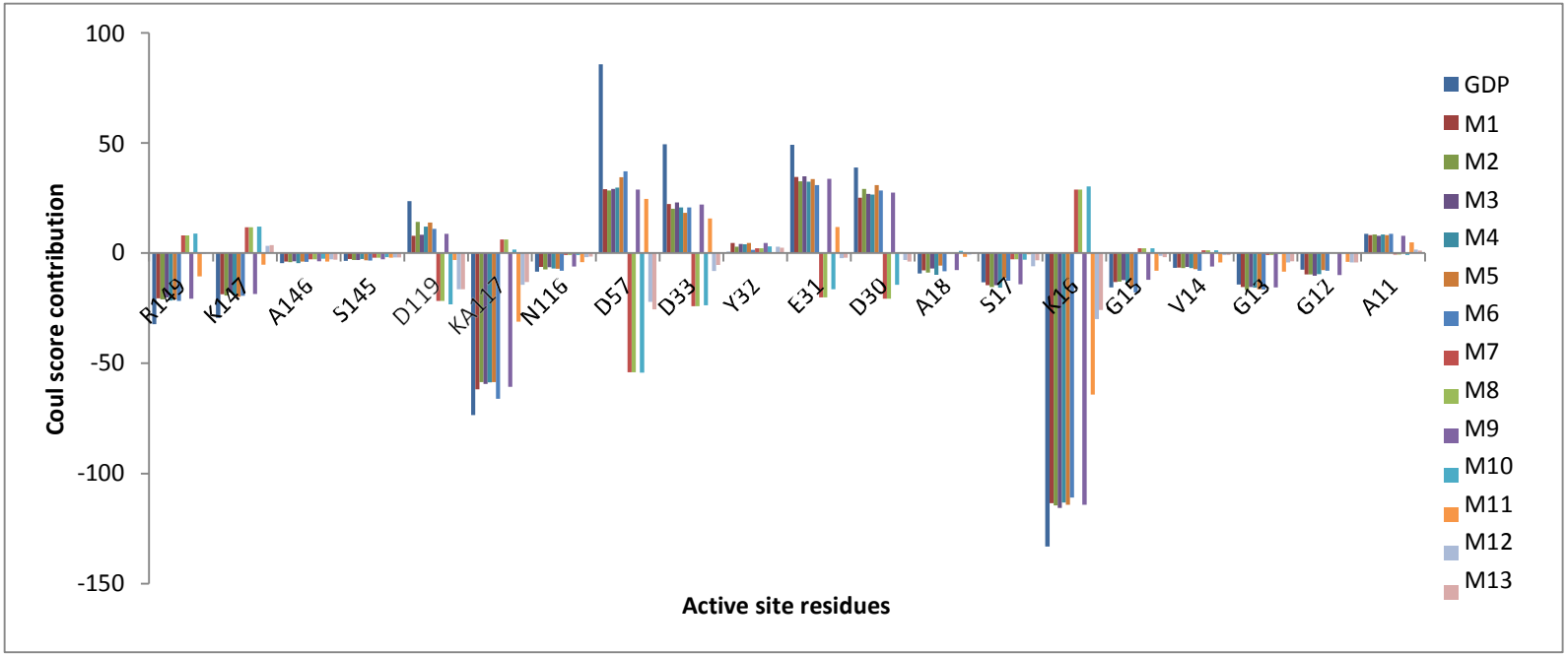

Figure S6: Contribution of Coulomb interaction of active site residues of the top 13 designed molecules for GDP bound conformation of K-Ras protein on glide docking.

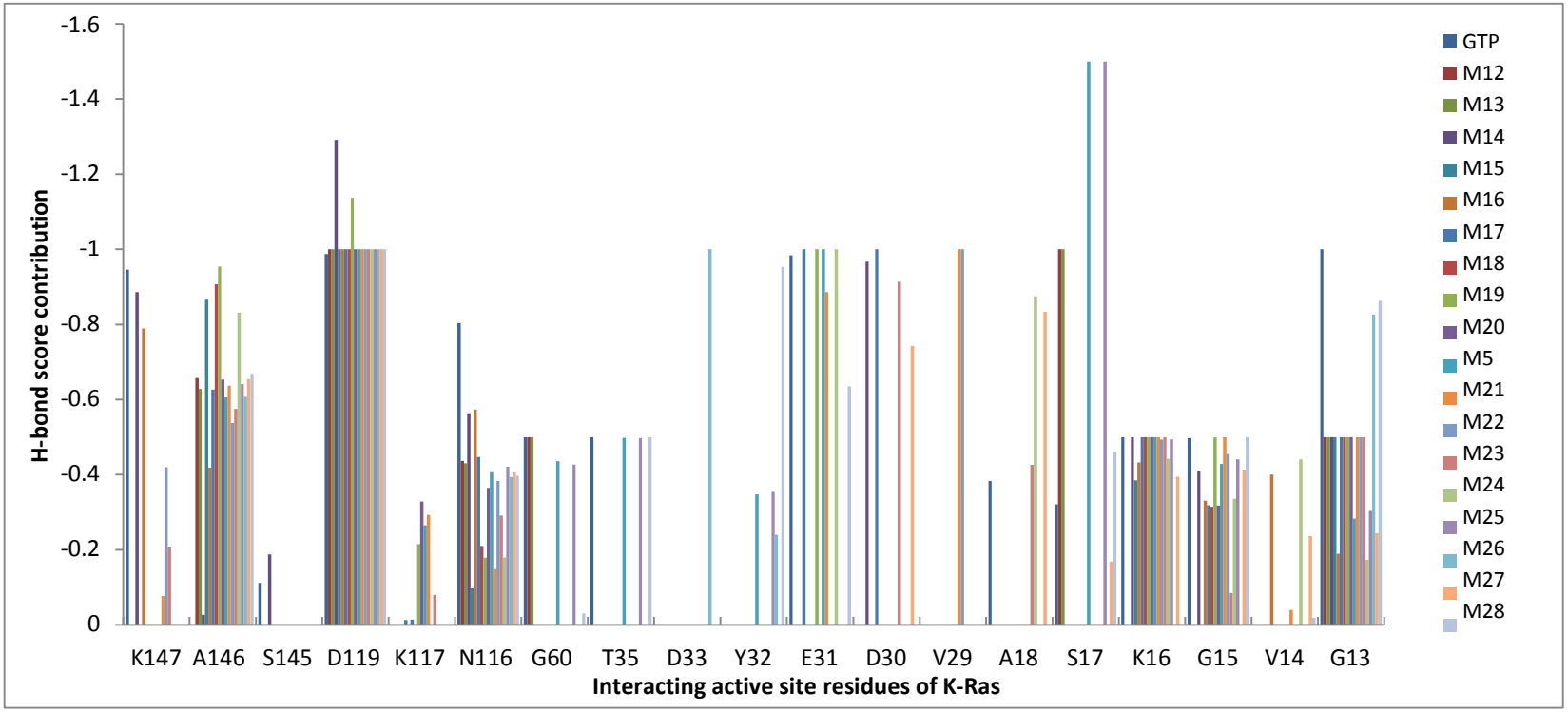

Figure S7: Contribution of H-Bond interaction of active site residues of the top 18 designed molecules for GTP bound conformation of K-Ras protein on glide docking.

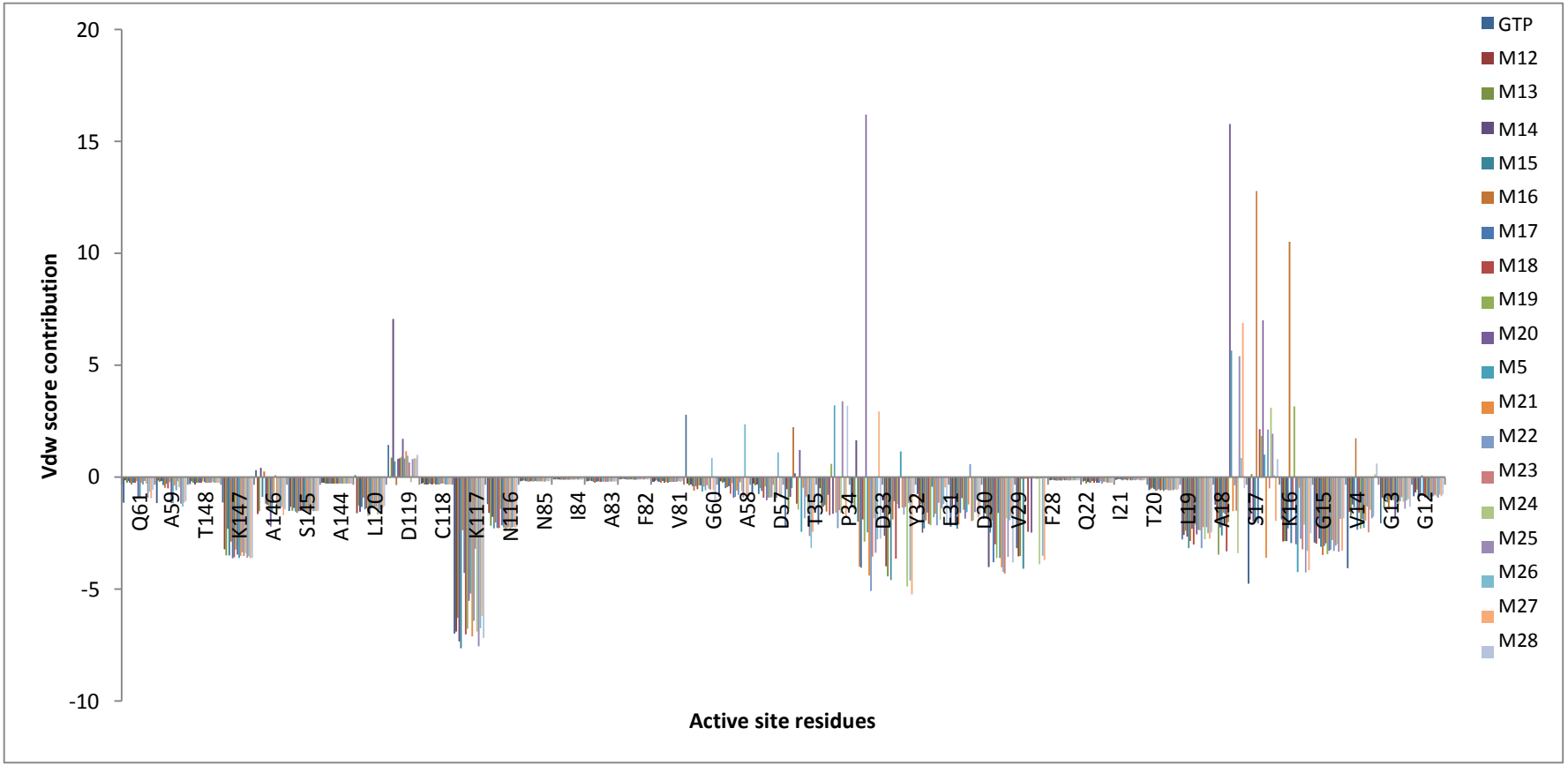

Figure S8: Contribution of Van der walls interaction of active site residues of the top 18 designed molecules for GTP bound conformation of K-Ras protein on glide docking.

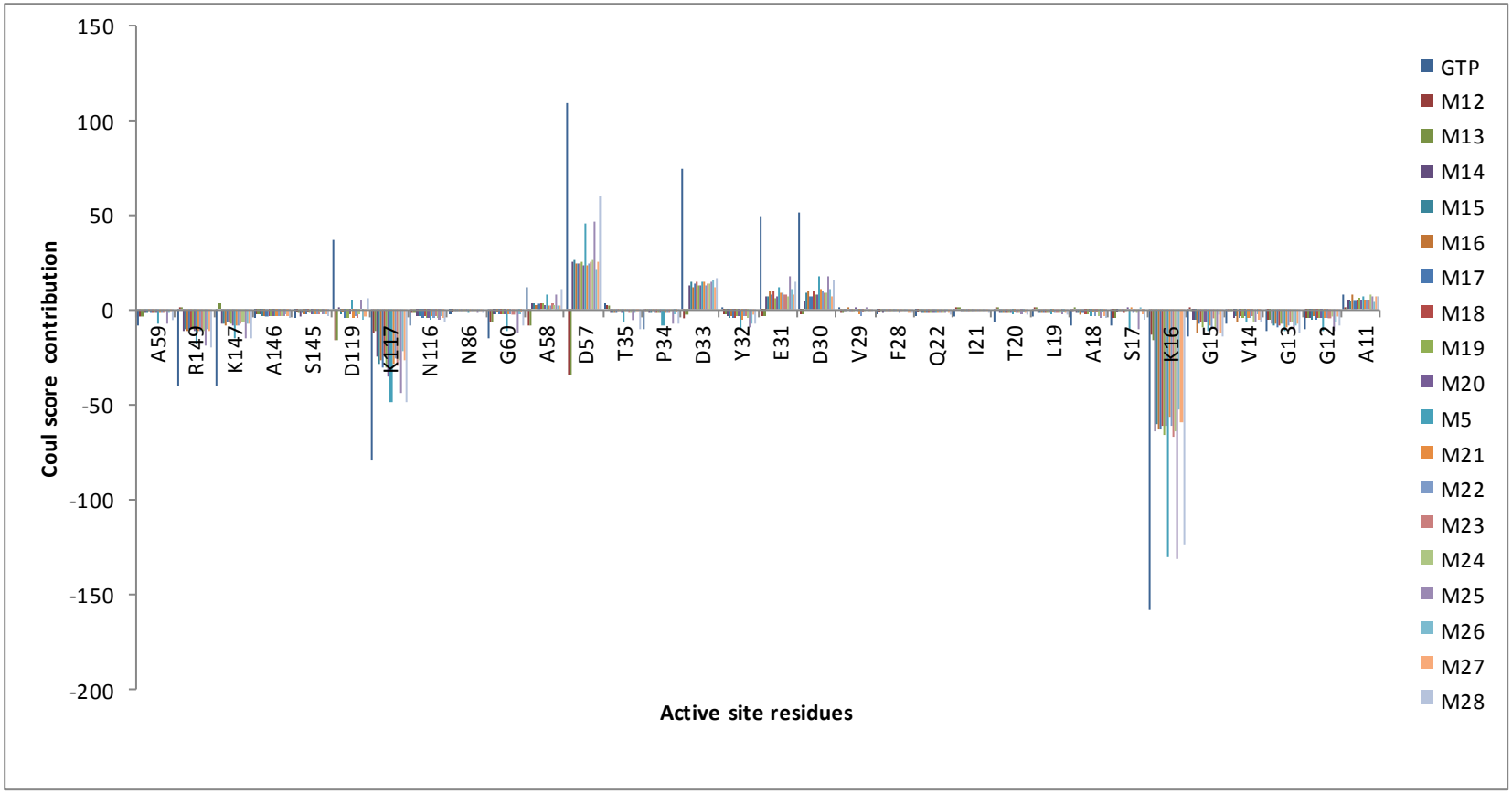

Figure S9: Contribution of Coulomb interaction of active site residues of the top 18 designed molecules for GTP bound conformation of K-Ras protein on glide docking

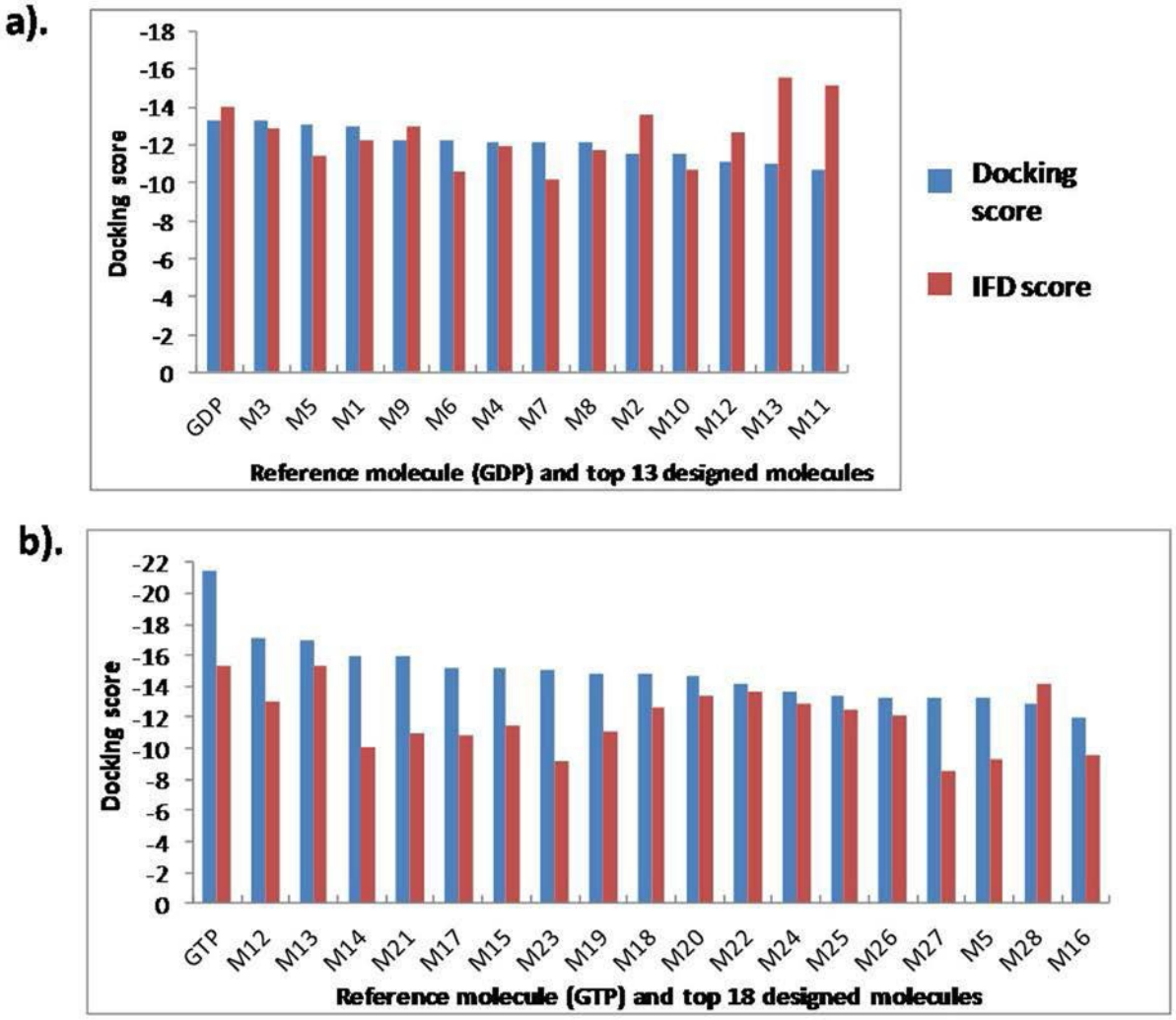

Figure S10: Comparison of docking methods (rigid and flexible docking) **a).** Top 13 designed molecules for GDP bound conformation of K-Ras protein. **b).** Top 18 designed molecules for GTP bound conformation of K-Ras protein

Tables

Table S1: Docking score and other energy parameters of top ranked compounds in docking

Molecules	Database		Mol_id	DockScore	LipophilicEvdW	PhobEn	PhobEnHB	PhobEnPairHB	HBond	Electro	Sitemap	LowMW	Penalties	ExposPenal	RotPenal	EpikStatePenalty
Reference molecule			GDP	-13.33	-1.89	0.00	-0.94	0.00	-4.47	-6.00	0.00	-0.03	0.00	0.00	0.00	0.00
Screened molecules from databases	NCI Diversity set		NSC 1945	-9.21	-0.64	0.00	0.00	0.00	-6.8	-2.00	0.00	-0.50	0.00	0.00	0.73	0.00
	Asinex		70014	-8.66	-2.06	0.00	0.00	-1.95	-2.36	-1.88	-0.27	-0.4	0.00	0.00	0.26	0.00
	Chembridge	kinaSet	5686	-8.42	-2.53	0.00	-1.00	-1.95	-1.98	-1.19	-0.37	-0.39	0.58	0.10	0.31	0.00
		kinaCore	6841	-7.88	-2.31	-0.17	0.00	-1.95	-1.96	-1.08	-0.4	-0.23	0.00	0.09	0.12	0.00
	DrugBank		DB000442	-7.61	-1.84	0.00	-1.00	0.00	-2.99	-1.09	-0.52	-0.50	0.00	0.13	0.20	0.00
	PubChem	HRAS Assay	1085315	-6.62	-2.50	0.00	-1.50	0.00	-2.01	-0.90	0.00	-0.18	0.00	0.10	0.37	0.00
		kinase inhibitor	3134	-5.11	-1.19	0.00	-1.50	0.00	-1.04	-0.43	-0.74	-0.50	0.00	0.00	0.00	0.29
	BindingDB		888706	-4.55	-1.66	0.00	0.00	0.00	-1.47	-1.25	0.00	-0.50	0.00	0.00	0.34	0.00

Dock score- Docking score, **Lipophilic EvdW**- Lipophilic term derived from hydrophobic grid potential at hydrophobic grid potential at the hydrophobic ligand atoms, **PhobEnHB**- Hydrophobic enclosure reward, **PhobEnPairHB**- Reward for hydrophobically packed H-bond**, PhobEnPairHB**- Rewards for hydrophobically packed correlated H-bond, **HBond**- chemScore H-bond pair term, **Electro**- Electrostatic rewards; includes coulomb and metal terms, **SiteMap**- SiteMap ligand-receptor non-H-bonding polar hydrophobic terms, **LowMW**- Reward for ligands with low molecular weight, **Penalties**- polar atom burial and desolvation penalties, and penalty for intra-ligand contacts

NCI Diversity set: https://dtp.cancer.gov/organization/dscb/obtaining/available_plates.htm

Asinex: http://www.asinex.com/download-zone.html

Chembridge: http://www.chembridge.com/screening_libraries/targeted_libraries/index.php

DrugBank: http://www.drugbank.ca/downloads#structures

PubChem: https://pubchem.ncbi.nlm.nih.gov/bioassay/759#section=Top, http://www.ncbi.nlm.nih.gov/pccompound/?term=kinase+inhibitors

BindingDB: https://www.bindingdb.org/jsp/dbsearch/PrimarySearch_ki.jsp?target=ras+protein&tag=tg&kiunit=nM&icunit=nM&column=ki&submit=Search&energyterm=kJ%2Fmole

Table S2: Contribution of interactions parameters in docking score of GDP and top 13 designed molecules

Mol	Dock Score	Lipophilic EvdW	PhobEn HB	PhobEn PairHB	HBond	Electro	Site map	Low MW	Penal ties	Expos Penalty	Rot Penalty	Epik State Penalty
GDP	-13.33	-1.89	-0.94	0.00	-4.47	-6.00	0.00	-0.03	0.0	0.00	0.00	0.00
M3	-13.30	-1.30	0.00	-1.95	-6.36	-3.50	-0.50	0.00	0.0	0.09	0.17	0.05
M5	-13.05	-1.69	0.00	-1.95	-5.69	-3.50	-0.51	0.00	0.0	0.04	0.18	0.07
M1	-12.94	-1.25	0.00	-1.95	-6.11	-3.50	-0.48	0.00	0.0	0.12	0.18	0.05
M9	-12.25	-1.24	0.00	-1.95	-5.43	-3.50	-0.48	0.00	0.0	0.11	0.18	0.05
M6	-12.21	-1.53	0.00	-1.95	-4.93	-3.50	-0.54	0.00	0.0	0.00	0.18	0.07
M4	-12.18	-1.86	-1.00	0.00	-5.95	-3.50	-0.47	0.00	0.0	0.27	0.27	0.06
M7	-12.12	-2.30	0.00	-1.82	-4.47	-3.30	-0.52	0.00	0.0	0.06	0.24	0.00
M8	-12.12	-2.30	0.00	-1.82	-4.47	-3.30	-0.52	0.00	0.0	0.06	0.24	0.00
M2	-11.51	-1.79	-1.00	0.00	-6.58	-3.50	-0.43	0.00	1.5	0.00	0.26	0.03
M10	-11.51	-2.14	0.00	-1.95	-3.44	-3.50	-0.54	-0.26	0.0	0.00	0.29	0.03
M12	-11.15	-2.03	0.00	-1.95	-3.61	-3.50	-0.52	-0.12	0.0	0.02	0.24	0.31
M13	-11.00	-2.26	0.00	-1.95	-3.27	-3.50	-0.55	0.00	0.0	0.01	0.21	0.31
M11	-10.65	-2.04	-1.00	0.00	-5.72	-2.00	-0.49	0.00	0.0	0.27	0.31	0.04

[#]Order of molecules are given based on docking score ranking

DockScore- Docking score, **Lipophilic EvdW-** Lipophilic term derived from hydrophobic grid potential at hydrophobic grid potential at the hydrophobic ligand atoms, **PhobEn HB-** Hydrophobic enclosure reward, **PhobEnPairHB-** Reward for hydrophobically packed H-bond**, PhobEnPairHB-** Rewards for hydrophobically packed correlated H-bond, **HBond-** chemScore H-bond pair term, **Electro-** Electrostatic rewards; includes coulomb and metal terms, **SiteMap-** SiteMap ligand-receptor non-H-bonding polar hydrophobic terms, **LowMW-** Reward for ligands with low molecular weight, **Penalties-** polar atom burial and desolvation penalties, and penalty for intra-ligand contacts.

Table S3: Contribution of interaction parameters in docking score of GTP and top 18 designed molecules.

Mol	DockScore	Lipophilic EvdW	PhobEn PairHB	HBond	Electro	Sitemap	LowMW	ExposPenal	RotPenal	EpikState Penalty
GTP	-21.47	-1.47	-3.29	-7.70	-7.0	0.00	0.00	0.00	0.00	0.00
M12	-17.06	-2.61	-5.06	-4.73	-4.5	-0.59	-0.12	0.00	0.24	0.31
M13	-17.00	-2.66	-5.11	-4.71	-4.5	-0.53	0.00	0.00	0.21	0.31
M14	-15.90	-1.75	-7.47	-4.50	-2.0	-0.43	-0.07	0.08	0.19	0.04
M21	-15.89	-2.28	-6.74	-4.61	-2.0	-0.51	0.00	0.00	0.21	0.04
M17	-15.17	-1.99	-7.03	-4.03	-2.0	-0.54	0.00	0.17	0.21	0.04
M15	-15.14	-2.52	-7.15	-3.34	-2.0	-0.35	-0.14	0.07	0.25	0.04
M23	-15.04	-2.34	-6.35	-4.21	-2.0	-0.30	-0.07	0.00	0.19	0.04
M19	-14.86	-1.87	-7.15	-3.88	-2.0	-0.24	-0.01	0.07	0.18	0.04
M18	-14.85	-2.48	-7.15	-3.05	-2.0	-0.09	-0.35	0.00	0.24	0.03
M20	-14.68	-2.41	-7.13	-2.97	-2.0	-0.32	-0.14	0.00	0.25	0.04
M22	-14.14	-2.49	-6.10	-3.46	-2.0	-0.29	-0.02	0.00	0.21	0.00
M24	-13.62	-1.77	-5.20	-4.35	-2.0	-0.62	-0.02	0.11	0.18	0.04
M25	-13.45	-2.14	-1.89	-7.18	-2.0	-0.45	0.00	0.00	0.18	0.03
M26	-13.31	-2.65	-5.09	-3.18	-2.0	-0.33	-0.27	0.00	0.21	0.00
M27	-13.29	-2.06	-5.01	-3.96	-2.0	-0.49	-0.04	0.07	0.19	0.00
M5	-13.24	-2.21	-1.85	-7.06	-2.0	-0.36	0.00	0.00	0.18	0.07
M28	-12.83	-1.87	-1.78	-7.08	-2.0	-0.35	0.00	0.00	0.19	0.06
M16	-12.05	-1.41	-5.20	-3.30	-2.0	-0.29	-0.03	0.00	0.19	0.00

#Order of molecules are given based on docking score ranking

DockScore- Docking score, **Lipophilic EvdW-** Lipophilic term derived from hydrophobic grid potential at hydrophobic grid potential at the hydrophobic ligand atoms, **PhobEnHB-** Hydrophobic enclosure reward, **PhobEnPairHB-** Reward for hydrophobically packed H-bond**, PhobEnPairHB-** Rewards for hydrophobically packed correlated H-bond, **HBond-** chemScore H-bond pair term, **Electro-** Electrostatic rewards; includes coulomb and metal terms, **SiteMap-** SiteMap ligand-receptor non-H-bonding polar hydrophobic terms, **LowMW-** Reward for ligands with low molecular weight, **Penalties-** polar atom burial and desolvation penalties, and penalty for intra-ligand contact

Table S4: Interaction map of GDP and top 13 designed molecules

Mol	G13	V14	G15	K16	S17	A18	F28	V29	D30	D33	I36	D57	T58	N116	K117	D119	A146
GDP	√	√	√	√, o	√	√	x		√					√	√, x	√	√
M1		√		√	√	√	x		√	√	√	o		√	√, x	√	√
M2		√		√	√	√	x	√		√	√	o		√	x	√	√
M3		√		√	√	√	x	√		√	√	o		√	√	√	√
M4		√		√	√	√	x			√	√	o		√	x	√	√
M5	√	√	√	√, o	√		x			√	√	o		√	x	√	√
M6	√		√	√, o	√	√	x	√				o		√	x, o	√	√
M7	√						x		√		√	o	√	√	√	√	√
M8				√	√		x		√		√	o	√	√	√	√	√
M9		√		√	√	√	x			√	√	o			√, x	√	√
M10	√				√						√		√	√		√	√
M11	√		√	√			x		√					√	√, x	√	√
M12	√			√	√									√	√	√	√
M13	√			√	√		x				√	o	√	√	√	√	√

'√' represents H-bond interaction, "x" represents hydrophobic interaction and "o" represents salt bridge

Table S5: Interaction map of GTP and top 18 designed molecules

Mol	G13	V14	G15	K16	S17	A18	F28	V29	D30	E31	Y32	D33	T35	I36	D57	T58	G60	N116	K117	D119	S145	A146	K147
GTP	√	√	√	√, o	√	√	X	√	√				√				√	√	√, x	√		√	
M12	√			o	√		x				x				√	√	√	√	√	√		√	
M13	√			√	√		x				√				√	√	√	√	x	√		√	
M14	√		√	√			x		√		√							√	√	√	√		√
M15	√		√	√			x			√	√							√	√	√		√	
M16		√	√	√			x			√								√	x	√		√	√
M17			√	√			x			√								√	√	√		√	
M18	√		√	√			x				x							√	x	√		√	
M19	√		√	√			x			√	x							√	x	√		√	
M20	√		√	√, o			x				√							√	√, x	√		√	
M5	√		√	√, o	√		x			√	√		√				√	√	x	√		√	
M21	√		√	√			x	√		√	√							√	√, x	√		√	√
M22	√		√	√, o			x	√			√							√		√		√	√
M23	√		√	√		√	x		√									√	x	√		√	√
M24		√	√	√		√	x			√								√	x	√		√	
M25	√		√	√, o	√		x					√	√				√	√	x	√		√	
M26				o			x				√							√	√	√		√	
M27	√	√	√	√		√	x		√		x							√		√		√	
M28	√		√	√, o	√		x			√	√	√	√		√		√	√	x	√		√	

'√' represents H-bonding interaction, "x" represents hydrophobic interaction and "o" represents salt bridge

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Table S6: ADME/T properties of designed and screened top 13 GDP molecules

Title	#stars	#amine	#acid	#rotor	#rtv FG	CNS	mol MW	dipole	SASA	FOSA	FISA	PISA	WPSA	volume	donor HB	accpt HB
4OBE _GDP	6	0	3	11	2	-2	443.20	17.98	612.74	80.37	493.50	035.65	03.23	1081.45	5	17.60
M1	7	1	3	16	2	-2	524.36	05.79	712.37	184.21	497.09	030.81	00.26	1334.74	7	17.95
M2	7	1	3	16	1	-2	522.39	11.00	721.00	217.35	449.59	053.41	00.65	1349.04	7	15.95
M3	6	1	3	15	2	-2	510.34	06.71	718.96	162.22	512.46	042.43	01.85	1302.92	7	17.95
M4	7	1	3	16	1	-2	512.35	03.63	706.41	240.18	436.44	029.46	00.33	1303.64	7	17.65
M5	9	1	3	16	1	-2	528.41	17.59	713.38	198.54	452.36	044.85	17.64	1331.37	7	16.45
M6	8	1	3	16	1	-2	528.41	15.74	716.82	203.42	442.46	043.12	27.82	1334.78	7	16.45
M7	7	1	0	12	0	-2	502.49	15.11	765.52	216.95	392.91	155.67	00.00	1408.21	8	17.30
M8	7	1	0	10	0	-2	472.46	16.18	739.89	169.86	410.98	159.05	00.00	1339.89	8	15.60
M9	7	1	3	16	2	-2	524.36	05.10	720.48	187.83	499.04	033.20	00.42	1339.68	7	17.95
M10	2	1	0	08	0	-2	370.37	11.45	658.32	129.90	355.14	173.28	00.00	1129.54	6	10.50
M11	2	0	1	11	0	-2	475.52	14.03	705.09	217.83	328.14	125.68	33.45	1319.93	6	13.10
M12	5	1	1	09	0	-2	414.38	16.65	682.89	80.58	423.46	178.85	00.00	1188.16	5	10.50
M13	4	1	1	09	0	-2	450.36	11.17	691.99	77.53	425.95	126.03	62.48	1214.96	5	10.50

Title	dip^2 /V	ACxDN ^.5/SA	glob	QPpolrz	QPlog PC16	QPlog Poct	QPlogPw	QPlog Po/w	QPlogS	CIQP logS	QPlog HERG	QPPC aco	QPlog BB	QPPM DCK	QPlogK p
4OBE _GDP	0.30	0.06	0.83	30.40	13.14	31.95	27.03	-2.69	-1.25	-2.05	1.00	0.00	-4.85	0.00	-9.43
M1	0.03	0.07	0.82	37.28	15.92	33.58	29.43	-4.14	-1.01	-2.20	0.15	0.00	-4.90	0.00	-11.10
M2	0.09	0.06	0.82	38.07	15.88	33.45	27.31	-3.08	-1.41	-2.84	-0.02	0.00	-4.47	0.00	-10.14
M3	0.03	0.07	0.80	36.76	15.88	33.56	29.85	-4.46	-1.25	-1.96	-0.24	0.00	-5.24	0.00	-11.44
M4	0.01	0.07	0.82	36.03	15.21	32.43	28.70	-3.80	-1.00	-2.09	0.06	0.00	-4.36	0.00	-09.99
M5	0.23	0.06	0.82	37.28	15.80	35.49	27.75	-3.29	-1.33	-2.78	0.05	0.00	-4.44	0.00	-10.23
M6	0.19	0.06	0.82	37.40	15.83	34.88	27.68	-3.17	-1.41	-2.78	0.01	0.00	-4.34	0.00	-10.05
M7	0.16	0.06	0.79	43.98	17.05	38.62	31.40	-2.57	-1.67	-2.35	-6.34	0.46	-3.92	0.14	-09.12
M8	0.20	0.06	0.79	42.57	16.57	37.80	30.25	-2.50	-1.97	-2.41	-6.34	0.31	-3.98	0.09	-09.64
M9	0.02	0.07	0.82	37.50	16.01	33.56	29.48	-4.15	-1.09	-2.20	0.02	0.00	-5.00	0.00	-11.13
M10	0.12	0.04	0.80	35.57	13.79	28.37	22.26	-1.30	-2.17	-2.39	-6.37	1.06	-3.25	0.33	-08.75
M11	0.15	0.05	0.83	40.81	15.27	32.09	23.78	0.27	-3.21	-4.45	-3.15	1.94	-3.23	1.12	-06.07
M12	0.23	0.03	0.79	37.33	14.67	29.46	21.14	-2.65	-3.07	-3.21	-4.63	0.06	-4.05	0.02	-09.89
M13	0.10	0.03	0.80	37.89	14.16	28.12	20.84	-2.33	-3.47	-3.87	-4.36	0.06	-3.91	0.04	-10.12

Title	IP(eV)	EA(eV)	#metab	QPlog Khsa	Human OralAbsorption	%Human OralAbsorption	SAfluorine	PSA	#NandO	RuleOf Five	RuleOf Three	#ring atoms	#in56	#nonconn	#nonHatm
4OBE_GDP	8.22	0.08	3	-2.04	1	0.00	0.00	264.45	16	2	1	14	14	4	28
M1	8.54	0.07	6	-1.87	1	0.00	0.00	288.22	16	3	1	14	14	4	34
M2	8.35	-0.08	6	-1.65	1	0.00	0.00	255.79	15	3	1	14	14	4	34
M3	8.67	0.18	6	-1.95	1	0.00	0.00	287.30	16	3	1	14	14	4	33
M4	8.30	-0.15	5	-1.91	1	0.00	0.00	259.12	16	3	1	14	14	4	33
M5	8.18	0.24	4	-1.73	1	0.00	0.00	257.97	15	3	1	14	14	4	33
M6	8.56	0.39	4	-1.73	1	0.00	0.00	256.00	15	3	1	14	14	4	33
M7	8.47	0.39	8	-1.14	1	0.00	0.00	248.24	15	3	2	20	20	4	36
M8	8.35	0.42	7	-0.98	1	0.00	0.00	239.36	14	2	2	20	20	4	34
M9	8.54	0.09	6	-1.89	1	0.00	0.00	289.00	16	3	1	14	14	4	34
M10	8.57	0.56	4	-0.67	1	0.00	0.00	198.13	11	2	1	15	15	0	27
M11	8.53	0.10	5	-0.82	1	7.73	0.00	186.40	11	2	1	20	20	4	33
M12	8.67	0.65	4	-0.72	1	0.00	0.00	238.46	13	2	1	15	15	0	30
M13	8.67	0.89	4	-0.66	1	0.00	62.48	237.77	13	2	1	15	15	0	32

Table S7: ADME/T properties of designed and screened top 18 GTP molecules

Title	#stars	#amine	#acid	#rotor	#rtvFG	CNS	mol MW	dipole	SASA	FOSA	FISA	PISA	WPSA	volume	donor HB	accptH B
4DSO_ GTP	7	0	4	14	3	-2	523.18	15.25	695.97	083.97	568.69	36.27	07.04	1229.07	5	21.60
M12	4	1	1	09	0	-2	414.38	07.43	690.40	084.61	438.06	167.73	00.00	1192.12	5	10.50
M13	5	1	1	09	0	-2	450.36	13.11	682.15	073.40	430.07	125.55	53.14	1201.29	5	10.50
M14	4	0	1	09	0	-2	431.40	16.84	640.90	117.50	356.99	166.41	00.00	1178.03	6	13.35
M15	0	0	1	09	0	-2	409.46	11.36	681.60	311.85	296.47	037.27	36.02	1202.78	5	11.40
M16	0	0	1	08	0	-2	441.50	11.23	695.59	191.12	296.13	205.11	03.23	1271.24	5	09.70
M17	2	0	1	07	0	-2	452.48	12.26	718.09	304.71	345.54	044.23	23.61	1289.54	5	12.20
M18	0	0	1	07	0	-2	345.38	08.35	598.14	109.01	290.67	162.46	35.99	1013.40	4	08.00
M19	0	0	1	08	0	-2	447.53	10.89	680.56	148.37	312.60	179.24	40.35	1238.71	5	10.20
M20	4	0	1	10	0	-2	409.40	14.83	666.96	253.25	368.71	045.01	00.00	1191.96	6	14.30
M5	7	1	3	16	1	-2	528.41	03.92	732.47	173.77	492.04	036.36	30.30	1372.01	7	16.45
M21	3	0	1	08	0	-2	452.42	07.72	694.92	275.90	385.26	033.76	00.00	1262.72	6	15.10
M22	1	0	1	07	0	-2	446.46	14.10	709.99	353.95	301.08	054.96	00.00	1298.20	5	11.70
M23	2	0	1	08	0	-2	431.47	11.43	650.22	093.39	336.28	187.01	33.54	1175.86	5	10.45
M24	0	0	1	08	0	-2	445.45	11.37	659.41	126.08	329.06	170.17	34.11	1212.42	5	13.40
M25	9	1	3	16	2	-2	524.36	16.93	741.83	164.13	533.60	042.19	01.91	1361.93	7	17.95
M26	0	0	1	08	0	-2	371.35	06.68	622.36	205.47	291.58	125.31	00.00	1091.45	4	09.00
M27	3	0	1	08	0	-2	439.43	13.40	702.53	146.83	351.93	203.77	00.00	1264.07	5	12.90
M28	7	1	3	16	1	-2	512.35	06.90	723.97	213.60	467.76	041.32	01.29	1341.07	7	17.65

Title	dip^2/V	ACxDN^.5/SA	glob	QPpolrz	QPlogPC16	QPlogPoct	QPlogPw	QPlogPo/w	QPlogS	CIQPlogS	QPlogHERG	QPPCaco	QPlogBB	QPPMDCK	QPlogKp
4DSO_GTP	0.19	0.07	0.80	34.39	15.12	34.20	31.02	-3.43	-0.78	-1.98	2.25	0.00	-6.23	0.00	-10.53
M12	0.05	0.03	0.79	37.38	14.74	26.94	21.18	-2.75	-3.17	-3.21	-4.69	0.04	-4.29	0.01	-10.20
M13	0.14	0.03	0.80	37.34	14.11	28.47	20.84	-2.47	-3.29	-3.87	-4.27	0.05	-3.92	0.03	-10.20
M14	0.24	0.05	0.84	36.80	14.22	32.21	24.77	-0.82	-2.60	-3.61	-3.08	1.03	-3.34	0.37	-6.65
M15	0.11	0.04	0.80	36.56	13.15	27.30	20.21	0.40	-3.59	-3.56	-3.10	3.87	-2.96	2.45	-5.99
M16	0.10	0.03	0.82	41.54	14.73	28.24	19.92	1.47	-4.14	-5.07	-3.68	3.90	-2.88	1.63	-5.49
M17	0.12	0.04	0.80	41.38	14.30	29.82	21.90	0.22	-4.19	-4.09	-3.21	1.33	-3.42	0.66	-7.06
M18	0.07	0.03	0.82	31.46	11.92	21.95	16.45	0.83	-3.45	-3.91	-3.48	4.40	-2.68	2.81	-5.63
M19	0.10	0.03	0.82	39.99	14.62	28.15	20.32	1.11	-3.99	-5.01	-3.50	2.72	-2.92	1.77	-5.88
M20	0.18	0.05	0.82	35.56	13.57	31.24	24.81	-1.35	-2.58	-2.58	-2.93	0.80	-3.74	0.28	-7.20
M5	0.01	0.06	0.82	38.83	16.49	33.23	28.01	-3.33	-1.59	-2.78	0.00	0.00	-4.86	0.00	-10.99
M21	0.05	0.05	0.81	39.57	14.28	31.34	26.14	-1.37	-3.09	-3.07	-2.91	0.56	-3.80	0.19	-7.73
M22	0.15	0.04	0.81	41.83	13.94	29.94	21.15	0.70	-4.08	-4.16	-3.05	3.50	-2.91	1.40	-6.20
M23	0.11	0.04	0.83	37.55	14.20	27.75	20.71	0.51	-3.50	-4.63	-3.39	1.62	-3.10	0.93	-6.29
M24	0.11	0.05	0.83	38.86	14.38	29.71	23.47	-0.24	-3.08	-3.88	-3.22	1.90	-2.99	1.11	-6.22
M25	0.21	0.06	0.80	38.48	16.58	36.66	29.83	-4.31	-1.31	-2.20	-0.26	0.00	-5.54	0.00	-11.73
M26	0.04	0.03	0.82	33.59	12.18	22.63	17.01	0.76	-3.28	-4.05	-3.17	4.31	-2.78	1.75	-5.68
M27	0.14	0.04	0.80	41.24	15.04	30.66	23.45	-0.10	-3.57	-3.94	-3.86	1.15	-3.54	0.42	-6.52
M28	0.04	0.06	0.81	37.64	15.88	33.52	29.03	-3.83	-1.18	-2.09	-0.07	0.00	-4.73	0.00	-10.52

Title	IP(eV)	EA(eV)	#metab	QPlogKhsa	HumanOralAbsorption	PercentHumanOralAbsorption	SAfluorine	PSA	#NandO	RuleOfFive	RuleOfThree	#ringatoms	#in56	#noncon	#nonHatm
4DSO_GTP	8.17	0.32	3	-2.74	1.00	00.00	00.00	313.09	19	3	1	14	14	4	32
M12	8.61	0.43	4	-0.72	1.00	00.00	00.00	237.31	13	2	1	15	15	0	30
M13	8.77	1.14	4	-0.68	1.00	00.00	53.14	235.26	13	2	1	15	15	0	32
M14	8.44	0.81	4	-0.97	1.00	00.00	00.00	200.31	12	2	1	20	20	4	31
M15	8.59	0.45	6	-0.79	2.00	39.78	00.00	165.85	10	0	1	14	14	4	28
M16	8.38	0.42	3	-0.36	2.00	46.12	00.00	160.95	09	0	1	20	20	4	31
M17	8.62	0.43	2	-0.64	1.00	17.46	00.00	198.42	12	1	1	19	19	8	31
M18	8.62	0.52	2	-0.62	2.00	43.31	00.00	144.62	08	0	1	15	15	0	24
M19	8.58	0.67	1	-0.49	1.00	41.25	00.00	162.24	09	0	1	20	20	4	30
M20	8.22	-0.21	8	-1.16	1.00	00.00	00.00	200.23	12	2	2	14	14	4	29
M5	8.46	0.22	4	-1.68	1.00	00.00	00.00	267.27	15	3	1	14	14	4	33
M21	8.54	0.04	4	-1.06	1.00	00.00	00.00	225.30	14	2	1	19	19	8	32
M22	8.09	-0.35	4	-0.53	2.00	27.82	00.00	188.58	12	1	1	19	19	8	32
M23	8.71	0.87	2	-0.63	1.00	33.68	00.00	175.88	10	0	1	20	20	4	30
M24	8.68	0.62	3	-0.90	1.00	17.59	00.00	190.54	11	1	1	20	20	4	31
M25	8.50	0.08	6	-1.91	1.00	00.00	00.00	291.84	16	3	1	14	14	4	34
M26	8.54	0.72	4	-0.61	2.00	42.75	00.00	161.08	10	0	1	15	15	0	27
M27	8.29	0.76	5	-0.81	1.00	14.51	00.00	194.62	11	1	1	20	20	4	32
M28	8.39	0.06	5	-1.87	1.00	00.00	00.00	270.13	16	3	1	14	14	4	33