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RESEARCH ARTICLE

Investigation of Anti-cancer Potential of *Solanum virginianum* L. Fruit and Leaf Extracts by *In Vitro* and *In Silico* Studies

Supplementary Figures and Tables:

Table S1. Identified phyto compounds in *S. virginianum* leaf aqueous extract

Name	Class	Formula	RT	m/z	Mass
8-Hydroxy-3-chlorodibenzofuran	Coumarone	$C_{12}H_7ClO_2$	0.803	241.0064	218.017
O-Demethylfonsecin	naphthopyranones	$C_{14}H_{12}O_6$	0.806	299.0489	276.057
4-Methoxybenzyl O-(2-sulfoglucoside)	glycosyl compounds	$C_{14}H_{20}O_{10}S$	1.076	381.0823	380.075
4-Fluoro-L-threonine	fluoroamino acid	$C_4H_8FNO_3$	1.159	138.0568	137.049
Isoamyl nitrite	o-nitroso compounds	$C_5H_{11}NO_2$	1.172	118.0877	117.080
N-(1-Deoxy-1-fructosyl)leucine	Amino acid derivative	$C_{12}H_{23}NO_7$	1.404	294.1574	293.149
Methyl N-methylanthranilate	benzoate ester	$C_9H_{11}NO_2$	1.779	166.0881	165.080
16-Ketoestradiol	Steroids	$C_{18}H_{22}O_3$	2.504	309.147	286.157
4-Hydroxycoumarin	Coumarin	$C_9H_6O_3$	2.998	163.0409	162.033
Indoleacrylic acid	unsaturated monocarboxylic acid	$C_{11}H_9NO_2$	3.236	188.0725	187.065
Tobramycin	Glycoside	$C_{18}H_{37}N_5O_9$	3.988	468.2623	467.256
Sulfamethopyrazine	sulfonamide	$C_{11}H_{12}N_4O_3S$	5.07	303.0526	280.063
2-Methylchrysene	carbopolycyclic	$C_{19}H_{14}$	5.688	265.0995	242.110
Fabianine	Alkaloid	$C_{14}H_{21}NO$	5.69	220.1716	219.164
Solasonine	Steroidal alkaloids	$C_{45}H_{73}NO_{16}$	5.766	884.5059	883.498
Koryoginsenoside R1	triterpenoids	$C_{46}H_{76}O_{15}$	6.095	868.5113	867.503
beta-Solamarine	Steroidal alkaloids	$C_{45}H_{73}NO_{15}$	6.131	868.511	867.503
Psychotridine	polyindoline alkaloid	$C_{55}H_{62}N_{10}$	6.391	884.5056	861.516
Laurelliptine	quinoline alkaloids	$C_{18}H_{19}NO_4$	7.435	314.1411	313.134
beta-Solanine	steroidal alkaloid	$C_{39}H_{63}NO_{11}$	7.439	722.4522	721.444
5alpha-Tomatidan-3-one	steroidal alkaloids	$C_{27}H_{43}NO_2$	8.949	414.3395	413.332
Veratramine	piperidine alkaloid	$C_{27}H_{39}NO_2$	9.974	410.3082	409.300
Aconine	Aconitum alkaloids	$C_{25}H_{41}NO_9$	5.3	500.2788	499.276
Kaempferol	Flavonoid	$C_{15}H_{10}O_6$	5.529	287.0575	286.050
Piperidolate	diarylmethane.	$C_{21}H_{25}NO_2$	9.403	324.198	323.190

Table S2. Identified phyto compounds in *S. virginianum* leaf hydro alcoholic extract

Name	Class of compound	Formula	RT	m/z	Mass
Chlorogenic acid	ester of caffeic acid and-quinic acid	$C_{16}H_{18}O_9$	3.995	353.0884	354.095 6
Quinic acid	a cyclohexanecarboxylic acid	$C_7H_{12}O_6$	4.195	191.0562	192.063 5
Nafoxidine	a nonsteroidal selective estrogen receptor modulator or partial antiestrogen	$C_{29}H_{31}NO_2$	4.39	470.2314	425.233 2
p-Coumaroyl quinic acid	Poly phenols,phenolics	$C_{16}H_{18}O_8$	4.905	337.0941	338.101 5
Gambiriin A3	It is a catachin, flavanoid	$C_{30}H_{28}O_{12}$	5.11	335.0785	580.160 6
Jubanine A	cyclopeptide alkaloids	$C_{40}H_{49}N_5O_6$	5.396	693.3546	694.361 6
Vicinin 2	flavonoid-8-o-glycosides.	$C_{27}H_{30}O_{17}$	5.463	625.1447	626.151 9
Allivicin	flavonoid-3-o-glycosides.	$C_{27}H_{30}O_{16}$	5.612	609.1497	610.156 9
N-Acetoxymethylflindersine	pyranoquinolines	$C_{17}H_{17}NO_4$	5.764	298.1098	299.117 1
Myricitrin	Flavonoid	$C_{21}H_{20}O_{12}$	6.245	463.0906	464.097 9
1,4-Di-O-caffeoylquinic acid	as quinic acids and derivatives.	$C_{25}H_{24}O_{12}$	6.245	515.1222	516.129 8
Mammeisin	prenylated neoflavonoids	$C_{25}H_{26}O_5$	6.331	405.1709	406.175 8
Isomaltulose	disaccharide carbohydrate composed of glucose and fructose.	$C_{12}H_{22}O_{11}$	1.052	341.1084	342.115 7
Brompheniramine	is an antihistamine drug of the propylamineclass.	$C_{16}H_{19}BrN_2$	1.109	377.0854	318.071 5
Fucosyllactose	oligosaccharide	$C_{18}H_{32}O_{15}$	1.11	533.1725	488.174 3
L-Malic acid	dicarboxylic acid	$C_4H_6O_5$	1.183	133.0137	134.021
4-Coumaroyl-2-hydroxy-putrescine	coumaric acids and derivatives.	$C_{13}H_{18}N_2O_3$	2.793	249.1242	250.131 4
Pedaliin	flavonoid o-glycosides.	$C_{22}H_{22}O_{12}$	6.415	477.1064	478.113 7
Aspulvinone H	cyclobutyrolactone lignan	$C_{27}H_{28}O_5$	6.806	431.187	432.194 2
Ferulic acid	Ferulic acid is a hydroxycinnamic acid	$C_{10}H_{10}O_4$	7.032	193.0514	194.058 7
Tricin 5-glucoside	flavonoid	$C_{23}H_{24}O_{12}$	7.126	491.122	492.129 4
Corchorifatty acid F	lineolic acids and derivatives.	$C_{18}H_{32}O_5$	8.778	327.2194	328.226 7
TR-Saponin C	glycosylated derivatives of triterpene sapogenins	$C_{54}H_{82}O_{21}$	9.018	1065.511 8	1066.51 7
Hordatine A	2-arylbenzofuran flavonoids.	$C_{28}H_{38}N_8O_4$	13.649	549.2863	550.292 1
Avermectin B1b aglycone	Avermectin B1b aglycone is a member of pyrans.	$C_{33}H_{46}O_8$	14.711	615.3183	570.317 9
Geranylfarnesyl diphosphate	Precursor for Sesterterpenoid	$C_{25}H_{44}O_7P_2$	16.424	577.2714	518.256 9
Harderoporphyrin	porphyrins	$C_{35}H_{36}N_4O_6$	17.419	607.2585	608.265 9
Ritterazine A	Natural cytotxic steroidal alkaloids	$C_{54}H_{76}N_2O_{10}$	20.305	971.5559	912.539 9
1-O-Sinapoylglucose	Glycoside. It derives from a hydroxycinnamic acid.	$C_{17}H_{22}O_{10}$	3.794	385.1142	386.121 3
Quercetin	Flavonoid	$C_{15}H_{10}O_7$	5.965	303.0477	302.040 4
Elatine	Alkaloid	$C_{38}H_{50}N_2O_{10}$	5.376	695.3613	694.354
Jubanine A	new cyclopeptide alkaloids	$C_{40}H_{49}N_5O_6$	5.536	696.364	695.356 5
Desglucomusennin	triterpenoid.	$C_{45}H_{72}O_{16}$	7.261	868.5012	867.493 9
Inundatine	sesquiterpenoid.	$C_{16}H_{23}NO_2$	6.69	262.1781	261.170 9

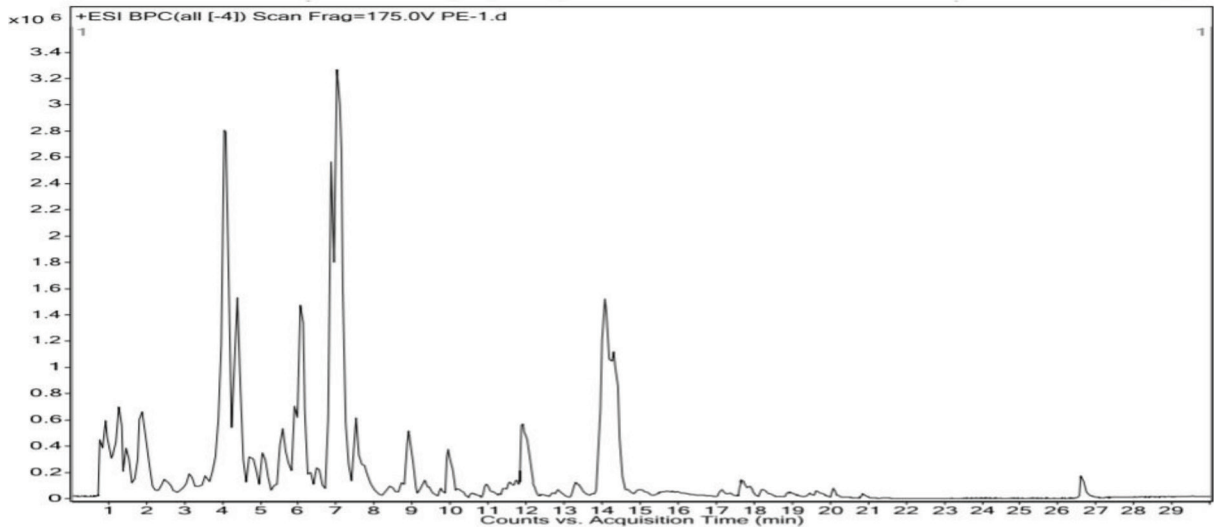


Figure S1. Chromatogram of *S. virginianum* leaf aqueous extract.

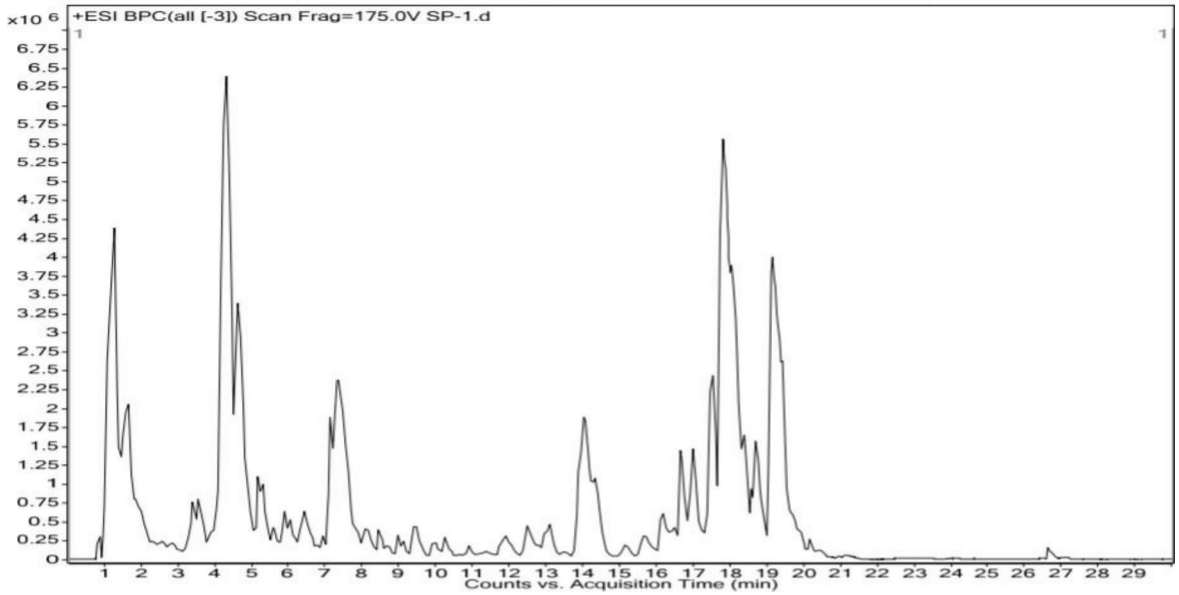


Figure S2. Chromatogram of *S. virginianum* leaf hydro alcoholic extract.

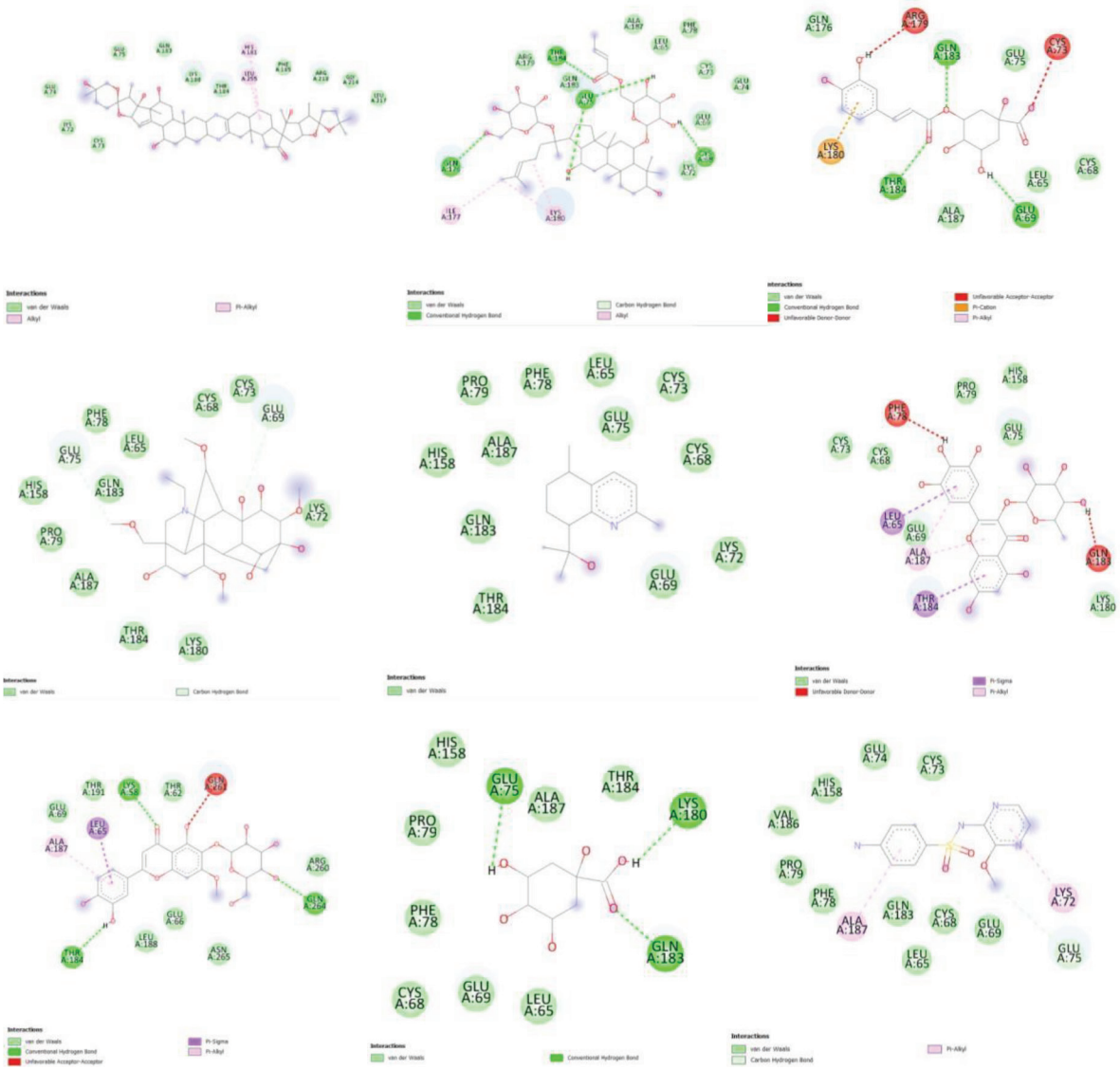


Figure S3. Target-ligand interaction between ligands - Ritterazine A, Koryoginesenoside R1, Caffeoyl quinic acid, Aconine, Fabianine, Myricitrin, Pedalin, Quinic acid, Sulfamethopyrazine and target Cyclin-D1 respectively.

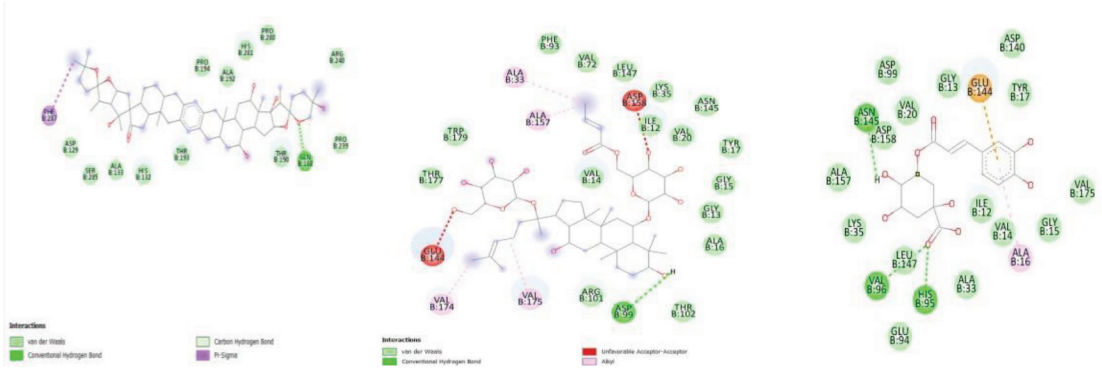
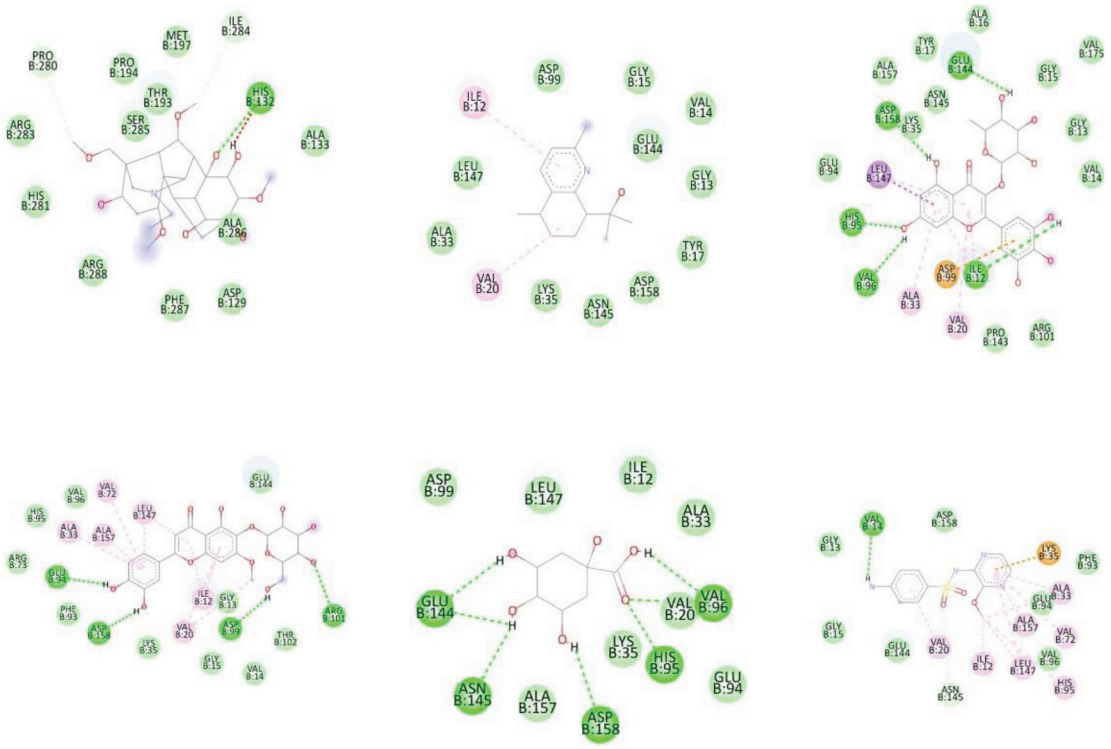


Figure S4. Target-ligand interaction between ligands - Ritterazine A, Koryoginesenoside R1, Caffeoyl quinic acid, Aconine, Fabianine, Myricitrin, Pedalin, Quinic acid, Sulfamethopyrazine and target Cyclin-D3 respectively.



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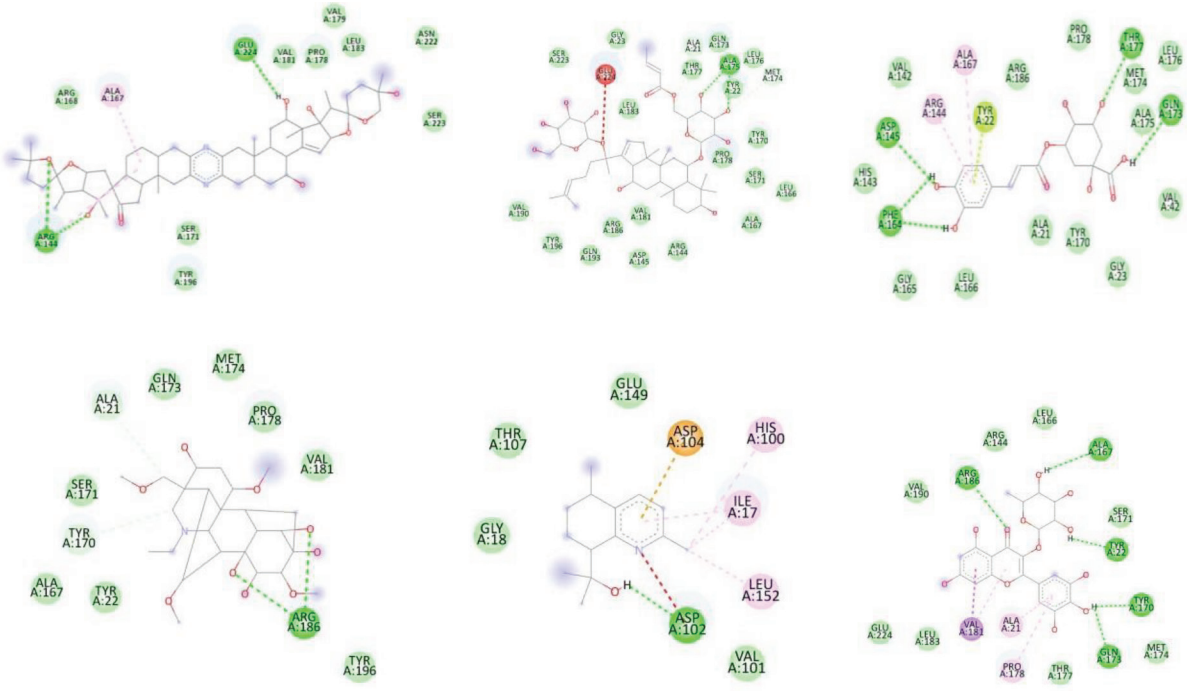
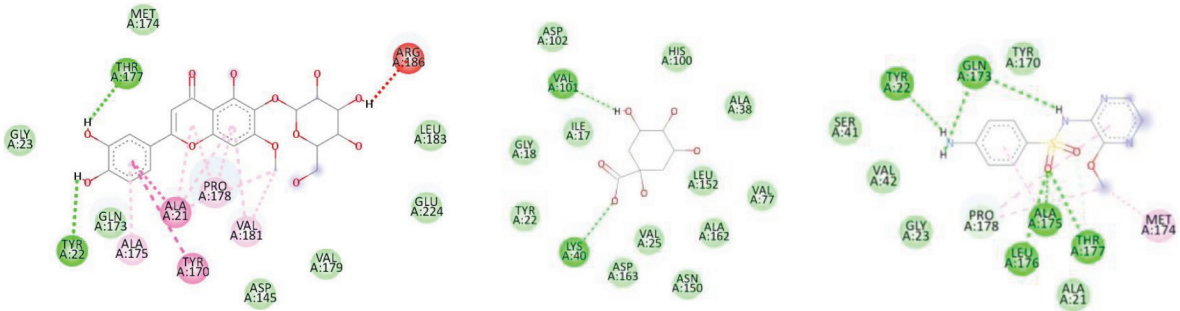


Figure S5. Target-ligand interaction between ligands - Ritterazine A, Koryoginesenoside R1, Caffeoyl quinic acid, Aconine, Fabianine, Myricitrin, Pedalin, Quinic acid, Sulfamethopyrazine and target CDK4 respectively.



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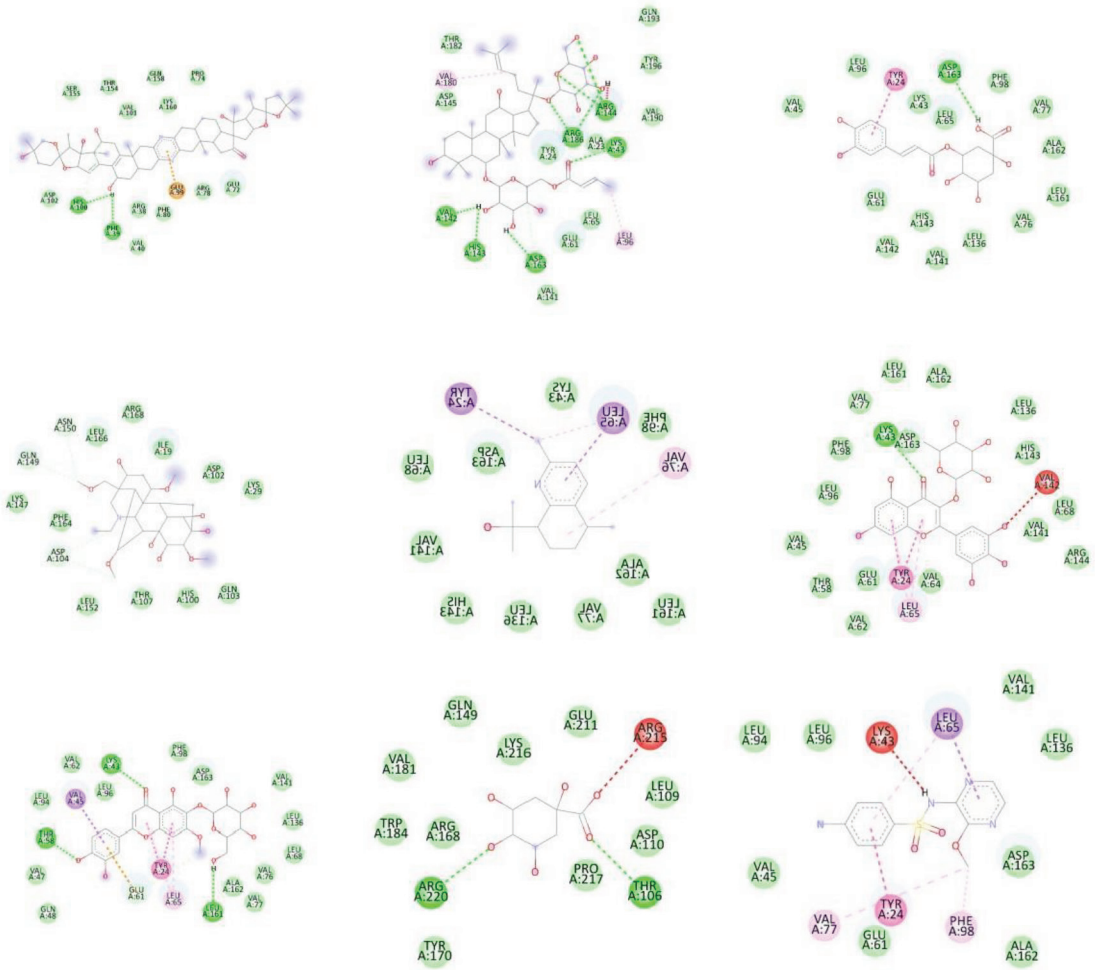


Figure S6. Target-ligand interaction between ligands - Ritterazine A, Koryoginesenoside R1, Caffeoyl quinic acid, Aconine, Fabianine, Myricitrin, Pedalin, Quinic acid, Sulfamethopyrazine and target CDK6 respectively.

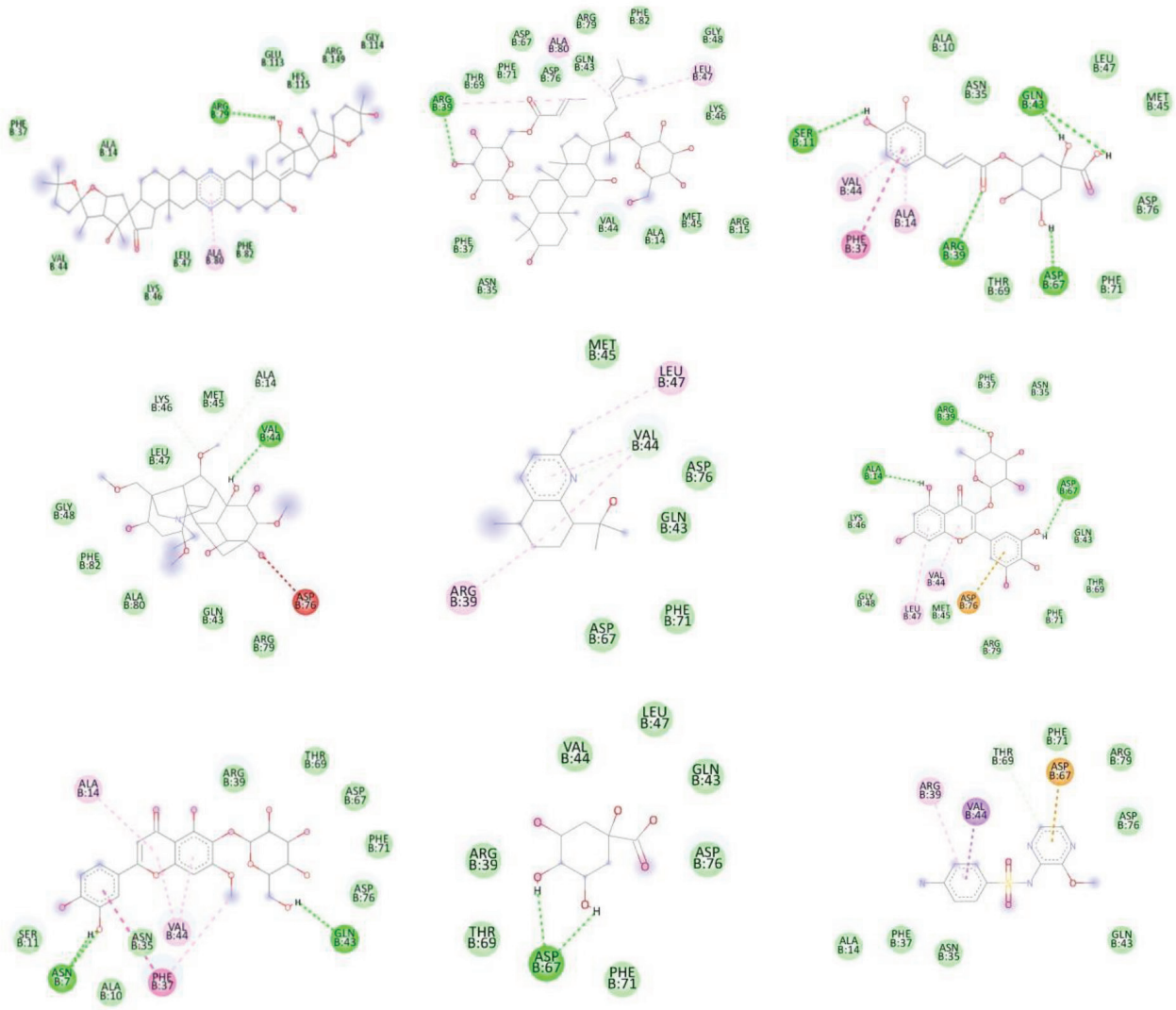


Figure S7. Target-ligand interaction between ligands - Ritterazine A, Koryoginesenoside R1, Caffeoyl quinic acid, Aconine, Fabianine, Myricitrin, Pedalin, Quinic acid, Sulfamethopyrazine and target p18 respectively.

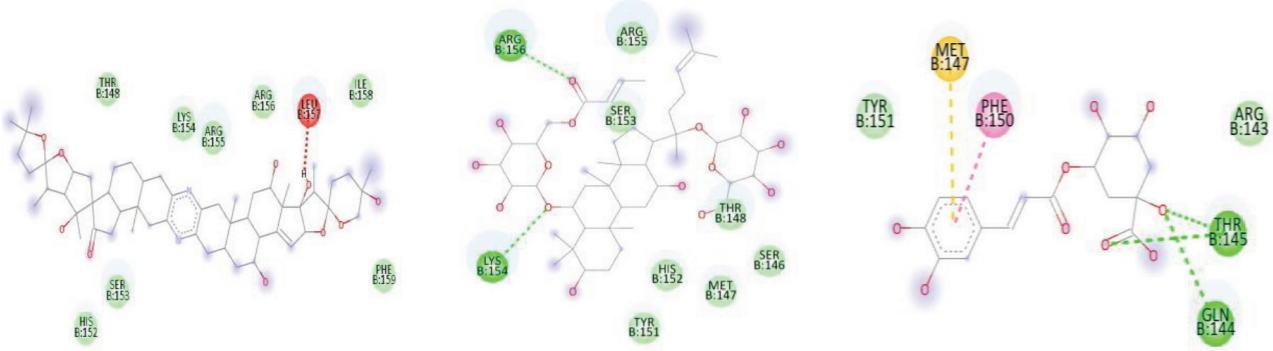
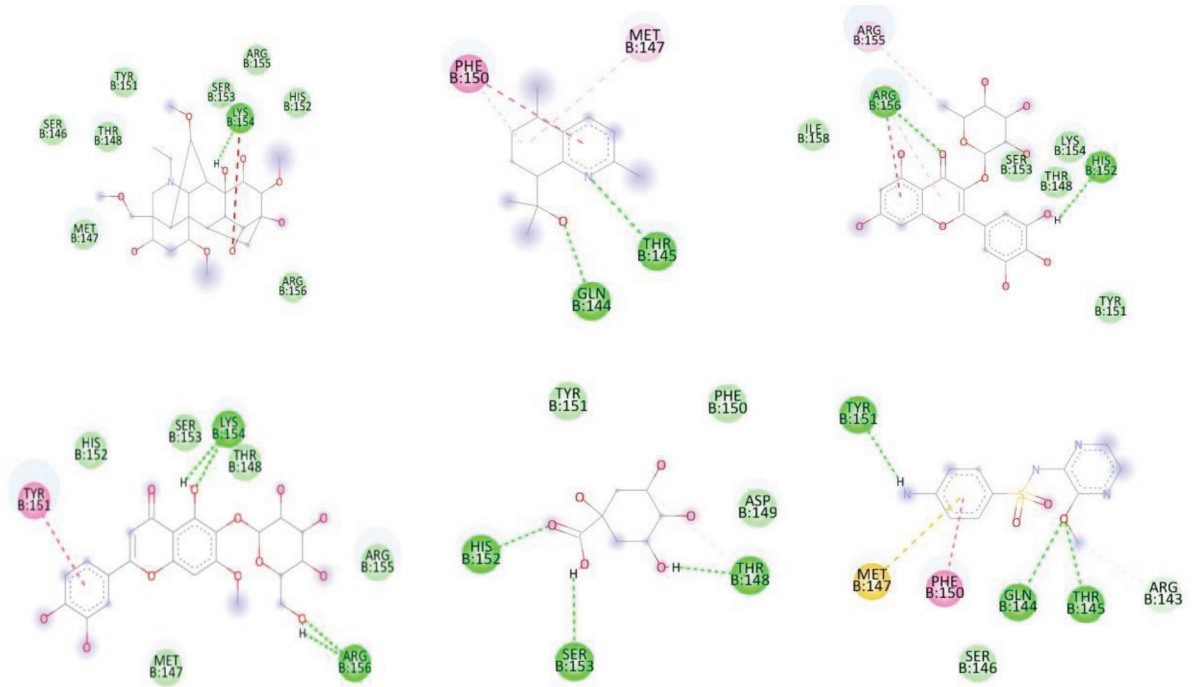


Figure S8. Target-ligand interaction between ligands - Ritterazine A, Koryoginesenoside R1, Caffeoyl quinic acid, Aconine, Fabianine, Myricitrin, Pedalin, Quinic acid, Sulfamethopyrazine and target p21 respectively.



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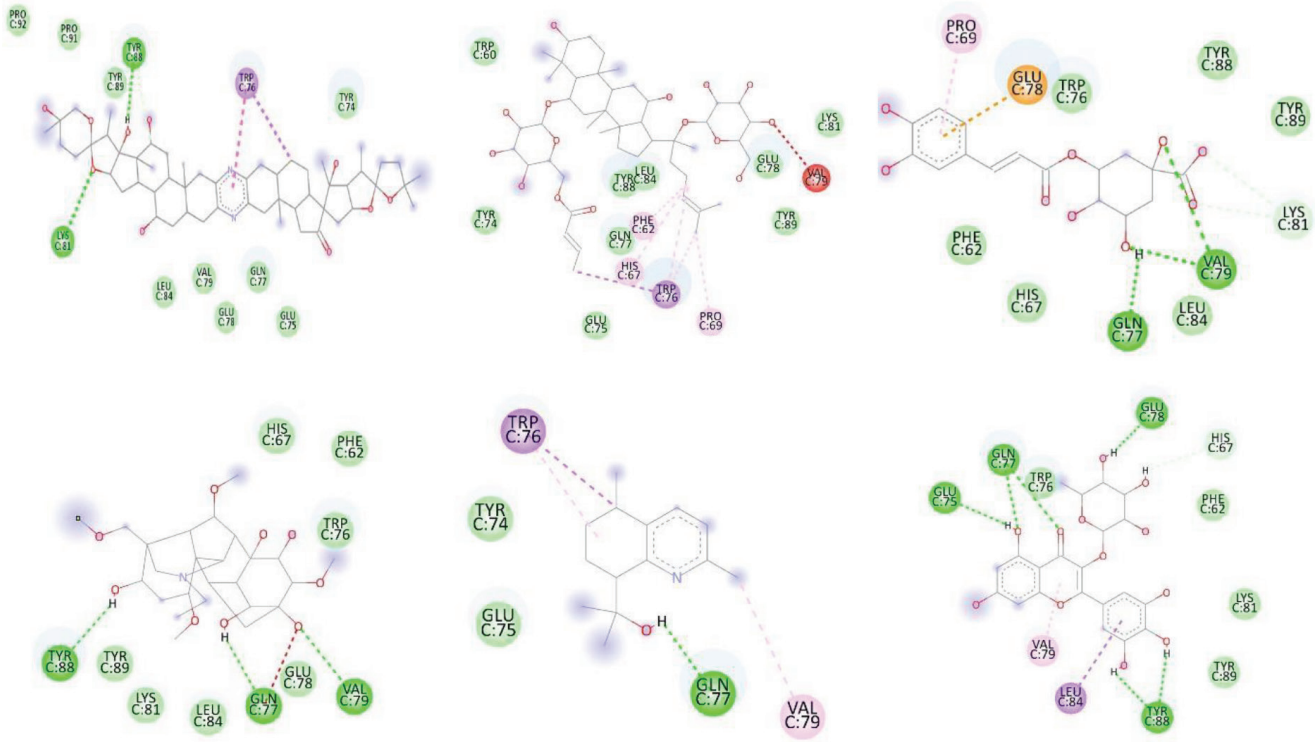
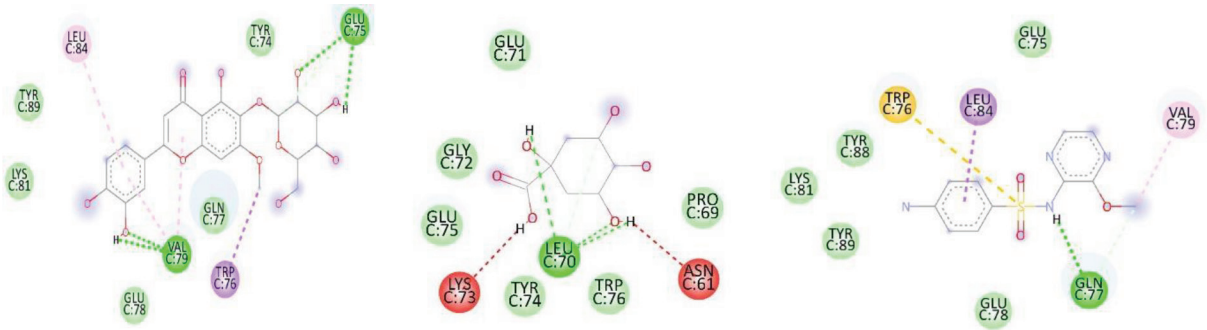


Figure S9. Target-ligand interaction between ligands - Ritterazine A, Koryoginesenoside R1, Caffeoyl quinic acid, Aconine, Fabianine, Myricitrin, Pedalin, Quinic acid, Sulfamethopyrazine and target p27 respectively.



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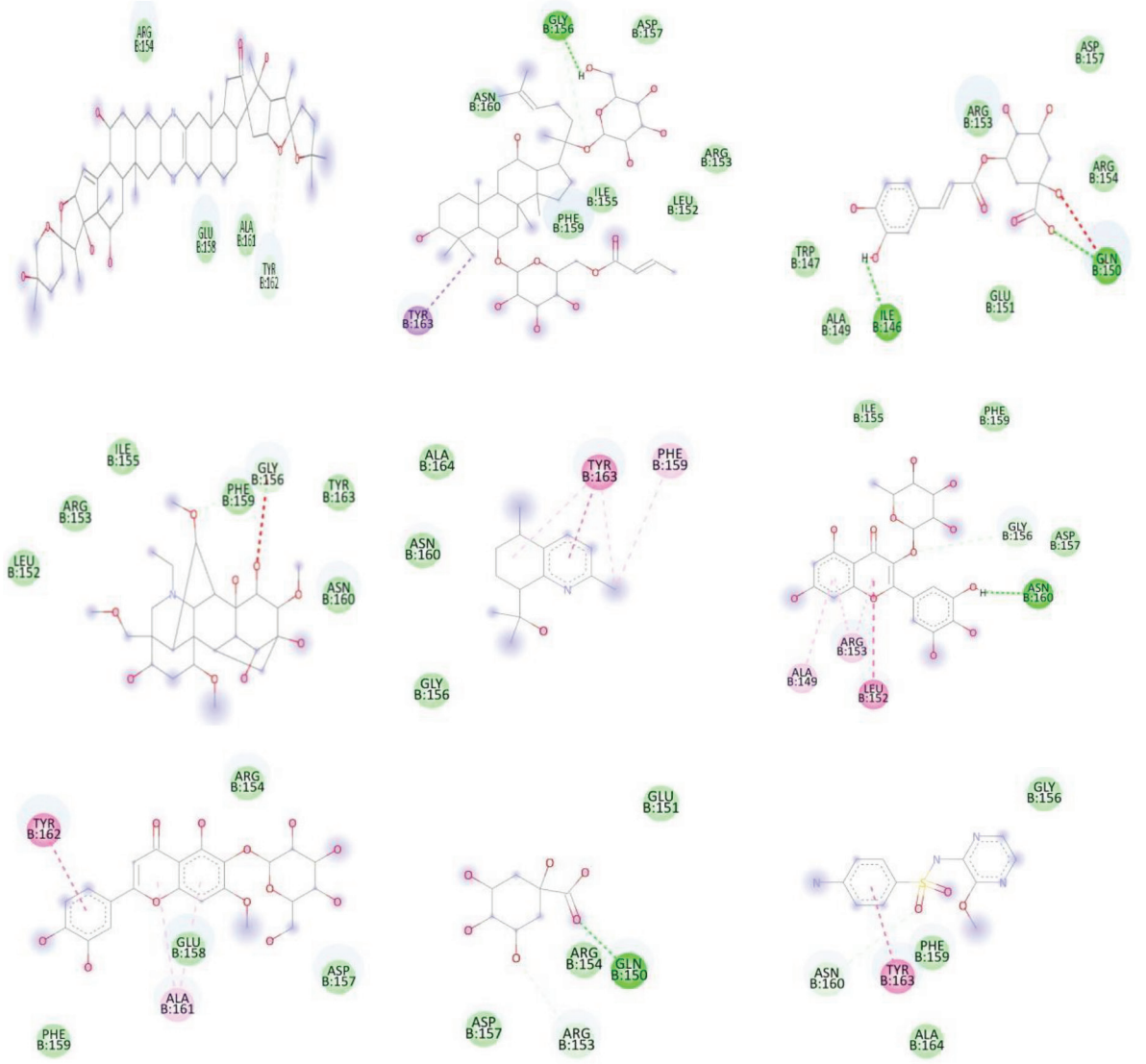


Figure S10. Target-ligand interaction between ligands - Ritterazine A, Koryoginesenoside R1, Caffeoyl quinic acid, Aconine, Fabianine, Myricitrin, Pedalin, Quinic acid, Sulfamethopyrazine and target BAX respectively.

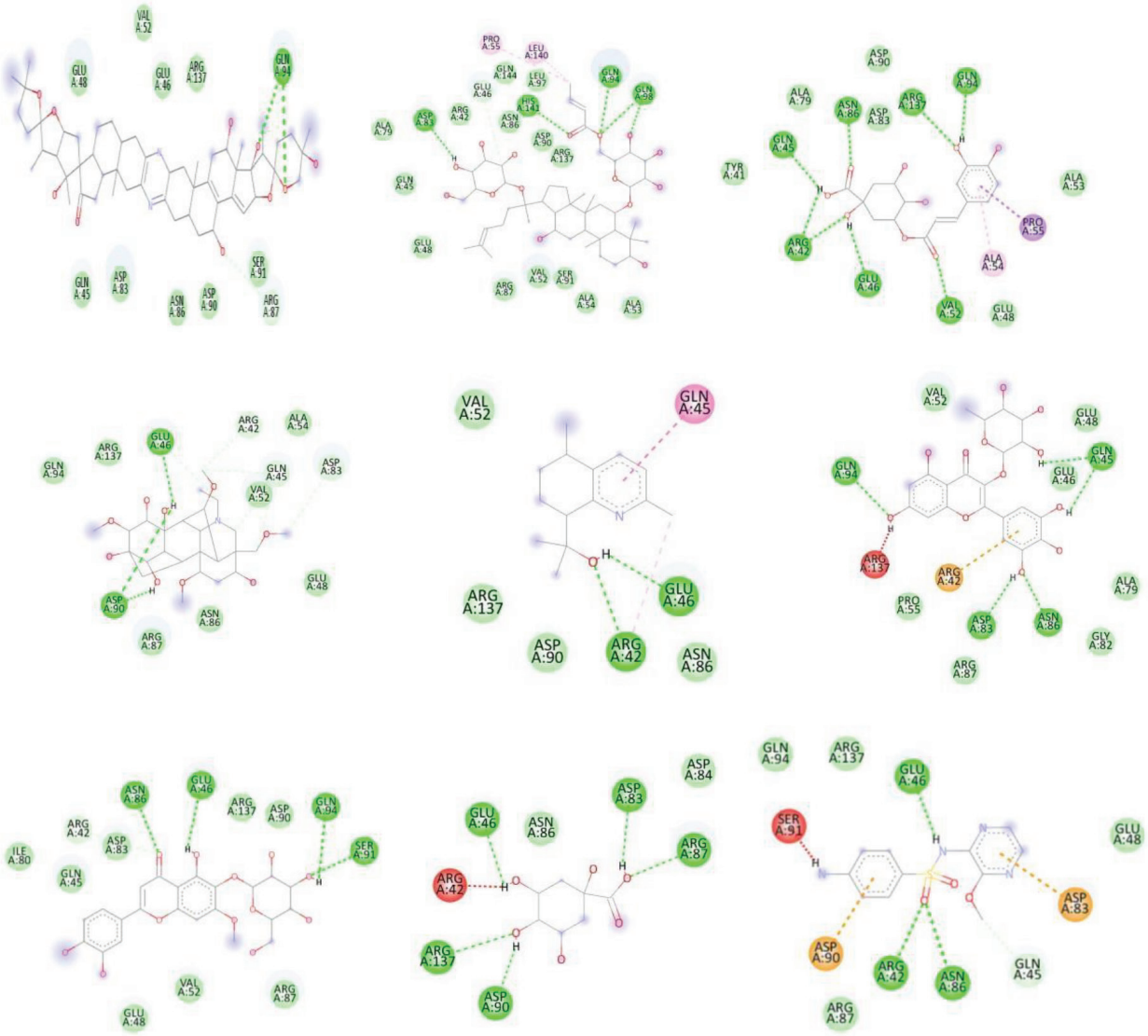


Figure S11. Target-ligand interaction between ligands - Ritterazine A, Koryoginesenoside R1, Caffeoyl quinic acid, Aconine, Fabianine, Myricitrin, Pedalin, Quinic acid, Sulfamethopyrazine and target BAK respectively.

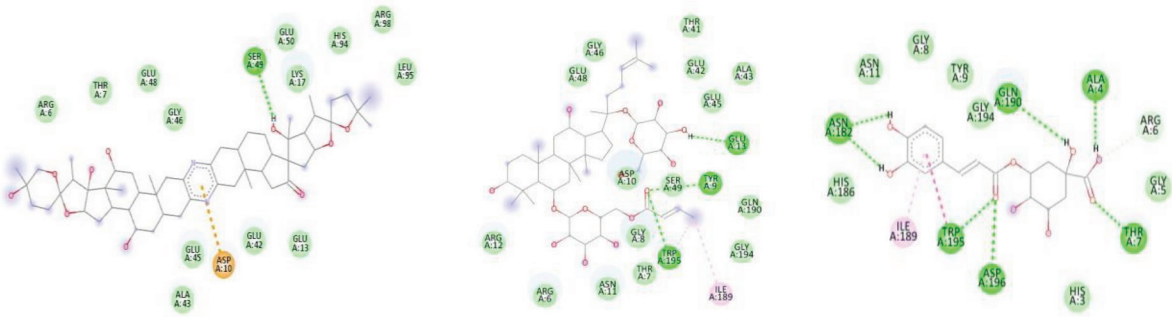
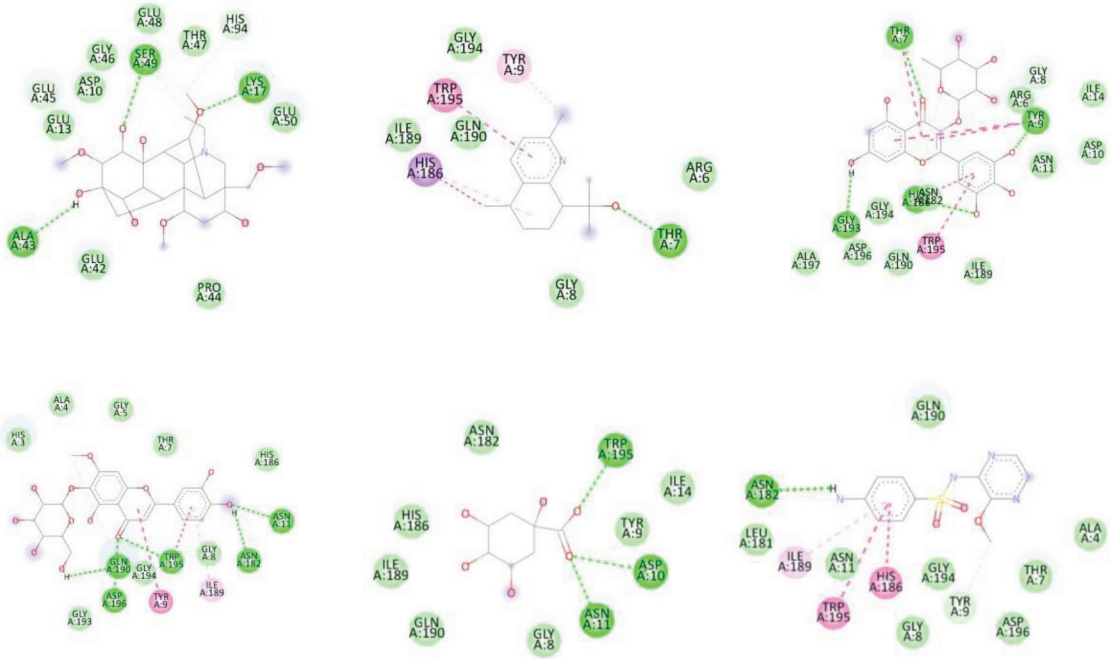


Figure S12. Target-ligand interaction between ligands - Ritterazine A, Koryoginesenoside R1, Caffeoyl quinic acid, Aconine, Fabianine, Myricitrin, Pedalin, Quinic acid, Sulfamethopyrazine and target Bcl-2 respectively.



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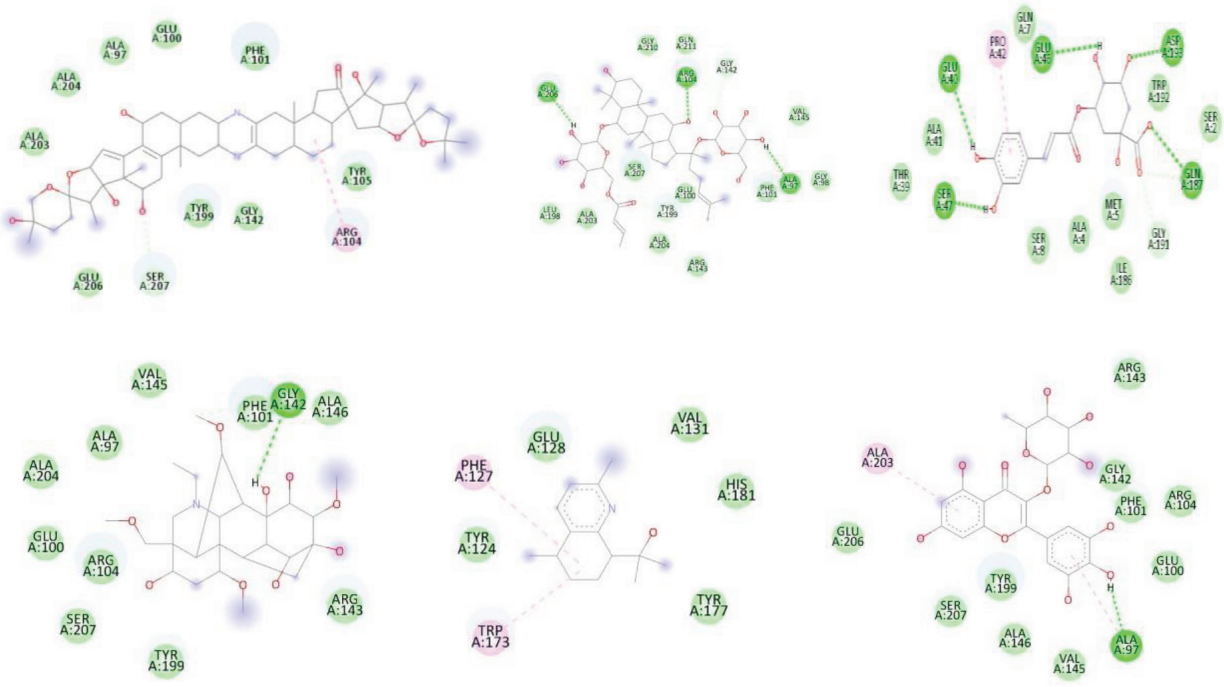
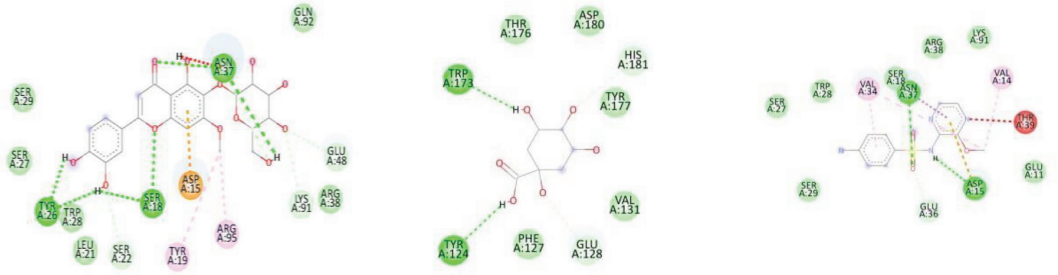


Figure S13. Target-ligand interaction between ligands - Ritterazine A, Koryoginesenoside R1, Caffeoyl quinic acid, Aconine, Fabianine, Myricitrin, Pedalin, Quinic acid, Sulfamethopyrazine and target Bcl-xl respectively.



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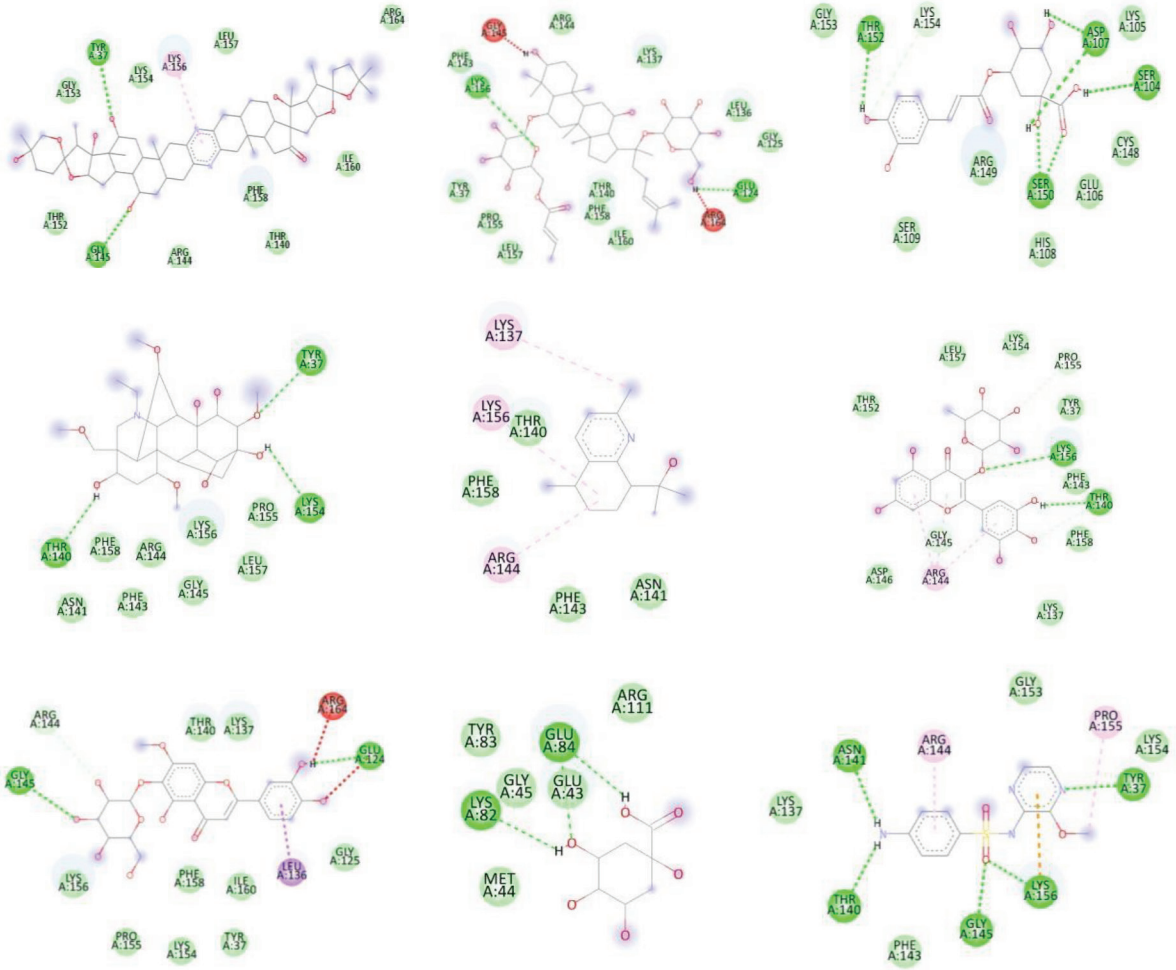

Figure S14. Target-ligand interaction between ligands - Ritterazine A, Koryoginesenoside R1, Caffeoyl quinic acid, Aconine, Fabianine, Myricitrin, Pedalin, Quinic acid, Sulfamethopyrazine and target Caspase-3 respectively.

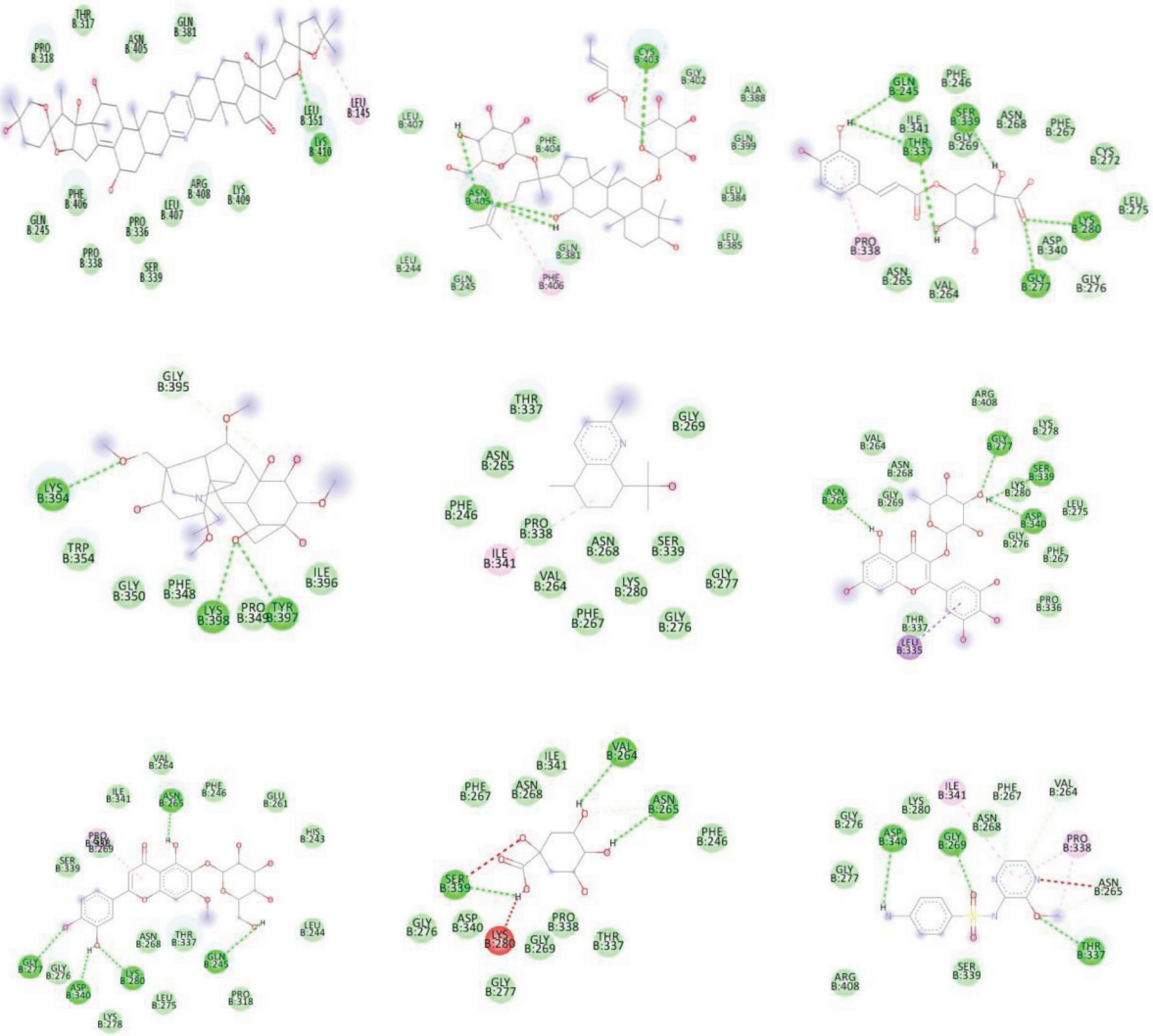

Figure S15. Target-ligand interaction between ligands - Ritterazine A, Koryoginesenoside R1, Caffeoyl quinic acid, Aconine, Fabianine, Myricitrin, Pedalin, Quinic acid, Sulfamethopyrazine and target Caspase-9 respectively.