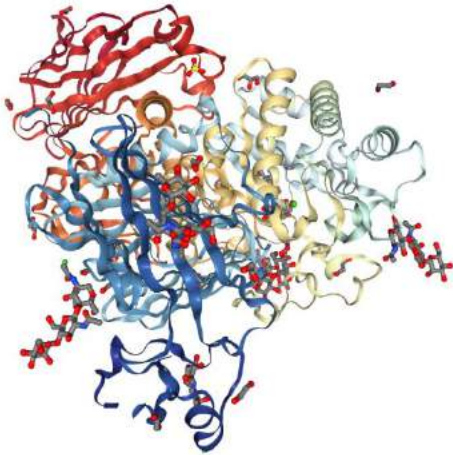
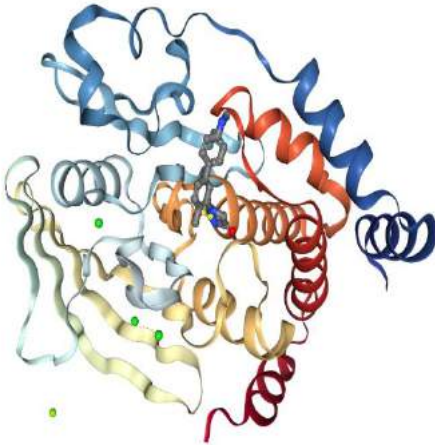


LAMPIRAN

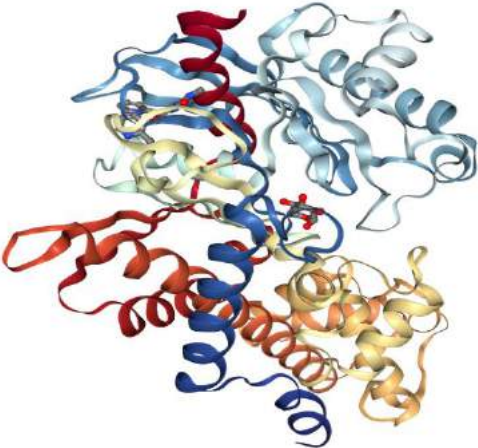
Lampiran 1. Struktur 3D Makromolekul



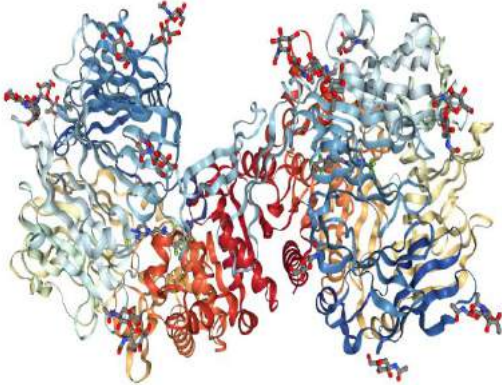
α -G (2QOE)



PTP1B (5T19)

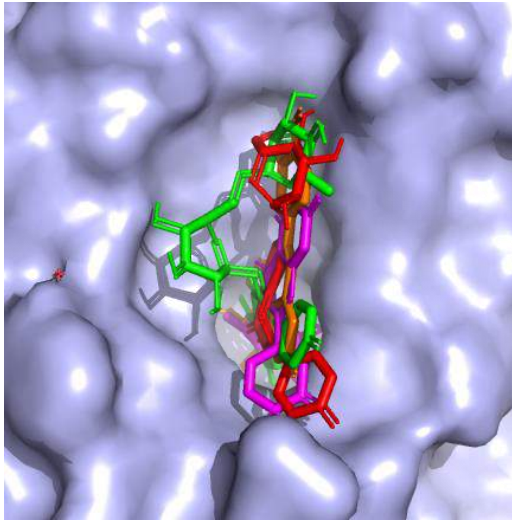


Glukokinase (4RCH)

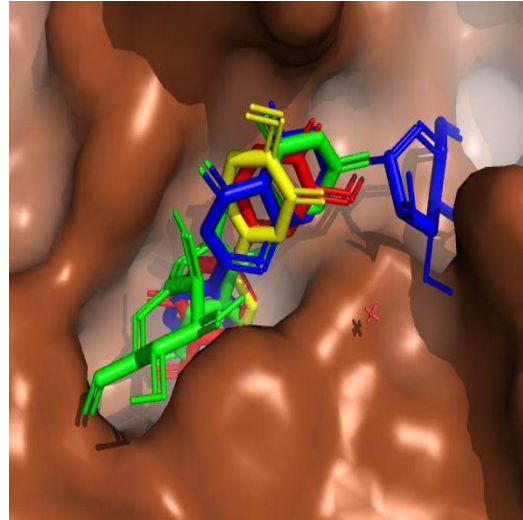


DPP4 (2QOE)

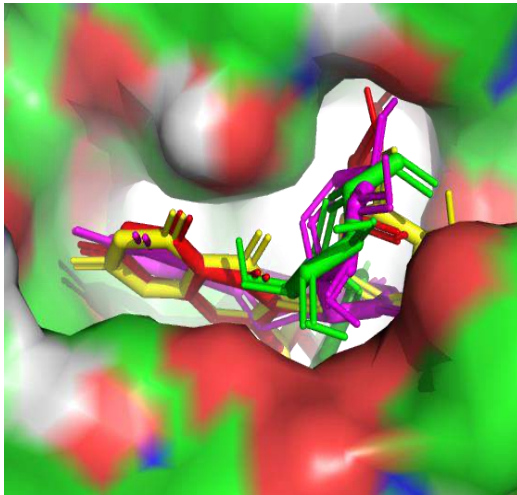
Lampiran 2. *Binding site* Target Makromolekul



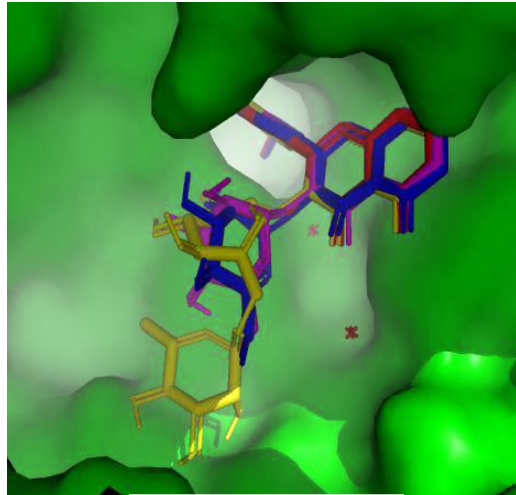
α - G (5NN8)



PTP-1B (5T19)



GK (4RCH)

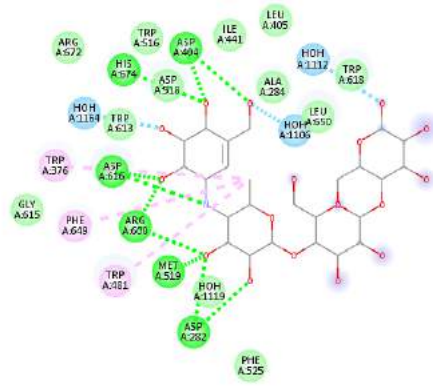
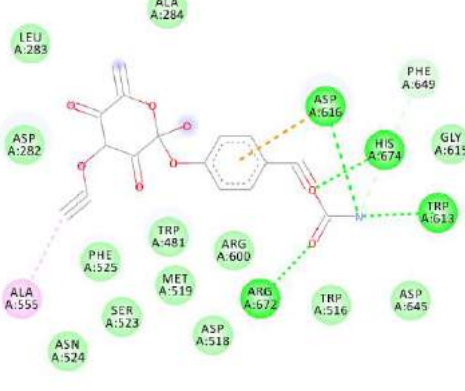
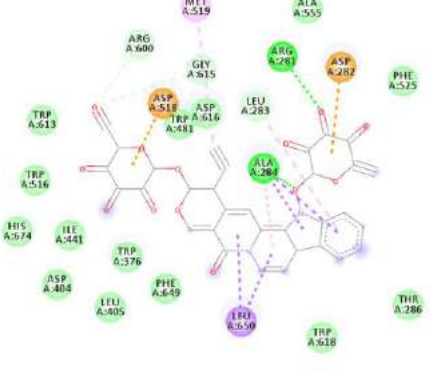
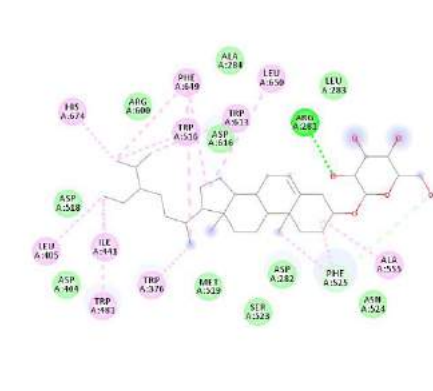


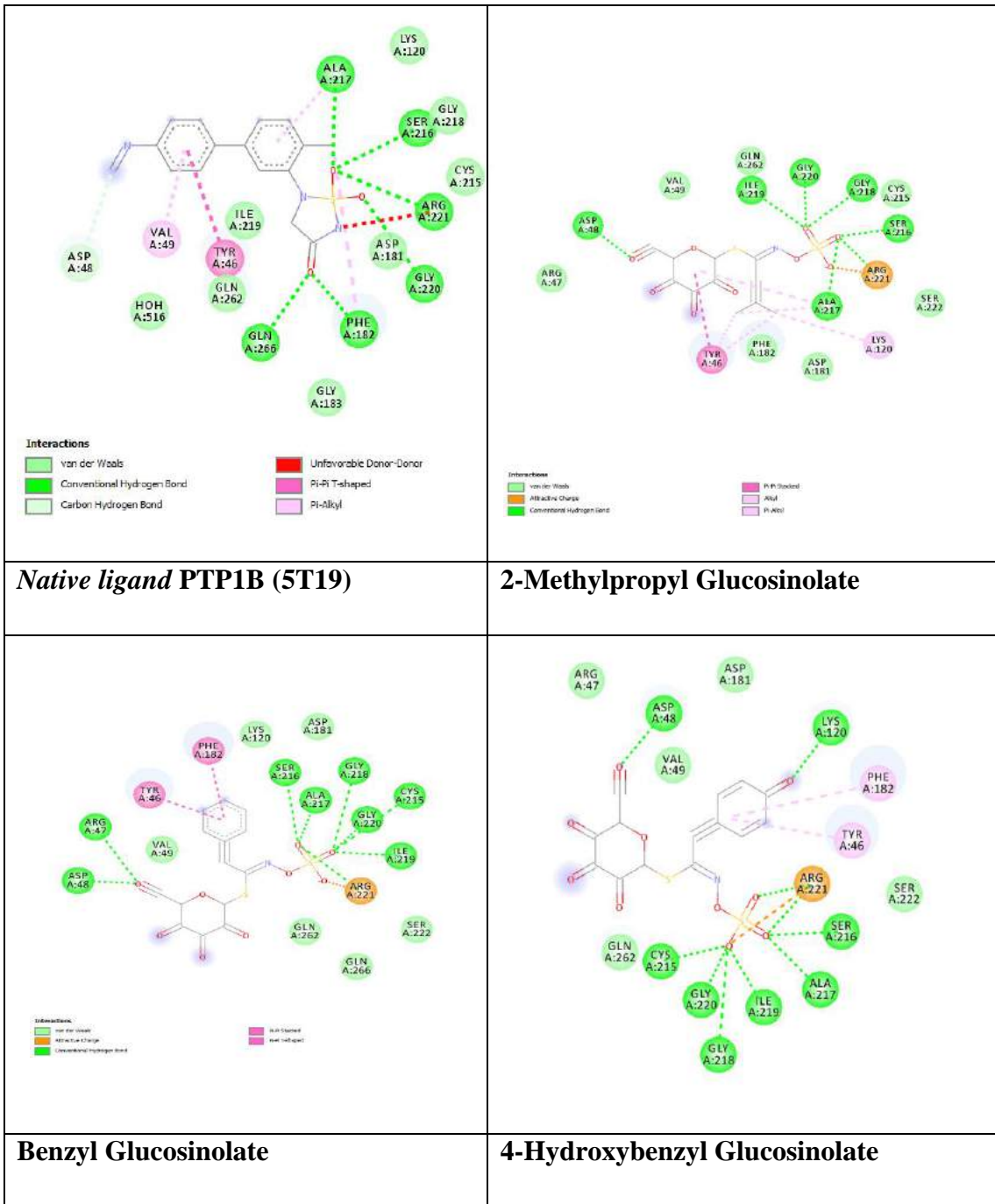
DPP4 (5T19)

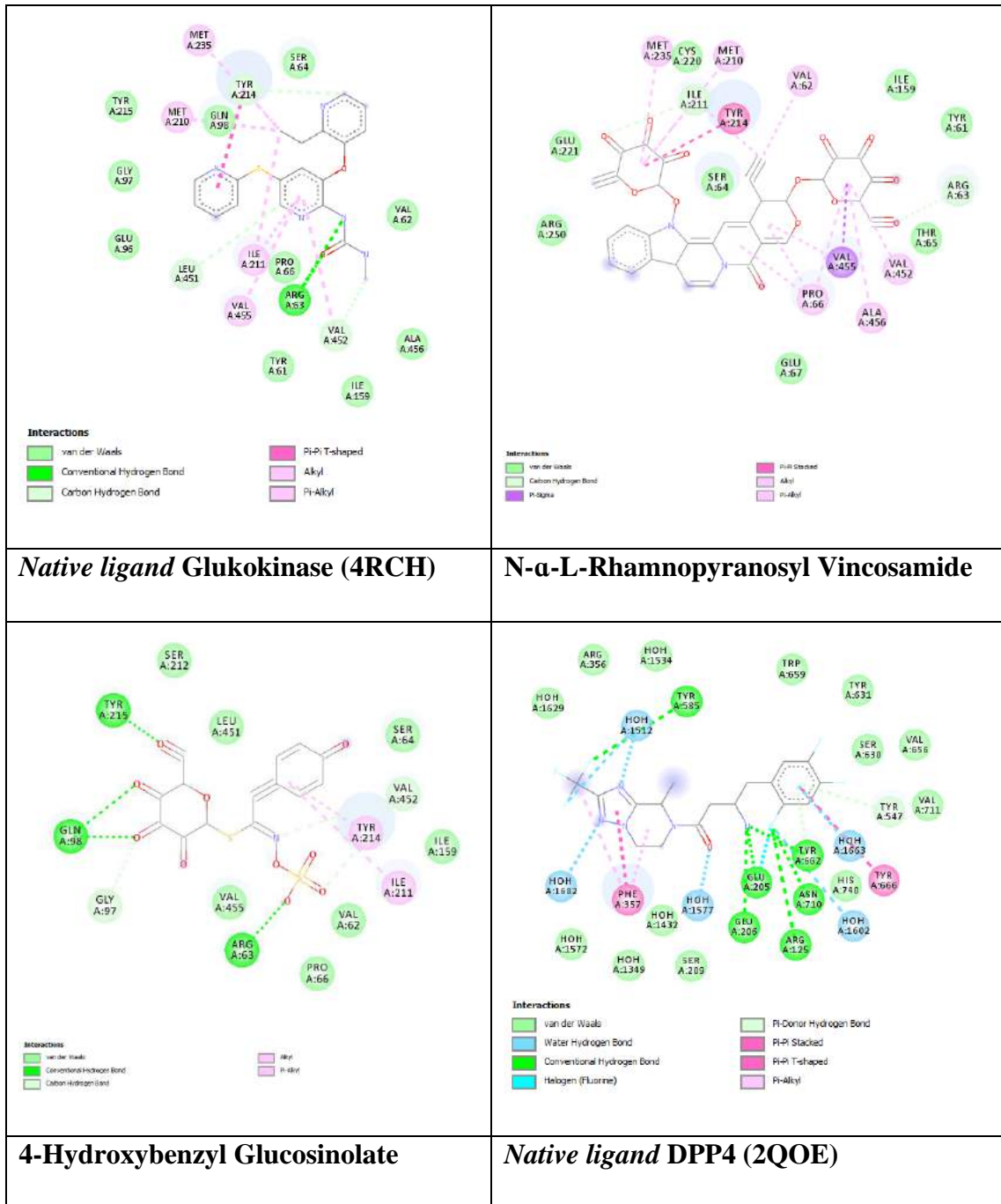
Lampiran 3. Hasil penambatan molekular

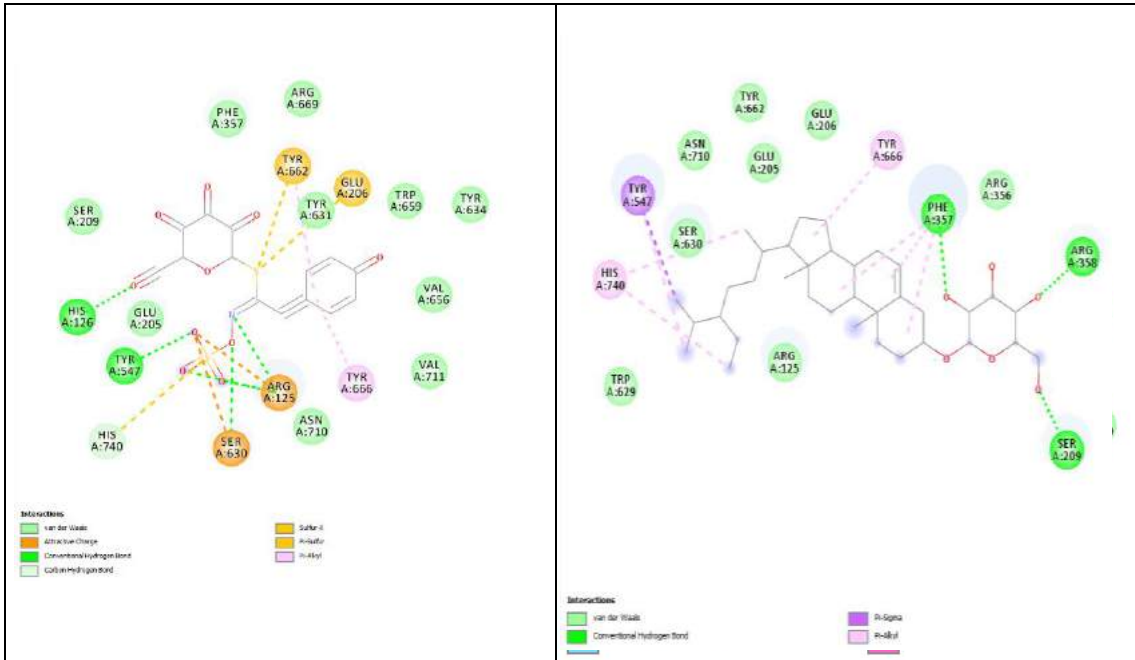
Senyawa Kimia	$\Delta G_{\text{binding}}$ (kcal/mol) \pm SD			
	PTP1B	GK	DPP4	AG
Ligan Asli	-11,6\pm0,00	-8,4\pm0,00	-8,2\pm0,00	-9,7\pm0,00
2-Methylpropyl Glucosinolate	-11,2 \pm 0,19	-7,4 \pm 0,00	-7,1 \pm 0,55	-5,5 \pm 0,16
3,5-Dihydroxy-6-methyl-2,3-dihydro-4H-pyran-4-one	-6,9 \pm 0,06	-4,6 \pm 0,00	-4,7 \pm 0,00	-4,8 \pm 0,13
Glucocochlearin	-10,5 \pm 0,09	-5,5 \pm 0,07	-5,7 \pm 0,07	-4,1 \pm 0,14
4-(α -L-Rhamnopyranosyloxy)benzyl Glucosinolate	-12,0 \pm 0,18	-8,9 \pm 0,08	-7,3 \pm 0,00	-7,0 \pm 0,10
Glucoconringiin	-9,9 \pm 0,06	-5,4 \pm 0,26	-5,9 \pm 0,78	-4,2 \pm 0,05
4-Hydroxyphenyl) acetonitrile	-5,3 \pm 0,18	-4,9 \pm 0,11	-4,7 \pm 0,06	-5,1 \pm 0,05
4-Hydroxybenzyl Glucosinolate	-11,5 \pm 0,00	-8,6 \pm 0,09	-8,9 \pm 0,00	-6,3 \pm 0,05
α -tokoferol	-7,6 \pm 0,00	-9,6 \pm 0,09	-7,4 \pm 0,05	-6,5 \pm 0,26
γ -tokoferol	-8,1 \pm 0,26	-9,3 \pm 0,09	-7,6 \pm 0,00	-7,0 \pm 0,05
Benzylamin	-4,5 \pm 0,00	-4,4 \pm 0,18	-4,9 \pm 0,05	-4,3 \pm 0,15
Benzyl glucosinolate	-10,6 \pm 0,14	-7,3 \pm 0,28	-8,0 \pm 0,00	-6,2 \pm 0,05
β -sitosterol 3-O- β -D-glucuronopyranoside	-9,4 \pm 0,00	-11,3 \pm 0,06	-7,9 \pm 0,06	-8,4 \pm 0,13
Quercetin	-9,0 \pm 0,19	-7,9 \pm 0,26	-7,5 \pm 0,05	-6,6 \pm 0,05
Rhamnetin	-7,2 \pm 0,10	-7,3 \pm 0,05	-7,0 \pm 0,18	-6,0 \pm 0,50
Kaempferol	-7,7 \pm 0,08	-7,9 \pm 0,23	-7,2 \pm 0,30	-6,2 \pm 0,08
N- α -L-Rhamnopyranosyl Vincosamide	-9,6 \pm 0,08	-10,8 \pm 0,07	-10,0 \pm 0,06	-10,1 \pm 0,10
O-ethyl-4-(α -l-rhamnosyloxy)benzyl carbamate	-8,9 \pm 0,22	-8,7 \pm 0,41	-7,1 \pm 0,66	-7,2 \pm 0,05
Niazimicin	-8,3 \pm 0,05	-9,1 \pm 0,15	-7,0 \pm 0,06	-6,8 \pm 0,08
Niaziminin	-8,2 \pm 0,00	-9,1 \pm 0,12	-6,5 \pm 0,00	-7,1 \pm 0,22
Niazimin	-8,4 \pm 0,19	-9,3 \pm 0,24	-7,1 \pm 0,06	-7,0 \pm 0,19

Lampiran 4. Interaksi Ligan Uji dengan masing-masing Makromolekul

 <p>Interactions</p> <ul style="list-style-type: none"> van der Waals Water Hydrogen Bond Conventional Hydrogen Bond Pi-Alkyl 	 <p>Interactions</p> <ul style="list-style-type: none"> van der Waals Conventional Hydrogen Bond Pi-Arene Pi-Donor Hydrogen Bond Alkyl
<p>Native ligand α-G (5NN8)</p>	<p>O-ethyl-4-(α-l-rhamnosyloxy)benzyl carbamate</p>
 <p>Interactions</p> <ul style="list-style-type: none"> van der Waals Conventional Hydrogen Bond Carbon Hydrogen Bond Pi-Arene Alkyl Alkyl 	 <p>Interactions</p> <ul style="list-style-type: none"> van der Waals Conventional Hydrogen Bond Pi-Donor Hydrogen Bond Alkyl Pi-Alkyl
<p>N-α-L-Rhamnopyranosyl Vincosamide</p>	<p>β-sitosterol 3-O-β-D-glucuronopyranoside</p>

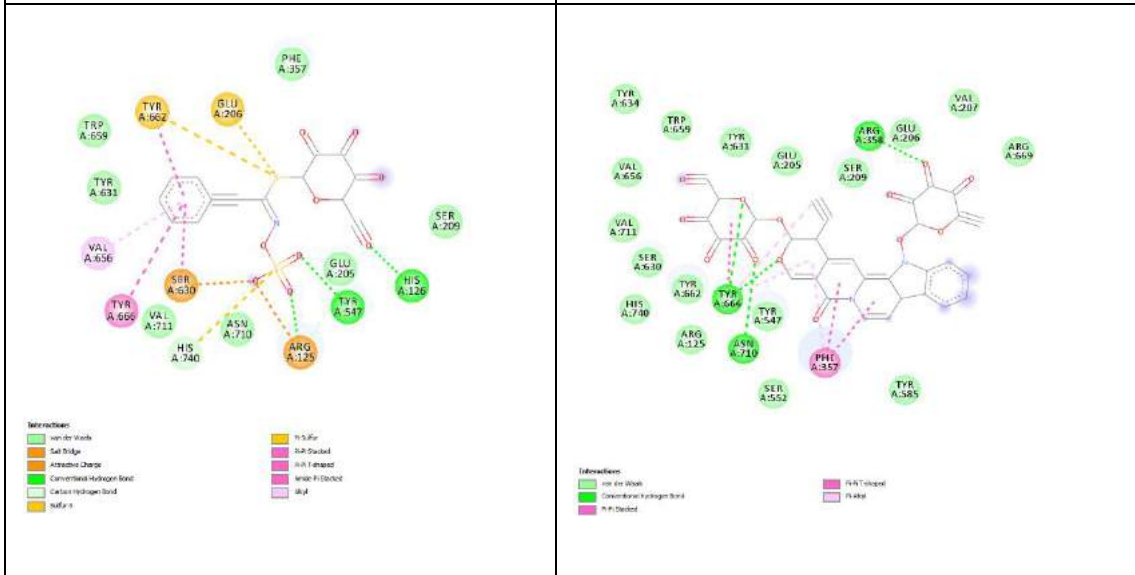






4-Hydroxybenzyl Glucosinolate

β-sitosterol 3-O-β-D-glucuronopyranoside



Benzyl glucosinolate

N-α-L-Rhamnopyranosyl Vincosamide