



UNIVERSITAT DE
BARCELONA

Non-glycosidic analogues of alpha-galactosylceramide: Design, synthesis and biological activity

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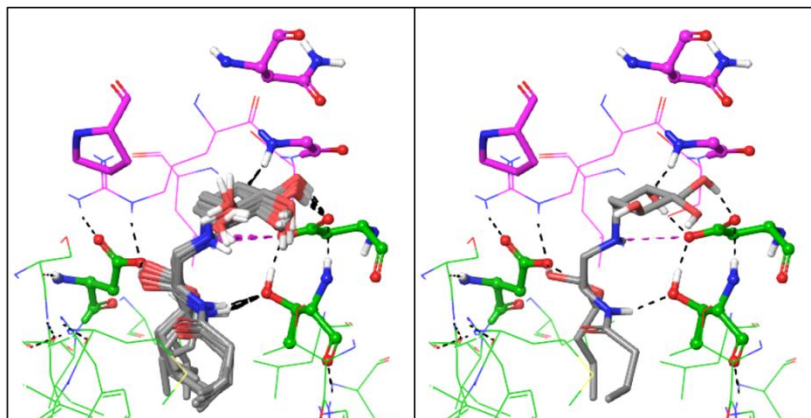
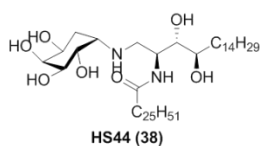
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ANNEX 2: Docking results summary

Summary of docking results of a selection of 20 ligands.

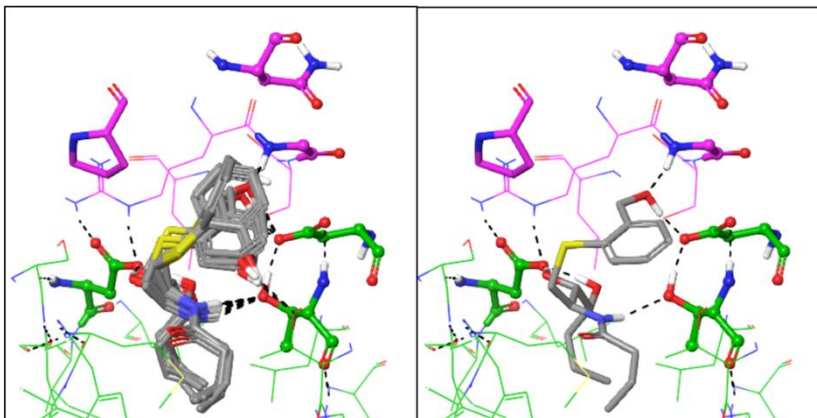
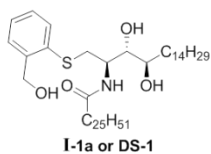
Superposition of 10 best scored docking poses on the left and best pose on the right, according to score ranking and presence of H-Bonding interactions considered important for activity. Tables indicate interactions of polar head and its substituents only; results of selected best pose are in bold.

- **HS44 (38):**



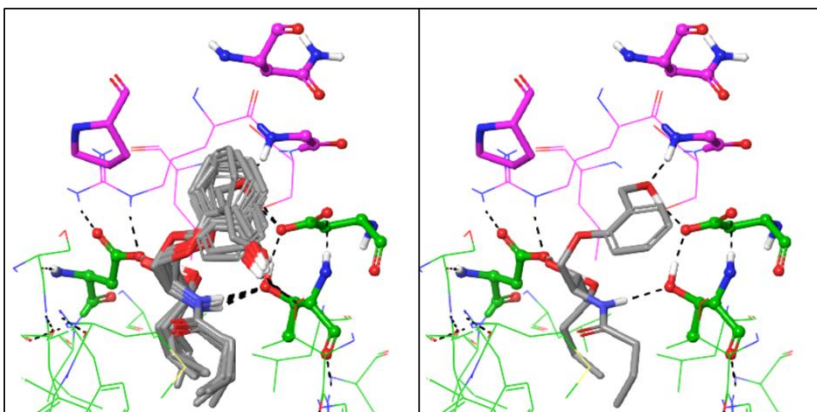
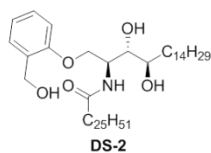
	Scores	Interactions
	-8,460	Asp153 _{CD1d} x2, Asp153 _{CD1d} salt, Gly96 _{αTCR}
	-8,318	Asp153 _{CD1d} x2, Asp153 _{CD1d} salt, Gly96 _{αTCR}
	-8,558	Asp153_{CD1d} x2, Asp153_{CD1d} salt, Gly96_{αTCR}
	-8,523	Asp153 _{CD1d} x2, Asp153 _{CD1d} salt, Gly96 _{αTCR}
	-8,442	Asp153 _{CD1d} x2, Asp153 _{CD1d} salt, Gly96 _{αTCR}
HS44	-8,598	Asp153 _{CD1d} x2, Asp153 _{CD1d} salt, Gly96 _{αTCR}
	-8,518	Asp153 _{CD1d} x2, Asp153 _{CD1d} salt, Gly96 _{αTCR}
	-9,085	Asp153 _{CD1d} x2, Asp153 _{CD1d} salt, Gly96 _{αTCR}
	-8,517	Asp153 _{CD1d} x2, Asp153 _{CD1d} salt, Gly96 _{αTCR}
	-8,998	Asp153 _{CD1d} x2, Asp153 _{CD1d} salt, Gly96 _{αTCR}

- DS-1:**



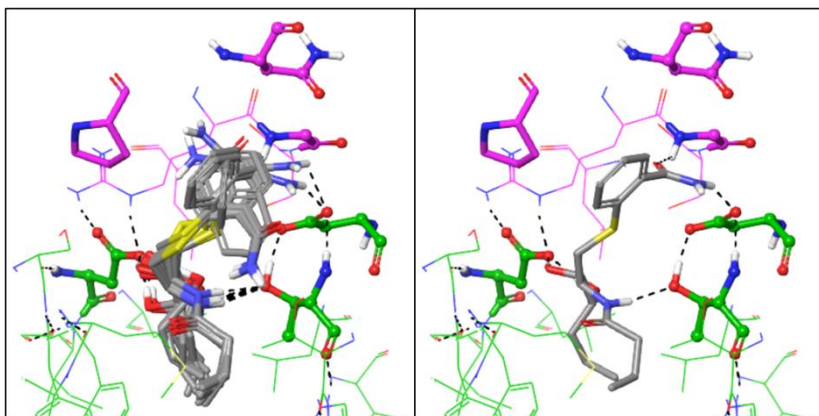
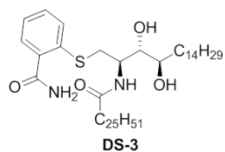
	Scores	Interactions
DS-1	-5,976	Gly96 _{αTCR}
	-6,811	Thr159 _{CD1d}
	-6,599	Thr159 _{CD1d}
	-5,754	Asp153 _{CD1d}
	-6,556	Asp153_{CD1d}, Gly96_{αTCR}
	-6,624	Thr159 _{CD1d}
	-6,810	Thr159 _{CD1d}
	-6,202	Asp153 _{CD1d} , Gly96 _{αTCR}
	-6,797	Asp153 _{CD1d}
-6,783	Thr159 _{CD1d}	

- DS-2:**



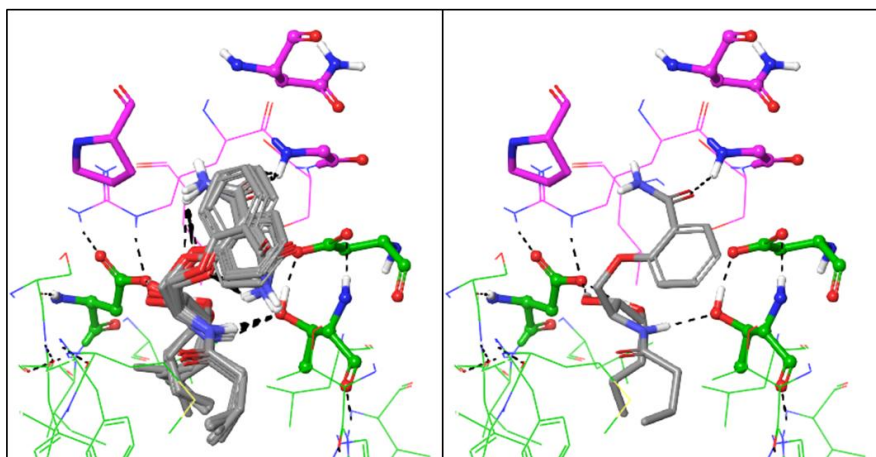
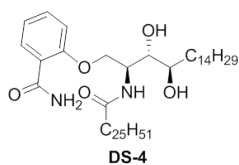
	Scores	Interactions
DS-2	-6,874	Thr159 _{CD1d}
	-6,776	Thr159 _{CD1d}
	-6,800	Thr159 _{CD1d}
	-7,045	Thr159 _{CD1d}
	-6,504	Thr159 _{CD1d}
	-6,465	Thr159 _{CD1d}
	-6,888	Thr159 _{CD1d}
	-6,530	-
	-6,919	Asp153_{CD1d}, Gly96_{αTCR}
	-6,605	Asp153 _{CD1d} , Gly96 _{αTCR}

- **DS-3:**



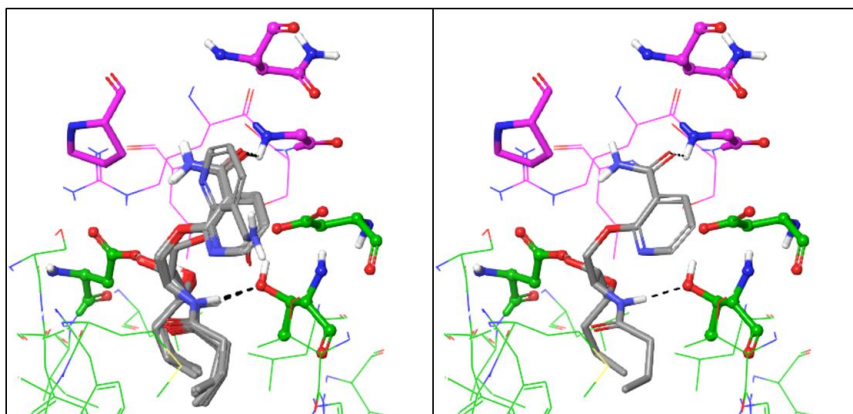
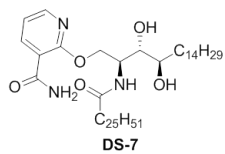
	Scores	Interactions
DS-3	-6,357	Asp94 _{αTCR}
	-5,719	Gly96 _{αTCR}
	-5,961	Asp153_{CD1d}, Gly96_{αTCR}
	-5,631	Asp153 _{CD1d} , Gly96 _{αTCR}
	-6,740	Thr159 _{CD1d}
	-6,773	Thr159 _{CD1d}
	-6,218	Thr159 _{CD1d}
	-6,085	Thr159 _{CD1d}
	-6,666	Thr159 _{CD1d}
	-6,440	Thr159 _{CD1d}

- **DS-4:**



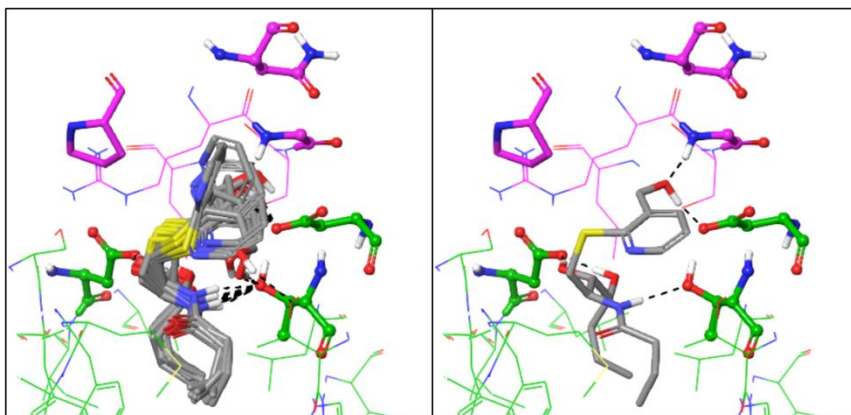
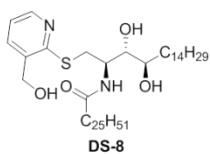
	Scores	Interactions
DS-4	-5,494	Asp94 _{αTCR} , Gly96 _{αTCR}
	-6,381	Thr159 _{CD1d}
	-6,328	Thr159 _{CD1d}
	-5,667	Asp94 _{αTCR} , Gly96 _{αTCR}
	-5,798	Asp94 _{αTCR} , Gly96 _{αTCR}
	-5,491	Asp94 _{αTCR} , Gly96 _{αTCR}
	-6,580	Thr159 _{CD1d}
	-6,395	Asp94_{αTCR}, Gly96_{αTCR}
	-5,578	Asp94 _{αTCR} , Gly96 _{αTCR}
	-6,333	Thr159 _{CD1d}

- **DS-7:**



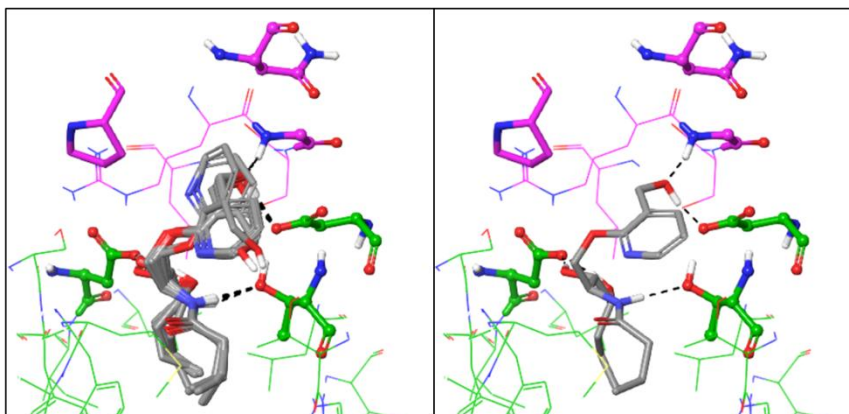
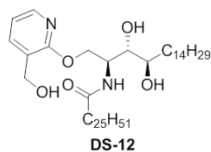
	Scores	Interactions
DS-7	-6,165	Asp94 _{αTCR} , Gly96 _{αTCR}
	-6,306	Asp94_{αTCR}, Gly96_{αTCR}
	-6,163	Thr159 _{CD1d}
	-6,359	Asp94 _{αTCR}
	-6,165	Asp94 _{αTCR} , Gly96 _{αTCR}
	-6,186	Asp94 _{αTCR} , Gly96 _{αTCR}
	-5,930	Asp94 _{αTCR}
	-6,291	Asp94 _{αTCR}
	-6,179	Asp94 _{αTCR} , Gly96 _{αTCR}
	-6,333	Asp94 _{αTCR}

- **DS-8:**



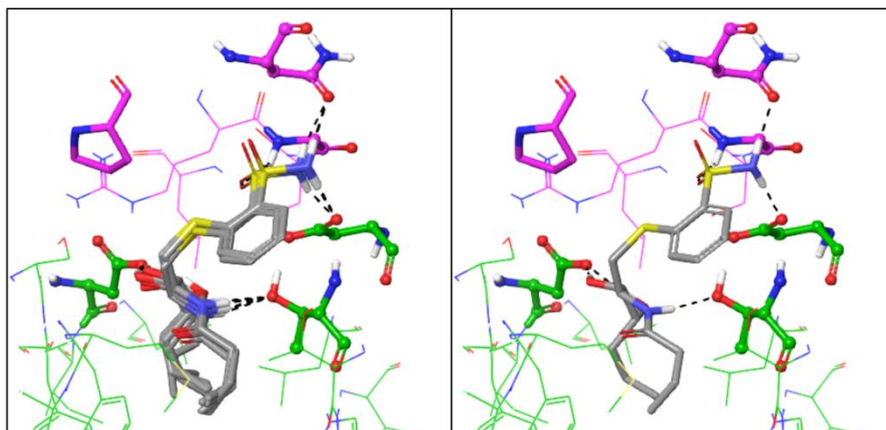
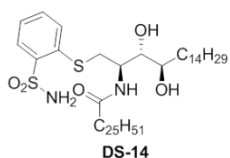
	Scores	Interactions
DS-8	-6,507	Asp153 _{CD1d} , Gly96 _{αTCR}
	-5,734	Thr156 _{CD1d}
	-6,444	Asp153 _{CD1d}
	-5,699	Asp153 _{CD1d}
	-6,553	Asp153_{CD1d}, Gly96_{αTCR}
	-6,510	Thr156 _{CD1d}
	-6,588	Thr159 _{CD1d}
	-6,503	Asp153 _{CD1d}
	-6,332	Asp153 _{CD1d}
	-6,933	Asp153 _{CD1d}

- DS-12:**



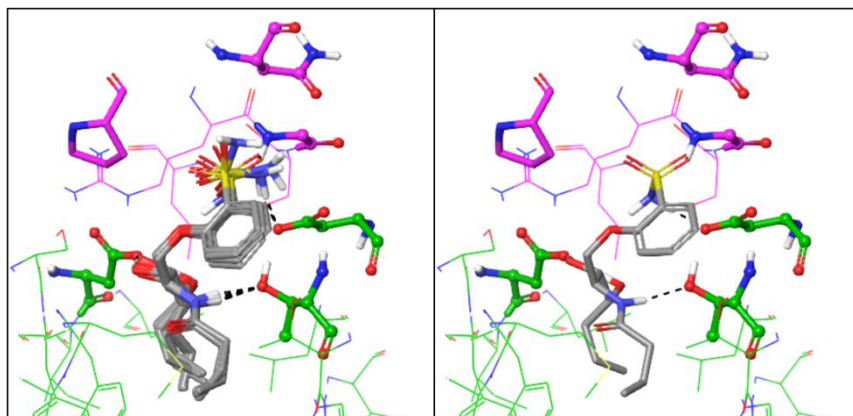
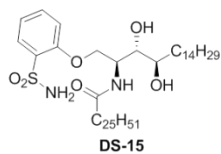
	Scores	Interactions
DS-12	-6,762	Asp153 _{CD1d}
	-6,732	Asp153 _{CD1d} , Gly96 _{αTCR}
	-6,888	Asp153 _{CD1d} , Gly96 _{αTCR}
	-6,393	Thr159 _{CD1d}
	-6,723	Asp153 _{CD1d}
	-6,955	Asp153_{CD1d}, Gly96_{αTCR}
	-6,952	Asp153 _{CD1d} , Gly96 _{αTCR}
	-6,886	Asp153 _{CD1d} , Gly96 _{αTCR}
	-6,841	Thr159 _{CD1d}
	-6,907	Asp153 _{CD1d} , Gly96 _{αTCR}

- DS-14:**



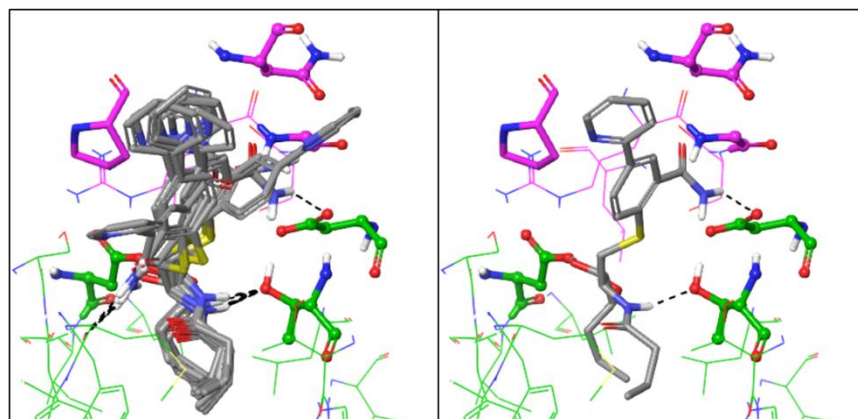
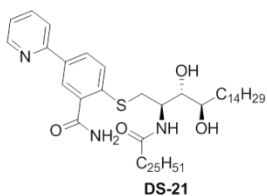
	Scores	Interactions
DS-14	-8,674	Asp153 _{CD1d} , Gly96 _{αTCR} , Asn30 _{αTCR}
	-8,557	Asp153 _{CD1d} , Gly96 _{αTCR} , Asn30 _{αTCR}
	-8,834	Asp153 _{CD1d} , Gly96 _{αTCR} , Asn30 _{αTCR}
	-8,706	Asp153 _{CD1d} , Gly96 _{αTCR} , Asn30 _{αTCR}
	-7,788	Asp153 _{CD1d} , Gly96 _{αTCR} , Asn30 _{αTCR}
	-8,406	Asp153 _{CD1d} , Gly96 _{αTCR} , Asn30 _{αTCR}
	-8,844	Asp153_{CD1d}, Gly96_{αTCR}, Asn30_{αTCR}
	-8,627	Asp153 _{CD1d} , Gly96 _{αTCR} , Asn30 _{αTCR}
	-8,570	Asp153 _{CD1d} , Gly96 _{αTCR} , Asn30 _{αTCR}
	-8,657	Asp153 _{CD1d} , Gly96 _{αTCR} , Asn30 _{αTCR}

- DS-15:**



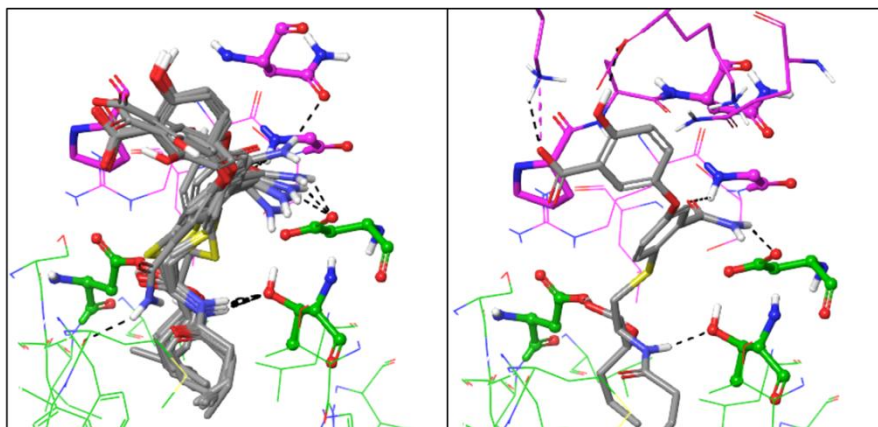
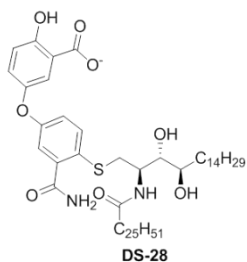
	Scores	Interactions
DS-15	-5,731	Close to "Asp153 _{CD1d} , Gly96 _{αTCR} "
	-6,082	Gly96 _{αTCR}
	-5,617	Close to "Asp153 _{CD1d} , Gly96 _{αTCR} "
	-5,337	Asp153 _{CD1d} , Gly96 _{αTCR}
	-5,313	Asp153 _{CD1d} , Gly96 _{αTCR}
	-5,492	Asp153_{CD1d}, Gly96_{αTCR}
	-5,940	Close to "Asp153 _{CD1d} , Gly96 _{αTCR} "
	-5,976	Close to "Asp153 _{CD1d} , Gly96 _{αTCR} "
	-5,995	Asp153 _{CD1d}
	-5,276	Asp153 _{CD1d}

- DS-21:**



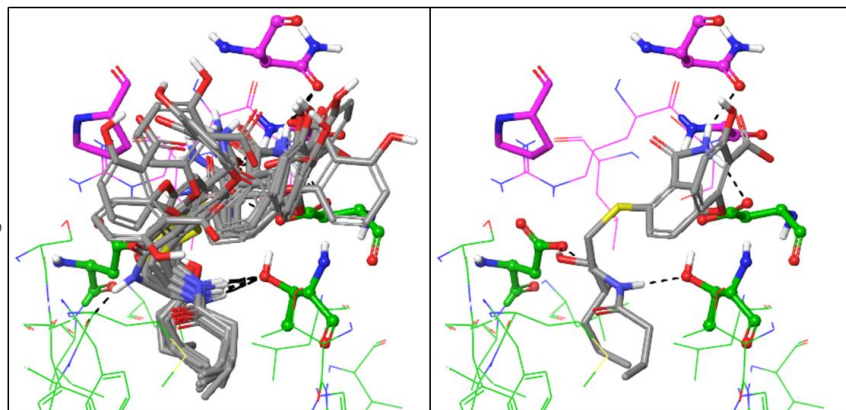
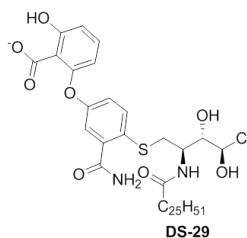
	Scores	Interactions
DS-21	-5,538	Met69 _{CD1d}
	-5,832	Asp29 _{αTCR} , Gly96 _{αTCR}
	-5,933	Met69 _{CD1d}
	-5,430	Asp153 _{CD1d}
	-7,470	Asp29 _{αTCR}
	-5,799	Met69 _{CD1d}
	-6,248	Asp94 _{αTCR} , Gly96 _{αTCR} , Lys68 _{αTCR} π-cat.
	-5,565	Asp153_{CD1d}
	-6,336	Met69 _{CD1d}
	-6,080	Asp94 _{αTCR}

- **DS-28:**



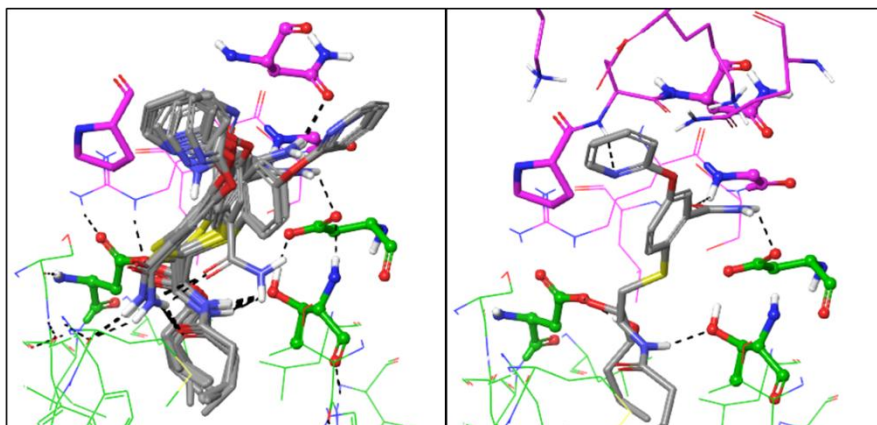
	Scores	Interactions
DS-28	-7,675	Asp29 _{αTCR} , Gly96 _{αTCR} , Lys71 _{αTCR} salt
	-8,007	Lys68 _{αTCR} , Lys71 _{αTCR}
	-8,808	Asp153 _{CD1d} , Gly96 _{αTCR} , Lys68 _{αTCR} , Lys71 _{αTCR}
	-7,191	Asp153 _{CD1d} , Gly96 _{αTCR} , Lys71 _{αTCR} salt
	-8,681	Asp153 _{CD1d} , Gly96 _{αTCR} , Lys68 _{αTCR} , Lys71 _{αTCR} salt
	-8,633	Asp153 _{CD1d} , Gly96 _{αTCR} , Lys68 _{αTCR} , Lys71 _{αTCR} salt
	-8,784	Met69 _{CD1d} , Lys68 _{αTCR} , Lys71 _{αTCR} salt
	-8,887	Asp153_{CD1d}, Gly96_{αTCR}, Lys68_{αTCR}, Lys71_{αTCR} salt
	-8,410	Asp153 _{CD1d} , Gly96 _{αTCR} , Lys68 _{αTCR} , Lys71 _{αTCR} , Lys71 _{αTCR} salt
	-8,519	Asn30 _{αTCR} , Lys68 _{αTCR} , Lys71 _{αTCR} salt

- **DS-29:**



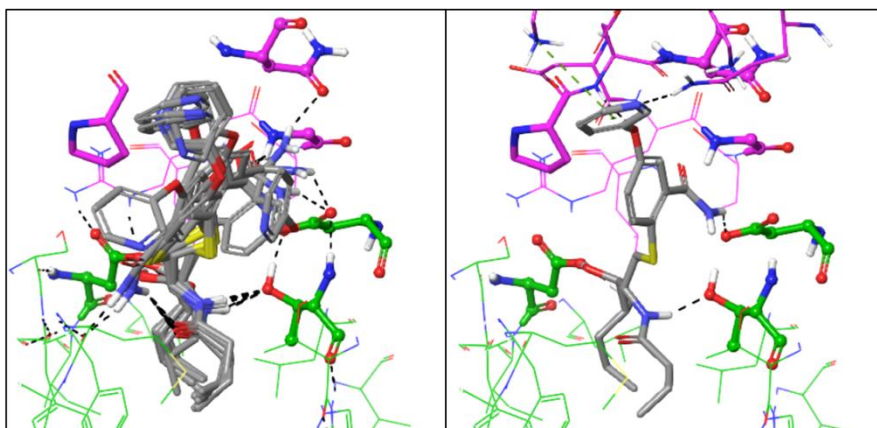
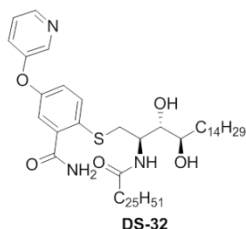
	Scores	Interactions
DS-29	-7,232	Asp153 _{CD1d} , Asp29 _{αTCR} , Lys68 _{αTCR} salt
	-7,500	-
	-8,568	Met69 _{CD1d} , Asp29 _{αTCR} x2, Lys68 _{αTCR} π-cat., Lys71 _{αTCR} salt
	-8,145	Asp153 _{CD1d} , Asp29 _{αTCR} , Lys68 _{αTCR} salt, Lys68 _{αTCR}
	-9,742	Asp94 _{αTCR} , Gly96 _{αTCR} , Lys68 _{αTCR} salt, Lys68 _{αTCR} , Gln52 _{αTCR}
	-7,984	Asp94 _{αTCR} , Gly96 _{αTCR} , Lys68 _{αTCR} salt,
	-8,963	Asp153_{CD1d}, Asn30_{αTCR}, Lys68_{αTCR} x2, Gln52_{αTCR}
	-7,879	Lys71 _{αTCR} salt
	-8,706	Gly96 _{αTCR} , Lys68 _{αTCR} salt, Lys68 _{αTCR} , Gln52 _{αTCR}
	-8,595	Asp153 _{CD1d} , Asn30 _{αTCR} , Lys68 _{αTCR} x2, Gln52 _{αTCR}

- **DS-31:**



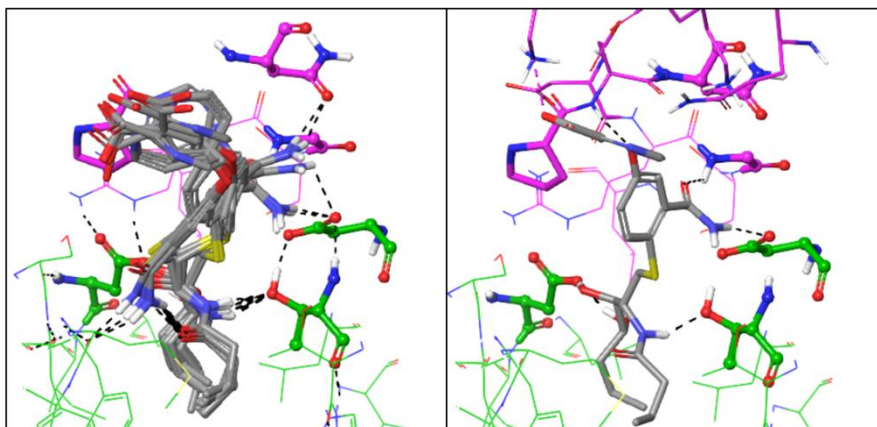
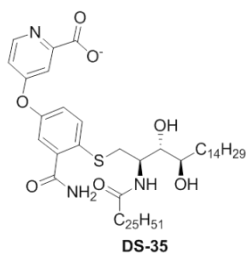
	Scores	Interactions
DS-31	-6,676	Asp153 _{CD1d} , Gly96 _{αTCR} , Asp29 _{αTCR}
	-6,331	Asp94 _{αTCR} , Lys68 _{αTCR} π-cat.
	-6,887	Met69 _{CD1d}
	-6,640	Asp29 _{αTCR} , Gly96 _{αTCR}
	-7,206	Met69 _{CD1d}
	-5,997	Close to "Asp153 _{CD1d} , Gly96 _{αTCR} "
	-6,615	-
	-6,818	Met69 _{CD1d}
	-6,503	Gly96 _{αTCR} , Asn30 _{αTCR}
	-6,853	Asp94 _{αTCR} , Lys68 _{αTCR}

- **DS-32:**



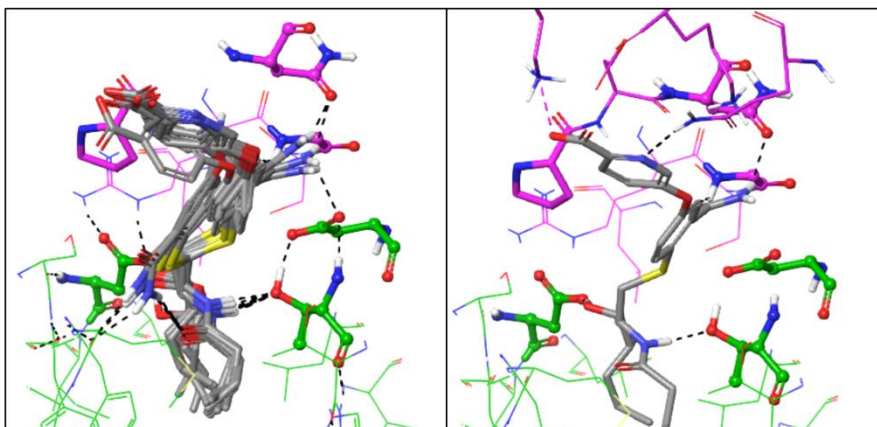
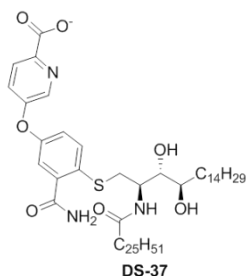
	Scores	Interactions
DS-32	-6,341	-
	-7,649	Asp29 _{αTCR} , Gln52 _{αTCR}
	-7,715	Asp153_{CD1d}, Asp29_{αTCR}, Gln52_{αTCR}, Lys71_{αTCR} π-cat.
	-7,594	Asp153 _{CD1d} , Asp29 _{αTCR} , Gln52 _{αTCR}
	-7,608	Asp153 _{CD1d} , Asp29 _{αTCR} , Gln52 _{αTCR}
	-6,466	Asp153 _{CD1d} , Gly96 _{αTCR}
	-7,746	Asp153 _{CD1d} , Asp29 _{αTCR} , Gln52 _{αTCR}
	-6,846	Met69 _{CD1d}
	-7,157	Met69 _{CD1d}
	-7,155	Gly96 _{αTCR} , Asn30 _{αTCR}

- **DS-35:**



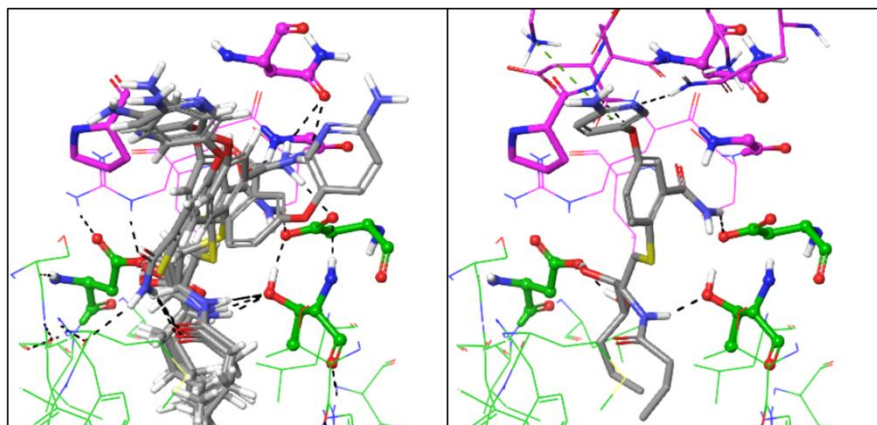
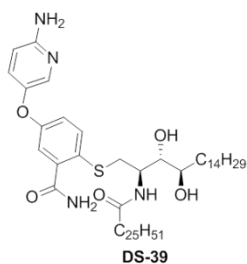
	Scores	Interactions
DS-35	-7,703	Asp153 _{CD1d} , Asp29 _{αTCR} , Lys71 _{αTCR} salt
	-6,853	Met69 _{CD1d} , Lys71 _{αTCR} salt, Lys71 _{αTCR}
	-7,174	Gly96 _{αTCR} , Gln52 _{αTCR}
	-6,965	Asp153 _{CD1d} , Gly96 _{αTCR} , Lys71 _{αTCR} salt
	-6,430	Gly96 _{αTCR} , Asn30 _{αTCR}
	-7,225	Met69 _{CD1d} , Lys71 _{αTCR} salt, Lys71 _{αTCR}
	-7,147	Gly96 _{αTCR} , Gln52 _{αTCR}
	-7,068	Gly96 _{αTCR} , Asn30 _{αTCR} , Gln52 _{αTCR} , Lys71 _{αTCR} salt
	-7,309	Met69 _{CD1d} , Lys71 _{αTCR} salt, Lys71 _{αTCR}
-7,822	Asp153_{CD1d}, Gly96_{αTCR}, Asp29_{αTCR}	

- **DS-37:**



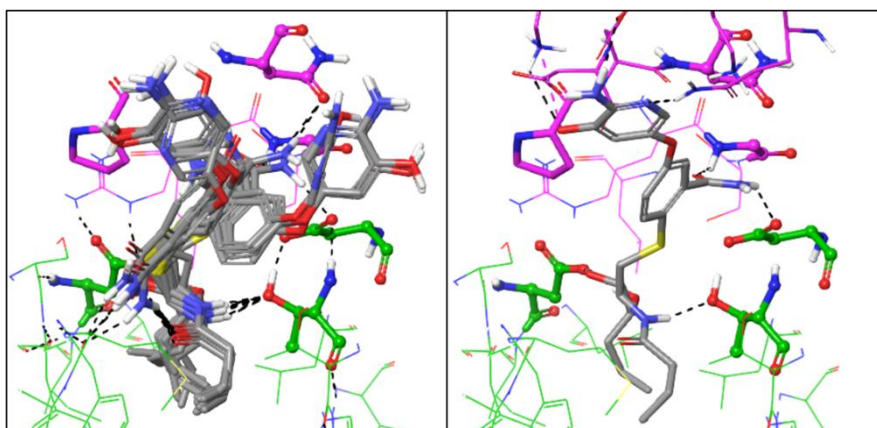
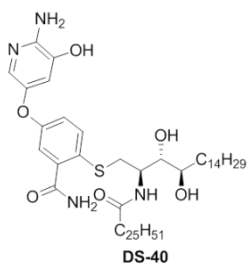
	Scores	Interactions
DS-37	-7,286	Gly96 _{αTCR} , Asp94 _{αTCR} , Lys71 _{αTCR} , Lys71 _{αTCR} salt
	-8,047	Met69 _{CD1d} , Lys71 _{αTCR} salt, Gln52 _{αTCR}
	-7,489	Gly96 _{αTCR} , Asn30 _{αTCR} , Lys71 _{αTCR} , Lys71 _{αTCR} salt
	-6,996	Gly96 _{αTCR} , Lys71 _{αTCR} salt
	-7,214	Asp153 _{CD1d} , Gly96 _{αTCR} , Lys71 _{αTCR} , Lys71 _{αTCR} salt
	-7,603	Gly96 _{αTCR} , Asp94 _{αTCR} , Gln52 _{αTCR} , Lys71 _{αTCR} salt
	-7,894	Met69 _{CD1d} , Lys71 _{αTCR} salt, Gln52 _{αTCR}
	-7,332	Met69 _{CD1d} , Lys71 _{αTCR} salt, Gln52 _{αTCR}
	-7,756	Gly96_{αTCR}, Asn30_{αTCR}, Gln52_{αTCR}, Lys71_{αTCR} salt
-7,628	Gly96 _{αTCR} , Asp94 _{αTCR} , Gln52 _{αTCR} , Lys71 _{αTCR} salt	

• **DS-39:**



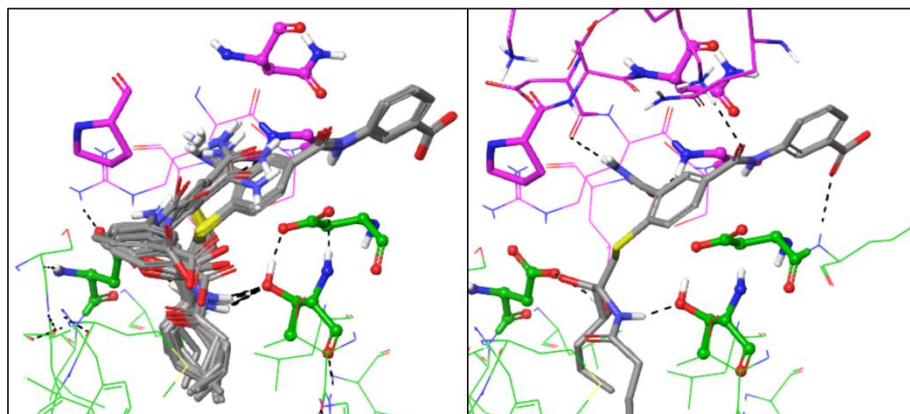
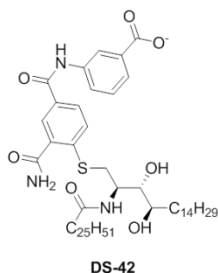
	Scores	Interactions
DS-39	-7,639	Met69 _{CD1d} , Lys68 _{αTCR}
	-8,001	Met69 _{CD1d} , Gln52 _{αTCR}
	-7,730	Gly96 _{αTCR} , Lys68 _{αTCR} , Gln52 _{αTCR}
	-6,986	Asn30 _{αTCR} , Gly96 _{αTCR}
	-8,134	Met69 _{CD1d} , Lys68 _{αTCR} , Gln52 _{αTCR}
	-7,111	Lys68 _{αTCR} , Gln52 _{αTCR}
	-7,068	Met69 _{CD1d} , Lys68 _{αTCR}
	-7,724	Asn30 _{αTCR} , Lys68 _{αTCR} , Gln52 _{αTCR}
	-8,230	Asp153_{CD1d}, Asp29_{αTCR}, Gln52_{αTCR}, Lys71_{αTCR} π-cat.
	-7,243	Asp153 _{CD1d} , Asn30 _{αTCR} , Lys68 _{αTCR} , Val50 _{αTCR}

• **DS-40:**



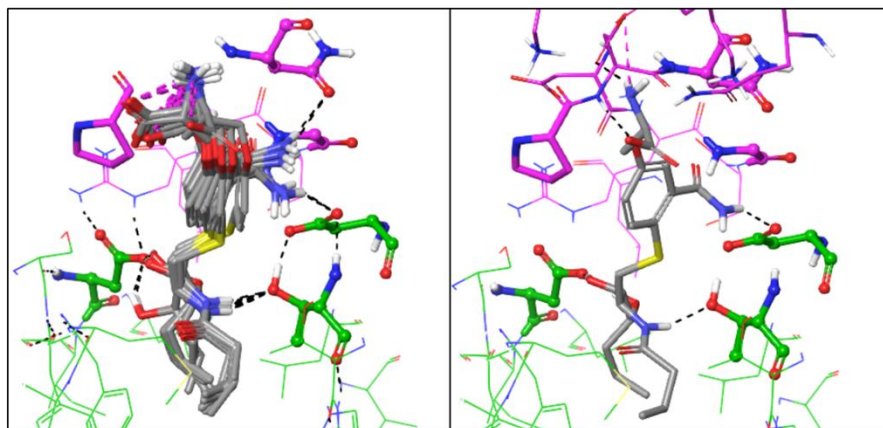
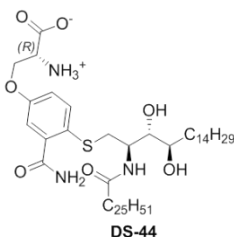
	Scores	Interactions
DS-40	-6,451	Gly96 _{αTCR} , Lys68 _{αTCR} , Val50 _{αTCR}
	-8,277	Met69 _{CD1d} , Lys68 _{αTCR} , Gln52 _{αTCR}
	-8,162	Met69 _{CD1d} , Lys68 _{αTCR} , Gln52 _{αTCR}
	-5,809	Gly96 _{αTCR} , Asp94 _{αTCR} , Lys68 _{αTCR} , Val50 _{αTCR}
	-6,118	Asp94 _{αTCR} , Lys68 _{αTCR} , Val50 _{αTCR}
	-6,199	Asp153 _{CD1d} , Asn30 _{αTCR} , Lys68 _{αTCR} , Val50 _{αTCR}
	-8,067	Met69 _{CD1d} , Lys68 _{αTCR} , Gln52 _{αTCR}
	-7,235	Asn30 _{αTCR} , Lys68 _{αTCR} , Gln52 _{αTCR}
	-6,681	Asp94 _{αTCR} , Lys68 _{αTCR} , Gln52 _{αTCR}
	-7,122	Met69 _{CD1d} , Asp29 _{αTCR} , Lys68 _{αTCR}

• **DS-42:**



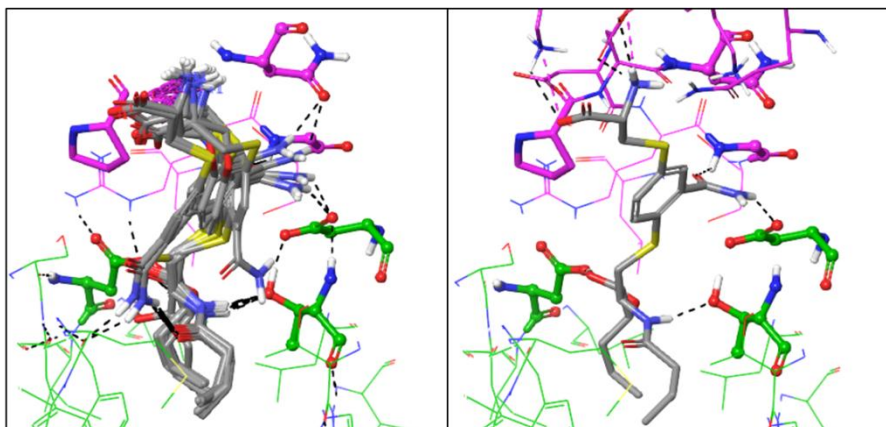
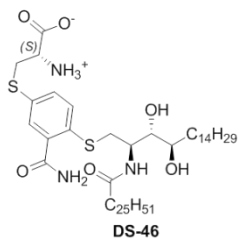
	Scores	Interactions
DS-42	-6,787	Lys65 _{CD1d} salt
	-8,173	Gln154 _{CD1d} , Gly96 _{αTCR} , Asp94 _{αTCR} , Lys68 _{αTCR}
	-7,887	Gln154 _{CD1d} , Gly96 _{αTCR} , Asp94 _{αTCR} , Lys68 _{αTCR}
	-7,118	-
	-7,627	Lys65 _{CD1d} salt
	-7,469	Lys65 _{CD1d} salt
	-9,294	Gln154_{CD1d}, Gly96_{αTCR}, Asp94_{αTCR}, Lys68_{αTCR}
	-9,045	Gln154 _{CD1d} , Gly96 _{αTCR} , Asp94 _{αTCR} , Lys68 _{αTCR}
	-6,955	Lys65 _{CD1d} salt
	-9,060	Gln154 _{CD1d} , Gly96 _{αTCR} , Asp94 _{αTCR} , Lys68 _{αTCR}

• **DS-44:**



	Scores	Interactions
DS-44	-7,410	Asp29 _{αTCR} , Lys68 _{αTCR} x2, Lys71 _{αTCR} salt
	-7,629	Asp153 _{CD1d} , Asp29 _{αTCR} x2, Asp29 _{αTCR} salt, Lys71 _{αTCR} salt
	-7,522	Asp29 _{αTCR} , Asp29 _{αTCR} salt, Asn30 _{αTCR} , Lys68 _{αTCR} , Lys71 _{αTCR} salt
	-7,469	Gly96 _{αTCR} , Asp29 _{αTCR} x2, Asp29 _{αTCR} salt, Lys71 _{αTCR} salt
	-7,498	Gly96 _{αTCR} , Asp94 _{αTCR} , Asp29 _{αTCR} x2, Asp29 _{αTCR} salt, Lys71 _{αTCR} salt
	-7,029	Asp29 _{αTCR} , Asp29 _{αTCR} salt, Lys68 _{αTCR} , Lys71 _{αTCR} salt
	-7,265	Asp153 _{CD1d} , Asp29 _{αTCR} , Asp29 _{αTCR} salt, Lys68 _{αTCR} , Lys71 _{αTCR} salt
	-8,122	Asp153_{CD1d}, Asp29_{αTCR}, Asp29_{αTCR} salt
	-7,193	Asp29 _{αTCR} , Asp29 _{αTCR} salt, Lys71 _{αTCR} salt
	-7,204	Asn30 _{αTCR} , Asp29 _{αTCR} , Asp29 _{αTCR} salt, Lys68 _{αTCR} , Lys71 _{αTCR} salt

• **DS-46:**



	Scores	Interactions
DS-46	-7,482	Gly96 _{αTCR} , Asp29 _{αTCR} , Asp29 _{αTCR} salt, Asn30 _{αTCR} , Lys68 _{αTCR} , Lys71 _{αTCR} salt
	-7,417	Asp29 _{αTCR} x2, Asp29 _{αTCR} salt, Lys71 _{αTCR} salt
	-7,552	Asp29 _{αTCR} , Asp29 _{αTCR} salt, Asn30 _{αTCR} , Lys68 _{αTCR} , Lys71 _{αTCR} salt
	-7,469	Gly96 _{αTCR} , Asp29 _{αTCR} x2, Asp29 _{αTCR} salt, Lys71 _{αTCR} salt
	-7,905	Gly96 _{αTCR} , Asp29 _{αTCR} , Asp29 _{αTCR} salt, Lys71 _{αTCR} salt
	-7,676	Gly96 _{αTCR} , Asp29 _{αTCR} , Asp29 _{αTCR} salt, Lys71 _{αTCR} salt
	-8,003	Gly96 _{αTCR} , Asp94 _{αTCR} , Asp29 _{αTCR} x3, Asp29 _{αTCR} salt, Lys71 _{αTCR} salt
	-8,430	Met69 _{CD1d} , Asp29 _{αTCR} x2, Asp29 _{αTCR} salt, Lys71 _{αTCR}
	-7,895	Asp153_{CD1d}, Gly96_{αTCR}, Asp29_{αTCR}, Asp29_{αTCR} salt, Lys68_{αTCR}, Lys71_{αTCR} salt
	-8,024	Met69 _{CD1d} , Asp29 _{αTCR} , Asp29 _{αTCR} salt, Lys68 _{αTCR} , Lys71 _{αTCR}