UNIVERSITAT de
BARCELONA

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

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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):**
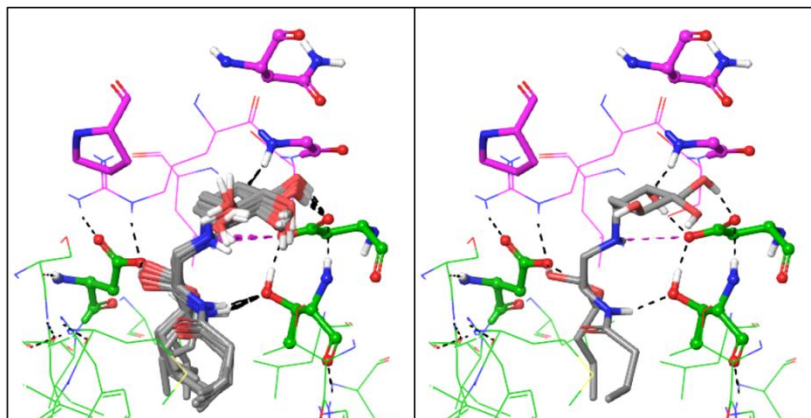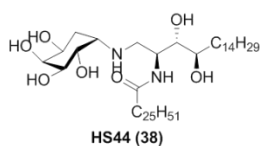
	Scores	Interactions
HS44	-8,460	Asp153$_{CD1d}$ x2, Asp153$_{CD1d}$ salt, Gly96$_{\alpha TCR}$
	-8,318	Asp153$_{CD1d}$ x2, Asp153$_{CD1d}$ salt, Gly96$_{\alpha TCR}$
	-8,558	**Asp153$_{CD1d}$ x2, Asp153$_{CD1d}$ salt, Gly96$_{\alpha TCR}$**
	-8,523	Asp153$_{CD1d}$ x2, Asp153$_{CD1d}$ salt, Gly96$_{\alpha TCR}$
	-8,442	Asp153$_{CD1d}$ x2, Asp153$_{CD1d}$ salt, Gly96$_{\alpha TCR}$
	-8,598	Asp153$_{CD1d}$ x2, Asp153$_{CD1d}$ salt, Gly96$_{\alpha TCR}$
	-8,518	Asp153$_{CD1d}$ x2, Asp153$_{CD1d}$ salt, Gly96$_{\alpha TCR}$
	-9,085	Asp153$_{CD1d}$ x2, Asp153$_{CD1d}$ salt, Gly96$_{\alpha TCR}$
	-8,517	Asp153$_{CD1d}$ x2, Asp153$_{CD1d}$ salt, Gly96$_{\alpha TCR}$
	-8,998	Asp153$_{CD1d}$ x2, Asp153$_{CD1d}$ salt, Gly96$_{\alpha TCR}$

- **DS-1:**
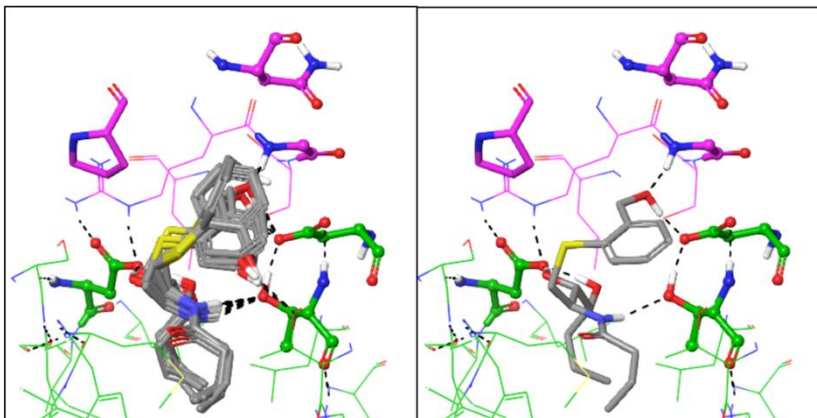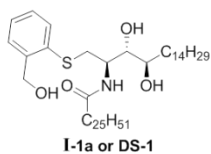
	Scores	Interactions
DS-1	-5,976	Gly96$_{\alpha TCR}$
	-6,811	Thr159$_{CD1d}$
	-6,599	Thr159$_{CD1d}$
	-5,754	Asp153$_{CD1d}$
	-6,556	**Asp153$_{CD1d}$, Gly96$_{\alpha TCR}$**
	-6,624	Thr159$_{CD1d}$
	-6,810	Thr159$_{CD1d}$
	-6,202	Asp153$_{CD1d}$, Gly96$_{\alpha TCR}$
	-6,797	Asp153$_{CD1d}$
	-6,783	Thr159$_{CD1d}$

- **DS-2:**
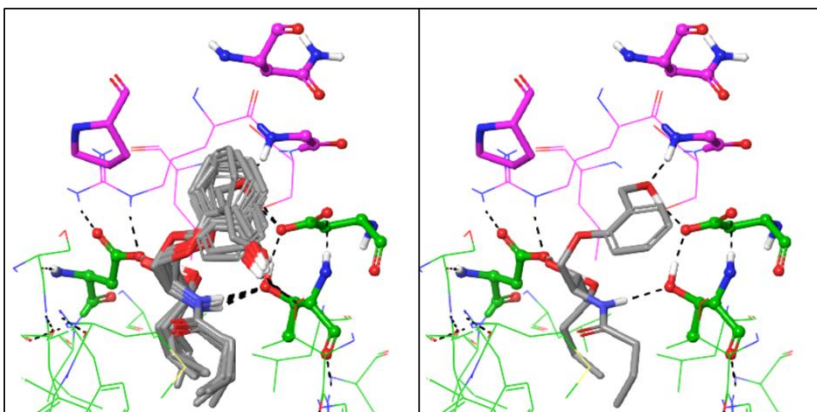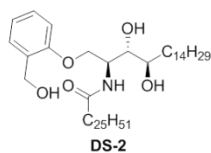
	Scores	Interactions
DS-2	-6,874	Thr159$_{CD1d}$
	-6,776	Thr159$_{CD1d}$
	-6,800	Thr159$_{CD1d}$
	-7,045	Thr159$_{CD1d}$
	-6,504	Thr159$_{CD1d}$
	-6,465	Thr159$_{CD1d}$
	-6,888	Thr159$_{CD1d}$
	-6,530	-
	-6,919	**Asp153$_{CD1d}$, Gly96$_{\alpha TCR}$**
	-6,605	Asp153$_{CD1d}$, Gly96$_{\alpha TCR}$

- **DS-3:**
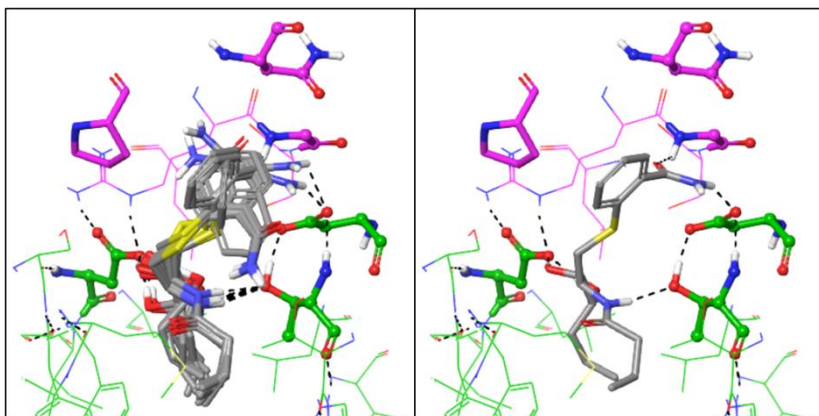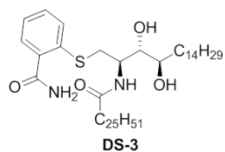
	Scores	Interactions
DS-3	-6,357	Asp94$_{\alpha TCR}$
	-5,719	Gly96$_{\alpha TCR}$
	-5,961	**Asp153$_{CD1d}$, Gly96$_{\alpha TCR}$**
	-5,631	Asp153$_{CD1d}$, Gly96$_{\alpha TCR}$
	-6,740	Thr159$_{CD1d}$
	-6,773	Thr159$_{CD1d}$
	-6,218	Thr159$_{CD1d}$
	-6,085	Thr159$_{CD1d}$
	-6,666	Thr159$_{CD1d}$
	-6,440	Thr159$_{CD1d}$

- **DS-4:**
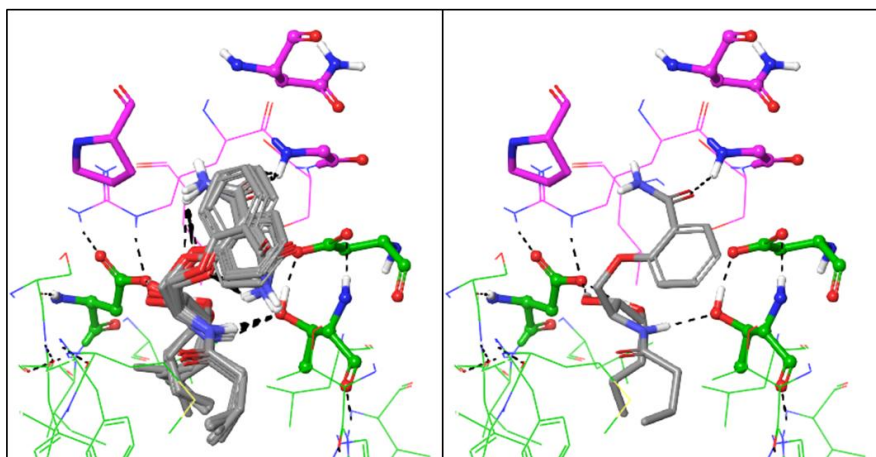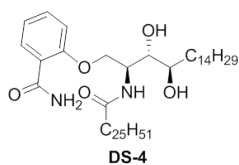
	Scores	Interactions
DS-4	-5,494	Asp94$_{\alpha TCR}$, Gly96$_{\alpha TCR}$
	-6,381	Thr159$_{CD1d}$
	-6,328	Thr159$_{CD1d}$
	-5,667	Asp94$_{\alpha TCR}$, Gly96$_{\alpha TCR}$
	-5,798	Asp94$_{\alpha TCR}$, Gly96$_{\alpha TCR}$
	-5,491	Asp94$_{\alpha TCR}$, Gly96$_{\alpha TCR}$
	-6,580	Thr159$_{CD1d}$
	-6,395	**Asp94$_{\alpha TCR}$, Gly96$_{\alpha TCR}$**
	-5,578	Asp94$_{\alpha TCR}$, Gly96$_{\alpha TCR}$
	-6,333	Thr159$_{CD1d}$

- **DS-7:**
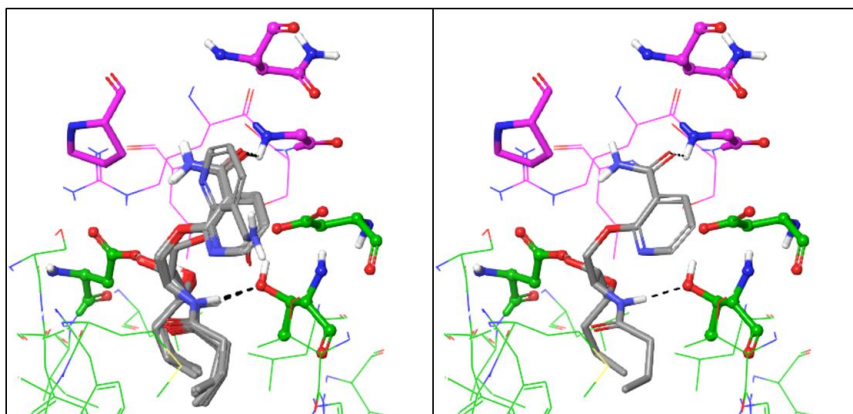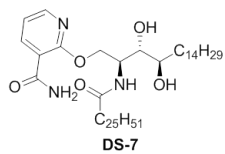
	Scores	Interactions
DS-7	-6,165	Asp94$_{\alpha TCR}$, Gly96$_{\alpha TCR}$
	-6,306	**Asp94$_{\alpha TCR}$, Gly96$_{\alpha TCR}$**
	-6,163	Thr159$_{CD1d}$
	-6,359	Asp94$_{\alpha TCR}$
	-6,165	Asp94$_{\alpha TCR}$, Gly96$_{\alpha TCR}$
	-6,186	Asp94$_{\alpha TCR}$, Gly96$_{\alpha TCR}$
	-5,930	Asp94$_{\alpha TCR}$
	-6,291	Asp94$_{\alpha TCR}$
	-6,179	Asp94$_{\alpha TCR}$, Gly96$_{\alpha TCR}$
	-6,333	Asp94$_{\alpha TCR}$

- **DS-8:**
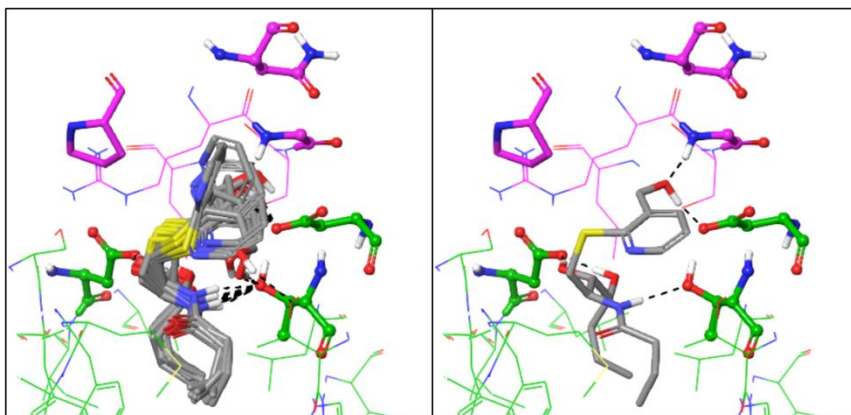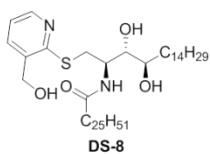
	Scores	Interactions
DS-8	-6,507	Asp153$_{CD1d}$, Gly96$_{\alpha TCR}$
	-5,734	Thr156$_{CD1d}$
	-6,444	Asp153$_{CD1d}$
	-5,699	Asp153$_{CD1d}$
	-6,553	**Asp153$_{CD1d}$, Gly96$_{\alpha TCR}$**
	-6,510	Thr156$_{CD1d}$
	-6,588	Thr159$_{CD1d}$
	-6,503	Asp153$_{CD1d}$
	-6,332	Asp153$_{CD1d}$
	-6,933	Asp153$_{CD1d}$

- **DS-12:**
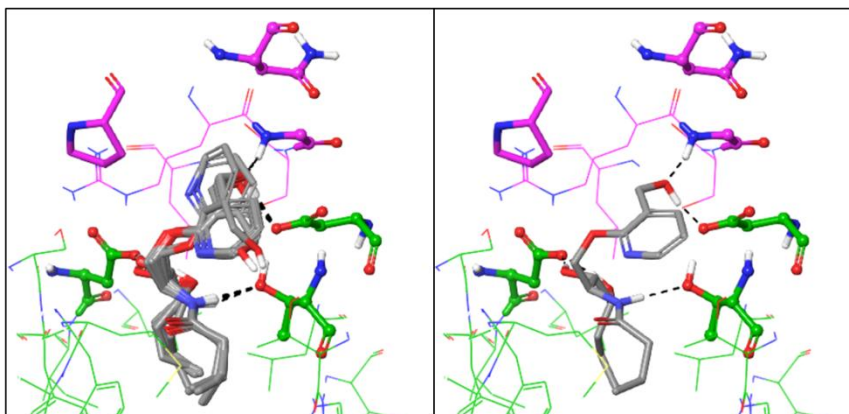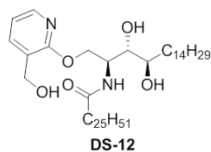
	Scores	Interactions
DS-12	-6,762	Asp153$_{CD1d}$
	-6,732	Asp153$_{CD1d}$, Gly96$_{\alpha TCR}$
	-6,888	Asp153$_{CD1d}$, Gly96$_{\alpha TCR}$
	-6,393	Thr159$_{CD1d}$
	-6,723	Asp153$_{CD1d}$
	-6,955	**Asp153$_{CD1d}$, Gly96$_{\alpha TCR}$**
	-6,952	Asp153$_{CD1d}$, Gly96$_{\alpha TCR}$
	-6,886	Asp153$_{CD1d}$, Gly96$_{\alpha TCR}$
	-6,841	Thr159$_{CD1d}$
	-6,907	Asp153$_{CD1d}$, Gly96$_{\alpha TCR}$
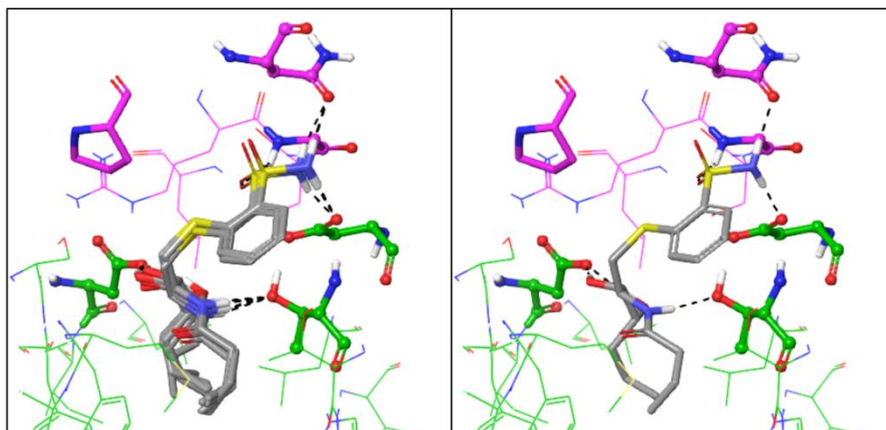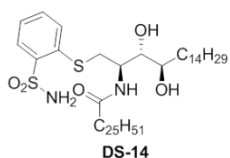
- **DS-14:**

	Scores	Interactions
DS-14	-8,674	Asp153$_{CD1d}$, Gly96$_{\alpha TCR}$, Asn30$_{\alpha TCR}$
	-8,557	Asp153$_{CD1d}$, Gly96$_{\alpha TCR}$, Asn30$_{\alpha TCR}$
	-8,834	Asp153$_{CD1d}$, Gly96$_{\alpha TCR}$, Asn30$_{\alpha TCR}$
	-8,706	Asp153$_{CD1d}$, Gly96$_{\alpha TCR}$, Asn30$_{\alpha TCR}$
	-7,788	Asp153$_{CD1d}$, Gly96$_{\alpha TCR}$, Asn30$_{\alpha TCR}$
	-8,406	Asp153$_{CD1d}$, Gly96$_{\alpha TCR}$, Asn30$_{\alpha TCR}$
	-8,844	**Asp153$_{CD1d}$, Gly96$_{\alpha TCR}$, Asn30$_{\alpha TCR}$**
	-8,627	Asp153$_{CD1d}$, Gly96$_{\alpha TCR}$, Asn30$_{\alpha TCR}$
	-8,570	Asp153$_{CD1d}$, Gly96$_{\alpha TCR}$, Asn30$_{\alpha TCR}$
	-8,657	Asp153$_{CD1d}$, Gly96$_{\alpha TCR}$, Asn30$_{\alpha TCR}$
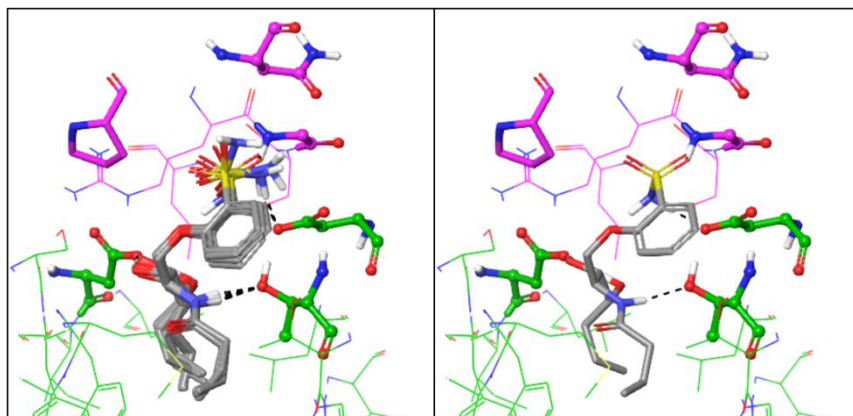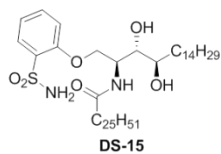
- **DS-15:**

	Scores	Interactions
DS-15	-5,731	Close to "Asp153$_{CD1d}$, Gly96$_{\alpha TCR}$"
	-6,082	Gly96$_{\alpha TCR}$
	-5,617	Close to "Asp153$_{CD1d}$, Gly96$_{\alpha TCR}$"
	-5,337	Asp153$_{CD1d}$, Gly96$_{\alpha TCR}$
	-5,313	Asp153$_{CD1d}$, Gly96$_{\alpha TCR}$
	-5,492	**Asp153$_{CD1d}$, Gly96$_{\alpha TCR}$**
	-5,940	Close to "Asp153$_{CD1d}$, Gly96$_{\alpha TCR}$"
	-5,976	Close to "Asp153$_{CD1d}$, Gly96$_{\alpha TCR}$"
	-5,995	Asp153$_{CD1d}$
	-5,276	Asp153$_{CD1d}$

- **DS-21:**
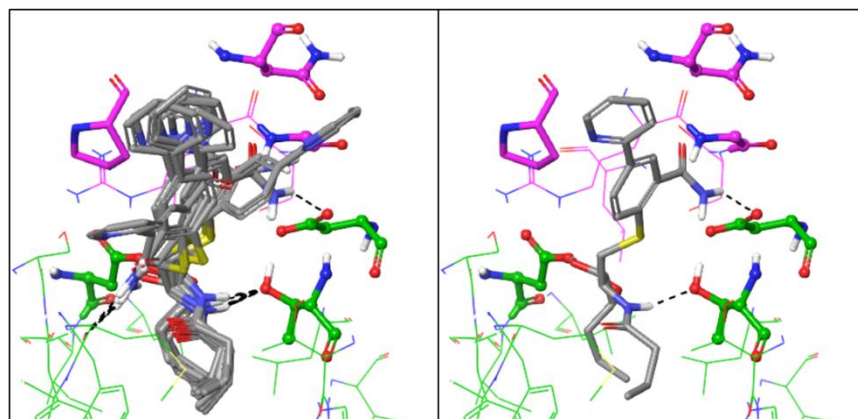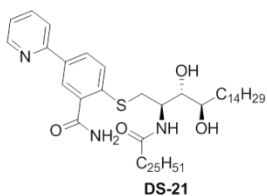
	Scores	Interactions
DS-21	-5,538	Met69$_{CD1d}$
	-5,832	Asp29$_{\alpha TCR}$, Gly96$_{\alpha TCR}$
	-5,933	Met69$_{CD1d}$
	-5,430	Asp153$_{CD1d}$
	-7,470	Asp29$_{\alpha TCR}$
	-5,799	Met69$_{CD1d}$
	-6,248	Asp94$_{\alpha TCR}$, Gly96$_{\alpha TCR}$, Lys68$_{\alpha TCR}$ π-cat.
	-5,565	**Asp153$_{CD1d}$**
	-6,336	Met69$_{CD1d}$
	-6,080	Asp94$_{\alpha TCR}$
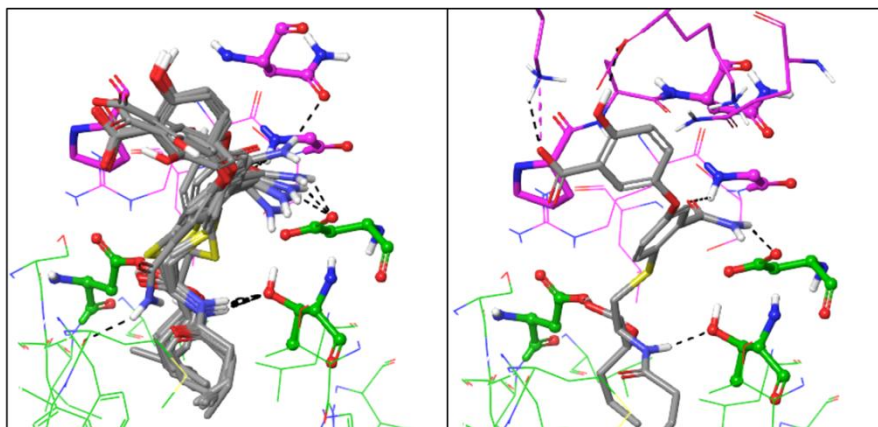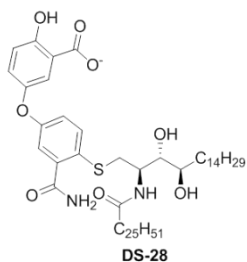
- **DS-28:**

	Scores	Interactions
DS-28	-7,675	Asp29$_{\alpha TCR}$, Gly96$_{\alpha TCR}$, Lys71$_{\alpha TCR}$ salt
	-8,007	Lys68$_{\alpha TCR}$, Lys71$_{\alpha TCR}$
	-8,808	Asp153$_{CD1d}$, Gly96$_{\alpha TCR}$, Lys68$_{\alpha TCR}$, Lys71$_{\alpha TCR}$
	-7,191	Asp153$_{CD1d}$, Gly96$_{\alpha TCR}$, Lys71$_{\alpha TCR}$ salt
	-8,681	Asp153$_{CD1d}$, Gly96$_{\alpha TCR}$, Lys68$_{\alpha TCR}$, Lys71$_{\alpha TCR}$ salt
	-8,633	Asp153$_{CD1d}$, Gly96$_{\alpha TCR}$, Lys68$_{\alpha TCR}$, Lys71$_{\alpha TCR}$ salt
	-8,784	Met69$_{CD1d}$, Lys68$_{\alpha TCR}$, Lys71$_{\alpha TCR}$ salt
	-8,887	**Asp153$_{CD1d}$, Gly96$_{\alpha TCR}$, Lys68$_{\alpha TCR}$, Lys71$_{\alpha TCR}$ salt**
	-8,410	Asp153$_{CD1d}$, Gly96$_{\alpha TCR}$, Lys68$_{\alpha TCR}$, Lys71$_{\alpha TCR}$, Lys71$_{\alpha TCR}$ salt
	-8,519	Asn30$_{\alpha TCR}$, Lys68$_{\alpha TCR}$, Lys71$_{\alpha TCR}$ salt
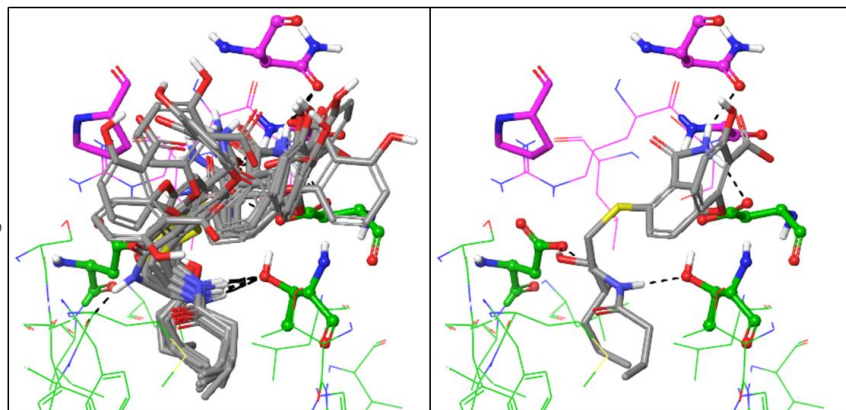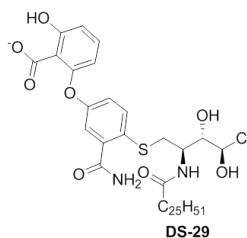
- **DS-29:**

	Scores	Interactions
DS-29	-7,232	Asp153$_{CD1d}$, Asp29$_{\alpha TCR}$, Lys68$_{\alpha TCR}$ salt
	-7,500	-
	-8,568	Met69$_{CD1d}$, Asp29$_{\alpha TCR}$ x2, Lys68$_{\alpha TCR}$ π-cat., Lys71$_{\alpha TCR}$ salt
	-8,145	Asp153$_{CD1d}$, Asp29$_{\alpha TCR}$, Lys68$_{\alpha TCR}$ salt, Lys68$_{\alpha TCR}$
	-9,742	Asp94$_{\alpha TCR}$, Gly96$_{\alpha TCR}$, Lys68$_{\alpha TCR}$ salt, Lys68$_{\alpha TCR}$, Gln52$_{\alpha TCR}$
	-7,984	Asp94$_{\alpha TCR}$, Gly96$_{\alpha TCR}$, Lys68$_{\alpha TCR}$ salt,
	-8,963	**Asp153$_{CD1d}$, Asn30$_{\alpha TCR}$, Lys68$_{\alpha TCR}$ x2, Gln52$_{\alpha TCR}$**
	-7,879	Lys71$_{\alpha TCR}$ salt
	-8,706	Gly96$_{\alpha TCR}$, Lys68$_{\alpha TCR}$ salt, Lys68$_{\alpha TCR}$, Gln52$_{\alpha TCR}$
	-8,595	Asp153$_{CD1d}$, Asn30$_{\alpha TCR}$, Lys68$_{\alpha TCR}$ x2, Gln52$_{\alpha TCR}$
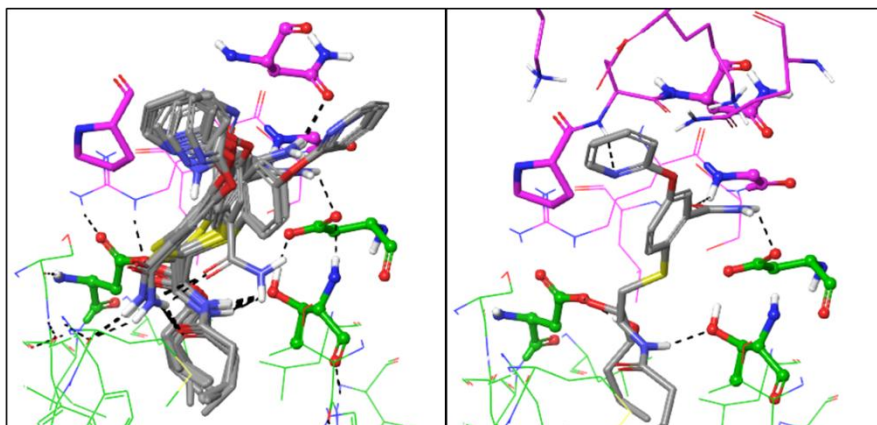
- **DS-31:**

	Scores	Interactions
DS-31	**-6,676**	**Asp153$_{CD1d}$, Gly96$_{\alpha TCR}$, Asp29$_{\alpha TCR}$**
	-6,331	Asp94$_{\alpha TCR}$, Lys68$_{\alpha TCR}$ π-cat.
	-6,887	Met69$_{CD1d}$
	-6,640	Asp29$_{\alpha TCR}$, Gly96$_{\alpha TCR}$
	-7,206	Met69$_{CD1d}$
	-5,997	Close to "Asp153$_{CD1d}$, Gly96$_{\alpha TCR}$"
	-6,615	-
	-6,818	Met69$_{CD1d}$
	-6,503	Gly96$_{\alpha TCR}$, Asn30$_{\alpha TCR}$
	-6,853	Asp94$_{\alpha TCR}$, Lys68$_{\alpha TCR}$
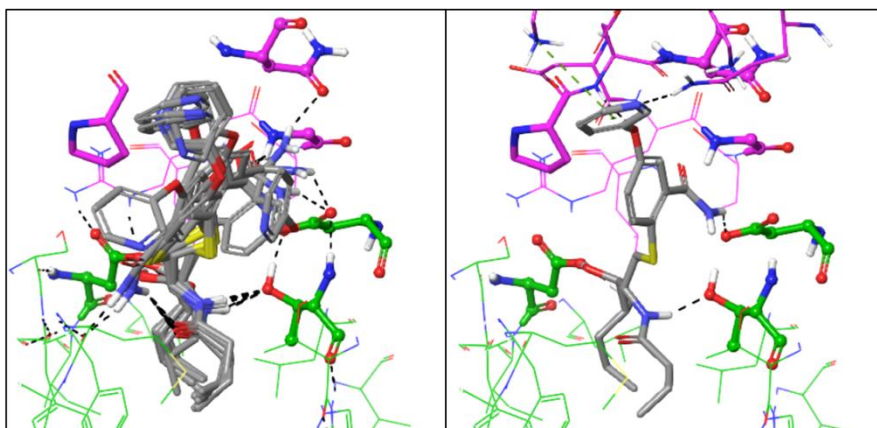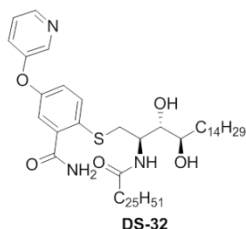
- **DS-32:**

	Scores	Interactions
DS-32	-6,341	-
	-7,649	Asp29$_{\alpha TCR}$, Gln52$_{\alpha TCR}$
	-7,715	**Asp153$_{CD1d}$, Asp29$_{\alpha TCR}$, Gln52$_{\alpha TCR}$, Lys71$_{\alpha TCR}$ π-cat.**
	-7,594	Asp153$_{CD1d}$, Asp29$_{\alpha TCR}$, Gln52$_{\alpha TCR}$
	-7,608	Asp153$_{CD1d}$, Asp29$_{\alpha TCR}$, Gln52$_{\alpha TCR}$
	-6,466	Asp153$_{CD1d}$, Gly96$_{\alpha TCR}$
	-7,746	Asp153$_{CD1d}$, Asp29$_{\alpha TCR}$, Gln52$_{\alpha TCR}$
	-6,846	Met69$_{CD1d}$
	-7,157	Met69$_{CD1d}$
	-7,155	Gly96$_{\alpha TCR}$, Asn30$_{\alpha TCR}$
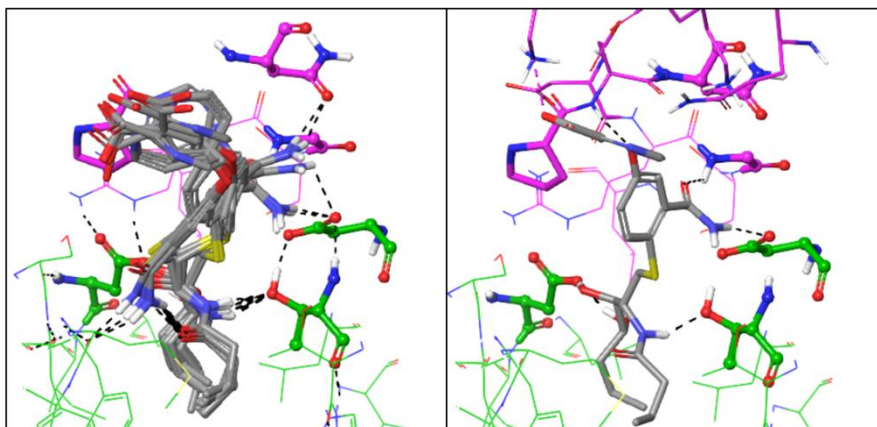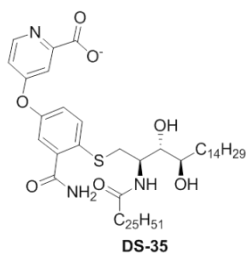
- **DS-35:**

	Scores	Interactions
	-7,703	Asp153$_{CD1d}$, Asp29$_{\alpha TCR}$, Lys71$_{\alpha TCR}$ salt
	-6,853	Met69$_{CD1d}$, Lys71$_{\alpha TCR}$ salt, Lys71$_{\alpha TCR}$
	-7,174	Gly96$_{\alpha TCR}$, Gln52$_{\alpha TCR}$
	-6,965	Asp153$_{CD1d}$, Gly96$_{\alpha TCR}$, Lys71$_{\alpha TCR}$ salt
DS-35	-6,430	Gly96$_{\alpha TCR}$, Asn30$_{\alpha TCR}$
	-7,225	Met69$_{CD1d}$, Lys71$_{\alpha TCR}$ salt, Lys71$_{\alpha TCR}$
	-7,147	Gly96$_{\alpha TCR}$, Gln52$_{\alpha TCR}$
	-7,068	Gly96$_{\alpha TCR}$, Asn30$_{\alpha TCR}$, Gln52$_{\alpha TCR}$, Lys71$_{\alpha TCR}$ salt
	-7,309	Met69$_{CD1d}$, Lys71$_{\alpha TCR}$ salt, Lys71$_{\alpha TCR}$
	-7,822	**Asp153$_{CD1d}$, Gly96$_{\alpha TCR}$, Asp29$_{\alpha TCR}$**

- **DS-37:**

	Scores	Interactions
	-7,286	Gly96$_{\alpha TCR}$, Asp94$_{\alpha TCR}$, Lys71$_{\alpha TCR}$, Lys71$_{\alpha TCR}$ salt
	-8,047	Met69$_{CD1d}$, Lys71$_{\alpha TCR}$ salt, Gln52$_{\alpha TCR}$
	-7,489	Gly96$_{\alpha TCR}$, Asn30$_{\alpha TCR}$, Lys71$_{\alpha TCR}$, Lys71$_{\alpha TCR}$ salt
	-6,996	Gly96$_{\alpha TCR}$, Lys71$_{\alpha TCR}$ salt
DS-37	-7,214	Asp153$_{CD1d}$, Gly96$_{\alpha TCR}$, Lys71$_{\alpha TCR}$, Lys71$_{\alpha TCR}$ salt
	-7,603	Gly96$_{\alpha TCR}$, Asp94$_{\alpha TCR}$, Gln52$_{\alpha TCR}$, Lys71$_{\alpha TCR}$ salt
	-7,894	Met69$_{CD1d}$, Lys71$_{\alpha TCR}$ salt, Gln52$_{\alpha TCR}$
	-7,332	Met69$_{CD1d}$, Lys71$_{\alpha TCR}$ salt, Gln52$_{\alpha TCR}$
	-7,756	**Gly96$_{\alpha TCR}$, Asn30$_{\alpha TCR}$, Gln52$_{\alpha TCR}$, Lys71$_{\alpha TCR}$ salt**
	-7,628	Gly96$_{\alpha TCR}$, Asp94$_{\alpha TCR}$, Gln52$_{\alpha TCR}$, Lys71$_{\alpha TCR}$ salt
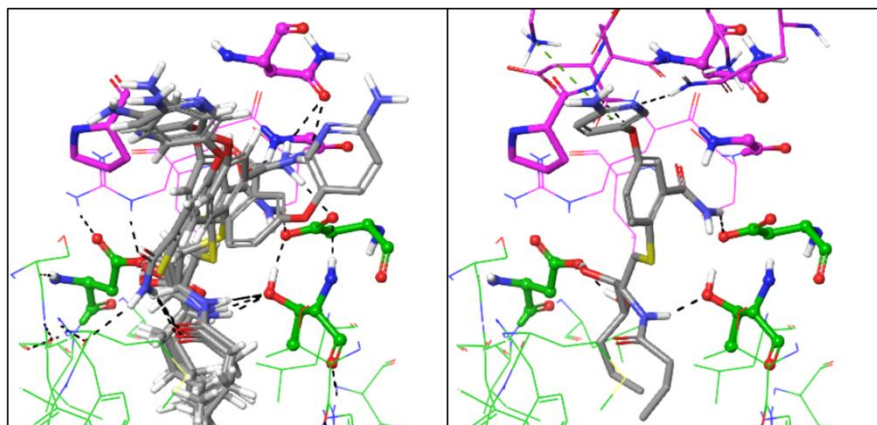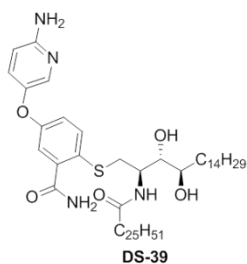
- **DS-39:**

	Scores	Interactions
DS-39	-7,639	Met69$_{CD1d}$, Lys68$_{\alpha TCR}$
	-8,001	Met69$_{CD1d}$, Gln52$_{\alpha TCR}$
	-7,730	Gly96$_{\alpha TCR}$, Lys68$_{\alpha TCR}$, Gln52$_{\alpha TCR}$
	-6,986	Asn30$_{\alpha TCR}$, Gly96$_{\alpha TCR}$
	-8,134	Met69$_{CD1d}$, Lys68$_{\alpha TCR}$, Gln52$_{\alpha TCR}$
	-7,111	Lys68$_{\alpha TCR}$, Gln52$_{\alpha TCR}$
	-7,068	Met69$_{CD1d}$, Lys68$_{\alpha TCR}$
	-7,724	Asn30$_{\alpha TCR}$, Lys68$_{\alpha TCR}$, Gln52$_{\alpha TCR}$
	-8,230	**Asp153$_{CD1d}$, Asp29$_{\alpha TCR}$, Gln52$_{\alpha TCR}$, Lys71$_{\alpha TCR}$ π-cat.**
	-7,243	Asp153$_{CD1d}$, Asn30$_{\alpha TCR}$, Lys68$_{\alpha TCR}$, Val50$_{\alpha TCR}$
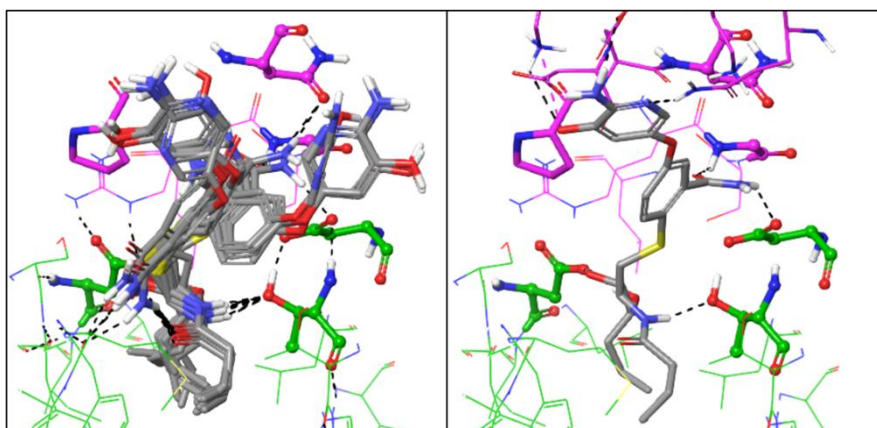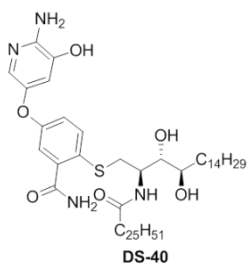
- **DS-40:**

	Scores	Interactions
DS-40	-6,451	Gly96$_{\alpha TCR}$, Lys68$_{\alpha TCR}$, Val50$_{\alpha TCR}$
	-8,277	Met69$_{CD1d}$, Lys68$_{\alpha TCR}$, Gln52$_{\alpha TCR}$
	-8,162	Met69$_{CD1d}$, Lys68$_{\alpha TCR}$, Gln52$_{\alpha TCR}$
	-5,809	Gly96$_{\alpha TCR}$, Asp94$_{\alpha TCR}$, Lys68$_{\alpha TCR}$, Val50$_{\alpha TCR}$
	-6,118	Asp94$_{\alpha TCR}$, Lys68$_{\alpha TCR}$, Val50$_{\alpha TCR}$
	-6,199	Asp153$_{CD1d}$, Asn30$_{\alpha TCR}$, Lys68$_{\alpha TCR}$, Val50$_{\alpha TCR}$
	-8,067	Met69$_{CD1d}$, Lys68$_{\alpha TCR}$, Gln52$_{\alpha TCR}$
	-7,235	Asn30$_{\alpha TCR}$, Lys68$_{\alpha TCR}$, Gln52$_{\alpha TCR}$
	-6,681	Asp94$_{\alpha TCR}$, Lys68$_{\alpha TCR}$, Gln52$_{\alpha TCR}$
	-7,122	Met69$_{CD1d}$, Asp29$_{\alpha TCR}$, Lys68$_{\alpha TCR}$
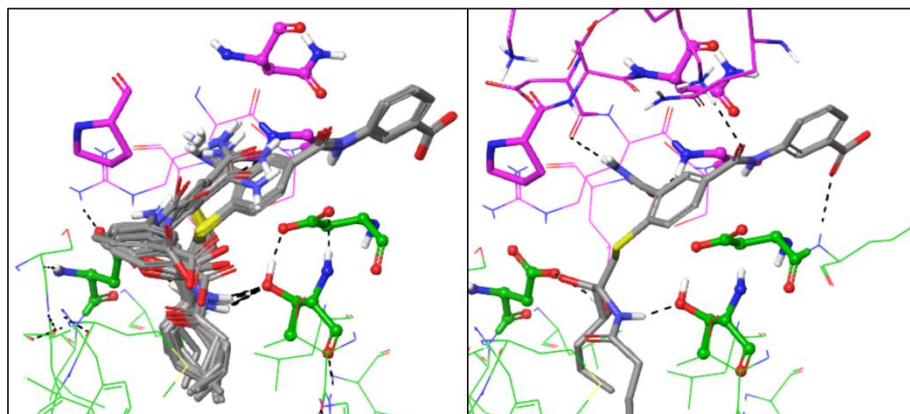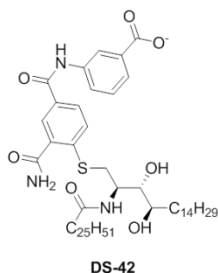
- **DS-42:**

Scores	Interactions
-6,787	$Lys65_{CD1d}$ salt
-8,173	$Gln154_{CD1d}$, $Gly96_{\alpha TCR}$, $Asp94_{\alpha TCR}$, $Lys68_{\alpha TCR}$
-7,887	$Gln154_{CD1d}$, $Gly96_{\alpha TCR}$, $Asp94_{\alpha TCR}$, $Lys68_{\alpha TCR}$
-7,118	-
-7,627	$Lys65_{CD1d}$ salt
-7,469	$Lys65_{CD1d}$ salt
-9,294	**$Gln154_{CD1d}$, $Gly96_{\alpha TCR}$, $Asp94_{\alpha TCR}$, $Lys68_{\alpha TCR}$**
-9,045	$Gln154_{CD1d}$, $Gly96_{\alpha TCR}$, $Asp94_{\alpha TCR}$, $Lys68_{\alpha TCR}$
-6,955	$Lys65_{CD1d}$ salt
-9,060	$Gln154_{CD1d}$, $Gly96_{\alpha TCR}$, $Asp94_{\alpha TCR}$, $Lys68_{\alpha TCR}$

(row label: **DS-42**)
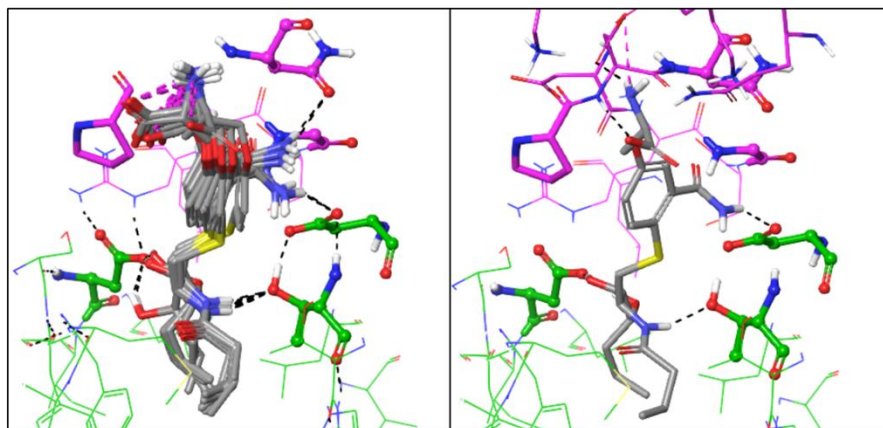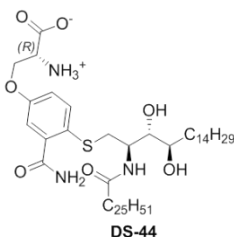
- **DS-44:**

Scores	Interactions
-7,410	$Asp29_{\alpha TCR}$, $Lys68_{\alpha TCR}$ x2, $Lys71_{\alpha TCR}$ salt
-7,629	$Asp153_{CD1d}$, $Asp29_{\alpha TCR}$ x2, $Asp29_{\alpha TCR}$ salt, $Lys71_{\alpha TCR}$ salt
-7,522	$Asp29_{\alpha TCR}$, $Asp29_{\alpha TCR}$ salt, $Asn30_{\alpha TCR}$, $Lys68_{\alpha TCR}$, $Lys71_{\alpha TCR}$ salt
-7,469	$Gly96_{\alpha TCR}$, $Asp29_{\alpha TCR}$ x2, $Asp29_{\alpha TCR}$ salt, $Lys71_{\alpha TCR}$ salt
-7,498	$Gly96_{\alpha TCR}$, $Asp94_{\alpha TCR}$, $Asp29_{\alpha TCR}$ x2, $Asp29_{\alpha TCR}$ salt, $Lys71_{\alpha TCR}$ salt
-7,029	$Asp29_{\alpha TCR}$, $Asp29_{\alpha TCR}$ salt, $Lys68_{\alpha TCR}$, $Lys71_{\alpha TCR}$ salt
-7,265	$Asp153_{CD1d}$, $Asp29_{\alpha TCR}$, $Asp29_{\alpha TCR}$ salt, $Lys68_{\alpha TCR}$, $Lys71_{\alpha TCR}$ salt
-8,122	**$Asp153_{CD1d}$, $Asp29_{\alpha TCR}$, $Asp29_{\alpha TCR}$ salt**
-7,193	$Asp29_{\alpha TCR}$, $Asp29_{\alpha TCR}$ salt, $Lys71_{\alpha TCR}$ salt
-7,204	$Asn30_{\alpha TCR}$, $Asp29_{\alpha TCR}$, $Asp29_{\alpha TCR}$ salt, $Lys68_{\alpha TCR}$, $Lys71_{\alpha TCR}$ salt

(row label: **DS-44**)
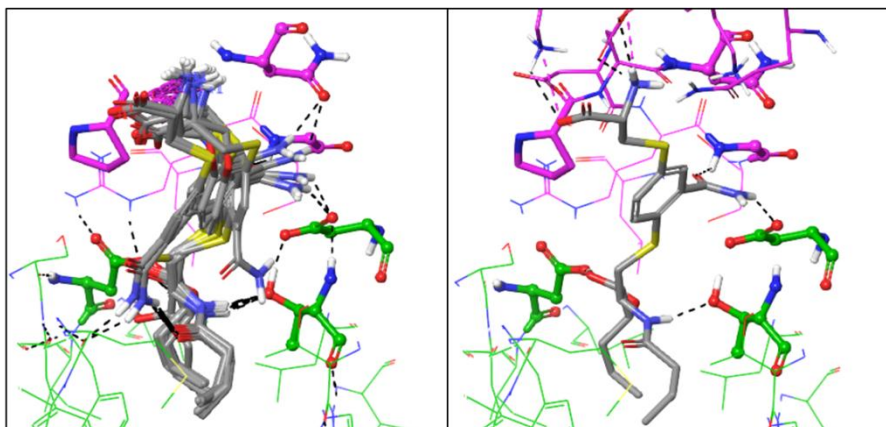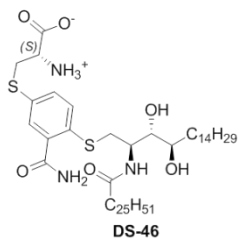
- **DS-46:**

	Scores	Interactions
DS-46	-7,482	$Gly96_{\alpha TCR}$, $Asp29_{\alpha TCR}$, $Asp29_{\alpha TCR}$ salt, $Asn30_{\alpha TCR}$, $Lys68_{\alpha TCR}$, $Lys71_{\alpha TCR}$ salt
	-7,417	$Asp29_{\alpha TCR}$ x2, $Asp29_{\alpha TCR}$ salt, $Lys71_{\alpha TCR}$ salt
	-7,552	$Asp29_{\alpha TCR}$, $Asp29_{\alpha TCR}$ salt, $Asn30_{\alpha TCR}$, $Lys68_{\alpha TCR}$, $Lys71_{\alpha TCR}$ salt
	-7,469	$Gly96_{\alpha TCR}$, $Asp29_{\alpha TCR}$ x2, $Asp29_{\alpha TCR}$ salt, $Lys71_{\alpha TCR}$ salt
	-7,905	$Gly96_{\alpha TCR}$, $Asp29_{\alpha TCR}$, $Asp29_{\alpha TCR}$ salt, $Lys71_{\alpha TCR}$ salt
	-7,676	$Gly96_{\alpha TCR}$, $Asp29_{\alpha TCR}$, $Asp29_{\alpha TCR}$ salt, $Lys71_{\alpha TCR}$ salt
	-8,003	$Gly96_{\alpha TCR}$, $Asp94_{\alpha TCR}$, $Asp29_{\alpha TCR}$ x3, $Asp29_{\alpha TCR}$ salt, $Lys71_{\alpha TCR}$ salt
	-8,430	$Met69_{CD1d}$, $Asp29_{\alpha TCR}$ x2, $Asp29_{\alpha TCR}$ salt, $Lys71_{\alpha TCR}$
	-7,895	**$Asp153_{CD1d}$, $Gly96_{\alpha TCR}$, $Asp29_{\alpha TCR}$, $Asp29_{\alpha TCR}$ salt, $Lys68_{\alpha TCR}$, $Lys71_{\alpha TCR}$ salt**
	-8,024	$Met69_{CD1d}$, $Asp29_{\alpha TCR}$, $Asp29_{\alpha TCR}$ salt, $Lys68_{\alpha TCR}$, $Lys71_{\alpha TCR}$