Supplementary information, Table S3 Covalent docking of the fatty acid chains with FabZ. S(hb_ext) and S(vdw_ext) denote the protein-ligand hydrogen bond energy (external H-bond) and van der Waals energy (external vdw) respectively. S(hb_int) denotes the ligand intramolecular hydrogen bond energy, and S(int) is the sum of the internal torsion and internal vdw terms. S(cov) is an additional constraint scoring contribution for covalent docking. Only the best conformations of different fatty acid chains were used for analysis. Note that the H-bond related energy terms of S(hb_ext) and S(hb_int) are almost all zero due to the lack of hydrogen-bond formation ability of fatty acid chains.

Chain length	GOLDScore					
	Fitness	S(hb_ext)	S(vdw_ext)	S(hb_int)	S(int)	S(cov)
4	-6.67	0.00	-2.76	0.00	-1.38	-1.50
6	1.59	0.00	3.78	0.00	-2.12	-1.48
8	5.24	0.00	8.73	0.00	-5.40	-1.36
10	10.67	0.14	13.33	0.00	-4.79	-3.00
12	15.14	0.00	17.03	0.00	-7.34	-0.94
14	19.06	0.00	23.91	0.00	-11.63	-2.19
16	10.42	0.00	21.08	0.00	-18.92	-0.64