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Supporting information for article:

Crystal structure of human brain-type fatty-acid-binding protein FABP7 complexed with palmitic acid

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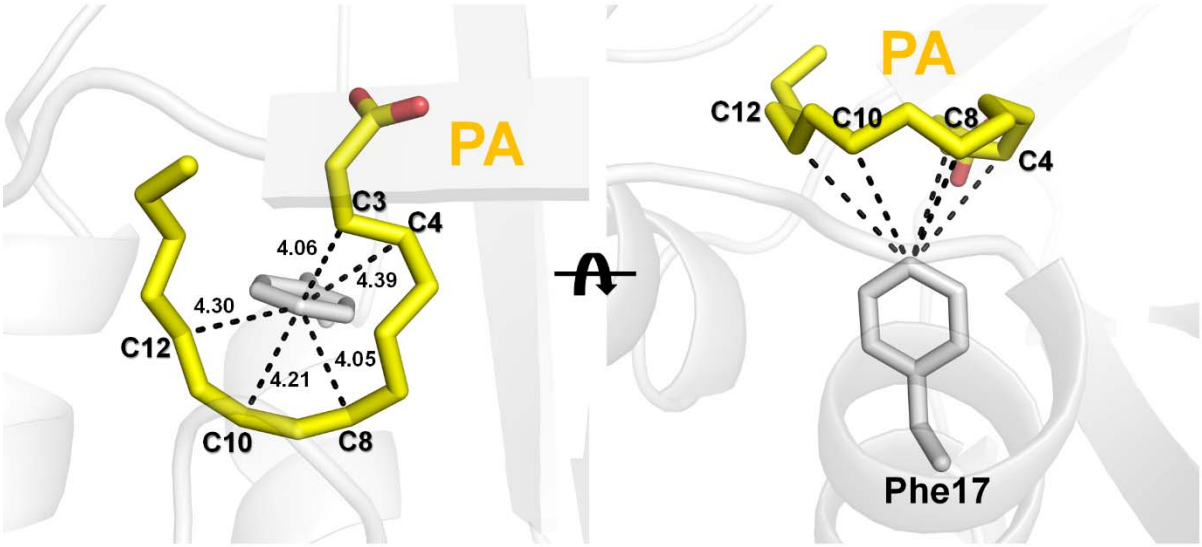

Figure S1 Interaction between palmitic acid (PA) and Phe17 in FA binding pocket of hFABP7.

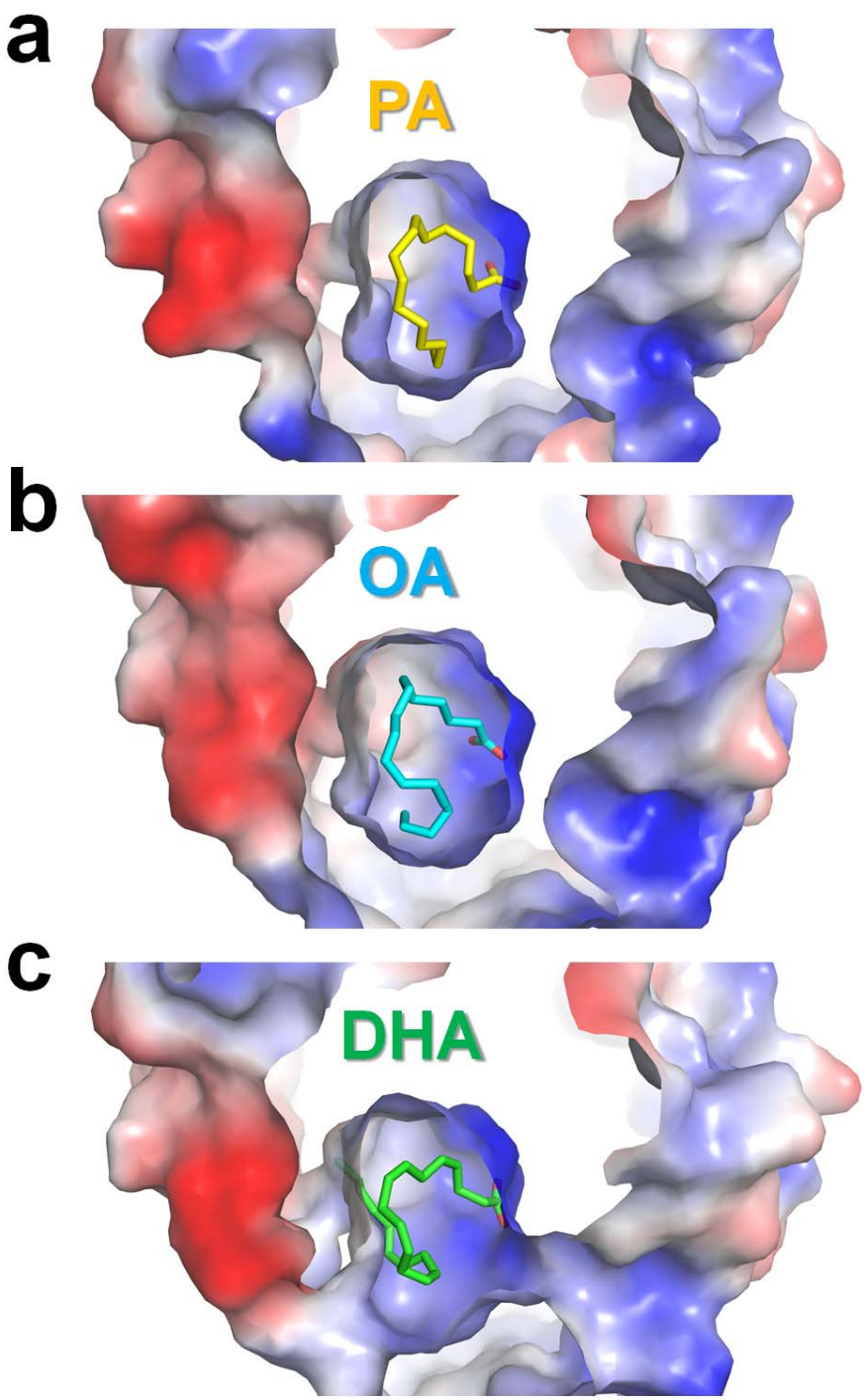

Figure S2 Electrostatic surface structure of the fatty acid binding pocket of (a) PA-, (b) OA- and (c) DHA-bound hFABP7.

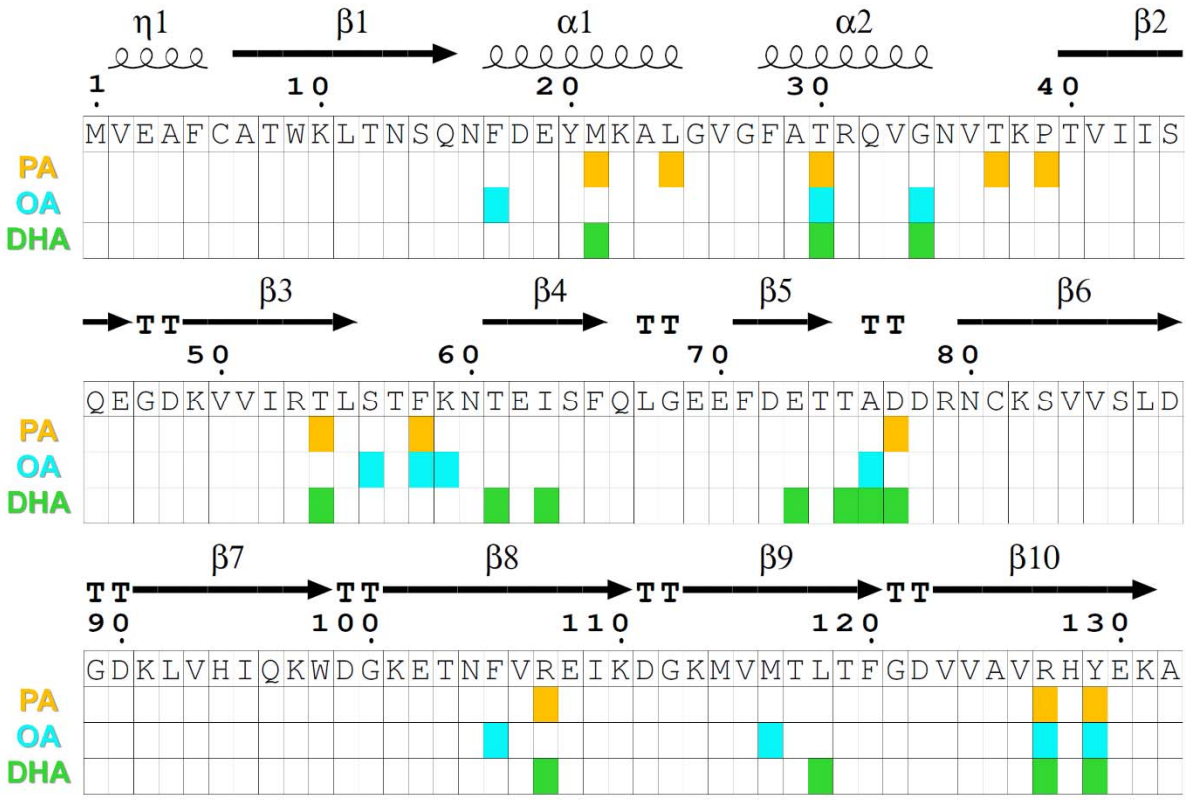

Figure S3 PA, OA, and DHA interaction residues in the hFABP7 amino acid sequence. Interatomic spacing less than 4.0 Å is marked.

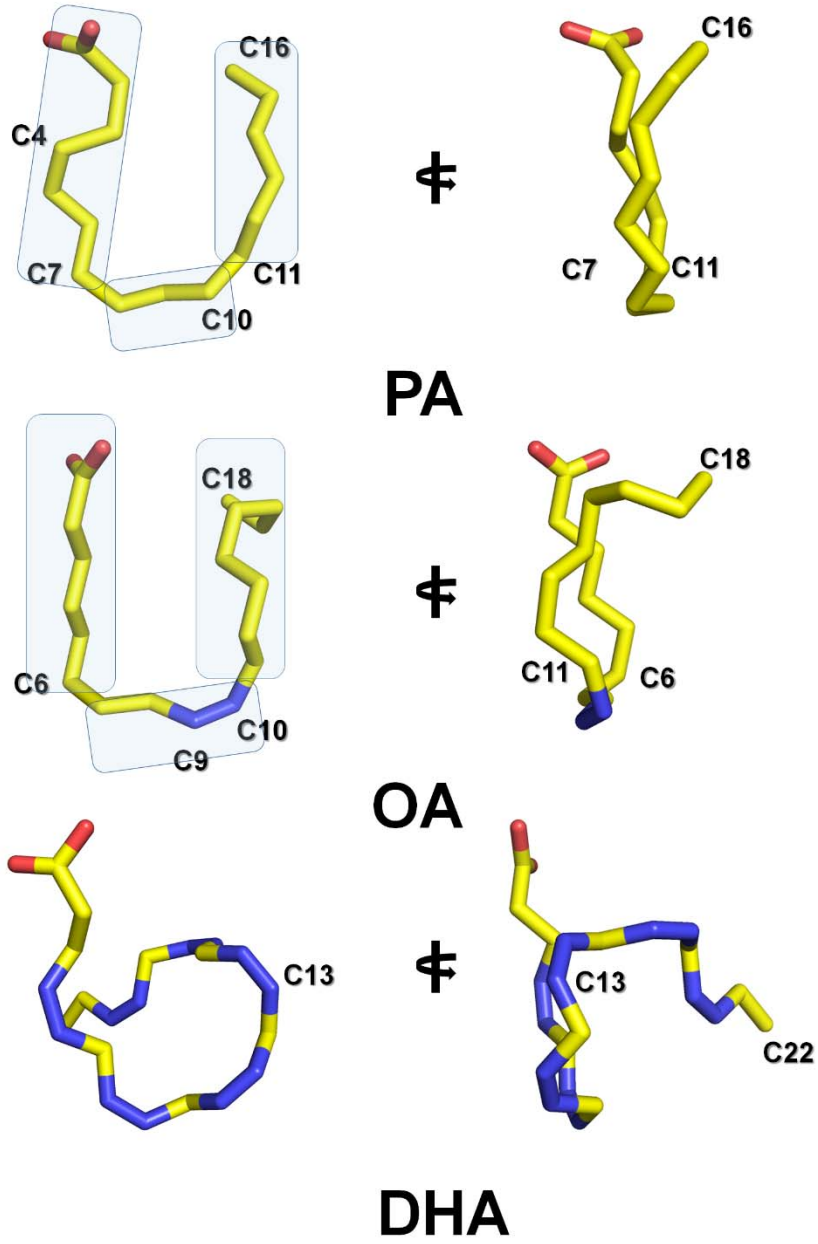

Figure S4 Conformations of PA, OA, and DHA in the PA binding pocket of hFABP7. The alkene bonds in OA or DHA are indicated by blue color.

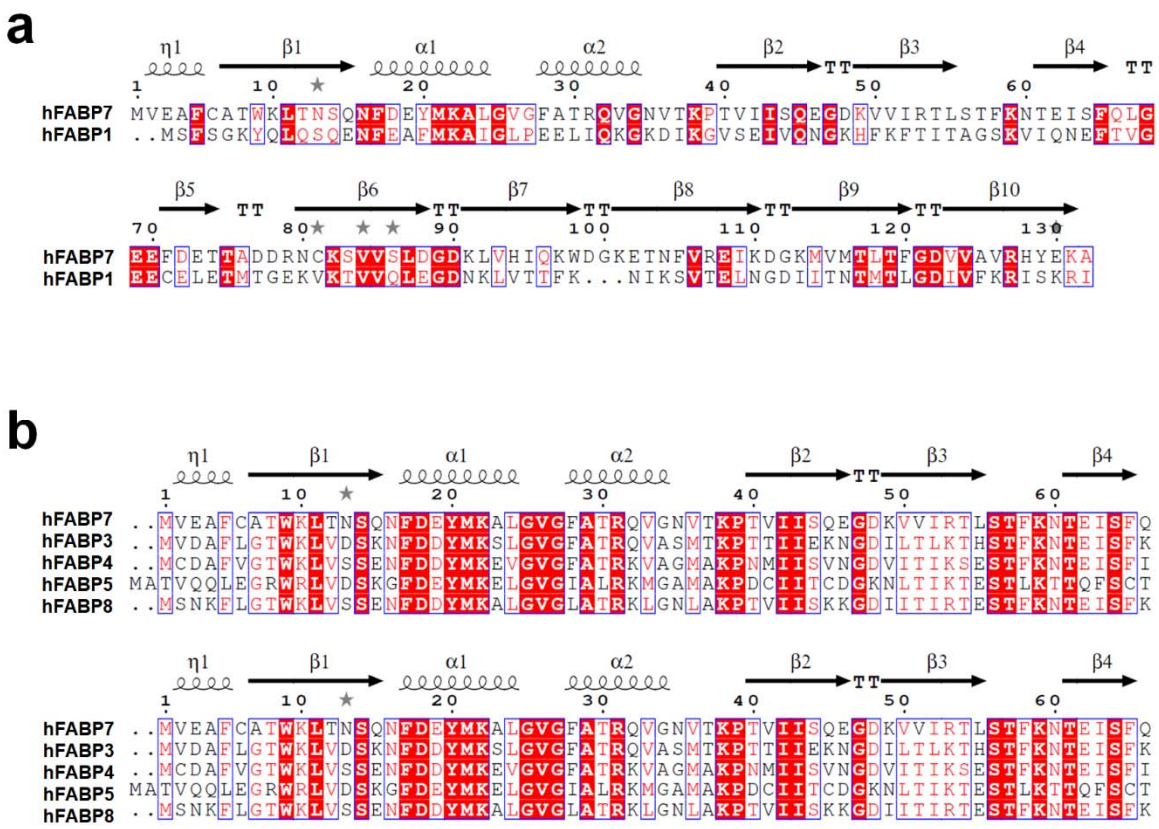

Figure S5 Sequence alignment of hFABP7 with other human FABP. (a) Sequence alignment of hFABP7 (Uniprot code: O15540) and hFABP1 (P07148). (b) Sequence alignment of hFABP7 with human FABP3 (P05413), hFABP4 (P15090), FABP5 (Q01469), and hFABP8 (P02689).

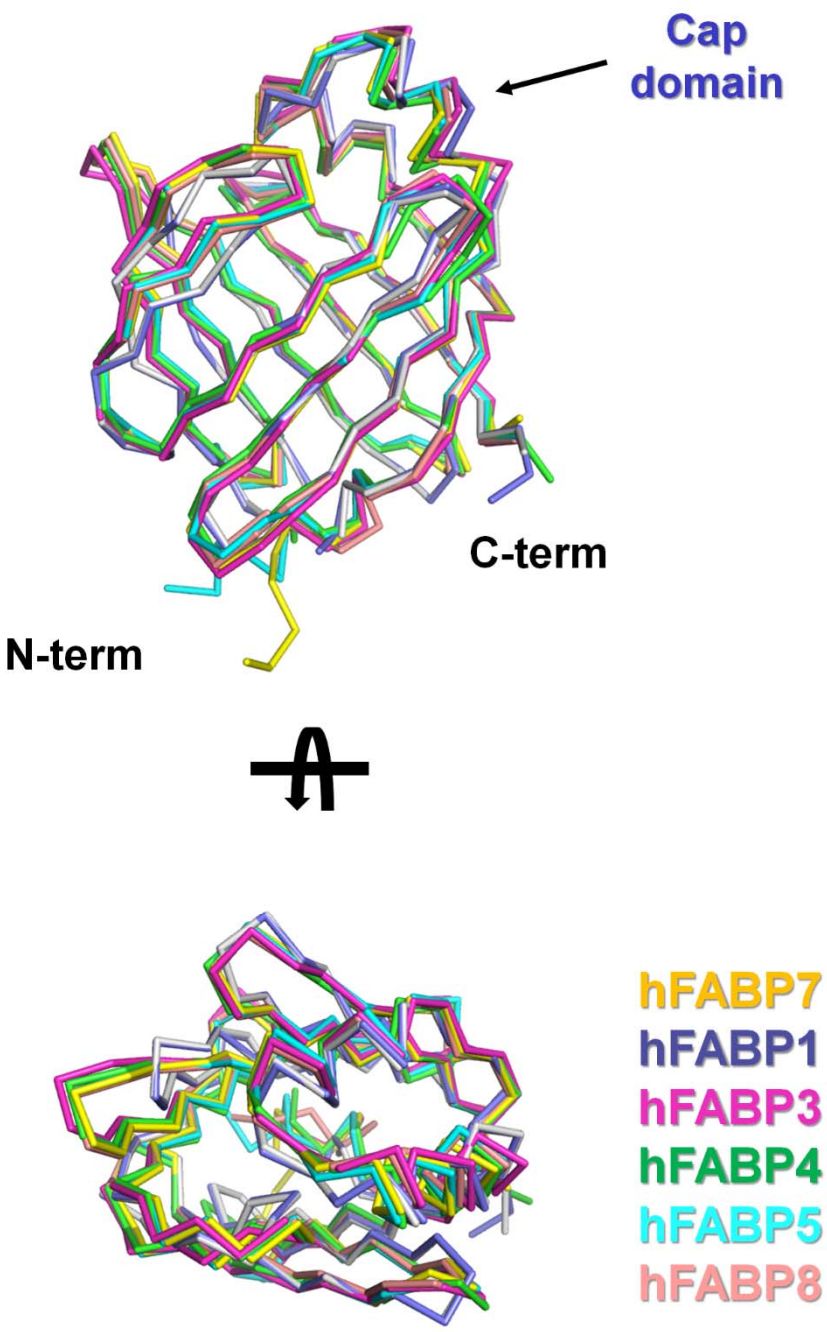

Figure S6 Superimposition of crystal structure of PA bound hFABL7, hFABP1, hFABP3, hFABP4, hFABP5 and hFABP8.

Table S1 Interatomic distances between OA and hFABP7.

Interatomic interaction less than 4.5 Å is listed (excluding water interactions).

OA atom	hFABP7 (residue atom)	Distance (Å)	OA atom	hFABP7 (residue atom)	Distance (Å)
O1	Thr54 OG1	3.85	C10	Val26 CG2	4.47
O1	Tyr129 OH	4.11	C10	Thr30 CG2	4.06
O2	Arg127 NE	4.44	C10	Asp77 CA	4.45
O2	Arg127 NH2	3.15	C10	Asp77 CB	3.60
O2	Tyr129 OH	2.92	C10	Asp77 CG	3.90
C1	Pro39 CG	4.26	C11	Thr30 CG2	3.86
C1	Val41 CG2	4.22	C12	Phe17 CE2	3.85
C1	Thr54 CG2	4.26	C12	Phe17 CZ	4.19
C1	Met116 CE	4.19	C12	Met21 SD	4.13
C1	Arg127 NH2	4.15	C12	Met21 CE	4.40
C2	Met116 CE	3.75	C13	Phe17 CE2	4.44
C4	Phe17 CZ	4.29	C13	Gly34 CA	3.62
C5	Phe105 CZ	4.49	C13	Thr37 CG2	4.34
C6	Phe105 CE1	4.48	C15	Thr37 CG2	4.22
C6	Phe105 CE2	4.42	C16	Thr37 CG2	4.21
C6	Phe105 CZ	3.76	C16	Ser56 CB	3.91
C7	Phe17 CZ	4.38	C16	Phe58 CD1	3.96
C7	Tyr20 CE1	4.43	C17	Phe58 CD1	3.86
C7	Leu24 CD2	4.26	C17	Phe58 CE1	4.34
C8	Asp77 CG	3.96	C17	Lys59 C	4.31
C9	Met29 SD	4.47	C17	Lys59 CA	4.36
C9	Met21 CG	4.33	C17	Lys59 CB	3.81
C10	Val26 CG2	4.24	C17	Ala76 CB	3.95
C9	Val26 CG1	4.44	C18	Thr54 CG2	4.35

C9	Val26 CG2	4.01	C18	Lys59 C	3.92
C9	Asp77 CB	4.04	C18	Lys59 CA	4.47
C9	Asp77 CG	3.86	C18	Lys59 CB	4.07
C10	Val26 CG1	4.11	C18	Ala76 CB	4.01

Table S2 Interatomic distances between DHA and hFABP7.

Interatomic interaction less than 4.5 Å is listed (excluding water interactions).

DHA atom	hFABP7 Chain A (residue atom)	Distance (Å)	DHA atom	hFABP7 Chain B (residue atom)	Distance (Å)
O1	Arg107 NH2	3.83	O1	Try129 OH	2.84
O1	Arg127 NH1	4.14	O2	Arg127 NH1	3.48
O1	Try129 OH	3.83	O2	Arg127 NH2	2.73
O2	Arg127 NH1	3.84	O2	Try129 OH	3.30
O2	Arg127 NH2	4.14	C1	Pro39 CG	4.18
O2	Try129 OH	2.31	C1	Val41 CG2	4.46
C1	Pro39 CG	4.34	C1	Met116 SD	4.50
C1	VAL41 CG2	3.86	C1	Arg127 CZ	3.95
C1	Thr54 CG2	4.04	C1	Tyr129 CE2	4.24
C1	Met116 SD	4.42	C1	Tyr129 CZ	4.05
C1	Tyr129 CE2	4.48	C2	Arg127 CZ	3.73
C1	Tyr129 CZ	3.91	C4	Phe105 CZ	4.38
C2	Arg127 CZ	4.13	C4	Met116 CE	4.14
C4	Leu118 CD2	4.11	C4	Met116 SD	4.42
C5	Phe17 CZ	4.50	C4	Leu118 CD2	3.73
C5	Phe105 CZ	4.19	C5	Phe17 CE1	4.31
C5	Leu118 CD2	3.96	C5	Phe17 CZ	4.34
C6	Phe17 CZ	4.42	C5	Phe105 CE1	4.25
C8	Leu24 CD2	4.34	C5	Phe105 CZ	4.01
C8	Asp77 CB	4.36	C5	Leu118 CD2	4.28
C8	Asp77 CG	3.74	C6	Phe17 CZ	4.28
C9	Ala76 C	4.25	C7	Leu24 CD2	4.09
C9	Ala76 CA	4.32	C8	Leu24 CD2	3.94
C9	Ala76 CB	3.54	C8	Val26 CG2	4.38

C9	Asp77 CA	4.33	C8	Asp77 CB	4.37
C9	Asp77 CB	3.87	C8	Asp77 CG	3.88
C9	Asp77 CG	3.75	C9	Ala76 CB	4.14
C10	Met21 SD	4.17	C9	Asp77 CA	4.39
C10	Thr30 CG2	4.37	C9	Asp77 CB	3.73
C10	Ala76 CB	4.37	C9	Asp77 CG	3.77
C10	Asp77 CB	4.45	C10	Met21 CG	4.21
C11	Met21 SD	4.23	C10	Met21 SD	3.88
C11	Thr30 CG2	3.90	C10	Val26 CG1	4.49
C11	Gly34 CA	4.40	C10	Val26 CG2	4.27
C11	Ala76 CB	4.34	C10	Thr30 CG2	4.13
C12	Thr30 CG2	4.14	C10	Asp77 CB	4.32
C12	Ala76 CB	3.48	C11	Met21 SD	3.83
C13	Gly34 CA	4.12	C11	Thr30 CG2	3.71
C13	Ala76 CB	4.38	C11	Gly34 CA	4.28
C14	Ala76 CB	4.49	C12	Thr30 CG2	3.99
C15	Ala76 CB	3.78	C12	Gly34 CA	4.49
C16	Thr61 CG2	3.64	C12	Ala76 CB	4.05
C16	Ala76 CB	3.18	C13	Gly34 CA	3.81
C17	Thr54 CB	4.46	C15	Ala76 CB	3.95
C17	Thr61 CB	3.89	C16	Thr54 CG2	4.29
C17	Thr61 CG2	2.51	C16	Ala76 CB	3.13
C17	Ala76 CA	4.14	C17	Thr54 CB	4.25
C17	Ala76 CB	3.06	C17	Thr61 CB	4.00
C18	Thr54 CB	4.30	C17	Thr61 CG2	3.88
C18	Thr61 CB	3.81	C17	Ala76 CA	4.10
C18	Thr61 CG2	2.85	C17	Ala76 CB	2.77
C18	Ala76 CA	4.44	C18	Thr54 CB	4.20

C18	Thr76 CB	3.53	C18	Thr54 CG2	4.13
C19	Thr61 CG2	3.88	C18	Thr61 CB	4.50
C19	Thr75 C	4.21	C18	Thr61 CG2	4.16
C19	Thr75 CA	4.46	C18	Ala76 CA	4.36
C19	Ala76 CA	3.55	C18	Thr76 CB	3.23
C19	Ala76 CB	2.88	C19	Thr61 CG2	4.40
C20	Thr75 C	3.78	C19	Thr75 C	4.40
C20	Thr75 CA	3.59	C19	Ala76 CA	3.51
C20	Thr75 CB	3.76	C19	Ala76 CB	2.65
C20	Thr75 CG2	4.36	C20	Thr75 C	3.90
C20	Ala76 CA	3.96	C20	Thr75 CA	3.85
C20	Ala76 CB	3.75	C20	Thr75 CB	4.00
C21	Thr61 CB	4.39	C20	Ala76 CA	3.83
C21	Ile63 CD1	4.39	C20	Ala76 CB	3.48
C21	Thr75 CA	4.08	C21	Thr75 CA	4.25
C21	Thr75 CB	4.44	C22	Glu73 CD	3.33
C22	Ile63 CD1	3.18	C22	Glu73 CG	3.82
C22	Ile63 CG1	4.10	C22	Thr75 C	4.42
C22	Glu73 CD	3.44	C22	Thr75 CA	3.59
C22	Glu73 CG	3.47	C22	Thr75 CB	4.00
C22	Thr74 C	4.34	C22	Thr75 CG2	3.80
C22	Thr75 C	4.49			
C22	Thr75 CA	3.51			
C22	Thr75 CB	3.84			
C22	Thr75 CG2	3.61			

Table S3 Analysis of bond lengths, bond angles and dihedral angles of PA, OA and DHA in FABP7.

Bond angle			
Type of bond	**PA**	**OA**	**DHA**
C1-C2-C3	115.00	112.91	110.61
C2-C3-C4	114.51	111.56	113.03
C3-C4-C5	114.67	110.90	127.75
C4-C5-C6	114.72	112.28	126.28
C5-C6-C7	115.56	112.26	114.61
C6-C7-C8	114.43	111.40	125.55
C7-C8-C9	114.38	129.77	127.33
C8-C9-C10	114.38	119.93	111.86
C9-C10-C11	113.41	122.30	127.77
C10-C11-C12	113.07	125.43	128.73
C11-C12-C13	113.03	111.73	111.36
C12-C13-C14	113.61	111.09	127.74
C13-C14-C15	112.40	111.79	127.44
C14-C15-C16	113.06	111.87	113.53
C15-C16-C17		111.81	126.25
C16-C17-C18		111.73	127.76
C17-C18-C19			112.21
C18-C19-C20			127.49
C19-C20-C21			126.41
C20-C21-C22			111.60
Dihedral angle			
Type of bond	**PA**	**OA**	**DHA**
C1-C2-C3-C4	41.24	-179.47	-112.75
C2-C3-C4-C5	109.66	178.04	-119.80
C3-C4-C5-C6	34.41	179.28	0.00
C4-C5-C6-C7	117.52	-66.34	-178.56
C5-C6-C7-C8	-136.59	-58.74	-170.95
C6-C7-C8-C9	-57.84	-179.03	1.47
C7-C8-C9-C10	140.67	-167.44	91.15
C8-C9-C10-C11	-137.43	81.84	-151.21
C9-C10-C11-C12	122.44	19.73	0.15

C10-C11-C12-C13	-161.09	-158.53	125.35
C11-C12-C13-C14	128.83	75.02	-109.20
C12-C13-C14-C15	-176.55	-178.90	0.06
C13-C14-C15-C16	119.44	70.41	-81.34
C14-C15-C16-C17		65.41	173.33
C15-C16-C17-C18		63.14	-0.71
C16-C17-C18-C19			-87.08
C17-C18-C19-C20			-143.79
C18-C19-C20-C21			1.21
C19-C20-C21-C22			169.51

Table S4 All-atom root mean square deviation (RMSD) calculation of PA in FABPs.

FABP (PDB code)	FABP1 (3STM)	FABP1 (3VG7:U)	FABP1 (3VG7:L)	FABP3 (2HMB)	FABP4 (2HNX)	FABP5 (1B56)	FABP7 (7E25)	FABP8 (2WUT)
FABP1 (3STM)		0.680	3.167	1.486	1.432	1.141	1.363	1.129
FABP1 (3VG7:A)	0.680		3.022	1.617	1.533	1.171	1.489	1.217
FABP1 (3VG7:B)	3.167	3.022		4.125	4.250	2.889	3.928	3.417
FABP3 (2HMB)	1.486	1.617	4.125		0.856	1.707	1.077	1.316
FABP4 (2HNX)	1.432	1.533	4.250	0.856		1.655	1.145	1.359
FABP5 (1B56)	1.141	1.171	2.889	1.707	1.655			1.108
FABP7 (7E25)	1.363	1.489	3.928	1.077	1.145	1.526		1.338
FABP8 (2WUT)	1.129	1.217	3.417	1.316	1.359	1.108	1.338	

*FABP1 (3VG7: U) and FABP1 (3VG7: L) indicate the U-shaped and liner PA molecule in FABP1.