

Folded structure and membrane affinity of the N-terminal domain of the three human isoforms of the mitochondrial voltage-dependent anion-selective channel

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SUPPORTING INFORMATION

Table S1. ^1H and ^{13}C resonance assignments for hVDAC1(1-25) in the presence dodecylphosphocholine micelles at a peptide/detergent molar ratio of 1:50 in phosphate buffer saline at pH 7.4.

Residue	^1H (ppm)			^{13}C (ppm)	
	H_N	H_α	Others	C_α	C_β
M1	---	4.08	2.14 β 2.54 γ 1.39 ϵ	54.65	32.65
A2	8.63	4.48	1.33 β	51.37	19.34
V3	8.32	4.25	2.03 β 0.95 γ	59.44	32.37
P4		4.38	--- β --- γ 2.95 δ	---	---
P5		4.41	2.34 β 2.06 γ' 1.97 γ'' 3.78 δ	---	---
T6	7.78	4.24	4.15 β 1.12 γ	62.01	69.64
Y7	8.13	4.40	3.09 β' 2.90 β'' 7.02 δ 6.77 ϵ	60.10	---
A8	8.85	4.40	1.36 β	52.05	19.00
D9	8.17	4.53	2.79 β' 2.78 β''	55.56	39.42
L10	7.92	4.14	1.86 β 1.79 γ' 1.70 γ'' 0.96 δ_1 0.93 δ_2	57.31	41.55
G11	7.90	3.82 3.75		45.24	
K12	7.97	4.01	1.95 β 1.54 γ' 1.47 γ'' 1.71 δ 2.98 ϵ --- ζ	59.14	31.99
S13	8.11	4.31	4.01 β' 3.89 β''	61.63	62.69
A14	8.39	4.01	1.47 β	54.58	18.00
R15	8.13	3.97	2.07 β'	59.24	---

			1.91 β'' 1.78 γ' 1.67 γ'' 3.21 δ 7.55 ε		
D16	8.20	4.51	2.96 β' 2.76 β''	56.26	39.33
V17	7.89	3.75	2.10 β 1.00 γ_1 0.75 γ_2	65.34	31.32
F18	8.00	4.39	3.26 β' 3.08 β'' 7.14 δ 7.24 ε --- ζ	59.41	39.05
T19	8.16	4.16	4.32 β 1.31 γ	63.92	67.98
K20	7.99	4.24	1.83 β 1.50 γ' 1.42 γ'' 1.63 δ 2.93 ε --- ζ	57.10	32.37
G21	8.11	3.78		---	
Y22	8.01	4.36	2.92 β' 2.77 β'' 6.97 δ 6.73 ε	58.34	38.71
G23	8.08	3.85 3.74		---	
F24	7.90	4.59	3.20 β' 2.94 β'' --- δ 7.27 ε --- ζ	57.32	39.45
G25	8.134	3.782		44.901	

Table S2. ^1H and ^{13}C resonance assignments for hVDAC2(12-36) in the presence dodecylphosphocholine micelles at a peptide/detergent molar ratio of 1:50 in phosphate buffer saline at pH 7.4.

Residue	^1H (ppm)			^{13}C (ppm)	
	H_N	H_α	Others	C_α	C_β
M1	---	---	---	---	---
C2	8.23	4.55	--- β	---	---
I3	8.21	4.17	1.75 β 1.51 γ_1' 1.16 γ_1'' --- γ_2 0.84 δ_1	---	---
P4		4.14	2.58 β 2.19 γ --- δ	---	---
P5		4.13	2.56 β 2.13 γ --- δ	---	---
S6	8.57	3.85		---	---
Y7	8.28	4.42	2.99 β' 2.71 β'' 7.17 δ --- ϵ	58.05	---
A8	8.15	4.11	1.43 β	54.74	17.99
D9	8.22	4.43	2.99 β' 2.73 β''	58.05	---
L10	8.47	4.36	1.88 β --- γ 0.95 δ	---	---
G11	8.05	3.88 3.78		---	
K12	7.96	3.99	1.96 β 1.59 γ' 1.46 γ'' 1.74 δ 3.00 ϵ --- ζ	59.53	---
A13	8.06	4.05	1.46 β	---	17.99
A14	8.41	4.00	1.50 β	---	17.99
R15	7.84	4.25	1.89 β 1.56 γ 2.96 δ --- ϵ	---	---
D16	---	4.53	2.88 β' 2.72 β''	57.65	28.11
I17	8.05	4.34	1.73 β 1.58 γ_1' 1.18 γ_1'' --- γ_2 0.85 δ_1	58.06	---
F18	8.30	4.44	3.13 β' 2.95 β''	58.06	---

			7.06 δ --- ε --- ζ		
N19	7.97	4.17	2.35 β' 2.07 β'' --- δ	61.17	---
K20	8.03	4.22	1.89 β 1.55 γ' 1.46 γ'' 1.65 δ 2.95 ε --- ζ	61.09	---
G21	8.13	3.94 3.83		---	
F22	8.31	4.16	3.28 β' 3.11 β'' 7.24 δ --- ε --- ζ	---	---
G23	8.09	3.81		---	
F24	8.01	4.59	3.21 β' 3.03 β'' --- δ 7.30 ε --- ζ	---	---
G25	---	---		---	

Table S3. ^1H and ^{13}C resonance assignments for hVDAC3(1-25) in the presence dodecylphosphocholine micelles at a peptide/detergent molar ratio of 1:50 in phosphate buffer saline at pH 7.4.

Residue	^1H (ppm)			^{13}C (ppm)	
	H_N	H_α	Others	C_α	C_β
M1	---	4.14	2.18 β 2.65 γ --- ε	54.81	32.75
C2	8.01	4.36	2.85 β	---	---
N3	8.62	---	2.80 β' 2.75 β'' 7.66 δ' 6.89 δ''	---	38.75
T4	8.09	4.49	4.13 β 1.24 γ	58.90	69.03
P5		4.58	2.29 β 1.97 γ' 1.84 γ'' 3.86 δ' 3.62 δ''	62.78	31.93
T6	8.38	4.41	4.46 β 1.25 γ	60.92	70.52
Y7	8.58	4.32	3.08 β 7.10 δ 6.80 ε	60.44	37.54
C8	8.23	4.18	2.92 β	---	---
D9	7.98	---	2.85 β	---	---
L10	8.19	4.09	1.88 β 1.80 γ' 1.61 γ'' 0.92 δ_1 0.88 δ_2	57.53	---
G11	8.49	3.82		44.82	
K12	7.92	3.98	1.94 β --- γ 1.58 δ 3.01 ε --- ζ	58.26	32.16
A13	7.87	4.23	1.52 β	54.45	17.93
A14	8.38	3.98	1.48 β	54.72	18.08
K15	8.02	3.95	1.86 β 1.54 γ' 1.45 γ'' 1.65 δ 2.95 ε --- ζ	59.67	---
D16	8.12	4.55	2.89 β' 2.70 β''	57.06	40.30
V17	7.98	3.74	2.18 β 1.06 γ_1 0.86 γ_2	65.82	31.30

F18	8.21	4.28	3.29 β' 3.09 β'' 7.19 δ 7.24 ε --- ζ	60.63	38.97
N19	8.43	4.54	2.97 β' 2.86 β'' 7.68 δ	54.94	38.59
K20	8.03	4.21	1.86 β 1.54 γ' 1.45 γ'' 1.66 δ --- ε --- ζ	57.22	32.50
G21	7.88	3.83 3.77		---	
Y22	8.07	4.33	2.86 β' 2.72 β'' 6.98 δ 6.77 ε	58.60	---
G23	8.03	3.79 3.70		45.23	
F24	7.95	4.53	3.18 β' 3.02 β'' --- δ 7.29 ε --- ζ	58.09	39.15
G25	8.04	3.71		---	