

Supplemental Table 1. Summary of d₀- and d₁₀-DMDSSO inter-linked cytochrome C peptides identified by LC MSⁿ

Peptide Sequence	AA Location	Mod. Position	Distance (α-α)	z	d ₀ -dmDSSO					d ₁₀ -dmDSSO				
					MS m/z	Δ ppm	MS2 m/z	z	Δ ppm	MS m/z	Δ ppm	MS2 m/z	z	Δ ppm
Ac-GDVEKGK KIFVQK	1-7 8-13	5T 8A	5.32	3	574.6436	1.00	874.400 415.761	1 2	2.9 1.5	577.9993	1.92	879.430 418.277	1 2	1.3 2.3
Ac-GDVEKGK KTGQAPGFSYTDANK	1-7 39-53	5T 39A	26.19	3	848.7386	1.27	874.400 826.901	1 2	2.9 2.0	852.0922	1.97	879.429 829.416	1 2	0.1 1.1
Ac-GDVEKGK KK*	1-7 87-88	5A 87	12.98	3	412.2164	0.10	421.716 375.207*	2 1*	1.5 --	415.571	0.74	424.233 380.239*	2 1*	2.3 --
Ac-GDVEKGK KKGGER	1-7 87-91	5T 87A	12.98	3	526.2721	0.85	874.398 343.204	1 2	0.6 2.3	529.6268	0.52	879.429 345.720	1 2	0.1 3.2
Ac-GDVEKGK KKGREDLIAYLK	1-7 87-99	5T 87 88A	13.03	4	631.335	1.02	874.399 544.311	1 3	1.7 1.3	633.8503	0.14	879.427 545.988	1 3	2.1 1.1
Ac-GDVEKGKK KK*	1-8 87-88	5 7A 87T	15.70	3	454.92					458.2704	3.02	488.280 380.239*	2 1*	3.0 --
Ac-GDVEKGKK KKGGER	1-8 87-91	5 7A 87 88A	15.73	4	426.9799	0.56	501.750 343.203	2 2	0.3 0.6	429.4966	2.28	504.266 361.706	2 2	0.9 2.9
Ac-GDVEKGKK KKGREDLIAYLK	1-8 87-99	5 7T 87 88A	15.73	5	530.8882	1.73	501.751 544.311	2 3	2.3 1.3	532.9012	0.54	504.265 545.988	2 3	1.1 1.1
KIFVQK GGKHK*	8-13 23-27	8A 25T	20.41	3	491.947	1.23	415.760 626.312*	2 1*	3.9 --	495.3013	1.31	418.279 631.342*	2 1*	4.3 --
KIFVQK KTGQAPGFSYTDANK	8-13 39-53	8T 39A	25.89	3	844.7656	1.09	862.487 826.901	1 2	1.7 2.0	848.12				
KIFVQK KK*	8-13 87-88	8A 87T	14.81	3	408.2464	1.52	415.760 375.207*	2 1*	3.9 --	411.601	2.34	418.277 380.24*	2 1*	2.1 --
KIFVQK KKGGER	8-13 87-91	8A 87 88T	15.72	4	391.978	0.36	415.761 359.190	2 2	1.5 2.1	394.4941	0.15	418.276 361.705	2 2	2.3 2.9

KIFVQK KGER*	8-13 88-91	8A 88T	15.72	3	479.6041	3.31	415.764 589.279*	2 1*	4.8 --	482.957	0.47	418.277 612.323*	2 1*	2.3 --
KIFVQK EDLIAYLKK	8-13 92-100	8T 99A	14.39	3	680.72					684.0757	3.07	867.513 583.346	1 2	4.5 2.4
KIFVQK GEREDLIAYLKK	8-13 89-100	8A 99T	14.39	4	596.3345	0.60	415.761 767.902	2 2	1.5 2.2	598.8497	0.10	418.277 770.417	2 2	2.3 1.3
GGKHK* HKTGPNLHGLFGR	23-27 26-38	25A 27T	6.29	5	429.8293	1.84	297.672* 511.929	2* 3	-- 4.6	431.8418	1.71	300.189* 513.607	2* 3	-- 4.4
GGKHK KTGQAPGFSYTDANK	23-27 39-53	25T 39A	19.25	3	766.0388	1.38	626.309 826.900	1 2	1.8 0.8	769.3952	0.04	631.341 829.416	1 2	2.7 1.1
GGKHK GITWGEETLMEYLENPKK	23-27 56-73	25T 72A	24.02	3	950.4685	3.67	626.308 1119.520	1 2	0.2 5.8	953.82				
KTGQAPGFSYTDANK KTGQAPGFSYTDANKNK	39-53 39-55	39A 53T	8.35	4	899.9332	2.83	826.900 963.955	2 2	0.8 0.7	902.45				
KTGQAPGFSYTDANK NKGITWGEETLMEYLENPKK	39-53 54-73	39A 55T	8.49	4	1038.2548	2.08	826.901 1240.599	2 2	2.0 2.9	1040.76				
KTGQAPGFSYTDANK GITWGEETLMEYLENPKK*	39-53 56-73	39A 72T	17.37	4	981.715	0.71	826.899 1127.52*	2 2*	5.6 --	984.23				
KTGQAPGFSYTDANK KYIPGTK	39-53 73-79	39A 73T	17.75	3	859.4291	0.11	826.900 906.477	2 1	0.8 1.8	862.78				
KTGQAPGFSYTDANK MIFAGIKK	39-53 80-87	39A 86T	24.17	3	893.12	2.42	826.901 1007.540	2 1	2.0 2.3	896.4719	0.05	829.416 1012.573	2 1	1.1 0.0
KTGQAPGFSYTDANK KGER*	39-53 88-91	39A 88T	23.26	3	753.6979	3.60	826.904 589.280*	2 1*	5.6 --	757.0514	2.58	829.419 594.311*	2 1*	4.7 --
KTGQAPGFSYTDANK EDLIAYLKK	39-53 92-100	39A 99T	15.09	3	954.8138	3.93	826.898 1192.630	2 1	1.7 1.5	958.1652	2.08	829.414 1197.663	2 1	1.3 2.8
KTGQAPGFSYTDANK GEREDLIAYLKK	39-53 89-100	39A 99T	15.09	4	801.65					804.4185	2.67	829.418 770.418	2 2	3.5 2.6

KTGQAPGFSYTDANK KATNE*	39-53 100-104	39T 100A	18.01	3	778.0289	1.72	842.887 630.311*	2 1*	3.2 --	781.3847	0.26	845.402 635.344*	2 1*	4.8 --
NKGITWGEETLMEYLENPK KYIPGTK	54-72 73-79	55A 73T	11.62	3	1081.8712	0.63	1176.548 874.505	2 1	0.0 2.0	1085.2223	0.70	1179.064 879.534	2 1	0.3 0.8
GITWGEETLMEYLENPKK MIFAGIKK	56-73 80-87	72T 86A	13.65	3	1077.54					1080.8999	0.86	1122.044 980.604	2 1	1.6 3.1
GITWGEETLMEYLENPKK M(ox)IFAGIKK	56-73 80-87	72A 86T	13.65	3	1082.8778	1.80	1119.523 991.571	2 1	3.1 6.6	1086.23				
KYIPGTK M(ox)IFAGIKK	73-79 80-87	73A 86T	13.22	3	633.69					637.0419	0.46	440.271 1012.574	2 1	0.1 1.0
MIFAGIKK KGER*	80-87 88-91	86T 88A	6.41	4	396.2183	1.42	504.275 279.157*	2 2*	3.2 --	398.7339	1.18	506.790 281.672*	2 2*	5.9 --
M(ox)IFAGIKK KGER*	80-87 88-91	86T 88A	6.41	4	400.2177					402.7331	2.34	514.787 281.673*	2 2*	4.9 --

All of the inter-linked peptides were identified by Batch-Tag, MS-Bridge, and LinkHunter. AA, amino acid; Mod., modification. MS3 m/z, m/z value of peptide sequenced in MS3.

*Peptide fragments were not sequenced in MS3, but confirmed through characteristic fragment pairs and MS-Bridge mass matching.

Inter-linked peptides were not selected for MSn analysis, but displays the expected isotopic doublet pattern in MS1; the isotopic counterpart was identified in MS3.