

# Supplementary Information for: Modeling van der Waals interactions between proteins and inorganic surfaces from time-dependent density functional theory calculations

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**Table 1**  $C_3$  coefficients calculated from TDDFT and from the proposed  $C_3$  model ( $\text{eV } \text{\AA}^3$ ).  $\Delta$  denotes the relative deviations of the coefficients obtained using the model with respect to the TDDFT coefficients.

Peptide	Si			SiO <sub>2</sub>		
	TDDFT	Model	$\Delta$ (%)	TDDFT	Model	$\Delta$ (%)
ala	1.457	1.471	1.0	0.924	0.932	0.8
arg	2.936	2.842	-3.2	1.859	1.807	-2.8
asn	2.045	2.075	1.5	1.297	1.313	1.3
asp	2.116	2.081	-1.7	1.331	1.310	-1.6
cys	1.942	1.982	2.1	1.218	1.241	1.9
gln	2.358	2.380	0.9	1.493	1.505	0.8
glu	2.467	2.385	-3.3	1.548	1.502	-3.0
gly	1.151	1.166	1.3	0.731	0.740	1.2
his	2.413	2.531	4.9	1.531	1.596	4.3
ile	2.387	2.385	-0.1	1.510	1.507	-0.2
leu	2.403	2.385	-0.8	1.519	1.507	-0.8
lys	2.558	2.577	0.7	1.622	1.635	0.8
met	2.590	2.592	0.1	1.624	1.625	0.0
phe	3.014	3.061	1.6	1.889	1.916	1.4
pro	1.952	2.021	3.5	1.237	1.274	3.0
ser	1.590	1.668	4.9	1.011	1.056	4.5
thr	1.905	1.972	3.5	1.209	1.248	3.2
trp	3.743	3.714	-0.8	2.337	2.323	-0.6
tyr	3.179	3.259	2.5	1.993	2.040	2.4
val	2.086	2.080	-0.3	1.320	1.315	-0.3
ala-leu	3.692	3.599	-2.5	2.327	2.273	-2.3
arg-met	5.372	5.177	-3.6	3.375	3.266	-3.2
asn-ser	3.429	3.486	1.7	2.170	2.203	1.5
asp-glu	4.439	4.209	-5.2	2.775	2.646	-4.6
cys-arg	4.702	4.567	-2.9	2.957	2.882	-2.5
gly-ala	2.408	2.380	-1.1	1.521	1.505	-1.1
gly-lys	3.522	3.486	-1.0	2.227	2.209	-0.8
his-pro	4.104	4.295	4.7	2.599	2.703	4.0
leu-ser	3.799	3.796	-0.1	2.400	2.397	-0.1
met-tyr	5.626	5.594	-0.6	3.514	3.499	-0.4
phe-cys	4.722	4.787	1.4	2.954	2.990	1.2
phe-his	5.258	5.336	1.5	3.302	3.346	1.3
pro-glu	4.338	4.149	-4.3	2.712	2.609	-3.8
thr-lys	4.290	4.292	0.1	2.712	2.717	0.2
thr-val	3.798	3.796	-0.1	2.398	2.397	-0.1
gln-asp	4.409	4.204	-4.7	2.760	2.649	-4.0
trp-asn	5.623	5.533	-1.6	3.519	3.470	-1.4
trp-gln	5.937	5.838	-1.7	3.717	3.662	-1.5
tyr-ile	5.319	5.387	1.3	3.343	3.381	1.1
val-ile	4.293	4.208	-2.0	2.707	2.656	-1.9
ala-gln-his	5.834	5.868	0.6	3.685	3.701	0.4
asn-cys-ala	5.040	5.015	-0.5	3.168	3.153	-0.5

**Table 1** (continued)

Peptide	Si			SiO <sub>2</sub>		
	TDDFT	Model	$\Delta$ (%)	TDDFT	Model	$\Delta$ (%)
asp-his-val	6.155	6.208	0.9	3.882	3.910	0.7
cys-thr-lys	5.925	5.989	1.1	3.737	3.771	0.9
gln-trp-ile	8.078	7.966	-1.4	5.066	5.003	-1.2
gly-pro-ser	4.258	4.341	2.0	2.691	2.737	1.7
leu-arg-gly	6.098	5.849	-4.1	3.844	3.701	-3.7
lys-met-asp	6.791	6.736	-0.8	4.270	4.237	-0.8
thr-phe-met	7.077	7.112	0.5	4.435	4.456	0.5
tyr-val-pro	6.841	6.846	0.1	4.293	4.297	0.1
asn-phe-gly-ala	7.056	7.004	-0.8	4.430	4.402	-0.6
cys-lys-phe-gly	7.949	7.987	0.5	4.993	5.012	0.4
glu-his-arg-leu	9.577	9.373	-2.1	6.034	5.914	-2.0
ile-gly-val-gln	7.415	7.241	-2.4	4.670	4.569	-2.2
leu-trp-asn-cys	9.532	9.387	-1.5	5.966	5.886	-1.4
met-asp-cys-lys	8.533	8.461	-0.8	5.354	5.312	-0.8
phe-ala-thr-val	7.919	7.815	-1.3	4.969	4.912	-1.1
ser-ile-lys-phe	8.856	8.891	0.4	5.577	5.595	0.3
thr-asn-pro-ile	8.856	8.891	0.4	5.577	5.595	0.3
val-met-leu-tyr	9.614	9.545	-0.7	6.028	5.989	-0.7

**Table 2**  $C_6$  coefficients calculated from TDDFT, from the pair-specific model, and from the species-specific model (eV Å<sup>6</sup>).  $\Delta$  denotes the relative deviations of the coefficients obtained using the models with respect to the TDDFT coefficients.

Peptide A	Peptide B	TDDFT	Pair-specific	$\Delta$ (%)	Species-specific	$\Delta$ (%)
ala	ala	1423.446	1447.124	1.7	1439.608	1.1
ala	arg	2865.177	2807.272	-2.0	2802.483	-2.2
ala	asn	1998.307	2041.531	2.2	2026.734	1.4
ala	asp	2054.682	2038.190	-0.8	2019.270	-1.7
ala	cys	1881.120	1933.619	2.8	1922.116	2.2
ala	gln	2301.514	2340.143	1.7	2330.543	1.3
ala	glu	2390.660	2336.802	-2.2	2323.079	-2.8
ala	gly	1126.375	1148.512	2.0	1135.798	0.8
ala	his	2358.565	2486.001	5.4	2489.050	5.5
ala	ile	2327.533	2342.959	0.7	2351.035	1.0
ala	leu	2341.127	2342.959	0.1	2351.035	0.4
ala	lys	2498.696	2539.355	1.6	2542.255	1.7
ala	met	2508.087	2530.843	0.9	2529.734	0.9
ala	phe	2917.096	2989.045	2.5	3018.036	3.5
ala	pro	1905.340	1981.910	4.0	1986.119	4.2
ala	ser	1557.217	1640.179	5.3	1623.364	4.2
ala	thr	1862.460	1938.791	4.1	1927.173	3.5
ala	trp	3613.017	3626.571	0.4	3664.108	1.4
ala	tyr	3078.426	3182.101	3.4	3201.792	4.0
ala	val	2033.761	2044.347	0.5	2047.226	0.7
ala	ala-leu	3589.260	3534.590	-1.5	3545.779	-1.2
ala	arg-met	5209.491	5082.621	-2.4	5087.354	-2.3
ala	asn-ser	3345.349	3426.217	2.4	3405.235	1.8
ala	asp-glu	4289.003	4119.500	-4.0	4097.485	-4.5
ala	cys-arg	4563.746	4485.398	-1.7	4479.736	-1.8
ala	gly-ala	2345.771	2340.143	-0.2	2330.543	-0.7
ala	gly-lys	3432.975	3432.374	-0.0	3433.191	0.0
ala	his-pro	4005.816	4212.418	5.2	4230.306	5.6
ala	leu-ser	3700.288	3727.646	0.7	3729.536	0.8

**Table 2** (continued)

Peptide A	Peptide B	TDDFT	Pair-specific	$\Delta$ (%)	Species-specific	$\Delta$ (%)
ala	met-tyr	5431.564	5457.450	0.5	5486.663	1.0
ala	phe-cys	4564.192	4667.171	2.3	4695.288	2.9
ala	phe-his	5098.450	5219.553	2.4	5262.222	3.2
ala	pro-glu	4191.862	4063.219	-3.1	4064.335	-3.0
ala	thr-lys	4181.576	4222.653	1.0	4224.565	1.0
ala	thr-val	3698.485	3727.646	0.8	3729.536	0.8
ala	gln-asp	4265.527	4122.840	-3.4	4104.950	-3.8
ala	trp-asn	5437.829	5412.609	-0.5	5445.979	0.1
ala	trp-gln	5743.302	5711.221	-0.6	5749.788	0.1
ala	tyr-ile	5160.063	5269.567	2.1	5307.964	2.9
ala	val-ile	4175.409	4131.814	-1.0	4153.398	-0.5
ala	ala-gln-his	5682.236	5762.281	1.4	5769.474	1.5
ala	asn-cys-ala	4889.815	4911.287	0.4	4898.731	0.2
ala	asp-his-val	5988.297	6088.772	1.7	6096.372	1.8
ala	cys-thr-lys	5763.756	5869.560	1.8	5871.265	1.9
ala	gln-trp-ile	7823.410	7798.687	-0.3	7855.960	0.4
ala	gly-pro-ser	4148.719	4259.615	2.7	4255.555	2.6
ala	leu-arg-gly	5929.783	5756.538	-2.9	5769.037	-2.7
ala	lys-met-asp	6590.133	6597.402	0.1	6601.533	0.2
ala	thr-phe-met	6850.226	6947.693	1.4	6985.217	2.0
ala	tyr-val-pro	6628.363	6697.372	1.0	6745.411	1.8
ala	asn-phe-gly-ala	6840.753	6859.732	0.3	6885.586	0.7
ala	cys-lys-phe-gly	7708.229	7812.833	1.4	7853.063	1.9
ala	glu-his-arg-leu	9309.140	9206.555	-1.1	9231.058	-0.8
ala	ile-gly-val-gln	7204.822	7109.482	-1.3	7130.013	-1.0
ala	leu-trp-asn-cys	9217.836	9178.201	-0.4	9229.403	0.1
ala	met-asp-cys-lys	8266.845	8275.528	0.1	8278.785	0.1
ala	phe-ala-thr-val	7672.793	7652.828	-0.3	7697.453	0.3
ala	ser-ile-lys-phe	8605.120	8713.841	1.3	8769.548	1.9
ala	thr-asn-pro-ile	8605.120	8713.841	1.3	8769.548	1.9
ala	val-met-leu-tyr	9308.915	9333.771	0.3	9395.197	0.9
arg	arg	5767.523	5457.532	-5.4	5389.765	-6.5
arg	asn	4022.410	3952.313	-1.7	3945.513	-1.9
arg	asp	4136.987	3933.404	-4.9	3964.970	-4.2
arg	cys	3787.646	3756.252	-0.8	3737.224	-1.3
arg	gln	4632.892	4533.555	-2.1	4527.207	-2.3
arg	glu	4813.853	4514.646	-6.2	4546.665	-5.5
arg	gly	2267.162	2226.030	-1.8	2220.789	-2.0
arg	his	4747.449	4808.990	1.3	4795.632	1.0
arg	ile	4685.298	4550.997	-2.9	4547.567	-2.9
arg	leu	4712.773	4550.997	-3.4	4547.567	-3.5
arg	lys	5029.496	4939.767	-1.8	4906.649	-2.4
arg	met	5050.032	4918.736	-2.6	4900.613	-3.0
arg	phe	5874.007	5775.177	-1.7	5822.549	-0.9
arg	pro	3835.274	3839.869	0.1	3848.347	0.3
arg	ser	3134.220	3177.131	1.4	3181.023	1.5
arg	thr	3748.803	3758.373	0.3	3762.718	0.4
arg	trp	7276.262	7001.715	-3.8	7051.208	-3.1
arg	tyr	6198.822	6145.037	-0.9	6201.089	0.0
arg	val	4093.921	3969.755	-3.0	3965.872	-3.1
arg	ala-leu	7226.035	6858.523	-5.1	6853.985	-5.2
arg	arg-met	10488.964	9876.522	-5.8	9794.313	-6.6
arg	asn-ser	6734.266	6629.698	-1.6	6630.471	-1.5

**Table 2** (continued)

Peptide A	Peptide B	TDDFT	Pair-specific	$\Delta$ (%)	Species-specific	$\Delta$ (%)
arg	asp-glu	8637.493	7948.303	-8.0	8015.570	-7.2
arg	cys-arg	9188.497	8714.038	-5.2	8630.924	-6.1
arg	gly-ala	4722.262	4533.555	-4.0	4527.207	-4.1
arg	gly-lys	6910.756	6666.050	-3.5	6631.373	-4.0
arg	his-pro	8063.592	8149.113	1.1	8147.913	1.1
arg	leu-ser	7449.058	7228.382	-3.0	7232.525	-2.9
arg	met-tyr	10938.220	10564.027	-3.4	10605.637	-3.0
arg	phe-cys	9190.967	9031.683	-1.7	9063.708	-1.4
arg	phe-his	10265.726	10084.422	-1.8	10122.116	-1.4
arg	pro-glu	8441.986	7854.768	-7.0	7898.946	-6.4
arg	thr-lys	8417.735	8198.394	-2.6	8173.302	-2.9
arg	thr-val	7445.525	7228.382	-2.9	7232.525	-2.9
arg	gln-asp	8590.037	7967.212	-7.2	7996.112	-6.9
arg	trp-asn	10950.384	10454.281	-4.5	10500.656	-4.1
arg	trp-gln	11565.339	11035.523	-4.6	11082.350	-4.2
arg	tyr-ile	10389.453	10196.288	-1.9	10252.591	-1.3
arg	val-ile	8405.868	8021.006	-4.6	8017.374	-4.6
arg	ala-gln-his	11439.106	11150.324	-2.5	11133.192	-2.7
arg	asn-cys-ala	9845.274	9516.344	-3.3	9493.090	-3.6
arg	asp-his-val	12055.776	11777.600	-2.3	11793.106	-2.2
arg	cys-thr-lys	11603.511	11389.956	-1.8	11355.699	-2.1
arg	gln-trp-ile	15753.158	15086.774	-4.2	15133.851	-3.9
arg	gly-pro-ser	8351.816	8243.538	-1.3	8258.029	-1.1
arg	leu-arg-gly	11938.053	11170.124	-6.4	11107.227	-7.0
arg	lys-met-asp	13268.440	12792.414	-3.6	12780.102	-3.7
arg	thr-phe-met	13793.638	13452.794	-2.5	13493.750	-2.2
arg	tyr-val-pro	13346.580	12955.169	-2.9	13023.178	-2.4
arg	asn-phe-gly-ala	13774.030	13261.553	-3.7	13303.139	-3.4
arg	cys-lys-phe-gly	15520.209	15133.044	-2.5	15140.254	-2.5
arg	glu-his-arg-leu	18741.892	17832.927	-4.8	17791.432	-5.1
arg	ile-gly-val-gln	14505.434	13781.098	-5.0	13773.240	-5.0
arg	leu-trp-asn-cys	18562.011	17762.038	-4.3	17793.316	-4.1
arg	met-asp-cys-lys	16645.366	16048.920	-3.6	16021.262	-3.8
arg	phe-ala-thr-val	15449.495	14811.339	-4.1	14865.427	-3.8
arg	ser-ile-lys-phe	17324.661	16878.891	-2.6	16910.830	-2.4
arg	thr-asn-pro-ile	17324.661	16878.891	-2.6	16910.830	-2.4
arg	val-met-leu-tyr	18744.155	18085.287	-3.5	18126.946	-3.3
asn	asn	2805.456	2878.828	2.6	2848.679	1.5
asn	asp	2885.016	2878.116	-0.2	2837.795	-1.6
asn	cys	2641.068	2730.083	3.4	2701.241	2.3
asn	gln	3231.125	3299.987	2.1	3280.623	1.5
asn	glu	3356.868	3299.275	-1.7	3269.739	-2.6
asn	gly	1581.298	1620.371	2.5	1594.790	0.8
asn	his	3311.168	3501.571	5.8	3507.246	5.9
asn	ile	3267.468	3305.008	1.1	3322.565	1.7
asn	leu	3286.583	3305.008	0.6	3322.565	1.1
asn	lys	3507.713	3579.520	2.0	3587.868	2.3
asn	met	3521.243	3572.401	1.4	3565.129	1.2
asn	phe	4095.862	4216.025	2.9	4272.470	4.3
asn	pro	2674.786	2795.734	4.5	2804.140	4.8
asn	ser	2186.120	2315.330	5.9	2281.154	4.3
asn	thr	2614.646	2736.489	4.7	2713.097	3.8
asn	trp	5073.413	5112.567	0.8	5185.457	2.2

**Table 2** (continued)

Peptide A	Peptide B	TDDFT	Pair-specific	$\Delta$ (%)	Species-specific	$\Delta$ (%)
asn	tyr	4322.472	4489.824	3.9	4526.890	4.7
asn	val	2855.082	2883.849	1.0	2890.621	1.2
asn	ala-leu	5039.060	4984.624	-1.1	5008.397	-0.6
asn	arg-met	7314.052	7162.799	-2.1	7169.740	-2.0
asn	asn-ser	4696.721	4832.243	2.9	4788.932	2.0
asn	asp-glu	6022.877	5815.476	-3.4	5766.633	-4.2
asn	cys-arg	6407.392	6320.481	-1.4	6305.853	-1.6
asn	gly-ala	3293.317	3299.987	0.2	3280.623	-0.4
asn	gly-lys	4819.540	4837.977	0.4	4841.757	0.5
asn	his-pro	5623.767	5935.390	5.5	5970.485	6.2
asn	leu-ser	5194.858	5258.424	1.2	5262.817	1.3
asn	met-tyr	7626.601	7700.310	1.0	7751.117	1.6
asn	phe-cys	6408.473	6584.192	2.7	6632.810	3.5
asn	phe-his	7158.550	7355.681	2.8	7438.815	3.9
asn	pro-glu	5886.520	5733.094	-2.6	5732.977	-2.6
asn	thr-lys	5870.514	5954.095	1.4	5960.064	1.5
asn	thr-val	5192.389	5258.424	1.3	5262.817	1.4
asn	gln-asp	5989.986	5816.188	-2.9	5777.517	-3.5
asn	trp-asn	7635.575	7629.480	-0.1	7693.235	0.8
asn	trp-gln	8064.367	8050.639	-0.2	8125.178	0.8
asn	tyr-ile	7244.798	7432.918	2.6	7508.553	3.6
asn	val-ile	5861.811	5826.943	-0.6	5872.284	0.2
asn	ala-gln-his	7977.585	8119.259	1.8	8132.800	1.9
asn	asn-cys-ala	6865.404	6926.612	0.9	6894.851	0.4
asn	asp-his-val	8407.448	8583.764	2.1	8597.101	2.3
asn	cys-thr-lys	8091.819	8278.205	2.3	8277.164	2.3
asn	gln-trp-ile	10984.697	10993.733	0.1	11106.842	1.1
asn	gly-pro-ser	5824.598	6007.606	3.1	5998.281	3.0
asn	leu-arg-gly	8325.138	8109.806	-2.6	8137.824	-2.2
asn	lys-met-asp	9252.390	9306.207	0.6	9308.989	0.6
asn	thr-phe-met	9618.070	9801.085	1.9	9868.893	2.6
asn	tyr-val-pro	9306.655	9445.577	1.5	9539.848	2.5
asn	asn-phe-gly-ala	9604.966	9671.011	0.7	9719.969	1.2
asn	cys-lys-phe-gly	10822.405	11016.197	1.8	11090.425	2.5
asn	glu-his-arg-leu	13069.832	12972.423	-0.8	13022.359	-0.4
asn	ile-gly-val-gln	10115.311	10023.472	-0.9	10065.894	-0.5
asn	leu-trp-asn-cys	12942.835	12940.741	-0.0	13035.238	0.7
asn	met-asp-cys-lys	11606.711	11674.375	0.6	11669.329	0.5
asn	phe-ala-thr-val	10773.041	10792.149	0.2	10880.218	1.0
asn	ser-ile-lys-phe	12081.263	12286.081	1.7	12398.112	2.6
asn	thr-asn-pro-ile	12081.263	12286.081	1.7	12398.112	2.6
asn	val-met-leu-tyr	13070.006	13165.338	0.7	13282.500	1.6
asp	asp	2970.284	2887.512	-2.8	2808.628	-5.4
asp	cys	2719.465	2724.133	0.2	2695.755	-0.9
asp	gln	3323.221	3297.264	-0.8	3272.580	-1.5
asp	glu	3457.266	3306.661	-4.4	3243.413	-6.2
asp	gly	1625.752	1619.042	-0.4	1584.485	-2.5
asp	his	3404.629	3500.042	2.8	3516.694	3.3
asp	ile	3360.645	3295.636	-1.9	3323.625	-1.1
asp	leu	3380.654	3295.636	-2.5	3323.625	-1.7
asp	lys	3606.629	3563.418	-1.2	3596.030	-0.3
asp	met	3625.699	3562.430	-1.8	3565.325	-1.7
asp	phe	4218.694	4221.923	0.1	4276.238	1.4

**Table 2** (continued)

Peptide A	Peptide B	TDDFT	Pair-specific	$\Delta$ (%)	Species-specific	$\Delta$ (%)
asp	pro	2750.598	2793.698	1.6	2800.904	1.8
asp	ser	2247.131	2315.369	3.0	2262.508	0.7
asp	thr	2688.282	2734.518	1.7	2697.293	0.3
asp	trp	5228.379	5121.028	-2.0	5198.375	-0.6
asp	tyr	4451.962	4499.102	1.1	4519.477	1.5
asp	val	2936.459	2876.487	-2.0	2888.840	-1.6
asp	ala-leu	5185.582	4973.858	-4.1	5011.721	-3.4
asp	arg-met	7529.915	7135.865	-5.2	7199.122	-4.4
asp	asn-ser	4831.114	4833.517	0.1	4769.130	-1.3
asp	asp-glu	6206.514	5834.204	-6.0	5720.868	-7.8
asp	cys-arg	6595.567	6297.568	-4.5	6329.552	-4.0
asp	gly-ala	3388.083	3297.264	-2.7	3272.580	-3.4
asp	gly-lys	4957.677	4822.492	-2.7	4849.341	-2.2
asp	his-pro	5783.920	5933.772	2.6	5986.424	3.5
asp	leu-ser	5344.354	5251.037	-1.8	5254.959	-1.7
asp	met-tyr	7858.322	7701.563	-2.0	7753.628	-1.3
asp	phe-cys	6601.581	6586.087	-0.2	6640.820	0.6
asp	phe-his	7370.837	7361.997	-0.1	7461.758	1.2
asp	pro-glu	6066.178	5740.390	-5.4	5713.144	-5.8
asp	thr-lys	6038.787	5937.968	-1.7	5962.150	-1.3
asp	thr-val	5342.106	5251.037	-1.7	5254.959	-1.6
asp	gln-asp	6171.924	5824.808	-5.6	5750.035	-6.8
asp	trp-asn	7866.130	7639.176	-2.9	7704.997	-2.0
asp	trp-gln	8307.285	8058.324	-3.0	8139.782	-2.0
asp	tyr-ile	7458.606	7434.769	-0.3	7511.928	0.7
asp	val-ile	6031.534	5812.155	-3.6	5881.291	-2.5
asp	ala-gln-his	8207.766	8115.560	-1.1	8146.196	-0.8
asp	asn-cys-ala	7067.940	6920.502	-2.1	6890.473	-2.5
asp	asp-his-val	8651.681	8585.500	-0.8	8595.782	-0.7
asp	cys-thr-lys	8326.186	8260.737	-0.8	8282.763	-0.5
asp	gln-trp-ile	11312.696	10993.992	-2.8	11132.233	-1.6
asp	gly-pro-ser	5992.290	6008.172	0.3	5985.549	-0.1
asp	leu-arg-gly	8567.186	8086.750	-5.6	8166.764	-4.7
asp	lys-met-asp	9524.396	9293.423	-2.4	9307.636	-2.3
asp	thr-phe-met	9905.550	9798.934	-1.1	9876.509	-0.3
asp	tyr-val-pro	9583.803	9449.350	-1.4	9546.873	-0.4
asp	asn-phe-gly-ala	9890.427	9677.366	-2.1	9724.266	-1.7
asp	cys-lys-phe-gly	11142.422	11007.216	-1.2	11115.019	-0.2
asp	glu-his-arg-leu	13451.094	12955.837	-3.7	13055.181	-2.9
asp	ile-gly-val-gln	10410.751	10008.524	-3.9	10076.008	-3.2
asp	leu-trp-asn-cys	13332.623	12939.008	-3.0	13062.029	-2.0
asp	met-asp-cys-lys	11951.267	11657.588	-2.5	11672.218	-2.3
asp	phe-ala-thr-val	11093.579	10791.214	-2.7	10888.119	-1.9
asp	ser-ile-lys-phe	12434.100	12275.046	-1.3	12420.912	-0.1
asp	thr-asn-pro-ile	12434.100	12275.046	-1.3	12420.912	-0.1
asp	val-met-leu-tyr	13459.661	13153.750	-2.3	13303.745	-1.2
cys	cys	2490.899	2574.349	3.4	2469.489	-0.9
cys	gln	3042.497	3129.104	2.9	3113.593	2.3
cys	glu	3165.581	3123.154	-1.3	3108.107	-1.8
cys	gly	1488.213	1534.597	3.1	1509.764	1.4
cys	his	3116.717	3329.267	6.8	3334.799	7.0
cys	ile	3077.442	3130.684	1.7	3159.171	2.7
cys	leu	3095.838	3130.684	1.1	3159.171	2.0

**Table 2** (continued)

Peptide A	Peptide B	TDDFT	Pair-specific	$\Delta$ (%)	Species-specific	$\Delta$ (%)
cys	lys	3302.244	3393.822	2.8	3404.291	3.1
cys	met	3321.210	3372.392	1.5	3294.193	-0.8
cys	phe	3863.710	4000.055	3.5	4081.615	5.6
cys	pro	2518.537	2649.739	5.2	2668.166	5.9
cys	ser	2056.893	2190.808	6.5	2161.749	5.1
cys	thr	2461.023	2589.829	5.2	2574.101	4.6
cys	trp	4788.418	4856.428	1.4	4954.806	3.5
cys	tyr	4076.953	4257.244	4.4	4321.249	6.0
cys	val	2688.906	2731.662	1.6	2746.819	2.1
cys	ala-leu	4748.881	4725.191	-0.5	4763.000	0.3
cys	arg-met	6896.390	6789.532	-1.6	6713.131	-2.7
cys	asn-ser	4422.773	4581.778	3.6	4544.704	2.8
cys	asp-glu	5683.175	5508.175	-3.1	5485.576	-3.5
cys	cys-arg	6040.316	5991.489	-0.8	5888.427	-2.5
cys	gly-ala	3102.144	3129.104	0.9	3113.593	0.4
cys	gly-lys	4539.486	4589.307	1.1	4595.768	1.2
cys	his-pro	5295.417	5639.894	6.5	5684.679	7.3
cys	leu-ser	4893.731	4982.379	1.8	5002.634	2.2
cys	met-tyr	7197.937	7290.523	1.3	7297.155	1.4
cys	phe-cys	6046.791	6235.291	3.1	6232.818	3.1
cys	phe-his	6749.789	6990.210	3.6	7098.128	5.2
cys	pro-glu	5554.427	5433.781	-2.2	5457.987	-1.7
cys	thr-lys	5529.346	5644.539	2.1	5660.105	2.4
cys	thr-val	4891.602	4982.379	1.9	5002.634	2.3
cys	gln-asp	5650.773	5514.125	-2.4	5491.062	-2.8
cys	trp-asn	7203.679	7247.398	0.6	7337.762	1.9
cys	trp-gln	7607.883	7646.420	0.5	7750.113	1.9
cys	tyr-ile	6830.553	7048.815	3.2	7162.133	4.8
cys	val-ile	5523.777	5523.234	-0.0	5587.704	1.2
cys	ala-gln-his	7515.108	7713.766	2.6	7733.935	2.9
cys	asn-cys-ala	6472.619	6559.826	1.4	6456.274	-0.2
cys	asp-his-val	7921.834	8147.799	2.9	8180.127	3.3
cys	cys-thr-lys	7624.784	7838.814	2.8	7771.982	1.9
cys	gln-trp-ile	10360.238	10437.992	0.8	10590.998	2.2
cys	gly-pro-ser	5486.407	5696.919	3.8	5703.107	4.0
cys	leu-arg-gly	7845.141	7702.347	-1.8	7730.260	-1.5
cys	lys-met-asp	8722.729	8812.123	1.0	8757.666	0.4
cys	thr-phe-met	9072.449	9284.052	2.3	9313.336	2.7
cys	tyr-val-pro	8776.871	8960.420	2.1	9099.662	3.7
cys	asn-phe-gly-ala	9057.031	9181.017	1.4	9259.877	2.2
cys	cys-lys-phe-gly	10204.701	10444.525	2.4	10470.974	2.6
cys	glu-his-arg-leu	12317.265	12322.021	0.0	12384.443	0.6
cys	ile-gly-val-gln	9533.766	9508.711	-0.3	9574.488	0.4
cys	leu-trp-asn-cys	12210.970	12274.206	0.5	12329.849	1.0
cys	met-asp-cys-lys	10946.185	11047.359	0.9	10908.869	-0.3
cys	phe-ala-thr-val	10159.618	10237.829	0.8	10369.792	2.1
cys	ser-ile-lys-phe	11386.703	11657.070	2.4	11812.641	3.7
cys	thr-asn-pro-ile	11386.703	11657.070	2.4	11812.641	3.7
cys	val-met-leu-tyr	12327.783	12474.645	1.2	12566.573	1.9
gln	gln	3721.495	3782.786	1.6	3770.281	1.3
gln	glu	3866.935	3780.063	-2.2	3762.239	-2.7
gln	gly	1821.167	1857.344	2.0	1840.884	1.1
gln	his	3813.516	4014.680	5.3	4018.044	5.4

**Table 2** (continued)

Peptide A	Peptide B	TDDFT	Pair-specific	$\Delta$ (%)	Species-specific	$\Delta$ (%)
gln	ile	3763.513	3788.538	0.7	3799.518	1.0
gln	leu	3785.586	3788.538	0.1	3799.518	0.4
gln	lys	4040.005	4104.511	1.6	4108.731	1.7
gln	met	4056.502	4094.701	0.9	4092.910	0.9
gln	phe	4718.465	4831.130	2.4	4868.592	3.2
gln	pro	3080.741	3204.289	4.0	3209.885	4.2
gln	ser	2517.656	2653.392	5.4	2631.714	4.5
gln	thr	3011.319	3136.191	4.2	3121.372	3.6
gln	trp	5844.928	5859.072	0.2	5907.184	1.1
gln	tyr	4979.418	5144.380	3.3	5169.763	3.8
gln	val	3288.495	3305.740	0.5	3309.860	0.7
gln	ala-leu	5804.439	5713.980	-1.6	5728.915	-1.3
gln	arg-met	8425.470	8213.555	-2.5	8218.971	-2.5
gln	asn-ser	5409.522	5538.679	2.4	5511.190	1.9
gln	asp-glu	6938.498	6662.626	-4.0	6633.673	-4.4
gln	cys-arg	7380.857	7247.958	-1.8	7239.654	-1.9
gln	gly-ala	3793.285	3782.786	-0.3	3770.281	-0.6
gln	gly-lys	5551.199	5547.154	-0.1	5548.470	-0.1
gln	his-pro	6477.264	6804.268	5.0	6826.782	5.4
gln	leu-ser	5983.602	6027.230	0.7	6030.086	0.8
gln	met-tyr	8786.434	8824.380	0.4	8861.527	0.8
gln	phe-cys	7382.870	7545.533	2.2	7581.039	2.7
gln	phe-his	8246.254	8431.109	2.2	8485.490	2.9
gln	pro-glu	6781.391	6569.651	-3.1	6570.977	-3.1
gln	thr-lys	6761.711	6826.001	0.9	6828.958	1.0
gln	thr-val	5980.776	6027.230	0.8	6030.086	0.8
gln	gln-asp	6900.374	6665.349	-3.4	6641.715	-3.8
gln	trp-asn	8796.298	8744.359	-0.6	8786.661	-0.1
gln	trp-gln	9290.251	9227.158	-0.7	9276.319	-0.1
gln	tyr-ile	8345.576	8518.217	2.1	8568.135	2.7
gln	val-ile	6752.118	6679.577	-1.1	6708.232	-0.7
gln	ala-gln-his	9188.769	9308.207	1.3	9316.575	1.4
gln	asn-cys-ala	7908.487	7939.833	0.4	7922.466	0.2
gln	asp-his-val	9684.142	9839.008	1.6	9848.179	1.7
gln	cys-thr-lys	9320.725	9489.679	1.8	9491.417	1.8
gln	gln-trp-ile	12654.179	12600.995	-0.4	12674.691	0.2
gln	gly-pro-ser	6708.825	6885.624	2.6	6880.190	2.5
gln	leu-arg-gly	9589.508	9299.310	-3.0	9315.330	-2.9
gln	lys-met-asp	10658.155	10667.075	0.1	10671.929	0.1
gln	thr-phe-met	11080.074	11232.620	1.4	11280.582	1.8
gln	tyr-val-pro	10721.011	10825.006	1.0	10887.215	1.6
gln	asn-phe-gly-ala	11064.445	11084.502	0.2	11117.204	0.5
gln	cys-lys-phe-gly	12466.953	12627.261	1.3	12678.375	1.7
gln	glu-his-arg-leu	15054.900	14872.734	-1.2	14903.569	-1.0
gln	ile-gly-val-gln	11651.809	11490.305	-1.4	11517.105	-1.2
gln	leu-trp-asn-cys	14910.484	14832.600	-0.5	14897.480	-0.1
gln	met-asp-cys-lys	13370.746	13381.478	0.1	13384.376	0.1
gln	phe-ala-thr-val	12410.234	12369.101	-0.3	12426.929	0.1
gln	ser-ile-lys-phe	13916.393	14082.744	1.2	14155.130	1.7
gln	thr-asn-pro-ile	13916.393	14082.744	1.2	14155.130	1.7
gln	val-met-leu-tyr	15056.645	15089.256	0.2	15168.613	0.7
glu	glu	4024.549	3787.448	-5.9	3735.913	-7.2
glu	gly	1891.506	1856.015	-1.9	1830.579	-3.2

**Table 2** (continued)

Peptide A	Peptide B	TDDFT	Pair-specific	$\Delta$ (%)	Species-specific	$\Delta$ (%)
glu	his	3961.331	4013.152	1.3	4027.491	1.7
glu	ile	3910.610	3779.166	-3.4	3800.579	-2.8
glu	leu	3934.015	3779.166	-3.9	3800.579	-3.4
glu	lys	4196.431	4088.409	-2.6	4116.893	-1.9
glu	met	4220.493	4084.730	-3.2	4093.107	-3.0
glu	phe	4911.125	4837.028	-1.5	4872.361	-0.8
glu	pro	3200.534	3202.253	0.1	3206.649	0.2
glu	ser	2614.300	2653.431	1.5	2613.068	-0.1
glu	thr	3127.800	3134.219	0.2	3105.568	-0.7
glu	trp	6087.489	5867.534	-3.6	5920.102	-2.8
glu	tyr	5182.583	5153.657	-0.6	5162.350	-0.4
glu	val	3416.976	3298.378	-3.5	3308.079	-3.2
glu	ala-leu	6035.152	5703.214	-5.5	5732.239	-5.0
glu	arg-met	8764.689	8186.621	-6.6	8248.353	-5.9
glu	asn-ser	5621.671	5539.952	-1.4	5491.388	-2.3
glu	asp-glu	7226.107	6681.355	-7.5	6587.908	-8.8
glu	cys-arg	7676.767	7225.046	-5.9	7263.353	-5.4
glu	gly-ala	3942.735	3780.063	-4.1	3762.239	-4.6
glu	gly-lys	5769.164	5531.669	-4.1	5556.054	-3.7
glu	his-pro	6730.234	6802.650	1.1	6842.721	1.7
glu	leu-ser	6219.346	6019.843	-3.2	6022.228	-3.2
glu	met-tyr	9149.253	8825.633	-3.5	8864.038	-3.1
glu	phe-cys	7685.512	7547.428	-1.8	7589.049	-1.3
glu	phe-his	8579.756	8437.426	-1.7	8508.433	-0.8
glu	pro-glu	7063.017	6576.947	-6.9	6551.144	-7.2
glu	thr-lys	7027.235	6809.874	-3.1	6831.043	-2.8
glu	thr-val	6216.823	6019.843	-3.2	6022.228	-3.1
glu	gln-asp	7185.673	6673.969	-7.1	6614.234	-8.0
glu	trp-asn	9157.699	8754.055	-4.4	8798.422	-3.9
glu	trp-gln	9671.114	9234.842	-4.5	9290.922	-3.9
glu	tyr-ile	8681.632	8520.069	-1.9	8571.510	-1.3
glu	val-ile	7019.494	6664.789	-5.0	6717.238	-4.3
glu	ala-gln-his	9551.668	9304.508	-2.6	9329.971	-2.3
glu	asn-cys-ala	8226.826	7933.723	-3.6	7918.087	-3.8
glu	asp-his-val	10068.848	9840.744	-2.3	9846.860	-2.2
glu	cys-thr-lys	9689.950	9472.212	-2.2	9497.016	-2.0
glu	gln-trp-ile	13168.990	12601.254	-4.3	12700.082	-3.6
glu	gly-pro-ser	6973.304	6886.190	-1.2	6867.459	-1.5
glu	leu-arg-gly	9970.681	9276.255	-7.0	9344.270	-6.3
glu	lys-met-asp	11085.821	10654.291	-3.9	10670.576	-3.8
glu	thr-phe-met	11531.128	11230.469	-2.6	11288.198	-2.1
glu	tyr-val-pro	11156.151	10828.779	-2.9	10894.241	-2.4
glu	asn-phe-gly-ala	11512.763	11090.857	-3.7	11121.501	-3.4
glu	cys-lys-phe-gly	12969.759	12618.281	-2.7	12702.969	-2.1
glu	glu-his-arg-leu	15655.067	14856.148	-5.1	14936.391	-4.6
glu	ile-gly-val-gln	12116.762	11475.358	-5.3	11527.219	-4.9
glu	leu-trp-asn-cys	15521.554	14830.866	-4.5	14924.270	-3.9
glu	met-asp-cys-lys	13911.763	13364.691	-3.9	13387.264	-3.8
glu	phe-ala-thr-val	12913.520	12368.165	-4.2	12434.830	-3.7
glu	ser-ile-lys-phe	14471.703	14071.709	-2.8	14177.930	-2.0
glu	thr-asn-pro-ile	14471.703	14071.709	-2.8	14177.930	-2.0
glu	val-met-leu-tyr	15668.211	15077.668	-3.8	15189.858	-3.0
gly	gly	891.346	911.539	2.3	889.704	-0.2

**Table 2** (continued)

Peptide A	Peptide B	TDDFT	Pair-specific	$\Delta$ (%)	Species-specific	$\Delta$ (%)
gly	his	1866.390	1972.891	5.7	1978.253	6.0
gly	ile	1841.623	1859.430	1.0	1874.081	1.8
gly	leu	1852.357	1859.430	0.4	1874.081	1.2
gly	lys	1977.166	2014.364	1.9	2021.392	2.2
gly	met	1984.182	2008.543	1.2	2001.952	0.9
gly	phe	2307.843	2373.940	2.9	2421.913	4.9
gly	pro	1507.633	1573.355	4.4	1580.374	4.8
gly	ser	1232.324	1302.117	5.7	1272.804	3.3
gly	thr	1473.803	1539.090	4.4	1518.898	3.1
gly	trp	2858.337	2880.065	0.8	2942.381	2.9
gly	tyr	2435.556	2527.545	3.8	2558.919	5.1
gly	val	1609.200	1622.457	0.8	1627.987	1.2
gly	ala-leu	2839.816	2805.234	-1.2	2825.261	-0.5
gly	arg-met	4121.541	4031.865	-2.2	4038.123	-2.0
gly	asn-ser	2647.175	2719.781	2.7	2682.976	1.4
gly	asp-glu	3393.334	3272.350	-3.6	3230.445	-4.8
gly	cys-arg	3610.743	3557.920	-1.5	3545.935	-1.8
gly	gly-ala	1856.114	1857.344	0.1	1840.884	-0.8
gly	gly-lys	2716.344	2723.196	0.2	2726.478	0.4
gly	his-pro	3169.745	3343.540	5.5	3374.009	6.4
gly	leu-ser	2927.806	2958.840	1.1	2962.267	1.2
gly	met-tyr	4296.907	4333.381	0.8	4376.253	1.9
gly	phe-cys	3610.780	3705.830	2.6	3747.059	3.8
gly	phe-his	4033.825	4144.124	2.7	4215.548	4.5
gly	pro-glu	3316.481	3226.663	-2.7	3226.335	-2.7
gly	thr-lys	3308.683	3350.747	1.3	3355.672	1.4
gly	thr-val	2926.383	2958.840	1.1	2962.267	1.2
gly	gln-asp	3374.890	3273.679	-3.0	3240.751	-4.0
gly	trp-asn	4302.161	4297.730	-0.1	4352.553	1.2
gly	trp-gln	4543.818	4534.702	-0.2	4598.647	1.2
gly	tyr-ile	4082.529	4184.268	2.5	4248.382	4.1
gly	val-ile	3303.559	3279.180	-0.7	3317.450	0.4
gly	ala-gln-his	4496.095	4573.333	1.7	4585.699	2.0
gly	asn-cys-ala	3868.755	3898.067	0.8	3871.116	0.1
gly	asp-his-val	4738.171	4833.527	2.0	4845.294	2.3
gly	cys-thr-lys	4560.339	4658.086	2.1	4657.012	2.1
gly	gln-trp-ile	6189.579	6191.425	0.0	6288.110	1.6
gly	gly-pro-ser	3282.736	3381.597	3.0	3373.646	2.8
gly	leu-arg-gly	4691.739	4567.034	-2.7	4591.532	-2.1
gly	lys-met-asp	5213.944	5236.535	0.4	5238.593	0.5
gly	thr-phe-met	5419.468	5516.158	1.8	5573.527	2.8
gly	tyr-val-pro	5244.131	5317.943	1.4	5398.043	2.9
gly	asn-phe-gly-ala	5412.312	5446.241	0.6	5488.351	1.4
gly	cys-lys-phe-gly	6098.472	6201.769	1.7	6265.113	2.7
gly	glu-his-arg-leu	7365.539	7306.244	-0.8	7349.847	-0.2
gly	ile-gly-val-gln	5700.454	5642.649	-1.0	5678.802	-0.4
gly	leu-trp-asn-cys	7292.546	7286.342	-0.1	7367.162	1.0
gly	met-asp-cys-lys	6540.267	6568.425	0.4	6563.739	0.4
gly	phe-ala-thr-val	6070.445	6075.877	0.1	6150.742	1.3
gly	ser-ile-lys-phe	6808.357	6917.179	1.6	7012.530	3.0
gly	thr-asn-pro-ile	6808.357	6917.179	1.6	7012.530	3.0
gly	val-met-leu-tyr	7364.624	7409.853	0.6	7509.084	2.0
his	his	3908.108	4252.538	8.8	4246.771	8.7

**Table 2** (continued)

Peptide A	Peptide B	TDDFT	Pair-specific	$\Delta$ (%)	Species-specific	$\Delta$ (%)
his	ile	3856.426	4025.330	4.4	4021.441	4.3
his	leu	3878.941	4025.330	3.8	4021.441	3.7
his	lys	4140.116	4360.358	5.3	4352.204	5.1
his	met	4155.425	4355.486	4.8	4356.393	4.8
his	phe	4833.364	5121.809	6.0	5117.637	5.9
his	pro	3156.965	3401.508	7.8	3401.595	7.8
his	ser	2580.314	2819.501	9.3	2829.260	9.7
his	thr	3086.034	3332.610	8.0	3340.057	8.2
his	trp	5986.585	6206.277	3.7	6197.372	3.5
his	tyr	5100.790	5455.310	7.0	5457.847	7.0
his	val	3369.708	3512.220	4.2	3510.644	4.2
his	ala-leu	5946.978	6067.118	2.0	6061.232	1.9
his	arg-met	8631.463	8720.264	1.0	8702.766	0.8
his	asn-ser	5543.202	5876.859	6.0	5887.247	6.2
his	asp-glu	7106.958	7068.982	-0.5	7094.926	-0.2
his	cys-arg	7561.605	7694.045	1.8	7681.172	1.6
his	gly-ala	3886.801	4014.680	3.3	4018.044	3.4
his	gly-lys	5688.156	5889.037	3.5	5881.197	3.4
his	his-pro	6637.460	7209.833	8.6	7199.108	8.5
his	leu-ser	6131.037	6400.618	4.4	6401.442	4.4
his	met-tyr	8999.473	9366.583	4.1	9364.982	4.1
his	phe-cys	7562.267	8006.864	5.9	8003.178	5.8
his	phe-his	8447.823	8930.135	5.7	8915.150	5.5
his	pro-glu	6946.123	6970.447	0.3	6979.827	0.5
his	thr-lys	6928.546	7248.756	4.6	7243.002	4.5
his	thr-val	6128.088	6400.618	4.5	6401.442	4.5
his	gln-asp	7068.286	7070.510	0.0	7085.479	0.2
his	trp-asn	9010.238	9263.635	2.8	9255.360	2.7
his	trp-gln	9516.302	9776.745	2.7	9766.157	2.6
his	tyr-ile	8549.742	9036.427	5.7	9030.029	5.6
his	val-ile	6918.070	7093.337	2.5	7082.826	2.4
his	ala-gln-his	9415.154	9864.794	4.8	9855.347	4.7
his	asn-cys-ala	8101.995	8428.414	4.0	8432.578	4.1
his	asp-his-val	9922.270	10431.732	5.1	10430.116	5.1
his	cys-thr-lys	9549.881	10078.455	5.5	10074.018	5.5
his	gln-trp-ile	12962.797	13357.862	3.0	13338.339	2.9
his	gly-pro-ser	6874.245	7305.476	6.3	7310.590	6.3
his	leu-arg-gly	9825.121	9863.431	0.4	9842.283	0.2
his	lys-met-asp	10919.058	11327.462	3.7	11326.773	3.7
his	thr-phe-met	11350.027	11921.482	5.0	11915.570	5.0
his	tyr-val-pro	10982.670	11480.613	4.5	11471.569	4.5
his	asn-phe-gly-ala	11334.744	11749.636	3.7	11744.410	3.6
his	cys-lys-phe-gly	12771.668	13396.333	4.9	13380.592	4.8
his	glu-his-arg-leu	15424.518	15767.373	2.2	15743.559	2.1
his	ile-gly-val-gln	11937.668	12192.485	2.1	12180.605	2.0
his	leu-trp-asn-cys	15273.123	15729.807	3.0	15713.083	2.9
his	met-asp-cys-lys	13697.052	14212.517	3.8	14212.314	3.8
his	phe-ala-thr-val	12713.157	13120.004	3.2	13109.611	3.1
his	ser-ile-lys-phe	14257.825	14939.005	4.8	14918.241	4.6
his	thr-asn-pro-ile	14257.825	14939.005	4.8	14918.241	4.6
his	val-met-leu-tyr	15423.708	16015.708	3.8	15998.549	3.7
ile	ile	3806.462	3793.549	-0.3	3781.896	-0.7
ile	leu	3828.815	3793.549	-0.9	3781.896	-1.2

**Table 2** (continued)

Peptide A	Peptide B	TDDFT	Pair-specific	$\Delta$ (%)	Species-specific	$\Delta$ (%)
ile	lys	4085.877	4114.328	0.7	4104.845	0.5
ile	met	4103.259	4097.743	-0.1	4113.078	0.2
ile	phe	4772.340	4834.361	1.3	4806.404	0.7
ile	pro	3115.743	3207.575	3.0	3203.354	2.8
ile	ser	2545.876	2654.366	4.3	2675.044	5.1
ile	thr	3045.256	3137.896	3.0	3151.998	3.5
ile	trp	5911.531	5866.088	-0.8	5829.289	-1.4
ile	tyr	5036.023	5145.767	2.2	5130.413	1.9
ile	val	3325.959	3310.019	-0.5	3304.942	-0.6
ile	ala-leu	5870.714	5722.657	-2.5	5707.333	-2.8
ile	arg-met	8521.898	8234.890	-3.4	8235.047	-3.4
ile	asn-ser	5470.413	5545.523	1.4	5572.011	1.9
ile	asp-glu	7016.883	6660.950	-5.1	6698.606	-4.5
ile	cys-arg	7465.153	7267.830	-2.6	7281.140	-2.5
ile	gly-ala	3836.236	3788.538	-1.2	3799.518	-1.0
ile	gly-lys	5614.244	5559.906	-1.0	5553.328	-1.1
ile	his-pro	6550.484	6819.053	4.1	6799.197	3.8
ile	leu-ser	6051.641	6034.064	-0.3	6031.342	-0.3
ile	met-tyr	8887.167	8829.659	-0.7	8817.894	-0.8
ile	phe-cys	7467.571	7551.193	1.1	7539.977	1.0
ile	phe-his	8340.003	8445.839	1.3	8402.247	0.8
ile	pro-glu	6857.979	6572.889	-4.2	6578.335	-4.1
ile	thr-lys	6838.471	6838.372	-0.0	6831.245	-0.1
ile	thr-val	6048.726	6034.064	-0.2	6031.342	-0.3
ile	gln-asp	6977.982	6670.323	-4.4	6697.545	-4.0
ile	trp-asn	8896.312	8757.246	-1.6	8726.256	-1.9
ile	trp-gln	9396.036	9240.776	-1.6	9203.210	-2.0
ile	tyr-ile	8440.761	8525.465	1.0	8486.711	0.5
ile	val-ile	6829.377	6689.717	-2.0	6661.240	-2.5
ile	ala-gln-his	9292.823	9329.125	0.4	9320.799	0.3
ile	asn-cys-ala	7998.560	7950.950	-0.6	7981.575	-0.2
ile	asp-his-val	9793.899	9854.505	0.6	9849.607	0.6
ile	cys-thr-lys	9427.050	9503.983	0.8	9514.024	0.9
ile	gln-trp-ile	12798.405	12620.473	-1.4	12559.508	-1.9
ile	gly-pro-ser	6784.698	6893.668	1.6	6901.284	1.7
ile	leu-arg-gly	9698.630	9325.051	-3.9	9301.554	-4.1
ile	lys-met-asp	10779.960	10680.005	-0.9	10690.353	-0.8
ile	thr-phe-met	11206.900	11242.298	0.3	11220.285	0.1
ile	tyr-val-pro	10843.218	10835.659	-0.1	10787.514	-0.5
ile	asn-phe-gly-ala	11190.144	11100.205	-0.8	11077.291	-1.0
ile	cys-lys-phe-gly	12609.441	12646.027	0.3	12616.914	0.1
ile	glu-his-arg-leu	15226.034	14907.488	-2.1	14874.689	-2.3
ile	ile-gly-val-gln	11784.611	11509.982	-2.3	11483.644	-2.5
ile	leu-trp-asn-cys	15080.811	14853.776	-1.5	14816.128	-1.8
ile	met-asp-cys-lys	13523.936	13396.838	-0.9	13423.926	-0.7
ile	phe-ala-thr-val	12551.750	12383.682	-1.3	12337.586	-1.7
ile	ser-ile-lys-phe	14075.049	14103.828	0.2	14040.602	-0.2
ile	thr-asn-pro-ile	14075.049	14103.828	0.2	14040.602	-0.2
ile	val-met-leu-tyr	15229.146	15105.525	-0.8	15053.537	-1.1
leu	leu	3851.336	3793.549	-1.5	3781.896	-1.8
leu	lys	4109.744	4114.328	0.1	4104.845	-0.1
leu	met	4127.789	4097.743	-0.7	4113.078	-0.4
leu	phe	4800.973	4834.361	0.7	4806.404	0.1

**Table 2** (continued)

Peptide A	Peptide B	TDDFT	Pair-specific	$\Delta$ (%)	Species-specific	$\Delta$ (%)
leu	pro	3133.985	3207.575	2.4	3203.354	2.2
leu	ser	2560.666	2654.366	3.7	2675.044	4.5
leu	thr	3063.023	3137.896	2.4	3151.998	2.9
leu	trp	5947.270	5866.088	-1.4	5829.289	-2.0
leu	tyr	5066.210	5145.767	1.6	5130.413	1.3
leu	val	3345.483	3310.019	-1.1	3304.942	-1.2
leu	ala-leu	5905.476	5722.657	-3.1	5707.333	-3.4
leu	arg-met	8572.692	8234.890	-3.9	8235.047	-3.9
leu	asn-ser	5502.539	5545.523	0.8	5572.011	1.3
leu	asp-glu	7059.230	6660.950	-5.6	6698.606	-5.1
leu	cys-arg	7509.546	7267.830	-3.2	7281.140	-3.0
leu	gly-ala	3858.833	3788.538	-1.8	3799.518	-1.5
leu	gly-lys	5647.266	5559.906	-1.6	5553.328	-1.7
leu	his-pro	6588.888	6819.053	3.5	6799.197	3.2
leu	leu-ser	6087.302	6034.064	-0.9	6031.342	-0.9
leu	met-tyr	8940.811	8829.659	-1.2	8817.894	-1.4
leu	phe-cys	7512.492	7551.193	0.5	7539.977	0.4
leu	phe-his	8389.776	8445.839	0.7	8402.247	0.1
leu	pro-glu	6899.352	6572.889	-4.7	6578.335	-4.7
leu	thr-lys	6878.693	6838.372	-0.6	6831.245	-0.7
leu	thr-val	6084.395	6034.064	-0.8	6031.342	-0.9
leu	gln-asp	7019.985	6670.323	-5.0	6697.545	-4.6
leu	trp-asn	8949.817	8757.246	-2.1	8726.256	-2.5
leu	trp-gln	9452.498	9240.776	-2.2	9203.210	-2.6
leu	tyr-ile	8491.048	8525.465	0.4	8486.711	-0.1
leu	val-ile	6869.751	6689.717	-2.6	6661.240	-3.0
leu	ala-gln-his	9347.622	9329.125	-0.2	9320.799	-0.3
leu	asn-cys-ala	8046.203	7950.950	-1.2	7981.575	-0.8
leu	asp-his-val	9851.824	9854.505	0.0	9849.607	-0.0
leu	cys-thr-lys	9482.773	9503.983	0.2	9514.024	0.3
leu	gln-trp-ile	12875.029	12620.473	-2.0	12559.508	-2.5
leu	gly-pro-ser	6824.663	6893.668	1.0	6901.284	1.1
leu	leu-arg-gly	9756.035	9325.051	-4.4	9301.554	-4.7
leu	lys-met-asp	10844.098	10680.005	-1.5	10690.353	-1.4
leu	thr-phe-met	11274.060	11242.298	-0.3	11220.285	-0.5
leu	tyr-val-pro	10908.062	10835.659	-0.7	10787.514	-1.1
leu	asn-phe-gly-ala	11256.988	11100.205	-1.4	11077.291	-1.6
leu	cys-lys-phe-gly	12684.647	12646.027	-0.3	12616.914	-0.5
leu	glu-his-arg-leu	15316.273	14907.488	-2.7	14874.689	-2.9
leu	ile-gly-val-gln	11854.511	11509.982	-2.9	11483.644	-3.1
leu	leu-trp-asn-cys	15171.457	14853.776	-2.1	14816.128	-2.3
leu	met-asp-cys-lys	13604.758	13396.838	-1.5	13423.926	-1.3
leu	phe-ala-thr-val	12626.791	12383.682	-1.9	12337.586	-2.3
leu	ser-ile-lys-phe	14158.530	14103.828	-0.4	14040.602	-0.8
leu	thr-asn-pro-ile	14158.530	14103.828	-0.4	14040.602	-0.8
leu	val-met-leu-tyr	15320.315	15105.525	-1.4	15053.537	-1.7
lys	lys	4386.276	4465.540	1.8	4443.908	1.3
lys	met	4402.935	4443.804	0.9	4446.017	1.0
lys	phe	5120.732	5232.907	2.2	5236.668	2.3
lys	pro	3344.676	3475.238	3.9	3476.290	3.9
lys	ser	2733.426	2874.465	5.2	2889.480	5.7
lys	thr	3269.295	3399.456	4.0	3410.343	4.3
lys	trp	6342.285	6348.854	0.1	6348.228	0.1

**Table 2** (continued)

Peptide A	Peptide B	TDDFT	Pair-specific	$\Delta$ (%)	Species-specific	$\Delta$ (%)
lys	tyr	5403.836	5568.017	3.0	5583.893	3.3
lys	val	3570.143	3589.337	0.5	3583.982	0.4
lys	ala-leu	6300.737	6204.474	-1.5	6192.184	-1.7
lys	arg-met	9144.992	8934.362	-2.3	8897.750	-2.7
lys	asn-ser	5872.231	6004.777	2.3	6022.432	2.6
lys	asp-glu	7528.629	7202.619	-4.3	7258.008	-3.6
lys	cys-arg	8011.359	7884.380	-1.6	7856.024	-1.9
lys	gly-ala	4117.721	4104.511	-0.3	4108.731	-0.2
lys	gly-lys	6026.288	6030.695	0.1	6010.384	-0.3
lys	his-pro	7031.748	7386.388	5.0	7373.578	4.9
lys	leu-ser	6495.549	6539.584	0.7	6539.409	0.7
lys	met-tyr	9534.799	9562.612	0.3	9574.993	0.4
lys	phe-cys	8012.217	8177.521	2.1	8186.043	2.2
lys	phe-his	8949.811	9144.056	2.2	9133.955	2.1
lys	pro-glu	7358.229	7114.439	-3.3	7138.267	-3.0
lys	thr-lys	7340.381	7415.787	1.0	7399.335	0.8
lys	thr-val	6492.360	6539.584	0.7	6539.409	0.7
lys	gln-asp	7487.374	7218.721	-3.6	7249.846	-3.2
lys	trp-asn	9545.498	9479.166	-0.7	9481.180	-0.7
lys	trp-gln	10081.789	10004.157	-0.8	10002.043	-0.8
lys	tyr-ile	9058.107	9233.136	1.9	9233.821	1.9
lys	val-ile	7329.771	7254.456	-1.0	7233.911	-1.3
lys	ala-gln-his	9974.502	10105.807	1.3	10093.358	1.2
lys	asn-cys-ala	8583.629	8614.281	0.4	8624.582	0.5
lys	asp-his-val	10511.767	10671.746	1.5	10676.229	1.6
lys	cys-thr-lys	10117.906	10303.352	1.8	10294.863	1.8
lys	gln-trp-ile	13733.321	13669.277	-0.5	13651.972	-0.6
lys	gly-pro-ser	7282.564	7465.651	2.5	7477.330	2.7
lys	leu-arg-gly	10409.235	10112.993	-2.9	10069.208	-3.3
lys	lys-met-asp	11568.572	11574.345	0.1	11576.123	0.1
lys	thr-phe-met	12025.171	12177.750	1.3	12183.196	1.3
lys	tyr-val-pro	11635.535	11734.175	0.8	11734.332	0.8
lys	asn-phe-gly-ala	12008.178	12018.521	0.1	12023.435	0.1
lys	cys-lys-phe-gly	13531.316	13701.959	1.3	13687.664	1.2
lys	glu-his-arg-leu	16341.310	16155.236	-1.1	16115.843	-1.4
lys	ile-gly-val-gln	12647.519	12474.915	-1.4	12454.202	-1.5
lys	leu-trp-asn-cys	16181.199	16088.900	-0.6	16080.483	-0.6
lys	met-asp-cys-lys	14512.035	14518.959	0.1	14525.497	0.1
lys	phe-ala-thr-val	13468.953	13413.430	-0.4	13408.500	-0.5
lys	ser-ile-lys-phe	15105.674	15282.565	1.2	15256.306	1.0
lys	thr-asn-pro-ile	15105.674	15282.565	1.2	15256.306	1.0
lys	val-met-leu-tyr	16341.352	16367.860	0.2	16353.988	0.1
met	met	4428.357	4416.992	-0.3	4349.756	-1.8
met	phe	5151.480	5230.265	1.5	5273.860	2.4
met	pro	3358.006	3466.848	3.2	3479.656	3.6
met	ser	2742.371	2866.932	4.5	2862.869	4.4
met	thr	3281.232	3389.232	3.3	3390.651	3.3
met	trp	6384.270	6349.440	-0.6	6398.261	0.2
met	tyr	5435.708	5566.355	2.4	5606.996	3.1
met	val	3585.188	3575.443	-0.3	3585.297	0.0
met	ala-leu	6331.791	6183.902	-2.3	6204.036	-2.0
met	arg-met	9195.120	8891.044	-3.3	8811.593	-4.2
met	asn-ser	5896.716	5994.649	1.7	5989.222	1.6

**Table 2** (continued)

Peptide A	Peptide B	TDDFT	Pair-specific	$\Delta$ (%)	Species-specific	$\Delta$ (%)
met	asp-glu	7576.981	7202.476	-4.9	7219.656	-4.7
met	cys-arg	8053.655	7846.444	-2.6	7756.030	-3.7
met	gly-ala	4136.053	4094.701	-1.0	4092.910	-1.0
met	gly-lys	6052.524	6007.662	-0.7	6009.193	-0.7
met	his-pro	7060.308	7377.650	4.5	7397.274	4.8
met	leu-ser	6524.857	6519.991	-0.1	6537.172	0.2
met	met-tyr	9597.078	9538.663	-0.6	9517.976	-0.8
met	phe-cys	8062.307	8157.973	1.2	8129.277	0.8
met	phe-his	8999.394	9141.067	1.6	9191.478	2.1
met	pro-glu	7405.294	7106.894	-4.0	7133.987	-3.7
met	thr-lys	7372.297	7388.352	0.2	7397.892	0.3
met	thr-val	6521.990	6519.991	-0.0	6537.172	0.2
met	gln-asp	7533.655	7212.447	-4.3	7219.459	-4.2
met	trp-asn	9604.460	9477.156	-1.3	9524.613	-0.8
met	trp-gln	10143.446	9999.457	-1.4	10052.395	-0.9
met	tyr-ile	9107.214	9219.414	1.2	9281.298	1.9
met	val-ile	7365.056	7228.502	-1.9	7259.599	-1.4
met	ala-gln-his	10019.791	10091.662	0.7	10101.485	0.8
met	asn-cys-ala	8629.938	8586.267	-0.5	8511.503	-1.4
met	asp-his-val	10562.068	10658.288	0.9	10682.284	1.1
met	cys-thr-lys	10166.284	10261.762	0.9	10200.488	0.3
met	gln-trp-ile	13813.229	13652.516	-1.2	13726.697	-0.6
met	gly-pro-ser	7314.924	7452.955	1.9	7466.926	2.1
met	leu-arg-gly	10459.969	10081.356	-3.6	10085.271	-3.6
met	lys-met-asp	11630.183	11533.858	-0.8	11483.546	-1.3
met	thr-phe-met	12096.426	12147.121	0.4	12136.715	0.3
met	tyr-val-pro	11702.161	11719.278	0.1	11794.397	0.8
met	asn-phe-gly-ala	12075.560	12007.999	-0.6	12054.347	-0.2
met	cys-lys-phe-gly	13606.080	13666.654	0.5	13646.874	0.3
met	glu-his-arg-leu	16422.581	16122.643	-1.8	16146.864	-1.7
met	ile-gly-val-gln	12711.469	12442.378	-2.1	12476.909	-1.9
met	leu-trp-asn-cys	16280.859	16057.923	-1.4	16054.332	-1.4
met	met-asp-cys-lys	14594.820	14461.565	-0.9	14338.963	-1.8
met	phe-ala-thr-val	13545.801	13391.731	-1.1	13463.214	-0.6
met	ser-ile-lys-phe	15182.022	15250.395	0.5	15326.677	0.9
met	thr-asn-pro-ile	15182.022	15250.395	0.5	15326.677	0.9
met	val-met-leu-tyr	16436.889	16322.481	-0.7	16338.799	-0.6
phe	phe	5993.879	6170.033	2.9	6045.477	0.9
phe	pro	3905.560	4091.845	4.8	4072.957	4.3
phe	ser	3189.611	3393.490	6.4	3452.068	8.2
phe	thr	3816.404	4008.595	5.0	4048.191	6.1
phe	trp	7429.601	7480.262	0.7	7324.677	-1.4
phe	tyr	6324.835	6574.477	4.0	6479.509	2.5
phe	val	4169.848	4219.255	1.2	4210.281	1.0
phe	ala-leu	7365.337	7291.550	-1.0	7253.083	-1.5
phe	arg-met	10697.052	10473.587	-2.1	10525.053	-1.6
phe	asn-ser	6859.405	7077.659	3.2	7153.182	4.3
phe	asp-glu	8818.256	8527.096	-3.3	8577.243	-2.7
phe	cys-arg	9368.972	9243.377	-1.3	9332.808	-0.4
phe	gly-ala	4811.199	4831.130	0.4	4868.592	1.2
phe	gly-lys	7040.100	7074.991	0.5	7087.225	0.7
phe	his-pro	8212.345	8681.799	5.7	8619.238	5.0
phe	leu-ser	7589.629	7695.995	1.4	7687.116	1.3

**Table 2** (continued)

Peptide A	Peptide B	TDDFT	Pair-specific	$\Delta$ (%)	Species-specific	$\Delta$ (%)
phe	met-tyr	11167.145	11272.887	0.9	11182.013	0.1
phe	phe-cys	9380.554	9638.232	2.8	9555.735	1.9
phe	phe-his	10470.573	10759.987	2.8	10591.757	1.2
phe	pro-glu	8618.738	8397.017	-2.6	8373.962	-2.8
phe	thr-lys	8575.270	8709.646	1.6	8713.503	1.6
phe	thr-val	7586.491	7695.995	1.4	7687.116	1.3
phe	gln-asp	8768.112	8521.197	-2.8	8573.474	-2.2
phe	trp-asn	11176.209	11164.431	-0.1	11025.790	-1.4
phe	trp-gln	11802.962	11779.536	-0.2	11621.913	-1.5
phe	tyr-ile	10595.221	10876.982	2.7	10714.557	1.1
phe	val-ile	8566.782	8521.761	-0.5	8445.328	-1.4
phe	ala-gln-his	11655.648	11878.274	1.9	11861.553	1.8
phe	asn-cys-ala	10040.029	10141.414	1.0	10229.408	1.9
phe	asp-his-val	12287.010	12562.983	2.2	12530.106	2.0
phe	cys-thr-lys	11825.476	12114.140	2.4	12155.100	2.8
phe	gln-trp-ile	16071.825	16082.041	0.1	15856.960	-1.3
phe	gly-pro-ser	8509.161	8795.564	3.4	8804.226	3.5
phe	leu-arg-gly	12167.802	11856.062	-2.6	11839.491	-2.7
phe	lys-met-asp	13529.617	13621.384	0.7	13644.054	0.8
phe	thr-phe-met	14073.715	14345.182	1.9	14224.815	1.1
phe	tyr-val-pro	13615.259	13821.866	1.5	13620.035	0.0
phe	asn-phe-gly-ala	14049.929	14153.476	0.7	14043.826	-0.0
phe	cys-lys-phe-gly	15829.003	16117.663	1.8	16002.942	1.1
phe	glu-his-arg-leu	19104.664	18972.810	-0.7	18904.882	-1.1
phe	ile-gly-val-gln	14787.182	14663.120	-0.8	14593.121	-1.3
phe	leu-trp-asn-cys	18943.770	18935.136	-0.1	18771.096	-0.9
phe	met-asp-cys-lys	16979.307	17089.584	0.7	17154.312	1.0
phe	phe-ala-thr-val	15760.084	15791.362	0.2	15607.915	-1.0
phe	ser-ile-lys-phe	17661.152	17971.518	1.8	17757.886	0.6
phe	thr-asn-pro-ile	17661.152	17971.518	1.8	17757.886	0.6
phe	val-met-leu-tyr	19123.104	19262.792	0.7	19055.985	-0.3
pro	pro	2550.473	2713.671	6.4	2710.701	6.3
pro	ser	2084.243	2247.538	7.8	2255.820	8.2
pro	thr	2492.925	2656.093	6.5	2661.565	6.8
pro	trp	4837.521	4963.247	2.6	4940.114	2.1
pro	tyr	4121.451	4357.473	5.7	4342.658	5.4
pro	val	2722.458	2799.020	2.8	2797.609	2.8
pro	ala-leu	4805.038	4838.508	0.7	4832.864	0.6
pro	arg-met	6974.480	6955.741	-0.3	6971.394	-0.0
pro	asn-ser	4477.970	4692.295	4.8	4703.351	5.0
pro	asp-glu	5742.319	5644.974	-1.7	5650.945	-1.6
pro	cys-arg	6109.798	6138.631	0.5	6159.905	0.8
pro	gly-ala	3140.114	3204.289	2.0	3209.885	2.2
pro	gly-lys	4595.494	4697.617	2.2	4700.056	2.3
pro	his-pro	5362.092	5764.202	7.5	5755.687	7.3
pro	leu-ser	4953.417	5104.136	3.0	5102.565	3.0
pro	met-tyr	7272.504	7473.344	2.8	7465.706	2.7
pro	phe-cys	6111.016	6390.607	4.6	6384.515	4.5
pro	phe-his	6825.686	7142.376	4.6	7117.944	4.3
pro	pro-glu	5612.266	5564.947	-0.8	5560.742	-0.9
pro	thr-lys	5597.585	5780.355	3.3	5781.246	3.3
pro	thr-val	4951.011	5104.136	3.1	5102.565	3.1
pro	gln-asp	5710.689	5647.010	-1.1	5654.180	-1.0

**Table 2** (continued)

Peptide A	Peptide B	TDDFT	Pair-specific	$\Delta$ (%)	Species-specific	$\Delta$ (%)
pro	trp-asn	7280.445	7408.004	1.8	7387.645	1.5
pro	trp-gln	7689.428	7816.559	1.6	7793.390	1.4
pro	tyr-ile	6908.184	7214.070	4.4	7189.403	4.1
pro	val-ile	5589.721	5655.618	1.2	5644.354	1.0
pro	ala-gln-his	7606.466	7885.753	3.7	7884.381	3.6
pro	asn-cys-ala	6546.325	6725.429	2.7	6745.207	3.0
pro	asp-his-val	8016.367	8334.947	4.0	8330.345	3.9
pro	cys-thr-lys	7715.966	8036.442	4.2	8049.350	4.3
pro	gln-trp-ile	10474.153	10673.157	1.9	10640.135	1.6
pro	gly-pro-ser	5553.567	5832.611	5.0	5833.678	5.0
pro	leu-arg-gly	7938.219	7876.171	-0.8	7875.404	-0.8
pro	lys-met-asp	8822.716	9033.832	2.4	9043.633	2.5
pro	thr-phe-met	9171.459	9512.833	3.7	9500.961	3.6
pro	tyr-val-pro	8874.129	9168.210	3.3	9137.751	3.0
pro	asn-phe-gly-ala	9158.268	9389.914	2.5	9373.764	2.4
pro	cys-lys-phe-gly	10319.785	10694.573	3.6	10684.508	3.5
pro	glu-his-arg-leu	12462.231	12598.274	1.1	12590.119	1.0
pro	ile-gly-val-gln	9645.328	9731.308	0.9	9721.395	0.8
pro	leu-trp-asn-cys	12341.506	12563.364	1.8	12545.947	1.7
pro	met-asp-cys-lys	11067.928	11332.594	2.4	11355.191	2.6
pro	phe-ala-thr-val	10272.417	10475.937	2.0	10448.424	1.7
pro	ser-ile-lys-phe	11519.966	11926.591	3.5	11895.141	3.3
pro	thr-asn-pro-ile	11519.966	11926.591	3.5	11895.141	3.3
pro	val-met-leu-tyr	12463.248	12777.985	2.5	12753.451	2.3
ser	ser	1703.807	1860.317	9.2	1819.154	6.8
ser	thr	2037.568	2198.380	7.9	2169.714	6.5
ser	trp	3950.100	4117.799	4.2	4195.964	6.2
ser	tyr	3366.169	3613.628	7.3	3647.858	8.4
ser	val	2224.585	2316.304	4.1	2324.484	4.5
ser	ala-leu	3925.419	4005.641	2.0	4033.954	2.8
ser	arg-met	5696.686	5755.160	1.0	5779.439	1.4
ser	asn-ser	3659.520	3886.744	6.2	3835.854	4.8
ser	asp-glu	4689.570	4679.897	-0.2	4611.122	-1.7
ser	cys-arg	4990.813	5079.035	1.8	5078.319	1.8
ser	gly-ala	2565.837	2653.392	3.4	2631.714	2.6
ser	gly-lys	3755.046	3887.678	3.5	3897.830	3.8
ser	his-pro	4382.003	4778.135	9.0	4820.626	10.0
ser	leu-ser	4047.280	4225.779	4.4	4229.744	4.5
ser	met-tyr	5938.211	6191.656	4.3	6246.274	5.2
ser	phe-cys	4990.193	5295.393	6.1	5349.364	7.2
ser	phe-his	5575.406	5924.087	6.2	6016.874	7.9
ser	pro-glu	4583.390	4612.065	0.6	4604.434	0.5
ser	thr-lys	4573.894	4783.941	4.6	4794.740	4.8
ser	thr-val	4045.285	4225.779	4.5	4229.744	4.6
ser	gln-asp	4664.246	4679.858	0.3	4629.768	-0.7
ser	trp-asn	5945.767	6144.225	3.3	6212.664	4.5
ser	trp-gln	6279.799	6482.287	3.2	6563.224	4.5
ser	tyr-ile	5642.814	5979.090	6.0	6058.449	7.4
ser	val-ile	4566.515	4681.766	2.5	4735.074	3.7
ser	ala-gln-his	6215.194	6535.265	5.2	6555.430	5.5
ser	asn-cys-ala	5347.355	5568.509	4.1	5537.359	3.5
ser	asp-his-val	6549.607	6907.749	5.5	6921.676	5.7
ser	cys-thr-lys	6303.792	6651.462	5.5	6657.703	5.6

**Table 2** (continued)

Peptide A	Peptide B	TDDFT	Pair-specific	$\Delta$ (%)	Species-specific	$\Delta$ (%)
ser	gln-trp-ile	8554.680	8847.749	3.4	8973.815	4.9
ser	gly-pro-ser	4537.964	4832.165	6.5	4818.870	6.2
ser	leu-arg-gly	6485.345	6521.424	0.6	6565.632	1.2
ser	lys-met-asp	7206.731	7478.958	3.8	7485.949	3.9
ser	thr-phe-met	7490.187	7880.994	5.2	7955.744	6.2
ser	tyr-val-pro	7248.060	7599.662	4.8	7699.255	6.2
ser	asn-phe-gly-ala	7480.623	7784.404	4.1	7836.028	4.8
ser	cys-lys-phe-gly	8429.098	8859.785	5.1	8948.407	6.2
ser	glu-his-arg-leu	10181.172	10437.718	2.5	10505.034	3.2
ser	ile-gly-val-gln	7879.482	8059.467	2.3	8110.684	2.9
ser	leu-trp-asn-cys	10078.625	10411.591	3.3	10520.550	4.4
ser	met-asp-cys-lys	9039.503	9380.862	3.8	9383.244	3.8
ser	phe-ala-thr-val	8390.152	8681.640	3.5	8776.269	4.6
ser	ser-ile-lys-phe	9410.892	9881.543	5.0	10008.053	6.3
ser	thr-asn-pro-ile	9410.892	9881.543	5.0	10008.053	6.3
ser	val-met-leu-tyr	10178.680	10584.518	4.0	10716.894	5.3
thr	thr	2436.903	2598.081	6.6	2577.989	5.8
thr	trp	4726.813	4864.305	2.9	4917.691	4.0
thr	tyr	4027.536	4268.183	6.0	4290.732	6.5
thr	val	2660.911	2738.194	2.9	2743.723	3.1
thr	ala-leu	4695.944	4734.997	0.8	4754.472	1.2
thr	arg-met	6815.580	6805.916	-0.1	6828.670	0.2
thr	asn-ser	4377.107	4593.179	4.9	4558.113	4.1
thr	asp-glu	5611.359	5527.047	-1.5	5478.162	-2.4
thr	cys-arg	5970.824	6006.513	0.6	6012.120	0.7
thr	gly-ala	3069.163	3136.191	2.2	3121.372	1.7
thr	gly-lys	4491.622	4596.856	2.3	4604.542	2.5
thr	his-pro	5241.234	5647.013	7.7	5676.923	8.3
thr	leu-ser	4841.325	4994.585	3.2	4997.013	3.2
thr	met-tyr	7105.855	7315.726	3.0	7356.684	3.5
thr	phe-cys	5971.150	6256.734	4.8	6297.593	5.5
thr	phe-his	6670.428	6999.515	4.9	7063.549	5.9
thr	pro-glu	5484.309	5448.622	-0.7	5442.434	-0.8
thr	thr-lys	5471.081	5655.847	3.4	5663.633	3.5
thr	thr-val	4838.971	4994.585	3.2	4997.013	3.3
thr	gln-asp	5580.779	5529.019	-0.9	5493.967	-1.6
thr	trp-asn	7114.305	7259.104	2.0	7306.090	2.7
thr	trp-gln	7513.936	7658.805	1.9	7714.365	2.7
thr	tyr-ile	6750.998	7064.389	4.6	7118.031	5.4
thr	val-ile	5462.808	5534.400	1.3	5571.022	2.0
thr	ala-gln-his	7434.515	7724.213	3.9	7739.204	4.1
thr	asn-cys-ala	6397.453	6581.730	2.9	6564.974	2.6
thr	asp-his-val	7834.881	8162.993	4.2	8172.754	4.3
thr	cys-thr-lys	7540.959	7862.936	4.3	7871.956	4.4
thr	gln-trp-ile	10235.399	10455.011	2.1	10541.664	3.0
thr	gly-pro-ser	5428.133	5710.182	5.2	5700.780	5.0
thr	leu-arg-gly	7758.214	7710.928	-0.6	7743.137	-0.2
thr	lys-met-asp	8621.949	8839.826	2.5	8848.889	2.6
thr	thr-phe-met	8962.030	9312.528	3.9	9367.433	4.5
thr	tyr-val-pro	8671.935	8979.090	3.5	9046.622	4.3
thr	asn-phe-gly-ala	8949.918	9197.895	2.8	9233.263	3.2
thr	cys-lys-phe-gly	10084.709	10470.849	3.8	10536.358	4.5
thr	glu-his-arg-leu	12179.584	12338.029	1.3	12386.244	1.7

**Table 2** (continued)

Peptide A	Peptide B	TDDFT	Pair-specific	$\Delta$ (%)	Species-specific	$\Delta$ (%)
thr	ile-gly-val-gln	9426.310	9526.301	1.1	9561.895	1.4
thr	leu-trp-asn-cys	12059.521	12303.449	2.0	12382.791	2.7
thr	met-asp-cys-lys	10815.406	11087.965	2.5	11098.291	2.6
thr	phe-ala-thr-val	10038.361	10258.592	2.2	10322.980	2.8
thr	ser-ile-lys-phe	11258.363	11678.206	3.7	11765.071	4.5
thr	thr-asn-pro-ile	11258.363	11678.206	3.7	11765.071	4.5
thr	val-met-leu-tyr	12178.691	12508.436	2.7	12603.007	3.5
trp	trp	9211.636	9065.199	-1.6	8868.448	-3.7
trp	tyr	7839.828	7971.490	1.7	7856.533	0.2
trp	val	5165.209	5119.583	-0.9	5107.562	-1.1
trp	ala-leu	9125.786	8845.096	-3.1	8794.093	-3.6
trp	arg-met	13256.358	12703.590	-4.2	12750.164	-3.8
trp	asn-ser	8497.490	8582.802	1.0	8682.117	2.2
trp	asp-glu	10933.378	10340.999	-5.4	10419.172	-4.7
trp	cys-arg	11609.835	11210.579	-3.4	11306.709	-2.6
trp	gly-ala	5960.478	5859.072	-1.7	5907.184	-0.9
trp	gly-lys	8721.320	8581.356	-1.6	8591.304	-1.5
trp	his-pro	10172.818	10521.959	3.4	10438.181	2.6
trp	leu-ser	9402.526	9336.323	-0.7	9325.949	-0.8
trp	met-tyr	13844.319	13673.365	-1.2	13555.489	-2.1
trp	phe-cys	11628.054	11689.126	0.5	11580.178	-0.4
trp	phe-his	12976.831	13038.975	0.5	12822.744	-1.2
trp	pro-glu	10686.403	10183.217	-4.7	10160.911	-4.9
trp	thr-lys	10623.131	10565.595	-0.5	10566.615	-0.5
trp	thr-val	9398.913	9336.323	-0.7	9325.949	-0.8
trp	gln-asp	10870.947	10332.537	-5.0	10406.255	-4.3
trp	trp-asn	13854.766	13530.202	-2.3	13354.601	-3.6
trp	trp-gln	14631.172	14276.708	-2.4	14076.328	-3.8
trp	tyr-ile	13130.329	13190.014	0.5	12986.518	-1.1
trp	val-ile	10613.744	10338.107	-2.6	10237.547	-3.5
trp	ala-gln-his	14440.443	14396.792	-0.3	14370.055	-0.5
trp	asn-cys-ala	12442.239	12300.438	-1.1	12405.762	-0.3
trp	asp-his-val	15223.968	15229.928	0.0	15188.424	-0.2
trp	cys-thr-lys	14651.254	14696.291	0.3	14738.392	0.6
trp	gln-trp-ile	19920.518	19495.233	-2.1	19206.313	-3.6
trp	gly-pro-ser	10541.944	10665.983	1.2	10679.850	1.3
trp	leu-arg-gly	15076.260	14374.573	-4.7	14340.545	-4.9
trp	lys-met-asp	16765.805	16524.195	-1.4	16546.254	-1.3
trp	thr-phe-met	17443.881	17398.878	-0.3	17242.019	-1.2
trp	tyr-val-pro	16875.062	16759.191	-0.7	16505.600	-2.2
trp	asn-phe-gly-ala	17413.459	17156.773	-1.5	17018.709	-2.3
trp	cys-lys-phe-gly	19616.748	19544.750	-0.4	19388.454	-1.2
trp	glu-his-arg-leu	23672.340	22998.922	-2.8	22900.058	-3.3
trp	ile-gly-val-gln	18322.755	17782.117	-3.0	17688.503	-3.5
trp	leu-trp-asn-cys	23482.733	22957.591	-2.2	22740.087	-3.2
trp	met-asp-cys-lys	21043.206	20733.059	-1.5	20801.756	-1.1
trp	phe-ala-thr-val	19533.118	19148.029	-2.0	18916.124	-3.2
trp	ser-ile-lys-phe	21883.888	21792.144	-0.4	21516.520	-1.7
trp	thr-asn-pro-ile	21883.888	21792.144	-0.4	21516.520	-1.7
trp	val-met-leu-tyr	23701.563	23363.909	-1.4	23093.731	-2.6
tyr	tyr	6674.211	7006.004	5.0	6925.576	3.8
tyr	val	4400.277	4491.212	2.1	4487.540	2.0
tyr	ala-leu	7772.170	7762.602	-0.1	7741.258	-0.4

**Table 2** (continued)

Peptide A	Peptide B	TDDFT	Pair-specific	$\Delta$ (%)	Species-specific	$\Delta$ (%)
tyr	arg-met	11287.680	11146.126	-1.2	11217.138	-0.6
tyr	asn-ser	7238.848	7538.186	4.1	7583.801	4.8
tyr	asp-glu	9305.556	9087.493	-2.3	9090.879	-2.3
tyr	cys-arg	9886.399	9837.015	-0.5	9931.390	0.5
tyr	gly-ala	5077.179	5144.380	1.3	5169.763	1.8
tyr	gly-lys	7429.227	7530.296	1.4	7551.864	1.6
tyr	his-pro	8666.497	9247.516	6.7	9209.558	6.3
tyr	leu-ser	8009.060	8194.129	2.3	8187.324	2.2
tyr	met-tyr	11783.421	12007.092	1.9	11941.624	1.3
tyr	phe-cys	9898.245	10266.454	3.7	10209.811	3.1
tyr	phe-his	11049.026	11464.520	3.8	11346.409	2.7
tyr	pro-glu	9095.122	8945.863	-1.6	8914.061	-2.0
tyr	thr-lys	9049.272	9270.934	2.5	9283.677	2.6
tyr	thr-val	8005.774	8194.129	2.4	8187.324	2.3
tyr	gln-asp	9252.924	9078.215	-1.9	9098.293	-1.7
tyr	trp-asn	11793.509	11896.047	0.9	11792.475	-0.0
tyr	trp-gln	12454.808	12550.603	0.8	12435.349	-0.2
tyr	tyr-ile	11180.423	11586.505	3.6	11465.041	2.5
tyr	val-ile	9039.914	9071.713	0.3	9027.005	-0.1
tyr	ala-gln-his	12299.998	12651.257	2.9	12647.508	2.8
tyr	asn-cys-ala	10594.624	10798.636	1.9	10868.036	2.6
tyr	asp-his-val	12966.155	13381.960	3.2	13355.409	3.0
tyr	cys-thr-lys	12478.753	12896.041	3.3	12941.538	3.7
tyr	gln-trp-ile	16959.452	17131.104	1.0	16974.815	0.1
tyr	gly-pro-ser	8979.639	9368.113	4.3	9367.541	4.3
tyr	leu-arg-gly	12840.111	12620.947	-1.7	12636.086	-1.6
tyr	lys-met-asp	14276.772	14502.940	1.6	14528.470	1.8
tyr	thr-phe-met	14850.660	15278.482	2.9	15195.343	2.3
tyr	tyr-val-pro	14367.228	14724.156	2.5	14573.879	1.4
tyr	asn-phe-gly-ala	14826.142	15078.148	1.7	14994.268	1.1
tyr	cys-lys-phe-gly	16703.081	17164.614	2.8	17098.286	2.4
tyr	glu-his-arg-leu	20160.312	20203.972	0.2	20178.858	0.1
tyr	ile-gly-val-gln	15604.054	15613.105	0.1	15573.792	-0.2
tyr	leu-trp-asn-cys	19989.675	20168.525	0.9	20062.242	0.4
tyr	met-asp-cys-lys	17916.638	18194.918	1.6	18258.772	1.9
tyr	phe-ala-thr-val	16630.478	16820.174	1.1	16686.731	0.3
tyr	ser-ile-lys-phe	18636.777	19139.220	2.7	18996.391	1.9
tyr	thr-asn-pro-ile	18636.777	19139.220	2.7	18996.391	1.9
tyr	val-met-leu-tyr	20178.758	20513.539	1.7	20377.682	1.0
val	val	2906.120	2888.128	-0.6	2885.703	-0.7
val	ala-leu	5129.601	4993.301	-2.7	4986.815	-2.8
val	arg-met	7446.041	7184.133	-3.5	7185.816	-3.5
val	asn-ser	4779.976	4839.088	1.2	4849.752	1.5
val	asp-glu	6131.108	5813.800	-5.2	5831.566	-4.9
val	cys-arg	6522.739	6340.353	-2.8	6347.339	-2.7
val	gly-ala	3352.014	3305.740	-1.4	3309.860	-1.3
val	gly-lys	4905.572	4850.729	-1.1	4846.616	-1.2
val	his-pro	5723.689	5950.175	4.0	5942.900	3.8
val	leu-ser	5287.742	5265.258	-0.4	5264.074	-0.5
val	met-tyr	7765.106	7705.590	-0.8	7707.484	-0.7
val	phe-cys	6524.752	6589.853	1.0	6591.747	1.0
val	phe-his	7287.183	7370.410	1.1	7355.572	0.9
val	pro-glu	5992.253	5736.333	-4.3	5740.335	-4.2

**Table 2** (continued)

Peptide A	Peptide B	TDDFT	Pair-specific	$\Delta$ (%)	Species-specific	$\Delta$ (%)
val	thr-lys	5975.273	5966.466	-0.1	5962.352	-0.2
val	thr-val	5285.199	5265.258	-0.4	5264.074	-0.4
val	gln-asp	6097.164	5821.162	-4.5	5833.347	-4.3
val	trp-asn	7773.222	7642.367	-1.7	7632.830	-1.8
val	trp-gln	8209.846	8064.257	-1.8	8052.069	-1.9
val	tyr-ile	7375.190	7440.166	0.9	7427.129	0.7
val	val-ile	5967.227	5837.082	-2.2	5825.293	-2.4
val	ala-gln-his	8119.843	8140.177	0.2	8137.024	0.2
val	asn-cys-ala	6988.834	6937.729	-0.7	6953.960	-0.5
val	asp-his-val	8557.642	8599.260	0.5	8598.529	0.5
val	cys-thr-lys	8237.011	8292.509	0.7	8299.771	0.8
val	gln-trp-ile	11182.696	11013.211	-1.5	10991.659	-1.7
val	gly-pro-ser	5928.321	6015.651	1.5	6019.374	1.5
val	leu-arg-gly	8474.335	8135.547	-4.0	8124.048	-4.1
val	lys-met-asp	9419.066	9319.137	-1.1	9327.413	-1.0
val	thr-phe-met	9792.032	9810.763	0.2	9808.595	0.2
val	tyr-val-pro	9474.342	9456.230	-0.2	9440.146	-0.4
val	asn-phe-gly-ala	9777.538	9686.714	-0.9	9680.056	-1.0
val	cys-lys-phe-gly	11017.566	11034.962	0.2	11028.963	0.1
val	glu-his-arg-leu	13304.008	13007.177	-2.2	12993.478	-2.3
val	ile-gly-val-gln	10296.954	10043.149	-2.5	10032.434	-2.6
val	leu-trp-asn-cys	13176.880	12961.918	-1.6	12953.886	-1.7
val	met-asp-cys-lys	11816.550	11689.735	-1.1	11708.879	-0.9
val	phe-ala-thr-val	10967.182	10806.731	-1.5	10790.875	-1.6
val	ser-ile-lys-phe	12298.245	12307.166	0.1	12283.584	-0.1
val	thr-asn-pro-ile	12298.245	12307.166	0.1	12283.584	-0.1
val	val-met-leu-tyr	13306.457	13181.607	-0.9	13167.424	-1.0
ala-leu	ala-leu	9056.734	8631.403	-4.7	8610.987	-4.9
ala-leu	arg-met	13149.330	12416.580	-5.6	12415.895	-5.6
ala-leu	asn-ser	8437.403	8364.421	-0.9	8400.225	-0.4
ala-leu	asp-glu	10831.856	10051.227	-7.2	10101.833	-6.7
ala-leu	cys-arg	11518.005	10957.868	-4.9	10974.859	-4.7
ala-leu	gly-ala	5917.338	5713.980	-3.4	5728.915	-3.2
ala-leu	gly-lys	8659.430	8383.864	-3.2	8375.320	-3.3
ala-leu	his-pro	10102.633	10279.782	1.8	10251.970	1.5
ala-leu	leu-ser	9334.572	9102.454	-2.5	9099.161	-2.5
ala-leu	met-tyr	13718.369	13320.659	-2.9	13303.168	-3.0
ala-leu	phe-cys	11525.756	11390.896	-1.2	11373.958	-1.3
ala-leu	phe-his	12869.474	12732.824	-1.1	12672.189	-1.5
ala-leu	pro-glu	10586.588	9915.877	-6.3	9922.977	-6.3
ala-leu	thr-lys	10547.691	10313.627	-2.2	10304.531	-2.3
ala-leu	thr-val	9330.311	9102.454	-2.4	9099.161	-2.5
ala-leu	gln-asp	10771.158	10061.993	-6.6	10098.510	-6.2
ala-leu	trp-asn	13731.285	13203.875	-3.8	13160.364	-4.2
ala-leu	trp-gln	14502.129	13933.231	-3.9	13880.882	-4.3
ala-leu	tyr-ile	13024.111	12859.414	-1.3	12806.465	-1.7
ala-leu	val-ile	10535.069	10090.114	-4.2	10052.022	-4.6
ala-leu	ala-gln-his	14334.544	14063.999	-1.9	14051.674	-2.0
ala-leu	asn-cys-ala	12341.745	11992.716	-2.8	12032.925	-2.5
ala-leu	asp-his-val	15108.827	14859.985	-1.6	14852.491	-1.7
ala-leu	cys-thr-lys	14542.331	14335.576	-1.4	14348.430	-1.3
ala-leu	gln-trp-ile	19751.082	19030.043	-3.6	18946.089	-4.1
ala-leu	gly-pro-ser	10465.355	10397.694	-0.7	10407.828	-0.6

**Table 2** (continued)

Peptide A	Peptide B	TDDFT	Pair-specific	$\Delta$ (%)	Species-specific	$\Delta$ (%)
ala-leu	leu-arg-gly	14962.027	14057.328	-6.0	14025.352	-6.3
ala-leu	lys-met-asp	16632.660	16110.545	-3.1	16123.689	-3.1
ala-leu	thr-phe-met	17295.257	16958.760	-1.9	16927.340	-2.1
ala-leu	tyr-val-pro	16733.139	16342.722	-2.3	16276.686	-2.7
ala-leu	asn-phe-gly-ala	17268.057	16738.465	-3.1	16706.143	-3.2
ala-leu	cys-lys-phe-gly	19456.920	19071.519	-2.0	19030.176	-2.2
ala-leu	glu-his-arg-leu	23490.164	22473.978	-4.3	22428.411	-4.5
ala-leu	ile-gly-val-gln	18181.166	17357.639	-4.5	17321.947	-4.7
ala-leu	leu-trp-asn-cys	23276.128	22400.034	-3.8	22346.446	-4.0
ala-leu	met-asp-cys-lys	20869.147	20209.891	-3.2	20244.564	-3.0
ala-leu	phe-ala-thr-val	19369.513	18676.905	-3.6	18613.772	-3.9
ala-leu	ser-ile-lys-phe	21714.797	21269.393	-2.0	21183.202	-2.5
ala-leu	thr-asn-pro-ile	21714.797	21269.393	-2.0	21183.202	-2.5
ala-leu	val-met-leu-tyr	23501.834	22784.928	-3.0	22713.065	-3.4
arg-met	arg-met	19094.336	17866.635	-6.4	17699.399	-7.3
arg-met	asn-ser	12247.770	12017.028	-1.9	12042.673	-1.7
arg-met	asp-glu	15734.037	14421.555	-8.3	14540.968	-7.6
arg-met	cys-arg	16724.540	15765.123	-5.7	15600.937	-6.7
arg-met	gly-ala	8590.230	8213.555	-4.4	8218.971	-4.3
arg-met	gly-lys	12570.502	12065.296	-4.0	12029.367	-4.3
arg-met	his-pro	14664.433	14775.074	0.8	14767.654	0.7
arg-met	leu-ser	13551.168	13089.118	-3.4	13107.980	-3.3
arg-met	met-tyr	19926.808	19136.239	-4.0	19122.224	-4.0
arg-met	phe-cys	16740.462	16362.188	-2.3	16331.678	-2.4
arg-met	phe-his	18688.610	18292.920	-2.1	18321.313	-2.0
arg-met	pro-glu	15377.794	14241.431	-7.4	14313.241	-6.9
arg-met	thr-lys	15311.599	14839.347	-3.1	14819.914	-3.2
arg-met	thr-val	13545.224	13089.118	-3.4	13107.980	-3.2
arg-met	gln-asp	15645.004	14448.490	-7.7	14511.586	-7.2
arg-met	trp-asn	19943.889	18965.459	-4.9	19013.398	-4.7
arg-met	trp-gln	21063.026	20016.215	-5.0	20062.629	-4.8
arg-met	tyr-ile	18912.345	18480.084	-2.3	18545.679	-1.9
arg-met	val-ile	15295.101	14518.092	-5.1	14514.357	-5.1
arg-met	ala-gln-his	20810.099	20214.579	-2.9	20196.079	-3.0
arg-met	asn-cys-ala	17921.371	17233.090	-3.8	17157.213	-4.3
arg-met	asp-his-val	21935.716	21352.597	-2.7	21381.902	-2.5
arg-met	cys-thr-lys	21112.895	20613.751	-2.4	20519.327	-2.8
arg-met	gln-trp-ile	28684.056	27350.173	-4.7	27391.169	-4.5
arg-met	gly-pro-ser	15192.639	14940.904	-1.7	14975.944	-1.4
arg-met	leu-arg-gly	21722.955	20227.218	-6.9	20147.260	-7.2
arg-met	lys-met-asp	24151.483	23159.409	-4.1	23095.452	-4.4
arg-met	thr-phe-met	25118.026	24368.685	-3.0	24352.303	-3.0
arg-met	tyr-val-pro	24300.487	23484.138	-3.4	23561.336	-3.0
arg-met	asn-phe-gly-ala	25076.633	24048.080	-4.1	24100.752	-3.9
arg-met	cys-lys-phe-gly	28254.156	27412.357	-3.0	27347.328	-3.2
arg-met	glu-his-arg-leu	34105.814	32315.504	-5.2	32260.960	-5.4
arg-met	ile-gly-val-gln	26398.062	24961.651	-5.4	24958.439	-5.5
arg-met	leu-trp-asn-cys	33806.626	32188.018	-4.8	32148.563	-4.9
arg-met	met-asp-cys-lys	30306.315	29048.010	-4.2	28902.077	-4.6
arg-met	phe-ala-thr-val	28128.908	26843.465	-4.6	26907.374	-4.3
arg-met	ser-ile-lys-phe	31528.685	30581.009	-3.0	30610.560	-2.9
arg-met	thr-asn-pro-ile	31528.685	30581.009	-3.0	30610.560	-2.9
arg-met	val-met-leu-tyr	34131.017	32753.400	-4.0	32730.075	-4.1

**Table 2** (continued)

Peptide A	Peptide B	TDDFT	Pair-specific	$\Delta$ (%)	Species-specific	$\Delta$ (%)
asn-ser	asn-ser	7863.380	8111.668	3.2	8047.765	2.3
asn-ser	asp-glu	10087.590	9766.149	-3.2	9683.498	-4.0
asn-ser	cys-arg	10729.186	10604.157	-1.2	10598.155	-1.2
asn-ser	gly-ala	5513.962	5538.679	0.5	5511.190	-0.1
asn-ser	gly-lys	8069.123	8117.239	0.6	8128.388	0.7
asn-ser	his-pro	9415.220	9961.835	5.8	10013.578	6.4
asn-ser	leu-ser	8697.714	8824.948	1.5	8830.844	1.5
asn-ser	met-tyr	12773.457	12925.515	1.2	12996.002	1.7
asn-ser	phe-cys	10732.718	11052.118	3.0	11120.866	3.6
asn-ser	phe-his	11987.682	12347.199	3.0	12463.409	4.0
asn-ser	pro-glu	9859.251	9624.928	-2.4	9617.719	-2.5
asn-ser	thr-lys	9828.719	9990.636	1.6	10003.524	1.8
asn-ser	thr-val	8693.677	8824.948	1.5	8830.844	1.6
asn-ser	gln-asp	10032.226	9764.876	-2.7	9703.299	-3.3
asn-ser	trp-asn	12787.932	12807.726	0.1	12894.028	0.8
asn-ser	trp-gln	13505.874	13514.161	0.1	13616.287	0.8
asn-ser	tyr-ile	12131.773	12476.390	2.8	12578.791	3.7
asn-ser	val-ile	9814.778	9777.292	-0.4	9844.743	0.3
asn-ser	ala-gln-his	13356.995	13627.116	2.0	13649.632	2.2
asn-ser	asn-cys-ala	11496.425	11625.600	1.1	11584.830	0.8
asn-ser	asp-his-val	14077.299	14408.222	2.4	14425.289	2.5
asn-ser	cys-thr-lys	13548.617	13891.699	2.5	13898.007	2.6
asn-ser	gln-trp-ile	18395.735	18452.365	0.3	18611.277	1.2
asn-ser	gly-pro-ser	9752.080	10084.181	3.4	10068.140	3.2
asn-ser	leu-arg-gly	13939.580	13606.968	-2.4	13658.217	-2.0
asn-ser	lys-met-asp	15493.241	15618.304	0.8	15626.743	0.9
asn-ser	thr-phe-met	16107.224	16450.848	2.1	16546.475	2.7
asn-ser	tyr-val-pro	15585.312	15854.930	1.7	15982.863	2.5
asn-ser	asn-phe-gly-ala	16084.653	16233.943	0.9	16299.263	1.3
asn-ser	cys-lys-phe-gly	18122.893	18488.641	2.0	18599.032	2.6
asn-ser	glu-his-arg-leu	21884.504	21770.075	-0.5	21850.057	-0.2
asn-ser	ile-gly-val-gln	16937.519	16821.113	-0.7	16884.868	-0.3
asn-ser	leu-trp-asn-cys	21676.143	21720.388	0.2	21856.702	0.8
asn-ser	met-asp-cys-lys	19436.761	19592.762	0.8	19594.426	0.8
asn-ser	phe-ala-thr-val	18040.892	18114.185	0.4	18235.220	1.1
asn-ser	ser-ile-lys-phe	20229.388	20619.348	1.9	20779.217	2.7
asn-ser	thr-asn-pro-ile	20229.388	20619.348	1.9	20779.217	2.7
asn-ser	val-met-leu-tyr	21887.786	22095.488	0.9	22263.725	1.7
asp-glu	asp-glu	12978.087	11786.336	-9.2	11614.518	-10.5
asp-glu	cys-arg	13780.109	12727.255	-7.6	12806.888	-7.1
asp-glu	gly-ala	7075.408	6662.626	-5.8	6633.673	-6.2
asp-glu	gly-lys	10352.457	9745.745	-5.9	9794.195	-5.4
asp-glu	his-pro	12076.022	11984.733	-0.8	12051.613	-0.2
asp-glu	leu-ser	11160.885	10611.624	-4.9	10615.470	-4.9
asp-glu	met-tyr	16431.119	15560.745	-5.3	15616.278	-5.0
asp-glu	phe-cys	13800.756	13306.048	-3.6	13368.561	-3.1
asp-glu	phe-his	15403.135	14866.854	-3.5	14977.911	-2.8
asp-glu	pro-glu	12685.397	11597.105	-8.6	11544.595	-9.0
asp-glu	thr-lys	12610.014	12000.443	-4.8	12041.912	-4.5
asp-glu	thr-val	11156.661	10611.624	-4.9	10615.470	-4.8
asp-glu	gln-asp	12904.818	11767.607	-8.8	11660.283	-9.6
asp-glu	trp-asn	16444.899	15427.251	-6.2	15491.548	-5.8
asp-glu	trp-gln	17366.254	16274.402	-6.3	16358.588	-5.8

**Table 2** (continued)

Peptide A	Peptide B	TDDFT	Pair-specific	$\Delta$ (%)	Species-specific	$\Delta$ (%)
asp-glu	tyr-ile	15584.958	15019.220	-3.6	15095.227	-3.1
asp-glu	val-ile	12597.804	11745.527	-6.8	11835.914	-6.0
asp-glu	ala-gln-his	17141.522	16392.661	-4.4	16437.569	-4.1
asp-glu	asn-cys-ala	14768.424	13984.704	-5.3	13961.179	-5.5
asp-glu	asp-his-val	18071.329	17342.953	-4.0	17349.154	-4.0
asp-glu	cys-thr-lys	17390.535	16694.981	-4.0	16742.920	-3.7
asp-glu	gln-trp-ile	23644.393	22206.129	-6.1	22362.936	-5.4
asp-glu	gly-pro-ser	12514.002	12138.774	-3.0	12103.997	-3.3
asp-glu	leu-arg-gly	17895.323	16338.743	-8.7	16465.795	-8.0
asp-glu	lys-met-asp	19899.769	18780.852	-5.6	18810.016	-5.5
asp-glu	thr-phe-met	20703.920	19798.172	-4.4	19886.546	-4.0
asp-glu	tyr-val-pro	20029.666	19087.820	-4.7	19184.874	-4.2
asp-glu	asn-phe-gly-ala	20669.360	19546.751	-5.4	19589.033	-5.2
asp-glu	cys-lys-phe-gly	23283.458	22238.156	-4.5	22378.188	-3.9
asp-glu	glu-his-arg-leu	28098.922	26171.920	-6.9	26314.236	-6.3
asp-glu	ile-gly-val-gln	21748.443	20222.057	-7.0	20311.517	-6.6
asp-glu	leu-trp-asn-cys	27871.661	26137.930	-6.2	26287.214	-5.7
asp-glu	met-asp-cys-lys	24975.878	23559.804	-5.7	23601.334	-5.5
asp-glu	phe-ala-thr-val	23184.535	21799.773	-6.0	21901.683	-5.5
asp-glu	ser-ile-lys-phe	25975.328	24798.479	-4.5	24971.894	-3.9
asp-glu	thr-asn-pro-ile	25975.328	24798.479	-4.5	24971.894	-3.9
asp-glu	val-met-leu-tyr	28130.951	26577.049	-5.5	26757.934	-4.9
cys-arg	cys-arg	14649.168	13910.168	-5.0	13733.335	-6.2
cys-arg	gly-ala	7524.907	7247.958	-3.7	7239.654	-3.8
cys-arg	gly-lys	11011.640	10646.941	-3.3	10615.942	-3.6
cys-arg	his-pro	12846.301	13037.317	1.5	13055.060	1.6
cys-arg	leu-ser	11870.504	11551.506	-2.7	11573.442	-2.5
cys-arg	met-tyr	17451.878	16888.099	-3.2	16901.404	-3.1
cys-arg	phe-cys	14661.681	14439.506	-1.5	14435.219	-1.5
cys-arg	phe-his	16369.128	16142.063	-1.4	16227.963	-0.9
cys-arg	pro-glu	13468.080	12568.318	-6.7	12637.241	-6.2
cys-arg	thr-lys	13412.824	13095.534	-2.4	13082.127	-2.5
cys-arg	thr-val	11865.241	11551.506	-2.6	11573.442	-2.5
cys-arg	gln-asp	13702.449	12750.168	-7.0	12783.189	-6.7
cys-arg	trp-asn	17467.519	16735.701	-4.2	16826.546	-3.7
cys-arg	trp-gln	18447.794	17663.178	-4.2	17760.347	-3.7
cys-arg	tyr-ile	16565.258	16309.486	-1.5	16426.514	-0.8
cys-arg	val-ile	13397.701	12812.824	-4.4	12842.462	-4.1
cys-arg	ala-gln-his	18229.152	17836.683	-2.1	17828.529	-2.2
cys-arg	asn-cys-ala	15697.333	15206.649	-3.1	15101.983	-3.8
cys-arg	asp-his-val	19214.696	18842.108	-1.9	18879.746	-1.7
cys-arg	cys-thr-lys	18493.879	18190.803	-1.6	18090.821	-2.2
cys-arg	gln-trp-ile	25123.293	24135.649	-3.9	24255.470	-3.5
cys-arg	gly-pro-ser	13308.524	13184.868	-0.9	13212.125	-0.7
cys-arg	leu-arg-gly	19028.114	17848.209	-6.2	17792.248	-6.5
cys-arg	lys-met-asp	21154.390	20437.674	-3.4	20369.572	-3.7
cys-arg	thr-phe-met	21999.669	21505.615	-2.2	21528.924	-2.1
cys-arg	tyr-val-pro	21284.081	20725.280	-2.6	20866.601	-2.0
cys-arg	asn-phe-gly-ala	21964.186	21221.098	-3.4	21306.282	-3.0
cys-arg	cys-lys-phe-gly	24747.445	24190.228	-2.2	24171.427	-2.3
cys-arg	glu-his-arg-leu	29874.549	28514.882	-4.5	28498.539	-4.6
cys-arg	ile-gly-val-gln	23122.819	22027.984	-4.7	22056.018	-4.6
cys-arg	leu-trp-asn-cys	29608.944	28404.301	-4.1	28424.080	-4.0

**Table 2** (continued)

Peptide A	Peptide B	TDDFT	Pair-specific	$\Delta$ (%)	Species-specific	$\Delta$ (%)
cys-arg	met-asp-cys-lys	26544.413	25633.804	-3.4	25471.983	-4.0
cys-arg	phe-ala-thr-val	24637.335	23689.562	-3.9	23813.953	-3.3
cys-arg	ser-ile-lys-phe	27616.870	26987.685	-2.3	27096.524	-1.9
cys-arg	thr-asn-pro-ile	27616.870	26987.685	-2.3	27096.524	-1.9
cys-arg	val-met-leu-tyr	29893.921	28905.564	-3.3	28957.849	-3.1
gly-ala	gly-ala	3866.724	3782.786	-2.2	3770.281	-2.5
gly-ala	gly-lys	5658.568	5547.154	-2.0	5548.470	-1.9
gly-ala	his-pro	6602.185	6804.268	3.1	6826.782	3.4
gly-ala	leu-ser	6099.515	6027.230	-1.2	6030.086	-1.1
gly-ala	met-tyr	8959.994	8824.380	-1.5	8861.527	-1.1
gly-ala	phe-cys	7528.316	7545.533	0.2	7581.039	0.7
gly-ala	phe-his	8407.596	8431.109	0.3	8485.490	0.9
gly-ala	pro-glu	6915.168	6569.651	-5.0	6570.977	-5.0
gly-ala	thr-lys	6892.487	6826.001	-1.0	6828.958	-0.9
gly-ala	thr-val	6096.691	6027.230	-1.1	6030.086	-1.1
gly-ala	gln-asp	7036.217	6665.349	-5.3	6641.715	-5.6
gly-ala	trp-asn	8969.459	8744.359	-2.5	8786.661	-2.0
gly-ala	trp-gln	9473.029	9227.158	-2.6	9276.319	-2.1
gly-ala	tyr-ile	8508.676	8518.217	0.1	8568.135	0.7
gly-ala	val-ile	6883.304	6679.577	-3.0	6708.232	-2.5
gly-ala	ala-gln-his	9366.818	9308.207	-0.6	9316.575	-0.5
gly-ala	asn-cys-ala	8063.007	7939.833	-1.5	7922.466	-1.7
gly-ala	asp-his-val	9872.237	9839.008	-0.3	9848.179	-0.2
gly-ala	cys-thr-lys	9501.759	9489.679	-0.1	9491.417	-0.1
gly-ala	gln-trp-ile	12902.431	12600.995	-2.3	12674.691	-1.8
gly-ala	gly-pro-ser	6838.697	6885.624	0.7	6880.190	0.6
gly-ala	leu-arg-gly	9775.928	9299.310	-4.9	9315.330	-4.7
gly-ala	lys-met-asp	10866.262	10667.075	-1.8	10671.929	-1.8
gly-ala	thr-phe-met	11297.673	11232.620	-0.6	11280.582	-0.1
gly-ala	tyr-val-pro	10931.151	10825.006	-1.0	10887.215	-0.4
gly-ala	asn-phe-gly-ala	11281.076	11084.502	-1.7	11117.204	-1.4
gly-ala	cys-lys-phe-gly	12710.845	12627.261	-0.7	12678.375	-0.3
gly-ala	glu-his-arg-leu	15347.849	14872.734	-3.1	14903.569	-2.9
gly-ala	ile-gly-val-gln	11878.722	11490.305	-3.3	11517.105	-3.0
gly-ala	leu-trp-asn-cys	15203.961	14832.600	-2.4	14897.480	-2.0
gly-ala	met-asp-cys-lys	13632.776	13381.478	-1.8	13384.376	-1.8
gly-ala	phe-ala-thr-val	12653.437	12369.101	-2.2	12426.929	-1.8
gly-ala	ser-ile-lys-phe	14187.401	14082.744	-0.7	14155.130	-0.2
gly-ala	thr-asn-pro-ile	14187.401	14082.744	-0.7	14155.130	-0.2
gly-ala	val-met-leu-tyr	15352.113	15089.256	-1.7	15168.613	-1.2
gly-lys	gly-lys	8280.944	8145.476	-1.6	8125.662	-1.9
gly-lys	his-pro	9661.911	9978.238	3.3	9970.054	3.2
gly-lys	leu-ser	8926.167	8839.168	-1.0	8839.959	-1.0
gly-lys	met-tyr	13110.594	12929.542	-1.4	12949.858	-1.2
gly-lys	phe-cys	11015.982	11055.883	0.4	11071.794	0.5
gly-lys	phe-his	12302.853	12355.613	0.4	12357.223	0.4
gly-lys	pro-glu	10118.123	9620.870	-4.9	9644.910	-4.7
gly-lys	thr-lys	10086.693	10019.135	-0.7	10003.727	-0.8
gly-lys	thr-val	8921.971	8839.168	-0.9	8839.959	-0.9
gly-lys	gln-asp	10295.193	9761.230	-5.2	9786.611	-4.9
gly-lys	trp-asn	13124.368	12810.917	-2.4	12821.862	-2.3
gly-lys	trp-gln	13861.356	13520.094	-2.5	13528.574	-2.4
gly-lys	tyr-ile	12451.051	12481.786	0.2	12493.993	0.3

**Table 2** (continued)

Peptide A	Peptide B	TDDFT	Pair-specific	$\Delta$ (%)	Species-specific	$\Delta$ (%)
gly-lys	val-ile	10073.213	9802.219	-2.7	9788.745	-2.8
gly-lys	ala-gln-his	13707.336	13651.733	-0.4	13640.459	-0.5
gly-lys	asn-cys-ala	11798.820	11642.826	-1.3	11648.317	-1.3
gly-lys	asp-his-val	14446.731	14421.982	-0.2	14428.036	-0.1
gly-lys	cys-thr-lys	13904.974	13923.470	0.1	13915.015	0.1
gly-lys	gln-trp-ile	18879.942	18471.585	-2.2	18470.703	-2.2
gly-lys	gly-pro-ser	10007.731	10091.659	0.8	10101.965	0.9
gly-lys	leu-arg-gly	14305.942	13655.765	-4.5	13615.501	-4.8
gly-lys	lys-met-asp	15901.222	15644.018	-1.6	15646.519	-1.6
gly-lys	thr-phe-met	16531.860	16462.677	-0.4	16478.562	-0.3
gly-lys	tyr-val-pro	15995.521	15861.810	-0.8	15876.136	-0.8
gly-lys	asn-phe-gly-ala	16507.458	16243.291	-1.6	16255.053	-1.5
gly-lys	cys-lys-phe-gly	18600.233	18516.387	-0.5	18512.976	-0.5
gly-lys	glu-his-arg-leu	22459.519	21821.415	-2.8	21788.354	-3.0
gly-lys	ile-gly-val-gln	17382.999	16855.738	-3.0	16841.294	-3.1
gly-lys	leu-trp-asn-cys	22247.329	21743.298	-2.3	21748.560	-2.2
gly-lys	met-asp-cys-lys	19949.224	19624.909	-1.6	19631.088	-1.6
gly-lys	phe-ala-thr-val	18515.782	18129.702	-2.1	18137.976	-2.0
gly-lys	ser-ile-lys-phe	20761.504	20651.467	-0.5	20641.888	-0.6
gly-lys	thr-asn-pro-ile	20761.504	20651.467	-0.5	20641.888	-0.6
gly-lys	val-met-leu-tyr	22464.960	22123.345	-1.5	22127.403	-1.5
his-pro	his-pro	11273.746	12222.346	8.4	12177.263	8.0
his-pro	leu-ser	10414.488	10845.499	4.1	10842.290	4.1
his-pro	met-tyr	15292.453	15873.477	3.8	15829.299	3.5
his-pro	phe-cys	12849.661	13570.003	5.6	13526.385	5.3
his-pro	phe-his	14352.410	15139.943	5.5	15040.813	4.8
his-pro	pro-glu	11802.788	11815.163	0.1	11820.876	0.1
his-pro	thr-lys	11768.821	12281.712	4.4	12272.968	4.3
his-pro	thr-val	10409.556	10845.499	4.2	10842.290	4.2
his-pro	gln-asp	12009.789	11986.350	-0.2	12035.673	0.2
his-pro	trp-asn	15309.589	15705.660	2.6	15631.133	2.1
his-pro	trp-gln	16169.331	16574.538	2.5	16487.431	2.0
his-pro	tyr-ile	14525.361	15314.879	5.4	15231.223	4.9
his-pro	val-ile	11752.133	12017.538	2.3	11964.564	1.8
his-pro	ala-gln-his	15992.996	16723.140	4.6	16701.130	4.4
his-pro	asn-cys-ala	13764.552	14284.322	3.8	14330.404	4.1
his-pro	asp-his-val	16855.135	17683.387	4.9	17666.973	4.8
his-pro	cys-thr-lys	16222.748	17076.930	5.3	17086.508	5.3
his-pro	gln-trp-ile	22024.273	22641.902	2.8	22509.095	2.2
his-pro	gly-pro-ser	11676.681	12382.498	6.0	12395.257	6.2
his-pro	leu-arg-gly	16690.493	16715.341	0.1	16672.448	-0.1
his-pro	lys-met-asp	18550.394	19194.431	3.5	19202.210	3.5
his-pro	thr-phe-met	19284.607	20203.083	4.8	20138.369	4.4
his-pro	tyr-val-pro	18659.674	19458.514	4.3	19353.080	3.7
his-pro	asn-phe-gly-ala	19257.325	19918.078	3.4	19861.439	3.1
his-pro	cys-lys-phe-gly	21698.550	22703.565	4.6	22625.299	4.3
his-pro	glu-his-arg-leu	26202.891	26725.581	2.0	26656.342	1.7
his-pro	ile-gly-val-gln	20279.885	20661.967	1.9	20610.289	1.6
his-pro	leu-trp-asn-cys	25951.202	26661.227	2.7	26559.944	2.4
his-pro	met-asp-cys-lys	23271.539	24082.635	3.5	24109.357	3.6
his-pro	phe-ala-thr-val	21599.714	22236.336	3.0	22136.769	2.5
his-pro	ser-ile-lys-phe	24221.424	25317.320	4.5	25186.434	4.0
his-pro	thr-asn-pro-ile	24221.424	25317.320	4.5	25186.434	4.0

**Table 2** (continued)

Peptide A	Peptide B	TDDFT	Pair-specific	$\Delta$ (%)	Species-specific	$\Delta$ (%)
his-pro	val-met-leu-tyr	26205.826	27139.326	3.6	27016.331	3.1
leu-ser	leu-ser	9621.787	9600.588	-0.2	9599.370	-0.2
leu-ser	met-tyr	14134.558	14054.864	-0.6	14062.779	-0.5
leu-ser	phe-cys	11876.096	12019.119	1.2	12028.033	1.3
leu-ser	phe-his	13262.685	13437.358	1.3	13426.841	1.2
leu-ser	pro-glu	10908.176	10464.723	-4.1	10463.076	-4.1
leu-ser	thr-lys	10872.608	10874.914	0.0	10874.705	0.0
leu-ser	thr-val	9617.301	9600.588	-0.2	9599.370	-0.2
leu-ser	gln-asp	11098.902	10619.011	-4.3	10623.328	-4.3
leu-ser	trp-asn	14148.997	13935.491	-1.5	13927.049	-1.6
leu-ser	trp-gln	14943.455	14704.297	-1.6	14694.318	-1.7
leu-ser	tyr-ile	13422.325	13568.937	1.1	13556.950	1.0
leu-ser	val-ile	10858.485	10640.066	-2.0	10633.699	-2.1
leu-ser	ala-gln-his	14775.584	14836.982	0.4	14837.630	0.4
leu-ser	asn-cys-ala	12719.195	12649.937	-0.5	12671.553	-0.4
leu-ser	asp-his-val	15572.903	15678.962	0.7	15677.795	0.7
leu-ser	cys-thr-lys	14988.917	15117.477	0.9	15134.868	1.0
leu-ser	gln-trp-ile	20353.346	20079.106	-1.4	20063.944	-1.4
leu-ser	gly-pro-ser	10787.573	10970.244	1.7	10971.143	1.7
leu-ser	leu-arg-gly	15421.250	14822.214	-3.9	14821.946	-3.9
leu-ser	lys-met-asp	17141.519	16992.101	-0.9	17008.106	-0.8
leu-ser	thr-phe-met	17822.183	17892.061	0.4	17897.867	0.4
leu-ser	tyr-val-pro	17243.699	17245.011	0.0	17230.529	-0.1
leu-ser	asn-phe-gly-ala	17795.427	17663.137	-0.7	17656.585	-0.8
leu-ser	cys-lys-phe-gly	20051.361	20118.471	0.3	20125.521	0.4
leu-ser	glu-his-arg-leu	24210.678	23705.140	-2.1	23702.387	-2.1
leu-ser	ile-gly-val-gln	18738.471	18307.624	-2.3	18302.618	-2.3
leu-ser	leu-trp-asn-cys	23984.178	23633.423	-1.5	23637.592	-1.4
leu-ser	met-asp-cys-lys	21505.912	21315.225	-0.9	21349.023	-0.7
leu-ser	phe-ala-thr-val	19960.598	19705.717	-1.3	19692.588	-1.3
leu-ser	ser-ile-lys-phe	22380.410	22437.095	0.2	22421.707	0.2
leu-ser	thr-asn-pro-ile	22380.410	22437.095	0.2	22421.707	0.2
leu-ser	val-met-leu-tyr	24218.211	24035.675	-0.8	24034.761	-0.8
met-tyr	met-tyr	20808.338	20579.304	-1.1	20458.211	-1.7
met-tyr	phe-cys	17477.967	17596.959	0.7	17477.780	-0.0
met-tyr	phe-his	19505.245	19673.019	0.9	19545.607	0.2
met-tyr	pro-glu	16059.469	15332.526	-4.5	15328.355	-4.5
met-tyr	thr-lys	15969.484	15911.887	-0.4	15930.289	-0.2
met-tyr	thr-val	14128.915	14054.864	-0.5	14062.779	-0.5
met-tyr	gln-asp	16336.782	15559.492	-4.8	15613.767	-4.4
met-tyr	trp-asn	20823.292	20407.225	-2.0	20305.217	-2.5
met-tyr	trp-gln	21990.677	21531.294	-2.1	21415.628	-2.6
met-tyr	tyr-ile	19736.819	19870.301	0.7	19758.129	0.1
met-tyr	val-ile	15955.644	15568.798	-2.4	15523.989	-2.7
met-tyr	ala-gln-his	21707.077	21715.512	0.0	21710.395	0.0
met-tyr	asn-cys-ala	18702.455	18515.382	-1.0	18532.158	-0.9
met-tyr	asp-his-val	22884.396	22956.957	0.3	22944.205	0.3
met-tyr	cys-thr-lys	22024.769	22119.836	0.4	22105.167	0.4
met-tyr	gln-trp-ile	29941.841	29394.503	-1.8	29232.133	-2.4
met-tyr	gly-pro-ser	15846.769	16065.479	1.4	16085.455	1.5
met-tyr	leu-arg-gly	22662.907	21678.042	-4.3	21676.118	-4.3
met-tyr	lys-met-asp	25202.352	24869.936	-1.3	24843.820	-1.4
met-tyr	thr-phe-met	26220.069	26194.373	-0.1	26053.896	-0.6

**Table 2** (continued)

Peptide A	Peptide B	TDDFT	Pair-specific	$\Delta$ (%)	Species-specific	$\Delta$ (%)
met-tyr	tyr-val-pro	25364.628	25253.124	-0.4	25112.036	-1.0
met-tyr	asn-phe-gly-ala	26173.575	25864.675	-1.2	25791.880	-1.5
met-tyr	cys-lys-phe-gly	29487.122	29443.927	-0.1	29305.360	-0.6
met-tyr	glu-his-arg-leu	35583.969	34686.549	-2.5	34648.386	-2.6
met-tyr	ile-gly-val-gln	27542.919	26793.657	-2.7	26758.992	-2.9
met-tyr	leu-trp-asn-cys	35295.455	34594.505	-2.0	34417.489	-2.5
met-tyr	met-asp-cys-lys	31631.458	31194.008	-1.4	31139.587	-1.6
met-tyr	phe-ala-thr-val	29360.160	28852.299	-1.7	28728.678	-2.1
met-tyr	ser-ile-lys-phe	32896.035	32841.339	-0.2	32696.120	-0.6
met-tyr	thr-asn-pro-ile	32896.035	32841.339	-0.2	32696.120	-0.6
met-tyr	val-met-leu-tyr	35626.614	35181.651	-1.2	34980.811	-1.8
phe-cys	phe-cys	14681.392	15046.055	2.5	14927.246	1.7
phe-cys	phe-his	16385.692	16817.628	2.6	16697.605	1.9
phe-cys	pro-glu	13488.355	13110.567	-2.8	13112.256	-2.8
phe-cys	thr-lys	13418.105	13606.787	1.4	13622.328	1.5
phe-cys	thr-val	11871.201	12019.119	1.2	12028.033	1.3
phe-cys	gln-asp	13721.671	13304.153	-3.0	13360.551	-2.6
phe-cys	trp-asn	17491.010	17445.850	-0.3	17351.680	-0.8
phe-cys	trp-gln	18471.893	18407.191	-0.3	18299.910	-0.9
phe-cys	tyr-ile	16580.775	16990.179	2.5	16888.480	1.9
phe-cys	val-ile	13405.812	13313.578	-0.7	13270.417	-1.0
phe-cys	ala-gln-his	18238.293	18564.632	1.8	18556.890	1.8
phe-cys	asn-cys-ala	15711.846	15831.719	0.8	15838.301	0.8
phe-cys	asp-his-val	19226.727	19627.491	2.1	19616.745	2.0
phe-cys	cys-thr-lys	18504.956	18914.987	2.2	18890.222	2.1
phe-cys	gln-trp-ile	25152.136	25130.916	-0.1	24978.579	-0.7
phe-cys	gly-pro-ser	13314.604	13736.894	3.2	13758.322	3.3
phe-cys	leu-arg-gly	19040.626	18534.148	-2.7	18524.512	-2.7
phe-cys	lys-met-asp	21172.903	21266.645	0.4	21233.523	0.3
phe-cys	thr-phe-met	22025.726	22398.003	1.7	22259.990	1.1
phe-cys	tyr-val-pro	21307.477	21591.977	1.3	21463.457	0.7
phe-cys	asn-phe-gly-ala	21987.239	22113.021	0.6	22046.969	0.3
phe-cys	cys-lys-phe-gly	24771.727	25174.847	1.6	25034.115	1.1
phe-cys	glu-his-arg-leu	29895.855	29654.765	-0.8	29611.989	-0.9
phe-cys	ile-gly-val-gln	23140.072	22910.005	-1.0	22875.899	-1.1
phe-cys	leu-trp-asn-cys	29647.898	29577.399	-0.2	29401.860	-0.8
phe-cys	met-asp-cys-lys	26572.626	26674.468	0.4	26605.034	0.1
phe-cys	phe-ala-thr-val	24664.072	24669.585	0.0	24556.441	-0.4
phe-cys	ser-ile-lys-phe	27637.468	28080.312	1.6	27943.579	1.1
phe-cys	thr-asn-pro-ile	27637.468	28080.312	1.6	27943.579	1.1
phe-cys	val-met-leu-tyr	29928.017	30083.069	0.5	29886.889	-0.1
phe-his	phe-his	18292.808	18757.553	2.5	18514.627	1.2
phe-his	pro-glu	15054.768	14647.233	-2.7	14634.096	-2.8
phe-his	thr-lys	14985.650	15211.004	1.5	15205.224	1.5
phe-his	thr-val	13257.057	13437.358	1.4	13426.841	1.3
phe-his	gln-asp	15316.471	14860.538	-3.0	14954.967	-2.4
phe-his	trp-asn	19522.795	19462.087	-0.3	19269.279	-1.3
phe-his	trp-gln	20617.874	20537.516	-0.4	20315.954	-1.5
phe-his	tyr-ile	18511.018	18977.791	2.5	18756.376	1.3
phe-his	val-ile	14969.123	14883.681	-0.6	14765.539	-1.4
phe-his	ala-gln-his	20367.896	20715.661	1.7	20678.302	1.5
phe-his	asn-cys-ala	17541.163	17700.307	0.9	17814.605	1.6
phe-his	asp-his-val	21469.975	21911.423	2.1	21866.734	1.9

**Table 2** (continued)

Peptide A	Peptide B	TDDFT	Pair-specific	$\Delta$ (%)	Species-specific	$\Delta$ (%)
phe-his	cys-thr-lys	20663.396	21154.628	2.4	21192.258	2.6
phe-his	gln-trp-ile	28076.748	28050.787	-0.1	27725.920	-1.2
phe-his	gly-pro-ser	14869.852	15345.450	3.2	15365.805	3.3
phe-his	leu-arg-gly	21261.166	20695.231	-2.7	20636.535	-2.9
phe-his	lys-met-asp	23638.196	23781.984	0.6	23802.631	0.7
phe-his	thr-phe-met	24585.443	25035.433	1.8	24862.224	1.1
phe-his	tyr-val-pro	23785.732	24112.170	1.4	23835.364	0.2
phe-his	asn-phe-gly-ala	24545.808	24681.640	0.6	24531.501	-0.1
phe-his	cys-lys-phe-gly	27654.304	28126.655	1.7	27943.733	1.1
phe-his	glu-his-arg-leu	33381.437	33100.117	-0.8	32971.105	-1.2
phe-his	ile-gly-val-gln	25836.984	25593.779	-0.9	25482.015	-1.4
phe-his	leu-trp-asn-cys	33091.289	33032.999	-0.2	32785.093	-0.9
phe-his	met-asp-cys-lys	29662.689	29839.625	0.6	29908.478	0.8
phe-his	phe-ala-thr-val	27532.837	27551.761	0.1	27296.260	-0.9
phe-his	ser-ile-lys-phe	30858.550	31362.247	1.6	31049.179	0.6
phe-his	thr-asn-pro-ile	30858.550	31362.247	1.6	31049.179	0.6
phe-his	val-met-leu-tyr	33406.818	33624.132	0.7	33318.865	-0.3
pro-glu	pro-glu	12401.794	11421.662	-7.9	11392.193	-8.1
pro-glu	thr-lys	12324.627	11842.830	-3.9	11861.009	-3.8
pro-glu	thr-val	10904.118	10464.723	-4.0	10463.076	-4.0
pro-glu	gln-asp	12615.272	11589.809	-8.1	11564.428	-8.3
pro-glu	trp-asn	16073.277	15196.079	-5.5	15174.196	-5.6
pro-glu	trp-gln	16973.660	16032.636	-5.5	16012.196	-5.7
pro-glu	tyr-ile	15232.328	14798.521	-2.9	14772.703	-3.0
pro-glu	val-ile	12312.511	11588.990	-5.9	11598.977	-5.8
pro-glu	ala-gln-his	16753.476	16162.854	-3.5	16175.754	-3.5
pro-glu	asn-cys-ala	14434.108	13789.631	-4.5	13815.914	-4.3
pro-glu	asp-his-val	17662.274	17092.400	-3.2	17083.717	-3.3
pro-glu	cys-thr-lys	16996.698	16470.686	-3.1	16509.507	-2.9
pro-glu	gln-trp-ile	23109.755	21885.294	-5.3	21870.838	-5.4
pro-glu	gly-pro-ser	12230.806	11963.212	-2.2	11952.125	-2.3
pro-glu	leu-arg-gly	17490.177	16128.164	-7.8	16174.434	-7.5
pro-glu	lys-met-asp	19449.142	18521.260	-4.8	18546.013	-4.6
pro-glu	thr-phe-met	20235.375	19512.071	-3.6	19510.998	-3.6
pro-glu	tyr-val-pro	19576.700	18806.680	-3.9	18775.752	-4.1
pro-glu	asn-phe-gly-ala	20201.761	19259.299	-4.7	19238.531	-4.8
pro-glu	cys-lys-phe-gly	22756.424	21925.513	-3.6	21947.677	-3.5
pro-glu	glu-his-arg-leu	27462.825	25814.357	-6.0	25849.174	-5.9
pro-glu	ile-gly-val-gln	21256.038	19944.840	-6.2	19956.904	-6.1
pro-glu	leu-trp-asn-cys	27241.323	25762.286	-5.4	25771.132	-5.4
pro-glu	met-asp-cys-lys	24410.302	23234.810	-4.8	23284.307	-4.6
pro-glu	phe-ala-thr-val	22660.013	21484.497	-5.2	21461.988	-5.3
pro-glu	ser-ile-lys-phe	25387.386	24450.024	-3.7	24446.124	-3.7
pro-glu	thr-asn-pro-ile	25387.386	24450.024	-3.7	24446.124	-3.7
pro-glu	val-met-leu-tyr	27494.413	26201.285	-4.7	26207.640	-4.7
thr-lys	thr-lys	12286.209	12324.235	0.3	12311.688	0.2
thr-lys	thr-val	10867.503	10874.914	0.1	10874.705	0.1
thr-lys	gln-asp	12540.317	12016.570	-4.2	12039.827	-4.0
thr-lys	trp-asn	15986.328	15772.291	-1.3	15775.399	-1.3
thr-lys	trp-gln	16884.010	16644.197	-1.4	16644.292	-1.4
thr-lys	tyr-ile	15166.134	15361.907	1.3	15363.642	1.3
thr-lys	val-ile	12269.746	12057.440	-1.7	12042.317	-1.9
thr-lys	ala-gln-his	16696.394	16802.613	0.6	16793.964	0.6

**Table 2** (continued)

Peptide A	Peptide B	TDDFT	Pair-specific	$\Delta$ (%)	Species-specific	$\Delta$ (%)
thr-lys	asn-cys-ala	14371.678	14326.489	-0.3	14342.175	-0.2
thr-lys	asp-his-val	17597.023	17751.448	0.9	17755.496	0.9
thr-lys	cys-thr-lys	16937.071	17128.320	1.1	17129.960	1.1
thr-lys	gln-trp-ile	22996.943	22735.171	-1.1	22724.257	-1.2
thr-lys	gly-pro-ser	12190.052	12420.244	1.9	12429.098	2.0
thr-lys	leu-arg-gly	17425.501	16799.659	-3.6	16767.106	-3.8
thr-lys	lys-met-asp	19368.615	19247.309	-0.6	19256.816	-0.6
thr-lys	thr-phe-met	20136.782	20259.048	0.6	20272.468	0.7
thr-lys	tyr-val-pro	19483.534	19522.957	0.2	19524.715	0.2
thr-lys	asn-phe-gly-ala	20107.127	19994.944	-0.6	19999.964	-0.5
thr-lys	cys-lys-phe-gly	22656.183	22785.467	0.6	22784.222	0.6
thr-lys	glu-his-arg-leu	27357.069	26853.200	-1.8	26824.751	-1.9
thr-lys	ile-gly-val-gln	21173.530	20739.390	-2.0	20724.387	-2.1
thr-lys	leu-trp-asn-cys	27098.608	26760.405	-1.2	26764.189	-1.2
thr-lys	met-asp-cys-lys	24299.300	24144.449	-0.6	24165.641	-0.6
thr-lys	phe-ala-thr-val	22553.355	22312.416	-1.1	22310.213	-1.1
thr-lys	ser-ile-lys-phe	25288.754	25412.494	0.5	25394.429	0.4
thr-lys	thr-asn-pro-ile	25288.754	25412.494	0.5	25394.429	0.4
thr-lys	val-met-leu-tyr	27363.635	27221.928	-0.5	27221.326	-0.5
thr-val	thr-val	9612.852	9600.588	-0.1	9599.370	-0.1
thr-val	gln-asp	11094.726	10619.011	-4.3	10623.328	-4.2
thr-val	trp-asn	14143.352	13935.491	-1.5	13927.049	-1.5
thr-val	trp-gln	14937.417	14704.297	-1.6	14694.318	-1.6
thr-val	tyr-ile	13416.493	13568.937	1.1	13556.950	1.1
thr-val	val-ile	10853.444	10640.066	-2.0	10633.699	-2.0
thr-val	ala-gln-his	14768.807	14836.982	0.5	14837.630	0.5
thr-val	asn-cys-ala	12713.668	12649.937	-0.5	12671.553	-0.3
thr-val	asp-his-val	15565.889	15678.962	0.7	15677.795	0.7
thr-val	cys-thr-lys	14982.008	15117.477	0.9	15134.868	1.0
thr-val	gln-trp-ile	20344.854	20079.106	-1.3	20063.944	-1.4
thr-val	gly-pro-ser	10782.610	10970.244	1.7	10971.143	1.8
thr-val	leu-arg-gly	15414.261	14822.214	-3.8	14821.946	-3.8
thr-val	lys-met-asp	17133.929	16992.101	-0.8	17008.106	-0.7
thr-val	thr-phe-met	17814.683	17892.061	0.4	17897.867	0.5
thr-val	tyr-val-pro	17236.437	17245.011	0.1	17230.529	-0.0
thr-val	asn-phe-gly-ala	17787.932	17663.137	-0.7	17656.585	-0.7
thr-val	cys-lys-phe-gly	20042.653	20118.471	0.4	20125.521	0.4
thr-val	glu-his-arg-leu	24199.840	23705.140	-2.0	23702.387	-2.1
thr-val	ile-gly-val-gln	18730.063	18307.624	-2.3	18302.618	-2.3
thr-val	leu-trp-asn-cys	23974.396	23633.423	-1.4	23637.592	-1.4
thr-val	met-asp-cys-lys	21496.622	21315.225	-0.8	21349.023	-0.7
thr-val	phe-ala-thr-val	19952.151	19705.717	-1.2	19692.588	-1.3
thr-val	ser-ile-lys-phe	22370.370	22437.095	0.3	22421.707	0.2
thr-val	thr-asn-pro-ile	22370.370	22437.095	0.3	22421.707	0.2
thr-val	val-met-leu-tyr	24207.915	24035.675	-0.7	24034.761	-0.7
gln-asp	gln-asp	12833.320	11758.988	-8.4	11687.765	-8.9
gln-asp	trp-asn	16351.644	15417.556	-5.7	15479.786	-5.3
gln-asp	trp-gln	17267.690	16266.717	-5.8	16343.985	-5.3
gln-asp	tyr-ile	15497.179	15017.368	-3.1	15091.853	-2.6
gln-asp	val-ile	12527.233	11760.315	-6.1	11826.907	-5.6
gln-asp	ala-gln-his	17046.550	16396.360	-3.8	16424.173	-3.6
gln-asp	asn-cys-ala	14685.227	13990.814	-4.7	13965.558	-4.9
gln-asp	asp-his-val	17970.794	17341.217	-3.5	17350.473	-3.5

**Table 2** (continued)

Peptide A	Peptide B	TDDFT	Pair-specific	$\Delta$ (%)	Species-specific	$\Delta$ (%)
gln-asp	cys-thr-lys	17293.321	16712.449	-3.4	16737.320	-3.2
gln-asp	gln-trp-ile	23510.672	22205.870	-5.5	22337.545	-5.0
gln-asp	gly-pro-ser	12444.887	12138.207	-2.5	12116.728	-2.6
gln-asp	leu-arg-gly	17795.360	16361.799	-8.1	16436.855	-7.6
gln-asp	lys-met-asp	19787.479	18793.636	-5.0	18811.369	-4.9
gln-asp	thr-phe-met	20586.097	19800.323	-3.8	19878.930	-3.4
gln-asp	tyr-val-pro	19916.504	19084.047	-4.2	19177.849	-3.7
gln-asp	asn-phe-gly-ala	20552.890	19540.396	-4.9	19584.736	-4.7
gln-asp	cys-lys-phe-gly	23151.811	22247.137	-3.9	22353.594	-3.5
gln-asp	glu-his-arg-leu	27941.841	26188.506	-6.3	26281.414	-5.9
gln-asp	ile-gly-val-gln	21626.480	20237.004	-6.4	20301.403	-6.1
gln-asp	leu-trp-asn-cys	27712.924	26139.664	-5.7	26260.423	-5.2
gln-asp	met-asp-cys-lys	24833.915	23576.591	-5.1	23598.446	-5.0
gln-asp	phe-ala-thr-val	23053.421	21800.709	-5.4	21893.781	-5.0
gln-asp	ser-ile-lys-phe	25829.760	24809.514	-4.0	24949.094	-3.4
gln-asp	thr-asn-pro-ile	25829.760	24809.514	-4.0	24949.094	-3.4
gln-asp	val-met-leu-tyr	27971.035	26588.638	-4.9	26736.688	-4.4
trp-asn	trp-asn	20840.416	20193.703	-3.1	20035.964	-3.9
trp-asn	trp-gln	22008.683	21308.582	-3.2	21129.390	-4.0
trp-asn	tyr-ile	19754.403	19687.314	-0.3	19506.861	-1.2
trp-asn	val-ile	15970.659	15433.633	-3.4	15347.216	-3.9
trp-asn	ala-gln-his	21729.798	21488.644	-1.1	21464.257	-1.2
trp-asn	asn-cys-ala	18719.311	18357.529	-1.9	18453.233	-1.4
trp-asn	asp-his-val	22907.529	22730.401	-0.8	22692.038	-0.9
trp-asn	cys-thr-lys	22046.037	21936.529	-0.5	21978.696	-0.3
trp-asn	gln-trp-ile	29967.247	29099.849	-2.9	28843.775	-3.8
trp-asn	gly-pro-ser	15863.703	15918.000	0.3	15929.119	0.4
trp-asn	leu-arg-gly	22684.941	21460.117	-5.4	21433.130	-5.5
trp-asn	lys-met-asp	25224.669	24663.540	-2.2	24687.047	-2.1
trp-asn	thr-phe-met	26241.128	25968.733	-1.0	25832.751	-1.6
trp-asn	tyr-val-pro	25386.411	25014.459	-1.5	24789.208	-2.4
trp-asn	asn-phe-gly-ala	26196.982	25606.312	-2.2	25481.943	-2.7
trp-asn	cys-lys-phe-gly	29512.548	29173.606	-1.1	29039.078	-1.6
trp-asn	glu-his-arg-leu	35618.387	34331.279	-3.6	34245.081	-3.9
trp-asn	ile-gly-val-gln	27568.763	26543.764	-3.7	26462.687	-4.0
trp-asn	leu-trp-asn-cys	35323.345	34266.389	-3.0	34076.240	-3.5
trp-asn	met-asp-cys-lys	31657.439	30944.959	-2.2	31012.938	-2.0
trp-asn	phe-ala-thr-val	29385.328	28580.573	-2.7	28375.076	-3.4
trp-asn	ser-ile-lys-phe	32926.894	32529.949	-1.2	32287.684	-1.9
trp-asn	thr-asn-pro-ile	32926.894	32529.949	-1.2	32287.684	-1.9
trp-asn	val-met-leu-tyr	35655.366	34874.879	-2.2	34640.562	-2.9
trp-gln	trp-gln	23242.606	22485.101	-3.3	22280.531	-4.1
trp-gln	tyr-ile	20862.772	20772.613	-0.4	20566.443	-1.4
trp-gln	val-ile	16867.400	16286.268	-3.5	16183.163	-4.1
trp-gln	ala-gln-his	22949.651	22677.592	-1.2	22648.032	-1.3
trp-gln	asn-cys-ala	19769.588	19370.749	-2.0	19480.847	-1.5
trp-gln	asp-his-val	24193.245	23985.645	-0.9	23943.116	-1.0
trp-gln	cys-thr-lys	23283.779	23148.003	-0.6	23192.949	-0.4
trp-gln	gln-trp-ile	31647.919	30707.111	-3.0	30411.625	-3.9
trp-gln	gly-pro-ser	16754.270	16796.018	0.2	16811.029	0.3
trp-gln	leu-arg-gly	23958.288	22649.621	-5.5	22610.635	-5.6
trp-gln	lys-met-asp	26640.261	26024.408	-2.3	26049.987	-2.2
trp-gln	thr-phe-met	27713.000	27400.268	-1.1	27244.440	-1.7

**Table 2** (continued)

Peptide A	Peptide B	TDDFT	Pair-specific	$\Delta$ (%)	Species-specific	$\Delta$ (%)
trp-gln	tyr-val-pro	26810.309	26393.888	-1.6	26136.576	-2.5
trp-gln	asn-phe-gly-ala	27666.306	27019.803	-2.3	26879.178	-2.9
trp-gln	cys-lys-phe-gly	31168.437	30784.671	-1.2	30627.028	-1.7
trp-gln	glu-his-arg-leu	37617.428	36231.590	-3.7	36126.291	-4.0
trp-gln	ile-gly-val-gln	29116.097	28010.597	-3.8	27913.897	-4.1
trp-gln	leu-trp-asn-cys	37303.987	36158.247	-3.1	35938.481	-3.7
trp-gln	met-asp-cys-lys	33433.600	32652.063	-2.3	32727.984	-2.1
trp-gln	phe-ala-thr-val	31033.605	30157.524	-2.8	29921.787	-3.6
trp-gln	ser-ile-lys-phe	34774.964	34326.611	-1.3	34044.702	-2.1
trp-gln	thr-asn-pro-ile	34774.964	34326.611	-1.3	34044.702	-2.1
trp-gln	val-met-leu-tyr	37655.507	36798.797	-2.3	36526.675	-3.0
tyr-ile	tyr-ile	18732.376	19176.352	2.4	18963.542	1.2
tyr-ile	val-ile	15149.326	15030.013	-0.8	14925.630	-1.5
tyr-ile	ala-gln-his	20612.566	20952.975	1.6	20929.709	1.5
tyr-ile	asn-cys-ala	17750.880	17880.064	0.7	18002.230	1.4
tyr-ile	asp-his-val	21727.439	22153.173	2.0	22111.528	1.8
tyr-ile	cys-thr-lys	20911.900	21362.057	2.1	21418.703	2.4
tyr-ile	gln-trp-ile	28411.230	28362.460	-0.2	28064.944	-1.2
tyr-ile	gly-pro-ser	15048.514	15506.192	3.0	15519.813	3.1
tyr-ile	leu-arg-gly	21516.374	20921.738	-2.8	20892.400	-2.9
tyr-ile	lys-met-asp	23921.399	24016.083	0.4	24050.627	0.5
tyr-ile	thr-phe-met	24878.656	25289.549	1.6	25137.466	1.0
tyr-ile	tyr-val-pro	24069.336	24369.505	1.2	24105.153	0.1
tyr-ile	asn-phe-gly-ala	24838.369	24956.881	0.5	24814.825	-0.1
tyr-ile	cys-lys-phe-gly	27985.035	28423.300	1.6	28275.400	1.0
tyr-ile	glu-his-arg-leu	33781.612	33471.395	-0.9	33376.211	-1.2
tyr-ile	ile-gly-val-gln	26146.859	25861.261	-1.1	25765.727	-1.5
tyr-ile	leu-trp-asn-cys	33484.774	33390.358	-0.3	33179.285	-0.9
tyr-ile	met-asp-cys-lys	30017.318	30129.281	0.4	30224.550	0.7
tyr-ile	phe-ala-thr-val	27861.260	27844.250	-0.1	27603.050	-0.9
tyr-ile	ser-ile-lys-phe	31228.669	31694.772	1.5	31410.045	0.6
tyr-ile	thr-asn-pro-ile	31228.669	31694.772	1.5	31410.045	0.6
tyr-ile	val-met-leu-tyr	33805.650	33964.695	0.5	33695.549	-0.3
val-ile	val-ile	12254.930	11795.382	-3.8	11723.918	-4.3
val-ile	ala-gln-his	16674.433	16441.895	-1.4	16419.224	-1.5
val-ile	asn-cys-ala	14355.583	14019.157	-2.3	14088.154	-1.9
val-ile	asp-his-val	17574.787	17370.474	-1.2	17354.648	-1.2
val-ile	cys-thr-lys	16916.242	16758.525	-0.9	16776.936	-0.8
val-ile	gln-trp-ile	22973.119	22244.568	-3.2	22081.788	-3.9
val-ile	gly-pro-ser	12173.702	12153.730	-0.2	12171.647	-0.0
val-ile	leu-arg-gly	17404.149	16436.337	-5.6	16380.363	-5.9
val-ile	lys-met-asp	19347.020	18832.280	-2.7	18849.569	-2.6
val-ile	thr-phe-met	20116.813	19821.830	-1.5	19750.718	-1.8
val-ile	tyr-val-pro	19463.016	19101.579	-1.9	18971.421	-2.5
val-ile	asn-phe-gly-ala	20085.165	19565.447	-2.6	19500.613	-2.9
val-ile	cys-lys-phe-gly	22631.791	22293.648	-1.5	22206.077	-1.9
val-ile	glu-his-arg-leu	27323.920	26274.600	-3.8	26190.832	-4.2
val-ile	ile-gly-val-gln	21148.513	20291.306	-4.0	20224.368	-4.4
val-ile	leu-trp-asn-cys	27072.647	26183.751	-3.3	26070.929	-3.7
val-ile	met-asp-cys-lys	24274.311	23624.097	-2.7	23674.658	-2.5
val-ile	phe-ala-thr-val	22529.574	21830.807	-3.1	21707.194	-3.6
val-ile	ser-ile-lys-phe	25258.889	24862.717	-1.6	24697.238	-2.2
val-ile	thr-asn-pro-ile	25258.889	24862.717	-1.6	24697.238	-2.2

**Table 2** (continued)

Peptide A	Peptide B	TDDFT	Pair-specific	$\Delta$ (%)	Species-specific	$\Delta$ (%)
val-ile	val-met-leu-tyr	27336.209	26632.764	-2.6	26485.291	-3.1
ala-gln-his	ala-gln-his	22690.482	22880.468	0.8	22864.200	0.8
ala-gln-his	asn-cys-ala	19532.869	19540.492	0.0	19559.013	0.1
ala-gln-his	asp-his-val	23915.123	24192.929	1.2	24187.692	1.1
ala-gln-his	cys-thr-lys	23017.506	23361.759	1.5	23362.980	1.5
ala-gln-his	gln-trp-ile	31257.303	30979.310	-0.9	30930.232	-1.1
ala-gln-his	gly-pro-ser	16566.225	16939.537	2.2	16948.313	2.3
ala-gln-his	leu-arg-gly	23681.849	22870.756	-3.4	22836.172	-3.6
ala-gln-his	lys-met-asp	26323.652	26258.215	-0.2	26263.843	-0.2
ala-gln-his	thr-phe-met	27369.632	27639.334	1.0	27625.046	0.9
ala-gln-his	tyr-val-pro	26481.562	26622.373	0.5	26591.717	0.4
ala-gln-his	asn-phe-gly-ala	27329.155	27250.926	-0.3	27233.731	-0.3
ala-gln-his	cys-lys-phe-gly	30792.549	31061.746	0.9	31032.429	0.8
ala-gln-his	glu-his-arg-leu	37179.863	36566.530	-1.6	36523.514	-1.8
ala-gln-his	ile-gly-val-gln	28776.027	28268.621	-1.8	28244.302	-1.9
ala-gln-his	leu-trp-asn-cys	36833.536	36476.721	-1.0	36441.795	-1.1
ala-gln-his	met-asp-cys-lys	33026.156	32944.573	-0.2	32959.180	-0.2
ala-gln-his	phe-ala-thr-val	30653.856	30422.723	-0.8	30391.460	-0.9
ala-gln-his	ser-ile-lys-phe	34368.794	34639.037	0.8	34589.023	0.6
ala-gln-his	thr-asn-pro-ile	34368.794	34639.037	0.8	34589.023	0.6
ala-gln-his	val-met-leu-tyr	37191.713	37129.999	-0.2	37091.021	-0.3
asn-cys-ala	asn-cys-ala	16820.884	16658.682	-1.0	16555.094	-1.6
asn-cys-ala	asp-his-val	20589.290	20653.753	0.3	20686.625	0.5
asn-cys-ala	cys-thr-lys	19816.323	19910.644	0.5	19846.691	0.1
asn-cys-ala	gln-trp-ile	26922.530	26452.178	-1.8	26615.042	-1.1
asn-cys-ala	gly-pro-ser	14260.285	14452.962	1.4	14458.921	1.4
asn-cys-ala	leu-arg-gly	20389.165	19520.168	-4.3	19546.643	-4.1
asn-cys-ala	lys-met-asp	22668.039	22382.008	-1.3	22331.796	-1.5
asn-cys-ala	thr-phe-met	23574.966	23570.369	-0.0	23611.123	0.1
asn-cys-ala	tyr-val-pro	22808.159	22722.751	-0.4	22872.442	0.3
asn-cys-ala	asn-phe-gly-ala	23537.048	23268.816	-1.1	23351.964	-0.8
asn-cys-ala	cys-lys-phe-gly	26518.683	26498.874	-0.1	26534.860	0.1
asn-cys-ala	glu-his-arg-leu	32011.873	31220.867	-2.5	31283.188	-2.3
asn-cys-ala	ile-gly-val-gln	24776.998	24118.014	-2.7	24186.975	-2.4
asn-cys-ala	leu-trp-asn-cys	31730.102	31129.262	-1.9	31196.320	-1.7
asn-cys-ala	met-asp-cys-lys	28444.413	28072.313	-1.3	27940.688	-1.8
asn-cys-ala	phe-ala-thr-val	26401.417	25963.596	-1.7	26104.930	-1.1
asn-cys-ala	ser-ile-lys-phe	29592.520	29560.440	-0.1	29726.405	0.5
asn-cys-ala	thr-asn-pro-ile	29592.520	29560.440	-0.1	29726.405	0.5
asn-cys-ala	val-met-leu-tyr	32034.131	31665.018	-1.1	31772.931	-0.8
asp-his-val	asp-his-val	25206.661	25582.067	1.5	25571.543	1.4
asp-his-val	cys-thr-lys	24260.345	24683.799	1.8	24708.044	1.9
asp-his-val	gln-trp-ile	32949.719	32756.858	-0.6	32699.235	-0.8
asp-his-val	gly-pro-ser	17460.138	17909.641	2.6	17910.340	2.6
asp-his-val	leu-arg-gly	24960.957	24166.893	-3.2	24166.940	-3.2
asp-his-val	lys-met-asp	27746.961	27748.951	0.0	27767.320	0.1
asp-his-val	thr-phe-met	28851.779	29217.682	1.3	29198.168	1.2
asp-his-val	tyr-val-pro	27915.045	28149.585	0.8	28097.307	0.7
asp-his-val	asn-phe-gly-ala	28808.184	28819.172	0.0	28788.410	-0.1
asp-his-val	cys-lys-phe-gly	32458.375	32834.025	1.2	32817.201	1.1
asp-his-val	glu-his-arg-leu	39188.603	38654.708	-1.4	38639.226	-1.4
asp-his-val	ile-gly-val-gln	30330.957	29876.427	-1.5	29861.145	-1.6
asp-his-val	leu-trp-asn-cys	38829.519	38566.122	-0.7	38534.796	-0.8

**Table 2** (continued)

Peptide A	Peptide B	TDDFT	Pair-specific	$\Delta$ (%)	Species-specific	$\Delta$ (%)
asp-his-val	met-asp-cys-lys	34813.518	34813.460	-0.0	34853.959	0.1
asp-his-val	phe-ala-thr-val	32313.069	32164.135	-0.5	32117.298	-0.6
asp-his-val	ser-ile-lys-phe	36225.927	36614.952	1.1	36563.063	0.9
asp-his-val	thr-asn-pro-ile	36225.927	36614.952	1.1	36563.063	0.9
asp-his-val	val-met-leu-tyr	39205.300	39244.140	0.1	39205.365	0.0
cys-thr-lys	cys-thr-lys	23350.777	23801.133	1.9	23739.872	1.7
cys-thr-lys	gln-trp-ile	31711.931	31614.019	-0.3	31670.114	-0.1
cys-thr-lys	gly-pro-ser	16804.721	17270.055	2.8	17290.346	2.9
cys-thr-lys	leu-arg-gly	24024.491	23348.057	-2.8	23327.805	-2.9
cys-thr-lys	lys-met-asp	26706.136	26749.917	0.2	26704.395	-0.0
cys-thr-lys	thr-phe-met	27768.739	28162.904	1.4	28153.825	1.4
cys-thr-lys	tyr-val-pro	26866.578	27149.058	1.1	27216.940	1.3
cys-thr-lys	asn-phe-gly-ala	27725.674	27806.089	0.3	27849.961	0.5
cys-thr-lys	cys-lys-phe-gly	31240.393	31672.457	1.4	31643.167	1.3
cys-thr-lys	glu-his-arg-leu	37717.800	37330.703	-1.0	37330.179	-1.0
cys-thr-lys	ile-gly-val-gln	29193.061	28830.355	-1.2	28851.645	-1.2
cys-thr-lys	leu-trp-asn-cys	37370.728	37203.391	-0.5	37190.983	-0.5
cys-thr-lys	met-asp-cys-lys	33507.474	33550.763	0.1	33439.518	-0.2
cys-thr-lys	phe-ala-thr-val	31099.585	31025.243	-0.2	31087.513	-0.0
cys-thr-lys	ser-ile-lys-phe	34866.919	35331.001	1.3	35385.901	1.5
cys-thr-lys	thr-asn-pro-ile	34866.919	35331.001	1.3	35385.901	1.5
cys-thr-lys	val-met-leu-tyr	37734.063	37840.393	0.3	37845.243	0.3
gln-trp-ile	gln-trp-ile	43095.356	41938.467	-2.7	41501.754	-3.7
gln-trp-ile	gly-pro-ser	22819.500	22934.097	0.5	22963.302	0.6
gln-trp-ile	leu-arg-gly	32629.716	30950.411	-5.2	30866.950	-5.4
gln-trp-ile	lys-met-asp	36280.076	35537.551	-2.0	35572.144	-1.9
gln-trp-ile	thr-phe-met	37737.089	37411.335	-0.9	37186.563	-1.5
gln-trp-ile	tyr-val-pro	36508.554	36039.238	-1.3	35667.850	-2.3
gln-trp-ile	asn-phe-gly-ala	37674.512	36898.536	-2.1	36699.735	-2.6
gln-trp-ile	cys-lys-phe-gly	42445.223	42043.357	-0.9	41804.142	-1.5
gln-trp-ile	glu-his-arg-leu	51231.492	49499.013	-3.4	49323.644	-3.7
gln-trp-ile	ile-gly-val-gln	39653.286	38258.754	-3.5	38105.832	-3.9
gln-trp-ile	leu-trp-asn-cys	50794.647	49380.080	-2.8	49055.524	-3.4
gln-trp-ile	met-asp-cys-lys	45528.934	44586.425	-2.1	44693.763	-1.8
gln-trp-ile	phe-ala-thr-val	42259.820	41181.600	-2.5	40838.106	-3.4
gln-trp-ile	ser-ile-lys-phe	47360.147	46882.163	-1.0	46458.356	-1.9
gln-trp-ile	thr-asn-pro-ile	47360.147	46882.163	-1.0	46458.356	-1.9
gln-trp-ile	val-met-leu-tyr	51276.814	50249.954	-2.0	49844.542	-2.8
gly-pro-ser	gly-pro-ser	12094.996	12535.195	3.6	12528.172	3.6
gly-pro-ser	leu-arg-gly	17289.712	16916.106	-2.2	16942.089	-2.0
gly-pro-ser	lys-met-asp	19218.012	19415.601	1.0	19431.783	1.1
gly-pro-ser	thr-phe-met	19981.125	20447.523	2.3	20473.909	2.5
gly-pro-ser	tyr-val-pro	19333.027	19705.197	1.9	19722.571	2.0
gly-pro-ser	asn-phe-gly-ala	19951.952	20177.615	1.1	20184.675	1.2
gly-pro-ser	cys-lys-phe-gly	22480.421	22981.445	2.2	23018.427	2.4
gly-pro-ser	glu-his-arg-leu	27144.286	27062.105	-0.3	27090.328	-0.2
gly-pro-ser	ile-gly-val-gln	21008.695	20909.773	-0.5	20927.461	-0.4
gly-pro-ser	leu-trp-asn-cys	26890.007	26997.410	0.4	27035.488	0.5
gly-pro-ser	met-asp-cys-lys	24110.850	24356.931	1.0	24385.878	1.1
gly-pro-ser	phe-ala-thr-val	22379.039	22514.245	0.6	22532.902	0.7
gly-pro-ser	ser-ile-lys-phe	25091.849	25628.761	2.1	25661.828	2.3
gly-pro-ser	thr-asn-pro-ile	25091.849	25628.761	2.1	25661.828	2.3
gly-pro-ser	val-met-leu-tyr	27151.788	27463.620	1.1	27508.091	1.3

**Table 2** (continued)

Peptide A	Peptide B	TDDFT	Pair-specific	$\Delta$ (%)	Species-specific	$\Delta$ (%)
leu-arg-gly	leu-arg-gly	24718.075	22883.998	-7.4	22785.512	-7.8
leu-arg-gly	lys-met-asp	27477.619	26232.576	-4.5	26230.766	-4.5
leu-arg-gly	thr-phe-met	28572.118	27599.823	-3.4	27577.421	-3.5
leu-arg-gly	tyr-val-pro	27643.917	26584.143	-3.8	26545.059	-4.0
leu-arg-gly	asn-phe-gly-ala	28527.959	27216.655	-4.6	27202.167	-4.7
leu-arg-gly	cys-lys-phe-gly	32143.390	31035.963	-3.5	30970.452	-3.6
leu-arg-gly	glu-his-arg-leu	38807.168	36562.076	-5.8	36459.617	-6.0
leu-arg-gly	ile-gly-val-gln	30036.093	28254.158	-5.9	28196.746	-6.1
leu-arg-gly	leu-trp-asn-cys	38452.945	36438.993	-5.2	36374.465	-5.4
leu-arg-gly	met-asp-cys-lys	34476.109	32910.662	-4.5	32915.787	-4.5
leu-arg-gly	phe-ala-thr-val	31999.272	30386.291	-5.0	30339.997	-5.2
leu-arg-gly	ser-ile-lys-phe	35873.785	34613.058	-3.5	34515.845	-3.8
leu-arg-gly	thr-asn-pro-ile	35873.785	34613.058	-3.5	34515.845	-3.8
leu-arg-gly	val-met-leu-tyr	38825.381	37090.118	-4.5	37011.242	-4.7
lys-met-asp	lys-met-asp	30548.410	30067.902	-1.6	30030.912	-1.7
lys-met-asp	thr-phe-met	31769.440	31661.344	-0.3	31640.097	-0.4
lys-met-asp	tyr-val-pro	30735.887	30522.185	-0.7	30563.124	-0.6
lys-met-asp	asn-phe-gly-ala	31717.906	31260.942	-1.4	31288.580	-1.4
lys-met-asp	cys-lys-phe-gly	35737.163	35601.147	-0.4	35569.956	-0.5
lys-met-asp	glu-his-arg-leu	43140.522	41953.585	-2.8	41963.216	-2.7
lys-met-asp	ile-gly-val-gln	33390.737	32402.166	-3.0	32423.699	-2.9
lys-met-asp	leu-trp-asn-cys	42758.054	41821.943	-2.2	41798.673	-2.2
lys-met-asp	met-asp-cys-lys	38332.306	37713.162	-1.6	37620.382	-1.9
lys-met-asp	phe-ala-thr-val	35578.247	34877.164	-2.0	34917.300	-1.9
lys-met-asp	ser-ile-lys-phe	39880.411	39711.454	-0.4	39750.000	-0.3
lys-met-asp	thr-asn-pro-ile	39880.411	39711.454	-0.4	39750.000	-0.3
lys-met-asp	val-met-leu-tyr	43169.373	42535.354	-1.5	42525.193	-1.5
thr-phe-met	thr-phe-met	33045.813	33342.370	0.9	33172.640	0.4
thr-phe-met	tyr-val-pro	31969.230	32139.616	0.5	31948.576	-0.1
thr-phe-met	asn-phe-gly-ala	32989.732	32916.426	-0.2	32817.967	-0.5
thr-phe-met	cys-lys-phe-gly	37168.162	37480.484	0.8	37306.573	0.4
thr-phe-met	glu-his-arg-leu	44860.586	44153.350	-1.6	44083.318	-1.7
thr-phe-met	ile-gly-val-gln	34722.656	34108.147	-1.8	34048.505	-1.9
thr-phe-met	leu-trp-asn-cys	44479.839	44032.621	-1.0	43810.049	-1.5
thr-phe-met	met-asp-cys-lys	39869.118	39714.165	-0.4	39675.271	-0.5
thr-phe-met	phe-ala-thr-val	37005.513	36722.474	-0.8	36551.576	-1.2
thr-phe-met	ser-ile-lys-phe	41471.207	41803.566	0.8	41595.738	0.3
thr-phe-met	thr-asn-pro-ile	41471.207	41803.566	0.8	41595.738	0.3
thr-phe-met	val-met-leu-tyr	44902.438	44784.972	-0.3	44526.453	-0.8
tyr-val-pro	tyr-val-pro	30928.657	30967.977	0.1	30639.297	-0.9
tyr-val-pro	asn-phe-gly-ala	31916.518	31711.832	-0.6	31534.619	-1.2
tyr-val-pro	cys-lys-phe-gly	35958.494	36119.468	0.5	35932.157	-0.1
tyr-val-pro	glu-his-arg-leu	43403.071	42529.292	-2.0	42407.784	-2.3
tyr-val-pro	ile-gly-val-gln	33594.012	32863.911	-2.2	32744.201	-2.5
tyr-val-pro	leu-trp-asn-cys	43030.373	42429.920	-1.4	42163.905	-2.0
tyr-val-pro	met-asp-cys-lys	38570.668	38292.296	-0.7	38406.546	-0.4
tyr-val-pro	phe-ala-thr-val	35800.978	35383.631	-1.2	35083.497	-2.0
tyr-val-pro	ser-ile-lys-phe	40123.218	40276.425	0.4	39921.220	-0.5
tyr-val-pro	thr-asn-pro-ile	40123.218	40276.425	0.4	39921.220	-0.5
tyr-val-pro	val-met-leu-tyr	43439.722	43164.395	-0.6	42827.218	-1.4
asn-phe-gly-ala	asn-phe-gly-ala	32936.420	32466.044	-1.4	32367.530	-1.7
asn-phe-gly-ala	cys-lys-phe-gly	37107.056	36986.440	-0.3	36892.141	-0.6
asn-phe-gly-ala	glu-his-arg-leu	44791.055	43537.835	-2.8	43476.138	-2.9

**Table 2** (continued)

Peptide A	Peptide B	TDDFT	Pair-specific	$\Delta$ (%)	Species-specific	$\Delta$ (%)
asn-phe-gly-ala	ile-gly-val-gln	34667.948	33653.246	-2.9	33592.700	-3.1
asn-phe-gly-ala	leu-trp-asn-cys	44403.789	43444.590	-2.2	43305.643	-2.5
asn-phe-gly-ala	met-asp-cys-lys	39802.164	39220.488	-1.5	39291.723	-1.3
asn-phe-gly-ala	phe-ala-thr-val	36944.477	36233.401	-1.9	36072.529	-2.4
asn-phe-gly-ala	ser-ile-lys-phe	41405.820	41243.790	-0.4	41057.232	-0.8
asn-phe-gly-ala	thr-asn-pro-ile	41405.820	41243.790	-0.4	41057.232	-0.8
asn-phe-gly-ala	val-met-leu-tyr	44826.374	44208.650	-1.4	44035.759	-1.8
cys-lys-phe-gly	cys-lys-phe-gly	41808.285	42133.698	0.8	41935.063	0.3
cys-lys-phe-gly	glu-his-arg-leu	50466.580	49631.662	-1.6	49521.328	-1.9
cys-lys-phe-gly	ile-gly-val-gln	39061.272	38347.997	-1.8	38269.964	-2.0
cys-lys-phe-gly	leu-trp-asn-cys	50025.752	49489.477	-1.1	49247.365	-1.6
cys-lys-phe-gly	met-asp-cys-lys	44844.949	44658.332	-0.4	44601.130	-0.5
cys-lys-phe-gly	phe-ala-thr-val	41623.478	41274.285	-0.8	41101.925	-1.2
cys-lys-phe-gly	ser-ile-lys-phe	46653.069	46993.216	0.7	46764.298	0.2
cys-lys-phe-gly	thr-asn-pro-ile	46653.069	46993.216	0.7	46764.298	0.2
cys-lys-phe-gly	val-met-leu-tyr	50504.804	50350.235	-0.3	50071.636	-0.9
glu-his-arg-leu	glu-his-arg-leu	60927.475	58443.739	-4.1	58314.063	-4.3
glu-his-arg-leu	ile-gly-val-gln	47156.820	45173.446	-4.2	45089.577	-4.4
glu-his-arg-leu	leu-trp-asn-cys	60375.539	58280.657	-3.5	58149.541	-3.7
glu-his-arg-leu	met-asp-cys-lys	54129.397	52635.540	-2.8	52670.323	-2.7
glu-his-arg-leu	phe-ala-thr-val	50241.186	48604.374	-3.3	48483.655	-3.5
glu-his-arg-leu	ser-ile-lys-phe	56322.001	55348.603	-1.7	55166.760	-2.0
glu-his-arg-leu	thr-asn-pro-ile	56322.001	55348.603	-1.7	55166.760	-2.0
glu-his-arg-leu	val-met-leu-tyr	60958.614	59321.083	-2.7	59161.882	-3.0
ile-gly-val-gln	ile-gly-val-gln	36498.879	34900.609	-4.4	34836.855	-4.5
ile-gly-val-gln	leu-trp-asn-cys	46731.424	45038.806	-3.6	44937.399	-3.8
ile-gly-val-gln	met-asp-cys-lys	41896.739	40649.051	-3.0	40706.477	-2.8
ile-gly-val-gln	phe-ala-thr-val	38886.747	37556.575	-3.4	37442.332	-3.7
ile-gly-val-gln	ser-ile-lys-phe	43592.648	42766.087	-1.9	42611.002	-2.2
ile-gly-val-gln	thr-asn-pro-ile	43592.648	42766.087	-1.9	42611.002	-2.2
ile-gly-val-gln	val-met-leu-tyr	47182.751	45823.137	-2.9	45691.650	-3.2
leu-trp-asn-cys	leu-trp-asn-cys	59872.961	58130.485	-2.9	57824.046	-3.4
leu-trp-asn-cys	met-asp-cys-lys	53661.824	52464.206	-2.2	52429.437	-2.3
leu-trp-asn-cys	phe-ala-thr-val	49808.848	48482.873	-2.7	48239.921	-3.1
leu-trp-asn-cys	ser-ile-lys-phe	55813.937	55194.295	-1.1	54887.031	-1.7
leu-trp-asn-cys	thr-asn-pro-ile	55813.937	55194.295	-1.1	54887.031	-1.7
leu-trp-asn-cys	val-met-leu-tyr	60437.946	59146.312	-2.1	58789.332	-2.7
met-asp-cys-lys	met-asp-cys-lys	48103.072	47298.047	-1.7	47071.103	-2.1
met-asp-cys-lys	phe-ala-thr-val	44647.171	43755.387	-2.0	43865.826	-1.8
met-asp-cys-lys	ser-ile-lys-phe	50039.594	49820.248	-0.4	49935.693	-0.2
met-asp-cys-lys	thr-asn-pro-ile	50039.594	49820.248	-0.4	49935.693	-0.2
met-asp-cys-lys	val-met-leu-tyr	54174.635	53355.631	-1.5	53356.096	-1.5
phe-ala-thr-val	phe-ala-thr-val	41440.915	40430.697	-2.4	40155.423	-3.1
phe-ala-thr-val	ser-ile-lys-phe	46444.606	46025.901	-0.9	45695.245	-1.6
phe-ala-thr-val	thr-asn-pro-ile	46444.606	46025.901	-0.9	45695.245	-1.6
phe-ala-thr-val	val-met-leu-tyr	50283.099	49323.501	-1.9	49014.606	-2.5
ser-ile-lys-phe	ser-ile-lys-phe	52065.169	52404.338	0.7	51987.782	-0.1
ser-ile-lys-phe	thr-asn-pro-ile	52065.169	52404.338	0.7	51987.782	-0.1
ser-ile-lys-phe	val-met-leu-tyr	56353.029	56155.779	-0.3	55766.410	-1.0
thr-asn-pro-ile	thr-asn-pro-ile	52065.169	52404.338	0.7	51987.782	-0.1
thr-asn-pro-ile	val-met-leu-tyr	56353.029	56155.779	-0.3	55766.410	-1.0
val-met-leu-tyr	val-met-leu-tyr	61013.511	60160.047	-1.4	59730.433	-2.1