

Electronic Supplementary Information

A Facile Approach to Cross-Reactively Colorimetric Sensor Arrays: An Application in the Recognition of 20 Natural Amino Acids

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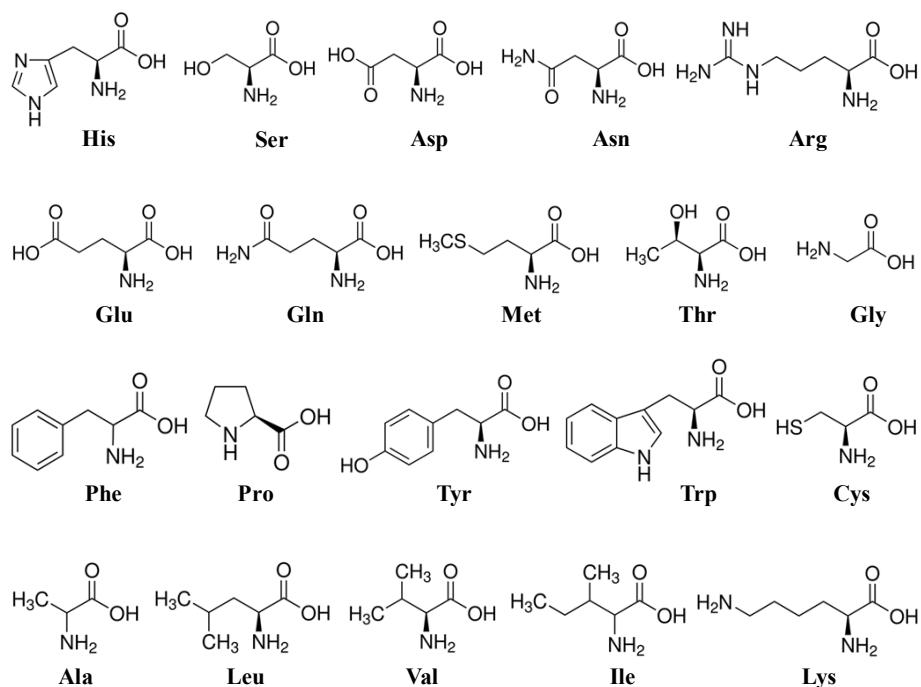


Figure S1. Chemical structures of the 20 natural amino acids and their name abbreviations.

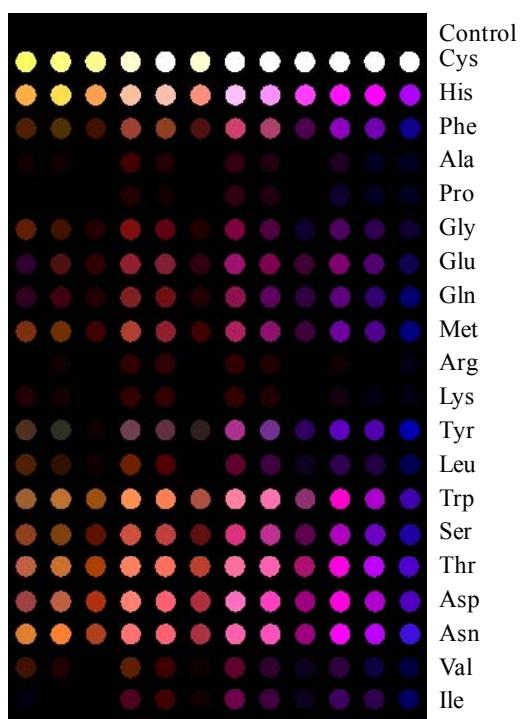


Figure S2. Color difference maps of the array for 20 natural amino acids at 100 μM and a control. For purposes of visualization, the color range of these difference maps was expanded from 4 to 8 bits per color (RGB range of 4-19 expanded to 0-255). A full database of the color differences see Tables S1. All of the experiments were performed in quadruplicate under physiological condition (10 mM HEPES buffer at pH 7.2).

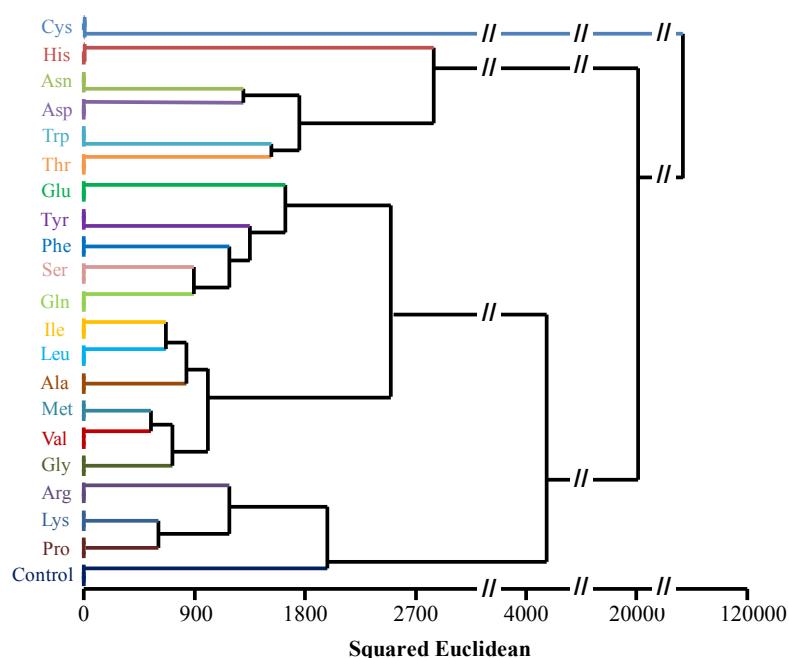


Figure S3. Hierarchical cluster analysis for the 20 natural amino acids at 100 μM and a control; no confusions or errors in classification were observed in 84 experiments. All of the experiments were performed in quadruplicate under physiological condition (10 mM HEPES buffer at pH 7.2).

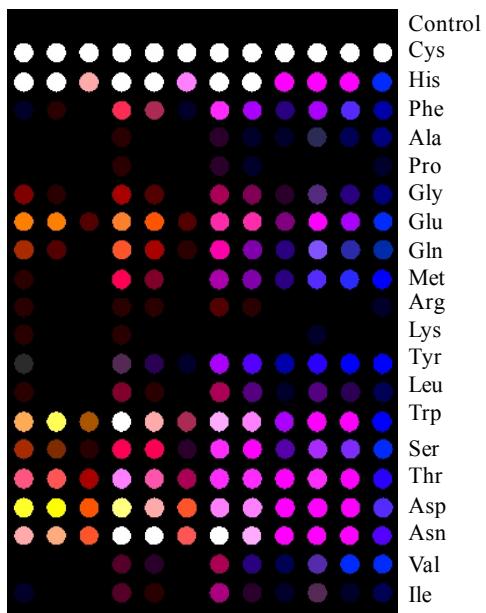


Figure S4. Color difference maps of the array for 20 natural amino acids at 50 μM and a control. For purposes of visualization, the color range of these difference maps was expanded from 3 to 8 bits per color (RGB range of 3-10 expanded to 0-255). A full database of the color differences see Tables S1. All of the experiments were performed in quadruplicate under physiological condition (10 mM HEPES buffer at pH 7.2).

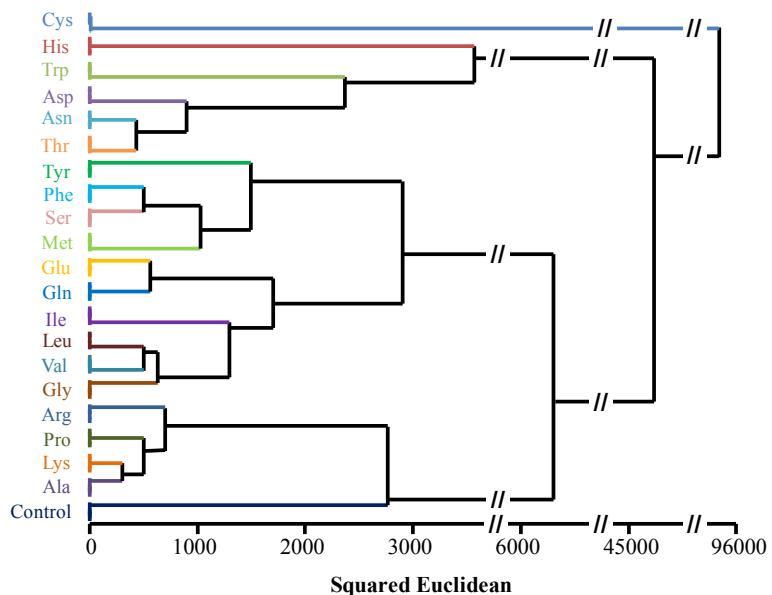


Figure S5. Hierarchical cluster analysis for 20 natural amino acids at 50 μM and a control; no confusions or errors in classification were observed in 84 experiments. All of the experiments were performed in quadruplicate under physiological condition (10 mM HEPES buffer at pH 7.2).

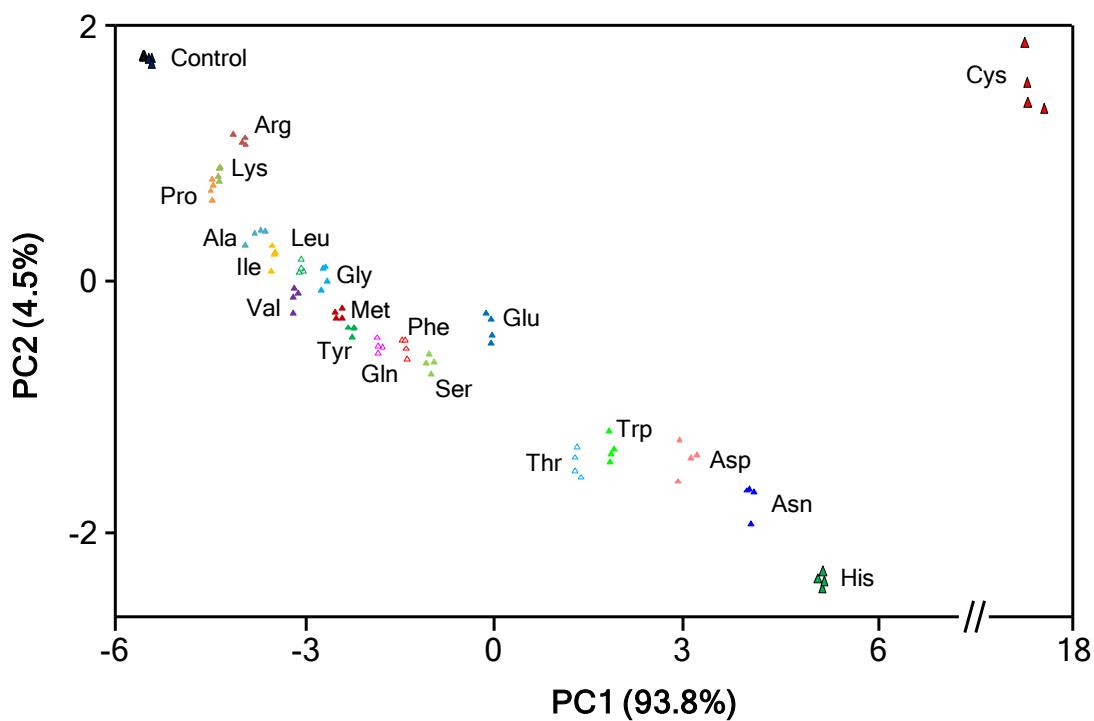


Figure S6. Two-dimensional principal component analysis plot of the array for 20 natural amino acids at 50 μM and a control. All of the experiments were performed in quadruplicate under physiological condition (10 mM HEPES buffer at pH 7.2).

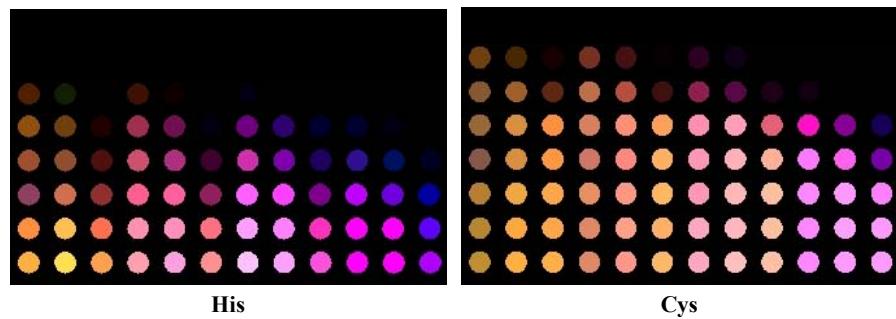


Figure S7. Color difference maps of the array for His and Cys at different concentrations and a control (control, 5, 10, 20, 30, 50, 80 and 100 μM were arranged from top to bottom). For purposes of visualization, the color range of these difference maps of His was expanded from 4 to 8 bits per color (RGB range of 4-19 expanded to 0-255); Cys was expanded from 5 to 8 bits per color (RGB range of 4-35 expanded to 0-255). All of the experiments were performed in quadruplicate under physiological condition (10 mM HEPES buffer at pH 7.2).

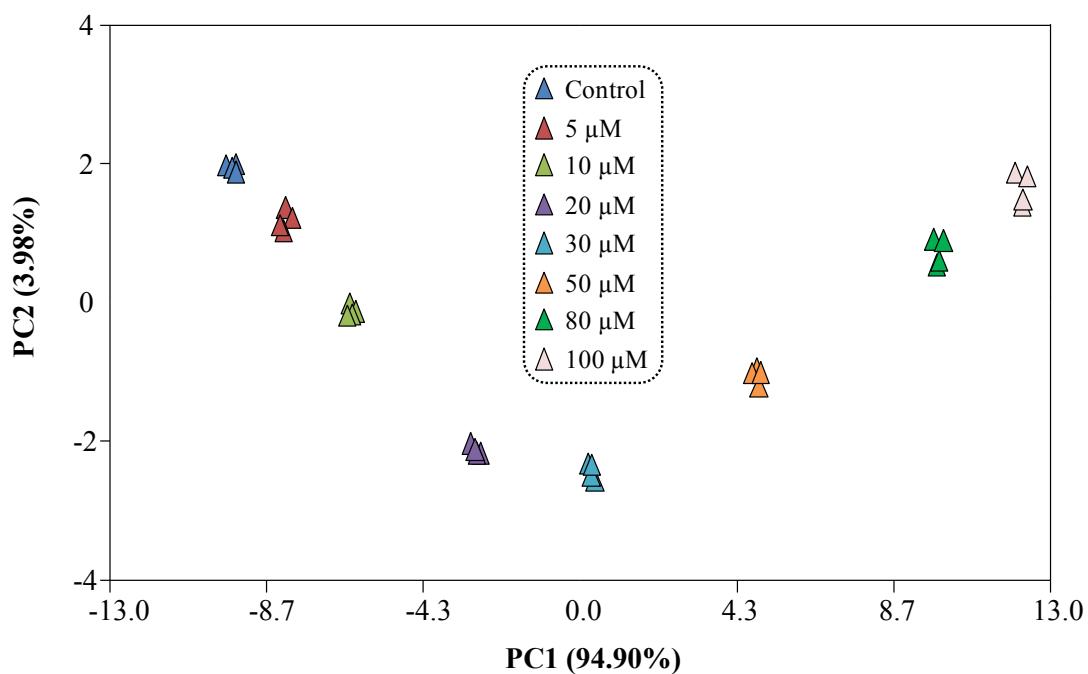


Figure S8 Two-dimensional principal component analysis plot of the developed array for His at different concentrations and a control. All of the experiments were performed in quadruplicate under physiological condition (10 mM HEPES buffer at pH 7.2).

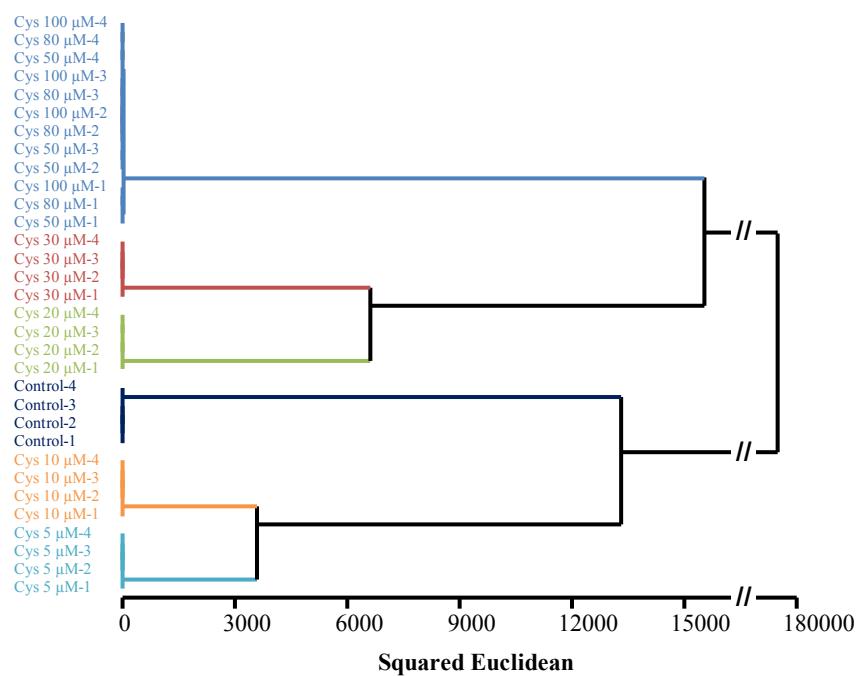


Figure S9. Hierarchical cluster analysis for Cys at different concentrations and a control. All of the experiments were performed in quadruplicate under physiological condition (10 mM HEPES buffer at pH 7.2).

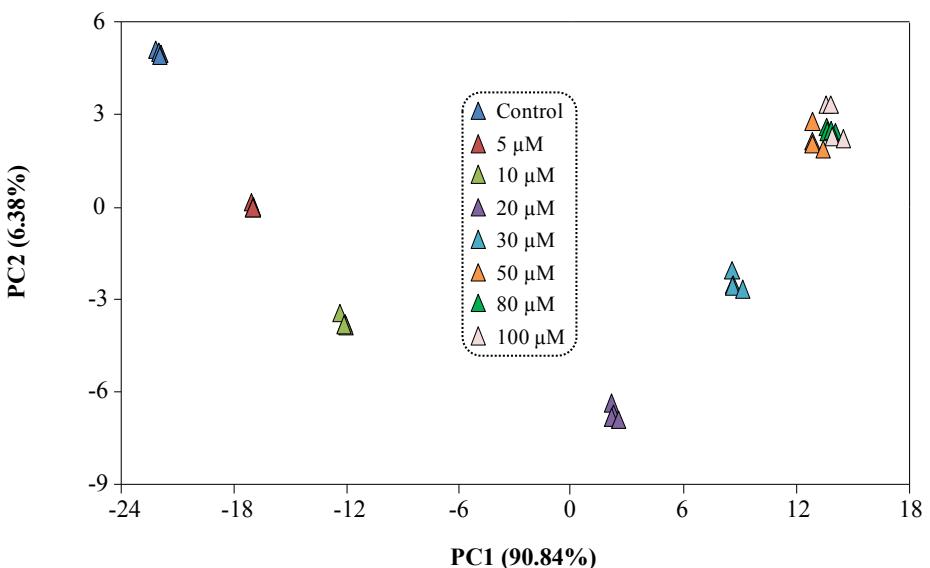


Figure S10. Two-dimensional principal component analysis plot of the developed array for Cys at different concentrations and a control. All of the experiments were performed in quadruplicate under physiological condition (10 mM HEPES buffer at pH 7.2).

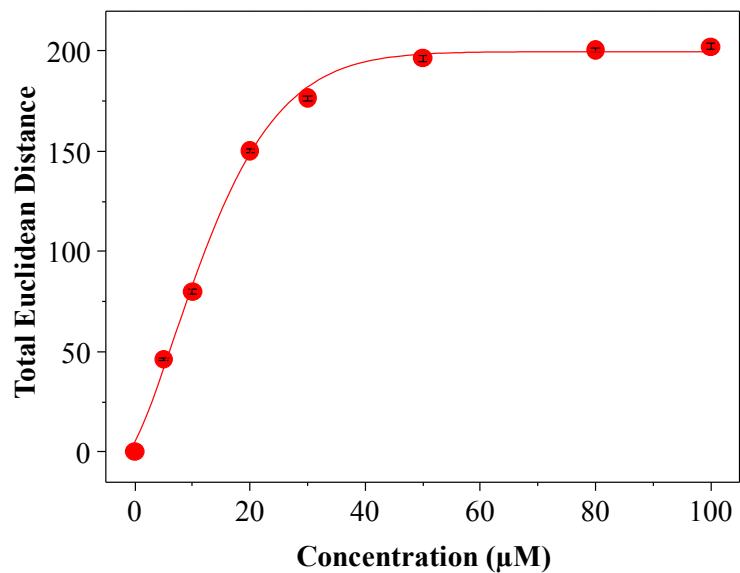


Figure S11. The total Euclidean distances of the array plotted versus different concentrations of Cys. All of the experiments were performed in quadruplicate under physiological condition (10 mM HEPES buffer at pH 7.2); the error bars shown were the standard deviation of quadruplicate experiments.

Table S1. Database for 20 natural amino acids at 50, 100 μ M and a control.

	R1	G1	B1	R2	G2	B2	R3	G3	B3	R4	G4	B4	R5	G5	B5	R6	G6	B6
Control-1	-0.980881	-0.585182	-0.066235	0.211678	0.413448	-0.604645	0.622738	0.54114	-0.02902	0.585526	0.87402	0.598499	-0.335268	-0.317173	-0.319904	0.326391	0.18368	-0.032774
Control-2	0.036873	-0.340389	0.313076	-0.189144	-0.252987	-0.593376	0.5746	0.594742	0.540115	-0.567646	0.218502	-0.957664	-0.963127	-0.861389	-0.557871	-0.525776	-0.36941	
Control-3	0.299419	0.202457	-0.038921	0.162514	-0.096619	-0.998634	0.280643	0.195288	0.400478	0.223969	0.155342	0.517239	-0.301468	-0.198704	-0.093208	-0.065552	-0.246159	-0.426085
Control-4	1.249573	1.027309	0.544212	0.58416	0.595768	-0.241379	0.247183	0.429499	0.46876	0.13554	0.262547	0.403893	0.719017	1.233868	0.708775	-0.439056	-0.339365	-0.808809
50 μ M Gly-	5.634343	3.779449	-0.853335	4.51178	3.458519	-1.342779	3.322636	1.527483	-1.120178	7.335609	3.55275	-2.994357	5.465687	2.717995	-3.420959	3.055992	1.053602	-2.656879
50 μ M Gly-	6.133831	3.750771	-1.42506	4.31649	2.889042	-1.482418	3.168318	1.376921	-1.287128	7.783886	3.829636	-3.167294	5.039946	2.308979	-2.865486	3.527483	1.861385	-2.118811
50 μ M Gly-	3.857976	4.206215	-1.486172	5.07238	3.861729	-1.281324	3.379652	1.701605	-1.163195	7.86787	3.798225	-3.5606	4.4534	1.766815	-3.978489	3.264595	1.35597	-2.74906
50 μ M Gly-	6.095222	3.790371	-1.62991	5.067261	3.339363	-1.874359	3.401844	1.41106	-1.234894	6.872654	2.871939	-4.004097	4.870262	1.944008	-3.336975	3.438034	1.346535	-2.617277
50 μ M Ala-	5.298203	1.958687	2.998291	1.483101	-2.153294	0.218164	1.06861	1.743265	3.651189	3.937511	1.834721	-3.400618	2.186413	0.721066	-1.53602			
50 μ M Ala-	3.759304	2.711506	-2.471836	3.195629	1.647659	-1.78969	2.129098	1.209627	-1.015364	5.583408	2.756912	-4.33359	4.136564	2.030045	-3.344143	2.590647	1.023216	-1.337999
50 μ M Ala-	4.023216	2.75555	2.745647	1.545461	2.745647	-1.562391	1.874359	1.993511	1.483101	1.288494	5.333811	-2.924206	4.464664	2.602936	-2.437347	2.371117	0.908501	-1.253328
50 μ M Ala-	3.815296	1.750771	-2.526115	2.16217	0.94026	-2.549335	1.782862	0.653807	-1.621031	4.90796	1.827927	-3.87402	3.037212	0.628883	-3.852165	2.01195	0.164219	-2.086824
50 μ M Val-	0.450247	1.639126	2.762035	3.062817	2.031754	-1.419939	2.573574	1.163197	-1.168318	5.479687	3.079891	-3.79174	3.844656	1.429497	-4.076138	2.911575	0.892799	-2.109934
50 μ M Val-	3.541142	1.379745	-3.044004	3.135544	1.59235	-2.337999	2.428474	0.974394	1.138271	5.453772	2.834415	-3.7337	4.785933	1.744965	-3.888699	2.91806	0.709457	-2.229431
50 μ M Val-	3.717312	1.34362	-2.90884	3.30386	2.172756	-1.833389	2.485149	0.896893	-1.170005	5.163536	1.961422	-4.858552	4.768862	2.290886	-4.088768	3.028679	0.967907	-1.975418
50 μ M Val-	3.788664	1.139297	-3.743599	2.985321	1.699215	-2.609083	2.271765	0.662001	1.264595	4.994881	3.050952	-3.880849	4.658928	1.752847	-4.007851	2.493	0.196312	-3.186413
50 μ M Leu-	3.854561	2.267326	-3.629096	2.779894	1.860363	-2.546601	2.525434	1.312735	-1.574259	6.502899	2.822807	-4.150902	4.56538	2.165241	-4.227379	3.488905	1.693752	-2.282349
50 μ M Leu-	4.310345	2.345169	3.335402	2.304506	1.718334	-2.61899	2.703995	1.397869	-1.881887	6.911234	2.944000	-4.31171	4.798098	2.346874	-3.931374	2.815294	0.974735	-2.901331
50 μ M Leu-	4.263229	1.852509	-3.373505	3.469784	2.220554	-2.566065	2.374872	1.130241	-1.779789	7.26767	3.272106	-4.245815	5.061111	2.893478	-3.58416	3.235575	1.344486	-2.309662
50 μ M Leu-	4.263229	1.630932	-2.872208	3.405602	2.255379	-2.819005	2.160807	0.973711	-1.907478	6.48003	3.247235	-4.13239	4.514168	1.974052	-4.056575	2.765448	1.212019	-2.704678
50 μ M Ile-1	6.145158	-0.650734	-4.809151	2.922157	0.874743	-2.867531	2.268692	0.869579	-1.766474	4.698193	1.563675	-5.182999	4.61079	1.811878	-3.767988	2.696825	0.628883	-2.620008
50 μ M Ile-2	1.919426	-0.231819	3.698909	2.780813	0.841927	-2.687948	1.854559	0.582792	-1.911232	5.669853	2.624786	-4.217478	4.223286	1.878113	-3.935471	2.72687	0.872652	-2.076136
50 μ M Ile-3	2.341072	0.33083	4.443153	2.606001	0.967224	-2.991808	2.036873	0.404384	1.993511	5.09962	4.956104	-4.56176	4.679874	2.406963	-3.260159	2.643906	0.812906	-2.351656
50 μ M Ile-4	3.130077	0.404915	4.741211	2.770912	0.764767	-3.20898	1.953906	0.639467	-2.055992	5.530556	2.006485	-4.50836	5.635418	0.804367	-4.395016	2.713896	0.735064	-3.159443
50 μ M Gln-	7.199047	4.675316	-2.834759	5.441105	3.195629	-2.669076	4.213726	1.272754	-1.534996	9.372822	4.148514	-5.023216	6.720041	3.618641	-5.441792	4.705019	1.641516	-2.665415
50 μ M Gln-	7.844315	4.653126	-2.905773	5.202801	3.521	-2.64698	3.803688	1.756231	-1.691021	9.542883	5.168999	-4.054451	7.319561	3.847389	-3.939228	4.850119	1.90044	-2.486174
50 μ M Gln-	8.862696	4.512459	-2.774666	4.819736	2.678047	-3.373505	3.65712	1.338682	-2.06487	4.924947	3.976177	-5.146866	8.244315	-5.157391	4.167635	3.818708	-3.608057	
50 μ M Met-	4.151585	1.675659	-3.333152	2.996588	1.199383	-3.14749	3.469103	1.443838	-1.792421	7.910892	3.313152	-4.303177	6.424745	2.143738	-4.170704	3.911575	1.196314	-3.111984
50 μ M Met-	4.697509	2.463299	3.051874	2.994074	1.974043	-2.31509	3.307403	1.51963	-2.036873	8.11779	3.694684	-5.089749	6.216864	2.184025	-4.791737	3.59679	1.223967	-3.401503
50 μ M Met-	5.32093	2.80608	-3.241718	3.851826	2.201092	-2.855242	3.739841	1.576307	-1.896553	8.410038	3.967224	-5.053555	6.517242	2.320605	-4.267666	4.077843	1.771791	-3.178558
50 μ M Met-	5.590988	3.214346	-2.748844	3.141346	4.051212	-2.233967	3.207099	1.400701	-1.834414	7.702229	7.470811	-5.424599	7.654172	2.304046	-3.932739	3.290884	0.744965	-3.329805
50 μ M Ser-	7.199047	4.675316	-2.834759	5.441105	3.195629	-2.669076	4.679071	2.125982	-1.534996	9.372822	4.148514	-5.023216	6.720041	-5.441792	4.705019	1.641516	-2.665415	
50 μ M Ser-	8.862696	4.512459	-2.774666	4.819736	2.678047	-3.373505	3.65712	1.338682	-2.06487	4.924947	3.976177	-5.146866	8.244315	-5.157391	4.167635	3.818708	-3.608057	
50 μ M Ser-	7.165245	3.683551	-4.503506	5.87402	2.875725	-4.053944	4.713213	1.861385	-2.031741	4.704111	2.109493	-3.02041	5.027657	-5.097301	4.851437	6.424745	2.143738	-3.111984
50 μ M Thr-	10.242929	6.263569	-7.64767	9.247868	5.818027	-5.503588	7.052608	3.617958	-2.038487	10.038504	6.302834	-7.864456	7.262728	-5.520218	-7.462616	7.772278	3.470461	-3.537304
50 μ M Thr-	9.2803	5.20314	-6.331512	6.833322	5.328781	-5.936155	7.043701	3.489244	-3.02873	11.772037	6.505306	-7.223967	7.505306	-5.121021	-7.980541	7.693069	3.486174	-5.824171
50 μ M Thr-	9.397976	4.859337	-4.744814	5.826563	6.044727	-5.733356	7.42267	3.457836	-3.839878	13.170471	6.414331	-8.297371	12.310343	5.178558	-8.113101	7.74394	3.226357	-6.02424
50 μ M Thr-	9.644588	4.854814	-4.744814	7.346195	9.169882	-6.944588	7.684212	3.939569	-4.215433	10.214079	6.474587	-8.073238	10.50872	-8.273472	7.566404	2.942886	-6.494709	
50 μ M Phe-	3.518951	2.349949	-4.816319	4.181973	3.035533	-3.775009	3.718674	1.700122	-2.031591	16.487198	8.686421	-8.489389	12.093548	-8.128371	-7.724819	7.32127	5.104132	-5.247524
50 μ M Phe-	3.412769	1.753841	-6.044044	3.473315	3.264841	-4.385798	4.100376	2.52919	-3.204021	8.5886	5.048481	-5.576986	7.397996	-4.358486	-5.269032	4.056334	2.576649	-3.551041
50 μ M Phe-	3.607716	2.28986	3.204824	3.762837	5.91806	-2.327282	6.381699	4.613178	-2.052264	5.036621	5.227228	-5.365311	7.272218	-5.422362	-5.582455	3.825878	2.298395	-4.097984
50 μ M Phe-	3.184394	2.732076	-3.743599	3.204696	5.917582	-4.282785	8.026563	5.907478	-4.509996	4.509375	6.209587	-5.906699	6.165128	-4.232116	-5.409355	3.493375	2.463296	-2.54558
50 μ M Phe-	10.324341	5.254356	-6.168488	1.779102	1.738136	-1.508362	1.508467	0.804686	-8.041858	9.24855	-3.92674	8.238478	-8.47559	11.269				

	R7	G7	B7	R8	G8	B8	R9	G9	B9	R10	G10	B10	R11	G11	B11	R12	G12	B12
Control-1	0.227722	-0.177876	-0.242401	-0.262547	-0.170364	-0.013313	0.091498	-0.111301	-0.243084	0.089791	0.410034	0.335609	0.107545	0.10413	0.09901	0.250256	0.479687	0.739159
Control-2	-0.479004	-0.928303	-0.14032	-0.3141	-0.131104	0.43906	-0.321611	-0.288496	-0.285423	-0.288836	0.019119	0.555473	-0.092678	-0.114716	-0.107204	0.032434	0.426085	0.86924
Control-3	-0.599863	-1.304882	-0.40287	-0.096279	-0.150902	0.04575	0.201776	0.030045	-0.095596	-0.073403	-0.032772	0.355759	0.034824	-0.005123	0.090477	0.288836	0.404234	0.738819
Control-4	-0.694777	-1.029362	-1.05394	-0.818026	-0.776375	-0.730282	0.303858	0.604984	0.71936	0.033459	0.488564	0.685905	-0.156709	-0.044041	-0.285419	-0.031751	0.102081	0.305222
50 µM Gly-	7.144075	2.23933	-5.793446	5.895527	1.44725	-6.020824	4.243087	0.27006	-4.19051	5.843291	-4.058723	-5.940595	4.359508	-3.748379	-6.44725	2.276203	-3.414133	-6.522705
50 µM Gly-	7.497099	2.85046	-5.63776	6.040691	1.856266	-5.281326	4.103107	0.231819	-4.767494	5.718334	-4.23489	-6.910549	4.349267	-3.736431	-6.317173	2.564356	-3.254013	-6.324345
50 µM Gly-	7.080233	2.423351	-5.872311	5.614887	1.443497	-5.599865	3.904063	-0.050188	-5.372482	5.249914	-4.119839	-7.218163	4.160465	-4.028679	-7.266304	2.175486	-3.845341	-7.377602
50 µM Gly-	6.930012	1.746326	-6.263573	5.61113	1.392624	-5.852512	3.553431	-0.478321	-5.892117	5.261865	-4.316494	-7.267666	4.074428	-4.455444	-7.219528	2.078184	-4.412428	-7.969955
50 µM Ala-	5.953228	1.653809	-4.328781	3.63776	0.859337	-0.992865	2.809151	0.36702	-4.257427	4.551042	-4.358481	-7.61353	3.130762	-5.410378	1.53875	-3.845341	-6.458858	
50 µM Ala-	5.514168	1.840904	-4.71936	3.835781	0.89621	-5.068626	2.957664	0.35268	-4.046772	4.776216	-3.950497	-5.3438	3.233526	-2.830318	-4.47943	1.535336	-3.838854	-5.884941
50 µM Ala-	5.054285	1.849785	-4.781837	3.799321	0.850462	-4.046772	3.799932	0.263336	-3.815294	4.567777	-4.192211	-5.17115	3.167634	-3.987575	-5.922846	1.389894	-3.736429	-5.420959
50 µM Ala-	5.530058	0.692043	-5.103107	3.827585	0.70536	-4.848072	2.650398	-0.155342	-4.194607	4.167293	-4.433599	-5.278255	0.828565	-3.52528	-5.314785	1.263571	-3.976101	-6.097645
50 µM Val-	6.678389	1.0628	-6.799591	4.780902	0.627518	-6.970978	3.195289	0.019802	-5.650051	5.725845	-5.158073	-7.94162	4.034142	-3.672924	-7.840561	1.762035	-4.15193	-7.708775
50 µM Val-	6.595499	1.512802	-6.534996	4.781729	1.105499	-5.911915	3.09423	-0.116079	-5.47081	5.147941	-5.801503	3.648003	-4.434277	-7.734722	1.385114	-4.681803	-8.354389	
50 µM Val-	7.431206	2.556164	-6.374633	4.80471	1.065891	-6.354385	2.958347	-0.327415	-5.726189	5.262466	-4.94503	-7.121204	3.557528	-4.857288	-8.201775	1.674974	-4.306931	-8.107204
50 µM Val-	6.732332	0.71526	-6.950497	4.369759	0.727176	-4.78379	-0.667217	-0.679074	2.809151	0.36702	-4.257427	4.551042	-4.358481	-7.791737	1.630591	-4.469103	-7.539433	
50 µM Leu-	7.508024	1.685558	-5.696623	5.017071	1.249912	-5.771938	3.629908	0.510412	-4.62035	5.751451	-3.987958	-5.922846	4.143052	-3.970935	-5.653465	1.845681	-3.762035	-5.889038
50 µM Leu-	7.661517	1.505978	-5.583852	5.11539	1.218129	-5.036869	3.535678	0.511348	-4.640835	5.700821	-4.04001	-3.271294	-5.187404	1.787299	-3.885626	-5.79208		
50 µM Leu-	7.633661	1.540115	-5.575385	4.9952	1.240696	-5.91806	3.494708	0.388529	-4.920452	5.663321	-4.044841	-6.065208	4.050871	-3.008877	-5.138271	1.762718	-3.957666	-5.942299
50 µM Leu-	7.334244	1.499146	-6.116425	4.951519	1.235577	-6.078526	2.993513	0.017071	-5.424377	5.445886	-4.085593	-6.580573	3.753841	-3.040997	-5.5606	1.333561	-4.274155	-6.264935
50 µM Ile-	7.952202	0.82349	-5.667805	4.972622	1.360535	-4.837206	3.580403	0.446911	-4.277491	5.36463	-4.94503	-7.26189	3.525098	-2.930691	-4.292248	1.643906	-3.521339	-5.379311
50 µM Ile-	7.026972	1.09116	-5.931717	4.929792	1.358486	-4.895187	3.56062	0.411743	-4.231819	5.29021	-3.99863	-5.42164	4.22137	-3.097503	-5.653465	1.845681	-3.762035	-5.889038
50 µM Ile-	6.425476	0.086376	-7.344486	4.696484	1.079446	-5.685558	3.154319	-0.051554	-4.753841	4.846023	-4.404915	-5.573574	3.284739	-3.427109	-5.875042	1.488904	-3.734039	-5.919426
50 µM Glu-	9.24889	3.094243	-7.703887	6.739161	2.18129	-7.036869	4.562308	0.433594	-5.065332	5.179439	-4.624104	-8.32236	5.083986	-4.694435	-7.926254	2.315464	-4.66678	-8.238308
50 µM Glu-	9.529569	2.883579	-7.716085	6.927279	1.95937	-7.355412	4.27552	0.046431	-4.637659	6.88665	-5.191875	-8.847981	5.119153	-4.461933	-7.740528	2.423694	-4.64732	-7.598156
50 µM Glu-	9.514509	2.147831	-7.426769	6.678389	1.850464	-7.366337	4.310345	0.21236	-6.220211	6.831001	-5.207577	-8.763741	4.793445	-4.528307	-7.181973	2.241379	-4.672585	-7.445202
50 µM Met-	7.923358	1.590302	-7.619663	6.935357	2.154696	-7.793102	4.095255	-0.248207	-6.06191	6.566064	-5.398087	-15.94539	4.620525	-5.01263	-8.177532	1.916695	-5.017071	-8.116081
50 µM Met-	7.353363	1.437012	-7.321217	6.322845	1.26152	-6.939571	4.604151	-0.100033	-5.86207	6.178218	-4.476955	-7.614514	3.884602	-5.630952	-8.334244	2.600546	-3.961761	-7.753159
50 µM Met-	7.450196	1.504269	-7.421204	6.060429	1.217484	-7.440765	4.621716	-0.086037	-6.271765	5.758706	-4.49036	-8.74359	4.589279	-4.314841	-8.157734	2.623079	-3.764425	-8.14954
50 µM Met-	8.101052	2.218845	-6.786957	6.023204	1.216294	-7.46502	4.474939	-0.056567	-5.933083	5.701945	-4.588972	-5.165863	4.275862	-5.080572	-8.604641	2.230113	-4.434618	-8.527485
50 µM Met-	7.363605	1.551384	-6.989057	5.905088	0.745647	-7.095598	4.081597	-0.077673	-6.327415	5.436792	-5.737111	-8.377603	4.428133	-4.02336	-8.407818	2.077501	-4.907818	-8.425404
50 µM Ser-	10.443497	3.154659	8.048481	2.108913	2.869375	8.269375	5.704708	0.043701	-4.967561	8.150905	-4.42028	-10.75931	6.573916	-4.515245	-9.31171	3.058723	-4.346193	-9.202797
50 µM Ser-	10.786276	3.632298	8.562309	2.082613	2.303565	8.170364	5.96839	-0.090475	-7.061796	7.683309	-5.531242	-10.29489	6.377262	-4.327076	-9.75111	3.201434	-4.208487	-9.152271
50 µM Ser-	11.246161	4.394333	7.960739	8.13998	2.181633	-8.428474	5.522074	-0.111984	-7.130421	7.489426	-4.244793	-9.62854	6.018094	-4.605328	-10.01502	3.006822	-4.135199	-9.300446
50 µM Ser-	11.677596	4.00478	-4.254753	4.824984	2.12786	-7.307956	5.437355	-0.598963	-7.317852	7.391624	-4.244804	-9.502362	6.125892	-4.232073	-9.157631	4.218846	-3.622396	-10.50768
50 µM Thr-	14.512461	4.422936	-7.112782	11.935814	4.191875	-11.25674	8.166952	0.860703	-9.810586	10.701604	-4.212357	-12.87709	8.394674	-3.826909	-11.57631	4.218846	-3.622396	-10.50768
50 µM Thr-	14.800274	4.912258	-7.112782	11.935812	4.092522	-11.31274	7.919427	0.682144	-10.02526	10.606691	-4.446911	-12.7197	8.384773	-4.585524	-13.07853	4.041652	-4.1789	-11.18402
50 µM Thr-	14.150904	3.985317	-12.41755	11.322294	2.939228	-12.21748	7.862411	0.210784	-10.60191	10.406281	-5.140241	-13.72024	8.290708	-4.8846	-13.14442	4.02424	-4.74189	-12.15466
50 µM Phe-	9.581429	4.388374	-7.222707	7.338682	3.350292	-8.298828	4.840219	0.310699	-6.965858	7.247866	-4.537247	-10.53994	6.363605	-4.166954	-9.417549	2.324844	-3.972345	-8.670876
50 µM Phe-	9.259474	4.305908	-7.887337	7.281668	3.546604	-8.31683	4.931436	0.222208	-6.240355	7.240355	-4.278686	-10.53994	6.152611	-3.635653	-9.562056	2.360261	-3.80532	-9.201091
50 µM Phe-	9.572552	4.12632	-6.869752	6.764427	3.92762	-8.199726	4.738819	0.105278	-6.910232	7.631032	-5.625777	-10.53994	6.569853	-3.294249	-9.65995	1.958006	-4.581085	-9.163879
50 µM Phe-	9.358446	4.350665	-7.274837	7.393695	3.626492	-8.695461	4.591988	0.238782	-7.041561	7.106826	-5.869924	-12.32459	7.118768	-3.189732	-11.37793	4.218846	-3.622396	-10.50768
50 µM Phe-	11.114372	4.221237	-7.288693	9.587914	3.899281	-7.390915	6.736397	0.155016	-5.682146	9.309506	-2.99556	-10.19256	8.421305	-2.903378	-9.520313	4.174121	-3.818369	-9.747009
50 µM Phe-	11.793106	4.657223	-7.813591	9.864799	4.952885	-7.162514	6.388787	0.104998	-5.604988	9.317172	-3.03141	-9.944008	8.045408	-				

	R1	G1	B1	R2	G2	B2	R3	G3	B3	R4	G4	B4	R5	G5	B5	R6	G6	B6
100 μM Gly	9.900311	6.205872	-2.612839	8.257767	5.662342	-3.830658	6.107546	3.077501	-2.141687	11.790031	5.933426	-5.543873	10.354389	5.163197	-4.622738	6.456812	3.145102	-3.731308
100 μM Gly	10.630589	6.322296	-2.8409	8.78013	5.884941	-3.61352	6.444178	3.335951	-1.962444	12.456127	5.956299	-5.320927	10.587915	4.85046	-5.014683	6.401503	3.098328	-3.443495
100 μM Gly	10.567085	5.962105	-2.846367	8.86548	5.854218	-3.606352	5.711186	3.218163	-2.265619	6.113476	-5.421989	10.059596	4.510071	-5.190849	6.544214	3.133152	-3.460566	
100 μM Gly	10.483101	5.994537	-3.364971	9.170364	5.904046	-3.781496	6.04575	2.880846	-2.307272	12.325367	5.761692	-5.425743	10.27791	4.603619	-5.153633	6.051554	2.721749	-3.849436
100 μM Ala	6.019119	3.250599	-2.501194	5.305908	3.966885	-1.842609	4.099352	2.333561	-0.99086	7.939571	4.044044	-3.236599	6.711504	3.759644	-3.124619	3.788664	2.234892	-1.748309
100 μM Ala	5.569817	3.332539	-2.558556	5.049164	3.907818	-2.17617	3.947422	2.171047	-1.046774	8.255035	4.250599	-3.681461	6.908844	3.820755	-3.091839	3.795494	2.27006	-1.724821
100 μM Ala	5.815979	3.232502	-2.616592	5.11301	3.722088	-2.232843	4.079208	2.10379	-0.986002	7.989418	3.867188	-3.775009	7.171047	3.390919	-2.920448	3.882895	2.165586	-1.745304
100 μM Ala	5.600204	3.279826	-2.591602	5.156364	3.81584	-2.004541	3.974974	2.177058	-1.054729	8.081257	4.001708	-3.769886	6.911301	3.826221	-3.088531	3.82144	2.187061	-1.752885
100 μM Val	7.723454	4.690678	-6.875727	5.141689	-0.87061	4.335609	2.435986	-2.129053	10.331852	5.762375	-4.114033	8.321955	3.688629	-4.901537	5.085354	2.848412	-2.740185	
100 μM Val	8.708088	5.466713	-2.671219	6.636736	4.939469	-3.210653	4.87898	2.575999	-1.915944	10.000343	5.024242	-4.195262	8.598446	3.899624	-4.536599	5.03076	2.687949	-2.770162
100 μM Val	8.399456	5.685902	-2.912197	6.772959	4.839195	-2.950908	5.192779	7.967026	4.951862	8.205262	3.700207	-4.806076	4.322294	1.721069	-3.555479			
100 μM Val	8.740185	5.524536	-2.542164	6.775009	4.991602	-3.251623	4.854647	2.55203	-0.24336	10.301128	5.12598	-5.291908	8.84568	3.923965	-4.97303	4.824856	2.117786	-3.485491
100 μM Leu	8.978832	5.70126	-2.603279	6.779787	4.775349	-3.612837	5.373165	2.941277	-1.785933	11.579723	3.857999	-3.855244	8.527483	4.543873	-5.155003	5.042336	2.52919	-3.205873
100 μM Leu	9.394333	6.046776	-2.141006	5.733968	5.700924	-2.580404	5.40321	2.965173	-1.665756	11.76067	6.28473	-4.417549	9.181633	4.859341	-4.612152	4.010584	1.581085	-4.078526
100 μM Leu	9.969616	6.419258	-1.939911	7.823637	5.725202	-2.81188	5.383747	2.920792	11.583477	6.172073	-4.153637	9.426959	4.90986	-4.22533	4.880846	2.275862	-3.307085	
100 μM Leu	9.888359	6.009764	-2.086376	6.785727	5.37624	-2.986002	5.184581	-2.975281	10.89449	5.762375	-4.114033	8.914959	4.811641	-4.790375	4.88426	2.026972	-3.642447	
100 μM Ile-	3.719357	1.311371	-1.5873	4.81871	3.12052	-3.63537	4.547626	2.180948	-1.9324	8.943325	4.180607	-5.631275	7.777054	3.403206	-4.793102	5.265278	2.379311	-3.48037
100 μM Ile-	3.114376	5.658585	5.413792	3.167974	5.179857	-4.179585	4.516558	2.950953	-1.921195	8.090105	4.453848	-3.61113	7.817345	3.188805	-4.976101	5.192217	2.530216	-3.467773
100 μM Ile-	3.391941	1.047115	-5.763058	4.881187	2.654835	-4.486856	4.593376	1.843973	-2.343803	9.2267	3.993172	-4.591818	8.092522	3.468671	-4.775005	5.185389	2.354048	-3.689655
100 μM Ile-	3.716969	1.251282	-6.026291	5.625473	3.05497	-4.572208	4.978151	2.184364	-2.480368	9.478321	4.589279	-5.670536	7.986687	3.269718	-5.444862	5.324343	2.128031	-3.815296
100 μM Glu	7.068283	3.206215	-6.584516	7.728785	4.471938	-6.025606	6.49392	3.162512	-2.916448	11.720296	5.140225	-4.107928	6.702629	4.315501	-4.240013			
100 μM Glu	6.937862	2.446228	-7.717084	7.97816	4.243036	-5.996364	5.535677	3.138613	-2.980198	13.90884	6.399799	-7.067817	10.99283	4.860703	-6.672924	6.811539	3.337317	-3.39843
100 μM Glu	6.708163	3.381016	-5.164946	8.099694	4.903381	-5.087231	6.358143	2.853191	-2.069307	11.226357	5.371113	-5.657223	6.920109	3.450325	-4.059748			
100 μM Glu	8.265961	3.934792	-6.636928	4.894496	4.749807	-5.479004	6.297276	2.678047	-3.267668	12.890747	5.99966	-7.240358	10.638169	6.202986	-6.56982	2.813931	-4.862816	
100 μM Me	8.024048	5.124791	-6.047447	11.671958	4.050873	-4.407648	8.09001	4.650734	-2.61251	15.270741	8.069469	-7.090816	13.91259	7.171104	-6.288494	8.125641	4.43121	-4.39126
100 μM Me	12.31649	7.677021	-5.055309	11.142473	7.85524	-4.711164	4.850323	4.76306	-3.089109	15.750427	8.89109	-7.356777	13.764425	6.961082	-7.097984	8.055651	4.361898	-4.757597
100 μM Me	12.412083	7.827927	-5.309319	11.42984	8.201096	-4.39365	8.545919	4.752132	-3.056334	15.55275	8.586891	-7.18573	13.978491	6.94162	-7.010925	8.04575	4.383747	-4.438375
100 μM Me	12.645271	7.774248	-6.128029	12.978832	7.772885	-5.045047	7.74875	6.054097	-6.163197	16.19374	8.494834	-6.986348	13.715533	6.953053	-7.059165	7.908501	4.294161	-7.92828
100 μM Ser	13.486855	8.131104	-6.486515	12.84568	8.19836	-5.786617	9.681461	5.064528	-4.06521	17.54287	6.948003	-7.347247	14.916464	6.788972	-8.349949	10.365995	5.344145	-5.472857
100 μM Ser	12.729599	8.130177	-6.494846	8.050765	8.258756	-5.931374	10.015364	4.938024	-4.23265	15.577374	6.923592	-8.863847	16.340046	7.784569	-8.486172	10.105837	4.923455	-5.800716
100 μM Tha	15.90099	10.24367	-5.853134	17.324684	7.174461	-4.44179	8.502218	5.391943	-5.153636	20.148514	11.736088	-10.38375	21.090134	11.197338	-10.5367	15.903357	4.876273	-7.259474
100 μM Tha	16.260838	10.34483	-8.132126	17.915329	11.581772	-7.602253	15.919765	8.310343	-4.952885	21.536018	12.796908	-10.5390	21.80809	11.457493	-10.15364	16.049505	8.292591	-7.538575
100 μM Tha	13.50933	11.030045	-7.635178	7.774248	7.744367	-4.424345	7.94875	6.054697	-6.054621	16.075113	12.913774	-10.476997	17.242847	11.28207	-10.3089	21.44827	11.978832	-16.283714
100 μM Pho	9.715453	7.303177	-4.330471	9.910206	7.365997	-4.414352	7.668488	4.74394	-3.733697	14.023012	8.676815	-11.645643	15.956452	12.892452	-11.12359	15.542847	8.03824	-8.508707
100 μM Pho	10.350971	7.185047	-5.129055	10.175827	7.272106	-5.006288	8.716969	5.616592	-3.92252	14.240747	9.516903	-6.875725	13.649029	8.007172	-6.641514	9.592693	6.326391	-5.147491
100 μM Pho	10.323662	7.384344	-5.982992	10.393993	7.174461	-4.544179	8.502218	5.391943	-3.668488	15.124275	9.703991	-7.407999	13.561881	8.031442	-7.210995	9.724138	5.79003	-6.252304
100 μM Glu	10.43428	3.267326	-7.281324	6.967948	6.037212	-5.68351	7.576988	3.915667	-3.218613	13.97377	6.376877	-7.346877	13.737767	6.80563	-7.186811	12.81118	3.038921	-5.456811
100 μM Glu	7.615566	3.027996	-7.586889	5.926802	5.573917	-5.760328	7.375119	3.60157	-3.457494	14.205604	5.985321	-6.126324	16.688972	6.689872	-6.653122	7.783884	3.907475	-5.325367
100 μM Asp	8.231136	3.554415	-8.945826	8.827587	5.053944	-5.9662	5.766674	3.876449	-3.736657	10.693057	7.678159	-7.794211	13.211712	6.756953	-7.480871	11.752132	3.758621	-5.331854
100 μM Asp	14.552406	10.918743	-6.441038	12.419254	7.797541	-5.153363	7.788668	-5.719749	-10.80505	12.456814	10.566573	10.98802	-12.356997	11.656881	-12.740574	14.688288	9.795492	-7.642642
100 μM Asp	14.706536	10.542164	-7.431889	13.881177	7.621776	-5.220887	9.808807	5.506317	10.69998	13.645114	-9.314785	20.940594	12.800957	-9.437351	15.197338	9.63059	-8.033798	
100 μM Asp	14.79044	11.014339	-7.229341	13.767923	9.170575	-7.040949	10.413184	5.639467	-5.531649	13.022998	13.630929	-10.05067	20.789656	12.802174	-10.10529	15.027211	9.423336	-8.171713
100 μM Asp	14.323567																	

	R7	G7	B7	R8	G8	B8	R9	G9	B9	R10	G10	B10	R11	G11	B11	R12	G12	B12	
100 μM Gly	12.372482	4.757938	-8.022873	9.196997	1.921474	-9.586208	7.007171	1.139639	-6.378286	9.5507	-4.092178	-9.985661	7.611813	-3.674974	-9.558895	3.732332	-3.93001	-9.869919	
100 μM Gly	12.746332	4.765789	-8.466337	9.621714	2.433937	-8.968933	5.903038	-0.607033	-7.732334	9.612838	-4.17617	-10.14817	7.334243	-3.858997	-9.600544	5.439057	-1.682486	-7.452713	
100 μM Gly	12.639128	4.427448	-8.700581	9.495049	2.435646	-9.029705	5.926596	-0.487881	-7.615568	9.483784	-4.254692	-10.39092	7.277911	-4.133152	-10.06316	3.415842	-4.133833	-9.883579	
100 μM Gly	12.144419	4.161831	-8.583473	9.028679	1.355751	-7.91492	6.269376	0.017412	-7.193924	8.936497	-4.768177	-10.69648	7.048668	-4.424036	-10.15364	3.770029	-4.055399	-10.01263	
100 μM Ala	7.618641	3.487198	-5.291908	6.080233	2.236254	-5.307953	4.410378	0.794128	-3.725504	6.336975	-3.303919	-6.718334	5.040402	-3.13315	-6.623081	2.792421	-2.996244	-6.793106	
100 μM Ala	7.544214	3.313759	-5.514511	6.172071	2.191193	-5.246841	4.35029	0.9911465	-3.728235	6.191193	-3.116081	-6.51656	4.872312	-2.920107	-6.432571	2.73438	-3.031069	-6.951859	
100 μM Ala	8.434961	3.517582	-5.993515	6.336292	2.16695	-5.320244	4.462957	0.70104	-3.910892	6.337317	-3.011951	-6.264595	4.944691	-3.23728	-6.242405	2.607716	-3.451008	-6.812222	
100 μM Ala	7.756229	3.25937	-5.514511	6.039946	1.935062	-5.2873	4.261079	0.86528	-4.048479	6.183681	-3.288527	-6.768181	4.876067	-3.091364	-6.59044	2.558211	-3.385524	-6.888392	
100 μM Val	10.41653	4.041653	-7.611813	7.732674	2.438377	-7.417889	5.530215	0.499146	-7.423477	5.90493	-4.742377	-10.45014	-9.450211	-6.262206	-9.234211	3.628542	-3.447725	-9.343121	
100 μM Val	10.176512	3.743938	-7.882896	7.808466	2.352647	-7.452406	5.574632	0.29464	-6.05121	7.547285	-4.709797	-9.402731	5.964152	-3.907476	-8.970467	3.281632	-3.543834	-8.996367	
100 μM Val	10.729259	3.390573	-7.909866	7.857288	2.390912	-7.32093	5.358826	-0.17412	-6.53875	6.52918	-5.065891	-7.95828	5.847879	-3.444521	-9.123592	3.322502	-4.009218	-9.210651	
100 μM Val	9.934041	3.930147	-7.964493	7.882827	2.508022	-7.440079	5.4676	-0.285421	-6.036497	7.26801	-4.610447	-9.531345	5.858928	-4.034755	-9.058519	3.303516	-3.496414	-8.840904	
100 μM Leu	10.754866	4.543873	-7.812565	8.403893	2.969273	-7.989758	5.845681	0.553774	-6.233187	7.844998	-4.028336	-9.541481	6.547968	-3.813246	-9.510075	3.889041	-3.544212	-9.807102	
100 μM Leu	10.786274	4.593033	-7.912598	8.489244	2.973026	-8.090134	5.981222	0.693411	-6.141685	7.891088	-3.421796	-9.466603	6.268692	-3.73742	-8.979176	3.211335	-3.557188	-9.731308	
100 μM Leu	10.714597	4.183338	-7.861042	8.267326	2.035242	-8.066235	5.781837	0.444521	-6.190166	7.673949	-3.963176	-9.176853	5.930352	-4.099691	-8.678387	2.941618	-3.864548	-9.301128	
100 μM Leu	10.752304	4.765648	-8.009216	7.945715	2.884941	-8.0422	4.60667	0.447798	-6.216253	7.445887	-4.039126	-9.680095	5.986002	-4.075623	-9.640491	3.394333	-4.079993	-9.356094	
100 μM Ile	10.466028	3.241039	-9.601231	6.808398	2.551041	-8.589962	5.86036	0.253328	-6.573574	8.617617	-3.528847	-10.48959	7.407989	-3.202118	-9.131786	4.068665	-4.09457	-10.09491	
100 μM Ile	10.712299	3.390573	-8.23079	7.820759	2.100716	-8.631615	6.055651	0.245134	-6.806417	8.715144	-4.100337	-10.74257	7.438034	-3.626493	-9.51622	3.868556	-3.780128	-10.02219	
100 μM Ile	11.104132	3.598843	-9.013313	8.23148	1.90065	-8.840218	5.89143	0.052919	-6.948446	8.305564	-3.692047	-10.365665	7.098669	-3.821080	-9.56572	3.841243	-4.081598	-10.02185	
100 μM Ile	10.998974	3.309662	-9.419598	8.16456	1.996929	-8.801636	5.732674	-0.11574	-7.030046	8.345852	-3.970638	-10.29123	6.626493	-4.392628	3.727893	-4.221918	-9.780128		
100 μM Glu	10.786596	5.87065	-9.39177	10.409355	2.987709	-10.22124	7.261522	1.186411	-7.003177	10.458177	-4.272277	-12.29601	7.720313	-4.790341	-12.23592	4.596449	-3.893822	-11.79413	
100 μM Glu	14.017752	5.303173	-9.941277	10.514511	2.666633	-11.01809	7.255377	0.74155	-8.182314	10.4493	-2.611614	-12.45151	7.802321	-4.327759	-12.29498	3.993513	-4.442814	-11.52475	
100 μM Glu	13.790712	5.002731	-9.89143	10.576647	2.497437	-10.72516	7.105839	0.62454	-8.058039	10.148173	-4.889385	-12.40938	7.736084	-4.167292	-11.34415	3.5898	-4.166269	-11.21133	
100 μM Glu	13.149538	4.344147	-10.33083	10.431547	2.38887	-10.92933	6.936156	0.393991	-8.20729	10.36975	-4.472515	-12.06077	7.630932	-4.696482	-12.06077	4.176852	-4.841583	-12.34824	
100 μM Me	10.466372	6.703312	-8.23079	5.285763	-10.8876	8.426767	2.331854	-7.974392	12.0676	-3.21113	-14.36114	10.04749	-2.94452	-10.24204	-13.21133	5.188801	-3.827929	-12.90543	
100 μM Me	10.707066	7.659745	-10.66541	13.1451	5.801296	-11.09457	8.379993	0.215793	-8.424717	11.75694	-3.434394	-14.2127	9.667805	-3.2943	-13.86378	4.755548	-3.825878	-12.60403	
100 μM Me	15.711849	8.646024	-10.48618	13.01915	5.610104	-10.86719	8.18846	1.718674	-8.626833	11.689653	-3.674976	-13.95015	9.506315	-3.876751	-14.29088	4.786617	-4.306248	-12.64254	
100 μM Me	15.717967	6.80321	-10.4592	12.897575	2.705121	-11.12154	10.474157	1.720313	-7.200572	11.791056	-3.665975	-13.96446	9.536634	-3.18334	-12.48849	4.822806	-4.404301	-12.93366	
100 μM Ser	18.77944	7.925915	-11.79208	16.050871	7.037212	-12.29191	9.829293	2.712872	-7.957597	15.213725	-3.733353	-15.9948	12.040628	-3.080231	-16.50563	6.826903	-4.112326	-14.94606	
100 μM Ser	18.69278	7.767498	-11.206211	7.06282	-13.02971	10.267204	2.717595	-9.934446	15.180609	-2.220121	-16.74016	11.841926	-2.993126	-16.17276	6.567088	-4.174463	-14.66337		
100 μM Ser	18.696827	7.723114	-12.44281	6.148378	7.367702	-12.49334	9.978088	2.846704	-8.946458	15.045408	-2.258793	-16.25162	11.757597	-2.92523	-16.14715	6.564698	-4.199387	-14.713131	
100 μM Ser	18.85937	7.88857	-12.38857	10.540559	7.172413	-12.96825	9.853192	-0.03745	-7.74059	10.3049	14.998566	-2.377945	-16.865693	11.767463	-3.041174	-16.50297	5.672891	-4.196825	-15.04005
100 μM Tha	25.39604	11.412769	-14.86958	12.339976	2.043427	-14.71287	14.94691	5.512461	-11.37351	22.39311	-3.12093	-19.17583	17.227039	-3.662342	-19.48549	9.757937	-4.077843	-17.71492	
100 μM Tha	26.184364	11.626835	-14.354054	23.406963	10.409698	-15.39672	15.02902	5.402185	-15.62581	22.461592	-1.554111	-18.67771	16.86924	-5.393776	-19.06077	9.405258	-3.992147	-17.31478	
100 μM Tha	26.182728	11.385799	-14.22875	23.822123	10.449986	-15.309605	15.001034	5.345852	-15.702204	20.70013	-1.500975	-19.694881	16.664469	-4.704085	-17.82759	9.373849	-3.987709	-16.64687	
100 μM Tha	25.156923	5.817345	-11.63708	12.080894	3.302492	-9.568794	8.100376	1.197082	-7.451006	12.101999	-3.502367	-11.77554	9.488222	-3.483099	-11.58894	5.424718	-3.25094	-9.810173	
100 μM Tha	15.019119	5.490269	-14.48754	21.91276	2.917036	-10.38614	8.225332	0.105693	-7.09457	12.16183	-3.87484	-11.38511	9.3875976	-3.457493	-11.42711	5.529191	-3.193922	-9.318197	
100 μM Asp	23.582451	11.629052	-14.704174	21.91278	2.142616	-13.61	14.6364	4.746723	-10.42169	11.36119	-2.059963	-12.59516	11.598156	-1.495049	-19.9604	9.200068	-4.363947	-16.9423	
100 μM Asp	24.23187	12.744961	-14.39194	21.839419	2.983714	-15.19802	14.016047	7.264254	-12.03176	20.889038	2.340005	-17.60703	15.442403	-5.029023	-15.42403	5.653465	-3.788666	-14.43257	
100 μM Asp	24.286174	12.76282	-14.70027	21.749037	1.991122	-15.04326	14.271082	7.302085	-12.09095	19.024925	-3.081926	-15.49883	15.527995	-18.0974	8.359781	-1.780914	-15.90816		
100 μM Asp	25.178217	11.248585	-14.400408	21.69553	2.147217	-12.34759	18.725574	1.036677	-12.02277	19.734644	-3.044147	-13.90988	15.097791	-4.227722	-18.82417	9.872312	-3.626493	-17.30632	
100 μM Asp	25.46876	11.102075	-16.0962	21.472176	1.724486	-12.461593	14.34415	1.											