Electronic Supplementary Material (ESI) for Molecular BioSystems.

Supplementary materials:

Features of S-Nitrosylation Based on Statistical Analysis and Molecular Dynamic Simulation: Cysteine Acidity, Surrounding Basicity, Steric Hindrance and Local Flexibility

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	3.5	4	4.5	5	5.5	6	6.5	7	7.5	8
Ser_C	0.250	0.925	0.485	0.377	0.909	0.892	0.647	0.877	0.769	0.458
Ser_O	0.516	0.777	0.114	0.376	0.892	0.810	0.845	0.756	0.886	0.236
Ser_N	0.896	0.531	0.100	0.203	0.204	0.340	0.919	0.187	0.778	0.509
Ser_CA	**0.014**	0.372	0.296	0.179	0.057	0.432	0.966	0.799	0.538	0.643
Ser_C*	0.082	0.520	0.087	0.253	0.729	0.376	0.537	0.184	0.591	0.321
Ser_O*	0.080	0.324	1.000	0.226	0.424	0.527	0.422	0.170	0.406	0.513
Thr_C	1.000	0.139	0.099	0.463	0.979	0.559	0.333	0.789	0.606	0.754
Thr_O	0.383	0.104	0.447	0.195	0.193	0.283	0.992	0.472	0.625	0.191
Thr_N	0.458	0.247	0.370	0.085	0.074	0.829	0.925	0.875	0.793	0.306
Thr_CA	1.000	0.996	0.362	**0.021**	0.115	0.363	0.297	0.543	0.411	0.625
Thr_C*	0.828	0.590	0.165	0.251	0.556	0.300	0.078	0.122	0.395	0.282
Thr_O*	0.180	0.921	0.600	0.292	0.234	0.168	0.172	0.368	0.360	0.652
Cys_C	0.066	**0.005**	**0.000**	**0.000**	**0.000**	**0.000**	**0.000**	**0.000**	**0.000**	**0.000**
Cys_O	**0.044**	**0.004**	**0.001**	**0.000**	**0.000**	**0.000**	**0.000**	**0.000**	**0.000**	**0.000**
Cys_N	0.508	0.055	**0.000**	**0.000**	**0.000**	**0.000**	**0.000**	**0.000**	**0.000**	**0.000**
Cys_CA	**0.000**	**0.000**	**0.000**	**0.000**	**0.000**	**0.000**	**0.000**	**0.000**	**0.000**	**0.000**
Cys_C*	**0.000**	**0.000**	**0.000**	**0.000**	**0.000**	**0.000**	**0.000**	**0.000**	**0.000**	**0.000**
Cys_S*	**0.000**	**0.000**	**0.000**	**0.000**	**0.000**	**0.000**	**0.000**	**0.000**	**0.000**	**0.000**
Pro_C	0.563	0.896	0.951	0.724	0.867	0.548	0.272	0.153	0.249	0.099
Pro_O	0.710	0.942	0.907	0.977	0.390	0.652	0.395	0.462	0.260	**0.044**
Pro_N	0.103	0.336	0.537	0.103	0.300	0.540	0.417	0.475	0.335	0.376
Pro_CA	0.563	0.912	0.617	0.652	0.764	0.584	0.754	0.382	0.342	0.341
Pro_C*	0.439	0.591	0.910	0.830	0.795	0.635	0.537	0.660	0.464	0.583
Asn_C	0.563	0.596	0.317	0.757	0.465	0.809	0.895	0.432	0.400	0.863
Asn_O	0.500	0.403	0.404	0.377	0.607	0.500	0.988	0.666	0.330	0.922
Asn_N	0.640	0.757	0.710	0.570	0.340	0.302	0.511	0.855	0.746	0.986
Asn_CA	0.563	0.509	0.672	0.970	0.526	0.830	0.828	0.931	0.618	0.923
Asn_C*	0.742	0.324	0.795	0.675	0.865	0.646	0.914	0.669	0.309	0.082
Asn_O*	0.832	0.289	0.175	0.175	0.266	0.361	0.442	0.061	**0.030**	**0.007**
Asn_N*	0.509	0.607	0.935	0.898	0.358	0.115	0.154	0.219	0.260	0.220
Gln_C	0.413	0.169	0.807	0.683	0.852	0.881	0.619	0.755	0.715	0.102
Gln_O	0.054	0.482	0.286	0.471	0.706	0.937	0.876	0.889	0.835	0.684
Gln_N	0.997	0.203	0.131	0.924	0.962	0.417	0.192	0.204	0.226	0.169

Gln_CA	1.000	0.316	0.214	0.906	0.820	0.859	0.739	0.500	0.260	0.356
Gln_C*	0.508	0.304	0.976	0.502	0.631	0.845	0.770	0.847	0.983	0.774
Gln_O*	0.219	0.839	0.342	0.958	0.457	0.940	0.508	0.917	0.704	0.727
Gln_N*	0.250	0.552	0.190	0.298	0.585	0.788	0.854	0.675	0.950	0.506

Supplementary Table S2 The hypothesis test for atoms of acidic amino acids. The atoms were categorized into eight types including carbon of main chain (C), alpha carbon of main chain (CA), nitrogen of main chain (N), oxygen of main chain (O), carbon of side chain (C*), nitrogen of side chain (N*), oxygen of side chain (O*) and sulfur of side chain (S*). The atoms were obtained with different distant thresholds (5, 5.5, 6, 6.5, 7, 7.5 and 8 Å), where the distance was from the atoms of neighboring residue to the sulfur of cysteine in protein structures.

	3.5	4	4.5	5	5.5	6	6.5	7	7.5	8
Asp_C	**0.005**	0.106	0.902	0.191	0.529	0.472	0.204	0.503	0.351	0.702
Asp_O	**0.018**	0.525	0.606	0.801	0.457	0.599	0.466	0.300	0.195	0.956
Asp_N	0.179	0.065	0.123	0.851	0.464	0.349	0.971	0.999	0.911	0.579
Asp_CA	**0.014**	0.183	0.394	0.246	0.886	0.981	0.644	0.728	0.998	0.446
Asp_C*	0.741	0.222	0.245	0.353	0.325	0.778	0.969	0.567	0.346	0.454
Asp_O*	0.326	0.289	0.350	0.651	0.526	0.205	0.267	0.890	0.864	0.721
Glu_C	0.997	0.900	0.699	0.234	0.321	0.840	0.182	0.143	0.074	0.260
Glu_O	0.790	0.814	0.457	0.677	0.722	0.628	0.409	0.170	0.188	0.095
Glu_N	0.719	0.847	0.481	0.883	0.546	0.113	0.104	**0.039**	**0.030**	**0.009**
Glu_CA	1.000	0.508	0.950	0.900	0.682	0.946	0.295	0.223	0.214	**0.022**
Glu_C*	0.384	0.672	0.495	0.396	0.546	0.996	0.589	0.301	0.804	0.730
Glu_O*	0.682	0.806	0.677	0.182	3.000	0.632	0.222	0.463	0.823	0.437

Supplementary Table S3 The hypothesis test for atoms of basic amino acids. The atoms were categorized into eight types including carbon of main chain (C), alpha carbon of main chain (CA), nitrogen of main chain (N), oxygen of main chain (O), carbon of side chain (C*), nitrogen of side chain (N*), oxygen of side chain (O*) and sulfur of side chain (S*). The atoms were obtained with different distant thresholds (5, 5.5, 6, 6.5, 7, 7.5 and 8 Å), where the distance was from the atoms of neighboring residue to the sulfur of cysteine in protein structures.

	3.5	4	4.5	5	5.5	6	6.5	7	7.5	8
Lys_C	0.441	0.812	0.338	0.742	0.448	0.729	0.905	0.437	0.388	0.242
Lys_O	0.328	0.725	0.516	0.497	0.480	0.528	0.318	0.220	0.250	0.301
Lys_N	0.123	0.062	0.629	0.418	0.436	0.486	0.880	0.909	0.581	0.321
Lys_CA	0.413	0.678	0.271	0.134	0.238	0.850	0.732	0.556	0.773	0.346
Lys_C*	0.180	0.182	0.600	0.970	0.664	0.897	0.704	0.813	0.617	0.896
Lys_N*	0.332	0.867	0.893	0.990	0.869	0.661	0.375	0.884	0.682	0.929
Arg_C	0.563	0.609	0.629	0.815	0.501	0.853	0.379	0.509	0.216	0.130
Arg_O	0.356	0.380	0.225	0.363	0.676	0.521	0.264	0.153	0.224	0.332
Arg_N	0.762	0.438	0.881	0.374	0.625	0.912	0.958	0.359	0.467	0.092
Arg_CA	1.000	0.418	0.342	0.367	0.405	0.824	0.283	0.535	0.291	0.285
Arg_C*	**0.014**	0.351	0.728	0.999	0.547	0.741	0.660	0.269	0.080	0.183
Arg_N*	0.551	0.960	0.299	0.694	0.669	0.575	0.333	0.419	0.893	0.791
His_C	**0.021**	**0.016**	0.064	**0.031**	0.095	0.528	0.858	0.842	0.597	0.589
His_O	0.867	0.272	0.937	0.705	0.438	0.781	0.489	0.998	0.797	0.964
His_N	0.102	0.415	0.771	0.532	0.691	0.768	0.973	0.610	0.774	0.620
His_CA	**0.014**	0.071	0.285	**0.019**	0.150	0.217	0.456	0.842	0.919	0.920
His_C*	0.180	0.298	0.788	0.430	0.476	0.281	0.267	0.582	0.787	0.960
His_N*	0.101	**0.004**	0.231	0.333	0.469	0.748	0.708	0.741	0.662	0.359

Supplementary Table S4 The hypothesis test for atoms of aromatic amino acids. The atoms were categorized into eight types including carbon of main chain (C), alpha carbon of main chain (CA), nitrogen of main chain (N), oxygen of main chain (O), carbon of side chain (C*), nitrogen of side chain (N*), oxygen of side chain (O*) and sulfur of side chain (S*). The atoms were obtained with different distant thresholds (5, 5.5, 6, 6.5, 7, 7.5 and 8 Å), where the distance was from the atoms of neighboring residue to the sulfur of cysteine in protein structures.

	3.5	4	4.5	5	5.5	6	6.5	7	7.5	8
Phe_C	0.563	0.521	**0.024**	0.169	0.118	0.063	**0.036**	0.082	0.076	0.134
Phe_O	0.337	0.063	0.069	0.081	0.237	0.107	0.108	0.164	**0.035**	**0.010**
Phe_N	0.332	0.135	0.258	0.187	0.274	0.053	**0.030**	**0.004**	**0.018**	**0.030**
Phe_CA	0.563	0.337	**0.036**	**0.015**	0.196	**0.013**	0.191	**0.044**	**0.016**	**0.008**
Phe_C*	0.629	0.623	**0.020**	**0.019**	**0.032**	**0.036**	**0.023**	**0.005**	**0.007**	**0.009**
Tyr_C	1.000	0.705	0.446	0.224	0.278	0.448	0.622	0.576	0.429	0.329
Tyr_O	0.477	0.057	0.131	0.098	0.079	0.102	0.288	0.676	0.473	0.504
Tyr_N	0.071	0.666	0.757	0.449	0.383	0.671	0.796	0.528	0.294	0.460
Tyr_CA	1.000	0.083	0.481	0.669	0.725	0.586	0.617	0.491	0.806	0.638
Tyr_C*	0.886	0.492	0.211	0.509	0.671	0.874	0.979	0.832	0.626	0.633
Tyr_O*	**0.034**	0.080	**0.044**	0.408	0.256	0.693	0.147	0.122	0.107	0.165
Trp_C	0.563	0.596	0.238	0.156	0.602	0.815	0.960	0.803	0.994	0.999
Trp_O	0.103	0.626	0.378	0.248	0.340	0.726	0.883	0.938	0.912	0.764
Trp_N	0.071	0.886	0.734	0.520	0.555	0.408	0.532	0.904	0.611	0.794
Trp_CA	1.000	0.710	0.910	0.939	0.311	0.552	0.818	0.904	0.795	0.821
Trp_C*	0.274	0.468	0.728	0.817	0.612	0.363	0.572	0.533	0.878	0.835
Trp_N*	0.219	0.117	0.070	0.171	0.257	0.952	0.484	0.528	0.685	0.909

Supplementary Table S5 The hypothesis test for atoms of aliphatic amino acids. The atoms were categorized into eight types including carbon of main chain (C), alpha carbon of main chain (CA), nitrogen of main chain (N), oxygen of main chain (O), carbon of side chain (C*), nitrogen of side chain (N*), oxygen of side chain (O*) and sulfur of side chain (S*). The atoms were obtained with different distant thresholds (5, 5.5, 6, 6.5, 7, 7.5 and 8 Å), where the distance was from the atoms of neighboring residue to the sulfur of cysteine in protein structures.

	3.5	4	4.5	5	5.5	6	6.5	7	7.5	8
Gly_C	0.557	0.613	0.505	0.839	0.761	0.813	0.698	0.914	0.631	0.484
Gly_O	0.938	0.809	0.672	0.275	0.463	0.457	0.609	0.379	0.898	0.885
Gly_N	**0.008**	0.054	0.216	0.082	**0.016**	**0.006**	**0.043**	0.162	0.300	0.796
Gly_CA	0.719	0.997	0.529	0.220	0.178	0.161	0.182	0.633	0.483	0.447
Ala_C	**0.021**	0.615	0.688	0.911	0.699	0.536	0.663	0.313	0.246	0.312
Ala_O	0.541	0.590	0.932	0.373	0.480	0.633	0.965	0.621	0.529	0.746
Ala_N	0.295	0.961	0.712	0.842	0.699	0.755	0.489	0.896	0.721	0.387
Ala_CA	0.084	0.833	0.708	0.757	0.617	0.577	0.731	0.997	0.427	0.559
Ala_C*	0.843	0.563	0.984	0.471	0.316	0.511	0.805	0.941	0.875	0.652
Val_C	0.416	0.663	0.620	0.549	0.334	0.327	0.509	0.718	0.501	0.999
Val_O	0.529	0.363	0.756	0.956	0.841	0.993	0.373	0.949	0.498	0.493
Val_N	0.349	0.222	0.272	0.195	0.106	0.063	0.496	0.846	0.962	0.749
Val_CA	1.000	0.898	0.384	0.697	0.295	0.753	0.419	0.424	0.999	0.979
Val_C*	**0.028**	0.398	0.415	0.411	0.554	0.605	0.739	0.704	0.543	0.784
Leu_C	0.413	0.816	0.344	0.461	0.450	0.684	0.201	0.627	0.365	0.178
Leu_O	0.710	0.778	0.697	0.699	0.758	0.731	0.626	0.326	0.433	0.294
Leu_N	0.165	0.447	0.953	0.437	**0.042**	**0.007**	**0.042**	**0.026**	**0.035**	0.057
Leu_CA	0.413	0.604	0.798	0.408	0.064	**0.033**	**0.019**	**0.035**	0.184	0.094
Leu_C*	0.610	0.134	0.061	**0.039**	**0.010**	**0.012**	**0.010**	**0.013**	**0.011**	**0.030**
Ile_C	0.416	0.653	0.789	0.574	0.338	0.412	0.272	0.411	0.428	0.407
Ile_O	0.607	0.956	0.704	0.472	0.584	0.332	0.348	0.624	0.297	0.228
Ile_N	0.509	0.802	0.239	0.443	0.245	0.114	0.111	0.136	0.234	0.210
Ile_CA	0.563	0.843	0.858	0.888	0.501	0.621	0.597	0.191	0.191	0.349
Ile_C*	0.249	0.600	0.589	0.837	0.496	0.506	0.861	0.472	0.152	0.177
Met_C	0.563	0.995	0.525	0.327	0.378	0.386	0.438	0.211	0.229	0.938
Met_O	0.567	0.852	0.707	0.616	0.194	0.258	0.360	0.485	0.555	0.269
Met_N	0.413	0.882	0.824	0.521	0.698	0.719	0.664	0.919	0.667	0.757
Met_CA	0.563	0.118	0.663	0.858	0.349	0.367	0.832	0.457	0.501	0.290
Met_C*	0.688	0.683	0.889	0.675	0.600	0.408	0.358	0.500	0.853	0.610
Met_S*	0.416	0.736	0.825	0.415	0.559	0.672	0.989	0.938	0.528	0.714

Supplementary Table S6.1 The percentage difference values of different types of atoms around the sulfur of cysteine with the distance of 3.5 Å. The atoms were categorized into eight types including carbon of main chain (C), alpha carbon of main chain (CA), nitrogen of main chain (N), oxygen of main chain (O), carbon of side chain (C*), nitrogen of side chain (N*), oxygen of side chain (O*) and sulfur of side chain (S*).

	C	O	N	CA	C*	O*	N*	S*
SER	0.41%	-0.63%	0.41%	0.62%	-0.93%	1.64%	-	-
THR	0.00%	0.82%	0.51%	0.00%	0.41%	0.92%	-	-
CYS	-1.35%	-1.24%	0.41%	-6.64%	-12.87%	-	-	-11.84%
PRO	-0.10%	0.30%	0.82%	-0.10%	0.93%	-	-	-
ASN	-0.10%	-0.42%	0.20%	-0.10%	0.00%	0.00%	-0.31%	-
GLN	-0.21%	-1.14%	0.00%	0.00%	-0.62%	-0.73%	0.41%	-
ASP	1.34%	2.06%	0.72%	0.62%	0.10%	1.03%	-	-
GLU	0.00%	0.20%	0.20%	0.00%	1.23%	-0.42%	-	-
LYS	0.31%	0.72%	1.13%	-0.21%	0.62%	-	-0.52%	-
ARG	-0.10%	0.62%	0.20%	0.00%	1.44%	-	0.51%	-
HIS	0.83%	-0.11%	1.44%	0.62%	0.51%	-	-0.93%	-
PHE	-0.10%	-1.05%	-0.52%	-0.10%	0.50%	-	-	-
TYR	0.00%	-0.52%	0.72%	0.00%	0.30%	1.13%	-	-
TRP	-0.10%	0.82%	0.72%	0.00%	1.34%	-	-0.73%	-
GLY	-0.42%	0.09%	2.37%	0.20%	-	-	-	-
ALA	0.83%	-0.63%	-0.83%	0.31%	-0.11%	-	-	-
VAL	0.21%	0.71%	-0.62%	0.00%	2.37%	-	-	-
LEU	-0.21%	-0.54%	1.13%	-0.21%	-0.43%	-	-	-
ILE	0.21%	0.51%	-0.31%	-0.10%	-1.14%	-	-	-
MET	-0.10%	0.41%	-0.21%	-0.10%	-0.01%	-	-	0.21%

Supplementary Table S6.2 The percentage difference values of different types of atoms around the sulfur of cysteine with the distance of 4 Å. The atoms were categorized into eight types including carbon of main chain (C), alpha carbon of main chain (CA), nitrogen of main chain (N), oxygen of main chain (O), carbon of side chain (C*), nitrogen of side chain (N*), oxygen of side chain (O*) and sulfur of side chain (S*).

	C	O	N	CA	C*	O*	N*	S*
SER	0.09%	-0.13%	1.12%	-0.94%	0.60%	1.43%	-	-
THR	1.44%	2.35%	1.23%	0.00%	1.94%	-0.12%	-	-
CYS	-3.01%	-3.32%	-2.81%	-11.63%	-13.61%	-	-	-12.90%
PRO	0.41%	0.29%	1.12%	-0.01%	1.61%	-	-	-
ASN	-0.31%	-0.84%	0.09%	-0.31%	-1.25%	-1.15%	0.51%	-
GLN	-1.04%	-0.73%	1.13%	-0.31%	-2.08%	0.20%	0.41%	-
ASP	1.54%	0.91%	2.36%	0.82%	1.12%	1.53%	-	-
GLU	-0.11%	0.19%	-0.22%	0.41%	0.70%	0.50%	-	-
LYS	-0.21%	-0.43%	2.26%	0.30%	2.66%	-	-0.11%	-
ARG	0.41%	-1.05%	1.12%	-0.52%	0.80%	-	-0.03%	-
HIS	1.55%	-1.15%	1.23%	1.03%	0.81%	-	4.02%	-
PHE	-0.52%	-2.71%	-1.67%	-0.83%	0.30%	-	-	-
TYR	0.61%	-1.98%	0.40%	1.23%	3.65%	1.64%	-	-
TRP	-0.31%	-0.63%	0.10%	-0.21%	-1.38%	-	-1.25%	-
GLY	0.91%	-0.45%	3.18%	0.28%	-	-	-	-
ALA	0.50%	0.69%	-0.02%	-0.22%	-1.48%	-	-	-
VAL	-0.64%	2.34%	-1.36%	0.20%	2.71%	-	-	-
LEU	0.09%	0.67%	0.91%	-0.53%	-5.80%	-	-	-
ILE	-0.42%	0.08%	0.30%	-0.11%	-2.86%	-	-	-
MET	0.00%	0.09%	-0.11%	0.93%	-0.65%	-	-	0.20%

Supplementary Table S6.3 The percentage difference values of different types of atoms around the sulfur of cysteine with the distance of 4.5 Å. The atoms were categorized into eight types including carbon of main chain (C), alpha carbon of main chain (CA), nitrogen of main chain (N), oxygen of main chain (O), carbon of side chain (C*), nitrogen of side chain (N*), oxygen of side chain (O*) and sulfur of side chain (S*).

	C	O	N	CA	C*	O*	N*	S*
SER	1.51%	-2.83%	2.65%	1.73%	3.26%	0.27%	-	-
THR	3.17%	1.92%	1.12%	1.12%	4.90%	0.70%	-	-
CYS	-7.27%	-5.71%	-8.94%	-12.47%	-14.97%	-	-	-13.12%
PRO	0.39%	0.28%	0.80%	-0.84%	0.11%	-	-	-
ASN	-1.47%	-1.16%	-0.63%	-0.42%	-1.06%	-1.77%	0.50%	-
GLN	-0.33%	-1.57%	1.74%	-1.15%	-1.38%	1.12%	1.23%	-
ASP	0.07%	1.51%	2.35%	1.02%	2.54%	3.69%	-	-
GLU	-0.75%	-1.37%	0.80%	-0.02%	0.25%	0.48%	-	-
LYS	1.62%	1.10%	0.70%	1.63%	1.80%	-	-0.11%	-
ARG	-0.44%	-2.10%	0.60%	1.12%	-0.90%	-	-3.88%	-
HIS	2.87%	0.19%	0.81%	1.64%	2.22%	-	3.59%	-
PHE	-3.65%	-3.34%	-1.57%	-2.70%	-6.27%	-	-	-
TYR	-0.95%	-2.19%	0.29%	1.12%	4.38%	2.56%	-	-
TRP	-1.25%	-1.15%	0.30%	0.10%	0.13%	-	-1.87%	-
GLY	1.79%	-0.89%	2.64%	2.43%	-	-	-	-
ALA	1.08%	-0.37%	0.79%	0.27%	0.04%	-	-	-
VAL	-0.26%	1.59%	-2.20%	-1.27%	6.62%	-	-	-
LEU	-3.27%	1.47%	0.16%	0.27%	-12.17%	-	-	-
ILE	0.06%	-1.49%	-2.09%	-0.22%	-2.05%	-	-	-
MET	-0.64%	0.70%	-0.22%	0.50%	-1.71%	-	-	-0.34%

Supplementary Table S6.4 The percentage difference values of different types of atoms around the sulfur of cysteine with the distance of 5 Å. The atoms were categorized into eight types including carbon of main chain (C), alpha carbon of main chain (CA), nitrogen of main chain (N), oxygen of main chain (O), carbon of side chain (C*), nitrogen of side chain (N*), oxygen of side chain (O*) and sulfur of side chain (S*).

	C	O	N	CA	C*	O*	N*	S*
SER	2.00%	-2.24%	2.63%	3.04%	3.14%	2.11%	-	-
THR	1.90%	4.89%	3.16%	4.50%	2.59%	1.51%	-	-
CYS	-17.34%	-11.11%	-14.03%	-15.28%	-15.81%	-	-	-14.99%
PRO	-0.36%	0.68%	2.84%	0.98%	2.02%	-	-	-
ASN	-0.76%	-1.69%	-1.07%	-0.23%	-0.77%	-2.30%	0.18%	-
GLN	0.69%	-1.17%	0.07%	0.08%	-0.99%	-0.12%	0.91%	-
ASP	-3.26%	1.18%	-0.56%	2.13%	4.28%	1.71%	-	-
GLU	-3.15%	-0.98%	0.47%	-0.04%	3.51%	2.32%	-	-
LYS	0.15%	-2.13%	1.70%	3.47%	1.03%	-	-0.02%	-
ARG	0.37%	-1.39%	-2.00%	1.62%	-4.47%	-	-2.05%	-
HIS	4.41%	1.21%	-0.13%	3.90%	5.09%	-	2.86%	-
PHE	-2.33%	-3.88%	-2.52%	-4.59%	-13.46%	-	-	-
TYR	-1.90%	-3.14%	1.21%	1.09%	7.27%	1.10%	-	-
TRP	-2.29%	-1.67%	0.81%	-0.12%	-1.78%	-	-1.67%	-
GLY	0.32%	-2.89%	5.91%	4.25%	-	-	-	-
ALA	0.11%	1.87%	-1.11%	0.32%	-1.74%	-	-	-
VAL	-1.44%	-0.10%	-3.58%	-1.31%	7.75%	-	-	-
LEU	-1.97%	2.26%	-1.84%	-2.77%	-21.88%	-	-	-
ILE	-1.21%	-2.15%	-2.33%	0.47%	-0.63%	-	-	-
MET	-0.65%	-0.75%	1.11%	0.08%	-4.54%	-	-	-1.48%

Supplementary Table S6.5 The percentage difference values of different types of atoms around the sulfur of cysteine with the distance of 5.5 Å. The atoms were categorized into eight types including carbon of main chain (C), alpha carbon of main chain (CA), nitrogen of main chain (N), oxygen of main chain (O), carbon of side chain (C*), nitrogen of side chain (N*), oxygen of side chain (O*) and sulfur of side chain (S*).

	C	O	N	CA	C*	O*	N*	S*
SER	0.21%	-0.72%	3.32%	4.86%	1.26%	1.26%	-	-
THR	0.74%	4.97%	4.98%	4.46%	3.99%	2.01%	-	-
CYS	-20.88%	-14.45%	-19.85%	-19.33%	-18.10%	-	-	-17.07%
PRO	-0.18%	2.82%	2.29%	1.16%	3.09%	-	-	-
ASN	2.01%	1.29%	2.02%	-1.91%	-1.11%	-2.20%	1.00%	-
GLN	0.47%	-0.88%	-0.26%	0.16%	1.15%	0.80%	-1.37%	-
ASP	1.36%	1.87%	-1.21%	0.34%	5.39%	2.20%	-	-
GLU	-3.38%	-0.49%	-1.31%	-1.41%	5.64%	1.99%	-	-
LYS	0.95%	-2.88%	1.06%	2.51%	2.61%	-	-0.23%	-
ARG	1.48%	-0.80%	-1.71%	1.80%	-3.38%	-	-2.91%	-
HIS	4.40%	2.54%	-0.35%	3.58%	9.18%	-	2.84%	-
PHE	-3.80%	-2.87%	-1.82%	-2.87%	-23.46%	-	-	-
TYR	-2.33%	-3.16%	1.60%	-1.10%	9.74%	2.13%	-	-
TRP	-1.16%	-1.78%	1.22%	-1.68%	-2.15%	-	-1.67%	-
GLY	2.65%	-2.20%	8.86%	6.18%	-	-	-	-
ALA	0.48%	3.05%	-1.99%	-1.60%	-2.61%	-	-	-
VAL	-4.47%	-0.87%	-6.21%	-4.27%	9.37%	-	-	-
LEU	-1.51%	-0.79%	-6.34%	-6.87%	-30.69%	-	-	-
ILE	-3.11%	-2.60%	-3.51%	-2.69%	-5.02%	-	-	-
MET	-0.87%	-2.01%	1.20%	-1.18%	-2.92%	-	-	-1.60%

Supplementary Table S6.6 The percentage difference values of different types of atoms around the sulfur of cysteine with the distance of 6 Å. The atoms were categorized into eight types including carbon of main chain (C), alpha carbon of main chain (CA), nitrogen of main chain (N), oxygen of main chain (O), carbon of side chain (C*), nitrogen of side chain (N*), oxygen of side chain (O*) and sulfur of side chain (S*).

	C	O	N	CA	C*	O*	N*	S*
SER	-1.36%	-1.77%	2.56%	1.63%	1.85%	3.00%	-	-
THR	2.15%	4.43%	0.91%	2.26%	5.18%	3.33%	-	-
CYS	-17.80%	-18.82%	-24.21%	-22.56%	-24.53%	-	-	-19.57%
PRO	1.03%	1.56%	1.54%	2.06%	2.62%	-	-	-
ASN	0.75%	2.72%	2.83%	-1.20%	1.34%	-2.32%	2.43%	-
GLN	0.87%	0.35%	-2.76%	0.56%	-2.09%	-0.24%	-1.07%	-
ASP	1.65%	0.93%	-2.17%	0.63%	2.97%	5.89%	-	-
GLU	-1.45%	-1.65%	-4.03%	0.22%	4.24%	2.16%	-	-
LYS	-0.11%	-3.00%	1.34%	-0.40%	0.38%	-	-0.13%	-
ARG	-0.20%	-0.92%	-0.19%	-0.81%	-4.78%	-	-4.18%	-
HIS	2.84%	1.71%	-0.26%	3.46%	11.00%	-	3.85%	-
PHE	-5.37%	-4.96%	-5.57%	-7.86%	-25.11%	-0.10%	-	-
TYR	-1.94%	-3.80%	0.75%	-1.84%	7.87%	0.67%	-	-
TRP	-0.96%	-0.96%	1.94%	-1.17%	-6.14%	-	0.29%	-
GLY	1.17%	-3.48%	11.61%	6.97%	-	-	-	-
ALA	3.01%	2.81%	-0.92%	-1.84%	-1.52%	-	-	-
VAL	-5.24%	-1.93%	-8.13%	-2.06%	8.71%	-	-	-
LEU	-1.45%	-1.97%	-9.92%	-7.55%	-46.42%	-	-	-
ILE	-3.35%	-3.97%	-6.44%	-1.60%	-4.25%	-	-	-
MET	-1.30%	-1.81%	-0.16%	-1.40%	-0.48%	-	-	-0.79%

Supplementary Table S6.7 The percentage difference values of different types of atoms around the sulfur of cysteine with the distance of 6.5 Å. The atoms were categorized into eight types including carbon of main chain (C), alpha carbon of main chain (CA), nitrogen of main chain (N), oxygen of main chain (O), carbon of side chain (C*), nitrogen of side chain (N*), oxygen of side chain (O*) and sulfur of side chain (S*).

	C	O	N	CA	C*	O*	N*	S*
SER	-0.27%	-1.08%	1.69%	-1.20%	1.31%	3.80%	-	-
THR	2.74%	0.06%	-0.48%	3.15%	6.36%	3.70%	-	-
CYS	-22.57%	-21.83%	-27.65%	-28.48%	-27.34%	-	-	-24.23%
PRO	3.07%	2.25%	2.34%	1.20%	5.54%	-	-	-
ASN	-0.20%	0.42%	1.87%	0.73%	-0.97%	1.69%	2.83%	-
GLN	2.50%	0.64%	-3.92%	-0.40%	-1.83%	0.88%	-0.26%	-
ASP	2.23%	2.44%	1.81%	-0.65%	2.82%	8.02%	-	-
GLU	-5.10%	-3.34%	-6.35%	-2.82%	4.69%	4.92%	-	-
LYS	-1.80%	-4.80%	0.16%	-0.24%	-0.32%	-	-1.28%	-
ARG	-2.91%	-3.84%	0.18%	-4.46%	-4.75%	-	-6.29%	-
HIS	2.20%	3.14%	1.69%	3.55%	11.57%	-	3.73%	-
PHE	-8.30%	-5.60%	-7.26%	-5.61%	-37.14%	-0.10%	-	-
TYR	-1.25%	-2.27%	0.72%	-2.28%	4.84%	3.34%	-	-
TRP	-0.66%	-0.45%	1.93%	-0.04%	-5.59%	-	1.62%	-
GLY	0.51%	-2.48%	8.57%	6.41%	-	-	-	-
ALA	0.99%	2.35%	-2.73%	-1.49%	0.81%	-	-	-
VAL	-4.58%	-6.01%	-4.90%	-6.06%	4.95%	-	-	-
LEU	-6.37%	-2.84%	-10.20%	-11.14%	-55.95%	-	-	-
ILE	-5.15%	-4.11%	-6.19%	-2.40%	-1.12%	-	-	-
MET	-1.52%	-1.72%	-0.39%	0.03%	-1.77%	-	-	0.03%

Supplementary Table S6.8 The percentage difference values of different types of atoms around the sulfur of cysteine with the distance of 7 Å. The atoms were categorized into eight types including carbon of main chain (C), alpha carbon of main chain (CA), nitrogen of main chain (N), oxygen of main chain (O), carbon of side chain (C*), nitrogen of side chain (N*), oxygen of side chain (O*) and sulfur of side chain (S*).

	C	O	N	CA	C*	O*	N*	S*
SER	0.93%	-1.33%	-4.46%	-1.64%	5.71%	6.03%	-	-
THR	1.25%	-4.01%	1.43%	1.24%	8.25%	2.42%	-	-
CYS	-25.38%	-21.24%	-30.26%	-32.85%	-29.42%	-	-	-29.84%
PRO	5.20%	2.62%	3.34%	4.58%	8.24%	-	-	-
ASN	-2.71%	-1.98%	0.07%	0.40%	2.39%	4.05%	2.71%	-
GLN	1.85%	1.13%	-4.05%	-0.94%	-2.71%	-0.68%	0.25%	-
ASP	1.37%	3.13%	1.88%	2.11%	-1.78%	3.11%	-	-
GLU	-4.53%	-4.63%	-9.60%	-3.89%	7.82%	4.67%	-	-
LYS	-4.63%	-6.28%	-0.82%	-0.18%	-5.79%	-	0.76%	-
ARG	-1.92%	-6.35%	-3.58%	-2.84%	-8.57%	-	-7.68%	-
HIS	1.98%	2.18%	4.04%	2.70%	12.76%	-	2.57%	-
PHE	-7.40%	-5.22%	-10.82%	-7.51%	-49.45%	-0.10%	-	-
TYR	-1.58%	-1.06%	-2.51%	-1.68%	4.89%	4.26%	-	-
TRP	-0.87%	-0.15%	0.78%	-0.15%	-4.01%	-	1.72%	-
GLY	-2.12%	-4.50%	7.88%	3.78%	-	-	-	-
ALA	-4.12%	0.53%	-0.12%	0.63%	2.40%	-	-	-
VAL	-4.34%	-3.39%	-1.57%	-5.60%	-4.83%	-	-	-
LEU	-2.63%	-7.05%	-12.15%	-12.26%	-64.87%	-	-	-
ILE	-3.66%	-0.85%	-5.85%	-6.79%	-6.71%	-	-	-
MET	-2.68%	-1.33%	0.52%	-0.92%	-2.04%	-	-	0.94%

Supplementary Table S6.9 The percentage difference values of different types of atoms around the sulfur of cysteine with the distance of 7.5 Å. The atoms were categorized into eight types including carbon of main chain (C), alpha carbon of main chain (CA), nitrogen of main chain (N), oxygen of main chain (O), carbon of side chain (C*), nitrogen of side chain (N*), oxygen of side chain (O*) and sulfur of side chain (S*).

	C	O	N	CA	C*	O*	N*	S*
SER	-0.15%	-0.23%	0.96%	-2.41%	3.29%	5.16%	-	-
THR	-2.53%	-2.41%	0.76%	1.82%	2.68%	2.79%	-	-
CYS	-31.00%	-23.02%	-32.86%	-33.39%	-33.17%	-	-	-33.48%
PRO	4.65%	5.07%	4.13%	5.79%	9.28%	-	-	-
ASN	-4.30%	-4.70%	0.66%	-2.11%	5.13%	5.98%	1.75%	-
GLN	-0.56%	0.59%	-4.91%	-2.51%	-0.30%	-1.22%	-0.18%	-
ASP	4.01%	5.57%	1.32%	0.21%	-3.61%	4.49%	-	-
GLU	-6.96%	-5.50%	-10.38%	-5.17%	4.12%	3.60%	-	-
LYS	-7.79%	-6.85%	-5.63%	-5.08%	-2.82%	-	2.50%	-
ARG	-5.48%	-5.57%	-3.21%	-4.43%	-20.88%	-	-5.77%	-
HIS	4.12%	2.38%	3.70%	2.27%	9.89%	-	3.47%	-
PHE	-7.65%	-8.78%	-9.42%	-9.31%	-59.21%	-0.10%	-	-
TYR	-1.19%	-2.12%	-3.99%	-0.88%	11.15%	4.13%	-	-
TRP	-0.36%	-0.05%	-0.68%	0.25%	-2.23%	-	2.64%	-
GLY	-2.91%	-2.70%	6.06%	5.38%	-	-	-	-
ALA	-5.95%	-3.35%	-1.85%	-3.57%	1.30%	-	-	-
VAL	-7.53%	2.52%	-0.61%	-1.12%	-11.83%	-	-	-
LEU	-4.79%	-4.96%	-13.81%	-10.08%	-69.09%	-	-	-
ILE	-1.98%	-3.81%	-4.58%	-6.32%	-23.57%	-	-	-
MET	-3.01%	-1.46%	-0.96%	-0.43%	3.69%	-	-	1.54%

Supplementary Table S6.10 The percentage difference values of different types of atoms around the sulfur of cysteine with the distance of 8 Å. The atoms were categorized into eight types including carbon of main chain (C), alpha carbon of main chain (CA), nitrogen of main chain (N), oxygen of main chain (O), carbon of side chain (C*), nitrogen of side chain (N*), oxygen of side chain (O*) and sulfur of side chain (S*).

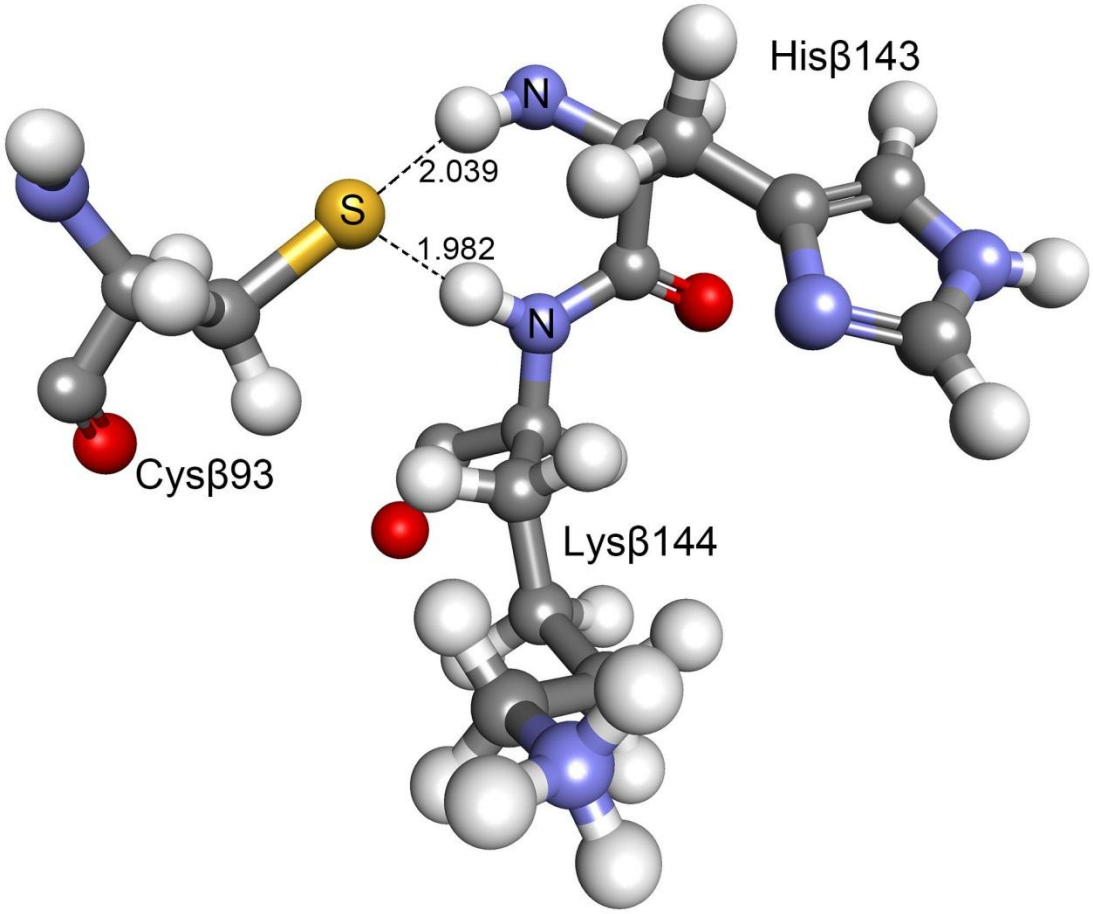
	C	O	N	CA	C*	O*	N*	S*
SER	-2.47%	-4.33%	-2.28%	-0.60%	6.34%	5.94%	-	-
THR	-3.41%	-7.95%	3.81%	1.46%	4.14%	1.09%	-	-
CYS	-31.75%	-26.77%	-33.81%	-34.03%	-35.47%	-	-	-38.05%
PRO	8.85%	8.75%	5.13%	5.35%	11.66%	-	-	-
ASN	-3.31%	-2.05%	-0.92%	-1.53%	9.09%	7.81%	2.45%	-
GLN	-5.34%	-1.62%	-6.07%	-2.64%	2.21%	-0.72%	1.34%	-
ASP	2.52%	0.25%	-0.47%	4.41%	-3.69%	2.04%	-	-
GLU	-5.98%	-8.86%	-12.79%	-10.39%	-1.88%	6.01%	-	-
LYS	-10.42%	-8.65%	-8.78%	-7.71%	-5.85%	-	1.13%	-
ARG	-8.41%	-6.96%	-8.41%	-4.26%	-24.72%	-	-7.61%	-
HIS	4.93%	2.87%	3.68%	2.97%	13.43%	-	6.22%	-
PHE	-6.77%	-11.72%	-9.56%	-12.35%	-73.67%	-0.31%	-	-
TYR	-3.40%	-2.36%	-3.60%	-1.84%	15.41%	3.90%	-	-
TRP	0.24%	0.14%	-0.28%	0.66%	-2.03%	-	1.49%	-
GLY	-3.30%	-2.25%	3.20%	7.06%	-	-	-	-
ALA	-6.23%	-0.95%	-5.32%	-2.92%	6.30%	-	-	-
VAL	-3.17%	3.05%	3.87%	-1.70%	-9.77%	-	-	-
LEU	-7.98%	-6.63%	-14.42%	-12.96%	-68.37%	-	-	-
ILE	-3.89%	-6.16%	-5.46%	-4.62%	-31.84%	-	-	-
MET	0.27%	-3.14%	0.47%	-3.04%	2.49%	-	-	1.62%

Supplementary Table S7 The S-nitrosylated cysteines with neighboring His in the distance threshold of 5Å.

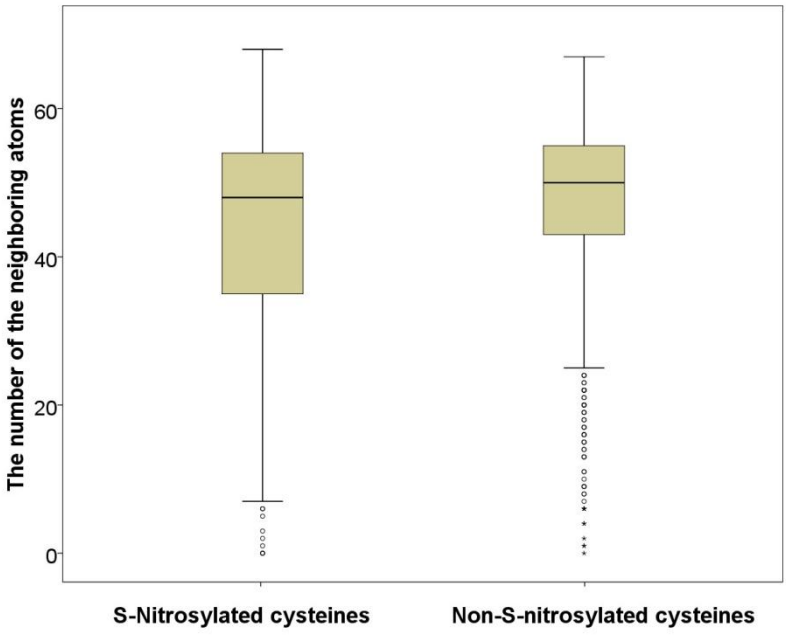
Protein No.	S-nitroso Site	PDB No.	Chain	Site	Neighboring His	Ref.
P03252	122	1AVP	A	122	HisA54	14525973
Q99KI0	126;410	1B0J	A	99;358	HisA98;HisA147,HisA167	19101475
P50247	195	1B3R	A	194	HisA352	20837516
P69905	105	1BZ1	A	105	HisA104	17350155
P02638	85	1CFP	A	84	HisA85	15590070
Q8BVI4	158	1DIR	A	157	HisA154	20837516
P68871	94	1DXT	B	94	HisB147	8637569;9843411
P25779	147	1EWP	A	25	HisA159	10753643
Q02293	299	1FT1	B	299	HisB362	16418269
P98170	327	1G73	C	327	HisC302,HisC320,	19273858
P09382	61	1GZW	B	60	HisB44,	18335467;19366988
P52197	230	1H4K	X	230	HisX229,HisX233,HisX234	12821142
P42123	164	1I0Z	A	163	HisA193	17629318
P0ACQ4	199	1I6A	A	199	HisA198,	14993439;15688001
P06213	1083	1IRK	A	1056	HisA1057,HisA1058	11225731
P26443	112;254	1L1F	A	59;201	HisA86;HisA199,	20837516
P14780	99	1L6J	A	99	HisA190,HisA401,HisA405,HisA411	12183632
P07237	53;56	1MEK	A	36;39	HisA38;HisA38	16724068
P16331	265	1PHZ	A	265	HisA264	20837516
Q9QUR7	115	1PIN	A	113	HisA59	16418269
P35505	396	1QQJ	A	396	HisA395	20837516
Q9QXF8	247	1R8X	A	246	HisA245	20837516
O35490	256	1UMY	A	256	HisA218	20837516
O75832	107	1UOH	A	107	HisA111	18395505
Q9DC50	210	1XMD	A	210	HisA207	20837516
P04406	152	1ZNQ	O	152	HisO179	17540725
Q8K2B3	238	1ZOY	A	196	HisA203	20837516
P0A7M9	37	2AW4	Z	37	HisZ41	19483679
P21399	437	2B3X	A	437	HisA178	7579417
Q9Y696	234	2D2Z	A	234	His196	16648260

P04271	85	2H61	A	84	His85	15590070
P15105	183	2UU7	A	183	HisA179	20837516
P69897	12	2XRP	A	12	HisA139	16418269
Q8VDN2	663	3B8E	A	656	HisA678	20837516
P63242	73	3CPF	A	73	HisA77	19101475
O15519	259	3H11	A	259	HisA283	16246840
P02088	94	3HRW/1HHO	B	93	HisB92	20837516
P21980	10	3LY6	A	10	HisA44	11305905
P63085	159	3O71	A	159	HisA123	19101475;19483679
P05202	187	3PD6	A	187	HisA373	19483679
O08749	484	3RNM	A	449	HisA450	20837516
P21980	277;336	3S3J	A	277;336	HisA335;HisA335	11305905
P68036	86	3SQV	C	86	HisC119	19483679
P11980	358	3SRF	C	357	HisC463	17629318;18335467;19366988
P07237	400	3UEM	A	400	HisA399	16724068
P02769	58	3V03	A	34	HisA39	11983891;12706341;17135341;18273439
Q05193	607	3ZVR	A	607	HisA584	16432212
P04642	163	4AJ4	A	162	HisA192	17629318
P43235	139	7PCK	A	25	HisA162	10521264

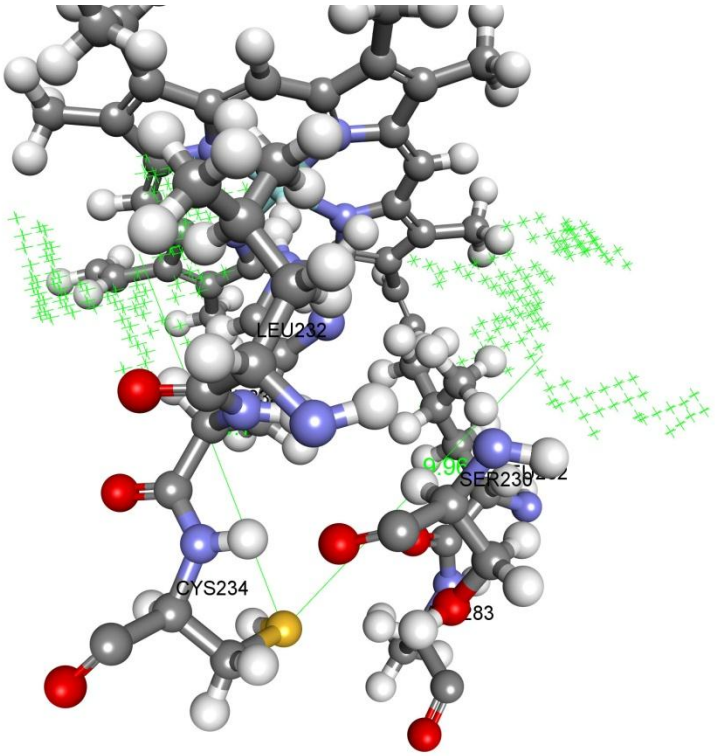
Supplementary Figure S1 The interactions between Cysβ93 and basic residues of Hisβ143, Lysβ144. The blue atoms were N; the red atoms were O; the white atoms were H; the gray atoms were C; the golden atoms were S.



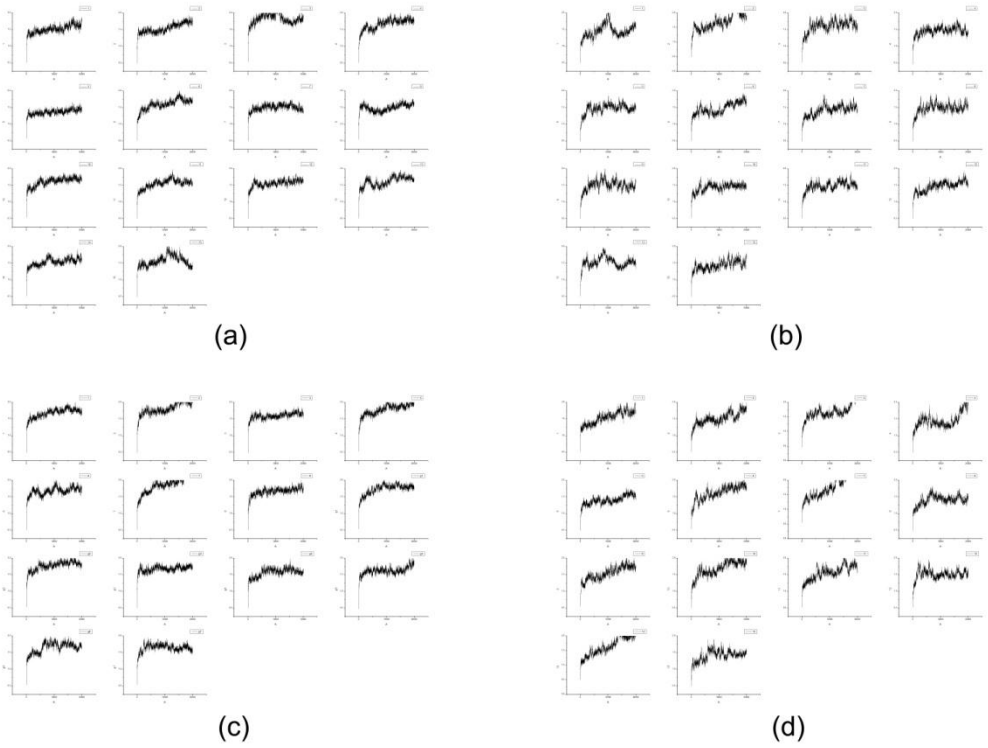
Supplementary Figure S2 The distribution of neighboring atoms in S-nitrosylated and non-S-nitrosylated cysteines.



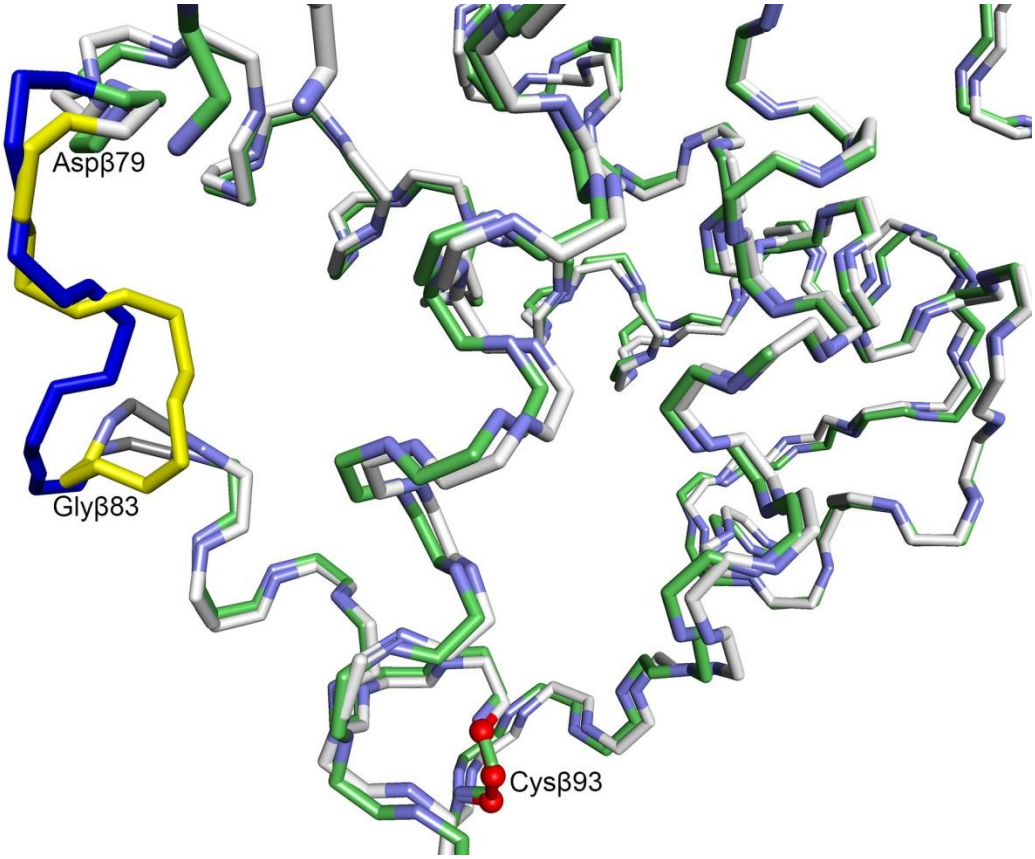
Supplementary Figure S3. The free space around the Cysβ93 in the R-state hemoglobin. The 'CYS234' was the Cysβ93 in hemoglobin. The green cross (+) represents the space in protein structure. The white atom was 'H'. The gray atom was 'C'. The blue atom was 'N'. The red atom was 'O'. The yellow atom was 'S'. The volume of green-cross space was **26.25 Å^3**. The space was analyzed using 1HHO.pdb.



Supplementary Figure S4 The RMSD of each trajectory of R-state (a), T-state (b), dep-R-state (c) and dep-T-state (d) hemoglobin. For each state of hemoglobin, the molecular dynamics simulation had been repeated 14 times.



Supplementary Figure S5 The average structures of the dep-T-state and T-state hemoglobins. The dep-T-state hemoglobin was colored in yellow. The T-state hemoglobin was colored in blue.



Supplementary Table S8 The S-nitrosylated cysteines used in the statistical analyses.

Protein No.	Site	PDB No.	Chain	Site	Reference/WebServer
P09211	102	12GS	A	101	SnoPred
P09211	48	12GS	A	47	SnoPred
P62826	112	1A2K	C	112	GPS-SNO
P62826	120	1A2K	C	120	GPS-SNO
P18031	32	1A5Y	A	32	GPS-SNO
P18031	92	1A5Y	A	92	GPS-SNO
P13448	113	1AHJ	A	113	GPS-SNO
Q9R0P5	23	1AK6	A	23	GPS-SNO
P02768	583	1AO6	A	559	SnoPred
P63329	228	1AUI	A	228	GPS-SNO
P03252	122	1AVP	A	122	SnoPred
P17918	135	1AXC	A	135	GPS-SNO
P17918	162	1AXC	A	162	GPS-SNO
Q99KI0	385	1B0J	A	358	20837516
Q99KI0	410	1B0J	A	383	20837516
Q99KI0	126	1B0J	A	99	20837516
P50247	195	1B3R	A	194	20837516
P50247	228	1B3R	A	227	20837516
P69905	105	1BZ1	A	105	GPS-SNO
P32020	495	1C44	A	71	20837516
P02638	85	1CFP	A	84	SnoPred
P47712	151	1CJY	A	151	GPS-SNO
P34914	230	1CQZ	A	230	20837516
P0A6L2	218	1DHP	A	218	GPS-SNO
Q8BVI4	158	1DIR	A	157	20837516
P30046	24	1DPT	A	23	GPS-SNO
Q8BH95	225	1DUB	A	225	20837516
P68871	94	1DXT	B	94	SnoPred
P15121	299	1EL3	A	298	GPS-SNO
Q60864	26	1ELW	A	26	GPS-SNO
P25779	147	1EWP	A	25	GPS-SNO
P17117	9	1F5V	A	9	GPS-SNO
Q91Y97	135	1FDJ	A	1134	20837516
Q91Y97	158	1FDJ	A	1157	20837516
Q91Y97	336	1FDJ	A	1335	20837516
P16015	187	1FLJ	A	188	20837516
Q02293	299	1FT1	B	299	GPS-SNO
P07335	254	1G0W	A	254	GPS-SNO
P07335	283	1G0W	A	283	GPS-SNO
P98170	327	1G73	C	327	GPS-SNO
P50398	317	1GND	A	317	GPS-SNO
P09382	61	1GZW	B	60	GPS-SNO

Q16665	800	1H2M	S	800	GPS-SNO
P52197	230	1H4K	X	230	GPS-SNO
P10242	130	1H88	C	130	GPS-SNO
P00493	106	1HMP	A	105	GPS-SNO
P42123	164	1I0Z	A	163	SnoPred
P0ACQ4	199	1I6A	A	199	GPS-SNO
P06213	1083	1IRK	A	1056	GPS-SNO
P06213	1165	1IRK	A	1138	GPS-SNO
P06213	1261	1IRK	A	1234	GPS-SNO
P06213	1272	1IRK	A	1245	GPS-SNO
P04797	154	1J0X	O	153	GPS-SNO
P04797	245	1J0X	O	244	GPS-SNO
P37040	472	1J9Z	A	472	20837516
P37040	566	1J9Z	A	566	20837516
P37040	630	1J9Z	A	630	20837516
P35754	79	1JHB	A	79	GPS-SNO
P35754	8	1JHB	A	8	GPS-SNO
P35754	83	1JHB	A	83	GPS-SNO
P0AGE9	124	1JKJ	A	123	GPS-SNO
P26443	172	1L1F	A	119	20837516
P26443	254	1L1F	A	201	20837516
P26443	112	1L1F	A	59	20837516
P14780	99	1L6J	A	99	GPS-SNO
P33198	305	1LWD	A	297	GPS-SNO
P33198	387	1LWD	A	379	GPS-SNO
P54071	113	1LWD	A	74	20837516
Q9D0F9	374	1LXT	A	373	20837516
P10111	161	1M9E	A	161	GPS-SNO
P17742	62	1M9E	A	62	20837516
P08133	114	1M9I	A	114	19854201
P07237	53	1MEK	A	36	GPS-SNO
P07237	56	1MEK	A	39	GPS-SNO
P05109	42	1MR8	A	42	GPS-SNO
P07014	75	1NEK	B	75	GPS-SNO
P29473	101	1NSE	A	101	SnoPred
P29473	96	1NSE	A	96	SnoPred
P11884	321	1O05	A	302	SnoPred
P47738	388	1O05	A	369	20837516
P47738	68	1O05	A	49	GPS-SNO
Q05962	160	1OKC	A	159	GPS-SNO
Q05962	257	1OKC	A	256	GPS-SNO
Q92854	135	1OLZ	A	114	19854201
P00586	248	1ORB	A	247	GPS-SNO
Q9JIF0	272	1ORH	A	254	GPS-SNO

Q05586	744	1PB7	A	236	GPS-SNO
P16331	265	1PHZ	A	265	20837516
Q9QUR7	115	1PIN	A	113	GPS-SNO
P62962	128	1PNE	A	127	20837516
Q05769	526	1PXX	A	540	SnoPred
P18760	139	1Q8G	A	139	GPS-SNO
P23528	80	1Q8G	A	80	SnoPred
Q9QUL6	91	1QDN	A	91	SnoPred
Q91X83	35	1QM4	A	35	20837516
Q91X83	377	1QM4	A	377	20837516
P32119	172	1QMV	A	172	SnoPred
P05062	269	1QO5	A	268	GPS-SNO
P35505	315	1QQJ	A	315	20837516
P35505	396	1QQJ	A	396	20837516
P35505	408	1QQJ	A	408	20837516
P0A862	82	1QXH	A	82	GPS-SNO
P48500	67	1R2R	A	66	GPS-SNO
Q9QXF8	147	1R8X	A	146	20837516
Q9QXF8	186	1R8X	A	185	20837516
Q9QXF8	247	1R8X	A	246	20837516
Q8R0Y6	17	1S3I	A	17	20837516
P12814	332	1SJJ	A	333	GPS-SNO
P49429	103	1SQI	A	103	20837516
O75874	297	1T09	A	297	SnoPred
O75874	379	1T09	A	379	SnoPred
Q99LC5	109	1T9G	R	109	20837516
P68372	12	1TUB	B	12	20837516
P63018	603	1UD0	A	603	GPS-SNO
O35490	131	1UMY	A	131	20837516
O35490	256	1UMY	A	256	20837516
O35490	299	1UMY	A	299	20837516
O35490	300	1UMY	A	300	20837516
O75832	107	1UOH	A	107	SnoPred
P0A7V8	32	1VS5	D	31	GPS-SNO
P0A7S3	27	1VS5	L	26	GPS-SNO
P0A7Q1	61	1VS6	3	60	GPS-SNO
P0A7L8	53	1VS6	W	52	GPS-SNO
P07355	133	1W7B	A	133	SnoPred
Q60676	77	1WAO	1	77	GPS-SNO
P05089	168	1WVA	A	168	GPS-SNO
P05089	303	1WVA	A	303	GPS-SNO
Q9DC50	210	1XMD	A	210	20837516
Q13838	165	1XTI	A	165	GPS-SNO
P50172	241	1Y5M	A	241	20837516

P50172	78	1Y5M	A	78	20837516
P25113	153	1YFK	A	153	GPS-SNO
P25113	55	1YFK	A	55	GPS-SNO
P05793	45	1YRL	A	45	GPS-SNO
Q00987	77	1Z1M	A	77	GPS-SNO
Q5XIF6	347	1Z2B	A	347	SnoPred
P05065	202	1ZAH	A	201	GPS-SNO
P04406	152	1ZNQ	O	152	SnoPred
Q8K2B3	238	1ZOY	A	196	20837516
Q8K2B3	266	1ZOY	A	224	20837516
P60422	188	2AW4	C	187	GPS-SNO
P0A7M9	16	2AW4	Z	16	GPS-SNO
P0A7M9	18	2AW4	Z	18	GPS-SNO
P0A7M9	37	2AW4	Z	37	GPS-SNO
P21399	437	2B3X	A	437	SnoPred
P51859	12	2B8A	A	12	GPS-SNO
P62260	192	2BR9	A	192	GPS-SNO
P27348	134	2BTP	A	134	GPS-SNO
P27348	25	2BTP	A	25	GPS-SNO
P63102	25	2C1J	A	25	GPS-SNO
P63102	94	2C1J	A	94	GPS-SNO
P0A853	298	2C44	A	298	GPS-SNO
P68510	112	2C63	A	112	GPS-SNO
P56965	222	2C6Z	A	221	SnoPred
P56965	274	2C6Z	A	273	SnoPred
Q99683	869	2CLQ	A	869	GPS-SNO
O88844	297	2CMJ	A	297	SnoPred
O88844	379	2CMJ	A	379	SnoPred
Q9Y696	234	2D2Z	A	234	GPS-SNO
P08249	89	2DFD	A	71	20837516
O14983	344	2DQS	A	344	GPS-SNO
O14983	349	2DQS	A	349	GPS-SNO
Q9WTX5	120	2E31	B	120	GPS-SNO
Q00981	152	2ETL	A	152	GPS-SNO
P0C8J8	149	2FIQ	A	149	GPS-SNO
P12658	100	2G9B	A	100	GPS-SNO
P09605	317	2GL6	A	317	GPS-SNO
P47942	248	2GSE	A	248	GPS-SNO
P04271	85	2H61	A	84	GPS-SNO
Q04206	38	2I9T	A	38	GPS-SNO
Q76MZ3	390	2IAE	A	390	GPS-SNO
P41567	69	2IF1	A	82	GPS-SNO
P10599	62	2IFQ	B	62	GPS-SNO
P10599	69	2IFQ	B	69	GPS-SNO

O94760	222	2JAJ	A	221	GPS-SNO
O94760	274	2JAJ	A	273	GPS-SNO
Q99836	216	2JS7	A	72	GPS-SNO
Q3U0V1	297	2JVZ	A	64	GPS-SNO
Q61990	109	2JZX	A	109	GPS-SNO
P08839	324	2KX9	A	324	GPS-SNO
P02639	86	2L0P	A	85	SnoPred
Q01405	180	2NUP	A	180	20837516
P33937	67	2NYA	A	31	GPS-SNO
P00966	132	2NZ2	A	132	GPS-SNO
P16460	97	2NZ2	A	97	20837516
Q8R0Y6	587	2O2P	A	587	20837516
Q8R0Y6	662	2O2P	A	662	20837516
P25372	92	2OE0	A	69	GPS-SNO
P11926	360	2OO0	A	360	GPS-SNO
P09373	123	2PFL	A	122	GPS-SNO
P06733	357	2PSN	A	356	SnoPred
P0A7M2	5	2QOV	Z	5	GPS-SNO
Q06830	52	2RII	A	52	GPS-SNO
P15105	183	2UU7	A	183	20837516
P15105	346	2UU7	A	346	20837516
P15105	99	2UU7	A	99	20837516
P28651	201	2W2J	A	200	GPS-SNO
Q03265	244	2W6E	A	201	20837516
P61620	13	2WWB	A	13	20837516
P10415	158	2XA0	A	158	GPS-SNO
P00558	108	2XE6	A	107	GPS-SNO
P00558	50	2XE6	A	49	GPS-SNO
P21817	314	2XOA	A	315	GPS-SNO
P21817	35	2XOA	A	36	GPS-SNO
P69897	12	2XRP	A	12	GPS-SNO
P69897	239	2XRP	A	241	GPS-SNO
P69897	303	2XRP	A	305	GPS-SNO
P69897	354	2XRP	A	356	GPS-SNO
P49185	116	2XS0	A	116	SnoPred
Q9ET01	446	2ZB2	A	445	20837516
P09411	50	2ZGV	A	49	20837516
P21708	179	2ZOQ	A	178	SnoPred
P12277	254	3B6R	A	254	SnoPred
Q8VDN2	663	3B8E	A	656	20837516
Q8VDN2	705	3B8E	A	698	20837516
Q05920	663	3BG3	A	663	20837516
Q05920	752	3BG3	A	752	20837516
P59215	140	3C7K	A	140	SnoPred

P63017	17	3C7N	B	17	20837516
Q16623	145	3C98	B	145	GPS-SNO
Q99MK8	120	3CIK	A	120	GPS-SNO
P25098	340	3CIK	A	340	19854201
Q99MK8	439	3CIK	A	439	GPS-SNO
Q99MK8	619	3CIK	A	619	GPS-SNO
Q99MK8	72	3CIK	A	72	GPS-SNO
P63242	73	3CPF	A	73	GPS-SNO
P29680	50	3CYV	A	50	GPS-SNO
Q07009	301	3DF0	A	301	GPS-SNO
P11517	126	3DHT	B	125	GPS-SNO
P11517	94	3DHT	B	93	GPS-SNO
P20337	137	3DZ8	A	137	SnoPred
Q9Z0X1	255	3GD3	A	255	20837516
O15519	254	3H11	A	254	GPS-SNO
O15519	259	3H11	A	259	GPS-SNO
P68370	295	3HKB	A	295	GPS-SNO
P68370	315	3HKB	A	315	GPS-SNO
P68370	316	3HKB	A	316	GPS-SNO
P68370	347	3HKB	A	347	GPS-SNO
P68370	376	3HKB	A	376	GPS-SNO
P02088	94	3HRW	B	93	20837516
P23284	202	3ICH	A	170	GPS-SNO
P0A7Z4	176	3IYD	A	176	GPS-SNO
O35215	24	3KER	A	23	20837516
O35215	57	3KER	A	56	20837516
Q9GZT4	113	3L6B	A	113	GPS-SNO
P21980	10	3LY6	A	10	GPS-SNO
Q92769	262	3MAX	A	266	GPS-SNO
Q92769	274	3MAX	A	278	GPS-SNO
P01009	256	3NE4	A	232	GPS-SNO
P29474	184	3NOS	A	184	SnoPred
P29474	201	3NOS	A	201	SnoPred
P29474	212	3NOS	A	212	SnoPred
P29474	235	3NOS	A	235	SnoPred
P29474	382	3NOS	A	382	SnoPred
P29474	94	3NOS	A	94	SnoPred
P29474	99	3NOS	A	99	SnoPred
P63085	159	3O71	A	159	GPS-SNO
P61080	85	3OJ4	A	85	GPS-SNO
P05202	106	3PD6	A	106	20837516
P05202	187	3PD6	A	187	20837516
P05202	295	3PD6	A	295	20837516
P56558	610	3PE3	A	610	GPS-SNO

Q91V92	623	3PFF	A	633	20837516
P61765	110	3PUJ	A	110	GPS-SNO
P07900	481	3Q6M	A	481	GPS-SNO
P07900	597	3Q6M	A	597	GPS-SNO
P07900	598	3Q6M	A	598	GPS-SNO
P00533	190	3QWQ	A	166	GPS-SNO
P00533	329	3QWQ	A	305	GPS-SNO
Q9I4E3	249	3RHY	A	249	GPS-SNO
O08749	484	3RNM	A	449	20837516
Q6P9V9	295	3RYC	A	295	SnoPred
Q6P9V9	347	3RYC	A	347	SnoPred
Q6P9V9	376	3RYC	A	376	SnoPred
P21980	143	3S3J	A	143	GPS-SNO
P21980	230	3S3J	A	230	GPS-SNO
P21980	269	3S3J	A	269	GPS-SNO
P21980	27	3S3J	A	27	GPS-SNO
P21980	277	3S3J	A	277	GPS-SNO
P21980	285	3S3J	A	285	GPS-SNO
P21980	336	3S3J	A	336	GPS-SNO
P21980	370	3S3J	A	370	GPS-SNO
P21980	371	3S3J	A	371	GPS-SNO
P21980	524	3S3J	A	524	GPS-SNO
P21980	545	3S3J	A	545	GPS-SNO
P21980	620	3S3J	A	620	GPS-SNO
P21980	98	3S3J	A	98	GPS-SNO
Q99020	104	3S7R	A	98	SnoPred
P05161	78	3SDL	C	78	GPS-SNO
Q99497	46	3SF8	B	46	SnoPred
Q99497	53	3SF8	B	53	SnoPred
P68036	86	3SQV	C	86	GPS-SNO
P14618	49	3SRD	A	49	SnoPred
P11980	326	3SRF	C	325	GPS-SNO
P11980	358	3SRF	C	357	GPS-SNO
P11980	423	3SRF	C	422	GPS-SNO
P11980	474	3SRF	C	473	GPS-SNO
P11980	49	3SRF	C	48	GPS-SNO
P49187	117	3TTJ	A	117	SnoPred
P60710	217	3U4L	A	217	GPS-SNO
P60710	257	3U4L	A	257	GPS-SNO
P60710	272	3U4L	A	272	GPS-SNO
P60710	285	3U4L	A	285	GPS-SNO
P07323	357	3UCC	A	356	GPS-SNO
P07237	400	3UEM	A	400	GPS-SNO
P02769	288	3V03	A	264	GPS-SNO

P02769	58	3V03	A	34	GPS-SNO
P02769	392	3V03	A	368	GPS-SNO
P02769	471	3V03	A	447	GPS-SNO
Q8CHT0	94	3V9J	A	95	20837516
Q05193	607	3ZVR	A	607	SnoPred
P04642	163	4AJ4	A	162	GPS-SNO
P06151	35	4AJ4	A	34	20837516
P05064	339	4ALD	A	338	GPS-SNO
P35557	371	4DCH	A	371	GPS-SNO
P42574	163	4EHH	A	163	GPS-SNO
P31749	224	4EJN	A	224	GPS-SNO
P31749	296	4EJN	A	296	GPS-SNO
P31749	310	4EJN	A	310	GPS-SNO
P01112	118	4Q21	A	118	SnoPred
O88989	137	5MDH	A	136	GPS-SNO
O88989	154	5MDH	A	153	GPS-SNO
P43235	139	7PCK	A	25	GPS-SNO