Electronic Supplementary Material (ESI) for Molecular BioSystems
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Supplementary materials:

Site Selectivity for Protein Tyrosine Nitration: Insights from Features of Structure and Topological Network

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Supplementary Table S1 The nitrated proteins and their structural information used in the predictive model as training data (From reference of GPS-YNO$_2$).

Protein and nitrated site	Protein structure and nitrated site	Experiment	Disease
B2RSH2_167	2ZJY_A_167	In vitro	-
O08553_182	2GSE_A_182	In vitro	-
O08553_431	2GSE_A_431	In vitro	-
O14737_73	2CRU_A_72	In vivo/vitro	
O35643_574	1W63_B_574	In vivo	Neurodegenerative disease
O43252_537	1X6V_B_537	In vitro	Jurkat lysate
O43719_327	2DIT_A_79	In vitro	Jurkat lysate
O43765_195	2VYI_A_195	In vitro	Jurkat lysate
O54922_409	2PFT_A_409	In vivo	Diabetic retinopathy
O60256_52	2JI4_A_52	In vitro	Jurkat lysate
O60506_373	2DGU_A_373	In vitro	Jurkat lysate
O75390_185	4CTS_A_158	In vitro	Jurkat lysate
O75390_345	4CTS_A_318	In vitro	-
O75396_33	2NUP_C_33	In vitro	Jurkat lysate
O75792_172	3PUF_A_172	In vitro	Jurkat lysate
O75832_138	1UOH_A_138	In vitro	Jurkat lysate
P00004_49	2PCB_B_48	In vitro	-
P00004_68	2PCB_B_67	In vitro	-
P00004_75	2PCB_B_74	In vitro	-
P00004_98	2PCB_B_97	In vitro	-
P00183_180	1GEK_A_179	In vitro	-
P00183_202	1GEK_A_201	In vitro	-
P00183_204	1GEK_A_203	In vitro	-
P00183_306	1GEK_A_305	In vitro	-
P00183_97	1GEK_A_96	In vitro	-
P00257_140	1L6V_A_82	In vitro	-
P00338_239	1I10_A_238	In vitro	Jurkat lysate
P00338_83	1I10_A_82	In vitro	Jurkat lysate
P00366_319	3MW9_A_262	In vitro	-
P00366_458	3MW9_A_401	In vitro	-
P00366_464	3MW9_A_407	In vitro	-
P00366_528	3MW9_A_471	In vitro	-
P00366_550	3MW9_A_493	In vitro	-
P00390_150	2AAQ_A_106	In vitro	-
P00390_158	2AAQ_A_114	In vitro	-
P00442_109	1COB_A_108	In vitro	-
P00489_162	2PYD_A_161	In vitro	-
P00489_186	2PYD_A_185	In vitro	-
P00489_204	2PYD_A_203	In vitro	-
P00489_227	2PYD_A_226	In vitro	-
P00489_234	2PYD_A_233	In vitro	-
P00489_281	2PYD_A_280	In vitro	-
P00489_298	2PYD_A_297	In vitro	-
P00489_405	2PYD_A_404	In vitro	-
P00489_473	2PYD_A_472	In vitro	-
P00489_512	2PYD_A_511	In vitro	-
P00489_525	2PYD_A_524	In vitro	-
P00489_549	2PYD_A_548	In vitro	-
P00489_554	2PYD_A_553	In vitro	-
P00489_614	2PYD_A_613	In vitro	-
P00489_649	2PYD_A_648	In vitro	-
P00489_727	2PYD_A_726	In vitro	-
P00489_75	2PYD_A_74	In vitro	-
P00489_76	2PYD_A_75	In vitro	-
P00489_778	2PYD_A_777	In vitro	-
P00489_781	2PYD_A_780	In vitro	-
P00489_792	2PYD_A_791	In vitro	-
P00489_821	2PYD_A_820	In vitro	-
P00489_84	2PYD_A_83	In vitro	-
P00489_85	2PYD_A_84	In vitro	-
P00489_91	2PYD_A_90	In vitro	-
P00558_161	2ZGV_A_160	In vitro	-
P00558_196	2ZGV_A_195	In vitro	Jurkat cells
P00558_76	2ZGV_A_75	In vitro	Jurkat cells
P00564_14	2CRK_A_14	In vivo	-
P00564_20	2CRK_A_20	In vivo	-
P00564_39	2CRK_A_39	In vivo	-
P00592_145	1HN4_A_123	In vitro	-
P00592_91	1HN4_A_69	In vitro	-
P00644_197	2EXZ_A_115	In vitro	-
P00698_38	3B6L_A_2020	In vitro	-
P00698_41	3B6L_A_2023	In vitro	-
P00698_71	3B6L_A_2053	In vitro	-
P00709_122	1HML_A_103	In vitro	-
P00709_37	1HML_A_18	In vitro	-

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P00730_308	1PYT_B_198	In vitro	-
P00730_358	1PYT_B_248	In vitro	-
P00749_44	2I9A_A_24	In vitro	-
P00766_146	2CGA_A_146	In vitro	-
P00766_171	2CGA_A_171	In vitro	-
P00781_103	1BH6_A_104	In vitro	-
P00781_205	1BH6_A_206	In vitro	-
P00781_208	1BH6_A_209	In vitro	-
P00781_21	1BH6_A_21	In vitro	-
P00781_213	1BH6_A_214	In vitro	-
P00781_237	1BH6_A_238	In vitro	-
P00781_261	1BH6_A_262	In vitro	-
P00781_262	1BH6_A_263	In vitro	-
P00781_56	1BH6_A_57	In vitro	-
P00781_90	1BH6_A_91	In vitro	-
P00784_194	1KHP_A_61	In vitro	-
P00784_236	1KHP_A_103	In vitro	-
P00784_249	1KHP_A_116	In vitro	-
P00807_96	1OME_A_105	In vitro	-
P00883_204	1ZAH_A_203	In vivo	-
P00883_223	1ZAH_A_222	In vitro	-
P00883_244	1ZAH_A_243	In vitro	-
P00883_328	1ZAH_A_327	In vivo	-
P00883_343	1ZAH_A_342	In vitro	-
P00924_191	1EBG_A_190	In vitro	-
P00924_259	1EBG_A_258	In vitro	-
P01006_106	2SIC_I_75	In vitro	-
P01009_162	3NE4_A_138	In vitro	-
P01009_184	3NE4_A_160	In vitro	-
P01009_211	3NE4_A_187	In vitro	-
P01009_268	3NE4_A_244	In vitro	-
P01009_321	3NE4_A_297	In vitro	-
P01009_62	3NE4_A_38	In vitro	-
P01024_686	2A73_B_664	In vitro	-
P01024_730	2A73_B_708	In vitro	-
P01031_700	3PRX_A_700	In vitro	-
P01050_3	1HRT_I_3	In vitro	-
P01050_63	1HRT_I_63	In vitro	-
P01112_137	4Q21_A_137	In vitro	-
P01112_157	4Q21_A_157	In vitro	-
P01112_40	4Q21_A_40	In vitro	-
P01112_96	4Q21_A_96	In vitro	-
P01180_80	1NPO_A_49	In vitro	-
P01426_24	1IQ9_A_24	In vitro	-
P01654_90	1H0D_A_85	In vivo	Atherosclerotic lesions
P01857_161	1HZH_H_291	In vitro	-
P01857_202	1HZH_H_338	In vitro	-
P01870_154	2VUO_A_278	In vitro	-
P02185_147	3A2G_A_146	In vitro	-
P02185_152	3A2G_A_151	In vitro	-
P02244_19	1I4Y_A_18	In vitro	-
P02244_68	1I4Y_A_67	In vitro	-
P02244_71	1I4Y_A_70	In vitro	-
P02564_134	4DB1_A_134	In vivo	-
P02564_142	4DB1_A_142	In vivo	-
P02647_260	2A01_A_236	In vitro	-
P02647_42	2A01_A_18	In vitro	-
P02647_53	2A01_A_29	In vitro	-
P02675_322	3GHG_B_292	In vivo	Prothrombotic
P02675_452	3GHG_B_422	In vivo	Prothrombotic
P02703_72	1PCO_A_55	In vitro	-
P02703_75	1PCO_A_58	In vitro	-
P02703_76	1PCO_A_59	In vitro	-
P02754_115	3PH5_A_115	In vitro	-
P02769_108	3V03_A_84	In vitro	-
P02769_161	3V03_A_137	In vitro	-
P02769_163	3V03_A_139	In vitro	-
P02769_171	3V03_A_147	In vitro	-
P02769_173	3V03_A_149	In vitro	-
P02769_179	3V03_A_155	In vitro	-
P02769_180	3V03_A_156	In vitro	-
P02769_184	3V03_A_160	In vitro	-
P02769_286	3V03_A_262	In vitro	-
P02769_342	3V03_A_318	In vitro	-
P02769_355	3V03_A_331	In vitro	-
P02769_357	3V03_A_333	In vitro	-
P02769_364	3V03_A_340	In vitro	-
P02769_376	3V03_A_352	In vitro	-
P02769_393	3V03_A_369	In vitro	-
P02769_424	3V03_A_400	In vitro	-

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P02769_434	3V03_A_410	In vitro	-
P02769_475	3V03_A_451	In vitro	-
P02769_520	3V03_A_496	In vitro	-
P02769_54	3V03_A_30	In vitro	-
P02945_144	1M0K_A_131	In vitro	-
P02945_146	1M0K_A_133	In vitro	-
P02945_77	1M0K_A_64	In vitro	-
P03040_26	1COP_D_26	In vitro	-
P03040_51	1COP_D_51	In vitro	-
P04177_423	1TOH_A_423	In vitro	-
P04177_428	1TOH_A_428	In vitro	-
P04177_432	1TOH_A_432	In vitro	-
P04179_217	1N0J_A_193	In vitro	-
P04179_58	1N0J_A_34	In vitro	-
P04179_69	1N0J_A_45	In vitro	-
P04806_340	3B8A_X_340	In vitro	-
P04806_346	3B8A_X_346	In vitro	-
P05064_174	4ALD_A_173	In vitro	-
P05181_318	3E4E_A_318	In vitro	-
P05181_381	3E4E_A_381	In vitro	-
P05181_423	3E4E_A_423	In vitro	-
P05181_71	3E4E_A_71	In vitro	-
P05202_316	3PD6_A_316	In vitro	-
P05202_67	3PD6_A_67	In vivo	Neurodegenerative disease
P05202_96	3PD6_A_96	In vitro	-
P05230_109	1RY7_A_109	In vitro	-
P05230_112	1RY7_A_112	In vitro	-
P05230_140	1RY7_A_140	In vitro	-
P05230_30	1RY7_A_30	In vitro	-
P05230_70	1RY7_A_70	In vitro	-
P05979_355	2OYE_P_355	In vitro	-
P05979_385	2OYE_P_385	In vitro	-
P05979_417	2OYE_P_417	In vitro	-
P06576_230	2W6E_D_180	In vivo	Familial amyotrophic lateral sclerosis
P06576_247	2W6E_D_197	In vitro	-
P06576_269	2W6E_D_219	In vitro	-
P06576_331	2W6E_D_281	In vitro	-
P06576_395	2W6E_D_345	In vitro	-
P06576_418	2W6E_D_368	In vitro	-
P06576_508	2W6E_D_458	In vitro	-
P06748_67	2P1B_A_67	In vitro	-
P06968_92	1DUP_A_93	In vitro	-
P07195_240	1I0Z_A_239	In vitro	-
P07195_84	1I0Z_A_83	In vitro	-
P07311_92	2VH7_A_91	In vitro	-
P07339_232	1LYA_B_168	In vitro	-
P07355_30	1W7B_A_30	In vitro	-
P07515_37	1PTF_A_37	In vitro	-
P07737_129	1CJF_A_128	In vitro	-
P07737_60	1CJF_A_59	In vitro	-
P07900_197	2FWY_A_197	In vitro	-
P07900_216	2FWY_A_216	In vitro	-
P07900_313	3Q6M_A_313	In vitro	-
P07954_54	3E04_A_54	In vitro	-
P07999_160	1GCO_A_158	In vitro	-
P07999_254	1GCO_A_253	In vitro	-
P08011_93	2H8A_A_92	In vitro	-
P08133_218	1M9I_A_218	In vitro	-
P08670_276	3TRT_A_276	In vitro	-
P08877_29	1KKL_H_29	In vitro	-
P08877_37	1KKL_H_37	In vitro	-
P09211_50	12GS_A_49	In vitro	-
P09237_167	2DDY_A_73	In vitro	-
P09429_78	2YRQ_A_85	In vitro	-
P09955_197	3GLJ_A_90	In vitro	-
P09955_306	3GLJ_A_198	In vitro	-
P09955_348	3GLJ_A_240	In vitro	-
P09955_356	3GLJ_A_248	In vitro	-
P09955_367	3GLJ_A_259	In vitro	-
P09955_385	3GLJ_A_277	In vitro	-
P0A0E3_37	1KA5_A_37	In vitro	-
P0A6A8_72	3EJB_A_91	In vitro	-
P0A786_241	1EKX_A_240	In vitro	-
P0A9C5_101	2GLS_A_100	In vitro	-
P0A9C5_115	2GLS_A_114	In vitro	-
P0A9C5_180	2GLS_A_179	In vitro	-
P0A9C5_288	2GLS_A_287	In vitro	-
P0A9C5_297	2GLS_A_296	In vitro	-
P0A9C5_327	2GLS_A_326	In vitro	-
P0A9C5_335	2GLS_A_334	In vitro	-

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P0A9C5_398	2GLS_A_397	In vitro	-
P0AGD3_35	1ISA_A_34	In vitro	-
P0C7M2_128	1L3K_A_128	In vitro	-
P0C7M2_167	1L3K_A_167	In vitro	-
P10145_40	1IL8_A_13	In vitro	-
P10153_60	1K2A_A_33	In vitro	-
P10276_208	3A9E_B_208	In vitro	-
P10276_277	3A9E_B_277	In vitro	-
P10276_362	3A9E_B_362	In vitro	-
P10768_202	3FCX_A_202	In vitro	-
P11142_115	3C7N_B_115	In vitro	-
P11142_134	3C7N_B_134	In vitro	-
P11142_149	3C7N_B_149	In vitro	-
P11142_183	3C7N_B_183	In vitro	-
P11142_41	3C7N_B_41	In vitro	-
P11413_401	1QKI_A_401	In vitro	-
P11586_258	1DIA_A_258	In vitro	-
P11586_52	1DIA_A_52	In vitro	-
P12004_60	1AXC_A_60	In vitro	-
P12724_60	1QMT_A_33	In vitro	-
P12758_169	1K3F_A_169	In vitro	-
P13010_295	1JEQ_B_295	In vitro	-
P13332_226	3FOA_A_226	In vitro	-
P13332_255	3FOA_A_255	In vitro	-
P13332_271	3FOA_A_271	In vitro	-
P13332_305	3FOA_A_305	In vitro	-
P13332_456	3FOA_A_456	In vitro	-
P13332_461	3FOA_A_461	In vitro	-
P13332_64	3FOA_A_64	In vitro	-
P13332_74	3FOA_A_74	In vitro	-
P13929_131	2XSX_A_131	In vitro	-
P13929_189	2XSX_A_189	In vitro	-
P13929_200	2XSX_A_200	In vitro	-
P13929_252	2XSX_A_252	In vitro	-
P13929_257	2XSX_A_257	In vitro	-
P13929_280	2XSX_A_280	In vitro	-
P13929_287	2XSX_A_287	In vitro	-
P13929_407	2XSX_A_407	In vitro	-
P13929_44	2XSX_A_44	In vitro	-
P13929_57	2XSX_A_57	In vitro	-
P14206_139	2ZKQ_B_138	In vivo	Neurodegenerative disease
P14618_105	3GQY_A_105	In vitro	-
P14618_148	3GQY_A_148	In vitro	-
P14649_86	1OE9_B_29	In vitro	-
P14779_335	3M4V_A_334	In vitro	-
P14902_15	2D0T_A_15	In vitro	-
P14902_345	2D0T_A_345	In vitro	-
P14902_353	2D0T_A_353	In vitro	-
P16276_151	1B0J_A_124	In vitro	-
P16276_472	1B0J_A_445	In vitro	-
P16276_71	1B0J_A_44	In vitro	-
P16284_713	2KY5_A_686	In vitro	-
P17183_252	1TE6_A_251	In vitro	-
P17183_270	1TE6_A_269	In vitro	-
P17183_44	1TE6_A_43	In vitro	-
P18669_142	1YFK_A_142	In vitro	-
P18669_50	1YFK_A_50	In vivo	Familial amyotrophic lateral sclerosis
P18669_92	1YFK_A_92	In vitro	-
P18872_69	3C7K_A_69	In vitro	-
P19338_351	2KRR_A_52	In vitro	-
P19338_525	2FC9_A_55	In vitro	-
P19652_109	3APU_A_91	In vitro	-
P19652_133	3APU_A_115	In vitro	-
P19652_145	3APU_A_127	In vitro	-
P19652_175	3APU_A_157	In vitro	-
P19652_45	3APU_A_27	In vitro	-
P19652_55	3APU_A_37	In vitro	-
P19652_68	3APU_A_50	In vitro	-
P19652_96	3APU_A_78	In vitro	-
P19784_13	3OFM_A_13	In vitro	-
P20618_158	1IRU_M_130	In vitro	-
P20700_482	2KPW_A_55	In vitro	-
P20813_111	3IBD_A_111	In vitro	-
P20813_190	3IBD_A_190	In vitro	-
P20813_203	3IBD_A_203	In vitro	-
P20813_235	3IBD_A_235	In vitro	-
P20813_244	3IBD_A_244	In vitro	-
P20813_268	3IBD_A_268	In vitro	-
P20813_348	3IBD_A_348	In vitro	-
P20813_354	3IBD_A_354	In vitro	-

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P20813_380	3IBD_A_380	In vitro	-
P21803_656	2PSQ_A_656	In vivo	Oxidative injury to the retinal pigment epithelium
P22102_417	2QK4_A_417	In vitro	-
P22234_22	2H31_A_22	In vitro	-
P23193_273	1TFI_A_22	In vitro	-
P23528_140	1Q8G_A_140	In vitro	-
P23528_68	1Q8G_A_68	In vitro	-
P24666_88	5PNT_A_87	In vitro	-
P25705_337	2W6E_A_294	In vitro	-
P25705_440	2W6E_A_397	In vitro	-
P25787_229	1IRU_B_228	In vivo	Human pituitary adenoma tissue
P25963_181	1IKN_D_181	In vitro	-
P26038_85	1E5W_A_85	In vitro	-
P26599_247	1SJR_A_110	In vitro	-
P26599_430	2ADC_A_430	In vitro	-
P27361_156	2ZOQ_A_156	In vitro	-
P27824_70	1JHN_A_71	In vitro	-
P28072_59	1IRU_H_25	In vitro	-
P29372_162	1F4R_A_162	In vitro	-
P29474_163	3NOS_A_163	In vitro	-
P29474_210	3NOS_A_210	In vitro	-
P29474_357	3NOS_A_357	In vitro	-
P29474_373	3NOS_A_373	In vitro	-
P29474_410	3NOS_A_410	In vitro	-
P29474_81	3NOS_A_81	In vitro	-
P30086_106	1BD9_A_106	In vitro	-
P30086_64	1BD9_A_64	In vitro	-
P30101_100	3F8U_A_100	In vitro	-
P30101_67	3F8U_A_67	In vitro	-
P30275_116	1QK1_A_77	In vitro	-
P30275_313	1QK1_A_274	In vitro	-
P31039_142	1ZOY_A_99	In vitro	-
P32969_180	2ZKR_E_180	In vitro	-
P34913_383	1S8O_A_383	In vivo	-
P34913_466	1S8O_A_466	In vivo	-
P35080_99	2V8C_A_98	In vitro	-
P35228_299	1NSI_A_299	In vitro	-
P35228_336	1NSI_A_336	In vitro	-
P35228_446	1NSI_A_446	In vitro	-
P35247_248	1PW9_A_228	In vitro	-
P35247_326	1PW9_A_306	In vitro	-
P35247_334	1PW9_A_314	In vitro	-
P35441_1126	1UX6_A_1108	In vitro	-
P35520_223	1JBQ_A_223	In vitro	-
P36959_318	2BLE_A_318	In vitro	-
P37837_206	1F05_A_206	In vitro	-
P37840_125	1XQ8_A_125	In vivo	Neurodegeneration
P37840_133	1XQ8_A_133	In vivo	Neurodegeneration
P37840_136	1XQ8_A_136	In vivo	Neurodegeneration
P37840_39	1XQ8_A_39	In vivo	Neurodegeneration
P39053_125	3ZVR_A_125	In vivo	Neurodegenerative disease
P39053_265	3ZVR_A_265	In vitro	-
P40142_275	3MOS_A_275	In vitro	-
P40926_161	2DFD_A_143	In vitro	-
P40926_56	2DFD_A_38	In vitro/vivo	-
P40926_80	2DFD_A_62	In vivo	-
P45452_338	1PEX_A_332	In vitro	-
P46406_312	1J0X_O_311	In vitro	-
P46406_318	1J0X_O_317	In vitro	-
P47813_106	1D7Q_A_119	In vitro	-
P51149_28	1T91_A_28	In vitro	-
P53041_434	1WAO_1_434	In vitro	-
P53396_213	3PFF_A_213	In vitro	-
P53396_227	3PFF_A_227	In vitro	-
P53396_384	3PFF_A_384	In vitro	-
P55072_644	3CF1_A_644	In vitro	-
P55769_11	2JNB_A_11	In vitro	-
P56574_311	1LWD_A_272	In vitro	-
P60301_32	1I02_A_11	In vitro	-
P60301_43	1I02_A_22	In vitro	-
P60301_72	1I02_A_51	In vitro	-
P60615_45	1IK8_A_24	In vitro	-
P60615_75	1IK8_A_54	In vitro	-
P60710_169	3BYH_A_169	In vitro	-
P60710_188	3BYH_A_188	In vitro	-
P60710_198	3BYH_A_198	In vitro	-
P60710_218	3BYH_A_218	In vivo/vitro	Neurodegenerative disease
P60710_240	3BYH_A_240	In vitro	-
P60710_294	3BYH_A_294	In vivo/vitro	-
P60710_362	3BYH_A_362	In vitro	-

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P60710_53	3BYH_A_53	In vitro	-
P60710_69	3BYH_A_69	In vitro	-
P60710_91	3BYH_A_91	In vitro	-
P60770_46	1V6P_A_25	In vitro	-
P60770_56	1V6P_A_35	In vitro	-
P60842_197	3EIQ_A_197	In vitro	-
P60842_70	3EIQ_A_70	In vitro	-
P61013_6	1FJK_A_6	In vitro	-
P61088_76	3HCT_B_76	In vitro	-
P61158_16	1K8K_A_16	In vitro	-
P61513_37	2ZKR_Z_37	In vitro	-
P61823_102	1C0B_A_76	In vitro	-
P61823_141	1C0B_A_115	In vitro	-
P61823_99	1C0B_A_73	In vitro	-
P61927_27	2ZKR_2_27	In vitro	-
P62136_255	1FJM_A_255	In vitro	-
P62158_100	3O77_A_368	In vitro	-
P62158_139	3O77_A_407	In vitro	-
P62249_115	2ZKQ_I_115	In vitro	-
P62259_131	3UBW_A_131	In vivo/vitro	-
P62259_214	3UBW_A_214	In vitro	-
P62259_85	3UBW_A_85	In vivo	Neurodegenerative disease
P62259_9	3UBW_A_9	In vitro	-
P62263_72	2ZKQ_K_72	In vitro	-
P62273_34	2ZKQ_N_34	In vitro	-
P62750_117	2ZKR_S_117	In vitro	-
P62750_144	2ZKR_S_144	In vitro	-
P62805_52	2HUE_C_51	In vivo/vitro	Mutatect tumor
P62805_73	2HUE_C_72	In vivo/vitro	Mutatect tumor
P62805_89	2HUE_C_88	In vivo/vitro	Mutatect tumor
P62826_147	1A2K_C_147	In vitro	-
P62917_133	2ZKR_A_133	In vitro	-
P62993_209	1GRI_A_209	In vitro	-
P63168_50	1F3C_A_50	In vitro	-
P63244_52	2ZKQ_A_52	In vitro	-
P63328_224	1AUI_A_224	In vivo	Neurodegenerative disease
P67775_284	3C5W_C_284	In vitro	-
P68699_73	1ATY_A_73	In vitro	-
P68871_131	1DXT_B_131	In vitro	-
P68871_146	1DXT_B_146	In vitro	-
P69542_26	1GVP_A_26	In vitro	-
P69542_41	1GVP_A_41	In vitro	-
P69542_56	1GVP_A_56	In vitro	-
P69687_140	3J06_A_139	In vitro	-
P69905_141	1BZ1_A_141	In vitro	-
P69905_25	1BZ1_A_25	In vitro	-
P69905_43	1BZ1_A_43	In vivo/vitro	-
P69924_123	1XIK_A_122	In vitro	-
P69924_290	1XIK_A_289	In vitro	-
P69924_3	2ALX_A_2	In vitro	-
P69924_63	1XIK_A_62	In vitro	-
P78417_108	1EEM_A_108	In vitro	-
P83731_11	2ZKR_U_11	In vitro	-
P84103_32	2I2Y_A_96	In vitro	-
P97427_290	1KCX_A_290	In vivo	-
Q01130_3	2LEA_A_3	In vitro	-
Q01518_419	1K8F_A_419	In vitro	-
Q02790_202	1QZ2_A_202	In vitro	-
Q03405_114	1YWH_A_92	In vitro	-
Q03405_171	1YWH_A_149	In vitro	-
Q03405_217	1YWH_A_195	In vitro	-
Q03405_258	1YWH_A_236	In vitro	-
Q03405_79	1YWH_A_57	In vitro	-
Q04206_152	1NFI_A_152	In vitro	-
Q04206_66	1NFI_A_66	In vitro	-
Q04447_269	1G0W_A_269	In vivo	Neurodegenerative disease
Q04447_39	1G0W_A_39	In vivo/vitro	Familial amyotrophic lateral sclerosis
Q06547_126	1AWC_B_126	In vitro	-
Q06830_194	2Z9S_A_194	In vitro	-
Q07955_170	1X4C_A_65	In vitro	-
Q07955_37	1X4A_A_44	In vitro	-
Q08211_200	1UIL_A_47	In vitro	-
Q09028_154	3GFC_A_154	In vitro	-
Q12996_159	2OOE_A_159	In vitro	-
Q13257_199	2V64_A_199	In vitro	-
Q13451_218	1KT0_A_218	In vitro	-
Q13765_120	3MCB_A_120	In vitro	-
Q14683_575	2WD5_A_575	In vitro	-
Q15019_129	2QA5_A_129	In vitro	-
Q15027_485	3JUE_A_485	In vivo	Human pituitary adenoma tissue

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Q15056_101	2DNG_A_100	In vitro	-
Q15056_86	2DNG_A_85	In vitro	-
Q15370_45	1VCB_A_45	In vitro	-
Q15427_16	1X5U_A_19	In vitro	-
Q16539_132	1BL6_A_132	In vitro	-
Q16539_258	1BL6_A_258	In vitro	-
Q16595_143	3S4M_A_143	In vitro	-
Q16647_430	3B6H_A_430	In vitro	-
Q16695_42	3A6N_A_41	In vivo/vitro	Mutatect tumors
Q3ULF4_505	2QZ4_A_505	In vivo	Neurodegenerative disease
Q5SIY4_36	1GC8_A_1036	In vitro	-
Q60468_218	1B10_A_218	In vitro	-
Q61644_437	2X3W_D_437	In vitro	-
Q61656_97	3FE2_A_97	In vivo	Neurodegenerative disease
Q62673_481	1Q4K_B_481	In vivo	Oxidative injury to the retinal pigment epithelium
Q64455_1034	3I36_A_1012	In vivo	Oxidative injury to the retinal pigment epithelium
Q71U36_103	3HKB_A_103	In vitro	-
Q71U36_224	3HKB_A_224	In vivo/vitro	Tubulin nitration in human gliomas
Q71U36_262	3HKB_A_262	In vitro	-
Q71U36_272	3HKB_A_272	In vitro	-
Q71U36_357	3HKB_A_357	In vivo/vitro	-
Q7TMM9_106	3DU7_B_108	In vivo/vitro	-
Q7TMM9_222	3DU7_B_224	In vivo/vitro	-
Q7TMM9_36	3DU7_B_36	In vitro	-
Q7TMM9_51	3DU7_B_53	In vitro	-
Q86VP6_723	4A0C_A_723	In vitro	-
Q8NHL6_122	1VDG_A_99	In vitro	-
Q8NHL6_58	1VDG_A_35	In vitro	-
Q8NHL6_99	1VDG_A_76	In vitro	-
Q8X1D8_398	2C12_A_398	In vitro	-
Q9CQV8_106	2BQ0_A_106	In vivo	Neurodegenerative disease
Q9CQV8_213	2BQ0_A_213	In vitro	-
Q9CQV8_84	2BQ0_A_84	In vivo	Neurodegenerative disease
Q9L422_51	3N5B_A_51	In vitro	-
Q9NPD3_12	2NN6_B_11	In vitro	-
Q9P2J5_336	2WFD_A_336	In vitro	-
Q9QUH6_505	3BXJ_A_490	In vivo	-
Q9QYG0_68	2QMQ_A_68	In vitro	-
Q9UKK9_36	2DSB_A_36	In vitro	-
Q9Y230_430	2XSZ_D_345	In vitro	-

Supplementary Table S2 The nitrated proteins and their structural information used as independent testing data.

Protein and site	Protein structure and site	Reference	Disease
D0VWU3_196	3DIV_A_196	PMID:17012782	-
D0VWU3_372	3DIV_A_372	PMID:17012782	-
P01764_99	2VXS_H_79	PMID:20676907	Kidney disease
P02768_108	1AO6_A_84	PMID:12927827	-
P02768_365	1AO6_A_341	PMID:12927827	-
P04637_107	1TSR_A_107	PMID:20499882	-
P04818_135	2RD8_A_135	PMID:22072032	-
P04818_213	2RD8_A_213	PMID:22072032	-
P04818_230	2RD8_A_230	PMID:22072032	-
P04818_258	2RD8_A_258	PMID:22072032	-
P04818_301	2RD8_A_301	PMID:22072032	-
P04818_33	2RD8_A_33	PMID:22072032	-
P04818_65	2RD8_A_65	PMID:22072032	-
P09936_80	2ETL_A_80	PMID:21706495	-
P11884_150	1CW3_A_131	PMID:14527943	-
P11884_158	1CW3_A_139	PMID:14527943	-
P14780_262	1L6J_A_262	PMID:21766372	-
P17751_118	1R2R_A_67	PMID:16800626	Neurodegenerative disease
P17751_259	1R2R_A_208	PMID:16800626	Neurodegenerative disease
P20029_161	3IUC_A_160	PMID:16800626	Neurodegenerative disease
P25942_82	3QD6_R_82	PMID:21832282	-
P50396_197	1LV0_A_197	PMID:15699043	Familial amyotrophic lateral sclerosis
Q13093_307	3D59_A_307	PMID:17210780	-
Q13093_335	3D59_A_335	PMID:17210780	-
Q14145_345	2DYH_A_345	PMID:21172423	-
Q14145_491	2DYH_A_491	PMID:21172423	-
Q14145_537	2DYH_A_537	PMID:21172423	-
Q62120_1021	4GL9_A_1021	PMID:17510231	Inflammatory response
Q8IWL3_128	3BVO_A_128	doi:10.1016/j.ijms	-
Q99PT1_156	1DOA_B_156	PMID:15699043	Familial amyotrophic lateral sclerosis
Q9Z1P2_241	1SJJ_A_242	PMID:15851474	-

Supplementary Table S3 The identity and positivity of the nitrated protein in BLAST by Discovery Studio 3.1.

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Protein	Identity	Positivity
B2RSH2	99	99
O08553	98	99
O14737	100	100
O35643	98	98
O43252	99	99
O43719	99	99
O43765	100	100
O54922	98	99
O60256	100	100
O60506	100	100
O75390	96	97
O75396	97	97
O75792	100	100
O75832	100	100
P00004	100	100
P00183	100	100
P00257	100	100
P00338	100	100
P00366	100	100
P00390	100	100
P00442	100	100
P00489	99	99
P00558	100	100
P00564	97	98
P00592	100	100
P00644	99	99
P00698	100	100
P00709	100	100
P00730	100	100
P00749	99	100
P00766	100	100
P00781	98	100
P00784	100	100
P00807	100	100
P00883	100	100
P00924	99	100
P01006	100	100
P01009	100	100
P01024	100	100
P01031	100	100
P01050	100	100
P01112	100	100
P01180	100	100
P01426	100	100
P01654	96	98
P01857	99	99
P01870	99	99
P02185	99	99
P02244	100	100
P02564	95	97
P02647	100	100
P02675	100	100
P02703	98	100
P02754	100	100
P02769	99	99
P02945	100	100
P03040	100	100
P04177	100	100
P04179	100	100
P04806	100	100
P05064	97	99
P05181	100	100
P05202	100	100
P05230	100	100
P05979	99	100
P06576	96	97
P06748	100	100
P06968	100	100
P07195	100	100
P07311	100	100
P07339	100	100
P07355	99	99
P07515	100	100
P07737	100	100
P07900	100	100
P07954	100	100
P07999	98	98
P08011	100	100
P08133	99	99

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P08670	100	100
P08877	98	98
P09211	100	100
P09237	100	100
P09429	100	100
P09955	100	100
P0A0E3	100	100
P0A6A8	100	100
P0A786	100	100
P0A9C5	97	99
P0AGD3	100	100
P0C7M2	100	100
P10145	100	100
P10153	100	100
P10276	100	100
P10768	99	99
P11142	100	100
P11413	99	99
P11586	100	100
P12004	100	100
P12724	99	99
P12758	100	100
P13010	100	100
P13332	98	99
P13929	100	100
P14206	99	99
P14618	100	100
P14649	99	100
P14779	99	99
P14902	100	100
P16276	99	99
P16284	98	100
P17183	98	99
P18669	100	100
P18872	100	100
P19338	100	100
P19652	99	99
P19784	99	99
P20618	100	100
P20700	100	100
P20813	99	100
P21803	99	99
P22102	99	100
P22234	98	98
P23193	100	100
P23528	100	100
P24666	100	100
P25705	97	98
P25787	100	100
P25963	100	100
P26038	100	100
P26599	100	100
P27361	99	99
P27824	95	99
P28072	100	100
P29372	100	100
P29474	100	100
P30086	100	100
P30101	99	99
P30275	97	99
P31039	96	98
P32969	100	100
P34913	100	100
P35080	99	100
P35228	100	100
P35247	99	99
P35441	97	98
P35520	99	100
P36959	99	99
P37837	100	100
P37840	100	100
P39053	97	99
P40142	95	98
P40926	99	99
P45452	100	100
P46406	99	99
P47813	100	100
P51149	99	99
P53041	100	100
P53396	100	100

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P55072	100	100
P55769	100	100
P56574	96	99
P60301	100	100
P60615	100	100
P60710	100	100
P60770	100	100
P60842	100	100
P61013	98	98
P61088	100	100
P61158	100	100
P61513	100	100
P61823	100	100
P61927	100	100
P62136	100	100
P62158	100	100
P62249	100	100
P62259	99	99
P62263	100	100
P62273	100	100
P62750	100	100
P62805	100	100
P62826	100	100
P62917	100	100
P62993	100	100
P63168	100	100
P63244	100	100
P63328	99	99
P67775	100	100
P68699	98	98
P68871	100	100
P69542	100	100
P69687	100	100
P69905	100	100
P69924	100	100
P78417	100	100
P83731	100	100
P84103	100	100
P97427	100	100
Q01130	100	100
Q01518	100	100
Q02790	100	100
Q03405	99	99
Q04206	99	99
Q04447	96	98
Q06547	98	100
Q06830	96	98
Q07955	100	100
Q08211	97	97
Q09028	100	100
Q12996	99	99
Q13257	100	100
Q13451	99	100
Q13765	100	100
Q14683	100	100
Q15019	100	100
Q15027	99	99
Q15056	98	98
Q15370	100	100
Q15427	98	100
Q16539	100	100
Q16595	100	100
Q16647	100	100
Q16695	100	100
Q3ULF4	96	98
Q5SIY4	99	99
Q60468	95	99
Q61644	100	100
Q61656	99	100
Q62673	95	98
Q64455	98	98
Q71U36	100	100
Q7TMM9	99	99
Q86VP6	99	99
Q8NHL6	100	100
Q8X1D8	100	100
Q9CQV8	98	99
Q9L422	100	100
Q9NPD3	100	100
Q9P2J5	96	96

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Q9QUH6	100	100
Q9QYG0	100	100
Q9UKK9	100	100
Q9Y230	97	97

Supplementary Table S4 All the structural features extracted from local protein structure. In the 'X_A', the X means the type of amino acids, and A means the type of atoms. The atoms are categorized into 8 types including carbon of main chain (C), alpha carbon (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*). 'S*' of 148 means the side-chain sulfur from Cys and Met. 'Atoms_8A' means the number of atoms in the distant threshold of 8 angstrom.

No.	Structral features
1	SER_C
2	SER_O
3	SER_N
4	SER_CA
5	SER_C*
6	SER_O*
7	THR_C
8	THR_O
9	THR_N
10	THR_CA
11	THR_C*
12	THR_O*
13	CYS_C
14	CYS_O
15	CYS_N
16	CYS_CA
17	CYS_C*
18	CYS_S*
19	PRO_C
20	PRO_O
21	PRO_N
22	PRO_CA
23	PRO_C*
24	ASN_C
25	ASN_O
26	ASN_N
27	ASN_CA
28	ASN_C*
29	ASN_O*
30	ASN_N*
31	GLN_C
32	GLN_O
33	GLN_N
34	GLN_CA
35	GLN_C*
36	GLN_O*
37	GLN_N*
38	ASP_C
39	ASP_O
40	ASP_N
41	ASP_CA
42	ASP_C*
43	ASP_O*
44	GLU_C
45	GLU_O
46	GLU_N
47	GLU_CA
48	GLU_C*
49	GLU_O*
50	LYS_C
51	LYS_O
52	LYS_N
53	LYS_CA
54	LYS_C*
55	LYS_N*
56	ARG_C
57	ARG_O
58	ARG_N
59	ARG_CA
60	ARG_C*
61	ARG_N*
62	HIS_C
63	HIS_O
64	HIS_N
65	HIS_CA
66	HIS_C*
67	HIS_N*
68	PHE_C

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69	PHE_O
70	PHE_N
71	PHE_CA
72	PHE_C*
73	TYR_C
74	TYR_O
75	TYR_N
76	TYR_CA
77	TYR_C*
78	TYR_O*
79	TRP_C
80	TRP_O
81	TRP_N
82	TRP_CA
83	TRP_C*
84	TRP_N*
85	GLY_C
86	GLY_O
87	GLY_N
88	GLY_CA
89	ALA_C
90	ALA_O
91	ALA_N
92	ALA_CA
93	ALA_C*
94	VAL_C
95	VAL_O
96	VAL_N
97	VAL_CA
98	VAL_C*
99	LEU_C
100	LEU_O
101	LEU_N
102	LEU_CA
103	LEU_C*
104	ILE_C
105	ILE_O
106	ILE_N
107	ILE_CA
108	ILE_C*
109	MET_C
110	MET_O
111	MET_N
112	MET_CA
113	MET_C*
114	MET_S*
115	All_C
116	All_O
117	All_N
118	All_CA
119	Polar_C
120	Polar_O
121	Polar_N
122	Polar_CA
123	Acid_C
124	Acid_O
125	Acid_N
126	Acid_CA
127	Basic_C
128	Basic_O
129	Basic_N
130	Basic_CA
131	Aromatic_C
132	Aromatic_O
133	Aromatic_N
134	Aromatic_CA
135	Aliphatic_C
136	Aliphatic_O
137	Aliphatic_N
138	Aliphatic_CA
139	Polar_C*
140	Polar_O*
141	Polar_N*
142	Acid_C*
143	Acid_O*
144	Basic_C*
145	Basic_N*
146	Aromatic_C*
147	Aliphatic_C*
148	S*

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149 Atoms_8A

Supplementary Table S5 The results of Mann-Whitney Test for AAPs. For polar, acid, basic, aromatic and aliphatic AAP, they are polar amino acids of S, T, C, P, N, Q, acidic amino acids of D, E, basic amino acids of K, R, H, aromatic amino acids of F, Y, W, and aliphatic amino acids of G, A, V, L, I, M.

Types of AAPs	P-value
Y-Ser	0.837
Y-Thr	0.939
Y-Cys	0.194
Y-Pro	0.529
Y-Asn	0.176
Y-Gln	0.385
Y-Asp	0.057
Y-Glu	0.286
Y-Lys	0.828
Y-Arg	0.056
Y-His	0.557
Y-Phe	0.016
Y-Tyr	0.000
Y-Trp	0.296
Y-Gly	0.884
Y-Ala	0.010
Y-Val	0.085
Y-Leu	0.032
Y-Ile	0.004
Y-Met	0.001
Y-Polar	0.248
Y-Acid	0.039
Y-Basic	0.265
Y-Aromatic	0.000
Y-Aliphatic	0.000

Supplementary Table S6 The results of Mann-Whitney Test for AATs. The table shows the P-value of Mann-Whitney test. For example, in the AAT of Phe-Y-X, the P-value is 0.840 when X is Ser.

AAT / X	Phe-Y-X	Tyr-Y-X	Ala-Y-X	Leu-Y-X	Ile-Y-X	Met-Y-X
S	0.840	0.011	0.017	0.090	0.651	0.025
T	0.871	0.010	0.223	0.820	0.197	0.043
C	0.097	0.054	0.018	0.205	0.007	0.025
P	0.748	0.100	0.647	0.900	0.907	0.509
N	0.230	0.003	0.677	0.177	0.768	0.279
Q	0.886	0.016	0.110	0.028	0.204	0.059
D	0.182	0.006	0.004	0.201	0.022	0.033
E	0.065	0.001	0.493	0.876	0.058	0.001
K	0.297	0.000	0.126	0.345	0.177	0.154
R	0.061	0.000	0.052	0.105	0.077	0.006
H	0.645	0.100	0.716	0.504	0.294	0.039
F	0.303	0.001	0.057	0.053	0.004	0.001
Y	0.001	0.000	0.000	0.000	0.000	0.023
W	0.306	0.337	0.321	0.458	0.095	0.808
G	0.287	0.078	0.819	0.737	0.463	0.014
A	0.057	0.000	0.166	0.021	0.016	0.009
V	0.091	0.000	0.257	0.051	0.012	0.009
L	0.053	0.000	0.021	0.293	0.006	0.000
I	0.004	0.000	0.016	0.006	0.544	0.001
M	0.001	0.023	0.009	0.000	0.001	0.031

Supplementary Table S7 The results of Mann-Whitney Test of structural features. The table shows the P-value of Mann-Whitney test in the structural features. For example, 'Ser-C*' means side-chain carbon from Ser. 'Aromatic-C*' means side-chain carbon of aromatic amino acids. There are polar amino acids of S, T, C, P, N, Q, acidic amino acids of D, E, basic amino acids of K, R, H, aromatic amino acids of F, Y, W, and aliphatic amino acids of G, A, V, L, I, M.

Type of Structral features	P-value
Ser-C*	0.507
Ser-O*	0.602
Thr-C*	0.797
Thr-O*	0.629
Cys-C*	0.300
Cys-S*	0.142
Pro-C*	0.904
Asn-C*	0.993
Asn-O*	0.640
Asn-N*	0.944
Gln-C*	0.330

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Gln-O*	0.767
Gln-N*	0.126
Asp-C*	0.259
Asp-O*	0.151
Glu-C*	0.002
Glu-O*	0.041
Acid-O*	0.013
Lys-C*	0.400
Lys-N*	0.752
Arg-C*	0.062
Arg-N*	0.370
His-C*	0.969
His-N*	0.841
Basic-N*	0.361
Phe-C*	0.194
Tyr-C*	0.000
Tyr-O*	0.008
Trp-C*	0.681
Trp-N*	0.916
Ala-C*	0.040
Val-C*	0.297
Leu-C*	0.002
Ile-C*	0.216
Met-C*	0.000
Met-S*	0.013
S* [a]	0.015
Aromatic-C*	0.002
Aliphatic-C*	0.000
Atom_8A	0.000

[a] 'S*' means side-chain sulfur from Met and Cys.

Supplementary Table S8 The nine clusters in predictive model using MDD method. For predictive model using MDD method, the column of 'Ps' is the conserved position in sequence used for clustering, and '+' means that the amino acid is in the downstream of the peptide, and vice versa. The column of 'Amino Acid' is the amino acid feature used for clustering. 'CP' is the condition positive; 'CN' is the condition negative.

Predictive Model	Cluster	Ps	Amino Acid	CP	CN
MDD	1	-4	Acid	89	494
	2	-2	Basic	73	434
	3	5	Basic	60	360
	4	6	Basic	49	328
	5	-3	Basic	42	293
	6	2	Basic	35	209
	7	-9	Acid	28	135
	8	-1	Acid	21	78
	9	-	-	118	608

Supplementary Table S9 The evaluation results of each cluster in predictive model using MDD method. 'NF' is the number of features used in the cluster. 'AC' is accuracy. 'SN' is sensitivity. 'SP' is specificity. Predictive model used the MDD method of sequence-based clustering. For Total and Balanced sensitivity and specificity, Total and Balanced SN = Total_TP/(Total_TP+Total_FN), Total and Balance SP = Total_TN/(Total_TN+Total_FP), where the Total_TP, Total_TN, Total_FN and Total_FP are the total number of TP, TN, FN and FP in nine clusters.

Predictive Model	Cluster	NF	AC (%)	SN (%)	SP (%)
MDD	1	14	88.16	68.54	91.70
	2	14	89.35	67.12	93.09
	3	11	91.43	83.33	92.78
	4	15	89.66	71.43	92.38
	5	16	90.45	69.05	93.52
	6	26	86.48	65.71	89.95
	7	23	94.48	96.43	94.07
	8	11	94.95	95.24	94.87
	9	11	75.34	33.90	83.39
	Total and Balanced		**77.75**	**64.85**	**90.64**

Supplementary Table S10 The evaluation results of each cluster only using sequence features in the predictive model using modified MDD method. 'NF' is the number of features used in the cluster. 'AC' is accuracy; 'SN' is sensitivity; 'SP' is specificity. Predictive model used the modified MDD method of structure-based clustering.

Predictive Model	Cluster	NF	AC (%)	SN (%)	SP (%)
Modified MDD	1	39	77.31	33.93	84.83
	2	13	83.41	32.53	91.09
	3	11	81.24	31.43	90.74

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	4	34	79.02	40.86	86.43
	5	21	79.53	39.13	85.81
	6	33	81.60	39.29	88.04
	7	31	80.67	38.46	87.83
	8	30	81.75	39.47	89.52
	9	12	83.94	33.87	91.06
	Total and Balanced		**62.36**	**36.12**	**88.60**

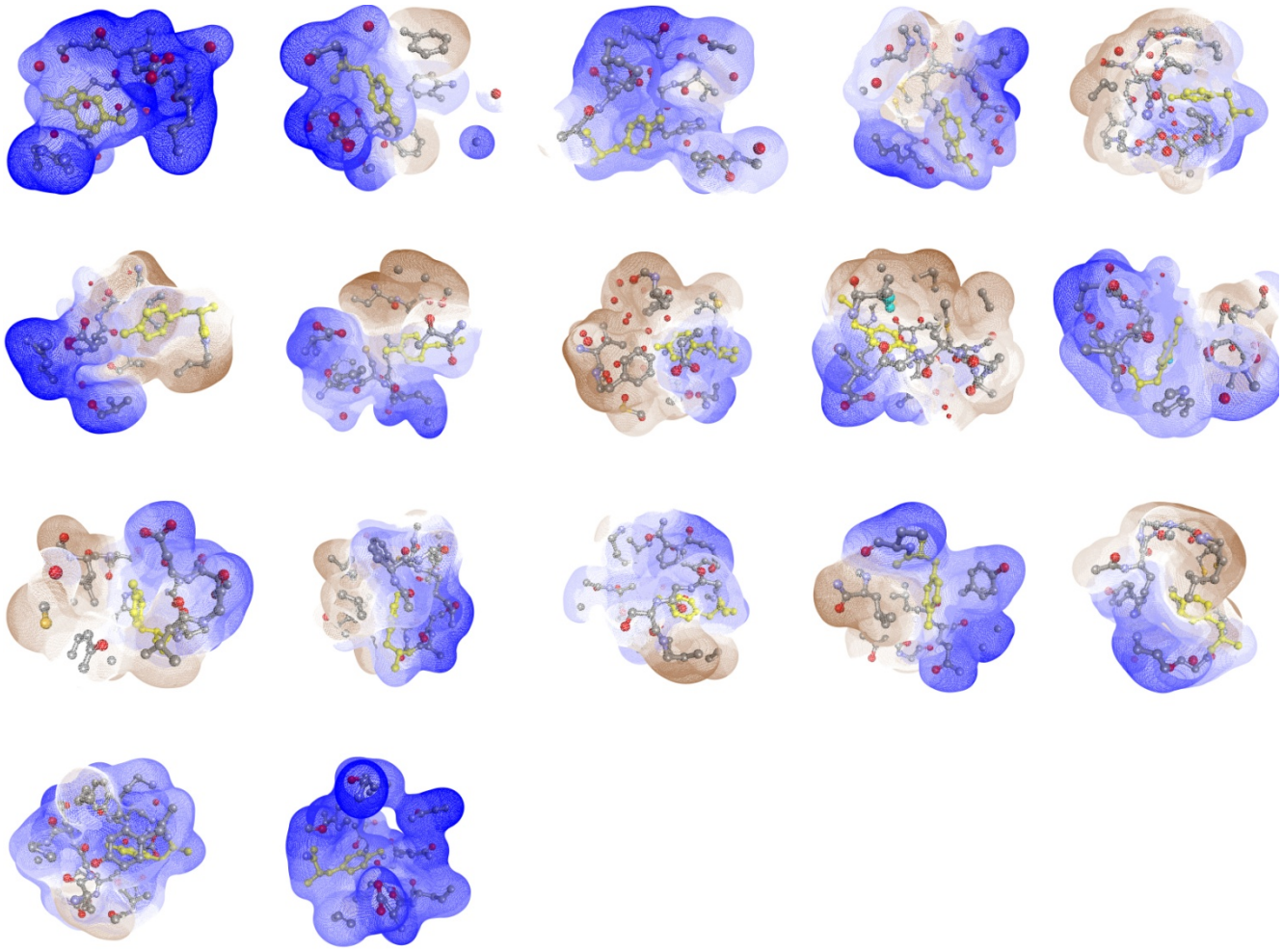

Figure S1. The hydrophobic/hydrophilic environment at the nitrated tyrosine. The environment of nitrated tyrosine (yellow) formed by oxygen (red), nitrogen (blue), carbon (gray) are shown. The color from hydrophilic to hydrophobic is from blue to brown.