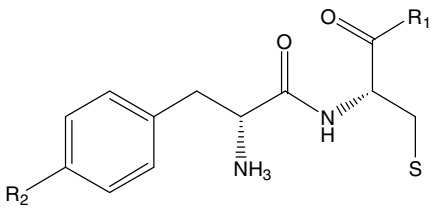
Supporting information to

Intramolecular addition of cysteine thiyl radical to phenylalanine and tyrosine in a model peptide, Phe(CysS$^{\bullet}$) and Tyr(CysS$^{\bullet}$): a computational study

by

Sergej Naumov and Christian Schöneich

Optimized cyclic structures in water at B3LYP/6-311g+/Pbf (Version 4.00, Jaguar 7.0) level of theory.**

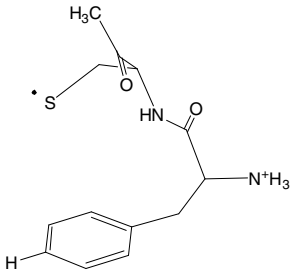


R_1= CH_3, NH_2, O^-

R_2= H, OH

R1=CH3; R2=H

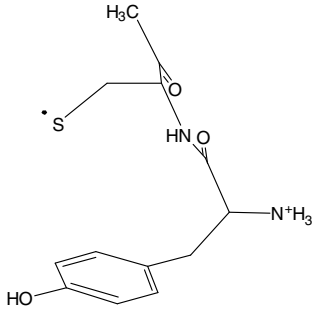
C1	-0.8063592412	-2.3060405938	0.0288424967
C2	-0.9170832067	-1.9705210424	-1.3260762306
C3	-2.1517500791	-1.6086342105	-1.8724181093
C4	-3.2921173987	-1.5730493259	-1.0697521059
C5	-3.1929184369	-1.9108336956	0.2804036039
C6	-1.9596151856	-2.2745601993	0.8236215872
C7	0.5252053543	-2.7181837774	0.6267128305
C8	1.1792309965	-1.6195030441	1.4919996383
C9	0.8274538693	1.8422279703	-1.4669709071
C10	1.6178837393	-0.4154611936	0.6440763464
C11	0.5544427921	3.1115180257	0.7364067143
C12	0.7193096536	4.4753019901	0.1265408061
C13	1.2069967738	1.9236881555	0.0268338972
H14	2.2905486481	2.0898029531	0.0735598205
H15	3.1527975436	-2.3637542951	1.4447986521
H16	2.2318293817	-3.0508819001	2.6318513756
H17	2.8164734141	-1.5289098062	2.8266415478
H18	0.1767321551	0.7761372430	1.4754009998
H19	-0.0415683014	-2.0194508064	-1.9681518754
H20	-2.2231332070	-1.3688749053	-2.9290352513
H21	-4.2527109659	-1.2987491682	-1.4960119838
H22	-4.0764023193	-1.8976118648	0.9121769825
H23	-1.8985770968	-2.5536113715	1.8725708442
H24	0.3829957034	-3.5971170869	1.2637025292
H25	1.2227026519	-3.0037577871	-0.1663848318
H26	0.5192855004	-1.3227882587	2.3074259934
H27	1.3685095721	1.0170391758	-1.9368179621
H28	1.1565486424	2.7415460819	-1.9996004332
H29	0.6008333742	5.2348977726	0.9006361979
H30	-0.0678694963	4.6357908418	-0.6209987844
H31	1.6815786891	4.5923110645	-0.3759574155
N32	2.4233408549	-2.1755291757	2.1388293238
N33	0.8872866140	0.7026964073	0.7565917301
O34	2.5844328578	-0.5323891769	-0.1112073488
O35	-0.0757871640	2.9334452494	1.7632105191
S36	-0.9417191562	1.6312645048	-1.8044016893



R1=CH3; R2=OH

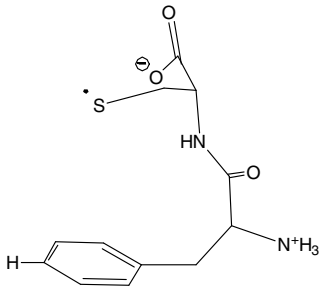
C1	-0.5206441099	-2.4043134206	0.0510238909
C2	-0.7413171862	-1.9955281649	-1.2697851263
C3	-2.0191551339	-1.6619498032	-1.7207354443

C4	-3.1016133484	-1.7335683717	-0.8415096568
C5	-2.9046998601	-2.1501530070	0.4765774527
C6	-1.6239014380	-2.4823752666	0.9096346674
C7	0.8589496418	-2.7865360821	0.5459973777
C8	1.4710681207	-1.7541896502	1.5235769046
C9	1.4651300587	1.7173795559	-1.3976711506
C10	1.9884918083	-0.5147769001	0.7786376337
C11	0.7296079344	2.9585953095	0.7172047816
C12	0.9018385147	4.3329904577	0.1369125116
C13	1.5730483275	1.8198933773	0.1354261869
H14	2.6179764702	2.0613348853	0.3719172460
H15	3.4425410016	-2.4886260584	1.5808147706
H16	2.4235074346	-3.2807555309	2.6231721086
H17	2.9784193293	-1.7761115938	2.9993324068
H18	0.4096526272	0.6150452312	1.4266280864
H19	0.0875356429	-1.9587940141	-1.9709622960
H20	-2.1823991008	-1.3592029386	-2.7500896522
O21	-4.3389421225	-1.3920127875	-1.3173169544
H22	-3.7520824934	-2.2226549285	1.1527521490
H23	-1.4902967430	-2.8212035997	1.9327048211
H24	0.7974930189	-3.7418674396	1.0775503830
H25	1.5418709955	-2.9312443165	-0.2958713820
H26	0.7558776417	-1.4866415737	2.3017330102
H27	2.1310610911	0.9319372061	-1.7615338986
H28	1.8124535703	2.6430591801	-1.8727503388
H29	0.5760550893	5.0781674132	0.8642466875
H30	0.2634109959	4.4260526772	-0.7501024053
H31	1.9320725549	4.5213476437	-0.1713805793
N32	2.6540910022	-2.3651167443	2.2269865727
N33	1.2078907248	0.5748663617	0.8025862352
O34	3.0588872792	-0.5788448516	0.1710217544
O35	-0.0467929342	2.7323723204	1.6279198310
S36	-0.2096377187	1.4096378635	-2.0196109870
H37	-5.0112708489	-1.4936543574	-0.6280871858



R1=O⁻; R2=H

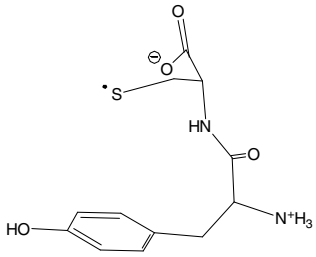
C1	-0.2850559342	-2.1482961852	-0.5714397641
C2	0.1389475285	-1.8255337088	-1.8650704268
C3	-0.7595003398	-1.3078460559	-2.8002541439
C4	-2.1002033953	-1.1131690348	-2.4533715712
C5	-2.5338990558	-1.4445395124	-1.1690882963
C6	-1.6335679445	-1.9590616492	-0.2376426634
C7	0.7007915536	-2.6692393613	0.4573728603
C8	1.1060631997	-1.5927750519	1.4915977339
C9	1.0229225698	1.8096946942	-1.5801781607
C10	1.7119965210	-0.3815611670	0.7747322872
C11	0.4802662376	3.0739219602	0.5494125495
C12	1.2617660651	1.8919580830	-0.0666120256
H13	1.4281121740	2.7065375599	-2.0552692294
H14	2.3263105482	2.0887762442	0.0913043473
H15	3.0616686875	-2.2103326016	1.9413680251
H16	1.9081682493	-3.0706608603	2.7701142690
H17	2.2855763258	-1.5363241289	3.2360126979
H18	0.0487509674	0.7191415446	1.1789955111
H19	1.1755320369	-1.9770946090	-2.1488832822
H20	-0.4179485962	-1.0633948230	-3.8004856792
H21	-2.7989495505	-0.7107669463	-3.1794707882
H22	-3.5736550086	-1.3007121574	-0.8933896451
H23	-1.9829597772	-2.2152533000	0.7582835154
H24	0.2705567203	-3.5155787180	1.0011340575
H25	1.6048632457	-3.0212129174	-0.0473437772
H26	0.2570735303	-1.3108102834	2.1141852337
H27	1.5463232219	0.9560680363	-2.0166715464
N28	0.9037165410	0.6688000243	0.6369794880
N29	2.1554177978	-2.1408954161	2.4190751133
O30	0.5987632943	4.1719833633	-0.0411167672
O31	2.8573307524	-0.4572858555	0.3176851824
O32	-0.2013879385	2.8414881080	1.5781698421
S33	-0.7252299515	1.7010495058	-2.0674467869



R1=O⁻; R2=OH

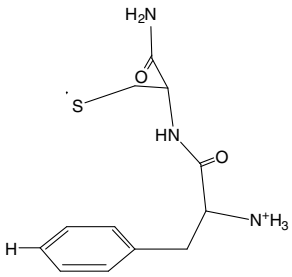
C1	-0.6291675247	-2.2988069123	0.1641026511
C2	-0.9148099975	-1.7569889836	-1.0953985425
C3	-2.2280081901	-1.5300055966	-1.5068641745

C4	-3.2837452724	-1.8513051108	-0.6510202661
C5	-3.0221015470	-2.3949551721	0.6080757095
C6	-1.7054433394	-2.6131393442	1.0033106612
C7	0.7894823661	-2.5878785211	0.6140615988
C8	1.3579964080	-1.5415064465	1.6064366713
C9	1.6660171016	1.9363027290	-1.4127750671
C10	1.9624532515	-0.3427310863	0.8628612435
C11	0.7210256693	3.1179125885	0.6375781354
O12	0.9323731825	4.2489101866	0.1448345333
C13	1.6239526481	1.9762364615	0.1172421177
H14	2.6402648253	2.1913500171	0.4644250983
H15	3.3183900505	-2.2511740136	1.8294686397
H16	2.2303105850	-3.0568297373	2.7938496666
H17	2.7325874718	-1.5406024529	3.2021035423
H18	0.3197330717	0.8072362761	1.2567258070
H19	-0.1048973460	-1.5268828544	-1.7816272623
H20	-2.4393181533	-1.1151666288	-2.4877075445
O21	-4.5609478930	-1.6249519156	-1.0900342618
H22	-3.8467775875	-2.6555611540	1.2653826678
H23	-1.5192422488	-3.0519807850	1.9787380137
H24	0.8076343857	-3.5613878933	1.1126218298
H25	1.4575570941	-2.6620946291	-0.2479787061
H26	0.5970262582	-1.2302382625	2.3221343189
H27	2.3690673006	1.1830454762	-1.7706204159
H28	2.0258331701	2.9028521410	-1.7837229719
N29	2.4800821735	-2.1406486827	2.4108705672
N30	1.1772537385	0.7241777053	0.7182900427
O31	3.1082037372	-0.4316865164	0.4091897907
O32	-0.1298379757	2.8205181593	1.5127712124
S33	0.0633023133	1.6756674950	-2.2139129059
H34	-5.2054323009	-1.9057373200	-0.4243593789



R1=NH_2; R2=H

C1	-0.5247002946	-2.3218056445	-0.5435765631
C2	-0.2733269540	-1.8137894345	-1.8285188311
C3	-1.3298283422	-1.5259249494	-2.7016526420
C4	-2.6529897485	-1.7489866051	-2.3045222774
C5	-2.9132427630	-2.2654706913	-1.0299806355
C6	-1.8560089490	-2.5490442238	-0.1578971233
C7	0.6120634676	-2.6486949368	0.4078893427
C8	0.9489190921	-1.5034016079	1.3917029761
C9	1.3210472604	2.0677299292	-1.4894674959
C10	1.6085651503	-0.3136136060	0.6712206922
C11	0.7946662316	3.2638319360	0.7186442082
C12	1.4766073598	2.0580704194	0.0489207757
H13	2.1137316993	4.6058077090	-0.1504637286
H14	2.5507531878	2.1052376221	0.2618864757
H15	2.8654090705	-2.1847681455	1.9571995685
H16	1.6439068331	-2.8761668860	2.8397329213
H17	2.1091943455	-1.3261649560	3.1537731182
H18	0.0727566105	0.9552210416	1.1836717683
H19	0.7517007578	-1.6627704694	-2.1604407410
H20	-1.1179103198	-1.1441618404	-3.6969955928
H21	-3.4723577201	-1.5334657932	-2.9862137316
H22	-3.9370114344	-2.4576446994	-0.7173459799
H23	-2.0671981151	-2.9640569758	0.8259588144
H24	0.3449400707	-3.5293637319	1.0037059119
H25	1.5177233872	-2.8950703429	-0.1570822309
H26	0.0677450891	-1.2013720977	1.9620201243
H27	1.8830999476	1.2266463967	-1.9124192986
H28	1.7771182886	2.9695929630	-1.9180154153
H29	0.8585390502	5.2989370456	0.8270694477
N30	1.2835580534	4.4747910127	0.4142578359
N31	0.9358446517	0.8477164212	0.6577329113
N32	1.9553185851	-2.0035529828	2.3986230061
O33	2.7123596840	-0.4732312508	0.1306141440
O34	-0.1686856531	3.0945096290	1.4830964433
S35	-0.3746411913	1.9627276572	-2.1126846550



R1=NH_2; R2=OH

C1	0.4172409213	-2.2628732547	-0.8263204369
C2	1.0808792384	-1.6430863882	-1.8909993166
C3	0.4080702358	-1.3051208337	-3.0652330639

C4	-0.9520821983	-1.6045567577	-3.1924614865
C5	-1.6280749642	-2.2367898034	-2.1472997976
C6	-0.9434235182	-2.5579586740	-0.9792303877
C7	1.1290882392	-2.6028595364	0.4659935202
C8	0.9440902052	-1.5238318110	1.5614446048
C9	1.3719117237	2.1203433703	-1.3740436594
C10	1.7543849208	-0.2647979246	1.2217678935
C11	1.2439331976	3.1925934479	0.9114329746
C12	1.6968360345	1.9480243655	0.1317535148
H13	3.1073373311	4.0670395492	0.7276556984
H14	2.7747930232	1.8305402393	0.2300080006
H15	2.4872016436	-2.1263088787	2.8581256301
H16	1.0801350923	-2.9766666068	3.0800080528
H17	1.2094818798	-1.4387786953	3.6544497289
H18	0.0625651036	0.6861379216	0.5862914451
H19	2.1426720779	-1.4271202857	-1.8165665409
H20	0.9325951121	-0.8352218878	-3.8911426231
O21	-1.5744154212	-1.2747670844	-4.3629228655
H22	-2.6799921940	-2.4840855333	-2.2572673853
H23	-1.4790835950	-3.0570006343	-0.1773441278
H24	0.7349278445	-3.5435068998	0.8619176478
H25	2.1993590770	-2.7450991708	0.2906036714
H26	-0.1125325036	-1.3031730499	1.7145037913
H27	1.9679409034	1.4062887925	-1.9520501975
H28	1.6735511615	3.1148238692	-1.7150898821
H29	1.8868366394	5.0423506179	1.4862894046
N30	2.1463279160	4.1798876424	1.0203797244
N31	1.0699607743	0.7531911208	0.6768390504
N32	1.4636797785	-2.0496955185	2.8724895535
O33	2.9718373088	-0.2684270436	1.4075437614
O34	0.0940158559	3.2712807840	1.3476081886
S35	-0.3466347987	1.8286565892	-1.8595064131
H36	-2.5064957139	-1.5376237159	-4.3385808273