

A New Generation of Cysteine Derivatives with Three Active Antioxidant Centers: Improving Reactivity and Stability

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Supporting Information

Materials

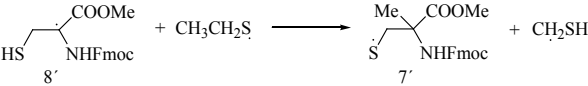
Cysteines were prepared following the standard procedures previously described that involving the corresponding commercially available cysteines and using classical protecting methodologies common in organic chemistry.

All compounds were identified by spectroscopic data and their purity (>99%) was chromatographically confirmed.

For antioxidant activity experiments, the supporting electrolyte, KCl (purity $\geq$ 99.5%, Panreac), 1,1-diphenyl-2-picrylhydrazyl (DPPH) radical (Sigma Aldrich), dry methanol (purity $\geq$ 99.8%, Panreac), Iron(II) sulphate heptahydrate (purity $\geq$ 99.5%, Acros Organics) and H₂O₂ (30% p/v, Panreac).

Table S1. Energy values for isodesmic reaction.

Isodesmic Species	E ₀ /Hartree	S ⁰ /cal·mol ⁻¹	ZPE/Hartree
CH ₃ CH ₂ S	-477.38605	67.6	0.06470
CH ₂ -SH	-438.04553	63.8	0.03140
1'	-952.61132	121.0	0.19175
2'	-913.30544	117.3	0.16112
7'	-1528.08910	174.1	0.36601
8'	-1488.78359	170.0	0.33548



Scheme S1. Isodesmic reaction to calculate the stabilization energy

Table S2. Geometrical parameters at B3LYP/6-31+G(d,p) in gas phase and using Polarizable Continuum Model (PCM) in different solvents.

No.	Solvent	<i>d</i> (O⋯HS)	Φ	ψ	χ ₁	<i>d</i> (O⋯HN)	θ
1	Gas-phase	2.080	-177.3	178.2	-94.8	2.067	112.0
	Heptane	2.066	-176.5	178.1	-93.5	2.066	112.1
	Metanol	2.040	-175.1	177.4	-90.9	2.065	112.1
	DMSO	2.039	-175.0	177.4	-90.8	2.065	112.1
	Water	2.039	-175.0	177.3	-96.7	2.065	112.1
2	Gas-phase	3.697	-107.9	161.5	-66.1	2.501	112.2
	Heptane	3.752	-103.8	166.5	-65.6	2.564	112.1
	Metanol	3.990	-103.4	165.8	-65.8	2.795	111.9
	DMSO	3.992	-103.6	166.2	-65.7	2.799	111.9
	Water	3.994	-107.2	161.1	-66.1	2.802	111.9
3	Gas-phase	2.078	-178.3	178.3	-96.4	2.067	112.0
	Heptane	2.059	-177.0	178.0	-94.5	2.059	112.0
	Metanol	2.029	-176.0	177.5	-92.1	2.060	112.1
	DMSO	2.028	-176.0	177.5	-92.0	2.060	112.1
	Water	2.027	-176.0	177.5	-92.0	2.059	112.1
4	Gas-phase	3.695	-107.4	161.6	-66.4	2.515	112.2
	Heptane	3.731	-107.4	161.3	-66.4	2.562	112.1
	Metanol	3.973	-104.1	165.0	-66.0	2.784	111.8
	DMSO	3.985	-103.8	165.4	-66.0	2.797	111.8
	Water	3.997	-103.5	165.9	-66.0	2.808	111.8
5	Gas-phase	2.109	-173.8	178.2	-92.9	2.093	112.1
	Heptane	2.098	-172.9	178.1	-91.7	2.091	112.1
	Metanol	2.087	-170.3	177.5	-88.4	2.082	112.1
	DMSO	2.087	-170.2	177.5	-88.4	2.082	112.1
	Water	2.087	-170.1	177.5	-88.3	2.082	112.1
6	Gas-phase	3.758	-103.5	161.8	-65.2	2.526	111.8
	Heptane	3.801	-102.6	161.8	-65.3	2.572	111.7
	Metanol	3.868	-104.6	166.2	-65.0	2.666	111.9
	DMSO	3.870	-104.7	166.5	-65.0	2.671	111.9
	Water	3.873	-104.8	166.9	-64.9	2.677	111.9
7	Gas-phase	2.128	-173.4	177.6	-91.7	2.087	112.1
	Heptane	2.126	-172.3	177.3	-90.3	2.086	112.1
	Metanol	2.126	-171.0	176.9	-88.0	2.082	112.0
	DMSO	2.126	-170.9	176.9	-88.0	2.082	112.0
	Water	2.127	-170.9	176.9	-87.9	2.082	112.0
8	Gas-phase	2.257	-142.4	166.9	-84.8	2.250	113.2
	Heptane	3.805	-104.3	163.0	-65.6	2.569	111.8
	Metanol	3.854	-107.4	165.0	-65.0	2.660	112.0
	DMSO	3.857	-107.5	165.2	-64.9	2.665	112.0
	Water	3.861	-107.6	165.5	-64.9	2.670	112.0

Table S3. Gas-phase Gibbs energies, $G^\circ_{(g)}$, calculated at B3LYP/6-31+G(d,p) level and PCM solvation energies in water and methanol of the species involved in the oxidation processes, values (kJ·mol⁻¹) at 298.15 K.

No.	$G^\circ_{(g)}$ /Hartree		$\Delta\Delta G^\circ_{solv}$	
	Red	Ox	H ₂ O	MeOH
1	-953.09275	-952.80272	-165.2	-162.7
2	-913.80677	-913.50952	-159.6	-157.5
3	-1070.96218	-1070.67737	-153.6	-150.1
4	-1031.67620	-1031.38434	-149.2	-146.3
5	-1146.19643	-1145.90619	-155.3	-152.4
6	-1106.91155	-1106.61389	-152.2	-149.3
7	-1528.41220	-1528.14114	-140.9	-137.9
8	-1489.12506	-1488.85222	-144.2	-142.4

Table S4. Gas-phase enthalpy energies, $H^\circ_{(g)}$, calculated at B3LYP/6-31+G(d,p) level of the species involved in the oxidation processes at 298.15 K.

No.	$H^\circ_{(g)}$ /Hartree				
	Neutral Compound	Sulphur Radical	Nitrogen Radical	C ^a Radical	C ^b Radical
1	-953.03520	-952.40446	-952.37233	-	-952.39218
2	-913.75000	-913.11718	-913.08586	-913.13025	-913.10521
3	-1070.89647	-1070.26610	-1070.22900	-	-1070.25364
4	-1031.61142	-1030.97937	-1030.94831	-1030.97345	-1030.96664
5	-1146.12770	-1145.49688	-1145.45953	-	-1145.48412
6	-1106.84394	-1106.21128	-1106.17863	-1106.20724	-1106.19900
7	-1528.32927	-1527.69809	-1527.66358	-	-1527.68563
8	-1489.04353	-1488.41067	-1488.37931	-1488.42418	-1488.40114

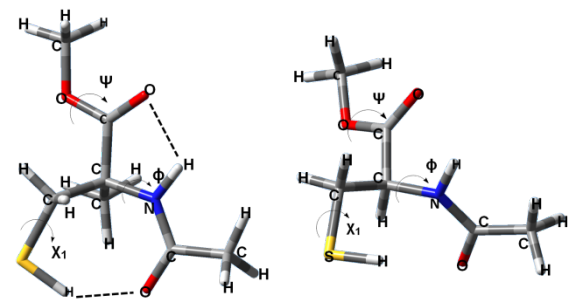


Fig S1. Optimized structures obtained by DFT calculations for compounds 1 and 2

Cartesian Coordinates for Optimized Geometries in Gas Phase Phase at B3lyp/6-31+G(d,p) Level of Neutral Compounds

(2R)-N-Ac-2-methylcysteine methyl ester (1)

C	-0.206959	0.002276	0.180137
C	-1.582244	-0.645984	-0.097628
O	-1.739073	-1.787425	-0.491845
C	-0.057145	1.211148	-0.808532
S	0.990276	2.633999	-0.308068
O	-2.594027	0.192904	0.158877
H	0.286157	0.820611	-1.769707
H	-1.038288	1.665044	-0.960575
H	2.104641	1.909711	-0.064852
N	0.753735	-1.072154	-0.112387
H	0.320376	-1.941806	-0.400888
C	2.107201	-1.032592	0.024353
C	2.826254	-2.341239	-0.262533
O	2.738173	-0.026361	0.356895
H	3.603124	-2.154975	-1.008701
H	3.324385	-2.670670	0.654212
H	2.168586	-3.139508	-0.616655
C	-0.155823	0.407464	1.668135
H	-0.421439	-0.448209	2.297172
H	0.852346	0.734672	1.922223
H	-0.848927	1.227370	1.864099
C	-3.925204	-0.326800	-0.052789
H	-4.096702	-1.194779	0.587294
H	-4.595872	0.489224	0.212132
H	-4.056007	-0.614175	-1.098230

N-Ac-methyl ester (2)

C	-0.145097	0.231790	0.094061
C	-1.496492	-0.423423	-0.213140
O	-1.686698	-1.214811	-1.115456
C	-0.161154	1.679372	-0.444923
S	1.301394	2.678994	0.030826
O	-2.454554	0.022763	0.615239
H	0.013711	0.244949	1.175009
H	-0.269194	1.676650	-1.534378
H	-1.017463	2.212288	-0.024159
H	2.223726	1.855072	-0.506418
N	0.922830	-0.557206	-0.489232
H	0.769725	-0.870752	-1.439725
C	1.772016	-1.311884	0.294182
C	2.685494	-2.258950	-0.462921
O	1.807764	-1.212175	1.514629
H	3.718086	-2.063129	-0.162512
H	2.445894	-3.284683	-0.167121
H	2.604033	-2.172371	-1.549862
C	-3.784514	-0.497121	0.394385
H	-3.786876	-1.583008	0.509858
H	-4.406596	-0.026027	1.154029
H	-4.130770	-0.237368	-0.608467

(2R)-N-Piv-2-methylcysteine methyl ester (3)

C	-0.221326	-0.005115	0.419056
C	-1.546696	-0.267352	-0.330917
O	-1.681646	-1.077469	-1.230046
C	0.177943	1.488345	0.143456
S	1.138380	2.395537	1.418100
O	-2.545562	0.495433	0.132173
H	0.708569	1.524624	-0.811038
H	-0.731290	2.084490	0.045336
H	2.155176	1.508135	1.477731
N	0.724192	-0.950962	-0.193995
H	0.312012	-1.526662	-0.917722
C	2.027657	-1.137632	0.140318
C	2.800378	-2.254246	-0.606827
O	2.605678	-0.462785	0.999243
C	-3.833917	0.312541	-0.495164
H	-4.175410	-0.716083	-0.361446
H	-4.499323	1.010783	0.010427
H	-3.770009	0.538736	-1.561660
C	-0.441926	-0.325131	1.912091
H	-0.860443	-1.331075	2.018766
H	0.511387	-0.279584	2.438337
H	-1.124445	0.398310	2.361240
C	1.972056	-3.007911	-1.664201
H	1.111516	-3.526830	-1.226434
H	1.615011	-2.346677	-2.462283
H	2.598281	-3.771076	-2.137907
C	3.294729	-3.252122	0.465025
H	3.919529	-4.021441	-0.002272
H	3.883466	-2.737321	1.227964
H	2.454841	-3.753935	0.959092
C	4.014742	-1.583709	-1.287924
H	4.616704	-1.041928	-0.554759
H	4.641586	-2.344434	-1.765932
H	3.695980	-0.874992	-2.060986

N-Piv-cysteine methyl ester (4)

C	-0.156067	0.234811	0.110045
C	-1.510662	-0.400947	-0.223278
O	-1.704673	-1.160219	-1.152021
C	-0.163319	1.700495	-0.376781
S	1.300250	2.676837	0.143637
O	-2.468328	0.022794	0.618033
H	-0.001160	0.208344	1.191054
H	-0.264440	1.738299	-1.466281
H	-1.019896	2.221683	0.057909
H	2.223133	1.864409	-0.409554
N	0.908760	-0.538598	-0.499710
H	0.763811	-0.796999	-1.466350
C	1.741687	-1.332282	0.258263
C	2.698407	-2.286577	-0.495168
O	1.749775	-1.272376	1.484192
C	-3.800434	-0.481804	0.377238
H	-3.809782	-1.570772	0.458772
H	-4.422179	-0.031030	1.149437
H	-4.142381	-0.189041	-0.617998
C	4.137025	-1.912110	-0.073205
H	4.236740	-1.935955	1.014406
H	4.849681	-2.621285	-0.508638
H	4.405040	-0.907739	-0.420461
C	2.374353	-3.718976	-0.012373
H	3.077002	-4.430705	-0.459863
H	2.452982	-3.784898	1.075387
H	1.360366	-4.017182	-0.302320
C	2.580239	-2.222552	-2.029651
H	1.588175	-2.527198	-2.384398
H	2.805472	-1.223421	-2.419621
H	3.301502	-2.913827	-2.477787

(2*R*)-*N*-Boc-2-methylcysteine methyl ester (5)

C	-1.422840	0.043585	0.196696
C	-2.407879	-1.107355	-0.114730
O	-2.081992	-2.202122	-0.533121
C	-1.782390	1.222808	-0.772591
S	-1.368997	2.940088	-0.265971
O	-3.677391	-0.761371	0.142204
H	-1.332309	1.007608	-1.744842
H	-2.866017	1.256669	-0.901161
H	-0.058003	2.717106	-0.032826
N	-0.107858	-0.532628	-0.100244
H	-0.115258	-1.496837	-0.412802
C	1.106046	0.040756	0.122640
O	1.295802	1.191859	0.504627
C	-4.675990	-1.776189	-0.100650
H	-4.481356	-2.652708	0.520989
H	-5.624714	-1.313565	0.167565
H	-4.669306	-2.068407	-1.152927
O	2.079228	-0.861966	-0.152640
C	3.511807	-0.512301	-0.067038
C	3.877567	-0.147709	1.375659
H	4.962008	-0.014685	1.452720
H	3.387699	0.775866	1.686515
H	3.585442	-0.953012	2.057581
C	3.840519	0.611706	-1.055489
H	4.924263	0.768078	-1.079187
H	3.515802	0.339100	-2.065048
H	3.359775	1.547699	-0.768245
C	4.192169	-1.818391	-0.486335
H	5.279576	-1.697226	-0.461108
H	3.917318	-2.632028	0.191598
H	3.897366	-2.099789	-1.501744
C	-1.563754	0.407732	1.689391
H	-1.450973	-0.490978	2.304110
H	-0.790731	1.124715	1.965744
H	-2.540086	0.855547	1.883004

N-Boc-cysteine methyl ester (6)

C	1.515422	0.278350	-0.042464
C	2.241962	-1.051440	0.197253
O	1.955483	-1.844604	1.071217
C	2.380304	1.426508	0.523294
S	1.744643	3.102217	0.132278
O	3.266403	-1.208210	-0.658932
H	1.379457	0.422504	-1.116636
H	2.491918	1.317419	1.606787
H	3.376423	1.385628	0.075983
H	0.525036	2.920953	0.678277
N	0.201157	0.246894	0.564612
H	0.143623	-0.138222	1.499986
C	-0.924724	0.071336	-0.213184
O	-0.947252	0.179825	-1.428504
C	4.052273	-2.409842	-0.500031
H	3.421444	-3.291607	-0.630911
H	4.813928	-2.360220	-1.276913
H	4.509371	-2.434615	0.491788
O	-1.978129	-0.200872	0.588092
C	-3.338921	-0.386430	0.039012
C	-3.362767	-1.595737	-0.901376
H	-4.396315	-1.802502	-1.198875
H	-2.770188	-1.412323	-1.798581
H	-2.972526	-2.482379	-0.391126
C	-3.803677	0.900687	-0.650223
H	-4.854746	0.797084	-0.940133
H	-3.724082	1.750789	0.035298
H	-3.213966	1.109291	-1.544006
C	-4.165958	-0.659395	1.297785
H	-5.214422	-0.817899	1.027286
H	-3.801208	-1.552751	1.813514
H	-4.110047	0.186968	1.989045

(2*R*)-*N*-Fmoc-2-methylcysteine methyl ester (7)

C	3.483537	-0.153806	0.151106
C	4.342880	1.091350	-0.170858
O	3.975869	2.021844	-0.863260
C	4.220044	-1.385915	-0.477976
S	3.915756	-3.051918	0.235235
O	5.547674	1.030326	0.411485
H	4.004482	-1.398092	-1.549393
H	5.296493	-1.254895	-0.351212
H	2.570325	-3.022189	0.132752
N	2.206034	0.124666	-0.514792
H	2.168504	0.992301	-1.038732
C	1.065289	-0.603602	-0.433438
O	0.919130	-1.679505	0.136845
C	3.319003	-0.249405	1.681559
H	2.947888	0.701106	2.077643
H	2.607121	-1.037794	1.926115
H	4.274885	-0.485237	2.152375
C	6.424372	2.156139	0.183451
H	5.965336	3.072410	0.560511
H	7.335615	1.924149	0.732678
H	6.629521	2.264275	-0.883676
O	0.065937	0.037965	-1.101618
C	-1.220517	-0.618126	-1.124059
H	-1.065159	-1.697631	-1.164646
H	-1.692919	-0.274622	-2.046491
C	-2.078211	-0.247081	0.097916
C	-3.393787	-1.012285	0.103835
H	-1.493354	-0.489691	0.995476
C	-2.546945	1.201062	0.126438
C	-3.609950	-2.387707	0.103268
C	-4.482535	-0.115785	0.113027
C	-1.798172	2.375382	0.150504
C	-3.957677	1.256821	0.129571
C	-4.926541	-2.867917	0.107692
H	-2.775671	-3.084335	0.109096
C	-5.794915	-0.596358	0.119128
C	-2.465438	3.607565	0.174325
H	-0.713396	2.341909	0.146294
C	-4.621503	2.486385	0.155420
C	-6.008213	-1.978222	0.114297
H	-5.109135	-3.938540	0.109427
H	-6.639287	0.087296	0.129131
C	-3.864781	3.661532	0.176848
H	-1.891093	4.529332	0.192237
H	-5.706989	2.533863	0.160899
H	-7.022923	-2.365929	0.118705
H	-4.366390	4.624855	0.197698

***N*-Fmoc-cysteine methyl ester (8)**

C	-3.609658	-0.237215	-0.069674
C	-4.278130	1.135005	-0.199441
O	-3.982965	2.106953	0.468177
C	-4.600476	-1.236475	0.580700
S	-4.276815	-3.008696	0.193803
O	-5.246500	1.120546	-1.125537
H	-4.596773	-1.079239	1.662851
H	-5.610058	-1.054151	0.205681
H	-2.929357	-2.933919	0.219006
N	-2.394233	-0.049728	0.704885
H	-2.343993	0.790439	1.269542
C	-1.236750	-0.717403	0.448376
O	-1.126293	-1.679792	-0.301268
C	-5.973883	2.356294	-1.309760
H	-5.290814	3.152576	-1.612415
H	-6.698255	2.146949	-2.095298
H	-6.476039	2.639706	-0.382262
O	-0.215743	-0.176218	1.160781
C	1.071863	-0.822413	1.034984
H	0.915452	-1.896419	0.920588
H	1.579150	-0.617735	1.979730
C	1.882738	-0.271203	-0.149946
C	3.196689	-1.021728	-0.312606
H	1.266383	-0.383319	-1.052079
C	2.351559	1.167121	0.019857
C	3.410089	-2.380920	-0.525376
C	4.285556	-0.129925	-0.222860
C	1.602692	2.328809	0.191762
C	3.761672	1.227955	-0.018062
C	4.725077	-2.850546	-0.644849
H	2.574697	-3.071344	-0.608544
C	5.596328	-0.599885	-0.343432
C	2.269287	3.553660	0.331023
H	0.518449	2.290696	0.221842
C	4.424662	2.450556	0.119238
C	5.807229	-1.966145	-0.553090
H	4.906059	-3.908043	-0.813583
H	6.440962	0.080415	-0.278446
C	3.667956	3.612742	0.295371
H	1.695018	4.465577	0.466651
H	5.509482	2.503027	0.088439
H	6.820590	-2.345474	-0.648934
H	4.169193	4.570402	0.403400
H	-3.350470	-0.593716	-1.071798

Cartesian Coordinates for Optimized Geometries in Methanol at B3lyp/6-31+G(d,p) Level of Neutral Compounds

***(2R)*-N-Ac-2-methylcysteine methyl ester (1)**

C	-0.214884	0.017354	0.181020
C	-1.593155	-0.630943	-0.104474
O	-1.740136	-1.764215	-0.531353
C	-0.083076	1.231485	-0.797038
S	1.049459	2.605764	-0.331440
O	-2.597987	0.194711	0.181200
H	0.196342	0.849277	-1.781139
H	-1.053636	1.721663	-0.887426
H	2.120940	1.825351	-0.064747
N	0.751281	-1.049545	-0.127933
H	0.318390	-1.907414	-0.452354
C	2.095846	-1.044309	0.036539
C	2.795804	-2.353188	-0.277654
O	2.745584	-0.056334	0.416321
H	3.581657	-2.162877	-1.013620
H	3.277101	-2.717782	0.634875
H	2.126989	-3.127821	-0.658551
C	-0.164628	0.405242	1.672941
H	-0.422590	-0.458663	2.292419
H	0.839733	0.738086	1.933823
H	-0.868719	1.213495	1.878514
C	-3.941360	-0.305723	-0.037798
H	-4.115057	-1.187923	0.580474
H	-4.599251	0.509073	0.257514
H	-4.079177	-0.552667	-1.091761

***N*-Ac-cysteine methyl ester (2)**

C	-0.149542	0.223436	0.084802
C	-1.486824	-0.472094	-0.218543
O	-1.643128	-1.351096	-1.044923
C	-0.187795	1.672180	-0.444572
S	1.241157	2.699304	0.082254
O	-2.465719	0.037037	0.539266
H	-0.018490	0.237555	1.169044
H	-0.260044	1.682656	-1.535549
H	-1.066092	2.181677	-0.044033
H	2.196960	2.000282	-0.561134
N	0.957366	-0.524597	-0.470591
H	1.015278	-0.603121	-1.477230
C	1.782408	-1.306395	0.283980
C	2.831154	-2.087939	-0.479296
O	1.692787	-1.368736	1.515938
H	3.818251	-1.829186	-0.086393
H	2.671647	-3.155237	-0.300050
H	2.814288	-1.901328	-1.555347
C	-3.797177	-0.498705	0.337677
H	-3.805750	-1.568145	0.555441
H	-4.431914	0.041655	1.037321
H	-4.119083	-0.324032	-0.690526

(2*R*)-N-Piv-2-methylcysteine methyl ester (3)

C	-0.215986	0.011196	0.422841
C	-1.536282	-0.266956	-0.339158
O	-1.642828	-1.070704	-1.250794
C	0.154182	1.505749	0.139659
S	1.199863	2.392566	1.367265
O	-2.543410	0.469170	0.126827
H	0.626075	1.559744	-0.843687
H	-0.760813	2.099204	0.108705
H	2.167382	1.450076	1.429789
N	0.748156	-0.922893	-0.182717
H	0.348065	-1.485509	-0.923949
C	2.036628	-1.141275	0.168739
C	2.800128	-2.253758	-0.592678
O	2.617330	-0.492202	1.055015
C	-3.835302	0.290705	-0.507527
H	-4.169010	-0.741356	-0.388506
H	-4.503170	0.975197	0.011476
H	-3.768056	0.543503	-1.566942
C	-0.445493	-0.308504	1.914023
H	-0.848761	-1.319889	2.020381
H	0.499606	-0.247657	2.453031
H	-1.148255	0.402779	2.351604
C	1.958471	-2.994347	-1.649211
H	1.095551	-3.505642	-1.207745
H	1.607320	-2.326065	-2.443691
H	2.576415	-3.761251	-2.126757
C	3.299810	-3.268386	0.461051
H	3.905243	-4.039024	-0.027864
H	3.913122	-2.774458	1.218741
H	2.461939	-3.764536	0.963530
C	4.010135	-1.584300	-1.284055
H	4.639453	-1.066996	-0.555564
H	4.615283	-2.345622	-1.787404
H	3.685029	-0.858098	-2.037586

N-Piv-cysteine methyl ester (4)

C	-0.187165	0.187647	0.087123
C	-1.563320	-0.451470	-0.158457
O	-1.789604	-1.326562	-0.972974
C	-0.180728	1.624169	-0.476604
S	1.307513	2.599888	-0.020733
O	-2.490022	0.103916	0.632159
H	-0.019719	0.220391	1.165547
H	-0.287713	1.612908	-1.564786
H	-1.022916	2.180980	-0.061370
H	2.210371	1.845208	-0.677375
N	0.865692	-0.621569	-0.488586
H	0.877900	-0.721029	-1.493575
C	1.685047	-1.414156	0.260104
C	2.715963	-2.290475	-0.487033
O	1.619847	-1.427777	1.495652
C	-3.850621	-0.372042	0.481869
H	-3.899244	-1.439201	0.705447
H	-4.434600	0.198996	1.201075
H	-4.201589	-0.186983	-0.534952
C	4.115705	-1.906514	0.044565
H	4.166297	-2.023057	1.129941
H	4.872444	-2.553904	-0.410898
H	4.363676	-0.868530	-0.203686
C	2.409167	-3.762421	-0.126000
H	3.155248	-4.417787	-0.587785
H	2.438017	-3.912301	0.956254
H	1.421074	-4.063903	-0.491077
C	2.690961	-2.125760	-2.018498
H	1.732139	-2.430262	-2.453987
H	2.913012	-1.098404	-2.327634
H	3.458247	-2.768816	-2.460810

(2*R*)-N-Boc-2-methylcysteine methyl ester (5)

C	-1.432404	0.065328	0.181795
C	-2.402576	-1.105328	-0.121911
O	-2.053044	-2.188583	-0.559629
C	-1.828486	1.225131	-0.789812
S	-1.329168	2.941563	-0.347708
O	-3.665055	-0.787240	0.159889
H	-1.445651	0.982946	-1.783500
H	-2.916467	1.285449	-0.849180
H	-0.028060	2.671237	-0.106482
N	-0.107864	-0.485347	-0.128023
H	-0.111485	-1.441447	-0.465231
C	1.106600	0.065934	0.136250
O	1.302292	1.206567	0.556416
C	-4.666830	-1.808746	-0.075887
H	-4.456973	-2.684666	0.540218
H	-5.611443	-1.351541	0.211637
H	-4.675580	-2.085754	-1.131324
O	2.073914	-0.837475	-0.144913
C	3.517838	-0.510822	-0.055297
C	3.890845	-0.180032	1.392667
H	4.977788	-0.073386	1.468785
H	3.424447	0.749453	1.721387
H	3.581488	-0.990033	2.061075
C	3.860191	0.622390	-1.026865
H	4.946012	0.759640	-1.050625
H	3.527959	0.371223	-2.039361
H	3.398480	1.563171	-0.724014
C	4.176239	-1.819881	-0.498251
H	5.264716	-1.713282	-0.472151
H	3.892769	-2.640581	0.167633
H	3.878012	-2.078266	-1.518840
C	-1.570222	0.430241	1.673862
H	-1.434649	-0.462910	2.290848
H	-0.812167	1.164018	1.946536
H	-2.556922	0.852682	1.872351

N-Boc-cysteina methyl ester (6)

C	1.517376	0.216648	-0.053397
C	2.270701	-1.105776	0.164793
O	1.938472	-1.970054	0.954628
C	2.349623	1.382934	0.522361
S	1.677810	3.043314	0.116831
O	3.356406	-1.170400	-0.614778
H	1.394750	0.361909	-1.128827
H	2.447082	1.287206	1.607119
H	3.351554	1.365781	0.089370
H	0.505100	2.906432	0.766850
N	0.196707	0.157389	0.529508
H	0.118738	-0.100390	1.505039
C	-0.930604	0.008334	-0.235172
O	-0.952599	0.098432	-1.458722
C	4.186590	-2.351501	-0.485391
H	3.609870	-3.242366	-0.740251
H	5.002736	-2.206316	-1.190509
H	4.566446	-2.431368	0.534720
O	-1.989950	-0.221611	0.566445
C	-3.369108	-0.370683	0.037601
C	-3.445406	-1.592851	-0.881407
H	-4.489858	-1.770054	-1.157117
H	-2.865090	-1.443575	-1.792889
H	-3.074700	-2.483449	-0.363927
C	-3.802234	0.921515	-0.660387
H	-4.862139	0.848941	-0.924587
H	-3.677684	1.778419	0.009434
H	-3.228588	1.096319	-1.571735
C	-4.184625	-0.598454	1.312449
H	-5.240345	-0.727512	1.056748
H	-3.842782	-1.496548	1.835722
H	-4.094333	0.256741	1.989090

(2*R*)-*N*-Fmoc-2-methylcysteine methyl ester (7)

C	3.486495	-0.158147	0.145949
C	4.292074	1.131204	-0.158018
O	3.880014	2.047366	-0.849280
C	4.276924	-1.332840	-0.517460
S	3.973664	-3.043269	0.093475
O	5.487452	1.116330	0.428113
H	4.103263	-1.297970	-1.595167
H	5.343982	-1.188259	-0.340109
H	2.627676	-3.018626	-0.000960
N	2.192785	0.074253	-0.508867
H	2.129428	0.936600	-1.039384
C	1.066877	-0.669273	-0.410352
O	0.938096	-1.740553	0.179973
C	3.339807	-0.293157	1.674347
H	2.926908	0.628584	2.094202
H	2.669454	-1.119333	1.909970
H	4.311807	-0.487512	2.131000
C	6.337730	2.271741	0.213554
H	5.846316	3.170150	0.590319
H	7.246186	2.063355	0.774904
H	6.555435	2.380748	-0.850206
O	0.055878	-0.059403	-1.088549
C	-1.231186	-0.715933	-1.085829
H	-1.079431	-1.796305	-1.093826
H	-1.704531	-0.403726	-2.018526
C	-2.086281	-0.302244	0.124736
C	-3.424800	-1.027929	0.125335
H	-1.517859	-0.546667	1.032083
C	-2.511722	1.159639	0.131303
C	-3.684061	-2.396703	0.136983
C	-4.486533	-0.098581	0.108463
C	-1.728313	2.312094	0.159203
C	-3.920605	1.258082	0.114426
C	-5.015979	-2.835682	0.130357
H	-2.873667	-3.120528	0.157445
C	-5.814481	-0.536972	0.103457
C	-2.359532	3.564555	0.161564
H	-0.645081	2.248003	0.178193
C	-4.549339	2.507254	0.118485
C	-6.070490	-1.912556	0.112848
H	-5.231623	-3.900046	0.141166
H	-6.636901	0.172812	0.093586
C	-3.757559	3.660344	0.140289
H	-1.758225	4.468858	0.182582
H	-5.632802	2.586678	0.107932
H	-7.096621	-2.268721	0.108735
H	-4.230435	4.638230	0.144395

***N*-Fmoc-cysteine methyl ester (8)**

C	-3.649785	-0.351782	0.161214
C	-3.977204	0.990970	-0.511339
O	-3.445656	2.050163	-0.235058
C	-4.815499	-0.756810	1.089163
S	-4.660927	-2.449661	1.783565
O	-4.944848	0.842935	-1.422547
H	-4.923553	-0.038503	1.906020
H	-5.746986	-0.764808	0.519959
H	-3.543791	-2.230120	2.504723
N	-2.393579	-0.269058	0.873237
H	-2.276624	0.468848	1.556326
C	-1.261343	-0.879376	0.424769
O	-1.203217	-1.675204	-0.506006
C	-5.387391	2.040381	-2.109717
H	-4.555098	2.483295	-2.659411
H	-6.166072	1.706613	-2.792737
H	-5.785361	2.758530	-1.390639
O	-0.199149	-0.500904	1.178845
C	1.083856	-1.083171	0.850340
H	0.931584	-2.113616	0.526005
H	1.641016	-1.071139	1.788703
C	1.824139	-0.281741	-0.234211
C	3.156478	-0.933472	-0.578633
H	1.175937	-0.241527	-1.119694
C	2.249336	1.117496	0.189256
C	3.411316	-2.220154	-1.047806
C	4.216994	-0.030063	-0.353960
C	1.467044	2.198131	0.592405
C	3.654465	1.242904	0.119835
C	4.738005	-2.603552	-1.291928
H	2.601261	-2.920765	-1.231732
C	5.539636	-0.412627	-0.599212
C	2.096496	3.403405	0.935917
H	0.386108	2.114370	0.641404
C	4.281261	2.445534	0.461284
C	5.791494	-1.706718	-1.068022
H	4.950039	-3.603161	-1.659766
H	6.361211	0.278140	-0.431819
C	3.491281	3.524549	0.872052
H	1.496343	4.251836	1.251722
H	5.361566	2.547019	0.407427
H	6.813525	-2.018820	-1.262602
H	3.962872	4.465689	1.139908
H	-3.535553	-1.106280	-0.619816

Cartesian Coordinates for Optimized Geometries in Water at B3lyp/6-31+G(d,p) Level of Neutral Compounds

(2*R*)-*N*-Ac-2-methylcysteine methyl ester (1)

C	-0.215245	0.017987	0.181203
C	-1.593603	-0.630245	-0.104696
O	-1.740278	-1.762845	-0.533587
C	-0.084178	1.232304	-0.796508
S	1.052038	2.604391	-0.332798
O	-2.598240	0.194699	0.182750
H	0.192434	0.850354	-1.781466
H	-1.054171	1.724033	-0.884321
H	2.121678	1.821596	-0.065439
N	0.751085	-1.048611	-0.128510
H	0.318209	-1.905617	-0.455326
C	2.095221	-1.044807	0.037341
C	2.794714	-2.353354	-0.278726
O	2.745580	-0.057842	0.419761
H	3.579455	-2.162576	-1.015794
H	3.277229	-2.718634	0.632879
H	2.125393	-3.127672	-0.659242
C	-0.164907	0.405141	1.673284
H	-0.422375	-0.459185	2.292330
H	0.839299	0.738309	1.934344
H	-0.869543	1.212793	1.879396
C	-3.941887	-0.304909	-0.037213
H	-4.115703	-1.188333	0.579244
H	-4.599489	0.509407	0.259987
H	-4.079799	-0.549252	-1.091753

***N*-Ac-cysteine methyl ester (2)**

C	-0.151931	0.220368	0.085205
C	-1.489355	-0.476212	-0.215667
O	-1.644143	-1.364566	-1.032369
C	-0.190428	1.669438	-0.443313
S	1.241103	2.694666	0.080483
O	-2.469764	0.042255	0.533497
H	-0.020191	0.234454	1.169437
H	-0.265017	1.681057	-1.534046
H	-1.067294	2.179293	-0.040261
H	2.193266	2.003138	-0.576210
N	0.954730	-0.527524	-0.470614
H	1.015723	-0.602231	-1.477354
C	1.786487	-1.301619	0.283405
C	2.839223	-2.077213	-0.480244
O	1.699630	-1.362619	1.516094
H	3.825439	-1.807739	-0.092280
H	2.690046	-3.145112	-0.295827
H	2.816721	-1.895232	-1.556936
C	-3.801564	-0.493867	0.333946
H	-3.812399	-1.560630	0.564313
H	-4.437612	0.055641	1.025183
H	-4.119814	-0.330550	-0.697213

(2*R*)-*N*-Piv-2-methylcysteine methyl ester (3)

C	-0.215911	0.011439	0.423304
C	-1.535964	-0.267066	-0.339263
O	-1.641591	-1.070476	-1.251368
C	0.153516	1.505977	0.139840
S	1.201717	2.392214	1.365929
O	-2.543363	0.468285	0.126756
H	0.623733	1.560406	-0.844250
H	-0.761529	2.099405	0.110772
H	2.167970	1.448325	1.428124
N	0.748742	-0.922433	-0.181866
H	0.348978	-1.484625	-0.923626
C	2.036858	-1.141336	0.169554
C	2.800117	-2.253646	-0.592284
O	2.617884	-0.492628	1.056288
C	-3.835072	0.290383	-0.508412
H	-4.168743	-0.741787	-0.390429
H	-4.503182	0.974318	0.010968
H	-3.767218	0.544449	-1.567467
C	-0.445950	-0.308224	1.914400
H	-0.848930	-1.319705	2.020682
H	0.498805	-0.247052	2.453992
H	-1.149285	0.402802	2.351499
C	1.957930	-2.994125	-1.648493
H	1.095217	-3.505330	-1.206551
H	1.606577	-2.325761	-2.442808
H	2.575685	-3.761024	-2.126254
C	3.300349	-3.268647	0.460858
H	3.904762	-4.039514	-0.028915
H	3.914999	-2.775419	1.217959
H	2.462705	-3.764375	0.964109
C	4.009717	-1.584104	-1.284327
H	4.639852	-1.067257	-0.556185
H	4.614306	-2.345403	-1.788346
H	3.684140	-0.857605	-2.037348

***N*-Piv-cysteine methyl ester (4)**

C	-0.188452	0.184470	0.086161
C	-1.565522	-0.456973	-0.150120
O	-1.792070	-1.349161	-0.945789
C	-0.182523	1.618552	-0.483385
S	1.306991	2.595246	-0.033268
O	-2.492269	0.115713	0.627928
H	-0.018766	0.221953	1.164191
H	-0.290838	1.603309	-1.571346
H	-1.023862	2.177195	-0.069165
H	2.208103	1.843662	-0.695772
N	0.863556	-0.626440	-0.488225
H	0.887853	-0.712778	-1.494202
C	1.679585	-1.422021	0.259675
C	2.716687	-2.291384	-0.486908
O	1.606354	-1.444299	1.495125
C	-3.853464	-0.361543	0.486647
H	-3.903574	-1.423843	0.731954
H	-4.437080	0.224766	1.193729
H	-4.203602	-0.196541	-0.533869
C	4.112808	-1.905690	0.053014
H	4.159577	-2.028914	1.137868
H	4.873647	-2.547642	-0.403269
H	4.358003	-0.865365	-0.188028
C	2.413090	-3.766269	-0.135436
H	3.162982	-4.416555	-0.598176
H	2.438370	-3.922606	0.946028
H	1.427406	-4.068724	-0.506189
C	2.698139	-2.118361	-2.017562
H	1.742023	-2.422989	-2.458808
H	2.918744	-1.088726	-2.319995
H	3.469181	-2.756863	-2.459896

(2*R*)-*N*-Boc-2-methylcysteine methyl ester (5)

C	-1.432747	0.066249	0.181506
C	-2.402252	-1.105098	-0.122294
O	-2.051823	-2.187740	-0.561072
C	-1.830265	1.225593	-0.789829
S	-1.328173	2.941869	-0.349801
O	-3.664532	-0.788253	0.160531
H	-1.449954	0.982725	-1.784293
H	-2.918316	1.286775	-0.846676
H	-0.027113	2.670349	-0.109690
N	-0.107851	-0.483367	-0.128911
H	-0.111389	-1.439012	-0.467432
C	1.106628	0.066911	0.137016
O	1.302630	1.207062	0.558750
C	-4.666139	-1.810058	-0.075534
H	-4.455513	-2.686283	0.539843
H	-5.610721	-1.353462	0.212959
H	-4.675422	-2.085926	-1.131242
O	2.073661	-0.836604	-0.144398
C	3.518008	-0.510868	-0.054909
C	3.891507	-0.180672	1.393030
H	4.978553	-0.075084	1.468908
H	3.426116	0.749235	1.721973
H	3.581504	-0.990462	2.061385
C	3.860758	0.622256	-1.026379
H	4.946613	0.759089	-1.050045
H	3.528466	0.371305	-2.038900
H	3.399441	1.563227	-0.723471
C	4.175455	-1.820274	-0.498208
H	5.263981	-1.714300	-0.472343
H	3.891741	-2.640871	0.167708
H	3.876897	-2.078295	-1.518795
C	-1.570500	0.430744	1.673657
H	-1.434229	-0.462389	2.290468
H	-0.812940	1.164989	1.946455
H	-2.557539	0.852295	1.872377

***N*-Boc-cysteine methyl ester (6)**

C	1.516924	0.210381	-0.056232
C	2.273254	-1.110713	0.161192
O	1.935510	-1.982474	0.940452
C	2.345965	1.379678	0.517904
S	1.668522	3.037538	0.111043
O	3.367173	-1.165577	-0.607327
H	1.393953	0.354301	-1.131888
H	2.444260	1.285845	1.602688
H	3.347646	1.365070	0.084425
H	0.500585	2.901929	0.769803
N	0.196413	0.148261	0.526166
H	0.117791	-0.100289	1.503980
C	-0.931426	0.000824	-0.237168
O	-0.954059	0.089571	-1.461128
C	4.200120	-2.345014	-0.479028
H	3.629788	-3.235377	-0.749562
H	5.024239	-2.190146	-1.172675
H	4.567810	-2.433153	0.544811
O	-1.990617	-0.226903	0.565078
C	-3.371472	-0.369514	0.038188
C	-3.454763	-1.590331	-0.881963
H	-4.500579	-1.762781	-1.155480
H	-2.875875	-1.442592	-1.794604
H	-3.086745	-2.483067	-0.366248
C	-3.799942	0.925410	-0.657483
H	-4.860438	0.857540	-0.920401
H	-3.670923	1.780893	0.013288
H	-3.226821	1.098973	-1.569409
C	-4.185864	-0.595141	1.314098
H	-5.242537	-0.718900	1.059820
H	-3.847462	-1.495582	1.835585
H	-4.090511	0.258748	1.991685

(2R)-N-Fmoc-2-methylcysteine methyl ester (7)

C	3.486220	-0.158091	0.145847
C	4.289745	1.132665	-0.158197
O	3.876308	2.047630	-0.850365
C	4.278942	-1.331062	-0.517548
S	3.975181	-3.042651	0.090221
O	5.484582	1.120100	0.428554
H	4.107549	-1.295030	-1.595548
H	5.345499	-1.186035	-0.337655
H	2.629318	-3.018520	-0.006041
N	2.192208	0.071959	-0.509281
H	2.127853	0.934043	-1.040116
C	1.066766	-0.671873	-0.409652
O	0.938414	-1.742554	0.182123
C	3.339756	-0.293363	1.674217
H	2.925070	0.627529	2.094088
H	2.671020	-1.120817	1.909928
H	4.312217	-0.485681	2.130765
C	6.333674	2.276466	0.213632
H	5.840869	3.174498	0.589421
H	7.241945	2.069645	0.775813
H	6.552090	2.384605	-0.850056
O	0.055459	-0.063586	-1.088778
C	-1.231624	-0.720014	-1.084713
H	-1.080124	-1.800428	-1.091721
H	-1.705296	-0.408836	-2.017582
C	-2.086323	-0.304888	0.125693
C	-3.425836	-1.028783	0.125900
H	-1.518400	-0.549748	1.033223
C	-2.509797	1.157564	0.131898
C	-3.687019	-2.397224	0.137647
C	-4.486330	-0.097987	0.108124
C	-1.724819	2.308980	0.160523
C	-3.918563	1.257929	0.114092
C	-5.019575	-2.834366	0.130368
H	-2.877705	-3.122239	0.158520
C	-5.814925	-0.534510	0.102435
C	-2.354393	3.562318	0.162366
H	-0.641693	2.243457	0.180707
C	-4.545672	2.507962	0.117619
C	-6.072834	-1.909776	0.112028
H	-5.236693	-3.898427	0.141226
H	-6.636343	0.176411	0.091840
C	-3.752313	3.660007	0.139936
H	-1.751887	4.465805	0.183983
H	-5.629014	2.588853	0.106324
H	-7.099450	-2.264522	0.107373
H	-4.223862	4.638529	0.143651

N-Fmoc-cysteine methyl ester (8)

C	-3.649160	-0.346689	0.161758
C	-3.978538	0.994486	-0.513247
O	-3.439807	2.052951	-0.248162
C	-4.812020	-0.751135	1.093555
S	-4.653572	-2.442773	1.790244
O	-4.955839	0.845653	-1.413812
H	-4.918444	-0.031937	1.909759
H	-5.745004	-0.760884	0.526958
H	-3.539961	-2.218967	2.515473
N	-2.390967	-0.263096	0.869763
H	-2.273815	0.470009	1.557899
C	-1.260628	-0.876434	0.422040
O	-1.204153	-1.671950	-0.509470
C	-5.401248	2.041266	-2.102496
H	-4.573369	2.477760	-2.663857
H	-6.188792	1.707034	-2.775017
H	-5.788450	2.764662	-1.382845
O	-0.197671	-0.501582	1.176769
C	1.084417	-1.085406	0.847702
H	0.930918	-2.115574	0.523046
H	1.641675	-1.074614	1.786015
C	1.825670	-0.284386	-0.236467
C	3.158154	-0.936398	-0.579901
H	1.178156	-0.244059	-1.122451
C	2.250771	1.114994	0.186673
C	3.413262	-2.223451	-1.047992
C	4.218614	-0.032826	-0.355403
C	1.468353	2.195843	0.589126
C	3.655932	1.240417	0.117522
C	4.740101	-2.606993	-1.291273
H	2.603415	-2.924392	-1.231540
C	5.541414	-0.415488	-0.599840
C	2.097724	3.401337	0.932160
H	0.387420	2.112039	0.638125
C	4.282676	2.443278	0.458409
C	5.793500	-1.709932	-1.067647
H	4.952319	-3.606908	-1.658160
H	6.362900	0.275386	-0.432511
C	3.492551	3.522514	0.868443
H	1.497511	4.249876	1.247551
H	5.362980	2.544780	0.404730
H	6.815619	-2.022153	-1.261541
H	3.964065	4.463794	1.135915
H	-3.537058	-1.102274	-0.618575

Cartesian Coordinates for Optimized Geometries in Gas-phase at B3lyp/6-31+G(d,p) Level of Radical Cations

(2R)-N-Ac-2-methylcysteine methyl ester radical cation (1)

C	0.300702	-0.049630	0.276137
C	1.704694	0.519721	-0.076989
O	1.883509	1.696124	-0.315524
C	0.028076	-1.264982	-0.645985
S	-1.535359	-2.131891	-0.205782
O	2.636490	-0.420987	-0.042294
H	-0.014242	-0.965754	-1.694435
H	0.829276	-1.994500	-0.514379
H	-2.154418	-2.042650	-1.401299
N	-0.616343	1.065450	0.003829
H	-0.136153	1.952232	-0.147665
C	-1.947908	1.038916	-0.037335
C	-2.695291	2.334816	-0.220868
O	-2.633102	-0.019986	0.070351
H	-3.333367	2.259732	-1.105172
H	-3.345429	2.488405	0.645291
H	-2.020140	3.187023	-0.322443
C	0.283859	-0.422977	1.776043
H	0.591933	0.435549	2.378063
H	-0.721403	-0.710992	2.094392
H	0.972610	-1.248328	1.971100
C	4.012446	0.006270	-0.288940
H	4.306823	0.735525	0.466564
H	4.604699	-0.902579	-0.212020
H	4.085324	0.444426	-1.284931

N-Ac-cysteine methyl ester radical cation (2)

C	0.308308	0.055323	-0.283520
C	1.730653	-0.490721	-0.024121
O	1.926545	-1.632930	0.332365
C	0.053045	1.336980	0.538031
S	-1.485519	2.172825	-0.027388
O	2.646763	0.434070	-0.261997
H	0.246578	0.301169	-1.352050
H	-0.014118	1.123872	1.606196
H	0.865967	2.043405	0.357548
H	-2.206598	2.078961	1.109701
N	-0.605463	-1.036409	0.020494
H	-0.140353	-1.903483	0.287425
C	-1.933490	-1.006113	-0.106643
C	-2.718917	-2.273629	0.101385
O	-2.568164	0.047163	-0.400796
H	-3.451570	-2.117396	0.897497
H	-3.269909	-2.496273	-0.817020
H	-2.074270	-3.119018	0.350675
C	4.044564	0.033468	-0.105309
H	4.268062	-0.777995	-0.798688
H	4.618232	0.925800	-0.344305
H	4.218392	-0.287647	0.922256

(2*R*)-*N*-Piv-2-methylcysteine methyl ester radical cation (3)

C	-1.053301	0.198478	0.289354
C	-2.108915	-0.886958	-0.064245
O	-1.805132	-2.042192	-0.279484
C	-1.262147	1.398580	-0.669903
S	-0.182568	2.826723	-0.244712
O	-3.338909	-0.392761	-0.060108
H	-1.079940	1.111878	-1.706799
H	-2.289904	1.752554	-0.572809
H	0.481178	2.926672	-1.414398
N	0.236403	-0.469531	0.070591
H	0.151017	-1.474768	-0.070663
C	1.451560	0.075087	0.073830
C	2.701706	-0.821401	-0.065101
O	1.645333	1.321542	0.182435
C	-4.426367	-1.334763	-0.312419
H	-4.425481	-2.105922	0.458803
H	-5.332121	-0.734368	-0.268031
H	-4.297981	-1.786497	-1.296729
C	-1.227804	0.588583	1.774955
H	-1.187719	-0.305032	2.402897
H	-0.428311	1.260511	2.096984
H	-2.192214	1.077961	1.929832
C	2.339712	-2.316824	-0.125129
H	1.828598	-2.662581	0.779941
H	1.735407	-2.571553	-1.003207
H	3.265948	-2.892876	-0.204289
C	3.601356	-0.545046	1.163936
H	4.511331	-1.145762	1.079354
H	3.886936	0.507606	1.220634
H	3.102456	-0.822358	2.098378
C	3.428596	-0.398323	-1.364138
H	3.716118	0.655117	-1.334418
H	4.336972	-0.997513	-1.474152
H	2.807268	-0.571107	-2.249645

***N*-Piv-cysteine methyl ester radical cation (4)**

C	-0.402949	-0.257634	0.379458
C	-1.678510	-0.379394	-0.482515
O	-1.711787	-1.039858	-1.499011
C	-0.023263	1.225428	0.584047
S	1.281017	1.395012	1.869491
O	-2.680843	0.303557	0.049415
H	-0.627782	-0.700666	1.358662
H	0.314284	1.685883	-0.346058
H	-0.893360	1.765950	0.961980
H	2.284124	1.850579	1.090742
N	0.617806	-1.048532	-0.291309
H	0.296577	-1.513564	-1.138449
C	1.850394	-1.278301	0.163536
C	2.785693	-2.255824	-0.575544
O	2.295307	-0.704108	1.199104
C	-3.965304	0.235955	-0.644433
H	-4.308036	-0.798983	-0.672935
H	-4.634617	0.856373	-0.053080
H	-3.854277	0.625072	-1.657182
C	3.964627	-1.421856	-1.134016
H	4.504327	-0.909720	-0.333875
H	4.664028	-2.092606	-1.641424
H	3.625607	-0.680430	-1.865799
C	3.302229	-3.278242	0.465288
H	3.995572	-3.965101	-0.027950
H	3.829922	-2.783446	1.283524
H	2.484139	-3.871412	0.886386
C	2.063985	-2.989691	-1.720730
H	1.213830	-3.583103	-1.367465
H	1.729698	-2.312683	-2.515179
H	2.768642	-3.687475	-2.181765

(2*R*)-*N*-Boc-2-methylcysteine methyl ester radical cation (5)

C	-1.428062	-0.058227	0.300367
C	-2.457410	-1.140466	-0.132158
O	-2.125023	-2.226971	-0.555096
C	-1.760785	1.235844	-0.499304
S	-0.648666	2.637753	-0.086231
O	-3.704438	-0.721000	0.045301
H	-1.712732	1.056673	-1.574431
H	-2.766110	1.568325	-0.232930
H	0.015969	2.718217	-1.257818
N	-0.134215	-0.611792	-0.087567
H	-0.152834	-1.576818	-0.414316
C	1.067258	-0.034991	0.097352
O	1.207955	1.181086	0.426480
C	-4.765386	-1.671889	-0.273203
H	-4.661116	-2.557381	0.354924
H	-5.690386	-1.142310	-0.056649
H	-4.704910	-1.949342	-1.326314
O	2.074841	-0.849068	-0.101440
C	3.544965	-0.449814	-0.049482
C	3.869621	0.024194	1.364211
H	4.948355	0.191361	1.439641
H	3.364106	0.961301	1.607008
H	3.596411	-0.735741	2.101948
C	3.809055	0.603647	-1.121801
H	4.886796	0.783803	-1.177326
H	3.479686	0.252901	-2.104504
H	3.322794	1.553161	-0.889591
C	4.228249	-1.775069	-0.375946
H	5.312303	-1.632206	-0.363591
H	3.973966	-2.539498	0.362898
H	3.939730	-2.133435	-1.367702
C	-1.535240	0.154092	1.826764
H	-1.397330	-0.799206	2.343403
H	-0.764532	0.843066	2.180744
H	-2.518343	0.551454	2.088701

***N*-Boc-cysteine methyl ester radical cation (6)**

C	1.477019	-0.379027	-0.338461
C	2.493372	-1.269730	0.406899
O	2.193131	-1.926579	1.379392
C	1.989365	1.083297	-0.379490
S	0.892382	2.155951	-1.386236
O	3.687809	-1.206618	-0.167252
H	1.403962	-0.747034	-1.369778
H	2.078274	1.503805	0.623948
H	2.961978	1.107269	-0.875747
H	0.242462	2.782767	-0.382645
N	0.208205	-0.529714	0.340479
H	0.199336	-1.148346	1.149443
C	-0.966081	-0.126470	-0.185499
O	-1.015928	0.658252	-1.179638
C	4.740266	-2.033416	0.417387
H	4.451249	-3.083491	0.359786
H	5.621218	-1.834050	-0.188375
H	4.899238	-1.742979	1.456599
O	-2.017644	-0.613048	0.419334
C	-3.463052	-0.249412	0.084501
C	-3.751691	-0.692957	-1.346339
H	-4.816902	-0.548208	-1.550473
H	-3.184627	-0.111056	-2.076221
H	-3.526983	-1.755291	-1.477622
C	-3.656756	1.246940	0.311963
H	-4.720156	1.481939	0.206516
H	-3.352978	1.531535	1.323909
H	-3.108585	1.845145	-0.418595
C	-4.228551	-1.084241	1.106993
H	-5.301047	-0.917809	0.973431
H	-4.027127	-2.150238	0.973205
H	-3.961239	-0.799782	2.128199

(2*R*)-*N*-Fmoc-2-methylcysteine methyl ester radical cation (7)

C	3.505711	-0.157870	0.182486
C	4.413246	1.047872	-0.185557
O	4.042764	1.984665	-0.866746
C	4.194334	-1.437325	-0.394765
S	3.747661	-3.063577	0.329253
O	5.627433	0.933086	0.348125
H	4.021357	-1.472292	-1.474310
H	5.269989	-1.368324	-0.225123
H	2.406767	-2.918708	0.218561
N	2.240173	0.150512	-0.498223
H	2.252165	1.008784	-1.042813
C	1.074052	-0.519269	-0.406225
O	0.863676	-1.581479	0.172473
C	3.339539	-0.189810	1.715642
H	3.007788	0.787991	2.077152
H	2.599717	-0.939284	1.999715
H	4.289230	-0.437861	2.193149
C	6.556062	2.019776	0.090342
H	6.157337	2.951308	0.495459
H	7.474020	1.733664	0.599844
H	6.718673	2.122430	-0.983810
O	0.090794	0.160644	-1.078610
C	-1.179512	-0.501570	-1.168672
H	-1.022367	-1.578341	-1.252691
H	-1.637453	-0.120900	-2.083879
C	-2.063461	-0.196385	0.060853
C	-3.350048	-1.000234	0.066053
H	-1.469644	-0.435791	0.952882
C	-2.585332	1.228047	0.121513
C	-3.530138	-2.372348	0.045941
C	-4.483159	-0.126919	0.108379
C	-1.892587	2.426241	0.150127
C	-4.018139	1.229735	0.142603
C	-4.842253	-2.877909	0.062552
H	-2.685236	-3.053700	0.028184
C	-5.799292	-0.645744	0.125277
C	-2.625052	3.625891	0.199227
H	-0.808841	2.448725	0.128853
C	-4.745343	2.442433	0.195709
C	-5.965743	-2.019748	0.100174
H	-4.998588	-3.952242	0.049840
H	-6.658310	0.016353	0.159000
C	-4.039268	3.632215	0.222972
H	-2.093227	4.572277	0.220694
H	-5.830296	2.440236	0.214679
H	-6.962183	-2.448648	0.112867
H	-4.566821	4.579336	0.263679

***N*-Fmoc-cysteine methyl ester radical cation (8)**

C	-3.604517	-0.197661	-0.173598
C	-4.369184	1.138002	-0.170938
O	-4.047099	2.092238	0.508989
C	-4.517208	-1.333865	0.351666
S	-4.065472	-3.021721	-0.222346
O	-5.412326	1.098981	-0.997291
H	-4.525949	-1.313207	1.445694
H	-5.538248	-1.187194	-0.005613
H	-2.723606	-2.851133	-0.171006
N	-2.410870	0.013310	0.633623
H	-2.416021	0.844558	1.216763
C	-1.235495	-0.619028	0.421247
O	-1.054407	-1.581200	-0.317706
C	-6.224657	2.300688	-1.078665
H	-5.617500	3.134254	-1.435581
H	-7.013617	2.060685	-1.788510
H	-6.638111	2.536656	-0.096720
O	-0.240720	-0.045077	1.161778
C	1.032348	-0.710461	1.120696
H	0.874601	-1.789030	1.065701
H	1.519267	-0.454107	2.063603
C	1.876010	-0.242878	-0.085232
C	3.164817	-1.030493	-0.229519
H	1.257254	-0.372208	-0.982973
C	2.391056	1.181351	0.021270
C	3.349551	-2.392295	-0.392334
C	4.293377	-0.151004	-0.190316
C	1.693633	2.368755	0.161466
C	3.822999	1.195404	-0.038513
C	4.662502	-2.882312	-0.510697
H	2.507799	-3.076137	-0.439826
C	5.610391	-0.654307	-0.310167
C	2.420379	3.570227	0.243239
H	0.610754	2.381544	0.213090
C	4.544241	2.410373	0.041465
C	5.781777	-2.018801	-0.467748
H	4.822673	-3.948138	-0.641647
H	6.465948	0.012490	-0.281618
C	3.833528	3.589150	0.182595
H	1.884823	4.508162	0.354516
H	5.628237	2.418092	-0.007077
H	6.778761	-2.435792	-0.563420
H	4.356416	4.537541	0.246953
H	-3.316512	-0.416636	-1.207866

Cartesian Coordinates for Optimized Geometries in Methanol at B3lyp/6-31+G(d,p) Level of Radical Cations

(2*R*)-*N*-Ac-2-methylcysteine methyl ester radical cation (1)

C	0.300209	-0.036105	0.262936
C	1.702282	0.523628	-0.094399
O	1.889191	1.679040	-0.427382
C	0.056879	-1.281704	-0.633179
S	-1.531645	-2.121823	-0.269411
O	2.640282	-0.401852	0.038559
H	0.075078	-1.019655	-1.690665
H	0.833677	-2.019670	-0.428763
H	-2.147759	-1.894313	-1.446844
N	-0.626674	1.055487	-0.049268
H	-0.172024	1.929959	-0.302589
C	-1.956938	1.021310	0.002598
C	-2.720523	2.294252	-0.247969
O	-2.616124	-0.030560	0.251801
H	-3.362768	2.154096	-1.121269
H	-3.361178	2.493729	0.614899
H	-2.056349	3.144290	-0.411044
C	0.269918	-0.373491	1.770315
H	0.550257	0.506828	2.353230
H	-0.733221	-0.678161	2.075356
H	0.970748	-1.181079	1.989834
C	4.012148	0.002720	-0.229515
H	4.304199	0.789670	0.466890
H	4.605119	-0.895447	-0.073592
H	4.096615	0.353817	-1.258544

***N*-Ac-methyl ester radical cation (2)**

C	0.305716	0.040771	-0.260557
C	1.725557	-0.492018	-0.002900
O	1.945772	-1.597782	0.452583
C	0.077484	1.351850	0.530197
S	-1.502458	2.146913	0.055816
O	2.638081	0.403517	-0.349963
H	0.223503	0.258508	-1.331630
H	0.082410	1.179459	1.606590
H	0.857471	2.066484	0.264177
H	-2.214006	1.872287	1.167832
N	-0.618309	-1.024308	0.085273
H	-0.197708	-1.854890	0.494570
C	-1.928023	-0.997175	-0.162095
C	-2.751797	-2.221991	0.122736
O	-2.498950	0.031056	-0.629110
H	-3.437705	-2.001673	0.945527
H	-3.349568	-2.455876	-0.761429
H	-2.131353	-3.081246	0.381309
C	4.033009	0.030369	-0.168770
H	4.259920	-0.844753	-0.778823
H	4.600736	0.895834	-0.502315
H	4.222898	-0.179752	0.884470

(2*R*)-*N*-Piv-2-methylcysteine methyl ester radical cation (3)

C	-0.285204	-0.106840	0.470243
C	-1.580998	-0.262530	-0.367008
O	-1.693294	-1.070317	-1.270437
C	0.142912	1.384337	0.381489
S	1.629260	1.758846	1.386877
O	-2.527693	0.566348	0.046583
H	0.336653	1.679573	-0.649636
H	-0.654987	2.004373	0.792407
H	2.486736	2.027204	0.381812
N	0.683031	-1.000079	-0.174138
H	0.288245	-1.565809	-0.921160
C	1.965940	-1.156861	0.143851
C	2.809424	-2.234538	-0.565870
O	2.540534	-0.446899	1.020177
C	-3.812379	0.494519	-0.632873
H	-4.236859	-0.502437	-0.508511
H	-4.430229	1.244975	-0.145300
H	-3.681187	0.723209	-1.691162
C	-0.573233	-0.556198	1.920330
H	-0.976240	-1.571580	1.920972
H	0.343776	-0.553676	2.512552
H	-1.299660	0.113474	2.384431
C	1.980096	-3.084119	-1.545472
H	1.164057	-3.617165	-1.046329
H	1.574391	-2.490802	-2.372175
H	2.635324	-3.839886	-1.987953
C	3.412689	-3.143537	0.531102
H	4.048468	-3.897305	0.057320
H	4.021151	-2.568167	1.232755
H	2.629450	-3.663363	1.092377
C	3.939151	-1.503448	-1.329446
H	4.558636	-0.913675	-0.649530
H	4.574877	-2.246575	-1.820105
H	3.534982	-0.840591	-2.101331

***N*-Piv-cysteine methyl ester radical cation (4)**

C	-0.406129	-0.259324	0.349156
C	-1.678191	-0.349888	-0.510815
O	-1.720301	-0.944652	-1.570794
C	-0.011295	1.221348	0.565898
S	1.317139	1.370165	1.818690
O	-2.687678	0.285154	0.066196
H	-0.635419	-0.706723	1.323111
H	0.312893	1.694412	-0.361345
H	-0.866002	1.759801	0.977988
H	2.335249	1.717026	1.004970
N	0.613044	-1.050660	-0.316951
H	0.344716	-1.429834	-1.220524
C	1.804042	-1.344044	0.203799
C	2.771455	-2.273068	-0.550055
O	2.176071	-0.854466	1.309340
C	-3.965465	0.264621	-0.630024
H	-4.308489	-0.765463	-0.734140
H	-4.639267	0.837432	0.002794
H	-3.857507	0.731102	-1.609872
C	3.894819	-1.374661	-1.125635
H	4.410201	-0.828601	-0.331203
H	4.625598	-2.008046	-1.637811
H	3.501429	-0.654356	-1.850016
C	3.366625	-3.271112	0.468539
H	4.090946	-3.910502	-0.044313
H	3.878384	-2.751579	1.281711
H	2.590140	-3.911715	0.898437
C	2.074875	-3.043326	-1.686536
H	1.241283	-3.651416	-1.320351
H	1.716440	-2.384461	-2.484867
H	2.801473	-3.721985	-2.142463

(2*R*)-*N*-Boc-methycysteine methyl ester radical cation (5)

C	-1.421696	-0.071571	0.307731
C	-2.456366	-1.144766	-0.122752
O	-2.141619	-2.233189	-0.565564
C	-1.733386	1.208911	-0.528672
S	-0.606374	2.605745	-0.167439
O	-3.697889	-0.722452	0.070823
H	-1.688265	0.999662	-1.597210
H	-2.730075	1.568498	-0.267365
H	0.092886	2.604453	-1.321201
N	-0.126386	-0.642303	-0.042760
H	-0.141918	-1.586873	-0.418562
C	1.068148	-0.061233	0.157233
O	1.202795	1.138060	0.523944
C	-4.769396	-1.645551	-0.269874
H	-4.678547	-2.550427	0.332175
H	-5.686575	-1.110838	-0.034072
H	-4.720668	-1.888796	-1.332019
O	2.082720	-0.876457	-0.064776
C	3.528040	-0.447788	-0.040363
C	3.890558	0.006857	1.372484
H	4.969376	0.183954	1.419140
H	3.377944	0.931769	1.643095
H	3.641140	-0.768907	2.102395
C	3.754222	0.630385	-1.098993
H	4.826945	0.835411	-1.166296
H	3.412539	0.286836	-2.079946
H	3.243997	1.561141	-0.845631
C	4.241774	-1.747807	-0.407207
H	5.321268	-1.574518	-0.419392
H	4.024611	-2.530467	0.325120
H	3.935037	-2.095228	-1.397808
C	-1.552720	0.171769	1.827220
H	-1.425499	-0.771594	2.363813
H	-0.785433	0.866858	2.173693
H	-2.536647	0.582110	2.061377

***N*-Boc-cysteine methyl ester radical cation (6)**

C	1.472278	-0.407476	-0.337570
C	2.505359	-1.282110	0.391423
O	2.239182	-1.947328	1.373421
C	1.938809	1.075143	-0.305744
S	0.841377	2.155455	-1.288707
O	3.691674	-1.203427	-0.196244
H	1.433802	-0.734499	-1.382548
H	1.987095	1.457179	0.714199
H	2.918477	1.148107	-0.781000
H	0.129895	2.700738	-0.280266
N	0.193812	-0.626104	0.297918
H	0.182995	-1.170569	1.155361
C	-0.968610	-0.212998	-0.238222
O	-1.006713	0.535935	-1.252000
C	4.769865	-1.983779	0.391074
H	4.516602	-3.044063	0.354495
H	5.640111	-1.769899	-0.225042
H	4.933190	-1.667391	1.422043
O	-2.031298	-0.673244	0.390797
C	-3.444003	-0.249106	0.071322
C	-3.790316	-0.704844	-1.345027
H	-4.852214	-0.513646	-1.527540
H	-3.209938	-0.164852	-2.095581
H	-3.612982	-1.778379	-1.458416
C	-3.574629	1.259786	0.270599
H	-4.628654	1.535961	0.170192
H	-3.242948	1.547310	1.272796
H	-3.003007	1.818523	-0.472272
C	-4.242790	-1.021743	1.119496
H	-5.307180	-0.805777	0.993143
H	-4.092233	-2.099088	1.007339
H	-3.947088	-0.726414	2.130175

(2*R*)-*N*-Fmoc-2-methylcysteine methyl ester radical cation (7)

C	3.488289	-0.148002	0.159131
C	4.313002	1.121612	-0.175340
O	3.918638	2.019520	-0.900240
C	4.269682	-1.353168	-0.458823
S	3.947590	-3.038594	0.207343
O	5.500458	1.110894	0.424865
H	4.105105	-1.352758	-1.538515
H	5.336800	-1.213207	-0.278298
H	2.606118	-3.023608	0.067558
N	2.204764	0.081817	-0.518830
H	2.161589	0.927524	-1.078175
C	1.073095	-0.645615	-0.414686
O	0.915187	-1.699648	0.195936
C	3.319046	-0.233155	1.688367
H	2.909334	0.705221	2.073030
H	2.638742	-1.046021	1.941593
H	4.282992	-0.421296	2.164134
C	6.368328	2.248298	0.183746
H	5.883853	3.164161	0.525743
H	7.267240	2.046447	0.762501
H	6.599678	2.319840	-0.880253
O	0.069828	-0.035014	-1.118259
C	-1.202218	-0.701552	-1.141432
H	-1.050174	-1.781496	-1.165716
H	-1.679653	-0.374105	-2.066144
C	-2.060345	-0.321088	0.085120
C	-3.395467	-1.040389	0.093931
H	-1.487496	-0.579374	0.984864
C	-2.491585	1.132351	0.124872
C	-3.668936	-2.394294	0.086791
C	-4.473041	-0.090132	0.113310
C	-1.729991	2.284663	0.154580
C	-3.927119	1.223764	0.133194
C	-5.015865	-2.804570	0.095421
H	-2.877389	-3.136164	0.080373
C	-5.827265	-0.515996	0.122932
C	-2.393999	3.525993	0.185056
H	-0.647206	2.247364	0.152785
C	-4.585327	2.481734	0.167397
C	-6.083645	-1.872437	0.112189
H	-5.245145	-3.865409	0.091309
H	-6.635255	0.207017	0.139744
C	-3.808929	3.622063	0.191219
H	-1.806311	4.438245	0.206631
H	-5.668085	2.539870	0.175187
H	-7.104913	-2.236692	0.119379
H	-4.273803	4.601328	0.217312

***N*-Fmoc-cysteine methyl ester radical cation (8)**

C	-3.651730	-0.354183	0.132898
C	-3.979118	0.998175	-0.521213
O	-3.437284	2.050860	-0.240376
C	-4.824645	-0.788518	1.037762
S	-4.663928	-2.493310	1.700405
O	-4.956586	0.864190	-1.423139
H	-4.950493	-0.087198	1.866706
H	-5.747950	-0.793303	0.455647
H	-3.574246	-2.273710	2.462268
N	-2.405746	-0.272337	0.864299
H	-2.311776	0.437836	1.579653
C	-1.265384	-0.866346	0.427852
O	-1.171839	-1.640817	-0.516258
C	-5.399799	2.070495	-2.094729
H	-4.571345	2.512612	-2.650785
H	-6.188930	1.747447	-2.770796
H	-5.784158	2.784618	-1.364420
O	-0.214963	-0.493799	1.213809
C	1.059665	-1.087659	0.912532
H	0.914346	-2.121868	0.597520
H	1.614207	-1.061978	1.851543
C	1.803491	-0.303370	-0.190038
C	3.129289	-0.945566	-0.549788
H	1.150795	-0.268871	-1.071482
C	2.234926	1.094940	0.208734
C	3.395911	-2.221024	-1.007503
C	4.204258	-0.012195	-0.355045
C	1.476931	2.173482	0.621763
C	3.663792	1.222665	0.101859
C	4.734336	-2.571920	-1.268712
H	2.605189	-2.944745	-1.173486
C	5.549849	-0.377585	-0.623204
C	2.138580	3.376423	0.934694
H	0.398790	2.107520	0.707043
C	4.319034	2.442675	0.417567
C	5.799949	-1.657338	-1.076364
H	4.957821	-3.570574	-1.630231
H	6.356905	0.331458	-0.476564
C	3.546927	3.508029	0.833079
H	1.554202	4.230822	1.261107
H	5.396310	2.531706	0.332161
H	6.814716	-1.972932	-1.291883
H	4.010500	4.455875	1.082957
H	-3.519177	-1.092909	-0.660415

Cartesian Coordinates for Optimized Geometries in Water at B3lyp/6-31+G(d,p) Level of Radical Cations

(2*R*)-*N*-Ac-2-methylcysteine methyl ester radical cation (1)

C	0.303088	-0.041124	0.260011
C	1.705346	0.520645	-0.092918
O	1.895987	1.682910	-0.399101
C	0.050191	-1.266112	-0.661618
S	-1.537952	-2.109971	-0.305501
O	2.639795	-0.412114	0.011221
H	0.061129	-0.980075	-1.712986
H	0.826429	-2.010562	-0.479822
H	-2.159554	-1.859839	-1.475472
N	-0.621591	1.060013	-0.023904
H	-0.165471	1.938618	-0.259350
C	-1.951814	1.028183	0.029678
C	-2.712028	2.308561	-0.191354
O	-2.613678	-0.026735	0.258057
H	-3.364750	2.185817	-1.059395
H	-3.341611	2.496788	0.682221
H	-2.045707	3.158120	-0.347943
C	0.280278	-0.409423	1.760383
H	0.570317	0.456964	2.359268
H	-0.722972	-0.713385	2.065847
H	0.977015	-1.225911	1.958965
C	4.011326	-0.007936	-0.257940
H	4.312595	0.761395	0.454073
H	4.601213	-0.912158	-0.127395
H	4.089704	0.366264	-1.279315

***N*-Ac-cysteine methyl ester radical cation (2)**

C	0.312127	0.040157	-0.258039
C	1.732402	-0.491479	-0.000850
O	1.955048	-1.604272	0.436101
C	0.075365	1.335459	0.555955
S	-1.506096	2.133252	0.092899
O	2.643118	0.414579	-0.324962
H	0.235853	0.277395	-1.325378
H	0.077934	1.142918	1.628944
H	0.853226	2.058023	0.305679
H	-2.219451	1.834292	1.197700
N	-0.610645	-1.033934	0.061865
H	-0.191320	-1.869625	0.461966
C	-1.918704	-1.005421	-0.193975
C	-2.741815	-2.236213	0.065502
O	-2.488555	0.029423	-0.647634
H	-3.423987	-2.034347	0.896190
H	-3.343185	-2.449500	-0.821368
H	-2.120693	-3.101264	0.301979
C	4.038239	0.046821	-0.136648
H	4.276118	-0.817988	-0.757161
H	4.603967	0.920292	-0.452300
H	4.219792	-0.177146	0.915272

**(2R)-N-Piv-2-methylcysteine methyl ester
radical cation (3)**

C	-1.052209	0.185961	0.271388
C	-2.116336	-0.891421	-0.063646
O	-1.831551	-2.044139	-0.331264
C	-1.267471	1.366370	-0.716002
S	-0.160892	2.788019	-0.371477
O	-3.343478	-0.398039	0.006938
H	-1.117164	1.048141	-1.747486
H	-2.283227	1.746160	-0.597426
H	0.545289	2.773233	-1.520246
N	0.234955	-0.481794	0.054413
H	0.155973	-1.473888	-0.153611
C	1.445258	0.067459	0.120305
C	2.699429	-0.813811	-0.043240
O	1.621524	1.306244	0.311161
C	-4.441637	-1.316381	-0.252421
H	-4.419814	-2.128374	0.475434
H	-5.341804	-0.716528	-0.140402
H	-4.358357	-1.710854	-1.265822
C	-1.216396	0.604060	1.749488
H	-1.170412	-0.278419	2.391817
H	-0.414987	1.283012	2.047246
H	-2.177914	1.099392	1.896708
C	2.358868	-2.310247	-0.160575
H	1.831997	-2.686580	0.722426
H	1.770631	-2.536349	-1.056582
H	3.293399	-2.872485	-0.243833
C	3.594755	-0.578371	1.195943
H	4.511070	-1.166511	1.089346
H	3.868554	0.474897	1.292293
H	3.092257	-0.894338	2.115902
C	3.428042	-0.336951	-1.322323
H	3.700295	0.718885	-1.251632
H	4.343399	-0.922906	-1.448777
H	2.807036	-0.480291	-2.212499

N-Piv-cysteine methyl ester radical cation (4)

C	-0.406202	-0.259834	0.349332
C	-1.679514	-0.352987	-0.508177
O	-1.724144	-0.952149	-1.565717
C	-0.011084	1.221608	0.561169
S	1.317414	1.373845	1.813189
O	-2.687661	0.285488	0.067422
H	-0.634135	-0.704609	1.324799
H	0.313247	1.691412	-0.367589
H	-0.865548	1.761506	0.971832
H	2.335065	1.721014	0.999067
N	0.612249	-1.052687	-0.315842
H	0.344509	-1.431394	-1.219691
C	1.804106	-1.343799	0.203954
C	2.771813	-2.272432	-0.549898
O	2.176332	-0.852739	1.308809
C	-3.965985	0.264247	-0.627285
H	-4.312032	-0.765485	-0.725062
H	-4.637758	0.842474	0.002776
H	-3.857963	0.724898	-1.609897
C	3.897720	-1.374847	-1.121580
H	4.412539	-0.831160	-0.325149
H	4.628248	-2.008469	-1.633875
H	3.506602	-0.652226	-1.844833
C	3.363259	-3.273290	0.468145
H	4.087759	-3.912866	-0.044264
H	3.874066	-2.755906	1.283326
H	2.584735	-3.913370	0.895149
C	2.076884	-3.039899	-1.689320
H	1.242411	-3.648441	-1.325861
H	1.720095	-2.378871	-2.486561
H	2.804054	-3.717850	-2.145456

**(2R)-N-Boc-2-methylcysteine methyl ester
radical cation (5)**

C	-1.421301	-0.073099	0.309822
C	-2.456314	-1.145044	-0.122761
O	-2.142248	-2.233925	-0.565136
C	-1.729978	1.207656	-0.527662
S	-0.602855	2.603717	-0.165067
O	-3.697627	-0.721232	0.068422
H	-1.682872	0.998026	-1.595987
H	-2.726889	1.568081	-0.268418
H	0.100902	2.599552	-1.316099
N	-0.125732	-0.645153	-0.037128
H	-0.141239	-1.587694	-0.417842
C	1.068436	-0.064301	0.164961
O	1.202649	1.133815	0.534690
C	-4.769717	-1.642485	-0.274871
H	-4.682239	-2.547288	0.327830
H	-5.686639	-1.106133	-0.041862
H	-4.718539	-1.886200	-1.336802
O	2.083493	-0.879350	-0.057999
C	3.527300	-0.447746	-0.040054
C	3.895026	0.010593	1.370382
H	4.973686	0.189792	1.412385
H	3.381758	0.935096	1.641061
H	3.649736	-0.763999	2.102975
C	3.746946	0.628921	-1.101763
H	4.818823	0.837197	-1.172775
H	3.403037	0.282201	-2.080804
H	3.234458	1.558606	-0.848997
C	4.242803	-1.746827	-0.407376
H	5.321829	-1.571057	-0.425496
H	4.031201	-2.528402	0.327792
H	3.931841	-2.097263	-1.395617
C	-1.555815	0.170758	1.828949
H	-1.431623	-0.772726	2.366056
H	-0.788189	0.864605	2.177030
H	-2.539566	0.582963	2.060504

N-Boc-cysteine methyl ester radical cation (6)

C	1.471819	-0.409316	-0.336868
C	2.505515	-1.284032	0.390766
O	2.240202	-1.952168	1.371165
C	1.936683	1.073836	-0.302593
S	0.842004	2.152621	-1.290310
O	3.691950	-1.202326	-0.196295
H	1.434217	-0.734955	-1.382242
H	1.979758	1.455638	0.717613
H	2.918113	1.148207	-0.773900
H	0.128688	2.701446	-0.285122
N	0.193056	-0.630241	0.296996
H	0.182072	-1.169647	1.157521
C	-0.968790	-0.216144	-0.239415
O	-1.006263	0.531066	-1.254214
C	4.771656	-1.981000	0.389990
H	4.521147	-3.041875	0.351346
H	5.641623	-1.763909	-0.225409
H	4.934044	-1.665862	1.421497
O	-2.032011	-0.674952	0.390490
C	-3.443576	-0.248789	0.071412
C	-3.791784	-0.704448	-1.344613
H	-4.853693	-0.512223	-1.526033
H	-3.211521	-0.165176	-2.095751
H	-3.615495	-1.778182	-1.457999
C	-3.572046	1.260415	0.270187
H	-4.625697	1.537997	0.169588
H	-3.239697	1.547673	1.272209
H	-2.999257	1.818026	-0.472631
C	-4.243523	-1.019844	1.119970
H	-5.307590	-0.802210	0.993760
H	-4.094644	-2.097476	1.008005
H	-3.947040	-0.724745	2.130495

(2*R*)-*N*-Fmoc-2-methylcysteine methyl ester radical cation (7)

C	3.486447	-0.143224	0.152982
C	4.300656	1.134944	-0.174834
O	3.899005	2.033345	-0.895154
C	4.277381	-1.337977	-0.472707
S	3.965803	-3.030536	0.180895
O	5.488191	1.130765	0.425208
H	4.113846	-1.331203	-1.552504
H	5.343273	-1.191828	-0.289892
H	2.623802	-3.021601	0.044931
N	2.200638	0.079554	-0.522806
H	2.149323	0.928855	-1.075956
C	1.073747	-0.655487	-0.418888
O	0.924446	-1.712959	0.188265
C	3.319514	-0.238752	1.681876
H	2.902356	0.693814	2.072474
H	2.646024	-1.058544	1.930855
H	4.285538	-0.421669	2.155502
C	6.347065	2.276172	0.189687
H	5.855155	3.186581	0.535557
H	7.247255	2.078967	0.768036
H	6.578540	2.354148	-0.873841
O	0.065702	-0.049285	-1.118594
C	-1.205143	-0.718700	-1.135439
H	-1.050829	-1.798411	-1.154033
H	-1.685318	-0.397426	-2.060861
C	-2.060819	-0.332570	0.091004
C	-3.396742	-1.050375	0.103836
H	-1.487101	-0.587643	0.991116
C	-2.490459	1.121495	0.125576
C	-3.671725	-2.403969	0.102972
C	-4.473229	-0.098862	0.118985
C	-1.727547	2.272989	0.152160
C	-3.925867	1.214512	0.133036
C	-5.019103	-2.812742	0.113670
H	-2.881090	-3.146796	0.099686
C	-5.827934	-0.523202	0.130867
C	-2.390181	3.515177	0.177863
H	-0.644813	2.234534	0.151816
C	-4.582669	2.473369	0.162012
C	-6.085820	-1.879401	0.126378
H	-5.249529	-3.873331	0.114310
H	-6.635004	0.200893	0.144548
C	-3.804976	3.612880	0.182307
H	-1.801445	4.426795	0.196967
H	-5.665350	2.532670	0.168857
H	-7.107500	-2.242441	0.135408
H	-4.268773	4.592742	0.204499

***N*-Fmoc-cysteine methyl ester radical cation (8)**

C	-3.650765	-0.345082	0.137717
C	-3.981544	1.010632	-0.507452
O	-3.441528	2.062599	-0.220305
C	-4.820362	-0.783832	1.045019
S	-4.655268	-2.490829	1.701029
O	-4.960286	0.880808	-1.408567
H	-4.943776	-0.085883	1.877095
H	-5.745693	-0.787496	0.466109
H	-3.566113	-2.271771	2.463770
N	-2.401647	-0.265946	0.863886
H	-2.301922	0.446934	1.575780
C	-1.265898	-0.869076	0.428029
O	-1.179889	-1.651252	-0.510752
C	-5.408014	2.091106	-2.070065
H	-4.582005	2.539339	-2.624857
H	-6.198030	1.771300	-2.746618
H	-5.792398	2.798645	-1.333393
O	-0.211362	-0.495819	1.207364
C	1.061167	-1.094360	0.905885
H	0.912496	-2.129029	0.593981
H	1.617071	-1.067535	1.844025
C	1.805966	-0.315405	-0.199724
C	3.135298	-0.956337	-0.548767
H	1.156737	-0.289102	-1.083966
C	2.231513	1.087257	0.190349
C	3.407816	-2.234149	-0.996206
C	4.206668	-0.018626	-0.355191
C	1.468484	2.167219	0.590207
C	3.660535	1.217989	0.089948
C	4.748478	-2.582901	-1.248786
H	2.620120	-2.961511	-1.160447
C	5.554635	-0.381990	-0.614105
C	2.125403	3.374229	0.897483
H	0.390056	2.099411	0.669802
C	4.310971	2.442075	0.399667
C	5.810517	-1.663988	-1.057598
H	4.976529	-3.583349	-1.602384
H	6.358900	0.330312	-0.467993
C	3.533926	3.508617	0.802742
H	1.537077	4.229632	1.214000
H	5.388405	2.533183	0.319004
H	6.827184	-1.978105	-1.266176
H	3.993743	4.459523	1.047835
H	-3.521569	-1.079659	-0.659948

Cartesian Coordinates for Optimized Geometries in Gas-phase at B3lyp/6-31+G(d,p) Level of Sulphur Neutral Radical

(2*R*)-*N*-Ac-2-methylcysteine methyl ester radical (1')

C	0.291726	-0.041828	0.262722
C	1.689698	0.503938	-0.093836
O	1.907656	1.640469	-0.472799
C	-0.015480	-1.237150	-0.699963
S	-1.381571	-2.337640	-0.233898
O	2.646988	-0.416667	0.077052
H	-0.170669	-0.834803	-1.706060
H	0.867547	-1.885538	-0.728557
N	-0.612509	1.084886	0.015265
H	-0.152106	1.941721	-0.269398
C	-1.968752	1.043816	0.073986
C	-2.684772	2.351343	-0.215604
O	-2.606579	0.021633	0.346429
H	-3.356088	2.200588	-1.065581
H	-3.302376	2.608799	0.649304
H	-2.008050	3.182101	-0.433028
C	0.283047	-0.447785	1.751121
H	0.615886	0.391126	2.370414
H	-0.728987	-0.731053	2.040840
H	0.944822	-1.300408	1.917813
C	3.999238	0.006444	-0.206464
H	4.279592	0.833664	0.449026
H	4.618568	-0.868212	-0.013489
H	4.084876	0.322137	-1.248287

***N*-Ac-cysteine methyl ester radical (2')**

C	0.296452	0.060085	-0.215088
C	1.715510	-0.459967	0.014061
O	1.979502	-1.528391	0.532659
C	0.026213	1.305785	0.678360
S	-1.338526	2.352105	0.083718
O	2.632828	0.414335	-0.418644
H	0.203386	0.367203	-1.262852
H	-0.143717	0.971142	1.706524
H	0.915848	1.945551	0.660832
N	-0.604282	-1.044532	0.059573
H	-0.188906	-1.852771	0.506924
C	-1.922235	-1.031274	-0.276019
C	-2.714981	-2.279698	0.060108
O	-2.448957	-0.058016	-0.820909
H	-3.498090	-2.013981	0.776114
H	-3.207214	-2.635731	-0.848711
H	-2.104327	-3.084293	0.478583
C	4.015653	0.035804	-0.234455
H	4.225808	-0.891609	-0.771205
H	4.594763	0.861411	-0.645041
H	4.230610	-0.100699	0.827504

(2*R*)-N-Piv-2-methylcysteine methyl ester radical (3')

C	-0.259028	-0.072480	0.438478
C	-1.571280	-0.263884	-0.348719
O	-1.721672	-1.069603	-1.249330
C	0.223020	1.399710	0.211228
S	1.476770	2.040013	1.356605
O	-2.541029	0.552470	0.084076
H	0.566144	1.489579	-0.824385
H	-0.638895	2.063919	0.339936
N	0.670062	-1.035042	-0.161766
H	0.262775	-1.616273	-0.883874
C	1.990105	-1.143192	0.129015
C	2.806095	-2.235772	-0.603698
O	2.550812	-0.409198	0.953004
C	-3.820597	0.431704	-0.575836
H	-4.215167	-0.578712	-0.449579
H	-4.463658	1.162902	-0.088269
H	-3.718154	0.652093	-1.640465
C	-0.520659	-0.400515	1.923026
H	-0.963225	-1.397586	2.013564
H	0.422408	-0.372928	2.468863
H	-1.199480	0.333609	2.362178
C	1.983469	-3.079399	-1.595214
H	1.169694	-3.623941	-1.102685
H	1.562912	-2.474817	-2.407279
H	2.634501	-3.827568	-2.059232
C	3.403224	-3.157113	0.484075
H	4.057328	-3.903703	0.020367
H	3.985726	-2.577054	1.203588
H	2.615746	-3.690185	1.029182
C	3.947207	-1.517270	-1.358753
H	4.540080	-0.908627	-0.672068
H	4.603323	-2.256075	-1.831895
H	3.554085	-0.862736	-2.145026

N-Piv-cysteine methyl ester radical (4')

C	-0.182871	0.181622	0.112283
C	-1.558871	-0.393694	-0.234317
O	-1.787725	-1.094736	-1.199989
C	-0.138057	1.659326	-0.349048
S	1.399184	2.539126	0.023110
O	-2.494479	0.018944	0.638031
H	-0.032003	0.133021	1.193077
H	-0.287890	1.724143	-1.436062
H	-0.961832	2.223296	0.105541
N	0.855725	-0.616789	-0.498813
H	0.732077	-0.853640	-1.472871
C	1.728884	-1.361140	0.258212
C	2.714855	-2.286040	-0.493065
O	1.742122	-1.289753	1.484246
C	-3.845558	-0.425932	0.384310
H	-3.893222	-1.516523	0.414330
H	-4.445897	0.009134	1.182032
H	-4.183118	-0.074441	-0.593239
C	4.140032	-1.868117	-0.067027
H	4.238930	-1.897263	1.020479
H	4.875302	-2.550851	-0.507332
H	4.373372	-0.852264	-0.404553
C	2.431872	-3.728088	-0.013186
H	3.156479	-4.418662	-0.458920
H	2.509082	-3.792919	1.074835
H	1.427940	-4.056016	-0.306545
C	2.598865	-2.222413	-2.027742
H	1.617760	-2.556928	-2.386536
H	2.794677	-1.215518	-2.413361
H	3.342307	-2.890116	-2.475412

(2*R*)-N-Boc-2-methylcysteine methyl ester radical (5')

C	-1.406307	-0.030428	0.272857
C	-2.424719	-1.131324	-0.090471
O	-2.127542	-2.249877	-0.464733
C	-1.630750	1.160723	-0.720443
S	-0.921866	2.768405	-0.268164
O	-3.689191	-0.713222	0.066356
H	-1.280749	0.851627	-1.710242
H	-2.708475	1.350620	-0.787680
N	-0.103672	-0.658791	0.064265
H	-0.112266	-1.626935	-0.234634
C	1.093867	-0.023416	0.160207
O	1.237424	1.165014	0.437919
C	-4.720912	-1.680067	-0.229183
H	-4.615113	-2.553142	0.418156
H	-5.660284	-1.164493	-0.034821
H	-4.657350	-1.992284	-1.273779
O	2.096081	-0.896537	-0.092727
C	3.513658	-0.475300	-0.084845
C	3.906032	0.015984	1.312477
H	4.985131	0.201169	1.341574
H	3.385937	0.939831	1.569360
H	3.672237	-0.745840	2.063365
C	3.753070	0.583843	-1.165904
H	4.825711	0.794079	-1.235048
H	3.416396	0.217034	-2.141075
H	3.229511	1.512705	-0.935944
C	4.242485	-1.777157	-0.427705
H	5.322454	-1.602493	-0.455651
H	4.033998	-2.546336	0.322018
H	3.925657	-2.152121	-1.405583
C	-1.613173	0.369141	1.748462
H	-1.563723	-0.519331	2.385643
H	-0.831249	1.068576	2.045512
H	-2.582836	0.853150	1.882819

N-Boc-cysteine methyl ester radical (6')

C	1.502216	0.202069	-0.082259
C	2.272595	-1.081380	0.247681
O	2.035323	-1.802180	1.195743
C	2.338991	1.415164	0.391710
S	1.633221	3.032879	-0.011070
O	3.281187	-1.281088	-0.619485
H	1.356172	0.264494	-1.162899
H	2.485640	1.375712	1.479317
H	3.341323	1.383694	-0.054442
N	0.195258	0.177132	0.530903
H	0.135400	-0.140579	1.490149
C	-0.940263	0.021180	-0.231402
O	-0.967736	0.084914	-1.450256
C	4.110403	-2.439239	-0.377533
H	3.507189	-3.348570	-0.419812
H	4.854554	-2.431414	-1.172708
H	4.587223	-2.365291	0.602455
O	-1.996435	-0.187776	0.585822
C	-3.366714	-0.340625	0.052835
C	-3.444171	-1.580087	-0.844661
H	-4.487186	-1.758012	-1.127518
H	-2.852877	-1.449647	-1.751962
H	-3.082798	-2.462968	-0.307248
C	-3.788755	0.938115	-0.678007
H	-4.844750	0.862991	-0.958792
H	-3.672384	1.807775	-0.023249
H	-3.196532	1.093136	-1.580845
C	-4.193642	-0.538554	1.325944
H	-5.249518	-0.666175	1.068049
H	-3.859320	-1.426831	1.870519
H	-4.099959	0.328392	1.986925

(2*R*)-*N*-Fmoc-2-methylcysteine methyl ester radical (7')

C	3.472167	-0.040177	0.245505
C	4.456876	1.053302	-0.220110
O	4.159498	1.983861	-0.944791
C	3.996375	-1.410156	-0.304557
S	3.340398	-2.923463	0.450944
O	5.685790	0.863302	0.279159
H	3.846279	-1.426132	-1.388559
H	5.074971	-1.462543	-0.114083
N	2.200820	0.332429	-0.374885
H	2.206943	1.172507	-0.942600
C	1.071513	-0.415080	-0.343428
O	0.941162	-1.499382	0.216276
C	3.380490	-0.003920	1.784470
H	3.128451	1.006720	2.120171
H	2.607232	-0.696740	2.117550
H	4.330542	-0.303478	2.231831
C	6.681057	1.846014	-0.084580
H	6.379316	2.834740	0.267254
H	7.596370	1.521614	0.408174
H	6.809350	1.868838	-1.168760
O	0.075258	0.208337	-1.028164
C	-1.187696	-0.491628	-1.104947
H	-0.991153	-1.562302	-1.182956
H	-1.649137	-0.129304	-2.025573
C	-2.088699	-0.200538	0.107407
C	-3.368309	-1.022496	0.052638
H	-1.515655	-0.449033	1.010760
C	-2.622331	1.223462	0.171586
C	-3.521496	-2.405311	0.001567
C	-4.496105	-0.175690	0.061619
C	-1.927044	2.427432	0.254875
C	-4.033780	1.217431	0.137418
C	-4.814771	-2.943125	-0.045485
H	-2.656837	-3.063842	0.008049
C	-5.785190	-0.713956	0.016524
C	-2.648515	3.628044	0.300239
H	-0.842042	2.440296	0.280180
C	-4.751715	2.415567	0.184728
C	-5.935392	-2.102969	-0.039271
H	-4.948796	-4.020247	-0.083089
H	-6.659571	-0.069156	0.026391
C	-4.048465	3.621053	0.265390
H	-2.116378	4.572794	0.364679
H	-5.838011	2.415915	0.161664
H	-6.931288	-2.535311	-0.074846
H	-4.592612	4.560459	0.303722

***N*-Fmoc-cysteine methyl ester radical (8')**

C	-3.577268	-0.065952	-0.274448
C	-4.466786	1.173375	-0.161741
O	-4.253581	2.105422	0.588602
C	-4.329025	-1.311957	0.280520
S	-3.679270	-2.900965	-0.321160
O	-5.519933	1.092485	-0.986177
H	-4.327992	-1.267656	1.373959
H	-5.366797	-1.276243	-0.071673
N	-2.354086	0.230660	0.442283
H	-2.356015	1.034253	1.058889
C	-1.227048	-0.512142	0.305826
O	-1.128940	-1.507762	-0.402308
C	-6.446372	2.201750	-0.950643
H	-5.935326	3.126220	-1.227199
H	-7.217959	1.952792	-1.677458
H	-6.872063	2.305492	0.049654
O	-0.221464	-0.000356	1.060163
C	1.040992	-0.705477	1.010305
H	0.841231	-1.775082	0.926722
H	1.517523	-0.488630	1.968150
C	1.921213	-0.231095	-0.157940
C	3.205124	-1.043660	-0.245905
H	1.335557	-0.346515	-1.079968
C	2.447696	1.190195	-0.016717
C	3.364851	-2.417351	-0.406327
C	4.328947	-0.197586	-0.144860
C	1.746297	2.388758	0.089658
C	3.859561	1.188145	-0.004561
C	4.661001	-2.947389	-0.461599
H	2.503015	-3.073203	-0.498226
C	5.620863	-0.727934	-0.201151
C	2.461945	3.587413	0.212566
H	0.661034	2.398751	0.081457
C	4.571644	2.384619	0.116050
C	5.777762	-2.108434	-0.358245
H	4.800292	-4.016937	-0.588888
H	6.492244	-0.083304	-0.126605
C	3.862261	3.584203	0.225679
H	1.924896	4.527769	0.297127
H	5.658145	2.388483	0.122560
H	6.775902	-2.534620	-0.403734
H	4.401854	4.522294	0.319762
H	-3.360942	-0.241134	-1.333979

Cartesian Coordinates for Optimized Geometries in Methanol at B3lyp/6-31+G(d,p) Level of Sulphur Neutral Radical

(2*R*)-*N*-Ac-2-methylcysteine methyl ester radical (1')

C	0.289854	-0.041674	0.264896
C	1.688735	0.510065	-0.095199
O	1.894654	1.652940	-0.468547
C	-0.005897	-1.235553	-0.698442
S	-1.400992	-2.313965	-0.256785
O	2.639736	-0.406440	0.070564
H	-0.136118	-0.841896	-1.710024
H	0.867747	-1.895919	-0.701394
N	-0.623719	1.078263	0.018286
H	-0.168225	1.944742	-0.247269
C	-1.972199	1.042331	0.065657
C	-2.688102	2.347147	-0.215224
O	-2.618739	0.009859	0.324264
H	-3.349300	2.207367	-1.075057
H	-3.311863	2.597522	0.647450
H	-2.007751	3.177195	-0.416724
C	0.290493	-0.442107	1.754695
H	0.634224	0.395905	2.367786
H	-0.719985	-0.714633	2.059277
H	0.950245	-1.296668	1.919103
C	4.002417	0.002406	-0.212792
H	4.289160	0.821955	0.448168
H	4.609076	-0.880043	-0.020390
H	4.088253	0.312783	-1.255290

***N*-Ac-cysteine methyl cysteine radical (2')**

C	0.298000	0.053605	-0.215733
C	1.719207	-0.469675	0.011482
O	1.975768	-1.545194	0.523728
C	0.035119	1.296038	0.682145
S	-1.349980	2.329086	0.106865
O	2.628609	0.404585	-0.416075
H	0.212808	0.356793	-1.264522
H	-0.122221	0.966385	1.712223
H	0.917638	1.943677	0.650536
N	-0.611627	-1.044358	0.055563
H	-0.210428	-1.849875	0.522048
C	-1.921239	-1.033291	-0.276896
C	-2.721051	-2.271401	0.061230
O	-2.447507	-0.053299	-0.834129
H	-3.526796	-1.993607	0.746709
H	-3.180018	-2.654453	-0.854364
H	-2.119091	-3.060031	0.517412
C	4.022275	0.043381	-0.235979
H	4.242345	-0.872610	-0.786589
H	4.587097	0.881566	-0.638625
H	4.236431	-0.094863	0.825008

**(2*R*)-*N*-Boc-2-methylcysteine methyl ester
radical (3')**

C	-1.412490	-0.025576	0.280399
C	-2.423191	-1.134950	-0.094250
O	-2.104925	-2.250015	-0.471354
C	-1.648874	1.163801	-0.708414
S	-0.916101	2.765806	-0.268043
O	-3.682003	-0.727637	0.059287
H	-1.319995	0.857699	-1.705050
H	-2.725467	1.363378	-0.753425
N	-0.102223	-0.639229	0.071715
H	-0.106516	-1.607758	-0.227218
C	1.093304	-0.005881	0.161963
O	1.237272	1.189459	0.433187
C	-4.724478	-1.688952	-0.244743
H	-4.623192	-2.563379	0.400027
H	-5.658379	-1.167407	-0.045460
H	-4.662454	-1.985914	-1.292944
O	2.094751	-0.875810	-0.084586
C	3.523227	-0.469791	-0.085496
C	3.925043	0.027398	1.305845
H	5.006927	0.193021	1.328844
H	3.424576	0.963939	1.556015
H	3.679799	-0.722454	2.064758
C	3.769792	0.573064	-1.179180
H	4.844943	0.764088	-1.256442
H	3.420357	0.202113	-2.148028
H	3.265754	1.514291	-0.955559
C	4.233715	-1.783838	-0.418117
H	5.314707	-1.619929	-0.451460
H	4.021489	-2.542279	0.341453
H	3.910639	-2.163686	-1.392089
C	-1.629735	0.357510	1.758615
H	-1.587018	-0.537238	2.386304
H	-0.849025	1.049871	2.074437
H	-2.600755	0.839094	1.891367

***N*-Boc-cysteine methyl ester radical (4')**

C	1.522582	0.340193	0.011185
C	2.144375	-1.066224	0.099971
O	1.698065	-1.985301	0.759612
C	2.432704	1.363045	0.719917
S	1.944318	3.092332	0.488532
O	3.255691	-1.137419	-0.643866
H	1.455490	0.596727	-1.048619
H	2.483839	1.163667	1.797484
H	3.459118	1.278918	0.343977
N	0.187200	0.371303	0.558912
H	0.075206	0.307190	1.562561
C	-0.903710	0.035319	-0.199348
O	-0.868120	-0.130329	-1.414733
C	3.966870	-2.400178	-0.642050
H	3.322199	-3.191673	-1.028257
H	4.823263	-2.247636	-1.296076
H	4.292739	-2.644391	0.370640
O	-1.993502	-0.052181	0.587976
C	-3.341685	-0.360368	0.046866
C	-3.341460	-1.753658	-0.588267
H	-4.366669	-2.023096	-0.861762
H	-2.723096	-1.784855	-1.486522
H	-2.973050	-2.498384	0.124462
C	-3.772691	0.735054	-0.932133
H	-4.814949	0.567299	-1.221995
H	-3.706225	1.719497	-0.457971
H	-3.156761	0.731507	-1.832549
C	-4.211262	-0.337940	1.305892
H	-5.249535	-0.558240	1.041291
H	-3.870659	-1.088824	2.025223
H	-4.176630	0.645878	1.783552

**(2*R*)-*N*-Fmoc-2-methylcysteine methyl ester
radical (7')**

C	3.461247	-0.016597	0.249714
C	4.419295	1.089239	-0.252846
O	4.087584	1.987470	-1.007639
C	4.033050	-1.385206	-0.245909
S	3.387135	-2.891391	0.535508
O	5.642793	0.947595	0.252389
H	3.915731	-1.441279	-1.331302
H	5.105672	-1.408263	-0.021344
N	2.182670	0.291808	-0.392051
H	2.163621	1.126972	-0.967273
C	1.072016	-0.474523	-0.347257
O	0.960780	-1.554224	0.236084
C	3.359668	0.082290	1.785256
H	3.087267	1.100414	2.077333
H	2.595894	-0.607045	2.146153
H	4.313291	-0.178237	2.248982
C	6.630392	1.938686	-0.130880
H	6.309170	2.928820	0.196513
H	7.544156	1.640287	0.378814
H	6.768222	1.927047	-1.213181
O	0.065339	0.109278	-1.046661
C	-1.197129	-0.595031	-1.102389
H	-1.002235	-1.666540	-1.168075
H	-1.663215	-0.248744	-2.026423
C	-2.092206	-0.284045	0.109939
C	-3.400954	-1.058457	0.035698
H	-1.535288	-0.559905	1.015132
C	-2.574466	1.157745	0.190158
C	-3.606414	-2.434412	-0.035378
C	-4.497524	-0.170387	0.045191
C	-1.836945	2.334542	0.306545
C	-3.985352	1.204066	0.143675
C	-4.919579	-2.922527	-0.099623
H	-2.769121	-3.127099	-0.034406
C	-5.806775	-0.657972	-0.017433
C	-2.515854	3.560211	0.367403
H	-0.752827	2.309008	0.350123
C	-4.661767	2.426508	0.206280
C	-6.008781	-2.040529	-0.091565
H	-5.093415	-3.993208	-0.153160
H	-6.655930	0.019506	-0.007443
C	-3.915702	3.604781	0.316537
H	-1.950762	4.483360	0.458038
H	-5.747000	2.466310	0.174135
H	-7.019805	-2.434468	-0.140793
H	-4.426079	4.562284	0.367514

N-Fmoc-cysteine methyl ester radical (8')

C	-3.580028	-0.052255	-0.266841
C	-4.437141	1.213075	-0.156162
O	-4.179963	2.148180	0.580827
C	-4.361176	-1.269420	0.308065
S	-3.744090	-2.882563	-0.265304
O	-5.497761	1.146300	-0.959405
H	-4.360751	-1.214255	1.399567
H	-5.396715	-1.219060	-0.047095
N	-2.340159	0.211747	0.434164
H	-2.319596	1.006292	1.062694
C	-1.232319	-0.548383	0.285648
O	-1.157655	-1.543132	-0.436140
C	-6.414170	2.271049	-0.931249
H	-5.894158	3.180701	-1.235723
H	-7.197275	2.016918	-1.642444
H	-6.825323	2.390677	0.072391
O	-0.213521	-0.071416	1.039899
C	1.046962	-0.780011	0.973211
H	0.847302	-1.847554	0.870324
H	1.522976	-0.585787	1.935767
C	1.928670	-0.281576	-0.184304
C	3.232498	-1.064657	-0.254519
H	1.358709	-0.404699	-1.114933
C	2.420512	1.151651	-0.036000
C	3.427635	-2.435120	-0.409483
C	4.335479	-0.192633	-0.135988
C	1.689985	2.335165	0.052087
C	3.832240	1.182285	-0.002269
C	4.737631	-2.934585	-0.444708
H	2.584506	-3.113535	-0.508806
C	5.641561	-0.691381	-0.172319
C	2.377043	3.550724	0.183326
H	0.605214	2.322462	0.020352
C	4.516608	2.394998	0.127022
C	5.833469	-2.068856	-0.326104
H	4.903836	-4.000810	-0.567005
H	6.495989	-0.026249	-0.084545
C	3.777719	3.579165	0.221609
H	1.817613	4.479071	0.253664
H	5.602394	2.423426	0.150928
H	6.841924	-2.471238	-0.355808
H	4.294347	4.529371	0.322043
H	-3.380041	-0.232386	-1.328014

Cartesian Coordinates for Optimized Geometries in Water at B3lyp/6-31+G(d,p) Level of Sulphur Neutral Radical

(2R)-N-Ac-2-methylcysteine methyl ester radical (1')

C	-0.248354	0.032961	0.244076
C	-1.637417	-0.560285	-0.087038
O	-1.819267	-1.715564	-0.433890
C	0.003036	1.220000	-0.739900
S	1.372426	2.342632	-0.330359
O	-2.608721	0.335431	0.072997
H	0.132609	0.815498	-1.747277
H	-0.888338	1.856214	-0.742464
N	0.691070	-1.066417	0.001205
H	0.253907	-1.950801	-0.234645
C	2.038486	-0.993525	0.017336
C	2.783932	-2.284461	-0.250425
O	2.663045	0.061622	0.238001
H	3.417591	-2.148366	-1.131363
H	3.437429	-2.494740	0.600851
H	2.122937	-3.138394	-0.412294
C	-0.238821	0.454642	1.728136
H	-0.551038	-0.383288	2.357954
O	0.768242	0.758245	2.014394
H	-0.918639	1.293809	1.890427
C	-3.964628	-0.113091	-0.182073
H	-4.223235	-0.921230	0.504055
H	-4.589976	0.759438	-0.005007
H	-4.055667	-0.452932	-1.214865

N-Ac-cysteine methyl ester radical (2')

C	0.298105	0.053063	-0.216303
C	1.719424	-0.470394	0.010404
O	1.975930	-1.546667	0.521173
C	0.035443	1.295261	0.681902
S	-1.348573	2.329402	0.106078
O	2.628471	0.404535	-0.415972
H	0.213034	0.356284	-1.265085
H	-0.122926	0.965559	1.711745
H	0.918246	1.942531	0.651220
N	-0.611776	-1.044729	0.054819
H	-0.210811	-1.850433	0.521260
C	-1.921416	-1.033164	-0.276088
C	-2.721456	-2.270973	0.062016
O	-2.448103	-0.052502	-0.832633
H	-3.529066	-1.992550	0.745020
H	-3.177728	-2.655909	-0.854175
H	-2.120161	-3.058445	0.520945
C	4.022441	0.044172	-0.235556
H	4.243456	-0.870919	-0.787247
H	4.586794	0.883270	-0.636904
H	4.236010	-0.094931	0.825419

(2*R*)-*N*-Piv-2-methylcysteine methyl ester radical (3')

C	3.460917	-0.016423	0.249684
C	4.418018	1.090325	-0.253120
O	4.085170	1.987910	-1.008354
C	4.034087	-1.384302	-0.246147
S	3.388441	-2.891387	0.534098
O	5.641305	0.950102	0.252268
H	3.917623	-1.440257	-1.331590
H	5.106492	-1.406759	-0.020657
N	2.181943	0.290911	-0.391825
H	2.162138	1.126673	-0.966174
C	1.071882	-0.475977	-0.347090
O	0.961464	-1.556101	0.236028
C	3.359823	0.082593	1.785262
H	3.087075	1.100573	2.077386
H	2.596511	-0.606978	2.146706
H	4.313808	-0.177350	2.248586
C	6.628360	1.942081	-0.130908
H	6.306050	2.931905	0.196293
H	7.542096	1.644454	0.379191
H	6.766470	1.930142	-1.213146
O	0.065017	0.106503	-1.047036
C	-1.197504	-0.597839	-1.101943
H	-1.002827	-1.669389	-1.167409
H	-1.663816	-0.251870	-2.025965
C	-2.092288	-0.286123	0.110484
C	-3.401791	-1.059286	0.035929
H	-1.535684	-0.562428	1.015724
C	-2.573159	1.156124	0.190618
C	-3.608620	-2.435061	-0.035209
C	-4.497522	-0.170113	0.044978
C	-1.834458	2.332181	0.307431
C	-3.984006	1.203859	0.143506
C	-4.922287	-2.921884	-0.099836
H	-2.772064	-3.128635	-0.034078
C	-5.807282	-0.656384	-0.018074
C	-2.512193	3.558567	0.367855
H	-0.750396	2.305570	0.351808
C	-4.659247	2.427008	0.205703
C	-6.010637	-2.038783	-0.092183
H	-5.097161	-3.992390	-0.153445
H	-6.655775	0.021930	-0.008454
C	-3.912009	3.604554	0.316229
H	-1.946210	4.481133	0.458827
H	-5.744415	2.467904	0.173027
H	-7.022027	-2.431716	-0.141787
H	-4.421442	4.562573	0.366895

***N*-Piv-cysteine methyl ester radical (4')**

C	-0.186699	0.186418	0.062126
C	-1.565074	-0.463373	-0.141467
O	-1.799897	-1.378955	-0.907123
C	-0.188303	1.611294	-0.532815
S	1.299080	2.581090	-0.175834
O	-2.483238	0.132362	0.630005
H	-0.006515	0.244426	1.137655
H	-0.312015	1.580901	-1.622998
H	-1.039251	2.182922	-0.144527
N	0.864562	-0.626057	-0.508070
H	0.918288	-0.684746	-1.514742
C	1.659866	-1.438405	0.243184
C	2.713037	-2.296100	-0.493971
O	1.556115	-1.482569	1.476056
C	-3.845541	-0.350227	0.520313
H	-3.890981	-1.404654	0.798268
H	-4.421083	0.256636	1.216570
H	-4.208568	-0.216589	-0.500259
C	4.098984	-1.901628	0.065979
H	4.133090	-2.030896	1.150682
H	4.870762	-2.534860	-0.384116
H	4.338899	-0.858030	-0.166100
C	2.417214	-3.775054	-0.153886
H	3.178387	-4.416749	-0.610104
H	2.429669	-3.936541	0.926993
H	1.438934	-4.083607	-0.538943
C	2.712184	-2.115660	-2.023871
H	1.761316	-2.419176	-2.476987
H	2.935393	-1.084543	-2.319319
H	3.489327	-2.750862	-2.460228

(2*R*)-*N*-Boc-2-methylcysteine methyl ester radical (5')

C	-1.412673	-0.025487	0.281249
C	-2.423039	-1.134939	-0.094557
O	-2.104013	-2.249767	-0.472011
C	-1.649042	1.164331	-0.706915
S	-0.915723	2.765963	-0.265803
O	-3.681699	-0.727952	0.058562
H	-1.320468	0.858898	-1.703809
H	-2.725570	1.364244	-0.751559
N	-0.102145	-0.638713	0.072732
H	-0.106395	-1.607142	-0.226585
C	1.093341	-0.005642	0.163077
O	1.237424	1.189892	0.434430
C	-4.724370	-1.688882	-0.246671
H	-4.623496	-2.563733	0.397553
H	-5.658184	-1.167277	-0.047291
H	-4.661998	-1.984727	-1.295146
O	2.094742	-0.875426	-0.083307
C	3.523530	-0.469666	-0.085571
C	3.926362	0.029124	1.304865
H	5.008389	0.193753	1.327083
H	3.426930	0.966508	1.553952
H	3.680782	-0.719403	2.064965
C	3.769368	0.571661	-1.180820
H	4.844418	0.762869	-1.258712
H	3.419657	0.199268	-2.149004
H	3.265243	1.513126	-0.958315
C	4.233481	-1.784268	-0.417054
H	5.314429	-1.620464	-0.451811
H	4.022076	-2.541568	0.343885
H	3.909364	-2.165411	-1.390174
C	-1.630747	0.356364	1.759642
H	-1.588702	-0.538895	2.386598
H	-0.850039	1.048156	2.076697
H	-2.601763	0.838012	1.892183

***N*-Boc-cysteine methyl ester radical (6')**

C	1.511126	0.218014	-0.053254
C	2.237011	-1.118861	0.175157
O	1.875432	-1.983004	0.951561
C	2.262814	1.377659	0.508924
S	1.729917	3.029874	0.123405
O	3.335527	-1.196591	-0.585872
H	1.396462	0.350680	-1.131288
H	2.452244	1.302445	1.599909
H	3.383711	1.328777	0.112794
N	0.188889	0.203788	0.523711
H	0.098663	0.068535	1.522335
C	-0.932680	-0.010403	-0.231839
O	-0.941838	-0.042624	-1.458941
C	4.142238	-2.393601	-0.453670
H	3.554398	-3.271224	-0.728264
H	4.973488	-2.256099	-1.142462
H	4.502151	-2.490354	0.572148
O	-2.001074	-0.152479	0.577603
C	-3.377252	-0.340013	0.051943
C	-3.457060	-1.641352	-0.750943
H	-4.501506	-1.836035	-1.014786
H	-2.871603	-1.581350	-1.669377
H	-3.095655	-2.483091	-0.151543
C	-3.792246	0.885576	-0.766506
H	-4.848839	0.794634	-1.038022
H	-3.670894	1.799049	-0.175549
H	-3.205068	0.973072	-1.681836
C	-4.205409	-0.442306	1.334681
H	-5.260250	-0.583882	1.082060
H	-3.877558	-1.292059	1.941075
H	-4.111483	0.470459	1.930750

(2*R*)-*N*-Fmoc-2-methylcysteine methyl ester radical (7')

C	3.460917	-0.016423	0.249684
C	4.418018	1.090325	-0.253120
O	4.085170	1.987910	-1.008354
C	4.034087	-1.384302	-0.246147
S	3.388441	-2.891387	0.534098
O	5.641305	0.950102	0.252268
H	3.917623	-1.440257	-1.331590
H	5.106492	-1.406759	-0.020657
N	2.181943	0.290911	-0.391825
H	2.162138	1.126673	-0.966174
C	1.071882	-0.475977	-0.347090
O	0.961464	-1.556101	0.236028
C	3.359823	0.082593	1.785262
H	3.087075	1.100573	2.077386
H	2.596511	-0.606978	2.146706
H	4.313808	-0.177350	2.248586
C	6.628360	1.942081	-0.130908
H	6.306050	2.931905	0.196293
H	7.542096	1.644454	0.379191
H	6.766470	1.930142	-1.213146
O	0.065017	0.106503	-1.047036
C	-1.197504	-0.597839	-1.101943
H	-1.002827	-1.669389	-1.167409
H	-1.663816	-0.251870	-2.025965
C	-2.092288	-0.286123	0.110484
C	-3.401791	-1.059286	0.035929
H	-1.535684	-0.562428	1.015724
C	-2.573159	1.156124	0.190618
C	-3.608620	-2.435061	-0.035209
C	-4.497522	-0.170113	0.044978
C	-1.834458	2.332181	0.307431
C	-3.984006	1.203859	0.143506
C	-4.922287	-2.921884	-0.099836
H	-2.772064	-3.128635	-0.034078
C	-5.807282	-0.656384	-0.018074
C	-2.512193	3.558567	0.367855
H	-0.750396	2.305570	0.351808
C	-4.659247	2.427008	0.205703
C	-6.010637	-2.038783	-0.092183
H	-5.097161	-3.992390	-0.153445
H	-6.655775	0.021930	-0.008454
C	-3.912009	3.604554	0.316229
H	-1.946210	4.481133	0.458827
H	-5.744415	2.467904	0.173027
H	-7.022027	-2.431716	-0.141787
H	-4.421442	4.562573	0.366895

***N*-Fmoc-cysteine methyl ester radical (8')**

C	-3.580127	-0.052469	-0.265637
C	-4.435491	1.214303	-0.156736
O	-4.176154	2.150621	0.578060
C	-4.362732	-1.267802	0.311032
S	-3.748046	-2.882438	-0.260642
O	-5.496635	1.147237	-0.958909
H	-4.361789	-1.211616	1.402431
H	-5.398367	-1.216650	-0.043718
N	-2.339735	0.210545	0.434770
H	-2.318119	1.005416	1.062870
C	-1.232562	-0.550103	0.285852
O	-1.158783	-1.545115	-0.436029
C	-6.411945	2.273058	-0.932529
H	-5.891219	3.181375	-1.239711
H	-7.195934	2.018082	-1.642416
H	-6.822112	2.395198	0.071181
O	-0.213155	-0.074016	1.039701
C	1.047265	-0.782552	0.972032
H	0.847702	-1.850029	0.868359
H	1.523529	-0.589247	1.934641
C	1.928685	-0.283016	-0.185271
C	3.233145	-1.065089	-0.255406
H	1.358891	-0.406066	-1.116006
C	2.419399	1.150553	-0.036396
C	3.429429	-2.435366	-0.410820
C	4.335449	-0.192285	-0.135935
C	1.687939	2.333562	0.051337
C	3.831109	1.182222	-0.001870
C	4.739853	-2.933829	-0.445684
H	2.586916	-3.114475	-0.510605
C	5.641979	-0.689998	-0.171866
C	2.374089	3.549597	0.183294
H	0.603209	2.320201	0.018658
C	4.514581	2.395399	0.128173
C	5.835001	-2.067293	-0.326207
H	4.906930	-3.999876	-0.568310
H	6.495878	-0.024289	-0.083361
C	3.774753	3.579036	0.222581
H	1.813952	4.477535	0.253379
H	5.600318	2.424617	0.152773
H	6.843770	-2.468891	-0.355607
H	4.290632	4.529582	0.323609
H	-3.380514	-0.233933	-1.326642

Cartesian Coordinates for Optimized Geometries in Gas-Phase at B3lyp/6-31+G(d,p) Level of Nitrogen Neutral Radical

(2*R*)-*N*-Ac-2-methylcysteine methyl ester radical (1')

C	0.029561	0.426220	0.184025
C	-1.157461	-0.549870	0.009512
O	-1.102777	-1.562725	-0.658417
C	-0.149243	1.498977	-0.937540
S	1.141576	2.798909	-1.015251
O	-2.273262	-0.110626	0.612727
H	-0.213670	0.998443	-1.906676
H	-1.087522	2.033115	-0.766826
H	2.176204	1.958819	-1.216167
N	1.288749	-0.248014	-0.054568
C	1.496543	-1.550737	0.391482
C	2.237872	-2.451022	-0.560629
O	1.188613	-1.864120	1.539351
H	2.390731	-3.425192	-0.093372
H	1.656049	-2.568281	-1.480667
H	3.202359	-2.006600	-0.826166
C	0.061455	1.076539	1.590304
H	0.097624	0.301920	2.356364
H	0.944222	1.711633	1.674593
H	-0.834116	1.688634	1.723680
C	-3.448191	-0.936562	0.450208
H	-3.261992	-1.934497	0.852108
H	-4.233305	-0.432047	1.011675
H	-3.712853	-1.013363	-0.606723

***N*-Ac-cysteine methyl ester radical (2')**

C	0.026633	0.476242	0.196194
C	-1.167880	-0.479886	0.009042
O	-1.099258	-1.585360	-0.483971
C	-0.209738	1.819522	-0.517561
S	1.089675	3.068626	-0.177511
O	-2.301172	0.078581	0.464148
H	0.118306	0.656272	1.279474
H	-0.295374	1.661296	-1.596239
H	-1.141799	2.262313	-0.162541
H	2.116906	2.334429	-0.650047
N	1.257020	-0.130878	-0.243719
C	1.644697	-1.329003	0.364494
C	2.238294	-2.359515	-0.557283
O	1.595884	-1.432431	1.586422
H	2.508209	-3.247213	0.016681
H	1.512167	-2.620753	-1.333273
H	3.125289	-1.949216	-1.051049
C	-3.496229	-0.728193	0.355251
H	-3.376824	-1.652345	0.924400
H	-4.294131	-0.115618	0.772320
H	-3.695133	-0.967146	-0.691602

(2*R*)-*N*-Piv-2-methylcysteine methyl ester radical (3')

C	-0.057841	0.132322	0.417272
C	-1.205955	-0.131559	-0.594291
O	-1.131806	-0.873623	-1.549183
C	0.074112	1.684328	0.605603
S	1.075894	2.275034	2.022248
O	-2.329058	0.523835	-0.245136
H	0.456837	2.106130	-0.326387
H	-0.922724	2.089527	0.785999
H	2.151133	1.487007	1.799896
N	1.140701	-0.334549	-0.265412
C	2.175090	-1.033969	0.313876
C	2.708085	-2.242053	-0.464650
O	2.713726	-0.582168	1.330199
C	-3.484310	0.287759	-1.079042
H	-3.750618	-0.771397	-1.063704
H	-4.279101	0.893780	-0.646153
H	-3.276690	0.594441	-2.106318
C	-0.405710	-0.611167	1.724157
H	-0.584254	-1.671727	1.519995
H	0.410280	-0.517867	2.440810
H	-1.307046	-0.182352	2.168252
C	1.531507	-3.153773	-0.875339
H	1.027925	-3.572502	0.003746
H	0.790440	-2.614716	-1.472390
H	1.909890	-3.991920	-1.470558
C	3.706604	-3.010040	0.416461
H	4.093008	-3.871766	-0.138513
H	4.548881	-2.378886	0.710721
H	3.231734	-3.378961	1.331218
C	3.420320	-1.707882	-1.732839
H	4.246427	-1.039219	-1.468938
H	3.832759	-2.550692	-2.298703
H	2.725567	-1.164252	-2.378334

***N*-Piv-cysteine methyl ester radical (4')**

C	0.080386	0.469342	0.239872
C	-1.101803	-0.472851	-0.054410
O	-1.030007	-1.506187	-0.684311
C	-0.091659	1.808253	-0.506333
S	1.152275	3.073678	-0.043896
O	-2.238591	0.021731	0.463688
H	0.072127	0.670562	1.321968
H	-0.066170	1.641063	-1.586625
H	-1.059408	2.243748	-0.250401
H	2.230556	2.341128	-0.387473
N	1.351677	-0.127742	-0.075922
C	1.632768	-1.395545	0.425929
C	2.492000	-2.311102	-0.449967
O	1.321588	-1.653810	1.588219
C	-3.430904	-0.767239	0.251729
H	-3.311321	-1.754042	0.703705
H	-4.232055	-0.212628	0.738096
H	-3.626194	-0.876625	-0.817243
C	3.972026	-1.982390	-0.128021
H	4.190367	-2.152595	0.930776
H	4.626370	-2.629380	-0.722908
H	4.210714	-0.941720	-0.369536
C	2.185917	-3.773765	-0.079678
H	2.829923	-4.441943	-0.661647
H	2.361338	-3.957355	0.983119
H	1.143594	-4.024528	-0.301037
C	2.212775	-2.065802	-1.945505
H	1.163704	-2.258547	-2.188222
H	2.450731	-1.037915	-2.236986
H	2.834539	-2.737617	-2.547714

(2*R*)-*N*-Boc-2-methylcysteine methyl ester radical (5')

C	-1.311567	0.238216	0.019749
C	-2.171474	-0.959990	-0.465290
O	-1.795806	-1.829423	-1.216435
C	-2.153105	1.548462	-0.175298
S	-1.470642	3.093275	0.536879
O	-3.393560	-0.942677	0.109508
H	-2.336596	1.683770	-1.243353
H	-3.112938	1.409155	0.324505
H	-0.297556	3.080203	-0.133525
N	-0.194239	0.309494	-0.909693
C	1.097017	0.601647	-0.483561
O	1.511705	1.752610	-0.456035
C	-4.255950	-2.053715	-0.214777
H	-3.795863	-2.993292	0.099485
H	-5.179147	-1.871586	0.334079
H	-4.443143	-2.085357	-1.290297
O	1.791041	-0.508655	-0.233131
C	3.262216	-0.491499	0.011302
C	3.564932	0.292663	1.290839
H	4.629415	0.193851	1.528358
H	3.330387	1.351859	1.175542
H	2.992829	-0.109904	2.132812
C	3.973397	0.084244	-1.215728
H	5.055580	-0.019248	-1.084533
H	3.686168	-0.465436	-2.117456
H	3.741313	1.141466	-1.354722
C	3.579389	-1.977191	0.185824
H	4.650723	-2.107880	0.367383
H	3.030373	-2.394037	1.035330
H	3.306034	-2.538774	-0.711923
C	-0.931942	-0.012708	1.493418
H	-0.379456	-0.951246	1.589778
H	-0.316177	0.808219	1.867805
H	-1.833554	-0.068023	2.108306

***N*-Boc-cysteine methyl ester radical (6')**

C	1.502247	0.721403	-0.092075
C	1.716003	-0.803637	-0.099393
O	0.926002	-1.621422	0.318703
C	2.538470	1.417519	0.813612
S	2.492877	3.247852	0.710136
O	2.916767	-1.108050	-0.624043
H	1.654177	1.069396	-1.126190
H	2.397461	1.102652	1.851146
H	3.544489	1.131524	0.501666
H	1.206702	3.377081	1.092555
N	0.169255	1.104359	0.295532
C	-0.886544	0.466407	-0.364045
O	-0.889178	0.320043	-1.579089
C	3.243870	-2.513996	-0.687332
H	2.513026	-3.041590	-1.303816
H	4.234505	-2.558380	-1.137651
H	3.253054	-2.945234	0.316099
O	-1.869967	0.194969	0.488607
C	-3.126112	-0.468958	0.052014
C	-2.805704	-1.824761	-0.583244
H	-3.741253	-2.365925	-0.760149
H	-2.286052	-1.708245	-1.535541
H	-2.182153	-2.423066	0.087401
C	-3.887861	0.462678	-0.895218
H	-4.868996	0.028560	-1.115417
H	-4.045851	1.439202	-0.426521
H	-3.350205	0.602031	-1.834469
C	-3.876129	-0.645160	1.373501
H	-4.844672	-1.120179	1.189706
H	-3.303484	-1.274662	2.060725
H	-4.048448	0.323216	1.852415

(2*R*)-*N*-Fmoc-2-methylcysteine methyl ester radical (7')

C	3.298907	-0.632259	0.603931
C	3.087143	0.861116	0.195291
O	2.692582	1.722306	0.950732
C	4.828948	-0.894908	0.540265
S	5.339771	-2.605949	0.967825
O	3.439691	1.074931	-1.078846
H	5.193830	-0.652354	-0.458461
H	5.340612	-0.251208	1.261672
H	4.698668	-3.200518	-0.059110
N	2.672777	-1.470776	-0.411685
C	1.291801	-1.643886	-0.406954
O	0.786876	-2.710030	-0.106387
C	2.718398	-0.858495	2.008446
H	1.661446	-0.586208	2.045215
H	2.831794	-1.906327	2.289831
H	3.249020	-0.233052	2.730236
C	3.275711	2.424626	-1.568200
H	3.896070	3.114134	-0.991425
H	3.596804	2.391377	-2.608244
H	2.228194	2.723719	-1.494057
O	0.622186	-0.560197	-0.849026
C	-0.795131	-0.745175	-1.130411
H	-0.939974	-1.770729	-1.473440
H	-1.007480	-0.046443	-1.941441
C	-1.685808	-0.457990	0.089045
C	-3.129434	-0.849034	-0.200911
H	-1.296883	-1.043675	0.932648
C	-1.817615	1.015540	0.453691
C	-3.645025	-2.089891	-0.564897
C	-3.979231	0.265548	-0.048928
C	-0.836780	1.923840	0.845179
C	-3.166896	1.420978	0.356955
C	-5.024141	-2.213727	-0.781161
H	-2.996715	-2.955969	-0.670492
C	-5.354504	0.139919	-0.264093
C	-1.211099	3.244229	1.131584
H	0.203700	1.630444	0.934576
C	-3.536892	2.737579	0.643630
C	-5.869237	-1.106758	-0.632875
H	-5.440849	-3.176526	-1.061828
H	-6.017626	0.992334	-0.145721
C	-2.548044	3.647289	1.029924
H	-0.453155	3.958005	1.440805
H	-4.574200	3.053076	0.572976
H	-6.936208	-1.219060	-0.802803
H	-2.820312	4.673798	1.258506

***N*-Fmoc-cysteine methyl ester radical (8')**

C	-3.605136	-0.688505	0.244662
C	-3.166443	0.430059	-0.719239
O	-2.094434	0.994903	-0.682813
C	-4.875568	-0.294635	1.023638
S	-5.565351	-1.657623	2.037154
O	-4.136934	0.700570	-1.606272
H	-4.671083	0.571839	1.658463
H	-5.663777	-0.024036	0.319217
H	-4.466629	-1.837769	2.797036
N	-2.559542	-1.072846	1.157398
C	-1.326052	-1.406133	0.596703
O	-1.223761	-2.150504	-0.367746
C	-3.843335	1.732622	-2.576441
H	-2.974869	1.448182	-3.173978
H	-4.735248	1.803859	-3.197049
H	-3.643999	2.679314	-2.070060
O	-0.317972	-0.928152	1.331744
C	1.025741	-1.289789	0.916730
H	1.006634	-2.311788	0.534483
H	1.613660	-1.245956	1.834985
C	1.590633	-0.325515	-0.139737
C	2.970664	-0.784254	-0.590597
H	0.891274	-0.302219	-0.985689
C	1.869977	1.078303	0.378163
C	3.347159	-1.988253	-1.179411
C	3.929496	0.215744	-0.325815
C	0.983945	2.022216	0.891488
C	3.247063	1.370606	0.274888
C	4.695157	-2.193019	-1.504173
H	2.611636	-2.758962	-1.395767
C	5.273124	0.010032	-0.650944
C	1.487134	3.259155	1.316831
H	-0.077859	1.808391	0.949799
C	3.745219	2.606026	0.697720
C	5.648259	-1.201507	-1.239923
H	5.002043	-3.126437	-1.966900
H	6.017859	0.776062	-0.453476
C	2.854677	3.546921	1.223049
H	0.807578	4.004717	1.719801
H	4.803937	2.837481	0.619094
H	6.689140	-1.374542	-1.498093
H	3.226030	4.511893	1.556442
H	-3.834426	-1.569112	-0.377477

Cartesian Coordinates for Optimized Geometries in Methanol at B3lyp/6-31+G(d,p) Level of Nitrogen Neutral Radical

(2*R*)-*N*-Ac-2-methylcysteine methyl ester radical (1')

C	0.038010	0.404180	0.223285
C	-1.127275	-0.612777	0.123198
O	-0.992378	-1.776018	-0.208164
C	-0.200716	1.482266	-0.877861
S	1.075189	2.794392	-0.996829
O	-2.299236	-0.044439	0.415357
H	-0.297545	0.996771	-1.851362
H	-1.134823	2.004419	-0.664455
H	2.089743	1.998450	-1.386517
N	1.308366	-0.232126	-0.037435
C	1.632037	-1.504532	0.413420
C	2.182509	-2.437237	-0.633720
O	1.621587	-1.761096	1.619087
H	2.055849	-3.468506	-0.298613
H	1.692630	-2.289650	-1.598953
H	3.252659	-2.235562	-0.758342
C	0.072192	1.040529	1.641995
H	0.159996	0.264141	2.402379
H	0.926803	1.714217	1.716024
H	-0.848857	1.607651	1.796167
C	-3.477168	-0.885986	0.321930
H	-3.398394	-1.714785	1.027419
H	-4.311687	-0.237095	0.579988
H	-3.582327	-1.267655	-0.694971

***N*-Ac-cysteine methyl ester radical (2')**

C	0.027024	0.467423	0.224696
C	-1.162856	-0.508732	0.084044
O	-1.053770	-1.673878	-0.245485
C	-0.231692	1.806539	-0.486403
S	1.072819	3.061933	-0.182444
O	-2.312773	0.092443	0.390620
H	0.135003	0.653089	1.306997
H	-0.342773	1.649592	-1.561725
H	-1.153696	2.248940	-0.108543
H	2.085741	2.382024	-0.754765
N	1.255377	-0.131609	-0.225710
C	1.684644	-1.321889	0.354137
C	2.226084	-2.349986	-0.600501
O	1.740055	-1.419303	1.581283
H	2.253604	-3.323980	-0.109166
H	1.621822	-2.399514	-1.509533
H	3.245303	-2.065625	-0.886333
C	-3.515070	-0.717846	0.317795
H	-3.445271	-1.548663	1.021729
H	-4.326584	-0.046340	0.590420
H	-3.647446	-1.094893	-0.697484

(2*R*)-*N*-Piv-2-methylcysteine methyl ester radical (3')

C	-0.043153	0.142413	0.381439
C	-1.191330	-0.063898	-0.649614
O	-1.057317	-0.527199	-1.764486
C	0.066316	1.699249	0.582876
S	1.082945	2.291594	1.989865
O	-2.361559	0.331134	-0.136538
H	0.428612	2.141013	-0.347059
H	-0.934845	2.083447	0.785173
H	2.171282	1.530820	1.735825
N	1.163205	-0.303589	-0.297600
C	2.218578	-0.976540	0.273656
C	2.704348	-2.235024	-0.455660
O	2.816853	-0.468834	1.231082
C	-3.528123	0.185536	-0.984177
H	-3.669918	-0.864228	-1.246578
H	-4.361326	0.550199	-0.386605
H	-3.409091	0.784466	-1.888713
C	-0.377402	-0.616496	1.679578
H	-0.570076	-1.671533	1.464929
H	0.452557	-0.544097	2.383012
H	-1.266428	-0.188927	2.146369
C	1.500885	-3.092881	-0.899383
H	0.931150	-3.457499	-0.037741
H	0.823256	-2.532771	-1.550356
H	1.862224	-3.964812	-1.454389
C	3.622959	-3.040854	0.478226
H	3.978143	-3.933027	-0.047866
H	4.491686	-2.454991	0.788882
H	3.091389	-3.366613	1.378230
C	3.499545	-1.766050	-1.701713
H	4.348537	-1.136945	-1.415261
H	3.887691	-2.643424	-2.230131
H	2.864216	-1.202515	-2.390707

***N*-Piv-cysteine methyl ester radical (4')**

C	0.074372	0.449044	0.271938
C	-1.108968	-0.501118	-0.003991
O	-1.012581	-1.589904	-0.535523
C	-0.096048	1.778342	-0.492508
S	1.155805	3.046574	-0.057084
O	-2.254522	0.043592	0.414317
H	0.058849	0.669534	1.351365
H	-0.075493	1.599821	-1.569874
H	-1.059078	2.221841	-0.236760
H	2.231714	2.370110	-0.504248
N	1.349754	-0.147469	-0.017457
C	1.655300	-1.410508	0.465939
C	2.498232	-2.309609	-0.442725
O	1.391063	-1.679301	1.641815
C	-3.463475	-0.730124	0.204195
H	-3.395406	-1.678507	0.739671
H	-4.267481	-0.116618	0.605668
H	-3.609343	-0.910557	-0.862104
C	3.983874	-1.983463	-0.138941
H	4.222493	-2.174465	0.911925
H	4.626018	-2.618820	-0.758313
H	4.217333	-0.938474	-0.365626
C	2.205443	-3.781744	-0.099705
H	2.836040	-4.431080	-0.715769
H	2.414384	-3.994821	0.951711
H	1.159046	-4.033522	-0.300599
C	2.198286	-2.035886	-1.929311
H	1.149256	-2.236763	-2.165221
H	2.421315	-0.999840	-2.202638
H	2.821080	-2.688089	-2.550879

(2*R*)-*N*-Boc-2-methylcysteine methyl ester radical (5')

C	-1.300745	0.243500	-0.002006
C	-2.174622	-0.942287	-0.497439
O	-1.831335	-1.756472	-1.331012
C	-2.159532	1.548741	-0.153974
S	-1.467649	3.090597	0.558281
O	-3.345274	-0.978518	0.149310
H	-2.380602	1.702649	-1.211736
H	-3.099799	1.394777	0.376969
H	-0.323055	3.115160	-0.157429
N	-0.201548	0.340834	-0.954258
C	1.099112	0.627159	-0.541248
O	1.517679	1.779212	-0.538378
C	-4.235174	-2.075923	-0.173255
H	-3.754452	-3.026937	0.062707
H	-5.114264	-1.922552	0.449649
H	-4.500023	-2.043034	-1.231394
O	1.780477	-0.481659	-0.282864
C	3.254587	-0.487360	0.012414
C	3.517230	0.298463	1.297652
H	4.569112	0.179210	1.575737
H	3.311969	1.362140	1.167802
H	2.903975	-0.087501	2.117485
C	4.010083	0.070260	-1.194244
H	5.084542	-0.053251	-1.026359
H	3.743164	-0.478398	-2.102668
H	3.804676	1.131572	-1.343951
C	3.538771	-1.976185	0.204845
H	4.600462	-2.118661	0.426470
H	2.954454	-2.379456	1.037007
H	3.295616	-2.538362	-0.701427
C	-0.889691	-0.033685	1.457867
H	-0.353620	-0.982852	1.533760
H	-0.247092	0.767624	1.828958
H	-1.777626	-0.080311	2.091875

***N*-Boc-cysteine methyl ester radical (6')**

C	1.507116	0.695066	-0.127191
C	1.747128	-0.828415	-0.101075
O	0.928991	-1.648070	0.268216
C	2.545795	1.438843	0.735149
S	2.450473	3.265829	0.590423
O	2.973930	-1.120408	-0.539612
H	1.633906	1.010604	-1.175534
H	2.442671	1.150622	1.783769
H	3.550434	1.173995	0.403740
H	1.213368	3.403298	1.106203
N	0.170867	1.058188	0.269551
C	-0.893649	0.435574	-0.390586
O	-0.927253	0.347127	-1.613125
C	3.343642	-2.523261	-0.564886
H	2.669842	-3.073111	-1.223959
H	4.361320	-2.542181	-0.949460
H	3.302833	-2.937073	0.443986
O	-1.850795	0.117062	0.471915
C	-3.154952	-0.481229	0.045631
C	-2.907040	-1.805689	-0.678214
H	-3.870607	-2.287390	-0.872067
H	-2.398698	-1.654454	-1.631779
H	-2.308628	-2.478791	-0.057222
C	-3.912673	0.533195	-0.813440
H	-4.919859	0.151432	-1.008219
H	-4.006725	1.487854	-0.286744
H	-3.415310	0.700520	-1.770189
C	-3.859450	-0.706959	1.383422
H	-4.846778	-1.143822	1.208509
H	-3.284542	-1.391294	2.014221
H	-3.989063	0.238564	1.918192

(2*R*)-*N*-Fmoc-2-methylcysteine methyl ester radical (7')

C	3.302492	-0.645313	0.604783
C	3.118565	0.868732	0.251650
O	2.780034	1.710821	1.057389
C	4.832363	-0.913339	0.548113
S	5.331511	-2.646814	0.897102
O	3.426914	1.114621	-1.022102
H	5.217931	-0.628163	-0.431046
H	5.335631	-0.309278	1.307037
H	4.821221	-3.185461	-0.228041
N	2.676927	-1.429970	-0.453743
C	1.301341	-1.639834	-0.445083
O	0.834329	-2.735637	-0.173645
C	2.706885	-0.920883	1.993486
H	1.652832	-0.638158	2.035586
H	2.802861	-1.980957	2.233065
H	3.244352	-0.338740	2.745163
C	3.336113	2.494448	-1.462070
H	4.037899	3.111126	-0.898064
H	3.601958	2.473226	-2.516986
H	2.317929	2.861780	-1.325214
O	0.601867	-0.570841	-0.851958
C	-0.818043	-0.769265	-1.133011
H	-0.958713	-1.802705	-1.450360
H	-1.028691	-0.093597	-1.962930
C	-1.702201	-0.449737	0.082405
C	-3.148322	-0.852363	-0.181921
H	-1.306966	-1.006728	0.942440
C	-1.835478	1.032584	0.410025
C	-3.665068	-2.102350	-0.514252
C	-4.001657	0.261439	-0.038894
C	-0.852959	1.956677	0.759623
C	-3.188519	1.429761	0.327682
C	-5.047874	-2.235529	-0.705646
H	-3.016782	-2.968234	-0.618774
C	-5.380743	0.127661	-0.228712
C	-1.228592	3.283026	1.019223
H	0.189791	1.667586	0.834412
C	-3.561889	2.751680	0.589022
C	-5.896321	-1.128947	-0.564433
H	-5.464418	-3.204918	-0.962718
H	-6.045052	0.979933	-0.117503
C	-2.570550	3.676528	0.933872
H	-0.470068	4.010983	1.292016
H	-4.601819	3.060222	0.529285
H	-6.965285	-1.248685	-0.715063
H	-2.844045	4.707257	1.140357

***N*-Fmoc-cysteine methyl ester radical (8')**

C	-3.612599	-0.694236	0.219252
C	-3.184320	0.444102	-0.732397
O	-2.060346	0.903966	-0.782472
C	-4.891444	-0.346116	1.002647
S	-5.545287	-1.742744	1.997298
O	-4.204384	0.835623	-1.496326
H	-4.715674	0.513938	1.652565
H	-5.687417	-0.089324	0.303262
H	-4.493139	-1.852954	2.831610
N	-2.556682	-1.078688	1.119500
C	-1.328772	-1.433977	0.564321
O	-1.228061	-2.229643	-0.360952
C	-3.935746	1.892212	-2.455207
H	-3.170173	1.565762	-3.160843
H	-4.883053	2.062381	-2.962561
H	-3.607479	2.792417	-1.933404
O	-0.318354	-0.922254	1.272304
C	1.032869	-1.302537	0.888558
H	1.013454	-2.329145	0.521163
H	1.601904	-1.252858	1.817929
C	1.621976	-0.354263	-0.168310
C	3.016783	-0.811449	-0.575081
H	0.948073	-0.350096	-1.035058
C	1.878560	1.062234	0.327901
C	3.417485	-2.026180	-1.126092
C	3.961136	0.203367	-0.312285
C	0.974590	2.010404	0.802779
C	3.255448	1.365520	0.247287
C	4.775342	-2.225283	-1.414793
H	2.695859	-2.810538	-1.338493
C	5.314823	0.004452	-0.601695
C	1.457317	3.262330	1.211184
H	-0.086613	1.789256	0.846481
C	3.734780	2.615200	0.652728
C	5.714106	-1.218075	-1.153080
H	5.101152	-3.166889	-1.846798
H	6.047945	0.781685	-0.405375
C	2.824842	3.560358	1.138589
H	0.762953	4.010098	1.583457
H	4.792690	2.854500	0.591037
H	6.762063	-1.387392	-1.383087
H	3.181007	4.535800	1.457375
H	-3.821988	-1.563625	-0.427031

Cartesian Coordinates for Optimized Geometries in Water at B3lyp/6-31+G(d,p) Level of Nitrogen Neutral Radical

(2*R*)-*N*-Ac-2-methylcysteine methyl ester radical (1')

C	0.038844	0.403887	0.225455
C	-1.125691	-0.614315	0.127185
O	-0.988271	-1.781408	-0.189594
C	-0.200722	1.482963	-0.874396
S	1.075958	2.794278	-0.993930
O	-2.299257	-0.043009	0.405623
H	-0.299062	0.998626	-1.848256
H	-1.134171	2.005447	-0.659293
H	2.087009	2.000425	-1.396637
N	1.309717	-0.231089	-0.034958
C	1.636718	-1.502820	0.414540
C	2.177903	-2.436996	-0.636171
O	1.637483	-1.757919	1.620789
H	2.050732	-3.467955	-0.300212
H	1.682543	-2.288168	-1.598374
H	3.247815	-2.238234	-0.767333
C	0.071907	1.038936	1.645041
H	0.162366	0.262215	2.404802
H	0.924484	1.715198	1.719215
H	-0.850845	1.603015	1.800128
C	-3.476921	-0.885473	0.315264
H	-3.402750	-1.705375	1.031558
H	-4.312783	-0.233251	0.560114
H	-3.575840	-1.279424	-0.697534

***N*-Ac-cysteine methyl ester radical (2')**

C	0.027580	0.467341	0.226990
C	-1.161837	-0.510077	0.088867
O	-1.050397	-1.678492	-0.228434
C	-0.232211	1.806528	-0.483385
S	1.072461	3.062054	-0.180305
O	-2.313219	0.093367	0.383922
H	0.136408	0.652877	1.309325
H	-0.344292	1.650046	-1.558609
H	-1.153815	2.248662	-0.104378
H	2.084074	2.385527	-0.758863
N	1.255806	-0.131081	-0.224257
C	1.687275	-1.321087	0.353740
C	2.223261	-2.349943	-0.603140
O	1.749595	-1.417902	1.580818
H	2.247316	-3.324876	-0.113421
H	1.618231	-2.395570	-1.511829
H	3.243497	-2.069493	-0.889225
C	-3.515120	-0.717905	0.313344
H	-3.448970	-1.541027	1.026601
H	-4.328108	-0.043662	0.574474
H	-3.641992	-1.105561	-0.698604

**(2*R*)-*N*-Piv-2-methylcysteine methyl ester
radical (3')**

C	-0.042513	0.143208	0.380777
C	-1.190379	-0.060772	-0.651328
O	-1.054223	-0.511519	-1.771206
C	0.066429	1.700278	0.582104
S	1.084394	2.292821	1.988152
O	-2.362077	0.322695	-0.133680
H	0.427721	2.142408	-0.348010
H	-0.934681	2.084081	0.785457
H	2.172633	1.532286	1.732958
N	1.164124	-0.302516	-0.297854
C	2.219452	-0.975623	0.273305
C	2.703798	-2.235207	-0.455075
O	2.819167	-0.467068	1.229493
C	-3.528683	0.180732	-0.982128
H	-3.665313	-0.866742	-1.256064
H	-4.363182	0.534379	-0.379822
H	-3.413368	0.790627	-1.879782
C	-0.376781	-0.615607	1.678794
H	-0.570905	-1.670311	1.464109
H	0.453832	-0.544481	2.381591
H	-1.264918	-0.187134	2.146366
C	1.499682	-3.091669	-0.899674
H	0.929010	-3.456078	-0.038640
H	0.822935	-2.530571	-1.550760
H	1.860480	-3.963594	-1.455003
C	3.620642	-3.042017	0.479703
H	3.974507	-3.935062	-0.045750
H	4.490360	-2.457485	0.790167
H	3.088063	-3.366380	1.379612
C	3.500672	-1.767651	-1.700643
H	4.350211	-1.139459	-1.413816
H	3.888116	-2.645756	-2.228315
H	2.866603	-1.203687	-2.390476

***N*-Piv-cysteine methyl ester radical (4')**

C	0.074558	0.448486	0.274207
C	-1.108024	-0.503325	0.000069
O	-1.009309	-1.596355	-0.522496
C	-0.097025	1.777036	-0.491258
S	1.154786	3.046143	-0.058214
O	-2.254960	0.044383	0.409703
H	0.058809	0.670023	1.353502
H	-0.077311	1.597693	-1.568452
H	-1.059962	2.220316	-0.235008
H	2.230083	2.373373	-0.512290
N	1.350415	-0.147191	-0.014214
C	1.658325	-1.409469	0.468832
C	2.498330	-2.308820	-0.442330
O	1.399217	-1.677454	1.646232
C	-3.463615	-0.730184	0.200077
H	-3.398215	-1.674888	0.742322
H	-4.268802	-0.113507	0.594184
H	-3.605334	-0.917489	-0.865572
C	3.984946	-1.985831	-0.139788
H	4.224458	-2.178767	0.910523
H	4.625102	-2.621537	-0.760824
H	4.220109	-0.940981	-0.365376
C	2.203443	-3.780993	-0.101103
H	2.832087	-4.430367	-0.719081
H	2.413728	-3.996163	0.949638
H	1.156357	-4.030720	-0.300999
C	2.197286	-2.032507	-1.928175
H	1.147714	-2.231409	-2.163342
H	2.421638	-0.996451	-2.200307
H	2.818430	-2.684867	-2.551194

**(2*R*)-*N*-Boc-2-methylcysteine methyl ester
radical (5')**

C	-1.300430	0.246007	-0.002305
C	-2.172605	-0.941461	-0.496906
O	-1.827737	-1.755213	-1.330615
C	-2.161555	1.549568	-0.154198
S	-1.470586	3.093233	0.555136
O	-3.342508	-0.979627	0.150001
H	-2.384890	1.702193	-1.211651
H	-3.100567	1.394851	0.378713
H	-0.326929	3.118542	-0.161958
N	-0.201886	0.344996	-0.955417
C	1.099306	0.629541	-0.542378
O	1.518664	1.781366	-0.538118
C	-4.231087	-2.078807	-0.171294
H	-3.748326	-3.028820	0.064405
H	-5.109532	-1.926706	0.452737
H	-4.497343	-2.046232	-1.229073
O	1.779513	-0.480201	-0.286044
C	3.253570	-0.488313	0.011901
C	3.514655	0.295067	1.298851
H	4.565736	0.173497	1.578863
H	3.311643	1.359327	1.170228
H	2.898928	-0.091069	2.116711
C	4.011656	0.070229	-1.192627
H	5.085622	-0.055052	-1.023069
H	3.745627	-0.476651	-2.102394
H	3.808014	1.132082	-1.340953
C	3.535257	-1.977800	0.202440
H	4.596321	-2.121972	0.425810
H	2.948886	-2.381551	1.032923
H	3.293242	-2.538196	-0.705264
C	-0.888120	-0.030136	1.457392
H	-0.351305	-0.978823	1.533643
H	-0.245796	0.771744	1.827711
H	-1.775634	-0.077120	2.091942

***N*-Boc-cysteine methyl ester radical (6')**

C	1.507112	0.692705	-0.129680
C	1.749610	-0.830582	-0.103938
O	0.929125	-1.652070	0.256463
C	2.546297	1.439419	0.729342
S	2.445559	3.266141	0.584432
O	2.980040	-1.119961	-0.532740
H	1.630879	1.007279	-1.178738
H	2.447287	1.151431	1.778387
H	3.550604	1.177234	0.395011
H	1.212727	3.401833	1.110744
N	0.170994	1.053389	0.269538
C	-0.894385	0.432726	-0.390971
O	-0.930090	0.348504	-1.613831
C	3.352506	-2.522263	-0.557949
H	2.684991	-3.071858	-1.223559
H	4.373213	-2.538472	-0.934445
H	3.304563	-2.937985	0.449790
O	-1.850204	0.111518	0.471982
C	-3.157273	-0.481690	0.046021
C	-2.914358	-1.805128	-0.681196
H	-3.879802	-2.282225	-0.876945
H	-2.404854	-1.653474	-1.634098
H	-2.319481	-2.482562	-0.061517
C	-3.913054	0.537056	-0.809541
H	-4.921868	0.158972	-1.002864
H	-4.002840	1.491003	-0.280827
H	-3.417244	0.704469	-1.767068
C	-3.860566	-0.708331	1.384247
H	-4.849232	-1.142188	1.209547
H	-3.286835	-1.395663	2.012882
H	-3.987124	0.236400	1.921146

(2*R*)-*N*-Fmoc-2-methylcysteine methyl ester radical (7')

C	3.303710	-0.646853	0.605215
C	3.120379	0.868959	0.258953
O	2.783825	1.707677	1.069145
C	4.833334	-0.915582	0.545493
S	5.331378	-2.651642	0.883441
O	3.426394	1.120125	-1.014114
H	5.218562	-0.625095	-0.432221
H	5.337687	-0.316348	1.307459
H	4.827643	-3.181989	-0.248523
N	2.676026	-1.426203	-0.456003
C	1.300710	-1.637808	-0.445124
O	0.835774	-2.733653	-0.169494
C	2.709858	-0.928088	1.993520
H	1.655930	-0.645279	2.038420
H	2.805778	-1.989198	2.228522
H	3.248808	-0.349497	2.746854
C	3.337801	2.502337	-1.447751
H	4.041714	3.114742	-0.881812
H	3.602276	2.485340	-2.503061
H	2.320515	2.870956	-1.307928
O	0.599598	-0.571614	-0.855188
C	-0.820620	-0.772351	-1.133880
H	-0.960733	-1.806895	-1.447797
H	-1.032668	-0.099586	-1.965763
C	-1.703503	-0.449480	0.081583
C	-3.149928	-0.852865	-0.180038
H	-1.307336	-1.003889	0.942829
C	-1.836468	1.033781	0.405042
C	-3.667083	-2.103819	-0.508163
C	-4.003146	0.261354	-0.039256
C	-0.853550	1.958877	0.750906
C	-3.189587	1.430771	0.322960
C	-5.050155	-2.237554	-0.697493
H	-3.018966	-2.970004	-0.611169
C	-5.382498	0.127067	-0.227033
C	-1.228834	3.286052	1.006891
H	0.189182	1.669694	0.825512
C	-3.562669	2.753511	0.580745
C	-5.898476	-1.130559	-0.558448
H	-5.466985	-3.207667	-0.951339
H	-6.046678	0.979665	-0.117599
C	-2.570906	3.679363	0.921774
H	-0.470038	4.014915	1.276506
H	-4.602623	3.061969	0.521131
H	-6.967611	-1.250732	-0.707475
H	-2.844131	4.710739	1.125338

***N*-Fmoc-cysteine methyl ester radical (8')**

C	-3.612059	-0.695038	0.217225
C	-3.183223	0.444402	-0.733229
O	-2.055805	0.895192	-0.790734
C	-4.892460	-0.350247	0.999267
S	-5.544278	-1.749076	1.992296
O	-4.205938	0.846494	-1.487440
H	-4.719624	0.509703	1.650018
H	-5.688220	-0.094912	0.299184
H	-4.495548	-1.854364	2.831507
N	-2.556545	-1.079238	1.118005
C	-1.328609	-1.436236	0.564134
O	-1.227574	-2.235006	-0.358507
C	-3.936946	1.903963	-2.445443
H	-3.179499	1.573739	-3.158041
H	-4.886920	2.082605	-2.944775
H	-3.598117	2.800147	-1.923518
O	-0.318406	-0.922584	1.271040
C	1.033228	-1.303575	0.889139
H	1.014179	-2.330719	0.523300
H	1.601414	-1.252561	1.818945
C	1.622953	-0.356699	-0.168585
C	3.018469	-0.813419	-0.573526
H	0.949964	-0.354505	-1.036062
C	1.877959	1.060931	0.325309
C	3.420703	-2.028931	-1.121750
C	3.961680	0.202928	-0.312439
C	0.972953	2.009091	0.798354
C	3.254588	1.365486	0.244550
C	4.778938	-2.227205	-1.409384
H	2.700085	-2.814588	-1.332685
C	5.315747	0.004895	-0.600835
C	1.454295	3.262305	1.204580
H	-0.088037	1.786970	0.842513
C	3.732586	2.616435	0.647766
C	5.716556	-1.218414	-1.149456
H	5.105940	-3.169429	-1.839125
H	6.047959	0.783295	-0.405783
C	2.821553	3.561612	1.131650
H	0.759088	4.009996	1.575412
H	4.790265	2.856671	0.585924
H	6.764789	-1.387130	-1.378615
H	3.176652	4.538002	1.448694
H	-3.819115	-1.563645	-0.430993

Cartesian Coordinates for Optimized Geometries in Gas-phase at B3lyp/6-31+G(d,p) Level of C[•] Neutral Radical

***N*-Ac-cysteine methyl ester radical (2')**

C	-0.278524	-0.004263	-0.298087
C	-1.611663	-0.585911	-0.207911
O	-1.825326	-1.794673	-0.316301
C	0.004170	1.442962	-0.137405
S	0.530283	1.904269	1.595801
O	-2.585719	0.329055	-0.006971
H	0.787255	1.782839	-0.813086
H	-0.909564	2.008939	-0.312587
H	1.803496	1.485969	1.444845
N	0.694923	-0.964333	-0.486695
H	0.302670	-1.900513	-0.557474
C	2.070236	-0.825260	-0.567088
C	2.829493	-2.112505	-0.820968
O	2.640193	0.254817	-0.445143
H	3.377568	-2.013955	-1.762832
H	3.568349	-2.244984	-0.025620
H	2.192639	-2.999249	-0.870860
C	-3.922783	-0.193997	0.098442
H	-3.992944	-0.891454	0.936466
H	-4.558492	0.674807	0.265777
H	-4.204706	-0.708538	-0.823407

N-Piv-cysteine methyl ester radical (4')

C	-0.306945	0.092361	-0.671431
C	-1.371402	-0.574016	0.080655
O	-1.454056	-1.779231	0.256362
C	-0.447037	1.454461	-1.245631
S	0.276690	2.791021	-0.149798
O	-2.308743	0.313077	0.508551
H	0.030855	1.528532	-2.228080
H	-1.495269	1.734901	-1.344981
H	1.529987	2.293658	-0.125822
N	0.864306	-0.601057	-0.930110
H	1.301535	-0.438207	-1.827647
C	1.576896	-1.380631	-0.006734
C	2.686096	-2.286280	-0.584355
O	1.298789	-1.363675	1.178516
C	-3.414855	-0.258166	1.228525
H	-3.057390	-0.785706	2.115997
H	-4.043840	0.586282	1.509541
H	-3.966449	-0.957056	0.594120
C	3.846580	-2.325911	0.429076
H	3.486884	-2.618388	1.417337
H	4.603247	-3.045826	0.099486
H	4.327183	-1.345479	0.521775
C	2.060698	-3.697306	-0.720118
H	2.814226	-4.400596	-1.092313
H	1.698641	-4.053361	0.247973
H	1.216716	-3.696319	-1.417674
C	3.219110	-1.826775	-1.956921
H	2.460405	-1.889185	-2.746392
H	3.619185	-0.805908	-1.923754
H	4.040196	-2.482381	-2.264296

N-Boc-cysteine methyl ester radical (6')

C	1.515839	0.141579	0.658051
C	2.041932	-1.042620	-0.019239
O	1.447029	-2.102309	-0.140255
C	2.375833	1.246595	1.153154
S	2.462301	2.695685	-0.030895
O	3.315881	-0.843688	-0.454471
H	2.030043	1.623458	2.121328
H	3.411449	0.923943	1.253407
H	1.140887	2.965324	-0.021068
N	0.161637	0.219107	0.926561
H	-0.135623	0.624892	1.806149
C	-0.872545	-0.153980	0.063048
O	-0.731502	-0.396319	-1.114909
C	3.928000	-1.972220	-1.101767
H	3.343538	-2.272424	-1.974752
H	4.919224	-1.631606	-1.400444
H	4.001155	-2.817477	-0.412265
O	-2.023192	-0.145394	0.769563
C	-3.322227	-0.445863	0.121238
C	-3.307896	-1.879013	-0.418889
H	-4.307321	-2.135566	-0.785997
H	-2.595205	-1.990344	-1.237122
H	-3.045142	-2.583787	0.376168
C	-3.613608	0.590536	-0.968552
H	-4.625708	0.431855	-1.355468
H	-3.564762	1.604042	-0.556730
H	-2.908216	0.507688	-1.796482
C	-4.308072	-0.308957	1.283586
H	-5.324050	-0.517419	0.934648
H	-4.064389	-1.015321	2.082756
H	-4.284825	0.704504	1.695898

N-Fmoc-cysteine methyl ester radical (8')

C	-3.631817	0.049901	0.112068
C	-4.544233	1.161698	0.335437
O	-4.216582	2.192473	0.924499
C	-3.987908	-1.177291	-0.640598
S	-3.465587	-1.128561	-2.436588
O	-5.785490	0.944635	-0.157545
H	-3.546604	-2.070501	-0.201031
H	-5.071742	-1.277260	-0.667894
H	-2.182061	-1.467837	-2.201390
N	-2.368419	0.307207	0.605859
H	-2.278533	1.210907	1.065762
C	-1.248904	-0.492895	0.566108
O	-1.176223	-1.601360	0.060403
C	-6.726365	2.017796	0.030301
H	-6.367222	2.927760	-0.456174
H	-7.651164	1.673186	-0.431238
H	-6.874423	2.213219	1.095186
O	-0.229700	0.151726	1.180858
C	1.036121	-0.550516	1.243468
H	0.836874	-1.612925	1.394381
H	1.535043	-0.135817	2.120933
C	1.885038	-0.335834	-0.020371
C	3.171776	-1.146795	0.046757
H	1.282663	-0.647436	-0.884183
C	2.405960	1.083494	-0.199294
C	3.336444	-2.522101	0.186176
C	4.292074	-0.296350	-0.055751
C	1.699793	2.274752	-0.346597
C	3.817656	1.086178	-0.210031
C	4.634448	-3.049033	0.227089
H	2.477297	-3.184712	0.252640
C	5.585675	-0.823902	-0.016552
C	2.410952	3.472688	-0.498147
H	0.614507	2.282069	-0.343919
C	4.525243	2.281498	-0.362883
C	5.747749	-2.205230	0.127549
H	4.777671	-4.120389	0.332508
H	6.454507	-0.176839	-0.098521
C	3.811217	3.474841	-0.505248
H	1.870141	4.407411	-0.613706
H	5.611628	2.288731	-0.374305
H	6.747405	-2.628963	0.159205
H	4.347193	4.411868	-0.625996

Cartesian Coordinates for Optimized Geometries in Methanol at B3lyp/6-31+G(d,p) Level of C[•] Neutral Radical

N-Ac-cysteine methyl ester radical (2')

C	-0.271487	-0.022583	-0.286954
C	-1.608526	-0.596580	-0.198348
O	-1.830631	-1.806836	-0.305414
C	0.002488	1.428999	-0.154058
S	0.477449	1.941616	1.581449
O	-2.571633	0.323779	0.003225
H	0.801341	1.753470	-0.817501
H	-0.905071	1.991451	-0.366894
H	1.723386	1.429108	1.529691
N	0.707647	-0.975414	-0.470931
H	0.330129	-1.915416	-0.563405
C	2.082238	-0.833796	-0.535538
C	2.845279	-2.103368	-0.837837
O	2.645326	0.250164	-0.371829
H	3.241262	-2.038514	-1.856886
H	3.695179	-2.173498	-0.154892
H	2.239056	-3.007771	-0.756440
C	-3.924711	-0.171895	0.094658
H	-4.017309	-0.866185	0.932410
H	-4.542010	0.709863	0.257997
H	-4.207848	-0.672571	-0.833609

N-Piv-cysteine methyl ester radical (4')

C	-0.333206	0.034591	-0.651653
C	-1.404133	-0.581971	0.129629
O	-1.534030	-1.786880	0.322279
C	-0.465321	1.382217	-1.264530
S	0.280663	2.734265	-0.201757
O	-2.290294	0.341212	0.574449
H	0.016373	1.428845	-2.244169
H	-1.509764	1.670696	-1.372174
H	1.567938	2.366599	-0.358883
N	0.819768	-0.683545	-0.917928
H	1.260695	-0.503281	-1.811862
C	1.548129	-1.445115	-0.005955
C	2.699238	-2.294160	-0.583718
O	1.253238	-1.459446	1.184108
C	-3.442398	-0.165631	1.279140
H	-3.131832	-0.706492	2.175668
H	-4.025854	0.713936	1.547010
H	-4.022855	-0.828044	0.632918
C	3.833455	-2.346845	0.458744
H	3.471239	-2.727033	1.416276
H	4.629195	-3.007120	0.099717
H	4.264733	-1.353824	0.625528
C	2.125125	-3.717437	-0.803076
H	2.914281	-4.373552	-1.185265
H	1.752223	-4.138467	0.135335
H	1.306562	-3.711463	-1.530352
C	3.256988	-1.755327	-1.917381
H	2.528477	-1.812744	-2.733947
H	3.612253	-0.722681	-1.826270
H	4.111351	-2.368470	-2.220025

N-Boc-cysteine methyl ester radical (6')

C	1.511887	0.097237	0.642509
C	2.081520	-1.065229	-0.031127
O	1.533734	-2.159458	-0.135595
C	2.342576	1.226078	1.137356
S	2.413192	2.656218	-0.071853
O	3.330126	-0.813118	-0.495000
H	1.968300	1.614718	2.087748
H	3.382263	0.928936	1.264031
H	1.123383	3.027901	0.050676
N	0.160749	0.127984	0.926185
H	-0.133813	0.603993	1.772015
C	-0.875295	-0.248868	0.071266
O	-0.729467	-0.532782	-1.104013
C	4.019360	-1.923106	-1.105669
H	3.461717	-2.286969	-1.971293
H	4.986282	-1.527633	-1.413155
H	4.149090	-2.734028	-0.385194
O	-2.023851	-0.212502	0.765219
C	-3.346679	-0.448873	0.122098
C	-3.407683	-1.880791	-0.414834
H	-4.424369	-2.088284	-0.763300
H	-2.718735	-2.026761	-1.248021
H	-3.167146	-2.596824	0.377236
C	-3.589179	0.603193	-0.962775
H	-4.612775	0.500034	-1.336474
H	-3.478376	1.611369	-0.551083
H	-2.901712	0.482314	-1.801346
C	-4.314232	-0.261492	1.291930
H	-5.341005	-0.414738	0.947300
H	-4.104964	-0.982613	2.087678
H	-4.234432	0.748996	1.703735

N-Fmoc-cysteine methyl ester radical (8')

C	-3.621894	0.068823	0.122508
C	-4.502152	1.214672	0.295296
O	-4.143390	2.264580	0.838986
C	-4.034269	-1.190477	-0.542865
S	-3.592857	-1.258637	-2.361395
O	-5.743548	1.010864	-0.189543
H	-3.593219	-2.065259	-0.069199
H	-5.119484	-1.272195	-0.522668
H	-2.277809	-1.487674	-2.175130
N	-2.347784	0.300253	0.596172
H	-2.217824	1.212983	1.026542
C	-1.250899	-0.532601	0.568952
O	-1.211412	-1.647449	0.069101
C	-6.676708	2.102902	-0.043447
H	-6.310098	2.987012	-0.569166
H	-7.603961	1.748729	-0.490680
H	-6.824530	2.335703	1.013220
O	-0.219164	0.084122	1.182691
C	1.043592	-0.628117	1.229308
H	0.840329	-1.692909	1.350677
H	1.540894	-0.242499	2.120326
C	1.892145	-0.375858	-0.027952
C	3.195953	-1.160677	0.031108
H	1.300177	-0.683207	-0.900344
C	2.383887	1.056663	-0.184899
C	3.390673	-2.534513	0.152826
C	4.299007	-0.285152	-0.056052
C	1.652990	2.235231	-0.322143
C	3.795854	1.089540	-0.191894
C	4.700821	-3.033477	0.188972
H	2.547521	-3.217384	0.212749
C	5.605151	-0.783699	-0.021309
C	2.340384	3.450220	-0.457037
H	0.567782	2.220357	-0.326340
C	4.480482	2.301288	-0.328393
C	5.796861	-2.164129	0.103487
H	4.866859	-4.102684	0.281584
H	6.459614	-0.116512	-0.090693
C	3.741469	3.481987	-0.458775
H	1.780665	4.374816	-0.564169
H	5.566410	2.331064	-0.337021
H	6.805318	-2.566499	0.132196
H	4.258255	4.431289	-0.566365

Cartesian Coordinates for Optimized Geometries in Water at B3lyp/6-31+G(d,p) Level of C^α Neutral Radical

N-Ac-cysteine methyl ester radical (2')

C	-0.271081	-0.023273	-0.286236
C	-1.608237	-0.596942	-0.197524
O	-1.830765	-1.807211	-0.304419
C	0.002653	1.428502	-0.155028
S	0.475048	1.943908	1.580424
O	-2.570960	0.323682	0.004208
H	0.802278	1.751948	-0.818005
H	-0.904560	1.990742	-0.369880
H	1.719129	1.426468	1.533754
N	0.708199	-0.975870	-0.470117
H	0.331148	-1.915926	-0.563951
C	2.082765	-0.834201	-0.533599
C	2.845810	-2.102927	-0.838734
O	2.645687	0.249622	-0.367176
H	3.233430	-2.039949	-1.861164
H	3.701016	-2.170079	-0.162231
H	2.241585	-3.008021	-0.750713
C	-3.924563	-0.171045	0.094365
H	-4.018270	-0.865951	0.931471
H	-4.541299	0.711014	0.258080
H	-4.207458	-0.670469	-0.834629

N-Piv-cysteine methyl ester radical (4')

C	-0.333724	0.033765	-0.651588
C	-1.405641	-0.582368	0.128525
O	-1.538473	-1.787721	0.317956
C	-0.464081	1.382813	-1.261747
S	0.285668	2.730401	-0.195897
O	-2.289011	0.341495	0.576923
H	0.017248	1.431096	-2.241379
H	-1.508076	1.673301	-1.368029
H	1.572602	2.365124	-0.361015
N	0.818508	-0.685298	-0.918443
H	1.260627	-0.503228	-1.811473
C	1.545966	-1.447672	-0.007182
C	2.698985	-2.294506	-0.584153
O	1.248903	-1.464831	1.182756
C	-3.443970	-0.164115	1.278128
H	-3.136695	-0.708222	2.173845
H	-4.025422	0.716333	1.547335
H	-4.025072	-0.822876	0.628832
C	3.833951	-2.342704	0.457823
H	3.473871	-2.723734	1.415873
H	4.631637	-3.000515	0.098652
H	4.262058	-1.348121	0.623441
C	2.128201	-3.719574	-0.800926
H	2.918649	-4.374226	-1.182841
H	1.757279	-4.140380	0.138424
H	1.309171	-3.716647	-1.527722
C	3.254829	-1.756536	-1.918920
H	2.525840	-1.816237	-2.734839
H	3.608427	-0.723201	-1.829398
H	4.109981	-2.368784	-2.221102

N-Boc-cysteine methyl ester radical (6')

C	1.511817	0.095432	0.641955
C	2.083302	-1.066580	-0.030606
O	1.537610	-2.162334	-0.133333
C	2.340698	1.226971	1.133880
S	2.405457	2.654742	-0.078462
O	3.330650	-0.812607	-0.496351
H	1.966646	1.616701	2.083821
H	3.381210	0.932462	1.259732
H	1.116516	3.027383	0.049923
N	0.160985	0.123348	0.927287
H	-0.133411	0.601953	1.771777
C	-0.875059	-0.253370	0.072582
O	-0.728907	-0.537754	-1.102913
C	4.023398	-1.922479	-1.103592
H	3.467454	-2.290362	-1.968626
H	4.989358	-1.525147	-1.411613
H	4.155168	-2.730797	-0.380610
O	-2.023457	-0.217520	0.766072
C	-3.347162	-0.449051	0.122402
C	-3.412015	-1.879657	-0.417507
H	-4.429471	-2.083895	-0.765571
H	-2.724203	-2.025535	-1.251672
H	-3.172726	-2.597988	0.372873
C	-3.586677	0.606114	-0.960055
H	-4.610508	0.506479	-1.334001
H	-3.473112	1.613004	-0.546058
H	-2.899530	0.485321	-1.798922
C	-4.314080	-0.261547	1.292698
H	-5.341261	-0.410836	0.947590
H	-4.107070	-0.985255	2.086689
H	-4.231153	0.747705	1.706859

N-Fmoc-cysteine methyl ester radical (8')

C	-3.626070	0.068159	0.123325
C	-4.498822	1.221765	0.281881
O	-4.129893	2.279979	0.802212
C	-4.051886	-1.202708	-0.510390
S	-3.633525	-1.310255	-2.332462
O	-5.745563	1.015263	-0.187927
H	-3.607907	-2.069031	-0.024058
H	-5.137079	-1.279914	-0.474820
H	-2.317151	-1.542082	-2.157721
N	-2.347068	0.301074	0.582798
H	-2.209400	1.219947	0.997319
C	-1.254286	-0.537368	0.560613
O	-1.222044	-1.657577	0.072499
C	-6.672053	2.114444	-0.053333
H	-6.304087	2.988269	-0.594997
H	-7.603952	1.758255	-0.489171
H	-6.812118	2.364481	1.000482
O	-0.218042	0.081290	1.164584
C	1.043424	-0.632810	1.212546
H	0.838751	-1.697927	1.328245
H	1.538509	-0.251678	2.106762
C	1.896781	-0.374751	-0.040591
C	3.200948	-1.158714	0.020876
H	1.308712	-0.677923	-0.917078
C	2.388062	1.059107	-0.187005
C	3.396488	-2.533232	0.133049
C	4.303579	-0.281375	-0.052347
C	1.656800	2.237502	-0.323482
C	3.799939	1.093698	-0.182552
C	4.706943	-3.031089	0.174091
H	2.553811	-3.217617	0.181361
C	5.610011	-0.778797	-0.012549
C	2.343631	3.454220	-0.444775
H	0.571718	2.220803	-0.337201
C	4.484100	2.307175	-0.305267
C	5.802533	-2.159925	0.102803
H	4.873499	-4.100869	0.258826
H	6.464155	-0.110190	-0.071514
C	3.744624	3.487757	-0.434029
H	1.783639	4.378754	-0.551032
H	5.570030	2.338332	-0.304499
H	6.811275	-2.561344	0.134745
H	4.261082	4.438391	-0.530993

Cartesian Coordinates for Optimized Geometries in Gas-phase at B3lyp/6-31+G(d,p) Level of C[⦿] Neutral Radical

(2*R*)-*N*-Ac-2-methylcysteine methyl ester
radical (1')

C	-0.224466	0.053090	0.202199
C	-1.591639	-0.612425	-0.079259
O	-1.730230	-1.750050	-0.488865
C	-0.129211	1.279115	-0.685435
S	1.154022	2.453692	-0.643788
O	-2.612598	0.208179	0.191558
H	-1.019803	1.622596	-1.197467
H	2.069215	1.659444	-0.024569
N	0.759428	-1.003083	-0.140189
H	0.336258	-1.833426	-0.539288
C	2.094277	-1.004979	0.098262
C	2.821915	-2.288012	-0.265028
O	2.716831	-0.046331	0.573745
H	3.596366	-2.051579	-1.000105
H	3.323746	-2.666478	0.629988
H	2.169599	-3.067175	-0.667552
C	-0.151938	0.385266	1.717946
H	-0.321667	-0.519074	2.311987
H	0.834305	0.780645	1.960847
H	-0.909670	1.129801	1.968139
C	-3.936543	-0.325698	-0.032976
H	-4.099980	-1.203932	0.595157
H	-4.618310	0.478645	0.239201
H	-4.058518	-0.601098	-1.082662

N-Ac-cysteine methyl ester radical (2')

C	-0.123908	0.242881	0.176721
C	-1.462929	-0.442299	-0.140103
O	-1.607562	-1.327775	-0.956430
C	-0.178821	1.684837	-0.266406
S	1.231563	2.705882	-0.298334
O	-2.456032	0.078661	0.598358
H	0.039954	0.168385	1.262914
H	-1.117331	2.220546	-0.183177
H	2.138248	1.710134	-0.400829
N	0.967528	-0.492007	-0.439149
H	0.854338	-0.703533	-1.422851
C	1.777712	-1.326321	0.302639
C	2.680078	-2.242407	-0.502594
O	1.782614	-1.317929	1.528522
H	3.681024	-2.223600	-0.065891
H	2.299702	-3.265591	-0.418127
H	2.737517	-1.975498	-1.561416
C	-3.771854	-0.476295	0.378624
H	-3.770850	-1.545099	0.602846
H	-4.428069	0.061696	1.061297
H	-4.078463	-0.322348	-0.658330

(2*R*)-*N*-Piv-2-methylcysteine methyl ester
radical (3')

C	-1.028206	0.195477	0.240386
C	-2.008930	-0.950889	-0.098029
O	-1.671364	-2.043266	-0.515154
C	-1.398025	1.377250	-0.635332
S	-0.710627	2.971356	-0.516099
O	-3.280929	-0.606550	0.133670
H	-2.322396	1.340158	-1.198828
H	0.423598	2.595484	0.136217
N	0.306194	-0.376471	-0.070248
H	0.258086	-1.296394	-0.490928
C	1.518273	0.151733	0.220406
C	2.767740	-0.702683	-0.109058
O	1.666494	1.272862	0.730124
C	-4.275402	-1.618030	-0.141320
H	-4.101114	-2.497181	0.482702
H	-5.229803	-1.153104	0.101341
H	-4.239186	-1.906244	-1.194037
C	-1.147261	0.494359	1.760120
H	-0.961432	-0.416297	2.339520
H	-0.410505	1.244605	2.046182
H	-2.147852	0.867771	1.984818
C	2.455816	-2.067721	-0.750188
H	1.856399	-2.709151	-0.093999
H	1.938748	-1.966311	-1.711365
H	3.393739	-2.597705	-0.946276
C	3.525825	-0.919828	1.220392
H	4.465091	-1.450937	1.030490
H	3.753452	0.037684	1.694705
H	2.934911	-1.519936	1.921913
C	3.642250	0.129914	-1.073666
H	3.877337	1.103580	-0.637586
H	4.579229	-0.400060	-1.277561
H	3.132285	0.295782	-2.029379

N-Piv-cysteine methyl ester radical (4')

C	-0.143045	0.230276	0.184086
C	-1.490859	-0.432925	-0.141027
O	-1.648075	-1.310769	-0.963311
C	-0.179504	1.679384	-0.236921
S	1.241620	2.686556	-0.235098
O	-2.478056	0.097388	0.599570
H	0.020190	0.137395	1.268770
H	-1.113010	2.223965	-0.155011
H	2.139539	1.683723	-0.343831
N	0.937954	-0.509053	-0.445209
H	0.827941	-0.687524	-1.433987
C	1.744188	-1.353297	0.284376
C	2.703889	-2.281107	-0.496472
O	1.730619	-1.350805	1.512811
C	-3.800954	-0.437556	0.374539
H	-3.815317	-1.507927	0.590789
H	-4.450493	0.104467	1.060463
H	-4.104576	-0.271794	-0.661520
C	4.140330	-1.930070	-0.047029
H	4.230849	-1.997683	1.039624
H	4.853797	-2.624758	-0.503787
H	4.417006	-0.914335	-0.352536
C	2.368845	-3.729644	-0.073010
H	3.072340	-4.425958	-0.542747
H	2.438313	-3.838728	1.011846
H	1.356003	-4.010147	-0.382783
C	2.598108	-2.156381	-2.027983
H	1.605236	-2.436625	-2.399357
H	2.836707	-1.145892	-2.379159
H	3.315934	-2.837297	-2.496901

**(2*R*)-*N*-Boc-2-methylcysteine methyl ester
radical (5')**

C	-1.450664	0.085789	0.188791
C	-2.420988	-1.090330	-0.074477
O	-2.080997	-2.189898	-0.465658
C	-1.887329	1.230903	-0.706718
S	-1.145153	2.805124	-0.761672
O	-3.690522	-0.756599	0.192272
H	-2.876214	1.200960	-1.147667
H	0.009834	2.464098	-0.134000
N	-0.125782	-0.464546	-0.160635
H	-0.139402	-1.401445	-0.547941
C	1.088141	0.065691	0.135511
O	1.286646	1.183852	0.613345
C	-4.676564	-1.791827	-0.015158
H	-4.465809	-2.647701	0.629652
H	-5.629842	-1.334760	0.246407
H	-4.672209	-2.113335	-1.058828
O	2.056917	-0.823818	-0.182385
C	3.492707	-0.496981	-0.053519
C	3.841974	-0.243191	1.416571
H	4.926367	-0.126203	1.516944
H	3.355655	0.659462	1.788433
H	3.534105	-1.093759	2.033509
C	3.846246	0.692149	-0.952847
H	4.932432	0.832595	-0.955994
H	3.526062	0.500617	-1.982118
H	3.377362	1.611766	-0.600458
C	4.164004	-1.776946	-0.558727
H	5.252201	-1.671041	-0.510605
H	3.870679	-2.634733	0.053833
H	3.880074	-1.979291	-1.595815
C	-1.522213	0.438376	1.700687
H	-1.286416	-0.443412	2.306163
H	-0.799827	1.221774	1.930305
H	-2.524624	0.790706	1.949987

***N*-Boc-cysteine methyl ester radical (6')**

C	1.509619	0.327517	-0.123806
C	2.181564	-1.039047	0.095211
O	1.764894	-1.900715	0.839397
C	2.414260	1.420502	0.394529
S	1.864320	3.058329	0.608865
O	3.300347	-1.148707	-0.641532
H	1.339551	0.439476	-1.205588
H	3.484761	1.316100	0.262463
H	0.553416	2.754267	0.731598
N	0.198920	0.356563	0.496554
H	0.151864	0.042677	1.458944
C	-0.930303	0.107054	-0.258196
O	-0.961731	0.141246	-1.478303
C	4.031296	-2.387199	-0.506118
H	3.405489	-3.228459	-0.811804
H	4.892703	-2.286382	-1.164962
H	4.347948	-2.527540	0.529769
O	-1.971837	-0.130805	0.565572
C	-3.332889	-0.383537	0.042012
C	-3.333669	-1.648807	-0.821595
H	-4.364628	-1.901215	-1.091537
H	-2.757479	-1.505131	-1.736548
H	-2.912111	-2.491141	-0.263771
C	-3.834211	0.846836	-0.720759
H	-4.883171	0.698098	-0.998213
H	-3.774733	1.738762	-0.088388
H	-3.253873	1.015308	-1.629049
C	-4.141868	-0.597945	1.323629
H	-5.188409	-0.797494	1.073637
H	-3.751355	-1.448980	1.889574
H	-4.100686	0.290354	1.961237

**(2*R*)-*N*-Fmoc-2-methylcysteine methyl ester
radical (7')**

C	3.501780	-0.162924	0.179286
C	4.360848	1.091446	-0.103369
O	3.985942	2.050142	-0.750428
C	4.220186	-1.349567	-0.437260
S	3.834928	-3.024793	-0.163859
O	5.572426	0.999189	0.457484
H	5.180044	-1.197190	-0.915977
H	2.541881	-2.841757	0.200324
N	2.209624	0.140528	-0.472475
H	2.193353	0.978891	-1.042720
C	1.071734	-0.584132	-0.381706
O	0.921901	-1.642109	0.227918
C	3.319205	-0.287797	1.714762
H	2.890045	0.634968	2.118494
H	2.643259	-1.112332	1.941813
H	4.284118	-0.475984	2.188160
C	6.452307	2.128429	0.260531
H	6.009289	3.030004	0.689006
H	7.373846	1.865469	0.777725
H	6.634217	2.283697	-0.804993
O	0.073846	0.028518	-1.074502
C	-1.209018	-0.635600	-1.087324
H	-1.046967	-1.714746	-1.101236
H	-1.677144	-0.317283	-2.020850
C	-2.076878	-0.240501	0.119618
C	-3.389512	-1.010716	0.131563
H	-1.498237	-0.461059	1.026783
C	-2.551377	1.205988	0.112638
C	-3.600447	-2.386685	0.157798
C	-4.481740	-0.118584	0.112579
C	-1.807118	2.383414	0.116868
C	-3.962288	1.256148	0.103516
C	-4.915146	-2.872078	0.161112
H	-2.763576	-3.079727	0.184522
C	-5.792250	-0.604277	0.117584
C	-2.479311	3.613116	0.108778
H	-0.722213	2.354219	0.121466
C	-4.630974	2.483322	0.097515
C	-6.000214	-1.986783	0.139927
H	-5.093638	-3.943173	0.183163
H	-6.639298	0.076020	0.105636
C	-3.878832	3.661599	0.099315
H	-1.908595	4.537297	0.110876
H	-5.716646	2.526634	0.093496
H	-7.013439	-2.378372	0.143485
H	-4.384208	4.623171	0.095185

N-Fmoc-cysteine methyl ester radical (8')

C	-3.599032	-0.163029	-0.154614
C	-4.456099	1.101657	-0.202962
O	-4.403506	1.987426	0.628144
C	-4.383298	-1.263903	0.508268
S	-4.191491	-2.946305	0.117951
O	-5.293051	1.089730	-1.248973
H	-5.088900	-1.039989	1.300899
H	-2.999155	-2.831003	-0.512133
N	-2.348256	0.186368	0.524463
H	-2.376700	0.906059	1.235787
C	-1.224677	-0.553447	0.351714
O	-1.129817	-1.517213	-0.403062
C	-6.205790	2.205088	-1.346787
H	-5.649800	3.140934	-1.434885
H	-6.792617	2.016369	-2.244453
H	-6.848130	2.245033	-0.464247
O	-0.210198	-0.074633	1.115206
C	1.056524	-0.763861	1.010380
H	0.866023	-1.831766	0.890157
H	1.552012	-0.578870	1.965306
C	1.907944	-0.237298	-0.157222
C	3.201679	-1.026795	-0.295108
H	1.306907	-0.330471	-1.071712
C	2.416076	1.186336	0.021838
C	3.378930	-2.391955	-0.502935
C	4.314755	-0.167487	-0.186166
C	1.698824	2.369757	0.179965
C	3.827794	1.205505	0.008631
C	4.681408	-2.900381	-0.598248
H	2.525230	-3.057662	-0.600366
C	5.613045	-0.676133	-0.282402
C	2.398943	3.574473	0.329703
H	0.613572	2.363141	0.191063
C	4.524235	2.408168	0.156116
C	5.787374	-2.048244	-0.487372
H	4.834151	-3.963024	-0.762661
H	6.476091	-0.021065	-0.202085
C	3.799201	3.592354	0.318036
H	1.849748	4.503228	0.454663
H	5.610499	2.428572	0.143602
H	6.790671	-2.457464	-0.564327
H	4.326447	4.535054	0.433591
H	-3.349164	-0.456236	-1.178185

Cartesian Coordinates for Optimized Geometries in Methanol at B3lyp/6-31+G(d,p) Level of C[⦿] Neutral Radical

(2R)-N-Ac-2-methylcysteine methyl ester radical (1')

C	-0.222626	0.045529	0.198945
C	-1.593112	-0.620392	-0.077813
O	-1.726811	-1.762749	-0.483001
C	-0.128811	1.268151	-0.694284
S	1.121243	2.479646	-0.602282
O	-2.604083	0.202027	0.189955
H	-0.995667	1.573522	-1.267651
H	2.046144	1.695225	0.014744
N	0.766692	-1.006181	-0.145219
H	0.346546	-1.848743	-0.522799
C	2.099337	-1.005002	0.079841
C	2.826391	-2.289215	-0.267214
O	2.725460	-0.031231	0.538322
H	3.631778	-2.057590	-0.969586
H	3.284098	-2.686761	0.643589
H	2.179454	-3.053793	-0.702015
C	-0.150539	0.379741	1.713146
H	-0.313028	-0.525705	2.305906
H	0.831124	0.785026	1.957883
H	-0.914770	1.116539	1.965972
C	-3.942978	-0.314042	-0.024175
H	-4.112140	-1.184581	0.611603
H	-4.608357	0.501552	0.251357
H	-4.073958	-0.583839	-1.073379

N-Ac-cysteine methyl ester radical (2')

C	-0.135970	0.212625	0.153809
C	-1.486013	-0.479411	-0.112939
O	-1.641242	-1.441925	-0.838564
C	-0.177609	1.639268	-0.330357
S	1.215644	2.686198	-0.274448
O	-2.465691	0.121182	0.571444
H	0.022678	0.172257	1.242220
H	-1.126172	2.162103	-0.353580
H	2.159788	1.722041	-0.298452
N	0.959678	-0.533434	-0.436202
H	1.028450	-0.537956	-1.445654
C	1.712617	-1.425394	0.272711
C	2.734410	-2.208975	-0.523053
O	1.580348	-1.575933	1.492756
H	3.717784	-2.073009	-0.065023
H	2.483151	-3.272104	-0.462347
H	2.783363	-1.915224	-1.573746
C	-3.800963	-0.421190	0.415381
H	-3.822772	-1.459531	0.750846
H	-4.437017	0.199965	1.043011
H	-4.110004	-0.359233	-0.629529

**(2*R*)-*N*-Piv-2-methylcysteine methyl ester
radical (3')**

C	-1.025736	0.190017	0.242790
C	-2.008258	-0.953351	-0.110353
O	-1.663278	-2.038561	-0.546974
C	-1.392381	1.377473	-0.627620
S	-0.754825	2.989215	-0.441349
O	-3.271526	-0.610945	0.129722
H	-2.275253	1.322949	-1.253043
H	0.384077	2.621464	0.206998
N	0.312732	-0.373610	-0.069346
H	0.269638	-1.300979	-0.475276
C	1.521801	0.156011	0.214778
C	2.771270	-0.698642	-0.109237
O	1.666431	1.287697	0.715183
C	-4.286159	-1.607717	-0.155051
H	-4.114974	-2.497355	0.453229
H	-5.229947	-1.134808	0.108718
H	-4.265644	-1.867657	-1.214664
C	-1.151134	0.475133	1.763325
H	-0.964750	-0.440082	2.333723
H	-0.419965	1.226289	2.060704
H	-2.153735	0.841295	1.990365
C	2.455465	-2.075613	-0.722866
H	1.864765	-2.704710	-0.047587
H	1.930623	-1.991549	-1.681176
H	3.393682	-2.605236	-0.916453
C	3.542237	-0.896672	1.216193
H	4.469958	-1.445771	1.023528
H	3.795351	0.065442	1.668448
H	2.951017	-1.473143	1.936559
C	3.637518	0.113481	-1.099079
H	3.887481	1.093917	-0.686148
H	4.568445	-0.426410	-1.301989
H	3.117510	0.261688	-2.052119

***N*-Piv-cysteine methyl ester radical (4')**

C	-0.161336	0.215921	0.116130
C	-1.523864	-0.479568	-0.062361
O	-1.711043	-1.482675	-0.722624
C	-0.213000	1.612863	-0.446984
S	1.184293	2.655534	-0.489003
O	-2.475684	0.169731	0.617302
H	0.035936	0.235743	1.198540
H	-1.160206	2.137874	-0.475066
H	2.124552	1.687365	-0.481531
N	0.908504	-0.569277	-0.471909
H	0.943296	-0.613811	-1.480728
C	1.673729	-1.430529	0.260065
C	2.712904	-2.290029	-0.493622
O	1.555458	-1.509070	1.489005
C	-3.819304	-0.368393	0.538506
H	-3.837787	-1.384438	0.936544
H	-4.429334	0.295424	1.148078
H	-4.162704	-0.366354	-0.497495
C	4.100155	-1.962030	0.104370
H	4.110858	-2.134747	1.183444
H	4.859590	-2.601290	-0.358004
H	4.376297	-0.918255	-0.082110
C	2.364892	-3.771268	-0.218749
H	3.113025	-4.417671	-0.689649
H	2.354277	-3.977635	0.854558
H	1.383976	-4.031472	-0.631486
C	2.743798	-2.047141	-2.014466
H	1.794441	-2.308575	-2.495895
H	2.996636	-1.010341	-2.262200
H	3.513163	-2.683006	-2.463463

**(2*R*)-*N*-Boc-2-methylcysteine methyl ester
radical (5')**

C	-1.455953	0.092339	0.183175
C	-2.419480	-1.091936	-0.083679
O	-2.063502	-2.183892	-0.491992
C	-1.908572	1.236593	-0.705797
S	-1.157705	2.810009	-0.768370
O	-3.681037	-0.772564	0.196172
H	-2.903473	1.211150	-1.133508
H	-0.000039	2.468328	-0.145853
N	-0.126123	-0.437131	-0.182115
H	-0.136161	-1.376606	-0.563798
C	1.087660	0.081524	0.136658
O	1.284080	1.200006	0.620973
C	-4.678806	-1.805090	-0.009703
H	-4.463596	-2.662765	0.629734
H	-5.624893	-1.344376	0.267085
H	-4.687904	-2.110655	-1.057203
O	2.053572	-0.810313	-0.170952
C	3.499459	-0.496013	-0.047721
C	3.854631	-0.245587	1.420454
H	4.940577	-0.144265	1.515530
H	3.384824	0.665184	1.793739
H	3.536795	-1.090541	2.039717
C	3.858303	0.686127	-0.952396
H	4.945410	0.814649	-0.959363
H	3.532837	0.493962	-1.979797
H	3.402029	1.612858	-0.601720
C	4.155702	-1.783208	-0.552774
H	5.244262	-1.685073	-0.506819
H	3.858724	-2.637068	0.063644
H	3.869600	-1.983634	-1.589725
C	-1.526547	0.436110	1.696405
H	-1.272022	-0.443590	2.296123
H	-0.821070	1.233917	1.928218
H	-2.534733	0.765599	1.952846

***N*-Boc-cysteine methyl ester radical (6')**

C	1.517529	0.323647	-0.078321
C	2.179979	-1.063078	0.040248
O	1.709359	-2.003855	0.649558
C	2.405742	1.375616	0.537592
S	1.892730	3.031093	0.723023
O	3.339004	-1.093614	-0.626237
H	1.382689	0.510600	-1.154591
H	3.480015	1.237975	0.516612
H	0.563665	2.792401	0.728267
N	0.190976	0.329081	0.502867
H	0.115449	0.163754	1.498949
C	-0.922711	0.048767	-0.249976
O	-0.927990	0.000359	-1.475700
C	4.077786	-2.340614	-0.598304
H	3.479577	-3.138231	-1.042290
H	4.973135	-2.155930	-1.188697
H	4.338801	-2.597100	0.429940
O	-1.982701	-0.125629	0.561154
C	-3.349991	-0.384000	0.039863
C	-3.370412	-1.702691	-0.737823
H	-4.405063	-1.949861	-0.996212
H	-2.789395	-1.634252	-1.658553
H	-2.970194	-2.515313	-0.123211
C	-3.818482	0.806112	-0.801302
H	-4.868975	0.661567	-1.073121
H	-3.740953	1.734789	-0.226888
H	-3.233281	0.903397	-1.716856
C	-4.172332	-0.499048	1.325272
H	-5.219654	-0.693137	1.076266
H	-3.806534	-1.321177	1.947791
H	-4.119770	0.428354	1.903503

(2R)-N-Fmoc-2-methylcysteine methyl ester radical (7')

C	3.486378	-0.130017	0.183908
C	4.337539	1.130778	-0.103991
O	3.942660	2.090179	-0.744048
C	4.193120	-1.306500	-0.464593
S	3.965194	-2.985635	-0.059964
O	5.550149	1.037286	0.436355
H	5.018094	-1.126331	-1.144026
H	2.694606	-2.887112	0.395016
N	2.180603	0.164905	-0.445303
H	2.136013	1.019842	-0.988827
C	1.073224	-0.605809	-0.380304
O	0.964818	-1.682265	0.208322
C	3.332423	-0.265185	1.719185
H	2.918885	0.658472	2.134450
H	2.654389	-1.084664	1.957556
H	4.303275	-0.461456	2.176654
C	6.442691	2.163514	0.239233
H	6.008095	3.063972	0.676396
H	7.362203	1.889629	0.752482
H	6.623292	2.313152	-0.826517
O	0.058238	-0.023056	-1.073842
C	-1.218718	-0.699657	-1.071747
H	-1.049920	-1.777487	-1.070009
H	-1.691560	-0.402655	-2.009608
C	-2.086626	-0.288806	0.130669
C	-3.415715	-1.031580	0.126659
H	-1.521360	-0.519898	1.043495
C	-2.530694	1.167564	0.124353
C	-3.657623	-2.403410	0.146000
C	-4.489011	-0.115990	0.094885
C	-1.762224	2.330044	0.151199
C	-3.940510	1.247840	0.095652
C	-4.983764	-2.859429	0.132097
H	-2.838302	-3.116696	0.177895
C	-5.811170	-0.571382	0.082434
C	-2.409303	3.574315	0.140338
H	-0.678479	2.279854	0.179584
C	-4.585088	2.488876	0.086344
C	-6.049750	-1.950011	0.099603
H	-5.185904	-3.926359	0.148739
H	-6.642441	0.127739	0.060865
C	-3.808208	3.652078	0.106928
H	-1.819745	4.486341	0.160471
H	-5.669355	2.554436	0.066674
H	-7.071207	-2.319242	0.089832
H	-4.293499	4.623856	0.100733

N-Fmoc-cysteine methyl ester radical (8')

C	-3.590395	-0.141278	-0.139126
C	-4.436612	1.132096	-0.218879
O	-4.318530	2.073799	0.545646
C	-4.363898	-1.195943	0.607179
S	-4.466895	-2.861553	0.120969
O	-5.338785	1.055663	-1.199306
H	-4.908830	-0.940210	1.509511
H	-3.441692	-2.858758	-0.757256
N	-2.315888	0.211711	0.485510
H	-2.311405	0.948747	1.179652
C	-1.215720	-0.562395	0.321697
O	-1.151959	-1.541767	-0.418196
C	-6.259782	2.168120	-1.327502
H	-5.708167	3.088864	-1.524838
H	-6.898611	1.913043	-2.170649
H	-6.848113	2.272165	-0.414014
O	-0.187223	-0.102075	1.078064
C	1.074389	-0.800664	0.969114
H	0.878654	-1.864876	0.829883
H	1.564220	-0.639215	1.930949
C	1.938494	-0.257199	-0.181905
C	3.242829	-1.032996	-0.301692
H	1.354778	-0.346588	-1.107860
C	2.429193	1.170700	0.012773
C	3.438548	-2.396019	-0.511793
C	4.345670	-0.163042	-0.167184
C	1.696925	2.347565	0.157314
C	3.841243	1.204354	0.026600
C	4.748857	-2.890242	-0.586273
H	2.595368	-3.072438	-0.623703
C	5.652140	-0.656583	-0.242376
C	2.382676	3.559314	0.325259
H	0.611831	2.332027	0.141358
C	4.524222	2.413438	0.192437
C	5.844534	-2.026655	-0.451645
H	4.915500	-3.950546	-0.751899
H	6.506554	0.006868	-0.142441
C	3.783703	3.590683	0.343827
H	1.821999	4.482506	0.439801
H	5.610144	2.444570	0.201446
H	6.853258	-2.424898	-0.512333
H	4.299316	4.537930	0.473322
H	-3.384139	-0.481206	-1.156861

Cartesian Coordinates for Optimized Geometries in Water at B3lyp/6-31+G(d,p) Level of C[•] Neutral Radical

(2R)-N-Ac-2-methylcysteine methyl ester radical (1')

C	-0.222544	0.044997	0.198679
C	-1.593278	-0.620597	-0.077888
O	-1.727155	-1.762987	-0.483101
C	-0.128325	1.267414	-0.694836
S	1.118549	2.481974	-0.598498
O	-2.603732	0.202114	0.189994
H	-0.992801	1.569424	-1.273563
H	2.044241	1.698512	0.018528
N	0.766714	-1.006846	-0.145442
H	0.346444	-1.850241	-0.521097
C	2.099379	-1.005020	0.078337
C	2.826699	-2.289353	-0.267324
O	2.725636	-0.030137	0.534990
H	3.633075	-2.058210	-0.968718
H	3.282945	-2.686767	0.644297
H	2.180208	-3.053961	-0.702635
C	-0.150342	0.379214	1.712811
H	-0.312994	-0.526226	2.305462
H	0.831358	0.784363	1.957642
H	-0.914458	1.116066	1.965814
C	-3.943160	-0.313188	-0.023563
H	-4.112445	-1.183580	0.612350
H	-4.607896	0.502758	0.252384
H	-4.074729	-0.582590	-1.072777

N-Ac-cysteine methyl ester radical (2')

C	-0.136202	0.211107	0.153445
C	-1.486458	-0.482226	-0.109494
O	-1.641185	-1.452011	-0.825639
C	-0.178060	1.637070	-0.332196
S	1.213756	2.685782	-0.273123
O	-2.466545	0.125173	0.567942
H	0.023156	0.172167	1.241872
H	-1.127164	2.158578	-0.360482
H	2.159774	1.723454	-0.294275
N	0.959430	-0.534972	-0.436559
H	1.036391	-0.529204	-1.445425
C	1.709541	-1.430315	0.270046
C	2.736947	-2.207128	-0.524928
O	1.570334	-1.589621	1.488616
H	3.718113	-2.069335	-0.062657
H	2.489389	-3.271409	-0.469590
H	2.788941	-1.908660	-1.574093
C	-3.802172	-0.417779	0.415977
H	-3.825201	-1.452466	0.762439
H	-4.438432	0.210455	1.036271
H	-4.109892	-0.366339	-0.629862

**(2*R*)-*N*-Piv-2-methylcysteine methyl ester
radical (3')**

C	-1.025267	0.188902	0.243965
C	-2.008522	-0.952922	-0.112247
O	-1.663952	-2.037600	-0.550679
C	-1.389597	1.378167	-0.625062
S	-0.759944	2.991825	-0.428061
O	-3.271455	-0.609660	0.127288
H	-2.265960	1.322041	-1.259462
H	0.379053	2.625603	0.220680
N	0.313121	-0.375259	-0.067525
H	0.270164	-1.303078	-0.472480
C	1.521911	0.154995	0.215815
C	2.771698	-0.698898	-0.108865
O	1.666004	1.287293	0.715475
C	-4.287294	-1.604507	-0.160501
H	-4.117584	-2.495749	0.445801
H	-5.230593	-1.131032	0.103909
H	-4.266532	-1.861598	-1.220788
C	-1.152006	0.471347	1.764789
H	-0.967855	-0.445337	2.333457
H	-0.419892	1.220626	2.064607
H	-2.154210	0.838748	1.991585
C	2.455873	-2.078819	-0.715830
H	1.867197	-2.705332	-0.036419
H	1.928957	-1.999451	-1.673397
H	3.394189	-2.608331	-0.909133
C	3.547878	-0.890640	1.214400
H	4.475723	-1.438953	1.020237
H	3.801284	0.073486	1.662211
H	2.960283	-1.465386	1.939072
C	3.633063	0.110556	-1.105238
H	3.884251	1.092646	-0.696912
H	4.563550	-0.429306	-1.310162
H	3.108901	0.254881	-2.056596

***N*-Piv-cysteine methyl ester radical (4')**

C	-0.160775	0.216988	0.112548
C	-1.522509	-0.483316	-0.054498
O	-1.707933	-1.498705	-0.696393
C	-0.216530	1.609929	-0.459364
S	1.176451	2.658349	-0.504038
O	-2.475225	0.175714	0.614127
H	0.039891	0.244487	1.194235
H	-1.165827	2.130571	-0.494974
H	2.121737	1.695238	-0.488602
N	0.908976	-0.569560	-0.473906
H	0.950793	-0.607419	-1.482742
C	1.670436	-1.433391	0.258044
C	2.712773	-2.290529	-0.493851
O	1.545565	-1.517055	1.486356
C	-3.817957	-0.366421	0.546085
H	-3.834174	-1.375042	0.962668
H	-4.428859	0.307197	1.143871
H	-4.162004	-0.383689	-0.489527
C	4.097169	-1.967233	0.113258
H	4.102307	-2.146508	1.191325
H	4.858391	-2.604457	-0.348941
H	4.375045	-0.922642	-0.065679
C	2.361325	-3.772699	-0.228357
H	3.110910	-4.417711	-0.698812
H	2.344981	-3.984909	0.843774
H	1.382220	-4.029411	-0.647602
C	2.752240	-2.040082	-2.013263
H	1.805318	-2.298174	-2.501222
H	3.007256	-1.002250	-2.254195
H	3.523528	-2.674389	-2.461130

**(2*R*)-*N*-Boc-2-methylcysteine methyl ester
radical (5')**

C	4.612556	-0.039306	0.102704
C	5.396078	0.234424	-1.186105
O	5.328309	-0.448977	-2.186593
C	5.590867	-0.445471	1.232184
S	4.937365	-0.195267	2.938089
O	6.179827	1.314459	-1.058939
H	5.878125	-1.490929	1.085779
H	6.490559	0.172163	1.180212
H	3.645253	-0.464678	2.647264
N	3.636074	-1.068531	-0.208768
H	3.793207	-1.569240	-1.076424
C	2.369023	-1.059241	0.294795
O	1.987384	-0.374441	1.233619
C	6.982119	1.642924	-2.210764
H	6.342019	1.846104	-3.072621
H	7.543075	2.533092	-1.927602
H	7.658008	0.818545	-2.450794
O	1.596672	-1.944619	-0.380239
C	0.237021	-2.089388	0.086549
H	0.226010	-2.019560	1.177446
H	-0.044136	-3.102739	-0.214104
H	4.096652	0.881292	0.396582
C	-0.686704	-1.048601	-0.539587
H	-0.358004	-0.058046	-0.211370
H	-0.577446	-1.091606	-1.631890
C	-2.149848	-1.290533	-0.146276
H	-2.412329	-2.330846	-0.383953
H	-2.270541	-1.181490	0.939171
C	-3.182476	-0.375547	-0.854668
C	-3.190075	1.079296	-0.396244
H	-2.993579	-0.430636	-1.938078
C	-4.610061	-0.809099	-0.547095
C	-2.194271	2.048724	-0.480176
C	-4.444057	1.408373	0.163273
C	-5.222512	-2.036086	-0.777880
C	-5.323866	0.236745	0.070114
C	-2.441500	3.331953	0.022312
H	-1.234640	1.828568	-0.938403
C	-4.690149	2.688223	0.663004
C	-6.554918	-2.216891	-0.388958
H	-4.681118	-2.848536	-1.257679
C	-6.652228	0.055828	0.460568
C	-3.677467	3.646981	0.594431
H	-1.665095	4.089903	-0.036845
H	-5.656062	2.940454	1.093365
C	-7.261890	-1.178699	0.227081
H	-7.044075	-3.170633	-0.568074
H	-7.207550	0.860025	0.936676
H	-3.854509	4.647474	0.980145
H	-8.295576	-1.333725	0.524799

N-Boc-cysteine methyl ester radical (6')

C	1.517535	0.322384	-0.077034
C	2.180213	-1.064806	0.036048
O	1.705890	-2.010403	0.635222
C	2.404413	1.372997	0.542741
S	1.892664	3.029047	0.726739
O	3.342959	-1.090187	-0.623608
H	1.383381	0.512719	-1.152854
H	3.478548	1.233856	0.527487
H	0.563182	2.792841	0.727155
N	0.190568	0.325703	0.503089
H	0.114069	0.168240	1.500335
C	-0.922603	0.044287	-0.249278
O	-0.926936	-0.008412	-1.475080
C	4.082529	-2.336964	-0.600787
H	3.487641	-3.131480	-1.054643
H	4.981286	-2.147128	-1.184288
H	4.337621	-2.600902	0.427029
O	-1.983417	-0.126899	0.561389
C	-3.351082	-0.383864	0.040147
C	-3.373944	-1.704517	-0.734138
H	-4.408987	-1.950013	-0.992476
H	-2.792342	-1.639827	-1.654785
H	-2.975997	-2.516489	-0.117166
C	-3.816785	0.805095	-0.804150
H	-4.867486	0.662037	-1.075855
H	-3.737378	1.735043	-0.232080
H	-3.231172	0.898828	-1.719827
C	-4.174198	-0.494004	1.325492
H	-5.221739	-0.686758	1.076462
H	-3.810306	-1.315276	1.950274
H	-4.120129	0.434837	1.901260

(2*R*)-*N*-Fmoc-2-methylcysteine methyl ester radical (7')

C	3.466642	-0.091389	0.207567
C	4.388493	1.103876	-0.137508
O	4.052693	2.047107	-0.833427
C	4.072980	-1.321515	-0.443342
S	4.029047	-2.950149	0.167033
O	5.592001	0.969947	0.415294
H	4.680184	-1.198191	-1.333669
H	2.844531	-2.884442	0.812226
N	2.166315	0.261345	-0.397878
H	2.145527	1.104569	-0.960401
C	1.064849	-0.522239	-0.362691
O	0.963164	-1.601759	0.217420
C	3.339828	-0.181239	1.745325
H	3.014698	0.783656	2.144248
H	2.596896	-0.931236	2.018090
H	4.298545	-0.448235	2.192241
C	6.549959	2.028541	0.160985
H	6.168205	2.976572	0.543590
H	7.450087	1.730939	0.694975
H	6.742884	2.106461	-0.910252
O	0.054425	0.056508	-1.068221
C	-1.213393	-0.636356	-1.089700
H	-1.030059	-1.711617	-1.113050
H	-1.684615	-0.323437	-2.023194
C	-2.095669	-0.267921	0.116296
C	-3.411012	-1.034024	0.089605
H	-1.531250	-0.508830	1.027034
C	-2.565998	1.179701	0.139102
C	-3.627735	-2.410121	0.079610
C	-4.500824	-0.137603	0.073004
C	-1.817903	2.354328	0.194186
C	-3.976972	1.235683	0.105440
C	-4.945246	-2.889966	0.051335
H	-2.795641	-3.108834	0.099971
C	-5.814436	-0.616810	0.045885
C	-2.486484	3.587143	0.206758
H	-0.733606	2.321326	0.226803
C	-4.643018	2.465387	0.119589
C	-6.027664	-1.999679	0.033698
H	-5.127892	-3.960510	0.045404
H	-6.658303	0.067269	0.035792
C	-3.886488	3.641218	0.168526
H	-1.913154	4.508708	0.248993
H	-5.728151	2.512857	0.096221
H	-7.042088	-2.387331	0.012620
H	-4.388638	4.604330	0.180693

N-Boc-cysteine methyl ester radical (8')

C	-3.621894	0.068823	0.122508
C	-4.502152	1.214672	0.295296
O	-4.143390	2.264580	0.838986
C	-4.034269	-1.190477	-0.542865
S	-3.592857	-1.258637	-2.361395
O	-5.743548	1.010864	-0.189543
H	-3.593219	-2.065259	-0.069199
H	-5.119484	-1.272195	-0.522668
H	-2.277809	-1.487674	-2.175130
N	-2.347784	0.300253	0.596172
H	-2.217824	1.212983	1.026542
C	-1.250899	-0.532601	0.568952
O	-1.211412	-1.647449	0.069101
C	-6.676708	2.102902	-0.043447
H	-6.310098	2.987012	-0.569166
H	-7.603961	1.748729	-0.490680
H	-6.824530	2.335703	1.013220
O	-0.219164	0.084122	1.182691
C	1.043592	-0.628117	1.229308
H	0.840329	-1.692909	1.350677
H	1.540894	-0.242499	2.120326
C	1.892145	-0.375858	-0.027952
C	3.195953	-1.160677	0.031108
H	1.300177	-0.683207	-0.900344
C	2.383887	1.056663	-0.184899
C	3.390673	-2.534513	0.152826
C	4.299007	-0.285152	-0.056052
C	1.652990	2.235231	-0.322143
C	3.795854	1.089540	-0.191894
C	4.700821	-3.033477	0.188972
H	2.547521	-3.217384	0.212749
C	5.605151	-0.783699	-0.021309
C	2.340384	3.450220	-0.457037
H	0.567782	2.220357	-0.326340
C	4.480482	2.301288	-0.328393
C	5.796861	-2.164129	0.103487
H	4.866859	-4.102684	0.281584
H	6.459614	-0.116512	-0.090693
C	3.741469	3.481987	-0.458775
H	1.780665	4.374816	-0.564169
H	5.566410	2.331064	-0.337021
H	6.805318	-2.566499	0.132196
H	4.258255	4.431289	-0.566365