Supplementary Data

Novel pyridinium-based tags: Synthesis and characterization for highly efficient analysis of thiol-containing peptides by mass spectrometry

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Table S1. Labeling efficiency of the thiol peptides from BSA derivatized by IMP and IPP.

No	Position	Peptide sequence	No of cysteines	Labeling efficiency/%	
				IMP	IPP
1	76-88	K.TCVADESHAGCEK.S	2	90.4	90.8
2	89-100	K.SLHTLFGDELCK.V	1	100	100
3	106-117	R.ETYGDMADCCEK.Q	2	100	100
4	118-130	K.QEPERNECFLSHK.D	1	100	66.2
5	118-138	K.QEPERNECFLSHKDDSPDLPK.L	1	100	100
6	123-130	R.NECFLSHK.D	1	100	100
7	123-138	R.NECFLSHKDDSPDLPK.L	1	100	100
8	139-151	K.LKPDPNTLCDEFK.A	1	100	100
9	139-155	K.LKPDPNTLCDEFKADEK.K	1	100	100
10	139-156	K.LKPDPNTLCDEFKADEKK.F	1	100	100
11	184-197	K.YNGVFQECCQAEDK.G	2		100
12	198-204	K.GACLLPK.I	1	100	100
13	223-228	R.CASIQK.F	1	100	100
14	267-285	K.ECCHGDLLECADDRADLAK.Y	3	100	100
15	286-297	K.YICDNQDTISSK.L	1	100	100
16	298-309	K.LKECCDKPLLEK.S	2	86.1	100
17	300-309	K.ECCDKPLLEK.S	2	100	100
18	310-318	K.SHCIAEVEK.D	1	100	100
19	310-340	K.SHCIAEVEKDAIPENLPPLTADFAEDKDVCK.N	2	100	

20	319-340	K.DAIPENLPPLTADFAEDKDVCK.N	1	100	100
21	375-386	K.EYEATLEECCAK.D	2	100	100
22	387-399	K.DDPHACYSTVFDK.L	1	100	100
23	387-401	K.DDPHACYSTVFDKLK.H	1	100	100
24	413-420	K.QNCDQFEK.L	1	100	100
25	456-468	K.VGTRCCTKPESER.M	2		100
26	460-468	R.CCTKPESER.M	2		92.6
27	469-482	R.MPCTEDYLSLILNR.L	1	65.7	100
28	483-489	R.LCVLHEK.T	1	100	100
29	483-495	R.LCVLHEKTPVSEK.V	1	100	100
30	496-507	K.VTKCCTESLVNR.R	2	100	100
31	499-507	K.CCTESLVNR.R	2	87.7	91.9
32	508-523	R.RPCFSALTPDETYVPK.A	1	100	100
33	529-544	K.LFTFHADICTLPDTEK.Q	1	100	
34	581-597	K.CCAADDKEACFAVEGPK.L	3	100	100
35	588-597	K.EACFAVEGPK.L	1	100	100

Table S2. The recognized thiol peptides from α-transferrin respectively derivatized by IAA, IMP, or IPP.

No	Position	Peptide sequence	No of cysteines	IAA	IMP	IPP
1	27-37	R.WCTISTHEANK.C	1	√	√	√
2	38-47	K.CASFRENVLR.I	1			√
3	48-59	R.ILESGPFVSCVK.K	1	√	√	√
4	48-60	R.ILESGPFVSCVKK.T	1	√	√	√
5	60-68	K.KTSHMDCIK.A	1			√
6	61-68	K.TSHMDCIK.A	1		√	
7	132-142	R.GKKSCHTGLGR.S	1		√	√
8	134-142	K. KSCHTGLGR.S	1			√
9	134-152	K.KSCHTGLGRSAGWNIPMAK.L	1			√
10	167-187	R.AAANFFSASCVPCADQSSFPK.L	2	√		
11	188-195	K.LCQLCAGK.G	1		√	√
12	196-216	K.GTDKCACSNHEPYFGYSGAFK.C	2	√		
13	244-256	R.KNYELLCGDNTRK.S	1	√		
14	245-255	K.NYELLCGDNTR.K	1	√	√	√
15	245-256	K.NYELLCGDNTRK.S	1	√	√	√
16	256-277	R.KSVDDYQECYLAMVPSHAVVAR.T	1	√	√	√
17	257-277	K. SVDDYQECYLAMVPSHAVVAR.T	1	√	√	√
18	351-365	R.ESKPPDSSKDECMVK.W	1	√	√	√
19	366-374	K.WCAIGHQER.T	1	√	√	√

20	366-376	K.WCAIGHQERTK.C	1		√	
21	377-402	K.CDRWSGFSGGAIECETAENTEECIAK.I	3	√		
22	380-402	R. WSGFSGGAIECETAENTEECIAK.I	2	√	√	
23	424-435	K.CGLVPVLAENYK.T	1	√	√	√
24	424-442	K.CGLVPVLAENYKTEGESCK.N	2	√		
25	494-513	K.INNCKFDEFFSAGCAPGSPR.N	2	√		
26	499-513	K.FDEFFSAGCAPGSPR.N	1	√	√	√
27	514-526	R.NSSLCALCIGSEK.G	2			√
28	514-530	R. NSSLCALCIGSEKGTGK.E	2		√	√
29	527-539	K.GTGKECVPNSNER.Y	1	√	√	
30	531-539	K.ECVPNSNER.Y	1		√	
31	549-560	R.CLVEKGDVAFVK.D	1		√	√
32	579-590	K.NLKKENFEVLCK.D	1	√	√	√
33	582-590	K.KENFEVLCK.D	1		√	√
34	583-590	K.ENFEVLCK.D	1	√	√	√
35	591-607	K.DGTRKPVTDAENCHLAR.G	1	√	√	√
36	595-607	R.KPVTDAENCHLAR.G	1	√	√	√
37	618-625	K.DKATCVEK.I	1		√	
38	620-625	K.ATCVEK.I	1		√	
39	637-653	K.SVTDCTSNFCLFQSNSK.D	2	√		
40	663-669	K.CLASIAK.K	1		√	
41	663-670	K.CLASIAKK.T	1			√

42	683-694	R.AMTNLRQCSTSK.L	1	√	√	√
43	695-704	K.LLEACTFHKP.	1	√	√	√

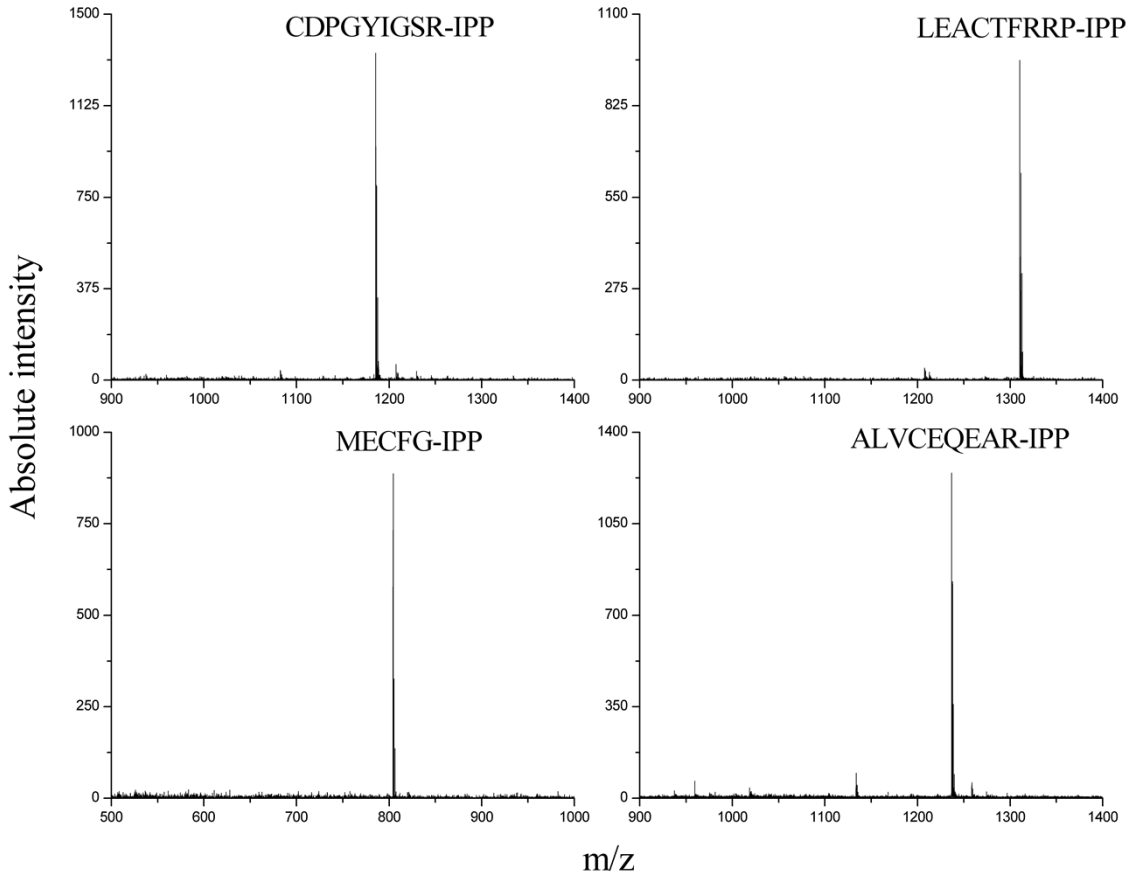

Figure S1. MALDI-TOF MS spectra of peptides CDPGYIGSR, LEACTFRRP, MECFG, and ALVCEQEAR respectively derivatized by IPP.

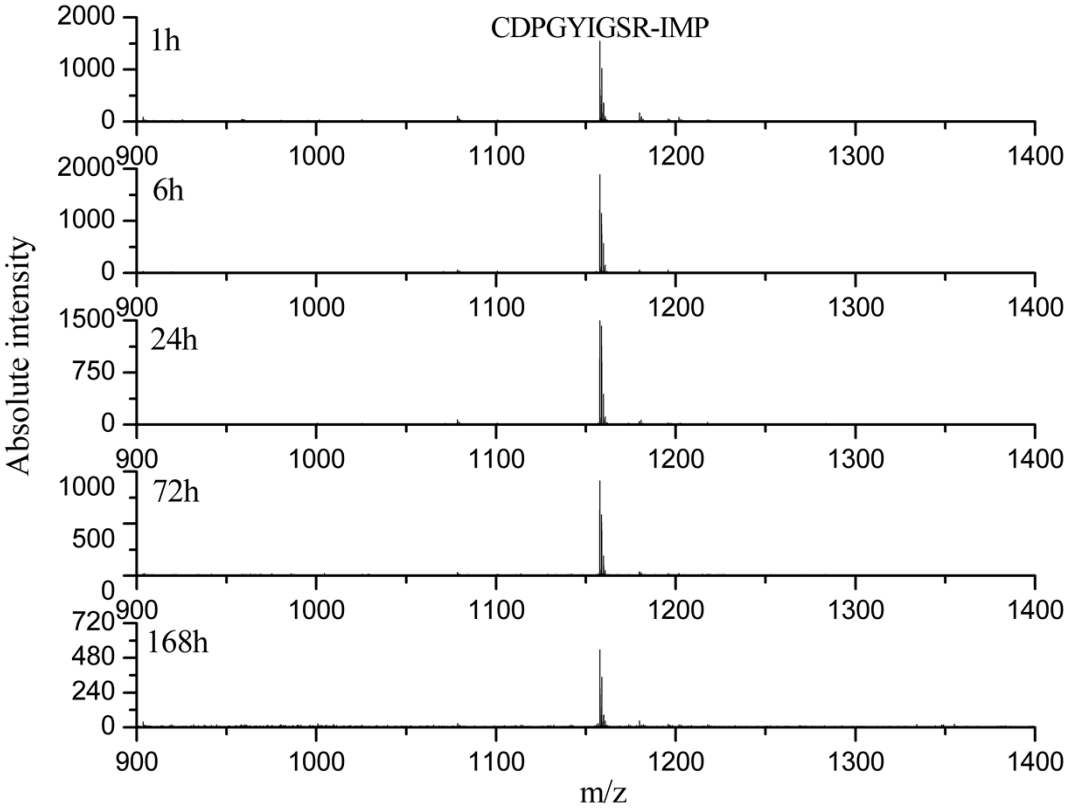

Figure S2. MALDI-TOF MS spectra of peptide CDPGYIGSR derivatized by IMP respectively stored at room temperature for 1 h, 6 h, 24 h, 72 h, and 168 h.

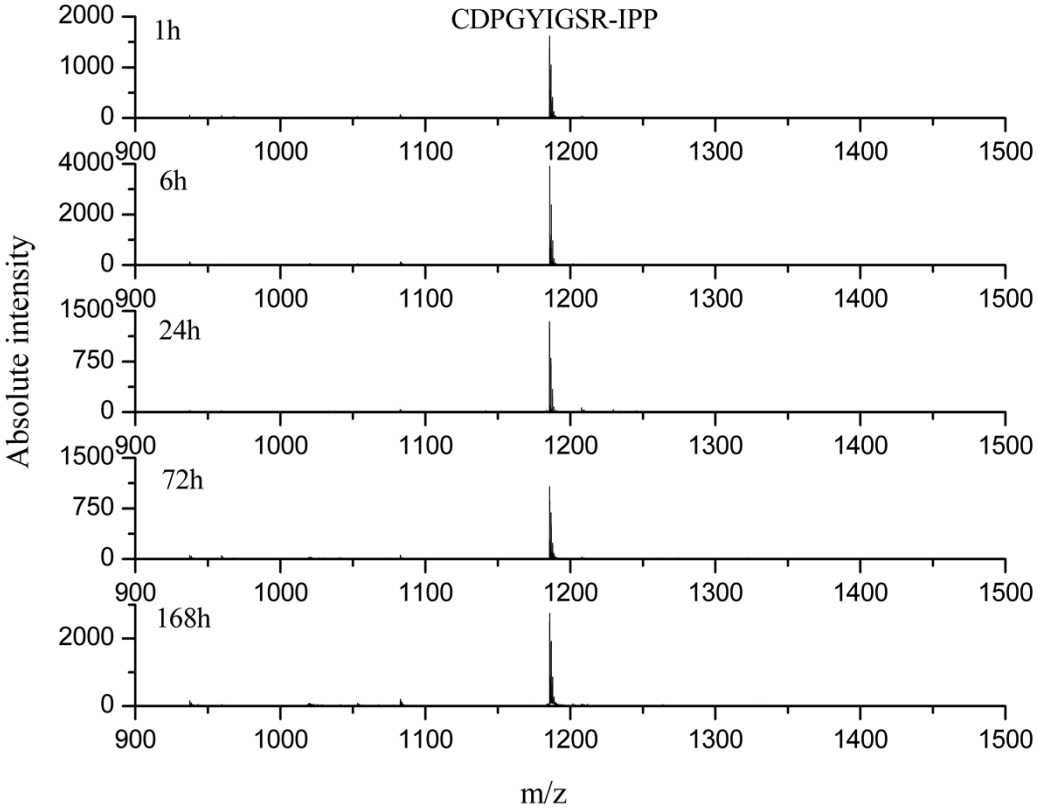

Figure S3. MALDI-TOF MS spectra of peptide CDPGYIGSR derivatized by IPP respectively stored at room temperature for 1 h, 6 h, 24 h, 72 h, and 168 h.

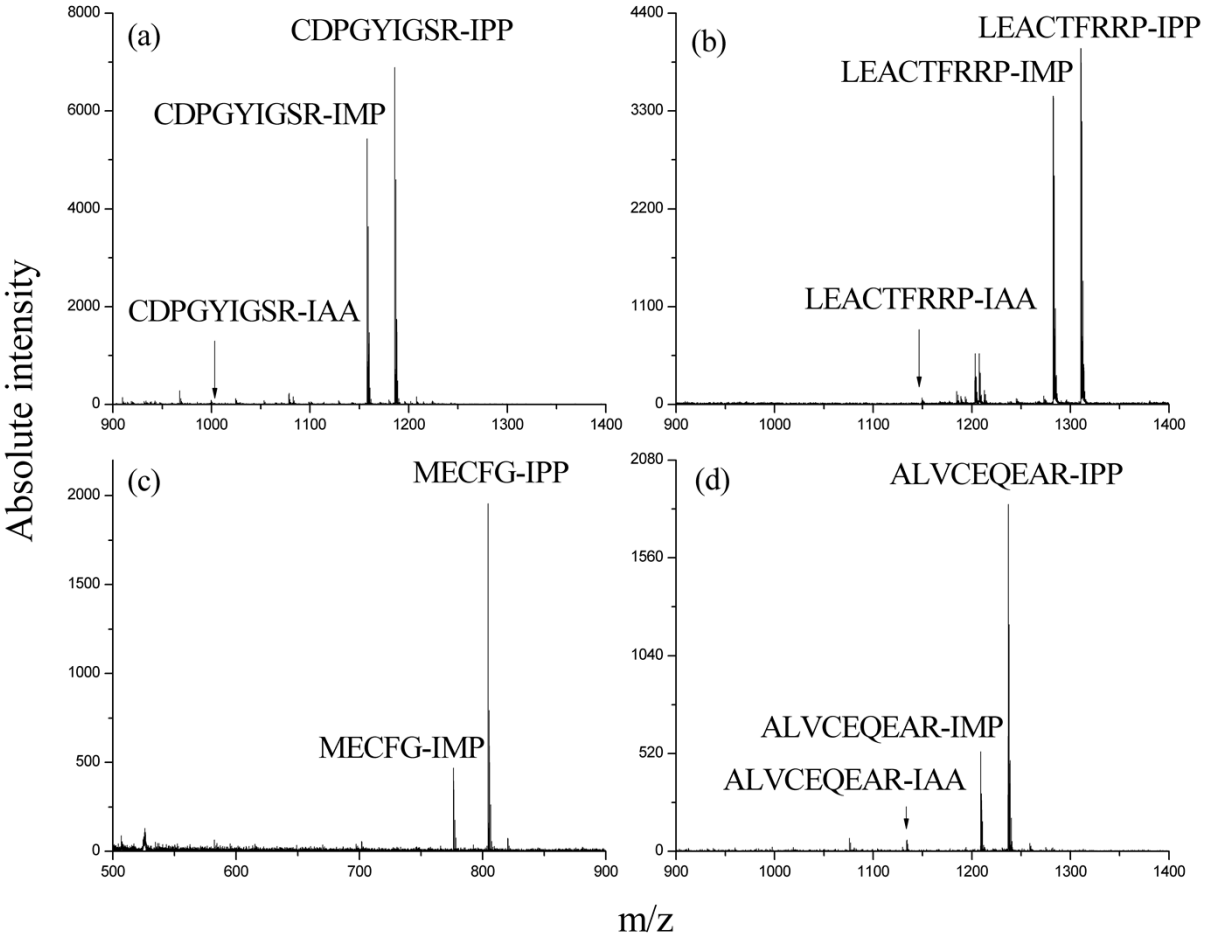

Figure S4. MALDI-TOF MS spectra of equimolar mixture of IAA, IMP, and IPP derivatized peptides CDPGYIGSR (a), LEACTFRRP (b), MECFG (c), and ALVCEQEAR (d).

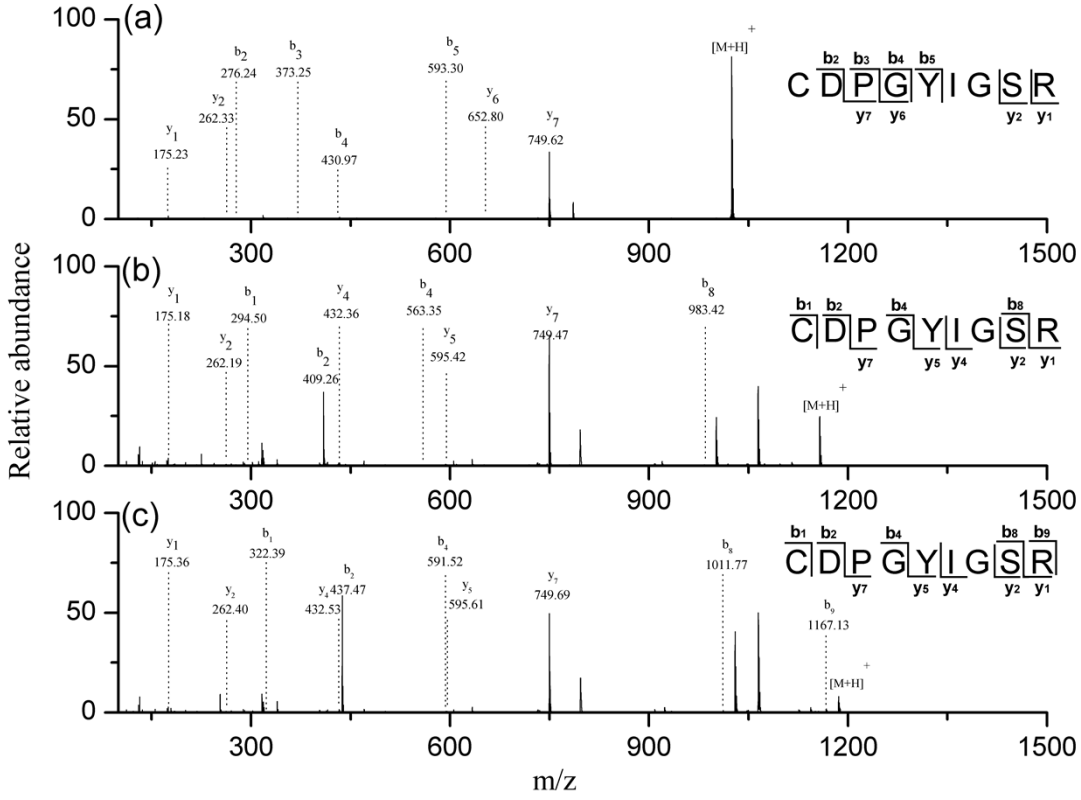

Figure S5. CID product ion mass spectra of the peptide CDPGYIGSR respectively derivatized by IAA (a), IMP (b), and IPP (c).