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Combined Mass Spectrometry-Guided Genome Mining and Virtual Screening for Acaricidal Active Secondary Metabolites of *Bacillus velezensis* W1

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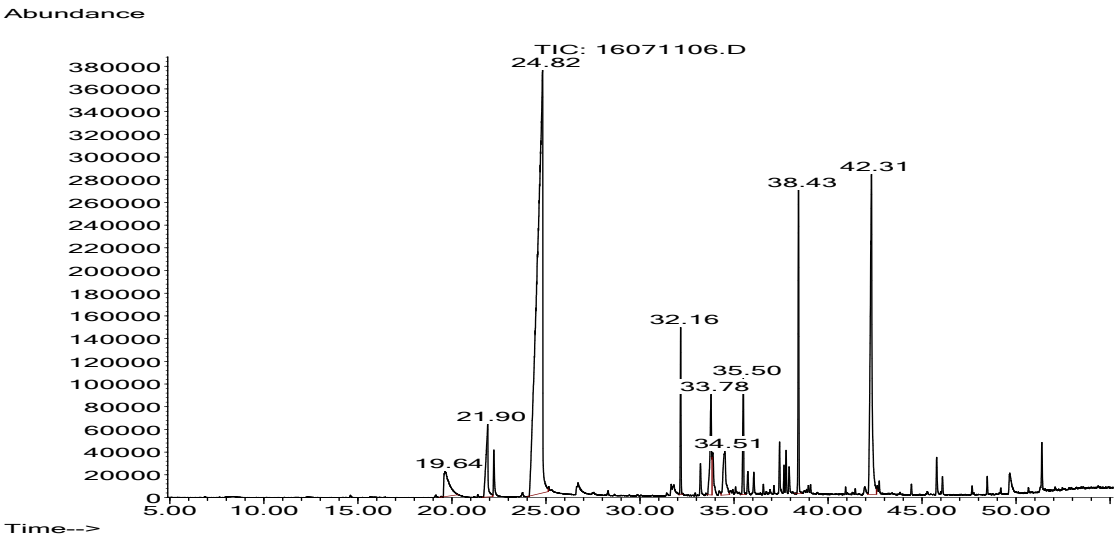
Content

Figure S1. GC-MS chromatogram of petroleum ether extraction part (PO98) of the crude extract of strain W1, including **S1.1:** total ion chromatograph (TIC), **S1.2:** area percent report, and **S1.3:** MS spectra of identified compound and the comparison of the MS spectra of its standard products.

S1.1: Total Ion Chromatograph (TIC)



S1.2: Area Percent Report

Data File : C:\MSDCHEM\1\DATA\16071106.D Vial: 1
Acq On : 11 Jul 2016 17:50 Operator:
Sample : P098 Inst : GCMS
Misc : Multiplr: 1.00
Sample Amount: 0.00
MS Integration Params: autoint1.e

Method : C:\MSDCHEM\1\METHODS\D-DDVP.M (Chemstation Integrator)
Title :

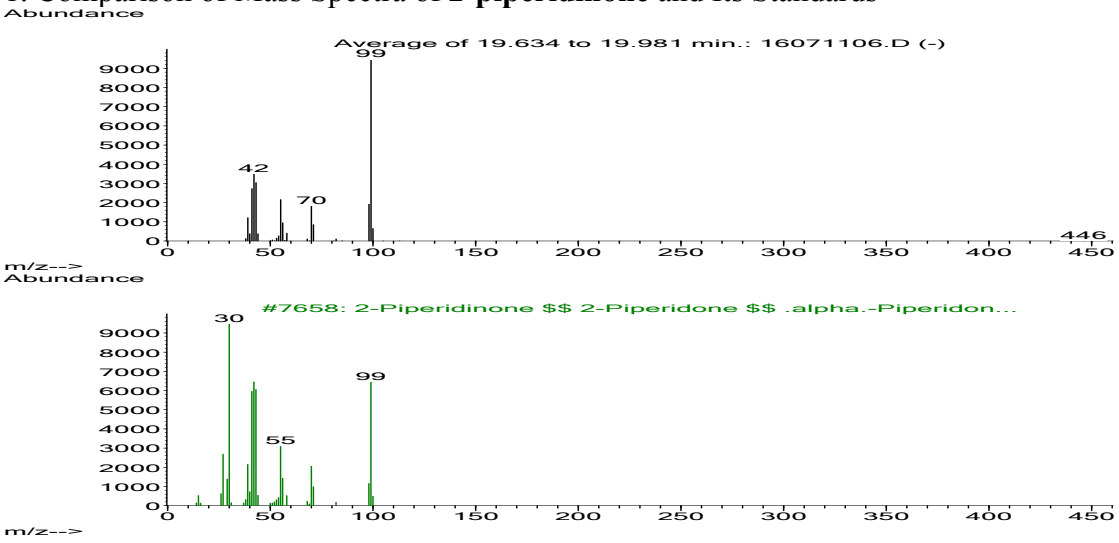
Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	19.639	3187	3212	3391	BB 4	22539	4921109	6.38%	3.183%
2	21.899	3555	3635	3686	PV	63739	5076274	6.58%	3.284%
3	22.235	3686	3698	3764	VB 2	40858	1649510	2.14%	1.067%
4	23.758	3901	3983	4009	BB 6	3621	251334	0.33%	0.163%
5	24.816	4015	4181	4238	BV 3	372590	77123138	100.00%	49.890%
6	25.152	4238	4244	4260	VV 9	5982	275448	0.36%	0.178%
7	25.302	4260	4272	4300	VB 9	2871	208920	0.27%	0.135%
8	26.707	4489	4535	4610	BB 5	9765	1248206	1.62%	0.807%
9	31.664	5449	5463	5472	VV 3	9904	420998	0.55%	0.272%
10	31.803	5472	5489	5540	VV 3	9119	897952	1.16%	0.581%
11	32.167	5540	5557	5576	PV	148323	3789323	4.91%	2.451%
12	33.219	5739	5754	5795	BV 3	28292	1134958	1.47%	0.734%
13	33.780	5822	5859	5869	VV 4	88560	5137624	6.66%	3.323%
14	33.865	5869	5875	5929	VV 3	37357	2387147	3.10%	1.544%
15	34.218	5929	5941	5958	PV 3	3831	222608	0.29%	0.144%
16	34.512	5958	5996	6042	VV	38756	3913411	5.07%	2.532%
17	35.084	6088	6103	6126	PV 8	6465	257646	0.33%	0.167%
18	35.495	6162	6180	6201	BV	102458	3668200	4.76%	2.373%
19	35.741	6201	6226	6255	VV 4	20582	888392	1.15%	0.575%
20	36.056	6255	6285	6313	PV 2	19559	782166	1.01%	0.506%
21	36.563	6358	6380	6393	BV	8849	240030	0.31%	0.155%
22	36.921	6424	6447	6473	VV	4369	242178	0.31%	0.157%
23	37.124	6473	6485	6513	VB 5	7918	247108	0.32%	0.160%
24	37.423	6514	6541	6575	BV	45893	1581550	2.05%	1.023%
25	37.658	6575	6585	6594	VV 2	25771	674153	0.87%	0.436%
26	37.771	6594	6606	6623	VV	38911	1236200	1.60%	0.800%
27	37.931	6623	6636	6663	VV 3	23813	948979	1.23%	0.614%
28	38.433	6708	6730	6759	PV	269532	7886157	10.23%	5.101%
29	38.957	6821	6828	6841	VV	7532	278026	0.36%	0.180%
30	39.074	6841	6850	6873	VV 6	8409	256730	0.33%	0.166%
31	41.959	7363	7390	7418	BV 4	7059	535459	0.69%	0.346%
32	42.306	7418	7455	7506	VV	280736	19836882	25.72%	12.832%
33	42.621	7506	7514	7525	VV 10	7596	317337	0.41%	0.205%

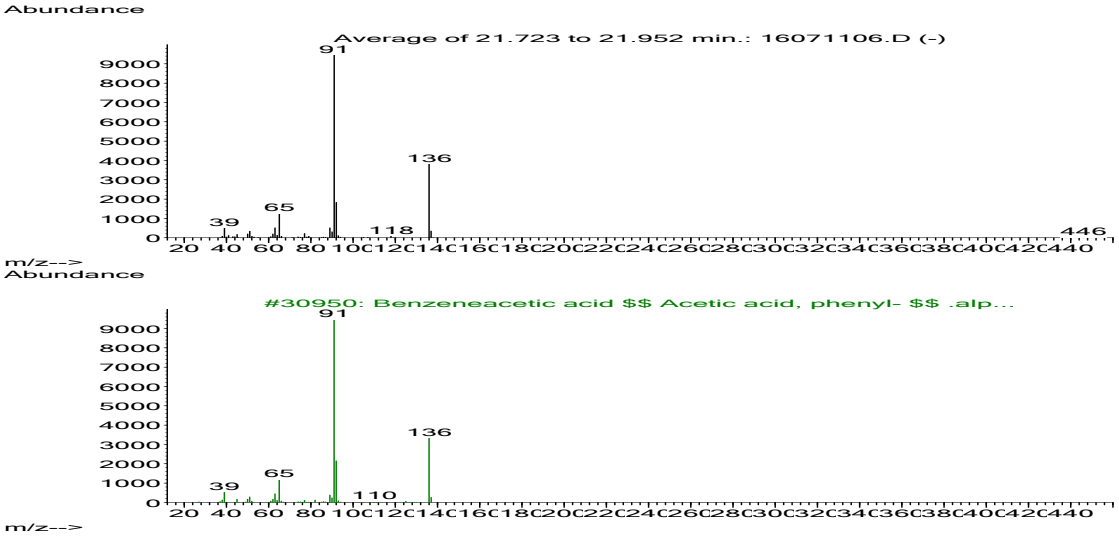
34	42.723	7525	7533	7562	VV	5	11490	406559	0.53%	0.263%
35	44.438	7828	7854	7886	BB	4	9591	284021	0.37%	0.184%
36	45.779	8057	8105	8138	BV	2	33010	1152655	1.49%	0.746%
37	46.089	8152	8163	8183	VB	6	16280	516667	0.67%	0.334%
38	48.466	8547	8608	8623	BV		16066	414358	0.54%	0.268%
39	49.187	8672	8743	8765	BB	7	5256	234943	0.30%	0.152%
40	49.668	8772	8833	8912	BV	7	18376	1751731	2.27%	1.133%
41	51.372	9056	9152	9176	BV	4	42452	1290516	1.67%	0.835%

S1.3: MS Spectra of identified Compound and the Comparison of the MS Spectra of Its Standard Products.

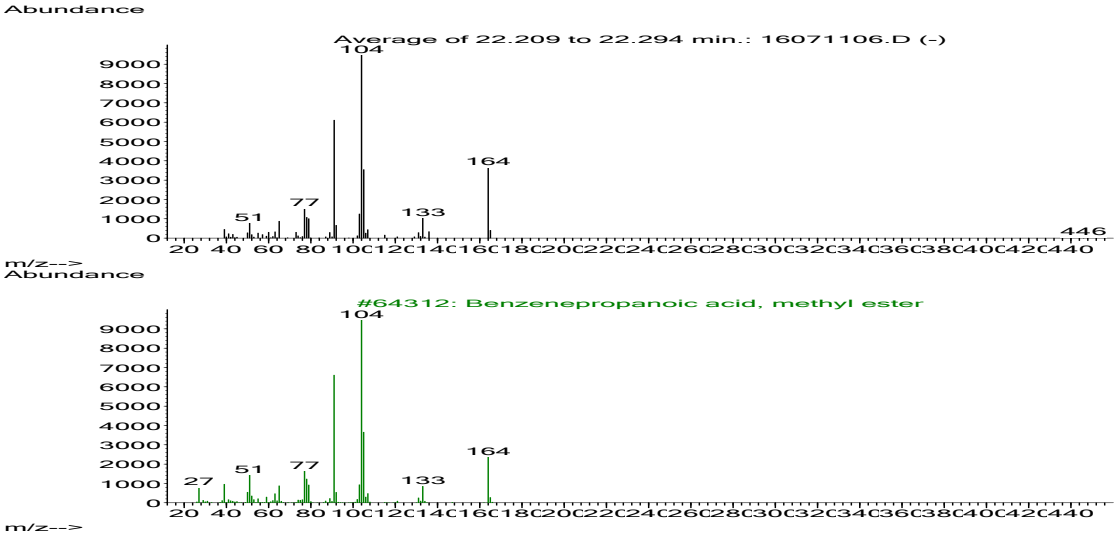
1. Comparison of Mass Spectra of **2-piperidinone** and Its Standards



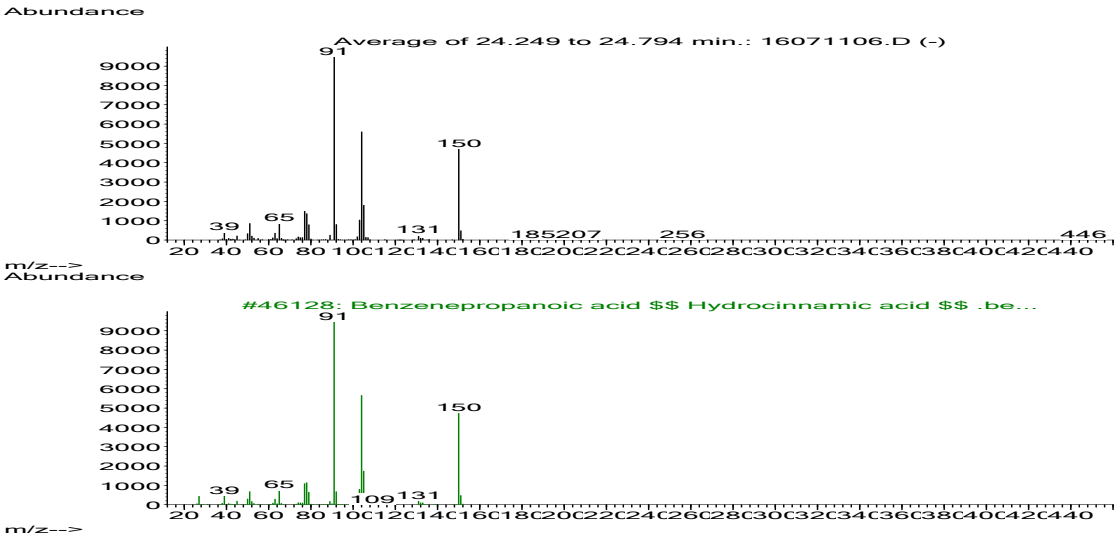
2. Comparison of Mass Spectra of **Benzeneacetic Acid** and Its Standards



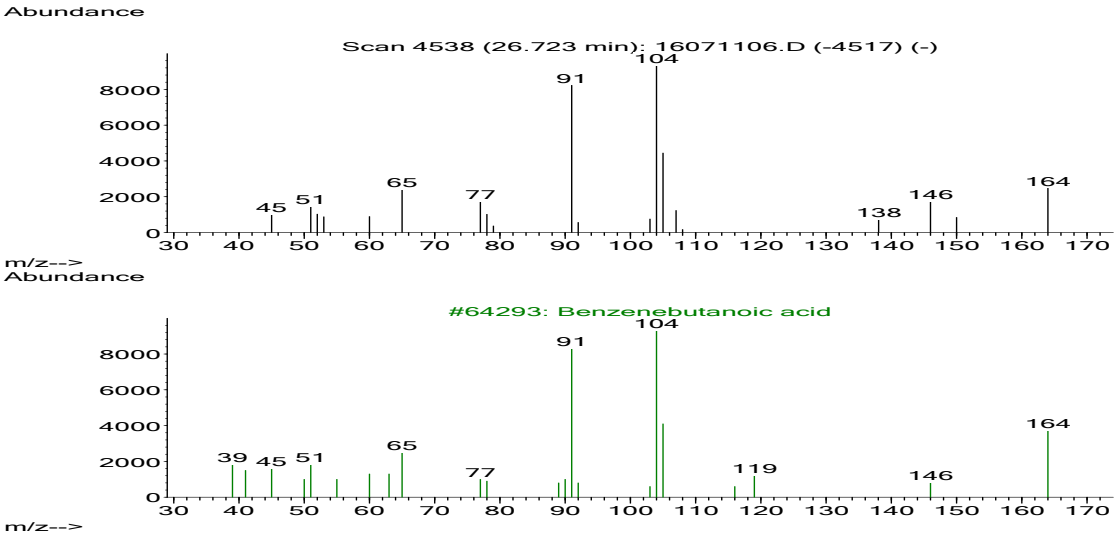
3. Comparison of Mass Spectra of **Methyl Ester Benzenepropanoic Acid** and Its Standards



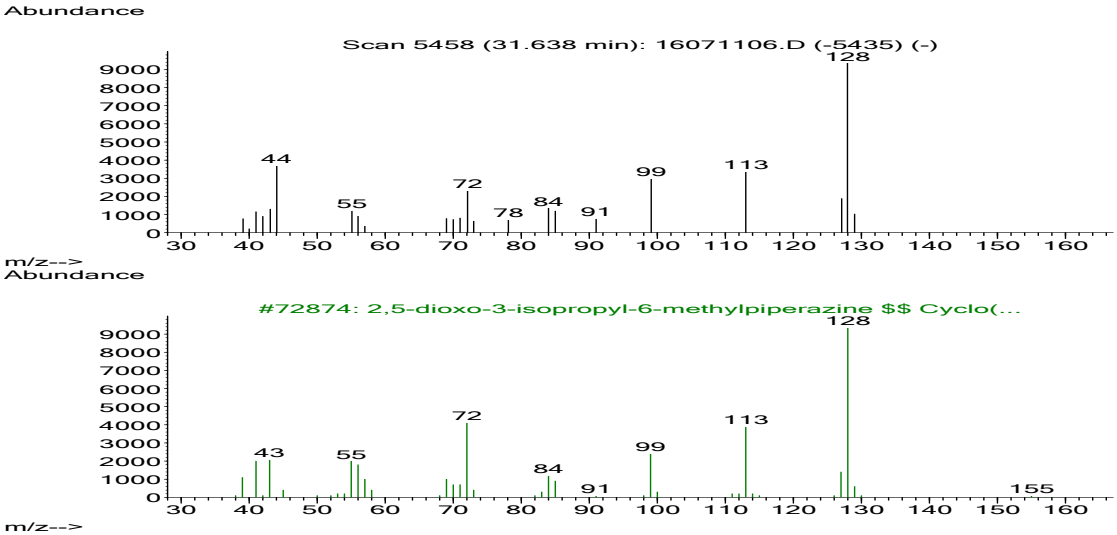
4. Comparison of Mass Spectra of **Benzenepropanoic Acid** and Its Standards



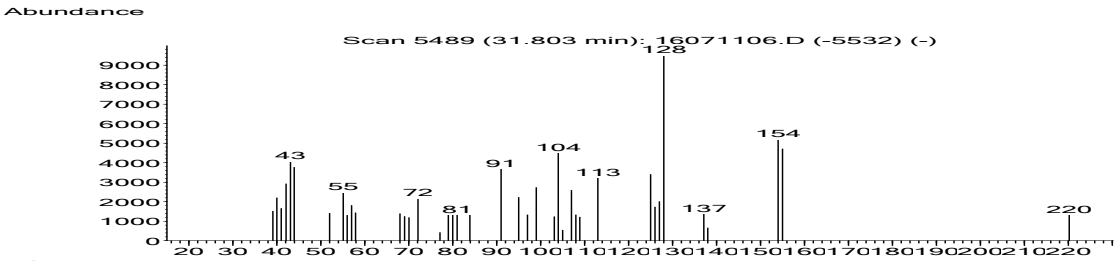
5. Comparison of Mass Spectra of **Benzenebutanoic Acid** and Its Standards



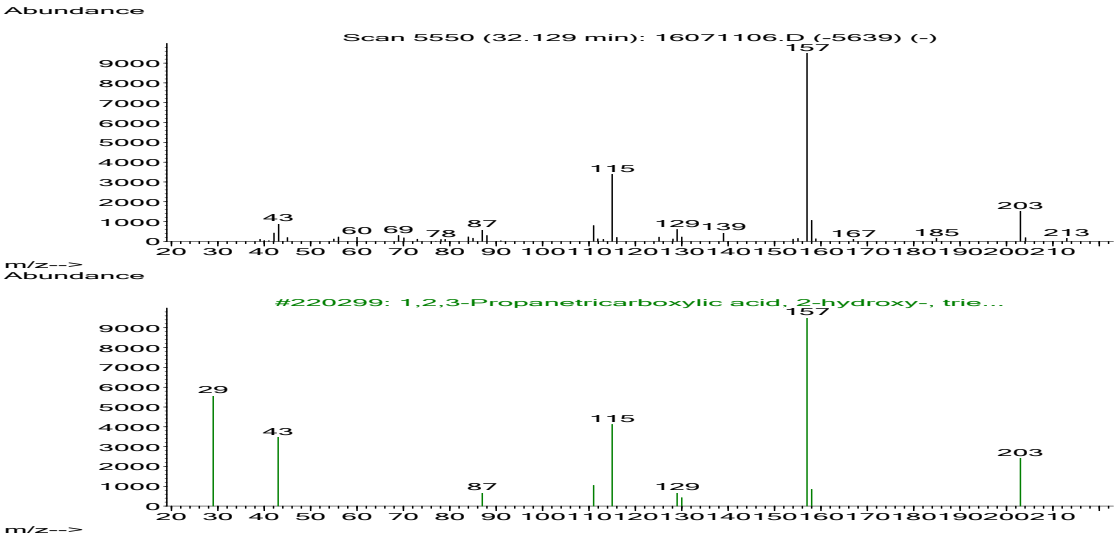
6. Comparison of Mass Spectra of **Cyclo(val-ala) Dipeptide** and Its Standards



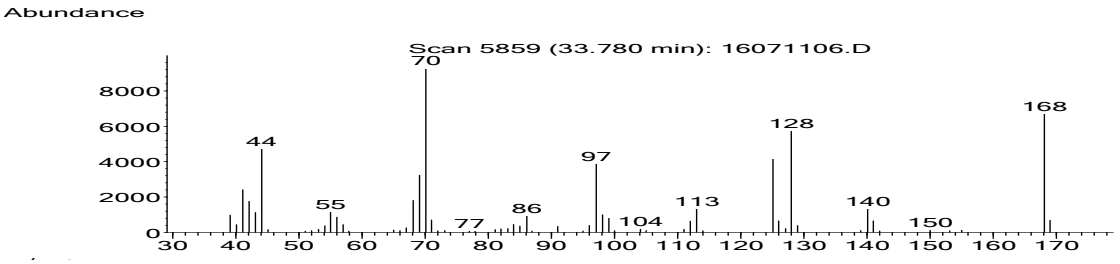
7. Mass Spectra of **Cyclo (Gly-L-Pro) Dipeptide**



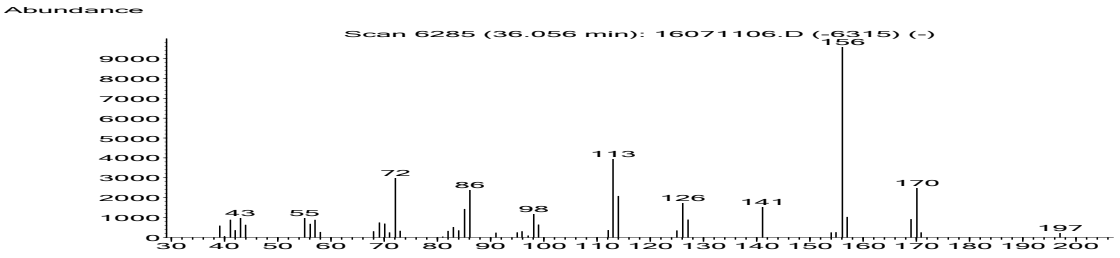
8. Comparison of Mass Spectra of **1,2,3-Propanetricarboxylic Acid,2-Hydroxy-,Triethyl Ester** and Its Standards



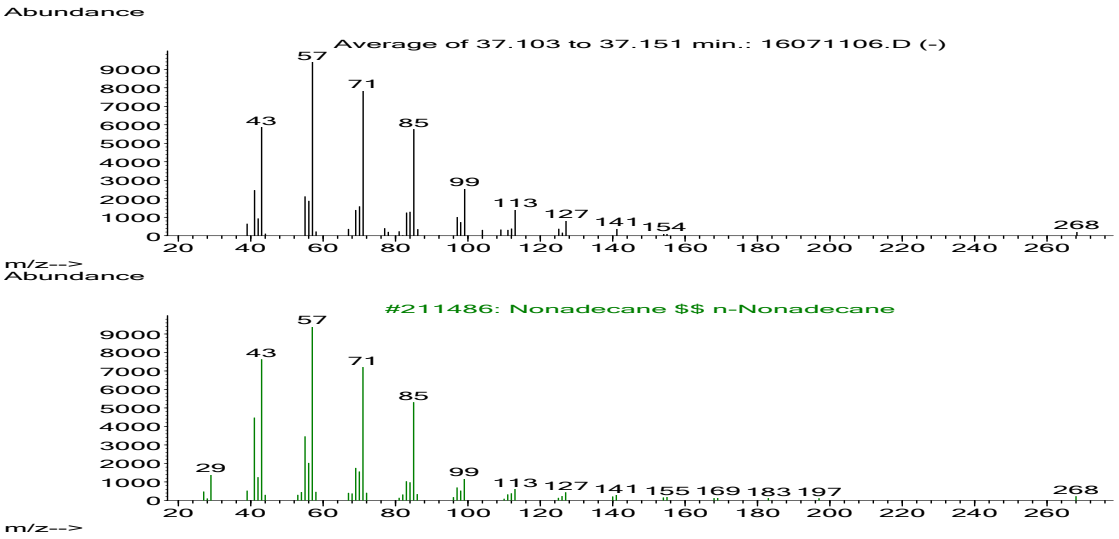
9. Mass Spectra of **Cyclo (L-Ala-L-Pro) Dipeptide**



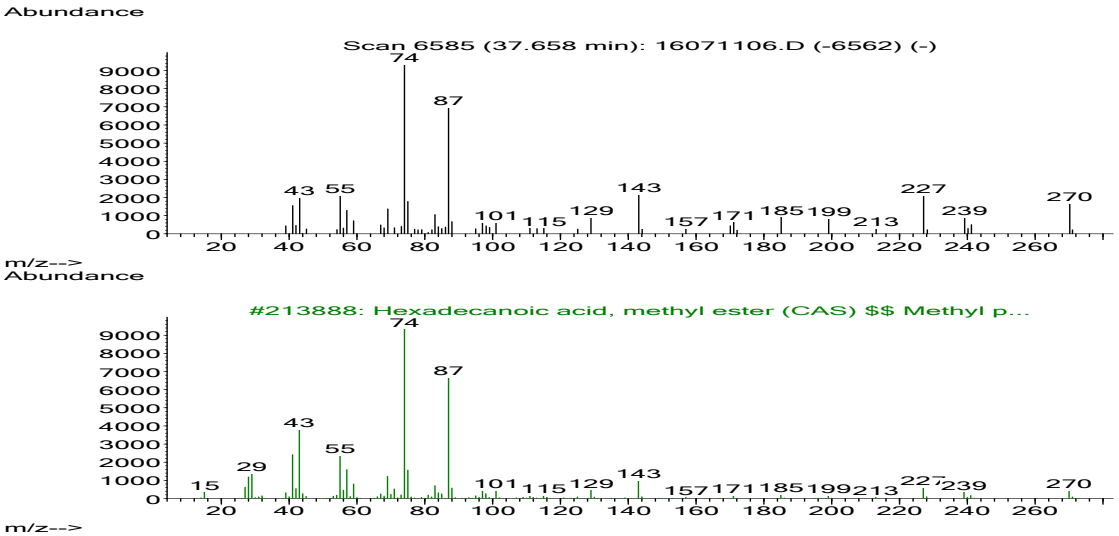
10. Mass Spectra of **Cyclo(gly-L-Val) Dipeptide**



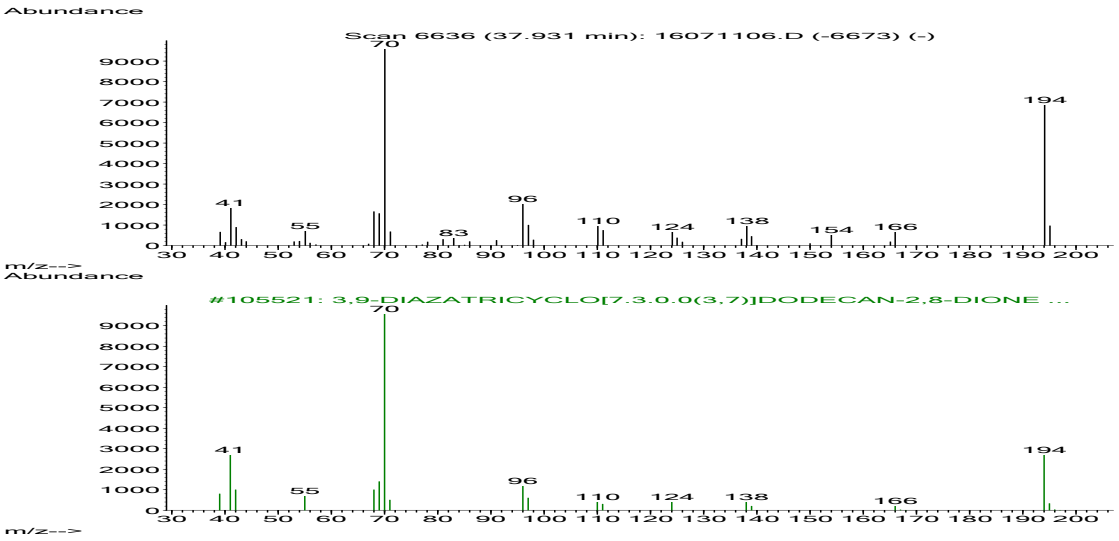
11. Comparison of Mass Spectra of **Nonadecane** and Its Standards



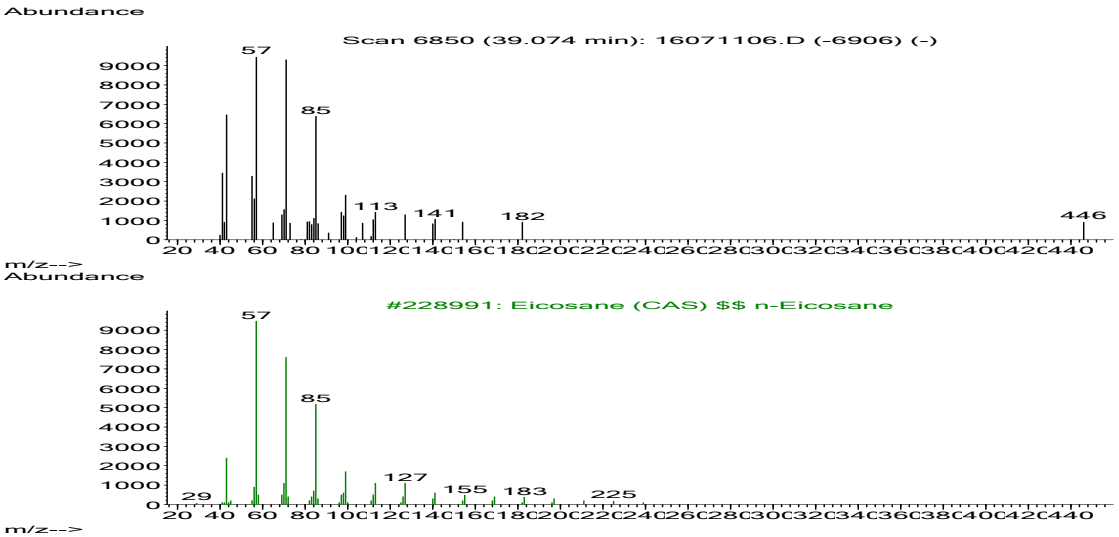
12. Comparison of Mass Spectra of **Hexadecanonic Acid, Methyl Ester** and Its Standards



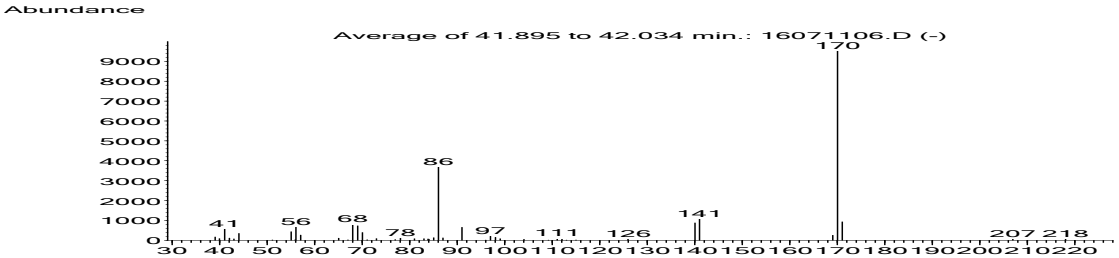
13 Comparison of Mass Spectra of **Cyclo (L-Pro-L-Pro) Dipeptide** and Its Standards



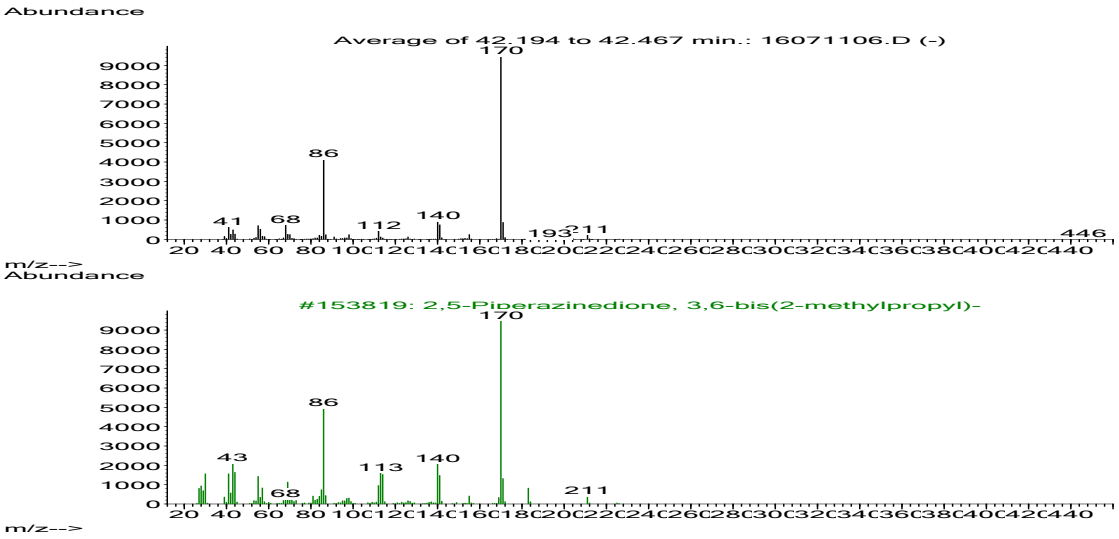
14. Comparison of Mass Spectra of **Icosane** and Its Standards



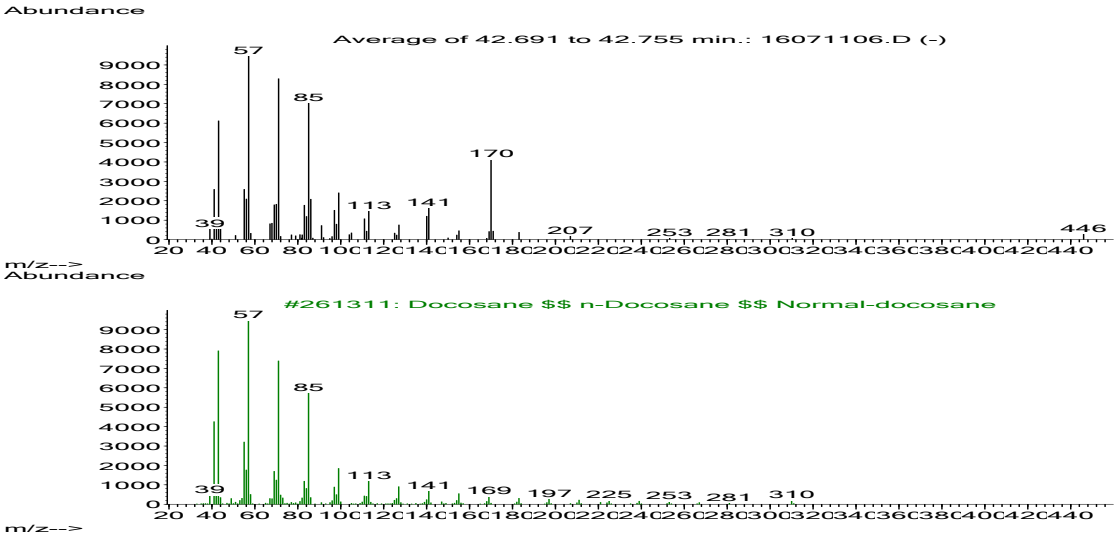
15. Mass Spectra of **Cyclo(Gly-L-Leu) Dipeptide**



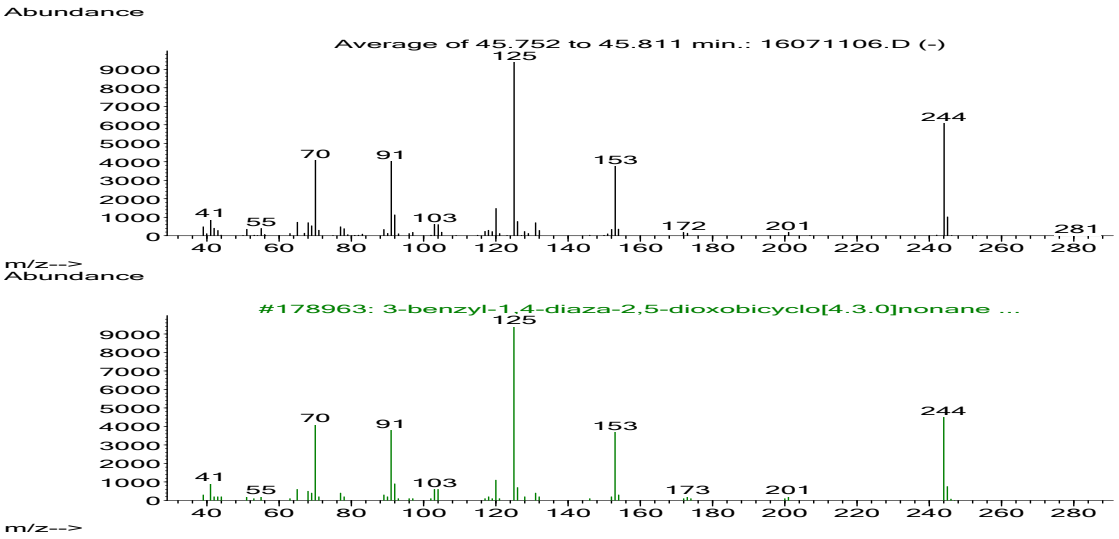
16. Comparison of Mass Spectra of **Cyclo (L-Leu-L-Leu) Dipeptide** and Its Standards



17. Comparison of Mass Spectra of **Docosane** and Its Standards



18. Comparison of Mass Spectra of **Cyclo (L-Phe-L-Pro) Dipeptide** and Its Standards



19. Comparison of Mass Spectra of **Cyclo (L-Phe-L-Leu) Dipeptide** and Its Standards

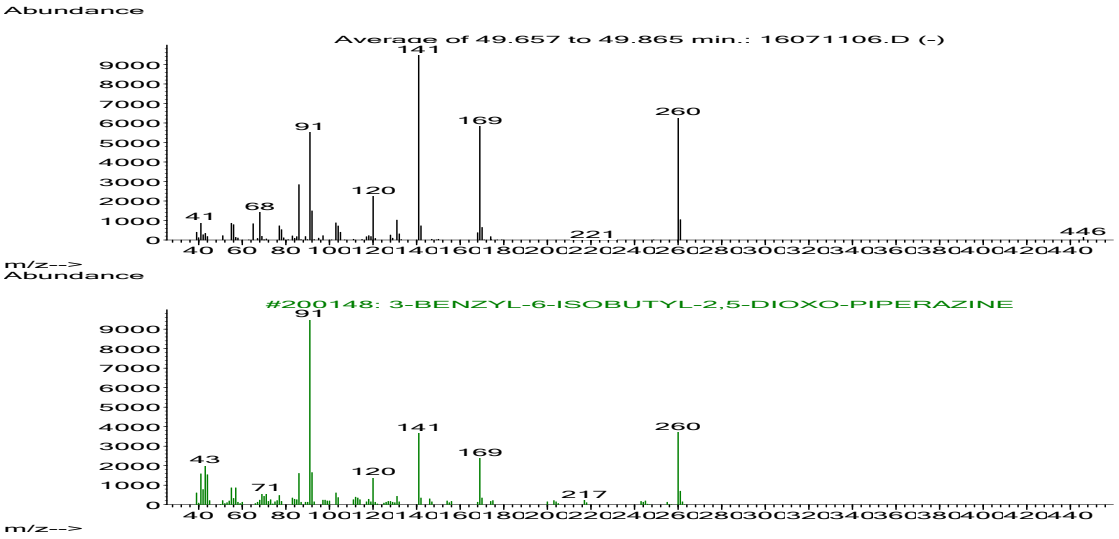
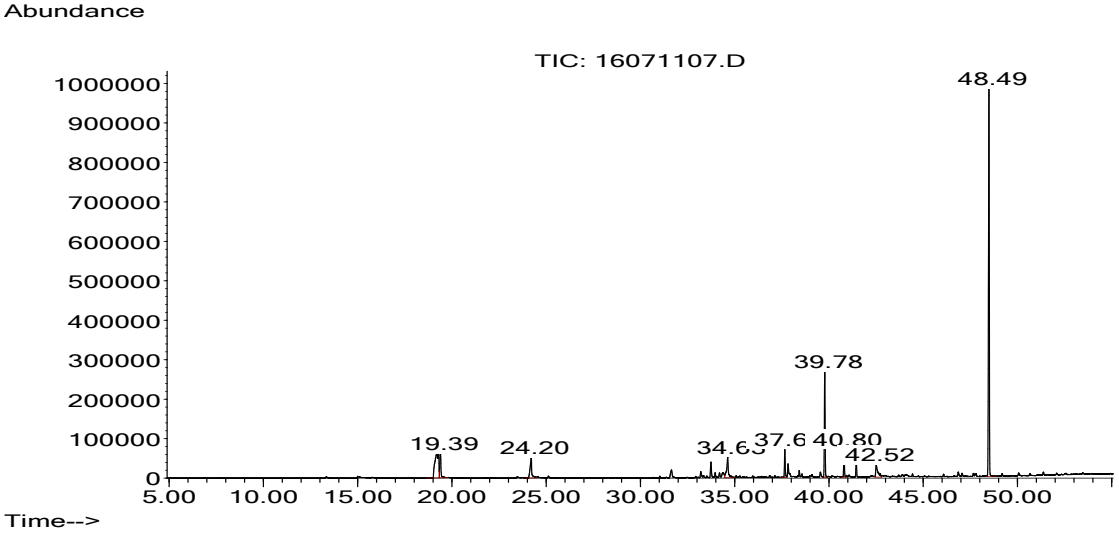


Figure S2. GC-MS chromatogram of ethyl acetate extraction part (PO99) of the crude extract of W1, including **S2.1:** total ion chromatograph (TIC), **S2.2:** area percent report, and **S2.3:** MS spectra of identified compound and the comparison of the MS spectra of its standard products.

S2.1: Total Ion Chromatograph (TIC)



S2.2: Area Percent Report

Data File : C:\MSDCHEM\1\DATA\16071107.D Vial: 1
Acq On : 11 Jul 2016 19:25 Operator:
Sample : P099 Inst : GCMS
Misc : Multiplr: 1.00
Sample Amount: 0.00
MS Integration Params: autoint1.e

Method : C:\MSDCHEM\1\METHODS\D-DDVP.M (Chemstation Integrator)
Title :

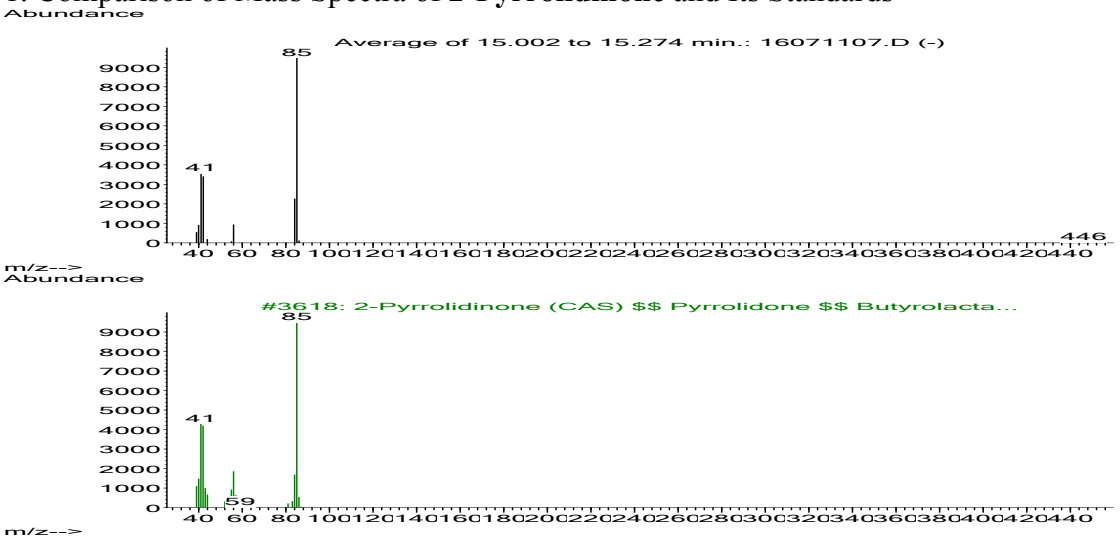
Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	% max.	% of total
1	13.346	1989	2034	2097	BB 4	3356	177106	0.59%	0.193%
2	15.018	2300	2347	2472	BV 2	4310	670757	2.25%	0.732%
3	15.771	2472	2488	2557	VB 6	2221	205971	0.69%	0.225%
4	19.201	3058	3130	3155	BV 5	64462	8722569	29.24%	9.525%
5	19.393	3155	3166	3238	VV	60053	2912780	9.76%	3.181%
6	19.821	3238	3246	3333	VB 6	1901	179980	0.60%	0.197%
7	23.475	3880	3930	3965	BV	3576	232640	0.78%	0.254%
8	24.201	4021	4066	4118	PV 2	50476	3206514	10.75%	3.502%
9	24.549	4118	4131	4215	VB 8	3355	329144	1.10%	0.359%
10	25.125	4221	4239	4271	BV 6	4662	180168	0.60%	0.197%
11	31.643	5436	5459	5509	VV 3	20206	1430975	4.80%	1.563%
12	32.936	5661	5701	5712	VV 7	4274	184078	0.62%	0.201%
13	33.208	5737	5752	5771	VV 7	15372	723590	2.43%	0.790%
14	33.347	5771	5778	5797	VV 9	6513	258213	0.87%	0.282%
15	33.523	5797	5811	5834	VV 6	5135	258432	0.87%	0.282%
16	33.743	5834	5852	5882	VV 3	40600	1597246	5.35%	1.744%
17	33.967	5882	5894	5922	VV 2	13237	559799	1.88%	0.611%
18	34.197	5922	5937	5951	VV 4	12968	505467	1.69%	0.552%
19	34.384	5951	5972	5989	VV 5	12675	1093597	3.67%	1.194%
20	34.624	5989	6017	6086	VV 4	51366	3559241	11.93%	3.887%
21	35.083	6086	6103	6116	VV 8	5639	238631	0.80%	0.261%
22	35.281	6116	6140	6157	VV 6	4587	316113	1.06%	0.345%
23	35.447	6157	6171	6199	VV 10	3026	233141	0.78%	0.255%
24	35.965	6249	6268	6310	VV 7	4412	302606	1.01%	0.330%
25	36.264	6310	6324	6350	VV 7	1808	185564	0.62%	0.203%
26	36.558	6369	6379	6420	VV 5	3040	218089	0.73%	0.238%
27	36.862	6420	6436	6470	VV 6	5501	318657	1.07%	0.348%
28	37.130	6470	6486	6507	VV 10	5141	219740	0.74%	0.240%
29	37.664	6565	6586	6604	VV 2	70634	2069365	6.94%	2.260%
30	37.835	6604	6618	6657	VV 3	33661	1816557	6.09%	1.984%
31	38.112	6657	6670	6703	VV 3	3235	349993	1.17%	0.382%
32	38.428	6703	6729	6740	VV	17925	704493	2.36%	0.769%

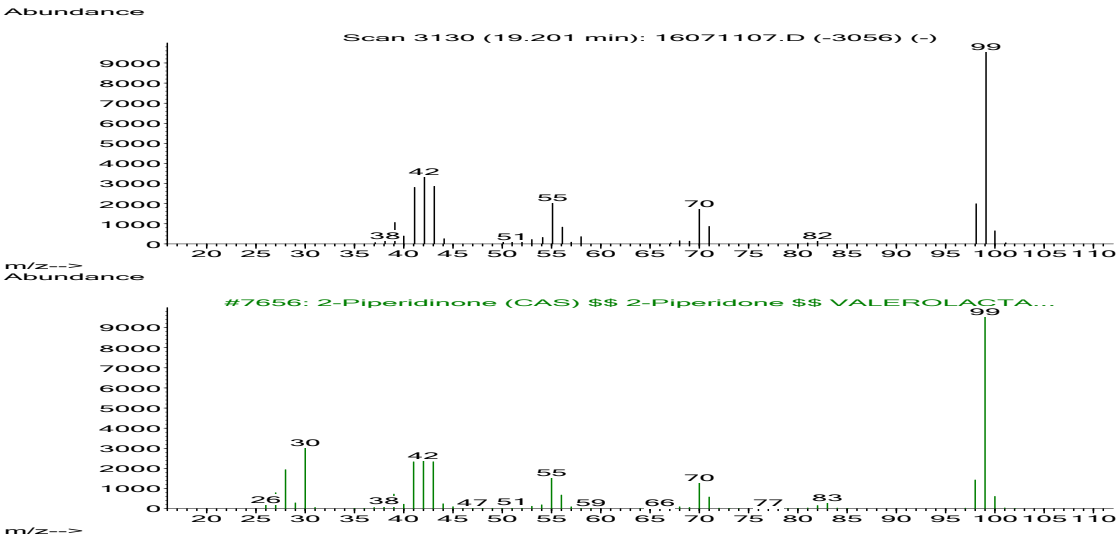
33	38.567	6740	6755	6787	VV	4	9269	413312	1.39%	0.451%
34	38.983	6819	6833	6844	VV	9	5112	184600	0.62%	0.202%
35	39.101	6844	6855	6904	VV	9	7385	468842	1.57%	0.512%
36	39.550	6929	6939	6965	VV	6	13514	595518	2.00%	0.650%
37	39.779	6965	6982	7007	VV		265525	7613305	25.52%	8.314%
38	39.966	7007	7017	7045	VV		2664	198700	0.67%	0.217%
39	40.169	7045	7055	7082	VV		3893	280936	0.94%	0.307%
40	40.479	7082	7113	7147	VV		2440	361230	1.21%	0.394%
41	40.805	7147	7174	7190	VV		69550	2060894	6.91%	2.251%
42	41.067	7209	7223	7266	VV	9	5435	377210	1.26%	0.412%
43	41.451	7266	7295	7322	VV	2	48329	1352206	4.53%	1.477%
44	42.312	7405	7456	7478	VV	2	4162	450795	1.51%	0.492%
45	42.514	7478	7494	7545	VV	7	29234	2515156	8.43%	2.747%
46	42.830	7545	7553	7565	VV	3	4169	227846	0.76%	0.249%
47	42.969	7565	7579	7632	VV	3	4473	516241	1.73%	0.564%
48	43.369	7632	7654	7701	VV	3	2614	341087	1.14%	0.372%
49	43.700	7701	7716	7735	VV	9	5048	245518	0.82%	0.268%
50	43.898	7735	7753	7768	VV	5	6341	377580	1.27%	0.412%
51	44.101	7768	7791	7841	VV	5	5443	784710	2.63%	0.857%
52	44.432	7841	7853	7867	VV	4	8003	266500	0.89%	0.291%
53	44.748	7898	7912	7955	VV	4	2567	212984	0.71%	0.233%
54	45.079	7955	7974	8006	VV	4	2357	183929	0.62%	0.201%
55	45.298	8006	8015	8101	PB	4	2101	218808	0.73%	0.239%
56	46.083	8144	8162	8176	PV	6	6691	225336	0.76%	0.246%
57	46.863	8285	8308	8335	VV	3	11761	570823	1.91%	0.623%
58	47.061	8335	8345	8363	VV	4	8329	336174	1.13%	0.367%
59	47.248	8363	8380	8418	VV	4	1936	194372	0.65%	0.212%
60	47.664	8439	8458	8466	VV	5	8326	277768	0.93%	0.303%
61	47.803	8466	8484	8507	VV	5	7377	435318	1.46%	0.475%
62	48.487	8589	8612	8698	VV		1023841	29831765	100.00%	32.577%
63	49.192	8734	8744	8799	VV	9	6981	309395	1.04%	0.338%
64	49.727	8799	8844	8893	PV	9	1442	218794	0.73%	0.239%
65	50.068	8893	8908	8939	VV	7	8038	397648	1.33%	0.434%
66	50.378	8939	8966	9004	VV	7	1721	202117	0.68%	0.221%
67	50.667	9004	9020	9071	VV	7	6083	359597	1.21%	0.393%
68	51.206	9071	9121	9143	PV	7	2528	374221	1.25%	0.409%
69	51.377	9143	9153	9174	VV	7	9029	375074	1.26%	0.410%
70	51.618	9174	9198	9231	VV	7	2491	286758	0.96%	0.313%
71	52.082	9231	9285	9309	VV	7	5752	460562	1.54%	0.503%
72	52.339	9309	9333	9345	VV	7	2597	182723	0.61%	0.200%
73	52.574	9345	9377	9411	VV	7	4319	506750	1.70%	0.553%
74	53.039	9411	9464	9501	VV	7	2326	542450	1.82%	0.592%
75	53.333	9501	9519	9532	VV	7	3093	216305	0.73%	0.236%
76	53.466	9532	9544	9577	VV	7	5212	396551	1.33%	0.433%
77	53.888	9597	9623	9639	VV	7	2676	257820	0.86%	0.282%
78	54.203	9673	9682	9731	VV	7	1535	231316	0.78%	0.253%
79	54.502	9731	9738	9794	VV	7	1491	173417	0.58%	0.189%

S2.3: MS spectra of identified compound and the comparison of the MS spectra of its standard products

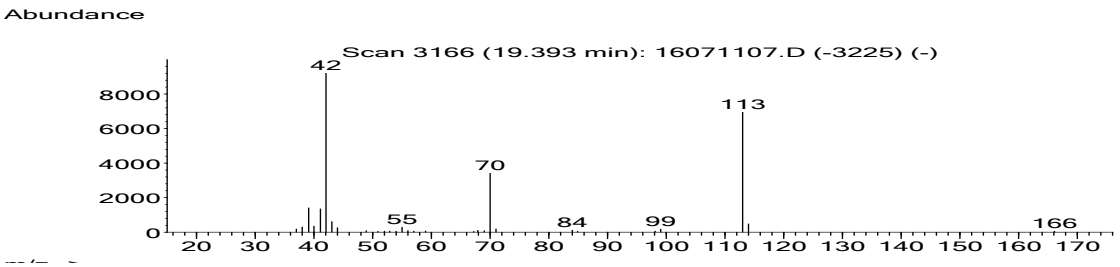
1. Comparison of Mass Spectra of **2-Pyrrolidinone** and Its Standards



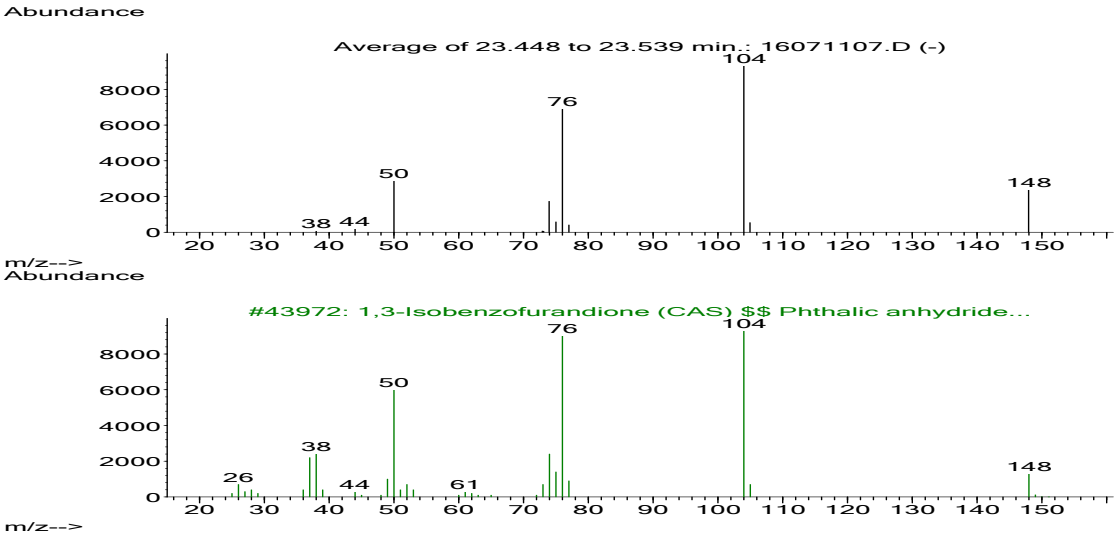
2. Comparison of Mass Spectra of **2-Piperidinone** and Its Standards



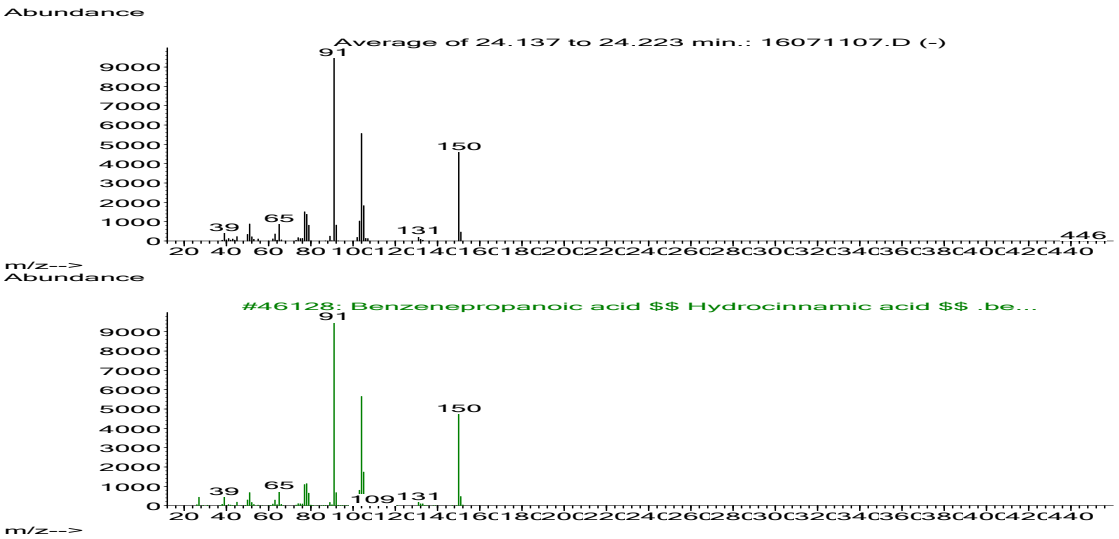
3. Mass Spectra of **Cyclo (Gly-Gly) Dipeptide**



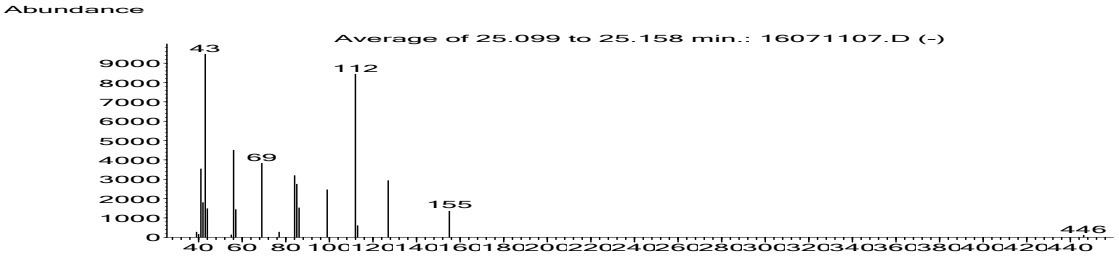
4. Comparison of Mass Spectra of **1,3-Isobenzofurandione** and Its Standards



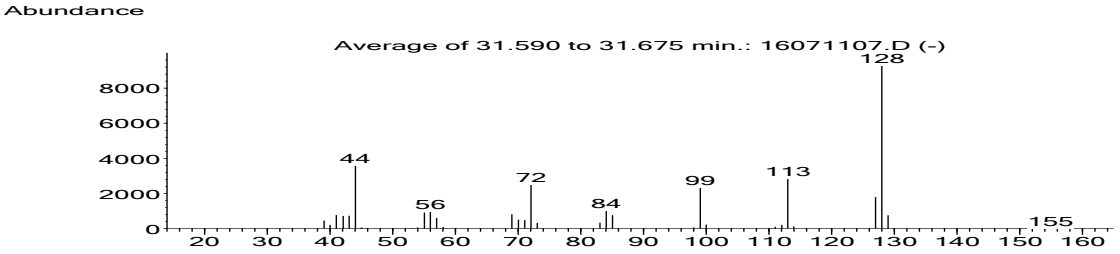
5. Comparison of Mass Spectra of **Benzenepropanoic Acid** and Its Standards



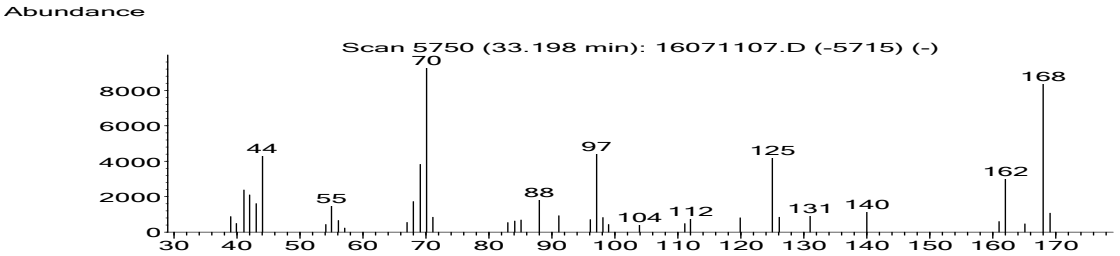
6. Mass Spectra of **Cyclo (Gly-L-Pro) Dipiptide**



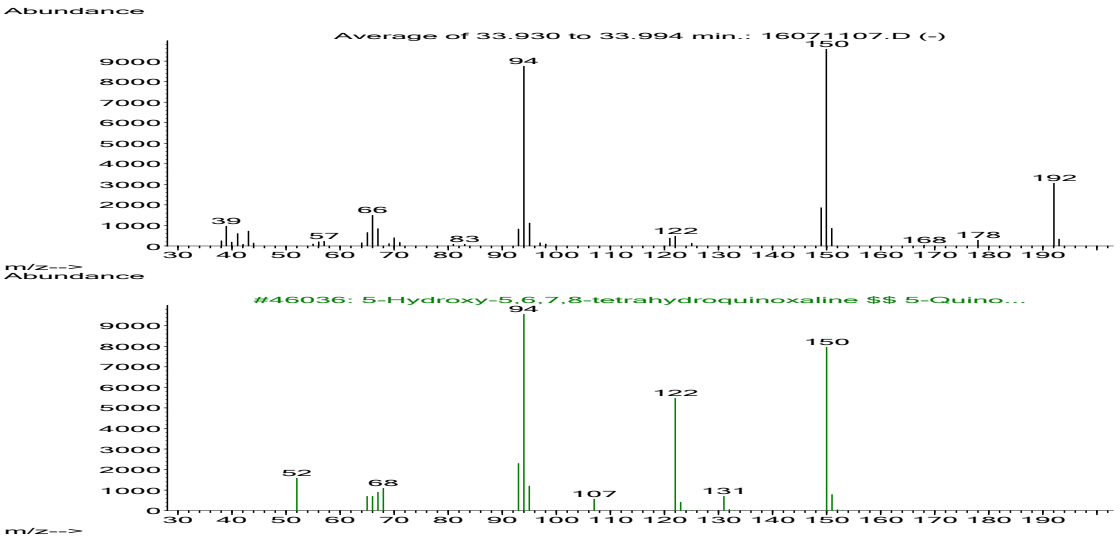
7. Mass Spectra of **Cyclo (Gly-L-Ala) Dipeptide**



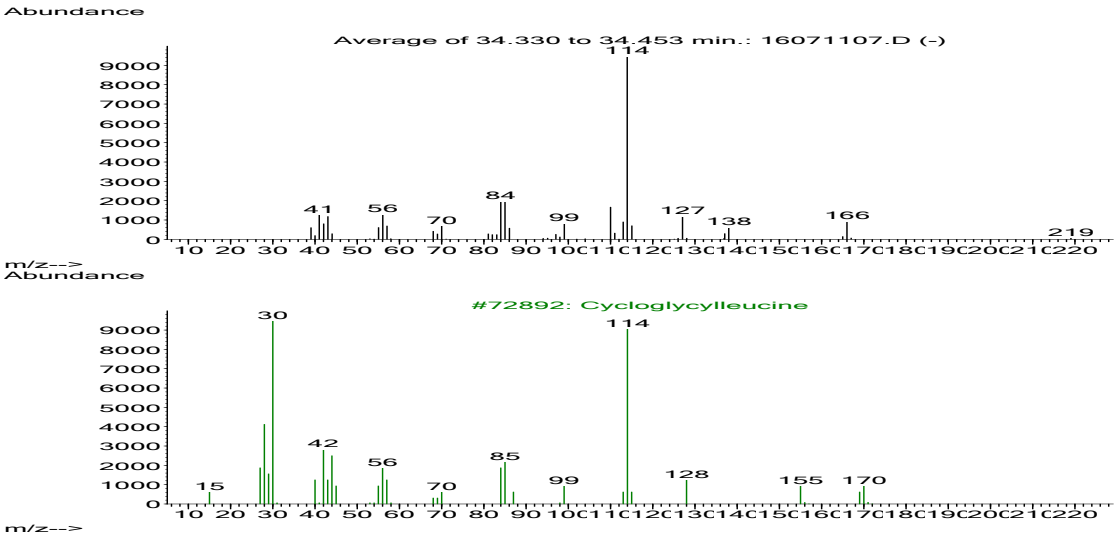
8. Mass Spectra of **Cyclo (L-Ala-L-Pro) Dipeptide**



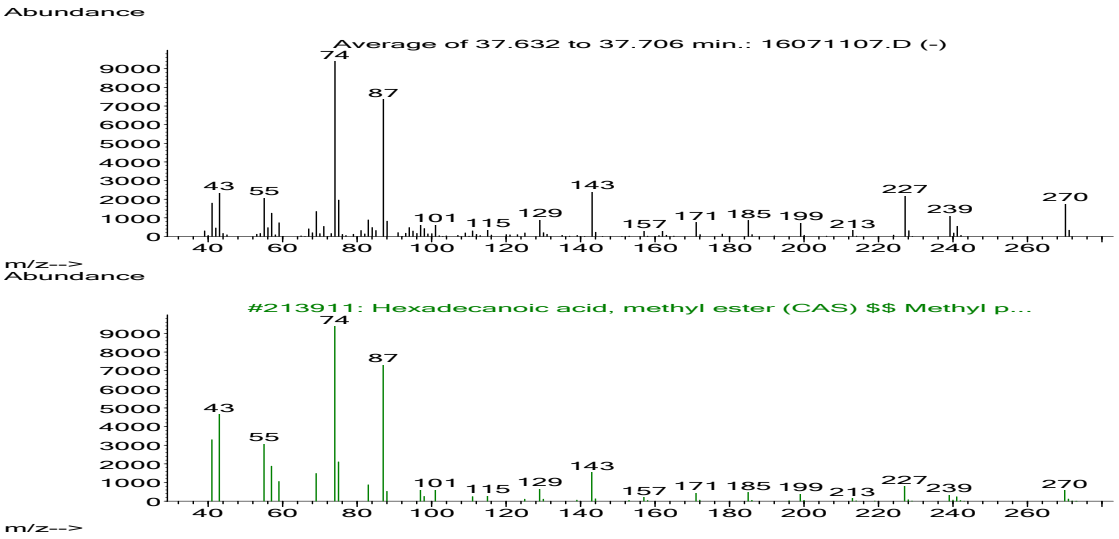
9. Comparison of Mass Spectra of **5-Hydroxy-5,6,7,8-Tetahydroquinoxaline** and Its Standards



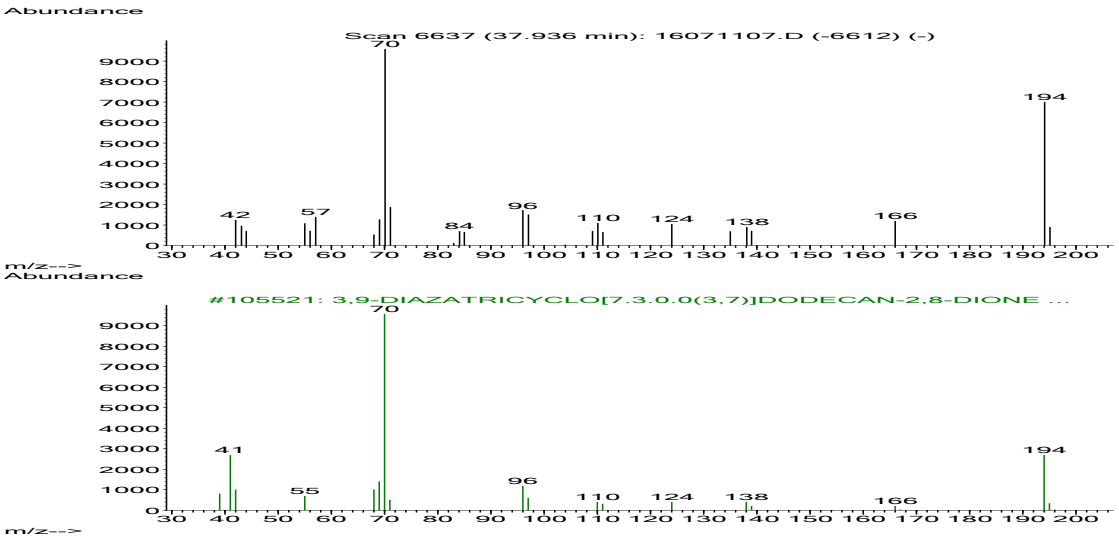
10. Comparison of Mass Spectra of **Cyclo (L-Gly-L-Leu) Dipeptide** and Its Standards



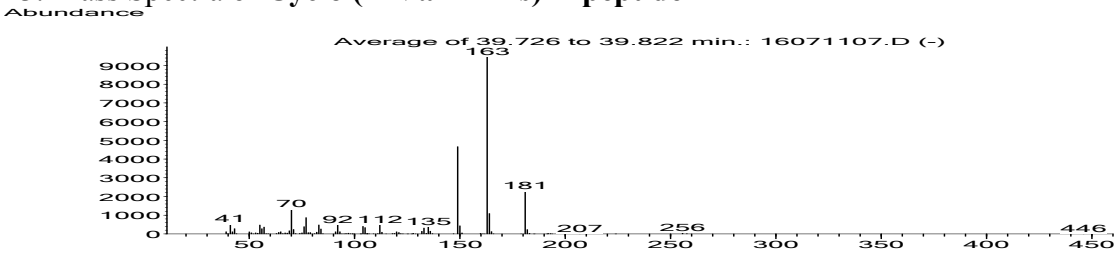
11 Comparison of Mass Spectra of **hexadecanoic acid, methyl ester** and Its Standards



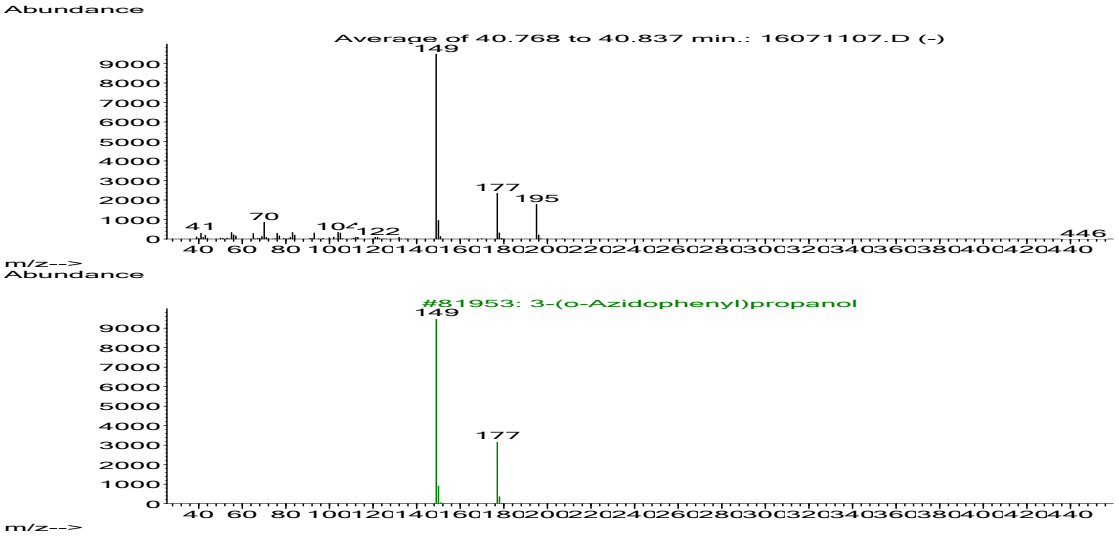
12 Comparison of Mass Spectra of **Cyclo (L-Pro-L-Pro) Dipeptide** and Its Standards



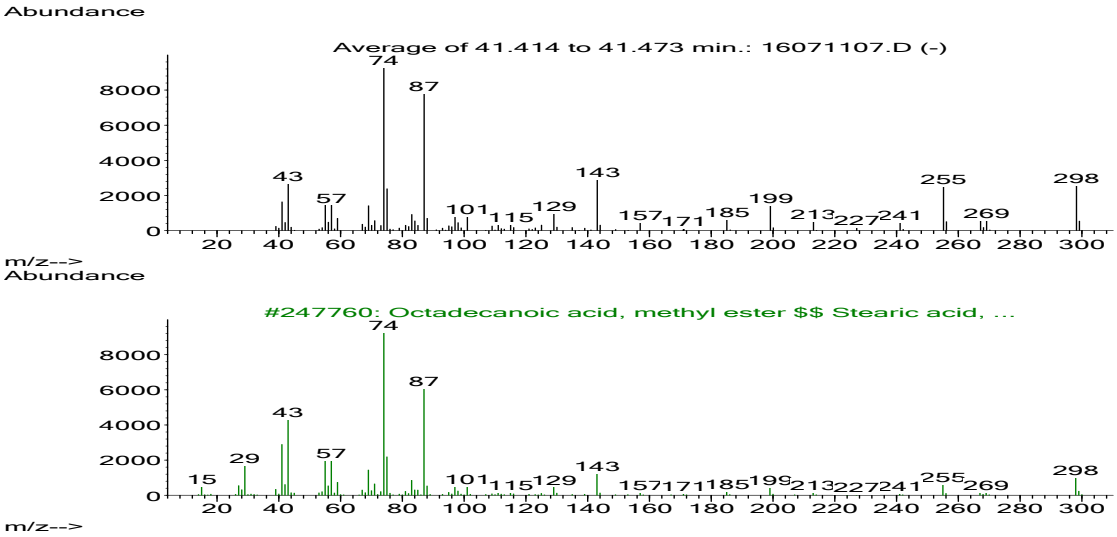
13. Mass Spectra of **Cyclo (L-Val-L-His) Dipeptide**



14. Comparison of Mass Spectra of **3-(o-azidophenyl) Propanol** and Its Standards



15. Comparison of Mass Spectra of **Octadecanoic Acid, Mrthyi Ester** and Its Standards



16. Comparison of Mass Spectra of **Cyclo (L-Pro-oh-L-Pro) Dipeptide** and Its Standards

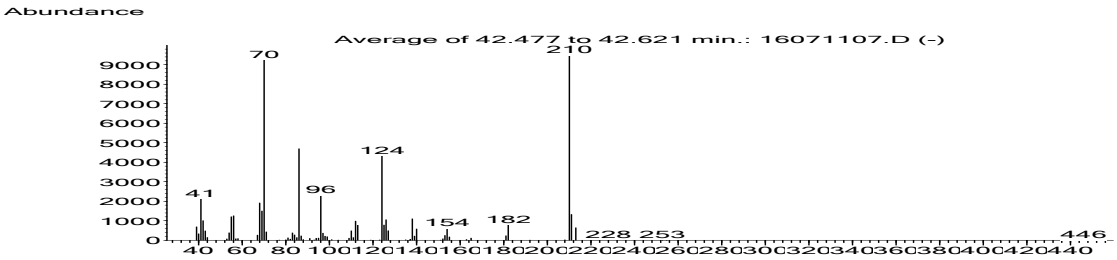
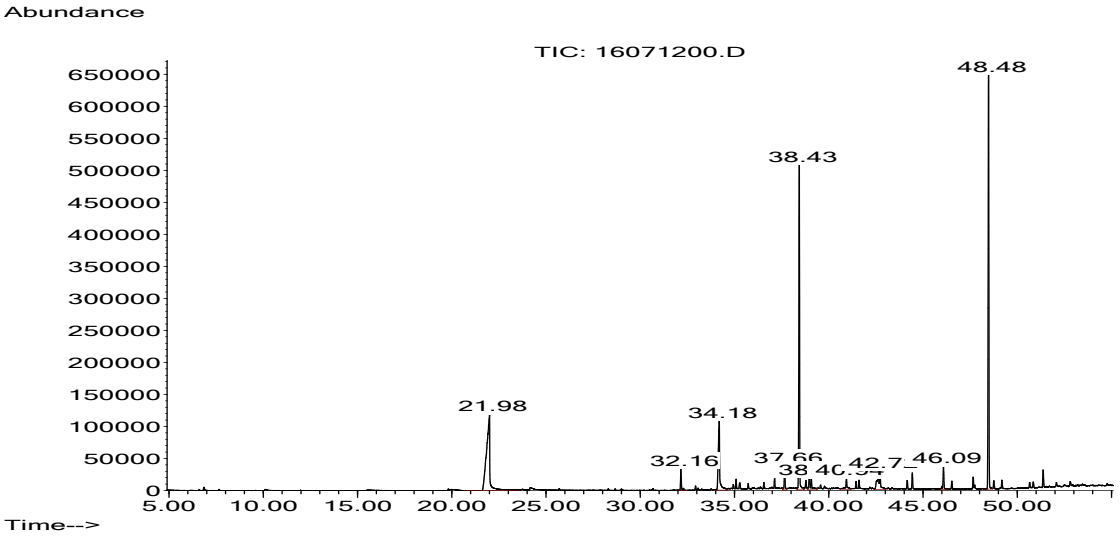


Figure S3. GC-MS chromatogram of acetone extraction part (PO100) of the crude extract of W1, including **S3.1:** total ion chromatograph (TIC), **S3.2:** area percent report, and **S3.3:** MS spectra of identified compound and the comparison of the MS spectra of its standard products.

S3.1: Total Ion Chromatograph (TIC)



S3.2: Area Percent Report

Data File : C:\MSDCHEM\1\DATA\16071200.D Vial: 1
Acq On : 12 Jul 2016 10:26 Operator:
Sample : P0100 Inst : GCMS
Misc : Multiplr: 1.00
Sample Amount: 0.00
MS Integration Params: autoint1.e

Method : C:\MSDCHEM\1\METHODS\D-DDVP.M (Chemstation Integrator)
Title :

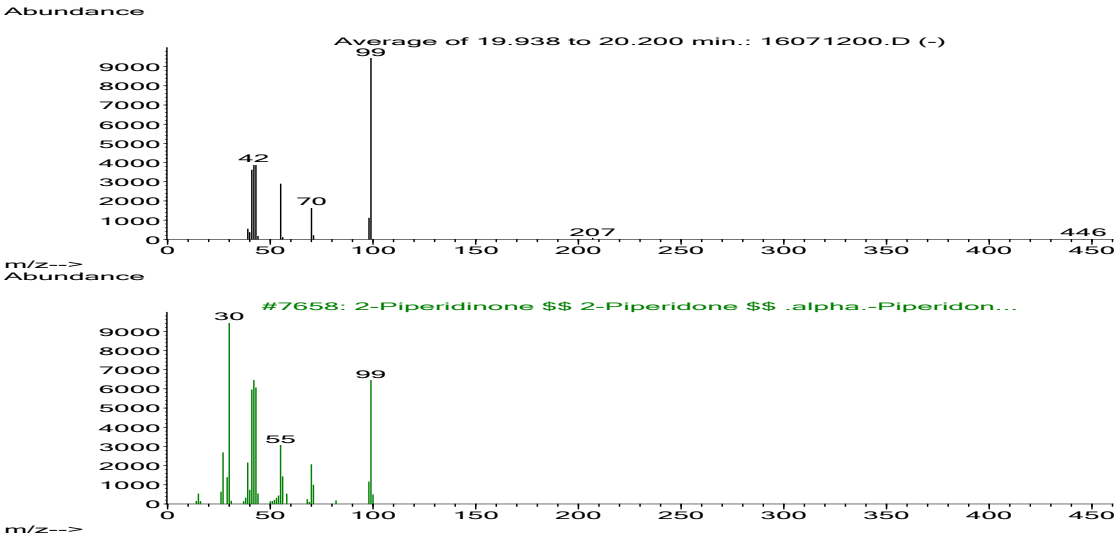
Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	21.995	3560	3653	3796	BV 2	114203	14266994	77.98%	19.377%
2	24.180	4031	4062	4163	BV 6	3823	499544	2.73%	0.678%
3	32.156	5537	5555	5574	VV	33545	940478	5.14%	1.277%
4	34.186	5901	5935	5982	VV 2	107963	5850488	31.98%	7.946%
5	34.939	6067	6076	6092	VV 5	8494	347545	1.90%	0.472%
6	35.084	6092	6103	6116	VV 2	16965	529439	2.89%	0.719%
7	35.281	6129	6140	6157	VV 6	11084	506398	2.77%	0.688%
8	35.725	6213	6223	6233	VV 2	10286	326280	1.78%	0.443%
9	36.376	6333	6345	6366	VV 2	4472	311992	1.71%	0.424%
10	36.558	6366	6379	6401	VV	11748	485223	2.65%	0.659%
11	36.873	6401	6438	6444	VV	3168	328640	1.80%	0.446%
12	36.985	6444	6459	6474	VV	4365	310102	1.70%	0.421%
13	37.130	6474	6486	6497	VV 3	17868	575880	3.15%	0.782%
14	37.658	6572	6585	6607	VV 3	37274	1189972	6.50%	1.616%
15	37.974	6622	6644	6665	VV 3	3550	395756	2.16%	0.538%
16	38.433	6710	6730	6777	VV	510972	14290056	78.11%	19.408%
17	38.791	6777	6797	6817	VV 4	14824	681525	3.73%	0.926%
18	38.967	6817	6830	6841	VV 7	18210	761190	4.16%	1.034%
19	39.074	6841	6850	6861	VV 3	17815	547577	2.99%	0.744%
20	39.170	6861	6868	6905	VV 3	3472	378837	2.07%	0.515%
21	39.566	6930	6942	6962	VV 6	7005	342230	1.87%	0.465%
22	39.779	6962	6982	6995	VV 4	5506	317032	1.73%	0.431%
23	40.939	7138	7199	7244	VV 3	16979	1228089	6.71%	1.668%
24	41.452	7281	7295	7308	VV 4	12916	422474	2.31%	0.574%
25	41.601	7308	7323	7345	VV 4	14986	585876	3.20%	0.796%
26	42.627	7476	7515	7524	VV 4	21251	1667650	9.12%	2.265%
27	42.723	7524	7533	7554	VV 4	28979	1050856	5.74%	1.427%
28	44.165	7785	7803	7825	VV 5	14031	455930	2.49%	0.619%
29	44.432	7825	7853	7893	VV 3	25904	813064	4.44%	1.104%
30	46.089	8152	8163	8188	VV 5	35371	1110578	6.07%	1.508%
31	46.532	8233	8246	8258	VV 5	12995	385219	2.11%	0.523%

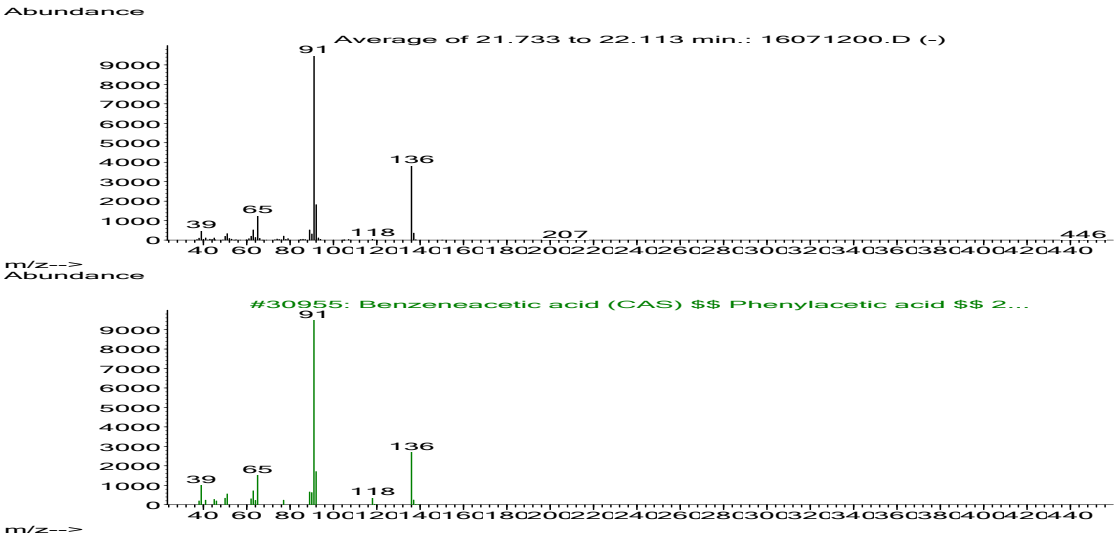
32	47.665	8440	8458	8467	VV	4	19041	567366	3.10%	0.771%	
33	48.477	8594	8610	8632	VV		648241	18294784	100.00%	24.847%	
34	48.760	8652	8663	8687	VV	6	13333	443997	2.43%	0.603%	
35	49.187	8712	8743	8762	VV	4	14063	533005	2.91%	0.724%	
36	50.662	8999	9019	9032	PV	6	9143	336415	1.84%	0.457%	
37	50.849	9041	9054	9083	VV	8	9562	376691	2.06%	0.512%	
38	51.372	9141	9152	9167	VV	2	27739	837458	4.58%	1.137%	
39	52.814	9407	9422	9441	VV	2	7760	335887	1.84%	0.456%	

S3.3: MS Spectra of Identified Compound and the Comparison of the MS Spectra of Its Standard Products.

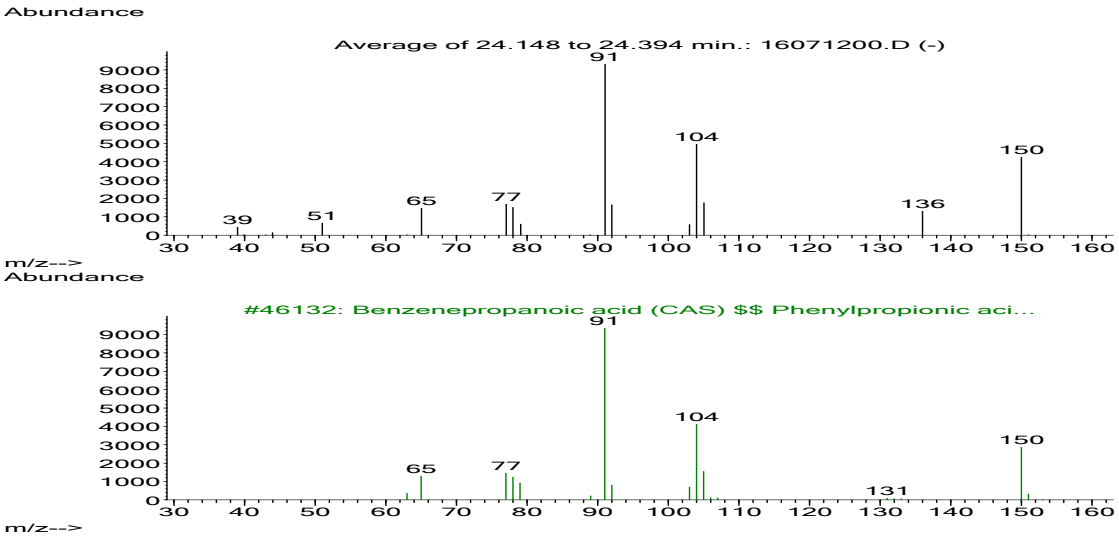
1. Comparison of Mass Spectra of **2-Piperidinone** and Its Standards



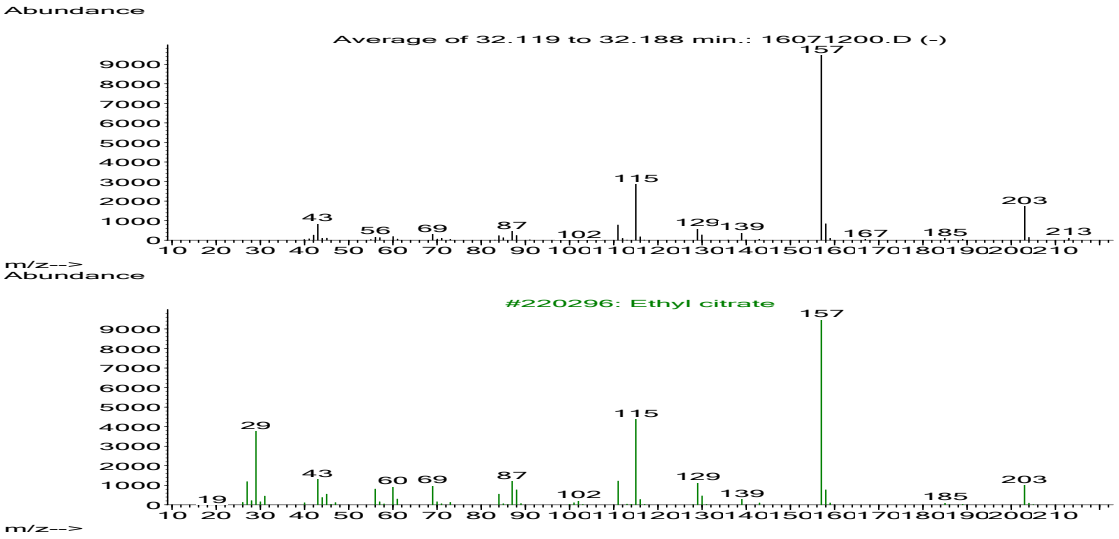
2. Comparison of Mass Spectra of **Benzeneacetic Acid** and Its Standards



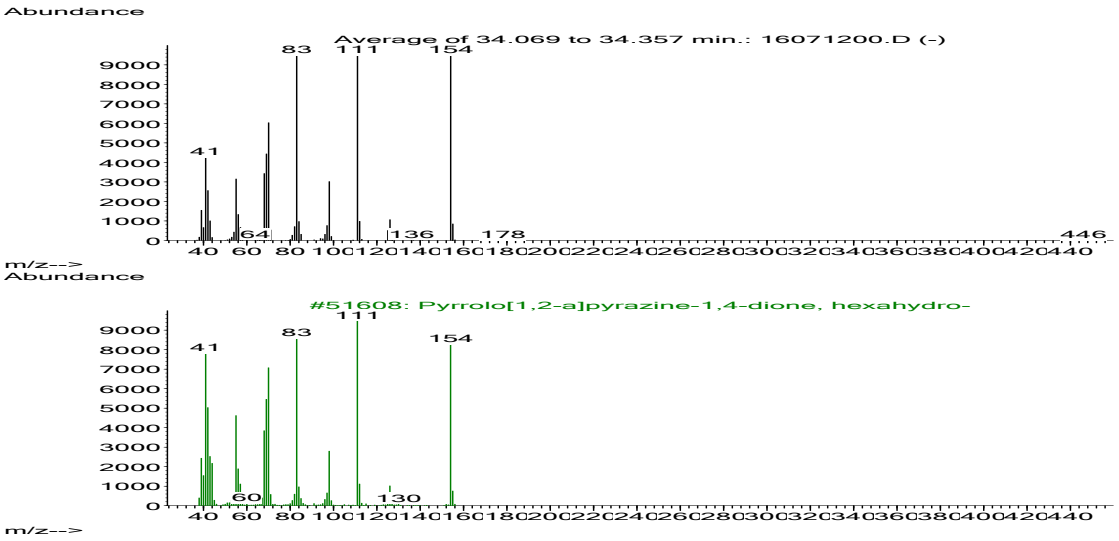
3. Comparison of Mass Spectra of **Benzenepropanoic Acid** and Its Standards



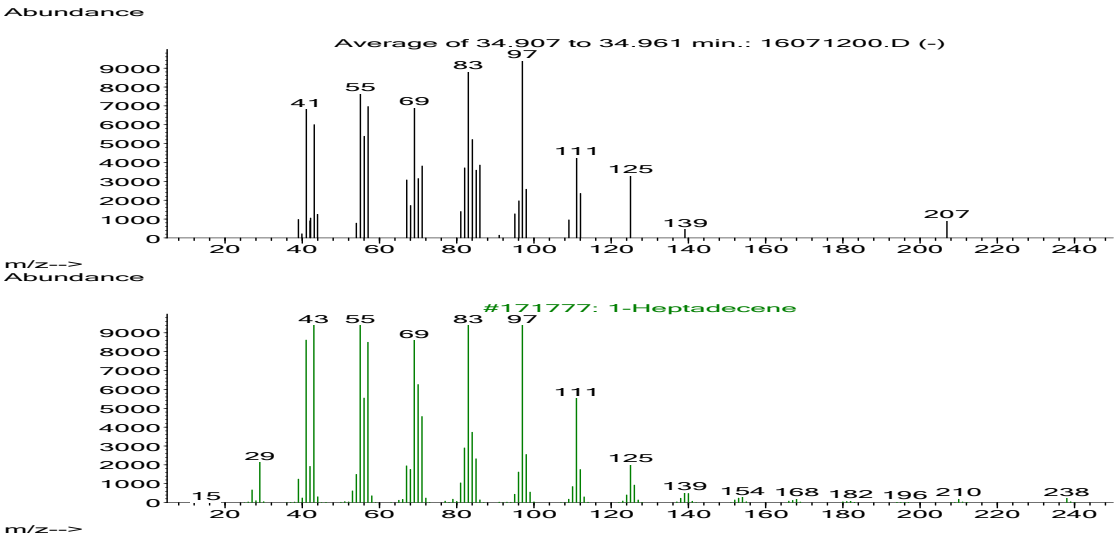
4. Comparison of Mass Spectra of **Etheyl Citrate** and Its Standards



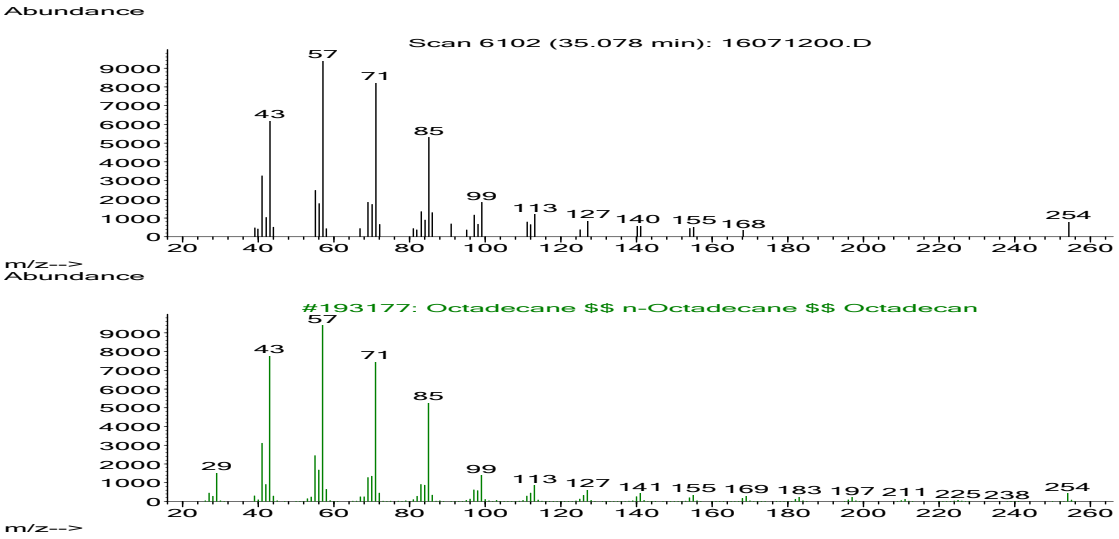
5. Comparison of Mass Spectra of **Cyclo (Gly-L-Pro) Dipeptide** and Its Standards



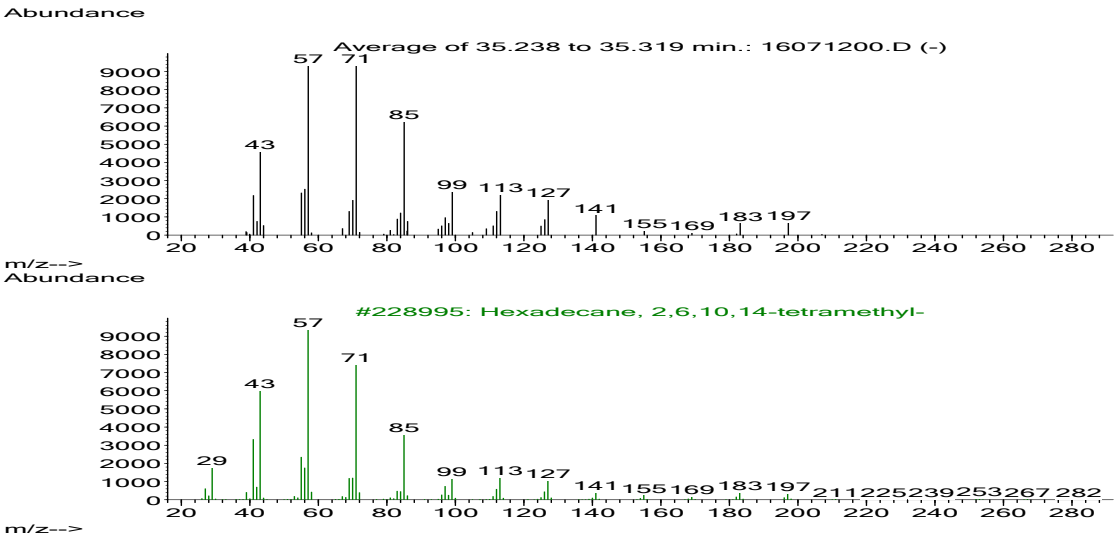
6. Comparison of Mass Spectra of **1-Heptadecene** and Its Standards



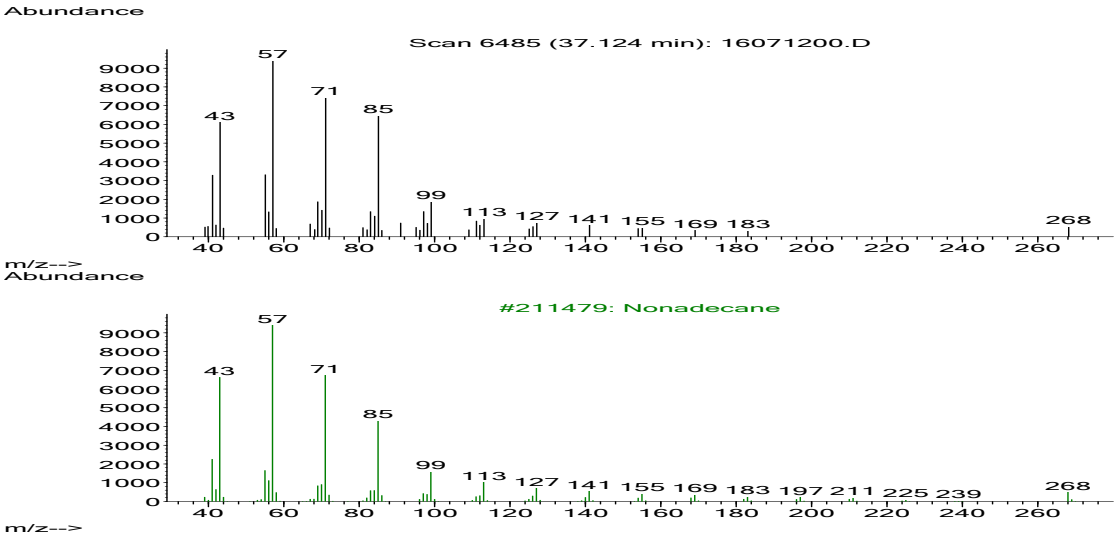
7. Comparison of Mass Spectra of **Octadecane** and Its Standards



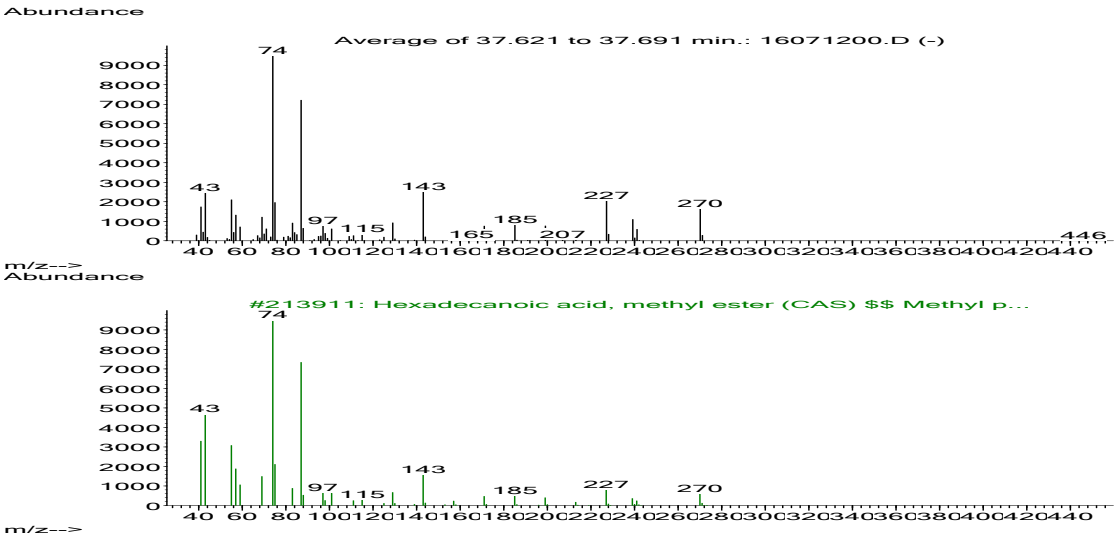
8. Comparison of Mass Spectra of **Hexadecane, 2,6,10,14-Tetramethyl-** and Its Standards



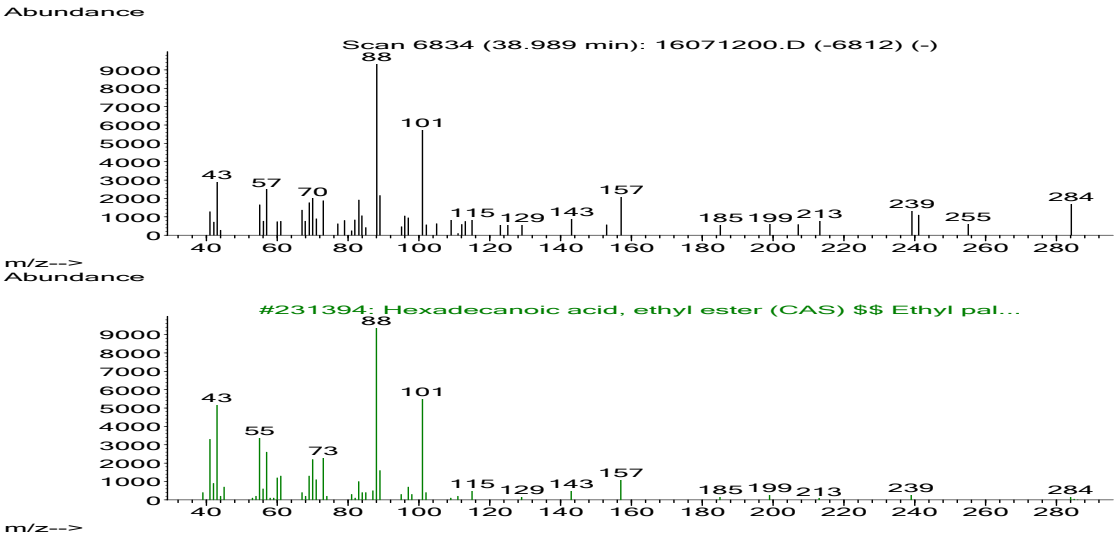
9. Comparison of Mass Spectra of **Nonadecane** and Its Standards



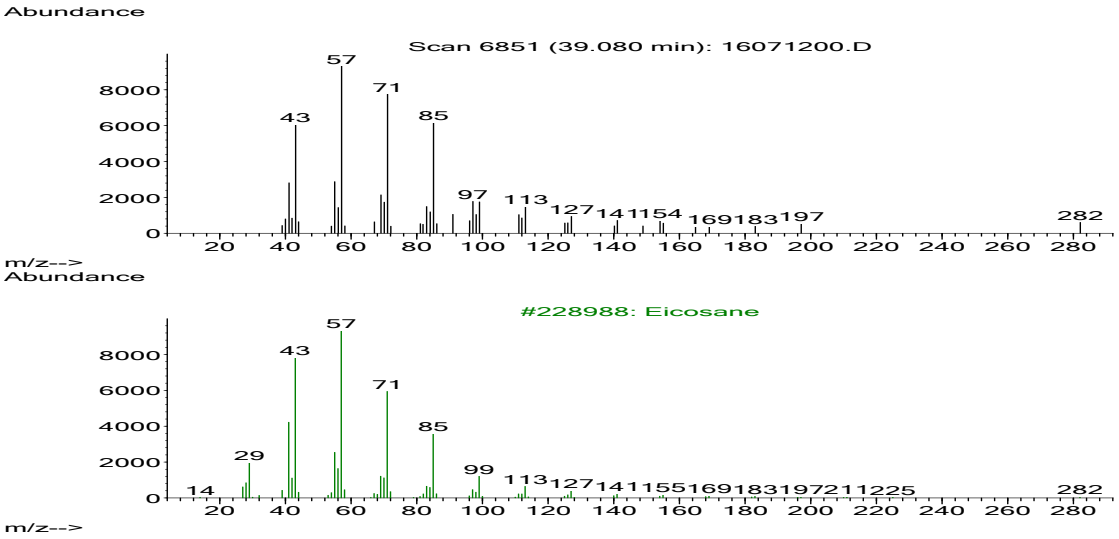
10. Comparison of Mass Spectra of **Hexadecanonic Acid, Methyl Ester** and Its Standards



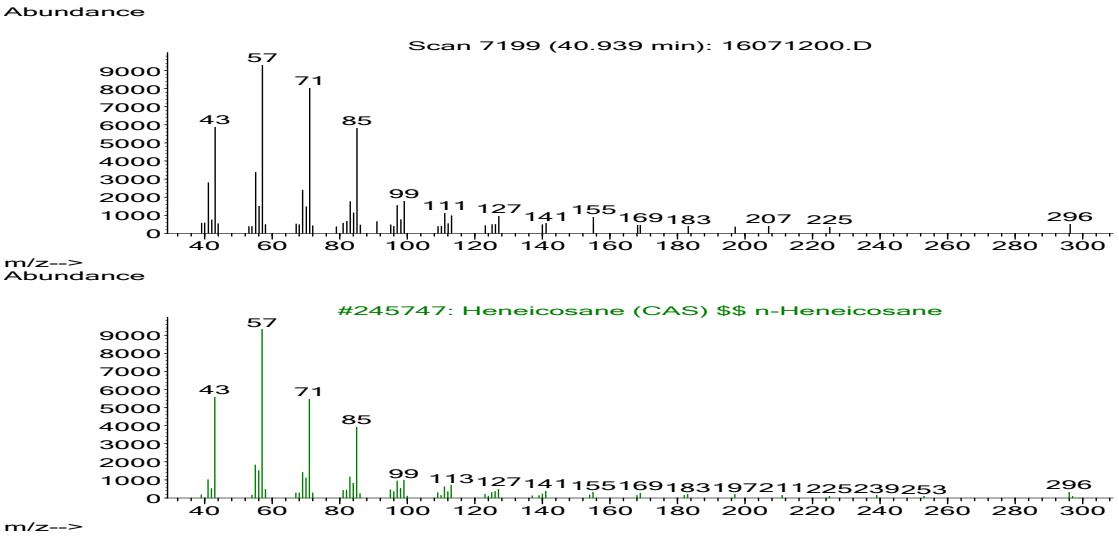
11. Comparison of Mass Spectra of **Hexadecanonic Acid, Ethyl Ester** and Its Standards



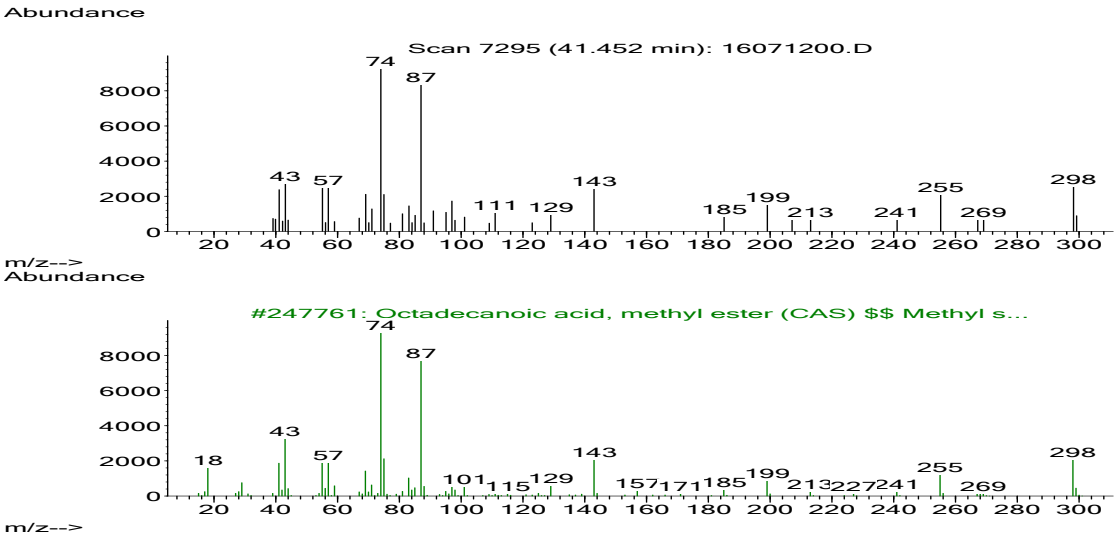
12. Comparison of Mass Spectra of **Icosane** and Its Standards



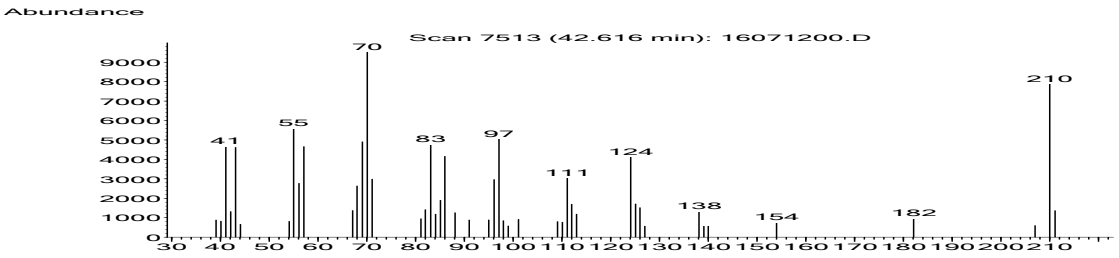
13. Comparison of Mass Spectra of **Heneicosane** and Its Standards



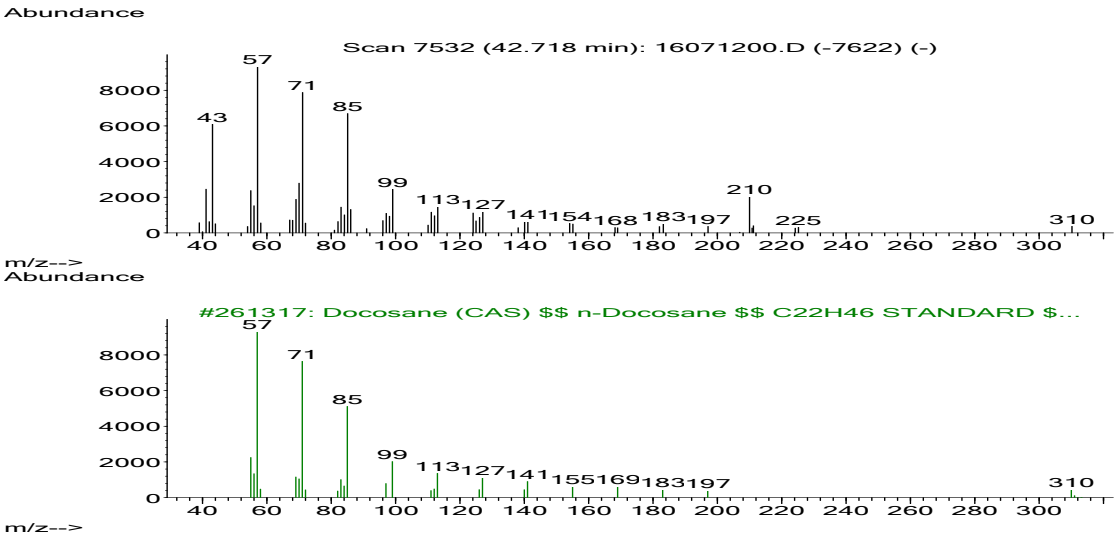
14. Comparison of Mass Spectra of **Octadecanoic Acid, Methyl Ester** and Its Standards



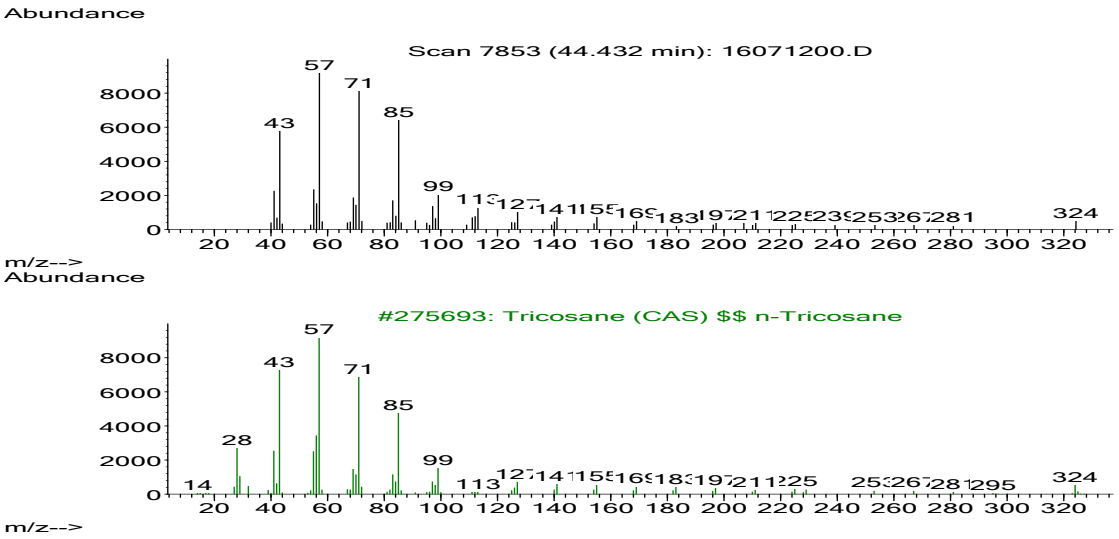
15. Mass Spectra of **Cyclo (L-Pro-oh-L-Pro) Dipeptide**



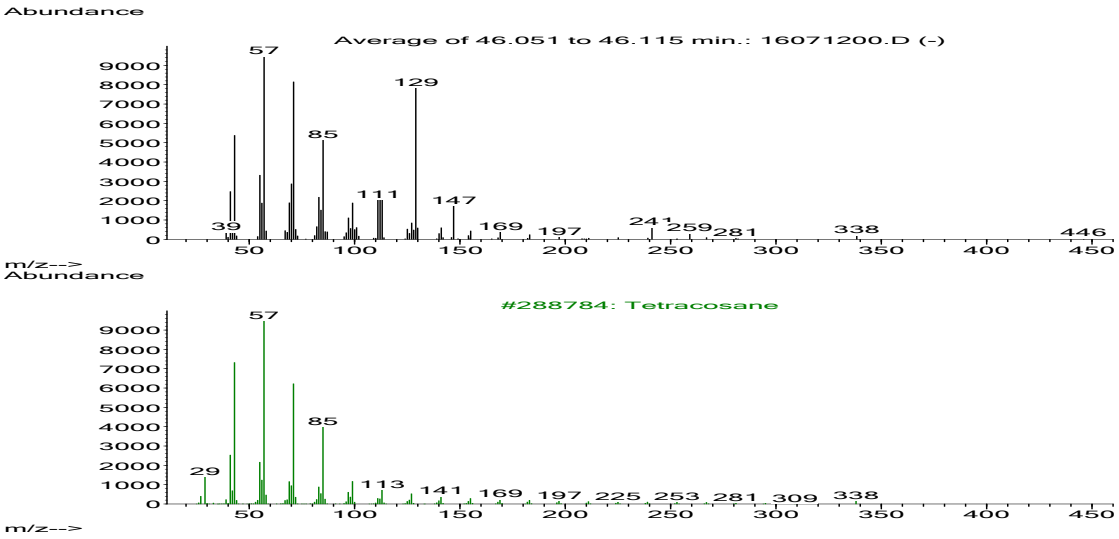
16. Comparison of Mass Spectra of **Docosane** and Its Standards



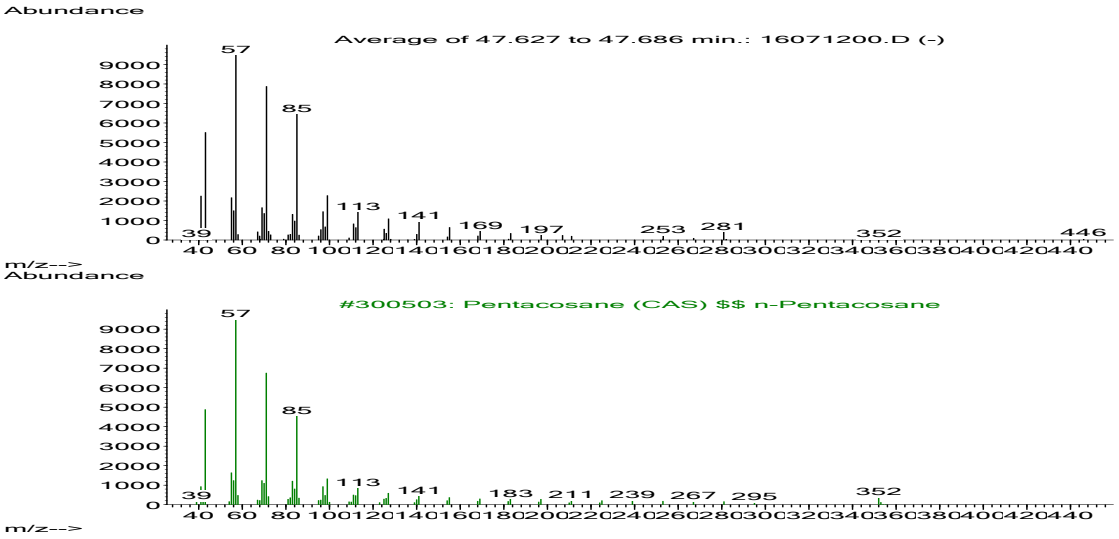
17. Comparison of Mass Spectra of **Tricosane** and Its Standards



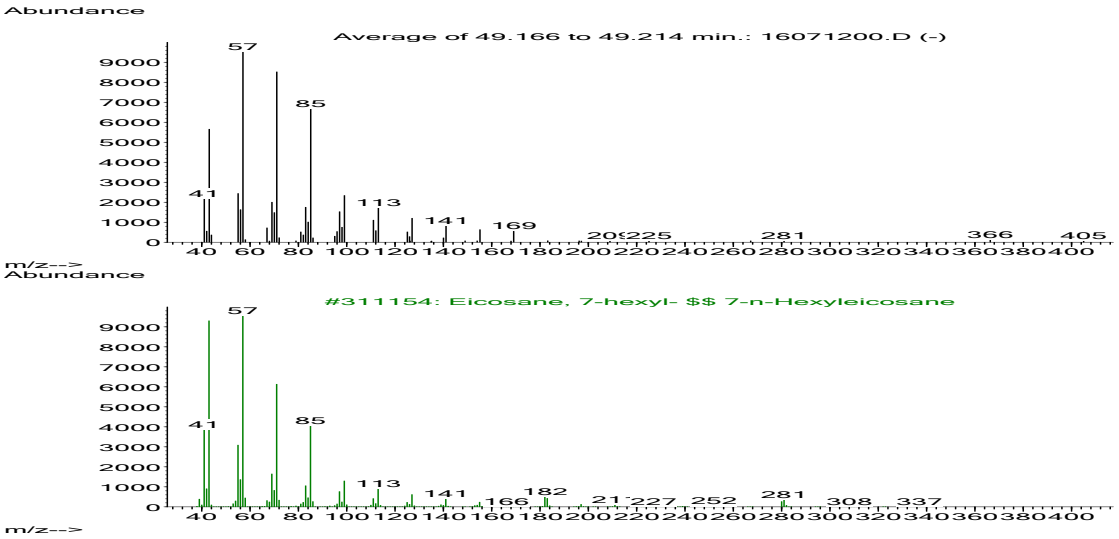
18. Comparison of Mass Spectra of **Tetracosane** and Its Standards



19. Comparison of Mass Spectra of **Pentacosane** and Its Standards



20. Comparison of Mass Spectra of **Eicosane,7-Hexyl-** and Its Standards



21. Comparison of Mass Spectra of **Heptacosane** and Its Standards

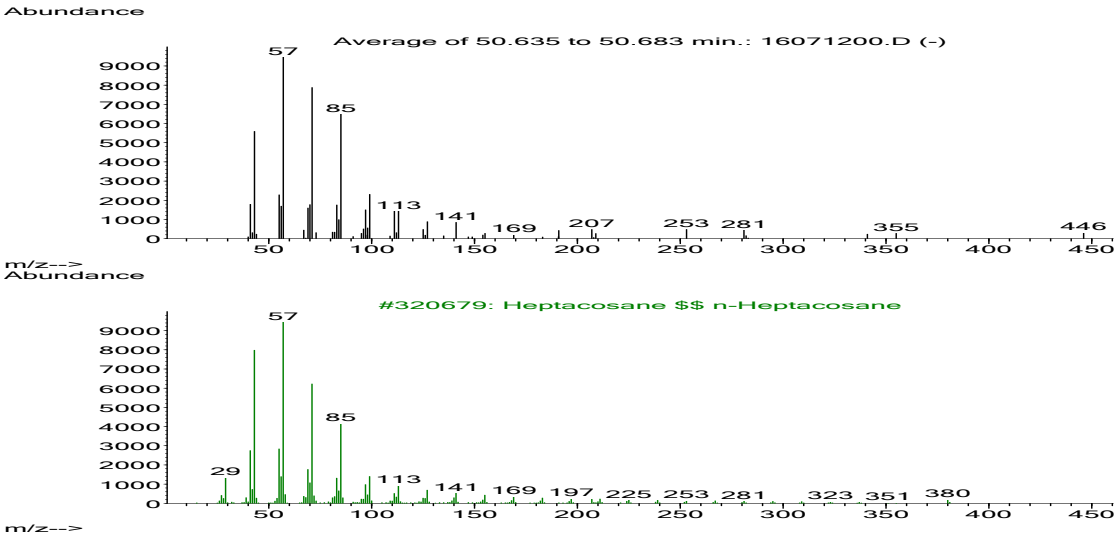
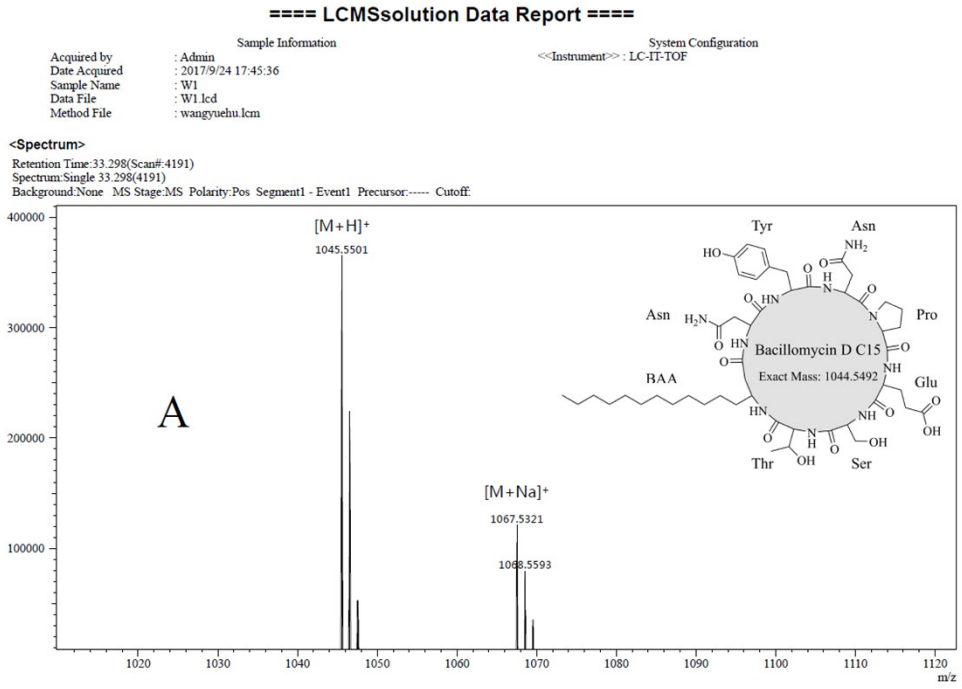


Figure S4 A: LC-ESI-MS spectrum and structure of the bacillomycin D C15. **B**: ESI-MS/MS spectrum of the precursor ion $[M + H]^+$ at m/z 1,045.5501 with fragment ions analysis.



==== LCMSsolution Data Report ====

Sample Information		System Configuration
Acquired by	: Admin	<<Instrument>> : LC-IT-TOF
Date Acquired	: 2017/9/24 17:45:36	
Sample Name	: W1	
Data File	: W1.lcd	
Method File	: wangyuehu.lcm	

<Spectrum>

Retention Time:33.298(Scan#:4192)
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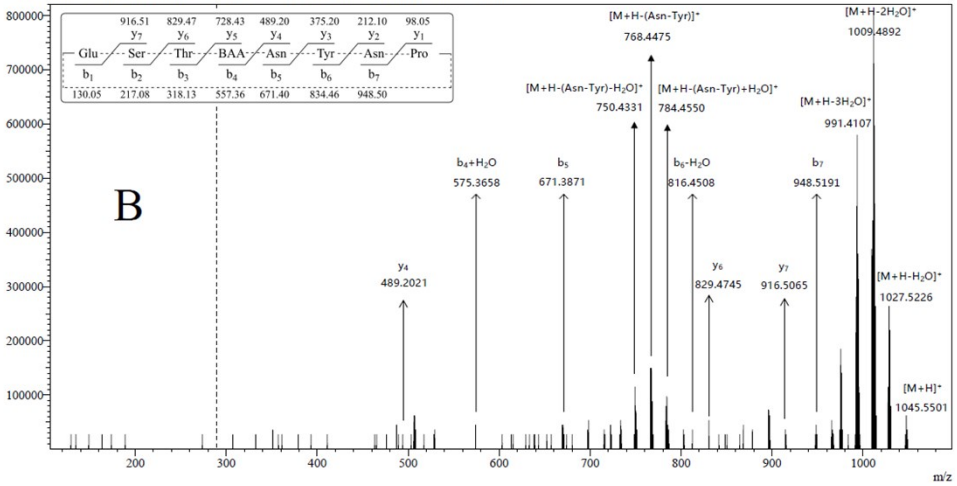
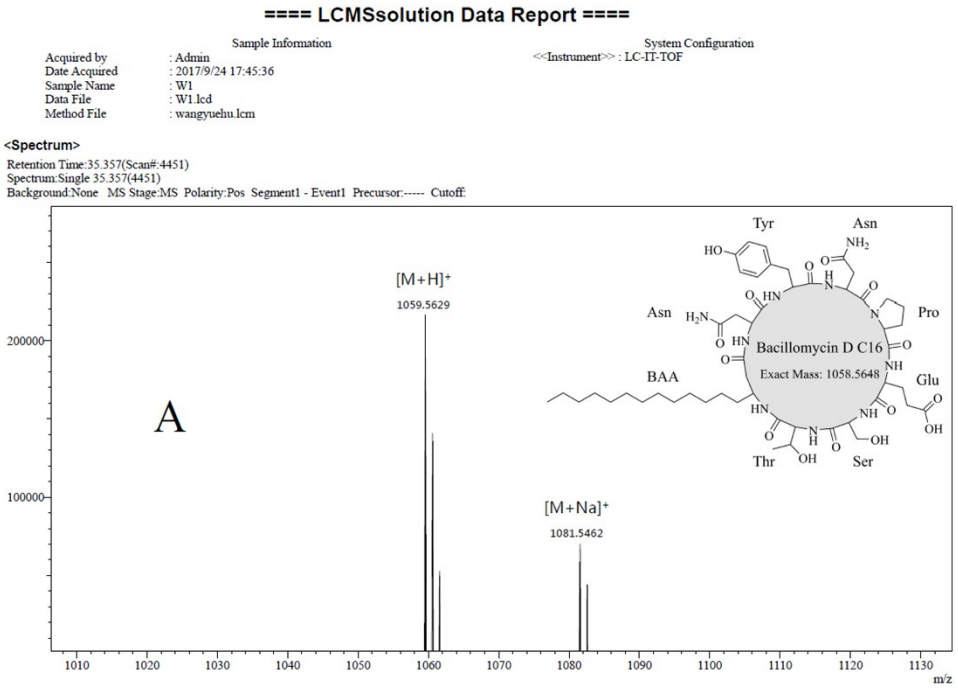


Figure S5 A: LC-ESI-MS spectrum and structure of the bacillomycin D C16. **B**: ESI-MS/MS spectrum of the precursor ion $[M + H]^+$ at m/z 1,059.5629 with fragment ions analysis.



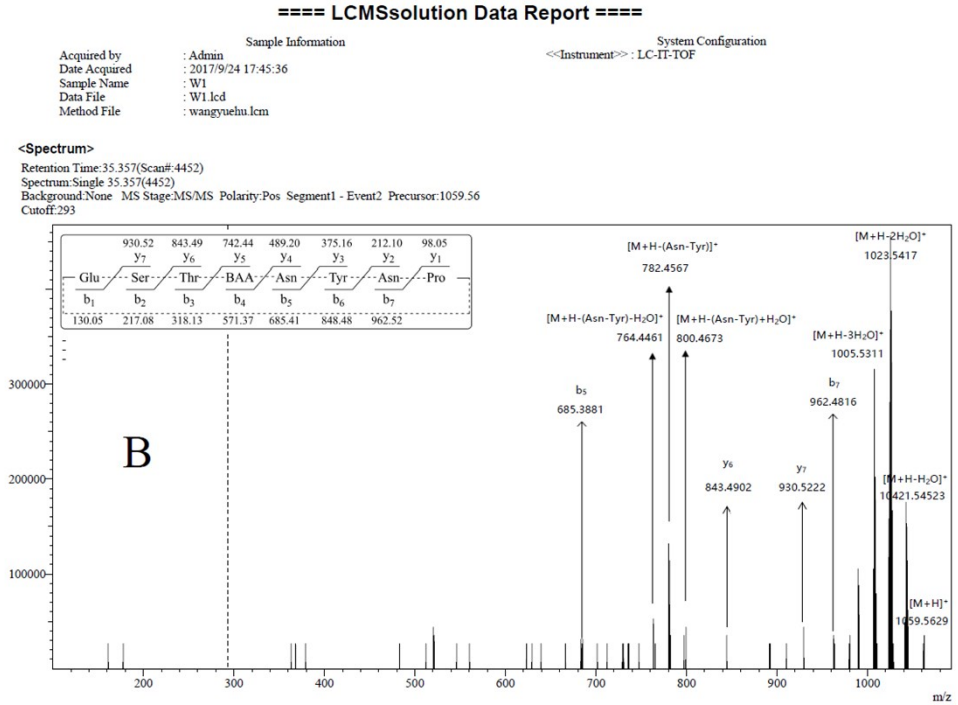


Figure S6 A: LC-ESI-MS spectrum and structure of the bacillomycin D C17.

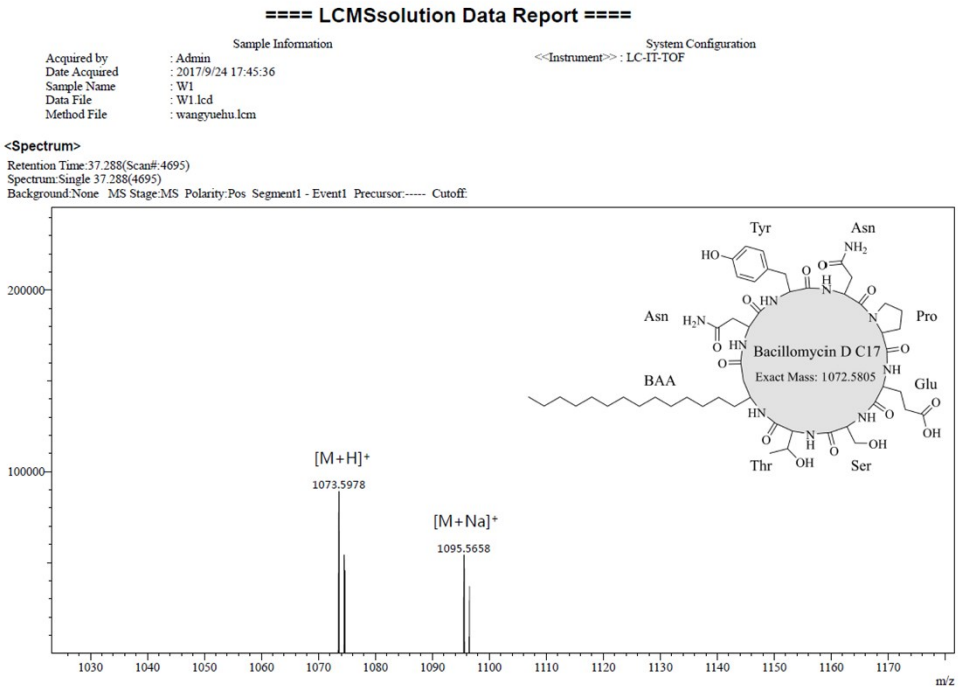


Table S1. Information of Known Acaricidal Compounds

NO.	Name	SMILES	Formula
1	Isomate-M	CCCC=CCCCCCCCO	$C_{26}H_{50}O_3$
2	(Z)-11-hexadecenal	CCCCC=CCCCCCCCCCC=O	$C_{16}H_{30}O$
3	Wintergreen oil	COC(=O)C1=CC=CC=C1O	$C_8H_8O_3$
4	Eucalyptus oil	CC1(C2CCC(O1)(CC2)C)C	$C_{10}H_{18}O$
5	Cyromazine	C1CC1NC2=NC(=NC(=N2)N)N	$C_6H_{10}N_6$
6	Diethyltoluamide	CCN(CC)C(=O)C1=CC=CC(=C1)C	$C_4H_{13}N_3$
7	Carbofuran	CC1(CC2=C(O1)C(=CC=C2)OC(=O)NC)C	$C_{12}H_{15}NO_3$
8	Sorbitol octanoate	CCCCCCCC(=O)OC(C(C(C(C(CO)O)O)O)O)O	$C_{14}H_{28}O_8$
9	Methoprene	CC(C)OC(=O)C=C(C)C=CCC(C)CCCC(C)(C)OC	$C_{19}H_{34}O_3$
10	Bifenazate	CC(C)OC(=O)NNC1=C(C=CC(=C1)C2=CC=CC=C2)OC	$C_{17}H_{20}N_2O_3$
11	Bioallethrin	CC1=C(C(=O)CC1OC(=O)C2C(C2(C)C)C=C(C)C)CC=C	$C_{19}H_{26}O_3$
12	Fenazaquin	CC(C)(C)C1=CC=C(C=C1)CCOC2=NC=NC3=CC=CC=C32	$C_{20}H_{22}N_2O$
13	Amitraz	CC1=CC(=C(C=C1)N=CN(C)C=NC2=C(C=C(C=C2)C)C)C	$C_{19}H_{23}N_3$
14	Acequinocyl	CCCCCCCCCCCCC1=C(C(=O)C2=CC=CC=C2C1=O)OC(=O)C	$C_{24}H_{32}O_4$
15	Pyrethroids	CC(=CC1C(C1(C)C)C(=O)OCC2=COC(=C2)CC3=CC=CC=C3)C	$C_{22}H_{26}O_3$
16	Spirotetramat	CCOC(=O)OC1=C(C(=O)NC12CCC(CC2)OC)C3=C(C=CC(=C3)C)C	$C_{21}H_{27}NO_5$
17	Fenpropathrin	CC1(C(C1(C)C)C(=O)OC(C#N)C2=CC(=CC=C2)OC3=CC=CC=C3)C	$C_{22}H_{23}NO_3$
18	Rotenone	CC(=C)C1CC2=C(O1)C=CC3=C2OC4COC5=CC(=C(C=C5C4C3=O)OC)OC	$C_{23}H_{22}O_6$
19	Spiromesifen	CC1=CC(=C(C(=C1)C)C2=C(C3(CCCC3)OC2=O)OC(=O)CC(C)(C)C)C	$C_{23}H_{30}O_4$
20	Fenpyroximate	CC1=NN(C(=C1C=NOCC2=CC=C(C=C2)C(=O)OC(C)(C)C)OC3=CC=CC=C3)C	$C_{24}H_{27}N_3O_4$
21	Dinocap	CCCCCCC(C)C1=CC(=C(C(=C1)[N+](=O)[O-])OC(=O)C=CC)[N+](=O)[O-]	$C_{18}H_{24}N_2O_6$
22	Spinosad	CCC1C(CCC2(O1)CC3CC(O2)CC=C(CC(C=CC=C4COC5C4(C(C=C(C5=NO)C)C(=O)O3)O)C)C)C	$C_{73}H_{110}N_2O_{17}$

23	Allosamidin	CC(=O)NC1C(C(C(OC1OC2C(OC(C(C2O)NC(=O)C)OC3C(C4C(C3O)N=C(O4)N(C)C)CO)CO)CO)O)O	$C_{25}H_{42}N_4O_{14}$
24	Moxidectin	CC1CC(=CCC2CC(CC3(O2)CC(=NOC)C(C(O3)C(=CC(C)C)C)C)OC(=O)C4C=C(C(C5C4(C(=CC=C1)CO5)O)O)C)C	$C_{37}H_{53}NO_8$
25	Spinosad	CCC1CCCC(C(C(=O)C2=CC3C4CC(CC4C=CC3C2CC(=O)O1)OC5C(C(C(C(O5)C)OC)OC)OC)C)OC6CCC(C(O6)C)N(C)C	$C_{73}H_{110}N_2O_{17}$
26	Pyrethrin	CC1=C(C(=O)CC1OC(=O)C2C(C2(C)C)C=C(C)C)CC=CC=C.CC1=C(C(=O)CC1OC(=O)C2C(C2(C)C)C=C(C)C(=O)OC)CC=CC=C	$C_{43}H_{56}O_8$
27	Abamectin	CC1C=CC=C2COC3C2(C(C=C(C3O)C)C(=O)OC4CC(CC=C(C1OC5CC(C(C(O5)C)OC6CC(C(C(O6)C)C)OC)OC)C)OC7(C4)C=CC(C(O7)C(C)C)C)O	$C_{48}H_{72}O_{13}$
28	Ivermectin	CCC(C)C1C(CCC2(O1)CC3CC(O2)CC=C(C(C(C=CC=C4COC5C4(C(C=C(C5O)C)C(=O)O3)O)C)OC6CC(C(C(O6)C)OC7CC(C(C(O7)C)O)OC)OC)C)C	$C_{48}H_{74}O_{14}$
29	Pheromone	CC(C)CC(C(=O)NC(CC1=CC=CC=C1)C(=O)NC(C(C)C)C(=O)NC(C(C)C)C(=O)NC(C(C)O)C(=O)NC(CC(C)C)C(=O)NC(C(C)C)C(=O)NCC(=O)O)N	$C_{42}H_{70}N_8O_{10}$
30	Avermectin	CCC(C)C1C(C=CC2(O1)CC3CC(O2)CC=C(C(C(C=CC=C4COC5C4(C(C=C(C5O)C)C(=O)O3)O)C)OC6CC(C(C(O6)C)OC7CC(C(C(O7)C)O)OC)OC)C)C	$C_{48}H_{72}O_{14}$
31	Doramectin	CC1C=CC=C2COC3C2(C(C=C(C3O)C)C(=O)OC4CC(CC=C(C1OC5CC(C(C(O5)C)OC6CC(C(C(O6)C)O)OC)OC)C)OC7(C4)C=CC(C(O7)C8CCCCC8)C)O	$C_{50}H_{74}O_{14}$
32	Eprinomectin	CCC(C)C1C(C=CC2(O1)CC3CC(O2)CC=C(C(C(C=CC=C4COC5C4(C(C=C(C5O)C)C(=O)O3)O)C)OC6CC(C(C(O6)C)OC7CC(C(C(O7)C)NC(=O)C)OC)OC)C)C	$C_{50}H_{75}NO_{14}$

Table S2. Compounds identified from Bacillus velezensis W1 and the maximum similarity

NO.	Compound name	SMILES	maximum similarity
1	2-Pyrrolidinone	C1CC(=O)NC1	0.22
2	2-Piperidinone	C1CCNC(=O)C1	0.22
3	Octadecane	CCCCCCCCCCCCCCCCCC	0.25
4	Nonadecane	CCCCCCCCCCCCCCCCCCC	0.25
5	Bacimethrin	COC1=NC=C(C(=N1)N)CO	0.18
6	Benzeneacetic acid	C1=CC=C(C=C1)CC(=O)O	0.3
7	Benzenepropanoic acid, methyl ester	COC(=O)CCC1=CC=CC=C1	0.31
8	Eicosane	CCCCCCCCCCCCCCCCCCCC	0.25
9	Benzenepropanoic acid	C1=CC=C(C=C1)CCC(=O)O	0.28
10	Cyclo (Gly-Pro)	C1CC2C(=O)NCC(=O)N2C1	0.37
11	Heneicosane	CCCCCCCCCCCCCCCCCCCCC	0.25
12	Benzenebutanoic acid	C1=CC=C(C=C1)CCCC(=O)O	0.28
13	Cyclo (Ala-Pro)	CC1C(=O)N2CCCC2C(=O)N1	0.38
14	Docosane	CCCCCCCCCCCCCCCCCCCCCC	0.25
15	Hexadecanonic acid, methyl ester	CCCCCCCCCCCCCCCC(OC)=O	0.44
16	Hexadecanonic acid, ethyl ester	CCCCCCCCCCCCCCCC(OCC)=O	0.54
17	Tricosane	CCCCCCCCCCCCCCCCCCCCCCC	0.25
18	Cyclo (Ala-Val)	CC1C(=O)NC(C(=O)N1)C(C)C	0.43
19	Octadecanoic acid, methyl ester	CCCCCCCCCCCCCCCCCC(=O)OC	0.44
20	Propanol,3-(O-Azi,dophenyl)	[N]=[N]=NC1=CC=CC=C1CCCO	——
21	Pentacosane	CCCCCCCCCCCCCCCCCCCCCCCCC	0.25
22	Cyclo (Pro-Pro)	C1CC2C(=O)N3CCCC3C(=O)N2C1	0.38

23	cyclo (Pro-trans-4-OH-Pro)	O=C(N1CC(O)CC12)C3CCCN3C2=O	0.48
24	Heptacosane	CCCCCCCCCCCCCCCCCCCCCCCCCCC	0.25
25	Eicosane,7-hexyl-	CCCCCCCCCCCCCC(CCCCCC)CCCCCC	0.25
26	Hexadecane, 2,6,10,14-tetramethyl-	CCC(C)CCCC(C)CCCC(C)CCCC(C)C	0.46
27	Cyclo (Gly-Phe)	C1C(=O)NC(C(=O)N1)CC2=CC=CC=C2	0.66
28	Cyclo (Leu-Leu)	CC(C)CC1C(=O)NC(C(=O)N1)CC(C)C	0.44
29	Etheyl citrate	O=C(OCC)CC(C(OCC)=O)(O)CC(OCC)=O	0.46
30	Cyclo (Gly-Tyr)	C1C(=O)NC(C(=O)N1)CC2=CC=C(C=C2)O	0.61
31	Cyclo (Phe-Pro)	C1CC2C(=O)NC(C(=O)N2C1)CC3=CC=CC=C3	0.66
32	Cyclo (Phe-Leu)	CC(C)CC1C(=O)NC(C(=O)N1)CC2=CC=CC=C2	0.75
33	Cyclo (Phe-trans-4-OH-Pro)	C1C(CN2C1C(=O)NC(C2=O)CC3=CC=CC=C3)O	0.73
34	Cyclo (Tyr-trans-4-OH-Pro)	O=C(NC(CC1=CC=C(O)C=C1)C2=O)C3N2CC(O)C3	0.68
35	Macrolactin A	CC1CCCC=CC=CC(CC(CC=CC=CC(CC=CC=CC(=O)O1)O)O)O	0.54
36	Macrolactin A, 7-O-malonyl-	CC1CCCC=CC=CC(CC(CC=CC=CC(CC=CC=CC(=O)O1)OC(=O)CC(=O)O)O)O	0.48
37	Surfactin C14	CC(C)CCCCCCCCC1CC(=O)NC(C(=O)NC(C(=O)NC(C(=O)NC(C(=O)NC(C(=O)NC(C(=O)O1)CC(C)C)CC(C)C)CC(=O)O)C(C)C)CC(C)C)CC(C)C)CCC(=O)O	0.48
38	Surfactin C15	CC(C)CCCCCCCCCC1CC(=O)NC(C(=O)NC(C(=O)NC(C(=O)NC(C(=O)NC(C(=O)NC(C(=O)O1)CC(C)C)CC(C)C)CC(=O)O)C(C)C)CC(C)C)CC(C)C)CCC(=O)O	0.48
39	Bacillomycin D C13	O=C(C(CC(NC(C(CC1=CC=C(C=C1)O)NC(C(CC(N)=O)NC(CC(N2)CCCCCCCCCC)=O)=O)=O)=O)N)N3C(C(NC(CCC(O)=O)C(NC(CO)C(NC(C(C)O)C2=O)=O)=O)=O)CCC3	0.67
40	Bacillomycin D C14	O=C(C(CC(NC(C(CC1=CC=C(C=C1)O)NC(C(CC(N)=O)NC(CC(N2)CCCCCCCCCCC)=O)=O)=O)=O)N)N3C(C(NC(CCC(O)=O)C(NC(CO)C(NC(C(C)O)C2=O)=O)=O)=O)CCC3	0.67
41	Bacillomycin D C15	O=C(C(CC(NC(C(CC1=CC=C(C=C1)O)NC(C(CC(N)=O)NC(CC(N2)CCCCCCCCCCCC)=O)=O)=O)=O)N)N3C(C(NC(CCC(O)=O)C(NC	0.67

		(CO)C(NC(C(C)O)C2=O)=O)=O)=O)CCC3	
42	Bacillomycin D C16	O=C(C(CC(NC(C(CC1=CC=C(C=C1)O)NC(C(CC(N)=O)NC(CC(N2)CCCCCCCCCCCCC)=O)=O)=O)=O)N)N3C(C(NC(CCC(O)=O)C(NC(CO)C(NC(C(C)O)C2=O)=O)=O)=O)CCC3	0.67
43	Bacillomycin D C17	O=C(C(CC(NC(C(CC1=CC=C(C=C1)O)NC(C(CC(N)=O)NC(CC(N2)CCCCCCCCCCCCCC)=O)=O)=O)=O)N)N3C(C(NC(CCC(O)=O)C(NC(CO)C(NC(C(C)O)C2=O)=O)=O)=O)CCC3	0.67