"Supplementary Data"

Nonlinear Mixture-wise Expansion Approach to Underdetermined Blind Separation of Nonnegative Dependent Sources

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Table S-1. Volumes of analytes and solvent used for the preparation of mixtures $\mathbf{X}_1$ to $\mathbf{X}_5$.

	Volume of components (μL)										Total volume (μL) of components	Volume (μL) of solvent (10% MeOH)
	$\mathbf{C}_1$	$\mathbf{C}_2$	$\mathbf{C}_3$	$\mathbf{C}_4$	$\mathbf{C}_5$	$\mathbf{C}_6$	$\mathbf{C}_7$	$\mathbf{C}_8$	$\mathbf{C}_9$	$\mathbf{C}_{10}$		
$\mathbf{X}_1$	10	50	40	55	45	20	35	30	25	15	325	625
$\mathbf{X}_2$	50	45	25	35	30	20	15	10	40	55	325	625
$\mathbf{X}_3$	10	45	40	50	55	15	35	25	30	20	325	625
$\mathbf{X}_4$	20	50	35	55	45	30	25	10	40	15	325	625
$\mathbf{X}_5$	55	10	20	15	25	50	35	40	45	30	325	625

Table S-2. Normalized correlation coefficients for analytes $\mathbf{C}_1$ to $\mathbf{C}_{10}$ shown in Figure S-1. Cross-correlation coefficients greater than 0.1 are in bold font. Analytes $\mathbf{C}_4$ and $\mathbf{C}_7$ have practically same mass spectra. Analytes $\mathbf{C}_4$ and $\mathbf{C}_5$, $\mathbf{C}_5$ and $\mathbf{C}_7$, $\mathbf{C}_3$ and $\mathbf{C}_9$, $\mathbf{C}_2$ and $\mathbf{C}_3$ as well as $\mathbf{C}_2$ and $\mathbf{C}_9$ are significantly correlated. $c_{nm} = \frac{\langle \mathbf{s}_n, \mathbf{s}_m \rangle}{\|\mathbf{s}_n\| \|\mathbf{s}_m\|}$, $n, m = 1, ..., 10$.

entry	$\mathbf{C}_1$	$\mathbf{C}_2$	$\mathbf{C}_3$	$\mathbf{C}_4$	$\mathbf{C}_5$	$\mathbf{C}_6$	$\mathbf{C}_7$	$\mathbf{C}_8$	$\mathbf{C}_9$	$\mathbf{C}_{10}$
$\mathbf{C}_1$	1.0000	0.0037	0.0576	0.0001	0.0005	0.0014	0.0004	0.0001	0.0001	0.0002
$\mathbf{C}_2$	0.0037	1.0000	**0.1540**	0.0012	0.0003	0.0733	0.0017	0.0009	**0.1362**	0.0001
$\mathbf{C}_3$	0.0576	**0.1540**	1.0000	0.0018	0.0021	0.0099	0.0022	0.0197	**0.3077**	0.0003
$\mathbf{C}_4$	0.0001	0.0012	0.0018	1.0000	**0.4775**	0.0037	**0.9543**	0.0015	0.0004	0.0000
$\mathbf{C}_5$	0.0005	0.0003	0.0021	**0.4775**	1.0000	0.0028	**0.3930**	0.0054	0.0005	0.0000
$\mathbf{C}_6$	0.0014	0.0733	0.0099	0.0037	0.0028	1.0000	0.0025	0.0023	0.0001	0.0026
$\mathbf{C}_7$	0.0004	0.0017	0.0022	**0.9543**	**0.3930**	0.0025	1.0000	0.0037	0.0003	0.0000
$\mathbf{C}_8$	0.0001	0.0009	0.0197	0.0015	0.0054	0.0023	0.0037	1.0000	0.0011	0.0037
$\mathbf{C}_9$	0.0001	**0.1362**	**0.3077**	0.0004	0.0005	0.0001	0.0003	0.0011	1.0000	0.0106
$\mathbf{C}_{10}$	0.0002	0.0001	0.0003	0.0000	0.0000	0.0026	0.0000	0.0037	0.0106	1.0000

Table S-3. Maximal normalized correlation coefficients between analytes $\mathbf{C}_1$ to $\mathbf{C}_{10}$ and components extracted by the NMU and NMF_L0 algorithms applied on LMM (1) composed of five mixtures $\mathbf{X}_1$ to $\mathbf{X}_5$. Mixture matrix has been scaled by $\arg\max_{n,t}\left\{\mathbf{X}_{nt}\right\}_{n,t=1}^{N,T}$. Columns from left to right: factorization method; normalized correlation coefficients: $c_{mm}=\left\langle \mathbf{s}_m,\hat{\mathbf{s}}_m\right\rangle / \left\|\mathbf{s}_m\right\| / \left\|\hat{\mathbf{s}}_m\right\|$, m=1,...,10. The NMU algorithm was run with number of sources set to M=T=2901 and the best matching results are shown in the table. The NMF_L0 algorithm was run with the following parameter setup: reverse sparse nonnegative least square (rsNNLS) sparse coder and alternating nonnnegative least square (ANLS) for dictionary update stage. NMF_L0 algorithm was cross-validated for values of $K\in\{3,4,5,6\}$. Number of sources was set to M=300 and number of iterations was set to 200. The best matching results are shown in the table. The asterisk sign denotes analytes in the library associated with the same extracted component. The best result is highlighted.

	$\mathbf{c}_{11}$	$\mathbf{c}_{22}$	$\mathbf{c}_{33}$	$\mathbf{c}_{44}$	$\mathbf{c}_{55}$	$\mathbf{c}_{66}$	$\mathbf{c}_{77}$	$\mathbf{c}_{88}$	$\mathbf{c}_{99}$	$\mathbf{c}_{10;10}$
NMU	0.0405 *	0.6922	0.6492 *	0.9846 x	0.4499 x	0.3641 +	0.9738 x	0.9956	0.9087 +	0.7334
NMF_L0, K=3, Update Err=2.3x10^{-3}	0.8566	0.7141	0.8772	0.7779 x	0.4348 x	0.9766	0.7498	0.5721	0.8558	0.7735
NMF_L0 K=4, Update Err=3.1x10^{-4}	0.9602	0.8799	0.7435	0.8650 x	0.4716 x	0.7639	0.7036 x	0.7438	0.9567	0.9070
NMF_L0, K=5, Update Err=7x10^{-6}	0.7269	0.9567	0.7448	0.8595	0.5616	0.9922	0.7117	0.6401	0.9924	0.9880
NMF_L0 K=6, Update Err=1.4x10^{-6}	0.3895	0.7619	0.8639	0.8646 x	0.6038	0.9747	0.7042 x	0.7181	0.9573	0.9075

Table S-4. Maximal normalized correlation coefficients between analytes $\mathbf{C}_1$ to $\mathbf{C}_{10}$ and components extracted by proposed dimensionality expansion method: $c_{mm} = \langle \mathbf{s}_m, \hat{\mathbf{s}}_m \rangle / \|\mathbf{s}_m\| / \|\hat{\mathbf{s}}_m\|$, m=1,...,10. Columns from left to right: combinations of mixture spectra; correlation coefficients; information of variance, σ^2, of the Gaussian kernel, type of factorization used with dimensionality expansion transform, type of scaling of the mixing matrix before mapping: x_{max} refers to $\arg\max_{n,t}\{\mathbf{X}_{nt}\}_{n,t=1}^{N,T}$ and $\|\mathbf{x}\|_1$ refers to $\arg\max_{t}\{\|\mathbf{x}_{\cdot t}\|_1\}_{t=1}^{T}$. The NMF_L0 algorithm was run with the following parameter setup: reverse sparse nonnegative least square (rsNNLS) sparse coder and alternating nonnnegative least square (ANLS) for dictionary update stage. The best result is obtained for number of overlapped sources equal to Q=50. Number of sources was set to P=200 and number of iterations was set to 100. The star '*' denotes analytes in the library associated with the same extracted component. The best result is highlighted.

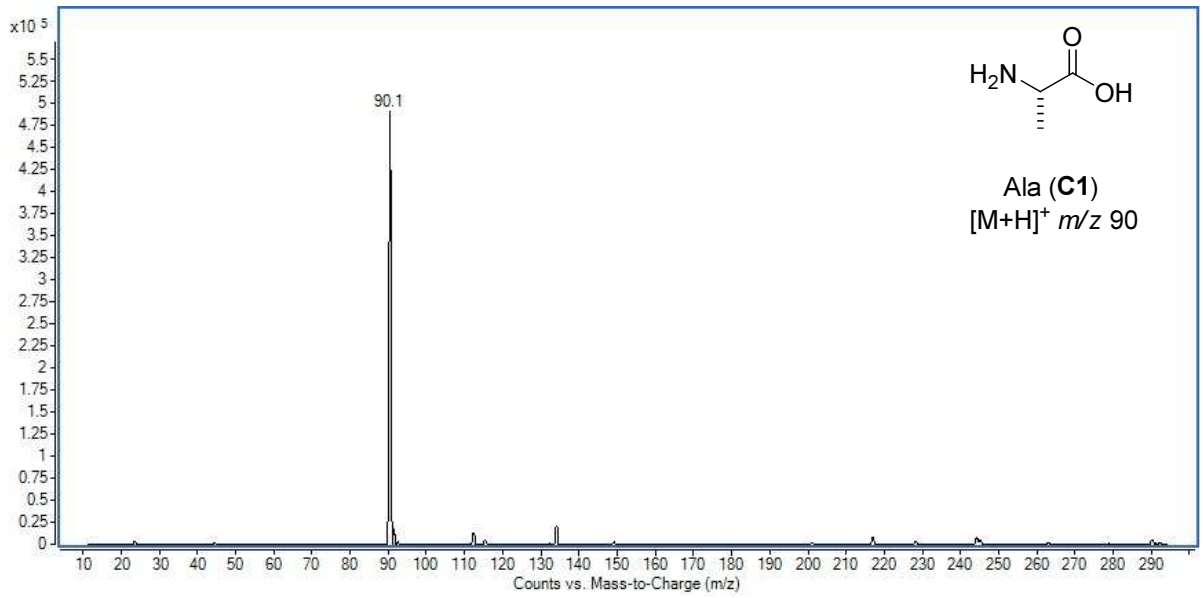
	$\mathbf{c}_{11}$	$\mathbf{c}_{22}$	$\mathbf{c}_{33}$	$\mathbf{c}_{44}$	$\mathbf{c}_{55}$	$\mathbf{c}_{66}$	$\mathbf{c}_{77}$	$\mathbf{c}_{88}$	$\mathbf{c}_{99}$	$\mathbf{c}_{10;10}$	**Mapping factorization**
$\mathbf{X}_1$ to $\mathbf{X}_5$	0.6114	0.9182	0.6351	0.7619	0.5606	0.6339	0.7784	0.8124	0.8812	0.8609	σ^2=1e0 NMF_L0, x_{max} Err=2.7x10^{-7}
$\mathbf{X}_1$ to $\mathbf{X}_5$	0.8974	0.9370	0.7808	0.9816 x	0.6956	0.9844	0.9684 x	0.9869	0.9194	0.9398	σ^2=1e0 NMU, x_{max}
$\mathbf{X}_1$ to $\mathbf{X}_5$	0.8792	0.9370	0.9160	0.9816 x	0.6994	0.9844	0.9684 x	0.9869	0.9194	0.9398	σ^2=1e0 NMU, x_{max} Denoising hard τ=1e-7
$\mathbf{X}_1$ to $\mathbf{X}_5$	0.7593	0.9253	0.6862	0.9753 x	0.5761	0.9732	0.9599 x	0.9954	0.8130	0.9684	σ^2=1e0 NMU, $\|\mathbf{x}\|_1$
$\mathbf{X}_1$ to $\mathbf{X}_5$	0.7222	0.9253	0.6862	0.9753	0.5621	0.9732	0.9599	0.9954	0.8130	0.9684	σ^2=1e0 NMU, $\|\mathbf{x}\|_1$

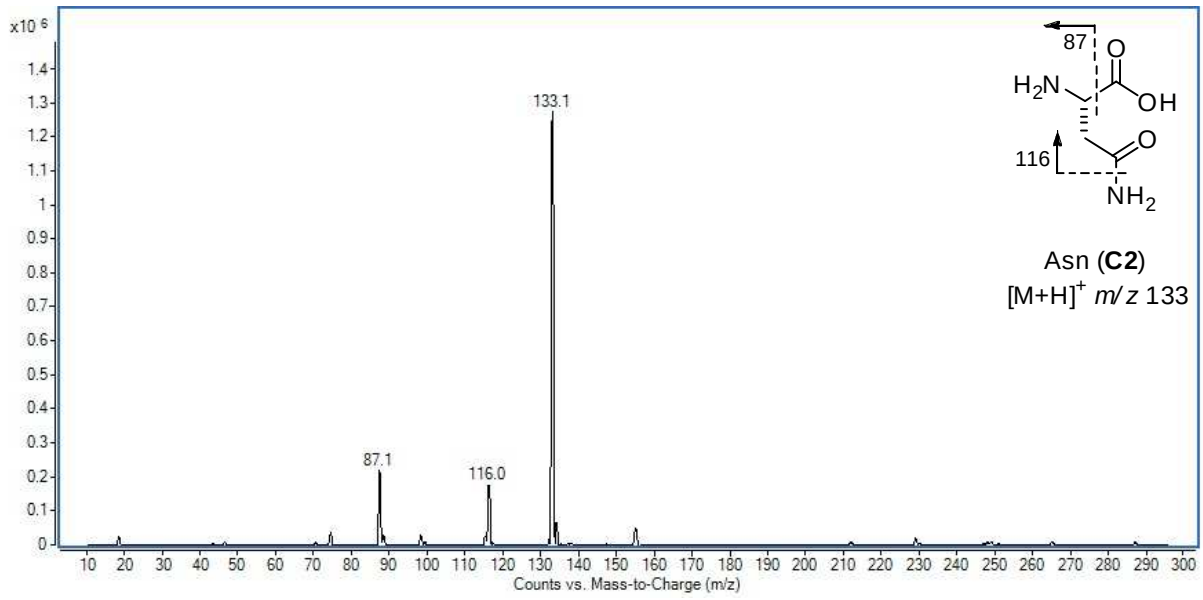
											Denoising hard τ=1e-7
$\mathbf{X_1}$ to $\mathbf{X_5}$	0.6249	0.8867	0.8983	0.9052 x	0.7466	0.9255	0.9448 x	0.9069	0.9163	0.9423	σ^2=1e-1 NMU, x_{max}
$\mathbf{X_1}$ to $\mathbf{X_5}$	0.6970	0.8867	0.9107	0.9052 x	0.6604	0.9255	0.9448 x	0.9069	0.9163	0.9423	σ^2=1e-1 NMU, x_{max} Denoising hard τ=1e-7
$\mathbf{X_1}$ to $\mathbf{X_5}$	0.9349	0.9596	0.7721	0.9559 x	0.6859	0.9435	0.9449 x	0.9895	0.9142	0.9553	σ^2=1e-1 NMU, $\|\mathbf{x}\|_1$
$\mathbf{X_1}$ to $\mathbf{X_5}$	0.8113	0.9596	0.6537	0.9559 x	0.5736	0.9435	0.9449 x	0.9895	0.9142	0.9553	σ^2=1e-1 NMU, $\|\mathbf{x}\|_1$ Denoising hard τ=1e-7
$\mathbf{X_1}$ to $\mathbf{X_5}$	0.9200	0.9218	0.7584	0.9757 x	0.4975	0.7507	0.9608 x	0.9953	0.8295	0.9158	σ^2=1e1 NMU, x_{max}
$\mathbf{X_1}$ to $\mathbf{X_5}$	0.8577	0.9218	0.7821	0.9757 x	0.5818	0.7990	0.9608 x	0.9953	0.8295	0.9158	σ^2=1e1 NMU, x_{max} Denoising hard τ=1e-7
$\mathbf{X_1}$ to $\mathbf{X_5}$	0.7083	0.9527	0.6815	0.9746	0.6144	0.9804	0.9584	0.9952	0.8815	0.9894	σ^2=1e1 NMU, $\|\mathbf{x}\|_1$
$\mathbf{X_1}$ to $\mathbf{X_5}$	0.8143	0.9527	0.6786	0.9746 x	0.6018	0.9804	0.9584 x	0.9952	0.8815	0.9894	σ^2=1e1 NMU, $\|\mathbf{x}\|_1$ Denoising harrd τ=1e-7
$\mathbf{X_{(1,3,4,5)}}$	0.8681	0.8484	0.9145	0.9008 x	0.4864	0.9160	0.8993 x	0.9826	0.8746	0.9359	σ^2=1e0 NMU, x_{max}
$\mathbf{X_{(1,3,4,5)}}$	0.8486	0.8484	0.9142	0.9008 x	0.6107	0.9160	0.8993 x	0.9826	0.8746	0.9359	σ^2=1e0 NMU, x_{max} Denoising hard τ=1e-7
$\mathbf{X_{(1,3,4,5)}}$	0.7637	0.9287	0.7860	0.9713 x	0.4970	0.9546	0.9634 x	0.9938	0.8811	0.8685	σ^2=1e0 NMU, $\|\mathbf{x}\|_1$
$\mathbf{X_{(1,3,4,5)}}$	0.6711	0.9287	0.8485	0.9713	0.6126	0.9546	0.9634	0.9938	0.8811	0.8685	σ^2=1e0

				x							NMU, $\|\mathbf{x}\|_1$ Denoising hard τ=1e-7
$\mathbf{X}_{(1,3,4,5)}$	0.6975	0.9446	0.8921	0.9057 x	0.6080	0.8391	0.9424 x	0.8997	0.9209	0.7865	σ^2=1e-1 NMU, x_{max}
$\mathbf{X}_{(1,3,4,5)}$	0.7005	0.9446	0.8919	0.9057 x	0.6570	0.8391	0.9424	0.8997	0.9209	0.7865	σ^2=1e-1 NMU, x_{max} Denoising hard τ=1e-7
$\mathbf{X}_{(1,3,4,5)}$	0.7928	0.8822	0.8927	0.8965 x	0.6274	0.8860	0.8950 x	0.9822	0.9080	0.9262	σ^2=1e-1 NMU, $\|\mathbf{x}\|_1$
$\mathbf{X}_{(1,3,4,5)}$	0.8348	0.8822	0.8926	0.8965 x	0.6275	0.8860	0.8950 x	0.9822	0.9080	0.9262	σ^2=1e-1 NMU, $\|\mathbf{x}\|_1$ Denoising hard τ=1e-7
$\mathbf{X}_{(1,3,4,5)}$	0.6685	0.8787	0.8537	0.9713 x	0.6439	0.9492	0.9633	0.9938	0.8833	0.9556	σ^2=1e1 NMU, x_{max}
$\mathbf{X}_{(1,3,4,5)}$	0.6432	0.8787	0.8395	0.9713 x	0.6169	0.9492	0.9633 x	0.9938	0.8833	0.9556	σ^2=1e1 NMU, x_{max} Denoising hard τ=1e-7
$\mathbf{X}_{(1,3,4,5)}$	0.7941	0.9357	0.7805	0.9712 x	0.5039	0.9044	0.9630 x	0.9936	0.9363	0.8031	σ^2=1e1 NMU, $\|\mathbf{x}\|_1$
$\mathbf{X}_{(1,3,4,5)}$	0.7997	0.9357	0.7805	0.9712 x	0.5515	0.9044	0.9630 x	0.9936	0.9363	0.8031	σ^2=1e1 NMU, $\|\mathbf{x}\|_1$ Denoising hard τ=1e-7
$\mathbf{X}_{(1,2,3)}$	0.6017	0.8855	0.7136	0.7474 x	0.5781	0.7958	0.7830	0.9671	0.9413	0.9826	σ^2=1e0 NMU, x_{max}
$\mathbf{X}_{(1,2,3)}$	0.7194	0.8855	0.6495	0.7474 x	0.5863	0.7958	0.7830 x	0.9671	0.9413	0.9826	σ^2=1e0 NMU, x_{max} Denoising hard τ=1e-7
$\mathbf{X}_{(1,2,3)}$	0.6309	0.8224	0.5365	0.8612 x	0.7049	0.6451	0.9231 x	0.9686	0.8400	0.9015	σ^2=1e0 NMU, $\|\mathbf{x}\|_1$

$\mathbf{X}_{(1,2,3)}$	0.5509	0.8224	0.4973	0.8612 x	0.7050	0.7498	0.9231 x	0.9686	0.8400	0.9015	σ^2=1e0 NMU, $\|\mathbf{x}\|_1$ Denoising hard τ=1e-7
$\mathbf{X}_{(1,2,3)}$	0.6191	0.9029	0.7897	0.7435 x	0.6542	0.7157	0.7525 x	0.8516	0.8639	0.8379	σ^2=1e-1 NMU, x_{max}
$\mathbf{X}_{(1,2,3)}$	0.6492	0.9029	0.6715	0.7435 x	0.6539	0.7157	0.7525 x	0.8516	0.8639	0.8379	σ^2=1e-1 NMU, x_{max} Denoising harrd τ=1e-7
$\mathbf{X}_{(1,2,3)}$	0.5934	0.8308	0.5123	0.8180 x	0.5791	0.7640	0.8597 x	0.9571	0.9267	0.9825	σ^2=1e-1 NMU, $\|\mathbf{x}\|_1$
$\mathbf{X}_{(1,2,3)}$	0.5449	0.8308	0.5434	0.8180 x	0.5751	0.7640	0.8597 x	0.9572	0.9267	0.9825	σ^2=1e-1 NMU, $\|\mathbf{x}\|_1$ Denoising hard τ=1e-7
$\mathbf{X}_{(1,2,3)}$	0.7234	0.8487	0.5026	0.8990 x	0.5603	0.8382	0.9217 x	0.9685	0.8288	0.8713	σ^2=1e1 NMU, x_{max}
$\mathbf{X}_{(1,2,3)}$	0.6652	0.8487	0.5449	0.8990 x	0.5932	0.8387	0.9217 x	0.9685	0.8288	0.8713	σ^2=1e1 NMU, x_{max} Denoising hard τ=1e-7
$\mathbf{X}_{(1,2,3)}$	0.6157	0.8866	0.4924	0.9547 x	0.6303	0.7579	0.9684 x	0.9676	0.9070	0.9905	σ^2=1e1 NMU, $\|\mathbf{x}\|_1$
$\mathbf{X}_{(1,2,3)}$	0.5855	0.8866	0.4924	0.9547 x	0.6303	0.7578	0.9684 x	0.9676	0.9070	0.9905	σ^2=1e1 NMU, $\|\mathbf{x}\|_1$ Denoising hard τ=1e-7
$\mathbf{X}_{(3,4)}$	0.5554	0.9107	0.6707	0.7453 x	0.6418	0.9166	0.7916 x	0.8869	0.8169	0.7617	σ^2=1e0 NMU, x_{max}
$\mathbf{X}_{(3,4)}$	0.4517	0.9107	0.6707	0.7453 x	0.6418	0.9166	0.7916 x	0.8869	0.8169	0.7621	σ^2=1e0 NMU, x_{max} Denoising hard τ=1e-7

$\mathbf{X}_{(3,4)}$	0.4873	0.7182	0.7689	0.7984 x	0.4657	0.9578	0.8249 x	0.9209	0.8092	0.7197	σ^2=1e0 NMU, $\|\mathbf{x}\|_{l_1}$
$\mathbf{X}_{(3,4)}$	0.5377	0.7179	0.7689	0.7984 x	0.4457	0.9578	0.8249 x	0.9209	0.8092	0.7197	σ^2=1e0 NMU, $\|\mathbf{x}\|_{l_1}$ Denoising hard τ=1e-7
$\mathbf{X}_{(3,4)}$	0.5309	0.7552	0.7321	0.8030 x	0.6653	0.8359	0.8349 x	0.9235	0.8051	0.7011	σ^2=1e-1 NMU, x_{max}
$\mathbf{X}_{(3,4)}$	0.5631	0.7552	0.7613	0.8030 x	0.6653	0.8359	0.8349 x	0.9235	0.8051	0.7011	σ^2=1e-1 NMU, x_{max} Denoising hard τ=1e-7
$\mathbf{X}_{(3,4)}$	0.5104	0.8479	0.6889	0.7308 x	0.5734	0.9386	0.7621 x	0.9318	0.7998	0.8085	σ^2=1e-1 NMU, $\|\mathbf{x}\|_{l_1}$
$\mathbf{X}_{(3,4)}$	0.6232	0.8479	0.6889	0.7308 x	0.6461	0.9386	0.7621 x	0.9318	0.7998	0.8085	σ^2=1e-1 NMU, $\|\mathbf{x}\|_{l_1}$ Denoising hard τ=1e-7
$\mathbf{X}_{(3,4)}$	0.5874	0.6050	0.6381	0.7070	0.6301	0.9400	0.7626	0.9448	0.7206	0.6451	Gauss, σ^2=1e1 NMU, x_{max}
$\mathbf{X}_{(3,4)}$	0.4638	0.6050	0.7164	0.7070	0.6329	0.9400	0.7626	0.9448	0.7206	0.6451	Gauss, σ^2=1e1 NMU, x_{max} Denoising hard τ=1e-7
$\mathbf{X}_{(3,4)}$	0.4973	0.7649	0.5762	0.7217 x	0.5866	0.9333	0.7067 x	0.9506	0.6622	0.6451	σ^2=1e1 NMU, $\|\mathbf{x}\|_{l_1}$
$\mathbf{X}_{(3,4)}$	0.4692	0.6605	0.5177	0.7217 x	0.5879	0.9333	0.7067	0.9506	0.6622	0.6594	σ^2=1e1 NMU, $\|\mathbf{x}\|_{l_1}$ Denoising hard τ=1e-7


x10 5
90.1
Counts vs. Mass-to-Charge (m/z)
Ala (C1)
[M+H]+ m/z 90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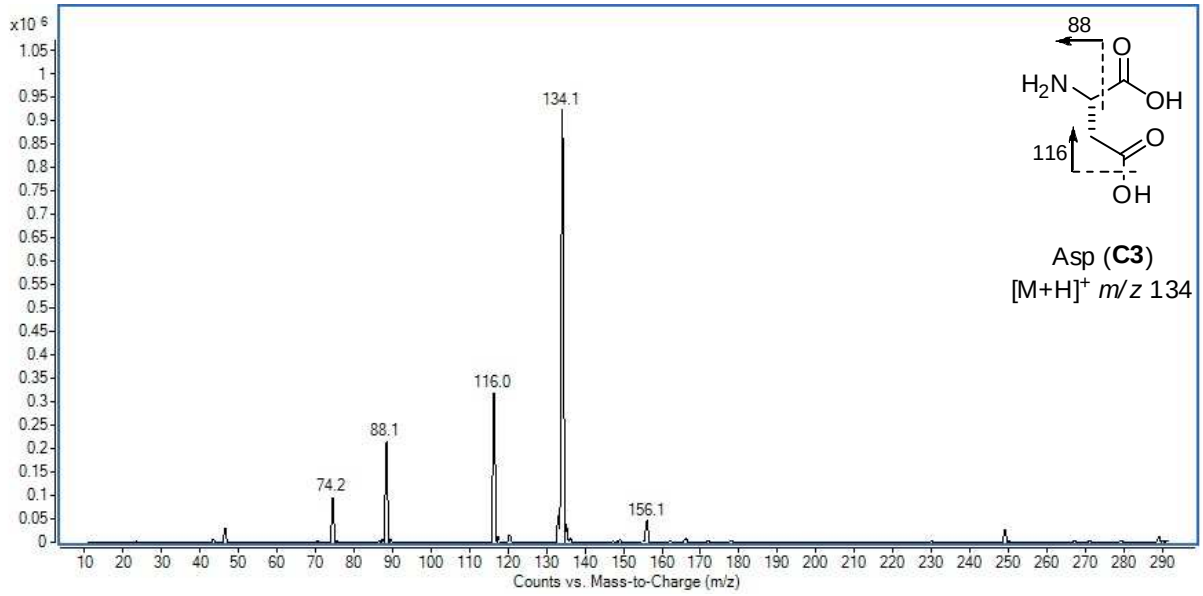
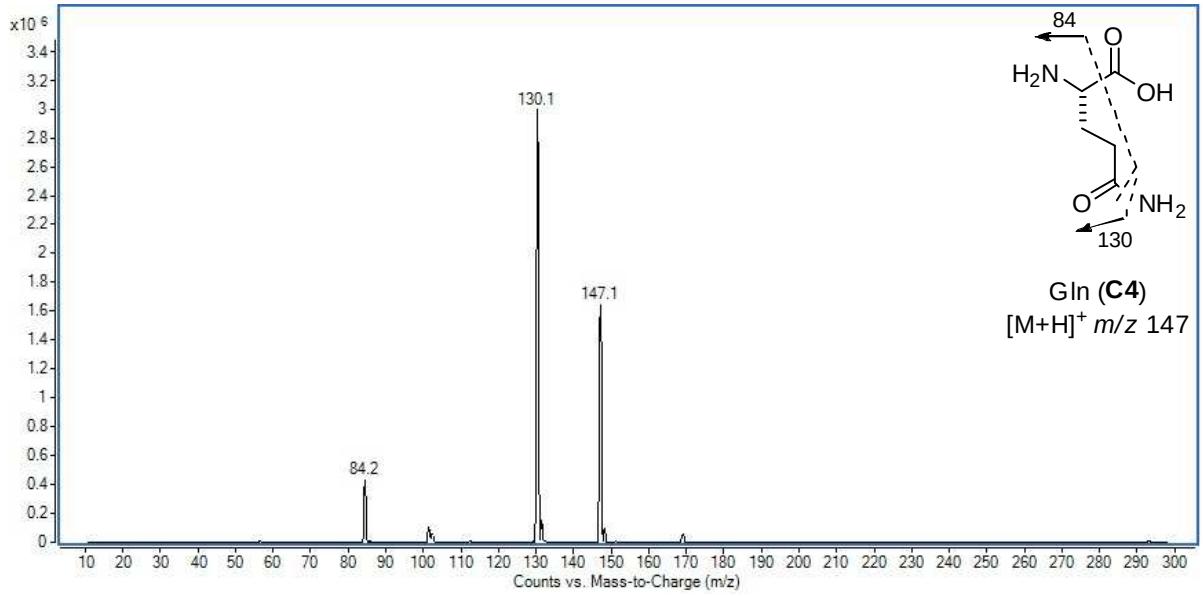
133.1
87.1
116.0
87
116
Counts vs. Mass-to-Charge (m/z)
Asn (C2)
[M+H]+ m/z 133


x10 6
134.1
116.0
88.1
74.2
156.1
Counts vs. Mass-to-Charge (m/z)
88
116
Asp (C3)
[M+H]+ m/z 134


x10 6
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147.1
84.2
Counts vs. Mass-to-Charge (m/z)
84
130
Gln (C4)
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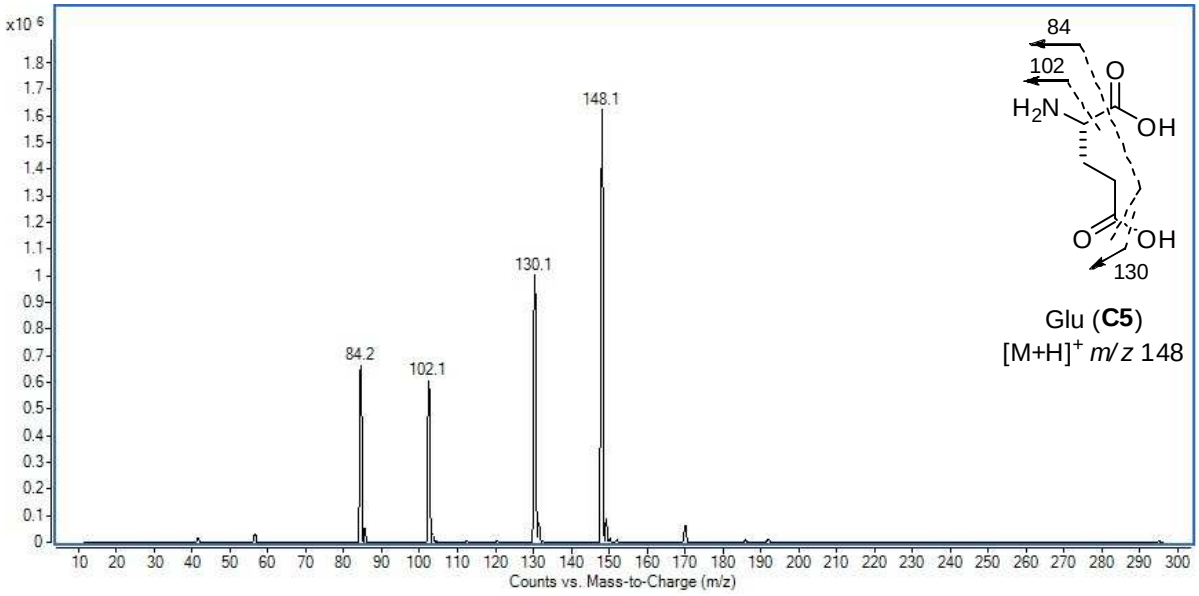
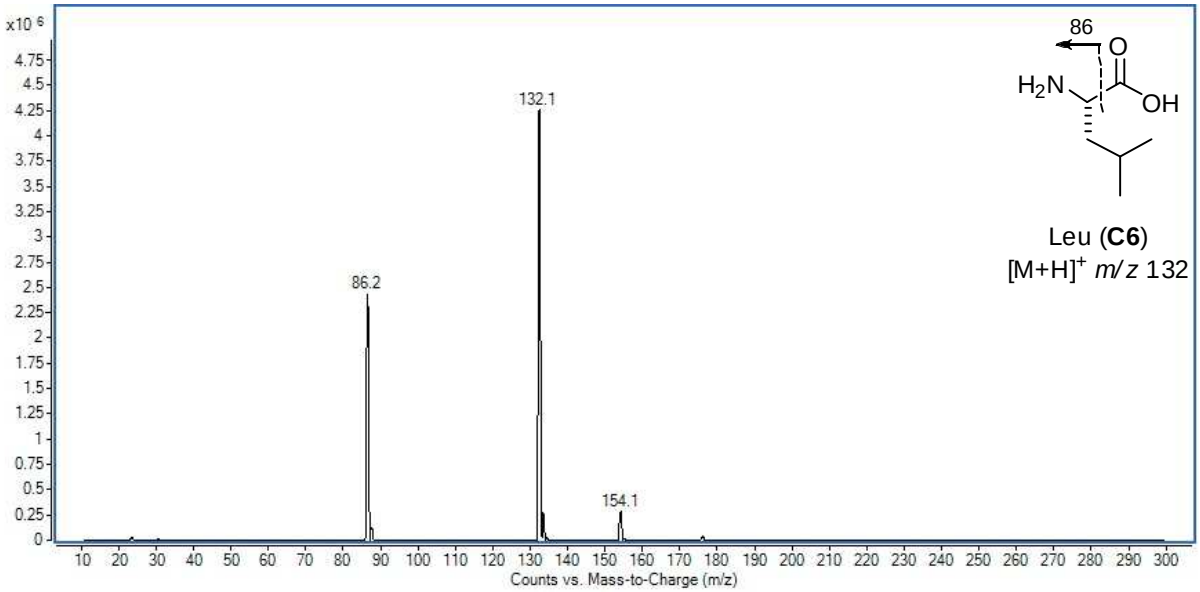
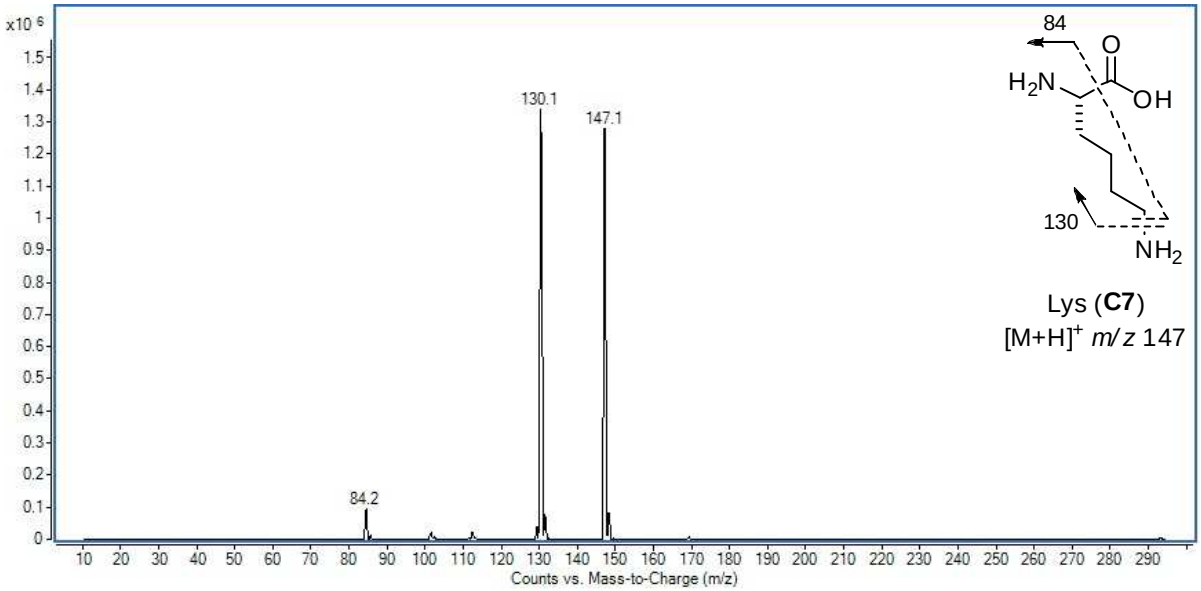
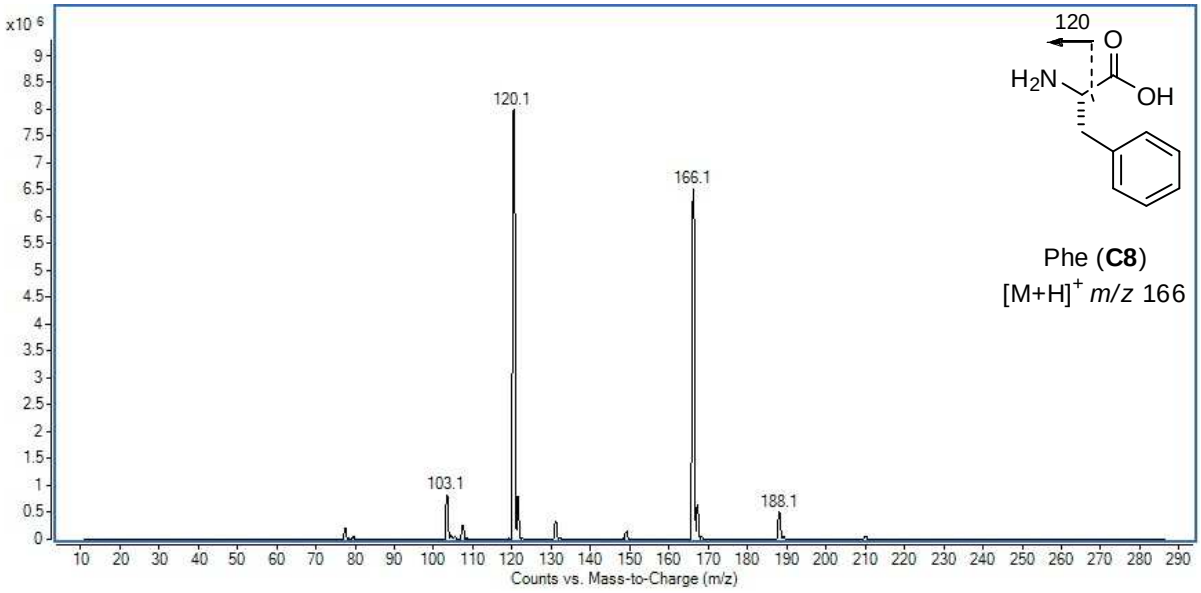

x10 6
148.1
130.1
84.2
102.1
Counts vs. Mass-to-Charge (m/z)
84
102
130
Glu (**C5**)
[M+H]+ *m/z* 148


x10 6
132.1
86.2
154.1
Counts vs. Mass-to-Charge (m/z)
86
Leu (**C6**)
[M+H]+ *m/z* 132


x10 6
130.1
147.1
84.2
Counts vs. Mass-to-Charge (m/z)
84
130
Lys (**C7**)
$[M+H]^+$ *m/z* 147


x10 6
120.1
166.1
103.1
188.1
Counts vs. Mass-to-Charge (m/z)
120
Phe (**C8**)
$[M+H]^+$ *m/z* 166

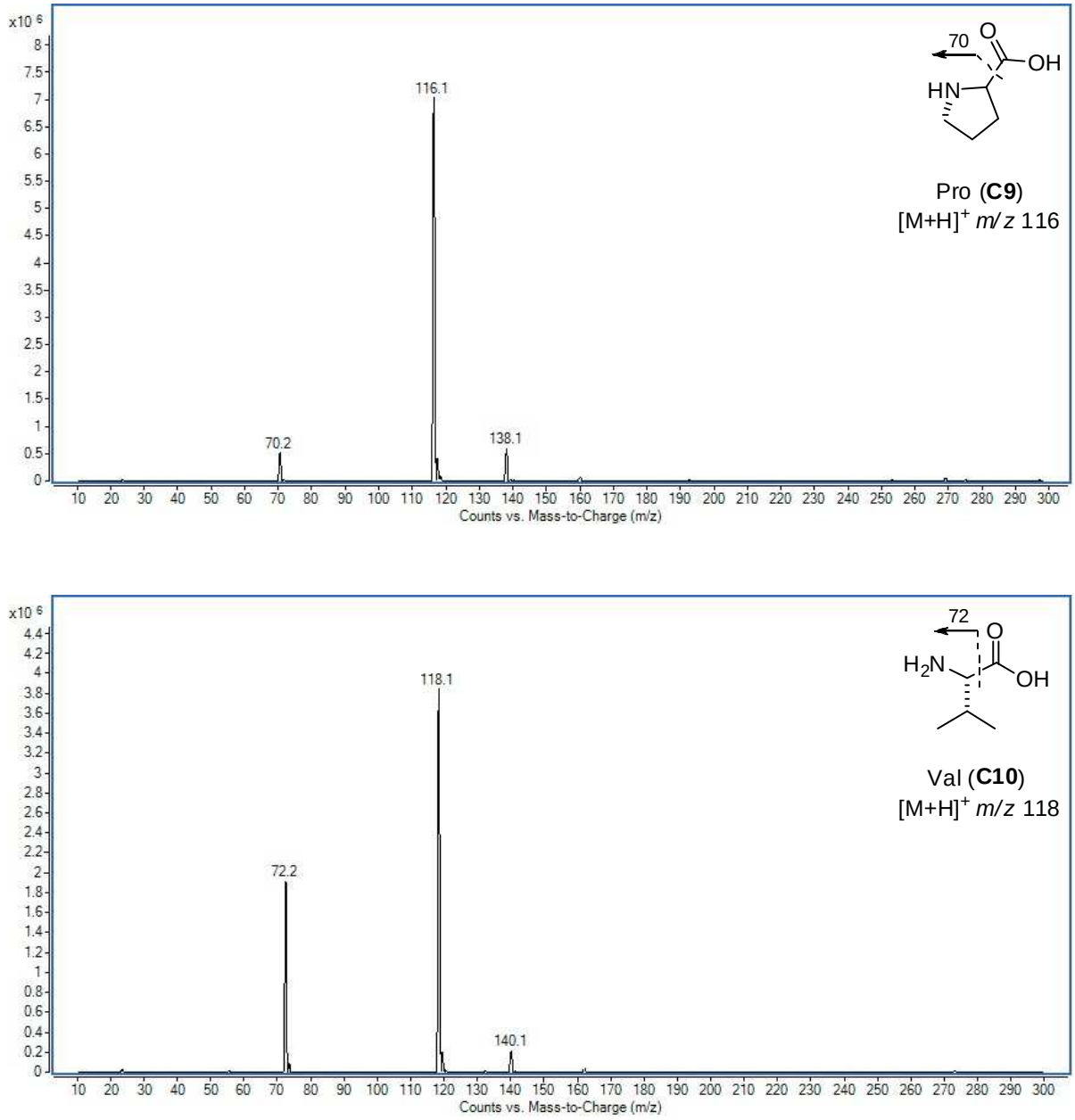
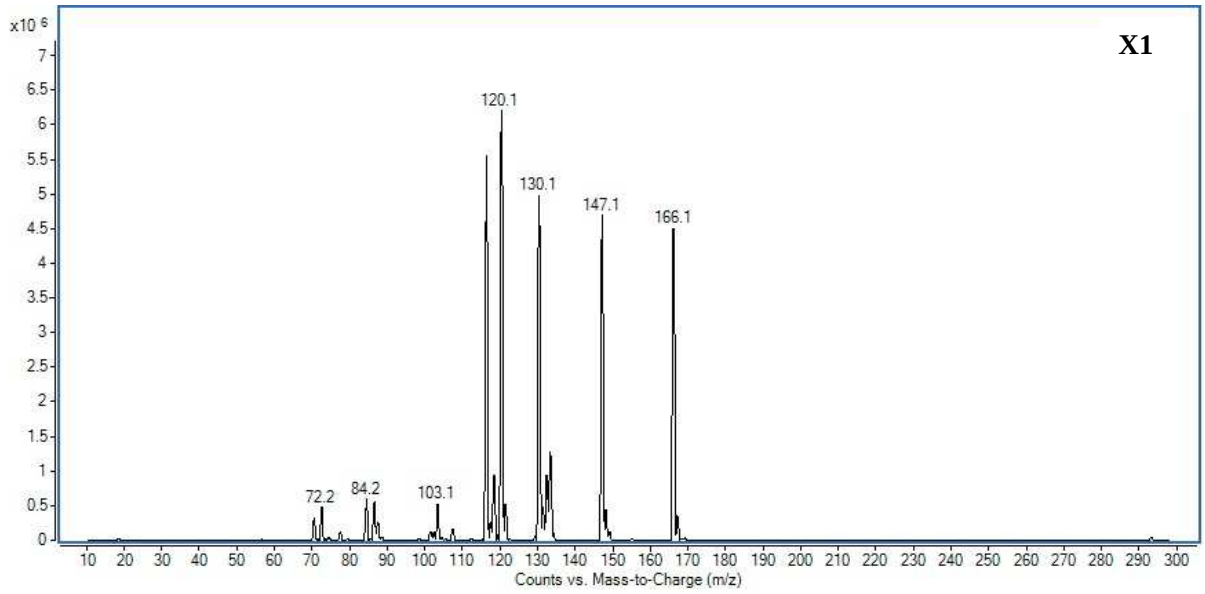
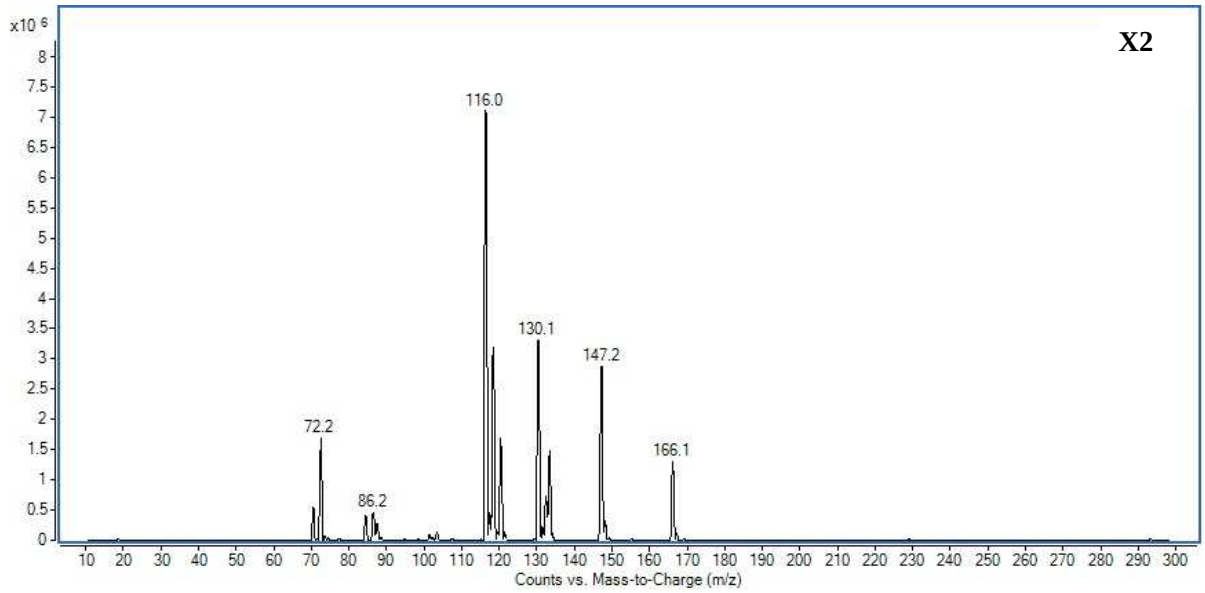
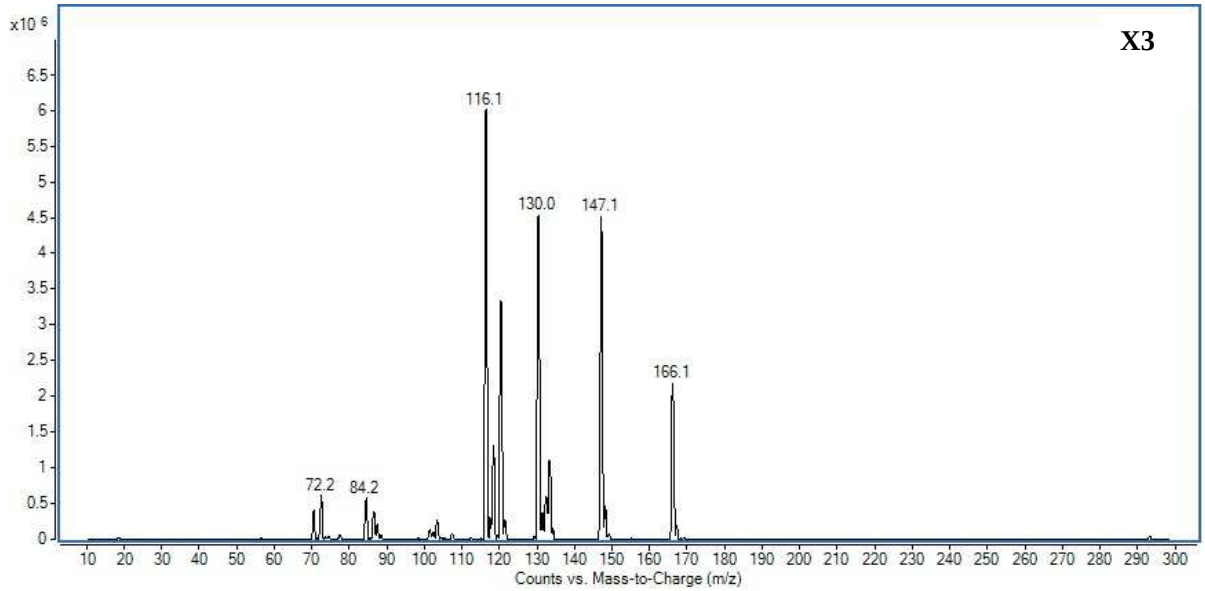
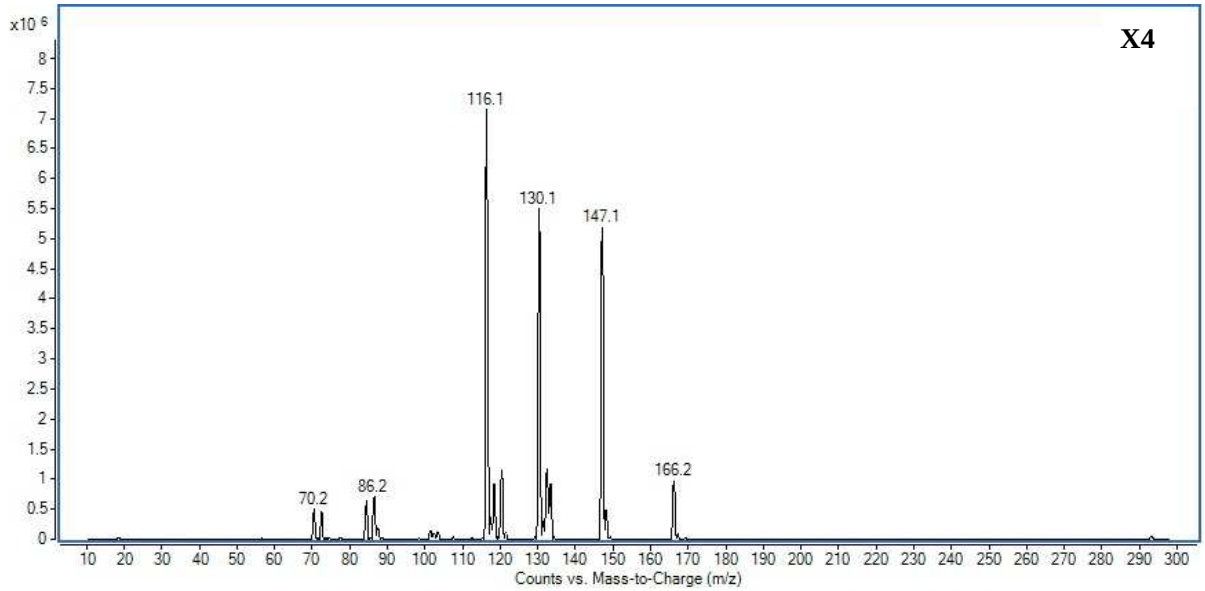

x10 6
116.1
70.2
138.1
70
O
OH
HN
Pro (C9)
[M+H]+ m/z 116
Counts vs. Mass-to-Charge (m/z)
x10 6
118.1
72.2
140.1
72
O
H2N
OH
Val (C10)
[M+H]+ m/z 118
Counts vs. Mass-to-Charge (m/z)

Figure S-1.


X1
x10 6
120.1
130.1
147.1
166.1
72.2
84.2
103.1
Counts vs. Mass-to-Charge (m/z)


X2
x10 6
116.0
130.1
147.2
166.1
72.2
86.2
Counts vs. Mass-to-Charge (m/z)


X3
x10 6
116.1
130.0
147.1
166.1
72.2
84.2
Counts vs. Mass-to-Charge (m/z)


X4
x10 6
116.1
130.1
147.1
166.2
70.2
86.2
Counts vs. Mass-to-Charge (m/z)

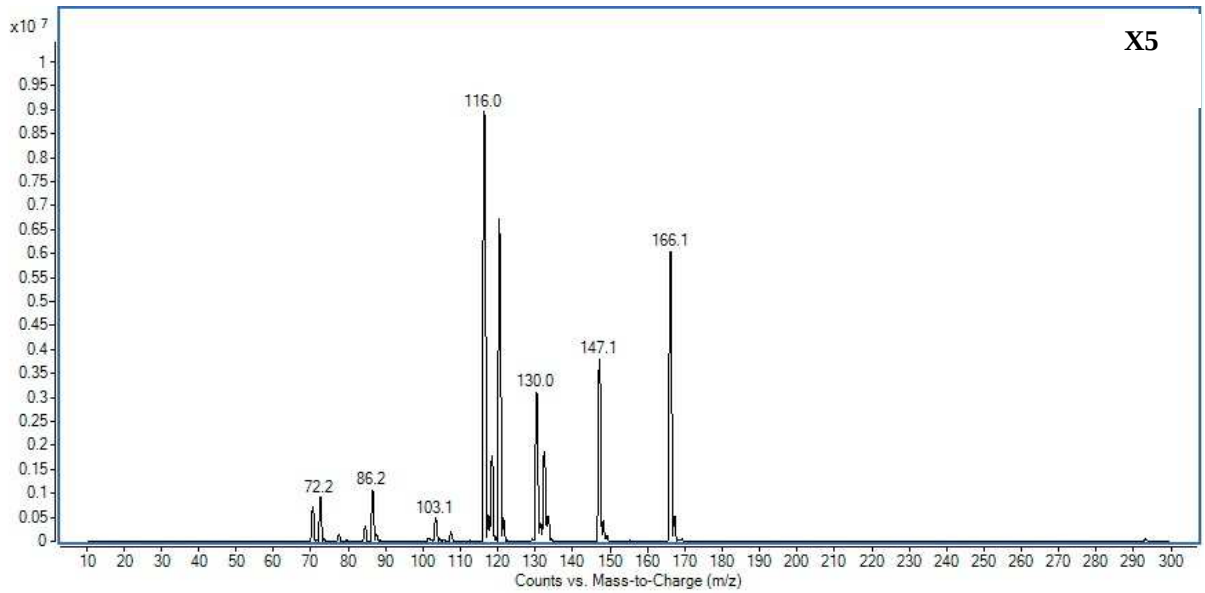
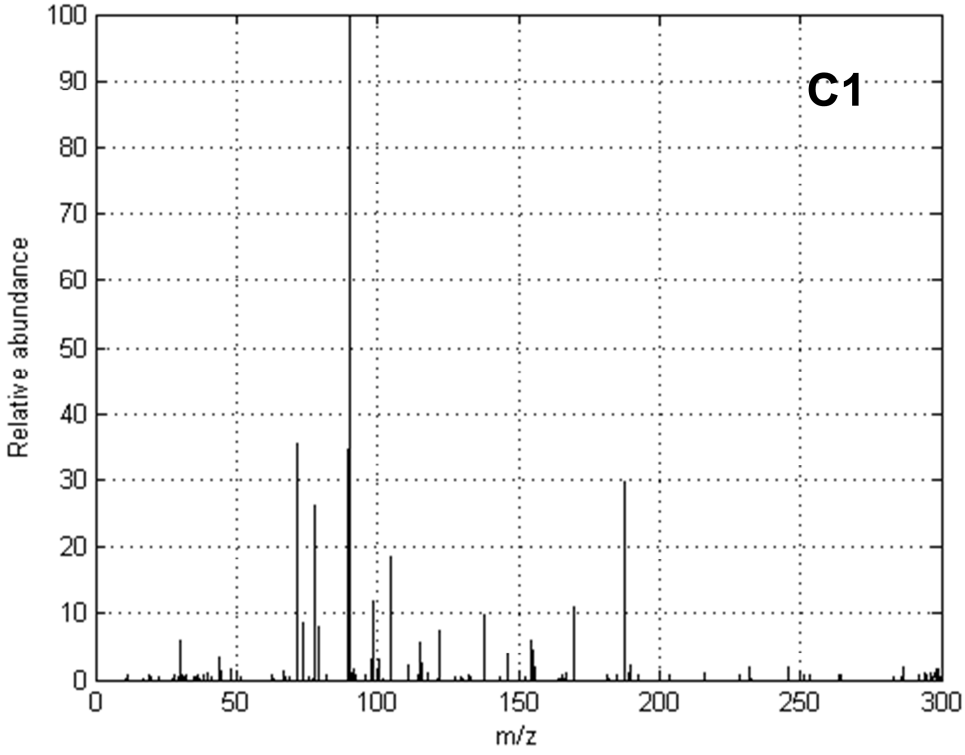
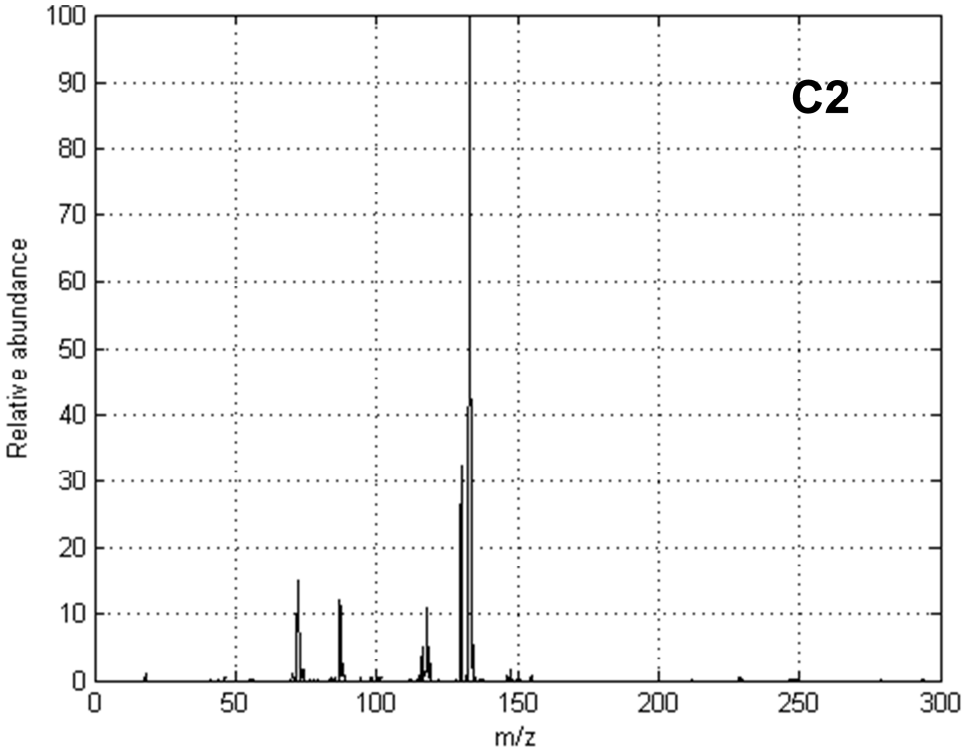
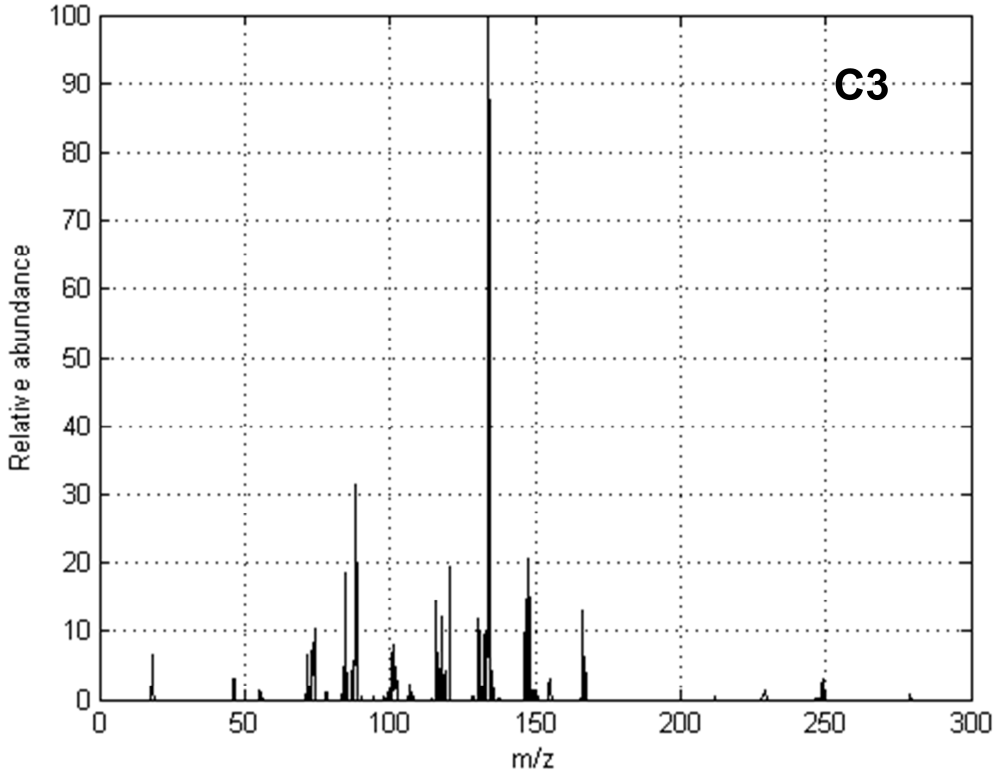
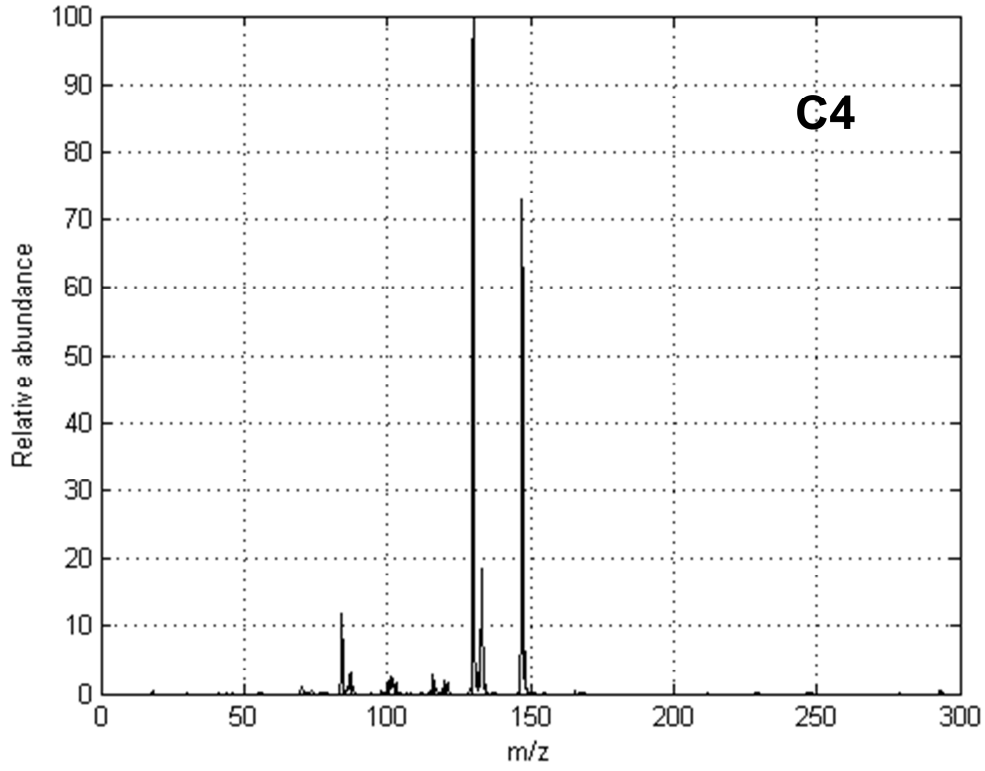

X5
x10 7
116.0
166.1
147.1
130.0
72.2
86.2
103.1
Counts vs. Mass-to-Charge (m/z)

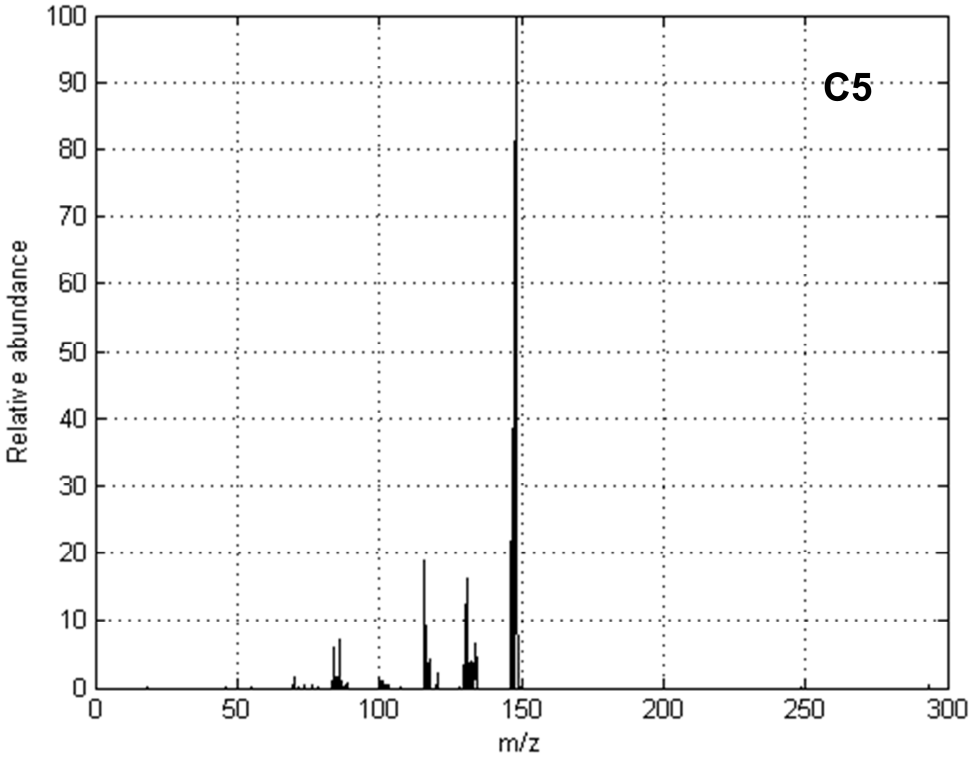
Figure S-2.

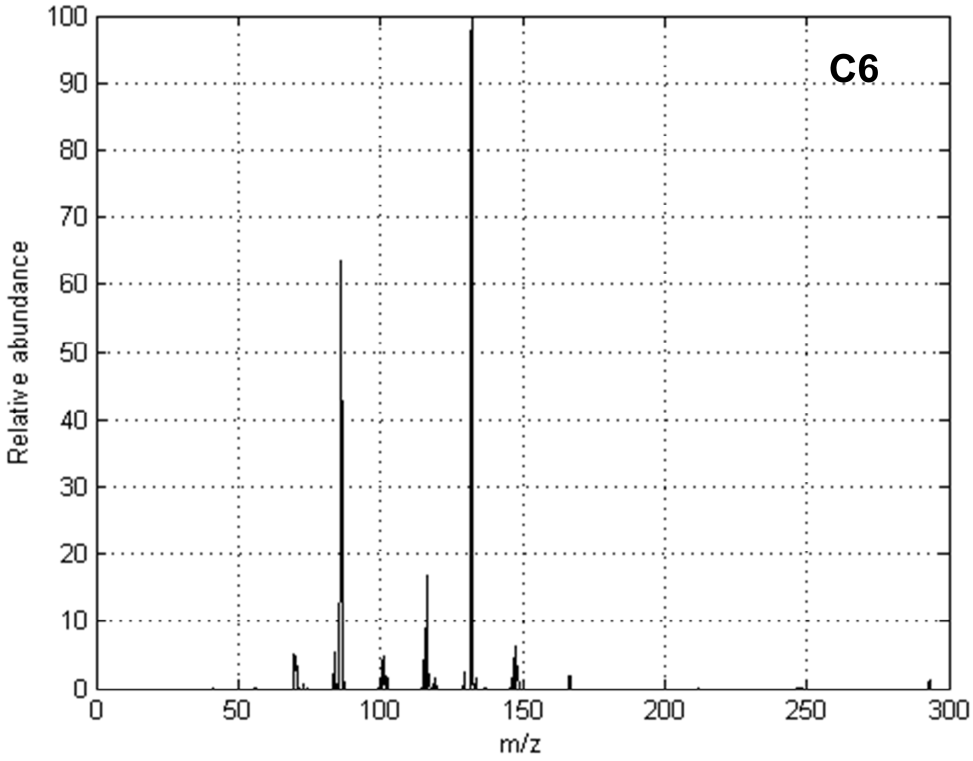

C1
Relative abundance
m/z
0
10
20
30
40
50
60
70
80
90
100
0
50
100
150
200
250
300

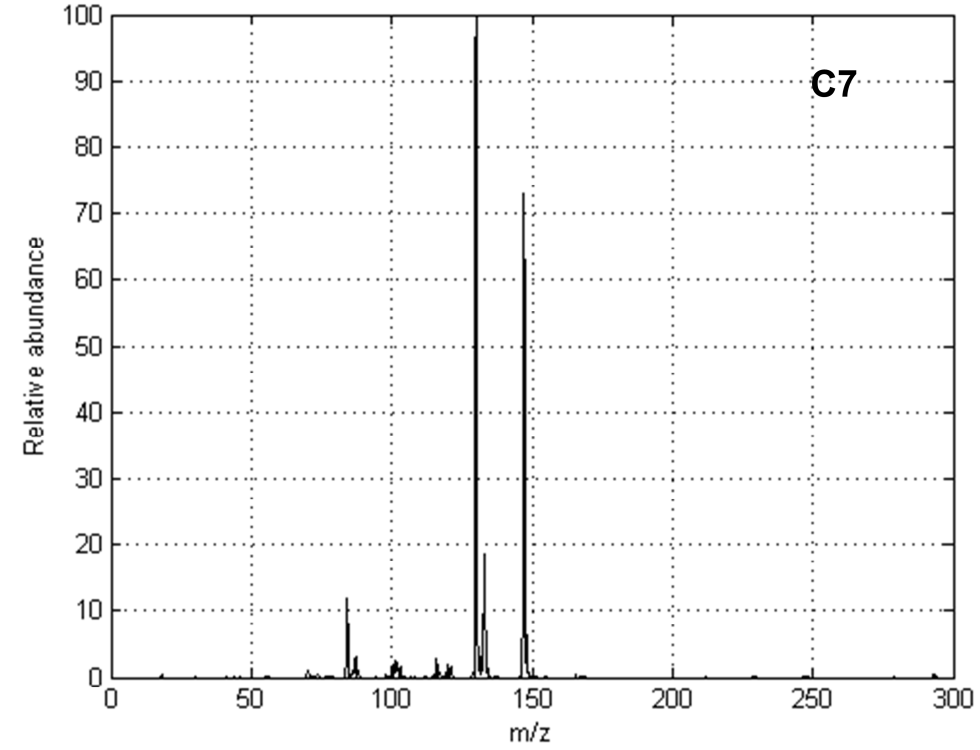

C2
Relative abundance
m/z
0
10
20
30
40
50
60
70
80
90
100
0
50
100
150
200
250
300

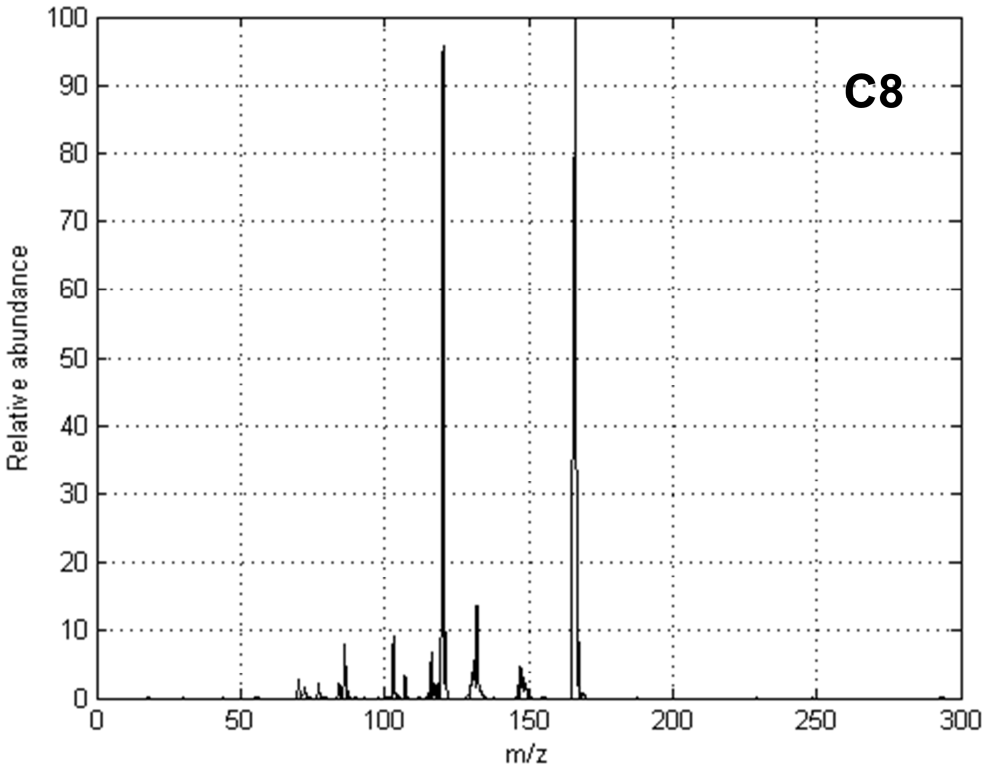

C3
Relative abundance
m/z
0
10
20
30
40
50
60
70
80
90
100
0
50
100
150
200
250
300

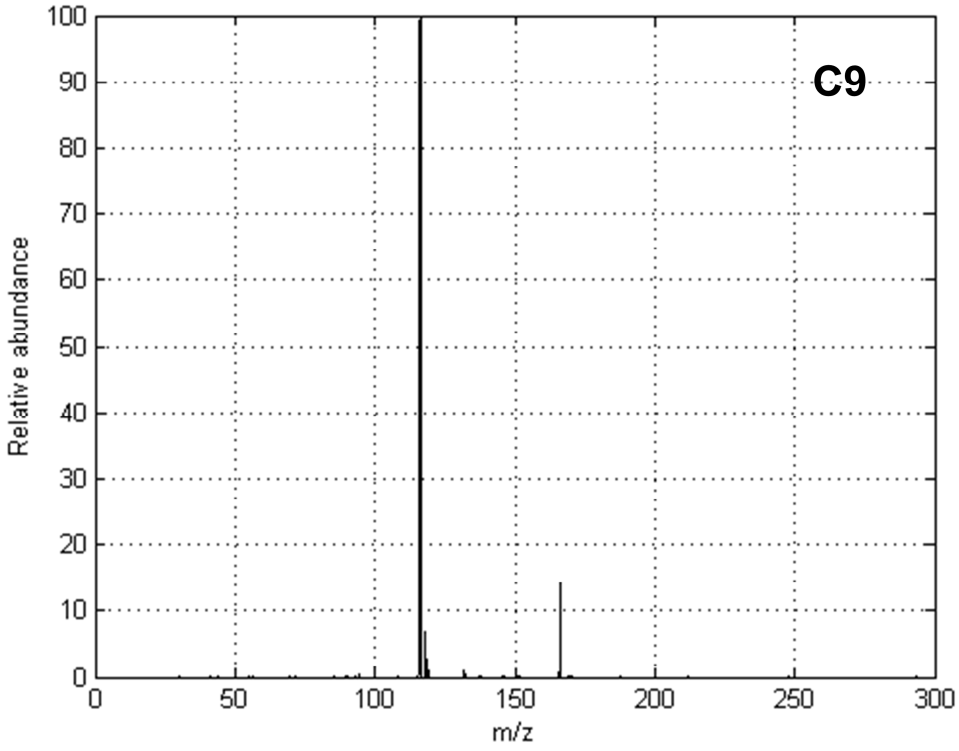

C4
Relative abundance
m/z
0
10
20
30
40
50
60
70
80
90
100
0
50
100
150
200
250
300


C5
Relative abundance
m/z
0
10
20
30
40
50
60
70
80
90
100
0
50
100
150
200
250
300


C6
Relative abundance
m/z
0
10
20
30
40
50
60
70
80
90
100
0
50
100
150
200
250
300


C7
Relative abundance
m/z
0
10
20
30
40
50
60
70
80
90
100
0
50
100
150
200
250
300


C8
Relative abundance
m/z
0
10
20
30
40
50
60
70
80
90
100
0
50
100
150
200
250
300


C9
Relative abundance
m/z
0
10
20
30
40
50
60
70
80
90
100
0
50
100
150
200
250
300

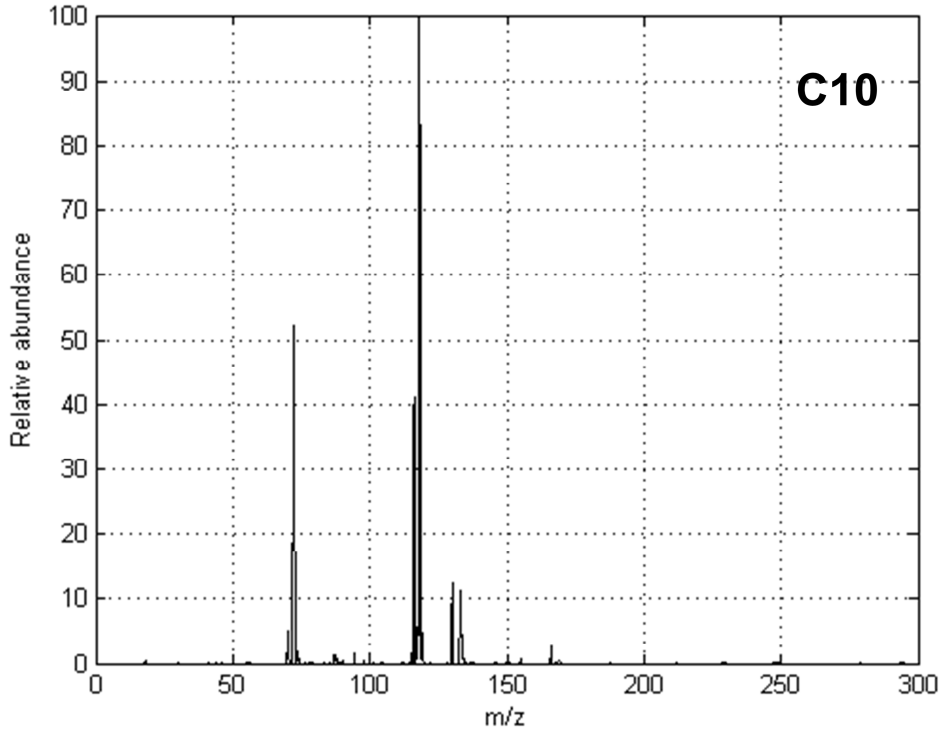

C10
Relative abundance
m/z
0
10
20
30
40
50
60
70
80
90
100
0
50
100
150
200
250
300

Figure S-3.