

Journal of The American Society for Mass Spectrometry
Supplementary Material

Benefit of the use of GCxGC/MS profiles for 1D GC/MS data treatment
illustrated by the analysis of pyrolysis products from East Asian handmade
papers

Bin Han, Silvia Lob, Michel Sablier*

Sorbonne Universités, Centre de Recherche sur la Conservation (USR 3224), Muséum national
d'Histoire naturelle, Ministère de la Culture et de la Communication, CNRS. 75005 Paris, France

*Corresponding authors

Email: michel.sablier@mnhn.fr

Address reprint requests to Dr. Michel Sablier

Tel: +33 1 40 79 53 23

Fax: +33 1 40 59 53 12

E-mail: michel.sablier@mnhn.fr

Address : Centre de recherche sur la conservation (CRC, USR 3224), Sorbonne Universités,
Muséum national d'Histoire naturelle, Ministère de la Culture et de la Communication, CNRS ; CP21,
36 rue Geoffroy-Saint-Hilaire, 75005 Paris, France

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Figure S1. Py-GCxGC/MS mass spectra (blue) and 1D AMDIS extracted spectra (red) for compound III (a), IV (b) and V (c) (unassigned peaks were not used for identification)

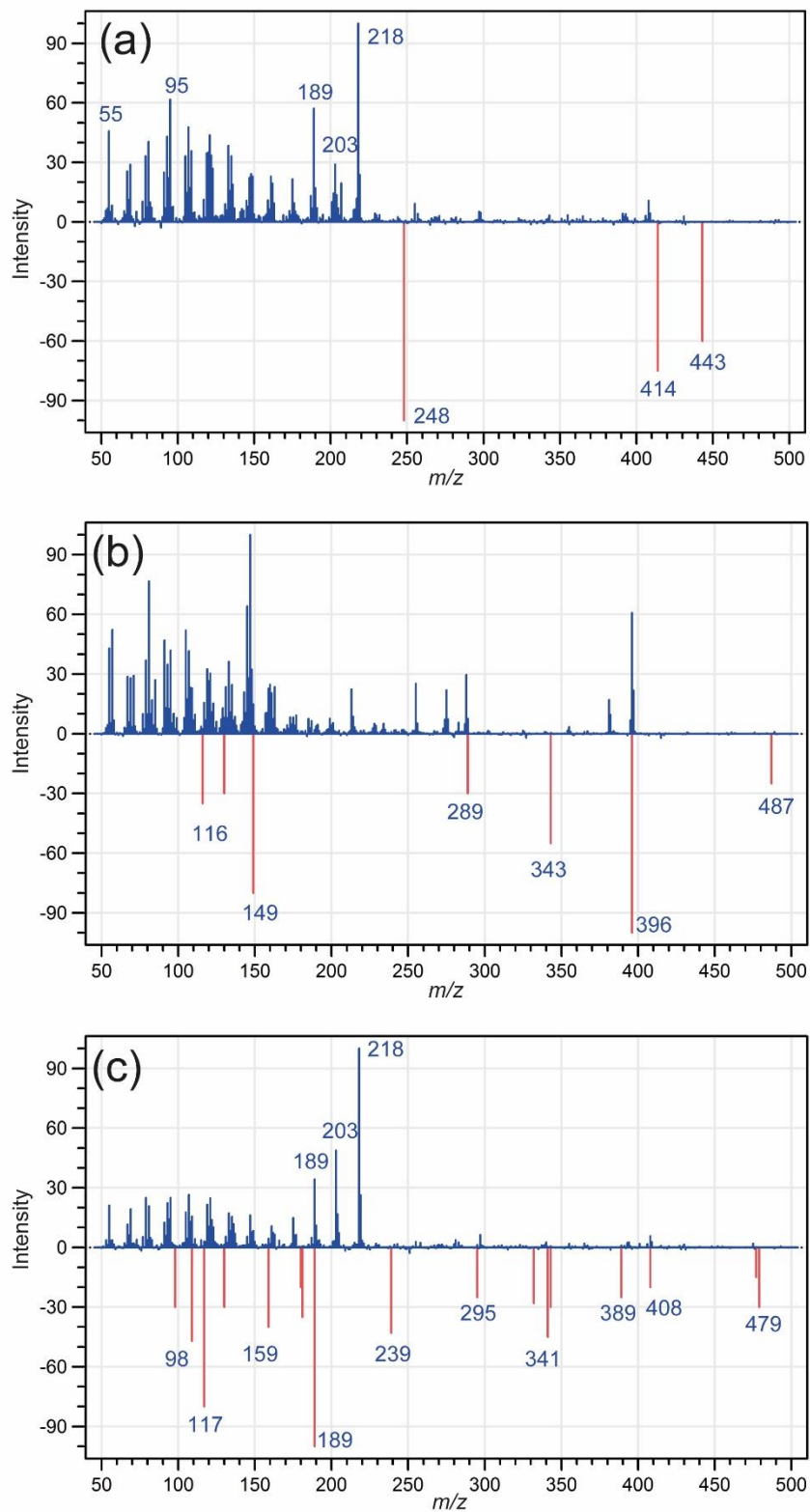


Figure S2. Compounds selected in the Py-GC/MS analysis in the marker region to test the performance of GCxGC/MS reintroduction for mass spectra analysis

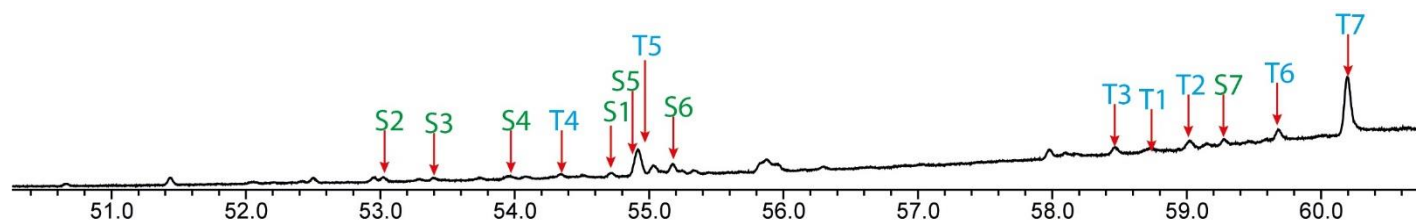


Figure S3. Procedure employed to derive the GCxGC mass spectra, 1D GC mass spectra using GCMS Postrun Analysis, AMDIS and GC Image to constitute the target library used in Part 3.3

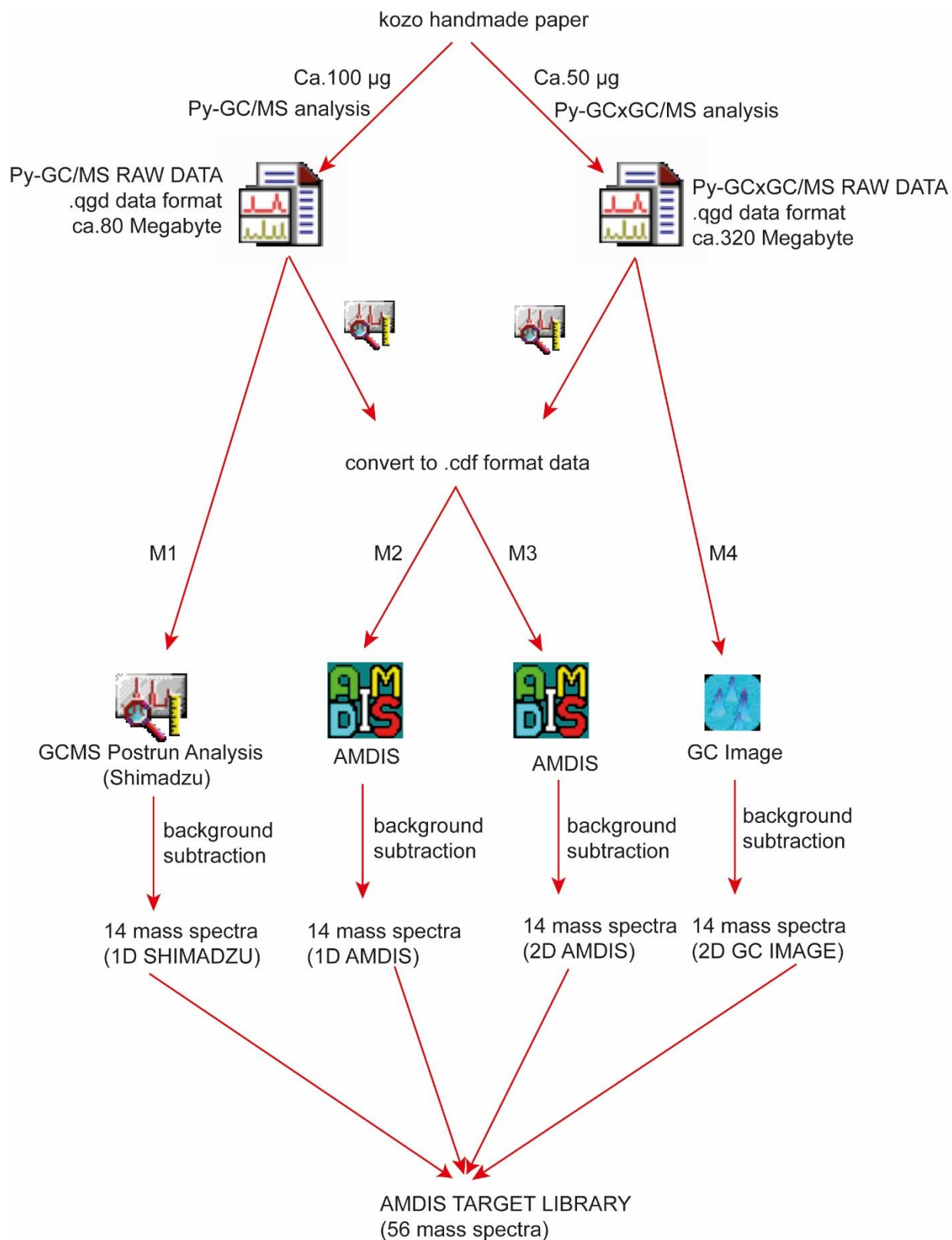


Figure S4. Target library of mass spectra collected from the procedure schematically reported in Figure S3 (the mass spectra are labeled in the format of 'Fig.S4-numbering-compound name-data source-treatment software' in accordance to the procedure described in Figure S3)

Figure S4-1-S1-1D-Shimadzu

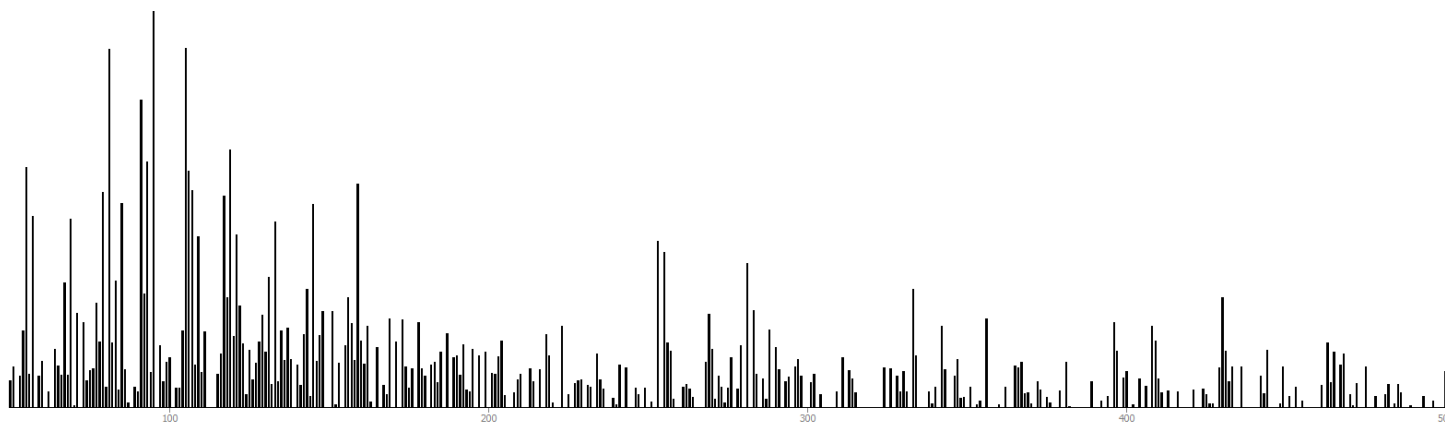


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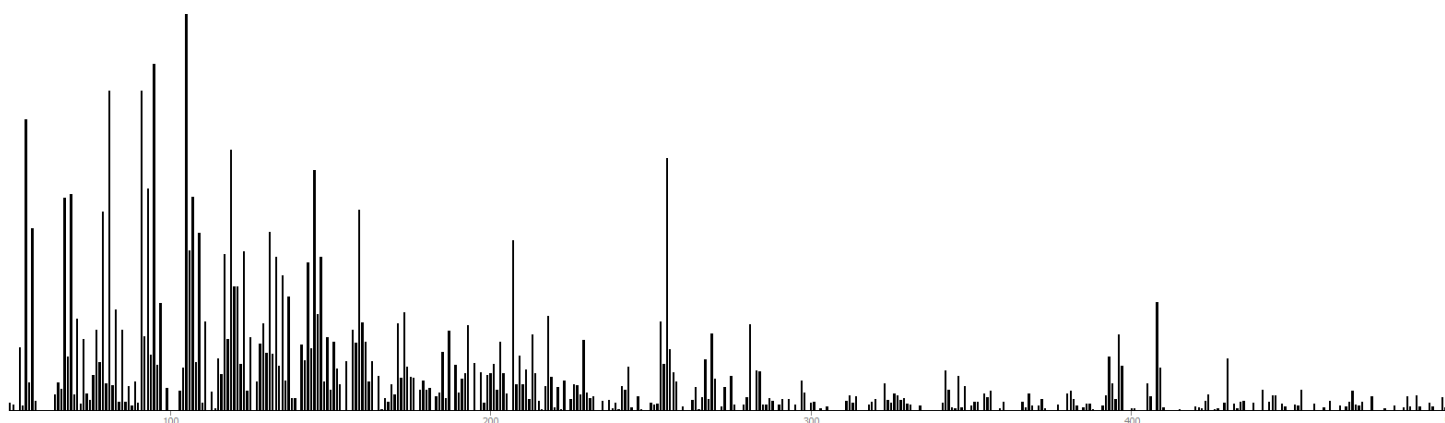


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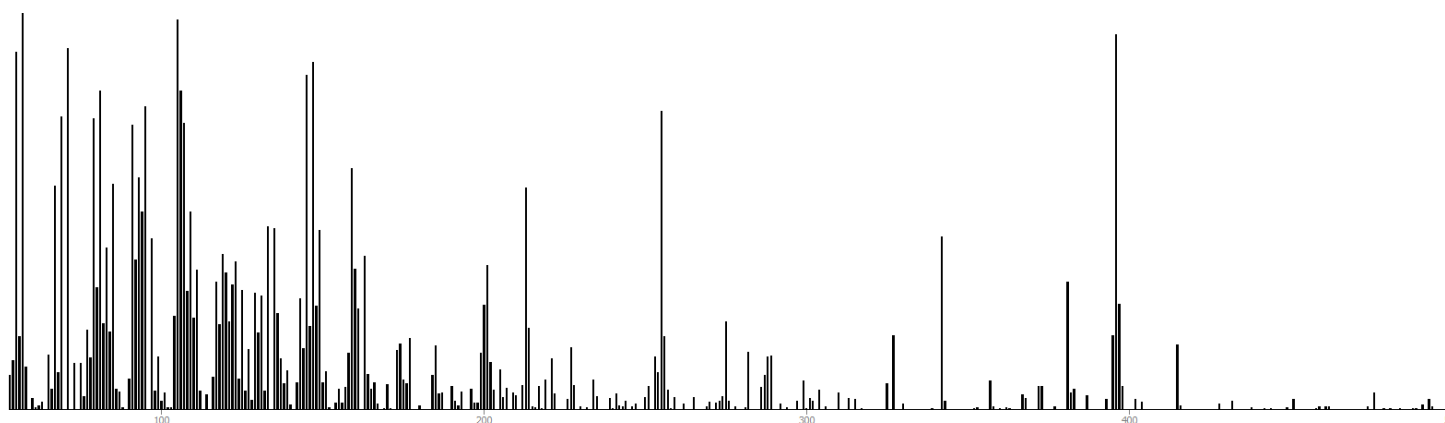


Figure S4-4-S1-2D-GC Image

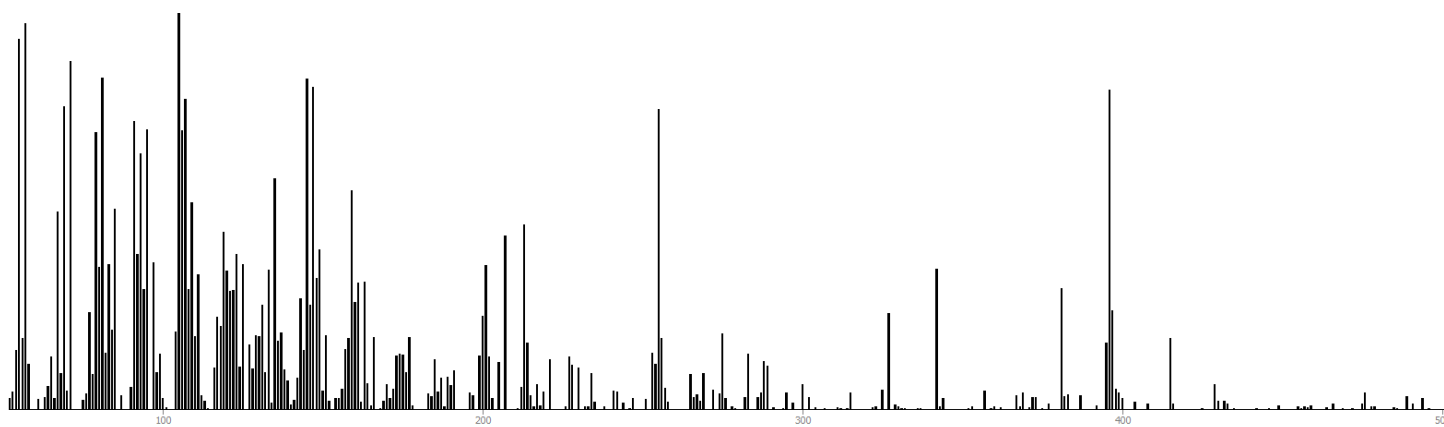


Figure S4-5-S2-1D-Shimadzu

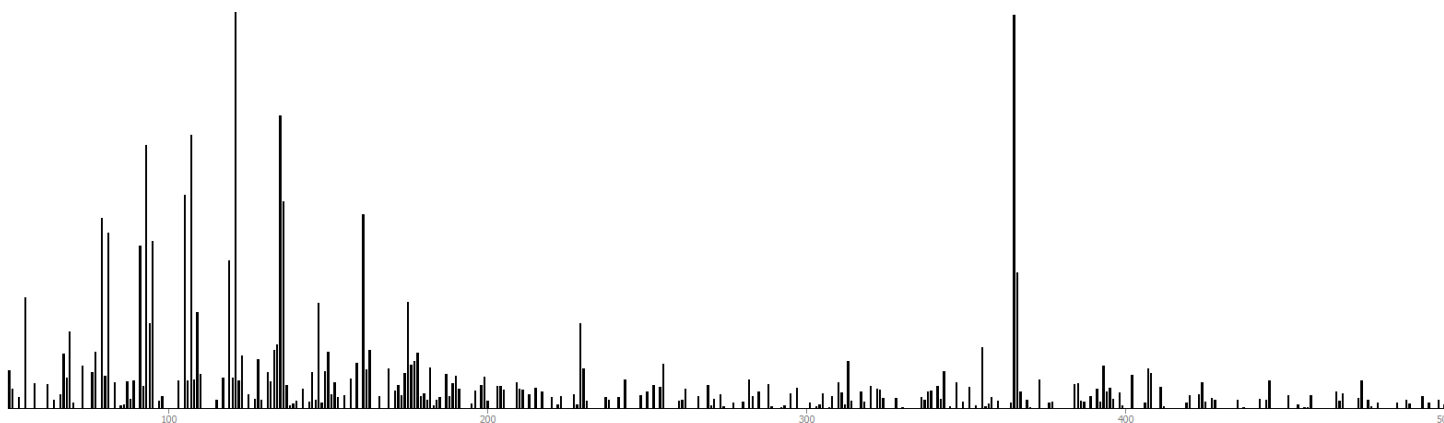


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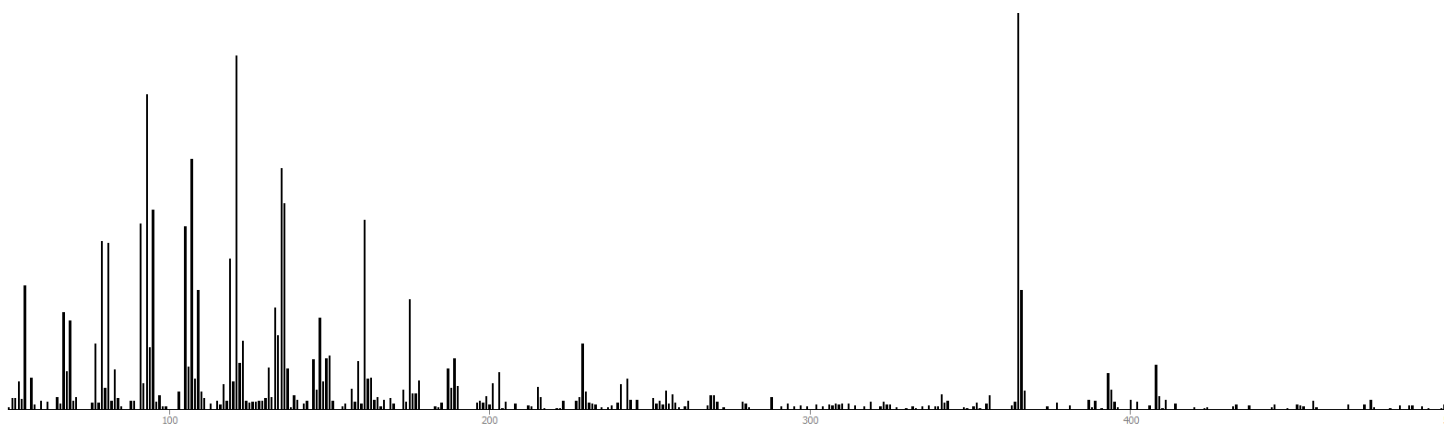


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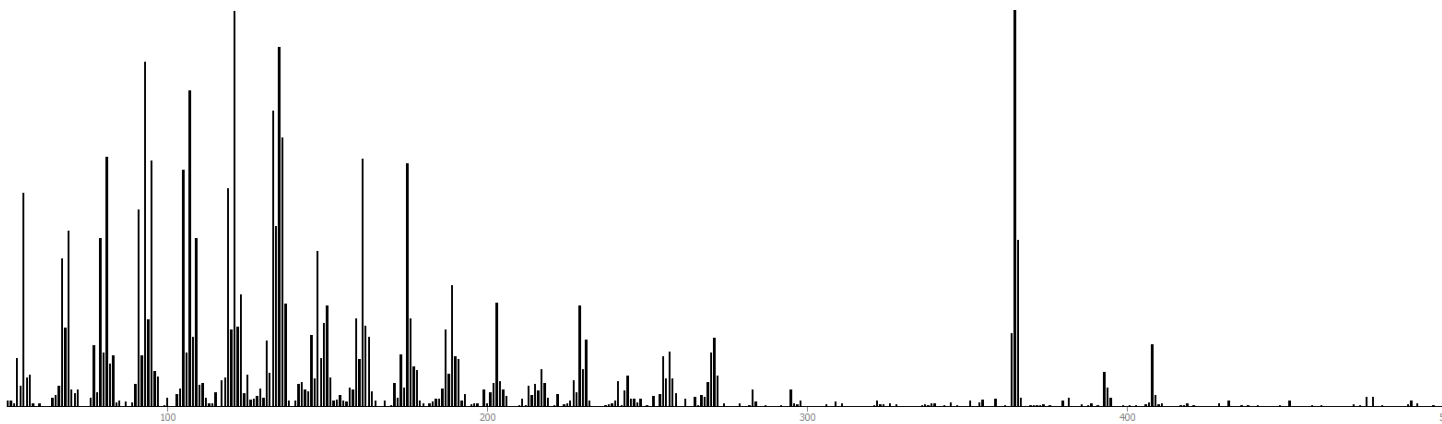


Figure S4-8-S2-2D-GC Image

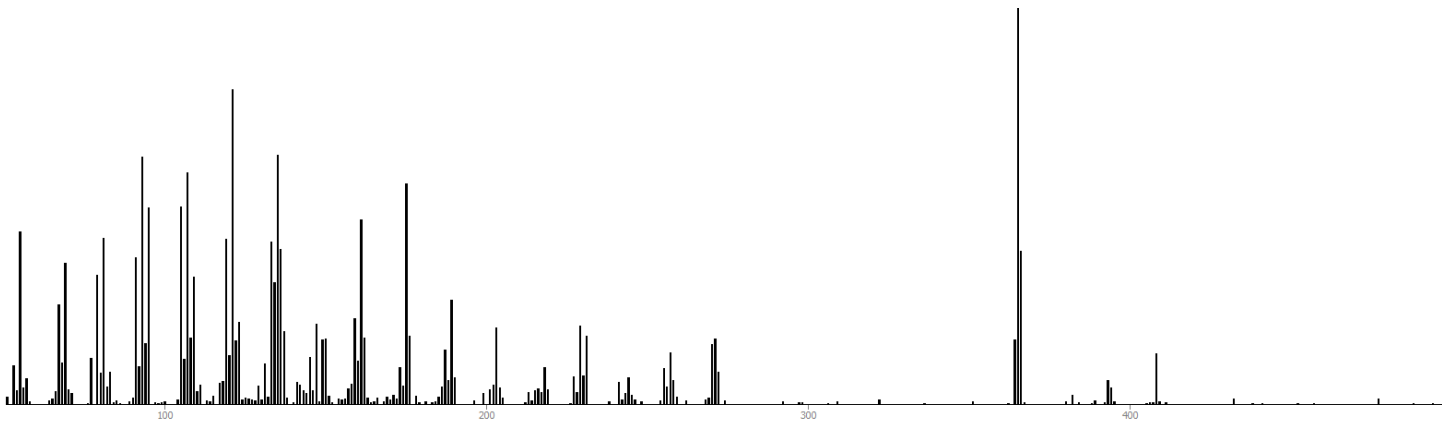


Figure S4-9-S3-1D- Shimadzu

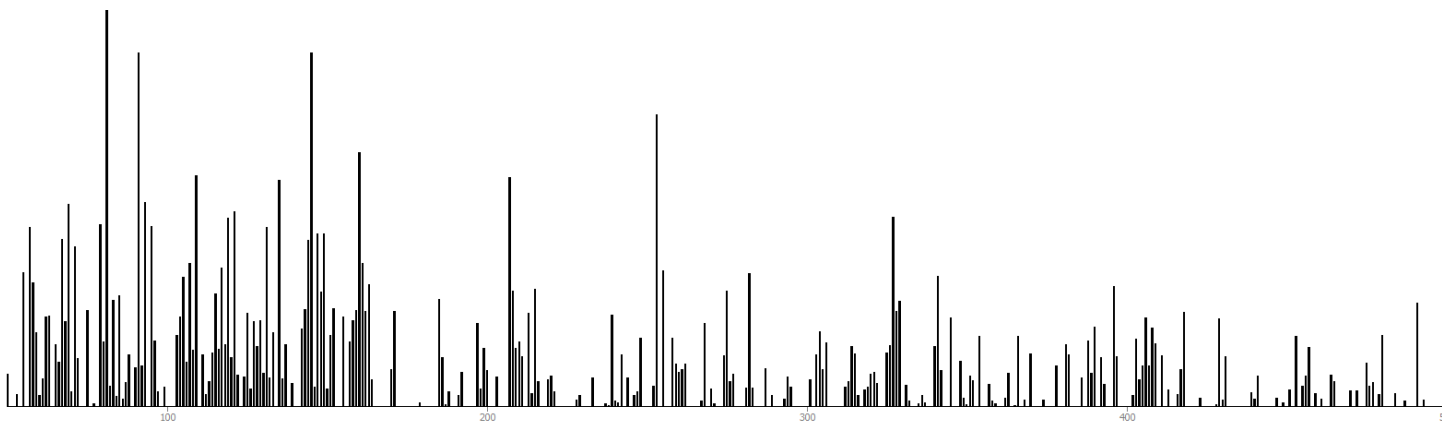


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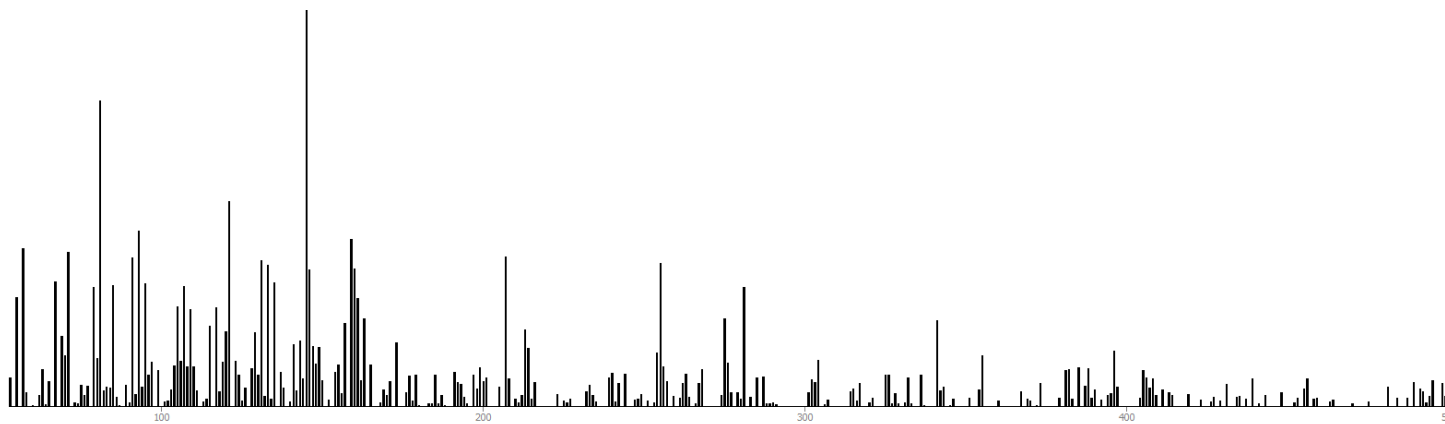


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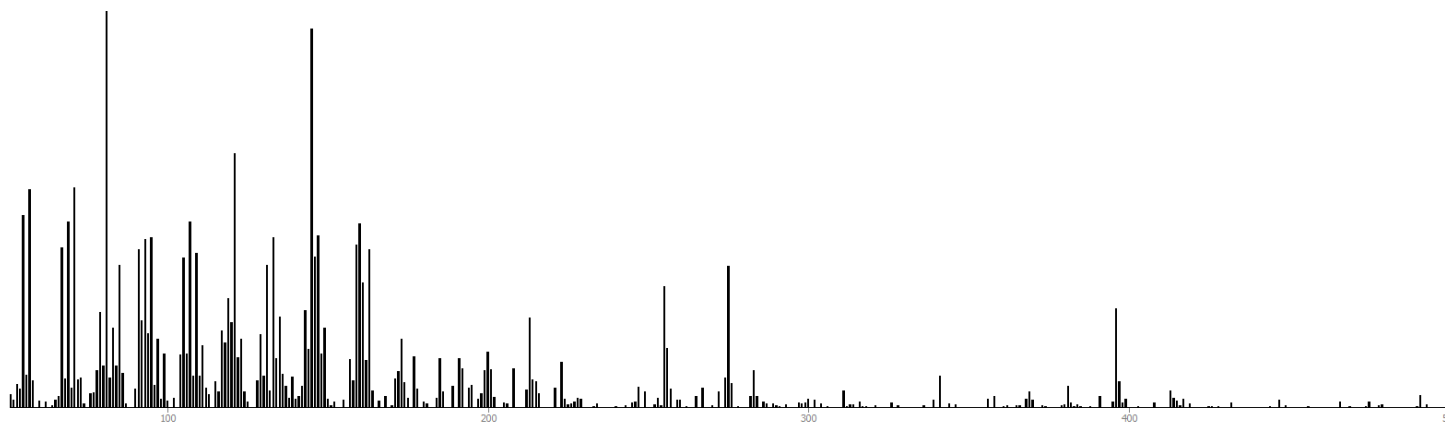


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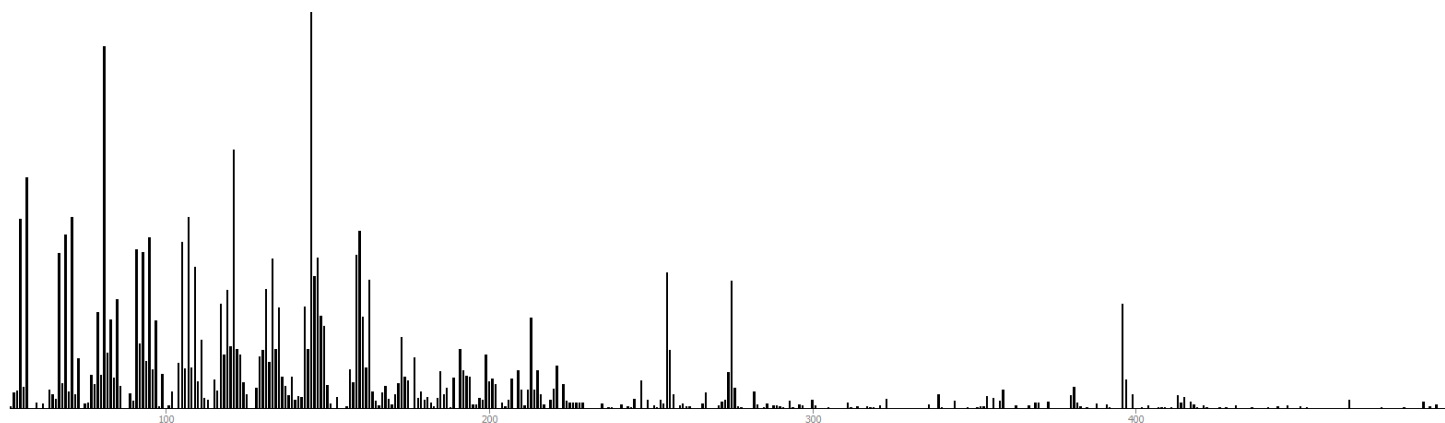


Figure S4-13-S4-1D- Shimadzu

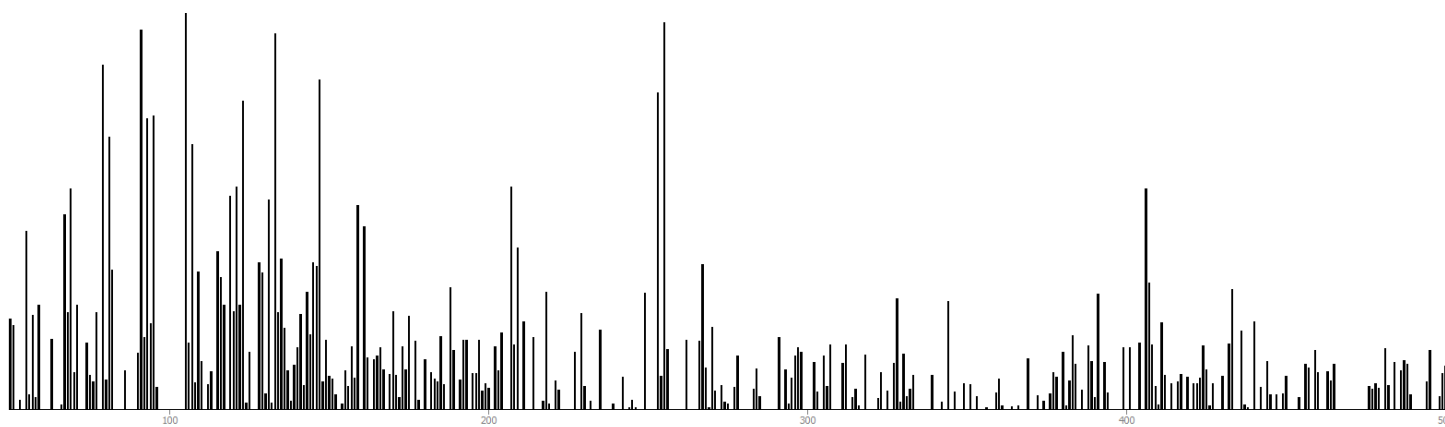


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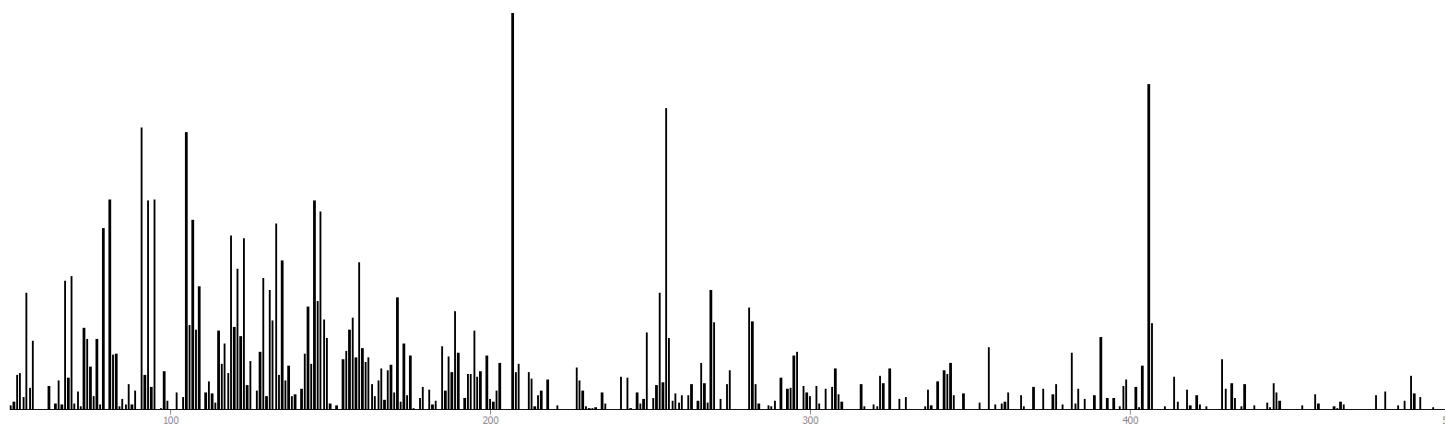


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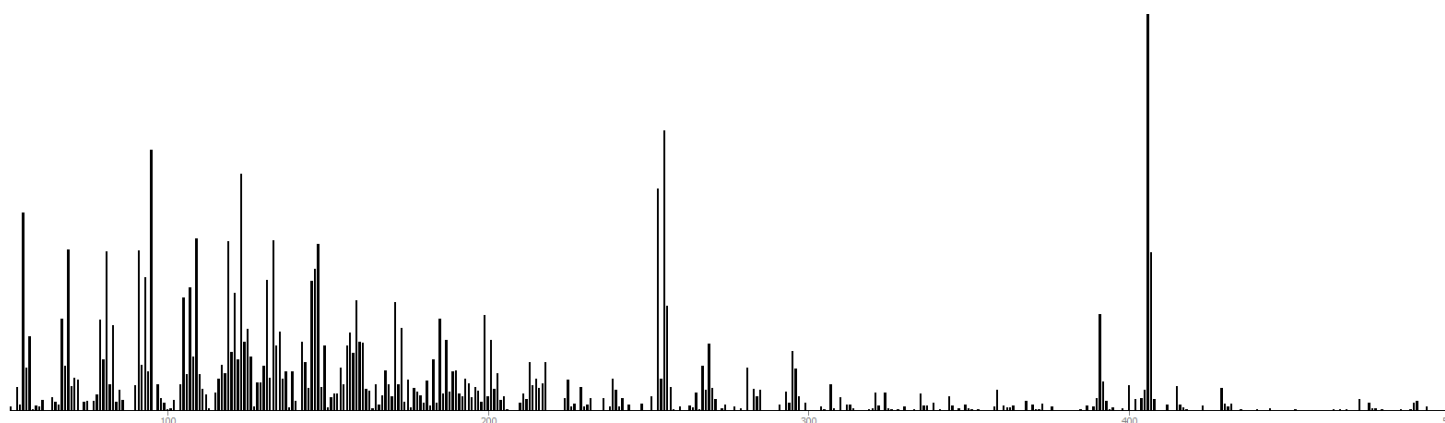


Figure S4-16-S4-2D-GC Image

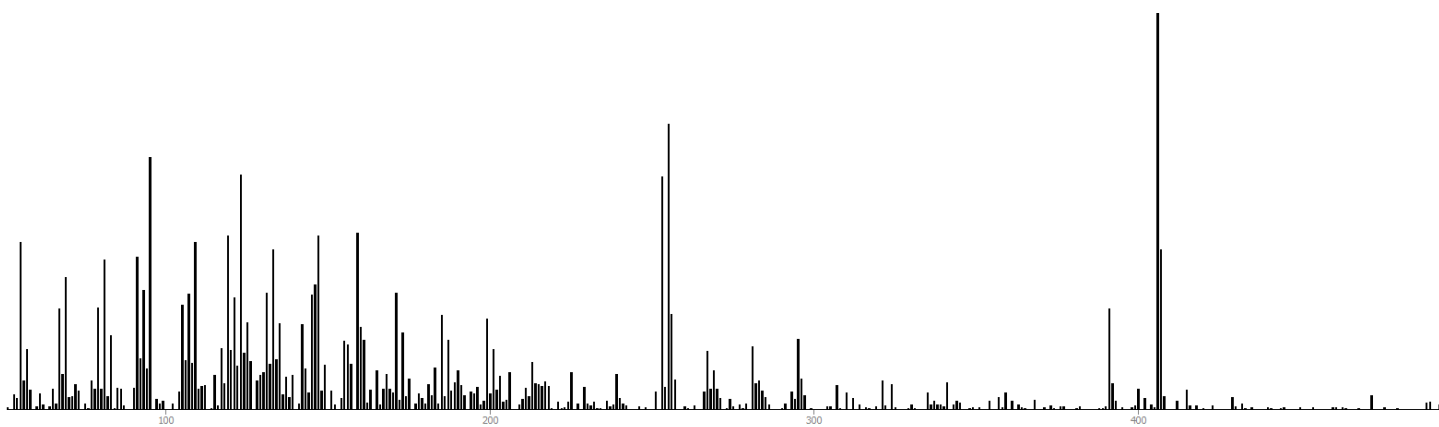


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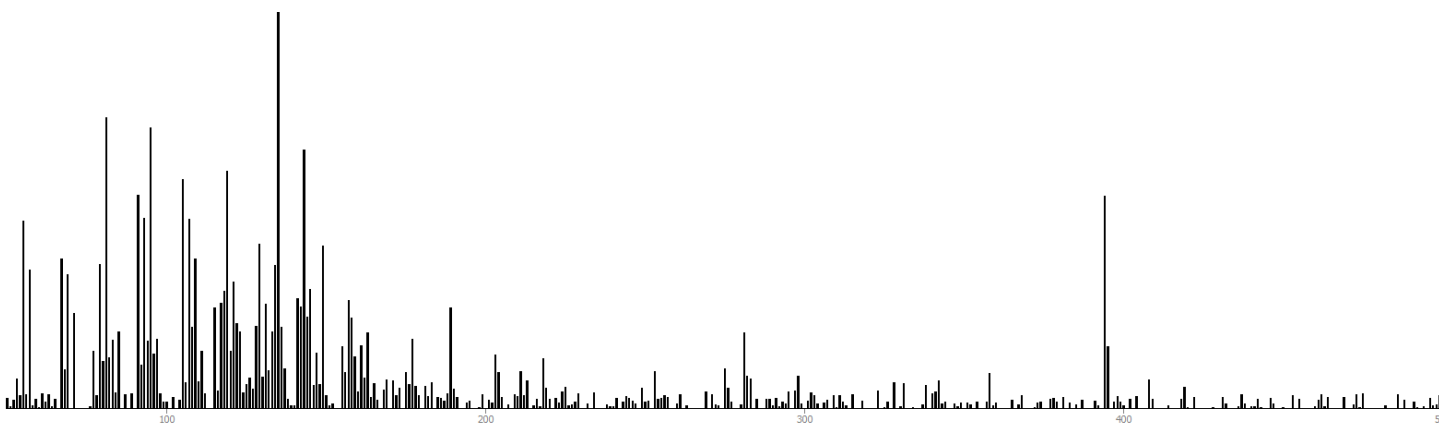


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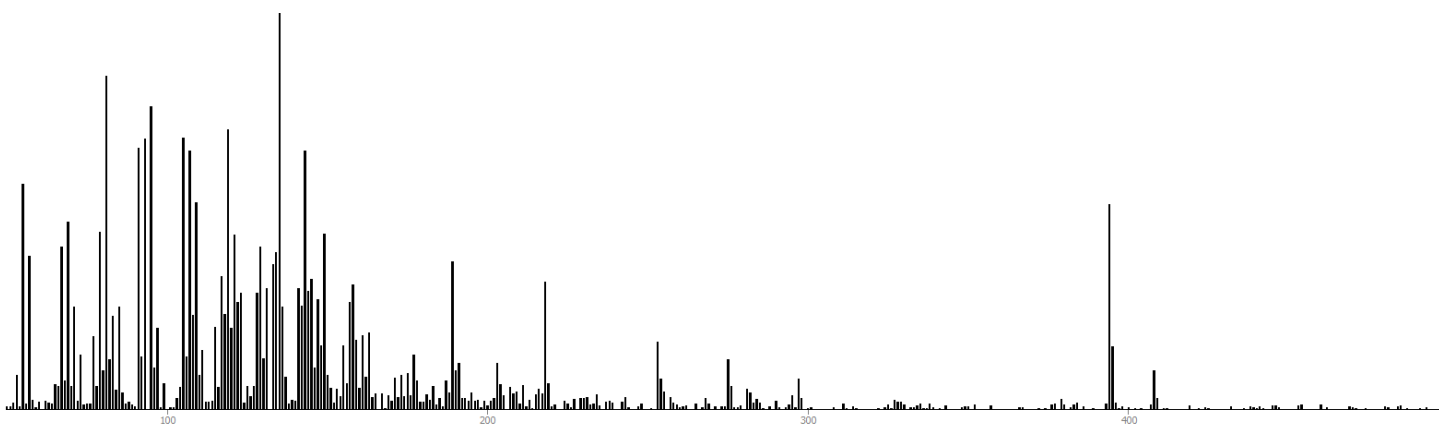


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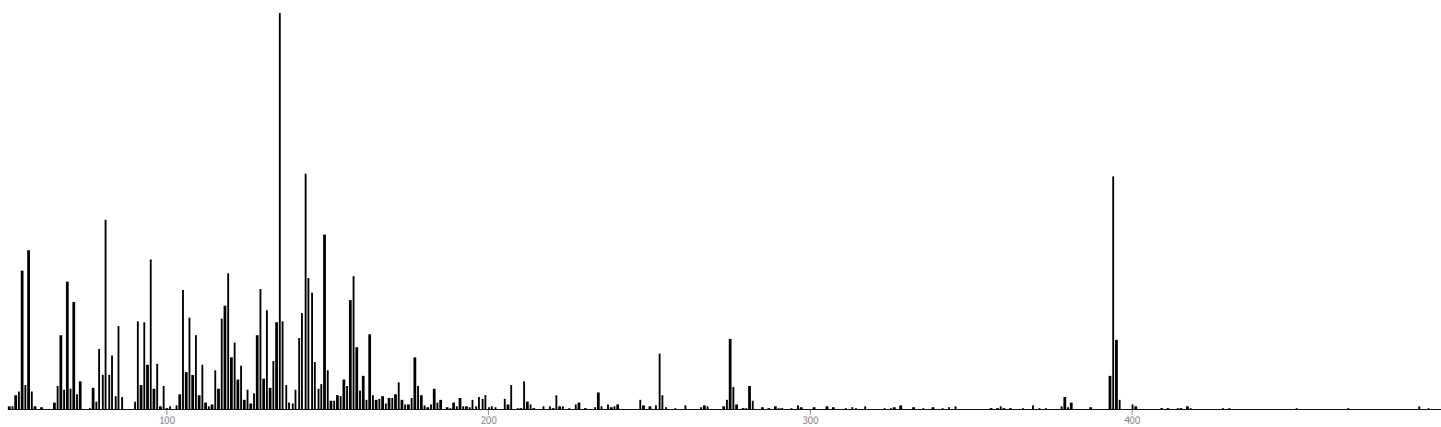


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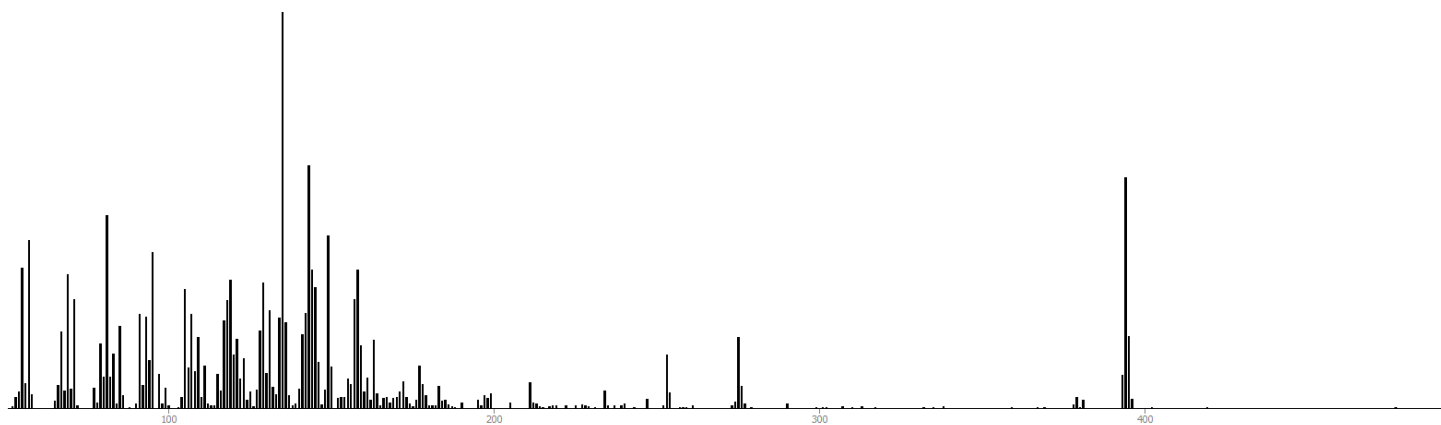


Figure S4-21-S6-1D-Shimadzu

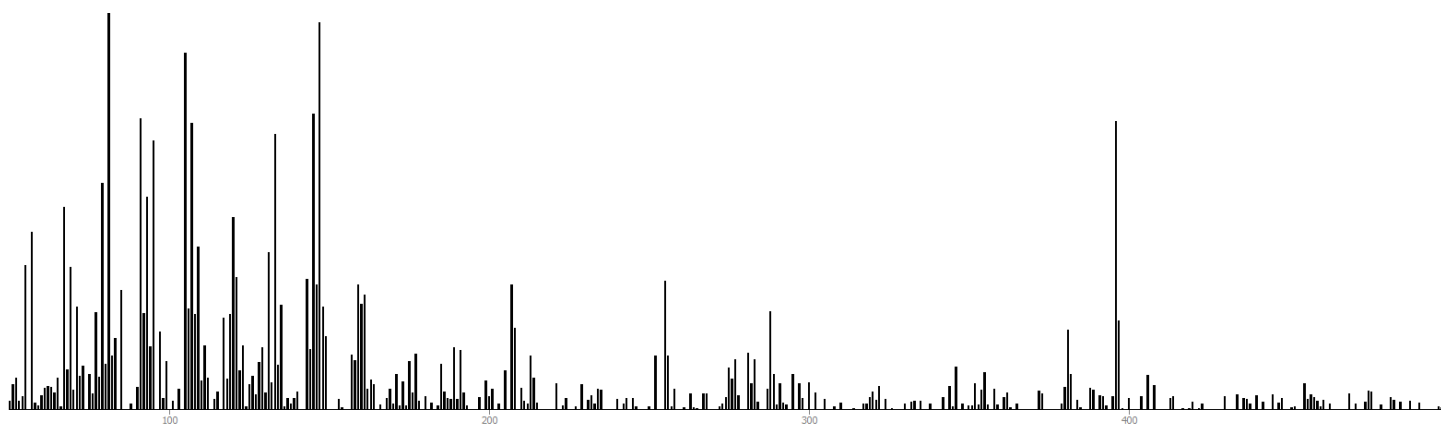


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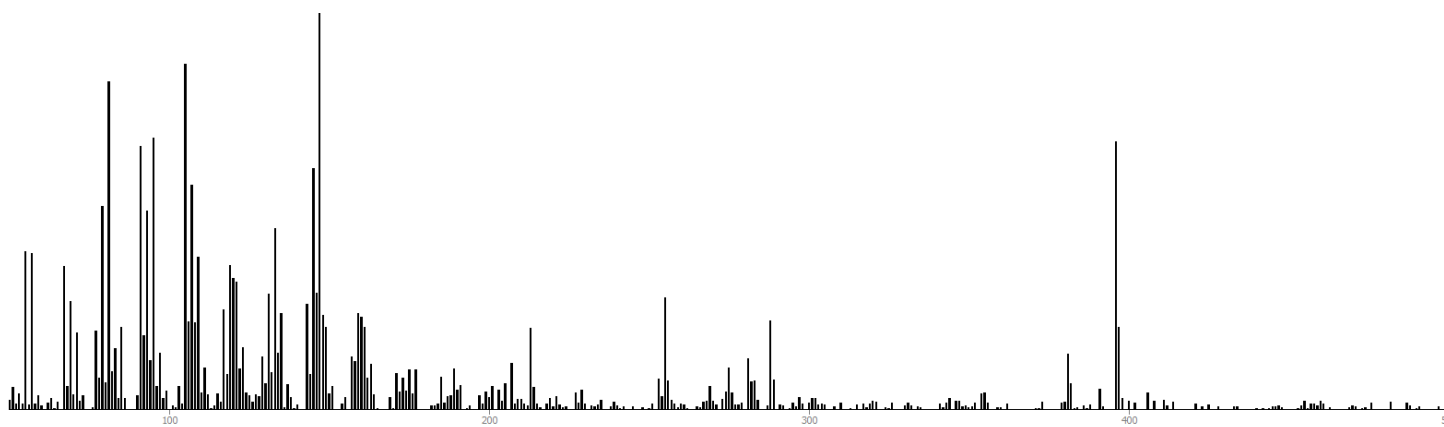


Figure S4-23-S6-2D-AMDIS

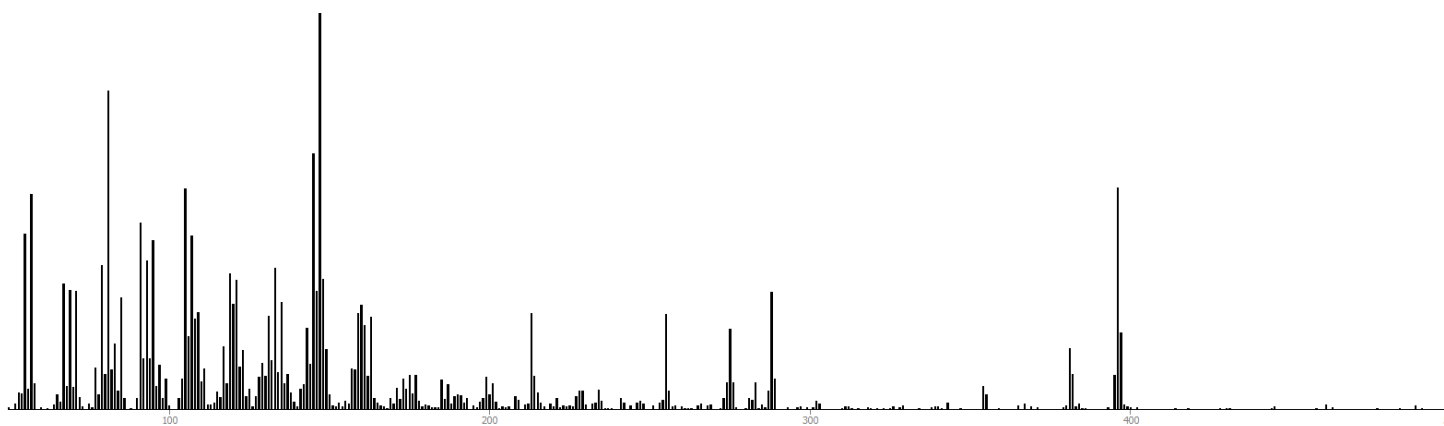


Figure S4-24-S6-2D-GC Image

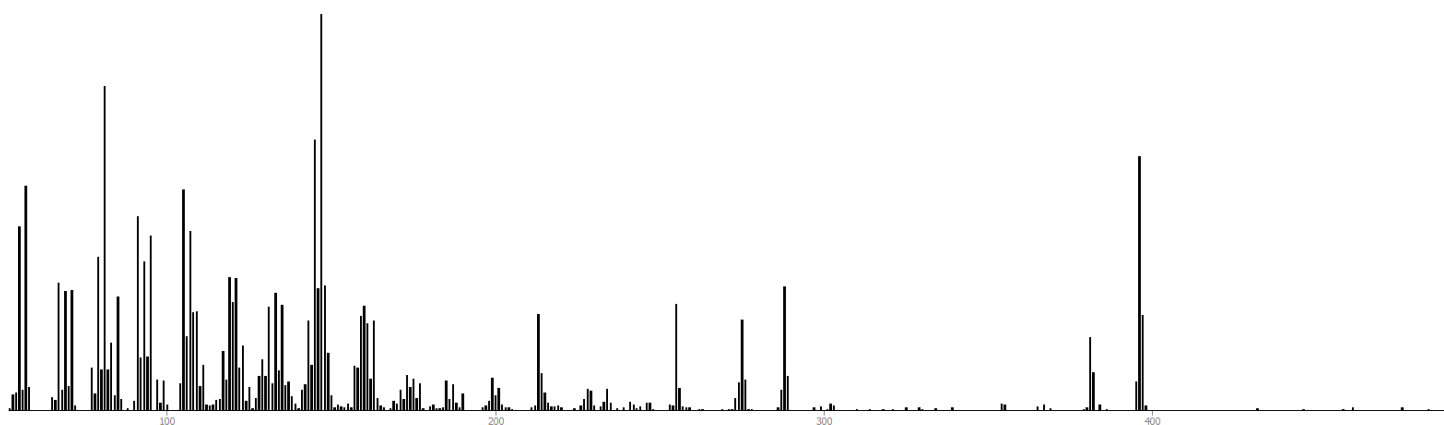


Figure S4-25-S7-1D-Shimadzu

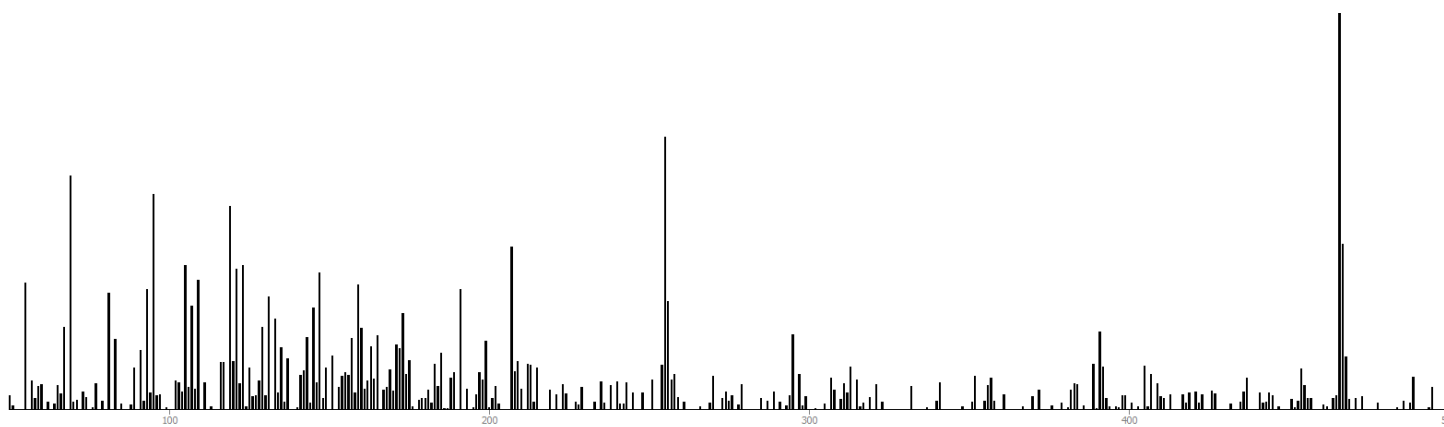


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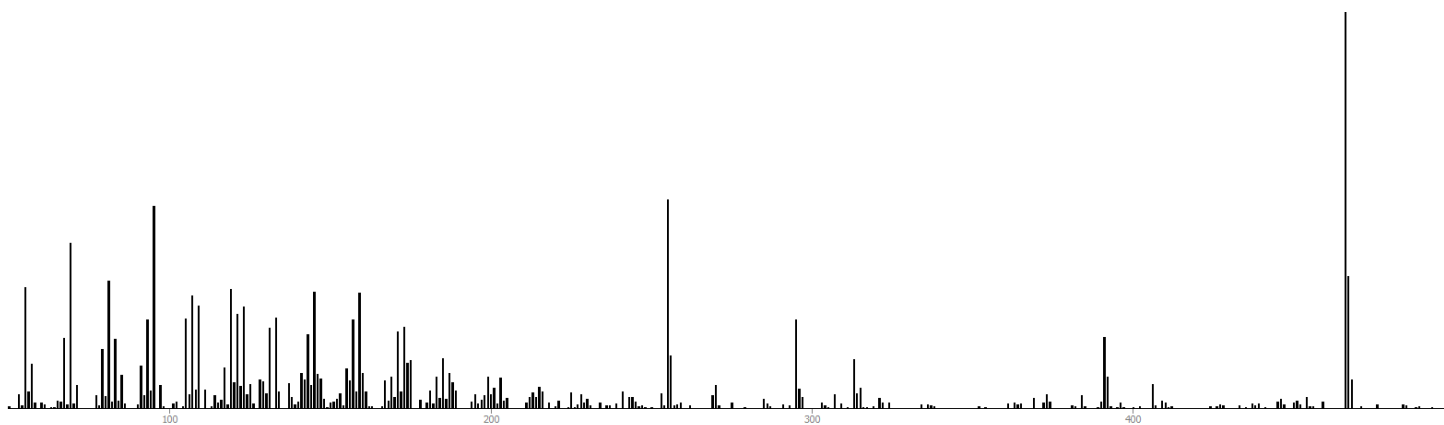


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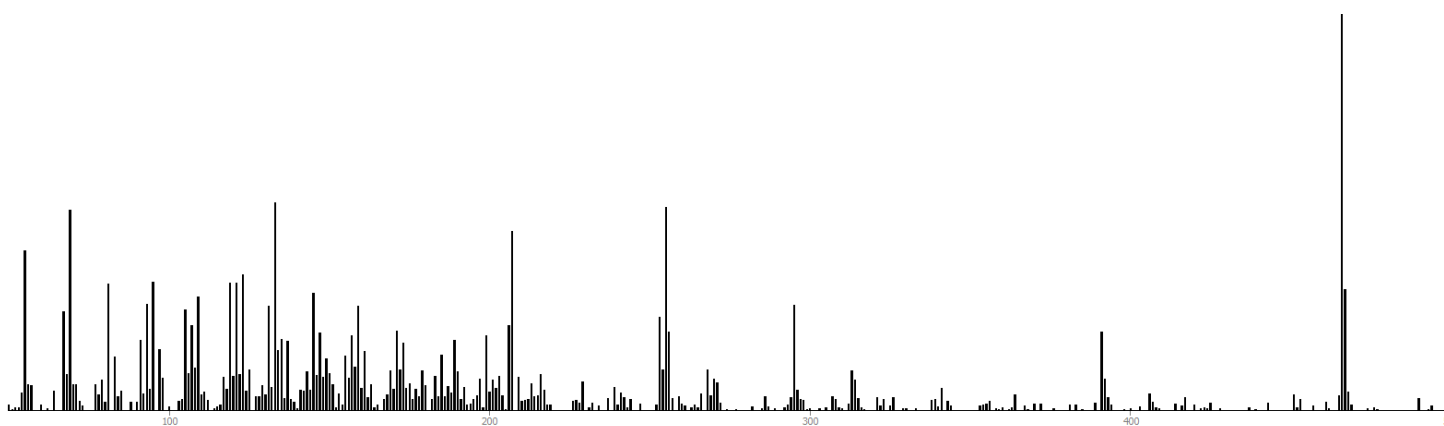


Figure S4-28-S7-2D-GC Image

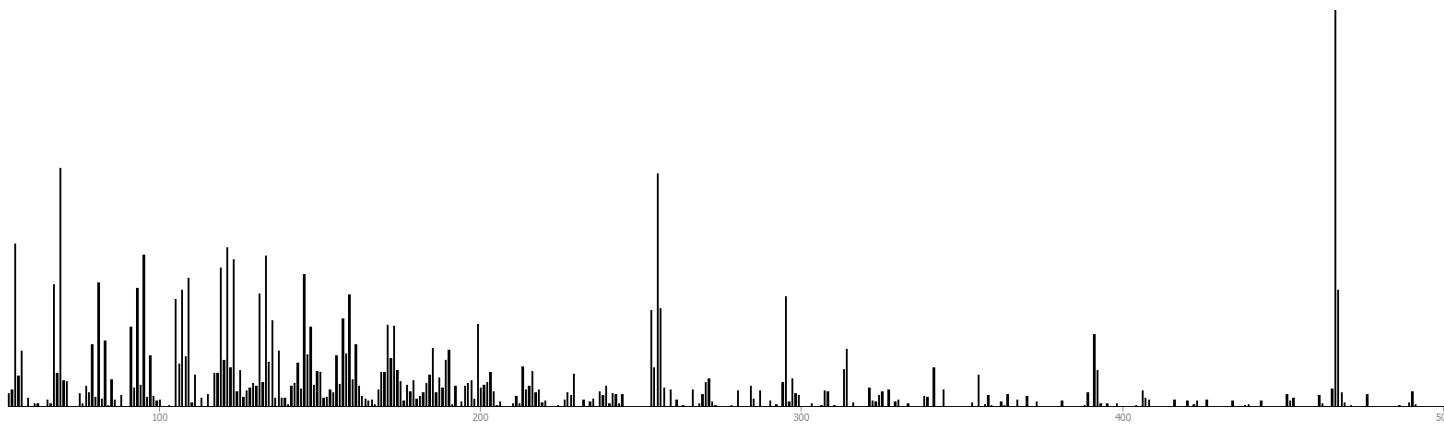


Figure S4-29-T1-1D-Shimadzu

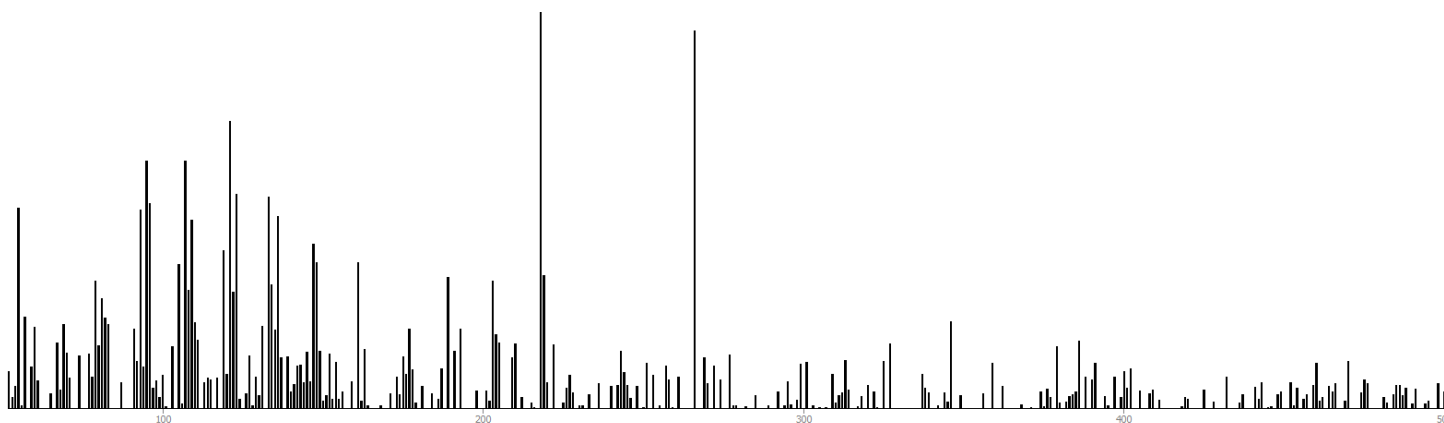


Figure S4-30-T1-1D-AMDIS

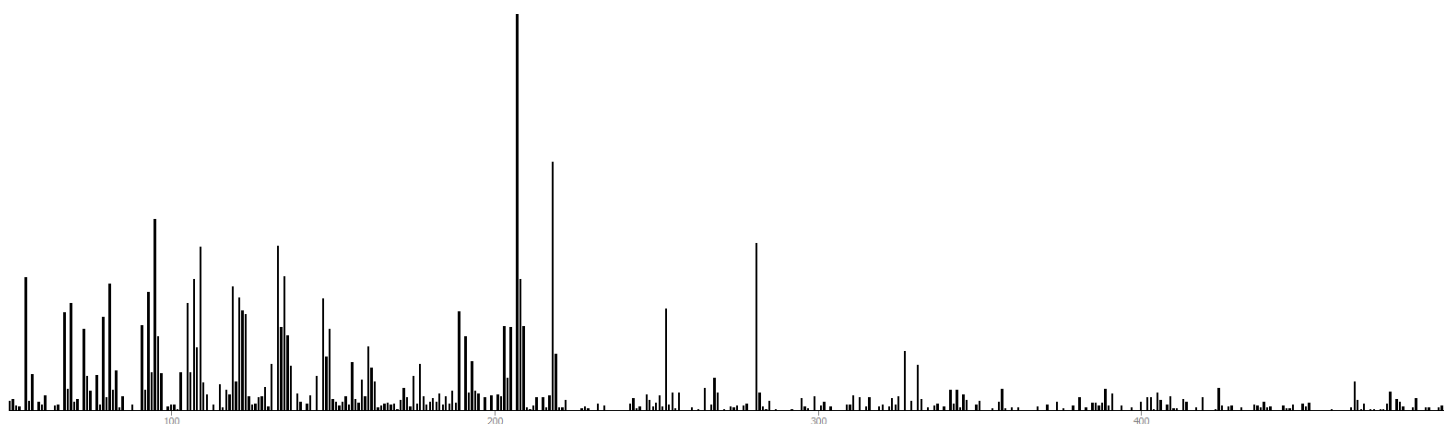


Figure S4-31-T1-2D-AMDIS

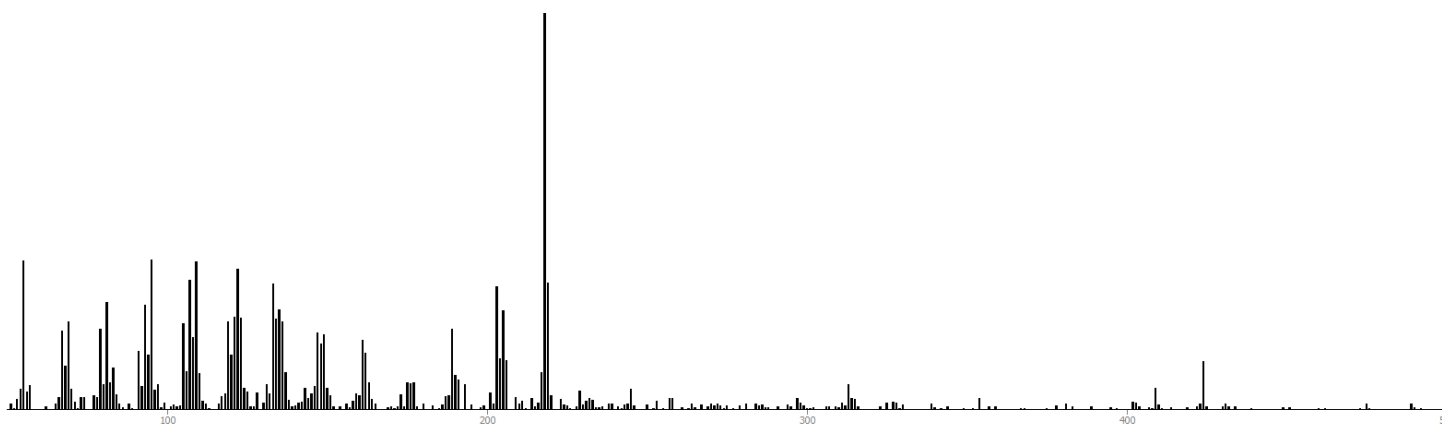


Figure S4-32-T1-2D-GC Image

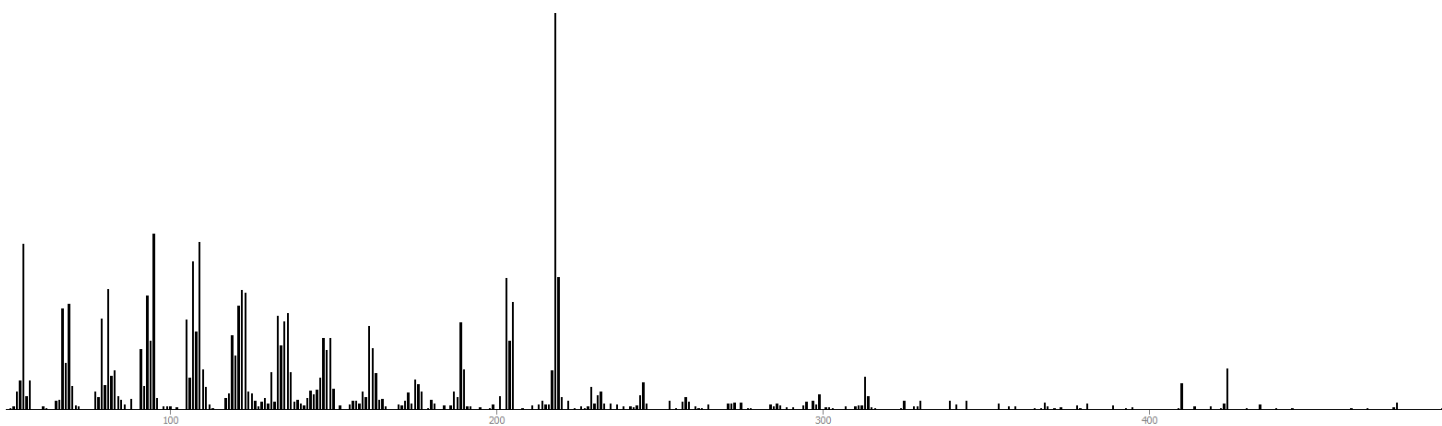


Figure S4-33-T2-1D-Shimadzu

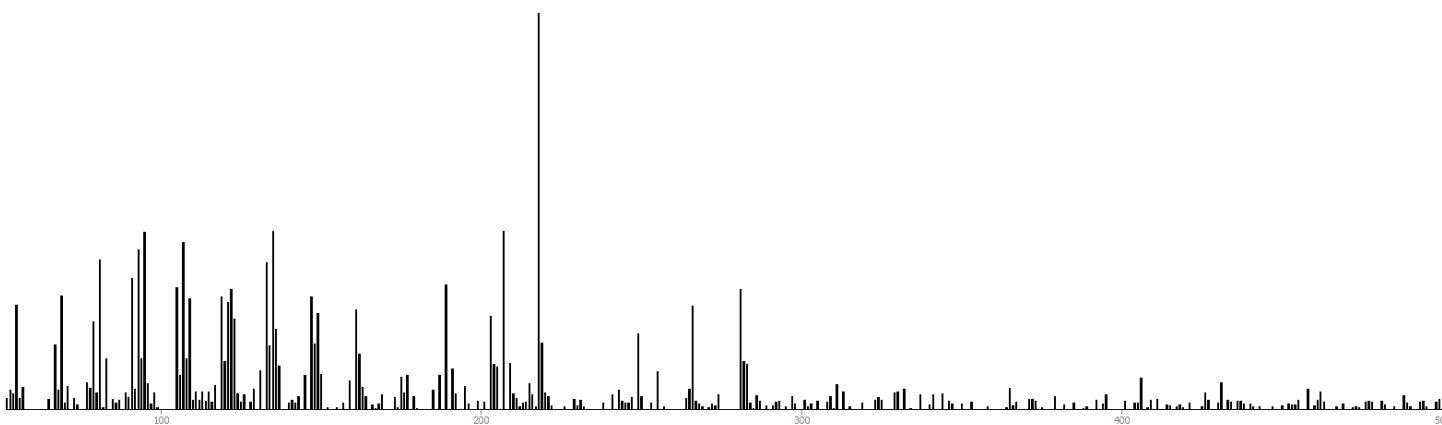


Figure S4-34-T2-1D-AMDIS

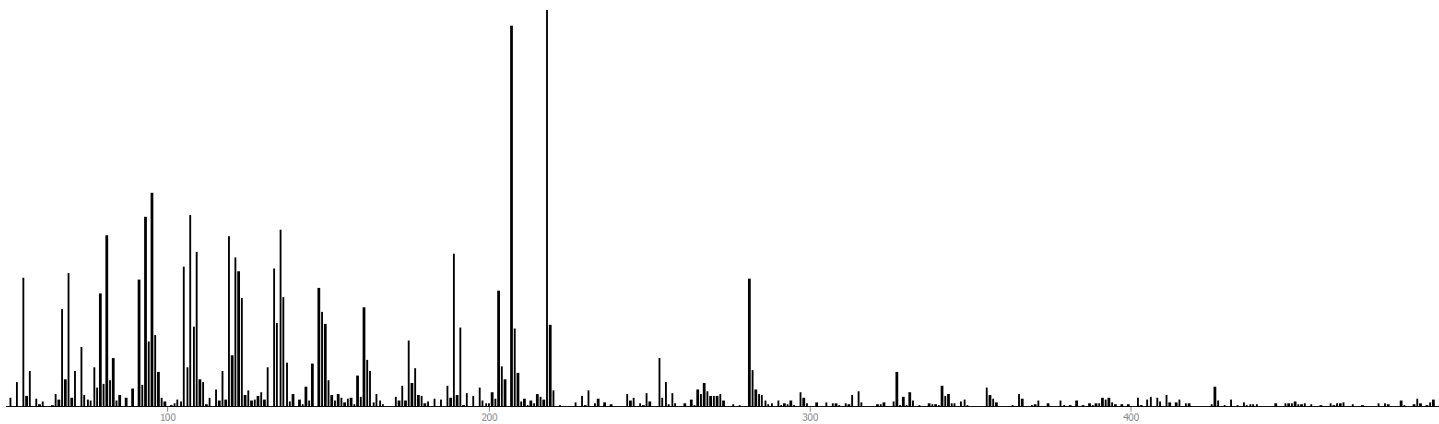


Figure S4-35-T2-2D-AMDIS

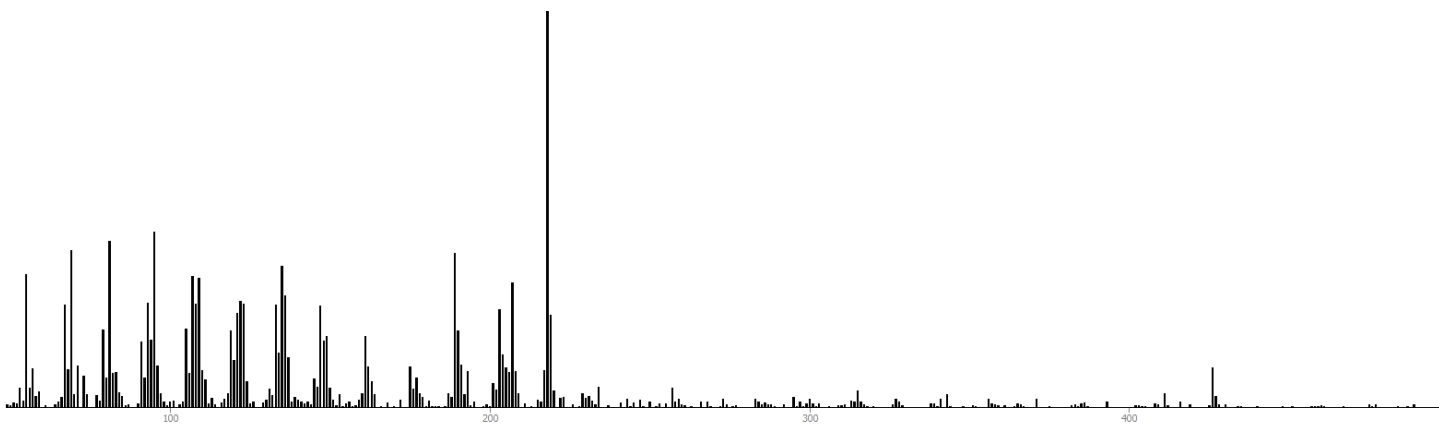


Figure S4-36-T2-2D-GC Image

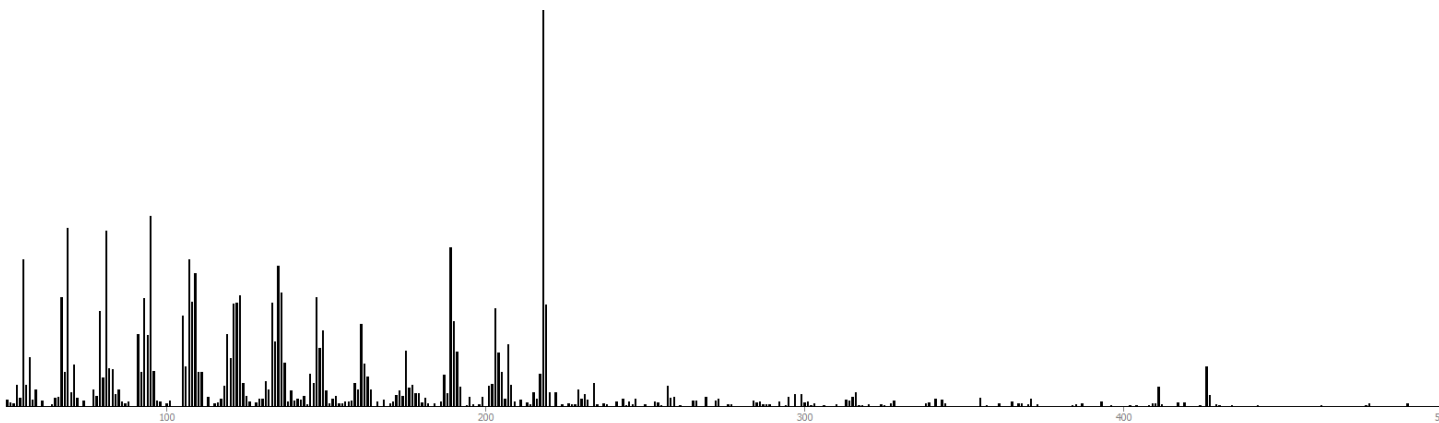


Figure S4-37-T3-1D-Shimadzu

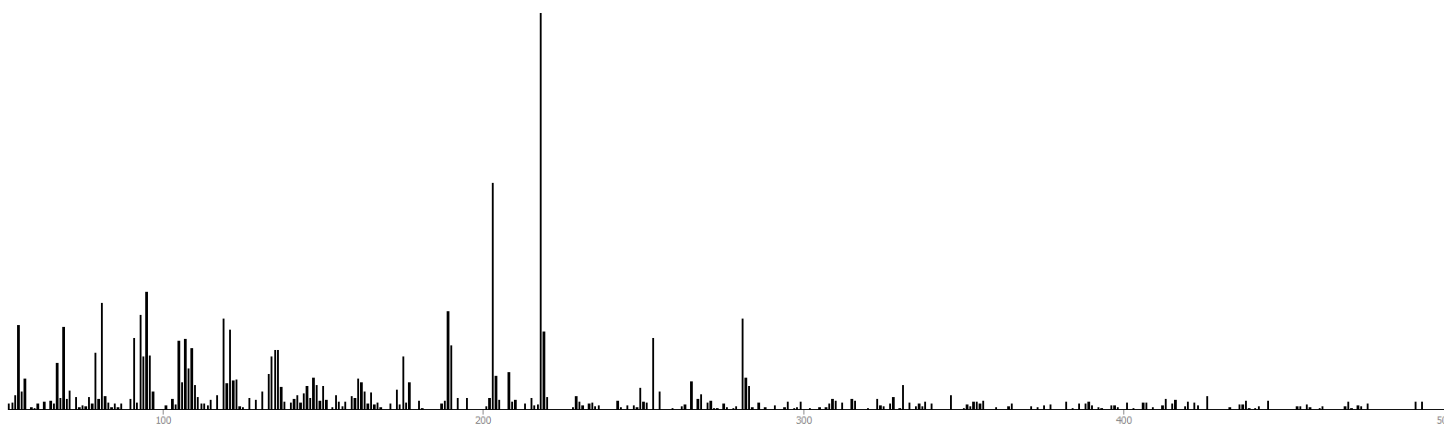


Figure S4-38-T3-1D-AMDIS

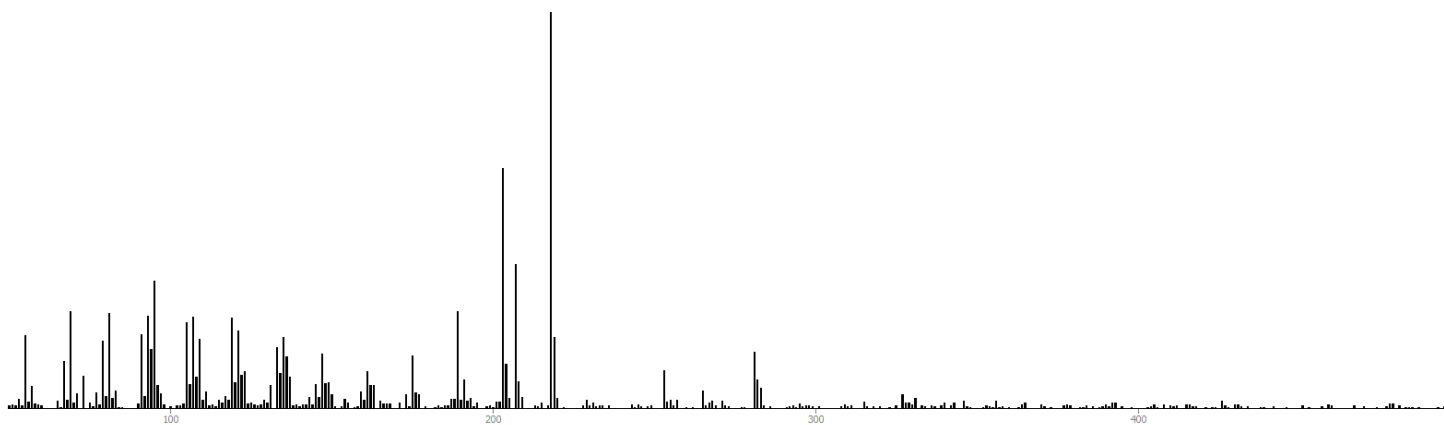


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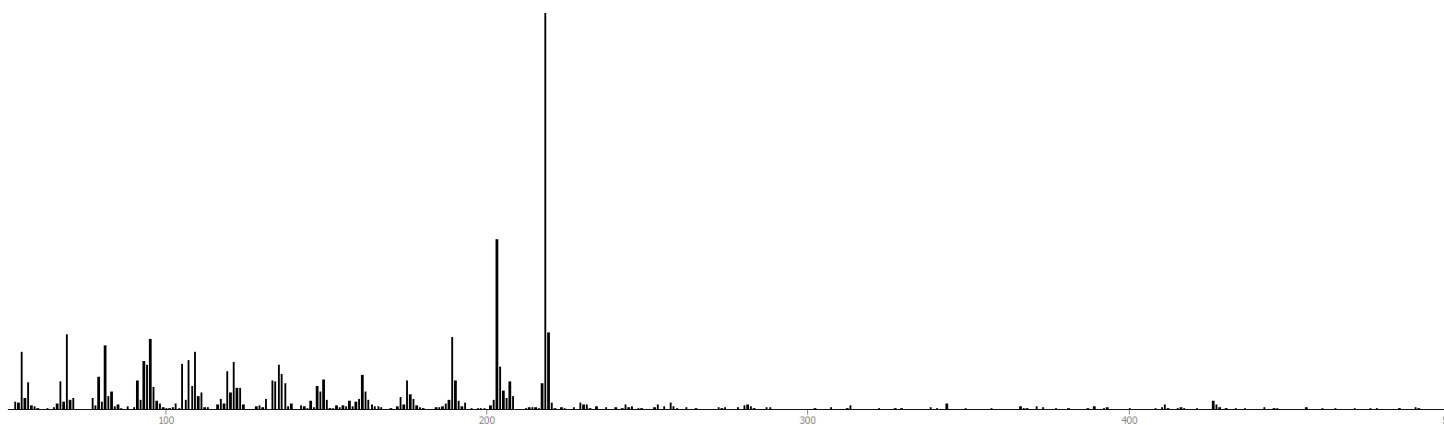


Figure S4-40-T3-2D-GC IMAGE

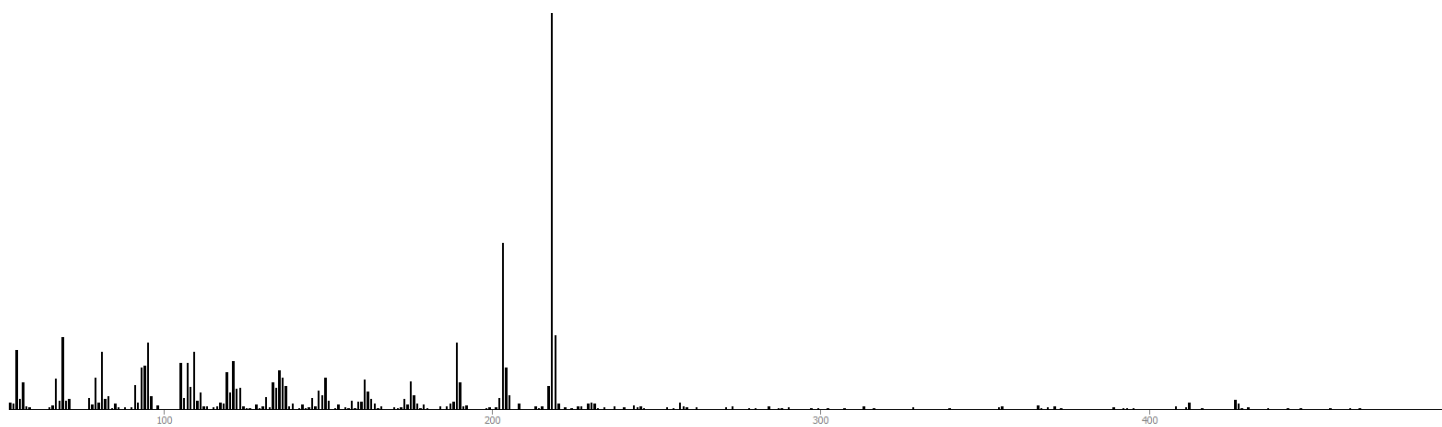


Figure S4-41-T4-1D-Shimadzu

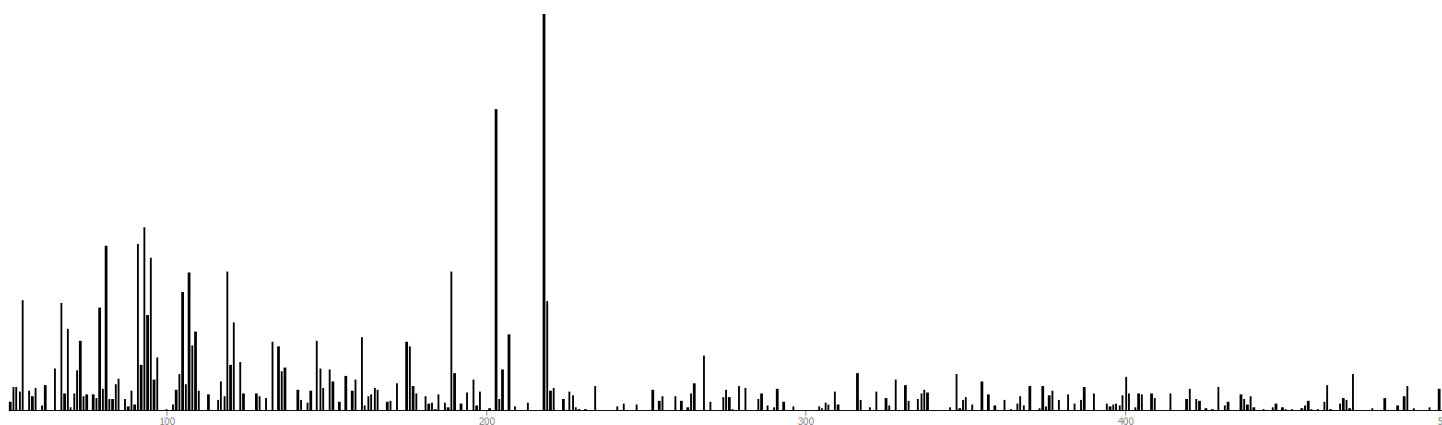


Figure S4-42-T4-1D-AMDIS

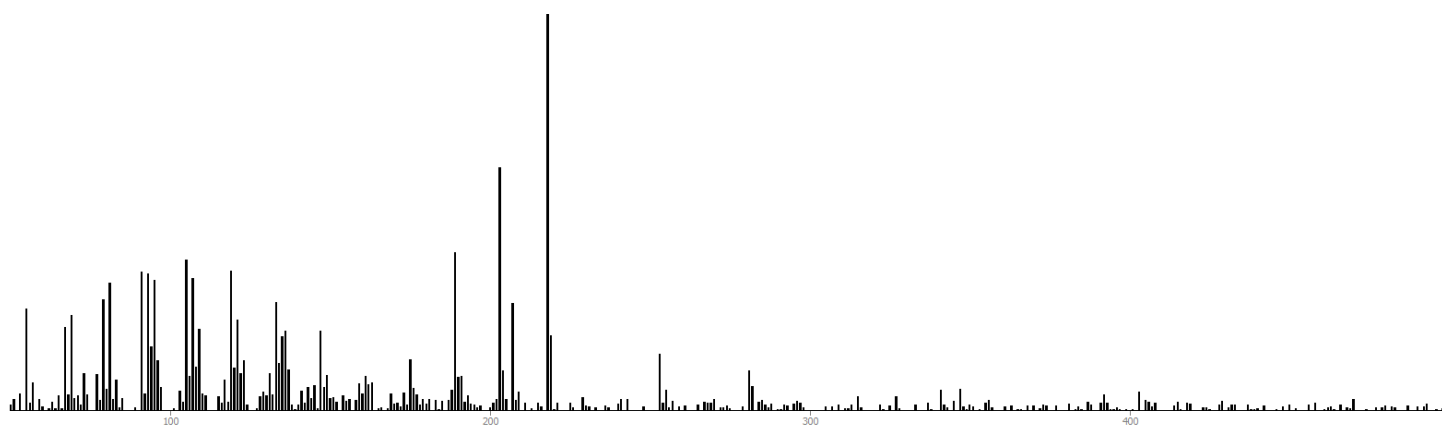


Figure S4-43-T4-2D-AMDIS

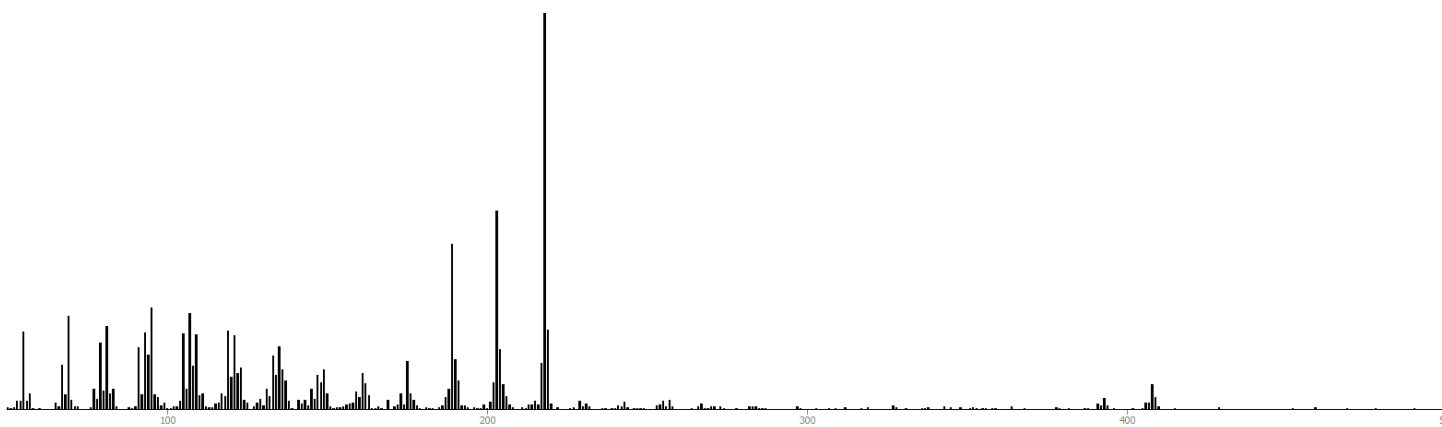


Figure S4-44-T4-2D-GC Image

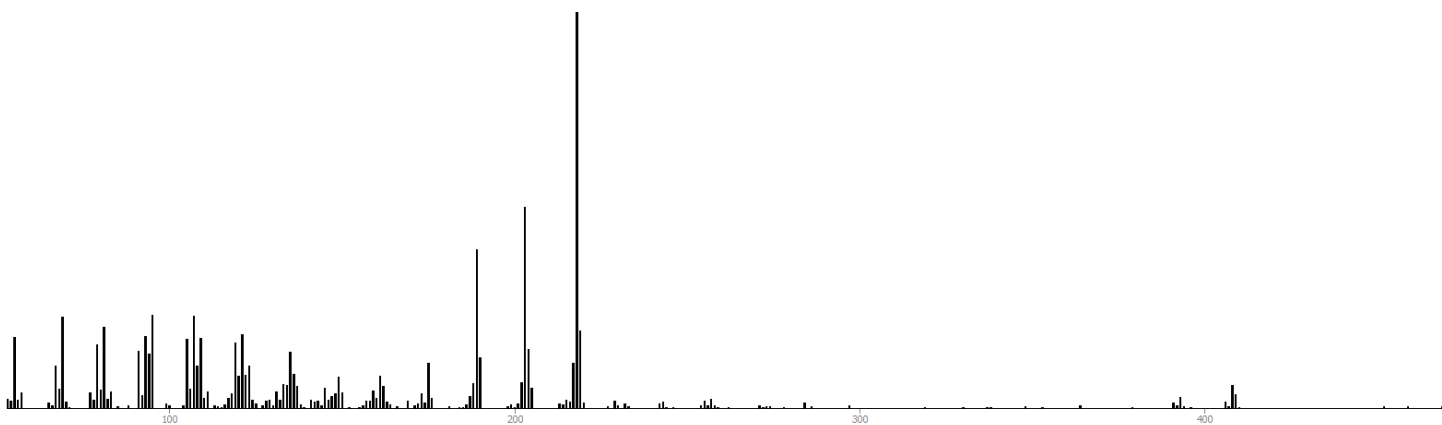


Figure S4-45-T5-1D-Shimadzu

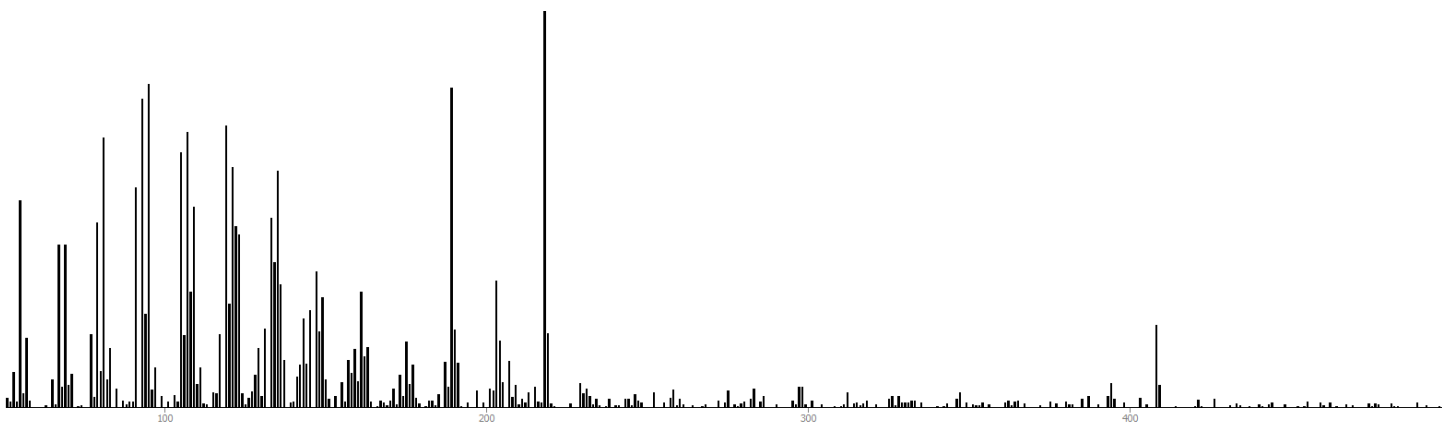


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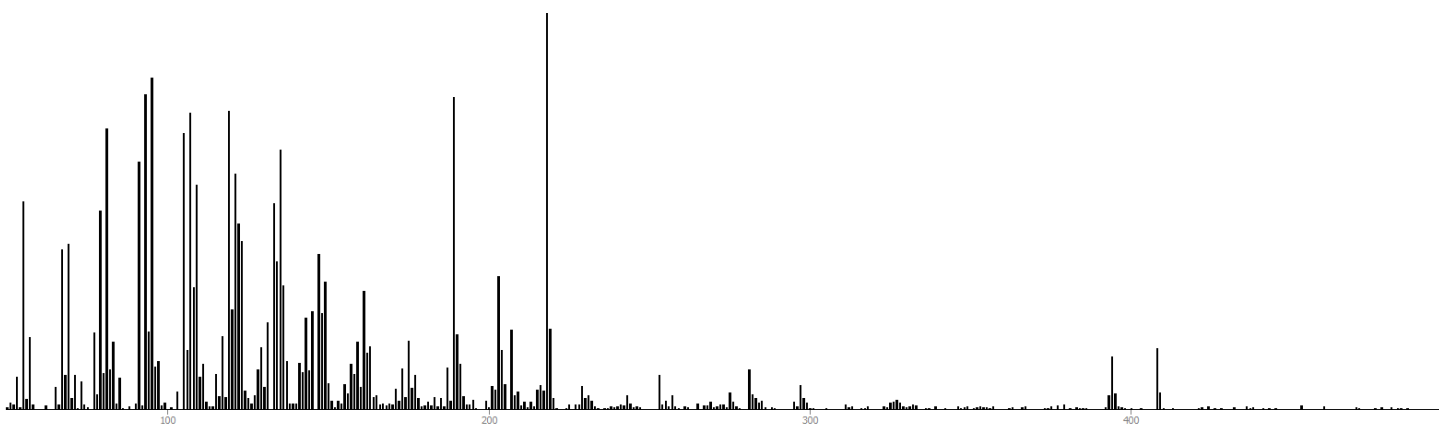


Figure S4-47-T5-2D-AMDIS

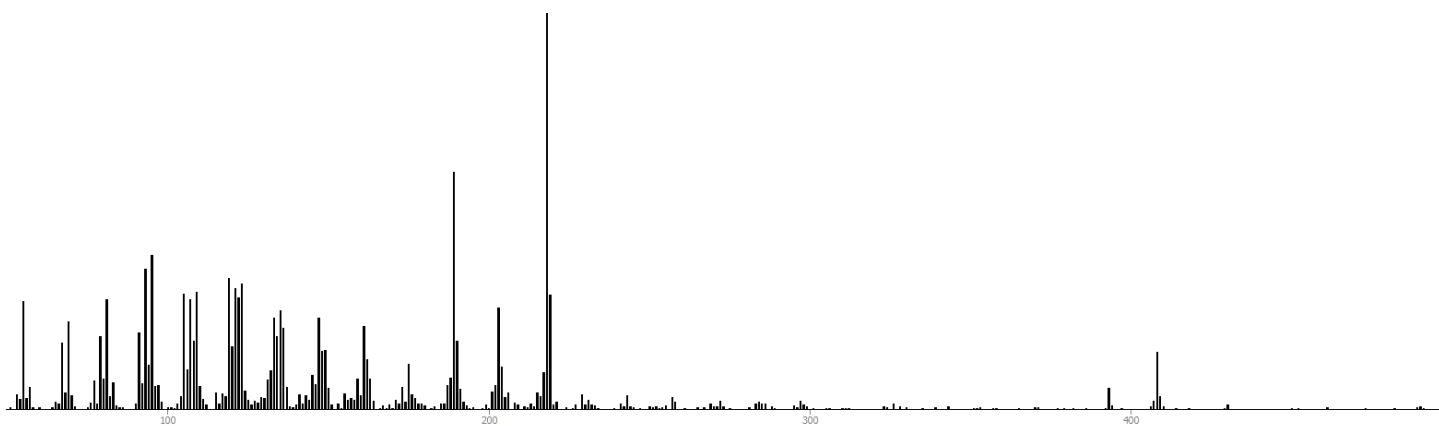


Figure S4-48-T5-2D-GC Image

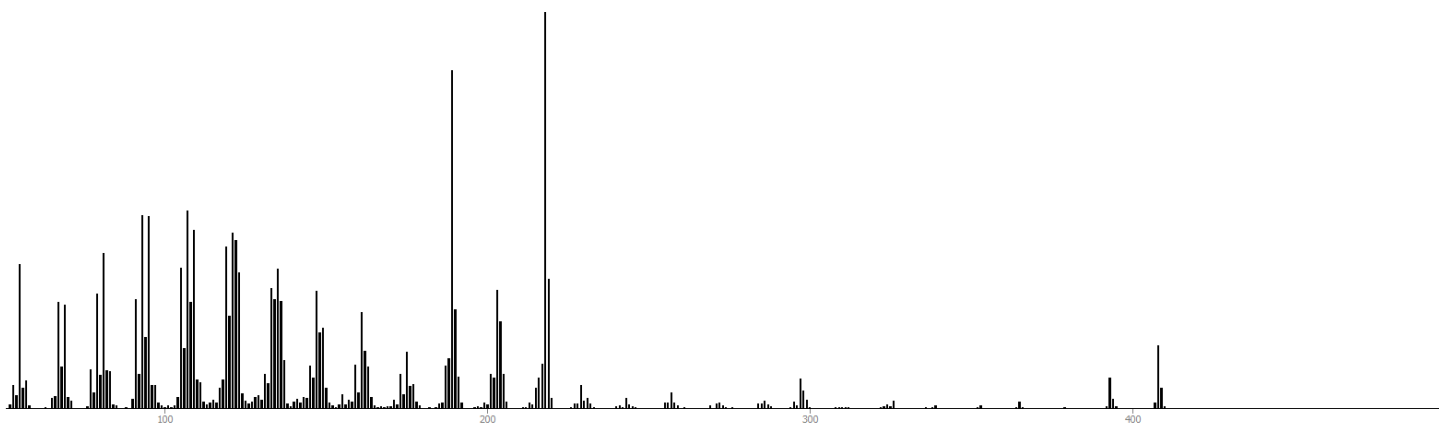


Figure S4-49-T6-1D-Shimadzu

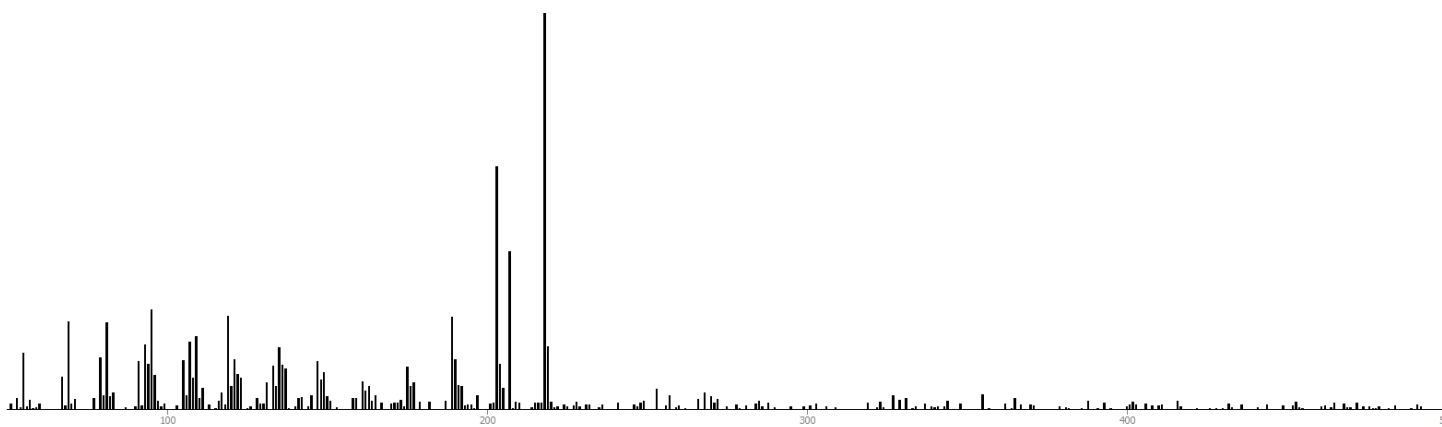


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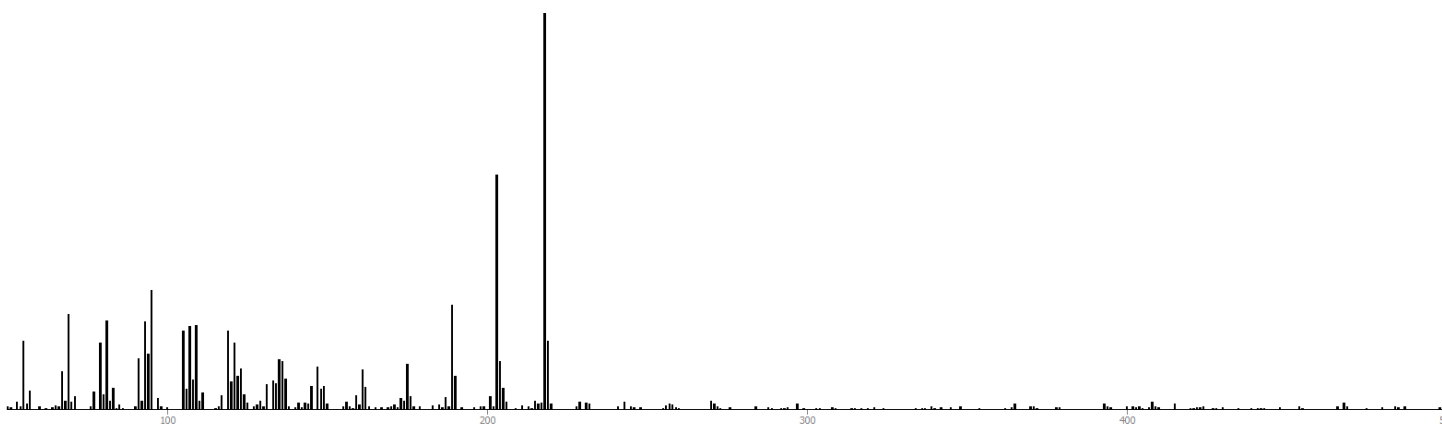


Figure S4-51-T6-2D-AMDIS

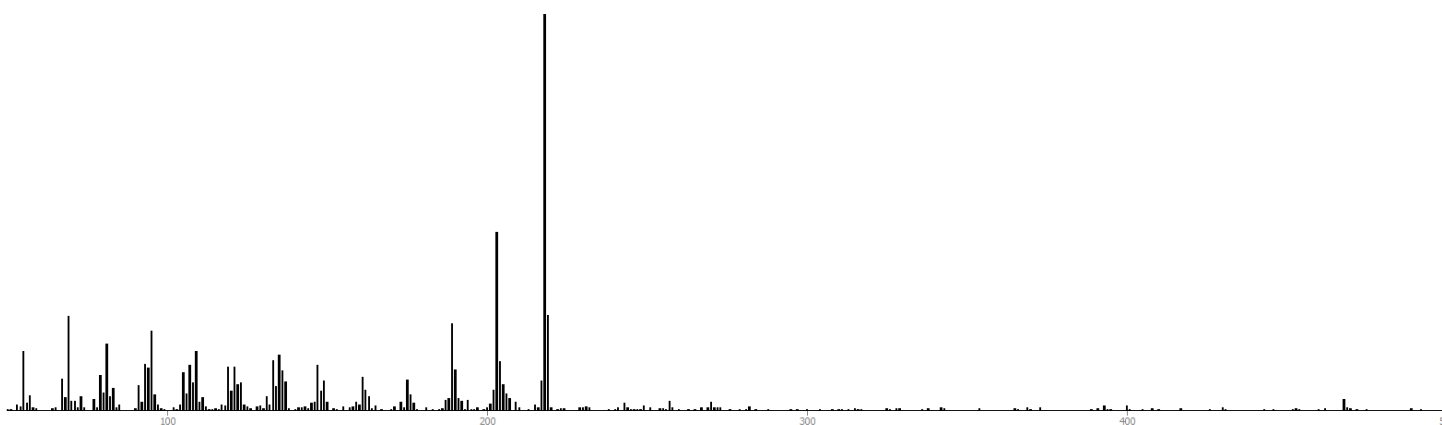


Figure S4-52-T6-2D-GC Image

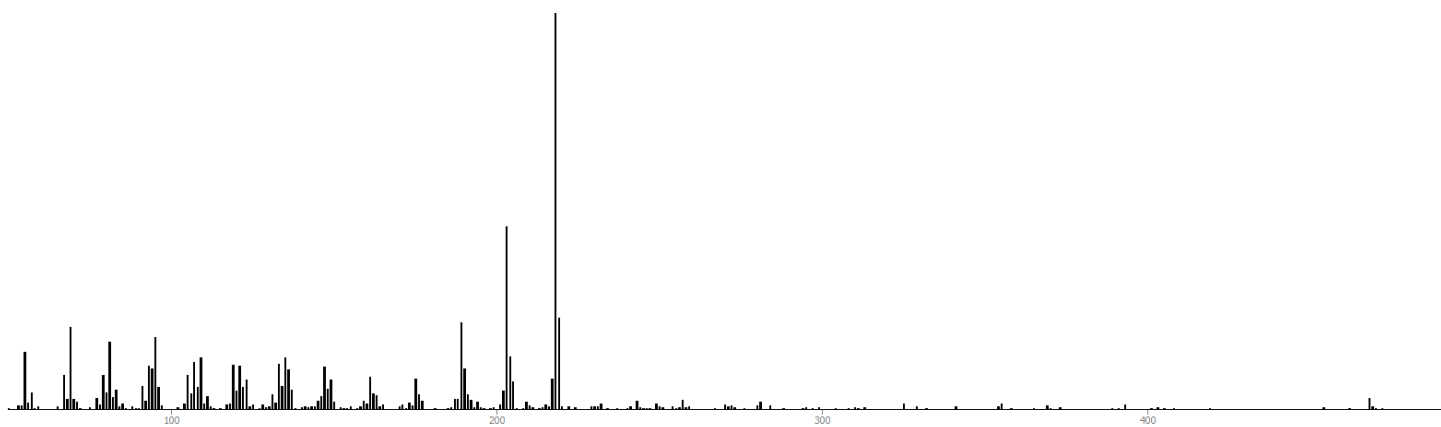


Figure S4-53-T7-1D-Shimadzu

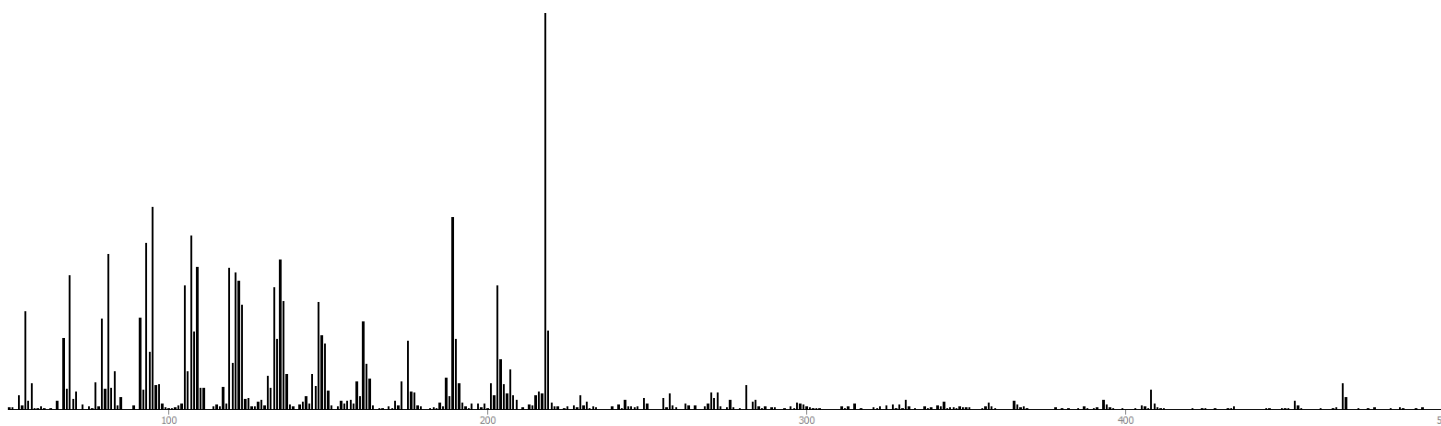


Figure S4-54-T7-1D-AMDIS

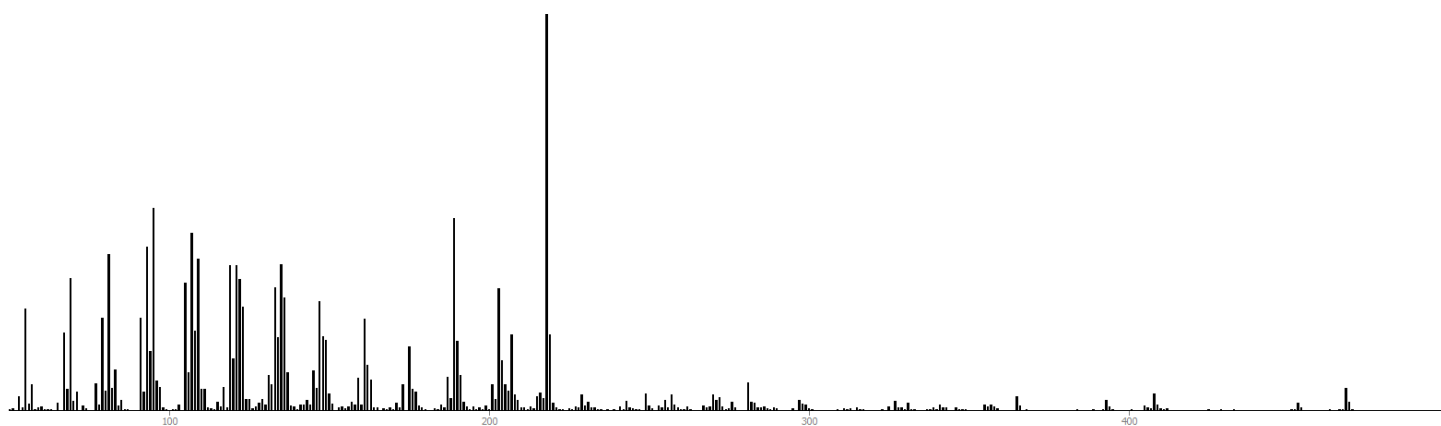


Figure S4-55-T7-2D-AMDIS

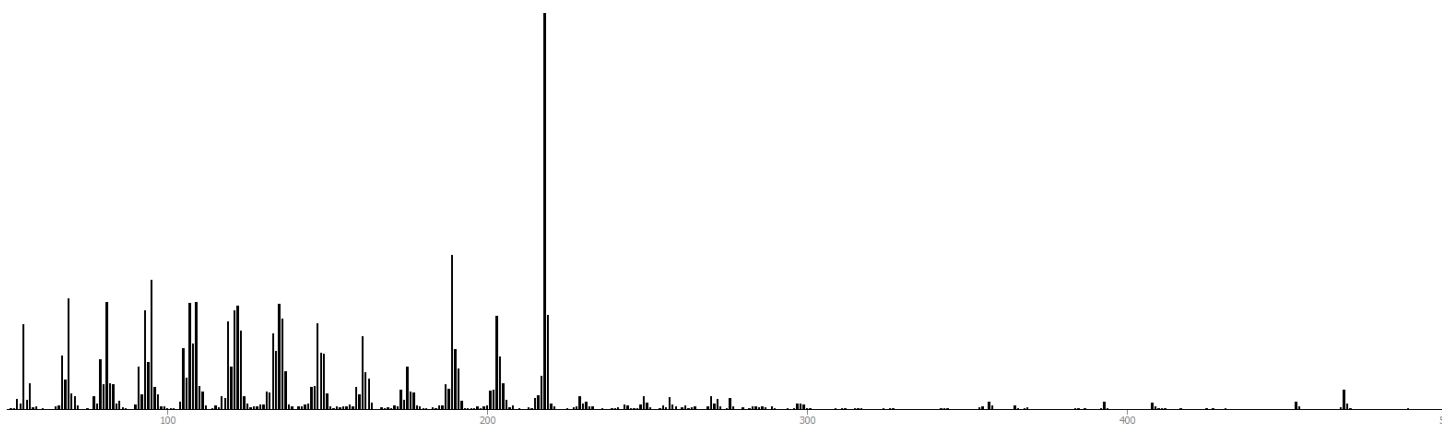


Figure S4-56-T7-2D-GC Image

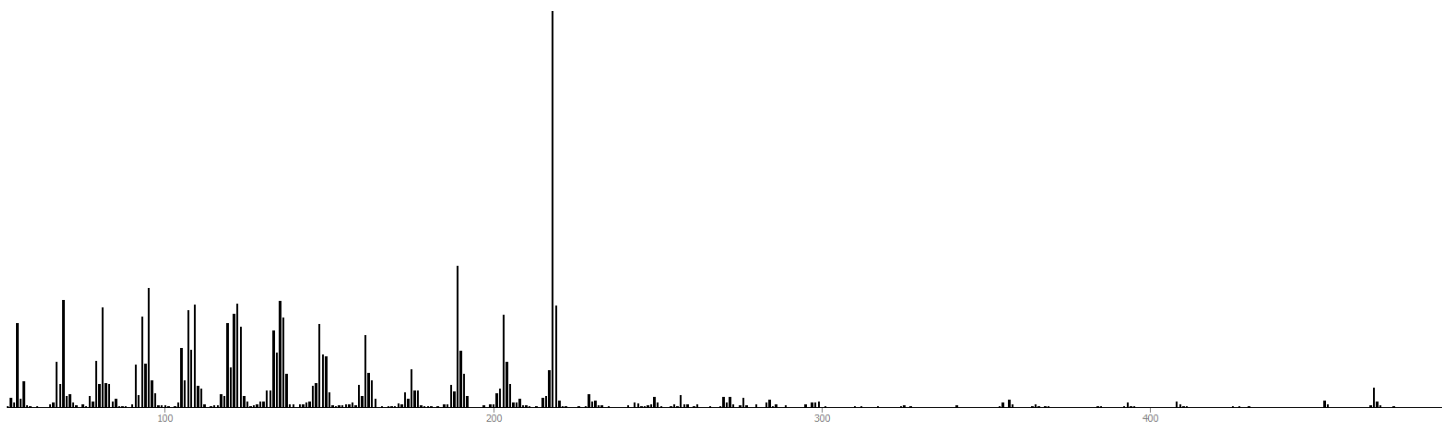


Figure S5. The standard derivation of mass spectra (base-peak normalized to 100) between M1-M2, M2-M3 and M3-M4 for compound S5 (a), T5 (b) and T7 (c). (M1, M2, M3 and M4 correspond to Figure S3)

