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Average Mass Scan of the Total Ion Chromatogram versus Percentage Chemical Composition in Multivariate Statistical Comparison of Complex Volatile Mixtures

Niko S. Radulović,*[a] Polina D. Blagojević[a] and Danielle Skropeta[b]

[a]Department of Chemistry, Faculty of Science and Mathematics, University of Niš, Višegradska 33, 18000 Niš, Serbia

[b]School of Chemistry, University of Wollongong, Wollongong NSW 2522, Australia

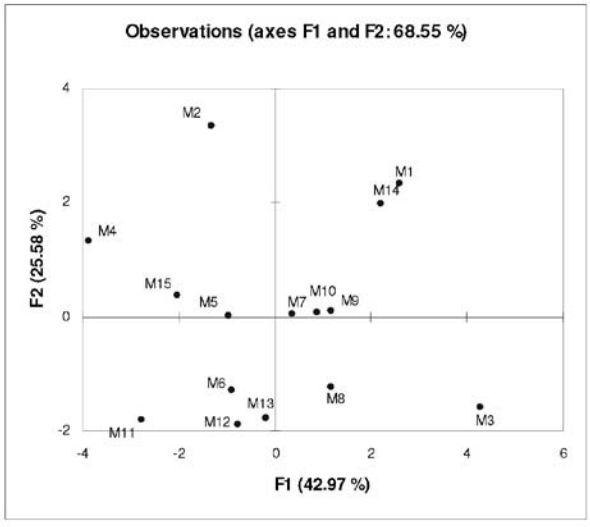

Figure S1. Principal component analysis (the original variables) ordination of 15 model complex mixtures (observations). Axes (F1 and F2 factors-the first and second principal component) refer to the ordination scores obtained from the samples. Axis F1 accounts for ca. 42% and axis F2 accounts for a further 26% of the total variance.

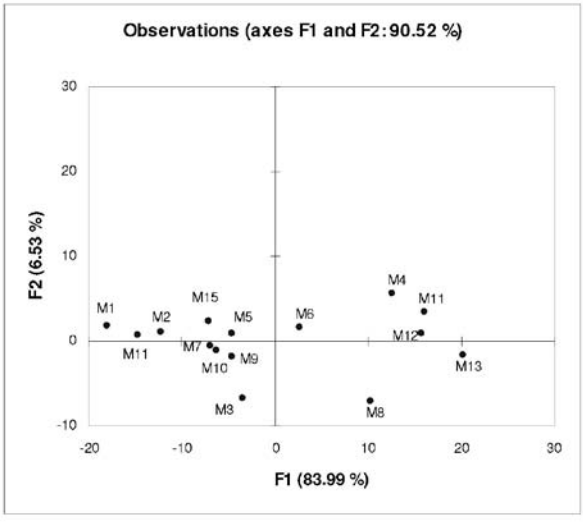

Figure S2. Principal component analysis (AMS relative abundances of *m*/*z* values as variables) ordination of 15 model complex mixtures (observations). Axes (F1 and F2 factors-the first and second principal component) refer to the ordination scores obtained from the samples. Axis F1 accounts for ca. 84% and axis F2 accounts for a further 7% of the total variance.

*e-mail: vangelis0703@yahoo.com

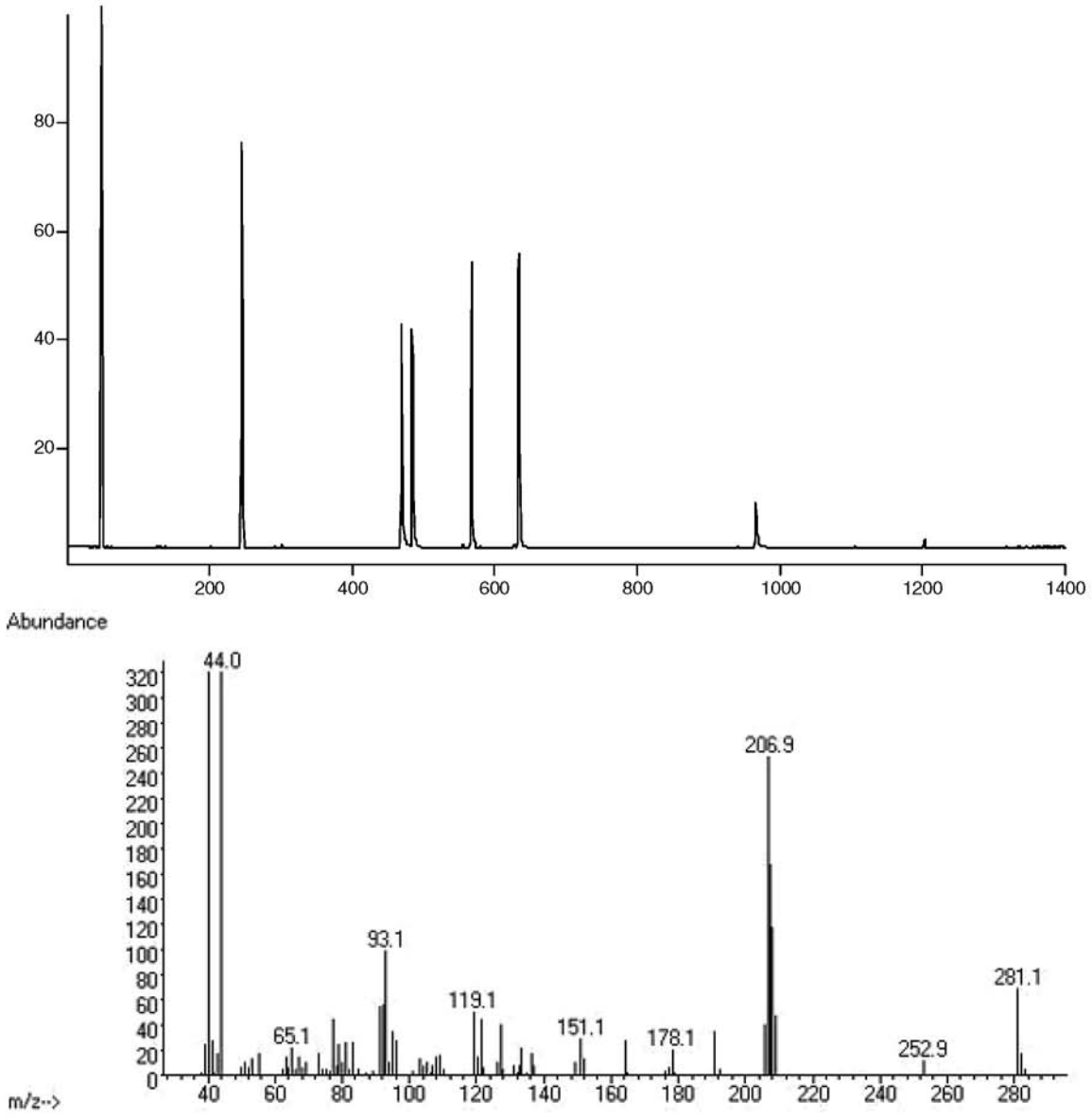

Figure S3. GC-MS (TIC) chromatogram (abscissa: scan number, ordinate: relative response of MS detector) and AMS profile (abscissa: *m*/*z* value, ordinate: response of MS detector) of model complex mixture M1.

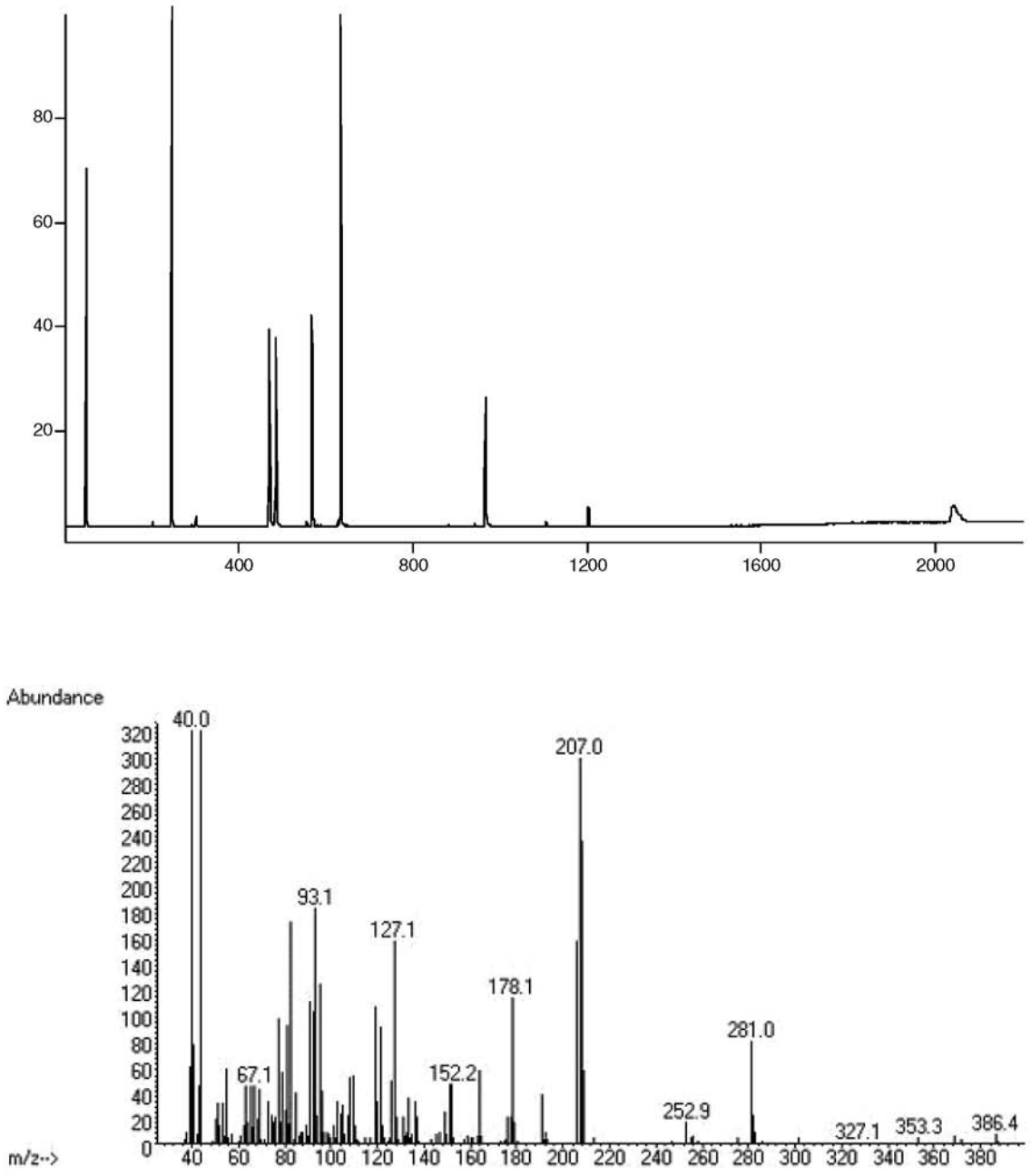

Figure S4. GC-MS (TIC) chromatogram (abscissa: scan number, ordinate: relative response of MS detector) and AMS profile (abscissa: *m*/*z* value, ordinate: response of MS detector) of model complex mixture M2.

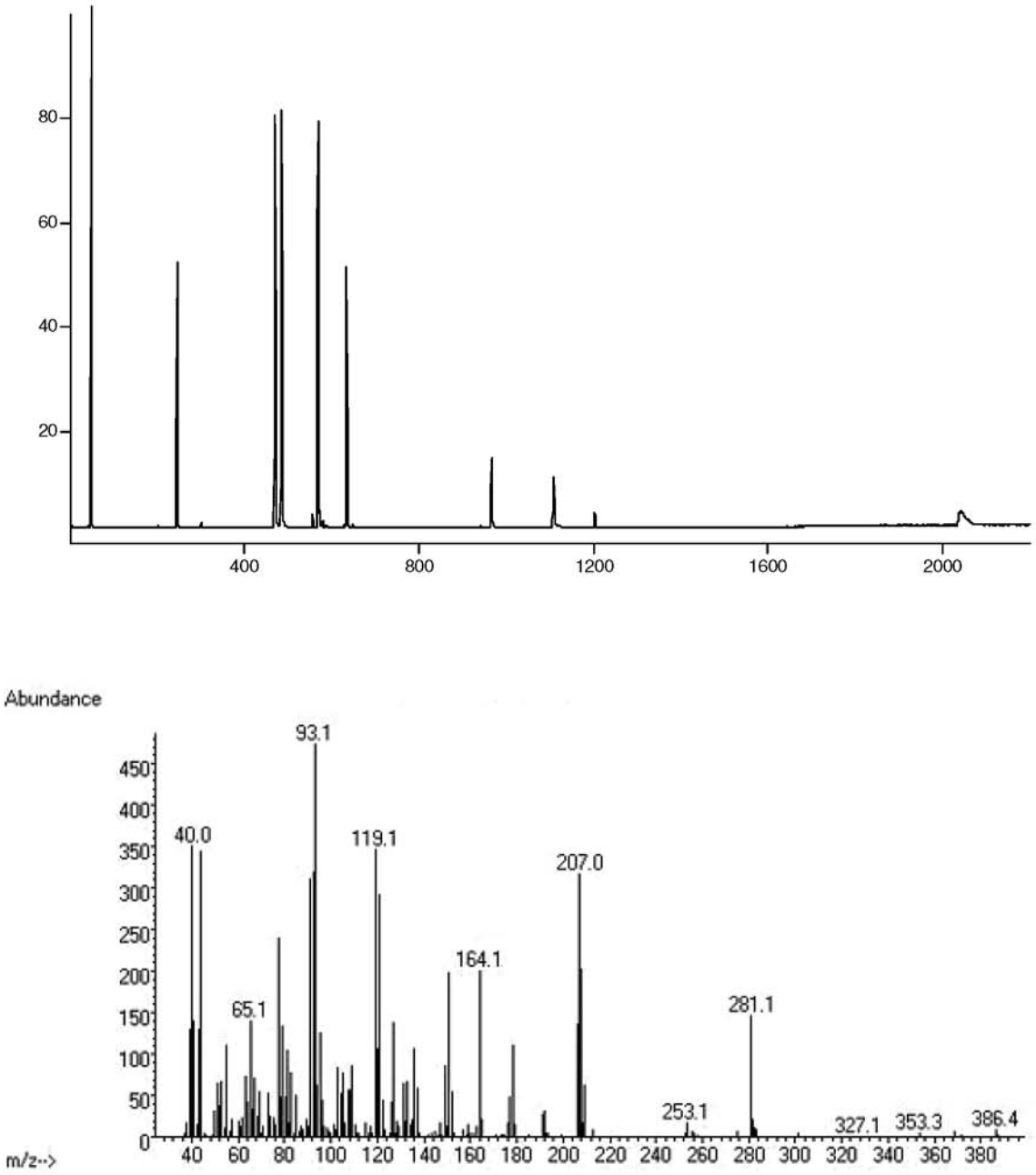

Figure S5. GC-MS (TIC) chromatogram (abscissa: scan number, ordinate: relative response of MS detector) and AMS profile (abscissa: *m*/*z* value, ordinate: response of MS detector) of model complex mixture M3.

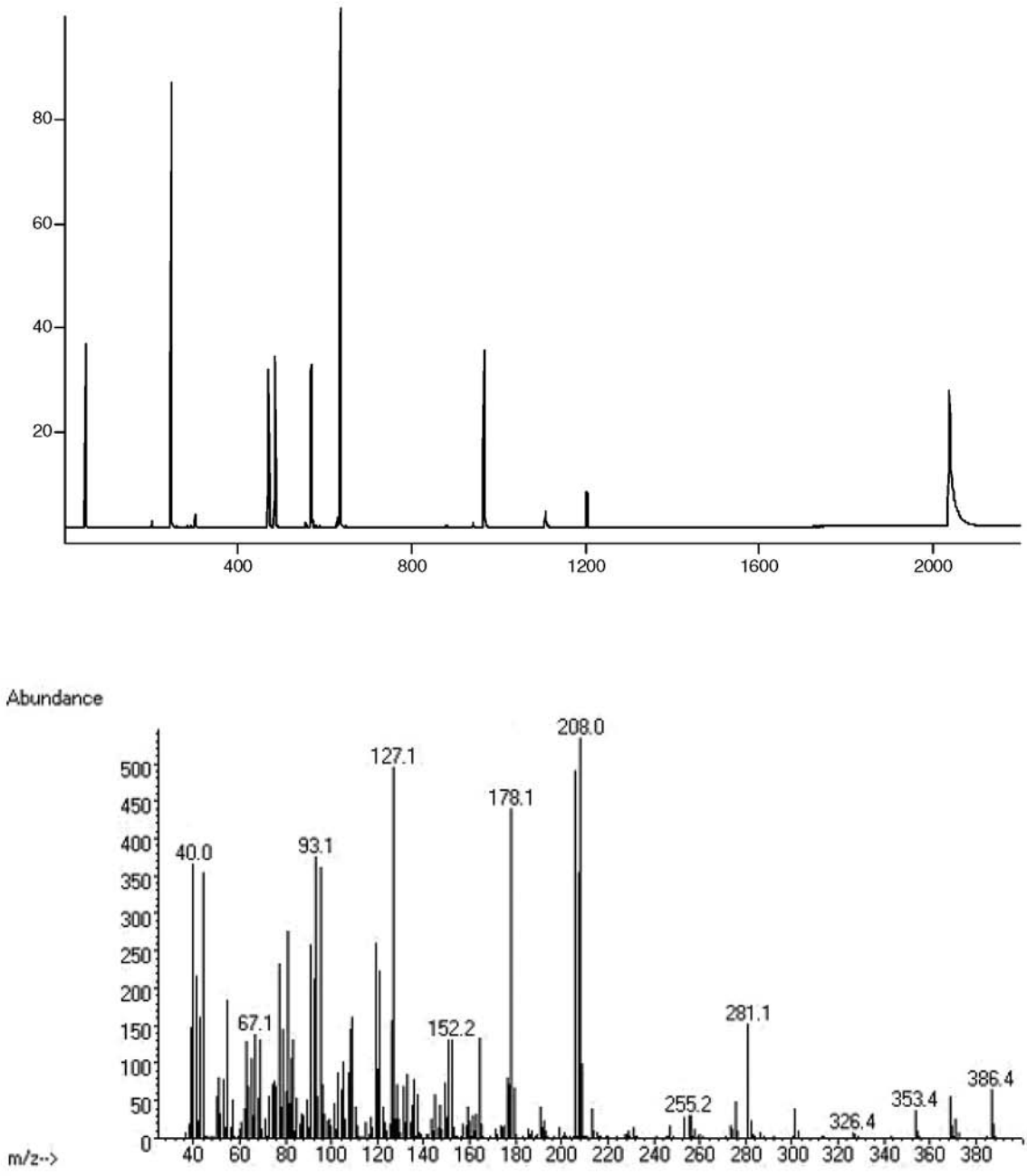

Figure S6. GC-MS (TIC) chromatogram (abscissa: scan number, ordinate: relative response of MS detector) and AMS profile (abscissa: *m*/*z* value, ordinate: response of MS detector) of model complex mixture M4.

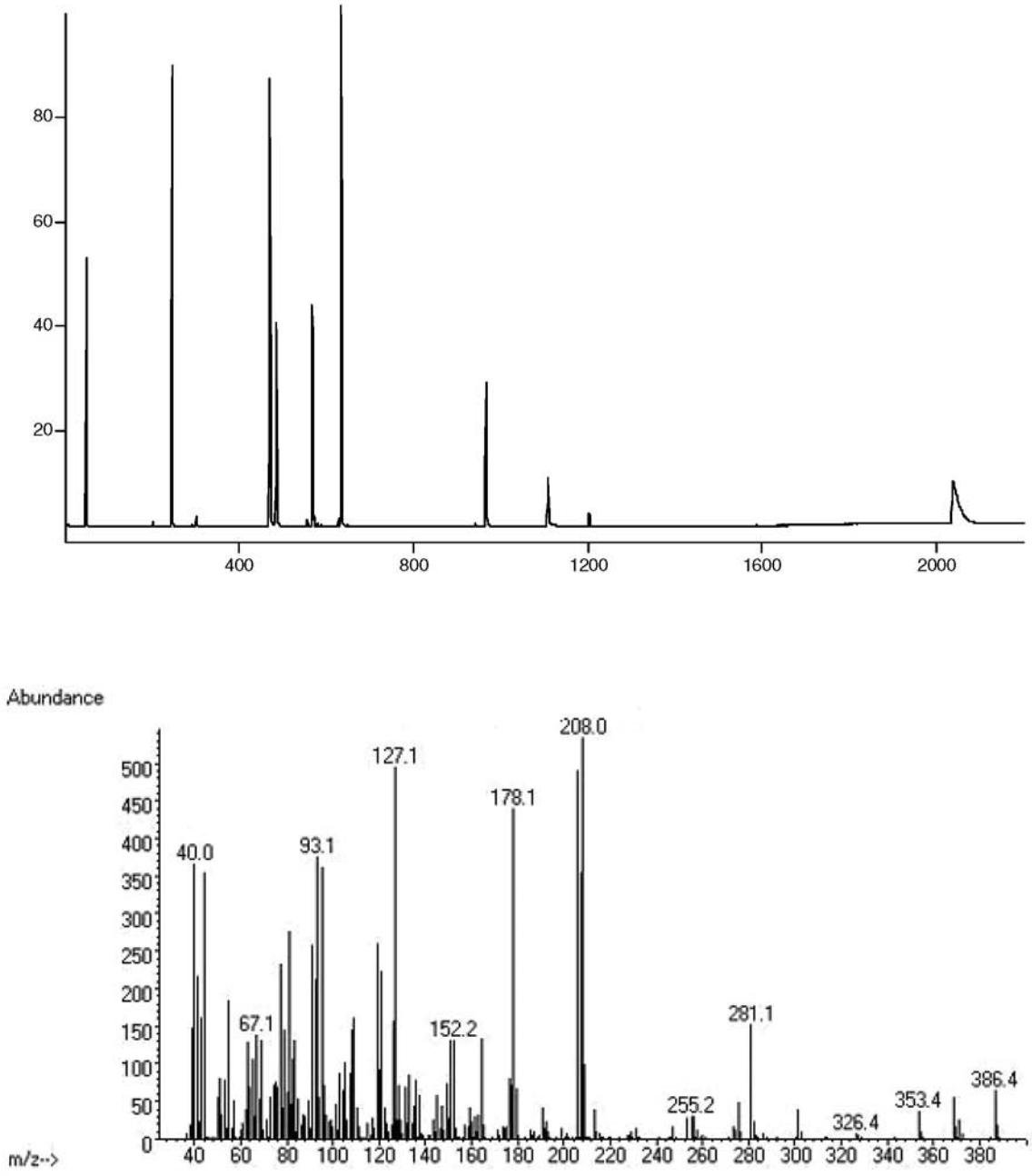

Figure S7. GC-MS (TIC) chromatogram (abscissa: scan number, ordinate: relative response of MS detector) and AMS profile (abscissa: *m*/*z* value, ordinate: response of MS detector) of model complex mixture M5.

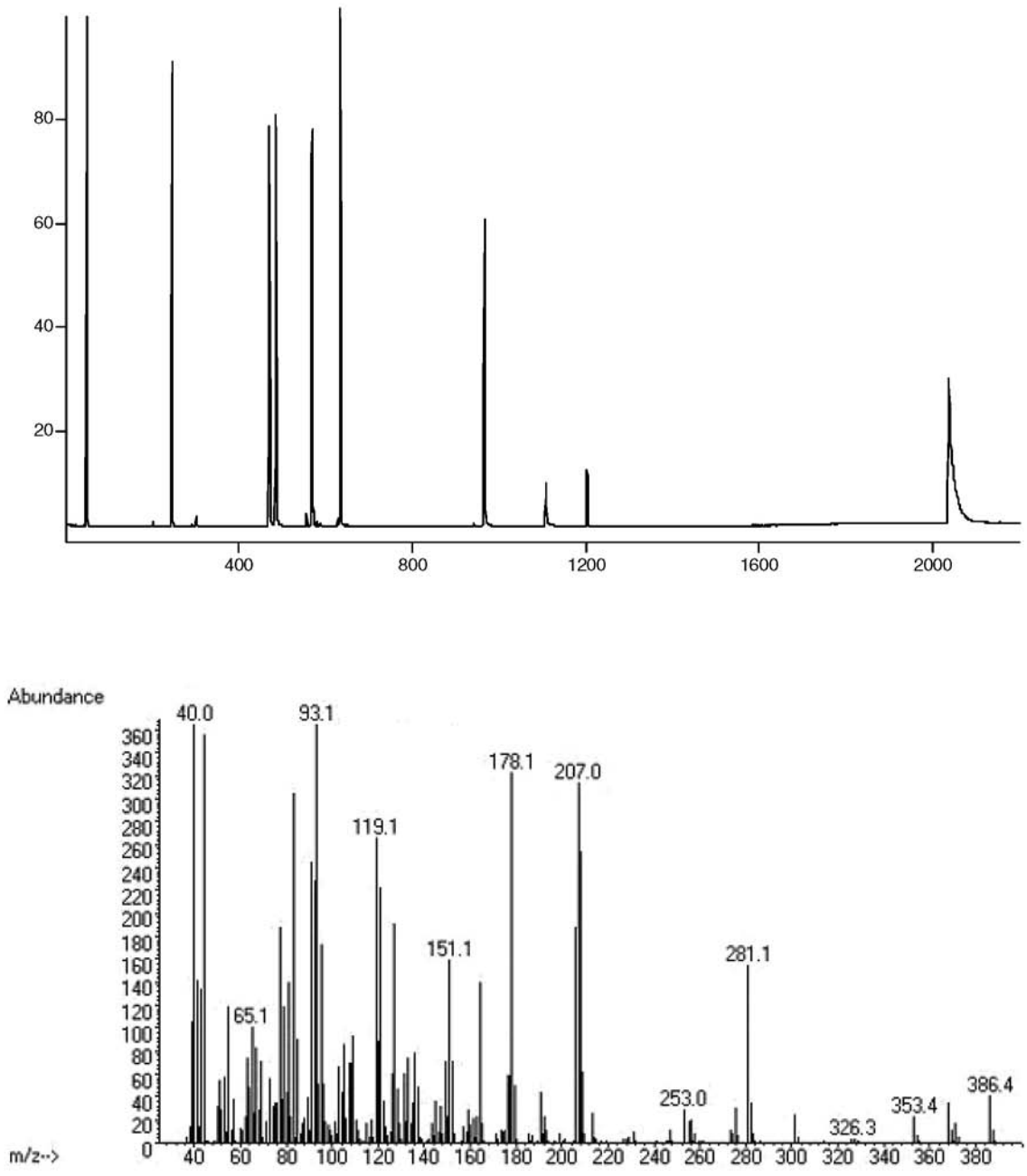

Figure S8. GC-MS (TIC) chromatogram (abscissa: scan number, ordinate: relative response of MS detector) and AMS profile (abscissa: *m*/*z* value, ordinate: response of MS detector) of model complex mixture M6.

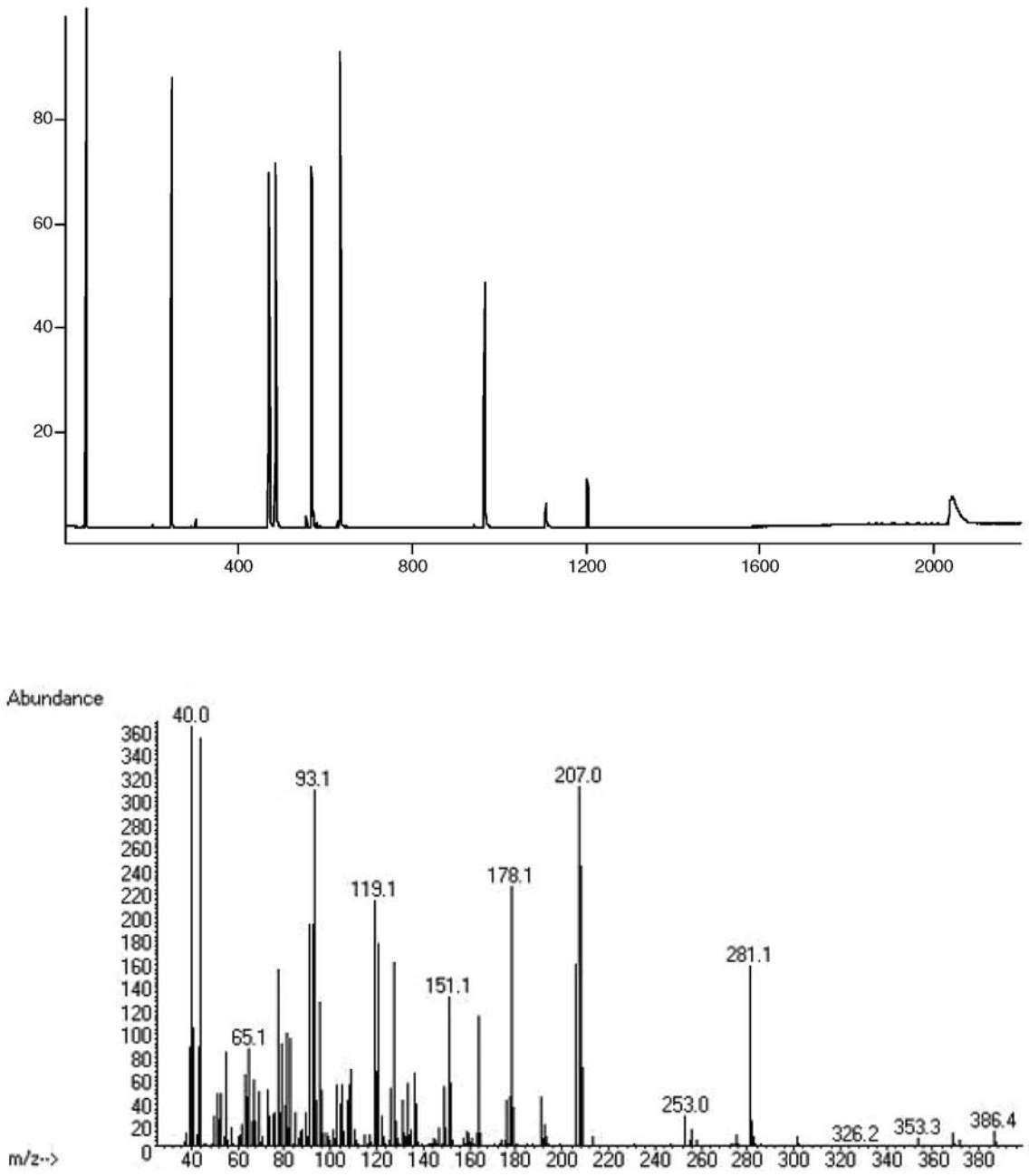

Figure S9. GC-MS (TIC) chromatogram (abscissa: scan number, ordinate: relative response of MS detector) and AMS profile (abscissa: *m*/*z* value, ordinate: response of MS detector) of model complex mixture M7.

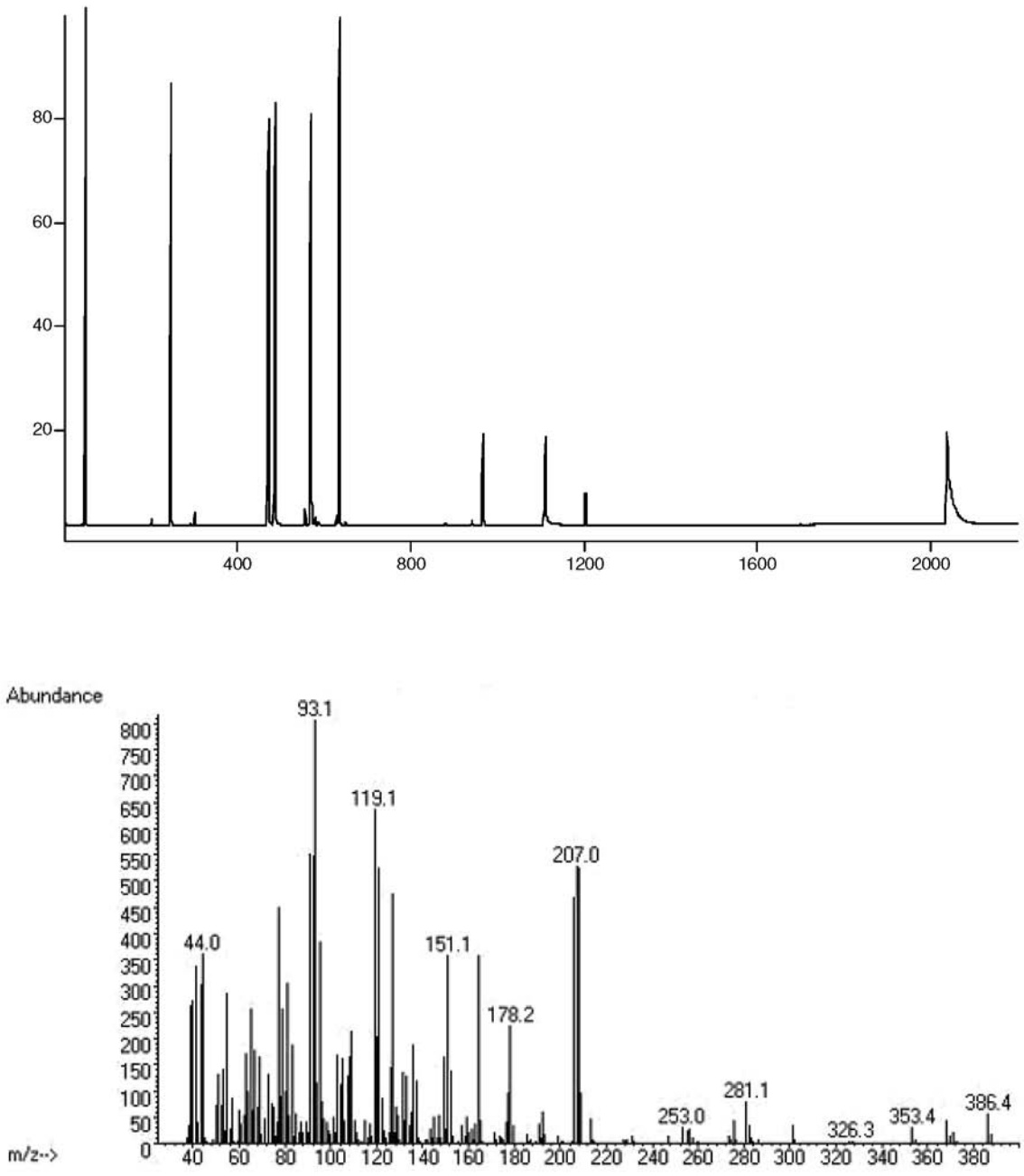

Figure S10. GC-MS (TIC) chromatogram (abscissa: scan number, ordinate: relative response of MS detector) and AMS profile (abscissa: *m*/*z* value, ordinate: response of MS detector) of model complex mixture M8.

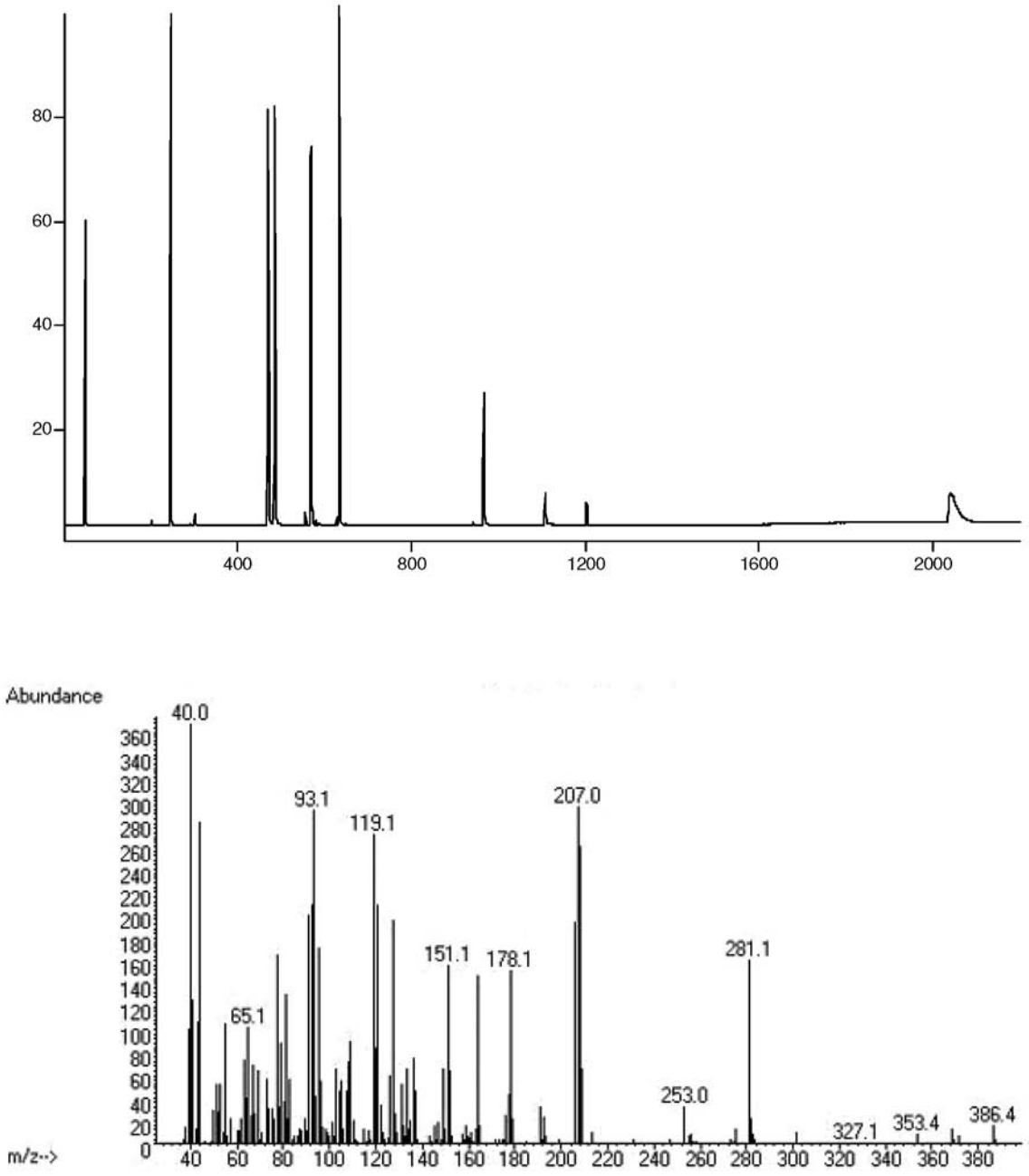

Figure S11. GC-MS (TIC) chromatogram (abscissa: scan number, ordinate: relative response of MS detector) and AMS profile (abscissa: *m*/*z* value, ordinate: response of MS detector) of model complex mixture M9.

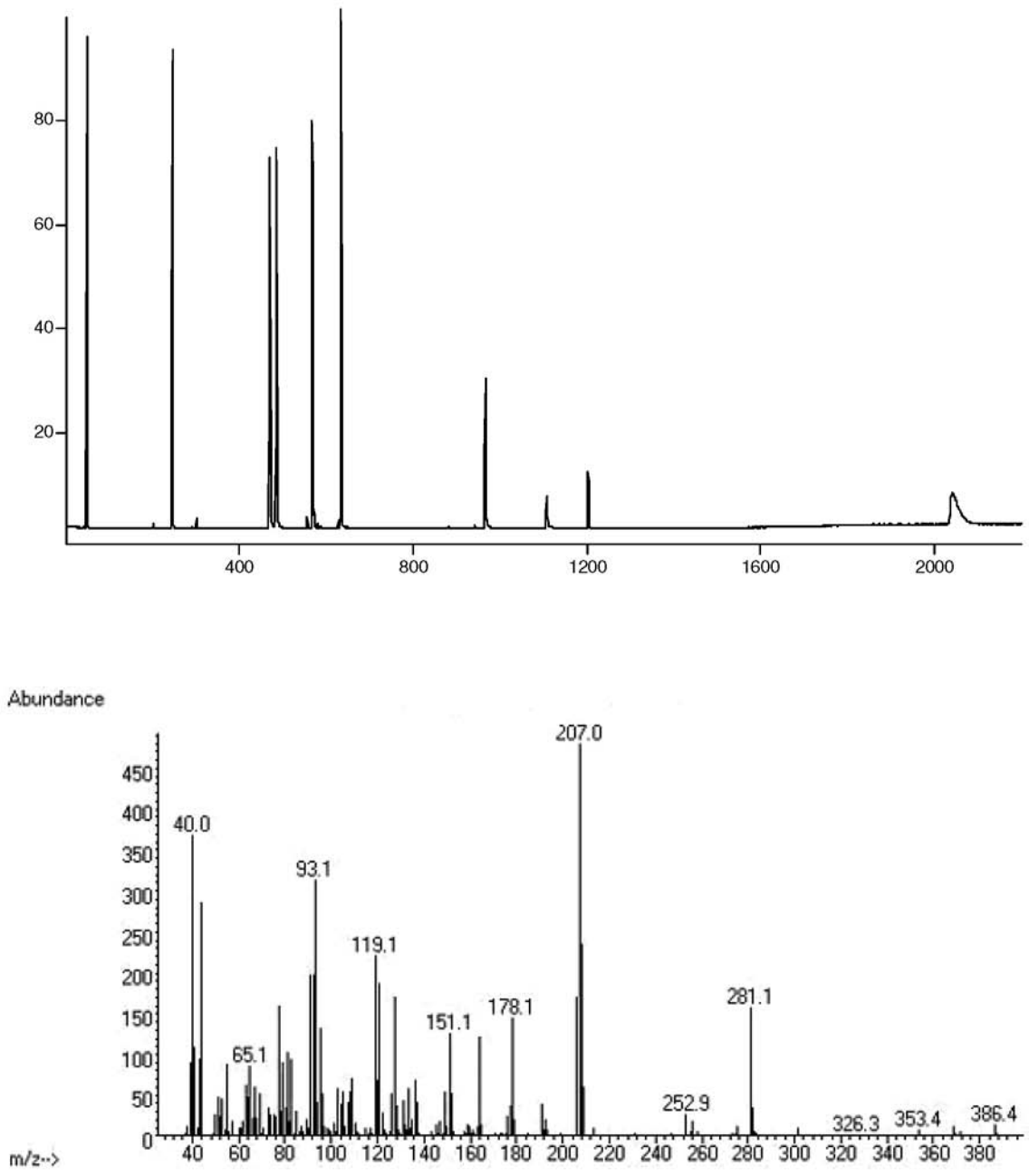

Figure S12. GC-MS (TIC) chromatogram (abscissa: scan number, ordinate: relative response of MS detector) and AMS profile (abscissa: *m*/*z* value, ordinate: response of MS detector) of model complex mixture M10.

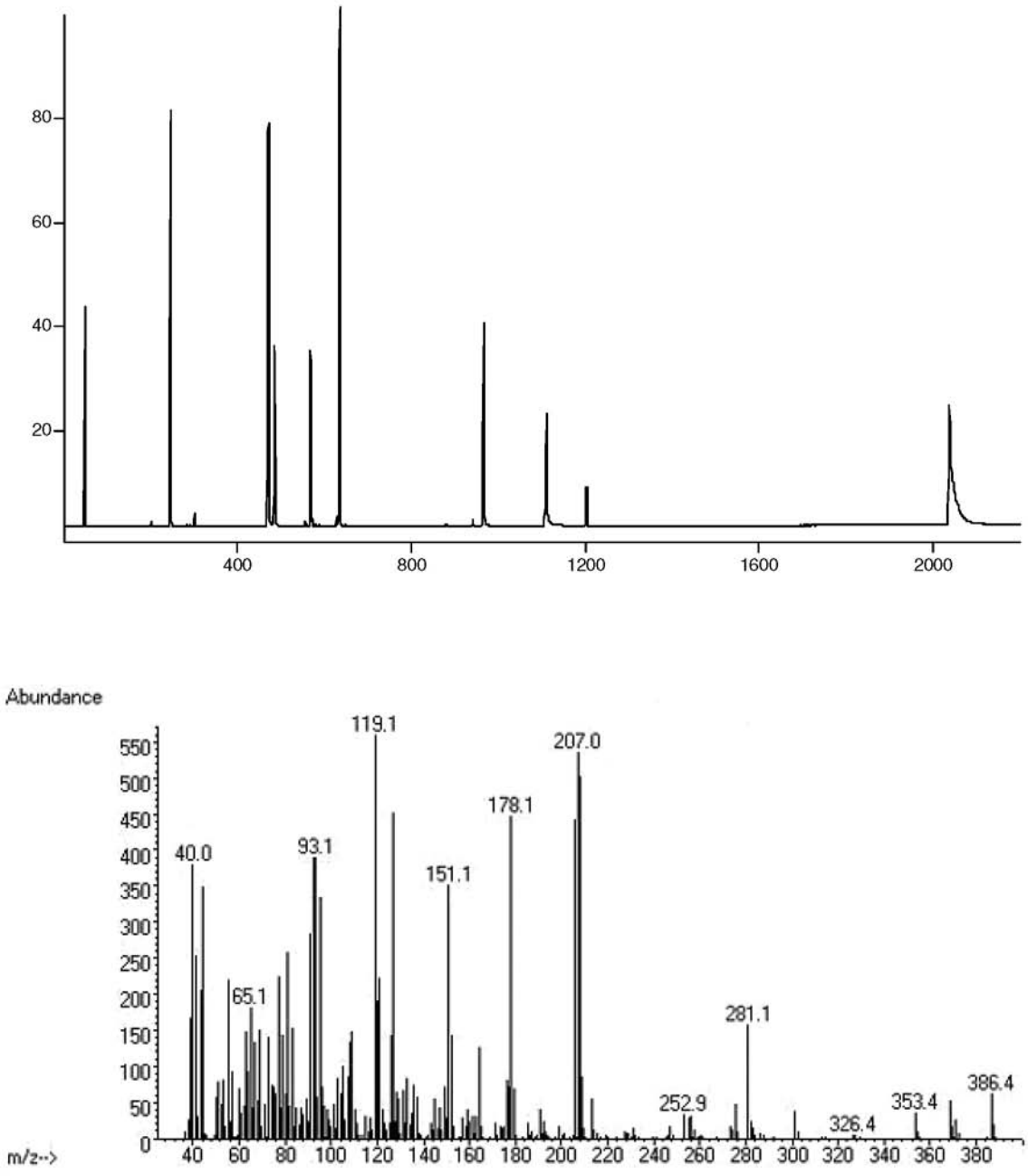

Figure S13. GC-MS (TIC) chromatogram (abscissa: scan number, ordinate: relative response of MS detector) and AMS profile (abscissa: *m*/*z* value, ordinate: response of MS detector) of model complex mixture M11.

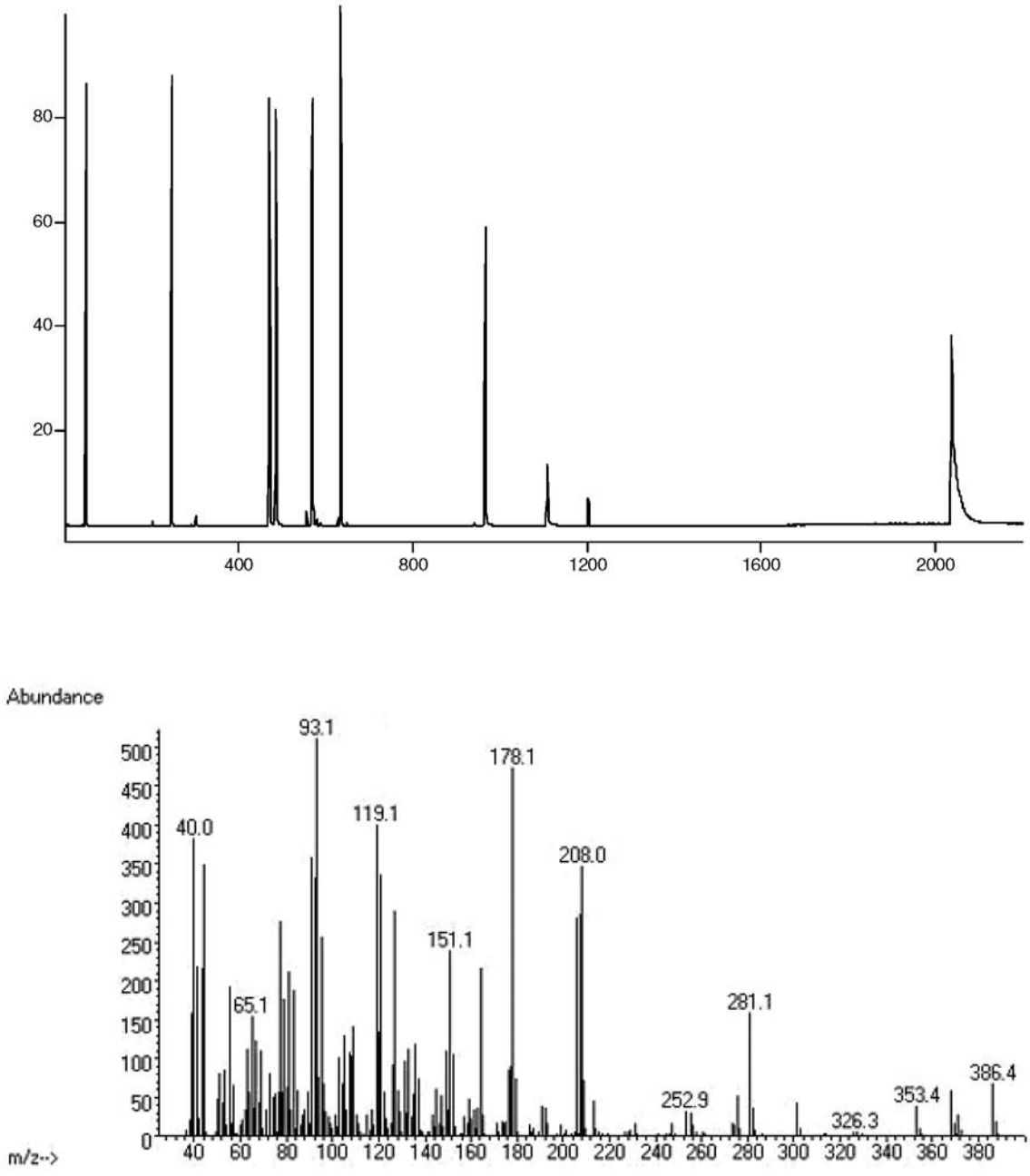

Figure S14. GC-MS (TIC) chromatogram (abscissa: scan number, ordinate: relative response of MS detector) and AMS profile (abscissa: *m*/*z* value, ordinate: response of MS detector) of model complex mixture M12.

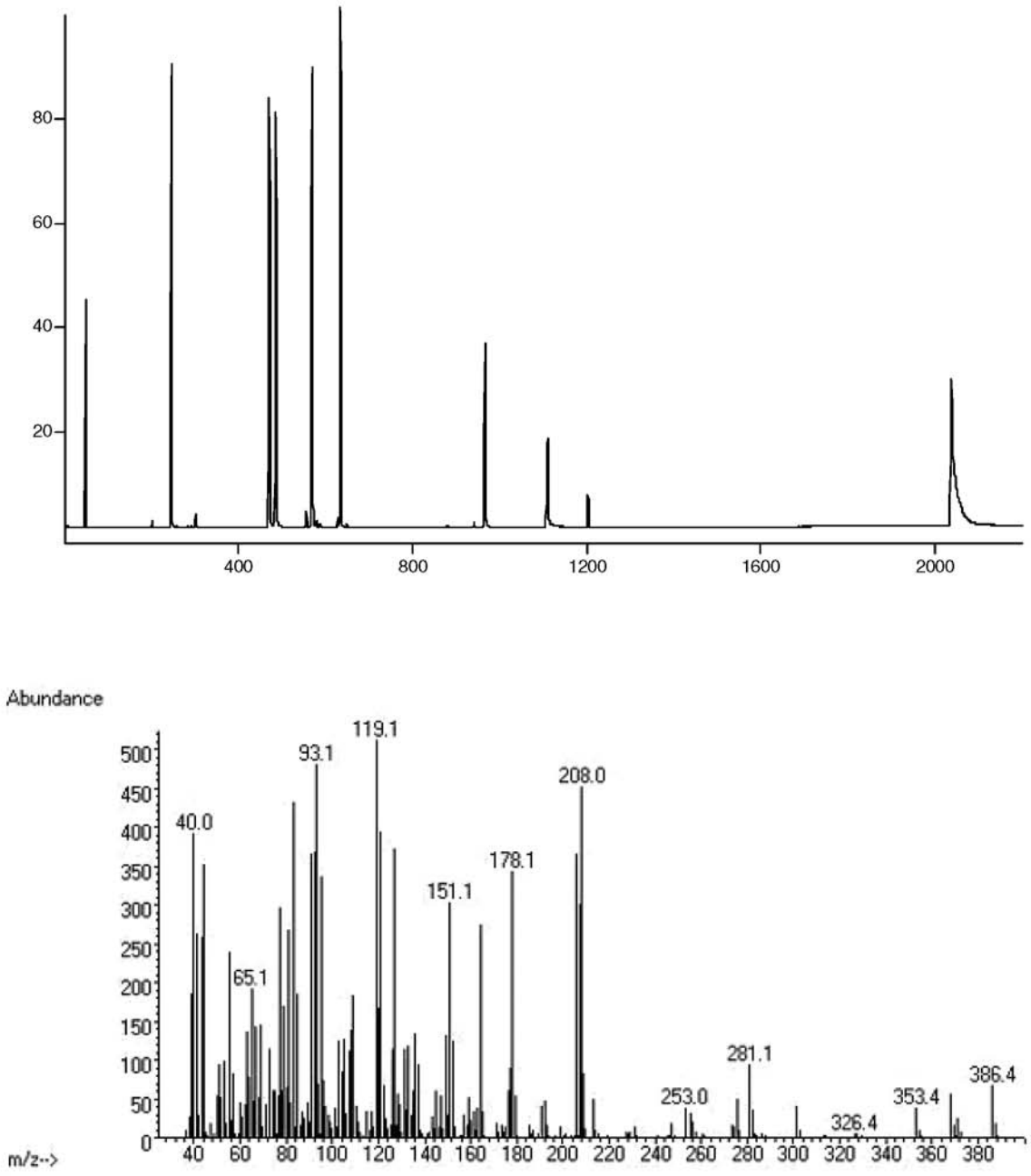

Figure S15. GC-MS (TIC) chromatogram (abscissa: scan number, ordinate: relative response of MS detector) and AMS profile (abscissa: *m*/*z* value, ordinate: response of MS detector) of model complex mixture M13.

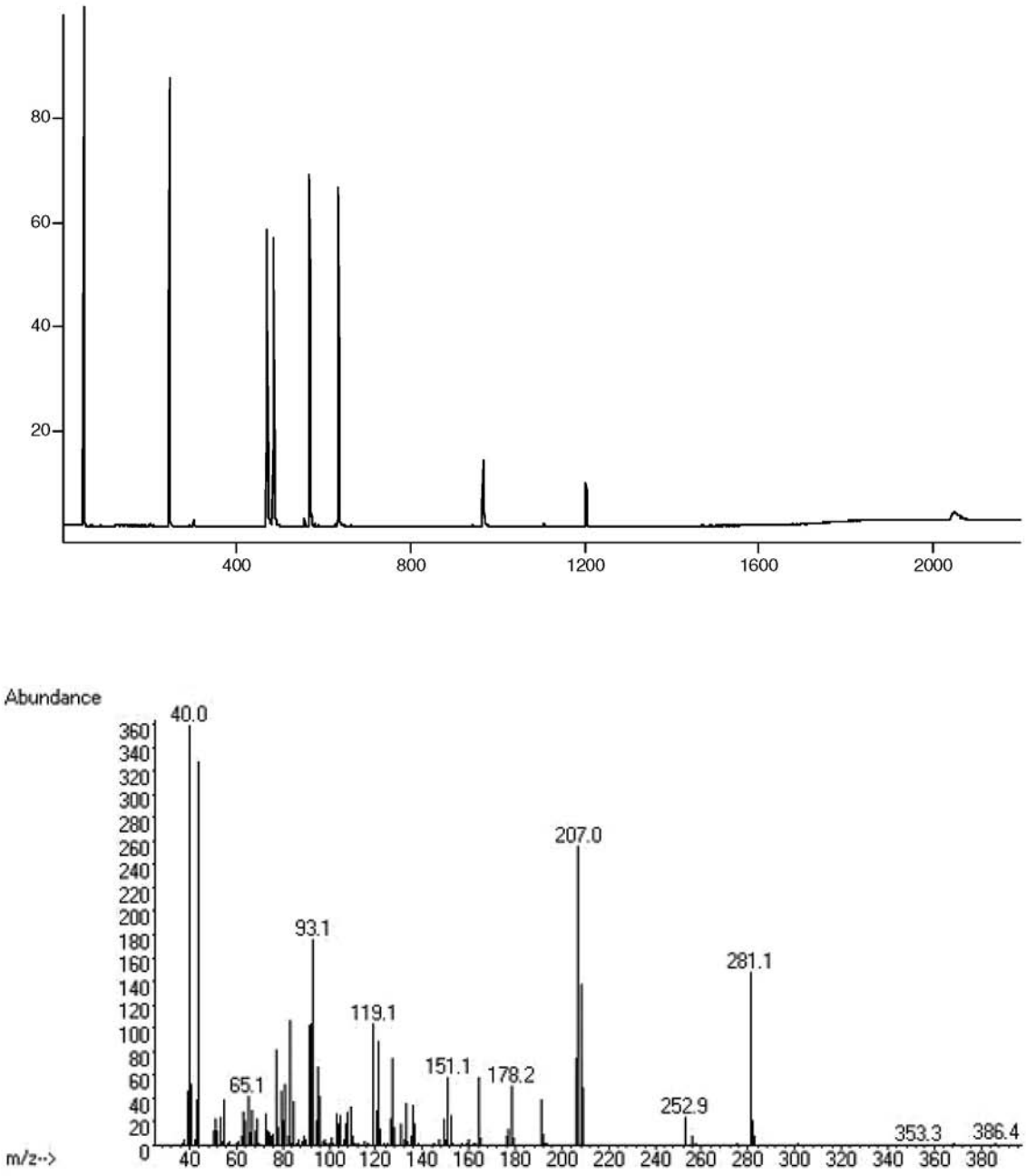

Figure S16. GC-MS (TIC) chromatogram (abscissa: scan number, ordinate: relative response of MS detector) and AMS profile (abscissa: *m*/*z* value, ordinate: response of MS detector) of model complex mixture M14.

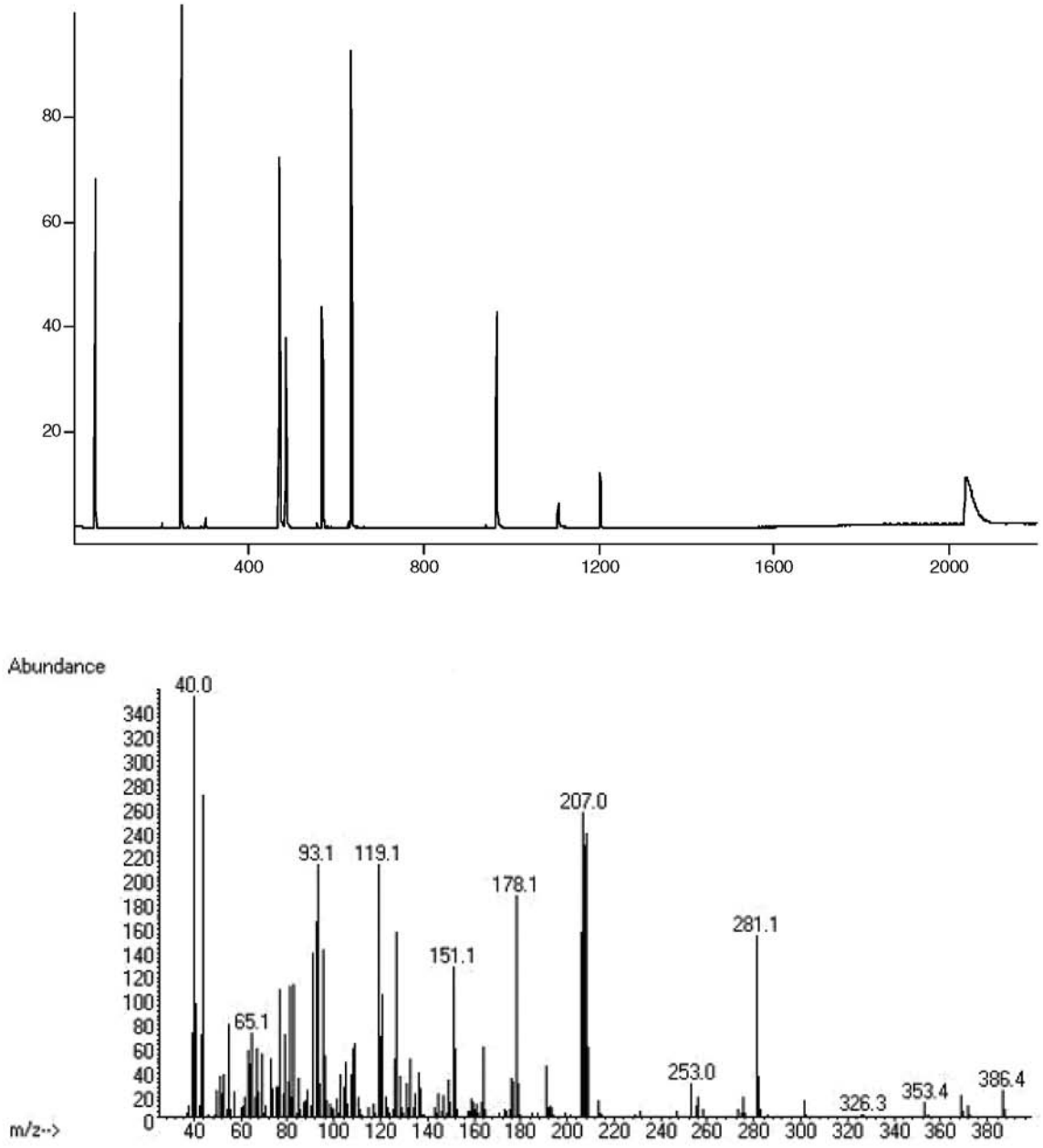

Figure S17. GC-MS (TIC) chromatogram (abscissa: scan number, ordinate: relative response of MS detector) and AMS profile (abscissa: *m*/*z* value, ordinate: response of MS detector) of model complex mixture M15.