

Supplementary Information

Dynamic Background Noise Removal on Overlapping GC-MS Peaks *via* Entropy Minimization Algorithm

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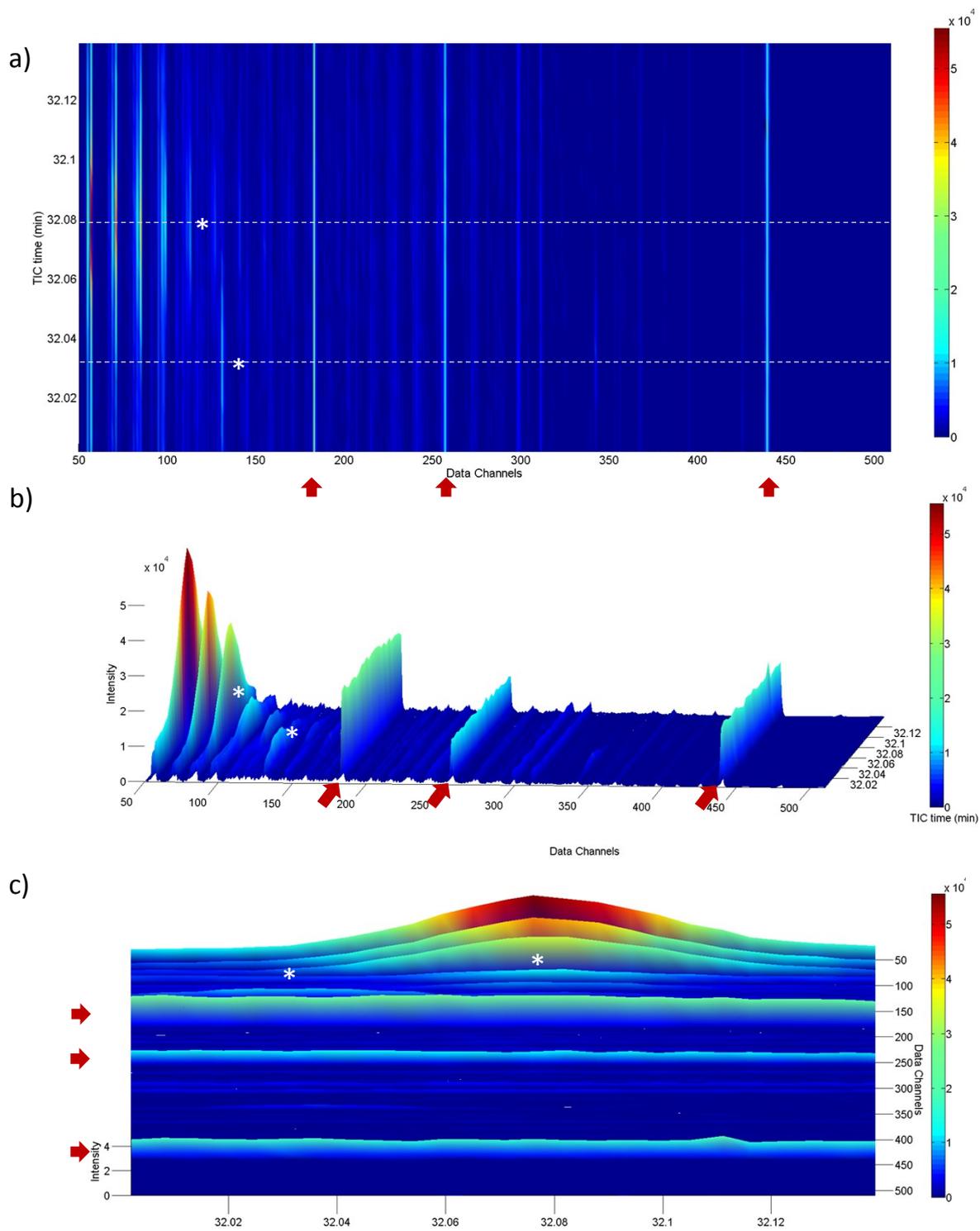


Figure S1. 3D plots of peak C27. (a) X-Y view. (b) Side view. (c) Top view. The two components were marked by white asterisks while the block of background noise was marked by red arrows. The intensity of the background noise is obvious from (b).

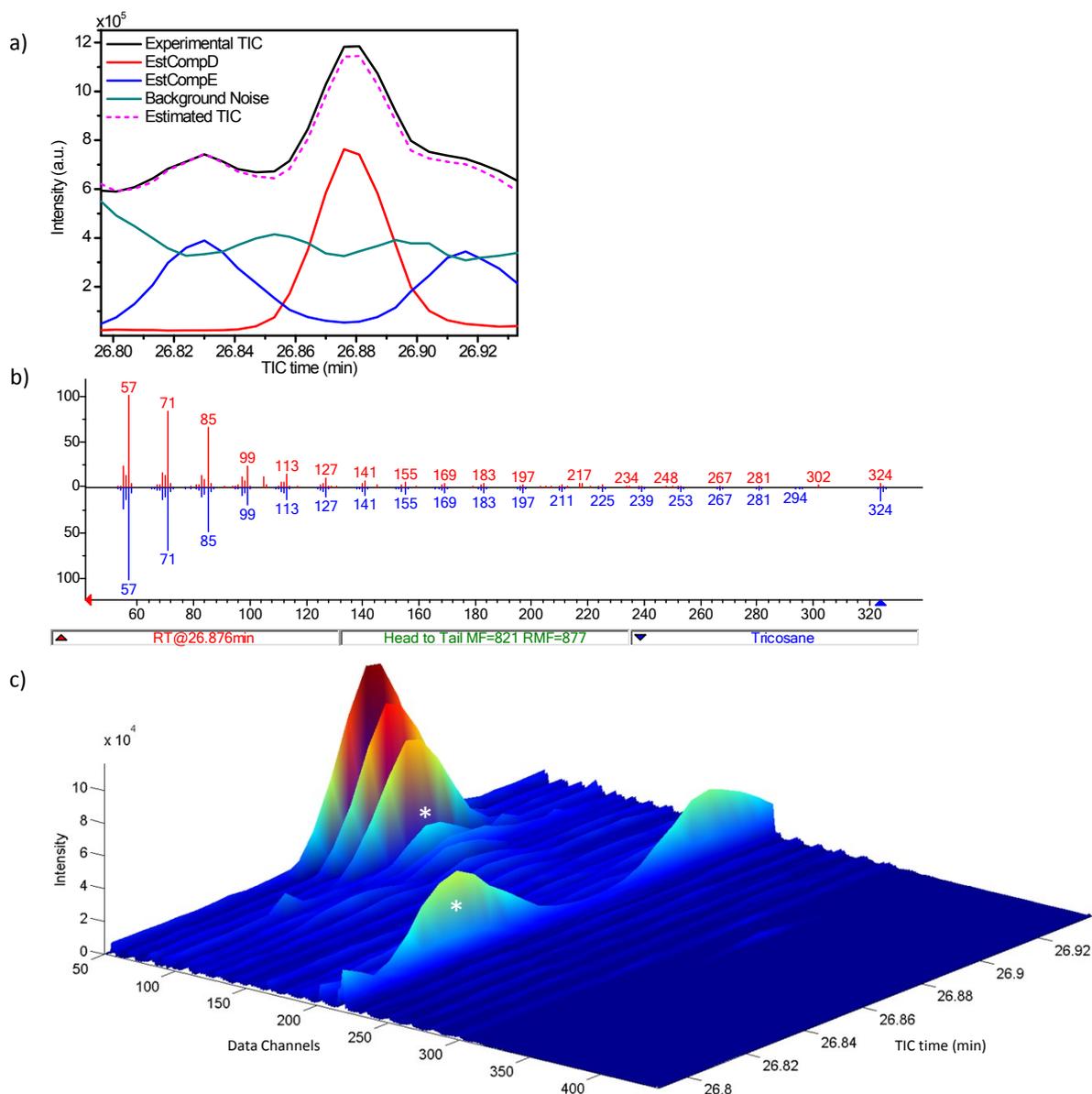


Figure S2. Analysis result of peak C23. (a) TIC profiles of the deconvoluted components and peak C23. Components EstCompD and EstCompE were identified. (b) Head-to-tail comparison mode in NIST mass spectral matching. The upper spectrum is EstCompD while the lower spectrum is of *n*-tricosane from NIST mass spectral library. (c) 3D plot of peak C23. Component EstCompD is marked by a white asterisks. EstCompE is marked by orange asterisk and is most likely an impurity.

The TIC profile of EstCompE has two peak apexes. A closer look at the 3D plot indicated a similar profile at *m/z* 216. Such TIC profile indicates the possible presence of isomeric compounds.¹

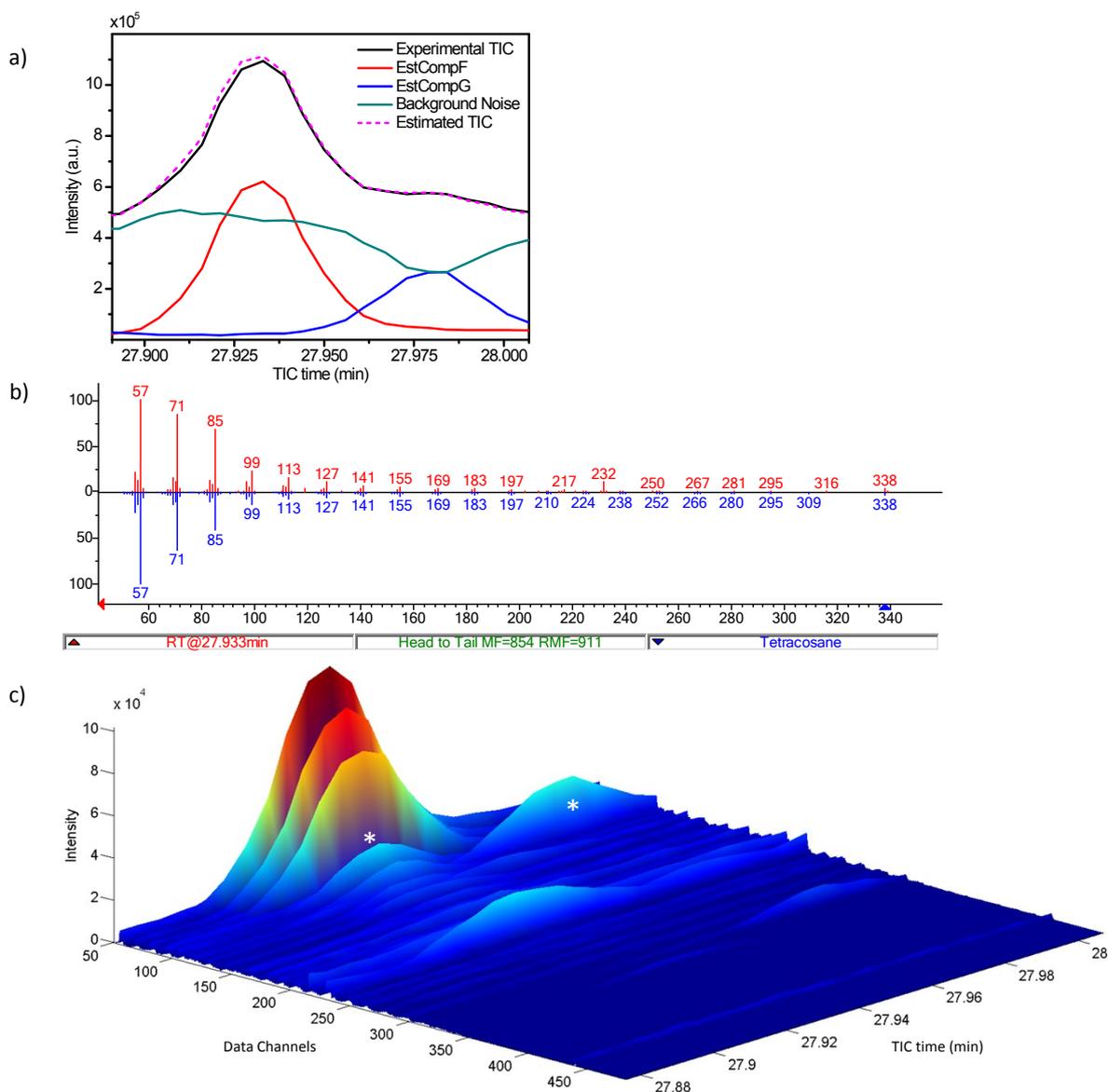


Figure S3. Analysis result of peak C24. (a) TIC profiles of the deconvoluted components and peak C24. Components EstCompF and EstCompG were identified. (b) Head-to-tail comparison mode in NIST mass spectral matching. The upper spectrum is EstCompF while the lower spectrum is of *n*-tetracosane from NIST mass spectral library. (c) 3D plot of peak C24. Component EstCompF and EstCompG are marked by white asterisks.

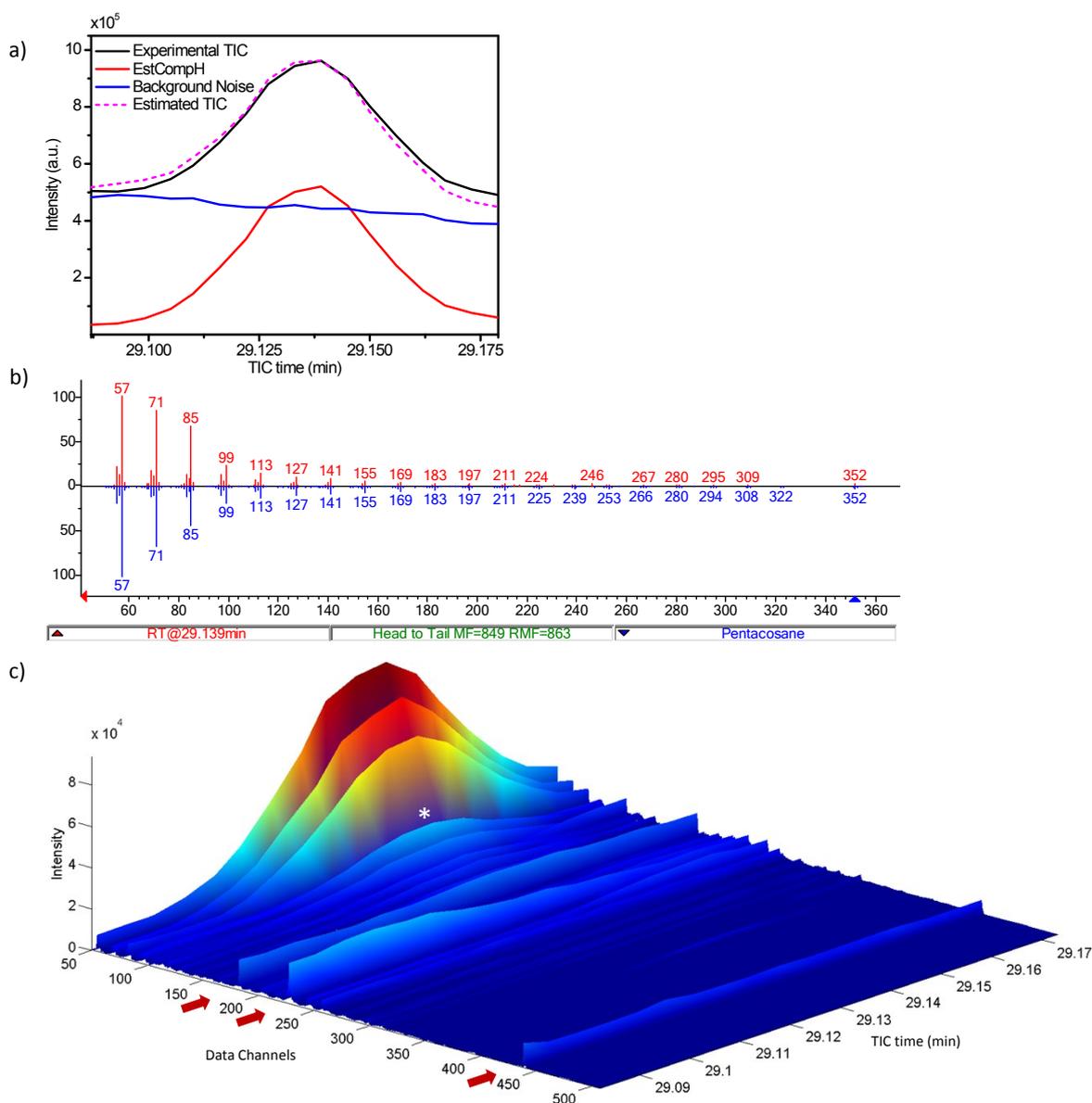


Figure S4. Analysis result of peak C25. (a) TIC profiles of the deconvoluted components and peak C25. Component EstCompH was identified. (b) Head-to-tail comparison mode in NIST mass spectral matching. The upper spectrum is EstCompH while the lower spectrum is of *n*-pentacosane from NIST mass spectral library. (c) 3D plot of peak C25. Component EstCompH is marked by a white asterisk. Blocks of background noise is obvious and marked by red arrows.

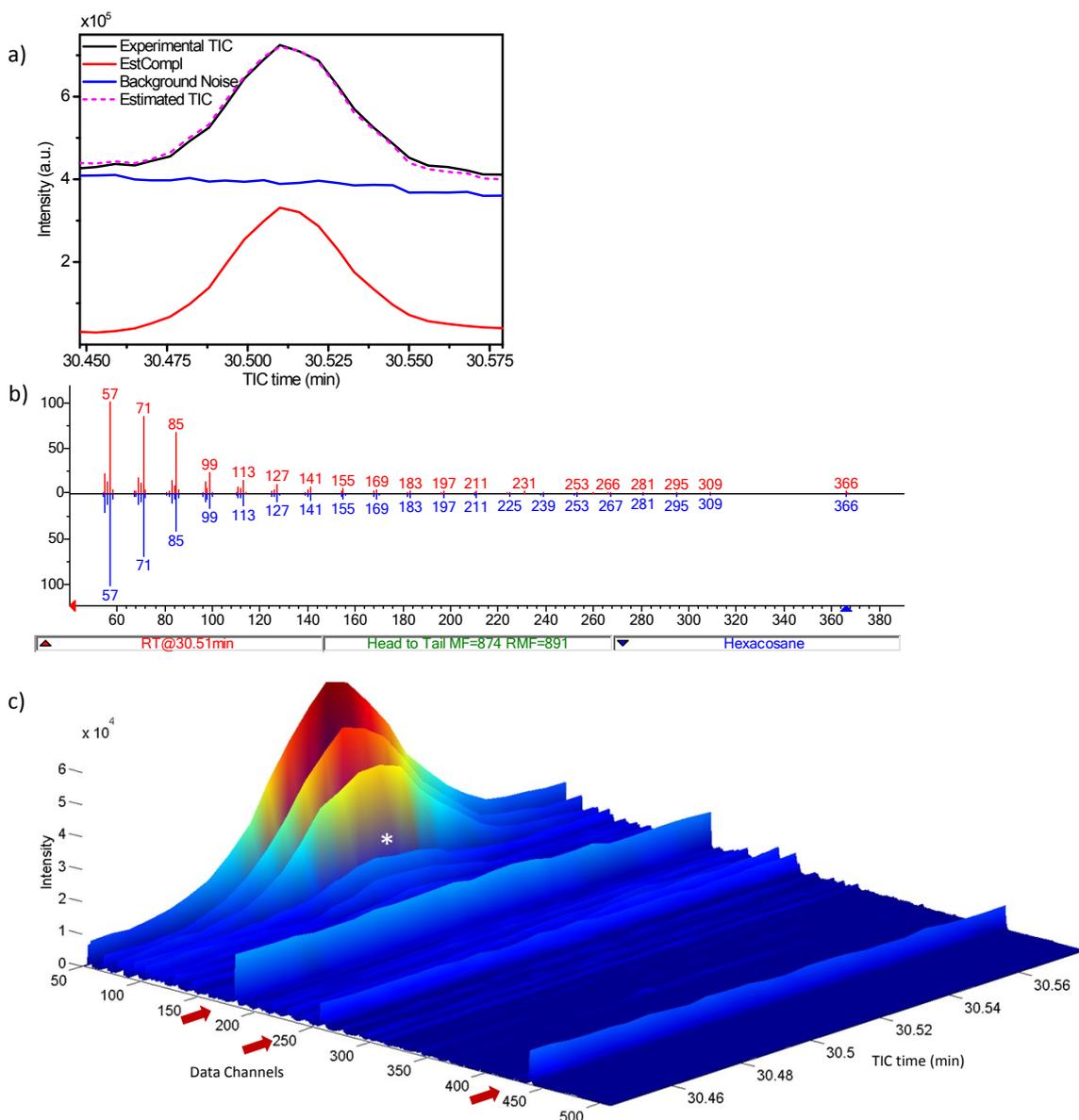


Figure S5. Analysis result of peak C26. (a) TIC profiles of the deconvoluted components and peak C26. Component EstCompl was identified. (b) Head-to-tail comparison mode in NIST mass spectral matching. The upper spectrum is EstCompl while the lower spectrum is of *n*-hexacosane from NIST mass spectral library. (c) 3D plot of peak C26. Component EstCompl is marked by a white asterisk. Blocks of background noise is obvious and marked by red arrows.

References

- (1) Lin, G. C.; Long, H. R.; Zhang, H. J.; Ji, X. W.; Lu, B.; Gu, X. Y. Analysis of unknown components in rose essential oil by entropy minimization algorithm. *J. Chinese Mass Spectrom. Soc.* **2015**, 36, 448-453.