

## Supporting Information

### Influence of Early Stages of Triglyceride Pyrolysis on the Formation of PAHs as Coke Precursors

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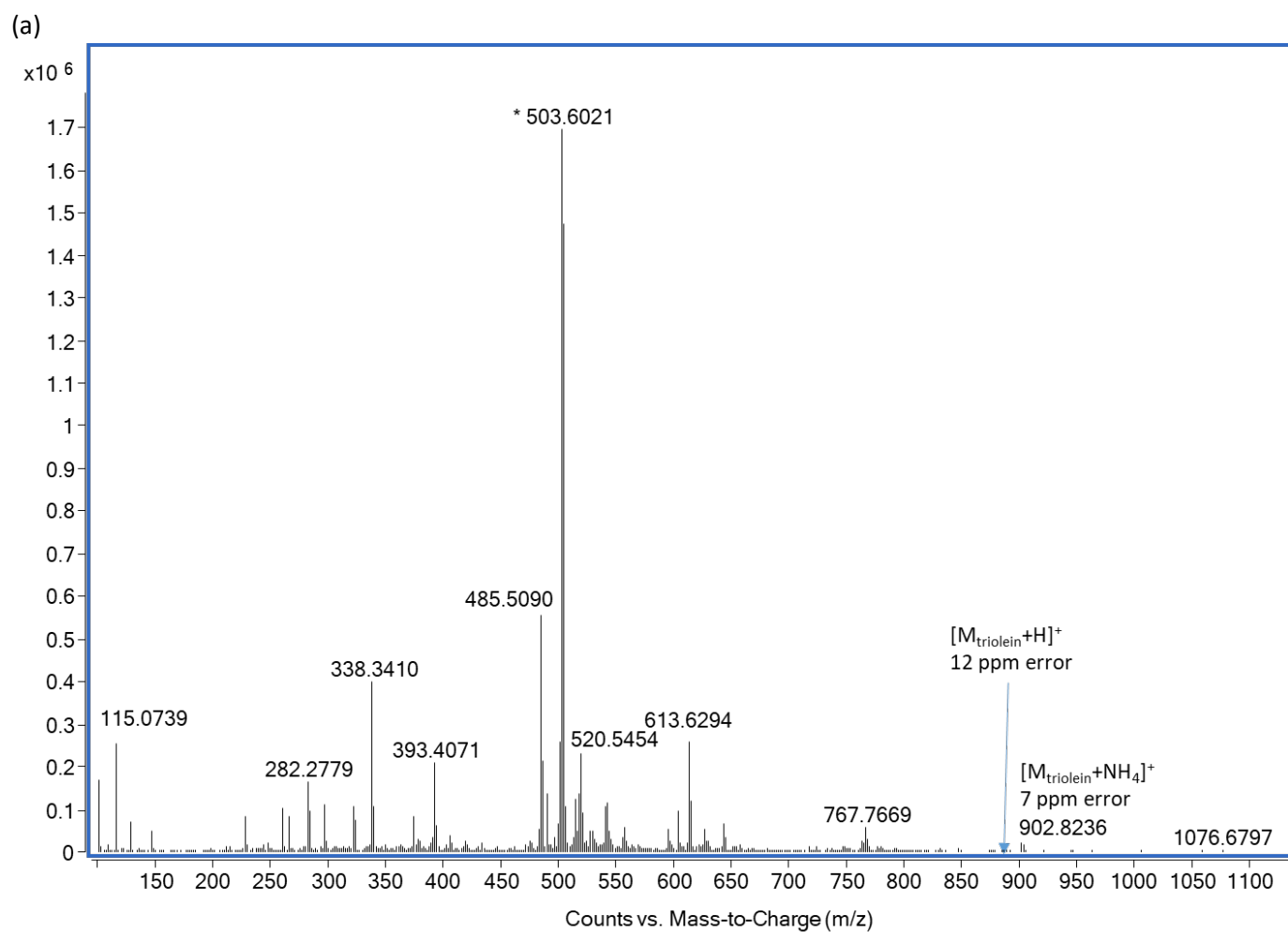
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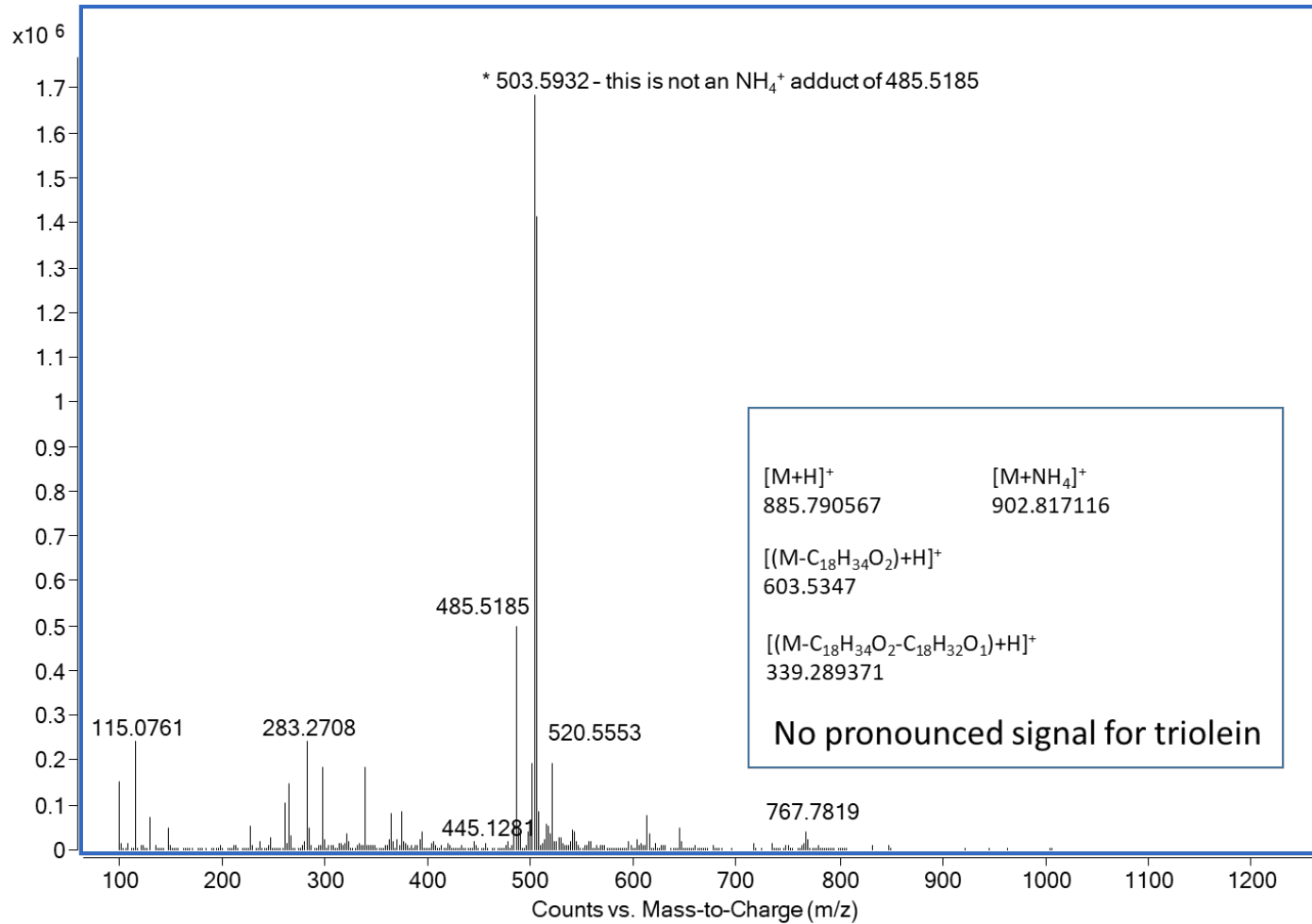
#### 1. Supporting Figures

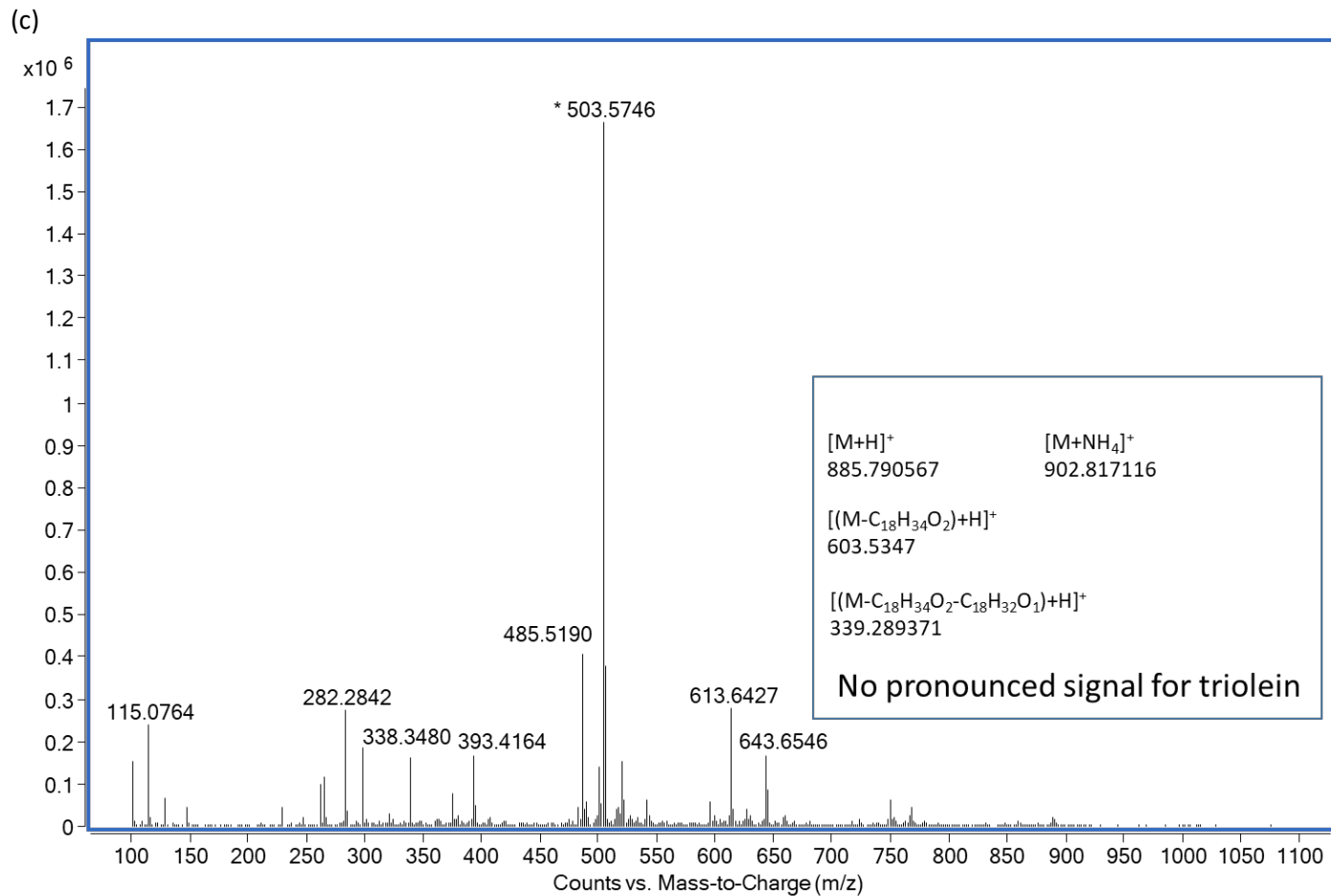
#### 2. Supporting Table

## 1. Supporting Figures

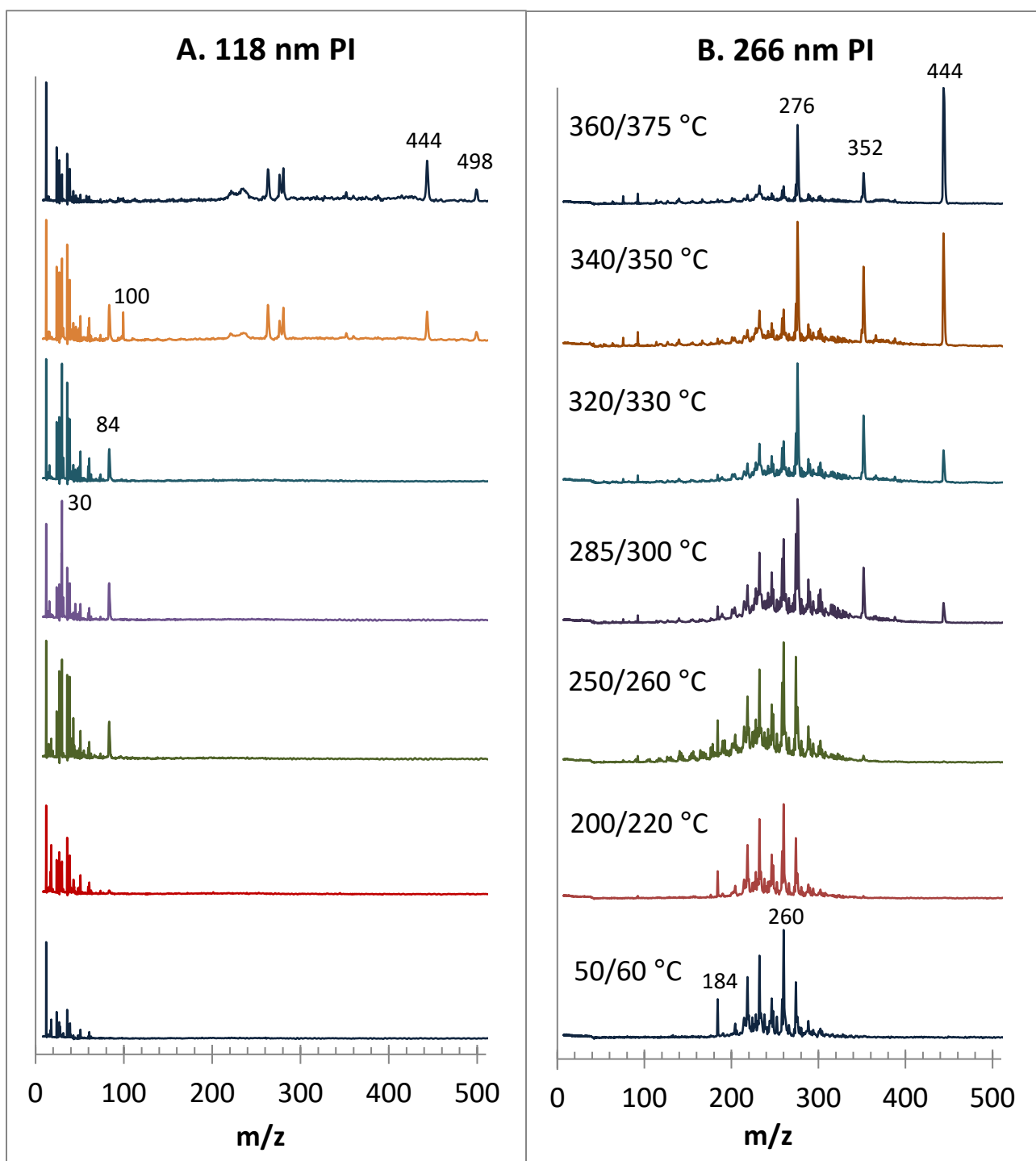


(b)





**Figure S1. APCI-TOF MS spectra of the cumulatively collected products that exited the MB gas expansion orifice, with pure He carrier gas at temperatures up to 400 °C (a) and up to 420 °C (b); with 10% H<sub>2</sub> in He up to 400 °C (c).**



**Figure S2.** Side by side TOFMS of triolein for A. 118 nm PI and B. 266 nm PI, at the same temperatures for each side. These TOFMS correspond to the pure He case of Figures 1-2 B/B' in the paper. Note the appearance of new pyrolysis products by 200/220 °C at 118 nm PI and by 250/260 °C at 266 nm PI.

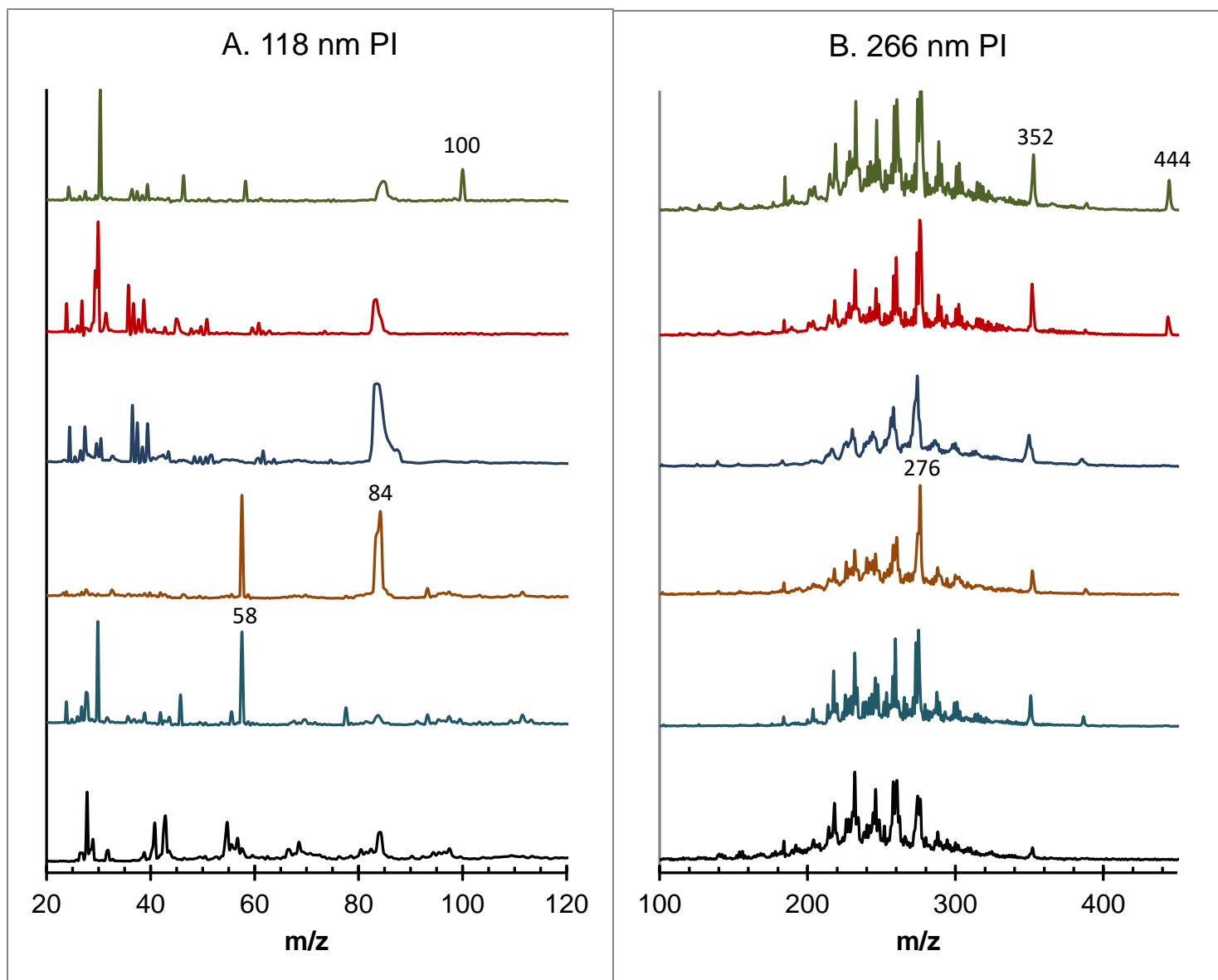


Figure S3. Comparative 118 nm (A) and 266 nm (B) PI MB-TOFMS of triolein at  $\sim 300$  °C over multiple separate experimental runs, encompassing various differences in sample holders and sample deposition conditions. In addition, temperature disparities in the various scans produce some relative differences in each case. In A a low  $m/z$  scan range has been chosen, to emphasize recognition of  $C_6$  and  $C_7$  peaks; in B a wider  $m/z$  range has been chosen, such that the appearance of higher mass associative chemistry PAHs can be correlated with the appearance of low mass peaks in A. In general, the appearance of a  $C_6$  peak in A, then followed by a  $C_7$  peak, is a prelude to incipient enhanced growth in B of the PAHs at  $m/z$  276, 352, and 444. Note that the actual effective temperature in the two bottom scan runs appears to be lower. This is evidenced by relatively weaker  $C_6/C_7$  product peaks at 118 nm PI accompanied by weaker overall emergence of “favored” PAH peaks at 266 nm PI.

## 2. Supporting Table

**Table S1. Molecular weights of less expected species for possible correlation with the observed MB-TOF low-MW (below 120 amu) peaks. The corresponding free radicals, potential intermediates, have MW less by 1 amu.**

| Species Types                                | C1        | C2        | C3        | C4           | C5           | C6           | C7           | C8           |
|--|-----------|-----------|-----------|--------------|--------------|--------------|--------------|--------------|
| <b>Hydrocarbons</b>                          |           |           |           |              |              |              |              |              |
| <b>Alkatrienes &amp; isomers</b>             | -         | -         | <b>38</b> | <b>52</b>    | <b>66</b>    | <b>80</b>    | <b>94</b>    | <b>108</b>   |
| $C_nH_{2n-4}$                                |           |           | $C_3H_2$  | $C_4H_4$     | $C_5H_6$     | $C_6H_8$     | $C_7H_{10}$  | $C_8H_{12}$  |
| <b>Alkatetraenes &amp; isomers</b>           | -         | -         | -         | <b>50</b>    | <b>64</b>    | <b>78*</b>   | <b>92*</b>   | <b>106*</b>  |
| $C_nH_{2n-6}$                                |           |           |           | $C_4H_2$     | $C_5H_4$     | $C_6H_6$     | $C_7H_8$     | $C_8H_{10}$  |
| <b>Alkapentaenes &amp; isomers</b>           | -         | -         | -         | -            | <b>62</b>    | <b>76</b>    | <b>90</b>    | <b>104*</b>  |
| $C_nH_{2n-8}$                                |           |           |           |              | $C_5H_2$     | $C_6H_4$     | $C_7H_6$     | $C_8H_8$     |
| <b>Alkahexaenes &amp; isomers</b>            | -         | -         | -         | -            | -            | <b>74</b>    | <b>88</b>    | <b>102</b>   |
| $C_nH_{2n-10}$                               |           |           |           |              |              | $C_6H_2$     | $C_7H_4$     | $C_8H_6$     |
| <b>Alkaheptaenes &amp; isomers</b>           | -         | -         | -         | -            | -            | -            | <b>86</b>    | <b>100</b>   |
| $C_nH_{2n-12}$                               |           |           |           |              |              |              | $C_7H_2$     | $C_8H_4$     |
| <b>Alcohols:</b>                             |           |           |           |              |              |              |              |              |
| <b>Saturated (alkanols)</b>                  | <b>32</b> | <b>46</b> | <b>60</b> | <b>74</b>    | <b>88</b>    | <b>102</b>   | <b>116</b>   |              |
| $C_nH_{2n+2}O$                               | $CH_4O$   | $C_2H_6O$ | $C_3H_8O$ | $C_4H_{10}O$ | $C_5H_{12}O$ | $C_6H_{14}O$ | $C_7H_{16}O$ |              |
| <b>Alkenols &amp; cycloalkanols</b>          | -         | <b>44</b> | <b>58</b> | <b>72</b>    | <b>86</b>    | <b>100</b>   | <b>114</b>   | <b>128</b>   |
| $C_nH_{2n}O$                                 |           |           | $C_3H_6O$ | $C_4H_8O$    | $C_5H_{10}O$ | $C_6H_{12}O$ | $C_7H_{14}O$ | $C_8H_{16}O$ |
| <b>Alkynols, cycloalkenols, alkadienols-</b> | <b>42</b> | <b>56</b> | <b>70</b> | <b>84</b>    | <b>98</b>    | <b>112</b>   |              |              |
| $C_nH_{2n-2}O$                               |           | $C_2H_2O$ | $C_3H_4O$ | $C_4H_6O$    | $C_5H_8O$    | $C_6H_{10}O$ | $C_7H_{12}O$ |              |
| <b>Alkatrienols &amp; isomers</b>            | -         | -         | -         | <b>68</b>    | <b>82</b>    | <b>96</b>    | <b>110</b>   |              |
| $C_nH_{2n-4}O$                               |           |           |           | $C_4H_4O$    | $C_5H_6O$    | $C_6H_8O$    | $C_7H_{10}O$ |              |
| <b>Saturated aldehydes/ketones</b>           | <b>30</b> | <b>44</b> | <b>58</b> | <b>72</b>    | <b>86</b>    | <b>100</b>   | <b>114</b>   | <b>128</b>   |
| $C_nH_{2n}O$                                 | $CH_2O$   | $C_2H_4O$ | $C_3H_6O$ | $C_4H_8O$    | $C_5H_{10}O$ | $C_6H_{12}O$ | $C_7H_{14}O$ | $C_8H_{16}O$ |
| <b>Monounsaturated aldehydes/ketones</b>     | <b>42</b> | <b>56</b> | <b>70</b> | <b>84</b>    | <b>98</b>    | <b>112</b>   |              |              |
| $C_nH_{2n-2}O$                               |           | $C_2H_2O$ | $C_3H_4O$ | $C_4H_6O$    | $C_5H_8O$    | $C_6H_{10}O$ | $C_7H_{12}O$ |              |

\* Could also be aromatic.