

# Supplementary Information for Characterization of Products from Fast and Isothermal Hydrothermal Liquefaction of Microalgae

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Table S1: Reactor Loadings for HTL Experiments

|                 | Fast, Low Loading   | Fast, High Loading  | Isothermal          |
|-----------------|---------------------|---------------------|---------------------|
| Dried Algae (g) | $0.0835 \pm 0.0001$ | $0.4997 \pm 0.0002$ | $0.4979 \pm 0.0001$ |
| Total Water (g) | $0.4705 \pm 0.0003$ | $2.7768 \pm 0.0005$ | $2.7732 \pm 0.0002$ |

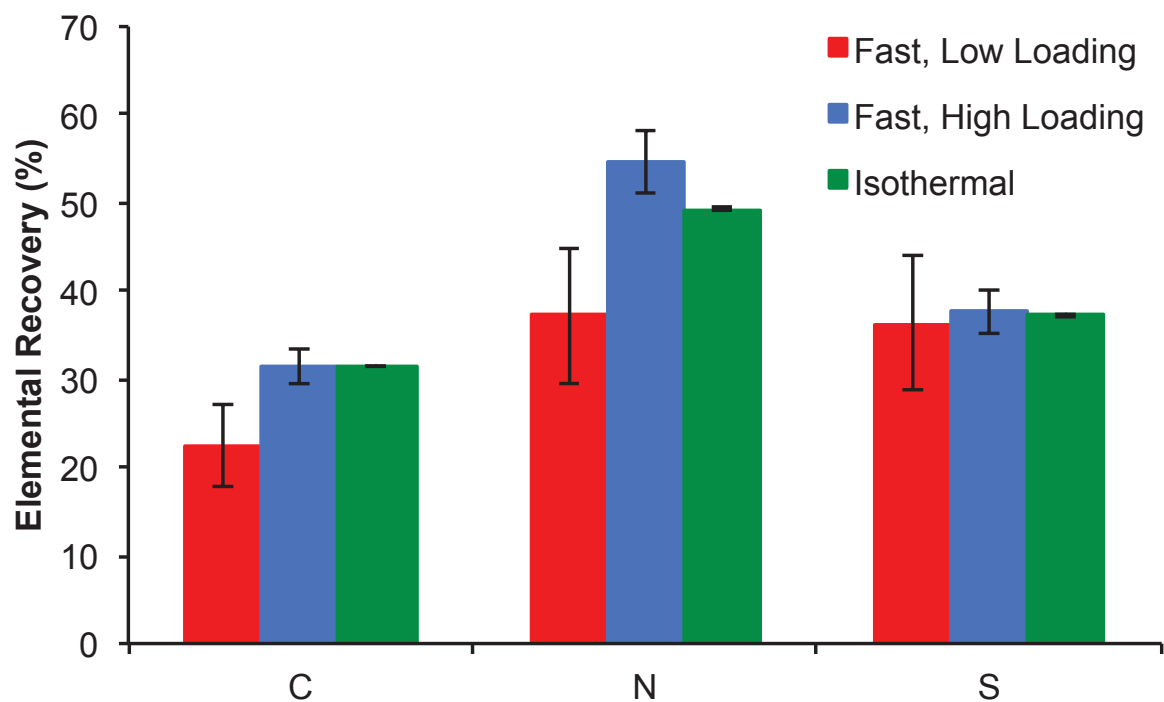


Figure S1: Recovery of C, N and S in the Aqueous Phase from HTL at Different Conditions

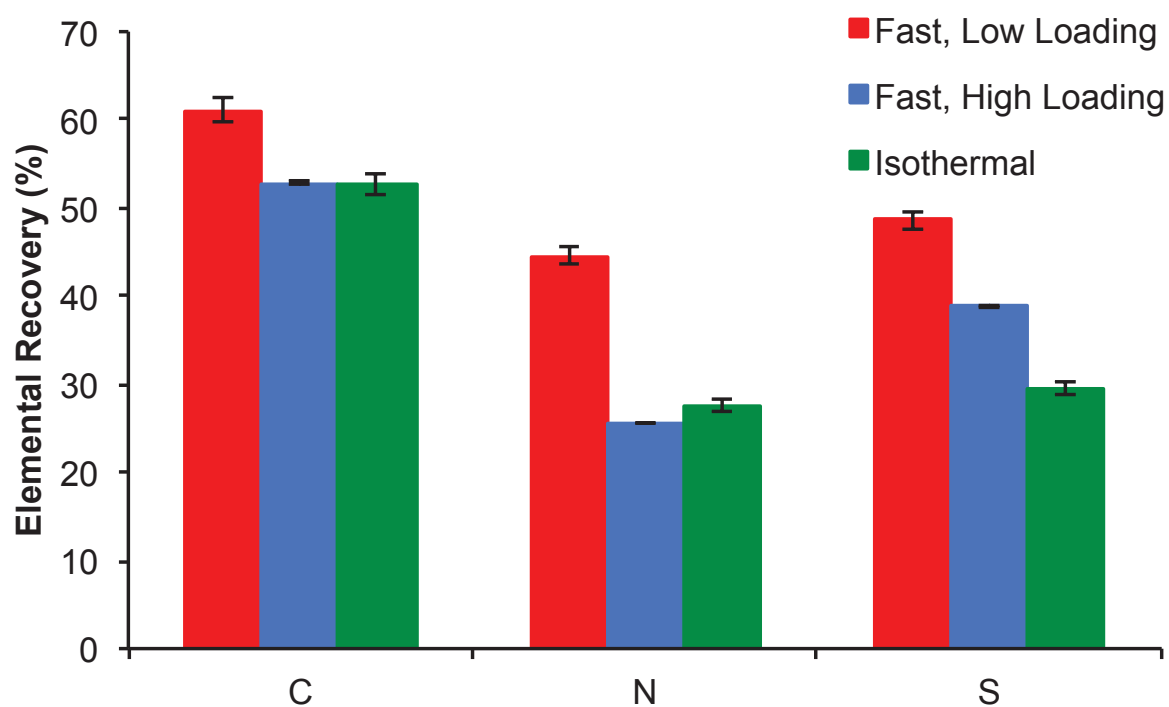


Figure S2: Recovery of C, N, and S in the Biocrude from HTL at Different Conditions

| Sample                        | Positive ESI | Negative ESI |
|-------------------------------|--------------|--------------|
| Fast, Low Loading - Aqueous   | 88.7%        | 69.5%        |
| Fast, High Loading - Aqueous  | 79.2%        | 83.8%        |
| Isothermal - Aqueous          | 93.3%        | 60.9%        |
| Fast, Low Loading - Biocrude  | 88.6%        | 94.4%        |
| Fast, High Loading - Biocrude | 90.2%        | 90.0%        |
| Isothermal - Biocrude         | 95.0%        | 92.1%        |

Table S2: Percentage of Peaks with Assigned Molecular Formulas for each Sample using each Ionization Method

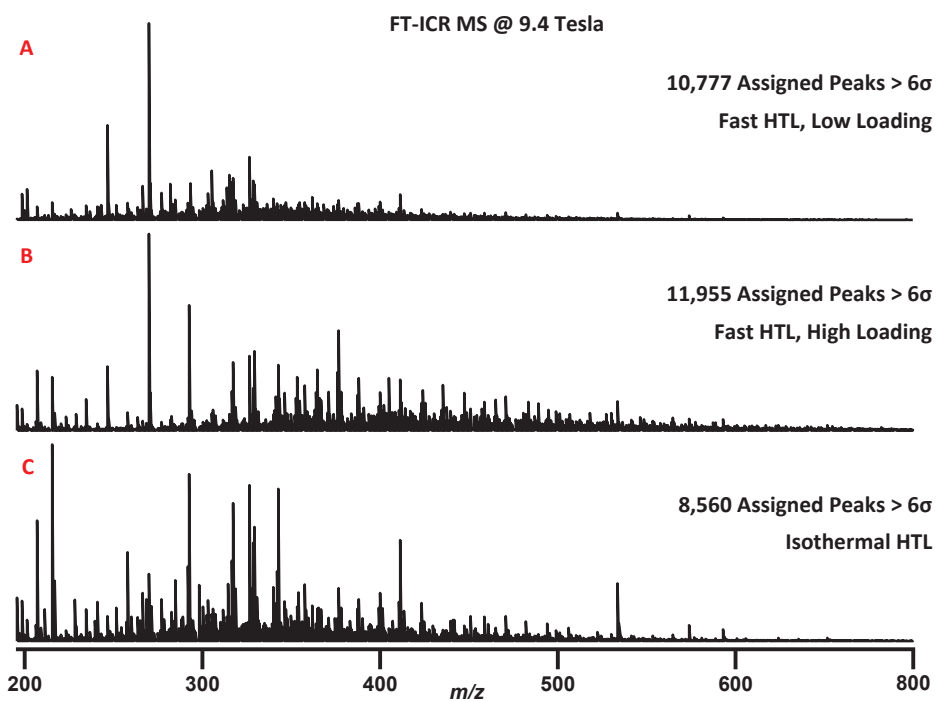


Figure S3: Negative ESI FT-ISR MS Broadband Spectra of Aqueous Phase Samples for HTL at Different Conditions

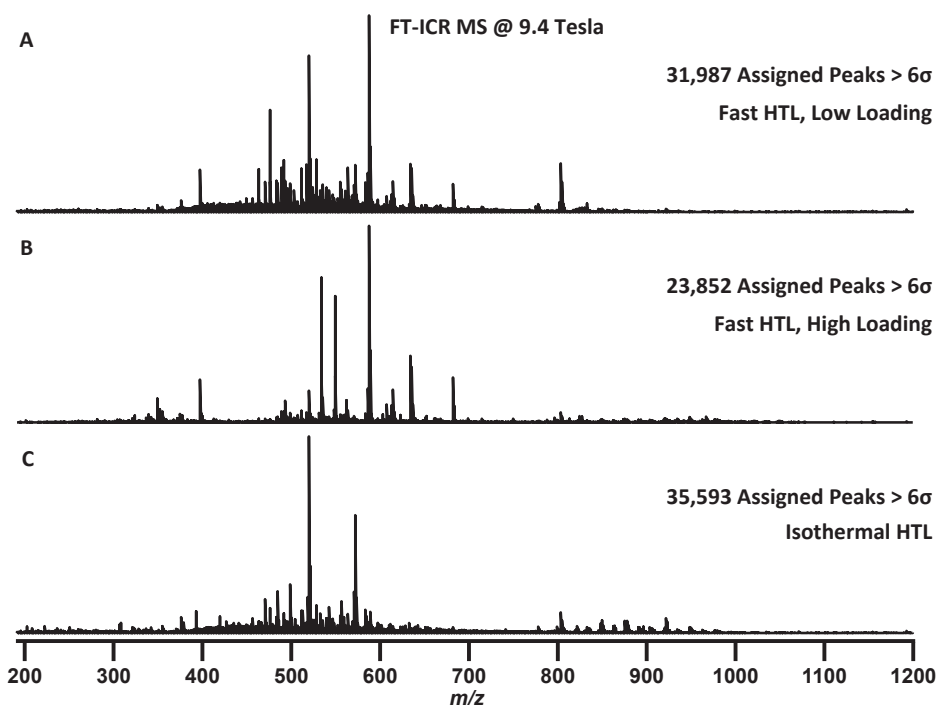


Figure S4: Positive ESI FT-ISR MS Broadband Spectra of Biocrude Samples for HTL at Different Conditions

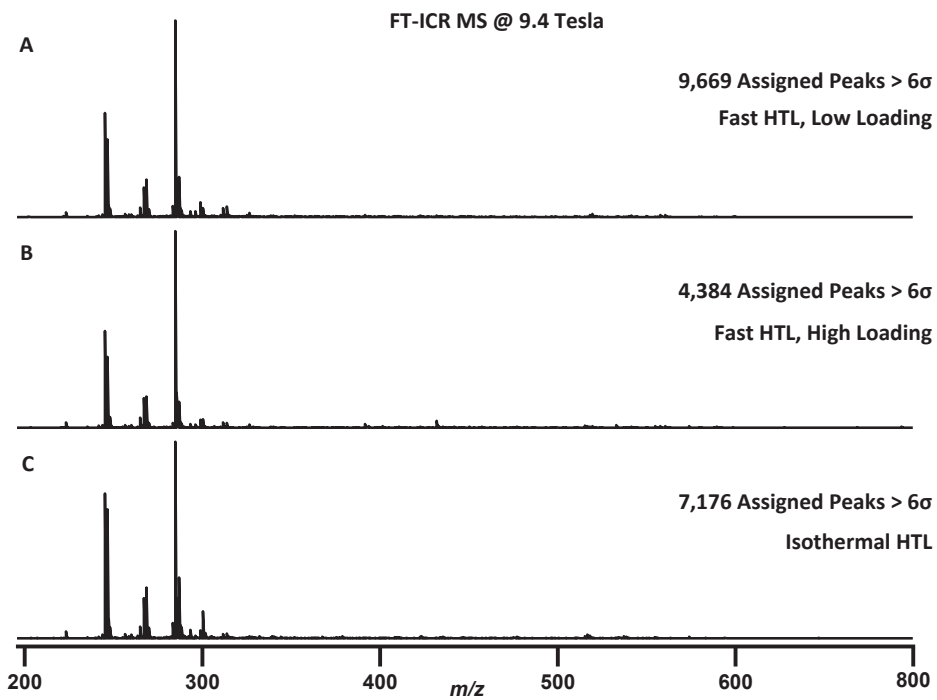


Figure S5: Negative ESI FT-ICR MS Broadband Spectra of Biocrude Samples for HTL at Different Conditions

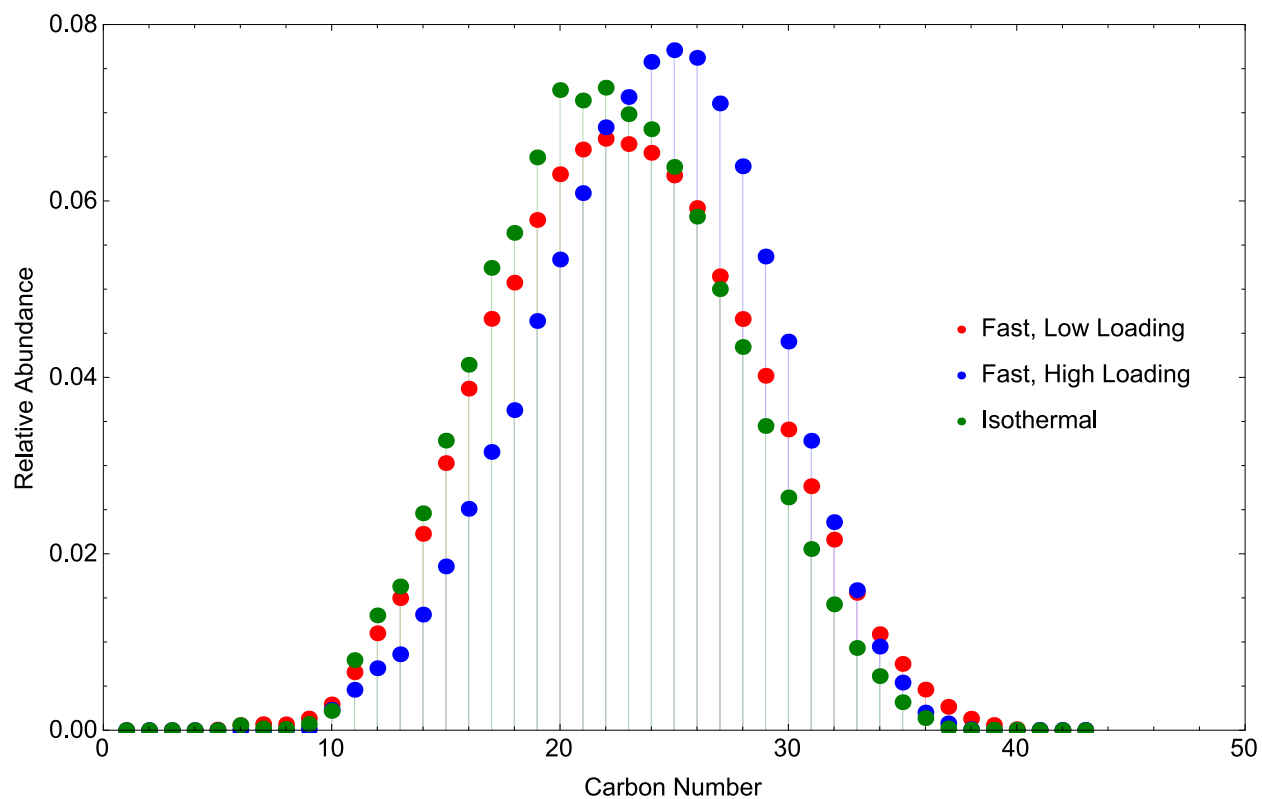


Figure S6: Carbon Number Distributions for Positive ESI Analysis of Aqueous Phase Samples

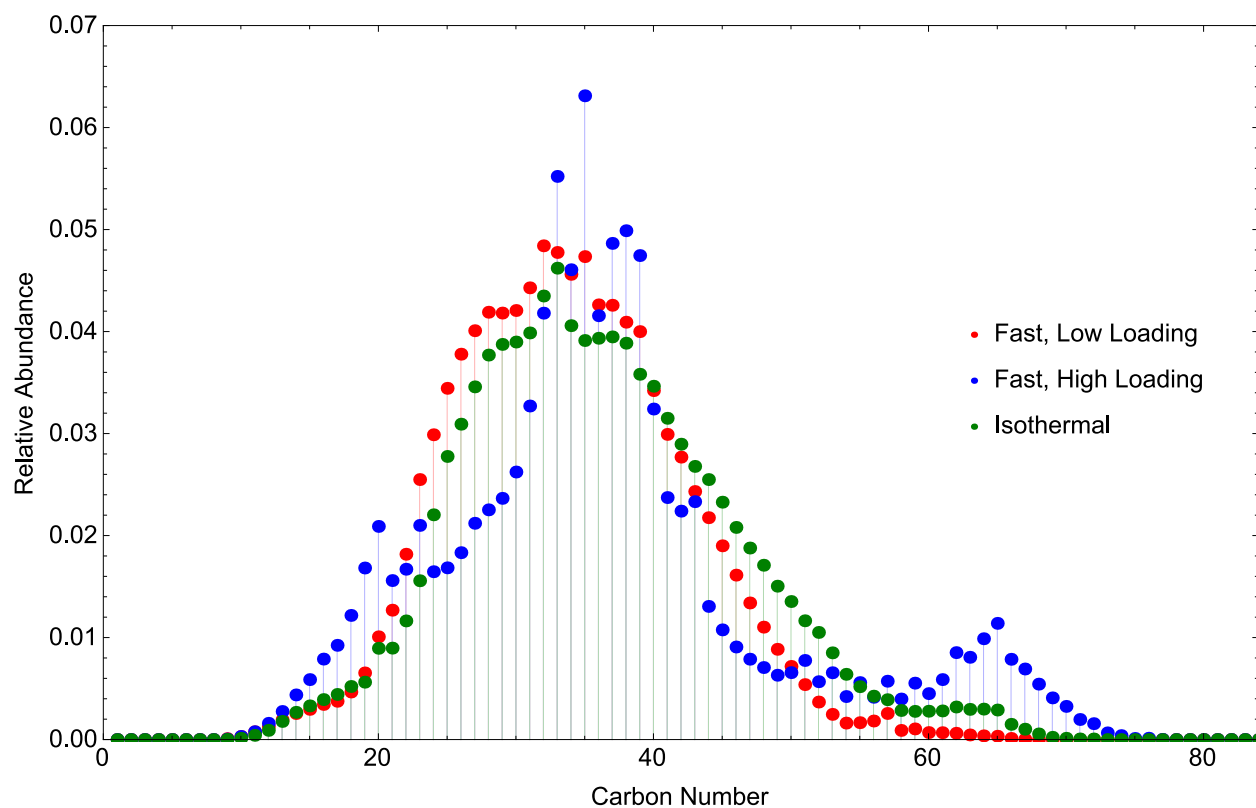


Figure S7: Carbon Number Distributions for Positive ESI Analysis of Biocrude Samples

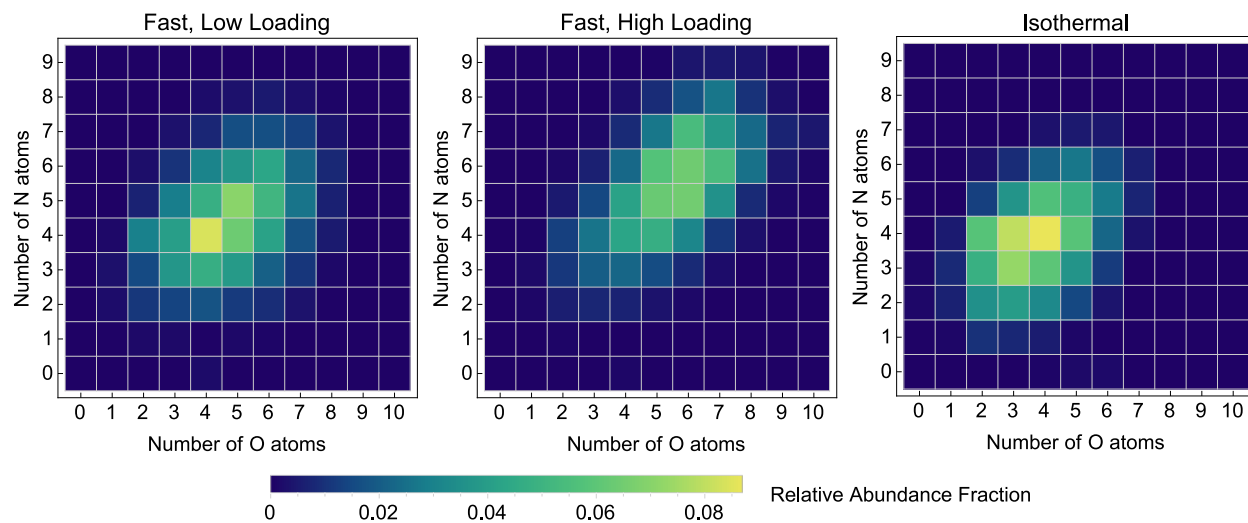


Figure S8: Heteroatom Density Graph for Positive ESI Analysis of Aqueous Phase Samples

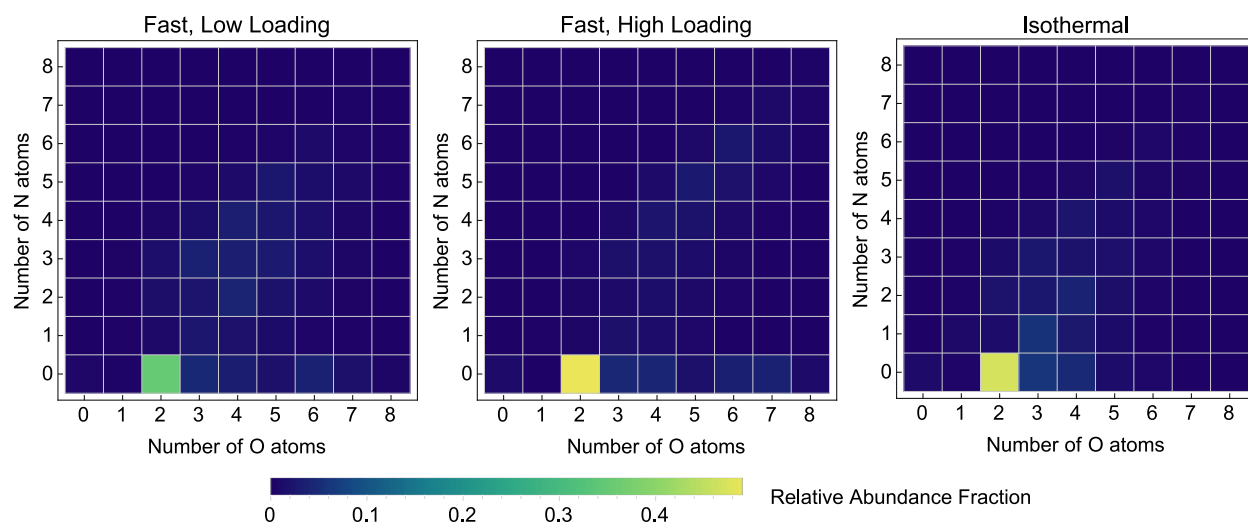


Figure S9: Heteroatom Density Graph for Negative ESI Analysis of Biocrude Samples

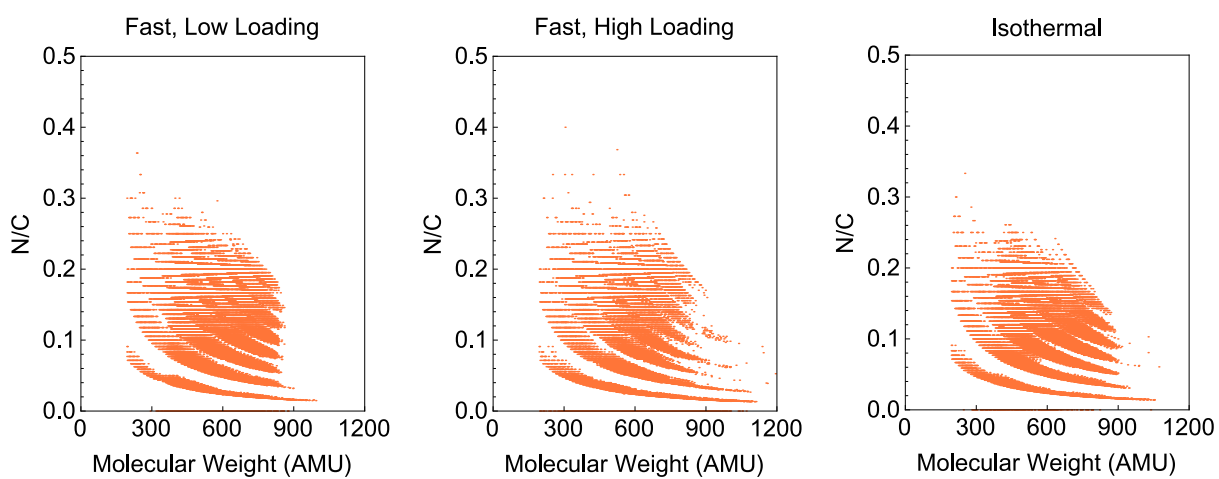
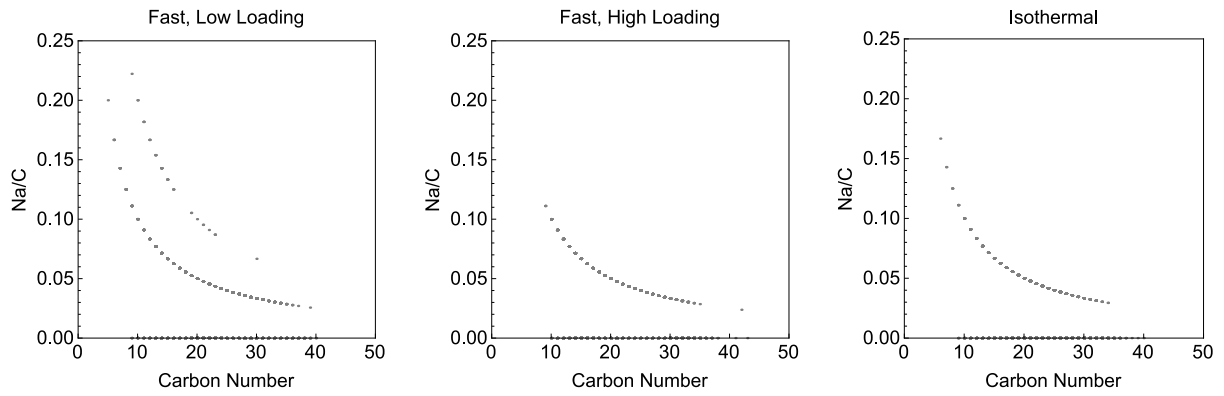
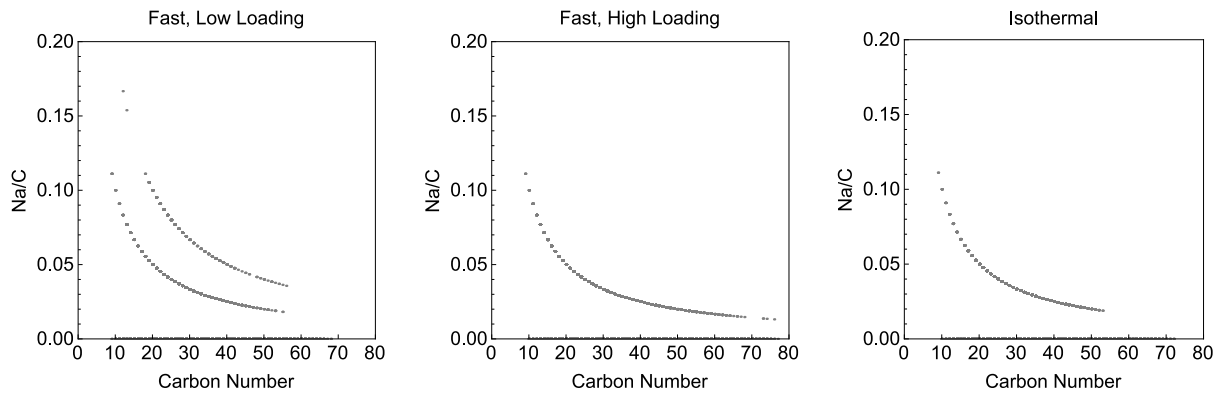


Figure S10: N:C Ratios vs. Average Molecular Weight for Positive ESI Analysis of Biocrude Samples



(a) Aqueous Phase (Positive ESI)



(b) Biocrude (Positive ESI)

Figure S11: Na:C Ratios vs. Carbon Number for Samples Analyzed Using Positive ESI Analysis

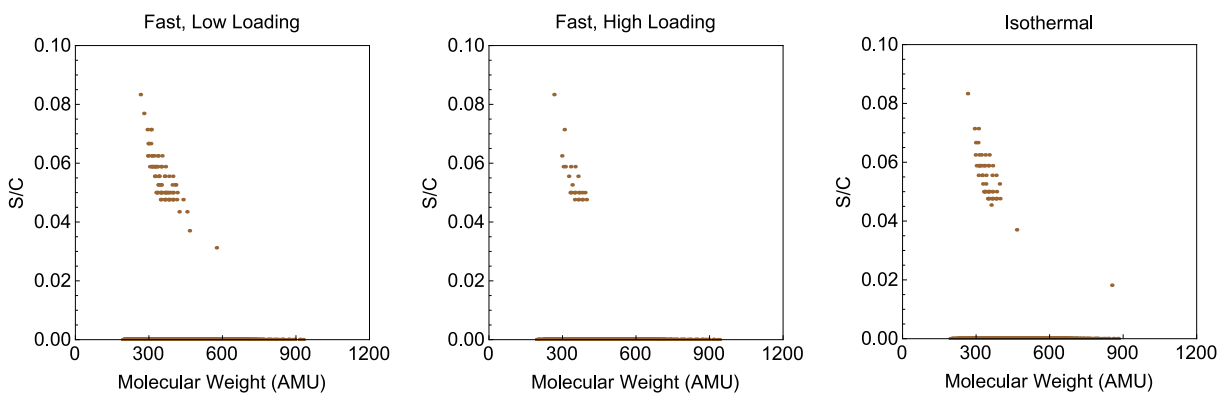


Figure S12: S:C Ratios vs. Average Molecular Weight for Biocrude Samples (Negative ESI)