Supporting Information

Systematic Study of Ionic Liquids-Based Coal Extraction: Selectivity in Extract

Molecular Weights and Targeted Functional Groups

Shuai Tan^a, Mitchell Ross Helling^b, Franco Basile^b, and Katie Dongmei Li-Oakey^{a*}

^a Department of Chemical Engineering, University of Wyoming, 1000 E, University Ave, Laramie,

Wyoming 82072, United States

^b Department of Chemistry, University of Wyoming, 1000 E, University Ave, Laramie, Wyoming 82072, United States



Figure S1. Extracted ion chromatograms (XIC) for the ions at m/z 192 (methylphenanthrene) for NIST-2684 coal extracts derived from different ILs. Red circles: the searched compounds with good NIST library matches.



Figure S2. Extracted ion chromatograms (XIC) for the ions at m/z 206 (phenanthrene with two additional carbons) for NIST-2684 coal extracts derived from different ILs. Red circles: the searched compounds with good NIST library matches.



Figure S3. Extracted ion chromatograms (XIC) for the ions at m/z 220 (phenanthrene with three additional carbons) for NIST-2684 coal extracts derived from different ILs. Red circles: the searched compounds with good NIST library matches.



Figure S4. Extracted ion chromatograms (XIC) for the ions at m/z 234 (phenanthrene with four additional carbons) for NIST-2684 coal extracts derived from different ILs. Red circles: the searched compounds with good NIST library matches.



Figure S5. Extracted ion chromatograms (XIC) for the ions at m/z 228 (4 ring PAHs) for NIST-2684 coal extracts derived from different ILs. Red circles: the searched compounds with good NIST library matches.



Figure S6. Extracted ion chromatograms (XIC) for the ions at m/z 242 (methylated 4 ring PAHs) for NIST-2684 coal extracts derived from different ILs. Red circles: the searched compounds with good NIST library matches.



Figure S7. Extracted ion chromatograms (XIC) for the ions at m/z 57 (alkanes) for NIST-2684 coal extracts derived from different ILs.



Figure S8. Extracted ion chromatograms (XIC) for the ions at m/z 117 (C₂₀+ FFAs) for NIST-2682 coal extracts derived from different ILs.



Figure S9. Extracted ion chromatograms (XIC) for the ions at m/z 234 (retene) for NIST-2682 coal extracts derived from different ILs.



Figure S10. Extracted ion chromatograms (XIC) for the ions at m/z 123 (bicyclic diterpanes) for NIST-2682 coal extracts derived from different ILs.



Figure S11. Extracted ion chromatograms (XIC) for the ions at m/z 123 (tricyclic diterpanes) for NIST-2682 coal extracts derived from different ILs. Red circles: the searched compounds with good NIST library matches.