Characterization of a Chinese lignite and the corresponding derivates using direct analysis in real time quadrupole time-of-flight mass spectrometry

Xing Fan,*[ab] Chu-Fan Wang,[a] Chun-Yan You,[a] Xian-Yong Wei,[a] Lu Chen,[a] Jing-Pei Cao,[a] Yun-Peng Zhao,[a] Wei Zhao,[a] Yu-Gao Wang,*[c] Jin-Li Lu[d]

[a]*Key Laboratory of Coal Processing and Efficient Utilization, Ministry of Education, China University of Mining & Technology, Xuzhou, Jiangsu 221116, China*

[b]*Key Laboratory for Mass Spectrometry and Instrumentation, East China Institute of Technology, Nanchang, Jiangxi 330013, China*

[c]*College of Chemistry and Chemical Engineering, Taiyuan University of Technology, Taiyuan 030024, Shanxi, China*

[d]*News Center of CUMT, China University of Mining & Technology, Jiangsu 221116, China*

* Corresponding author Xing Fan at: School of Chemical Engineering and Technology, China University of Mining & Technology, Xuzhou, Jiangsu 221116, China. Tel.: +86-516-83885951; E-mail: fanxing@cumt.edu.cn; Yu-Gao Wang at: College of Chemistry and Chemical Engineering, Taiyuan University of Technology, Taiyuan, Shanxi 030024, China. +86-13653602168; E-mail: wyg_cumt@163.com

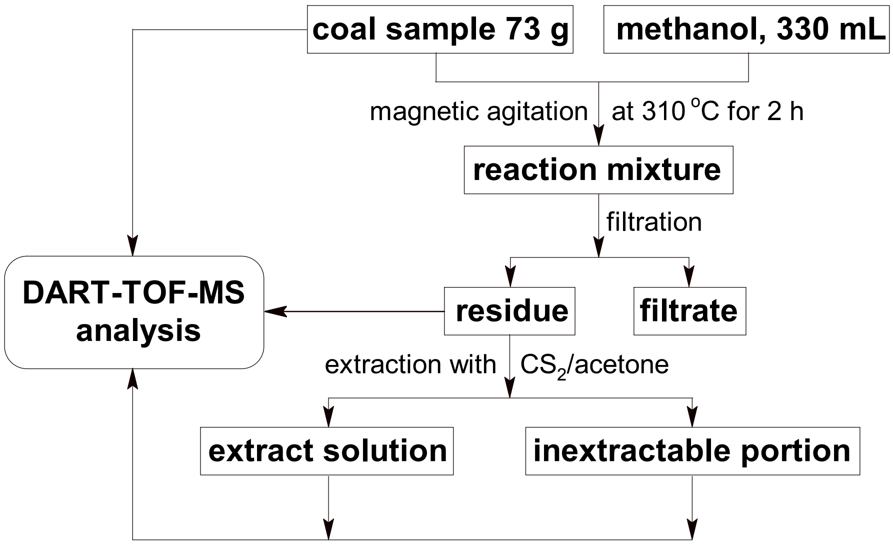

Figure S1 The experimental procedure

Table S1 Fragments of the precursor ion at m/z 680.48

Measure m/z	Ion species	Calculated m/z	Calculated molecular weight (u)	Formula	Mass error (ppm)
383.13769	$(M+H)^+$	383.13902	382.13174	$C_{24}H_{18}N_2O_3$	2.48
439.20074	$(M+H)^+$	439.20162	438.19434	$C_{28}H_{26}N_2O_3$	2.05
495.26534	$(M+H)^+$	495.26422	494.25806	$C_{32}H_{34}N_2O_3$	-2.27
551.32649	$(M+H)^+$	551.32682	550.31921	$C_{36}H_{42}N_2O_3$	0.6
607.39011	$(M+H)^+$	607.38942	606.38214	$C_{40}H_{50}N_2O_3$	-1.14
663.45352	$(M+H)^+$	663.45202	662.44474	$C_{44}H_{58}N_2O_3$	-2.26
680.48000	$(M+NH_4)^+$	680.47857	678.44474	$C_{44}H_{58}N_2O_3$	-2.16