Electronic Supplementary Information

White fluorescence of polyaromatics derived from methanol conversion in Ca^{2+}-exchanged small-pore zeolites

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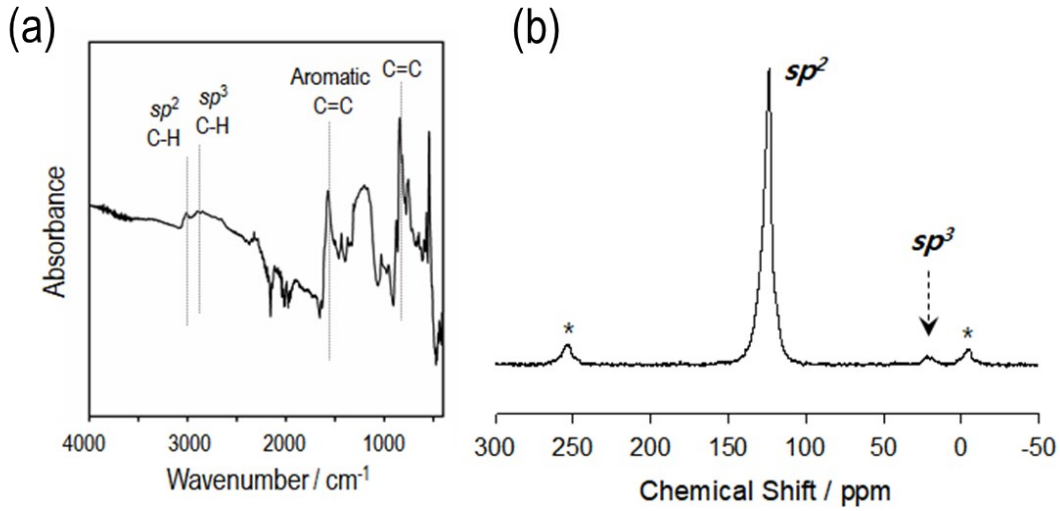

Fig. S1. Characterizations of the product from methanol conversion in Ca-LTA zeolite. (a) ATR-FTIR spectrum displays the presence of sp^3 C-H, sp^2 C-H and sp^2 C=C. (b) ^{13}C CP/MAS NMR spectrum exhibits a peak covering from 120 to 140 ppm, corresponding to sp^2-carbon and an additional sp^3-carbon peak at 19 ppm. The spectrum was acquired at spinning rate of 13 kHz, and asterisks indicate spinning side bands.

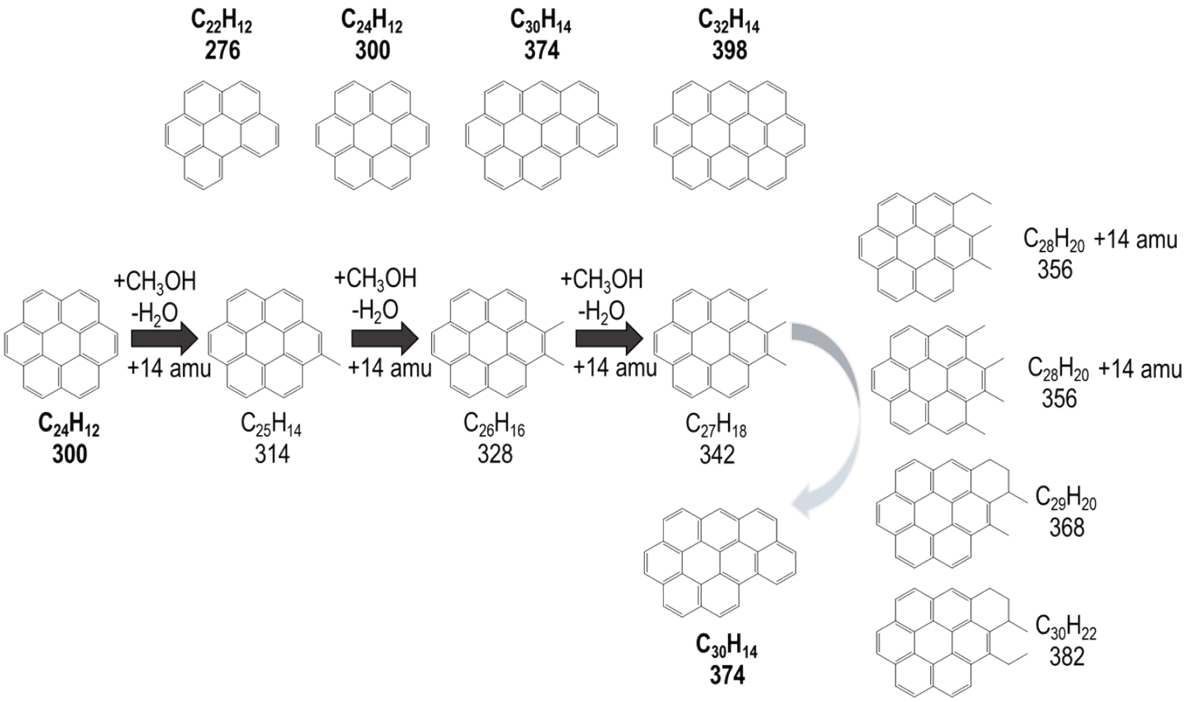

Fig. S2. Examples of PAH candidate with an atomic composition corresponding to the mass peaks (upper) and an example of PAH growth during the methanol conversion (down). As a result, the mass spectrum displayed 14 mass intervals between the products: 14 (Δ mass) = [addition of a methanol molecule (mass = 32)]– [loss of a water molecule (mass = 18)].

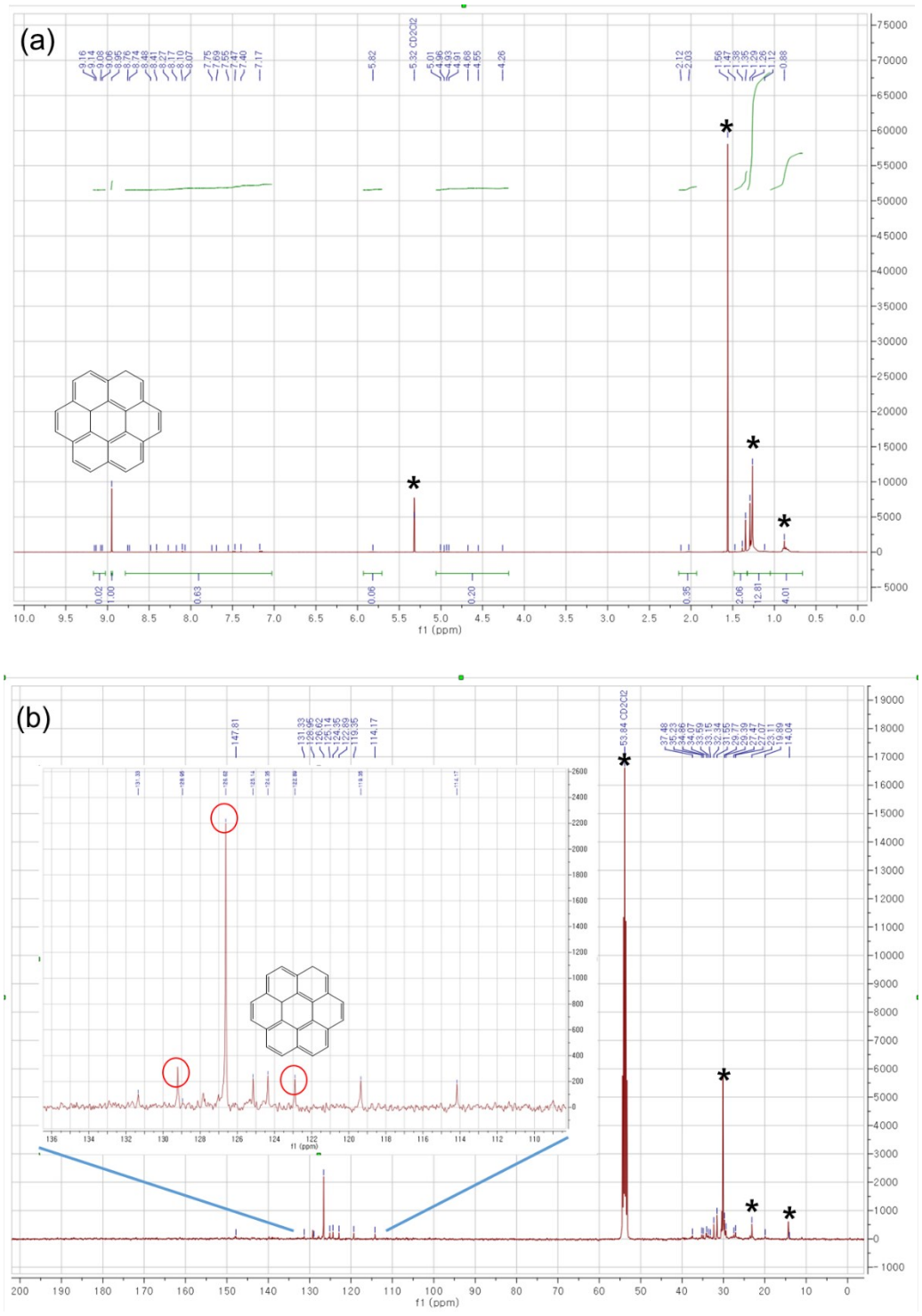

Fig. S3. (a) ^{1}H and (b) ^{13}C solution-state NMR spectra of the blue-emitting component. Asterisks represent peaks from the deuterated solvent.

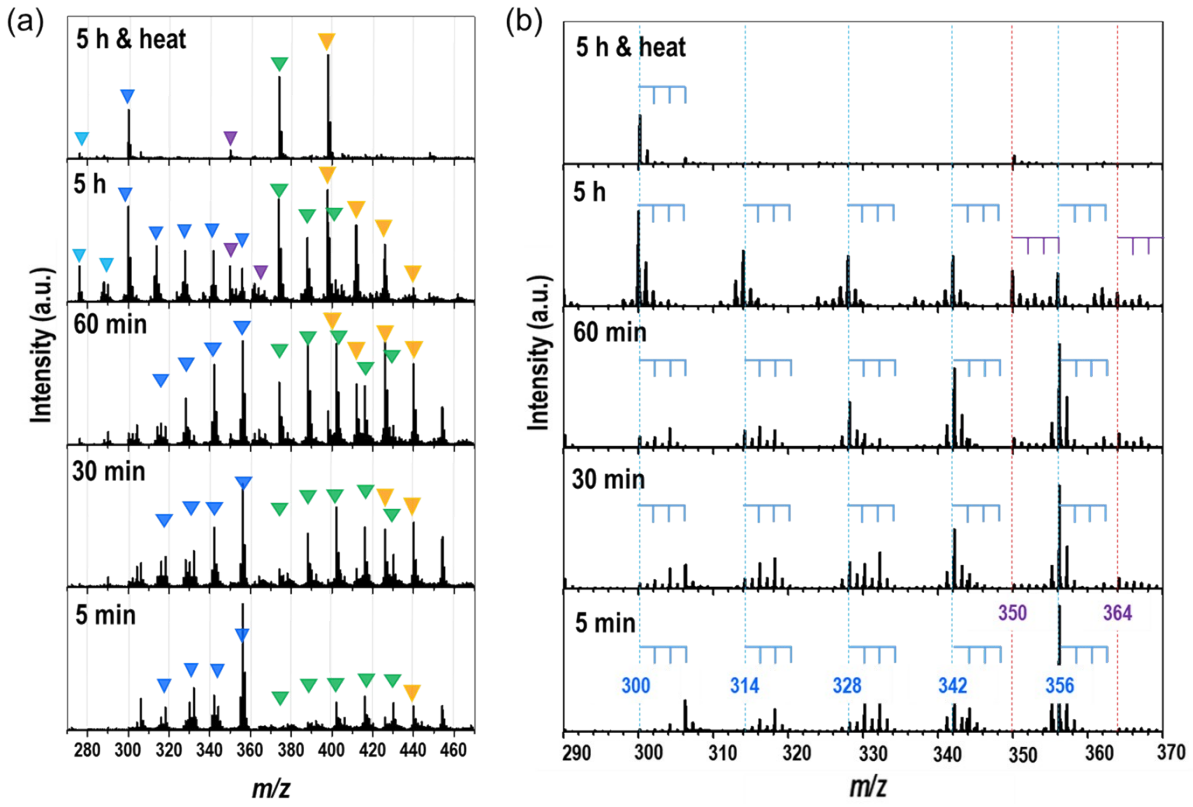

Fig. S4. (a) Mass spectra of the products collected at certain time over the reaction course and (b) the expanded view of the mass spectra for the selected peak regions. The colored triangles and vertical lines serve as a guide for the eye to highlight the observed trend.

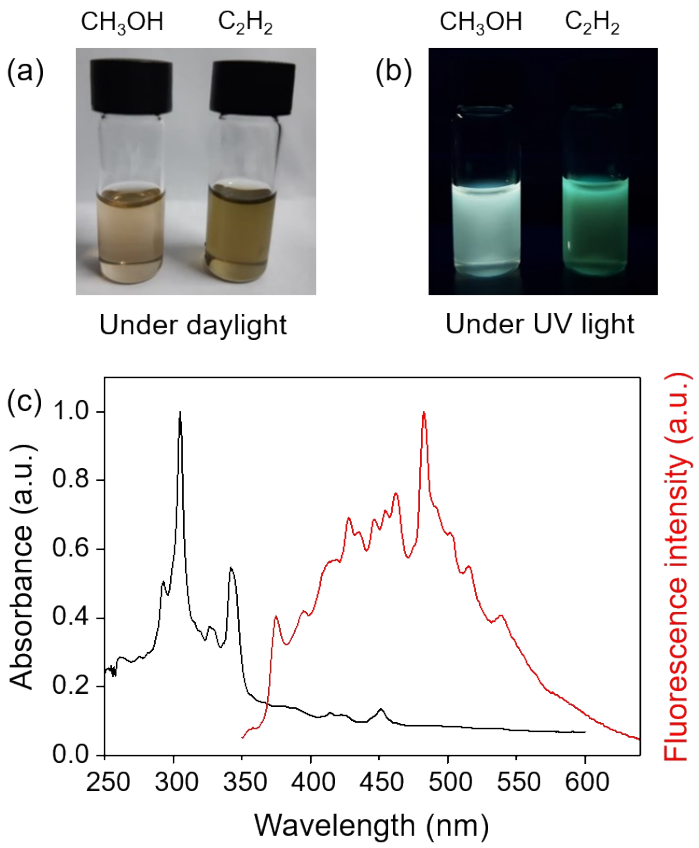

Fig. S5. Photographs of the NMP solutions containing methanol- and acetylene-derived products, which are illuminated under (a) daylight and (b) UV light (λ = 365 nm). (c) Absorption and fluorescence spectra of the acetylene-derived product dissolved in NMP (see Fig. 1 for the white fluorescence of the methanol-derived product).

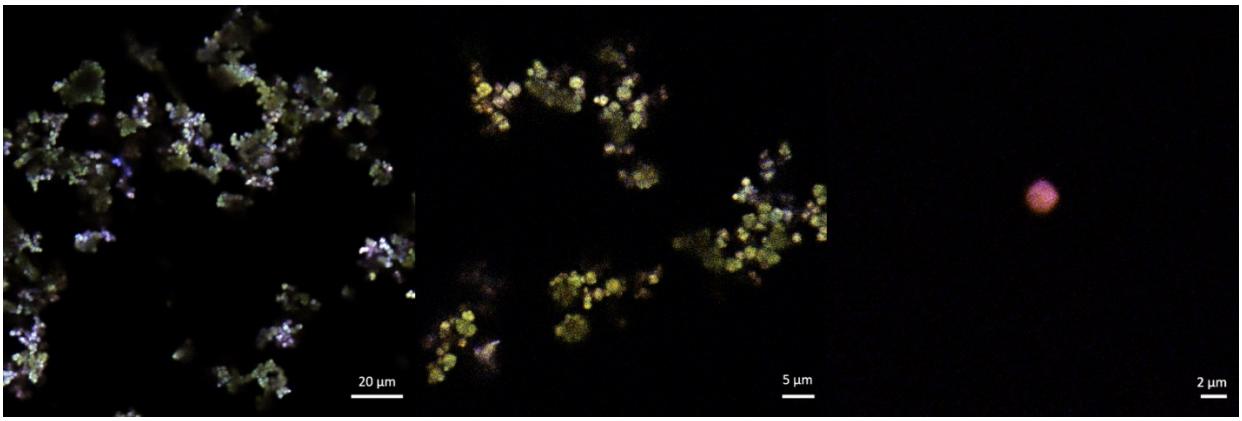

Fig. S6. Additional confocal images of methanol-derived PAH/zeolite composite sample taken at different magnifications. These images are the merged images measured under three distinct excitation light wavelengths (λ = 405, 488, and 555 nm).

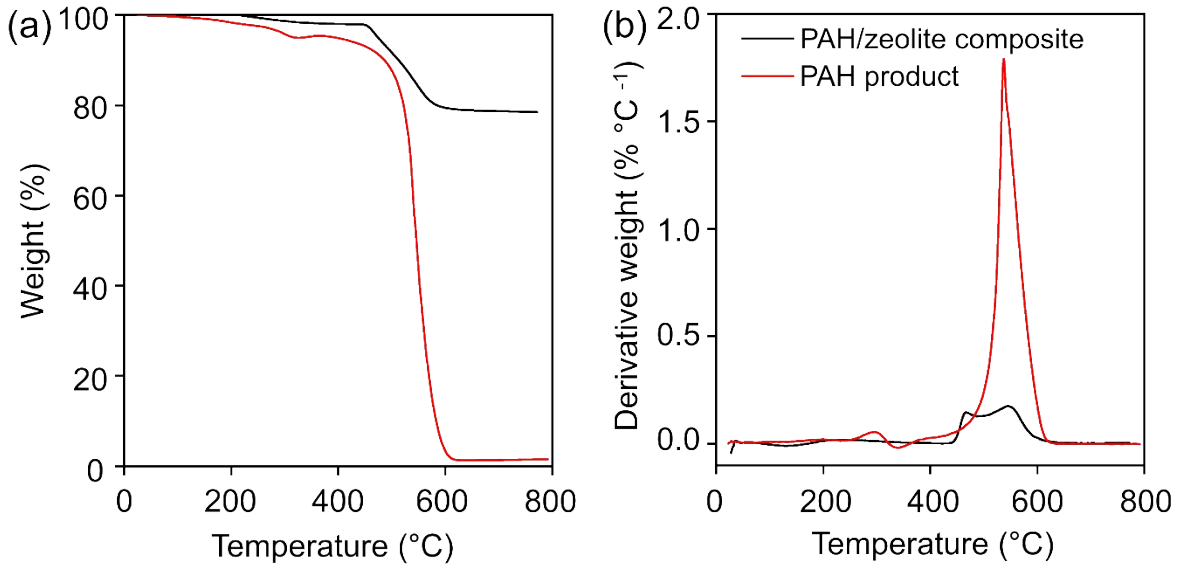

Fig. S7. (a) TGA profiles of methanol-derived PAH/zeolite composite sample and PAH itself. (b) The corresponding DTG curves show characteristic decomposition temperatures of the organics in a N_2/air mixture.

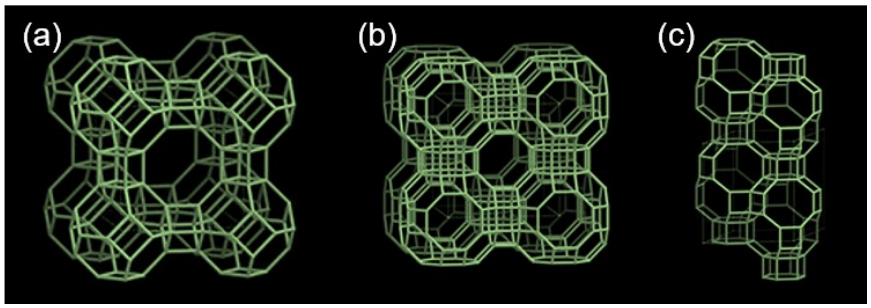

Fig. S8. Framework model for (a) LTA, (b) RHO, and (c) CHA zeolites. Each of the zeolite framework types was viewed along (a) [100], (b) [001], and (c) [001] zone axes. These model images were taken from the database of zeolite structures of the International Zeolite Association (see the website, http://www.iza-structure.org/databases/).

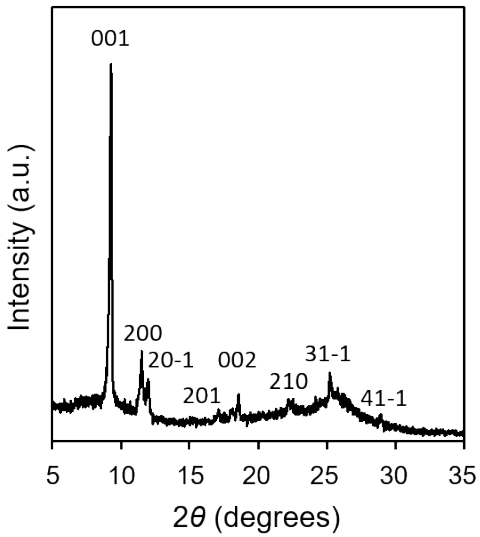

Fig. S9. XRD pattern of the PAH product from using methanol and RHO zeolite, after a recrystallization process using dichloromethane as a solvent. Miller indices of coronene structure are shown as a set of three integers in the XRD pattern, indicating the structure of the recrystallized product is identical to that of coronene.

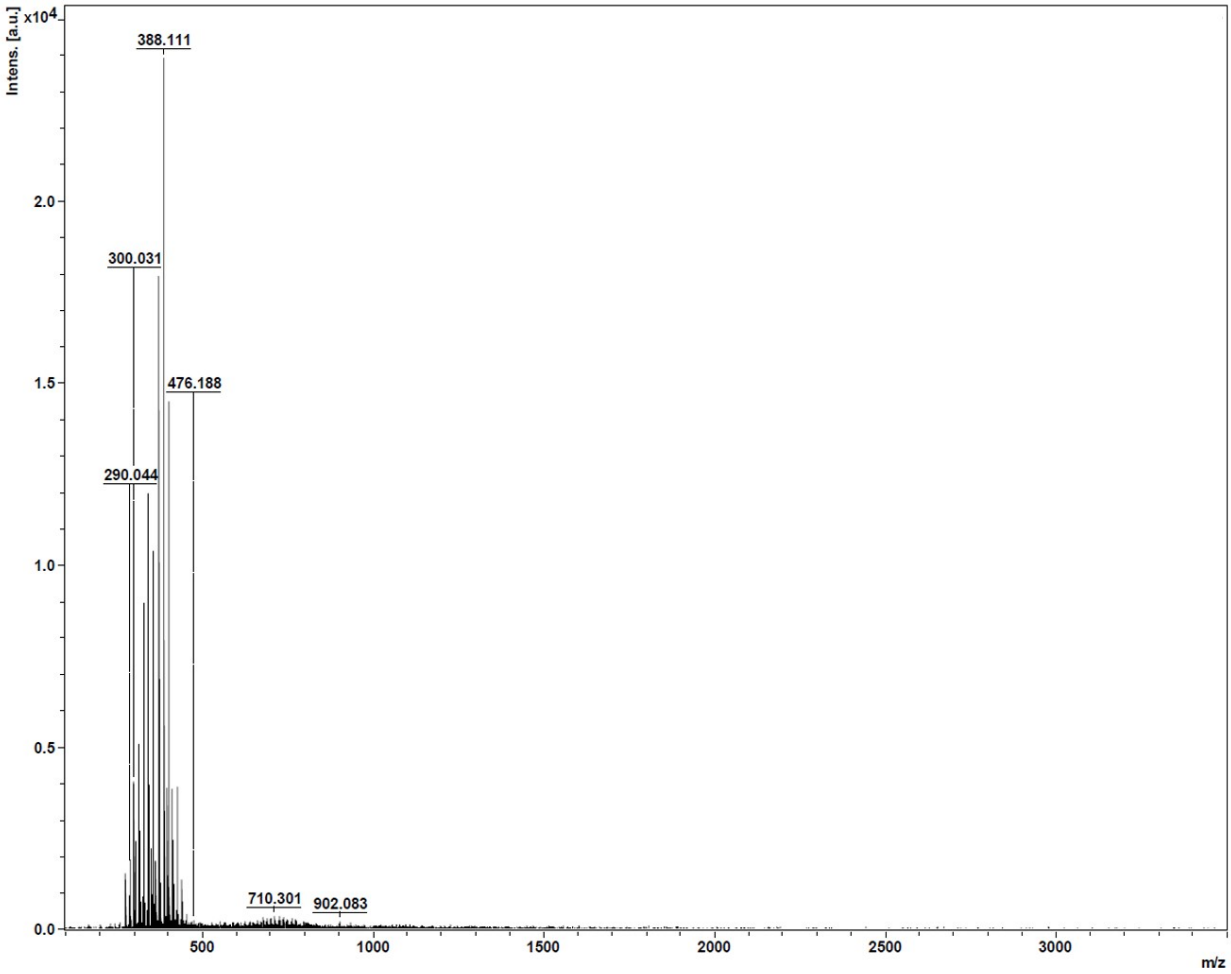

Fig. S10. Full-range LDI-TOF MS mass spectrum of the product obtained from methanol conversion in Ca-LTA zeolite (see Fig. 2 for the enlarged spectrum).

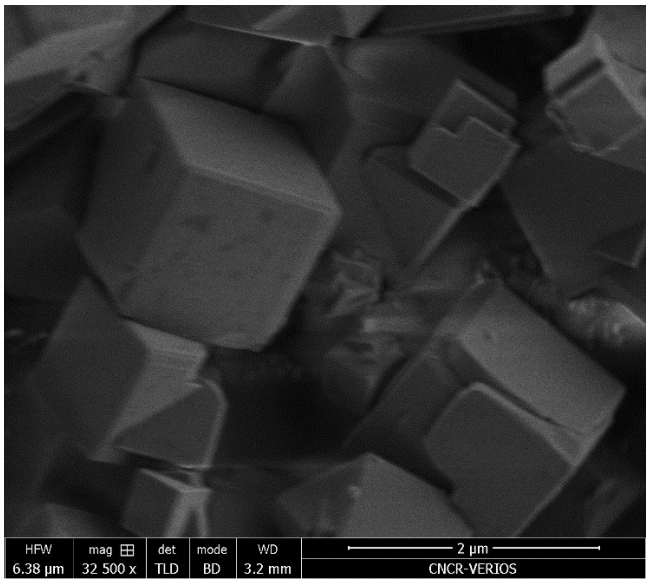

Fig. S11. Scanning electron microscope image of the PAH/zeolite composite sample obtained from methanol conversion.