Porous Metal-Organic Frameworks Based on 3,6-bis(4-benzoic acid)-N-(4-benzoic acid)carbazole for HPLC Separation of Small Organic Molecules

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Table S1. Selected bond lengths (Å) and angles (deg) for YCZ-1

YCZ-1			
Cu(1)-O(6)	1.954(2)	Cu(3)-O(2)#6	1.946(3)
Cu(1)-O(6)#1	1.954(2)	Cu(3)-O(2)#7	1.946(3)
Cu(1)-O(6)#2	1.954(2)	Cu(3)-N(4)	2.175(5)
Cu(1)-O(6)#3	1.954(2)	Cu(3)-Cu(4)	2.6326(10)
Cu(1)-N(2)	2.158(5)	Cu(4)-O(1)#5	1.981(3)
Cu(1)-Cu(2)	2.6314(10)	Cu(4)-O(1)	1.982(3)
Cu(2)-O(5)	1.965(3)	Cu(4)-O(4)#6	2.000(3)
Cu(2)-O(5)#2	1.966(3)	Cu(4)-O(4)#7	2.000(3)
Cu(2)-O(5)#1	1.966(3)	Cu(4)-N(5)	2.181(7)
Cu(2)-O(5)#3	1.966(3)	Cu(4)-O(1)	1.982(3)
Cu(2)-N(3)#4	2.144(6)	Cu(4)-O(4)#6	2.000(3)
Cu(3)-O(3)	1.929(3)	Cu(4)-O(4)#7	2.000(3)
Cu(3)-O(3)#5	1.929(3)	Cu(4)-N(5)	2.181(7)
O(6)-Cu(1)-O(6)#1	90.59(15)	O(3)-Cu(3)-O(3)#5	90.3(2)
O(6)-Cu(1)-O(6)#2	88.19(14)	O(3)-Cu(3)-O(2)#6	88.82(18)
O(6)#1-Cu(1)-O(6)#2	168.15(15)	O(3)#5-Cu(3)-O(2)#6	169.82(16)
O(6)-Cu(1)-O(6)#3	168.14(15)	O(3)-Cu(3)-O(2)#7	169.82(16)
O(6)#1-Cu(1)-O(6)#3	88.19(14)	O(3)#5-Cu(3)-O(2)#7	88.82(18)
O(6)#2-Cu(1)-O(6)#3	90.59(15)	O(2)#6-Cu(3)-O(2)#7	90.2(2)
O(6)-Cu(1)-N(2)	95.93(7)	O(3)-Cu(3)-N(4)	95.69(15)
O(6)#1-Cu(1)-N(2)	95.93(7)	O(3)#5-Cu(3)-N(4)	95.68(15)
O(6)#2-Cu(1)-N(2)	95.93(7)	O(2)#6-Cu(3)-N(4)	94.49(14)
O(6)#3-Cu(1)-N(2)	95.93(7)	O(2)#7-Cu(3)-N(4)	94.49(14)
O(6)-Cu(1)-Cu(2)	84.07(7)	O(3)-Cu(3)-Cu(4)	85.73(11)
O(6)#1-Cu(1)-Cu(2)	84.07(7)	O(3)#5-Cu(3)-Cu(4)	85.73(11)
O(6)#2-Cu(1)-Cu(2)	84.07(7)	O(2)#6-Cu(3)-Cu(4)	84.09(9)
O(6)#3-Cu(1)-Cu(2)	84.07(7)	O(2)#7-Cu(3)-Cu(4)	84.09(9)
N(2)-Cu(1)-Cu(2)	180	N(4)-Cu(3)-Cu(4)	177.98(14)

O(5)-Cu(2)-O(5)#2	88.05(16)	O(1)#5-Cu(4)-O(1)	91.4(2)
O(5)-Cu(2)-O(5)#1	90.65(16)	O(1)#5-Cu(4)-O(4)#6	165.56(15)
O(5)#2-Cu(2)-O(5)#1	167.81(16)	O(1)-Cu(4)-O(4)#6	88.47(17)
O(5)-Cu(2)-O(5)#3	167.81(16)	O(1)#5-Cu(4)-O(4)#7	88.47(17)
O(5)#2-Cu(2)-O(5)#3	90.65(16)	O(1)-Cu(4)-O(4)#7	165.56(15)
O(5)#1-Cu(2)-O(5)#3	88.06(16)	O(4)#6-Cu(4)-O(4)#7	88.1(2)
O(5)-Cu(2)-N(3)#4	96.09(8)	O(1)#5-Cu(4)-N(5)	96.3(2)
O(5)#2-Cu(2)-N(3)#4	96.10(8)	O(1)-Cu(4)-N(5)	96.3(2)
O(5)#1-Cu(2)-N(3)#4	96.10(8)	O(4)#6-Cu(4)-N(5)	98.0(2)
O(5)#3-Cu(2)-N(3)#4	96.10(8)	O(4)#7-Cu(4)-N(5)	98.0(2)
O(5)-Cu(2)-Cu(1)	83.91(8)	O(1)#5-Cu(4)-Cu(3)	82.68(11)
O(5)#2-Cu(2)-Cu(1)	83.90(8)	O(1)-Cu(4)-Cu(3)	82.68(11)
O(5)#1-Cu(2)-Cu(1)	83.90(8)	O(4)#6-Cu(4)-Cu(3)	82.98(9)
O(5)#3-Cu(2)-Cu(1)	83.90(8)	O(4)#7-Cu(4)-Cu(3)	82.98(9)
N(3)#4-Cu(2)-Cu(1)	180	N(5)-Cu(4)-Cu(3)	178.6(3)

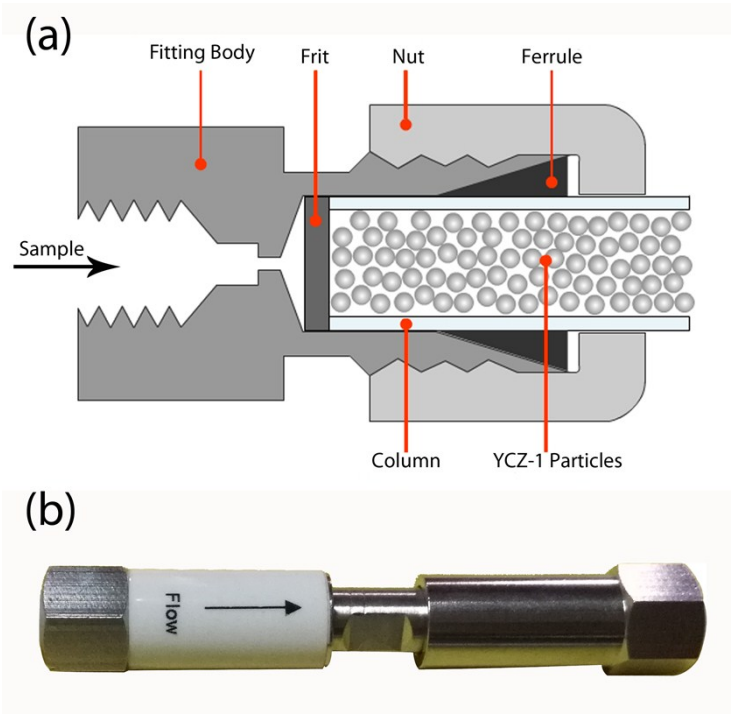

Fig. S1 (a) Internal structure of the YCZ-1 packed column; (b) Photograph of the YCZ-1 packed column.

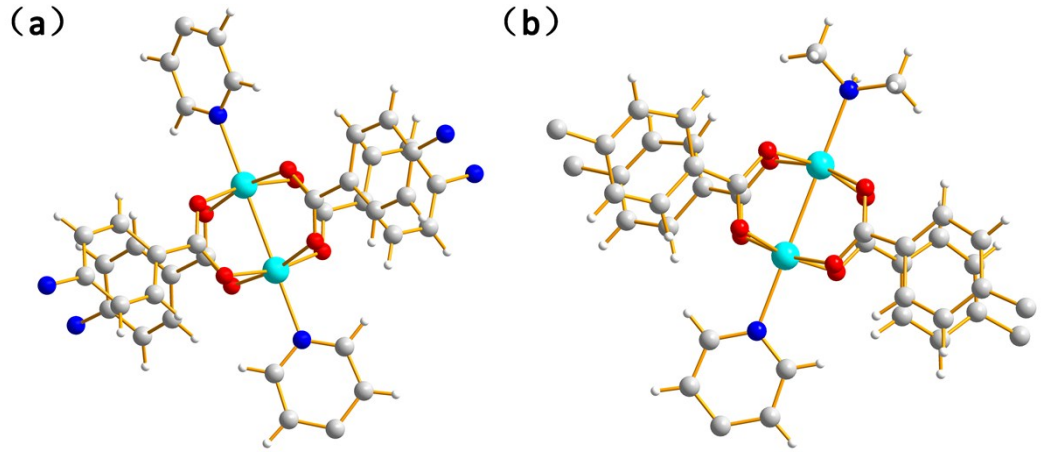

Fig. S2 (a) View of **Cu-pdw-1**; (b) View of **Cu-pdw-2**.

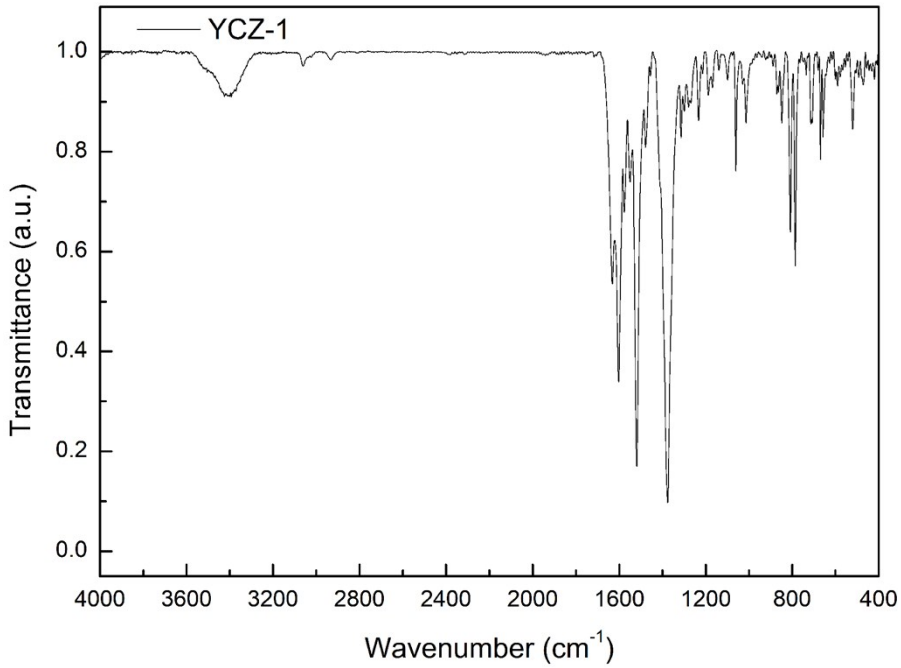

Fig. S3. Infrared spectra after baseline normalization for YCZ-1.

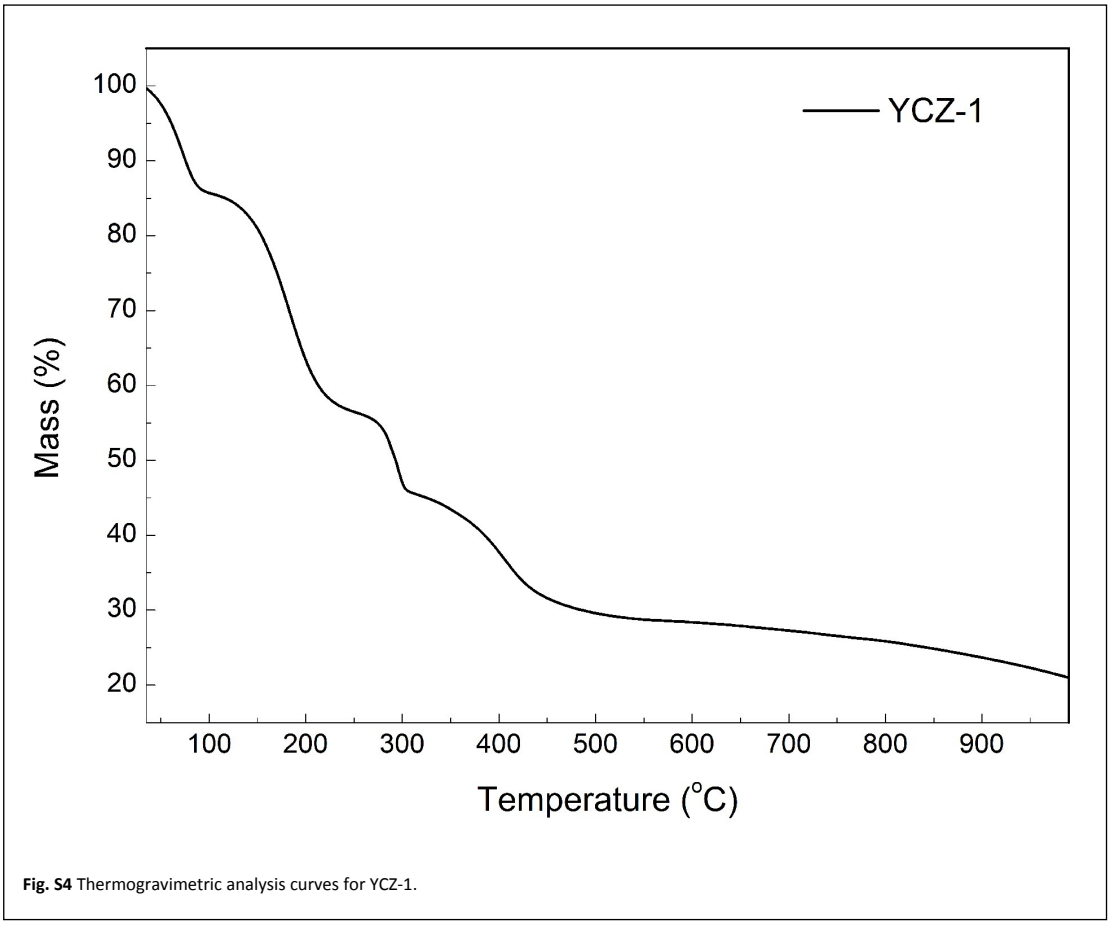

Fig. S4 Thermogravimetric analysis curves for YCZ-1.

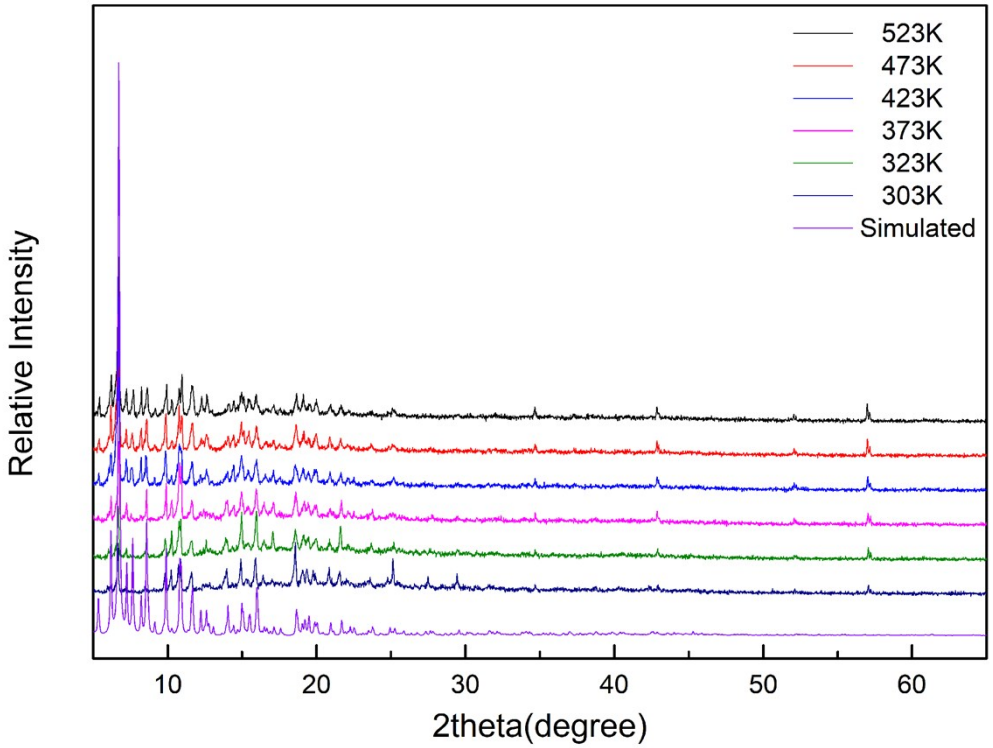

Fig. S5 Simulated (purple), experimental powder X-ray diffraction (PXRD) patterns for YCZ-1 at 303K(dark blue), 323K(green), 373K(pink), 423K(blue), 473K(red) and 523K(black).

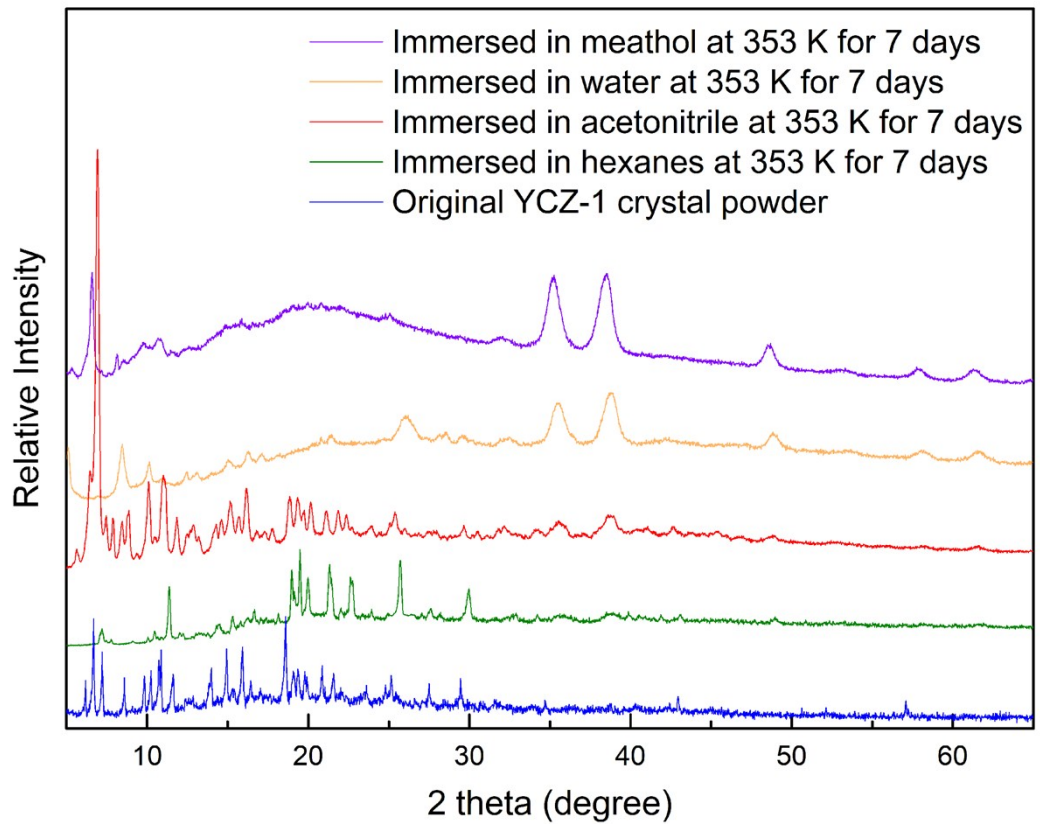

Fig. S6 X-ray diffraction (PXRD) patterns of original YCZ-1 powder and the powder immersed in hexanes (green), acetonitrile (red), water (orange) and meathol (purple) at 353 K for 7 days.

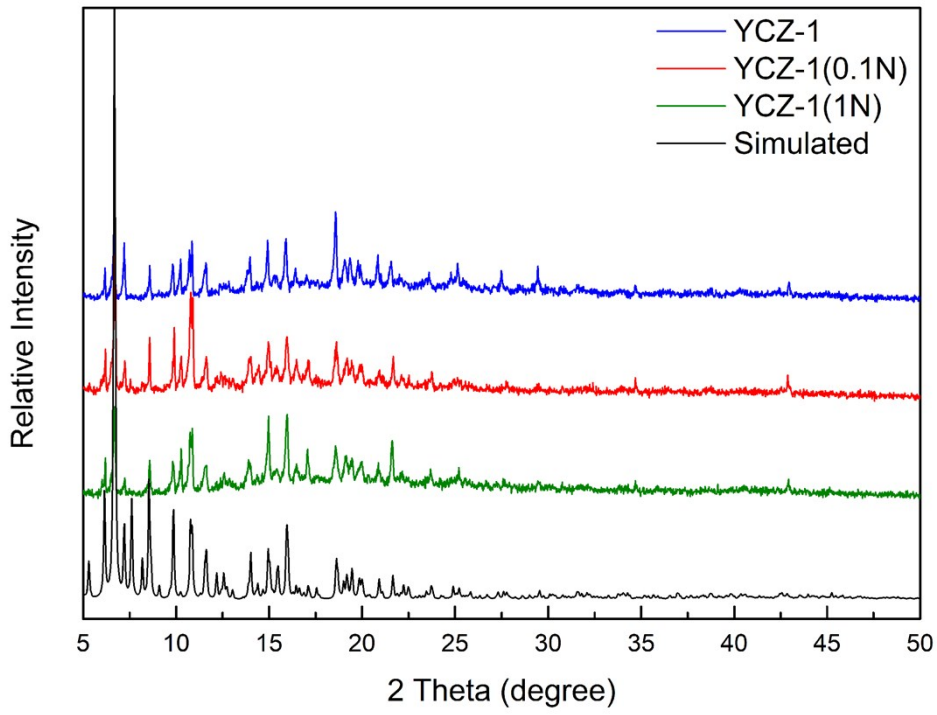

Fig. S7 Simulated (black), experimental powder X-ray diffraction (PXRD) patterns for YCZ-1 (blue), YCZ-1(0.1N) (red) and YCZ-1(1N) (green)

Equation S1. Resolution *R* was calculated based on the following equation:

$$R = 1.18 \times \frac{t_{R2} - t_{R1}}{w_2 - w_1}$$

where *R*: resolution between compounds 1 and 2 separated by the material

t_{R1}, t_{R2}: retention time of compounds 1 and 2

w_1, w_2: full width at haft maximum of peak 1 and 2.

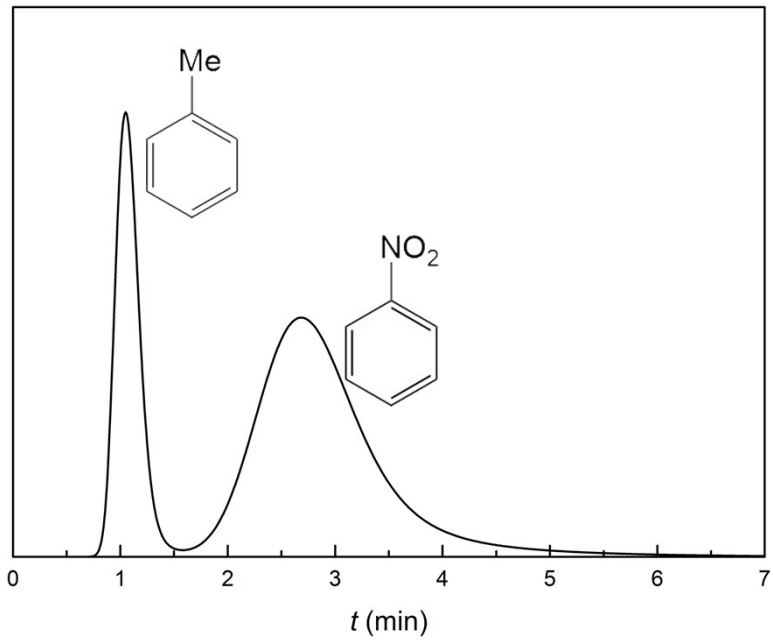

Fig. S8 Liquid-phase separation of a mixture of toluene and nitrobenzene on the YCZ-1 packed column with hexanes/methanol (98:2) as the eluent at a flow rate 0.5mL/min.

In order to measuring the separated ability of **YCZ-1** as stationary phases for HPLC, a series of small molecules was selected and put to the test at first. Nitrobenzene and toluene, both of them in the region of the pore size in **YCZ-1**, are selected to test **YCZ-1** packed column. A mixture of nitrobenzene and toluene was passed through **YCZ-1** packed column with hexanes/methanol (98:2) as eluent. As shown in Fig. S8, an obvious baseline separation was obtained. And the retention times for nitrobenzene and toluene is 1.06 and 2.68 min, respectively. Moreover, the resolution (***R***) between toluene and nitrobenzene is calculated and the value is 1.53. The high R value achieved by a 30 × 2.1 mm **YCZ-1** packed column reveals the efficient ability of separating toluene and nitrobenzene by **YCZ-1** material.