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Electronic Supplementary Information

Hydroxyl-functionalized pillar[5]arene with high separation performance for gas chromatography

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List of Contents:

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1. ^{1}H NMR spectrum, Infrared spectrum and ESI-MS spectrum of the compounds

2. The parameters of the Golay equations for the capillary columns

3. Resolution for the isomers on the columns

4. Structures and properties of the analytes

5.Chromatograms of commercial reagent samples

6. Repeatability, reproducibility and long-term stability of the P5A-C10-OH capillary column

1. ^{1}H NMR spectrum, Infrared spectrum and ESI-MS spectrum of the compounds

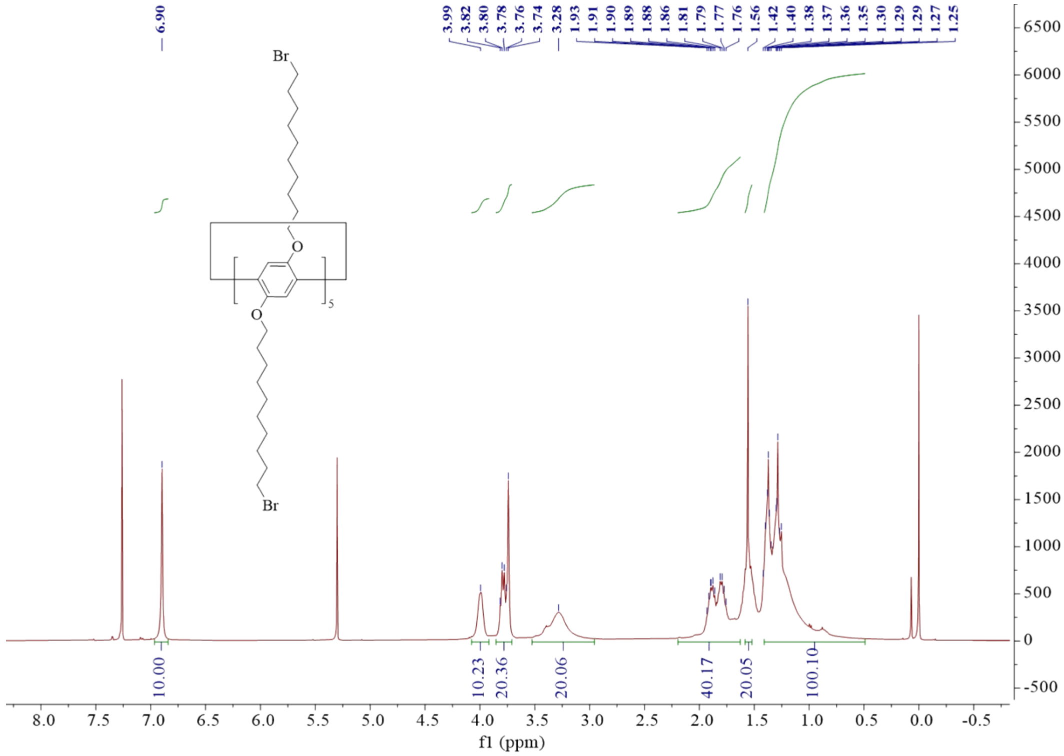


Fig. S1 ^{1}H NMR spectrum of P5A-C10-FBr.

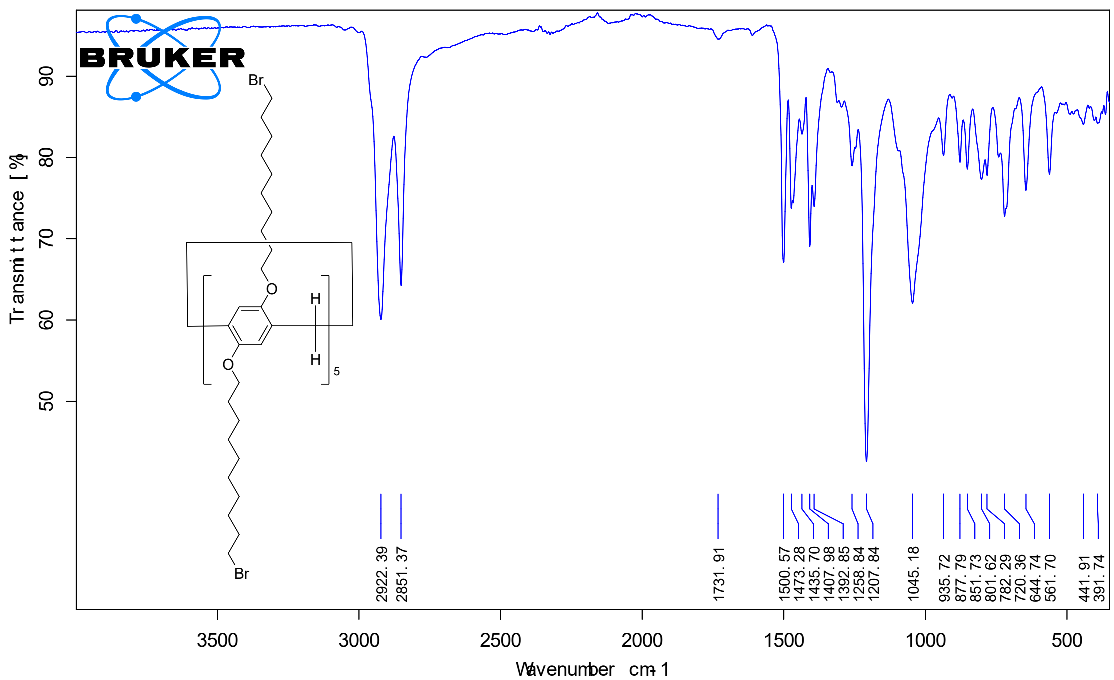


Fig. S2 Infrared spectrum of P5A-C10-FBr.

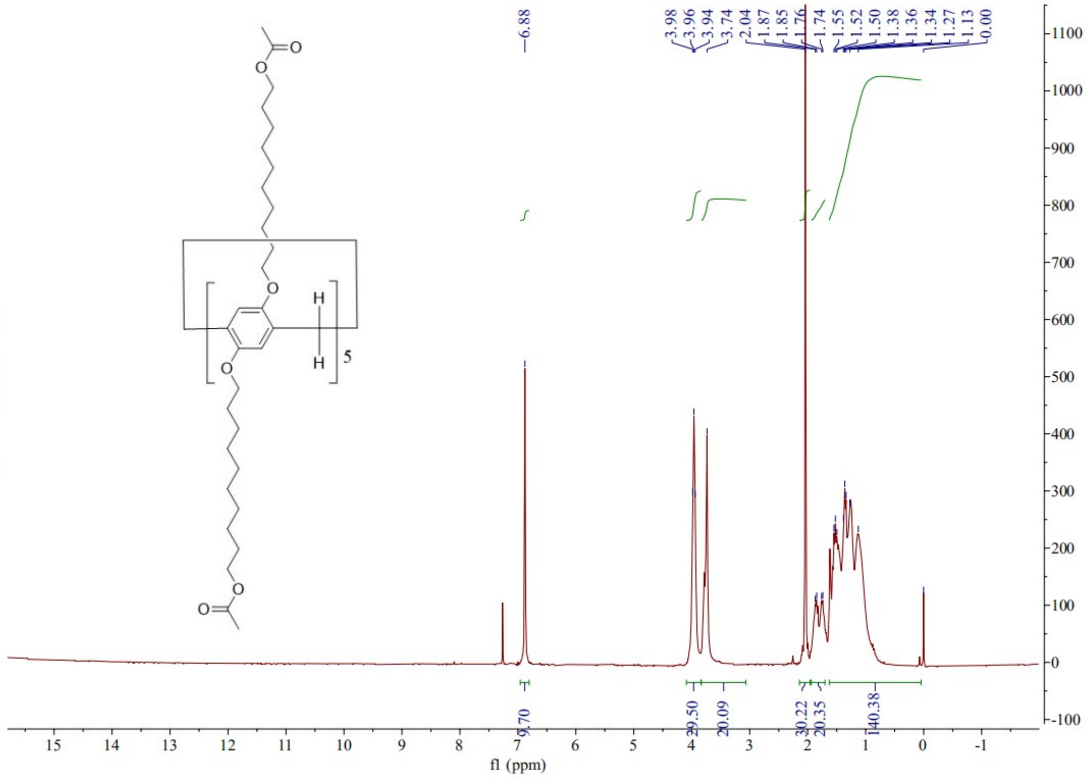


Fig. S3 [1]H NMR spectrum of P5A-C10-OAc.

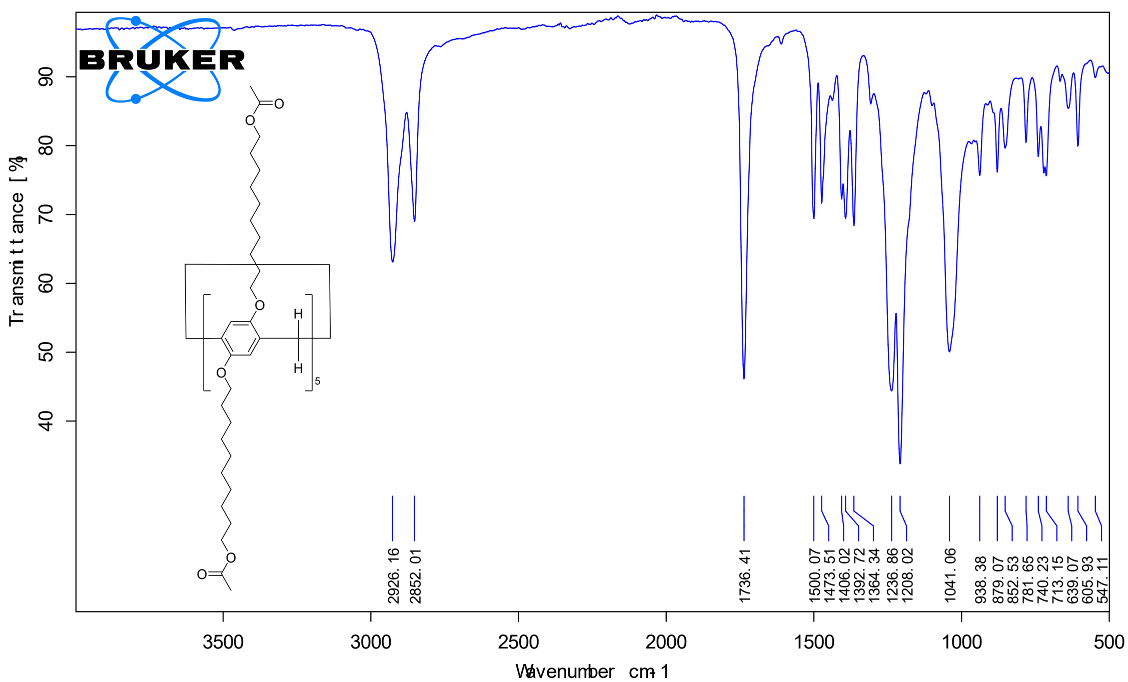


Fig. S4 Infrared spectrum of P5A-C10-OAc.

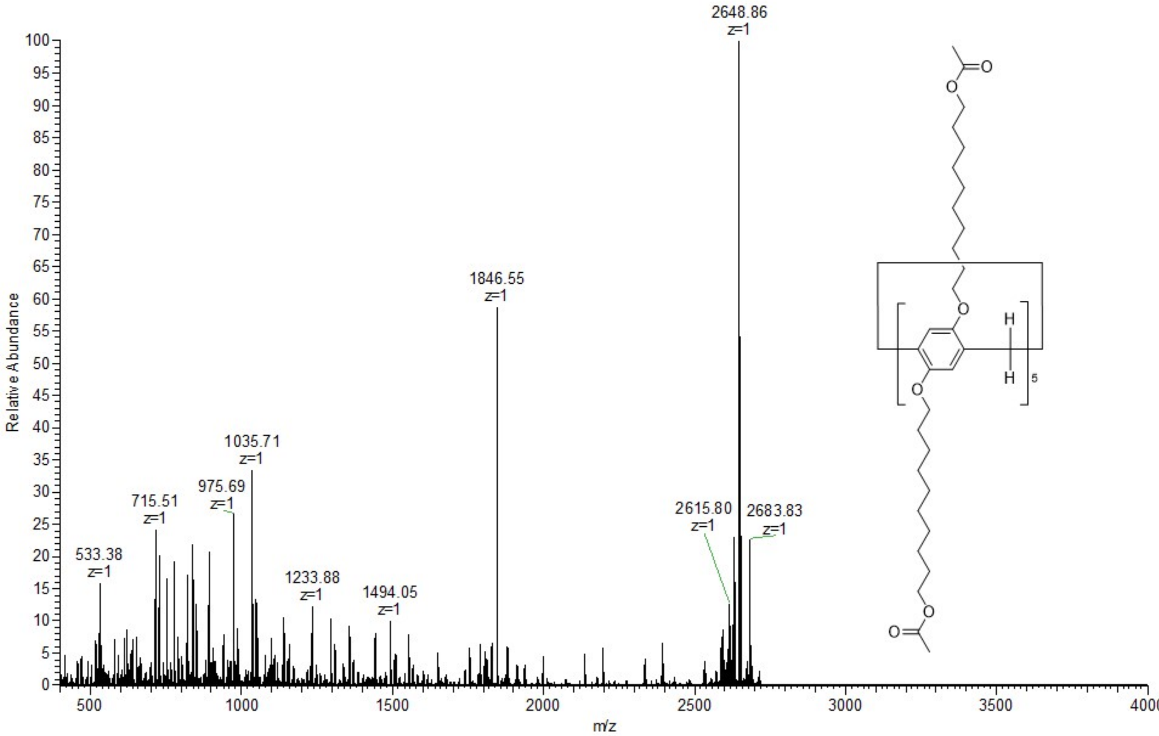


Fig. S5 ESI-MS spectrum of P5A-C10-OAc.

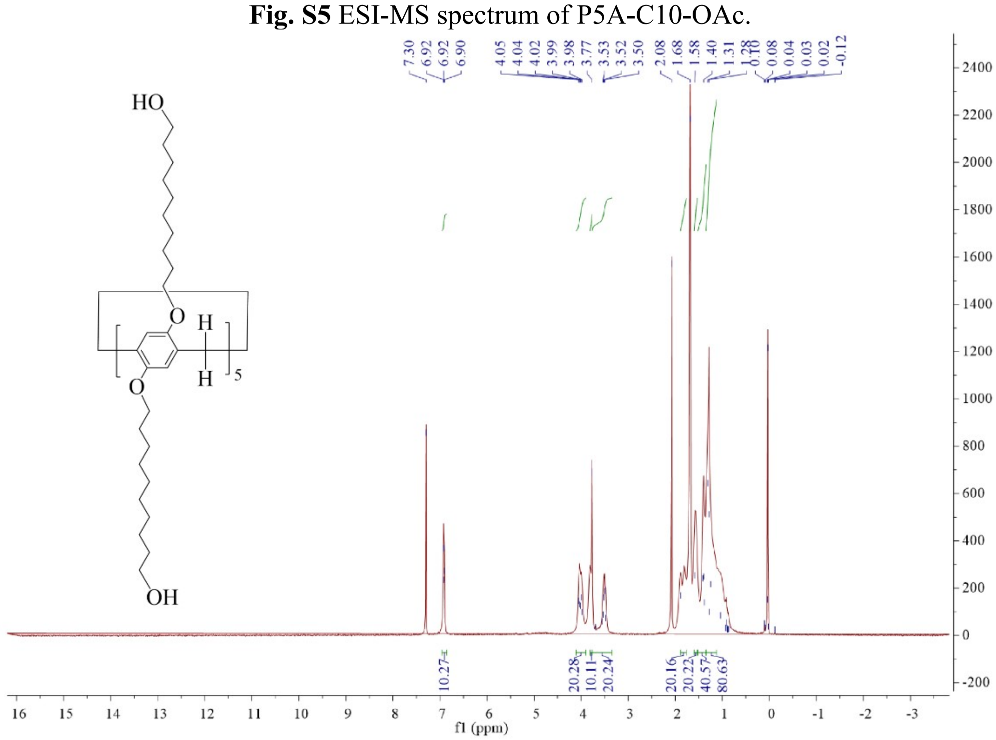


Fig. S6 ^{1}H NMR spectrum of P5A-C10-OH.

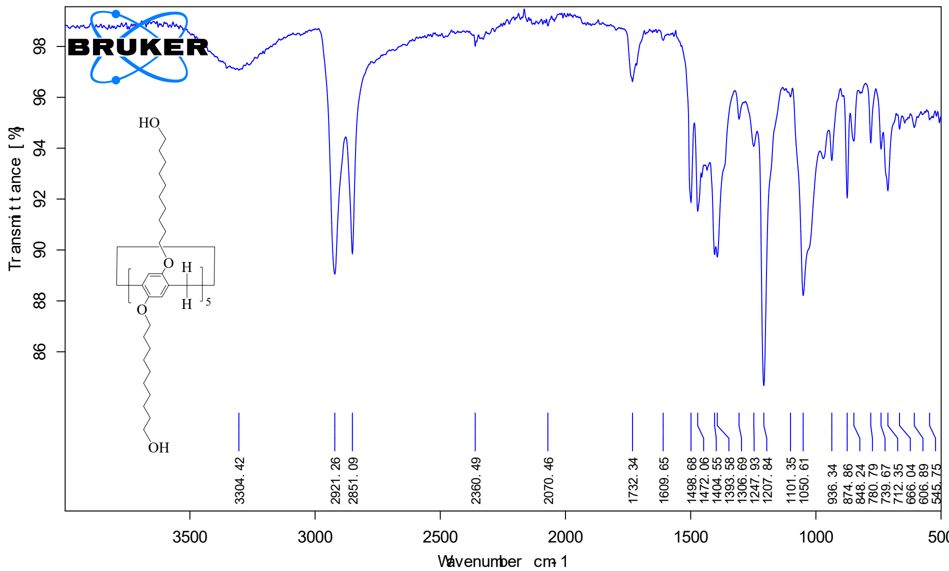


Fig. S7 Infrared spectrum of P5A-C10-OH.

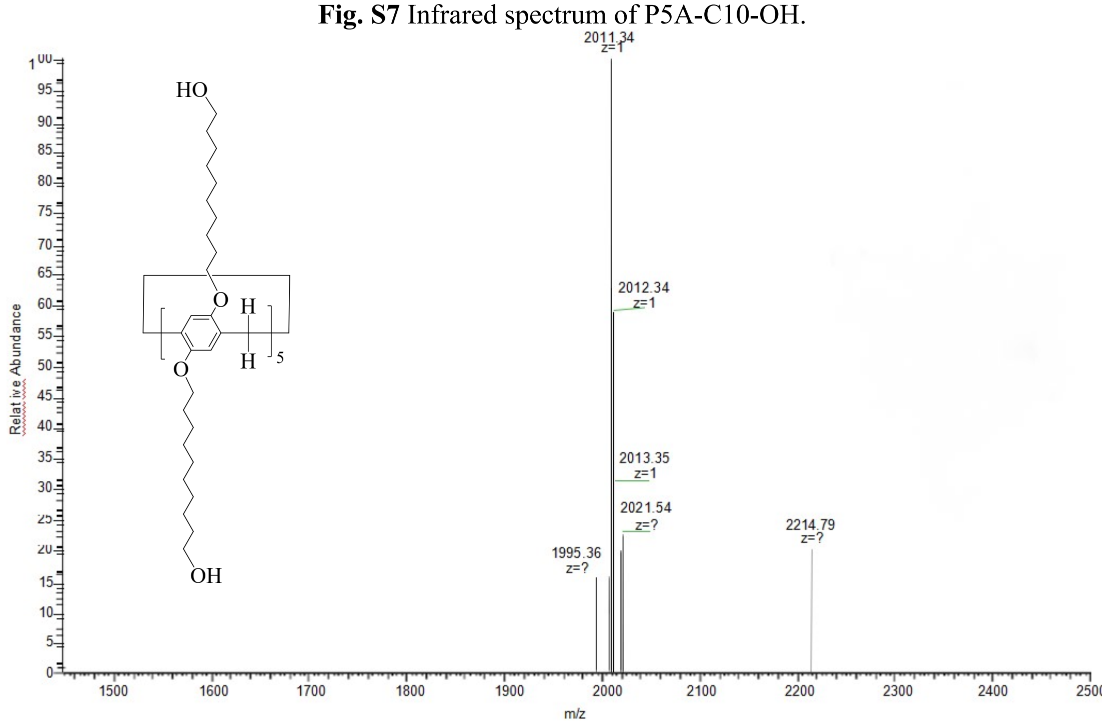


Fig. S8 ESI-MS spectrum of P5A-C10-OH.

2. The parameters of the Golay equations for the capillary columns

Table S1. The minimum plate height (H_{min}), column efficiency (*n*), retention factor (*k*) and the coefficients (*B*, *C*) of the Golay equations for the P5A-C10-OH and P5A-C10 capillary columns determined by *n*-dodecane at 120 °C.

Parameters	P5A-C10-OH	P5A-C10
H_{min} (mm)	0.31	0.46
n (plates/m)	3233	2172
u_{opt} (cm/s)	15.08	8.76
k (at u_{opt})	2.35	4.96
B (±SD) (mm × cm/s)	5.31 (±1.86)	8.05 (± 1.46)
C (±SD) (mm × s/cm)	0.034 (± 0.005)	0.068 (±0.005)

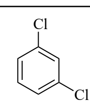
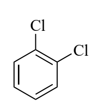
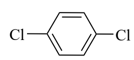
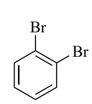
3. Resolution for the isomers on the columns

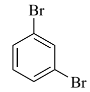
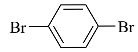
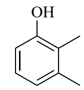
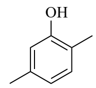
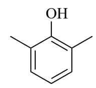
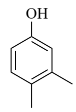
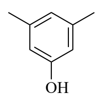
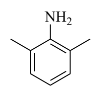
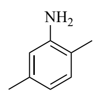
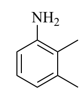
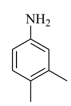
Table S2. Resolution (*R*) for the isomers on P5A-C10-OH, P5A-C10 and HP-35 columns.

Analytes	P5A-C10-OH		P5A-C10		HP-35	
	Elution order	*R*	Elution order	*R*	Elution order	*R*
	m-	-	*m*-	-	*m*-	-
dichlorobenzene	*o*-	3.33	*p*-	co-eluted	*p*-	3.47
	p-	2.31	*o*-	1.05	*o*-	5.62
	m-	-	*m*-	-	*m*-	-
dibromobenzene	*o*-	4.27	*p*-	co-eluted	*p*-	1.80
	p-	5.16	*o*-	1.30	*o*-	5.57
	m-	-	*m*-	-	*m*-	-
chloronitrobenzene	*o*-	4.32	*o*-	0.56	*p*-	4.04
	p-	21.54	*p*-	2.03	*o*-	1.93
	m-	-	*m*-	-	*m*-	-
bromonitrobenzene	*o*-	3.36	*o*-	co-eluted	*p*-	3.31
	p-	27.94	*p*-	12.23	*o*-	1.05
	2,6-	-	2,6-	-	2,6-	-
	2,5-	17.43	2,5-	3.80	2,5-	8.71
xylenol	2,3-	5.63	2,3-	2.30	3,5-	5.29
	3,5-	2.92	3,5-	0.45	2,3-	2.78
	3,4-	4.24	3,4-	0.99	3,4-	4.05
	o-	-	*o*-	-	*o*-	-
chloroaniline	*p*-	18.83	*m*-	5.44	*m*-	18.50
	m-	2.05	*p*-	co-eluted	*p*-	0.47
	o-	-	*o*-	-	*o*-	-
bromoaniline	*m*-	19.62	*m*-	6.67	*m*-	14.55
	p-	2.21	*p*-	0.48	*p*-	co-eluted
	o-	-	*o*-	-	*o*-	-
iodoaniline	*m*-	17.49	*m*-	8.72	*m*-	16.86
	p-	2.32	*p*-	1.76	*p*-	0.65
	o-	-	*o*-	-	*o*-	-
phenylenediamine	*p*-	9.33	*p*-	2.88	*p*-	11.78
	m-	4.06	*m*-	0.89	*m*-	7.28
	2,6-	-	2,6-	-	2,6-	-
dimethylaniline	2,5-	3.07	2,5-	0.37	2,5-	0.63
	2,3-	4.16	2,3-	1.73	3,4-	5.98
	3,4-	1.84	3,4-	co-eluted	2,3-	1.49

4. Structures and properties of the analytes

Table S3. Structures and properties of the analytes.

Compound	Structure	Boiling point	Dipole moment
o-dichlorobenzene		180.4 °C	3.50Debye
m-dichlorobenzene		173 °C	2.27Debye
p-dichlorobenzene		174.1 °C	0Debye
o-dibromobenzene		224 °C	2.14Debye

m-dibromobenzene		219.5 ℃	1.43Debye
p-dibromobenzene		219 ℃	0Debye
2,3-xylenol		218 ℃	2.17Debye
2,5-xylenol		212 ℃	1.58Debye
2,6-xylenol		203 ℃	1.74Debye
3,4-xylenol		225 ℃	1.78Debye
3,5-xylenol		219 ℃	1.51Debye
2,6-dimethylaniline		216 ℃	2.35Debye
2,5-dimethylaniline		218 ℃	2.06Debye
2,3-dimethylaniline		212 ℃	2.14Debye
3,4-dimethylaniline		226 ℃	1.79Debye

5. Chromatograms of commercial reagent samples

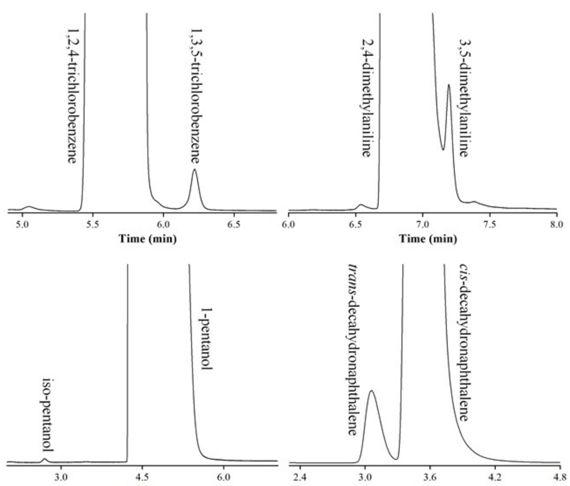


Fig. S9 Applications of the P5A-C10-OH column for the determination of minor impurities in the real samples of 1,2,4-trichlorobenzene, 2,4-dimethylaniline, 1-pentanol and *cis*-decahydronaphthalene, respectively.

6. Repeatability, reproducibility, and long-term stability of the P5A-C10-OH capillary column

Table S4. Repeatability and reproducibility of the P5A-C10-OH capillary column on the retention times (t_R, min).

Analytes	run-to-run (n = 5)		day-to-day (n = 4)		column-to-column (n = 3)	
	t_R (min)	RSD (%)	t_R (min)	RSD (%)	t_R (min)	RSD (%)
n-tetradecane	8.58	0.03	8.57	0.11	8.89	2.48
n-pentadecane	9.32	0.01	9.31	0.06	9.52	1.23
n-hexadecane	10.01	0.02	10.01	0.03	10.17	0.88
1-nonanol	8.93	0.01	8.93	0.04	9.13	2.09
1-decanol	9.68	0.01	9.69	0.08	9.73	0.49
1-undecanol	10.41	0.01	10.43	0.19	10.36	0.23
1-dodecanol	11.35	0.03	11.38	0.21	11.24	0.53
methyl decanoate	8.98	0.02	8.98	0.03	9.16	1.71
methyl undecanoate	9.66	0.02	9.67	0.06	9.71	0.44
methyl laurate	10.37	0.01	10.38	0.12	10.36	0.21

Table S5. Long-term stability of the P5A-C10-OH column on the retention times of the indicated isomer analytes over the time period.

Analyte	Retention time (min)			RSD (%)
	0 month	1 month	6 month	
n-tetradecane	8.55	8.64	8.56	0.55
n-pentadecane	9.29	9.38	9.31	0.56
n-hexadecane	9.98	10.07	10.01	0.48
2,6-xylenol	7.34	7.47	7.46	1.00
2,5-xylenol	8.94	9.08	9.06	0.82
2,3-xylenol	9.42	9.57	9.54	0.81
3,5-xylenol	9.68	9.83	9.81	0.83
3,4-xylenol	10.10	10.25	10.25	0.86
o-bromoaniline	7.68	7.81	7.79	0.96
m-bromoaniline	9.65	9.81	9.76	0.83
p-bromoaniline	9.85	10.01	9.97	0.82

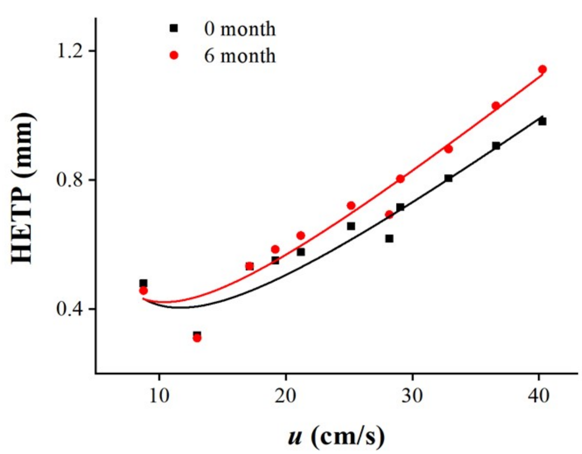


Fig. S10 Long-term stability of the P5A-C10-OH column on the column efficiency over the time period.