

Electronic Supplementary Information (ESI)

1. Reagents and Chemicals

Bulk MoS₂ powder (1-2 μm) was purchased from Aladdin Chemicals (Shanghai, China). Poly(dimethylsiloxane) was purchased from J&K Scientific Ltd. (Guangzhou, China). Fused-silica capillary was purchased from Yongnian Optic Fiber Factory (Hebei, China). All of the tested chemicals are of GC grade and purchased from Aladdin Chemicals (Shanghai, China). All water used in this work was 18 MΩ-cm deionized water (DIW) produced with a water purification system (PCWJ-10, Pure Technology Co. Ltd., Chengdu, China). All standards and stock solutions were stored at 4 °C in the dark until use.

2. Instrumentation

An Agilent (Santa Clara, USA) GC-7820A system with a capillary control unit, a split injection port, and a flame ionization detector was used for all GC separations. Highly pure N₂ gas (99.999%) was used as the carrier gas with a linear velocity of 10-25 cm/s. The injection split ratio was 200:1. The instrument control and data acquisition were carried out with a ChemStation software (Agilent, USA). The SEM images were obtained from a JEOL JSM-7500F scanning electron microscope (Akishima, Japan) at 30.0 kV. The transmission electron microscopy images were obtained from a FEI Tecnai G2 F20 S-TWIN transmission electron microscope (Oregon, USA). The atomic force microscopy images were obtained from a SPA-400 model atomic force microscope (Kyoto, Japan).

3. Preparation of MoS₂/PDMS-modified open tubular columns

Fused-silica capillary was at first filled with 1 M NaOH and kept for 1 h. The capillary was then washed with ultrapure water for 1 h, followed by rinsing with a flow of 0.1 M HCl for 2 h, until the pH of the outflow was around 7. The obtained capillary was then purged with N₂ flow at 150 °C for 5 h.

The MoS₂-coated column was prepared by a dynamic coating method similar to previously reported^[1]. 0.1 mL suspension of MoS₂ nanosheet was introduced into the modified capillary mentioned above, and then pushed all through the capillary with a rate of 0.6 cm/s in order to coat a wet layer on the inner wall of the capillary. During the coating process, a 2-m long buffering tube was connected to the outlet end of the capillary column to avoid sudden flow change of the introduced suspension. Subsequently, the coated open tubular column was blown with N₂ for 1 h and then kept under an increased temperature (30 °C-300°C, 2 °C/min) and a thereafter steady temperature (300°C, 6 h) for conditioning prior to use. PDMS-column was prepared with the same procedure using 4.7% w.t.% PDMS in CH₂Cl₂.

4. Calculation of thermodynamics

The adsorption enthalpies were calculated based on the van't Hoff equation^[2]:

$$\ln k' = -\frac{\Delta H}{RT} + \frac{\Delta S}{R} + \ln \Phi$$

k' stands for retention factor, calculated by equation:

$$k' = \frac{t - t_0}{t_0}$$

t stands for retention time and t_0 stands for dead time, measured by butane as model molecule.

R stands for gas constant equal to 8.314 J/(mol•K)

T stands for thermodynamic temperature

Φ stands for compare, calculated by equation:

$$\Phi = \frac{V_{COL} - t_0 v}{t_0 v}$$

V_{COL} stands for the physical volume of column and v stands for the speed of carry gas.

The slope was obtained from the van't Hoff plots and the Gibbs free energies were calculated from the equation:

$$\Delta G = \Delta H - T\Delta S$$

5. Figures and tables



Fig.S1 Left: the suspension of layered MoS₂ nanosheets dispersed in a mixture of water and ethanol. Right: Tyndall effect observed from the MoS₂ suspension.

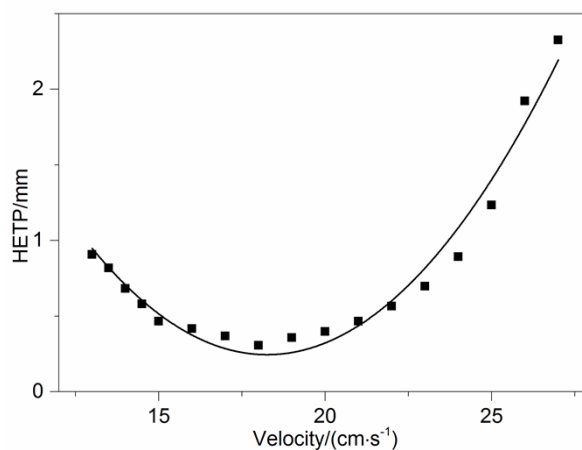


Fig. S2 Van Deemter plot of dodecane at 120 °C (H_{\min} : 0.31 mm at 18.0 cm/s).

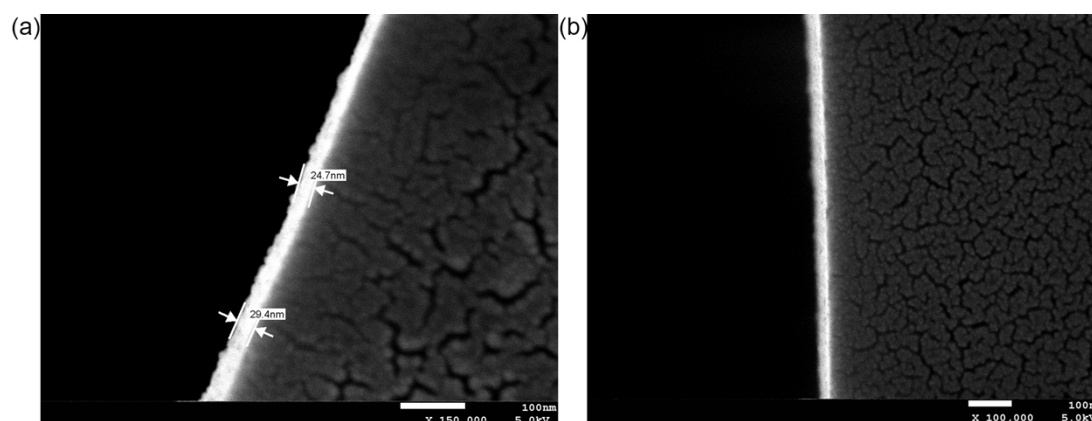


Fig. S3 SEM images of cross section of capillary open tubular column coated with MoS₂ nanosheets.

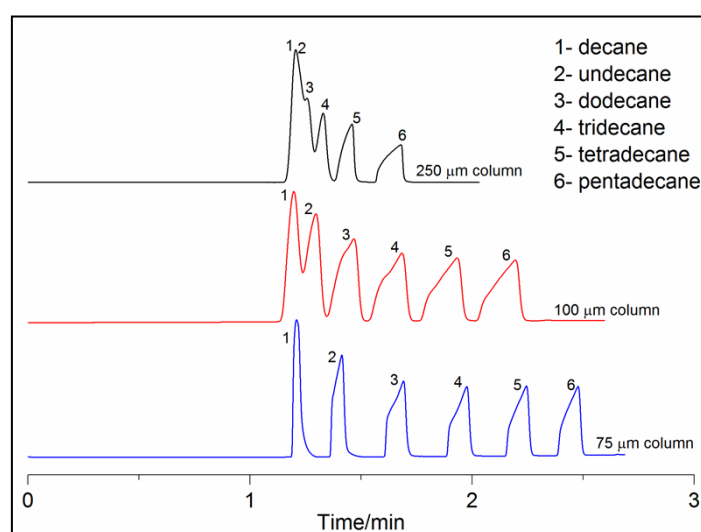


Fig. S4 Chromatogram of alkane mixture obtained from MoS₂-coated column with different inner diameters in the same separation conditions.

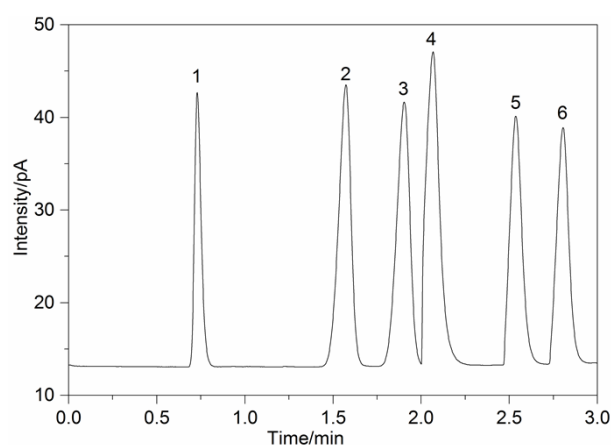


Fig. S5 Chromatogram of Grob's test mixture obtained from MoS₂-coated column: 1. Carbon dichloride; 2. Decane; 3. Undecane; 4. 2,6-dimethylaniline; 5. Methyl undecanoate; 6. Methyl dodecanoate. Temperature program: 60 °C for 0.5 min, then 45 °C/min from 60 °C to 180 °C, and at 180 °C until end.

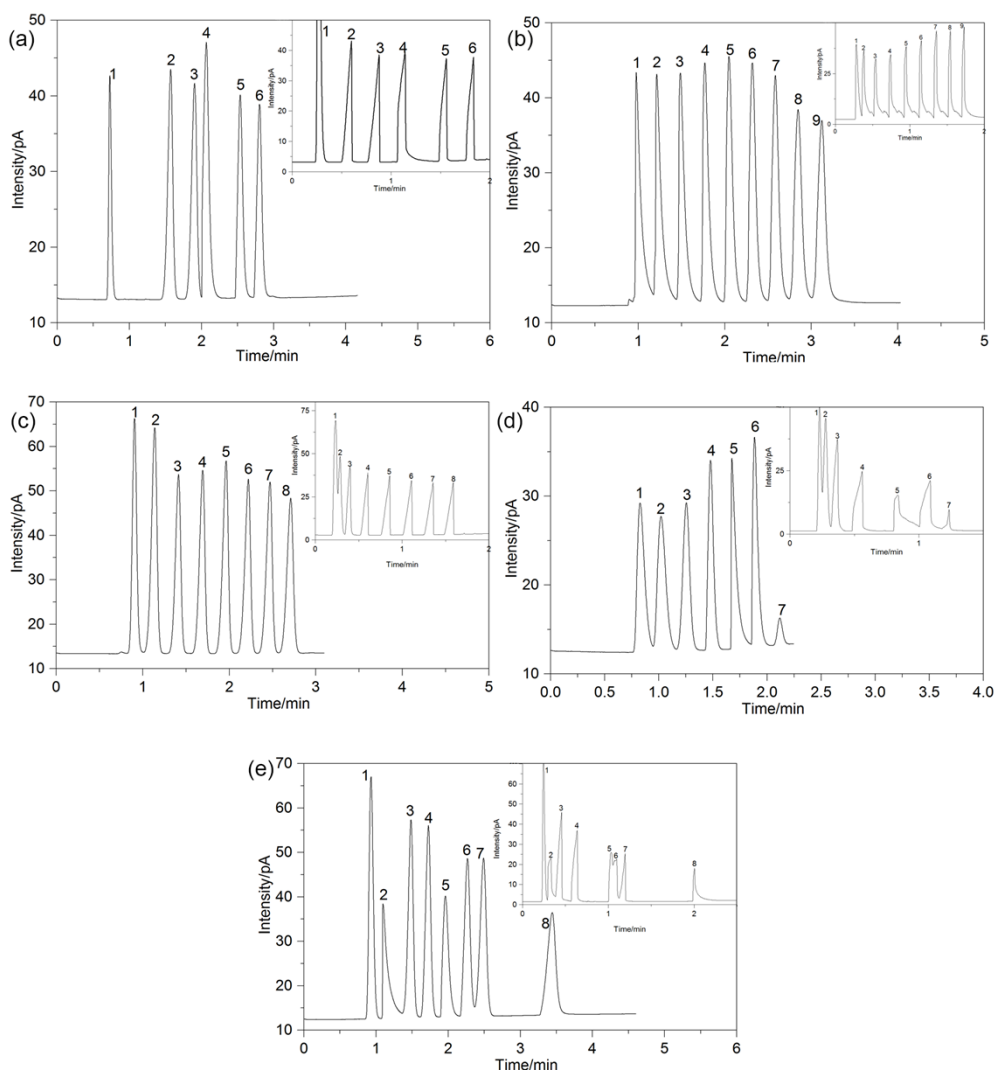


Fig. S6 Chromatogram obtained in the same separation conditions from MoS₂-coated column and PDMS-coated column (inset): (a) 1. Carbon dichloride; 2. Decane; 3. Undecane; 4. 2,6-dimethylaniline; 5. Methyl undecanoate; 6. Methyl dodecanoate. (b) 1. Butanol; 2. Pentanol; 3. Hexanol; 4. Heptanol; 5. Octanol; 6. Nonanol; 7. Decanol; 8. Undecanol; 9. Dodecanol. (c) 1. Octane; 2. Nonane; 3. Decane; 4. Undecane; 5. Dodecane; 6. Tridecane; 7. Tetradecane; 8. Pentadecane. (d) 1. Benzene; 2. Toluene; 3. Chlorobenzene; 4. Anisole; 5. Aniline; 6. Acetophenone; 7. Naphthalene. (e) 1. benzene; 2. Butanol; 3. Chlorobenzene; 4. Anisole; 5. Phenol; 6. Methyl benzoate; 7. Naphthalene; 8. 2-naphthol.

Table S1Chromatographic data of the MoS₂-coated column obtained from the tested molecules

	Boiling point (°C)	Retention factor (k)	N (plates/m)
butanol	117.4	2.42	1650
pentanol	137.3	3.25	2260
hexanol	157	4.21	2900
heptanol	175.8	5.19	3540
octanol	196	6.17	4010
nonanol	214	7.12	4650
decanol	232.9	8.05	5260
undecanol	241	8.97	5150
dodecanol	255	9.93	5780
octane	125.8	2.17	1480
nonane	150.8	2.99	1440
decane	174.1	3.95	2330
undecane	196	4.92	3290
dodecane	216.2	5.87	4290
tridecane	234	6.77	5160
tetradecane	253.5	7.65	6010
pentadecane	268	8.48	6230
2,6-dimethylaniline	214	6.24	3070
methyl undecanoate	247	7.88	6340
methyl dodecanoate	262	8.82	7640
benzene	80.1	1.99	1450
toluene	110.6	2.83	900
chlorobenzene	131.7	3.97	1380
anisole	153.8	4.99	2190
aniline	184	5.86	2560
acetophenone	202	6.85	3230
naphthalene	218	7.94	4010

Table S2McReynolds constants obtained from MoS₂-coated column and PDMS-coated column at 120 °C^[a]

Phase	McReynolds constant values					ΔI
	x'	y'	z'	u'	s'	
MoS ₂ nanosheets	49.8	11	94.3	76.3	64.1	79.2
1						
DB-1	16	55	44	65	42	44

[a]: x': benzene; y': 1-butanol; z': 2-pentanone; u': nitropropane; s': pyridine

Reference

- ¹. Z.-Y. Gu and X.-P. Yan, *Angew. Chem. Int. Ed.* **49** (2010) 1477.
- ². M. Karwa and S. Mitra, *Anal. Chem.* **78** (2006) 2064.