

Supporting Information

Pillar[5]arene promoted selective spreading of chlormequat droplets on hydrophobic surface

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1. The synthesis route of HO-P5

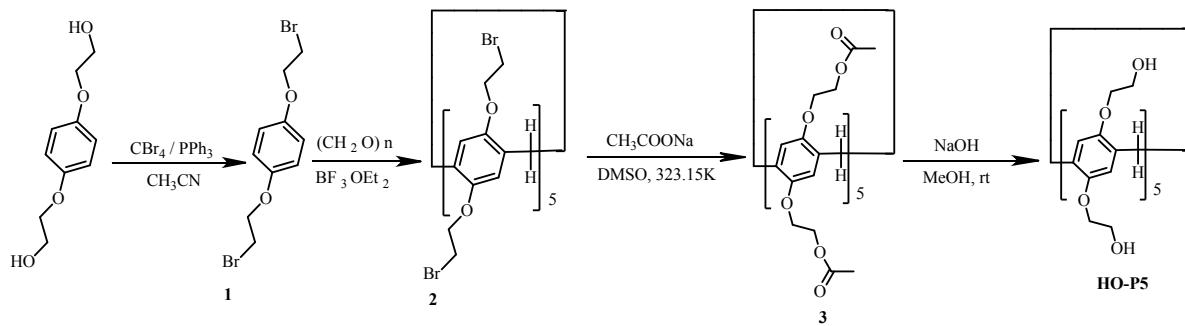


Figure S1. The synthesis route of HO-P5.

The compound **2** was synthesized according to the synthesis route of Yong et al. paper¹. To a solution of 1,4-bis-(2-hydroxyethoxy)-benzene (5.0 g, 25.2 mmol), Triphenylphosphine (16g, 60 mmol) in dry acetonitrile (250 mL) was cooled with an ice bath and stirring. Under vigorous stirring, carbon tetrabromide (20 mg, 60 mmol) dissolved in 30 mL of acetonitrile was slowly added. The mixture was stirred at room temperature for 4 hours. Then cold water (200 mL) was added to the reaction mixture to form white precipitation. The solid was collected by filtration, washed with methanol/water (3:2, 3 × 100 mL), then was recrystallized from methanol, and dried under vacuum to afford desired product **1** as white crystals, yield 7.25 g, 94%. ¹H NMR (400 MHz, CDCl₃, rt) δ (ppm): 6.86 (s, 4H), 4.25 (t, J = 6.3 Hz, 4H), 3.62 (t, J = 6.8 Hz, 4H).

1,4-bis(2-bromoethoxy) benzene **1** (4.86g, 15 mmol) and paraformaldehyde (1.35 g, 45 mmol) in 1,2-dichloroethane (100 mL) under nitrogen, was cooled with an ice bath. Boron trifluoride diethyl etherate (3.45 g, 23.30 mmol) was added to the solution, and then the mixture was stirred at room temperature for 45minutes. Green color appeared, and the reaction was controlled by TLC (PE/DCM = 12:8) until the start material was finished in the reaction mixture. The mixture was then washed with water (2 × 50 mL). The solvent was dried with Na₂SO₄, evaporated to provide a crude product, which was purified by column chromatography (eluent: petroleum ether/Dichloromethane, 4:1) to afford a white solid compound **2**, yield 2.8 g, 52%. ¹H NMR (400 MHz, CDCl₃, rt) δ (ppm): 6.93 (s, 10 H), 4.24 (t, J = 5.7 Hz, 20 H), 3.86 (s, 10 H), 3.65 (t, J = 5.6 Hz, 20 H).

Compound **2** (2 g, 12.4 mmol) and sodium acetate (2.0 g, 240 mmol) in dimethylsulfoxide (80 mL), the mixture was stirred at the temperature of 50°C for 3

hours, TLC was used to control the total consumption of start reagents. Water was added (3 times of the volume of DMSO). Then ethyl acetate (100 mL) was used for extraction, and the mixture was vigorously shaken. Organic and water layers were separated using the separatory funnel, and the organic layer was dried with Na₂SO₄. The solvent was evaporated, and a viscous product (compound **3**) was obtained, then was directly used for the next step. In a 100 mL flask, compound **3** (1.5 g, 1.0 mmol), sodium hydroxide (0.48 mg, 12 mmol) were stirred for 2 hours. Rotator was used to remove the methanol solvent; the solid was recrystallized from water, filtered and dried. White powder (HO-P5) was obtained with a yield of 0.72 g, 67.2%. ¹H NMR (600 MHz, CD₃OD): δ 6.94 (s, 10 H), 3.94 (d, J = 4.9 Hz, 20 H), 3.89 – 3.85 (m, 20 H), 3.81 (s, 10 H).

2. The synthesis of diethoxybenzene pillar[5]arene (DEP5)

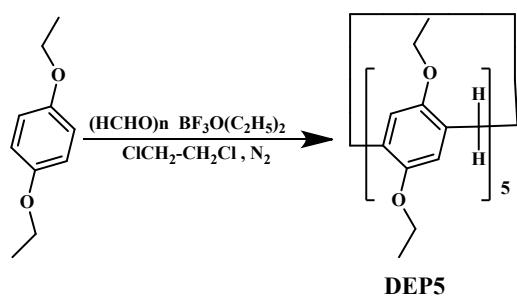


Figure S2. The synthetic route of DEP5.

To a solution of 1,4-diethoxybenzene (1.46 g, 8.70 mmol) in 1,2-dichloroethane (50 mL), paraformaldehyde (0.81 g, 26.35 mmol) was added to a nitrogen atmosphere, stirred for about 30 min. Boron trifluoride etherate (1.4 mL, 11.34 mmol) was added to the solution, and the mixture was stirred at room temperature under TLC control until the start reagent was consumed. The solution was poured into methanol and the resulting precipitate collected by filtration to obtain a white solid, which was purified by column chromatography (eluent: petroleum ether/Dichloromethane, 5:4) to afford a clear white solid diethoxy pillar[5]arene (DEP5) . Yield 0.8 g. ¹H NMR (600 MHz, CDCl₃): δ 6.81 (s, 10 H), 3.89 (d, J = 13.8, 6.8 Hz, 20 H), 3.80 (s, 10 H), 1.35 (t, J = 6.9 Hz, 30 H).

3. The ^1H NMR and ^{13}C NMR spectrum of HO-P5 and DEP5

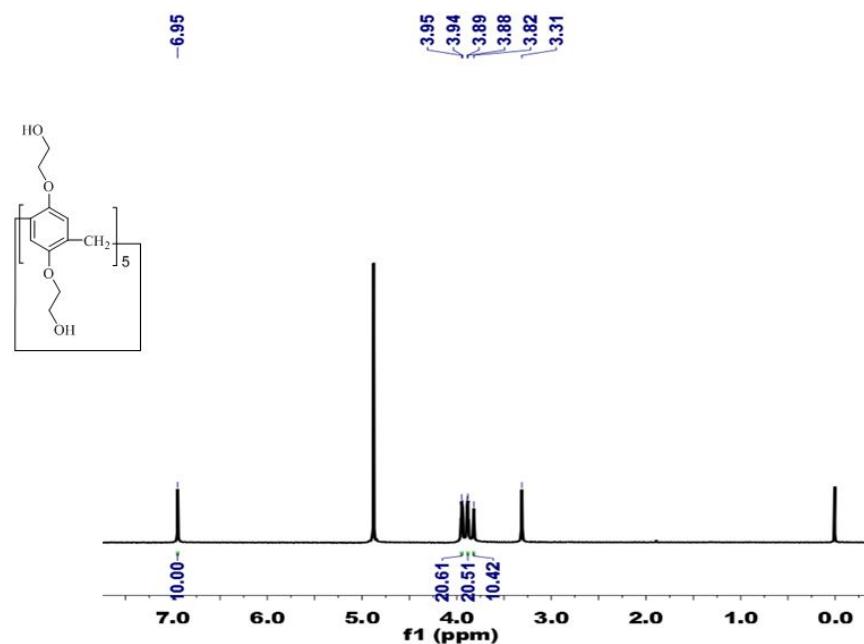


Figure S3. The ^1H NMR spectrum (600 MHz, CD_3OD , 298 K) of HO-P5.

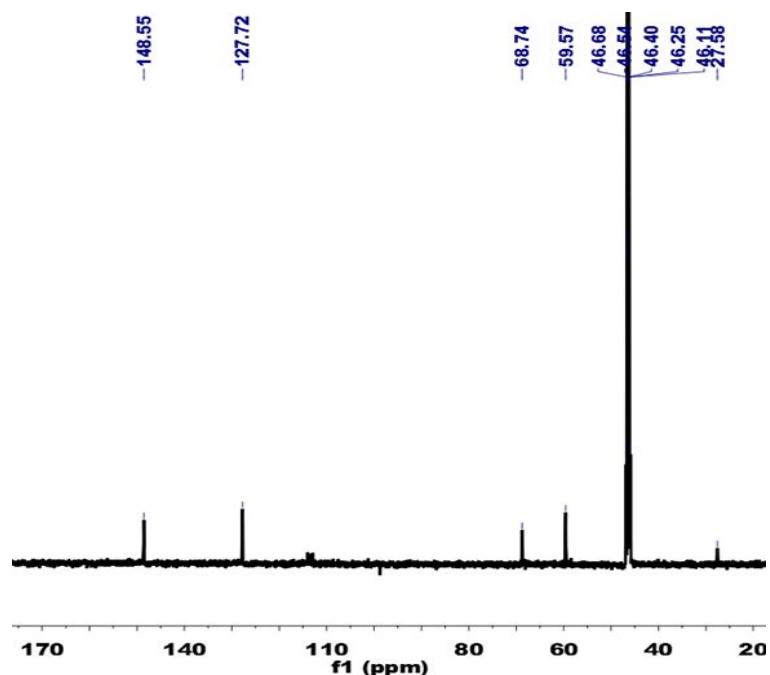


Figure S4. The ^{13}C NMR spectrum (150 MHz, CD_3OD , 298 K) of HO-P5.

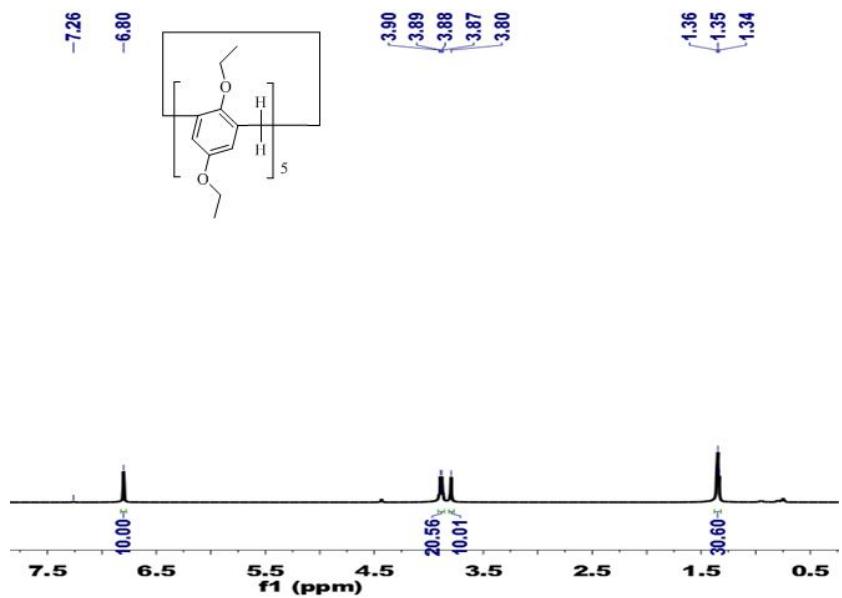


Figure S5. The ^1H NMR spectrum (600 MHz, CDCl_3 , 298 K) of DEP5.

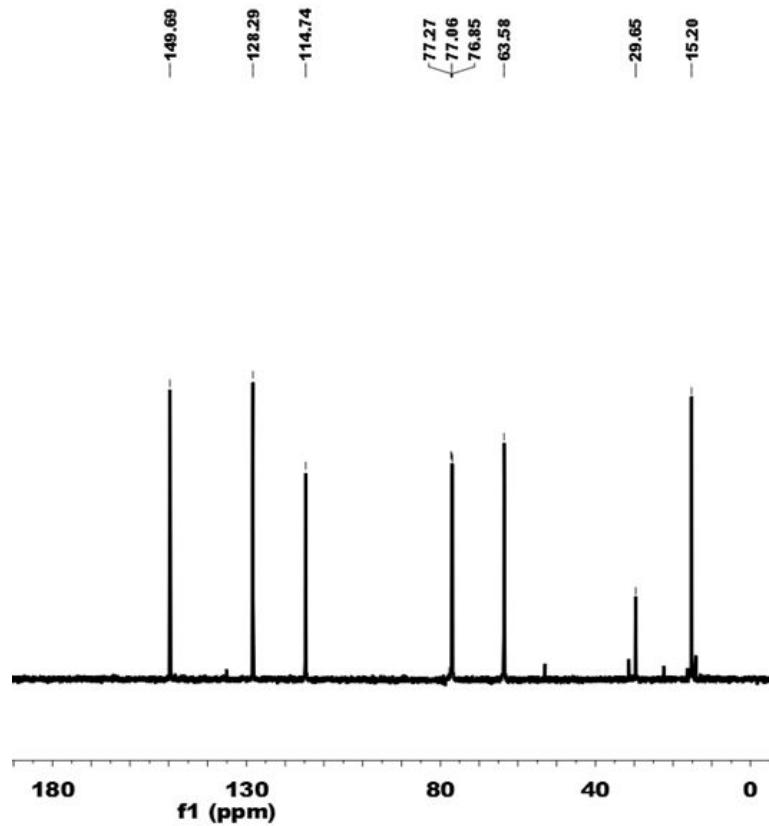


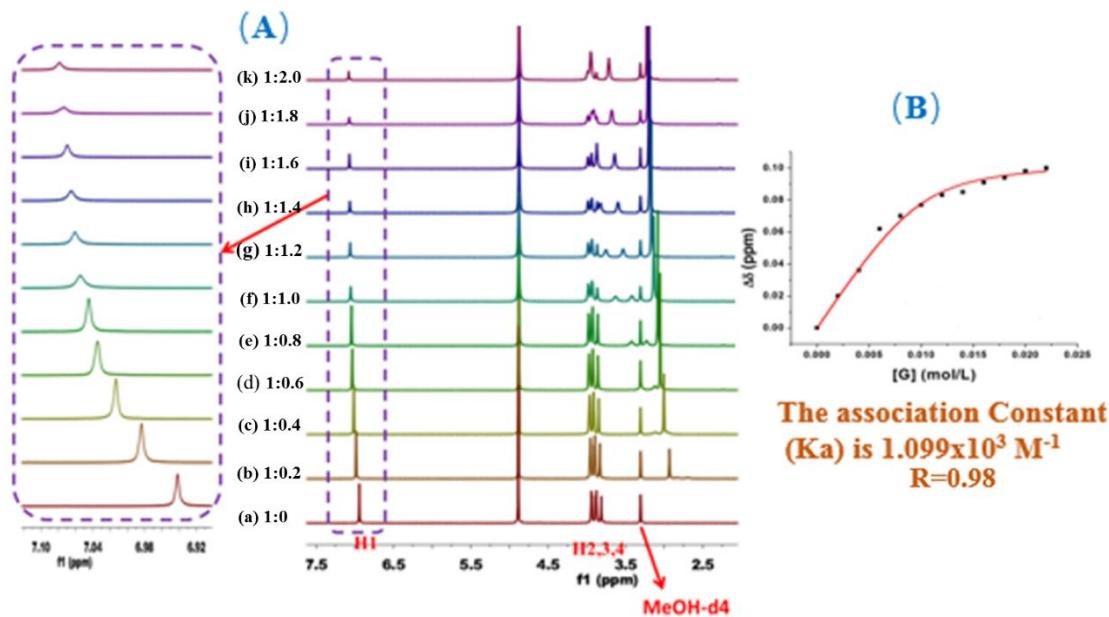
Figure S6. The ^{13}C NMR spectrum (150 MHz, CDCl_3 , 298 K) of DEP5.

4. The ^1H NMR titrations of HO-P5 and guest

To determine the stoichiometry and association constant between HO-P5 and guest molecules, ^1H NMR titrations were done with the following method: A heavy aqueous solution of chlormequat (1.0×10^{-1} M, 5 μL , 10 μL , 20 μL to 100 μL) was added to a heavy aqueous HO-P5 solution (0.5 mL, 10.0×10^{-3} M). After each addition, NMR spectrum was checked. By a non-linear curve-fitting method, the association constant between the guest and HO-P5 was calculated. By a mole ratio plot, a 1:1 stoichiometry was obtained; the guest was shown to form a 1:1 complex with HO-P5. The non-linear curve-fitting was based on the equation: S1

$$\Delta\delta = (\Delta\delta_\infty/[G]_0) (0.5[H]_0 + 0.5([G]_0+1/K_a) - (0.5 ([H]_0^2 + 2[H]_0(1/K_a - [G]_0)) + (1/K_a + [G]_0)^{0.5})) \quad (\text{Eq. S1})$$

Where $\Delta\delta$ is the chemical shift change of H1 on HO-P5 at $[H]_0$, $\Delta\delta_\infty$ is the chemical shift change of H1 when the guest is completely complexed, $[G]_0$ is the fixed initial concentration of the guest, and $[H]_0$ is the varying concentrations of HO-P5.



^1H NMR titration of HO-P5 and chlormequat

Figure S7. (A) ^1H NMR (MeOH-d_4 , 293 K, 600 MHz) titration of HO-P5 at a concentration of 2 mM upon different concentrations of chlormequat. (B) The chemical shift changes of H1 on HO-P5 upon addition of chlormequat. The red solid line was

obtained from the non-linear curve-fitting using Eq. S1. The association constant (K_a) for chlormequat was calculated as 1099 M^{-1} .

5. The modified process of the HO-P5-modified surface.

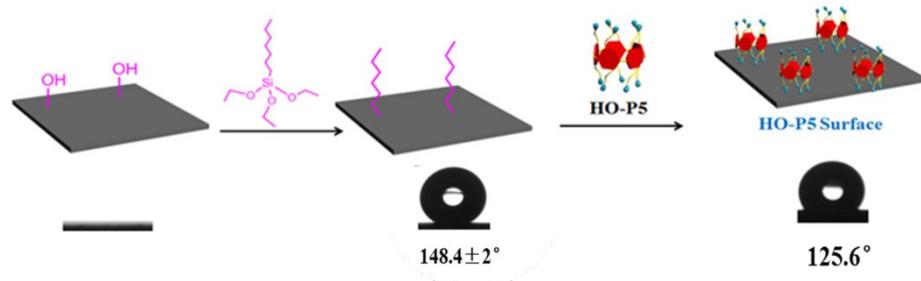


Figure S8. The construction and contact angle changes of the water droplet on the HO-P5 functional surface before and after each step of modification.

6. The Relationship between the CAs and the concentration of various guest.

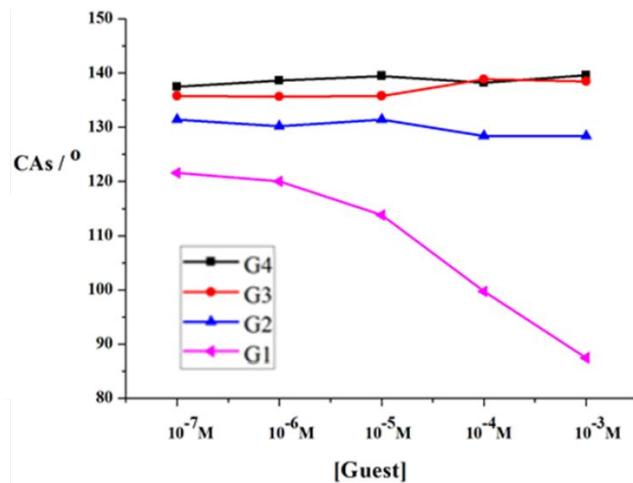


Figure S9. The Relationship between the contact angle and the concentration. The contact angle decreased with the increasing concentration of the guests (from 10^{-7} M to 10^{-3} M).

7. The theoretical size cavity of pillar[n]arenes

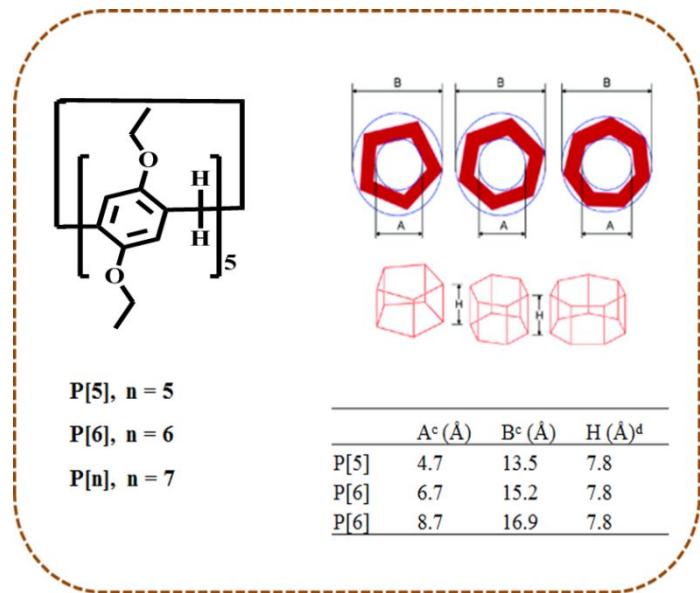


Figure S10. Size cavity of pillar[n]arene and the X-ray crystal structures were reported in the paper of Xue¹.

8. The Size determination of the different guests using Gaussian calculation.

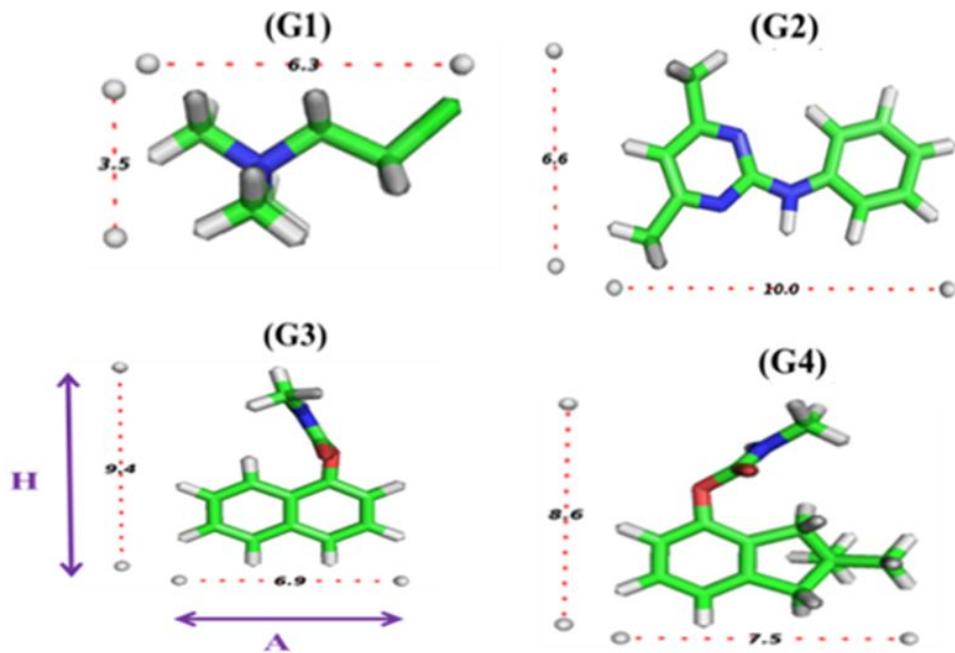


Figure S11. Size of the different guests according to the Gaussian calculation. (G1) chlormequat, (G2) pyrimethanil, (G3) carbaryl, and (G4) carbofuran.

9. Selective recognition of DEP5 interface with various guest.

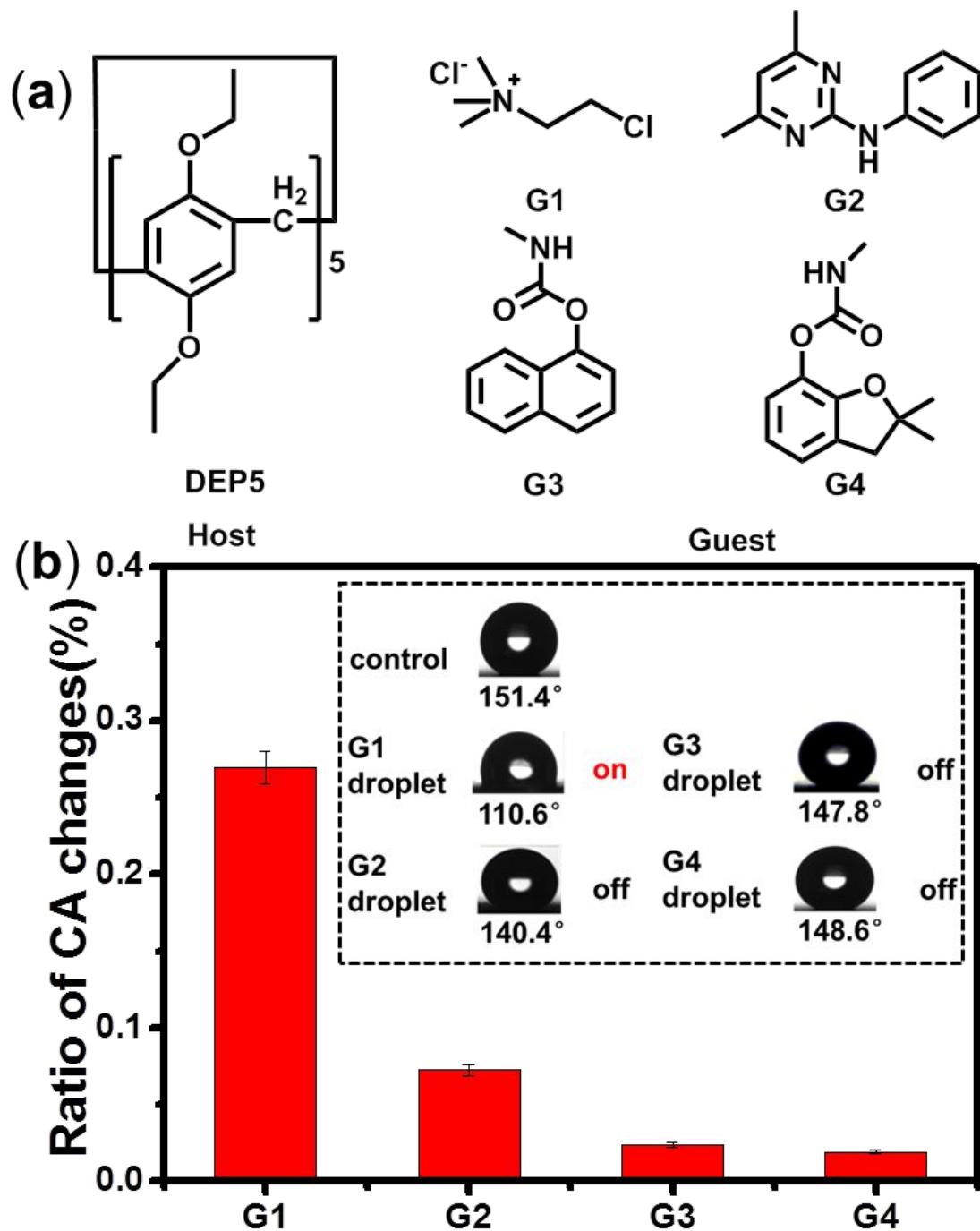


Figure S12. (a) Chemical structure of the host and guests. (b) Selective spreading of DEP5 interface with different pesticides dropping onto the surface. The ratio of CA changes represent $|(\theta_G - \theta_S)/\theta_S|$ means the contact angle changes before and after the guest droplet drop onto the surface.

10. Three-dimensional coordinates of G1 binding with HO-P5 or DEP5.

A. Three-dimensional coordinates of DEP5 and G1.

Cartesian Co-ordinates (XYZ format)

C	-2.56215900	3.43489400	-1.02713100
C	-1.33843400	4.08853100	-0.93837200
C	-0.69806200	4.28971300	0.26892500
C	-1.35262300	3.85296900	1.42726700
C	-2.56257400	3.18864900	1.33694300
C	-3.18225400	2.94895100	0.11056600
C	0.67713400	4.93926700	0.32330500
C	1.81414400	3.92542000	0.28500000
C	2.26517300	3.33792600	1.46652700
C	3.26023300	2.37652500	1.47359500
C	3.83715800	1.94739900	0.27239900
C	3.41051400	2.55789600	-0.89222500
C	2.42087000	3.53504600	-0.89689700
C	4.89230400	0.85093500	0.23945900
C	4.30263500	-0.54880300	0.12523000
C	4.14303200	-1.18559700	-1.09295100
C	3.53824300	-2.43634800	-1.15995300
C	3.08687300	-3.09744100	-0.03350800
C	3.30406400	-2.48218200	1.20633500
C	3.88668500	-1.22893100	1.27045700
C	2.36192000	-4.43038500	-0.14833600
C	0.84633600	-4.28277700	-0.20751500
C	0.16239700	-4.15219100	-1.40439300
C	-1.21550400	-3.96656400	-1.41068100
C	-1.95541000	-3.89685600	-0.24446800
C	-1.27195300	-4.07005000	0.96491500
C	0.10039400	-4.25217300	0.97058200

C	-3.45041000	-3.61519700	-0.28504600
C	-3.77534900	-2.12819500	-0.21596600
C	-3.95505800	-1.35821400	-1.35210800
C	-4.18642100	0.00899400	-1.24712800
C	-4.26320800	0.65146200	-0.02544300
C	-4.13134800	-0.13442300	1.12575500
C	-3.88166000	-1.49143000	1.02034400
C	-4.48126800	2.15603100	0.05328300
O	-3.11732600	3.22765900	-2.26795400
O	2.02581000	4.07465600	-2.09818500
O	4.52676200	-0.56994900	-2.25866600
O	0.84130300	-4.14449600	-2.59776400
O	-3.86622900	-1.92345400	-2.60090900
O	-0.73674200	4.11117700	2.60410100
O	3.72640900	1.80364400	2.60691700
O	2.91240600	-3.17264500	2.30158100
O	-2.02038500	-4.04451900	2.09131100
O	-4.25934000	0.50381500	2.31180500
H	-0.87134700	4.43351400	-1.84332600
H	-3.04329100	2.82090800	2.21944400
H	0.77168200	5.61919300	-0.51216500
H	0.76170800	5.52805000	1.22636600
H	1.80199000	3.64071200	2.38222900
H	3.85617800	2.27158600	-1.82861000
H	5.49319200	0.90720100	1.13669000
H	5.55084000	1.03184300	-0.59861600
H	3.40512500	-2.89205800	-2.12471800
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H	2.62078500	-5.05409800	0.69634600
H	2.70901000	-4.93686800	-1.03850900
H	-1.71768600	-3.85752200	-2.35543800

H	0.62604000	-4.35586500	1.89670600
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H	-3.74854100	-2.08500600	1.90084300
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H	-5.05472700	2.46606300	-0.80944900
C	5.75654700	-1.00724700	-2.80349300
C	6.04720800	-0.16132700	-4.02501300
O	7.23009300	-0.65817200	-4.57879000
H	5.69655100	-2.05206300	-3.08570800
H	6.55207800	-0.89827600	-2.07563600
H	6.14707500	0.88096200	-3.73204700
H	5.21613800	-0.23511200	-4.72334900
H	7.51224100	-0.11224100	-5.29880800
C	0.77288500	-5.34102400	-3.34839800
C	1.65553700	-5.17332000	-4.56702800
O	1.50410700	-6.33477700	-5.32933000
H	-0.24679300	-5.53752500	-3.65927800
H	1.11251800	-6.18043700	-2.75284800
H	2.68688300	-5.02939700	-4.25456900
H	1.34610900	-4.28846400	-5.11933800
H	2.11039400	-6.33394300	-6.05629000
C	-5.10097400	-2.20518900	-3.23058600
C	-4.80313400	-2.90610900	-4.53916100
O	-6.03370100	-3.10721400	-5.17014900
H	-5.64802600	-1.28883300	-3.42047000
H	-5.71168500	-2.83866800	-2.59801700
H	-4.29373800	-3.84621500	-4.34230300
H	-4.14155100	-2.28610400	-5.14064800
H	-5.92177300	-3.62667600	-5.95355300

C	-3.80591500	4.33407200	-2.81870500
C	-4.44679200	3.88457400	-4.11481600
O	-5.05327800	5.01489700	-4.66887900
H	-3.11931900	5.15042700	-3.01154000
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H	-5.17002900	3.09873900	-3.91152100
H	-3.68485500	3.47557100	-4.77538000
H	-5.55713700	4.77761600	-5.43434700
C	2.86465000	5.09238600	-2.61122000
C	2.21914300	5.63914000	-3.86695300
O	3.10100200	6.59310000	-4.38100000
H	3.84471200	4.69316400	-2.84543200
H	2.98660700	5.88302200	-1.88045900
H	1.25360700	6.07463600	-3.62153000
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H	2.71143100	7.03955400	-5.11927200
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H	-3.29478100	-0.69290700	3.67564800
H	-5.01715400	-1.01033900	3.47683900
H	-5.54113900	1.18680100	4.46965900
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H	-4.72486200	0.50432800	6.56136400
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C	-2.51691900	-4.31033900	4.38265400
O	-1.87843200	-4.55528600	5.60426600
H	-0.70759800	-3.50611800	3.57632700
H	-0.90629100	-5.24145600	3.33698900
H	-3.23451800	-5.08916800	4.14108700
H	-3.03942100	-3.35821500	4.39225200

H	-2.51135000	-4.54569900	6.30839500
C	3.21294100	-2.68067100	3.58393900
C	2.81239400	-3.73728400	4.59163000
O	3.13216400	-3.20959000	5.84828400
H	2.66624300	-1.76513700	3.77827000
H	4.27406400	-2.48078600	3.67676700
H	3.35589500	-4.65634600	4.39183000
H	1.74998100	-3.94612100	4.50849400
H	2.86419900	-3.81008300	6.52952700
C	3.27646600	2.25684200	3.85907600
C	4.06944800	1.53186700	4.92577000
O	3.59373500	2.01342700	6.15118300
H	2.22064400	2.04575800	3.98369800
H	3.43335200	3.32470800	3.95779600
H	5.12813500	1.73799700	4.79679400
H	3.91864000	0.46006700	4.83556500
H	4.02634100	1.56650600	6.86503600
C	-1.38812000	3.82053700	3.81523900
C	-0.53441600	4.36330200	4.94175000
O	-1.21545900	4.05122700	6.12432800
H	-1.51098000	2.75017100	3.93497400
H	-2.36484200	4.28920500	3.84590500
H	-0.40977400	5.43558700	4.82081500
H	0.44874500	3.90240300	4.91723900
H	-0.71072800	4.33479800	6.87352700
Cl	-0.07861000	-0.01983200	1.25010500
C	0.17165000	-0.55507800	-0.43391500
C	-0.12535500	0.63006000	-1.34342500
N	0.05510900	0.36311700	-2.82411100
C	-0.18186700	1.65545000	-3.53941900
C	1.43765900	-0.10746100	-3.13083000

C	-0.92861400	-0.64226600	-3.32046000
H	1.19221000	-0.88581900	-0.50003000
H	-0.49494900	-1.38289900	-0.59346500
H	-1.14566500	0.95055500	-1.21200500
H	0.52961800	1.45022900	-1.10007000
H	-0.08399100	1.47886100	-4.60070600
H	-1.17611500	2.00753700	-3.31330000
H	0.55039000	2.37840700	-3.21530300
H	1.56163600	-0.12136700	-4.20359200
H	1.57565100	-1.10186900	-2.74354900
H	2.15144800	0.56509500	-2.68688700
H	-1.92622000	-0.31048100	-3.09177200
H	-0.80574500	-0.73781600	-4.38944700
H	-0.74210500	-1.59357100	-2.85394500

B. Three-dimensional coordinates of DEP5 and G1.

Cartesian Co-ordinates (XYZ format)

C	3.15843800	-2.89970900	-1.01161700
C	2.04654000	-3.73428400	-0.96979400
C	1.41201700	-4.05907600	0.21286300
C	1.95641800	-3.54954100	1.39896000
C	3.05302300	-2.70635700	1.35758300
C	3.66646500	-2.35285700	0.15419800
C	0.17090500	-4.93978700	0.21506400
C	-1.13559800	-4.15651200	0.17678200
C	-1.75693300	-3.77120300	1.36490000

C -2.91872700 -3.01830400 1.37238600
C -3.50104900 -2.60674100 0.16798100
C -2.90475400 -3.02714400 -1.00457700
C -1.74243100 -3.78948900 -1.01279900
C -4.72660000 -1.70523500 0.13608300
C -4.36643900 -0.22512700 0.12289700
C -4.22552100 0.48982800 -1.05417000
C -3.81372800 1.81763200 -1.02747900
C -3.54449800 2.47950800 0.15565500
C -3.73821100 1.77467000 1.34968400
C -4.13201600 0.44814800 1.32163400
C -3.05202500 3.91901200 0.15079100
C -1.53413500 4.03707500 0.11626200
C -0.83275000 4.12478100 -1.07385100
C 0.55627600 4.17068900 -1.07084100
C 1.29068300 4.14240100 0.10004900
C 0.58158300 4.10670800 1.30729700
C -0.80138700 4.04432300 1.30301200
C 2.81229100 4.13624300 0.06547300
C 3.40604200 2.73303900 0.06773300
C 3.67855400 2.04603300 -1.10372400

C	4.15685300	0.74159600	-1.05986200
C	4.38147400	0.08038800	0.13341600
C	4.15062600	0.78822700	1.31917300
C	3.66514900	2.08411600	1.27513700
C	4.83289100	-1.37277000	0.14714700
O	3.70455400	-2.58600400	-2.23109600
O	-1.17730600	-4.11827500	-2.22246700
O	-4.43890200	-0.10981400	-2.27190600
O	-1.49420500	4.11748900	-2.27708700
O	3.42064500	2.61727000	-2.32501800
O	1.35267600	-3.92798700	2.54817500
O	-3.54743800	-2.63184300	2.50618300
O	-3.51304400	2.45904400	2.49478400
O	1.32117700	4.13271600	2.43972200
O	4.41926900	0.13348000	2.47174700
H	1.66729000	-4.13087400	-1.89432300
H	3.44702700	-2.28817800	2.26098000
H	0.21929800	-5.59926300	-0.64103200
H	0.17803100	-5.56334700	1.09857100
H	-1.29233500	-4.05504000	2.28671900
H	-3.34007200	-2.73897400	-1.94467600

H	-5.34766700	-1.91115500	0.99672800
H	-5.30715600	-1.94368700	-0.74447900
H	-3.69188600	2.33793800	-1.96095900
H	-4.24307400	-0.10164500	2.23368600
H	-3.42416300	4.42644600	1.02994400
H	-3.46999100	4.42171400	-0.71062700
H	1.07211600	4.21892000	-2.01294100
H	-1.34177600	3.97884400	2.22500900
H	3.19215500	4.67980000	0.91955600
H	3.13814500	4.66289500	-0.82110100
H	4.34246900	0.22908200	-1.98733000
H	3.45538200	2.61289000	2.18202700
H	5.44903500	-1.54910300	1.01780900
H	5.44715500	-1.55138300	-0.72439300
C	-5.71163100	0.12463000	-2.85095600
C	-5.78223200	-0.62063900	-4.16751000
H	-1.39579800	-6.33903800	-4.68635600
H	-5.84992400	1.19031900	-3.00130600
H	-6.48508300	-0.21551700	-2.17027700
H	-5.64665300	-1.68557200	-4.01374100
H	-5.01389300	-0.27059600	-4.84871800

H	5.79705200	-3.74022300	-4.53871000
C	-1.66976700	5.38446200	-2.88833900
C	-2.42932200	5.18743900	-4.18369300
H	4.91020600	4.15599600	-4.86520500
H	-0.70011500	5.83505000	-3.07314800
H	-2.21370100	6.03757000	-2.21384500
H	-3.40185500	4.74611500	-3.99557300
H	-1.88018200	4.53539000	-4.85444900
H	-2.57739600	6.14033500	-4.68018800
C	4.54453000	3.15156200	-3.00411000
C	4.07151400	3.74199700	-4.31602900
H	-6.74798600	-0.46393900	-4.63566900
H	5.27246500	2.36519900	-3.17442000
H	5.01454800	3.90769800	-2.38372800
H	3.35218600	4.53503100	-4.14359900
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H	1.59886000	-4.16997800	5.83912300
C	4.60137100	-3.54401900	-2.76701600
C	5.10882100	-3.02759600	-4.09717100
H	-3.91434800	-3.10376000	5.75991500
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H 5.42009700 -3.70068500 -2.07224800
H 5.62894200 -2.08462200 -3.96969100
H 4.28604300 -2.87519700 -4.78735600
H -3.95545500 2.58052900 5.77105800
C -1.73925600 -5.24741900 -2.87114300
C -0.98595900 -5.48139700 -4.16402300
H 1.34386400 4.66406000 5.70553400
H -2.79179200 -5.06717200 -3.06356300
H -1.66702700 -6.11067400 -2.21803400
H 0.06376300 -5.67114700 -3.96896500
H -1.06340200 -4.61779200 -4.81607200
H 4.93287800 0.37147900 5.73120400
C 4.40246500 0.82012800 3.70173200
C 4.92311500 -0.12404200 4.76616400
H 3.39031400 1.13734100 3.93135600
H 5.02879300 1.70364100 3.63652800
H 5.93221000 -0.44229900 4.53249500
H 4.29409900 -1.00397300 4.84121500
C 0.69821300 4.31438000 3.69006400
C 1.78566400 4.51122300 4.72654400
H 0.09287500 3.44580200 3.92873500

H	0.04742000	5.18162000	3.65220200
H	2.39136200	5.37632300	4.48362500
H	2.43189700	3.64216000	4.77672800
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H	-3.25231900	1.03710500	3.94702500
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H	-4.18706300	-1.62382200	4.85015900
C	1.94957300	-3.63861300	3.79078900
C	1.16132800	-4.36020500	4.86475700
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H	2.98166500	-3.97329300	3.78770600
H	1.16709000	-5.42934900	4.68802900
H	0.13230500	-4.01965300	4.88147900

C1	-0.09299700	0.01213000	1.21569900
C	0.56494500	0.22629100	-0.42965800
C	-0.50297900	-0.23363100	-1.41235100
N	-0.12322300	-0.13475600	-2.87528300
C	-1.27459200	-0.67396300	-3.66345400
C	0.12397400	1.27963200	-3.28384300
C	1.08133700	-0.95906500	-3.18482400
H	0.80621800	1.26871200	-0.53009400
H	1.46021200	-0.36592700	-0.47723600
H	-0.74572800	-1.26679400	-1.23010000
H	-1.39452300	0.35895900	-1.28957200
H	-1.05289300	-0.55926300	-4.71434400
H	-1.39543100	-1.71865200	-3.42511200
H	-2.17213000	-0.13363600	-3.40819500
H	0.27121500	1.29901300	-4.35396600
H	1.01269600	1.64968000	-2.80073000
H	-0.72677700	1.88689900	-3.01982300
H	0.89982100	-1.97247400	-2.86977000
H	1.24956000	-0.92745200	-4.25129600
H	1.94088200	-0.56158400	-2.67572500

11. Reference

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