Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Asymmetric Liquid Crystalline Dibenzo[a,h]anthracenes for Organic Semiconductors with High Mobility and Thermal Stability

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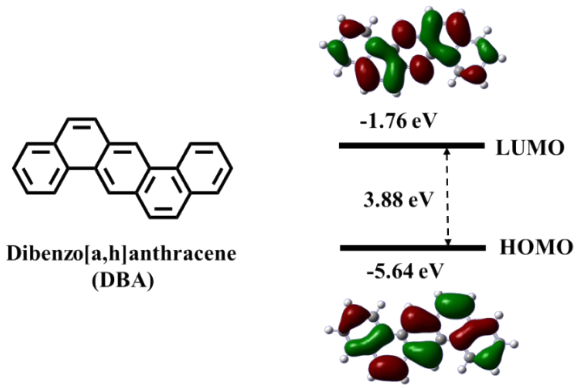


Fig. S1 Calculated frontier molecular orbitals of dibenzo[a,h]anthracene (DBA)

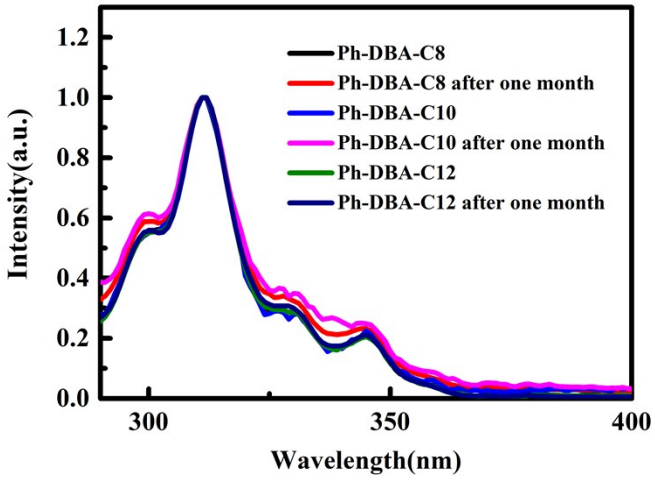


Fig. S2 Time-dependent UV-vis spectra of Ph-DBA-Cn in dilute $CHCl_3$

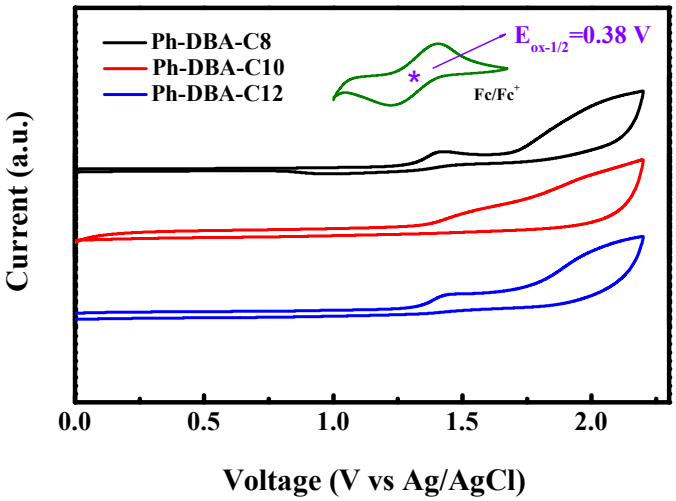


Fig. S3 The CVs of Ph-DBA-Cn in CH_2Cl_2 solution (Cyclic voltammograms measured in 0.1 M tetrabutylammonium hexafluorophosphate solutions with the ferrocene/ferrocenium (Fc/Fc^+) redox couple as the external standard and Ag/AgCl as reference electrode at a scanning ramp of 50 mV s^{-1})

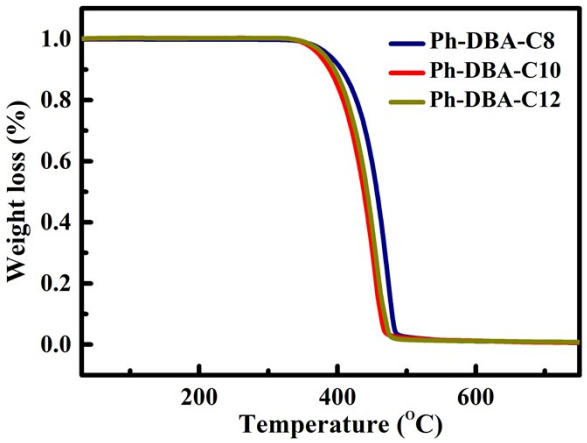


Fig. S4 TGA thermograms of Ph-DBA-Cn at a heating rate of 10 °C/min under N_2 atmosphere

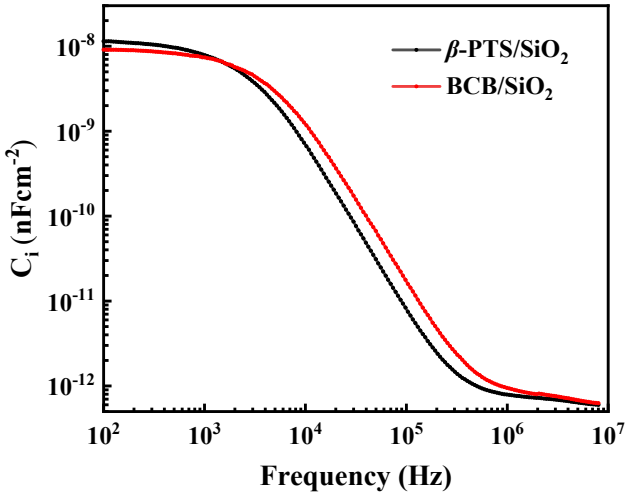


Fig. S5 Frequency dependence of capacitance (C_i) for β-PTS/SiO_2 and BCB/SiO_2 dielectrics measured from the sandwich structure (Au/insulator/heavily *p*-doped Si), showing C_i of 11.5 and 9.1 nF cm^{-2} for β-PTS/SiO_2 and BCB/SiO_2 dielectrics, respectively, at 100 Hz.

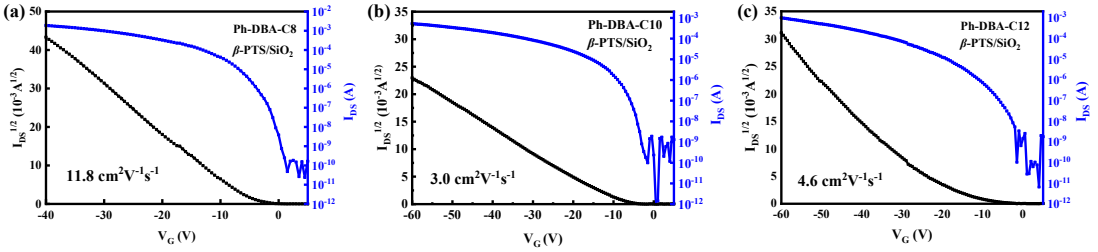


Fig. S6 Transfer curves of Ph-DBA-Cn OTFTs on the β-PTS/SiO_2 dielectric

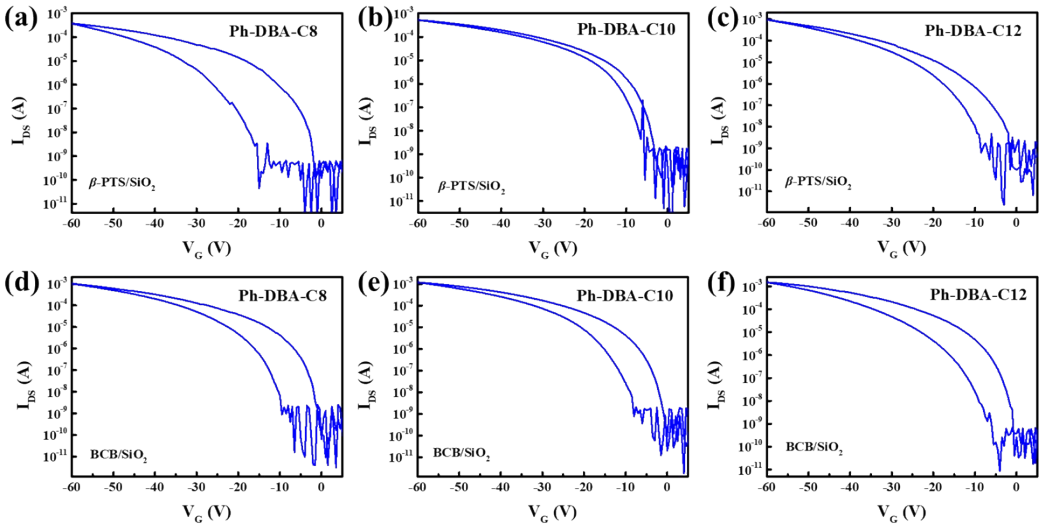


Fig. S7 Transfer curves of Ph-DBA-Cn OTFTs during forward and the forward and reverse scanning

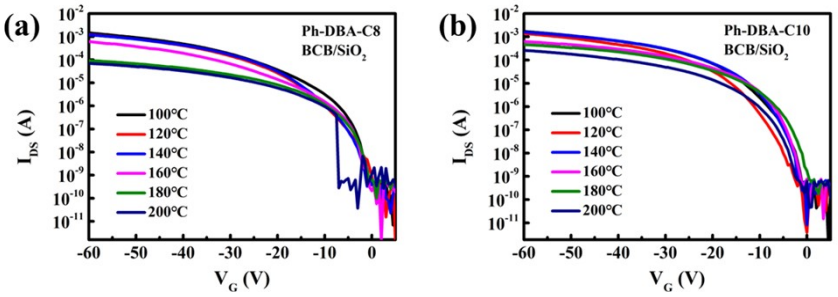


Fig. S8 Temperature-related transfer characteristics OTFTs on the BCB/SiO2 dielectric (a) Ph-DBA-C8, (b) Ph-DBA-C10

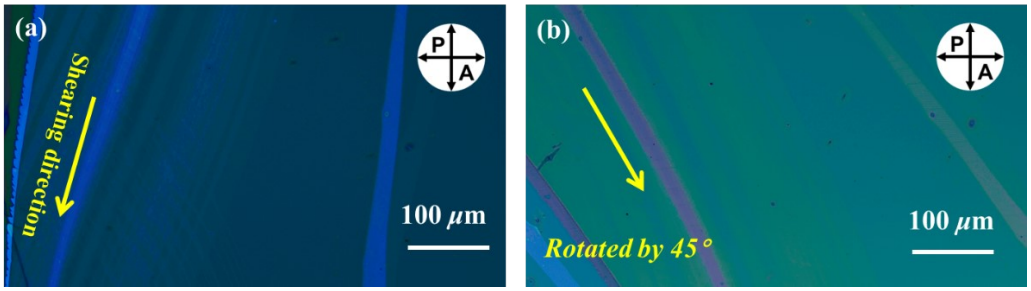


Fig. S9 POM textures of the blade-coated Ph-DBA-C10 film on the BCB-covered substrate (a) 0°, and (b) 45°.

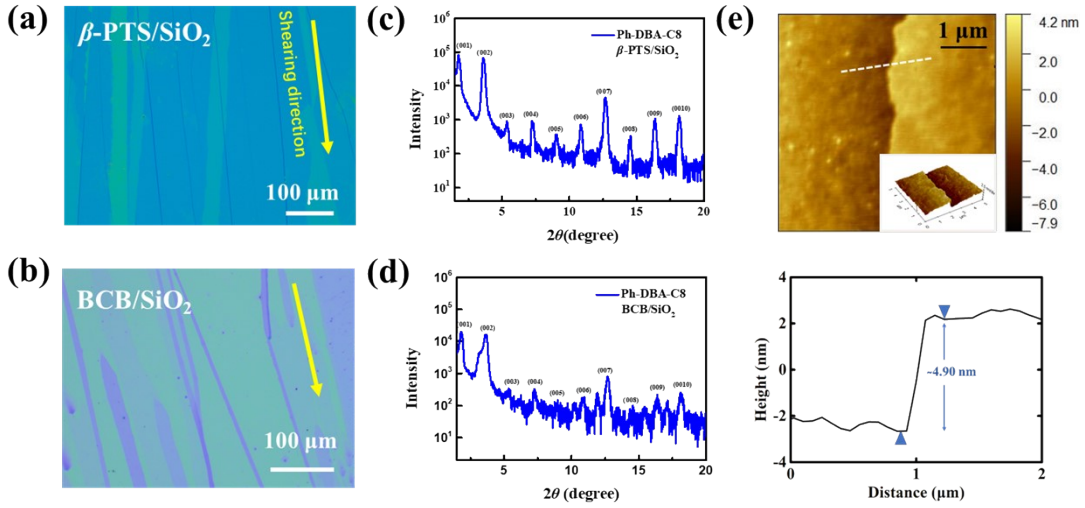


Fig. S10 Optical microscopy images and XRD patterns of the blade-coated Ph-DBA-C8 films on the β-PTS/SiO_2 (a,c) and BCB/SiO_2 (b,d) dielectrics. (e) AFM topographic image and corresponding cross-sectional height profile of the blade-coated Ph-DBA-C8 film on the BCB/SiO_2 dielectric.

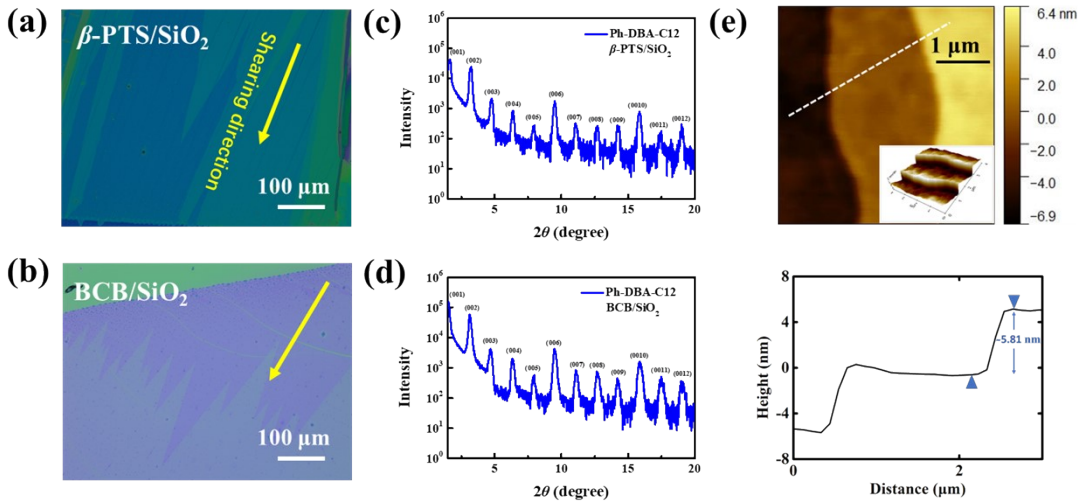


Fig. S11 Optical microscopy images and XRD patterns of the blade-coated Ph-DBA-C12 films on the β-PTS/SiO_2 (a,c) and BCB/SiO_2 (b,d) dielectrics. (e) AFM topographic image and corresponding cross-sectional height profile of the blade-coated Ph-DBA-C12 film on the BCB/SiO_2 dielectric.

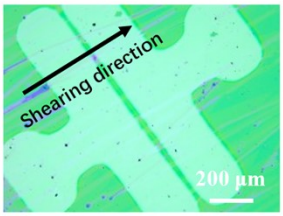


Fig. S12 The optical microscopy image of source/drain electrodes on the blade-coated film

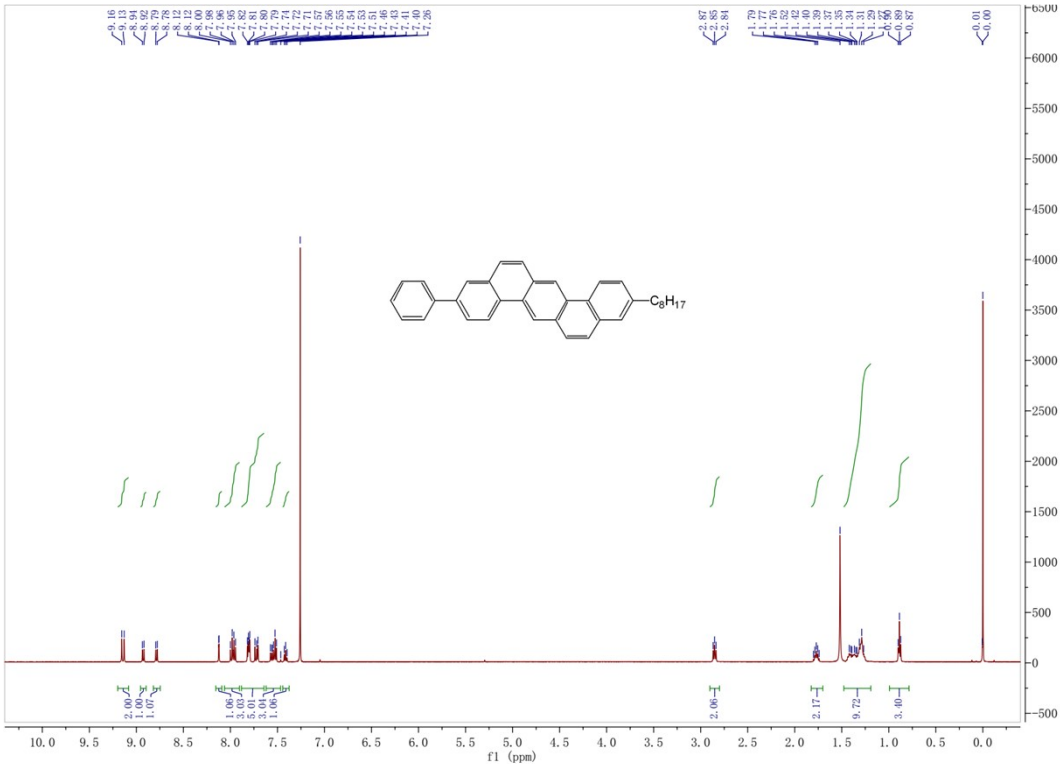
Table S1 Summary of thermal behaviors of phase-transition temperatures (°C) with corresponding transitions enthalpies (ΔH/KJmol^{-1}) and phases of Ph-DBA-Cn determined by the DSC curves and POM textures during the second heating process at a rate of 10 °C/min.

Compound	Phase Transition T/°C (ΔH/KJmol^{-1})
Ph-DBA-C8	C_{r1} 131 (-) C_{r2} 207 (0.37) SmE 279 (1.70) SmA 339 (1.28) Iso
Ph-DBA-C10	C_{r1} 129 (-) C_{r2} 197 (0.46) SmE 276 (1.56) SmA 332 (1.20) Iso
Ph-DBA-C12	C_{r1} 121 (0.47) C_{r2} 191 (0.31) SmE 273(1.37) SmA 322 (1.03) Iso
Crystalline: Cr, Smectic: Sm, Isotropic: Iso.	

Table S2 Structural parameters of the blade-coated Ph-DBA-Cn films

Compound	Dielectrics	d_{001} (Å)[a]	L (Å)[b]	θ_{tilt} (°)[c]
Ph-DBA-C8	β-PTS/SiO_2	50.1	27.2	~23
	BCB/SiO_2	49.1		~26
Ph-DBA-C10	β-PTS/SiO_2	50.1	29.4	~32
	BCB/SiO_2	51.0		~30
Ph-DBA-C12	β-PTS/SiO_2	52.8	32.3	~35
	BCB/SiO_2	—		—

[a]Interlayer distance determined from the (001) reflection of the XRD patterns. [b]Molecular length estimated from the DFT-Optimized structures. [c]Molecular inclination angle with respect to the substrate normal, defined as $\theta_{tilt} = \cos^{-1}(d_{001}/2L)$.



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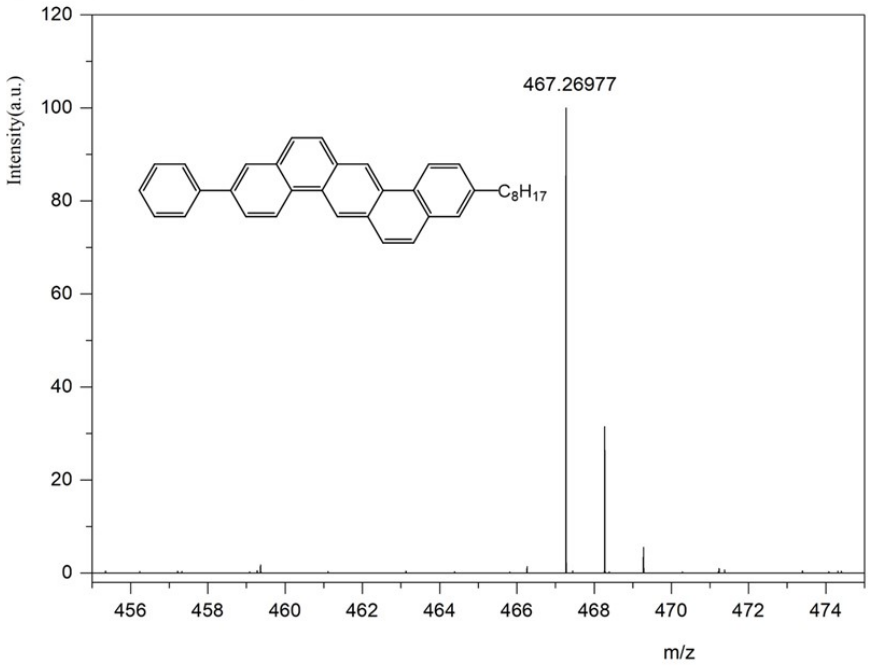
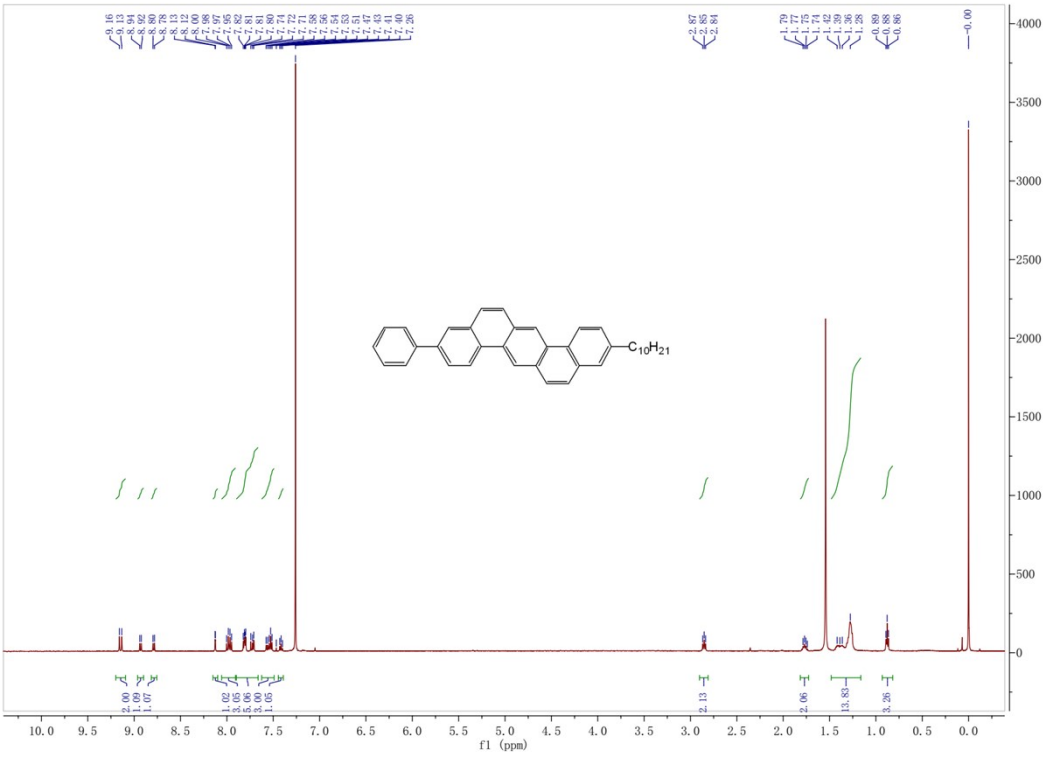
T:_FTMS + p APCI corona Full ms [50.0000-750.0000]





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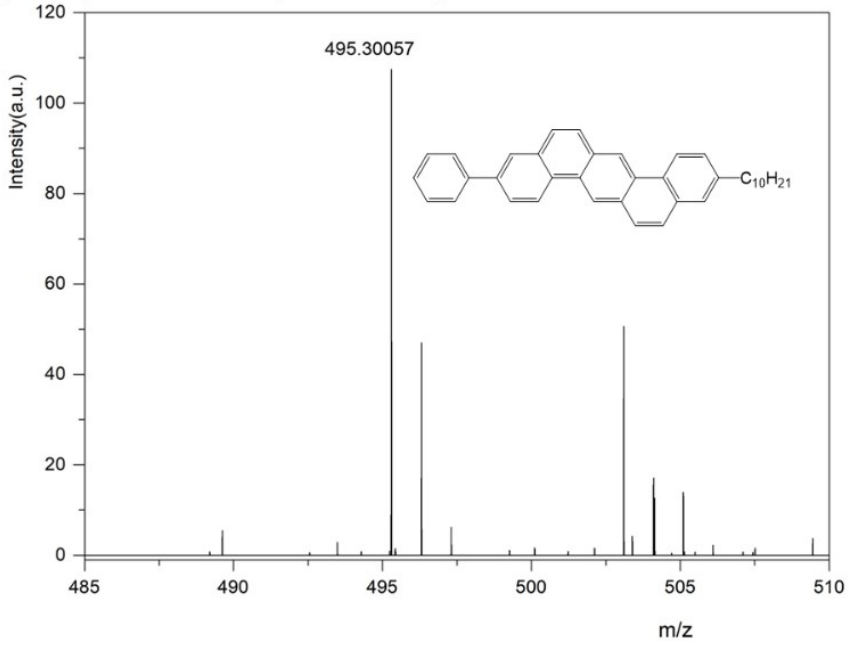
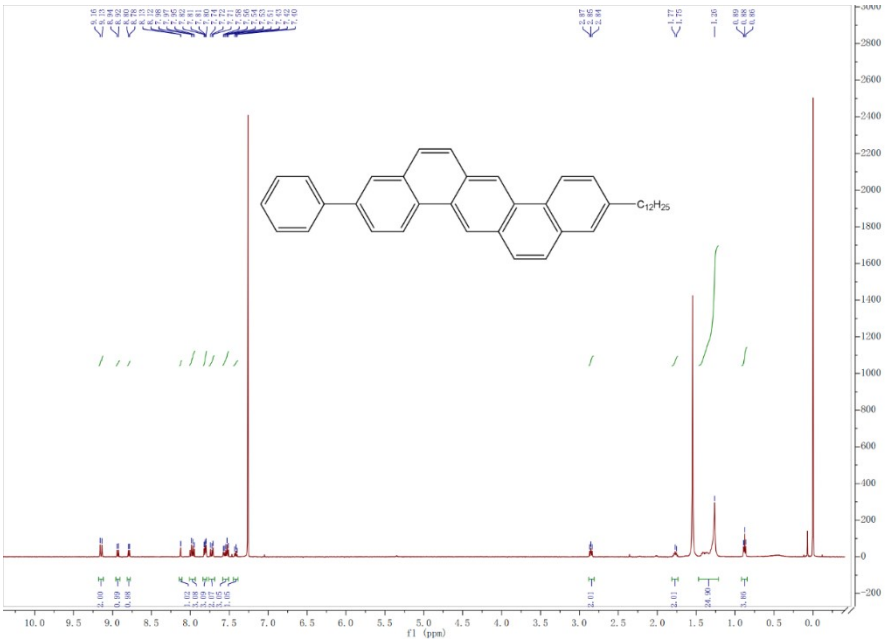
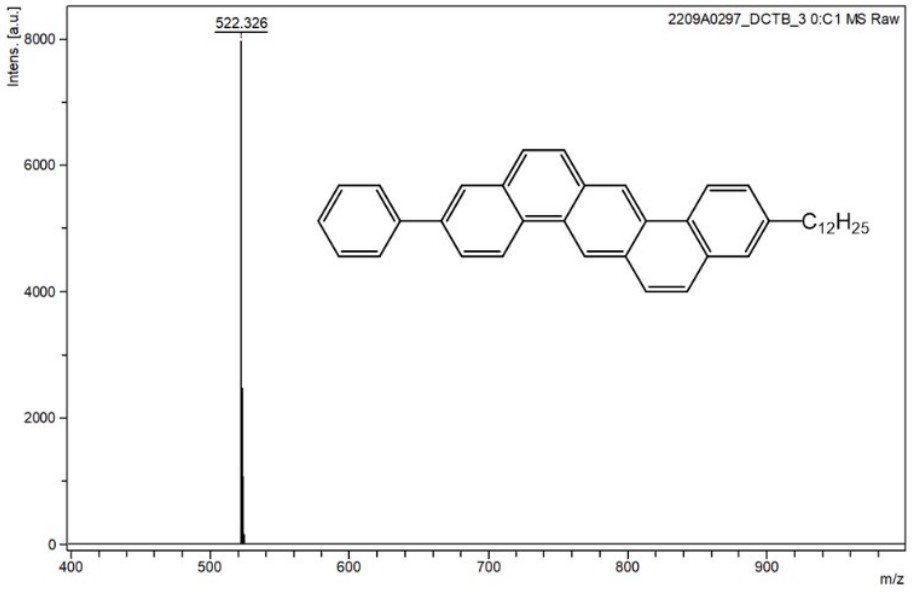
T:_FTMS + p APCI corona Full ms [50.0000-750.0000]



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