Electronic Supplementary Material (ESI) for ChemComm.

Separation and Electric Characterisation of all 18 Isomers BisPCBM

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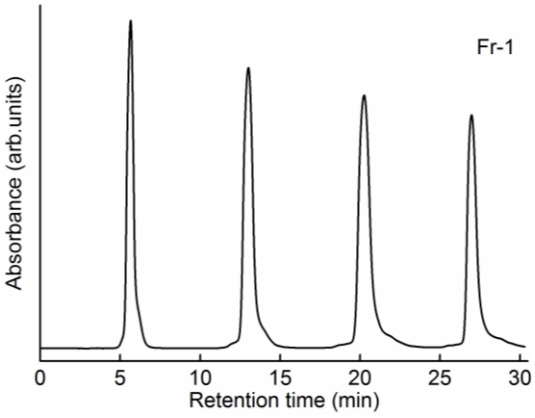
S1 The HPLC spectra during purification process

The HPLC spectra are listed according to the fraction purifications. They demonstrate the whole purification procedure for isolating all 18 isomers from the BisPCBM mixture. Pure Fr-1 to Fr-7 were purified from different stages via various columns, followed with purification test to show >99% purity. Fr-1, Fr-4, Fr-6 and Fr-7 were easily purified out with silica column. Other fractions with more isomers were purified out through recycling via more stages with 5PBB and 5PYE column due to the reduction time per cycle.

(A) Stage 2



(B) Purity test

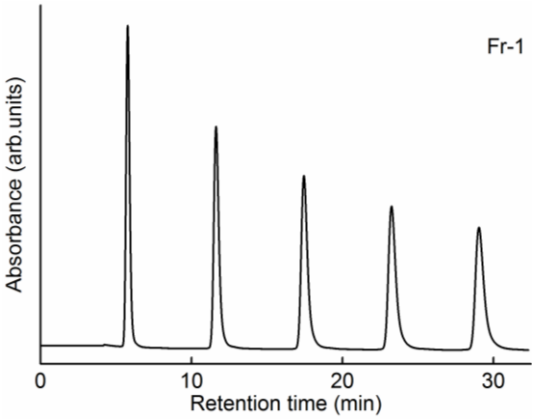
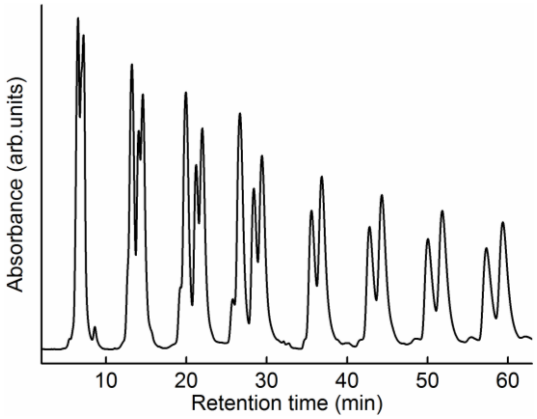
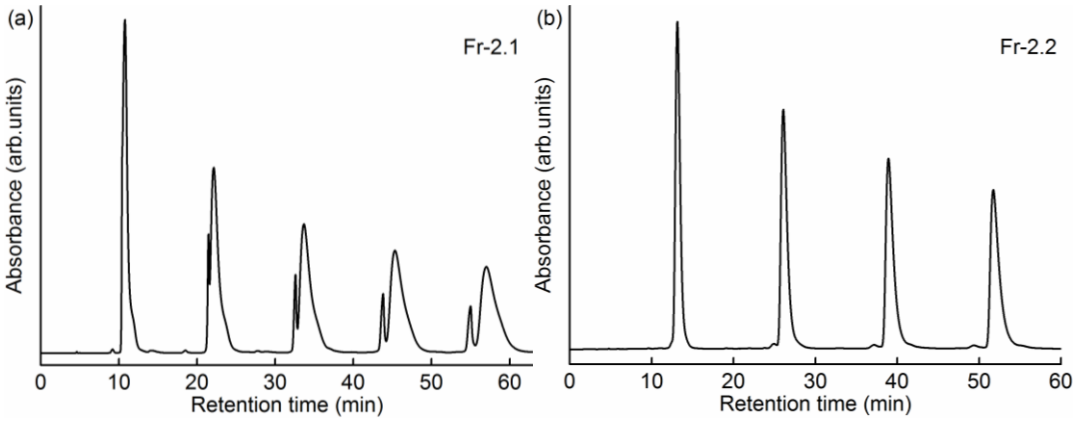


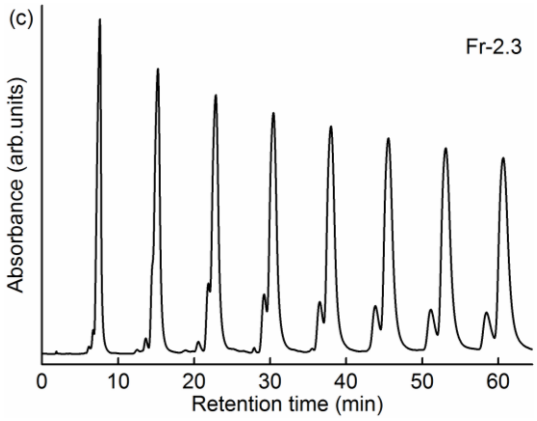
Fig.1 Purification process of Fr-1

(A) Stage 2

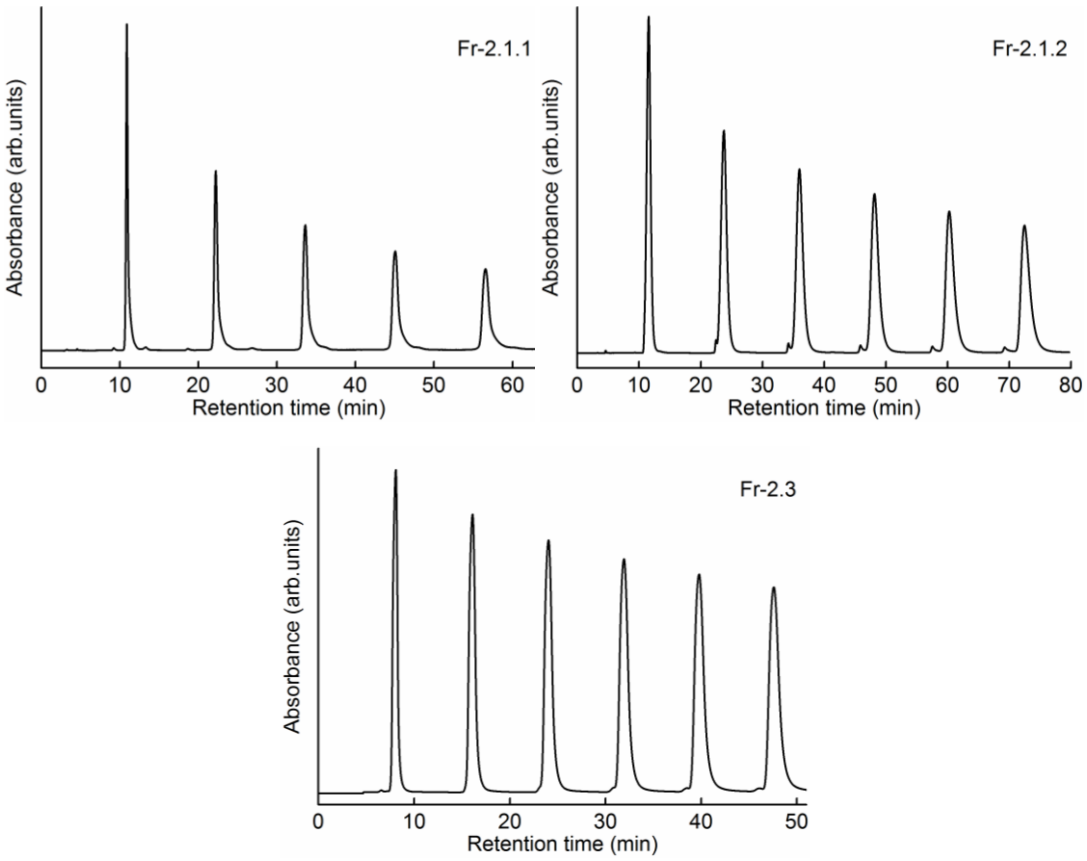


(B) Stage 3





(C) Stage 4



(D) Purity test

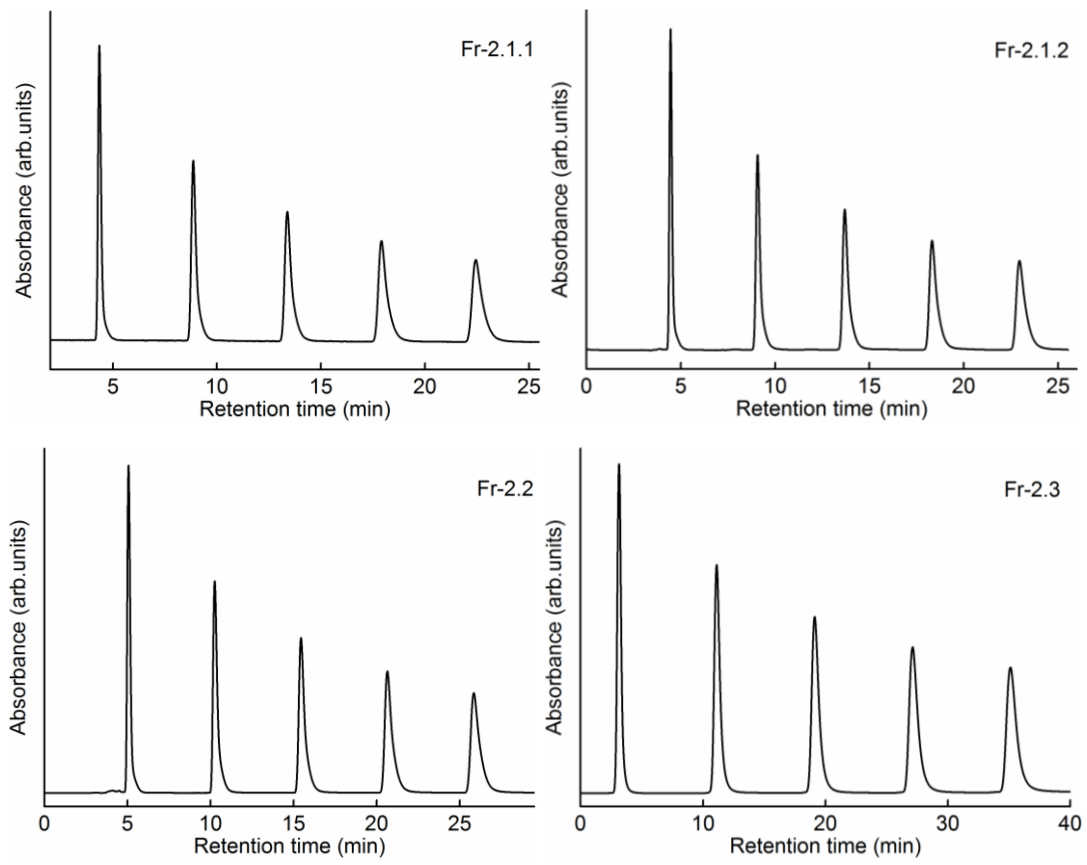
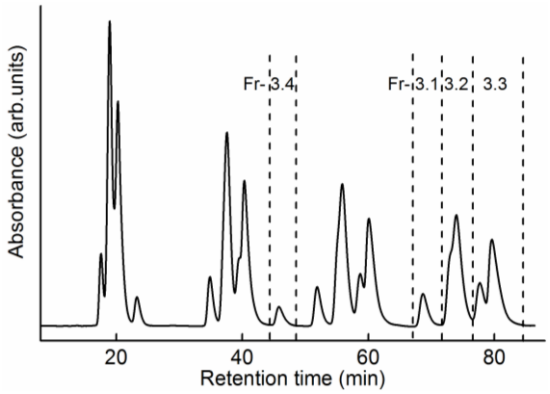
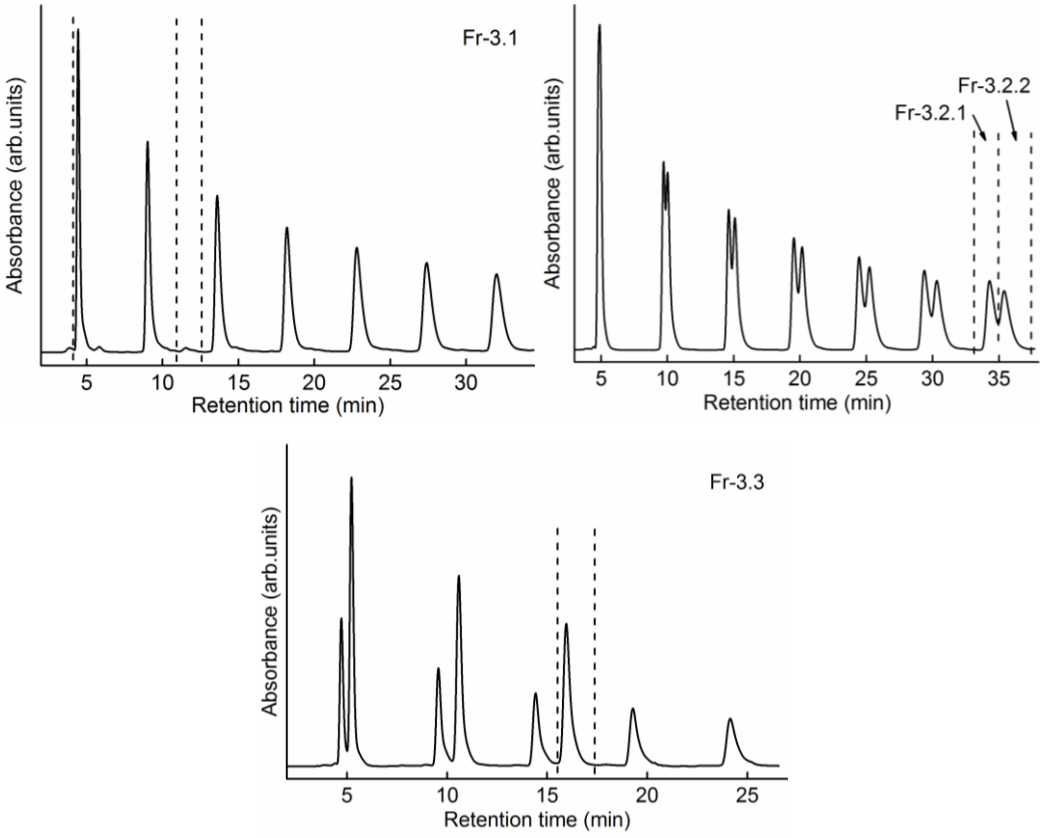


Fig.2 Purification process of Fr-2

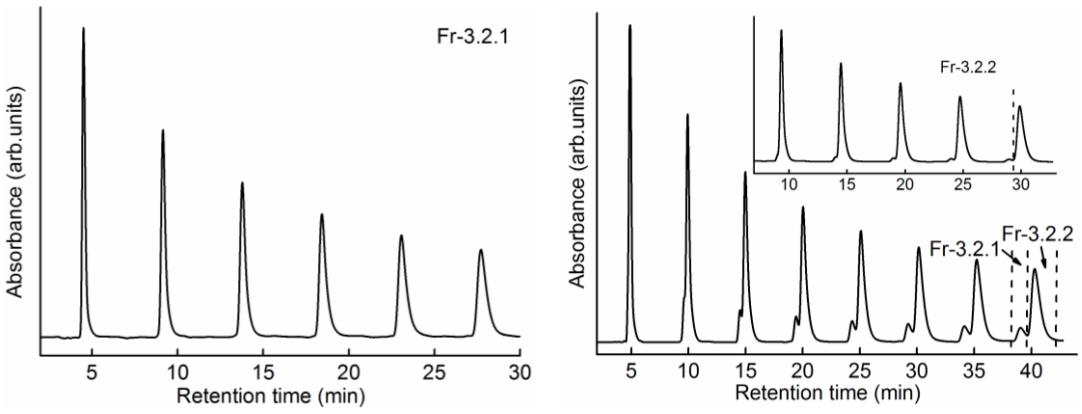
(A) Stage 2



(B) Stage 3



(C) Stage 4



(D) Purity Test

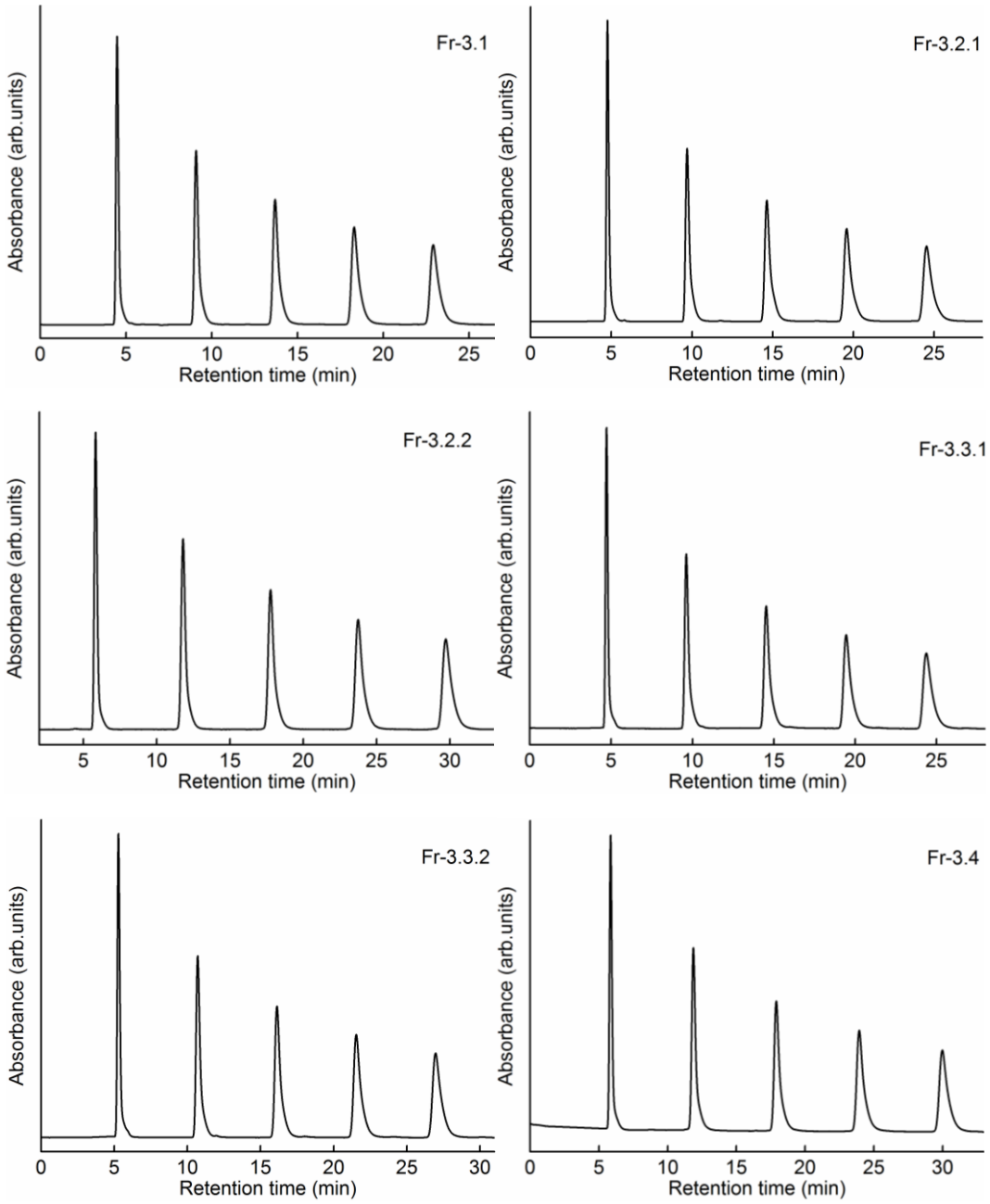


Fig.3 Purification process of Fr-3

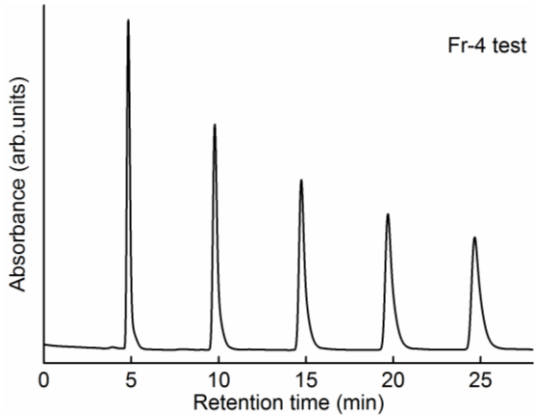
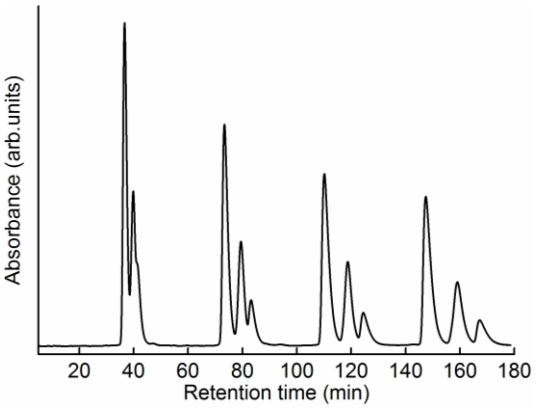
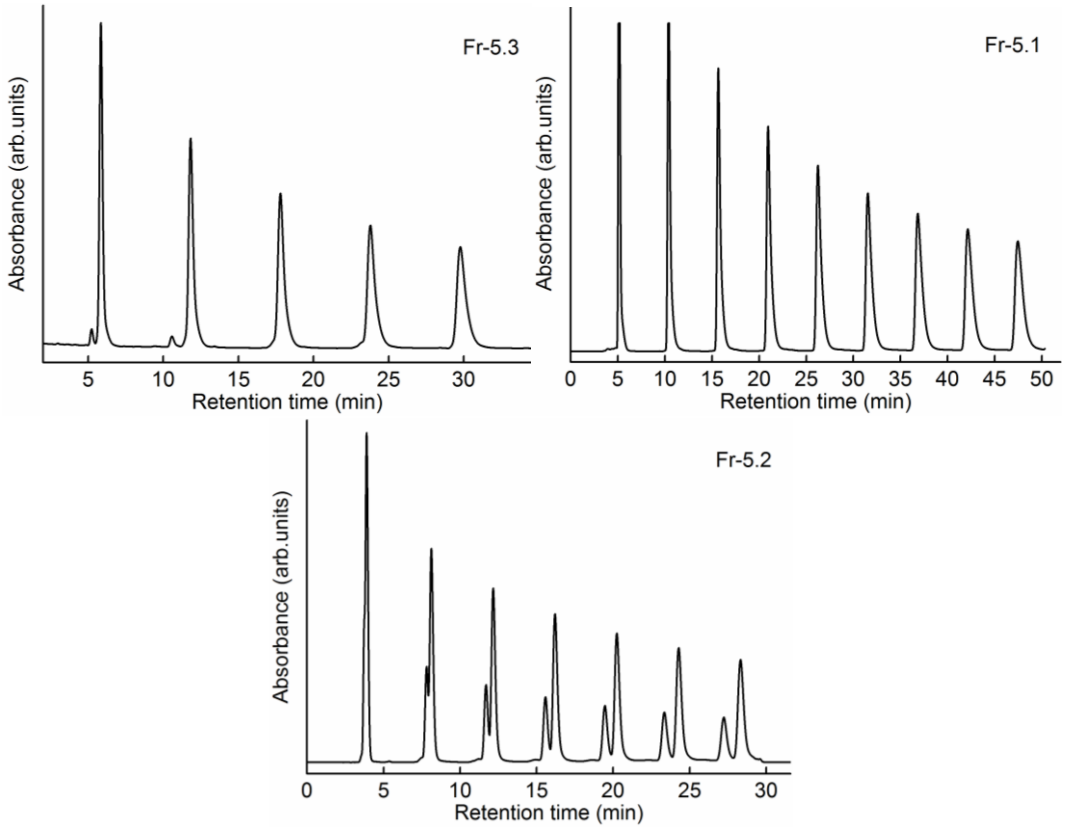


Fig.4 Purification process of Fr-4

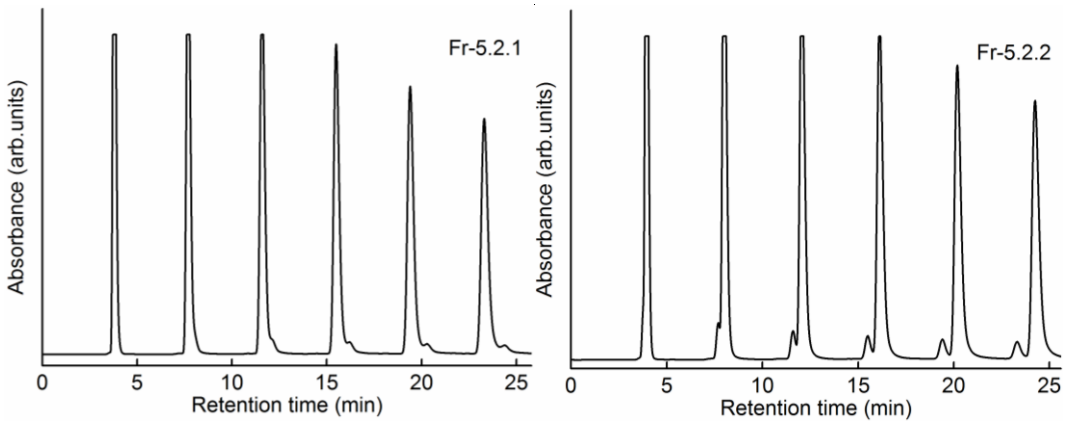
(A) Stage 2



(B) Stage 3



(C) Stage 4



(D) Purity test

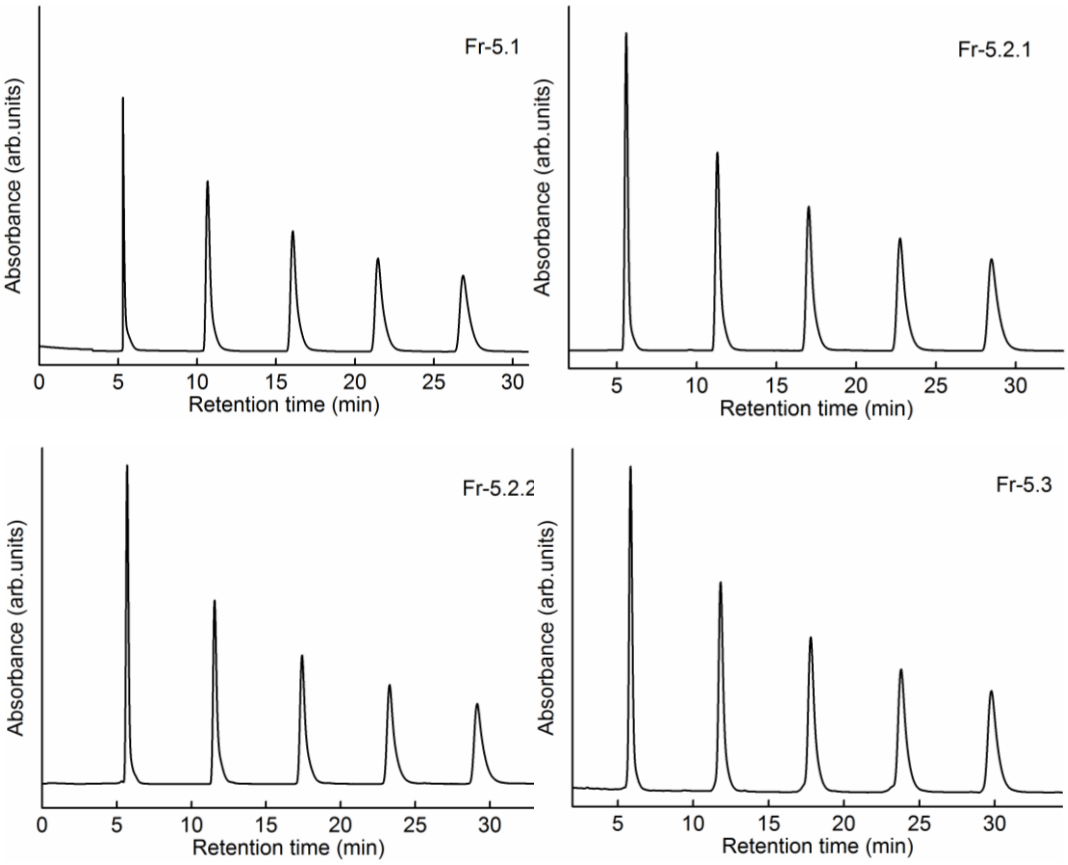
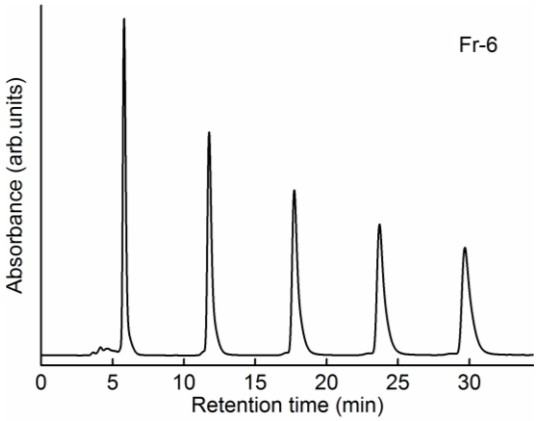


Fig.5 Purification process of Fr-5

(A) Stage 2



(B) Purity test

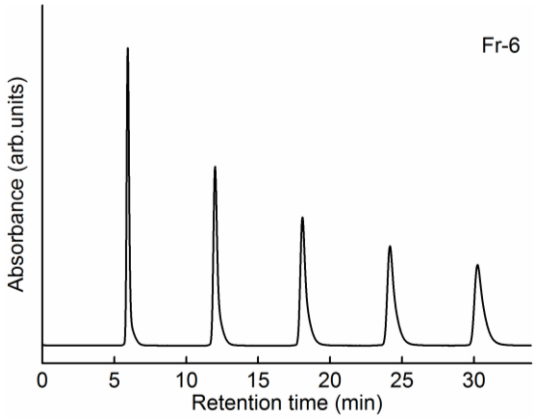
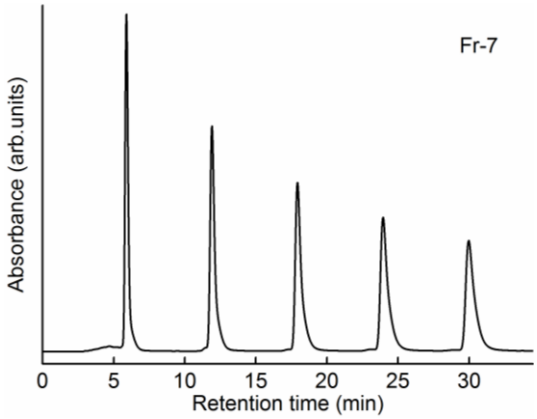


Fig.6 Purification process of Fr-6

(A) Stage 2



(B) Purity test

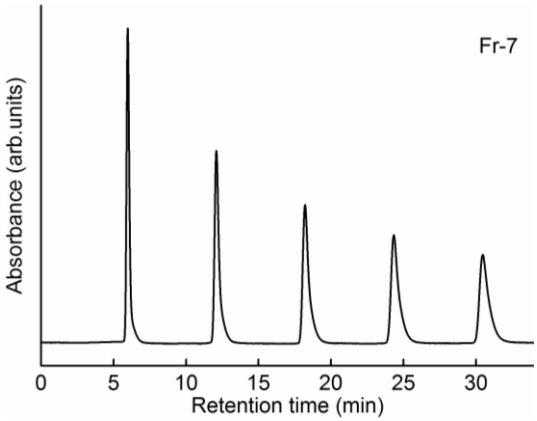
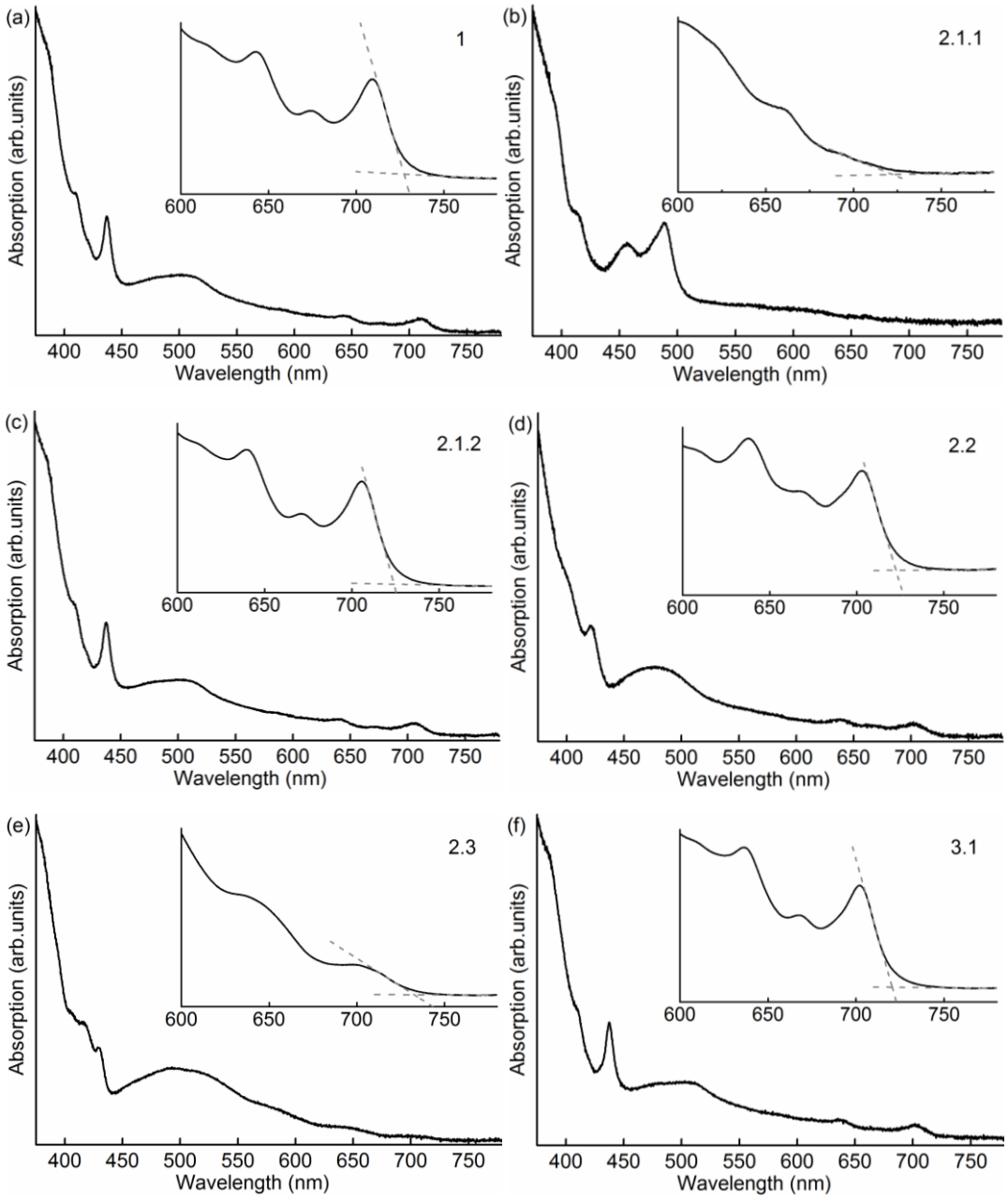
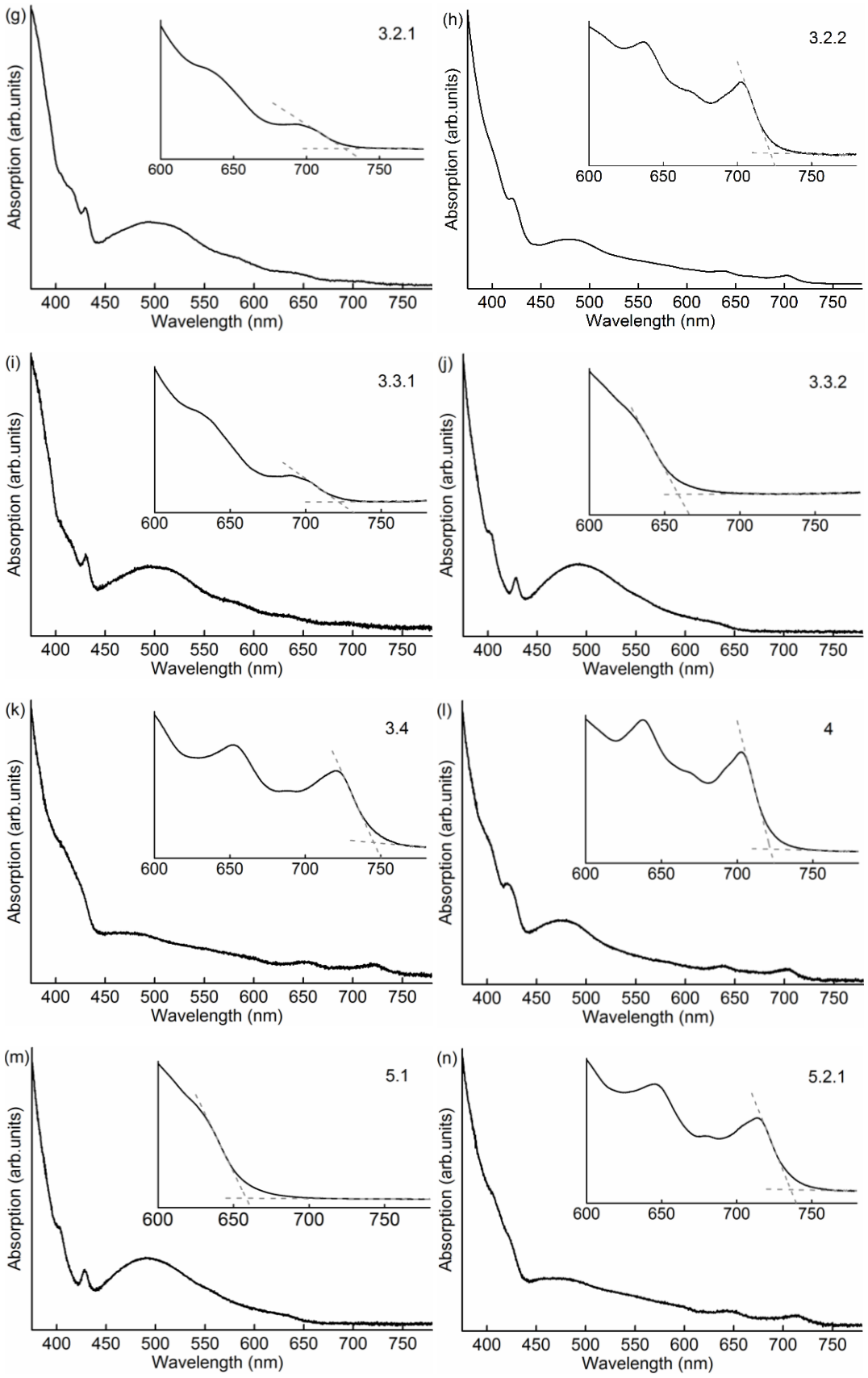


Fig.7 Purification process of Fr-7

S2 UV-Vis spectra for 18 isomers, BisPCBM mixture and PCBM

The UV-Vis spectra show absorption of individual isomer from Fr-1 to Fr-7, PCBM and BisPCBM full mixture, range from the 350-780nm with the same test parameters. The inserted figures on the right top of each picture display the HOMO-LUMO gap calculation according to the first onset of peaks scanning started from 780nm. The absorption similarities and differences for all spectra are quite clear, which can be applied for further discussions about the molecular structural determination.




(g)
3.2.1
(h)
3.2.2
(i)
3.3.1
(j)
3.3.2
(k)
3.4
(l)
4
(m)
5.1
(n)
5.2.1
Absorption (arb.units)
Wavelength (nm)
400 450 500 550 600 650 700 750
600 650 700 750

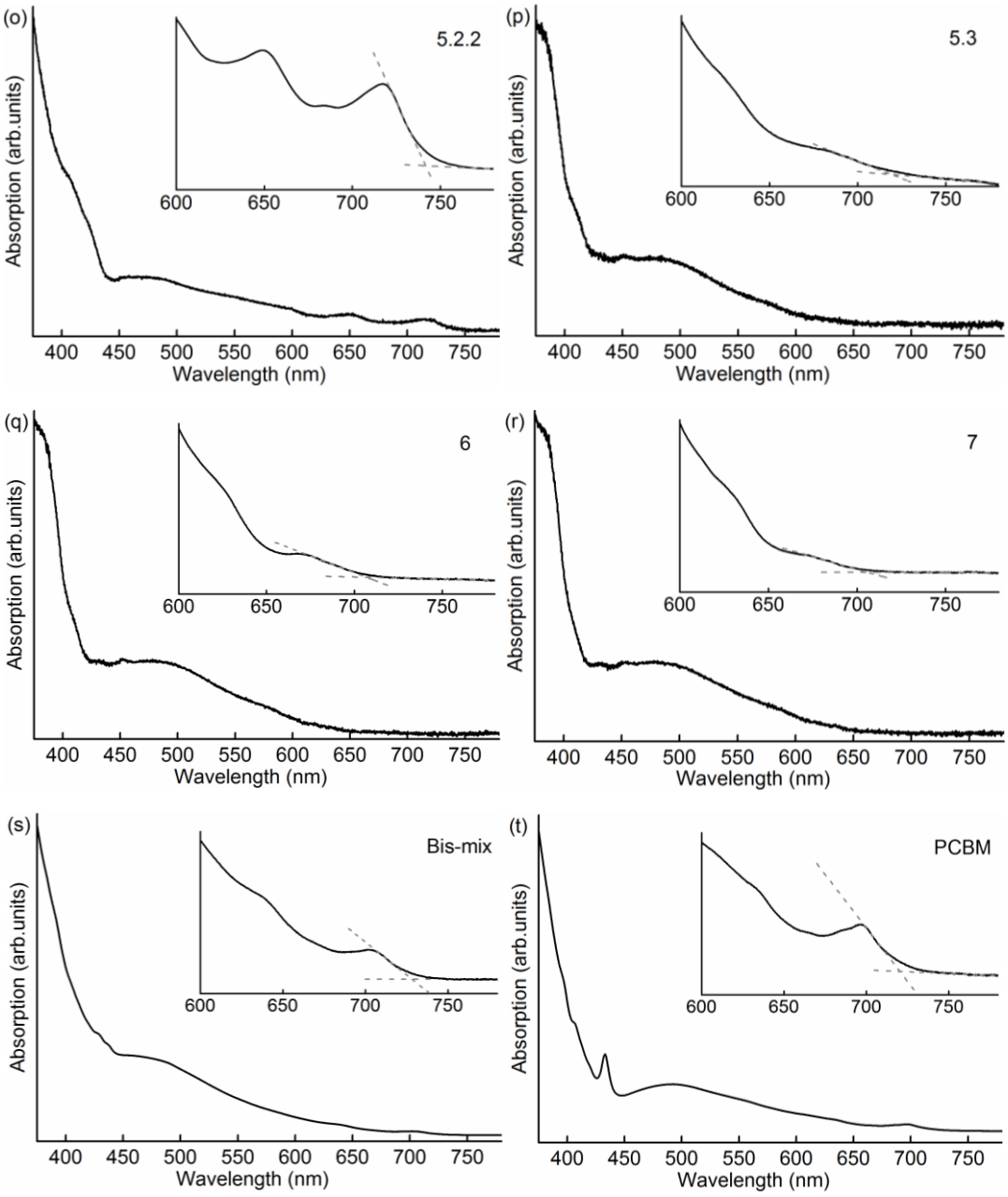
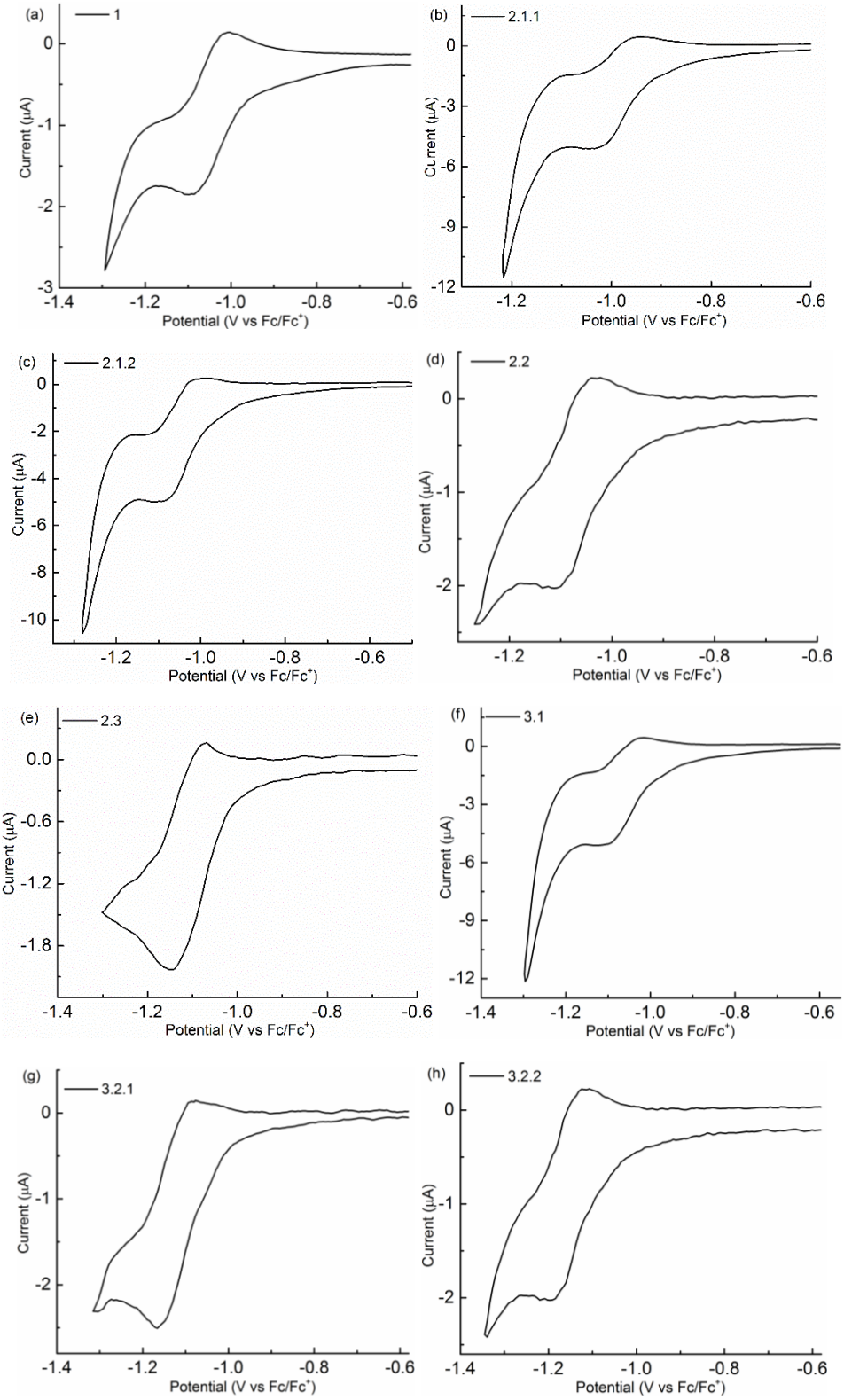
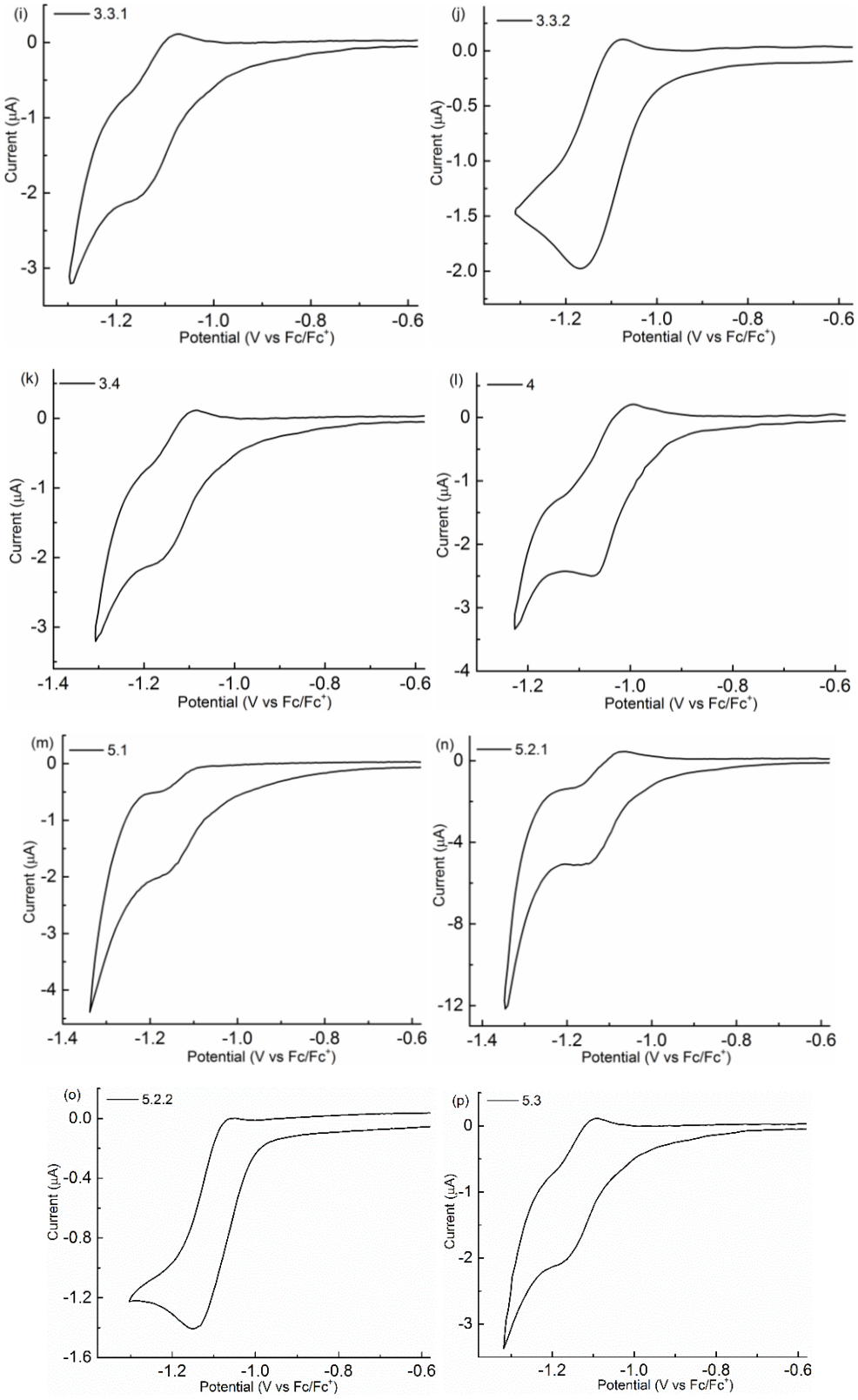


Fig. 8 UV-Vis spectra for 18 isomers, BisPCBM mixture and PCBM

S3 Cyclic Voltammograms of 18 isomers, BisPCBM mixture and PCBM

All cyclic voltammograms display the reversible reduction and oxidation process of all the isomers, PCBM and BisPCBM mixture from 0.8 to -0.8 V. All the data refers to the average of Ferrocene peak couple (Fc 1/2) as zero point. The onsets of first reduction peaks are the LUMO levels of all the samples. The isomer LUMO levels are quite different from each other ranging from -3.7 to 3.9 eV, compared to the PCBM -3.91 eV and BisPCBM -3.82 eV.




(i)
3.3.1
Current (μA)
Potential (V vs Fc/Fc+)
(j)
3.3.2
Current (μA)
Potential (V vs Fc/Fc+)
(k)
3.4
Current (μA)
Potential (V vs Fc/Fc+)
(l)
4
Current (μA)
Potential (V vs Fc/Fc+)
(m)
5.1
Current (μA)
Potential (V vs Fc/Fc+)
(n)
5.2.1
Current (μA)
Potential (V vs Fc/Fc+)
(o)
5.2.2
Current (μA)
Potential (V vs Fc/Fc+)
(p)
5.3
Current (μA)
Potential (V vs Fc/Fc+)

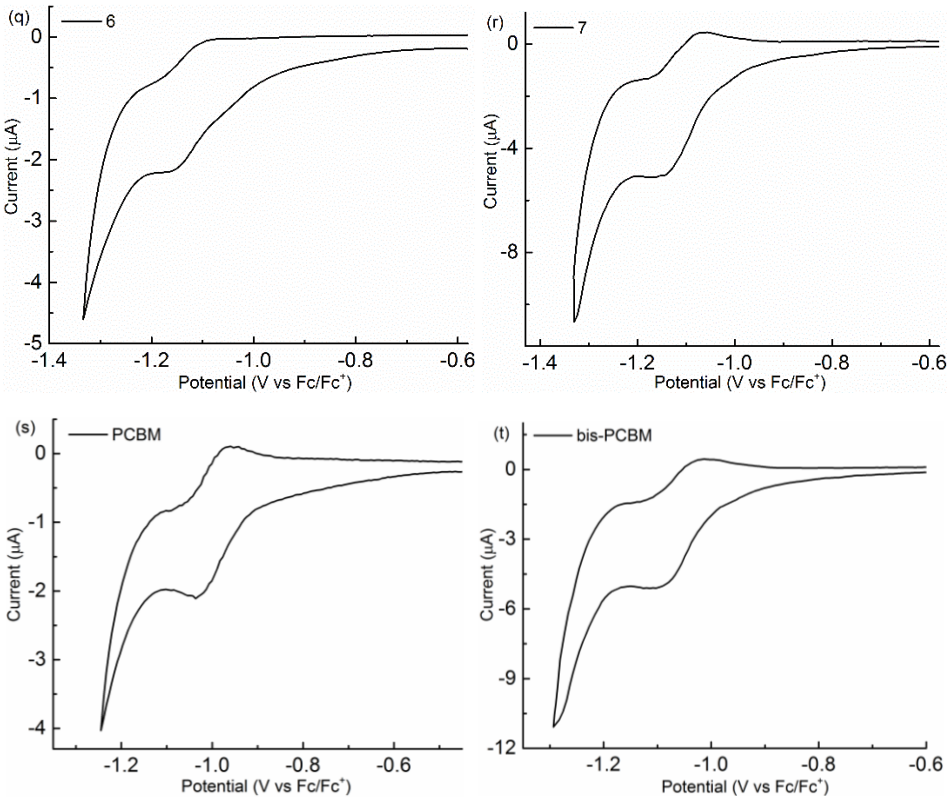


Fig.9 CV of 18 isomers, BisPCBM mixture and PCBM