

Novel Diketopyrrolopyrrole-based π -Conjugated Molecules Synthesized via One-Pot Direct Arylation Reaction

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Supplementary Information

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1.DFT-optimized geometries

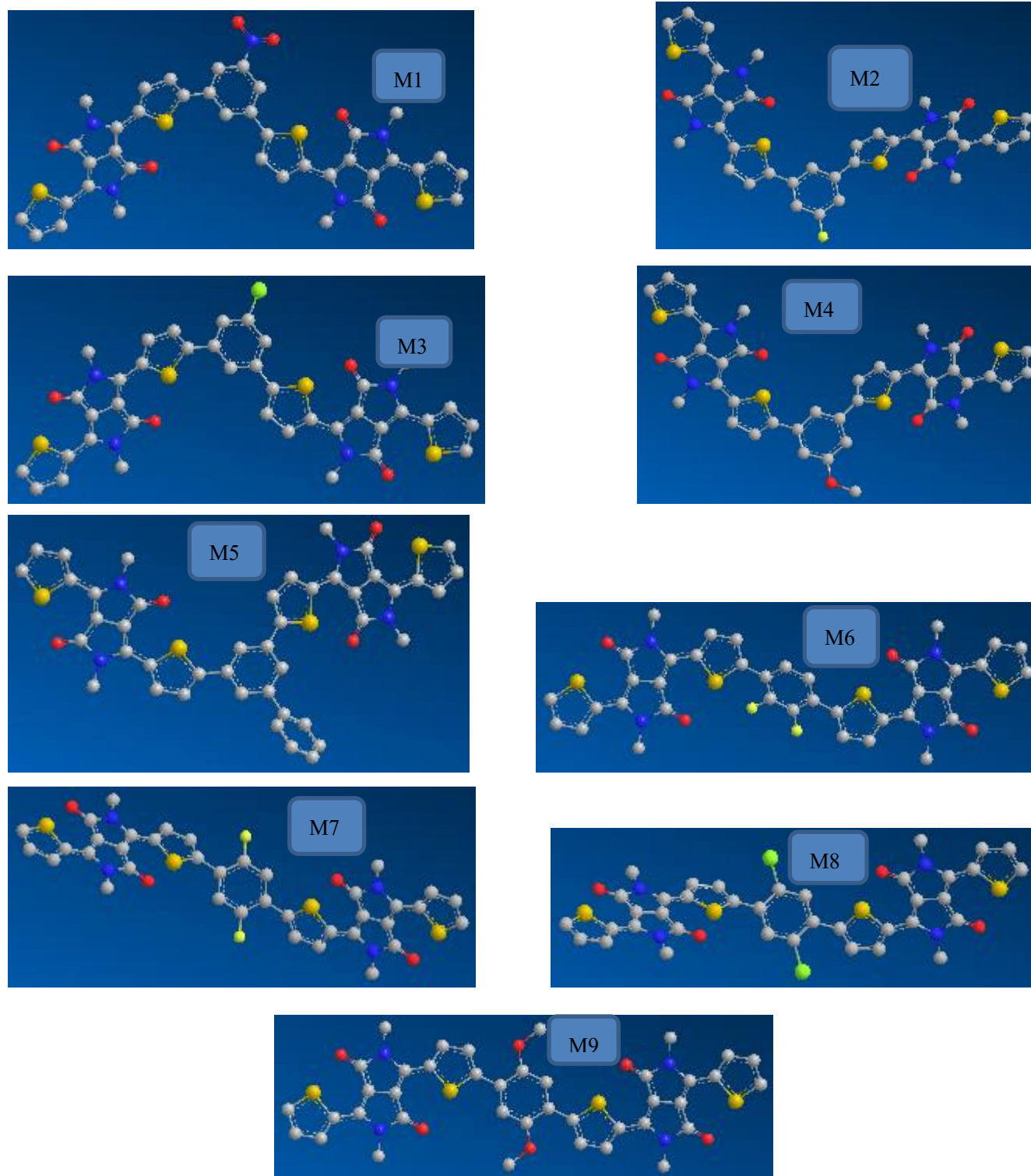
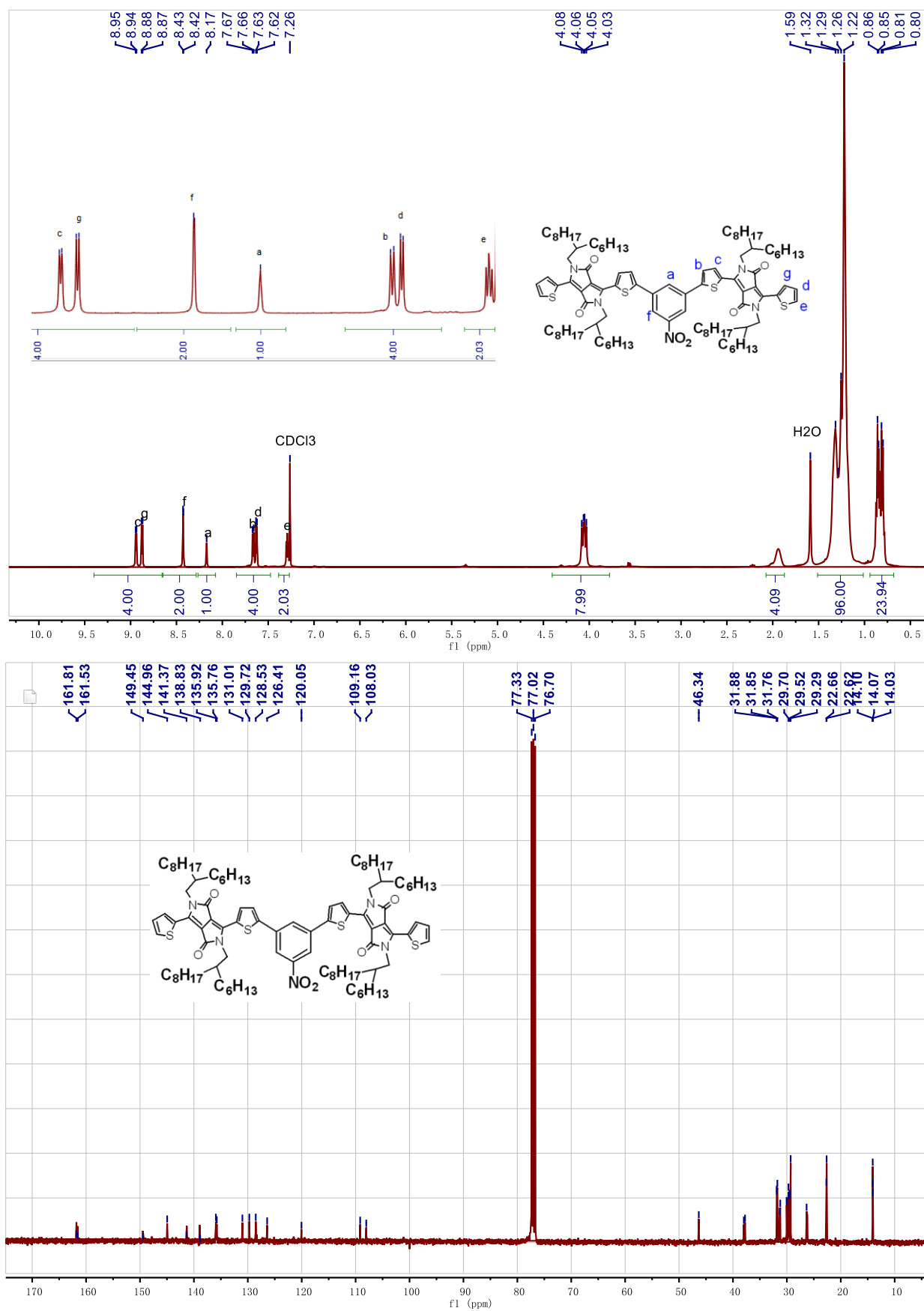
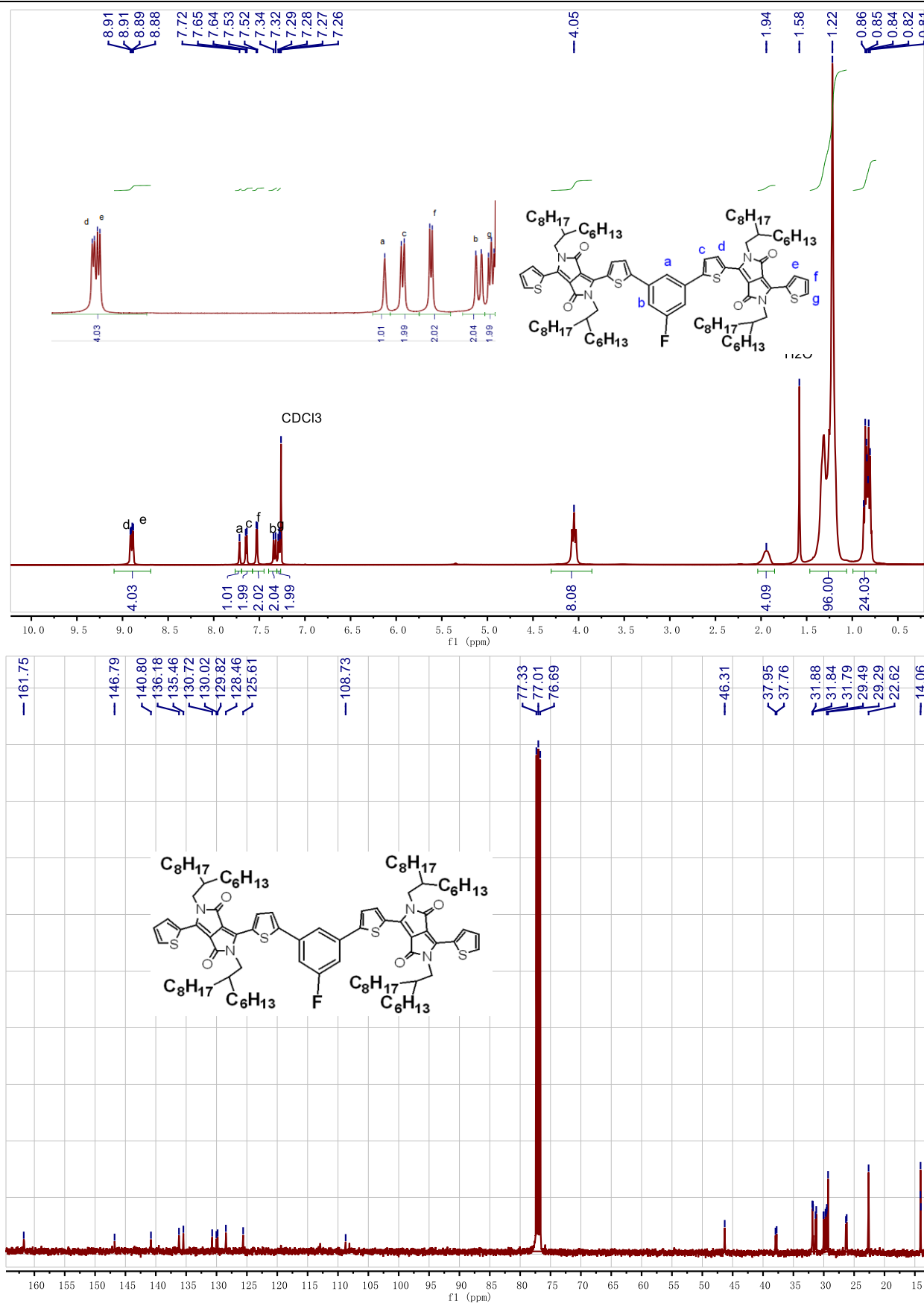
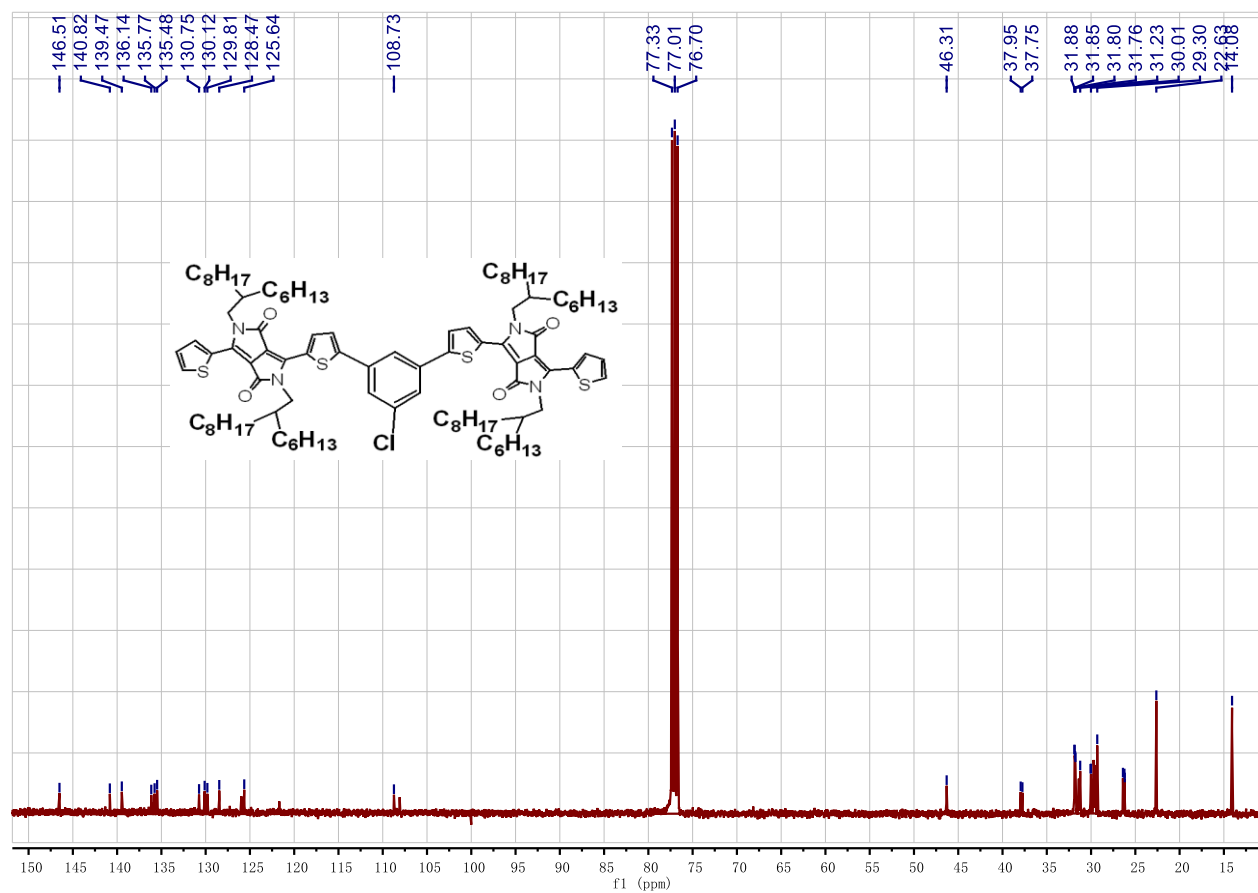
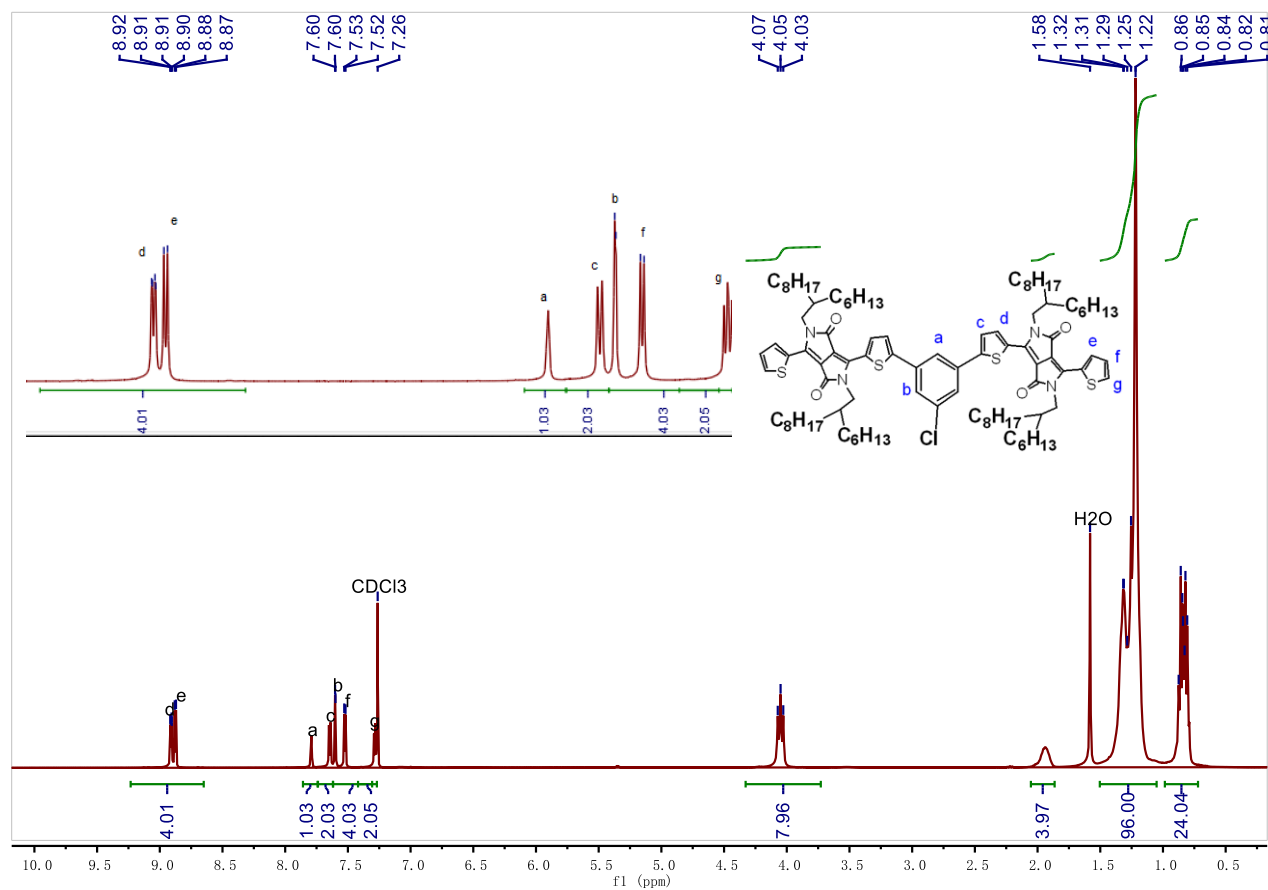


Figure S1 DFT-optimized geometries of Molecules **Ms1~9** (the alkyl chains replaced by methyl groups).

2. ^1H and ^{13}C NMR spectraFigure S2 ^1H and ^{13}C NMR spectra of M1 in CDCl_3 .

**Figure S3** ^1H and ^{13}C NMR spectra of M2 in CDCl_3 .

**FigureS4** ¹H and ¹³C NMR spectra of M3 in CDCl₃.

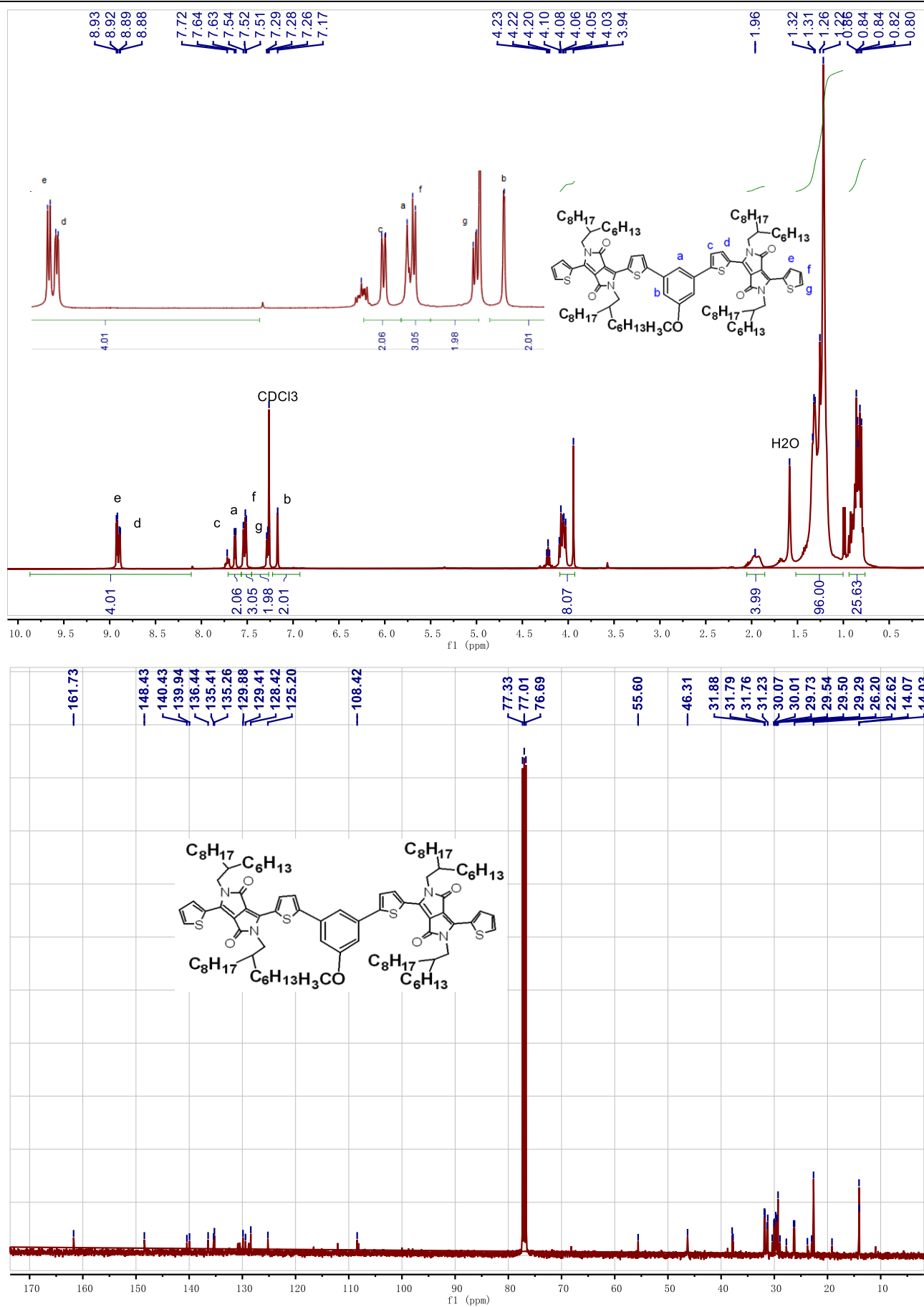
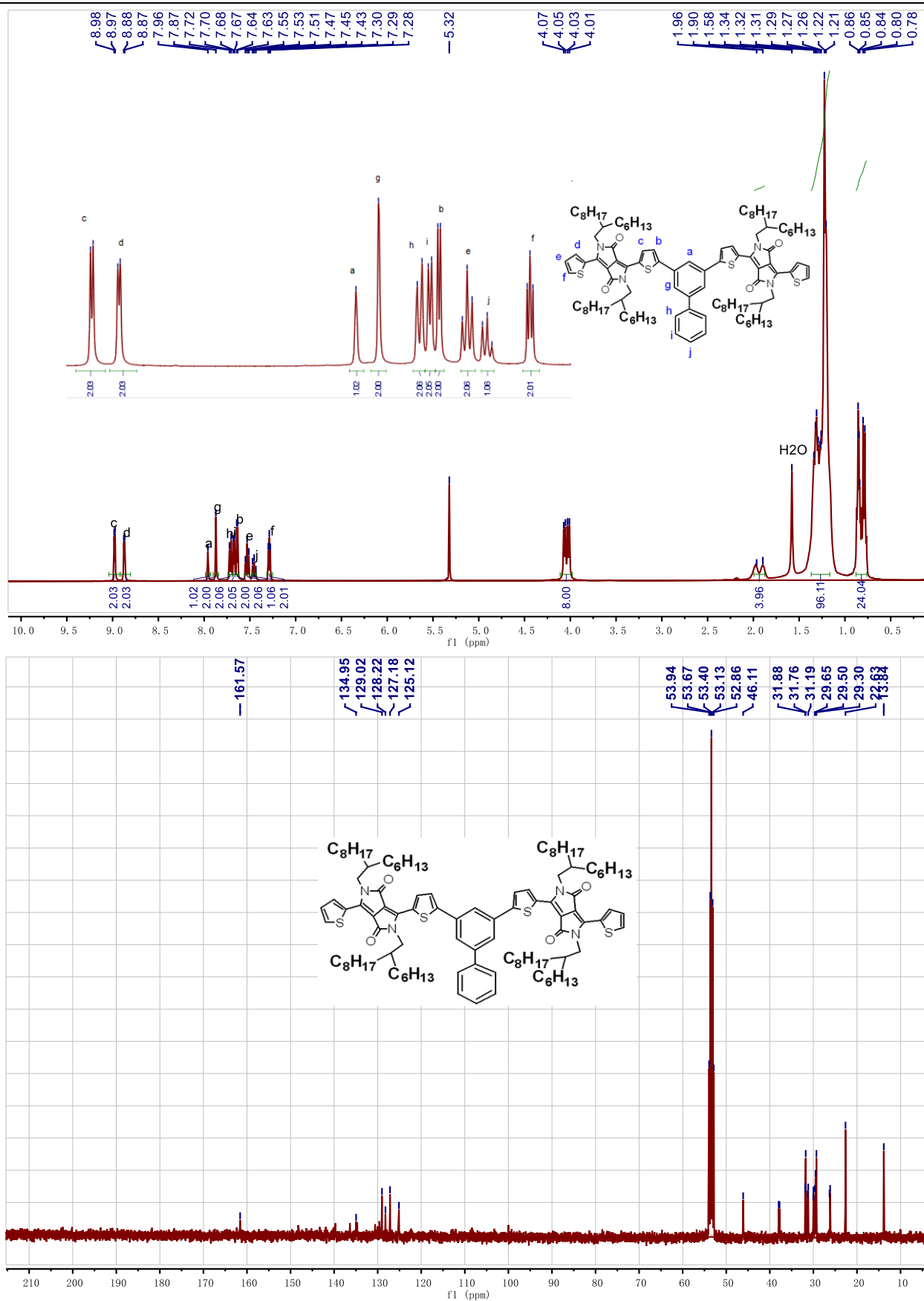
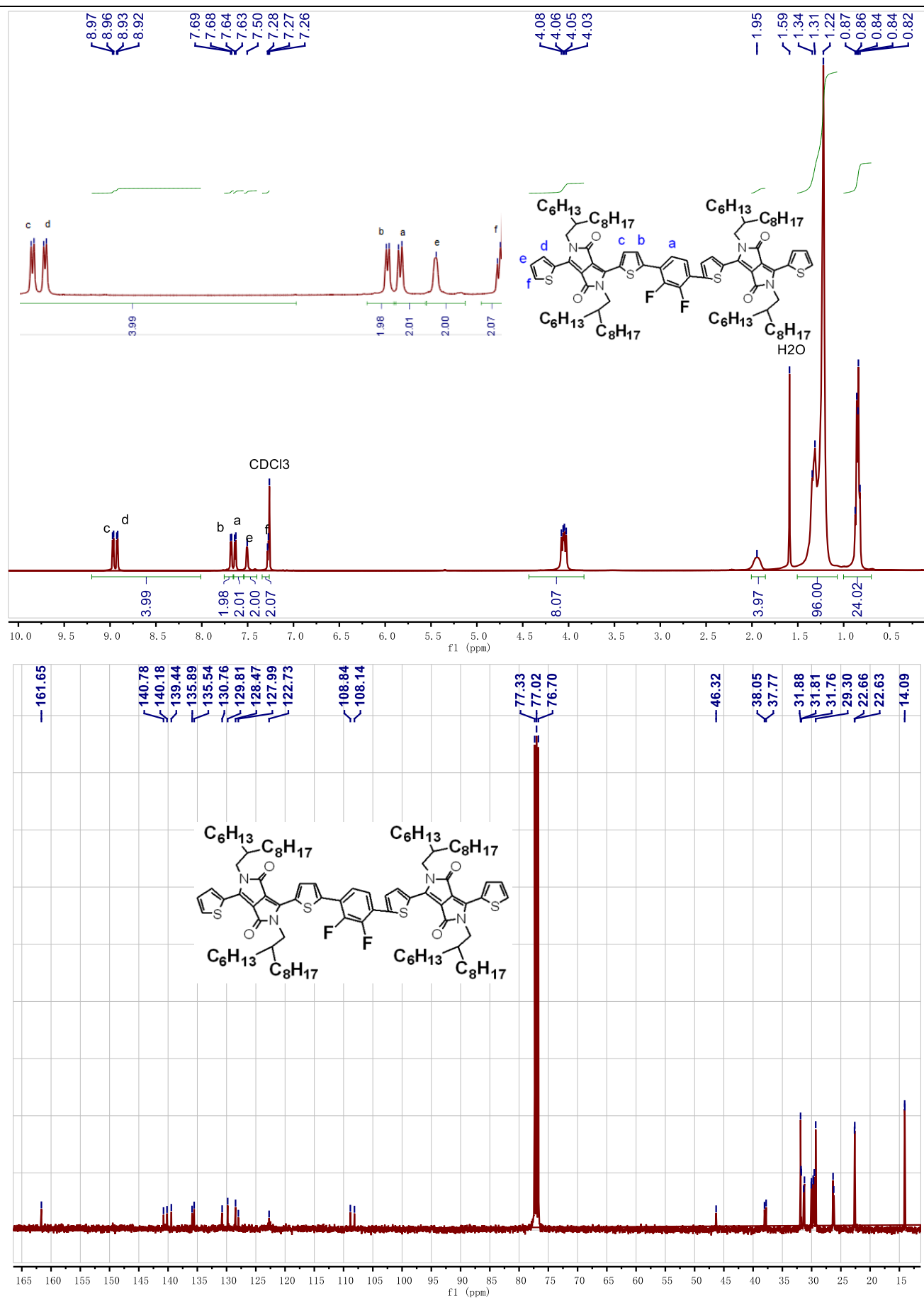
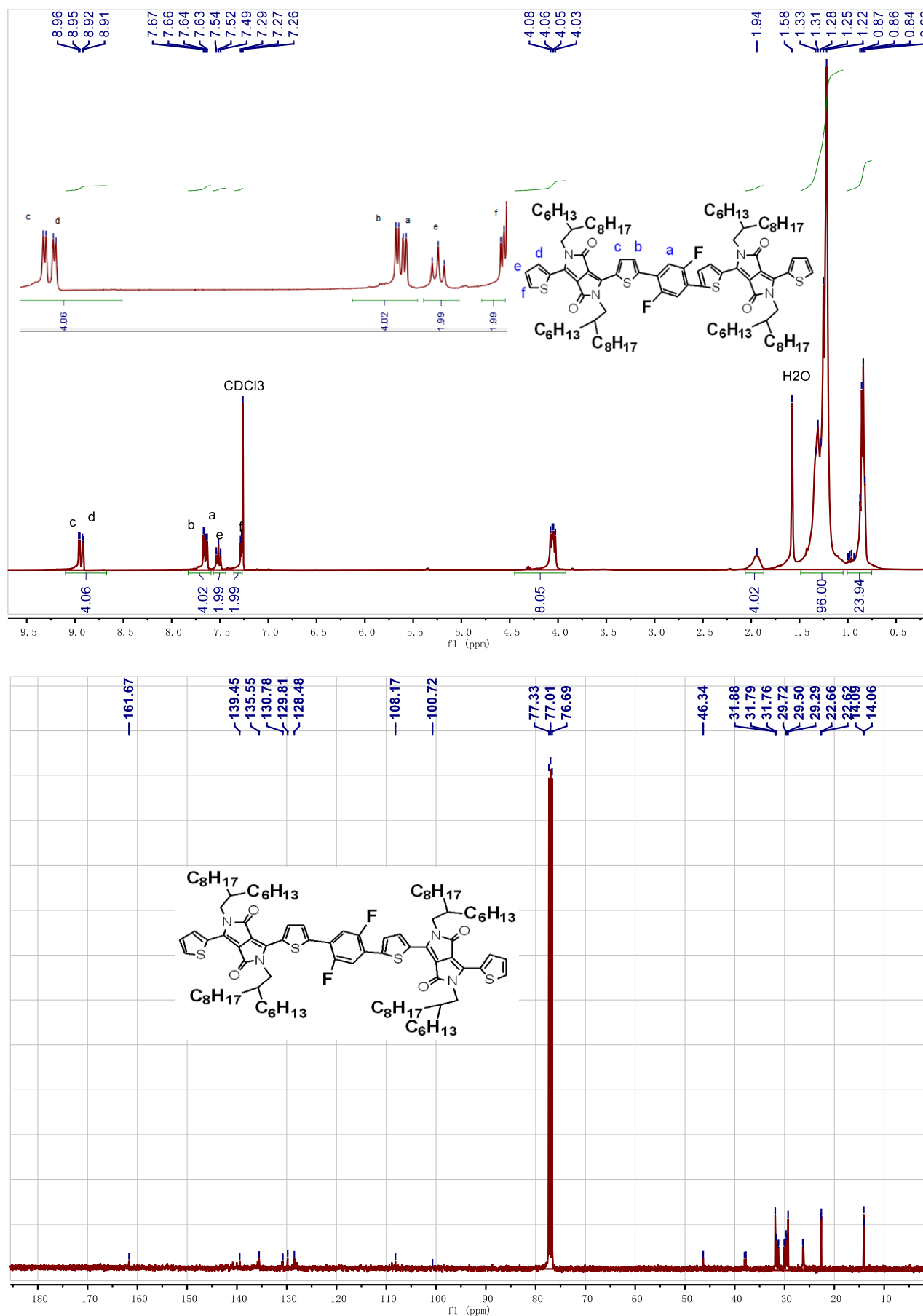


Figure S5 ^1H and ^{13}C NMR spectra of **M4** in CDCl_3 .

**Figure S6** ^1H and ^{13}C NMR spectra of M5 in CDCl_3 .

**Figure S7** ^1H and ^{13}C NMR spectra of **M6** in CDCl_3 .

**Figure S8** ^1H and ^{13}C NMR spectra of M7 in CDCl_3 .

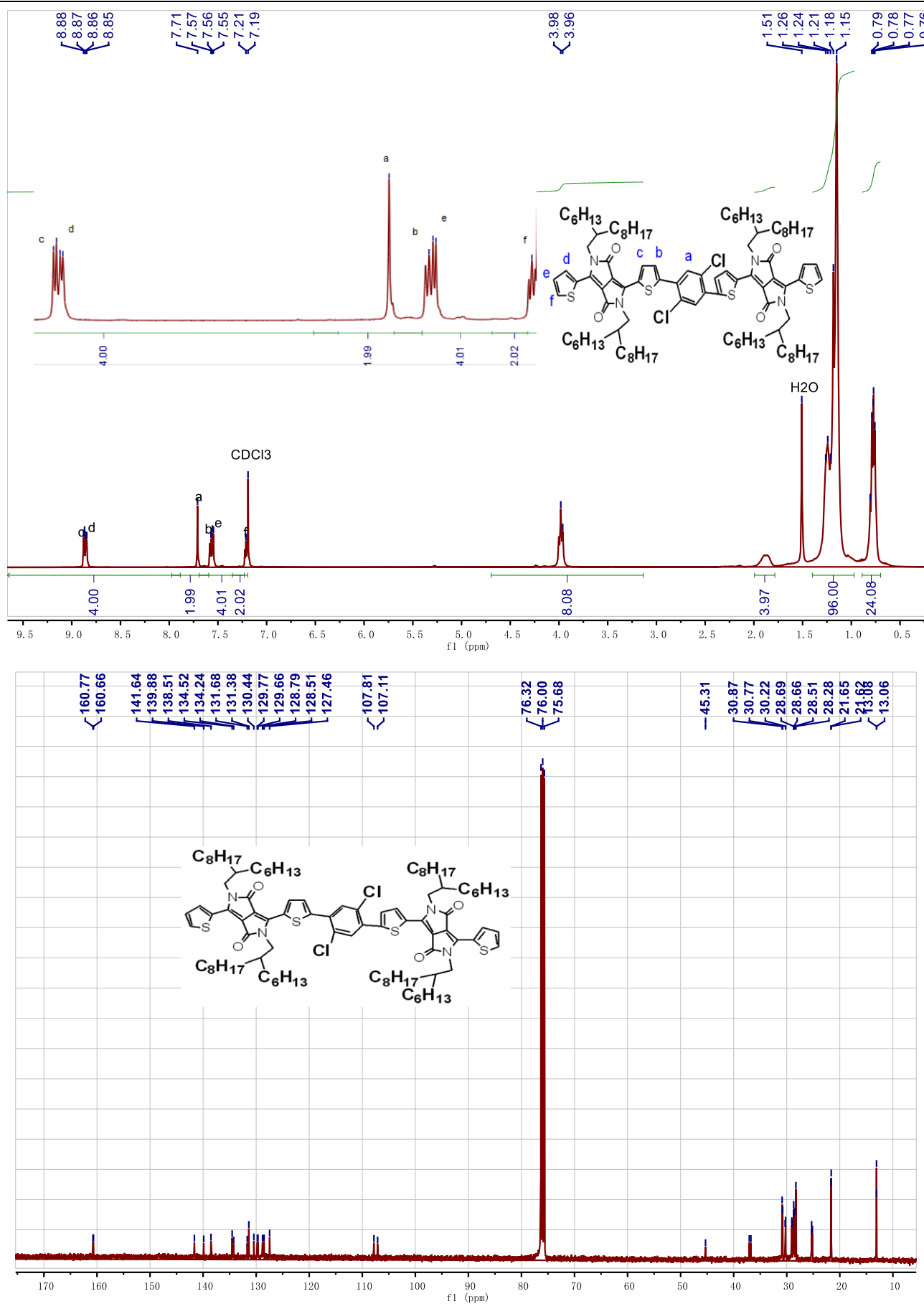


Figure S9 ^1H and ^{13}C NMR spectra of **M8** in CDCl_3 .

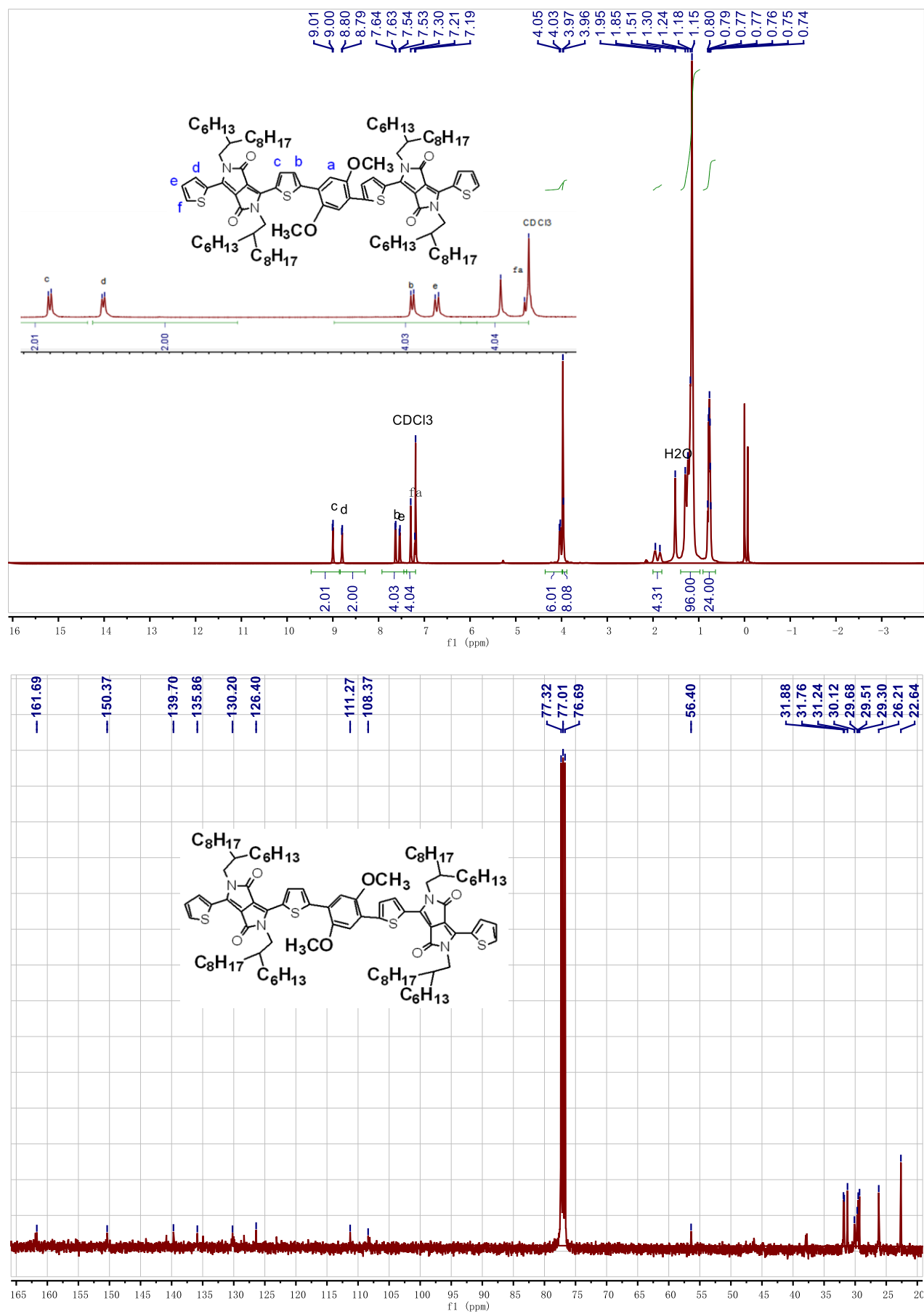
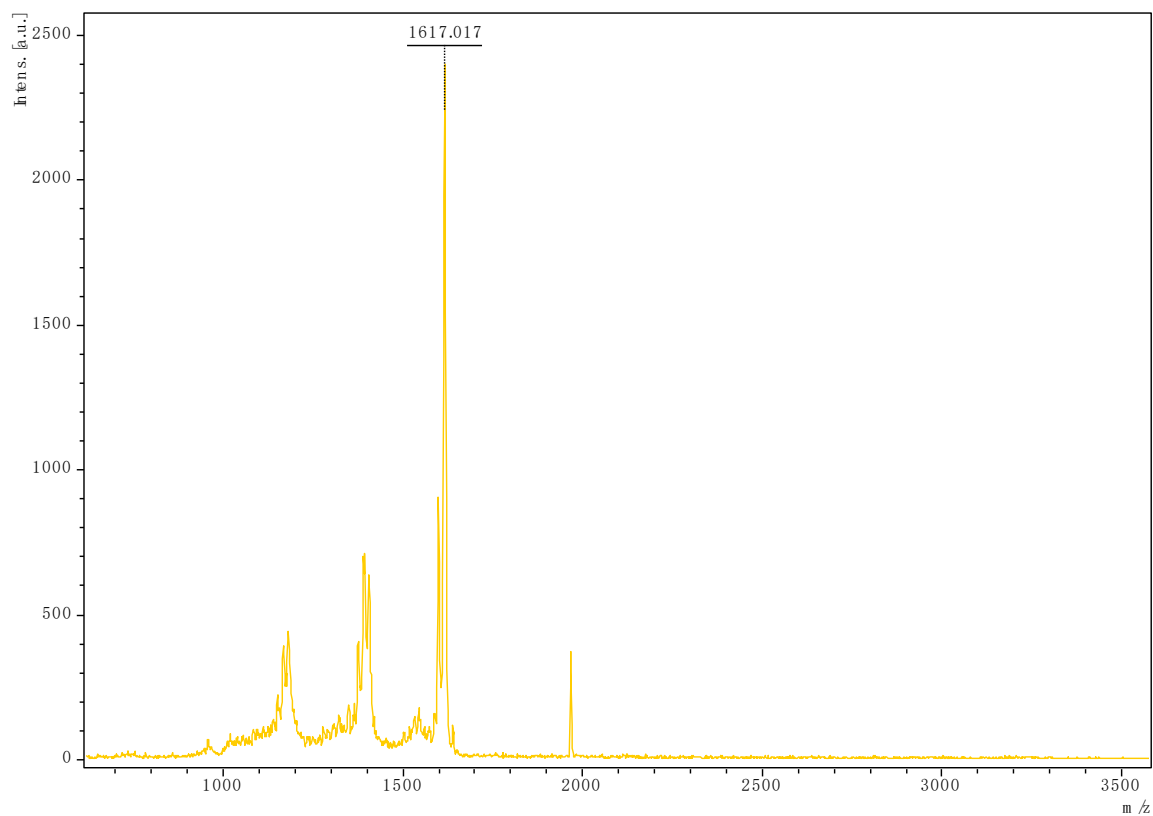
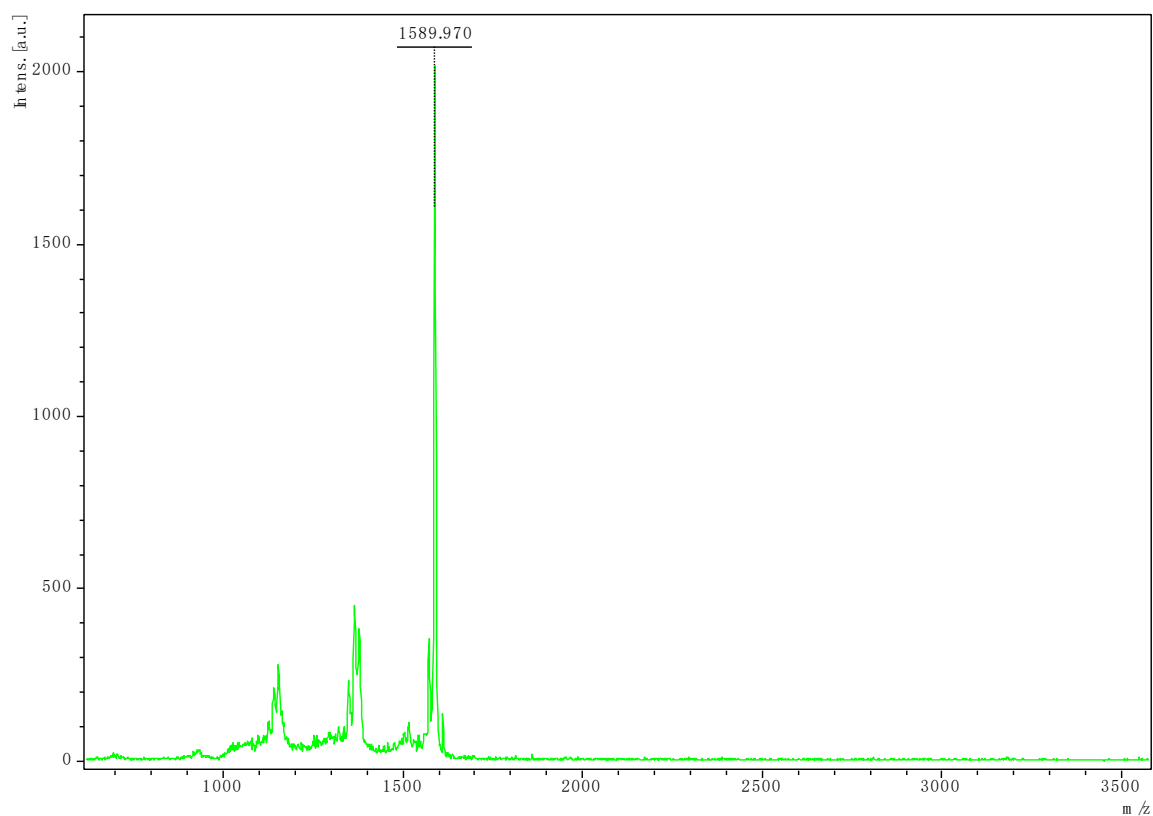


Figure S10 ^1H and ^{13}C NMR spectra of **M9** in CDCl_3 .

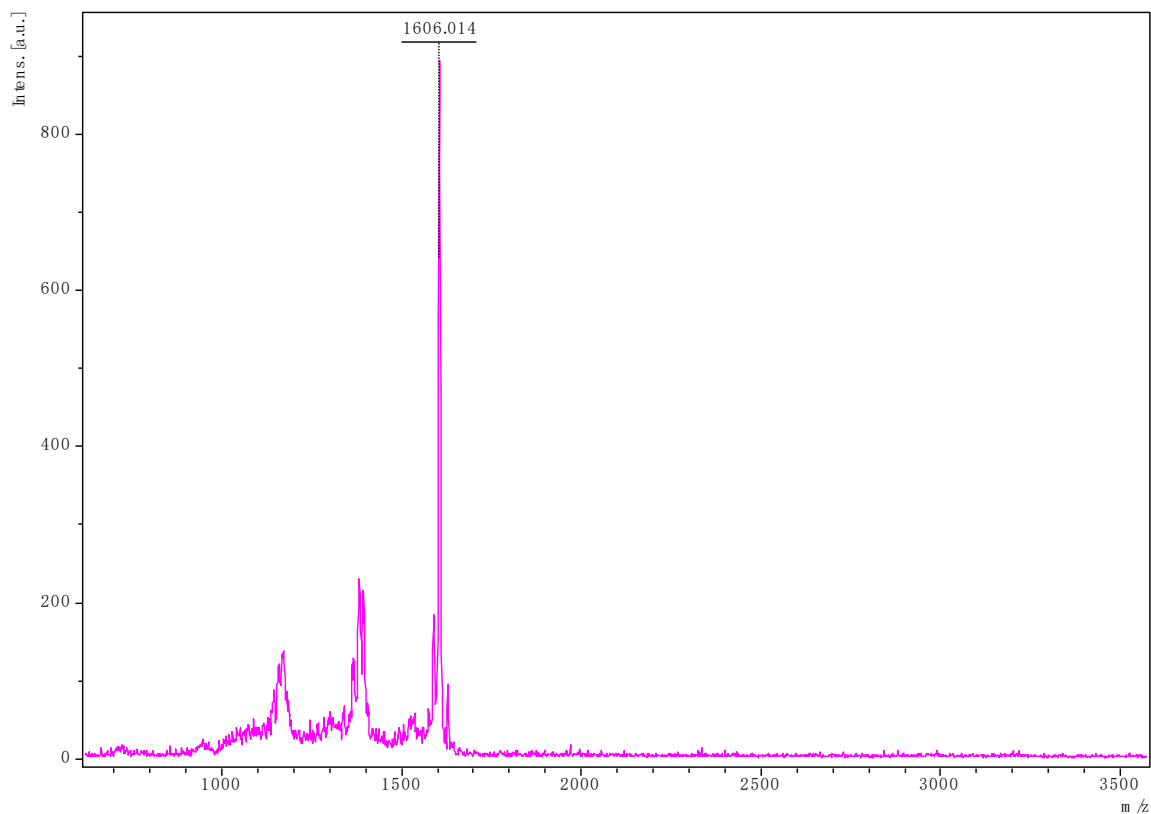
3. MALDI-TOF MS spectra



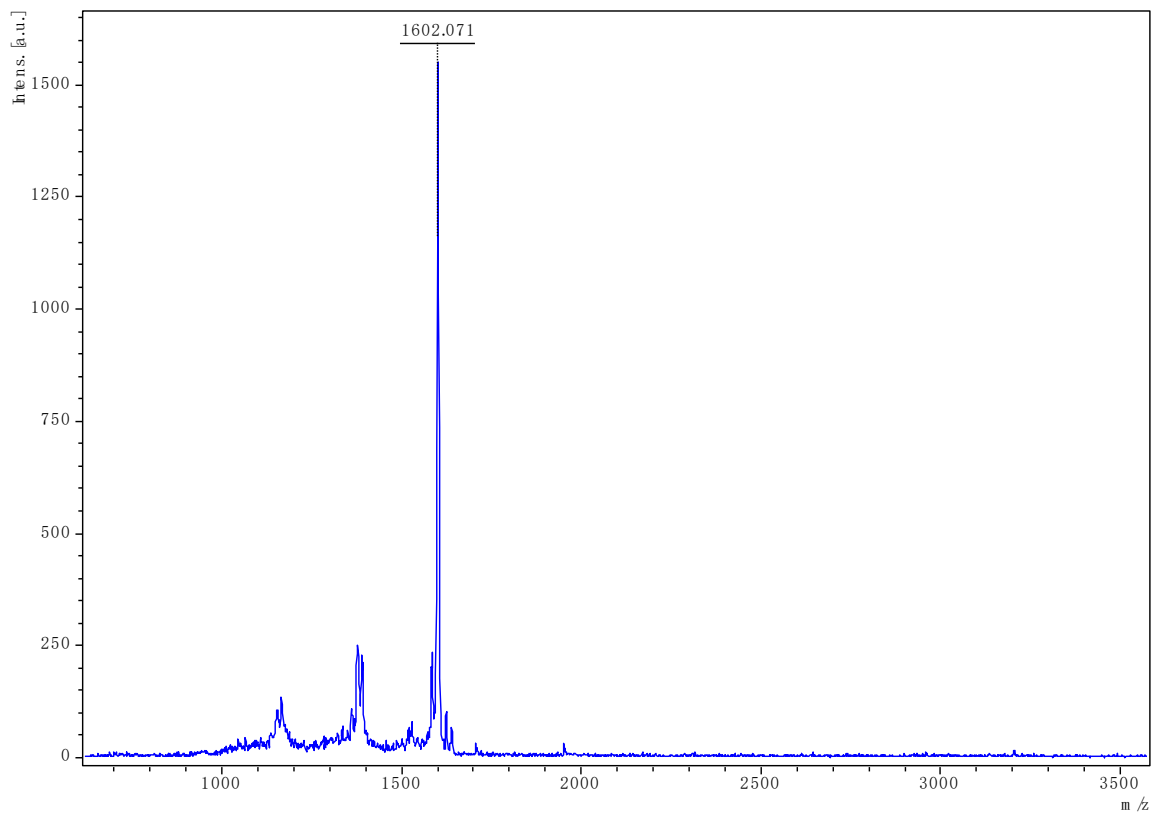
FigureS11 MALDI-TOF MS spectrum of **M1**, calcd. 1617.5070, found 1617.0710 .



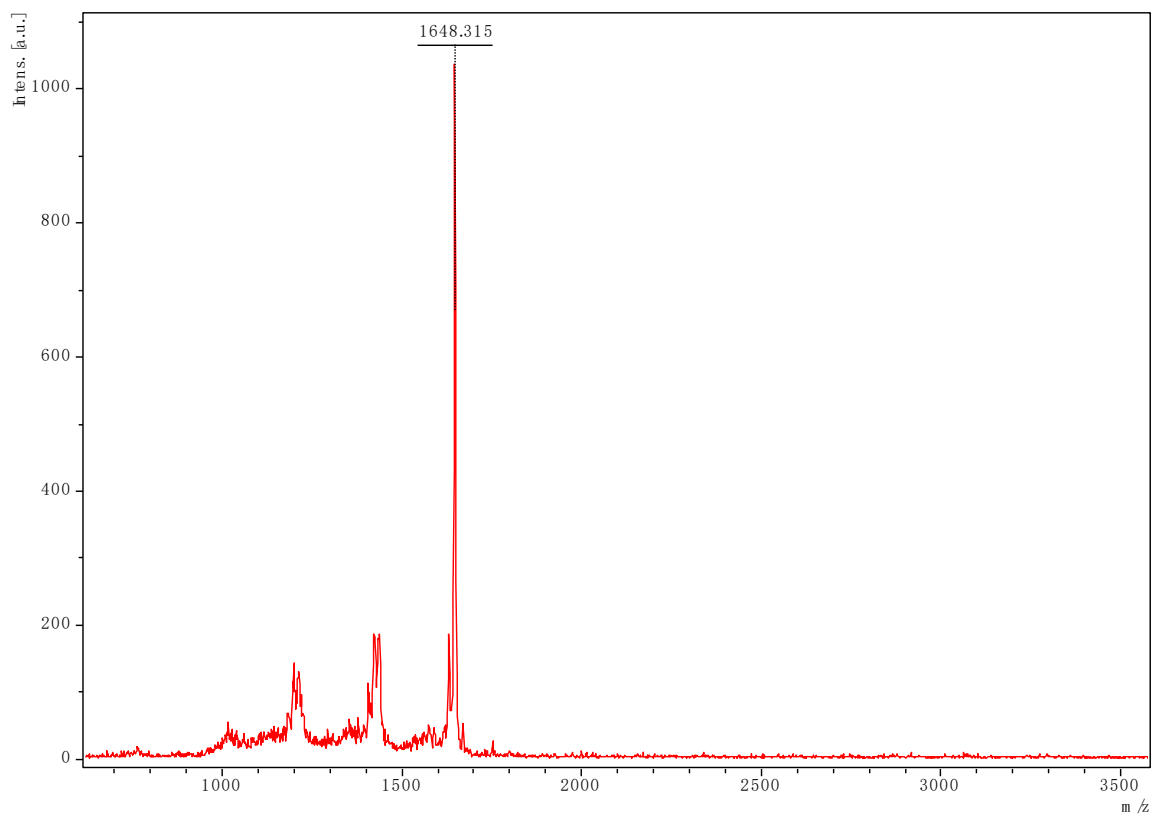
FigureS12 MALDI-TOF MS spectrum of **M2**, calcd. 1590.5004, found 1589.9700.



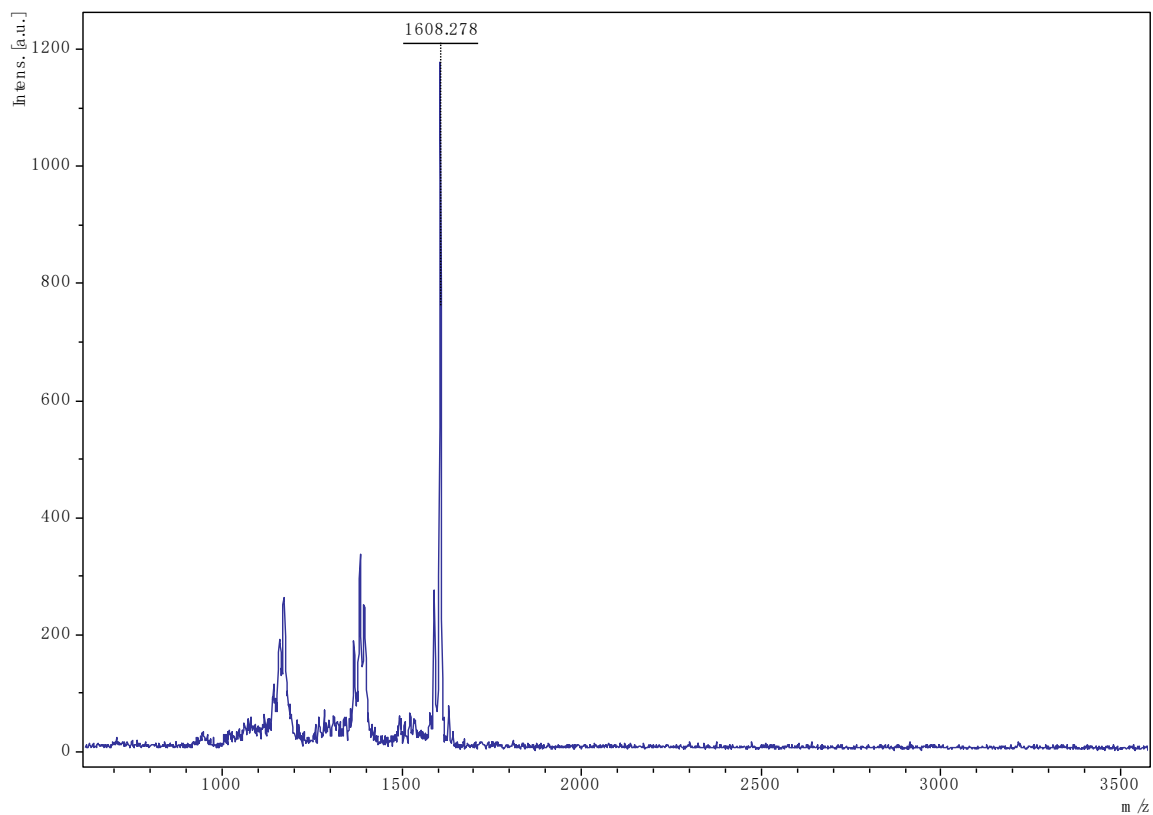
FigureS13 MALDI-TOF MS spectrum of **M3**, calcd.1606.9520, found 1606.0140.



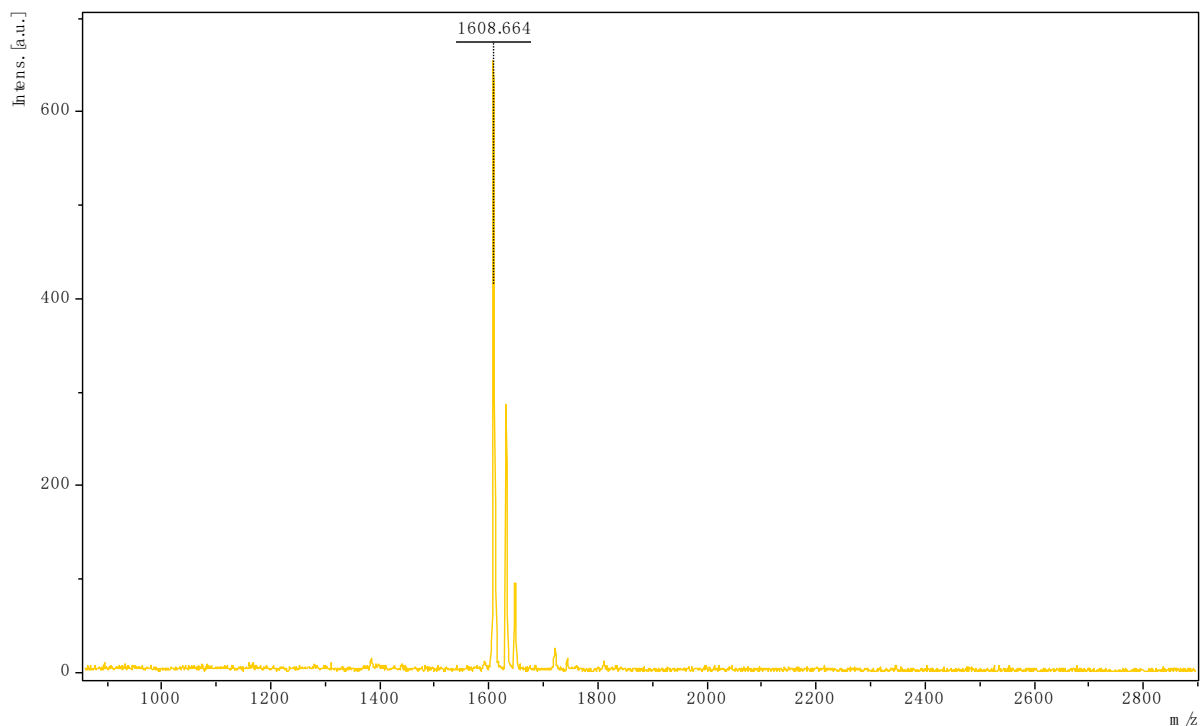
FigureS14 MALDI-TOF MS spectrum of **M4**, calcd. 1602.5360, found 1602.0710.



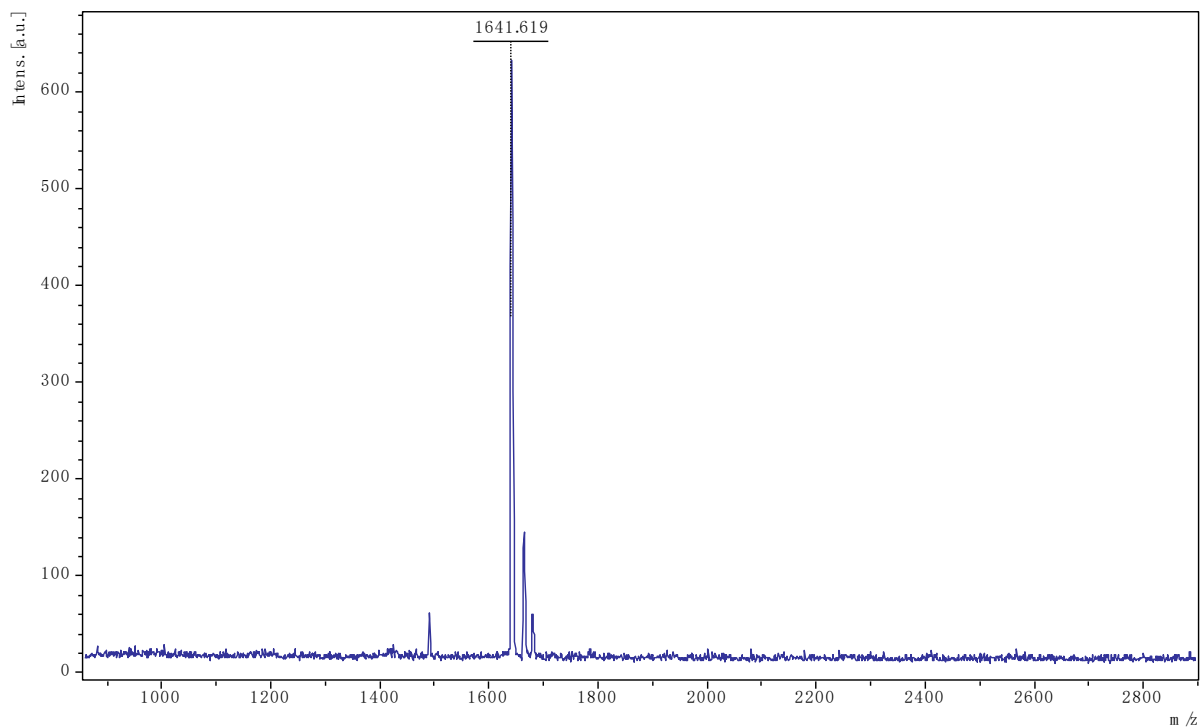
FigureS15 MALDI-TOF MS spectrum of **M5**, calcd. 1648.6080, found 1648.3150.



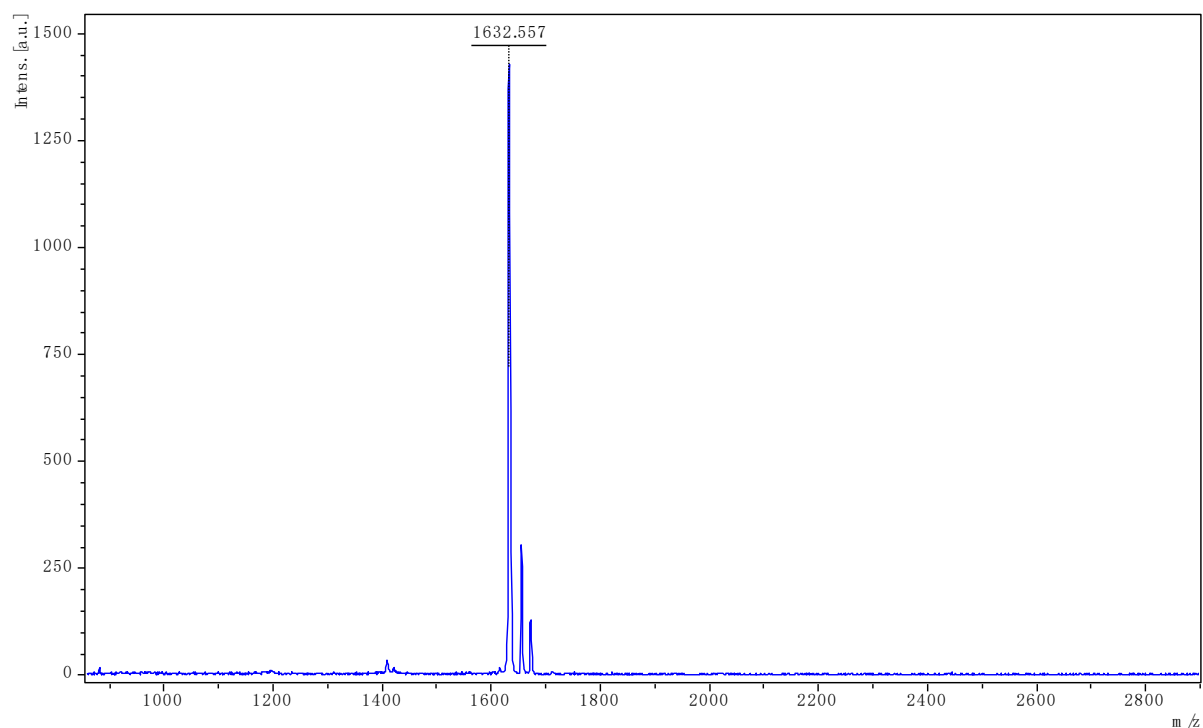
FigureS16 MALDI-TOF MS spectrum of **M6**, calcd.1608.4900, found 1608.2780.



FigureS17 MALDI-TOF MS spectrum of **M7**, calcd. 1608.4700, found 1608.6640.



FigureS18 MALDI-TOF MS spectrum of **M8**, calcd. 1641.3800, found 1641.6190.



FigureS19 MALDI-TOF MS spectrum of **M9**, calcd. 1632.5400, found 1632.5570.