

# Electronic Supplementary Material

## Unravelling the bottleneck of phosphonic acid anchoring groups aiming towards enhancing the stability and efficiency of mesoscopic solar cells

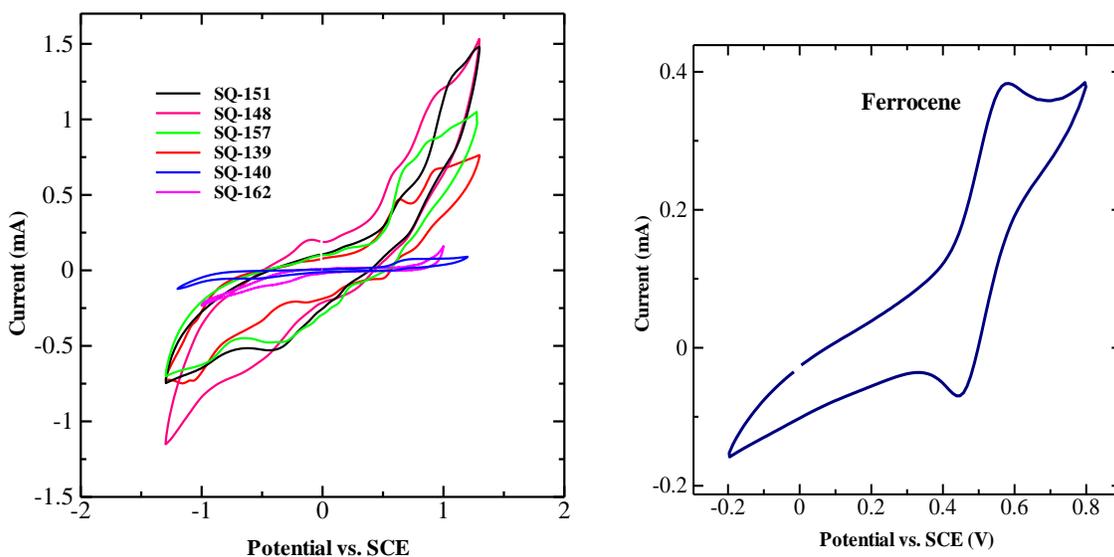
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<sup>2</sup> i-Powered Energy System Research Center (i-PERC), The University of Electro-Communications, Tokyo 182-8585, Japan

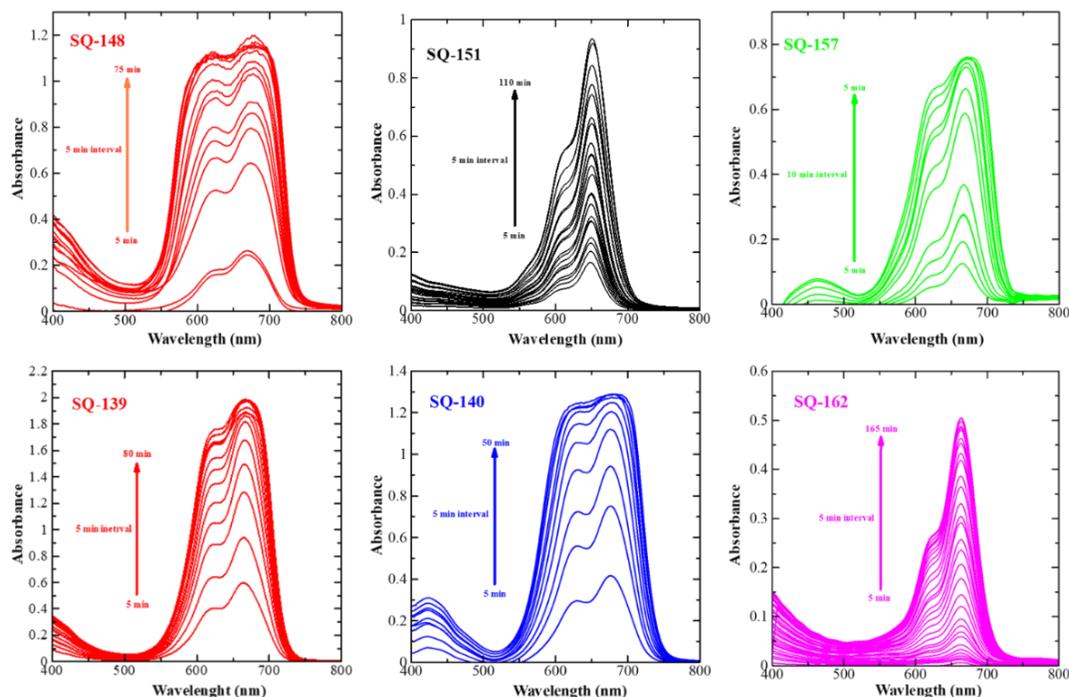
E-mail: [shyam@life.kyutech.ac.jp](mailto:shyam@life.kyutech.ac.jp)

### Electrochemical characterization



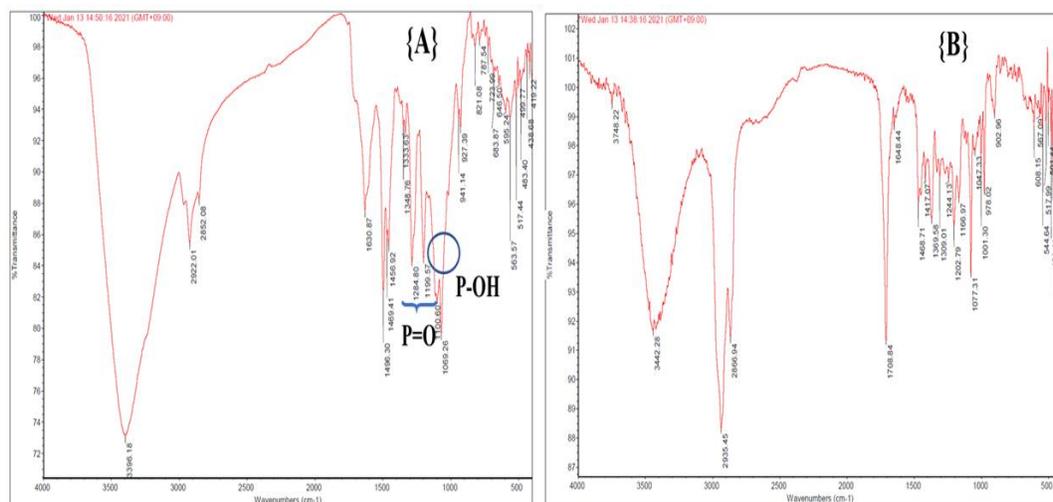
**Figure. S1.** Cyclic voltammogram of unsymmetrical squaraine dyes and ferrocene (2 mM) in DMF using 200 mM of Tetrabutylammoniumhexafluorophosphate as electrolyte recorded at 20 mV/s. In every case, Pt foil, Pt wire, and saturated calomel electrode (SCE) were used as a counter, working, and reference electrodes, respectively.

## Dye adsorption behavior on thin films of mesoporous TiO<sub>2</sub>

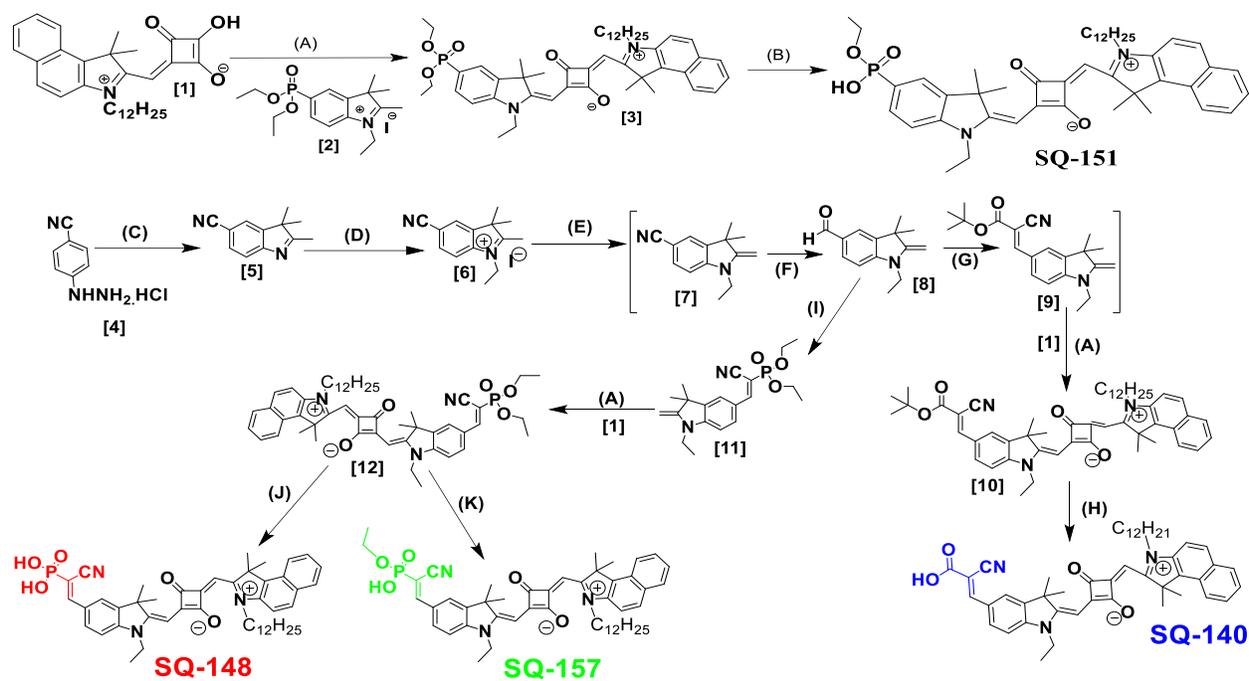


**Figure S2.** Electronic absorption spectra of unsymmetrical squaraine dyes adsorbed on the thin films of mesoporous TiO<sub>2</sub> (4 nm) measured after their adsorption for different times until saturation. In case, a dye solution of 0.1 mM in ethanol was used for the time-dependent dye adsorption studies at room temperature.

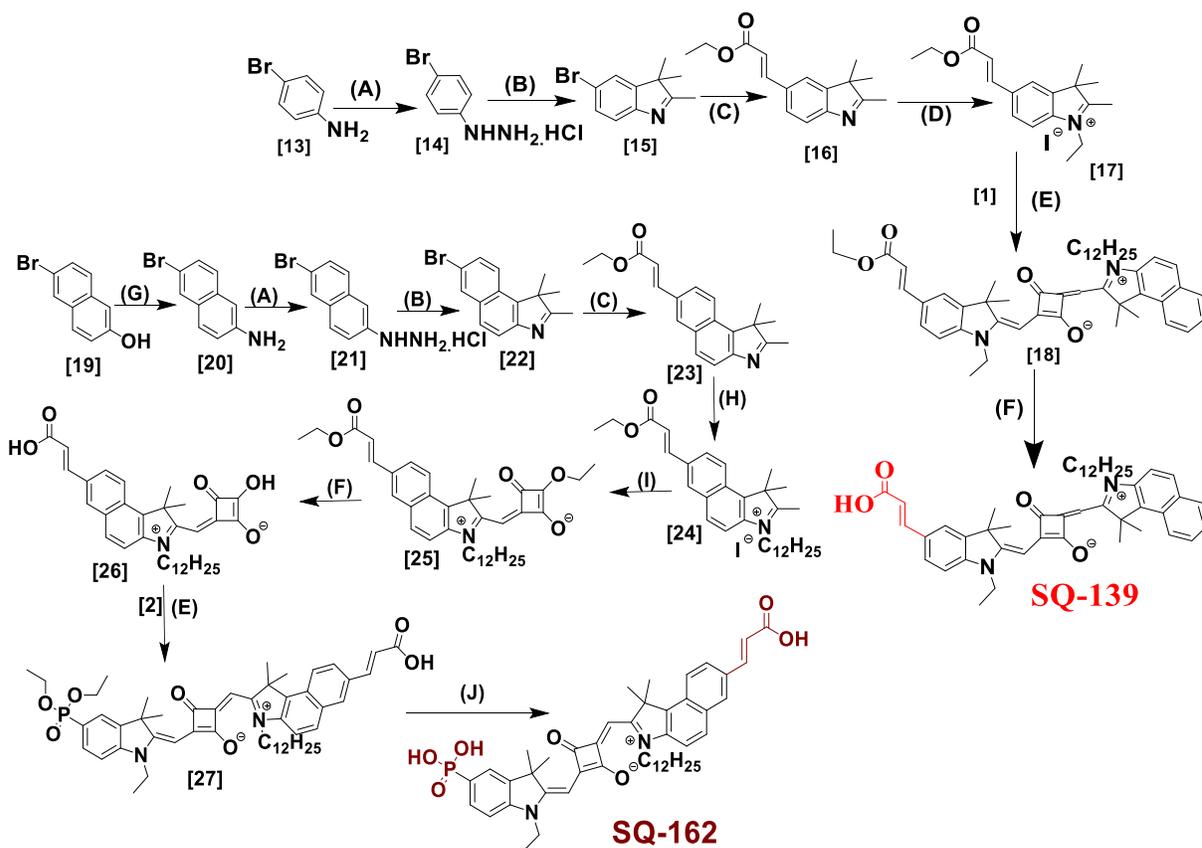
## FTIR spectra for the binding mode of SQ-162 on TiO<sub>2</sub>



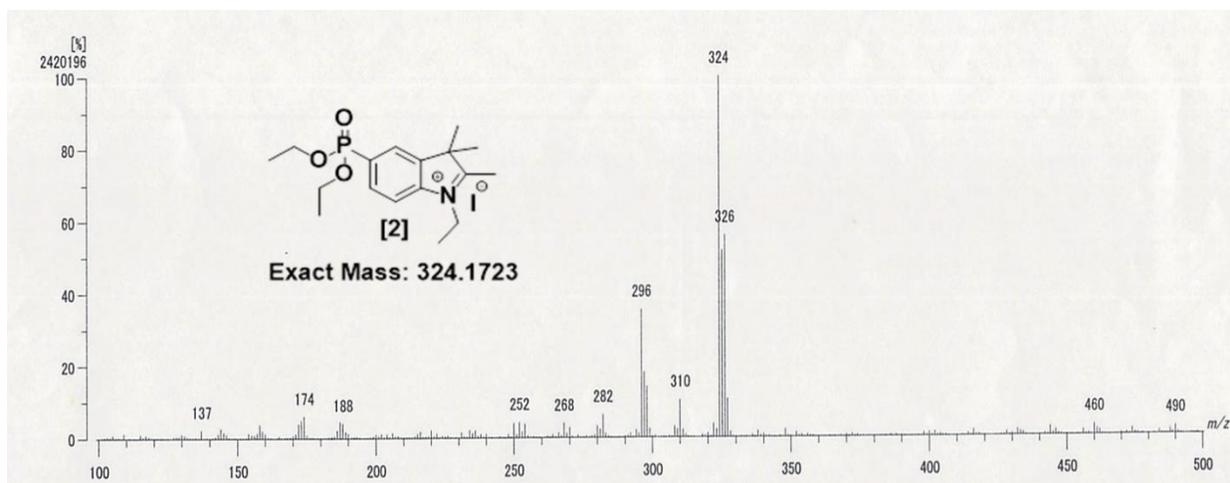
**Figure S3** Fourier Transform Infrared spectra for the dye SQ-162: Free dye {A} and after its binding with TiO<sub>2</sub> {B}.



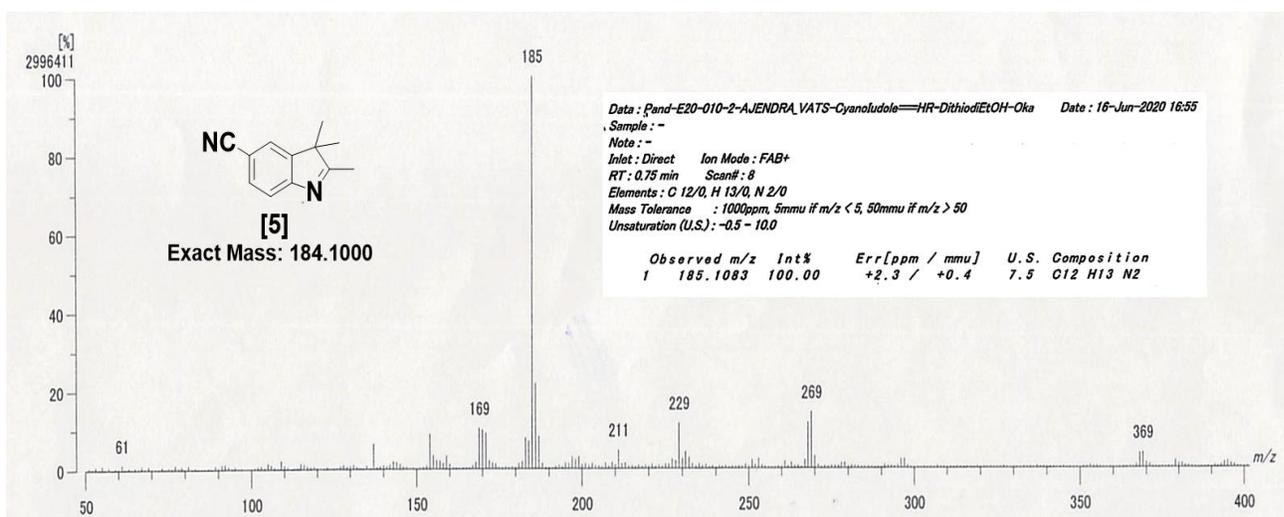
Synthetic Scheme-1



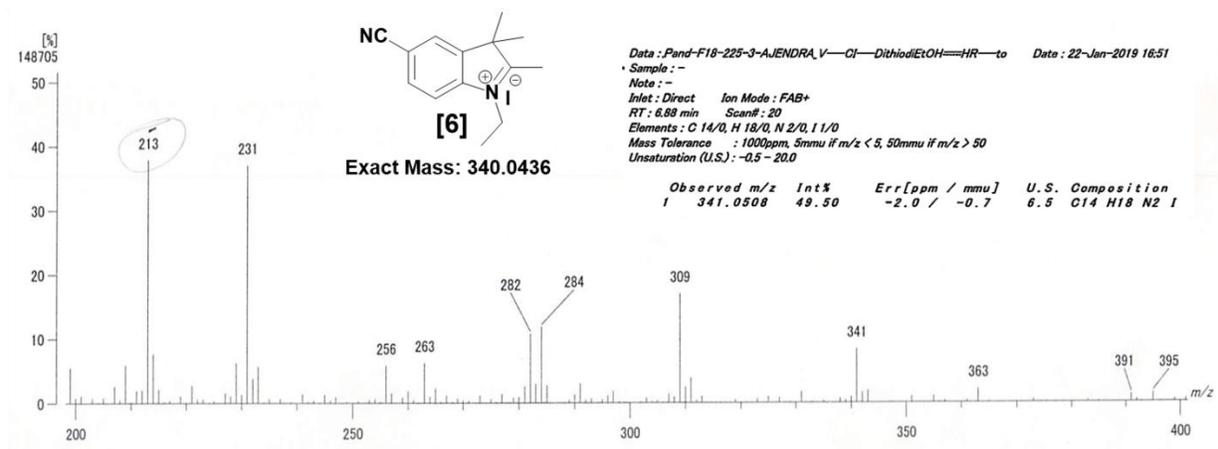
Synthetic Scheme-2



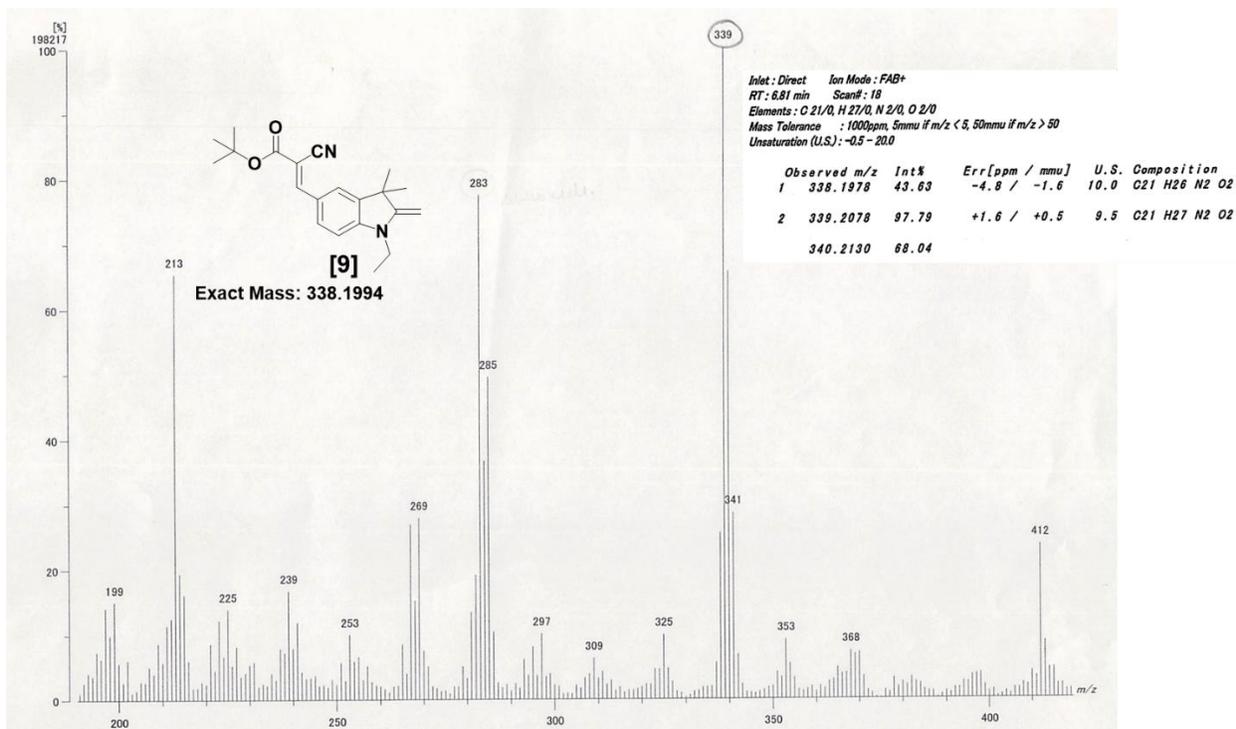
FAB-MS of the intermediate (2)



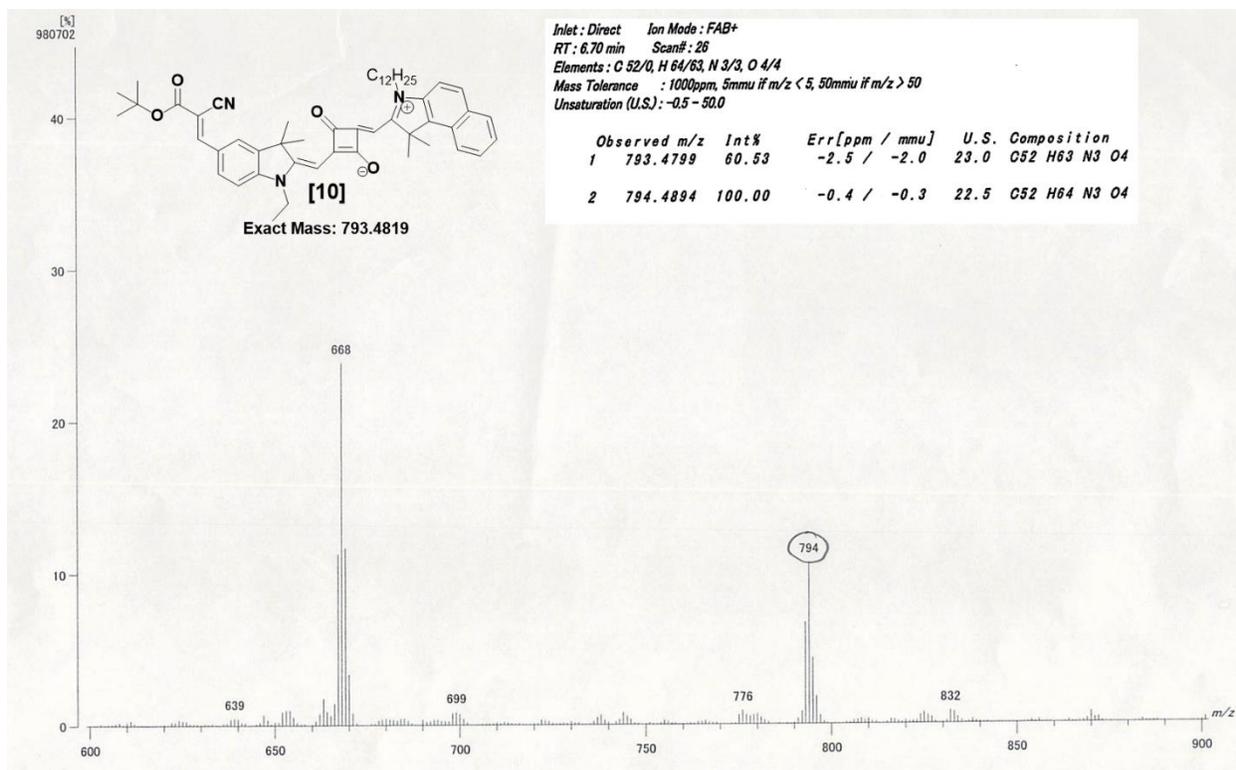
FAB-MS & HR FAB-MS of the intermediate (5)



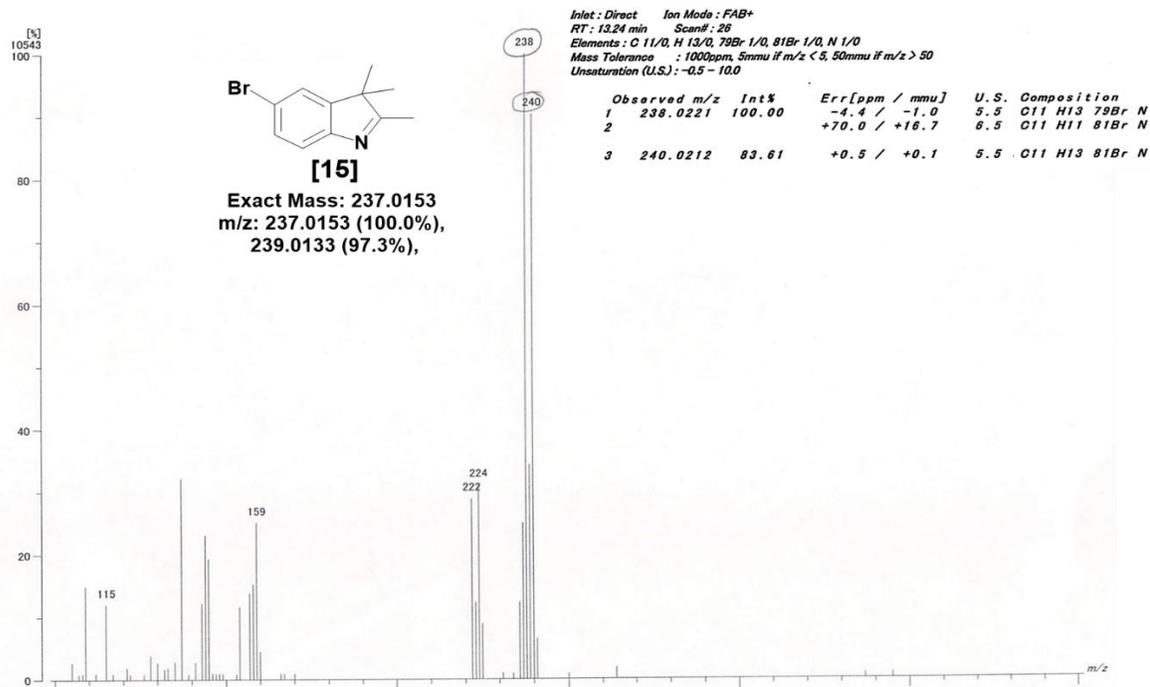
FAB-MS & HR FAB-MS of the intermediate (6)



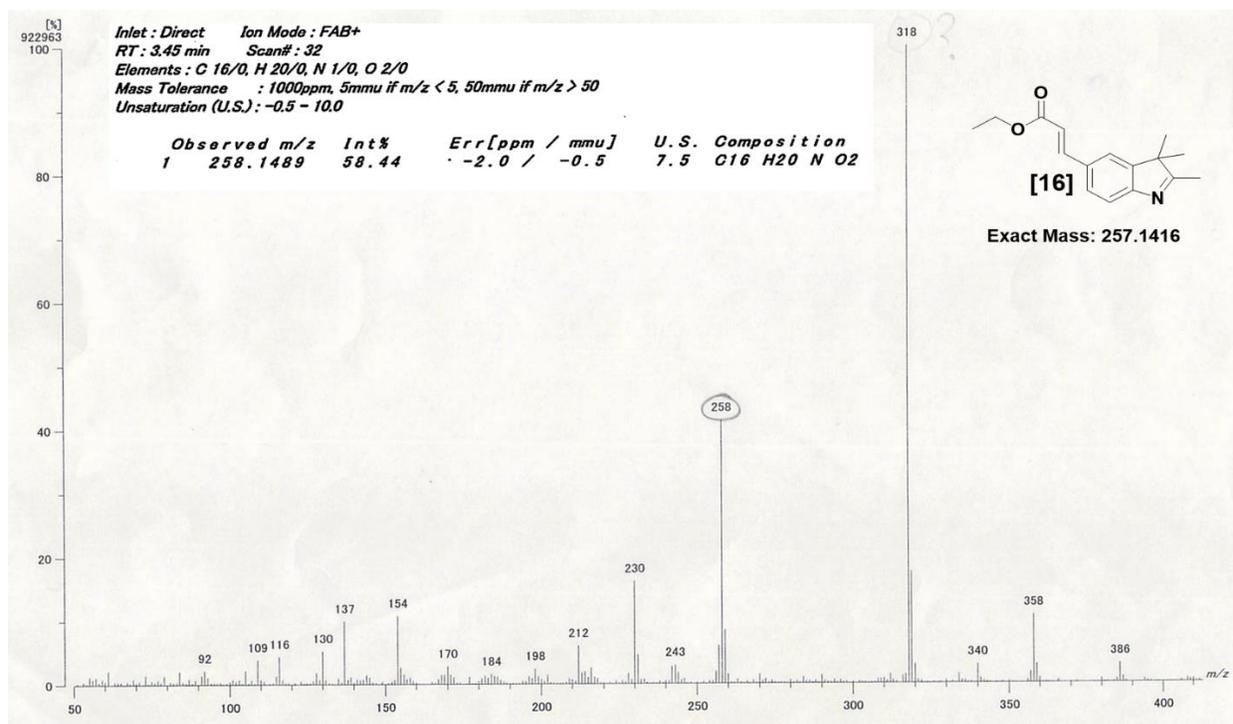
FAB-MS & HR FAB-MS of the intermediate (9)



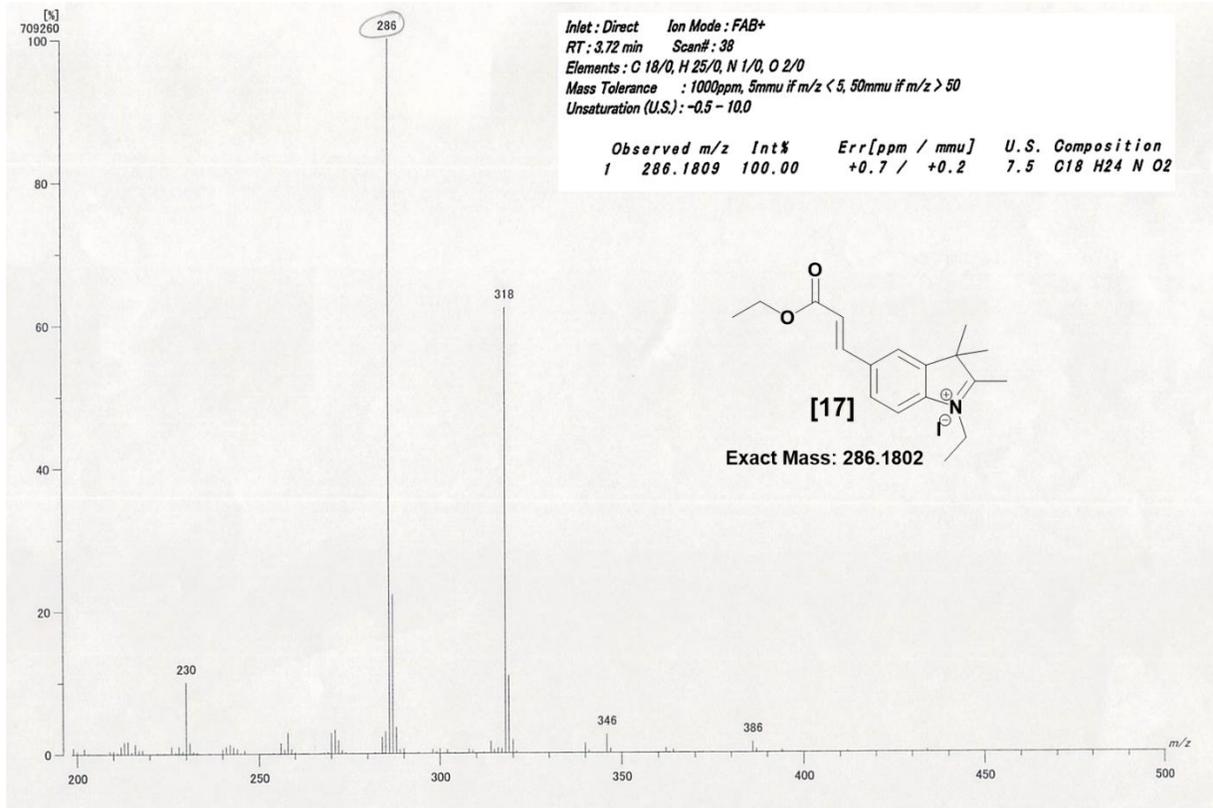
FAB-MS & HR FAB-MS of the intermediate (10)



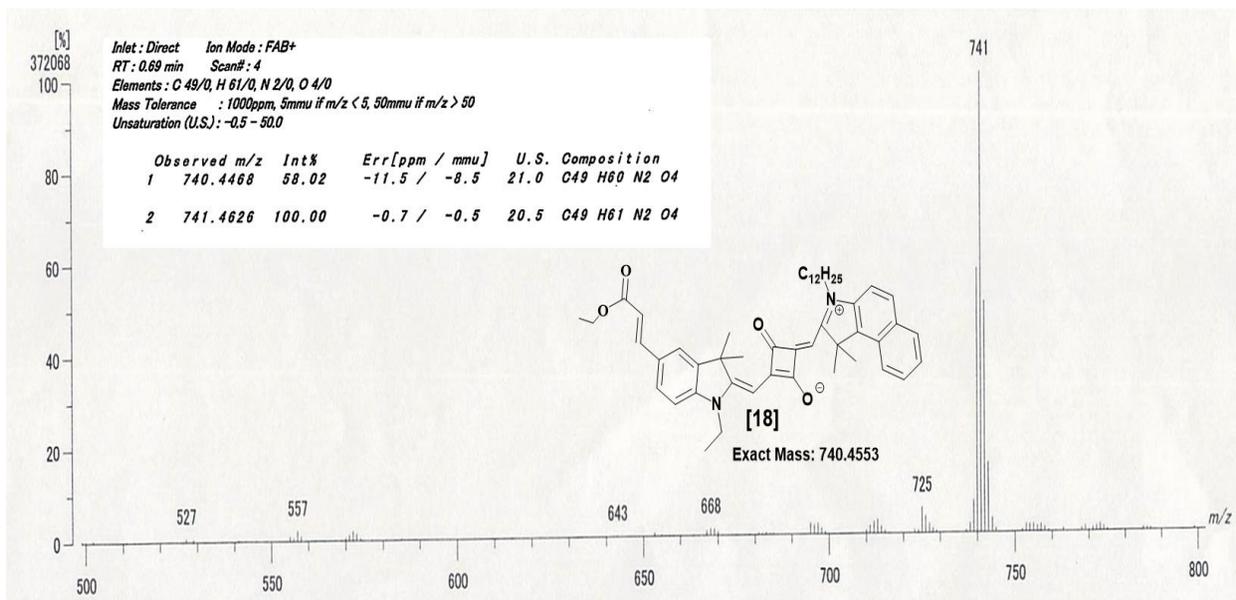
FAB-MS & HR FAB-MS of the intermediate (15)



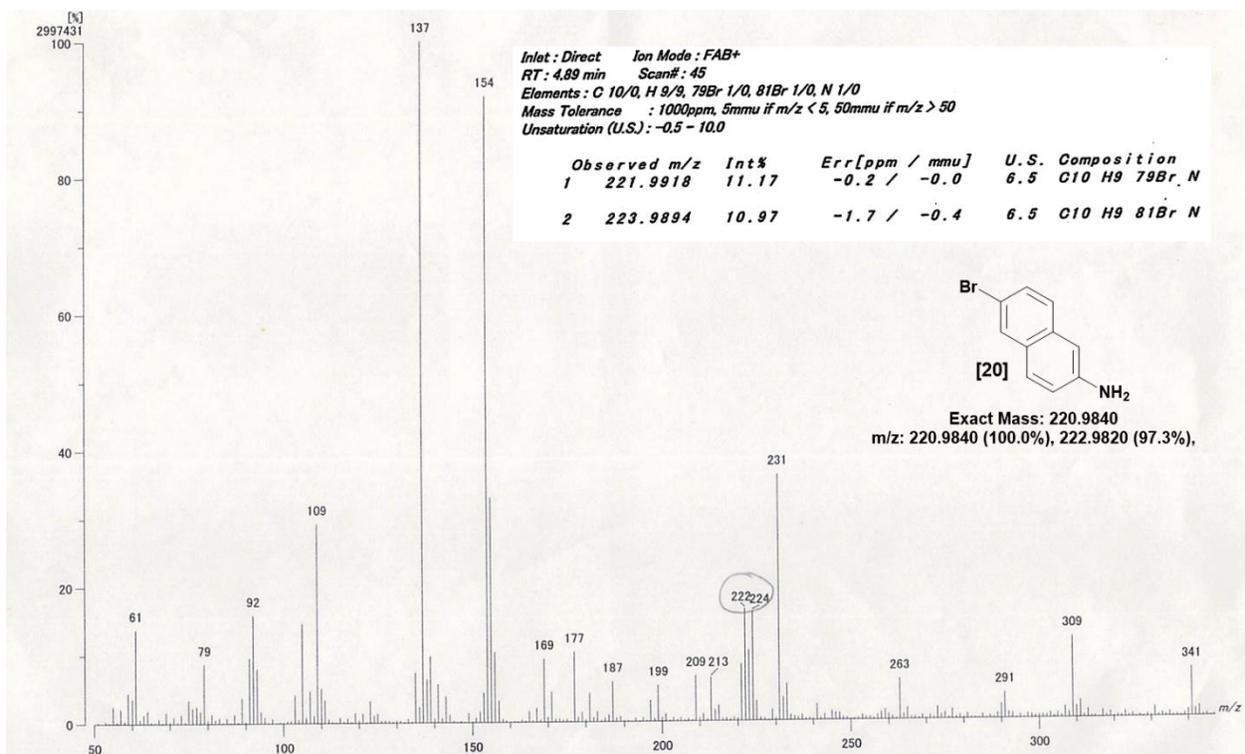
FAB-MS & HR FAB-MS of the intermediate (16)



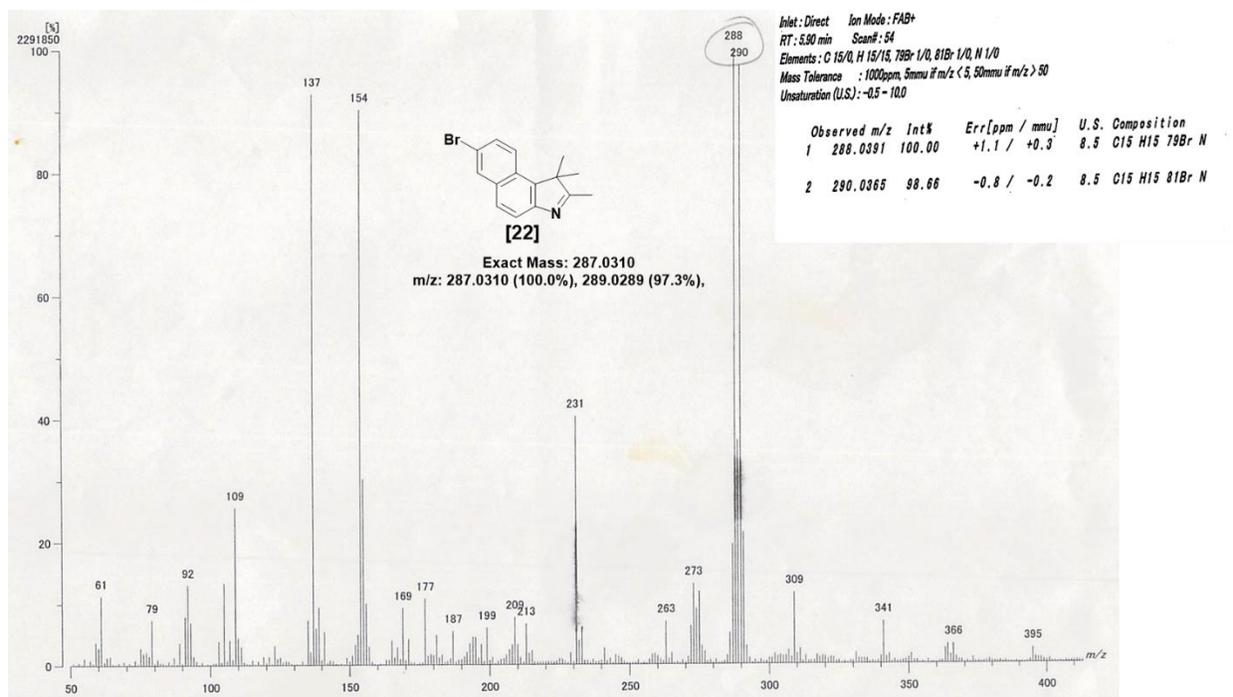
FAB-MS & HR FAB-MS of the intermediate (17)



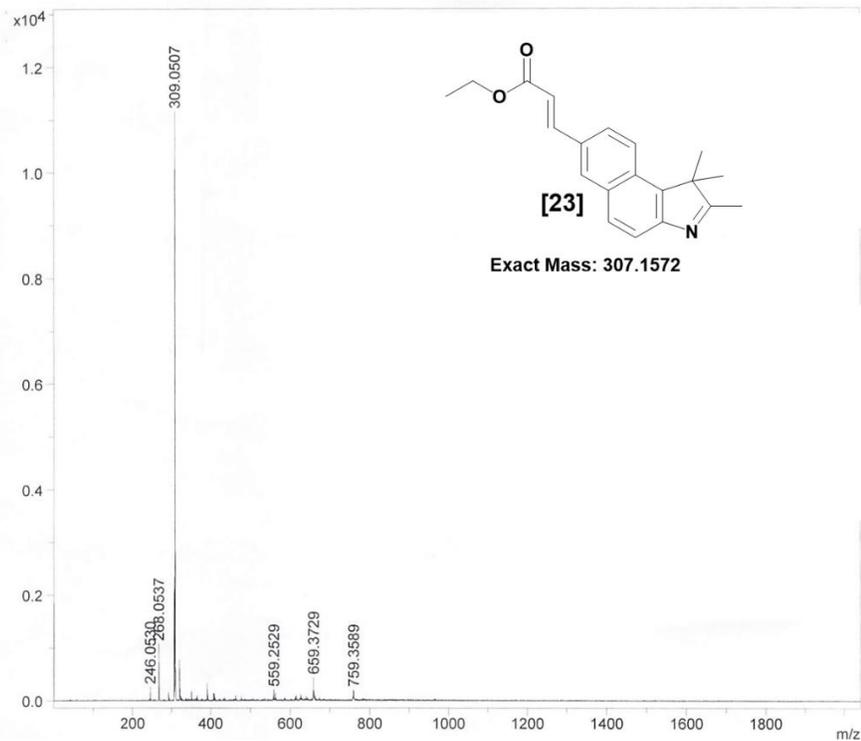
FAB-MS & HR FAB-MS of the intermediate (18)



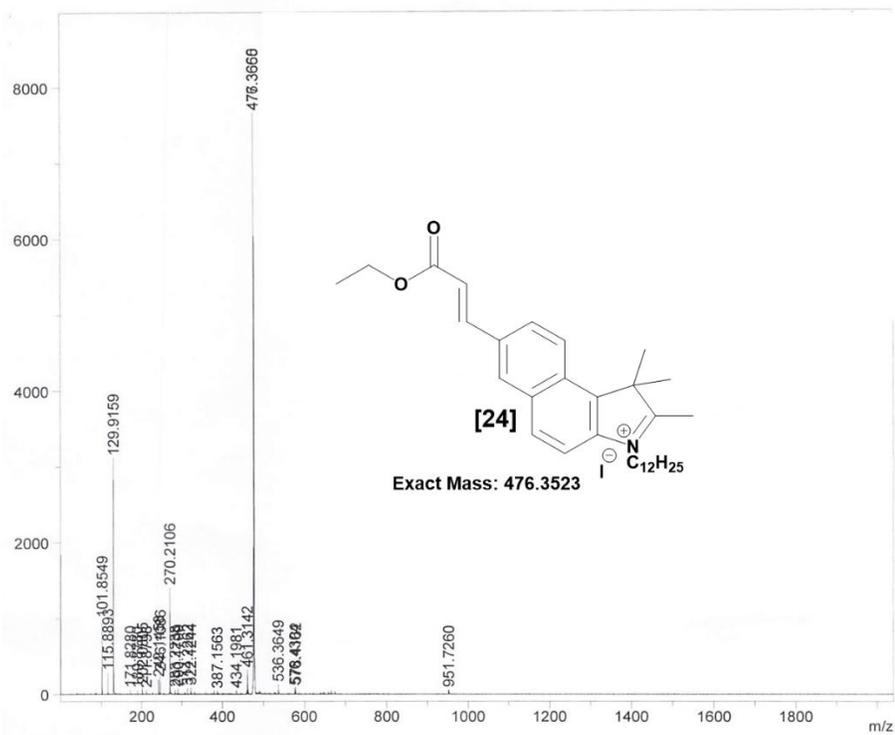
FAB-MS & HR FAB-MS of the intermediate (20)



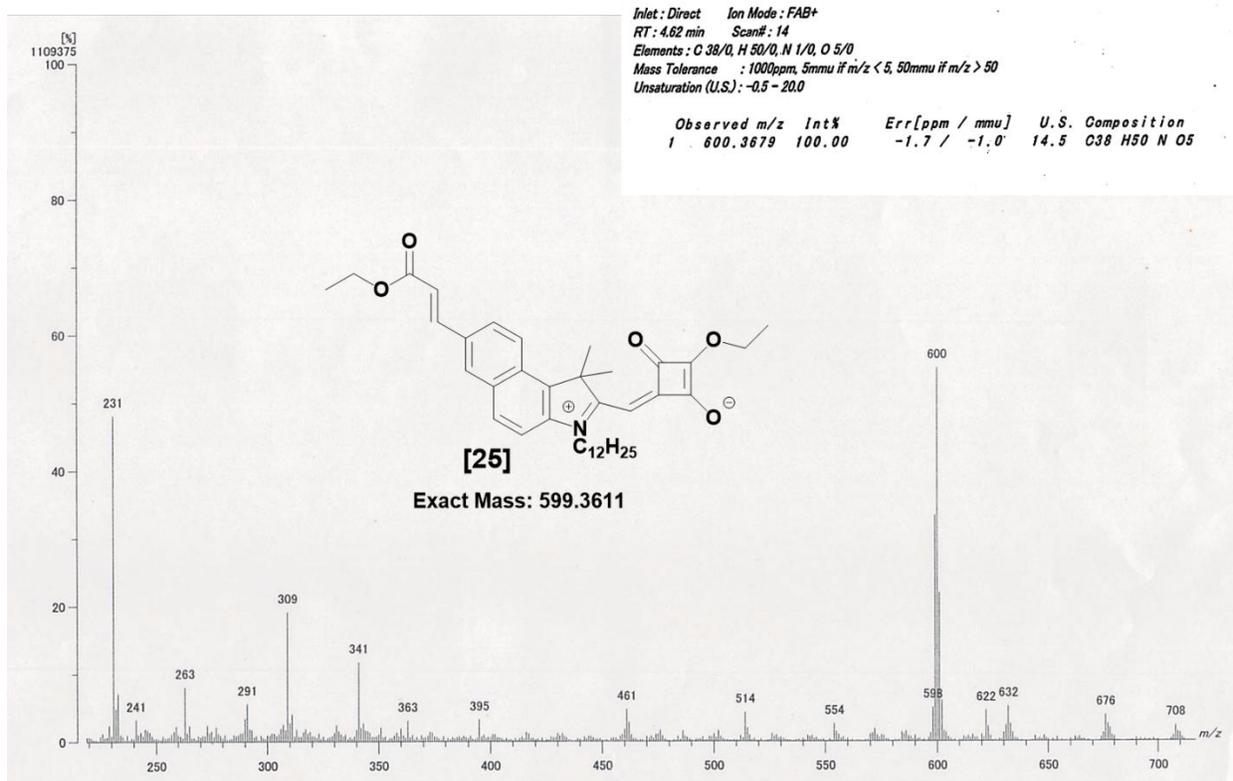
FAB-MS & HR FAB-MS of the intermediate (22)



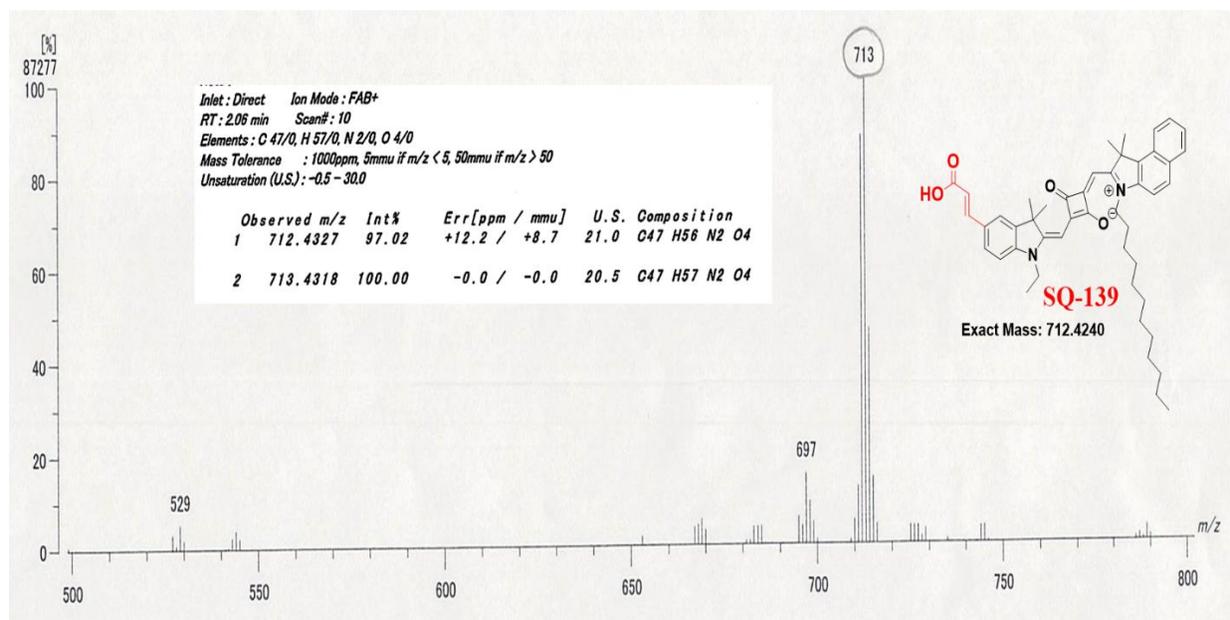
LALDI TOFMS of the intermediate (23)



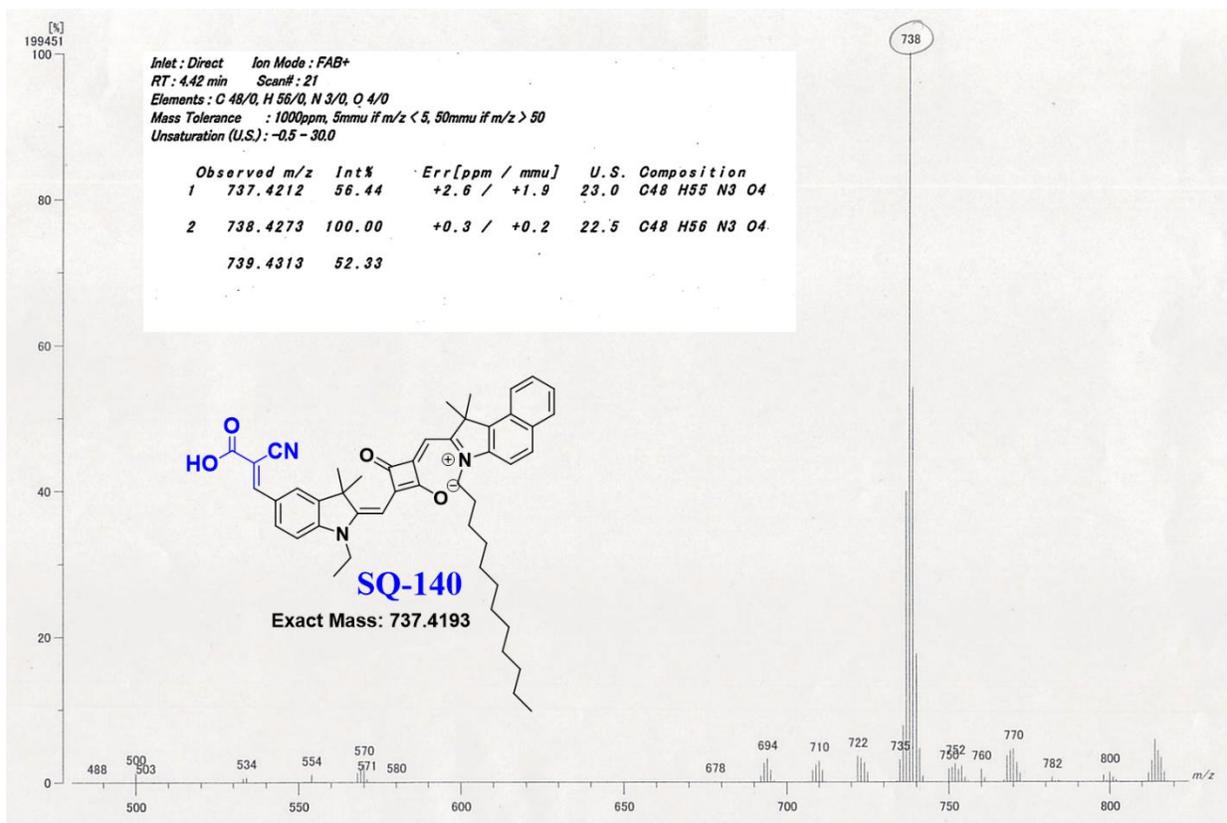
LALDI TOFMS of the intermediate (24)



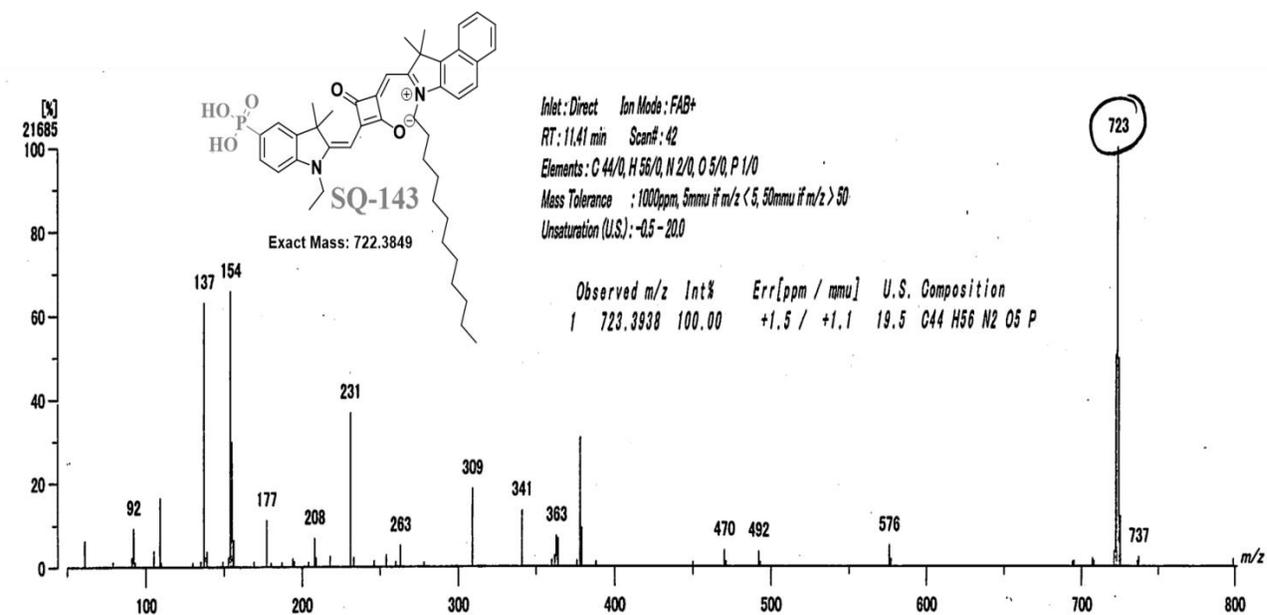
FAB-MS & HR FAB-MS of the intermediate (25)



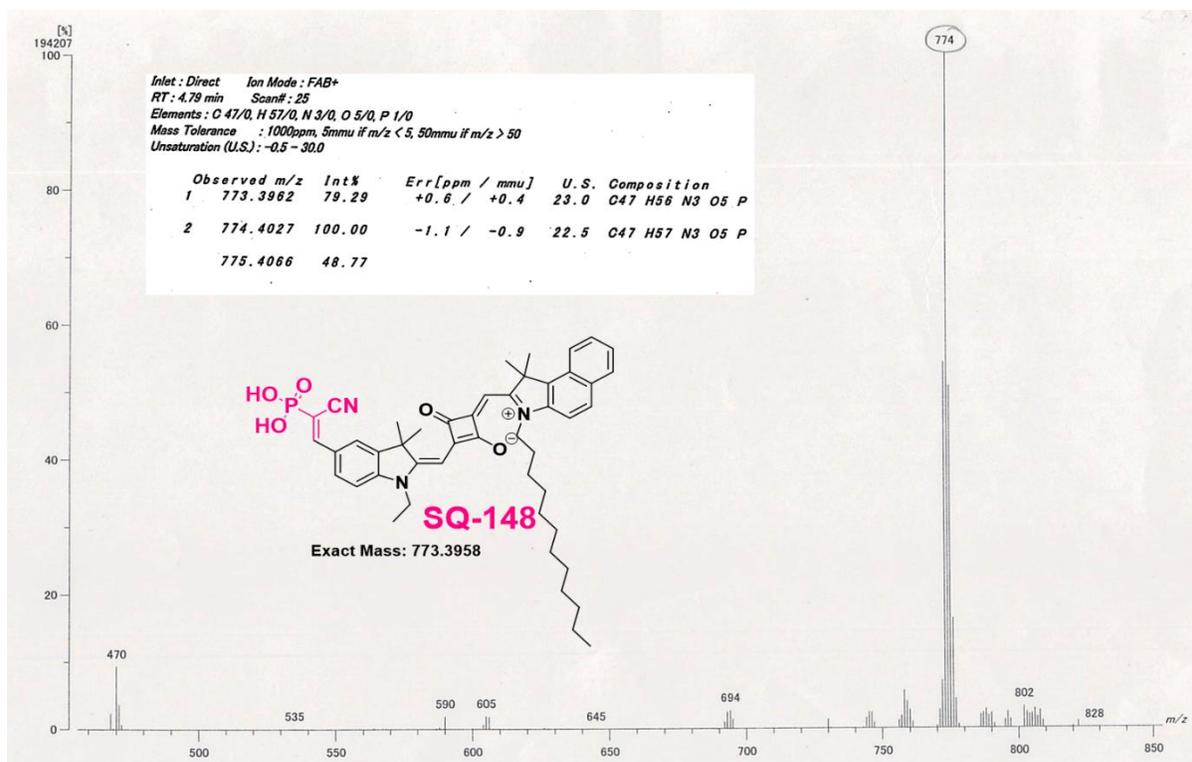
FAB-MS & HR FAB-MS of the Squaraine dye SQ-139



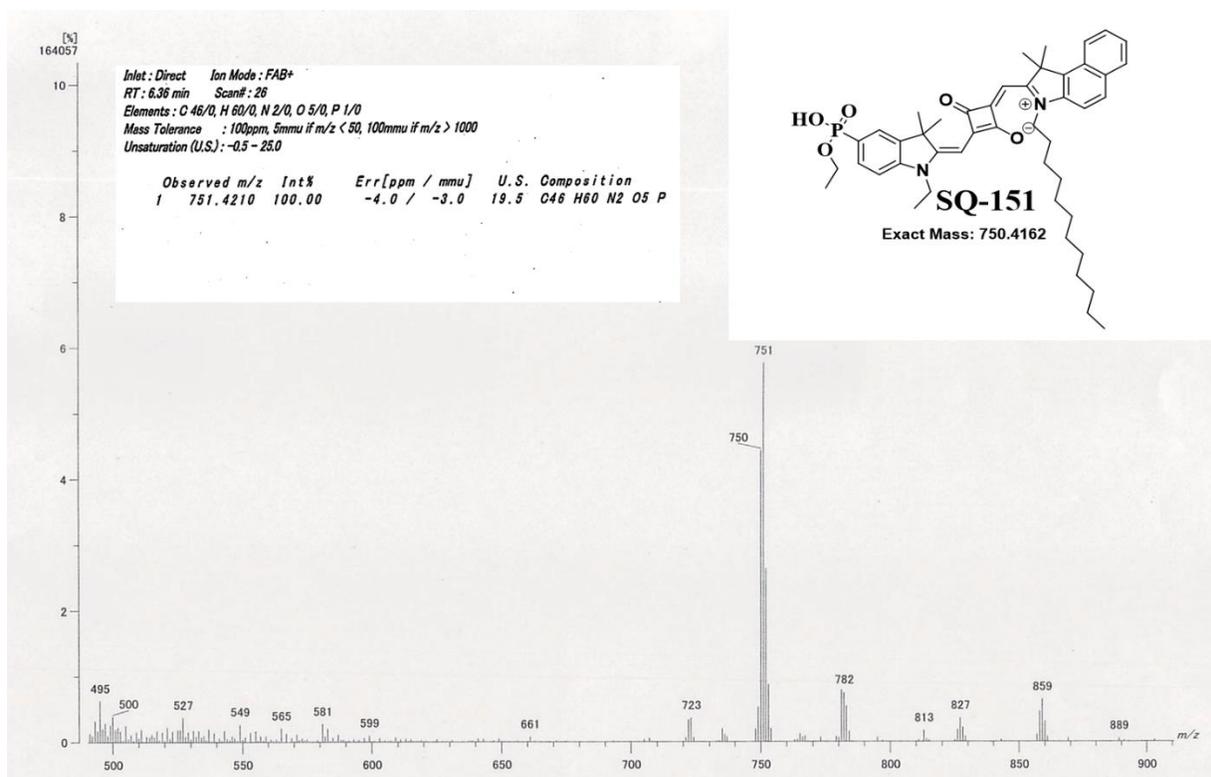
FAB-MS & HR FAB-MS of the Squaraine dye SQ-140



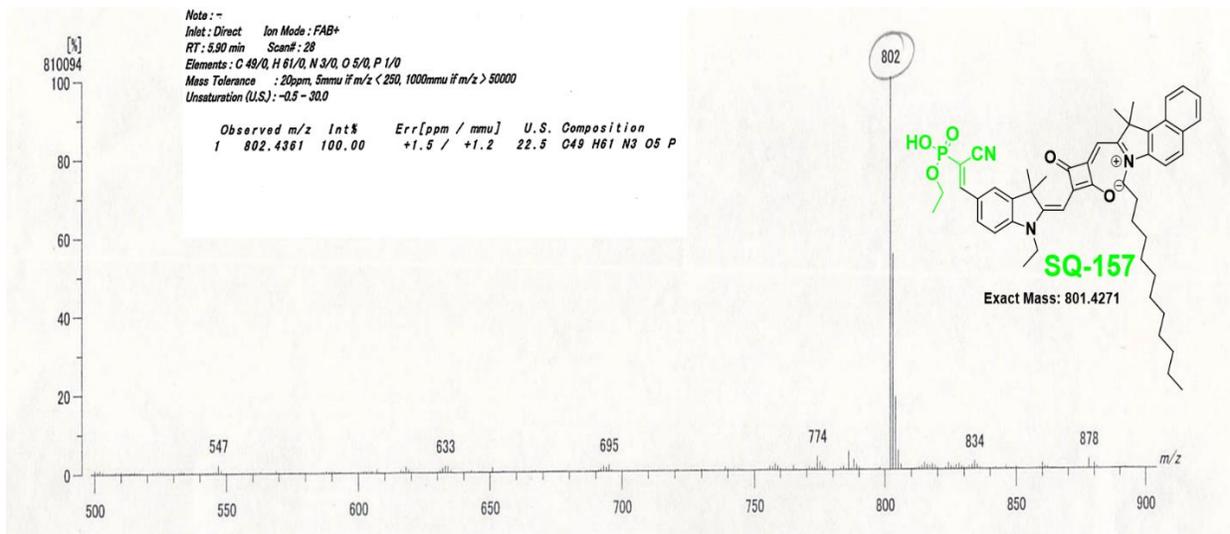
FAB-MS & HR FAB-MS of the Squaraine dye SQ-143



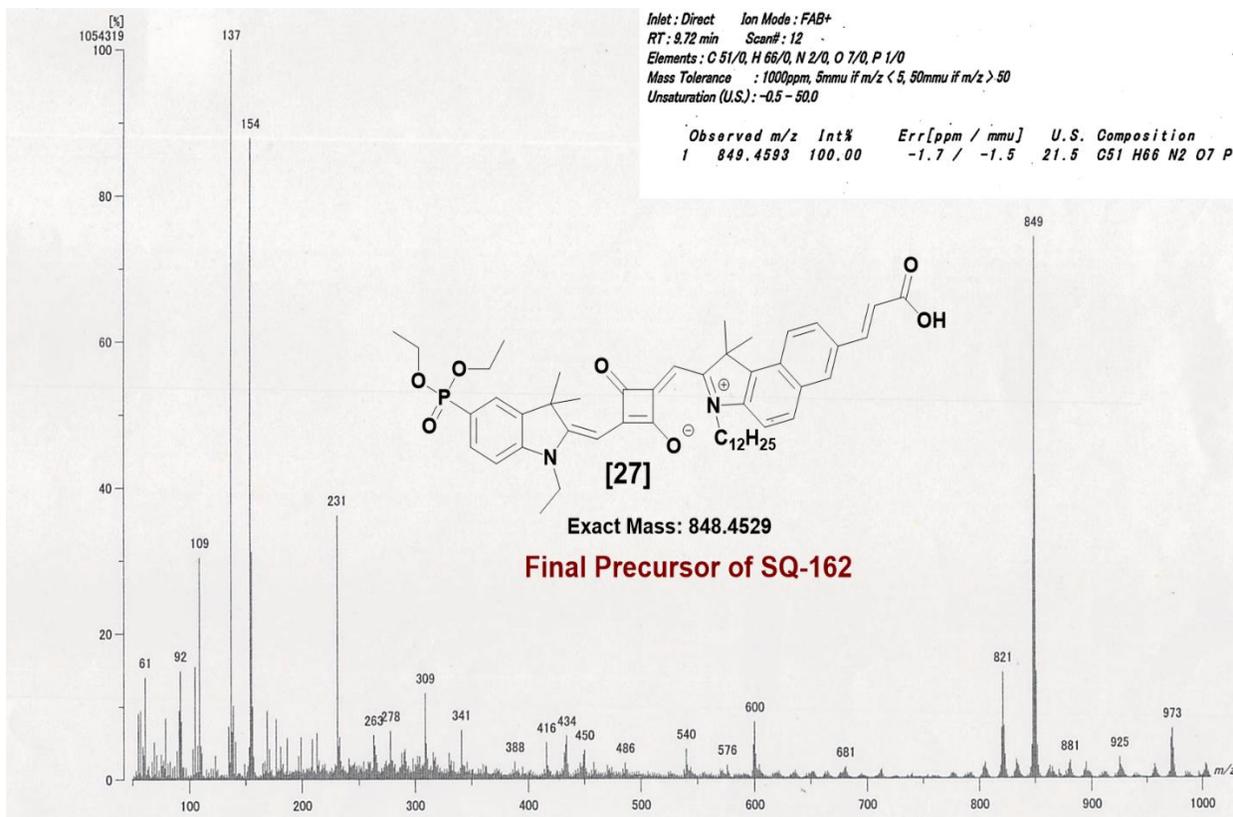
FAB-MS & HR FAB-MS of the Squaraine dye SQ-148



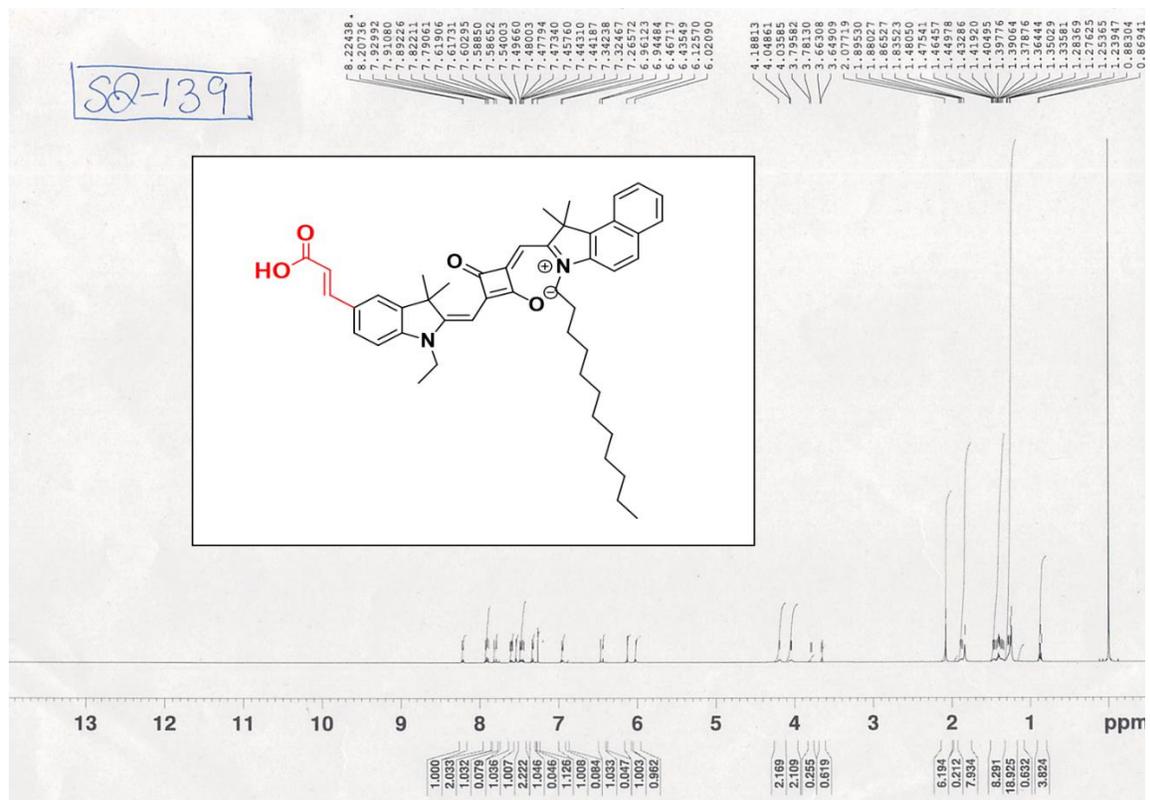
FAB-MS & HR FAB-MS of the Squaraine dye SQ-151



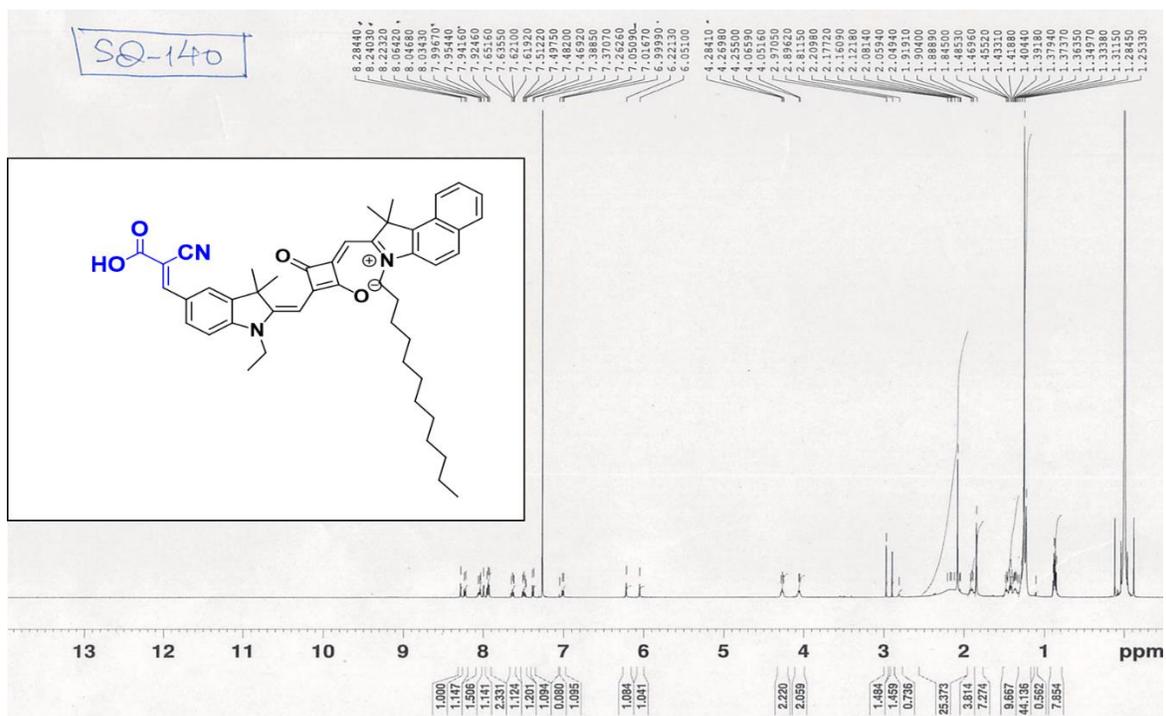
FAB-MS & HR FAB-MS of the Squaraine dye SQ-157



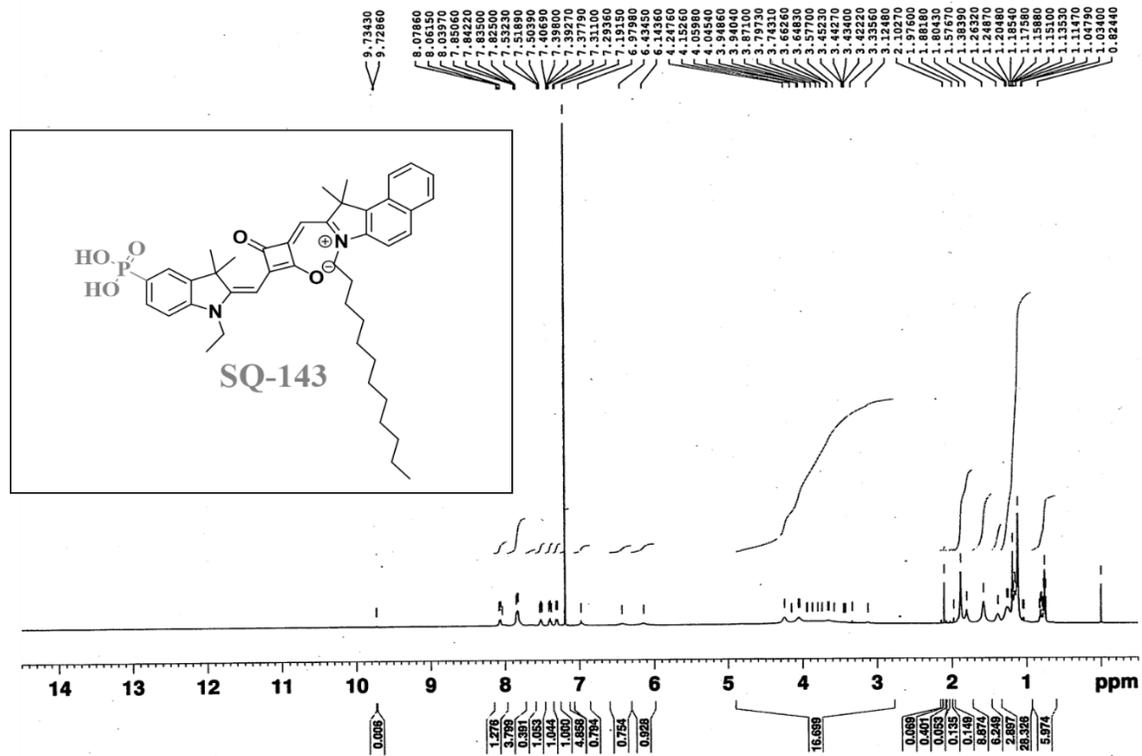
FAB-MS & HR FAB-MS of the Squaraine dye SQ-162



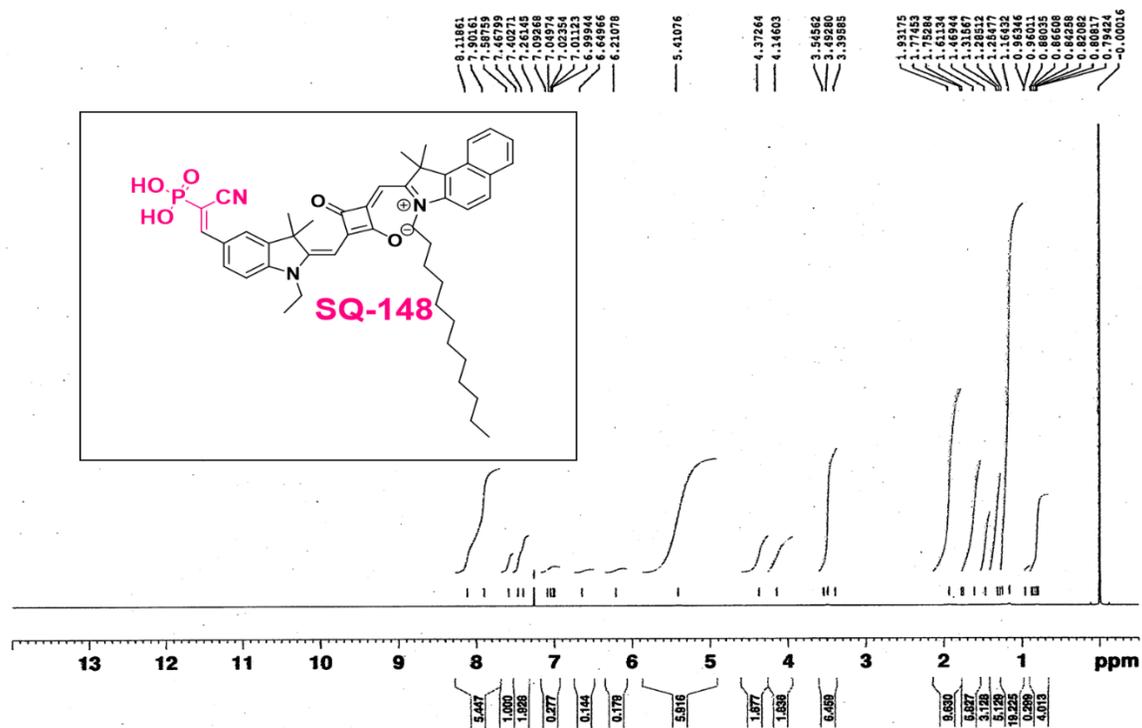
Proton NMR of the Squaraine dye SQ-139



Proton NMR of the Squaraine dye SQ-140



Proton NMR of the Squaraine dye SQ-143



Proton NMR of the Squaraine dye SQ-148

