

Synthesis and Structure-activity Relationship of Palmatine Derivatives as a Novel Class of Antibacterial Agents against *Helicobacter pylori*

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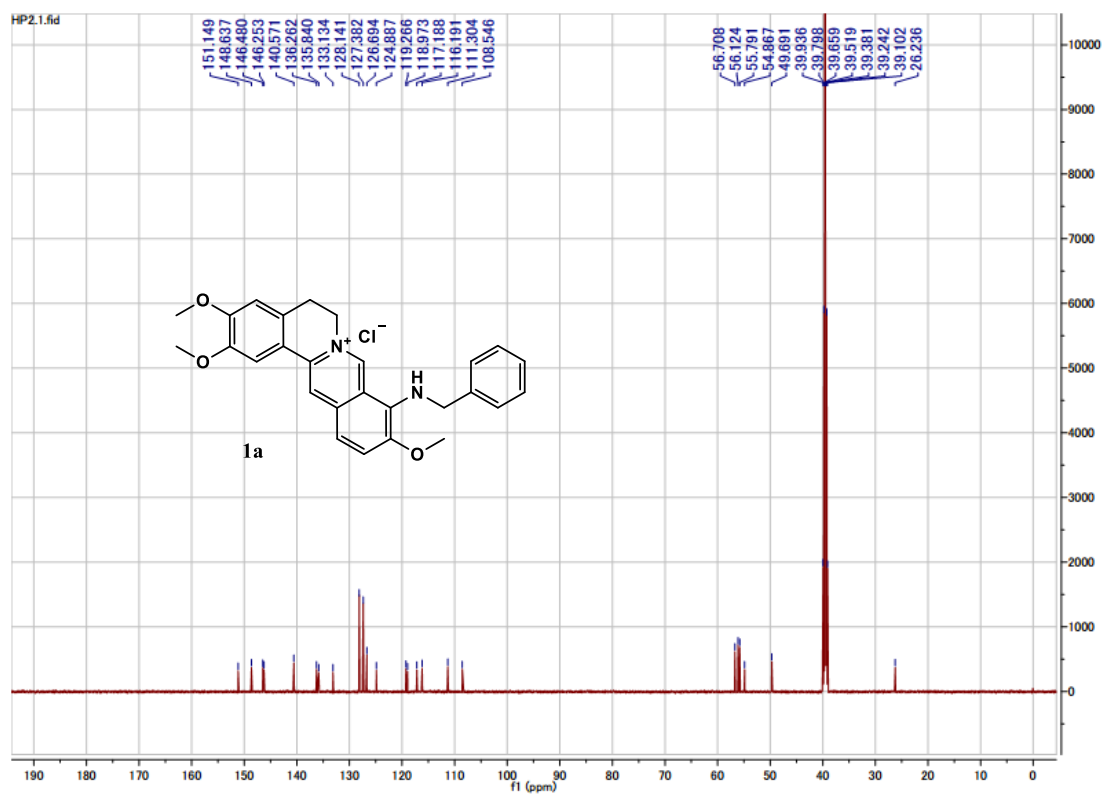
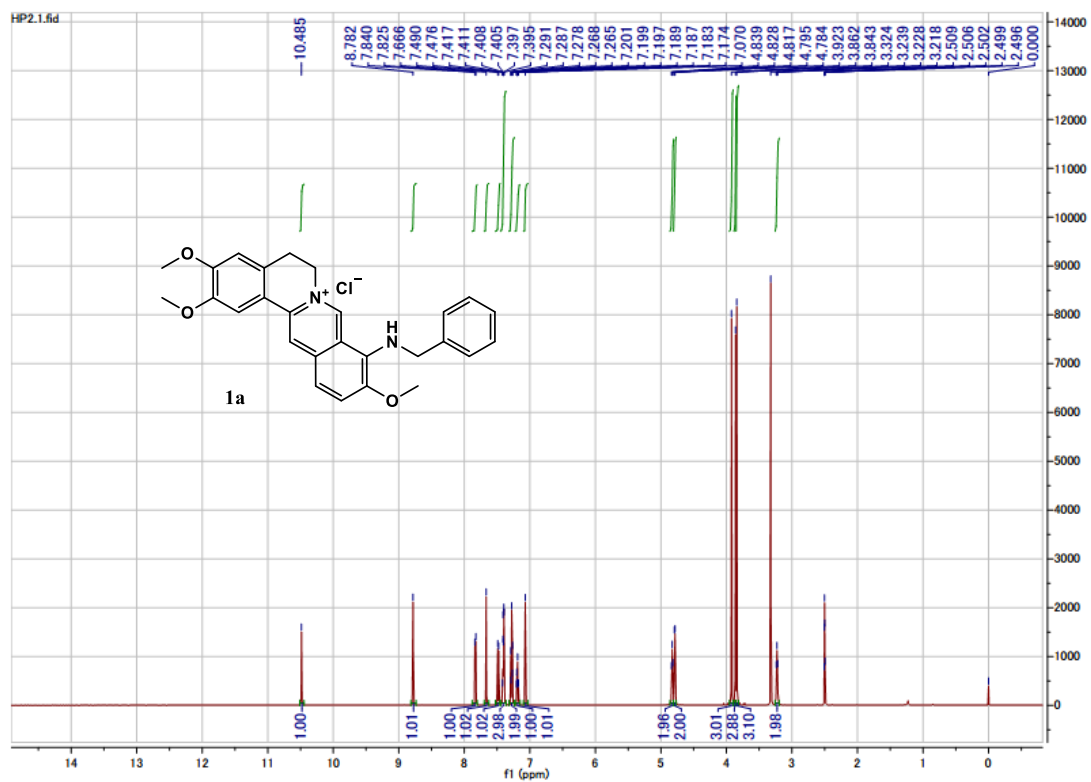
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Table SI. The reaction time and temperature of each target compound.

Code	reaction time (h)	reaction temperature (°C)	yield (%)
1a	6	110	41
1b	4	110	43
1c	4	110	48
1d	6	110	57
1e	8	110	35
1f	7	110	54
1g	7	110	44
1h	72	120	19
1i	72	95	35
2	6	110	52
3	24	25	73
4a	6	71	37
4b	3	71	45
4c	6	71	49
4d	8	71	37
4e	8	71	40
4f	24	71	42
4g	24	71	47
4h	8	71	35
4i	24	71	36

Figure S1: ^1H NMR, ^{13}C NMR, HRMS-ESI spectra of compound **1a**



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T: FTMS + c ESI Full ms [100.00-700.00]

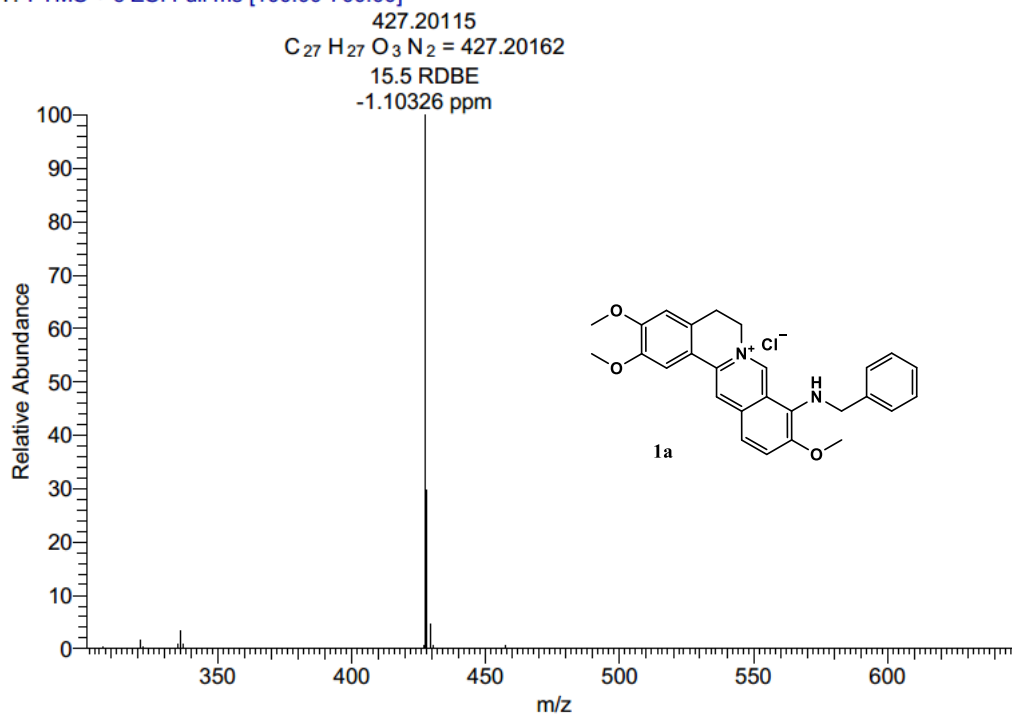
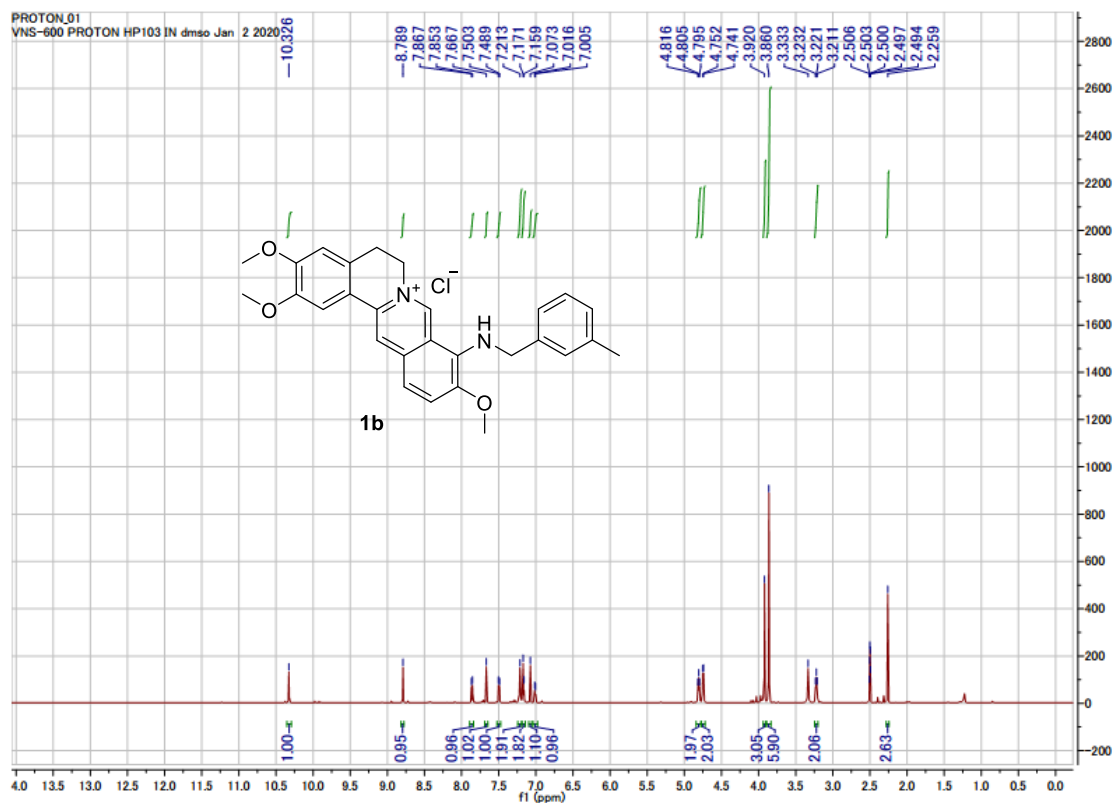
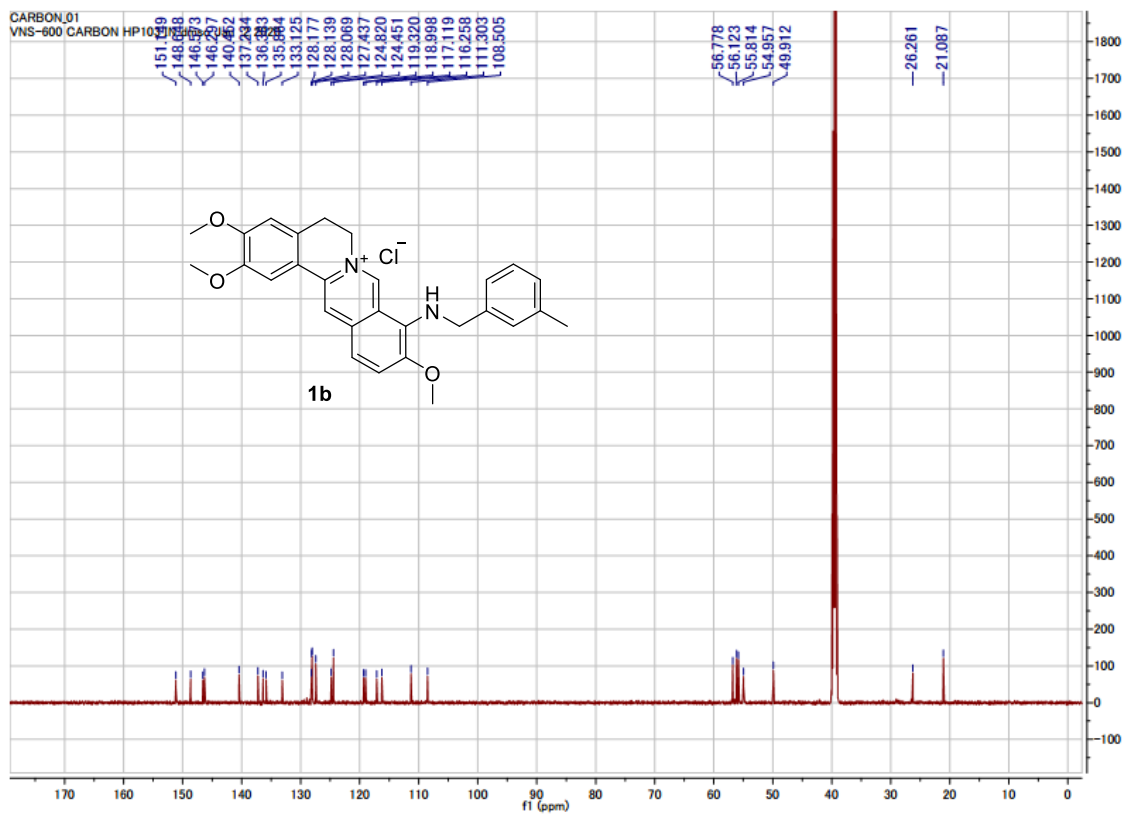


Figure S2: ¹H NMR, ¹³C NMR, HRMS-ESI spectra of compound **1b**





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HP103_191213160724 #30 RT: 0.30 AV: 1 NL: 2.08E7
T: FTMS + c ESI Full ms [100.00-2000.00]

441.21698
C₂₈ H₂₉ O₃ N₂ = 441.21727
-0.65566 ppm

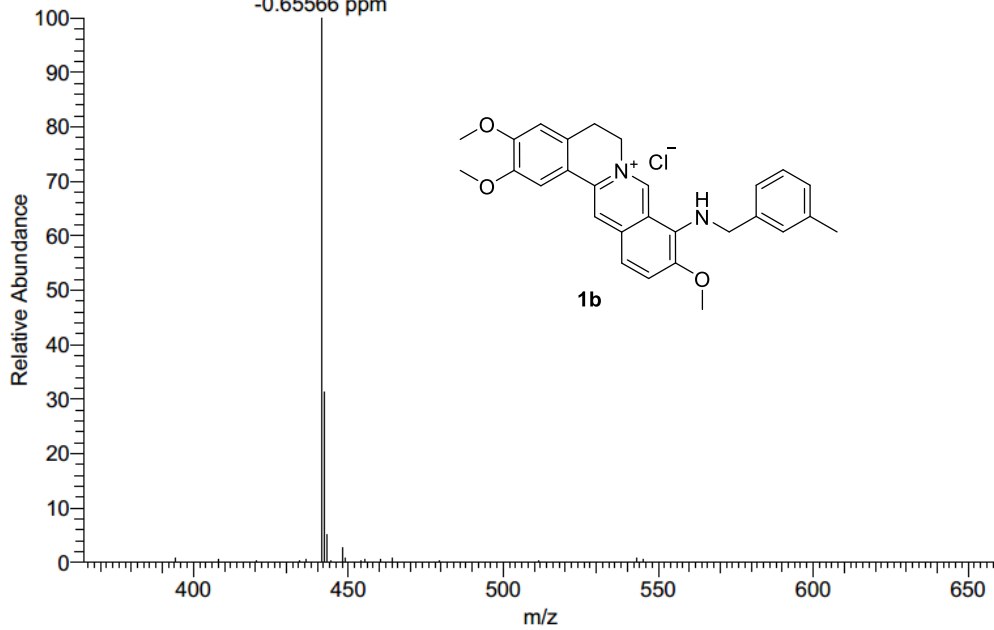
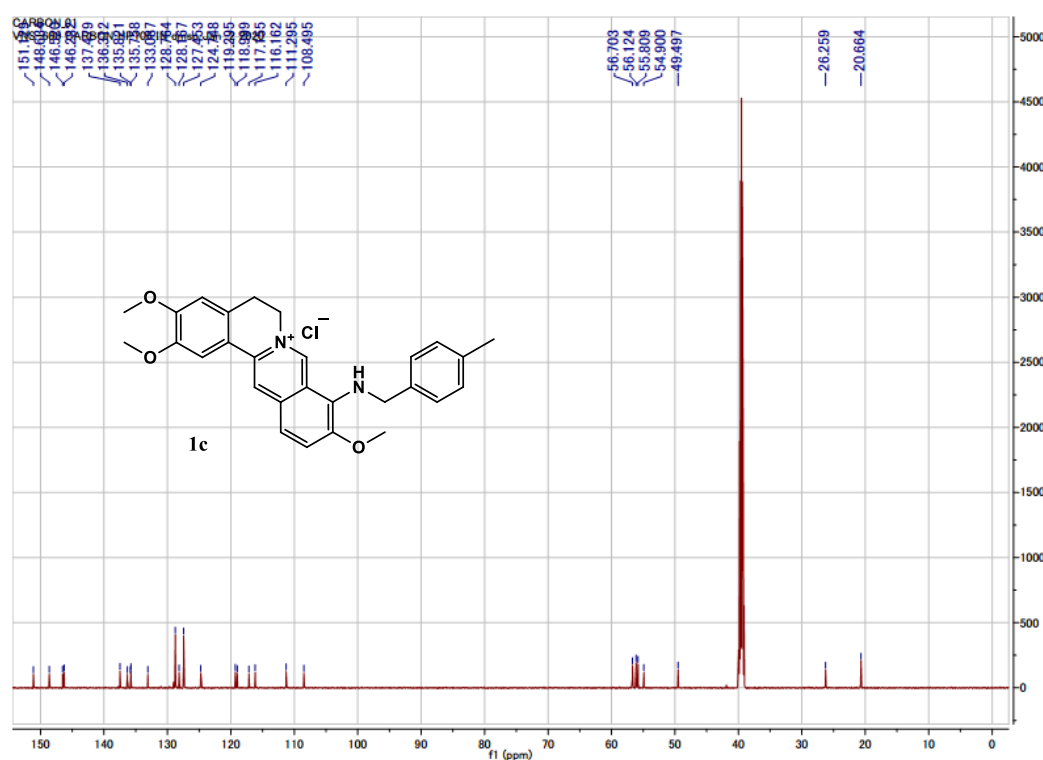
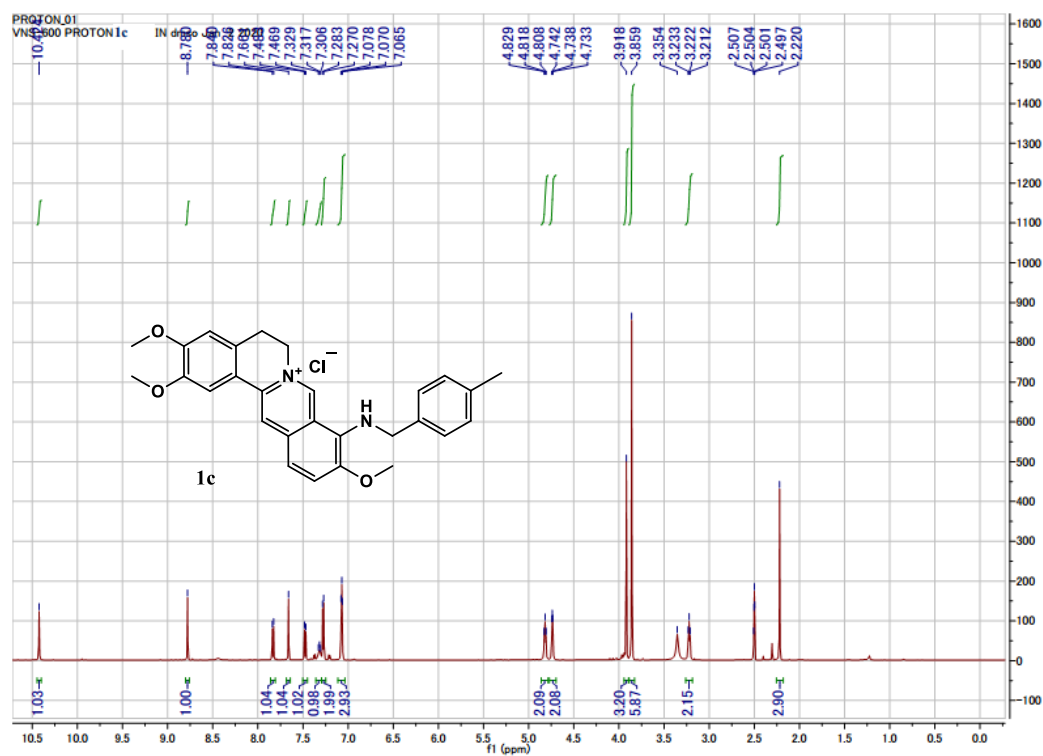


Figure S3: ^1H NMR, ^{13}C NMR, HRMS-ESI spectra of compound **1c**



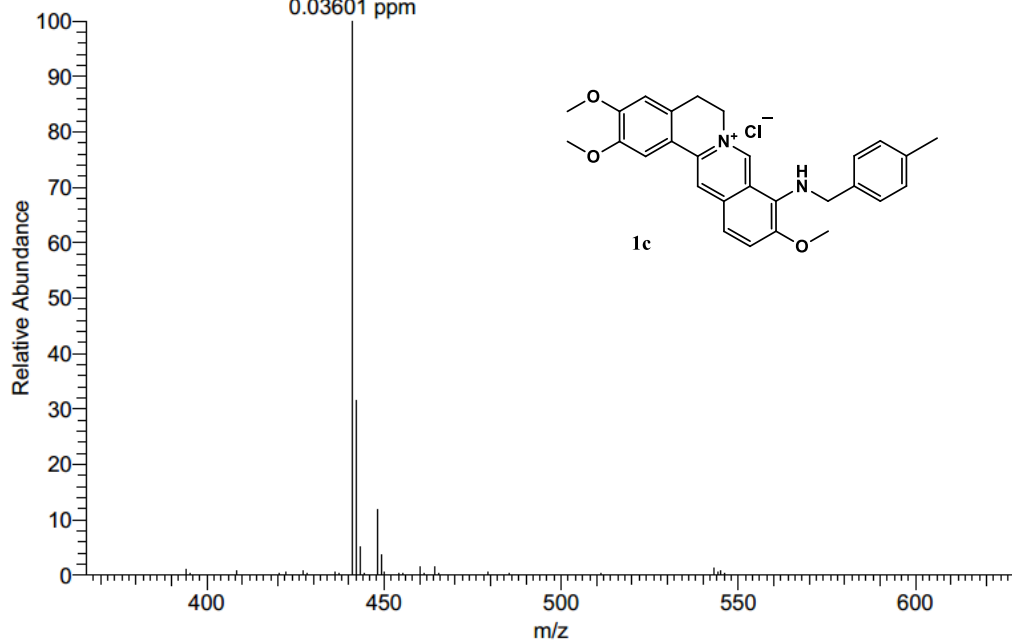
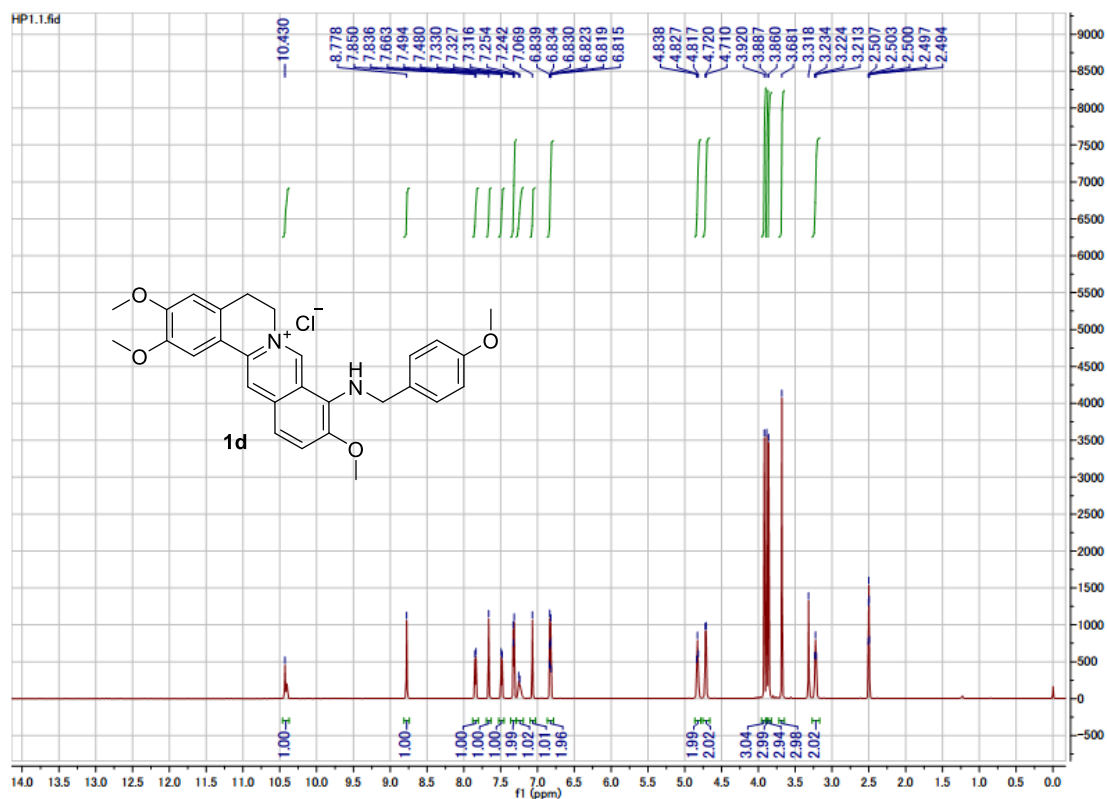
Ic _191213160724 #57 RT: 0.63 AV: 1 NL: 1.55E7

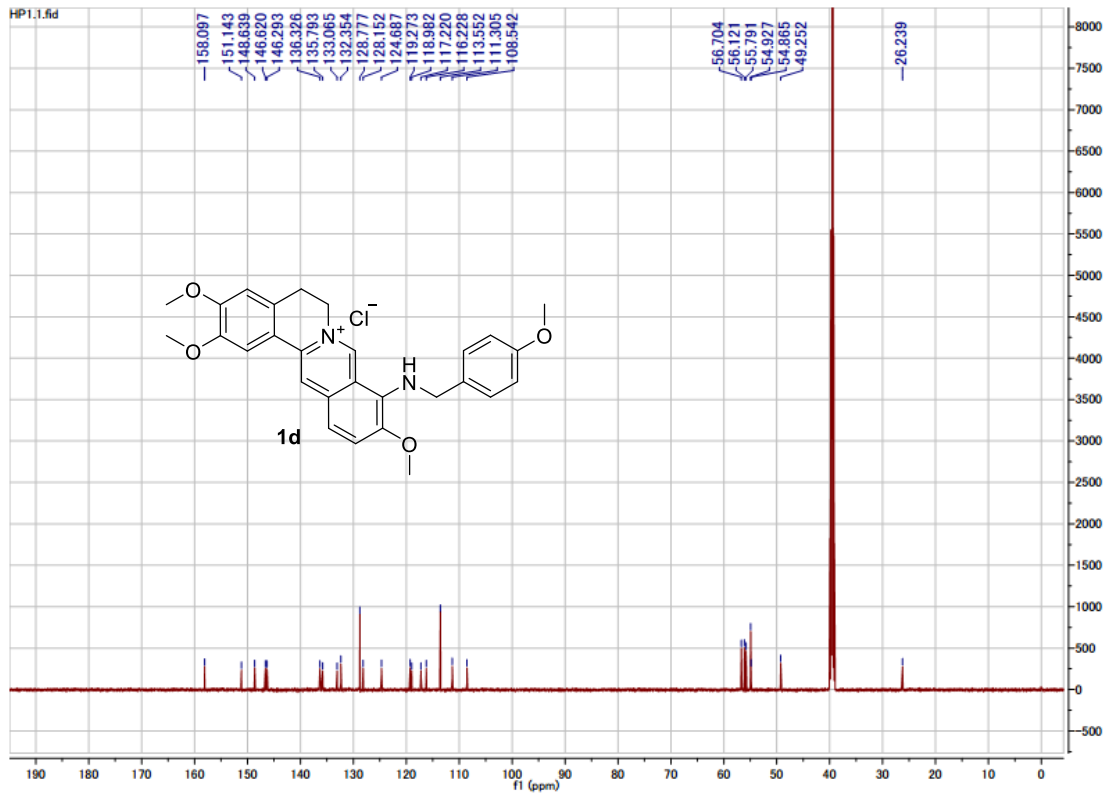
T: FTMS + c ESI Full ms [100.00-2000.00]

441.21729

C₂₈H₂₉O₃N₂ = 441.21727

0.03601 ppm

Figure S4: ¹H NMR, ¹³C NMR, HRMS-ESI spectra of compound 1d



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HP1_ESI+ #23 RT: 0.13 AV: 1 SB: 2 0.91, 0.91 NL: 1.02E8
T: FTMS + c ESI Full ms [100.00-700.00]

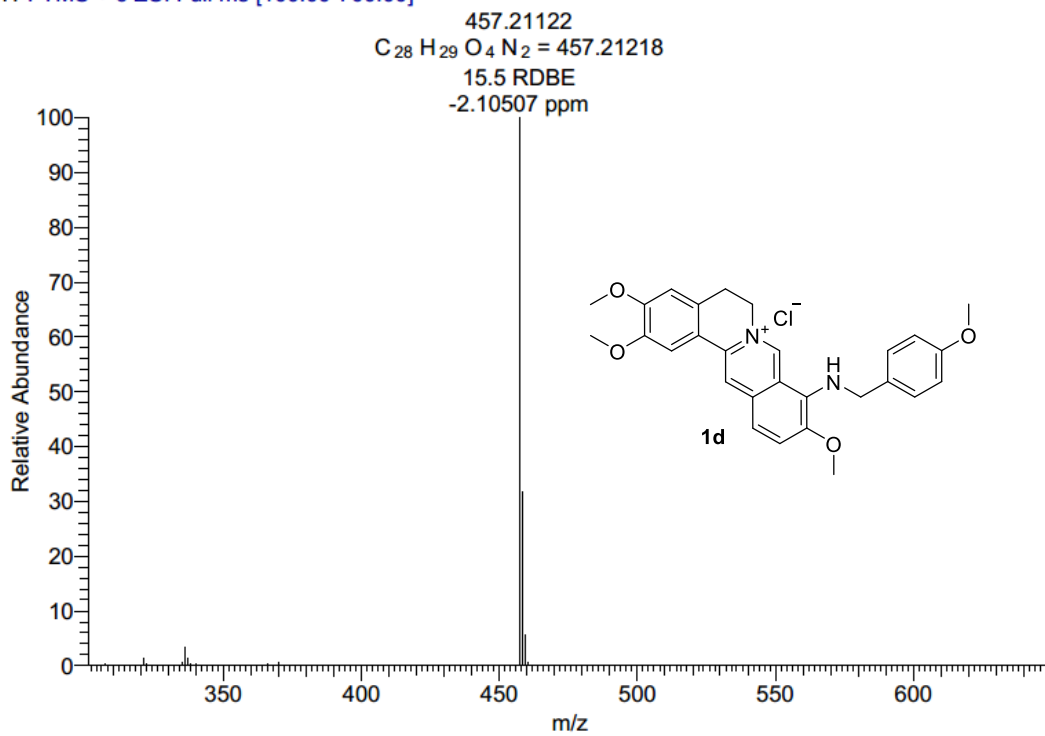
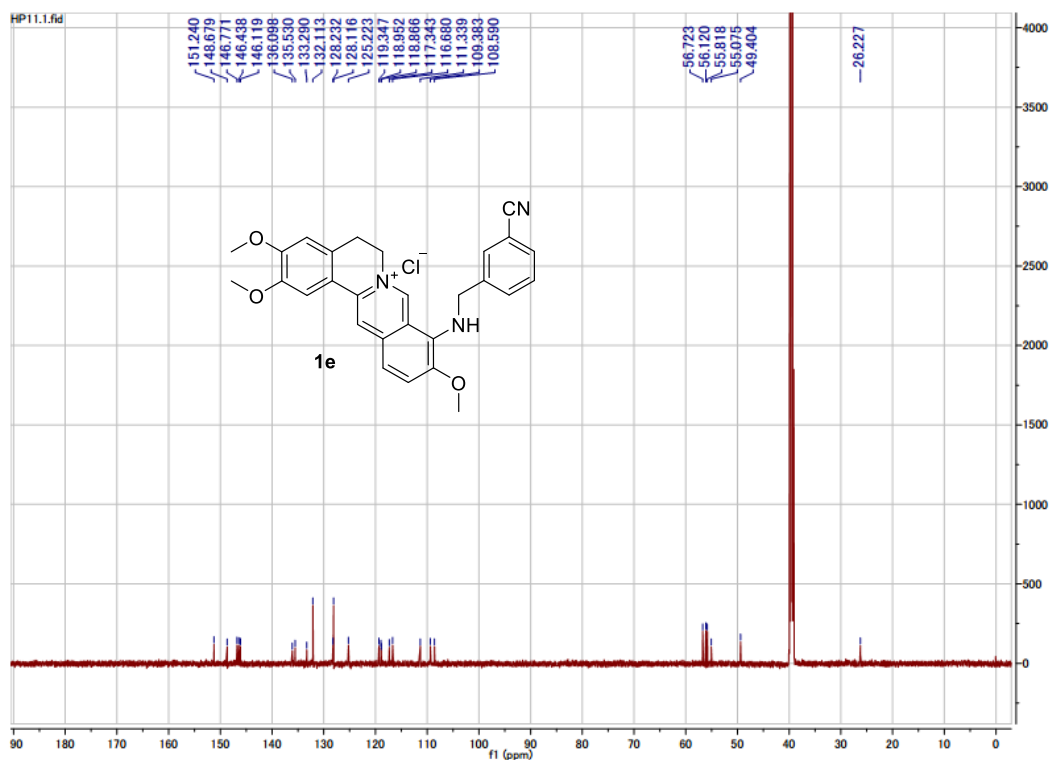
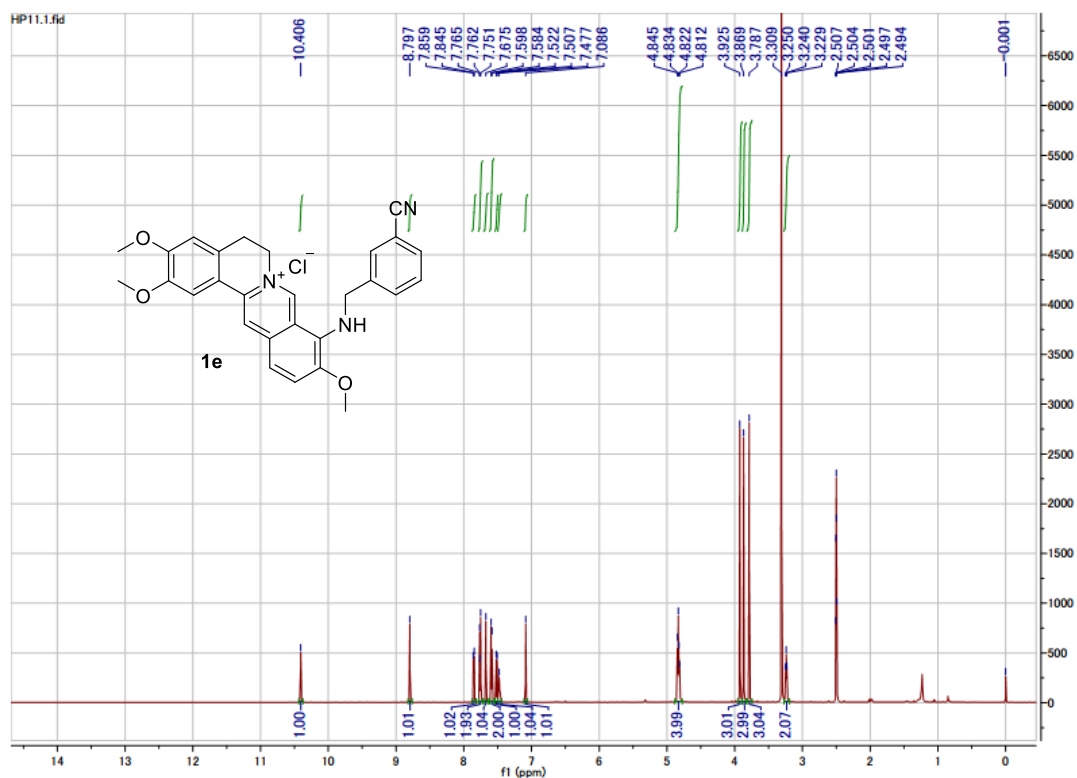


Figure S5: ^1H NMR, ^{13}C NMR, HRMS-ESI spectra of compound **1e**



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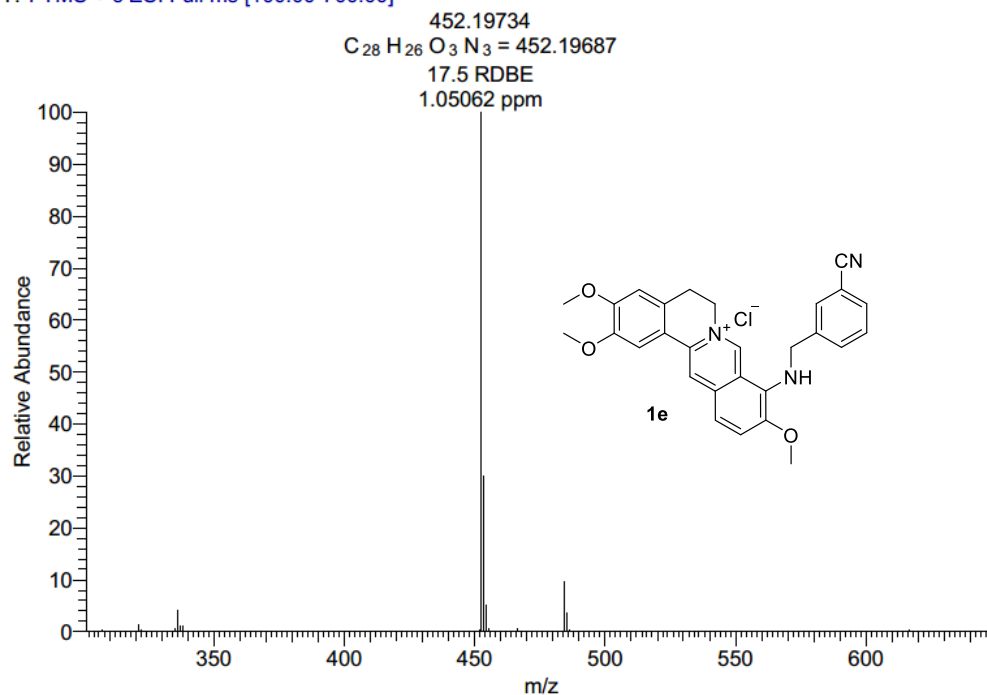
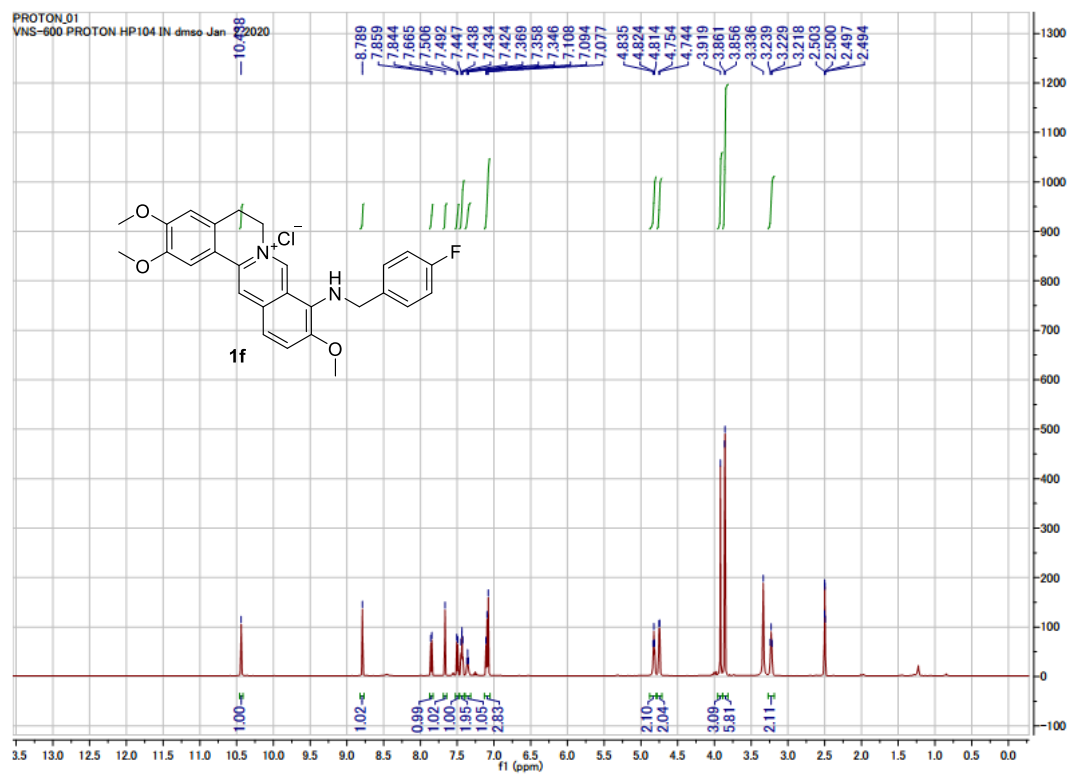
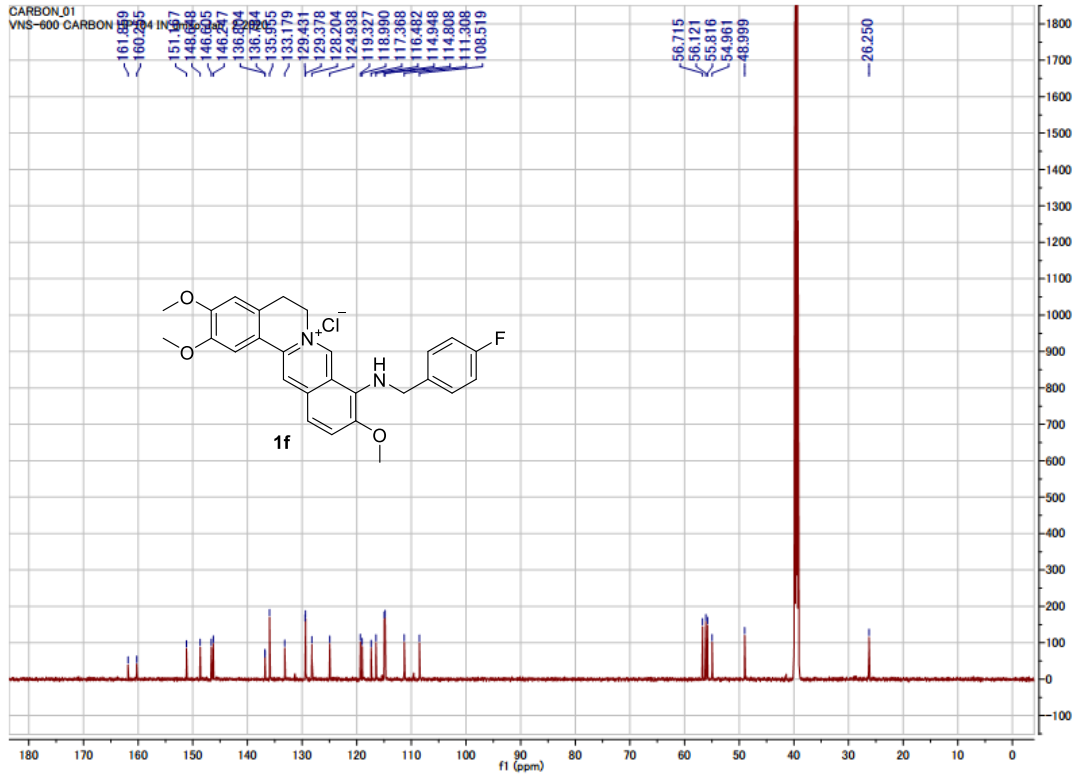


Figure S6: 1H NMR, ^{13}C NMR, HRMS-ESI spectra of compound 1f





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HP104_191213160724 #32 RT: 0.31 AV: 1 NL: 1.08E7
T: FTMS + c ESI Full ms [100.00-2000.00]

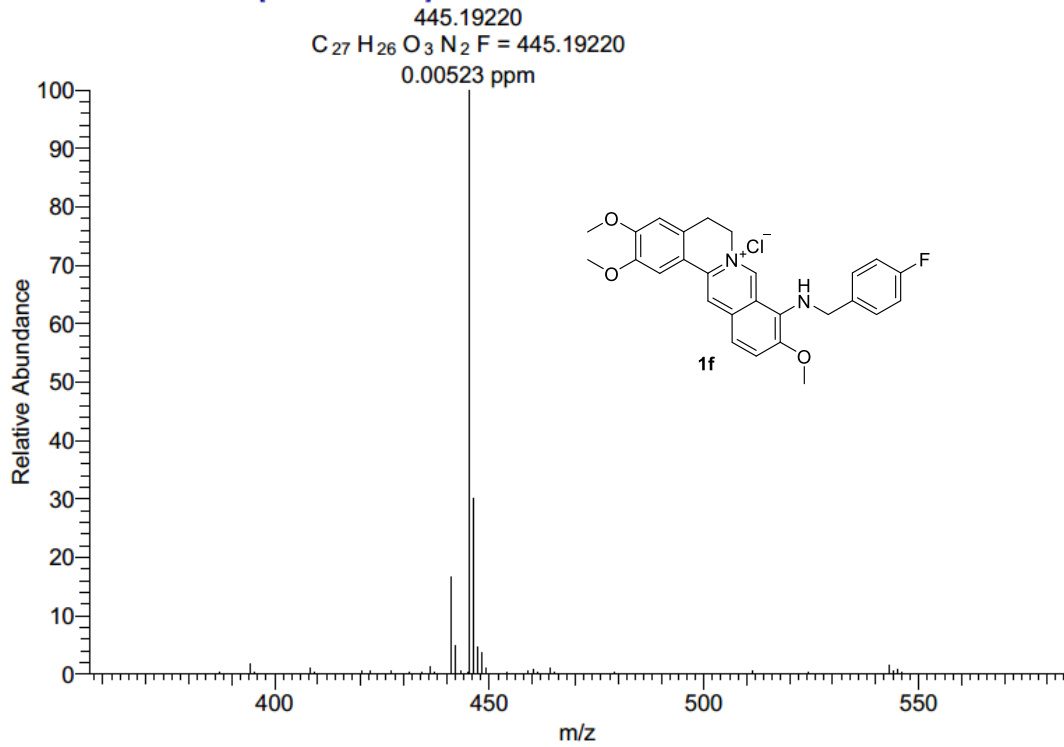
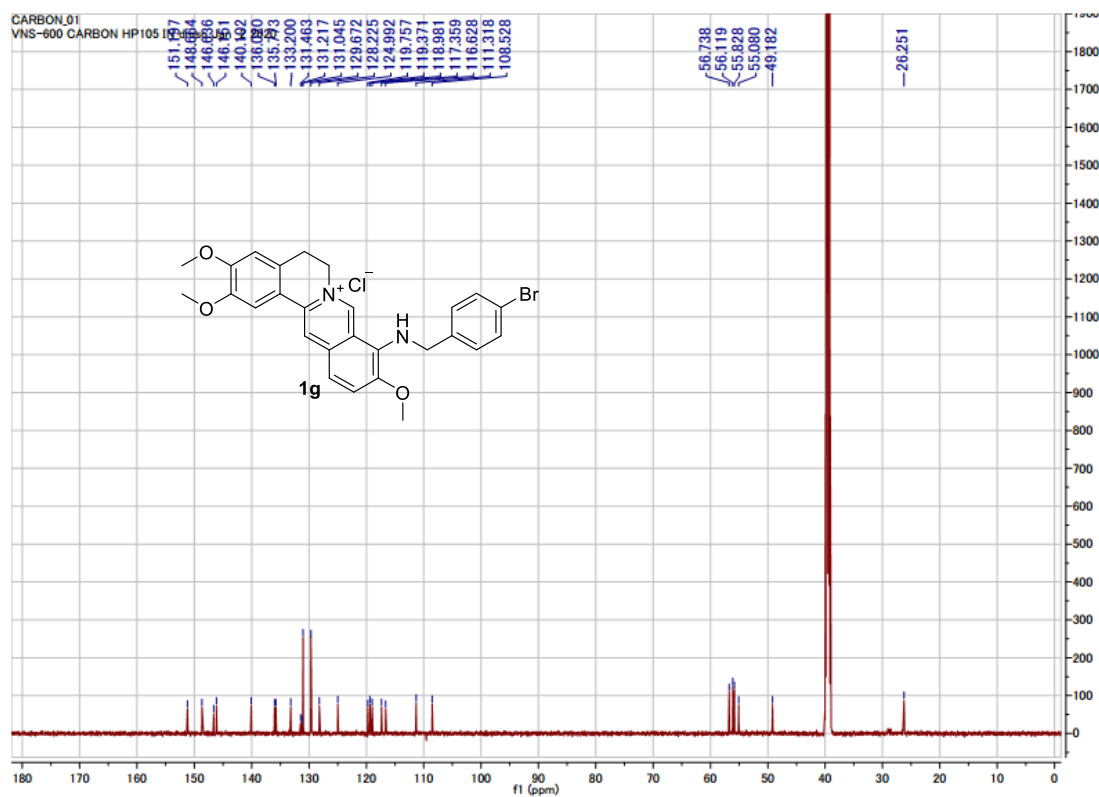
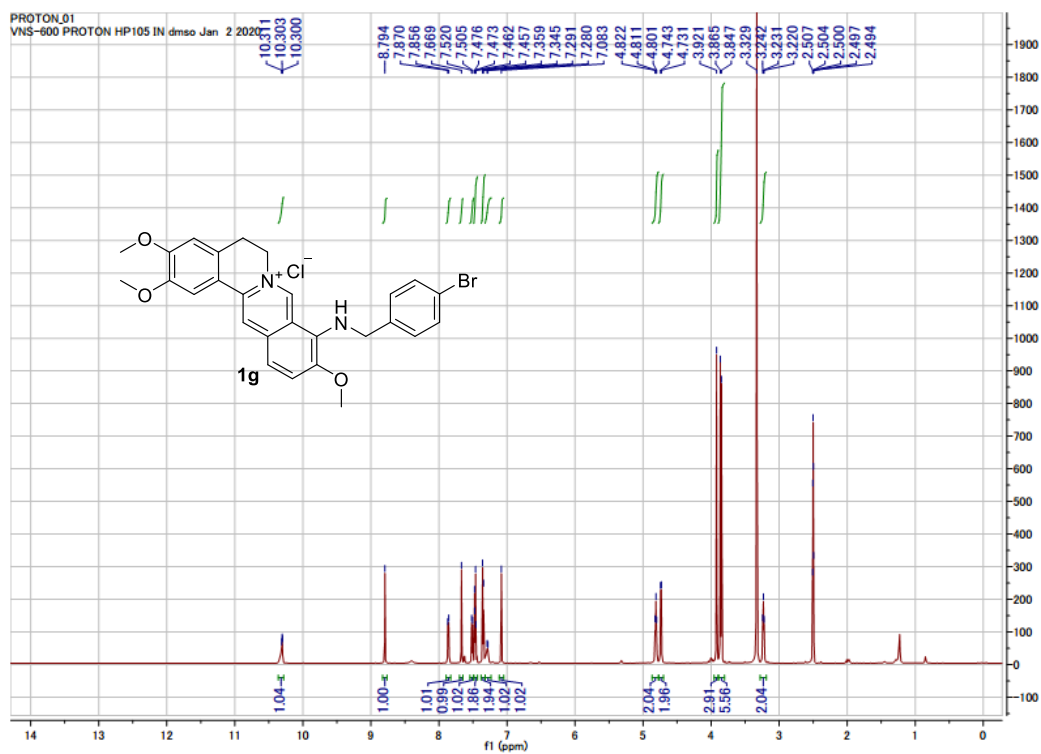


Figure S7: ^1H NMR, ^{13}C NMR, HRMS-ESI spectra of compound **1g**



HP105_191213160724 #20 RT: 0.19 AV: 1 NL: 9.39E7
T: FTMS + c ESI Full ms [100.00-2000.00]

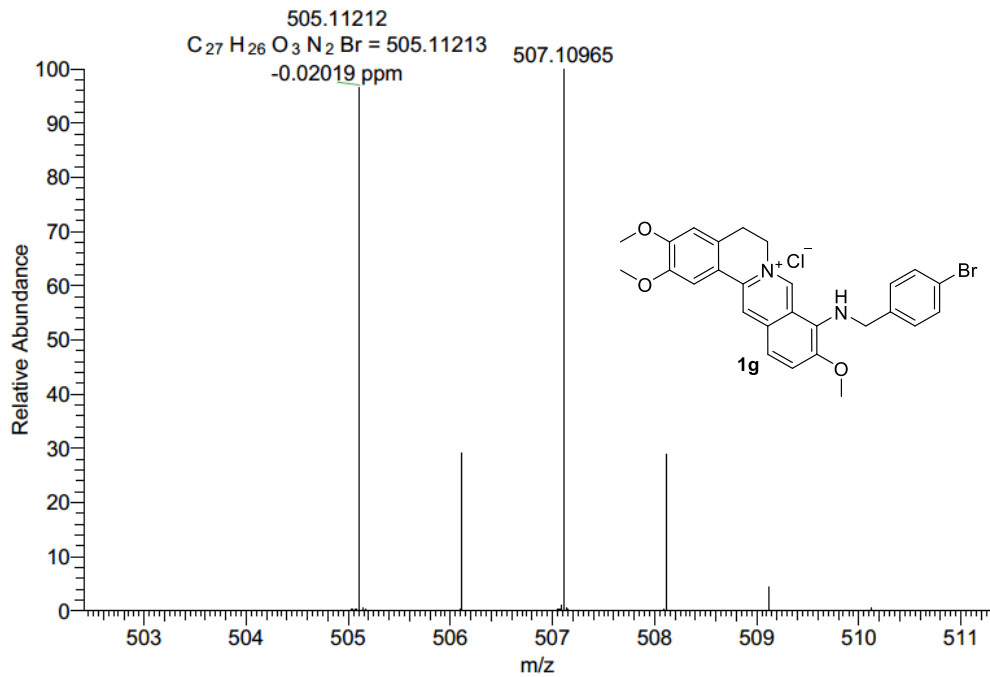
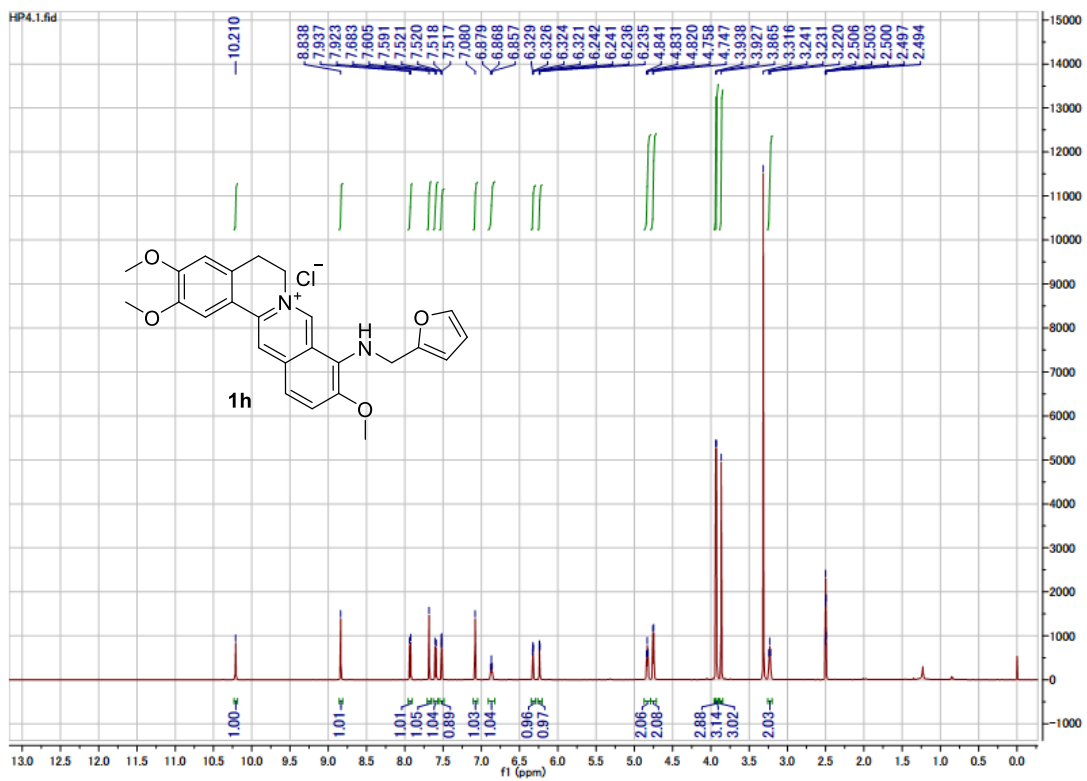
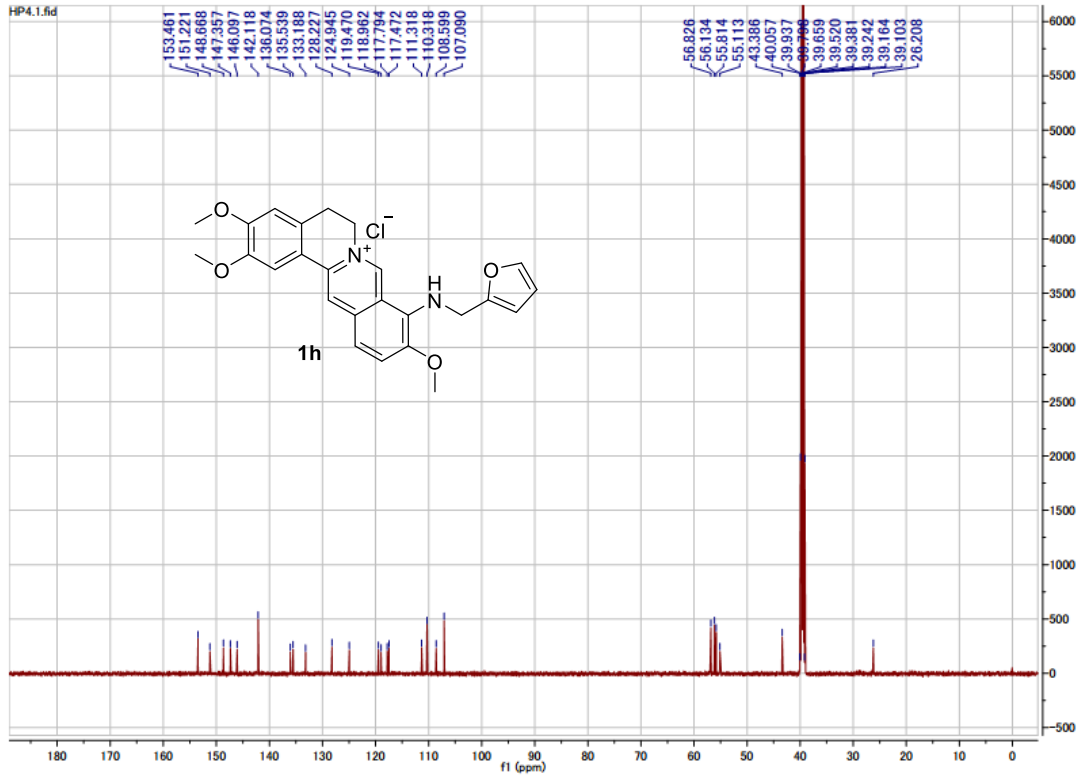


Figure S8: ¹H NMR, ¹³C NMR, HRMS-ESI spectra of compound **1h**





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HP4_ESI+ #47 RT: 0.26 AV: 1 SB: 2 0.60, 0.60 NL: 2.28E8
T: FTMS + c ESI Full ms [100.00-700.00]

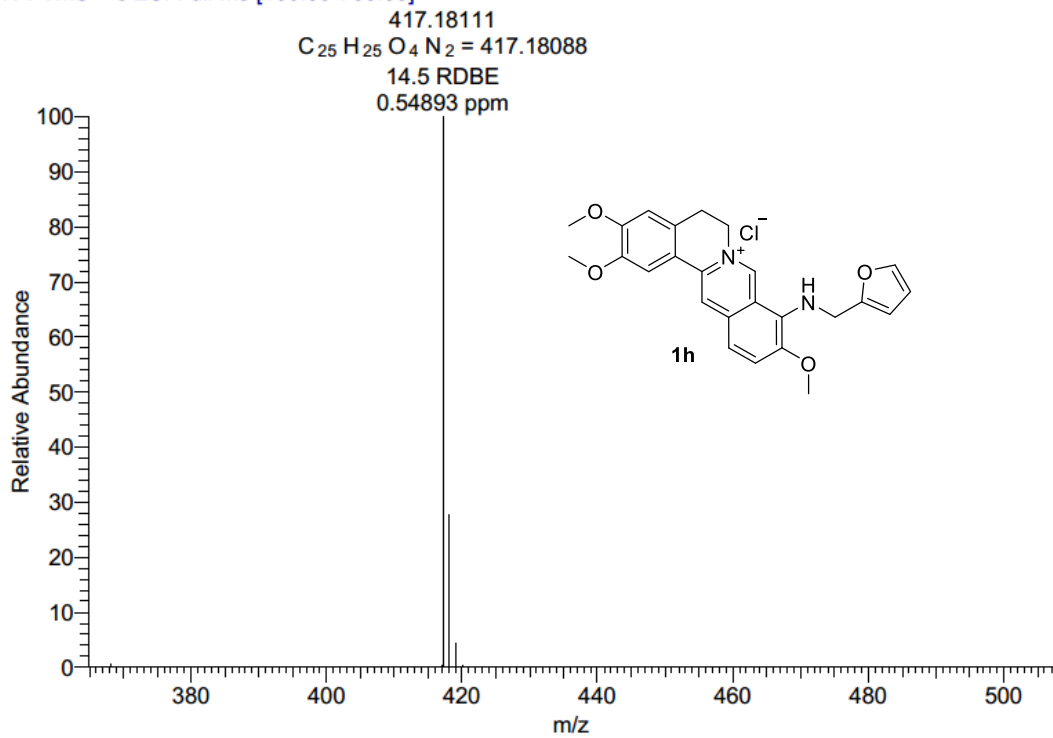
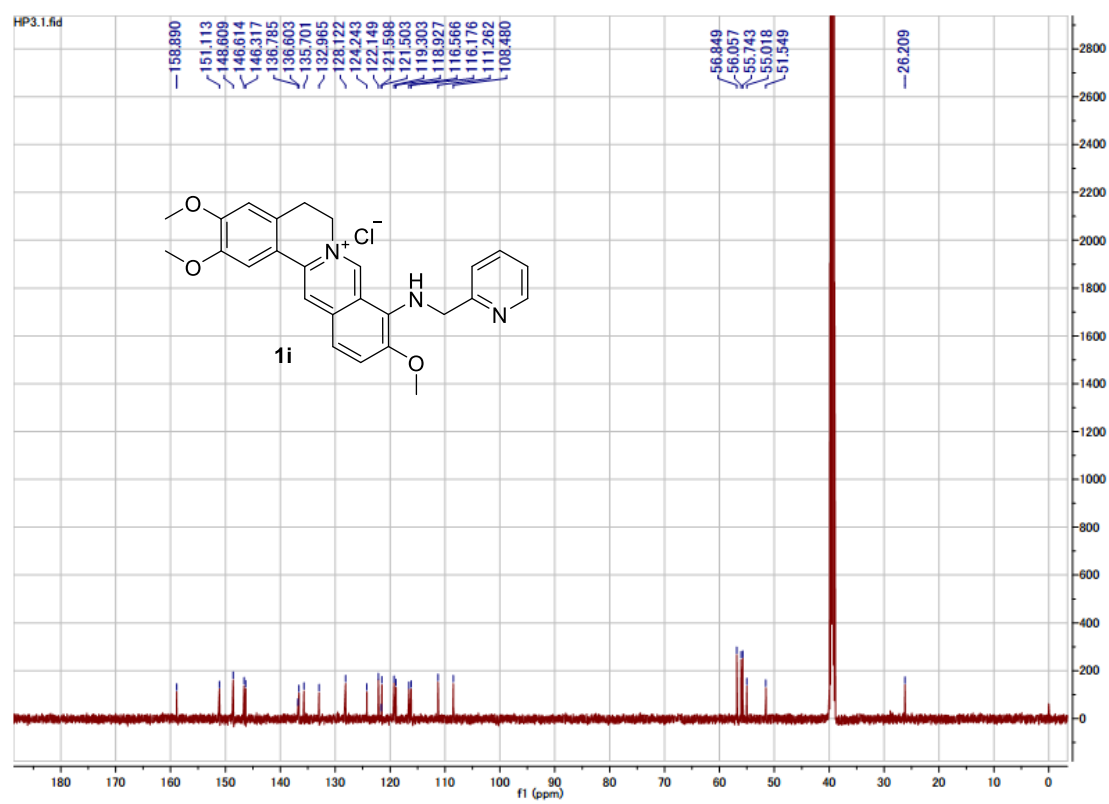
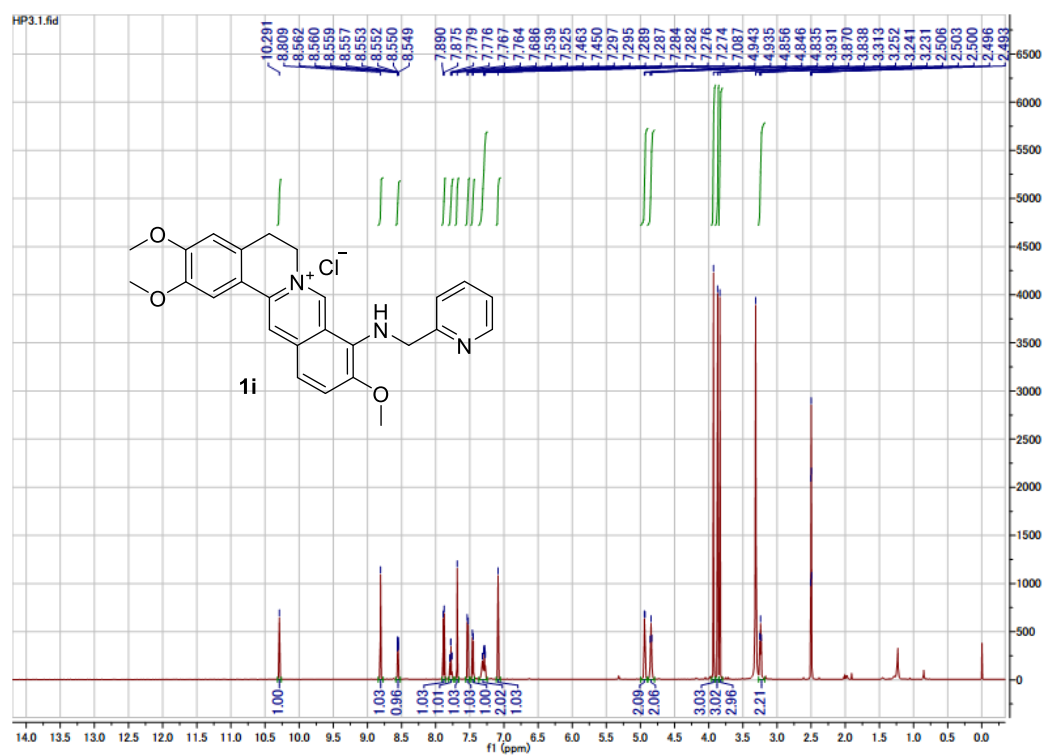


Figure S9: ^1H NMR, ^{13}C NMR, HRMS-ESI spectra of compound **1i**



HP3_ESI+ #30 RT: 0.17 AV: 1 SB: 2 0.34, 0.34 NL: 7.23E7
 T: FTMS + c ESI Full ms [100.00-700.00]

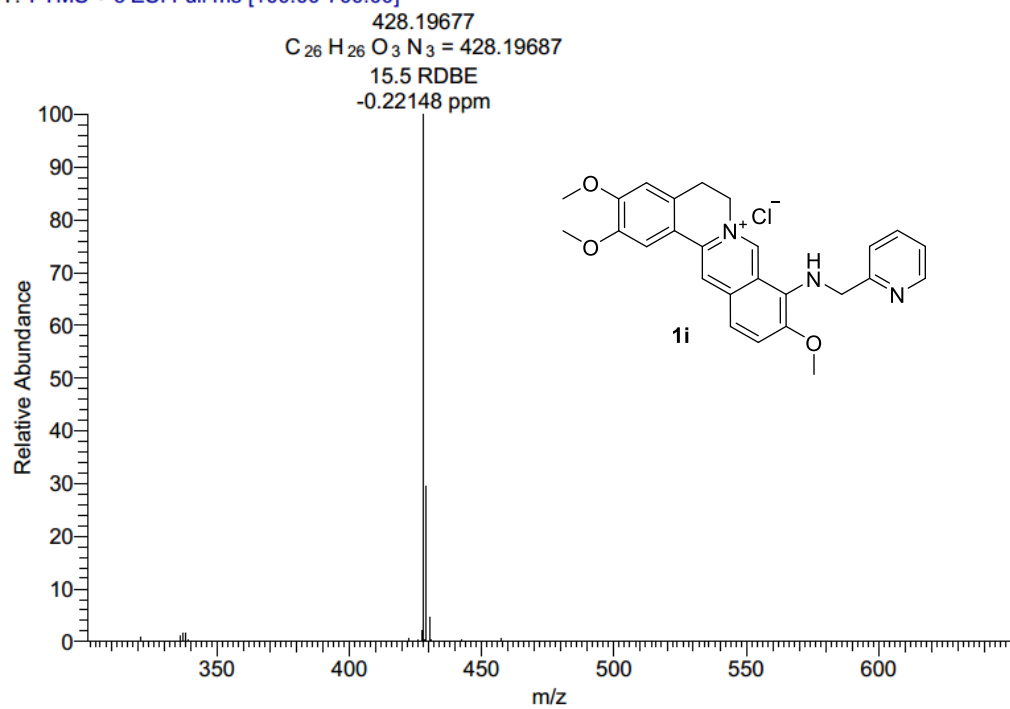
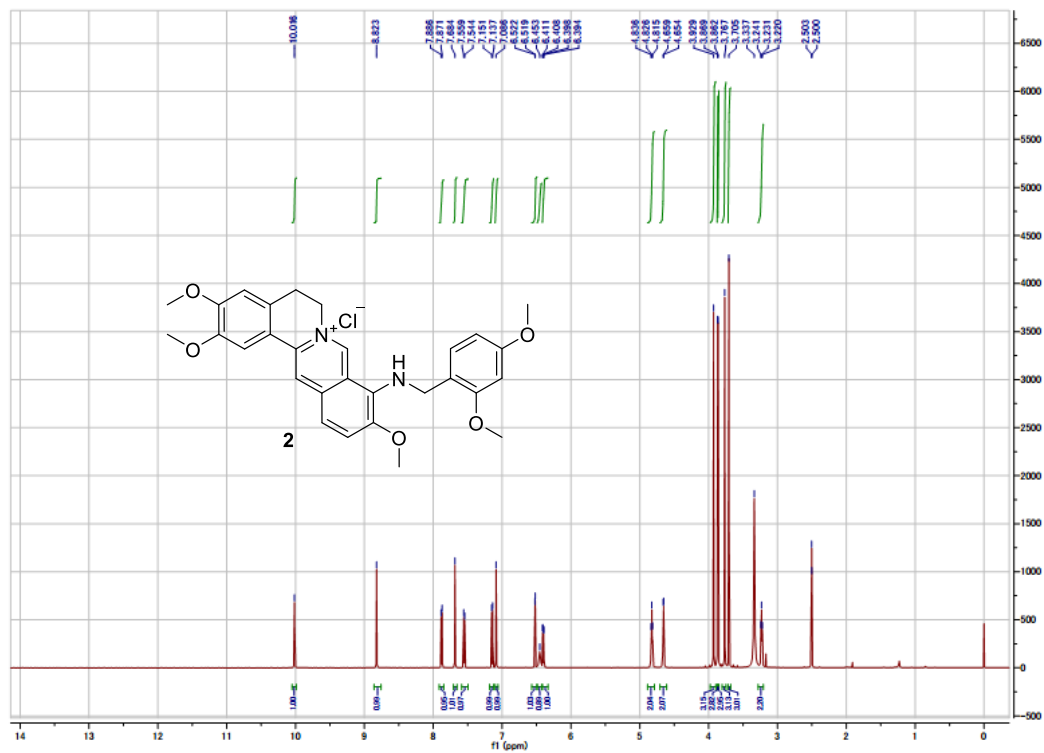
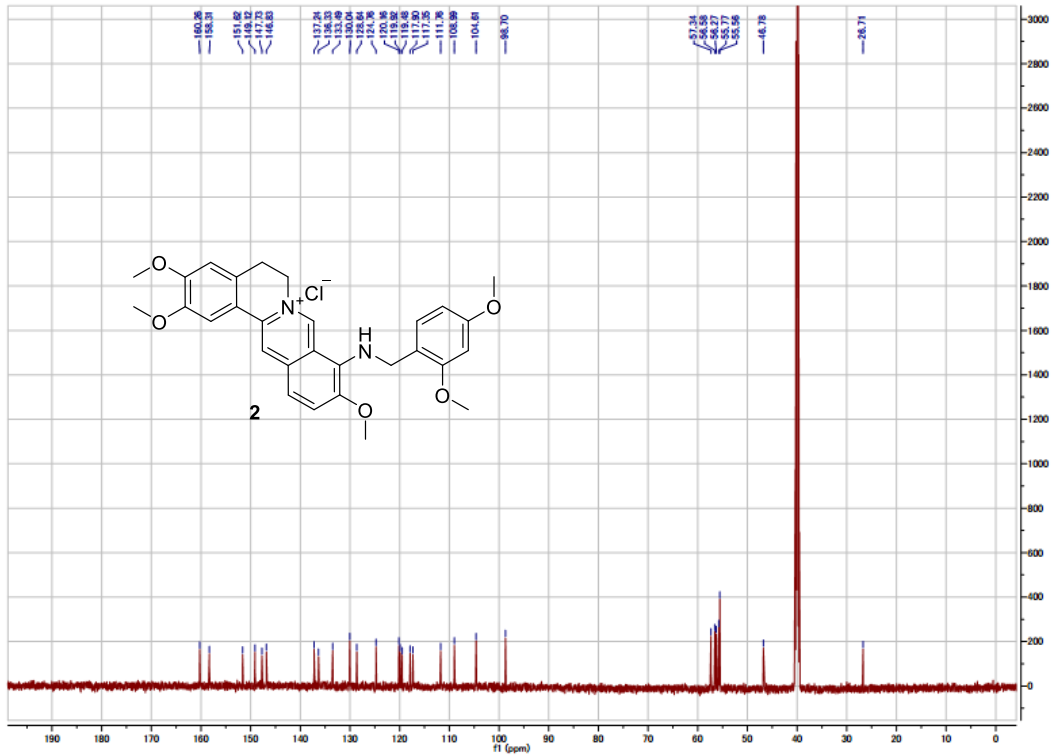


Figure S10: 1H NMR, ^{13}C NMR, HRMS-ESI spectra of compound 2





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PN1 #35 RT: 0.42 AV: 1 NL: 3.42E8
 T: FTMS + c ESI Full ms [100.00-1000.00]

487.22269
 C₂₉ H₃₁ O₅ N₂ = 487.22275
 -0.12676 ppm

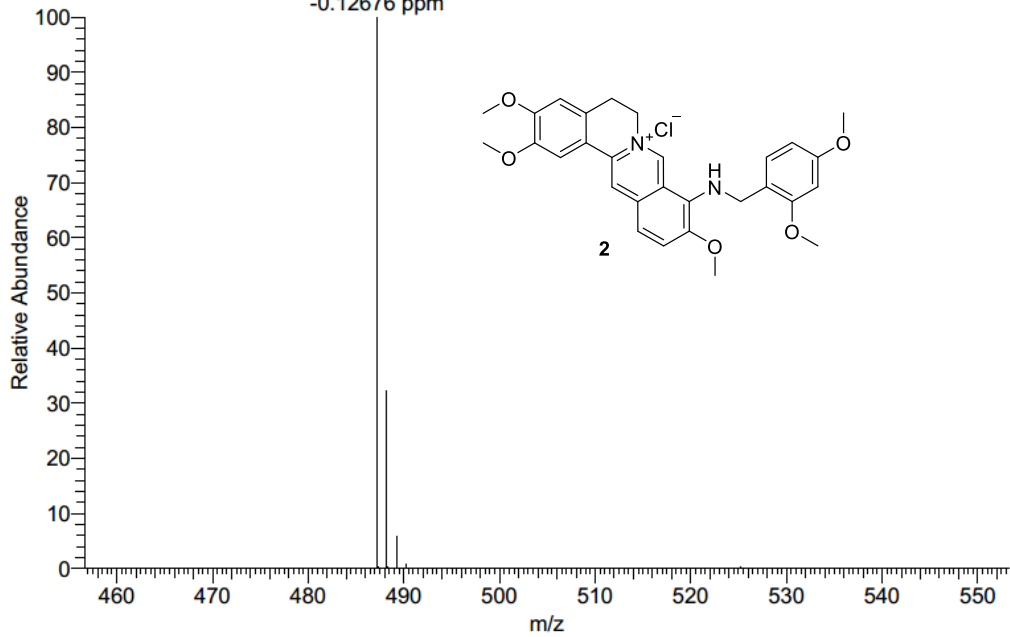
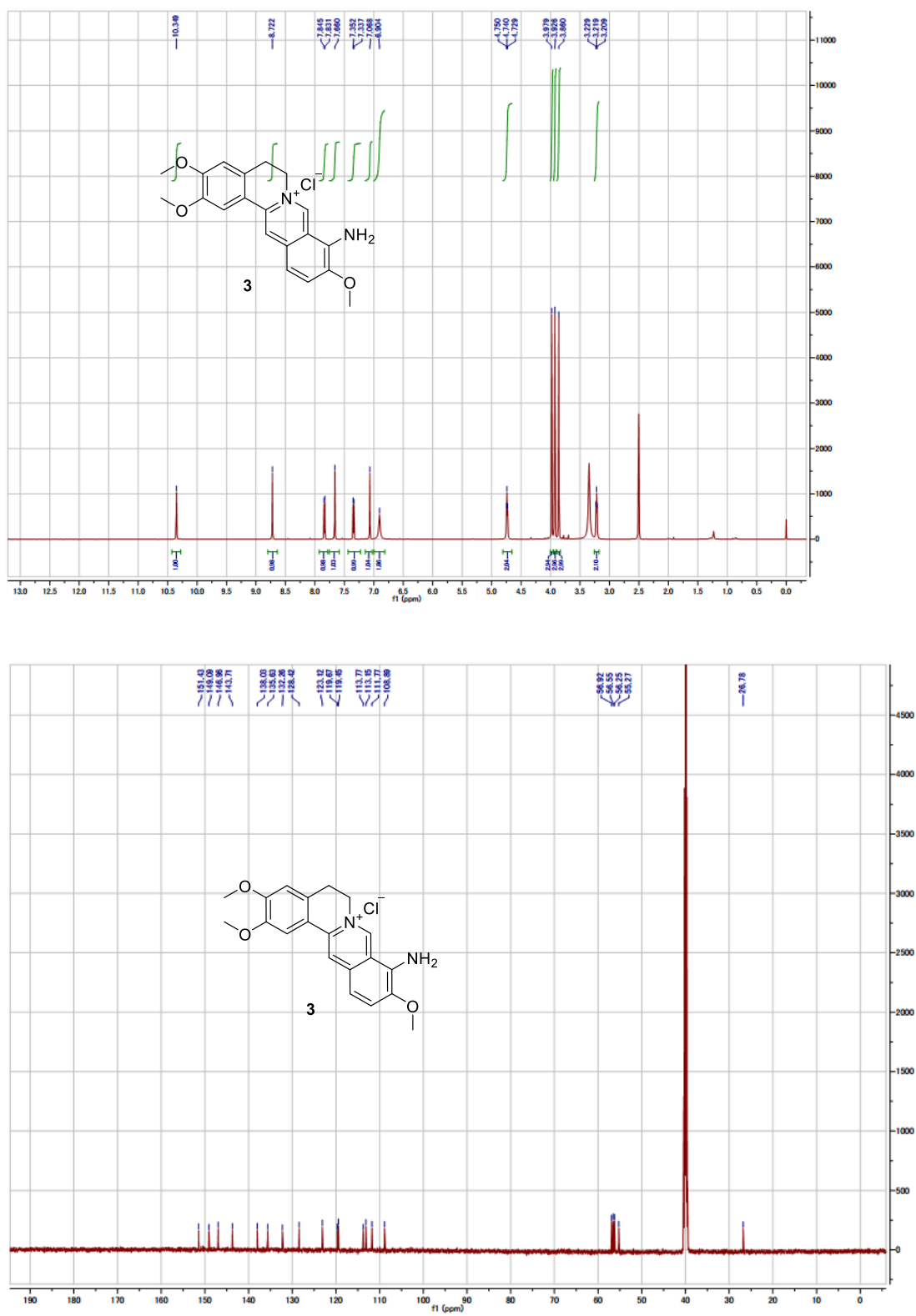
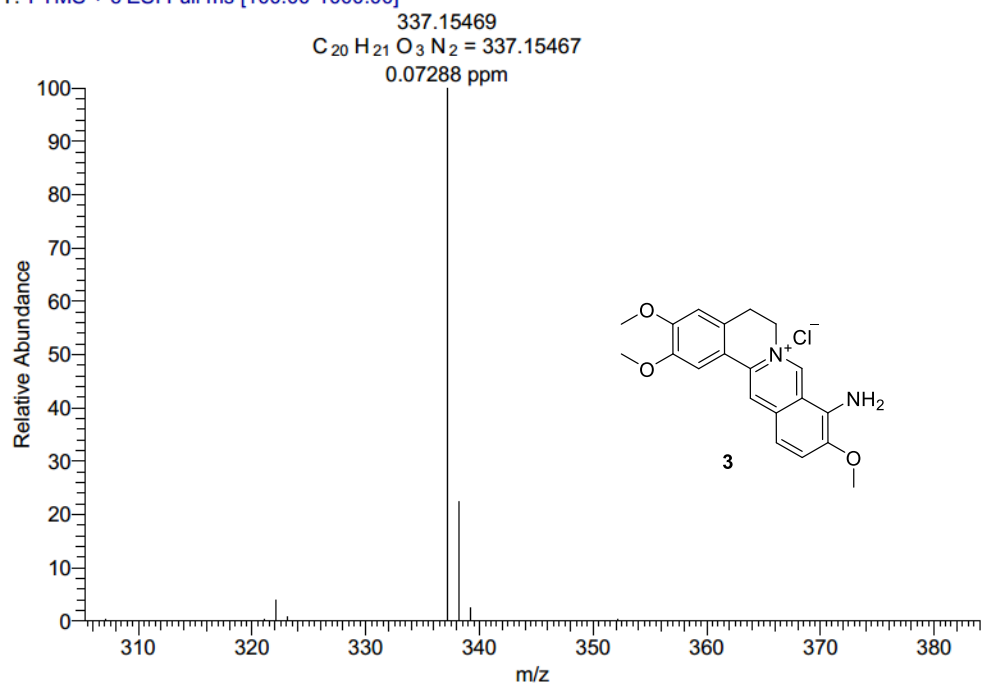
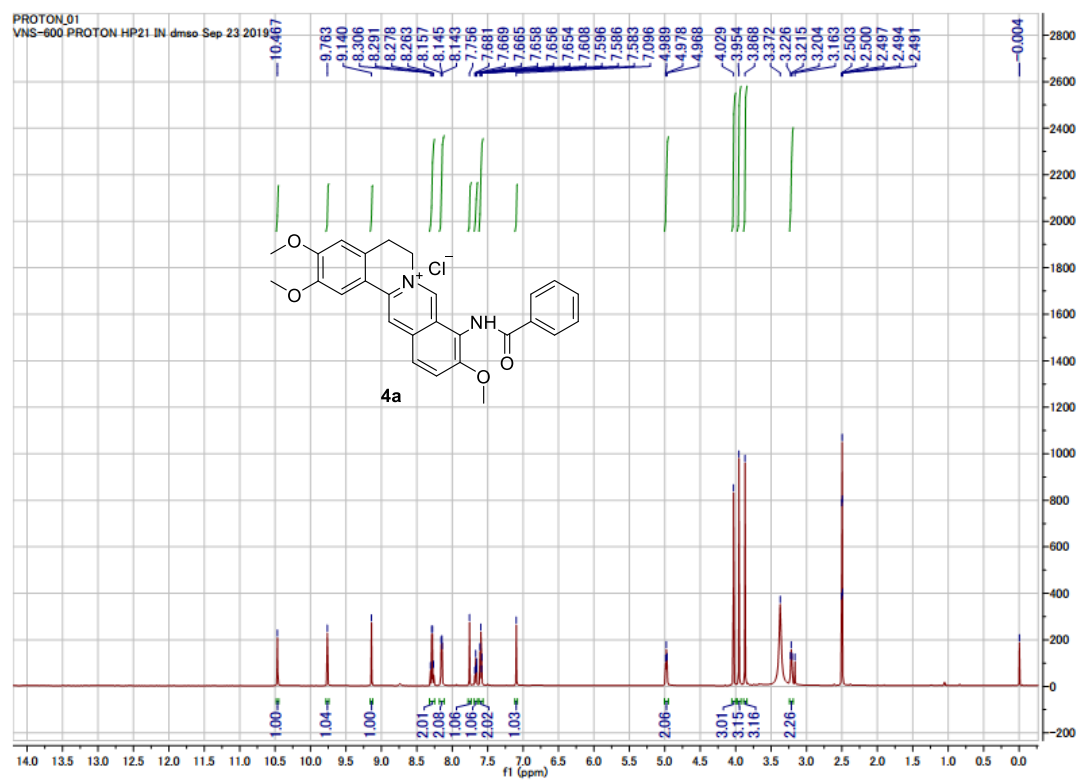


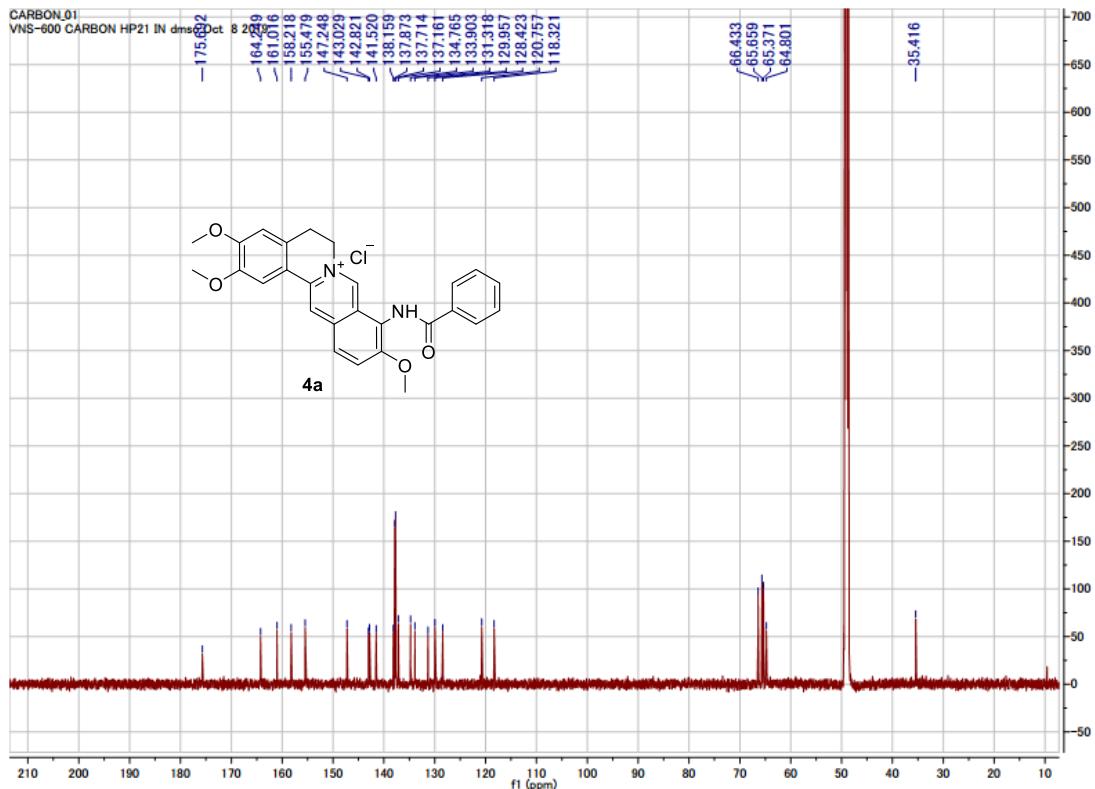
Figure S11: ^1H NMR, ^{13}C NMR, HRMS-ESI spectra of compound **3**



PN2 #32 RT: 0.33 AV: 1 NL: 1.79E8

T: FTMS + c ESI Full ms [100.00-1000.00]

Figure S12: ¹H NMR, ¹³C NMR, HRMS-ESI spectra of compound 4a



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HP21_191014141139 #30 RT: 0.28 AV: 1 NL: 4.32E8
T: FTMS + c ESI Full ms [150.00-1000.00]

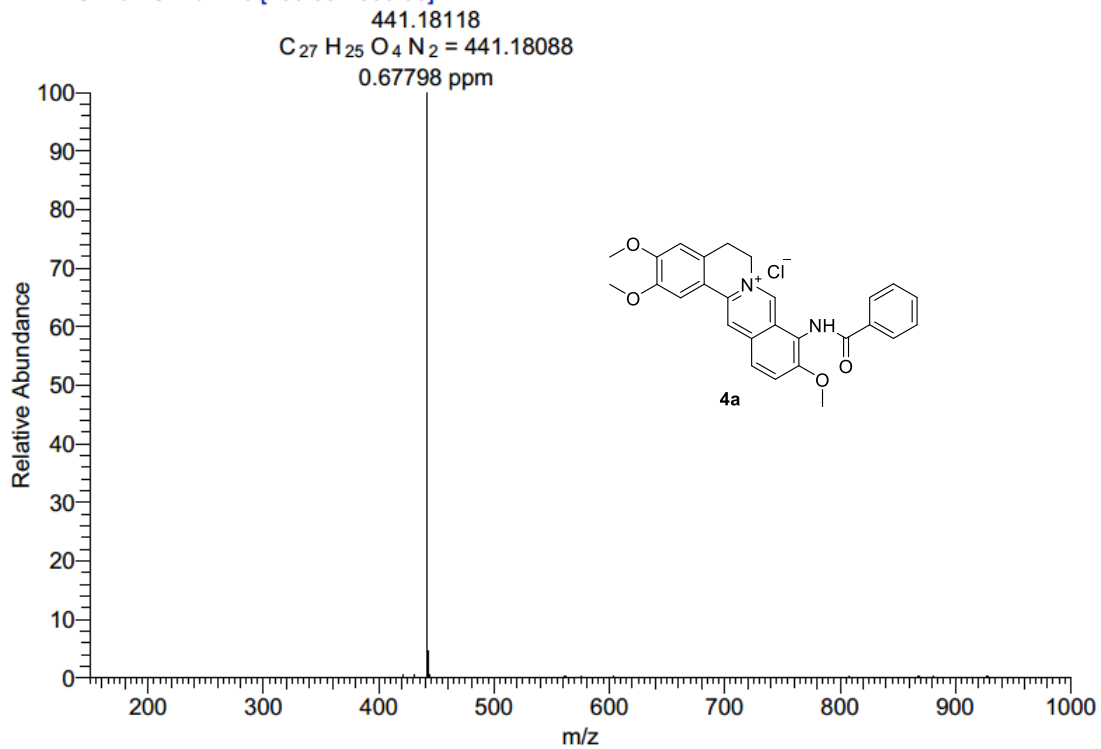
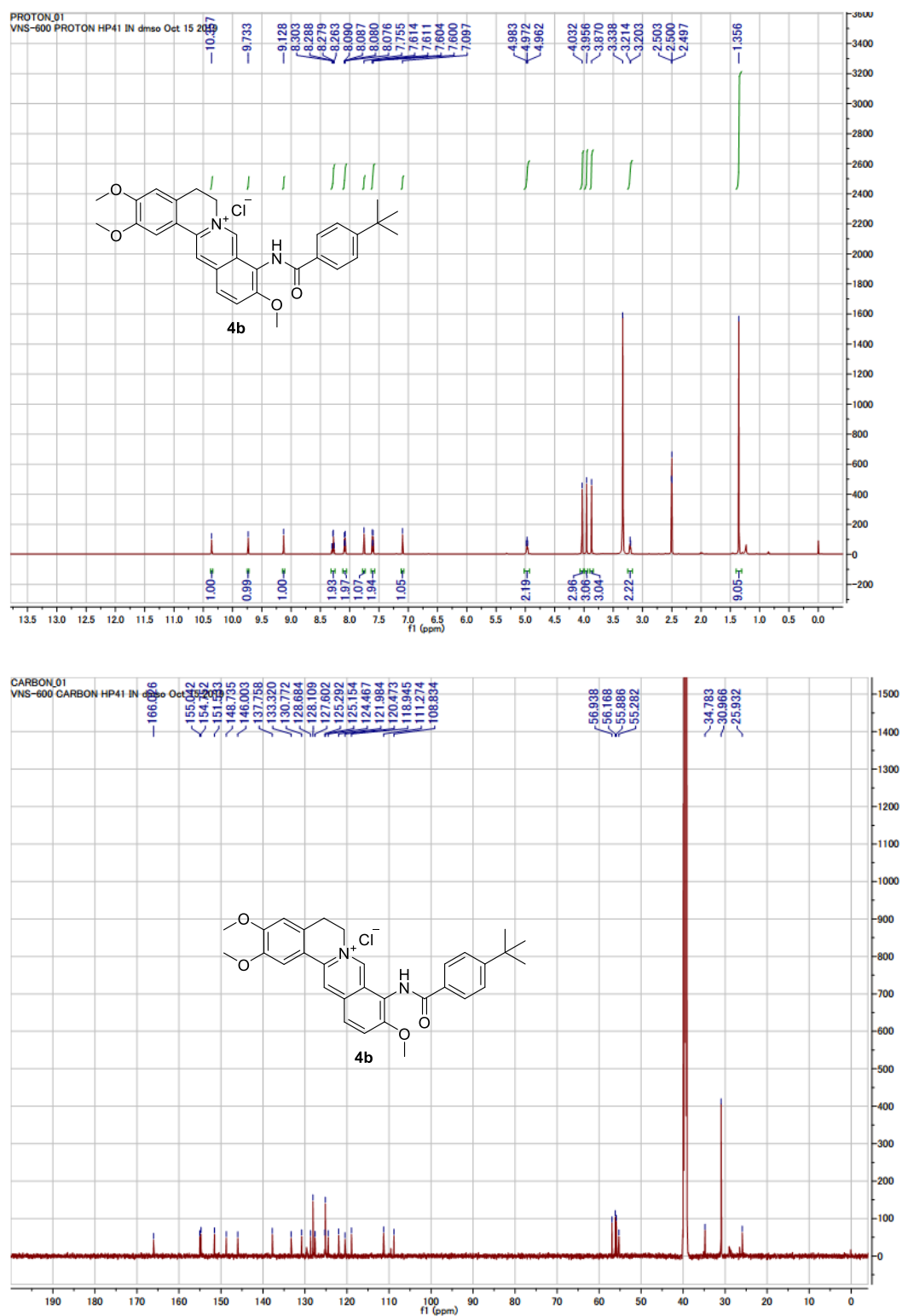
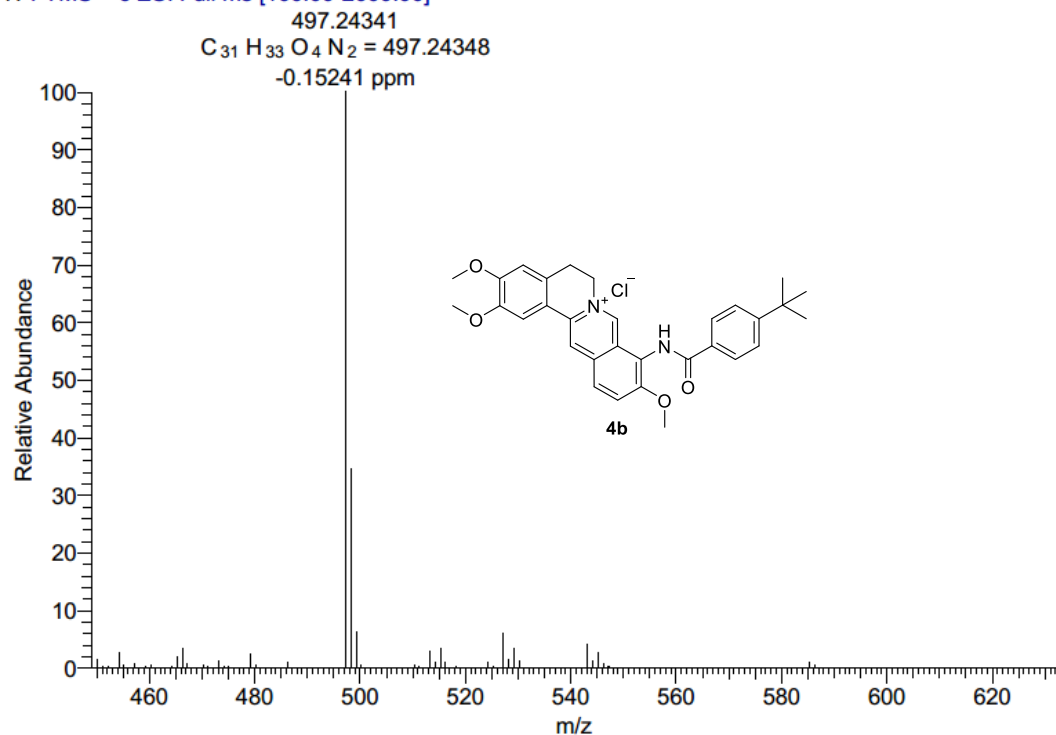
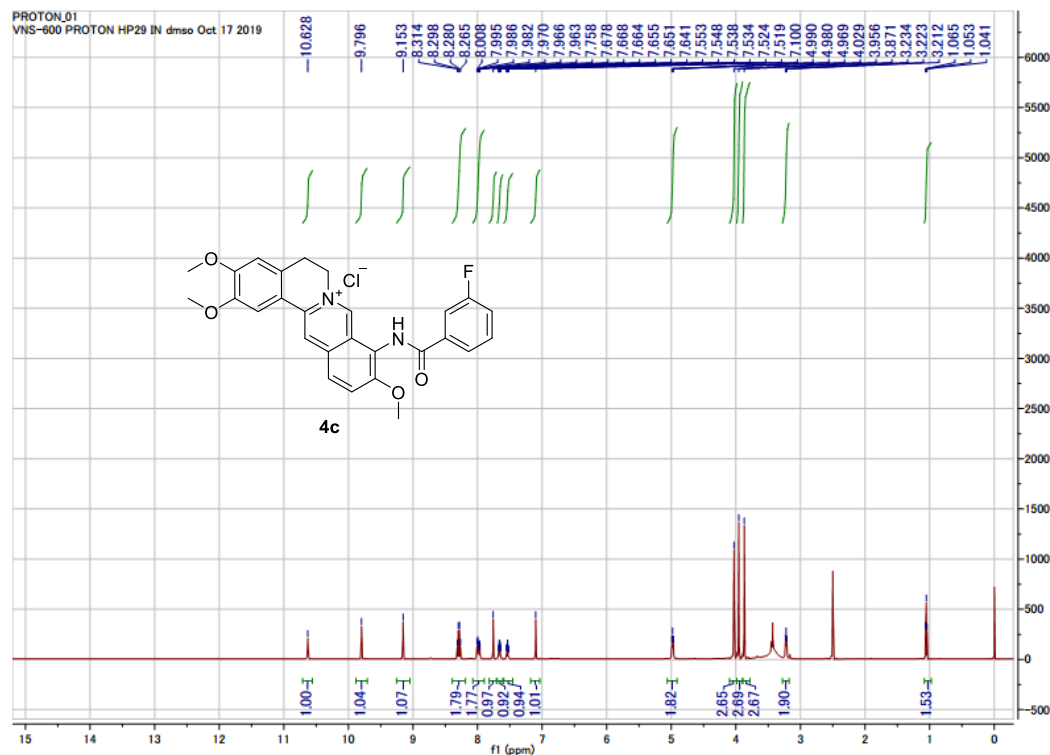
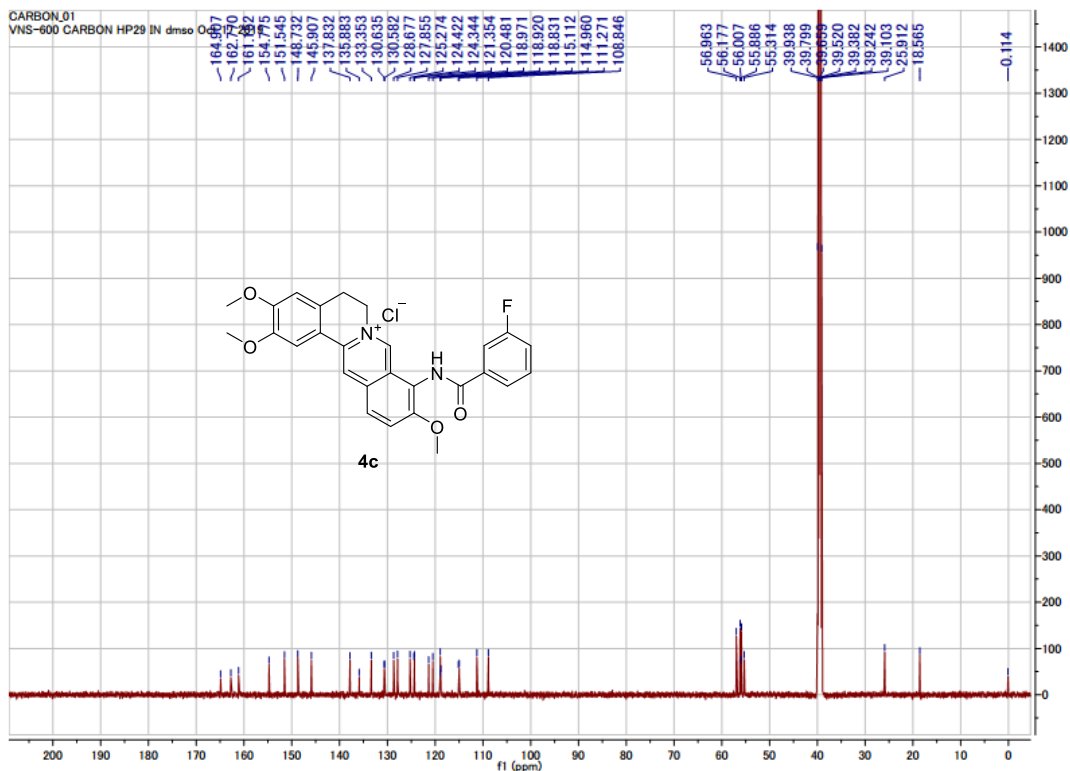


Figure S13: ^1H NMR, ^{13}C NMR, HRMS-ESI spectra of compound **4b**



HP41_191213160724 #39 RT: 0.36 AV: 1 NL: 1.05E7
T: FTMS + c ESI Full ms [100.00-2000.00]Figure S14: 1H NMR, ^{13}C NMR, HRMS-ESI spectra of compound **4c**



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HP29_191213160724 #18 RT: 0.19 AV: 1 NL: 1.59E8
T: FTMS + c ESI Full ms [100.00-2000.00]

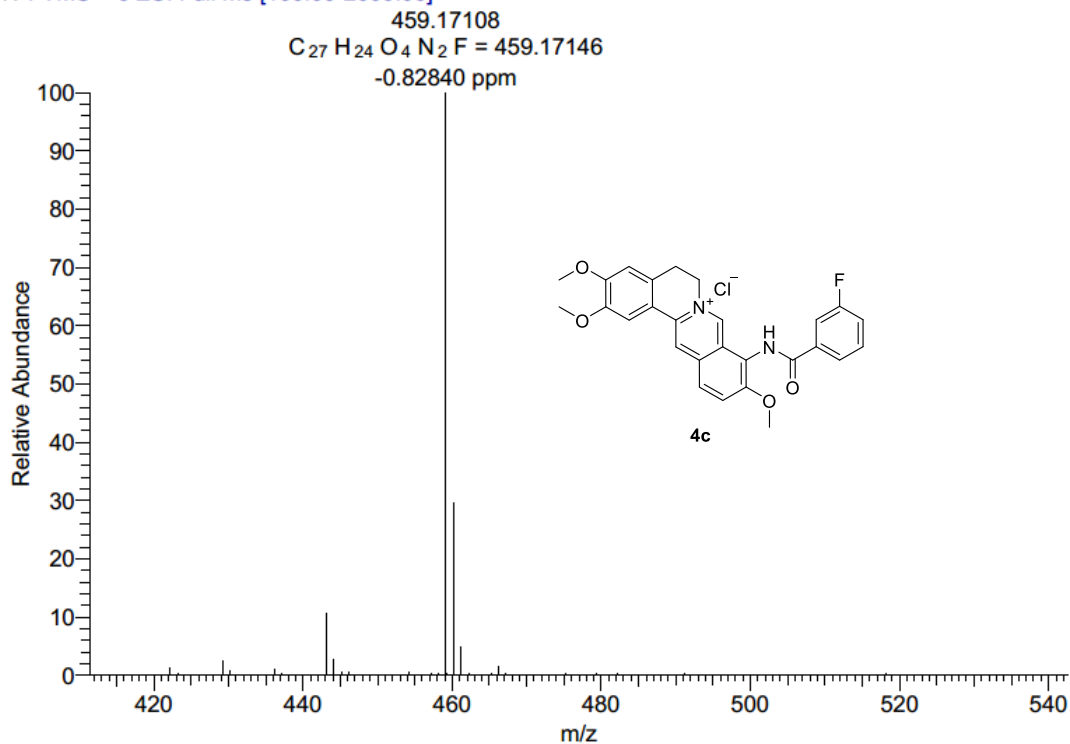
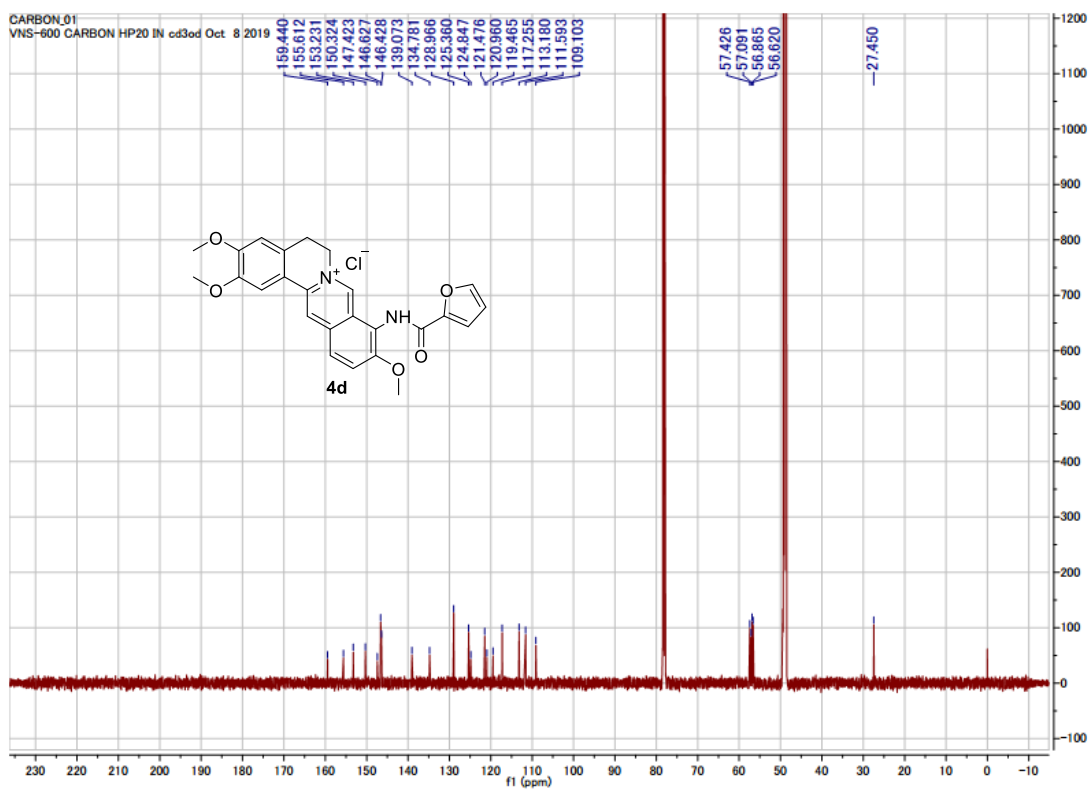
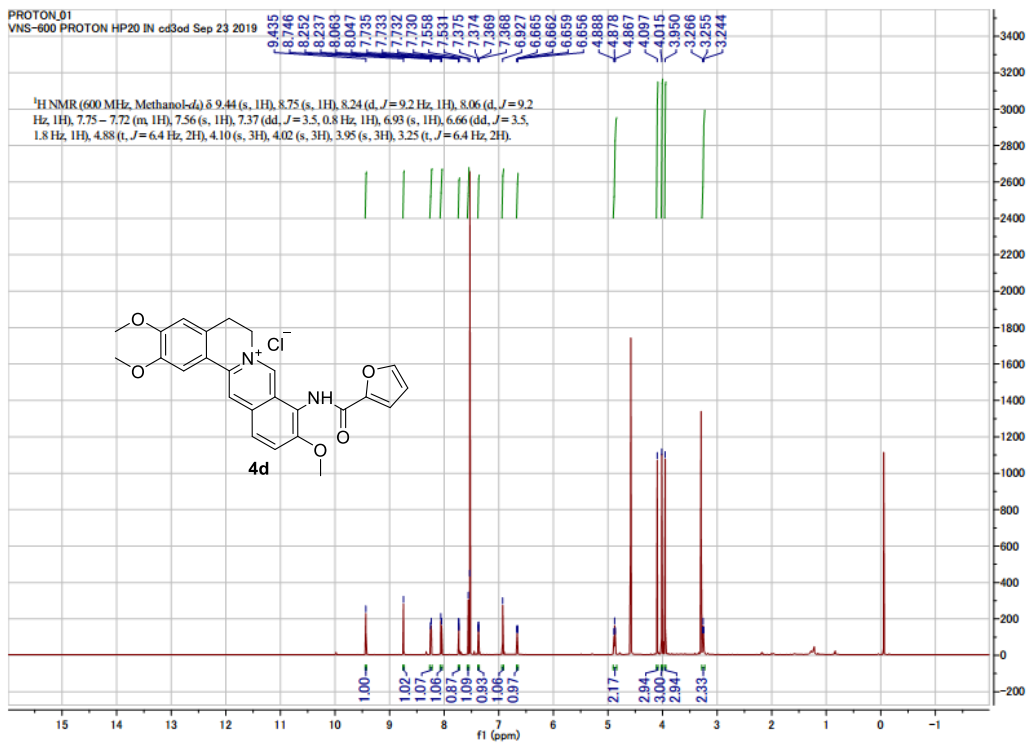


Figure S15: ¹H NMR, ¹³C NMR, HRMS-ESI spectra of compound **4d**



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T: FTMS + c ESI Full ms [150.00-1000.00]

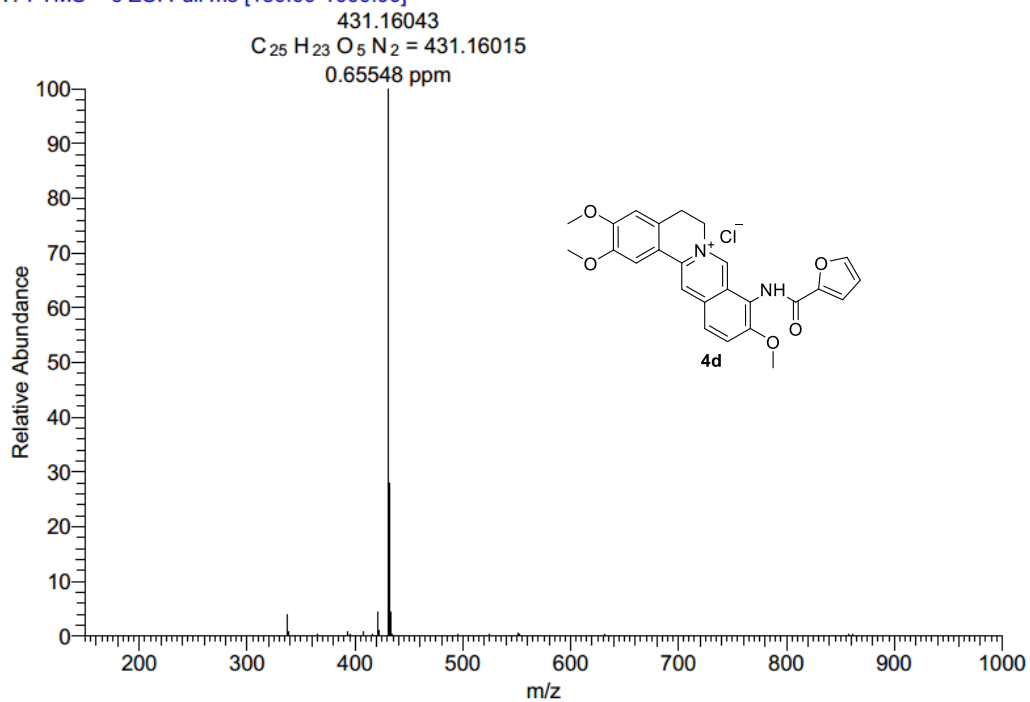
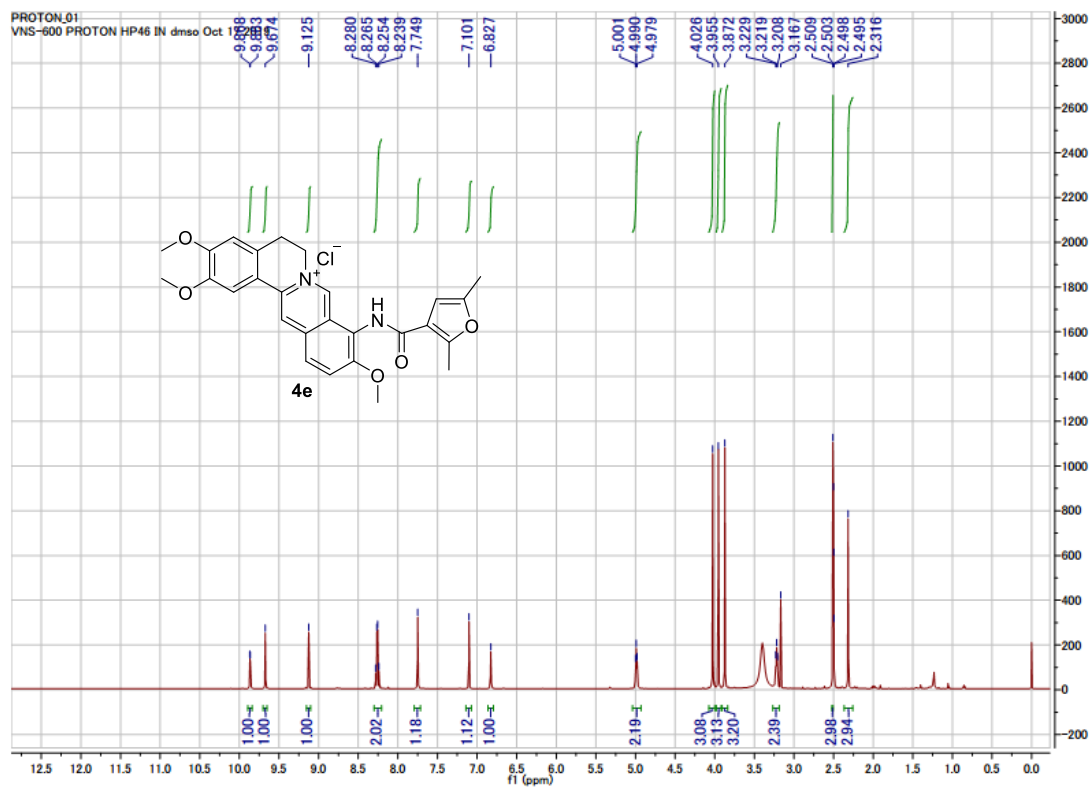
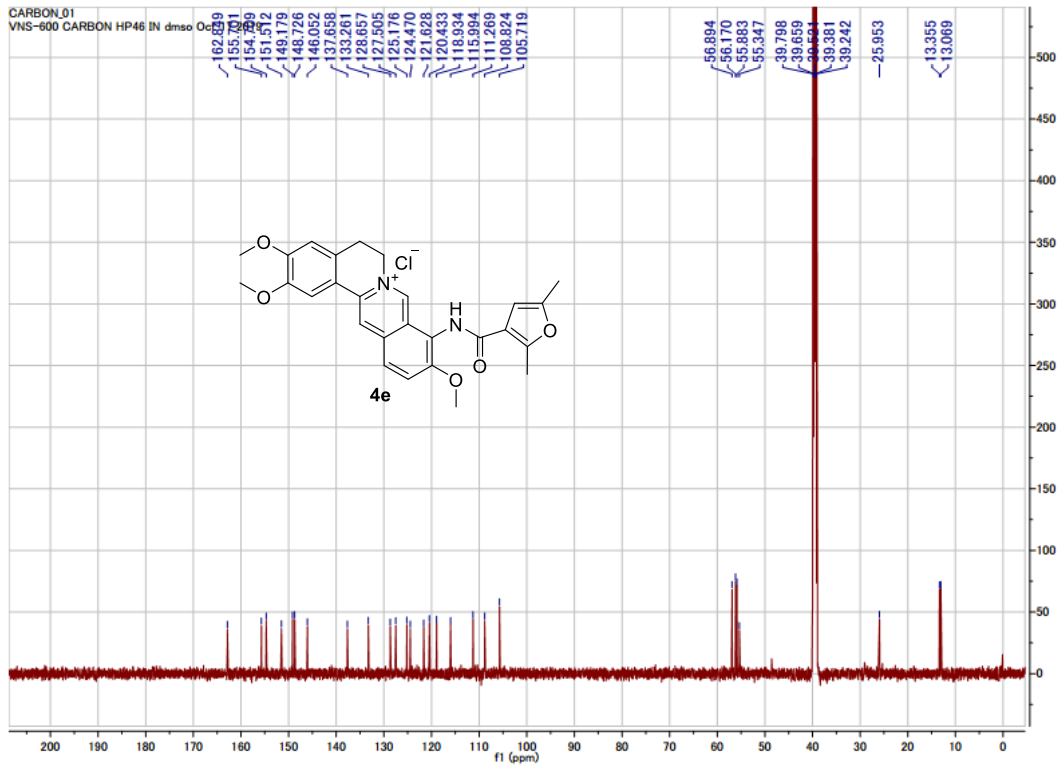


Figure S16: 1H NMR, ^{13}C NMR, HRMS-ESI spectra of compound **4e**





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HP46_191213160724 #14 RT: 0.14 AV: 1 NL: 1.90E8
T: FTMS + c ESI Full ms [100.00-2000.00]

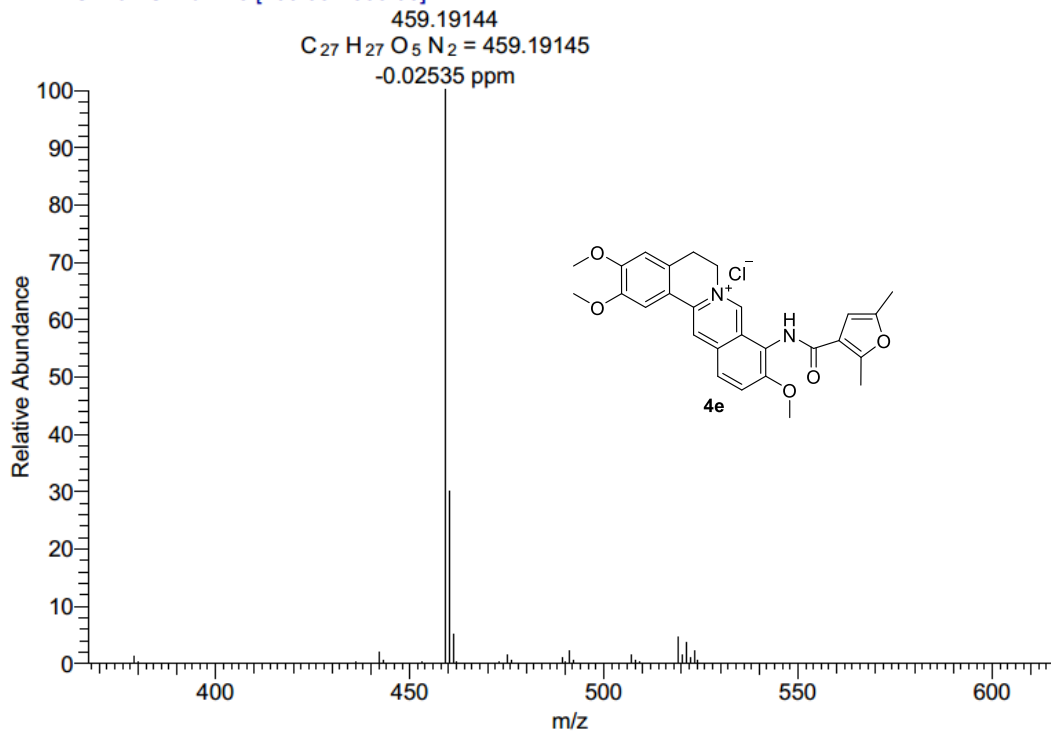
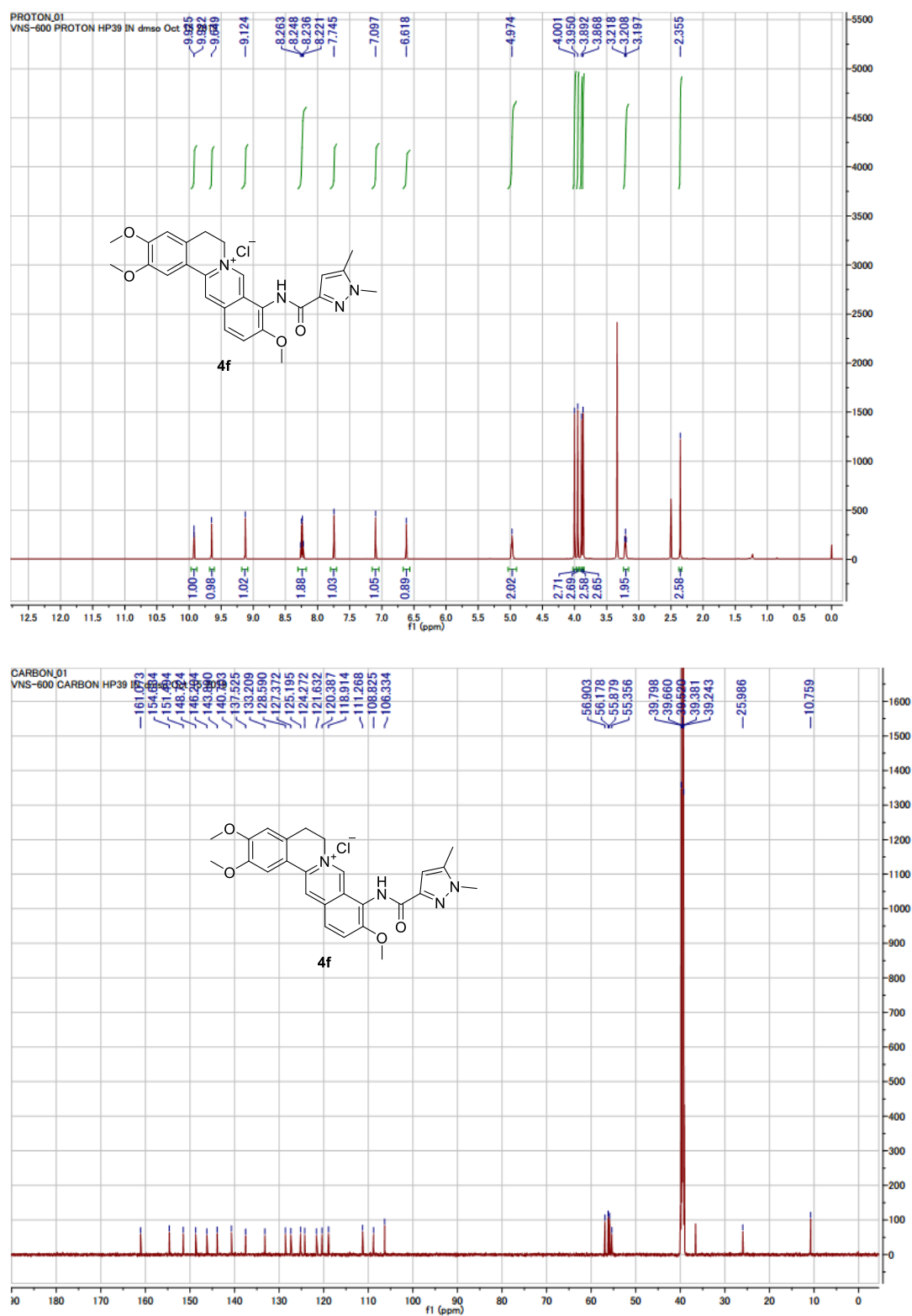


Figure S17: ^1H NMR, ^{13}C NMR, HRMS-ESI spectra of compound **4f**



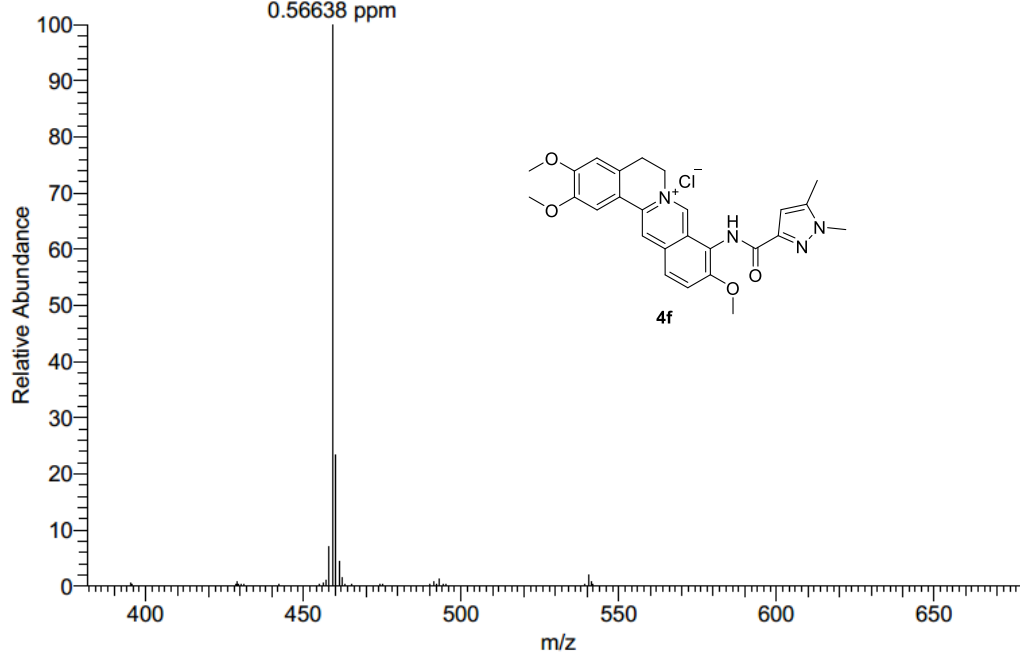
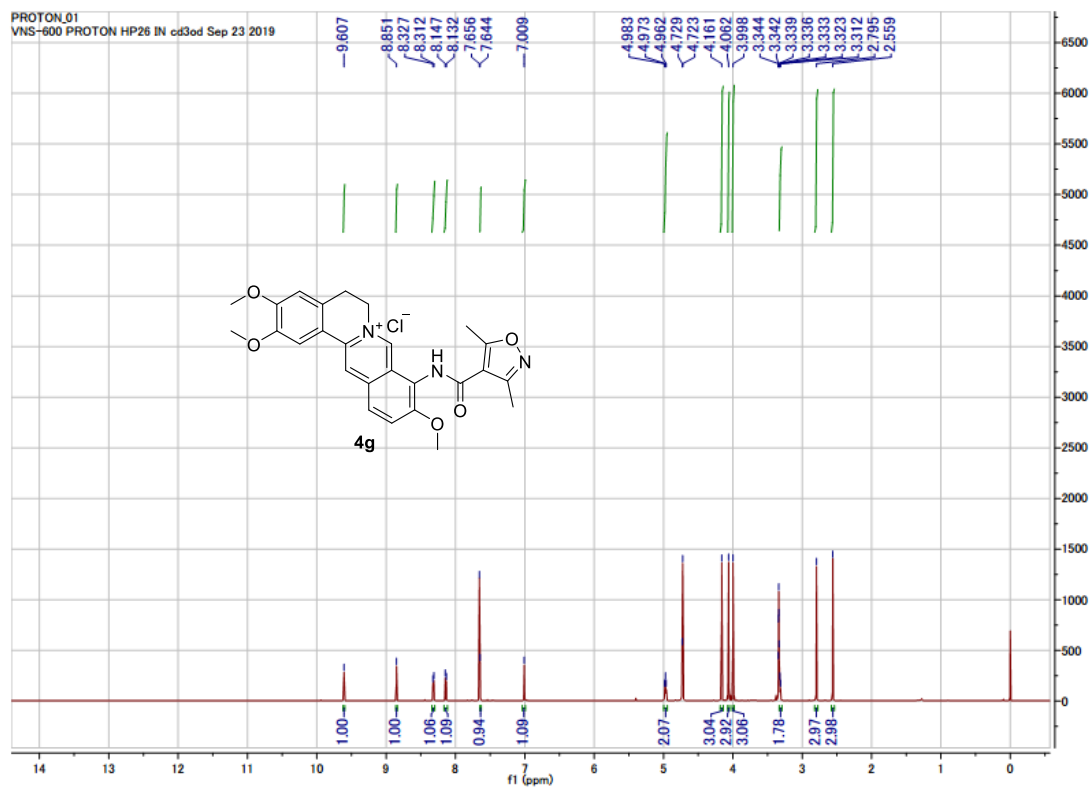
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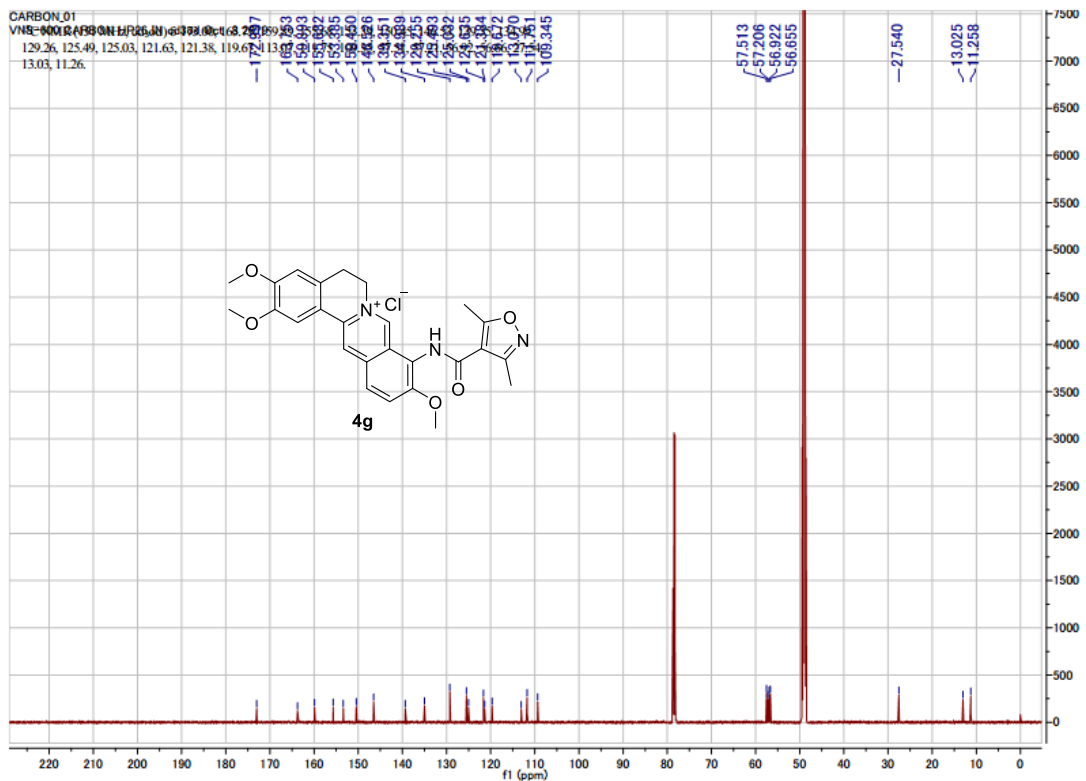
T: FTMS + c ESI Full ms [100.00-2000.00]

459.20294

C₂₆ H₂₇ O₄ N₄ = 459.20268

0.56638 ppm

Figure S18: ¹H NMR, ¹³C NMR, HRMS-ESI spectra of compound 4g



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HP26_191014141139 #34 RT: 0.31 AV: 1 NL: 4.21E8
T: FTMS + c ESI Full ms [150.00-1000.00]

460.18695
 $C_{26}H_{26}O_5N_3 = 460.18670$
0.55044 ppm

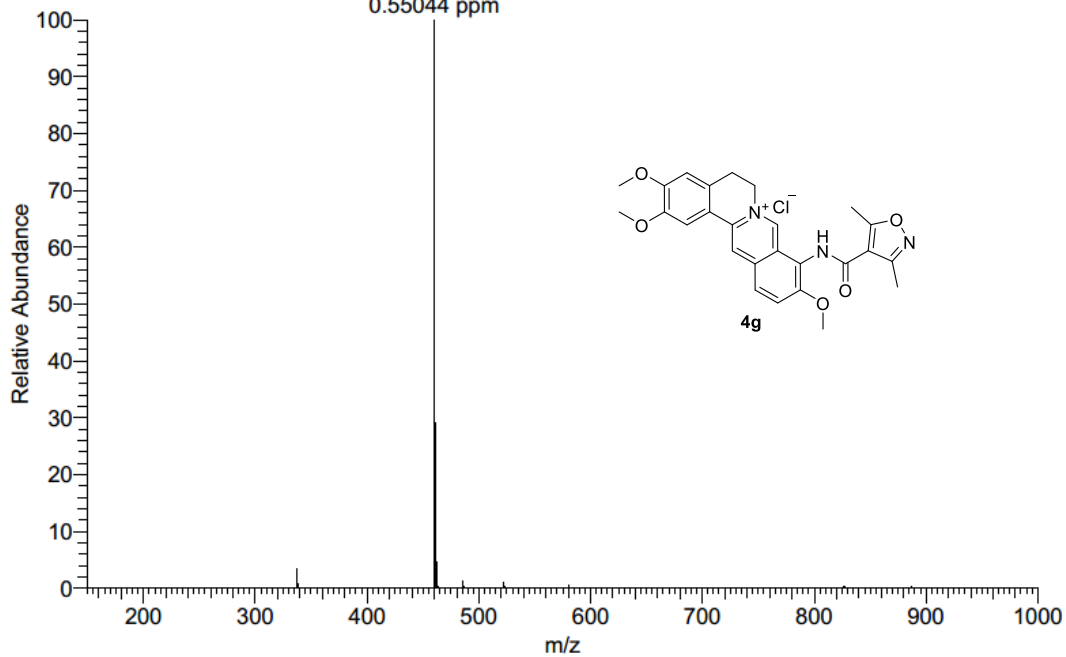
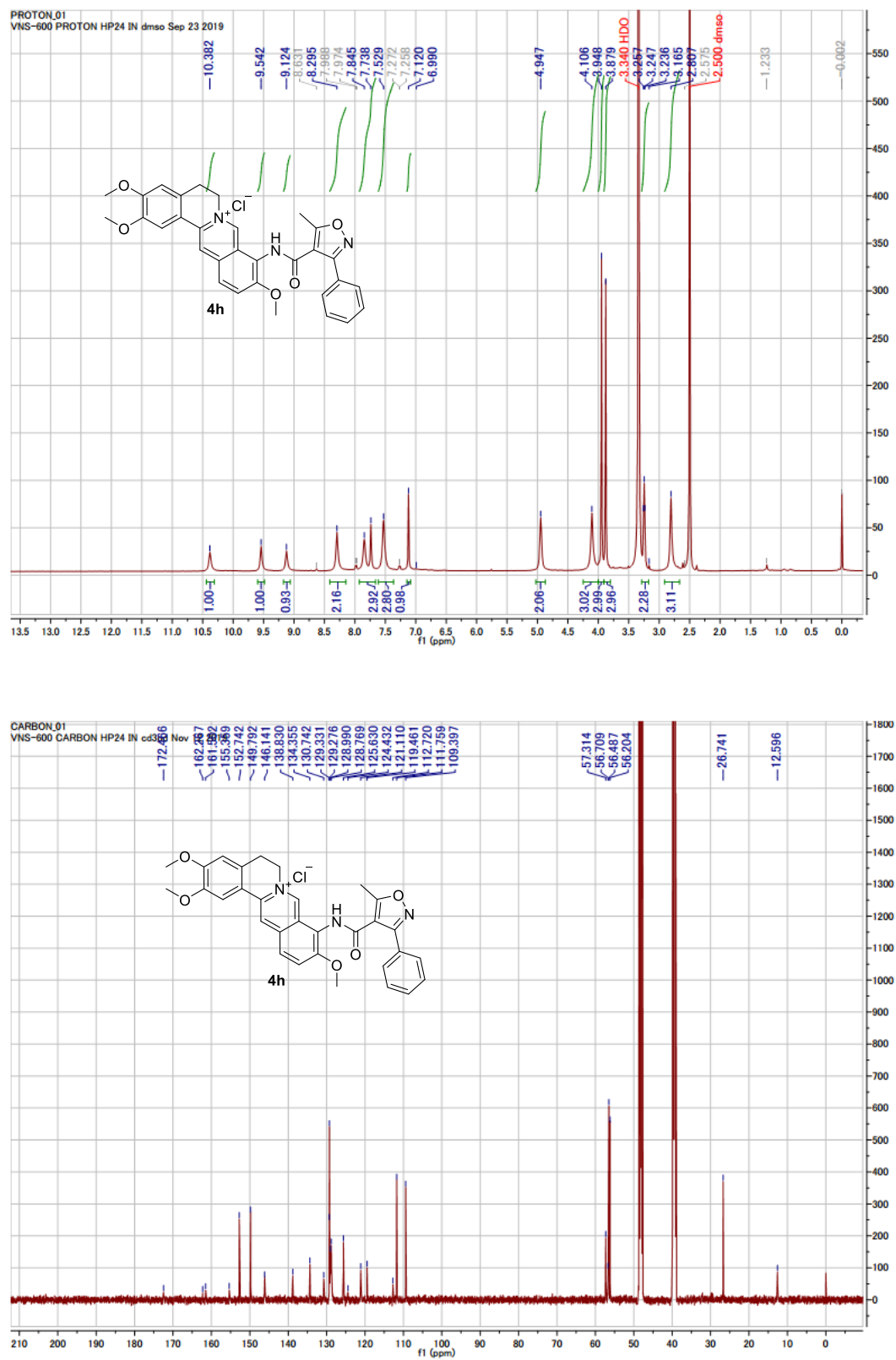


Figure S19: ^1H NMR, ^{13}C NMR, HRMS-ESI spectra of compound **4h**



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T: FTMS + c ESI Full ms [150.00-1000.00]

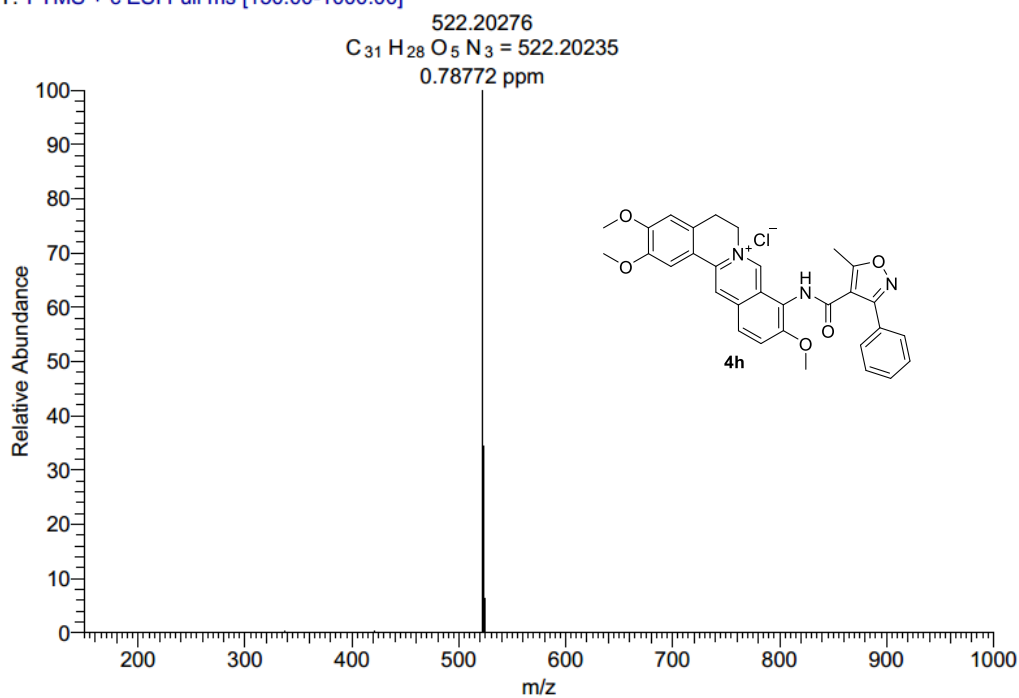
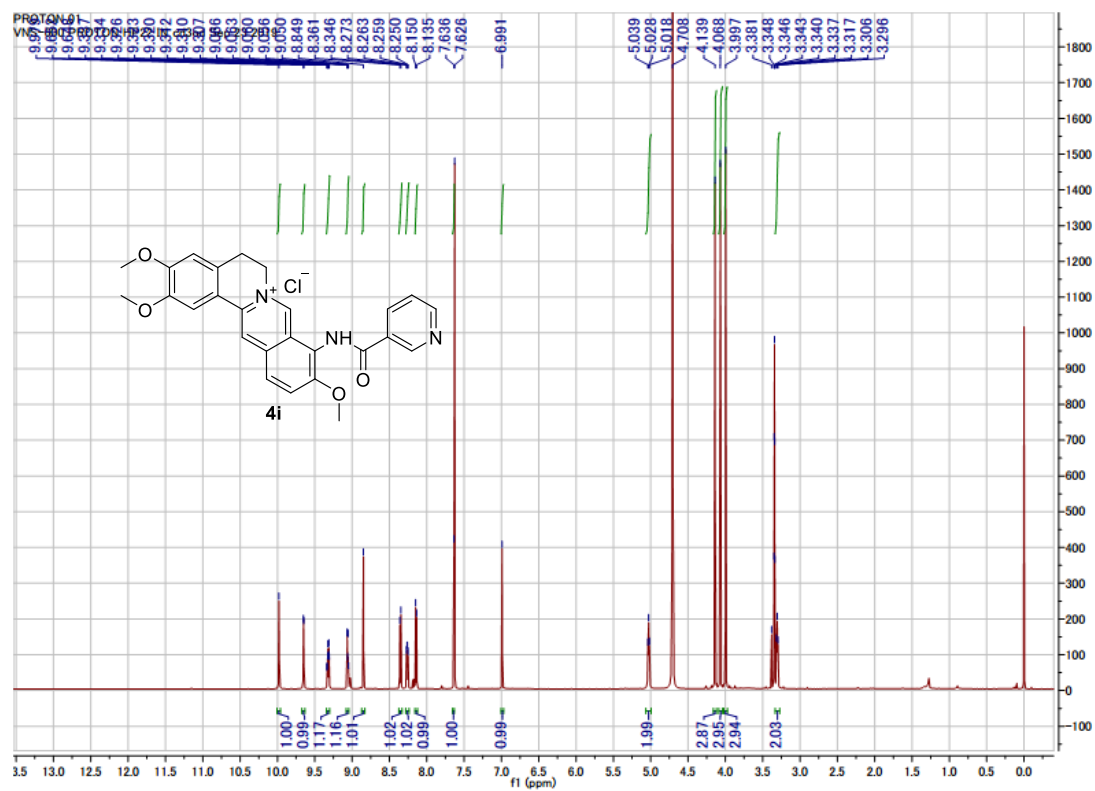
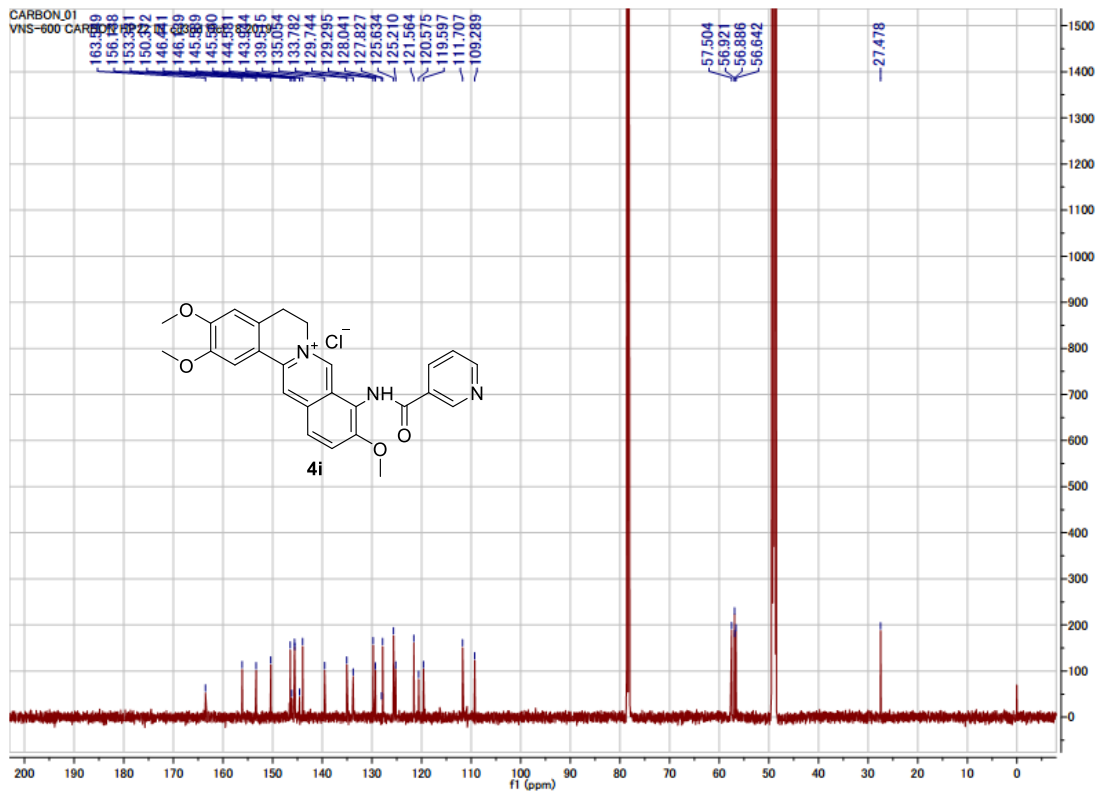


Figure S20: 1H NMR, ^{13}C NMR, HRMS-ESI spectra of compound 4i





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HP22_191014141139 #32 RT: 0.31 AV: 1 NL: 1.30E8
T: FTMS + c ESI Full ms [150.00-1000.00]

