

Supplementary Information For

Development of a Convergent Large-Scale Synthesis for Venetoclax, a First-in-Class BCL-2 Selective Inhibitor

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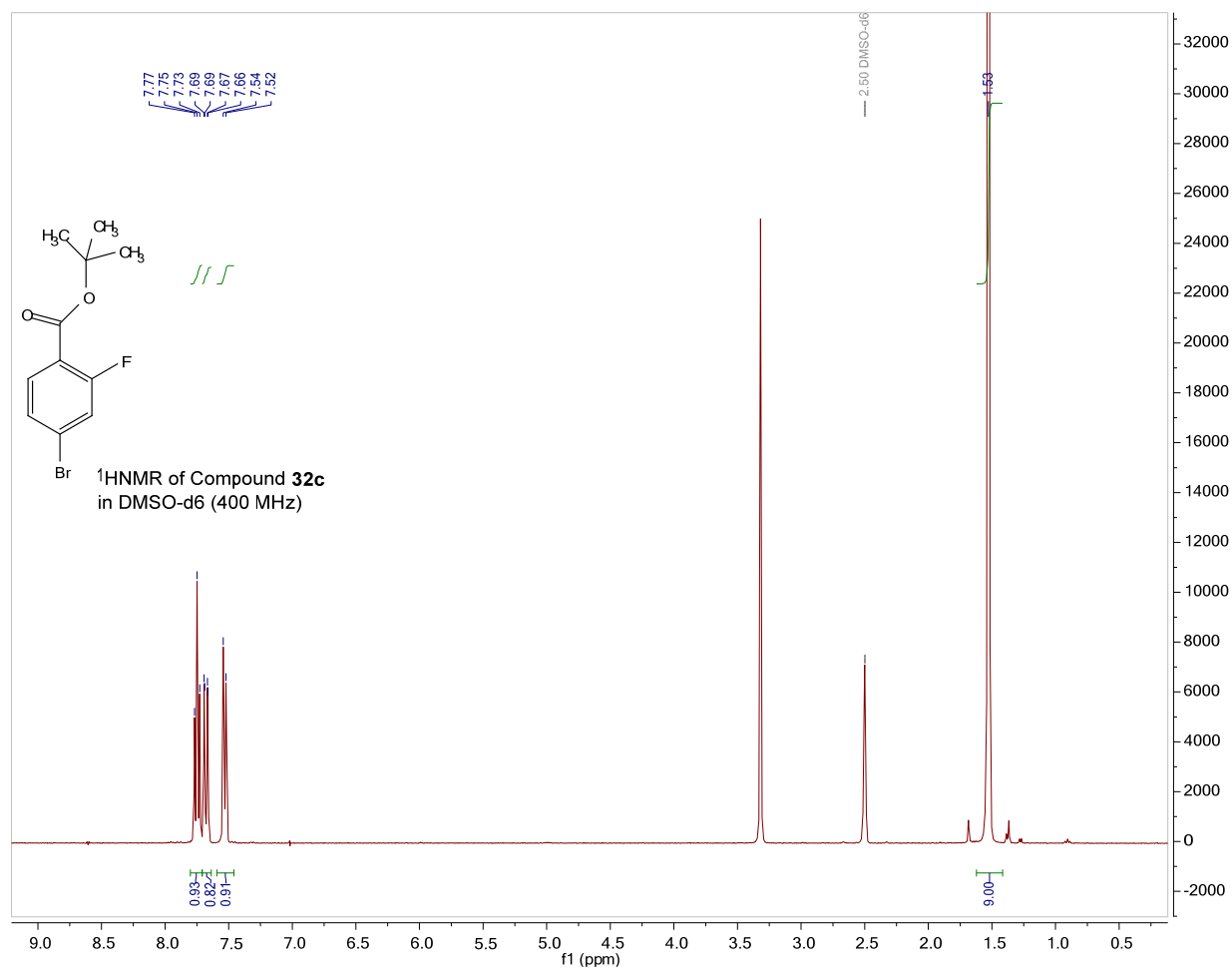
* Yiyin.ku@abbvie.com

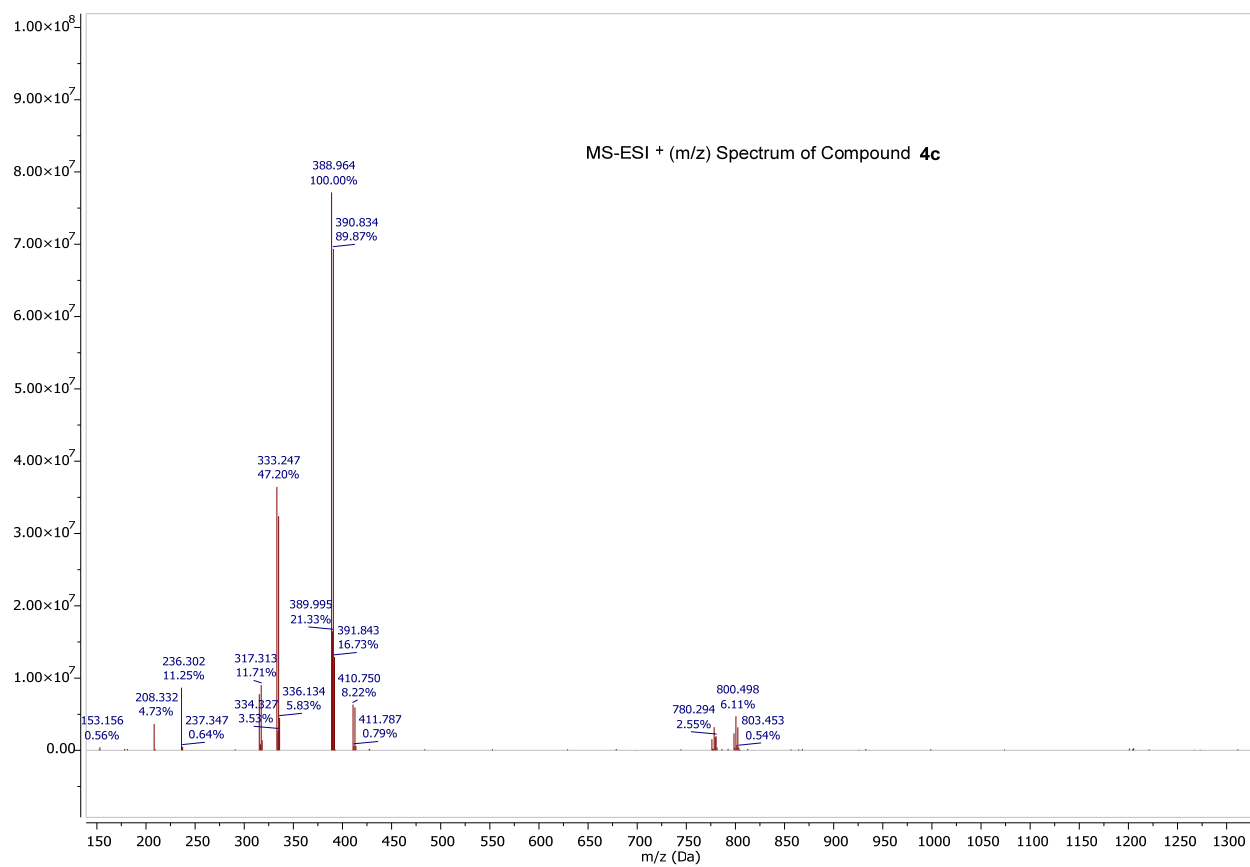
Spectrum Information

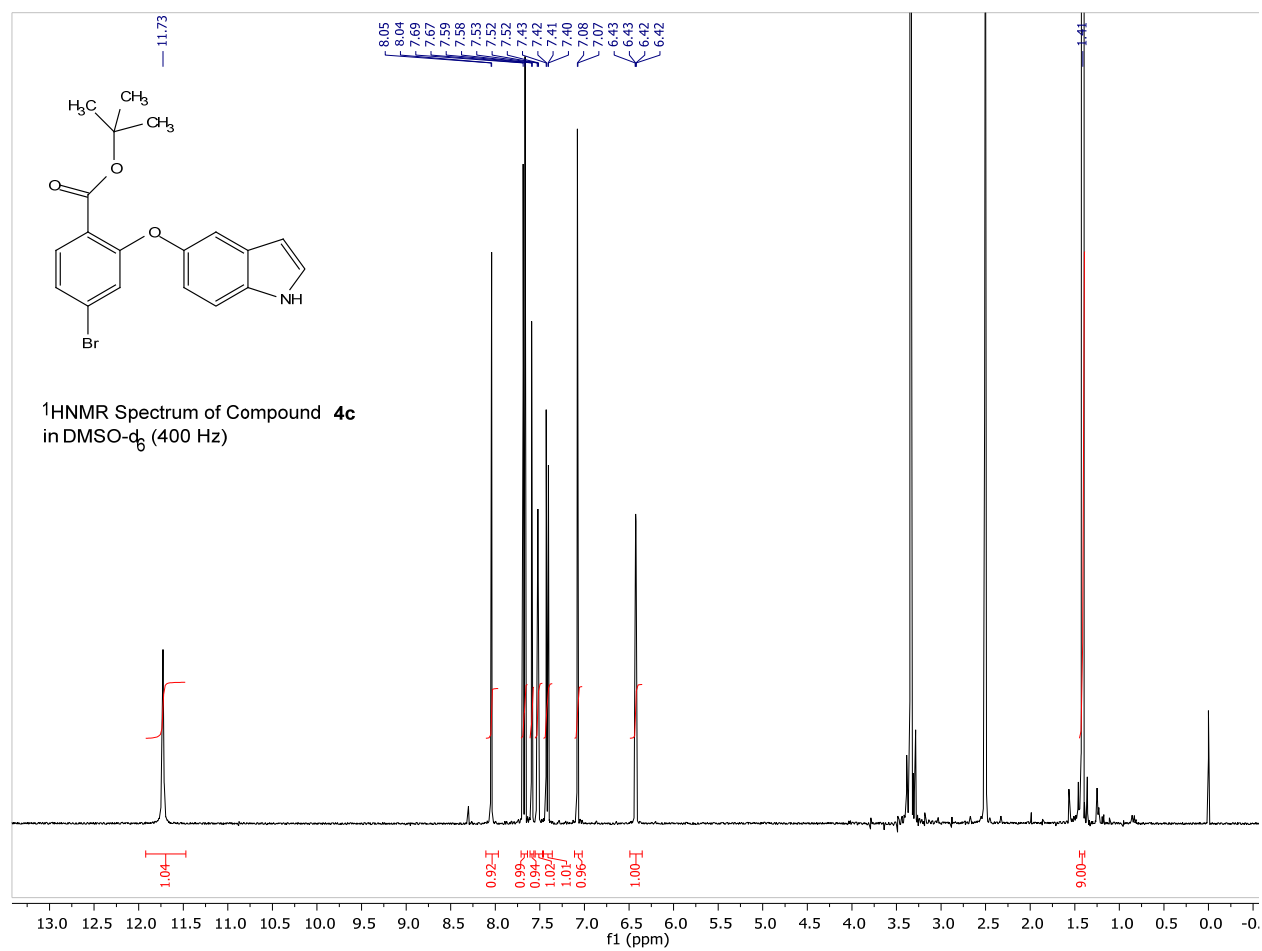
¹ H NMR Spectrum of 32c	S4
MS-ESI ⁺ Spectrum of Compound 4c	S5
¹ H NMR Spectrum of 4c	S6
¹³ C NMR Spectrum of 4c	S7
¹³ C NMR DEPT Spectrum of 4c	S8
¹ H NMR Spectrum of 12	S9
¹ H NMR Spectrum of 5	S10
MS-ESI ⁺ Spectrum of Compound 29	S11
¹ H NMR Spectrum of 29	S12
¹³ C NMR Spectrum of 29	S13
¹³ C NMR DEPT Spectrum of 29	S14
MS-ESI ⁺ Spectrum of Compound 26	S15

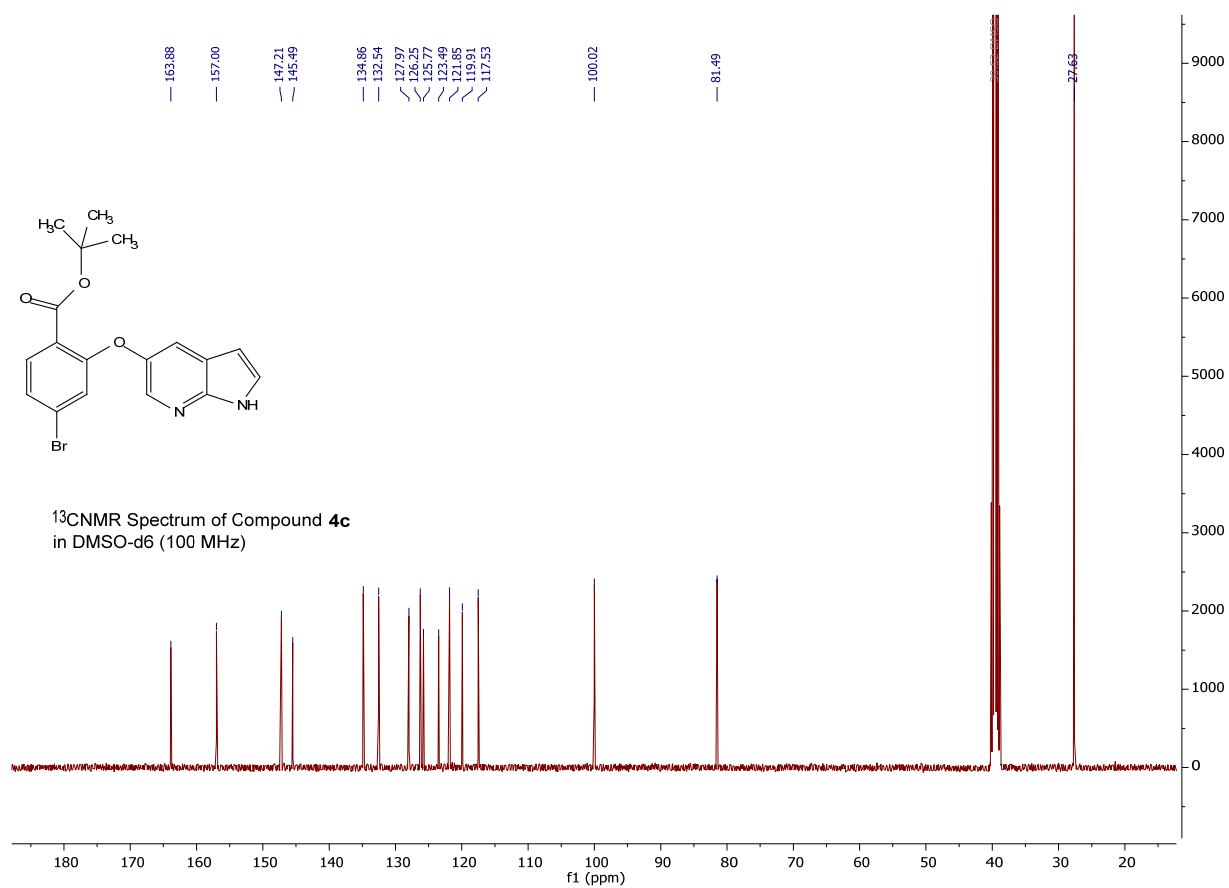
¹ H NMR Spectrum of 26	S16
¹³ C NMR Spectrum of 26	S17
¹³ C NMR DEPT Spectrum of 26	S18
¹ H NMR Spectrum of 26 (Freebase).....	S19
MS-ESI ⁺ Spectrum of Compound 23c	S20
¹ H NMR Spectrum of 23c	S21
¹³ C NMR Spectrum of 23c	S22
¹³ C NMR DEPT Spectrum of 23c	S23
MS-ESI ⁺ Spectrum of Compound 2	S24
¹ H NMR Spectrum of 2	S25
¹³ C NMR Spectrum of 2	S26
¹³ C NMR DEPT Spectrum of 2	S27
MS-ESI ⁺ Spectrum of Compound 3	S28
¹ H NMR Spectrum of 3	S29
¹³ C NMR Spectrum of 3	S30
¹³ C NMR DEPT Spectrum of 3	S31
MS-ESI ⁺ Spectrum of Compound 1	S32
¹ H NMR Spectrum of 1	S33
¹³ C NMR Spectrum of 1	S34
¹³ C NMR DEPT Spectrum of 1	S35
MS-ESI ⁺ Spectrum of Compound 38	S36
¹ H NMR Spectrum of 38	S37
¹³ C NMR Spectrum of 38	S38
¹³ C NMR DEPT Spectrum of 38	S39
MS-ESI ⁺ Spectrum of Compound 39	S40
¹ H NMR Spectrum of 39	S41
¹³ C NMR Spectrum of 39	S42
¹³ C NMR DEPT Spectrum of 39	S43

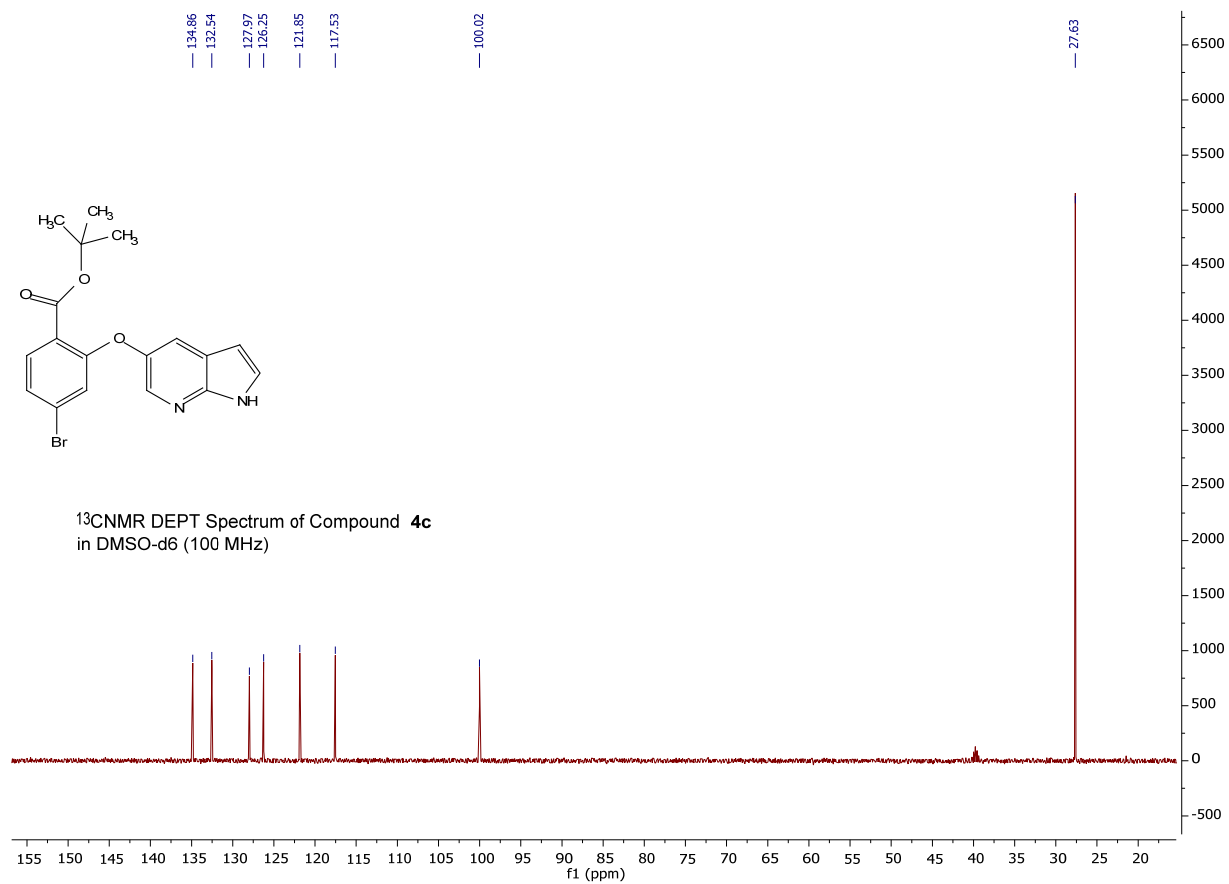
MS-ESI ⁺ Spectrum of Compound 40	S44
¹ H NMR Spectrum of 40	S45
¹³ C NMR Spectrum of 40	S46
¹³ C NMR DEPT Spectrum of 40	S47
APCI Spectrum of Compound 41	S48
¹ H NMR Spectrum of 41	S49
¹³ C NMR Spectrum of 41	S50
¹³ C NMR DEPT Spectrum of 41	S51

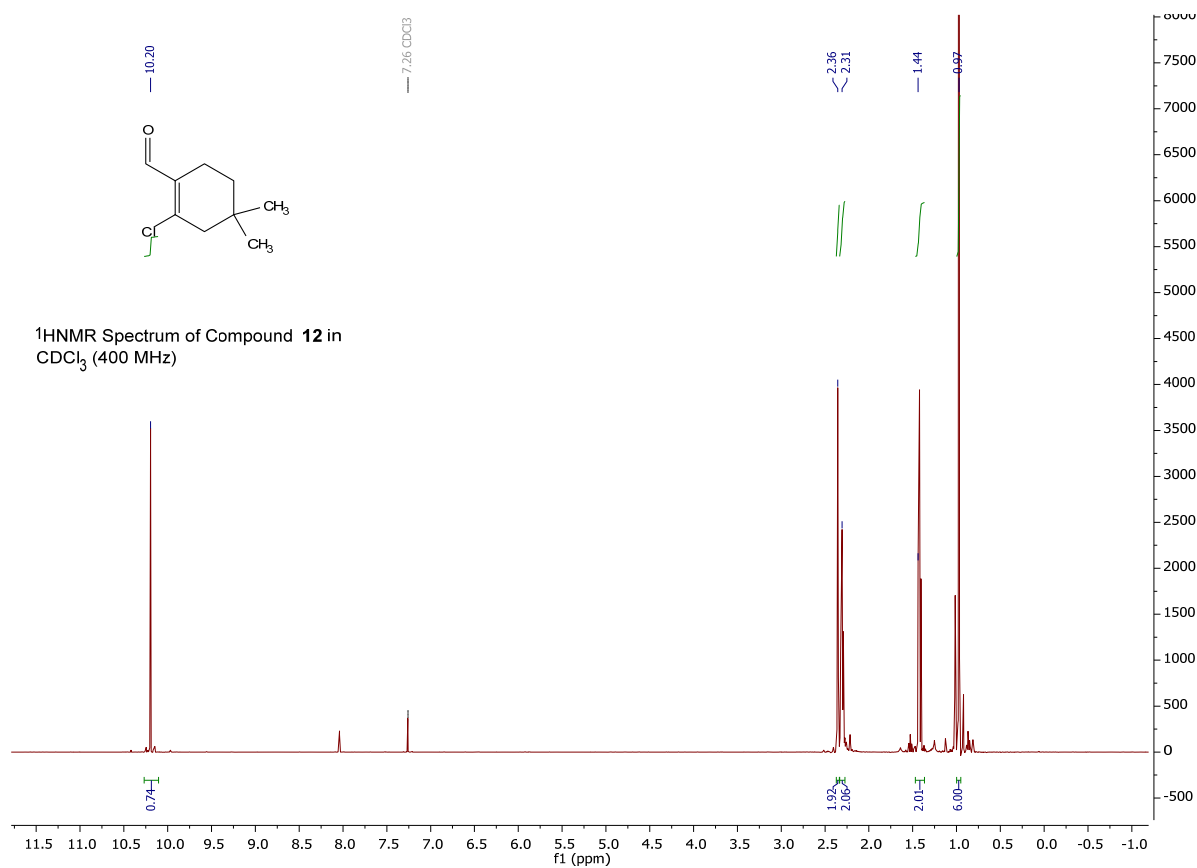


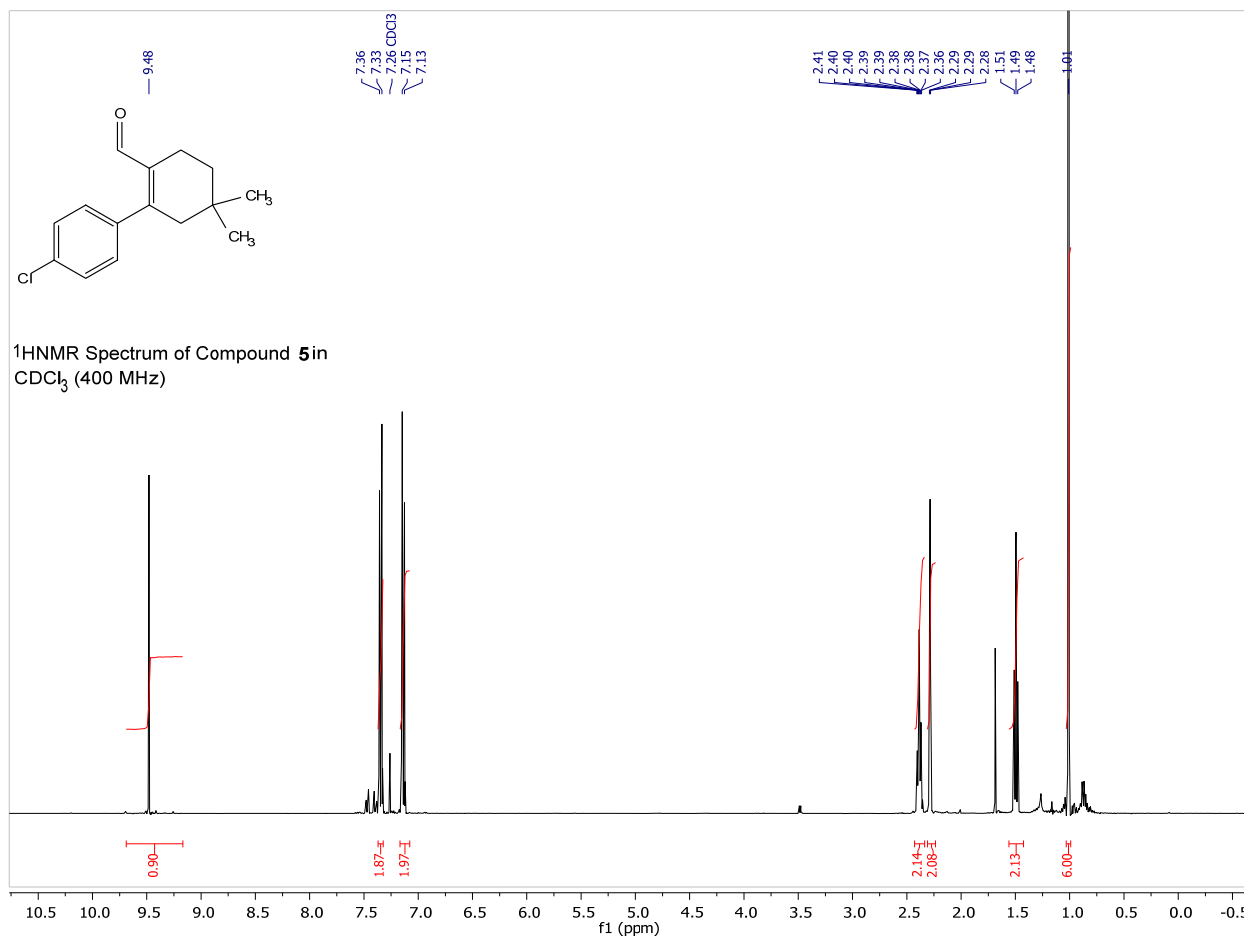


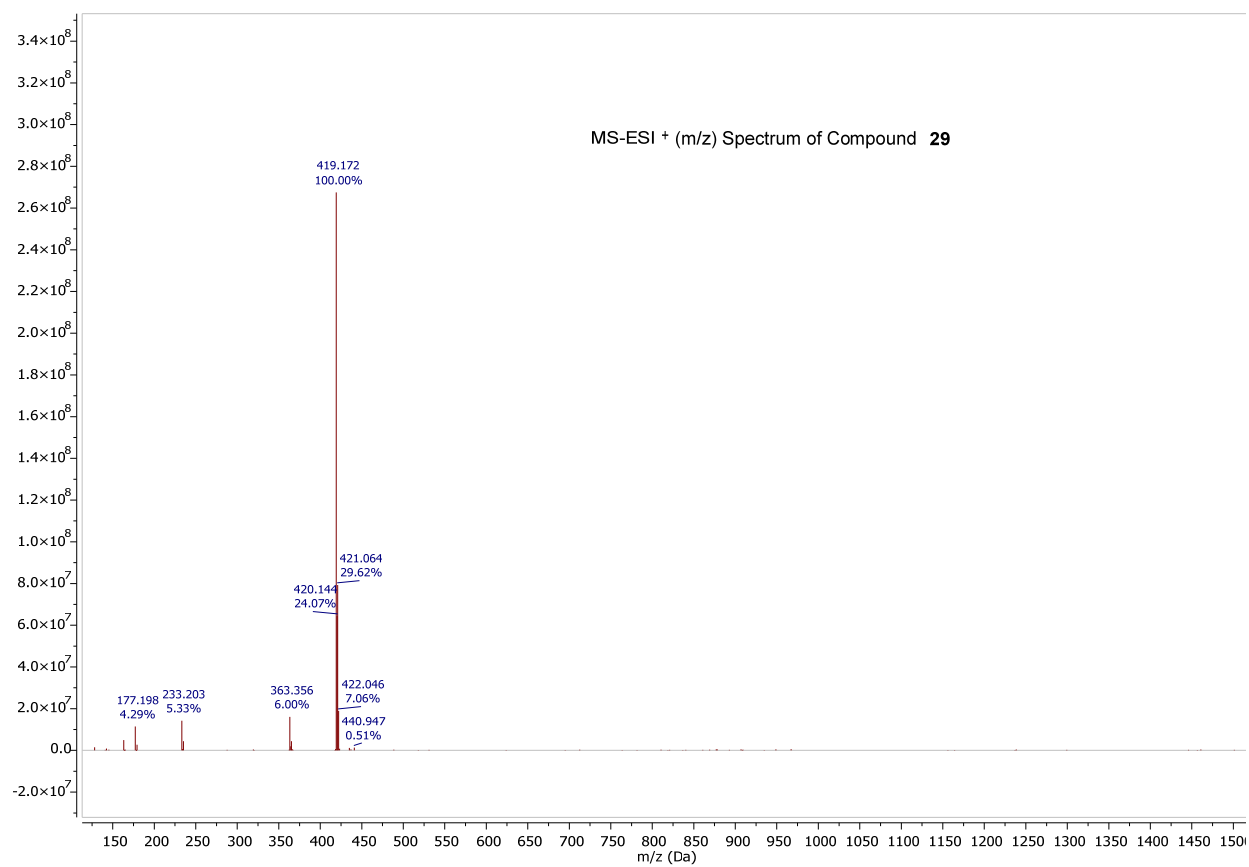


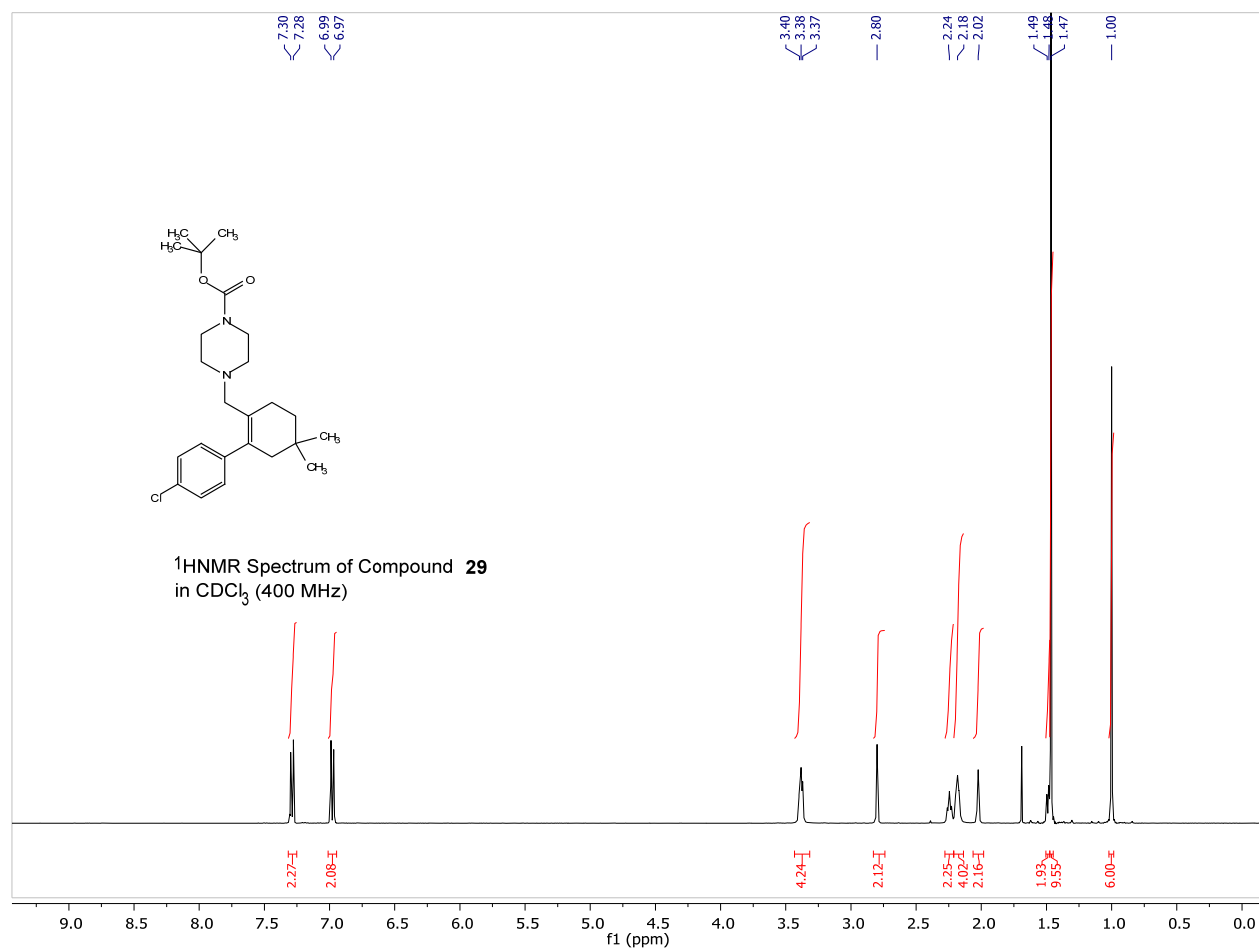


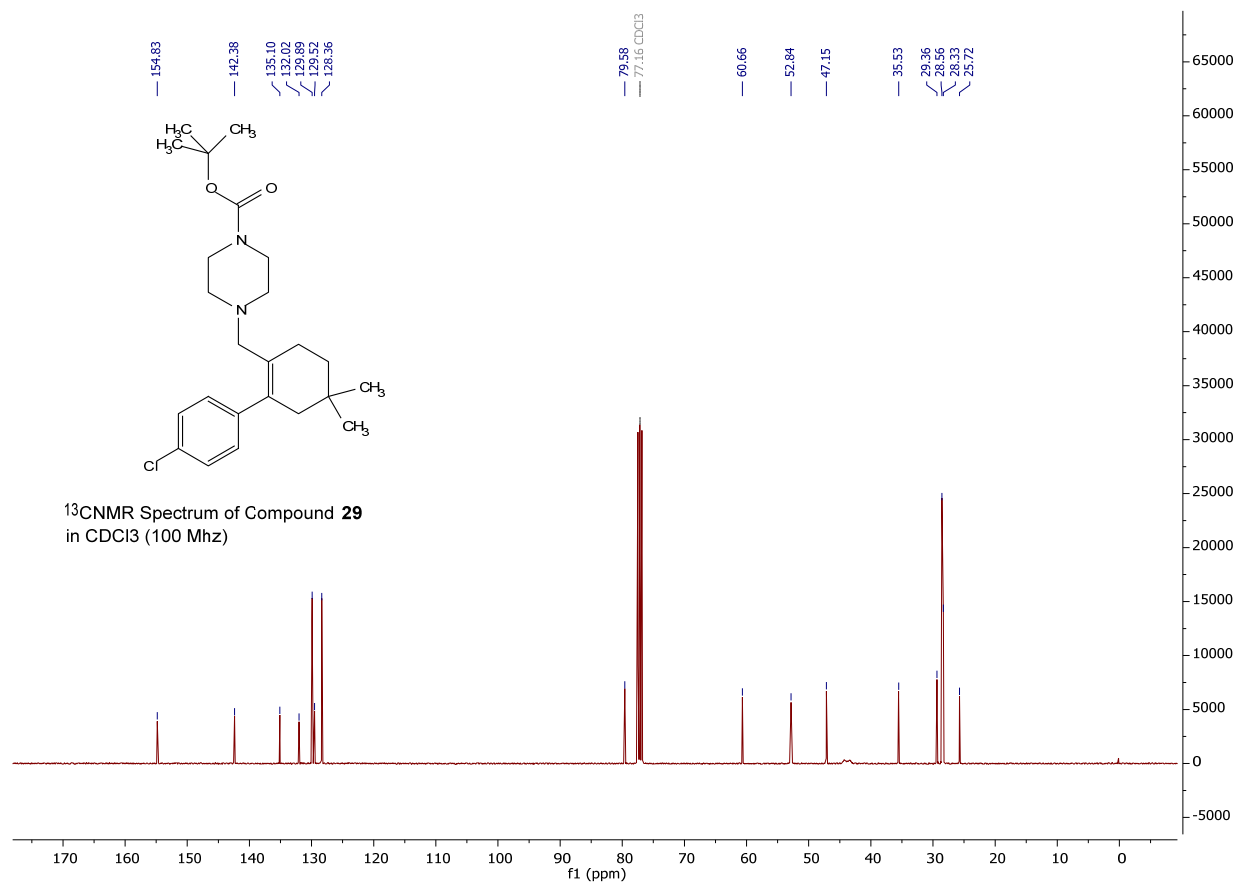


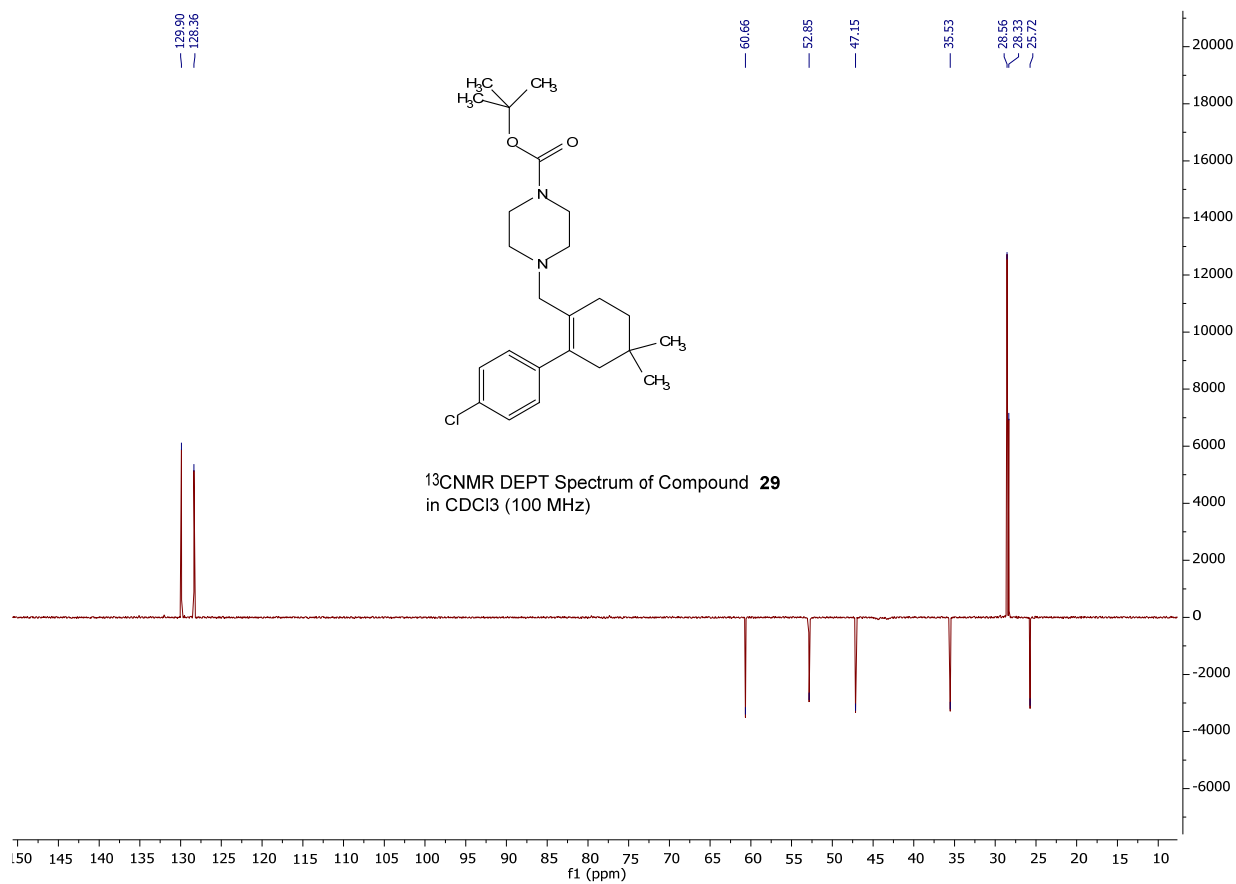


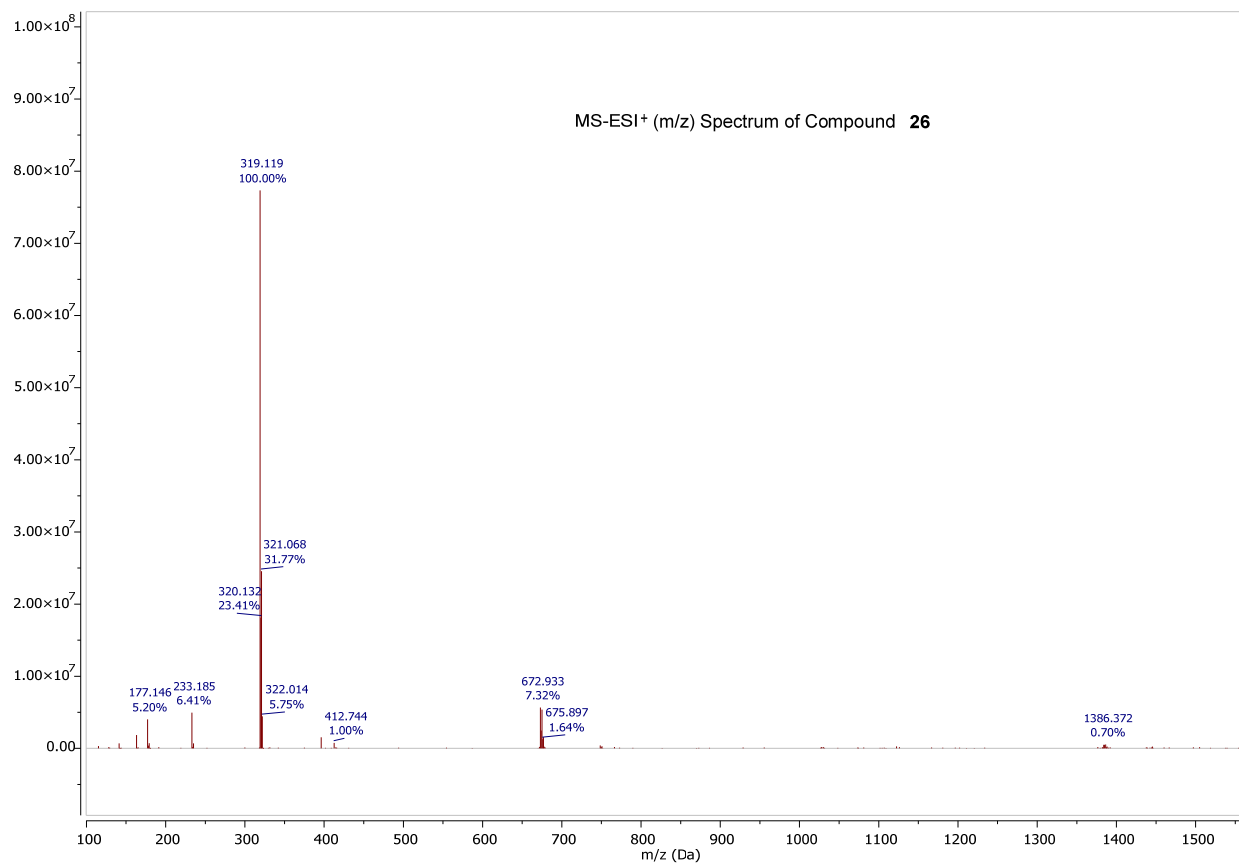


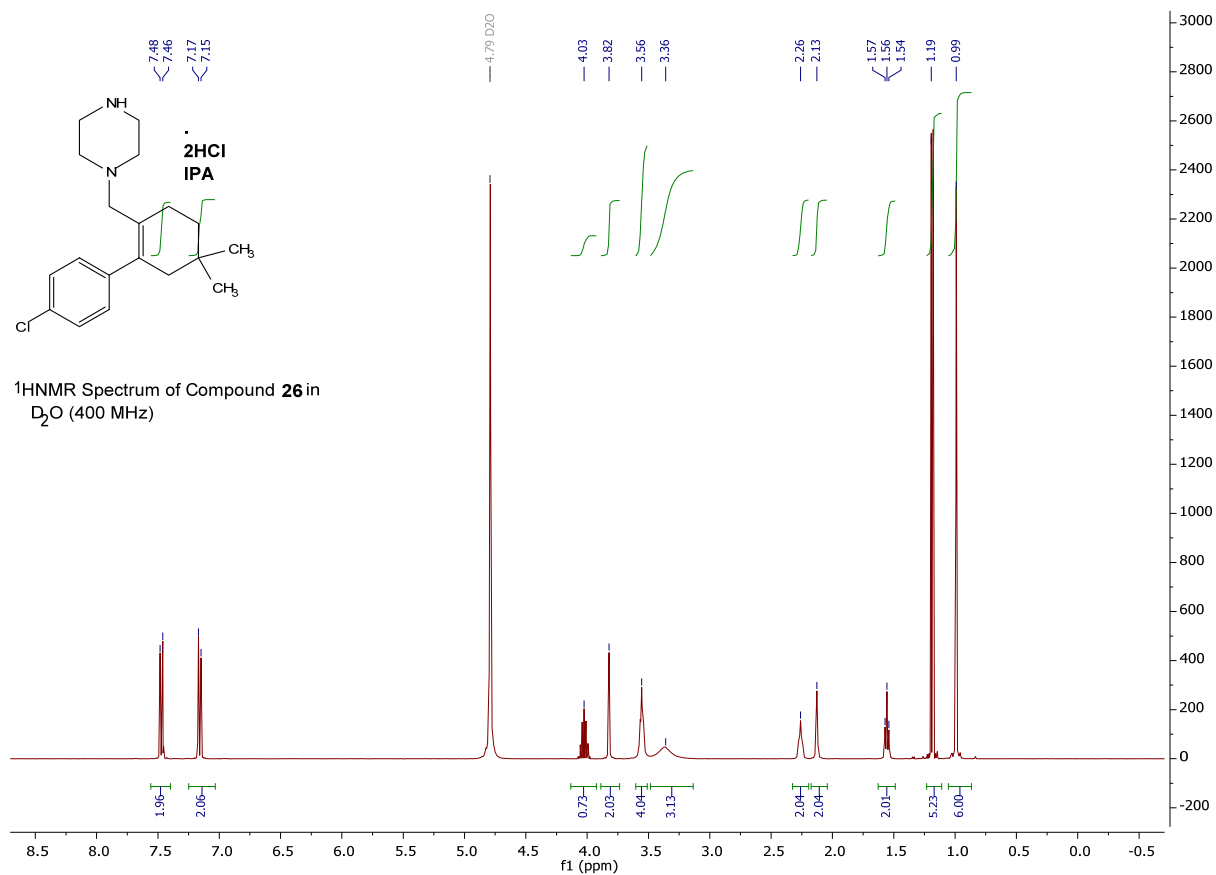


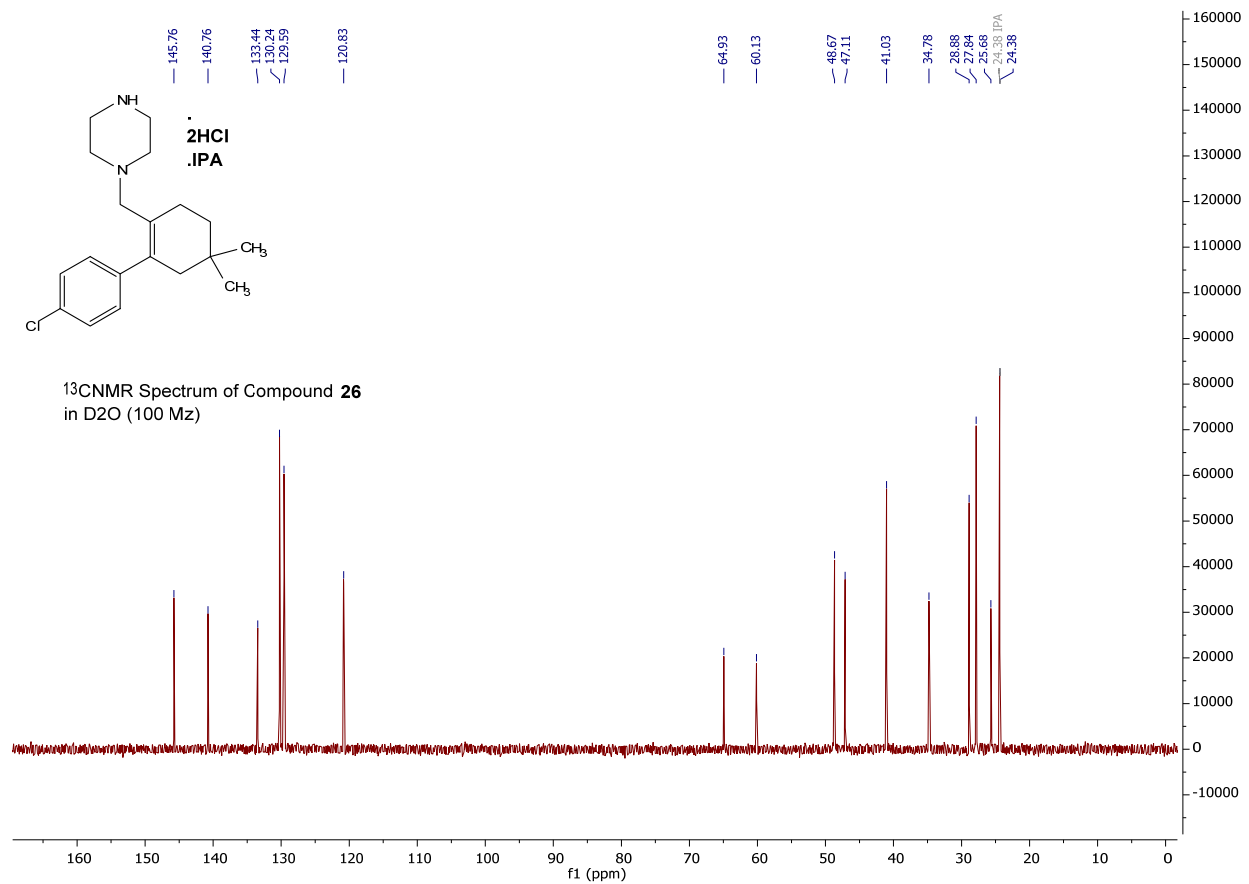


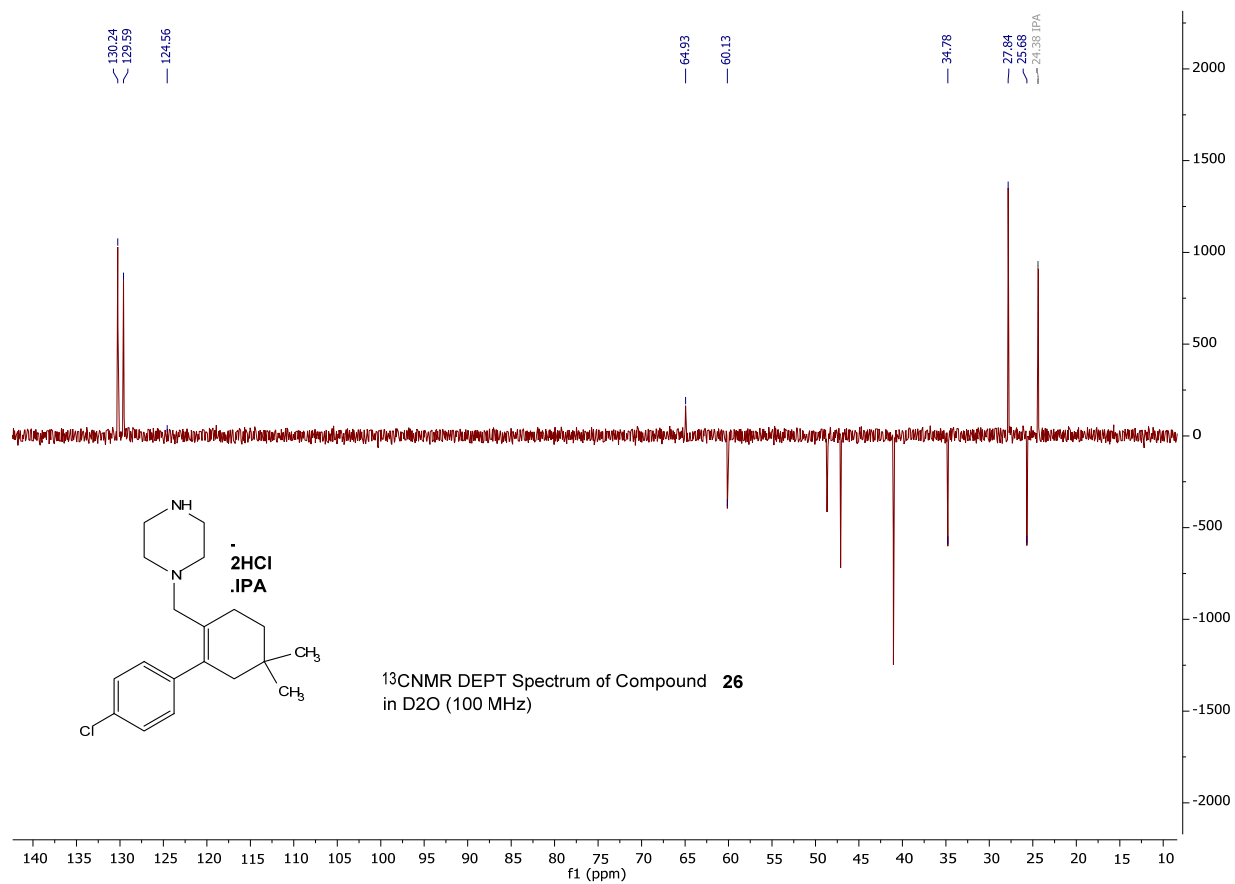


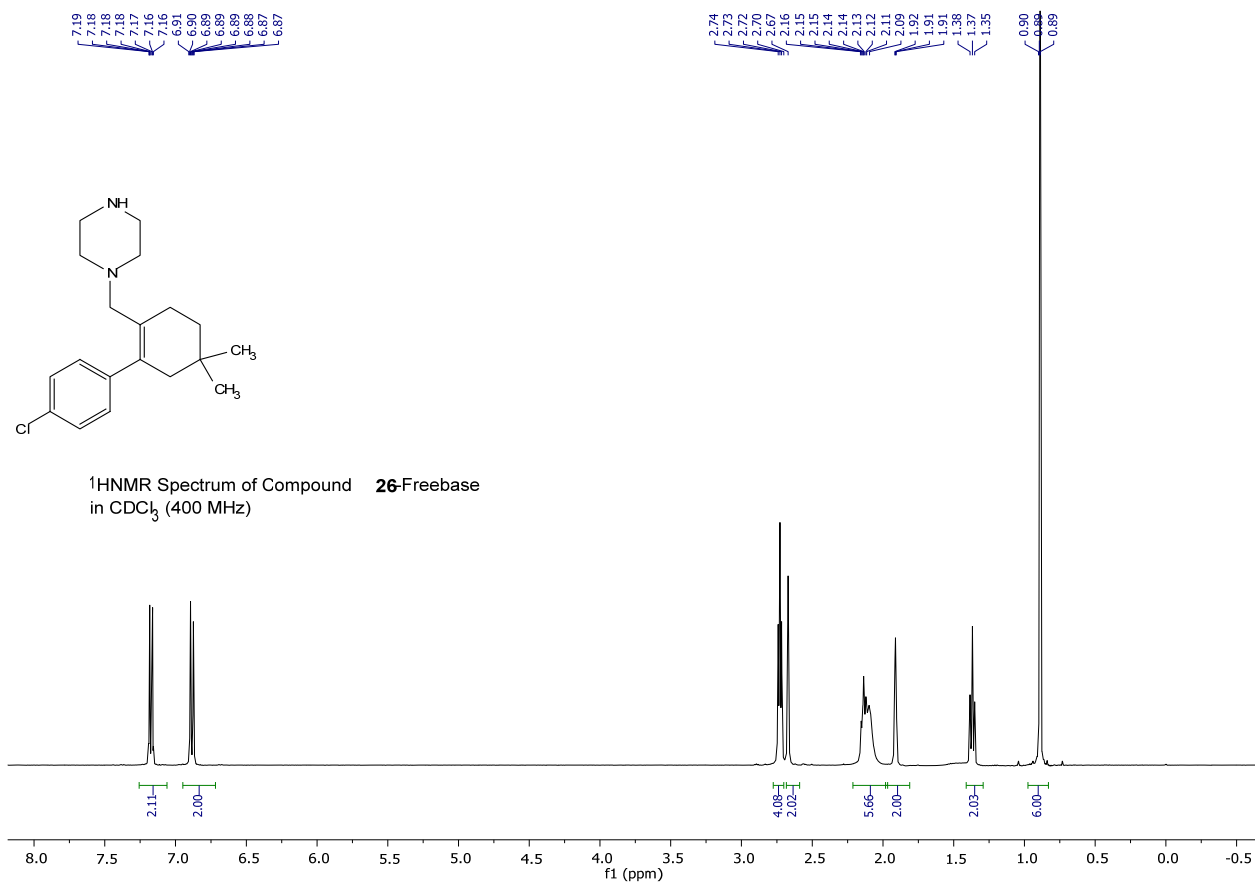


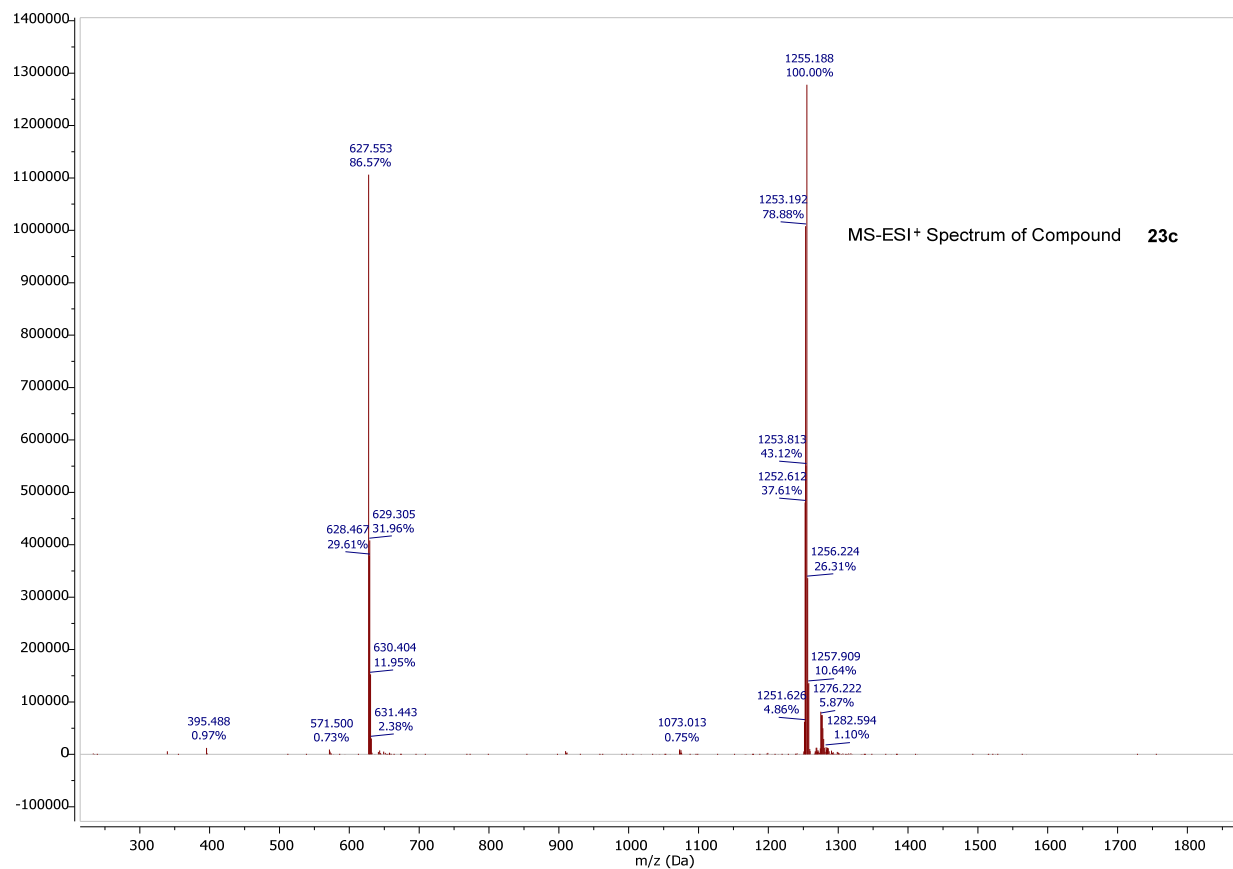


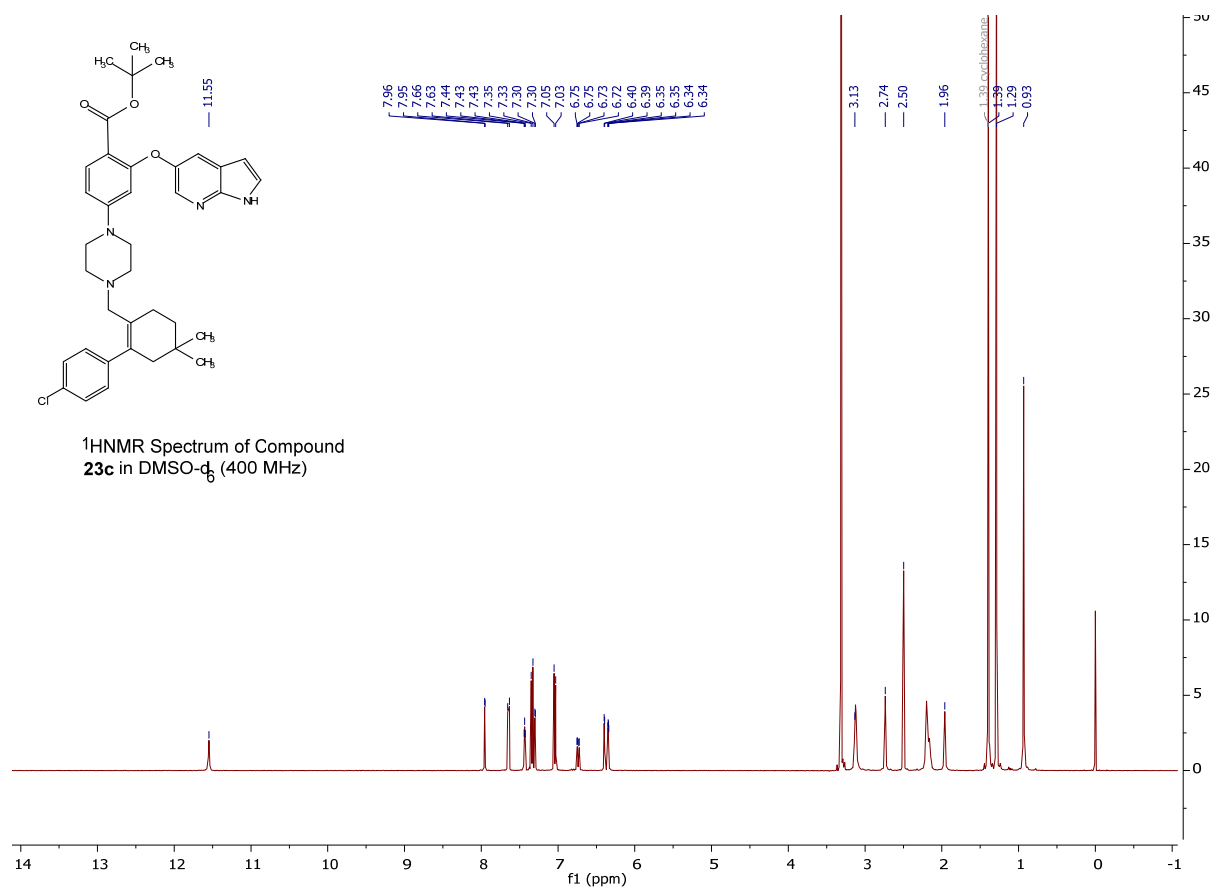


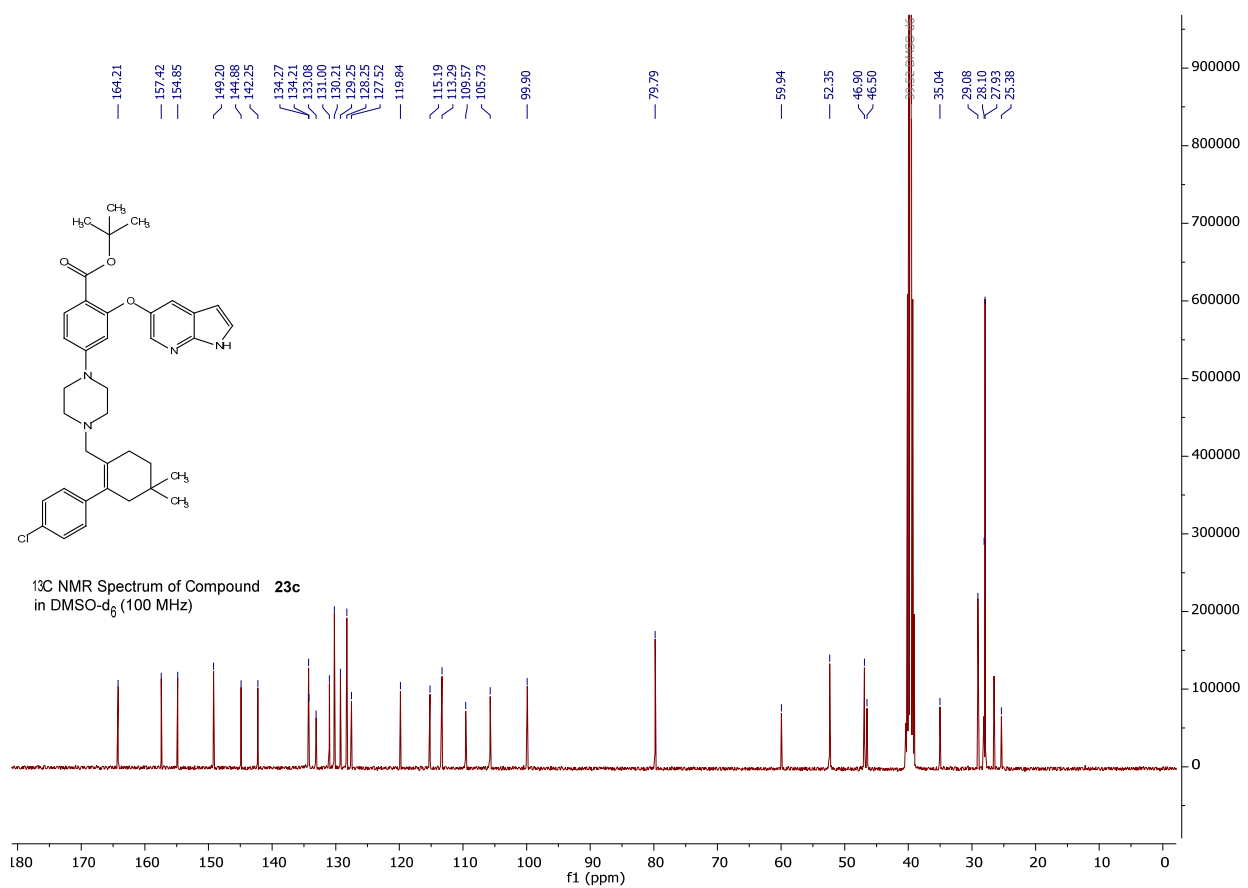


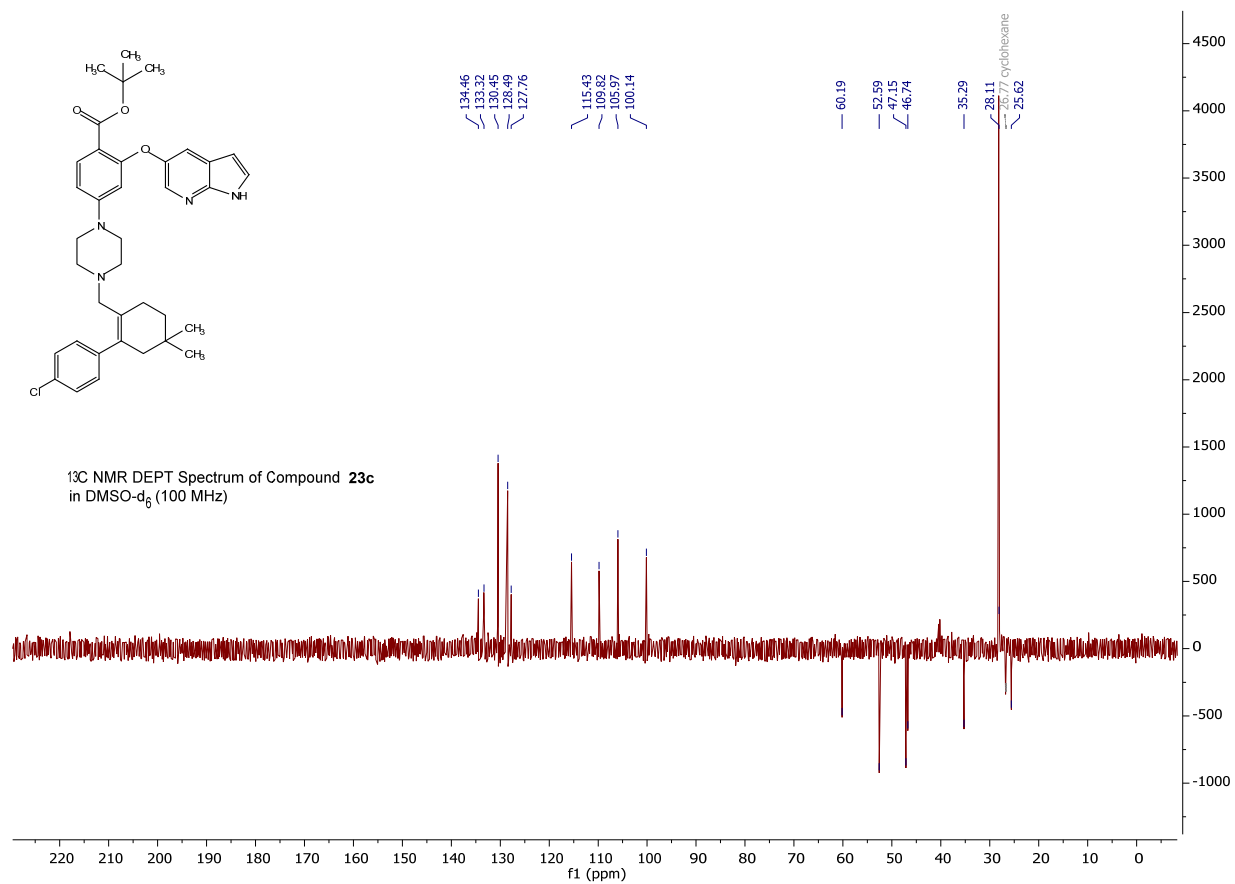


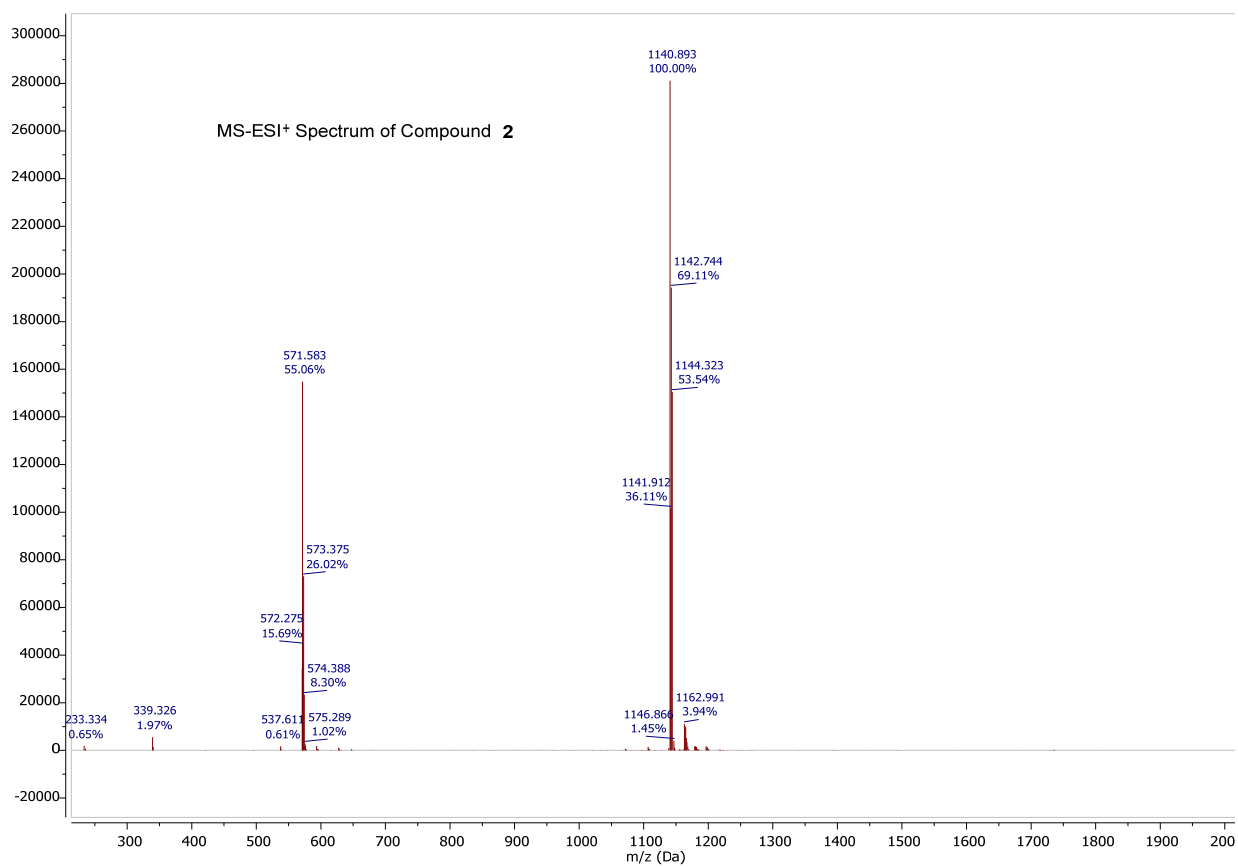


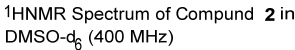


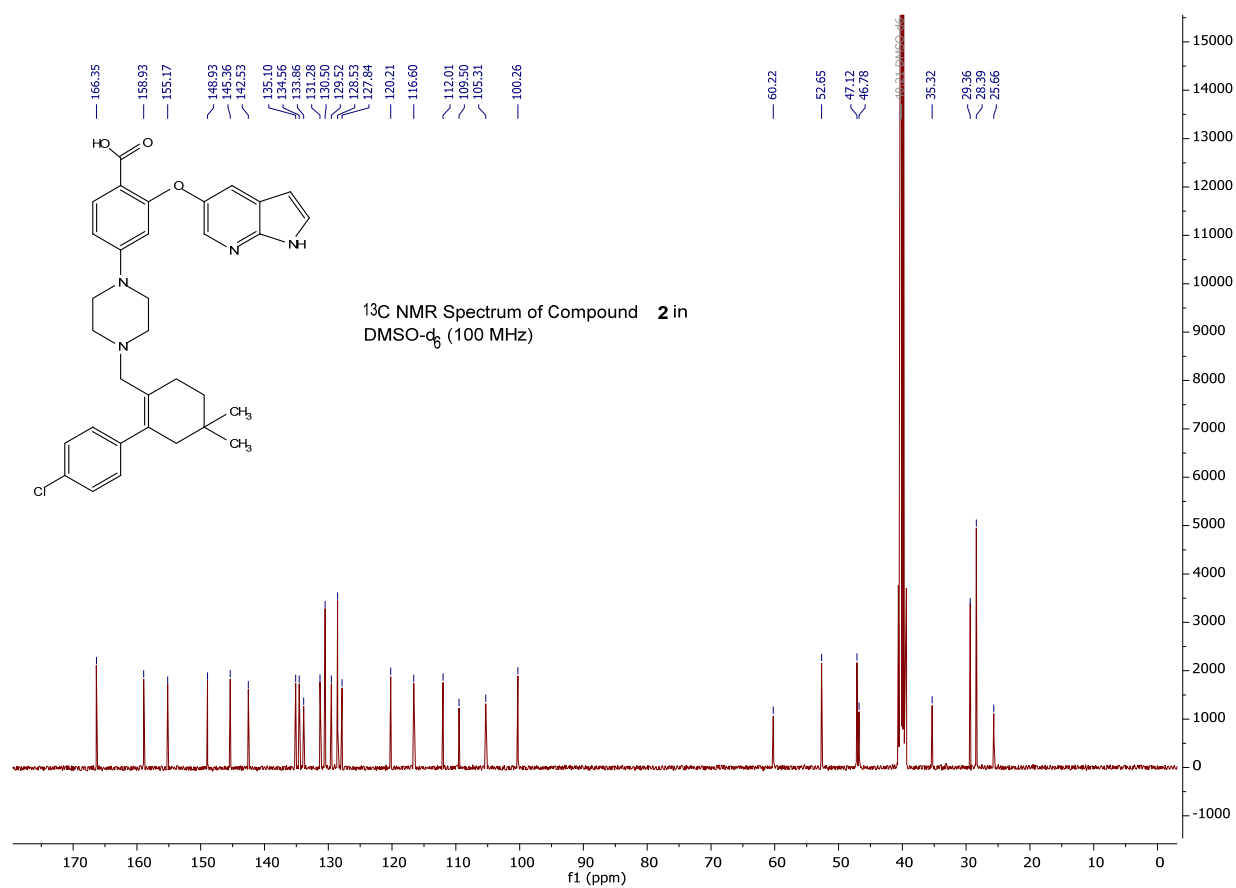


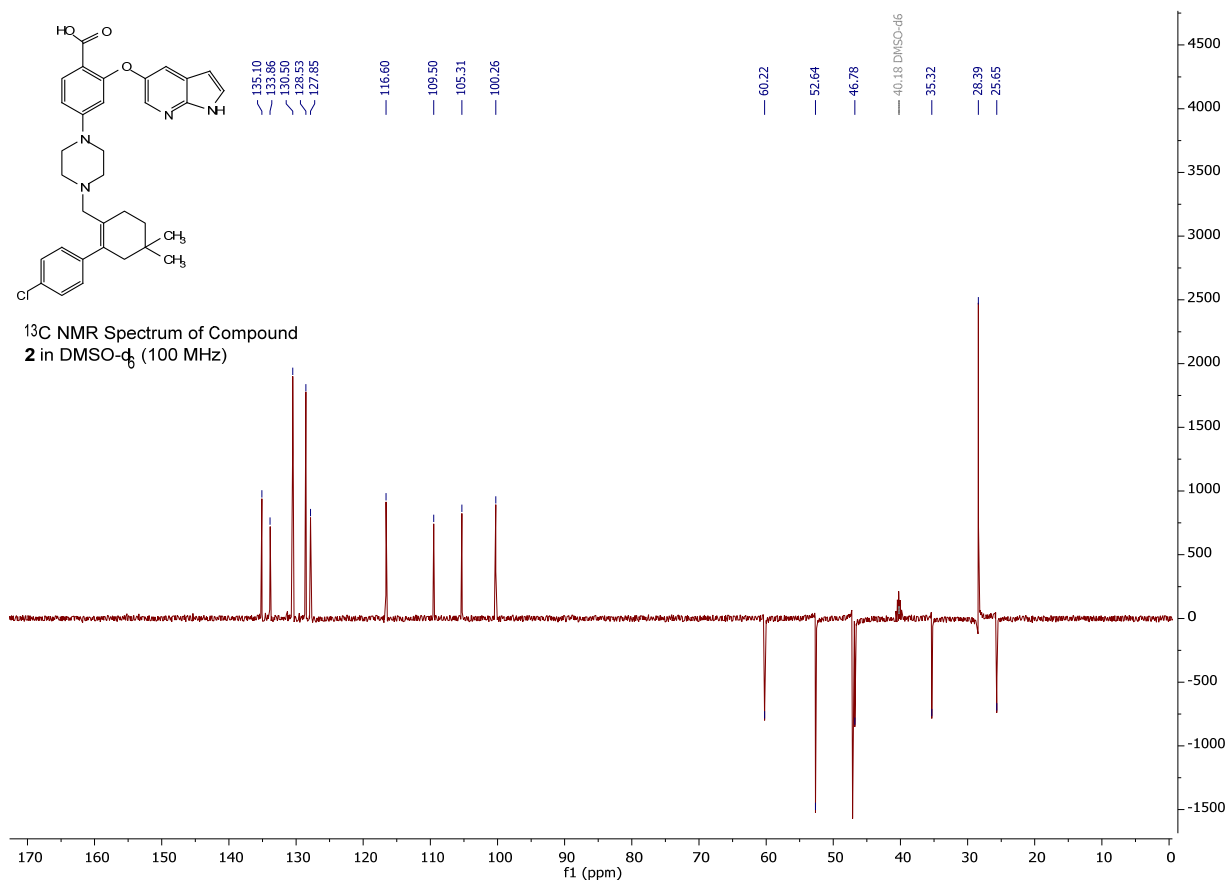


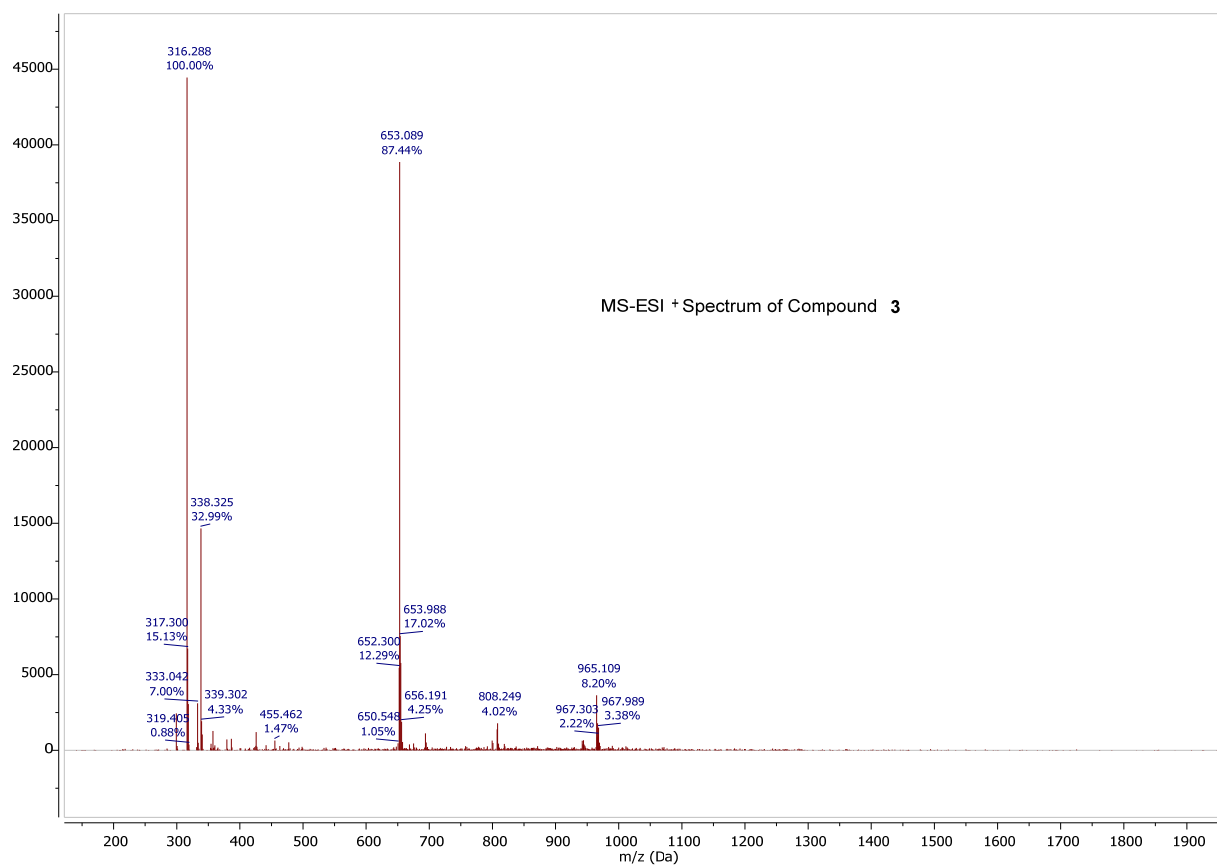


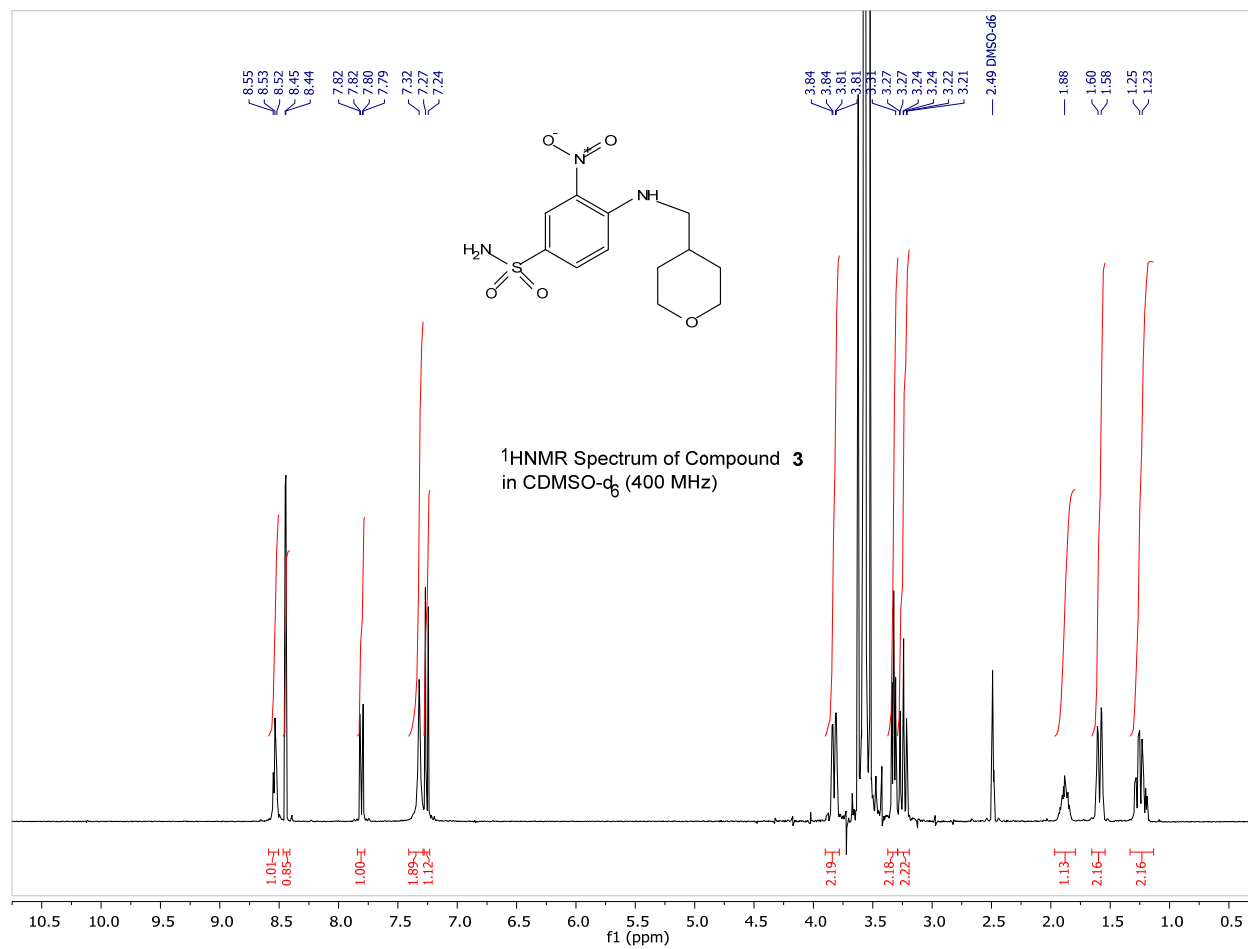


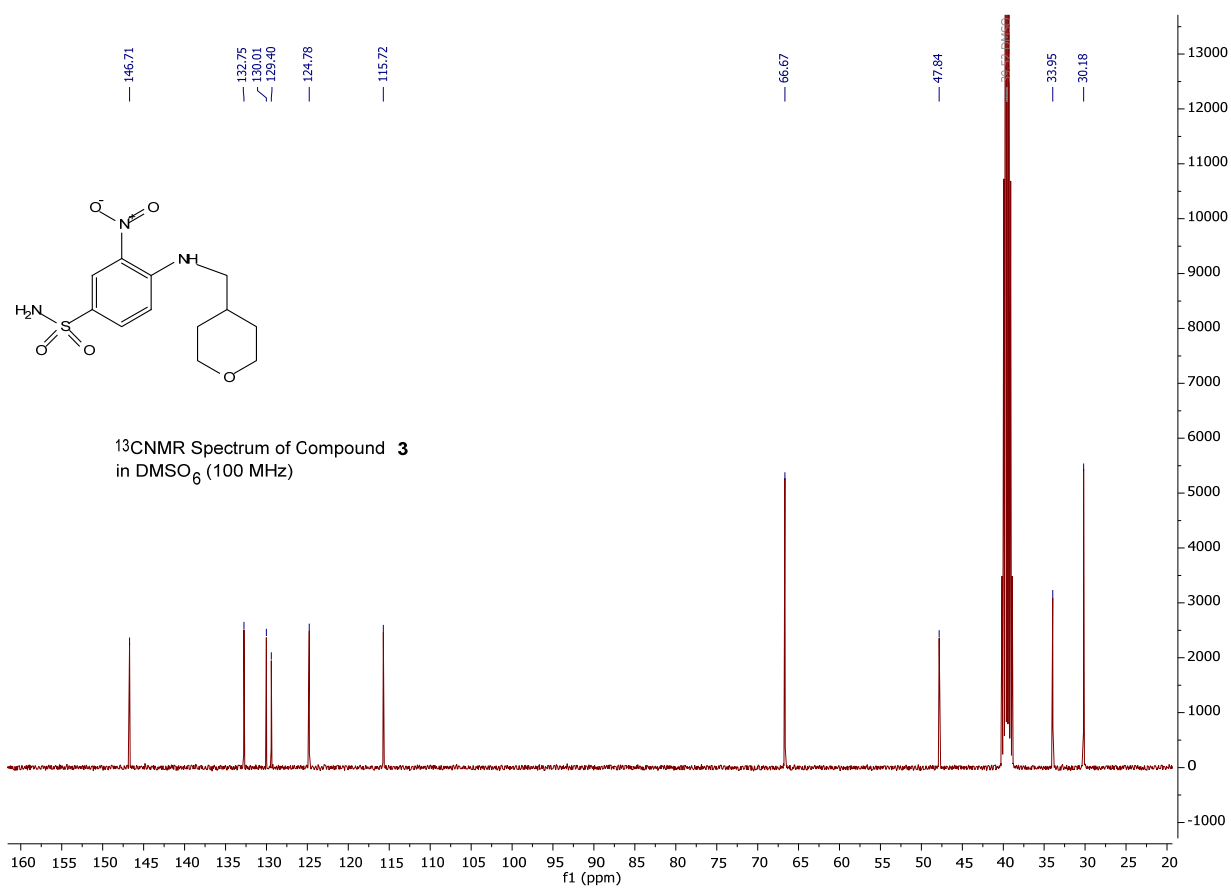


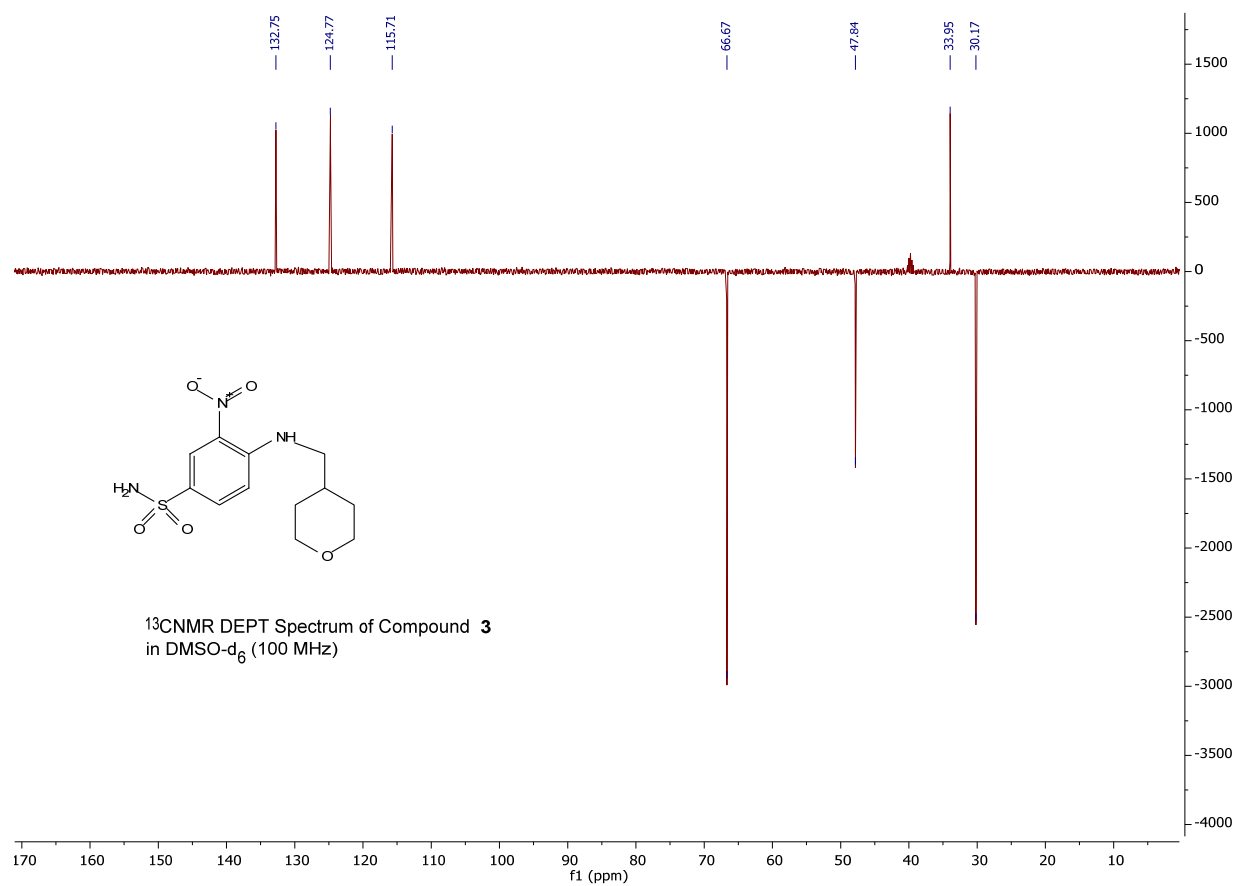


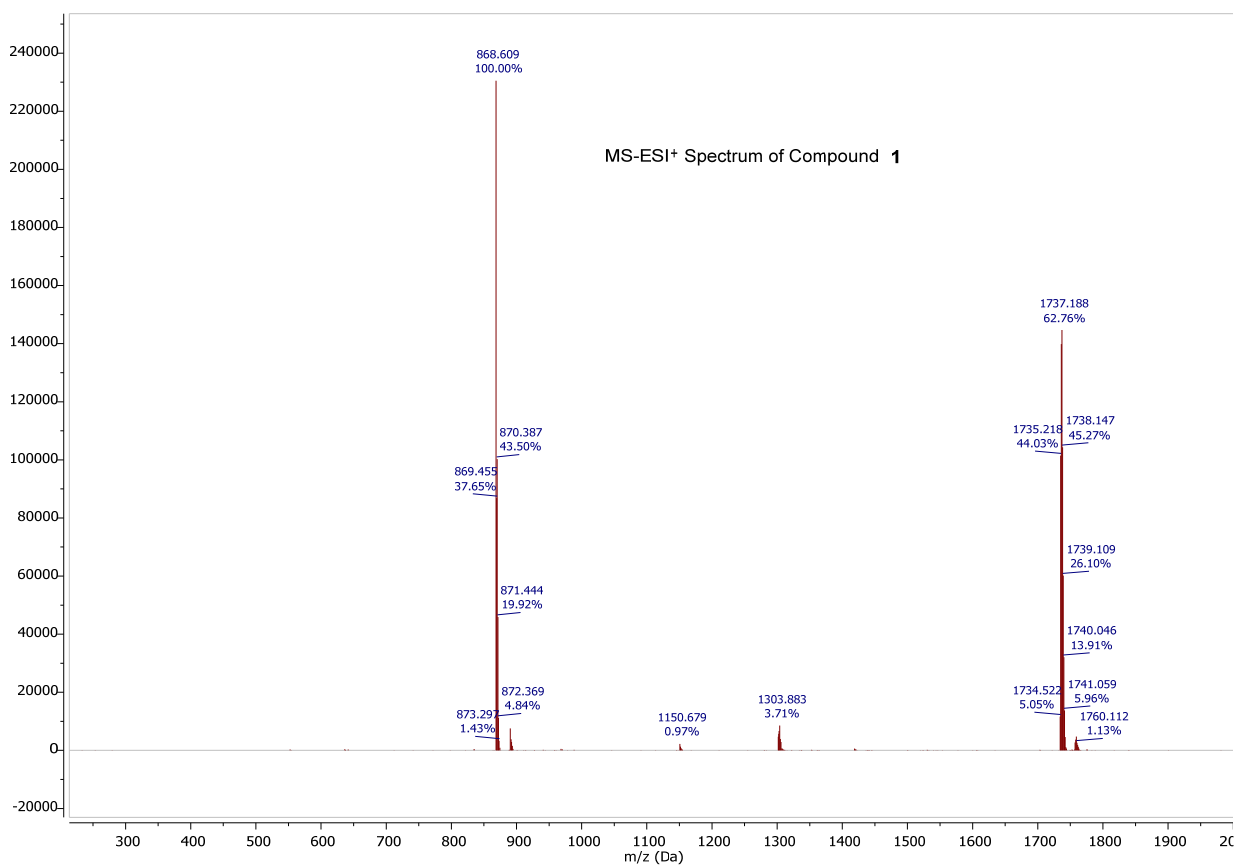


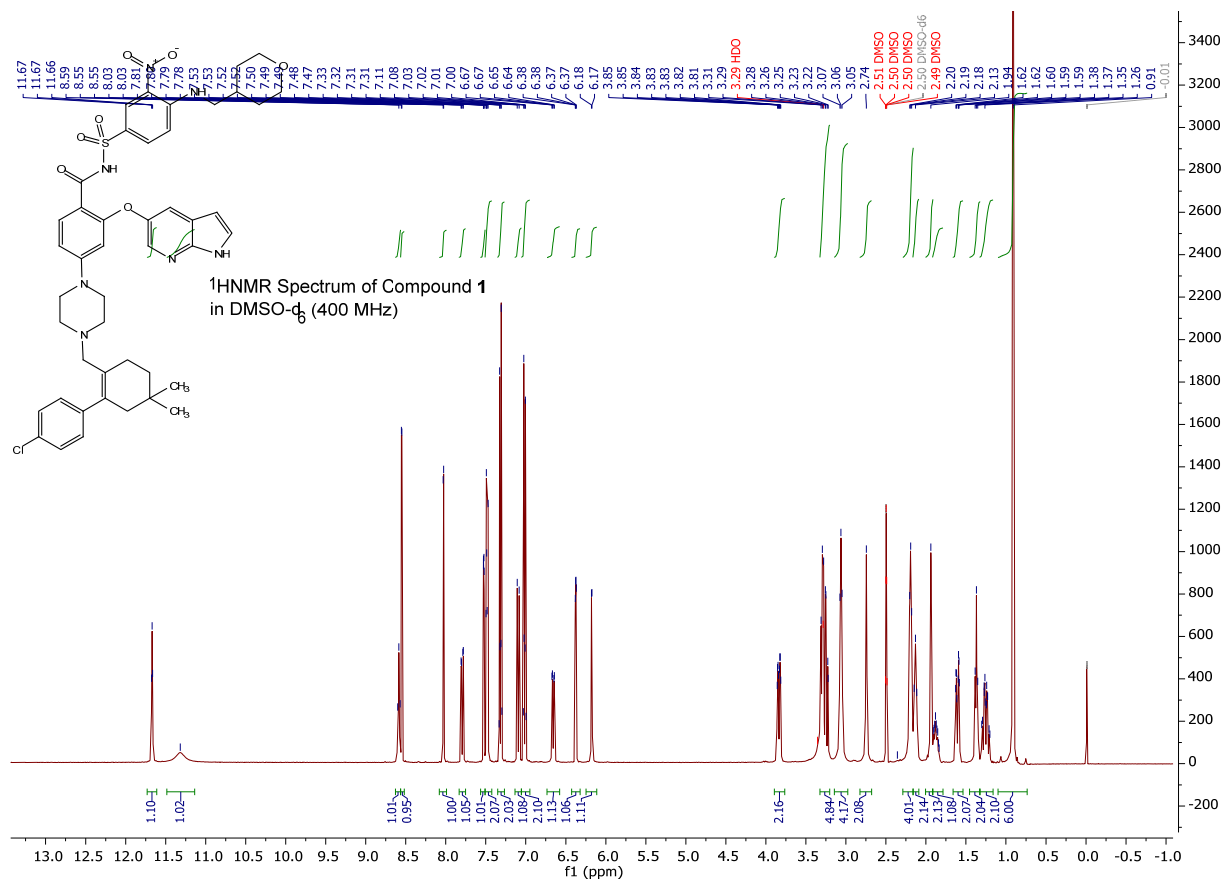


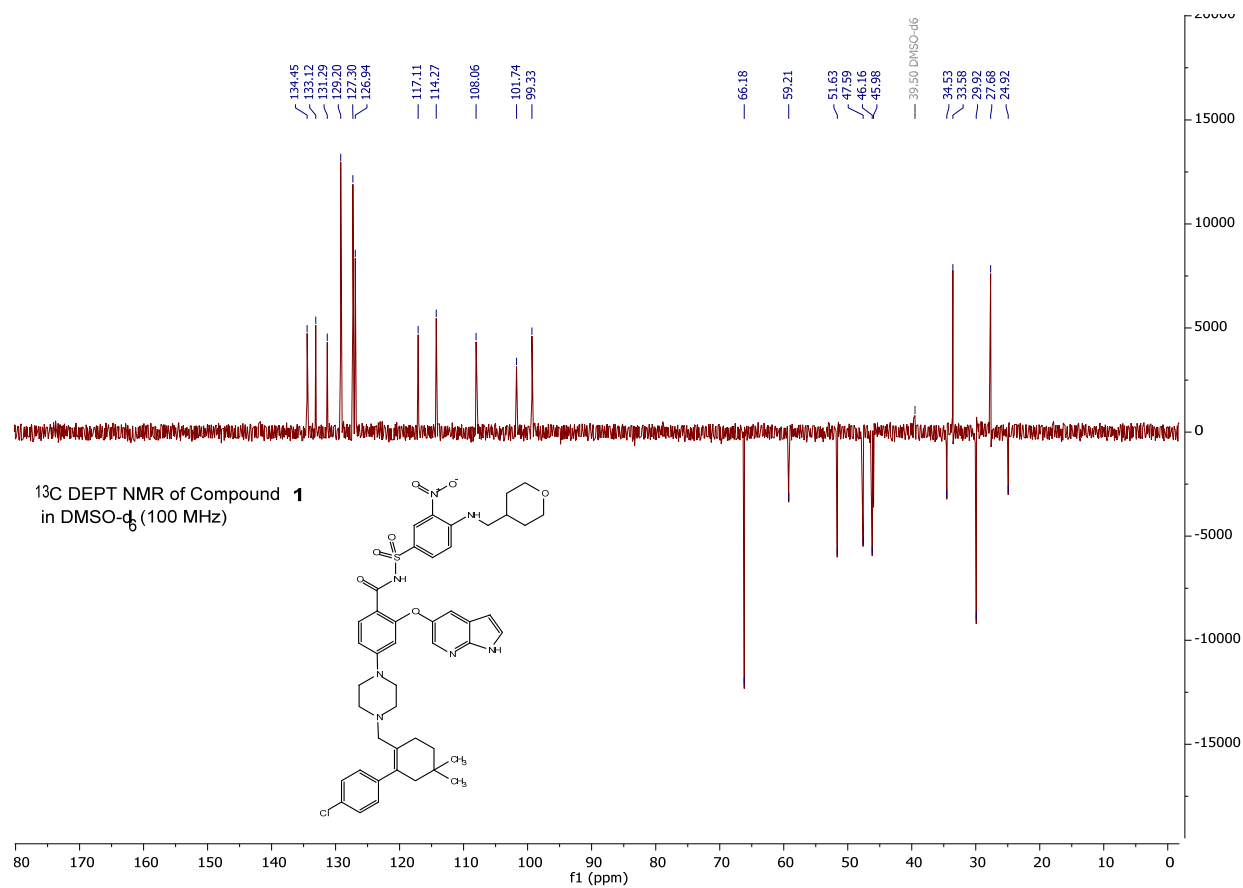


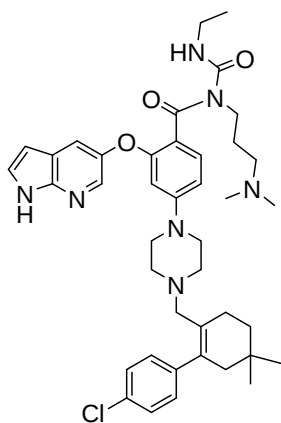








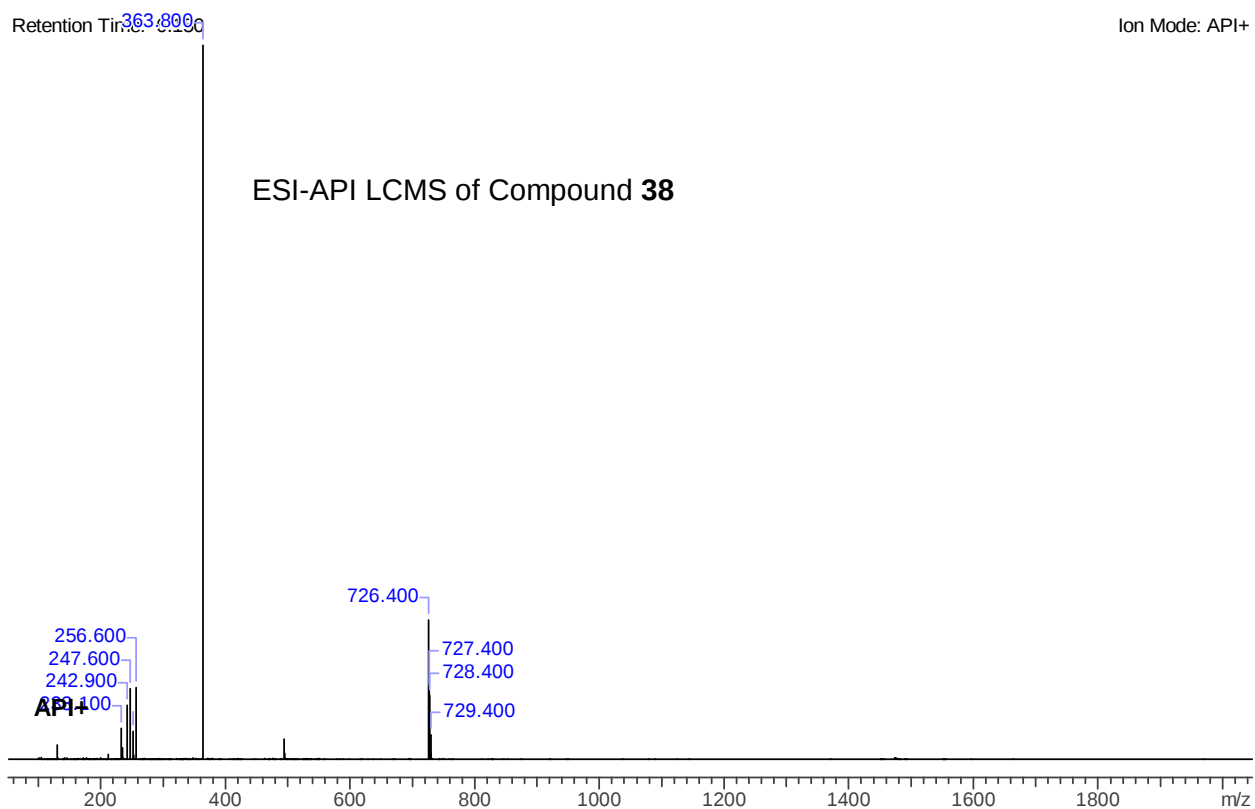


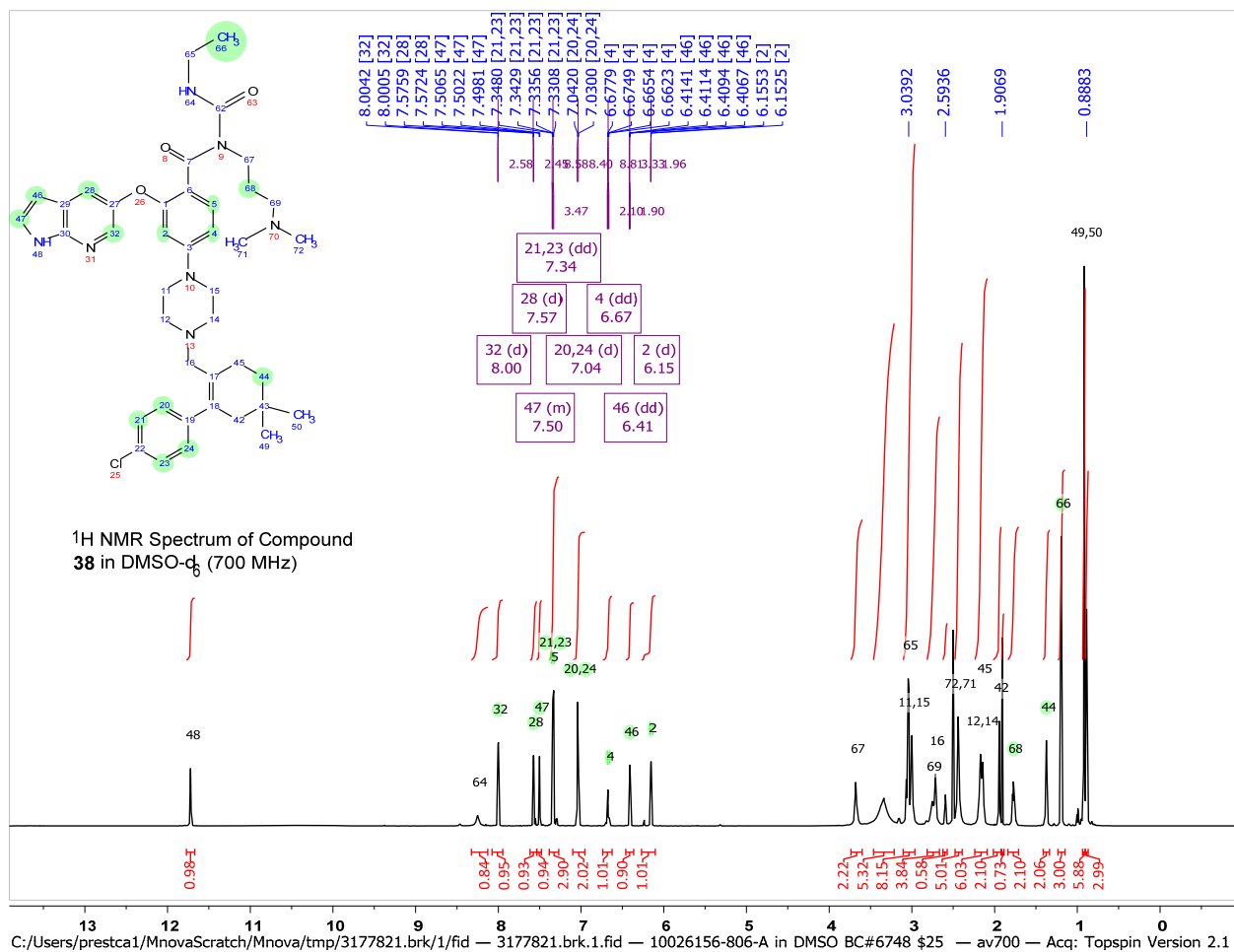


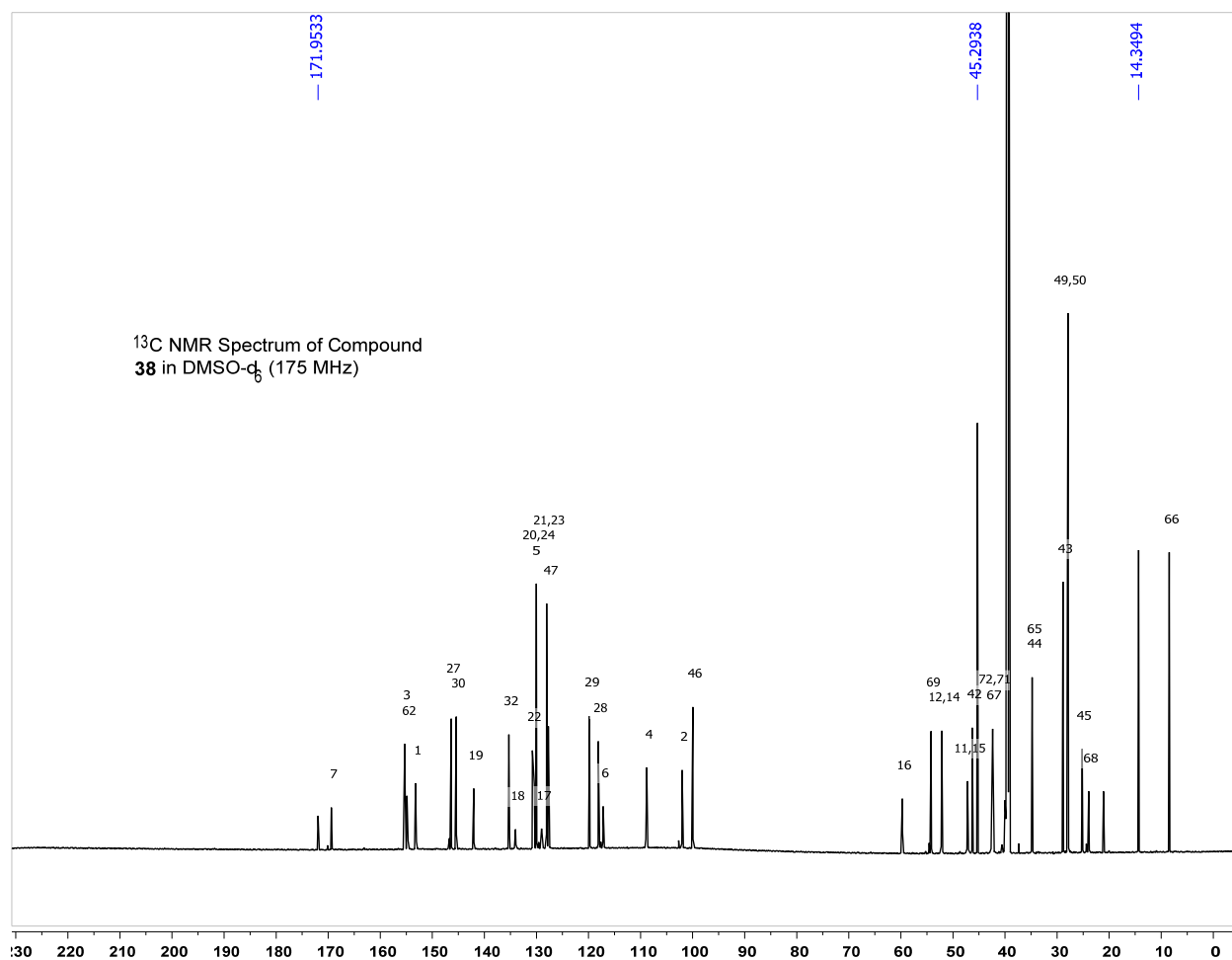
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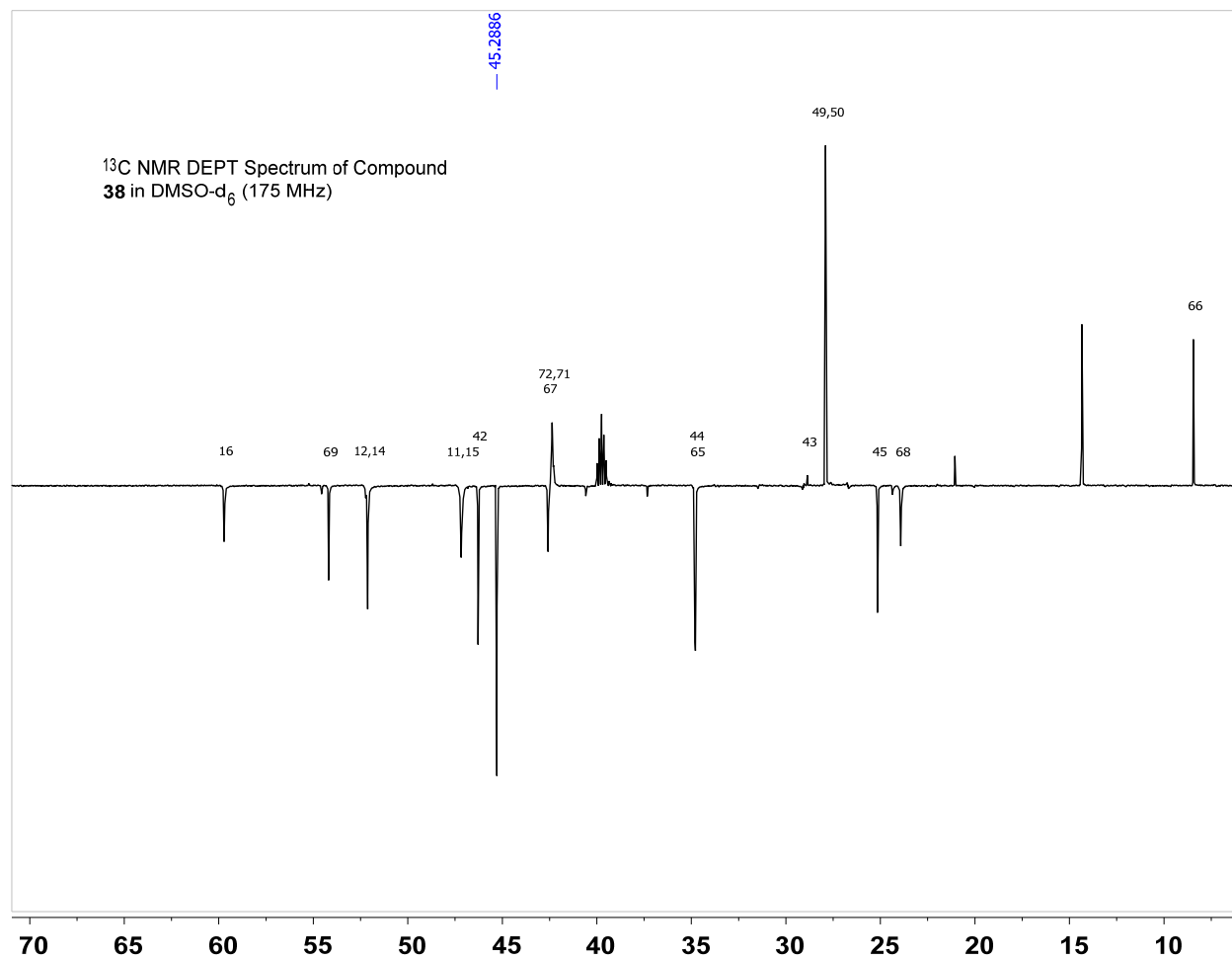
Chemical Formula: $C_{41}H_{52}ClN_7O_3$

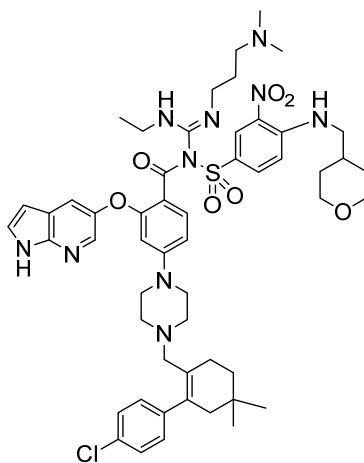
Exact Mass: 725.38







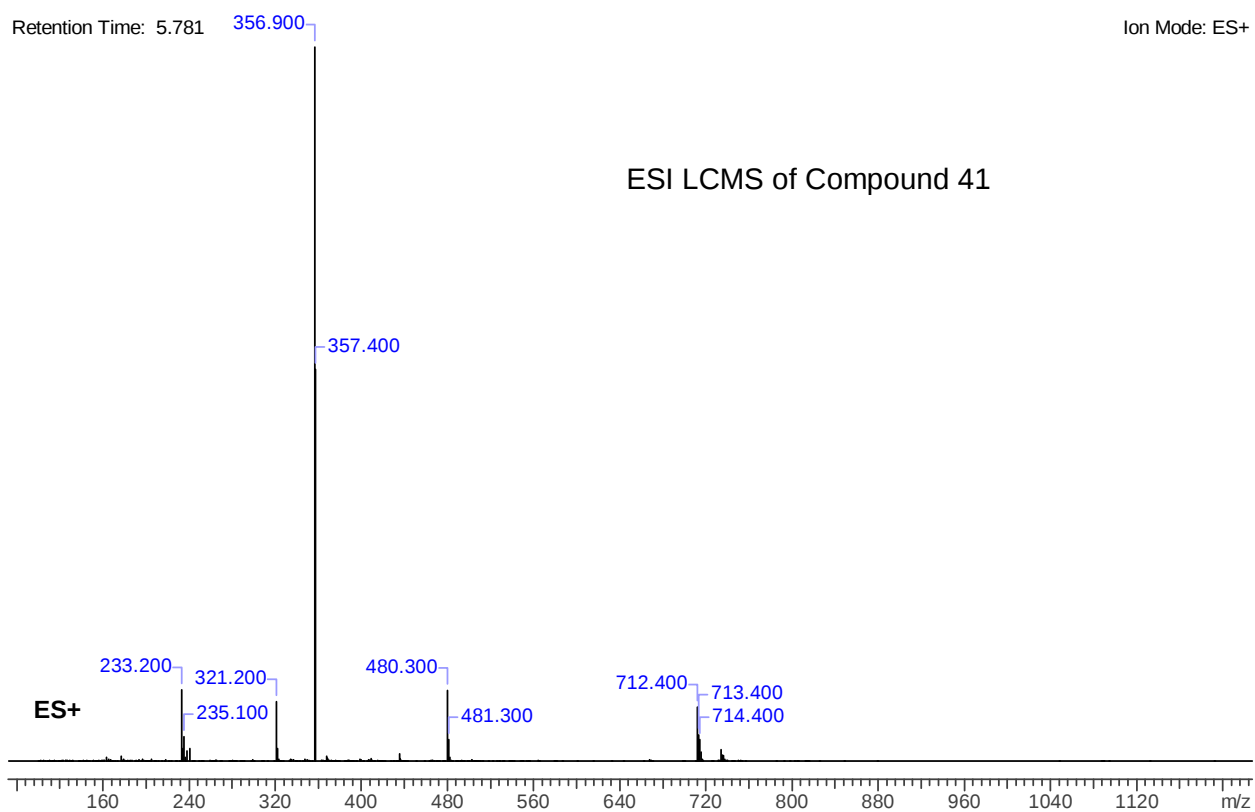


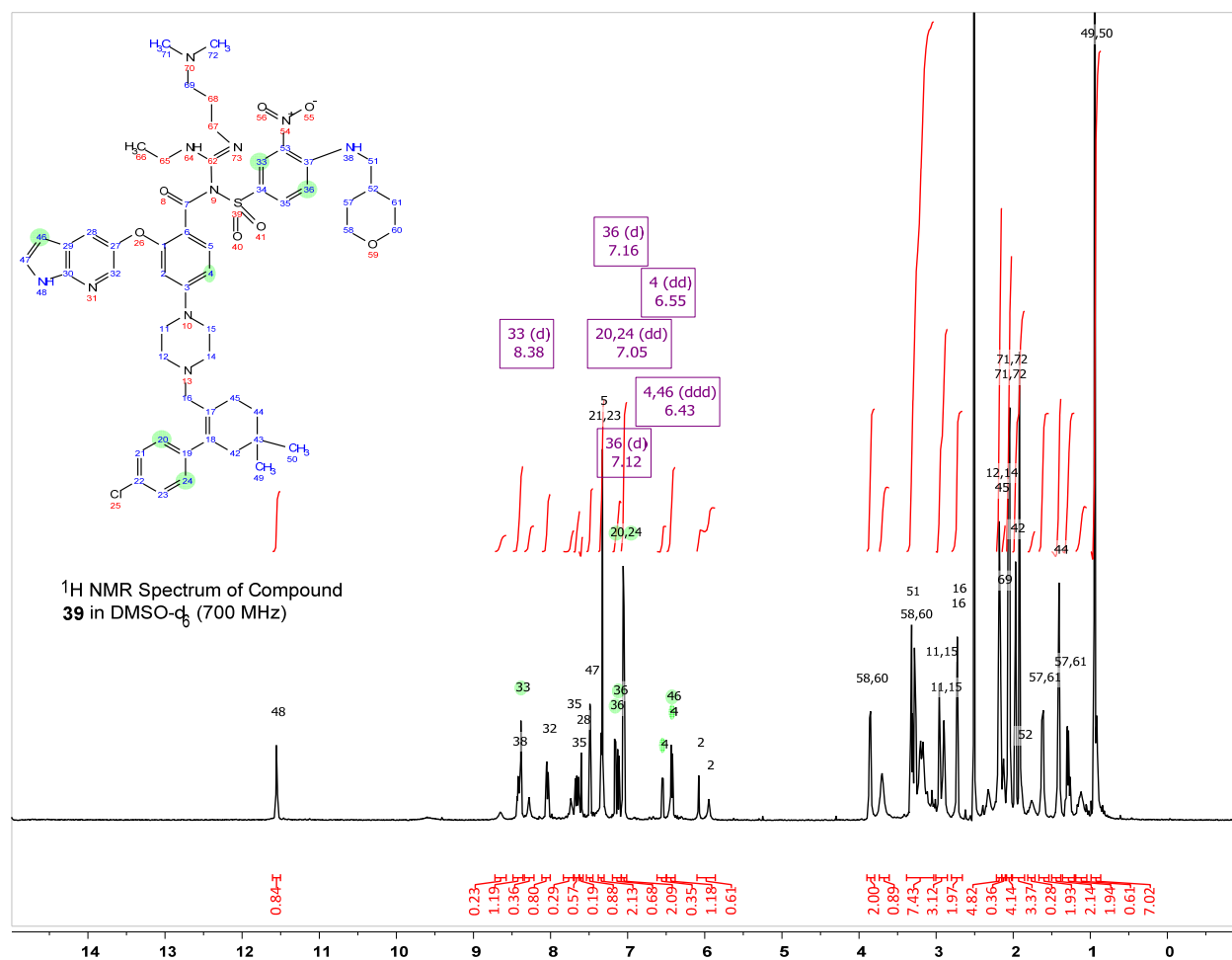


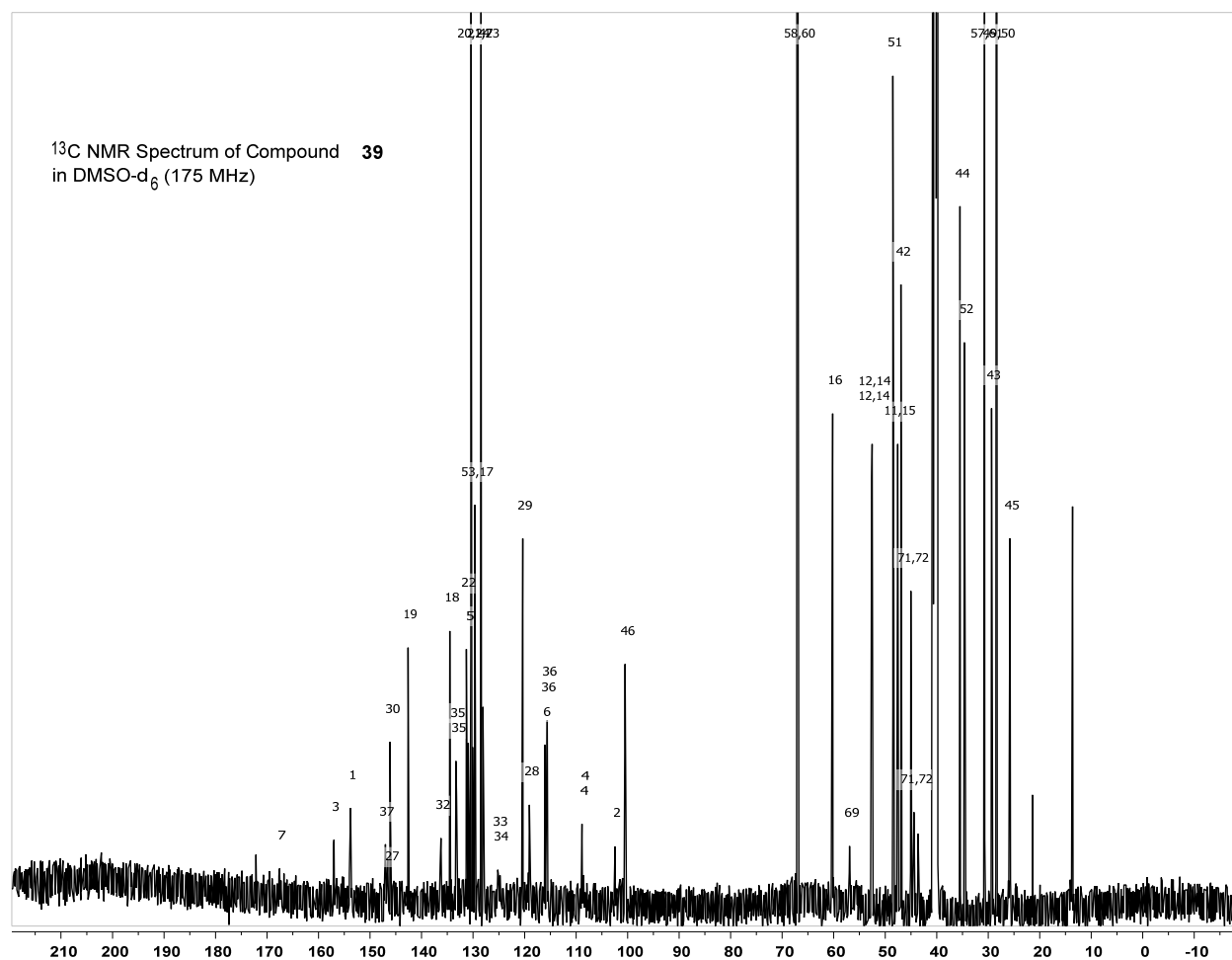
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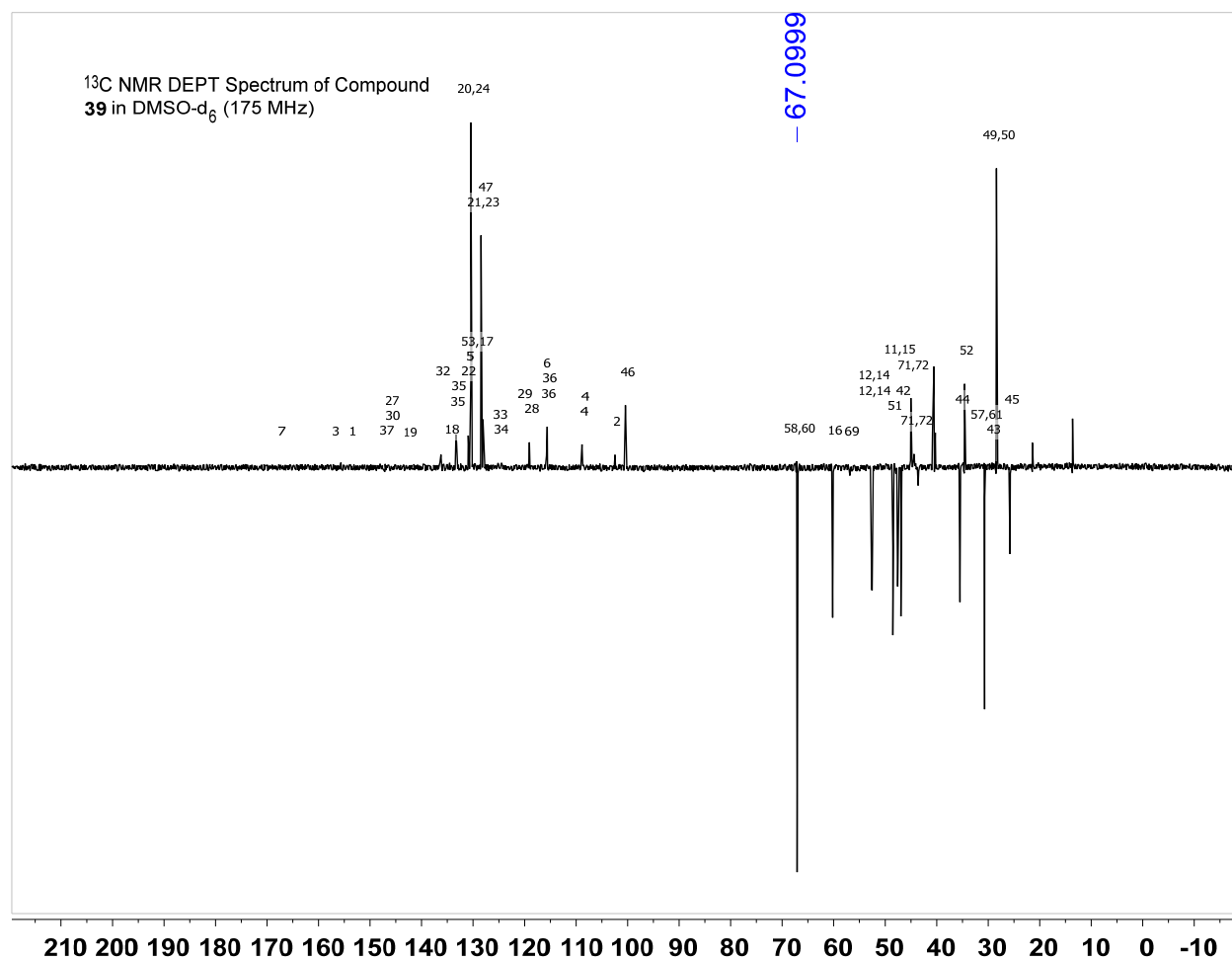
Chemical Formula: $C_{53}H_{67}ClN_{10}O_7S$

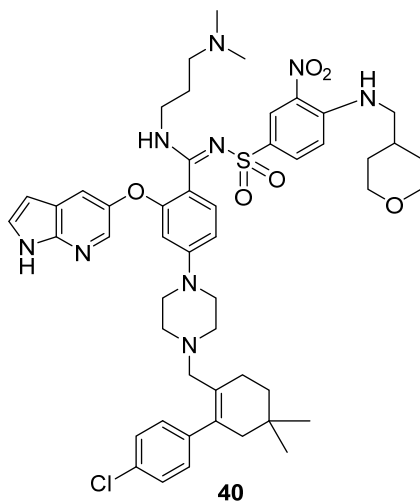
Exact Mass: 1022.46



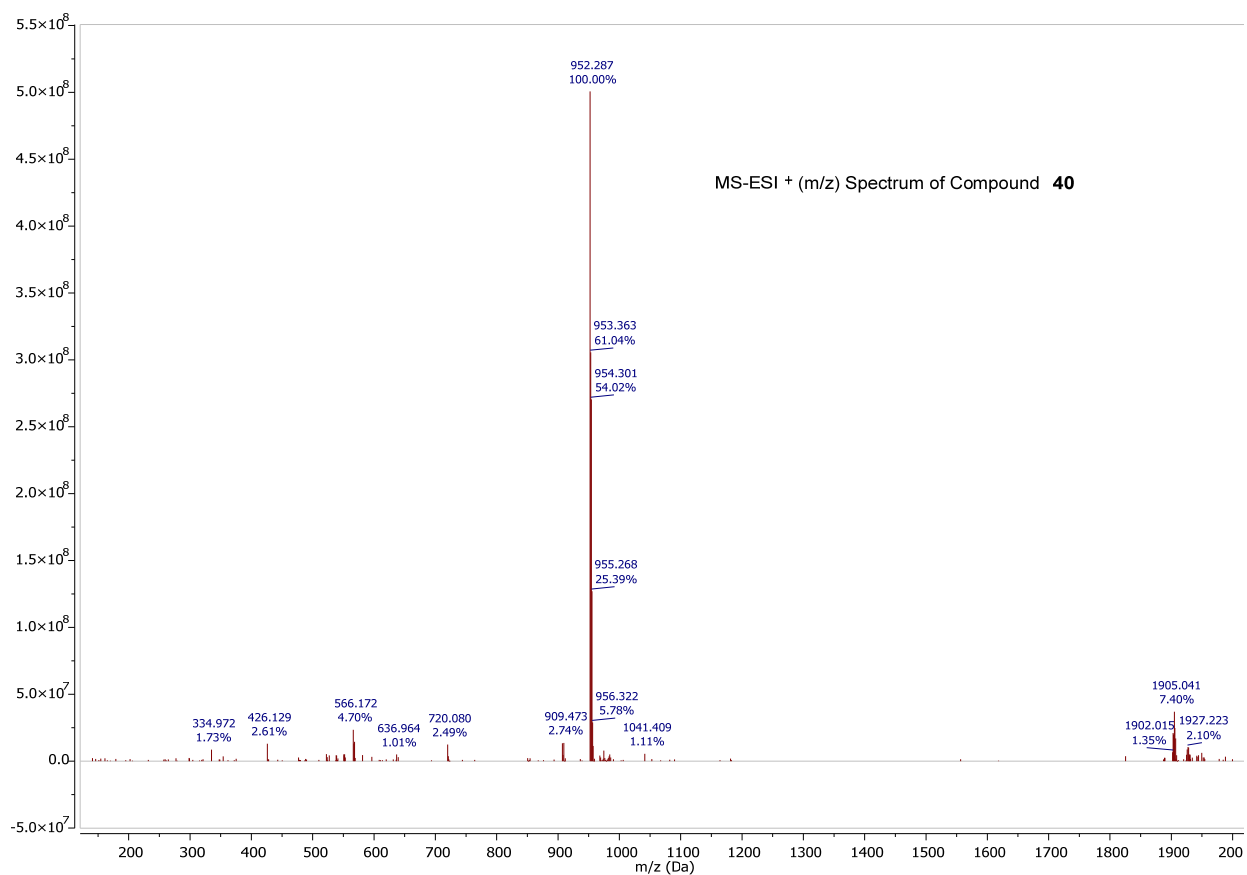


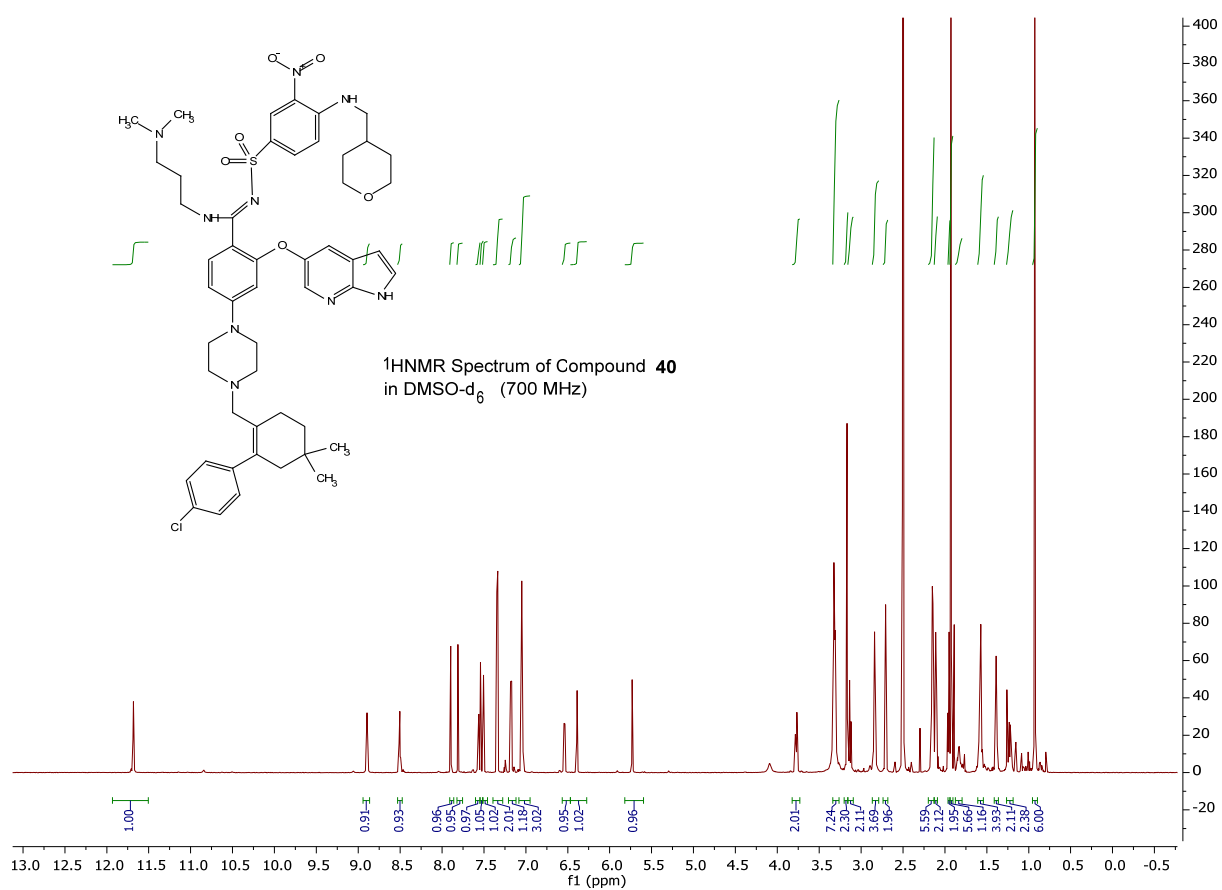


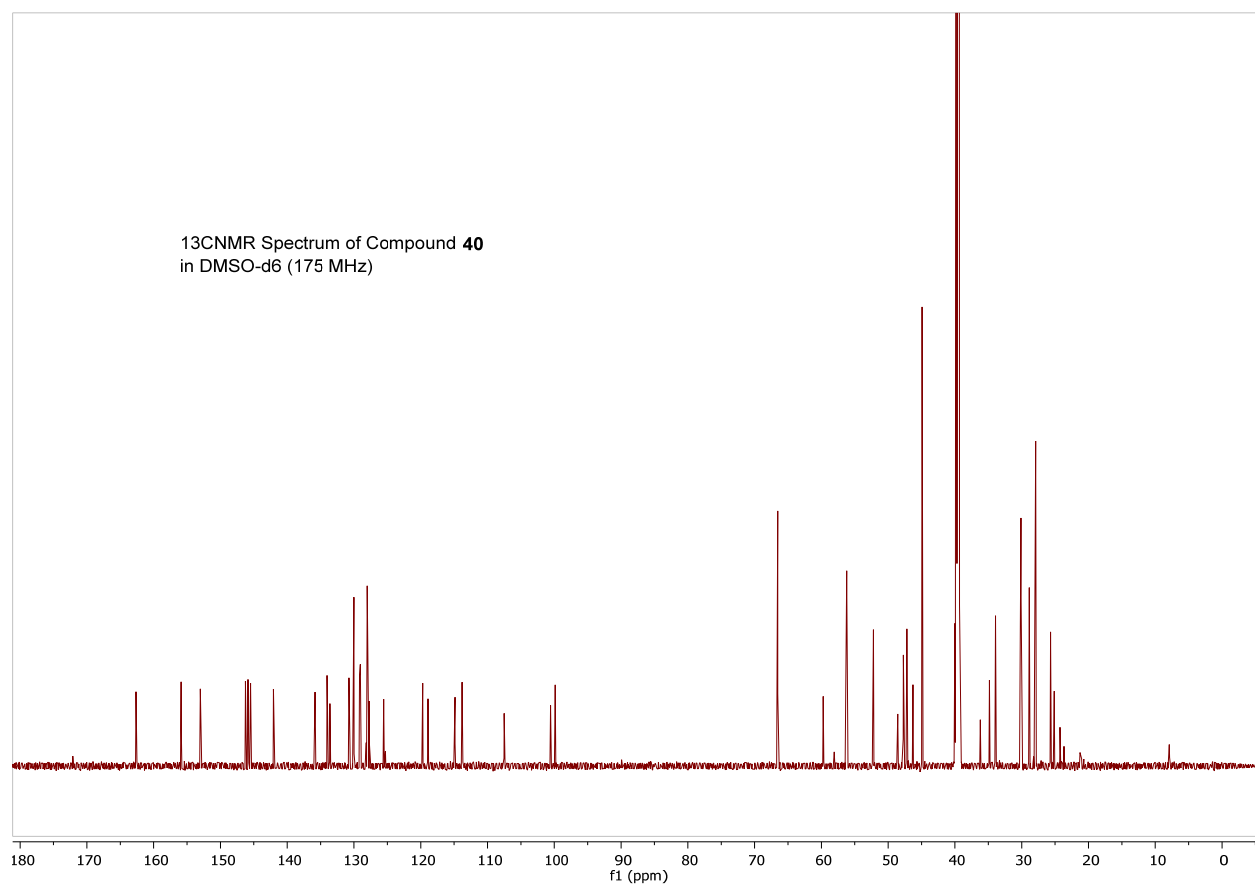


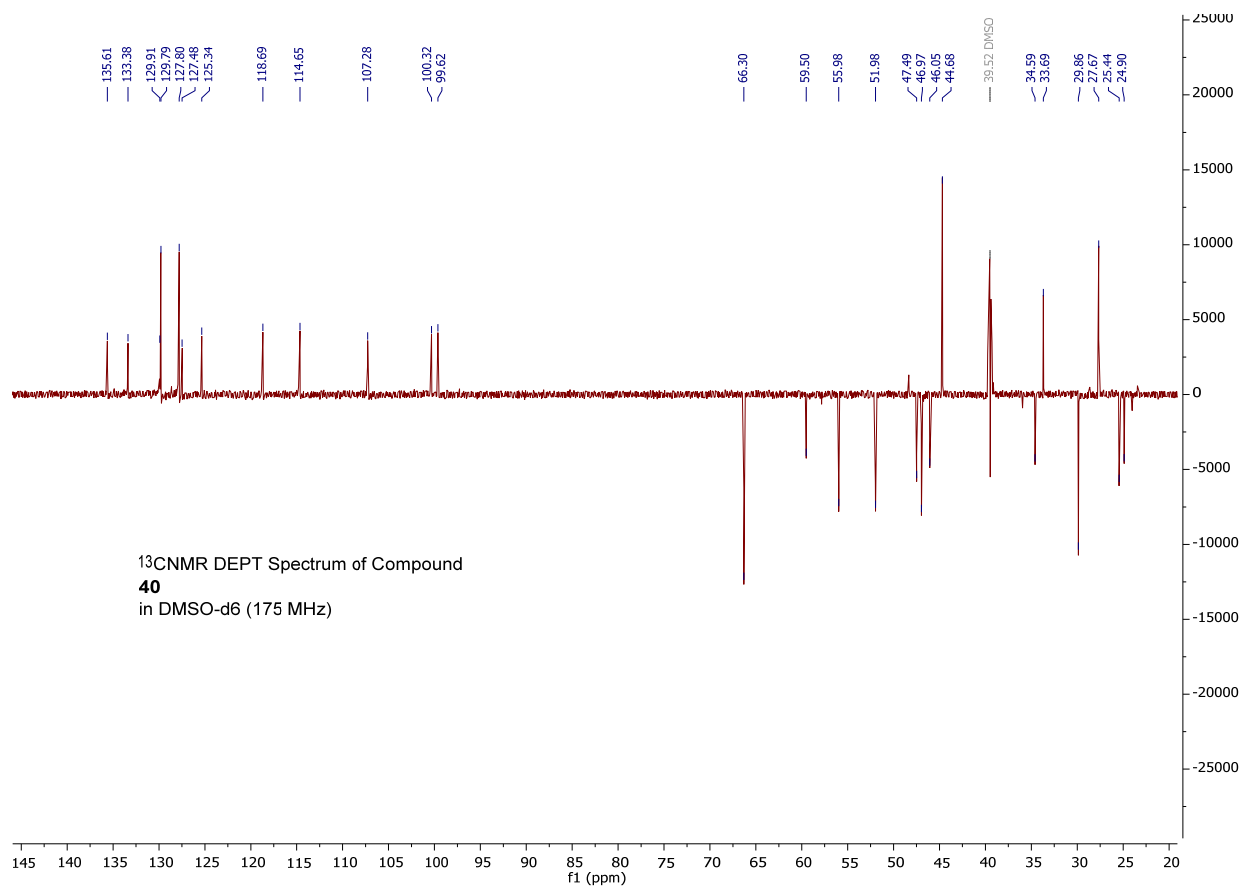


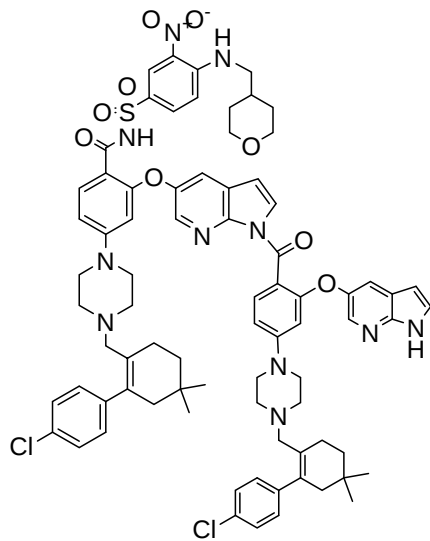
Chemical Formula: $C_{50}H_{62}ClN_9O_6S$
Exact Mass: 951.42











41

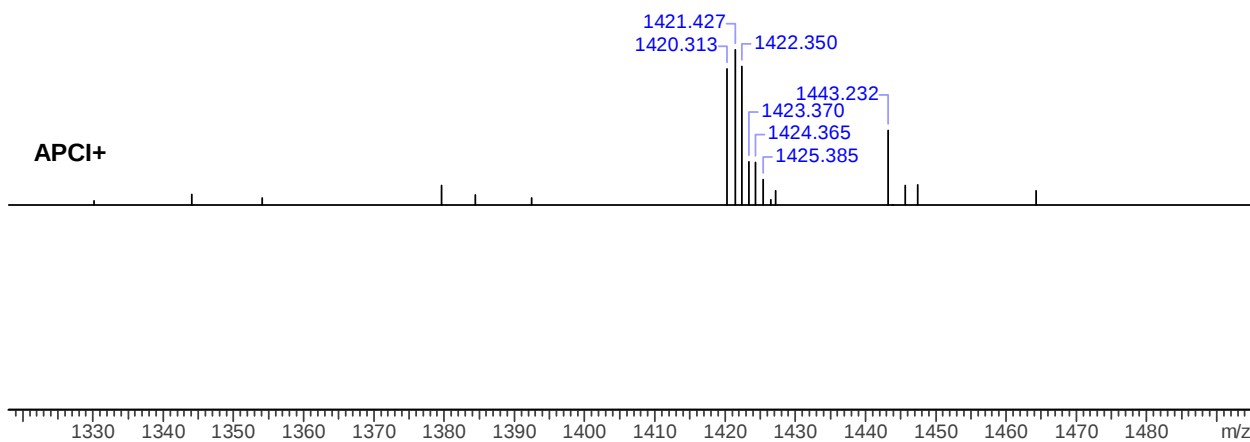
Chemical Formula: $C_{78}H_{83}Cl_2N_{11}O_9S$

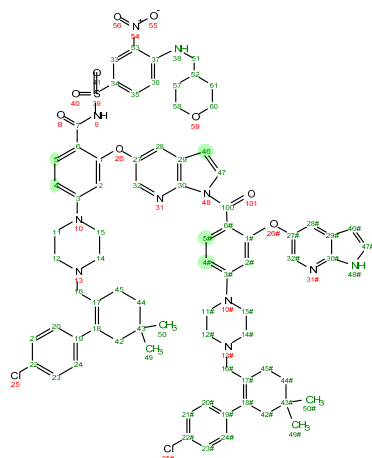
Exact Mass: 1419.55

Retention Time: 26.741

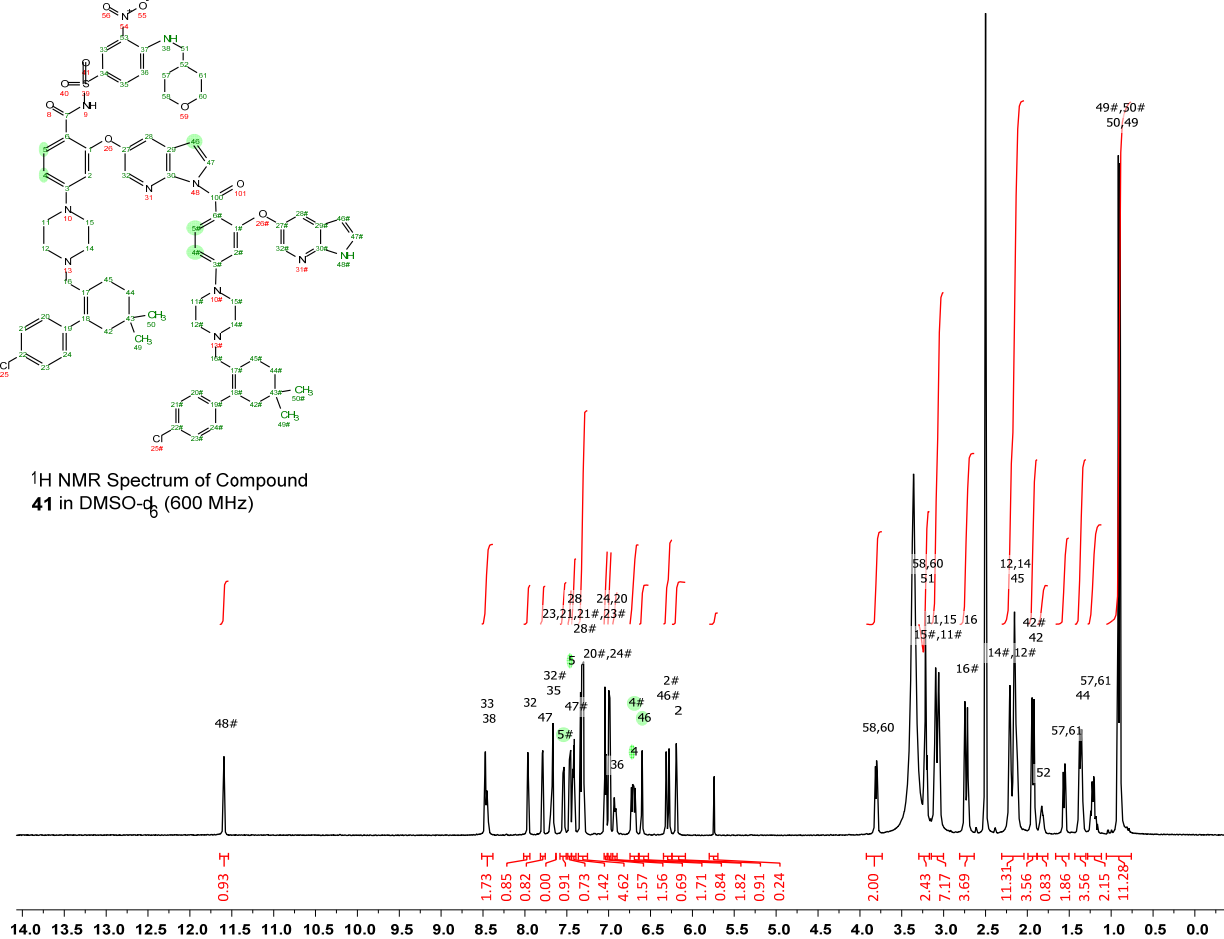
Ion Mode: APCI+

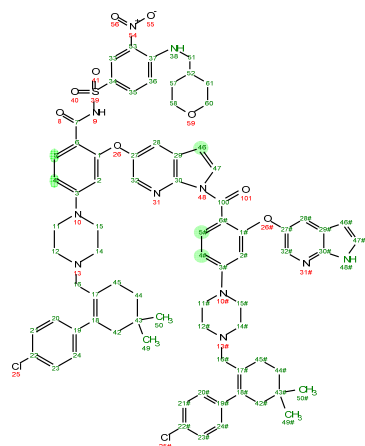
APCI LCMS Spectrum of Compound **41**





¹H NMR Spectrum of Compound 41 in DMSO-*d*₆ (600 MHz)





^{13}C NMR Spectrum of Compound
41 in $\text{DMSO}-d_6$ (150 MHz)

