

Supplementary Materials: Synthesis and Biological Evaluation of a Fluorine-18-Labeled COX Inhibitor [¹⁸F]Fluorooctyl Fenbufen Amide for Imaging of Brain Tumors

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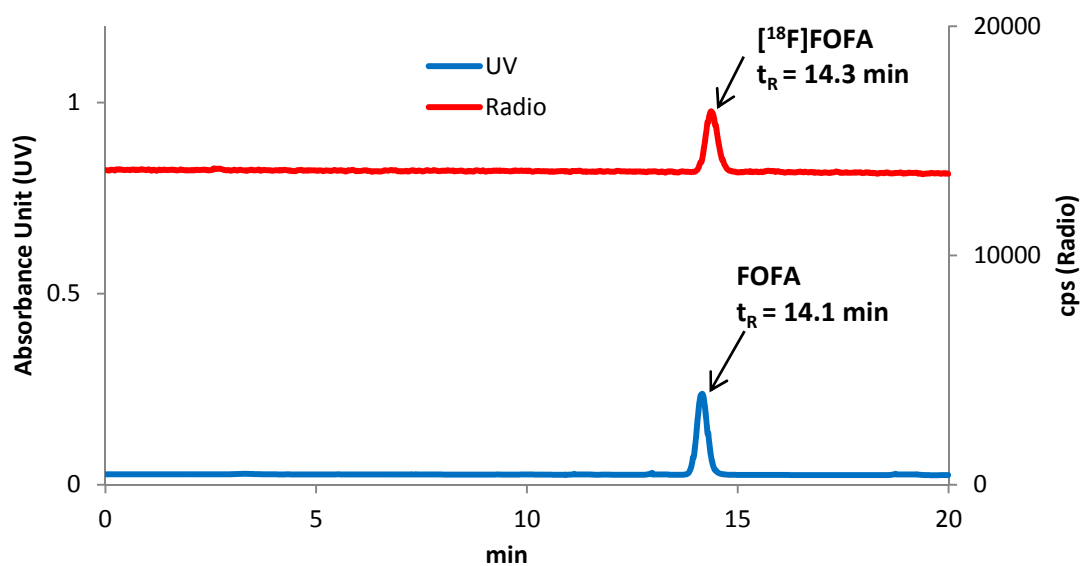


Figure S1. The HPLC chromatogram of the purified [¹⁸F]FOFA{[¹⁸F]-1} along with the authentic sample FOFA 1 for purity assessment using semipreparative RP-HPLC. The injection contained a radioactivity of 40 uCi mixed with a concentration of 0.02 mg/0.2 mL of FOFA 1.

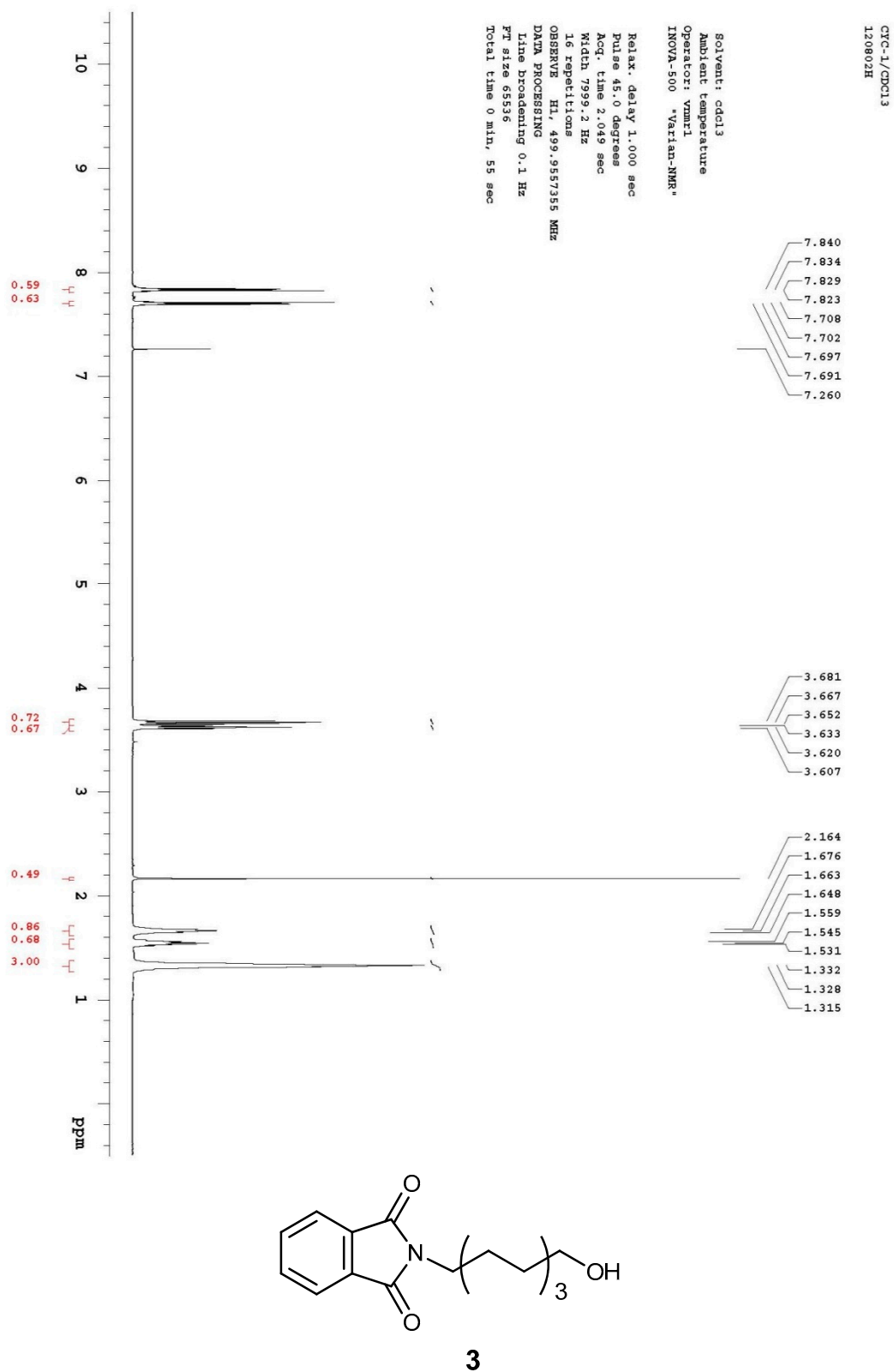


Figure S2. ¹H-NMR of 2-(8-Hydroxyoctyl)isoindoline-1,3-dione **3**.

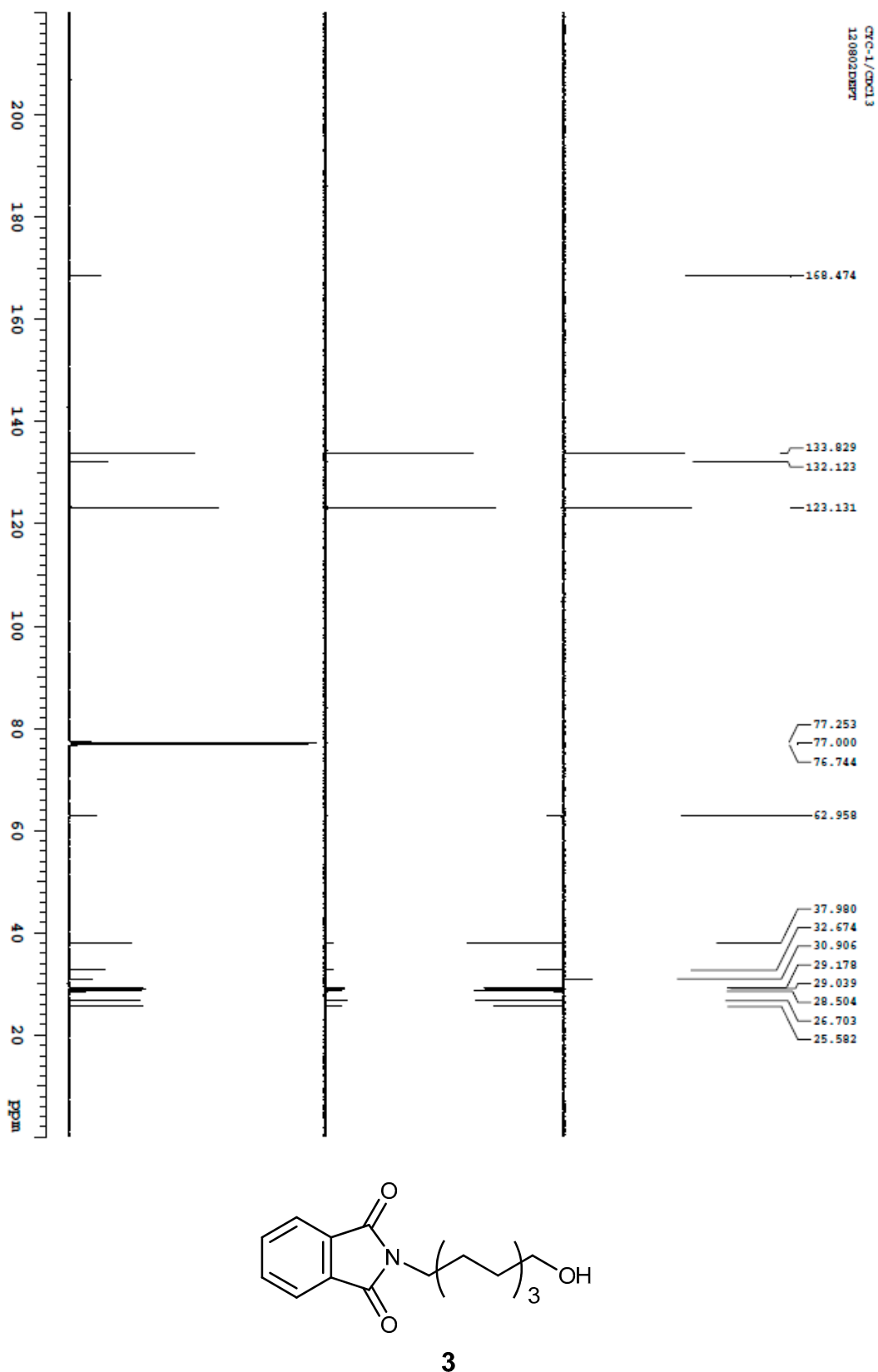


Figure S3. ¹³C-DEPT of 2-(8-Hydroxyoctyl)isoindoline-1,3-dione 3.

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元素分析儀Heraeus CHN-O Rapid 服務報告

姓名: 張育嘉

單位: 清大醫環俞鑑山LAB

收件日: 102.6.25

完成日: 102.6.26

實測值:

樣品名	CYC-1	CYC-1						
N%	5.36	5.44						
C%	69.46	69.48						
H%	7.81	8.11						

樣品名								
N%								
C%								
H%								

推測值:

樣品名	CYC-1							
N%	5.09							
C%	69.79							
H%	7.69							

所使用之標準品: Acetanilide

	理論值	測出值
N%	10.36	10.33
C%	71.09	70.89
H%	6.71	6.66

備註:

儀器負責人簽章: 謝育容

技術員簽章: 技士李慈明

Figure S4. Elemental analysis of 2-(8-Hydroxyoctyl)isoindoline-1,3-dione 3.

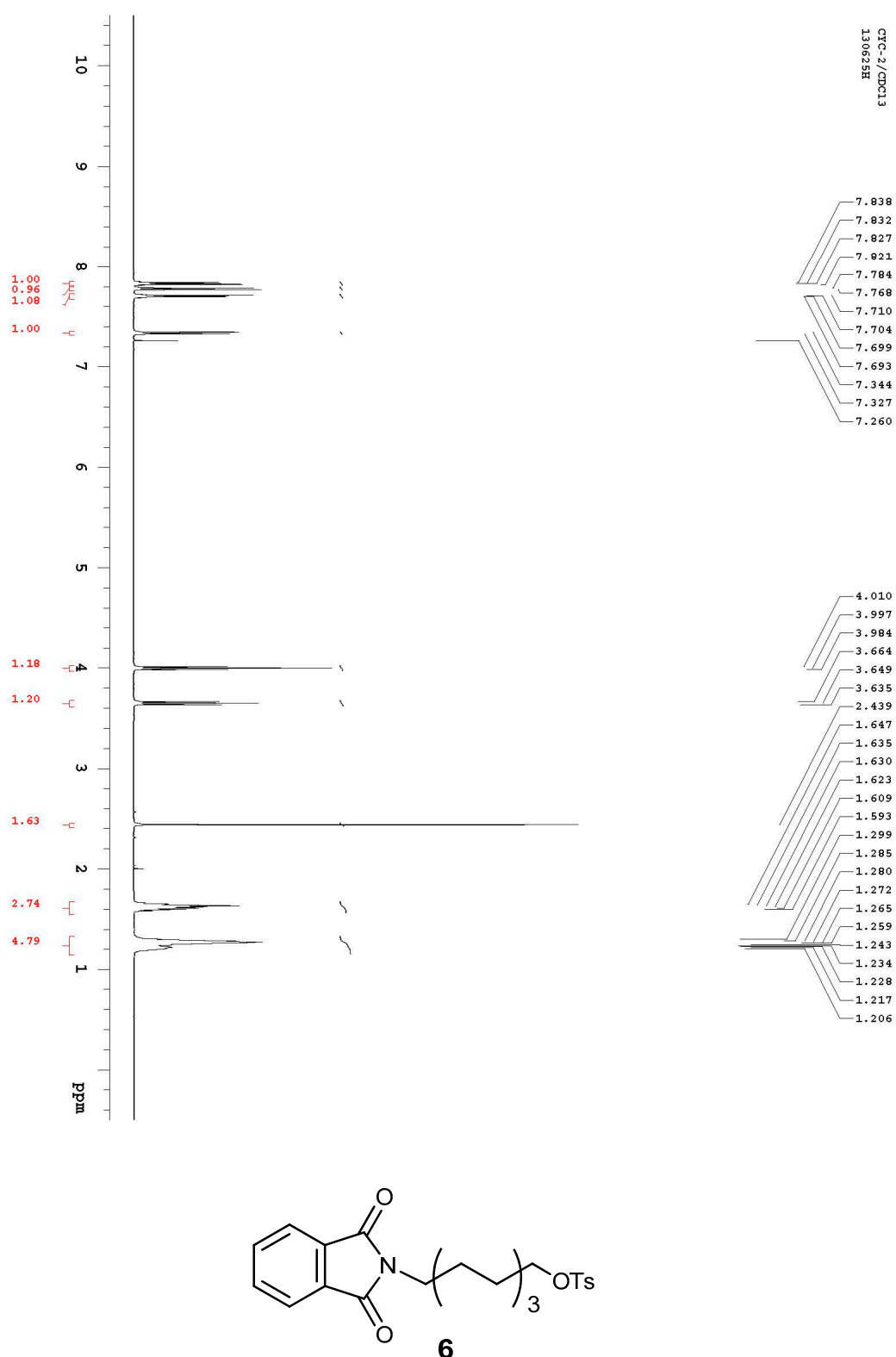


Figure S5. ¹H-NMR of 8-(1,3-Dioxoisindolin-2-yl)octyl 4-methylbenzenesulfonate **6**.

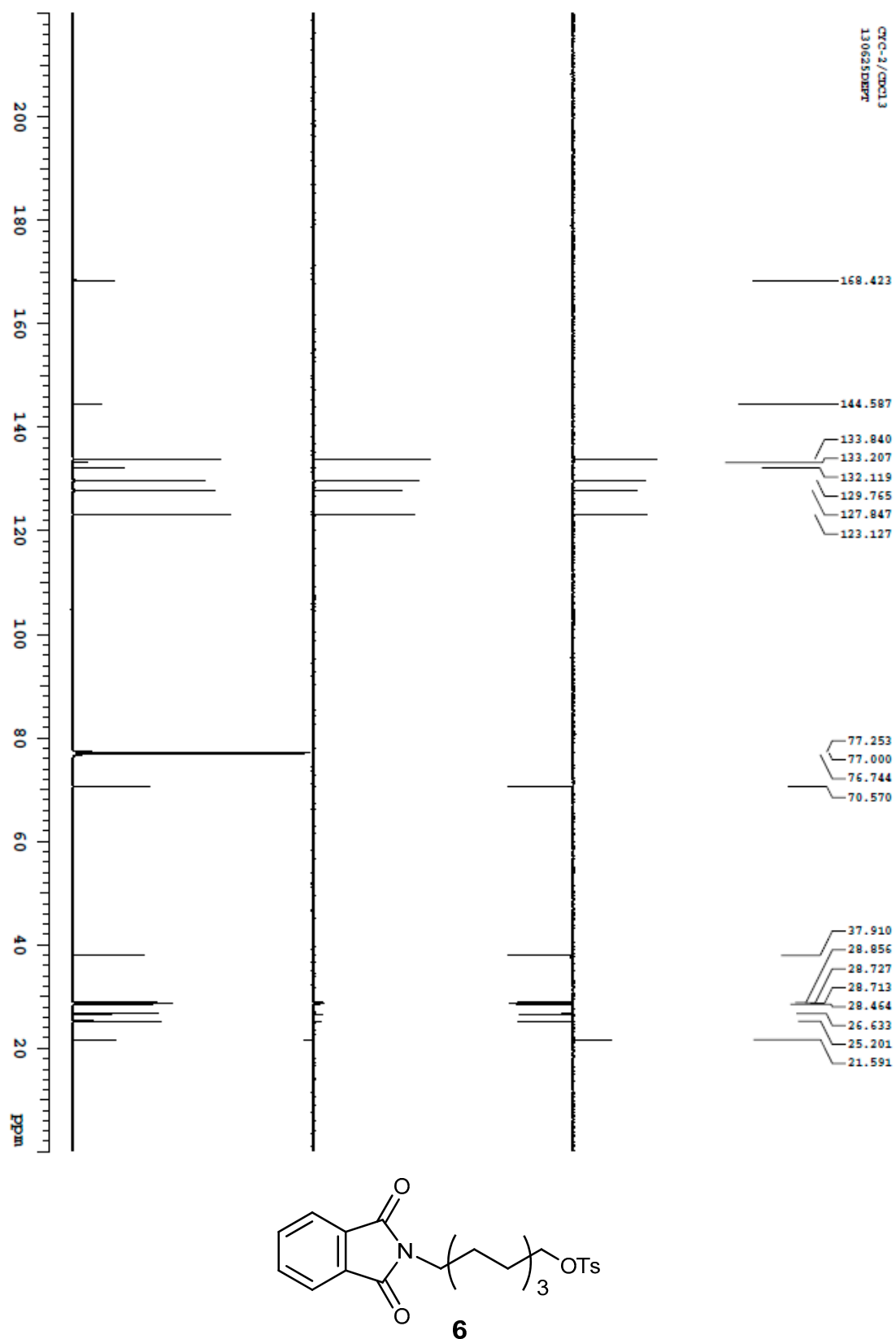


Figure S6. ¹³C-DEPT of 8-(1,3-Dioxisoindolin-2-yl)octyl 4-methylbenzenesulfonate 6.

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實測值:

樣品名	CYC-2	CYC-2						
N%	3.40	3.51						
C%	64.32	64.24						
H%	6.33	5.99						

樣品名								
N%								
C%								
H%								

推測值:

樣品名	CYC-2							
N%	3.26							
C%	64.31							
H%	6.34							

所使用之標準品: Acetanilide

	理論值	測出值
N%	10.36	10.33
C%	71.09	70.89
H%	6.71	6.66

備註:

儀器負責人簽章: 張育嘉

技術員簽章: 技士李慈明

Figure S7. Elemental analysis of 8-(1,3-Dioxoisindolin-2-yl)octyl 4-methylbenzenesulfonate 6.

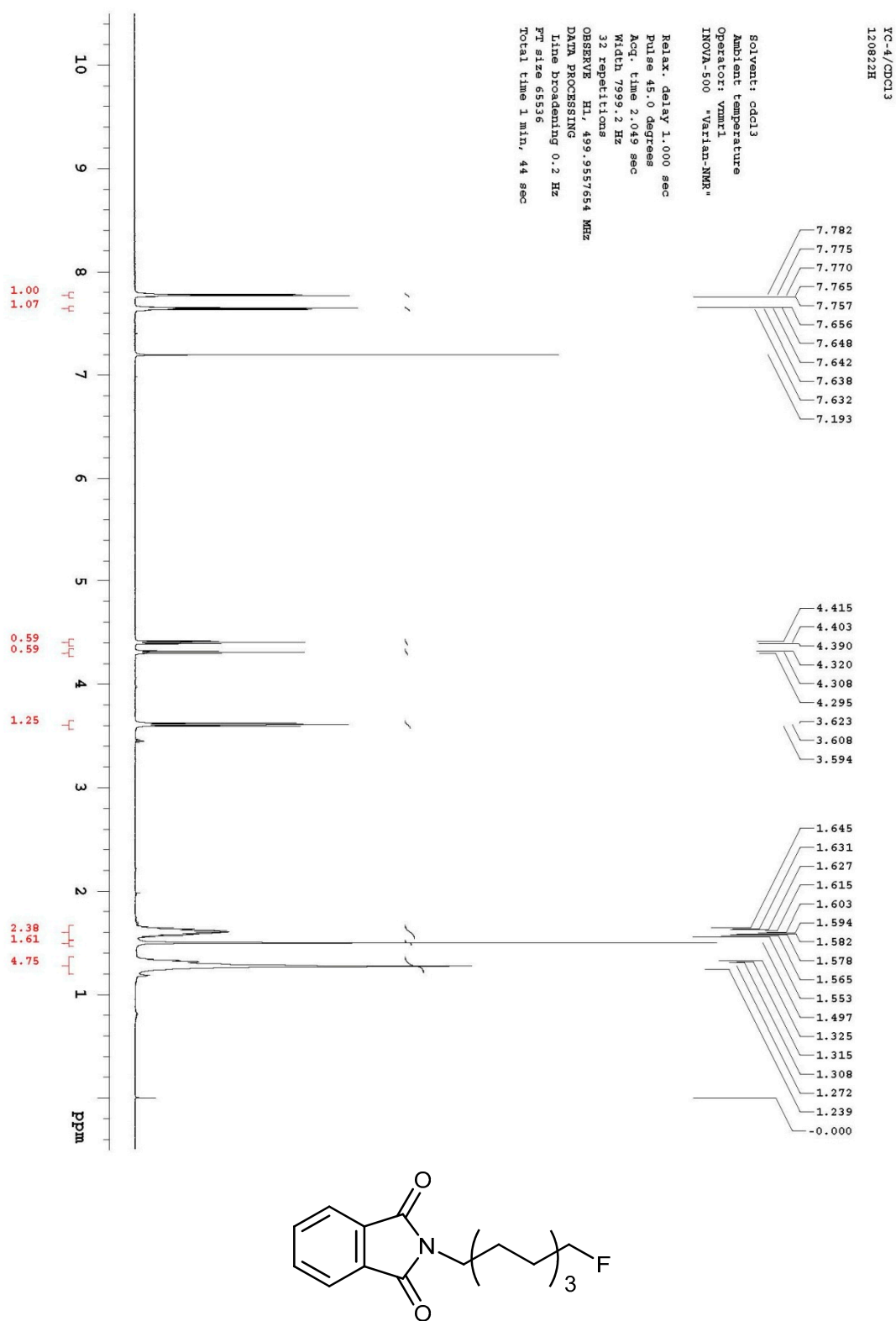
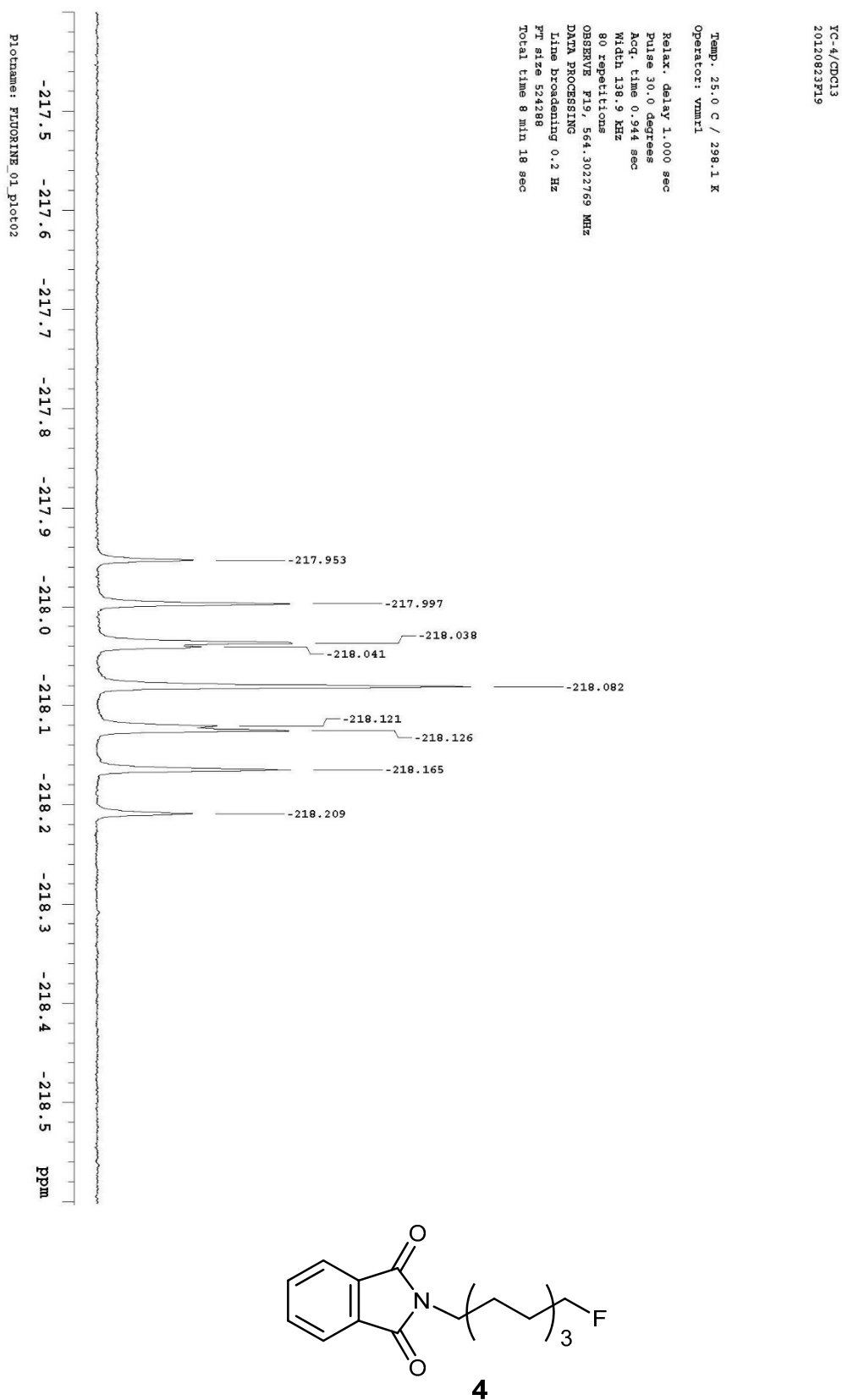


Figure S8. ¹H-NMR of 2-(8-Fluorooctyl)isoindoline-1,3-dione **4**.

Figure S10. ¹⁹F-NMR of 2-(8-Fluorooctyl)isoindoline-1,3-dione **4**.

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實測值:

樣品名	CYC-4	CYC-4						
N%	5.37	5.40						
C%	69.27	69.35						
H%	7.34	7.31						

樣品名								
N%								
C%								
H%								

推測值:

樣品名	CYC-4							
N%	5.05							
C%	69.29							
H%	7.27							

所使用之標準品: Acetanilide

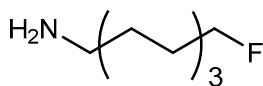
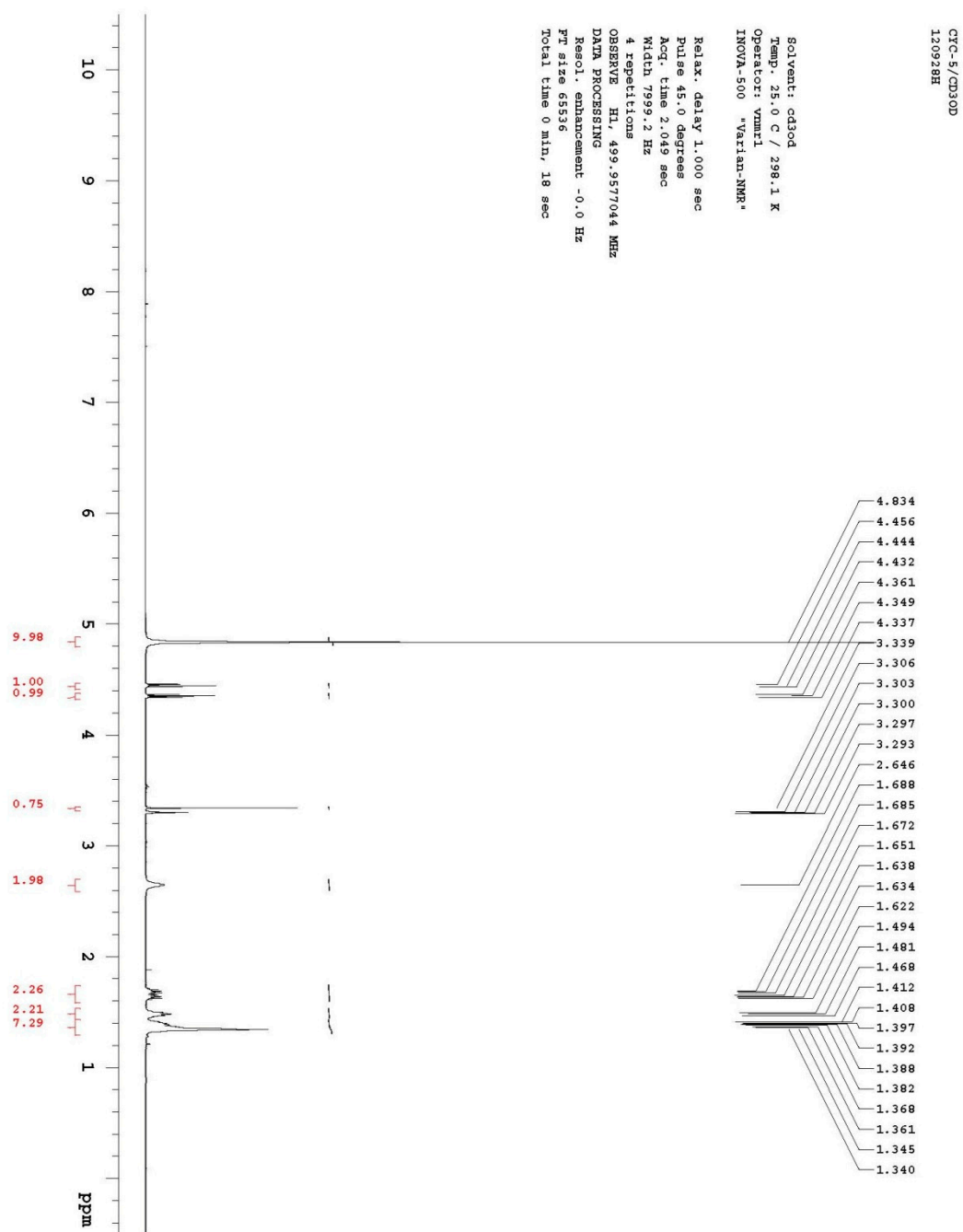
	理論值	測出值
N%	10.36	10.33
C%	71.09	70.89
H%	6.71	6.66

備註:

儀器負責人簽章: 謝育嘉

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Figure S11. Elemental analysis of 2-(8-Fluorooctyl)isoindoline-1,3-dione **4**.

**5**Figure S12. ¹H-NMR of 8-Fluorooctan-1-amine 5.

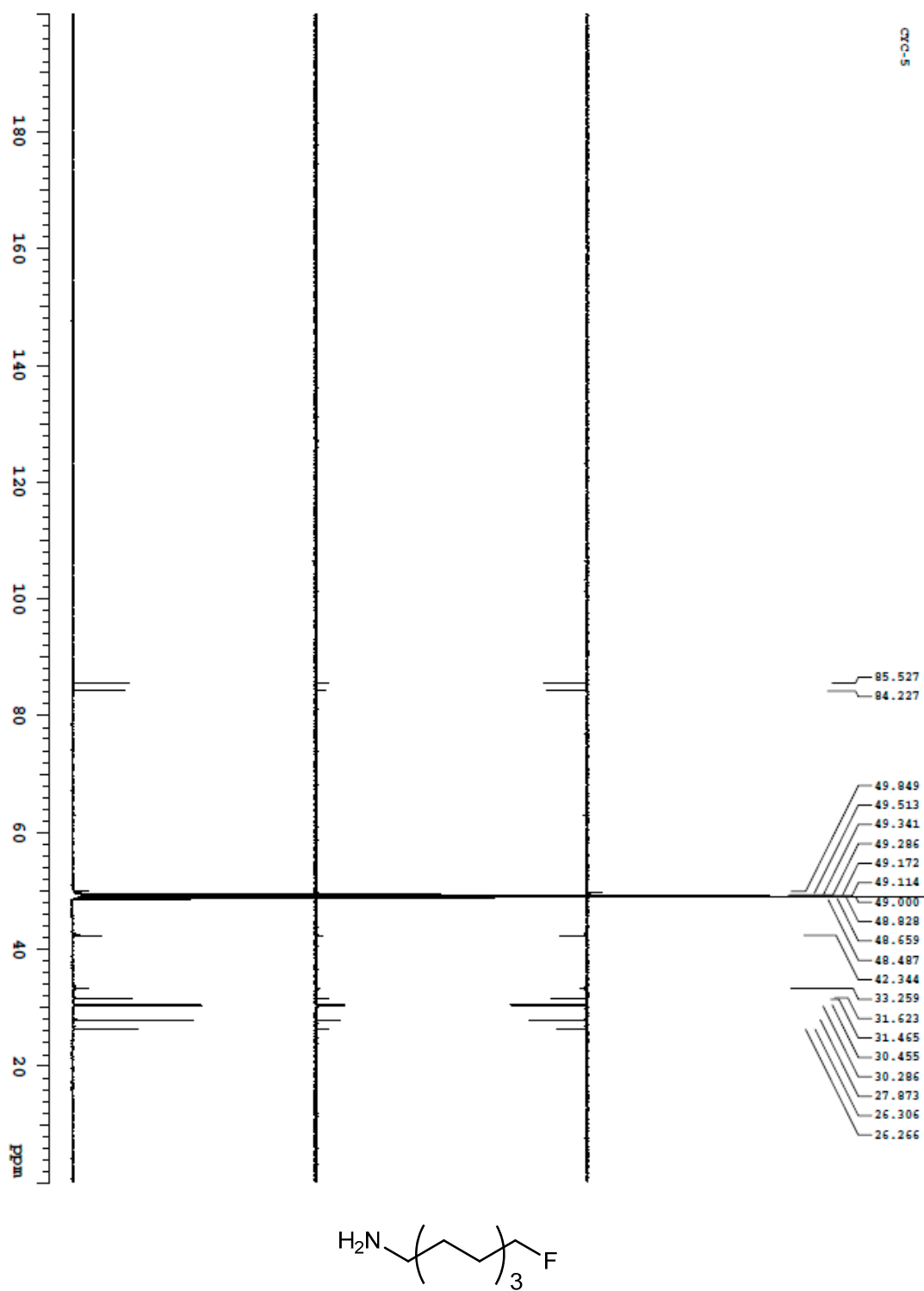


Figure S13. ^{13}C -DEPT of 8-Fluorooctan-1-amine 5.

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收件日: 102.6.25

完成日: 102.6.26

實測值:

樣品名	CYC-5	CYC-5						
N%	9.72	9.68						
C%	65.52	65.16						
H%	12.14	12.16						

樣品名								
N%								
C%								
H%								

推測值:

樣品名	CYC-5							
N%	9.51							
C%	65.26							
H%	12.32							

所使用之標準品: Acetanilide

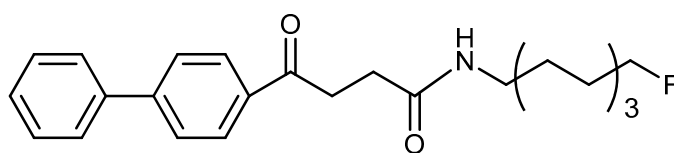
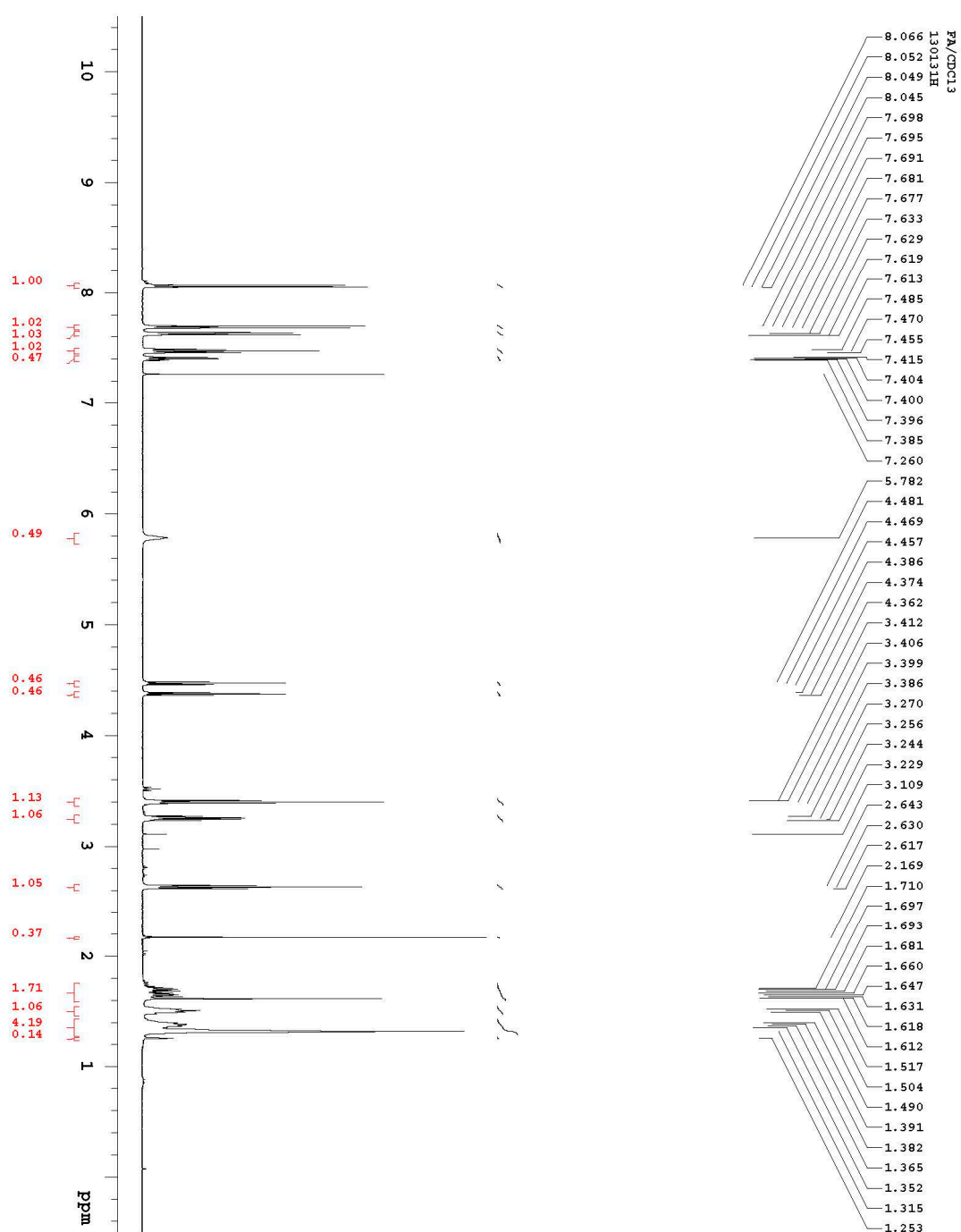
	理論值	測出值
N%	10.36	10.33
C%	71.09	70.89
H%	6.71	6.66

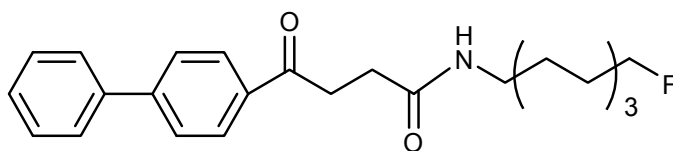
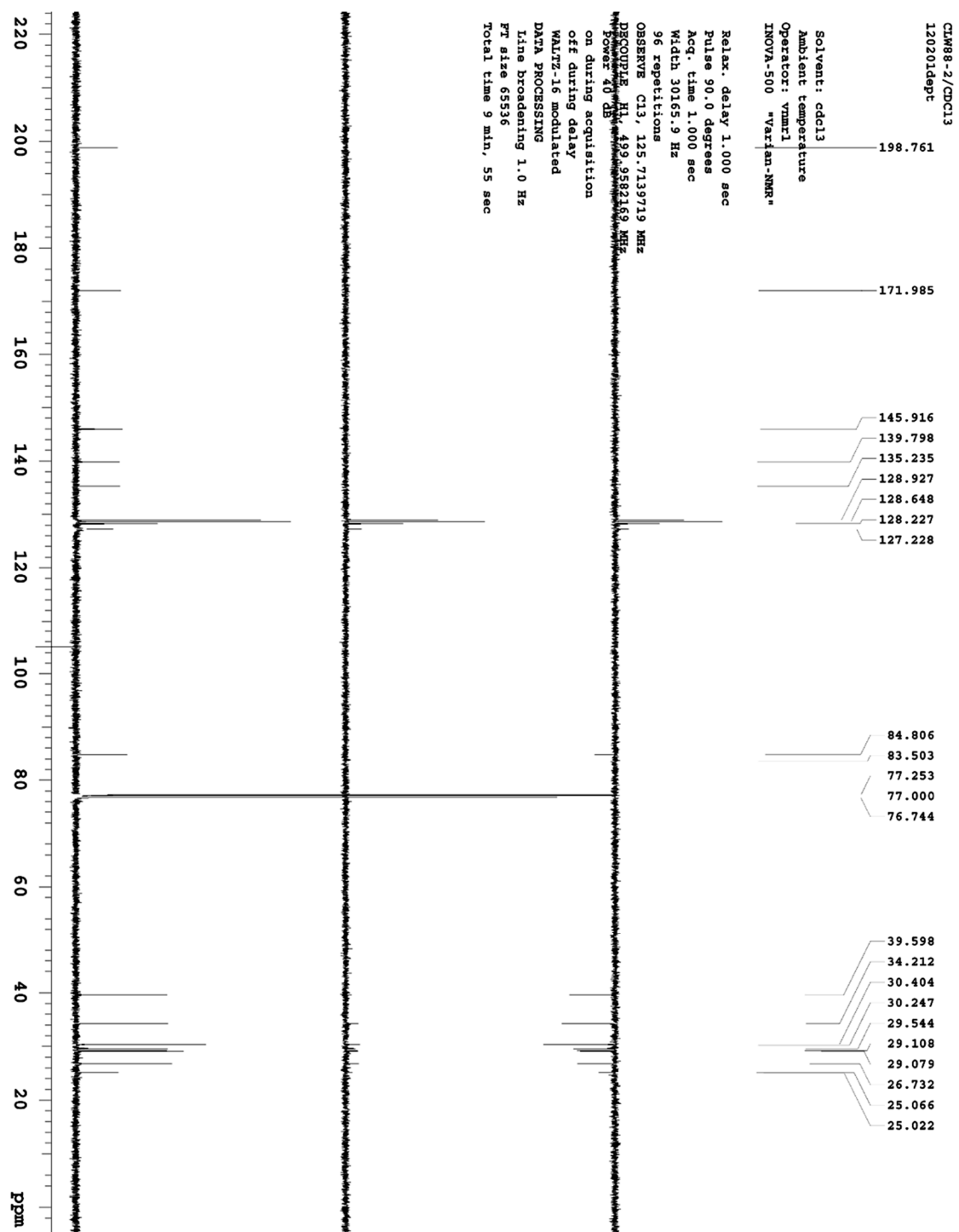
備註:

儀器負責人簽章: 謝育嘉

技術員簽章: 技士李茲明

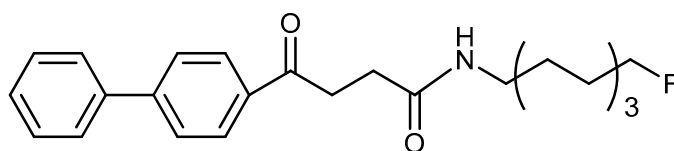
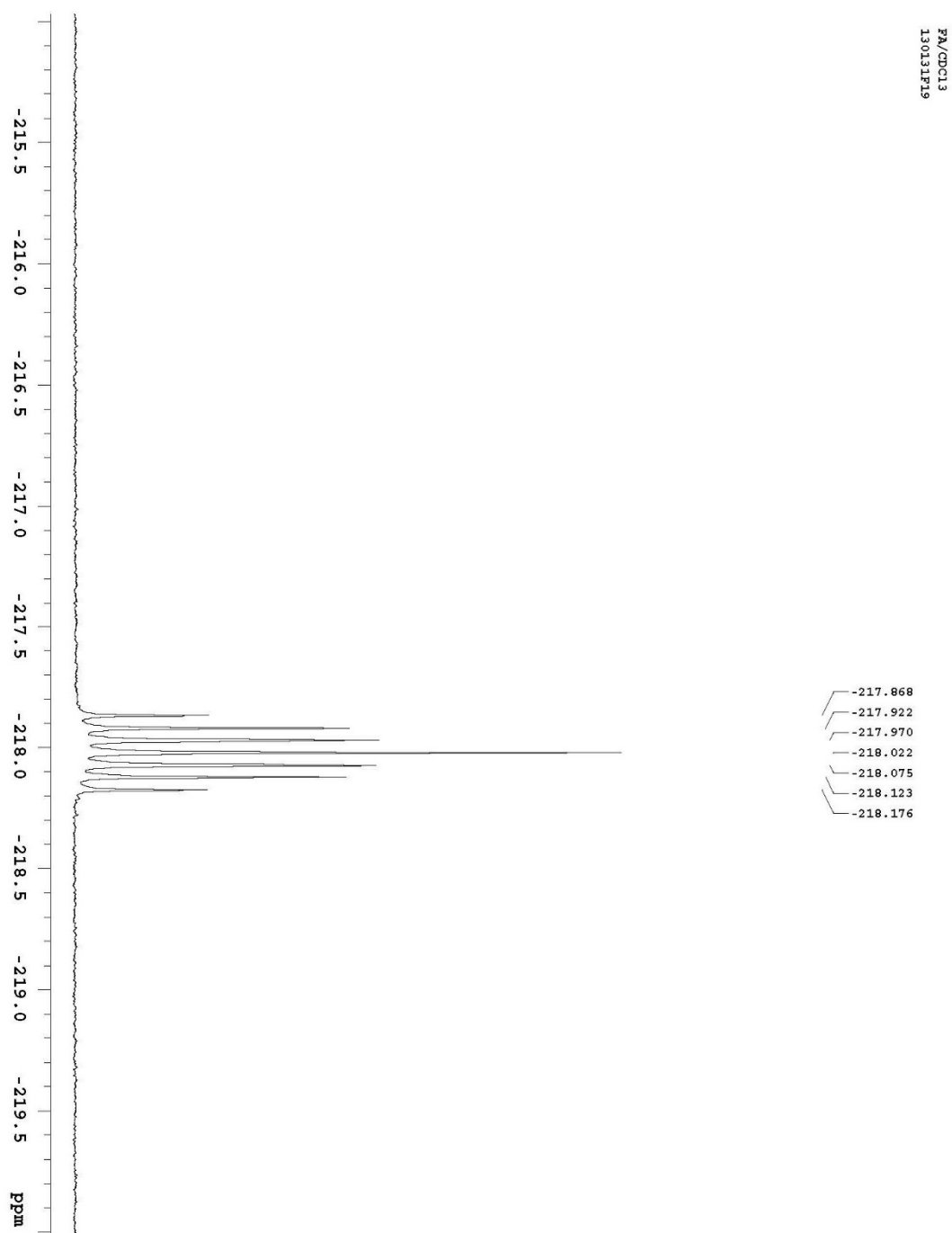
Figure S14. Elemental analysis of 8-Fluorooctan-1-amine 5.

**FOFA, 1****Figure S16.** ¹H-NMR of 8-Fluorooctyl fenbufen amide 1.



FOFA, 1

Figure S17. ¹³C-NMR of 8-Fluorooctyl fenbufen amide 1.

**FOFA, 1****Figure S18.** ¹⁹F-NMR of 8-Fluorooctyl fenbufen amide 1.

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收件日: 102.6.25

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實測值:

樣品名	FOFA	FOFA						
N%	3.77	3.41						
C%	75.28	75.04						
H%	7.74	7.52						

樣品名								
N%								
C%								
H%								

推測值:

樣品名	FOFA							
N%	3.65							
C%	75.16							
H%	7.88							

所使用之標準品: Acetanilide

	理論值	測出值
N%	10.36	10.33
C%	71.09	70.89
H%	6.71	6.66

備註:

儀器負責人簽章: 謝育嘉

技術員簽章: 技士李慈明

Figure S19. Elemental analysis of 8-Fluorooctyl fenbufen amide 1.