

Support information

1-(Piperidin-3-yl)thymine amides as inhibitors of *M. tuberculosis* thymidylate kinase

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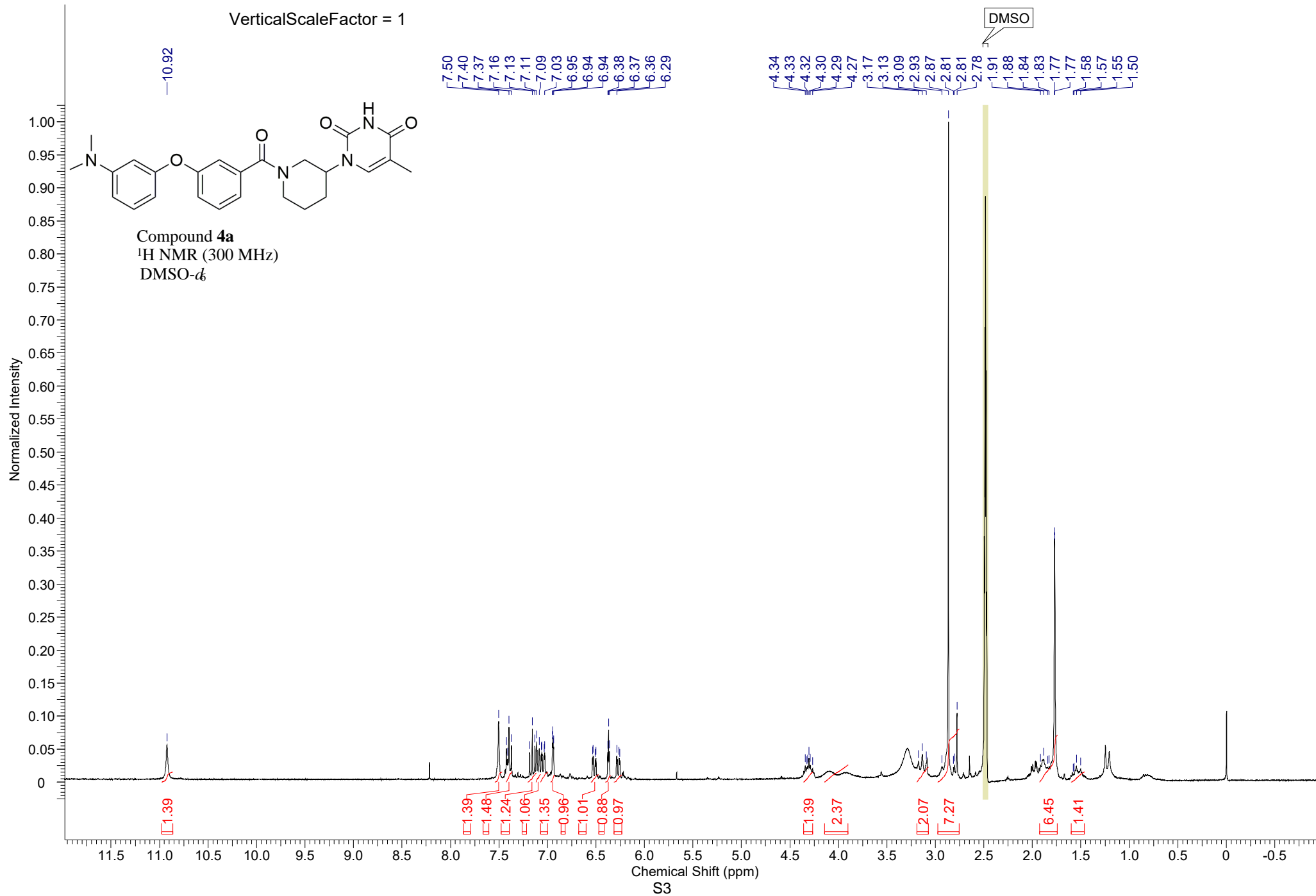
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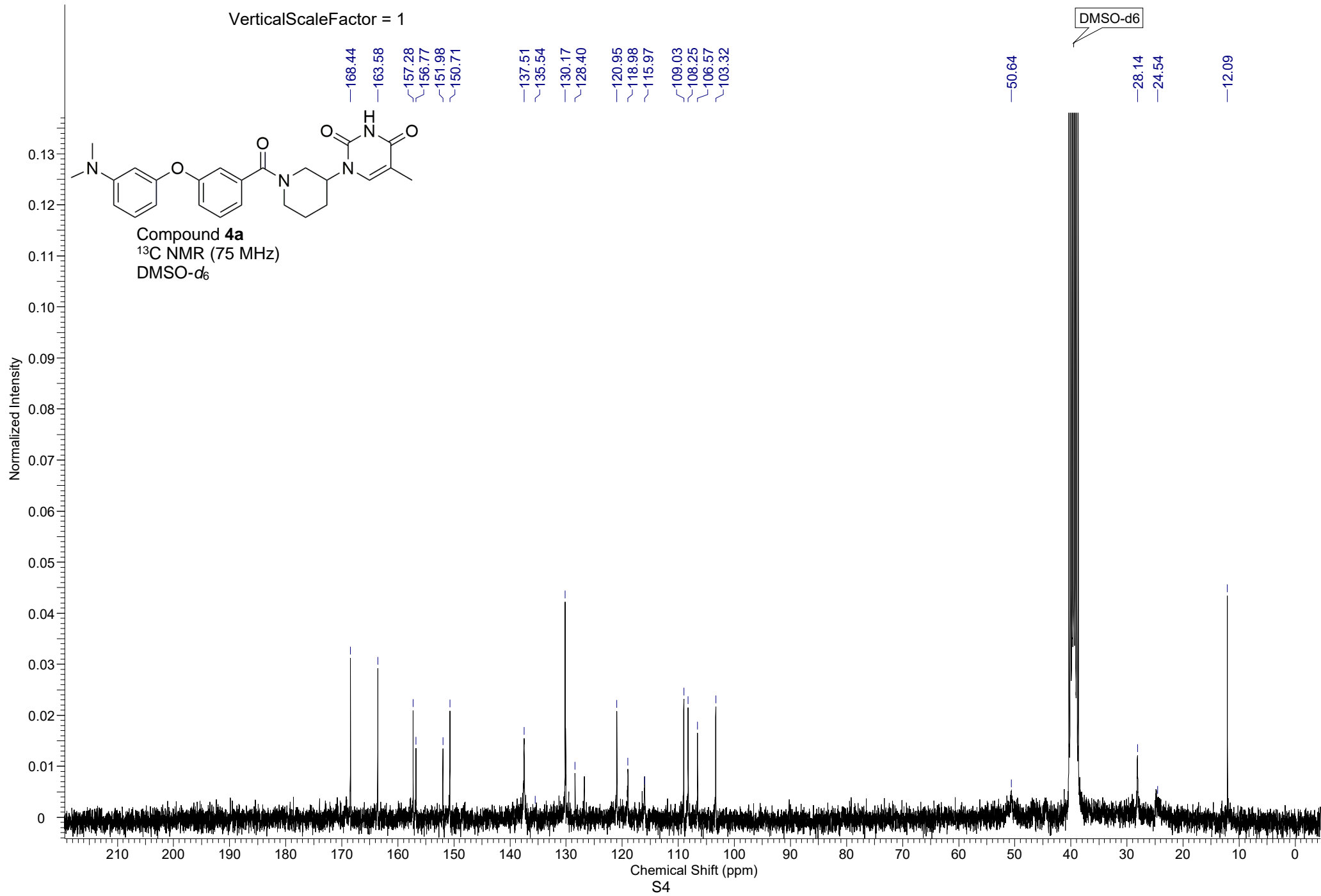
^c Laboratory for Microbiology, Parasitology and Hygiene (LMPH), Department of Pharmaceutical Sciences, University of Antwerp, Campus Drie Eiken, Universiteitsplein 1, Belgium

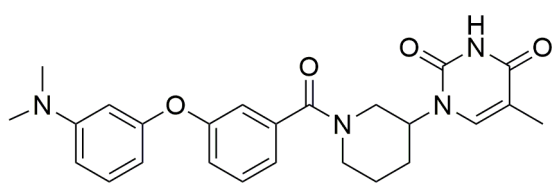
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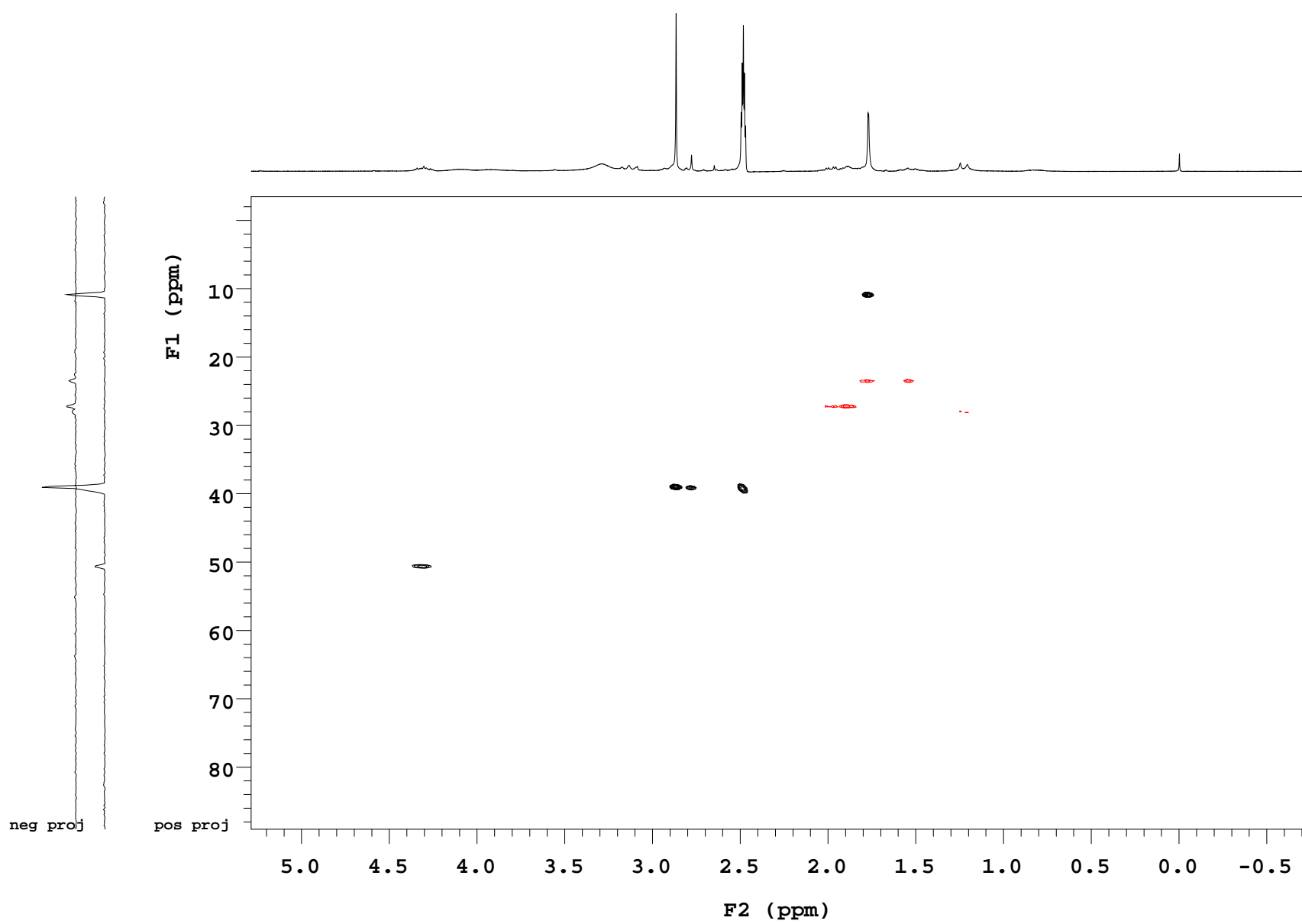
¹ H-NMR spectrum compound 4a	S3
¹³ C-NMR spectrum compound 4a	S4
HSQC spectrum compound 4a	S5
¹ H-NMR spectrum compound 4b	S6
¹³ C-NMR spectrum compound 4b	S7
HSQC spectrum compound 4b	S8
¹ H-NMR spectrum compound 4c	S9
¹³ C-NMR spectrum compound 4c	S9
¹³ C-NMR spectrum compound 4c	S10
HSQC spectrum compound 4c	S11
¹ H-NMR spectrum compound 4d	S12
¹³ C-NMR spectrum compound 4d	S13
HSQC spectrum compound 4d	S14
¹ H-NMR spectrum compound 4e	S15
¹³ C-NMR spectrum compound 4e	S16
HSQC spectrum compound 4e	S17
¹ H-NMR spectrum compound 4f	S18
¹³ C-NMR spectrum compound 4f	S19
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¹ H-NMR spectrum compound 4g	S21
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¹³ C-NMR spectrum compound 4j	S31
HSQC spectrum compound 4j	S32
¹ H-NMR spectrum compound 4k	S33
¹³ C-NMR spectrum compound 4k	S34
HSQC spectrum compound 4k	S35

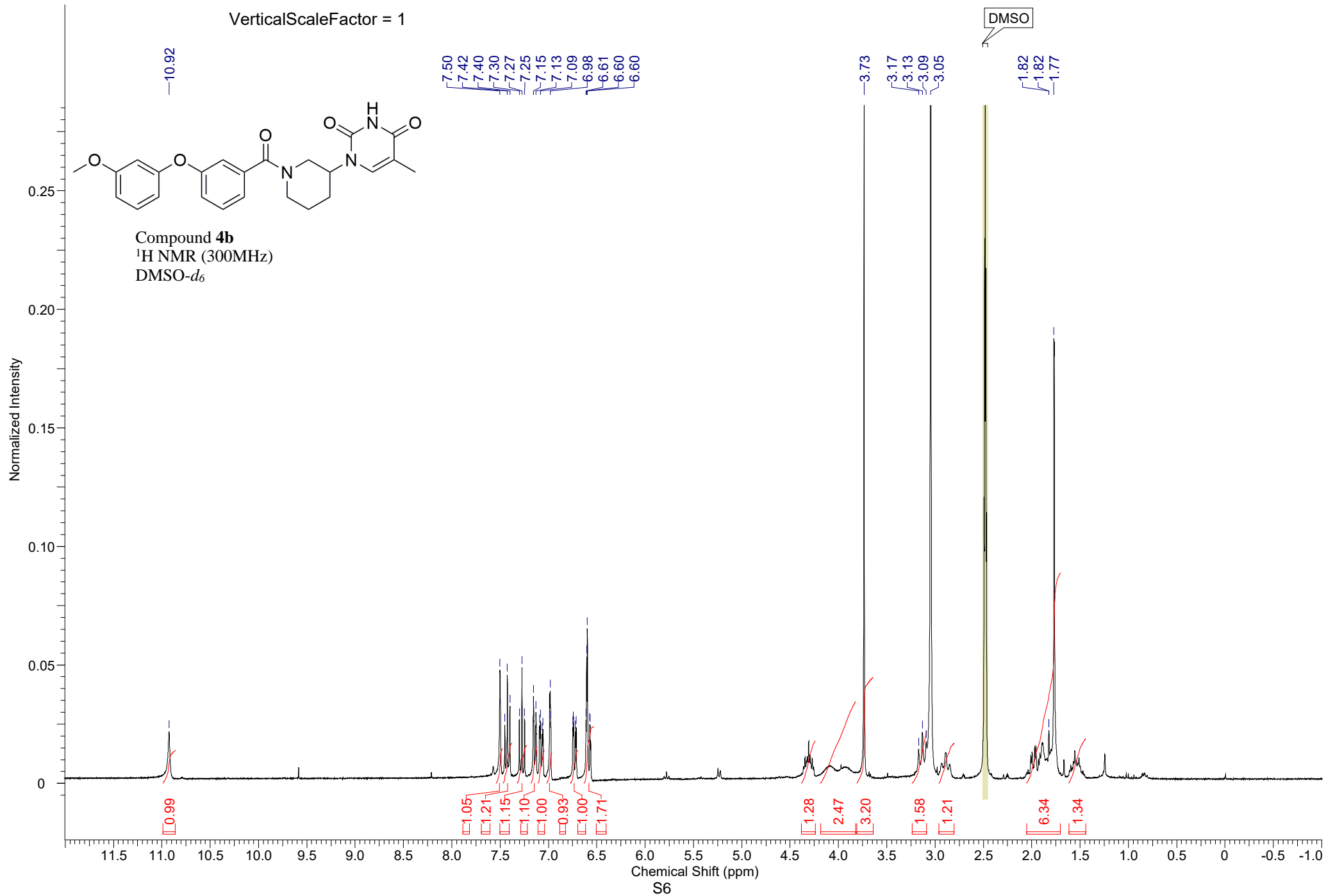


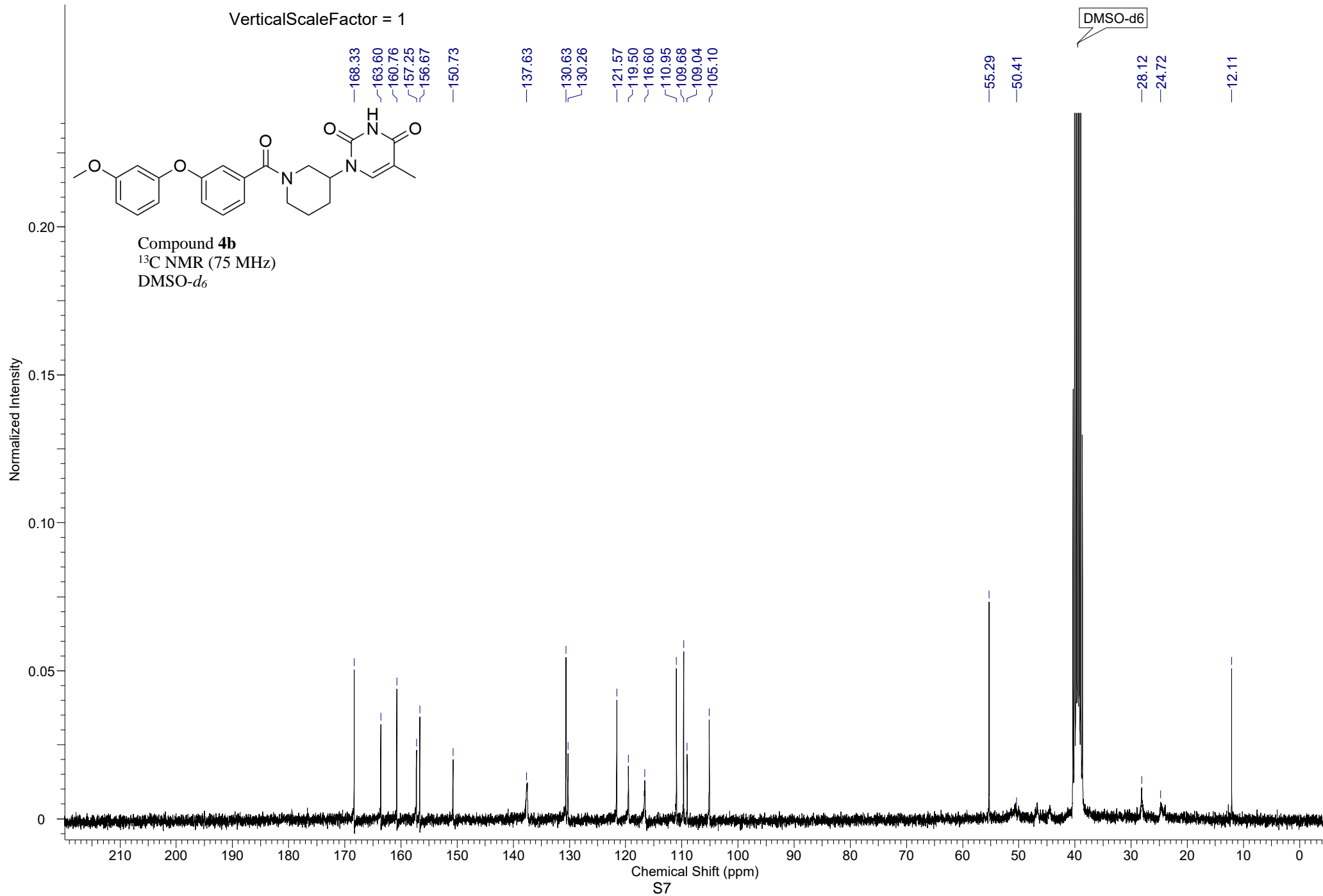


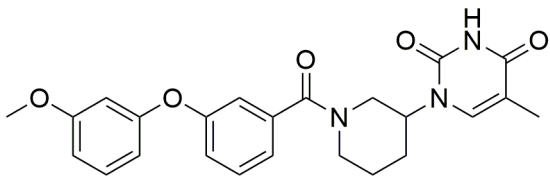


Compound **4a**
HSQC
DMSO-*d*₆

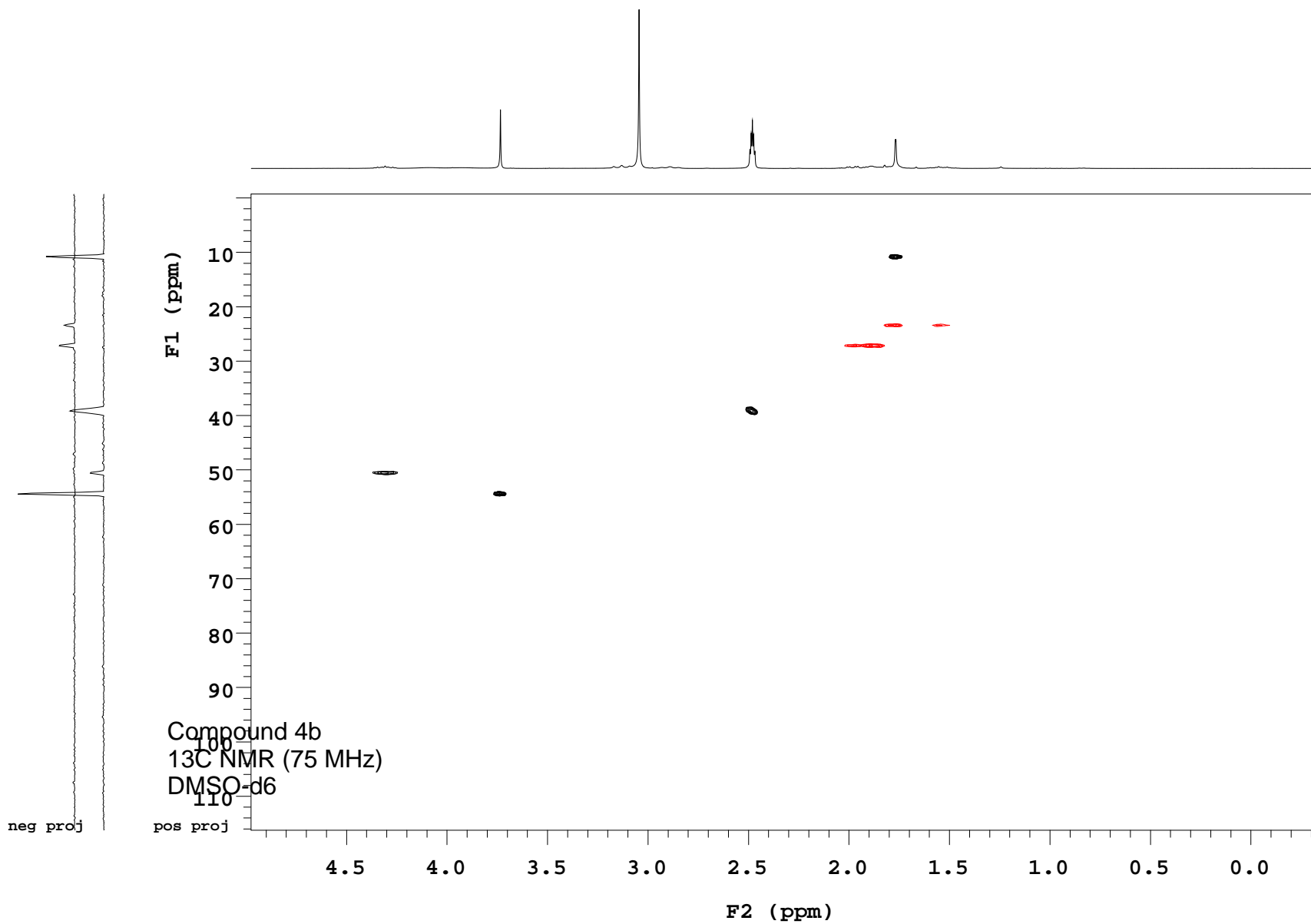




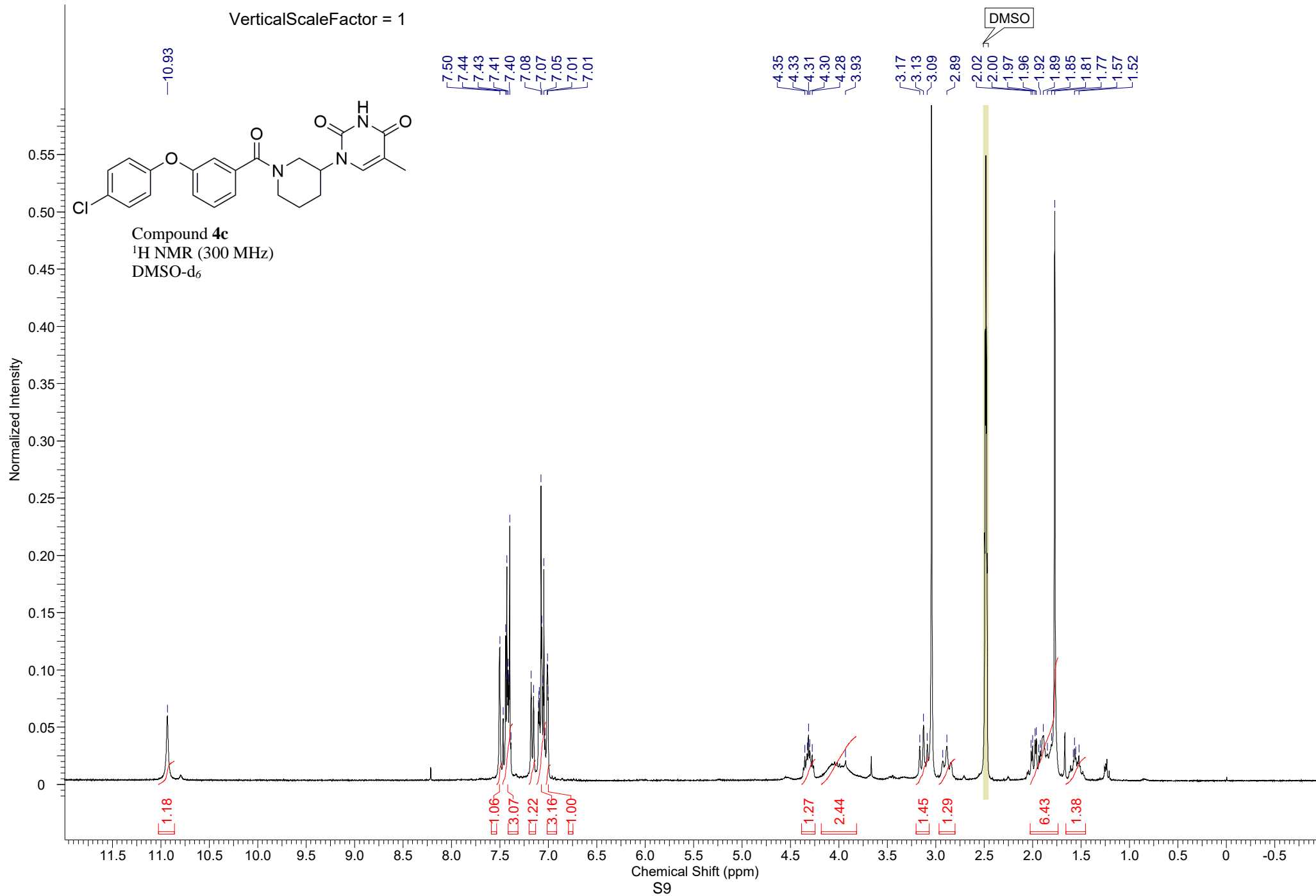


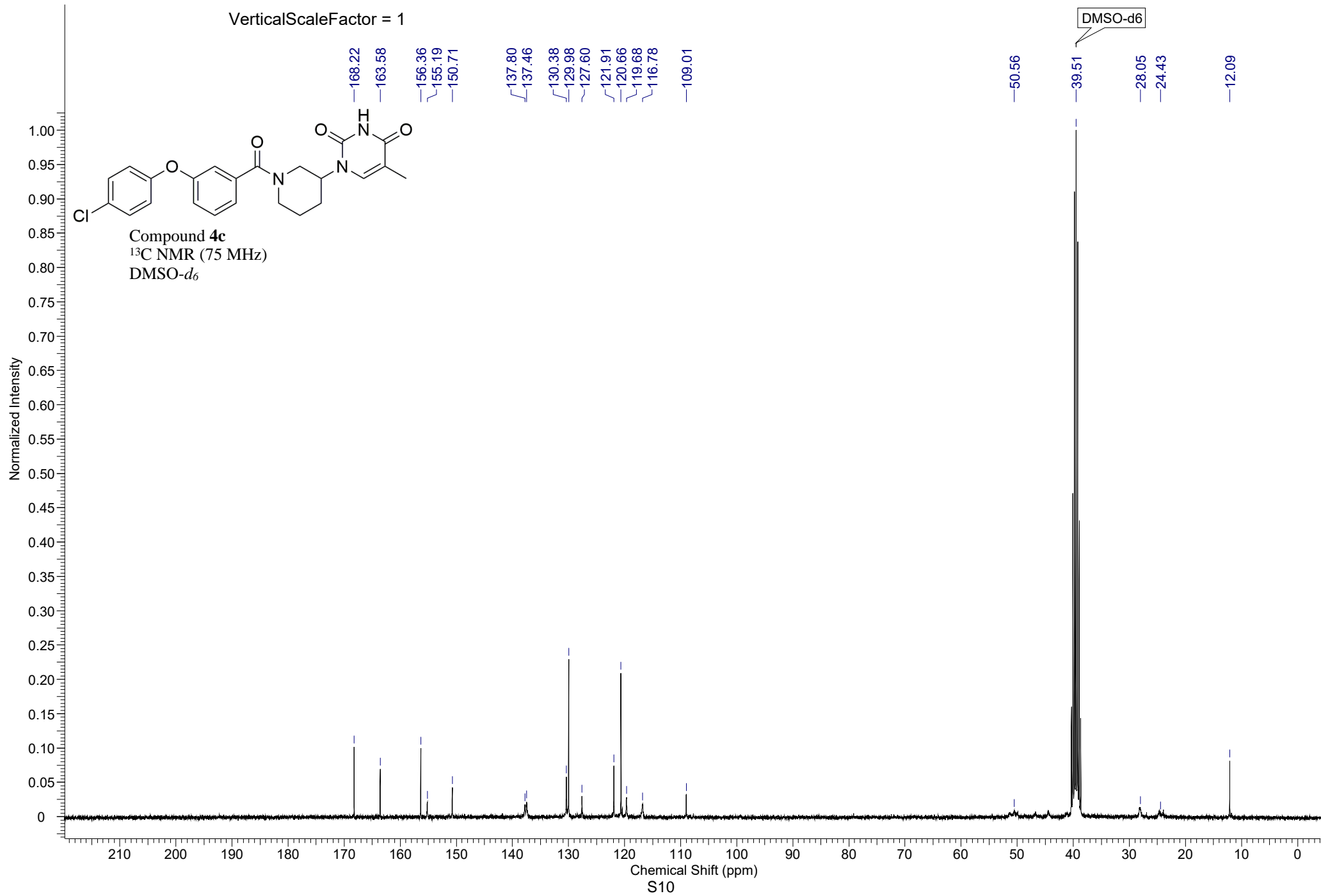


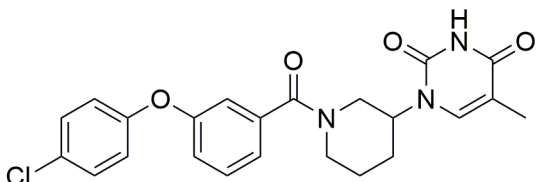
Compound **4b**
HSQC
DMSO-*d*₆



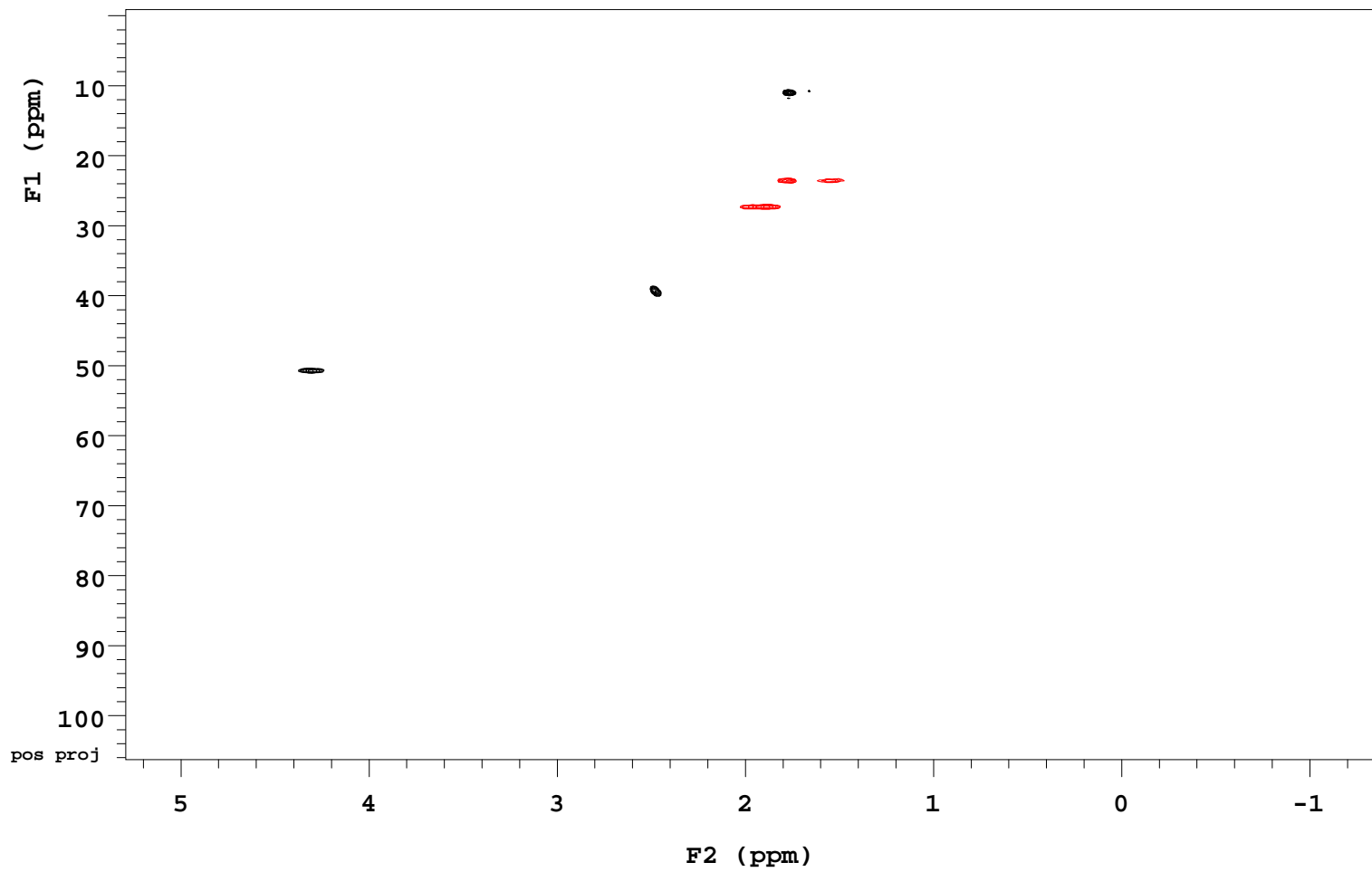
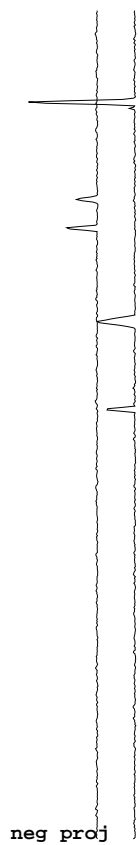
Compound 4b
13C NMR (75 MHz)
DMSO-*d*₆

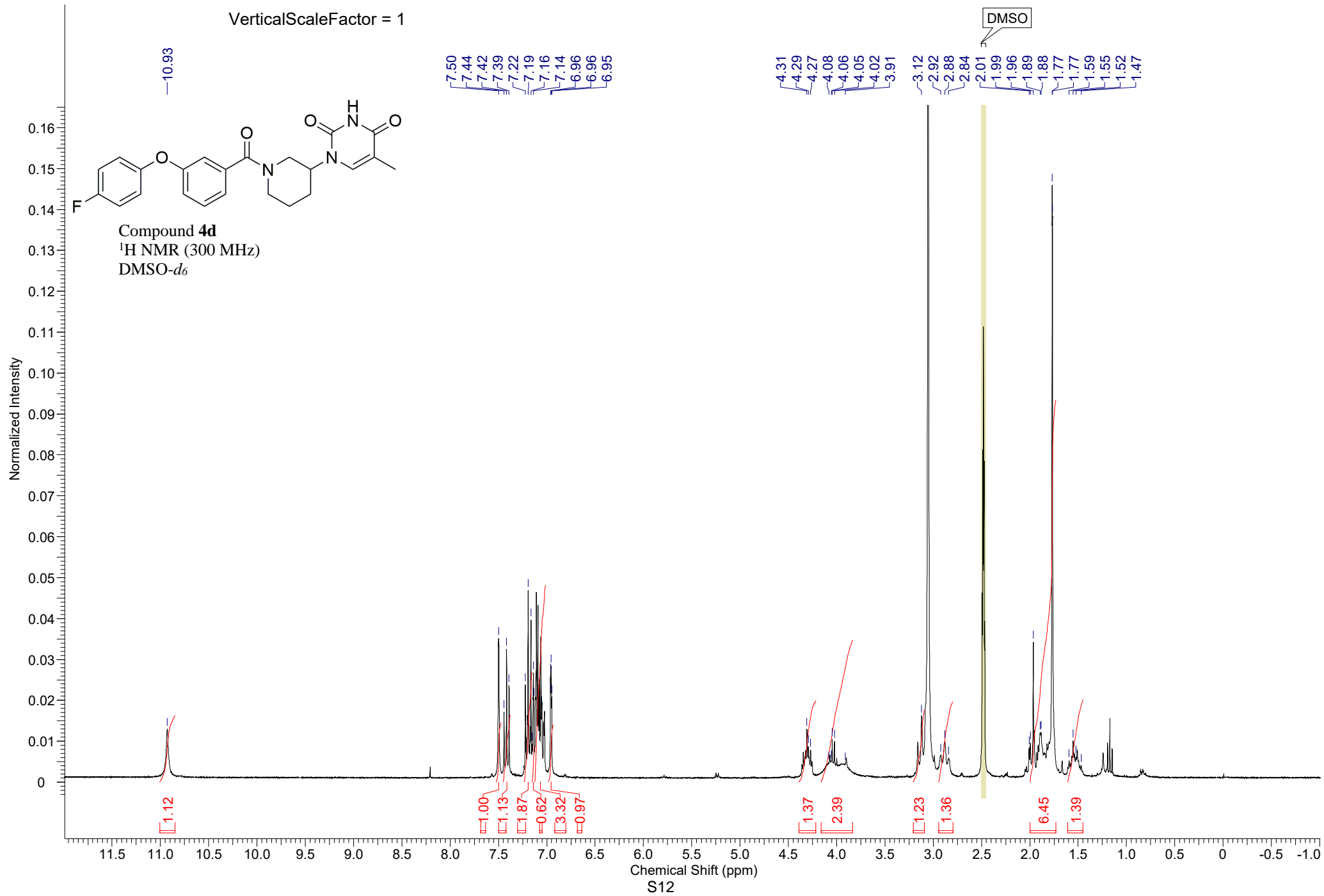


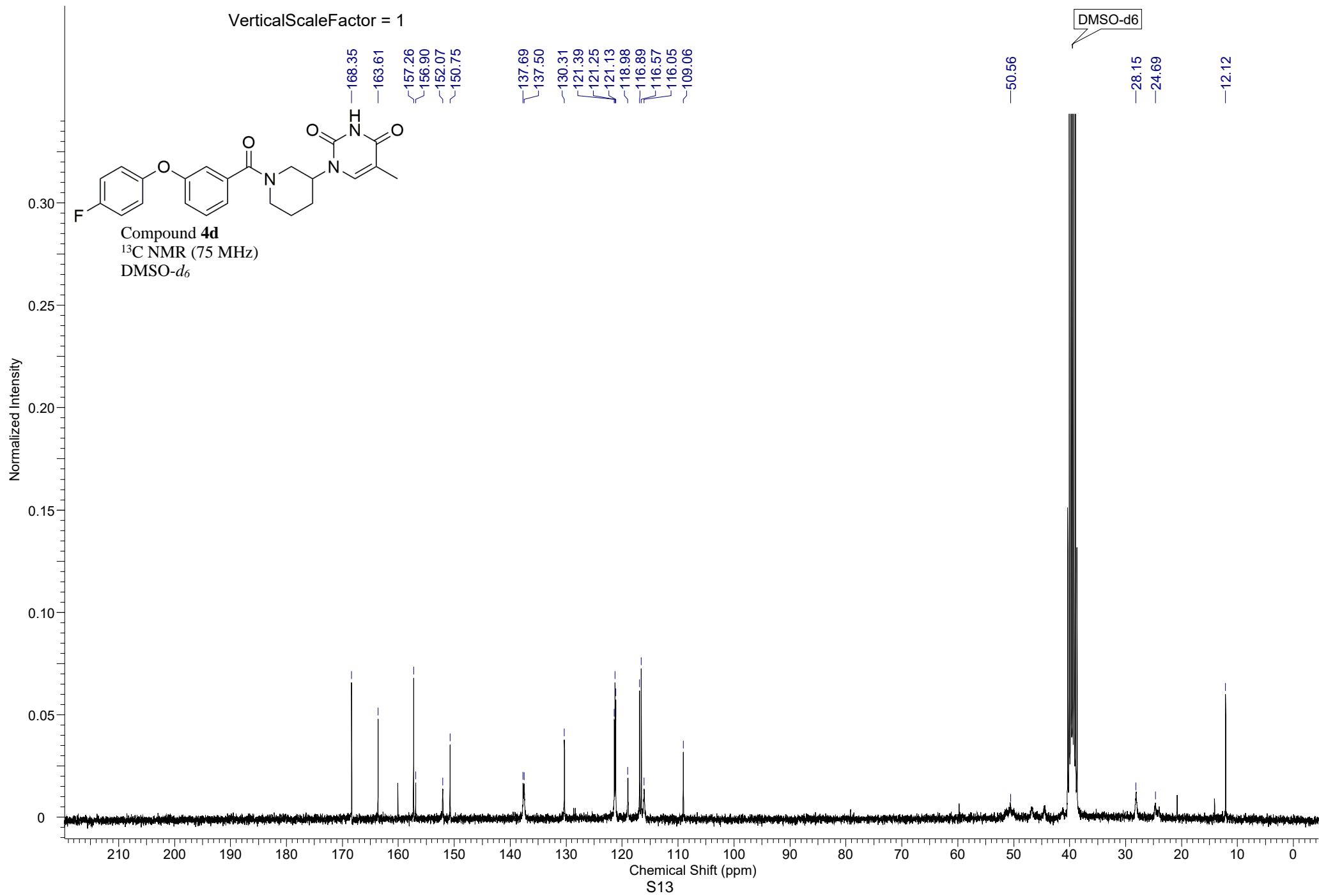


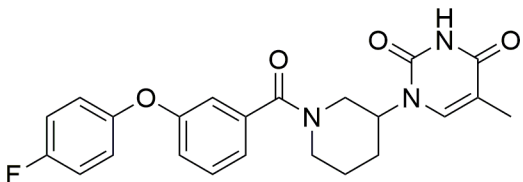


Compound **4c**
HSQC
DMSO-*d*₆

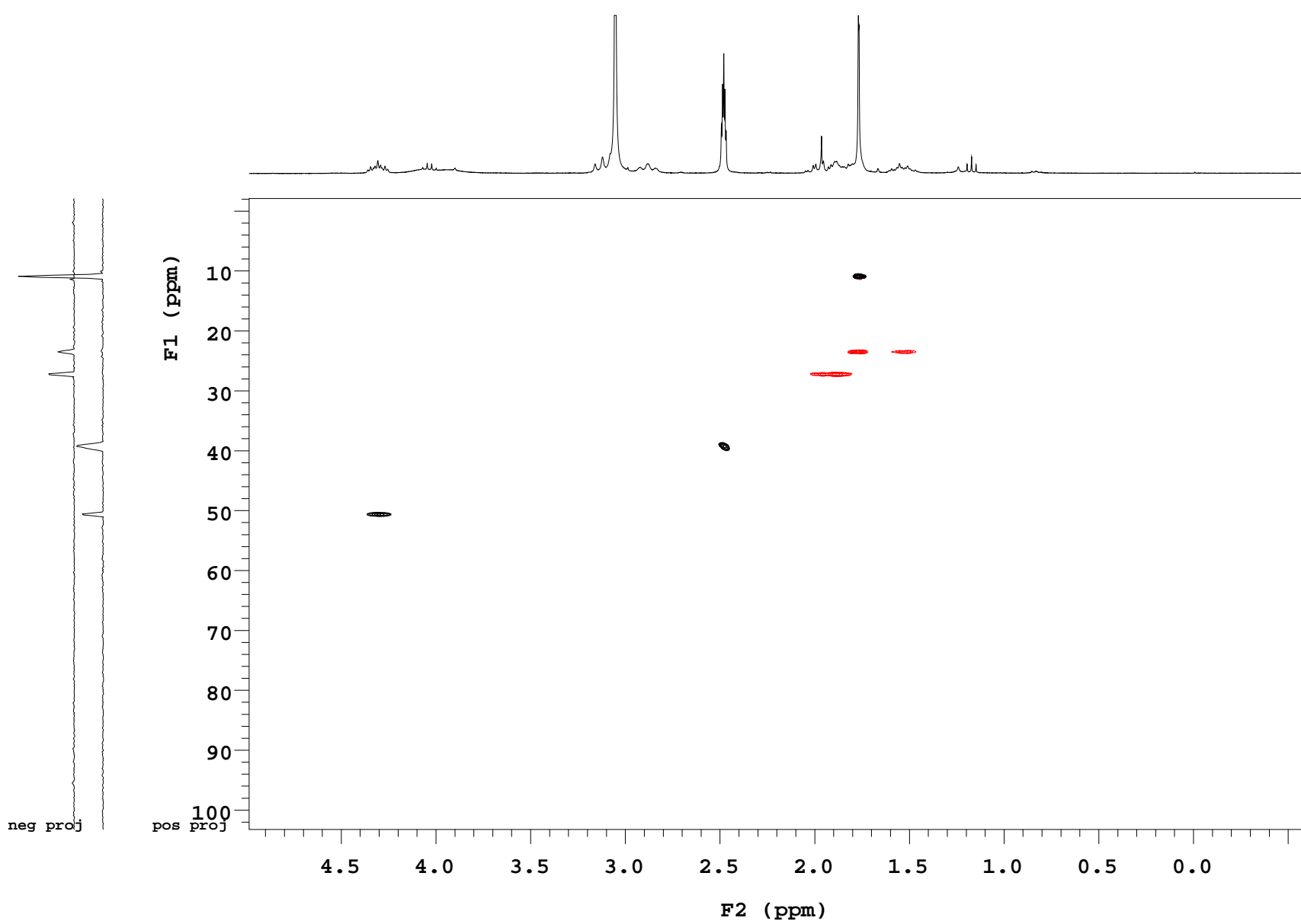


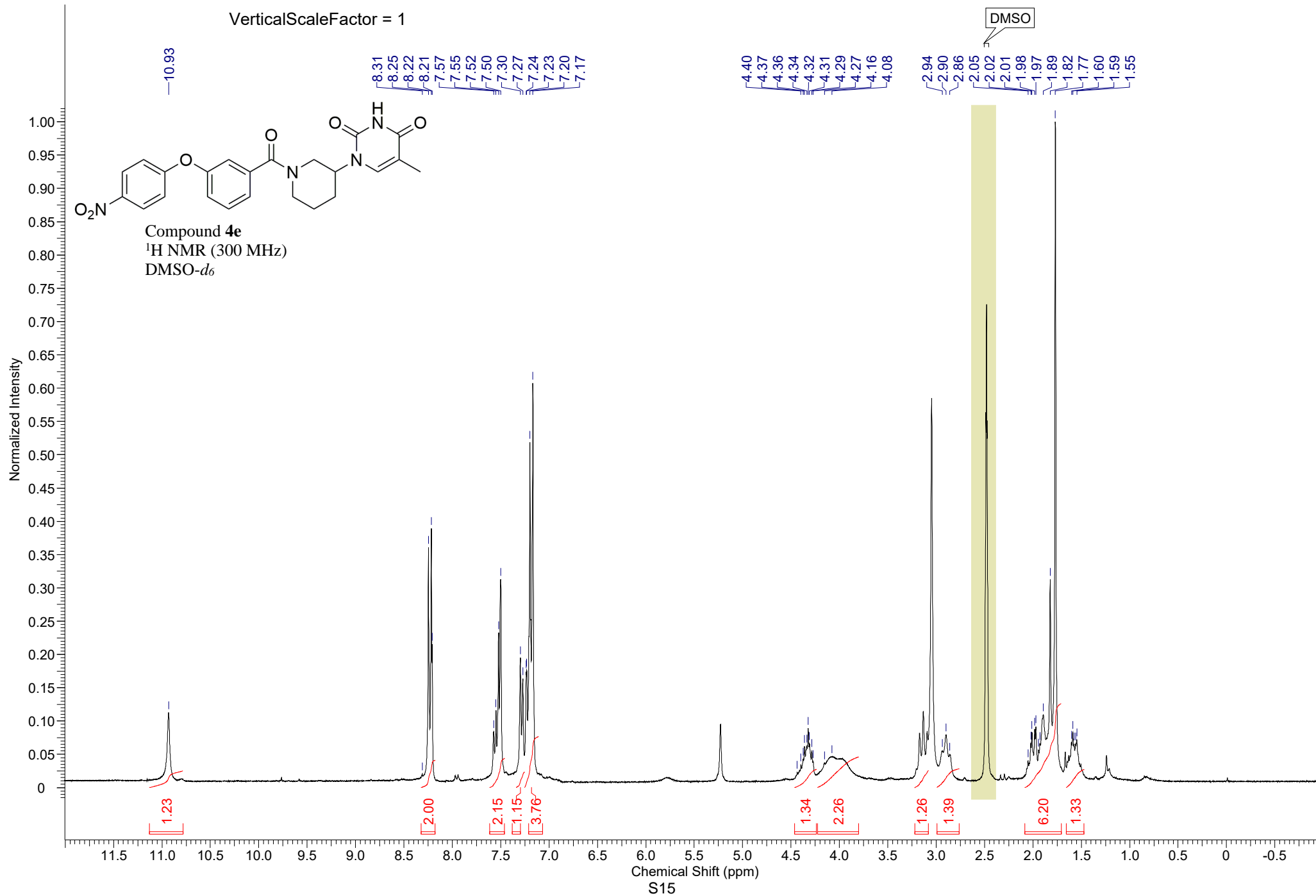


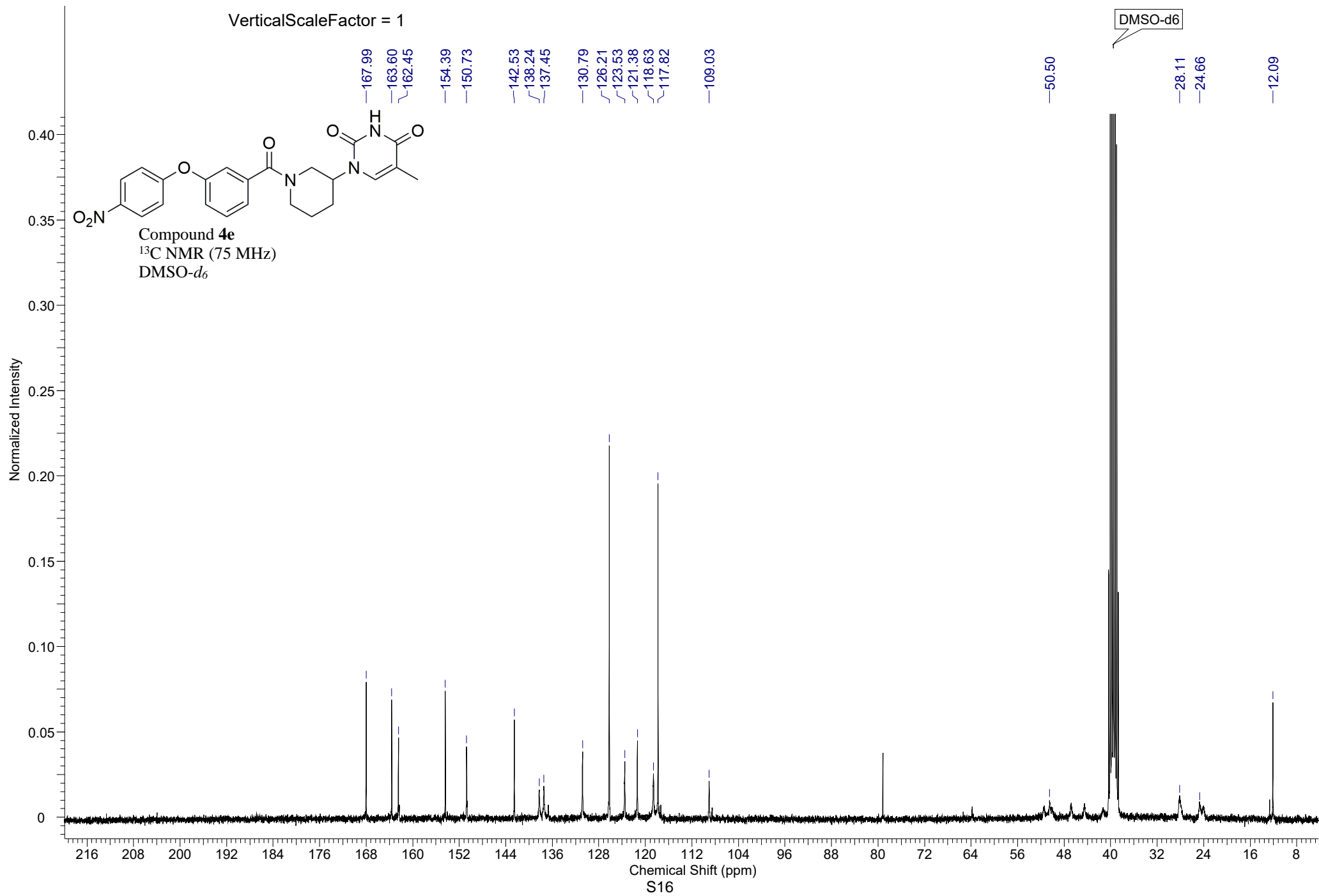


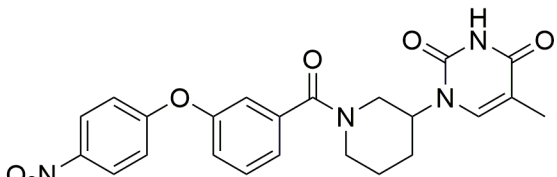


Compound **4d**
HSQC
DMSO-*d*₆

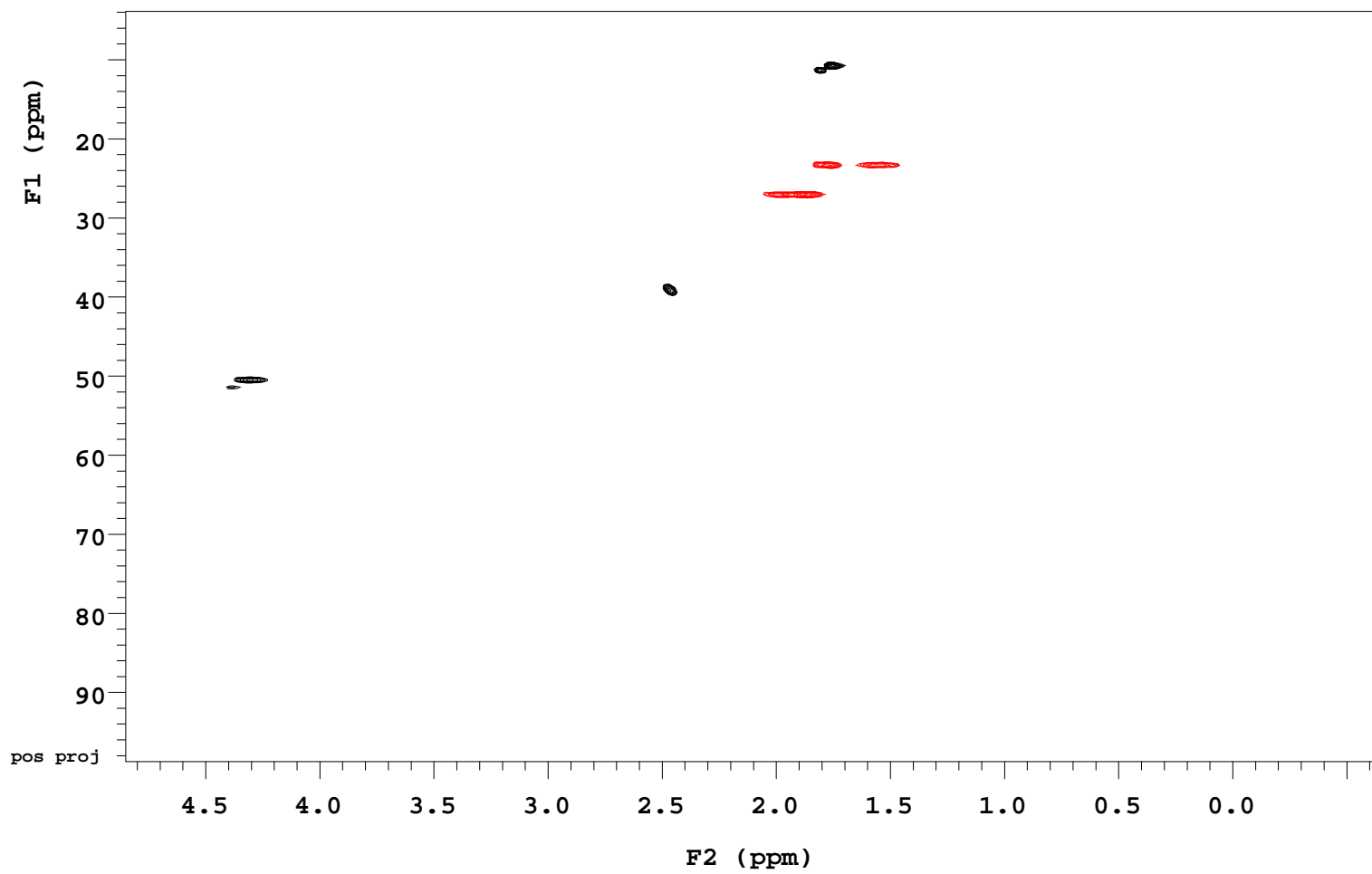
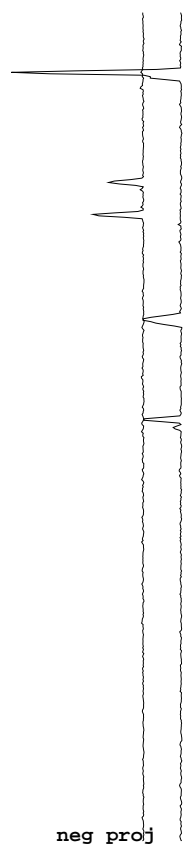


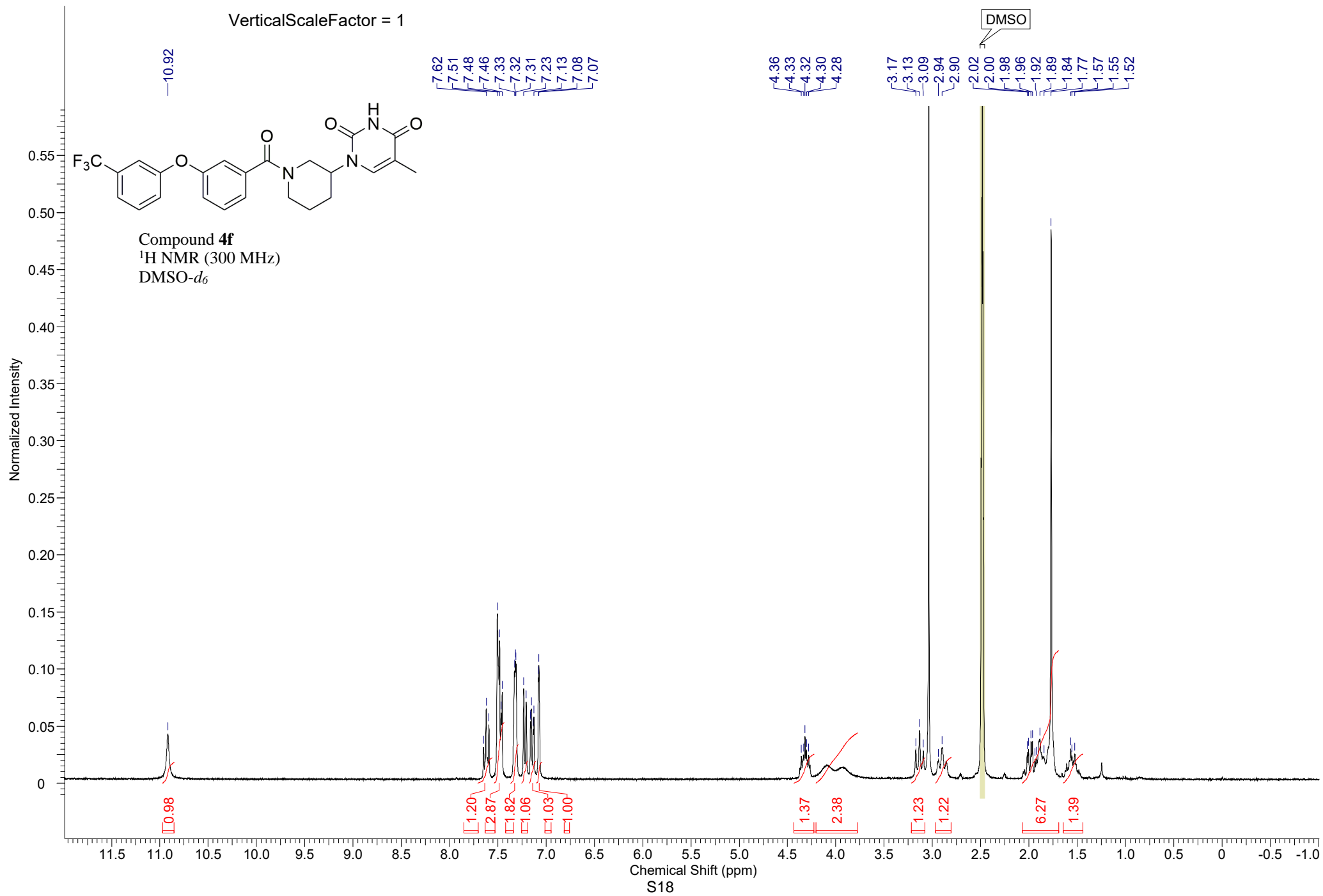


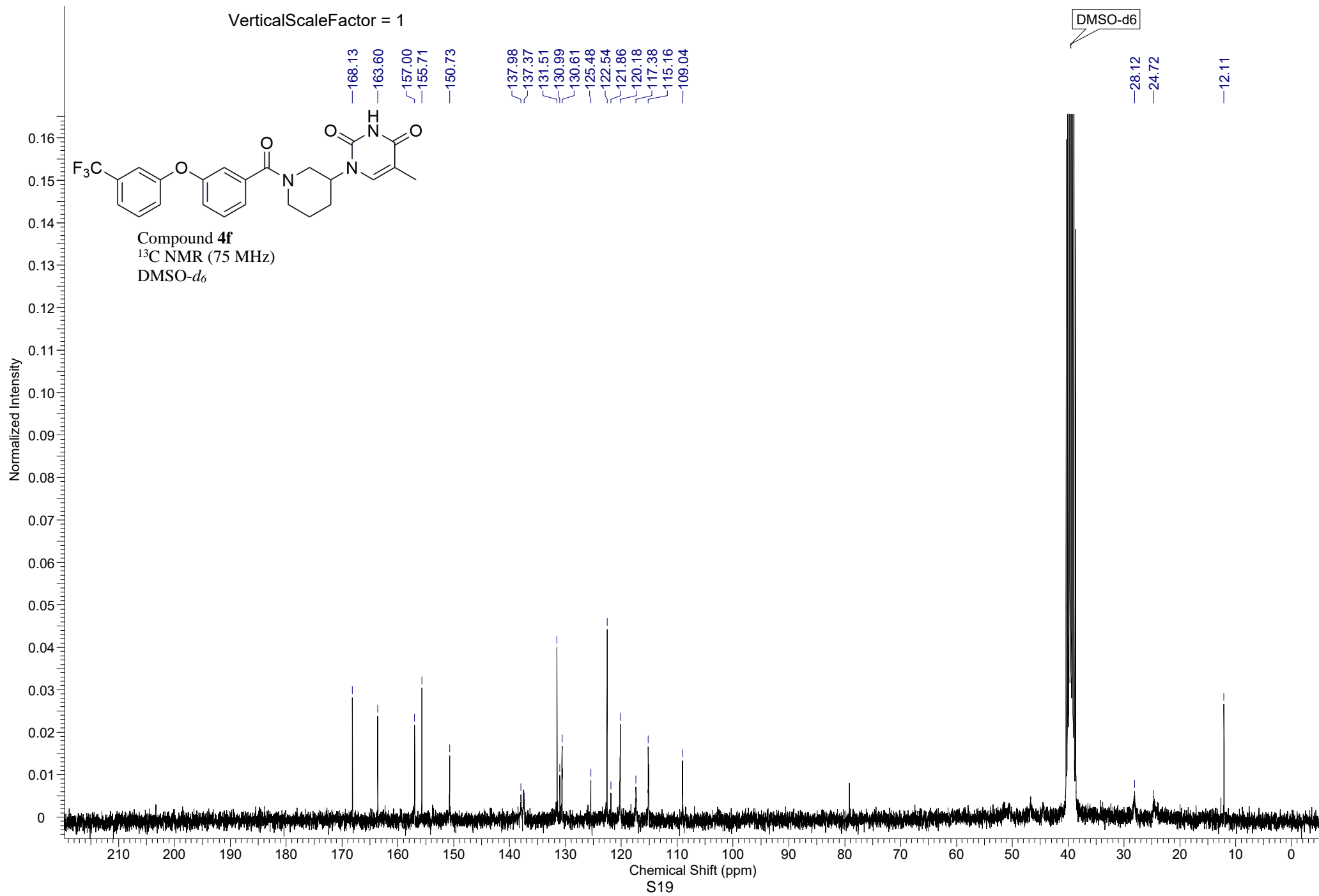


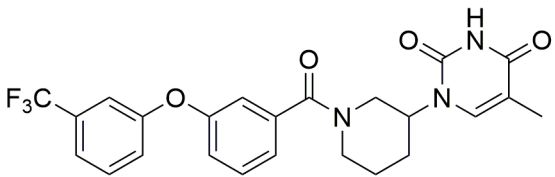


Compound 4e
HSQC
DMSO-*d*₆

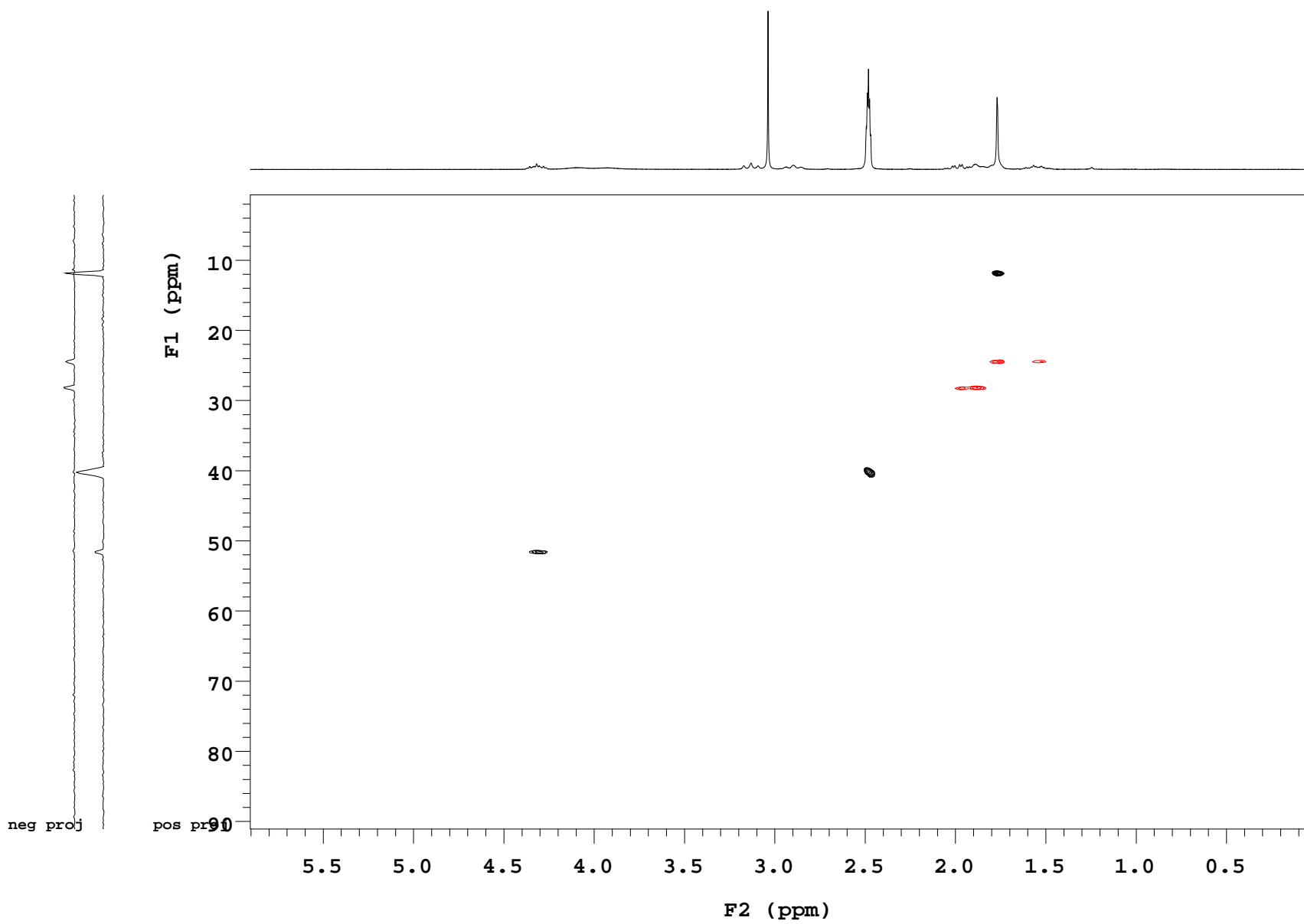


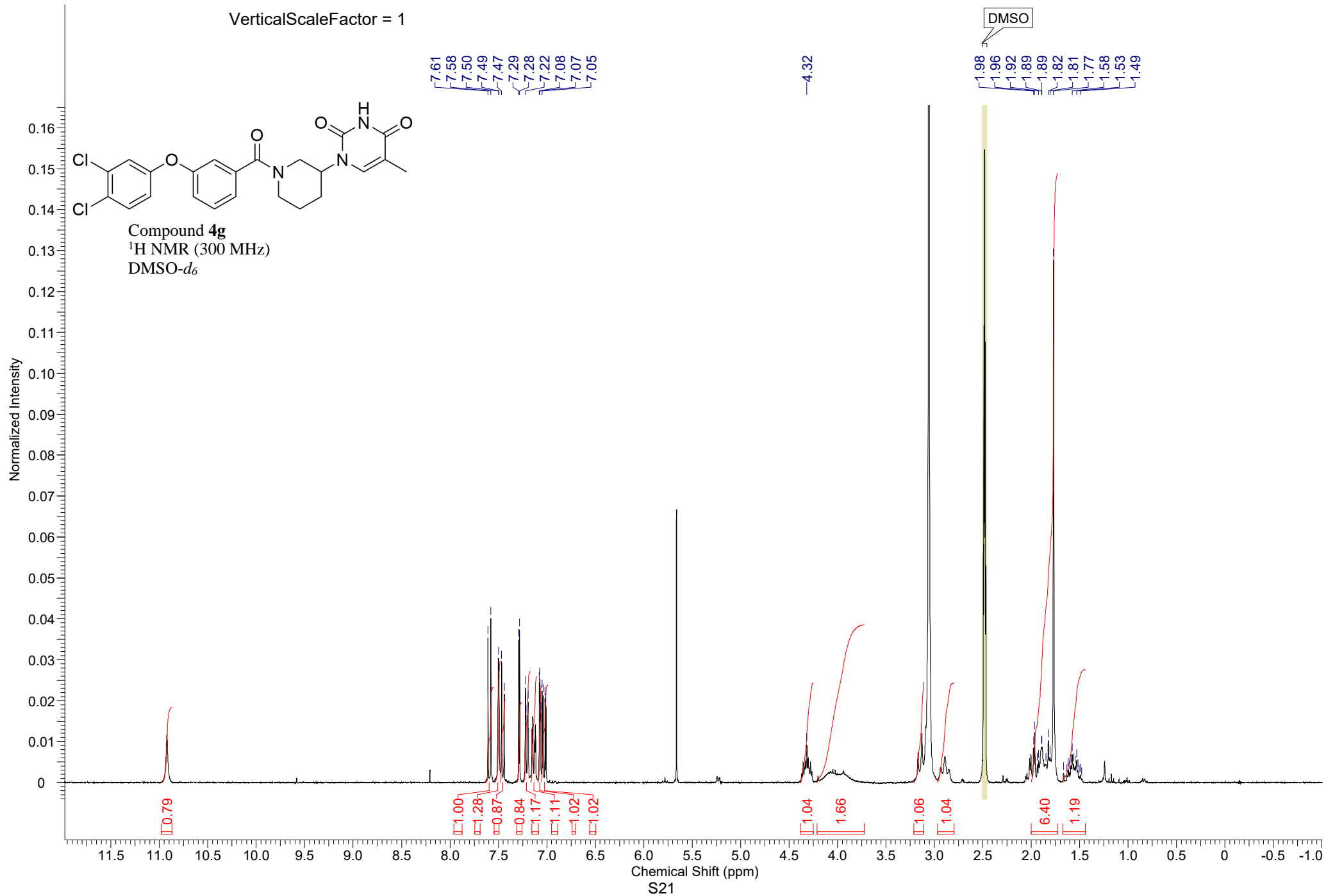


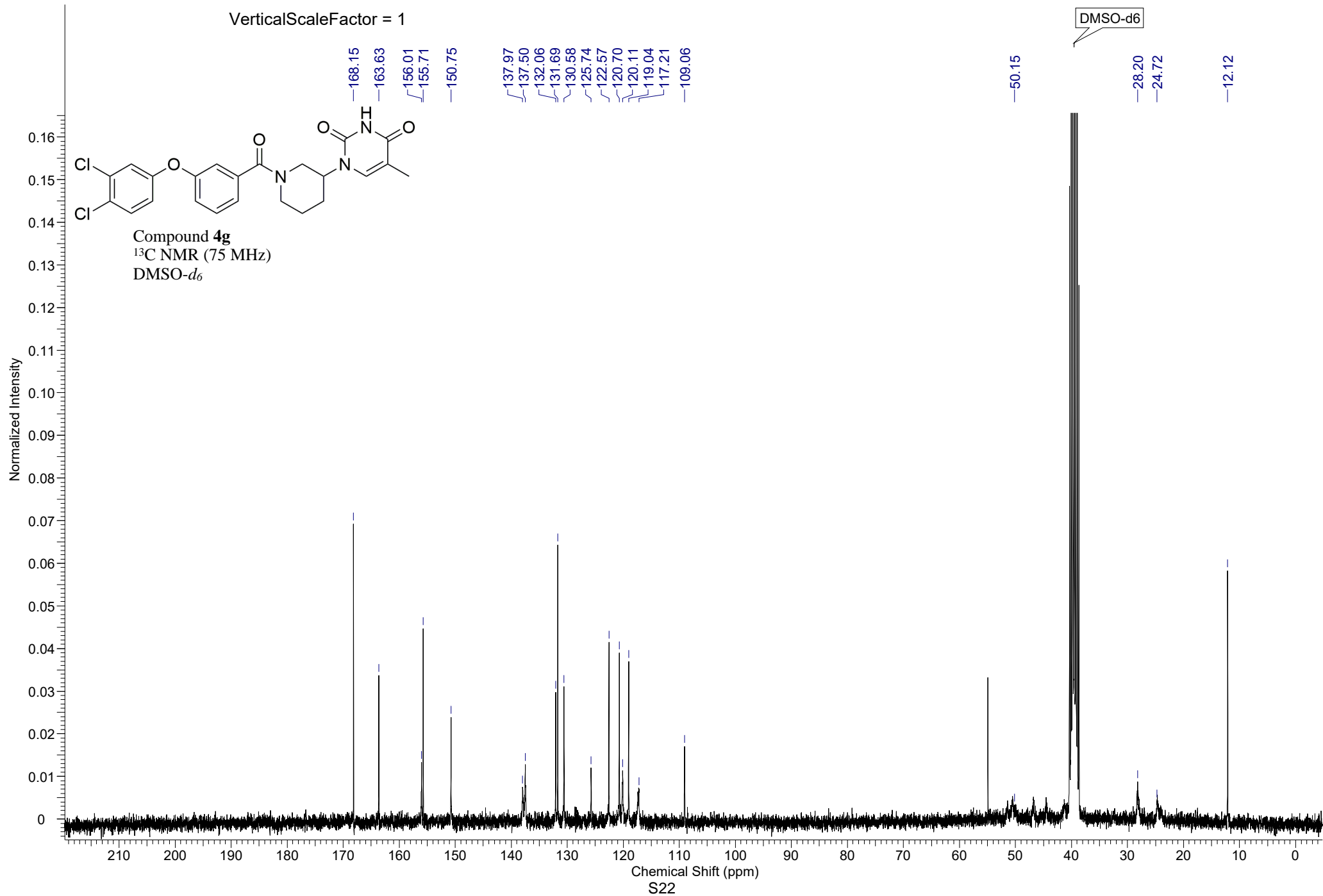


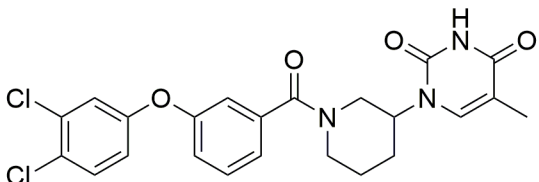


Compound **4f**
HSQC
DMSO-*d*₆

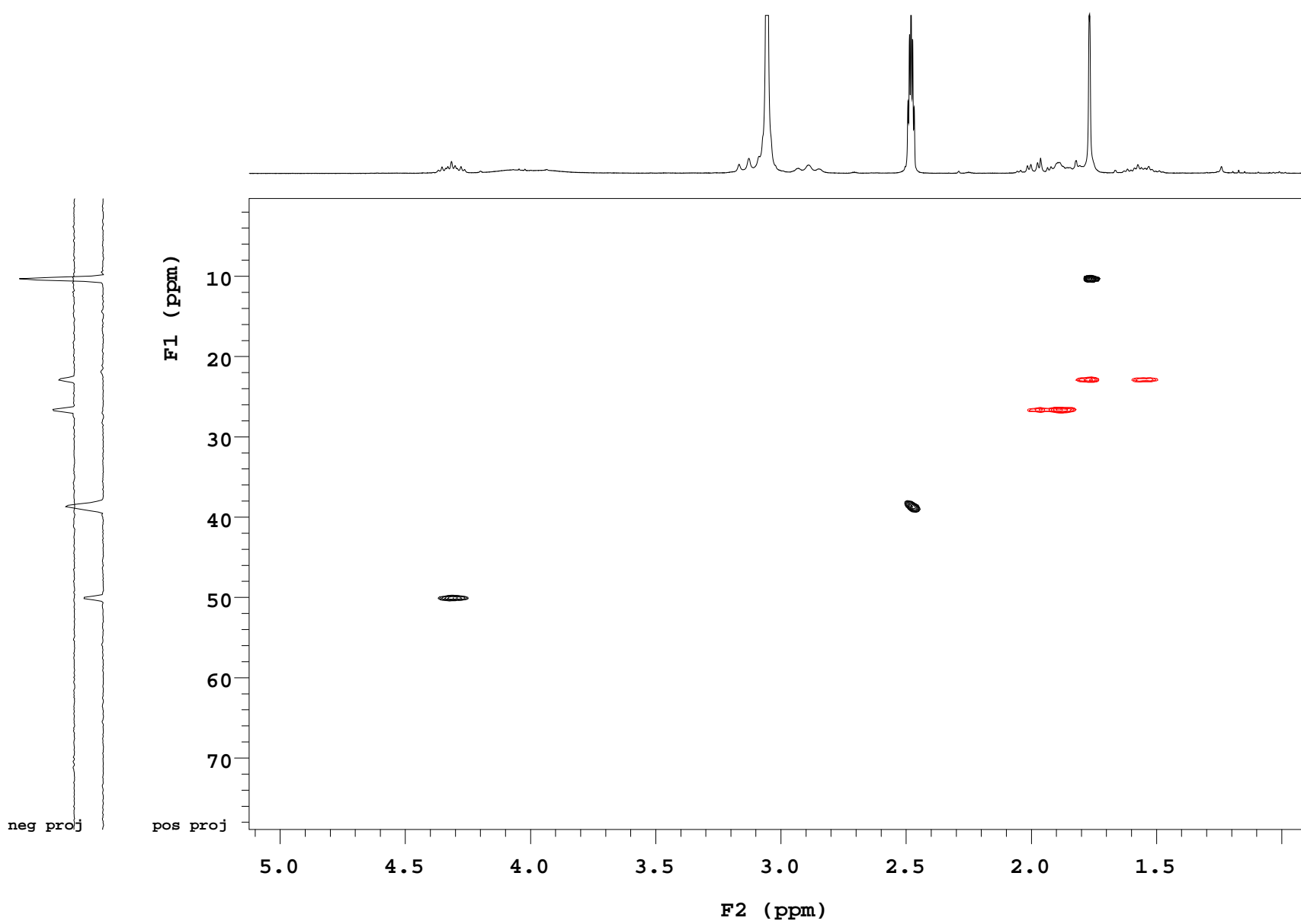


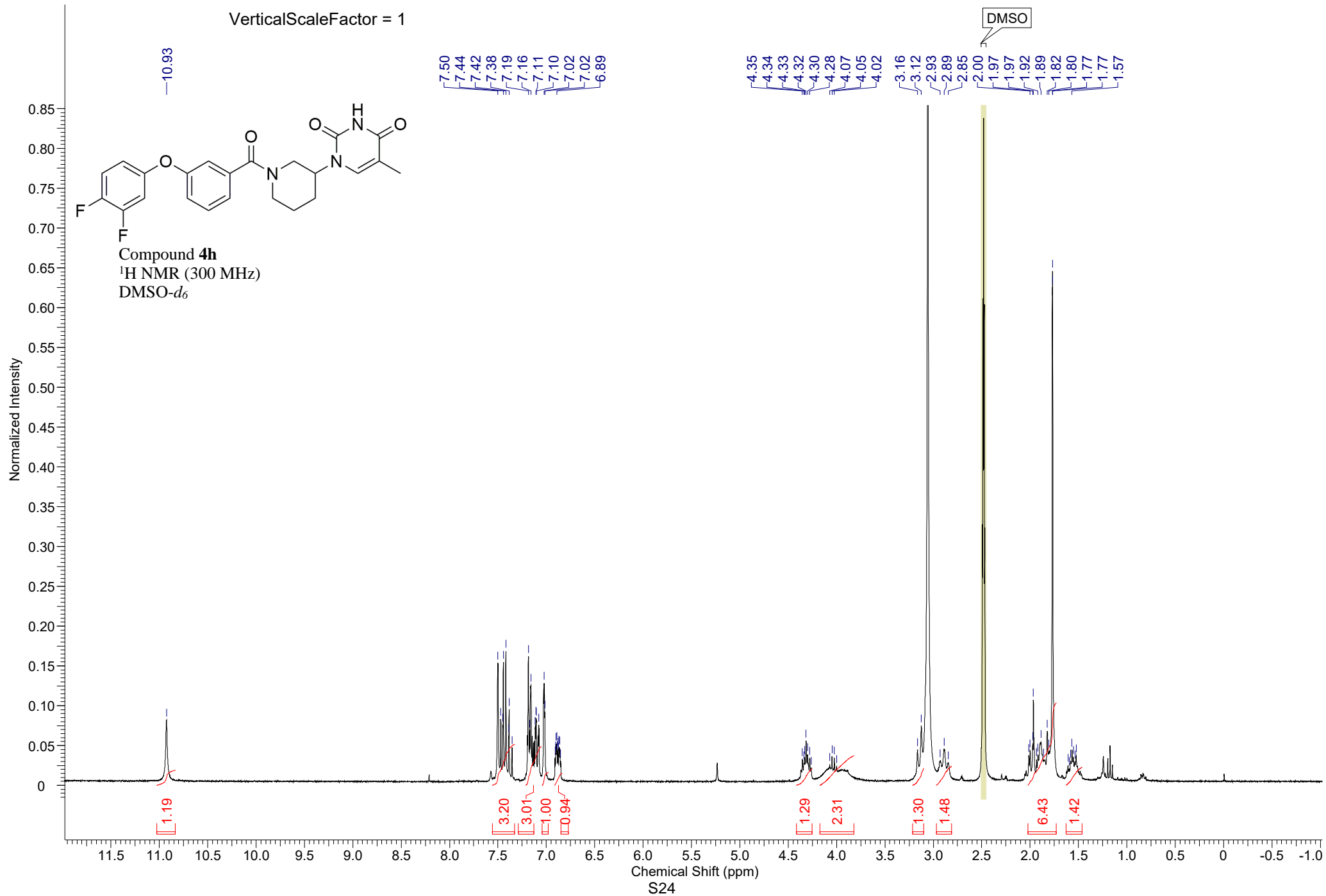


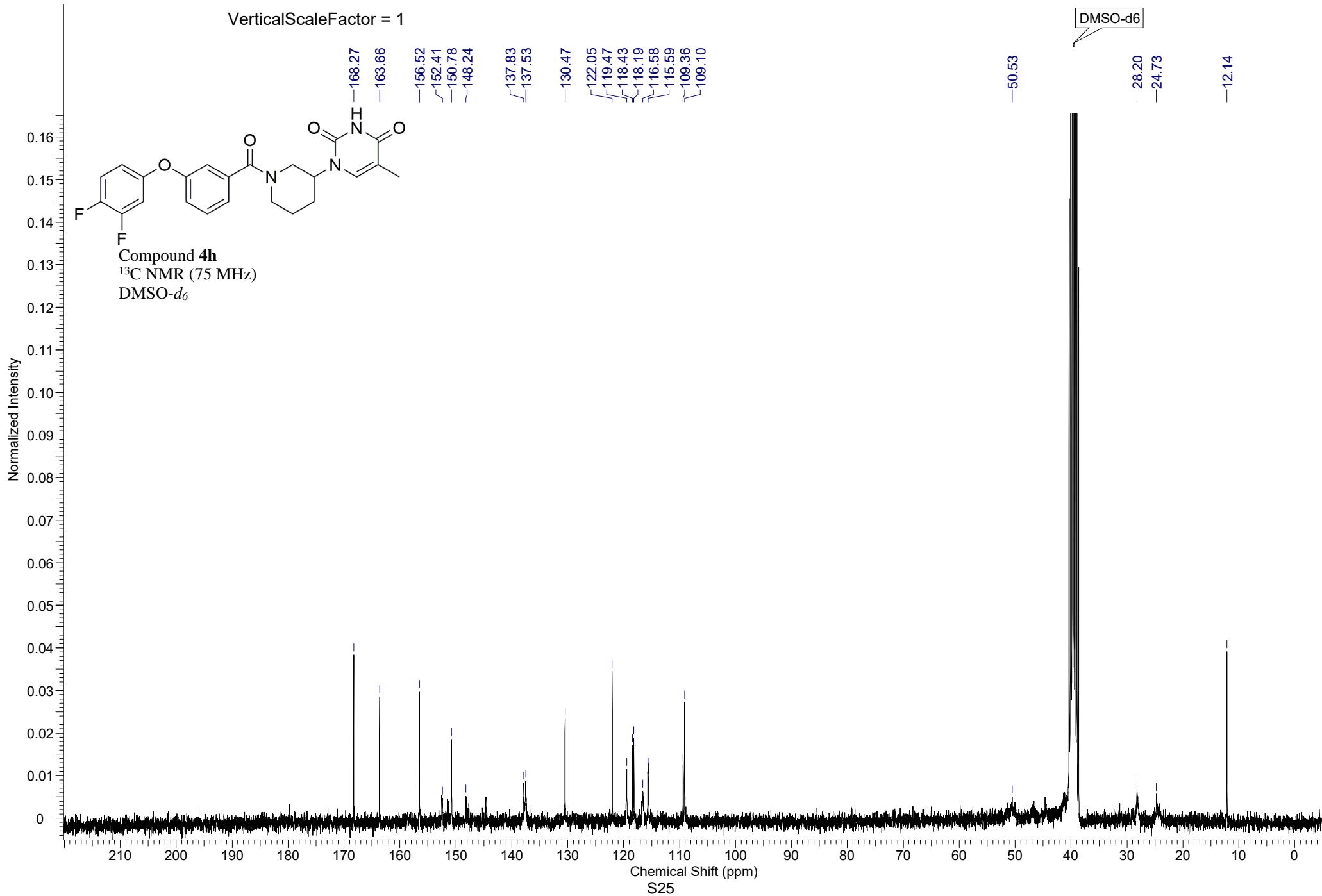


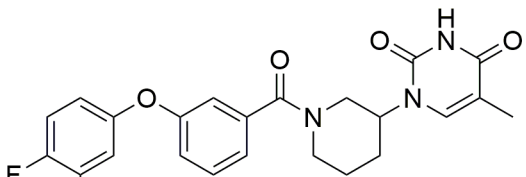


Compound **4g**
HSQC
DMSO-*d*₆









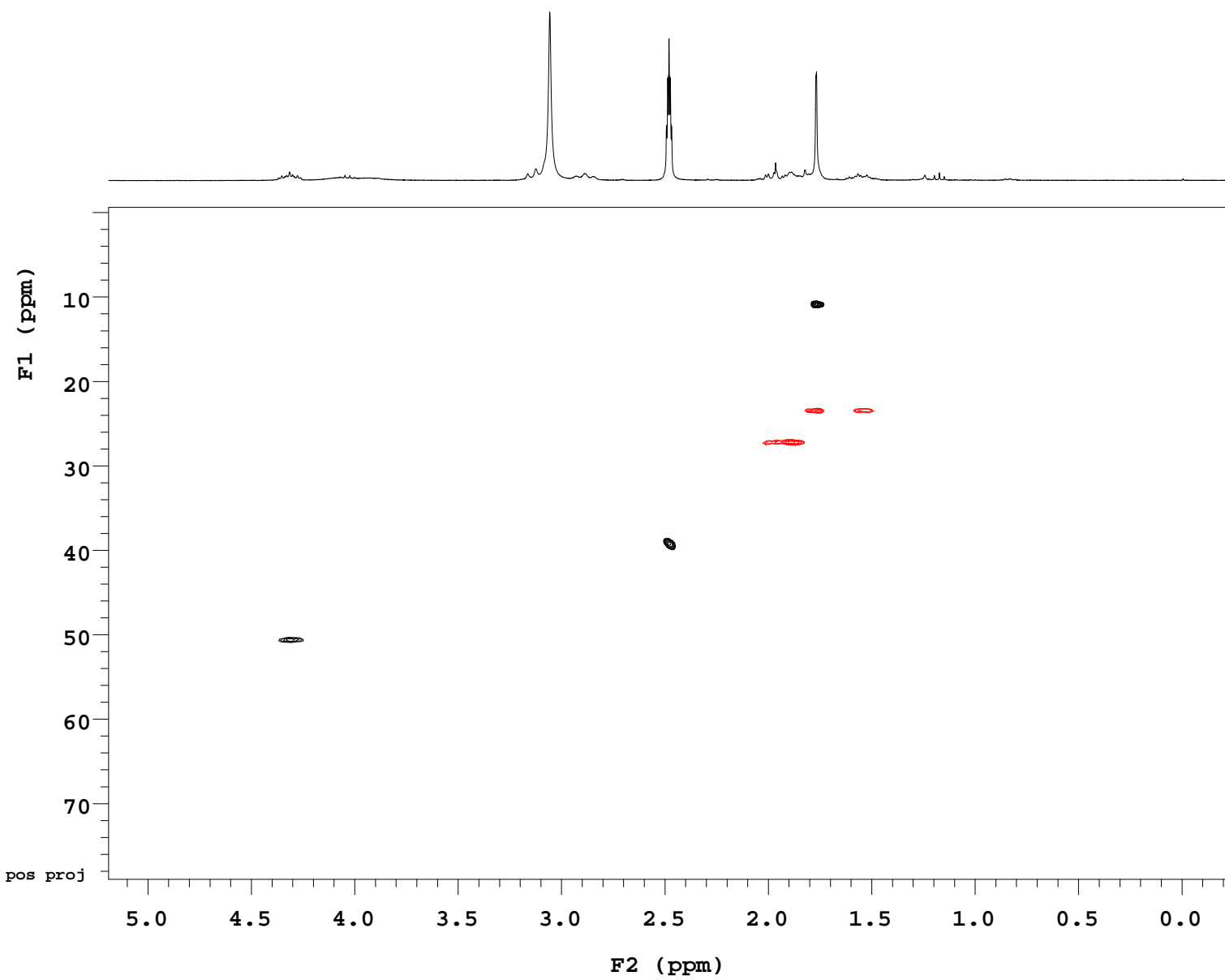
Compound **4h**

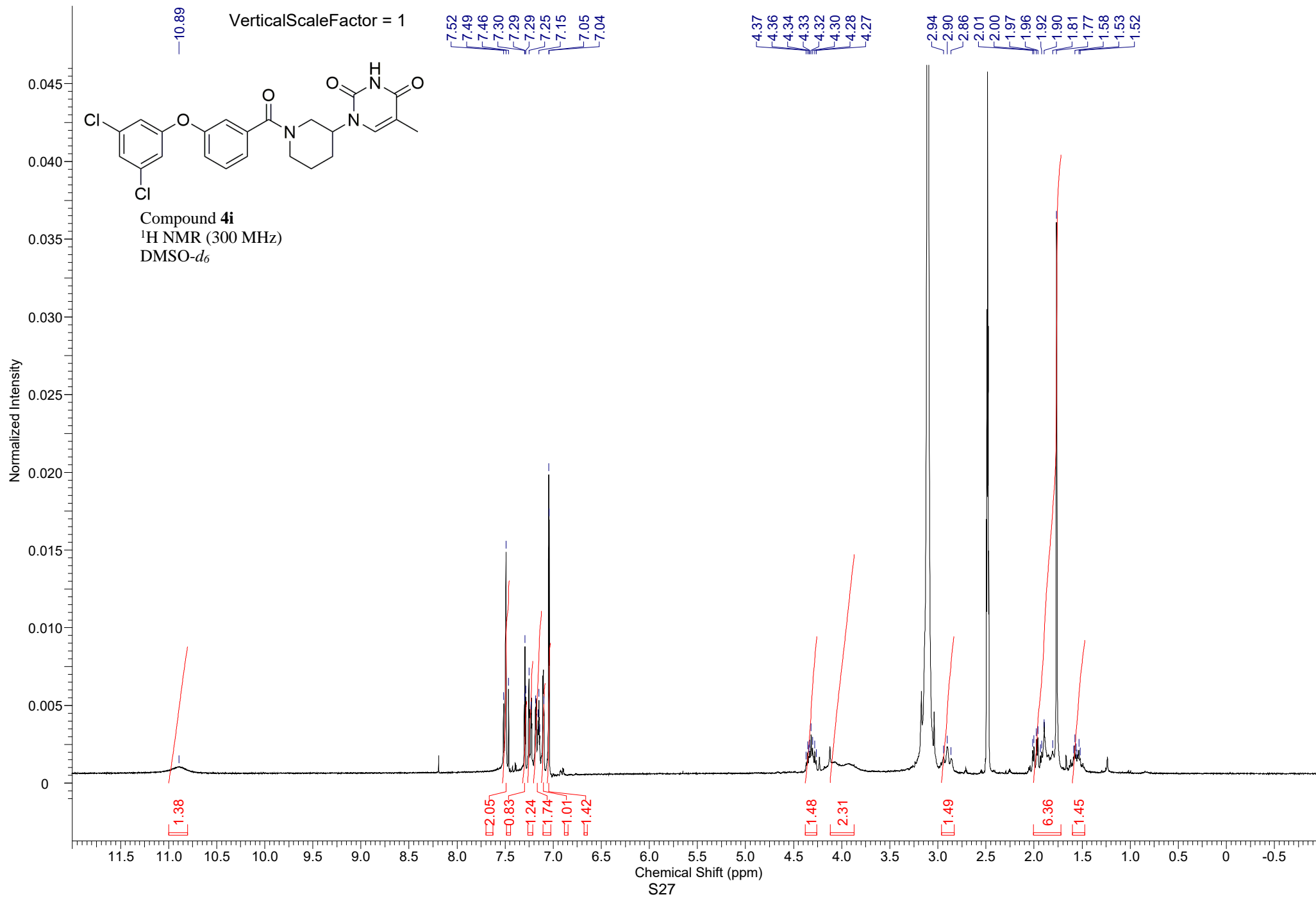
HSQC

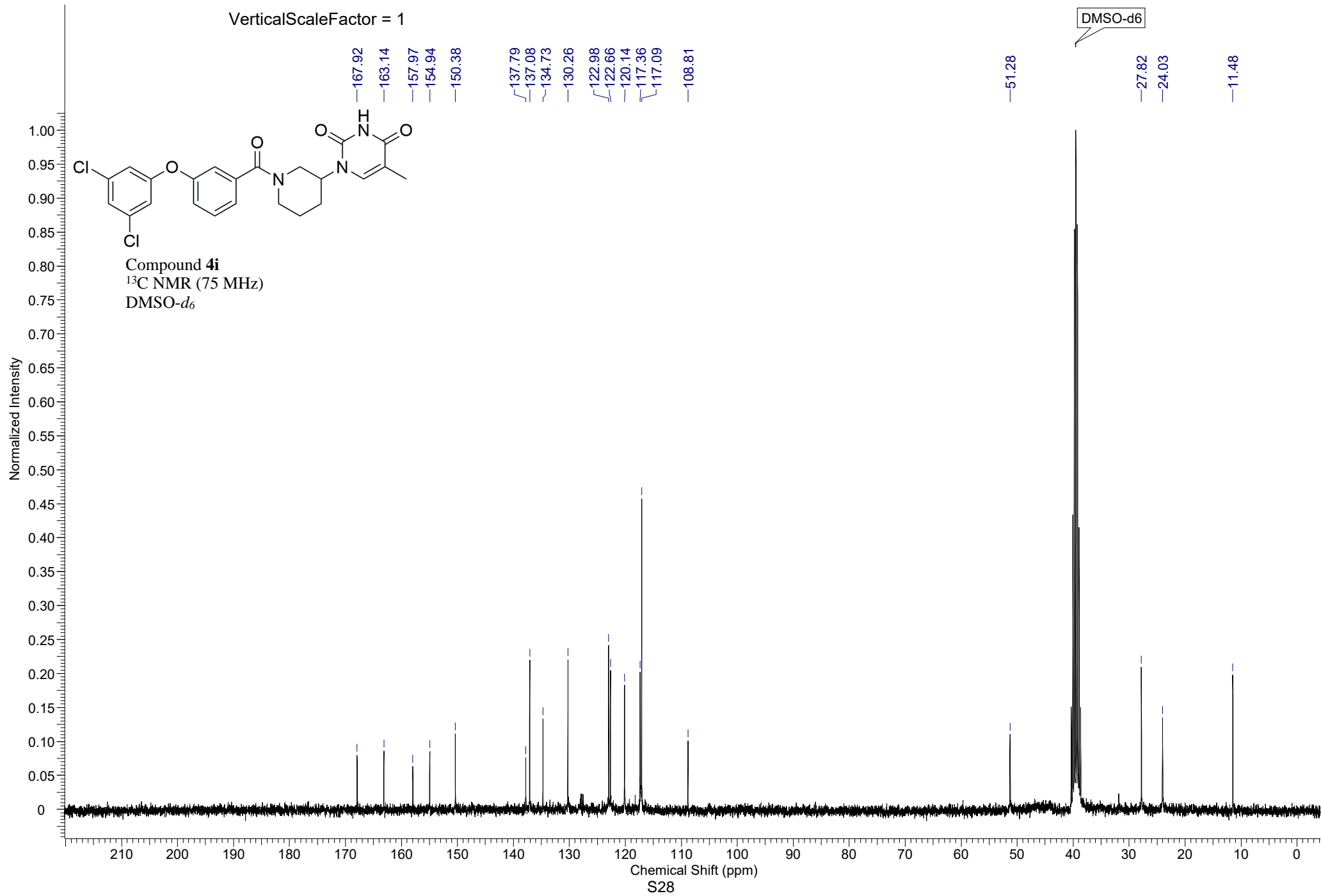
DMSO-*d*₆

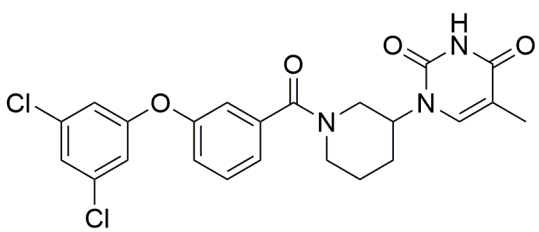
neg proj

pos proj

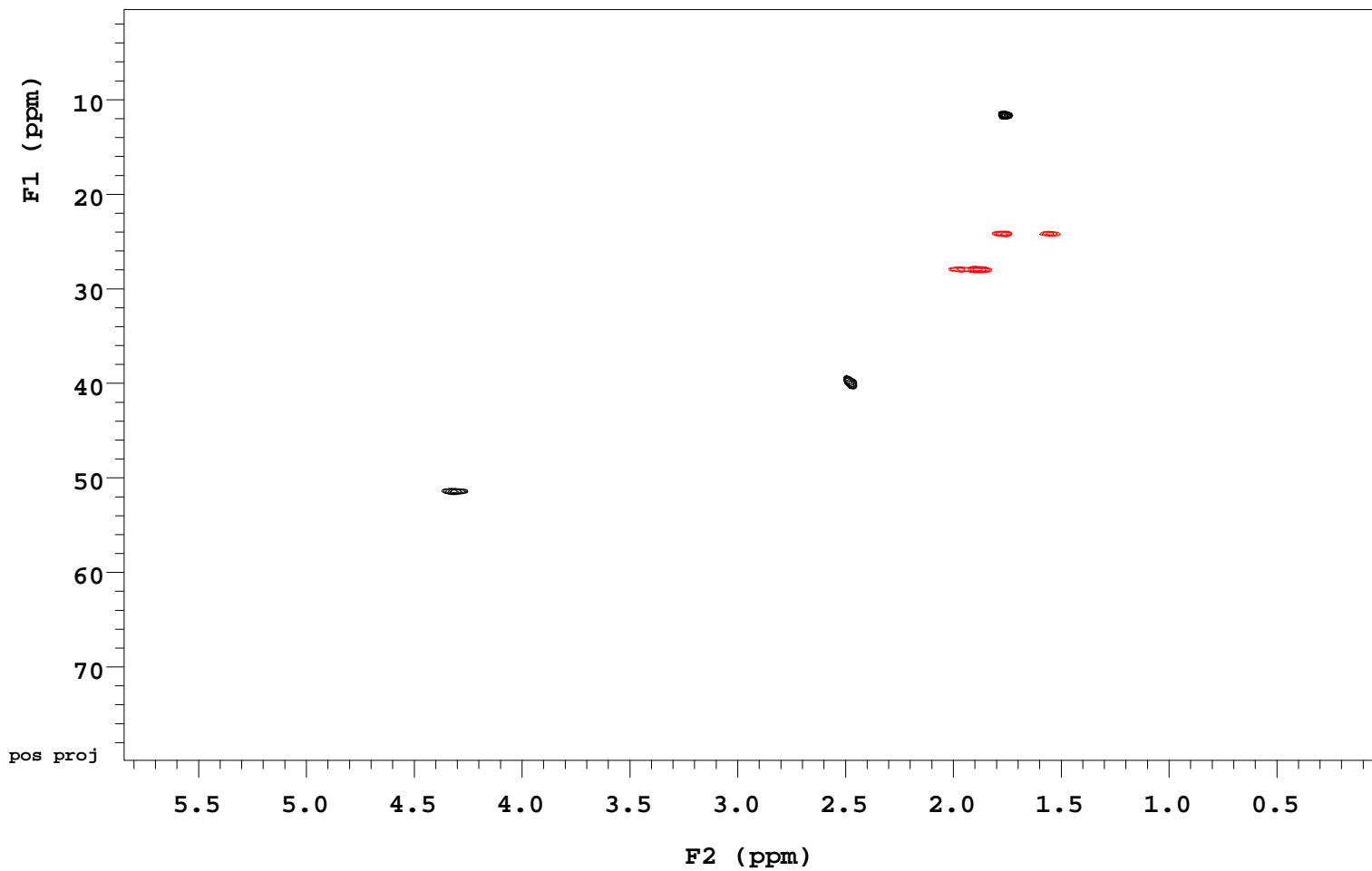
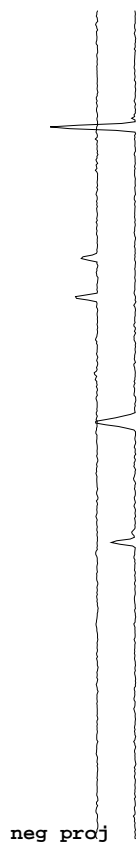


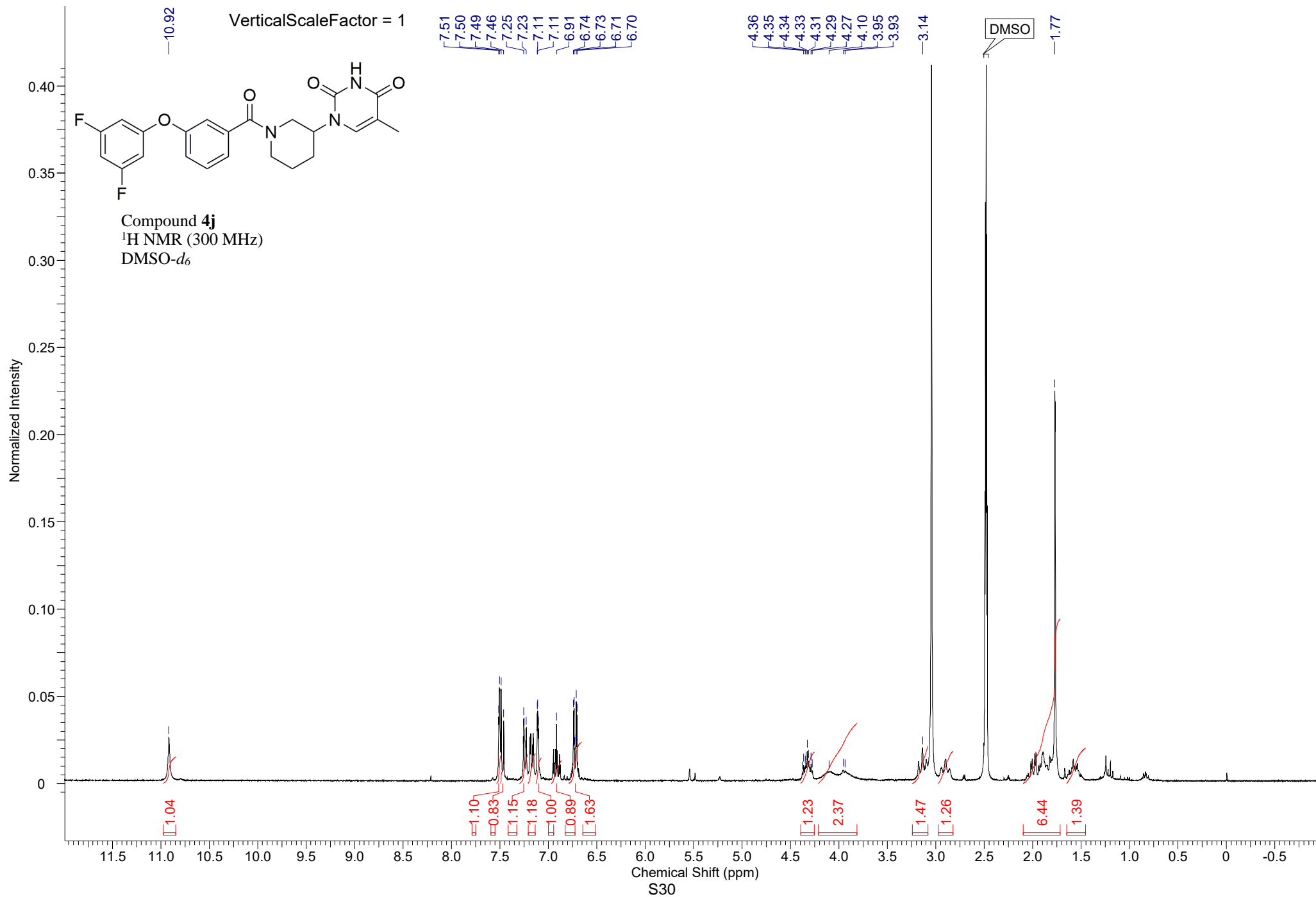


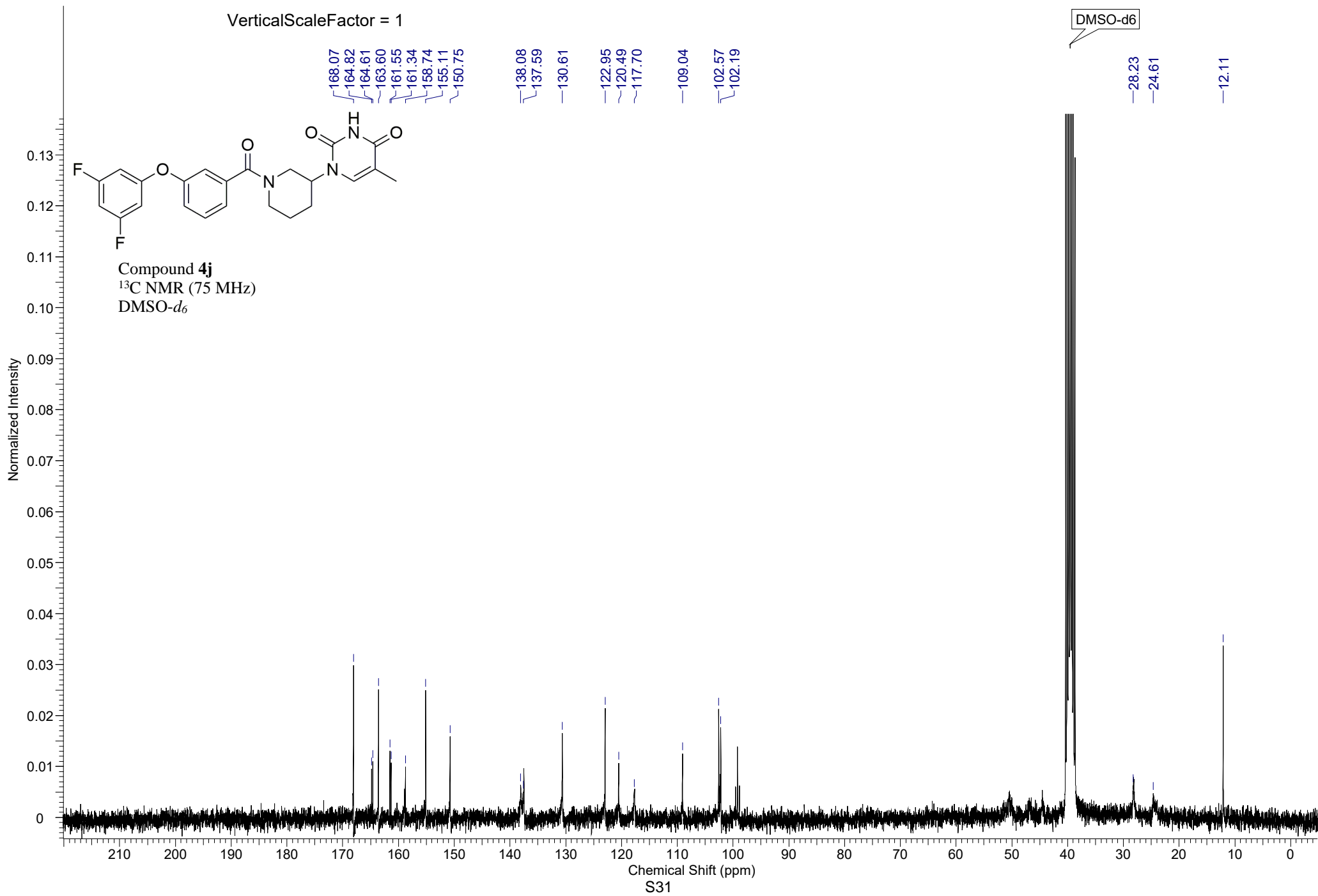


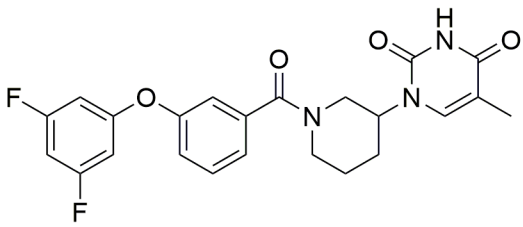


Compound **4i**
HSQC
DMSO-*d*₆

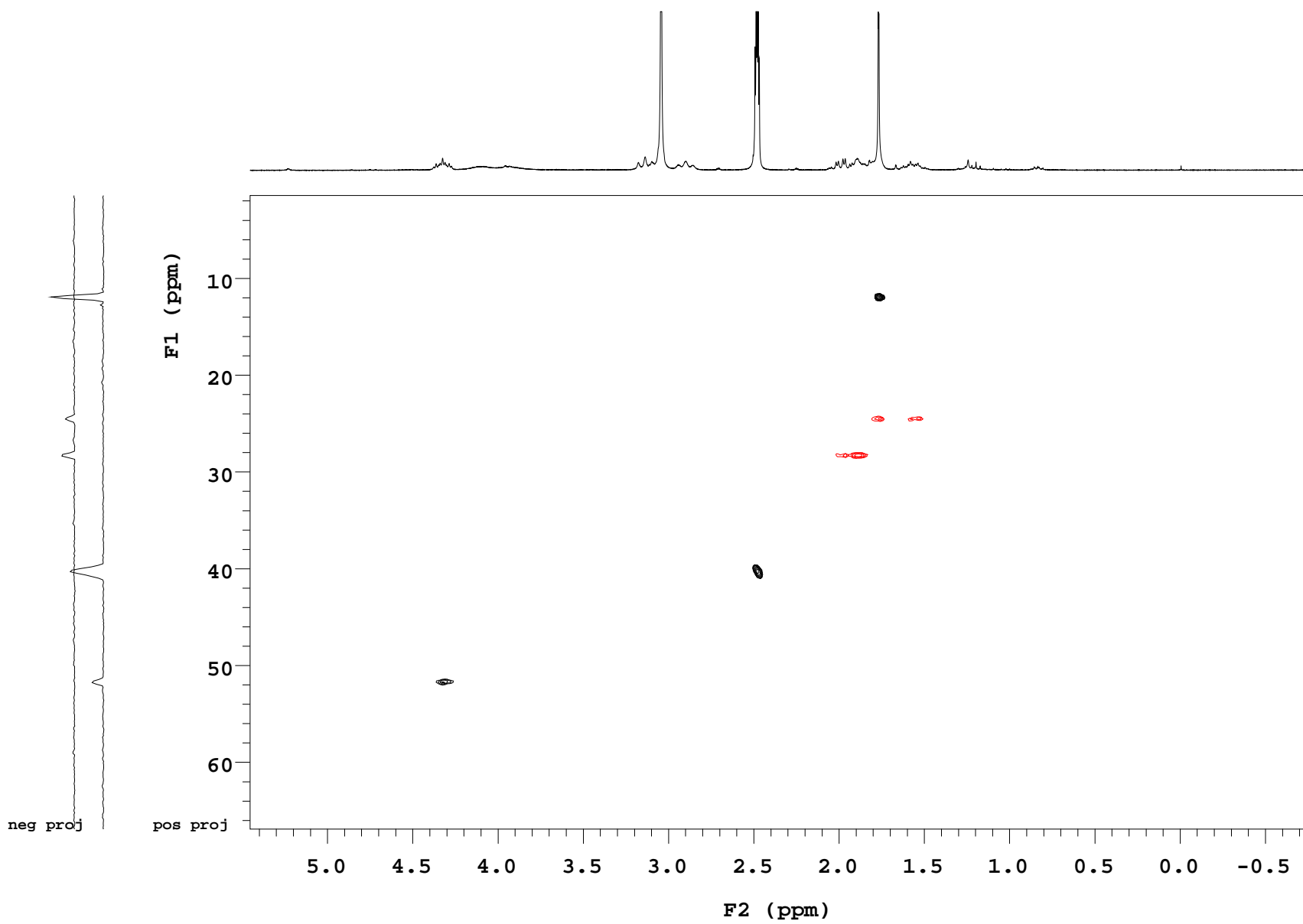


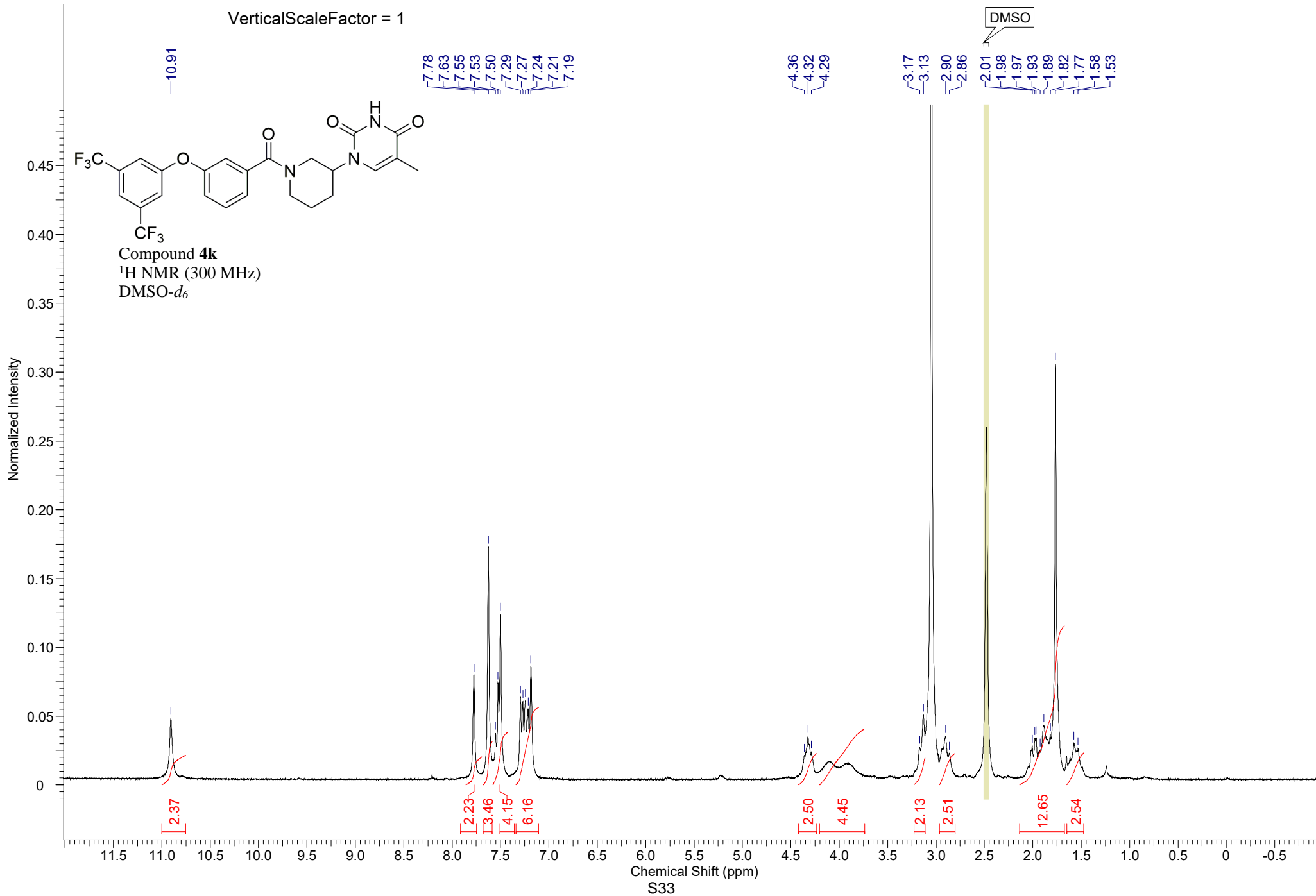


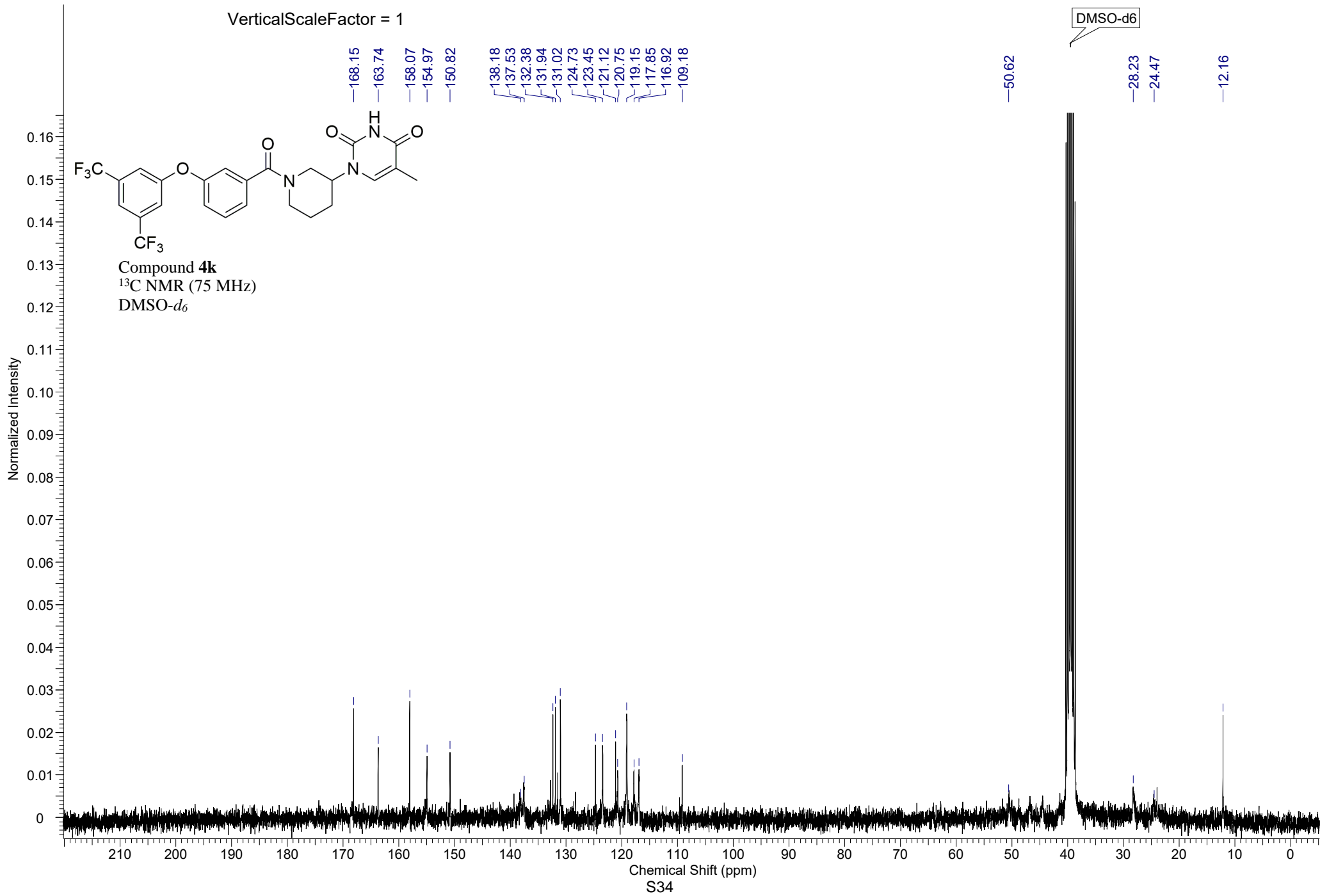


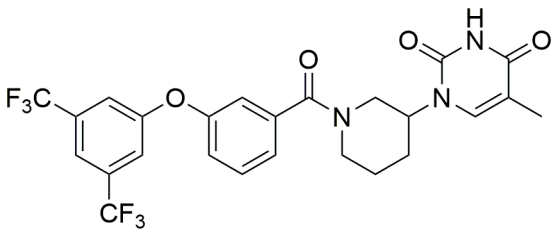


Compound **4j**
HSQC
DMSO-*d*₆









Compound 4h
HSQC
DMSO-*d*₆

