

Supporting Information

Synthesis of Novel Fluoro Analogues of MKC442 as Microbicides

Yasser M. Loksha,^{‡, #} Erik B. Pedersen,^{, ‡} Roberta Loddo,[†] Giuseppina Sanna,[†] Gabriella Collu,[†] Gabriele Giliberti[†] and Paolo La Colla^{*, †}*

^{*}Nucleic Acid Center, Department of Physics, Chemistry and Pharmacy, University of Southern Denmark, Campusvej 55, DK-5230 Odense M, Denmark.

[†]Dipartimento di Scienze Biomediche, Università di Cagliari, Cittadella Universitaria, 09042 Monserrato (CA), Italy

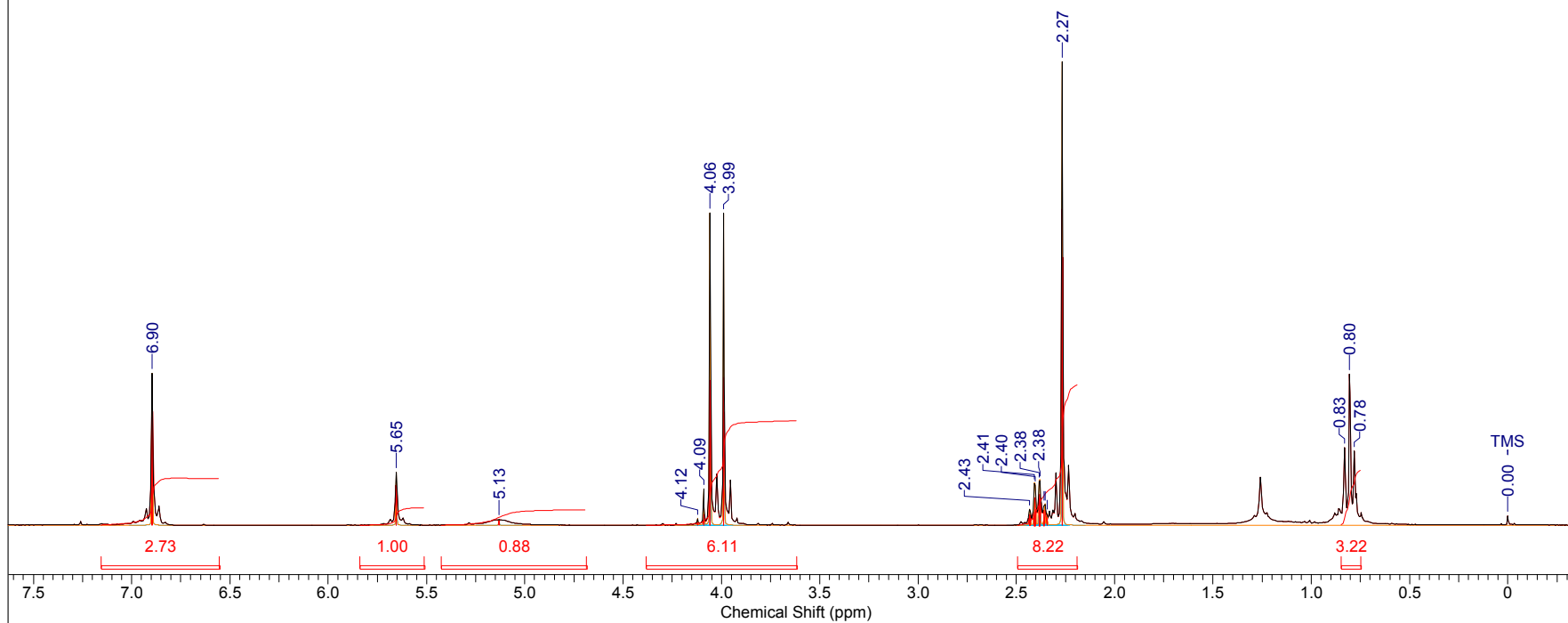
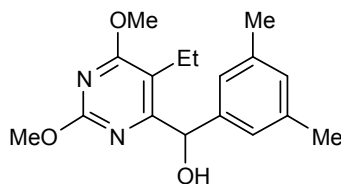
[#]Faculty of Pharmacy and Pharmaceutical Industries, Sinai University, North Sinai, Al-Arish, Egypt

Table of Contents

¹ H NMR (CDCl ₃) of compound 2	S3
¹³ C NMR (CDCl ₃) of compound 2	S4
¹ H NMR (CDCl ₃) of compound 3	S5
¹³ C NMR (CDCl ₃) of compound 3	S6
¹ H NMR (DMSO- <i>d</i> ₆) of compound 4a	S7
¹³ C NMR (DMSO- <i>d</i> ₆) of compound 4a	S8
¹ H NMR (DMSO- <i>d</i> ₆) of compound 4b	S9
¹³ C NMR (DMSO- <i>d</i> ₆) of compound 4b	S10
¹ H NMR (DMSO- <i>d</i> ₆) of compound 5	S11
¹³ C NMR (DMSO- <i>d</i> ₆) of compound 5	S12
¹ H NMR (CDCl ₃) of compound 9a	S13
¹³ C NMR (CDCl ₃) of compound 9a	S14
¹ H NMR (CDCl ₃) of compound 9b	S15
¹³ C NMR (CDCl ₃) of compound 9b	S16
¹ H NMR (CDCl ₃) of compound 9c	S17
¹³ C NMR (CDCl ₃) of compound 9c	S18
¹ H NMR (CDCl ₃) of compound 11a	S19
¹³ C NMR (CDCl ₃) of compound 11a	S20
¹ H NMR (CDCl ₃) of compound 11b	S21
¹³ C NMR (CDCl ₃) of compound 11b	S22
¹ H NMR (CDCl ₃) of compound 12 , YML220	S23
¹³ C NMR (CDCl ₃) of compound 12 , YML220	S24
¹ H NMR (CDCl ₃) of compound 13	S25
¹³ C NMR (CDCl ₃) of compound 13	S26

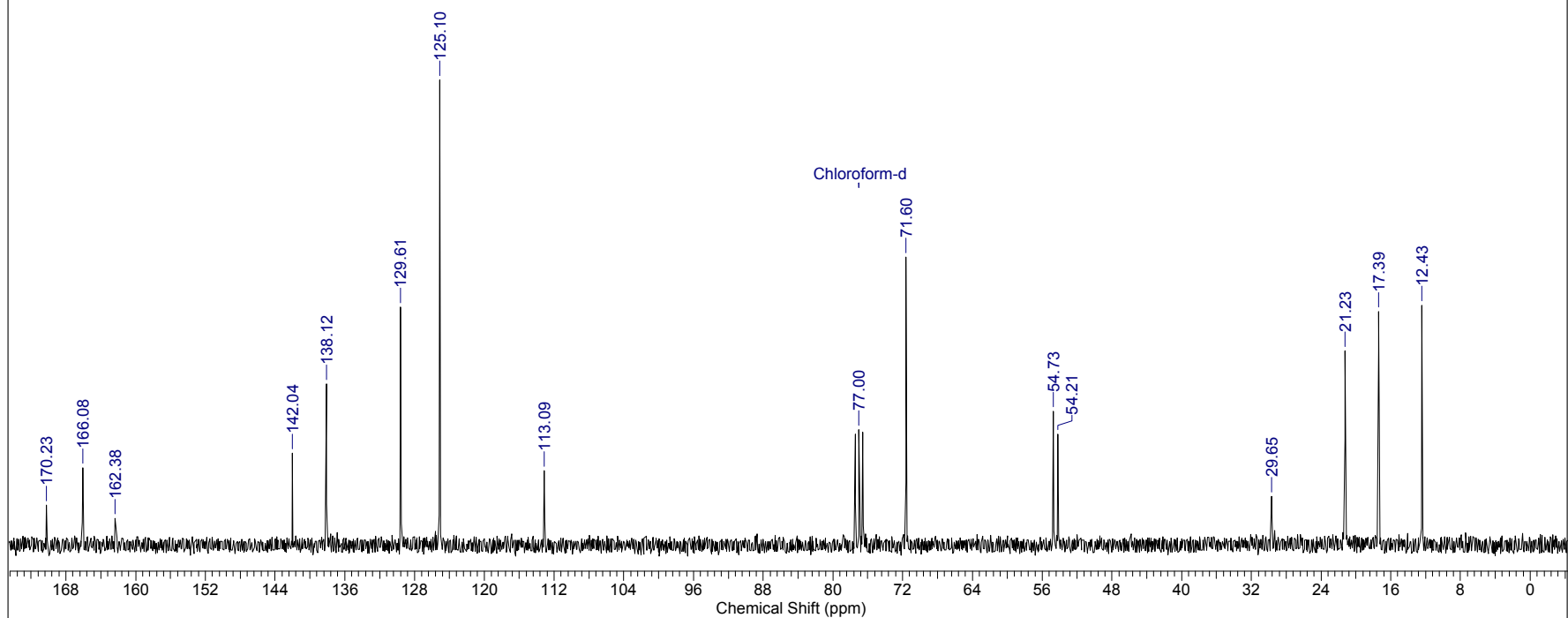
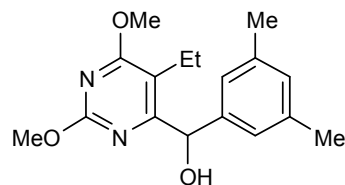
Acquisition Time (sec)	3.0027	Comment	yml 038	Date	Aug 27 2004	File Name	D:\01_Research\SHIVA\NMR\Data\Yasser\YML038\yml0827H		
Frequency (MHz)	300.09	Nucleus	1H	Number of Transients	8	Original Points Count	18016	Points Count	32768
Pulse Sequence	s2pul	Solvent	CHLOROFORM-D			Sweep Width (Hz)	6000.00	Temperature (degree C)	25.000

¹H NMR Spectrum of Compound **2** in CDCl₃



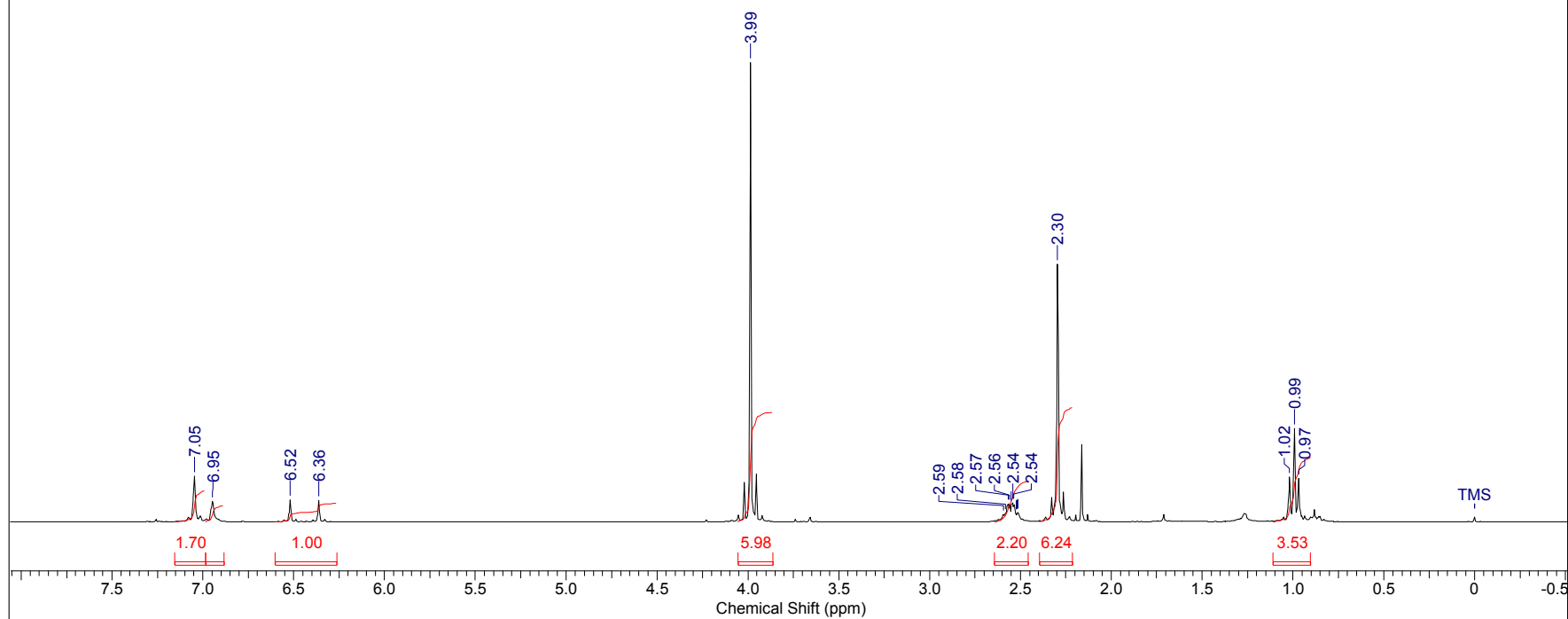
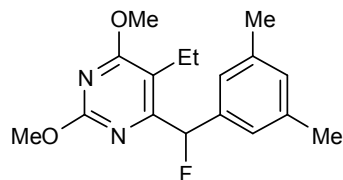
Acquisition Time (sec)	1.8148	Comment	ym1 038	Date	Aug 27 2004	File Name	D:\01_Research\SHIVA\NMR\Data\Yasser\YML038\ym10827C		
Frequency (MHz)	75.46	Nucleus	13C	Number of Transients	256	Original Points Count	34048	Points Count	65536
Pulse Sequence	s2pul	Solvent	CHLOROFORM-D			Sweep Width (Hz)	18761.73	Temperature (degree C)	25.000

¹³C NMR Spectrum of Compound **2** in CDCl₃



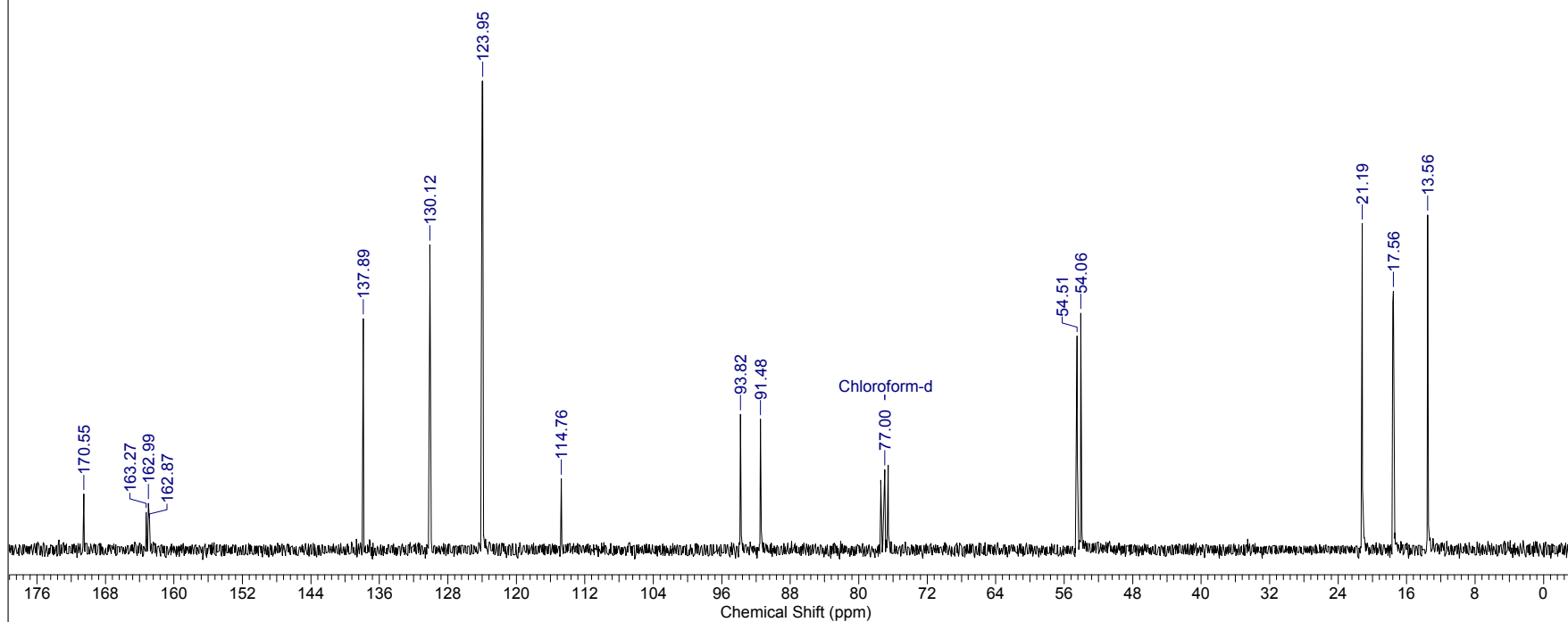
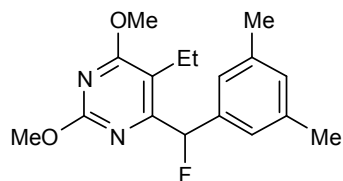
Acquisition Time (sec)	3.0027	Comment	ym1 031	Date	Aug 24 2004	File Name	D:\01_Research\SHIVA\NMR\Data\Yasser\YML031\ym10824H		
Frequency (MHz)	300.09	Nucleus	1H	Number of Transients	8	Original Points Count	18016	Points Count	32768
Pulse Sequence	s2pul	Solvent	CHLOROFORM-D			Sweep Width (Hz)	6000.00	Temperature (degree C)	25.000

¹H NMR Spectrum of Compound **3** in CDCl₃



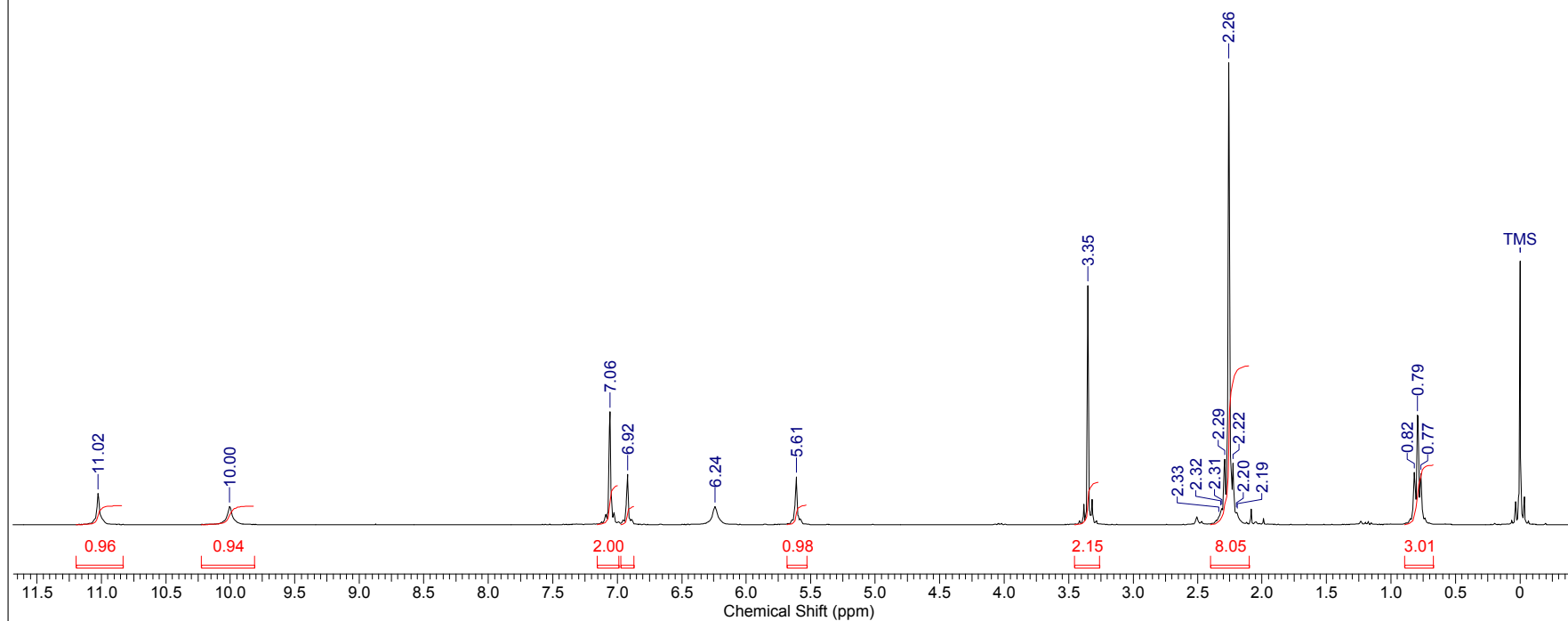
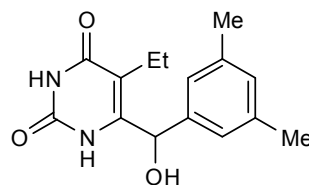
Acquisition Time (sec)	1.8148	Comment	yml 031	Date	Aug 23 2004	File Name	D:\01_Research\SHIVA\NMR\Data\Yasser\YML031\yml0823C		
Frequency (MHz)	75.46	Nucleus	13C	Number of Transients	256	Original Points Count	34048	Points Count	65536
Pulse Sequence	s2pul	Solvent	CHLOROFORM-D			Sweep Width (Hz)	18761.73	Temperature (degree C)	25.000

¹³C NMR Spectrum of Compound 3 in CDCl₃



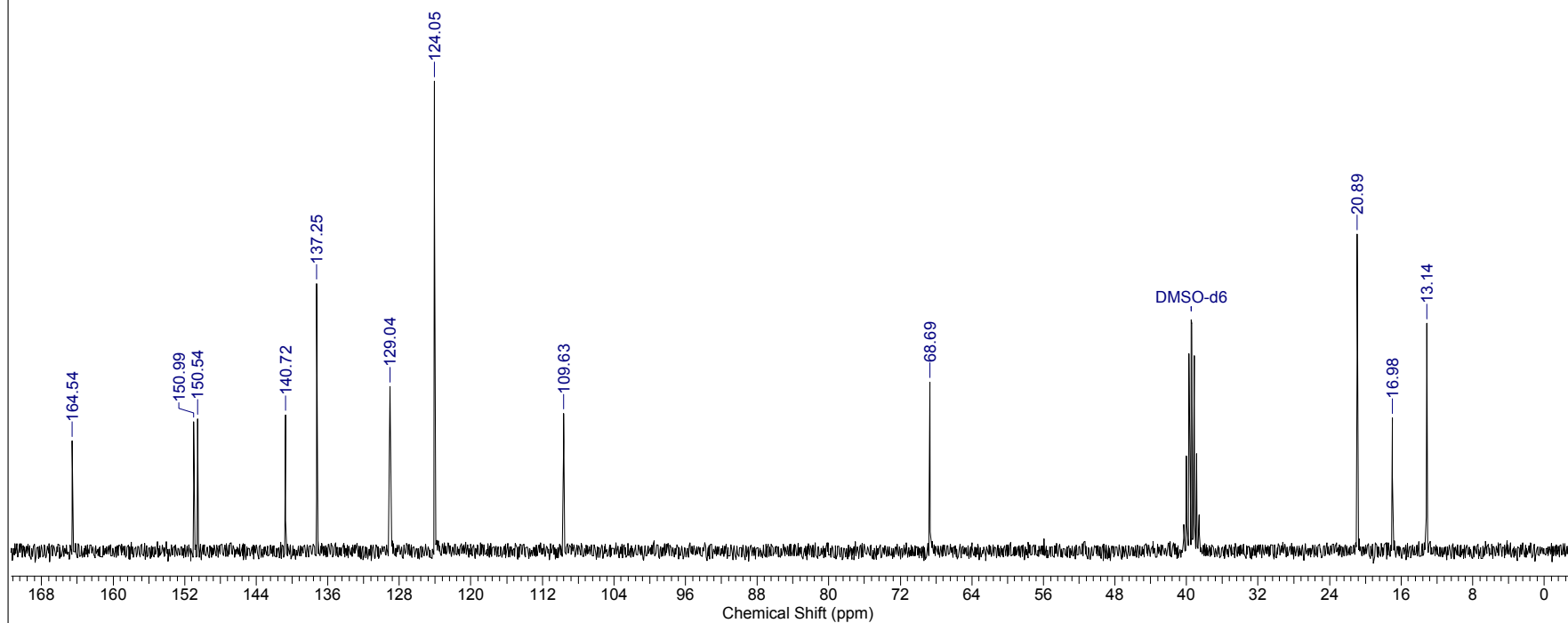
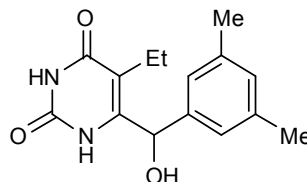
Acquisition Time (sec)	3.0027	Comment	ym1 042	Date	Sep 4 2004	File Name	D:\01_Research\SHIVA\NMR\Data\Yasser\YML042\ym10904H		
Frequency (MHz)	300.09	Nucleus	1H	Number of Transients	8	Original Points Count	18016	Points Count	32768
Pulse Sequence	s2pul	Solvent	DMSO-D6	Sweep Width (Hz)	6000.00	Temperature (degree C)	25.000		

¹H NMR Spectrum of Compound **4a** in DMSO-*d*₆



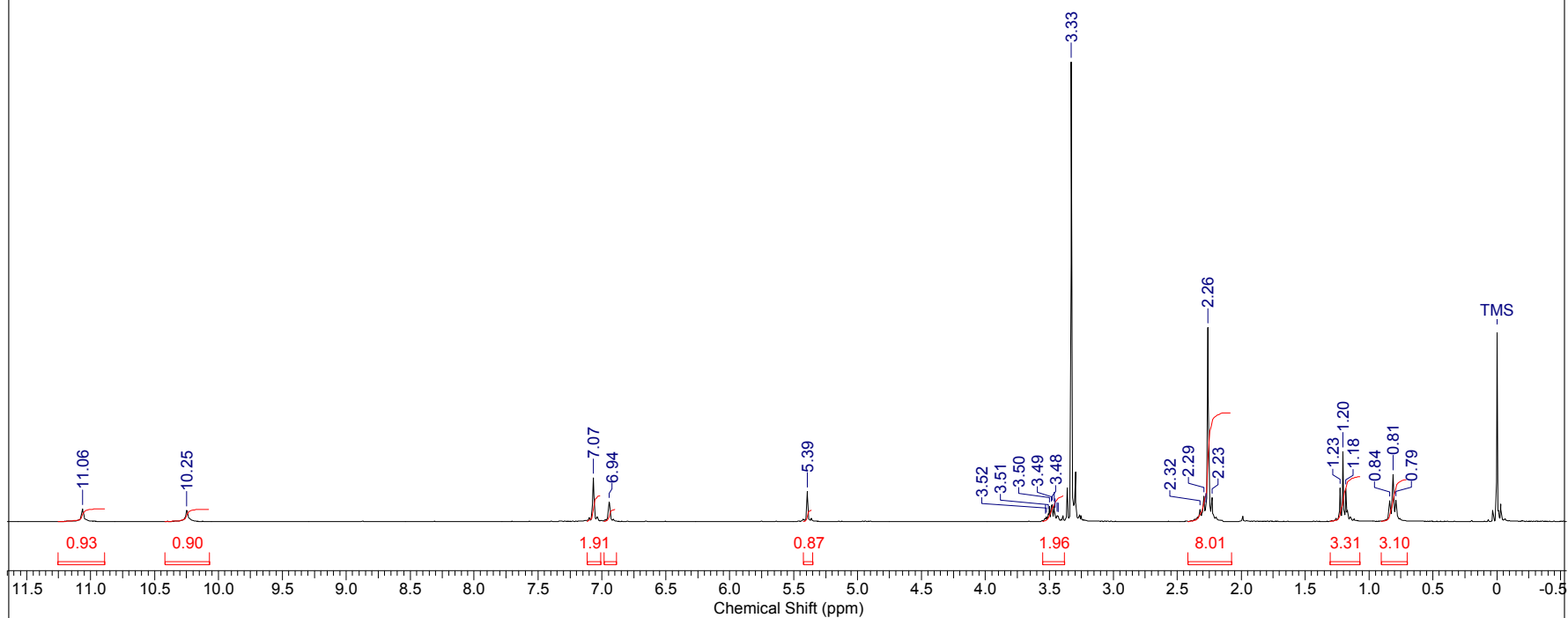
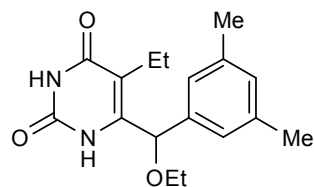
Acquisition Time (sec)	1.8148	Comment	ym1 042	Date	Sep 4 2004	File Name	D:\01_Research\SHIVA\NMR\Data\Yasser\YML042\ym10904C		
Frequency (MHz)	75.46	Nucleus	¹³ C	Number of Transients	256	Original Points Count	34048	Points Count	65536
Pulse Sequence	s2pul	Solvent	DMSO-D6	Sweep Width (Hz)	18761.73	Temperature (degree C)	25.000		

¹³C NMR Spectrum of Compound **4a** in DMSO-*d*₆



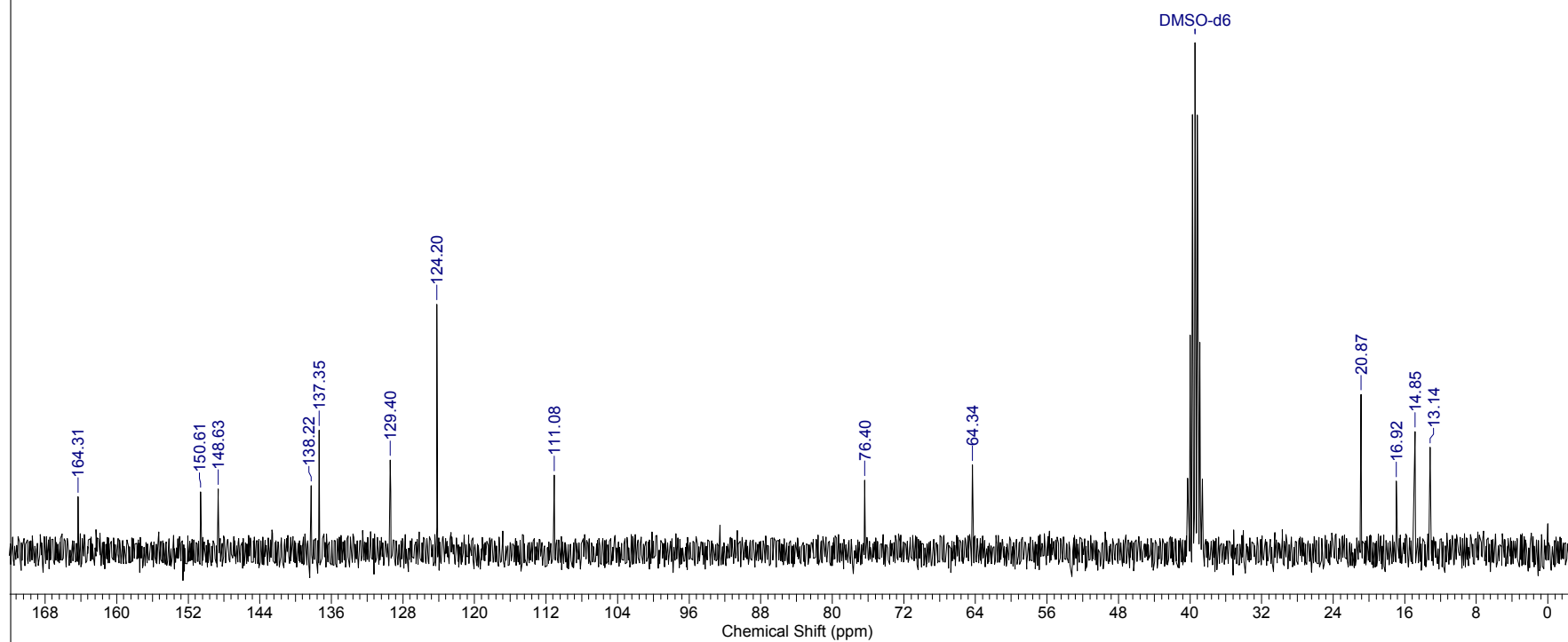
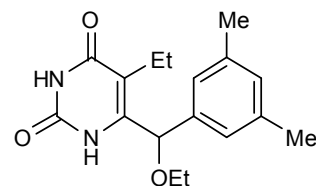
Acquisition Time (sec)	3.0027	Comment	ym1 041	Date	Sep 4 2004	File Name	D:\01_Research\SHIVA\NMR\Data\Yasser\YML041\ym10904H		
Frequency (MHz)	300.09	Nucleus	1H	Number of Transients	8	Original Points Count	18016	Points Count	32768
Pulse Sequence	s2pul	Solvent	DMSO-D6	Sweep Width (Hz)	6000.00	Temperature (degree C)	25.000		

¹H NMR Spectrum of Compound **4b** in DMSO-d₆



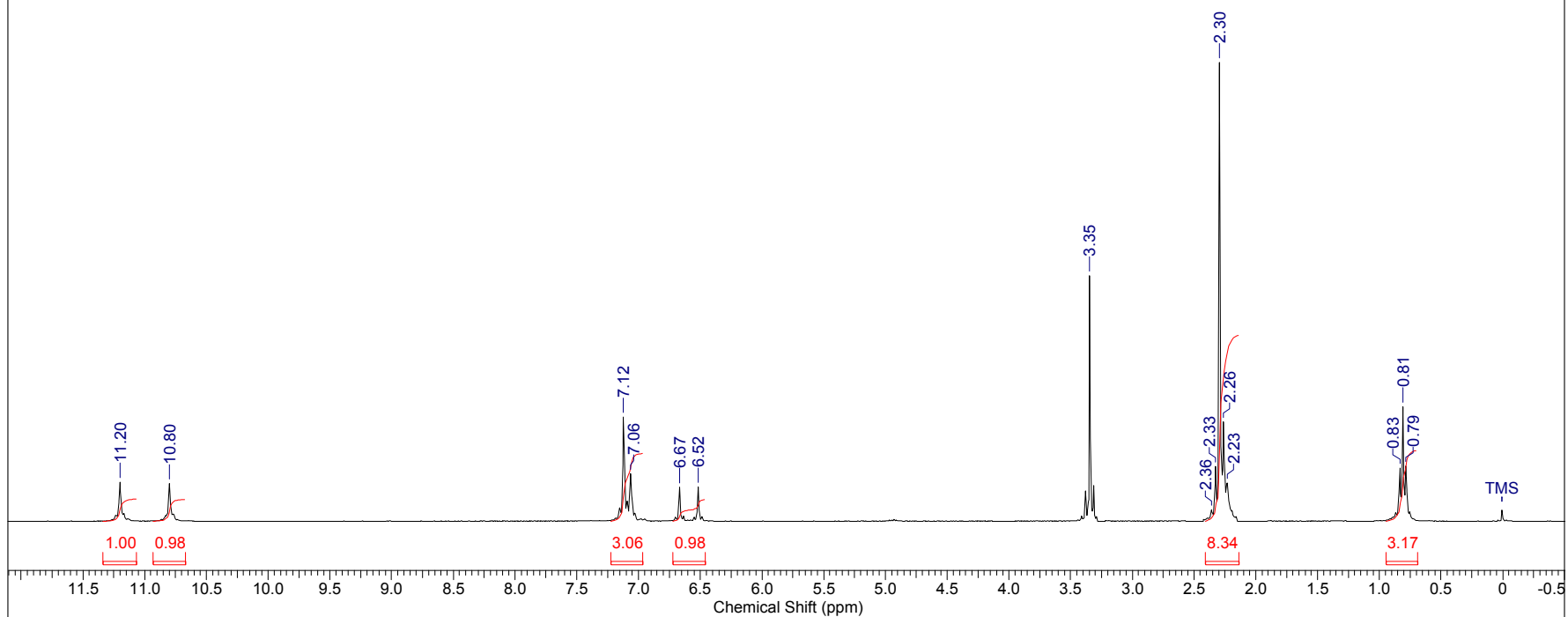
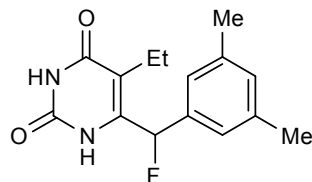
Acquisition Time (sec)	1.8148	Comment	ym1 041	Date	Sep 4 2004	File Name	D:\01_Research\SHIVA\NMR\Data\Yasser\YML041\ym10904C		
Frequency (MHz)	75.46	Nucleus	13C	Number of Transients	256	Original Points Count	34048	Points Count	65536
Pulse Sequence	s2pul	Solvent	DMSO-D6	Sweep Width (Hz)	18761.73	Temperature (degree C)	25.000		

^{13}C NMR Spectrum of Compound **4b** in $\text{DMSO-}d_6$



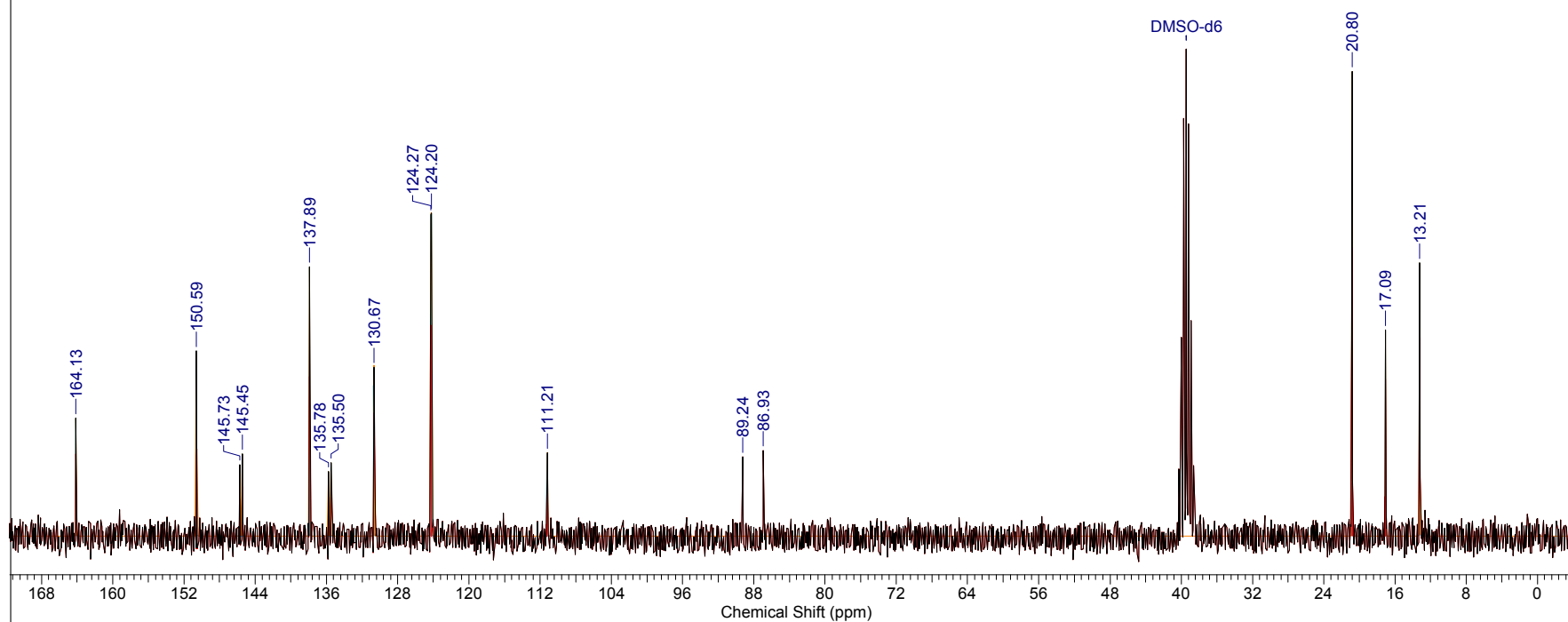
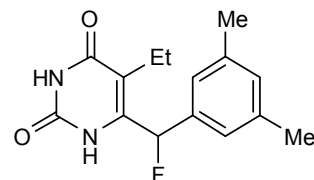
Acquisition Time (sec)	3.0027	Comment	ym1 05b	Date	Oct 1 2004	File Name	D:\01_Research\SHIVA\NMR\Data\Yasser\YML056\ym11001H		
Frequency (MHz)	300.09	Nucleus	1H	Number of Transients	8	Original Points Count	18016	Points Count	32768
Pulse Sequence	s2pul	Solvent	DMSO-D6	Sweep Width (Hz)	6000.00	Temperature (degree C)	25.000		

¹H NMR Spectrum of Compound **5** in DMSO-*d*₆



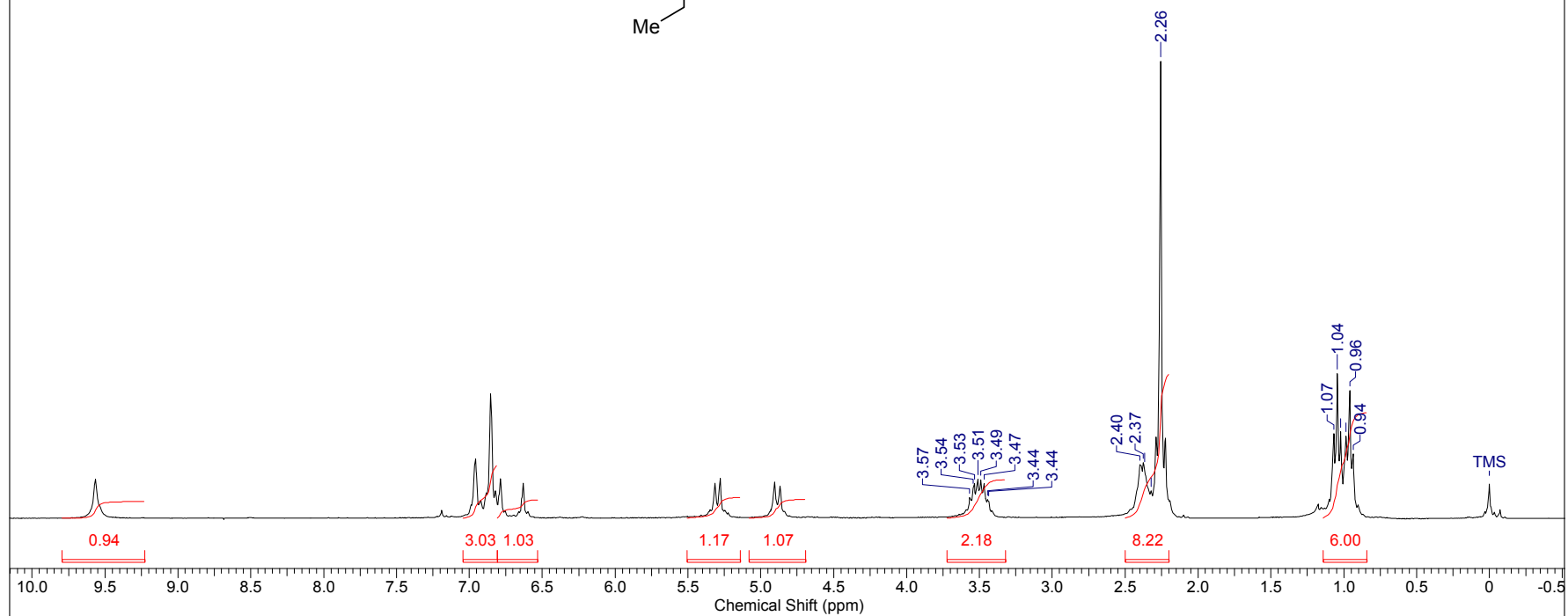
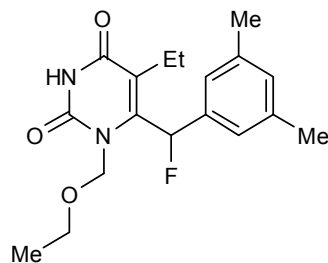
Acquisition Time (sec)	1.8148	Comment	yml 05b	Date	Oct 1 2004	File Name	D:\01_Research\SHIVA\NMR\Data\Yasser\YML056\yml1002C		
Frequency (MHz)	75.46	Nucleus	13C	Number of Transients	256	Original Points Count	34048	Points Count	65536
Pulse Sequence	s2pul	Solvent	DMSO-D6	Sweep Width (Hz)	18761.73	Temperature (degree C)	25.000		

¹³C NMR Spectrum of Compound **5** in DMSO-*d*₆



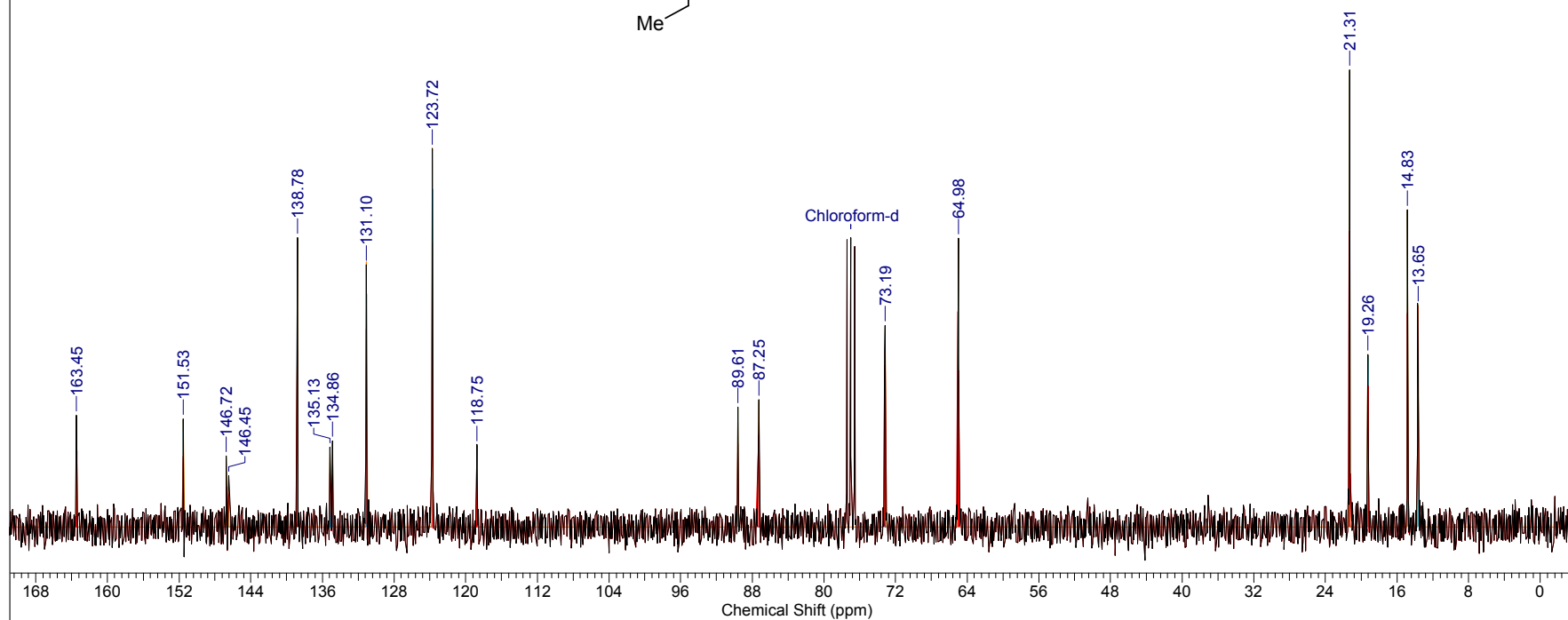
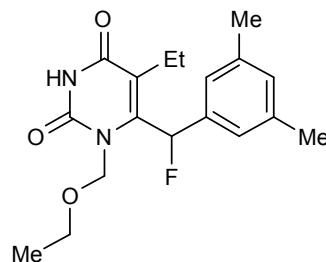
Acquisition Time (sec)	3.0027	Comment	yml 063	Date	Oct 8 2004	File Name	D:\01_Research\SHIVA\NMR\Data\Yasser\YML063\yml1008H		
Frequency (MHz)	300.09	Nucleus	1H	Number of Transients	8	Original Points Count	18016	Points Count	32768
Pulse Sequence	s2pul	Solvent	CHLOROFORM-D			Sweep Width (Hz)	6000.00	Temperature (degree C)	25.000

¹H NMR Spectrum of Compound **9a** in CDCl₃



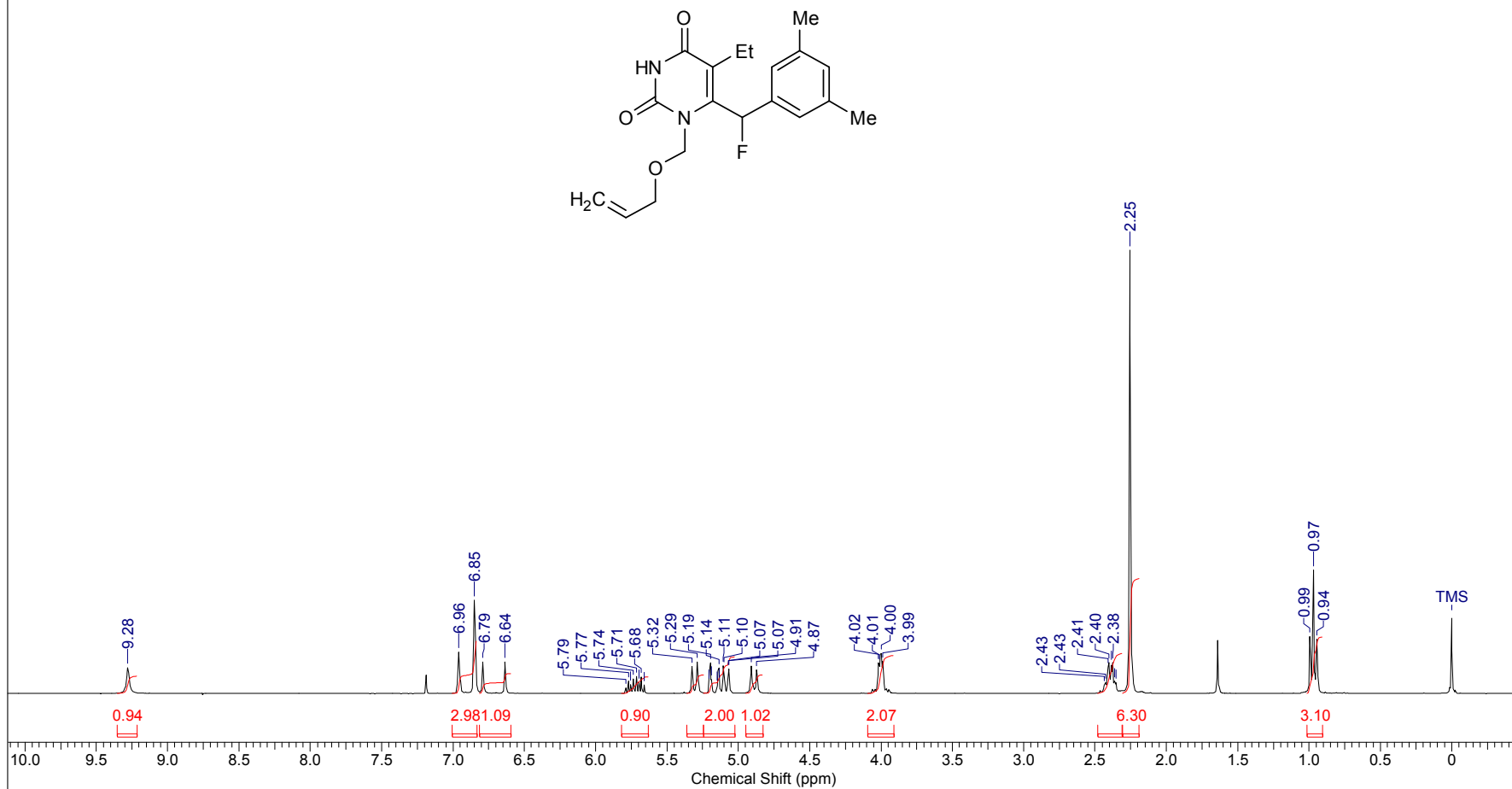
Acquisition Time (sec)	1.8148	Comment	yml 063	Date	Oct 8 2004	File Name	D:\01_Research\SHIVA\NMR\Data\Yasser\YML063\yml1008C		
Frequency (MHz)	75.46	Nucleus	13C	Number of Transients	256	Original Points Count	34048	Points Count	65536
Pulse Sequence	s2pul	Solvent	CHLOROFORM-D			Sweep Width (Hz)	18761.73	Temperature (degree C)	25.000

¹³C NMR Spectrum of Compound **9a** in CDCl₃



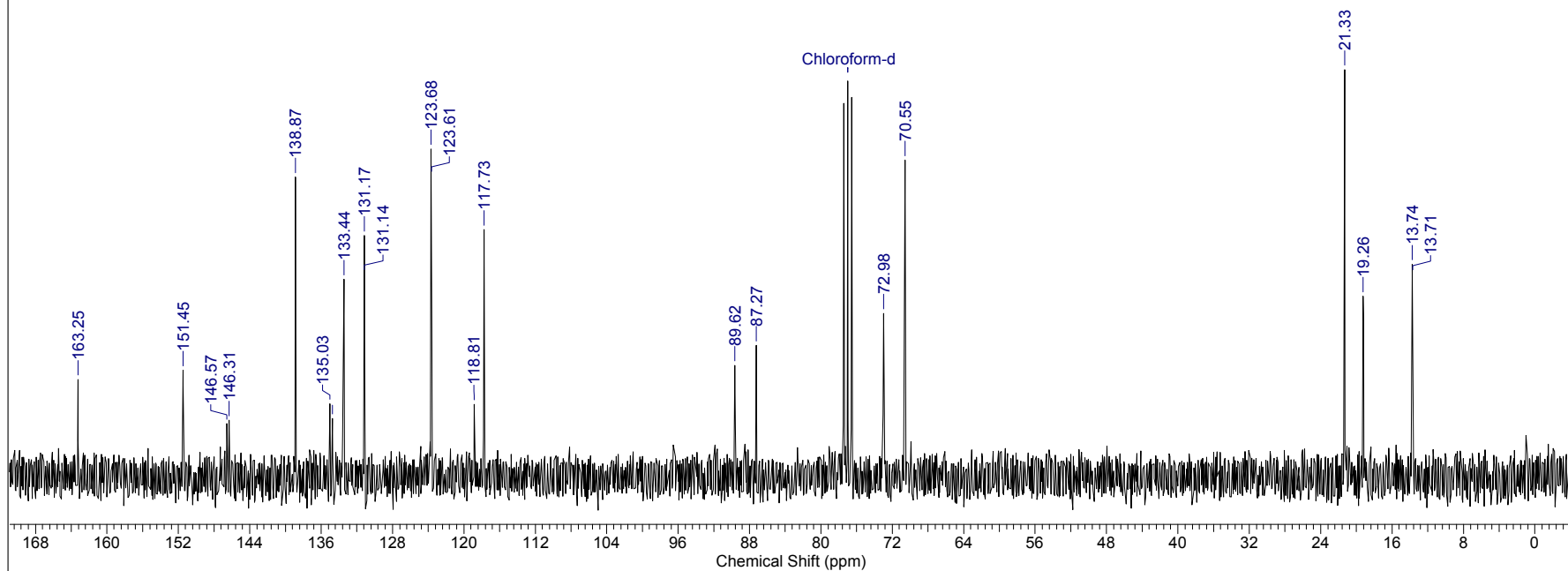
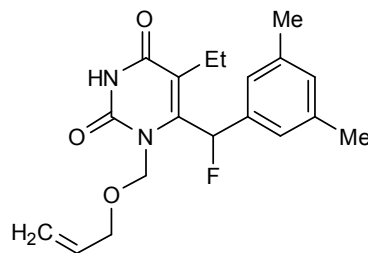
Acquisition Time (sec)	3.0027	Comment	yml 073	Date	Oct 29 2004	File Name	D:\01_Research\SHIVA\NMR\Data\Yasser\YML073\yml1029H		
Frequency (MHz)	300.09	Nucleus	1H	Number of Transients	8	Original Points Count	18016	Points Count	32768
Pulse Sequence	s2pul	Solvent	CHLOROFORM-D			Sweep Width (Hz)	6000.00	Temperature (degree C)	25.000

¹H NMR Spectrum of Compound **9b** in CDCl₃



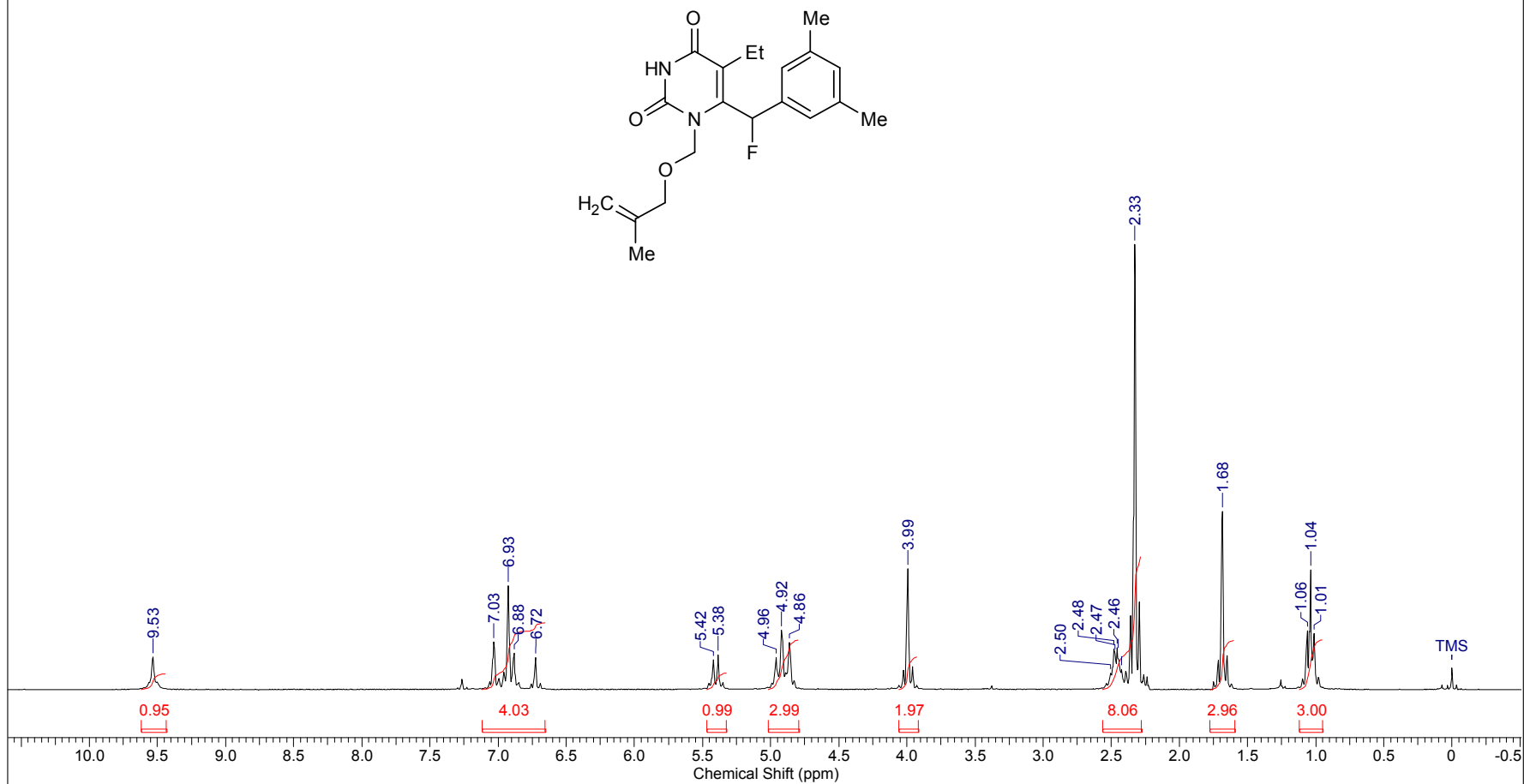
Acquisition Time (sec)	1.8148	Comment	yml 073	Date	Oct 29 2004	File Name	D:\01_Research\SHIVA\NMR\Data\Yasser\YML073\yml1029C		
Frequency (MHz)	75.46	Nucleus	¹³ C	Number of Transients	256	Original Points Count	34048	Points Count	65536
Pulse Sequence	s2pul	Solvent	CHLOROFORM-D			Sweep Width (Hz)	18761.73	Temperature (degree C)	25.000

¹³C NMR Spectrum of Compound **9b** in CDCl₃



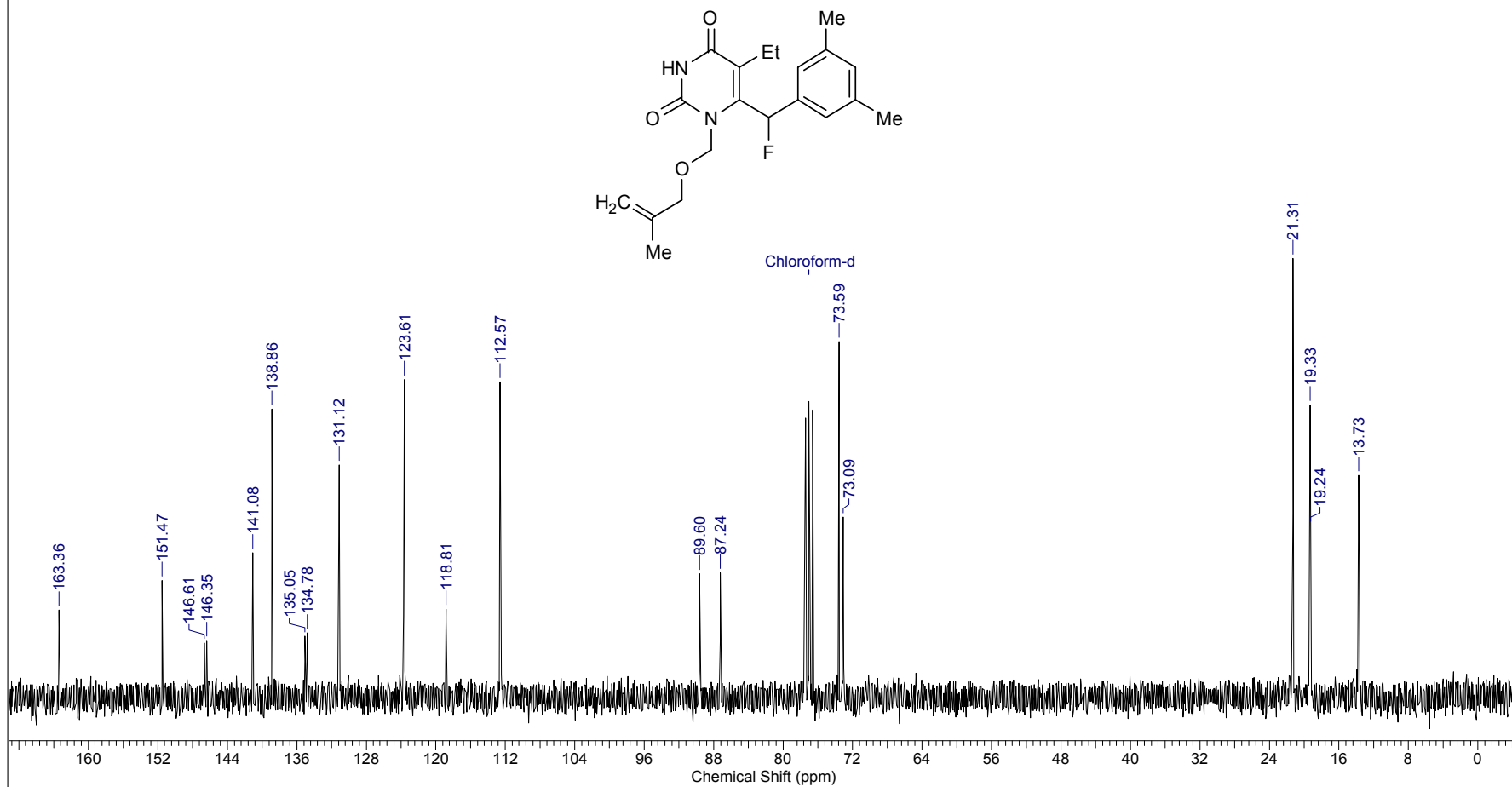
Acquisition Time (sec)	3.0027	Comment	yml 072	Date	Oct 22 2004	File Name	D:\01_Research\SHIVA\NMR\Data\Yasser\YML072\yml1022H		
Frequency (MHz)	300.09	Nucleus	1H	Number of Transients	8	Original Points Count	18016	Points Count	32768
Pulse Sequence	s2pul	Solvent	CHLOROFORM-D			Sweep Width (Hz)	6000.00	Temperature (degree C)	25.000

¹H NMR Spectrum of Compound **9c** in CDCl₃



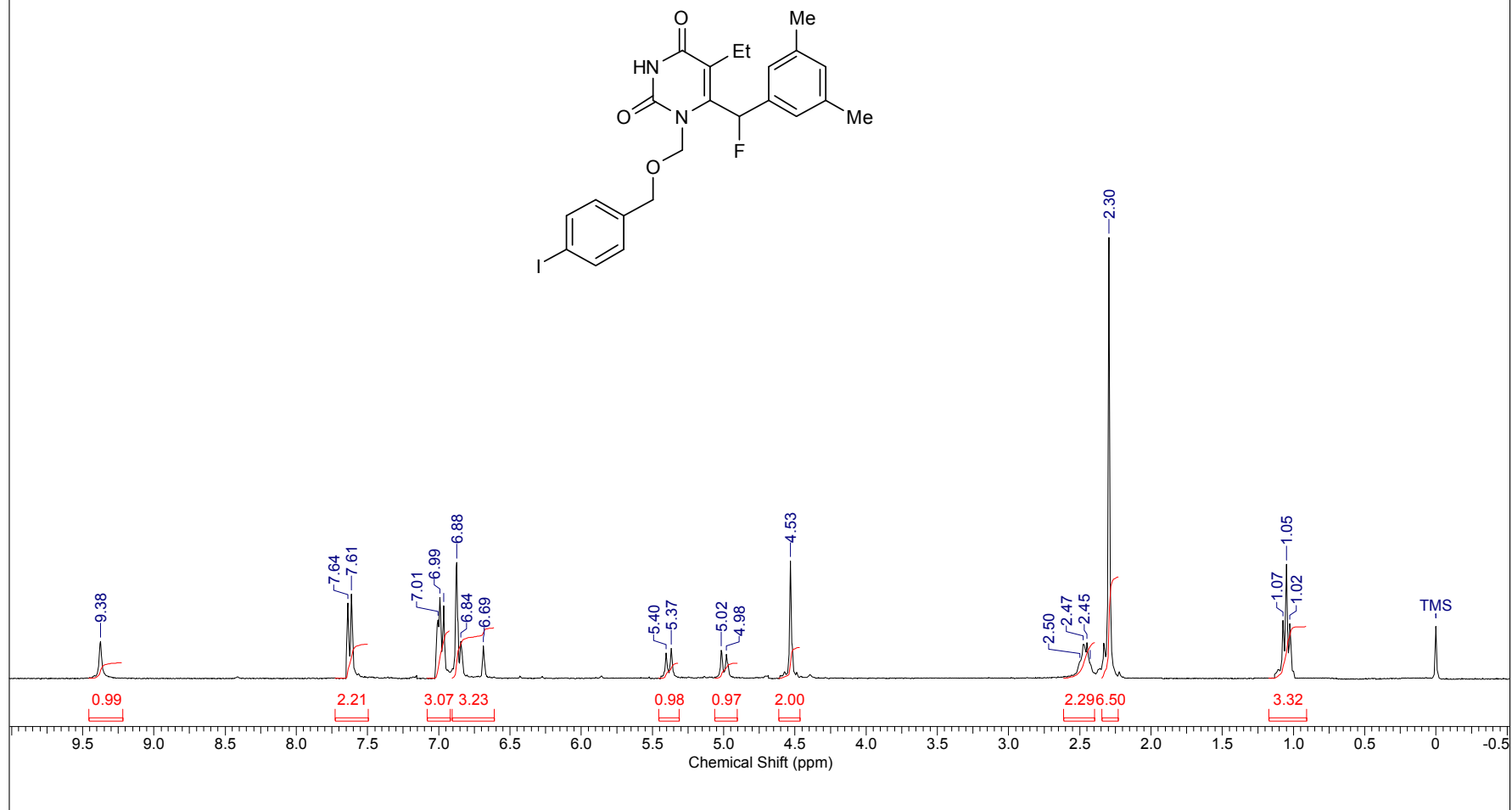
Acquisition Time (sec)	1.8148	Comment	yml 072	Date	Oct 22 2004	File Name	D:\01_Research\SHIVA\NMR\Data\Yasser\YML072\yml1022C		
Frequency (MHz)	75.46	Nucleus	¹³ C	Number of Transients	256	Original Points Count	34048	Points Count	65536
Pulse Sequence	s2pul	Solvent	CHLOROFORM-D			Sweep Width (Hz)	18761.73	Temperature (degree C)	25.000

¹³C NMR Spectrum of Compound **9c** in CDCl₃



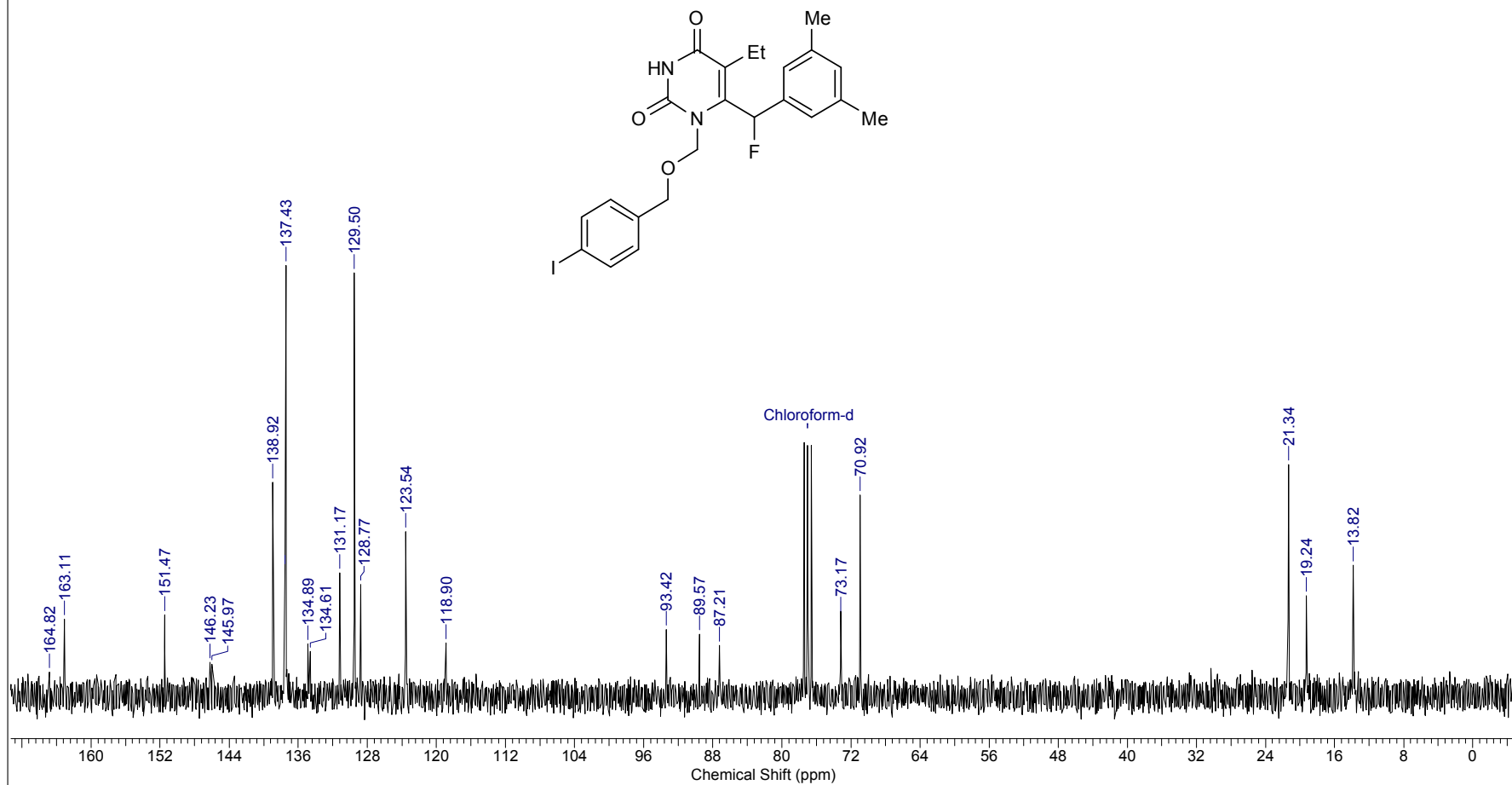
Acquisition Time (sec)	3.0027	Comment	yml 218	Date	Sep 16 2005	File Name	D:\01_Research\SHIVA\NMR\Data\Yasser\YML218\yml0916H		
Frequency (MHz)	300.09	Nucleus	1H	Number of Transients	8	Original Points Count	18016	Points Count	32768
Pulse Sequence	s2pul	Solvent	CHLOROFORM-D			Sweep Width (Hz)	6000.00	Temperature (degree C)	25.000

¹H NMR Spectrum of Compound **11a** in CDCl₃



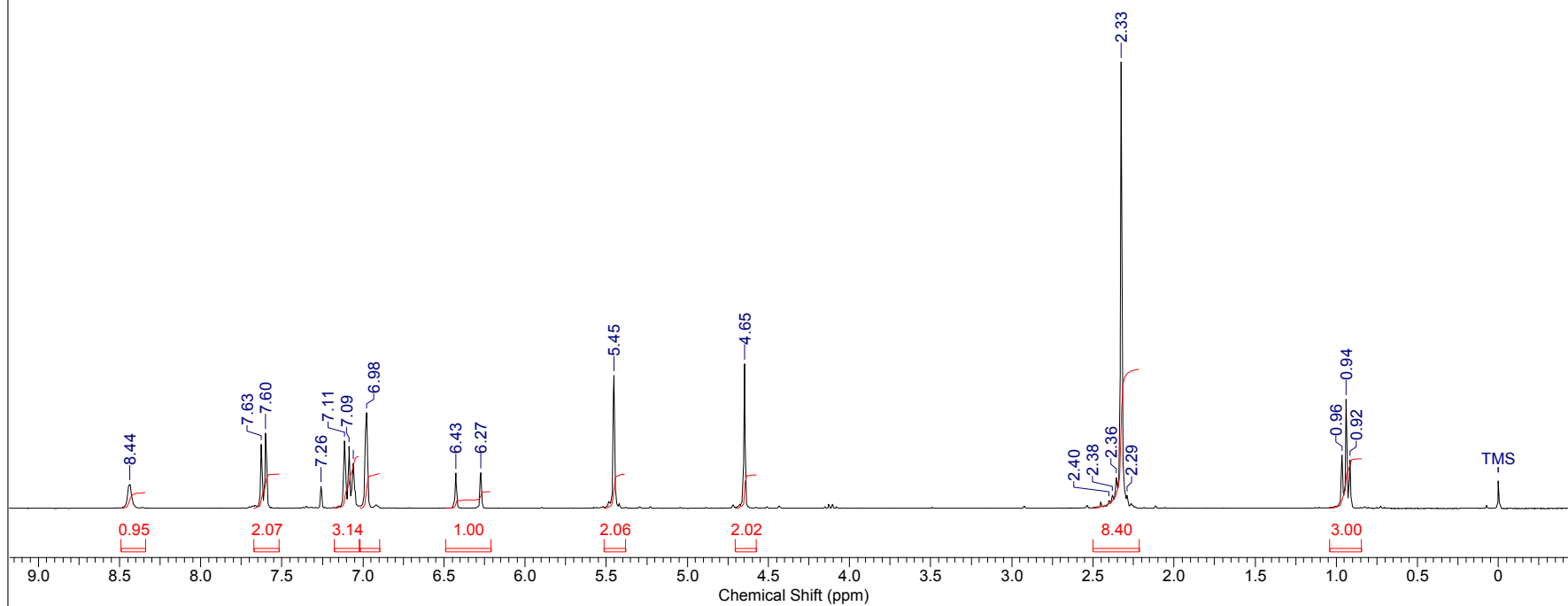
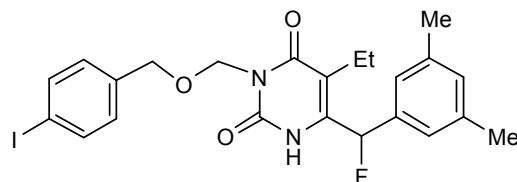
Acquisition Time (sec)	1.8148	Comment	yml 218	Date	Sep 16 2005	File Name	D:\01_Research\SHIVA\NMR\Data\Yasser\YML218\yml0916C		
Frequency (MHz)	75.46	Nucleus	¹³ C	Number of Transients	256	Original Points Count	34048	Points Count	65536
Pulse Sequence	s2pul	Solvent	CHLOROFORM-D			Sweep Width (Hz)	18761.73	Temperature (degree C)	25.000

¹³C NMR Spectrum of Compound **11a** in CDCl₃



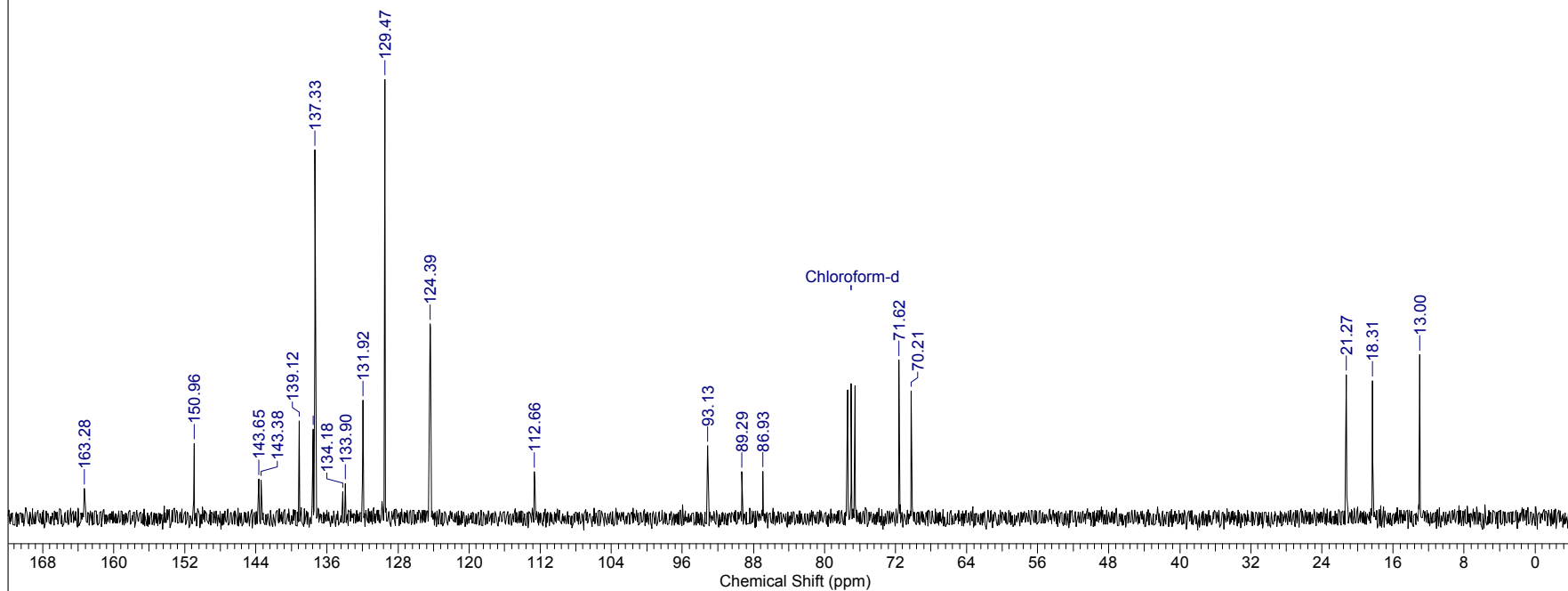
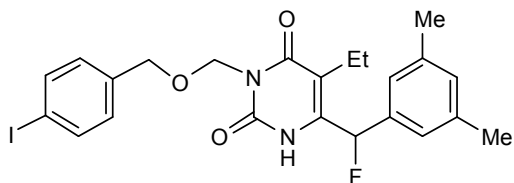
Acquisition Time (sec)	3.0027	Comment	ym1 304	Date	Feb 8 2007		
File Name	D:\01_Research\SHIVAN\NMR\Data\Yasser_01_01_2007\YML304\ym10208H				Frequency (MHz)	300.09	Nucleus 1H
Number of Transients	8	Original Points Count	18016	Points Count	32768	Pulse Sequence	s2pul
Solvent	CHLOROFORM-D			Sweep Width (Hz)	6000.00	Temperature (degree C)	25.000

¹H NMR Spectrum of Compound **11b** in CDCl₃



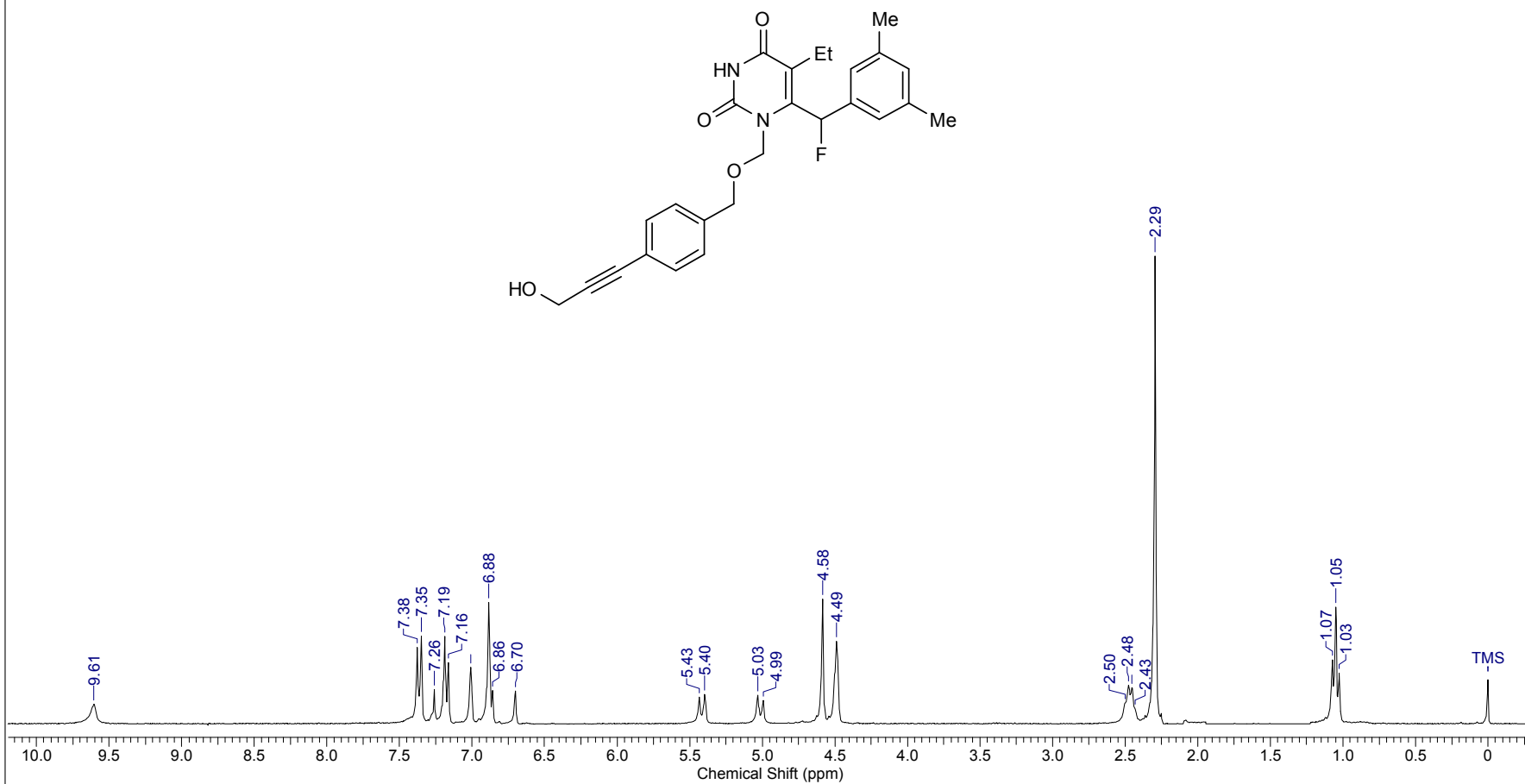
Acquisition Time (sec)	1.8148	Comment	yml 304	Date	Feb 8 2007
File Name	D:\01_Research\SHIVA\NMR\Data\Yasser_01_01_2007\YML304\yml0208C			Frequency (MHz)	75.46
Nucleus	¹³ C	Number of Transients	256	Original Points Count	34048
Pulse Sequence	s2pul	Solvent	CHLOROFORM-D	Points Count	65536
Temperature (degree C)	25.000			Sweep Width (Hz)	18761.73

¹³C NMR Spectrum of Compound **11b** in CDCl₃



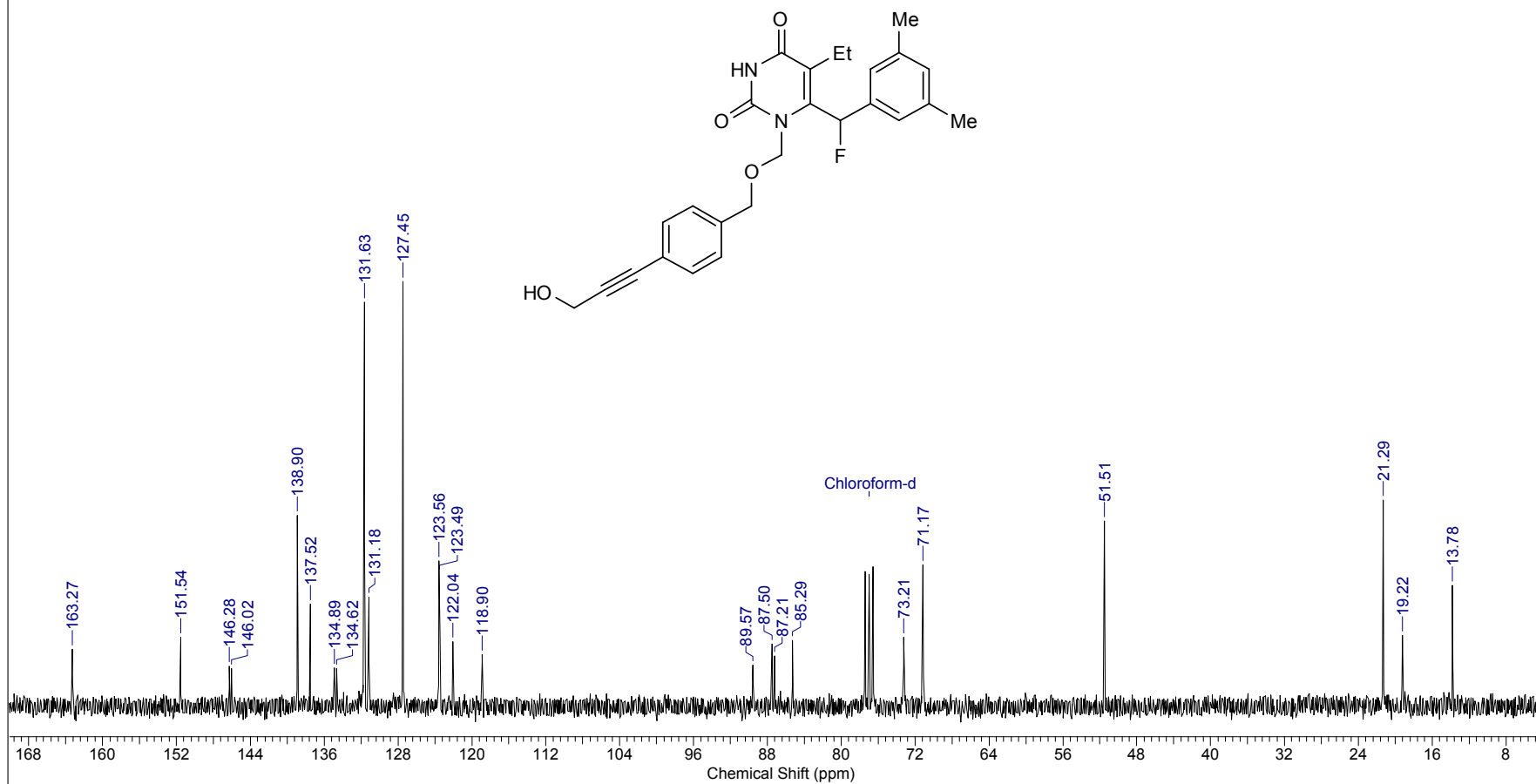
Acquisition Time (sec)	3.0027	Comment	ym1 220	Date	Feb 13 2007		
File Name	D:\01_Research\SHIVA\NMR\Data\Yasser_01_01_2007\YML220\ym10213H				Frequency (MHz)	300.09	Nucleus 1H
Number of Transients	8	Original Points Count	18016	Points Count	32768	Pulse Sequence	s2pul
Solvent	CHLOROFORM-D			Sweep Width (Hz)	6000.00	Temperature (degree C)	25.000

¹H NMR Spectrum of Compound **12 (YML220)** in CDCl₃



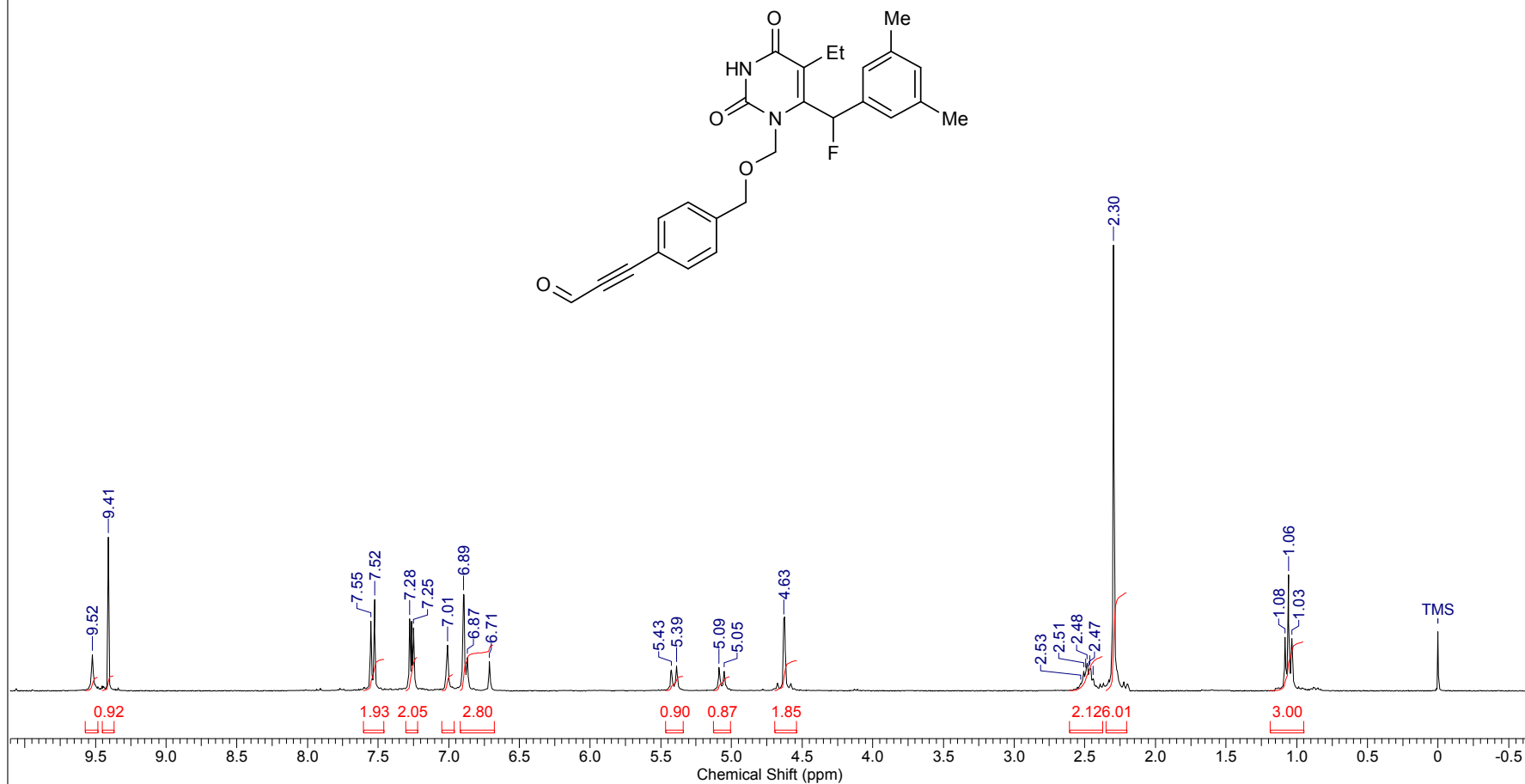
Acquisition Time (sec)	1.8148	Comment	yml 220	Date	Feb 13 2007	
File Name	D:\01_Research\SHIVA\NMR\Data\Yasser_01_01_2007\YML220\yml0213C				Frequency (MHz)	75.46
Nucleus	¹³ C	Number of Transients	256	Original Points Count	34048	Points Count 65536
Pulse Sequence	s2pul	Solvent	CHLOROFORM-D		Sweep Width (Hz)	18761.73
Temperature (degree C)	25.000					

¹³C NMR Spectrum of Compound **12** (YML220) in CDCl₃



Acquisition Time (sec)	3.0027	Comment	yml 222	Date	Sep 23 2005	File Name	D:\01_Research\SHIVA\NMR\Data\Yasser\YML222\yml0923H		
Frequency (MHz)	300.09	Nucleus	1H	Number of Transients	8	Original Points Count	18016	Points Count	32768
Pulse Sequence	s2pul	Solvent	CHLOROFORM-D			Sweep Width (Hz)	6000.00	Temperature (degree C)	25.000

¹H NMR Spectrum of Compound **13** in CDCl₃



Acquisition Time (sec)	1.8148	Comment	yml 222	Date	Sep 23 2005	File Name	D:\01_Research\SHIVA\NMR\Data\Yasser\YML222\yml0923C		
Frequency (MHz)	75.46	Nucleus	¹³ C	Number of Transients	256	Original Points Count	34048	Points Count	65536
Pulse Sequence	s2pul	Solvent	CHLOROFORM-D			Sweep Width (Hz)	18761.73	Temperature (degree C)	25.000

¹³C NMR Spectrum of Compound **13** in CDCl₃

