

Supporting Information for:

(Synthesis and) Structure Activity Relationships of Schweinfurthin Indoles

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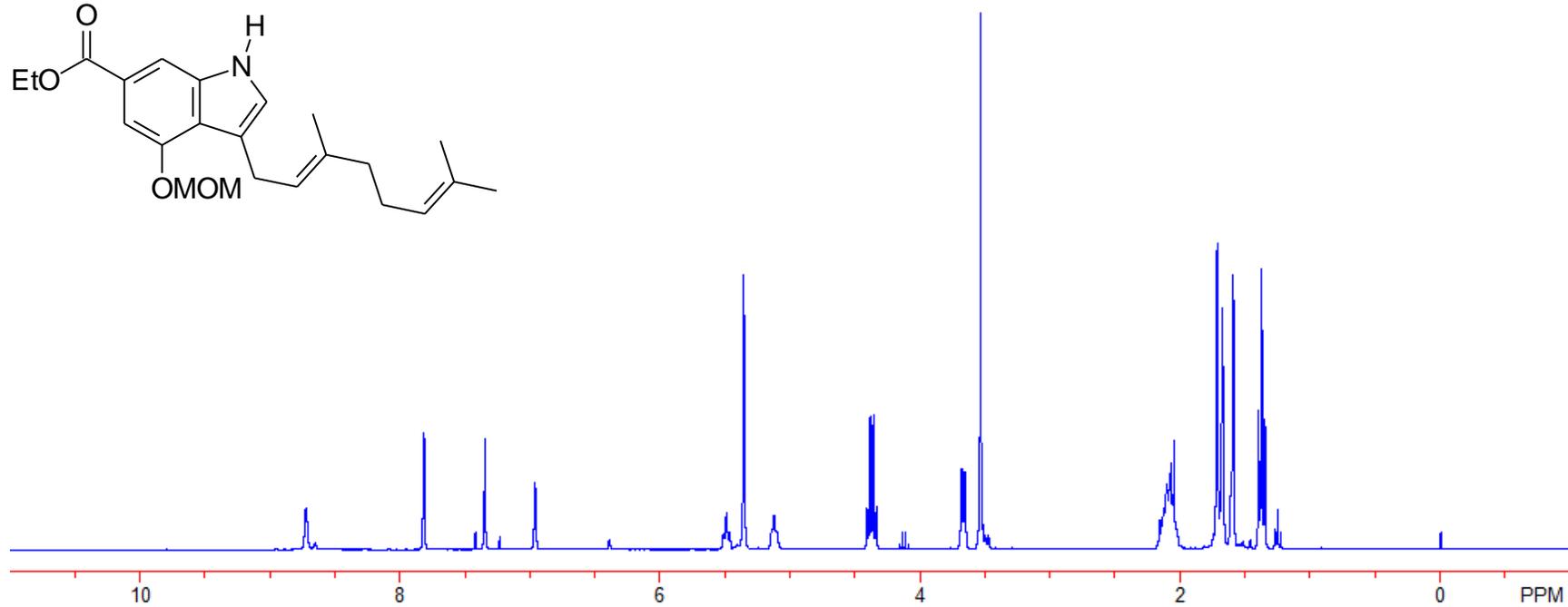
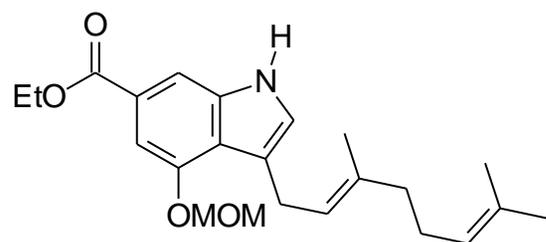
^b*Molecular Targets Laboratory, Center for Cancer Research, NCI-Frederick, Frederick, MD 21702*

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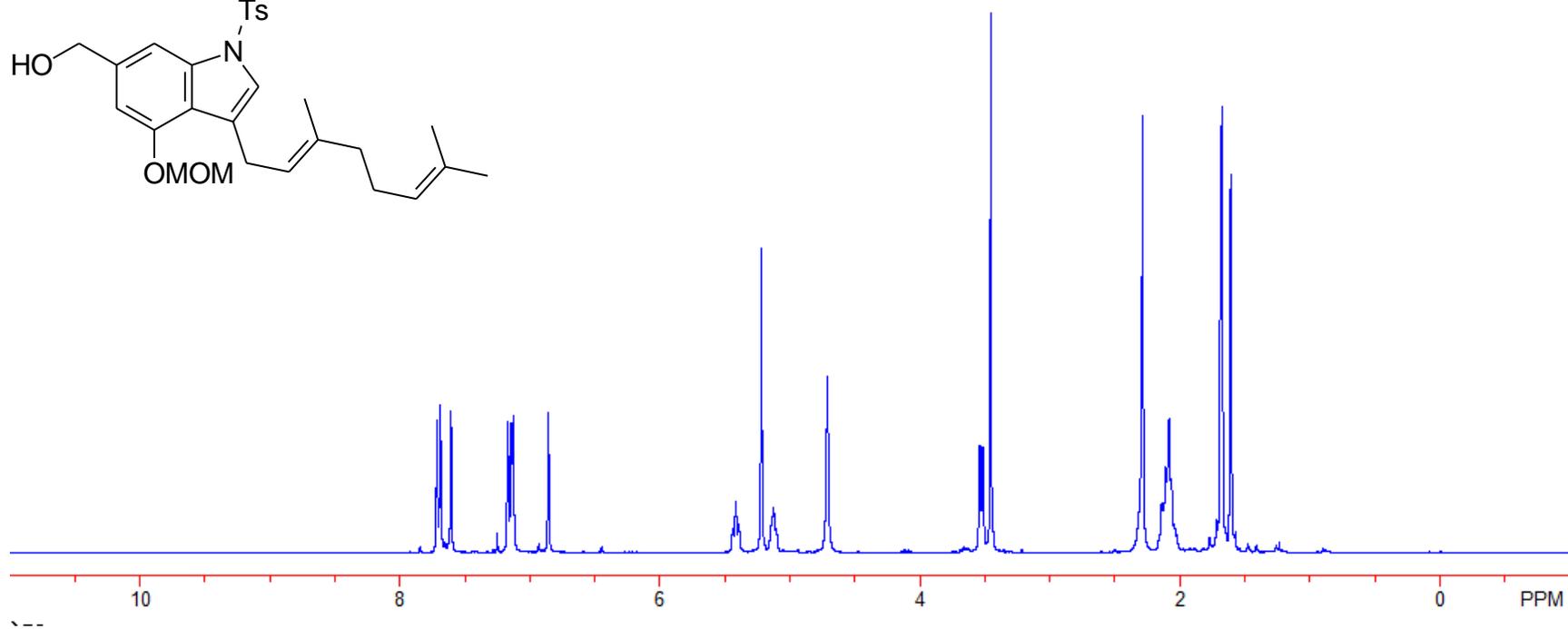
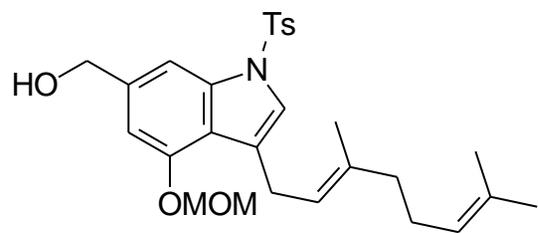
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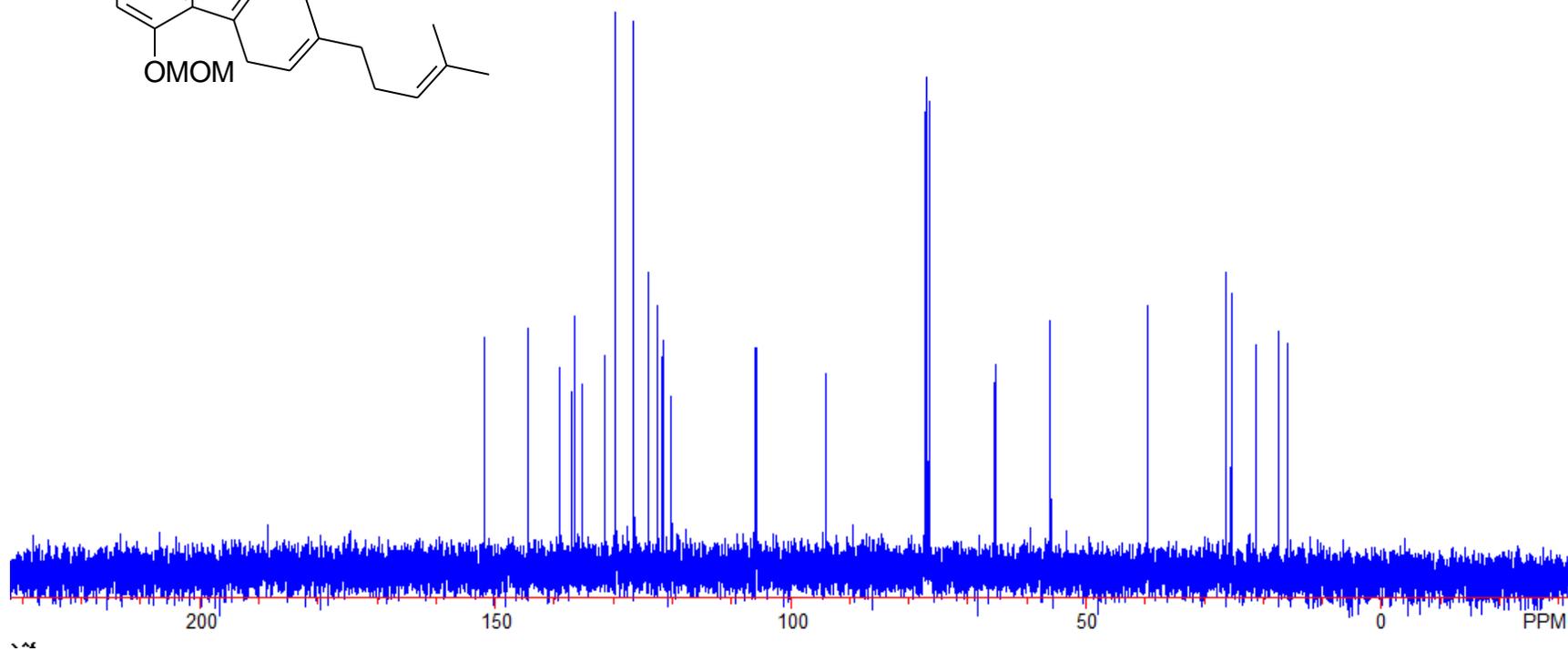
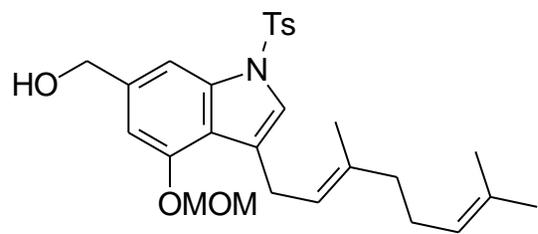
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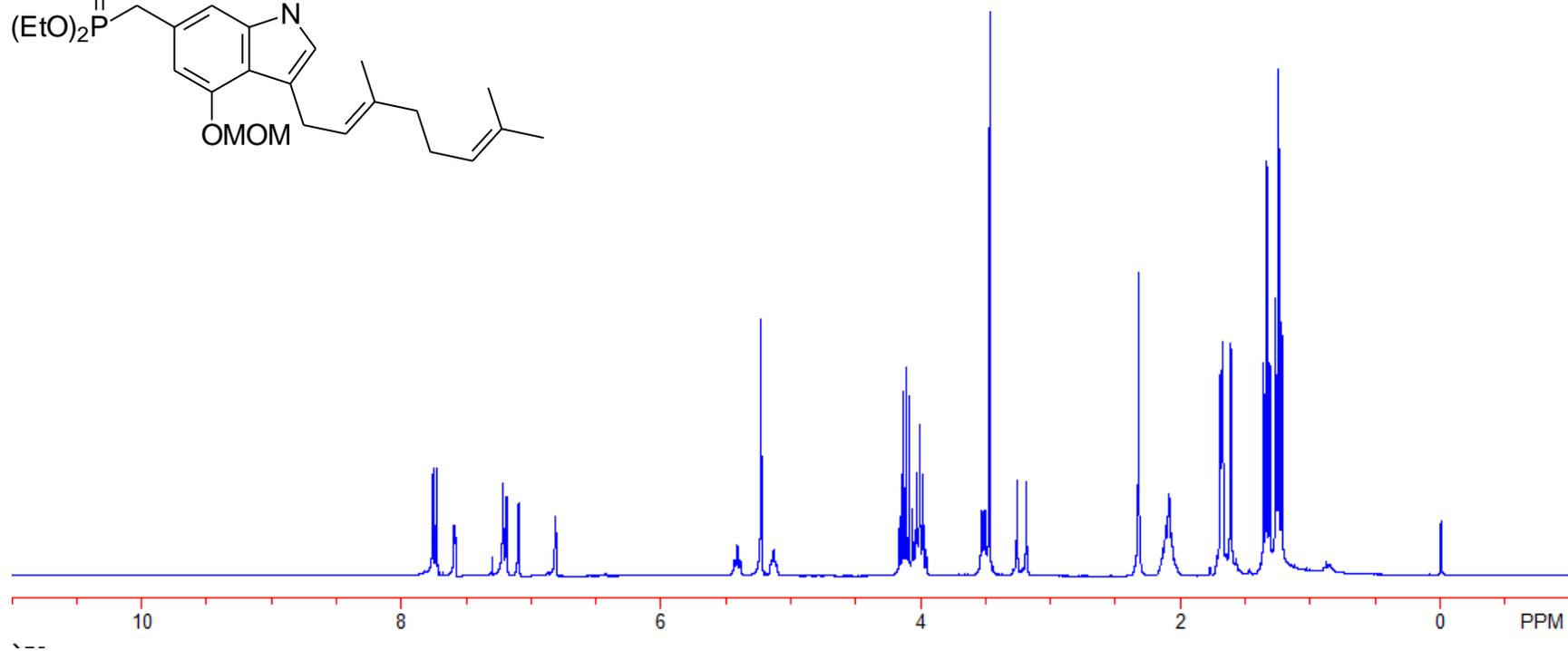
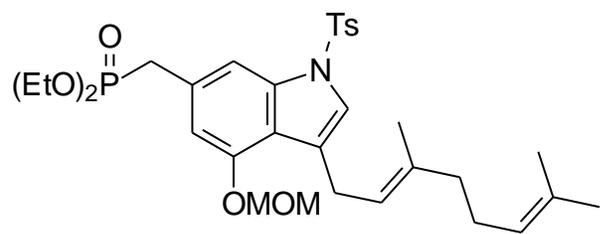


300 MHz ¹H NMR Spectrum for Compound 12

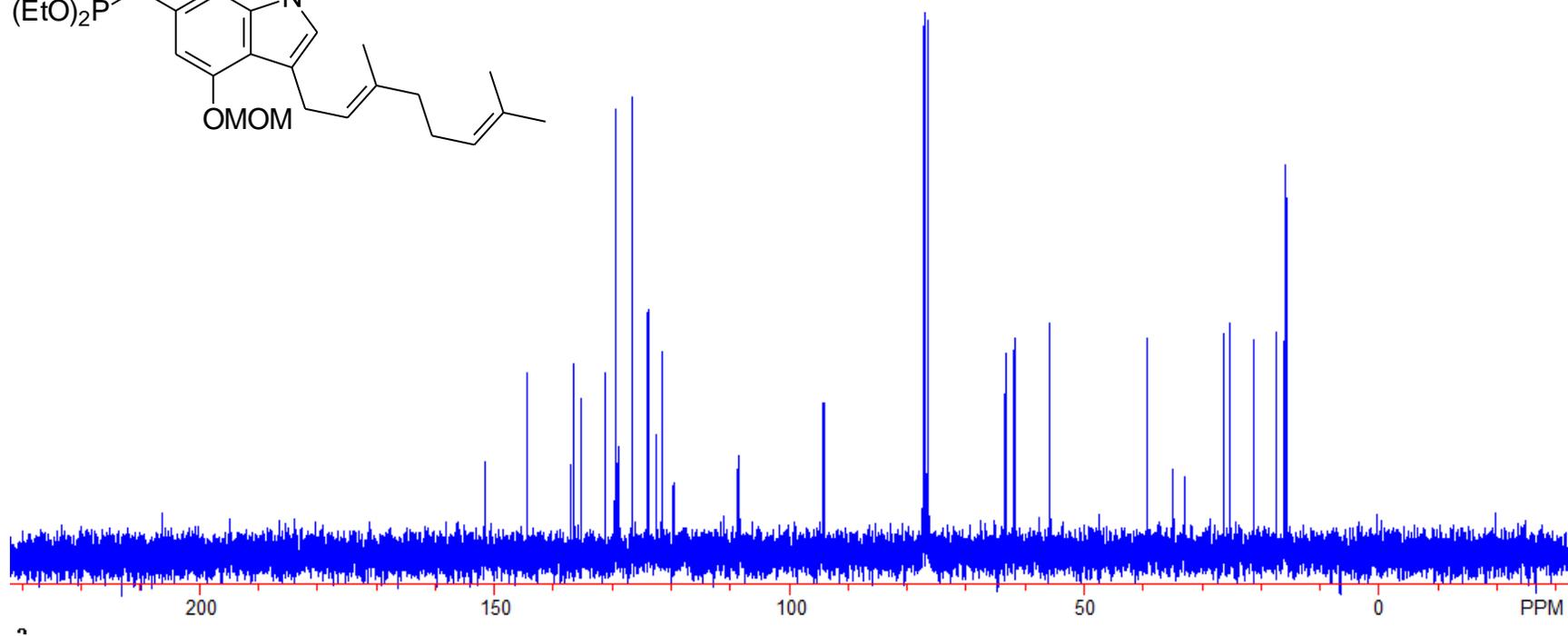
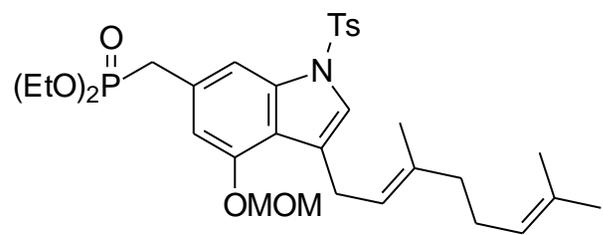




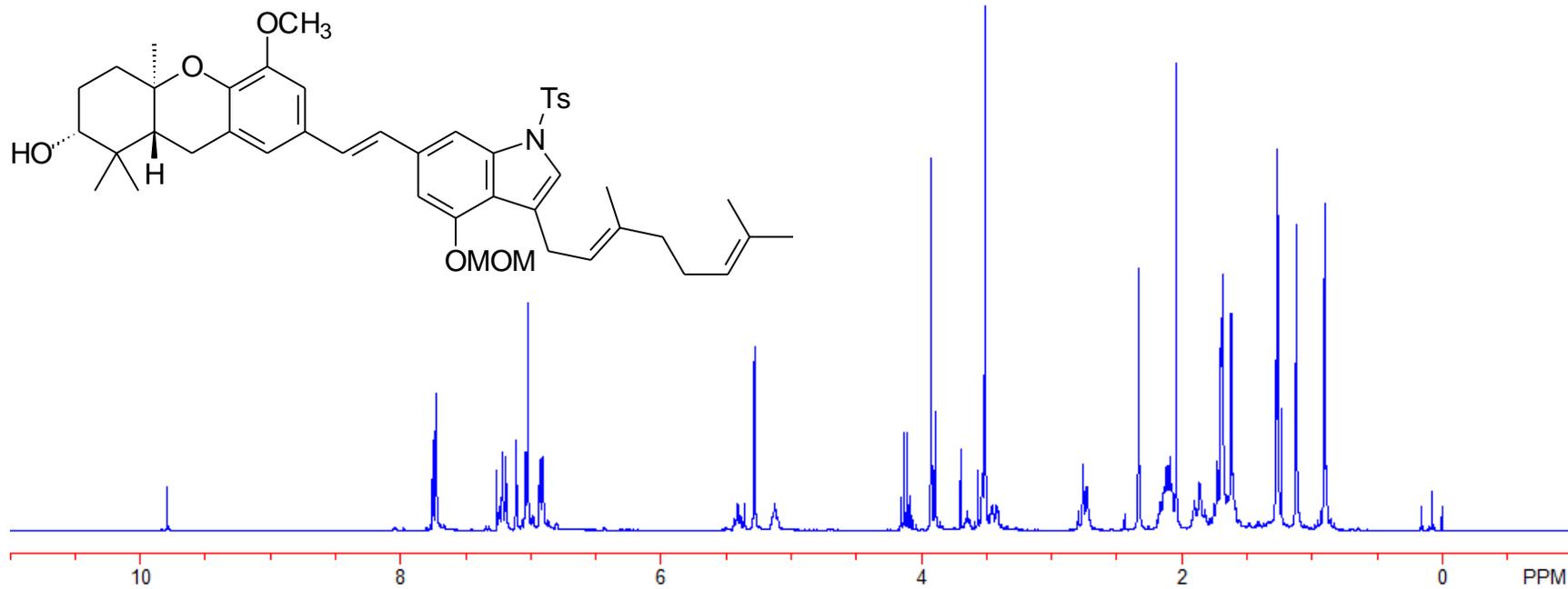
75 MHz ¹³C NMR Spectrum for Compound 13



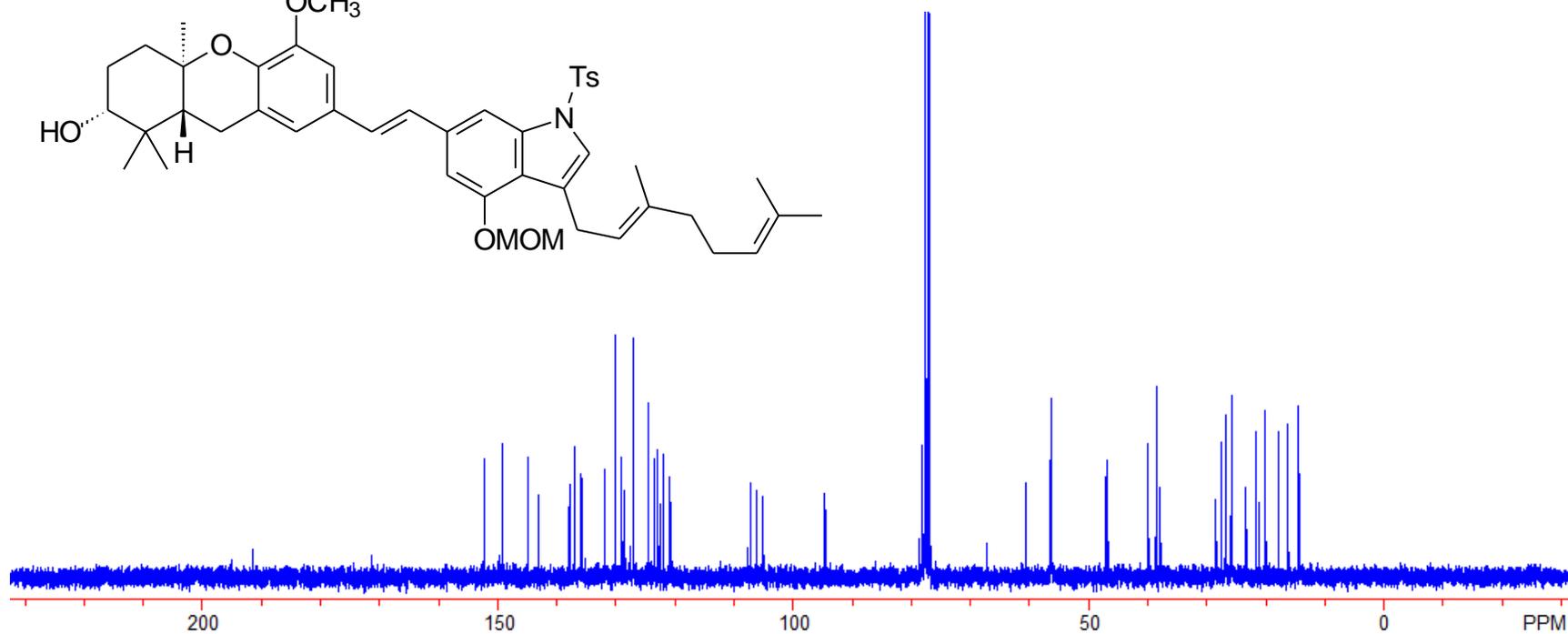
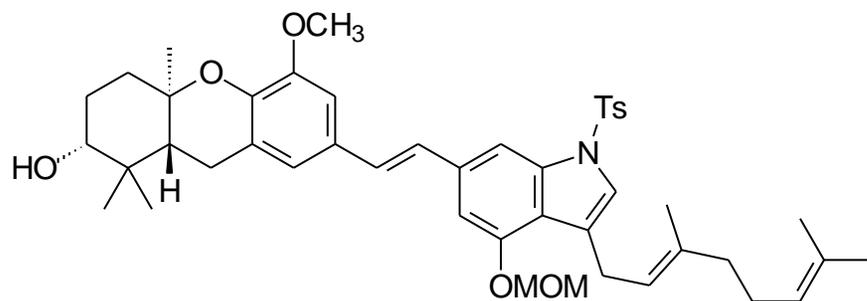
300 MHz ¹H NMR Spectrum for Compound 14



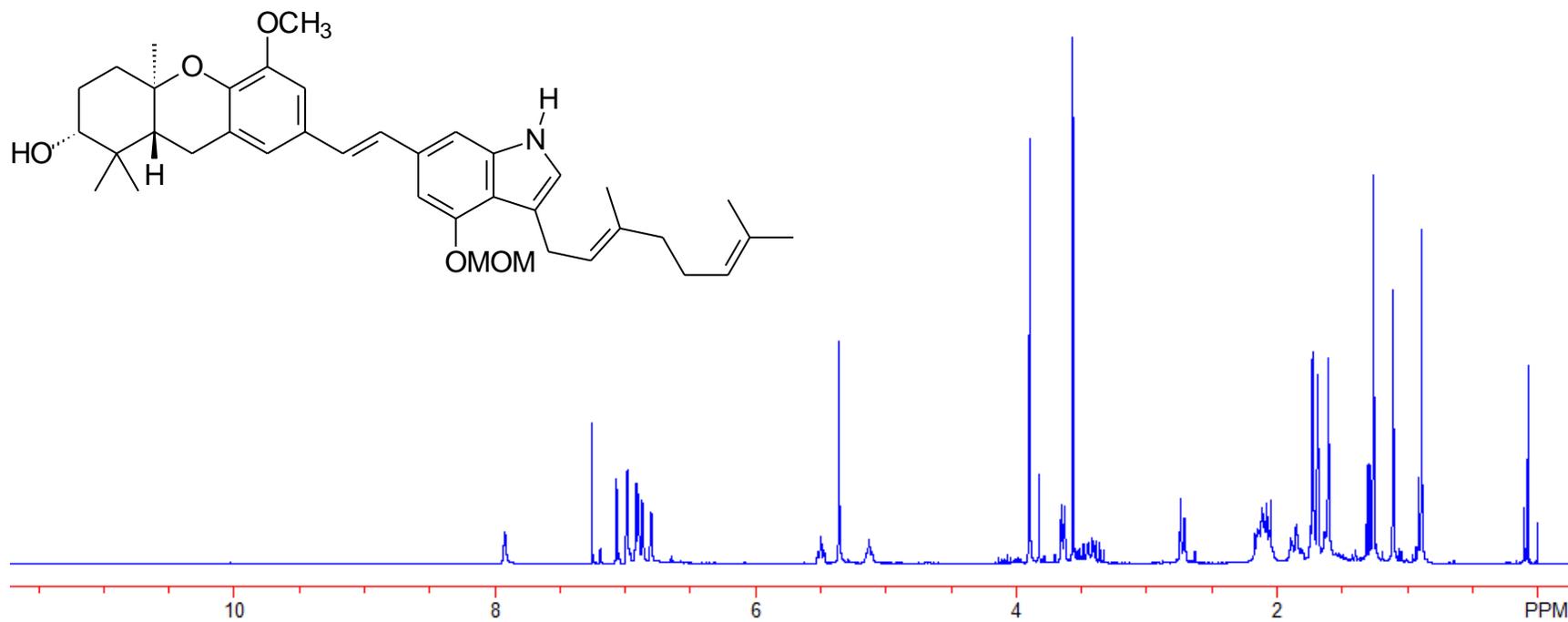
75 MHz ¹³C NMR Spectrum for Compound 14



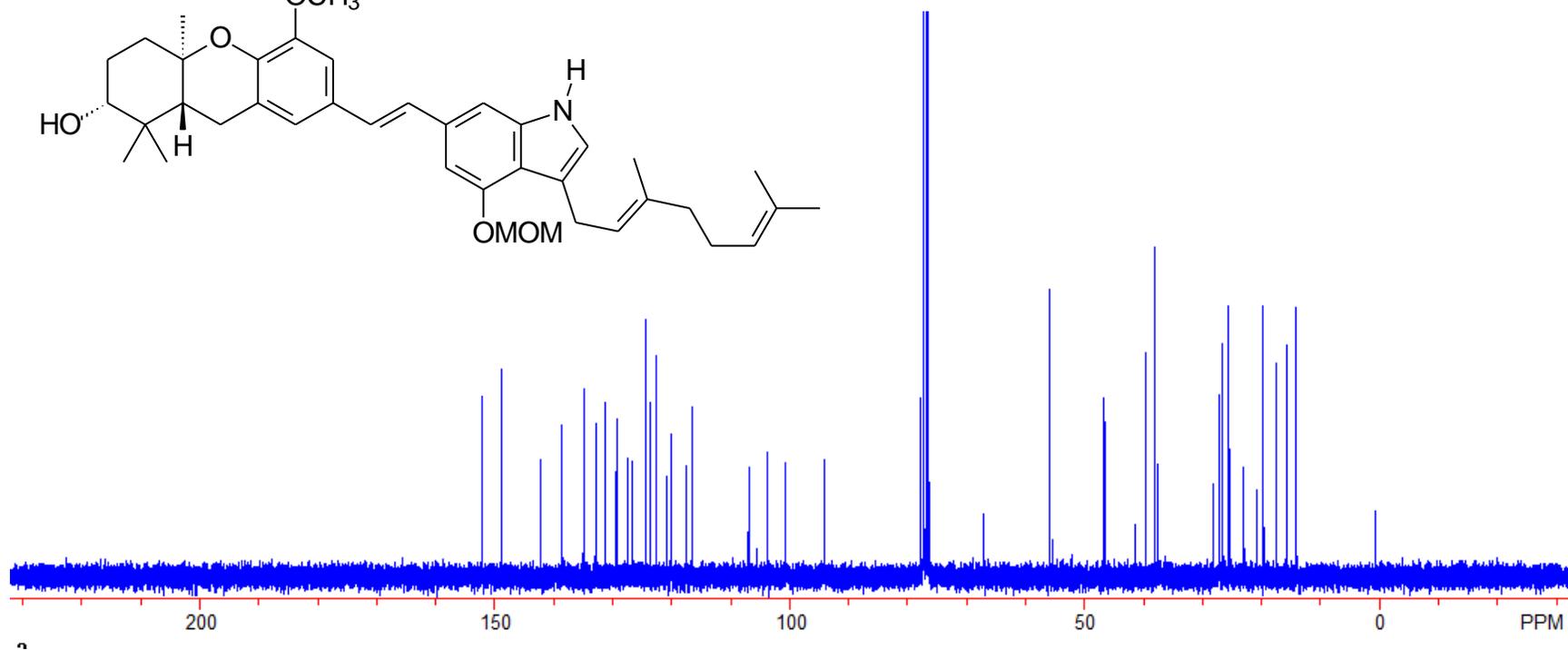
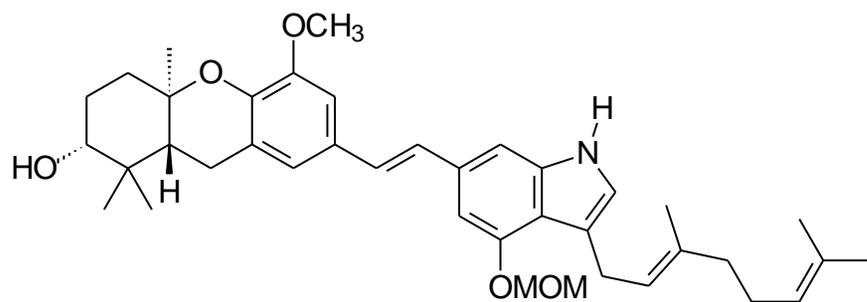
300 MHz ¹H NMR Spectrum for Compound 16



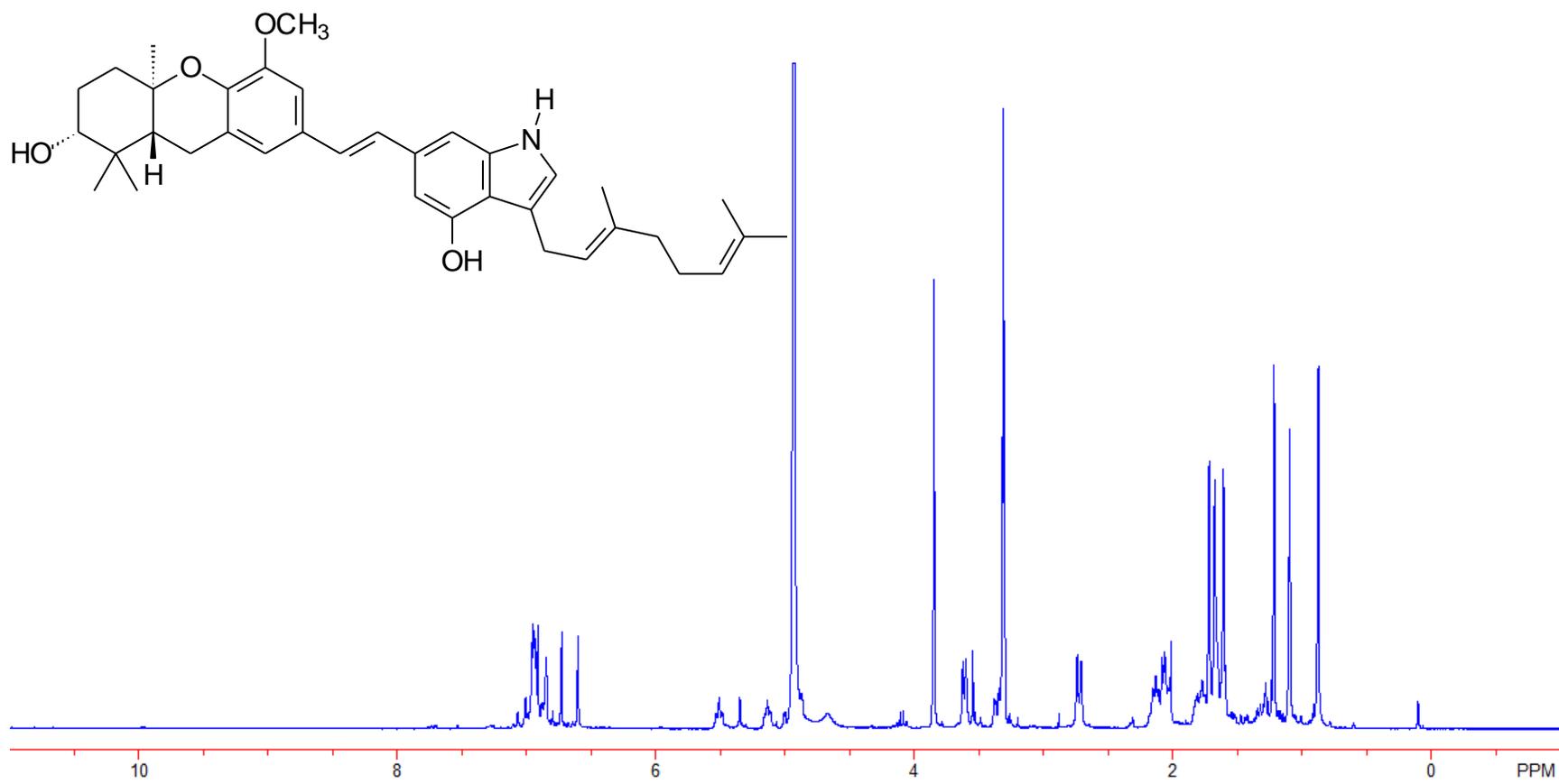
75 MHz ¹³C NMR Spectrum for Compound 16



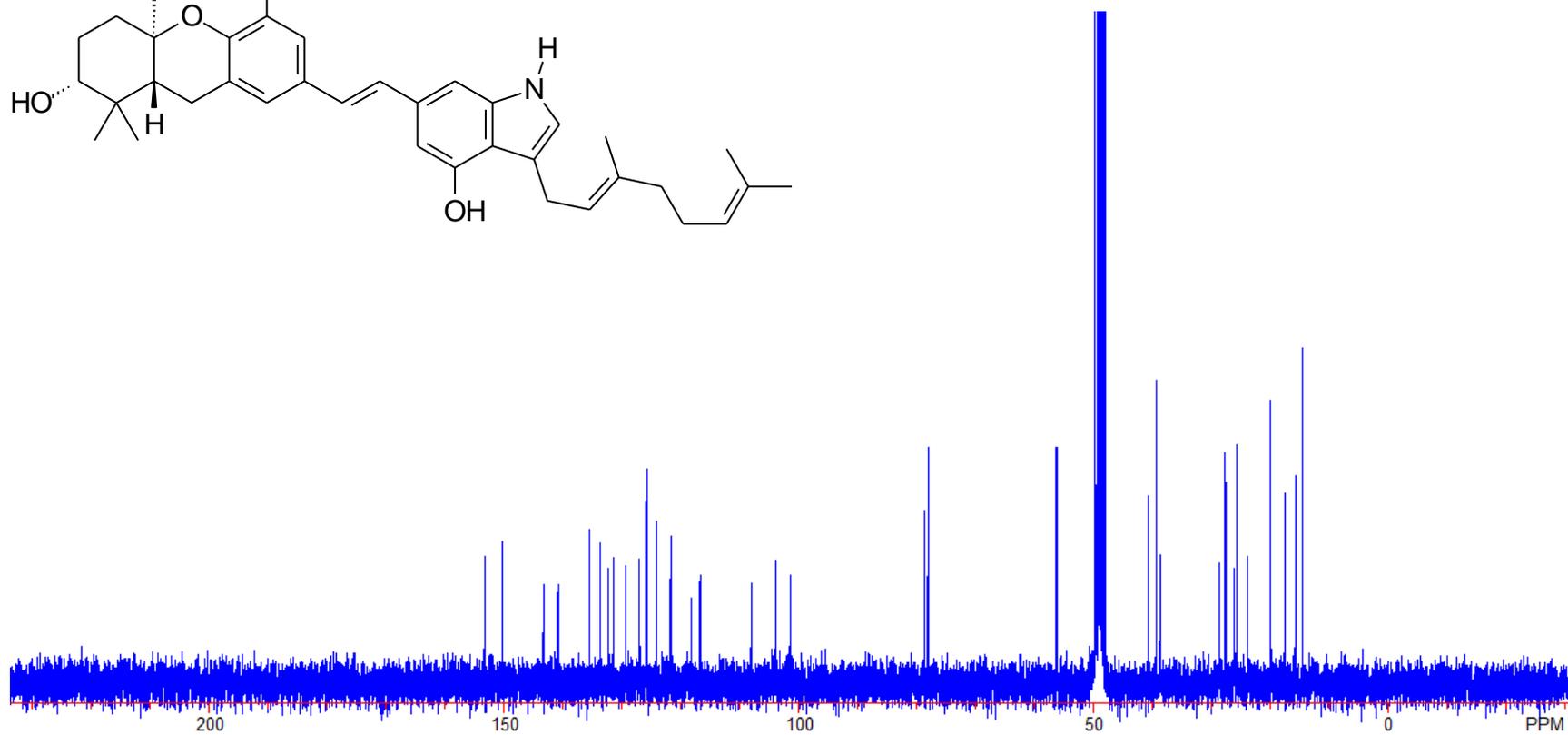
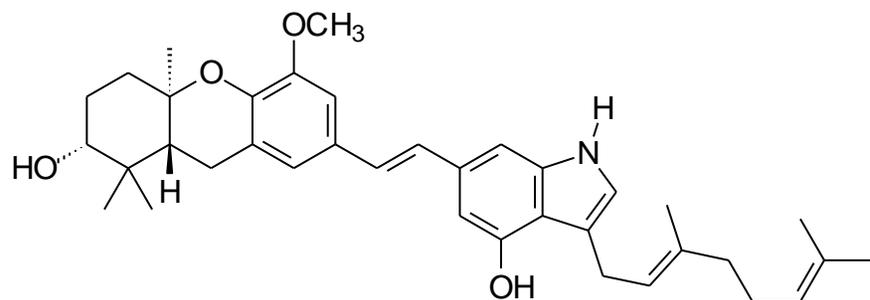
300 MHz ¹H NMR Spectrum for Compound 17



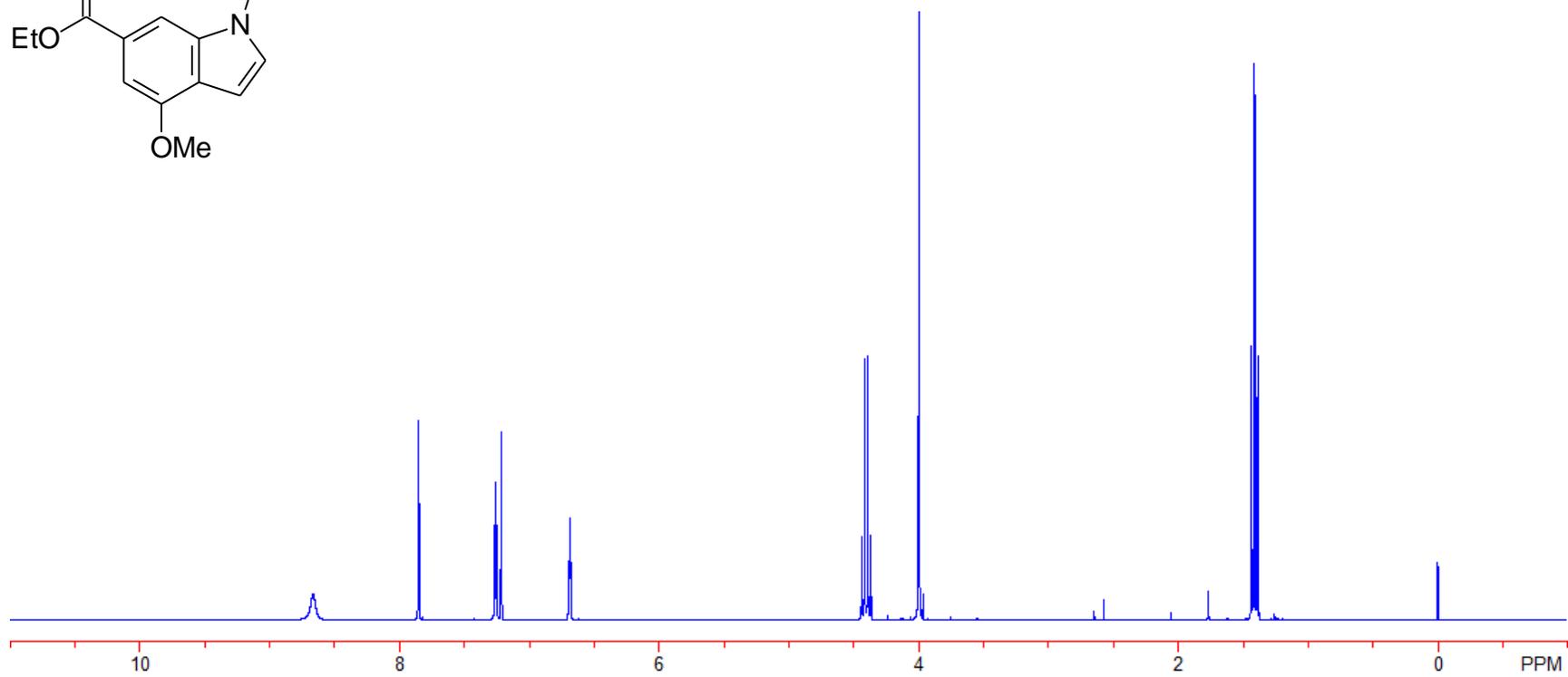
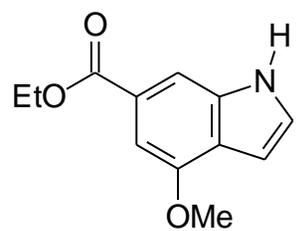
75 MHz ¹³C NMR Spectrum for Compound 17



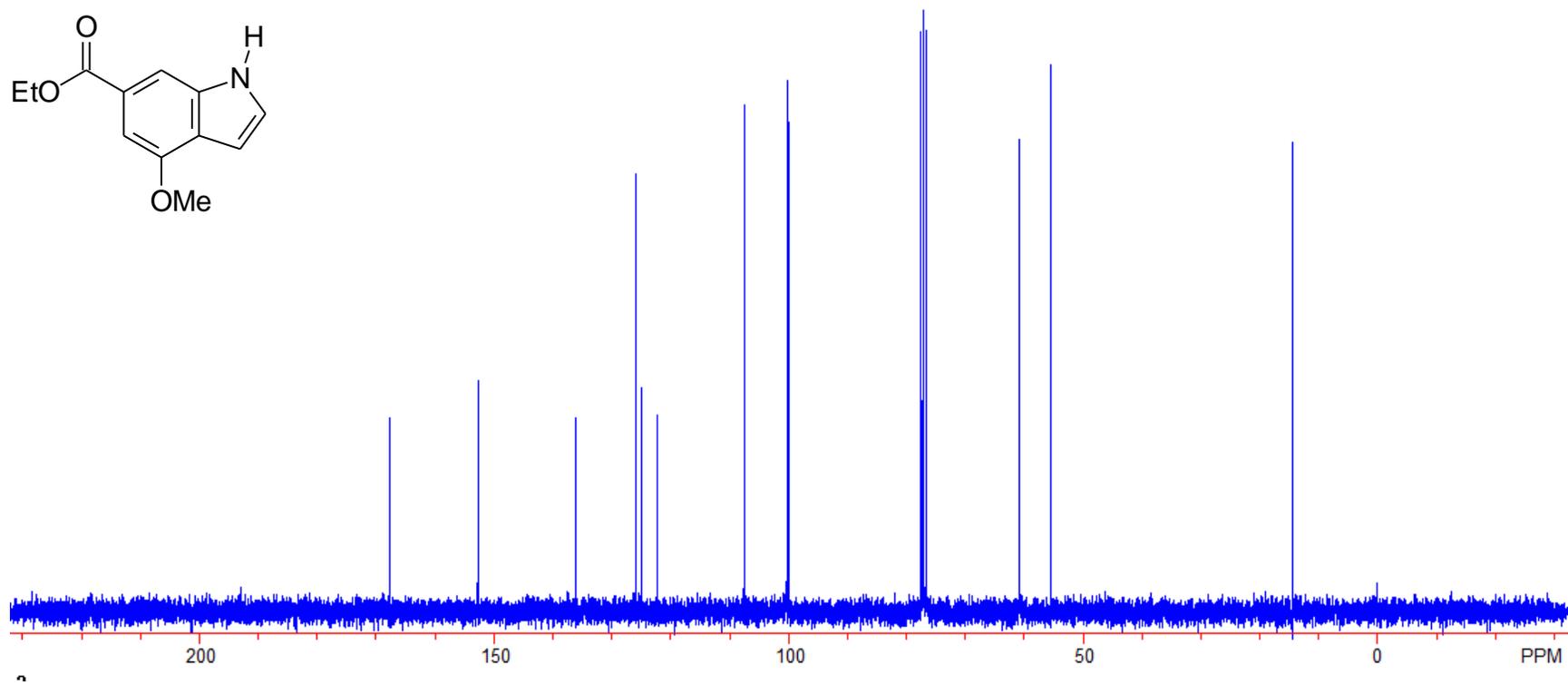
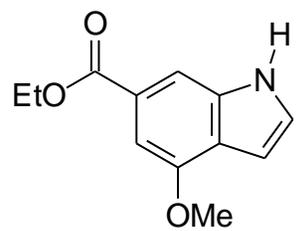
300 MHz ¹H NMR Spectrum (CD₃OD) for Compound **18**



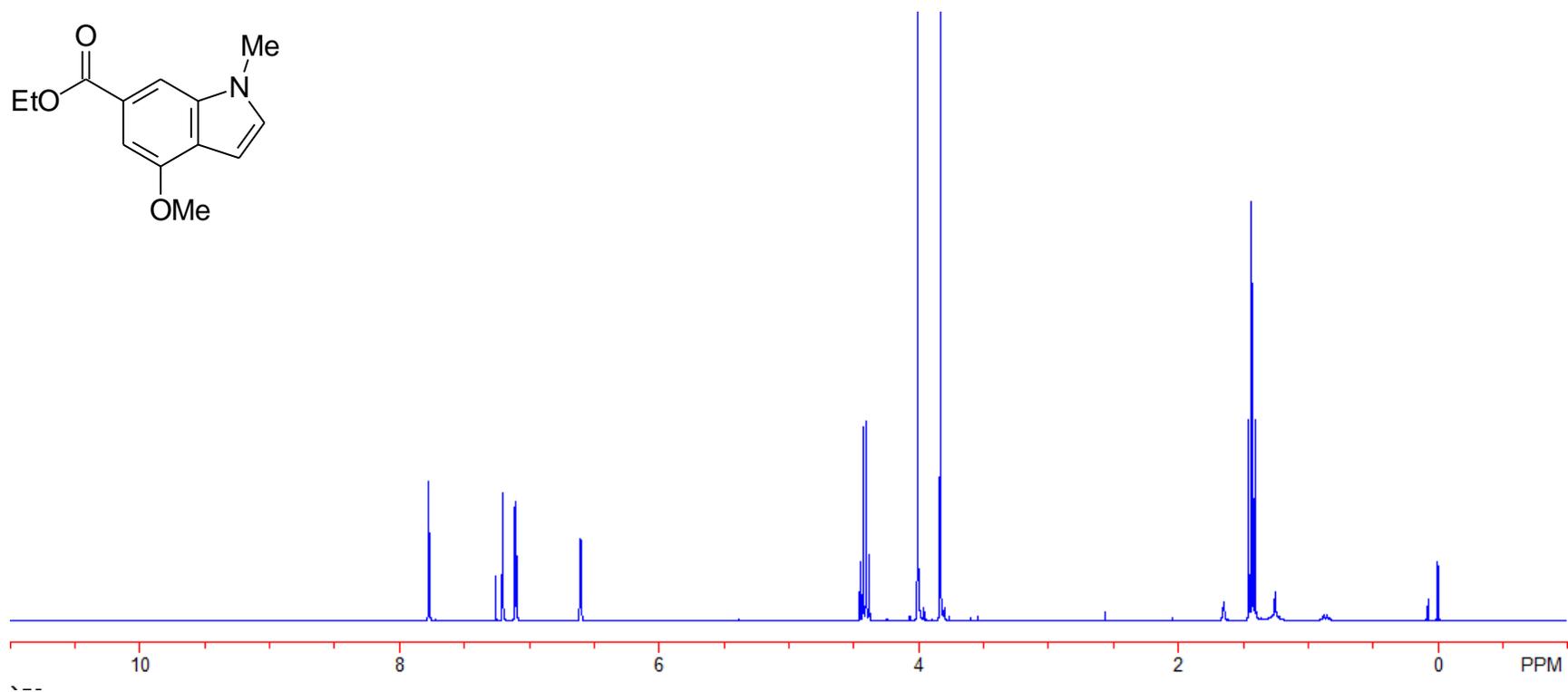
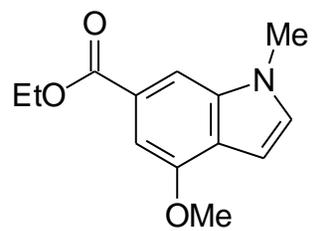
75 MHz ¹³C NMR Spectrum (CD₃OD) for Compound 18



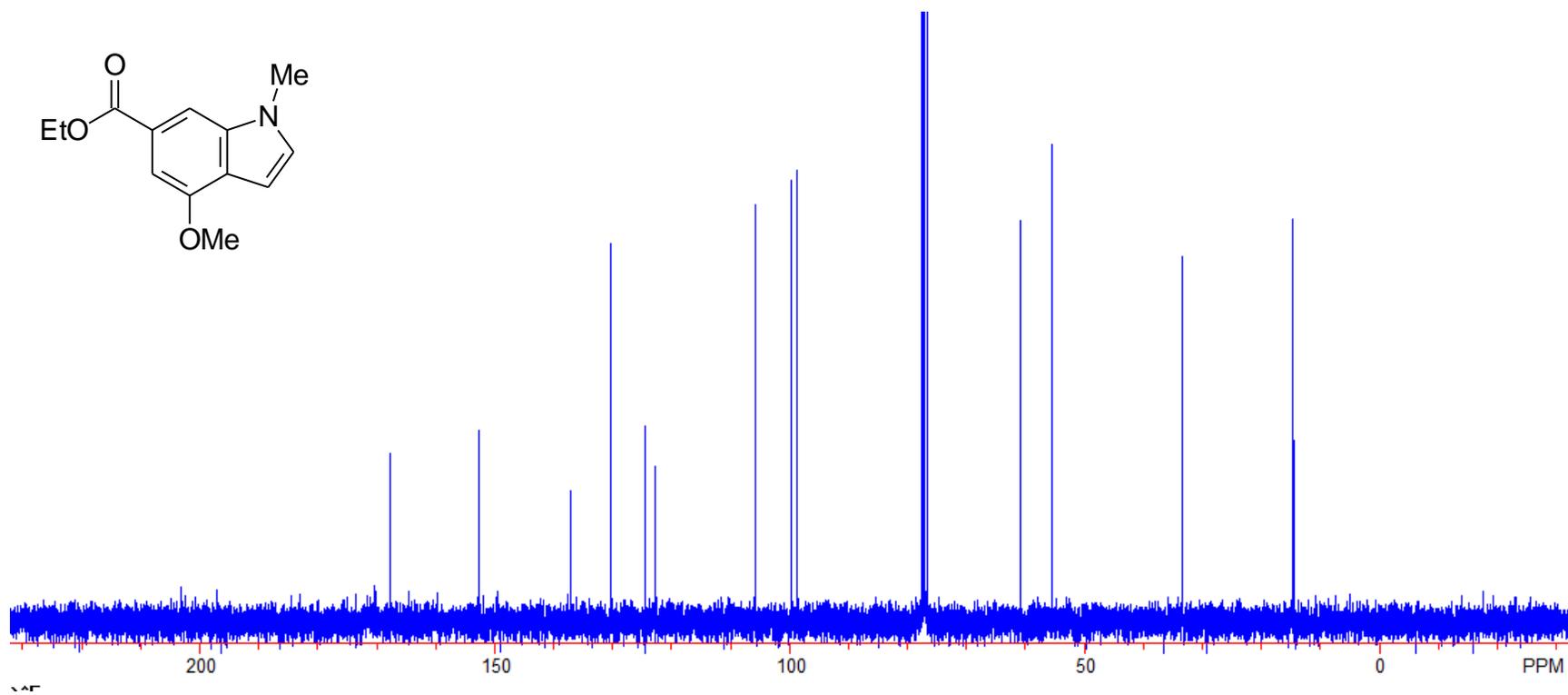
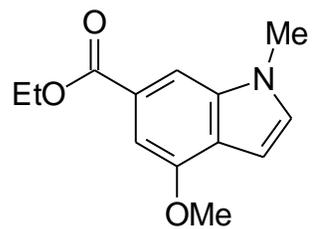
300 MHz ¹H NMR Spectrum for Compound 23



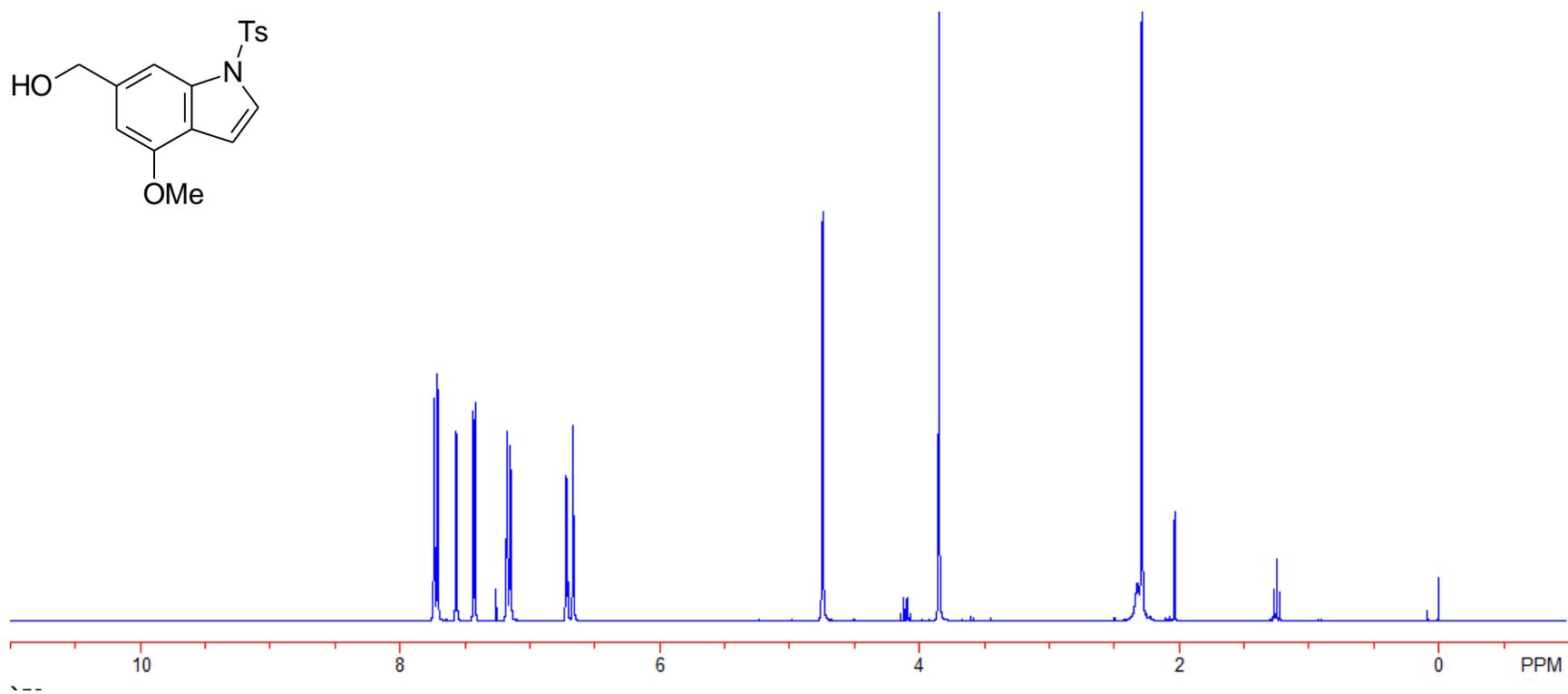
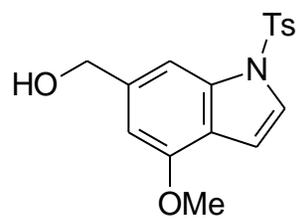
75 MHz ¹³C NMR Spectrum for Compound 23



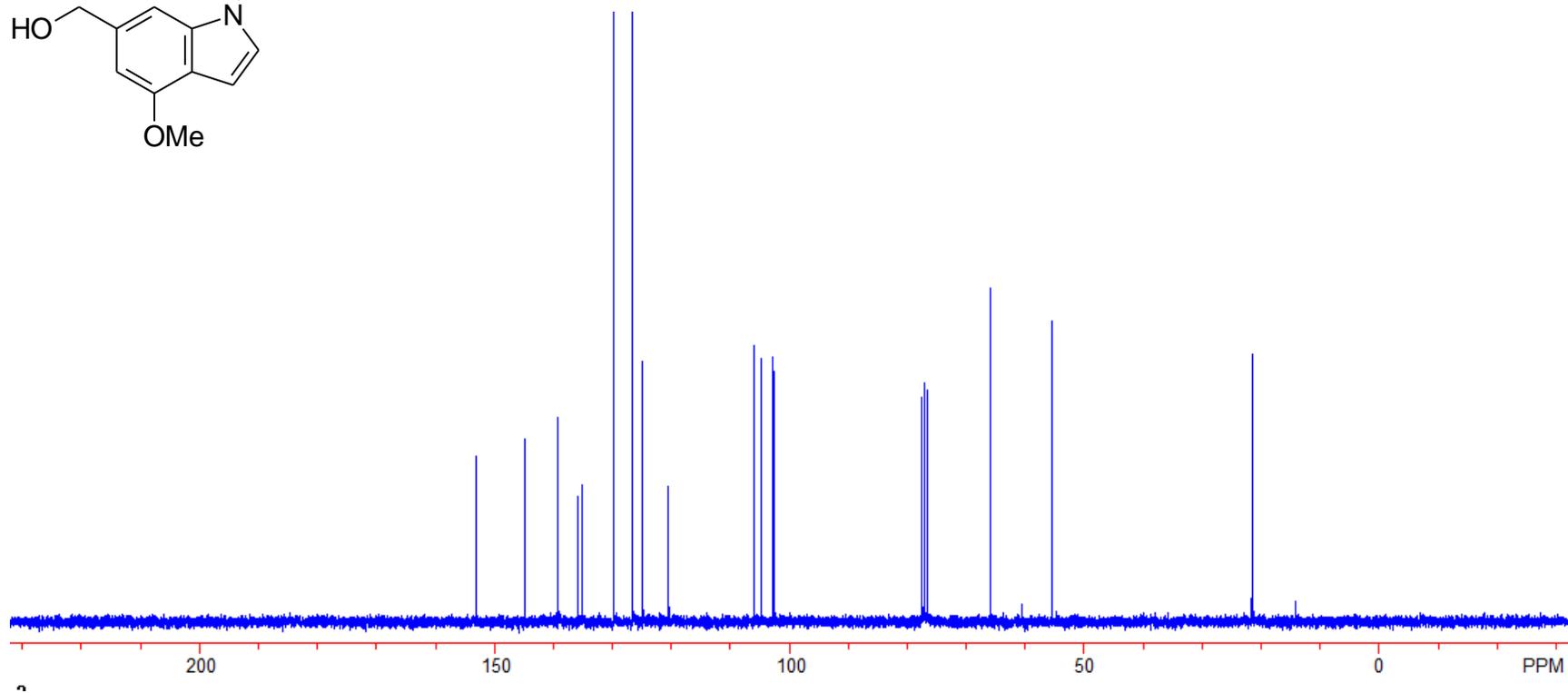
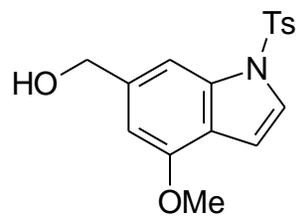
300 MHz ¹H NMR Spectrum for Compound 31



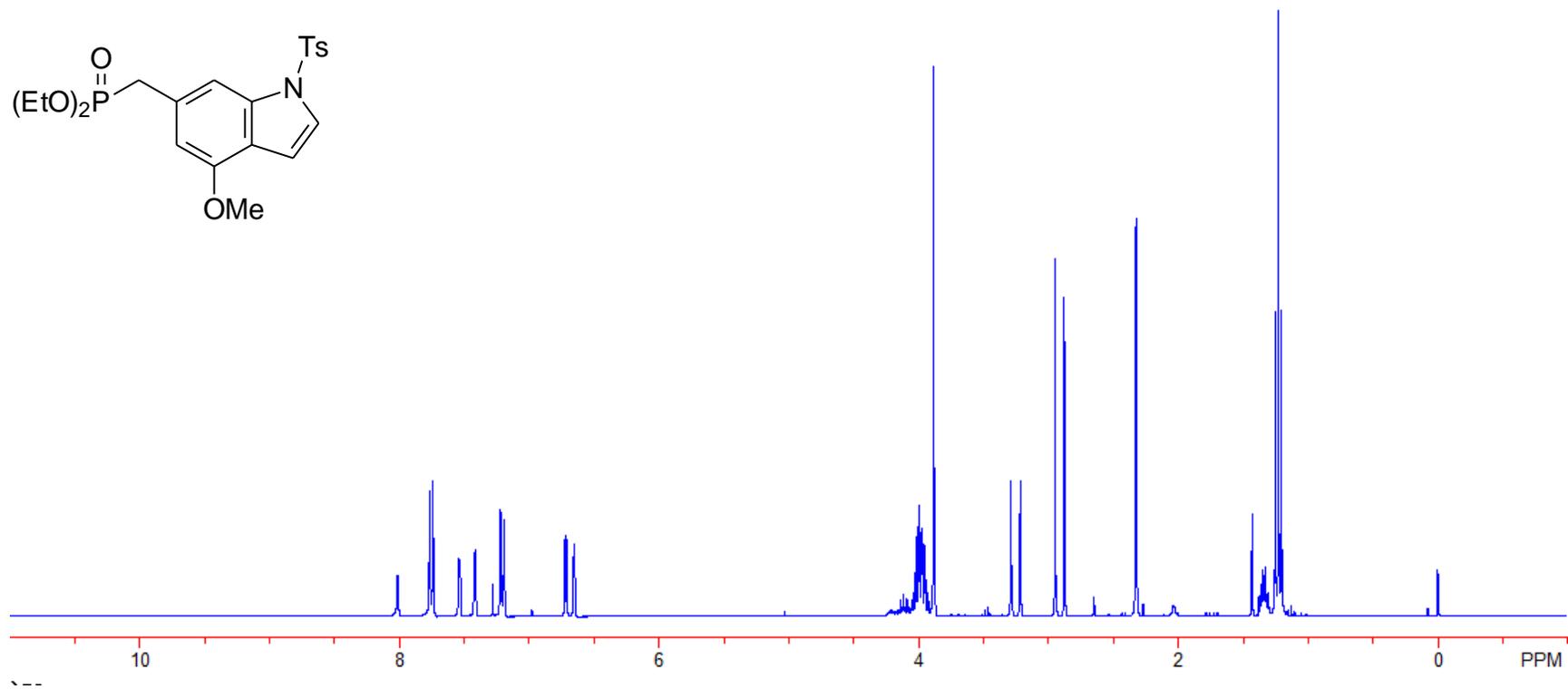
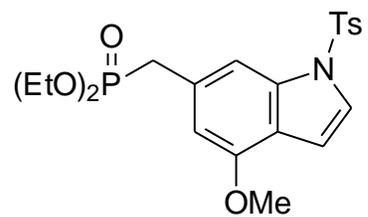
75 MHz ^{13}C NMR Spectrum for Compound **31**



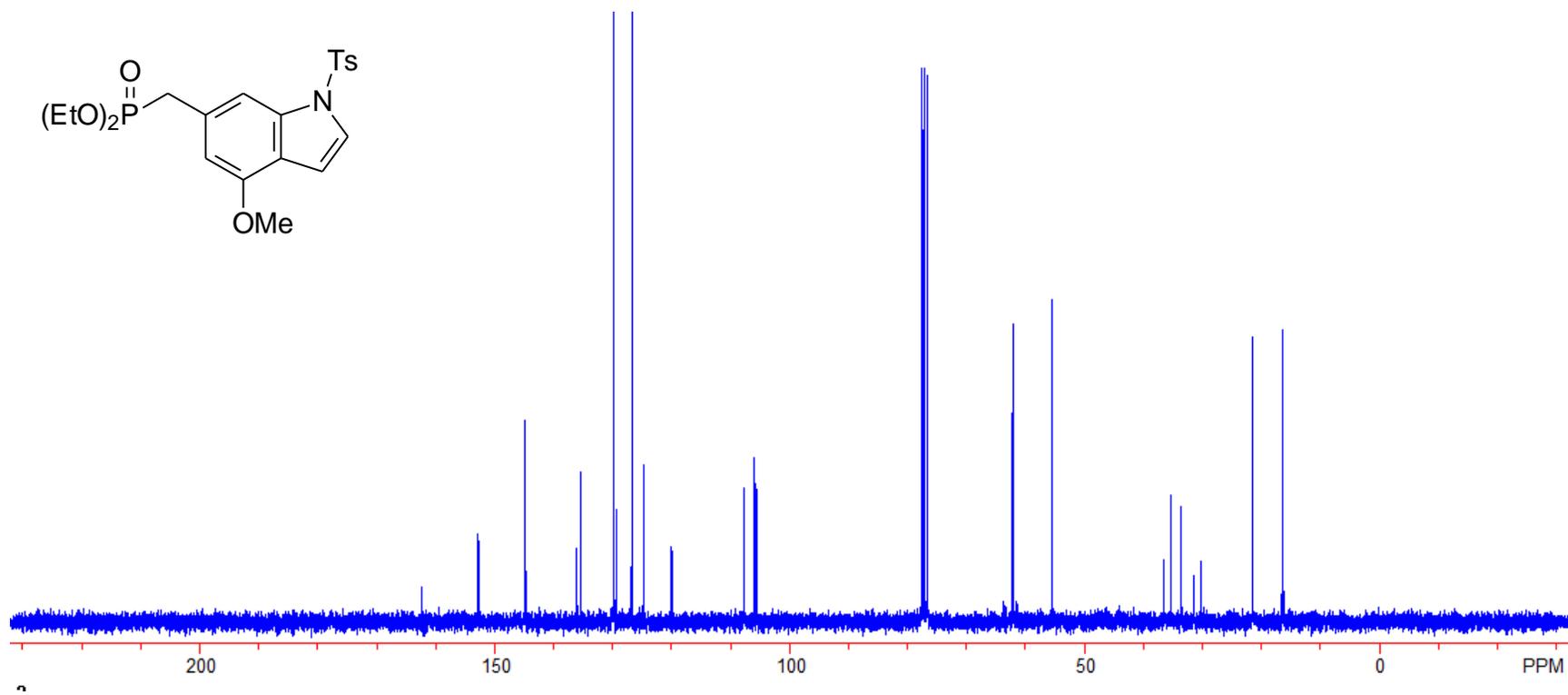
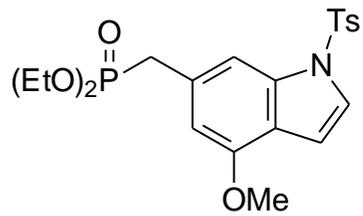
300 MHz ¹H NMR Spectrum for Compound 24



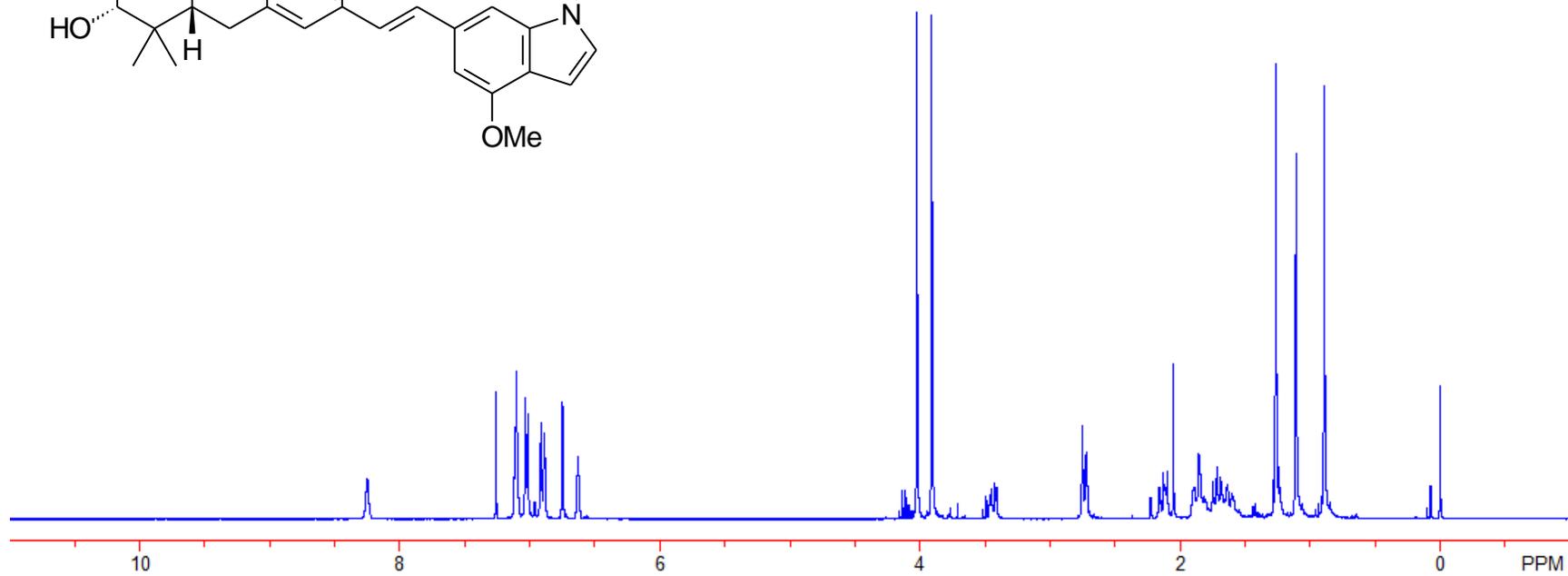
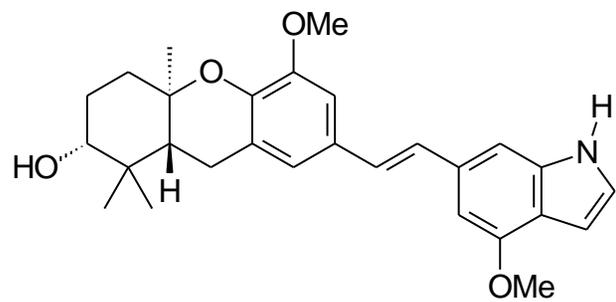
75 MHz ¹³C NMR Spectrum for Compound 24



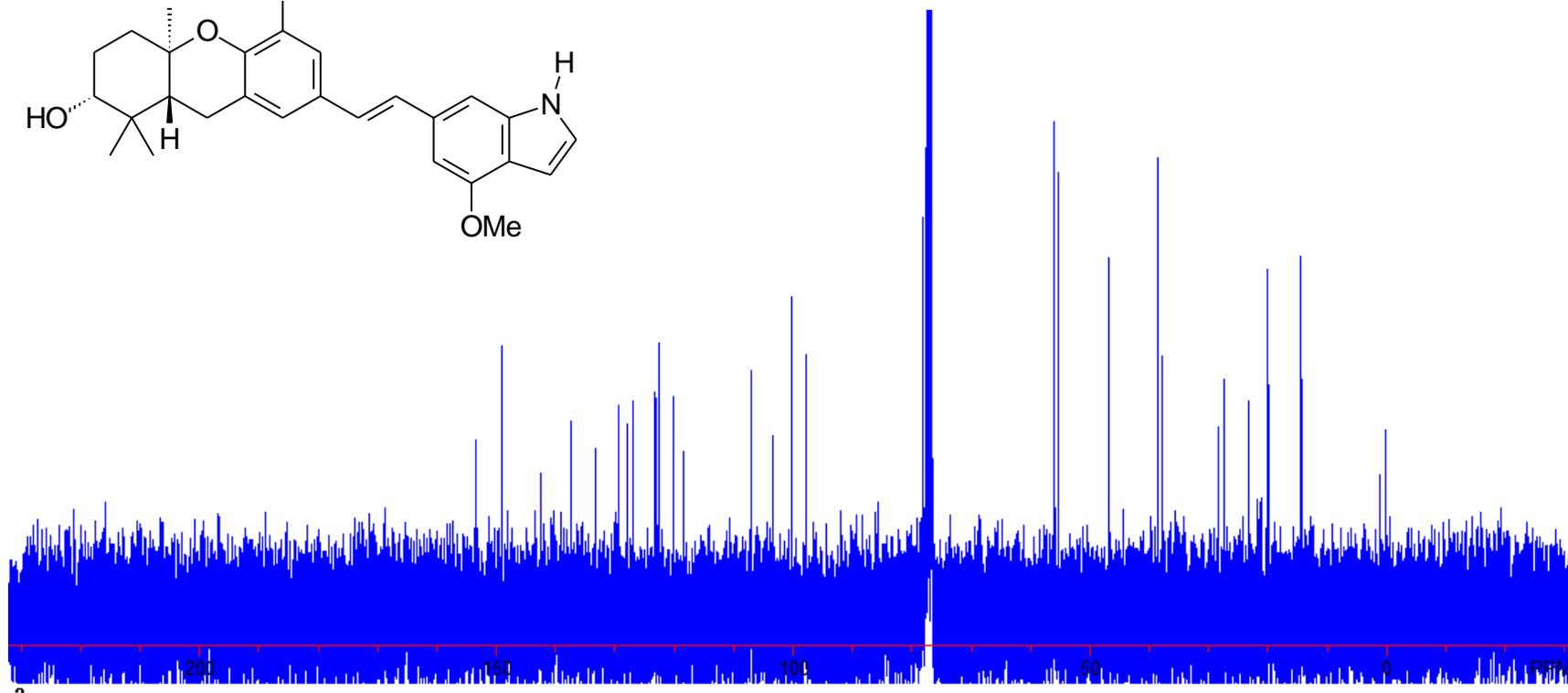
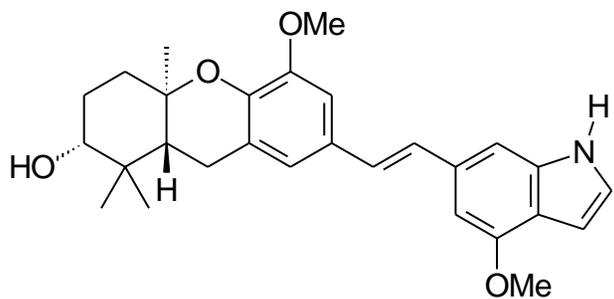
300 MHz ¹H NMR Spectrum for Compound 25



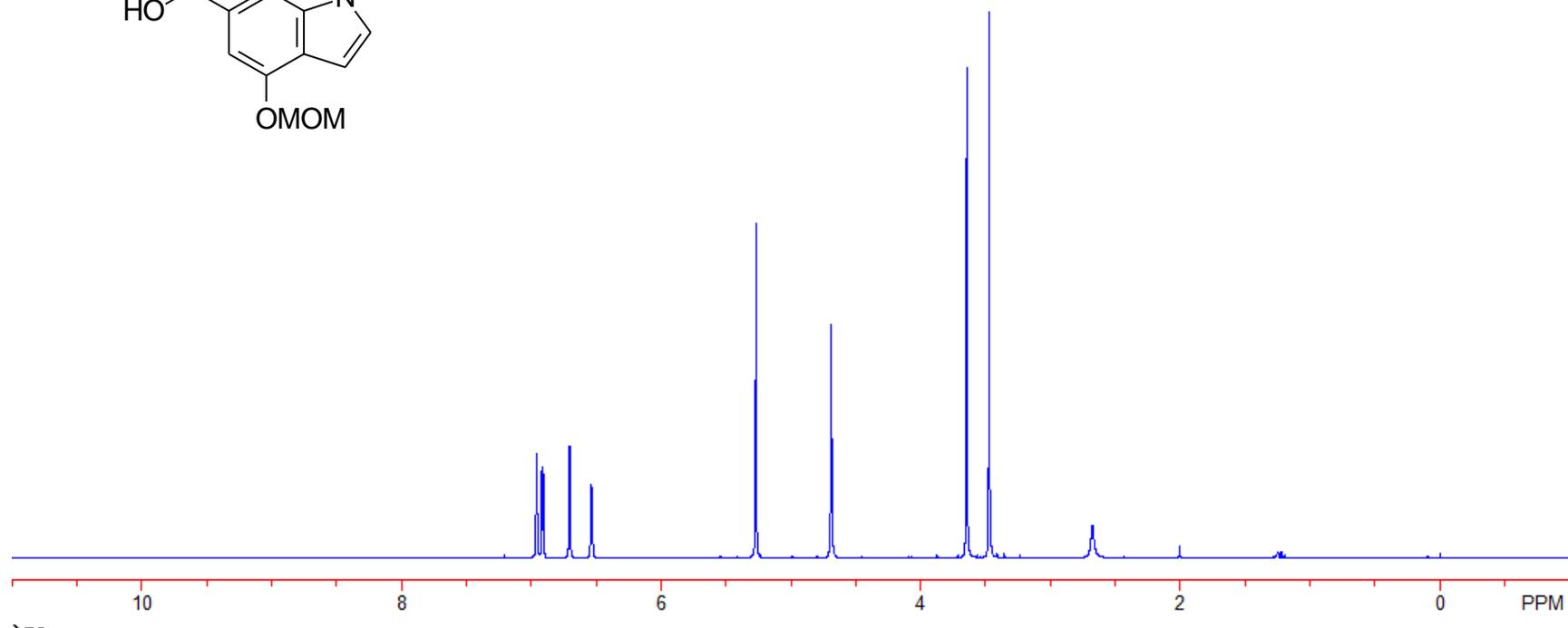
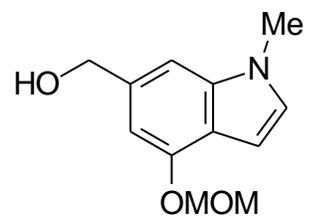
75 MHz ¹³C NMR Spectrum for Compound 25



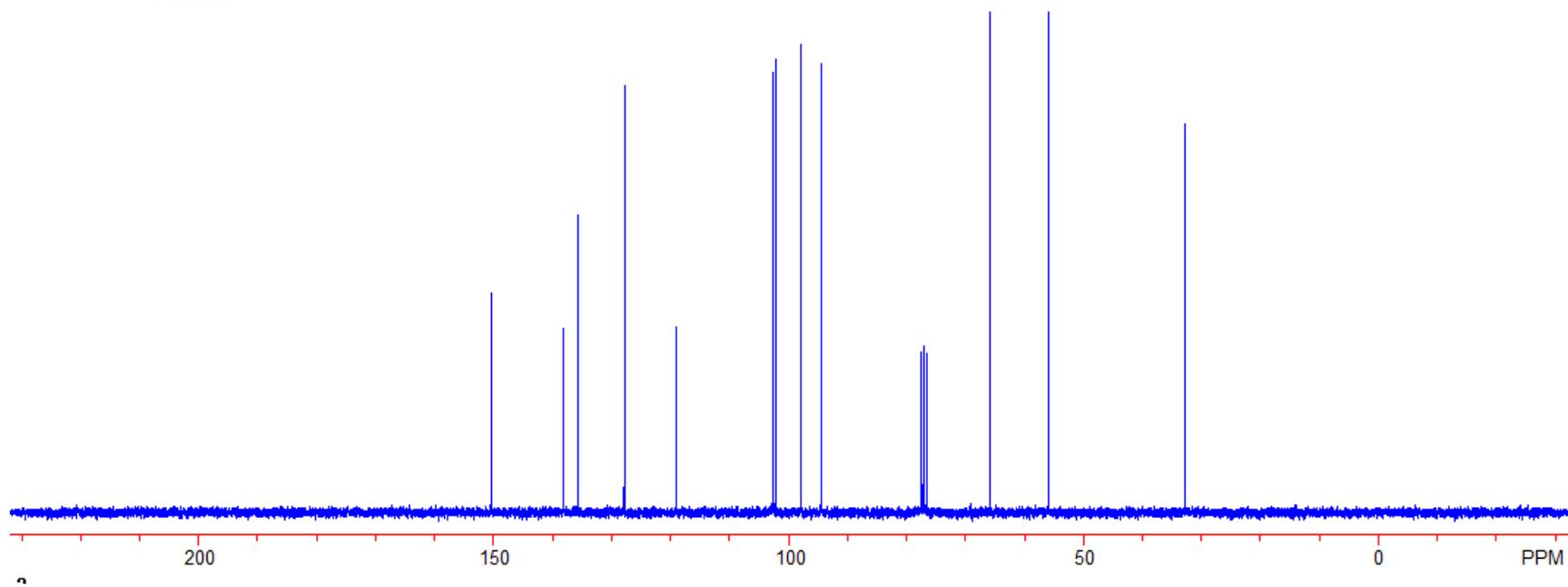
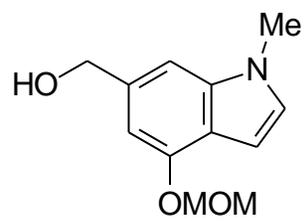
300 MHz ¹H NMR Spectrum for Compound 19



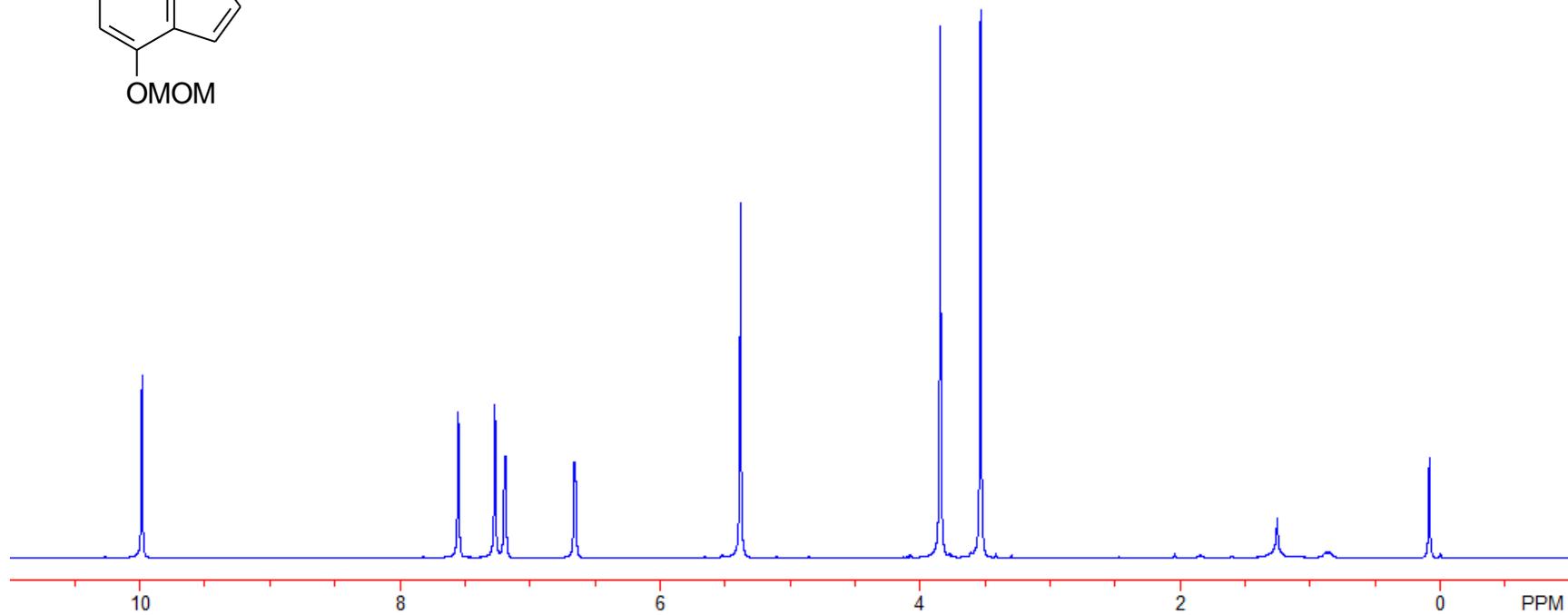
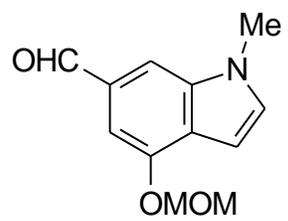
75 MHz ¹³C NMR Spectrum for Compound 19



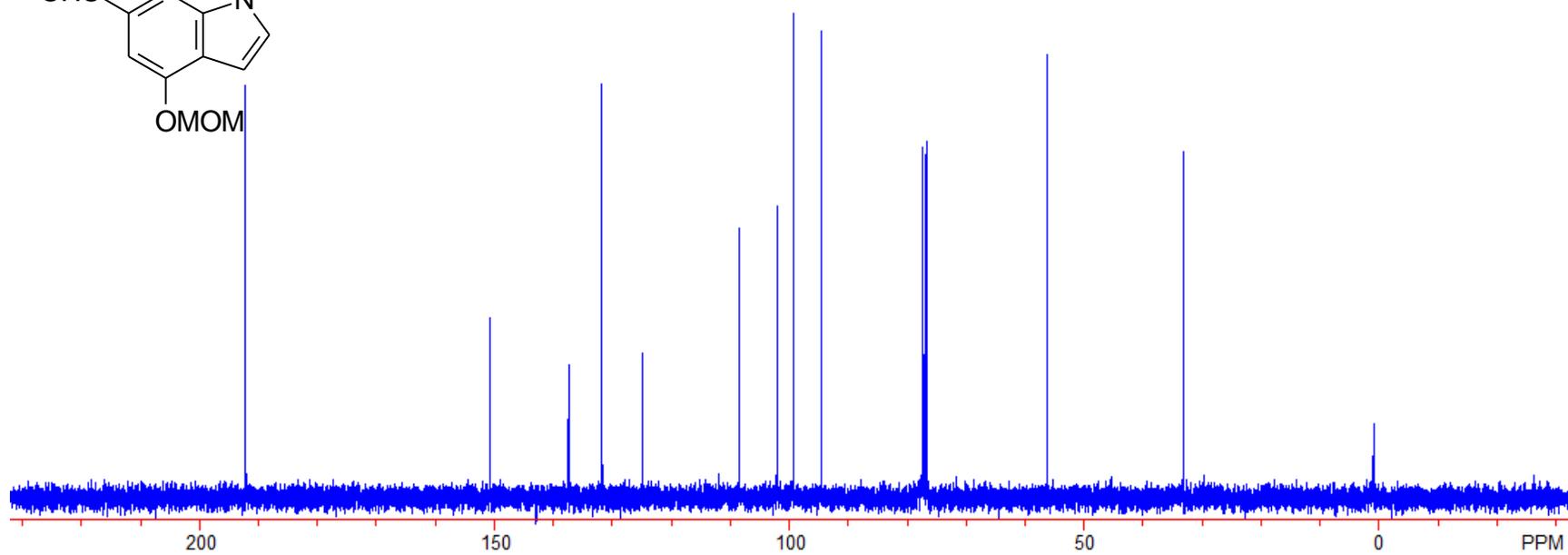
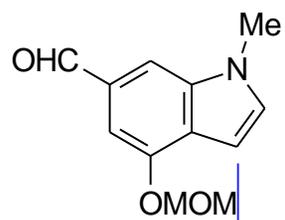
300 MHz ¹H NMR Spectrum for Compound **27**



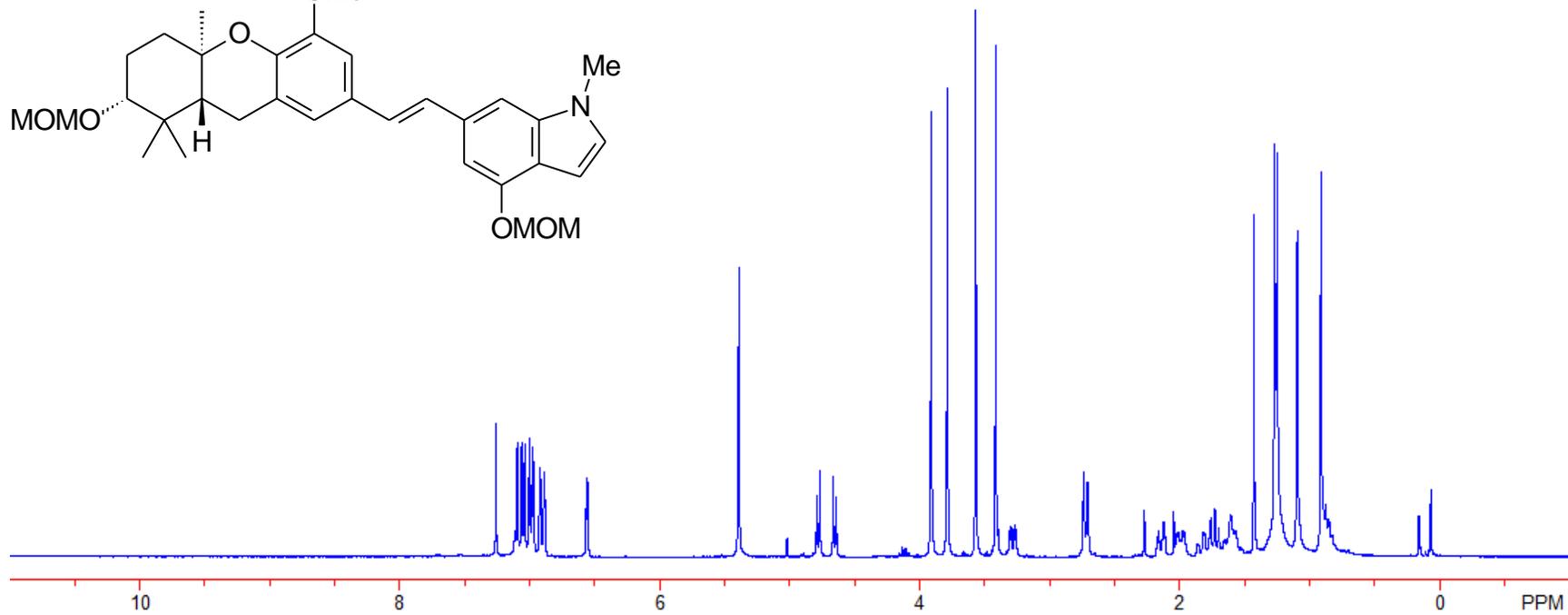
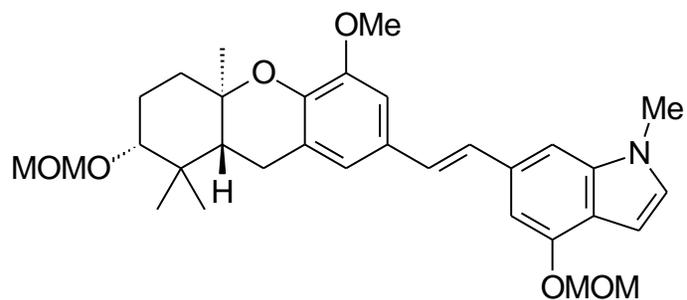
75 MHz ¹³C NMR Spectrum for Compound 27



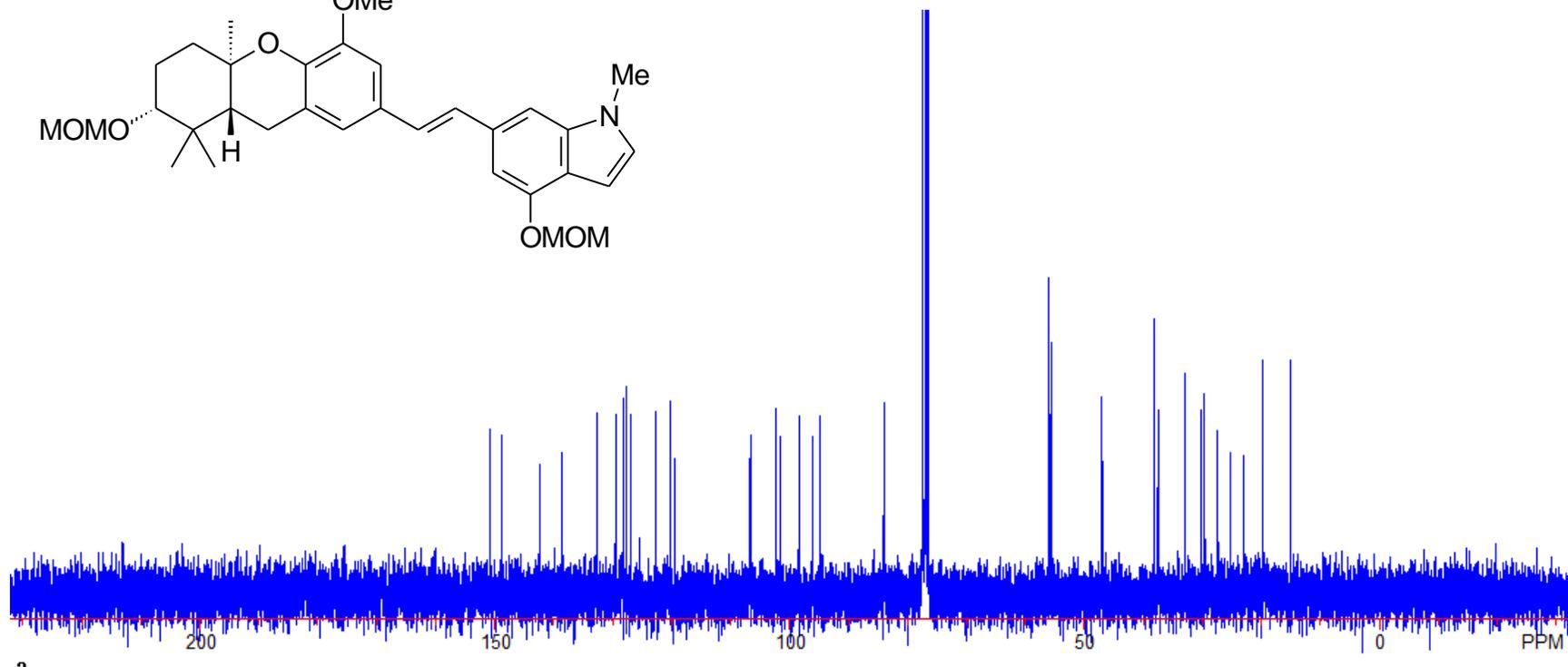
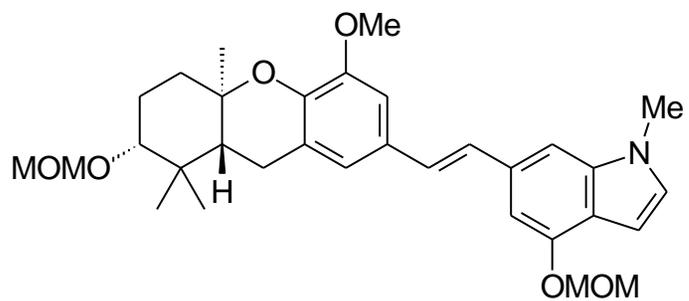
300 MHz ^1H NMR Spectrum for Compound **28**



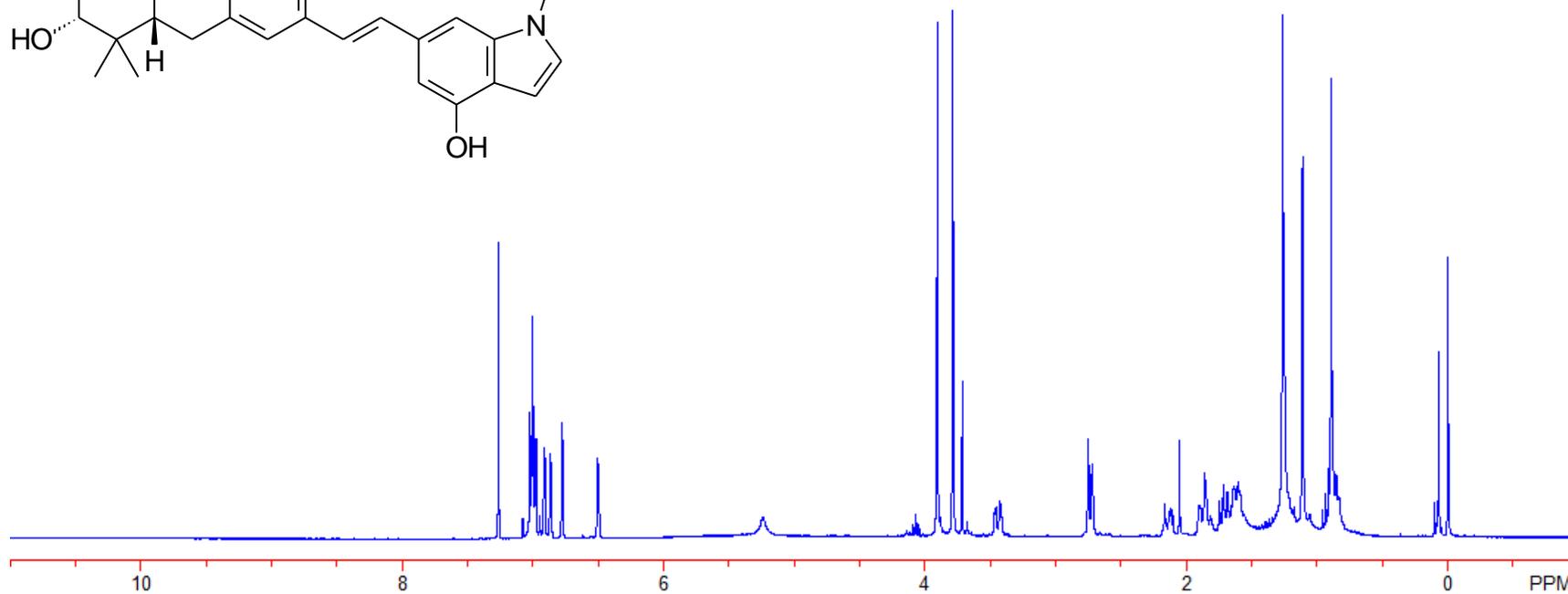
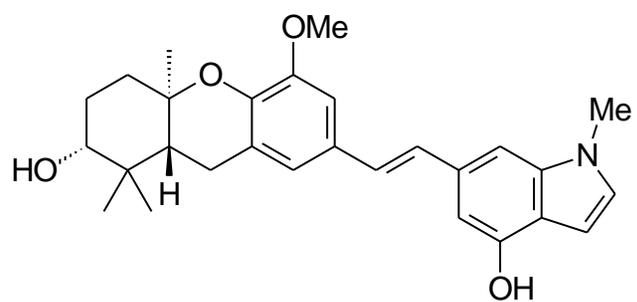
75 MHz ^{13}C NMR Spectrum for Compound 28



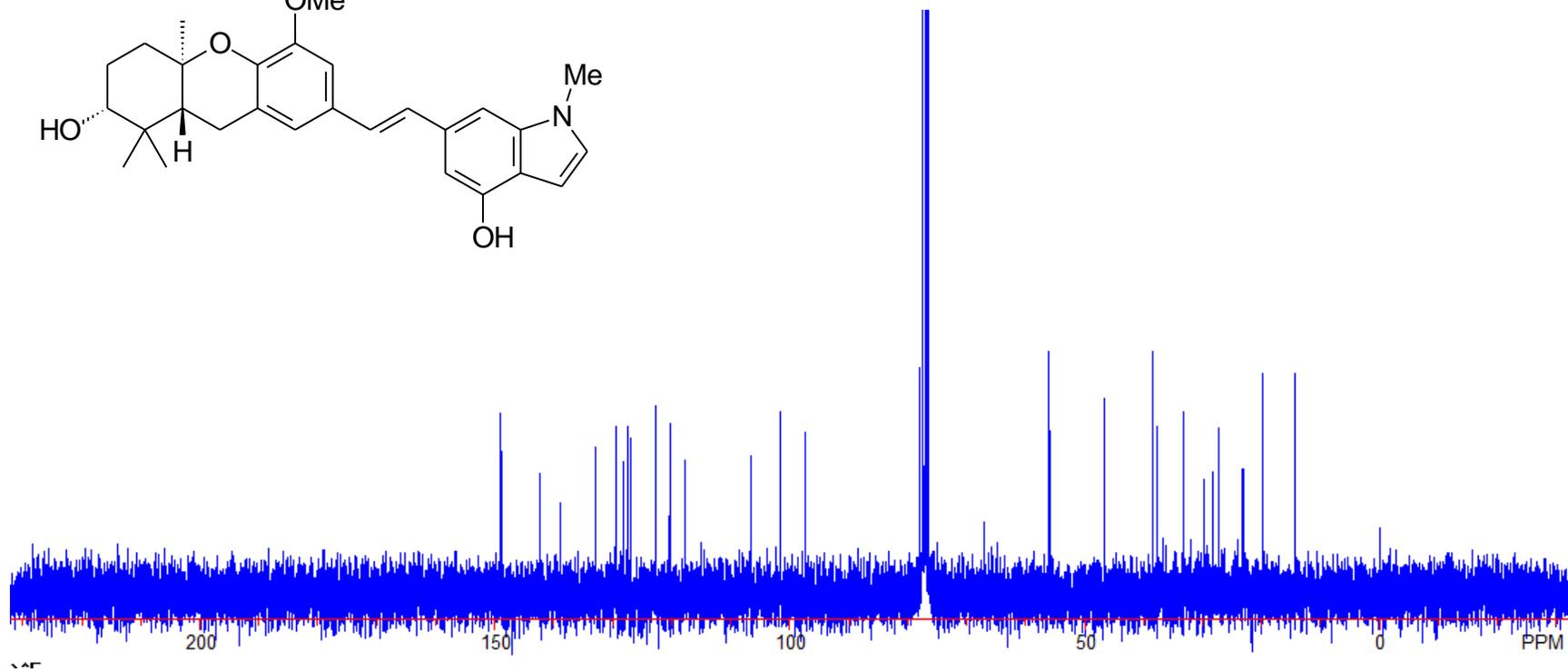
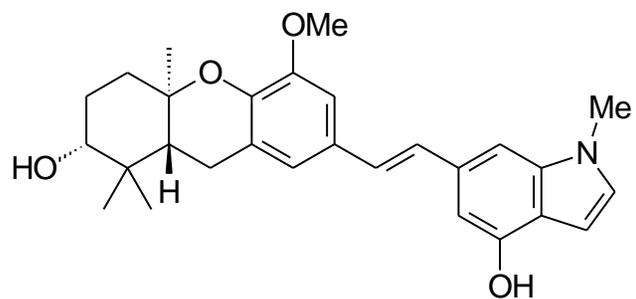
300 MHz ¹H NMR Spectrum for Compound 30



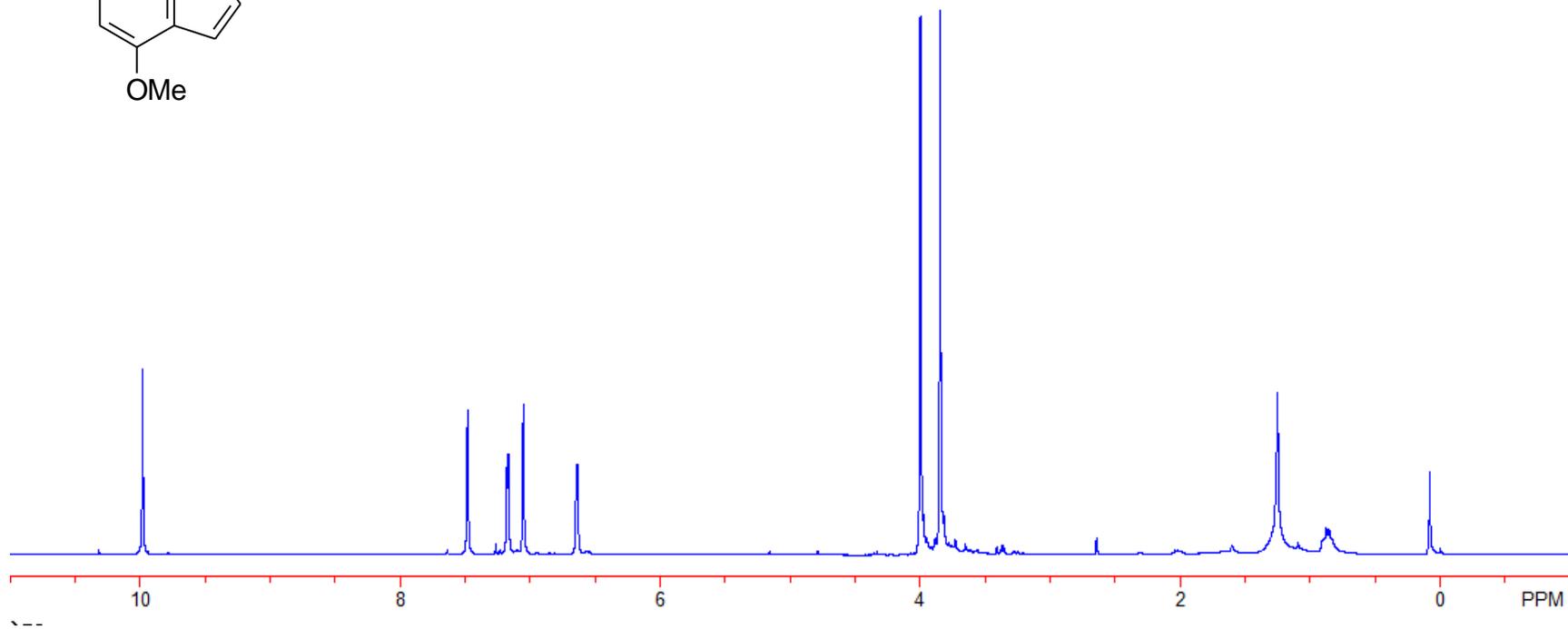
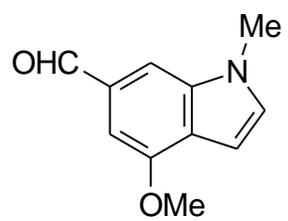
75 MHz ¹³C NMR Spectrum for Compound 30



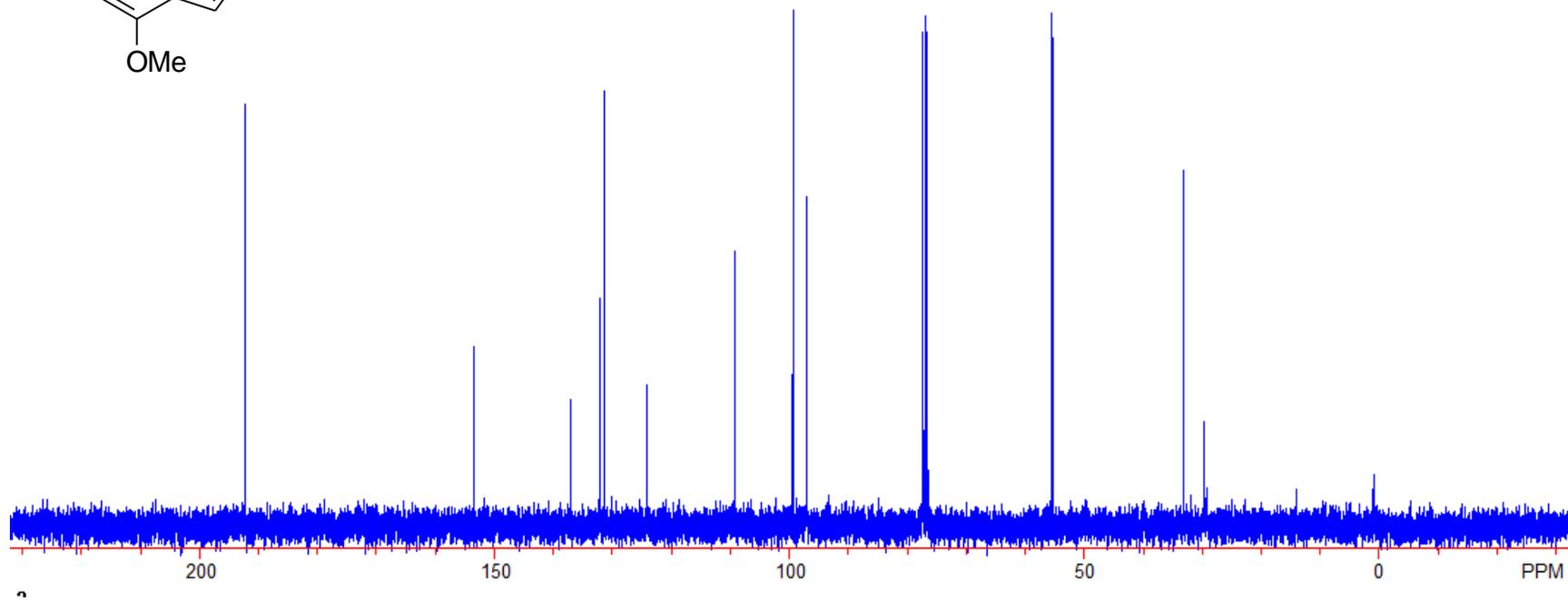
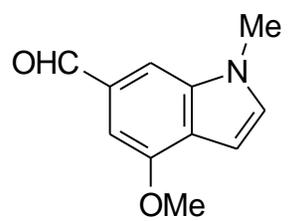
300 MHz ¹H NMR Spectrum for Compound **20**



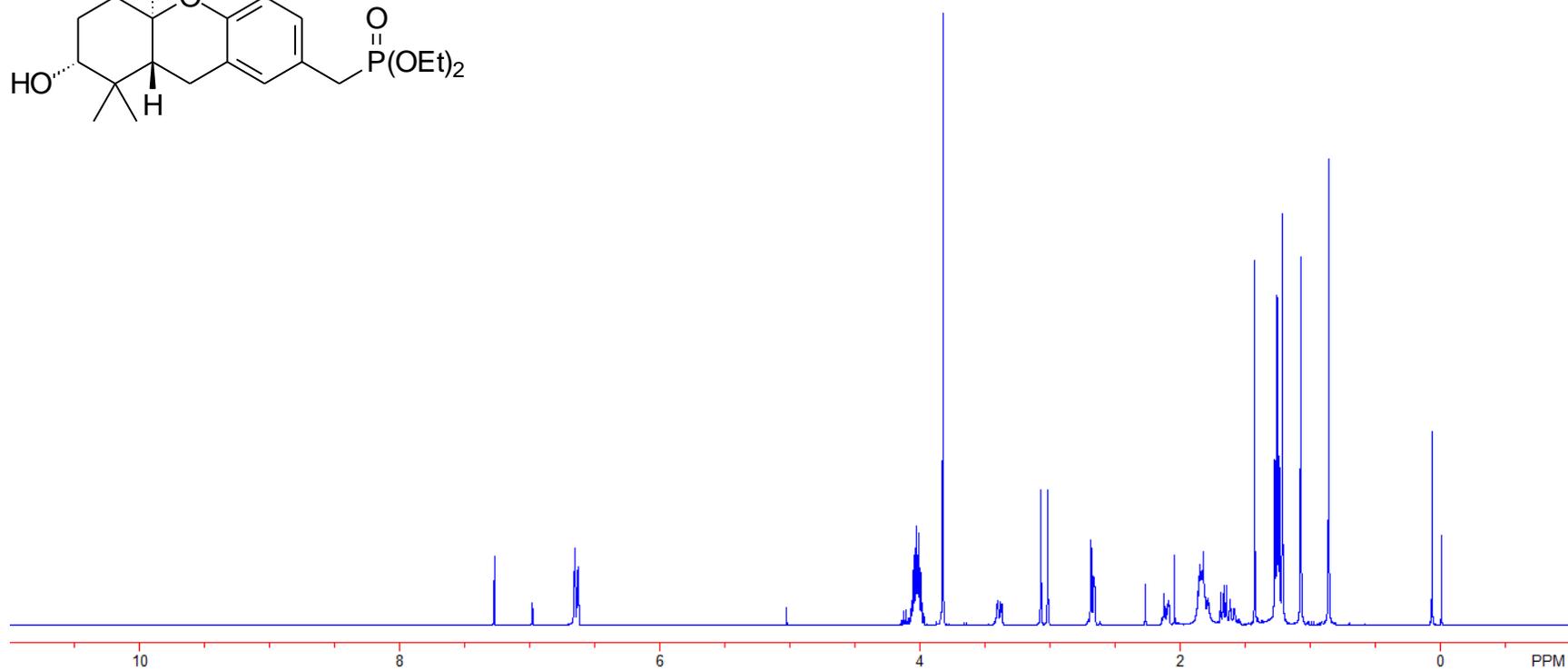
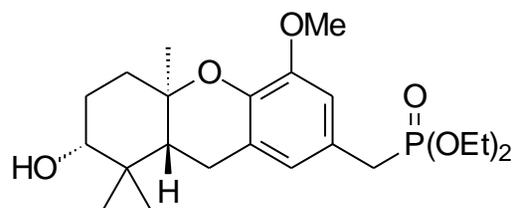
75 MHz ¹³C NMR Spectrum for Compound 20



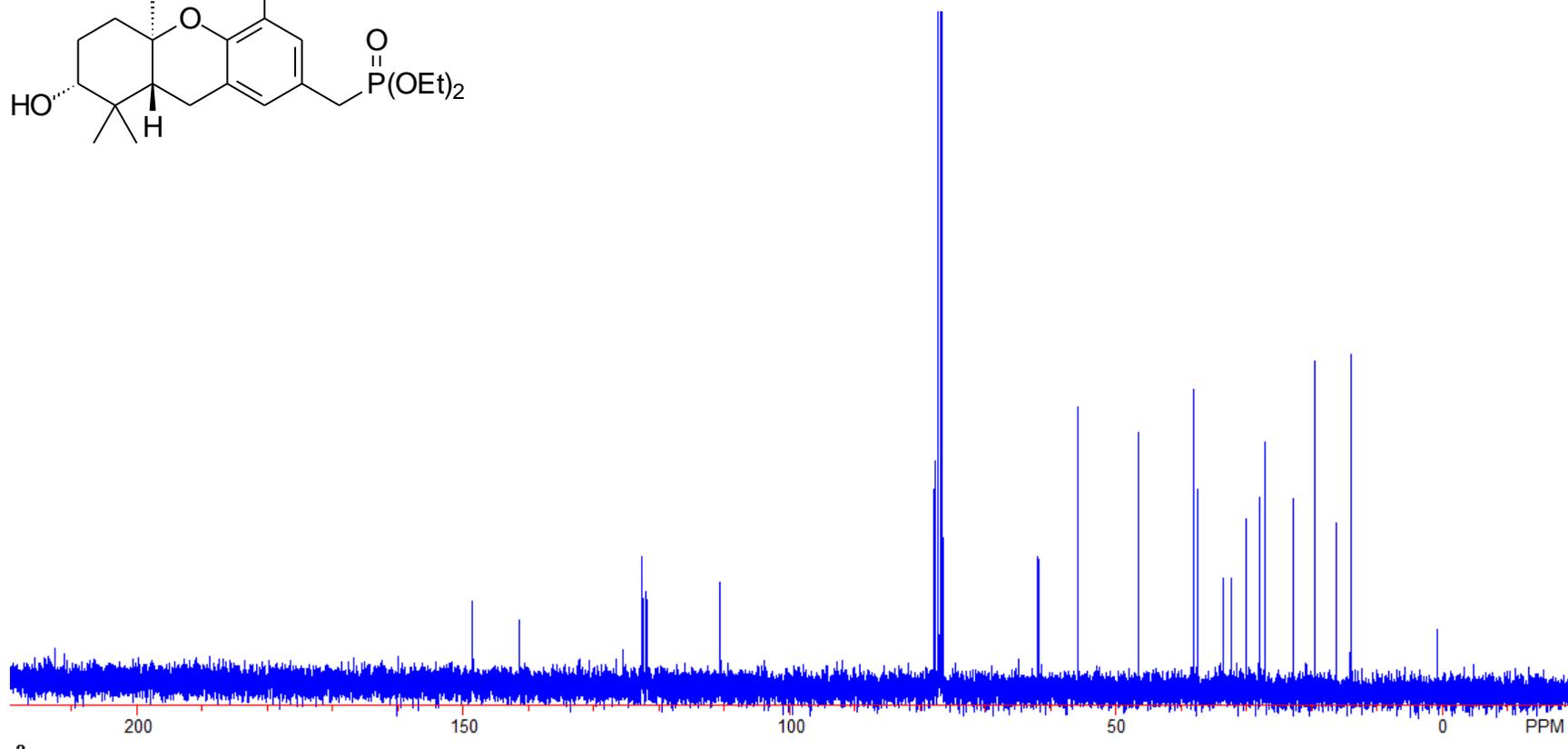
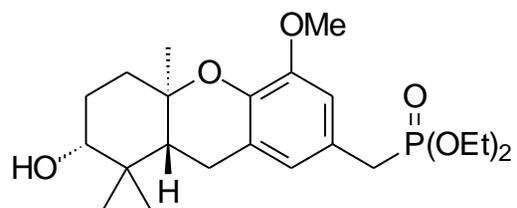
300 MHz ¹H NMR Spectrum for Compound **32**



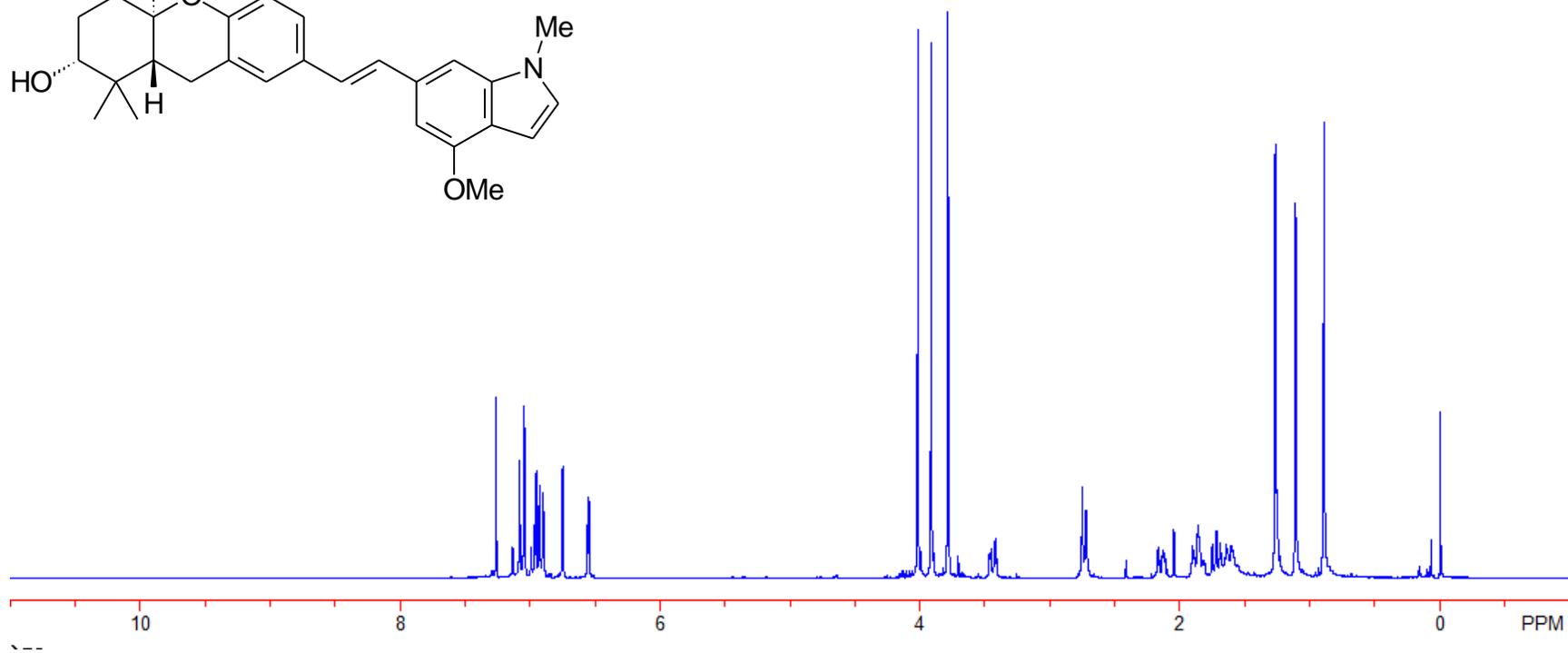
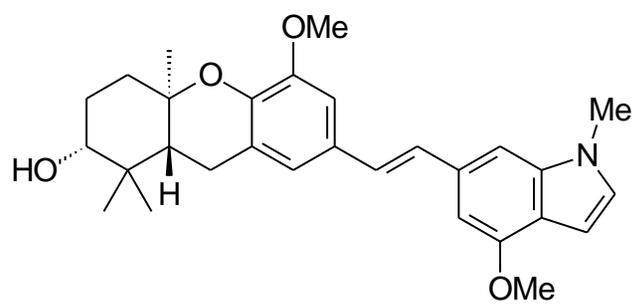
75 MHz ¹³C NMR Spectrum for Compound 32



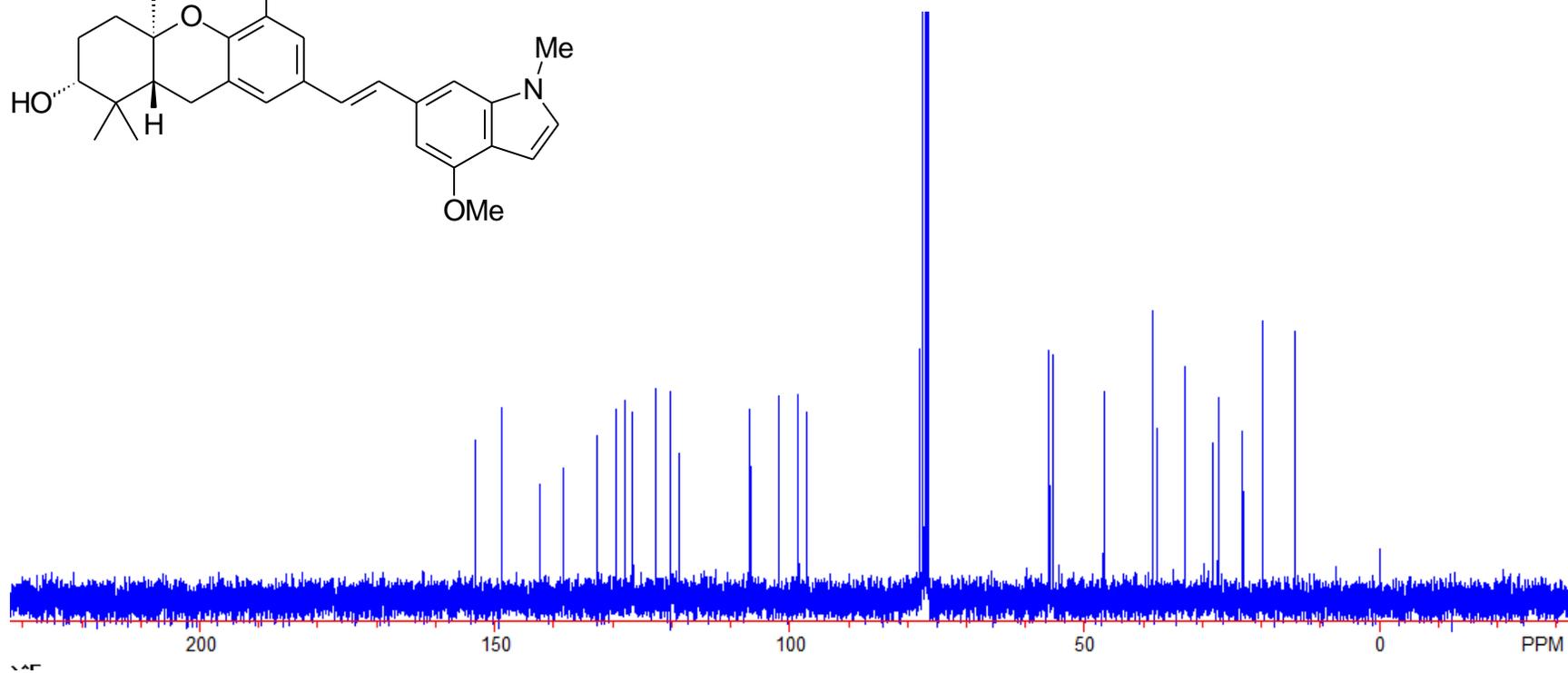
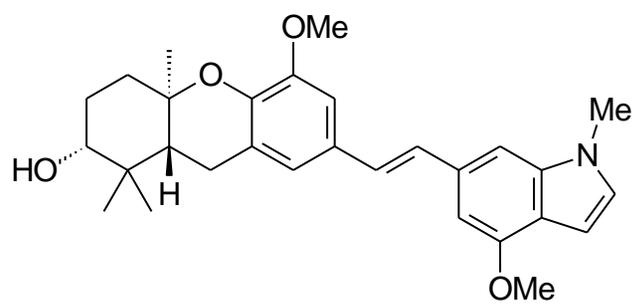
300 MHz ¹H NMR Spectrum for Compound 33



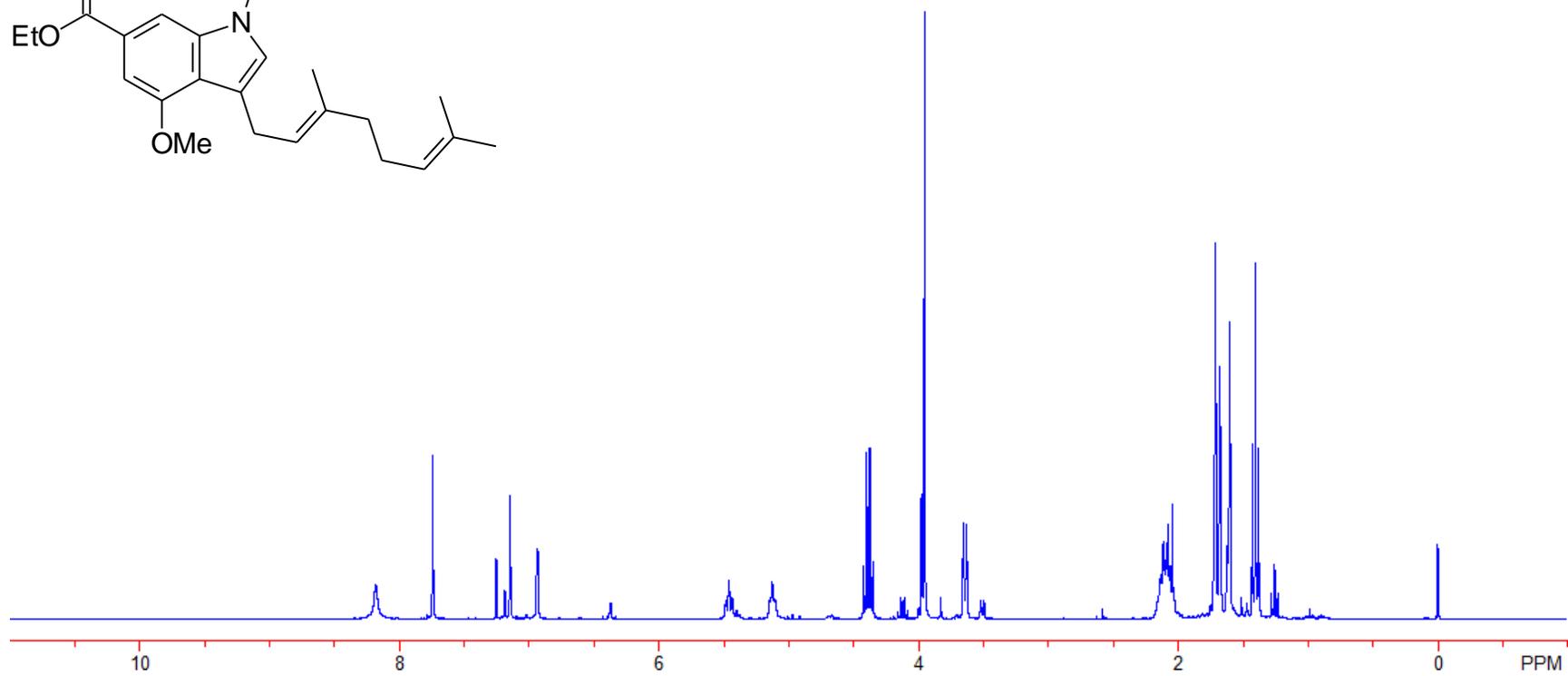
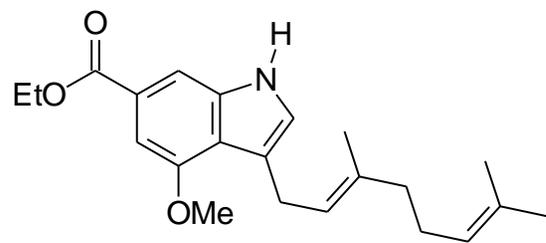
75 MHz ¹³C NMR Spectrum for Compound 33



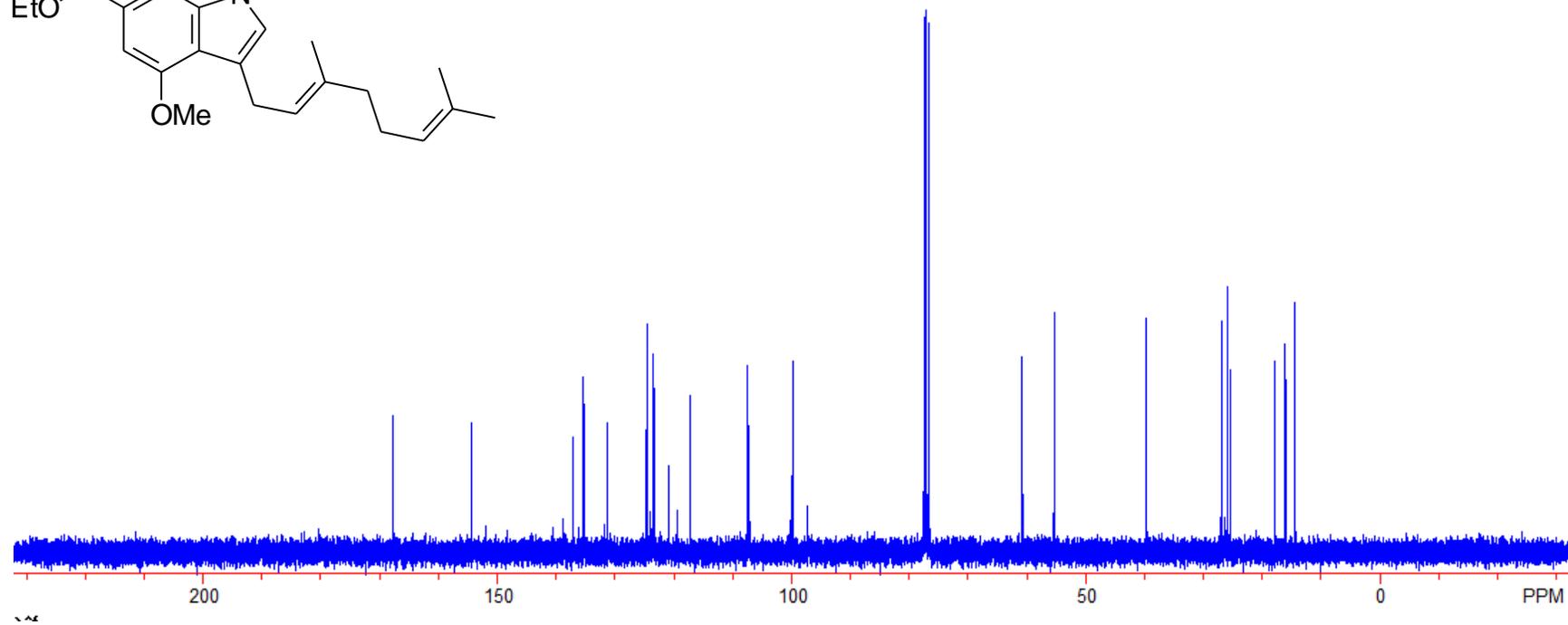
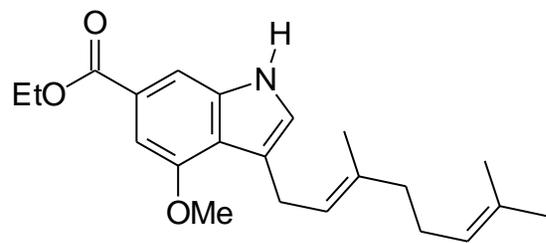
300 MHz ¹H NMR Spectrum for Compound 21



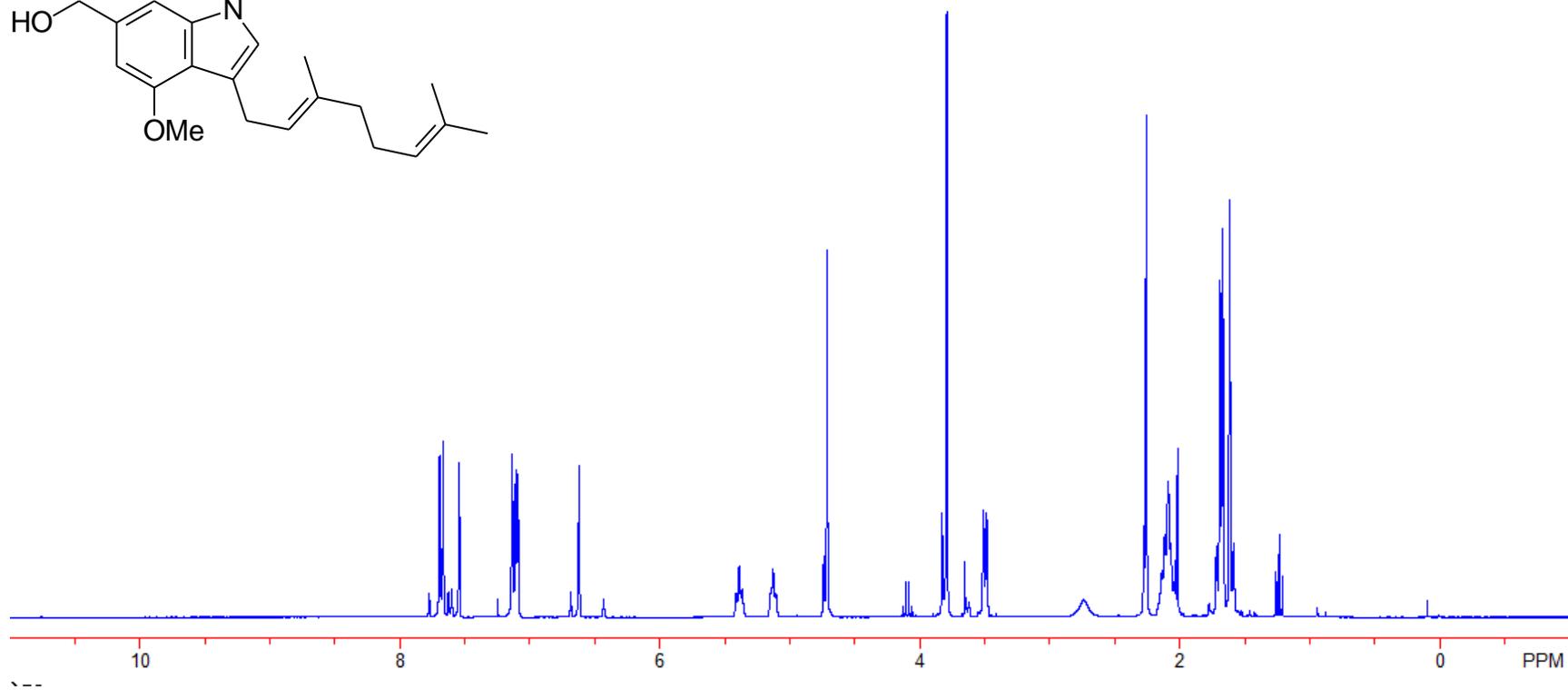
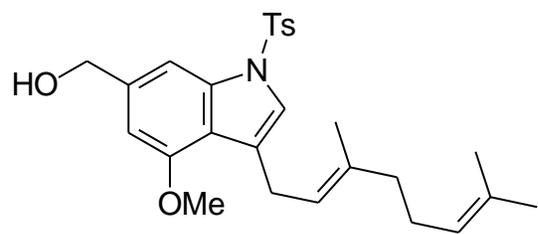
75 MHz ¹³C NMR Spectrum for Compound 21



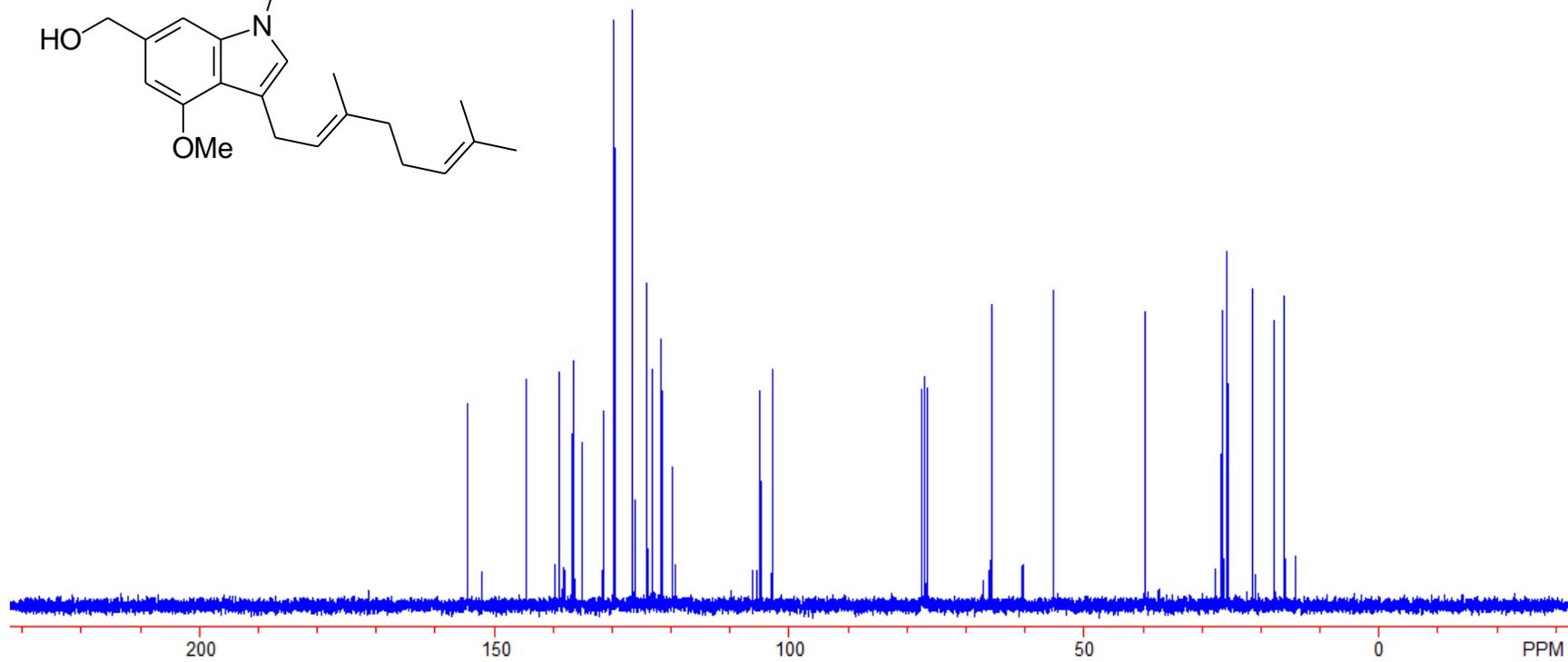
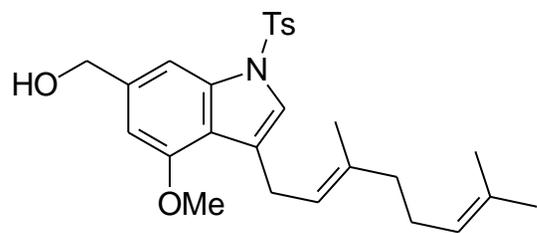
300 MHz ^1H NMR Spectrum for Compound 34



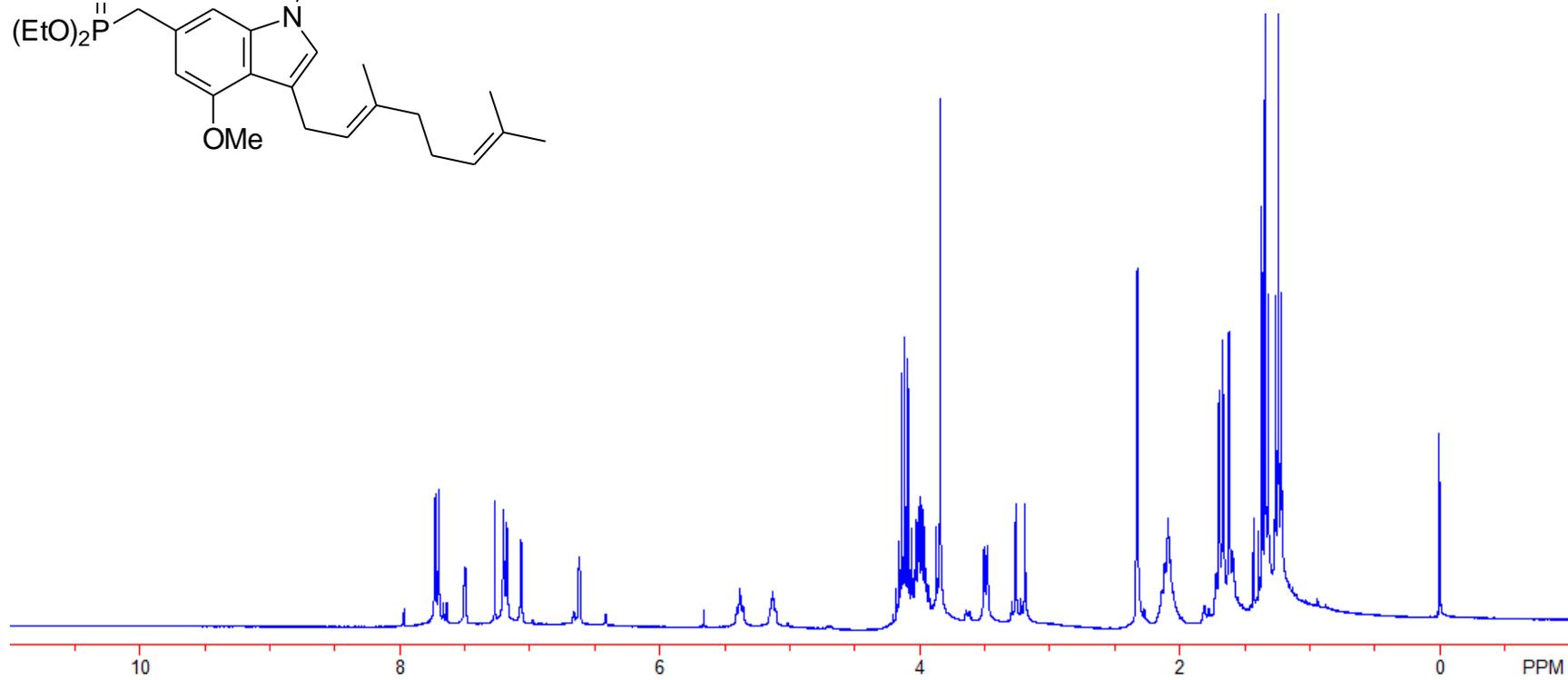
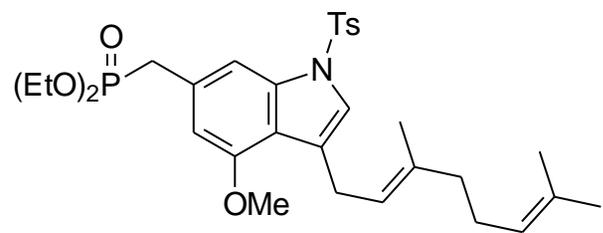
75 MHz ¹³C NMR Spectrum for Compound **34**



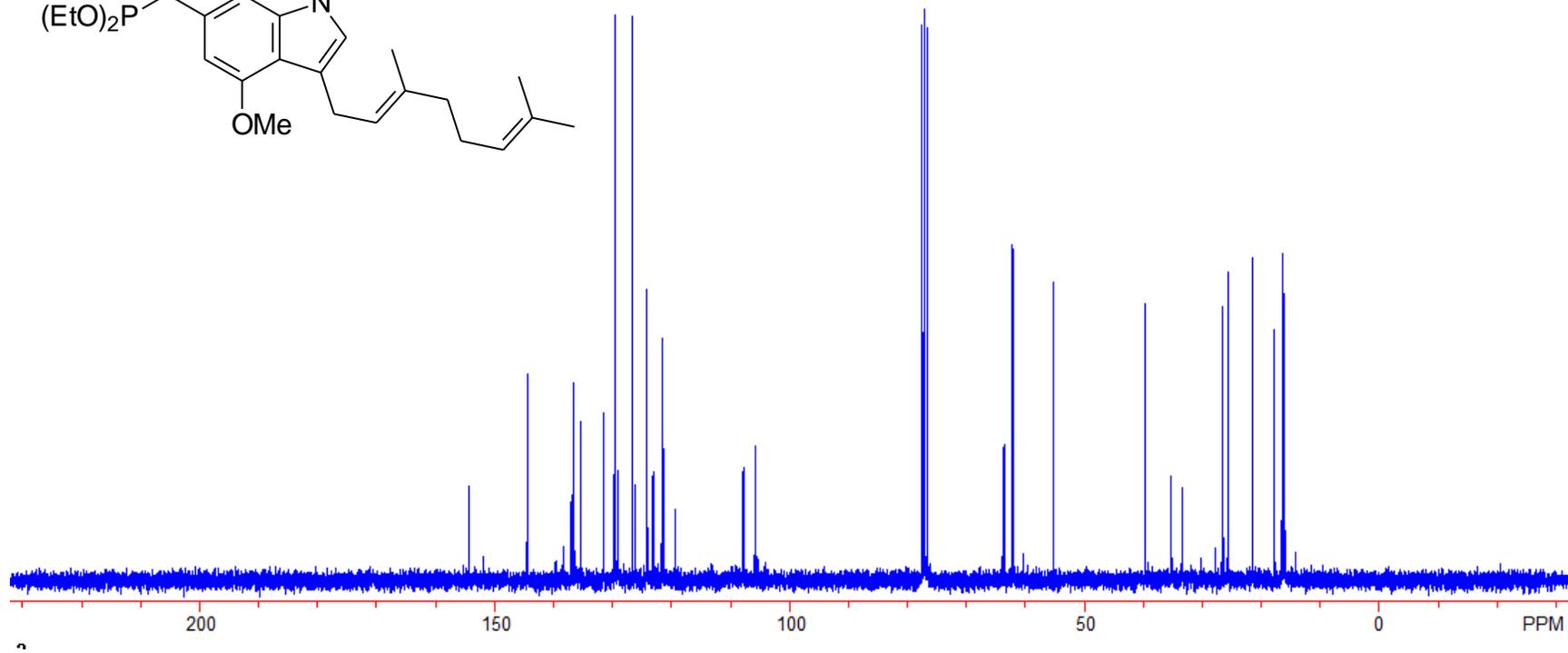
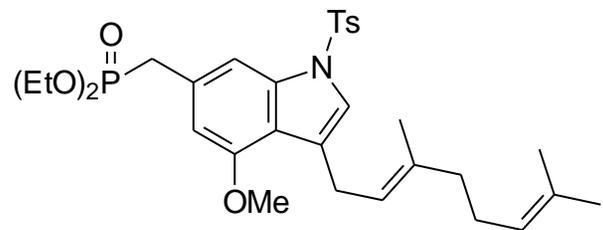
300 MHz ¹H NMR Spectrum for Compound 35



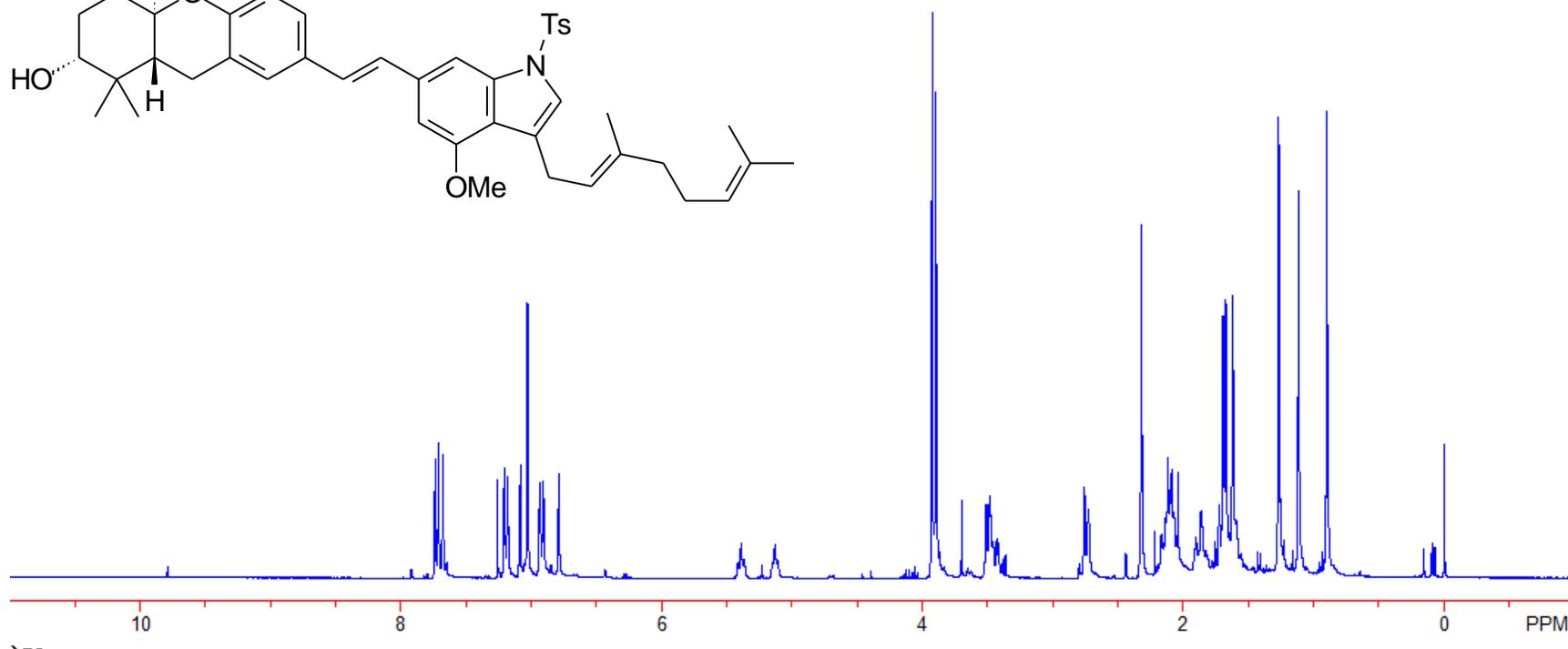
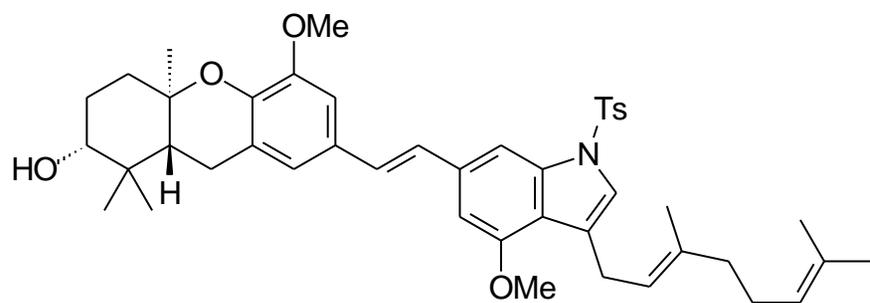
75 MHz ¹³C NMR Spectrum for Compound 35



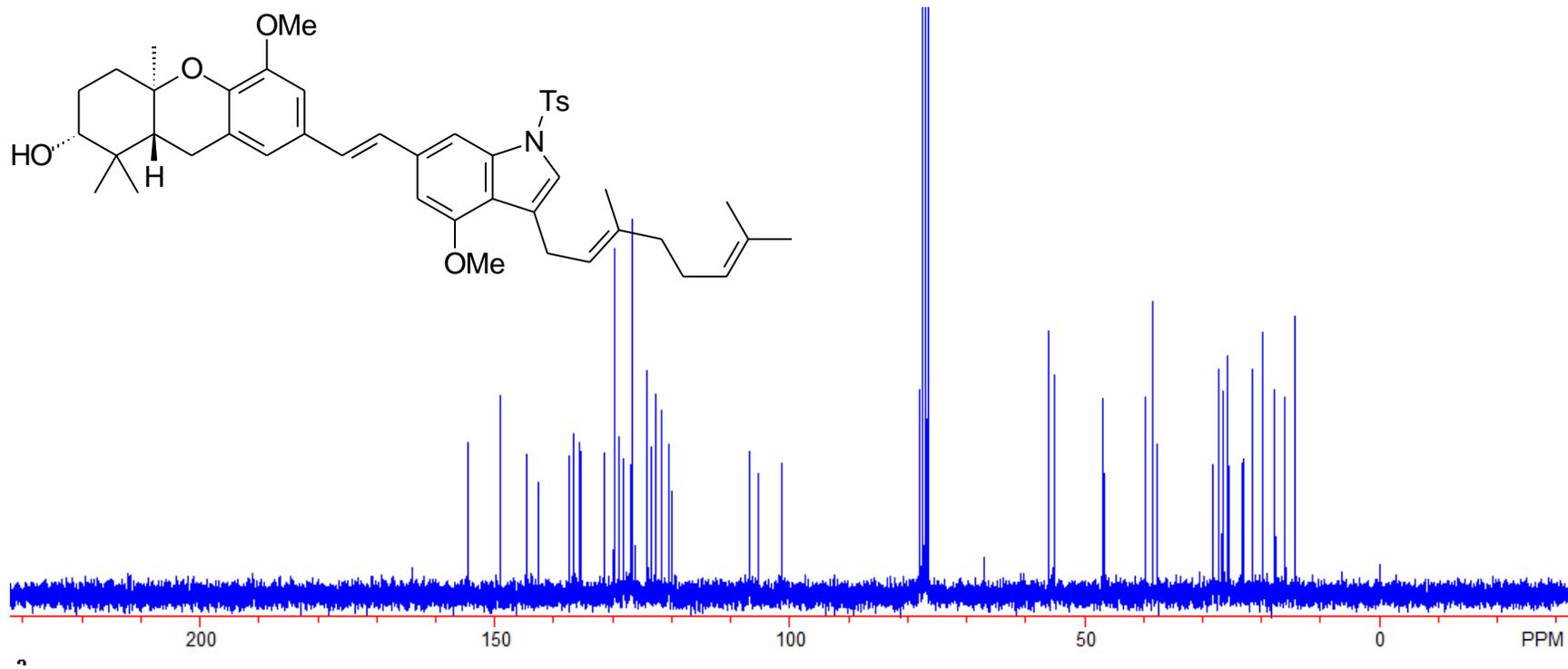
300 MHz ¹H NMR Spectrum for Compound 36

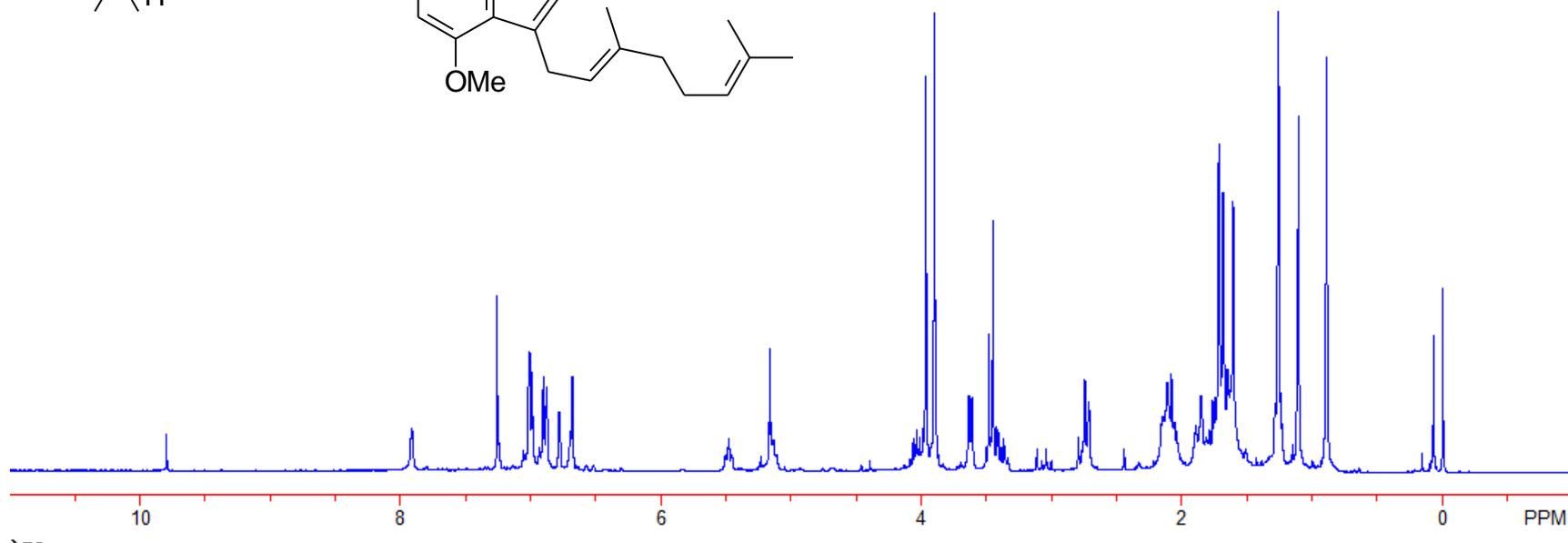
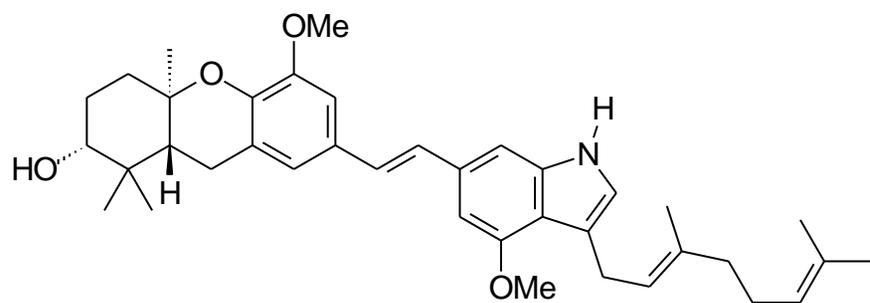


75 MHz ¹³C NMR Spectrum for Compound 36

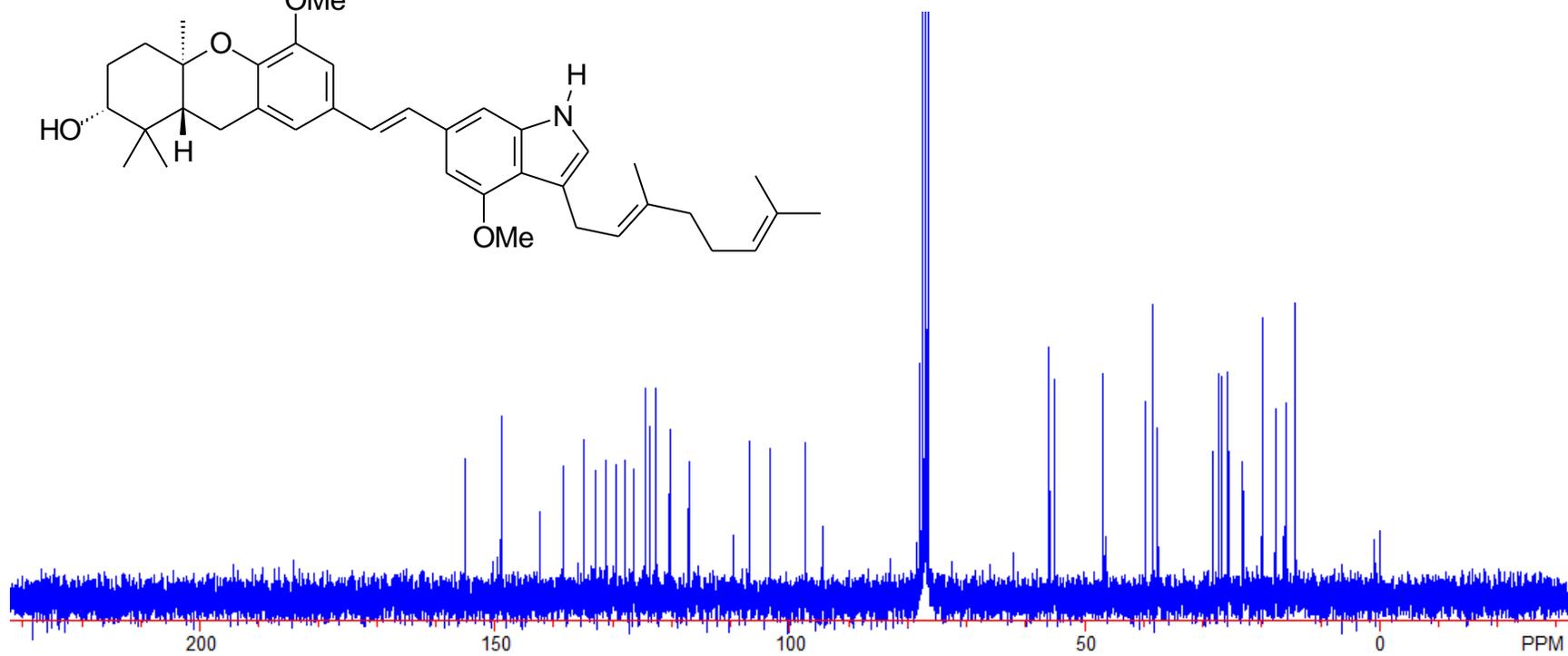
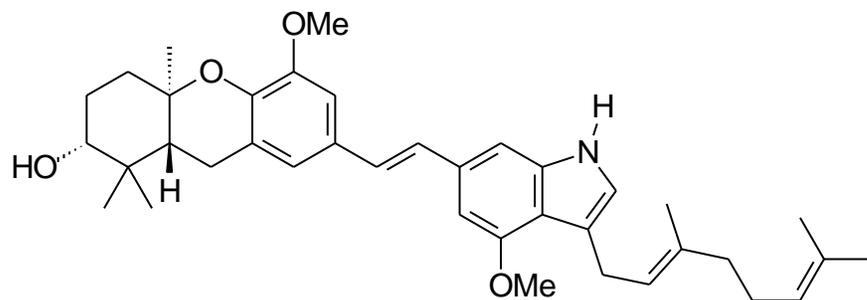


300 MHz ¹H NMR Spectrum for Compound 37

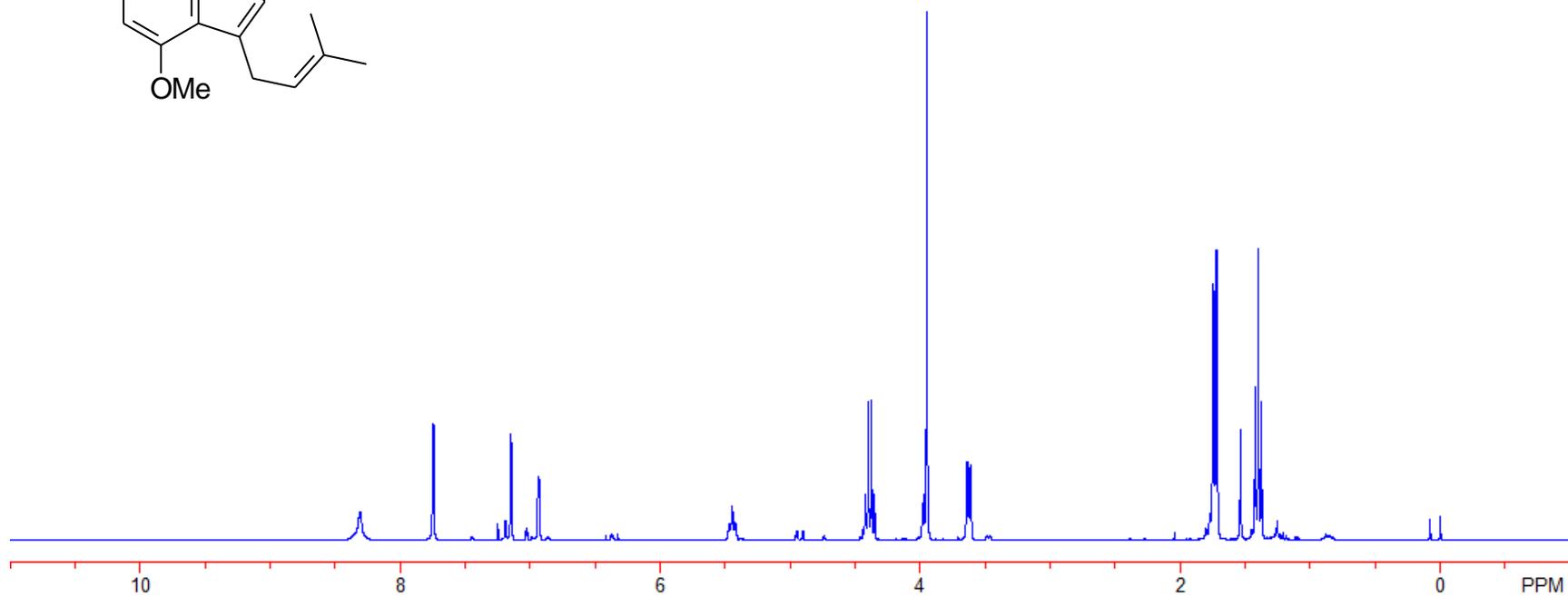
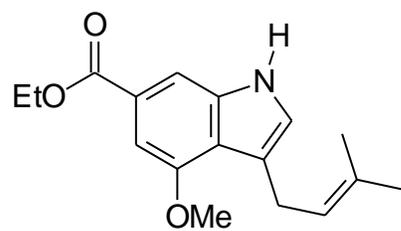




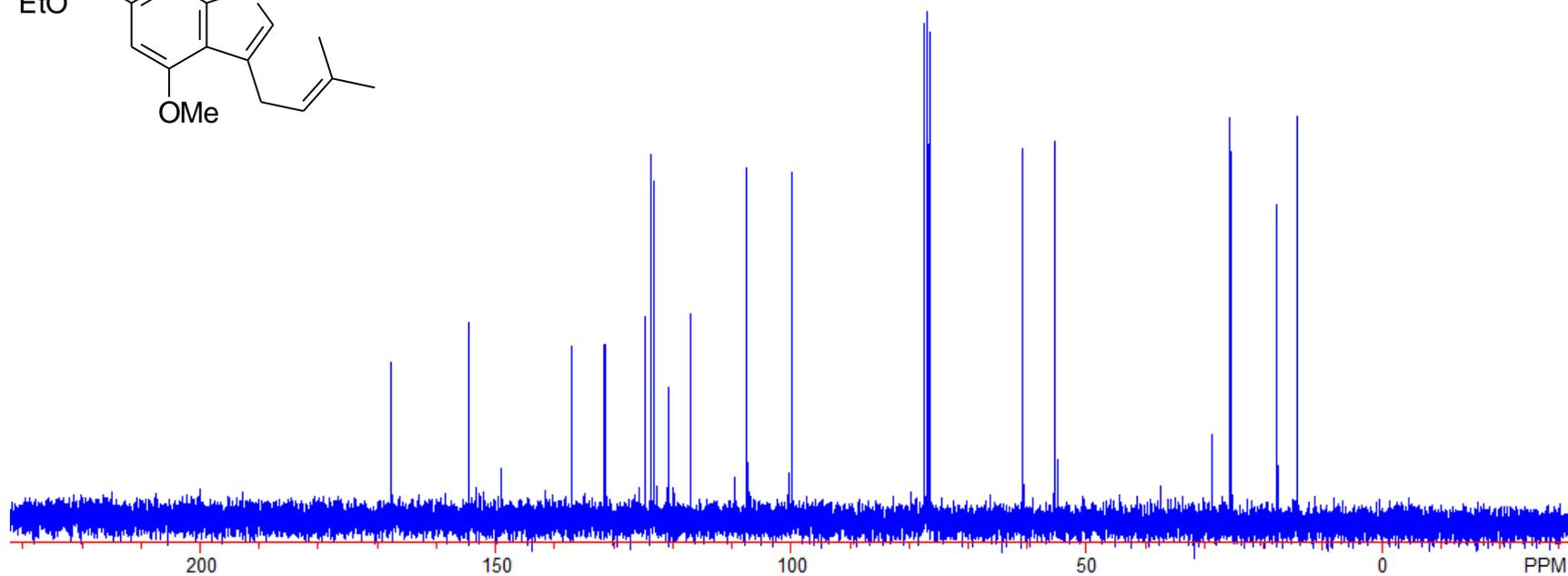
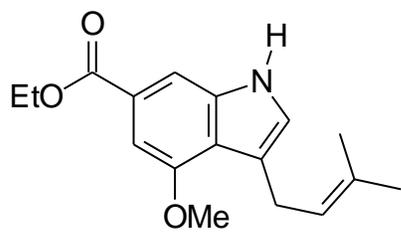
300 MHz ¹H NMR Spectrum for Compound 38



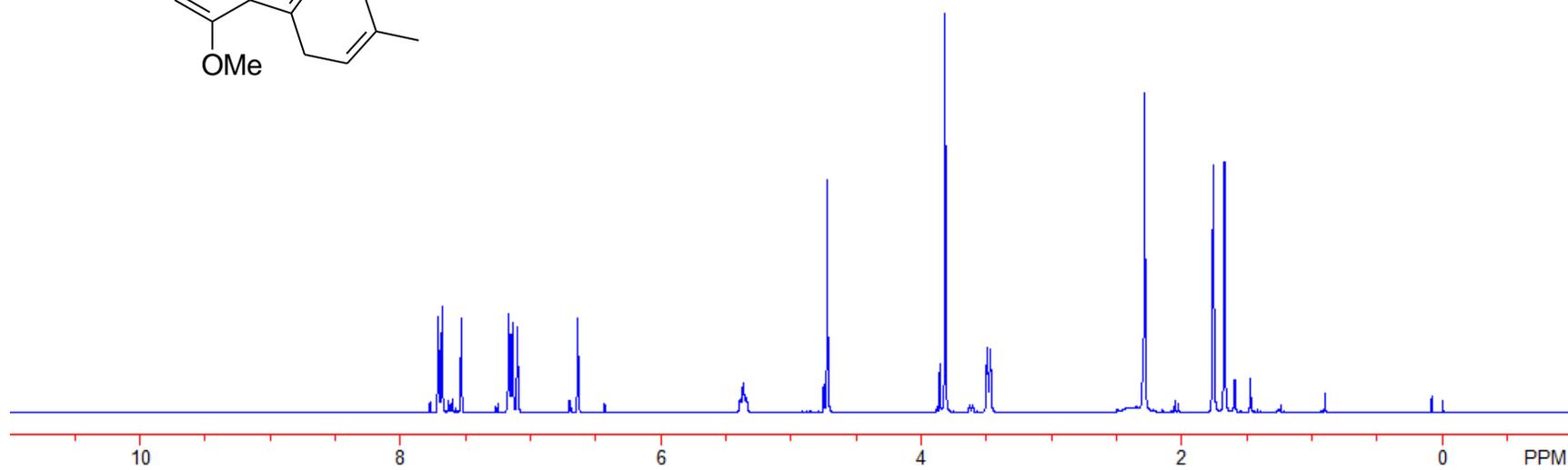
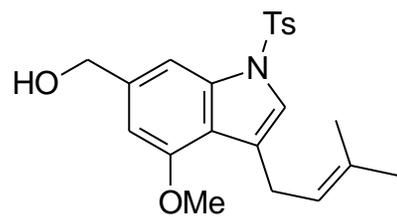
75 MHz ¹³C NMR Spectrum for Compound 38



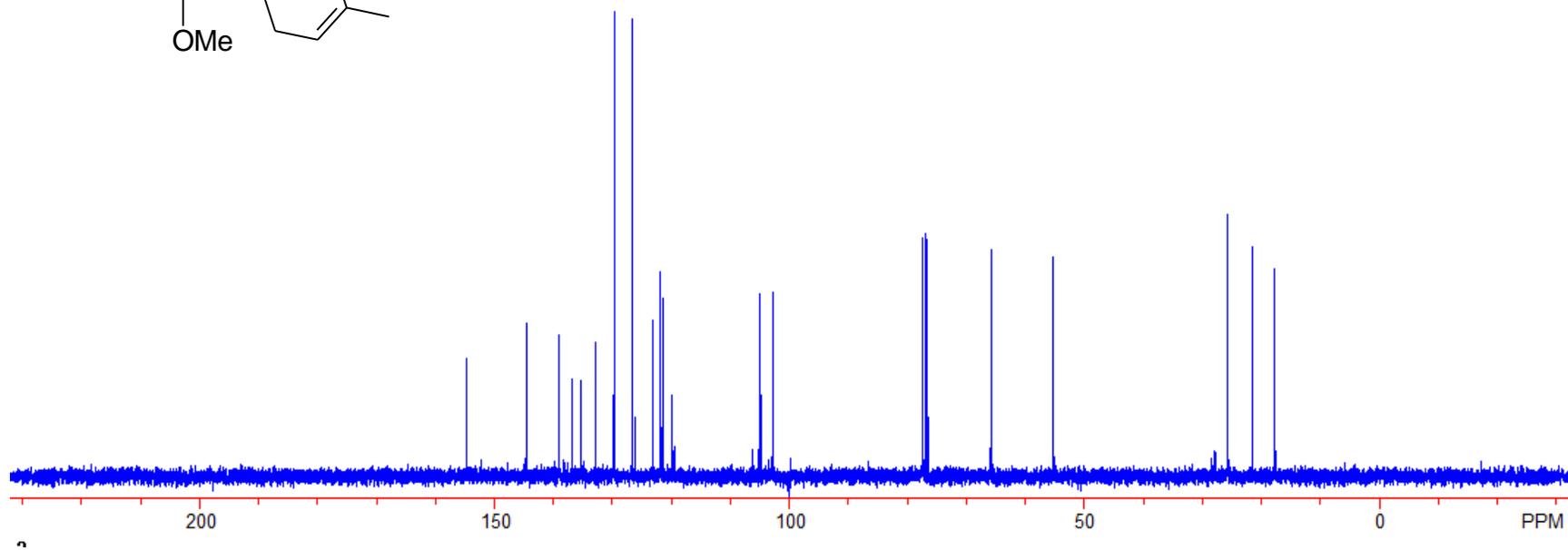
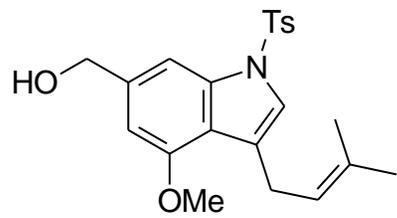
300 MHz ^1H NMR Spectrum for Compound **39**



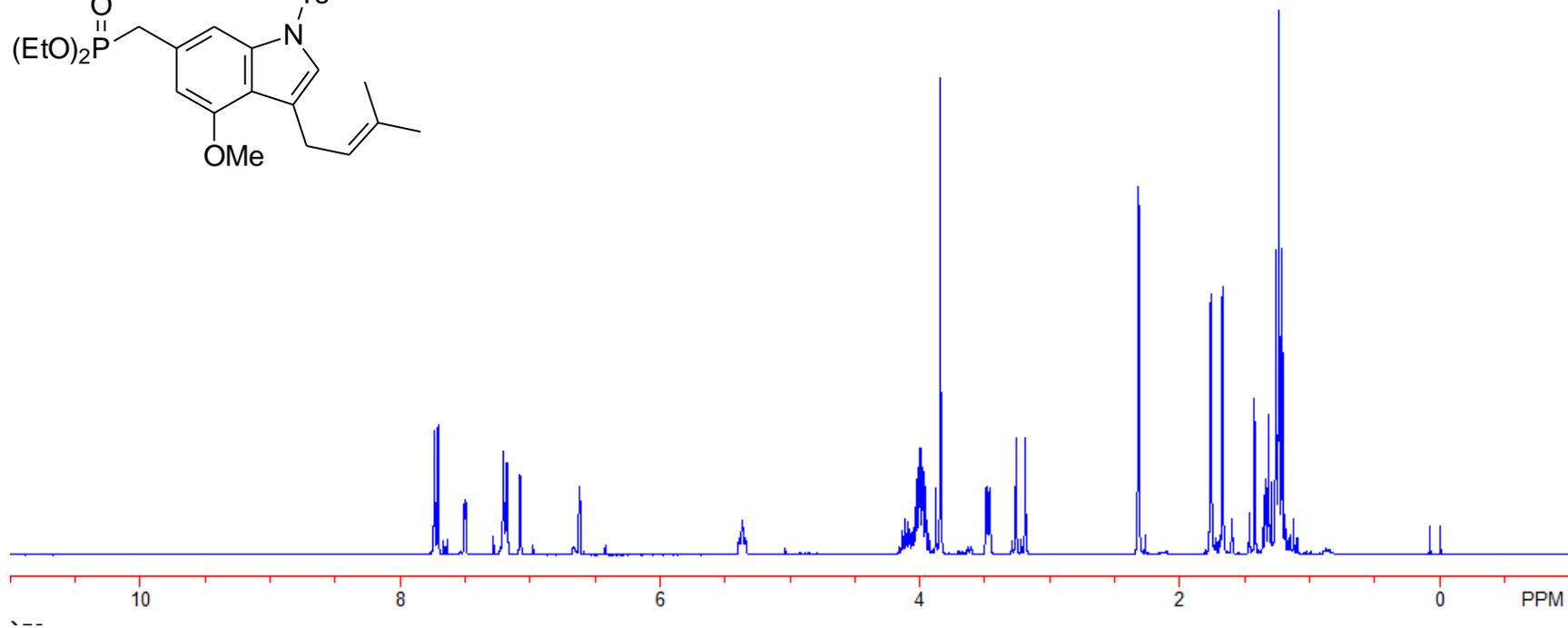
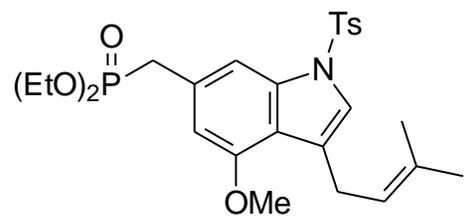
75 MHz ^{13}C NMR Spectrum for Compound 39



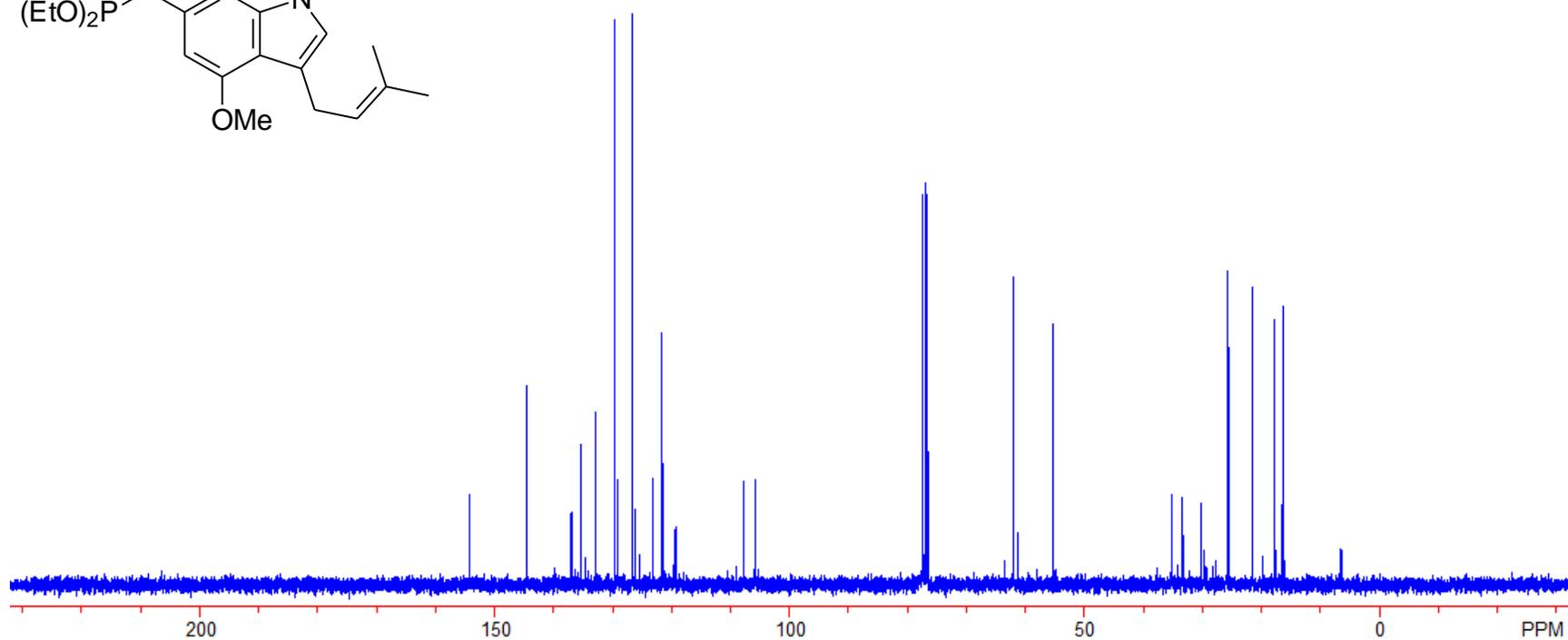
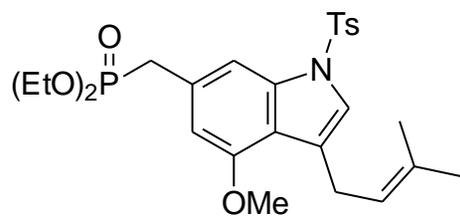
300 MHz ¹H NMR Spectrum for Compound 40



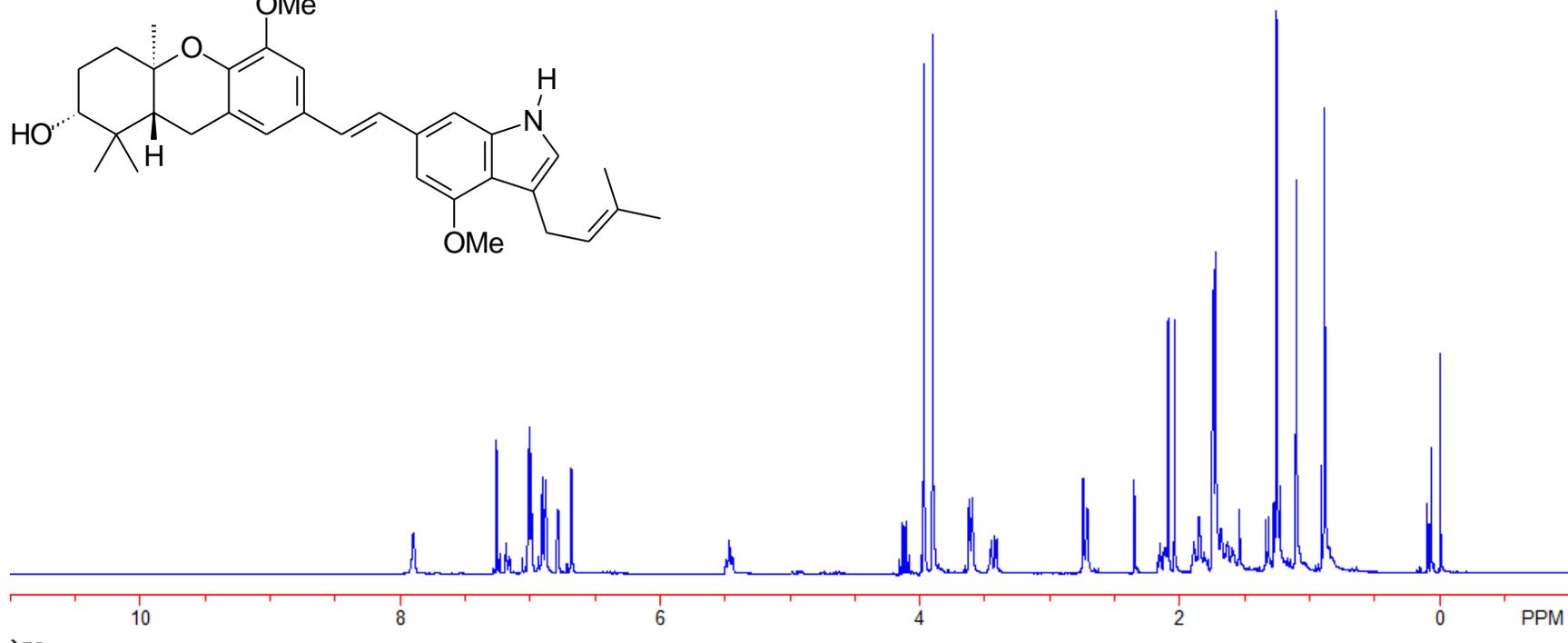
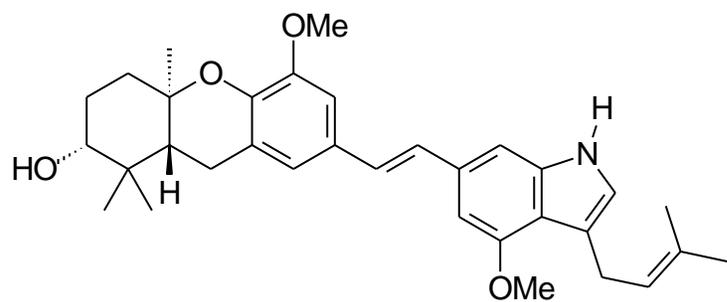
75 MHz ¹³C NMR Spectrum for Compound 40



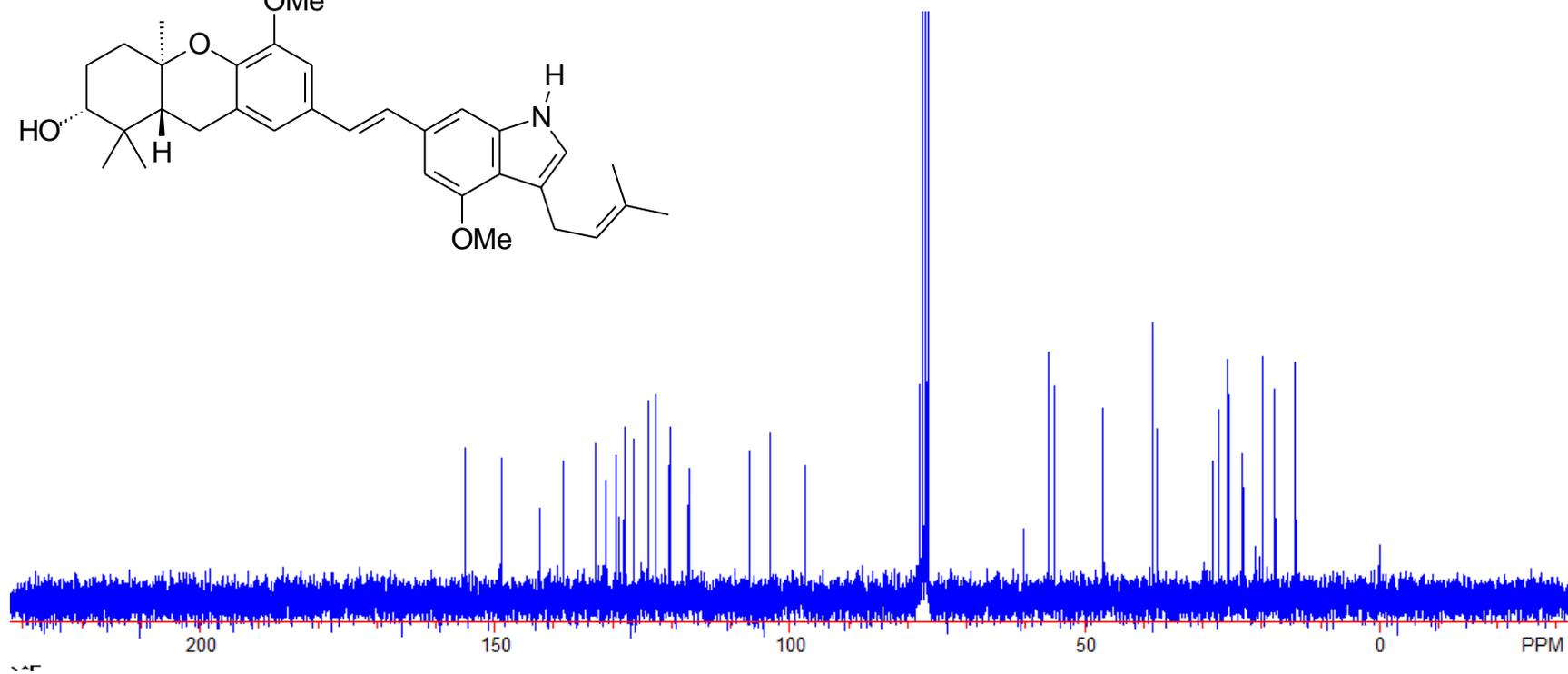
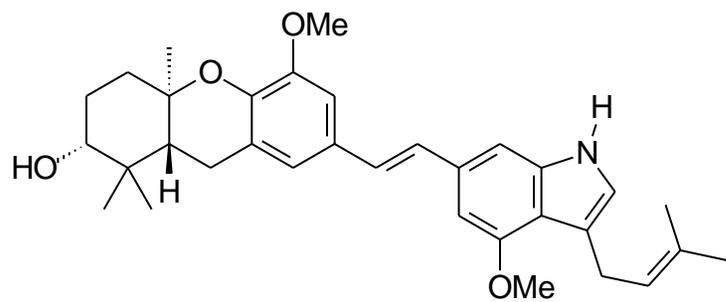
300 MHz ¹H NMR Spectrum for Compound 41



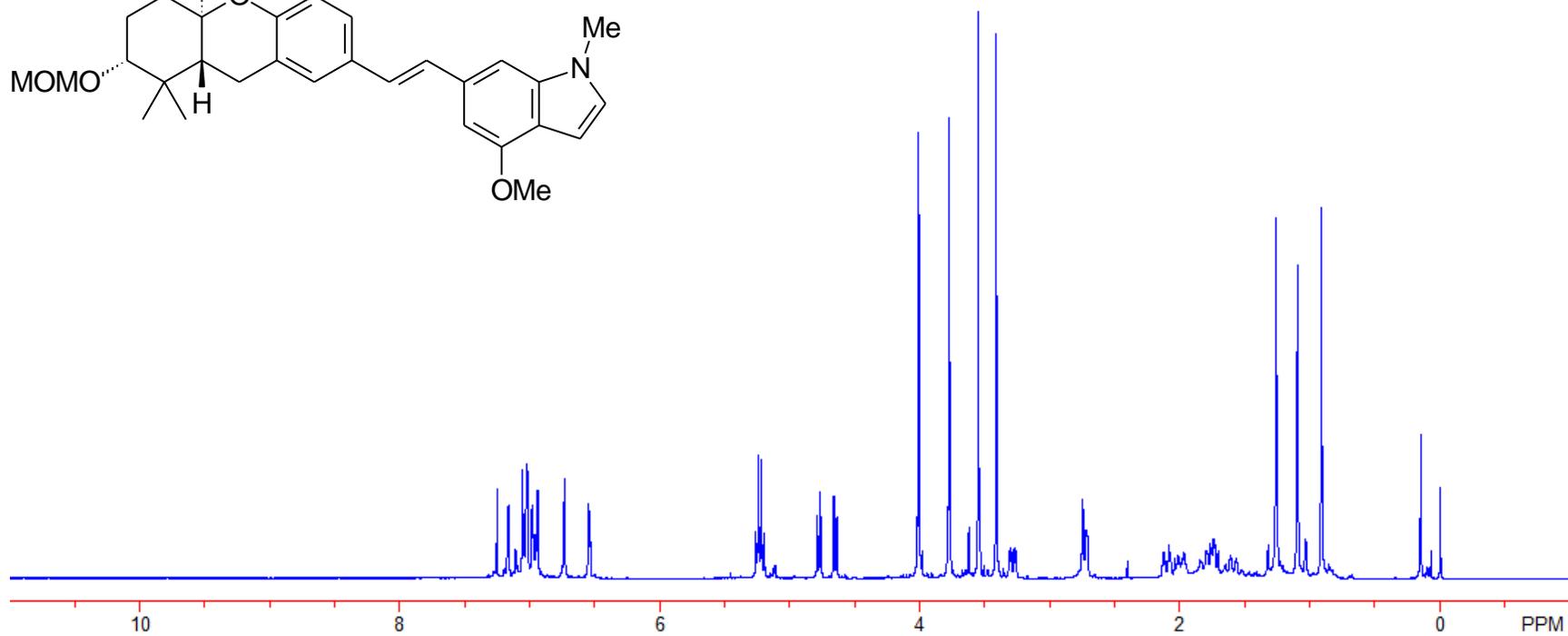
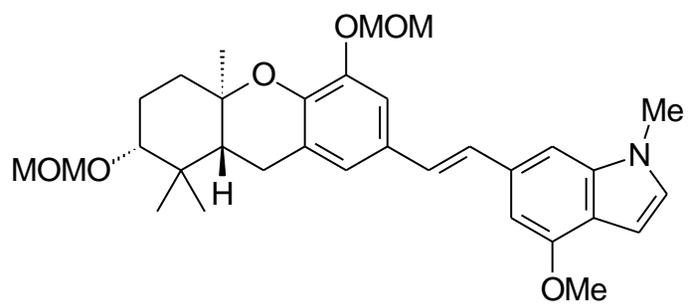
75 MHz ¹³C NMR Spectrum for Compound 41



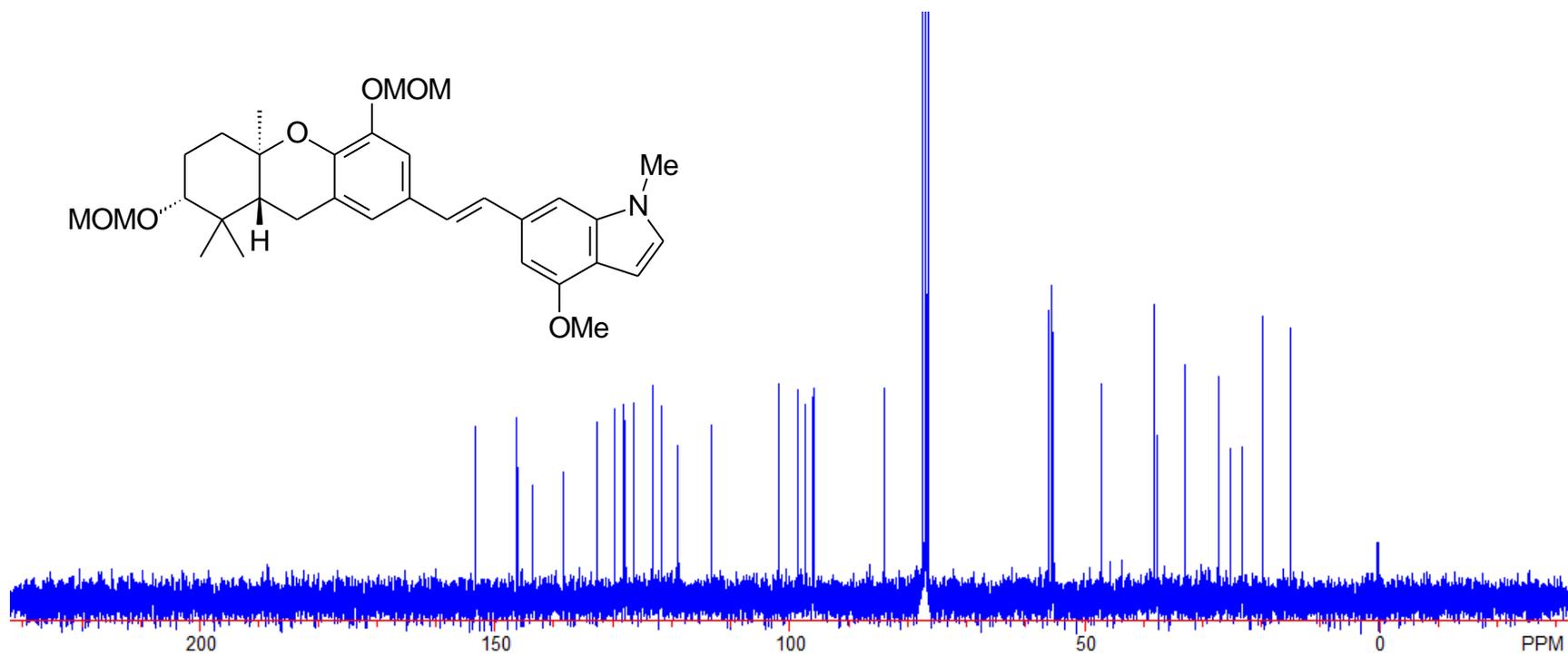
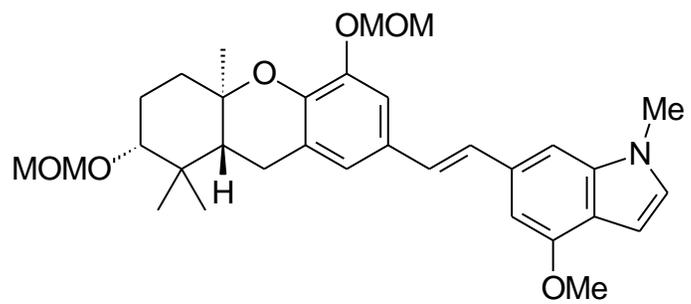
300 MHz ¹H NMR Spectrum for Compound 43



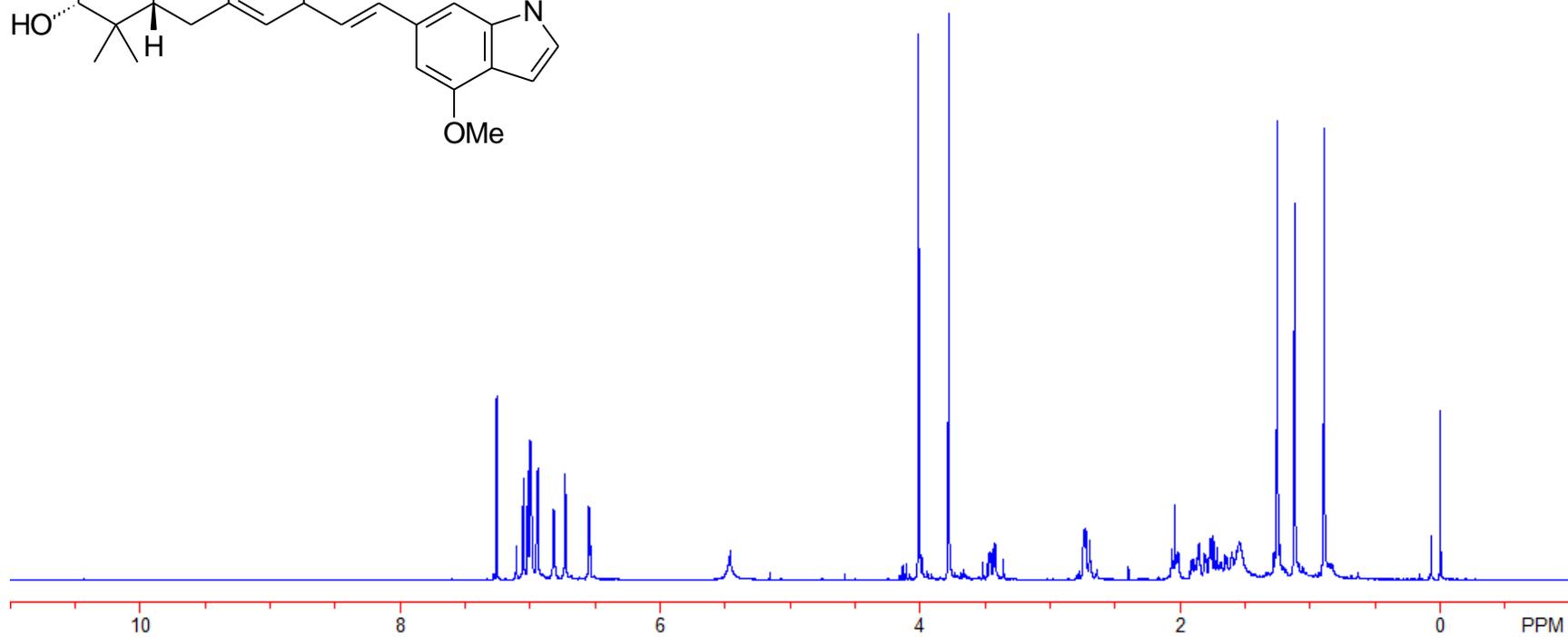
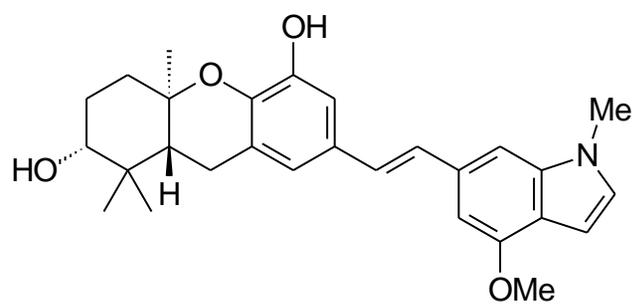
75 MHz ^{13}C NMR Spectrum for Compound 43



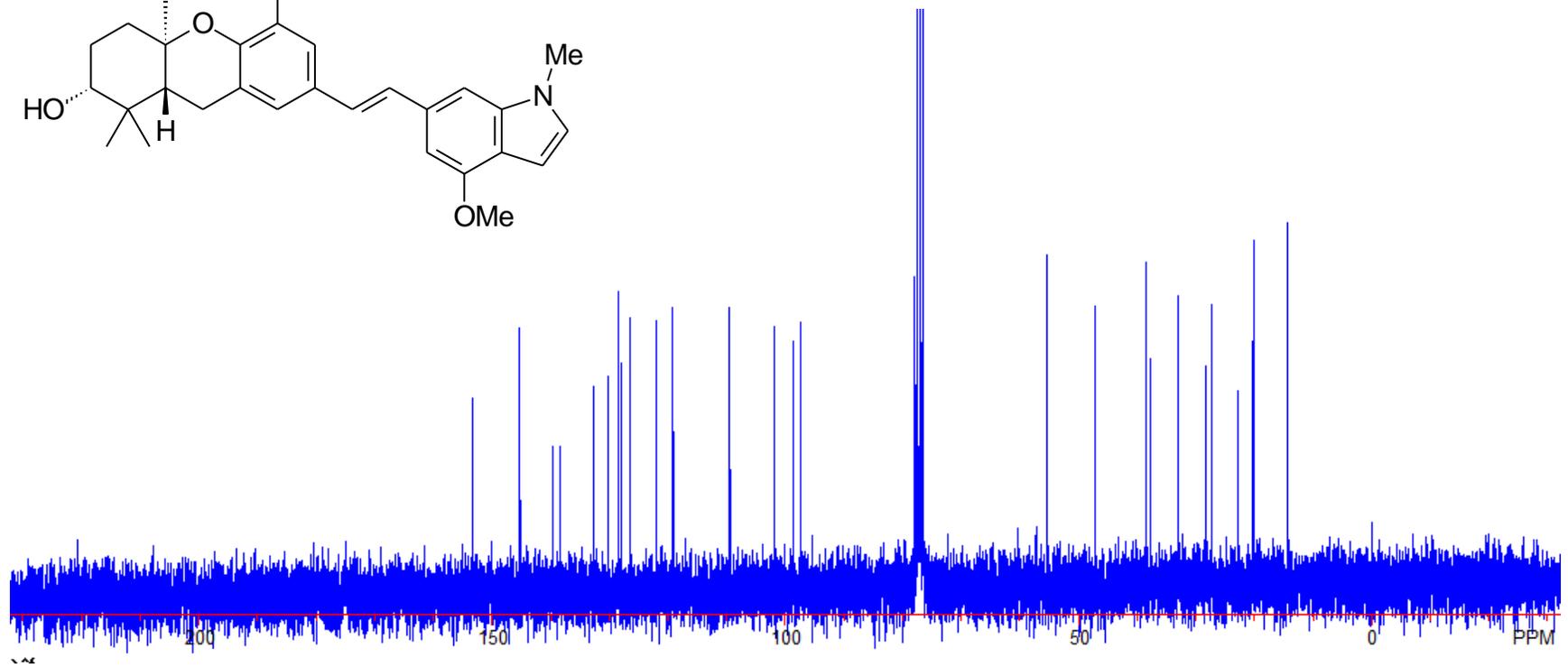
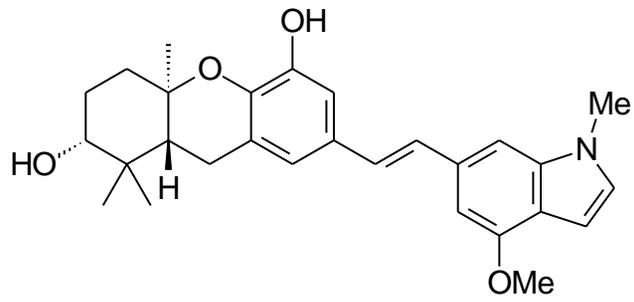
300 MHz ¹H NMR Spectrum for Compound 46



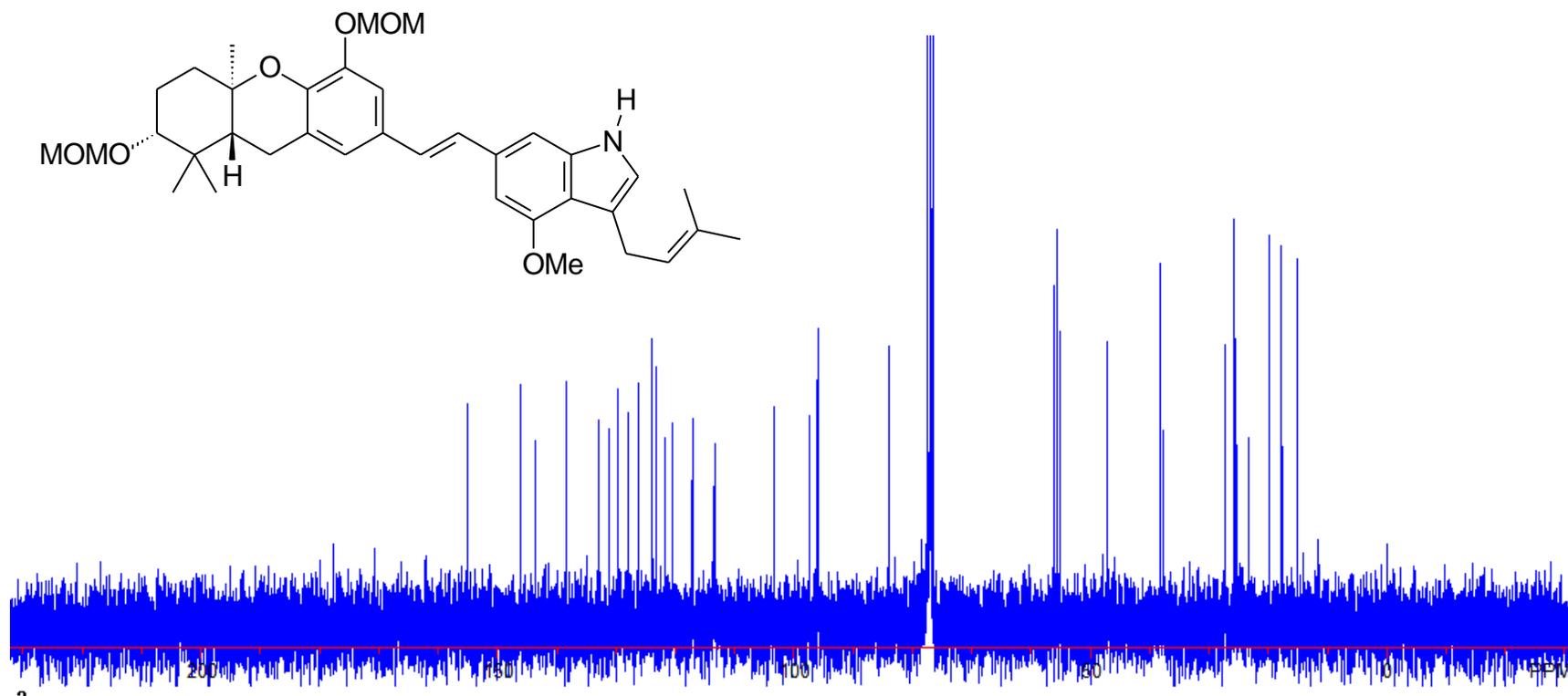
75 MHz ¹³C NMR Spectrum for Compound 46



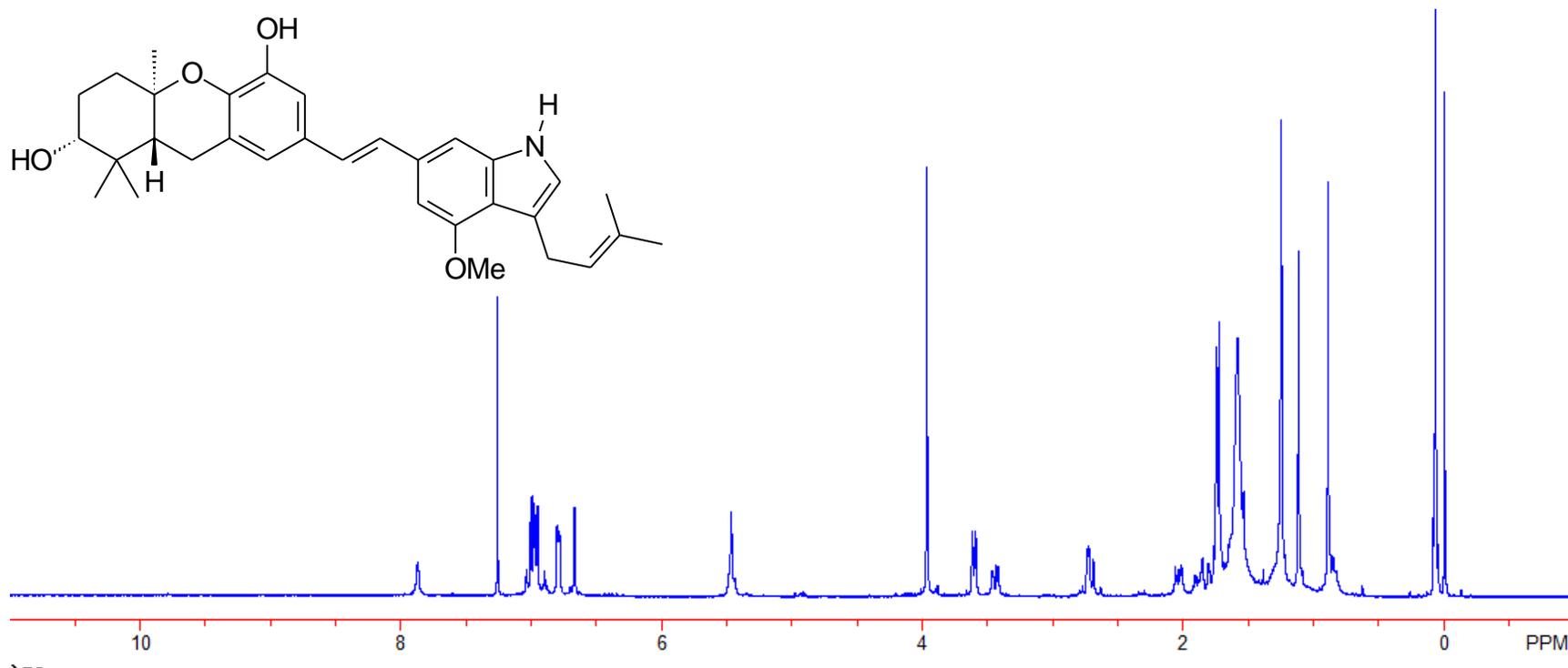
300 MHz ¹H NMR Spectrum for Compound 47



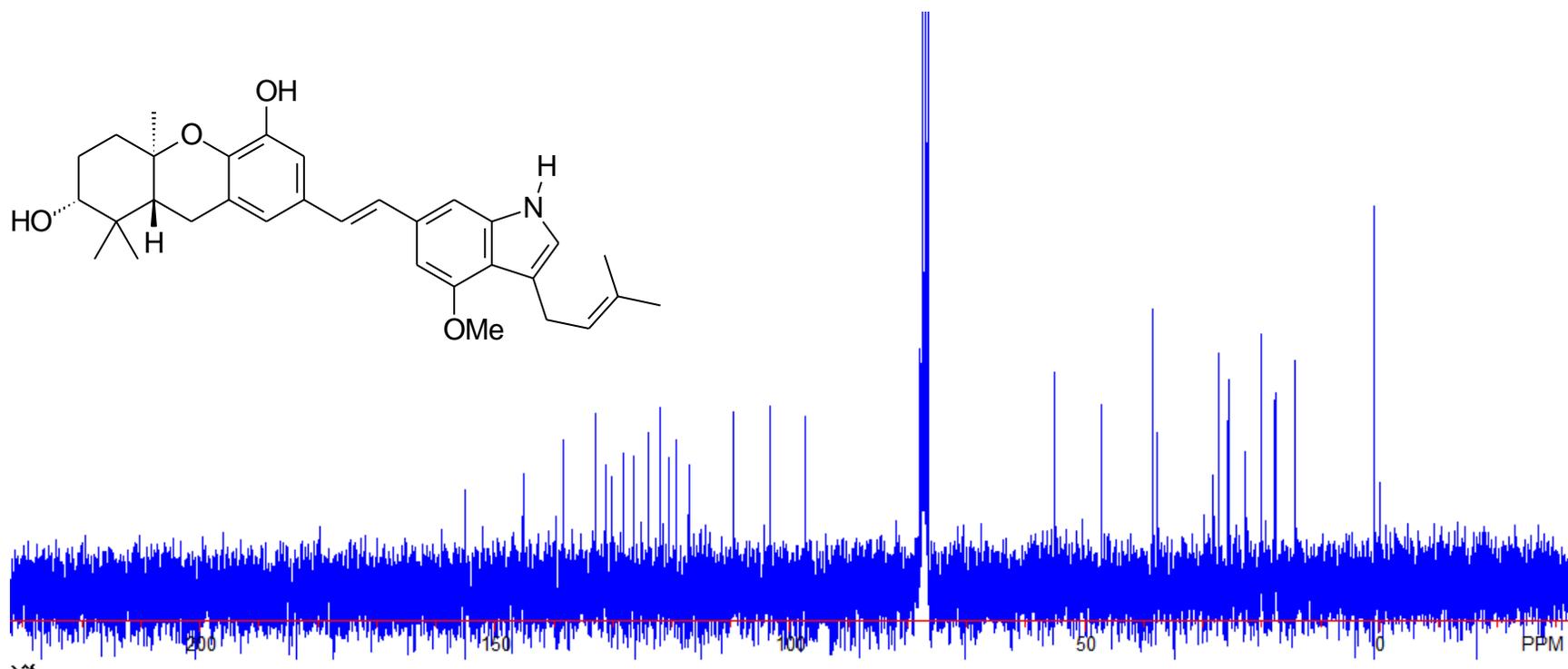
75 MHz ^{13}C NMR Spectrum for Compound 47



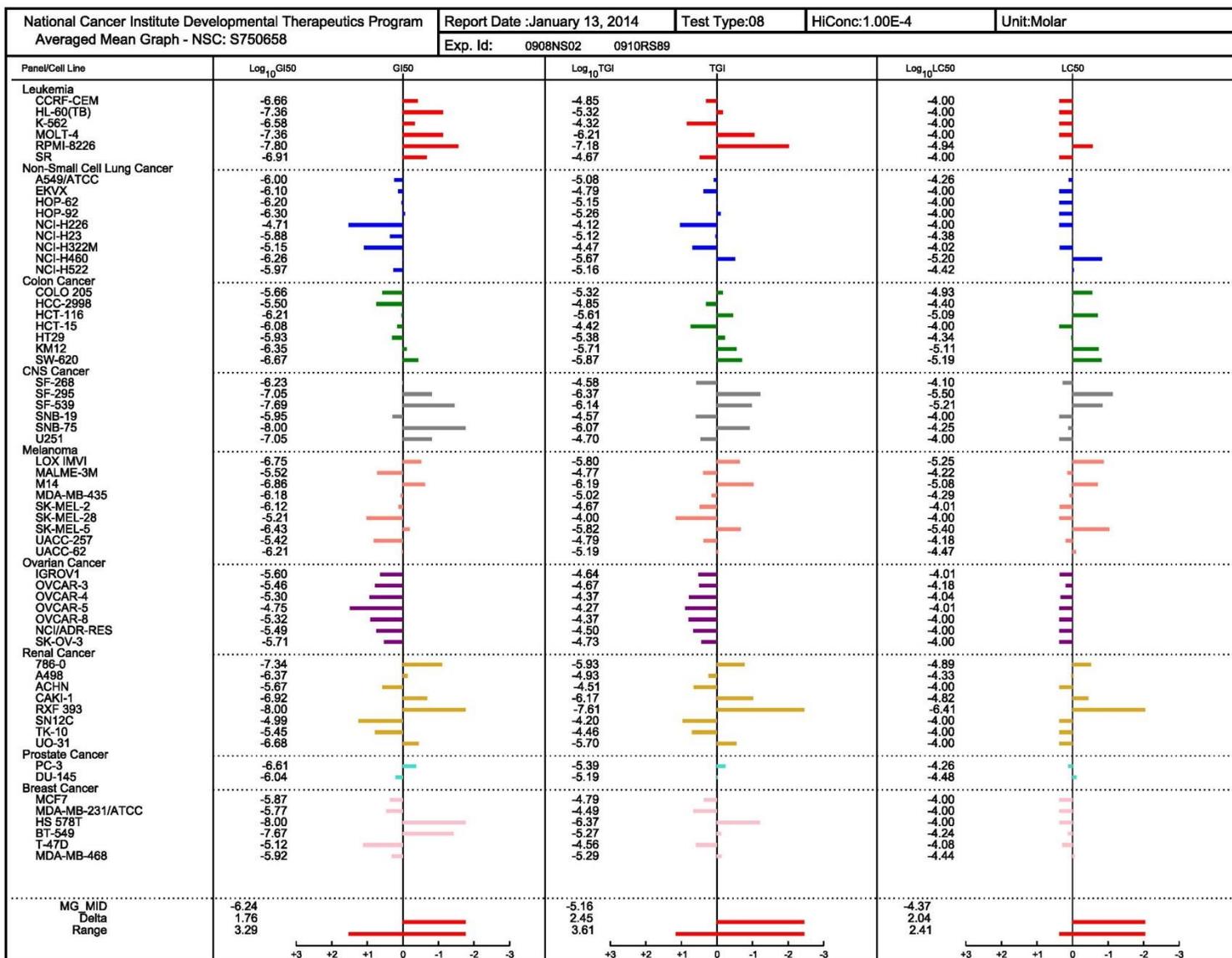
75 MHz ¹³C NMR Spectrum for Compound 49



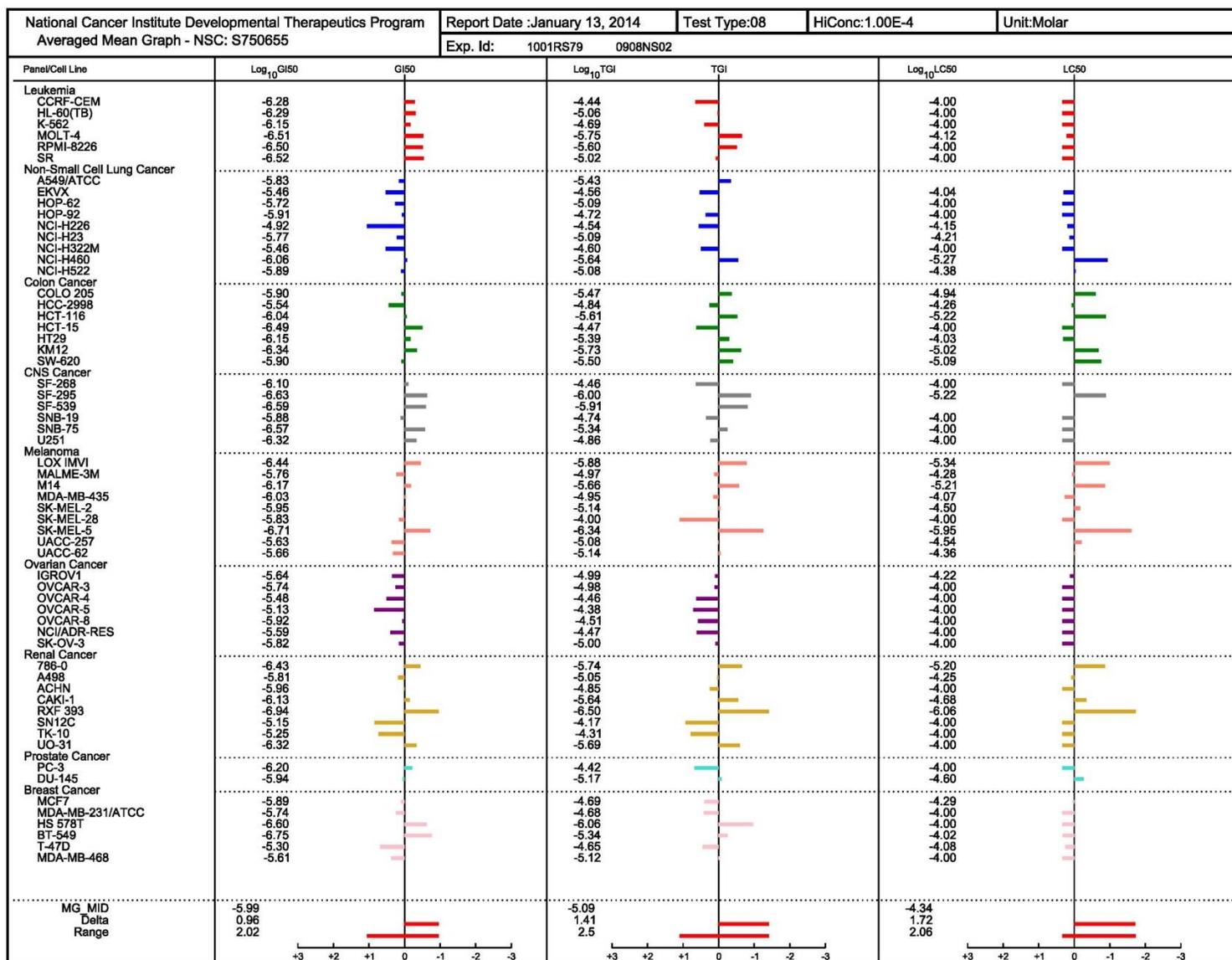
300 MHz ^1H NMR Spectrum for Compound **50**



75 MHz ^{13}C NMR Spectrum for Compound 50



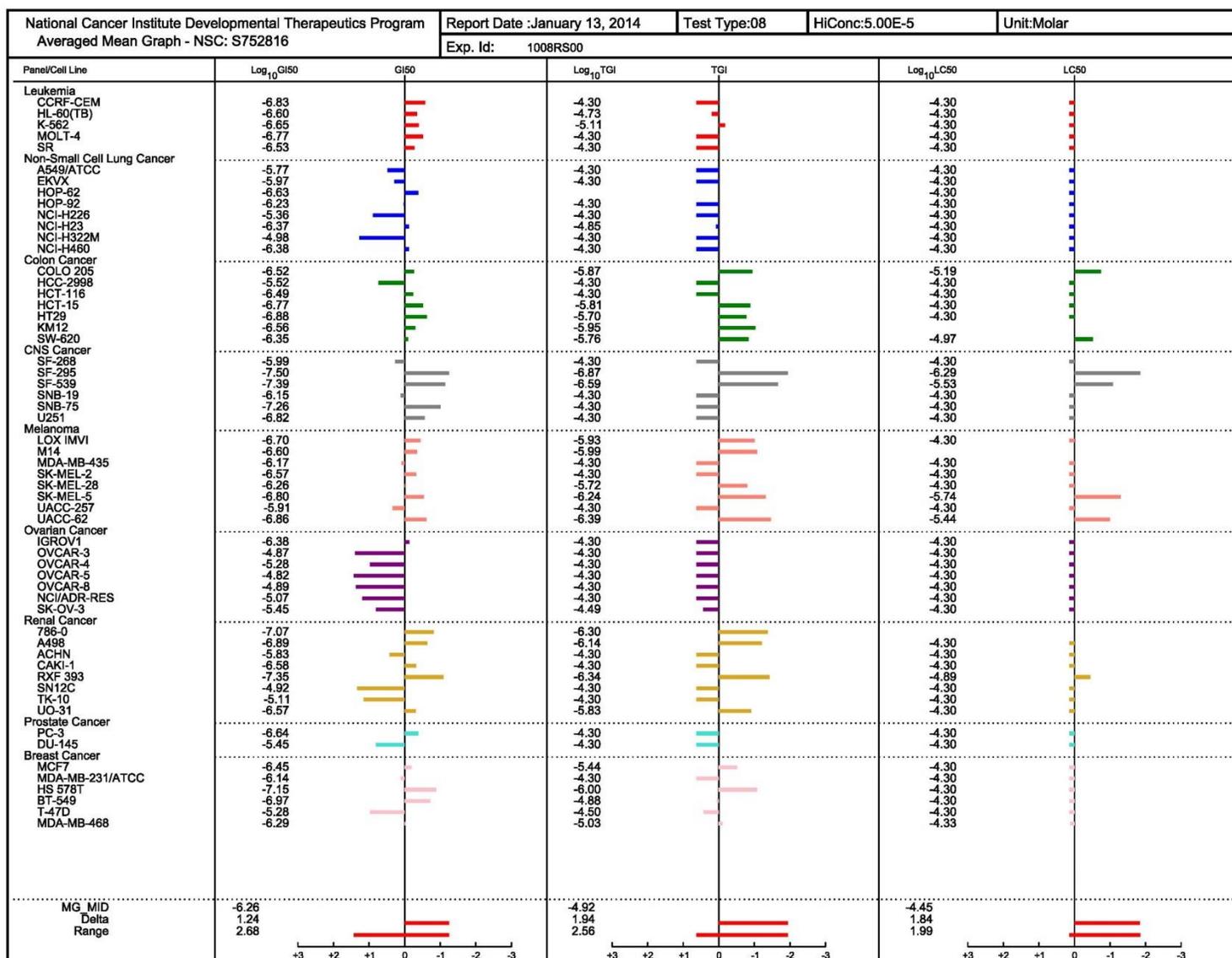
Average Mean Graph NCI 60 cell line data for compound 5



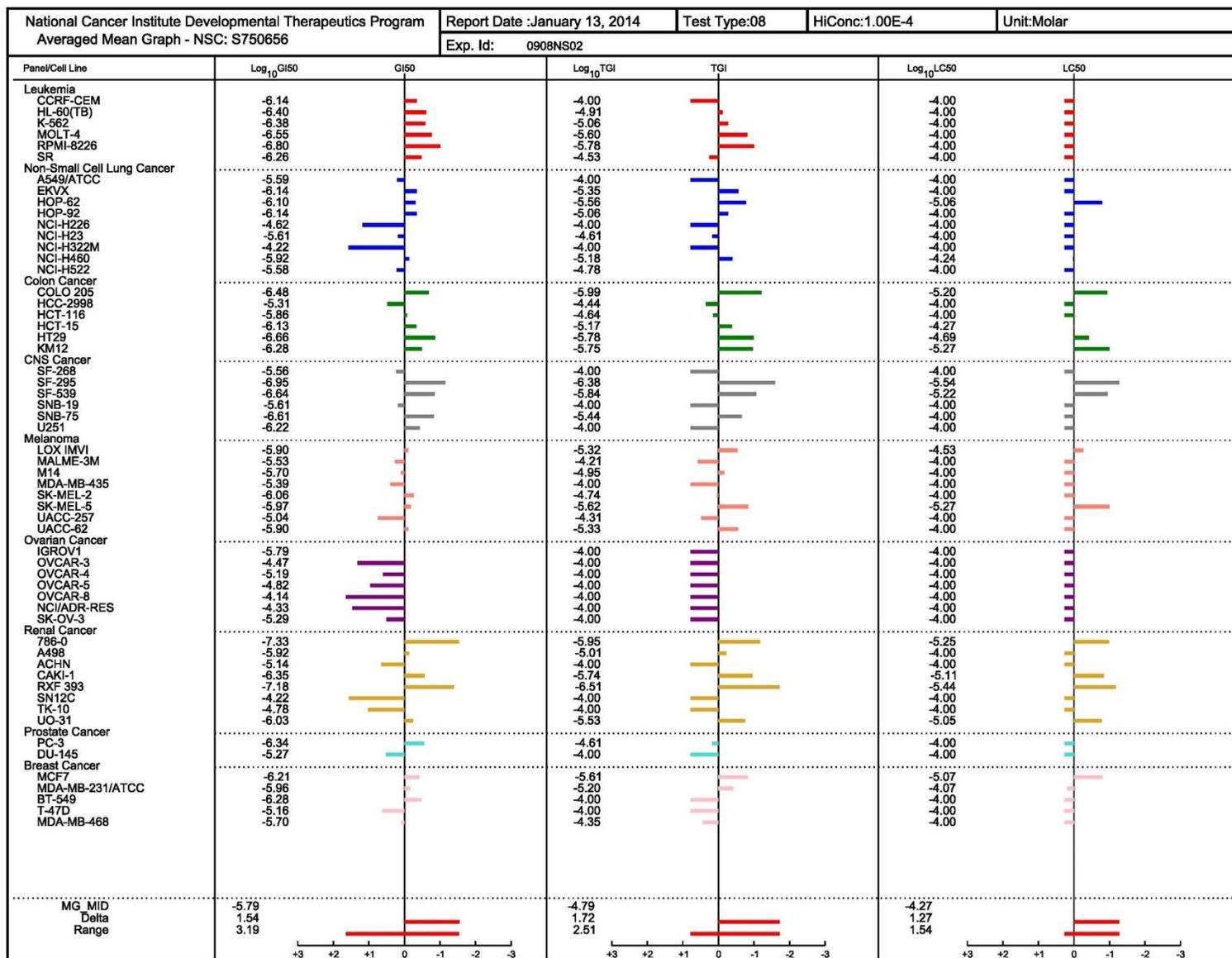
Average Mean Graph NCI 60 cell line data for compound 6

National Cancer Institute Developmental Therapeutics Program		Report Date :January 13, 2014		Test Type:08		HiConc:1.00E-4		Unit:Molar	
Averaged Mean Graph - NSC: S752116		Exp. Id: 1003NS03 1005RS58							
Panel/Cell Line	Log ₁₀ GI50	GI50	Log ₁₀ TGI	TGI	Log ₁₀ LC50	LC50			
Leukemia									
CCRF-CEM	-6.13		-4.00		-4.00				
HL-60(TB)	-4.73		-4.00		-4.00				
K-562	-5.69		-4.00		-4.00				
MOLT-4	-6.09		-4.00		-4.00				
RPMI-8226	-6.55		-4.49		-4.00				
SR	-6.12		-4.00		-4.00				
Non-Small Cell Lung Cancer									
A549/ATCC	-5.20		-4.00		-4.00				
EKVX	-5.32		-4.00		-4.00				
HOP-62	-6.08		-4.33		-4.00				
HOP-92	-5.86		-4.37		-4.00				
NCI-H226	-4.24		-4.00		-4.00				
NCI-H23	-5.20		-4.00		-4.00				
NCI-H322M	-4.49		-4.00		-4.00				
NCI-H460	-5.48		-4.00		-4.00				
NCI-H522	-5.31		-4.36		-4.00				
Colon Cancer									
COLO 205	-5.56		-5.08		-4.65				
HCC-2998	-5.02		-4.00		-4.00				
HCT-116	-5.63		-4.00		-4.00				
HCT-15	-5.84		-4.76		-4.00				
HT29	-5.58		-4.73		-4.10				
KM12	-5.69		-4.98		-4.13				
SW-620	-5.69		-5.08		-4.40				
CNS Cancer									
SF-268	-5.37		-4.00		-4.00				
SF-295	-6.54		-5.82		-4.29				
SF-539	-6.49		-5.56		-4.08				
SNB-19	-5.58		-4.00		-4.00				
SNB-75	-6.31		-4.00		-4.00				
U251	-6.22		-4.00		-4.00				
Melanoma									
LOX IMVI	-5.55		-4.12		-4.00				
MALME-3M	-5.31		-4.00		-4.00				
M14	-5.78		-5.03		-4.20				
MDA-MB-435	-5.42		-4.00		-4.00				
SK-MEL-2	-5.71		-4.00		-4.00				
SK-MEL-28	-5.33		-4.30		-4.04				
SK-MEL-5	-5.85		-5.50		-5.14				
UACC-257	-4.92		-4.09		-4.00				
UACC-62	-6.02		-5.12		-4.00				
Ovarian Cancer									
IGROV1	-5.30		-4.00		-4.00				
OVCAR-3	-4.36		-4.00		-4.00				
OVCAR-4	-4.54		-4.00		-4.00				
OVCAR-5	-4.59		-4.00		-4.00				
OVCAR-8	-4.00		-4.00		-4.00				
NCI/ADR-RES	-4.19		-4.00		-4.00				
SK-OV-3	-5.47		-4.00		-4.00				
Renal Cancer									
786-O	-6.44		-4.96		-4.00				
A498	-5.99		-4.64		-4.00				
ACHN	-5.15		-4.00		-4.00				
CAKI-1	-5.39		-4.03		-4.00				
RXF 393	-7.08		-6.35		-4.95				
SN12C	-4.23		-4.00		-4.00				
TK-10	-4.72		-4.00		-4.00				
UC-31	-6.32		-5.23		-4.00				
Prostate Cancer									
PC-3	-5.99		-4.00		-4.00				
DU-145	-5.09		-4.00		-4.00				
Breast Cancer									
MCF7	-5.61		-4.30		-4.00				
MDA-MB-231/ATCC	-5.57		-4.20		-4.00				
HS 578T	-6.51		-4.00		-4.00				
BT-549	-5.43		-4.30		-4.00				
T-47D	-4.53		-4.00		-4.00				
MDA-MB-468	-5.52		-4.57		-4.00				
Summary Statistics									
MG MID	-5.5		-4.34		-4.07				
Delta	1.58		2.02		1.08				
Range	3.08		2.35		1.14				

Average Mean Graph NCI 60 cell line data for compound 7



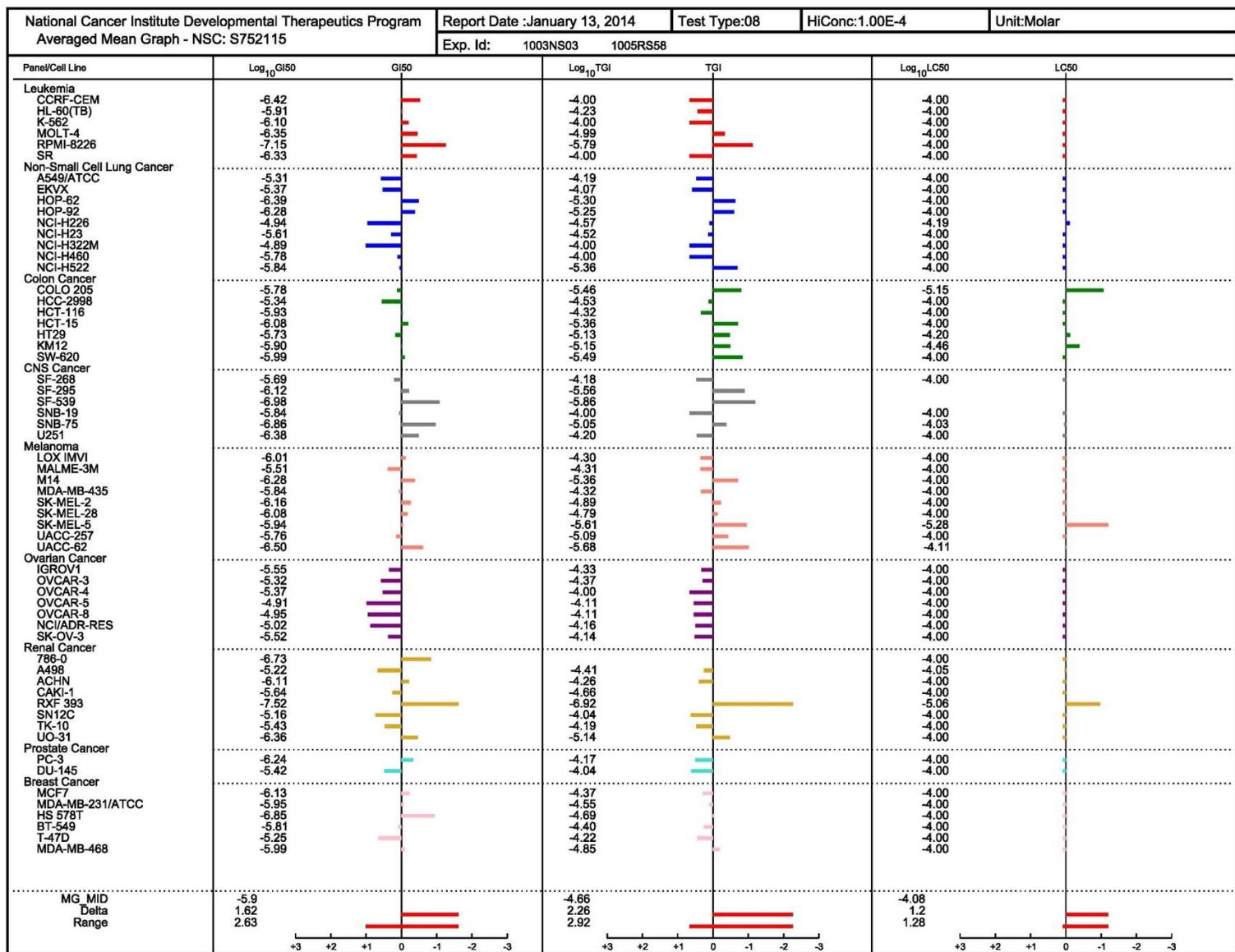
Average Mean Graph NCI 60 cell line data for compound 8



Average Mean Graph NCI 60 cell line data for compound 18

National Cancer Institute Developmental Therapeutics Program Averaged Mean Graph - NSC: S751060		Report Date :January 13, 2014	Test Type:08	HiConc:1.00E-4	Unit:Molar	
		Exp. Id: 0910NS96				
Panel/Cell Line	Log ₁₀ GI50	GI50	Log ₁₀ TGI	TGI	Log ₁₀ LC50	LC50
Leukemia						
CCRF-CEM	-6.82				-4.00	
HL-60(TB)	-6.86				-4.00	
K-562	-6.49				-4.00	
MOLT-4	-7.04				-4.00	
RPMI-8226	-7.55				-4.00	
SR	-6.52				-4.00	
Non-Small Cell Lung Cancer						
A549/ATCC	-6.06				-4.00	
EKVX	-6.27				-4.00	
HOP-62	-6.30				-5.02	
NCI-H226	-5.76				-4.23	
NCI-H23	-6.16				-4.00	
NCI-H322M	-5.45				-4.00	
NCI-H460	-6.42				-4.43	
NCI-H522	-6.15				-4.00	
Colon Cancer						
COLO 205	-6.66				-6.05	
HCC-2998	-5.55				-4.31	
HCT-116	-6.27				-5.22	
HCT-15	-6.40				-4.00	
HT29	-6.54				-4.00	
KM12	-6.72				-5.44	
SW-620	-6.51				-5.26	
CNS Cancer						
SF-268	-6.55				-4.00	
SF-295	-7.26				-6.10	
SF-539	-6.85				-5.51	
SNB-19	-6.17				-4.00	
SNB-75	-7.03				-6.33	
U251	-6.48				-4.50	
Melanoma						
LOX IMVI	-6.41				-5.35	
MALME-3M	-6.24				-4.00	
M14	-6.76				-6.13	
MDA-MB-435	-6.45				-4.00	
SK-MEL-2	-6.51				-4.00	
SK-MEL-28	-6.68				-6.11	
SK-MEL-5	-6.75				-6.45	
UACC-257	-6.53				-6.12	
UACC-62	-6.79				-6.40	
Ovarian Cancer						
IGROV1	-6.01				-4.00	
OVCAR-3	-5.92				-5.09	
OVCAR-4	-6.06				-4.00	
OVCAR-5	-6.00				-4.00	
OVCAR-8	-5.44				-4.00	
NCI/ADR-RES	-5.68				-4.00	
SK-OV-3	-6.47				-5.89	
Renal Cancer						
786-0	-7.14				-5.52	
A498	-6.61				-6.09	
ACHN	-6.24				-5.16	
CAKI-1	-7.10				-6.07	
RXF-393	-7.02				-6.50	
SN12C	-5.21				-4.29	
TK-10	-5.81				-4.96	
UO-31	-6.73				-6.01	
Prostate Cancer						
PC-3	-6.72				-4.00	
DU-145	-5.97				-4.04	
Breast Cancer						
MCF7	-6.41				-5.70	
MDA-MB-231/ATCC	-6.07				-4.00	
HS 578T	-7.29				-6.11	
BT-549	-6.64				-4.00	
T-47D	-5.55				-4.30	
MDA-MB-468	-6.20				-5.35	
MG MID						
Delta	-6.42				-4.5	
Range	1.2				2	
	2.42				2.5	

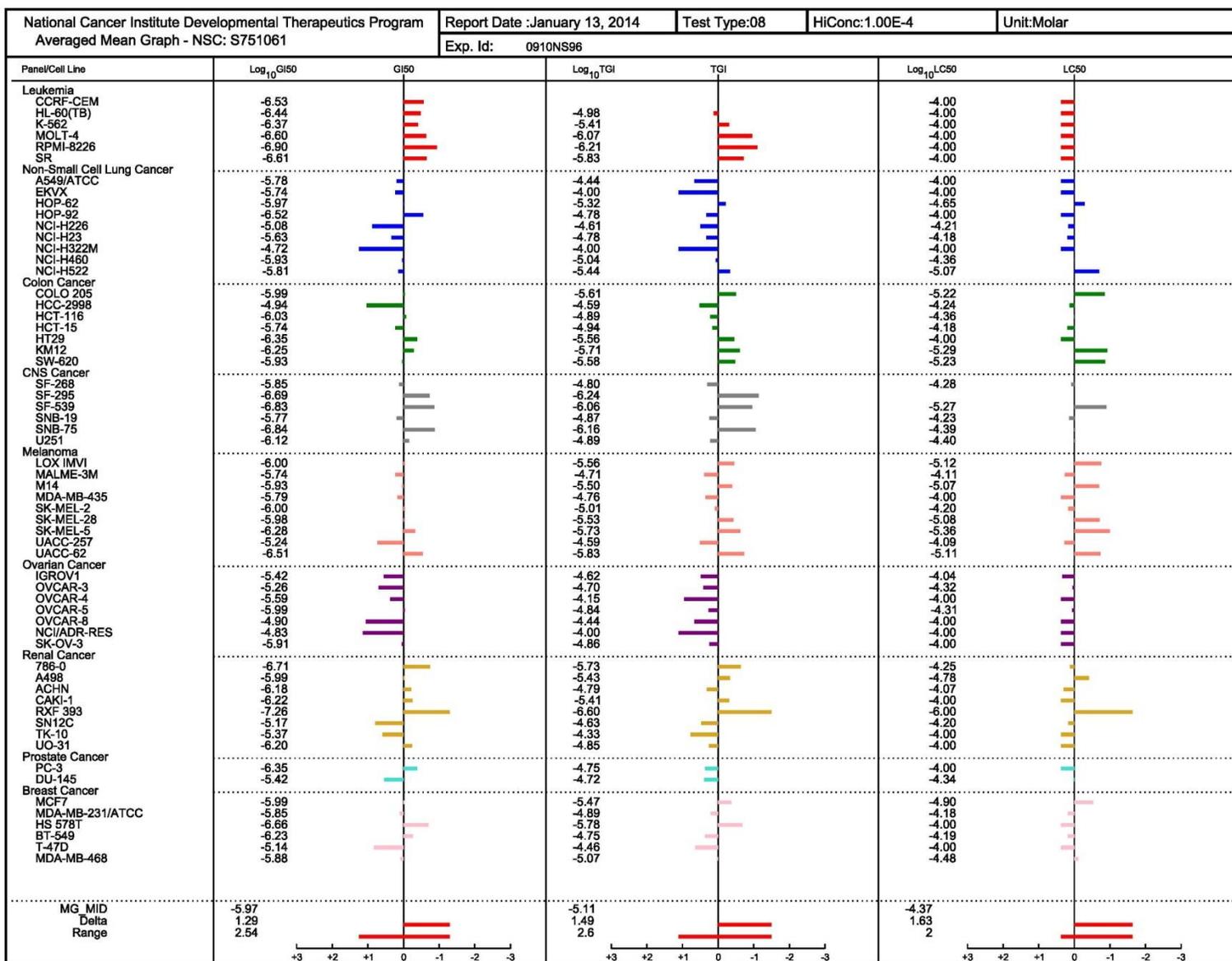
Average Mean Graph NCI 60 cell line data for compound 19



Average Mean Graph NCI 60 cell line data for compound 20

National Cancer Institute Developmental Therapeutics Program Averaged Mean Graph - NSC: S752114		Report Date :January 13, 2014	Test Type:08	HiConc:1.00E-4	Unit:Molar	
		Exp. Id: 1003NS03	1005RS58			
Panel/Cell Line	Log ₁₀ GI50	GI50	Log ₁₀ TGI	TGI	Log ₁₀ LC50	LC50
Leukemia						
CCRF-CEM	-6.34		-5.03		-4.00	
HL-60(TB)	-5.92		-4.41		-4.00	
K-562	-6.00		-4.48		-4.00	
MOLT-4	-6.36		-5.07		-4.00	
RPMI-8226	-6.77		-5.70		-4.00	
SR	-6.29		-4.00		-4.00	
Non-Small Cell Lung Cancer						
A549/ATCC	-5.72		-4.00		-4.00	
EKVX	-5.80		-4.31		-4.00	
HOP-62	-6.21		-5.42		-4.54	
HOP-92	-5.92		-5.24		-4.00	
NCI-H226	-5.22		-4.00		-4.00	
NCI-H23	-5.57		-4.24		-4.00	
NCI-H322M	-4.74		-4.00		-4.00	
NCI-H460	-5.97		-4.92		-4.21	
NCI-H522	-5.74		-5.09		-4.00	
Colon Cancer						
COLO 205	-5.96		-5.52		-5.18	
HCC-2998	-5.28		-4.60		-4.12	
HCT-116	-5.91		-4.82		-4.29	
HCT-15	-5.94		-5.20		-4.19	
HT29	-5.90		-5.25		-4.36	
KM12	-5.70		-4.95		-4.38	
SW-620	-5.89		-5.47		-4.98	
CNS Cancer						
SF-268	-5.68		-4.16		-4.00	
SF-295	-6.77		-6.27		-5.15	
SF-539	-6.67		-5.26		-4.24	
SNB-19	-5.86		-4.00		-4.00	
SNB-75	-6.44		-4.94		-4.00	
U251	-6.45		-4.81		-4.16	
Melanoma						
LOX IMVI	-5.79		-4.77		-4.10	
MALME-3M	-5.42		-4.32		-4.00	
M14	-6.24		-4.78		-4.34	
MDA-MB-435	-5.99		-4.88		-4.04	
SK-MEL-2	-6.07		-4.69		-4.00	
SK-MEL-28	-5.76		-4.76		-4.19	
SK-MEL-5	-6.29		-5.97		-5.85	
UACC-257	-5.61		-4.45		-4.00	
UACC-62	-6.45		-5.66		-4.63	
Ovarian Cancer						
IGROV1	-5.65		-4.34		-4.02	
OVCAR-3	-5.19		-4.63		-4.24	
OVCAR-4	-5.41		-4.00		-4.00	
OVCAR-5	-5.34		-4.42		-4.00	
OVCAR-8	-5.03		-4.00		-4.00	
NCI/ADR-RES	-5.19		-4.00		-4.00	
SK-OV-3	-5.59		-4.40		-4.00	
Renal Cancer						
786-0	-6.67		-5.62		-4.00	
A498	-6.39		-5.09		-4.00	
ACHN	-6.00		-4.06		-4.00	
CAKI-1	-6.16		-5.32		-4.00	
RXF 393	-7.35		-6.56		-5.37	
SN12C	-5.22		-4.00		-4.00	
TK-10	-5.50		-4.03		-4.00	
UO-31	-6.30		-5.52		-4.00	
Prostate Cancer						
PC-3	-6.16		-4.08		-4.00	
DU-145	-5.61		-4.18		-4.00	
Breast Cancer						
MCF7	-5.82		-4.84		-4.18	
MDA-MB-231/ATCC	-5.83		-4.47		-4.00	
HS 578T	-6.45		-5.30		-4.00	
BT-549	-5.55		-4.51		-4.00	
T-47D	-5.36		-4.41		-4.00	
MDA-MB-468	-5.91		-4.98		-4.00	
Summary Statistics						
MG MID	-5.9		-4.77		-4.18	
Delta	1.45		1.79		1.47	
Range	2.61		2.56		1.65	

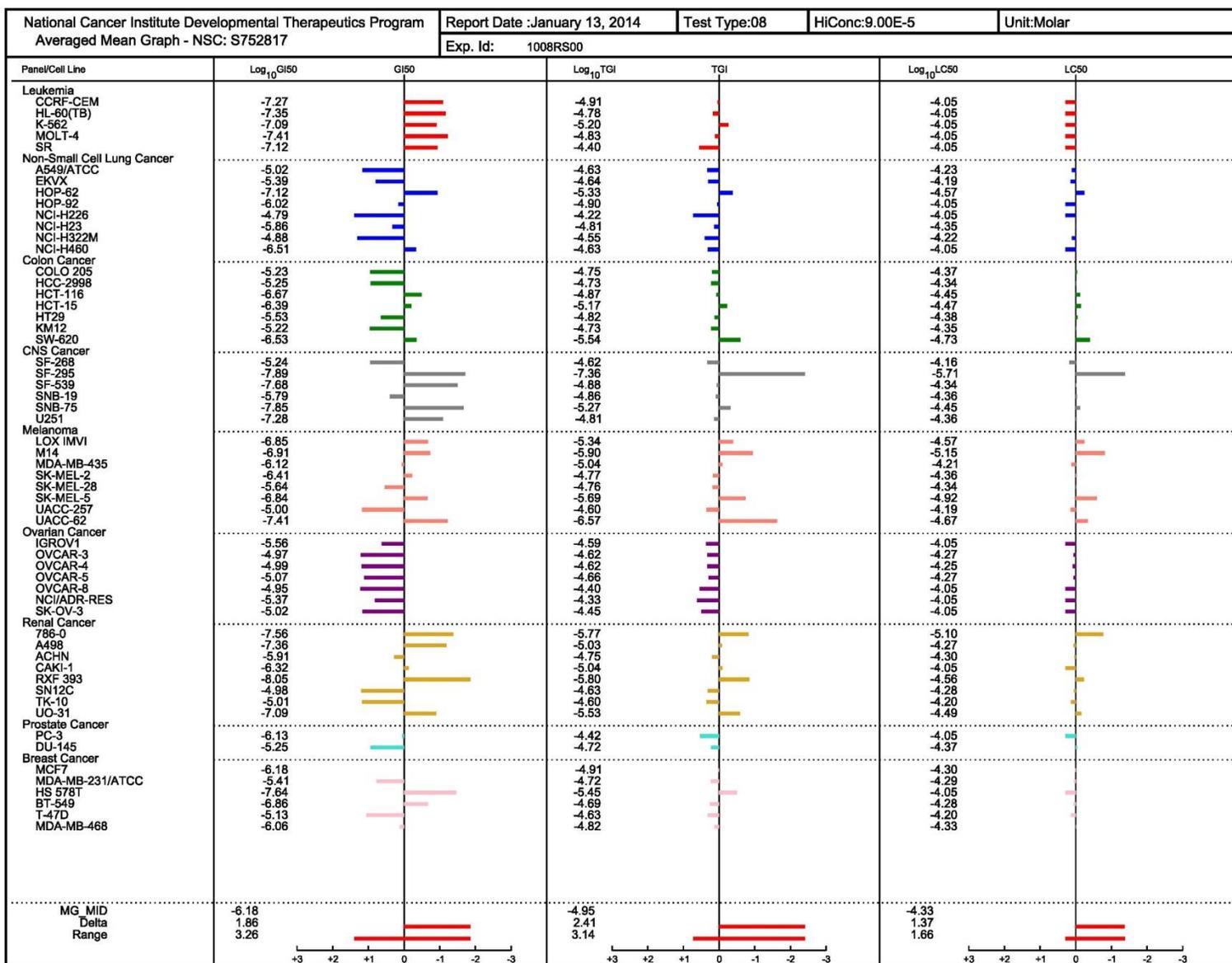
Average Mean Graph NCI 60 cell line data for compound 21



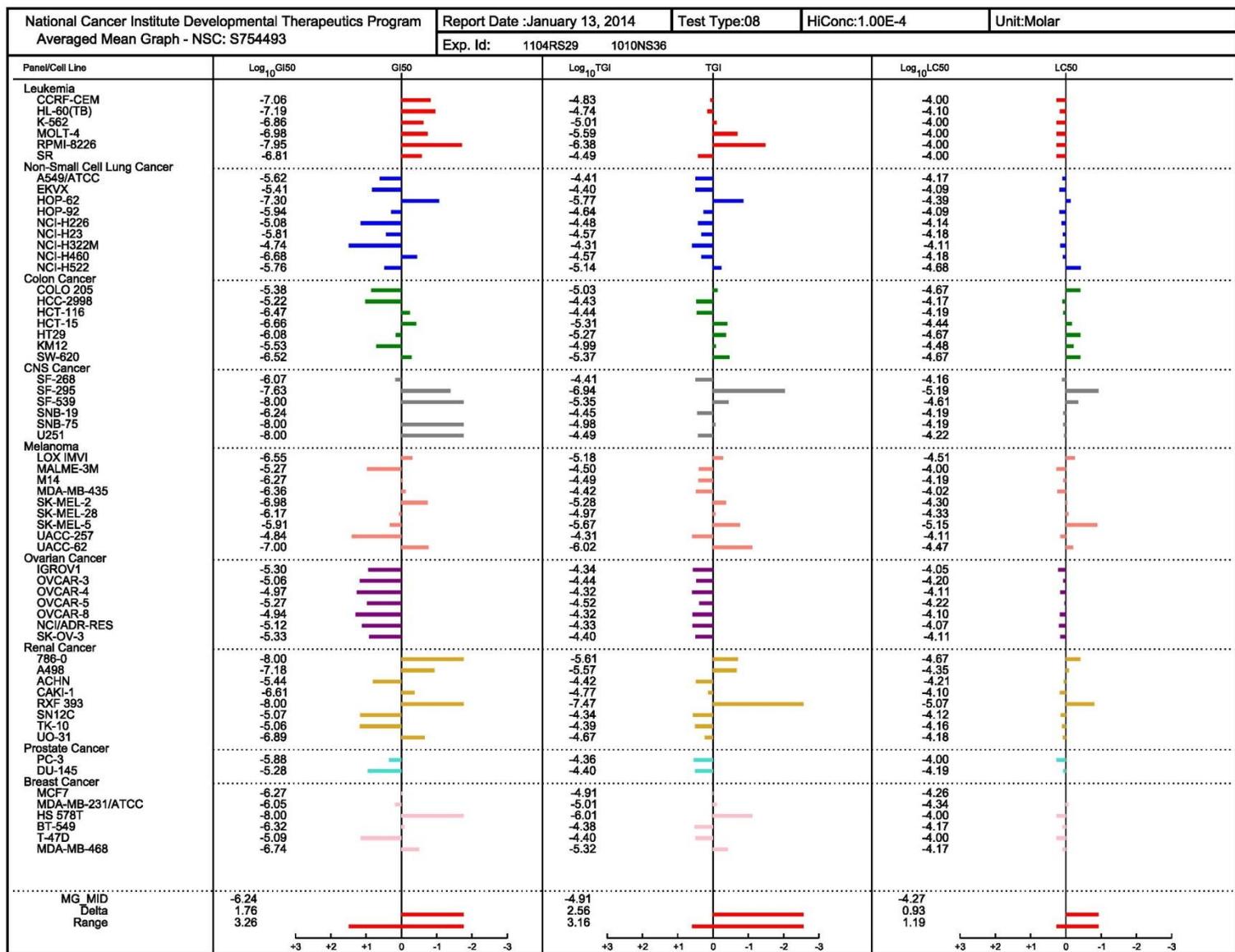
Average Mean Graph NCI 60 cell line data for compound 38

National Cancer Institute Developmental Therapeutics Program Averaged Mean Graph - NSC: S754492		Report Date :January 13, 2014	Test Type:08	HiConc:1.00E-4	Unit:Molar	
		Exp. Id: 1104RS29	1010NS36			
Panel/Cell Line	Log ₁₀ GI50	GI50	Log ₁₀ TGI	TGI	Log ₁₀ LC50	LC50
Leukemia						
CCRF-CEM	-6.68		-6.07		-4.00	
HL-60(TB)	-6.72		-5.61		-4.07	
K-562	-6.51		-5.86		-4.00	
MOLT-4	-6.81		-6.18		-4.00	
RPMI-8226	-7.11		-6.45		-4.00	
SR	-6.49		-5.26		-4.00	
Non-Small Cell Lung Cancer						
A549/ATCC	-6.28		-4.89		-4.30	
EKVX	-6.08		-5.18		-4.00	
HOP-62	-7.06		-6.32		-5.63	
HOP-92	-6.75		-5.25		-4.03	
NCI-H226	-5.57		-5.01		-4.49	
NCI-H23	-6.19		-5.45		-4.57	
NCI-H322M	-5.20		-4.40		-4.00	
NCI-H460	-6.43		-5.66		-4.77	
NCI-H522	-6.19		-5.70		-5.28	
Colon Cancer						
COLO 205	-6.66		-6.32		-5.81	
HCC-2998	-5.60		-4.80		-4.27	
HCT-116	-6.38		-4.90		-4.24	
HCT-15	-6.76		-5.87		-5.21	
HT29	-6.97		-6.15		-5.55	
KM12	-6.45		-5.77		-5.10	
SW-620	-6.54		-5.95		-5.39	
ONS Cancer						
SF-268	-5.95		-4.84		-4.04	
SF-295	-7.32		-6.66		-6.06	
SF-539	-7.30		-6.51		-5.60	
SNB-19	-6.40		-5.38		-4.55	
SNB-75	-7.05		-5.57		-4.12	
U251	-7.12		-5.64		-4.89	
Melanoma						
LOX IMVI	-6.53		-5.89		-5.35	
MALME-3M	-5.70		-5.06		-4.04	
M14	-6.28		-5.55		-4.33	
MDA-MB-435	-6.19		-5.04		-4.13	
SK-MEL-2	-6.48		-5.80		-4.96	
SK-MEL-28	-6.46		-5.65		-4.80	
SK-MEL-5	-6.58		-6.17		-5.83	
UACC-257	-5.68		-4.89		-4.31	
UACC-62	-6.64		-6.18		-5.04	
Ovarian Cancer						
IGROV1	-5.78		-4.38		-4.00	
OVCAR-3	-5.55		-4.92		-4.42	
OVCAR-4	-5.61		-4.48		-4.00	
OVCAR-5	-5.81		-5.14		-4.29	
OVCAR-8	-5.42		-4.63		-4.13	
NCI/ADR-RES	-5.54		-4.54		-4.00	
SK-OV-3	-6.11		-5.14		-4.17	
Renal Cancer						
786-0	-7.30		-6.52		-6.05	
A498	-6.66		-6.22		-5.28	
ACHN	-5.90		-4.82		-4.31	
CAKI-1	-6.46		-5.66		-4.27	
RXF 393	-7.58		-6.98		-6.14	
SN12C	-5.60		-4.72		-4.28	
TK-10	-5.56		-4.76		-4.18	
UO-31	-6.36		-5.16		-4.25	
Prostate Cancer						
PC-3	-6.62		-4.76		-4.00	
DU-145	-5.69		-4.82		-4.33	
Breast Cancer						
MCF7	-6.40		-5.43		-4.72	
MDA-MB-231/ATCC	-6.57		-5.62		-4.51	
HS 578T	-7.27		-6.16		-4.00	
BT-549	-6.45		-4.81		-4.17	
T-47D	-6.76		-4.77		-4.00	
MDA-MB-468	-6.71		-5.96		-4.98	
MG_MID						
Delta	-6.37		-5.47		-4.59	
Range	1.22		1.51		1.55	
	2.38		2.6		2.14	

Average Mean Graph NCI 60 cell line data for compound 43



Average Mean Graph NCI 60 cell line data for compound 47



Average Mean Graph NCI 60 cell line data for compound 50