Supporting Information for

Nitropyrrolins A-E, Farnesyl-α-Nitropyrroles from a Marine-Derived Bacterium Related to the Genus *Streptomyces*

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[†]Korea Institute of Science and Technology, Gangneung.

[‡]Scripps Institution of Oceanography.

[§]Contributed equally to this work.

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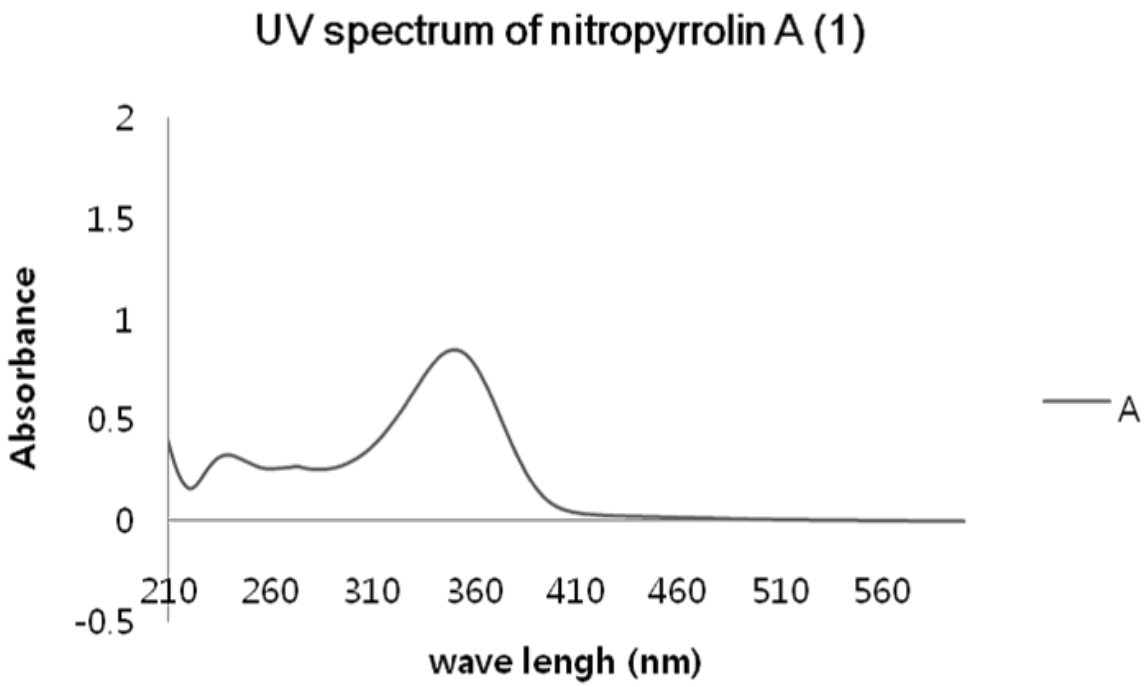
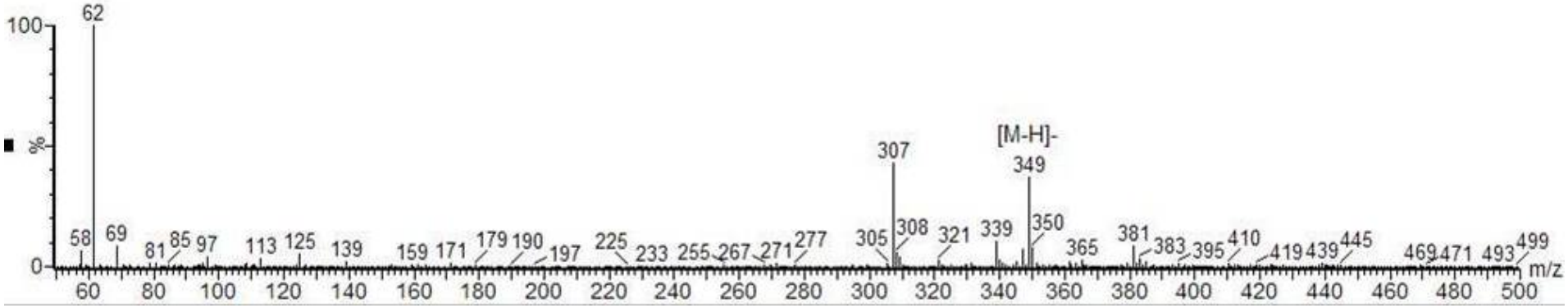


Figure S1 UV spectrum of nitropyrrolin A (**1**) in CH_3OH (10^{-4} M).



Selected Isotopes : $C_{0-50}H_{0-100}O_{0-10}N_{0-5}$ **Error Limit : 20 ppm**

Measured Mass	*% Base*	*Formula*	*Calculated Mass*	*Error*
349.2124	94.7%	$C_{24}H_{29}O_2$	349.2167	12.0
		$C_{16}H_{31}O_7N$	349.2100	-6.7
		$C_{19}H_{29}O_4N_2$	349.2127	0.9
		$C_{22}H_{27}ON_3$	349.2154	8.6
		$C_{14}H_{29}O_6N_4$	349.2087	-11.0
		$C_{17}H_{27}O_3N_5$	349.2114	-3.0

Figure S2 MS data of nitropyrrolin A (**1**) (Upper, positive ESI MS; Middle, negative ESI MS; Bottom, negative HR-FAB MS).

Table S1. NMR data for nitropyrrolin A (**1**) in $CDCl_3$

Position	δ_H mult (*J* in Hz)	δ_C	COSY	HMBC	Key NOE
1	9.49, br s		5		
2		137.5			
3	7.06, br s	111.2	5, 1'	2, 4, 5, 1'	
4		124.3			
5	6.90, br s	122.2	3, 1'	2, 3, 4	
1'	2.73, br dd (15.0, 2.0) 2.53, dd (15.0, 10.5)	28.8	2'	3, 4, 5, 2', 3'	4', 15'
2'	3.58, br dd (10.5, 2.0)	78.3	1'	4, 1', 3' , 4', 15'	15'
3'		74.6			
4'	1.73, br ddd (14.0, 10.5, 6.0) 1.49, br ddd (14.0, 10.5, 6.0)	36.2	5'	2', 3', 5'	1'
5'	2.20, m 2.14, m	22.0	4', 6'	3', 4', 6', 7'	
6'	5.18, br t (7.0)	124.1	5', 14'	4', 5', 8', 14'	8'
7'		136.0			
8'	2.01, m	39.7	9'	6', 7', 9', 10', 14'	6'
9'	2.09, m	26.6	8' , 10'	8', 10', 11'	
10'	5.10, tq (7.0, 1.0)	124.1	9', 12' , 13'	8', 9', 12', 13'	12'
11'		131.6			
12'	1.69, br d (1.0)	25.7	10'	10', 11', 13'	10'
13'	1.61, s	17.7	10'	10', 11', 12'	
14'	1.65, s	16.1	6'	6', 7', 8'	
15'	1.27, s	23.4		2', 3', 4'	1', 2'

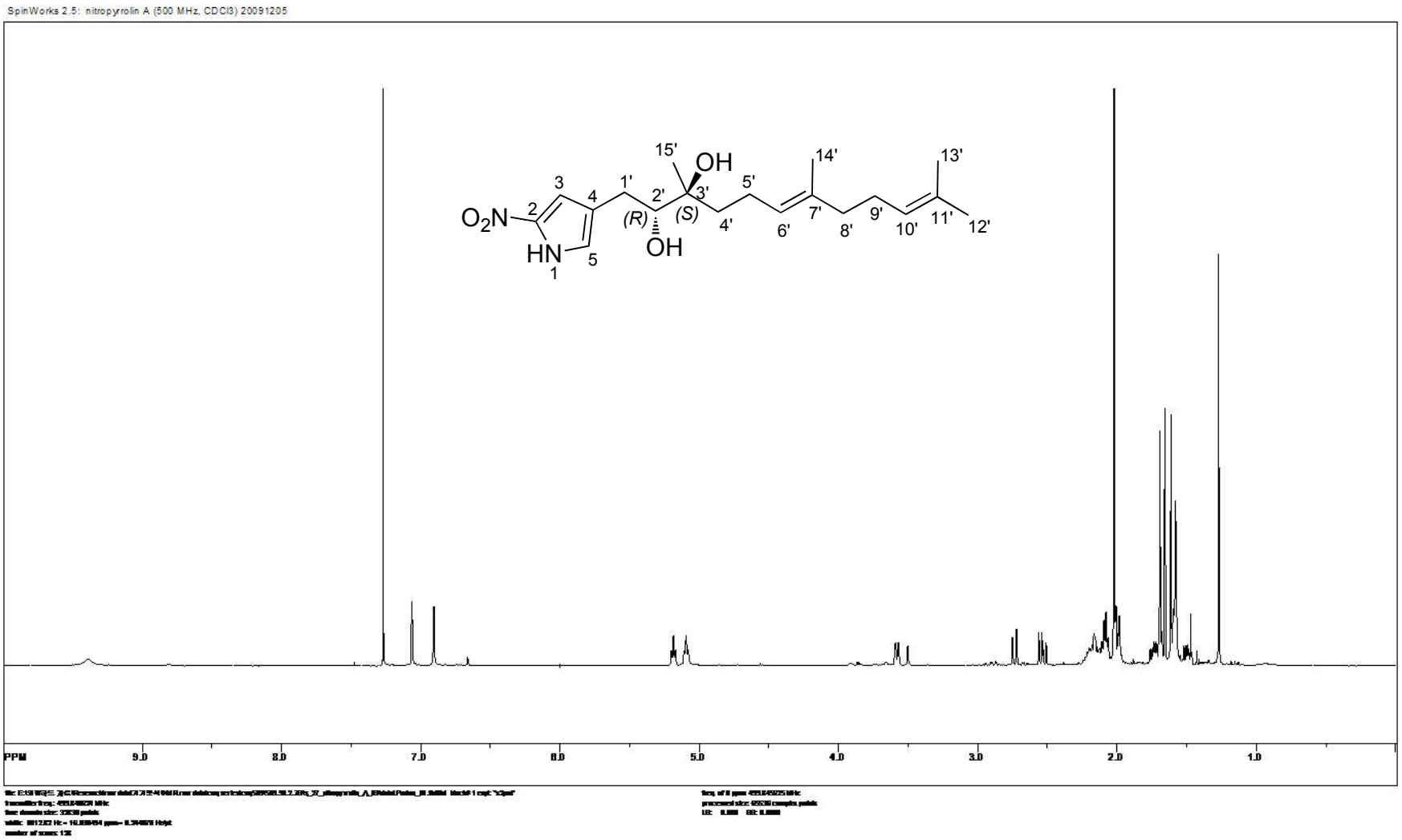


Figure S3 ^{1}H NMR spectrum of nitropyrrolin A (**1**) in $CDCl_3$ (500 MHz), a reference signal: $CDCl_3$ at δ_H 7.27.

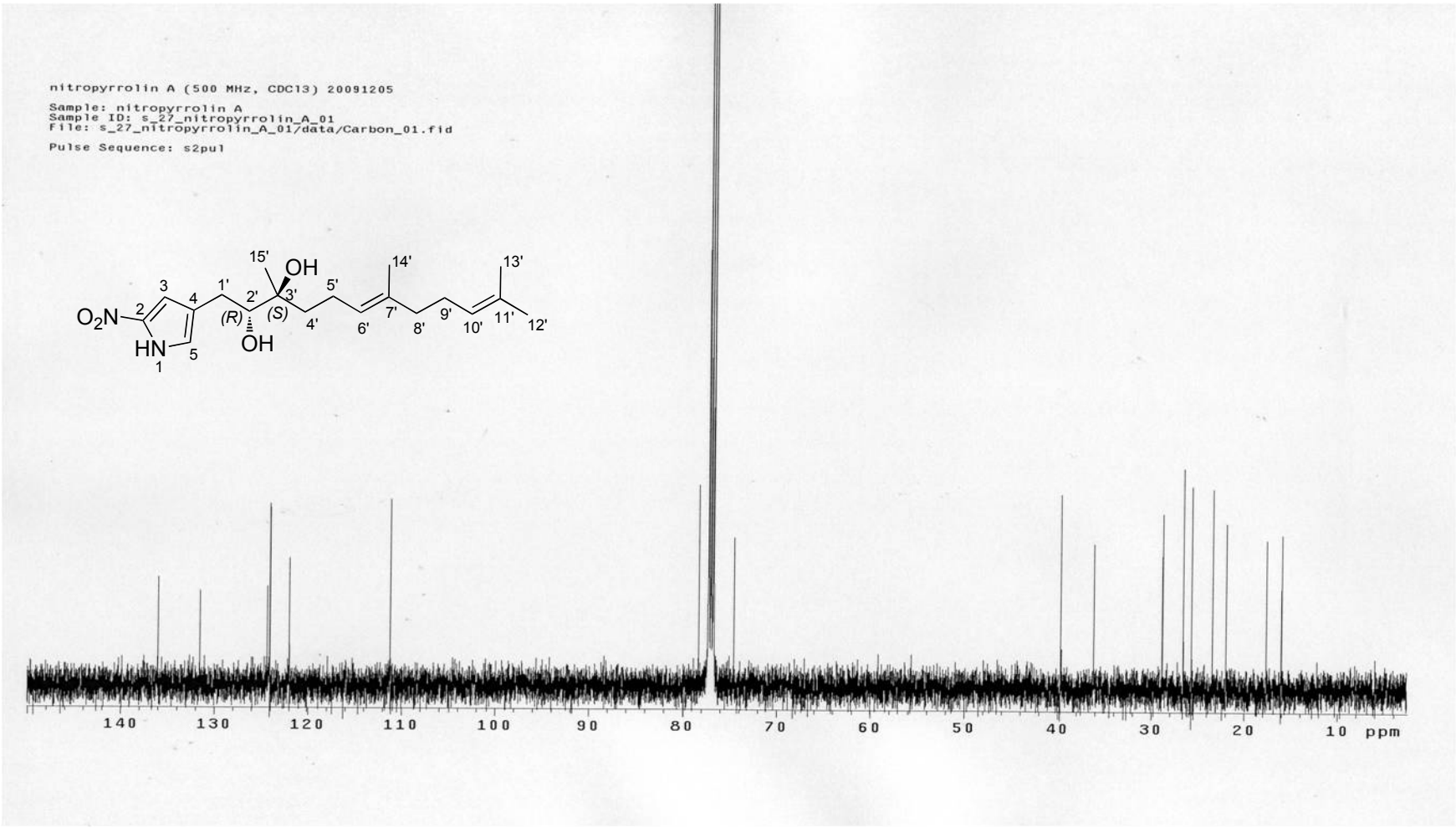


Figure S4 ^{13}C NMR spectrum of nitropyrrolin A (**1**) in $CDCl_3$ (125 MHz), a reference signal: $CDCl_3$ at δ_C 77.0.

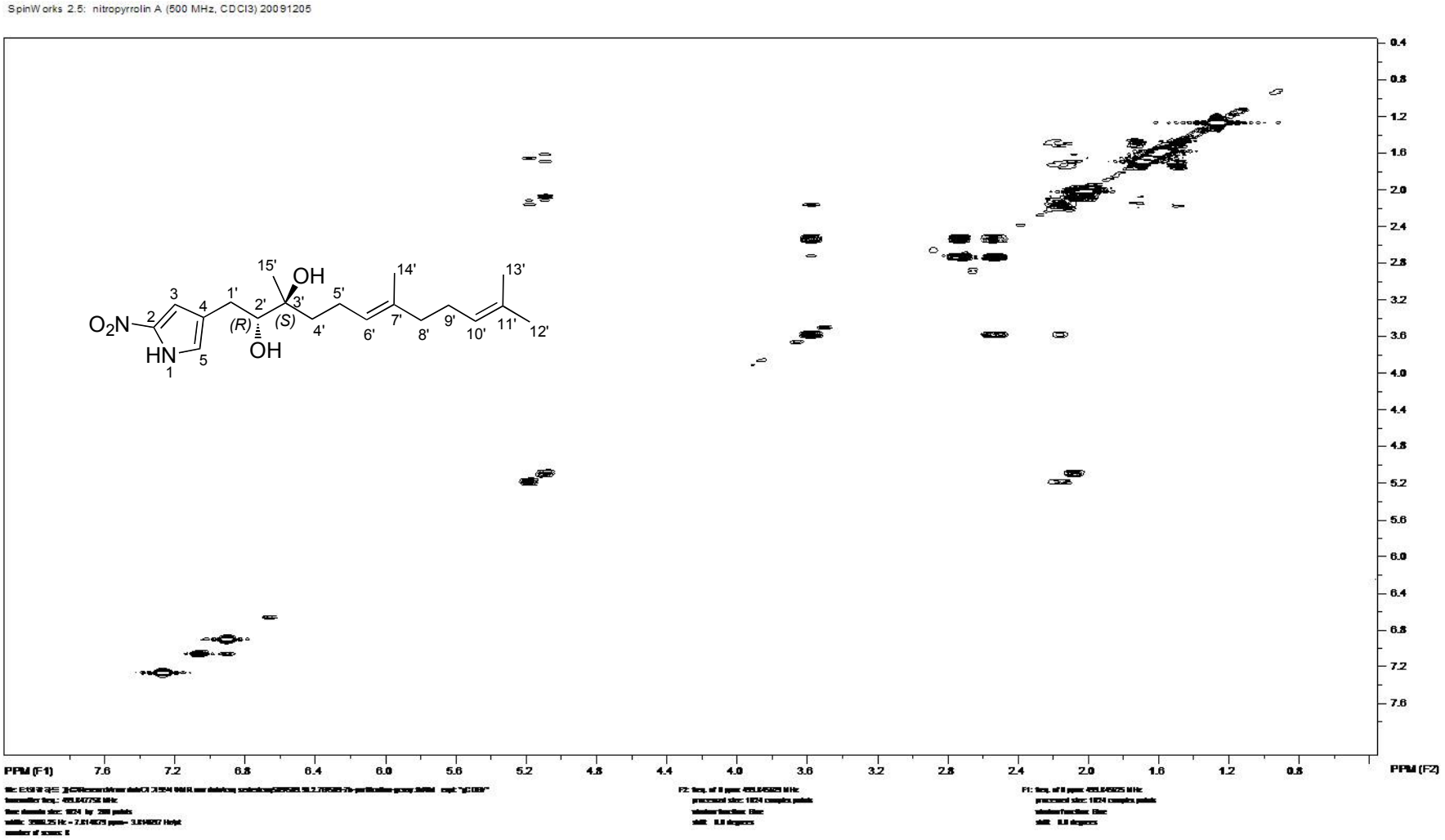


Figure S5 ^{1}H-^{1}H gCOSY spectrum of nitropyrrolin A (**1**) in $CDCl_3$ (500 MHz).

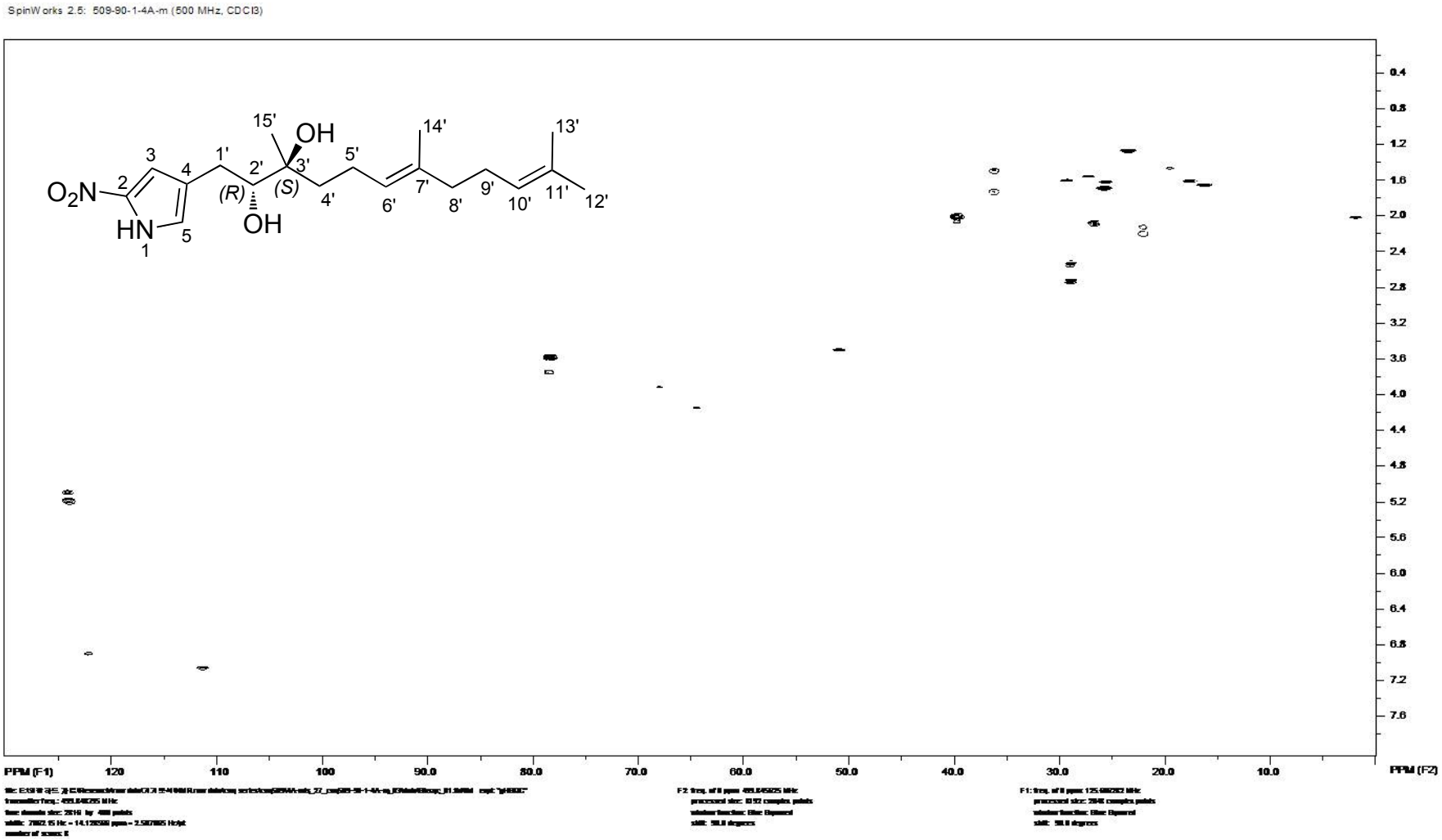


Figure S6 gHSQC spectrum of nitropyrrolin A (**1**) in $CDCl_3$ (500 MHz).

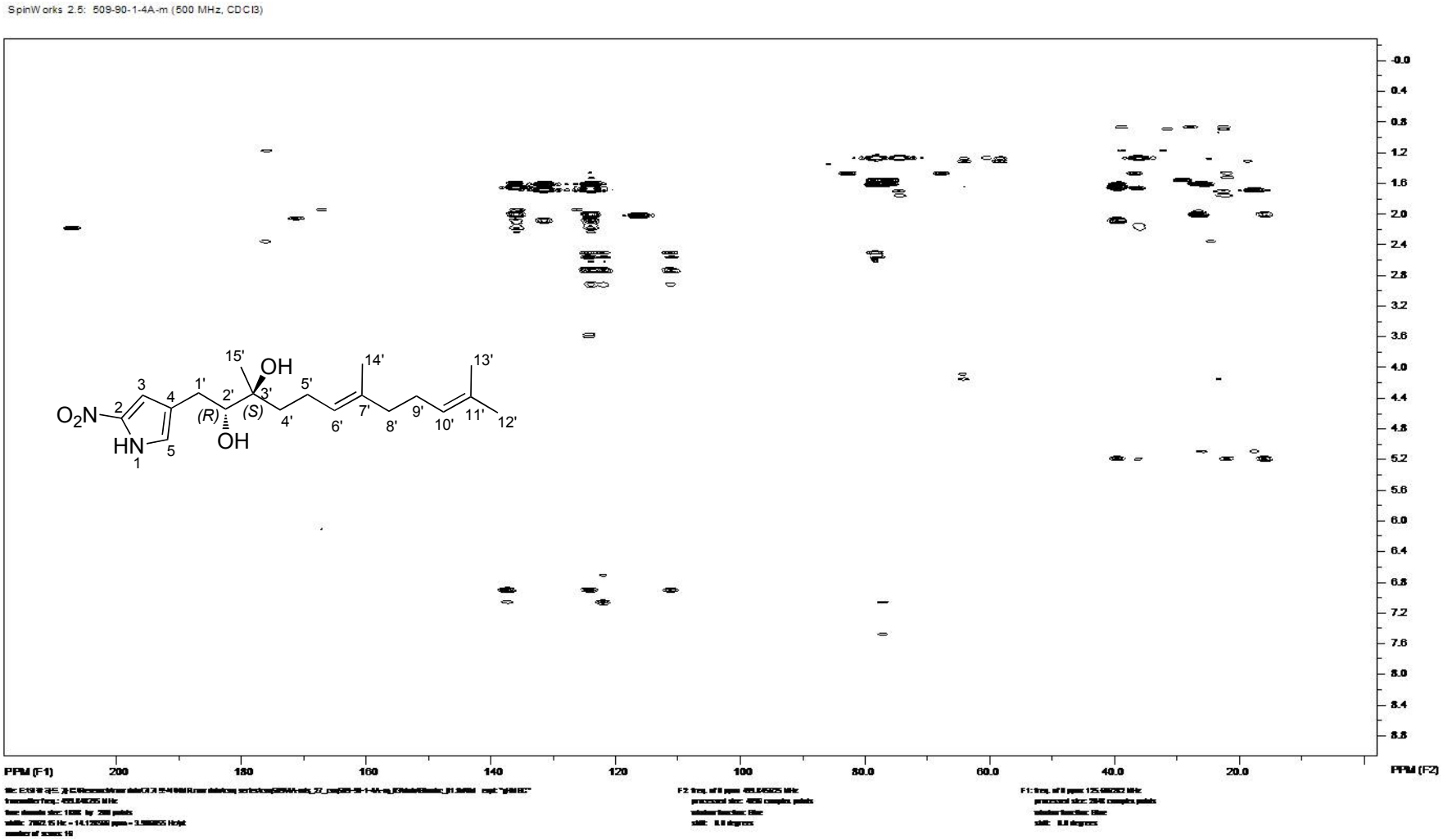


Figure S7 gHMBC spectrum of nitropyrrolin A (**1**) in $CDCl_3$ (500 MHz).

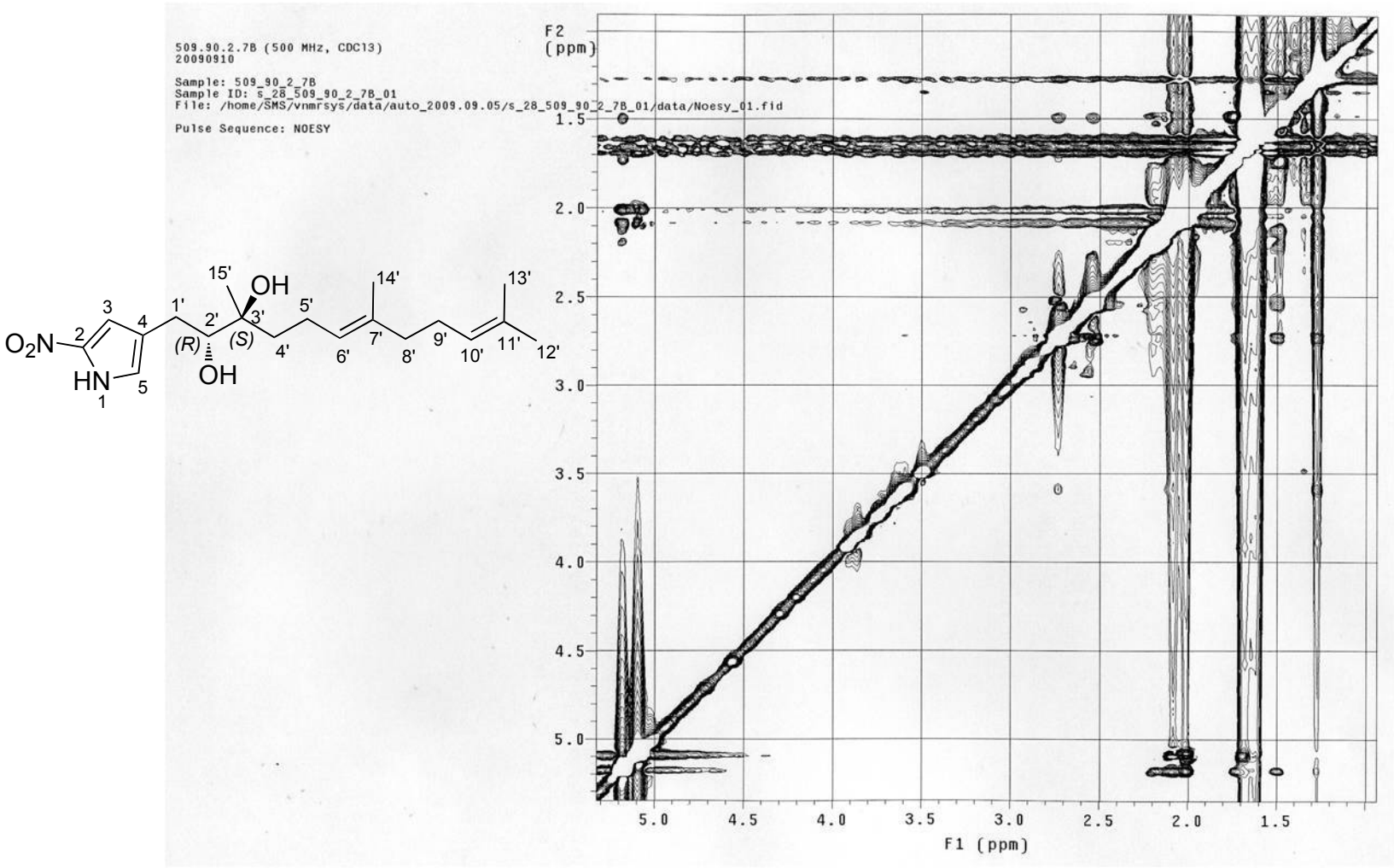


Figure S8 2D NOESY spectrum of nitropyrrolin A (**1**) in $CDCl_3$ (500 MHz).

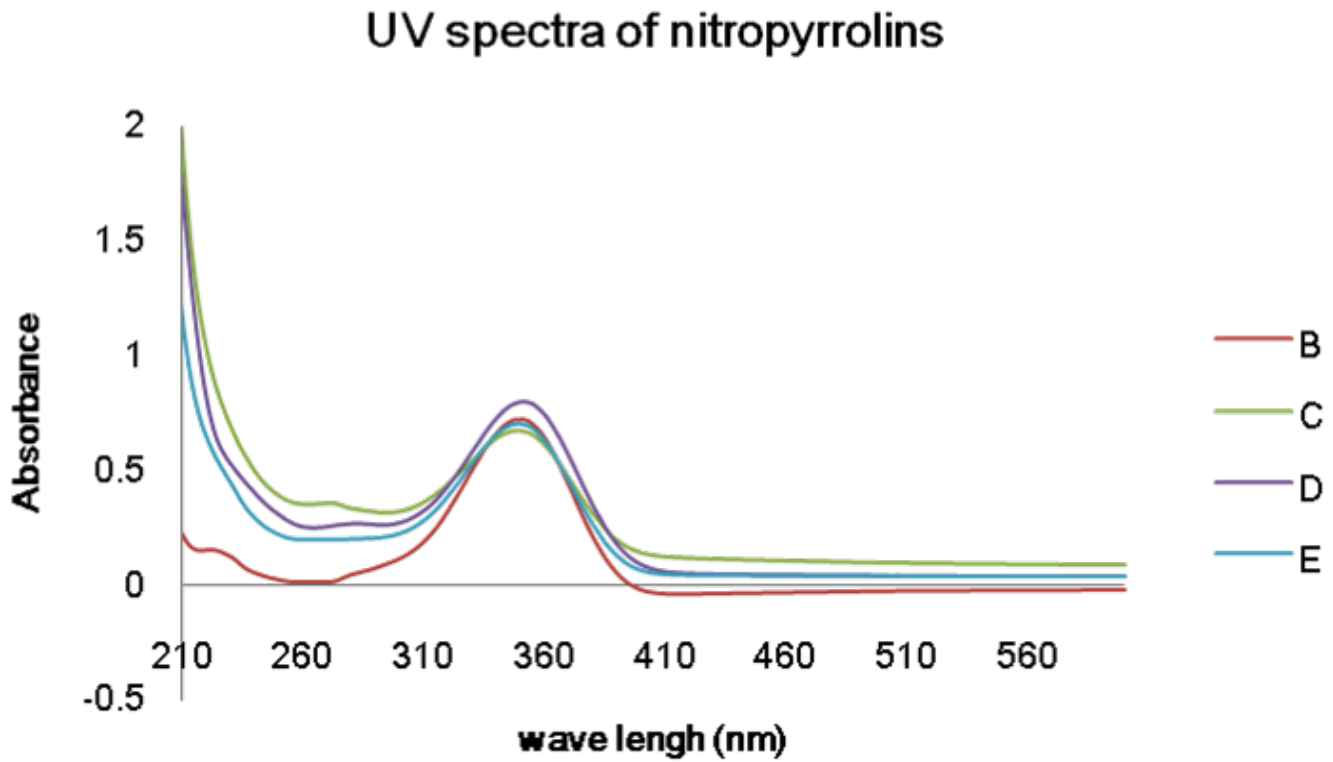
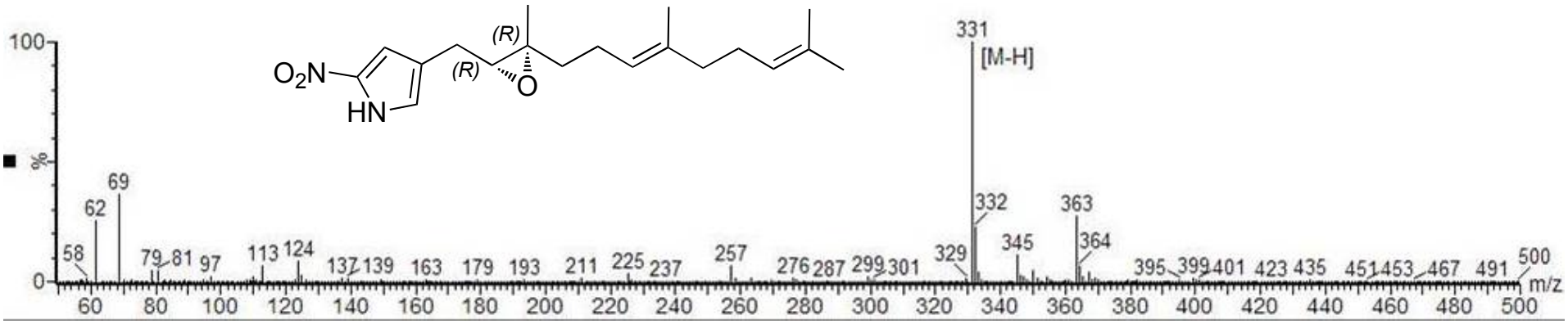


Figure S9 UV spectra of nitropyrrolins B (**2**), C (**3**), D (**4**) and E (**5**) in CH_3OH (10^{-4} M).



Selected Isotopes : $C_{0\text{-}50}H_{0\text{-}100}O_{0\text{-}10}N_{0\text{-}5}$ **Error Limit : 20 ppm**

Measured Mass	*% Base*	*Formula*	*Calculated Mass*	*Error*
331.2029	38.2%	$C_{24}H_{27}O$	331.2062	9.9
		$C_{16}H_{29}O_6N$	331.1995	-10.0
		$C_{19}H_{27}O_3N_2$	331.2021	-2.3
		$C_{22}H_{25}N_3$	331.2048	5.8
		$C_{14}H_{27}O_5N_4$	331.1981	-14.0
		$C_{17}H_{25}O_2N_5$	331.2008	-6.4

Figure S10 MS data of nitropyrrolin B (**2**) (Upper, positive ESI MS; Middle, negative ESI MS; Bottom, negative HR-FAB MS).

Table S2. NMR data for nitropyrrolin B (**2**) in $CDCl_3$

Position	δ_H mult (*J* in Hz)	δ_C	COSY	HMBC	Key NOE
1	9.51, br s	137.4			
2					
3	7.03, br s	110.9	5	2, 4, 5	
4		123.0			
5	6.87, br s	121.6	3, 1'	2, 3, 4	
1'	2.71, dd (15.0, 6.0) 2.68, dd (15.0, 6.0)	26.7	5, 2'	2, 3, 5, 2', 3'	
2'	2.94, dd (6.0, 6.0)	63.1	1'	2, 1', 4'	4', 15'
3'		61.5			
4'	1.70, ddd (13.5, 8.0, 6.0) 1.49, ddd (13.5, 9.5, 6.5)	38.6	5'		2'
5'	2.11, m	23.7	4', 6'	4', 6'	
6'	5.08, m[a]	123.3	5', 14'	5', 14'	
7'		135.8			
8'	2.05, m	26.7	9', 10'	7', 9', 10'	
9'	1.96, br dd (8.0, 7.0)	39.7	8', 10'	7', 8', 10', 11', 13'	
10'	5.08, m[a]	124.2	9', 12', 13'	9', 12'	
11'		131.6			
12'	1.68, br d (1.0)	25.8	10'	10', 11', 13'	
13'	1.60, s	17.8	10'	9', 10', 11', 12'	
14'	1.60, s	16.1	6'	6', 7'	
15'	1.38, s	16.8		2', 3', 4'	2'

[a] The multiplicity of this signal was unresolved due to peak overlapping and the chemical shift was assigned by interpretation of HSQC and HMBC spectroscopic data.

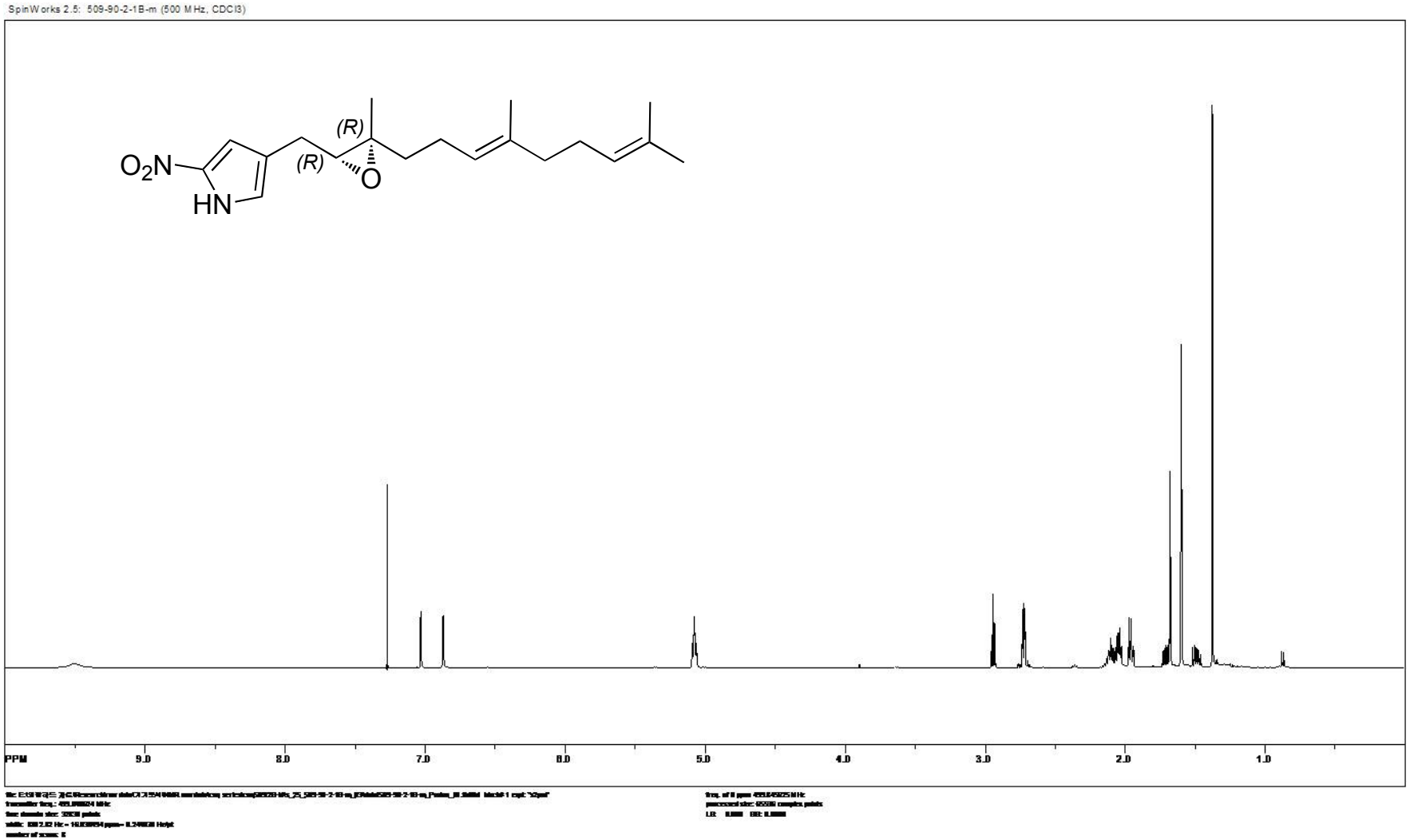


Figure S11 ^{1}H NMR spectrum of nitropyrrolin B (**2**) in $CDCl_3$ (500 MHz).

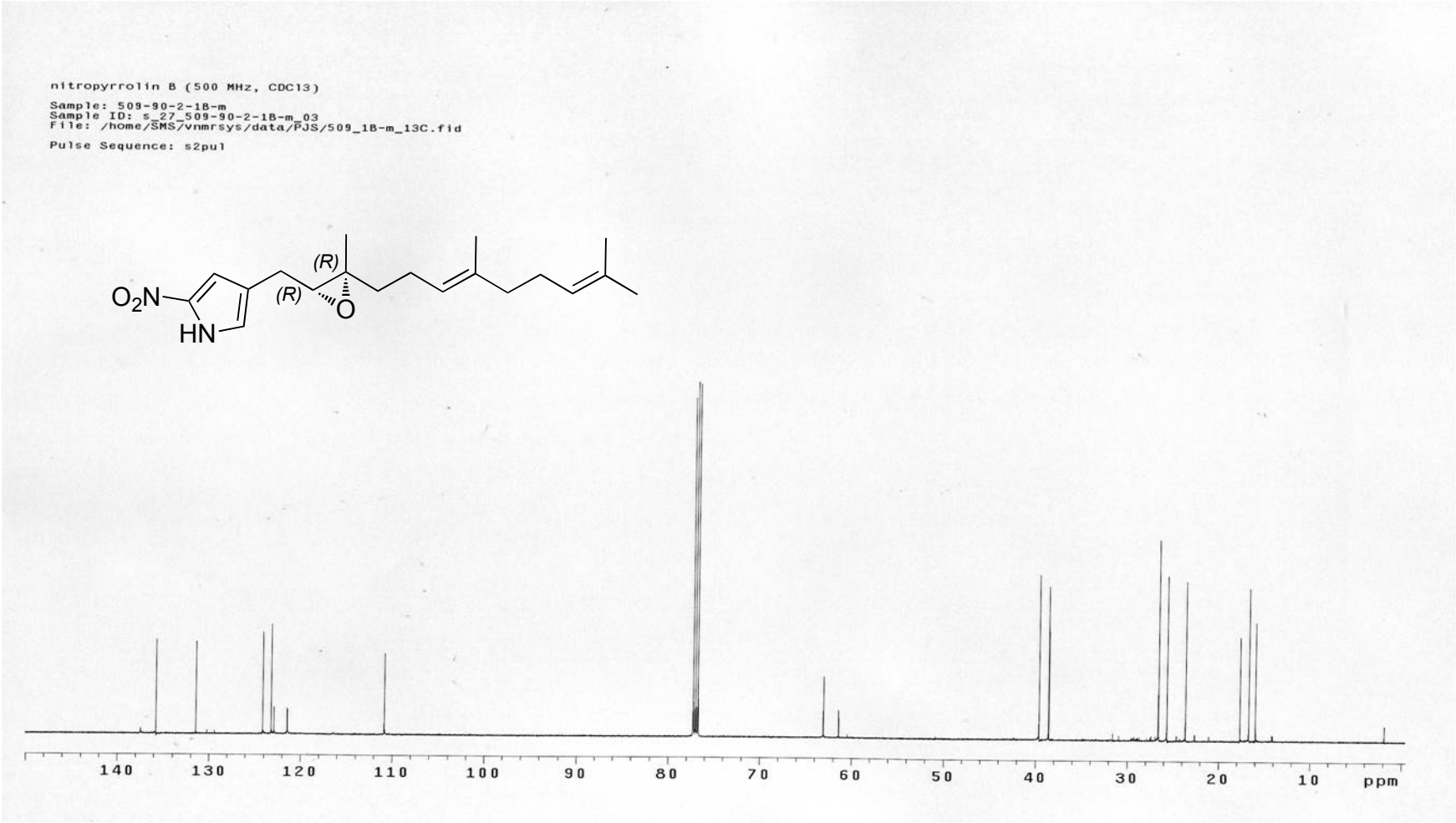


Figure S12 ^{13}C NMR spectrum of nitropyrrolin B (**2**) in $CDCl_3$ (125 MHz).

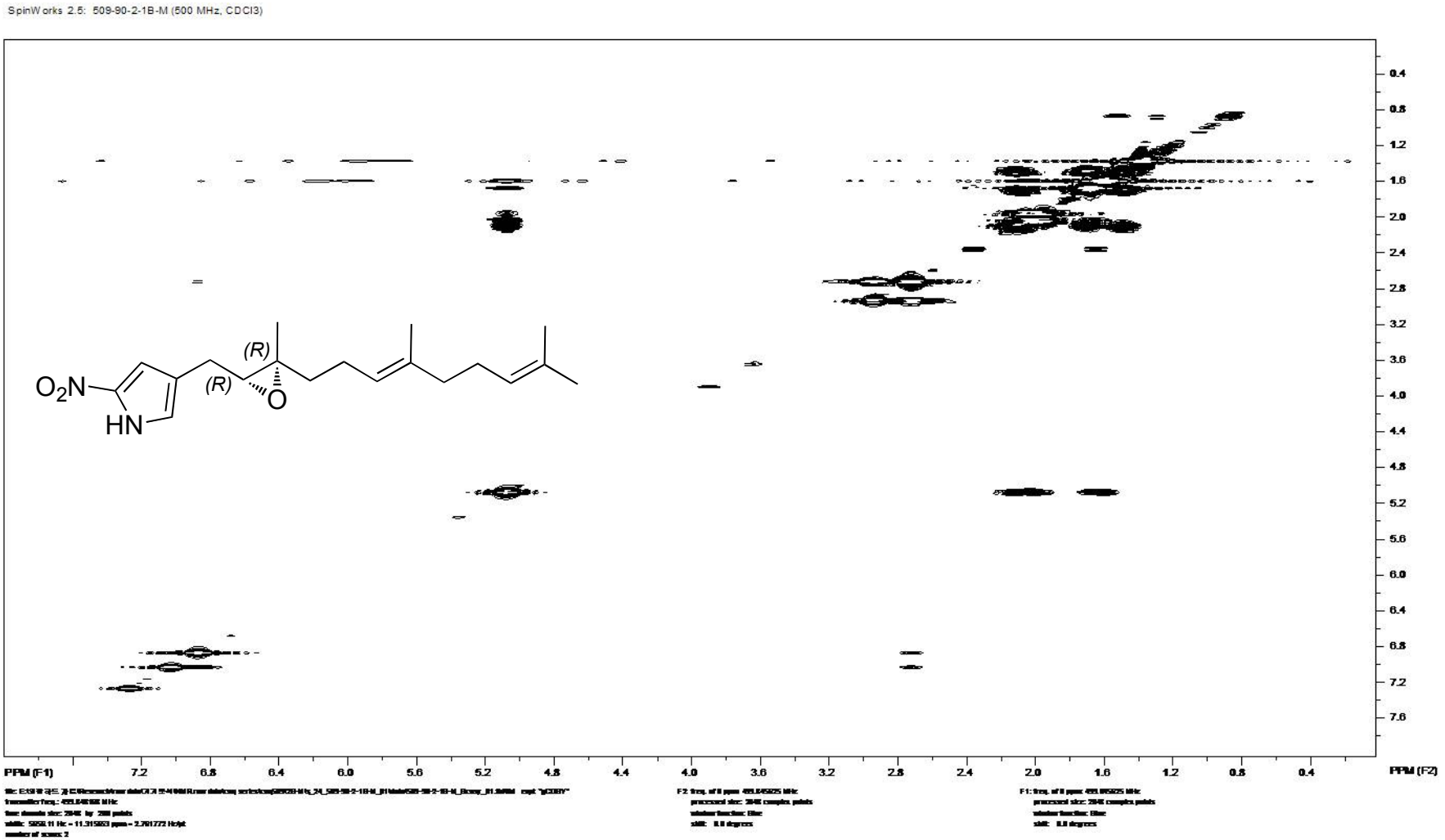


Figure S13 ^{1}H-^{1}H gCOSY spectrum of nitropyrrolin B (**2**) in $CDCl_3$ (500 MHz).

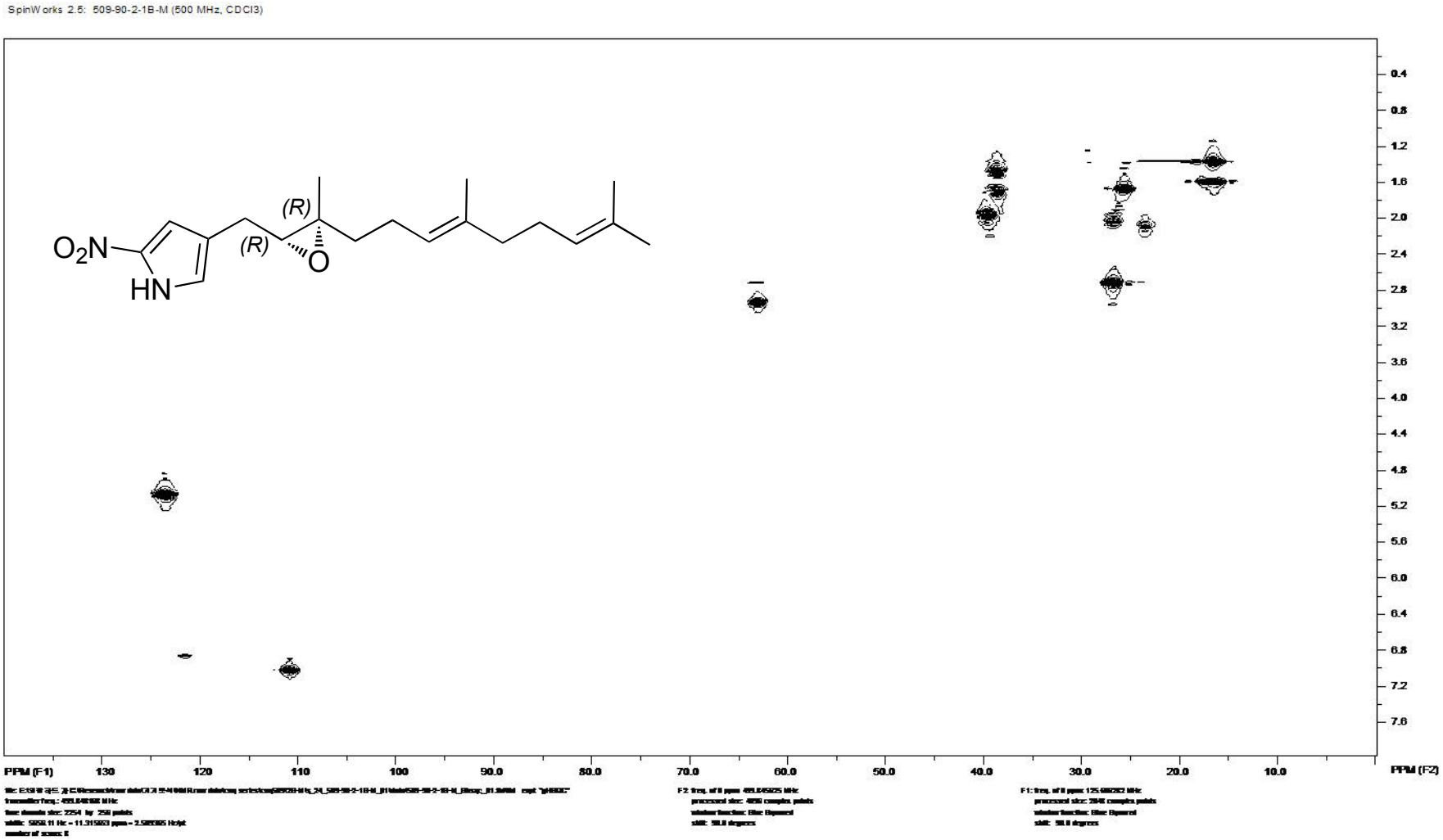


Figure S14 gHSQC spectrum of nitropyrrolin B (**2**) in $CDCl_3$ (500 MHz).

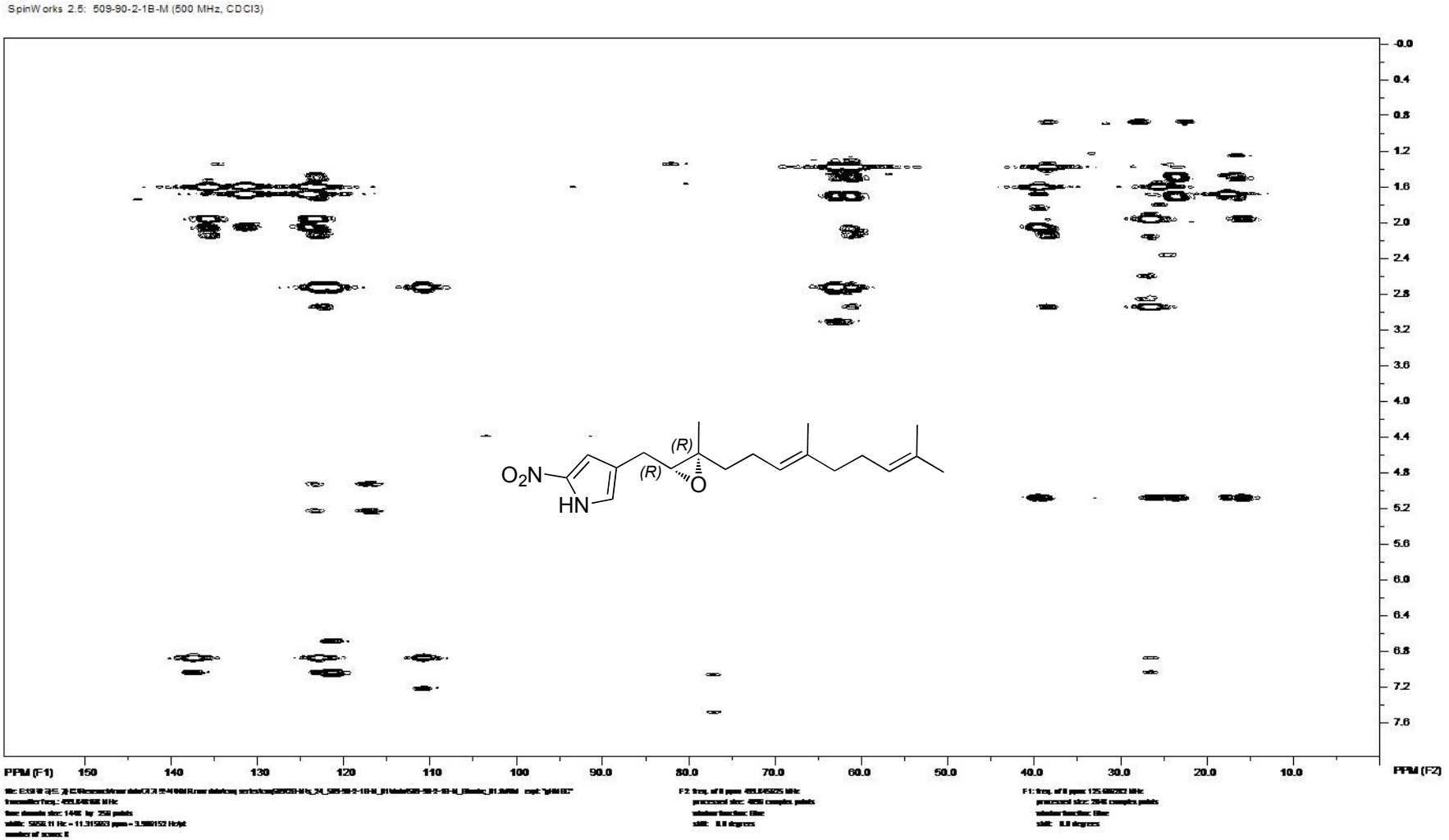


Figure S15 gHMBC spectrum of nitropyrrolin B (**2**) in $CDCl_3$ (500 MHz).

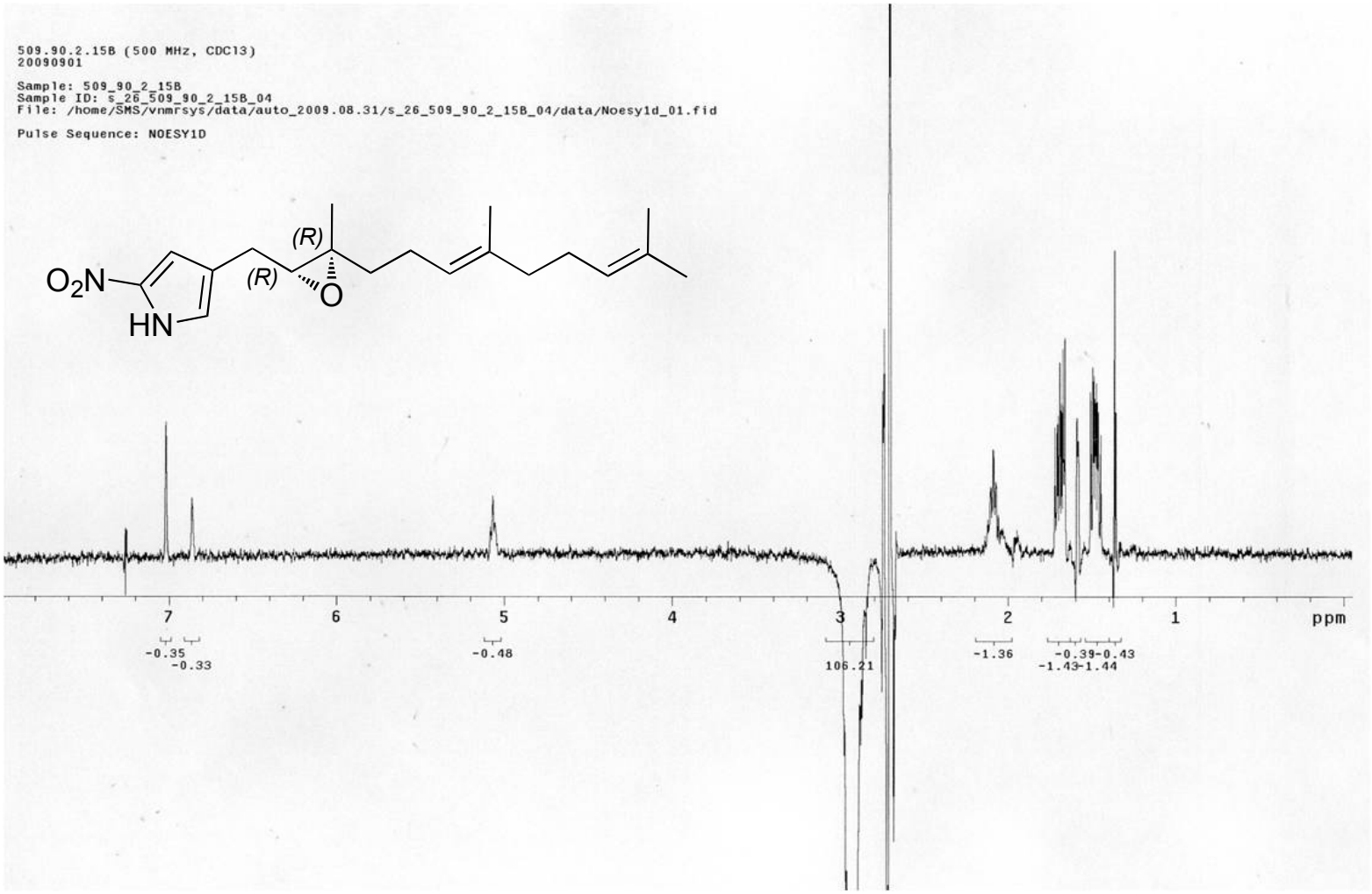
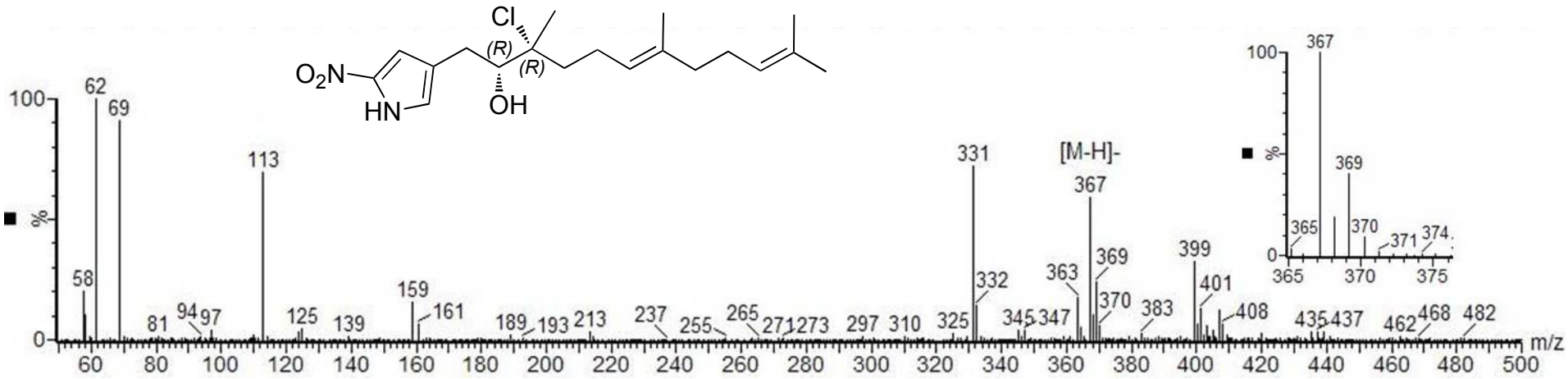


Figure S16 Selective 1D NOESY spectrum of nitropyrrolin B (**2**) in $CDCl_3$ (500 MHz), irradiation of H-2' signal at d_H 2.94



Selected Isotopes : $H_{0\text{-}50}C_{0\text{-}50}N_{0\text{-}5}O_{0\text{-}5}Cl_{0\text{-}2}{}^{37}Cl_{0\text{-}2}$ **Error Limit : 20 ppm**

Measured Mass	*% Base*	*Formula*	*Calculated Mass*	*Error*
367.1791	43.5%	$C_{23}H_{21}N_5$	367.1797	1.6
		$C_{25}H_{23}N_2O$	367.1810	5.2
		$C_{20}H_{23}N_4O_3$	367.1770	-5.8
		$C_{22}H_{25}NO_4$	367.1783	-2.1
		$C_{16}H_{25}N_5O_5$	367.1855	17.0
		$C_{22}H_{26}N_3Cl$	367.1815	6.6
		$C_{24}H_{28}OCl$	367.1829	10.0
		$C_{17}H_{26}N_5O_2Cl$	367.1775	-4.4
		$C_{19}H_{28}N_2O_3Cl$	367.1788	-0.8
		$C_{14}H_{28}N_4O_5Cl$	367.1748	-12.0
		$C_{21}H_{31}NCl_2$	367.1833	12.0

Figure S17 MS data of nitropyrrolin C (**3**). (Upper, negative ESI MS; Bottom, negative HR-FAB MS)

Table S3. NMR data for nitropyrrolin C (**3**) in $CDCl_3$

Position	δ_H mult (*J* in Hz)	δ_C	COSY	HMBC	Key NOE[a]
1	9.48, br s		5		
2		137.5			
3	7.07, br s	111.3	5	2, 4, 5	
4		124.0			
5	6.92, br s	122.2	1, 3	2, 3, 4	
1'	2.93, dd (15.0, 1.5) 2.60, dd (15.0, 10.5)	29.2	2'	3, 4, 5, 2'	15'
2'	3.75, dd (10.5, 1.5)	78.4	1'	4, 5, 1', 4', 15'	4', 15'
3'		78.0			
4'	2.00, m 1.75, ddd (14.0, 11.0, 5.0)	39.6	5', 6'	3'	2'
5'	2.28, m 2.19, m	23.0	4', 6'	4', 6', 7'	
6'	5.15, td (7.0, 1.0)	123.0	5', 8', 14'	4', 5', 14'	
7'		136.3			
8'	1.99, m	39.7	9', 10'		
9'	2.08, dd (7.5, 7.5)	26.6	8', 10'		
10'	5.09, tq (7.0, 1.5)	124.1	9', 12', 13'	9', 13'	
11'		131.5			
12'	1.69, s	25.7	10'	10', 11', 13'	
13'	1.61, s	17.7	10'	10', 11', 12'	
14'	1.63, s	16.1	6'	6', 7', 8'	
15'	1.64, s	25.6			1' , 2'

[a] NOE data was recorded in DMSO-d_6

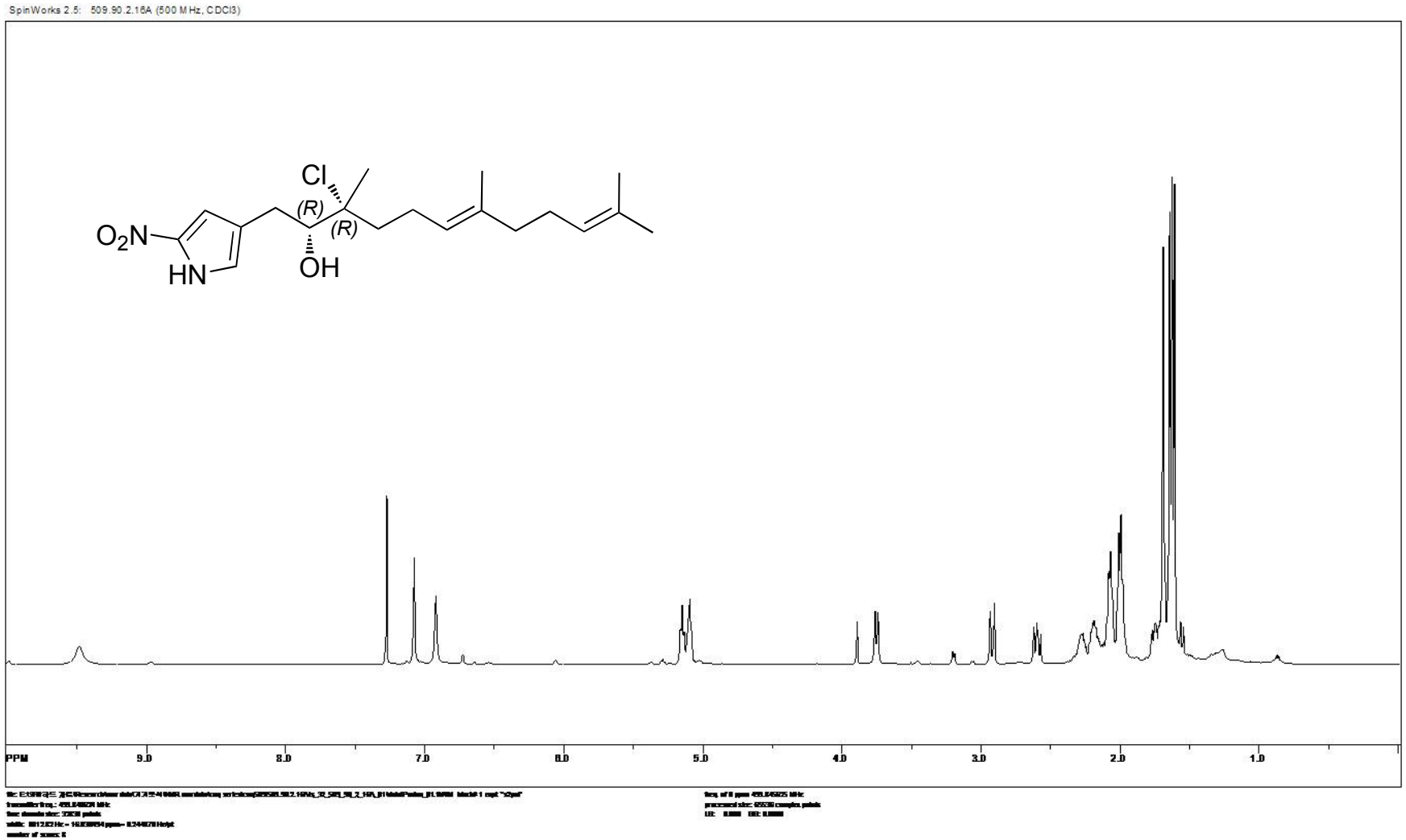


Figure S18 ^{1}H NMR spectrum of nitropyrrolin C (**3**) in $CDCl_3$ (500 MHz).

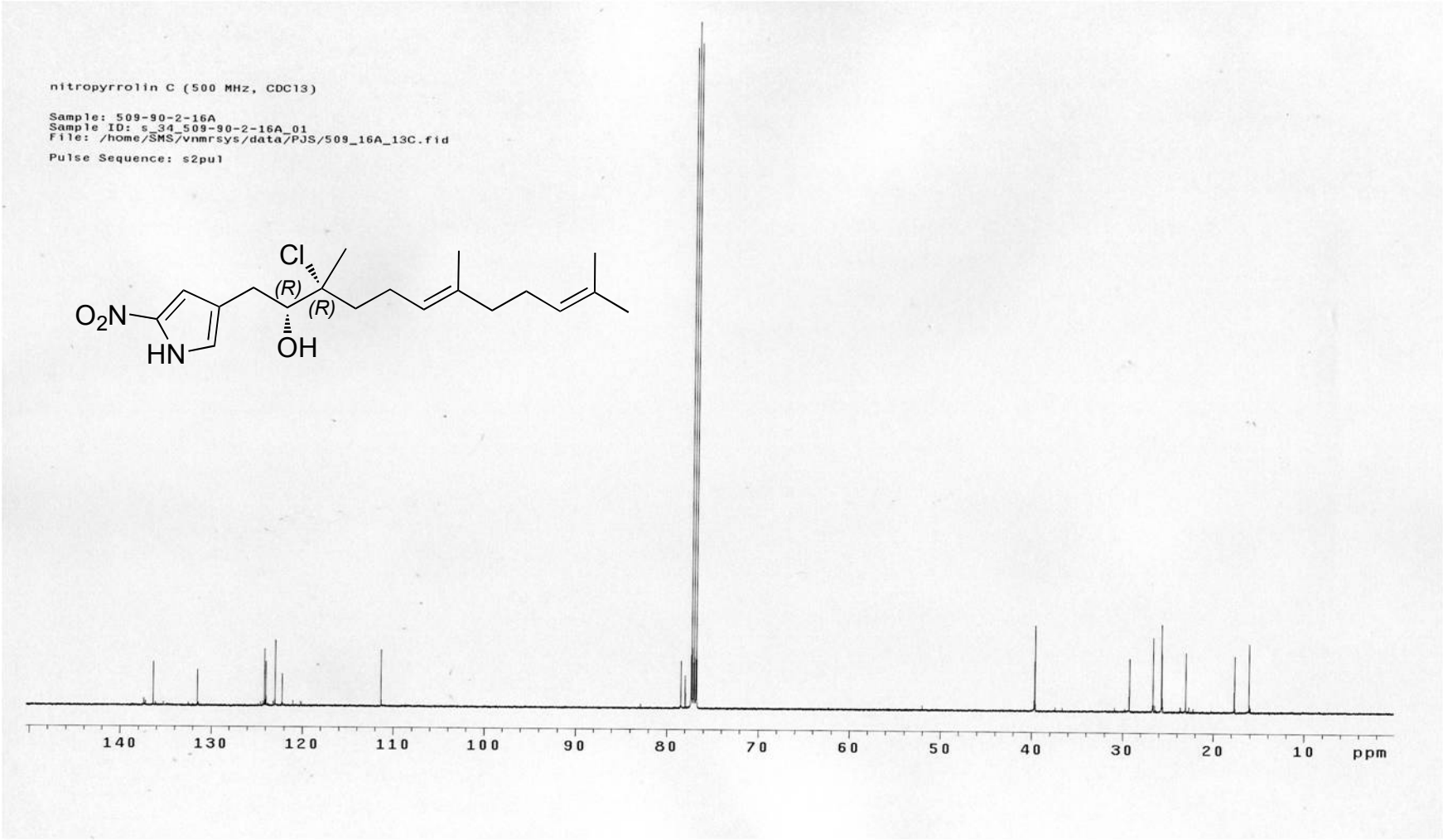


Figure S19 ^{13}C NMR spectrum of nitropyrrolin C (**3**) in $CDCl_3$ (125 MHz).

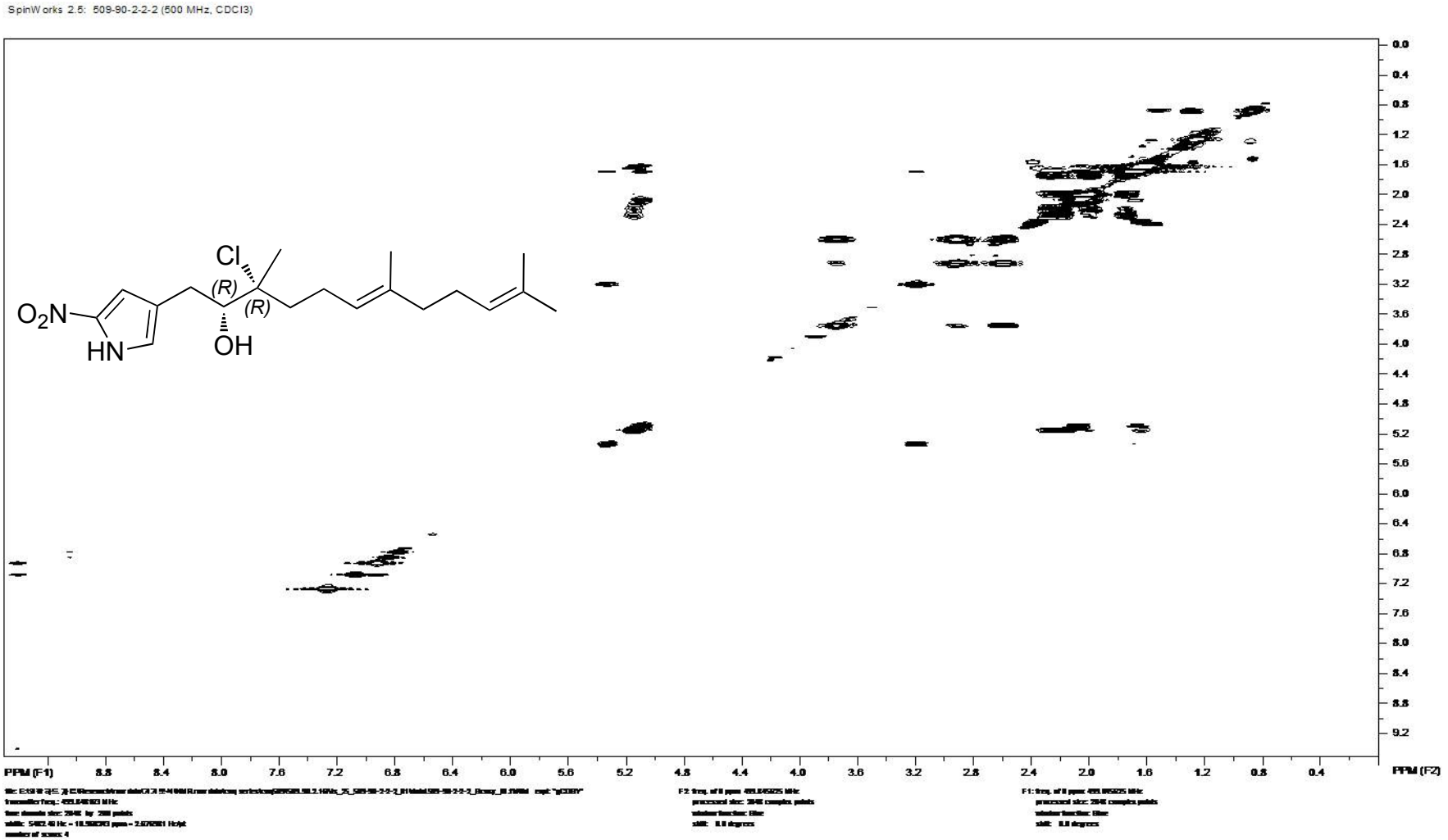


Figure S20 ^{1}H-^{1}H gCOSY spectrum of nitropyrrolin C (**3**) in $CDCl_3$ (500 MHz).

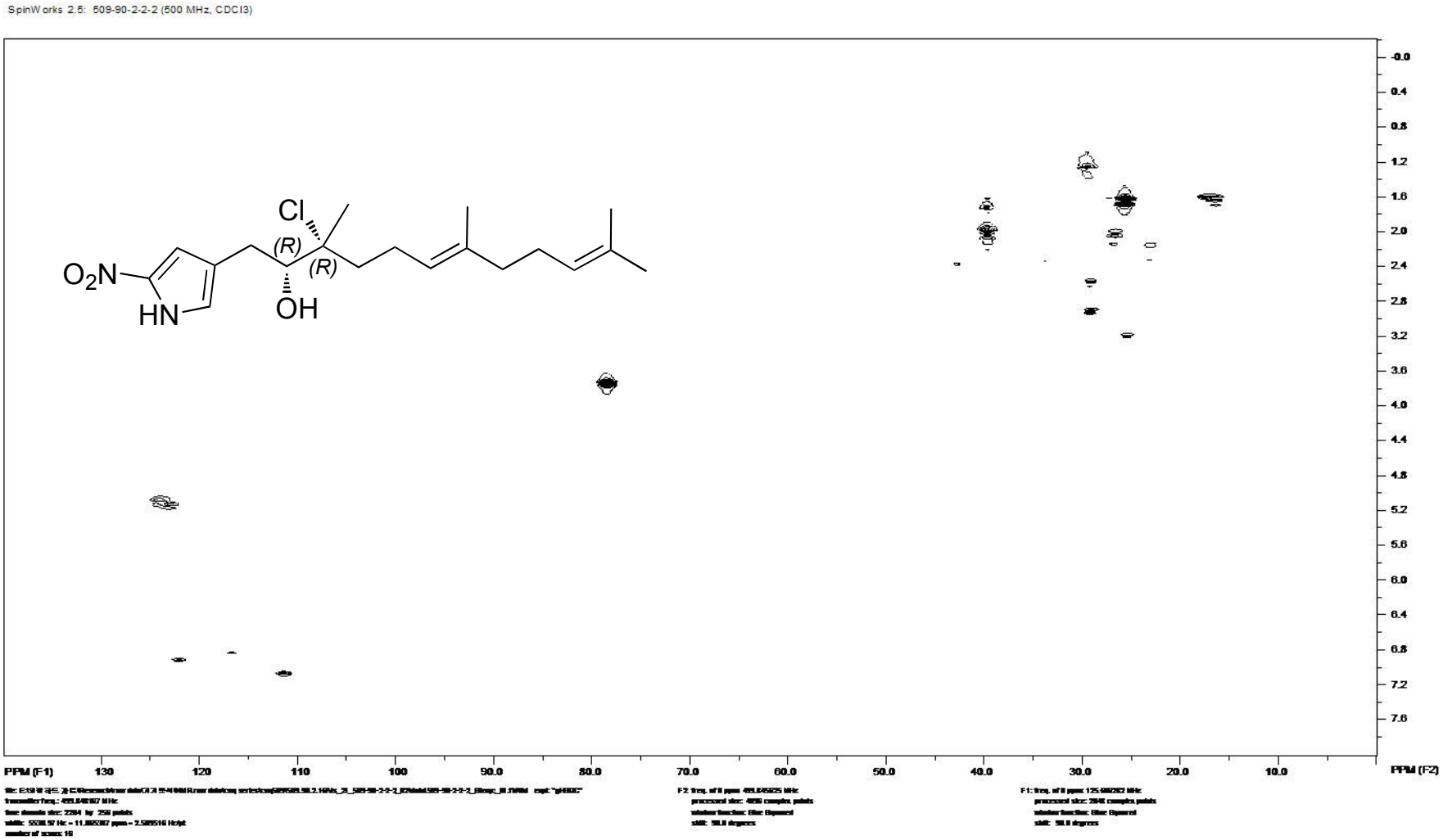


Figure S21 gHSQC spectrum of nitropyrrolin C (**3**) in $CDCl_3$ (500 MHz).

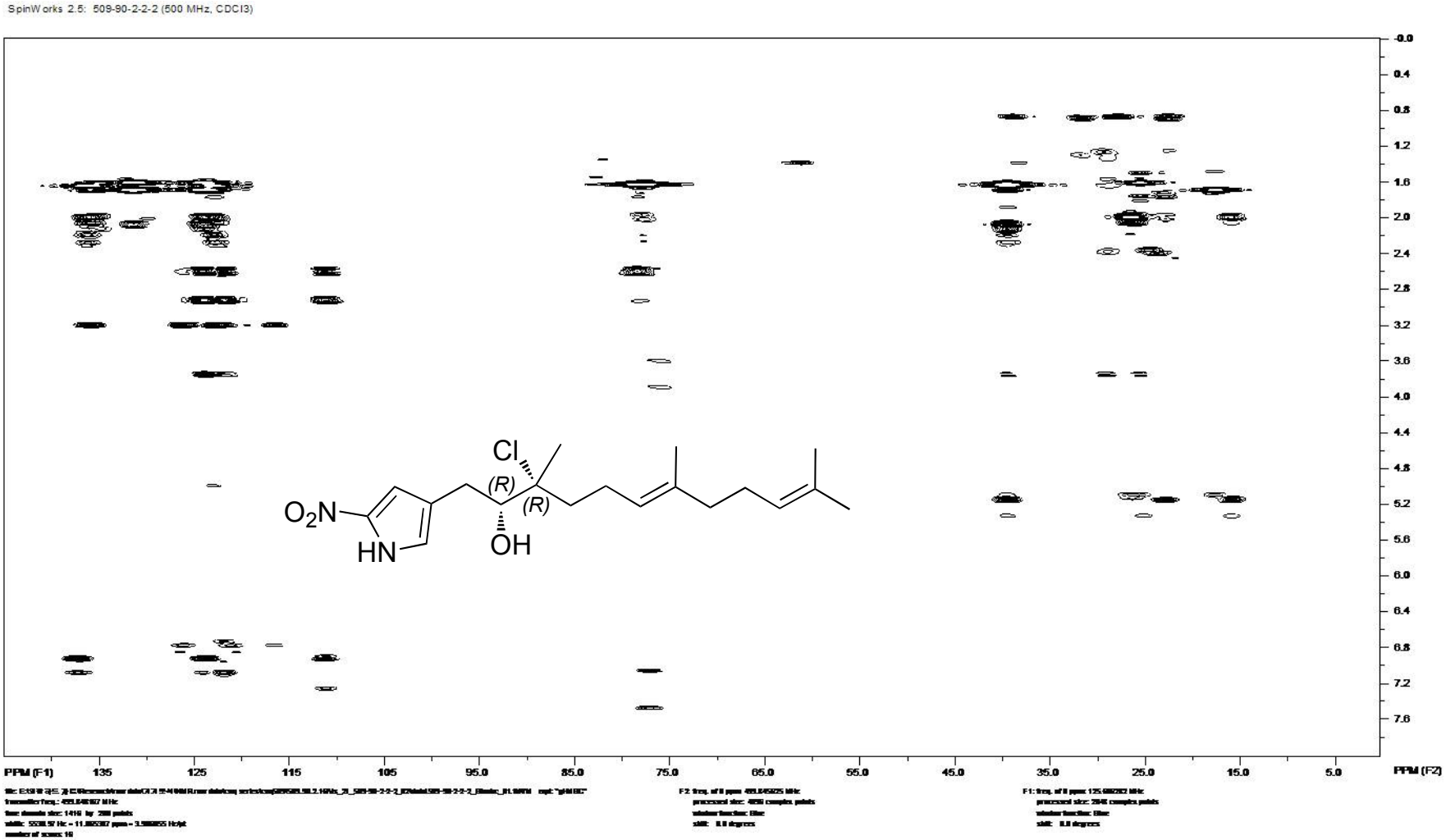


Figure S22 gHMBC spectrum of nitropyrrolin C (**3**) in $CDCl_3$ (500 MHz).

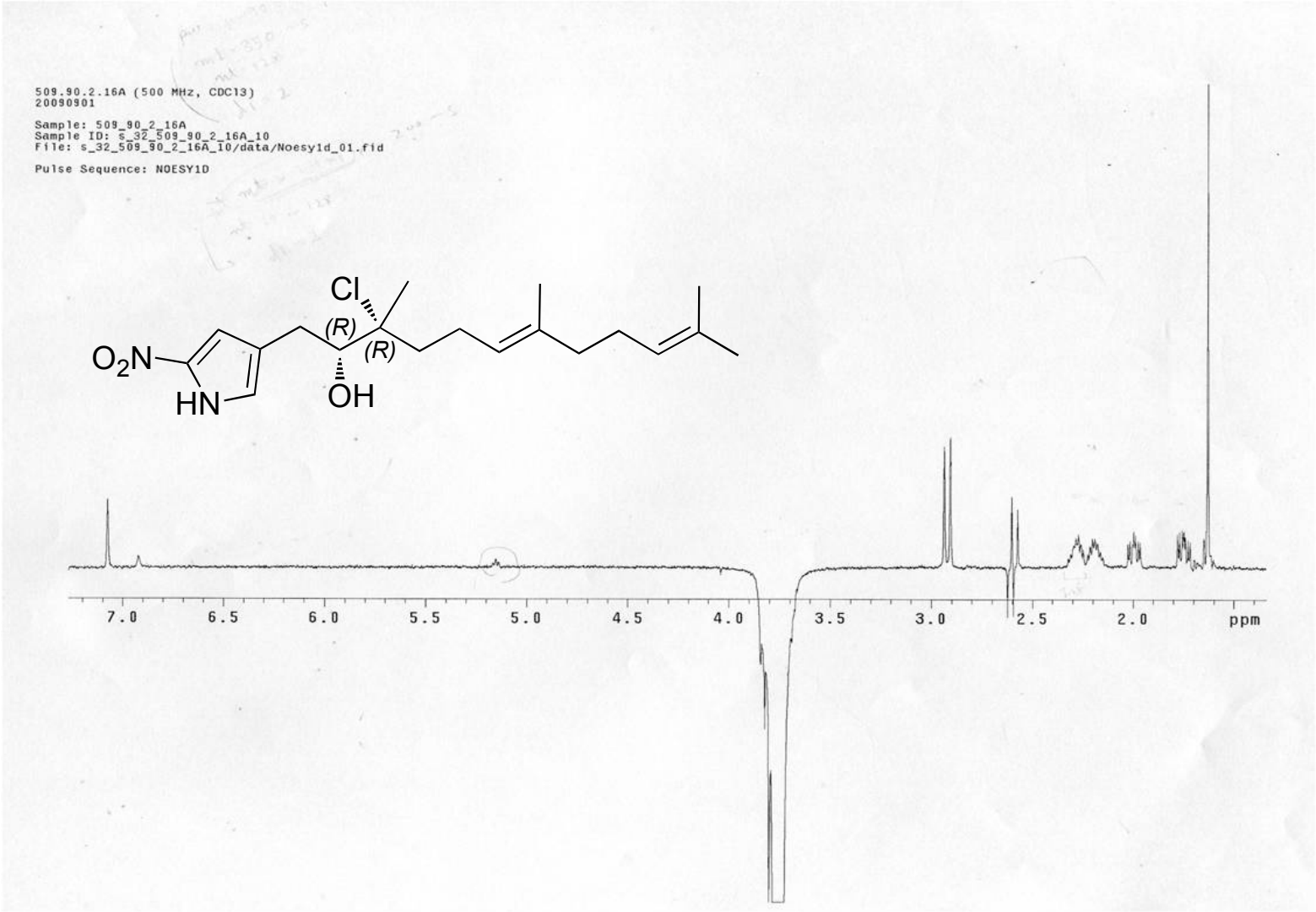


Figure S23 Selective 1D NOESY spectrum of nitropyrrolin C (**3**) in $CDCl_3$ (500 MHz), irradiation of H-2' signal at δ_H 3.75.

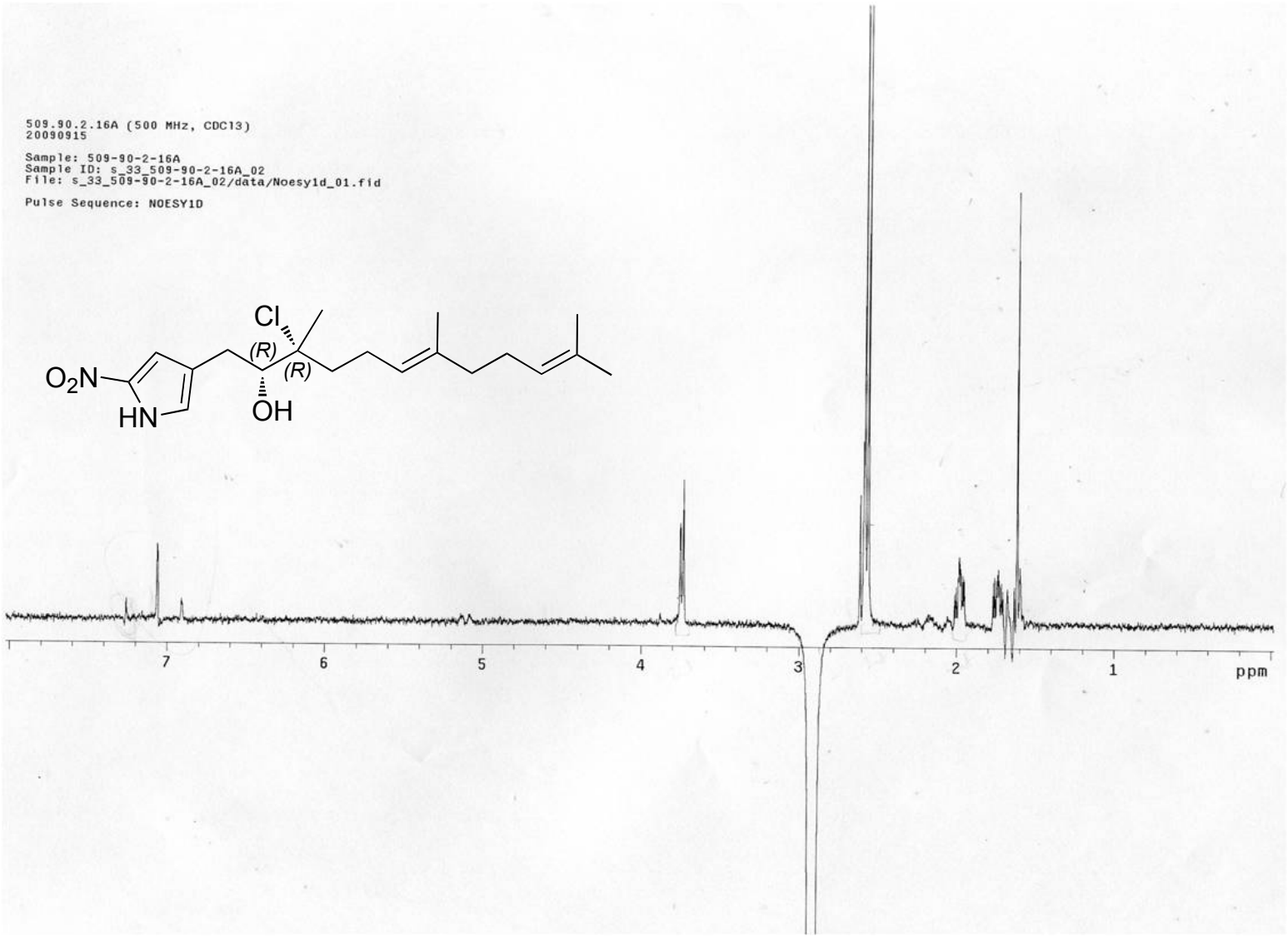


Figure S24 Selective 1D NOESY spectrum of nitropyrrolin C (**3**) in $CDCl_3$ (500 MHz), irradiation of H_2-1'a signal at δ_H 2.93.

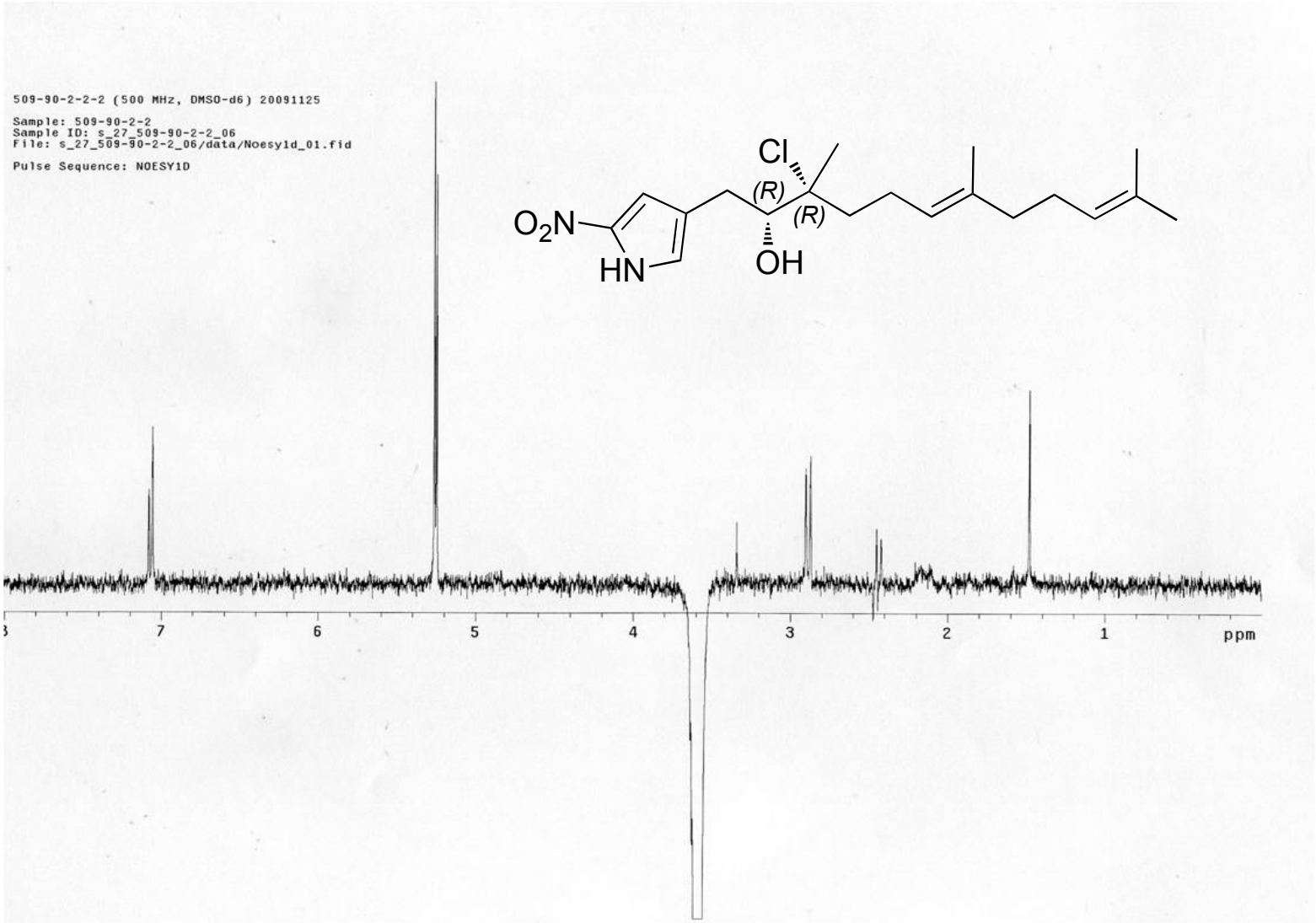


Figure S25 Selective 1D NOESY spectrum of nitropyrrolin C (**3**) in DMSO-d_6 (500 MHz), irradiation of H-2' signal

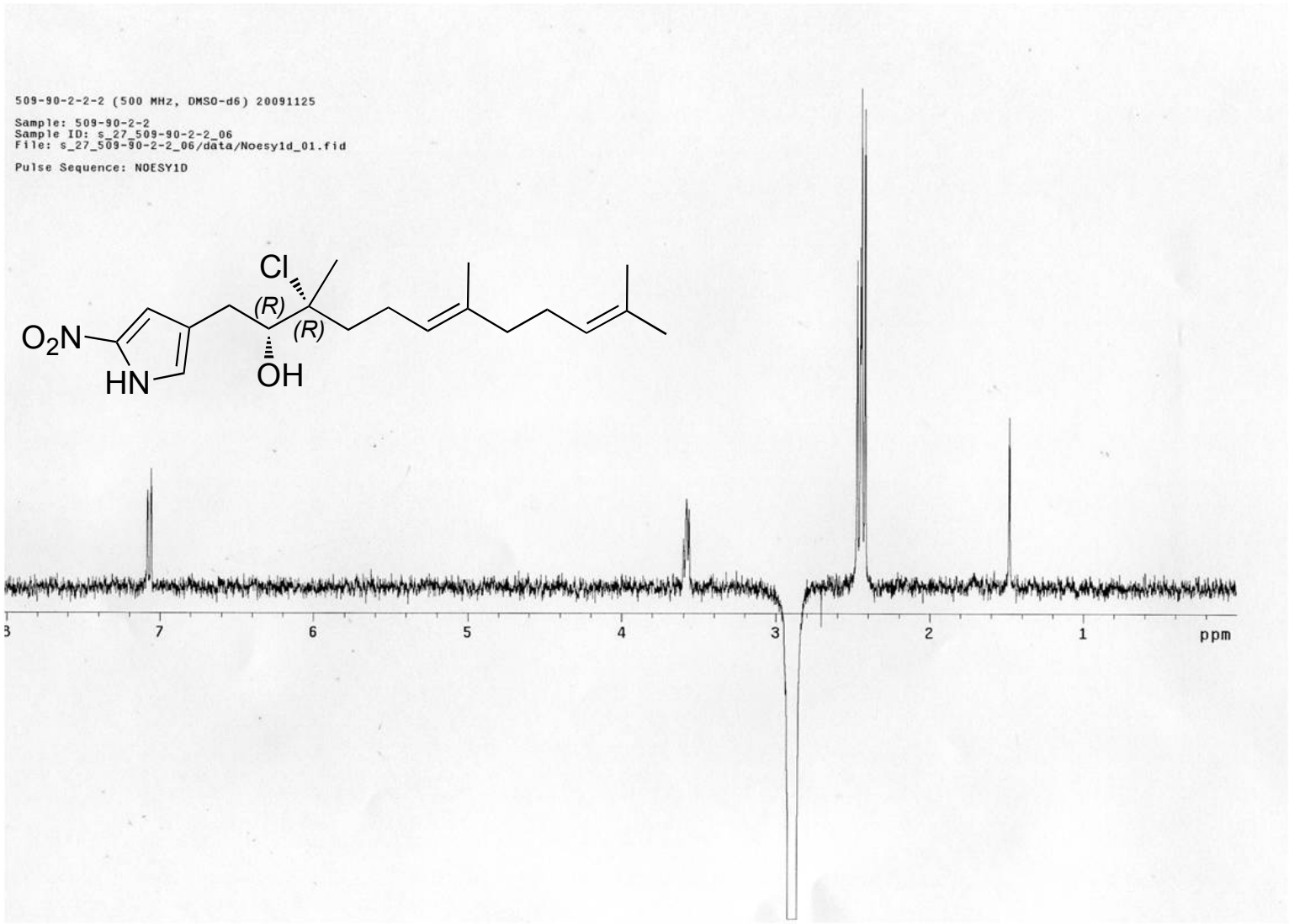


Figure S26 Selective 1D NOESY spectrum of nitropyrrolin C (**3**) in DMSO-d_6 (500 MHz), irradiation of H-1'a signal

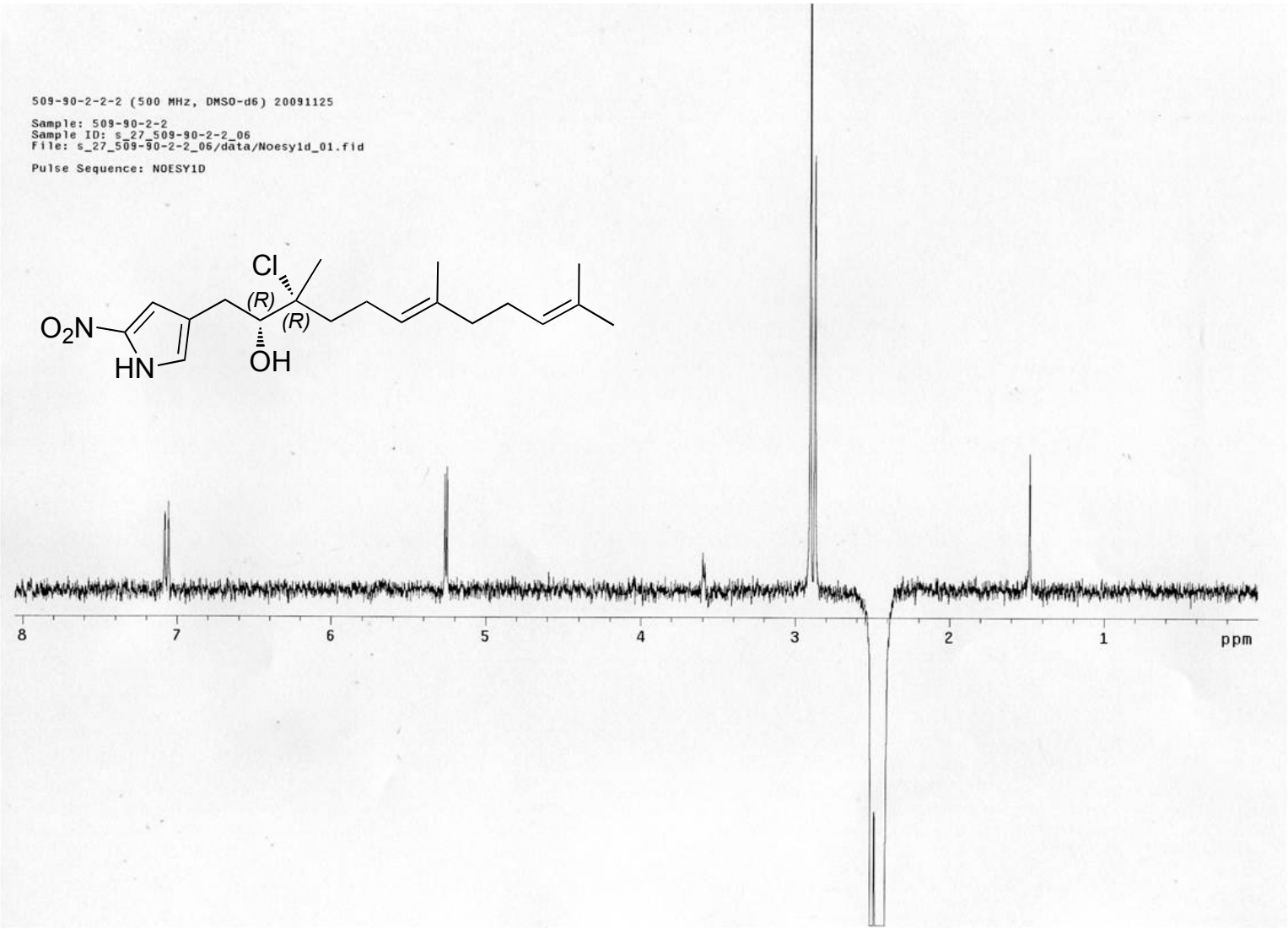
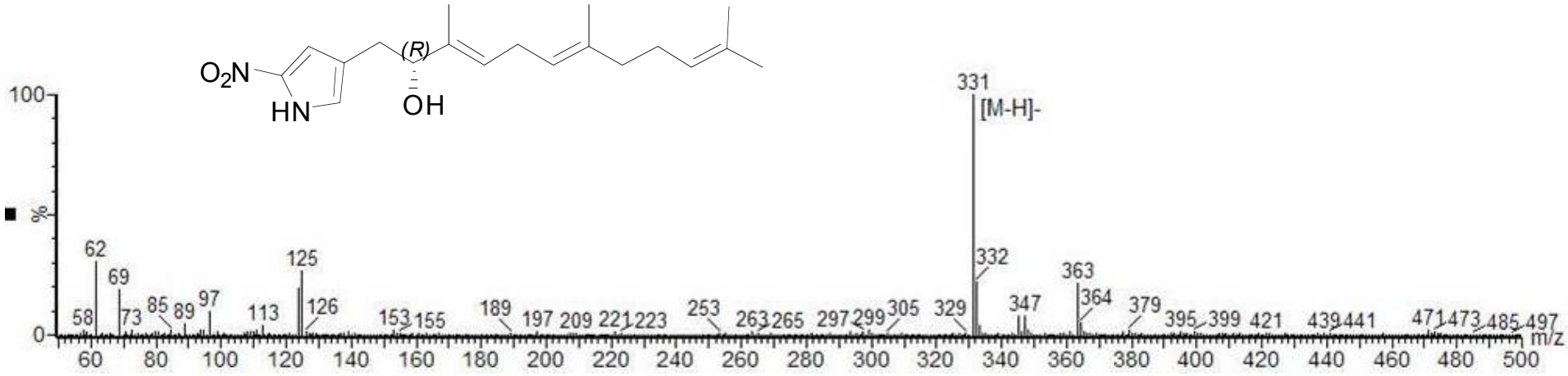


Figure S27 Selective 1D NOESY spectrum of nitropyrrolin C (**3**) in DMSO-d_6 (500 MHz), irradiation of H-1'b signal



Selected Isotopes : $C_{0-50}H_{0-100}O_{0-10}N_{0-5}$ **Error Limit : 20 ppm**

Measured Mass	*% Base*	*Formula*	*Calculated Mass*	*Error*
331.2023	78.9%	$C_{24}H_{27}O$	331.2062	12.0
		$C_{16}H_{29}O_6N$	331.1995	-8.6
		$C_{19}H_{27}O_3N_2$	331.2021	-0.5
		$C_{22}H_{25}N_3$	331.2048	7.7
		$C_{14}H_{27}O_5N_4$	331.1981	-13.0
		$C_{17}H_{25}O_2N_5$	331.2008	-4.5

Figure S28 MS data of nitropyrrolin D (**4**) (Upper, positive ESI MS; Middle, negative ESI MS; Bottom, negative HR-FAB MS).

Table S4. NMR data for nitropyrrolin D (**4**) in $CDCl_3$

Position	δ_H mult (*J* in Hz)	δ_C	COSY	HMBC	Key NOE
1	9.38, br s				
2		137.5			
3	7.01, br s	111.5	5, 1'	2, 5	
4		123.7			
5	6.84, br s	122.1	3	2, 3, 4	
1'	2.72, m[a]	32.7	3, 2'	3, 4, 2'	
2'	4.18, dd (6.5, 6.5)	77.6	1'	4, 1', 3', 4', 15'	4'
3'		136.0			
4'	5.38, dd (7.0, 7.0)	126.3	5', 15'	2', 5', 6', 15'	2'
5'	2.73, m[a]	26.9	4', 6'	3', 4', 6', 7'	
6'	5.08, m[a]	121.9	5'	4'	8'
7'		135.9			
8'	1.99, m	39.6	10'	6', 7', 9', 10'	6'
9'	2.07, m	26.7	10'	8', 10', 11'	
10'	5.09, m[a]	124.2	9', 12', 13'		
11'		131.5			
12'	1.69, s	25.7	10'	10', 11'	
13'	1.61, s	17.7	10'	10', 11'	
14'	1.63, s	16.1	6'	6', 7'	
15'	1.71, s	11.8	4'	3', 4'	

[a] The multiplicity of this signal was unresolved due to peak overlapping and the chemical shift was assigned by interpretation of HSQC and HMBC spectroscopic data.

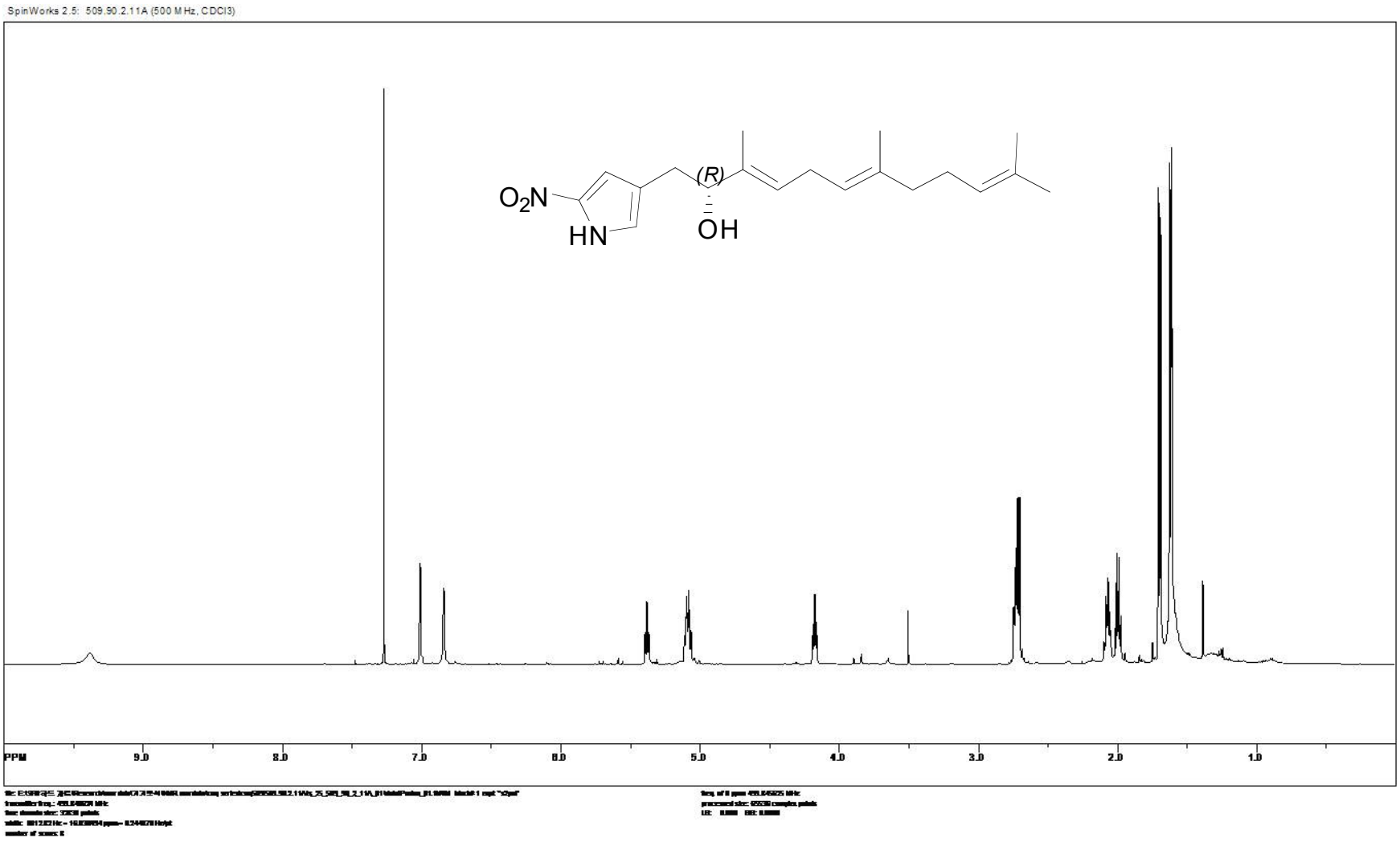


Figure S29 ^{1}H NMR spectrum of nitropyrrolin D (**4**) in $CDCl_3$ (500 MHz).

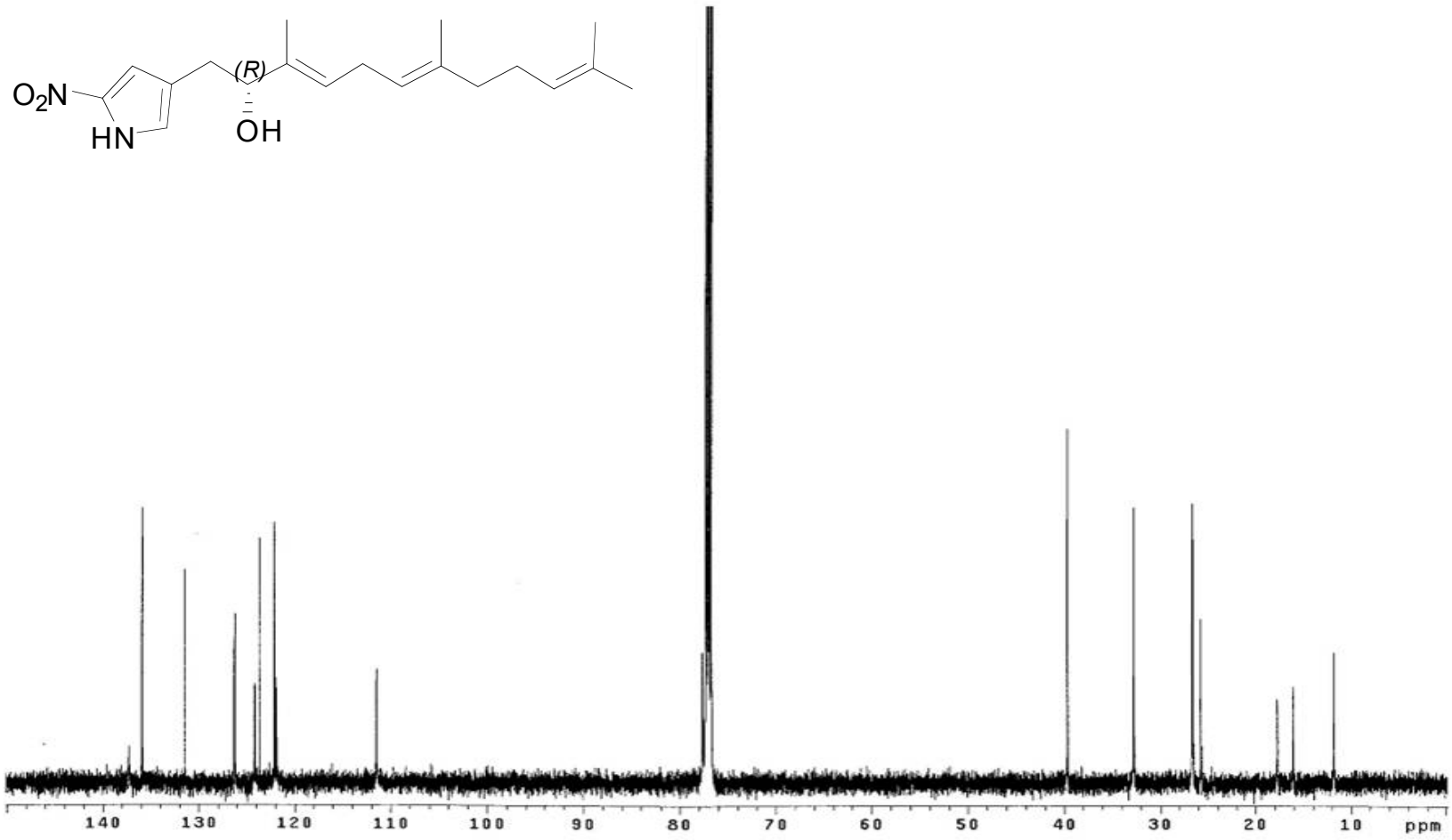


Figure S30 ^{13}C NMR spectrum of nitropyrrolin D (**4**) in $CDCl_3$ (125 MHz).

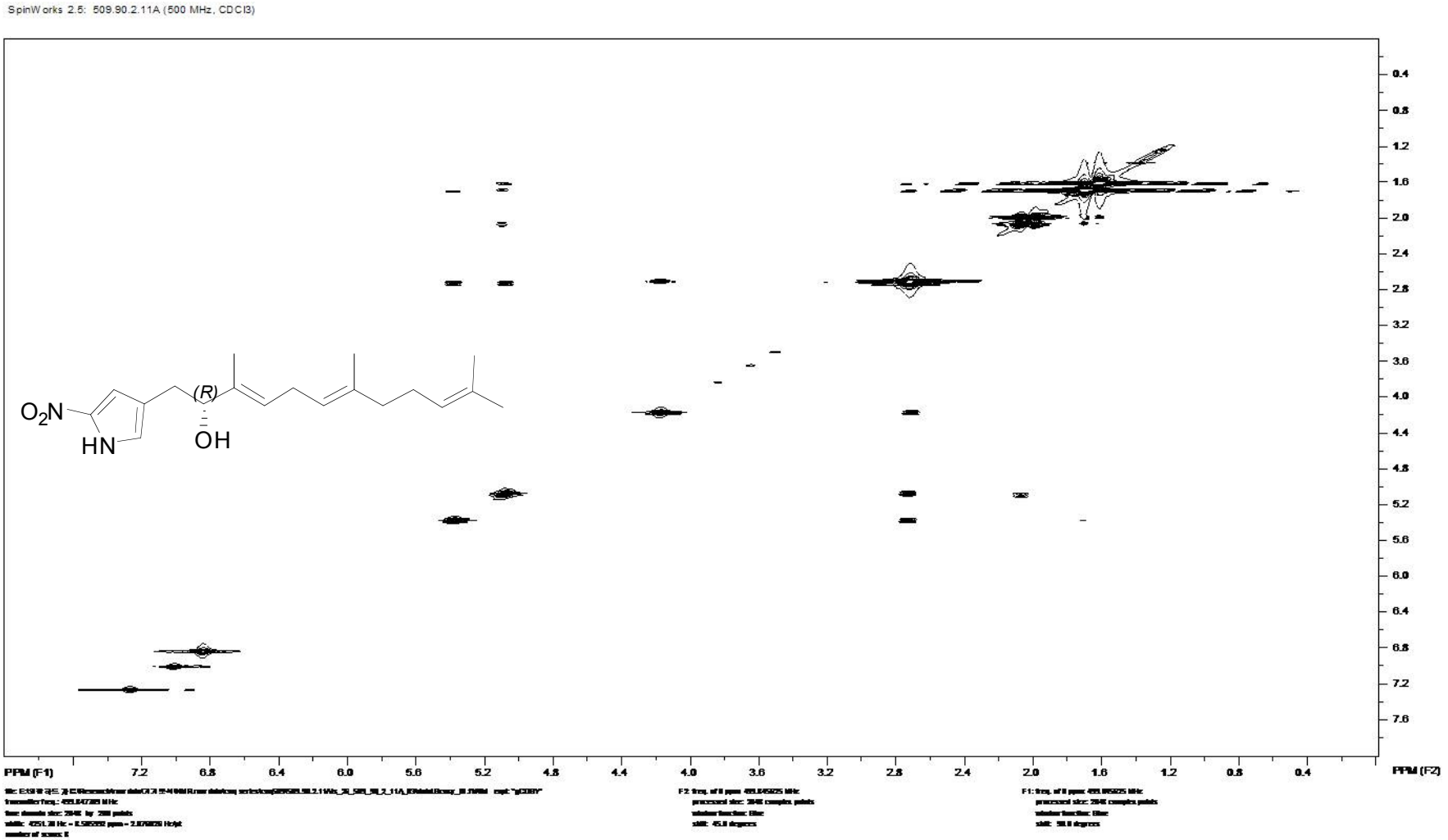


Figure S31 ^{1}H-^{1}H gCOSY spectrum of nitropyrrolin D (**4**) in $CDCl_3$ (500 MHz).

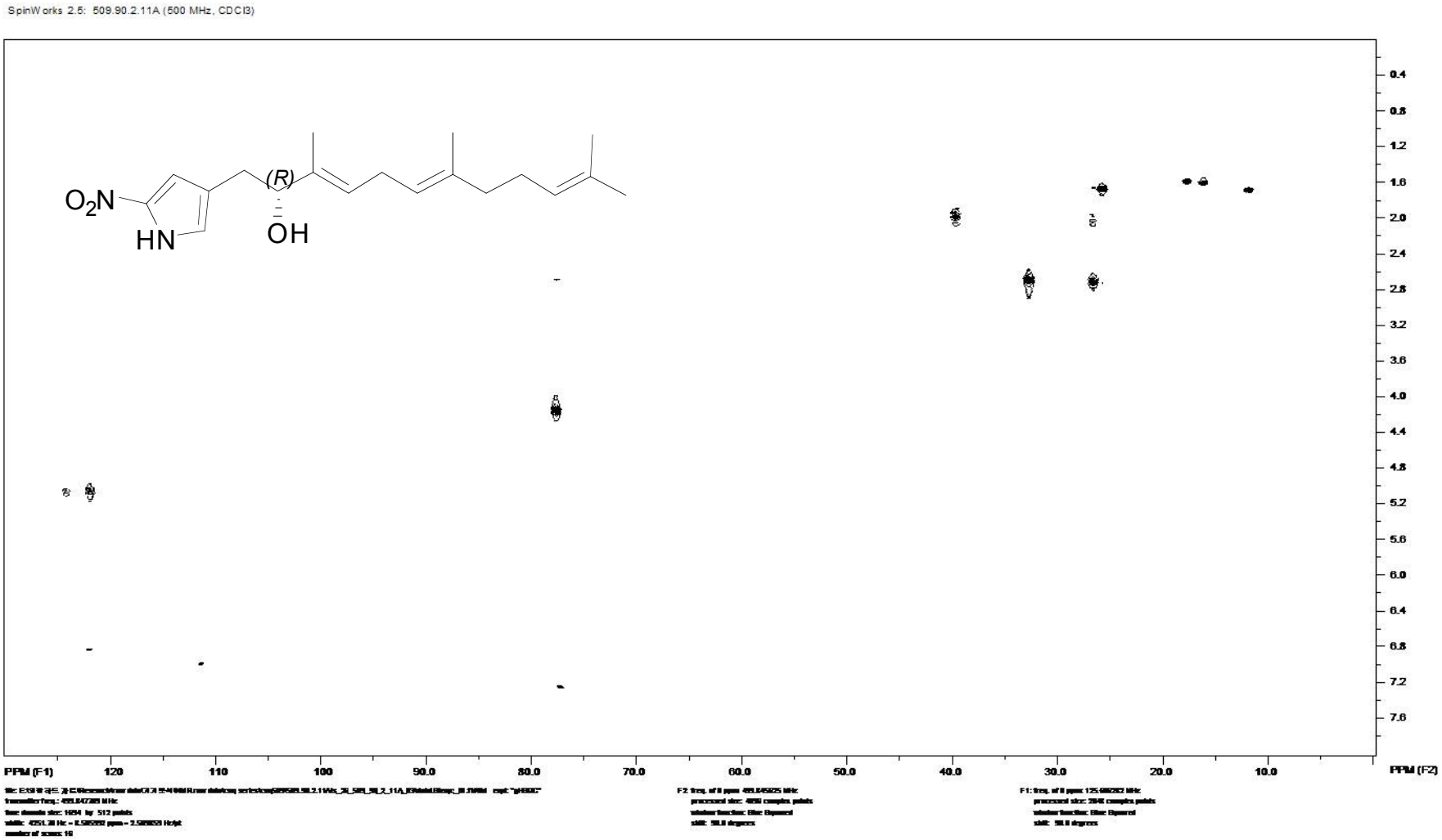


Figure S32 gHSQC spectrum of nitropyrrolin D (**4**) in $CDCl_3$ (500 MHz).

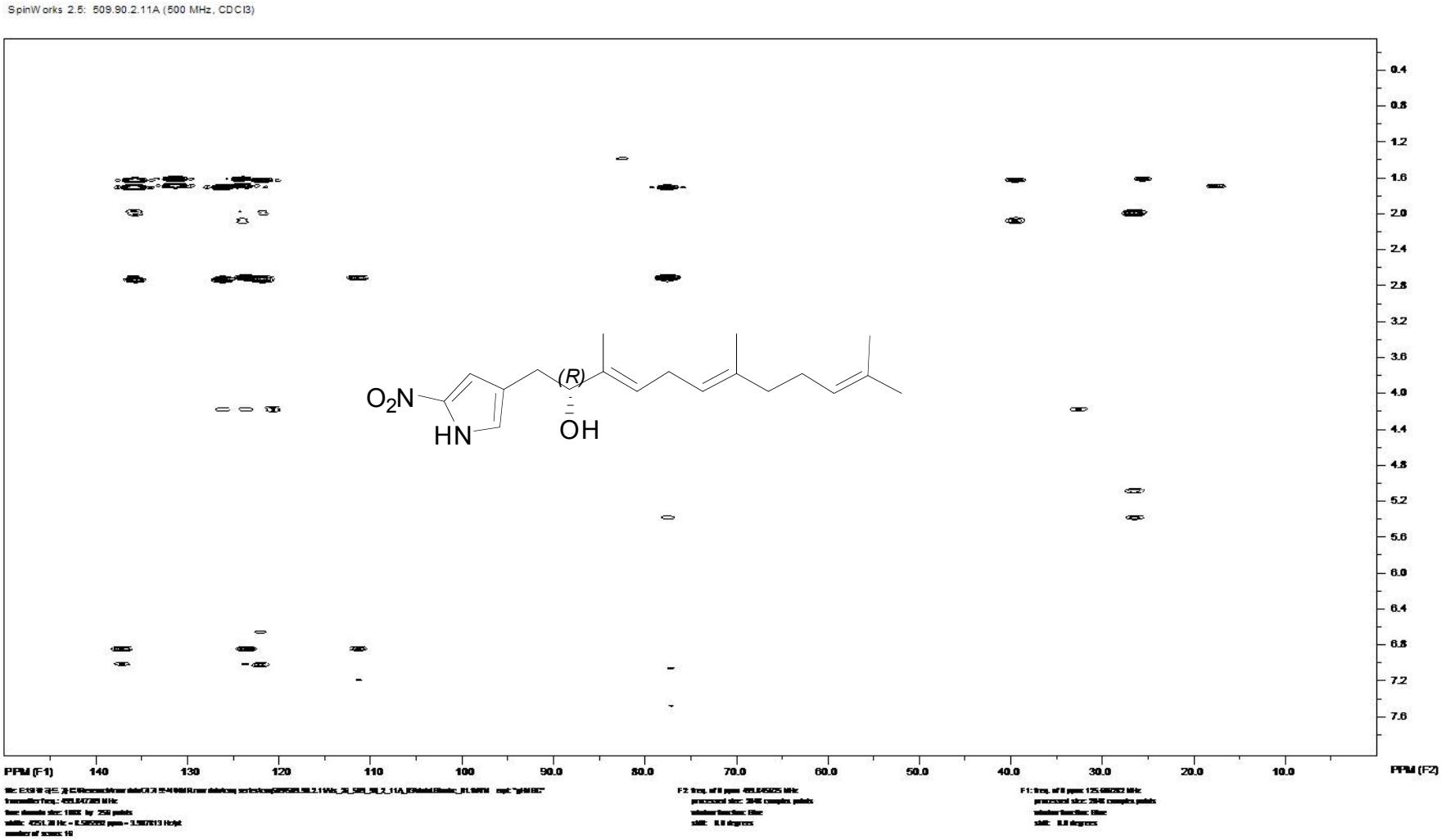


Figure S33 gHMBC spectrum of nitropyrrolin D (**4**) in $CDCl_3$ (500 MHz).

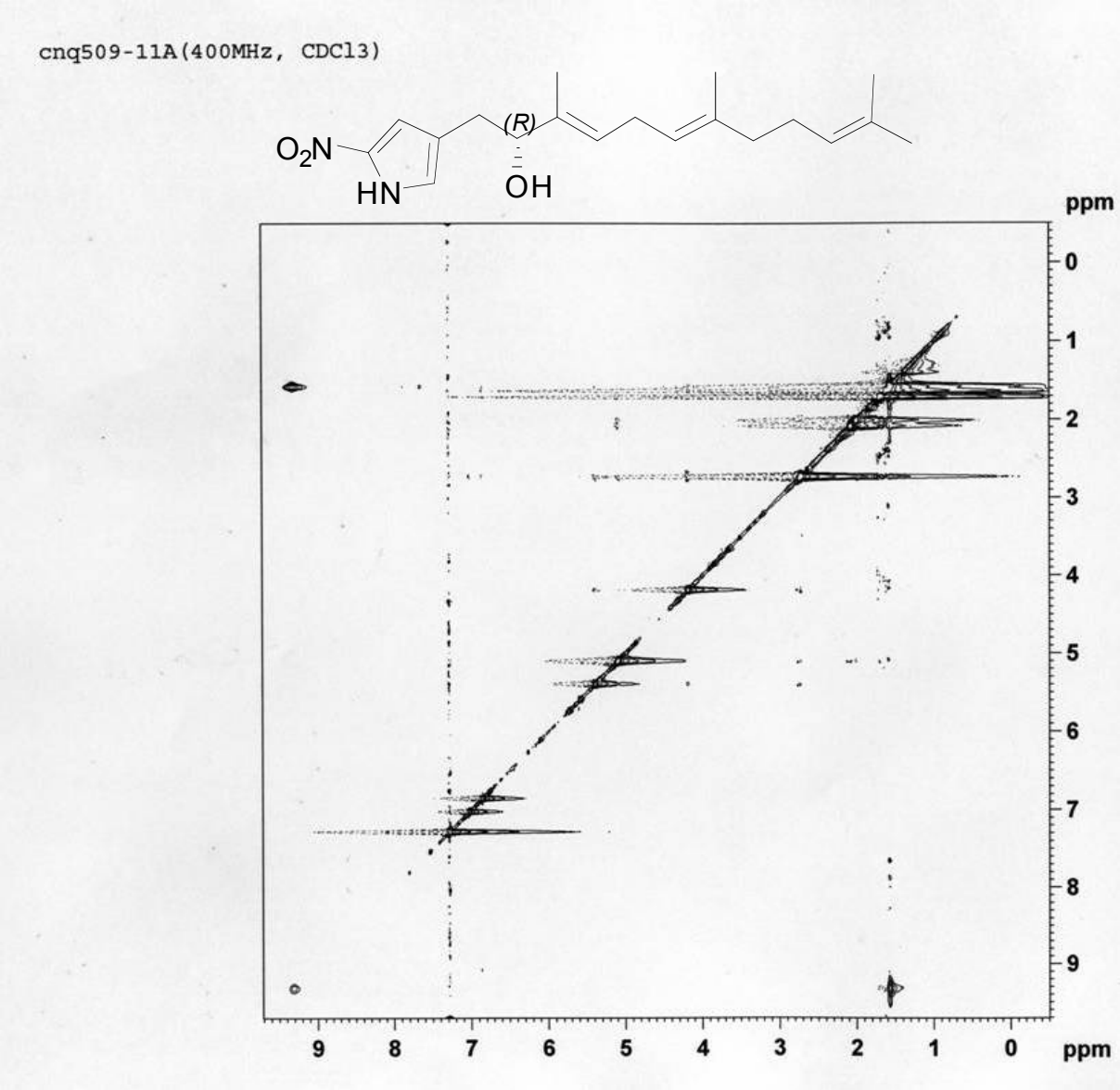
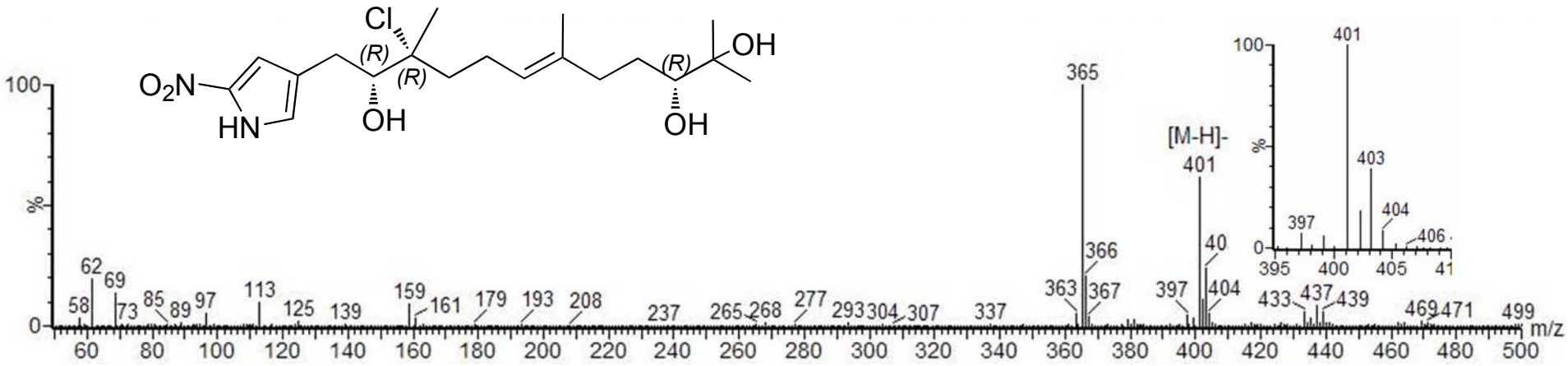


Figure S34 2D NOESY spectrum of nitropyrrolin D (**4**) in $CDCl_3$ (500 MHz).



Selected Isotopes : $H_{0-50}C_{0-50}N_{0-3}O_{3-7}Cl_{0-2}{}^{37}Cl_{0-2}$ **Error Limit : 20 ppm**

Measured Mass	*% Base*	*Formula*	*Calculated Mass*	*Error*
401.1837	36.8%	$C_{25}H_{25}N_2O_3$	401.1865	7.0
		$C_{22}H_{27}NO_6$	401.1838	0.3
		$C_{24}H_{30}O_3Cl$	401.1883	12.0
		$C_{23}H_{28}NO_3Cl$	401.1757	-20.0
		$C_{19}H_{30}N_2O_5Cl$	401.1843	1.5
		$C_{16}H_{33}N_3O_4Cl_2$	401.1848	2.7

Figure S35 MS data of nitropyrrolin E (**5**) (Upper, positive ESI MS; Middle, negative ESI MS; Bottom, negative HR-FAB MS).

Table S5. NMR data for nitropyrrolin E (**5**) in $CDCl_3$

Position	δ_H mult (*J* in Hz)	δ_C	COSY	HMBC	Key NOE
1	9.58, br s		3, 5		
2		137.4			
3	7.08, br s	111.5	1, 5	2, 5	
4		123.9			
5	6.92, br s	122.2	1, 3	2, 3, 4	
1'	2.94, dd (15.0, 2.0) 2.60, dd (15.0, 10.5)	29.8		3, 4, 5, 2'	2'
2'	3.76, br d (10.5)	78.3	1'		1', 4', 15'
3'		77.9			
4'	1.98, ddd (14.0, 11.0, 5.0) 1.72, ddd (14.0, 11.0, 5.0)	39.9	5'		2'
5'	2.29, m[a] 2.19, m[a]	23.5	4', 6'	6', 7'	
6'	5.22, dd (7.0, 7.0)	123.9	5', 14'	5', 8', 14'	8'
7'		136.1			
8'	2.27, m[a] 2.09, ddd (15.0, 8.0, 8.0)	36.9	9'	6', 7', 9'	6', 10'
9'	1.60, m[a] 1.42, dddd (14.0, 10.0. 8.0, 5.0)	29.9	8', 10'	8'	
10'	3.36, dd (10.0, 1.5)	78.2	9'		8', 12', 13'
11'		73.2			
12'	1.22, s	26.2		10', 11', 13'	10'
13'	1.18, s	23.6		10', 11', 12'	10'
14'	1.66, s	16.1		6', 7', 8'	
15'	1.62, s	25.9		3'	2'

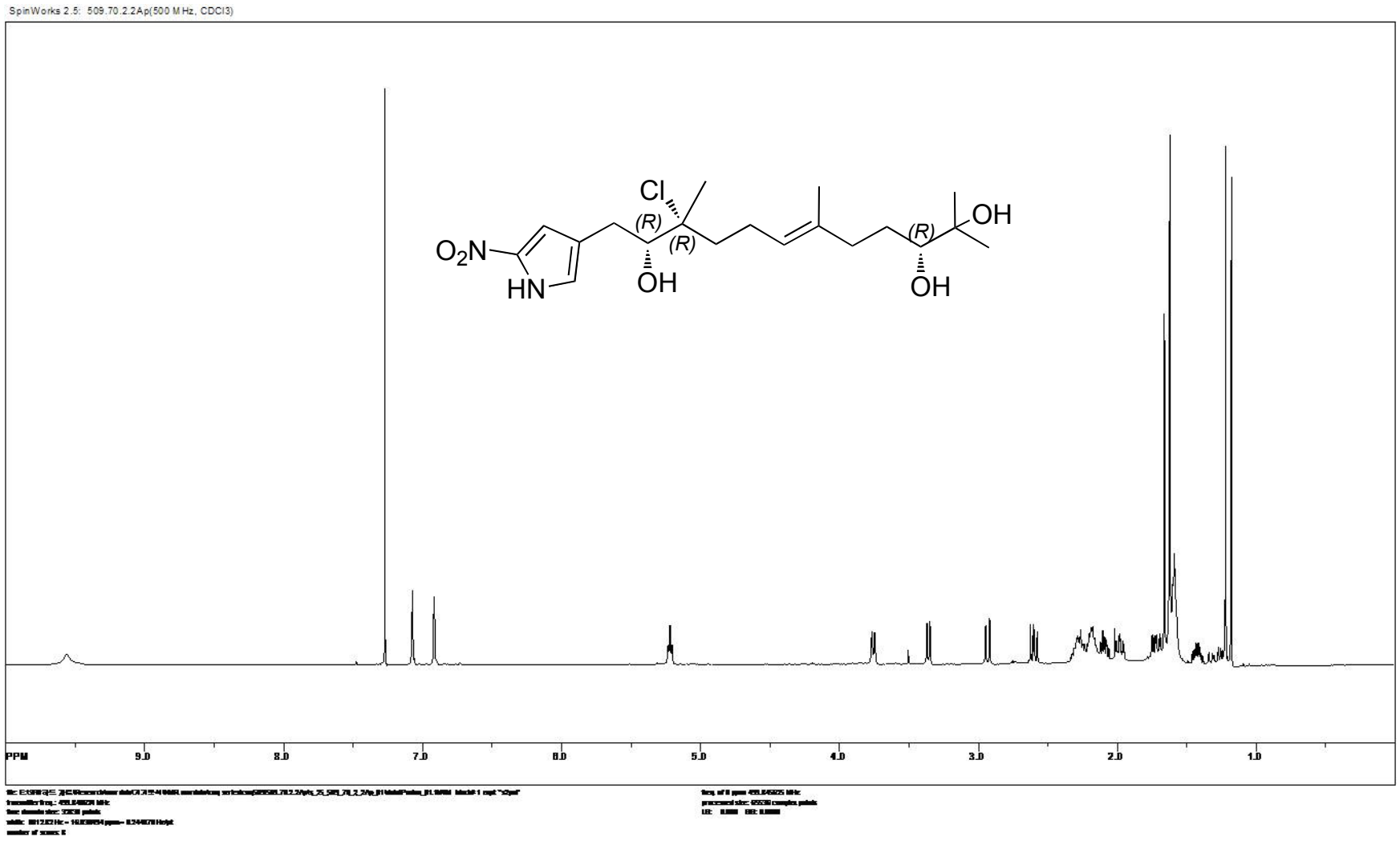


Figure S36 ^{1}H NMR spectrum of nitropyrrolin E (**5**) in $CDCl_3$ (500 MHz).

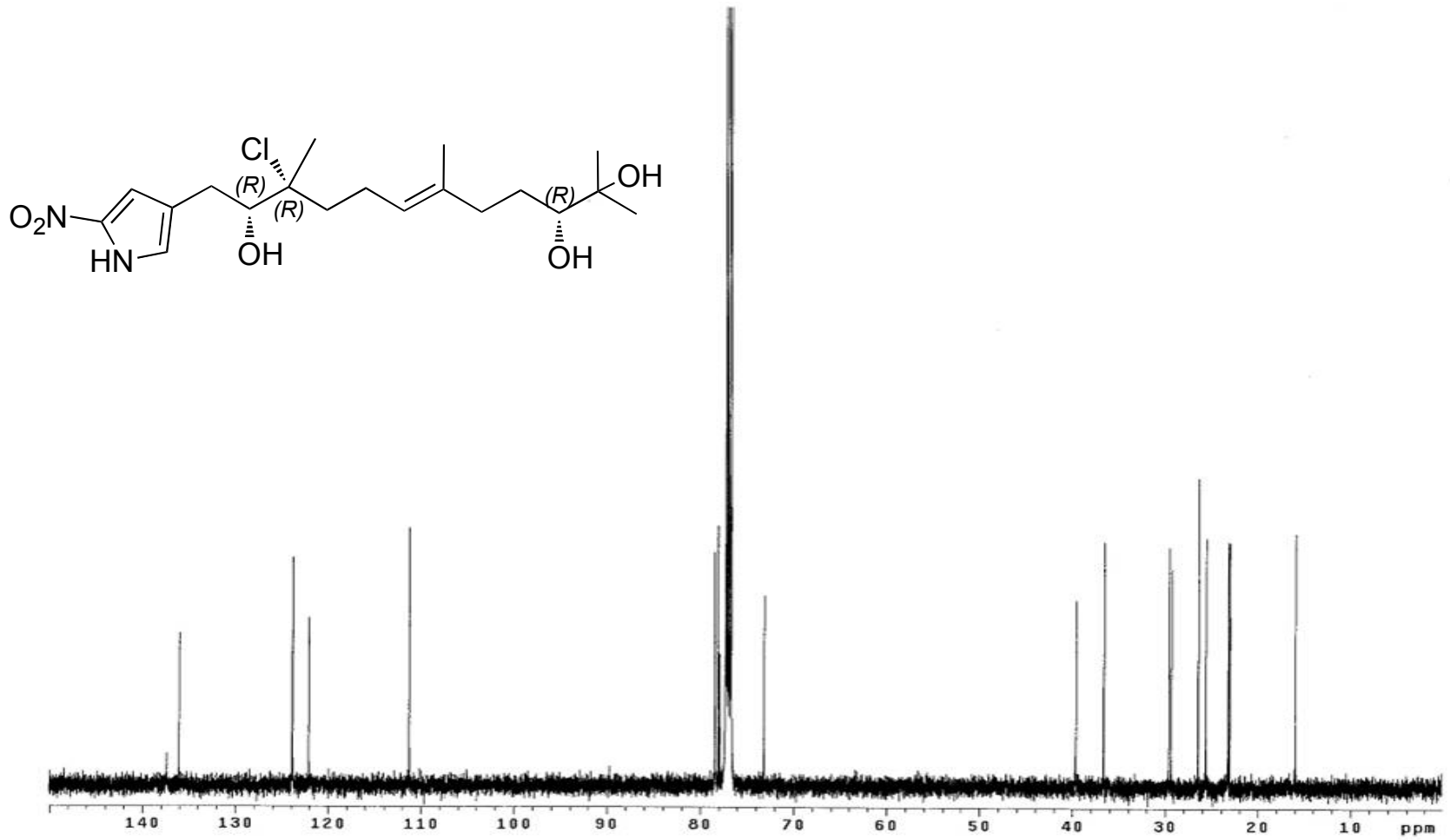


Figure S37 ^{13}C NMR spectrum of nitropyrrolin E (**5**) in $CDCl_3$ (125 MHz).

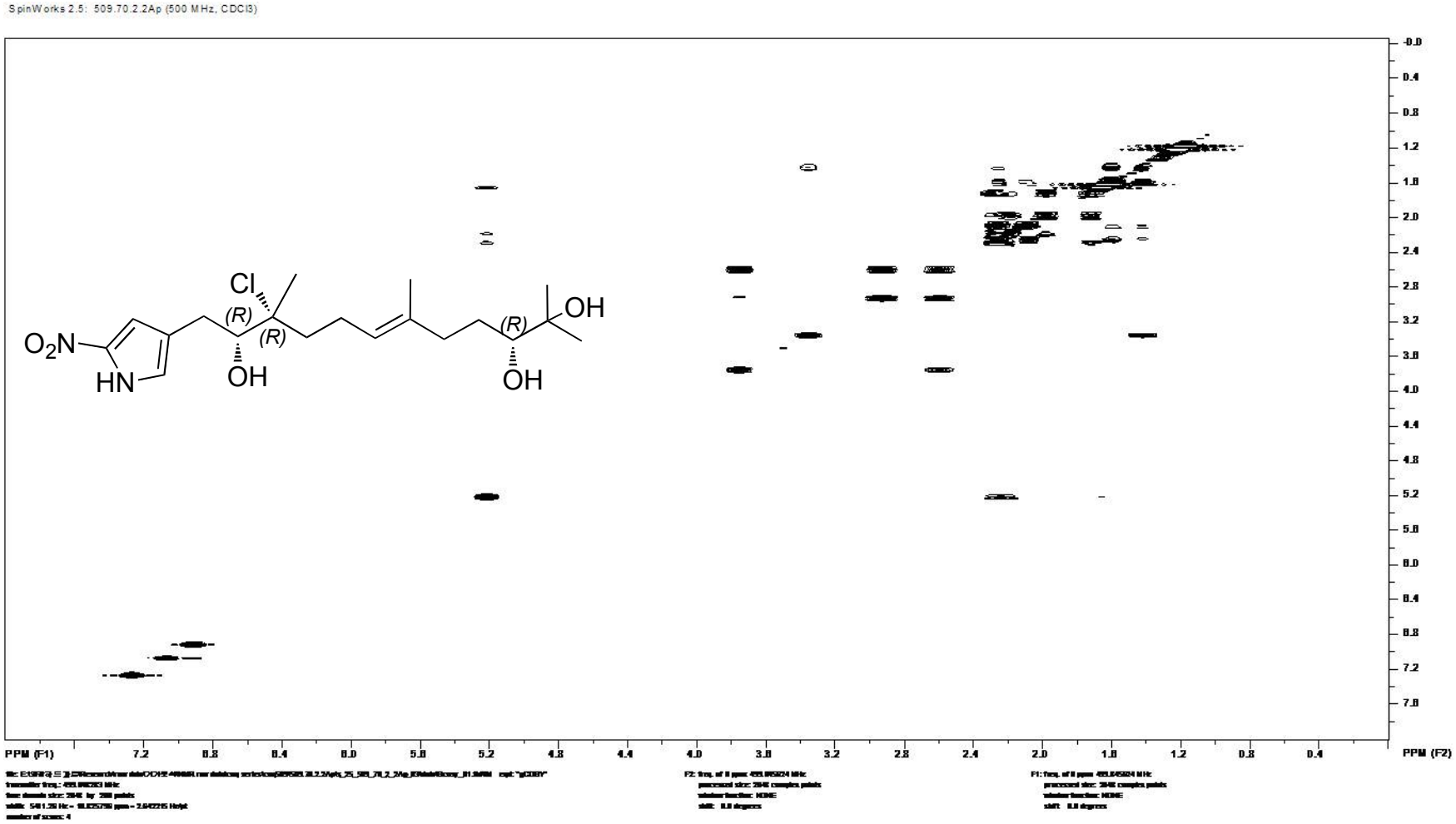


Figure S38 ^{1}H-^{1}H gCOSY spectrum of nitropyrrolin E (**5**) in $CDCl_3$ (500 MHz).

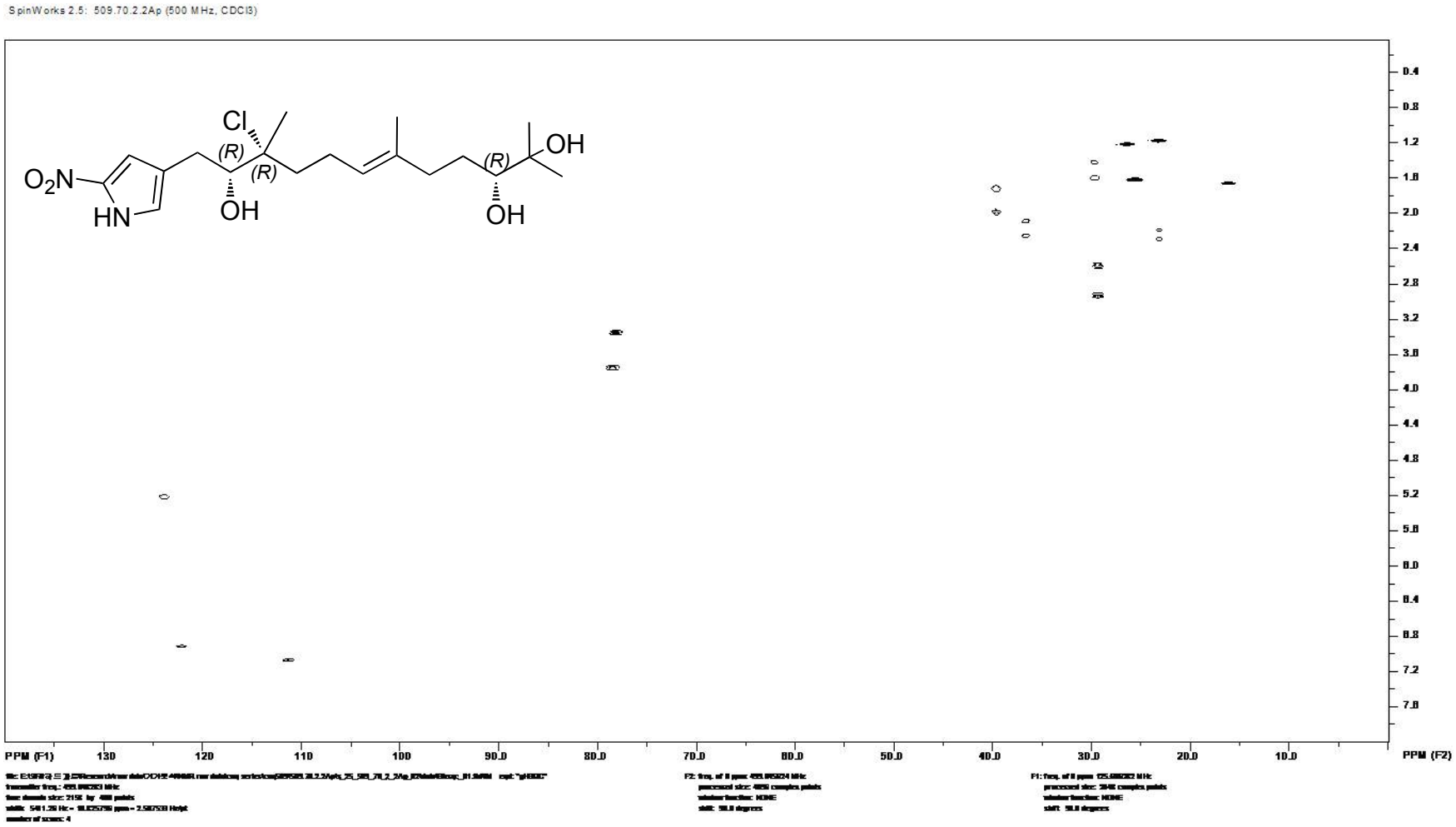


Figure S39 gHSQC spectrum of nitropyrrolin E (**5**) in $CDCl_3$ (500 MHz).

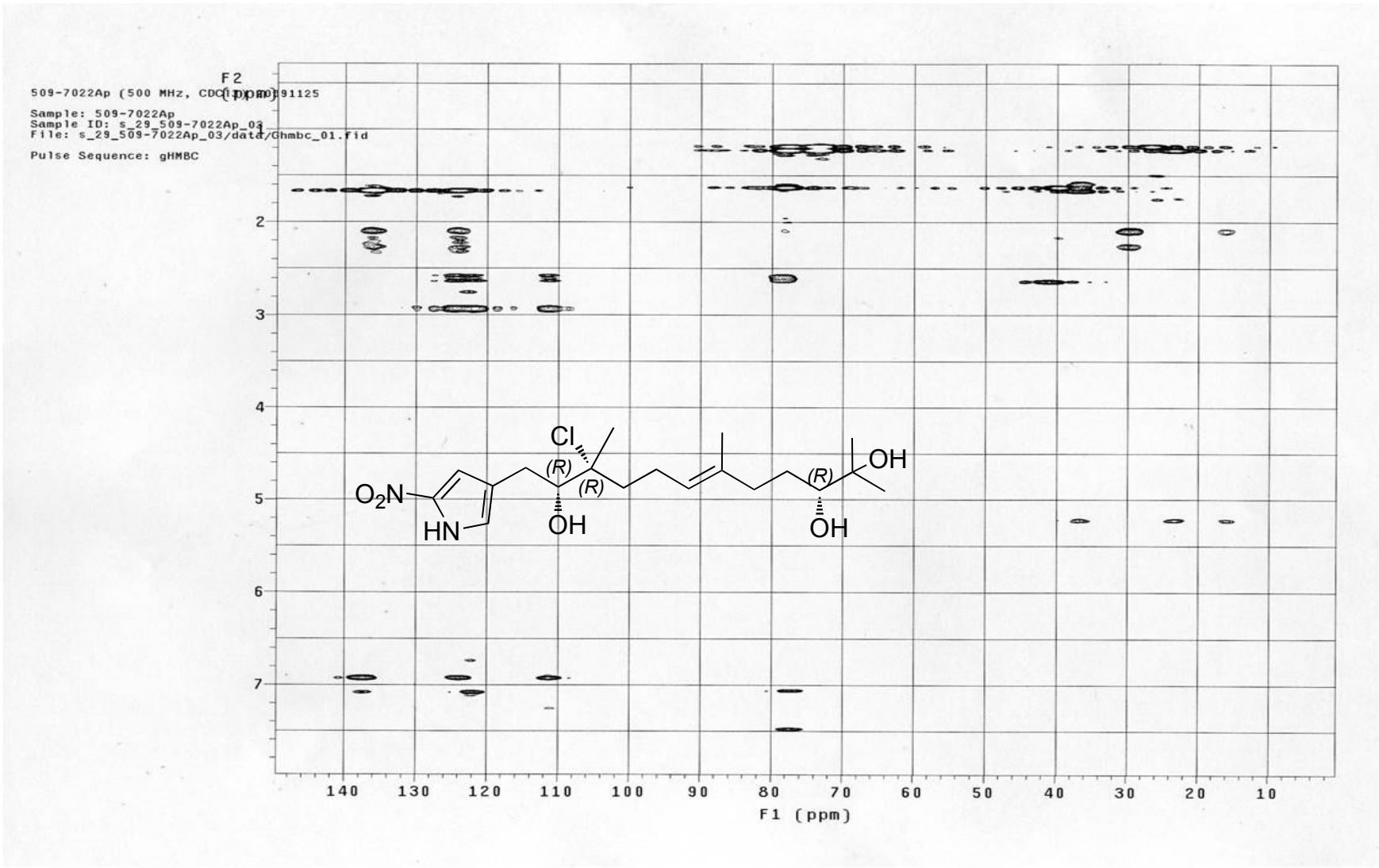


Figure S40 gHMBC spectrum of nitropyrrolin E (**5**) in $CDCl_3$ (500 MHz).

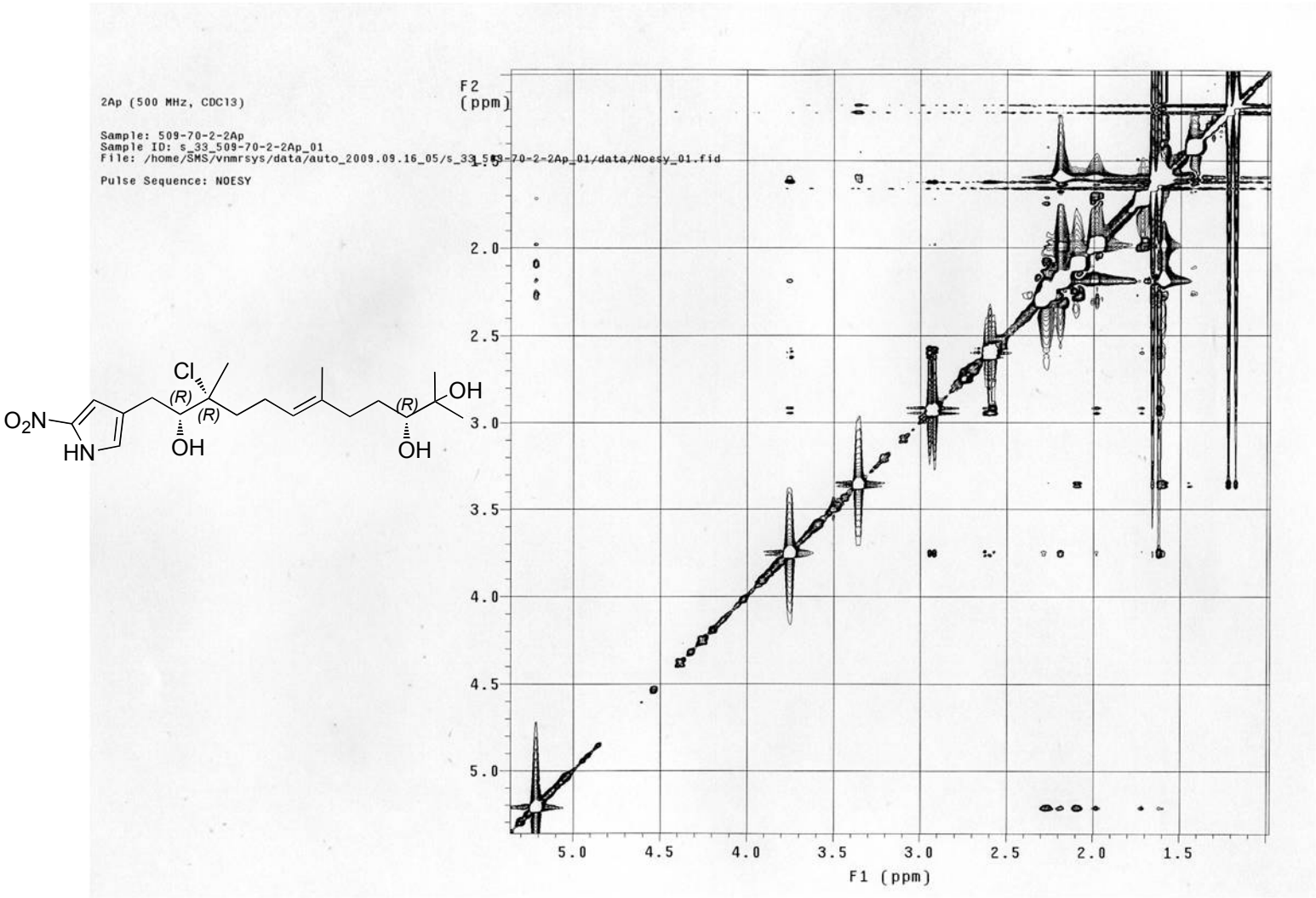


Figure S41 2D NOESY spectrum of nitropyrrolin E (**5**) in $CDCl_3$ (500 MHz).

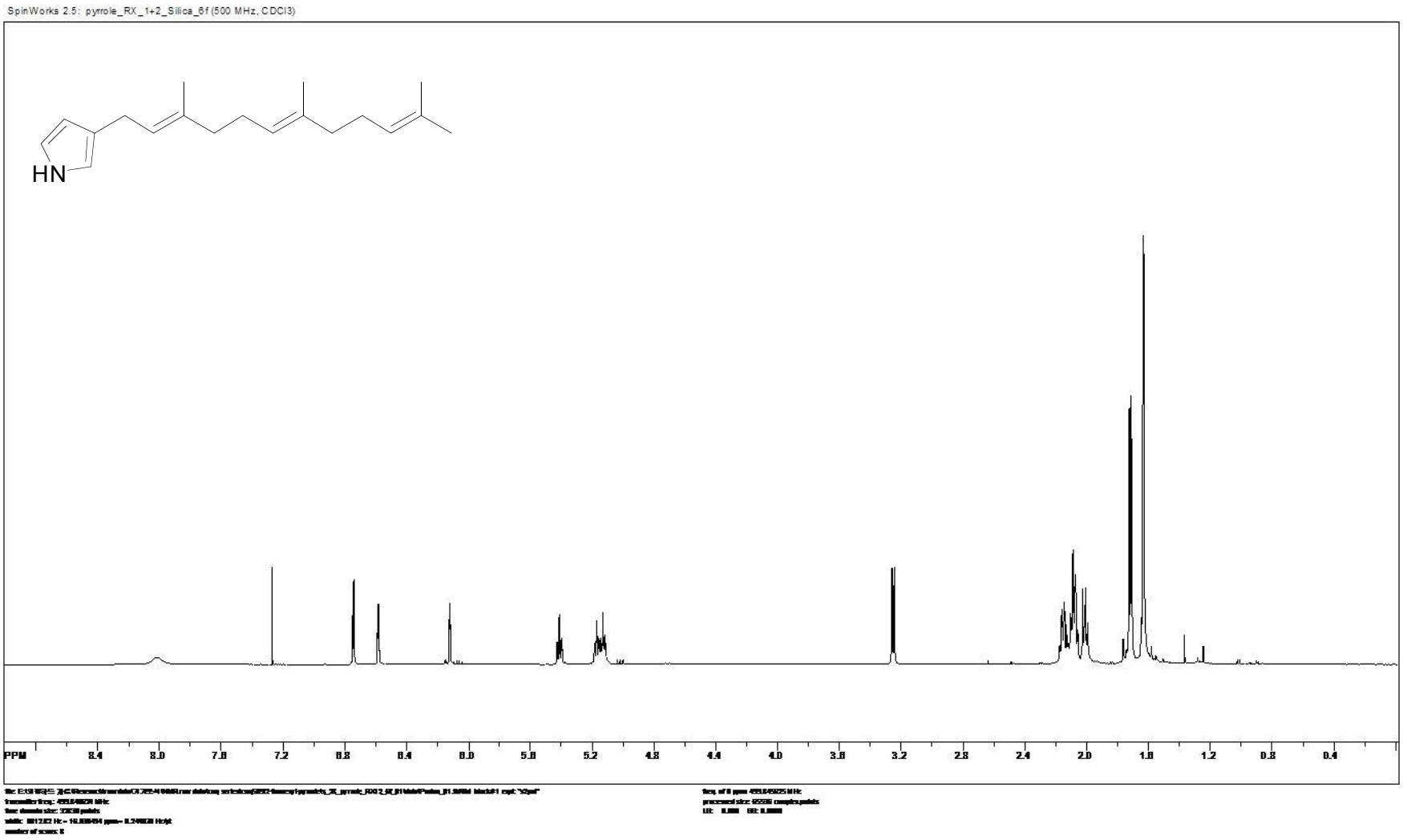


Figure S42 ^{1}H NMR spectrum of 3-farnesyl-pyrrole (**6**) in $CDCl_3$ (500 MHz).

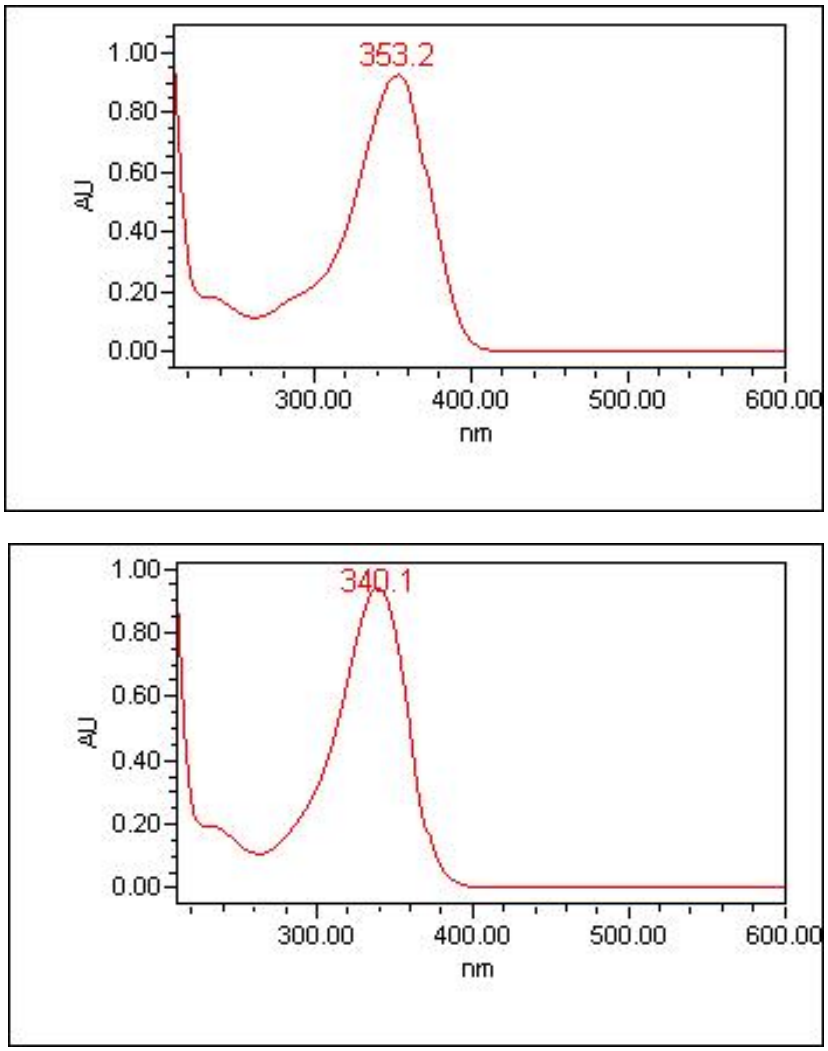


Figure S43 UV spectra (PDA detector) of γ-farnesyl-α-nitropyrrole (**7**) (upper) and β-farnesyl-α-nitropyrrole (**8**) (bottom) (acetonitril-water solvent mixture).

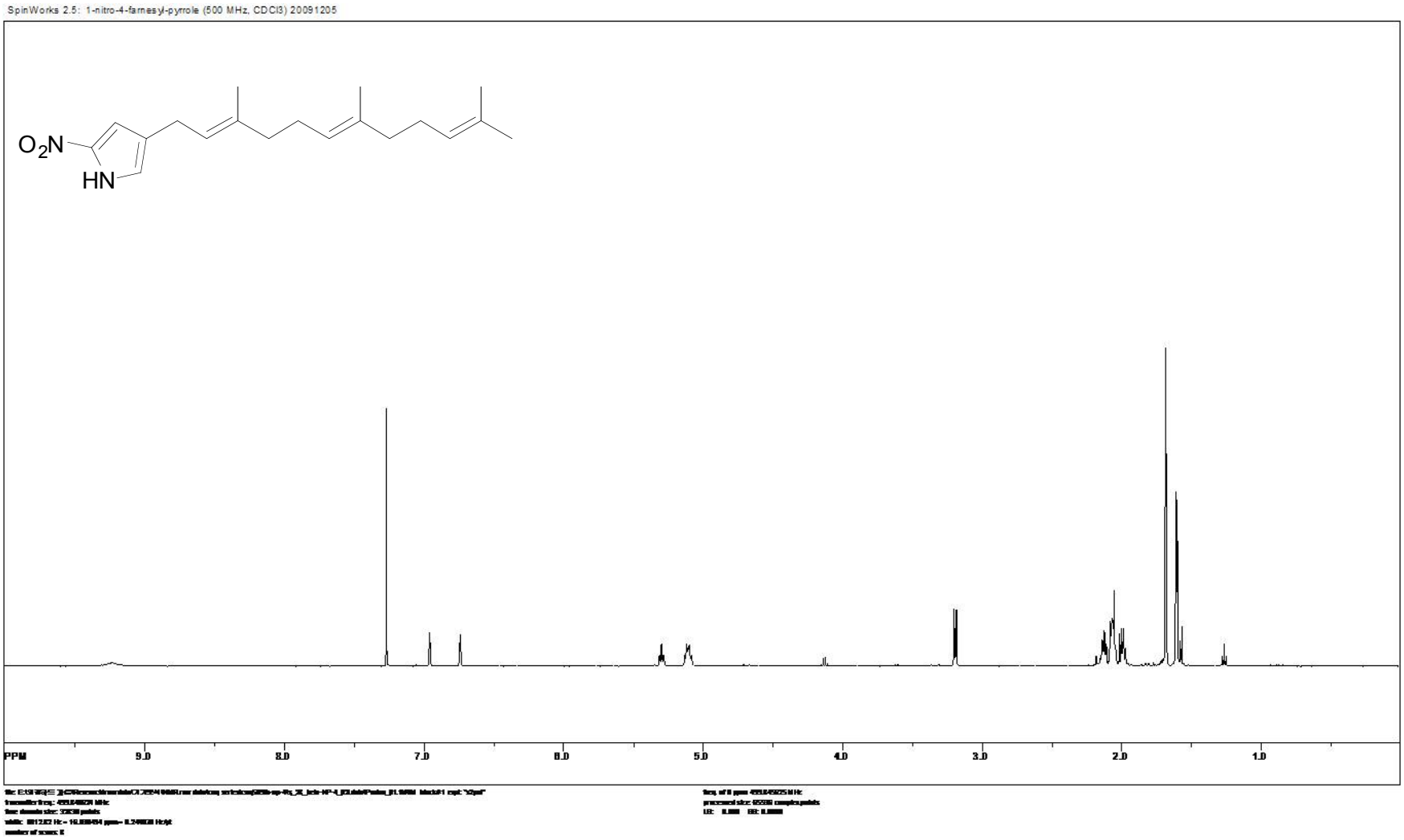


Figure S44 ^{1}H NMR spectrum of γ-farnesyl-α-nitropyrrole (**7**) in $CDCl_3$ (500 MHz).

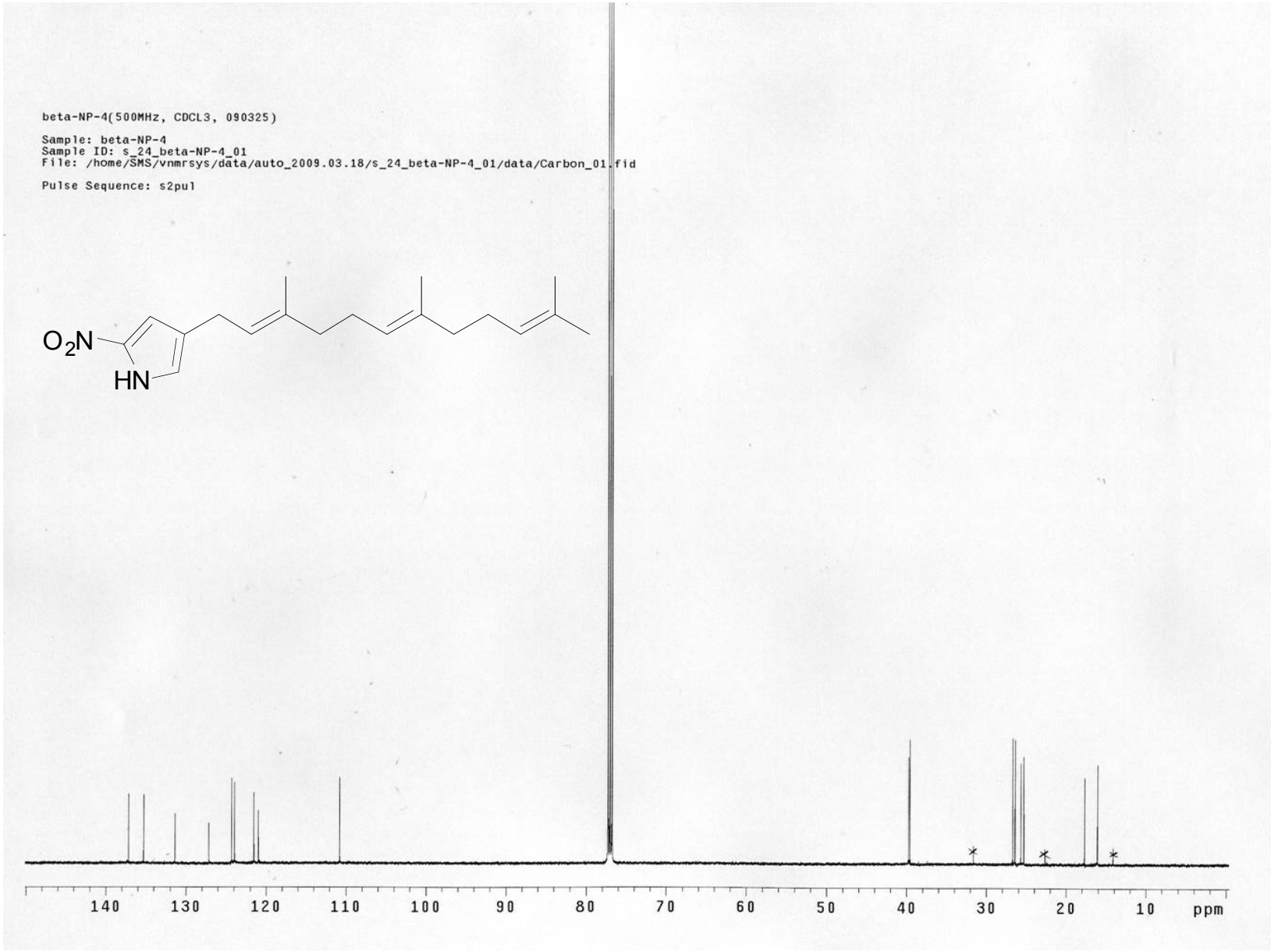


Figure S45 ^{13}C NMR spectrum of γ-farnesyl-α-nitropyrrole (**7**) in $CDCl_3$ (125 MHz).

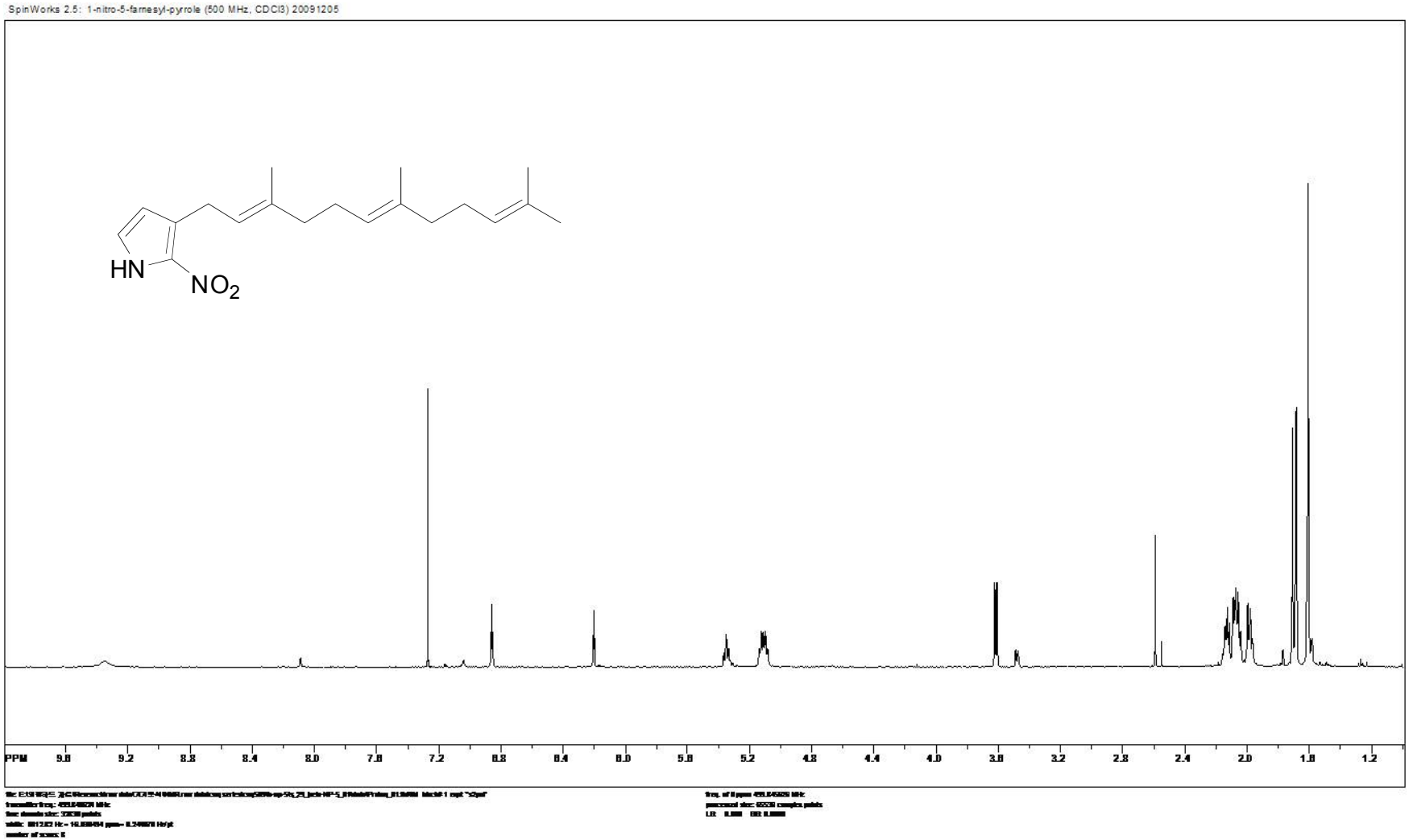


Figure S46 ^{1}H NMR spectrum of β-farnesyl-α-nitropyrrole (**8**) in $CDCl_3$ (500 MHz).

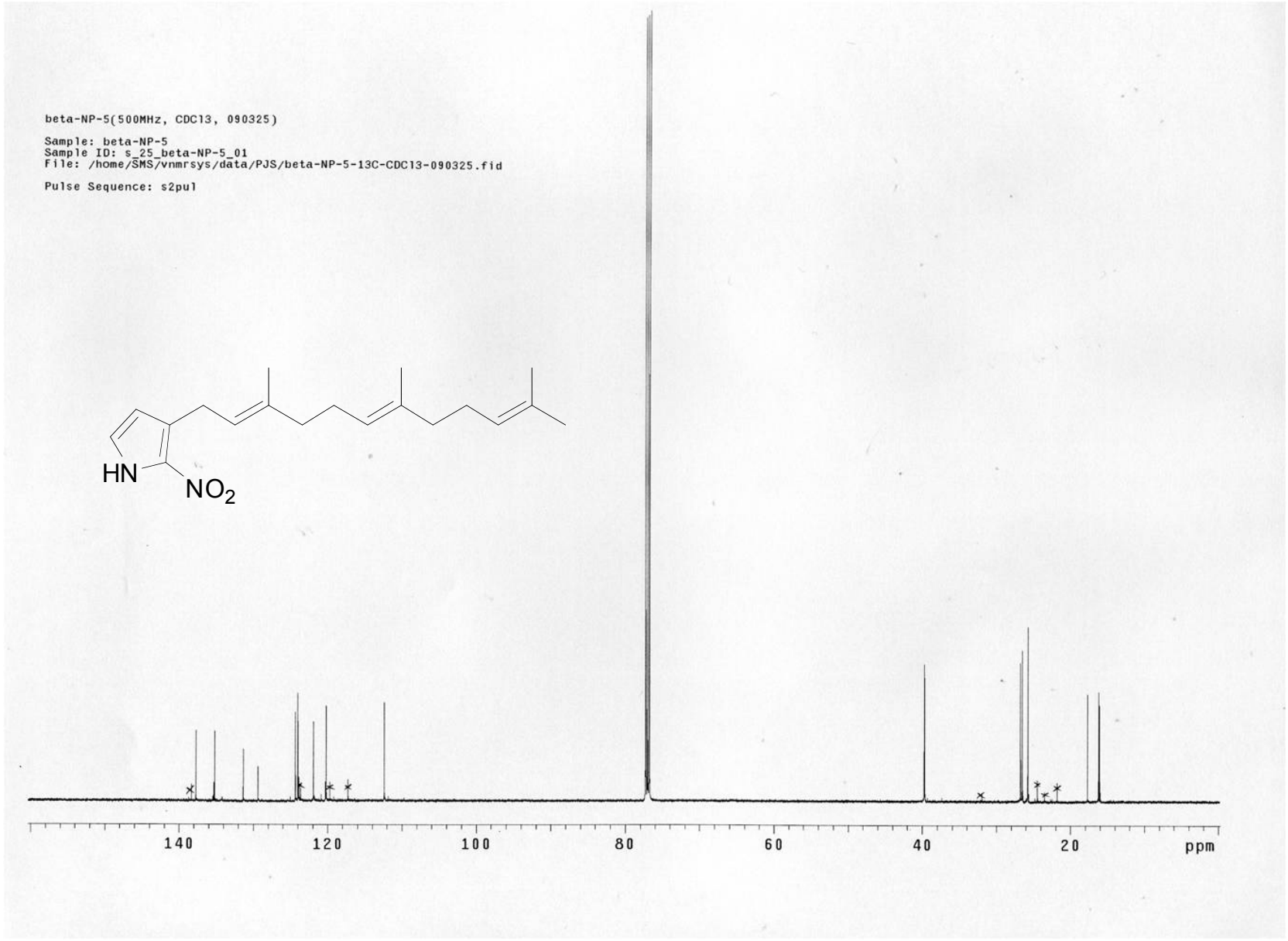


Figure S47 ^{13}C NMR spectrum of β-farnesyl-α-nitropyrrole (**8**) in $CDCl_3$ (125 MHz).

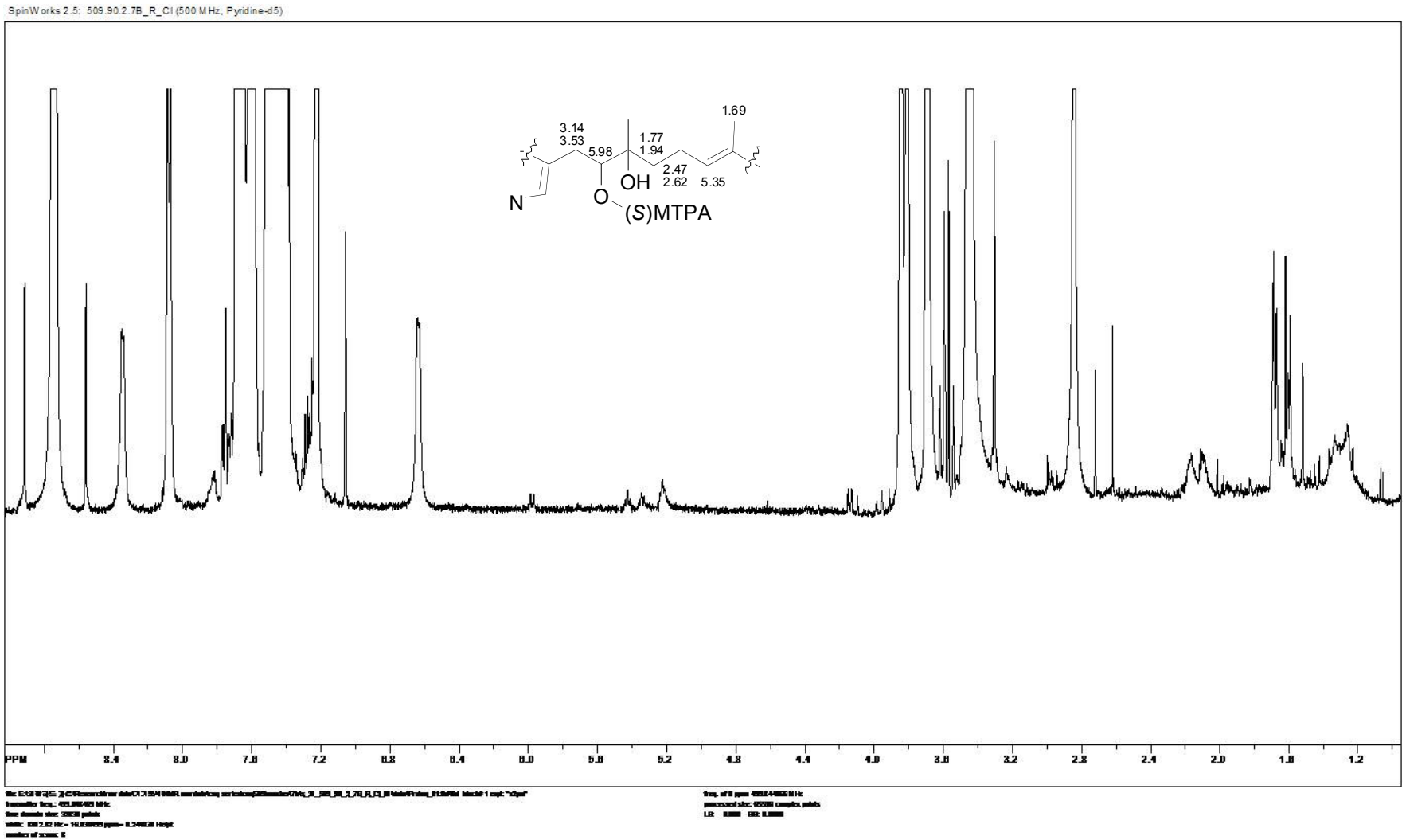


Figure S48 ^{1}H NMR spectrum of the (*S*)-Mosher ester of **1** (**9a**) in pyridine-d_5 (500 MHz).

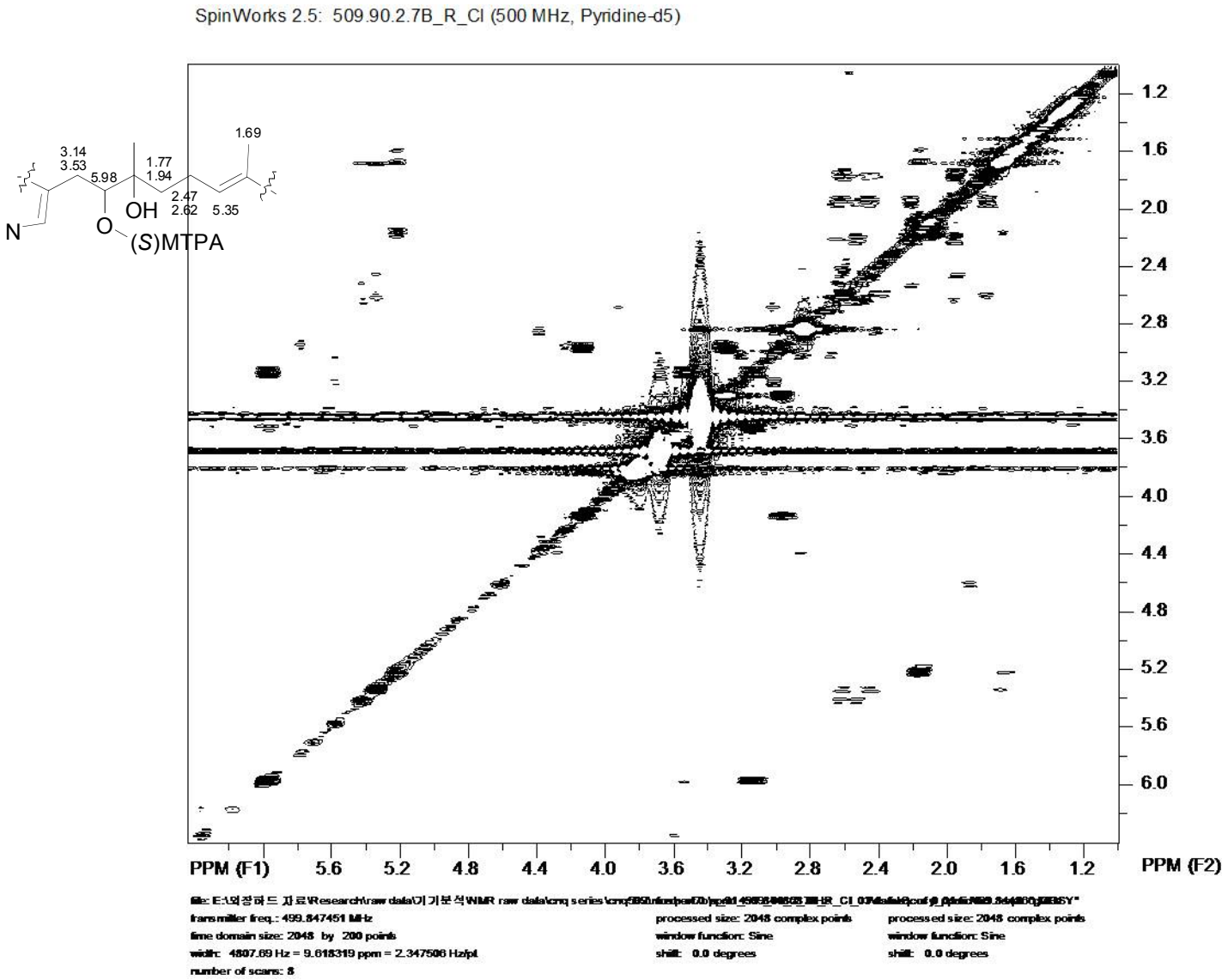


Figure S49 ^{1}H-^{1}H gCOSY spectrum of the (*S*)-Mosher ester of **1** (**9a**) in pyridine-d_5 (500 MHz).

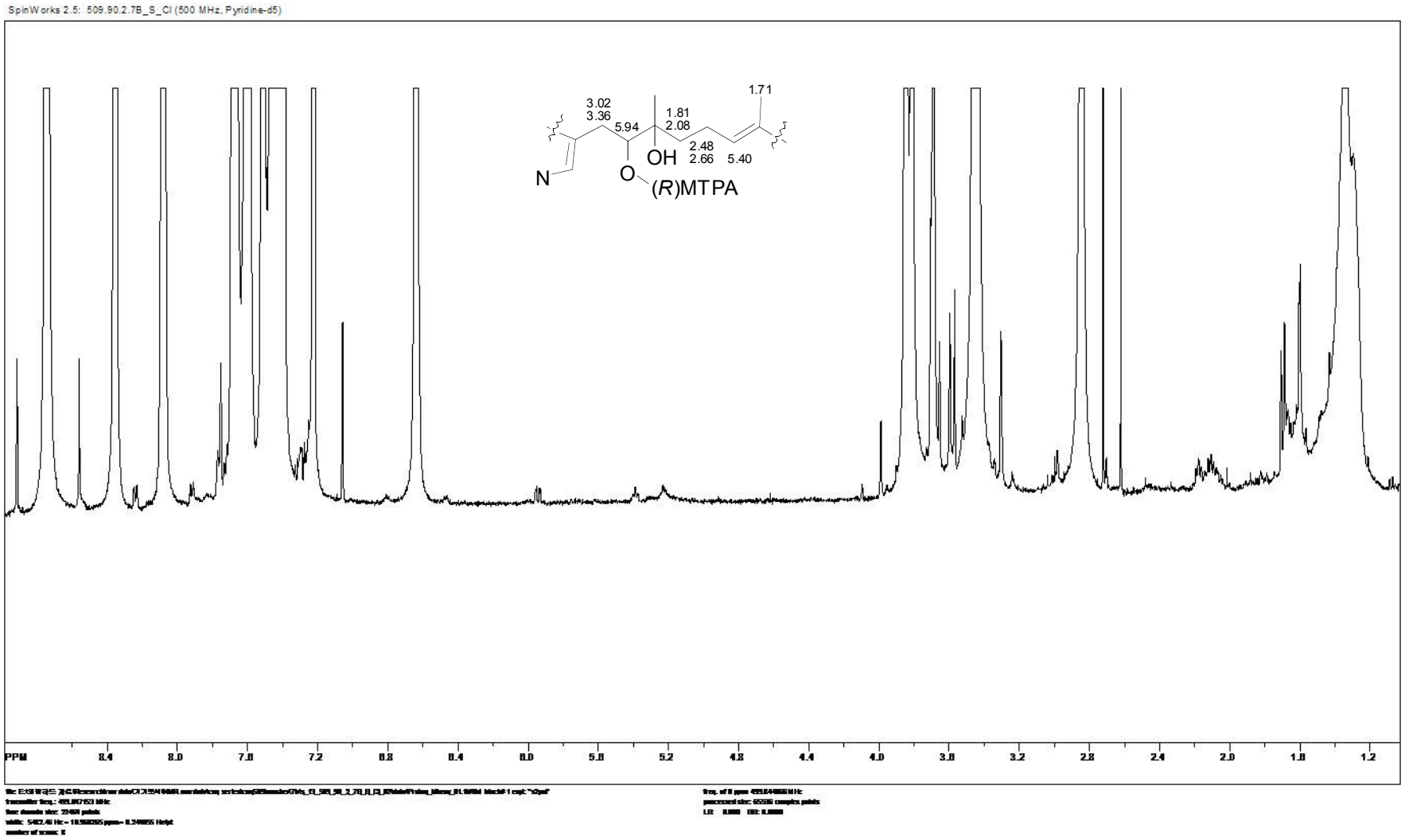


Figure S50 ^{1}H NMR spectrum of the (*R*)-Mosher ester of **1** (**9b**) in pyridine-d_5 (500 MHz).

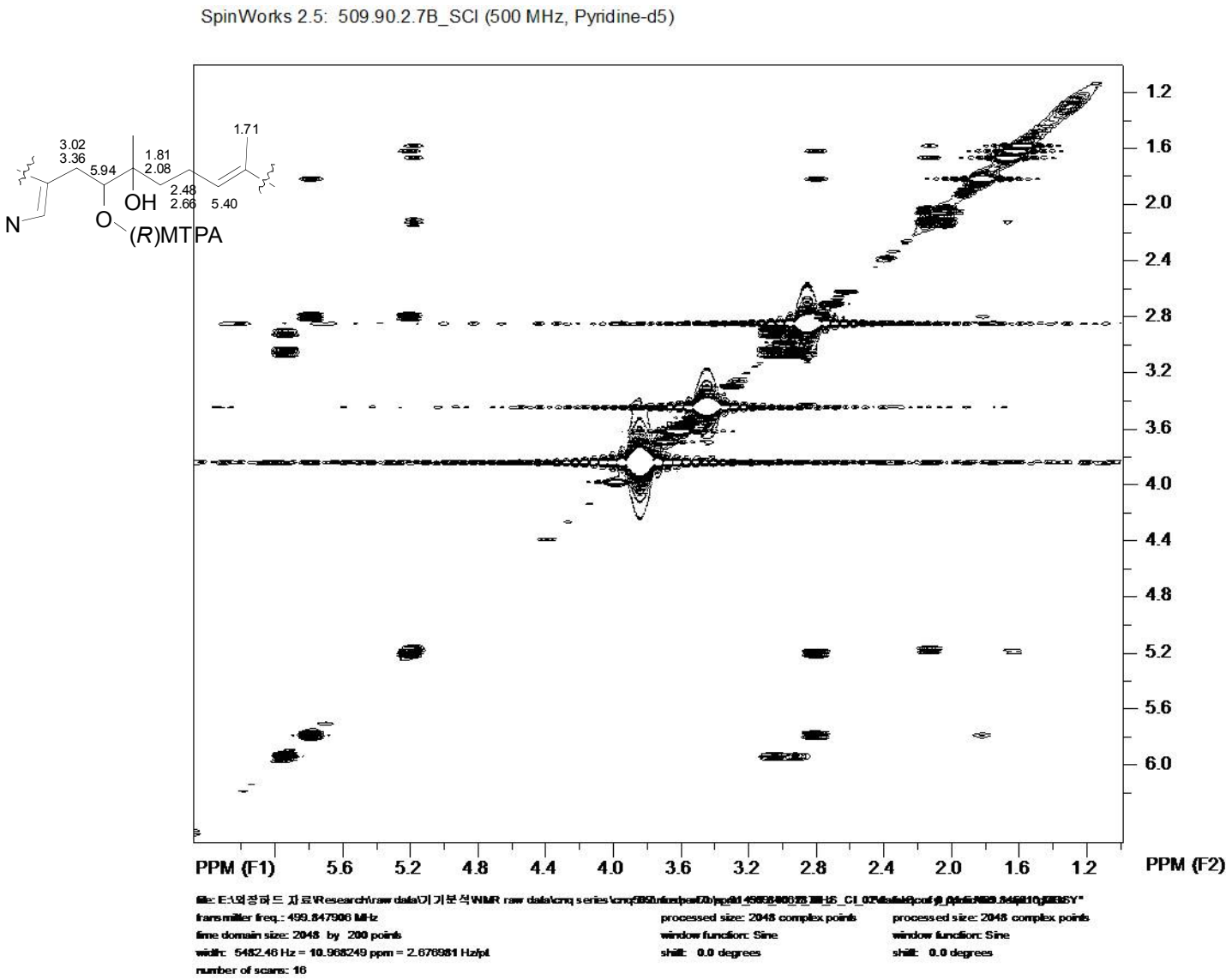


Figure S51 ^{1}H-^{1}H gCOSY spectrum of the (*R*)-Mosher ester of **1** (**9b**) in pyridine-d_5 (500 MHz).

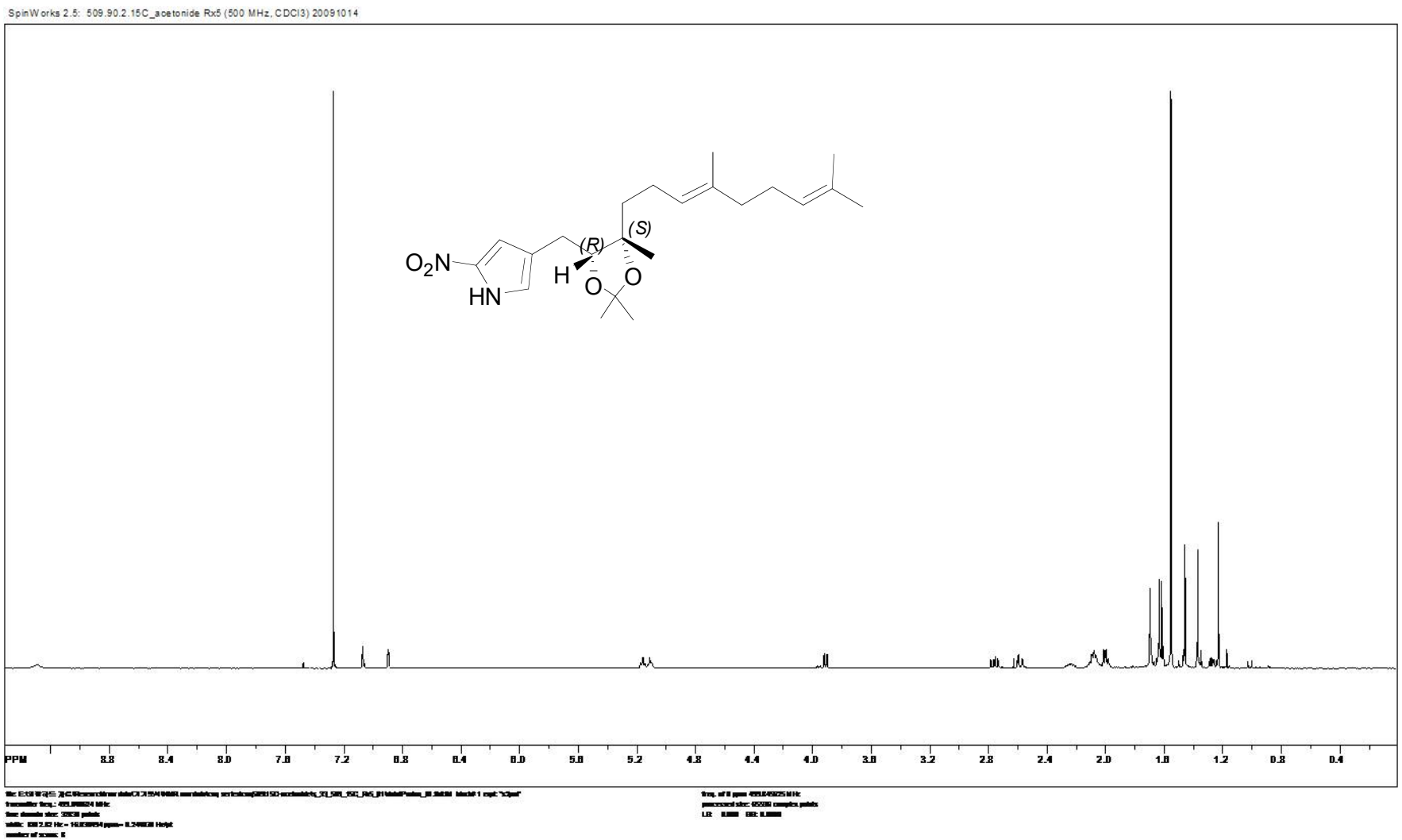


Figure S52 ^{1}H NMR spectrum of the acetonide derivative of **2** (**10**) in $CDCl_3$ (500 MHz).

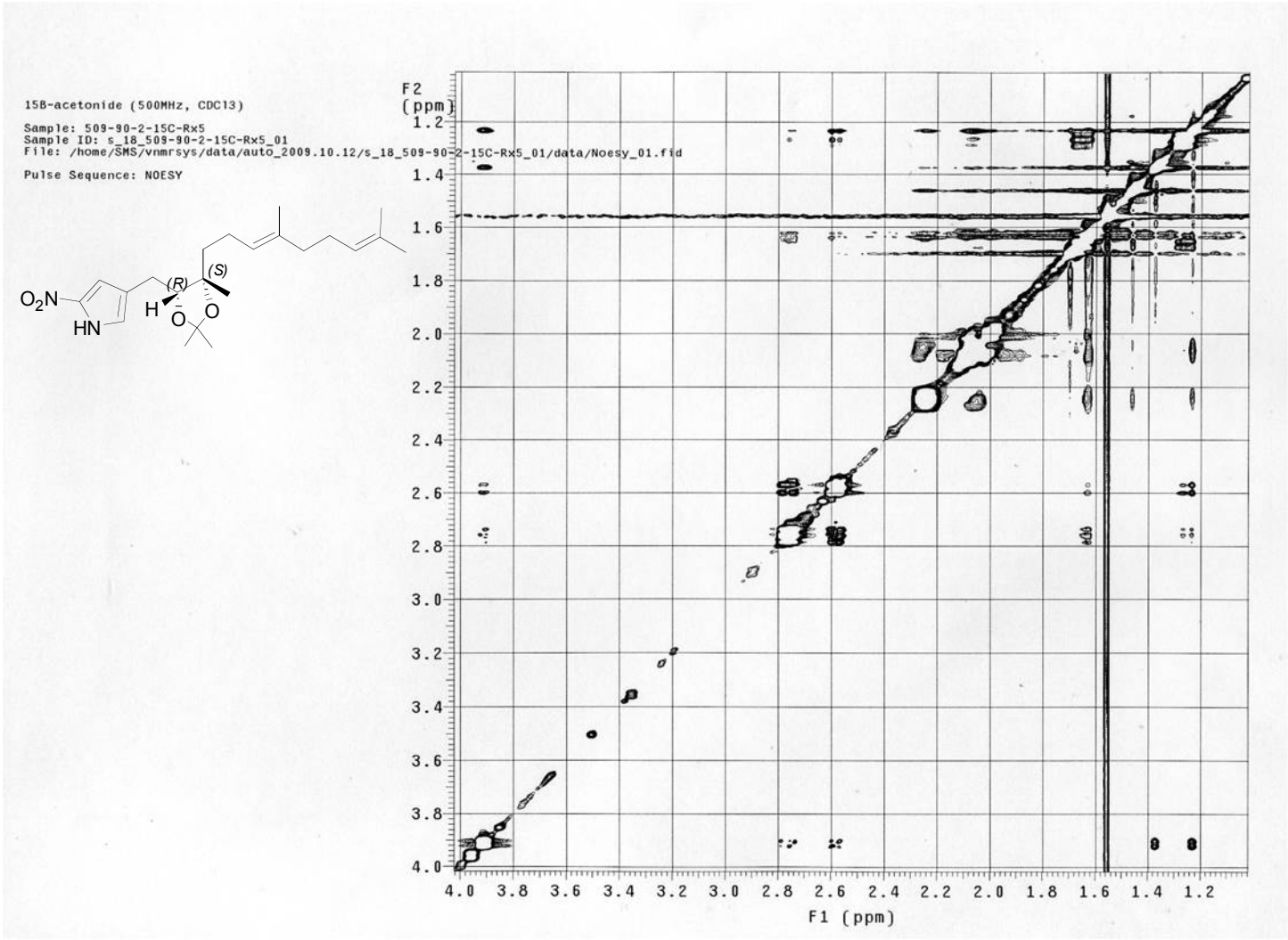


Figure S53 2D NOESY spectrum of the acetonide derivative of **2** (**10**) in $CDCl_3$ (500 MHz).

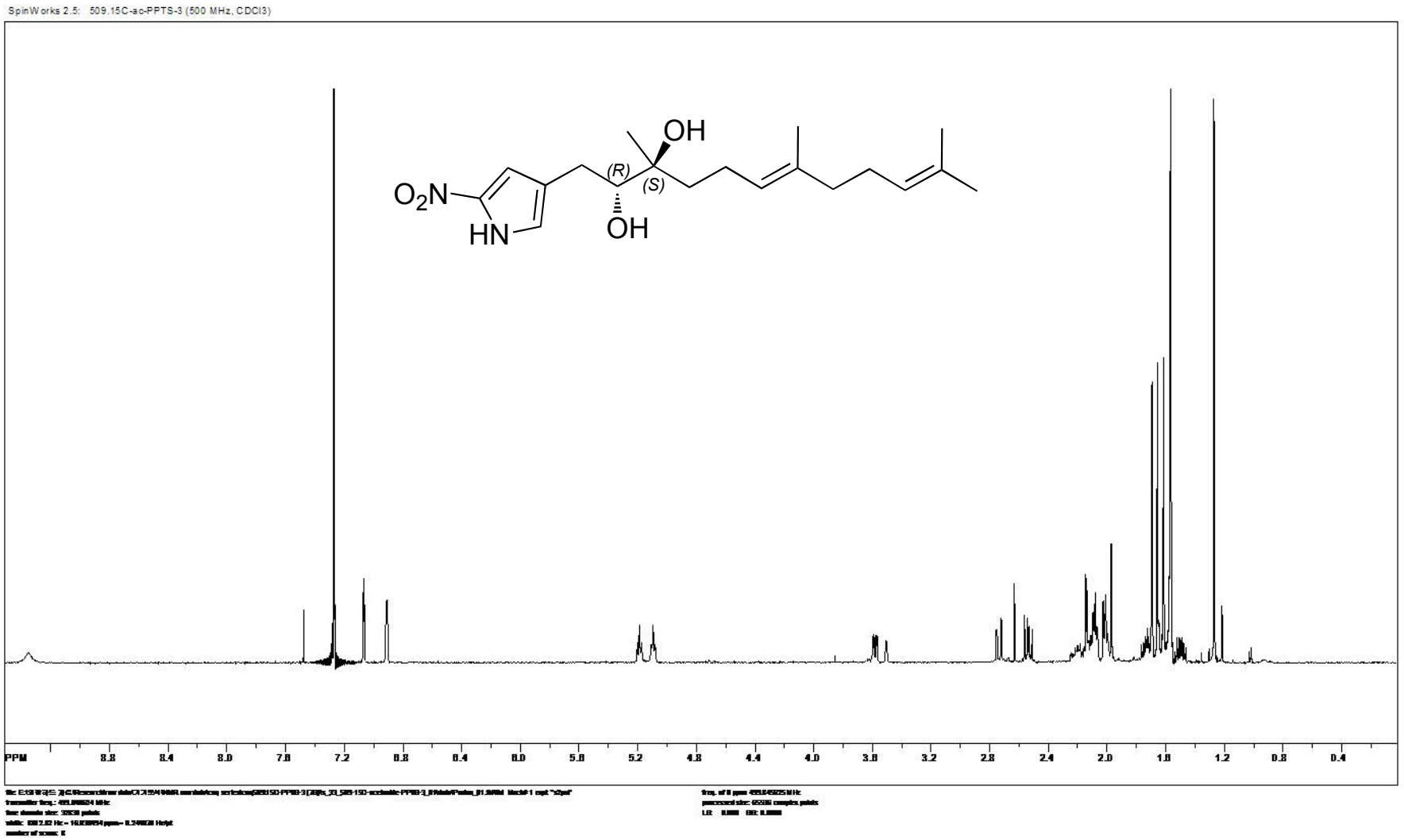


Figure S54 ^{1}H NMR spectrum of the diol derivative of **2** (**11**) in $CDCl_3$ (500 MHz).

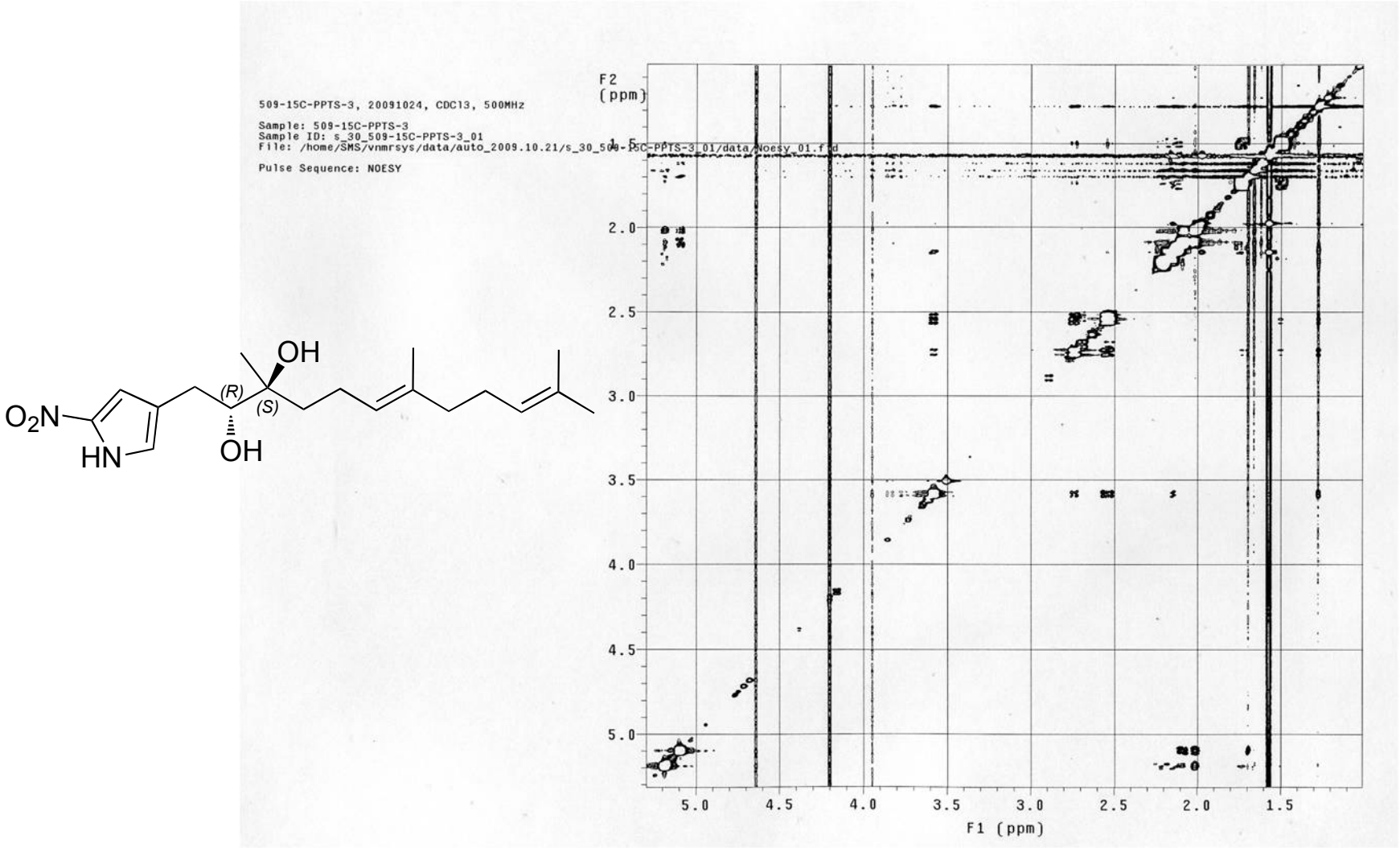


Figure S55 2D NOESY spectrum of the diol derivative of **2** (**11**) in $CDCl_3$ (500 MHz).

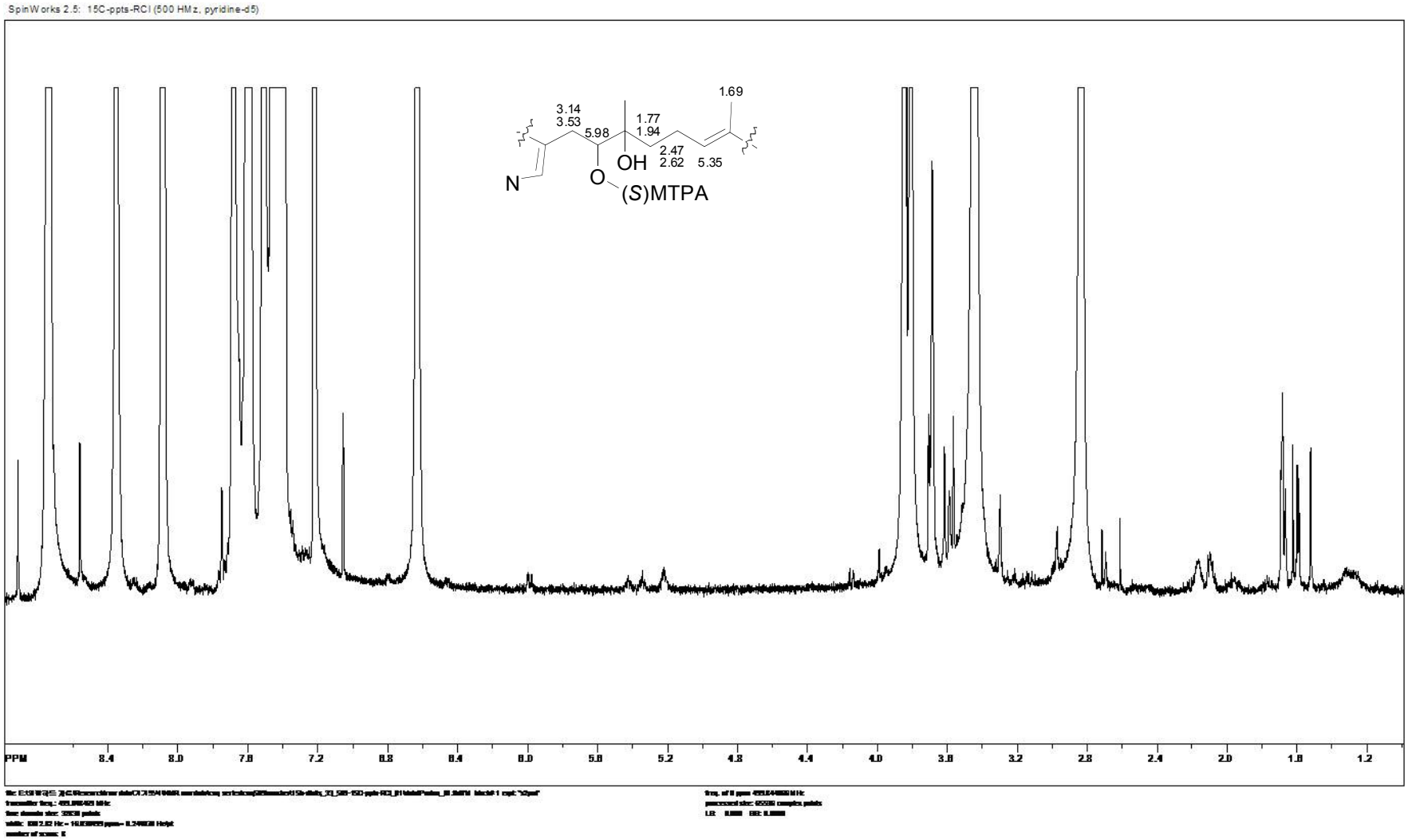


Figure S56 ^{1}H NMR spectrum of the (S)-Mosher ester of **11** in pyridine-d_5 (500 MHz).

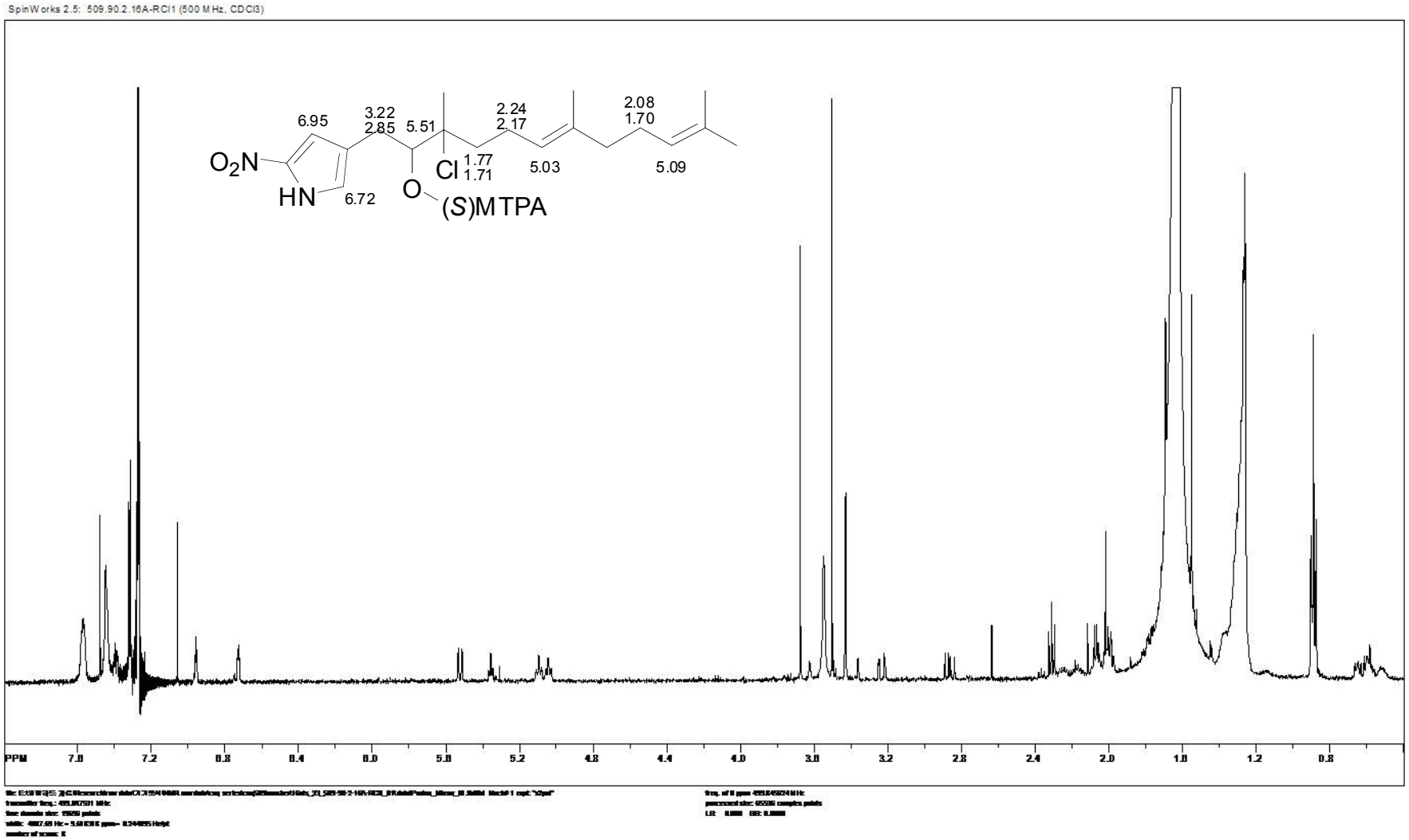


Figure S57 ^{1}H NMR spectrum of the (*S*)-Mosher ester of **3** (**12a**) in pyridine-d_5 (500 MHz).

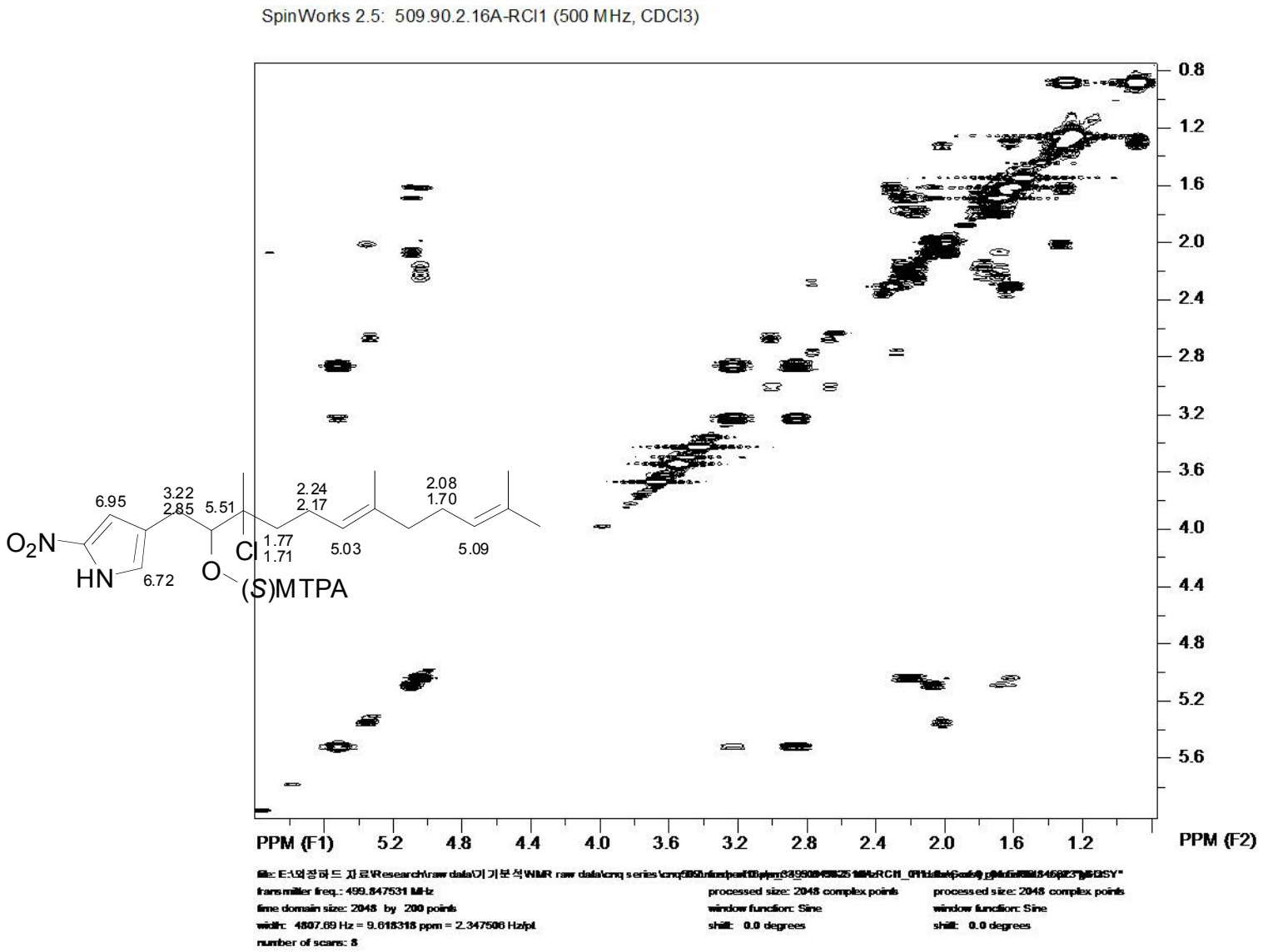


Figure S58 ^{1}H-^{1}H gCOSY spectrum of the (*S*)-Mosher ester of **3** (**12a**) in pyridine-d_5 (500 MHz).

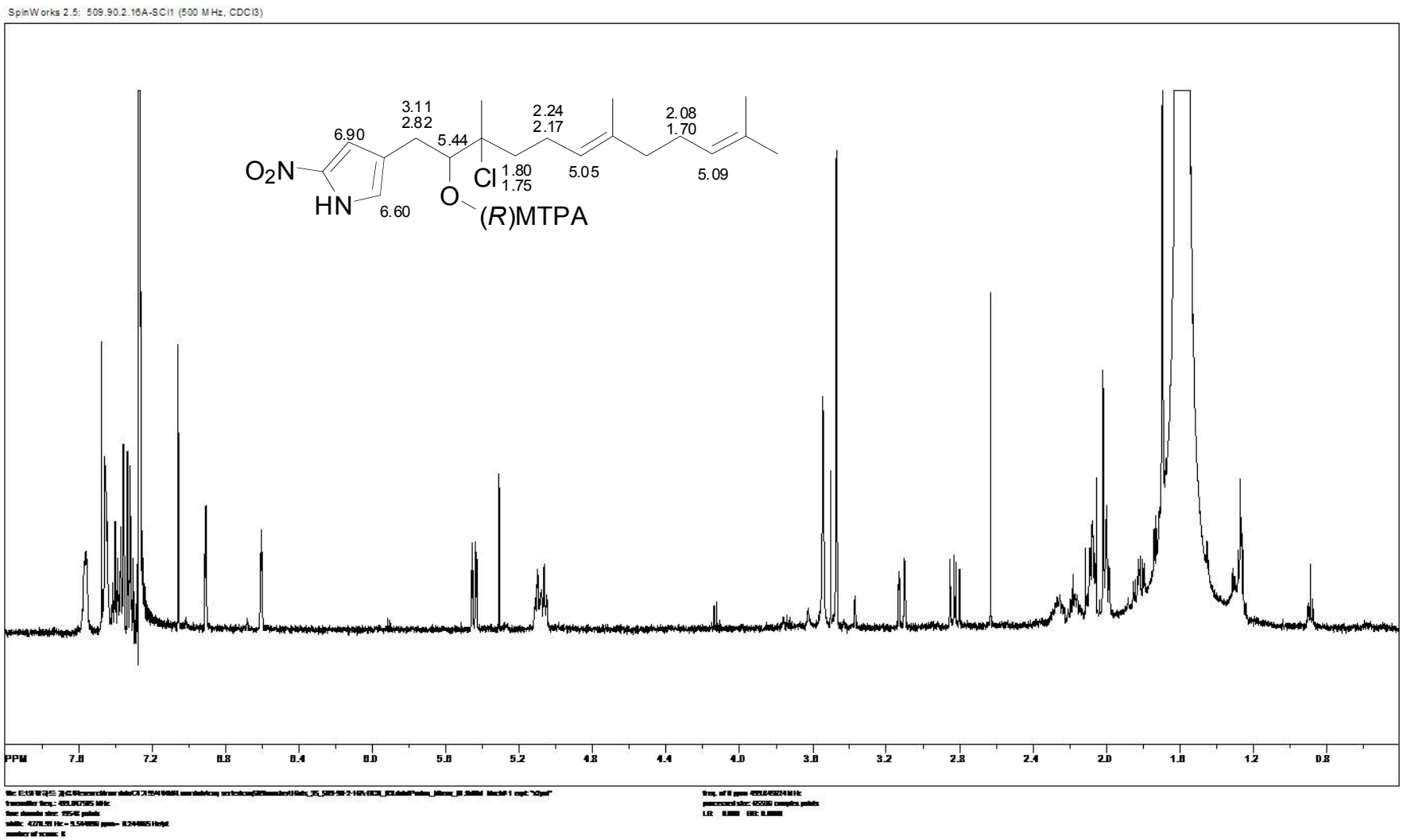


Figure S59 ^{1}H NMR spectrum of the (*R*)-Mosher ester of **3** (**12b**) in pyridine-d_5 (500 MHz).

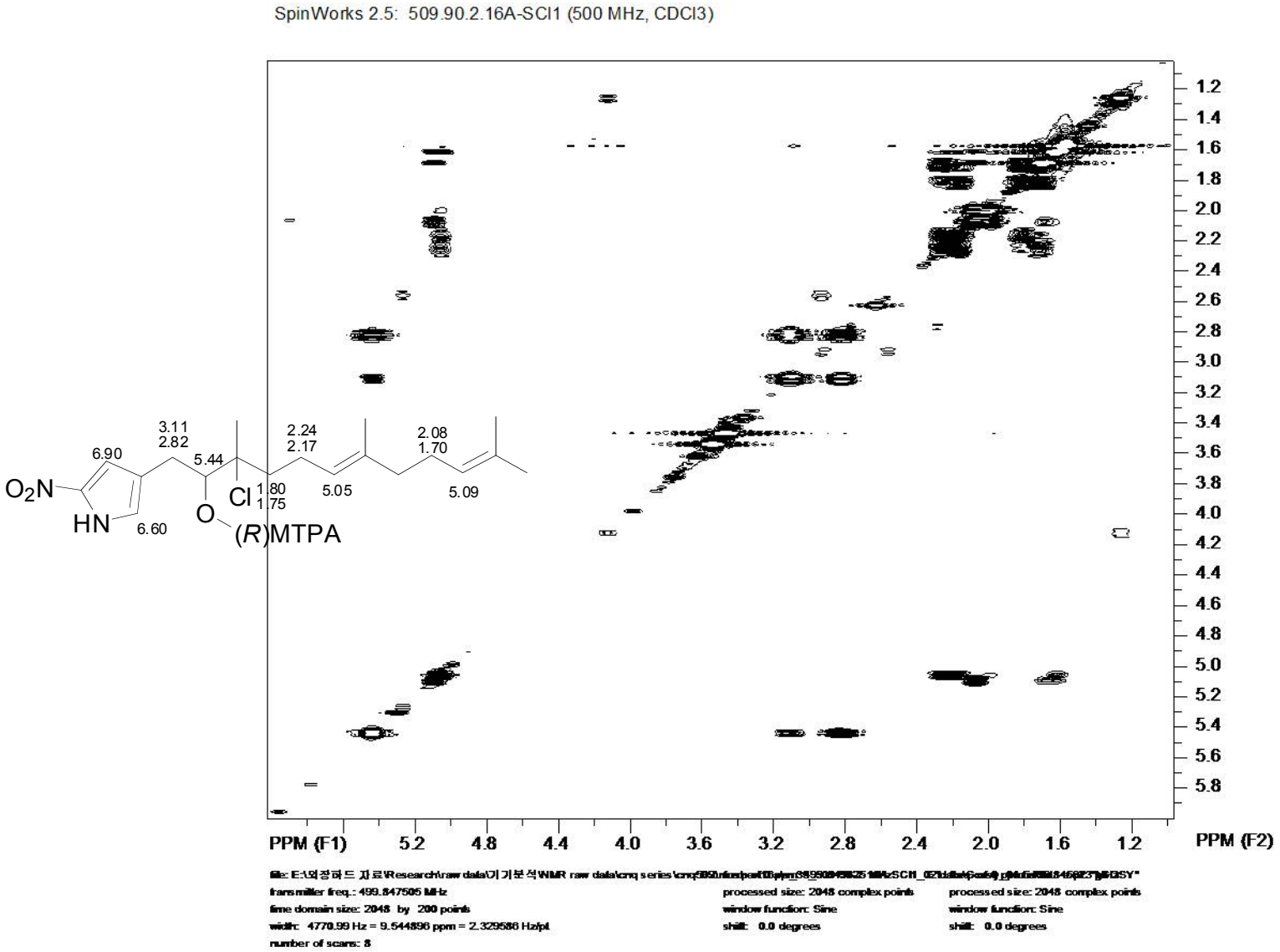


Figure S60 ^{1}H-^{1}H gCOSY spectrum of the (*R*)-Mosher ester of **3** (**12b**) in pyridine-d_5 (500 MHz).

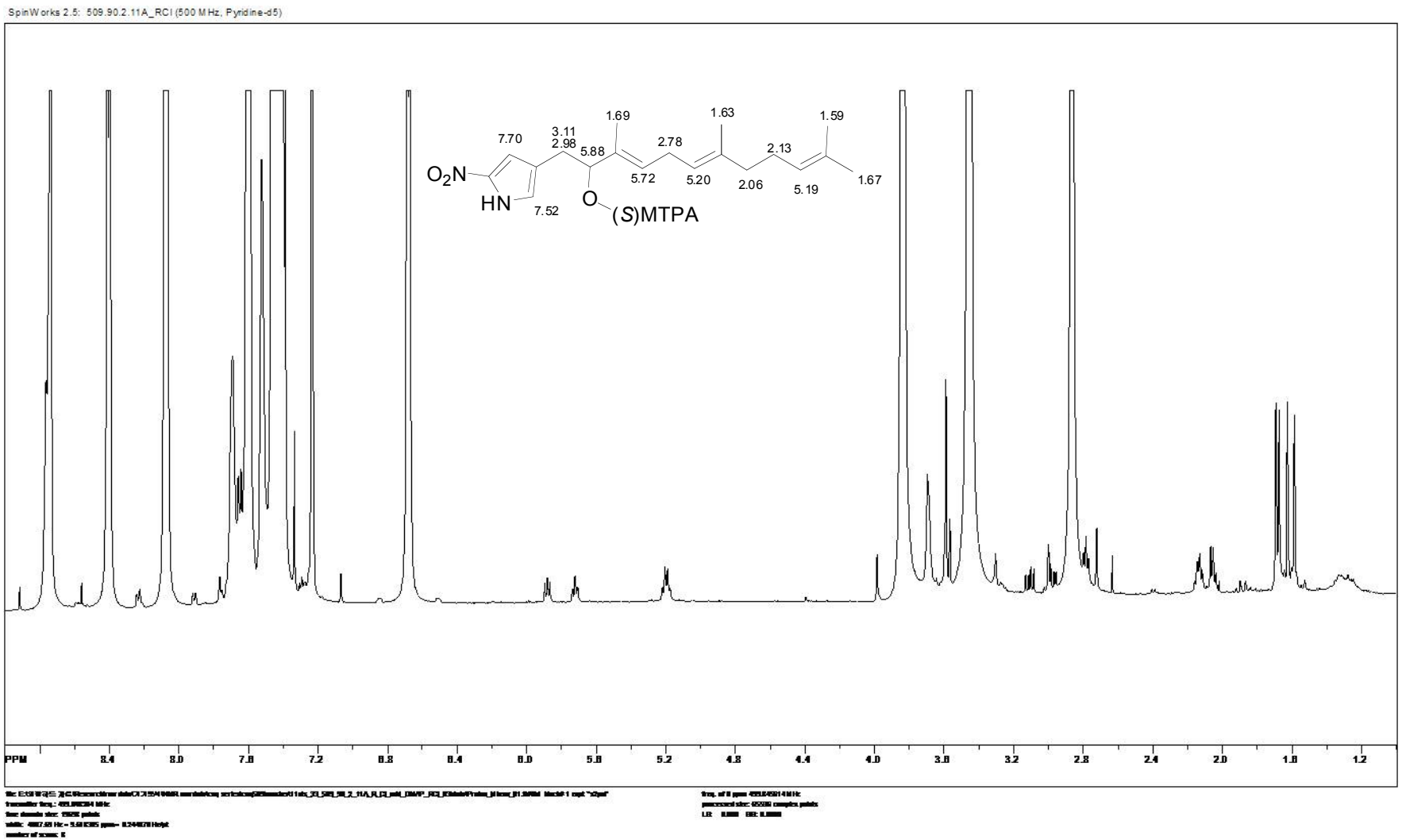


Figure S61 ^{1}H NMR spectrum of the (*S*)-Mosher ester of **4** (**13a**) in pyridine-d_5 (500 MHz).

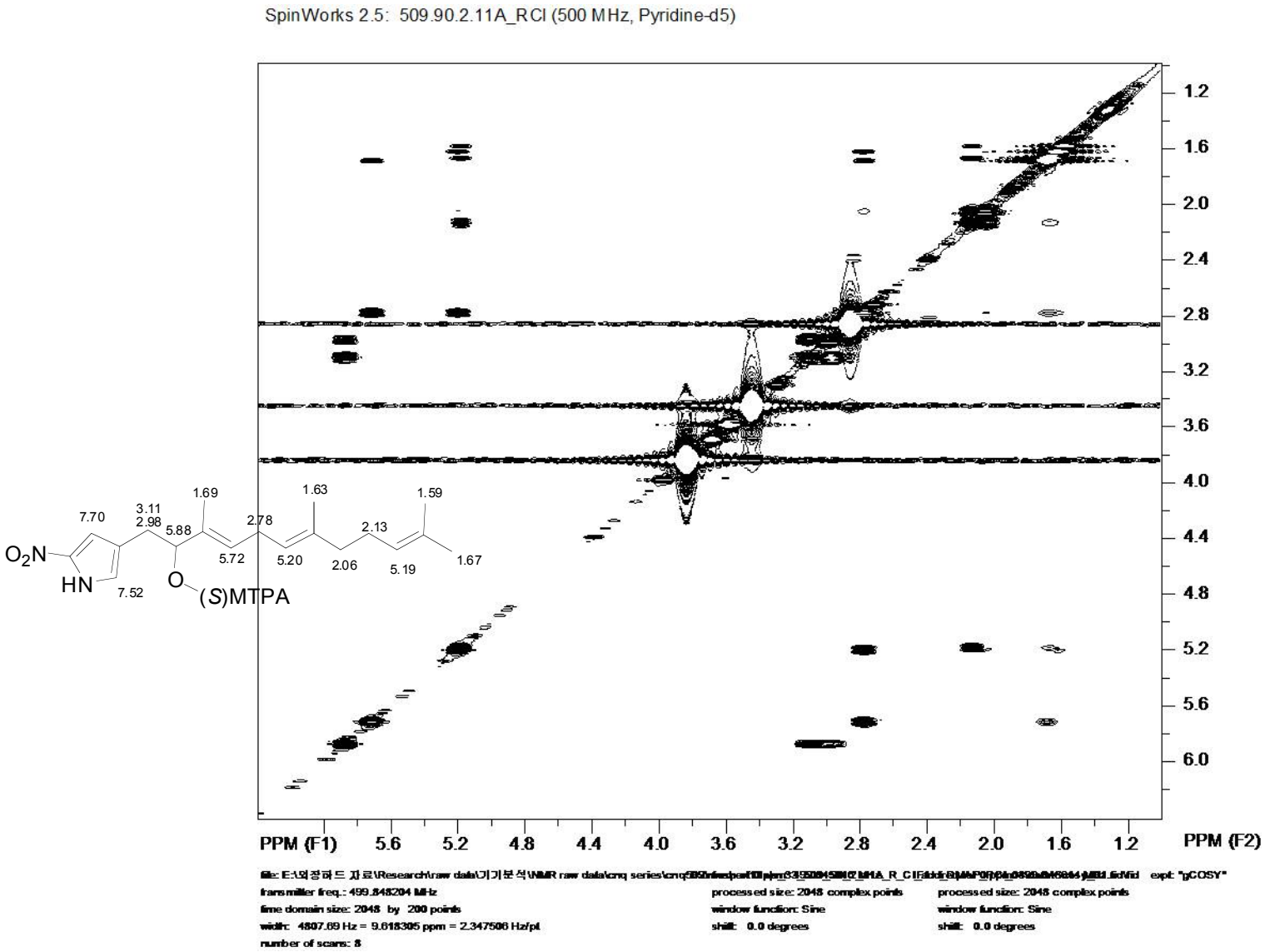


Figure S62 ^{1}H-^{1}H gCOSY spectrum of the (*S*)-Mosher ester of **4** (**13a**) in pyridine-d_5 (500 MHz).

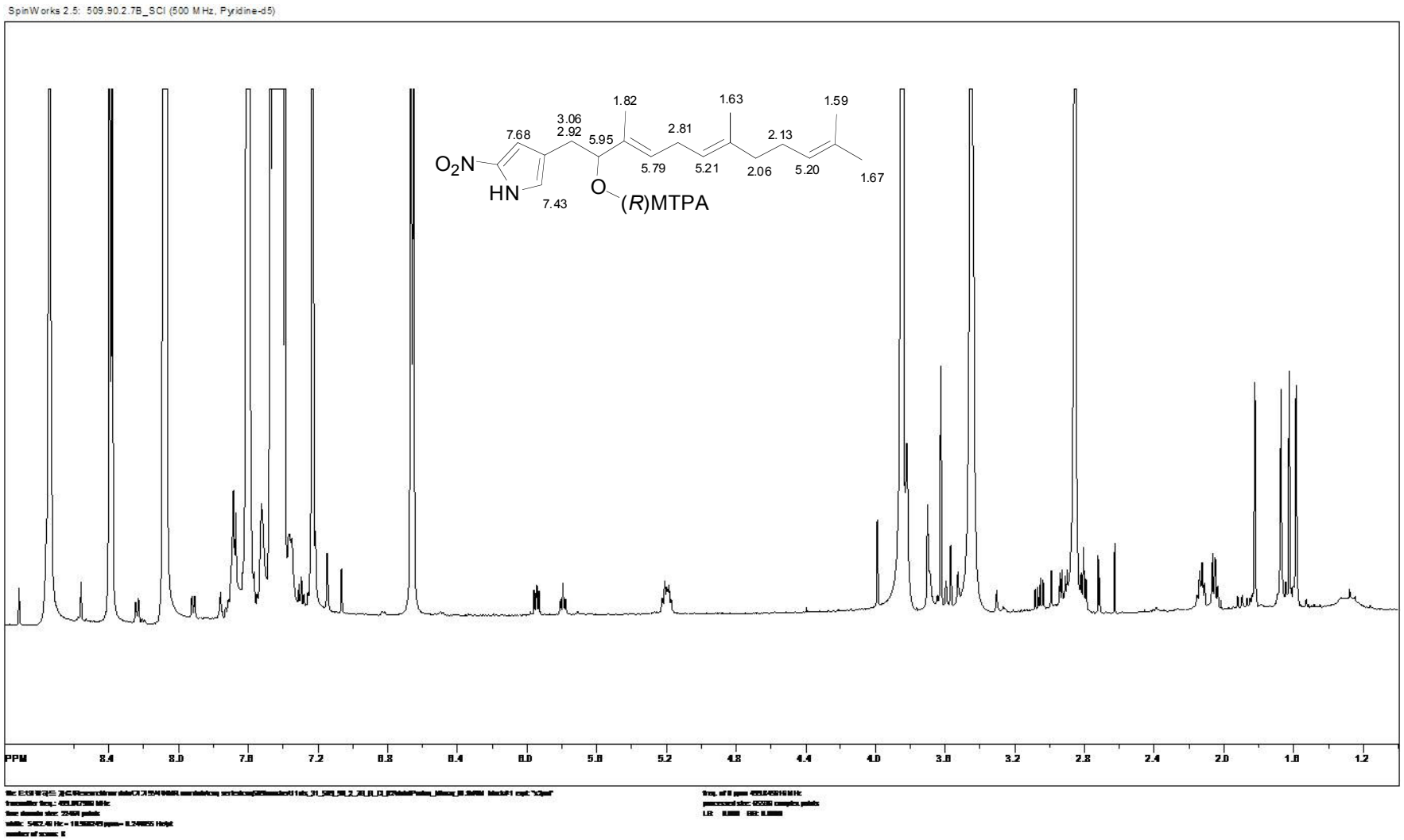


Figure S63 ^{1}H NMR spectrum of the (*R*)-Mosher ester of **4** (**13b**) in pyridine-d_5 (500 MHz).

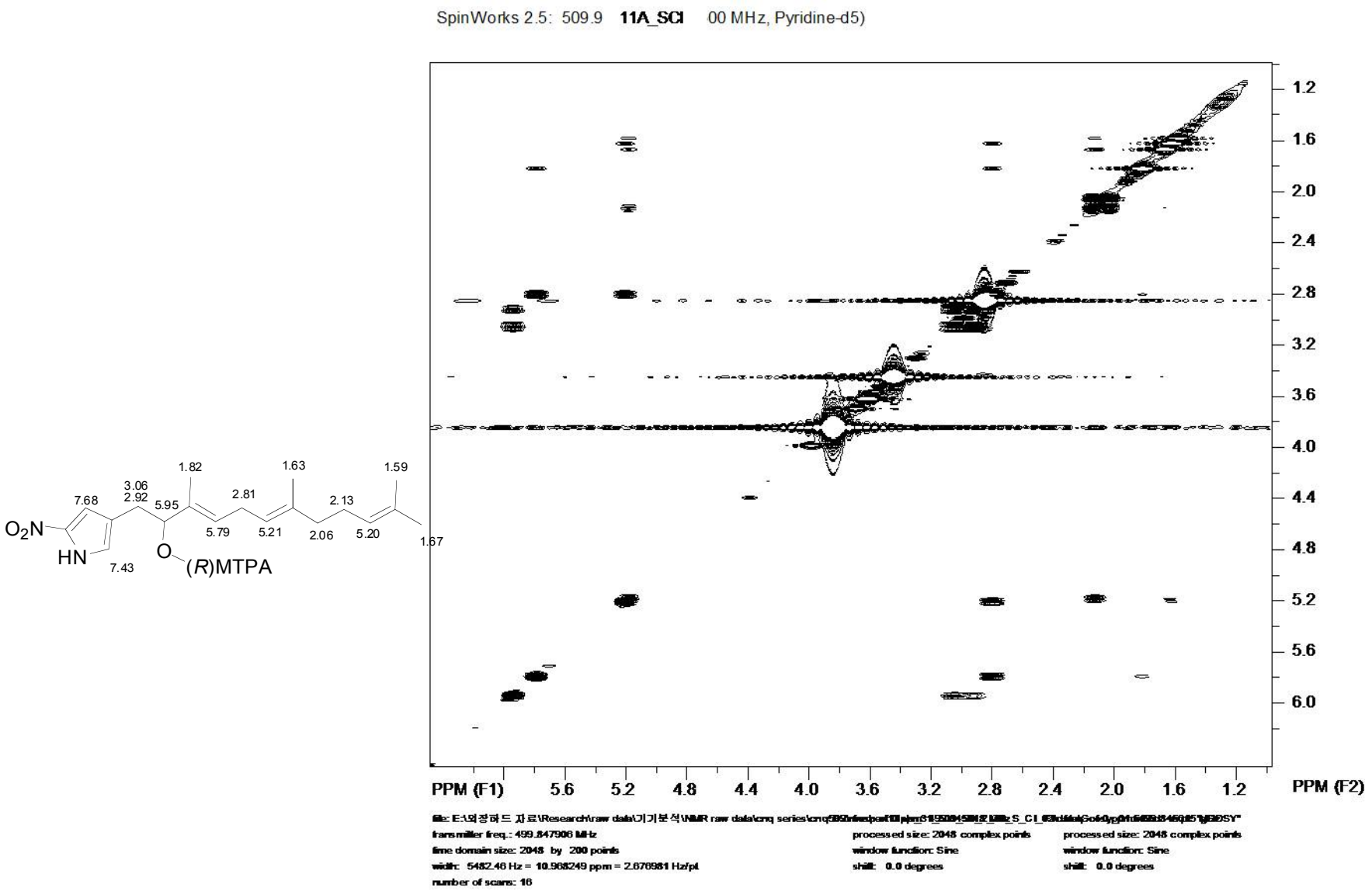


Figure S64 ^{1}H-^{1}H gCOSY spectrum of the (*R*)-Mosher ester of **4** (**13b**) in pyridine-d_5 (500 MHz).

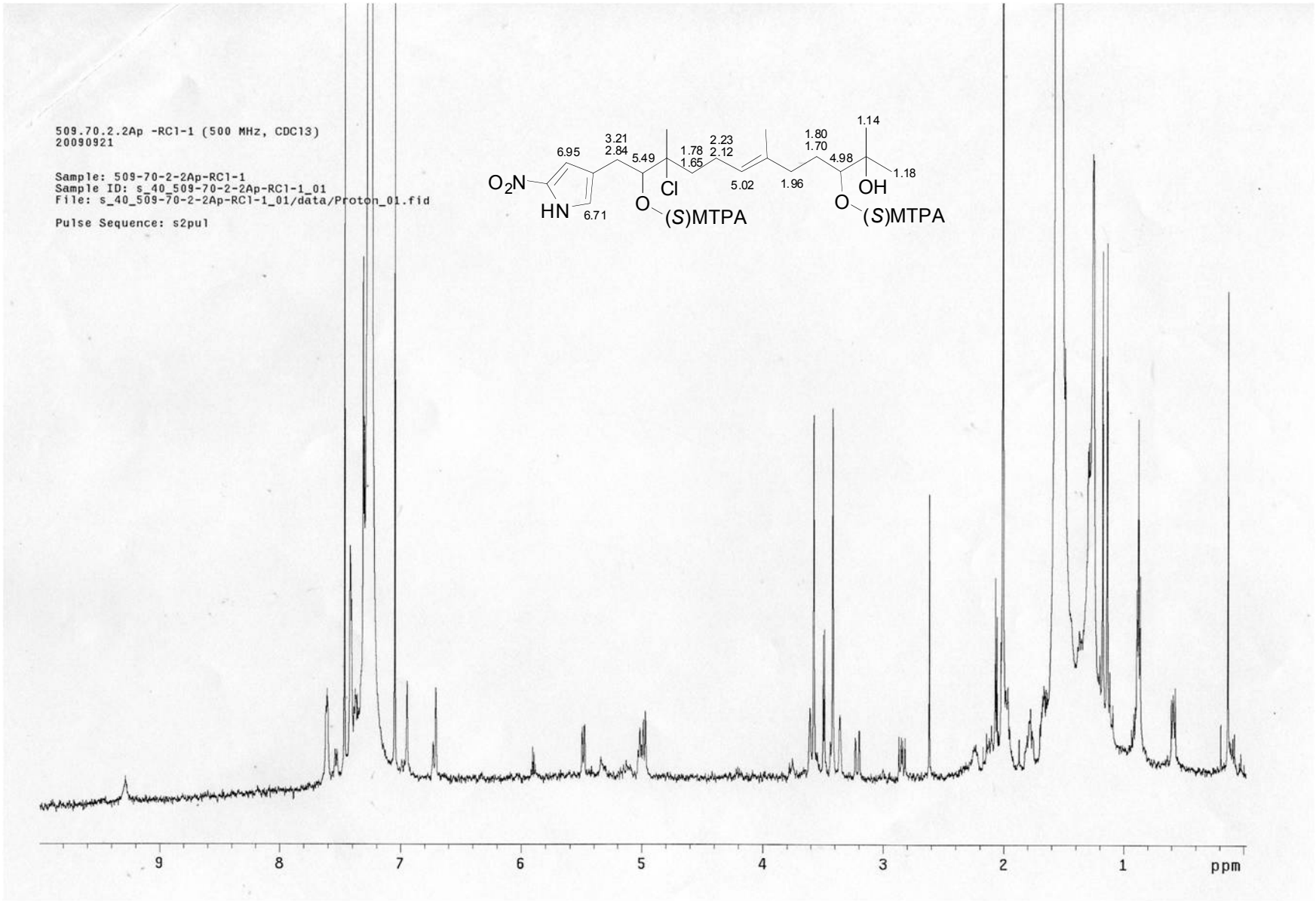


Figure S65 ^{1}H NMR spectrum of the *bis*-(*S*)-Mosher ester of **5** (**14a**) in pyridine-d_5 (500 MHz).

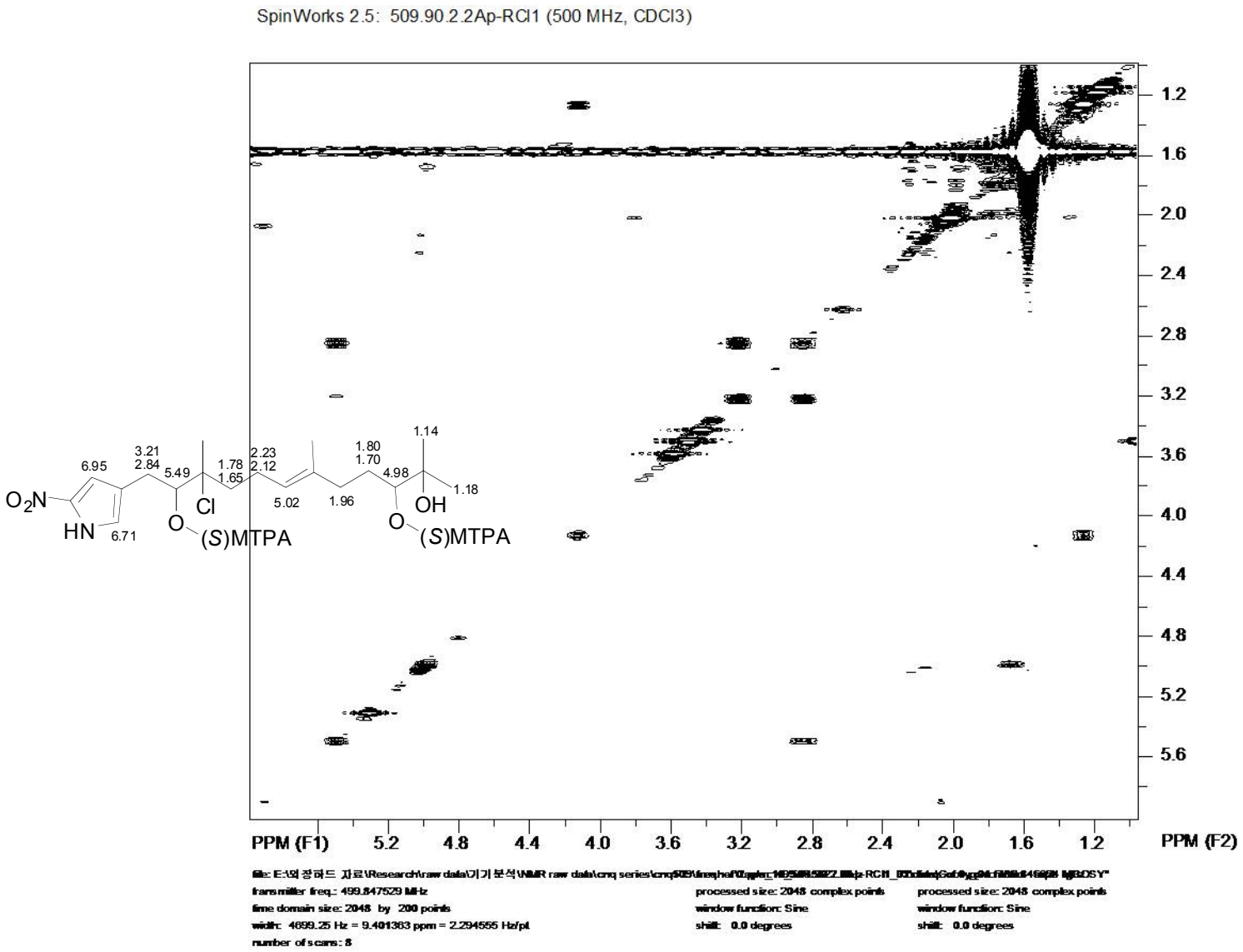


Figure S66 ^{1}H-^{1}H gCOSY spectrum of the *bis*-(*S*)-Mosher ester of **5** (**14a**) in pyridine-d_5 (500 MHz).

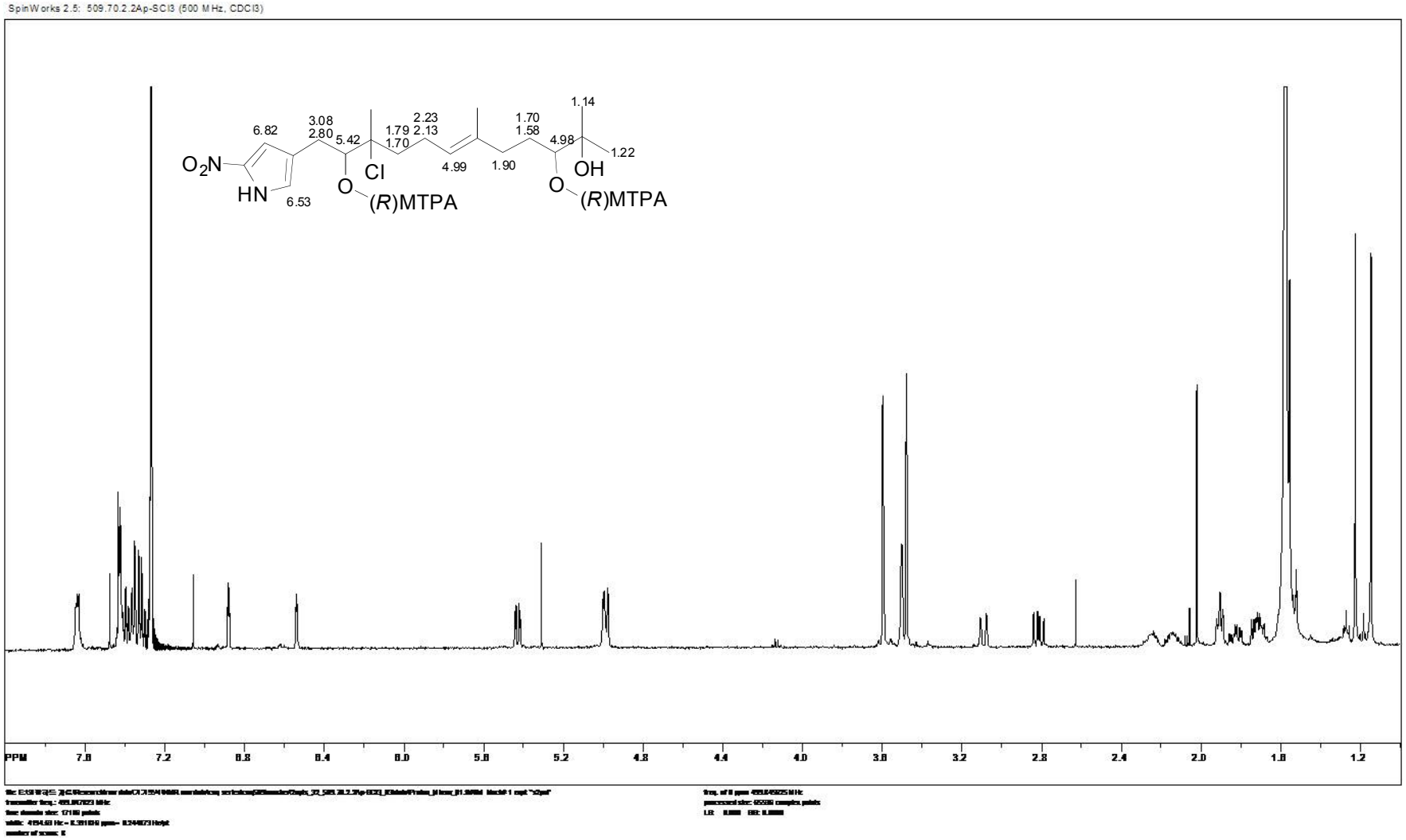


Figure S67 ^{1}H NMR spectrum of the *bis*-(*R*)-Mosher ester of **5** (**14b**) in pyridine-d_5 (500 MHz).

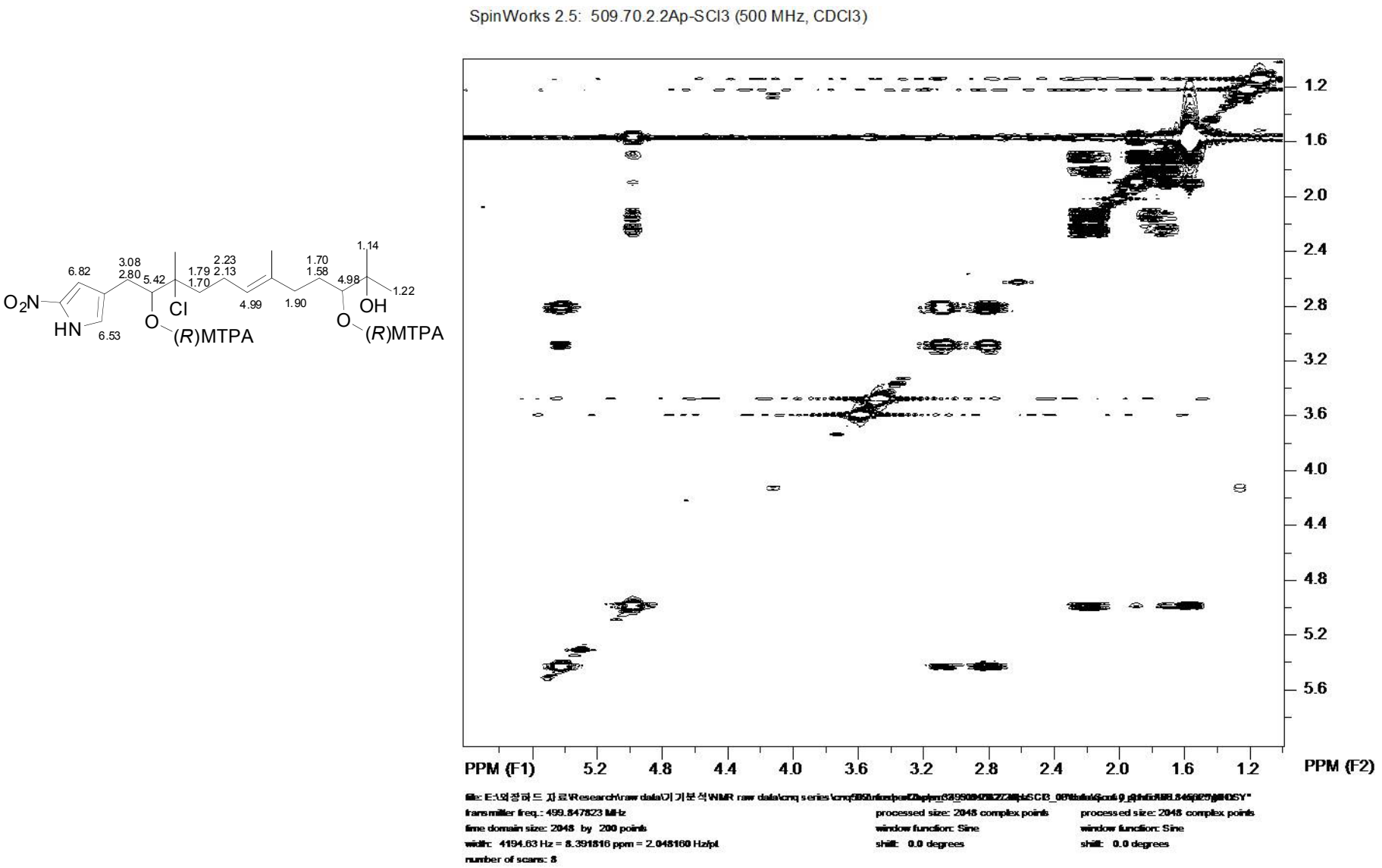


Figure S68 ^{1}H-^{1}H gCOSY spectrum of the *bis*-(*R*)-Mosher ester of **5** (**14b**) in pyridine-d_5 (500 MHz).