

# Supporting information

## Anti-Infective Discorhabdins from a Deep-Water Alaskan Sponge of the Genus *Latrunculia* †

MinKyun Na,<sup>‡,§</sup> Yuanqing Ding,<sup>‡</sup> Bin Wang,<sup>‡</sup> Babu L. Tekwani,<sup>‡</sup> Raymond F. Schinazi,<sup>⊥</sup> Scott Franzblau,<sup>||</sup> Michelle Kelly,<sup>▽</sup> Robert Stone,<sup>○</sup> Xing-Cong Li,<sup>‡</sup> Daneel Ferreira,<sup>‡</sup> and Mark T. Hamann<sup>‡,\*</sup>

*Department of Pharmacognosy and the National Center for Natural Products Research (NCNPR), School of Pharmacy, The University of Mississippi, University, MS 38677, USA, College of Pharmacy, Yeungnam University, Gyeongsan, Gyeongbuk 712-749, South Korea, Department of Pediatrics, Emory University/VA Medical Center, Decatur, GA 30033, USA, Institute for Tuberculosis Research, College of Pharmacy, University of Illinois at Chicago, Chicago, Illinois 60607, USA, National Centre for Aquatic Biodiversity and Biosecurity, National Institute of Water and Atmospheric Research (NIWA), Private Bag 109695, Auckland, New Zealand, Auke Bay Laboratories, Alaska Fisheries Science Center, NOAA Fisheries, 17109 Point Lena Loop Road, Juneau, AK 99801, USA*

† Dedicated to the late Dr. John W. Daly of NIDDK, NIH, Bethesda, Maryland and to the late Dr. Richard E. Moore of the University of Hawaii at Manoa for their pioneering work on bioactive natural products.

\* To whom correspondence should be addressed. Tel: +1-662-915-5730. Fax: +1-662-915-6975. E-mail: [mthamann@olemiss.edu](mailto:mthamann@olemiss.edu).

‡ The University of Mississippi.

§ Yeungnam University.

⊥ Emory University/VA Medical Center.

|| University of Illinois at Chicago.

▽ NIWA.

○ Alaska Fisheries.

# LC-MS spectrum of dihydrodiscorhabdin B (1)

## Display Report

### Analysis Info

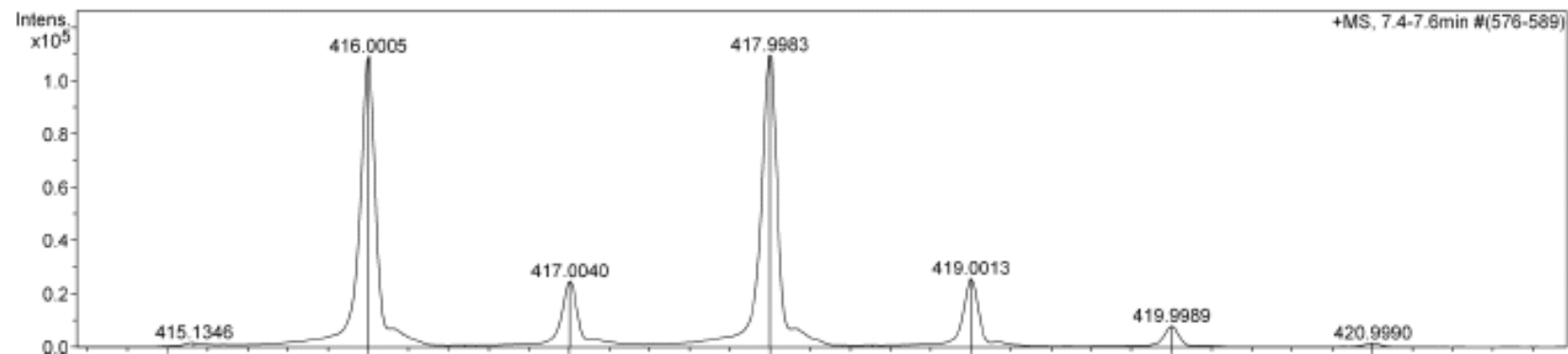
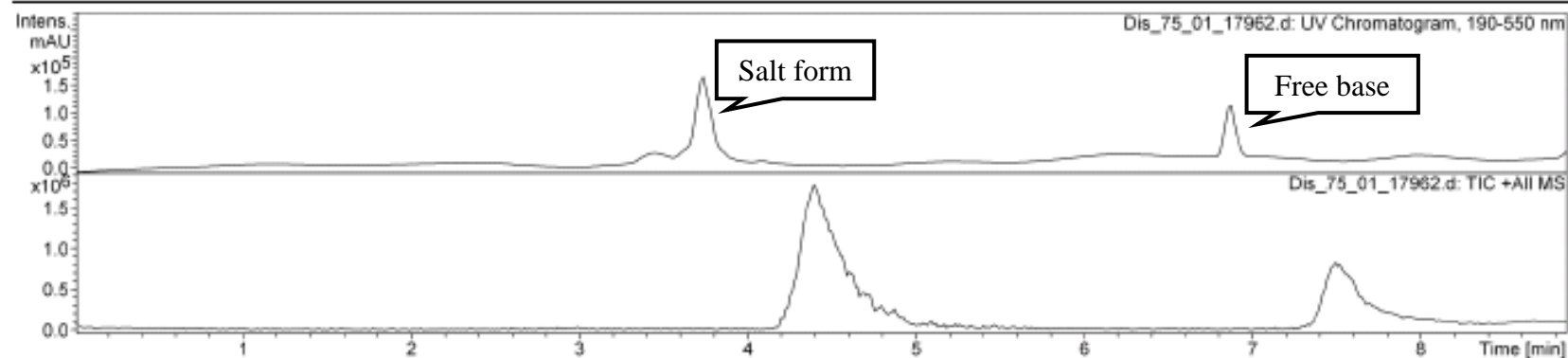
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Method Compound test.m  
Sample Name Dis  
Comment

Acquisition Date 6/18/2008 2:54:17 PM

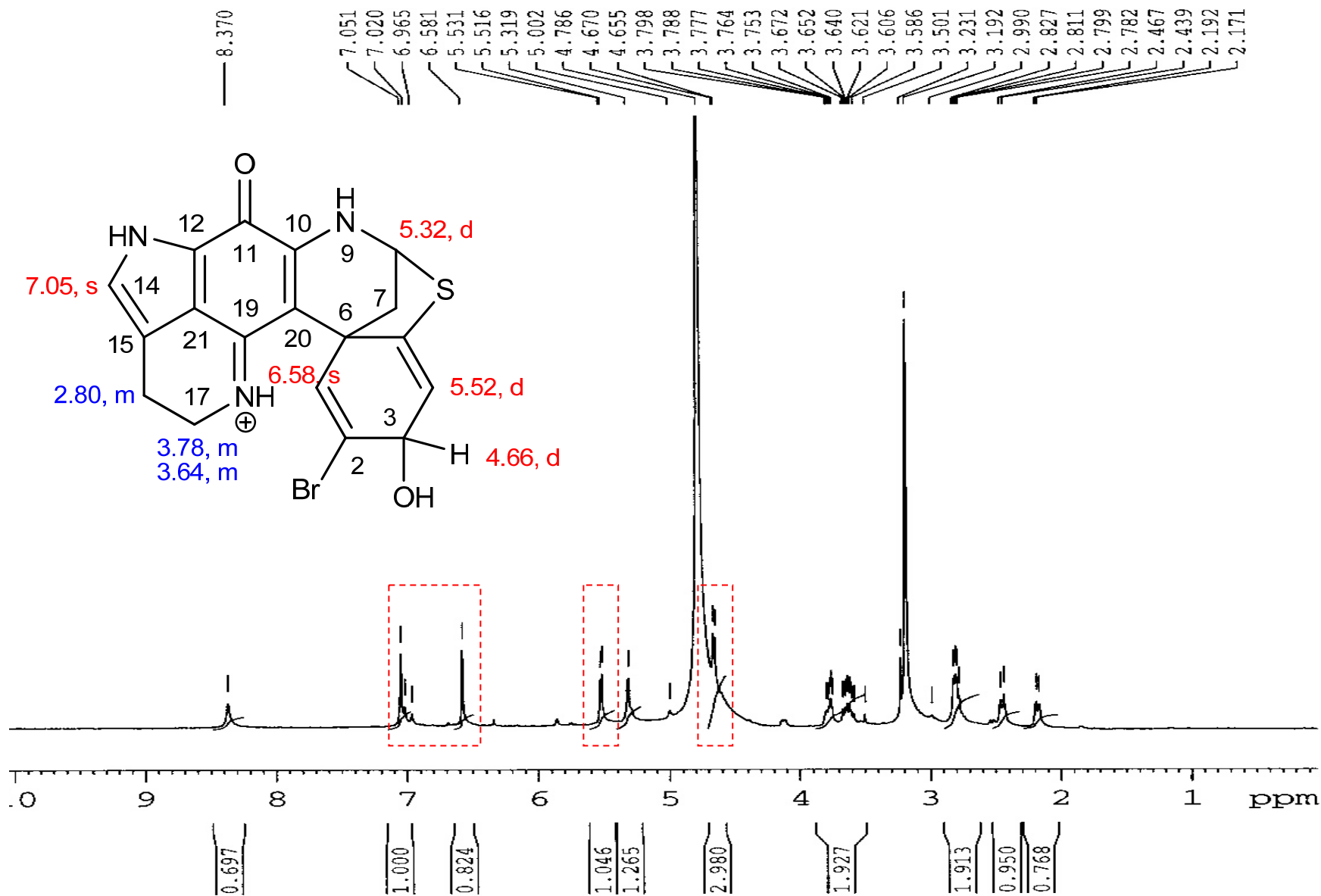
Operator Administrator  
Instrument micrOTOF 93

### Acquisition Parameter

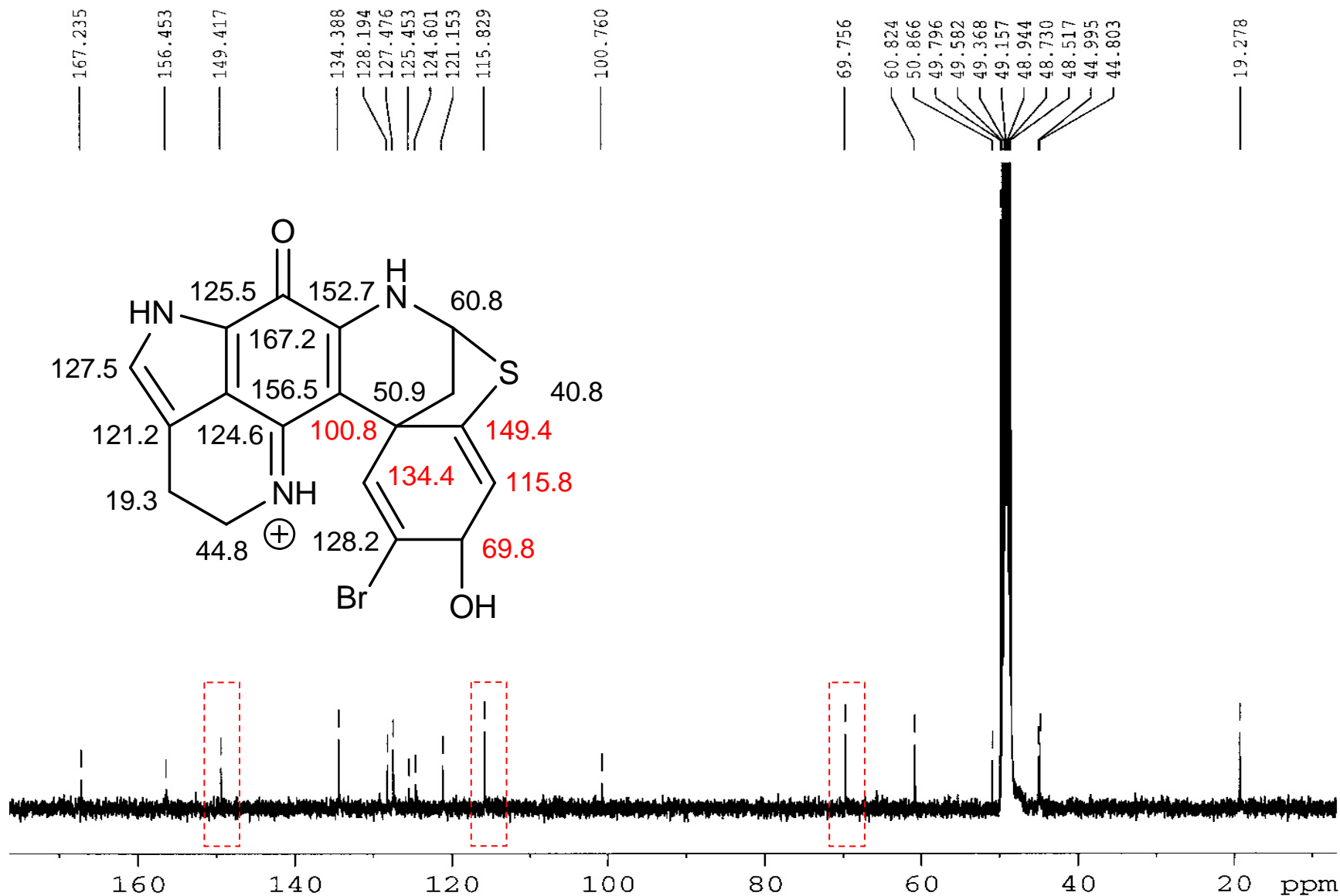
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Scan Begin	50 m/z	Hexapole RF	250.0 V	Set Pulsar Push	402 V
Scan End	3000 m/z	Skimmer 1	40.0 V	Set Reflector	1305 V
		Hexapole 1	20.8 V	Set Flight Tube	9000 V
				Set Detector TOF	2150 V



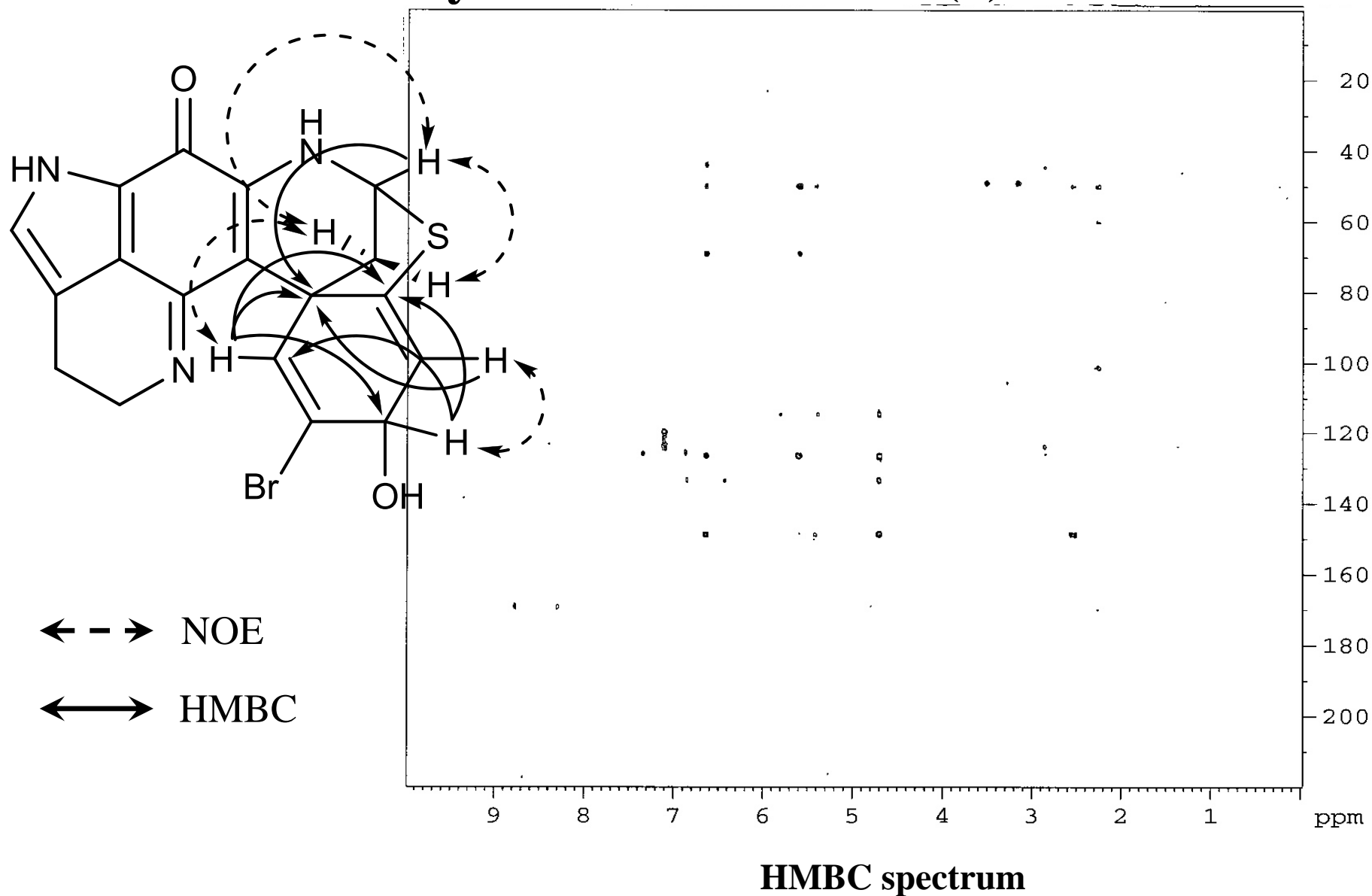
# <sup>1</sup>H-NMR spectrum of dihydrodiscorhabdin B (1)



# $^{13}\text{C}$ -NMR spectrum of dihydrodiscorhabdin B (1)

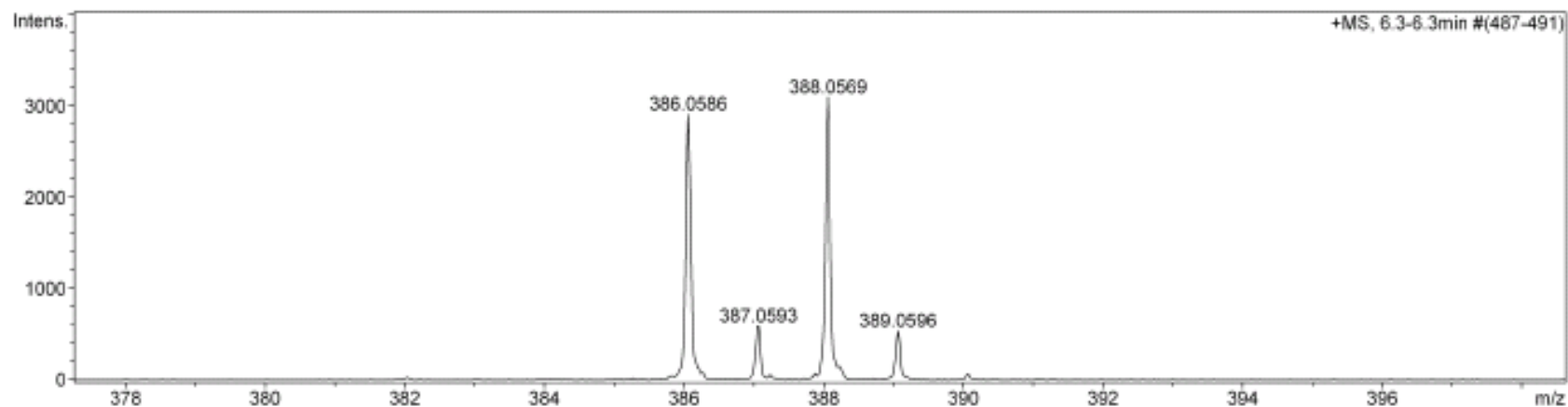
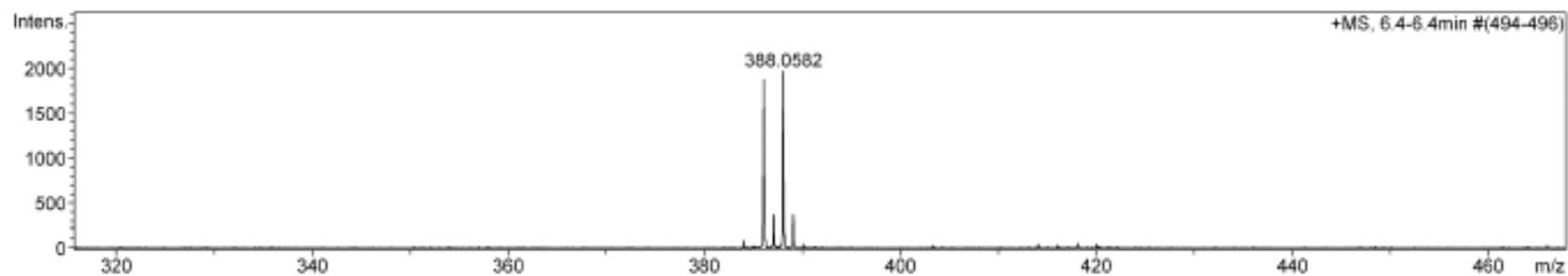
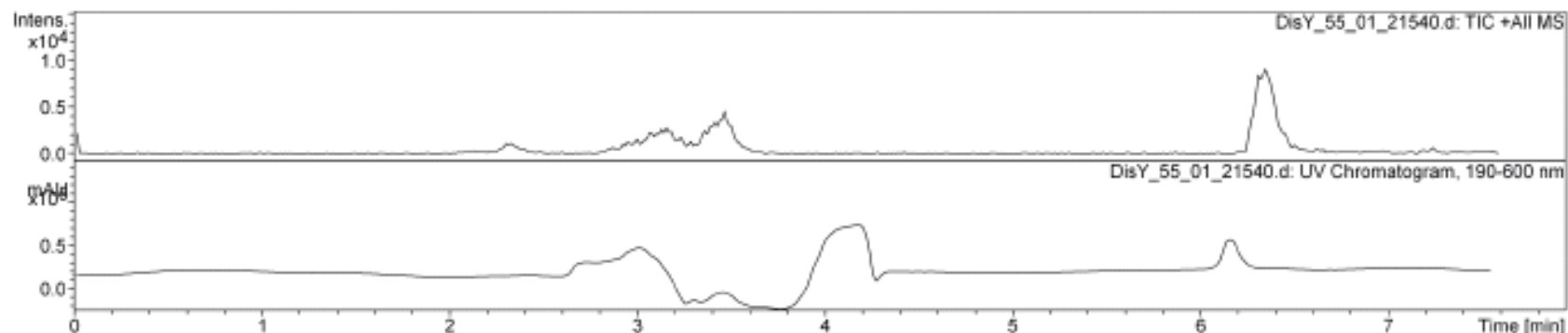


# Key HMBC and NOE correlations of dihydrodiscorhabdin B (1)

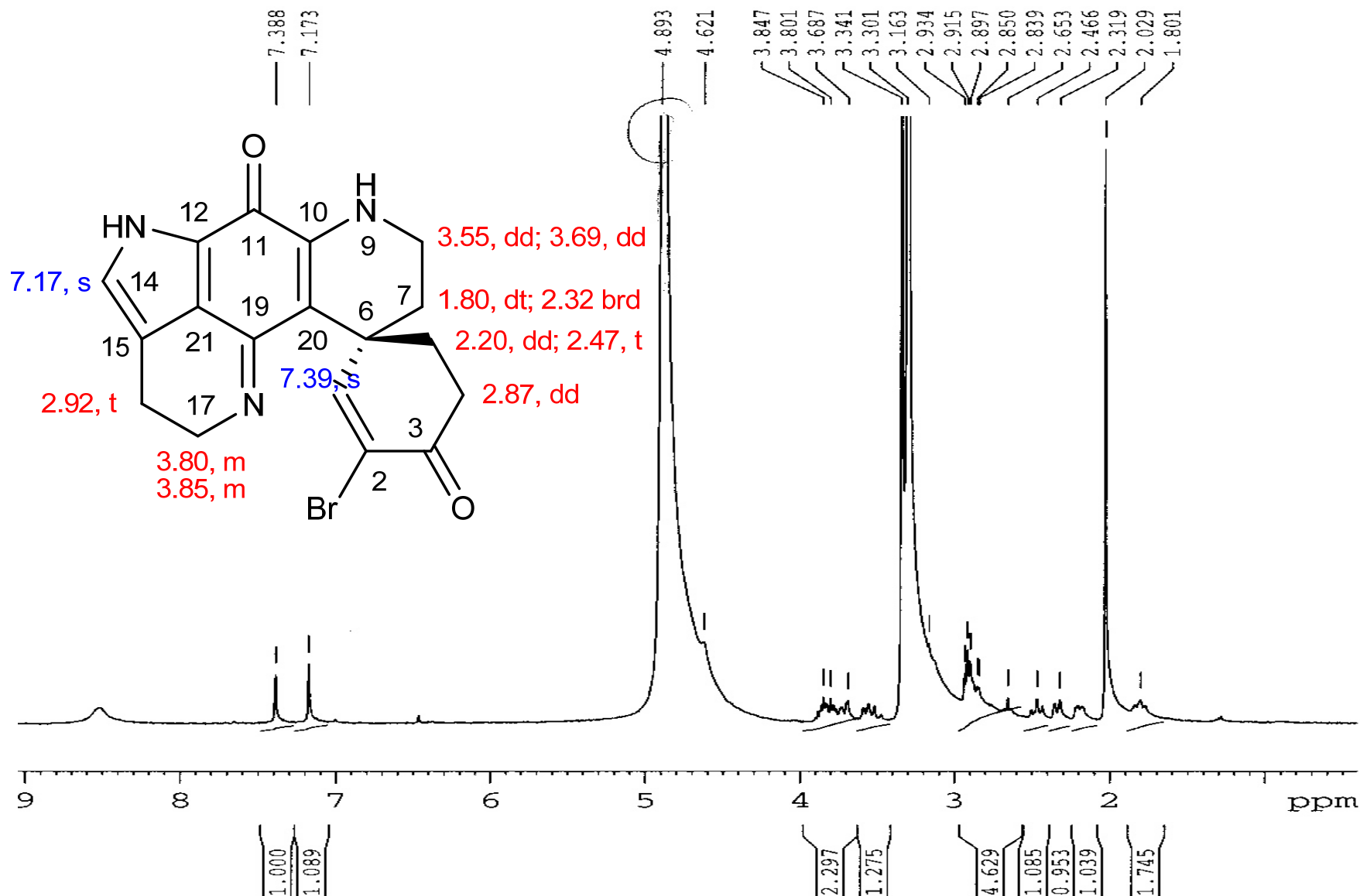


# LC-MS spectrum of discorhabdin Y (2)

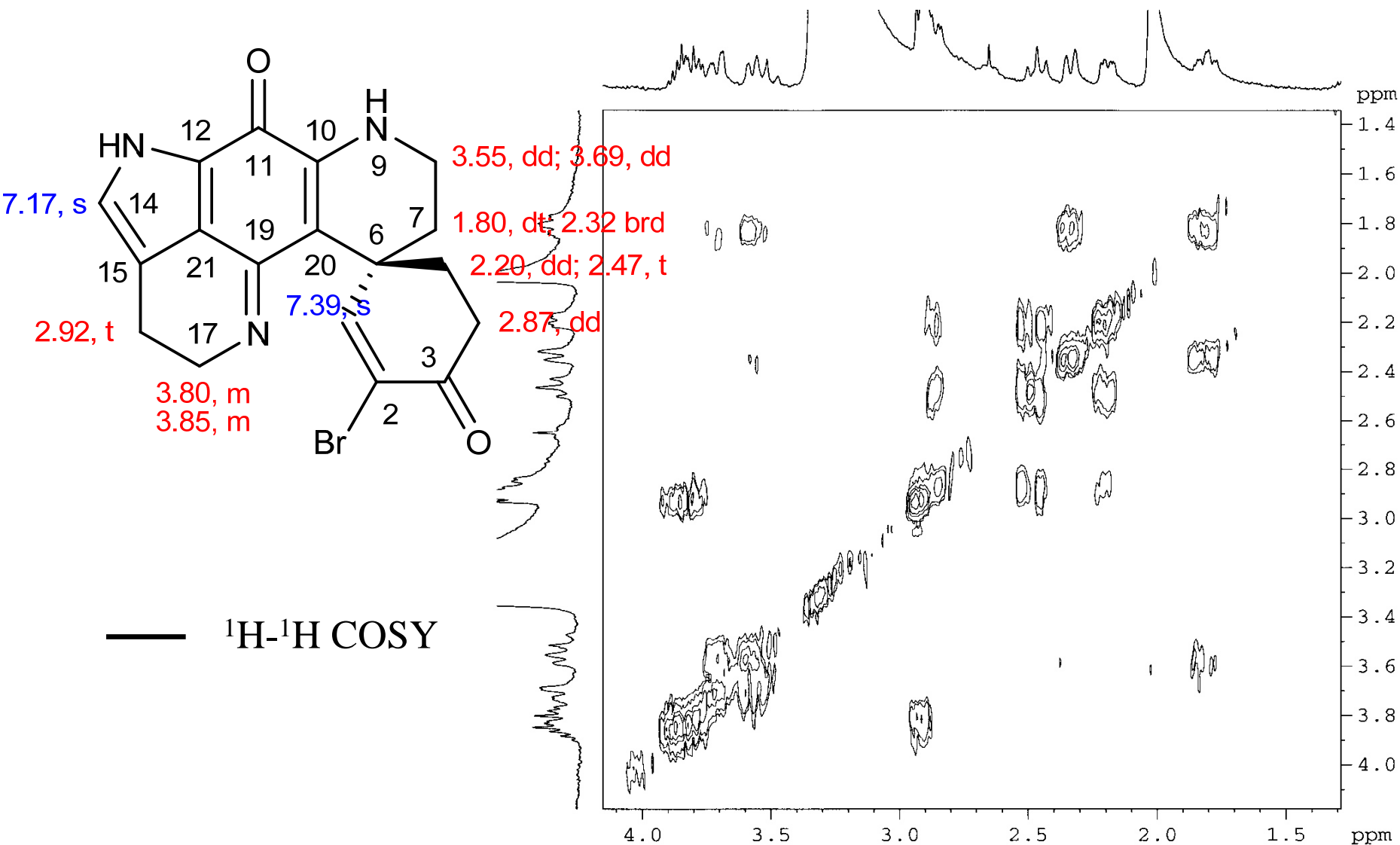
## Generic Display Report (all)



# <sup>1</sup>H-NMR spectrum of discorhabdin Y (2)

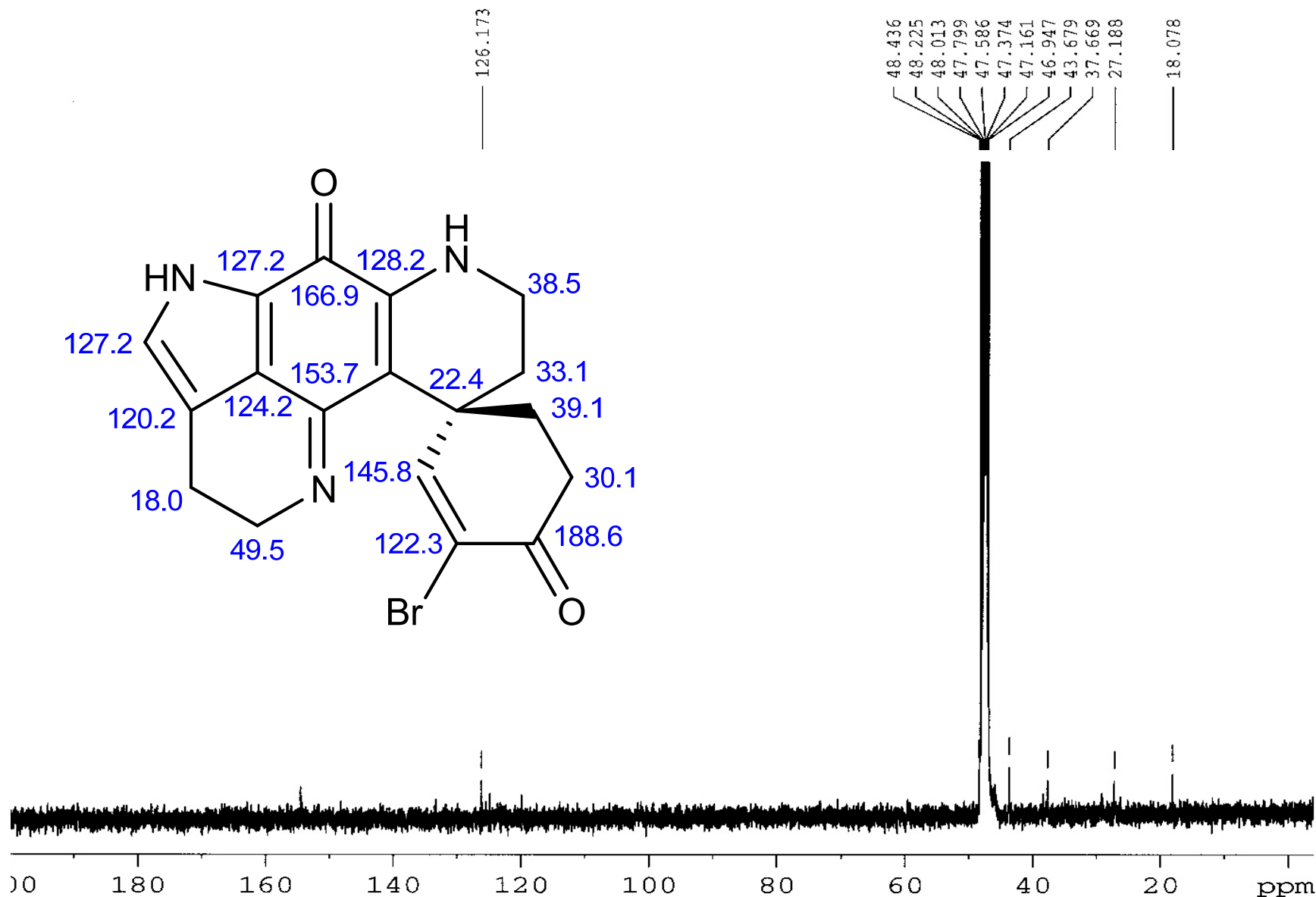


# $^1\text{H}$ - $^1\text{H}$ COSY spectrum of discorhabdin Y (2)





# $^{13}\text{C}$ -NMR spectrum of discorhabdin Y (2)



# LC-MS spectrum of discorhabdin A (3)

## Display Report

### Analysis Info

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Method LCMS-rutin-pos.m  
Sample Name 04AK018-8-4-3  
Comment

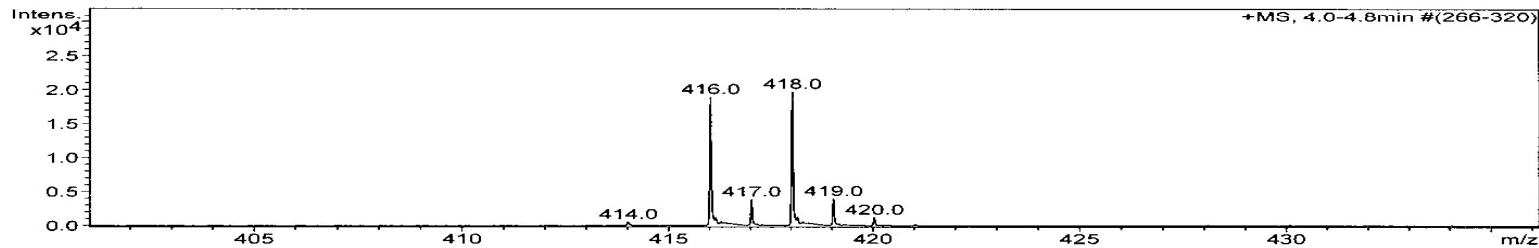
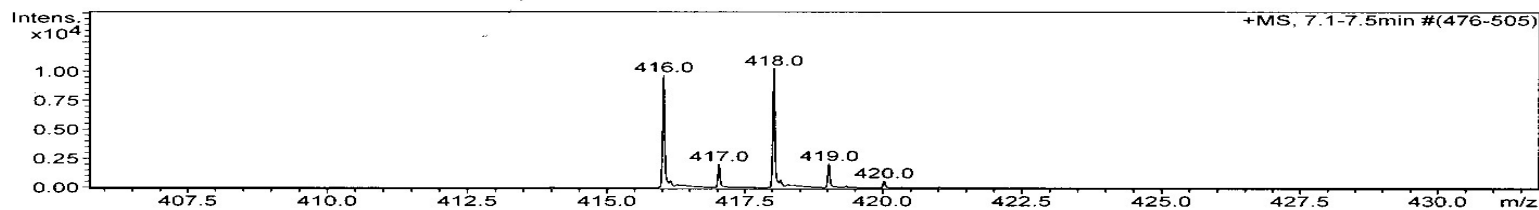
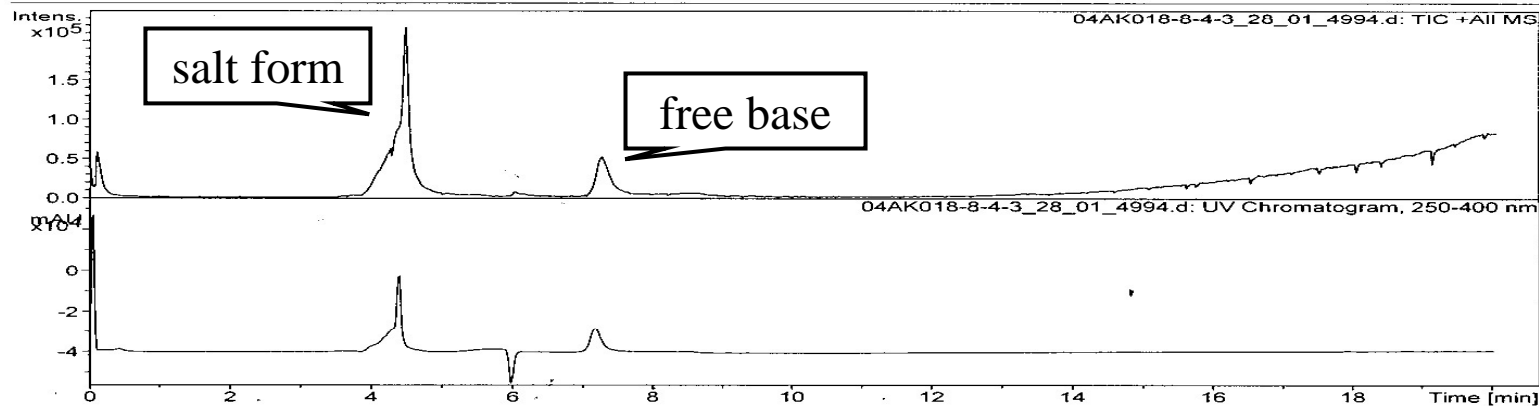
Acquisition Date 10/11/2006 3:02:24 AM

Operator Administrator  
Instrument microTOF 93

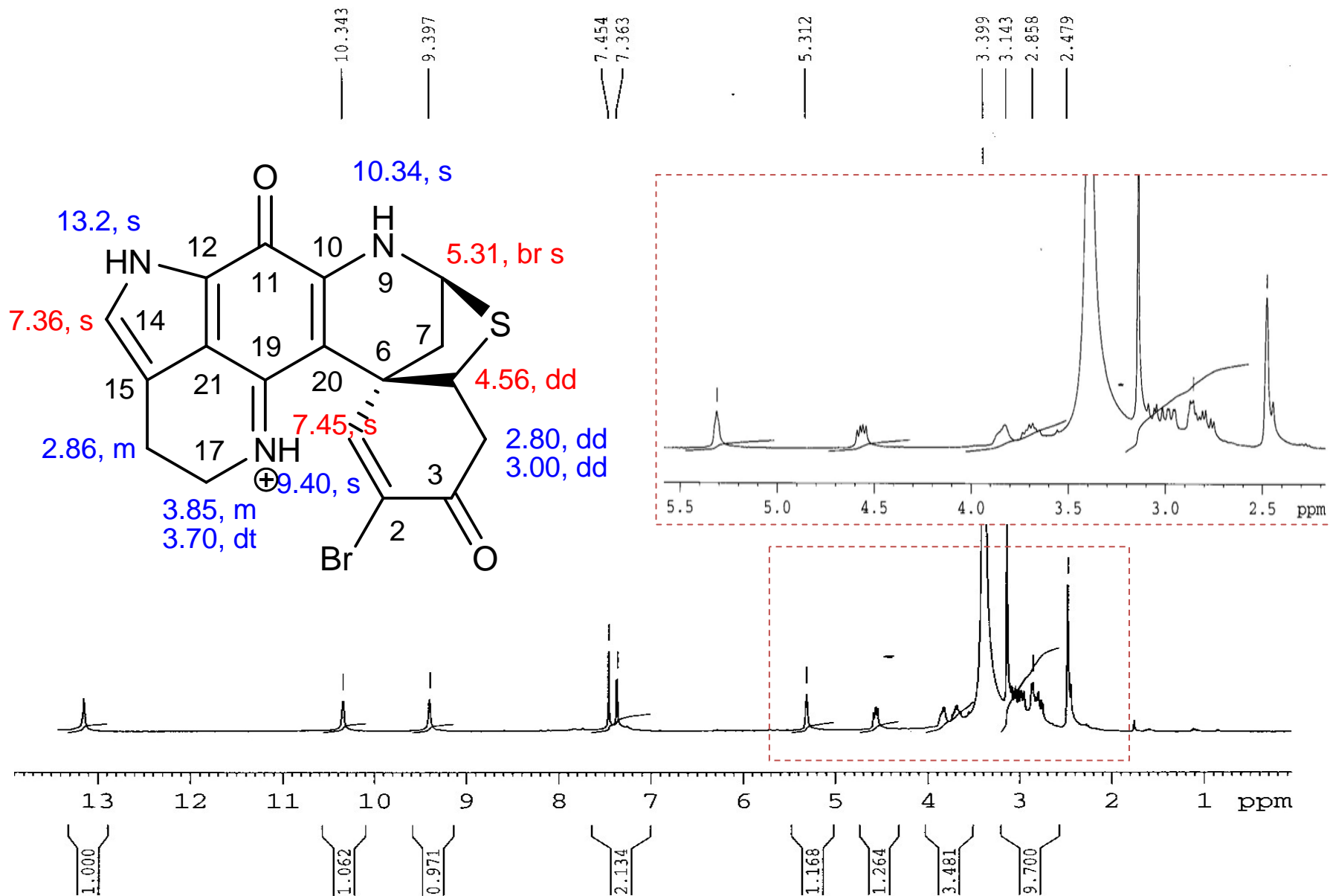
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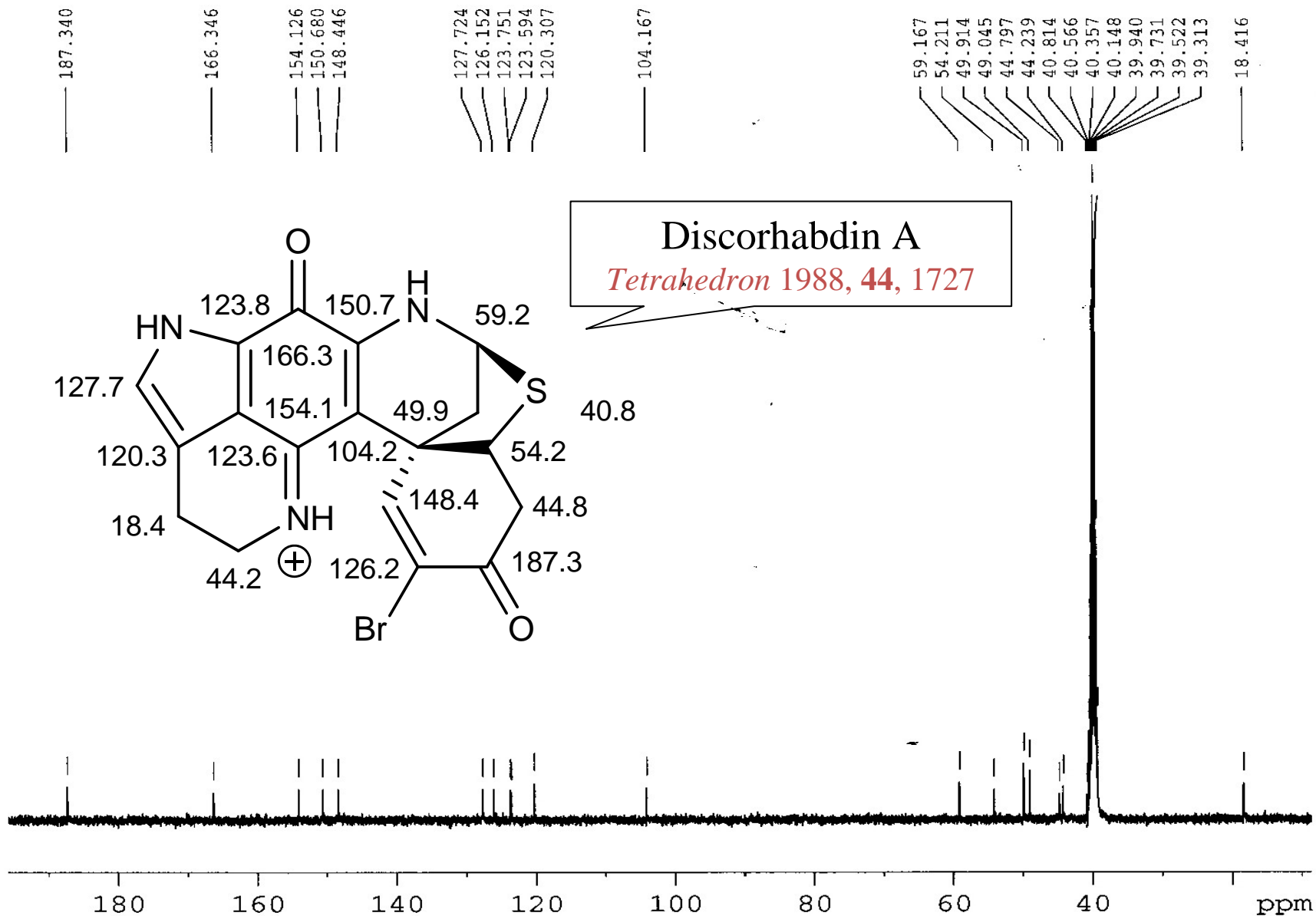
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Set Reflector	1300 V
Set Flight Tube	9000 V
Set Detector TOF	2135 V



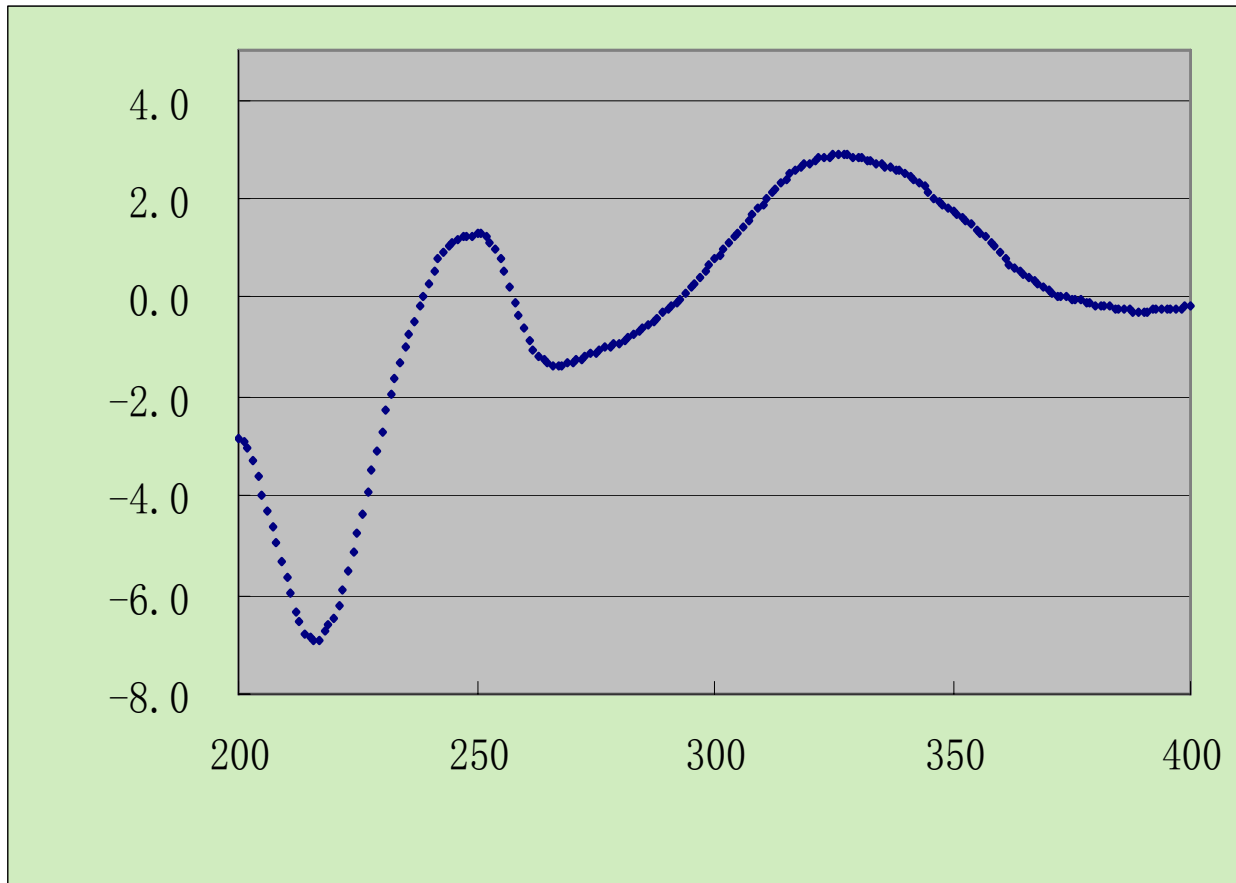
# <sup>1</sup>H-NMR spectrum of discorhabdin A (3)



# <sup>13</sup>C-NMR spectrum of discorhabdin A (3)



# Experimental CD data of discorhabdin A (3)



# LC-MS spectrum of discorhabdin C (4)

## Display Report

### Analysis Info

Analysis Name D:\Data\Na\04ak018f8-5-3-1\_81\_01\_4602.d  
Method LCMS-rutin-pos.m  
Sample Name 04ak018f8-5-3-1  
Comment

Acquisition Date 9/20/2006 4:21:23 PM

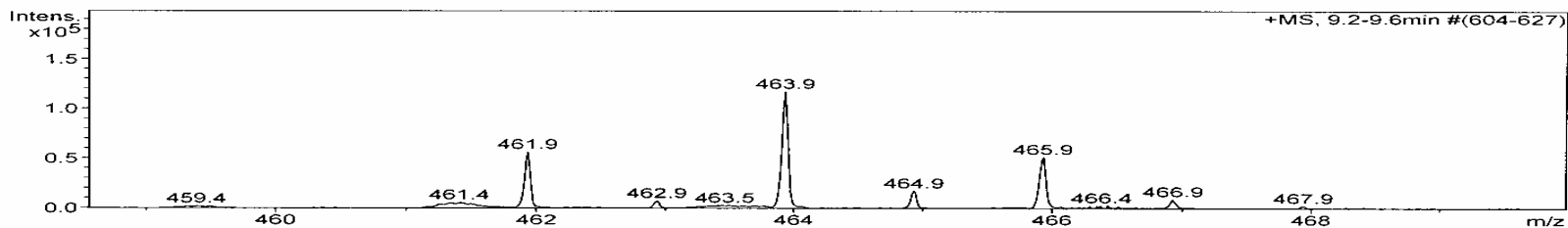
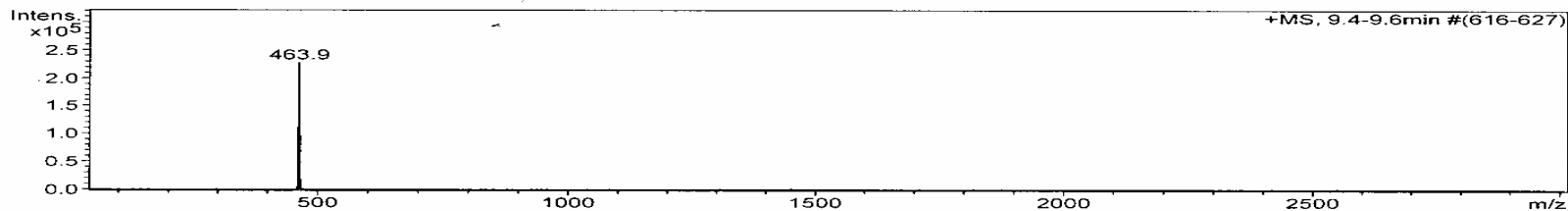
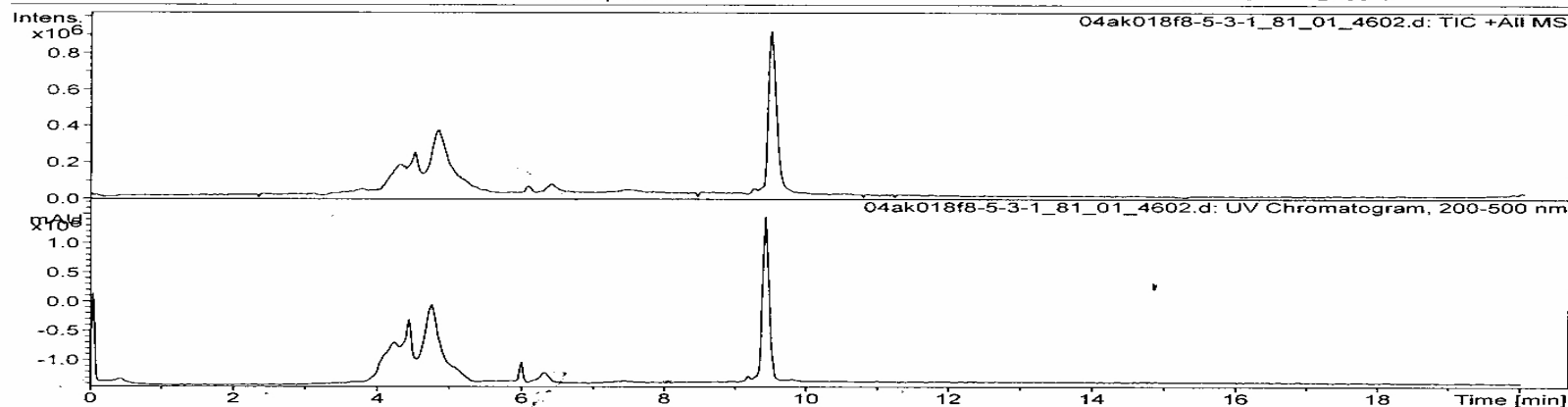
Operator Administrator  
Instrument microTOF 93

### Acquisition Parameter

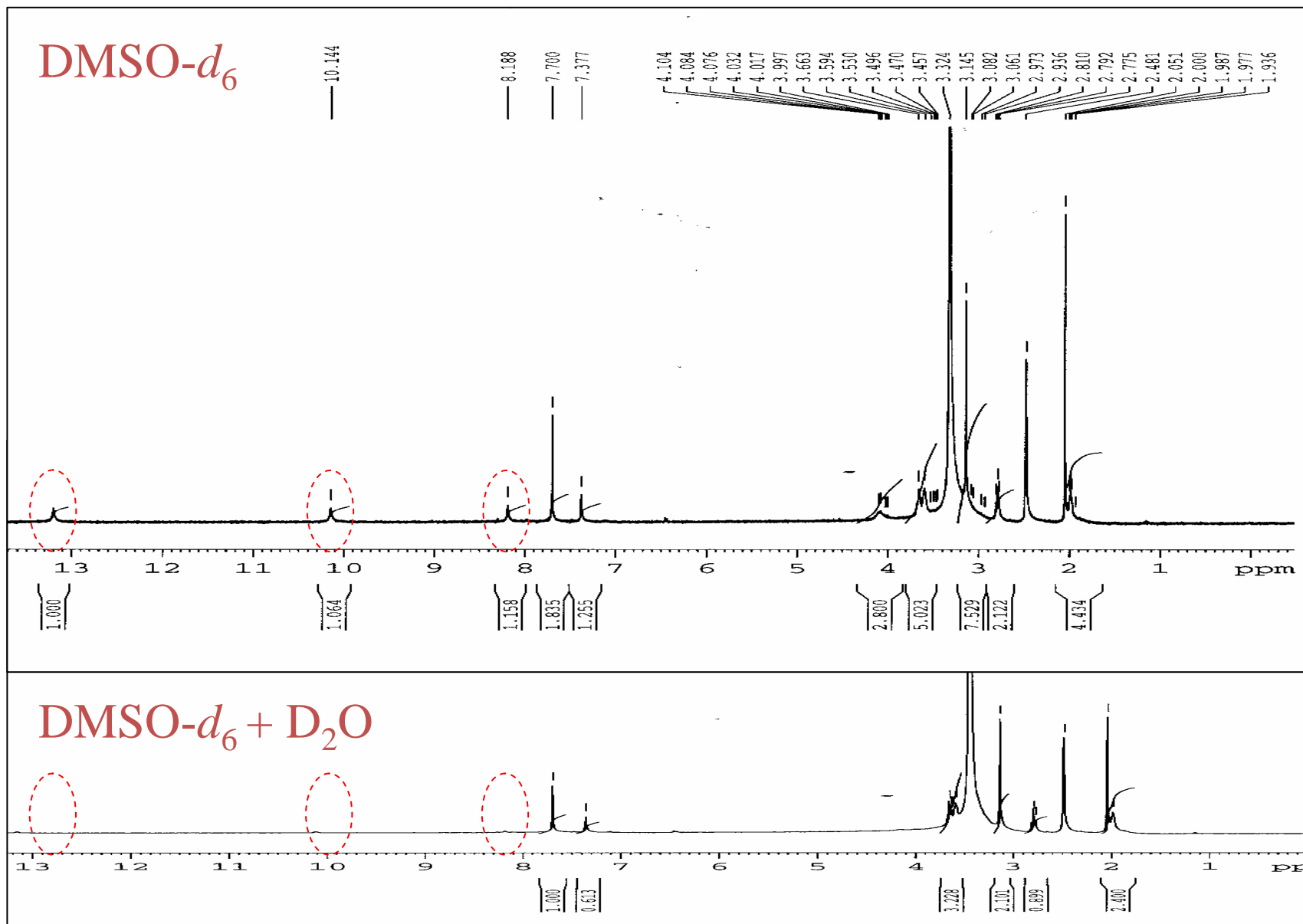
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Ion Polarity Positive  
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Skimmer 1 50.0 V  
Hexapole 1 21.9 V

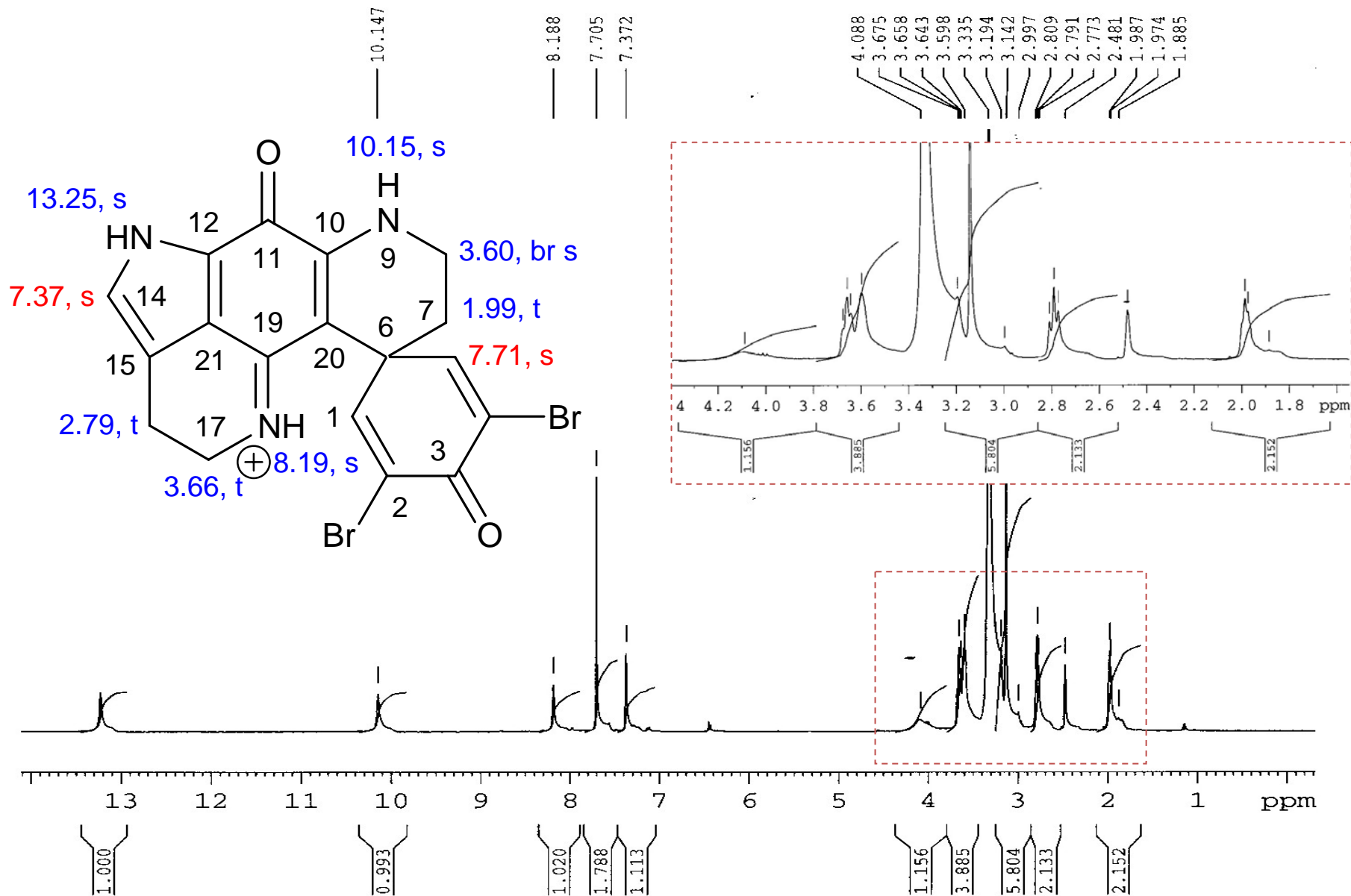
Set Corrector Fill 46 V  
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# $^1\text{H-NMR}$ spectrum of discorhabdin C (4)

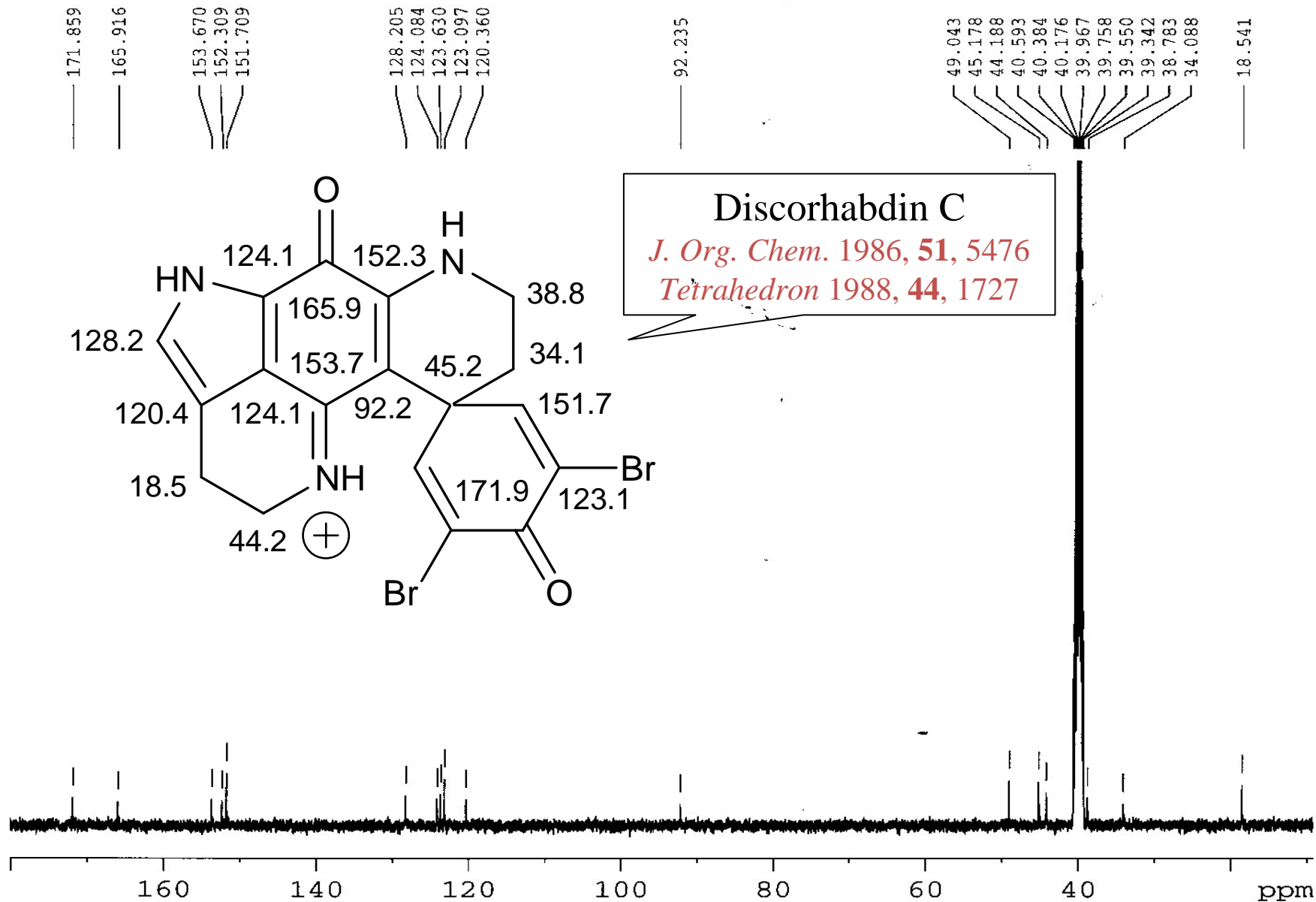


# <sup>1</sup>H-NMR spectrum of discorhabdin C (4)





# <sup>13</sup>C-NMR spectrum of discorhabdin C (4)



# LC-MS spectrum of discorhabdin E (5)

## Display Report

### Analysis Info

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Method LCMS-rutin-pos.m  
Sample Name 04AK08-8-5-6-3  
Comment

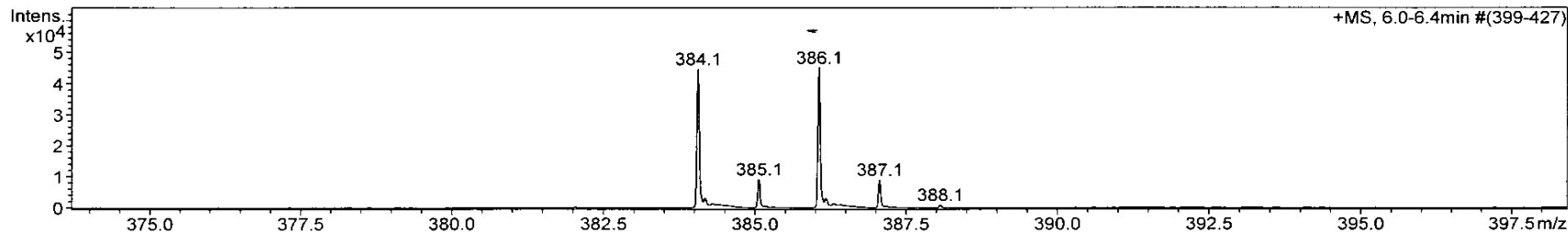
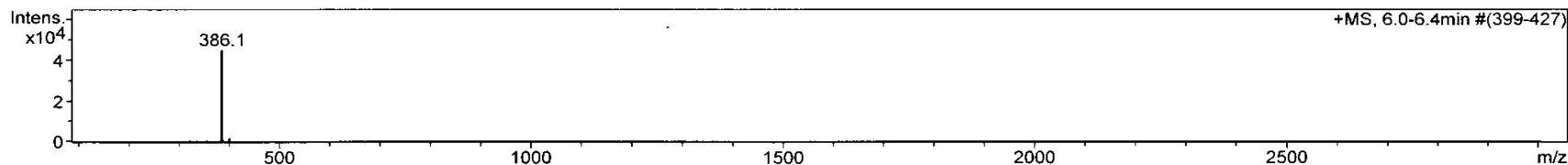
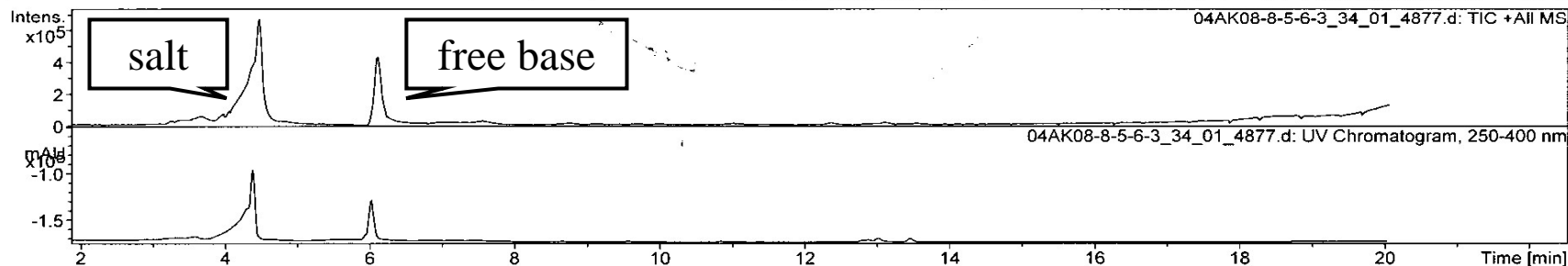
Acquisition Date 10/5/2006 10:51:23 PM

Operator Administrator  
Instrument micrOTOF 93

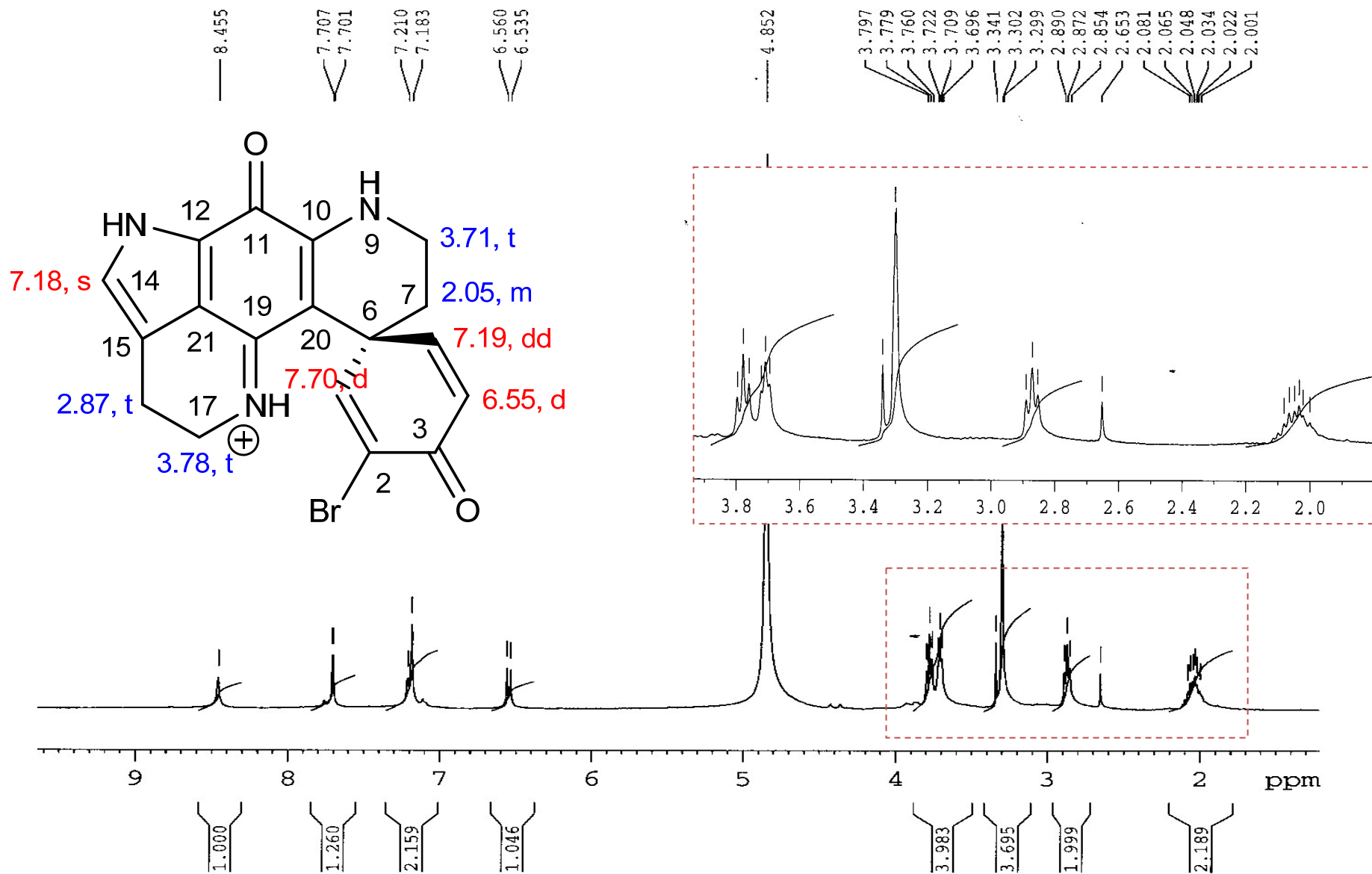
### Acquisition Parameter

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Capillary Exit 80.0 V  
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Skimmer 1 50.0 V  
Hexapole 1 21.9 V

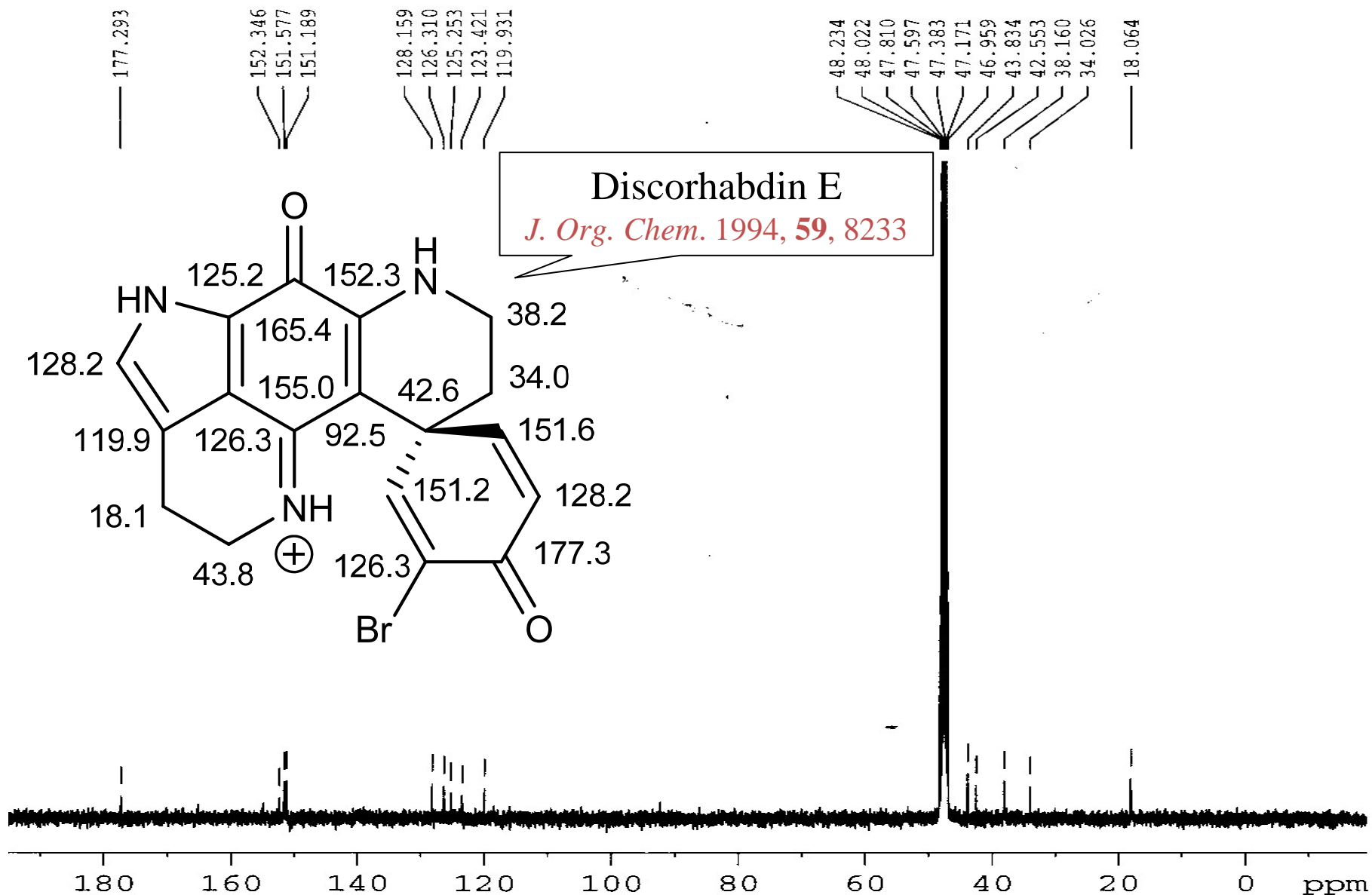
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Set Reflector 1300 V  
Set Flight Tube 9000 V  
Set Detector TOF 2135 V



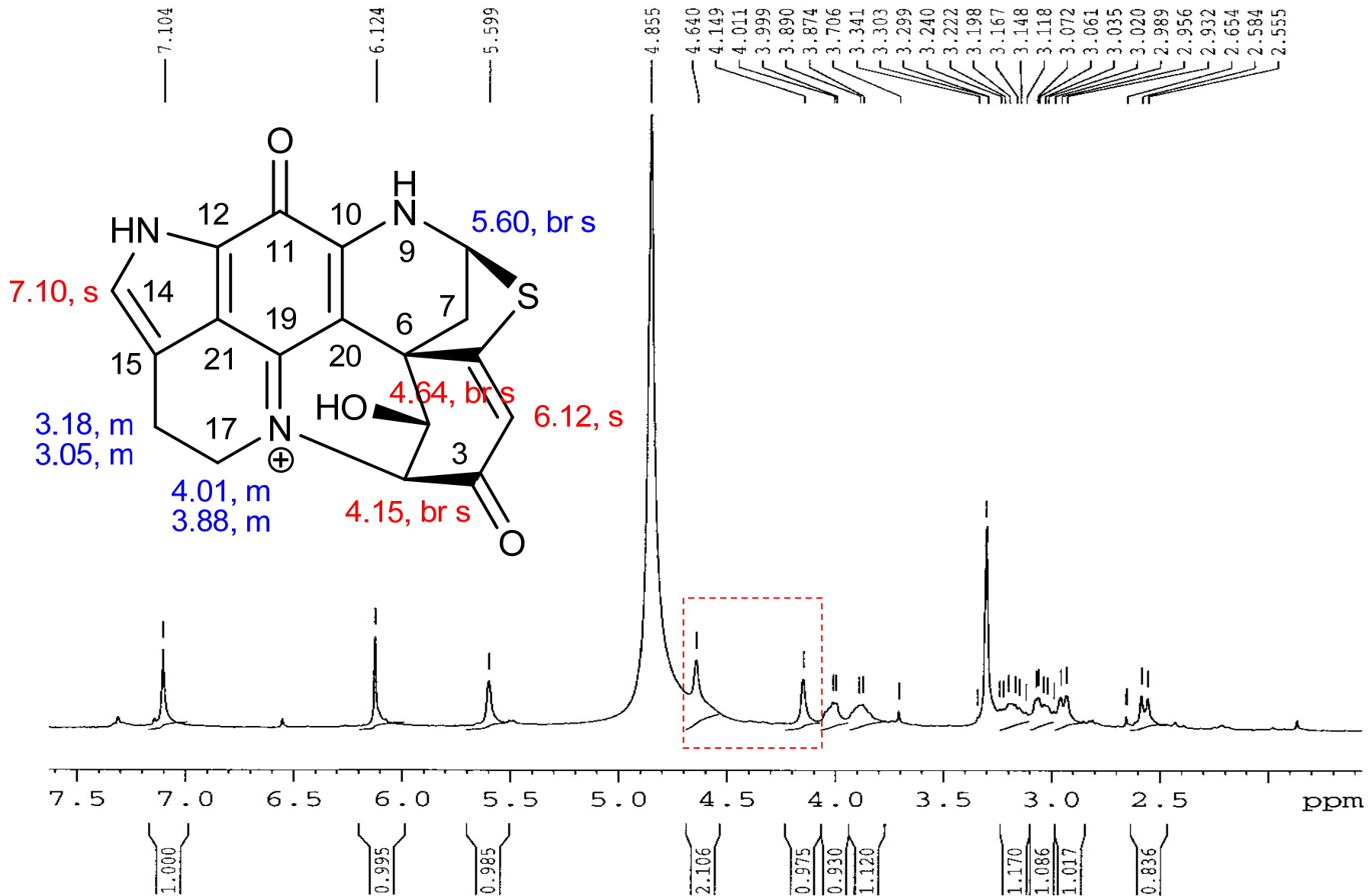
# <sup>1</sup>H-NMR spectrum of discorhabdin E (5)



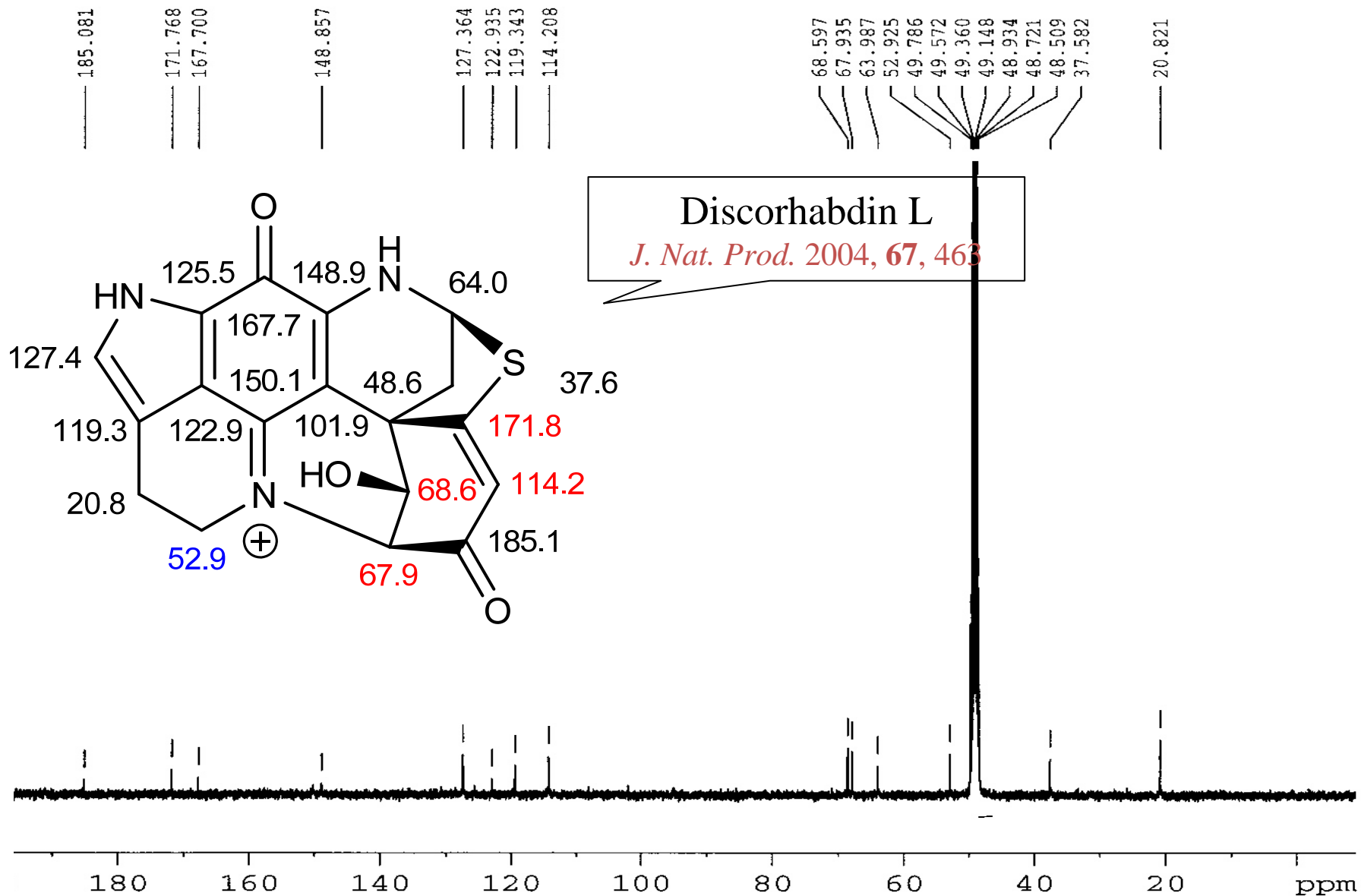
# <sup>13</sup>C-NMR spectrum of discorhabdin E (5)



# $^1\text{H-NMR}$ spectrum of discorhabdin L (6)



# $^{13}\text{C}$ -NMR spectrum of discorhabdin L (6)



# LC-MS spectrum of dihydrodiscorhabdin C (7)

## Display Report

### Analysis Info

Analysis Name H:\Na\AK-8-4-4\_36\_01\_4880.d  
Method LCMS-rutin-pos.m  
Sample Name AK-8-4-3  
Comment

Acquisition Date 10/6/2006 8:14:02 AM

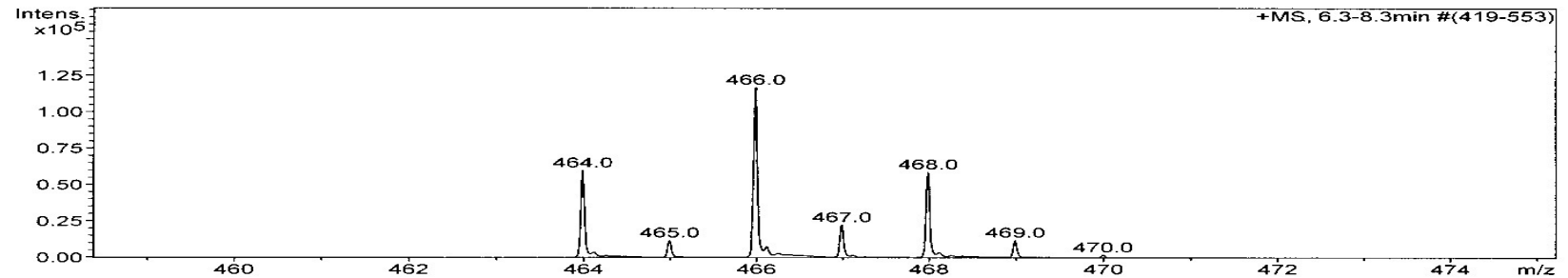
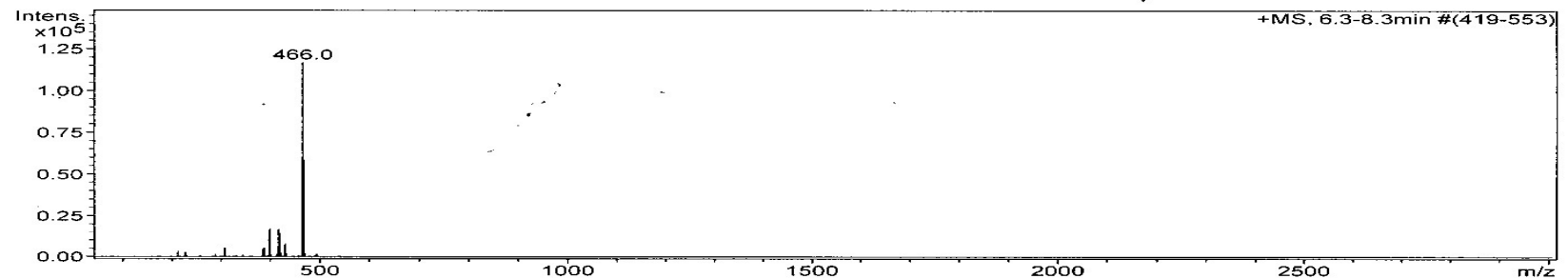
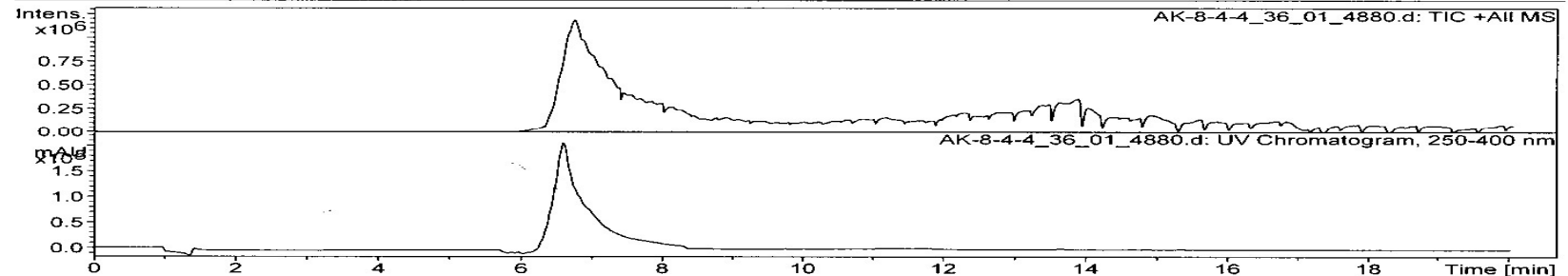
Operator Administrator  
Instrument micrOTOF 93

### Acquisition Parameter

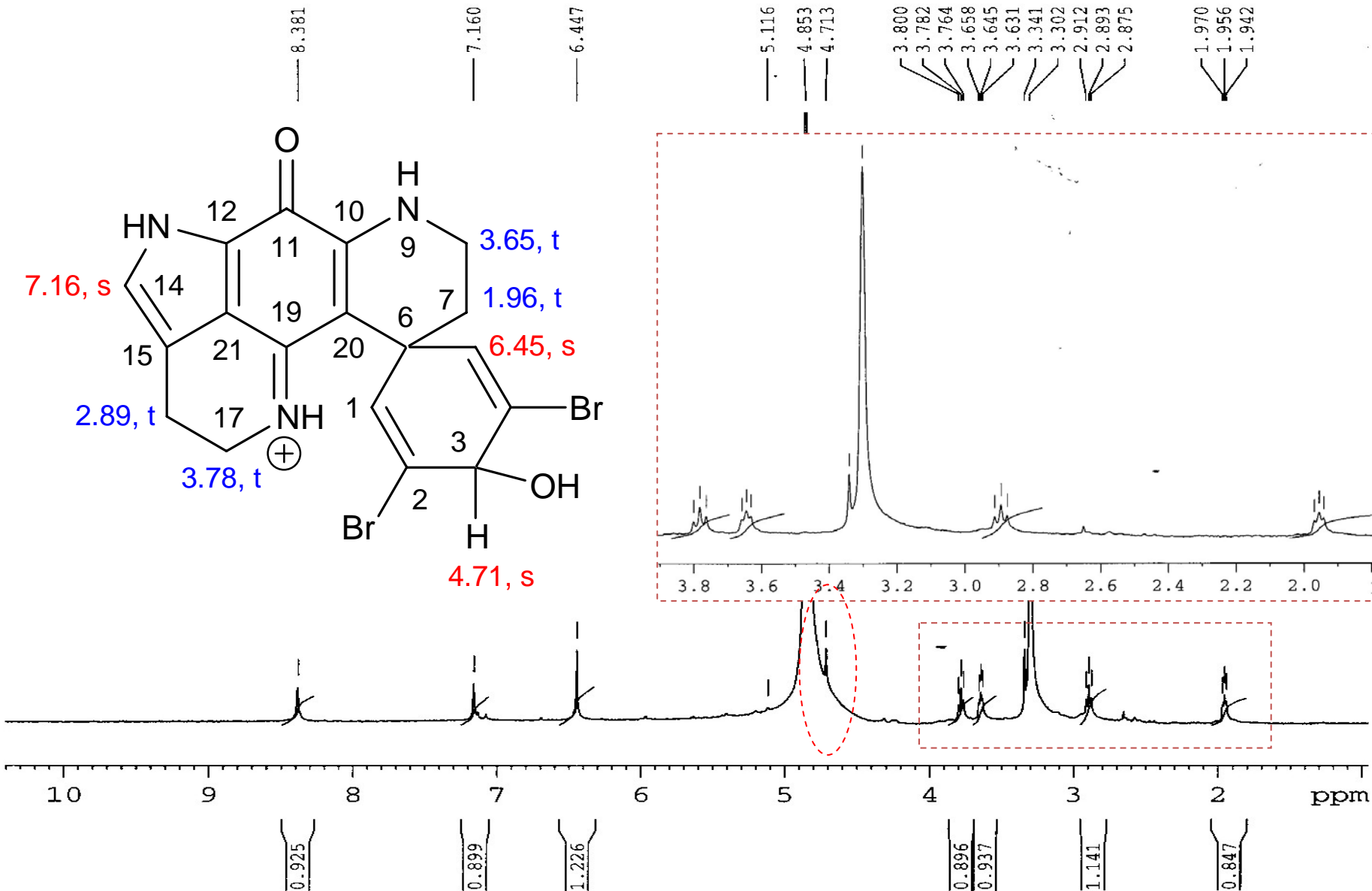
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Ion Polarity Positive  
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Skimmer 1 50.0 V  
Hexapole 1 21.9 V

Set Corrector Fill 48 V  
Set Pulsar Pull 401 V  
Set Pulsar Push 401 V  
Set Reflector 1300 V  
Set Flight Tube 9000 V  
Set Detector TOF 2135 V

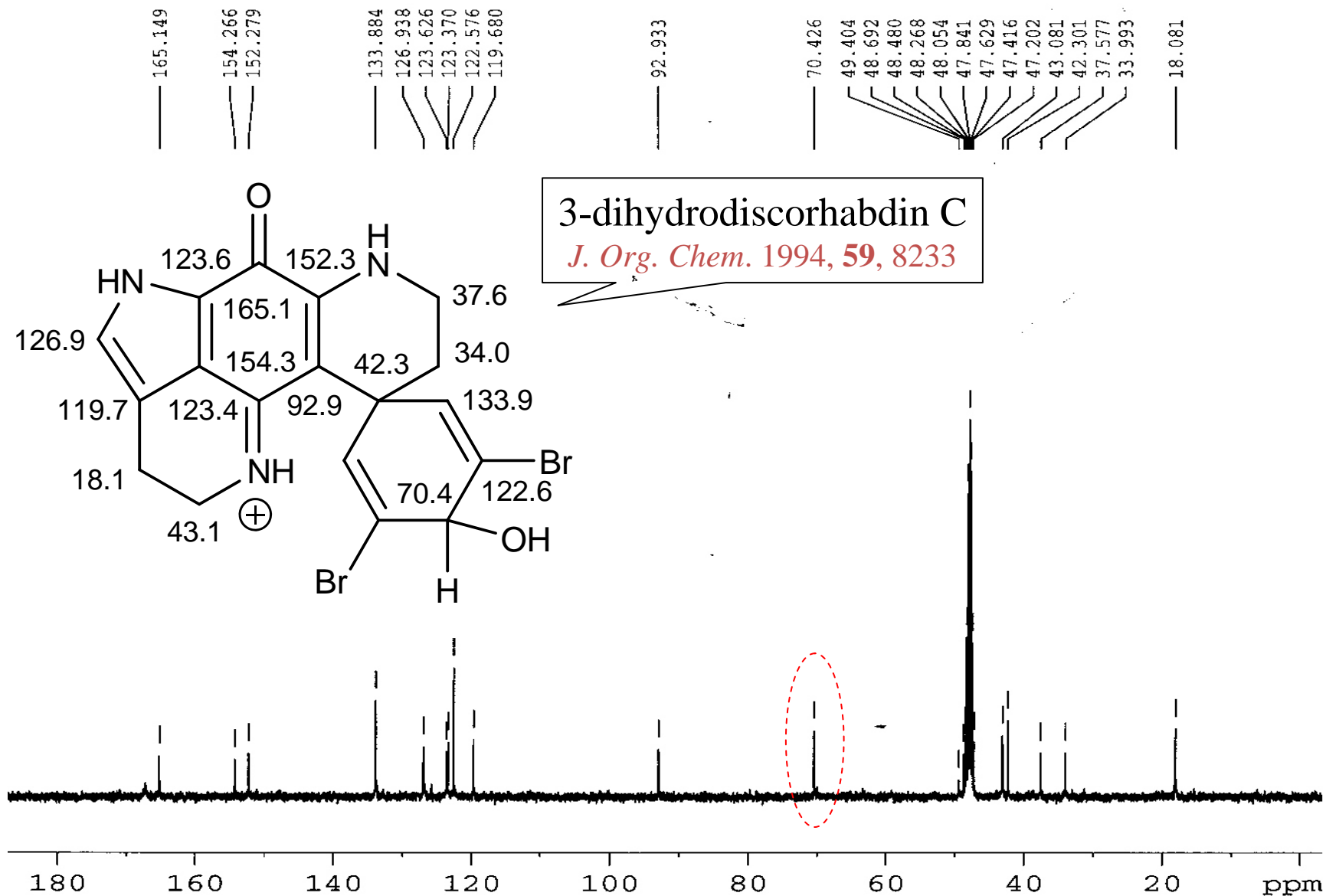


# $^1\text{H-NMR}$ spectrum of dihydrodiscorhabdin C (7)





# $^{13}\text{C}$ -NMR spectrum of dihydrodiscorhabdin C (7)



# LC-MS spectrum of compound 8

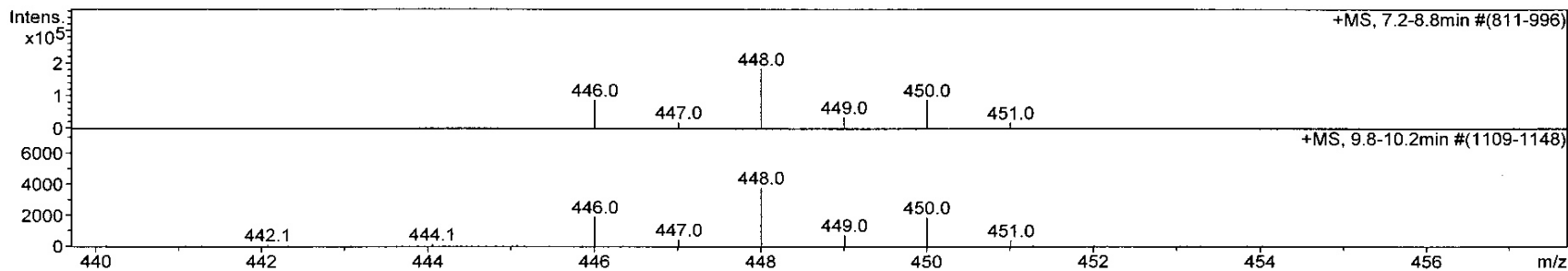
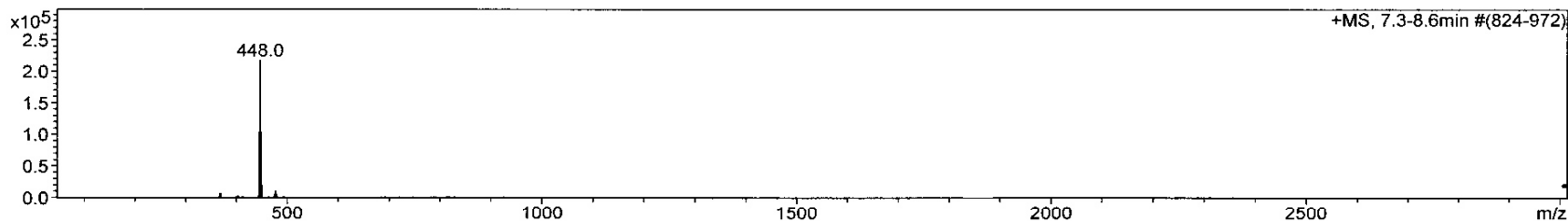
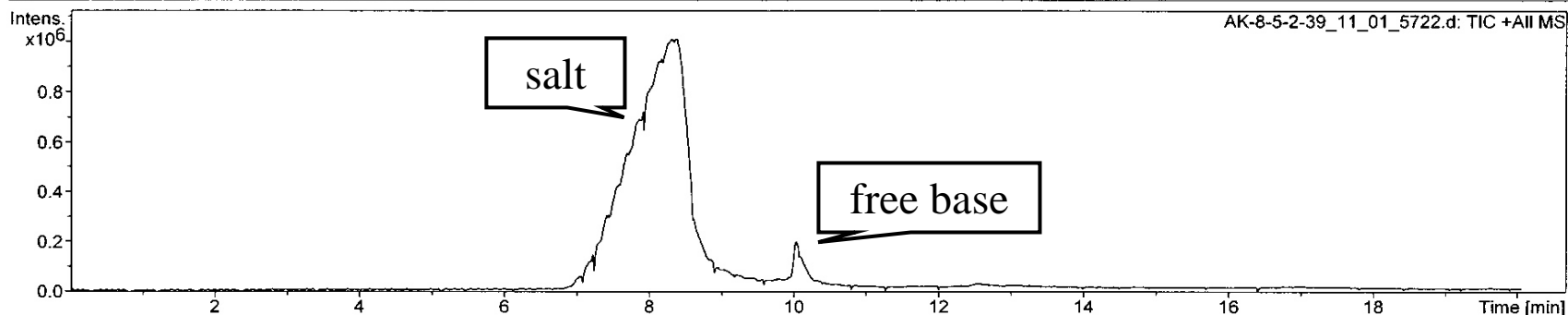
## Generic Display Report

### Analysis Info

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Method LCMS-rutin-pos.m  
Sample Name AK-8-5-2-39  
Comment

Acquisition Date 11/7/2006 4:14:17 PM

Operator Administrator  
Instrument micrOTOF



# $^1\text{H-NMR}$ spectrum of compound 8

