

Supporting Information for

Use of Cyclohexylisocyanide and Methyl 2-Isocynoacetate as Convertible Isocyanides for Microwave -Assisted Fluorous Synthesis of 1,4-Benzodiazepine-2,5-dione Library

Hongyu Zhou,^{†,‡} Wei Zhang,[§] and Bing Yan^{*,†,‡}

St. Jude Children's Research Hospital, Memphis, Tennessee, 38105 U.S.A.

*School of Chemistry and Chemical Engineering, Shandong University, Jinan, 250100,
China*

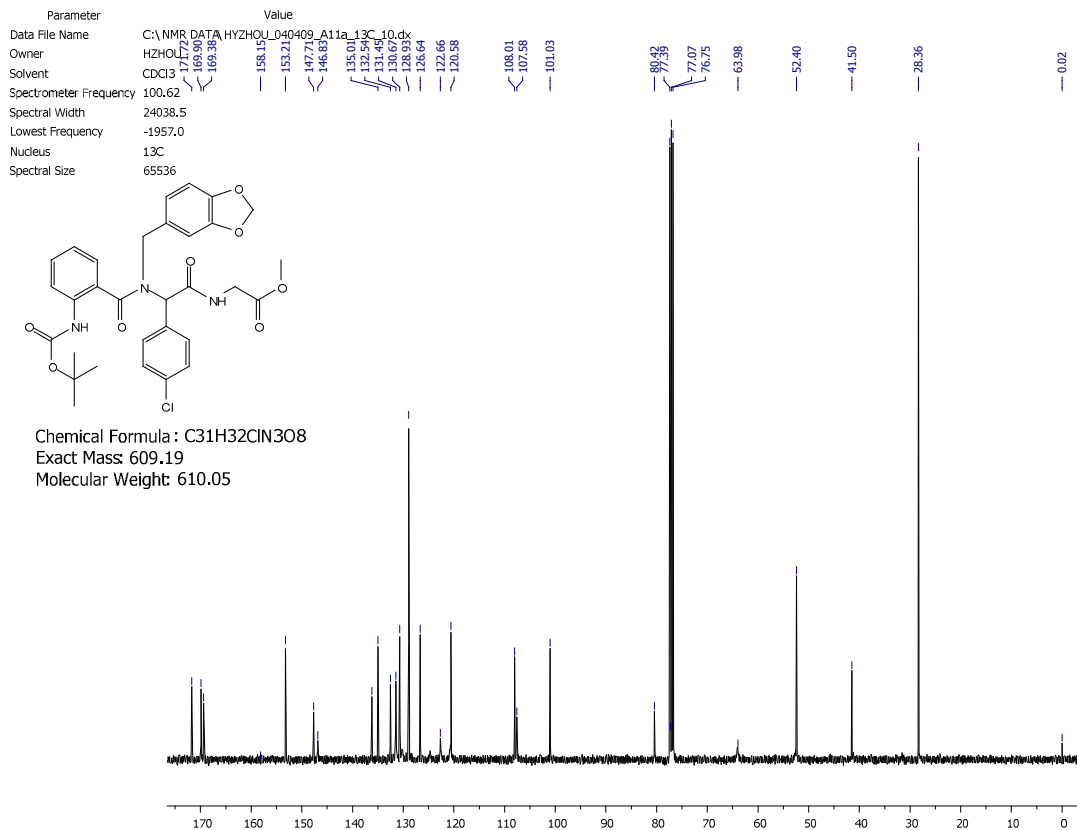
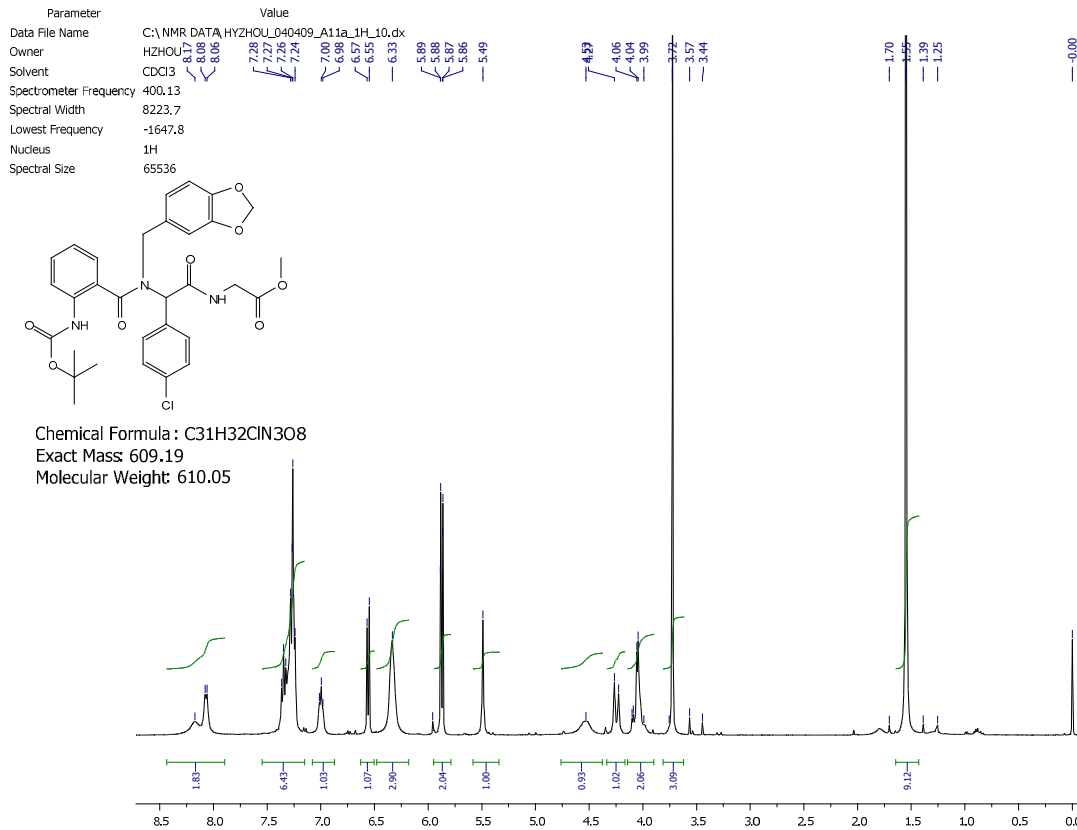
*Department of Chemistry, University of Massachusetts Boston, 100 Morrissey Boulevard
Boston, Massachusetts 02125 U.S.A.*

¹H, ¹³C NMR and HRMS data for selected intermediates and final products.

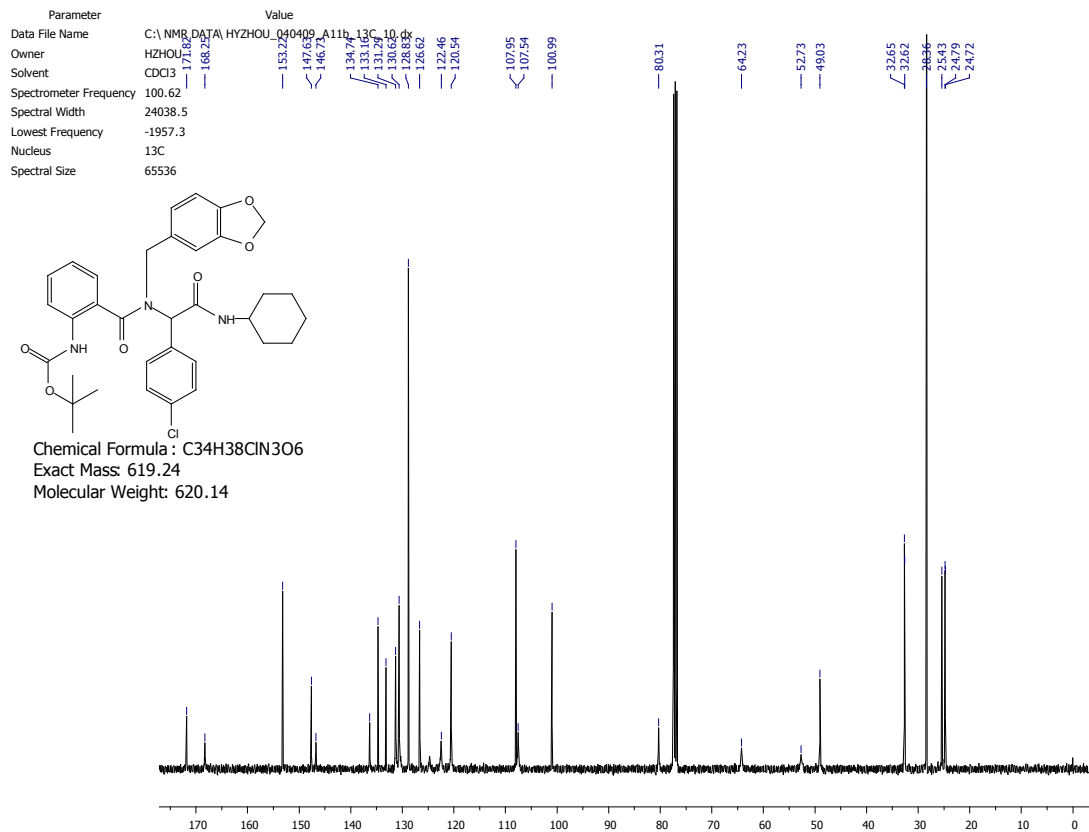
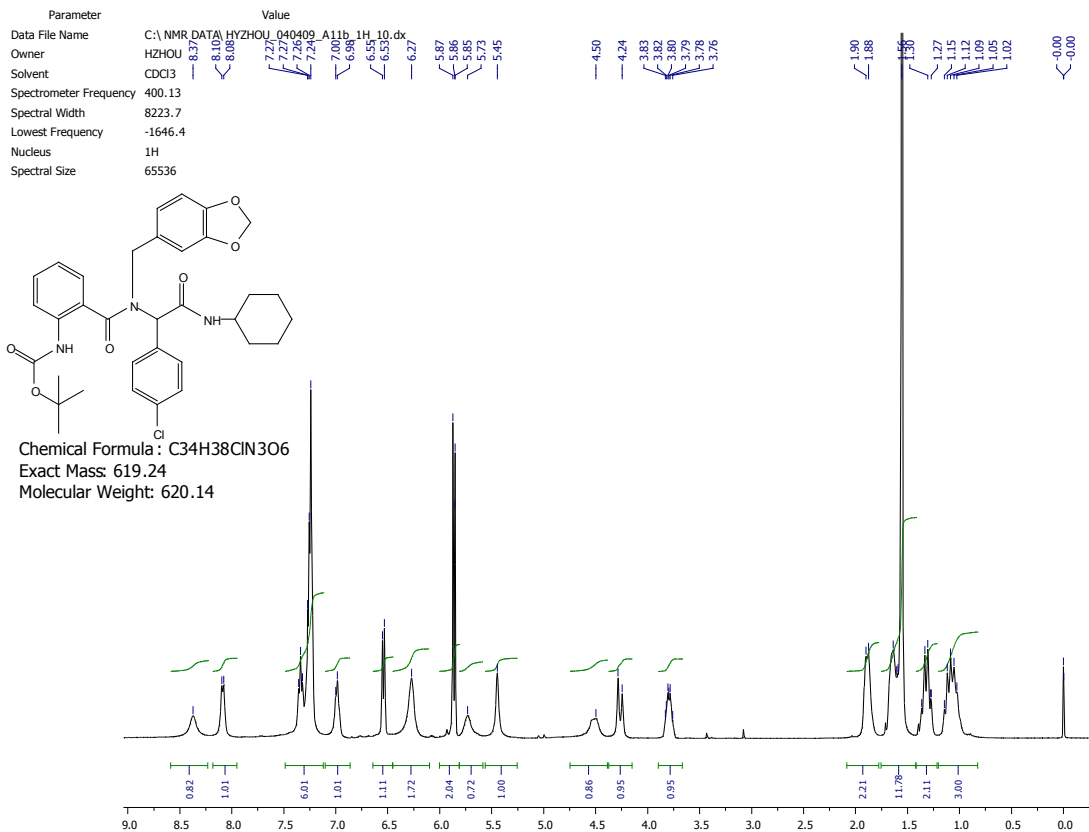
Table of Contents:

5a – ^1H and ^{13}C NMR.....	3
5b – ^1H and ^{13}C NMR.....	4
6a – ^1H and ^{13}C NMR.....	5
6{2,1,1} – ^1H and ^{13}C NMR.....	6
6{2,1,3} – ^1H and ^{13}C NMR.....	7
6{2,2,1} – ^1H and ^{13}C NMR.....	8
6{2,2,3} – ^1H and ^{13}C NMR.....	9
6{1,1,1} – ^1H and ^{13}C NMR.....	10
6{3,1,1} – ^1H and ^{13}C NMR.....	11
6{1,1,3} – ^1H and ^{13}C NMR.....	12
6{1,2,1} – ^1H and ^{13}C NMR.....	13
6{3,2,1} – ^1H and ^{13}C NMR.....	14
6{1,1,2} – ^1H and ^{13}C NMR.....	15
6{3,1,4} – ^1H and ^{13}C NMR.....	16
6{4,1,2} – ^1H and ^{13}C NMR.....	17
6{1,2,5} – ^1H and ^{13}C NMR.....	18
6{4,2,4} – ^1H and ^{13}C NMR.....	19
6{2,2,2} – ^1H and ^{13}C NMR.....	20
6{2,2,4} – ^1H and ^{13}C NMR.....	21
8{2,1,3,1} – ^1H NMR.....	22
8{2,2,1,2} – ^1H NMR	22
8{2,2,3,6} – ^1H NMR	23
8{1,1,1,5} – ^1H NMR	23
8{1,1,1,2} – ^1H NMR	24
8{1,1,3,2} – ^1H NMR	24
8{1,1,3,3} – ^1H NMR	25
8{3,2,1,5} – ^1H NMR	25
8{4,1,2,6} – ^1H NMR	26
8{4,2,4,6} – ^1H NMR	26
8{2,1,1,1} – ^1H NMR and HRMS.....	27
8{1,1,1,4} – ^1H NMR and HRMS.....	28
8{3,2,1,6} – ^1H NMR and HRMS.....	29
8{1,1,2,1} – ^1H NMR and HRMS.....	30
8{1,1,2,3} – ^1H , ^{13}C NMR and HRMS.....	31,32
8{1,1,2,4} – ^1H NMR and HRMS.....	33
8{3,1,4,4} – ^1H NMR and HRMS.....	34
8{3,1,4,5} – ^1H NMR and HRMS.....	35
8{4,1,2,1} – ^1H NMR and HRMS.....	36
8{1,2,5,3} – ^1H NMR and HRMS.....	37

5a – ¹H and ¹³C NMR

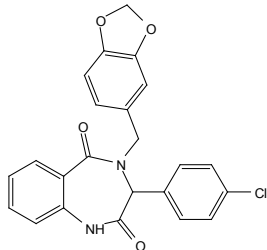


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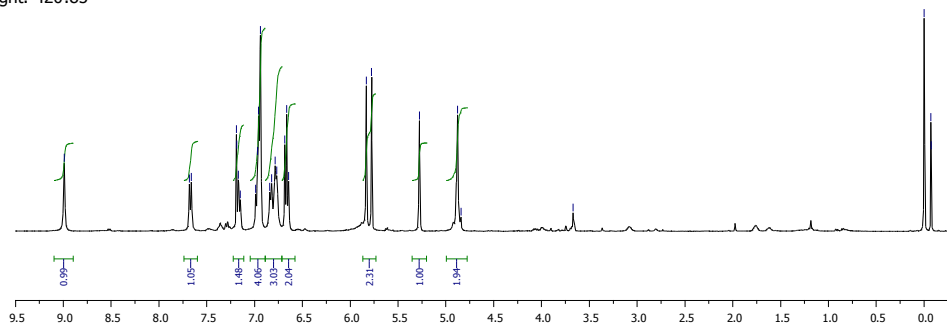


6a – ¹H and ¹³C NMR

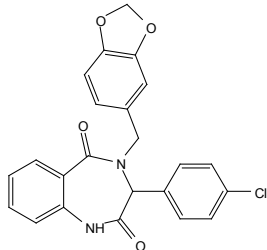
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Lowest Frequency	-1678.8
Nucleus	¹ H
Spectral Size	65536



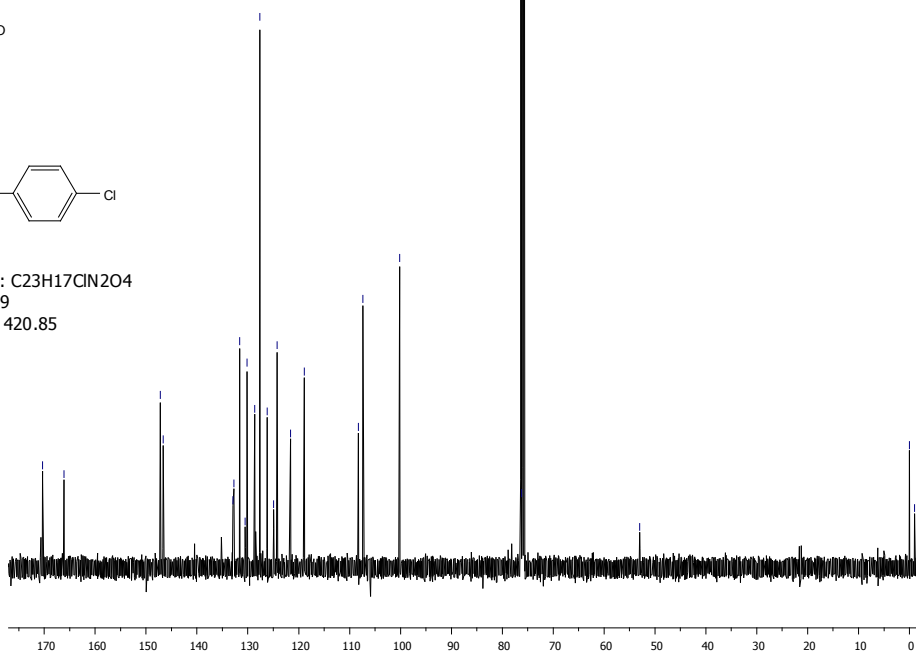
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 Molecular Weight: 420.85



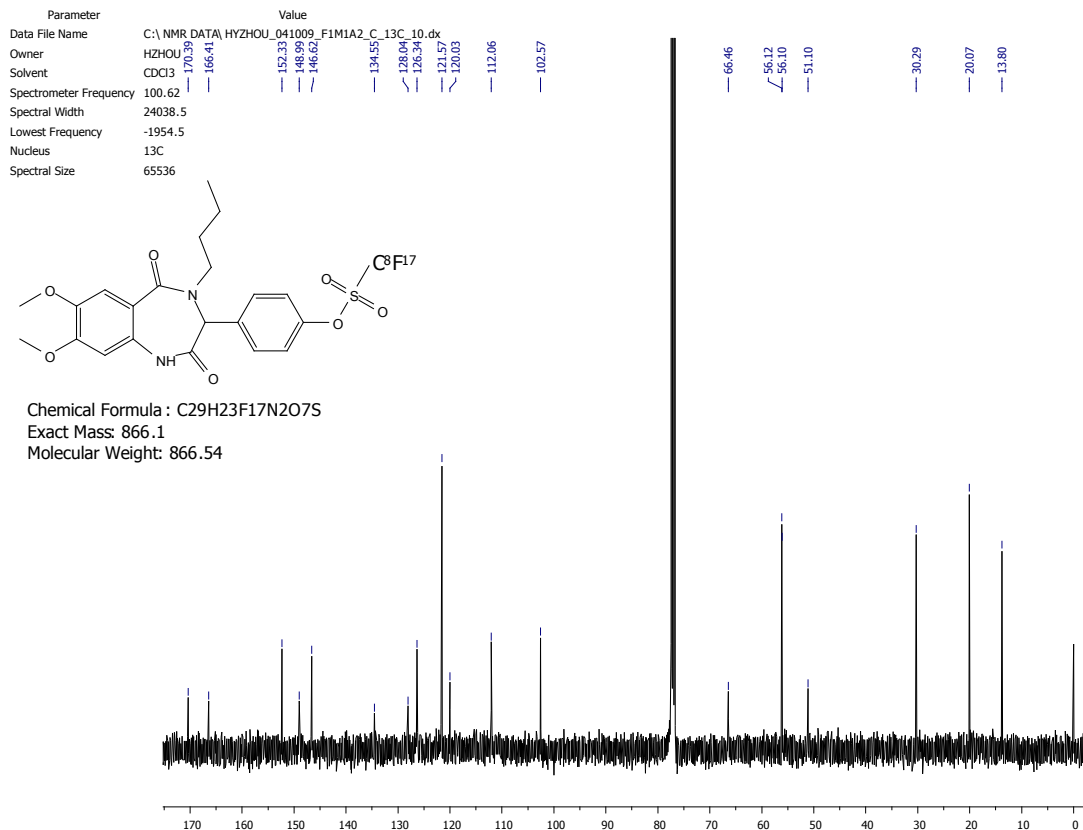
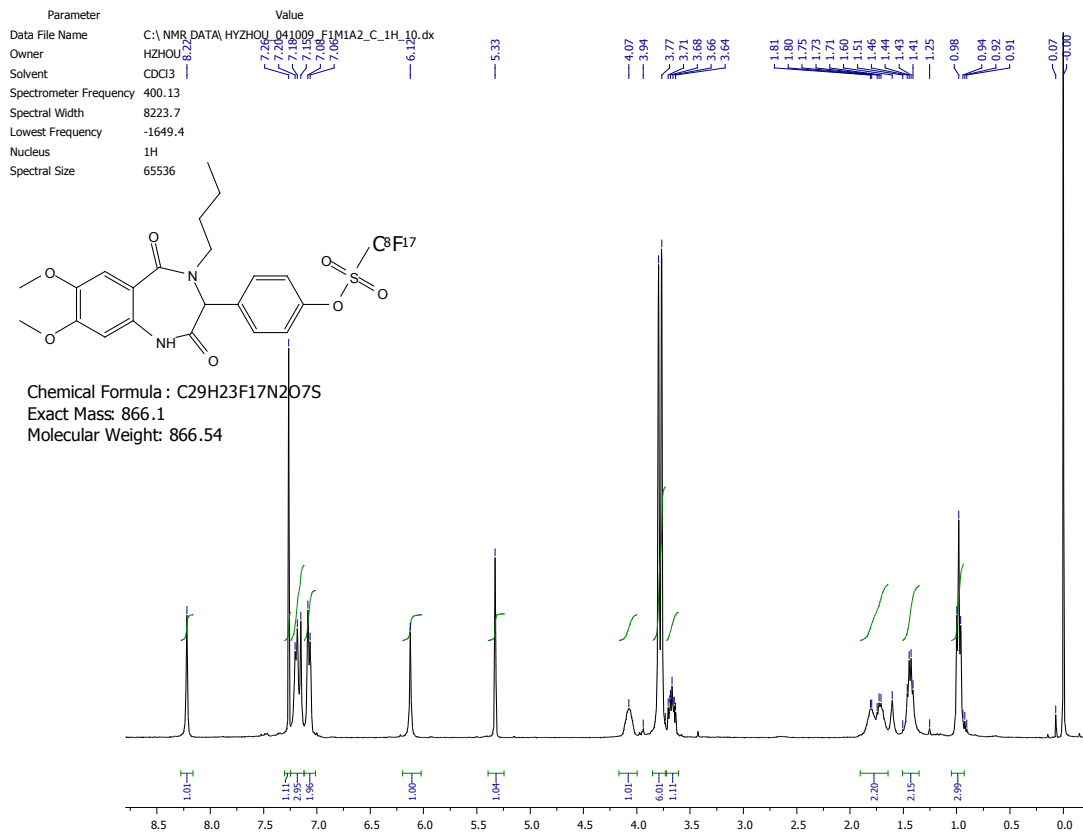
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Chemical Formula : C₂₃H₁₇ClN₂O₄
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 Molecular Weight: 420.85

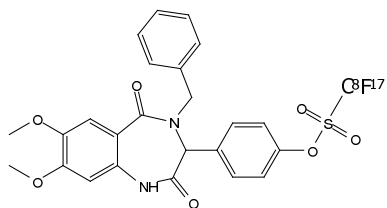


6{2,1,1} – ¹H and ¹³C NMR

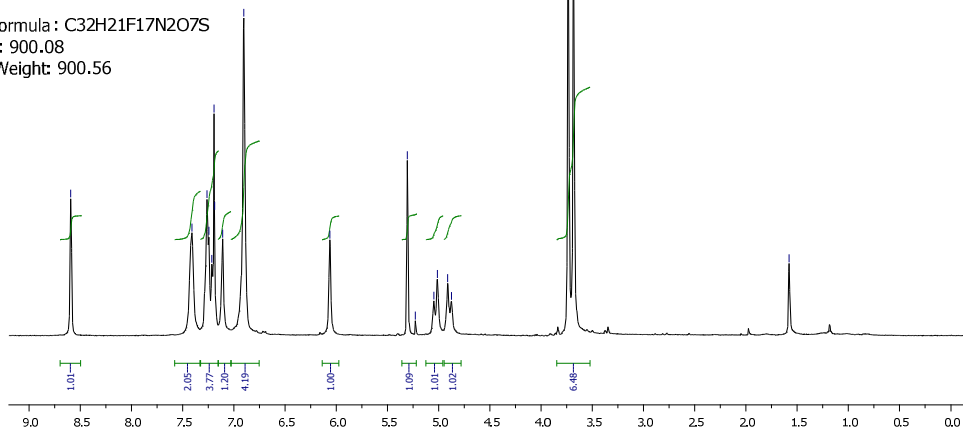


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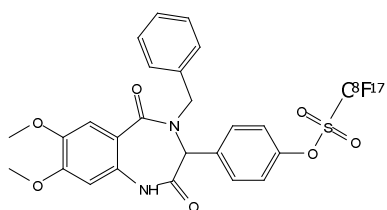
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Nucleus	¹ H
Spectral Size	65536



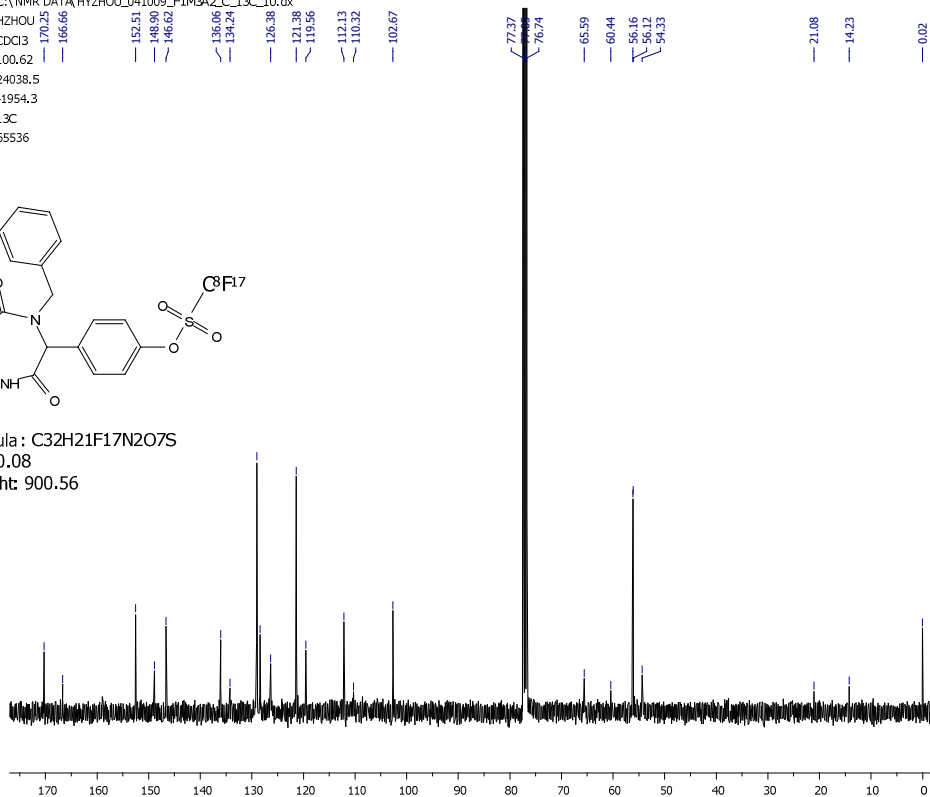
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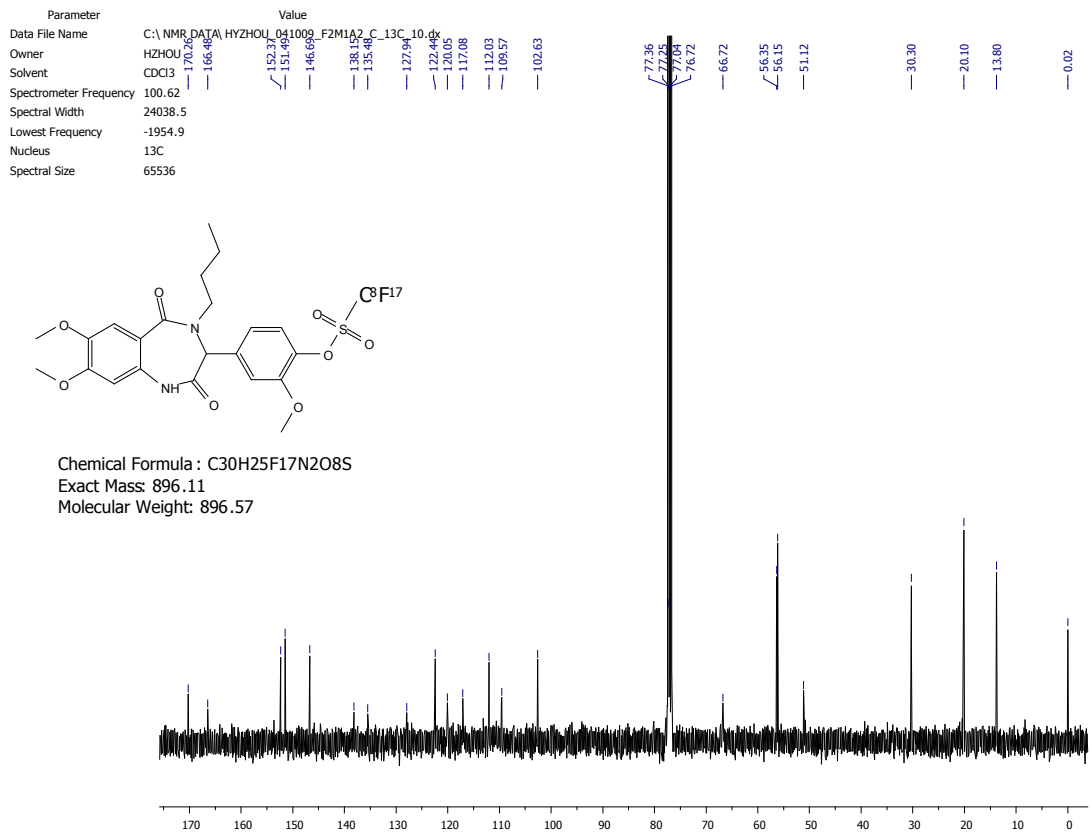
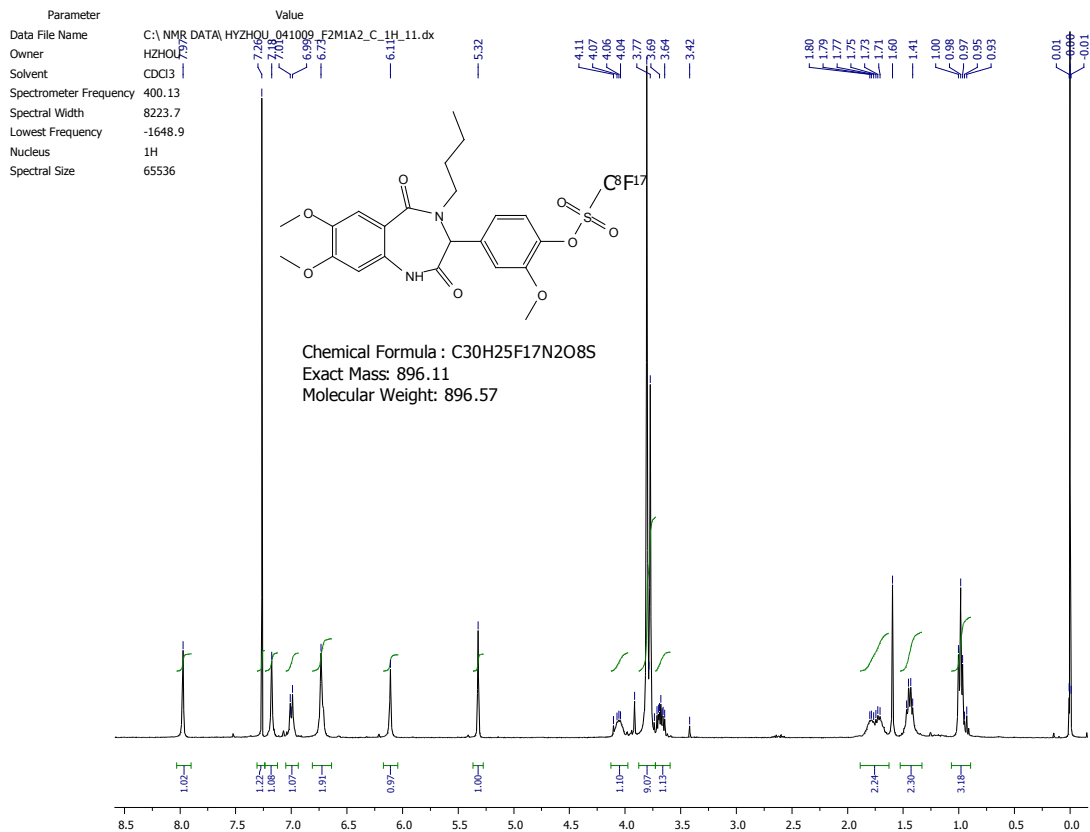
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Nucleus	¹³ C
Spectral Size	65536



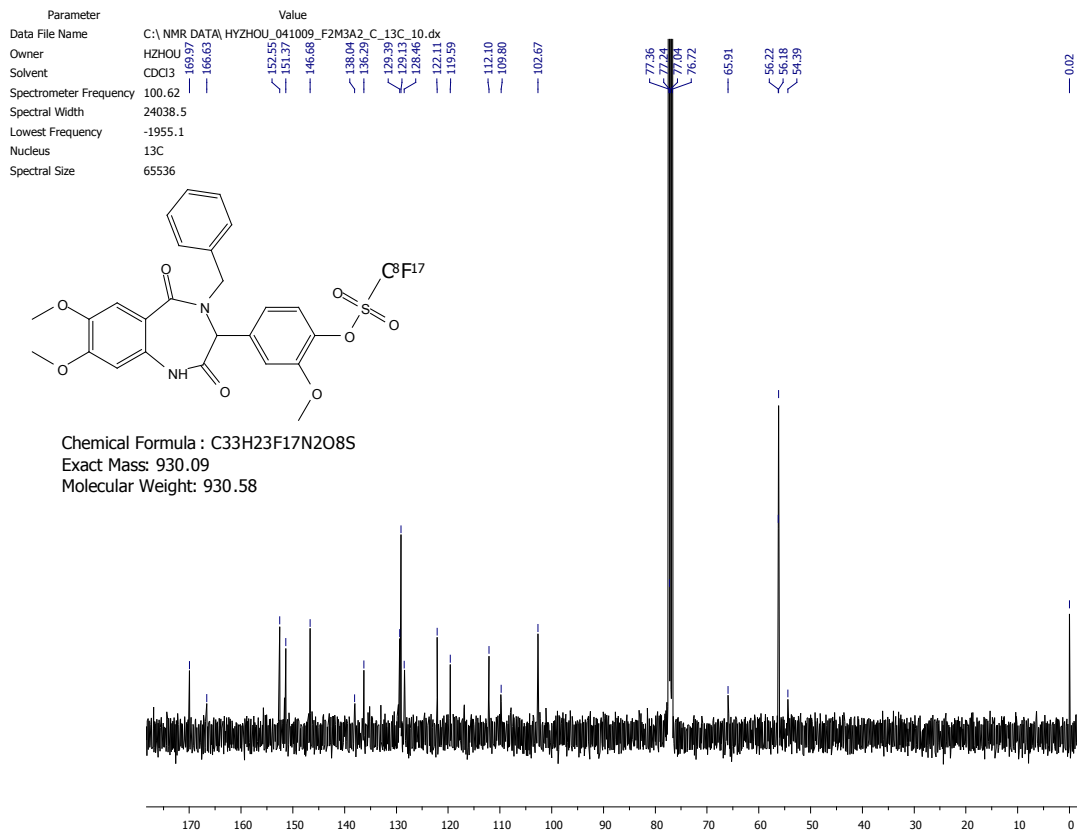
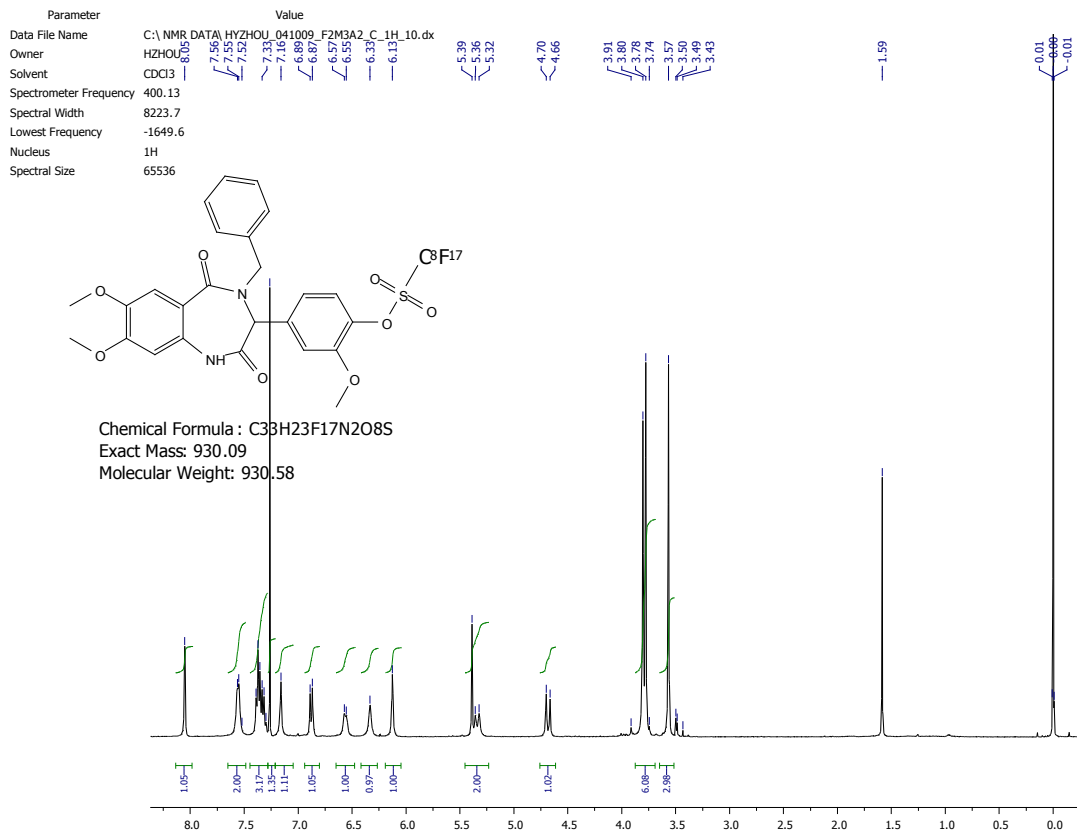
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 Molecular Weight: 900.56



6{2,2,1} – ¹H and ¹³C NMR

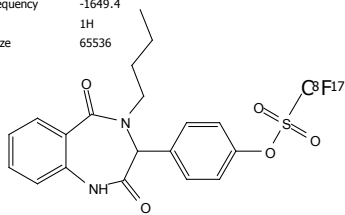


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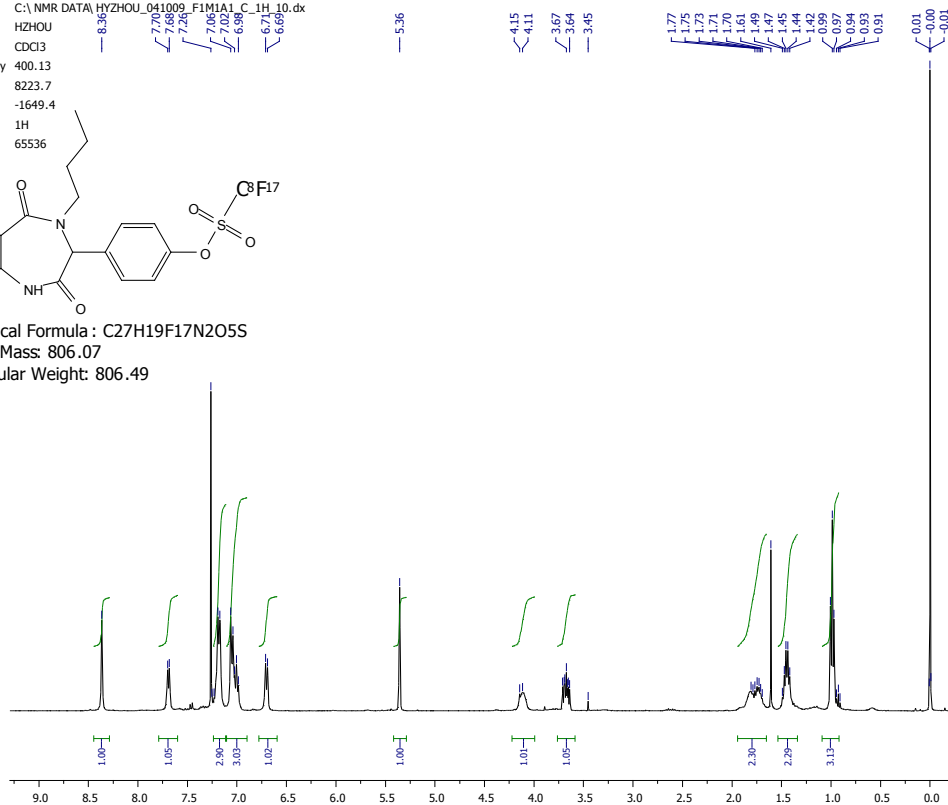


6{1,1,1} – ¹H and ¹³C NMR

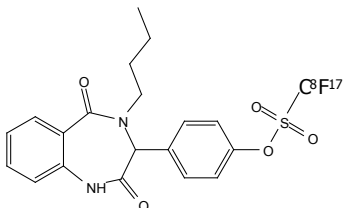
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Nucleus	¹ H
Spectral Size	65536



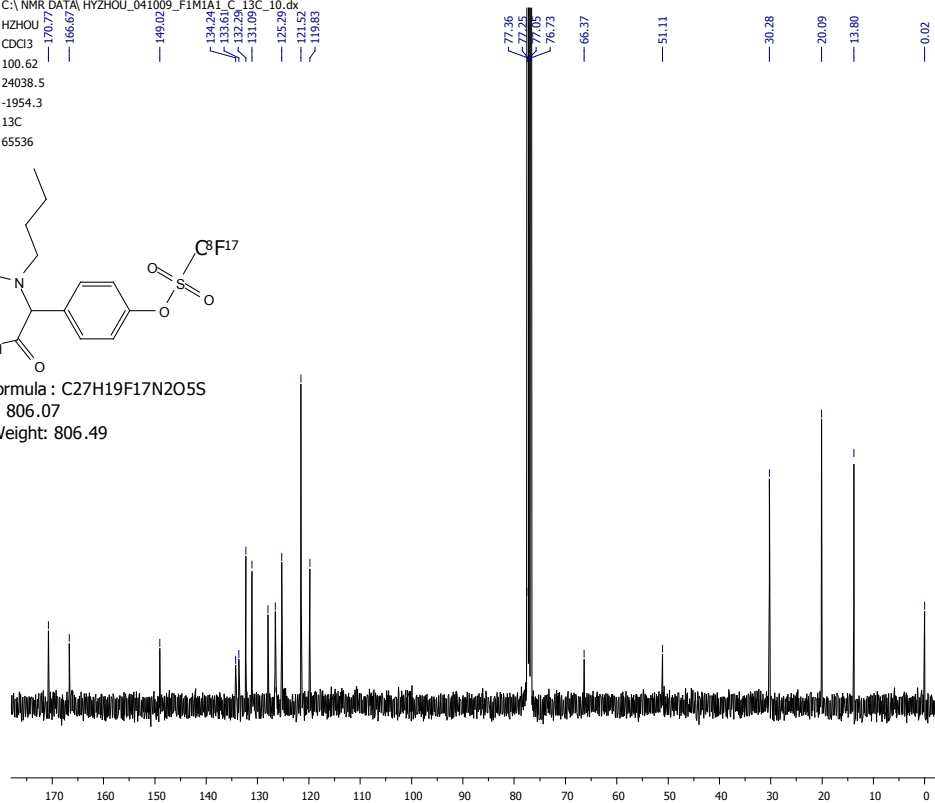
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Nucleus	¹³ C
Spectral Size	65536

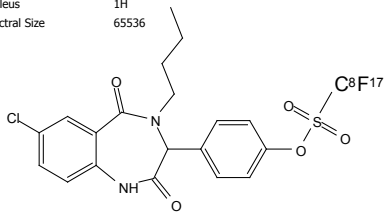


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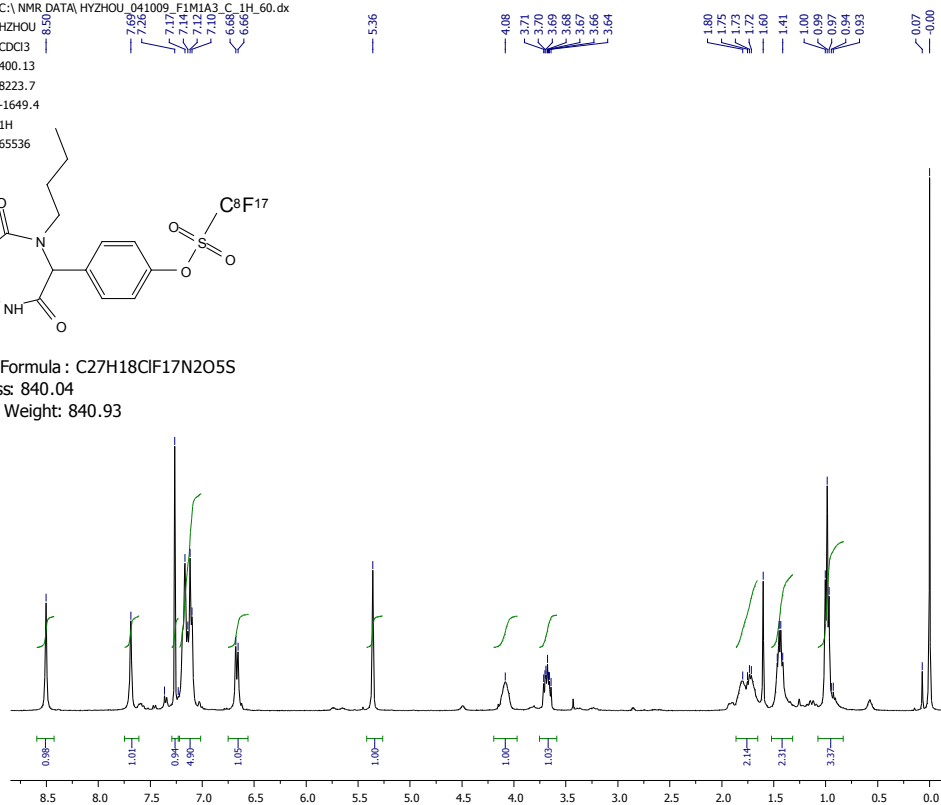


6{3,1,1} – ¹H and ¹³C NMR

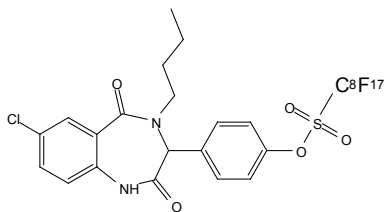
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Lowest Frequency	-1649.4
Nucleus	¹ H
Spectral Size	65536



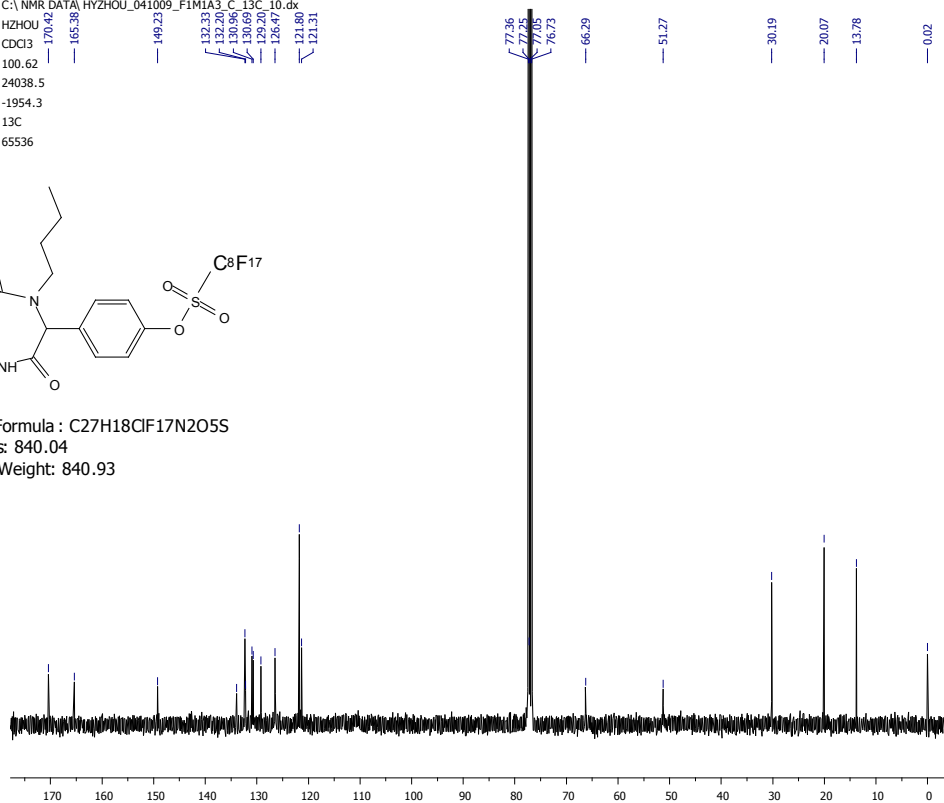
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 Molecular Weight: 840.93



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Nucleus	¹³ C
Spectral Size	65536

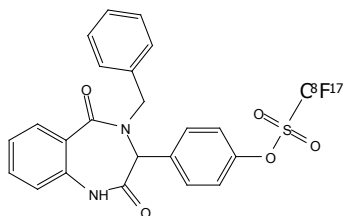


Chemical Formula : C₂₇H₁₈ClF₁₇N₂O₅S
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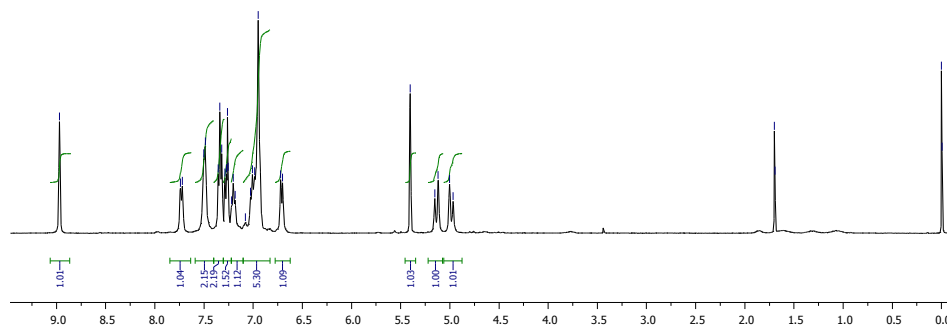


6{1,1,3} – ¹H and ¹³C NMR

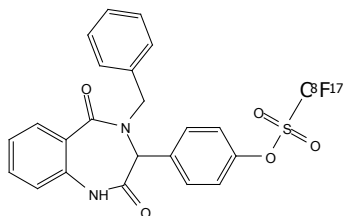
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Lowest Frequency	-1650.8
Nucleus	¹ H
Spectral Size	65536



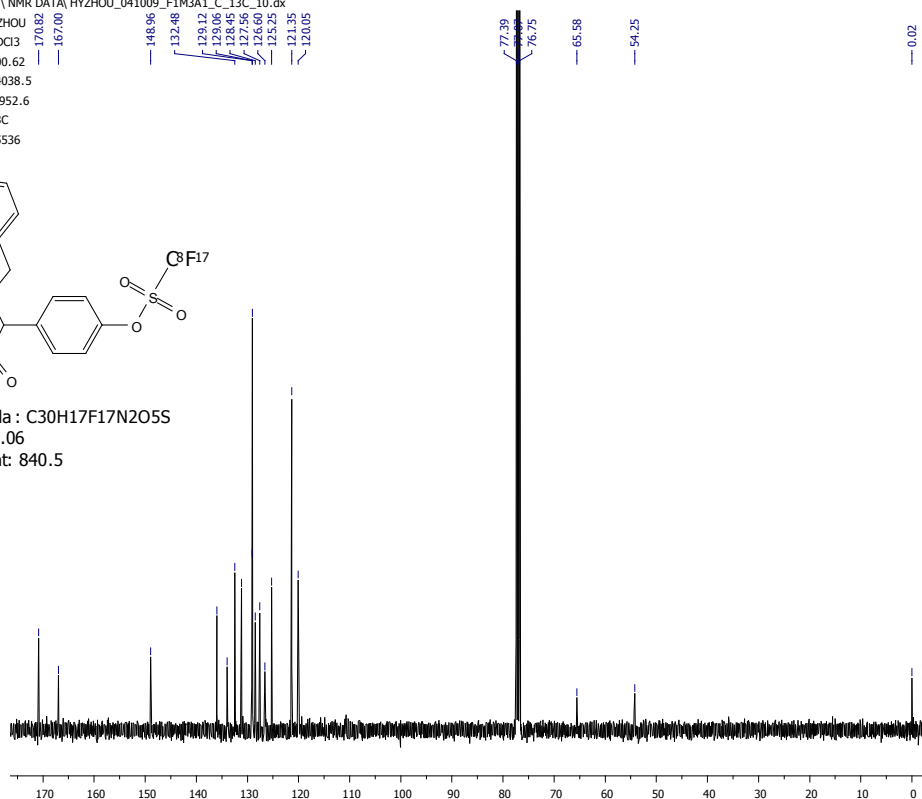
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 Molecular Weight: 840.5



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Spectral Size	65536

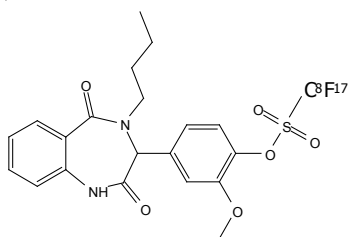


Chemical Formula : C₃₀H₁₇F₁₇N₂O₅
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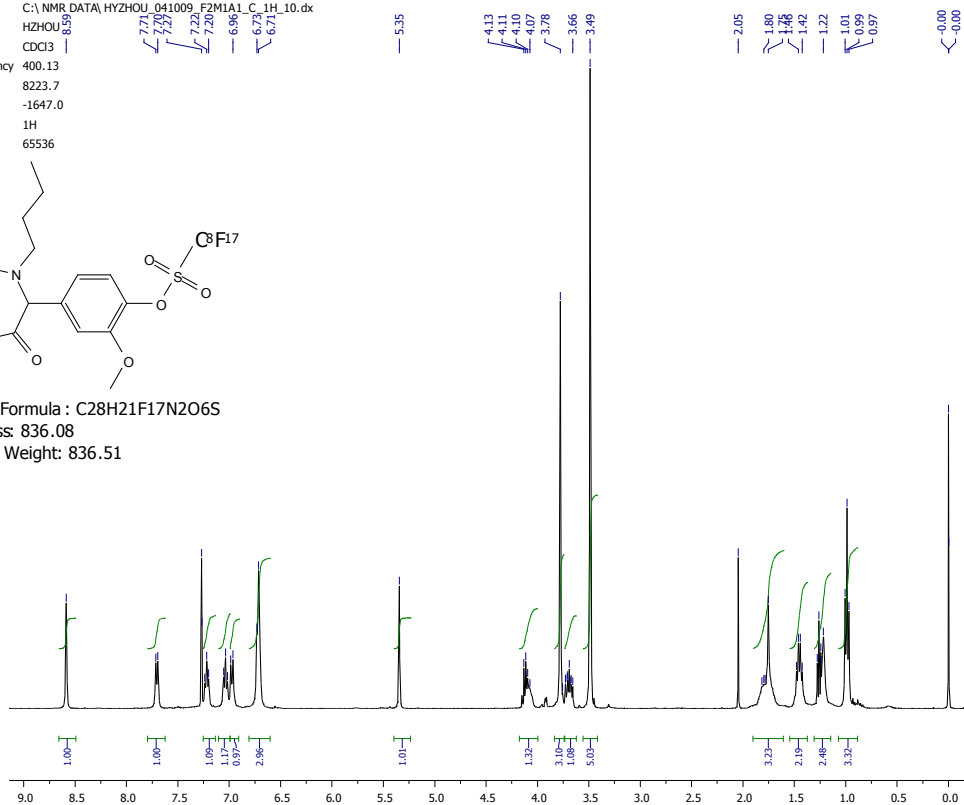


6{1,2,1} – ¹H and ¹³C NMR

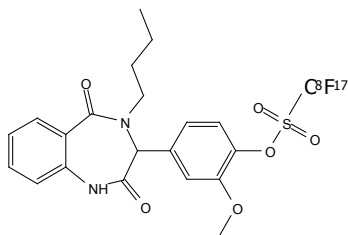
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Nucleus	¹ H
Spectral Size	65536



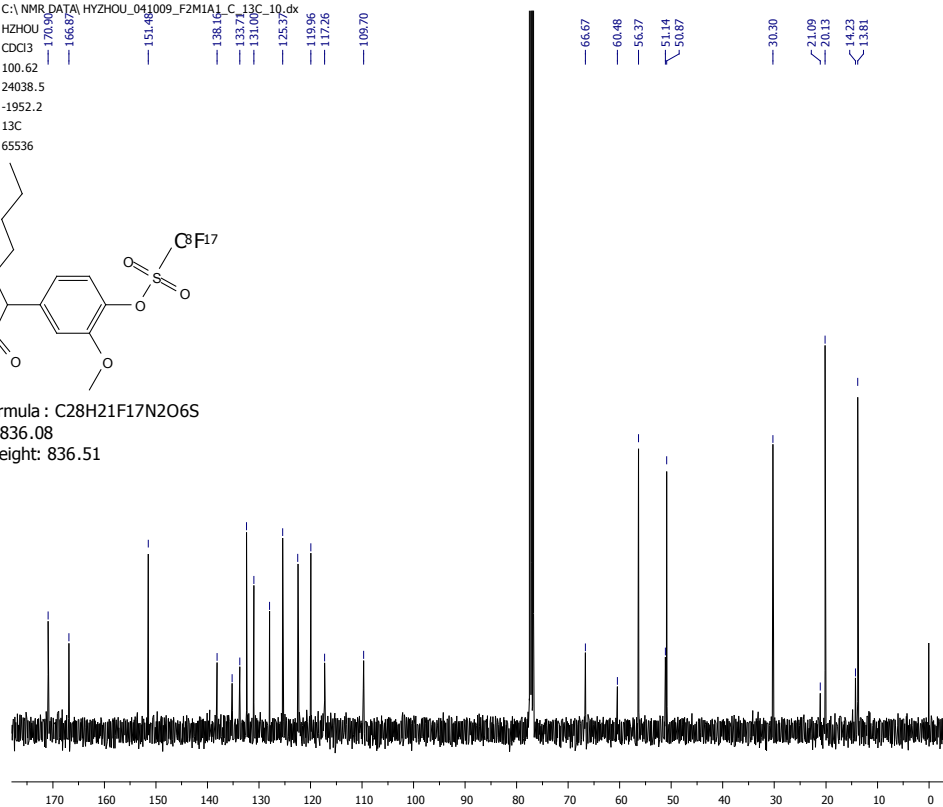
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 Molecular Weight: 836.51



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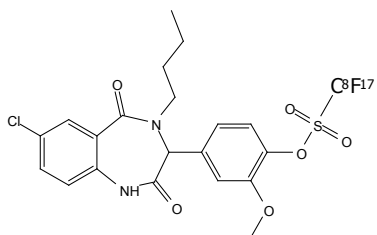


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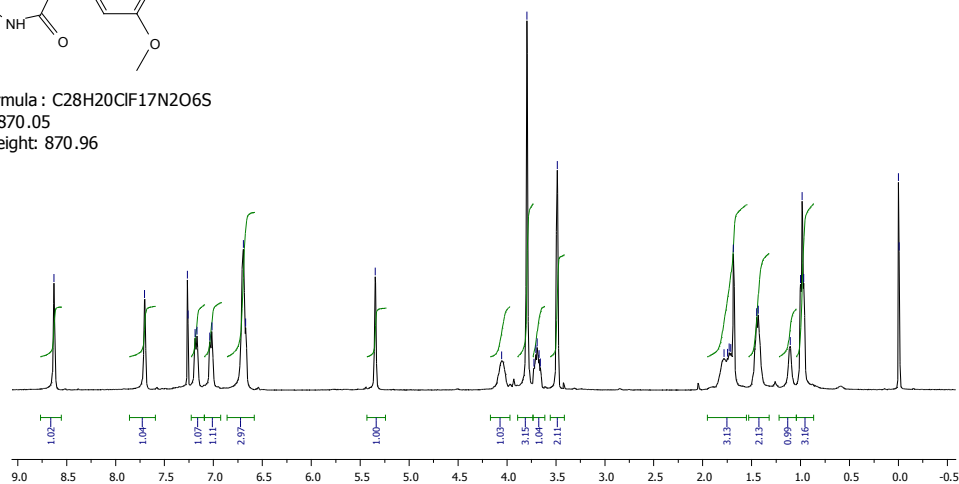


6{3,2,1} – ¹H and ¹³C NMR

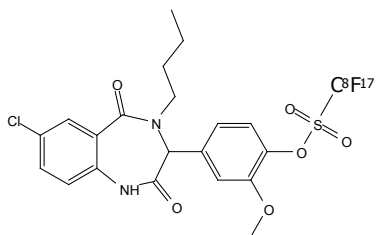
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Nucleus	¹ H
Spectral Size	65536



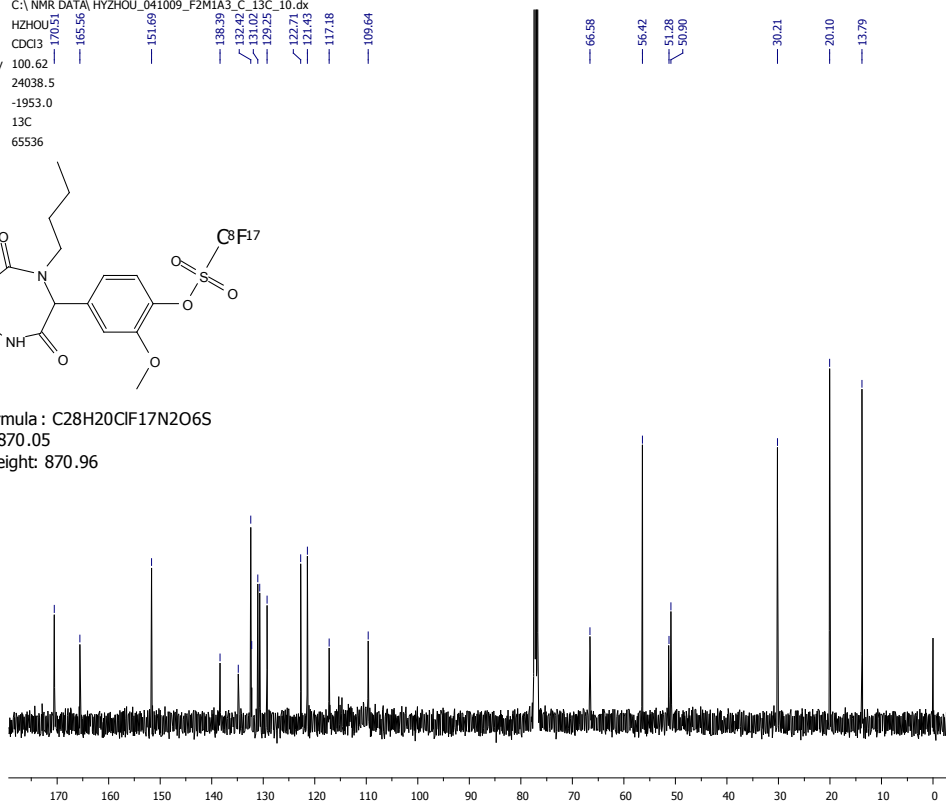
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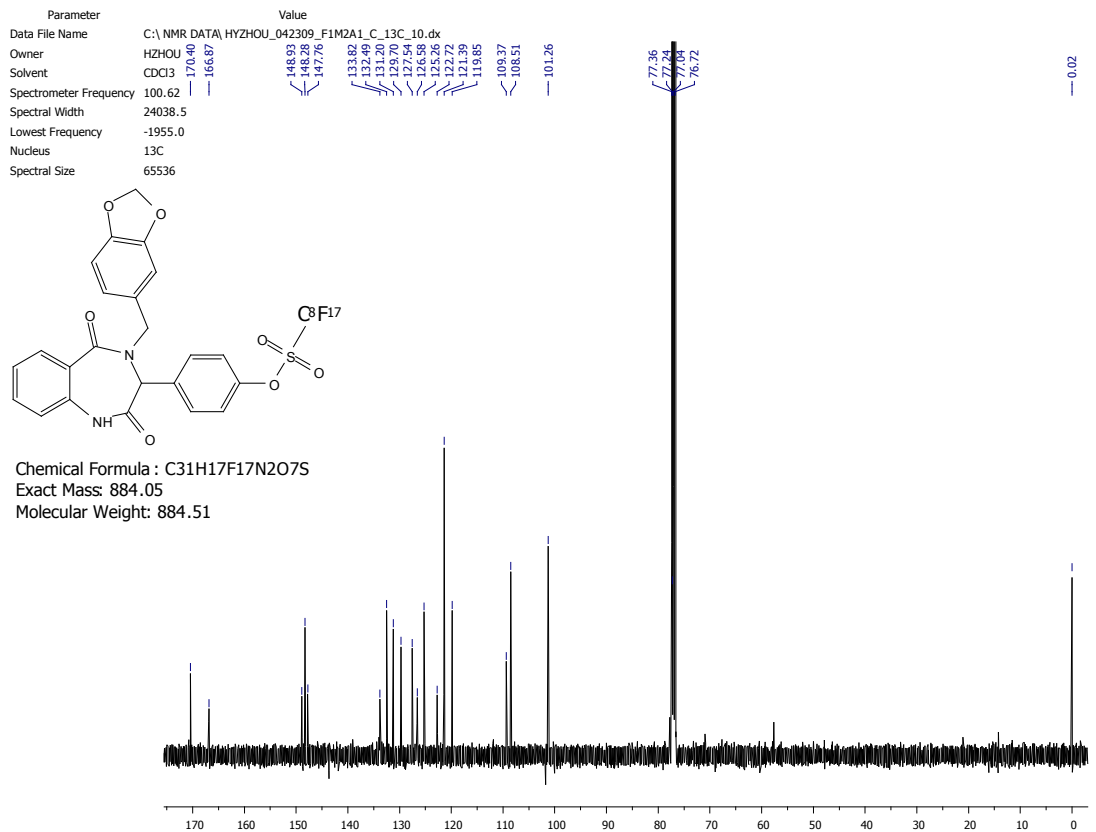
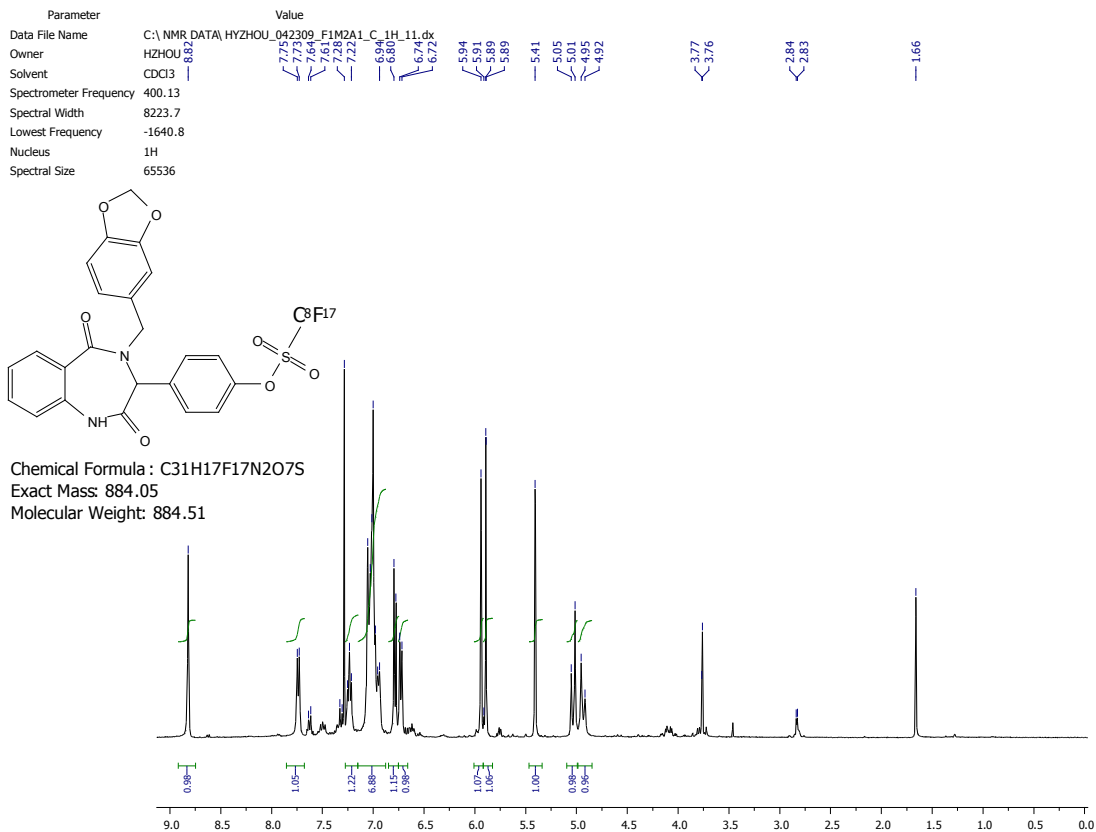
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Nucleus	¹³ C
Spectral Size	65536



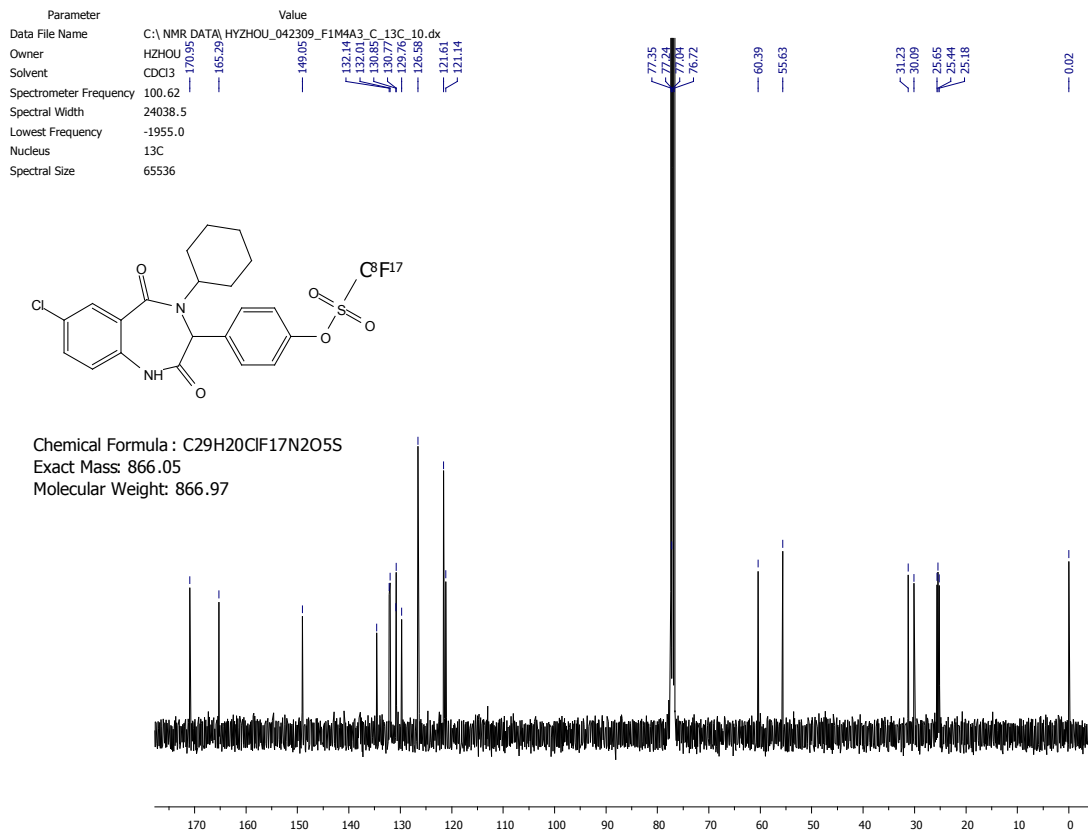
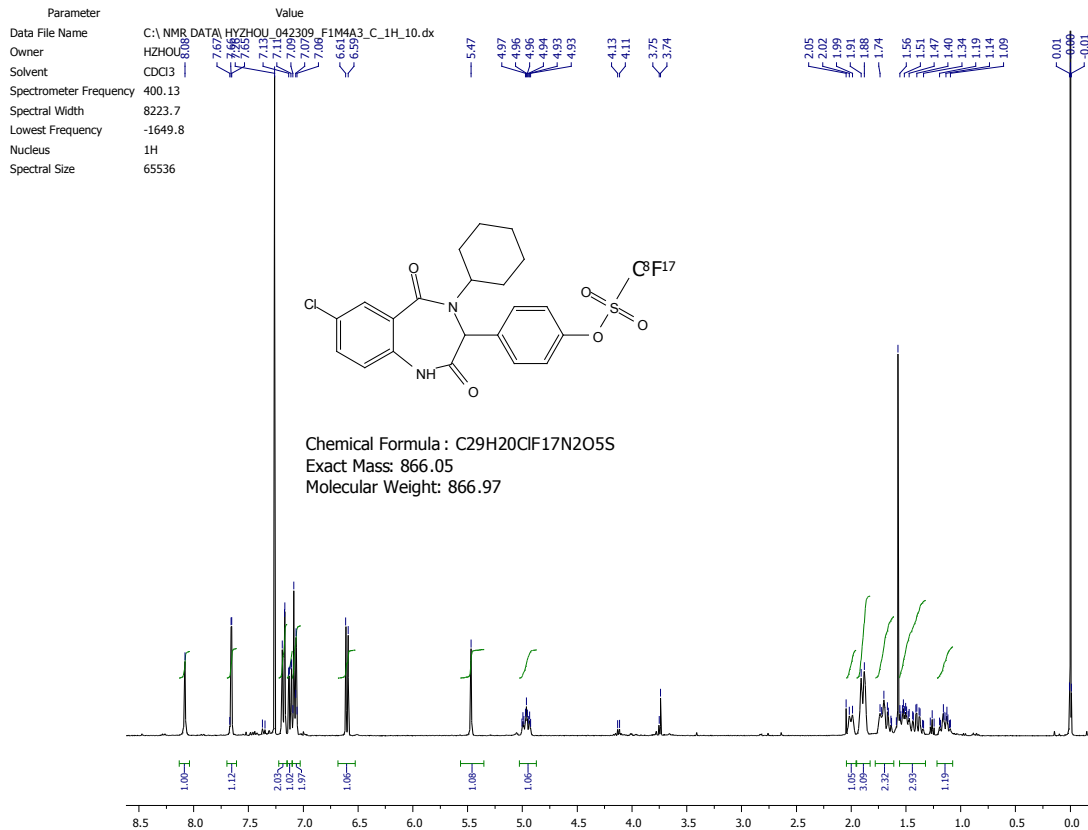
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 Molecular Weight: 870.96



6{1,1,2} – ¹H and ¹³C NMR

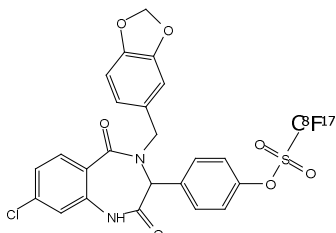


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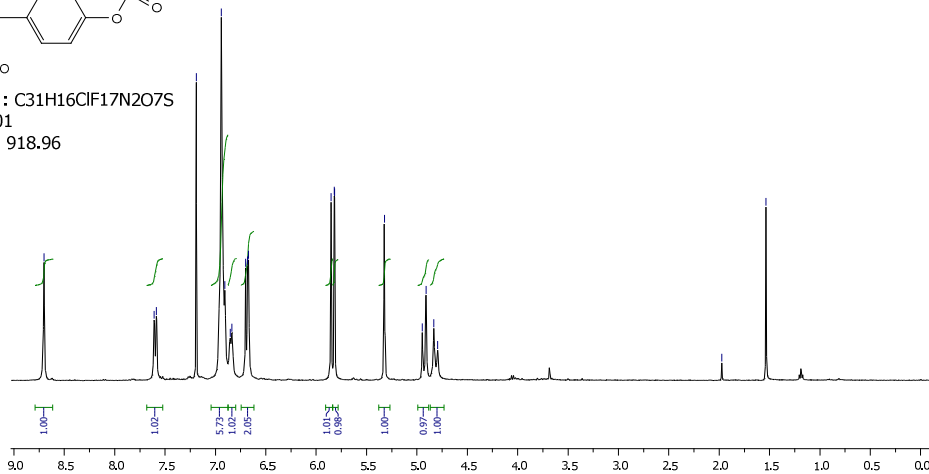


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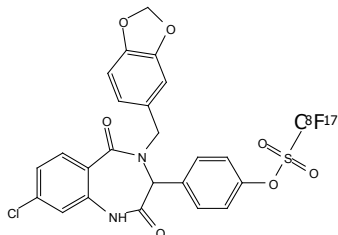
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Spectral Width	8223.7
Lowest Frequency	-1678.4
Nucleus	¹ H
Spectral Size	65536



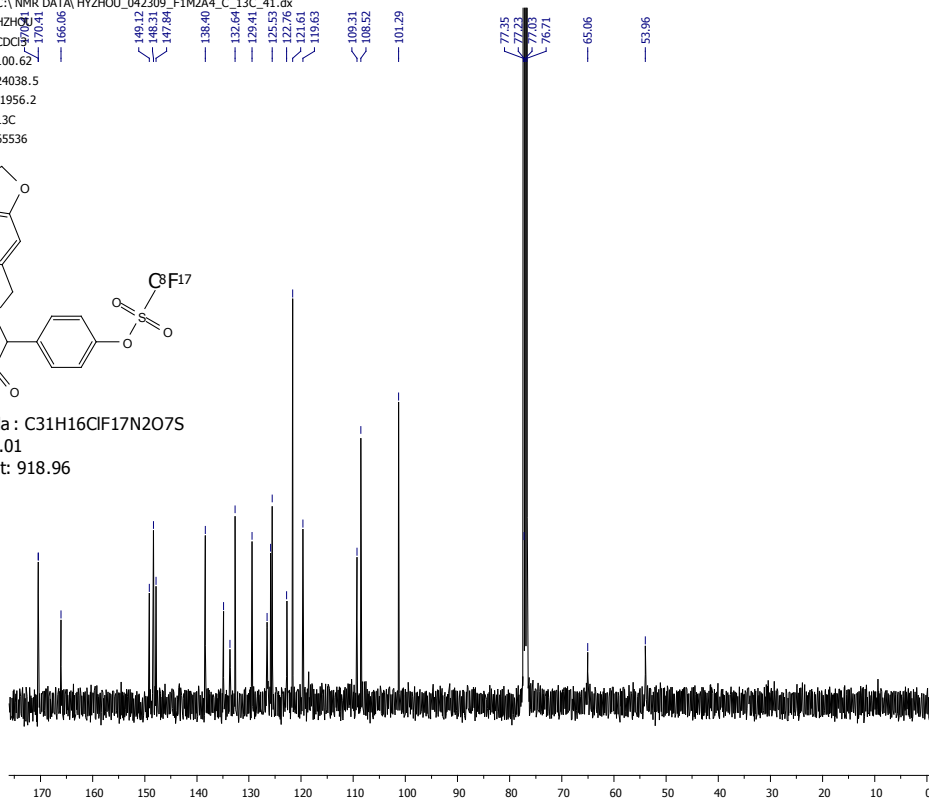
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 Molecular Weight: 918.96



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Spectral Size	65536

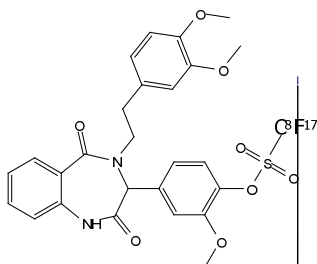


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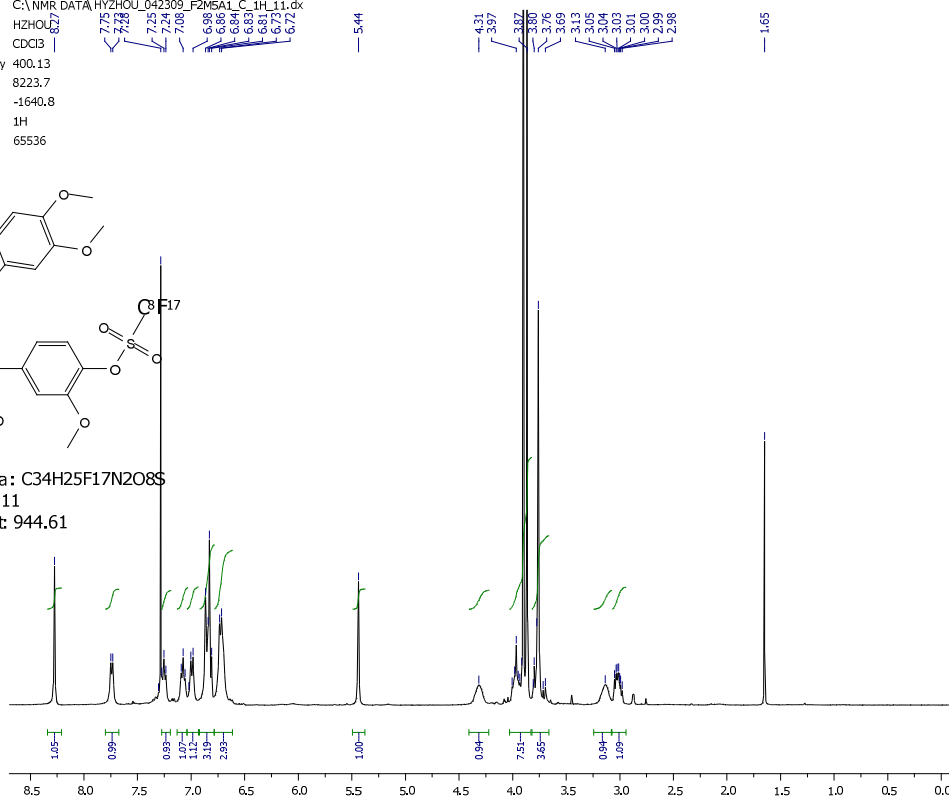


6{1,2,5} – ¹H and ¹³C NMR

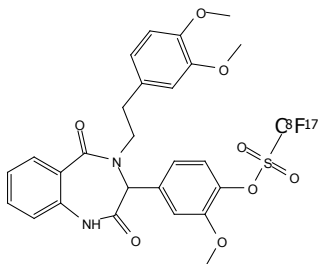
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Nucleus	1H
Spectral Size	65536



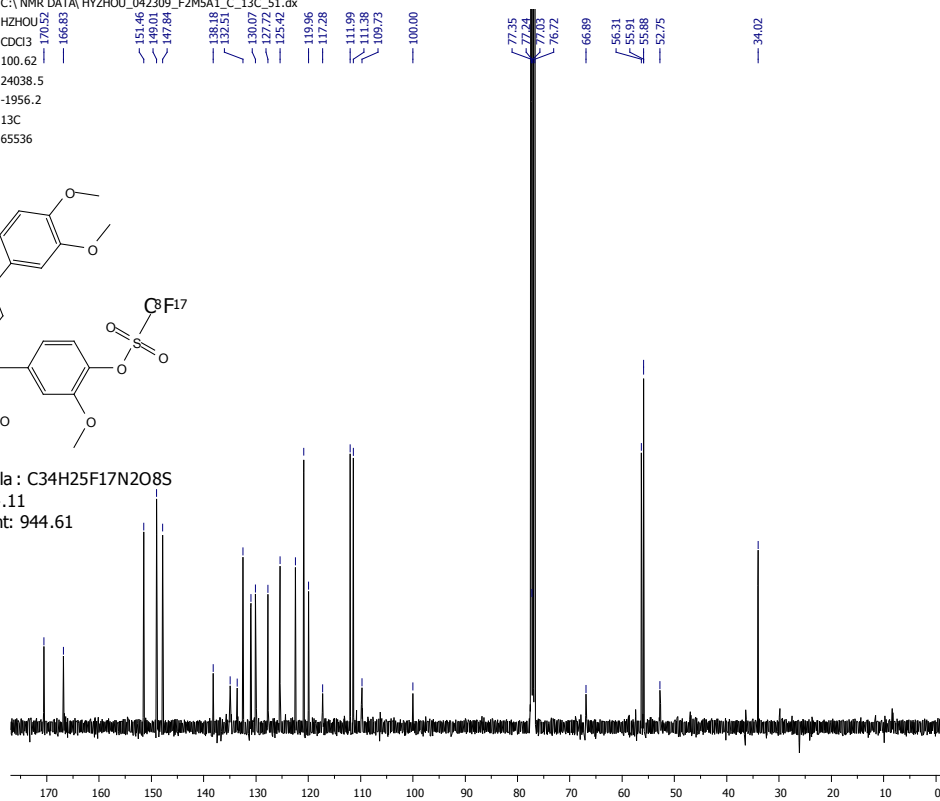
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Solvent	CDCl3
Spectrometer Frequency	100.62
Spectral Width	24038.5
Lowest Frequency	-1956.2
Nucleus	13C
Spectral Size	65536

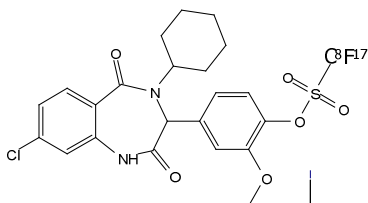


Chemical Formula : C₃₄H₂₅F₁₇N₂O₈S
 Exact Mass: 944.11
 Molecular Weight: 944.61

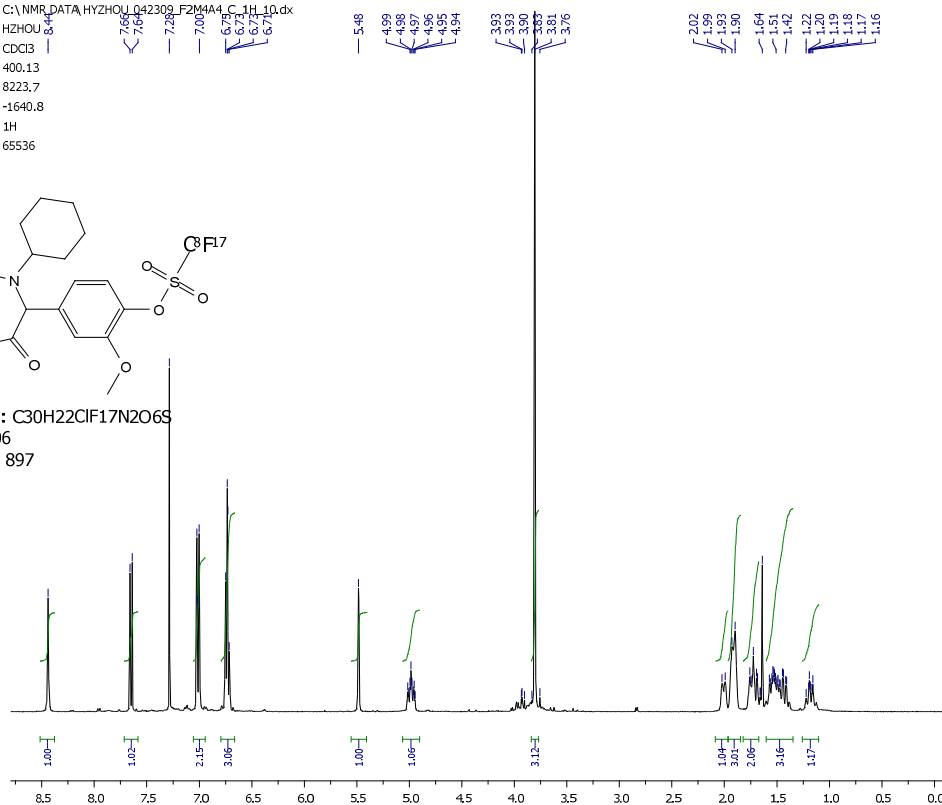


6{4,2,4} – ¹H and ¹³C NMR

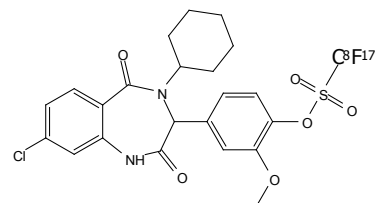
Parameter Value
 Data File Name C:\NMR_DATA\HZHOU_042309_F2M4A4_C_1H_10.dx
 Owner HZHOU 84
 Solvent CDCl3
 Spectrometer Frequency 400.13
 Spectral Width 8223.7
 Lowest Frequency -1640.8
 Nucleus 1H
 Spectral Size 65536



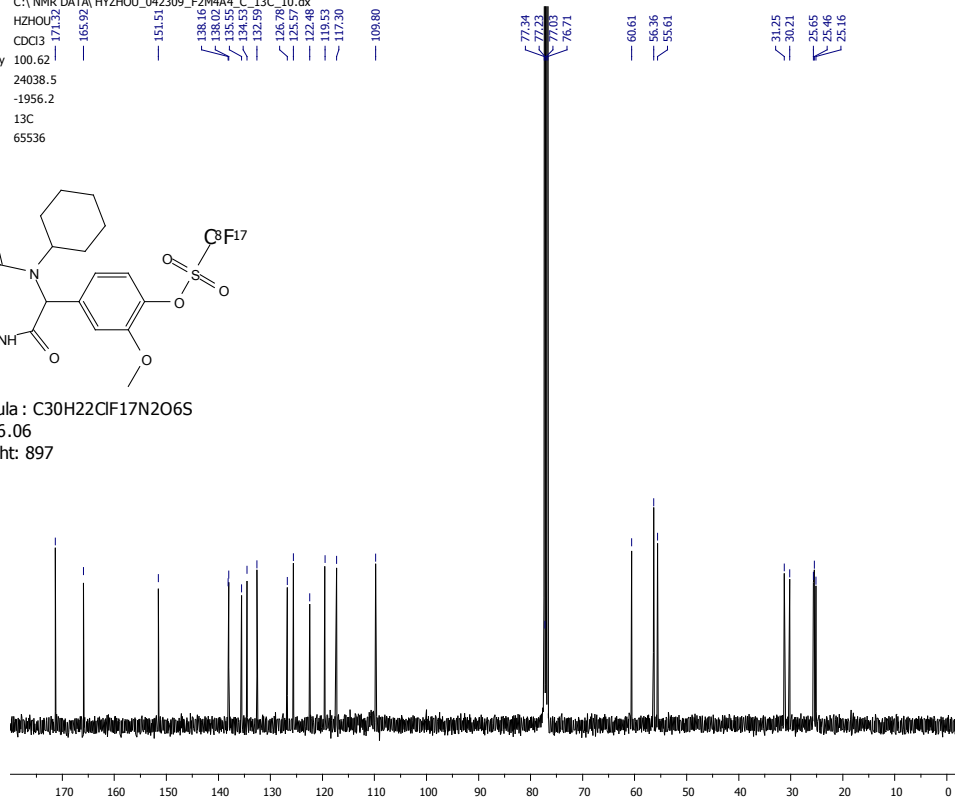
Chemical Formula: C₃₀H₂₂ClF₁₇N₂O₆S
 Exact Mass: 896.06
 Molecular Weight: 897



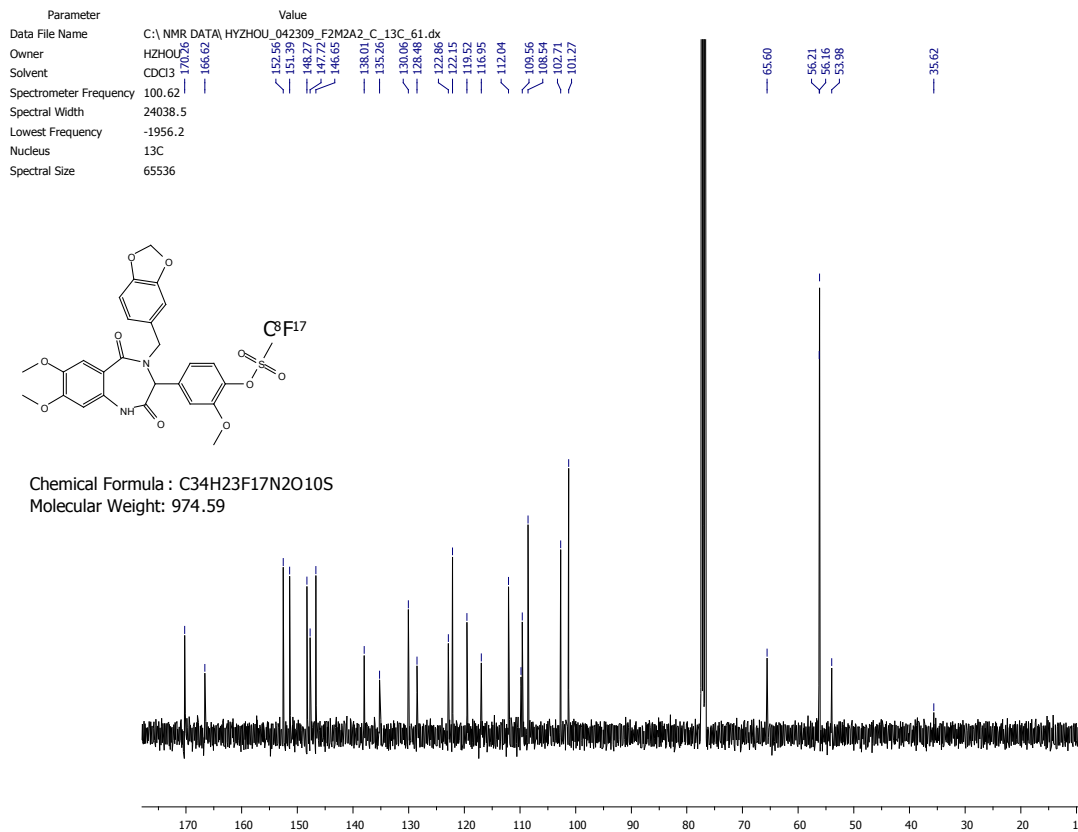
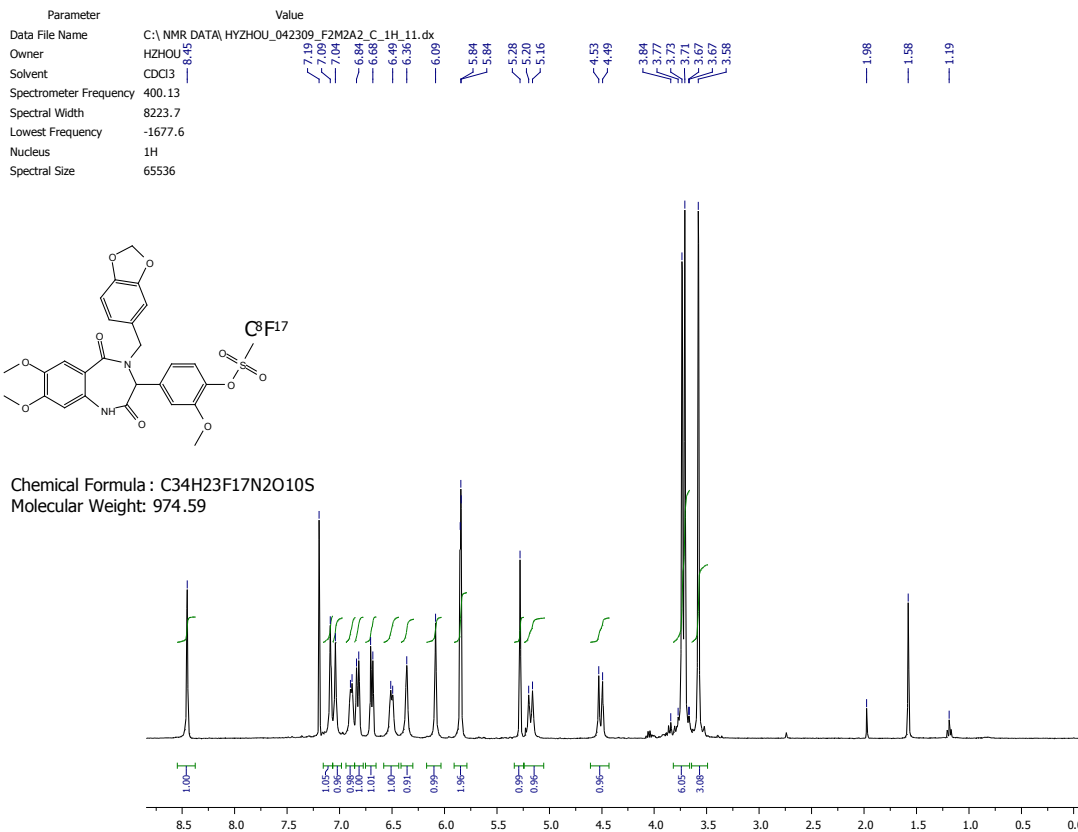
Parameter Value
 Data File Name C:\NMR_DATA\HZHOU_042309_F2M4A4_C_13C_10.dx
 Owner HZHOU 84
 Solvent CDCl3
 Spectrometer Frequency 100.62
 Spectral Width 24038.5
 Lowest Frequency -1956.2
 Nucleus 13C
 Spectral Size 65536



Chemical Formula: C₃₀H₂₂ClF₁₇N₂O₆S
 Exact Mass: 896.06
 Molecular Weight: 897

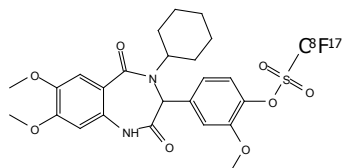


6{2,2,2} – ¹H and ¹³C NMR

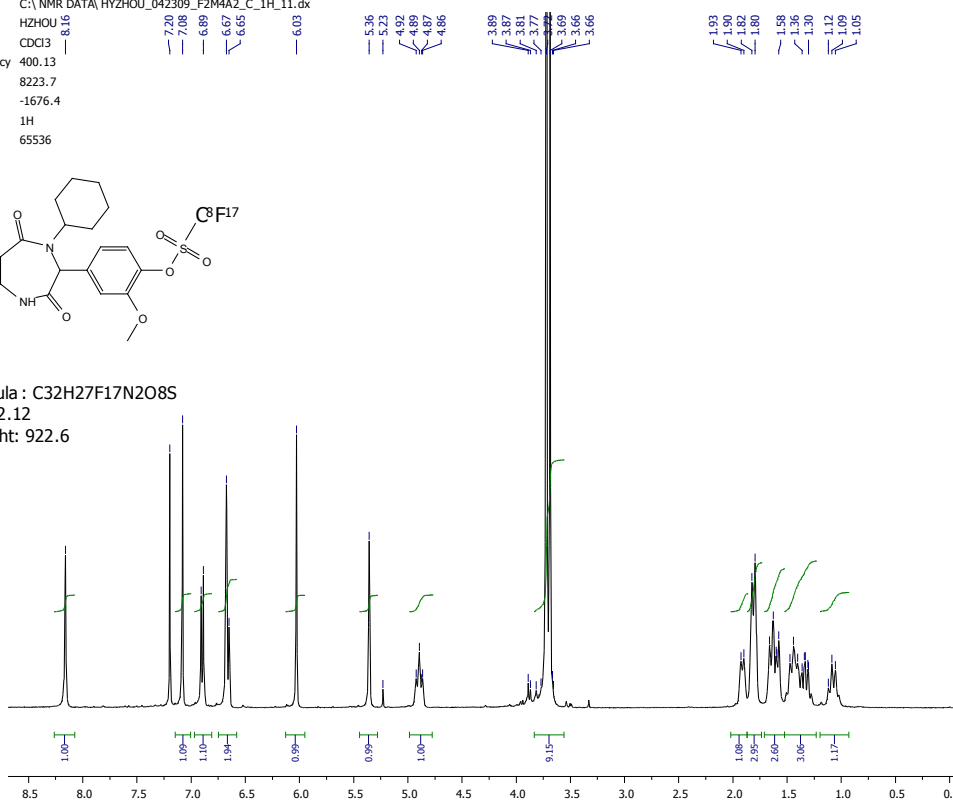


6{2,2,4} – ¹H and ¹³C NMR

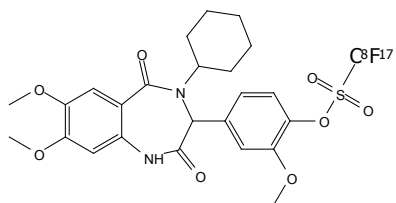
Parameter	Value
Data File Name	C:\NMR DATA\HYZHOU_042309_F2M4A2_C_1H_11.dx
Owner	HZHOU
Solvent	CDCl3
Spectrometer Frequency	400.13
Spectral Width	8223.7
Lowest Frequency	-1676.4
Nucleus	¹ H
Spectral Size	65536



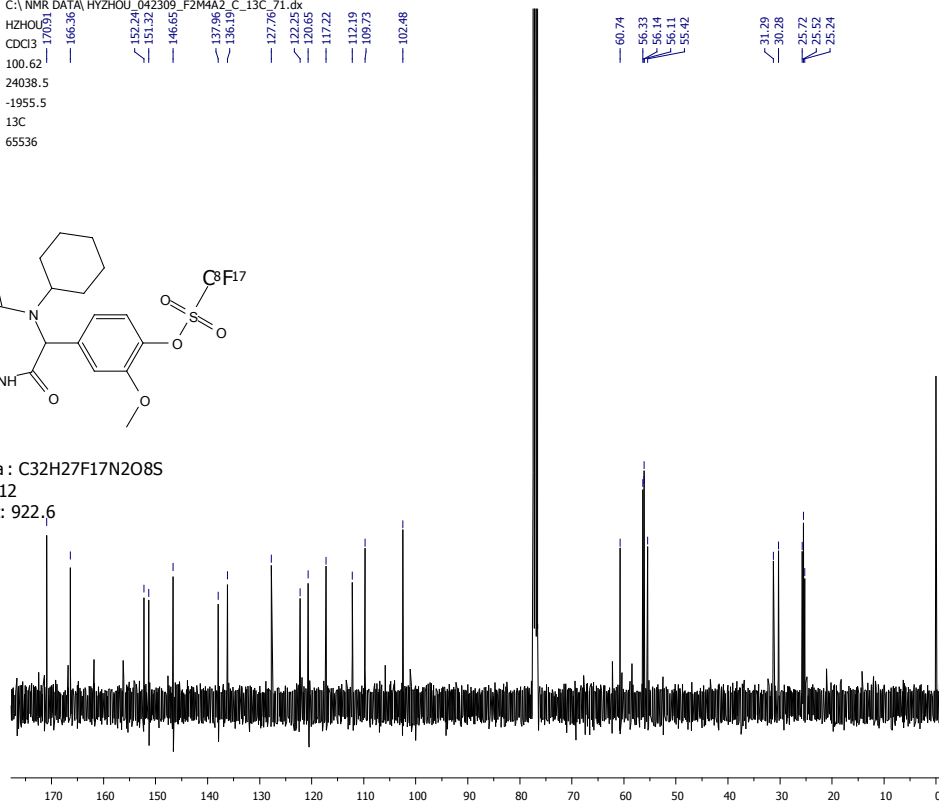
Chemical Formula : C₃₂H₂₇F₁₇N₂O₈
 Exact Mass: 922.12
 Molecular Weight: 922.6



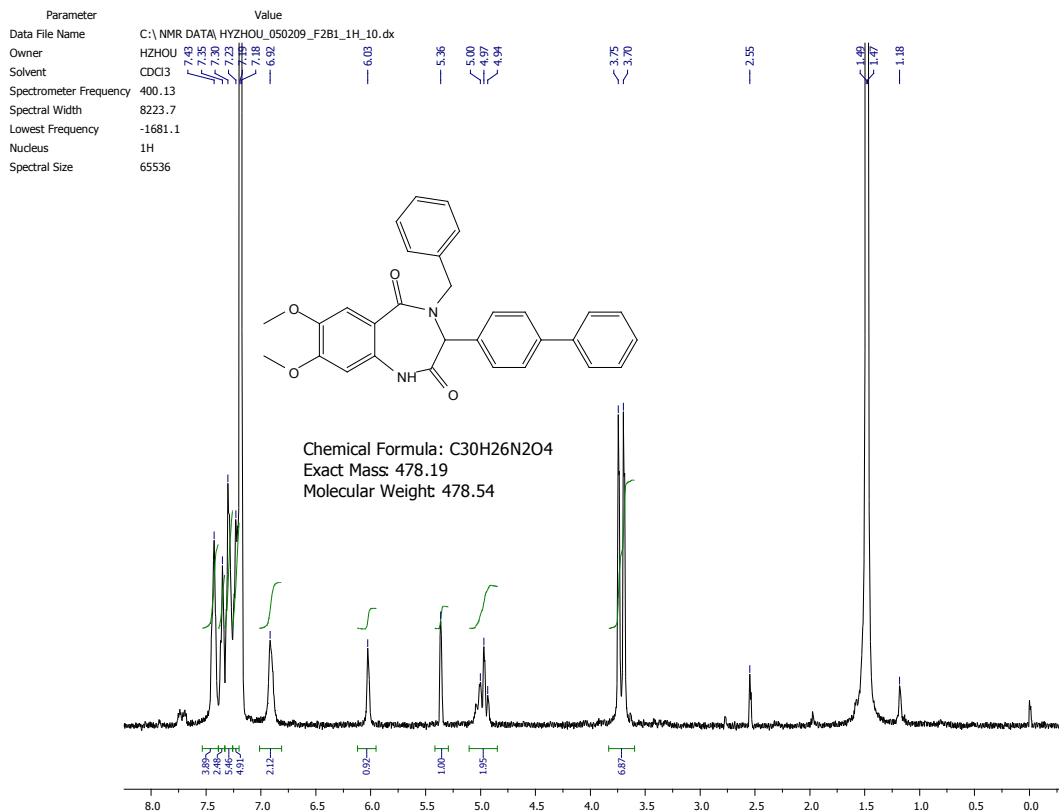
Parameter	Value
Data File Name	C:\NMR DATA\HYZHOU_042309_F2M4A2_C_13C_71.dx
Owner	HZHOU
Solvent	CDCl3
Spectrometer Frequency	100.62
Spectral Width	24038.5
Lowest Frequency	-1955.5
Nucleus	¹³ C
Spectral Size	65536



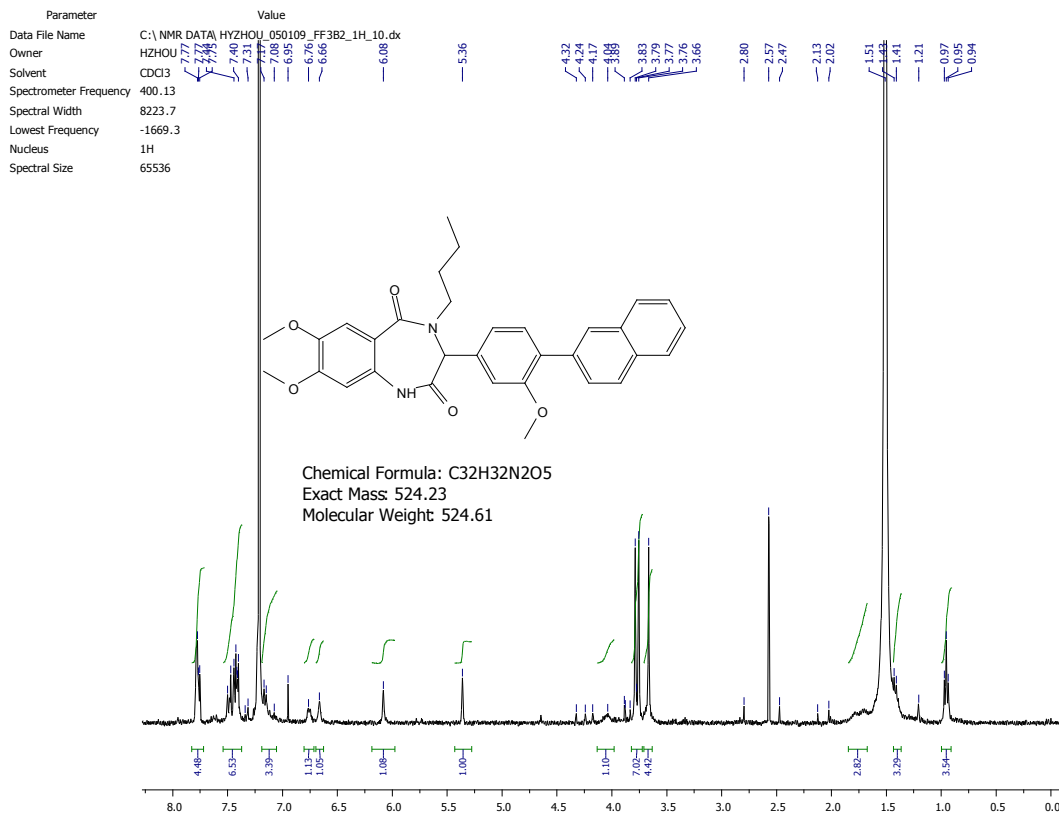
Chemical Formula : C₃₂H₂₇F₁₇N₂O₈
 Exact Mass: 922.12
 Molecular Weight: 922.6



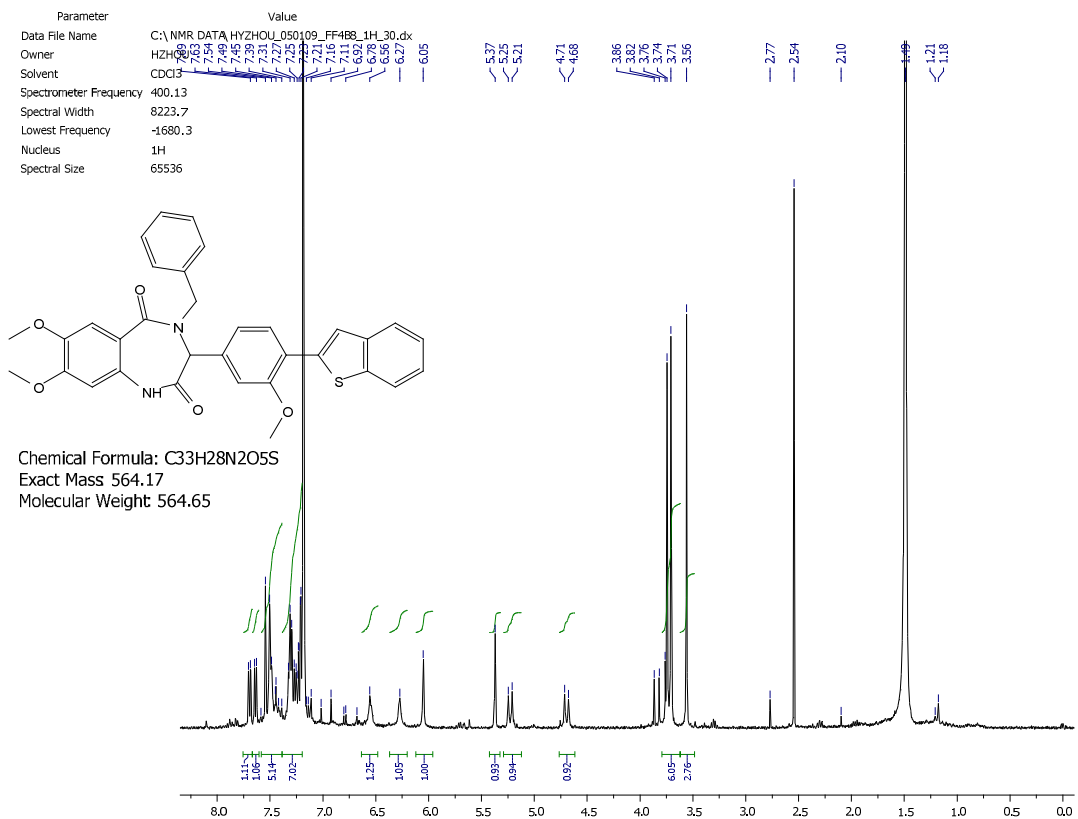
8{2,1,3,1} - ¹H NMR



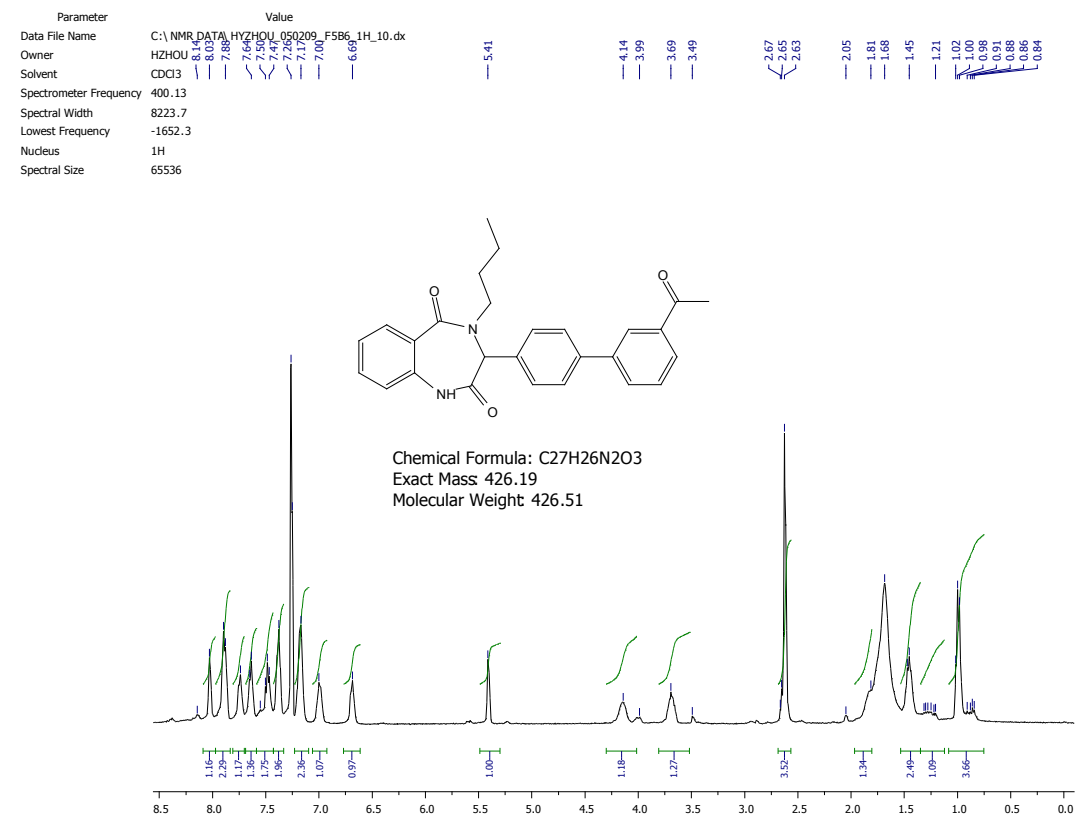
8{2,2,1,2} - ¹H NMR



8{2,2,3,6} - ¹H NMR

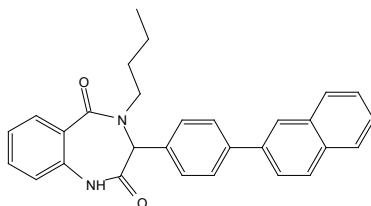


8{1,1,1,5} - ¹H NMR

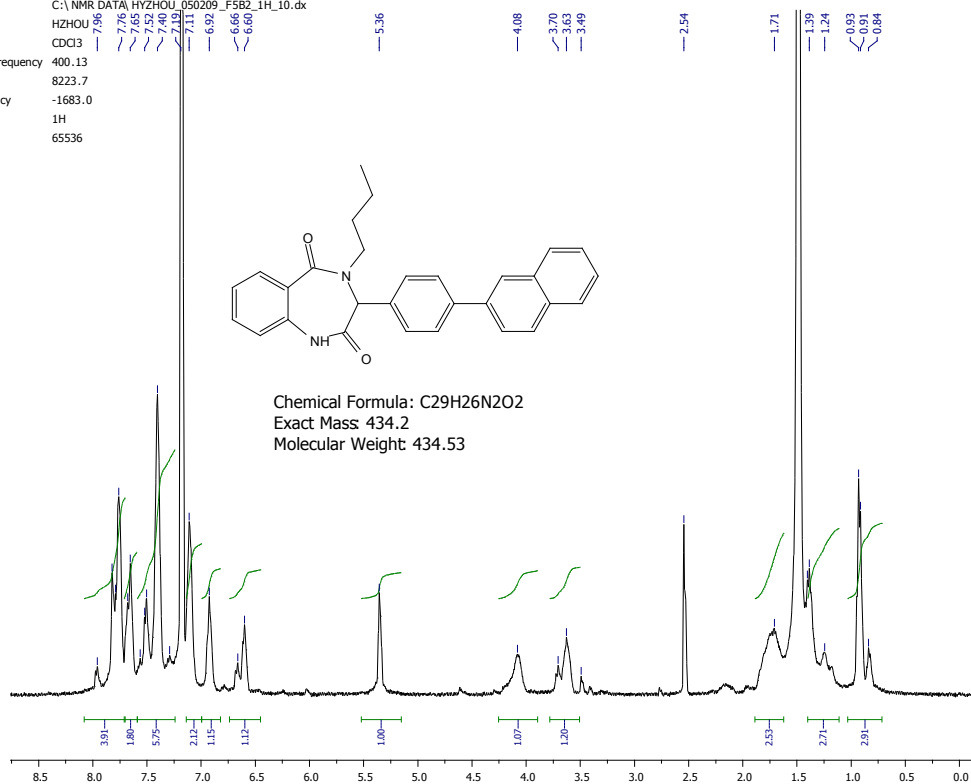


8{1,1,1,2} - ¹H NMR

Parameter	Value
Data File Name	C:\NMR DATA\HYZHOU_050209_FF582_1H_10.dx
Owner	HZHOU
Solvent	CDCl ₃
Spectrometer Frequency	400.13
Spectral Width	8223.7
Lowest Frequency	-1683.0
Nucleus	¹ H
Spectral Size	65536

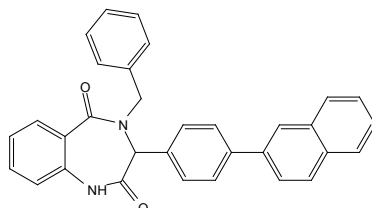


Chemical Formula: C₂₉H₂₆N₂O₂
 Exact Mass: 434.2
 Molecular Weight: 434.53

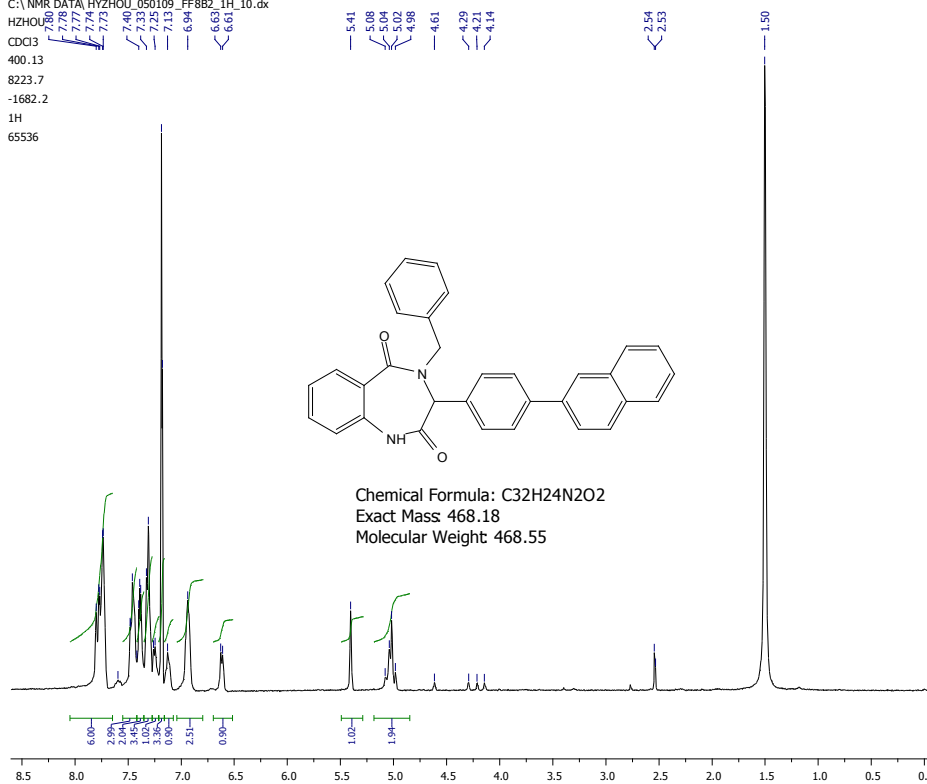


8{1,1,3,2} - ¹H NMR

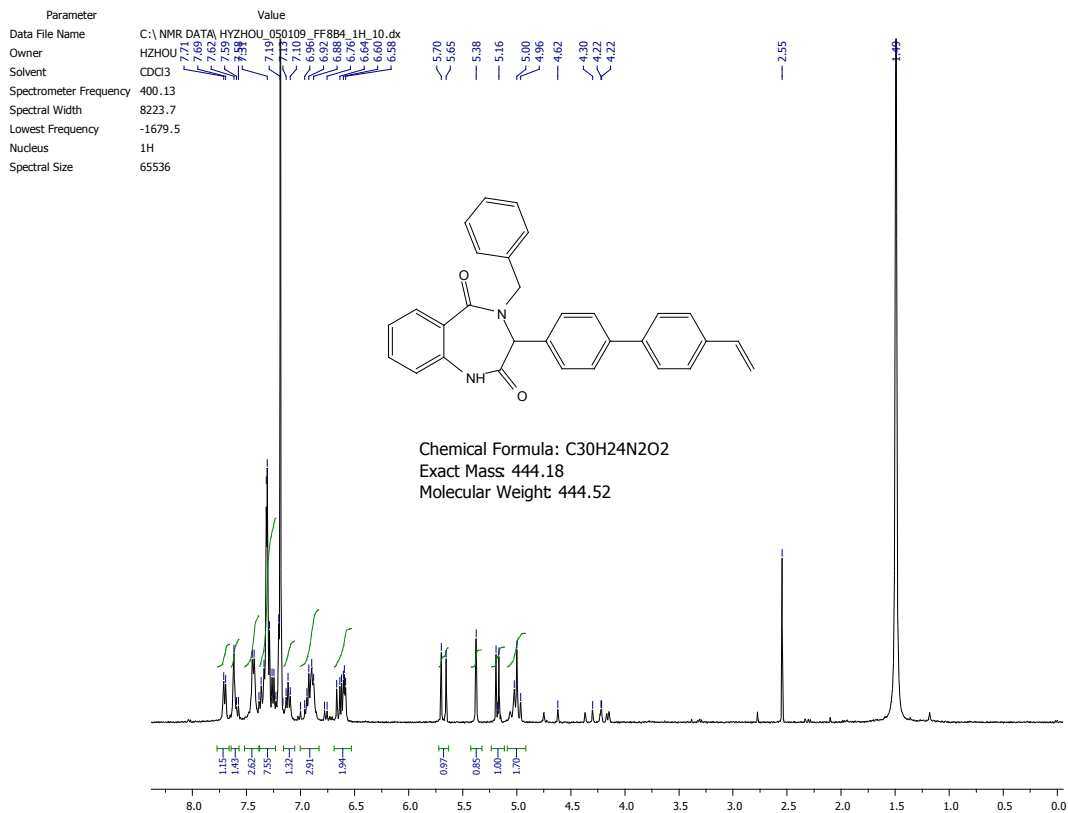
Parameter	Value
Data File Name	C:\NMR DATA\HYZHOU_050109_FF882_1H_10.dx
Owner	HZHOU
Solvent	CDCl ₃
Spectrometer Frequency	400.13
Spectral Width	8223.7
Lowest Frequency	-1682.2
Nucleus	¹ H
Spectral Size	65536



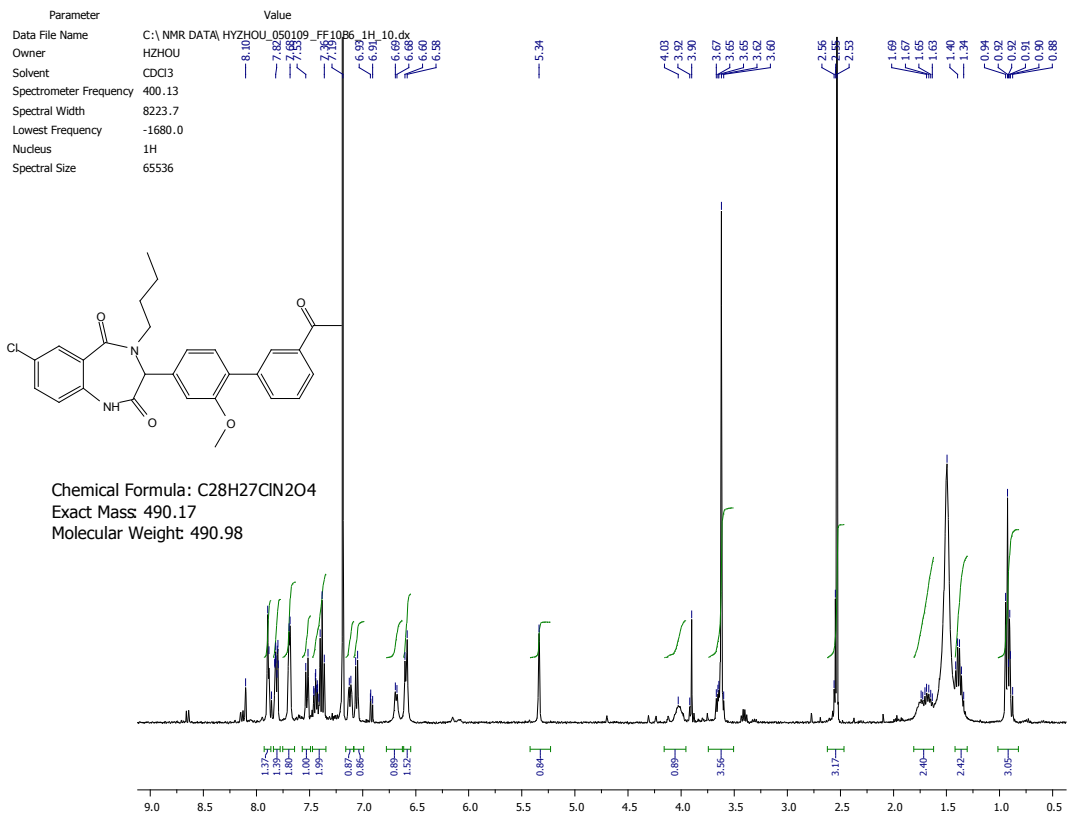
Chemical Formula: C₃₂H₂₄N₂O₂
 Exact Mass: 468.18
 Molecular Weight: 468.55



8{1,1,3,3} - ¹H NMR

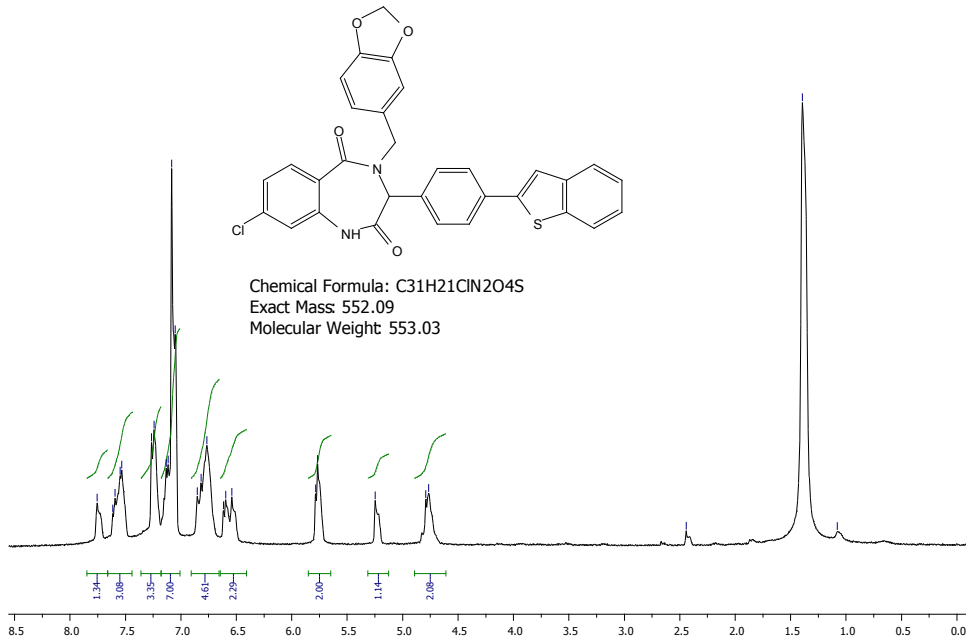


8{3,2,1,5} - ¹H NMR



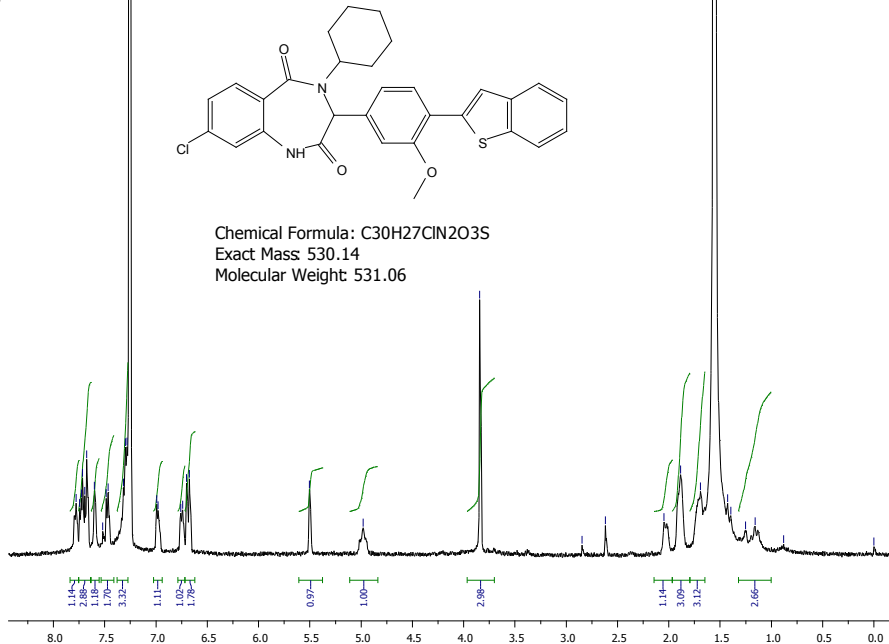
8{4,1,2,6} - ¹H NMR

Parameter	Value
Data File Name	C:\NMR DATA\HYZHOU_050209_F1688_1H_10.dx
Owner	HZHOU
Solvent	CDCl ₃
Spectrometer Frequency	400.13
Spectral Width	8223.7
Lowest Frequency	-1728.7
Nucleus	¹ H
Spectral Size	65536

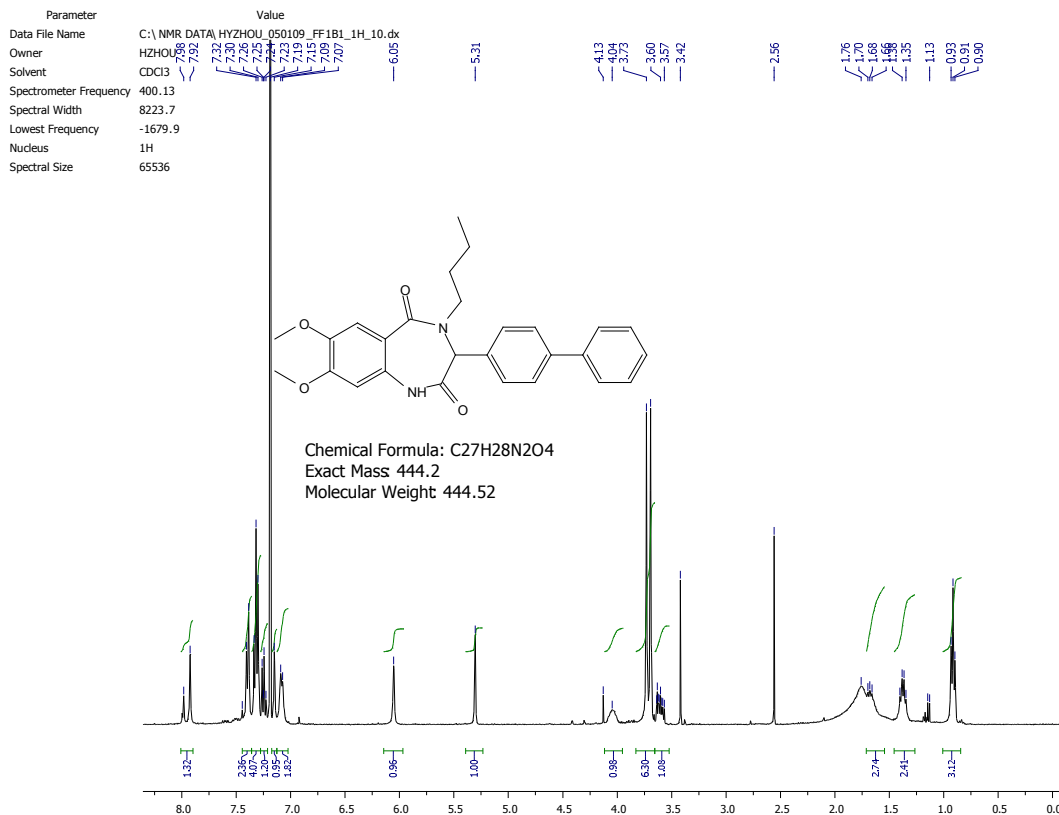


8{4,2,4,6} - ¹H NMR

Parameter	Value
Data File Name	C:\NMR DATA\HYZHOU_050209_F1888_1H_10.dx
Owner	HZHOU
Solvent	CDCl ₃
Spectrometer Frequency	400.13
Spectral Width	8223.7
Lowest Frequency	-1652.6
Nucleus	¹ H
Spectral Size	65536



8{2,1,1,1} - ¹H NMR and HRMS



Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

47 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-80 H: 0-150 N: 1-3 O: 3-5

Zhou, Hongyu, FF1B1

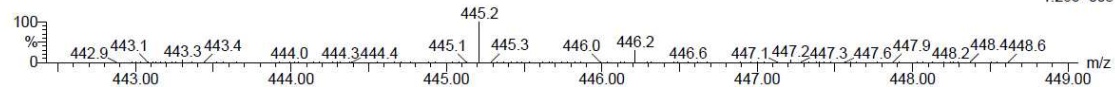
University of Illinois, SCS, Mass Spectrometry Lab

Qtof_25249 41 (2.935) AM (Cen,3, 80.00, Ar,13000.0,716.46,0.70,LS 3); Sm (SG, 2x3.00)

Q-tof UE521

1: TOF MS ES+

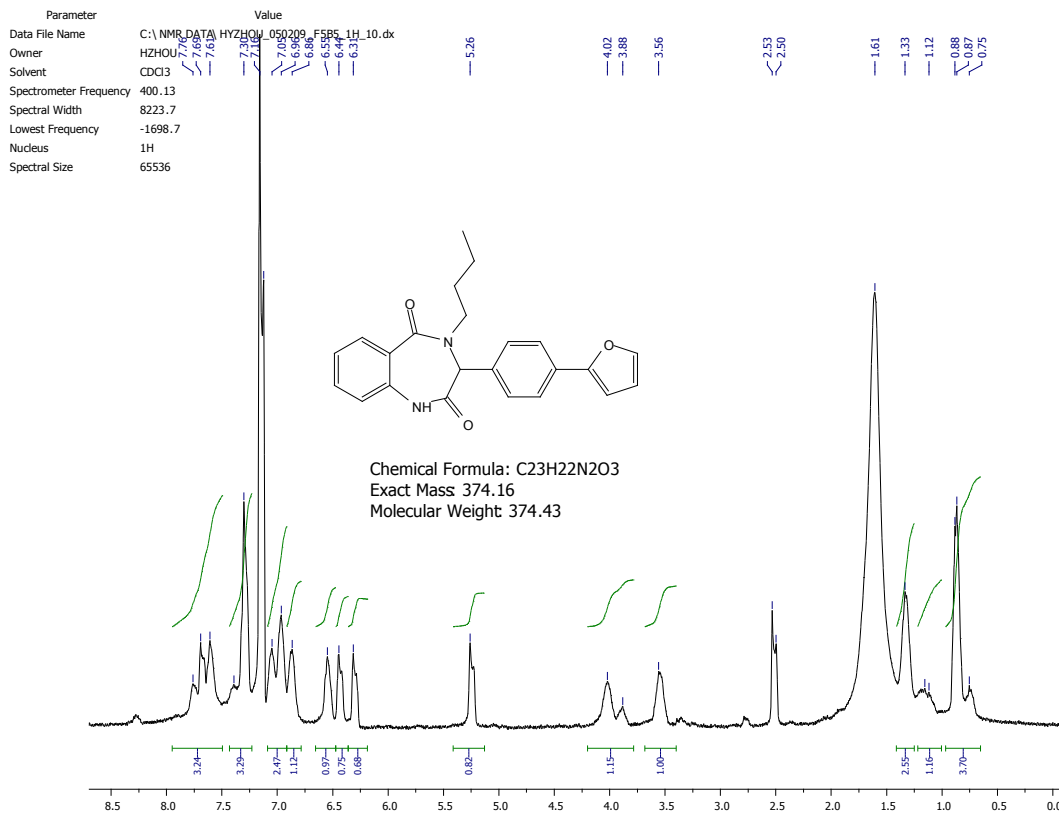
1.26e+003



Minimum: -1.5
 Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
445.2124	445.2127	-0.3	-0.7	14.5	0.4	C ₂₇ H ₂₉ N ₂ O ₄

8{1,1,1,4} - ¹H NMR and HRMS



Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

39 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

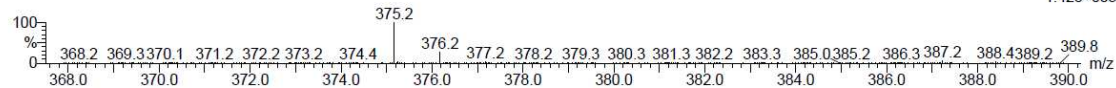
C: 0-80 H: 0-150 N: 1-3 O: 3-5

Zhou, Hongyu, FF1B5

University of Illinois, SCS, Mass Spectrometry Lab

Qtof_25250_37 (2.649) AM (Cen,3, 80.00, Ar,13000.0,716.46,0.70,LS 3); Sm (SG, 2x3.00)

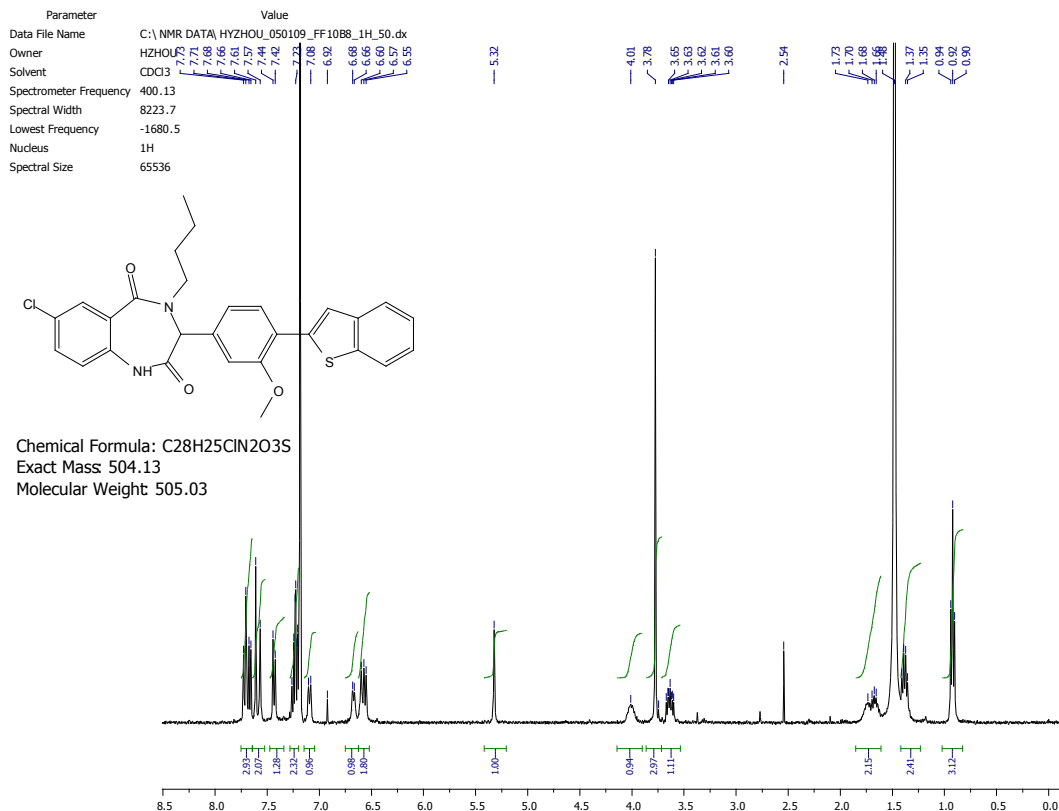
Q-tof UE521
 1: TOF MS ES+
 1.42e+003



Minimum: -1.5
 Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
375.1703	375.1709	-0.6	-1.6	13.5	1.0	C ₂₃ H ₂₃ N ₂ O ₃

8{3,2,1,6} - ¹H NMR and HRMS



Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

50 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

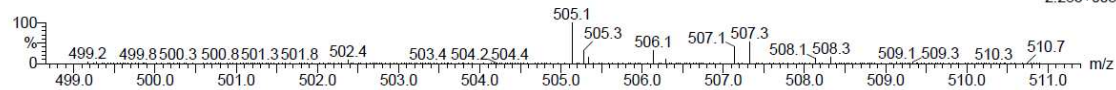
C: 0-80 H: 0-150 N: 1-3 O: 2-4 S: 1-1 Cl: 1-1

Zhou, Hongyu, FF10B8

University of Illinois, SCS, Mass Spectrometry Lab

Qtof_2525130 (2.150) AM (Cen,3, 80.00, Ar,13000.0,716.46,0.70,LS 3); Sm (SG, 2x3.00)

Q-tof UE521
1: TOF MS ES+
2.28e+003



Minimum:

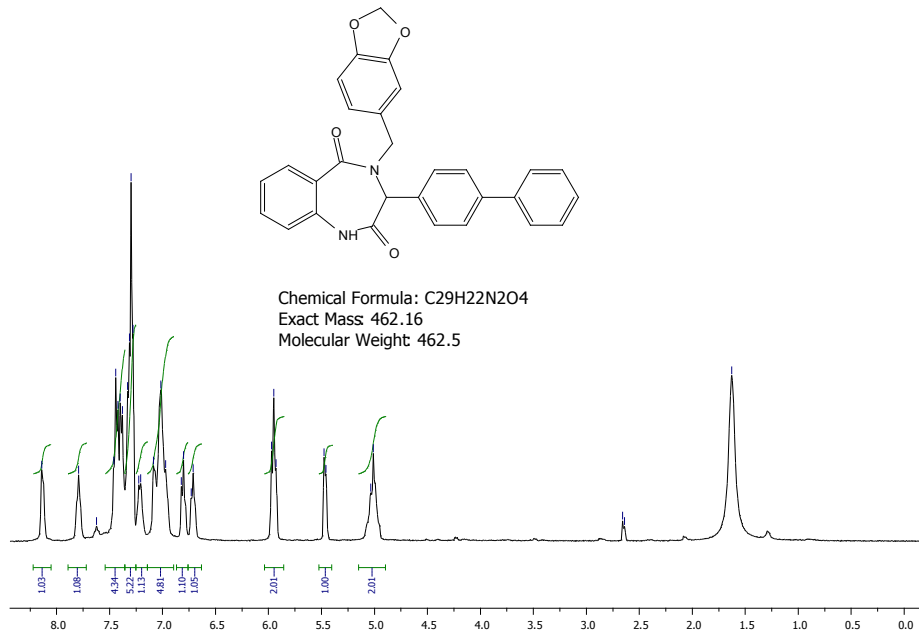
Maximum: 5.0 10.0 -1.5

Mass Calc. Mass mDa PPM DBE i-FIT Formula

505.1344 505.1353 -0.9 -1.8 16.5 1.3 C₂₈ H₂₆ N₂ O₃ S Cl

8{1,1,2,1} - ¹H NMR and HRMS

Parameter	Value
Data File Name	C:\NMR DATA\HYZHOU_050209_F14B1_1H_10.dx
Owner	HZHOU
Solvent	CDCl ₃
Spectrometer Frequency	400.13
Spectral Width	8223.7
Lowest Frequency	-1640.8
Nucleus	¹ H
Spectral Size	65536



Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

68 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

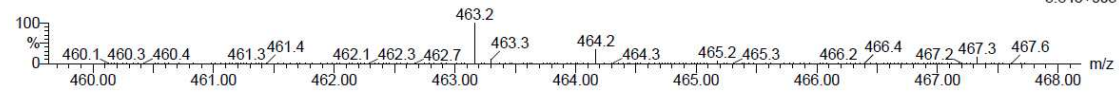
C: 0-80 H: 0-150 N: 1-3 O: 2-5

Zhou, Hongyu, FF14B1

University of Illinois, SCS, Mass Spectrometry Lab

Qtof_2525237 (2.649) AM (Cen,3, 80.00, Ar,13000.0,716.46,0.70,LS 3); Sm (SG, 2x3.00); Cm (37:38)

Q-tof UE521
 1: TOF MS ES+
 3.84e+003

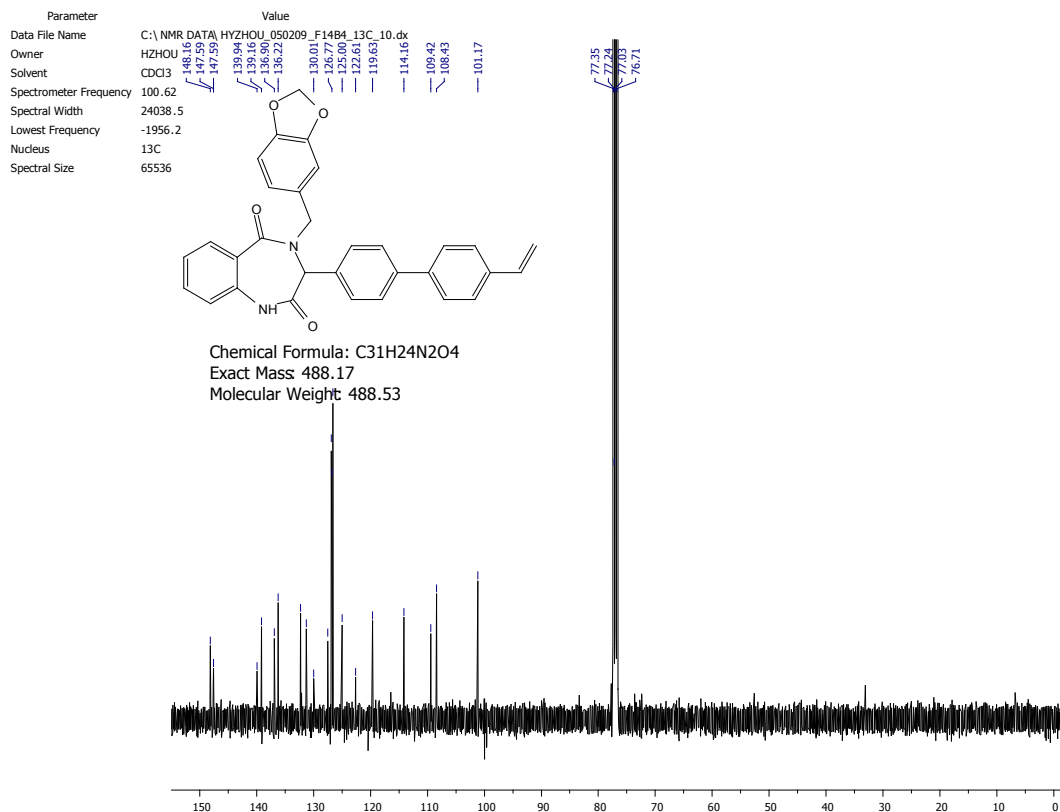
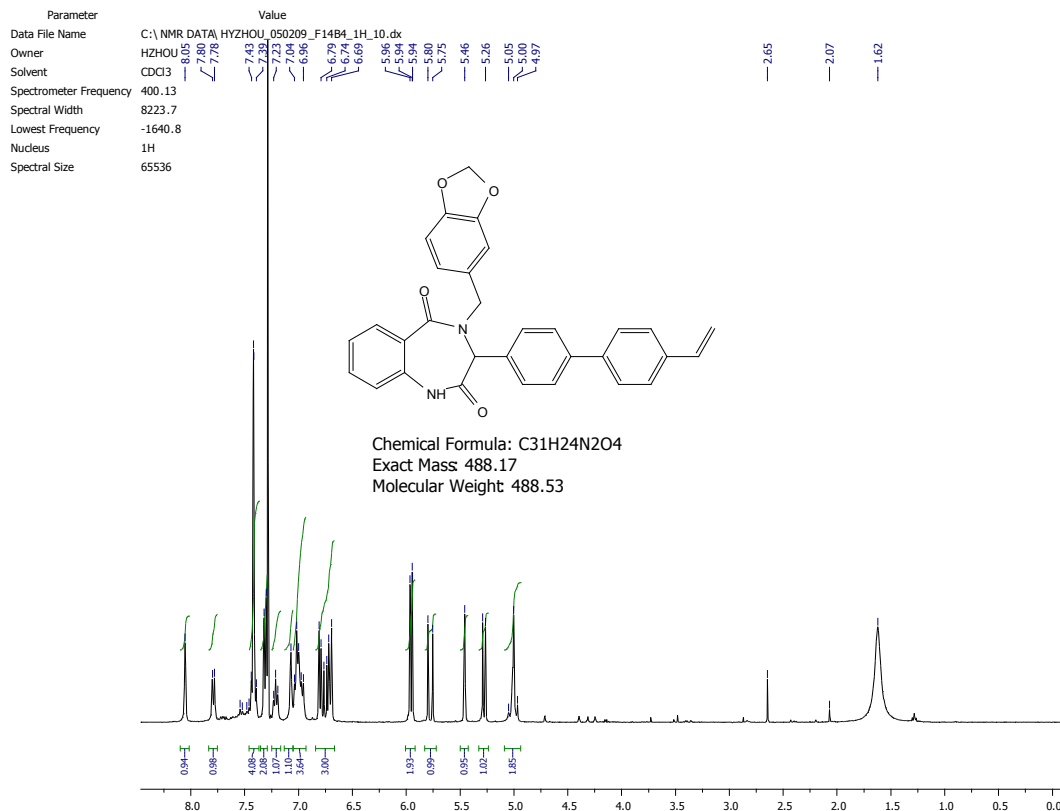


Minimum:

Maximum: 5.0 10.0 -1.5 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
463.1648	463.1658	-1.0	-2.2	19.5	1.4	C ₂₉ H ₂₃ N ₂ O ₄

8{1,1,2,3} - ¹H, ¹³C NMR and HRMS



Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

71 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-80 H: 0-150 N: 1-3 O: 2-5

Zhou, Hongyu, FF14B4

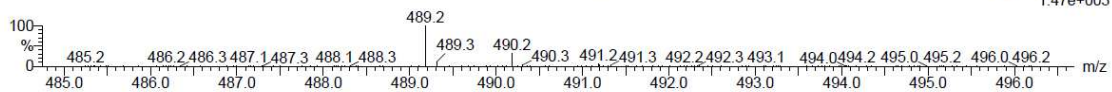
University of Illinois, SCS, Mass Spectrometry Lab

Qtof_25253 22 (1.578) AM (Cen,3, 80.00, Ar,13000.0,716.46,0.70,LS 3); Sm (SG, 2x3.00)

Q-tof UE521

1: TOF MS ES+

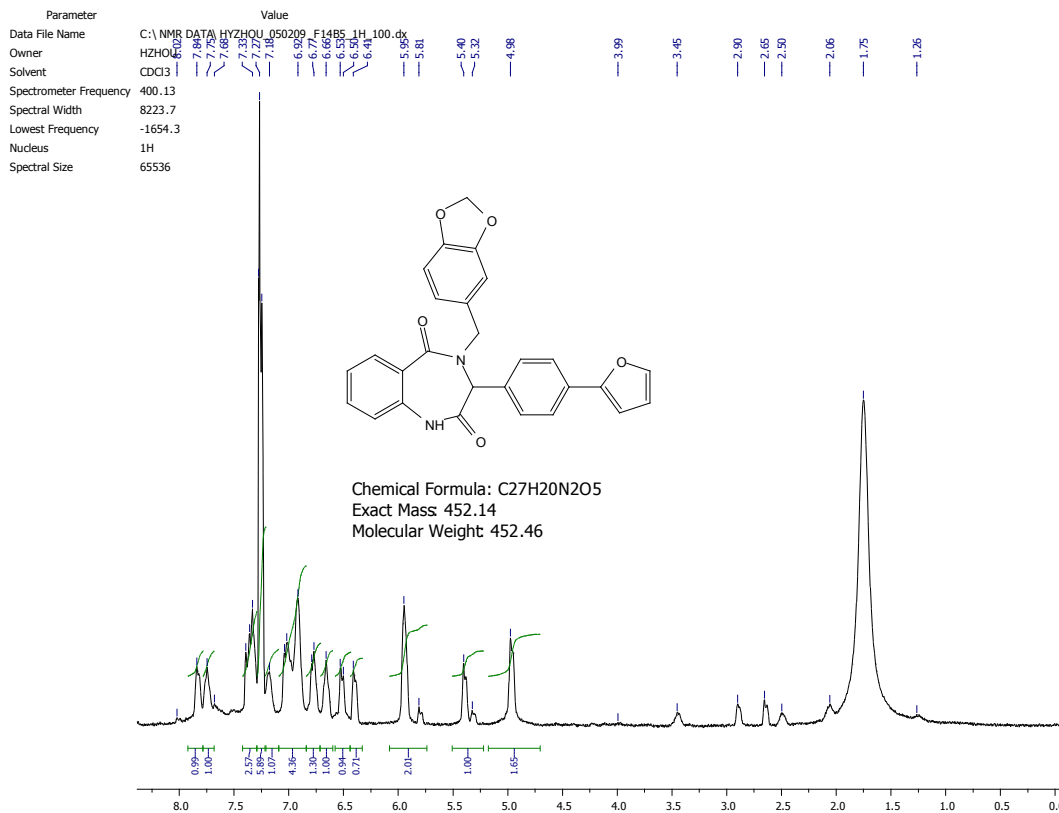
1.47e+003



Minimum: -1.5
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
489.1803	489.1814	-1.1	-2.2	20.5	4.7	C31 H25 N2 O4

8{1,1,2,4} - ¹H NMR and HRMS



Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

69 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

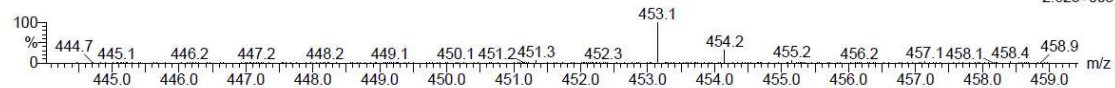
C: 0-80 H: 0-150 N: 1-3 O: 2-5

Zhou, Hongyu, FF14B5

University of Illinois, SCS, Mass Spectrometry Lab

Qtof_25254 23 (1.650) AM (Cen,3, 80.00, Ar,13000.0,716.46,0.70,LS 3), Sm (SG, 2x3.00)

Q-tof UE521
 1: TOF MS ES+
 2.62e+003



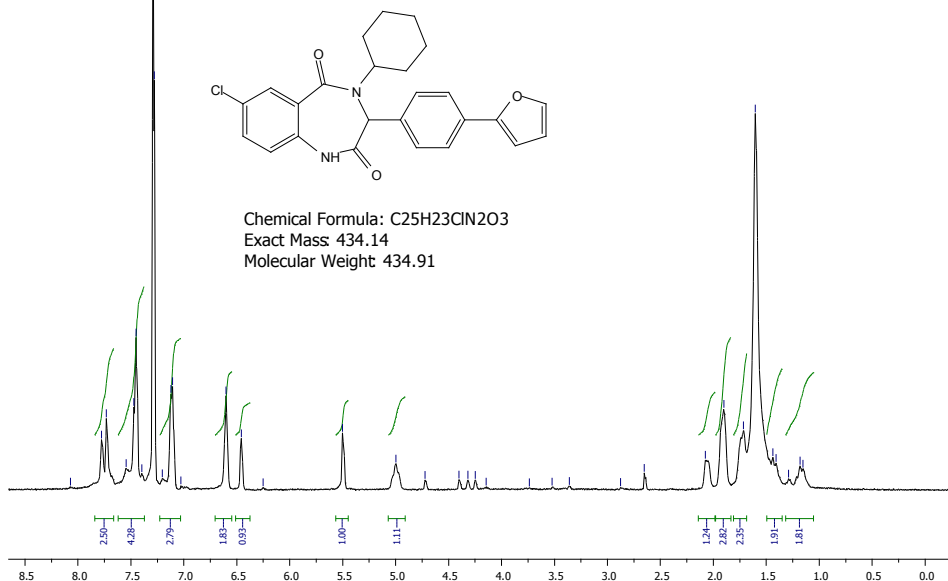
Minimum:

Maximum: 5.0 10.0 -1.5 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
453.1463	453.1450	1.3	2.9	18.5	2.1	C ₂₇ H ₂₁ N ₂ O ₅

8{3,1,4,4} - ¹H NMR and HRMS

Parameter	Value
Data File Name	C:\NMR DATA\HYZHOU_050209_FF15B5_1H_10.dx
Owner	HZHOU
Solvent	CDCl ₃
Spectrometer Frequency	400.13
Spectral Width	8223.7
Lowest Frequency	-1640.8
Nucleus	¹ H
Spectral Size	65536



Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

57 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-80 H: 0-150 N: 1-3 O: 2-5 Cl: 1-1

Zhou, Hongyu, FF15B5

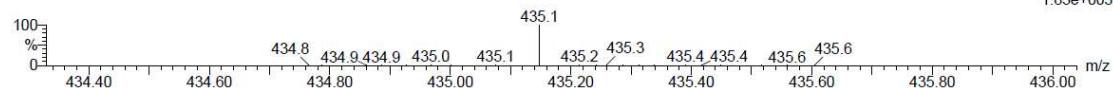
University of Illinois, SCS, Mass Spectrometry Lab

Qtof_25255_33 (2.364) AM (Cen,3, 80.00, Ar,13000.0,716.46,0.70,LS 3); Sm (SG, 2x3.00)

Q-tof UE521

1: TOF MS ES+

1.83e+003



Minimum:

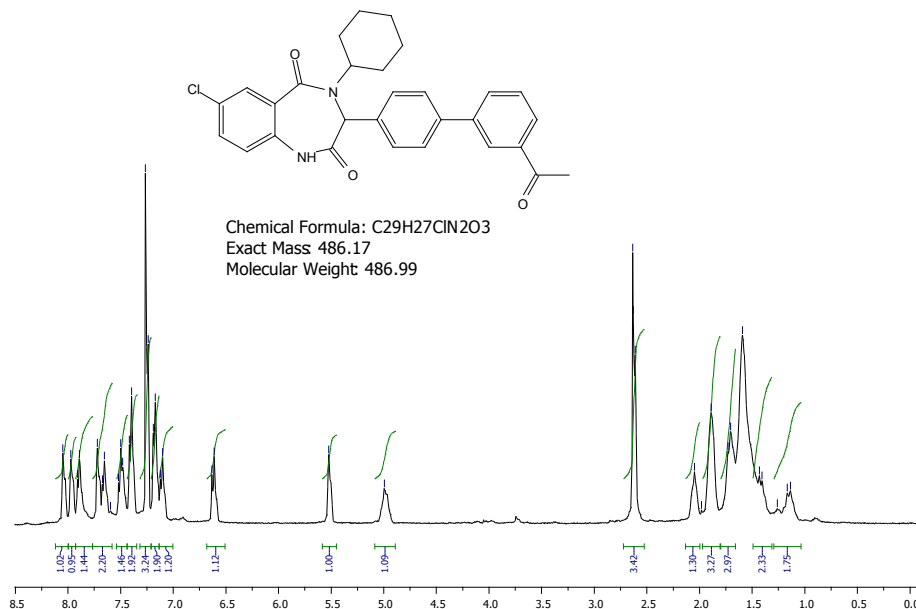
Maximum:

	5.0	10.0	-1.5
			50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
435.1479	435.1475	0.4	0.9	14.5	n/a	C ₂₅ H ₂₄ N ₂ O ₃ Cl

8{3,1,4,5} - ¹H NMR and HRMS

Parameter	Value
Data File Name	C:\NMR DATA\HYZHOU_050209_FF15B6_1H_10.dx
Owner	HZHOU
Solvent	CDCl ₃
Spectrometer Frequency	400.13
Spectral Width	8223.7
Lowest Frequency	-1652.4
Nucleus	¹ H
Spectral Size	65536



Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

66 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

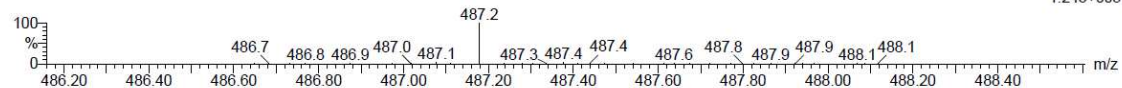
C: 0-80 H: 0-150 N: 1-3 O: 2-5 Cl: 1-1

Zhou, Hongyu, FF15B6

University of Illinois, SCS, Mass Spectrometry Lab

Qtof_25256_39 (2.792) AM (Cen,3, 80.00, Ar,13000.0,716.46,0.70,LS 3); Sm (SG, 2x3.00)

Q-tof UE521
 1: TOF MS ES+
 1.24e+003

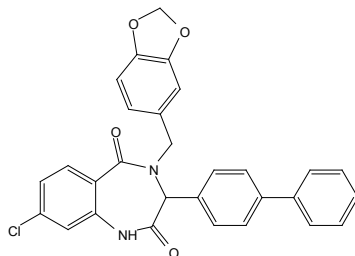


Minimum: -1.5
 Maximum: 50.0

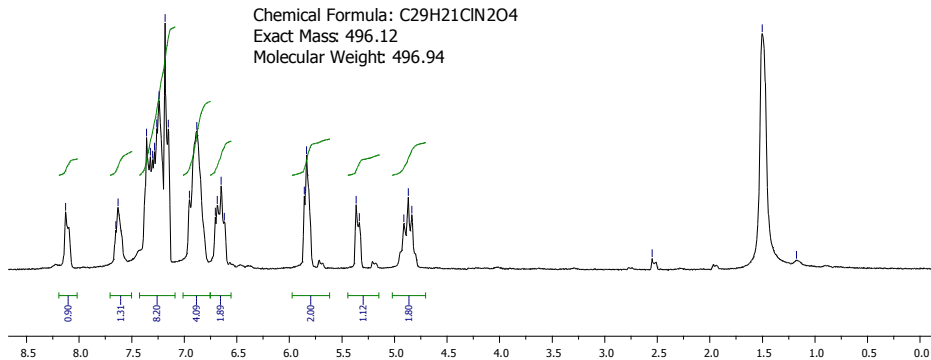
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
487.1780	487.1788	-0.8	-1.6	16.5	n/a	C ₂₉ H ₂₈ N ₂ O ₃ Cl

8{4,1,2,1} - ¹H NMR and HRMS

Parameter	Value
Data File Name	C:\NMR DATA\HYZHOU_050209_F16B1_1H_10.dx
Owner	HZHOU
Solvent	CDCl ₃
Spectrometer Frequency	400.13
Spectral Width	8223.7
Lowest Frequency	-1689.6
Nucleus	¹ H
Spectral Size	65536



Chemical Formula: C₂₉H₂₁ClN₂O₄
 Exact Mass: 496.12
 Molecular Weight: 496.94



Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

67 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

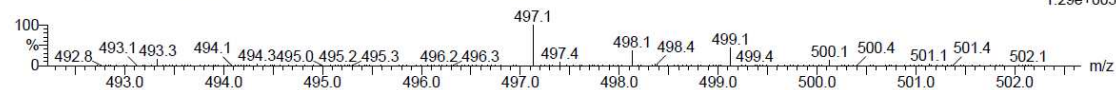
C: 0-80 H: 0-150 N: 1-3 O: 2-5 Cl: 1-1

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Qtof_25257_35 (2.507) AM (Cen,3, 80.00, Ar,13000.0,716.46,0.70,LS 3); Sm (SG, 2x3.00)

Q-tof UE521
 1: TOF MS ES+
 1.29e+003



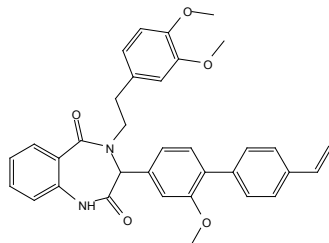
Minimum:

Maximum:

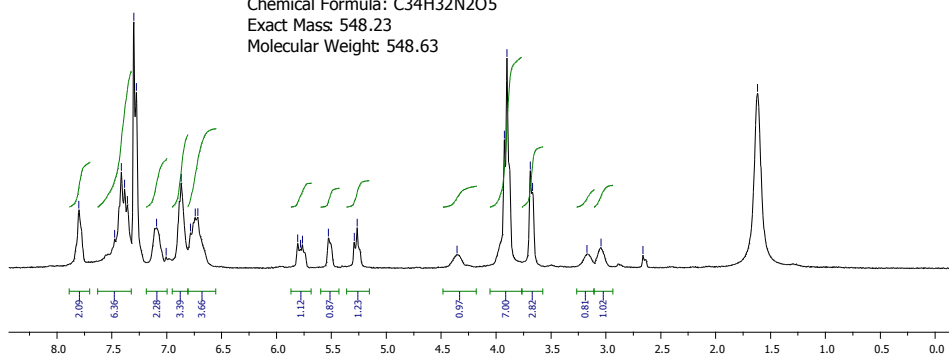
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
497.1266	497.1268	-0.2	-0.4	19.5	4.2	C ₂₉ H ₂₂ N ₂ O ₄ Cl

8{1,2,5,3} - ¹H NMR and HRMS

Parameter	Value
Data File Name	C:\NMR_DATA\HZHOU_050209_FF17B4_1H_10.dk
Owner	HZHOU
Solvent	CDCl ₃
Spectrometer Frequency	400.13
Spectral Width	8223.7
Lowest Frequency	-1640.8
Nucleus	¹ H
Spectral Size	65536



Chemical Formula: C₃₄H₃₂N₂O₅
 Exact Mass: 548.23
 Molecular Weight: 548.63



Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
 Element prediction: Off
 Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

83 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

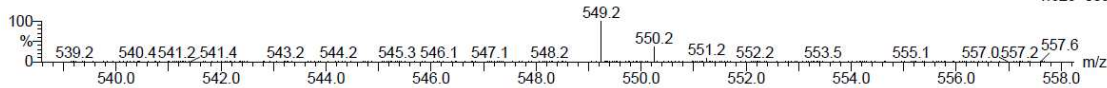
C: 0-80 H: 0-150 N: 1-3 O: 2-5

Zhou, Hongyu, FF17B4

University of Illinois, SCS, Mass Spectrometry Lab

Qtof_25258 22 (1.578) AM (Cen,3, 80.00, Ar,13000.0,716.46,0.70,LS 3); Sm (SG, 2x3.00)

Q-tof UE521
 1: TOF MS ES+
 1.62e+003



Minimum:

Maximum:

5.0 10.0 -1.5
 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
549.2371	549.2389	-1.8	-3.3	19.5	1.6	C ₃₄ H ₃₃ N ₂ O ₅