

Supporting information

Gerberdriasins A–F, six undescribed coumarin derivatives from *Gerbera anandria* (Linn) Sch-Bip with their protective effects on scopolamine-induced PC12 cells

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China

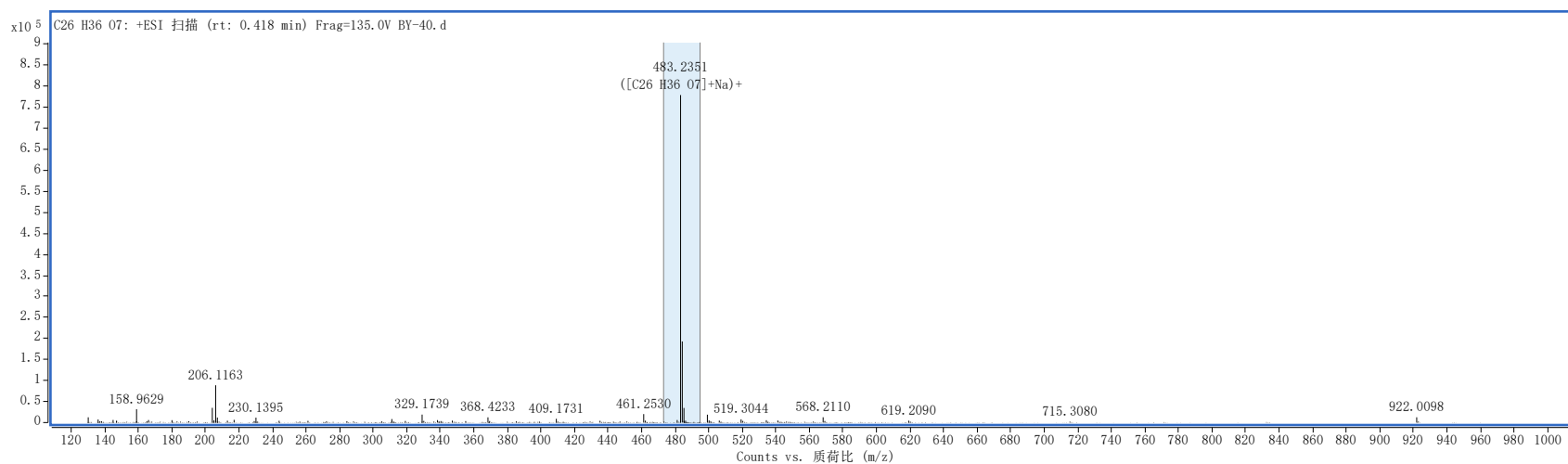
^c School of Animal Science, Xichang College, Xichang, Sichuan 615000, P.R. China

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峰高总百分比 (Calc)	峰高 (计算值)	峰高百分数(计算值)	m/z (Calc)	Diff (mDa)	峰高	峰高百分数	峰高总百分比	m/z	Diff (ppm)
74.5	749957.1	100	483.2353	0.2	779032.4	100	77.4	483.2351	0.38

最佳	ID 来源	分子式	种类	m/z	分数	Diff (ppm)	分数 (MFG)
TRUE	MFG	C26 H36 O7	(M+Na)+	483.2351	96.71	0.74	96.71

Figure S1. HRESIMS spectrum of *Gerberdriasins A (1)*

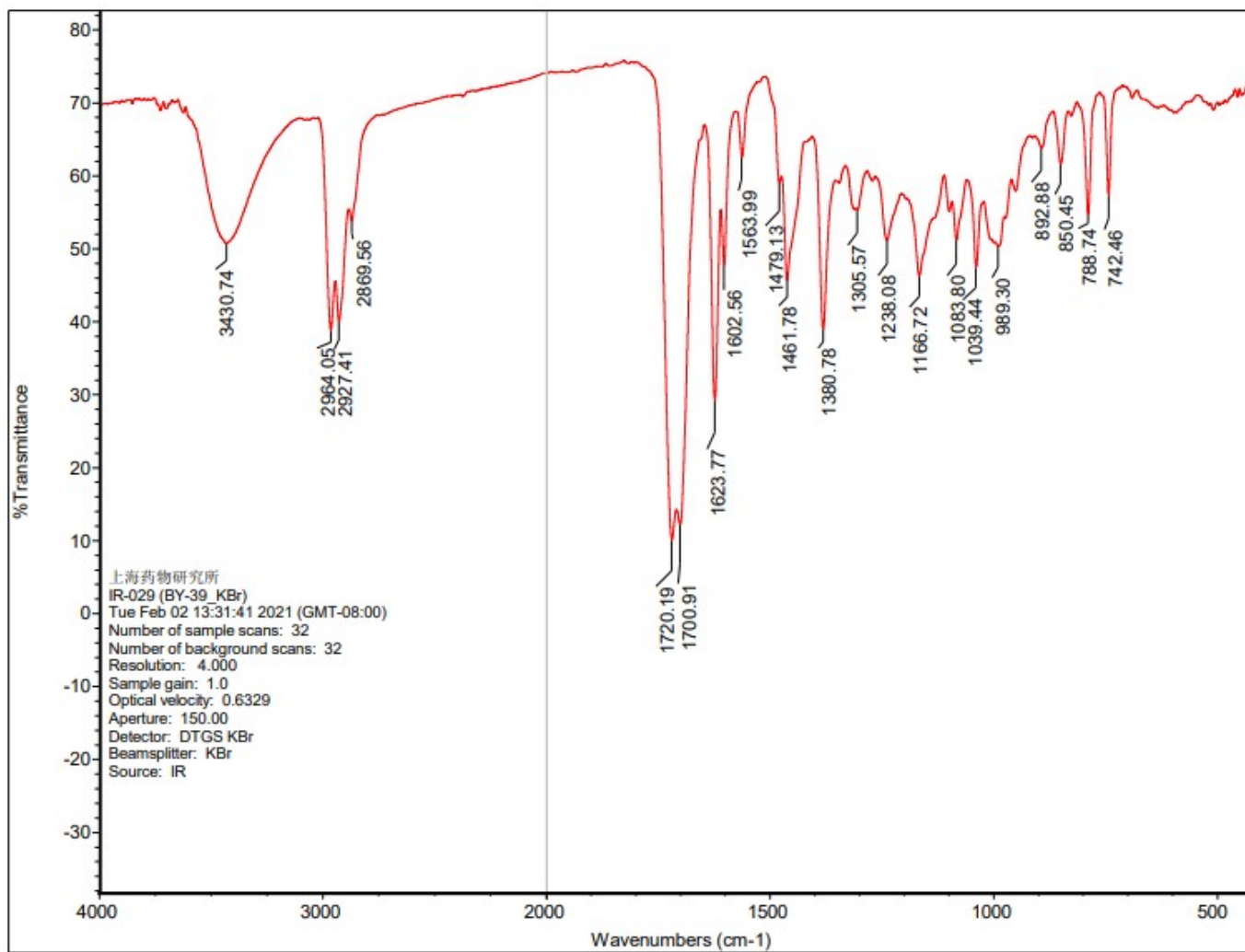


Figure S2. IR spectrum of *Gerberdriasins A (1)*

Rudolph Research Analytical

Thursday, 11/05/2020

This sample was measured on an Autopol VI, serial number 90079,
manufactured by Rudolph Research Analytical, Hackettstown, NJ.

LotID : BY-39
Set Temperature : 20.0
Temp Corr : OFF

n	Average	Std.Dev.	Maximum	Minimum
6	-15.834	0.8335	-15.000	-16.667

S.No	Sample ID	Time	Result	Scale	OR ° Arc	WLG	Lg.mm	Conc.	Temp.	Comment
1	BY-39	04:12:51 PM	-16.667	SR	-0.010	589	100.00	0.060	20.1	
2	BY-39	04:12:57 PM	-16.667	SR	-0.010	589	100.00	0.060	20.1	
3	BY-39	04:13:04 PM	-15.000	SR	-0.009	589	100.00	0.060	20.0	
4	BY-39	04:13:10 PM	-15.000	SR	-0.009	589	100.00	0.060	20.0	
5	BY-39	04:13:16 PM	-15.000	SR	-0.009	589	100.00	0.060	20.0	
6	BY-39	04:13:23 PM	-16.667	SR	-0.010	589	100.00	0.060	20.0	

Signature

Figure S3. OR Value of *Gerberdriasins A (1)* in CH₃OH

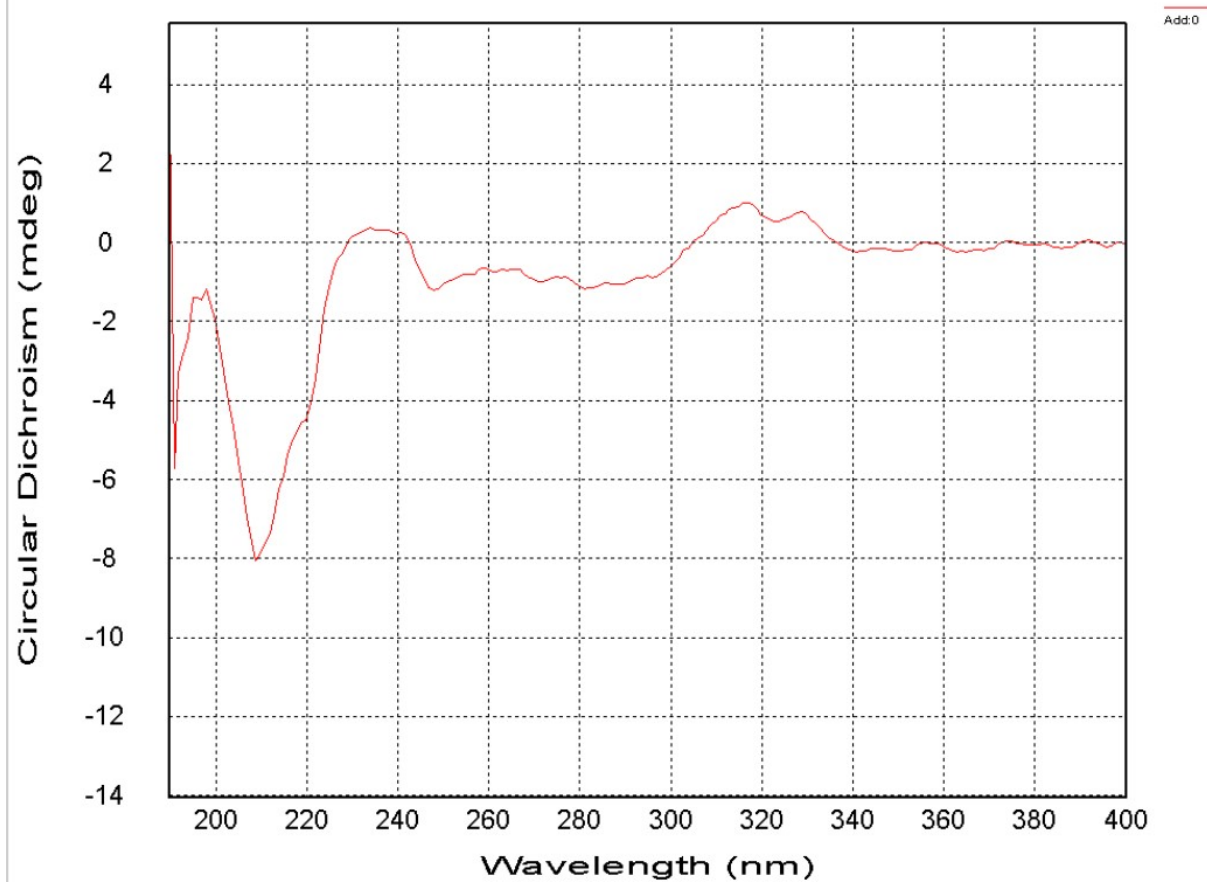


Figure S4. CD spectra of *Gerberdriasins A (1)* in CH₃OH

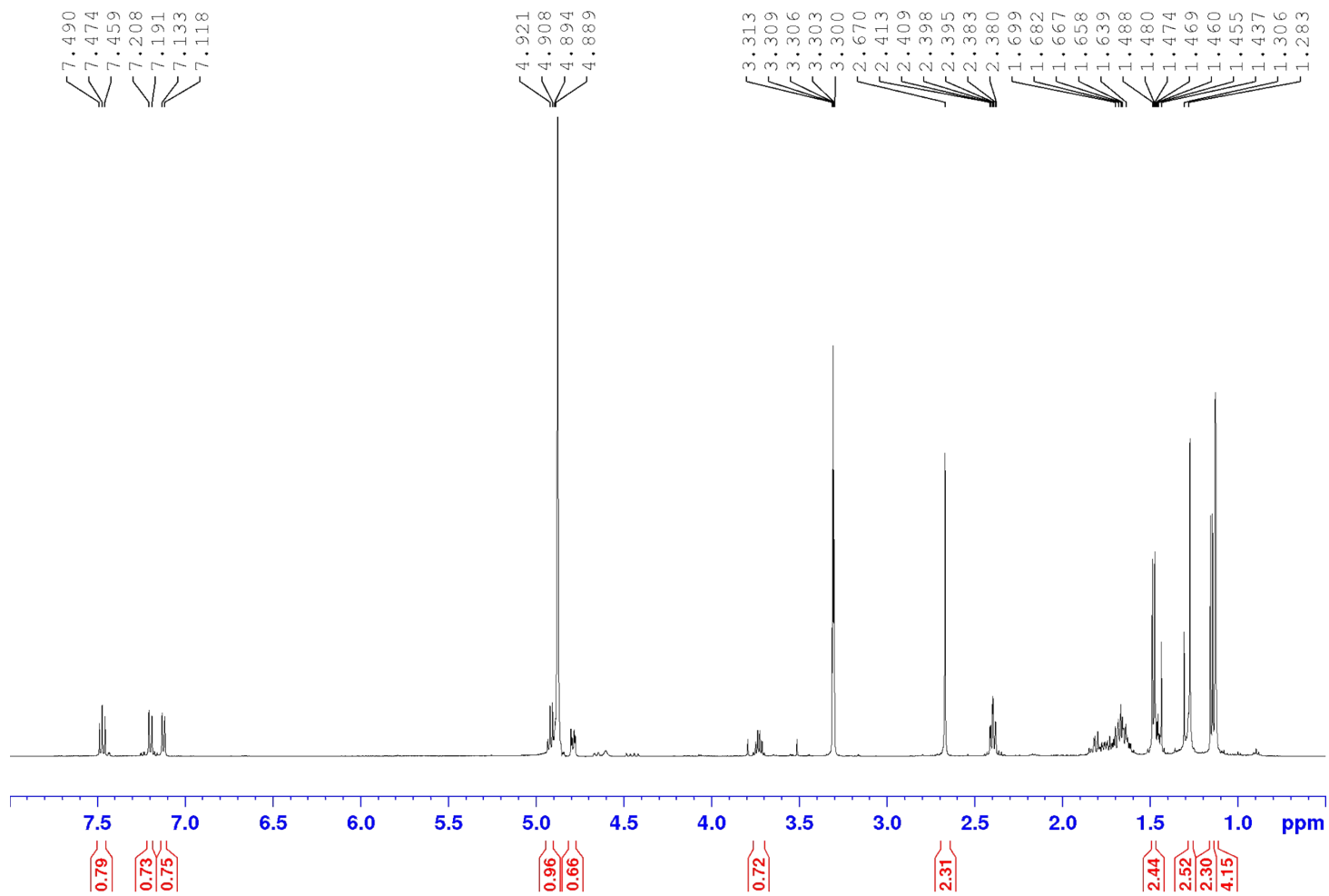


Figure S5. ^1H - NMR spectrum of *Gerberdriasins A (1)* in CD_3OD

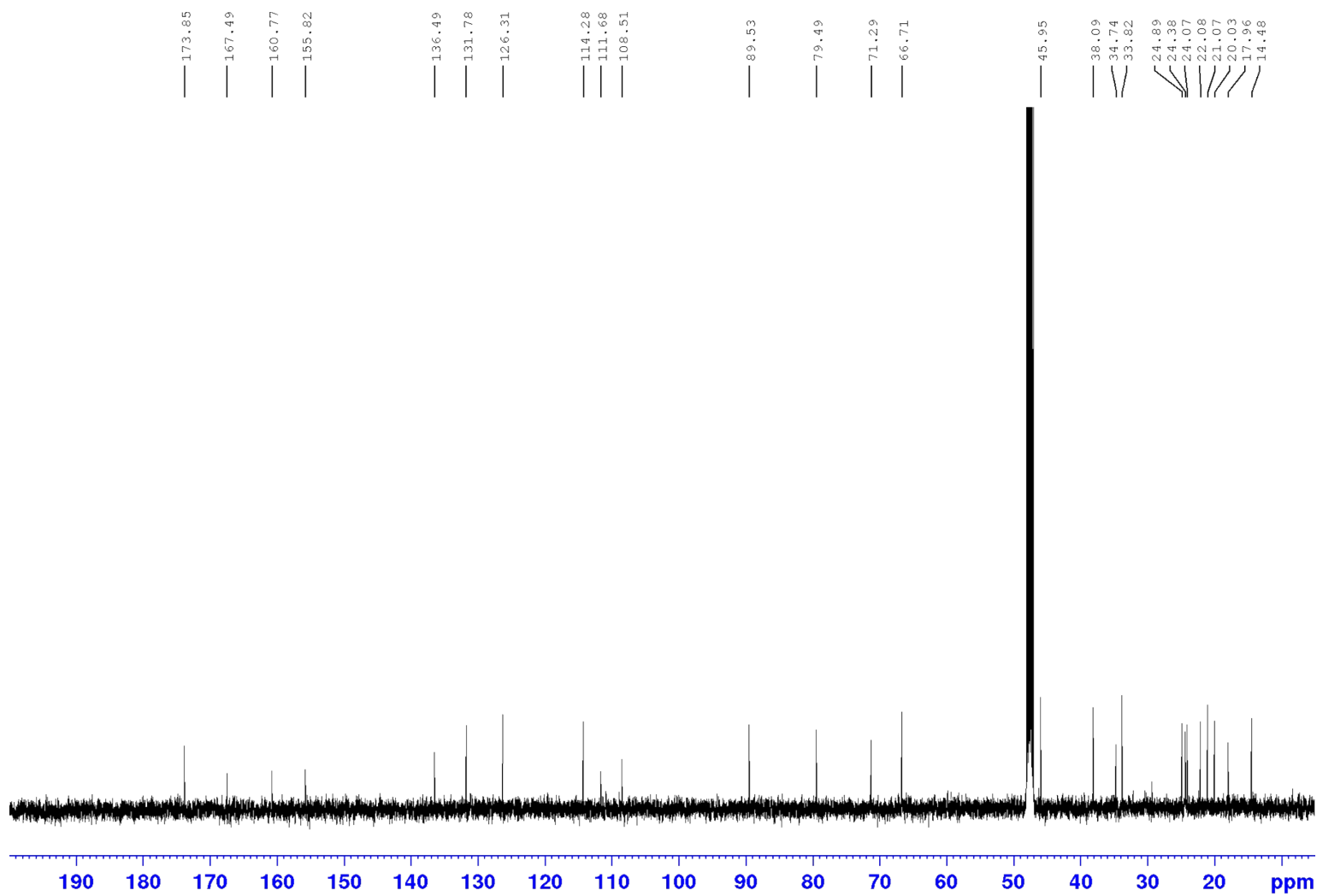


Figure S6. ^{13}C NMR spectrum of *Gerberdriasins A (1)* in CD_3OD

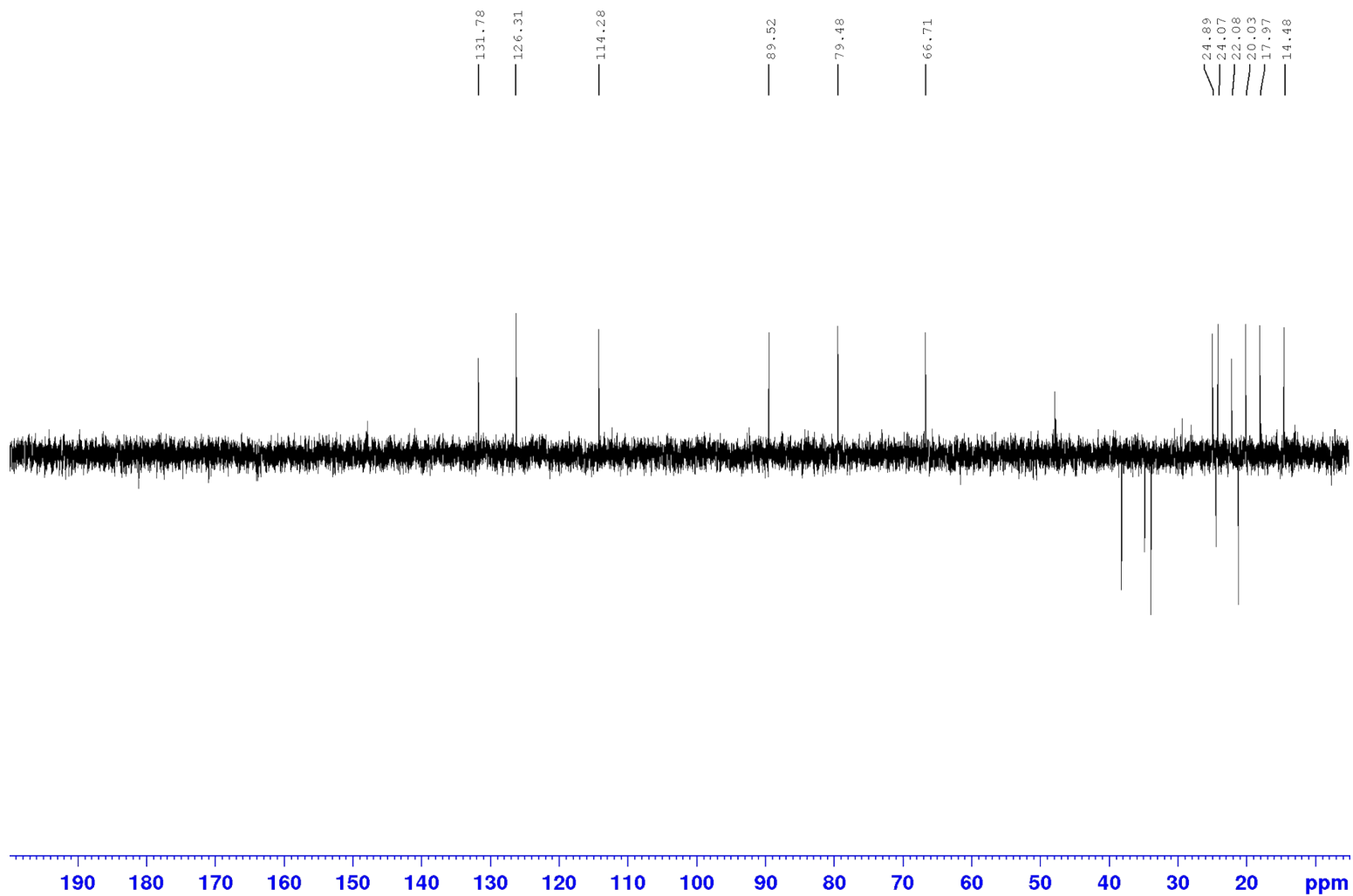


Figure S7. DEPT-135 NMR spectrum of *Gerberdriasins A (1)* in CD₃OD

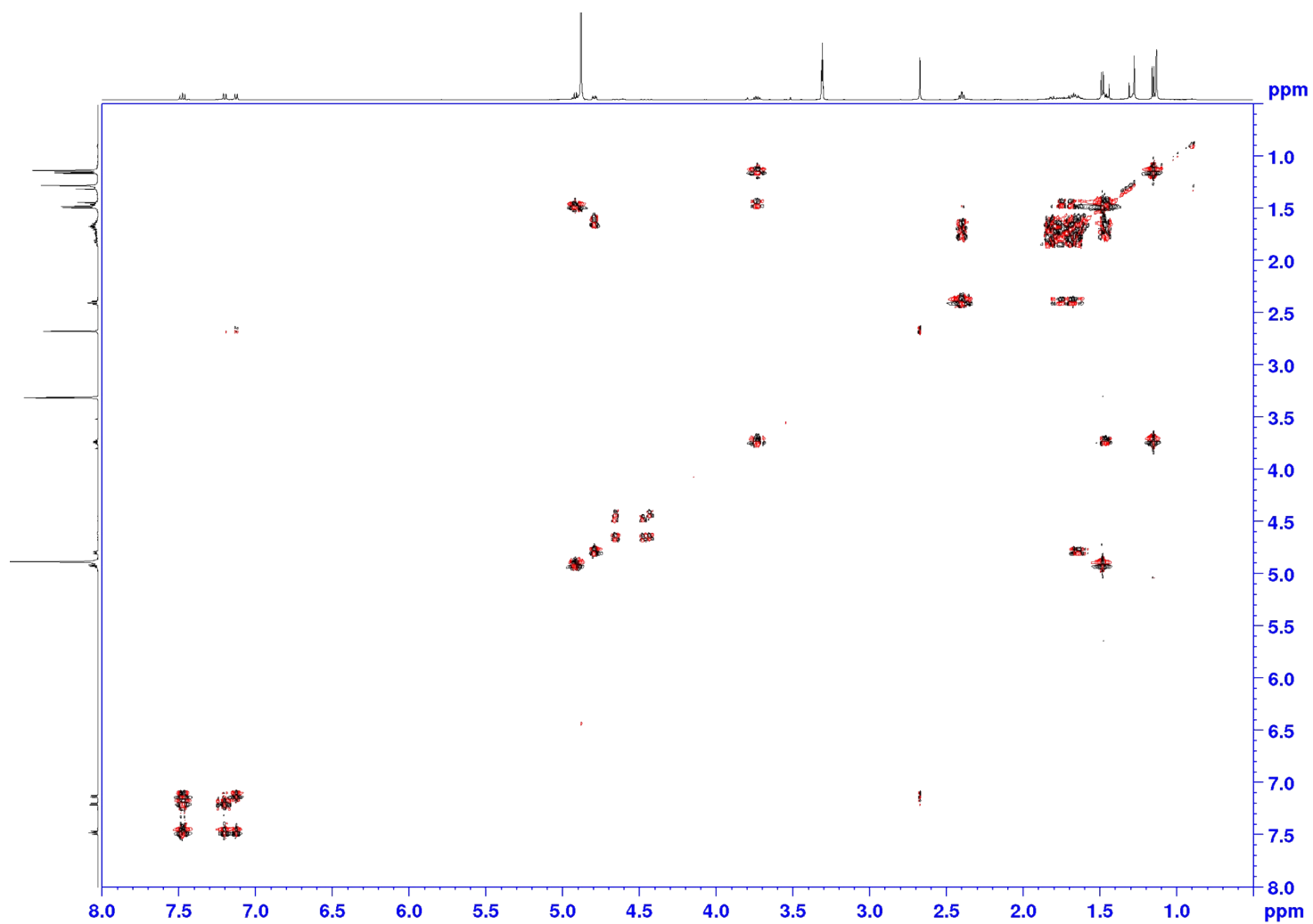


Figure S8. ^1H - ^1H COSY spectrum of *Gerberdriasins A (1)* in CD_3OD

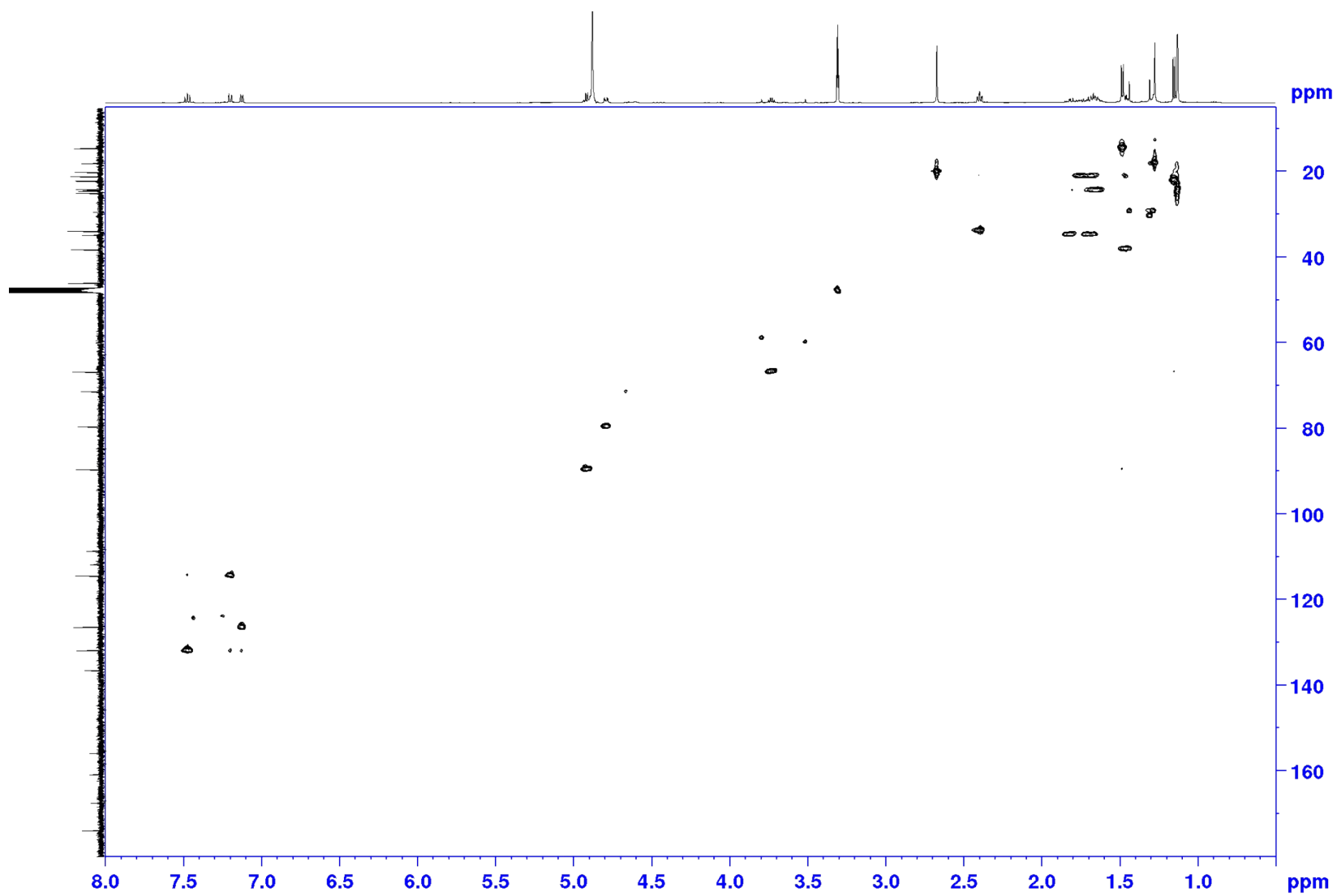


Figure S9. HSQC spectrum of *Gerberdriasins A (1)* in CD₃OD

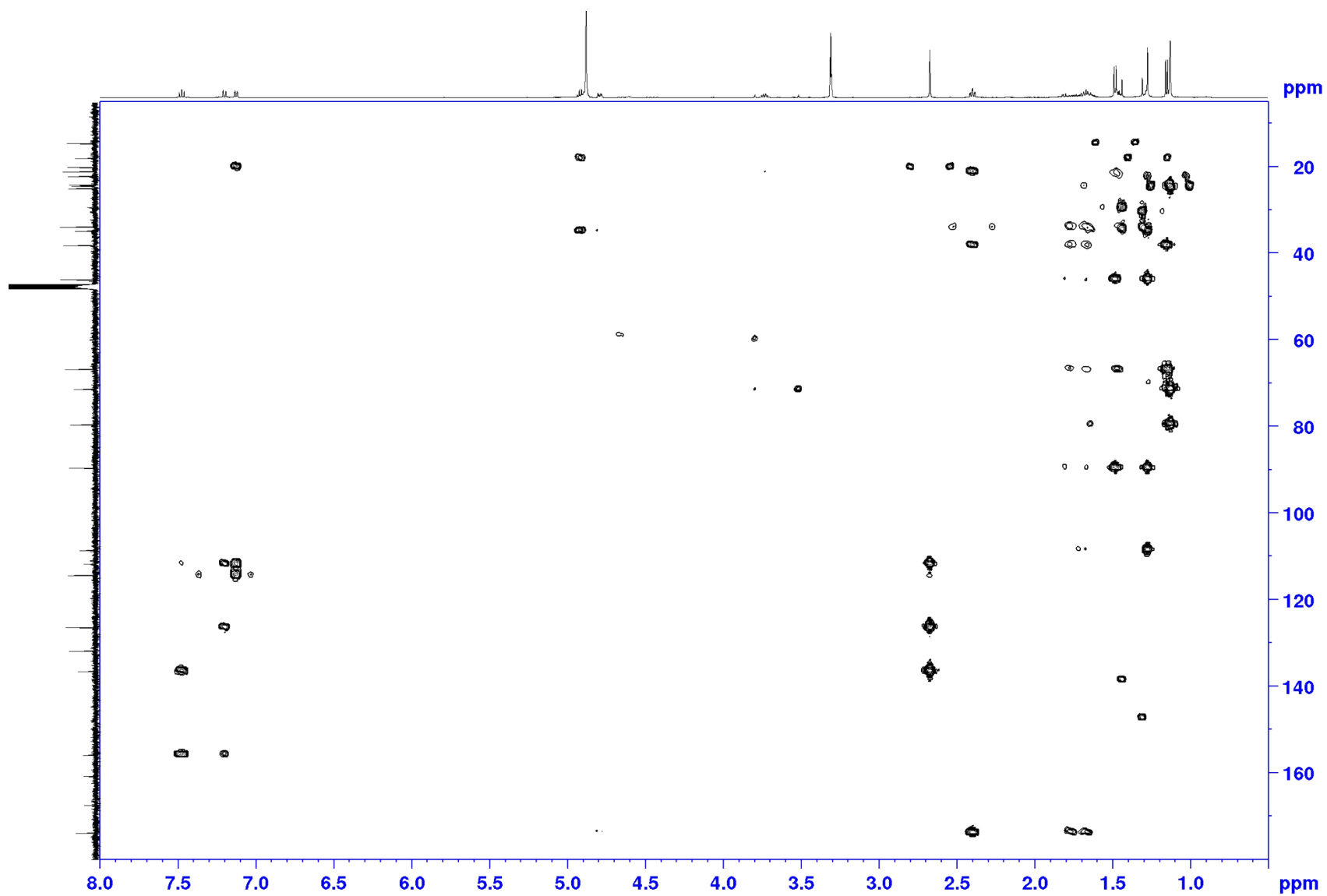


Figure S10. HMBC spectrum of *Gerberdriasins A (1)* in CD₃OD

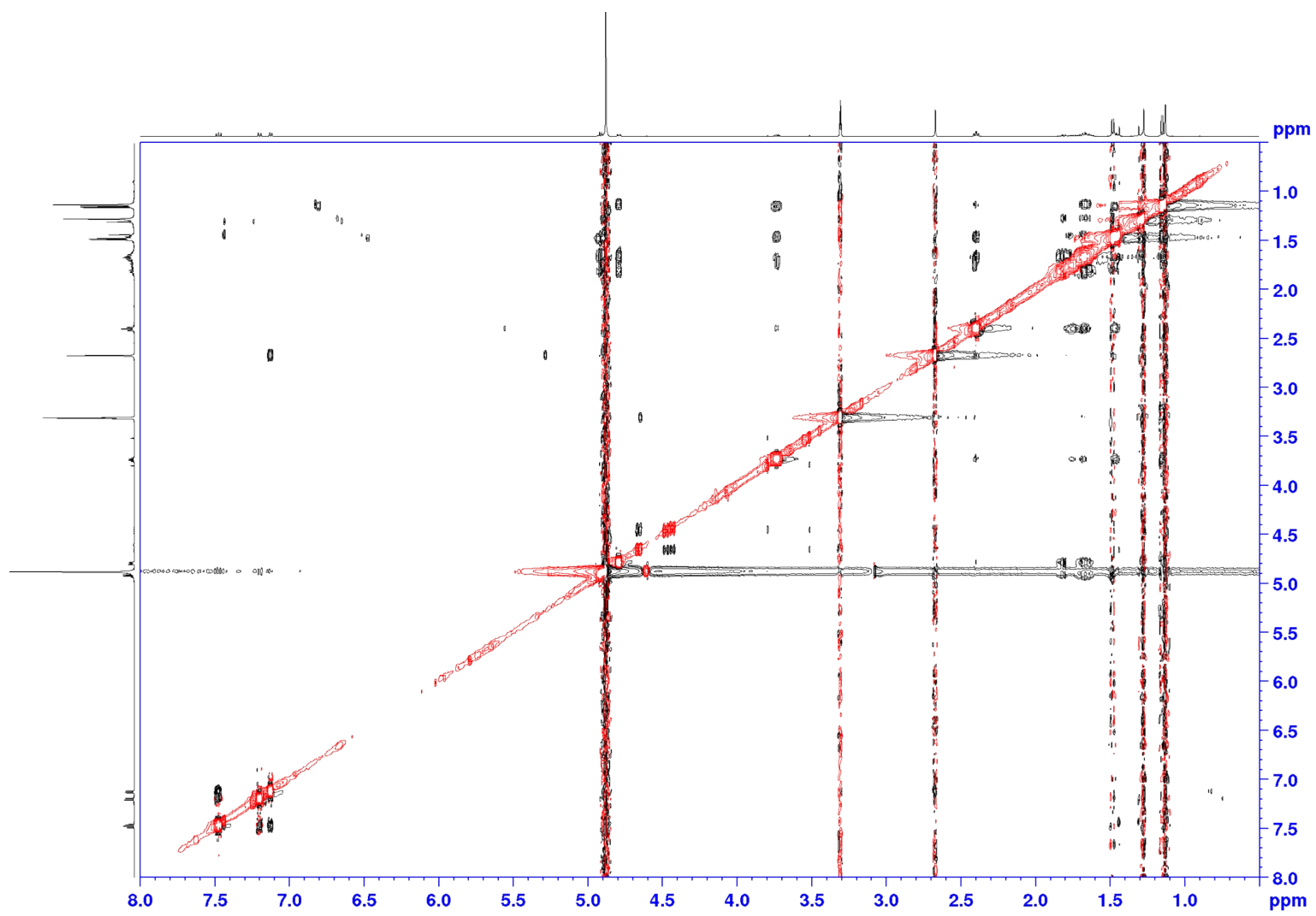
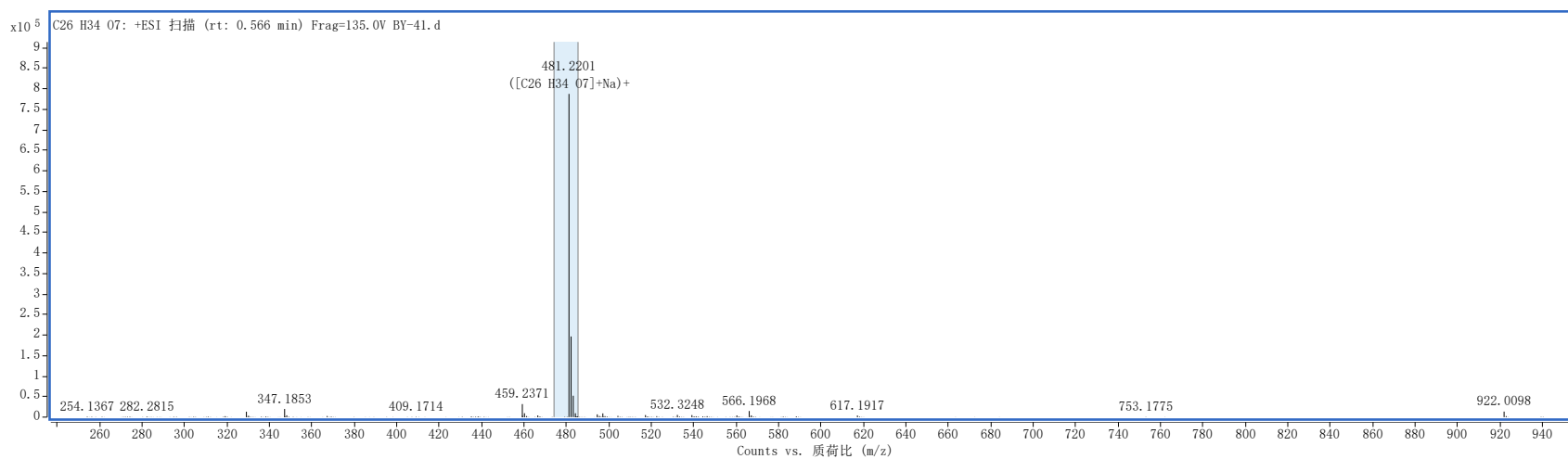


Figure S11. NOESY spectrum of *Gerberdriasin A (1)* in CD₃OD



峰高总百分比 (Calc)	峰高 (计算值)	峰高百分数(计算值)	m/z (Calc)	Diff (mDa)	峰高	峰高百分数	峰高总百分比	m/z	Diff (ppm)
74.1	774564.7	100	481.2197	-0.4	787452.4	100	75.3	481.2201	-0.8

最佳	ID 来源	分子式	种类	m/z	分数	Diff (ppm)	分数 (MFG)
TRUE	MFG	C26 H34 O7	(M+Na)+	481.2201	93.63	-0.99	93.63

Figure S12. HRESIMS spectrum of *Gerberdriasin B* (2)

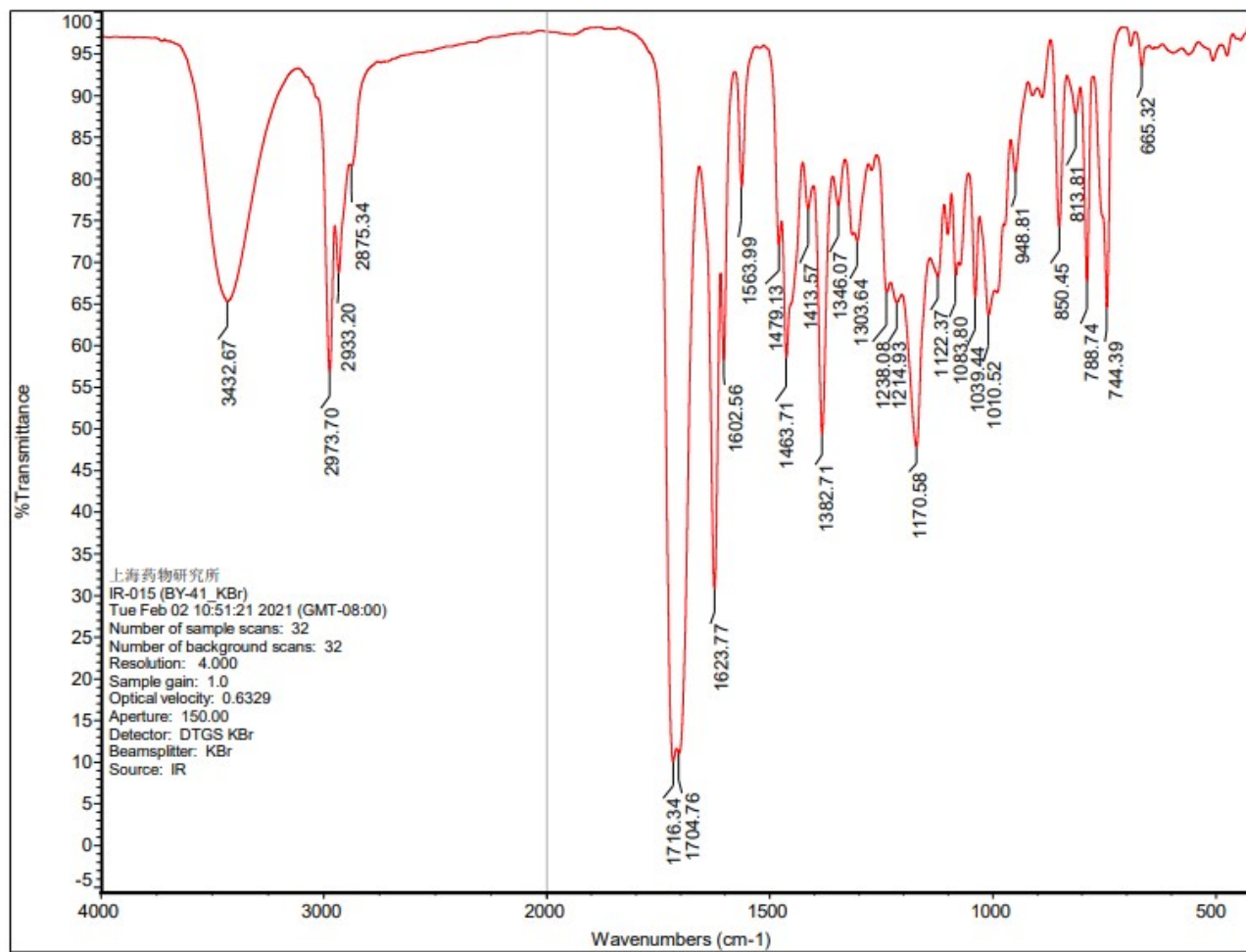


Figure S13. IR spectrum of *Gerberdriasin B* (2)

Rudolph Research Analytical

Thursday, 11/05/2020

This sample was measured on an Autopol VI, serial number 90079,
manufactured by Rudolph Research Analytical, Hackettstown, NJ.

LotID : BY-41
Set Temperature : 20.0
Temp Corr : OFF

n	Average	Std.Dev.	Maximum	Minimum
6	-14.445	0.4972	-13.333	-14.667

S.No	Sample ID	Time	Result	Scale	OR °Arc	WLG	Lg.mm	Conc.	Temp.	Comment
1	BY-41	05:02:08 PM	-14.667	SR	-0.011	589	100.00	0.075	20.0	
2	BY-41	05:02:14 PM	-14.667	SR	-0.011	589	100.00	0.075	20.0	
3	BY-41	05:02:20 PM	-14.667	SR	-0.011	589	100.00	0.075	19.9	
4	BY-41	05:02:27 PM	-14.667	SR	-0.011	589	100.00	0.075	19.9	
5	BY-41	05:02:33 PM	-14.667	SR	-0.011	589	100.00	0.075	19.9	
6	BY-41	05:02:39 PM	-13.333	SR	-0.010	589	100.00	0.075	19.9	

Signature

Figure S14. OR Value of *Gerberdriasin B (2)* in CH₃OH

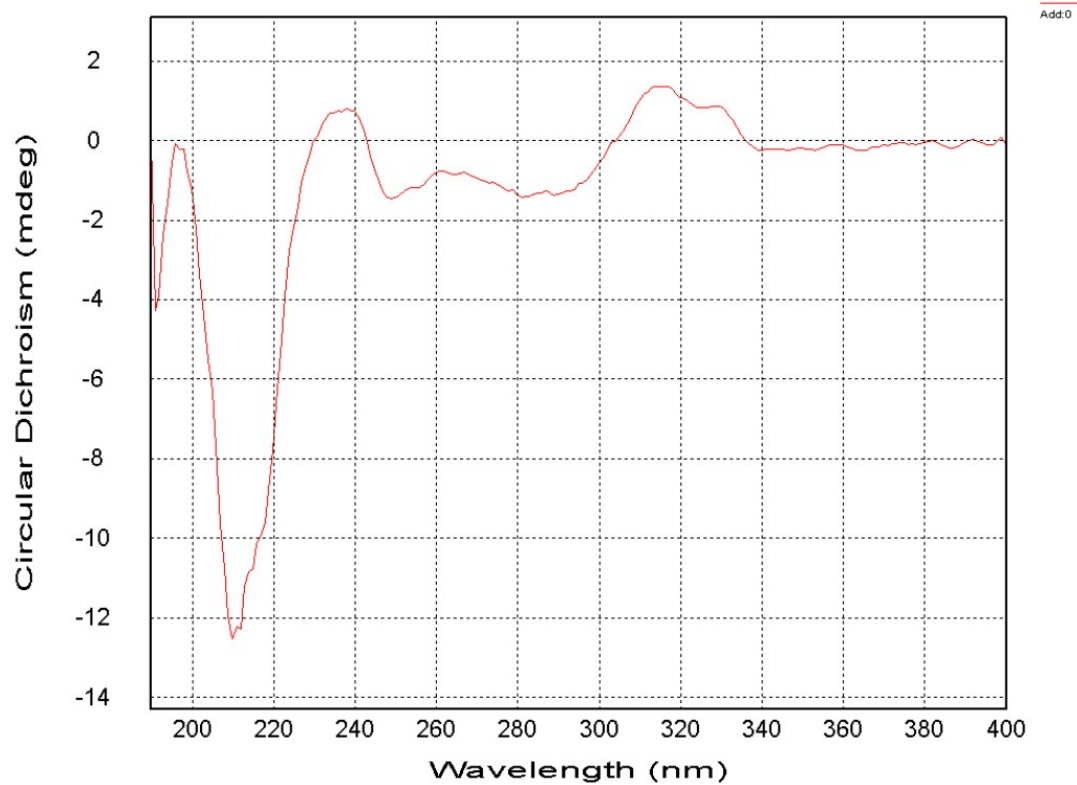


Figure S15. CD spectra of *Gerberdriasin B (2)* in CH₃OH

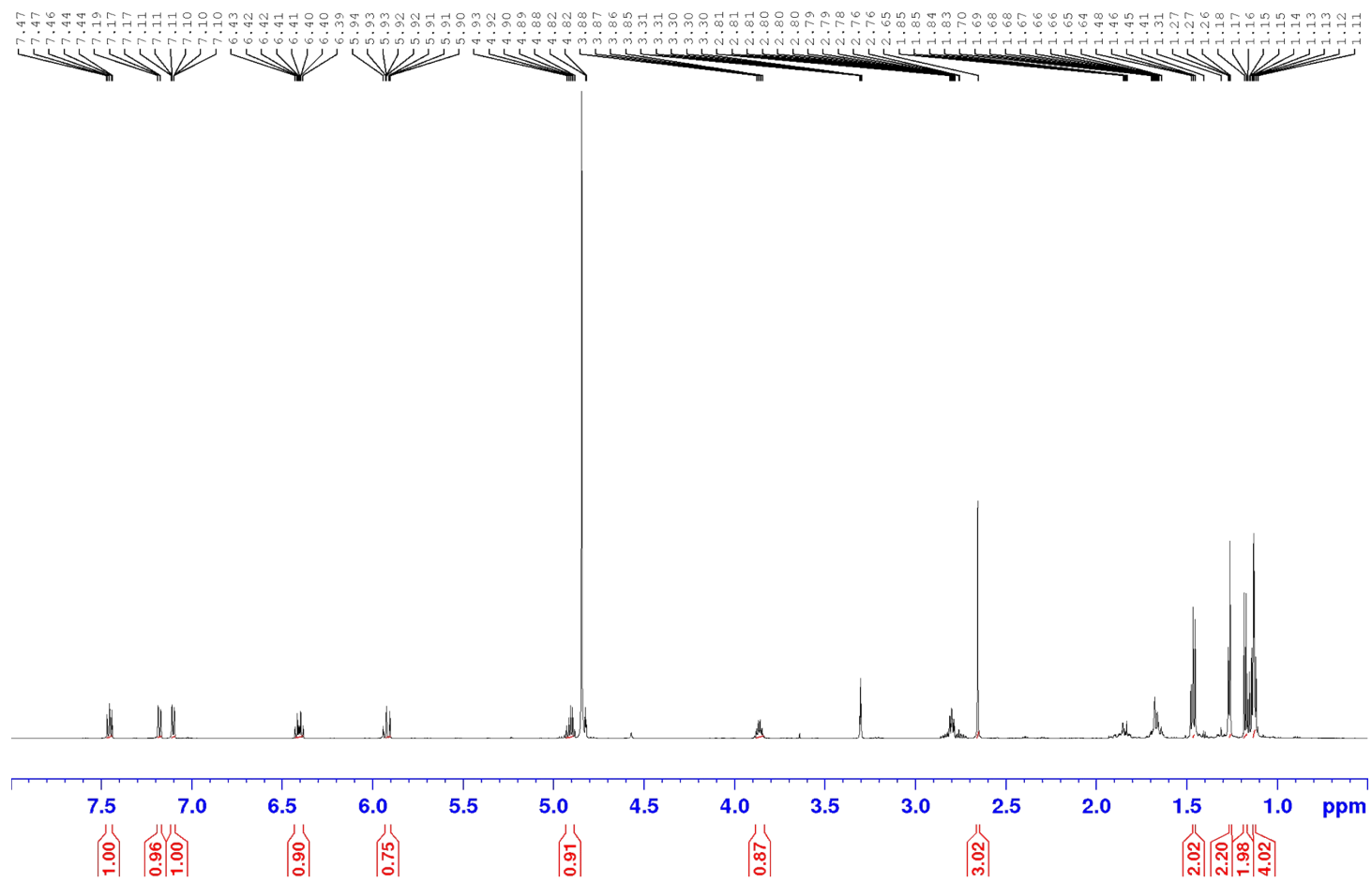


Figure S16. ¹H NMR spectrum of *Gerberdriasin B (2)* in CD₃OD

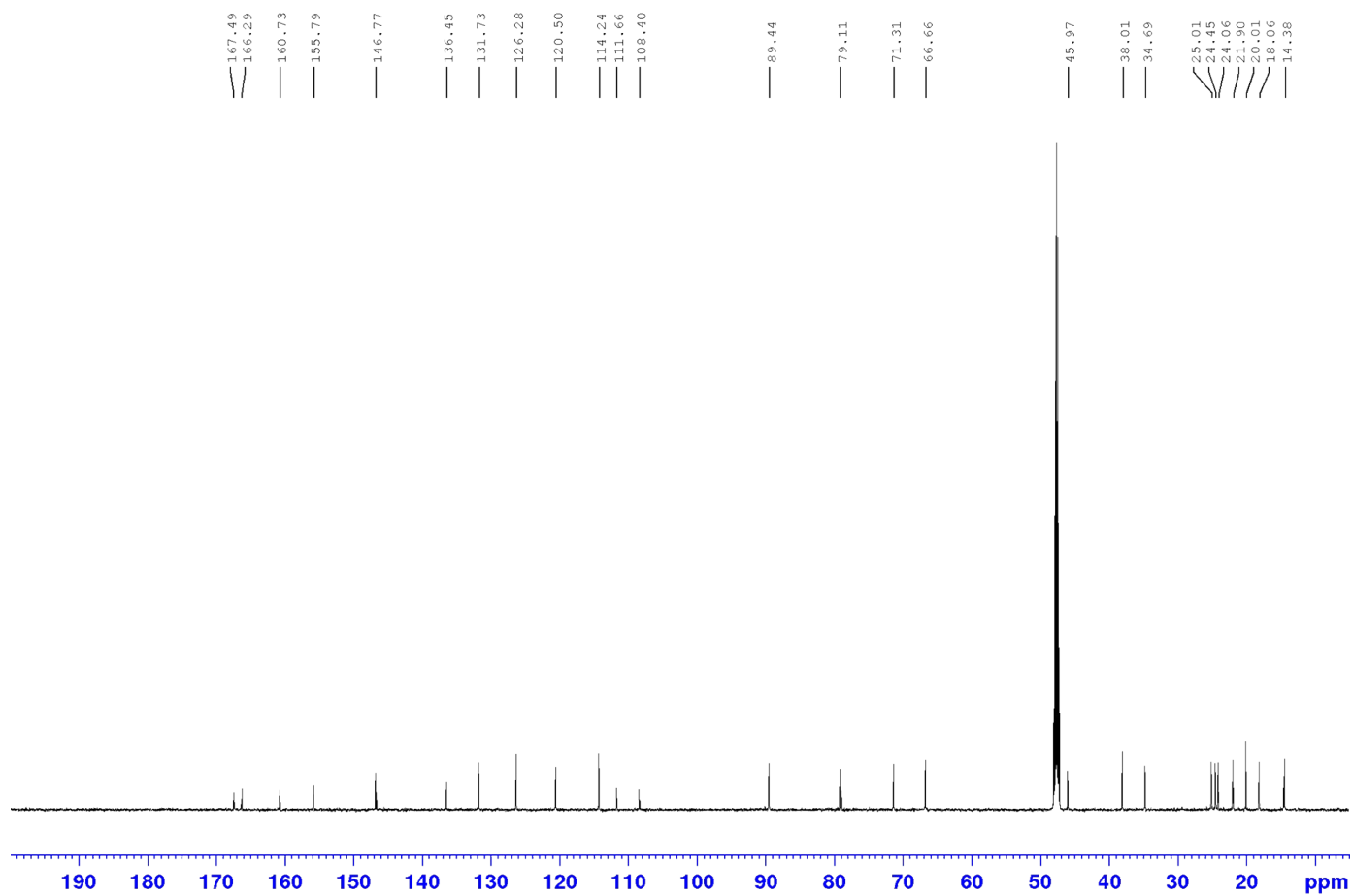


Figure S17. ¹³C NMR spectrum of *Gerberdriasin B (2)* in CD₃OD

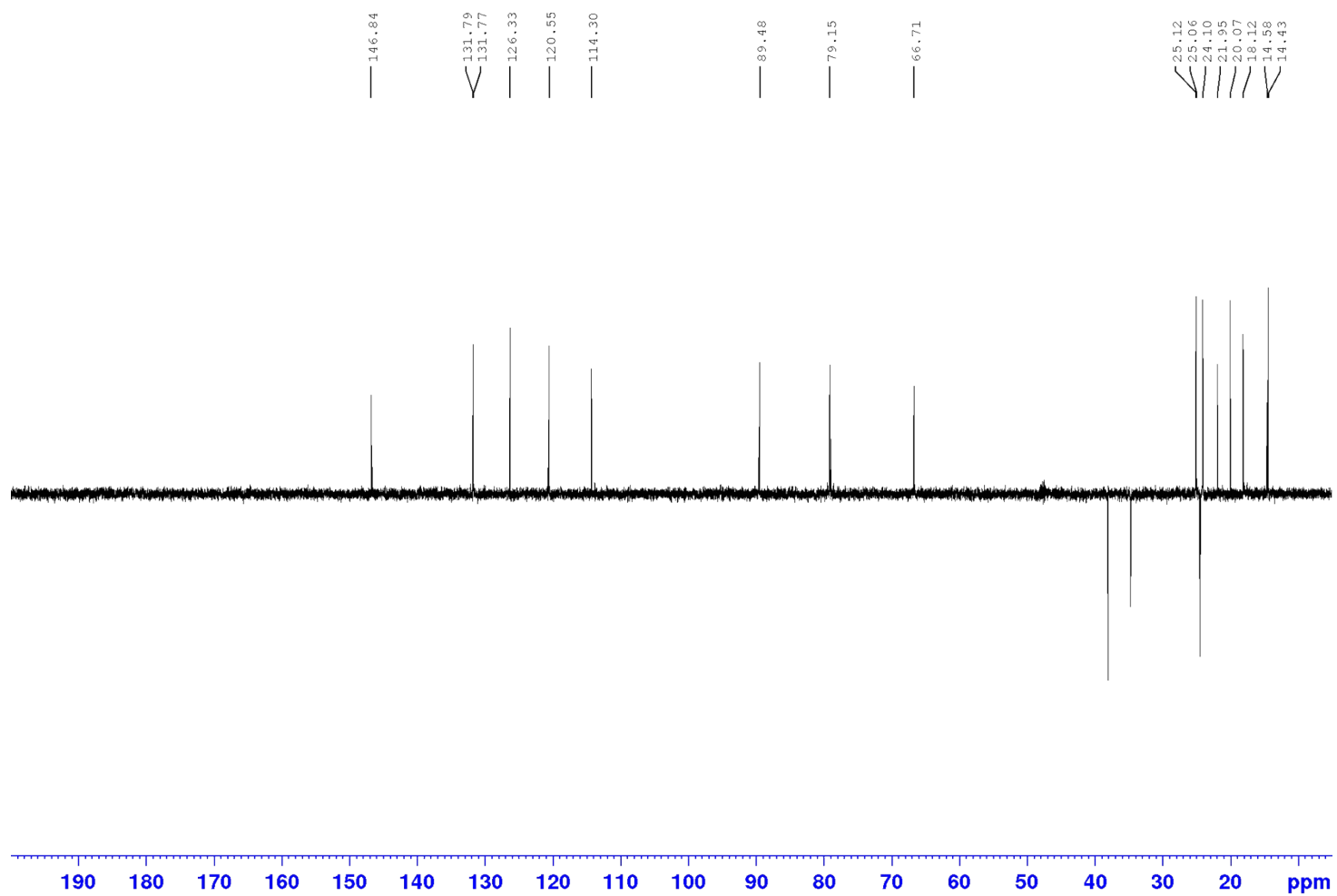


Figure S18. DEPT-135 NMR spectrum of *Gerberdriasin B (2)* in CD_3OD

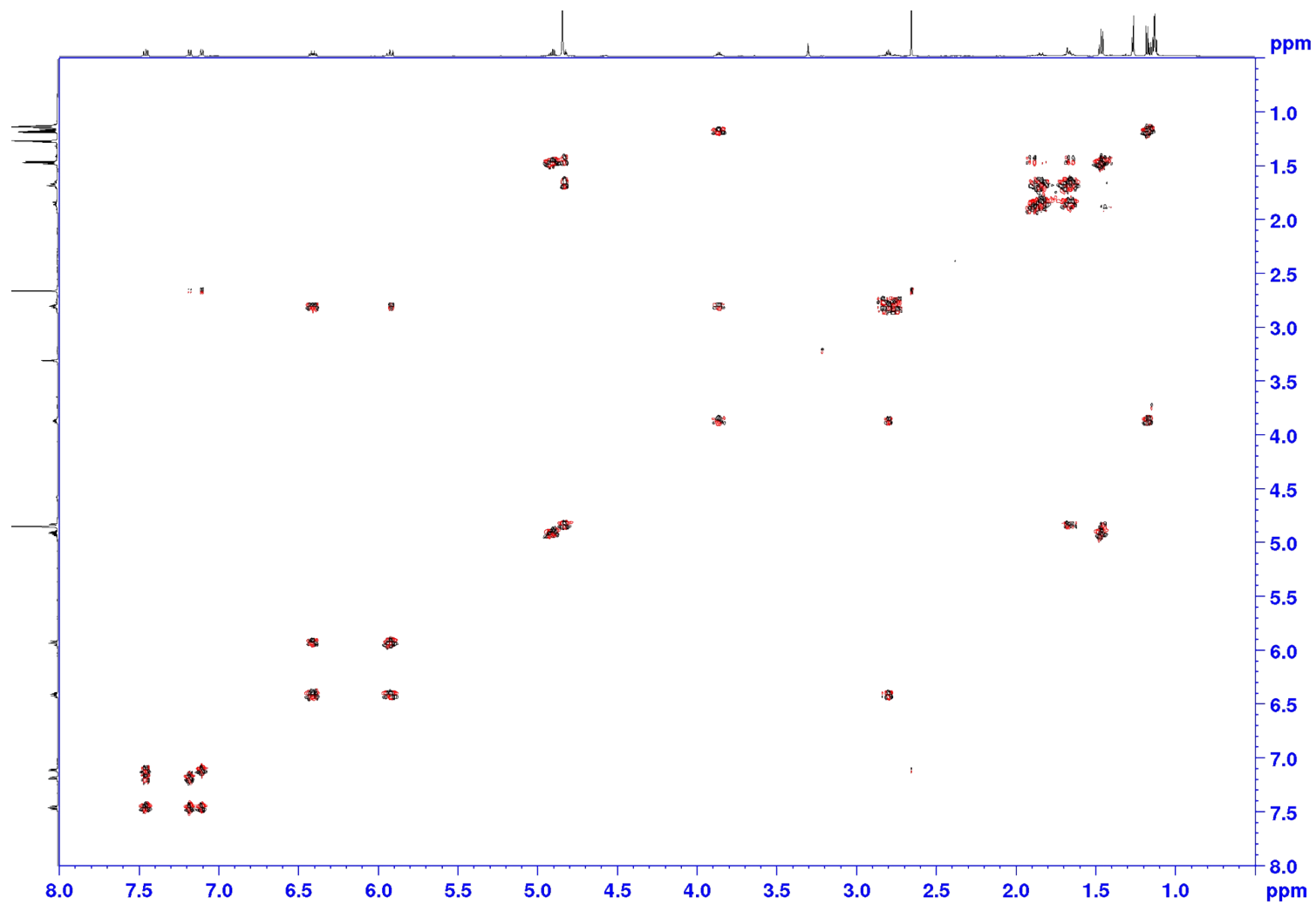


Figure S19. ^1H - ^1H COSY spectrum of *Gerberdriasin B* (2) in CD_3OD

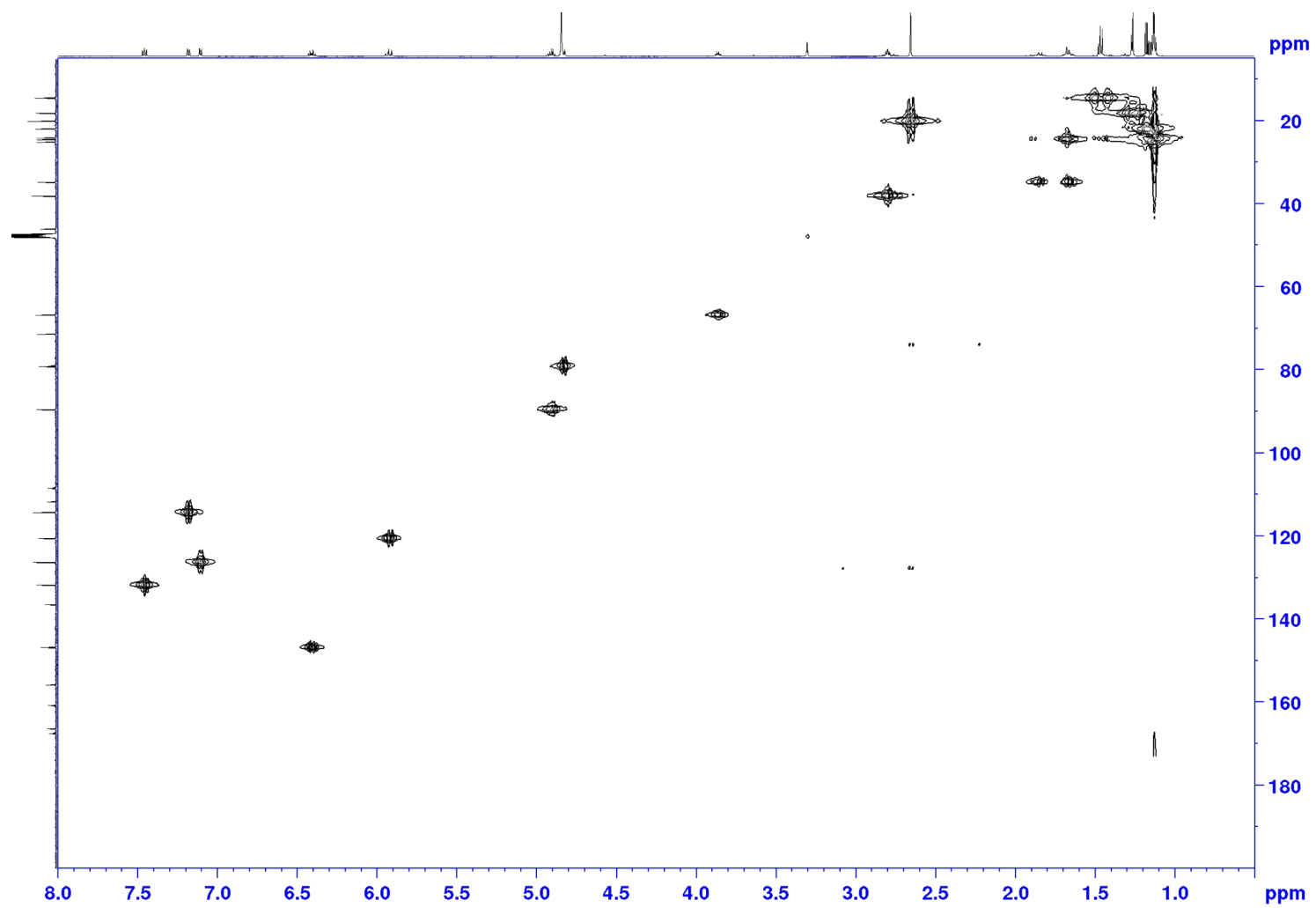


Figure S20. HSQC spectrum of *Gerberdriasin B (2)* in CD₃OD

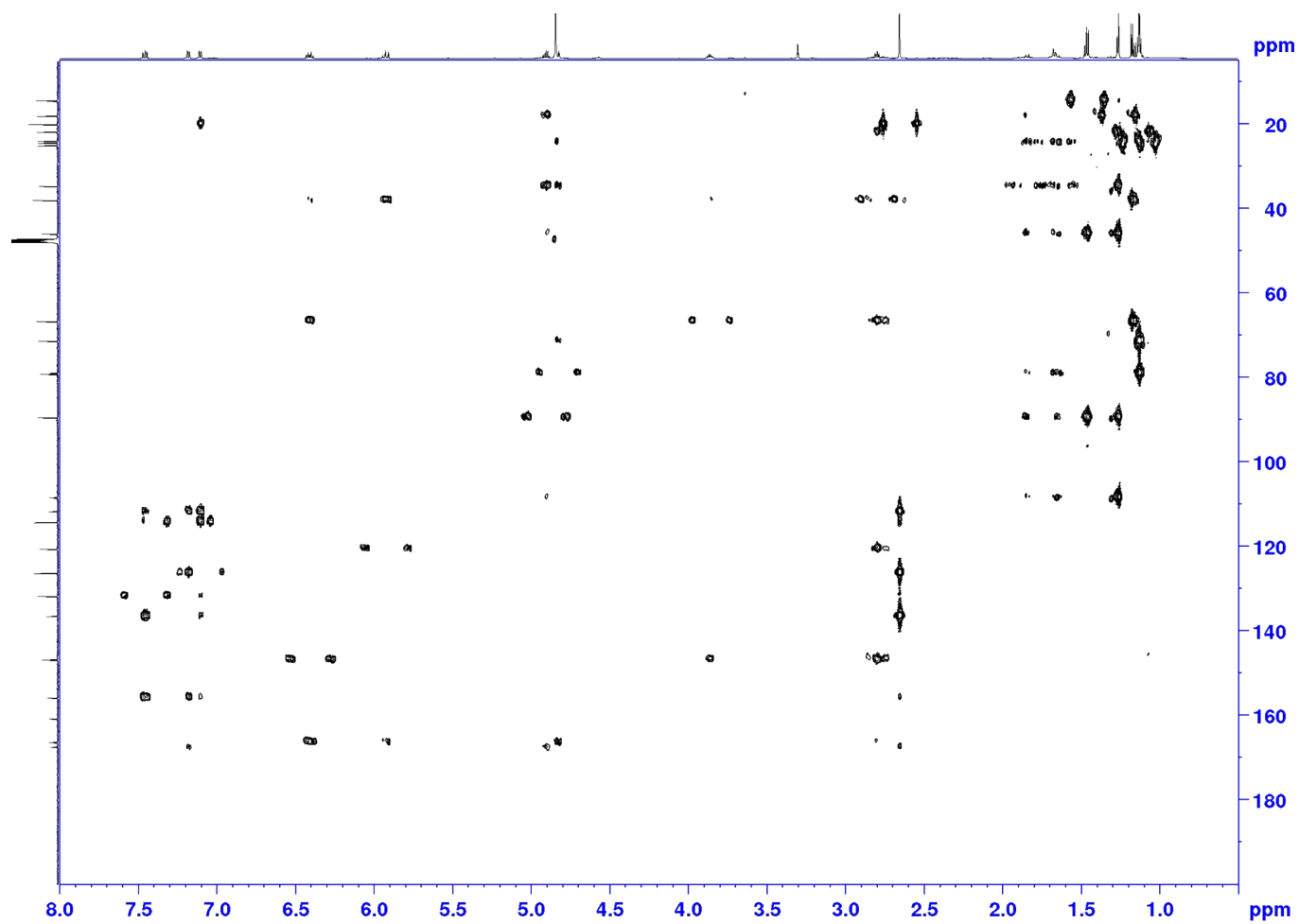


Figure S21. HMBC spectrum of *Gerberdriasin B* (2) in CD₃OD

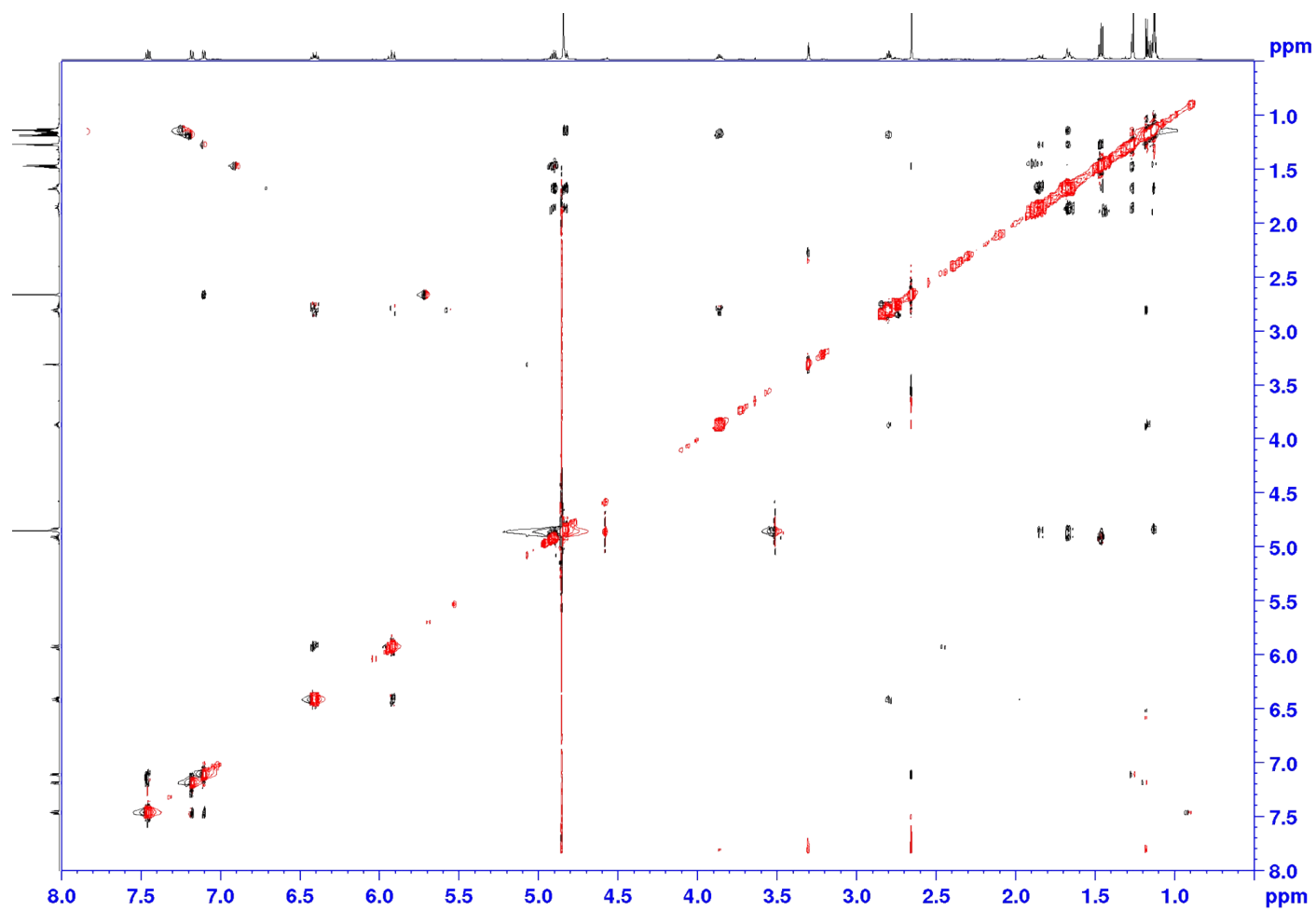
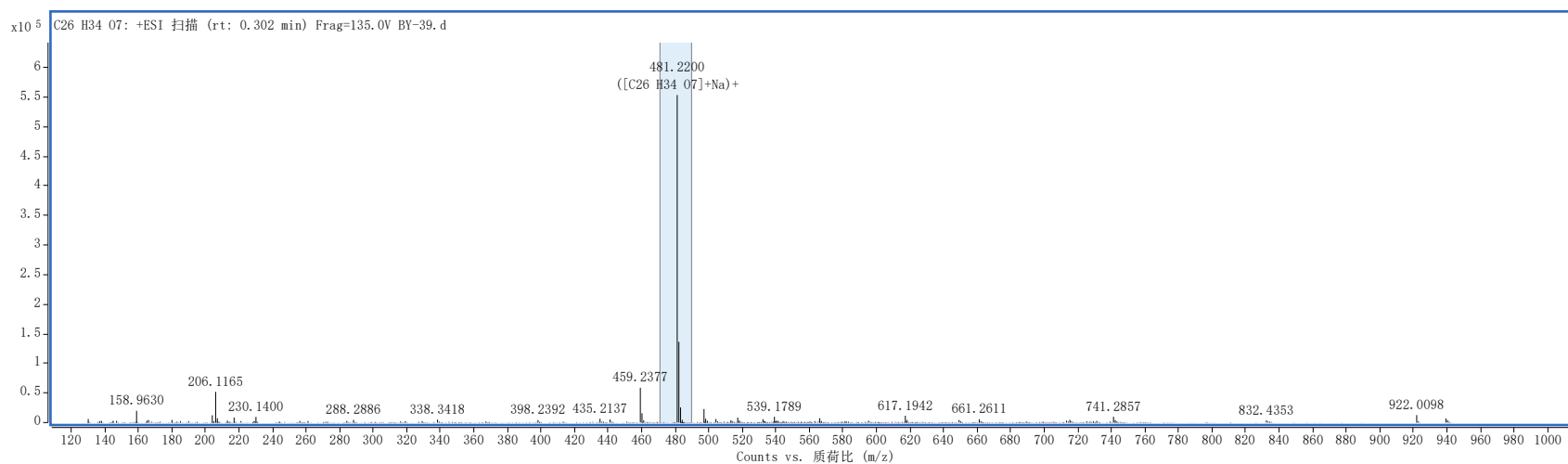


Figure S22. NOESY spectrum of *Gerberdriasin B (2)* in CD_3OD



峰高总百分比 (Calc)	峰高 (计算值)	峰高百分数(计算值)	m/z (Calc)	Diff (mDa)	峰高	峰高百分数	峰高总百分比	m/z	Diff (ppm)
74.5	533033.5	100	481.2197	-0.3	553444.9	100	77.4	481.22	-0.67

ID 来源	分子式	种类	m/z	分数	Diff (ppm)	分数 (MFG)
MFG	C26 H34 O7	(M+Na)+	481.2200	96.7	-0.55	96.7

Figure S23. HRESIMS spectrum of *Gerberdriasin C (3)*

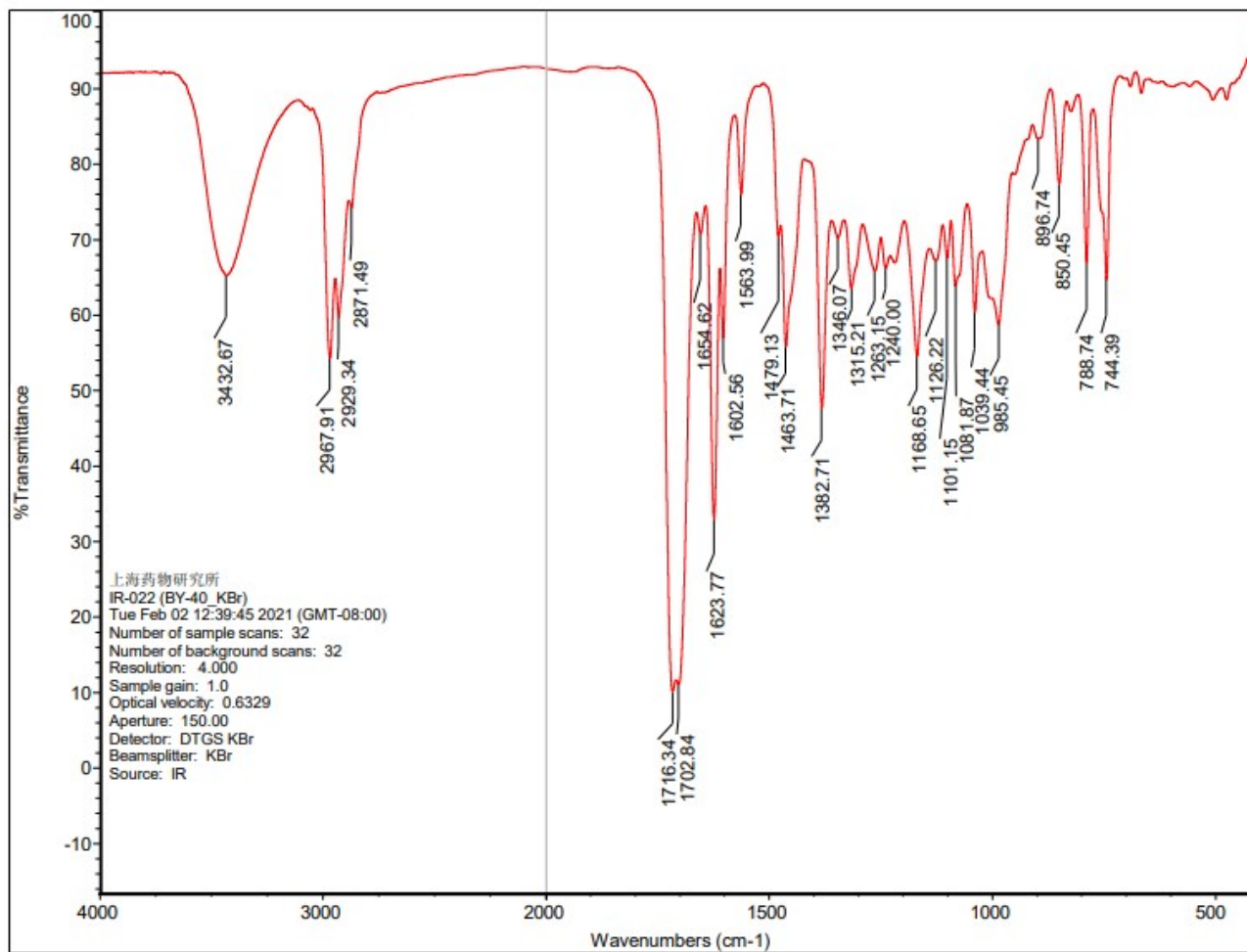


Figure S24. IR spectrum of *Gerberdriasin C (3)*

Rudolph Research Analytical

Thursday, 11/05/2020

This sample was measured on an Autopol VI, serial number 90079,
manufactured by Rudolph Research Analytical, Hackettstown, NJ.

LotID : BY-40
Set Temperature : 20.0
Temp Corr : OFF

n	Average	Std.Dev.	Maximum	Minimum
6	-5.278	0.6213	-5.000	-6.667

S.No	Sample ID	Time	Result	Scale	OR ° Arc	WLG	Lg.mm	Conc.	Temp.	Comment
1	BY-40	04:42:59 PM	-5.000	SR	-0.003	589	100.00	0.060	20.0	
2	BY-40	04:43:06 PM	-6.667	SR	-0.004	589	100.00	0.060	20.0	
3	BY-40	04:43:11 PM	-5.000	SR	-0.003	589	100.00	0.060	20.0	
4	BY-40	04:43:17 PM	-5.000	SR	-0.003	589	100.00	0.060	20.0	
5	BY-40	04:43:23 PM	-5.000	SR	-0.003	589	100.00	0.060	20.0	
6	BY-40	04:43:29 PM	-5.000	SR	-0.003	589	100.00	0.060	19.9	

Signature

Figure S25. OR Value of *Gerberdriasin C (3)* in CH₃OH

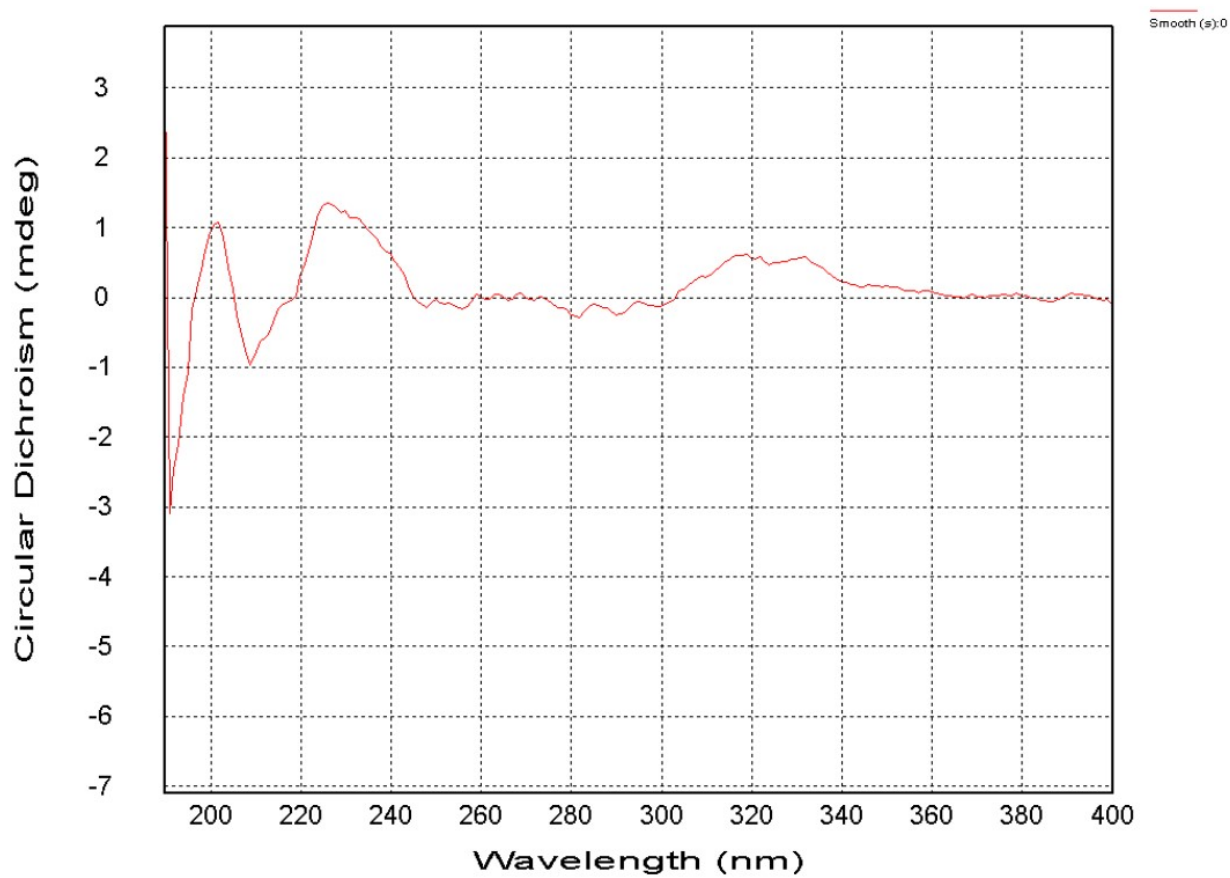


Figure S26. CD spectra of *Gerberdriasin C* (**3**) in CH₃OH

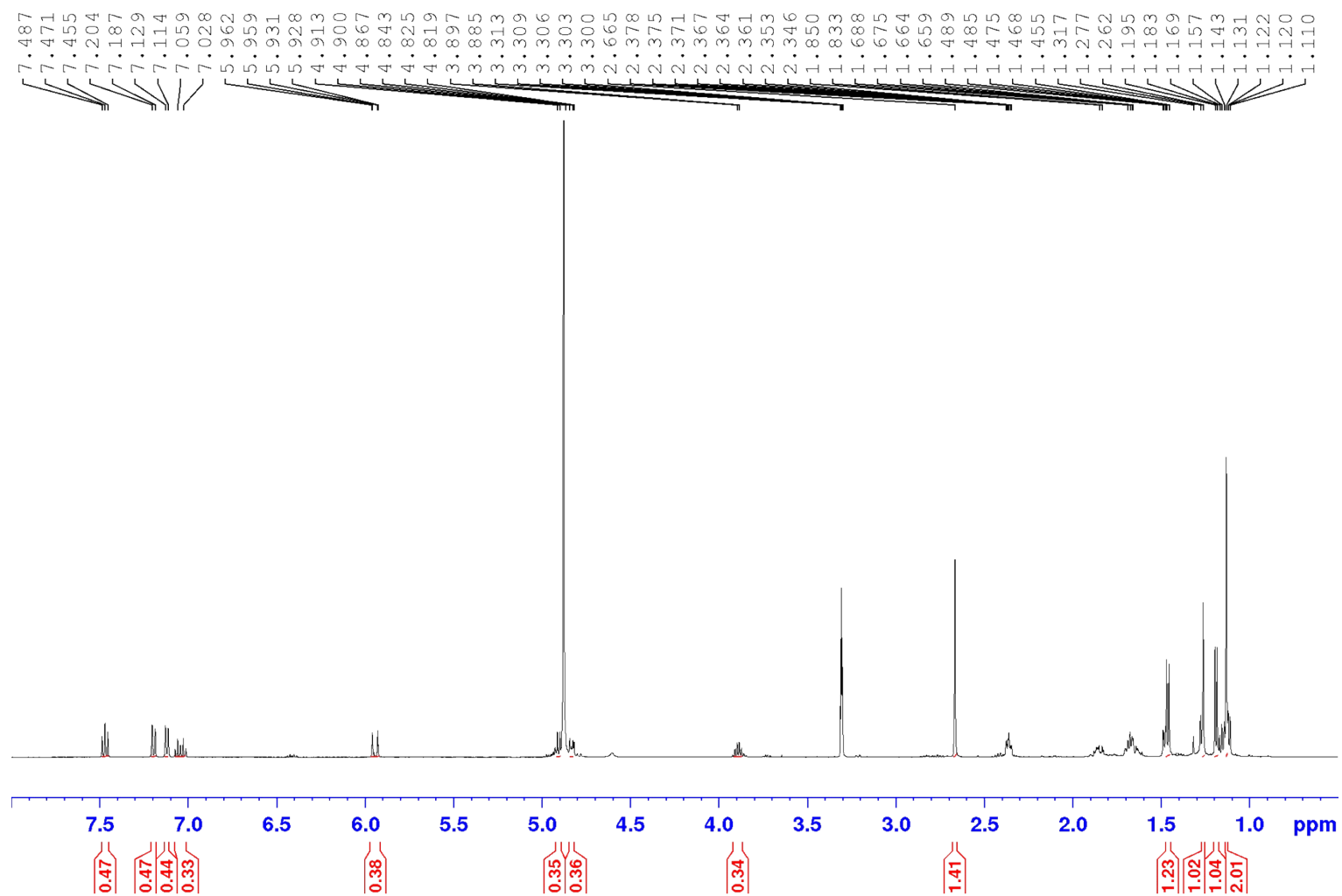


Figure S27. ¹H NMR spectrum of *Gerberdriasin C* (**3**) in CD₃OD

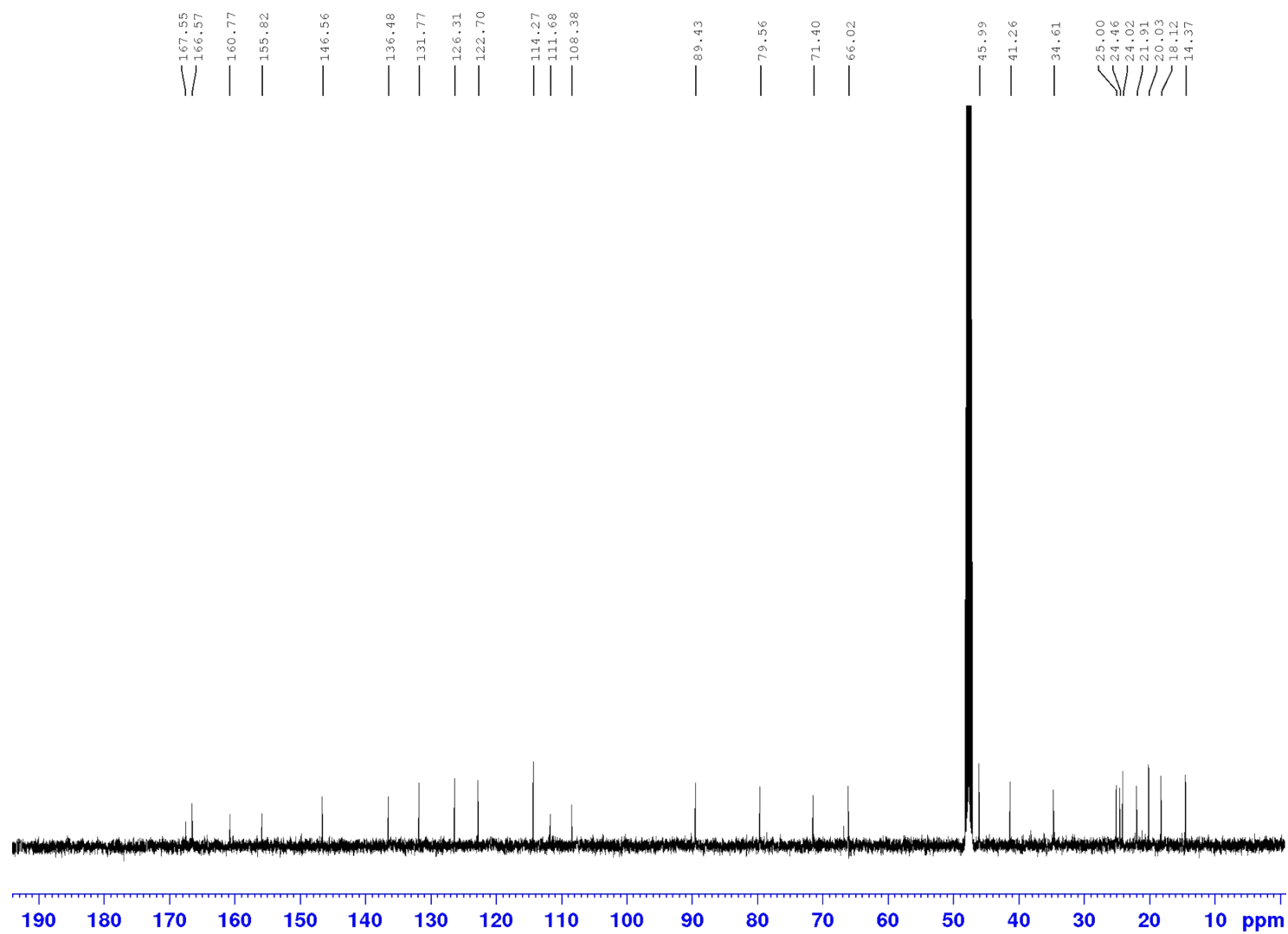


Figure S28. ^{13}C NMR spectrum of *Gerberdriasin C (3)* in CD_3OD

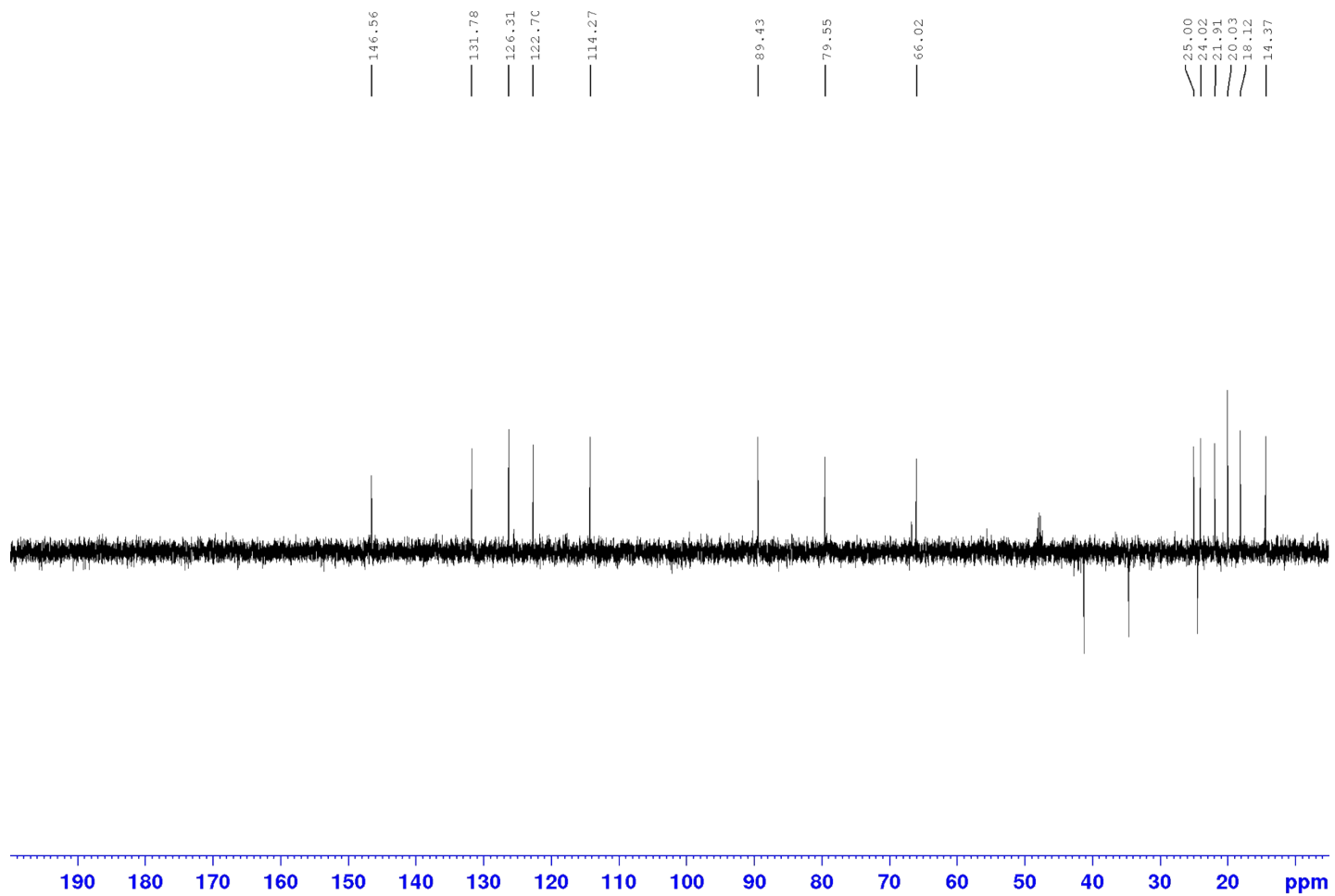


Figure S29. DEPT-135 NMR spectrum of *Gerberdriasin C (3)* in CD₃OD

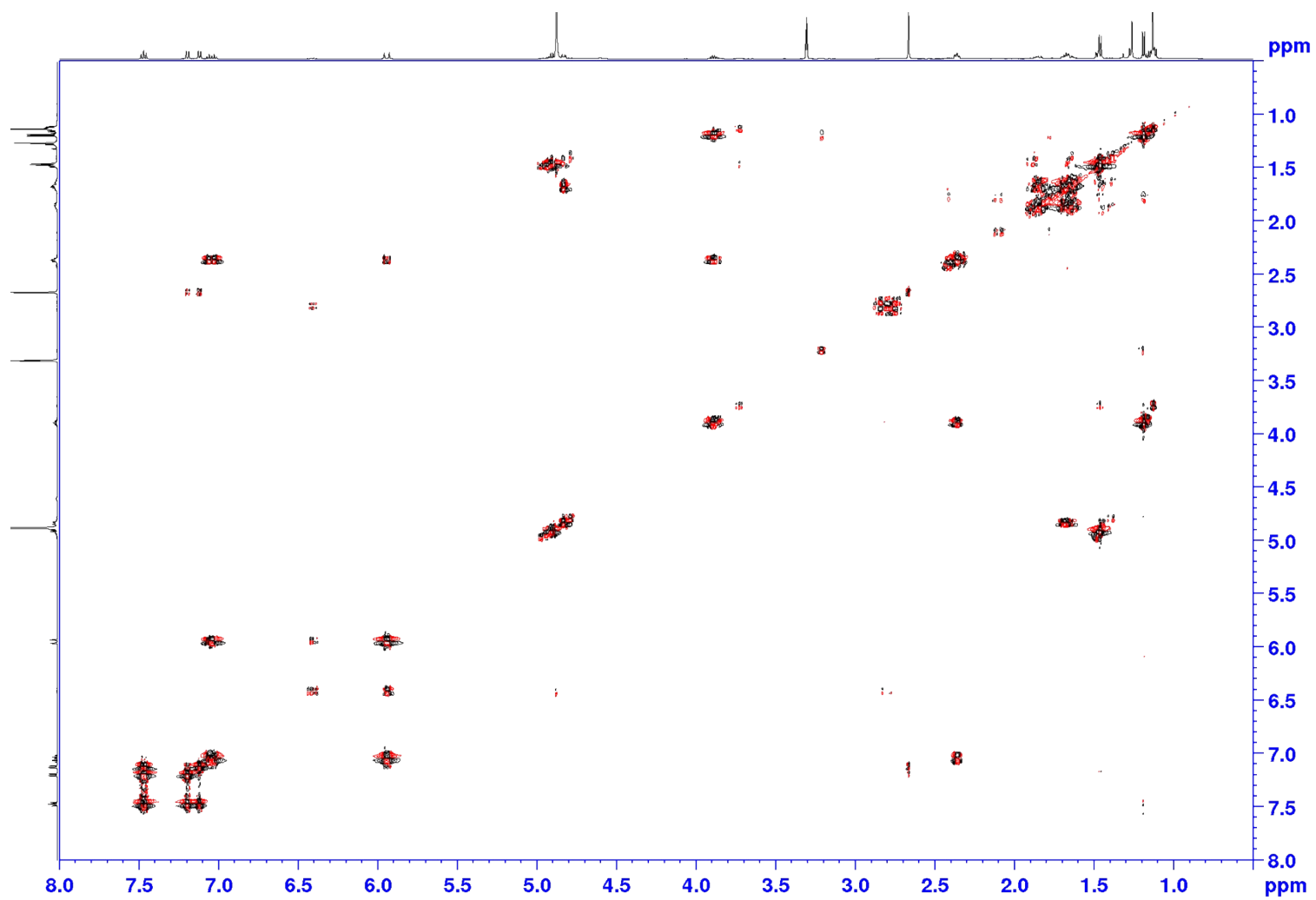


Figure S30. ^1H - ^1H COSY spectrum of *Gerberdriasin C* (**3**) in CD_3OD

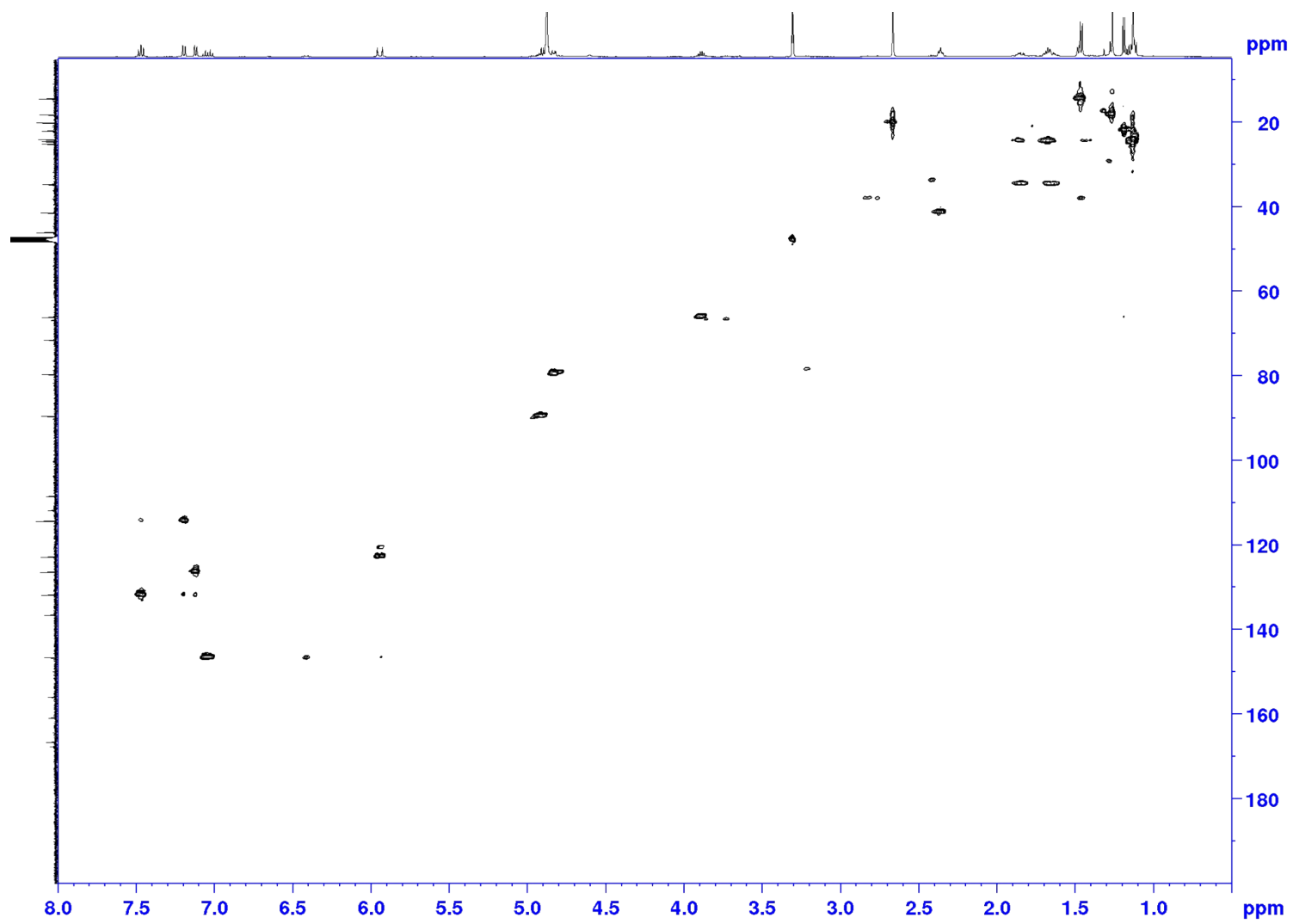


Figure S31. HSQC spectrum of *Gerberdriasin C (3)* in CD₃OD

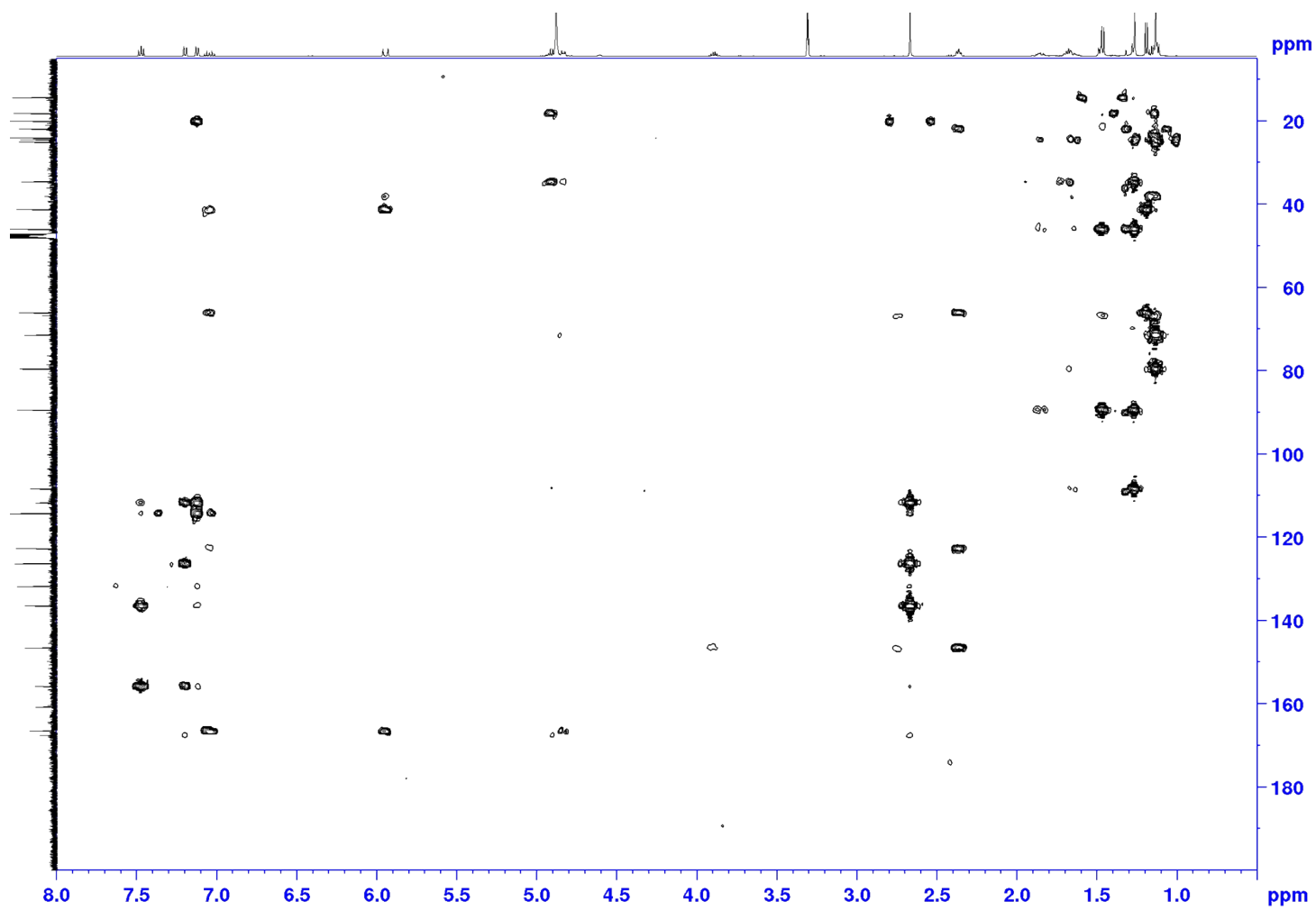


Figure S32. HMBC spectrum of *Gerberdriasin C* (**3**) in CD₃OD

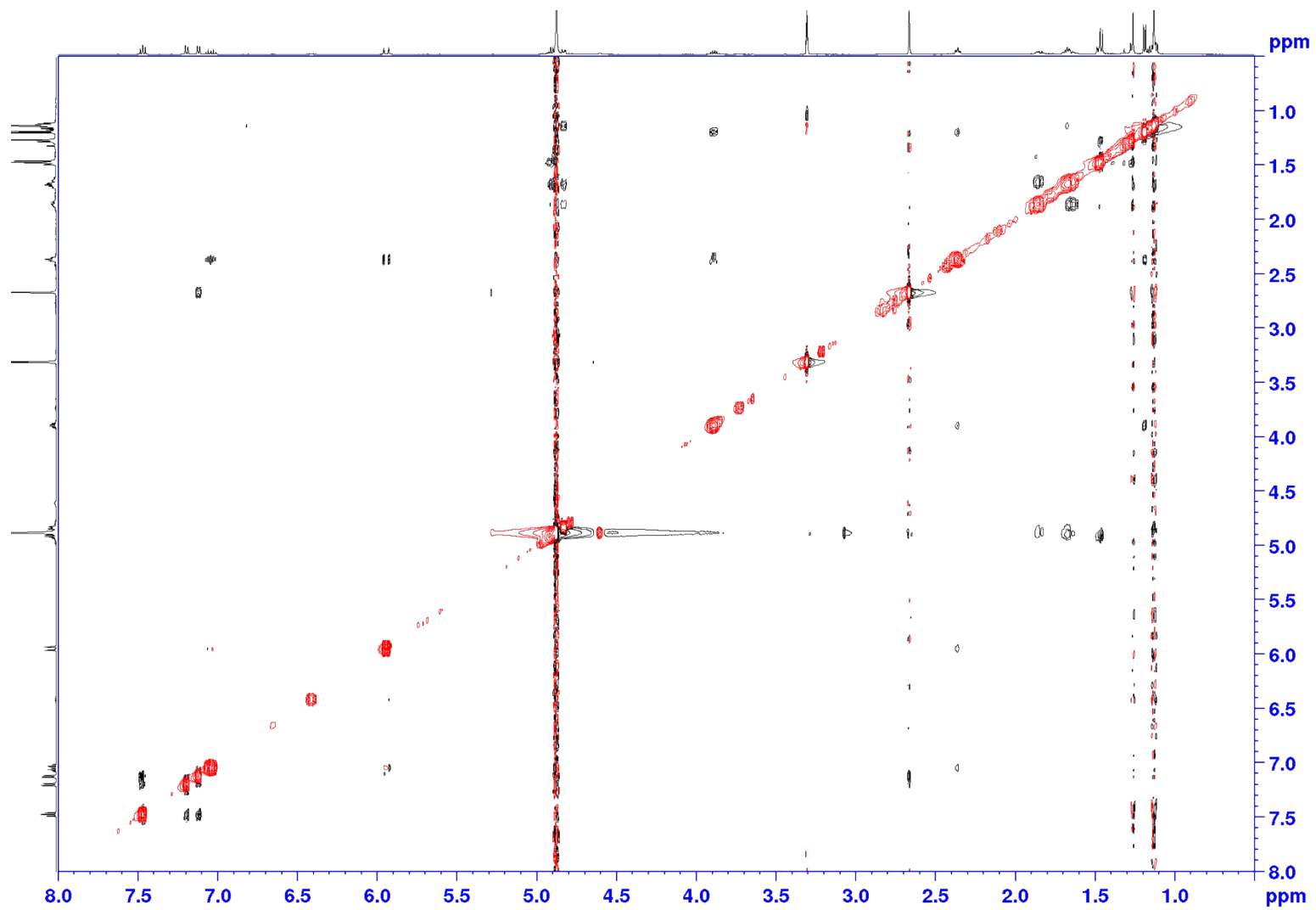
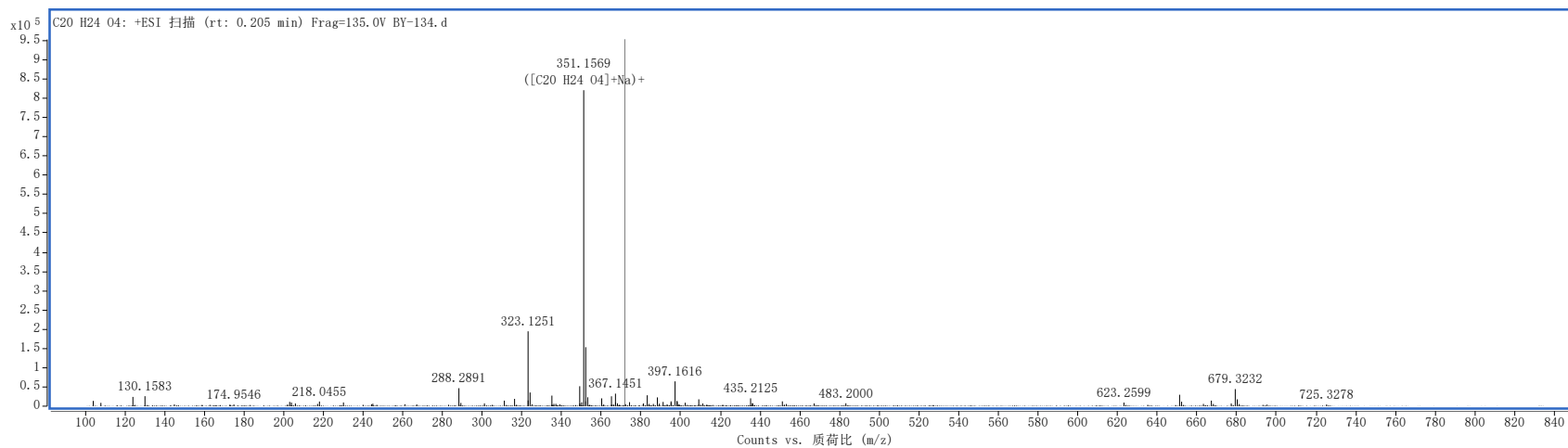


Figure S33. NOESY spectrum of *Gerberdriasin C* (3) in CD₃OD



峰高总百分比 (Calc)	峰高 (计算值)	峰高百分数(计算值)	m/z (Calc)	Diff (mDa)	峰高	峰高百分数	峰高总百分比	m/z	Diff (ppm)
79.9	796654.4	100	351.1567	-0.2	821034.6	100	82.3	351.1569	-0.67

最佳	ID 来源	分子式	种类	m/z	分数	Diff (ppm)	分数 (MFG)
TRUE	MFG	C20 H24 O4	(M+Na)+	351.1569	96.79	-0.27	96.79

Figure S34. HRESIMS spectrum of *Gerberdriasin D (4)*

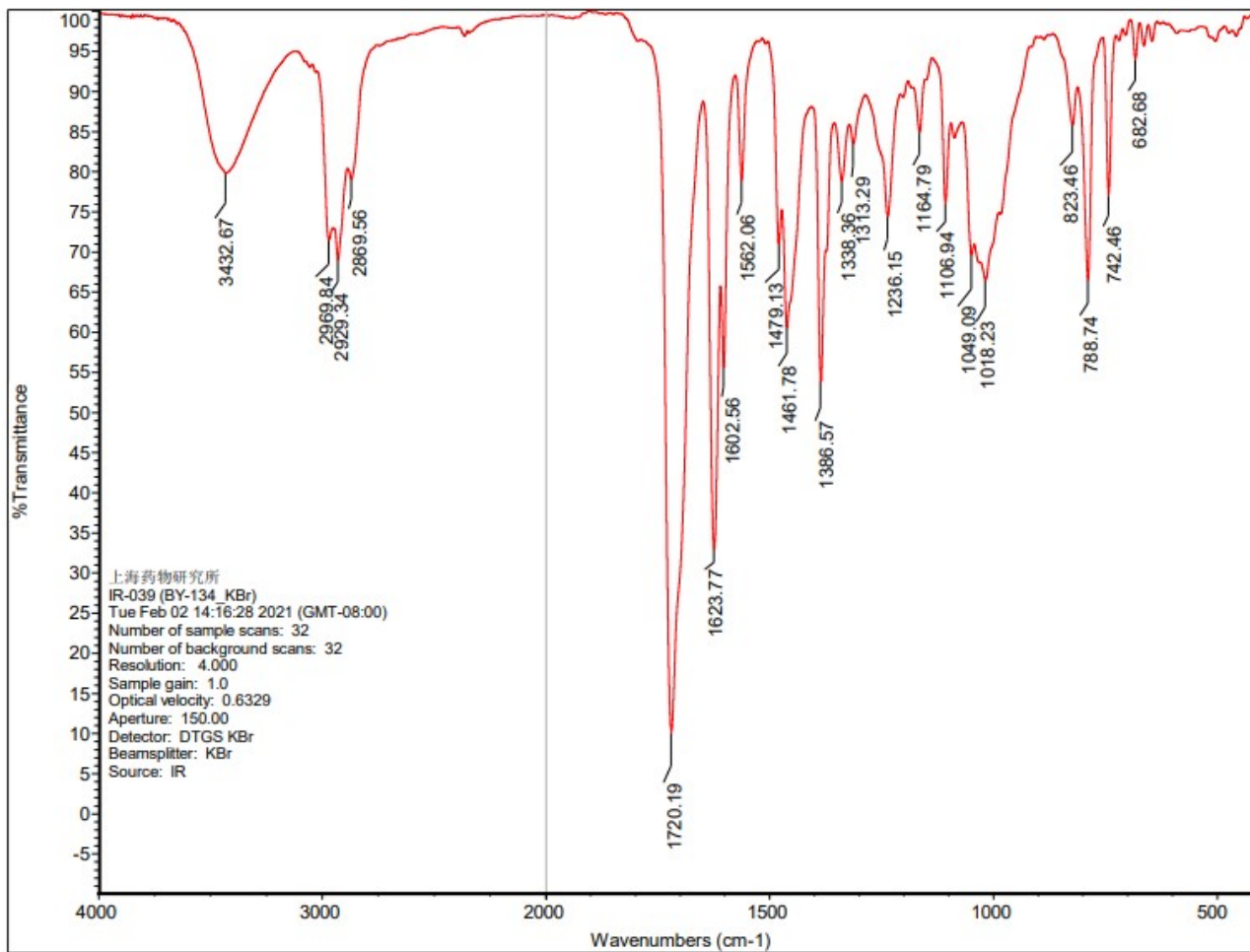


Figure S35. IR spectrum of *Gerberdriasin D* (4)

Rudolph Research Analytical

Thursday, 02/04/2021

This sample was measured on an Autopol VI, serial number 90079,
manufactured by Rudolph Research Analytical, Hackettstown, NJ.

LotID : BY-134
Set Temperature : 20.0
Temp Corr : OFF

n	Average	Std.Dev.	Maximum	Minimum
6	13.333	0.0000	13.333	13.333

S.No	Sample ID	Time	Result	Scale	OR ° Arc	WLG	Lg.mm	Conc.	Temp.	Comment
1	BY-134	10:59:06 AM	13.333	SR	0.008	589	100.00	0.060	20.3	
2	BY-134	10:59:12 AM	13.333	SR	0.008	589	100.00	0.060	20.3	
3	BY-134	10:59:19 AM	13.333	SR	0.008	589	100.00	0.060	20.3	
4	BY-134	10:59:25 AM	13.333	SR	0.008	589	100.00	0.060	20.3	
5	BY-134	10:59:32 AM	13.333	SR	0.008	589	100.00	0.060	20.3	
6	BY-134	10:59:39 AM	13.333	SR	0.008	589	100.00	0.060	20.3	

Signature

Figure S36. OR Value of *Gerberdriasin D (4)* in CH₃OH

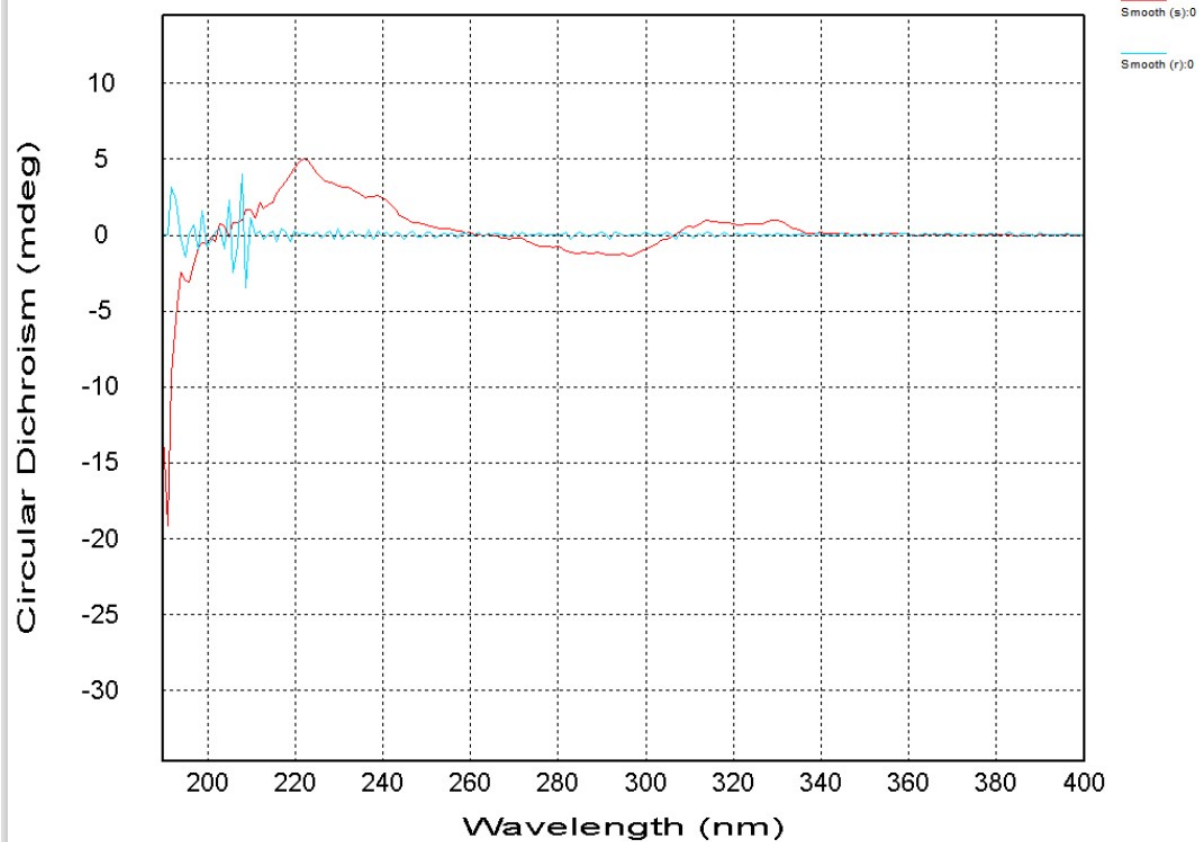


Figure S37. CD spectra of *Gerberdriasin D (4)* in CH₃OH

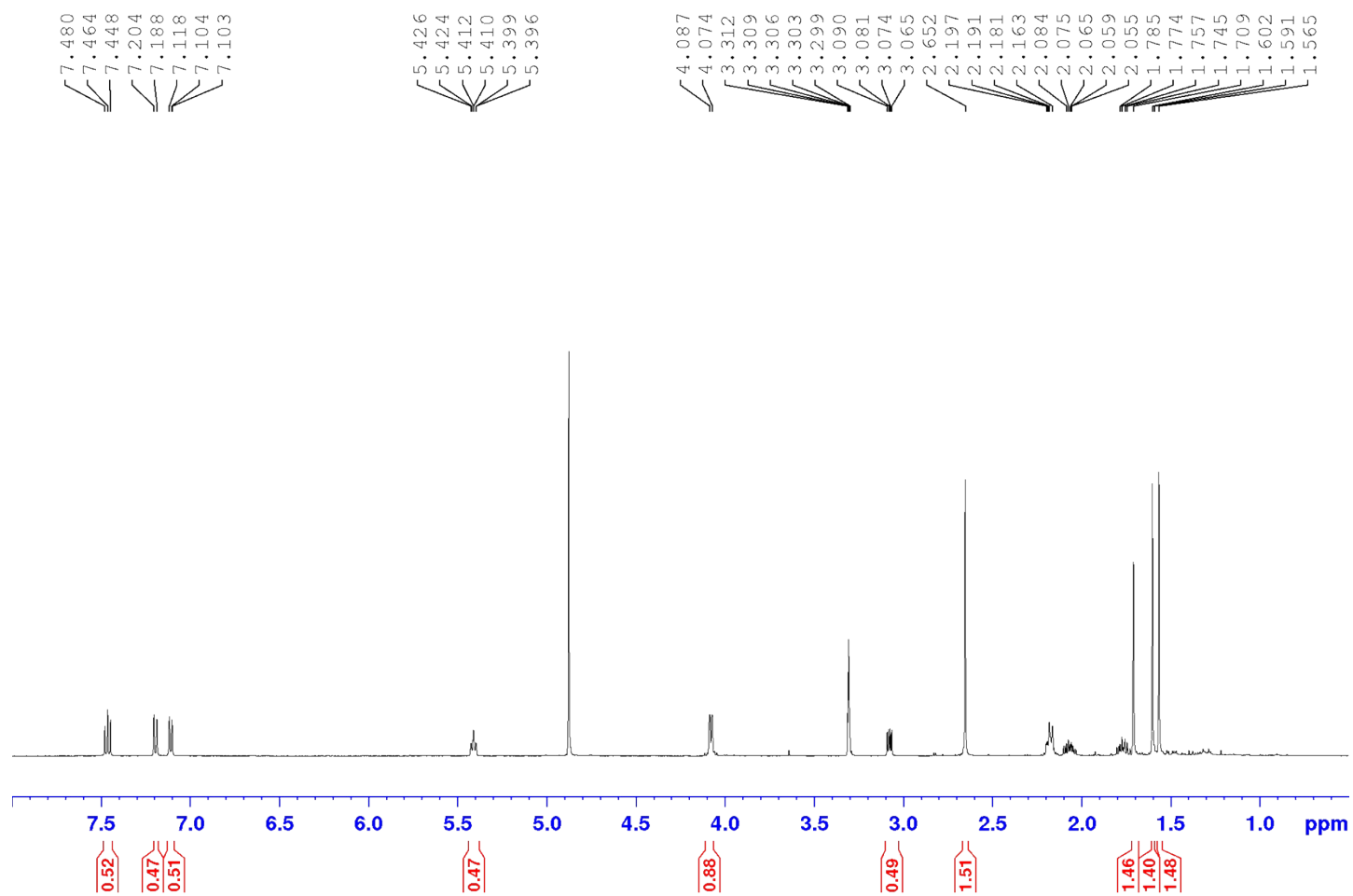


Figure S38. ^1H NMR spectrum of *Gerberdriasin D (4)* in CD_3OD

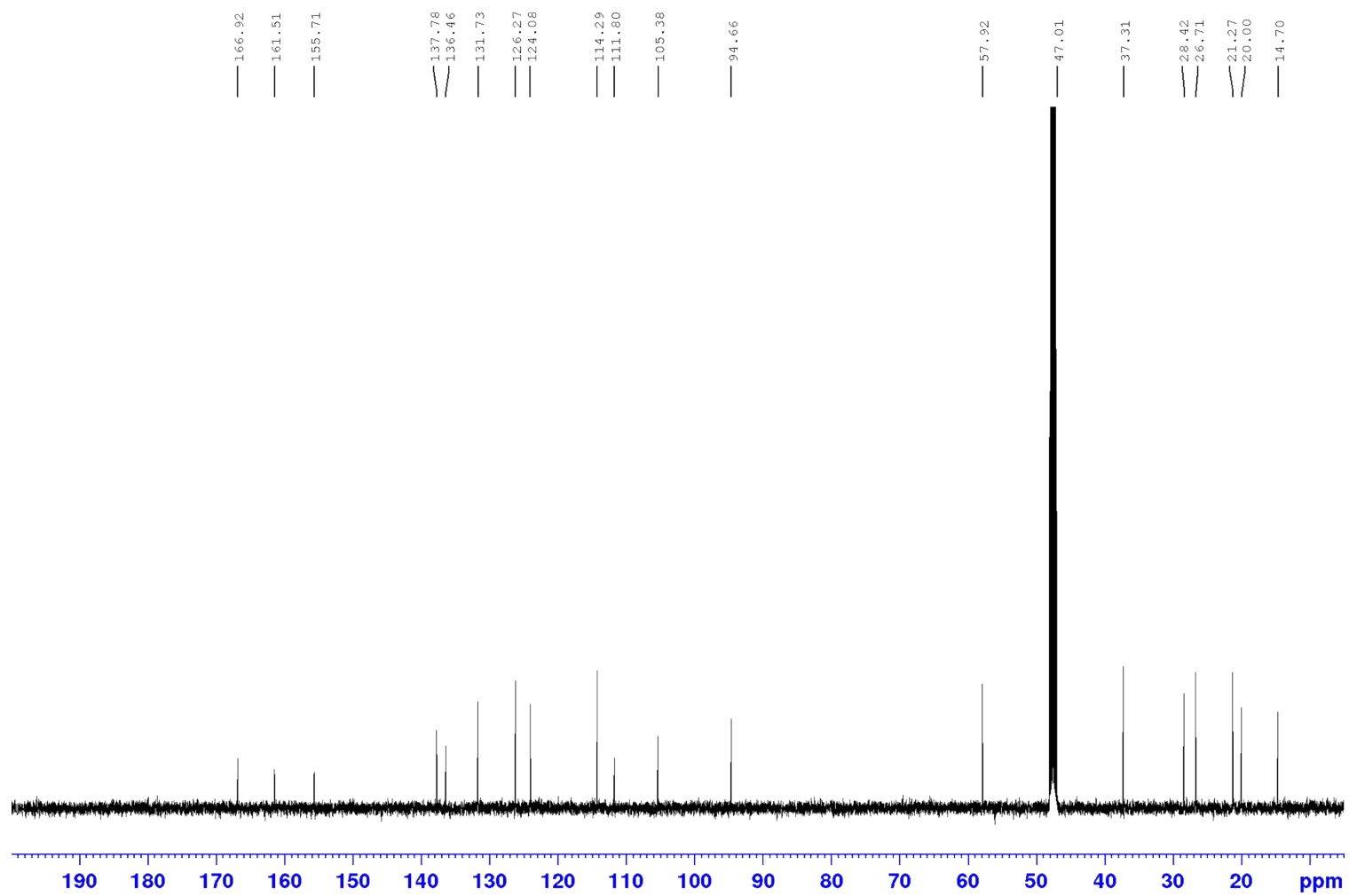


Figure S39. ^{13}C NMR spectrum of *Gerberdriasin D (4)* in CD_3OD

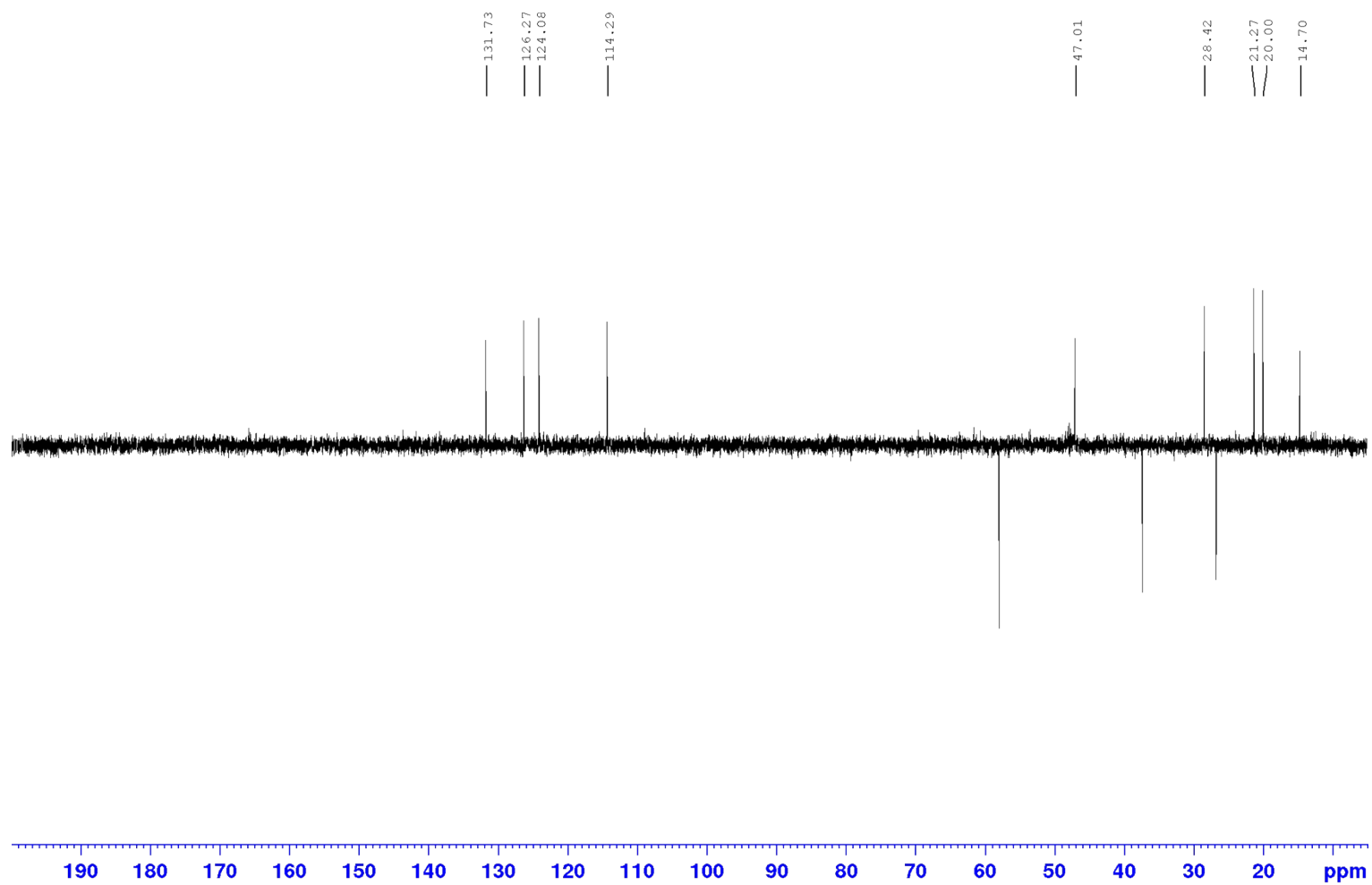


Figure S40. DEPT-135 NMR spectrum of *Gerberdriasin D (4)* in CD₃OD

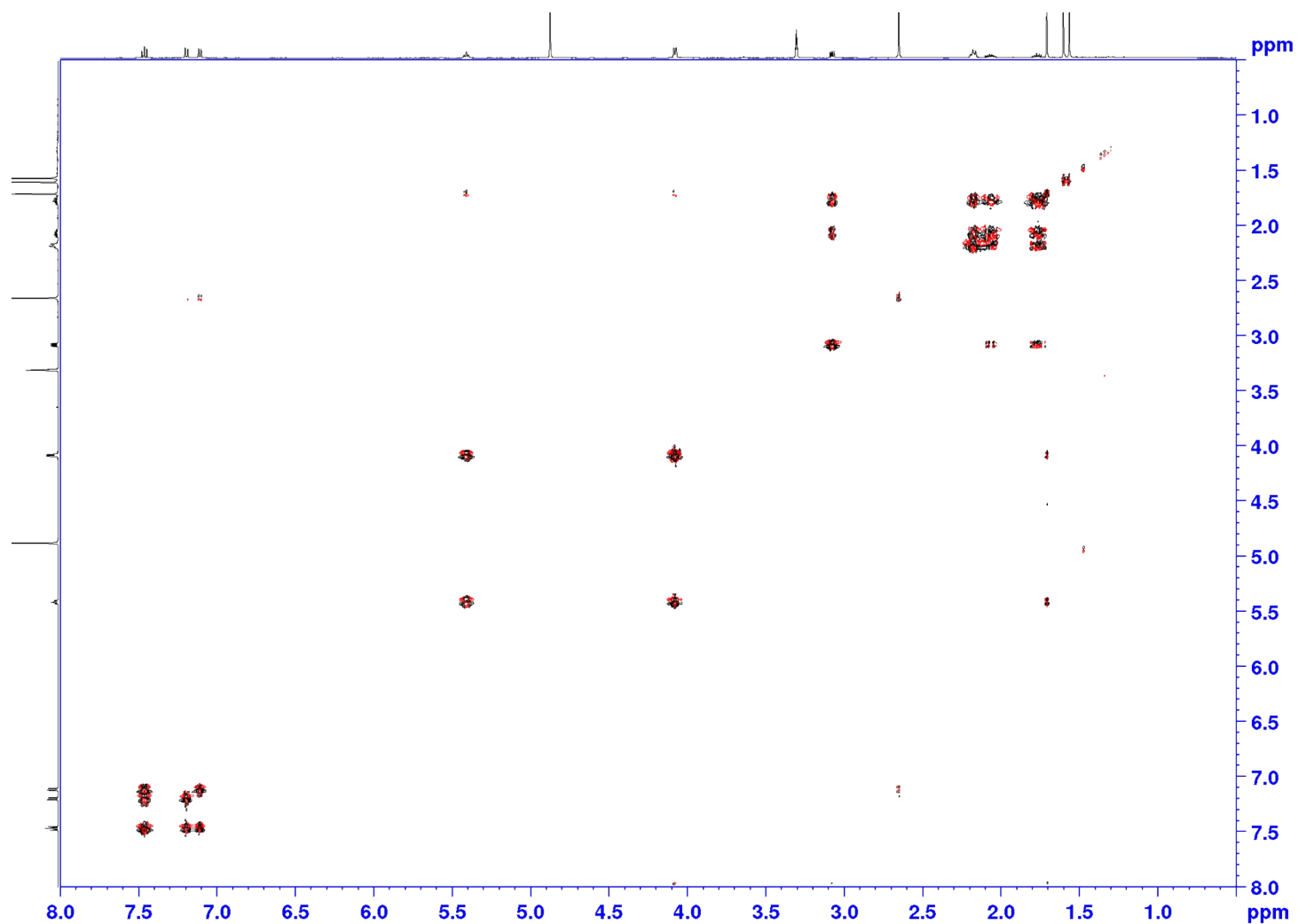


Figure S41. ^1H - ^1H COSY spectrum of *Gerberdriasin D* (4) in CD_3OD

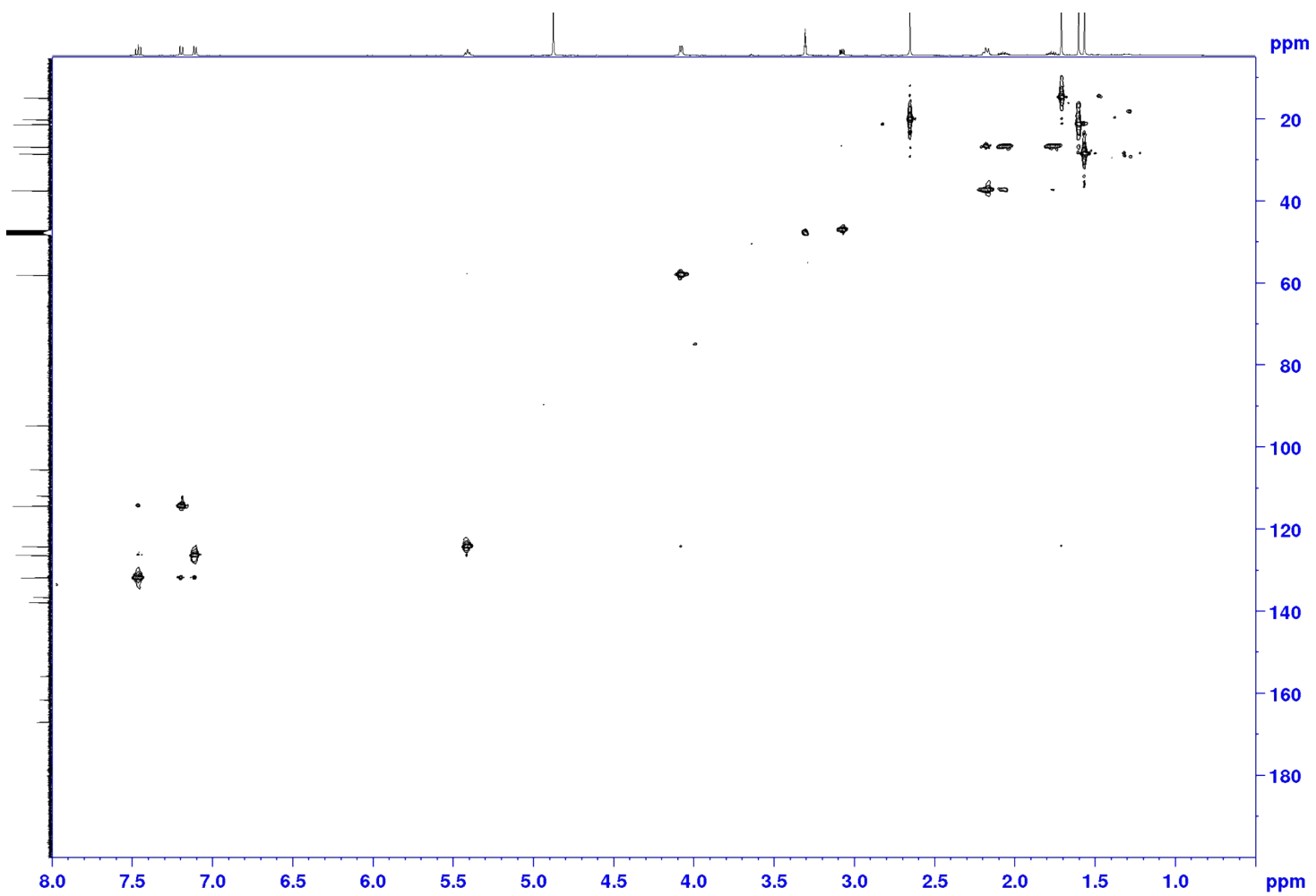


Figure S42. HSQC spectrum of *Gerberdriasin D (4)* in CD₃OD

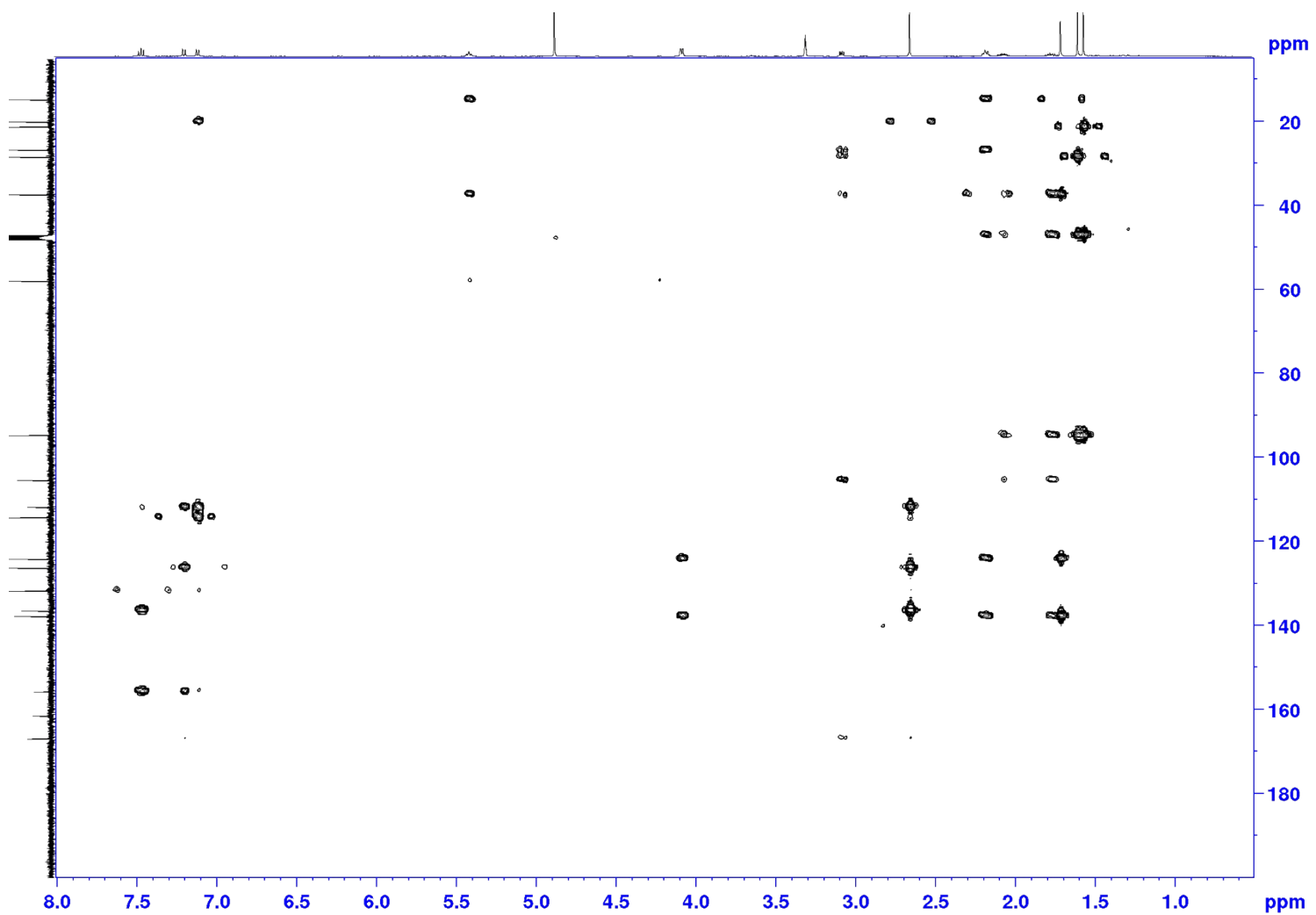


Figure S43. HMBC spectrum of *Gerberdriasin D (4)* in CD_3OD

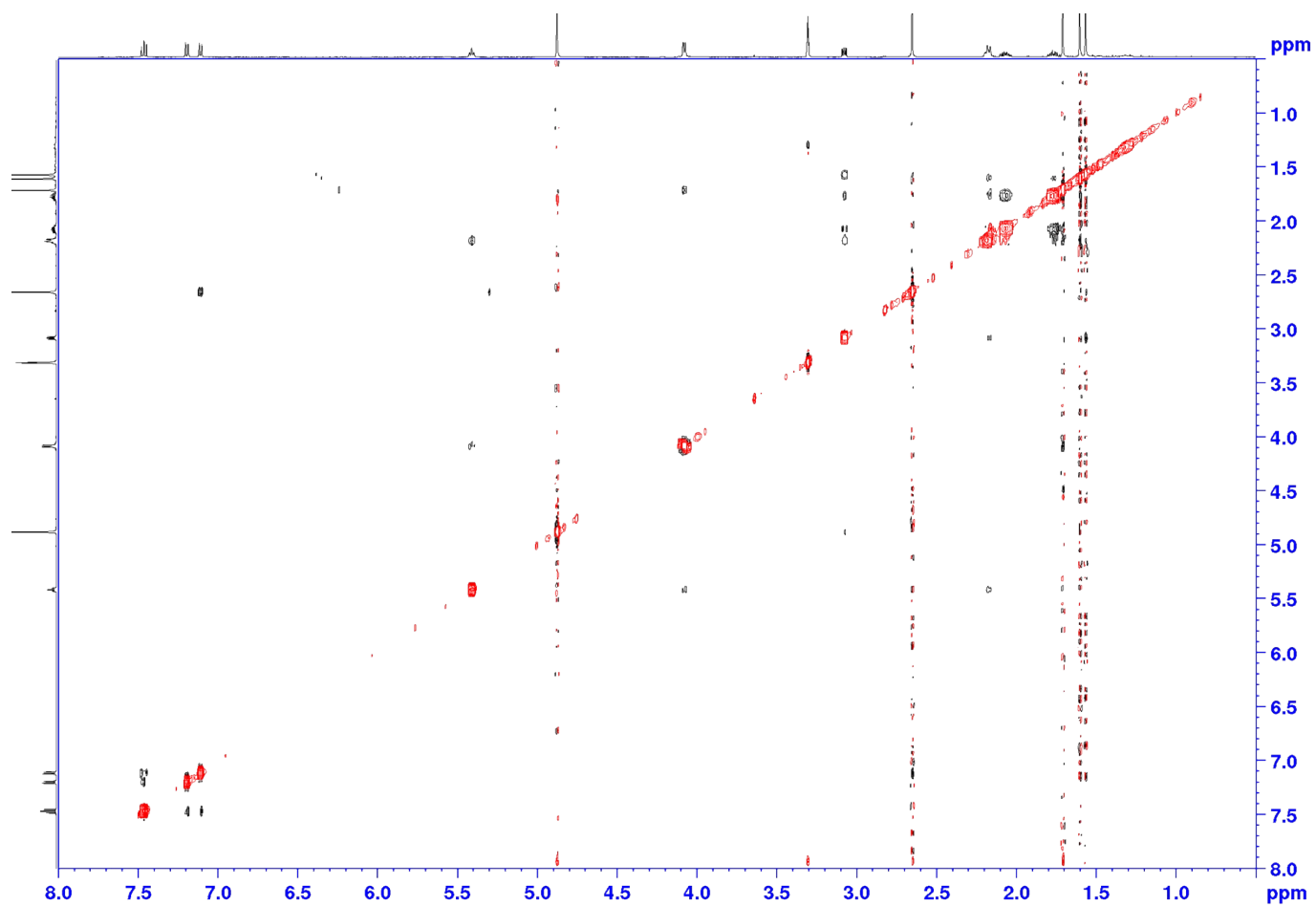
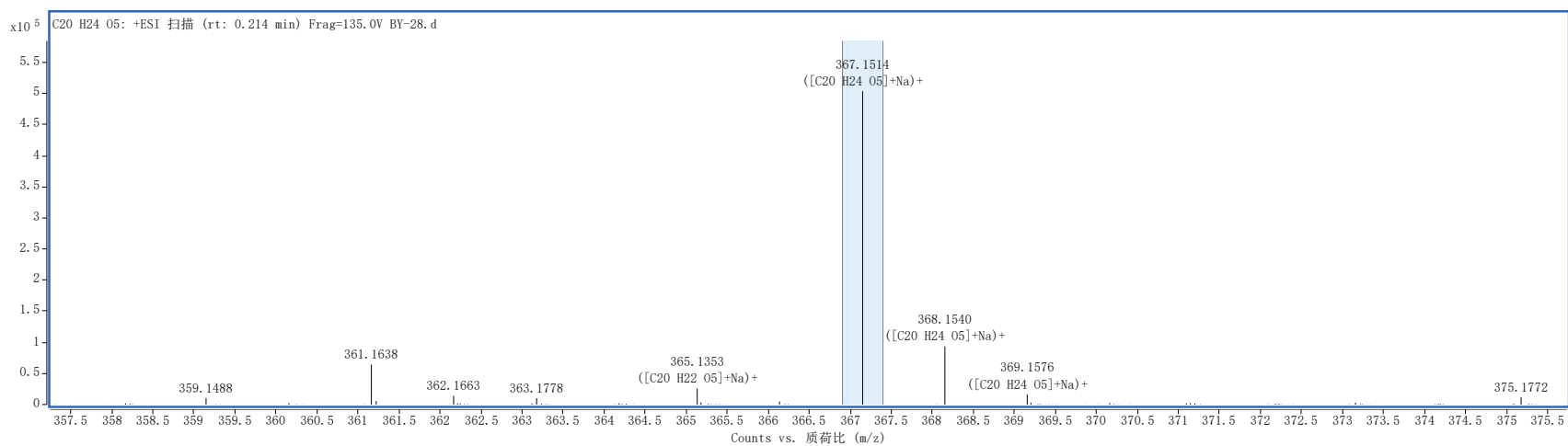


Figure S44. NOESY spectrum of *Gerberdriasin D (4)* in CD₃OD



峰高总百分比 (Calc)	峰高 (计算值)	峰高百分数(计算值)	m/z (Calc)	Diff (mDa)	峰高	峰高百分数	峰高总百分比	m/z	Diff (ppm)
79.7	489192.6	100	367.1516	0.2	503858	100	82.1	367.1514	0.48

最佳	ID 来源	分子式	种类	m/z	分数	Diff (ppm)	分数 (MFG)
TRUE	MFG	C20 H24 O5	(M+Na)+	367.1514	96.32	0.86	96.32

Figure S45. HRESIMS spectrum of *Gerberdriasin E (5)*

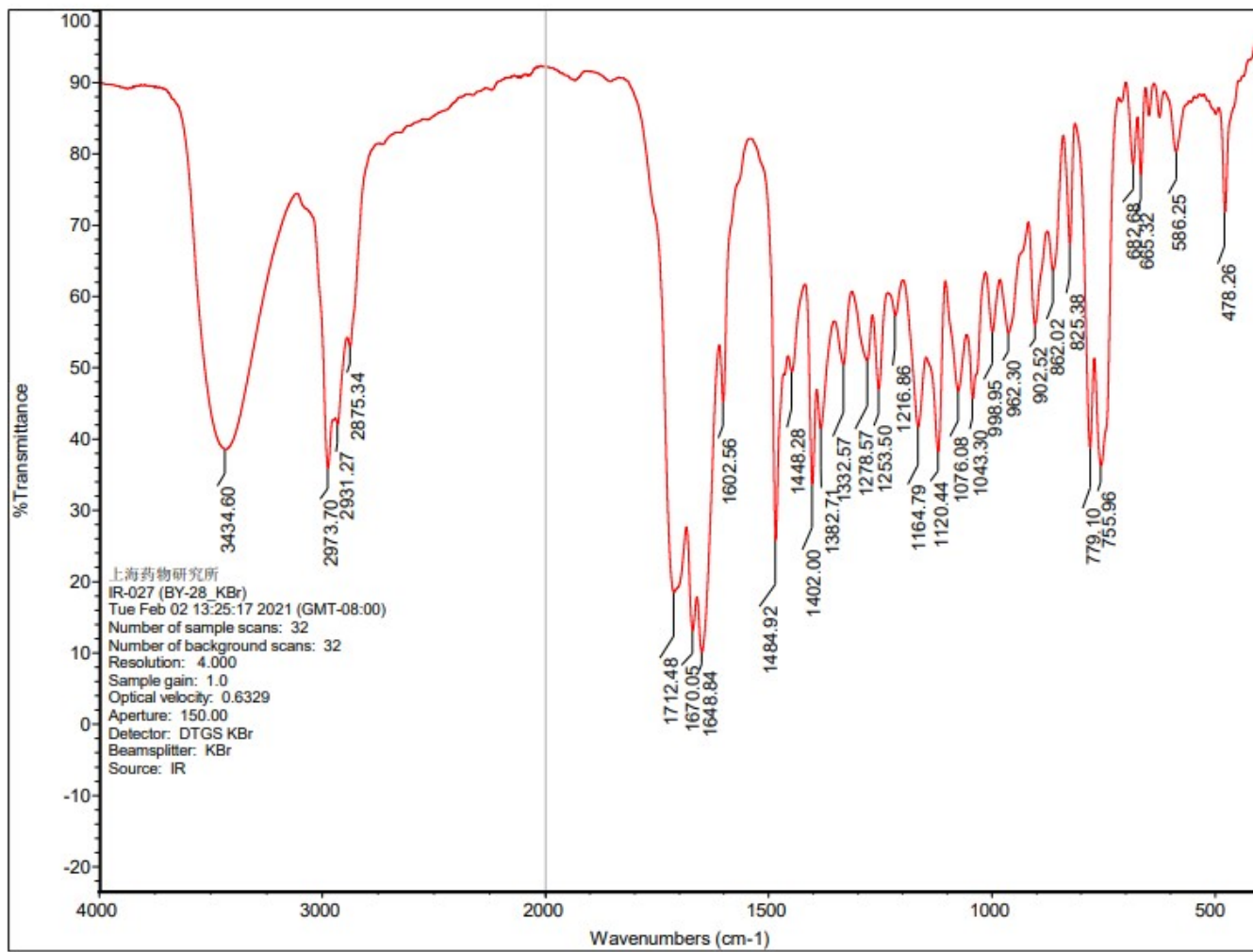


Figure S46. IR spectrum of *Gerberdriasin E* (5)

Rudolph Research Analytical

Thursday, 02/24/2022

This sample was measured on an Autopol VI, serial number 90079, manufactured by Rudolph Research Analytical, Hackettstown, NJ.

LotID : 28-1

Set Temperature : 20.0

Temp Corr : OFF

n	Average	Std.Dev.	Maximum	Minimum											
6	-16.000	0.0000	-16.000	-16.000	S.No	Sample ID	Time	Result	Scale	OR ° Arc	WLG	Lg.mm	Conc.	Temp.	Comment
1	28-1	10:47:06 AM	-16.000	SR	-0.004	589	100.00	0.025	20.2						
2	28-1	10:47:12 AM	-16.000	SR	-0.004	589	100.00	0.025	20.2						
3	28-1	10:47:12 AM	-16.000	SR	-0.004	589	100.00	0.025	20.2						
4	28-1	10:47:18 AM	-16.000	SR	-0.004	589	100.00	0.025	20.1						
5	28-1	10:47:24 AM	-16.000	SR	-0.004	589	100.00	0.025	20.1						
6	28-1	10:47:30 AM	-16.000	SR	-0.004	589	100.00	0.025	20.1						

Signature

Figure S47. OR Value of *Gerberdriasin E (5)* in CH₃OH

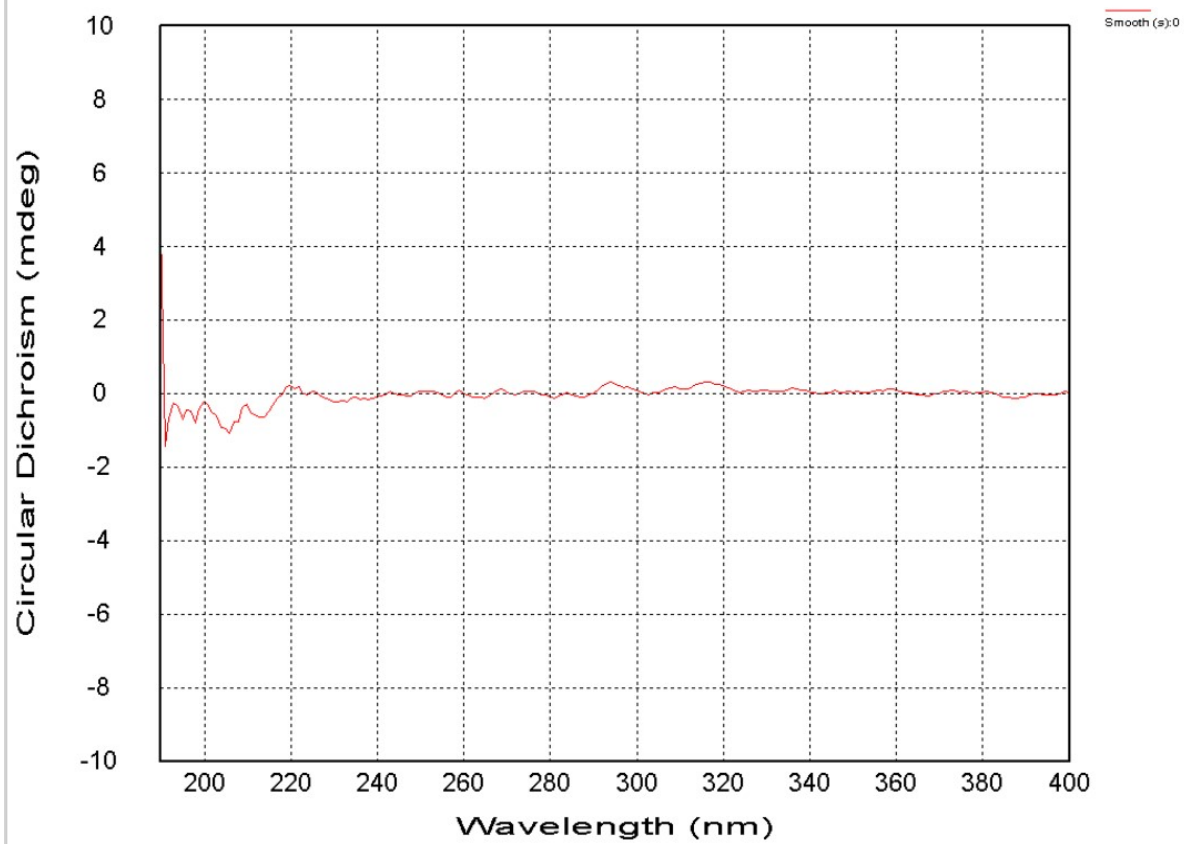


Figure S48. CD spectra of *Gerberdriasin E (5)* in CH₃OH

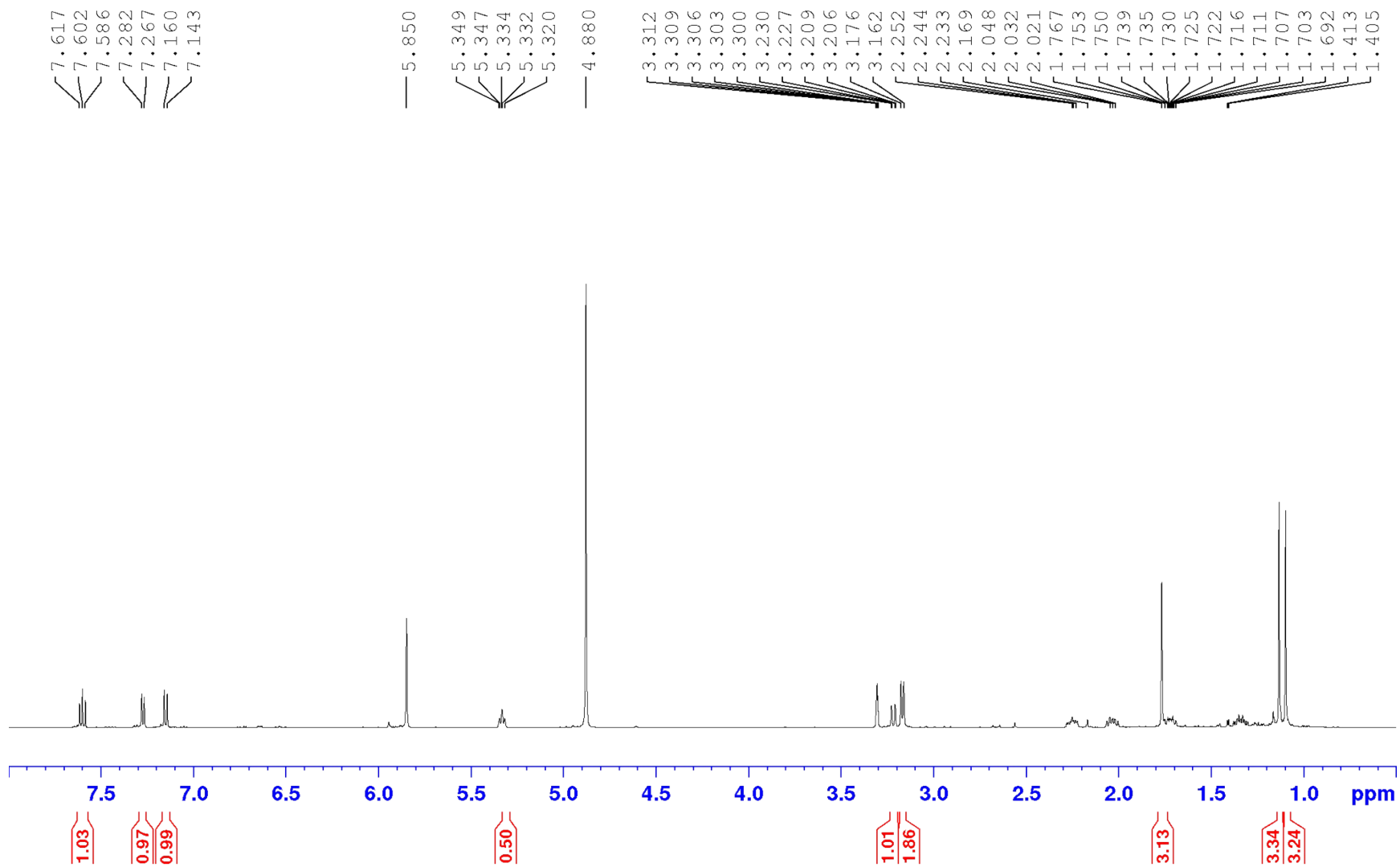


Figure S49. ¹H NMR spectrum of *Gerberdriasin E (5)* in CD₃OD

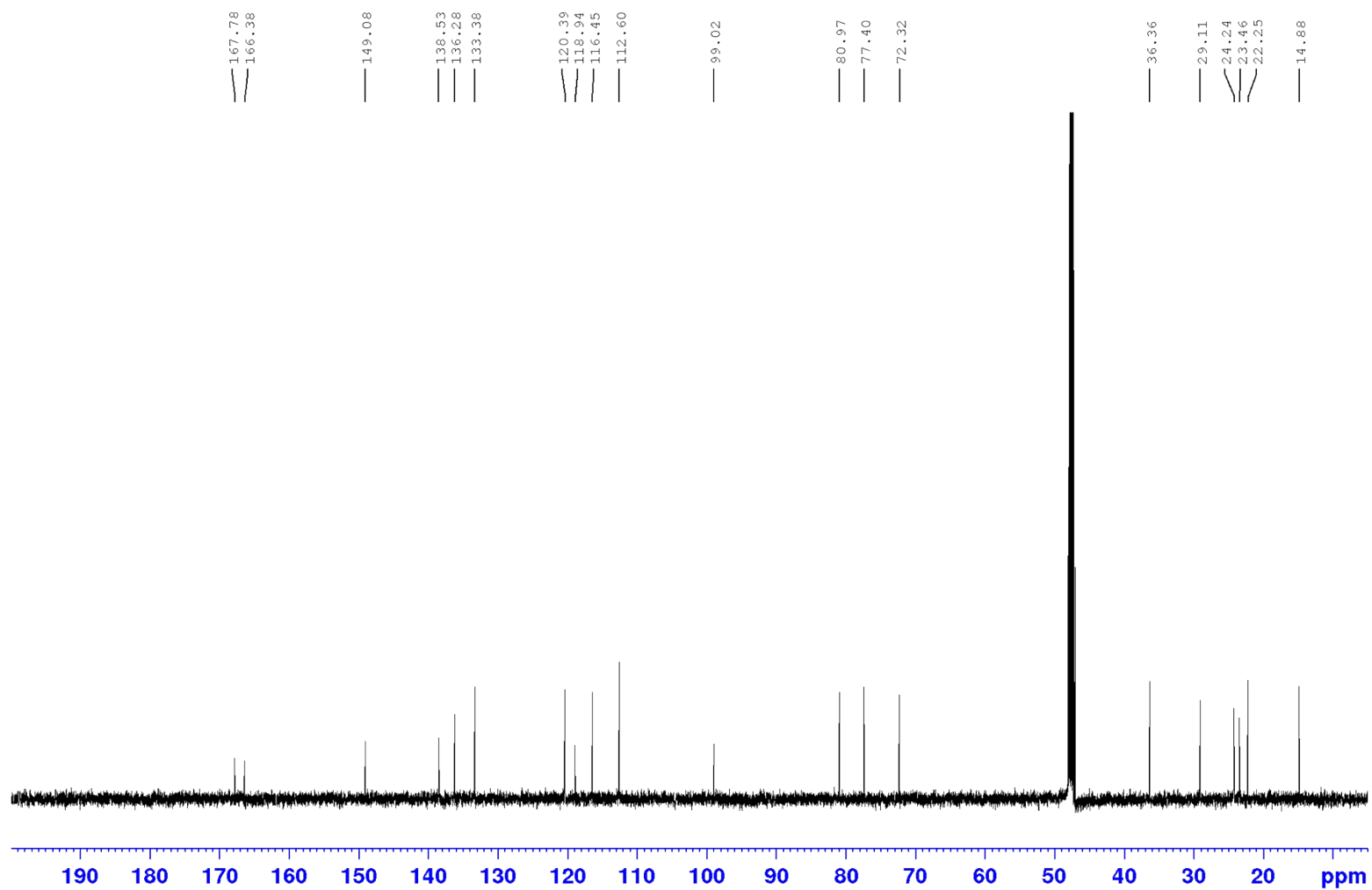


Figure S50. ^{13}C NMR spectrum of *Gerberdriasin E (5)* in CD_3OD

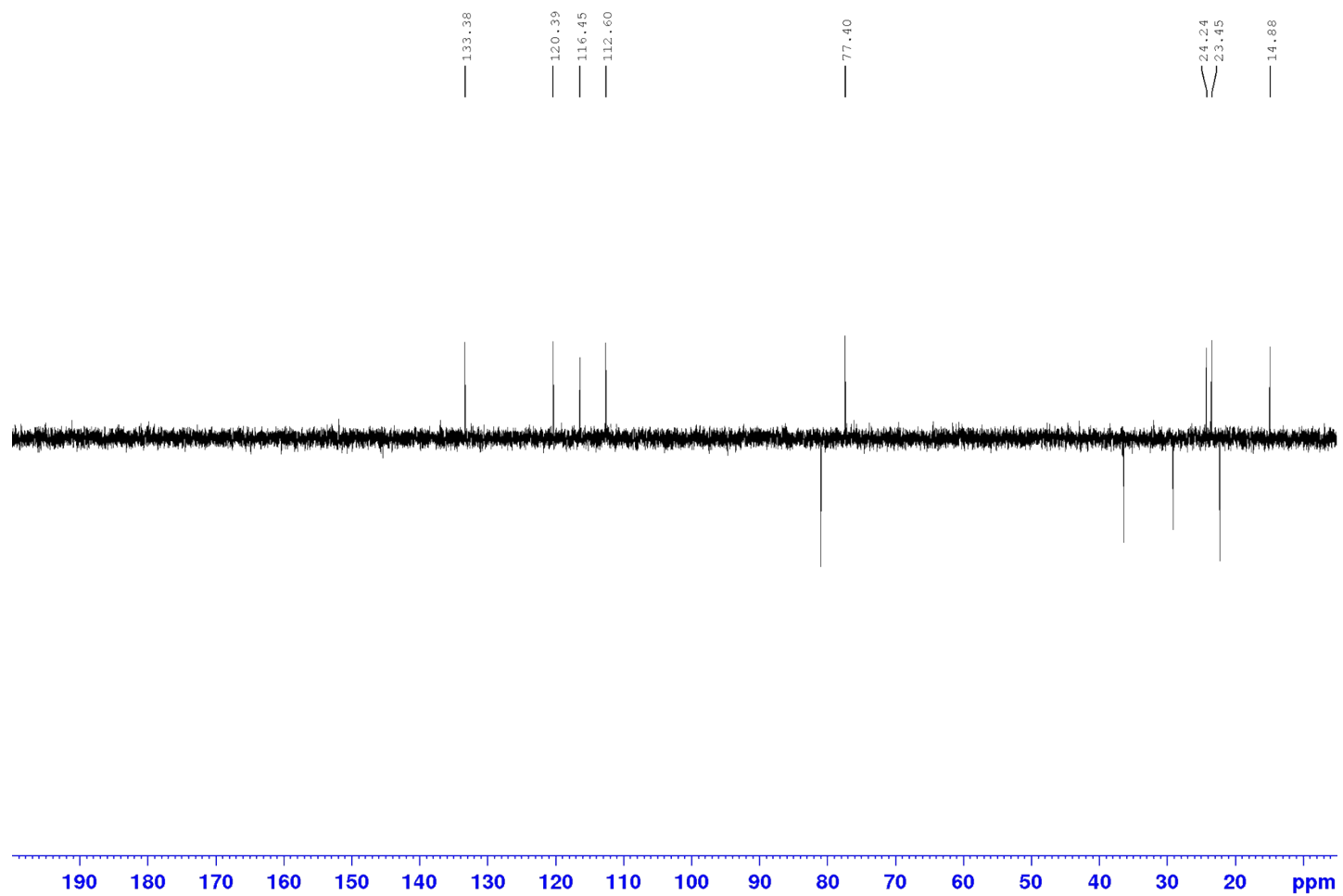


Figure S51. DEPT-135 NMR spectrum of *Gerberdriasin E (5)* in CD₃OD

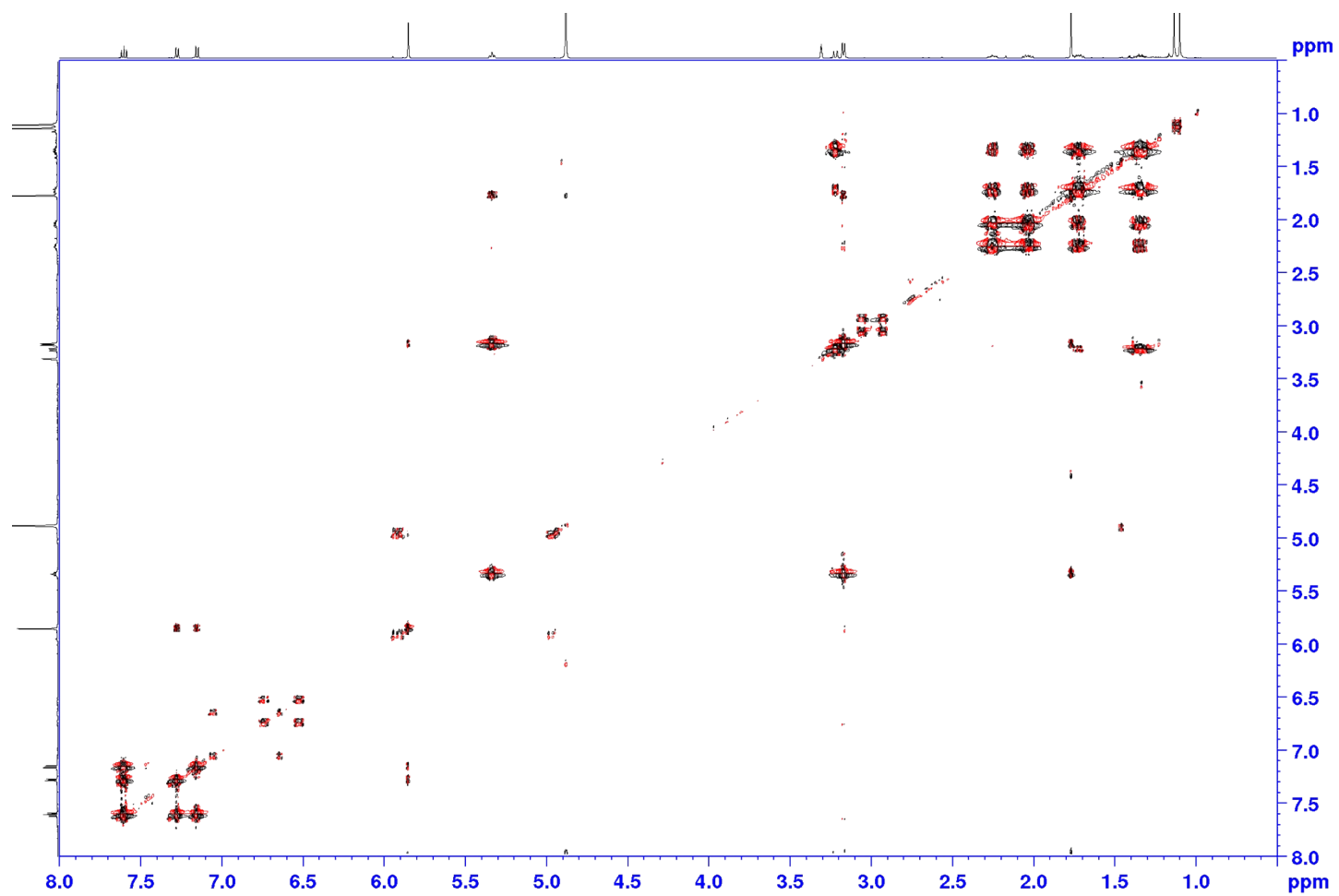


Figure S52. ^1H - ^1H COSY spectrum of *Gerberdriasin E (5)* in CD_3OD

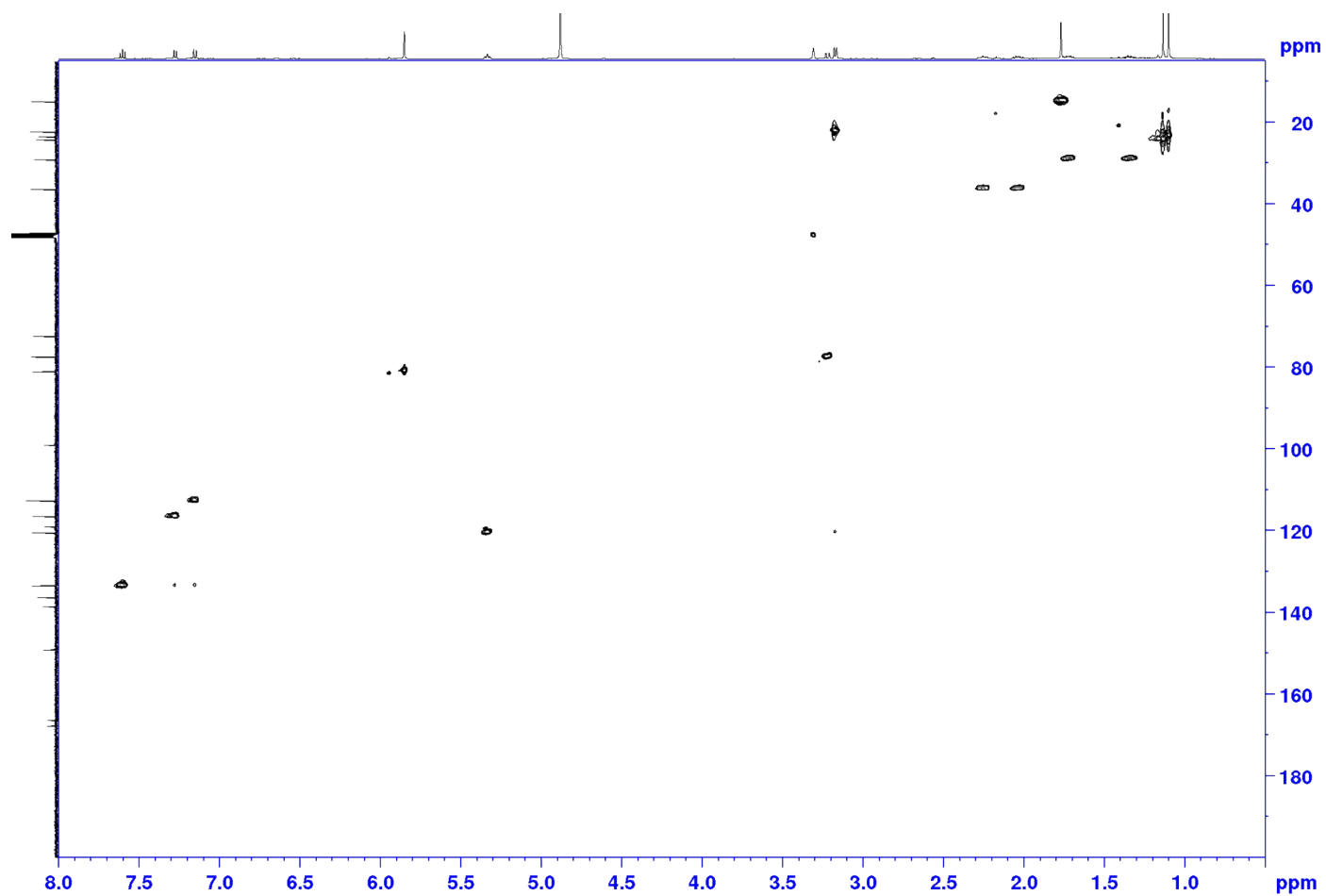


Figure S53. HSQC spectrum of *Gerberdriasin E (5)* in CD₃OD

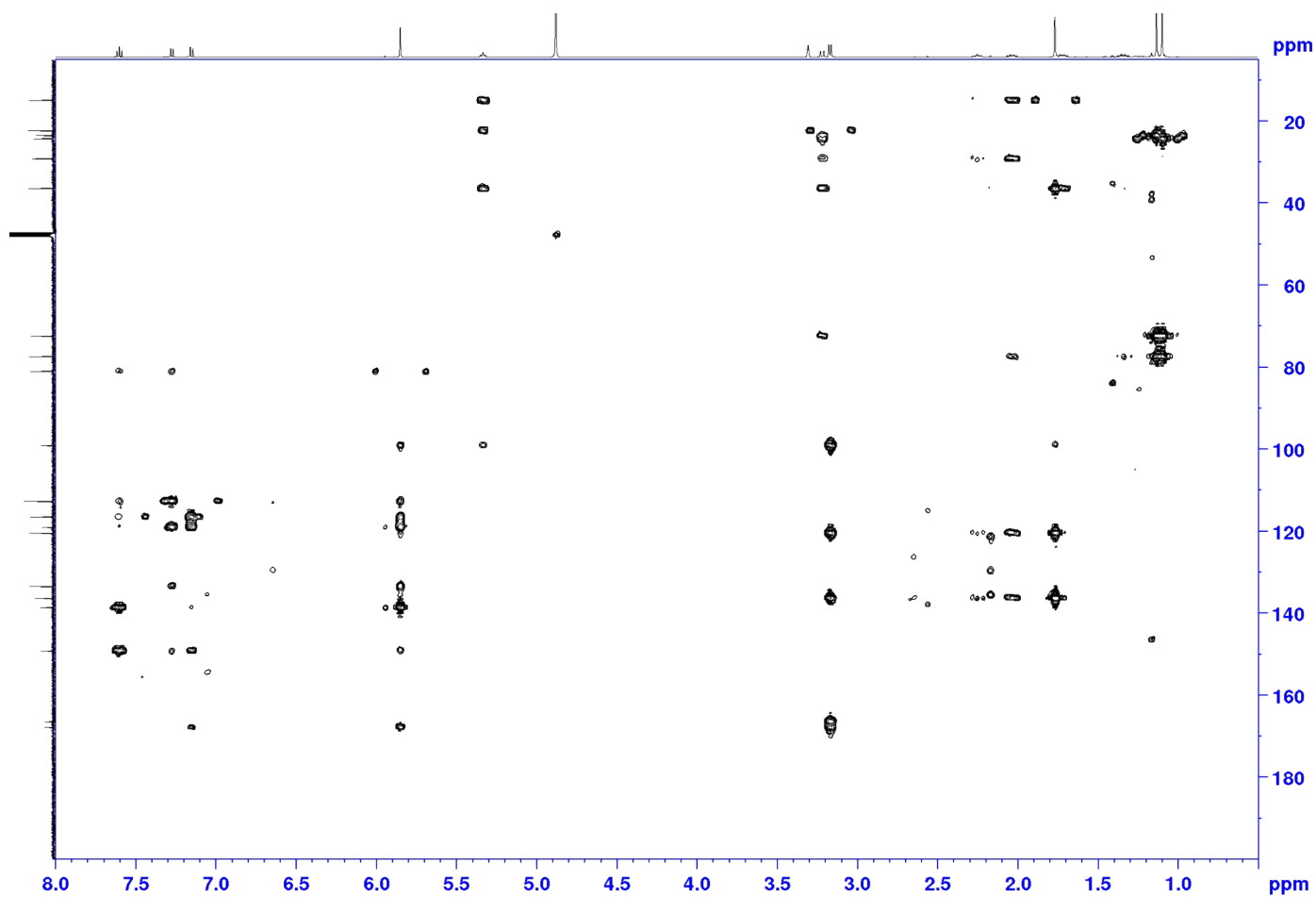


Figure S54. HMBC spectrum of *Gerberdriasin E (5)* in CD_3OD

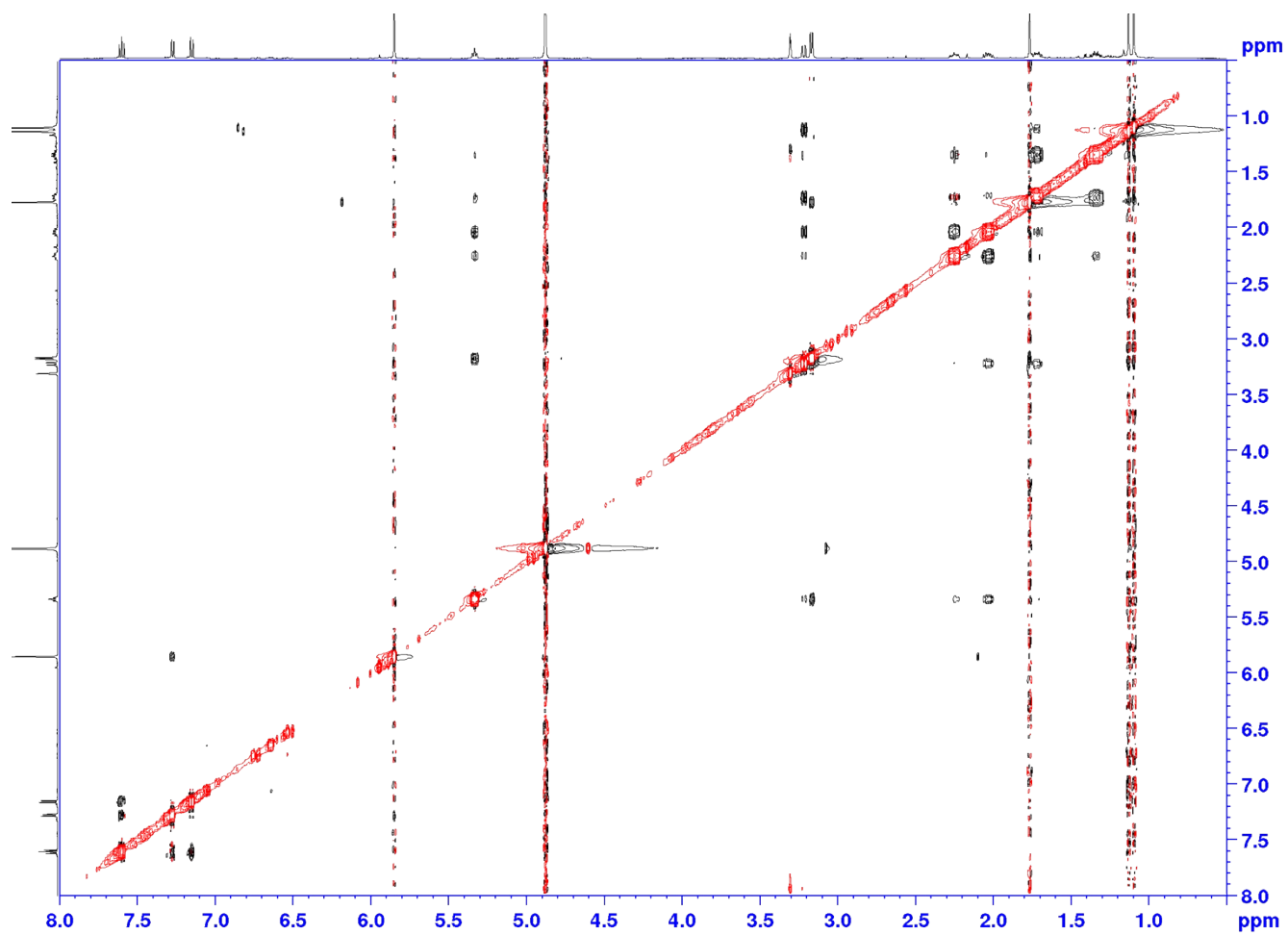
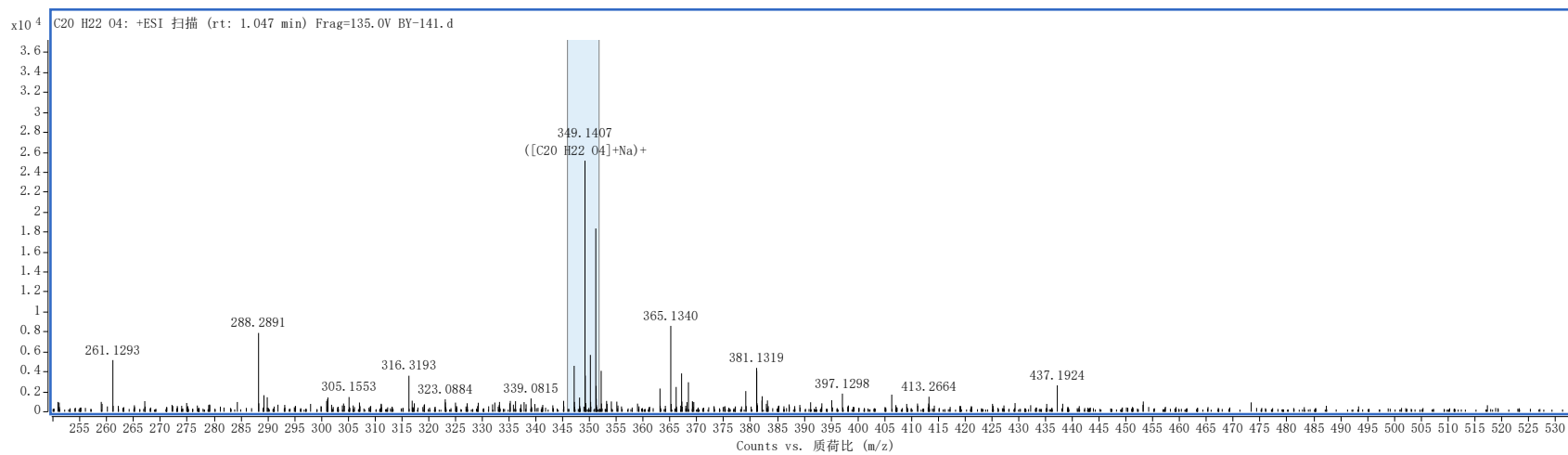


Figure S55. NOESY spectrum of *Gerberdriasin E (5)* in CD₃OD



峰高总百分比 (Calc)	峰高 (计算值)	峰高百分数(计算值)	m/z (Calc)	Diff (mDa)	峰高	峰高百分数	峰高总百分比	m/z	Diff (ppm)
81.9	25291.4	100	349.141	0.3	25171.2	100	81.6	349.1407	1

最佳	ID 来源	分子式	种类	m/z	分数	Diff (ppm)	分数 (MFG)
TRUE	MFG	C ₂₀ H ₂₂ O ₄	(M+Na) ⁺	349.1407	84.32	0.83	84.32

Figure S56. HRESIMS spectrum of *Gerberdriasin F* (6)

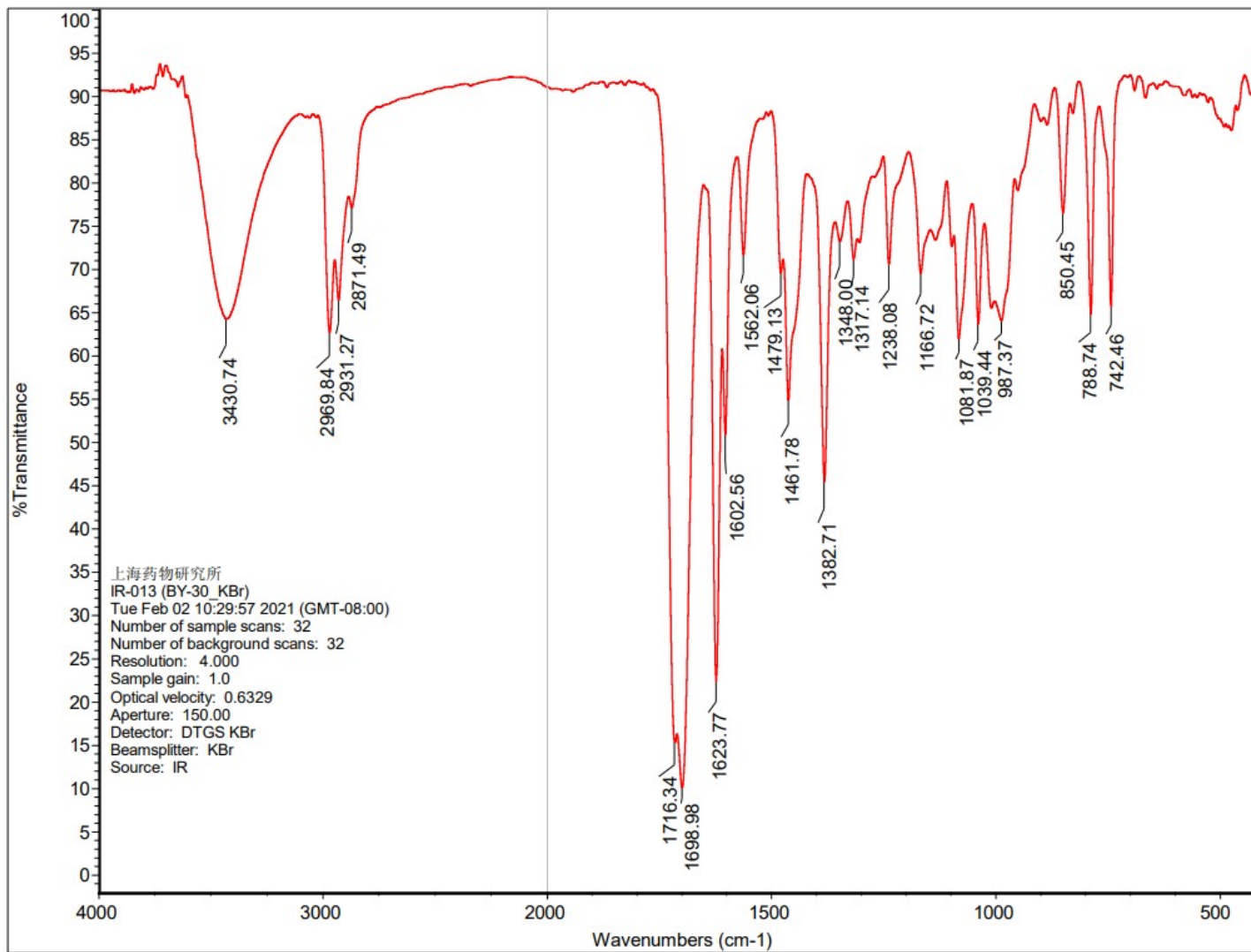


Figure S57. IR spectrum of Gerberdriasin F (6)

Rudolph Research Analytical

Thursday, 02/24/2022

This sample was measured on an Autopol VI, serial number 90079,
manufactured by Rudolph Research Analytical, Hackettstown, NJ.

LotID : BY-141
Set Temperature : 20.0
Temp Corr : OFF

n	Average	Std.Dev.	Maximum	Minimum						
6	-9.167	1.8634	-5.000	-10.000						
S.No	Sample ID	Time	Result	Scale	OR ° Arc	WLG	Lg.mm	Conc.	Temp.	Comment
1	BY-141	11:02:54 AM	-10.000	SR	-0.002	589	100.00	0.020	19.7	
2	BY-141	11:03:00 AM	-10.000	SR	-0.002	589	100.00	0.020	19.7	
3	BY-141	11:03:06 AM	-10.000	SR	-0.002	589	100.00	0.020	19.7	
4	BY-141	11:03:12 AM	-10.000	SR	-0.002	589	100.00	0.020	19.7	
5	BY-141	11:03:17 AM	-10.000	SR	-0.002	589	100.00	0.020	19.7	
6	BY-141	11:03:23 AM	-5.000	SR	-0.001	589	100.00	0.020	19.8	

Signature

Figure S58. OR Value of *Gerberdriasin F (6)* in CH₃OH

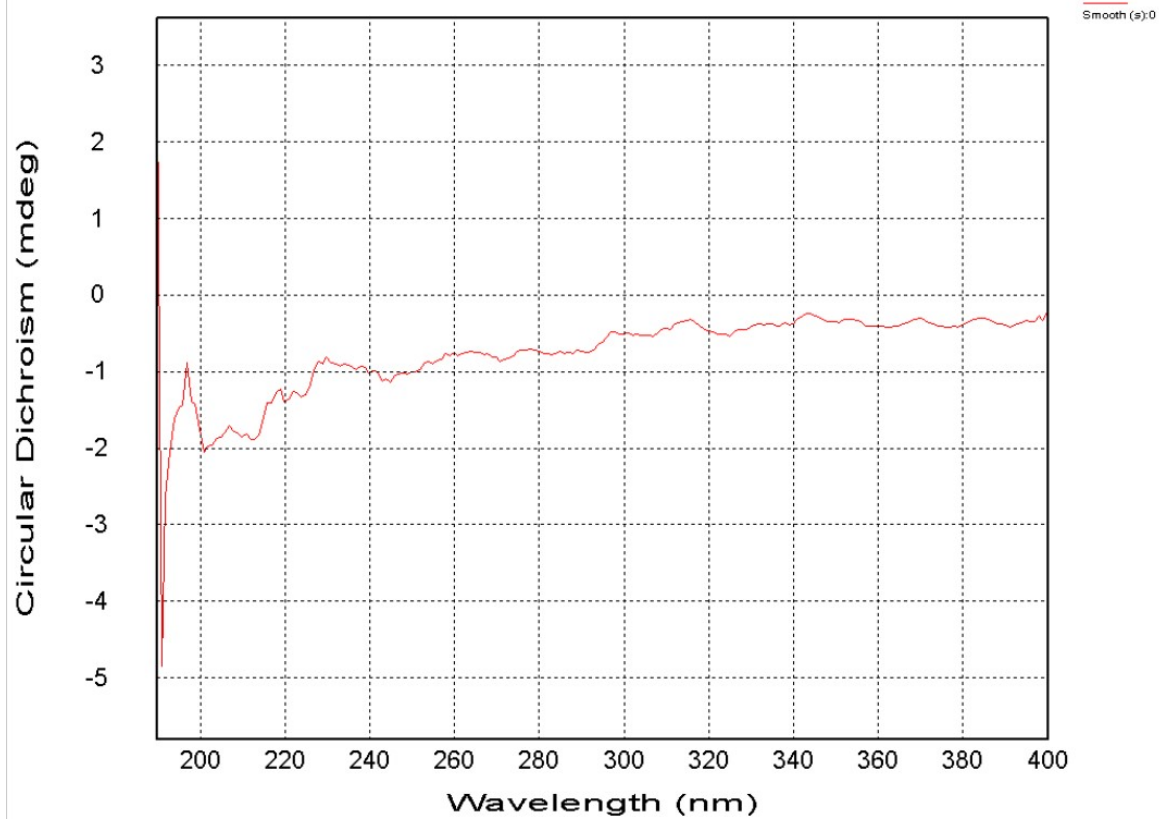


Figure S59. CD spectra of *Gerberdriasin F (6)* in CH₃OH

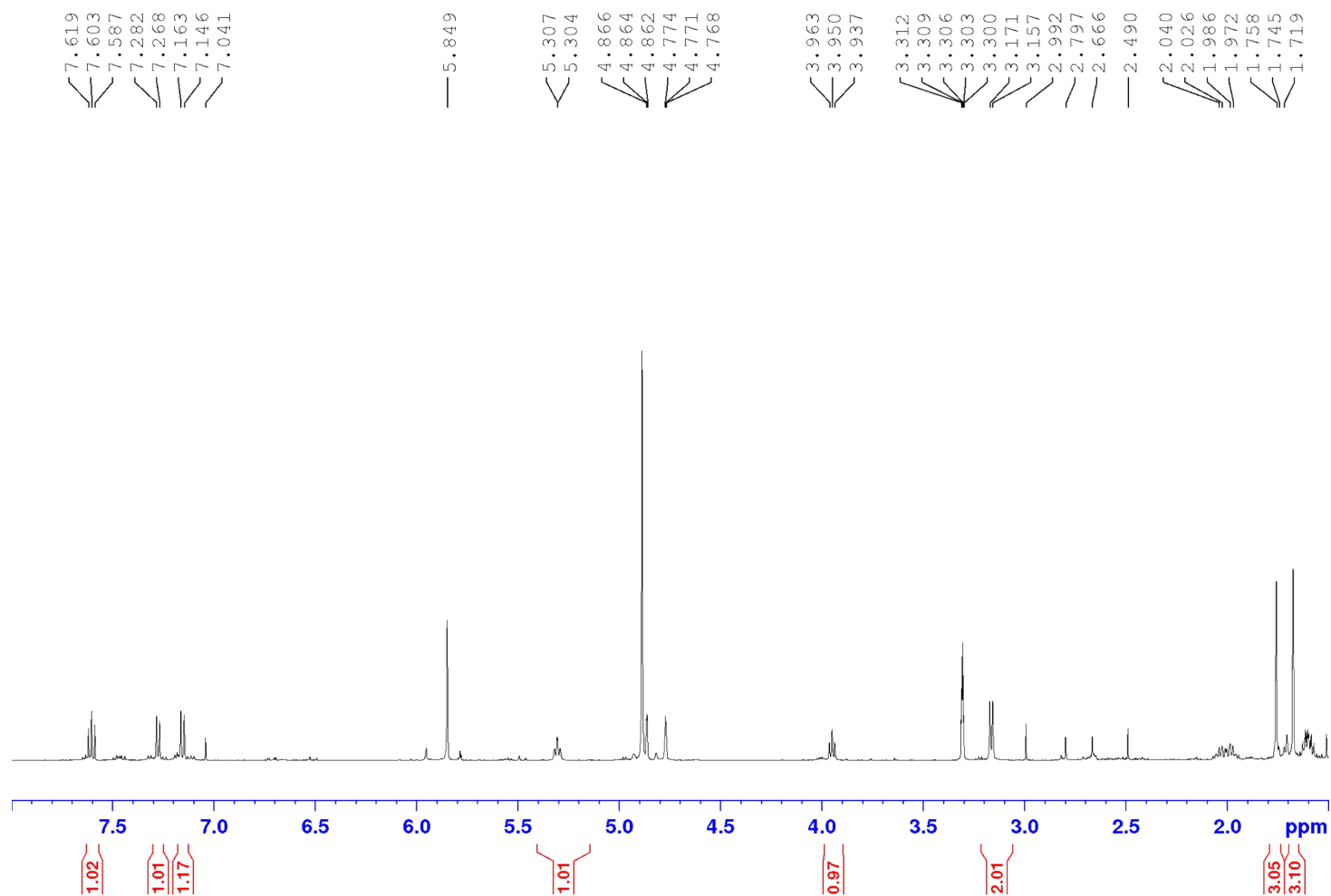


Figure S60. ^1H NMR spectrum of *Gerberdriasin F (6)* in CD_3OD

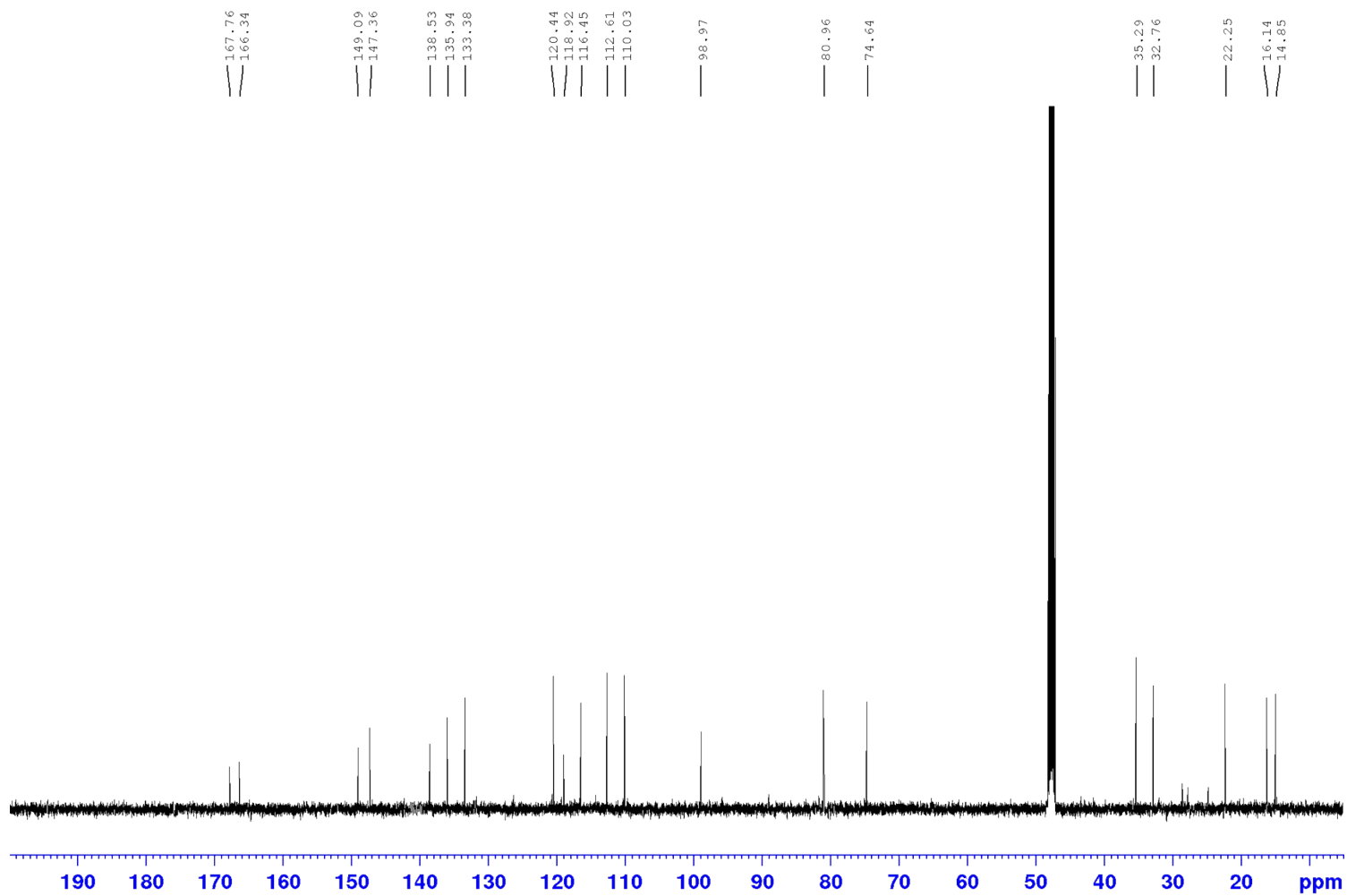


Figure S61. ^{13}C NMR spectrum of *Gerberdriasin F (6)* in CD_3OD

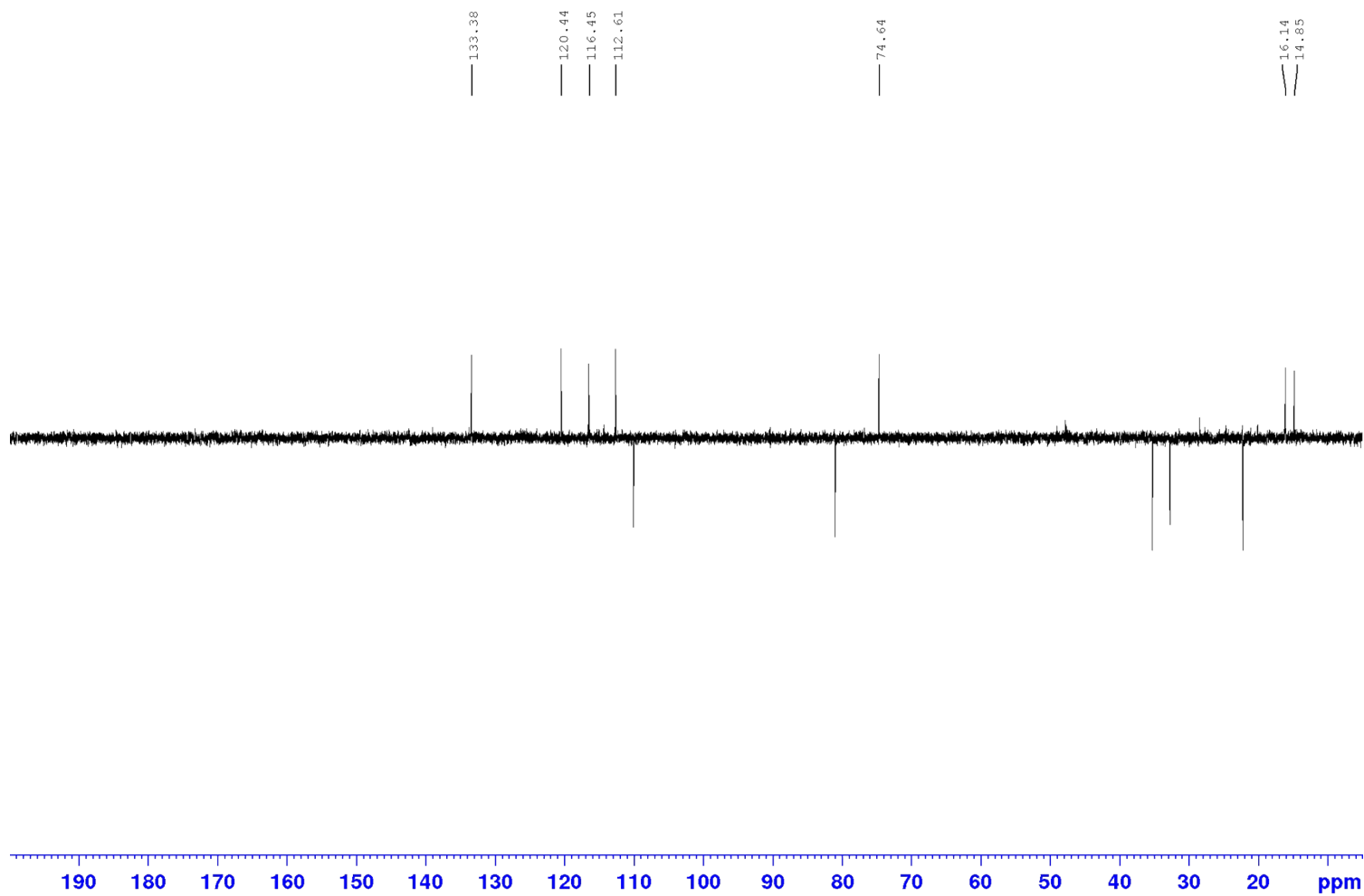


Figure S62. DEPT-135 NMR spectrum of *Gerberdriasin F (6)* in CD₃OD

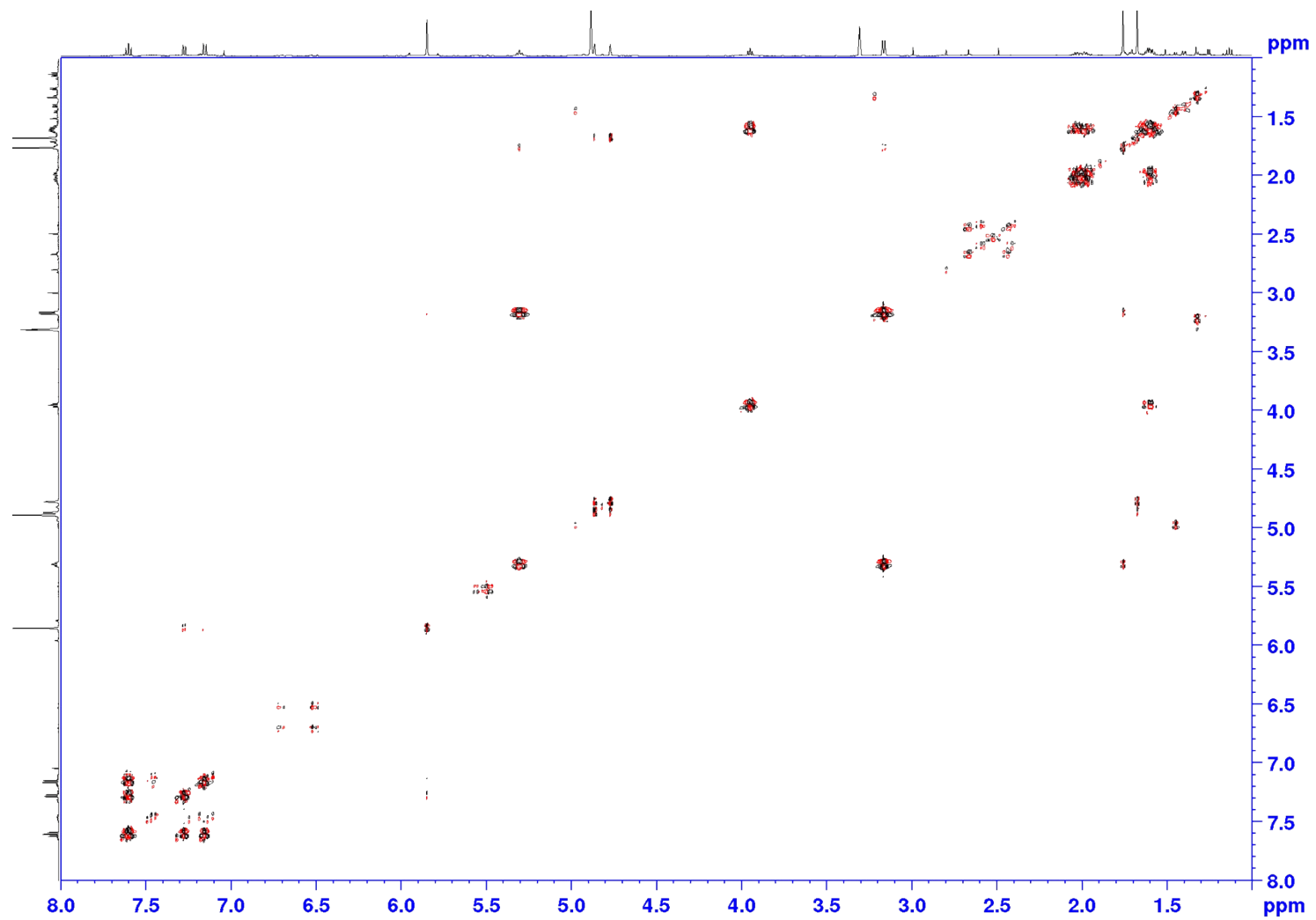


Figure S63. ^1H - ^1H COSY spectrum of *Gerberdriasin F* (6) in CD_3OD

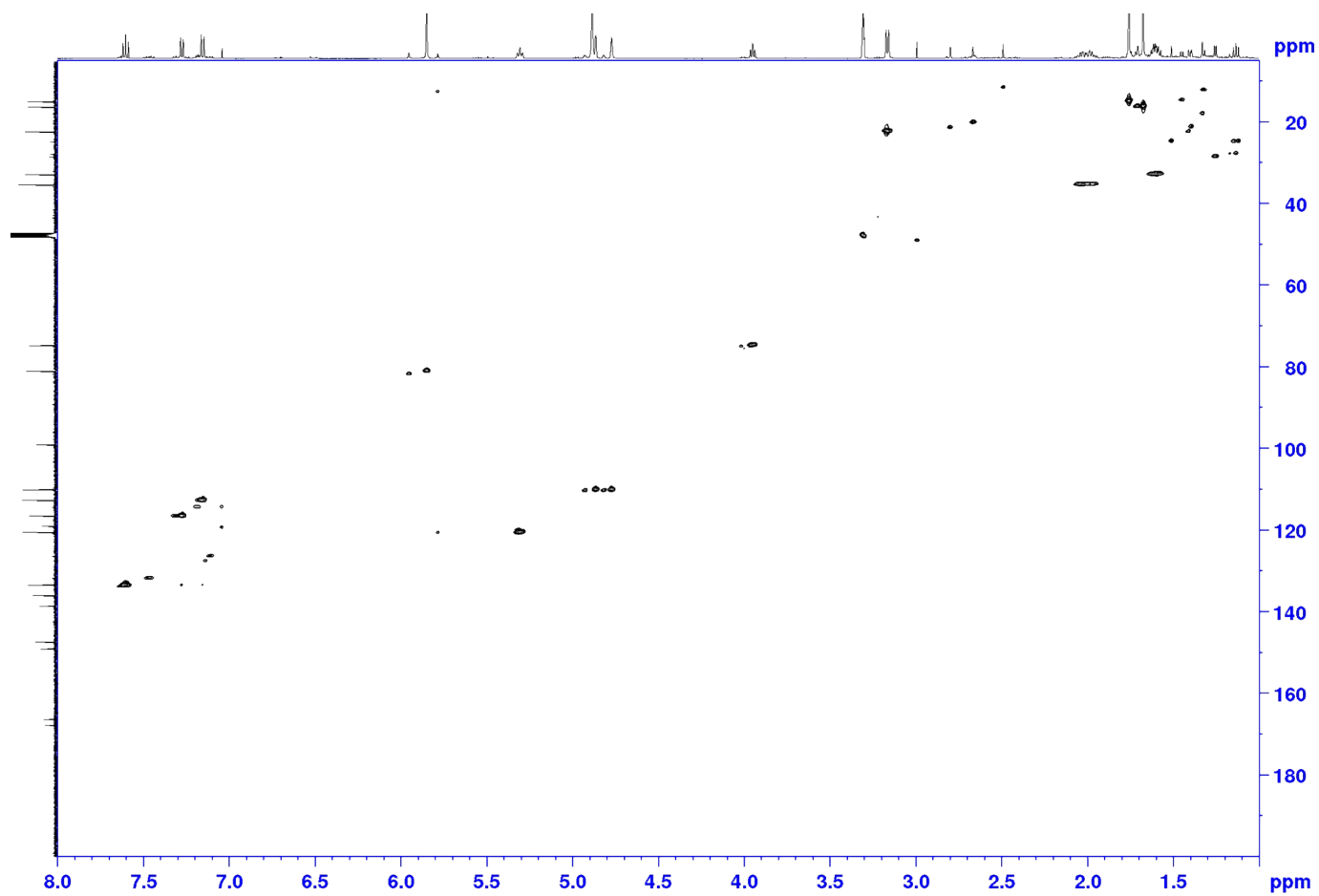


Figure S64. HSQC spectrum of *Gerberdriasin F (6)* in CD_3OD

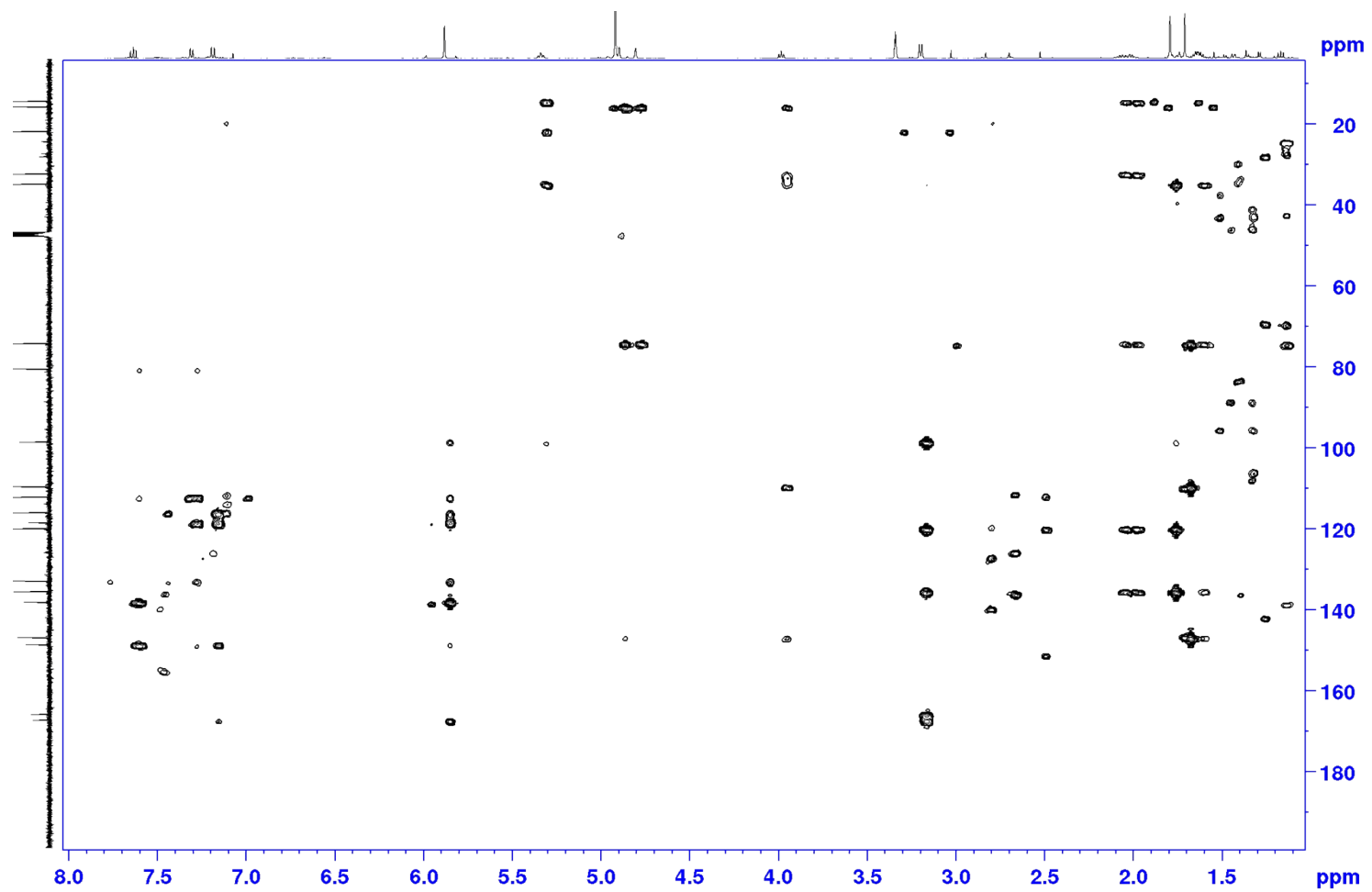


Figure S65. HMBC spectrum of *Gerberdriasin F (6)* in CD_3OD

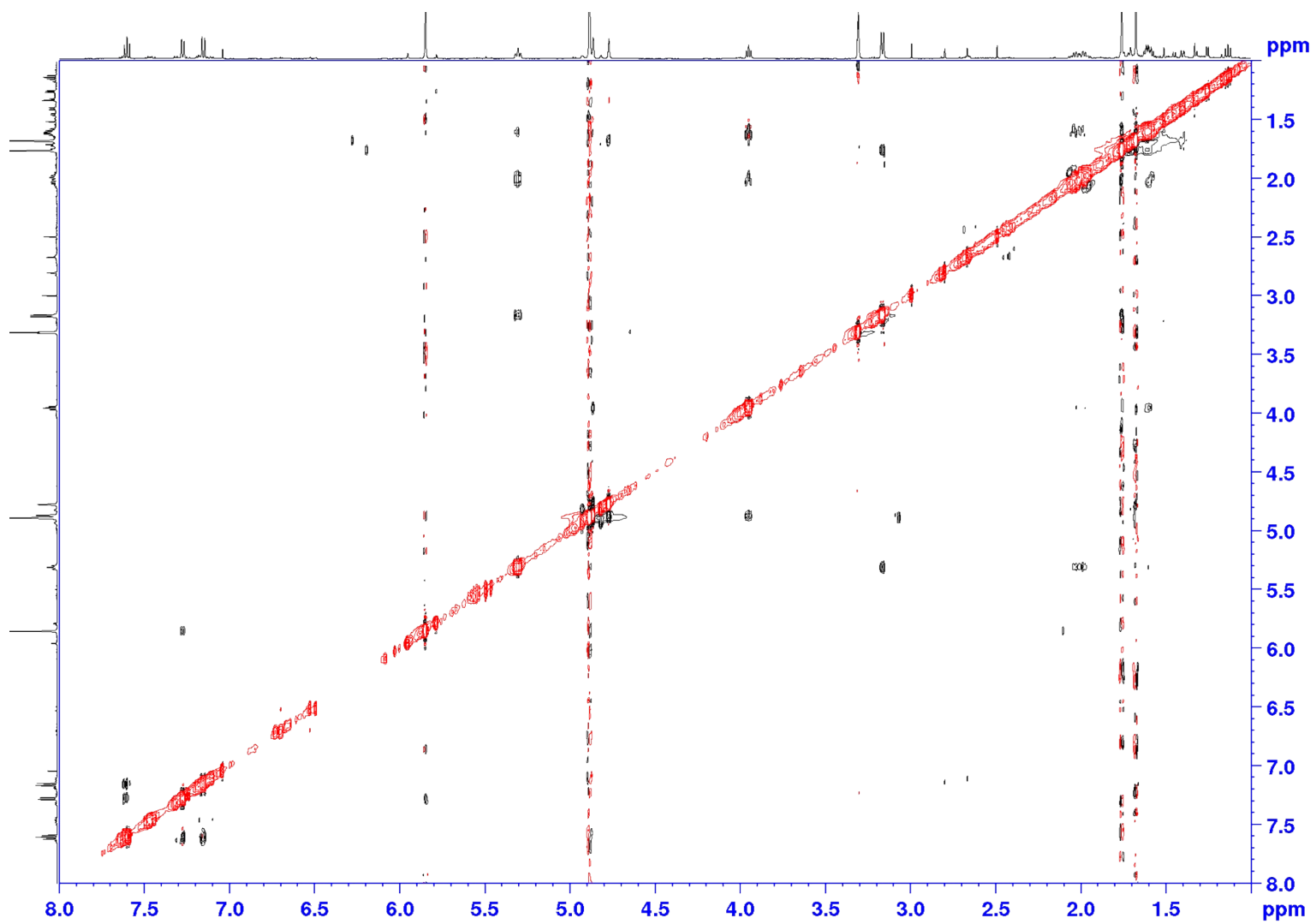


Figure S66. NOESY spectrum of *Gerberdriasin F (6)* in CD₃OD

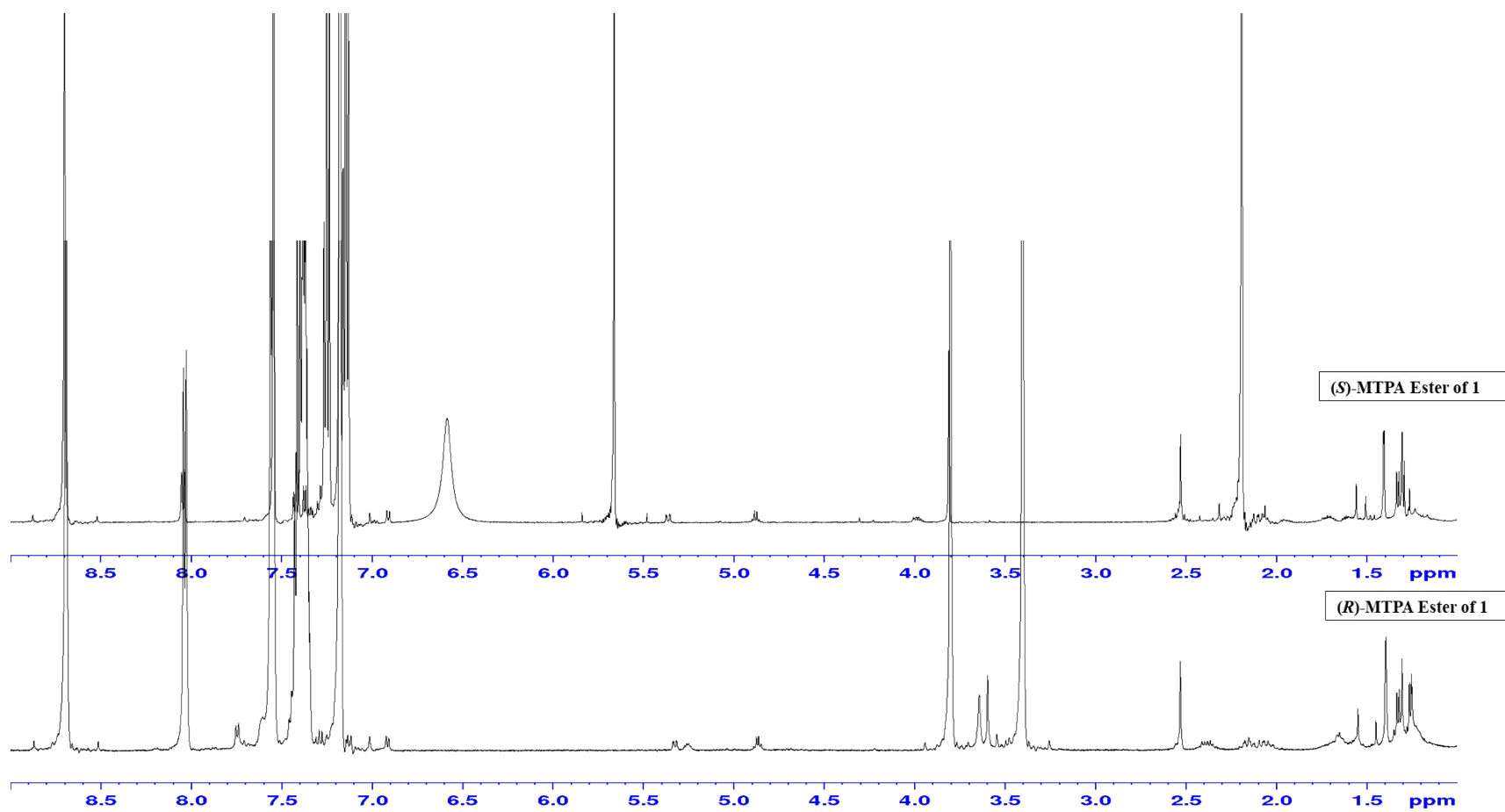


Figure S67: Chemical shift differences ($\Delta\delta_H$ (*S-R*)) between (*S*)-MTPA and (*R*)-MTPA of 1.

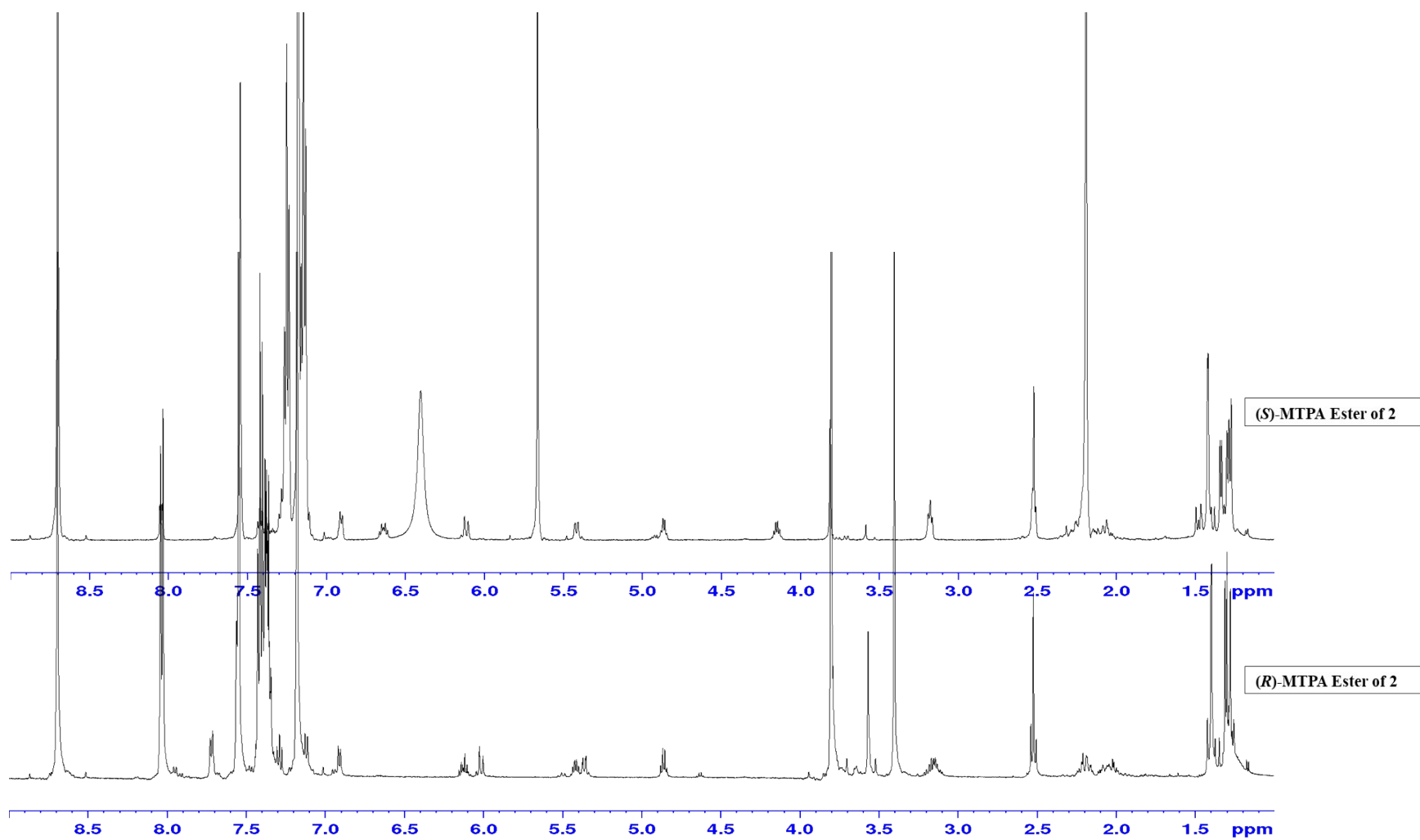


Figure S68: Chemical shift differences ($\Delta\delta_{\text{H}}(S-R)$) between (S)-MTPA and (R)-MTPA of 2.

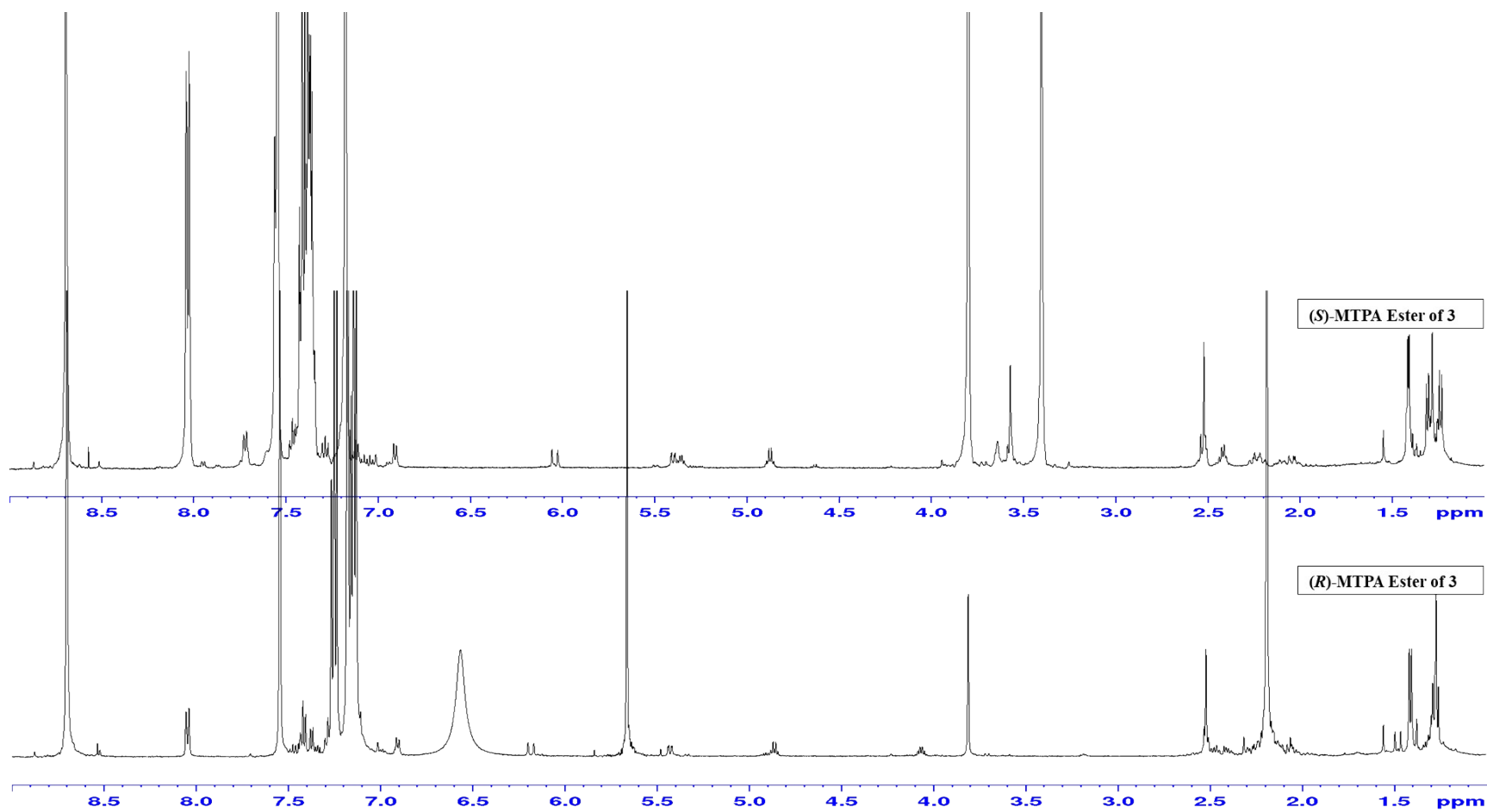


Figure S69: Chemical shift differences ($\Delta\delta_{\text{H}}$ (*S-R*)) between (*S*)-MTPA and (*R*)-MTPA of 3.

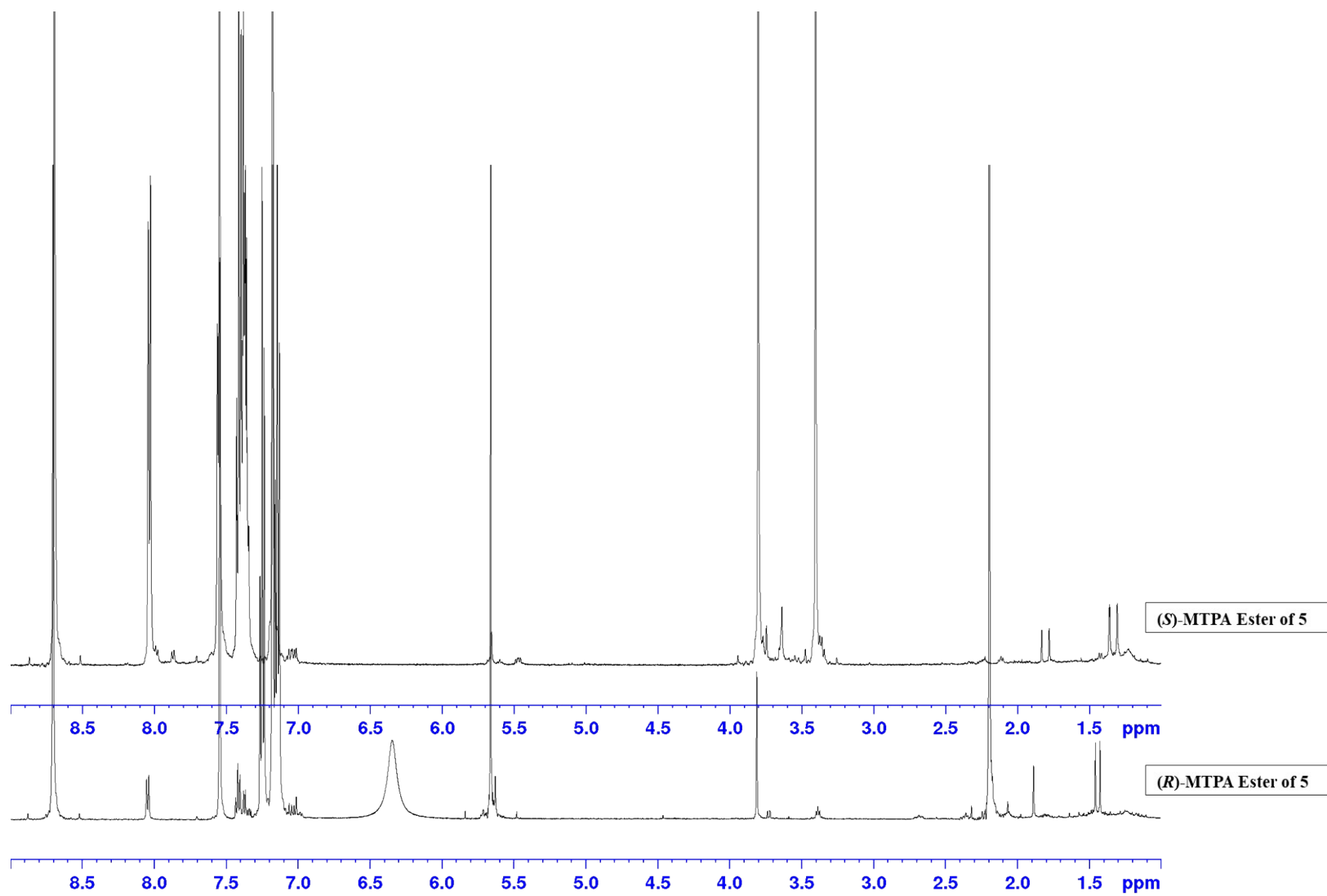


Figure S70: Chemical shift differences ($\Delta\delta_H$ (*S-R*)) between (*S*)-MTPA and (*R*)-MTPA of 5.