Дополнительные материалы

Синтез и биологические свойства 7(7,11)—гидропроизводных олигомицина А

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Supplemental data

Synthesis and biological activity of 7(7,11)—hydro derivatives of oligomycin A

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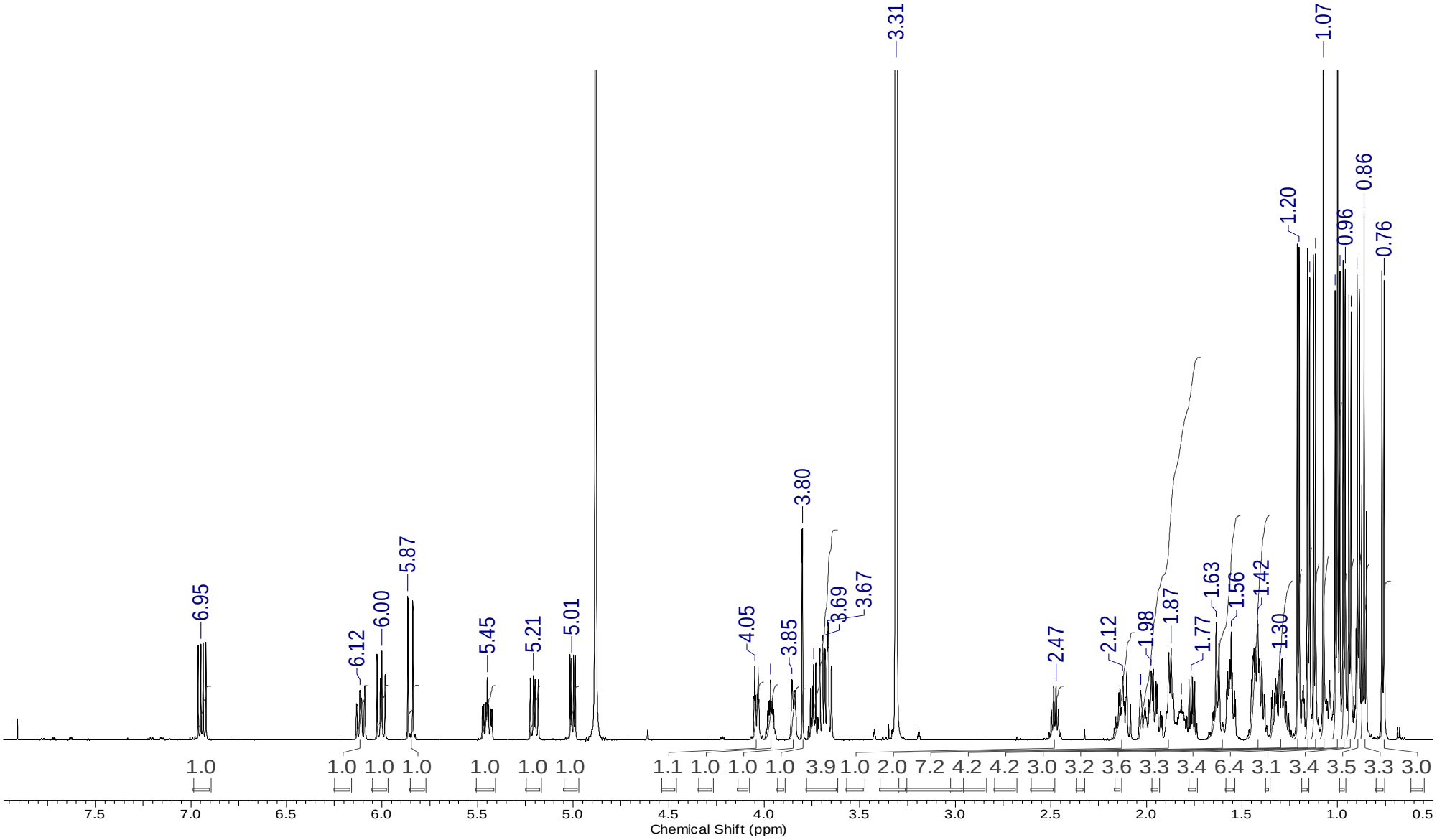


Рис. Д1. Спектр ЯМР ^{1}H (600 МГц, CD_3OD, 25 °C) (7*S*)-дигидроолигомицина А (**2**)

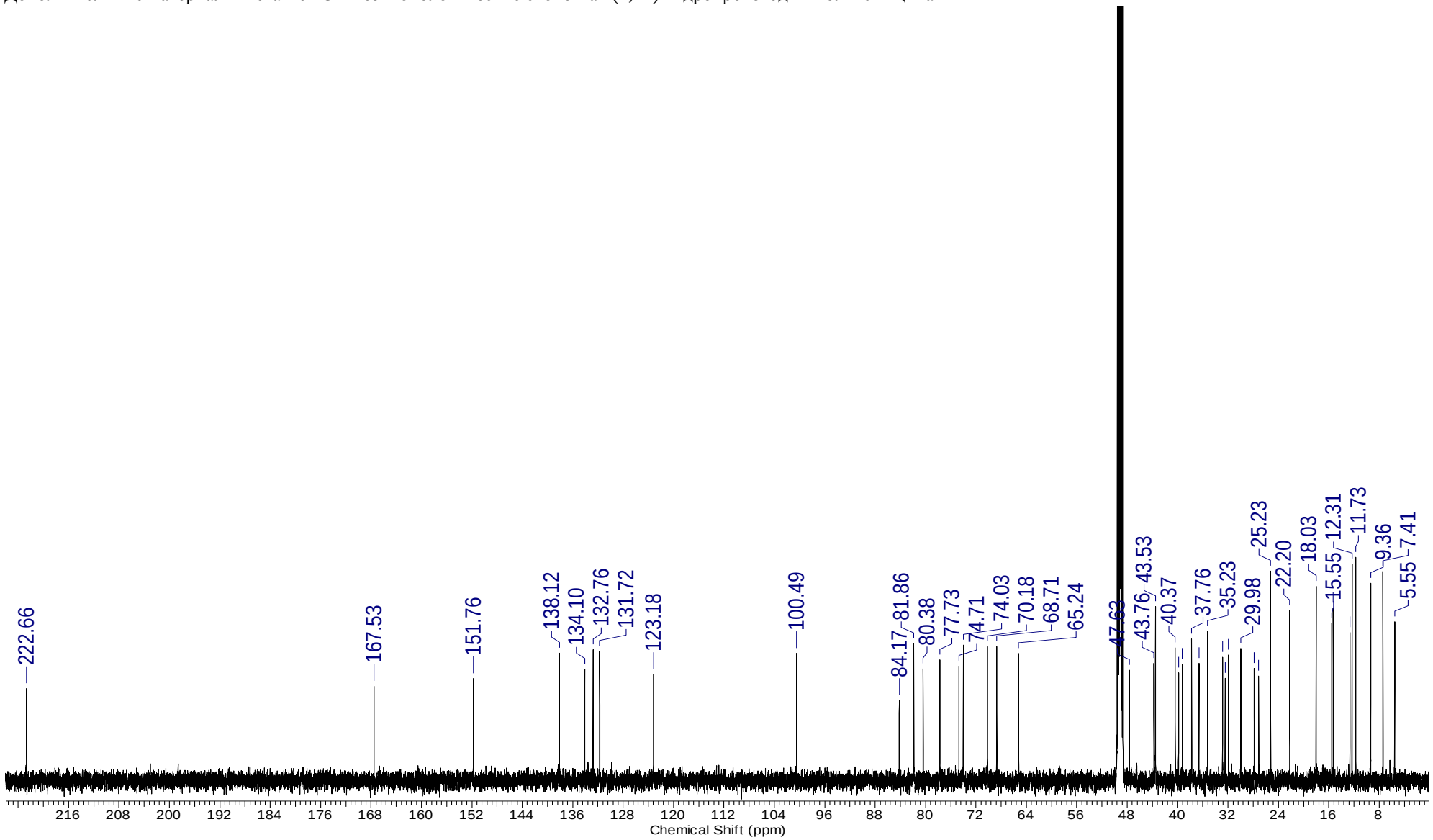


Рис. Д2. Спектр ЯМР ^{13}C (150 МГц, CD_3OD, 25 °C) образца **2**

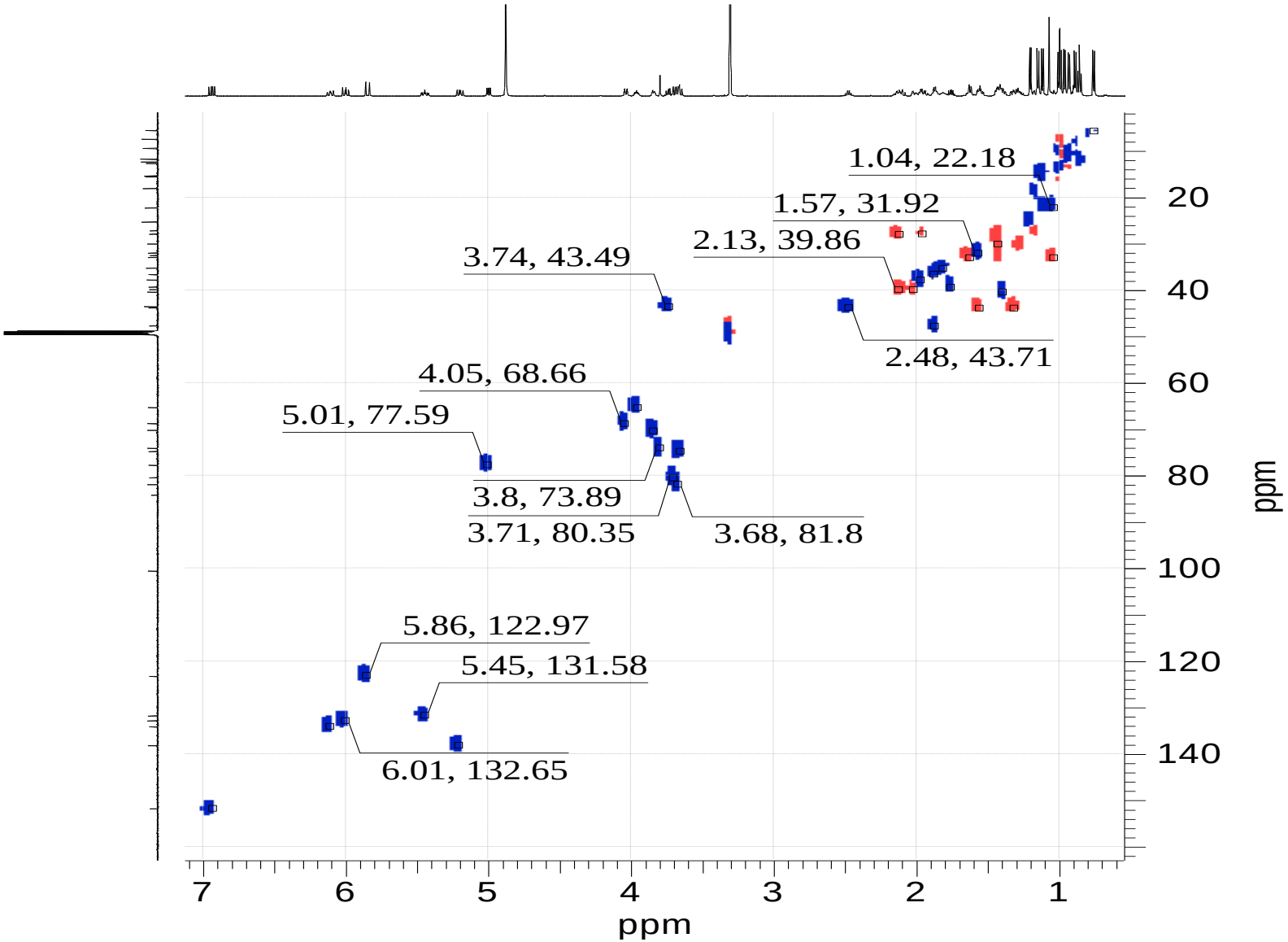


Рис. Д3. Спектр ЯМР ^{1}H-^{13}C HSQC (CD_3OD, 25 °C) образца **2**

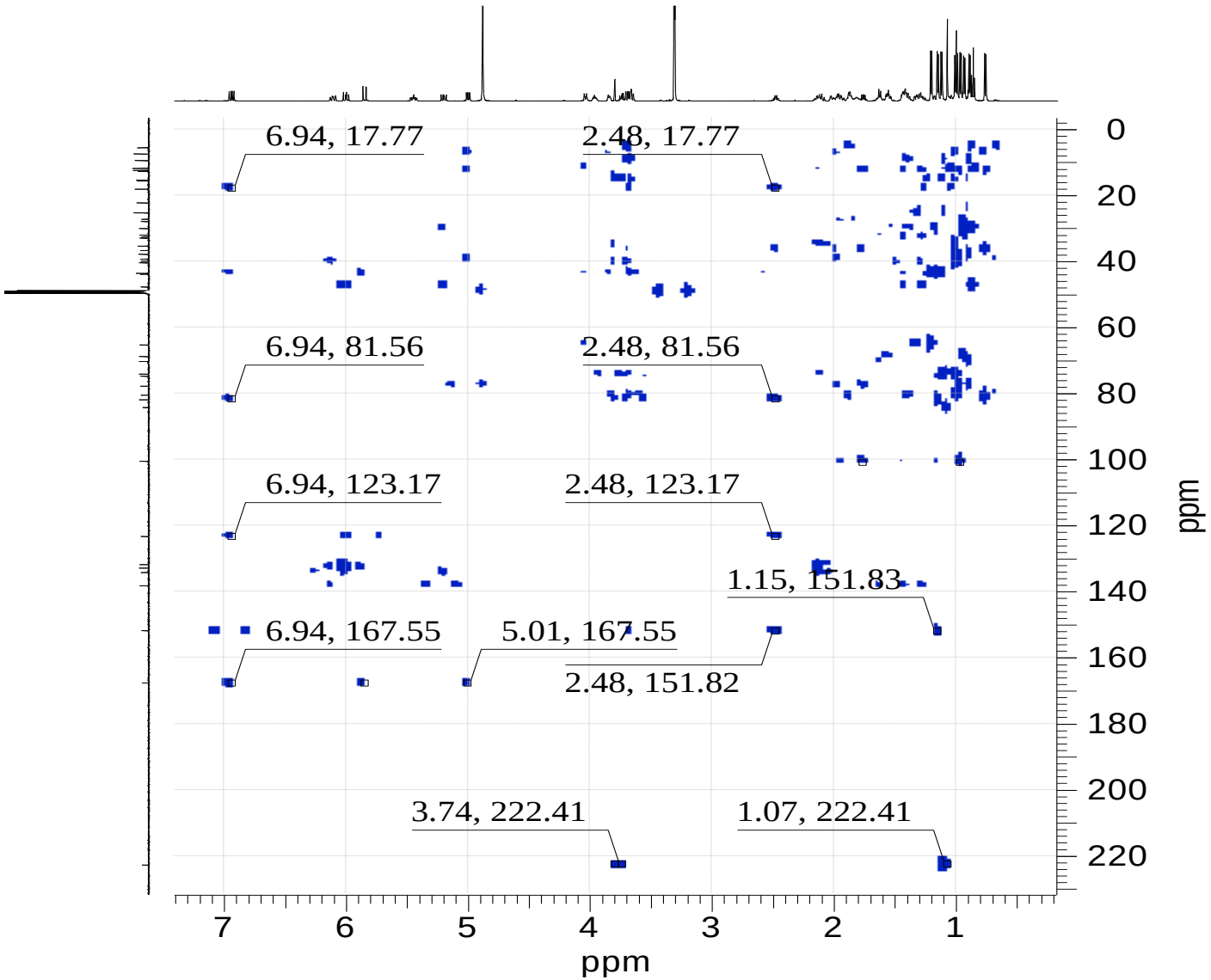


Рис. Д4. Спектр ЯМР ^{1}H-^{13}C HMBC (CD_3OD, 25 °C) образца **2**

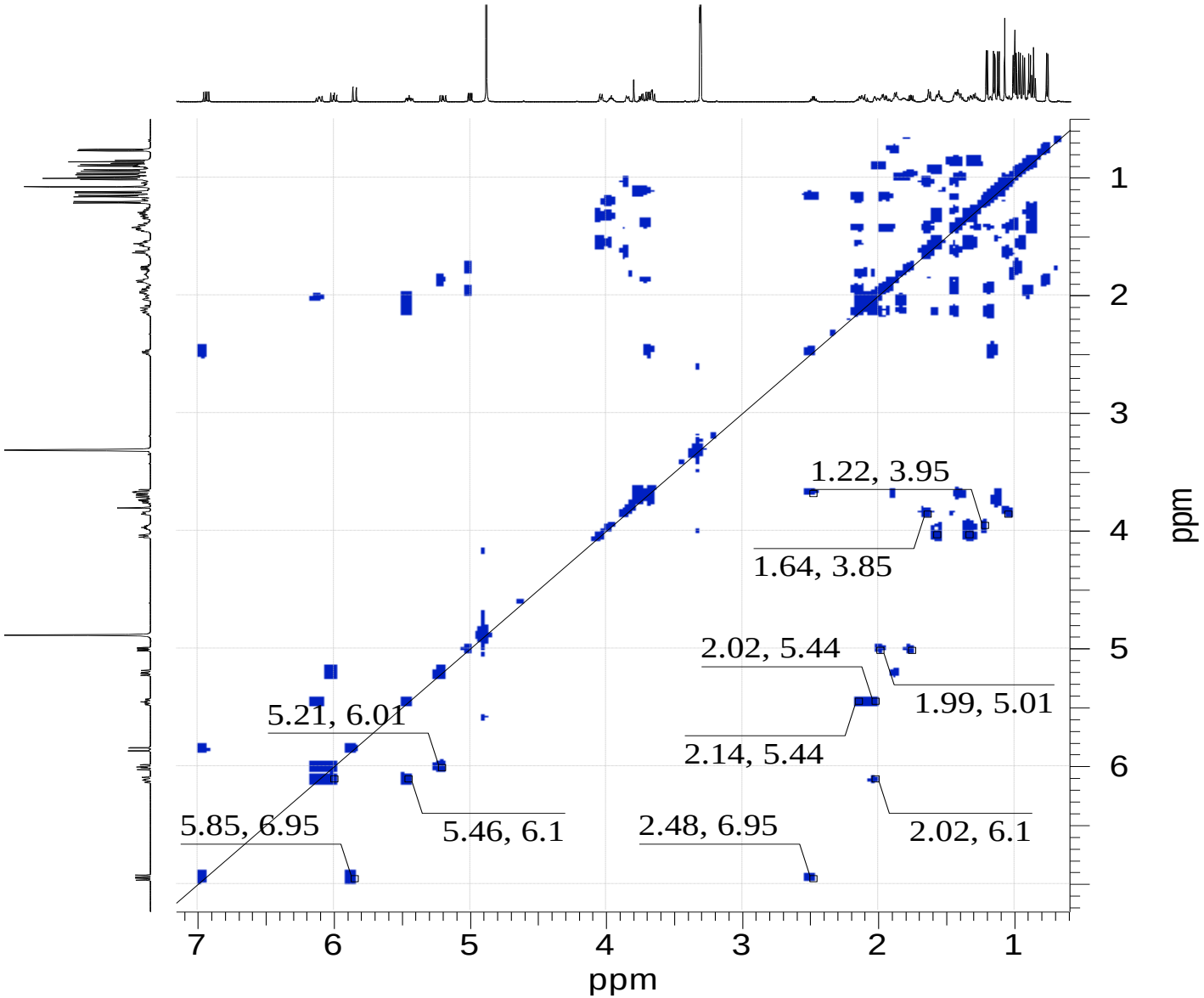


Рис. Д5. Спектр ЯМР ^{1}H-^{1}H COSY (CD_3OD, 25 °C) образца **2**

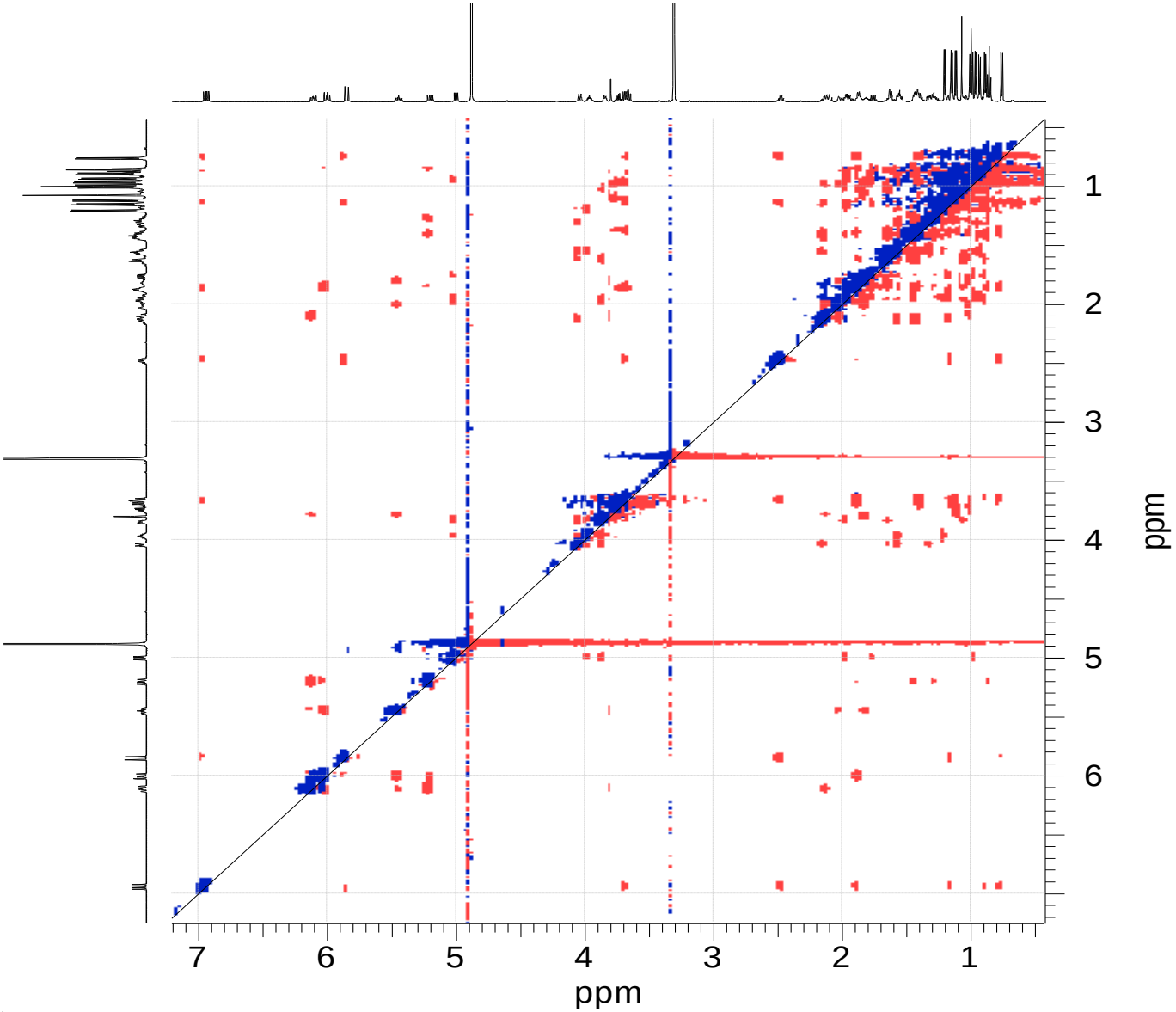


Рис. Д6. Спектр ЯМР ^{1}H-^{1}H ROESY (CD_3OD, 25 °C) образца **2**

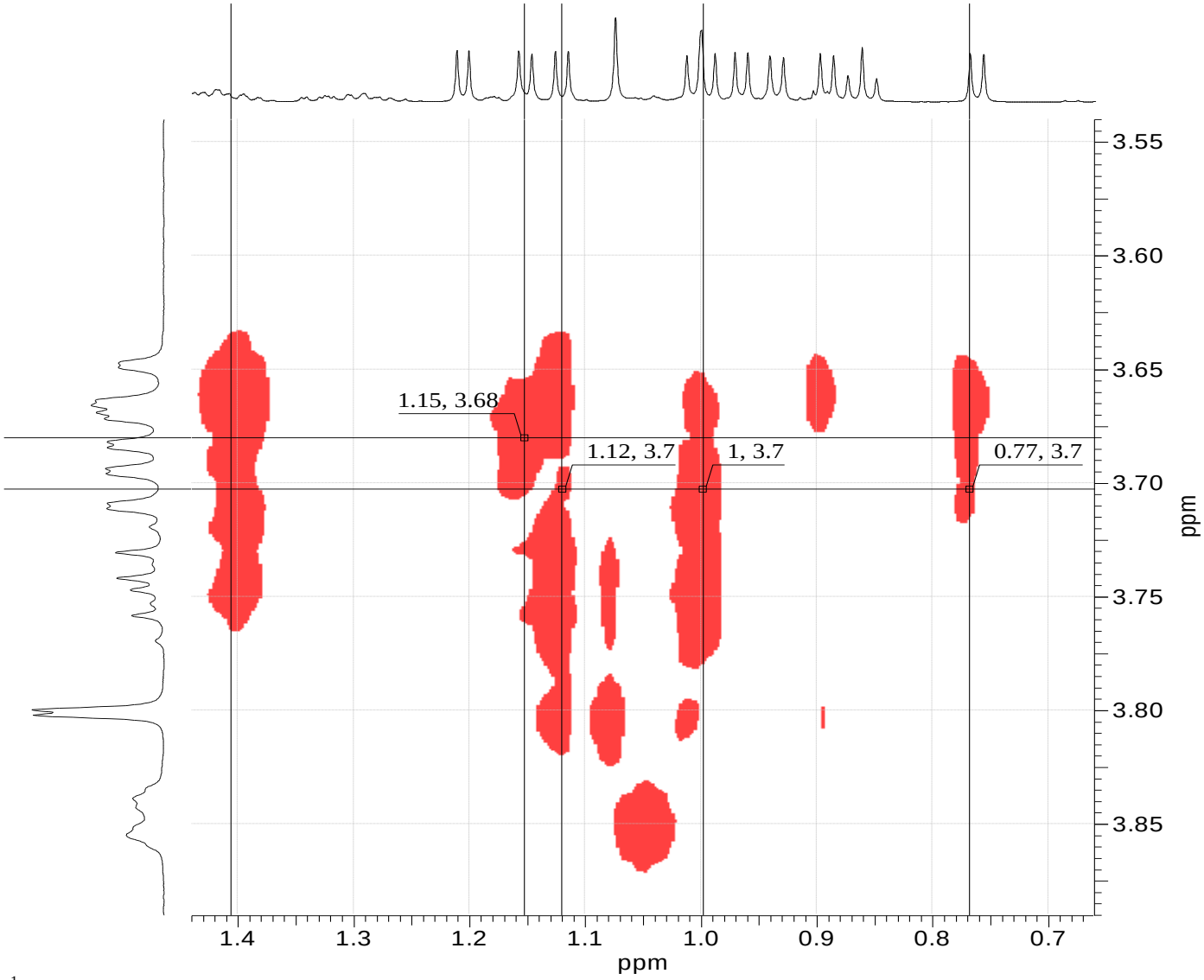


Рис. Д7. Спектр ЯМР ^{1}H-^{1}H ROESY (CD_3OD, 25 °C) образца **2** (увеличенный фрагмент)

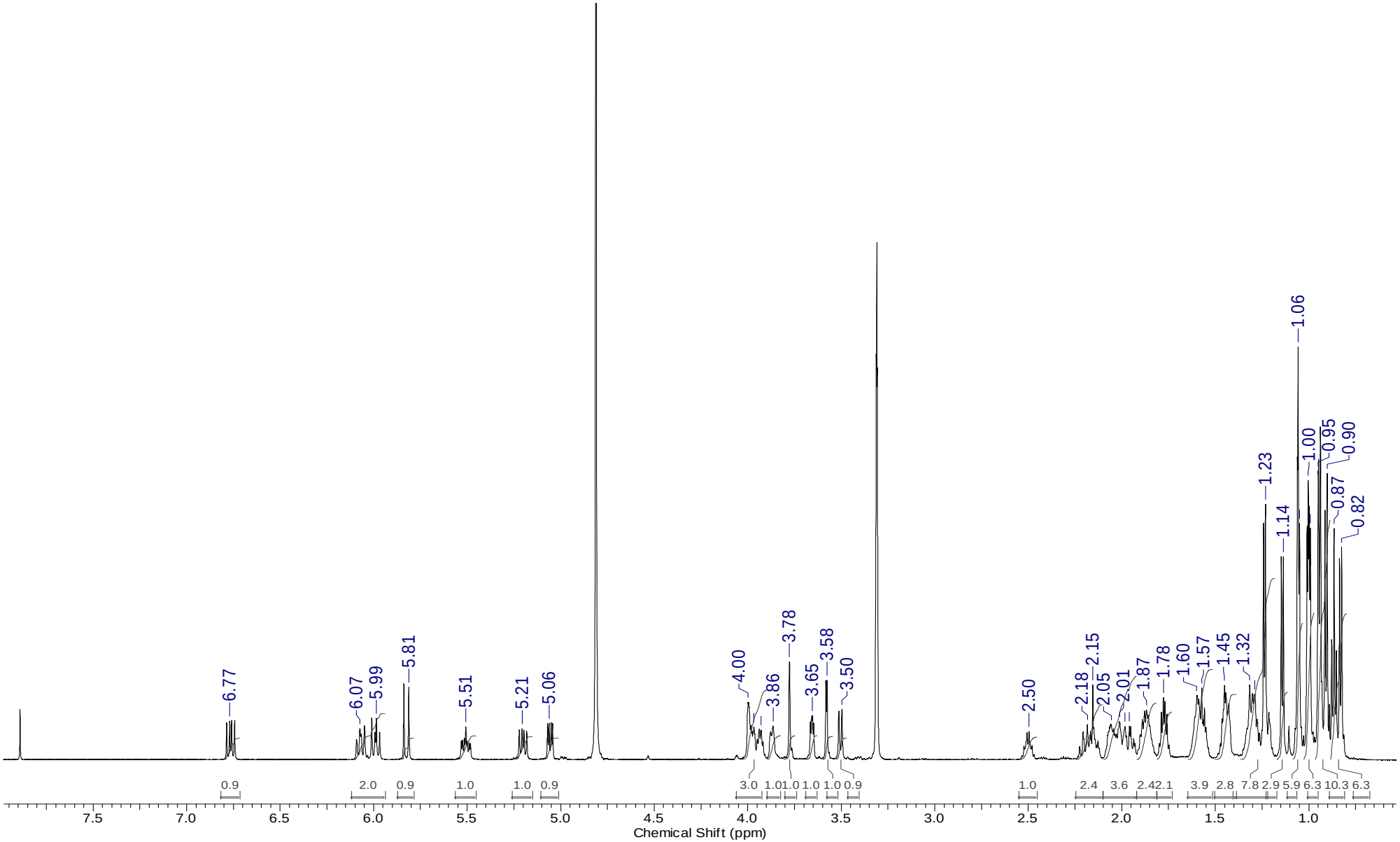


Рис. Д8. Спектр ЯМР ^{1}H (600 МГц, CD_3OD, 25 °C) (7S, 11R)-7,11-тетрагидроолигомицина А (**3**)

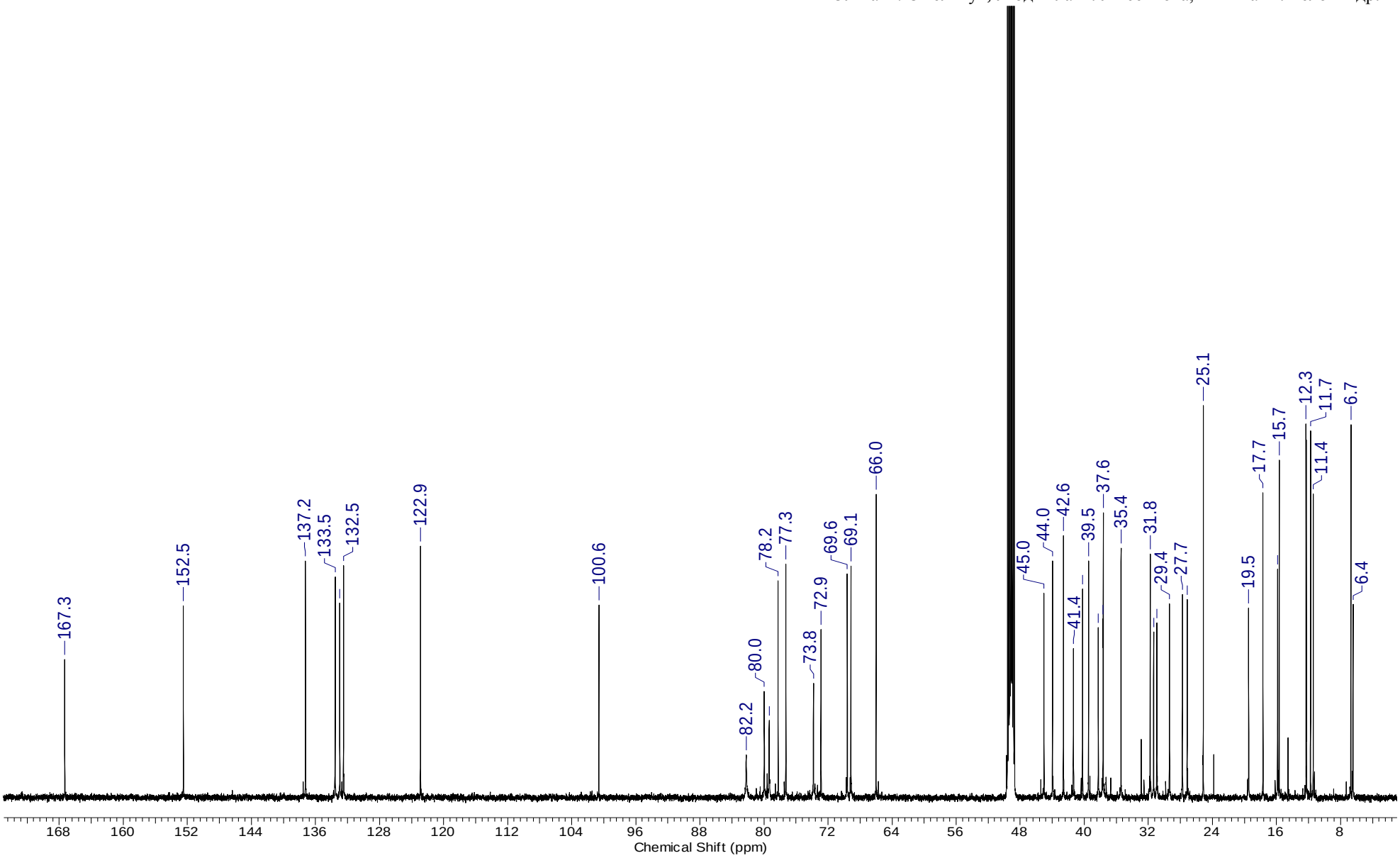


Рис. Д9. Спектр ЯМР ^{13}C (150 МГц, CD_3OD, 25 °C) образца **3** (увеличенный фрагмент)

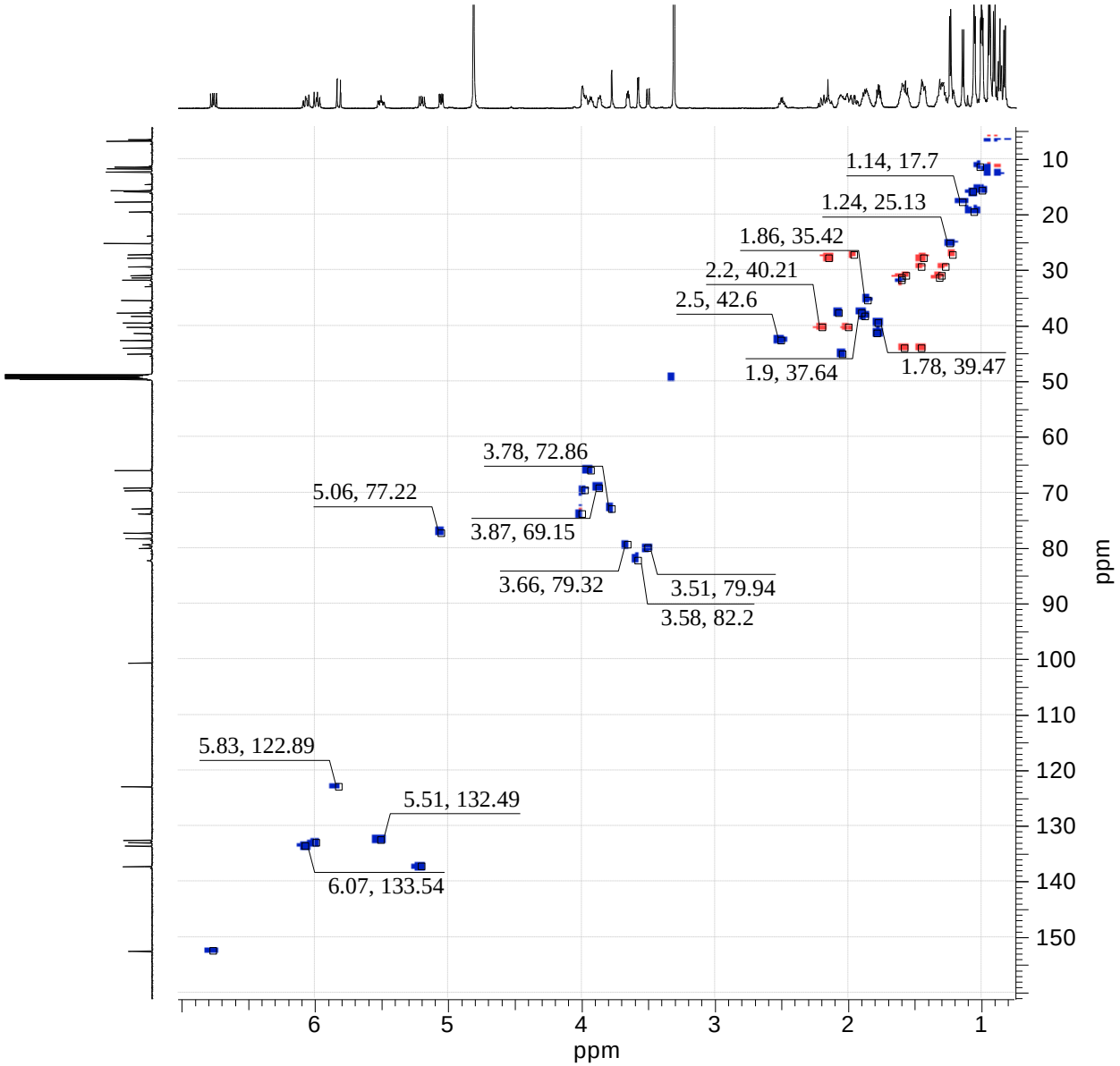


Рис. Д10. Спектр ЯМР ^{1}H-^{13}C HSQC (CD_3OD, 25 °C) образца **3**

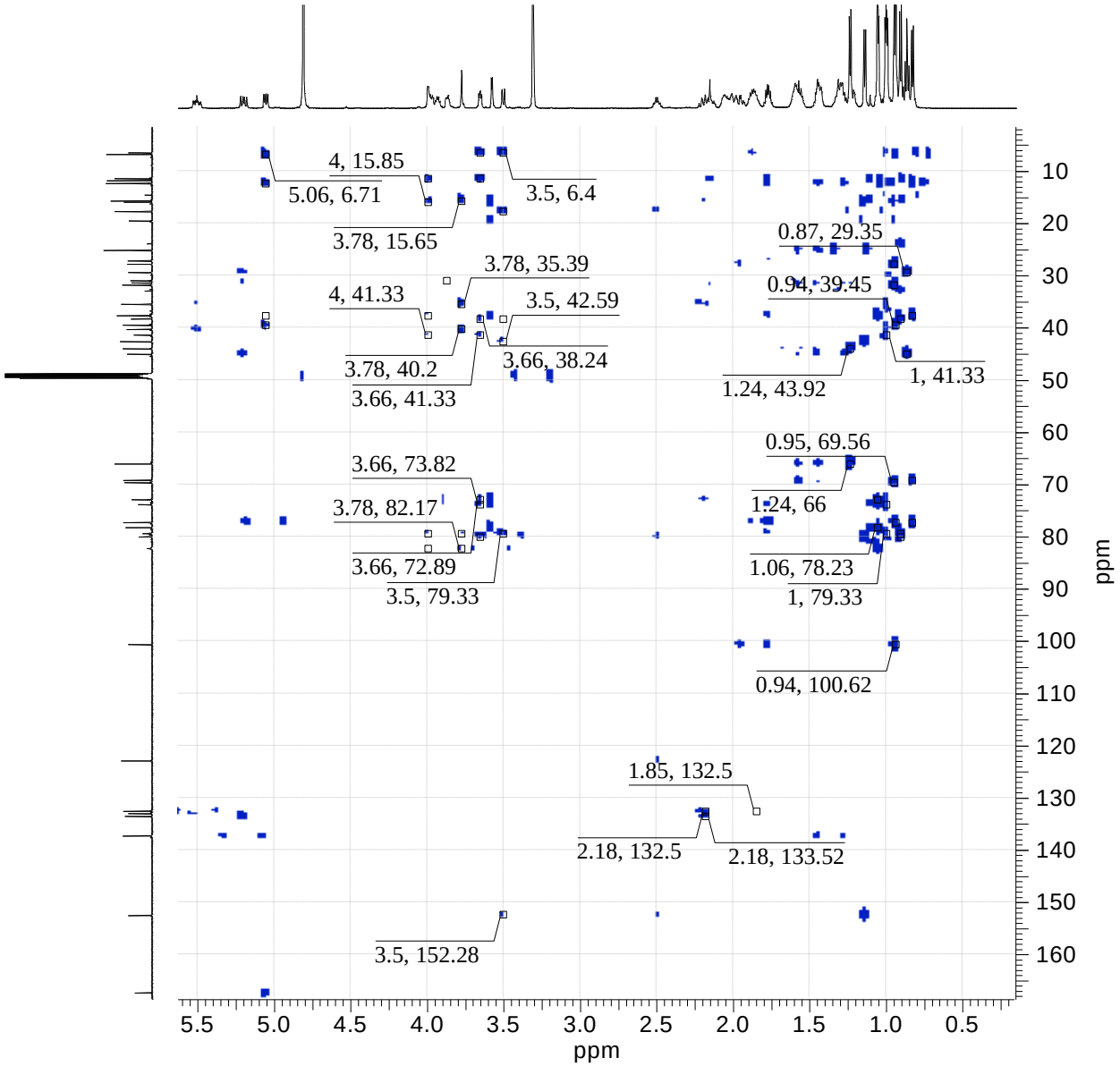


Рис. Д11. Спектр ЯМР ^{1}H-^{13}C HMBC (CD_3OD, 25 °C) образца **3**

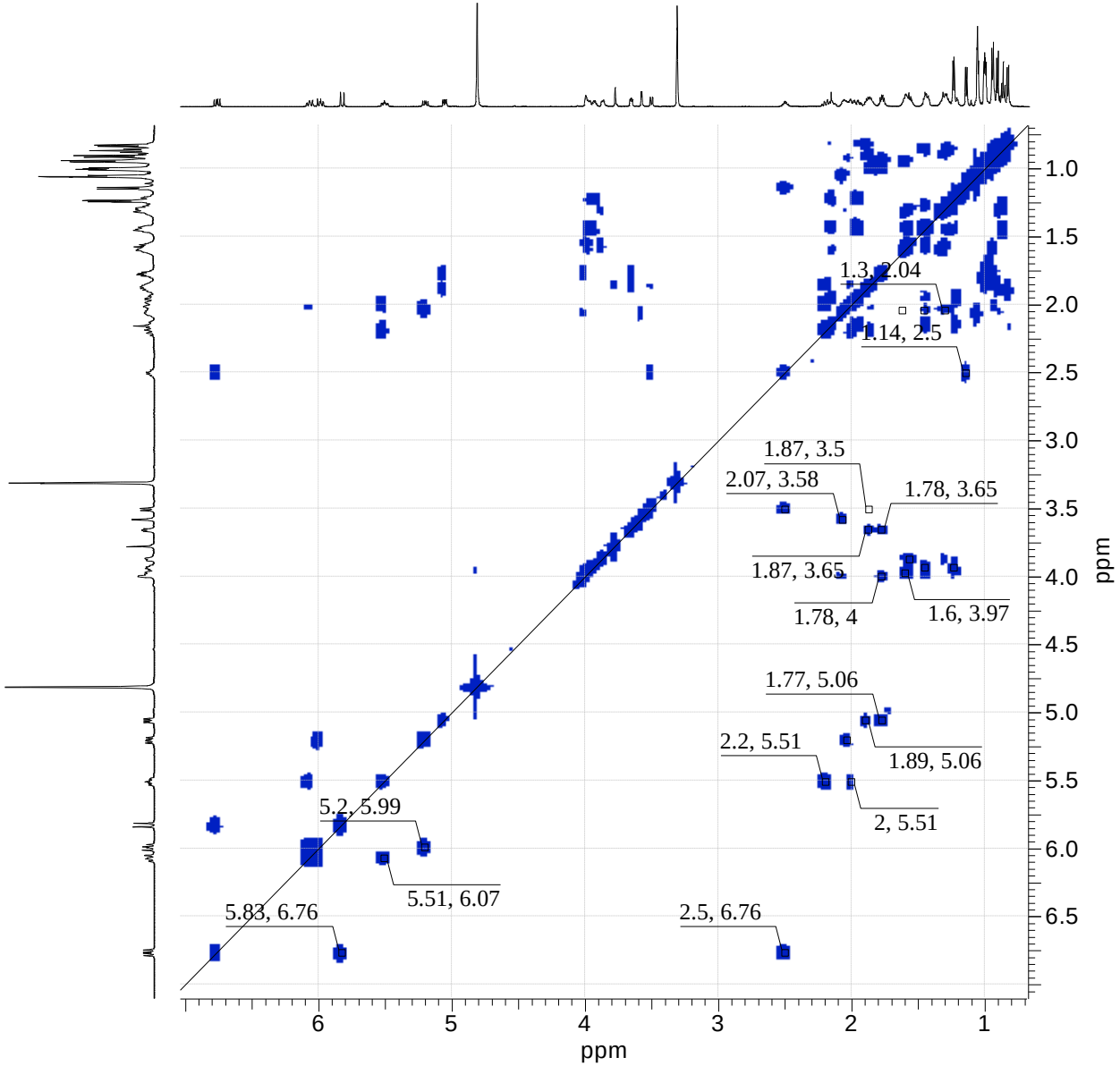


Рис. Д12. Спектр ЯМР ^{1}H-^{1}H COSY (CD_3OD, 25 °C) образца **3**

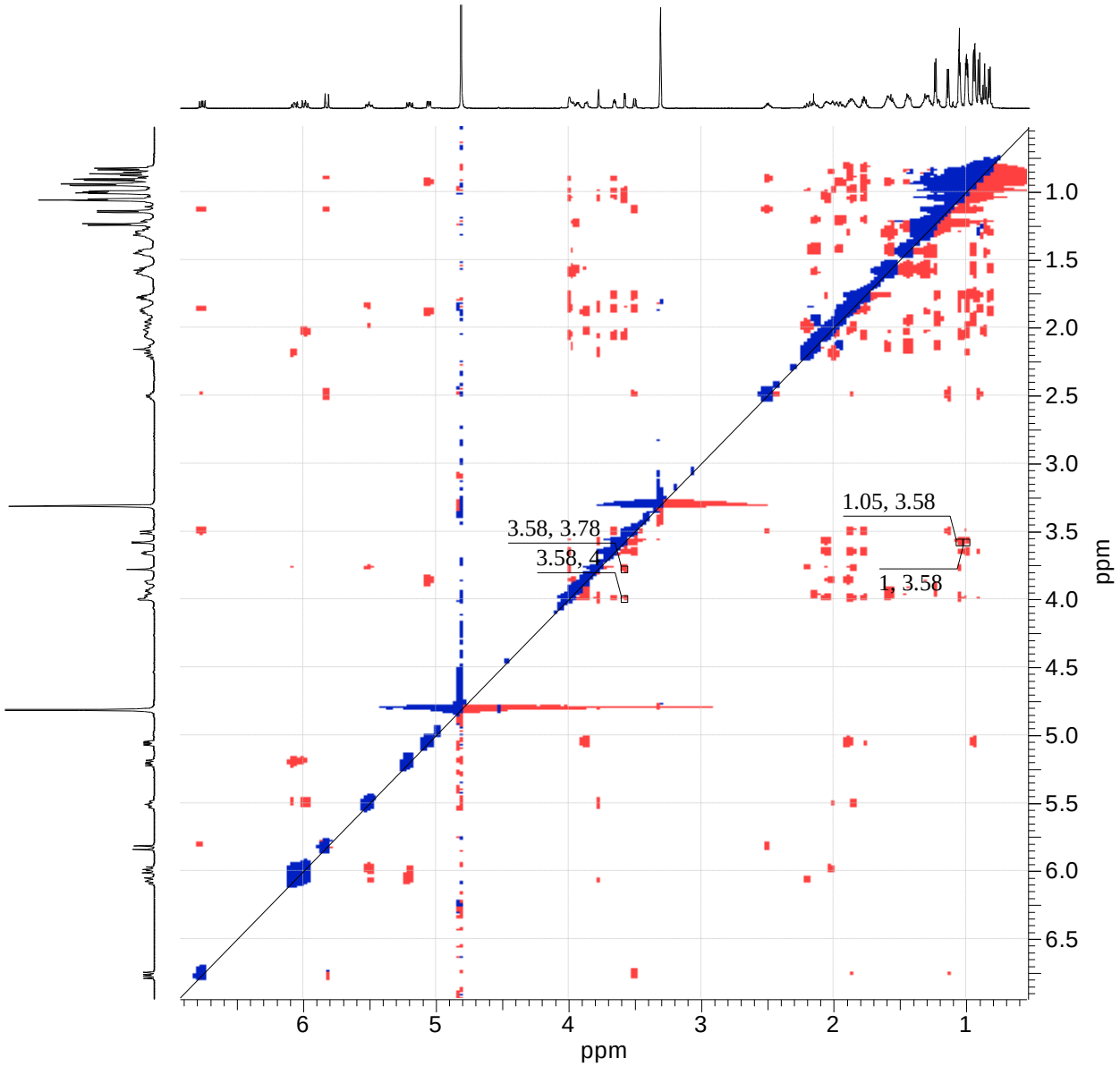


Рис. Д13. Спектр ЯМР ^{1}H-^{1}H ROESY (CD_3OD, 25 °C) образца **3**

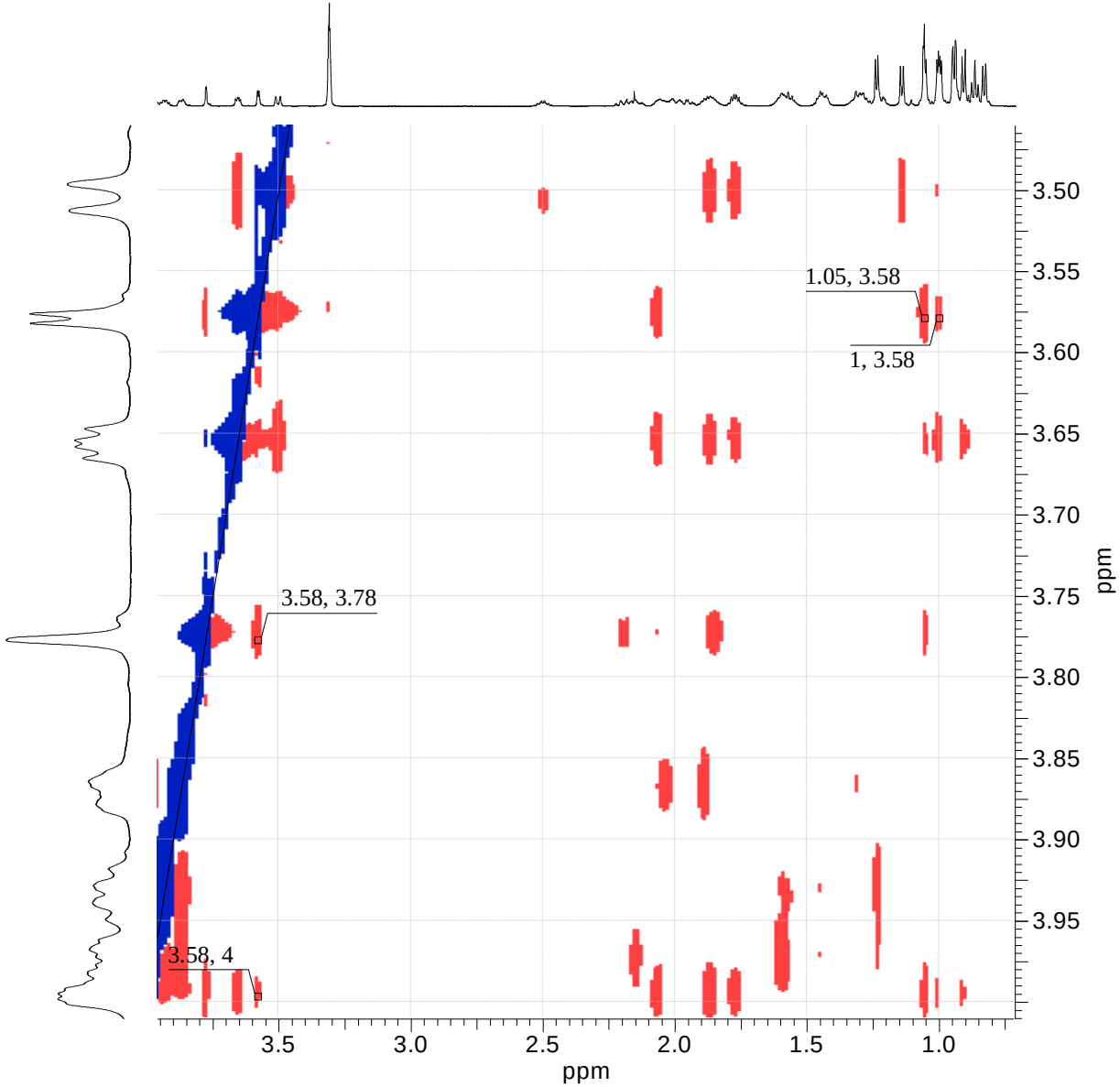


Рис. Д14. Спектр ЯМР ^{1}H-^{1}H ROESY (CD_3OD, 25 °C) образца **3** (увеличенный фрагмент)

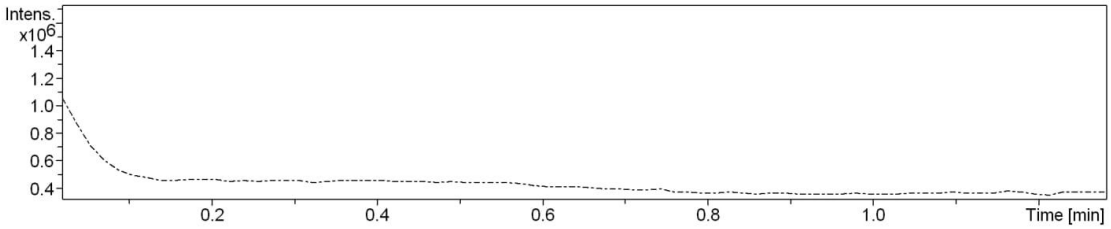
Compound Spectrum List Report

Analysis Info

Analysis Name	D:\Data\OO\OO-19_CHCl3+EtOH_neg_tune_wide.d	Acquisition Date	30.01.2017 11:05:51
Method	tune_wide.m	Operator	Korolev
Sample Name		Instrument / Ser#	micrOTOF-Q II 10225
Comment			

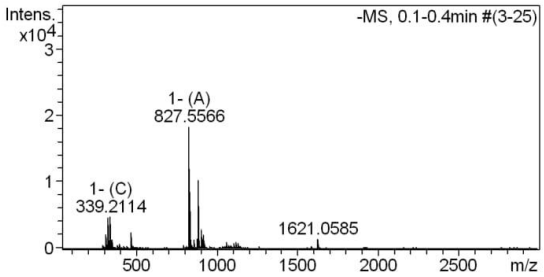
Acquisition Parameter

Source Type	ESI	Ion Polarity	Negative	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4000 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	550.0 Vpp	Set Divert Valve	Source

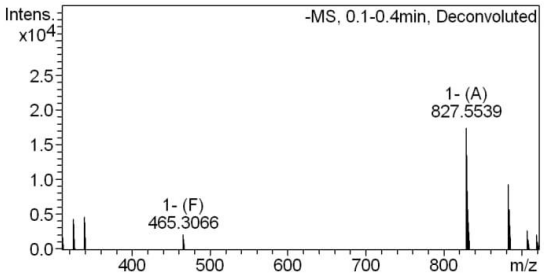


#	RT [min]	Area	Int. Type	Intens.	S/N	Chromatogram	Max. m/z
n.a.	0.2	n.a.	Average spectrum	n.a.	n.a.	n.a.	827.5066

-MS, 0.1-0.4min #(3-25)



#	m/z	Res.	S/N	I	I %
1	325.1969	7877	407.5	4574	25.0
2	339.2114	8077	403.8	4806	26.3
3	465.3068	9502	137.8	2375	13.0
4	827.5566	8618	653.2	18286	100.0
5	828.5113	7283	303.8	8531	46.7
6	829.5048	7811	290.4	8176	44.7
7	830.5066	8077	137.8	3895	21.3
8	881.5617	8068	323.8	10187	55.7
9	882.5629	7885	172.7	5452	29.8
10	905.5259	8093	84.2	2792	15.3



#	m/z	Res.	S/N	I	I %
1	311.1826			2052	11.2
2	325.1963			4573	25.0
3	339.2109			4806	26.3
4	465.3066			2374	13.0
5	827.5539			18285	100.0
6	881.5612			10187	55.7
7	905.5242			2792	15.3
8	917.5275			2076	11.4

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Рис. Д15. HRMS ESI Масс-спектр (7*S*)-дигидроолигомицина А (**2**)

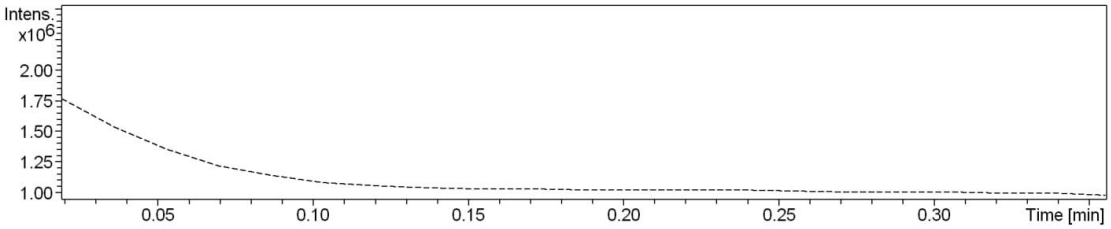
Compound Spectrum List Report

Analysis Info

Analysis Name	D:\Data\OO\OO-22-1_AcCN+H2O_pos_tune_wide.d	Acquisition Date	30.06.2017 10:42:53
Method	tune_wide.m	Operator	Korolev
Sample Name		Instrument / Ser#	micrOTOF-Q II 10225
Comment			

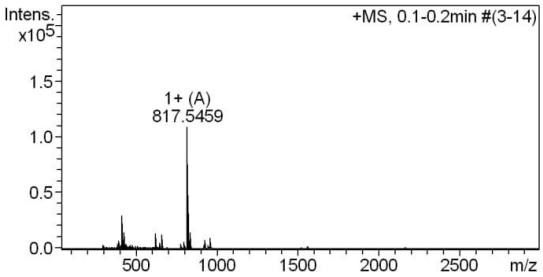
Acquisition Parameter

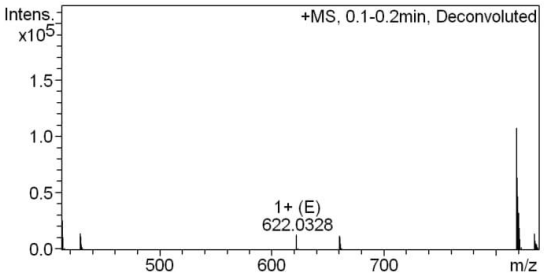
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	550.0 Vpp	Set Divert Valve	Source



#	RT [min]	Area	Int. Type	Intens.	S/N	Chromatogram	Max. m/z
n.a.	0.1	n.a.	Average spectrum	n.a.	n.a.	n.a.	817.5459

+MS, 0.1-0.2min #(3-14)





#	m/z	Res.	S/N	I	I %
1	413.2685	9771	568.0	29556	27.1
2	429.2412	9140	251.1	13739	12.6
3	622.0326	9552	167.6	12894	11.8
4	659.9885	9024	161.0	12744	11.7
5	817.5459	13181	1390.1	108992	100.0
6	818.5481	11561	612.7	48047	44.1
7	819.5579	11098	418.5	32815	30.1
8	820.5621	9051	120.9	9519	8.7
9	833.5228	9346	176.6	13763	12.6
10	959.9624	11444	139.2	9610	8.8

#	m/z	Res.	S/N	I	I %
1	413.2682			29555	27.1
2	429.2421			13738	12.6
3	622.0328			12893	11.8
4	659.9877			12744	11.7
5	817.5469			108991	100.0
6	833.5232			13763	12.6

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Рис. Д16. HRMS ESI Масс-спектр (7S, 11R)-7,11-тетрагидроолигомицина А (**3**).

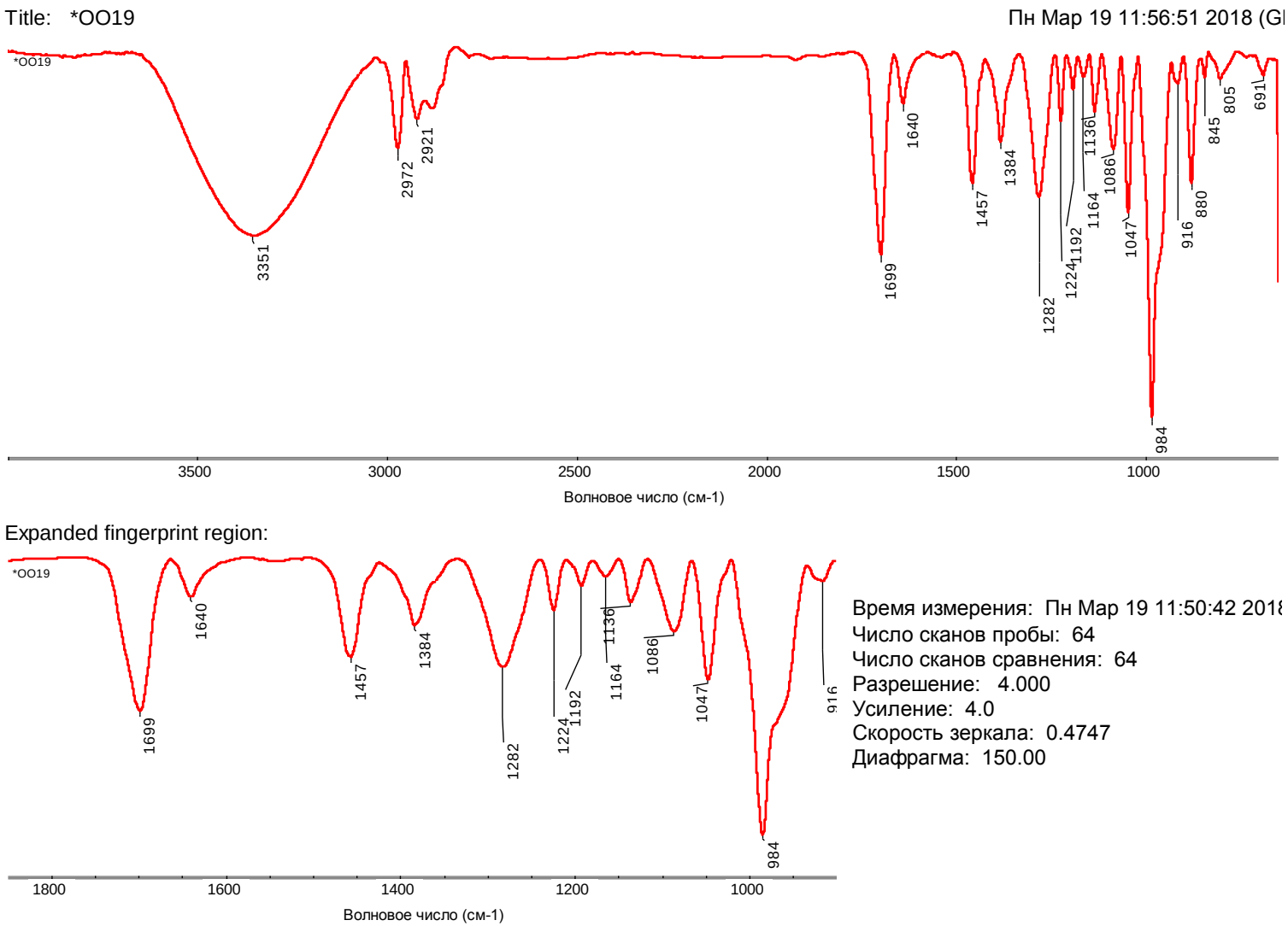

Рис. Д17. ИК-спектр (7*S*)-дигидроолигомицина А (**2**)

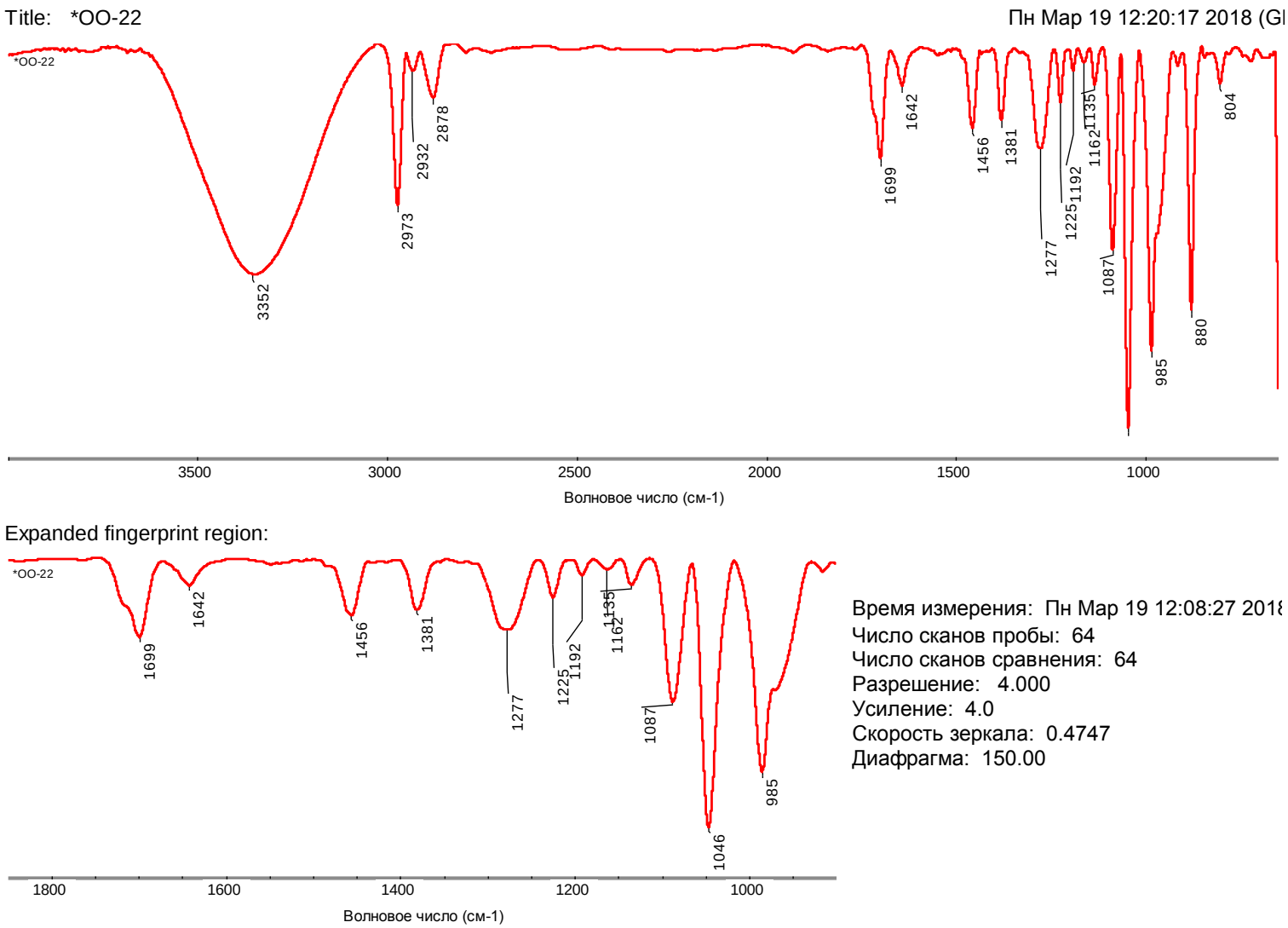

Рис. Д18. ИК-спектр (7S, 11R)-7,11-тетрагидроолигомицина А (**3**).