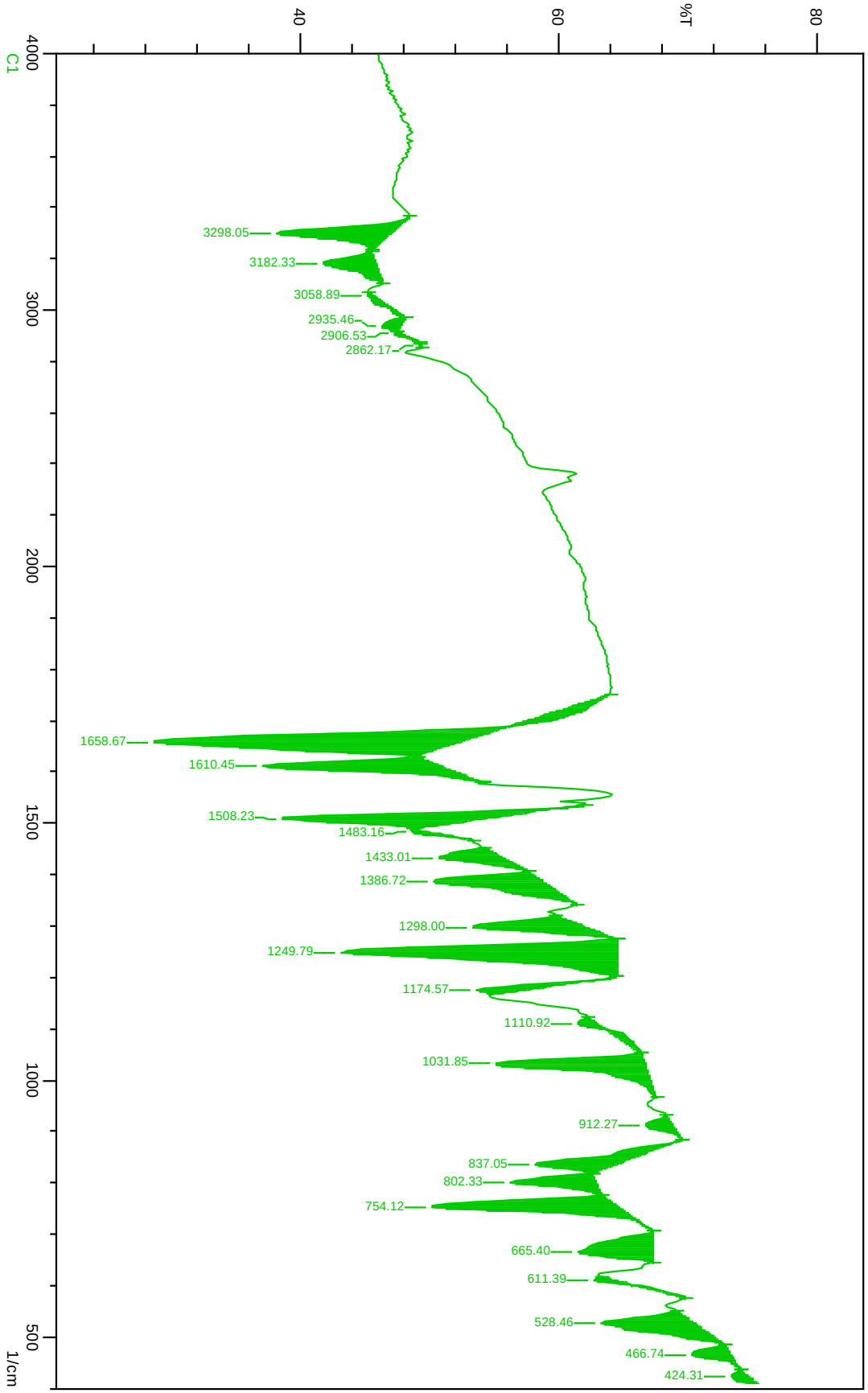
Larvicidal Activities of 2-Aryl-2,3-Dihydroquinazolin-4-ones Against Malaria Vector *Anopheles arabiensis*, In Silico ADMET Prediction and Molecular Target Investigation

Katharigatta N. Venugopala [1,2,*], Pushpalatha Ramachandra [3], Christophe Tratrat [1], Raquel M. Gleiser [4], Subhrajyoti Bhandary [5], Deepak Chopra [5], Mohamed A. Morsy [1,6], Bandar E. Aldhubiab[1], Mahesh Attimarad [1], Anroop B. Nair [1], Nagaraja Sreeharsha [1], Rashmi Venugopala [7], Pran Kishore Deb [8], Sandeep Chandrashekharappa [9], Hany Ezzat Khalil [1,10], Osama I. Alwassil [11], Sara Nidal Abed [8], Yazan A. Bataineh [8], Ramachandra Palenge [3], Michelyne Haroun [1], Shinu Pottathil [13], Meravanige B. Girish [14], Sabah H. Akrawi [1] and Viresh Mohanlall [2]

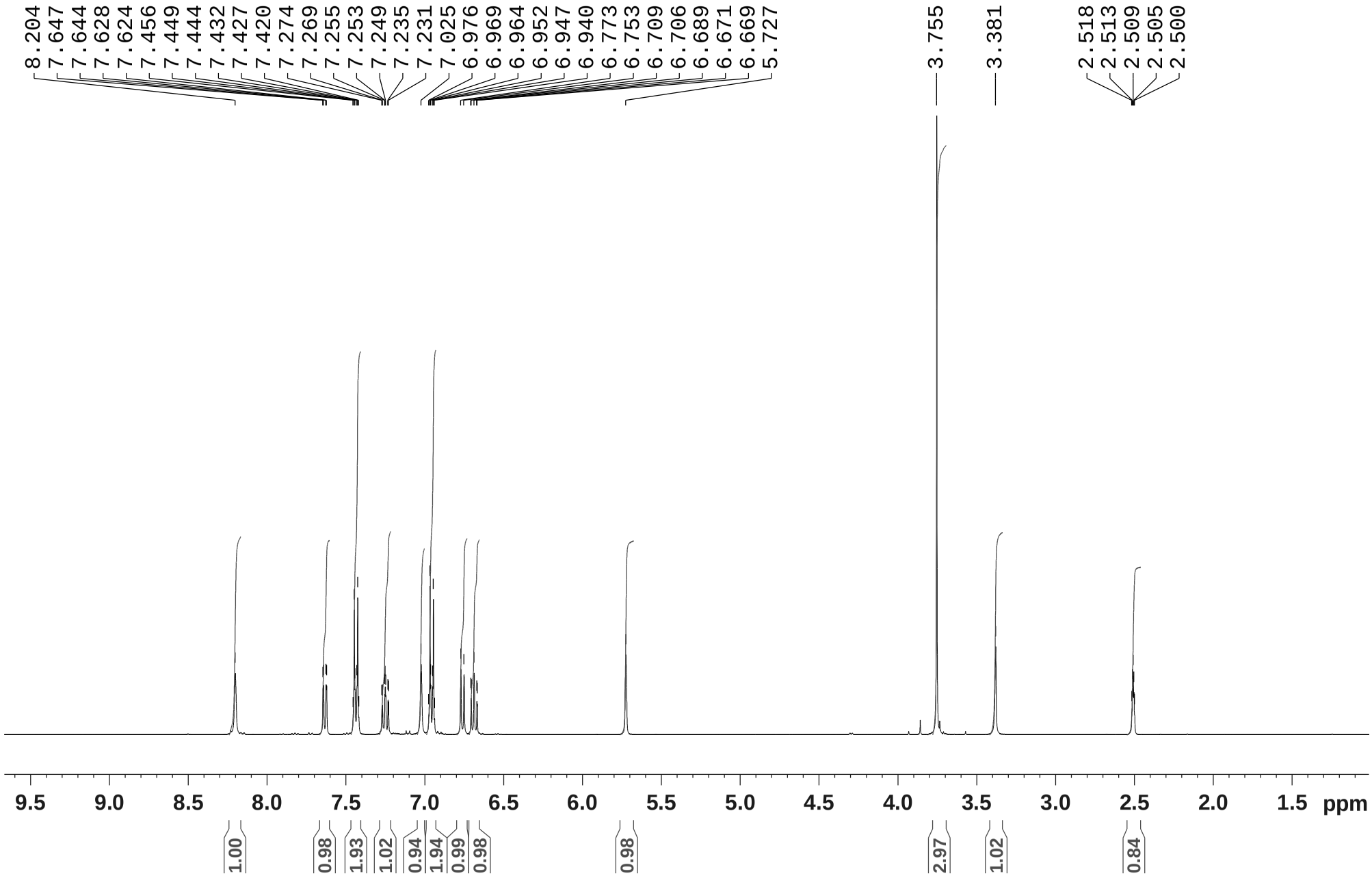
[1] Department of Pharmaceutical Sciences, College of Clinical Pharmacy, King Faisal University, Al-Ahsa 31982, Kingdom of Saudi Arabia; momorsy@kfu.edu.sa (M.A.M.); baldhubiab@kfu.edu.sa (B.E.A.); mattimarad@kfu.edu.sa (M.A.); anair@kfu.edu.sa (A.B.N.); sharsha@kfu.edu.sa (N.S.); heahmed@kfu.edu.sa (H.E.K.); mharoun@kfu.edu.sa (M.H.); sakrawi@kfu.edu.sa (S.H.A.)
[2] Department of Biotechnology and Food Technology, Durban University of Technology, Durban 4001, South Africa; vireshm@dut.ac.za (V.M.)
[3] Department of Chemistry, School of Applied Sciences, REVA University, Bangalore 560 064, India; pushpalatha@reva.edu.in (P.R.); ramachandrap@reva.edu.in (R.P.)
[4] CREAN-IMBIV (CONICET-UGC), AV Valparaiso s.n., and FCEFyN, AV. Sarsfield 299, Universidad Nacional de Cordoba, Cordoba 5000, Argentina; raquel.gleiser@unc.edu.ar (R.M.G.)
[5] Department of Chemistry, Indian Institute of Science Education and Research Bhopal, Indore By-pass Road, Bhauri, Bhopal 462 066, Madhya Pradesh, India; bhandarysj@gmail.com (S.B.); dchopra@iiserb.ac.in (D.C.)
[6] Department of Pharmacology, Faculty of Medicine, Minia University, El-Minia 61511, Egypt
[7] Department of Public Health Medicine, University of KwaZulu-Natal, Howard College Campus, Durban 4001, South Africa; venugopalar@ukzn.ac.za (R.V.)
[8] Department of Pharmaceutical Sciences, Faculty of Pharmacy, Philadelphia University, PO Box 1, Amman 19392, Jordan; pdeb@philadelphia.edu.jo (P.K.D.); sousanidal95@gmail.com (S.N.A.); YBatineh@philadelphia.edu.jo (Y.A.B.)
[9] Institute for Stem Cell Biology and Regenerative Medicine, NCBS, TIFR, GKVK, Bellary Road, Bangalore 560 065, India; sandeepc@instem.res.in (S.C.)
[10] Department of Pharmacognosy, Faculty of Pharmacy, Minia University, Minia 61519, Egypt
[11] Department of Pharmaceutical Sciences, College of Pharmacy, King Saud bin Abdulaziz University for Health Sciences, Riyadh 11481, Kingdom of Saudi Arabia; wassilo@ksau-hs.edu.sa
[12] Department of Pharmaceutical Chemistry, Shri Vishnu College of Pharmacy, Vishnupur, Bhimavaram 534 202, West Godavari Dist., Andhra Pradesh, India; raghumrp@svcp.edu.in
[13] Department of Biomedical Sciences, College of Clinical Pharmacy, King Faisal University, Al-Ahsa 31982, Kingdom of Saudi Arabia; spottathail@kfu.edu.sa (S.P.)
[14] Department of Biomedical Sciences, College of Medicine, King Faisal University, Al-Ahsa 31982, Kingdom of Saudi Arabia; gmeravanige@kfu.edu.sa (M.B.G.)
* Correspondence: kvenugopala@kfu.edu.sa (K.N.V.)

TABLE OF CONTENTS

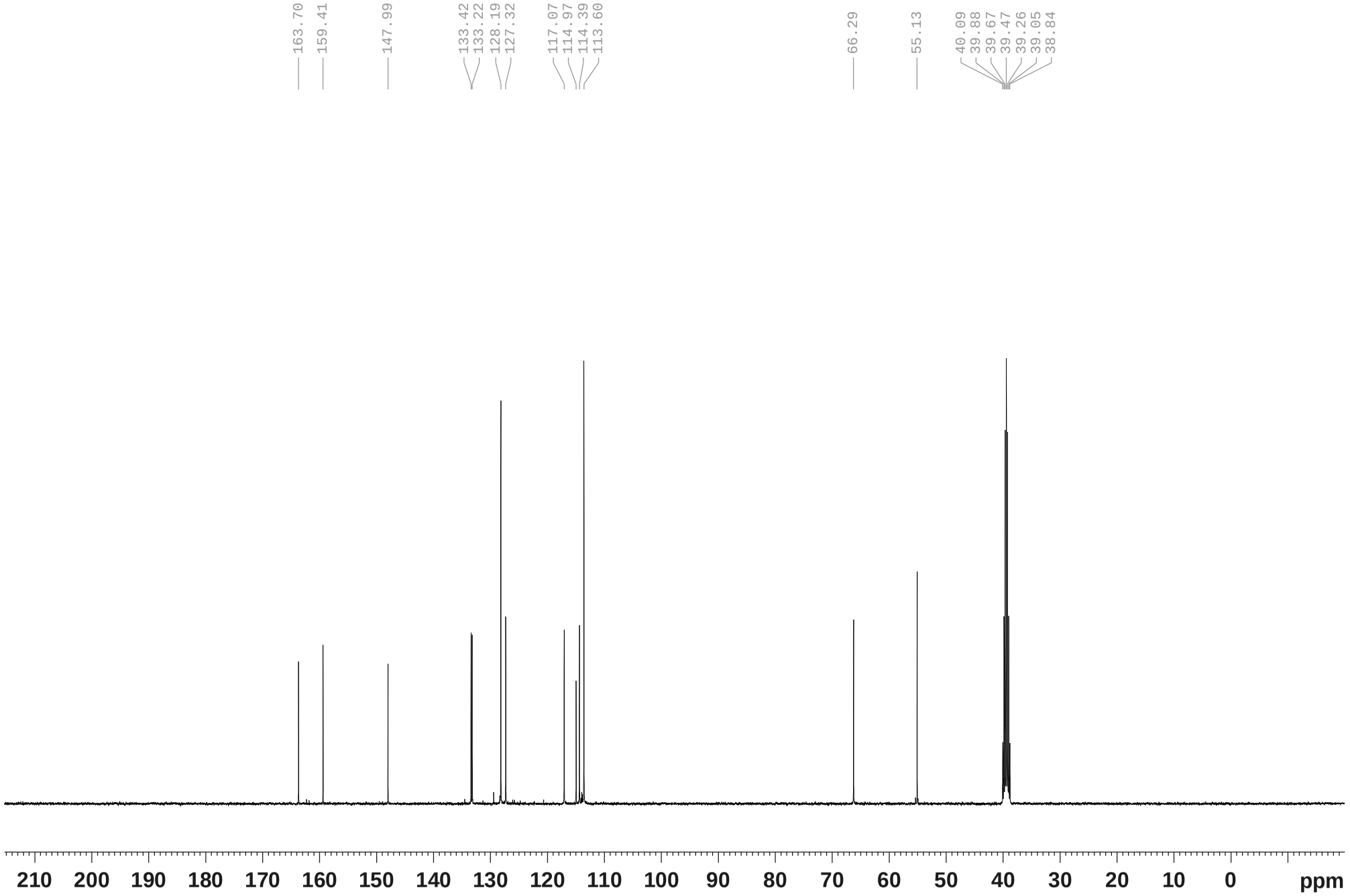
S17	^{1}H-NMR of 2-(4-chlorophenyl)-2,3-dihydroquinazolin-4(1*H*)-one (**3f**)
S18	^{13}C-NMR of 2-(4-chlorophenyl)-2,3-dihydroquinazolin-4(1*H*)-one (**3f**)
S19	FT-IR of 2-(3,4-dimethoxyphenyl)-2,3-dihydroquinazolin-4(1*H*)-one (**3g**)
S20	^{1}H-NMR of 2-(3,4-dimethoxyphenyl)-2,3-dihydroquinazolin-4(1*H*)-one (**3g**)
S21	^{13}C-NMR of 2-(3,4-dimethoxyphenyl)-2,3-dihydroquinazolin-4(1*H*)-one (**3g**)
S22	FT-IR of 2-(4-(dimethylamino)phenyl)-2,3-dihydroquinazolin-4(1*H*)-one (**3h**)
S23	^{1}H-NMR of 2-(4-(dimethylamino)phenyl)-2,3-dihydroquinazolin-4(1*H*)-one (**3h**),
S24	^{13}C-NMR of 2-(4-(dimethylamino)phenyl)-2,3-dihydroquinazolin-4(1*H*)-one (**3h**)
S21	FT-IR of 2-(3-nitrophenyl)-2,3-dihydroquinazolin-4(1*H*)-one (**3i**)
S26	^{1}H-NMR of 2-(3-nitrophenyl)-2,3-dihydroquinazolin-4(1*H*)-one (**3i**)
S27	^{13}C-NMR of 2-(3-nitrophenyl)-2,3-dihydroquinazolin-4(1*H*)-one (**3i**)
S28	FT-IR of 2-(4-fluorophenyl)-2,3-dihydroquinazolin-4(1*H*)-one (**3j**)
S29	^{1}H-NMR of 2-(4-fluorophenyl)-2,3-dihydroquinazolin-4(1*H*)-one (**3j**)
S30	^{13}C-NMR of 2-(4-fluorophenyl)-2,3-dihydroquinazolin-4(1*H*)-one (**3j**)
S31	FT-IR of 2-(1*H*-imidazol-4-yl)-2,3-dihydroquinazolin-4(1*H*)-one (**3k**)
S32	^{1}H-NMR of 2-(1*H*-imidazol-4-yl)-2,3-dihydroquinazolin-4(1*H*)-one (**3k**)

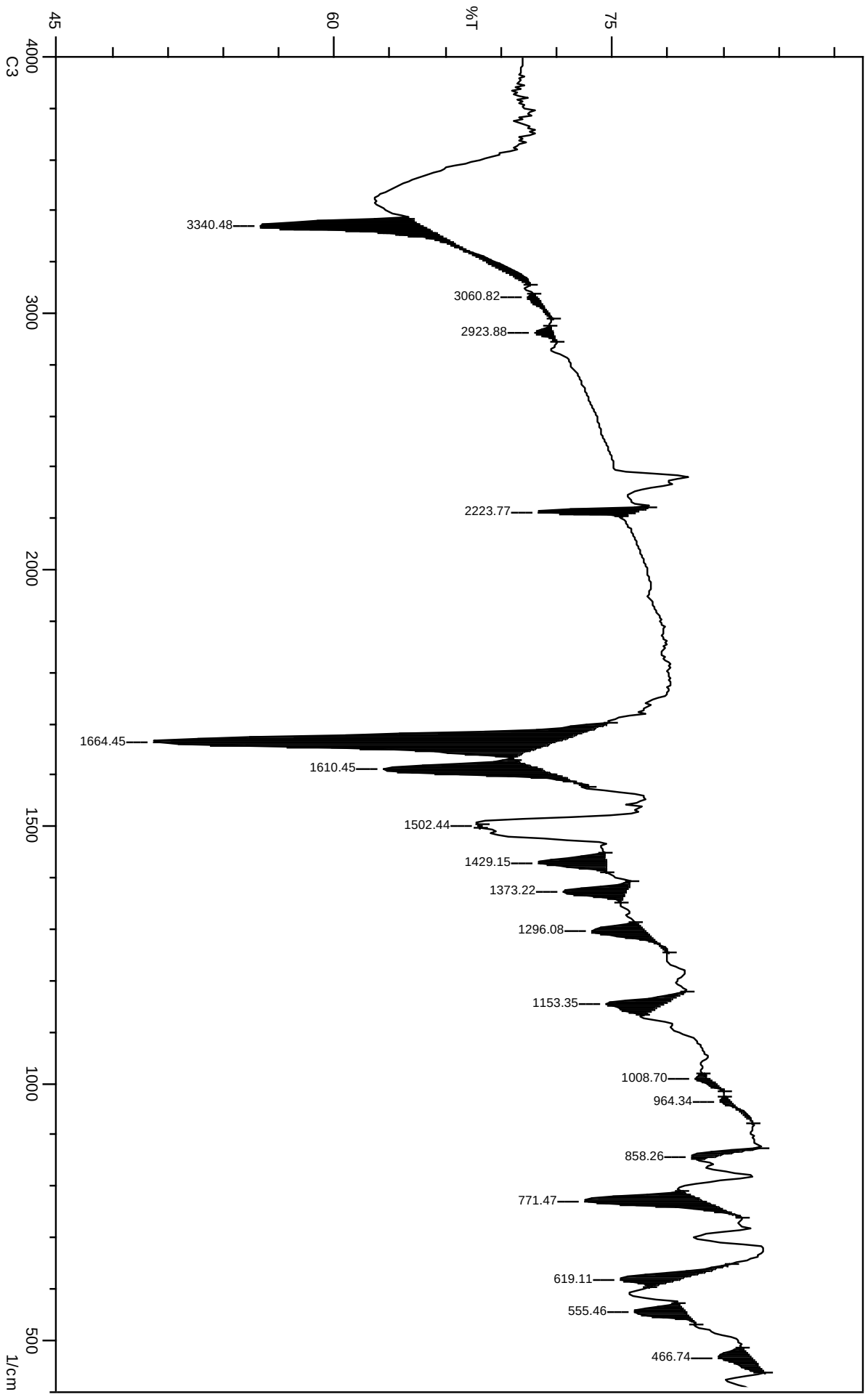

%T
40
60
80
4000
3000
2000
1500
1000
500
1/cm
C1
3298.05
3182.33
3058.89
2935.46
2906.53
2862.17
1658.67
1610.45
1508.23
1483.16
1433.01
1386.72
1298.00
1249.79
1174.57
1110.92
1031.85
912.27
837.05
802.33
754.12
665.40
611.39
528.46
466.74
424.31

PROTON DMSO {C:\Bruker\TOPSPIN\KFUCCP} nmr 12

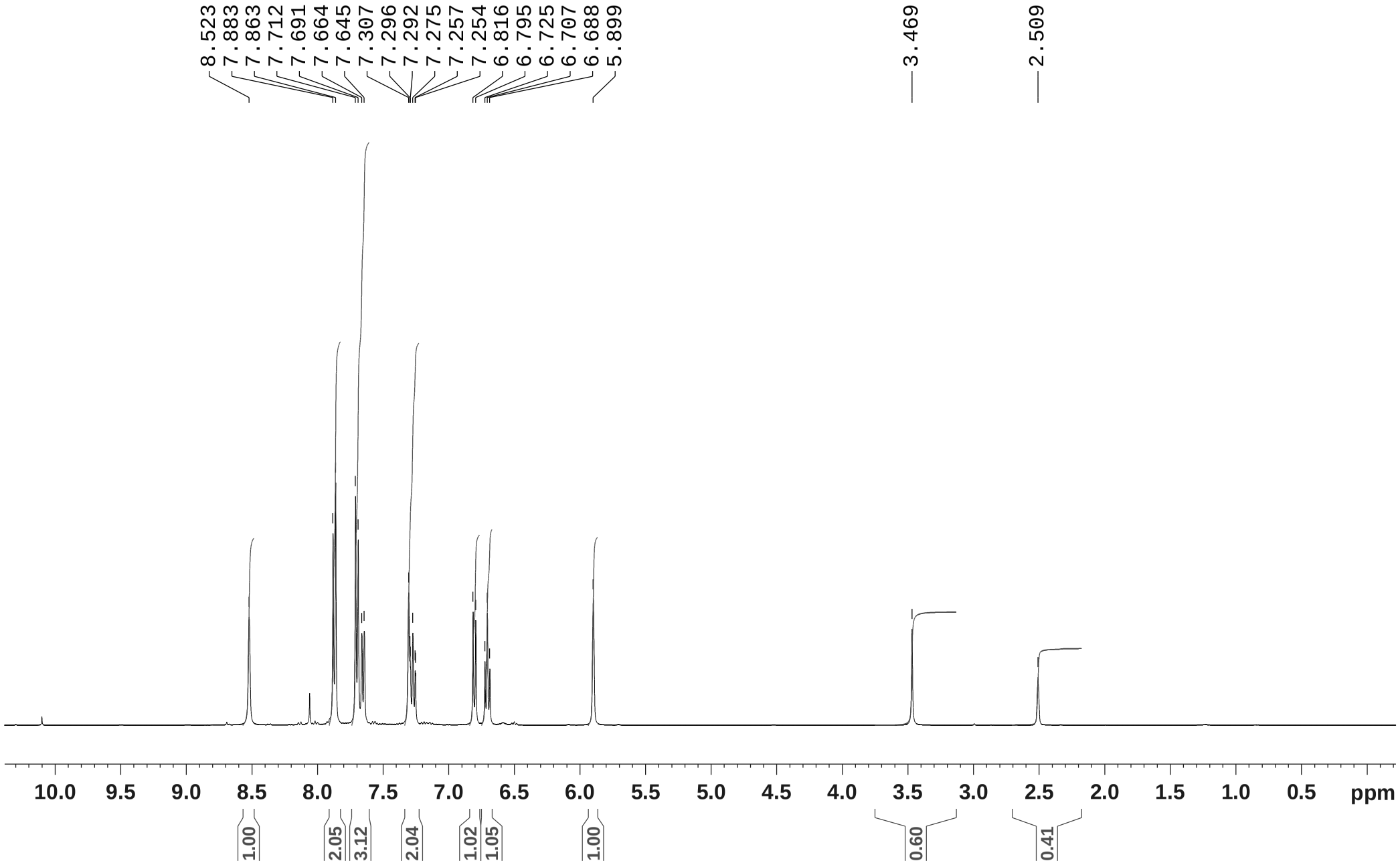


C13CPD DMSO {C:\Bruker\TOPSPIN\KFUCCP} nmr 12

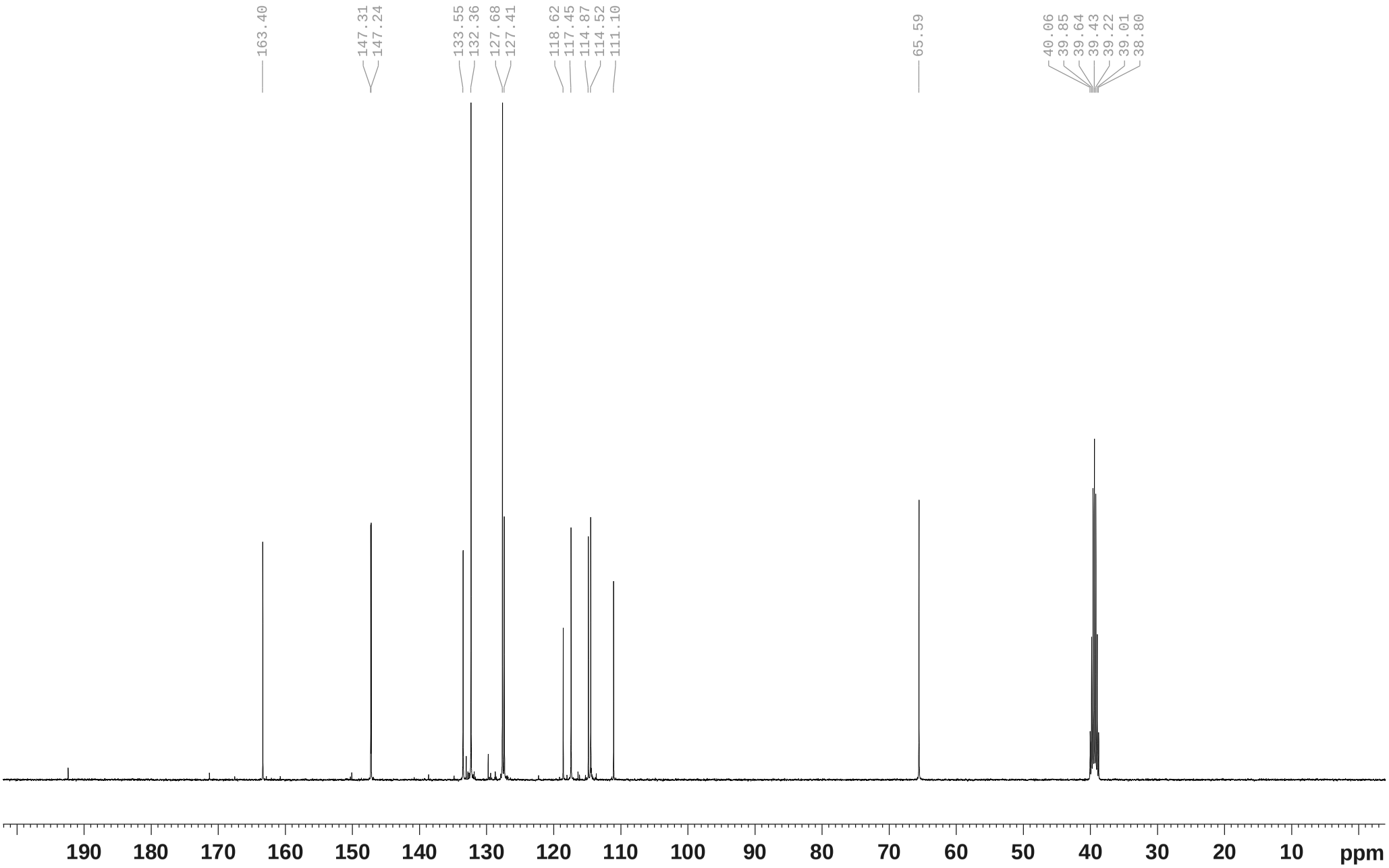


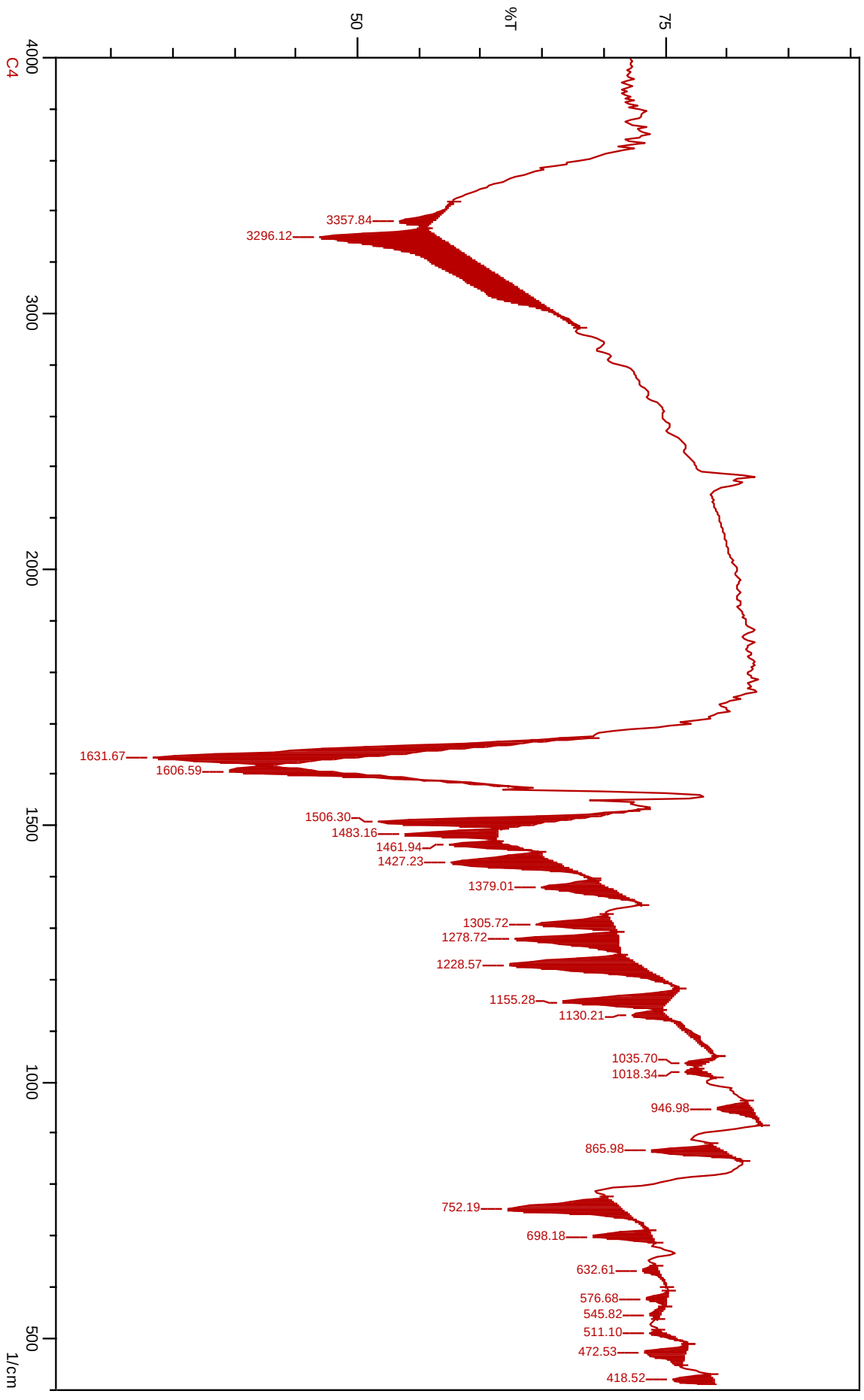

45
60
%T
75
4000
3000
2000
1500
1000
500
1/cm
C3
3340.48
3060.82
2923.88
2223.77
1664.45
1610.45
1502.44
1429.15
1373.22
1296.08
1153.35
1008.70
964.34
858.26
771.47
619.11
555.46
466.74

PROTON DMSO {C:\Bruker\TOPSPIN\KFUCCP} nmr 6

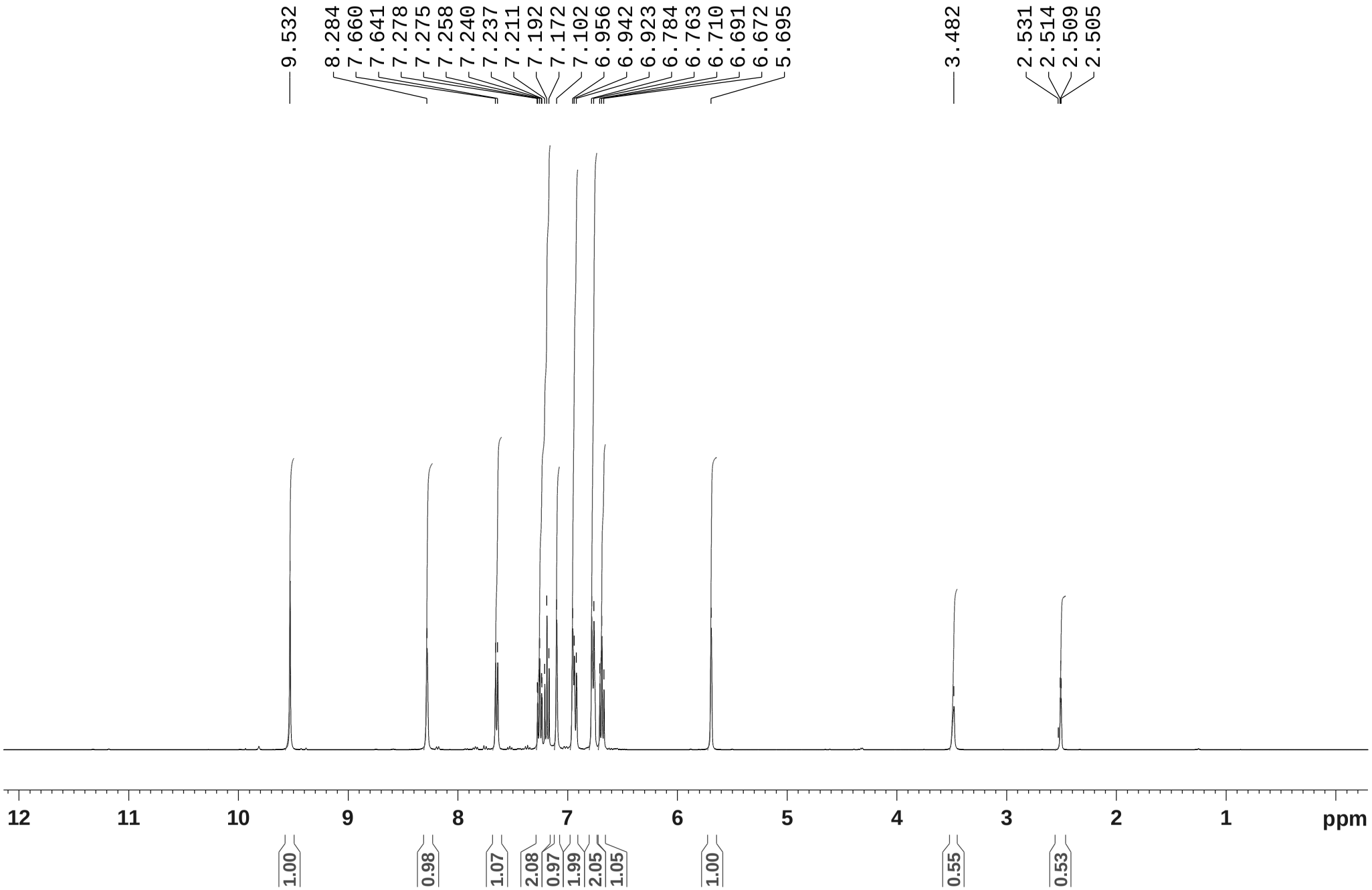


C13CPD DMSO {C:\Bruker\TOPSPIN\KFUCCP} nmr 6

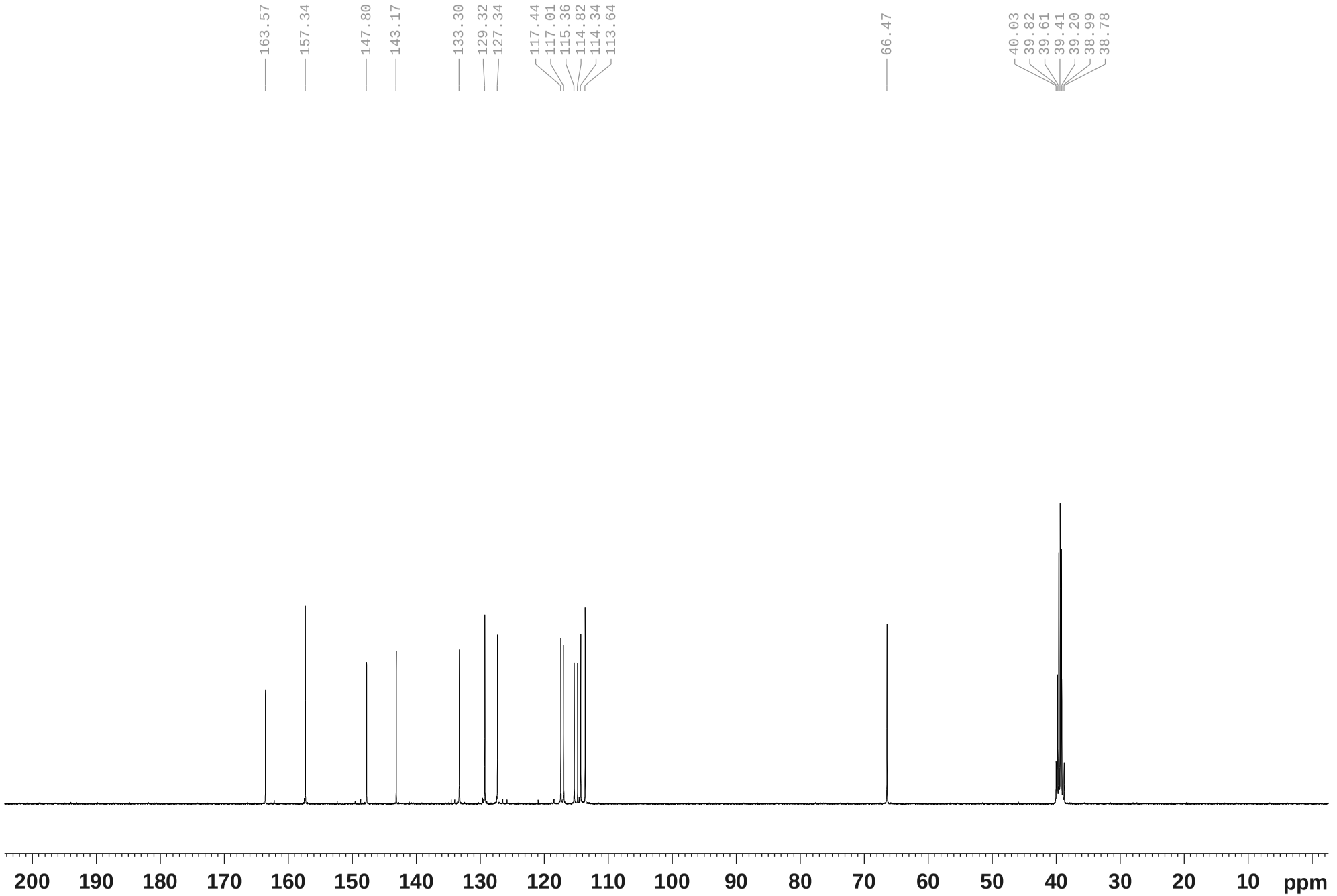


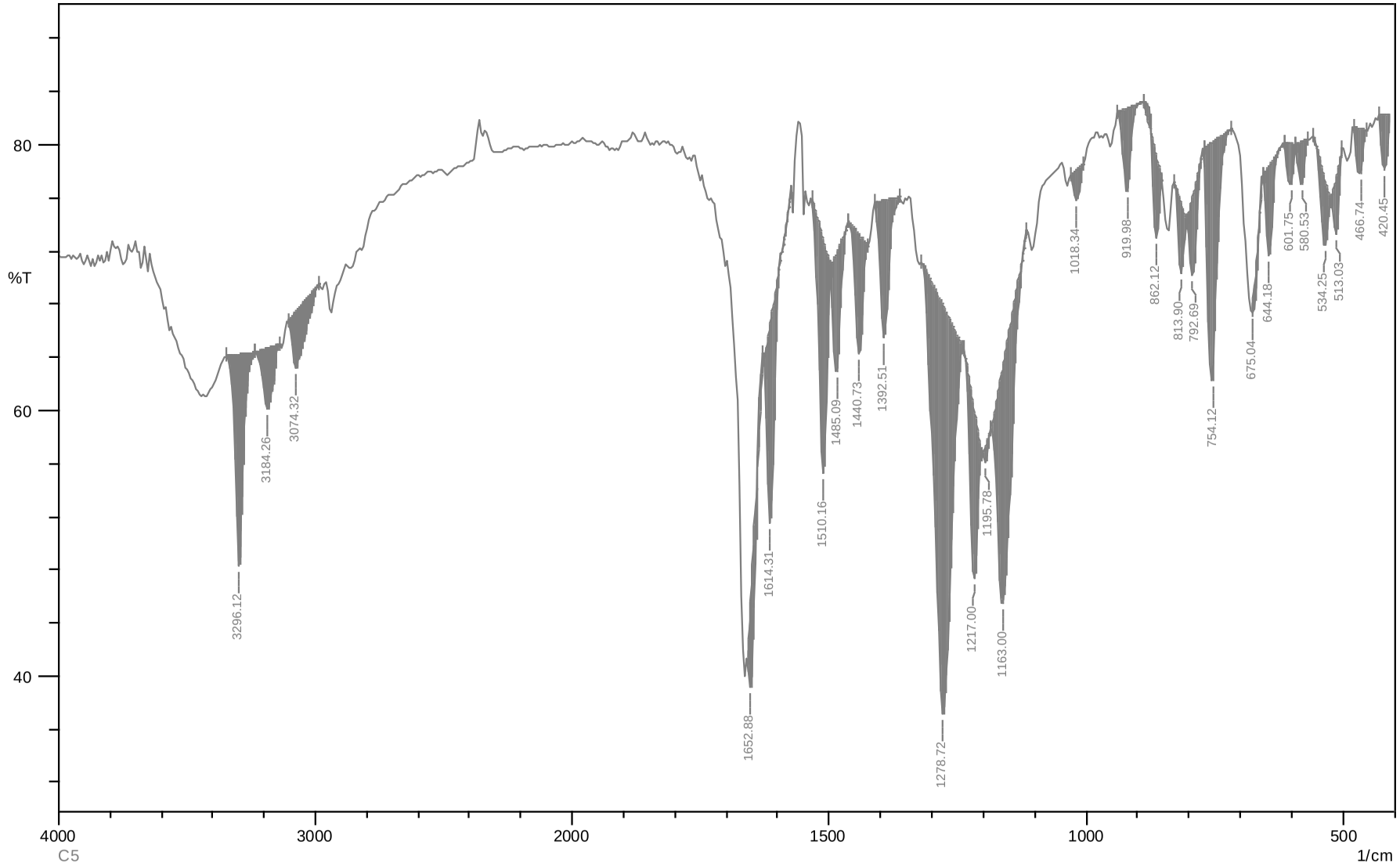

C4
%T
50
75
4000
3000
2000
1500
1000
500
1/cm
3357.84
3296.12
1631.67
1606.59
1506.30
1483.16
1461.94
1427.23
1379.01
1305.72
1278.72
1228.57
1155.28
1130.21
1035.70
1018.34
946.98
865.98
752.19
698.18
632.61
576.68
545.82
511.10
472.53
418.52

PROTON DMSO {C:\Bruker\TOPSPIN\KFUCCP} nmr 10

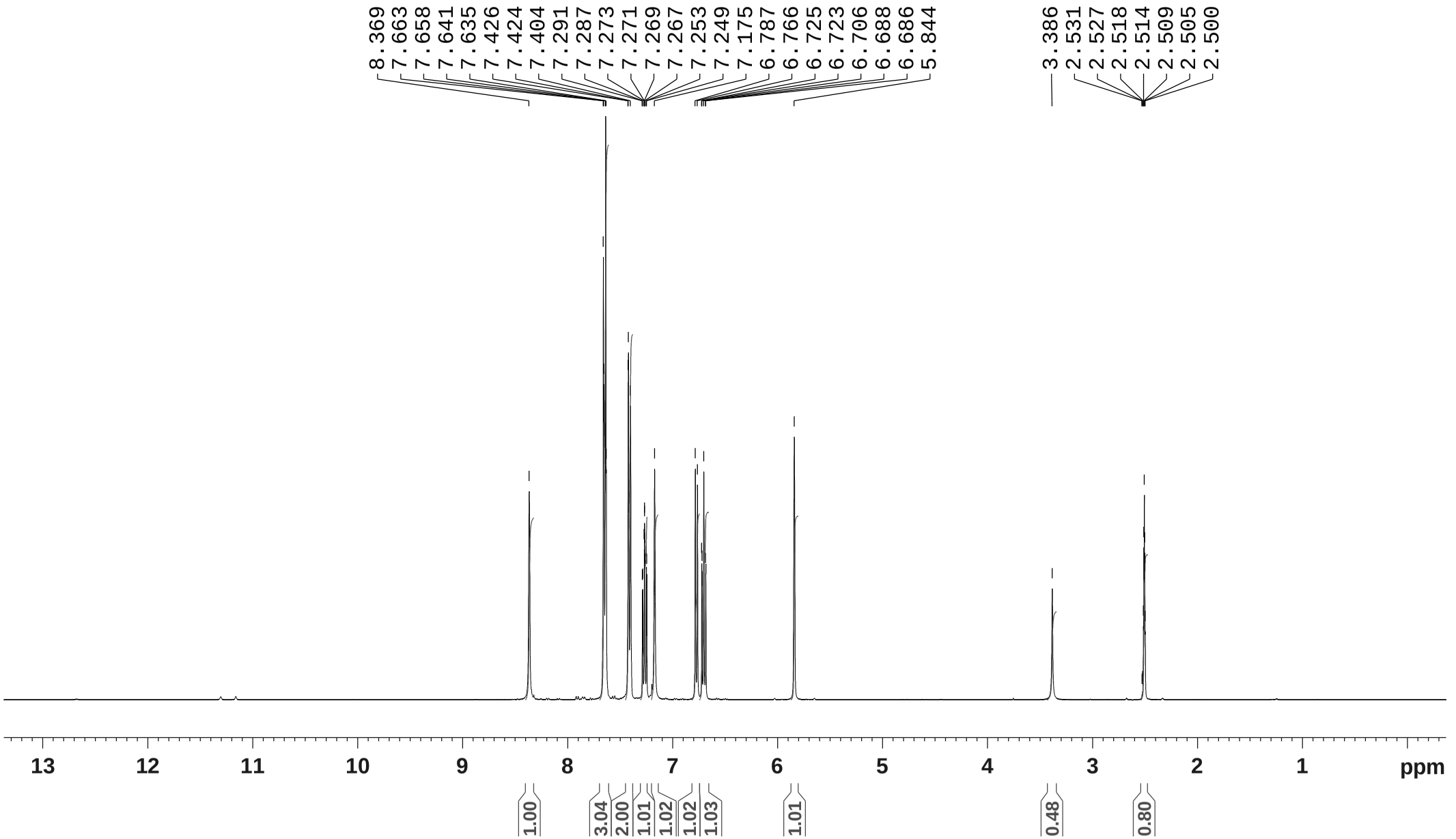


C13CPD DMSO {C:\Bruker\TOPSPIN\KFUCCP} nmr 10

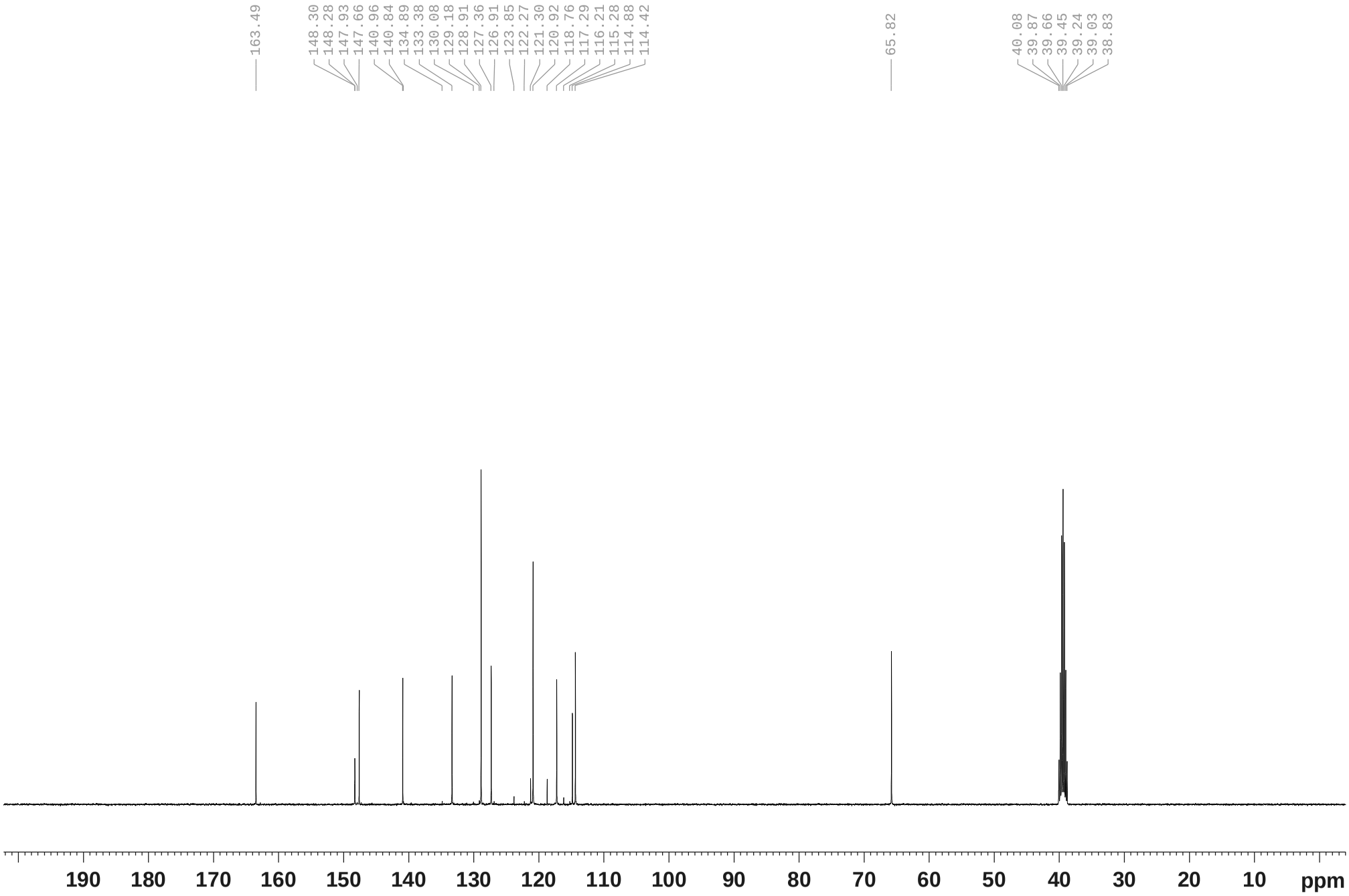


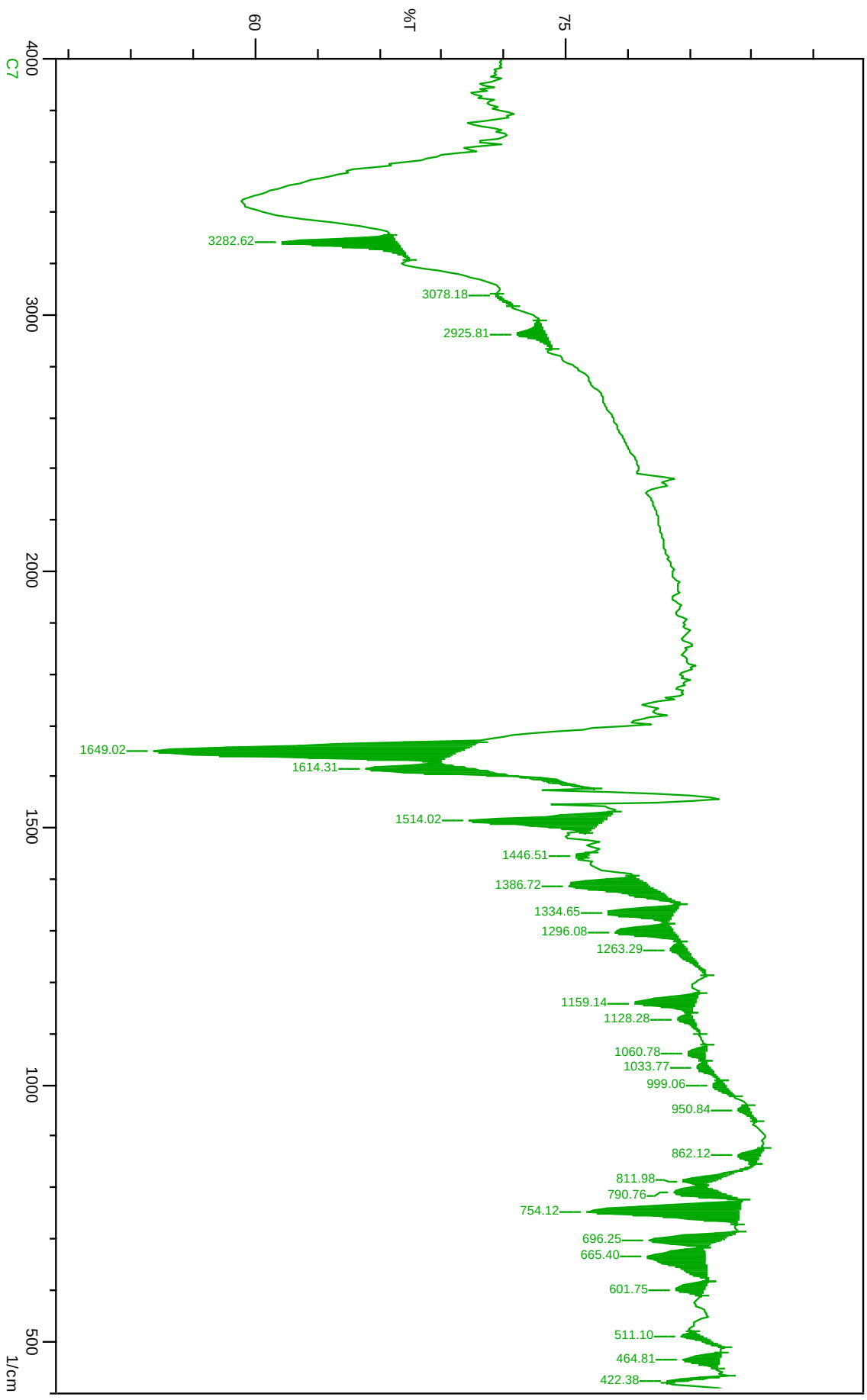

%T
80
60
40
4000
3000
2000
1500
1000
500
1/cm
C5
3296.12
3184.26
3074.32
1652.88
1614.31
1510.16
1485.09
1440.73
1392.51
1278.72
1217.00
1195.78
1163.00
1018.34
919.98
862.12
813.90
792.69
754.12
675.04
644.18
601.75
580.53
534.25
513.03
466.74
420.45

PROTON DMSO {C:\Bruker\TOPSPIN\KFUCCP} nmr 11

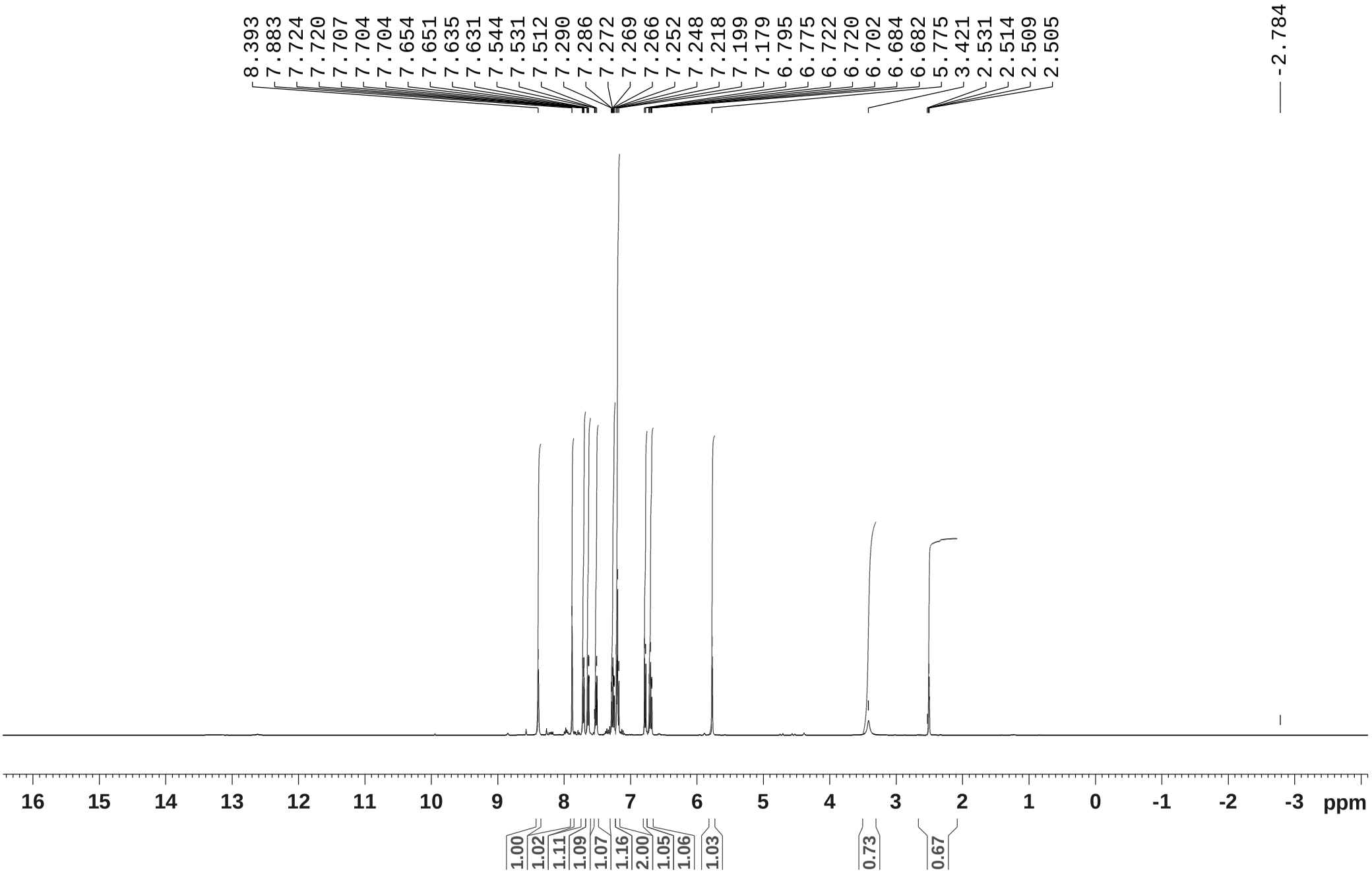


C13CPD DMSO {C:\Bruker\TOPSPIN\KFUCCP} nmr 11

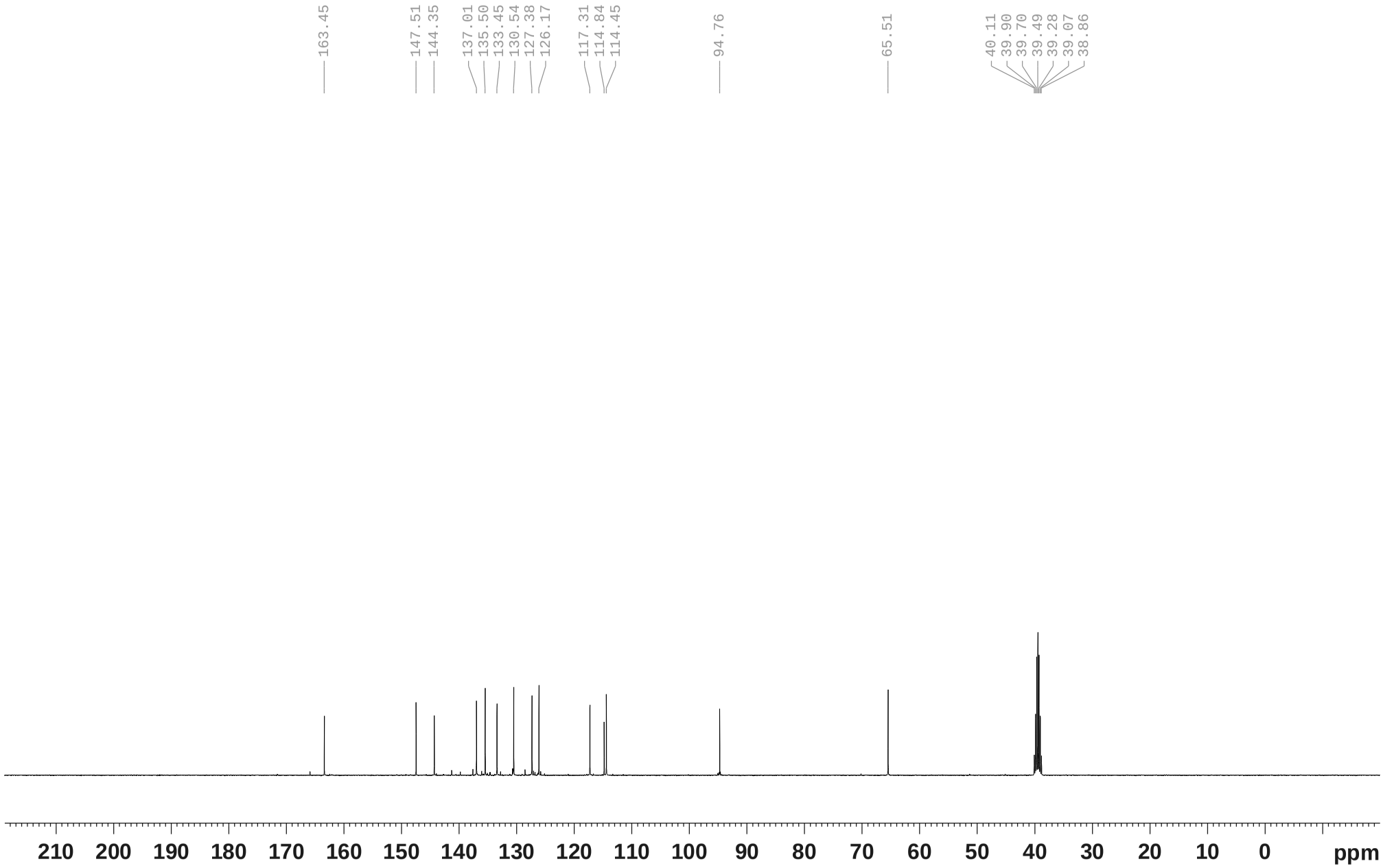


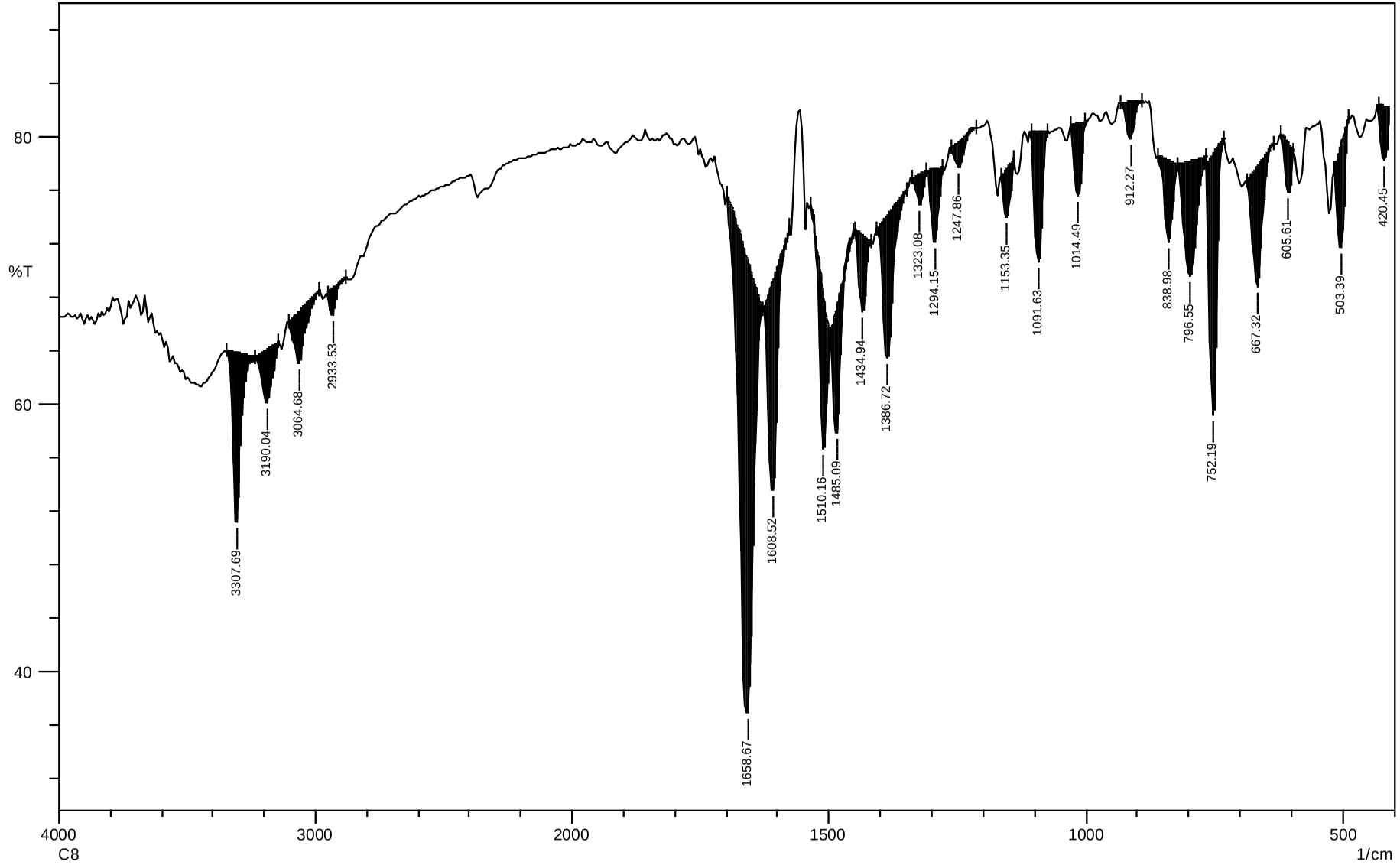

C7
%T
60
75
4000
3000
2000
1500
1000
500
1/cm
3282.62
3078.18
2925.81
1649.02
1614.31
1514.02
1446.51
1386.72
1334.65
1296.08
1263.29
1159.14
1128.28
1060.78
1033.77
999.06
950.84
862.12
811.98
790.76
754.12
696.25
665.40
601.75
511.10
464.81
422.38

PROTON DMSO {C:\Bruker\TOPSPIN\KFUCCP} nmr 16

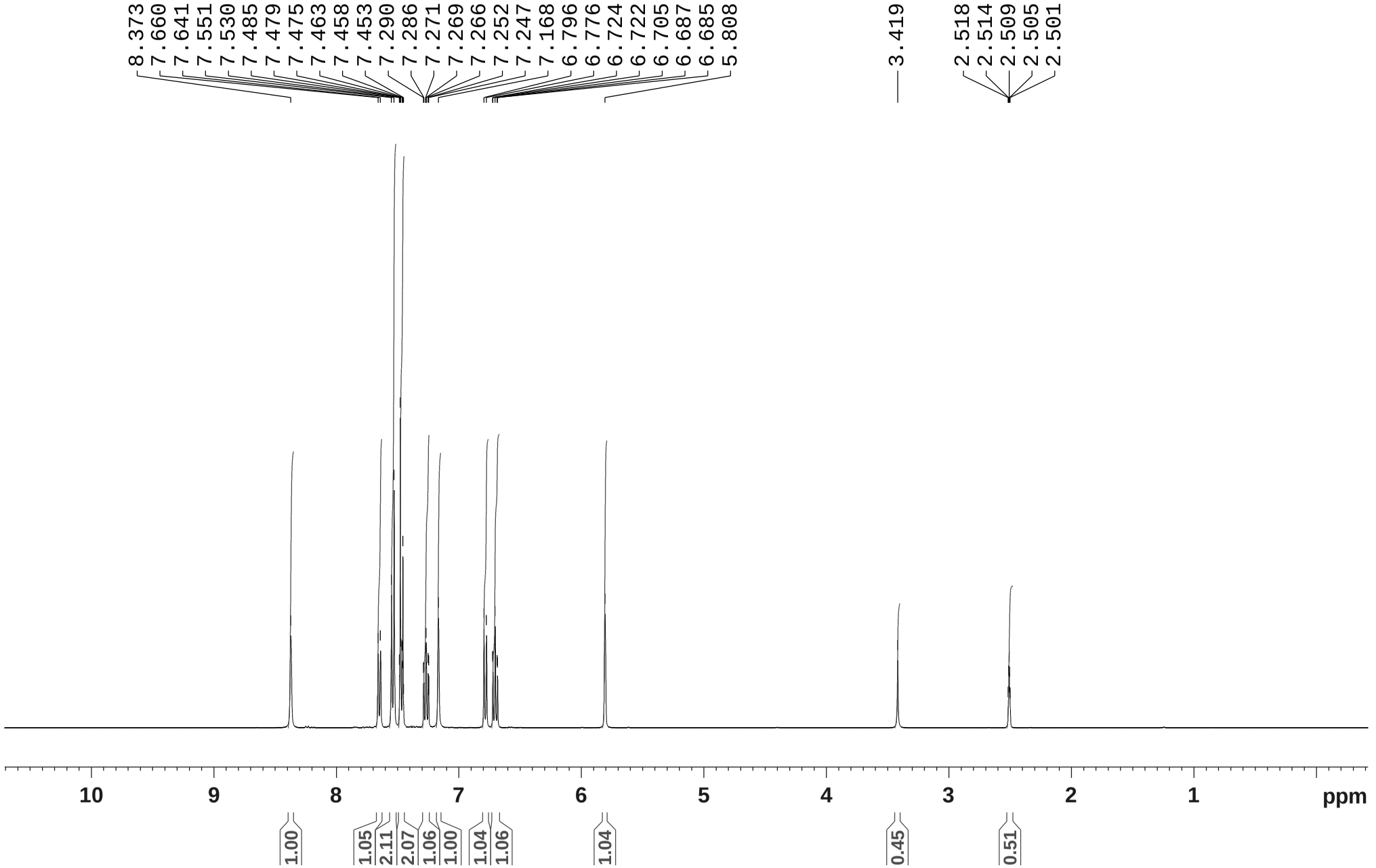


C13CPD DMSO {C:\Bruker\TOPSPIN\KFUCCP} nmr 16

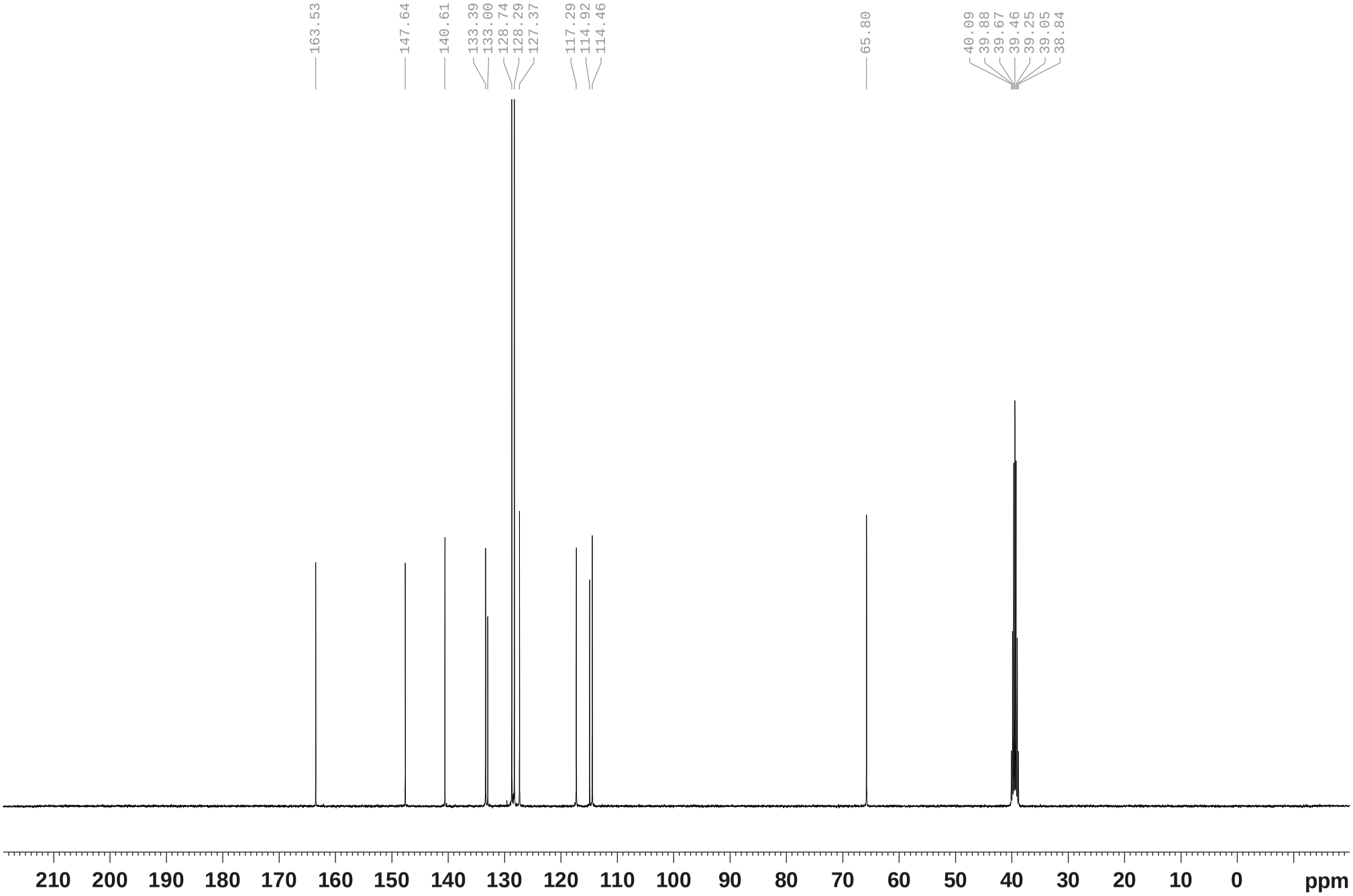



80
60
40
%T
3307.69
3190.04
3064.68
2933.53
1658.67
1608.52
1510.16
1485.09
1434.94
1386.72
1323.08
1294.15
1247.86
1153.35
1091.63
1014.49
912.27
838.98
796.55
752.19
667.32
605.61
503.39
420.45
4000
3000
2000
1500
1000
500
C8
1/cm

PROTON DMSO {C:\Bruker\TOPSPIN\KFUCCP} nmr 8

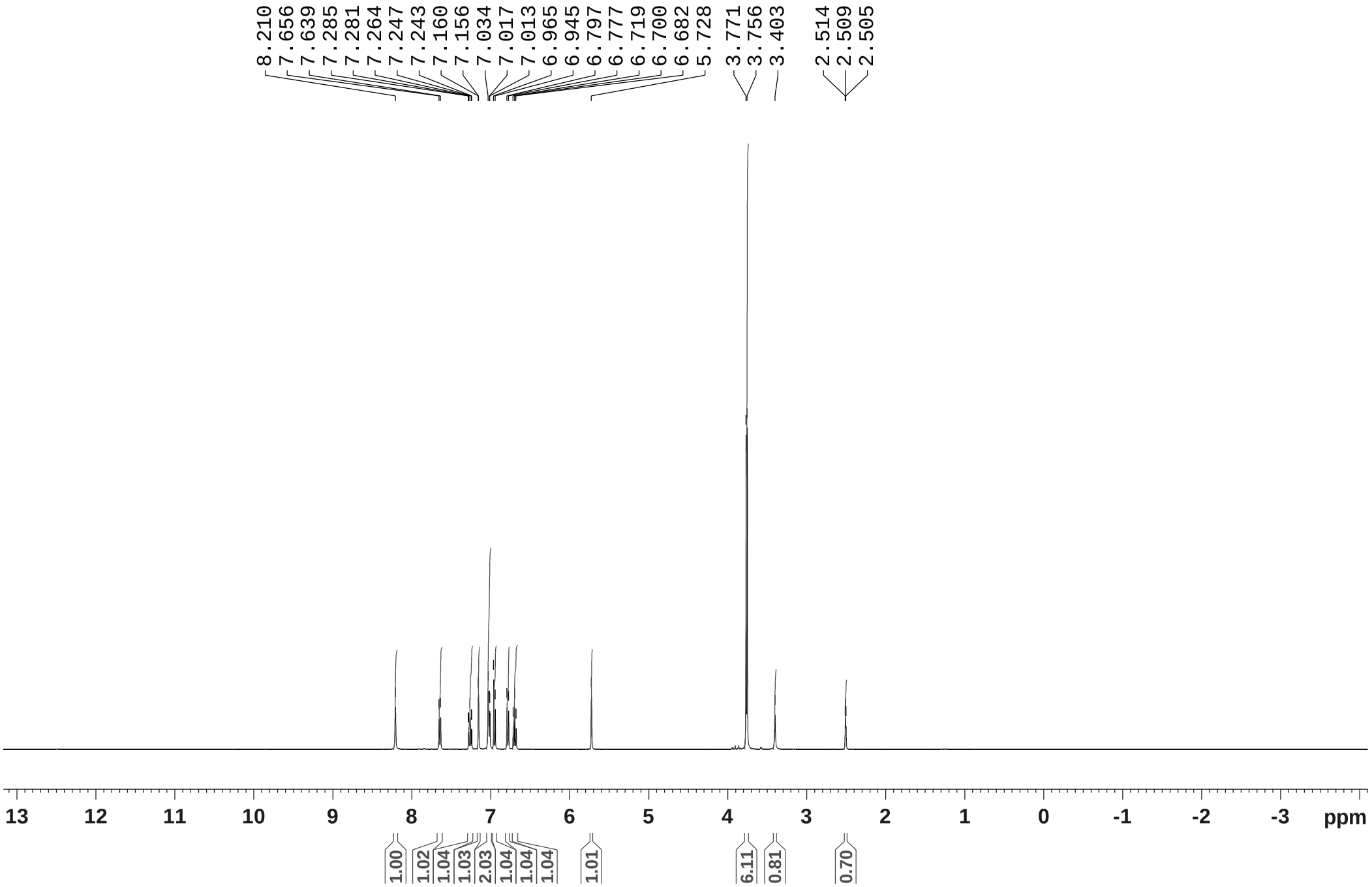


C13CPD DMSO {C:\Bruker\TOPSPIN\KFUCCP} nmr 8

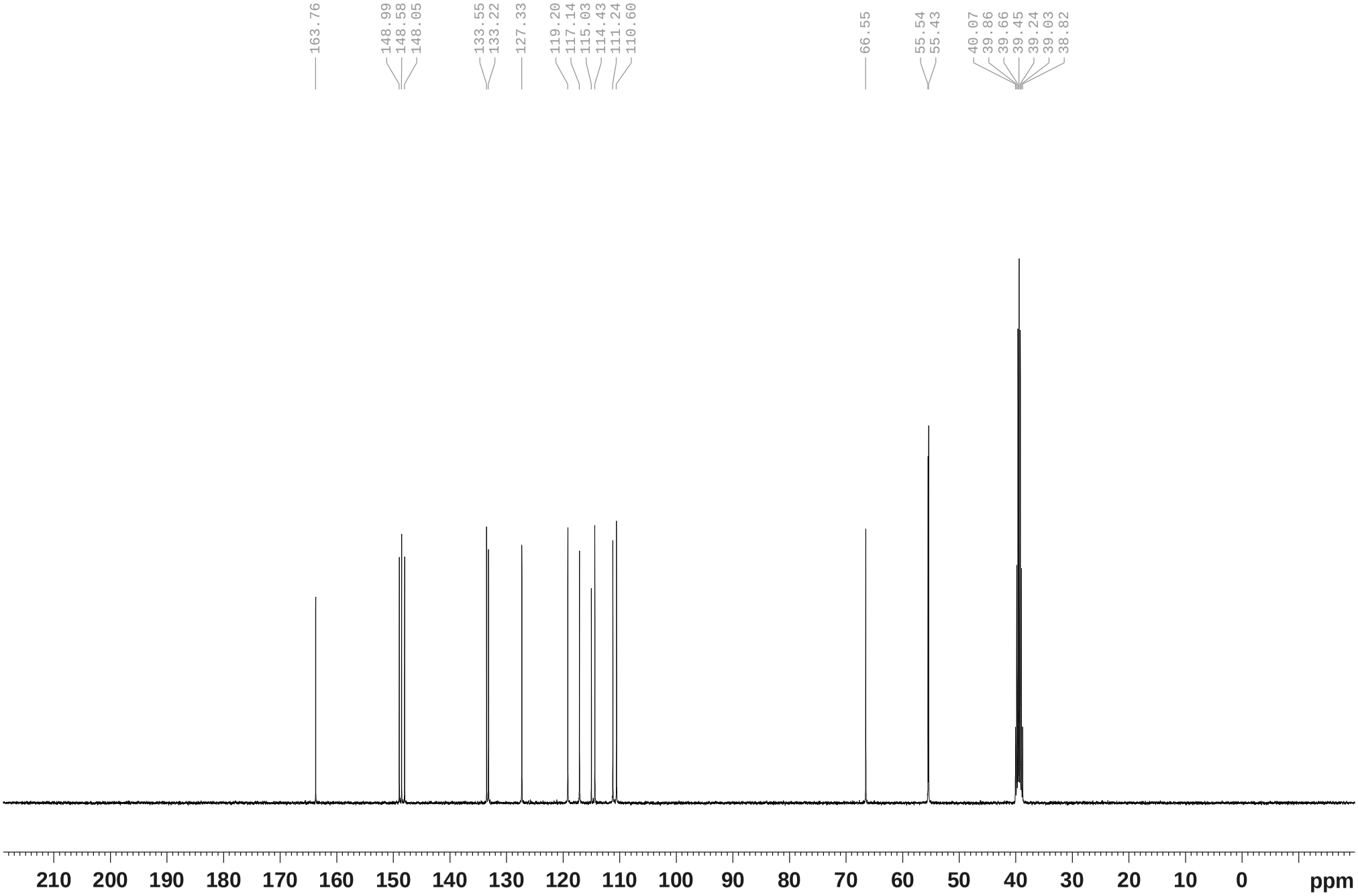


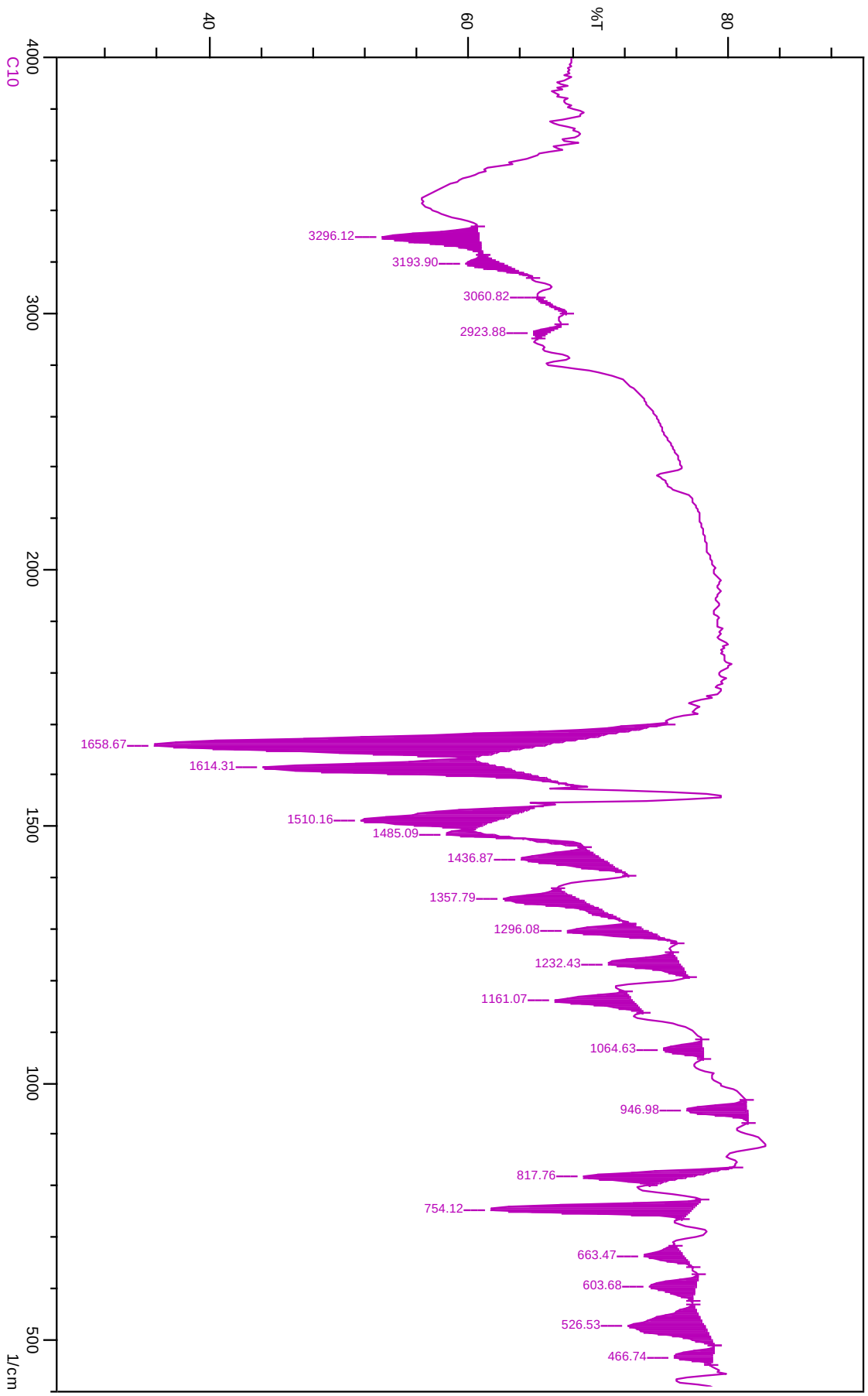
C9
%T
50
75
4000
3000
2000
1500
1000
500
1/cm
3330.84
3299.98
3006.82
2933.53
1660.60
1610.45
1510.16
1488.94
1458.08
1369.37
1309.58
1263.29
1232.43
1139.85
1024.13
887.19
854.41
810.05
757.97
702.04
622.96
574.75
514.96
470.60
418.52

PROTON DMSO {C:\Bruker\TOPSPIN\KFUCCP} nmr 7

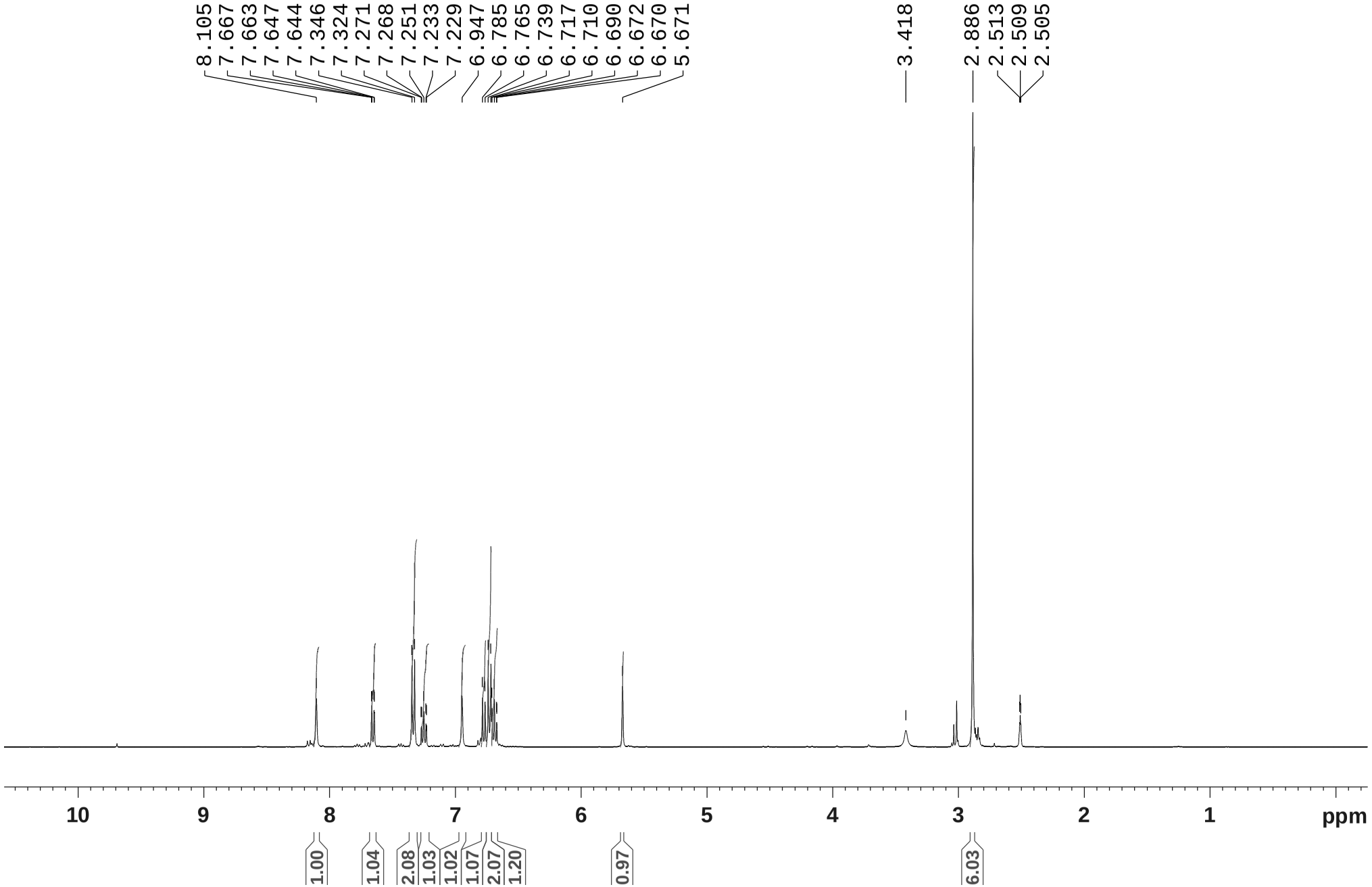


C13CPD DMSO {C:\Bruker\TOPSPIN\KFUCCP} nmr 7

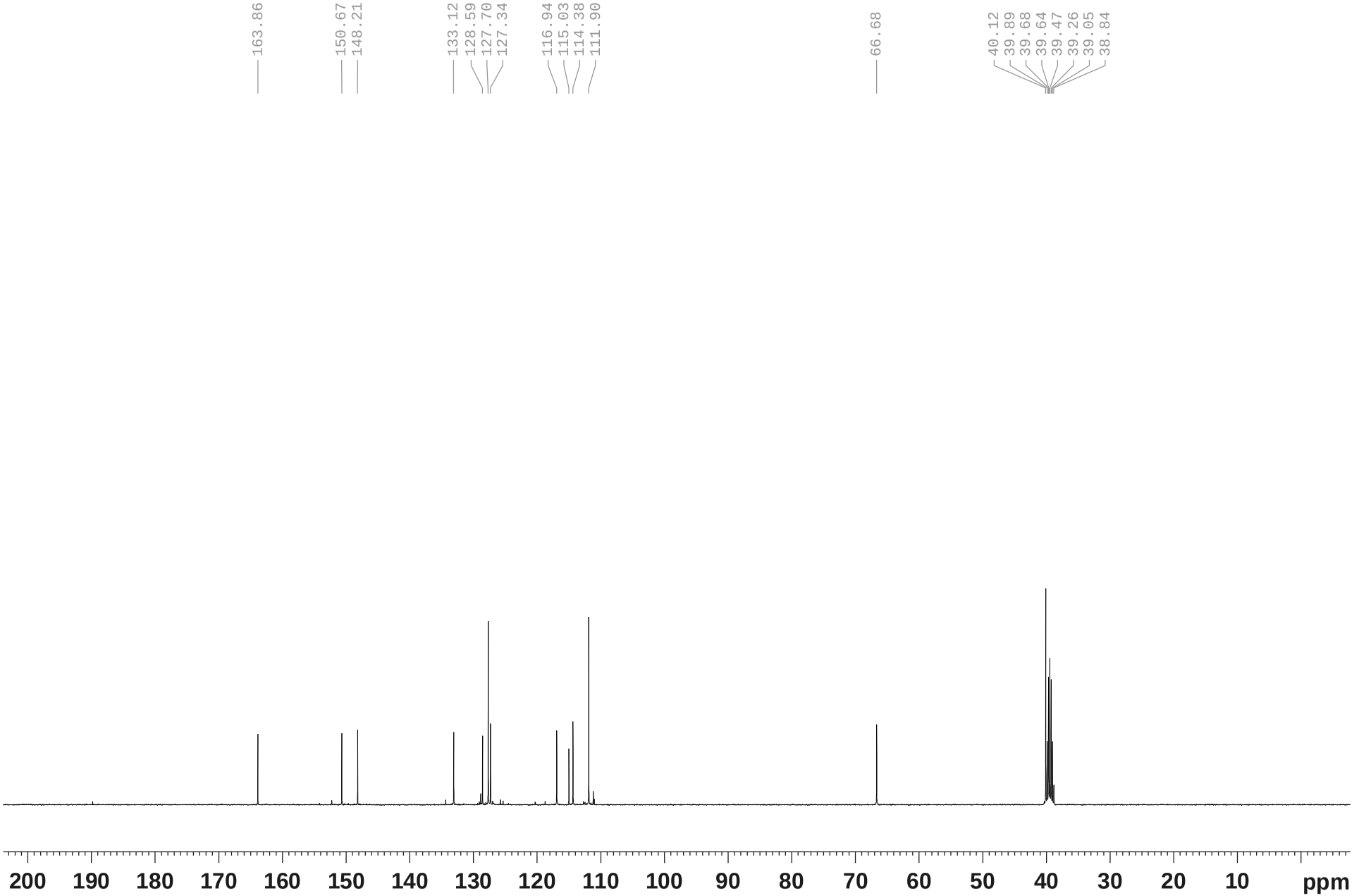


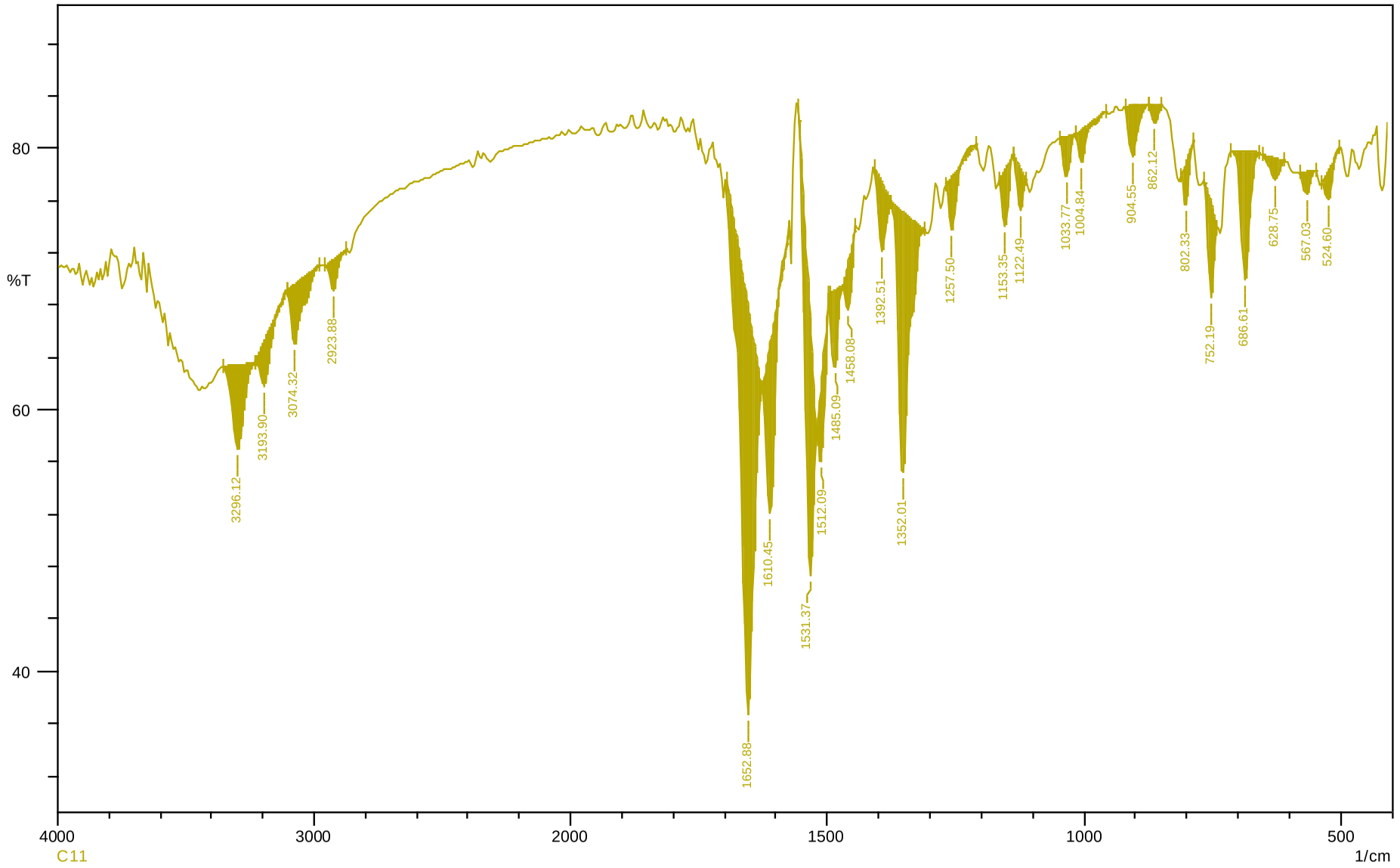

%T
40
60
80
4000
3000
2000
1500
1000
500
1/cm
C10
3296.12
3193.90
3060.82
2923.88
1658.67
1614.31
1510.16
1485.09
1436.87
1357.79
1296.08
1232.43
1161.07
1064.63
946.98
817.76
754.12
663.47
603.68
526.53
466.74

PROTON DMSO {C:\Bruker\TOPSPIN\KFUCCP} nmr 14

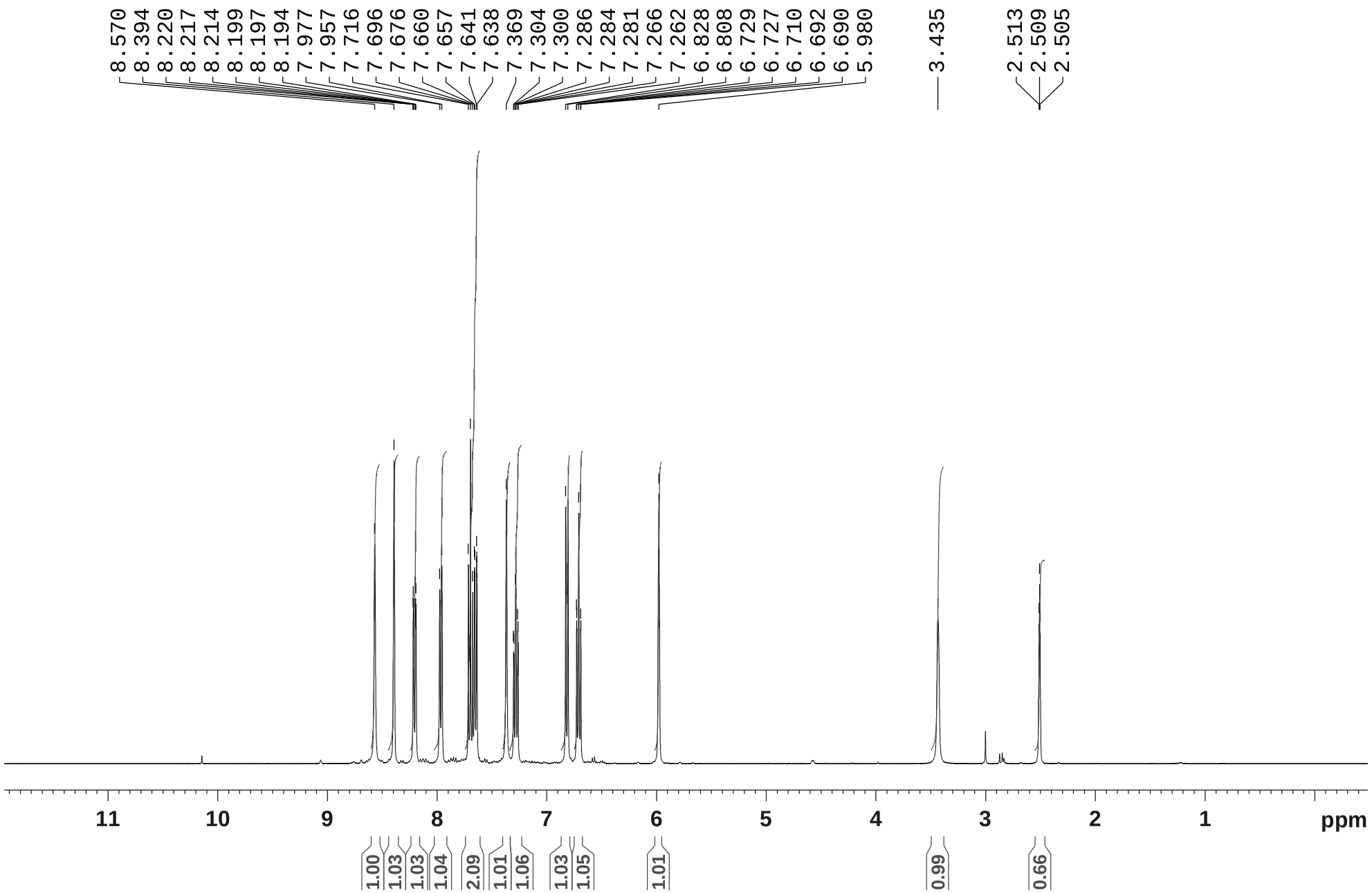


C13CPD DMSO {C:\Bruker\TOPSPIN\KFUCCP} nmr 14

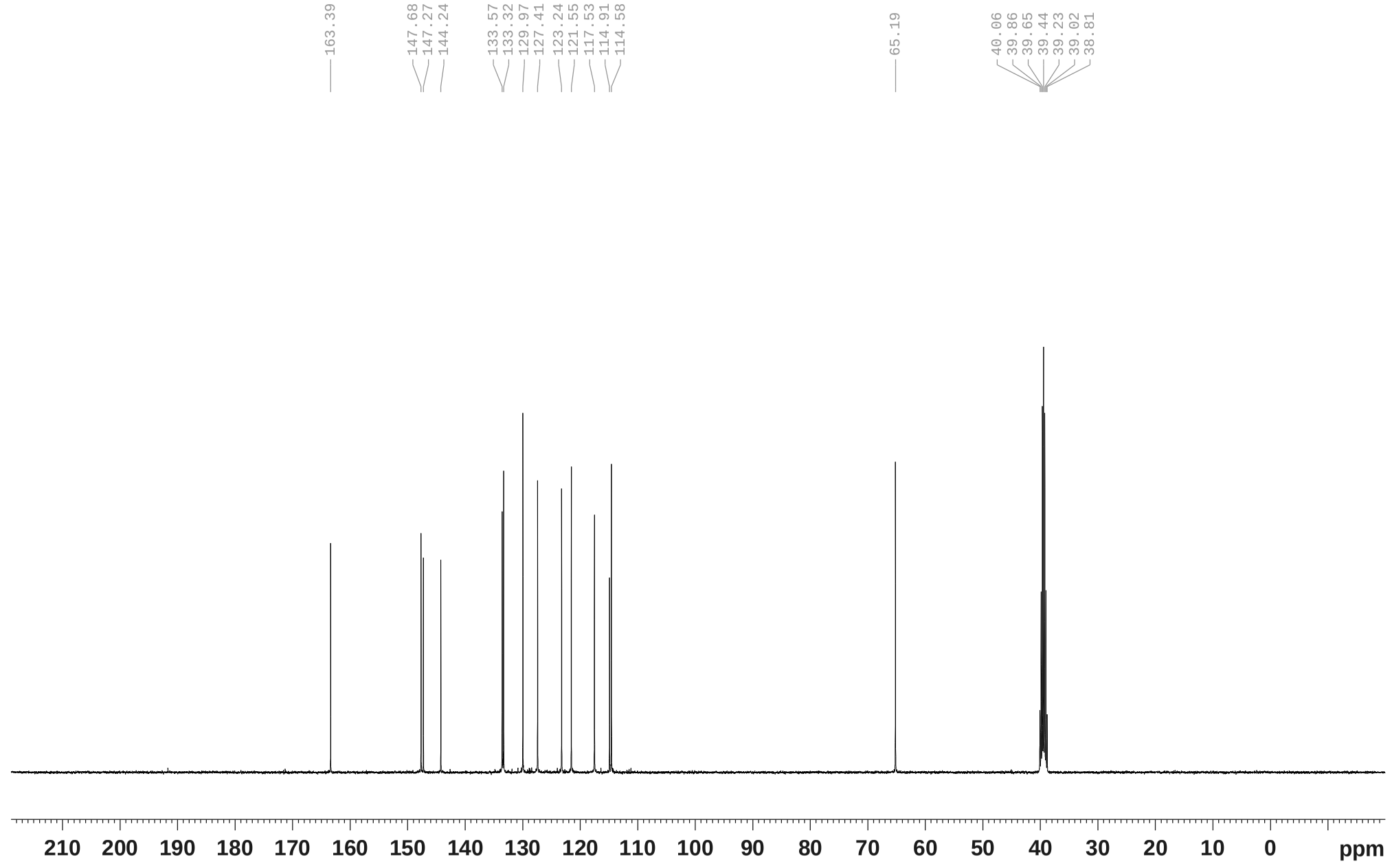



80
60
40
%T
3296.12
3193.90
3074.32
2923.88
1652.88
1610.45
1531.37
1512.09
1485.09
1458.08
1392.51
1352.01
1257.50
1153.35
1122.49
1033.77
1004.84
904.55
862.12
802.33
752.19
686.61
628.75
567.03
524.60
4000
3000
2000
1500
1000
500
1/cm
C11

PROTON DMSO {C:\Bruker\TOPSPIN\KFUCCP} nmr 15

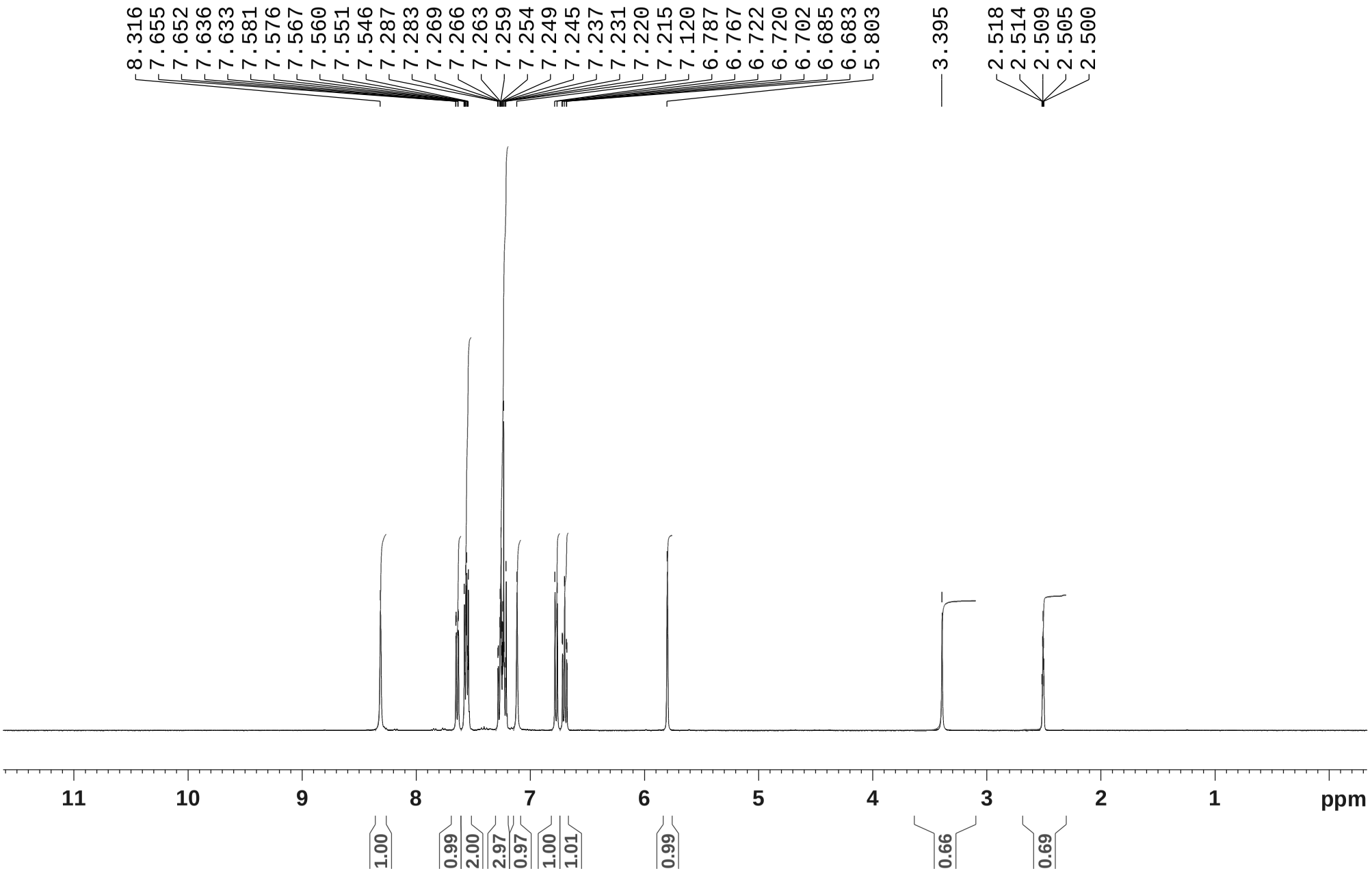


C13CPD DMSO {C:\Bruker\TOPSPIN\KFUCCP} nmr 15

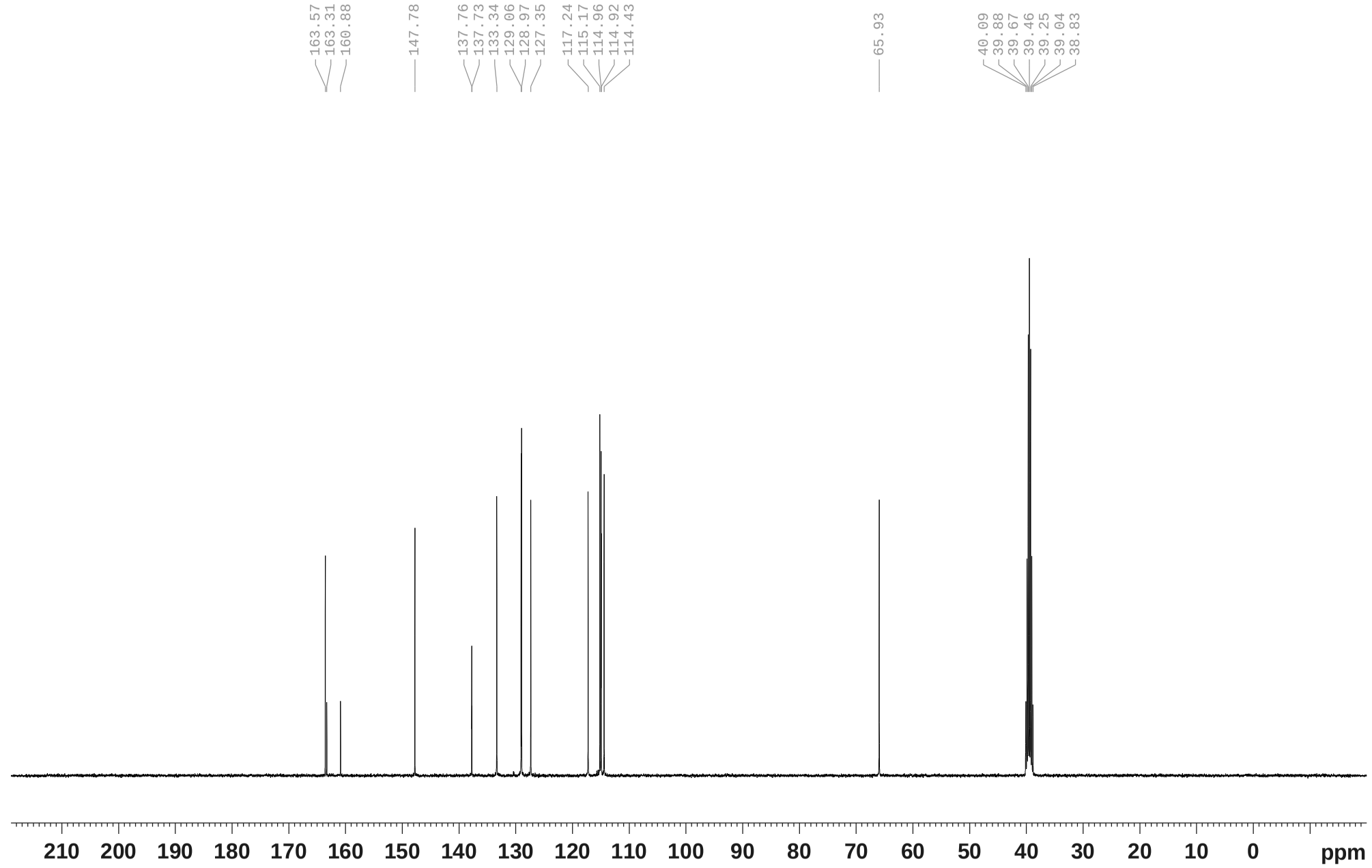


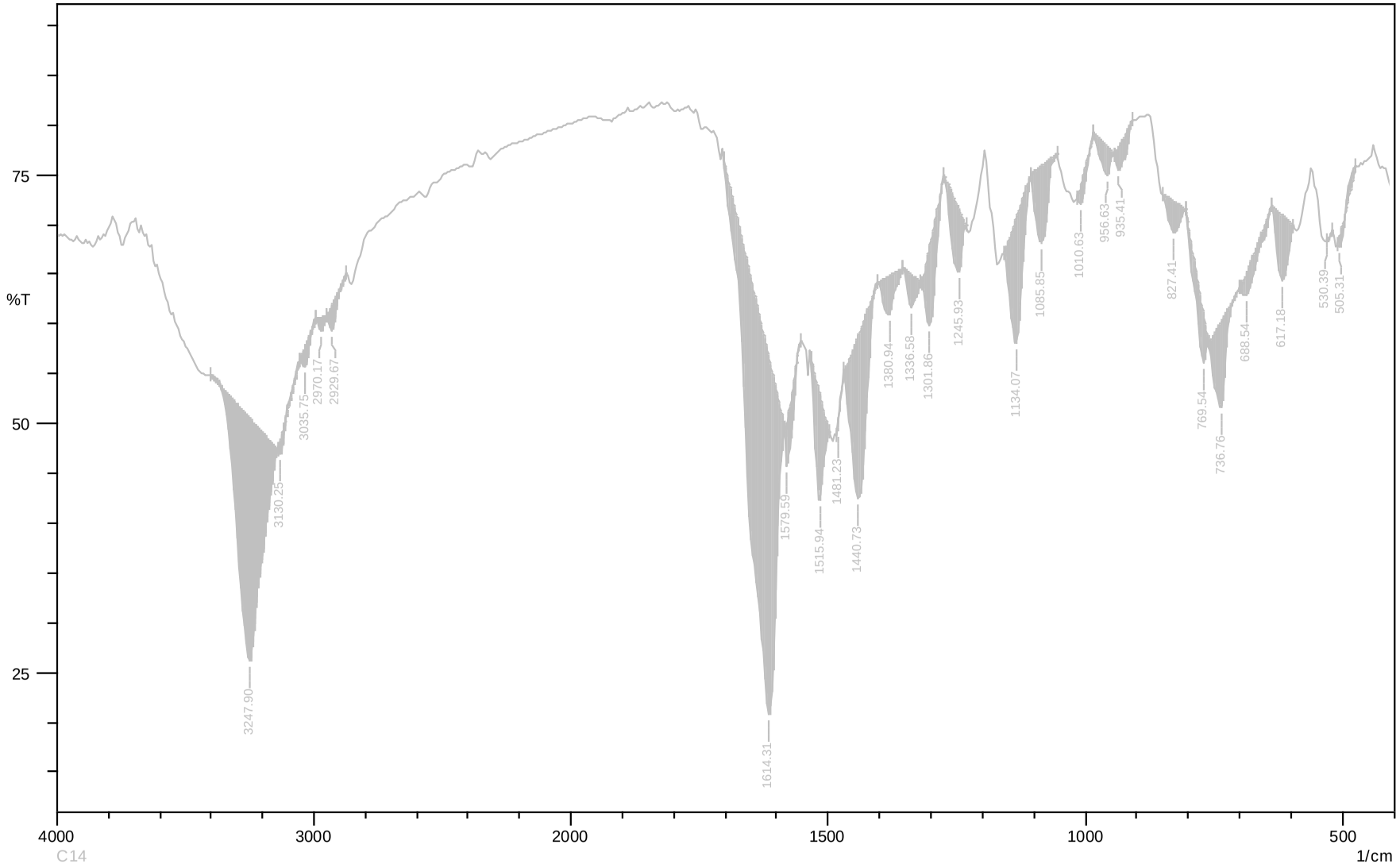
%T
25
50
75
4000
3000
2000
1500
1000
500
1/cm
C12
3299.98
3184.26
3130.25
3066.61
2931.60
1658.67
1610.45
1508.23
1485.09
1436.87
1388.65
1296.08
1234.36
1159.14
1097.42
919.98
838.98
806.19
750.26
675.04
609.46
520.74
420.45

PROTON DMSO {C:\Bruker\TOPSPIN\KFUCCP} nmr 9

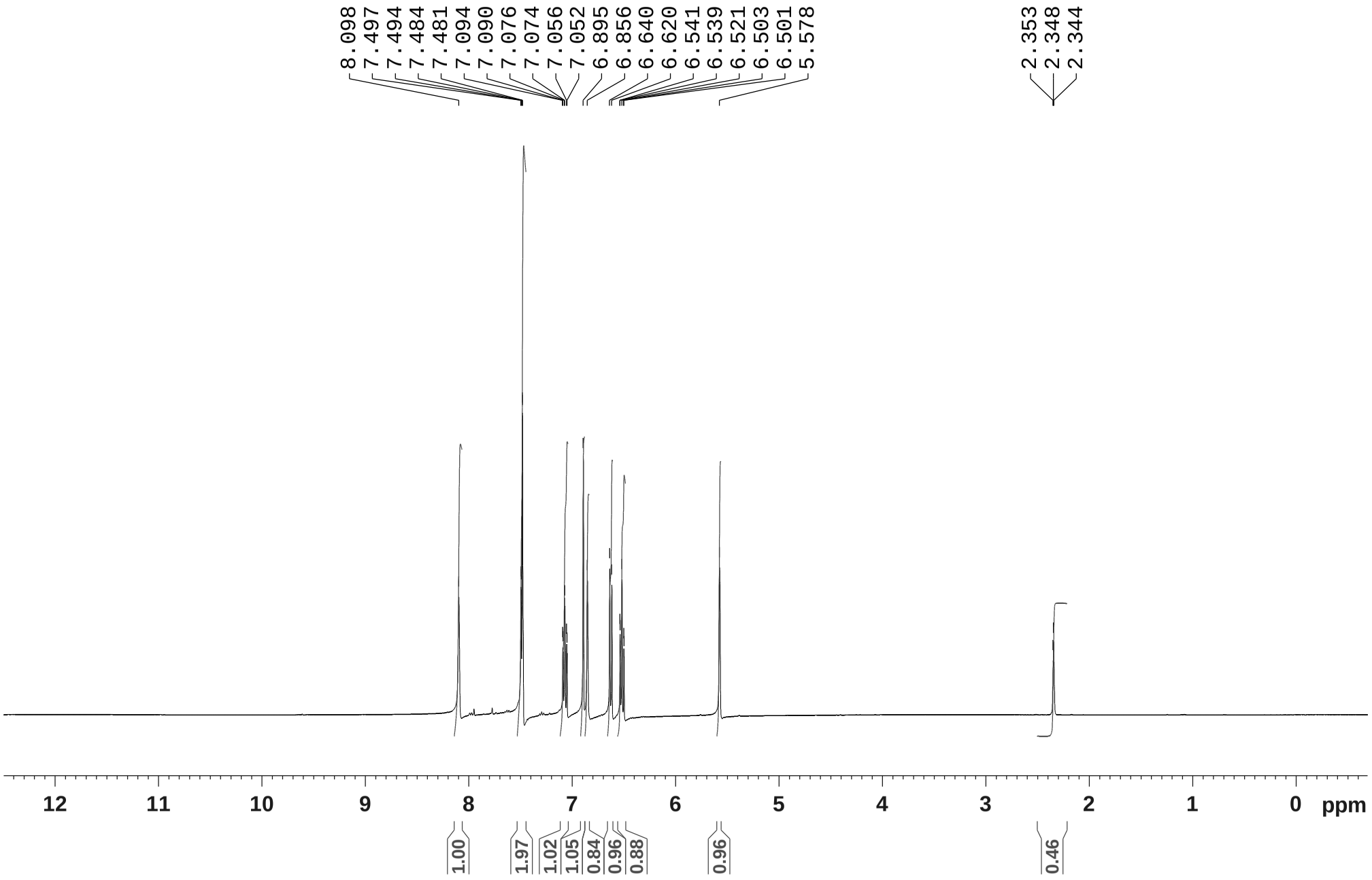


C13CPD DMSO {C:\Bruker\TOPSPIN\KFUCCP} nmr 9

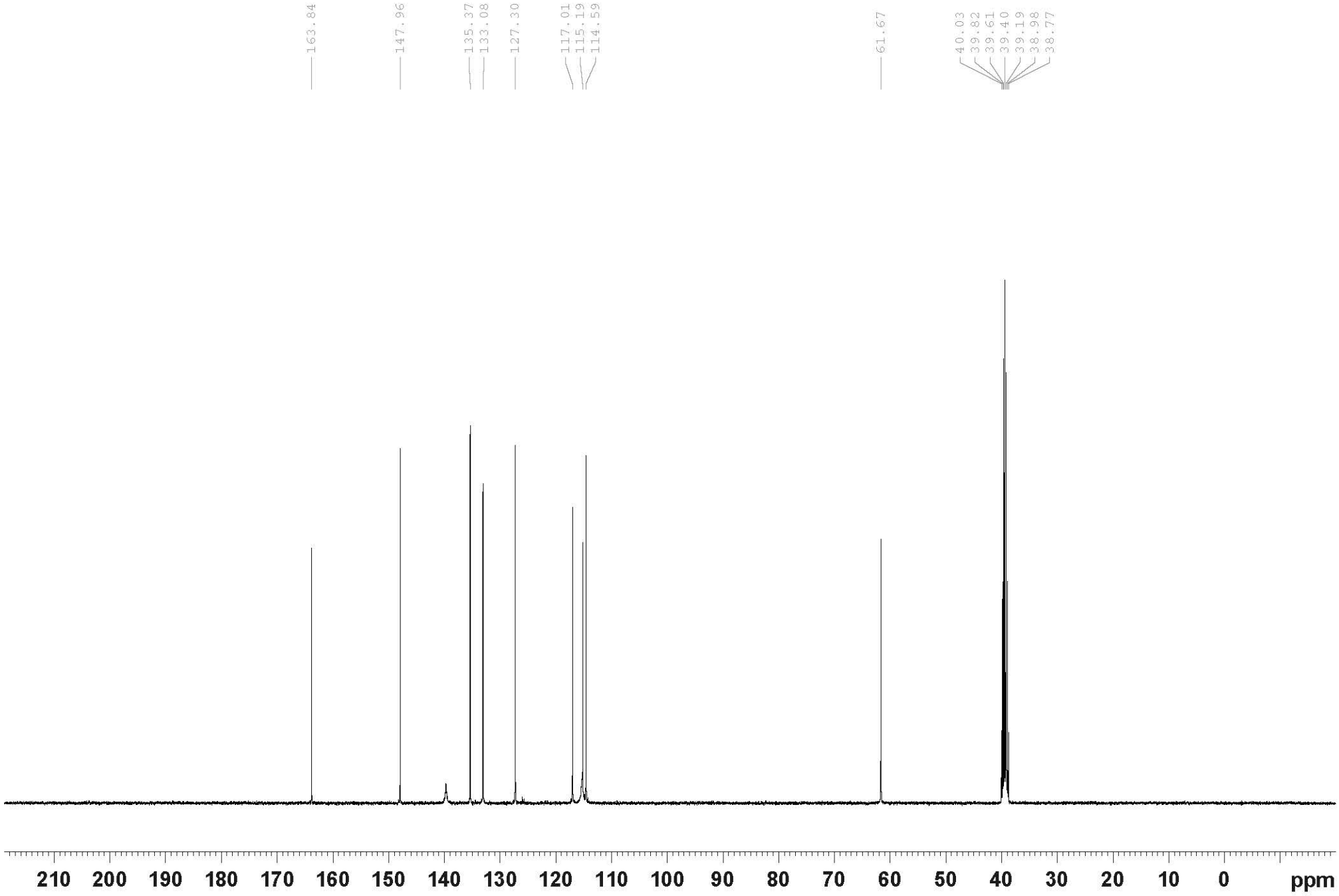


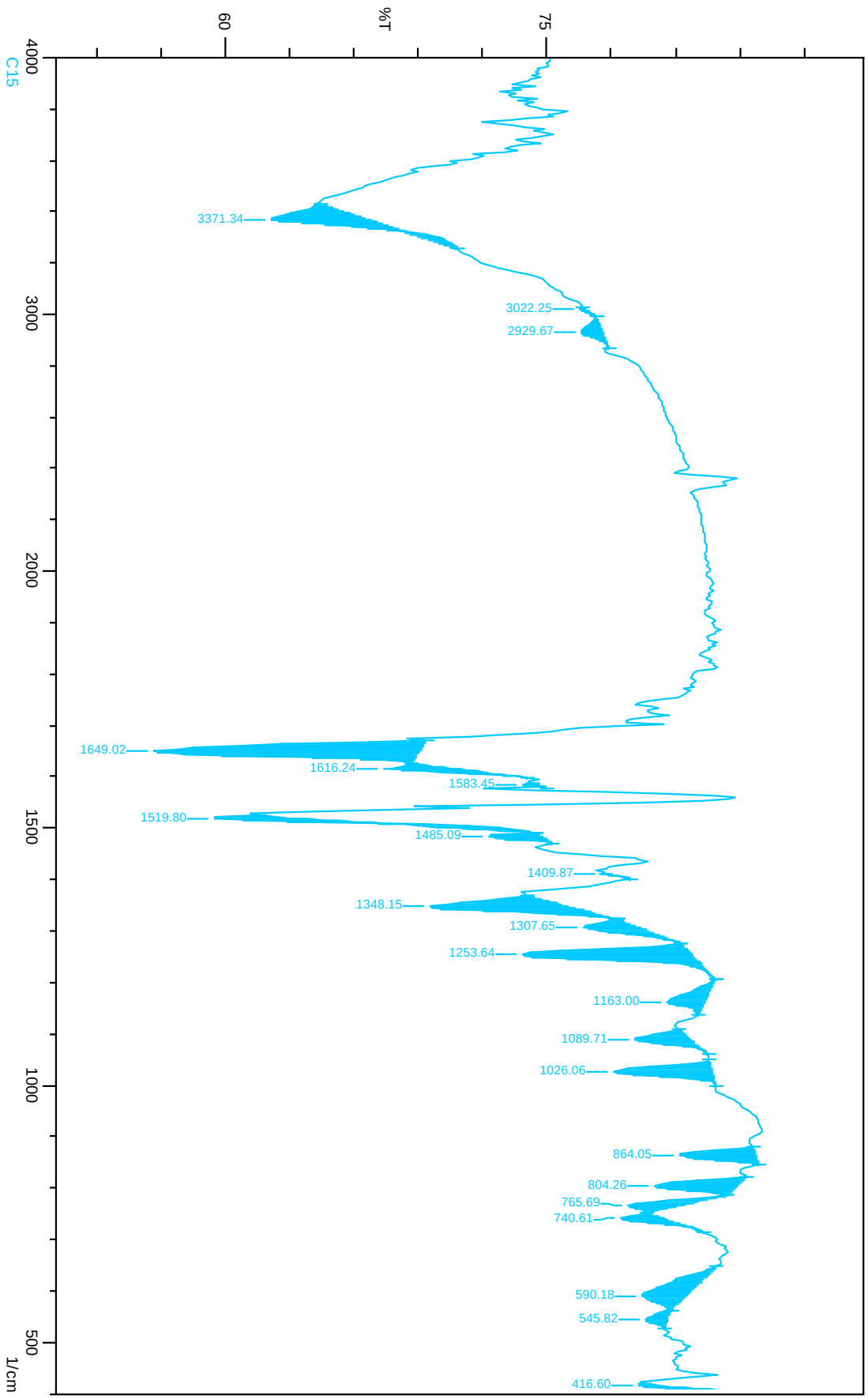

%T
75
50
25
4000
3000
2000
1500
1000
500
1/cm
C14
3247.90
3130.25
3035.75
2970.17
2929.67
1614.31
1579.59
1515.94
1481.23
1440.73
1380.94
1336.58
1301.86
1245.93
1134.07
1085.85
1010.63
956.63
935.41
827.41
769.54
736.76
688.54
617.18
530.39
505.31

PROTON DMSO {C:\Bruker\TOPSPIN\KFUCCP} nmr 3

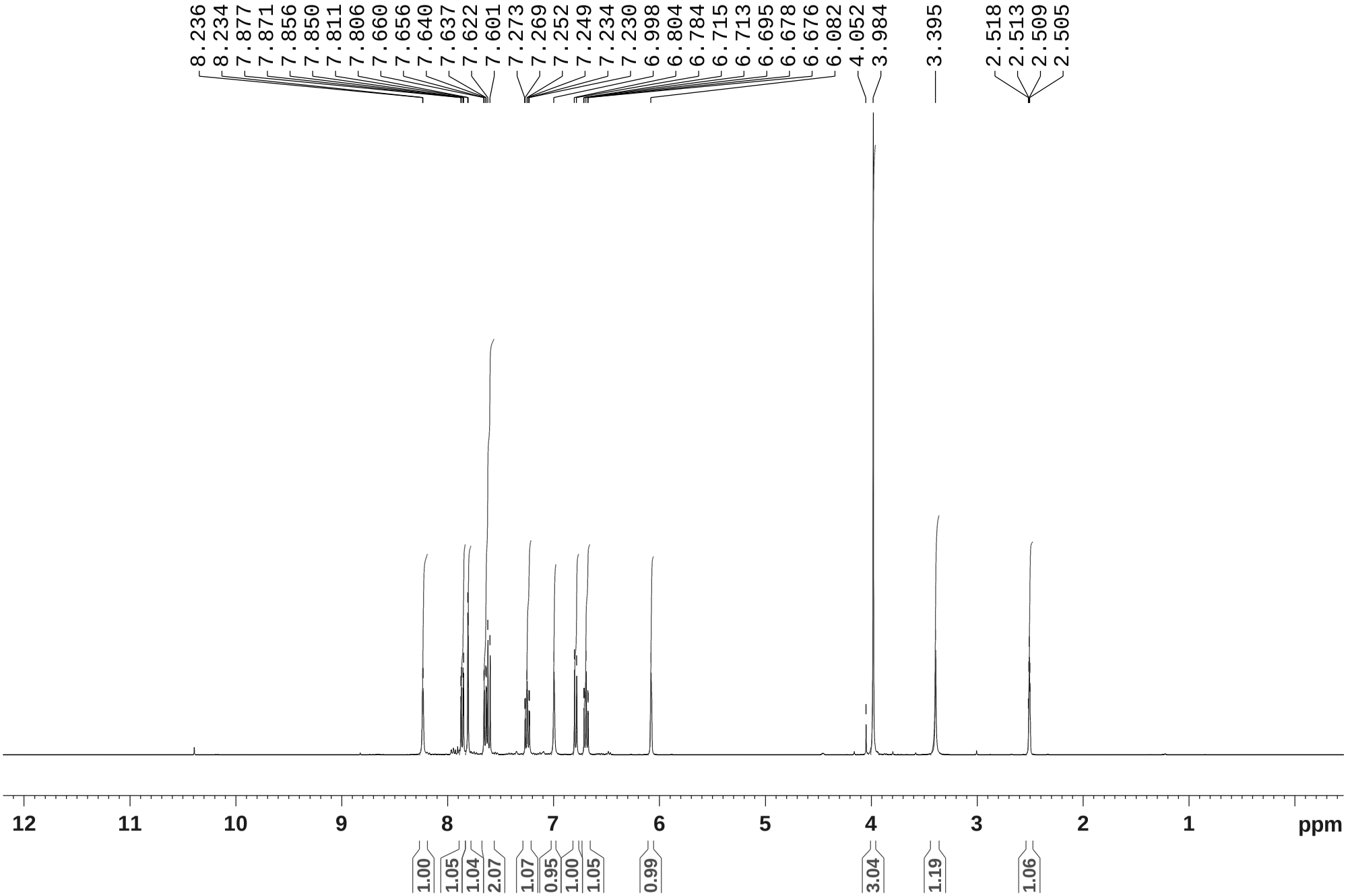


C13CPD DMSO {C:\Bruker\TOPSPIN\KFUCCP} nmr 3

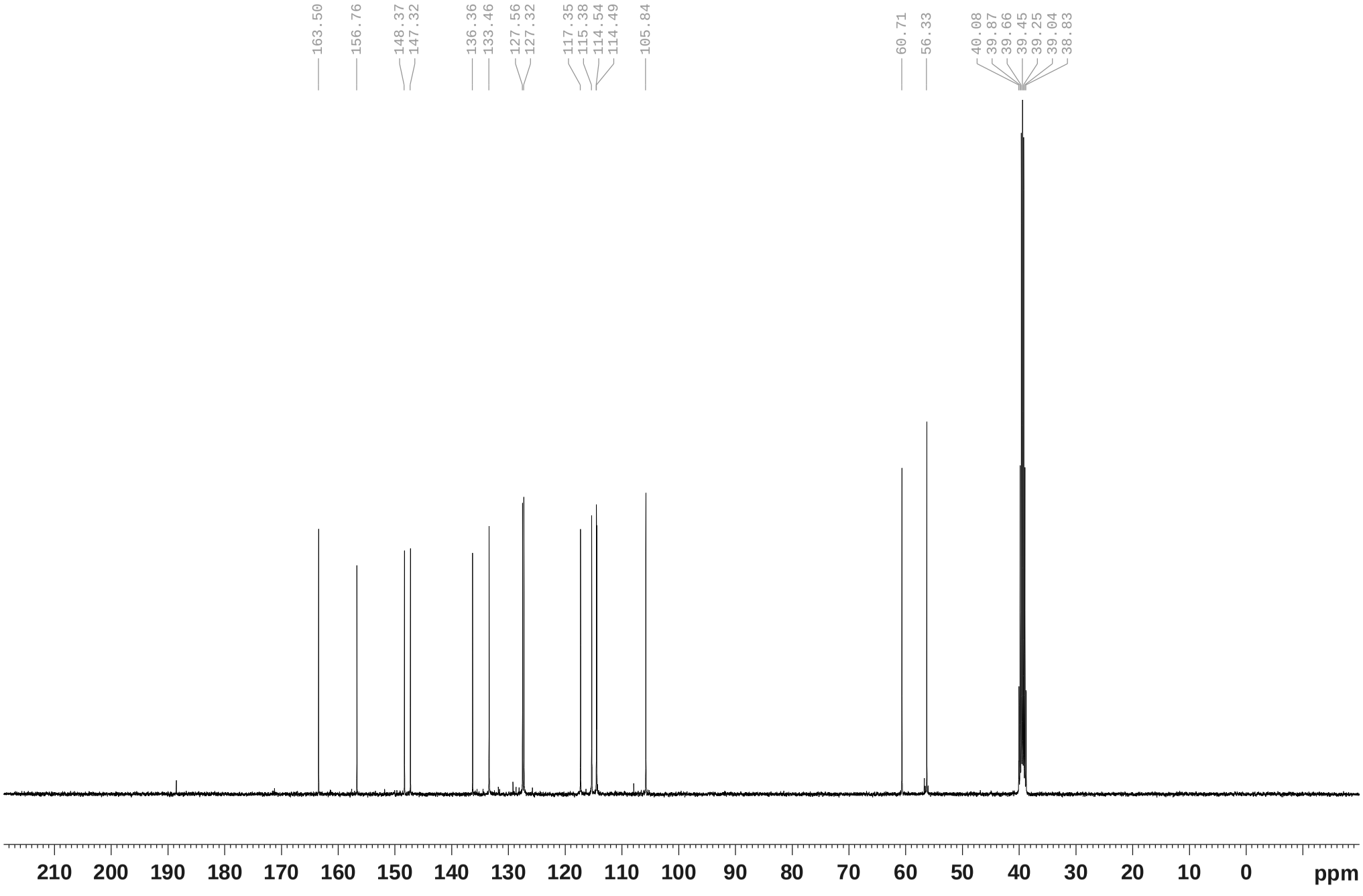


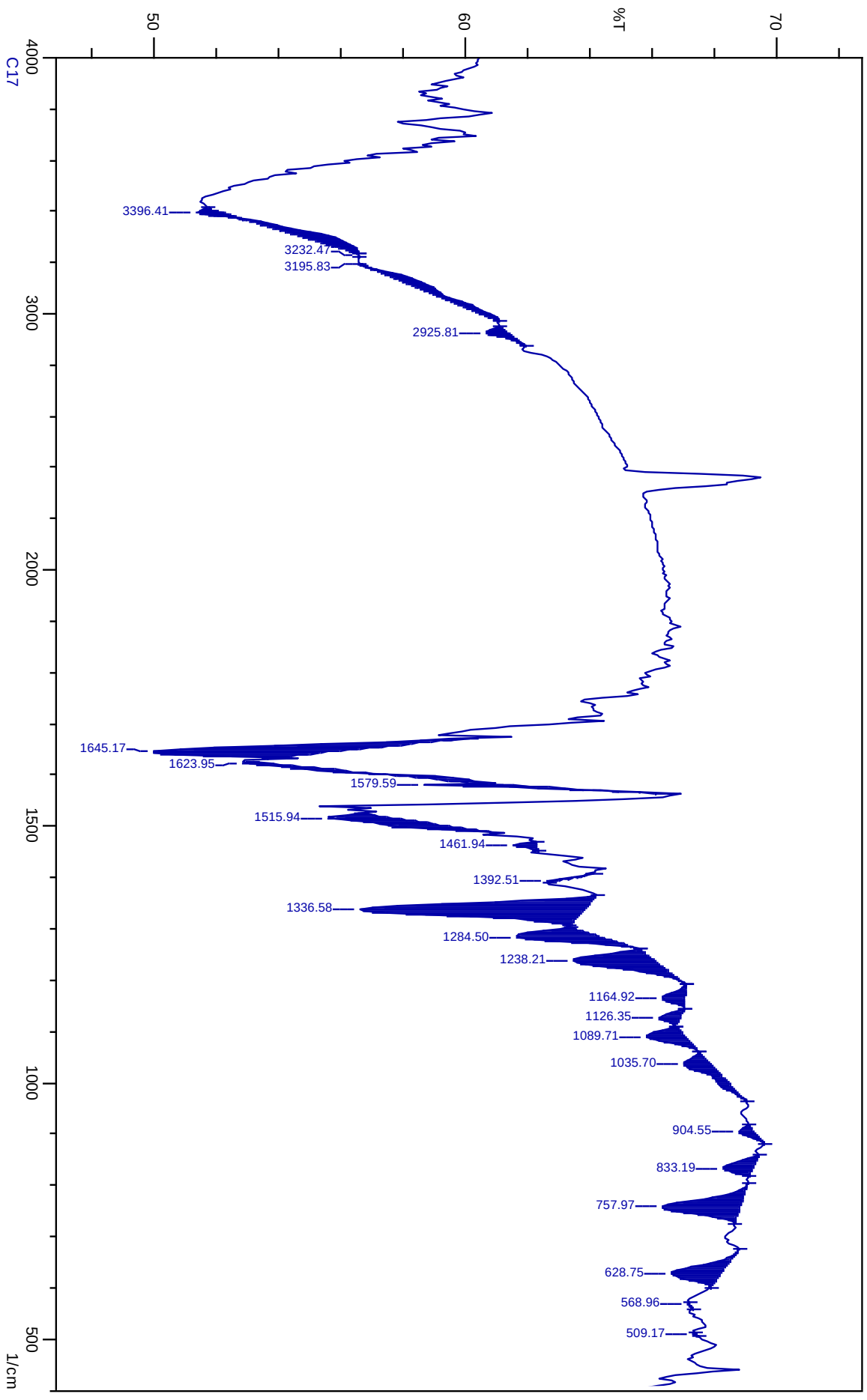

C15
60
%T
75
4000
3000
2000
1500
1000
500
1/cm
3371.34
3022.25
2929.67
1649.02
1616.24
1583.45
1519.80
1485.09
1409.87
1348.15
1307.65
1253.64
1163.00
1089.71
1026.06
864.05
804.26
765.69
740.61
590.18
545.82
416.60

PROTON DMSO {C:\Bruker\TOPSPIN\KFUCCP} nmr 4

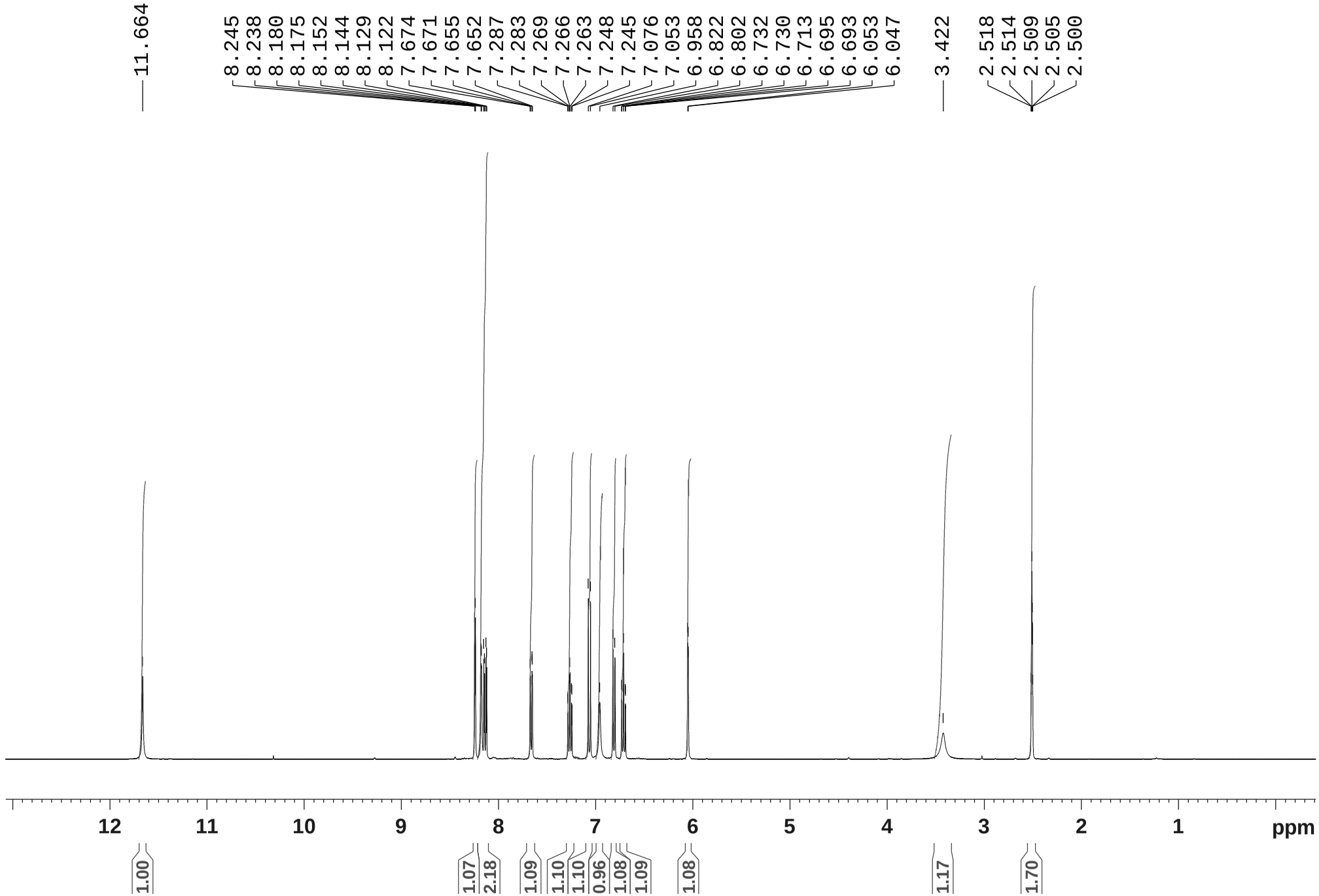


C13CPD DMSO {C:\Bruker\TOPSPIN\KFUCCP} nmr 4

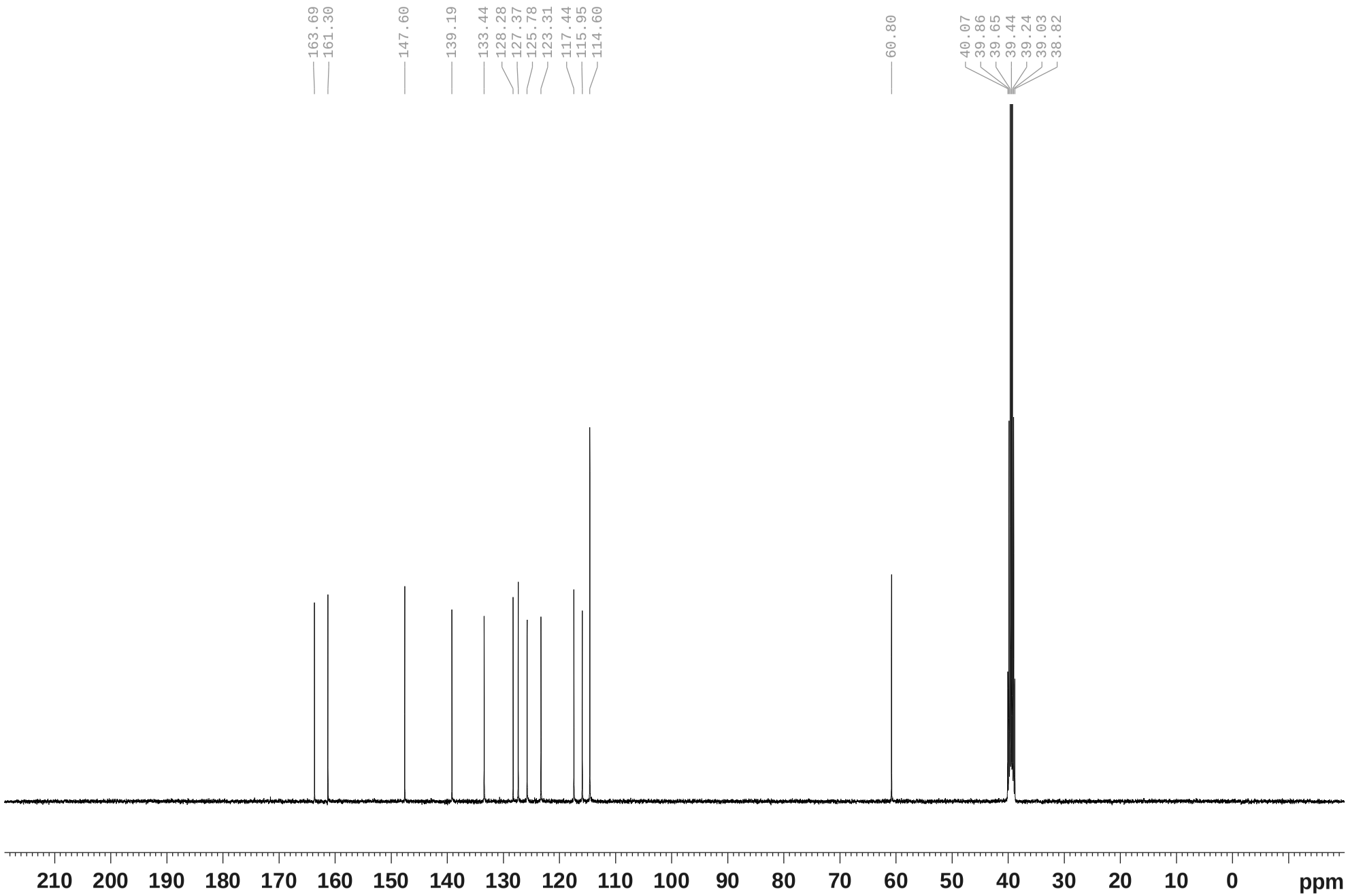


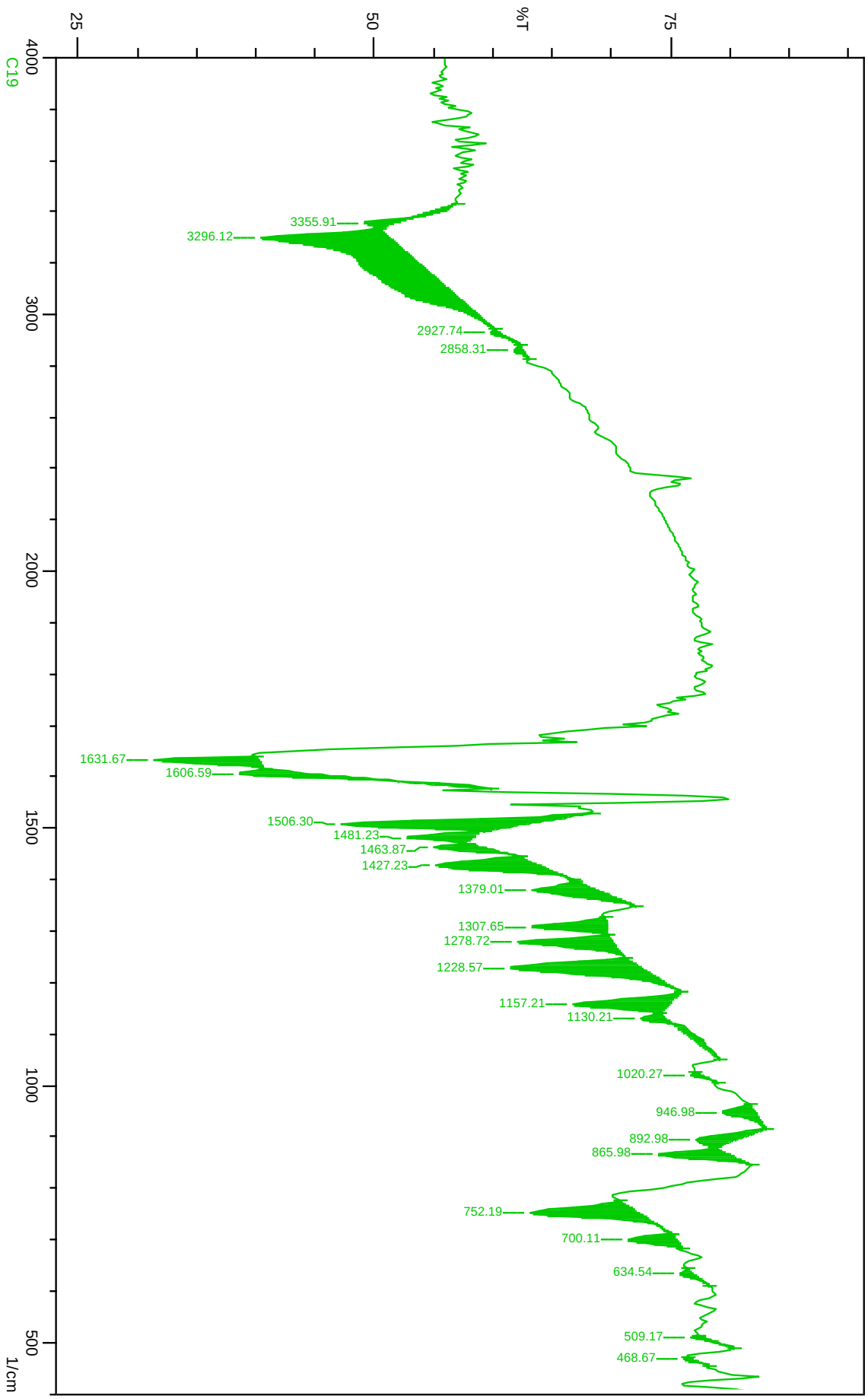

C17
%T
50
60
70
4000
3000
2000
1500
1000
500
1/cm
3396.41
3232.47
3195.83
2925.81
1645.17
1623.95
1579.59
1515.94
1461.94
1392.51
1336.58
1284.50
1238.21
1164.92
1126.35
1089.71
1035.70
904.55
833.19
757.97
628.75
568.96
509.17

PROTON DMSO {C:\Bruker\TOPSPIN\KFUCCP} nmr 2

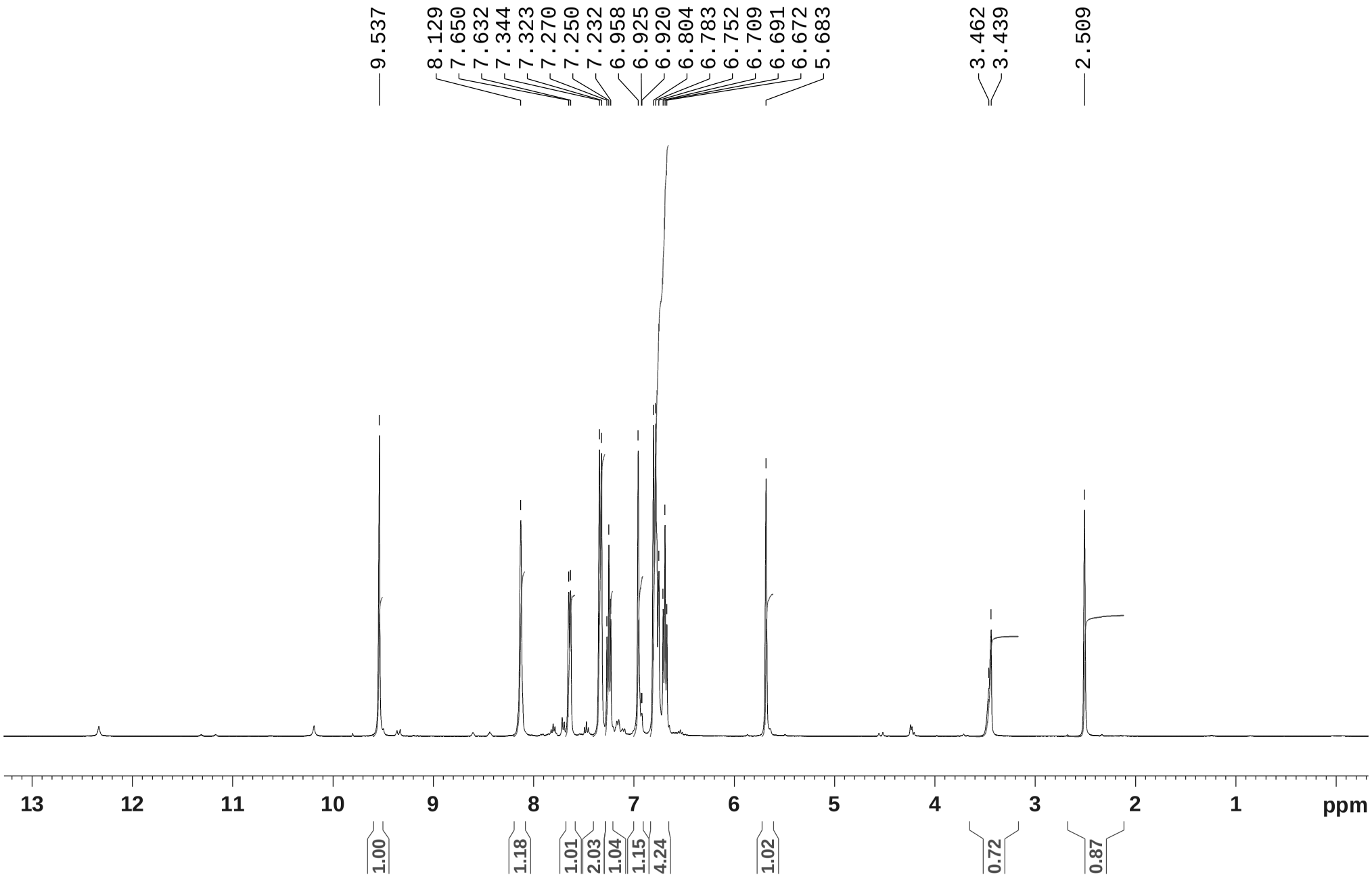


C13CPD DMSO {C:\Bruker\TOPSPIN\KFUCCP} nmr 2




25
50
%T
75
4000
3000
2000
1500
1000
500
1/cm
C19
3355.91
3296.12
2927.74
2858.31
1631.67
1606.59
1506.30
1481.23
1463.87
1427.23
1379.01
1307.65
1278.72
1228.57
1157.21
1130.21
1020.27
946.98
892.98
865.98
752.19
700.11
634.54
509.17
468.67

PROTON DMSO {C:\Bruker\TOPSPIN\KFUCCP} nmr 5



C13CPD DMSO {C:\Bruker\TOPSPIN\KFUCCP} nmr 5