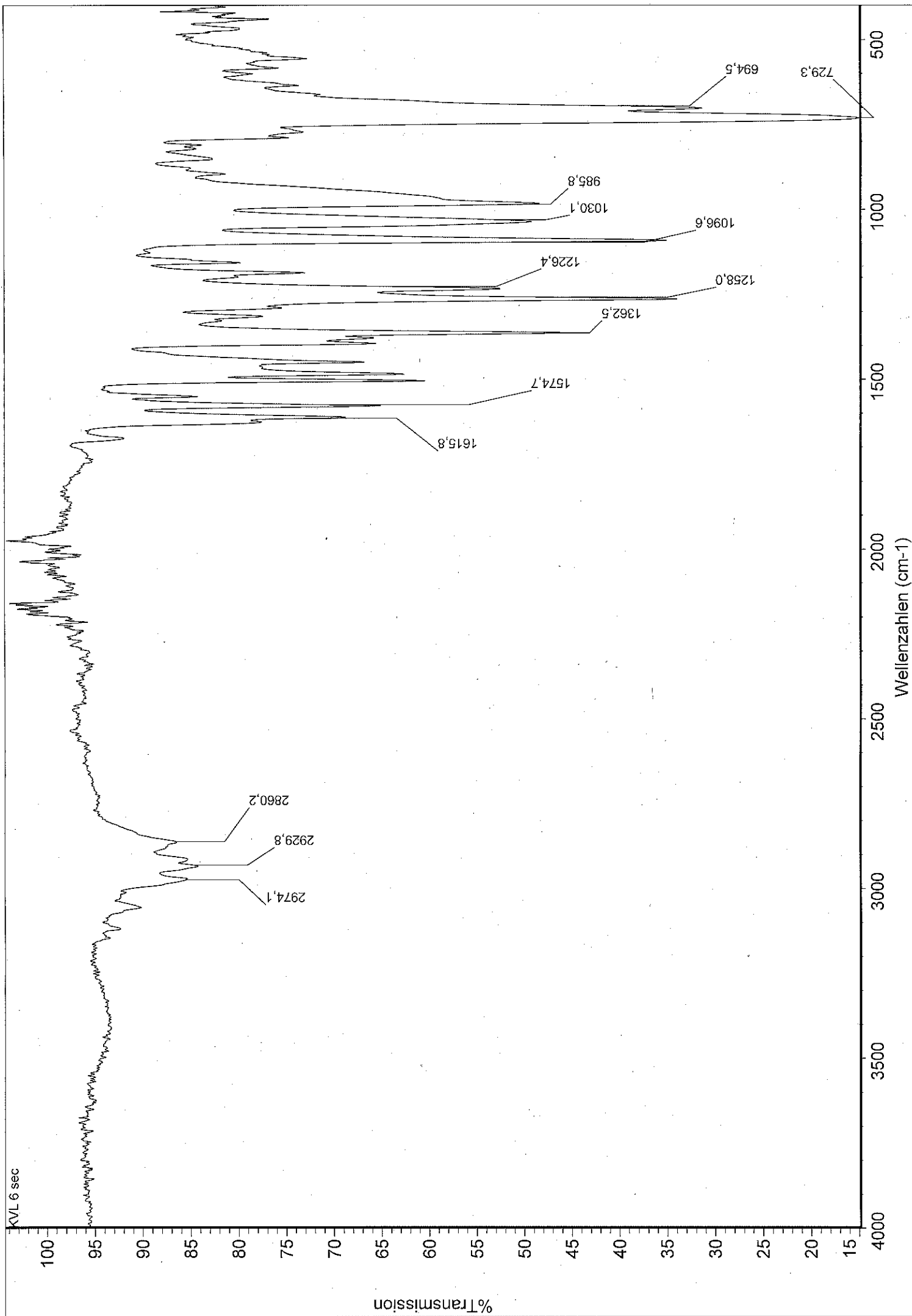


COMPOUND 1



Analysis Report

Analysis Info

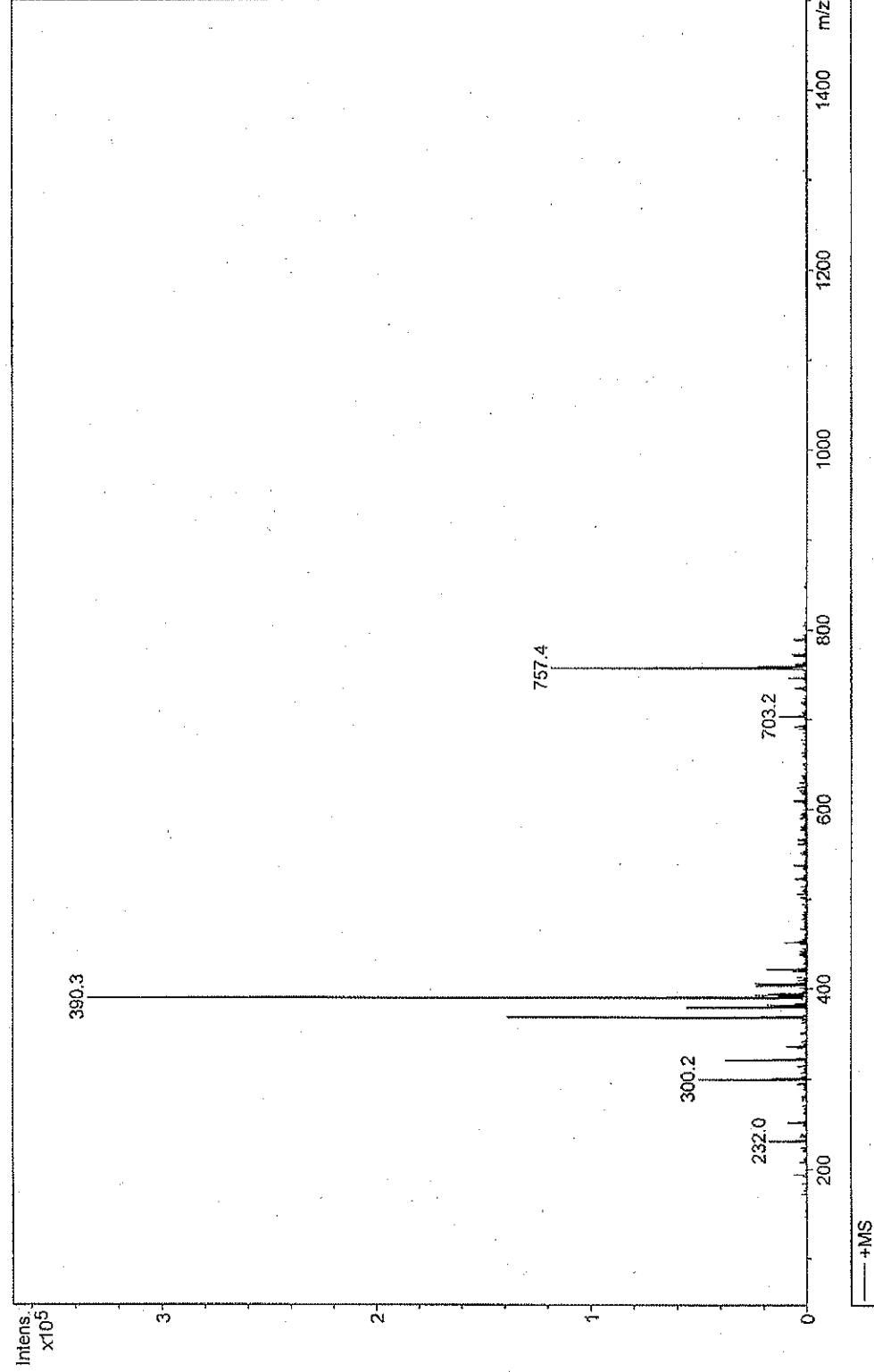
Analysis Name OC3_KenmogneAr_0822_AKVL6_01.d
Method Tune-nan.MS
Workgroup OC3

Esquire 3000



Operator S.Heitkamp
Acquisition Date 24.08.2016 15:36:01
Print Date 24.08.2016 15:38:28

Comment Ar. Kenmogne, OC3, AKVL6, ACN

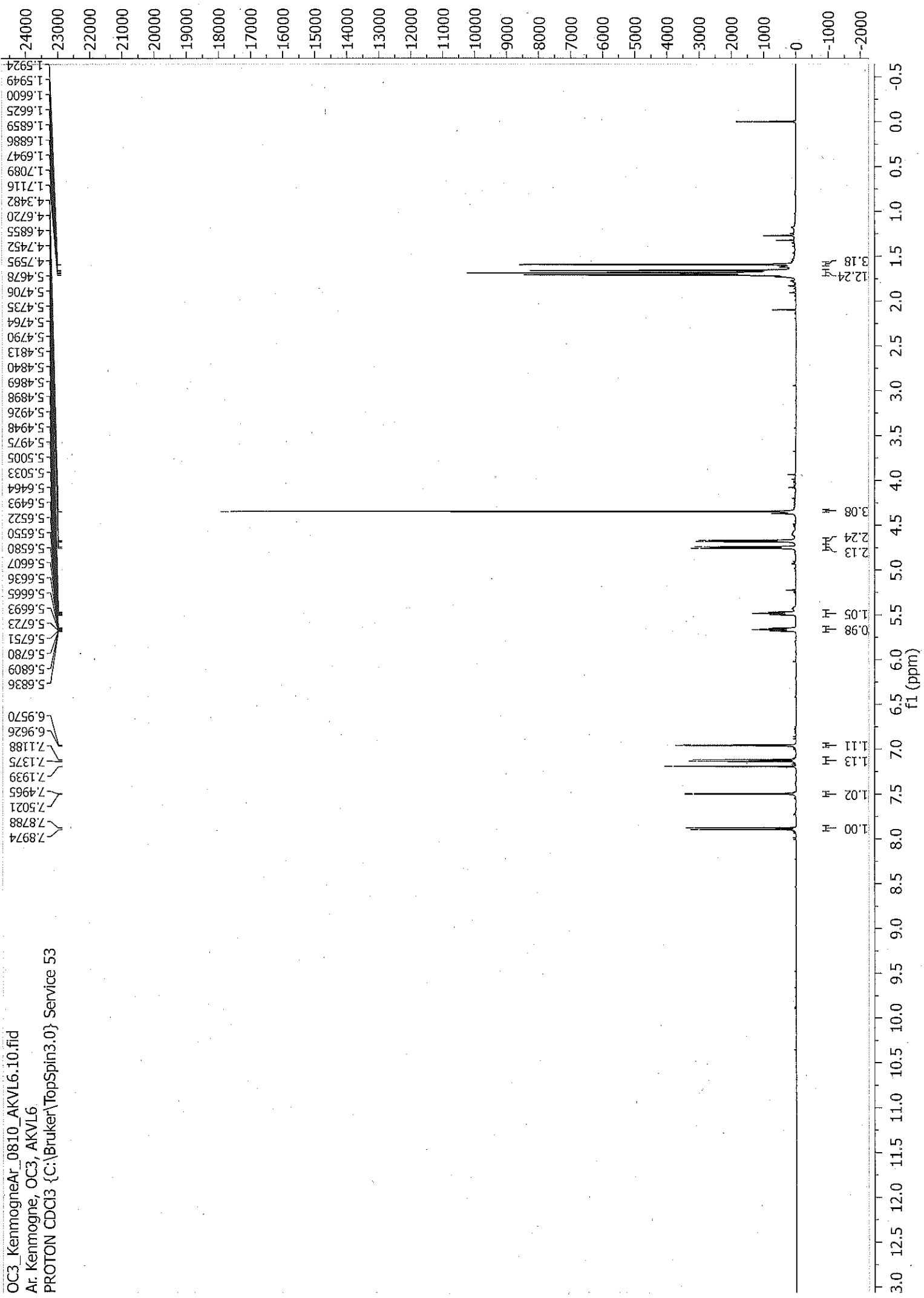


Acquisition Parameter

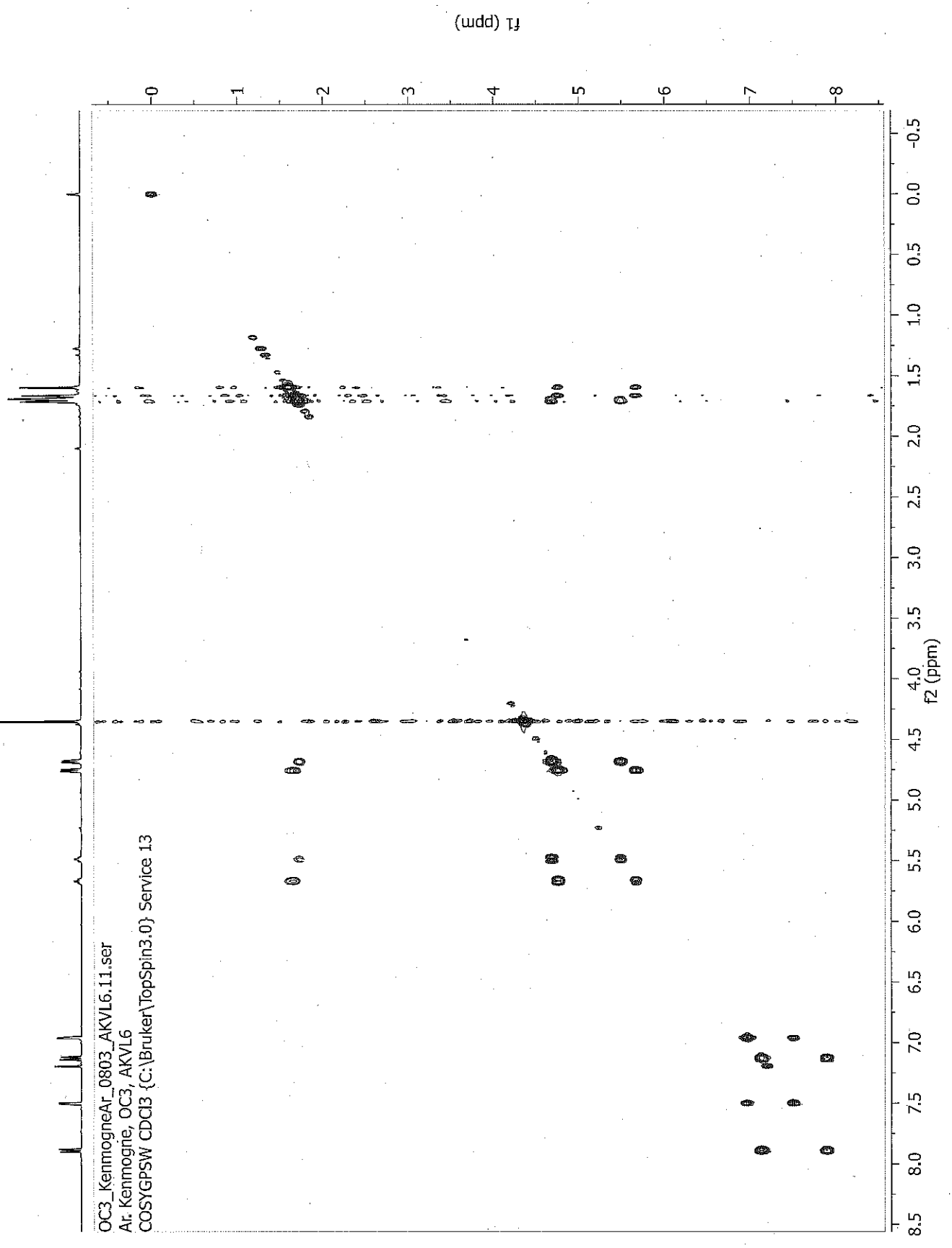
Mode NanoESI, off-line
Ion Source Type Positive
Ion Polarity Std/Normal
Mass Range Mode 50 m/z
Scan Begin 1500 m/z
Scan End 20 Spectra
Averages on
Rolling, Averages 2 cis
Tune SPS
Target Mass 400 m/z
Compound Stability 40 %
Smart Parameter Setting active

Tune Instrument
Trap Drive 40.8
Octopole RF Amplitude 120.0 Vpp
Lens 2 -60.0 Volt
Capillary Exit 91.8 Volt
Skim 1 22.9 Volt
Skim 2 6.0 Volt
Lens 1 -5.0 Volt
Cap Exit Offset 68.9 Volt
Octopole 2.54 Volt
Octopole Delta 2.40 Volt
Dry Temp (Set) 100 °C
Nebulizer (Set) 2.00 psi
Dry Gas (Set) 2.00 l/min
Accumulation Time 666 µs
ICC Target 5000
Charge Control on

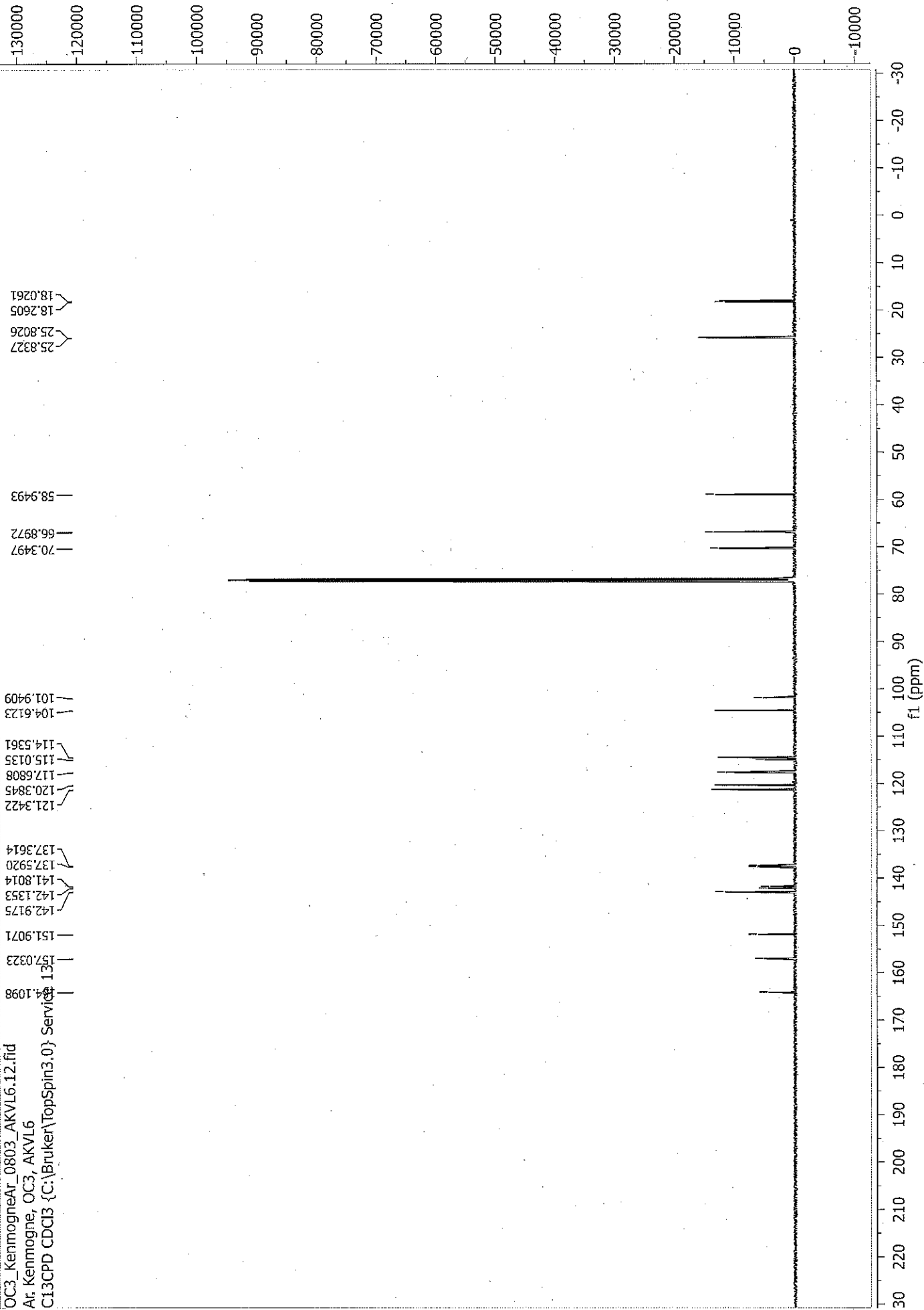
OC3_KenmogneAr_0810_AKVL6.10.fid
Ar: Kenmogne, OC3, AKVL6
PROTON CDCl3 {C:\Bruker\TopSpin3.0} Service 53



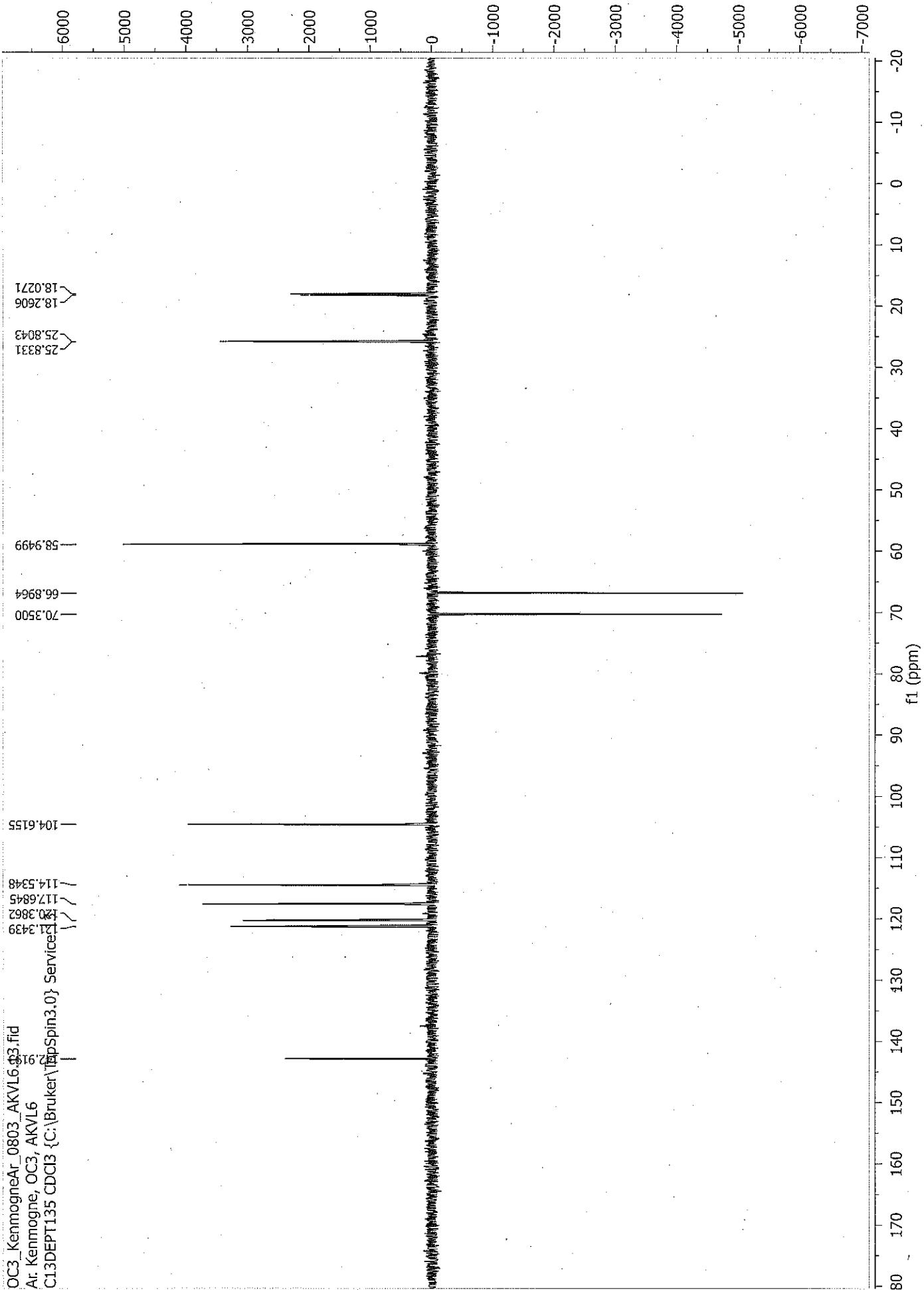
OC3_KennognreA1_0803_AKVL6.11.ser
A1: Kennognre, OC3, AKVL6
COSYGPSW CDCl3 {C:\Bruker\TopSpin3.0} Service 13



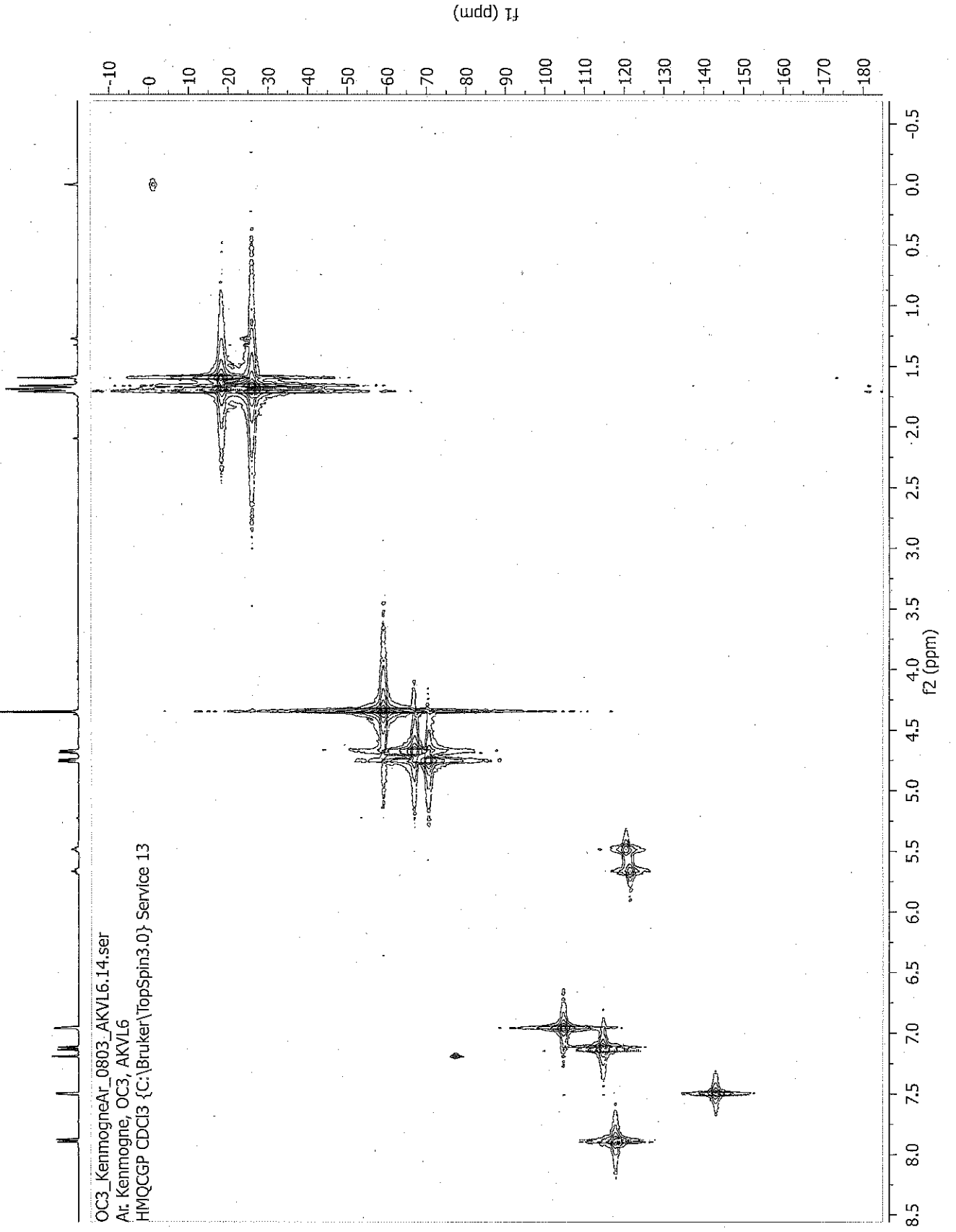
OC3_KenmogneAr_0803_AKVL6.12.fid
At: Kenmogne, OC3, AKVL6
C13CPD CDC13 {C:\Bruker\TopSpin3.0} Service 1.3



OC3_KenmogneAr_0803_AKVL6_03.fid
Ar: Kenmogne, OC3, AKVL6
C13DEPT135 CDCIB {C:\Bruker\TopSpin3.0} Services

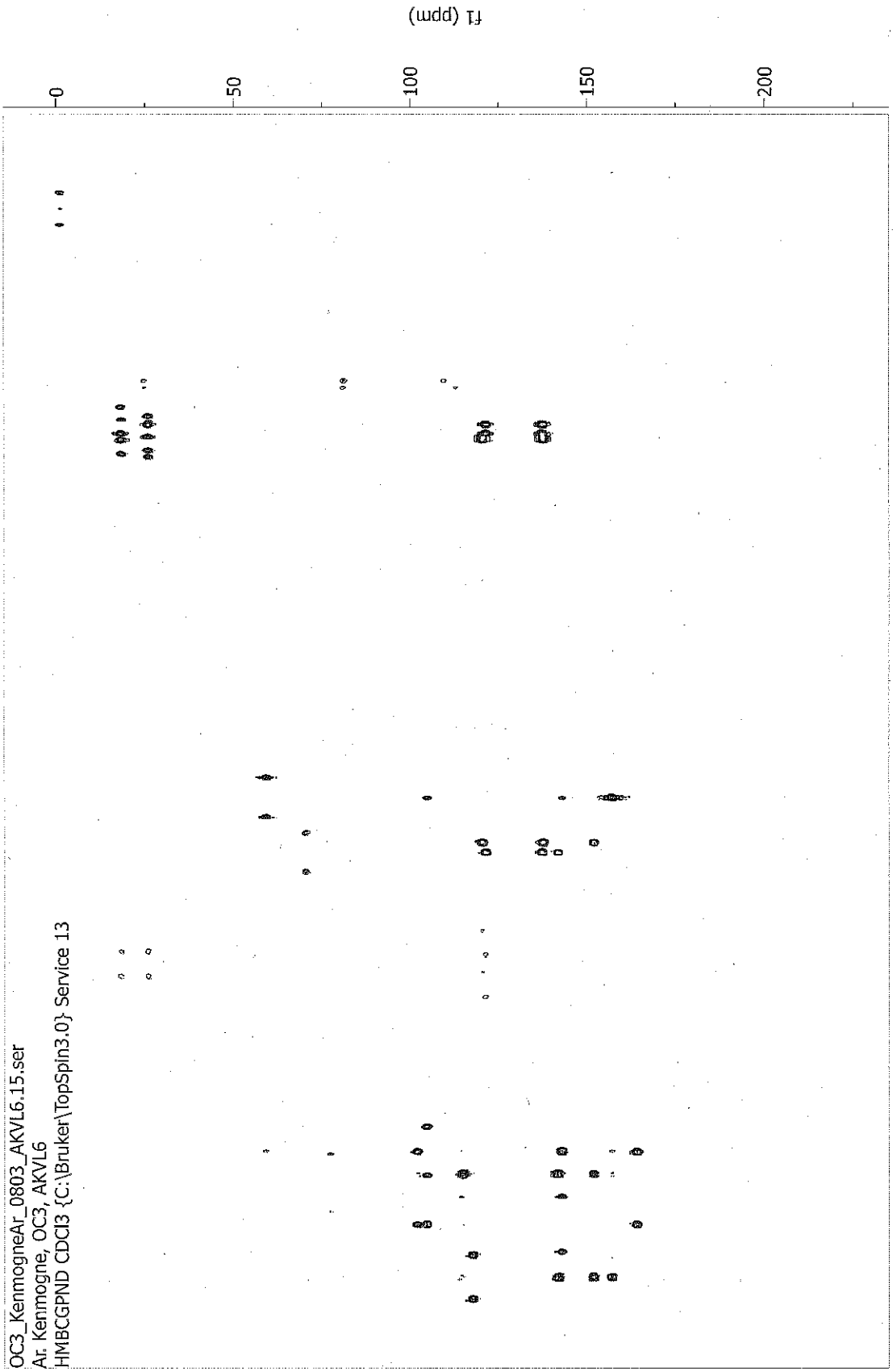


OC3_KemogneA1_0803_AKVL6.14.ser
A1: Kemogne, OC3, AKVL6
HMQCGP CDCl3 {C:[Bruker\TopSpin3.0]} Service 13

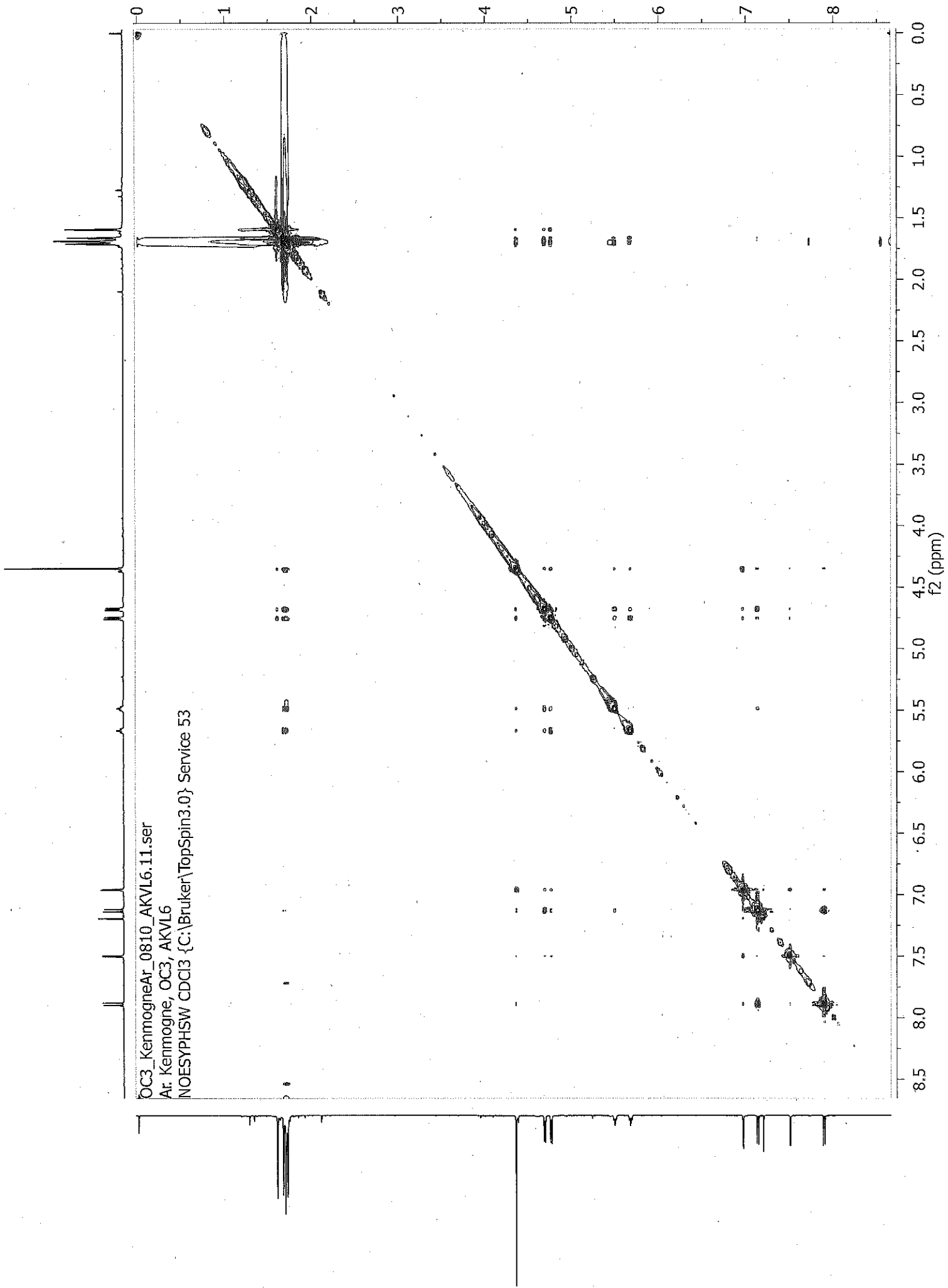


(uidd) F1

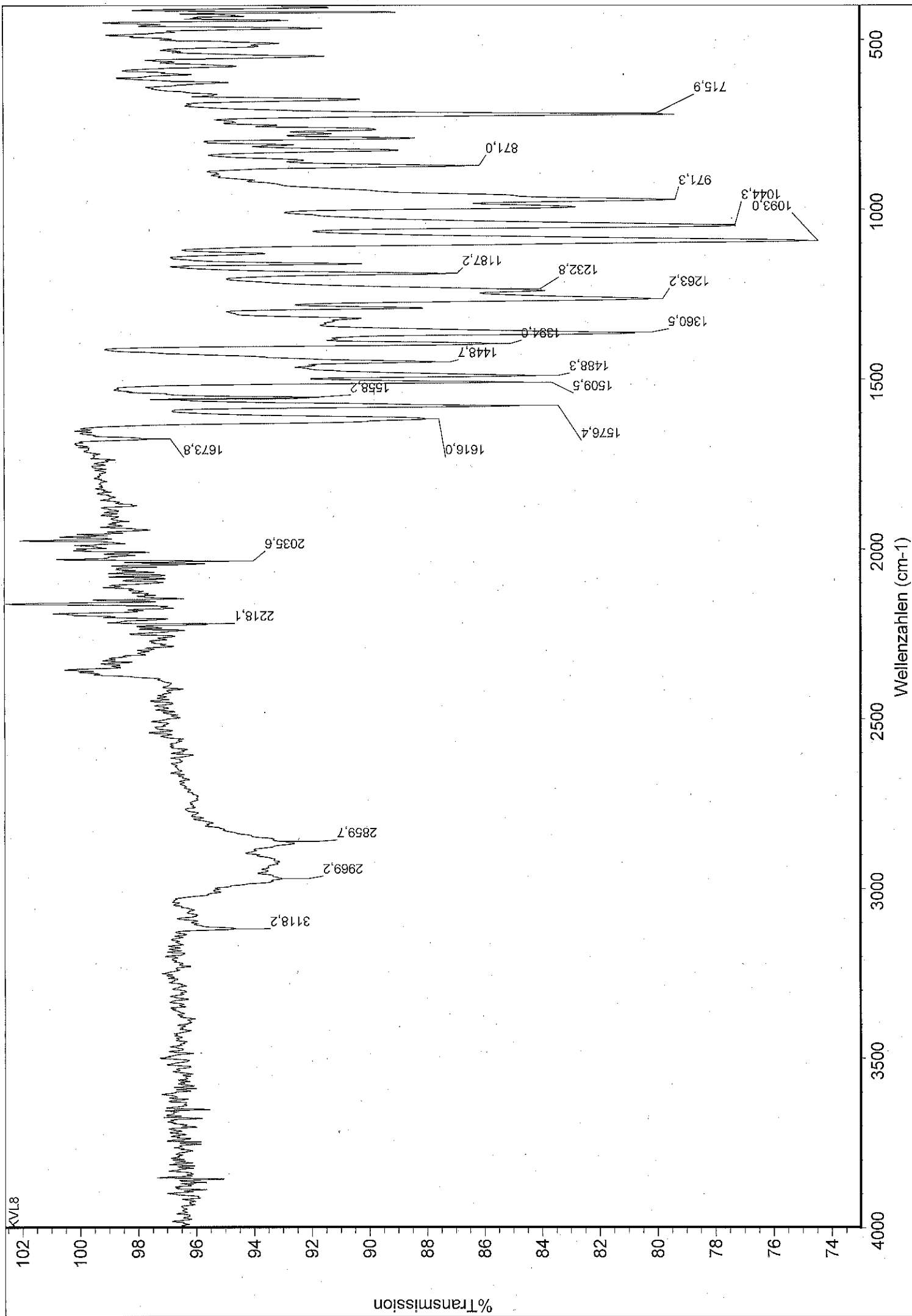
OC3_KenmogneA1_0803_AKVL6.15.ser
A1: Kenmogne, OC3, AKVL6
HMBCGPND CDC13 {C:\Bruker\TopSpin3.0} Service 13



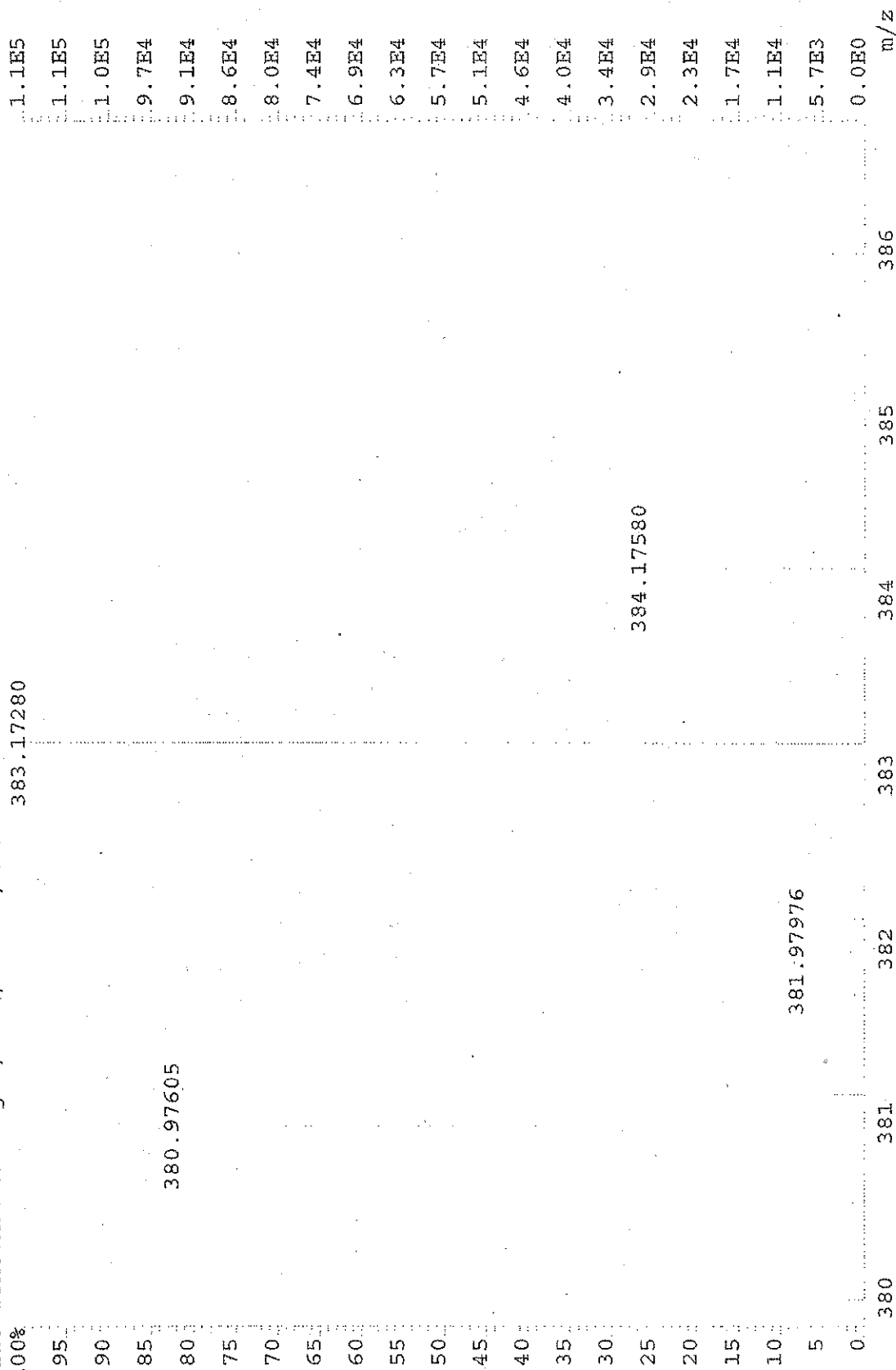
OC3_KenmogneAr_0810_AKVL6.11.ser
Ar: Kenmogne, OC3, AKVL6
NOESYPHSW CDCI3 {C:\Bruker\TopSpin3.0} Service 53



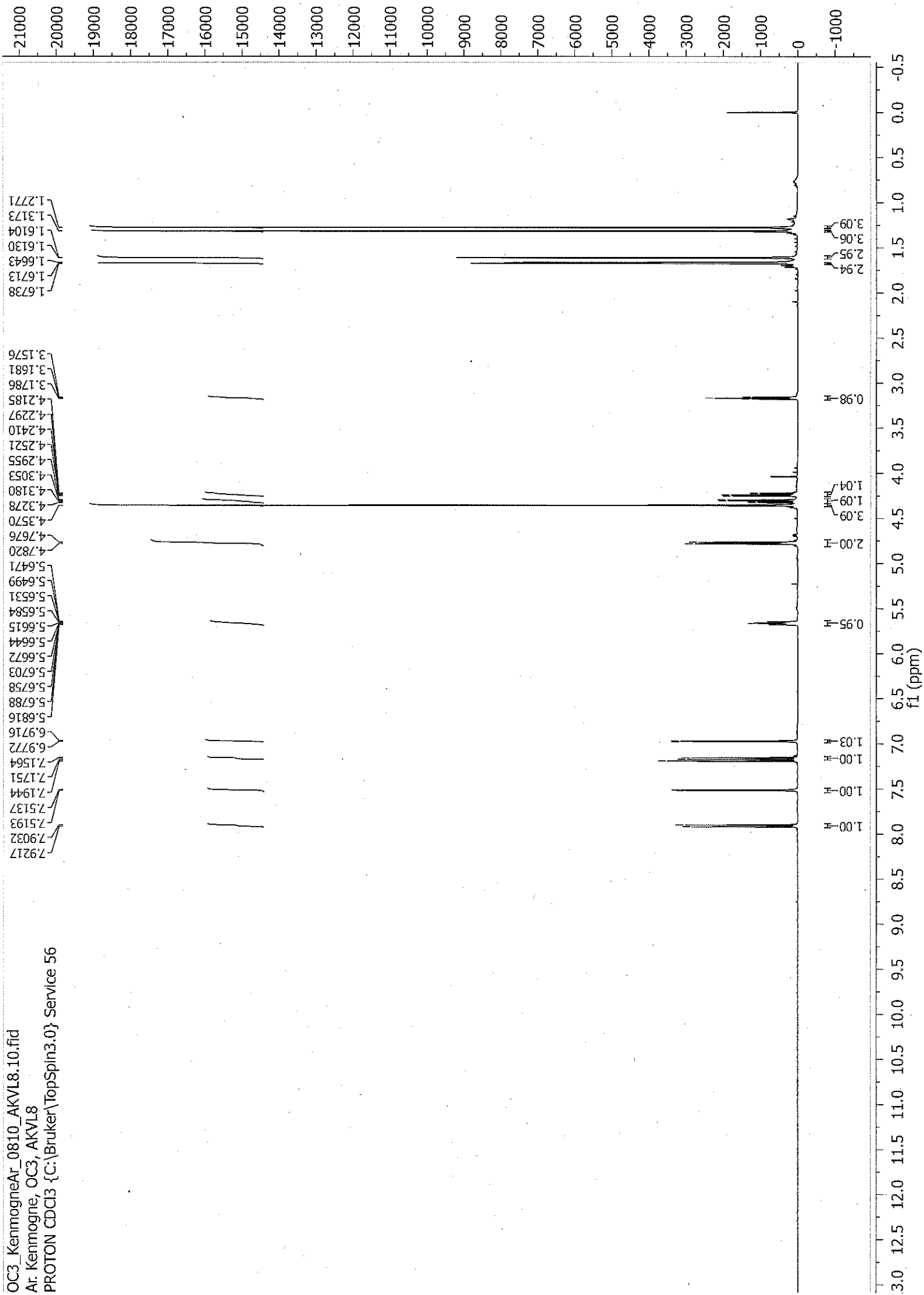
COMPOUND 2



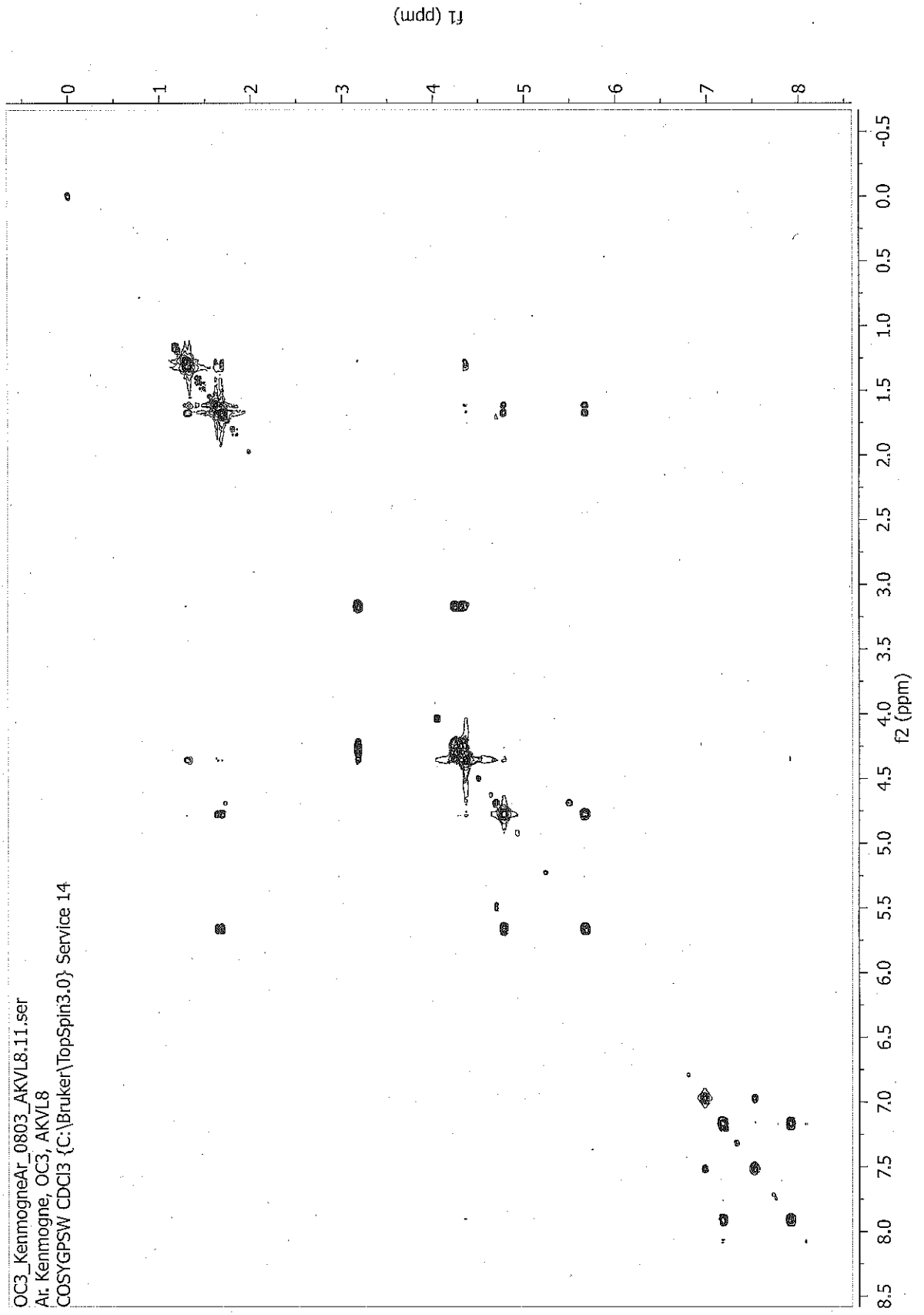
File:MFB2016_109 Ident:48 52 SMO(1,7) PKD(7,3,7,0.50%,0.0,0.00%,F,F) SPEC(Heights, Centroid) Acq>
 AutoSpec EI+ Voltage BpM:383 BpI:114236 TIC:359861 Flags:NORM
 File Text:Ar. Kenmogne, OC3, AKVL8, HWP



OC3_KenmogneAr_0810_AKVL8.10.fid
Ar: Kenmogne, OC3, AKVL8
PROTON CDCl3 {C:\Bruker\TopSpin3.0} Service 56



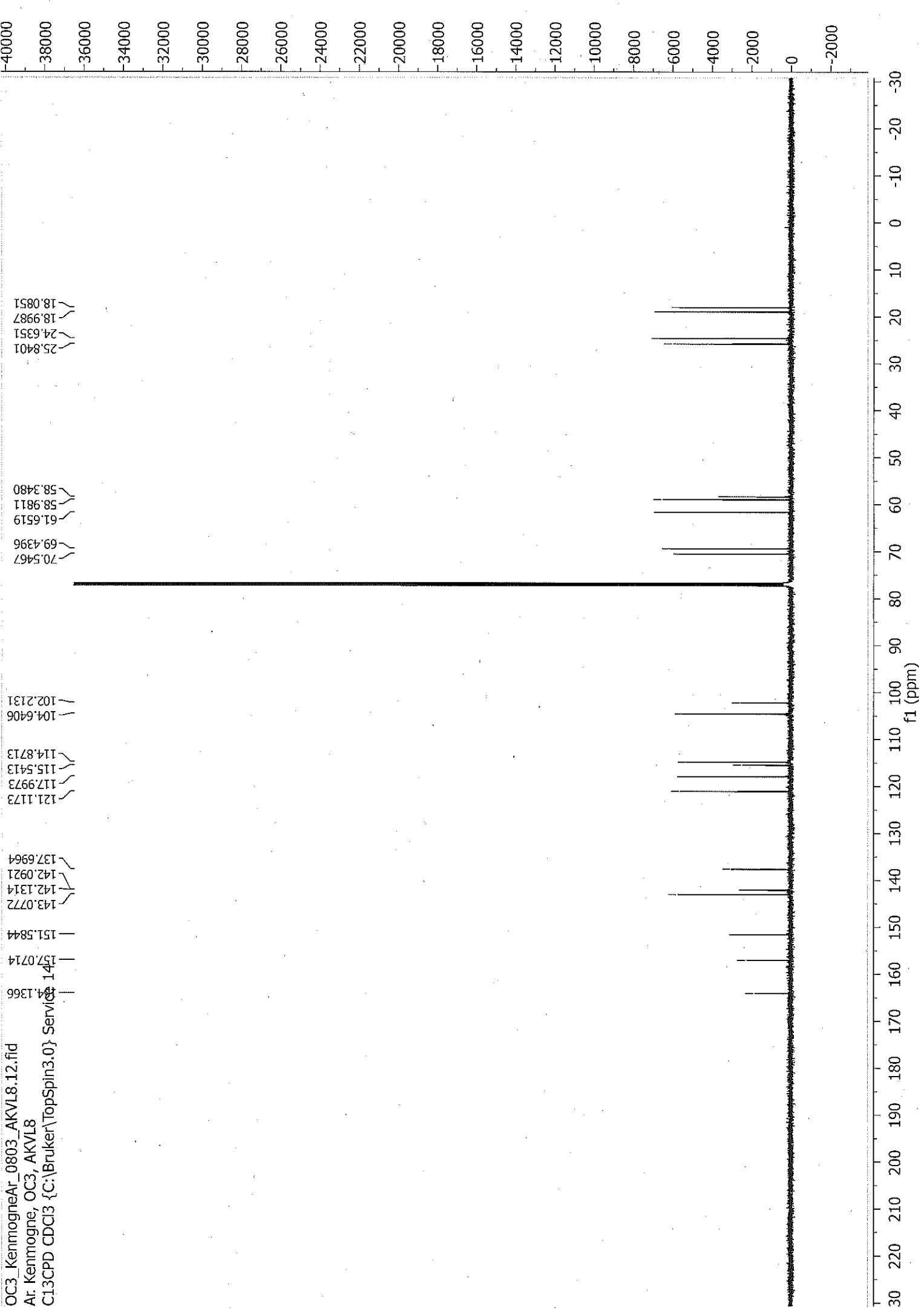
OC3_KennogneAr_0803_AKVL8.11.ser
Ar, Kennogne, OC3, AKVL8
COSYGPSW CDCl3 {c:\Bruker\TopSpin3.0} Service 14



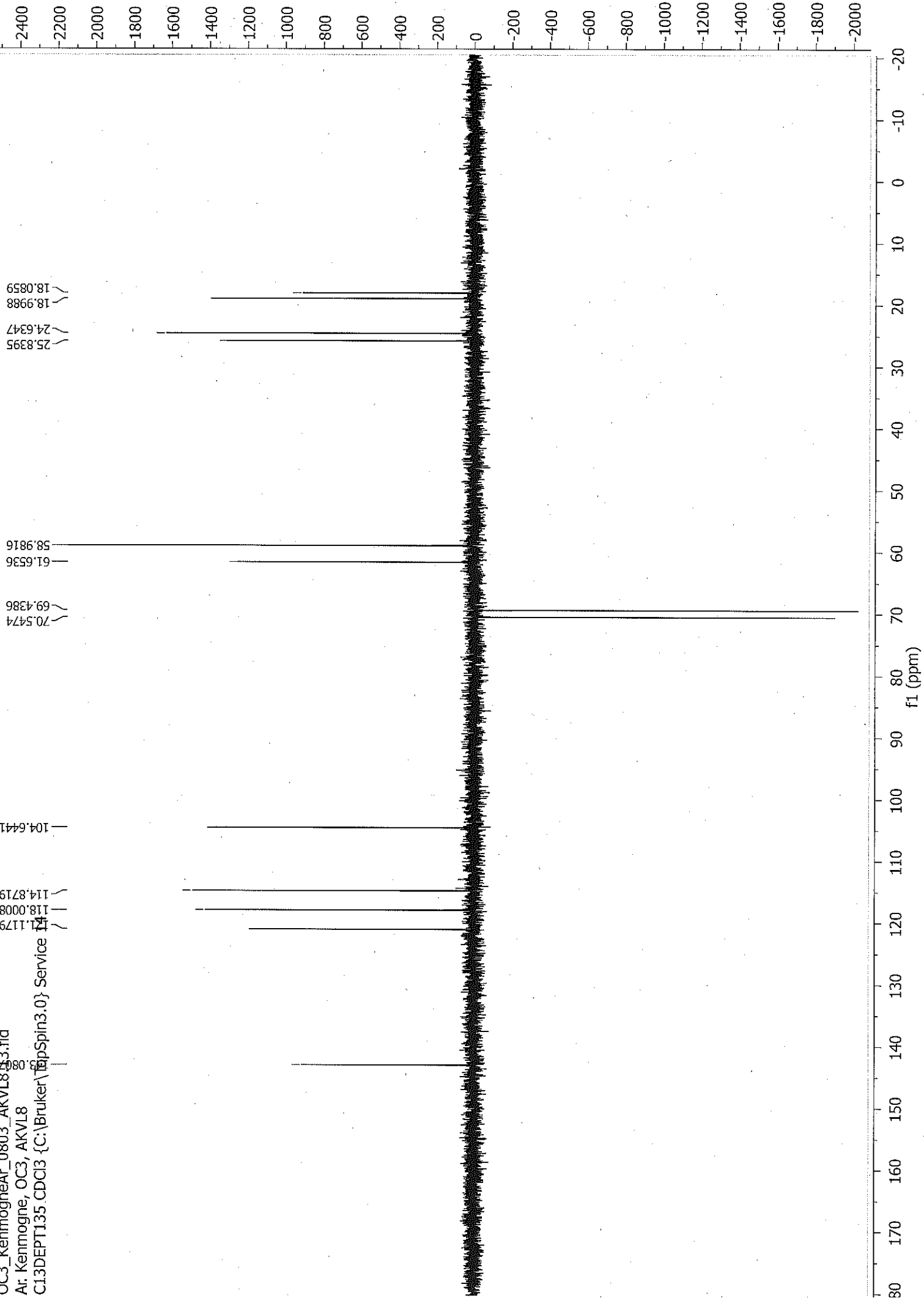
f1 (ppm)

f2 (ppm)

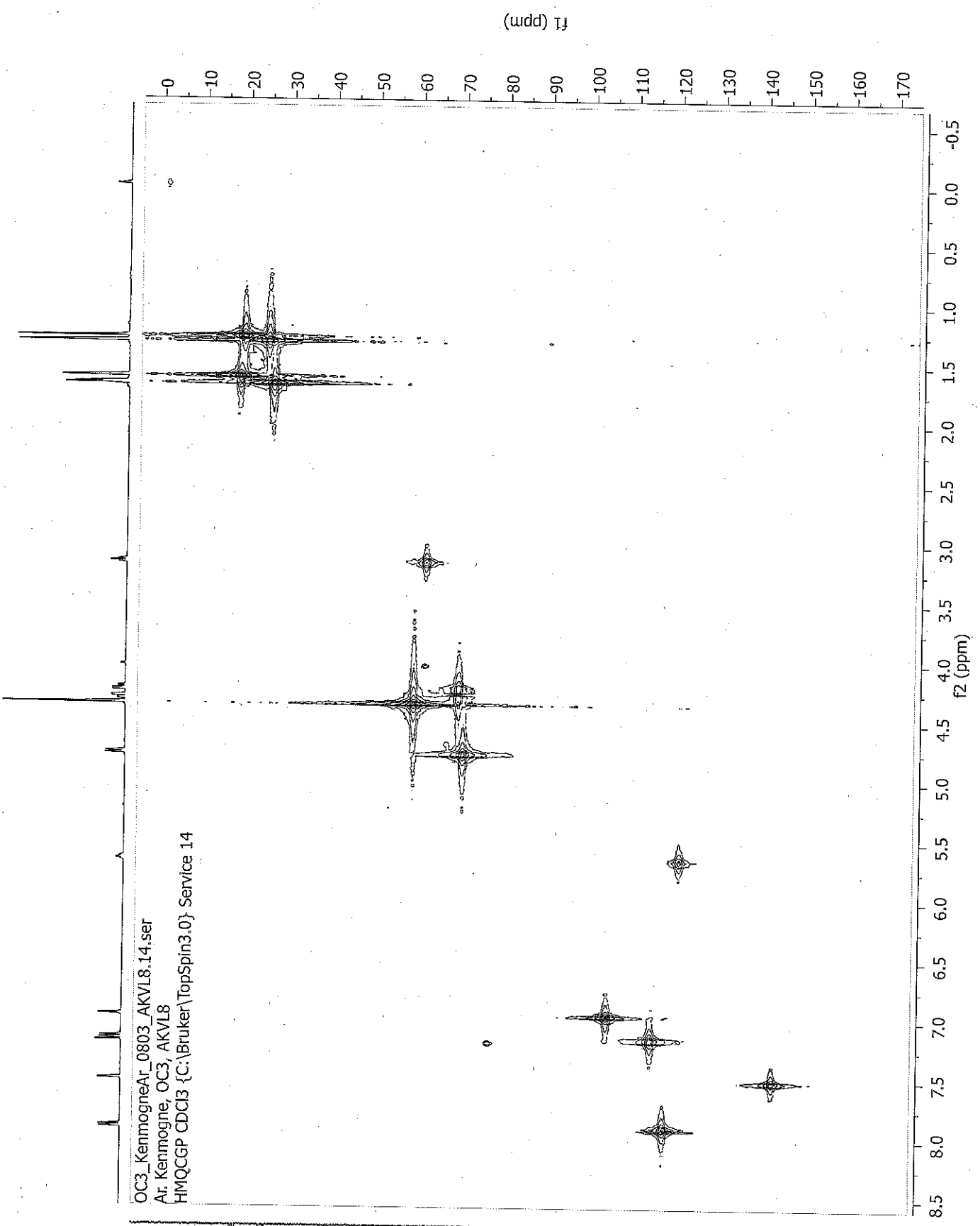
OC3_KenmogneAr_0803_AKV18.12.fid
Ar: Kenmogne, OC3, AKV18
C13CPD CDCl3 {C:\Bruker\TopSpin3.0} Service



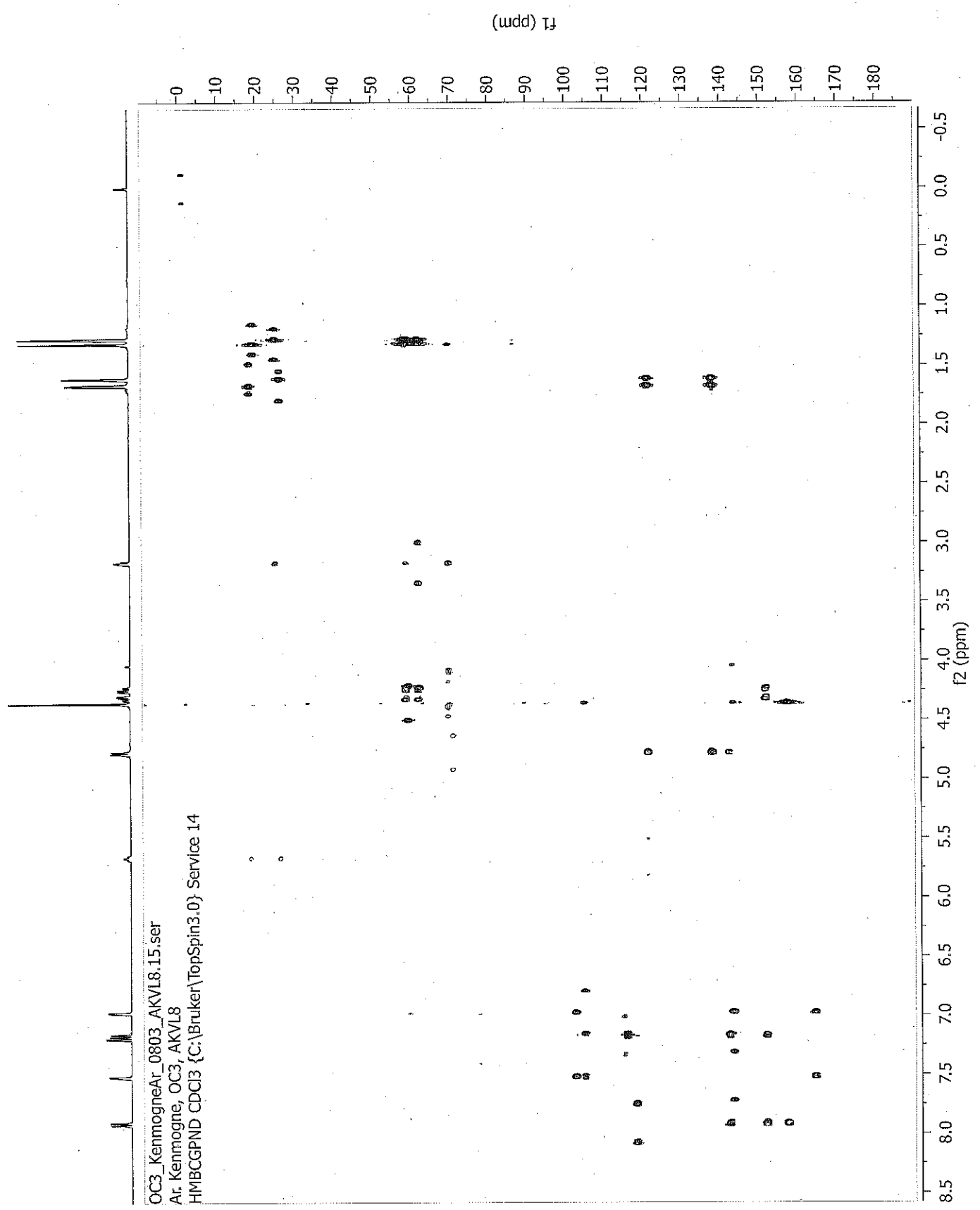
OC3_KenmogneAr_0803_AKVL853.fid
Ar: Kenmogne, OC3, AKVL8
C13DEPT135.CDC3 {C:\Bruker\TopSpin3.0} Service 14



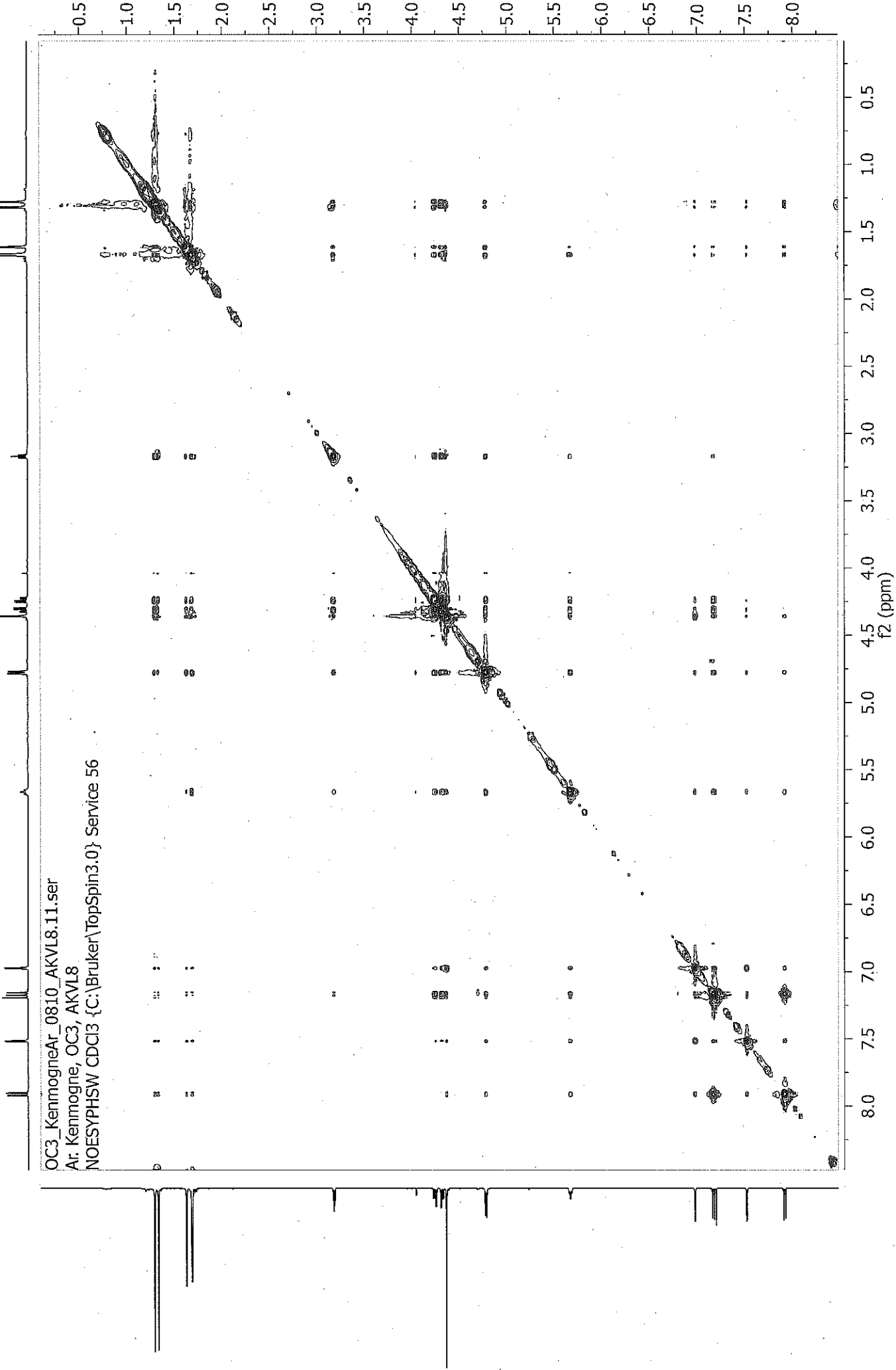
OC3_KenmogneAr_0803_AKVL8.14.ser
Ar: Kenmogne, OC3, AKVL8
HMQCQP CDC13 {C:\Bruker\TopSpin3.0} Service 14



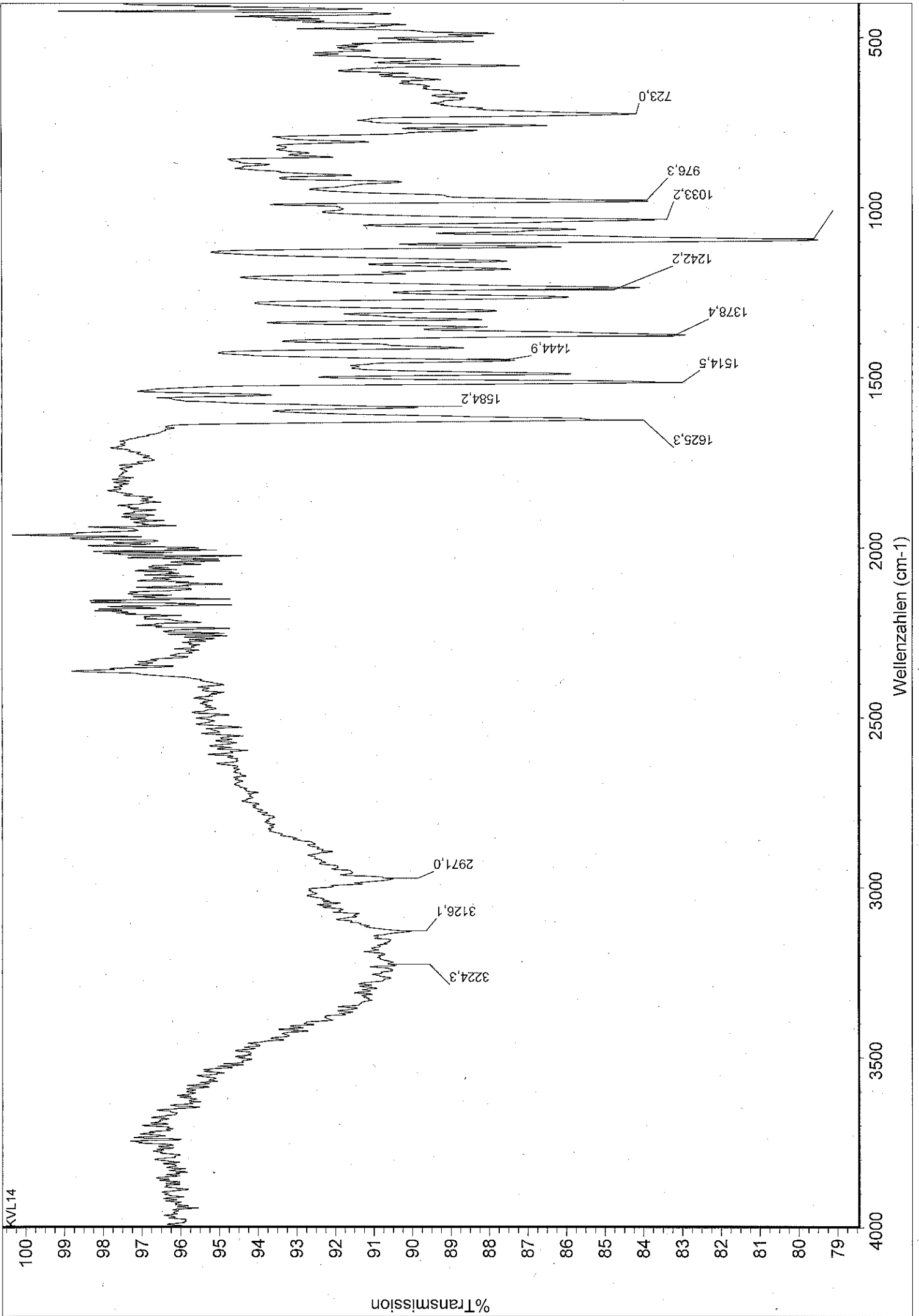
OC3_KenmogneAr_0803_AKVL8.15.ser
Ar: Kenmogne, OC3, AKVL8
HMBCGPND CDCl3 {C:\Bruker\TopSpin3.0} Service 14



OC3_KenmogneAr_0810_AKVL8.11.ser
Ar. Kenmogne, OC3, AKVL8
NOESYPHSW CDCI3 {C:\Bruker\TopSpin3.0} Service 56

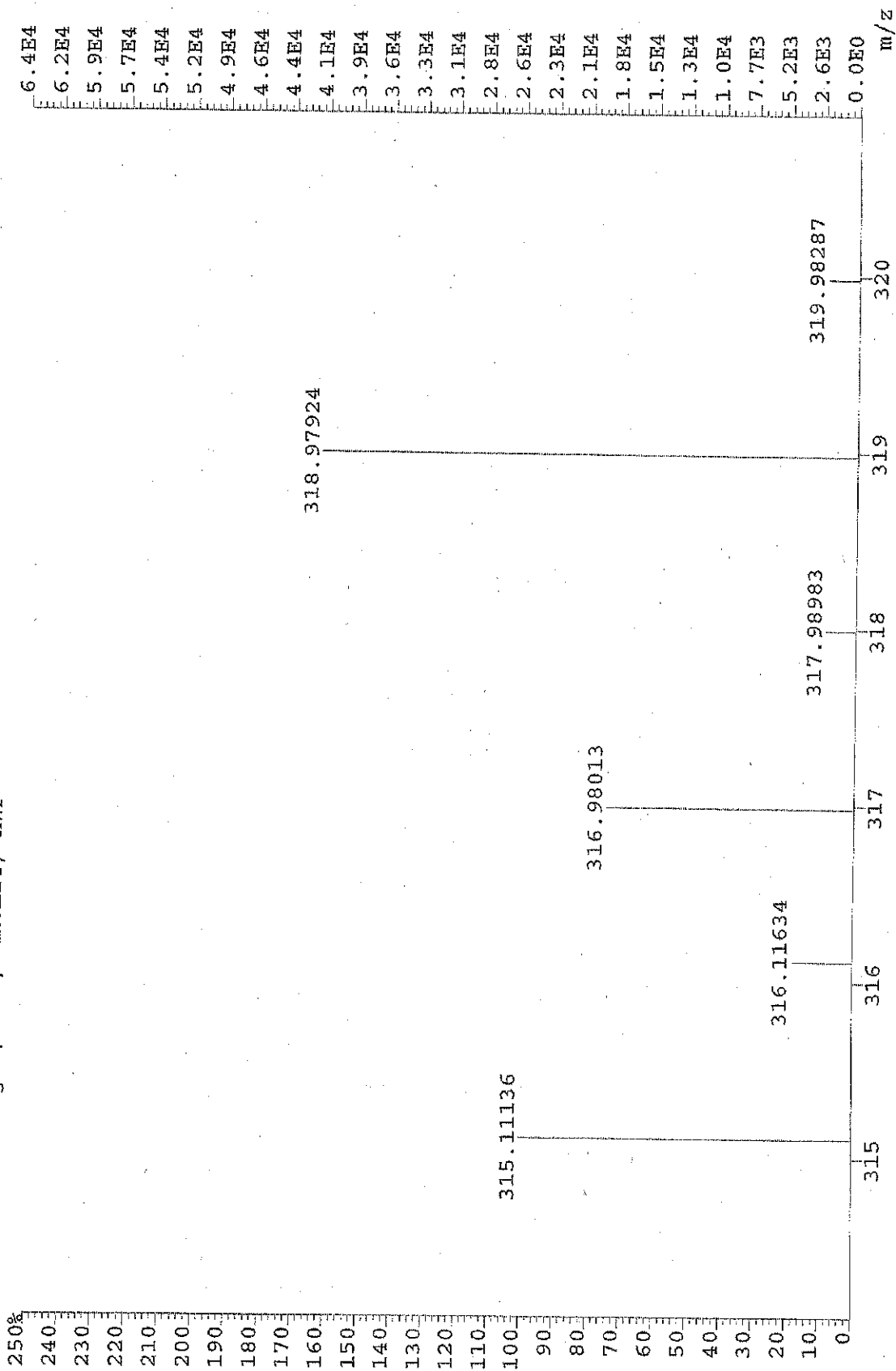


COMPOUND 3

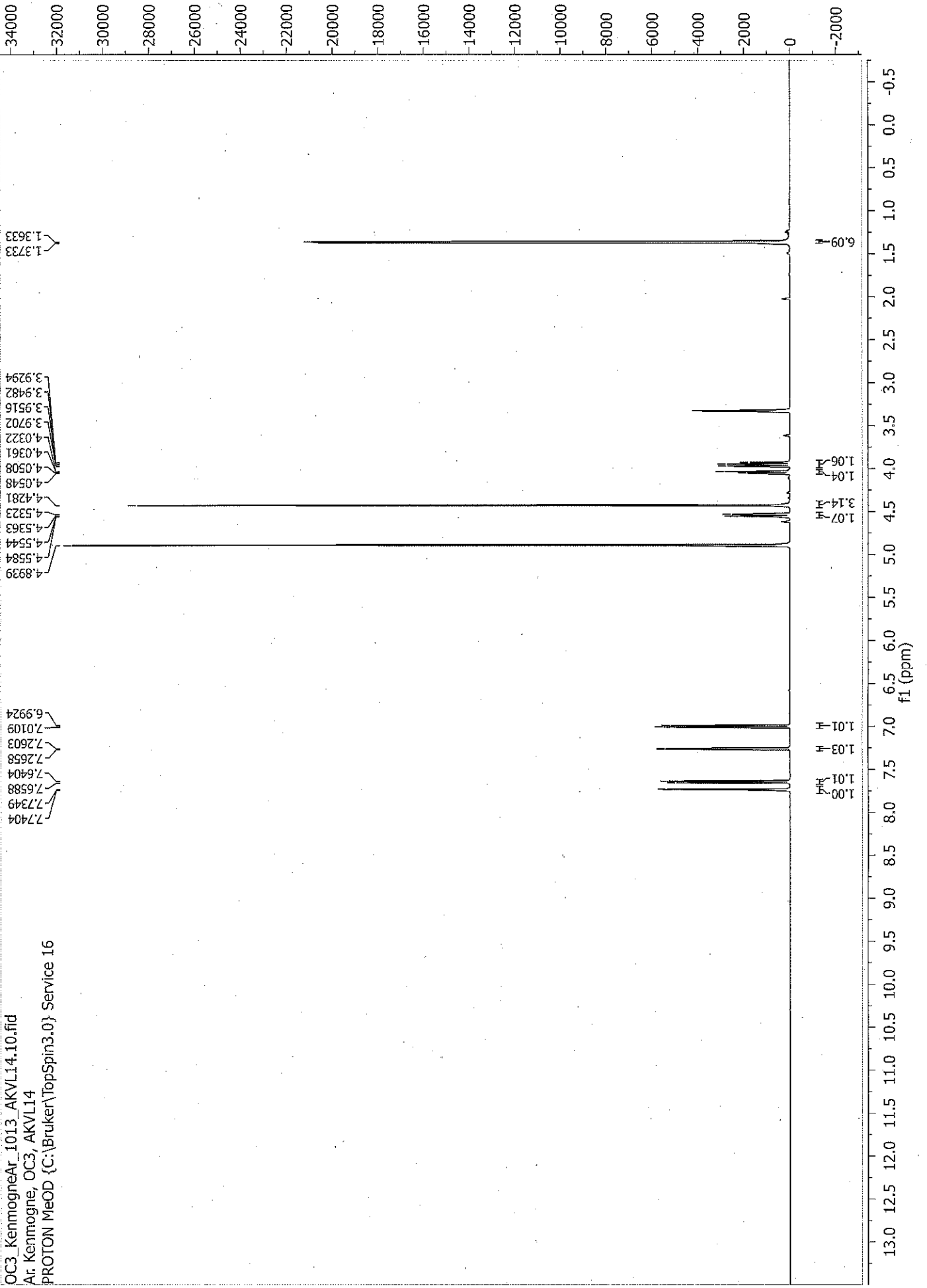


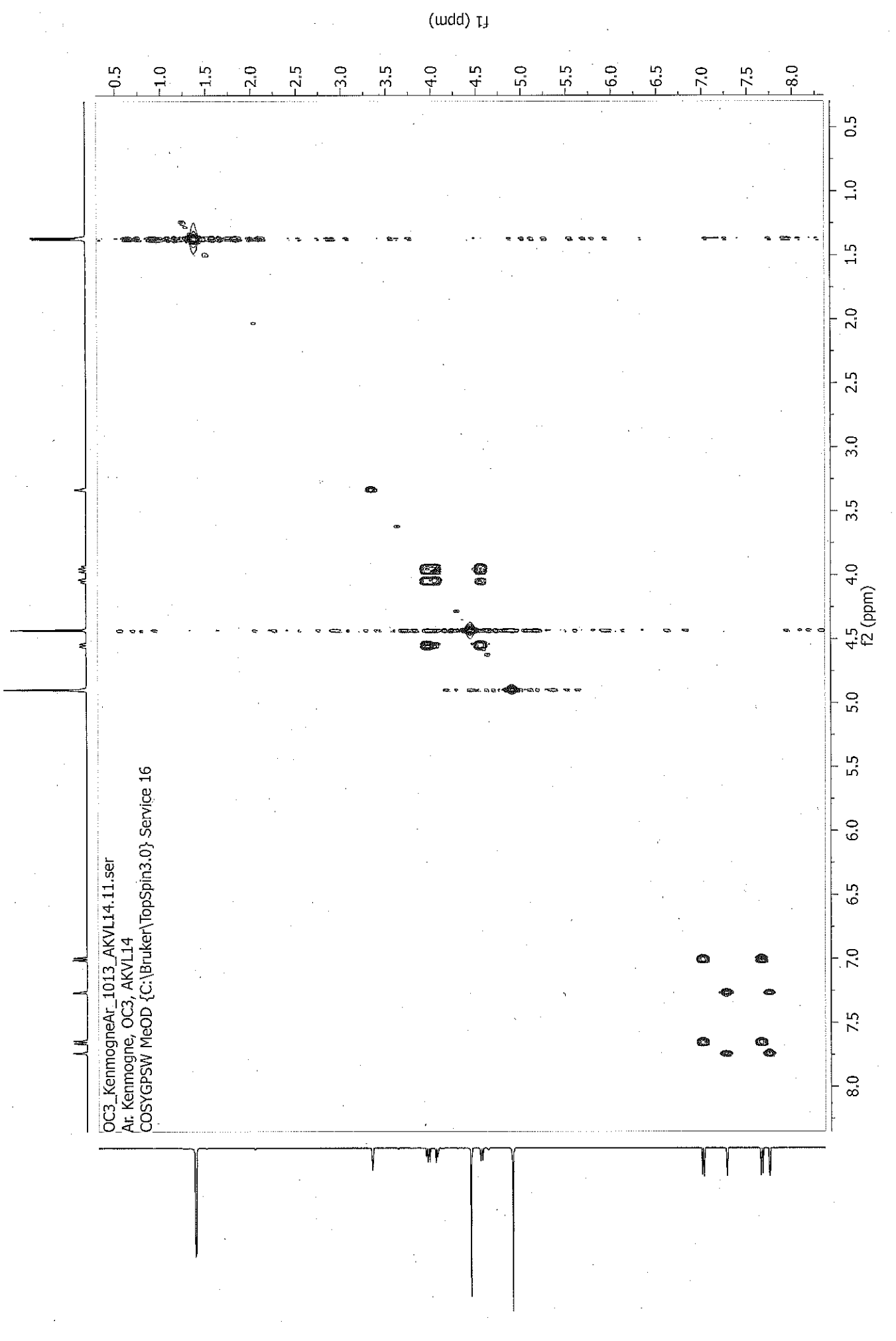
KVL14

File:MFB2016_123X Ident:40_50 SMO(1,7) PKD(7,3,7,0.50%,0.0,0.00%,F,F) SPEC(Heights, Centroid) Ac>
AutoSpec EI+ Voltage BpM:319 BpI:41690 TIC:159279 Flags:NORM
File Text:Ar. Kenmogne, OC3, AKVLI14, HWP



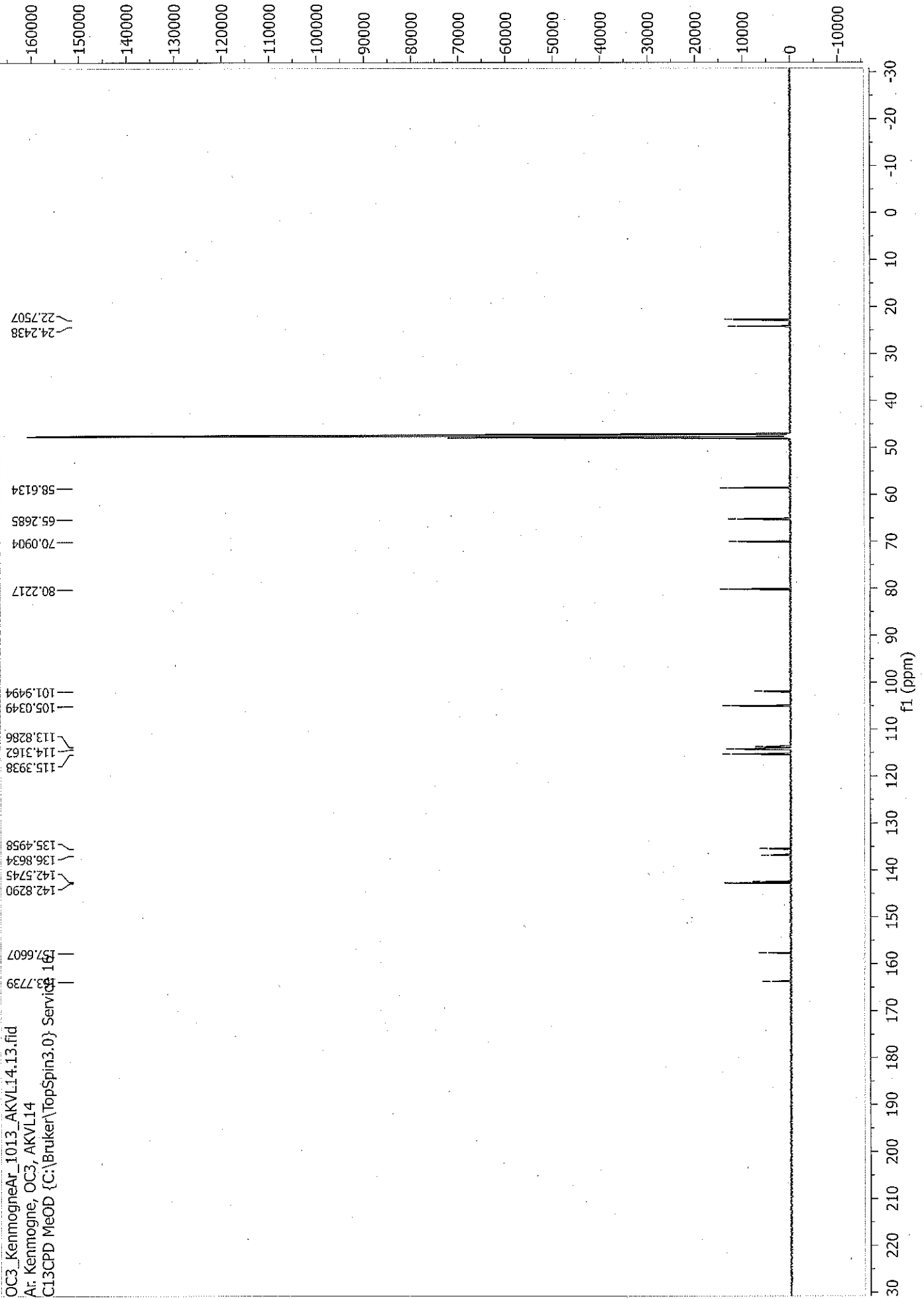
OC3_KenmogneAr_1013_AKVL14.10.fid
Ar. Kenmogne, OC3, AKVL14
PROTON MeOD {C:\Bruker\TopSpin3.0} Service 16

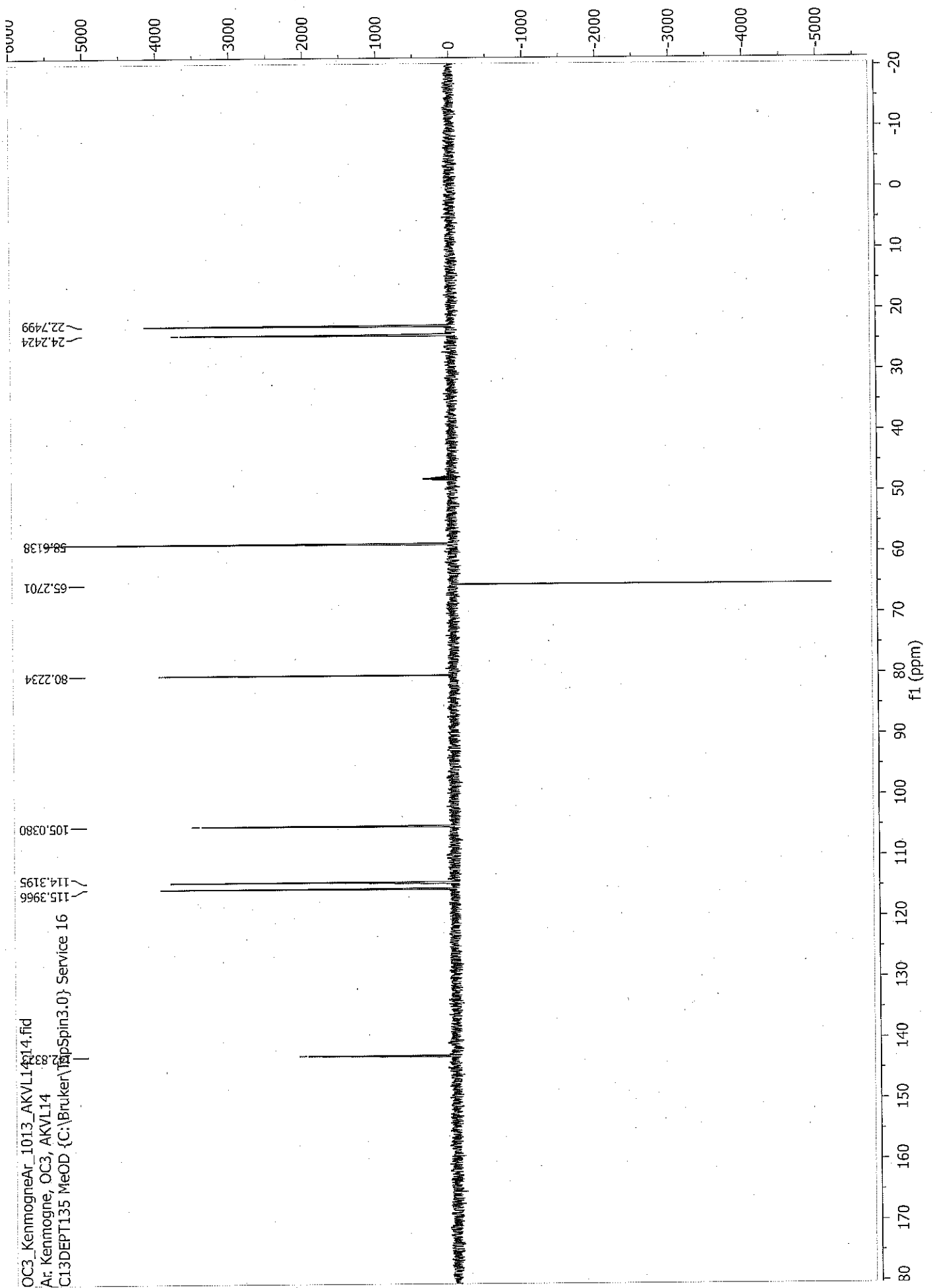




OC3_KennogneAr_1013_AKVL14_11.ser
Ar: Kennogne, OC3, AKVL14
COSYGPSW MeOD {C:\Bruker\TopSpin3.0} Service 16

OC3_KenmogneAr_1013_AKVL14.13.fid
Ar: Kenmogne, OC3, AKVL14
C13CPD MeOD (C:\Bruker\TopSpin3.0) Service 16





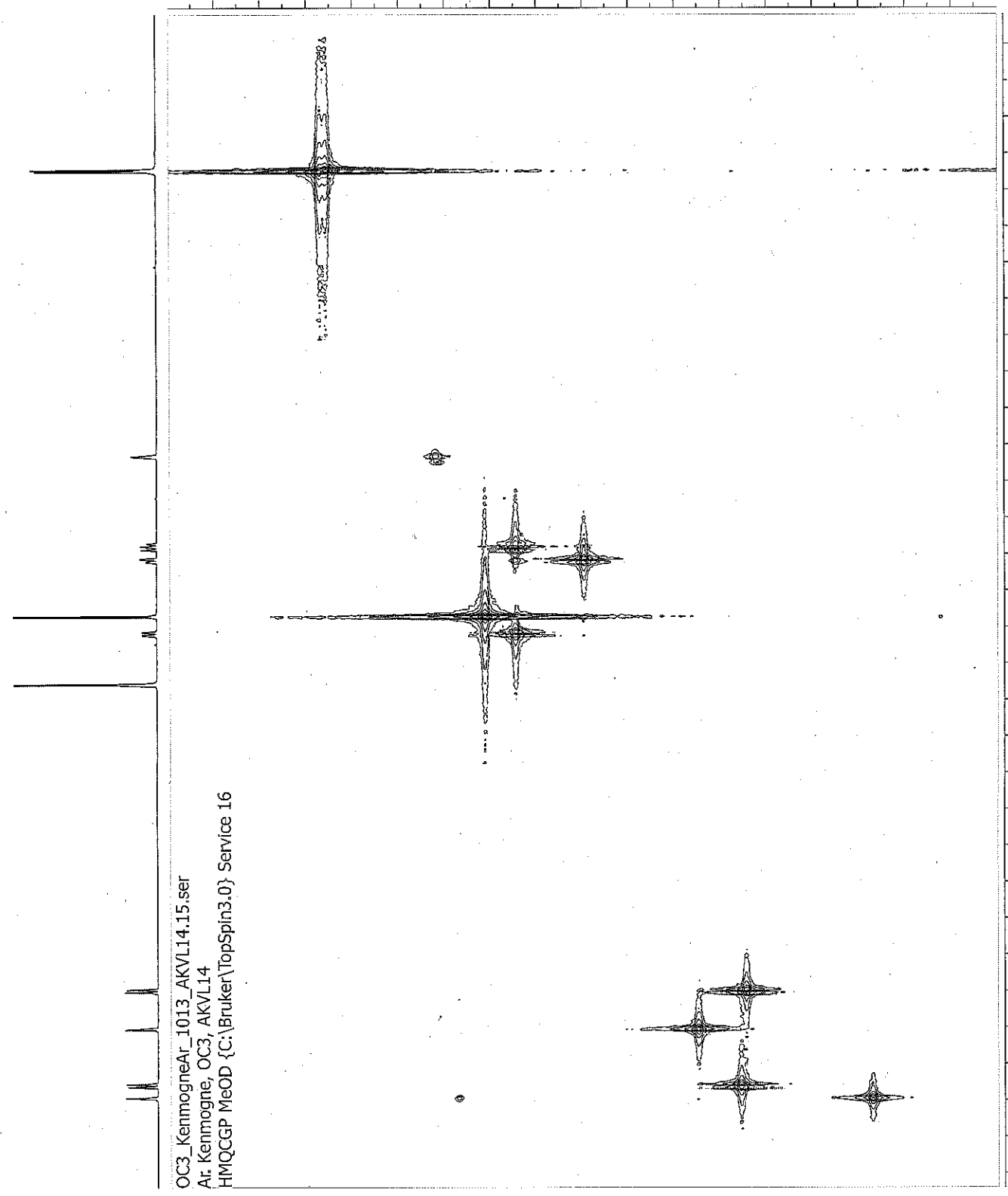
OC3_KennogneAr_1013_AKVL14.15.ser
Ar. Kennogne, OC3, AKVL14
HMQCGP MeOD {C:\Bruker\TopSpin3.0} Service 16

F1 (ppm)

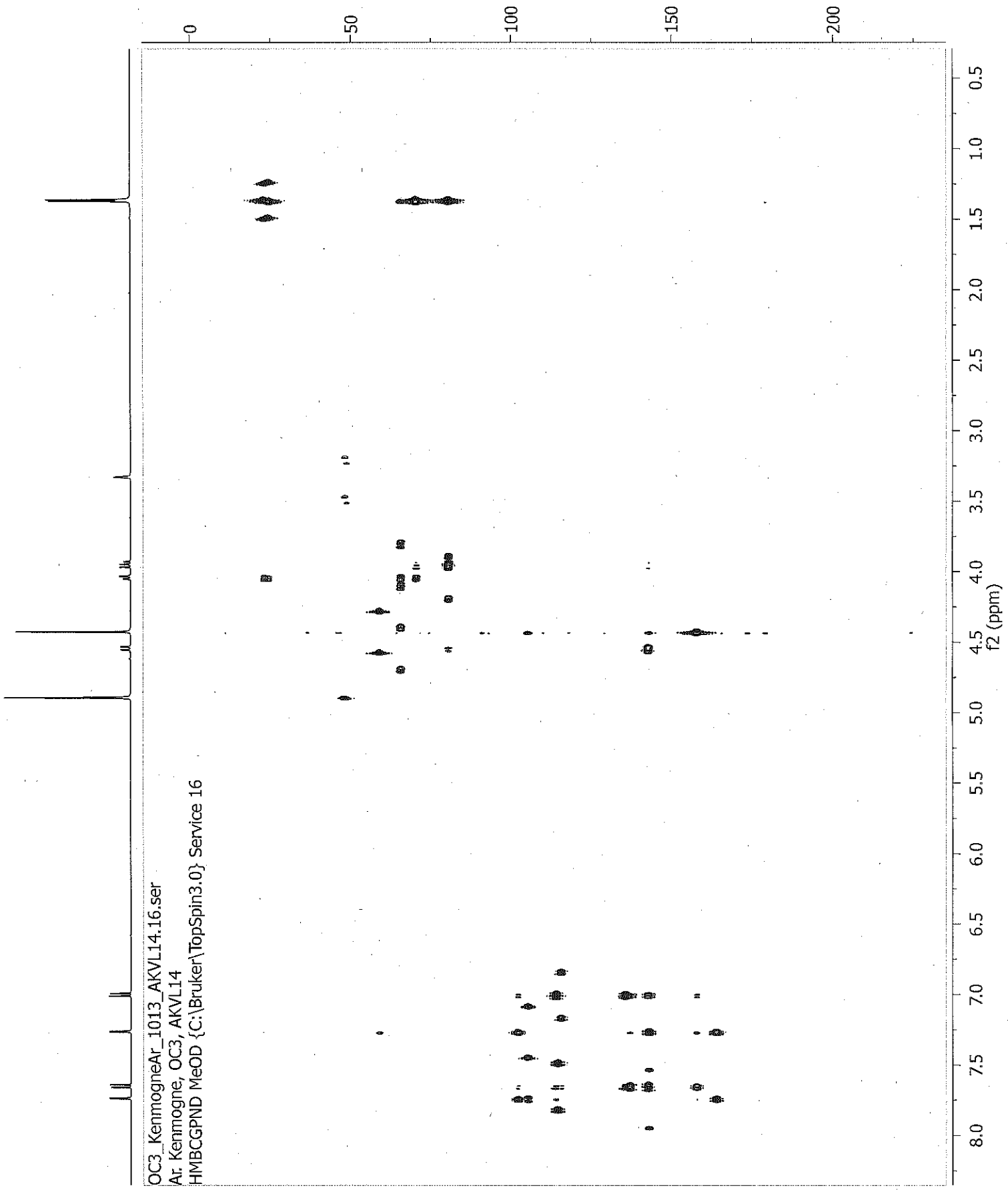
0
-10
-20
30
-40
-50
-60
-70
80
90
-100
-110
-120
-130
-140
-150
-160

0.5
1.0
1.5
2.0
2.5
3.0
3.5
4.0
4.5
5.0
5.5
6.0
6.5
7.0
7.5
8.0

f2 (ppm)



OC3_KenmogneAr_1013_AKVL14.16.ser
Ar: Kenmogne, OC3, AKVL14
HMBCGPND MeOD {C:\Bruker\TopSpin3.0} Service 16



OC3_KenmogneAr_1013_AKVL14.17.ser
Ar: Kenmogne, OC3, AKVL14
NOESYPHSW MeOD {C:\Bruker\TopSpin3.0} Service 16

