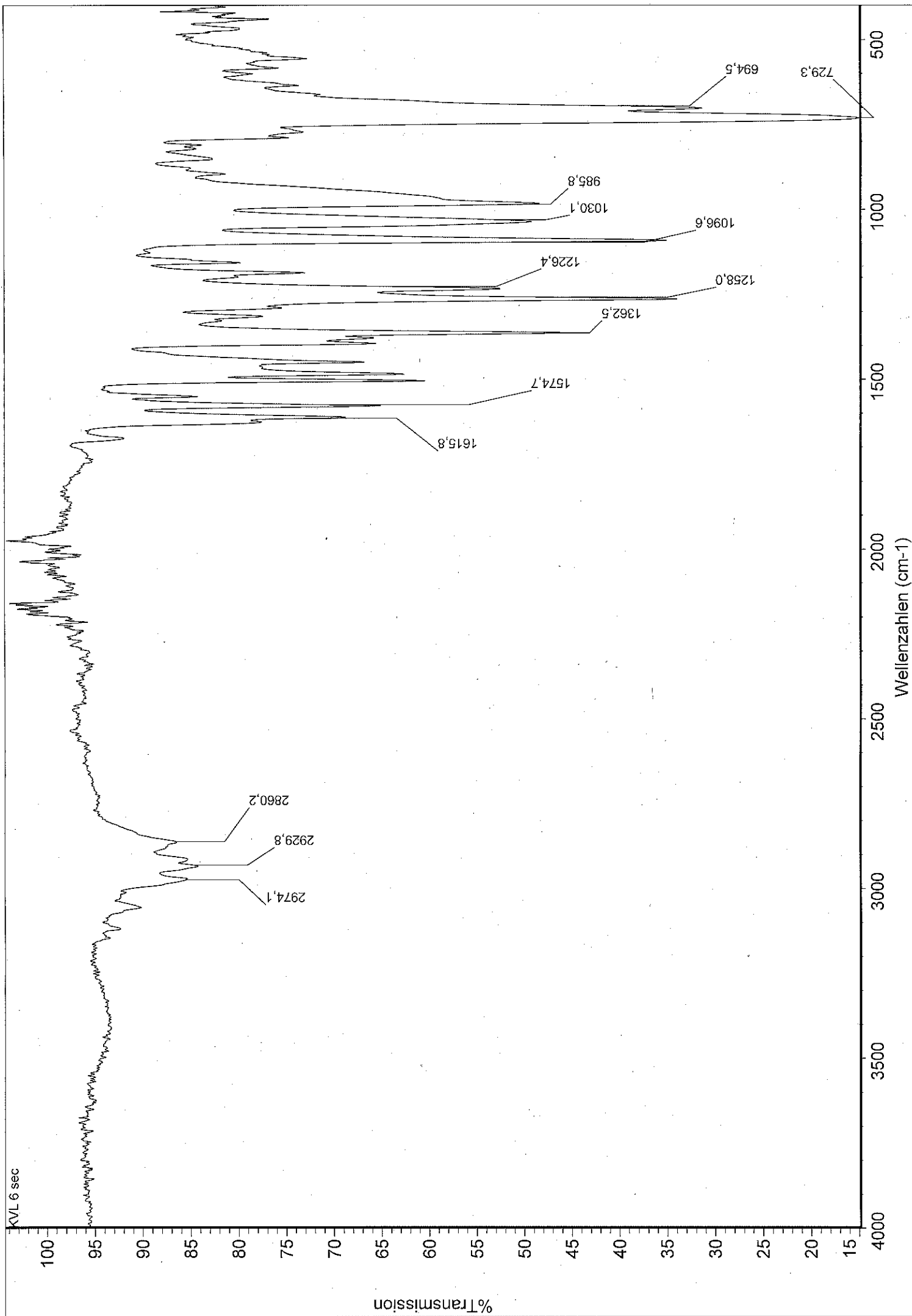


# COMPOUND 1



# Analysis Report

## Analysis Info

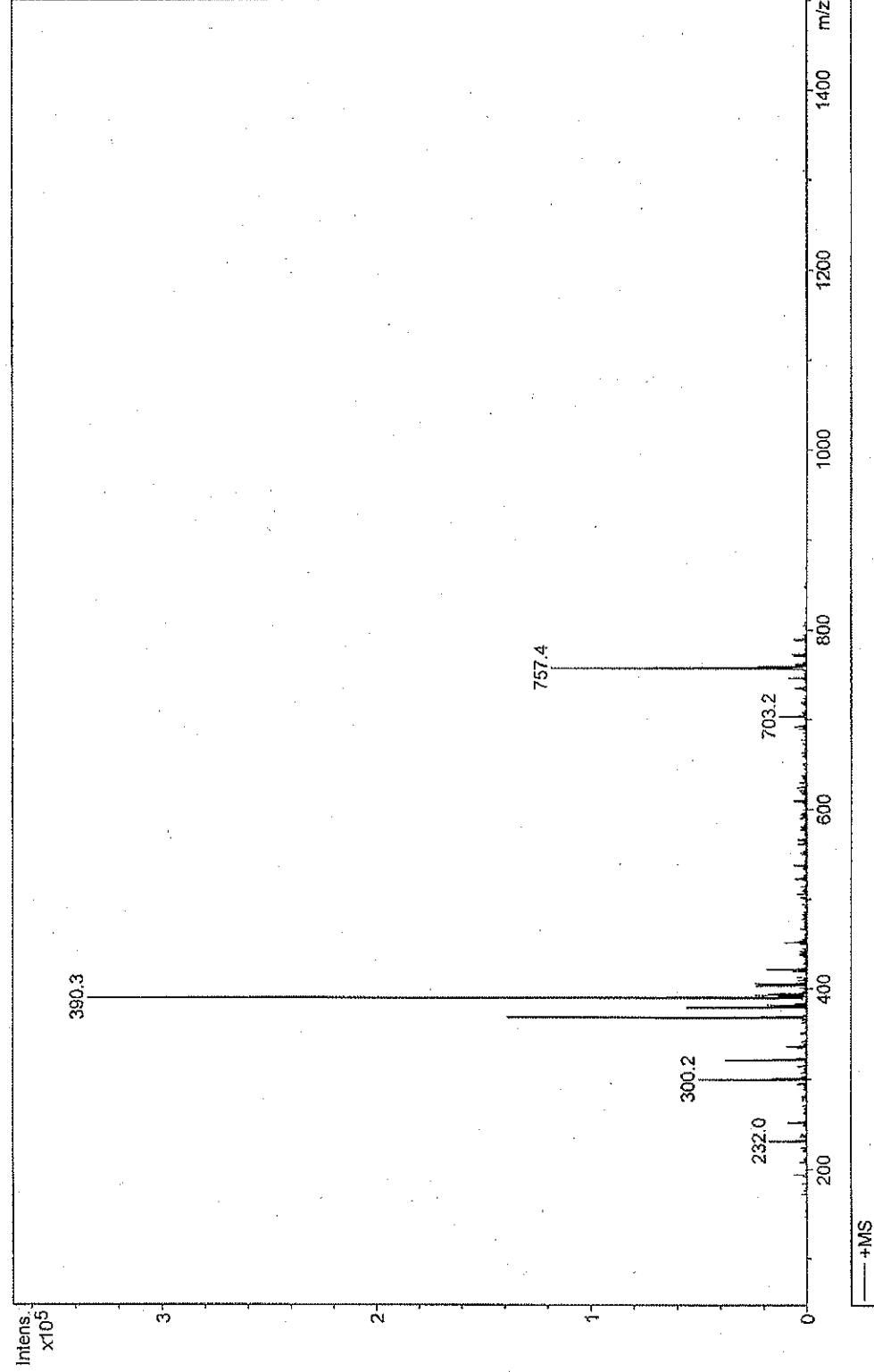
Analysis Name OC3\_KenmogneAr\_0822\_AKVL6\_01.d  
Method Tune-nan.MS  
Workgroup OC3

## 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

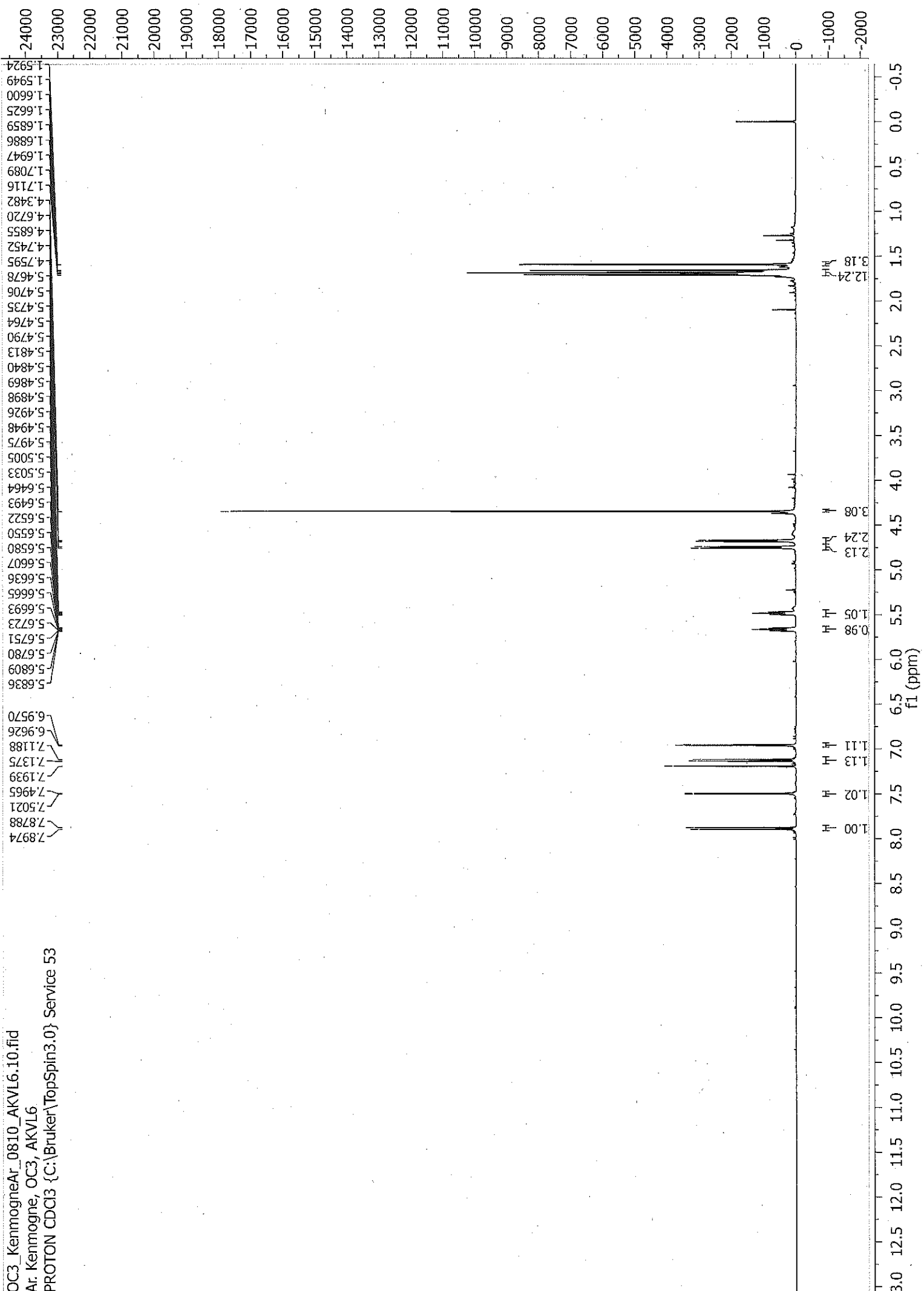


## Acquisition Parameter

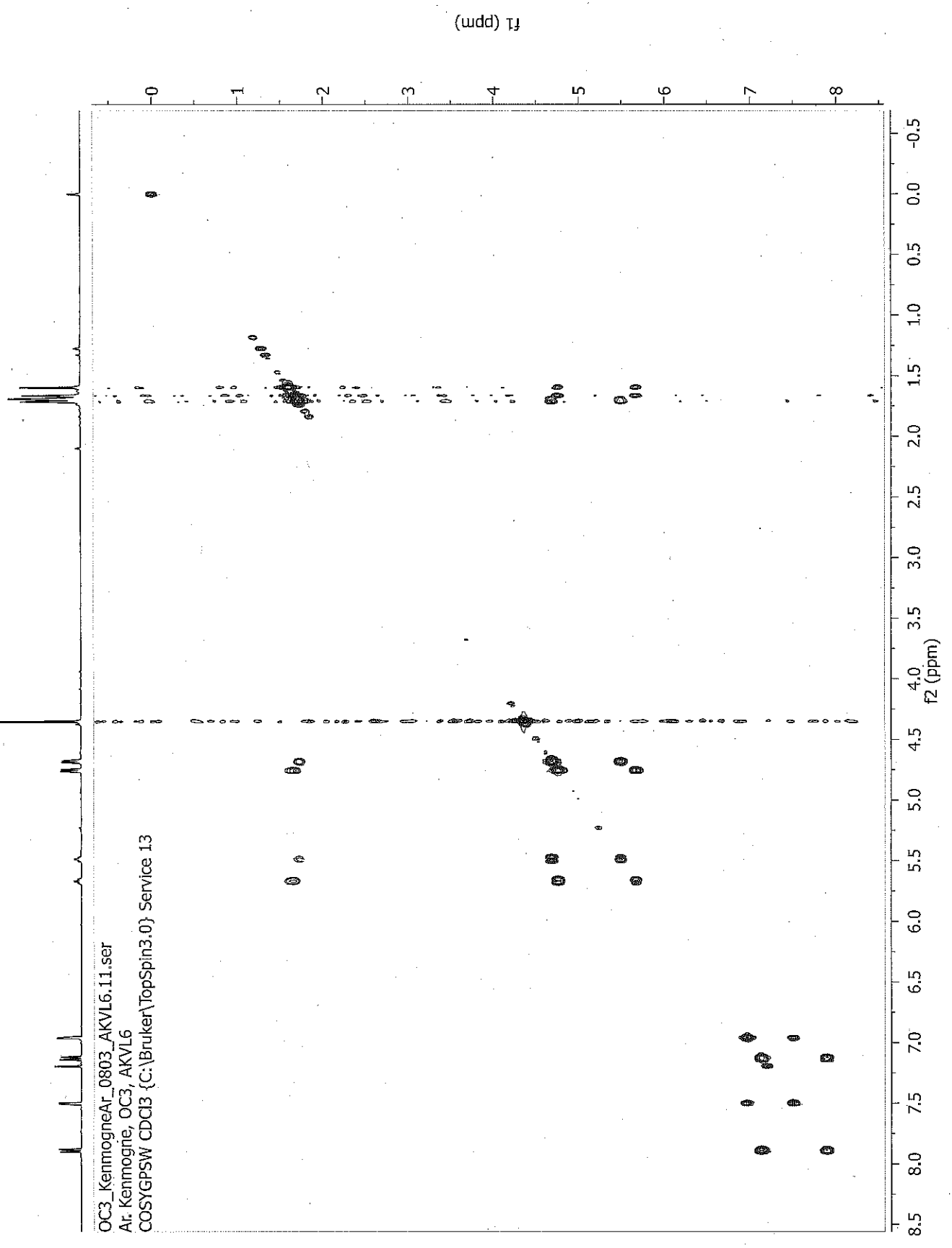
Mode NanoESI, off-line  
Ion Source Type Positive  
Ion Polarity Std/Normal  
Mass Range Mode 50 m/z  
Scan Begin 1500 m/z  
Scan End 20 Spectra  
Averages on  
Rolling, Averages 2 cis  
Tune SPS  
Target Mass 400 m/z  
Compound Stability 40 %  
Smart Parameter Setting active

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

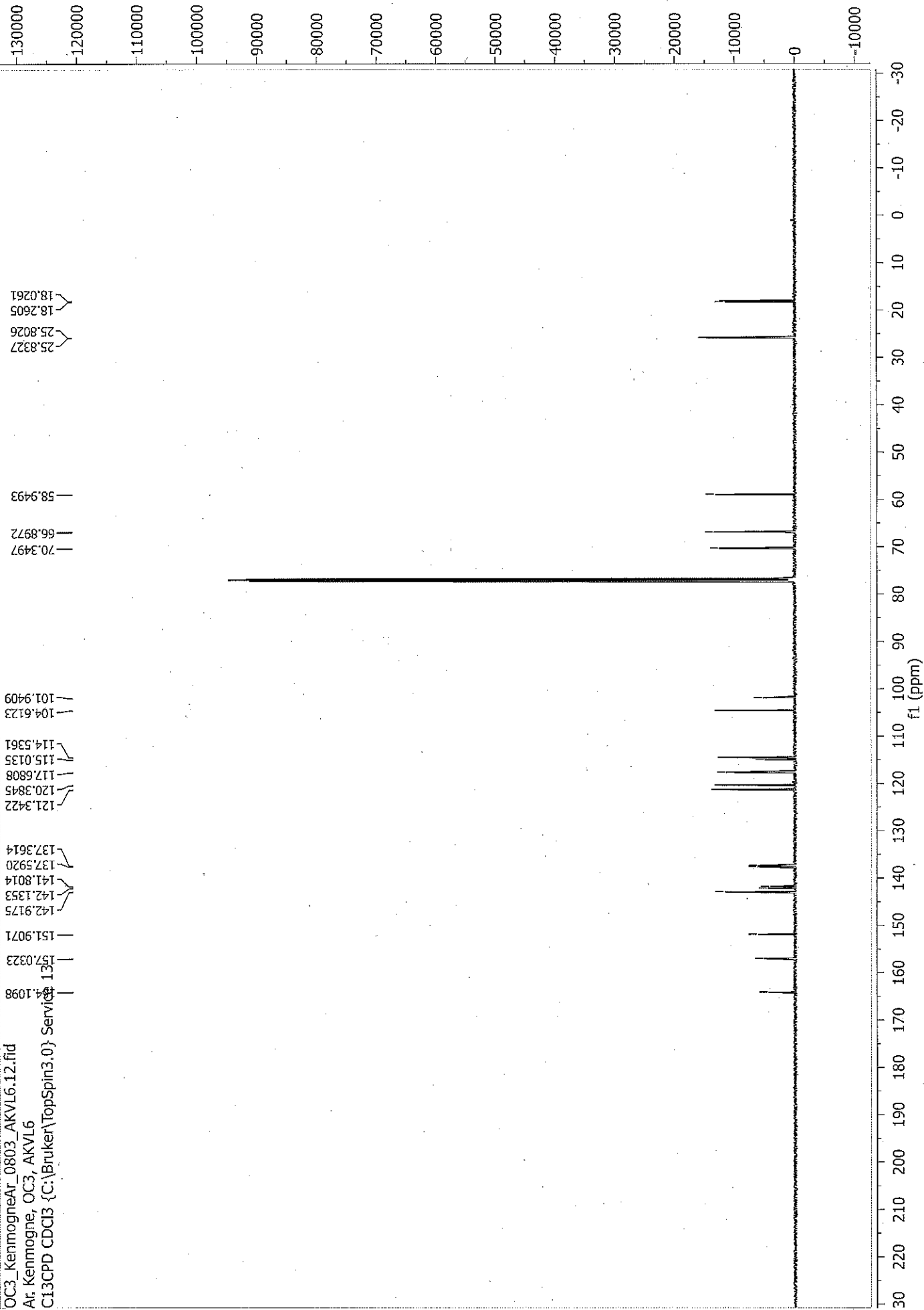
OC3\_KenmogneAr\_0810\_AKVL6.10.fid  
Ar: Kenmogne, OC3, AKVL6  
PROTON CDCl3 {C:\Bruker\TopSpin3.0} Service 53



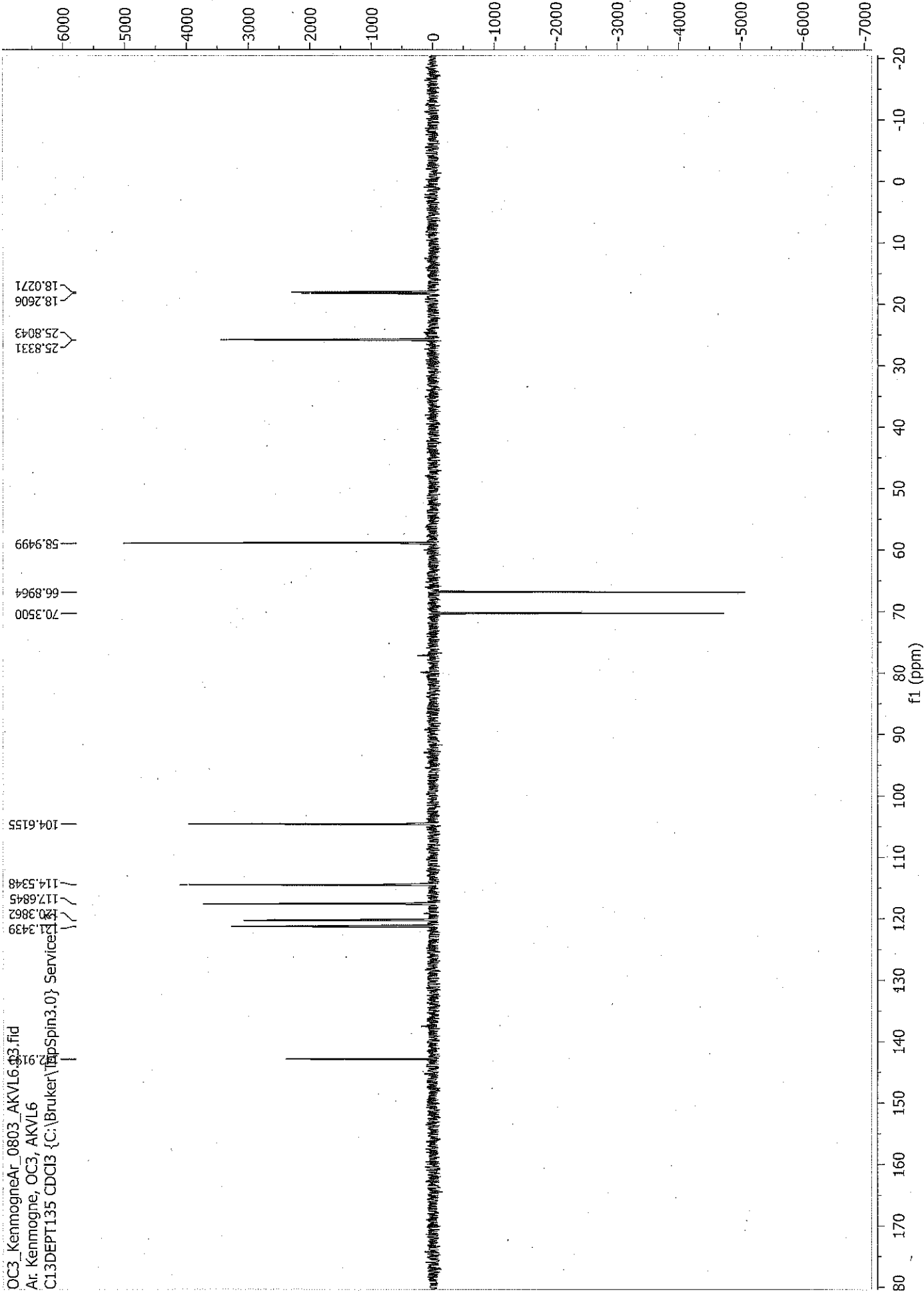
OC3\_KennognreA1\_0803\_AKVL6.11.ser  
A1: Kennognre, OC3, AKVL6  
COSYGPSW CDCl3 {C:\Bruker\TopSpin3.0} Service 13



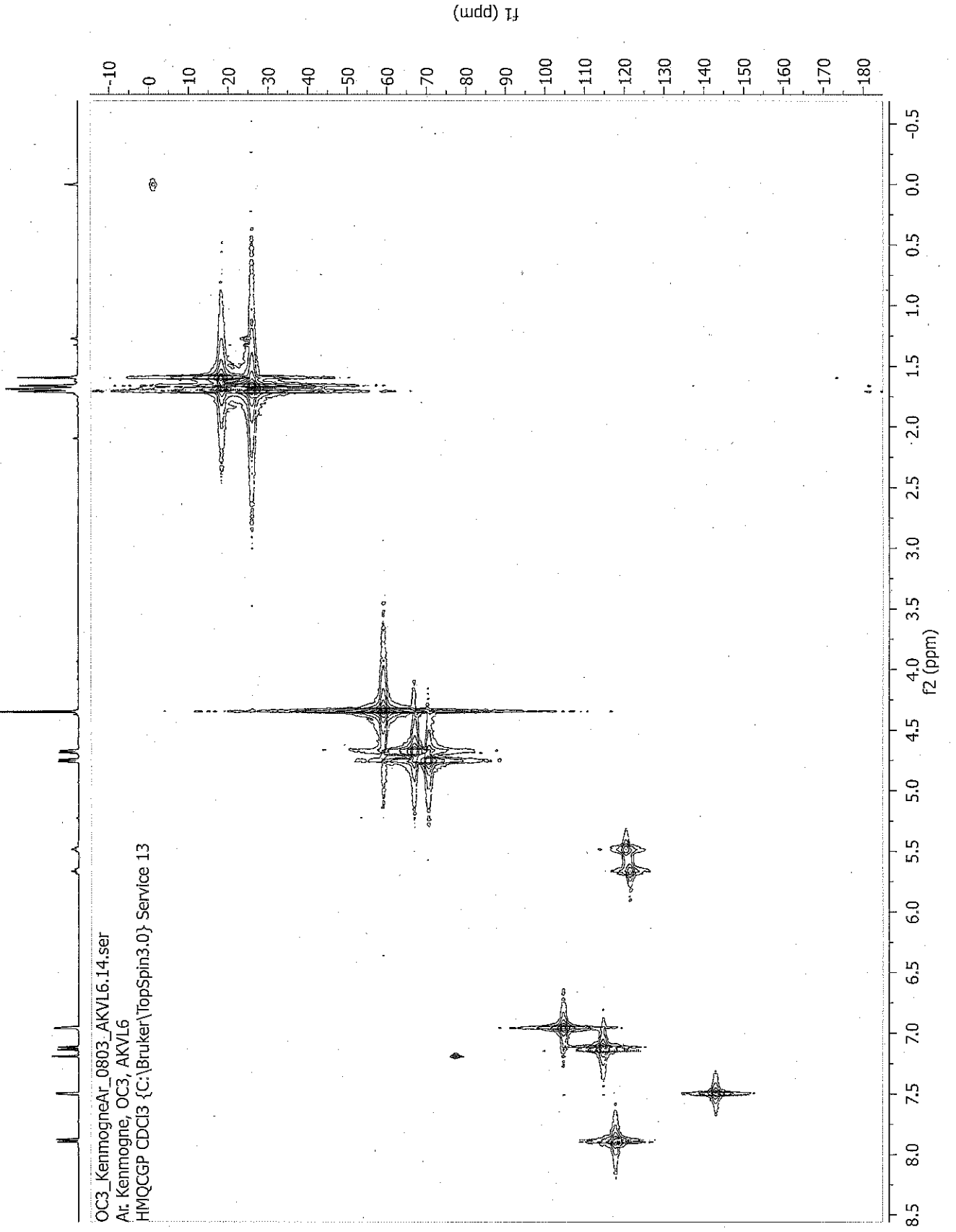
OC3\_KenmogneAr\_0803\_AKVL6.12.fid  
At: Kenmogne, OC3, AKVL6  
C13CPD CDC13 {C:\Bruker\TopSpin3.0} Service 1.3



OC3\_KenmogneAr\_0803\_AKVL6\_03.fid  
Ar: Kenmogne, OC3, AKVL6  
C13DEPT135 CDCIB {C:\Bruker\TopSpin3.0} Services



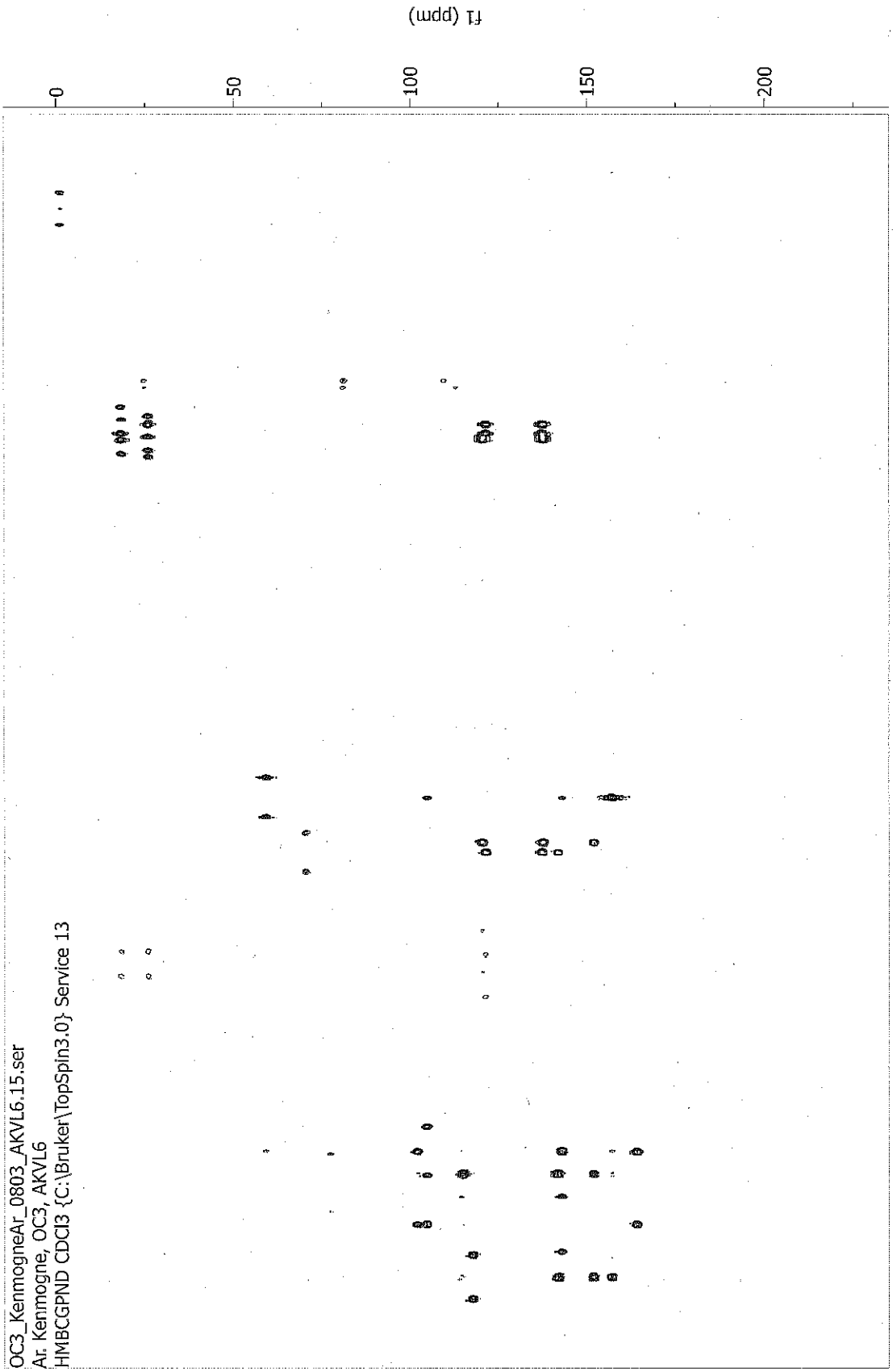
OC3\_KemogneA1\_0803\_AKVL6.14.ser  
A1: Kemogne, OC3, AKVL6  
HMQCGP CDCl3 {C:[Bruker\TopSpin3.0} Service 13



(uidd) F1



OC3\_KenmogneA1\_0803\_AKVL6.15.ser  
A1: Kenmogne, OC3, AKVL6  
HMBCGPND CDC13 {C:\Bruker\TopSpin3.0} Service 13

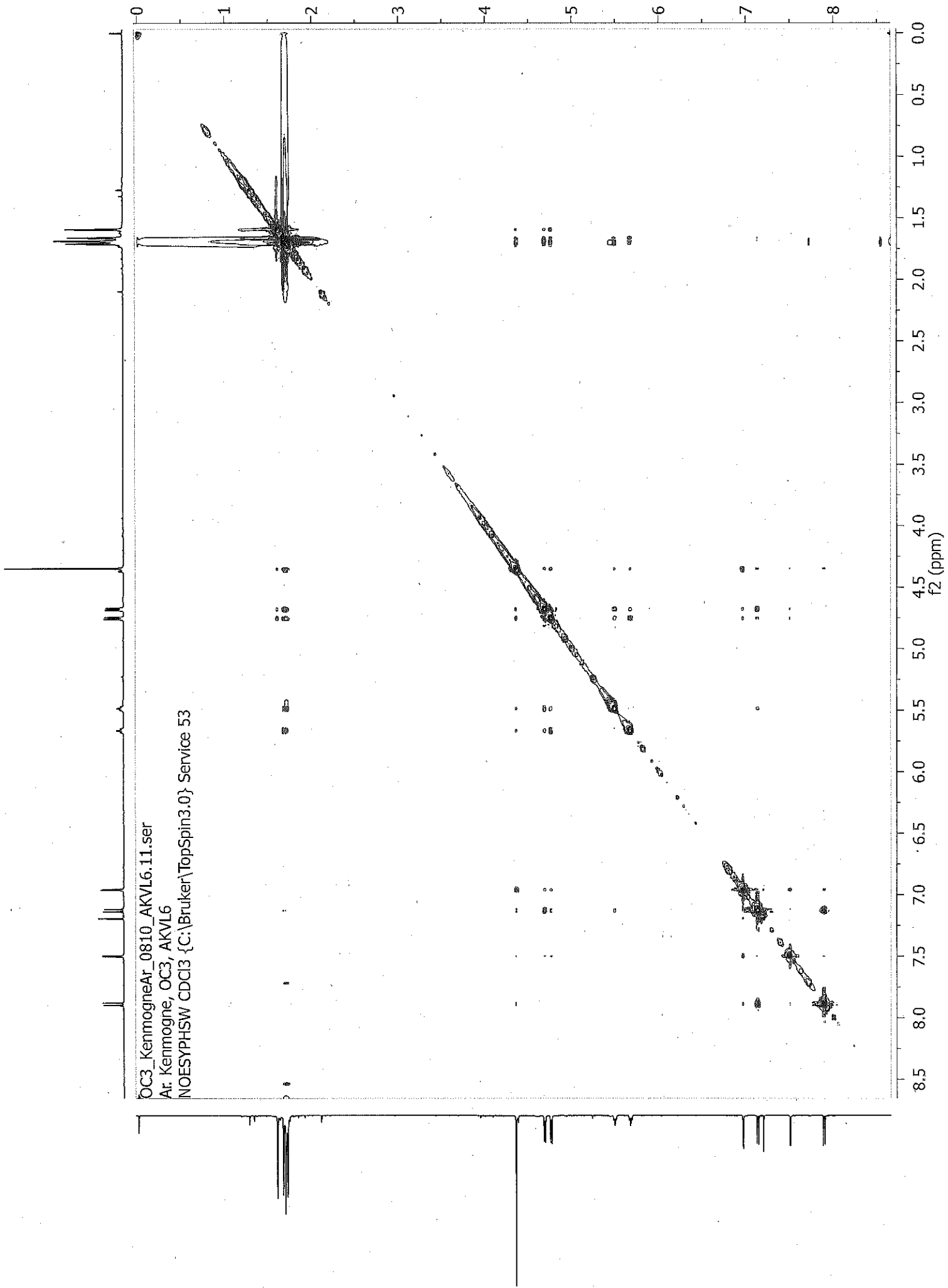


8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5

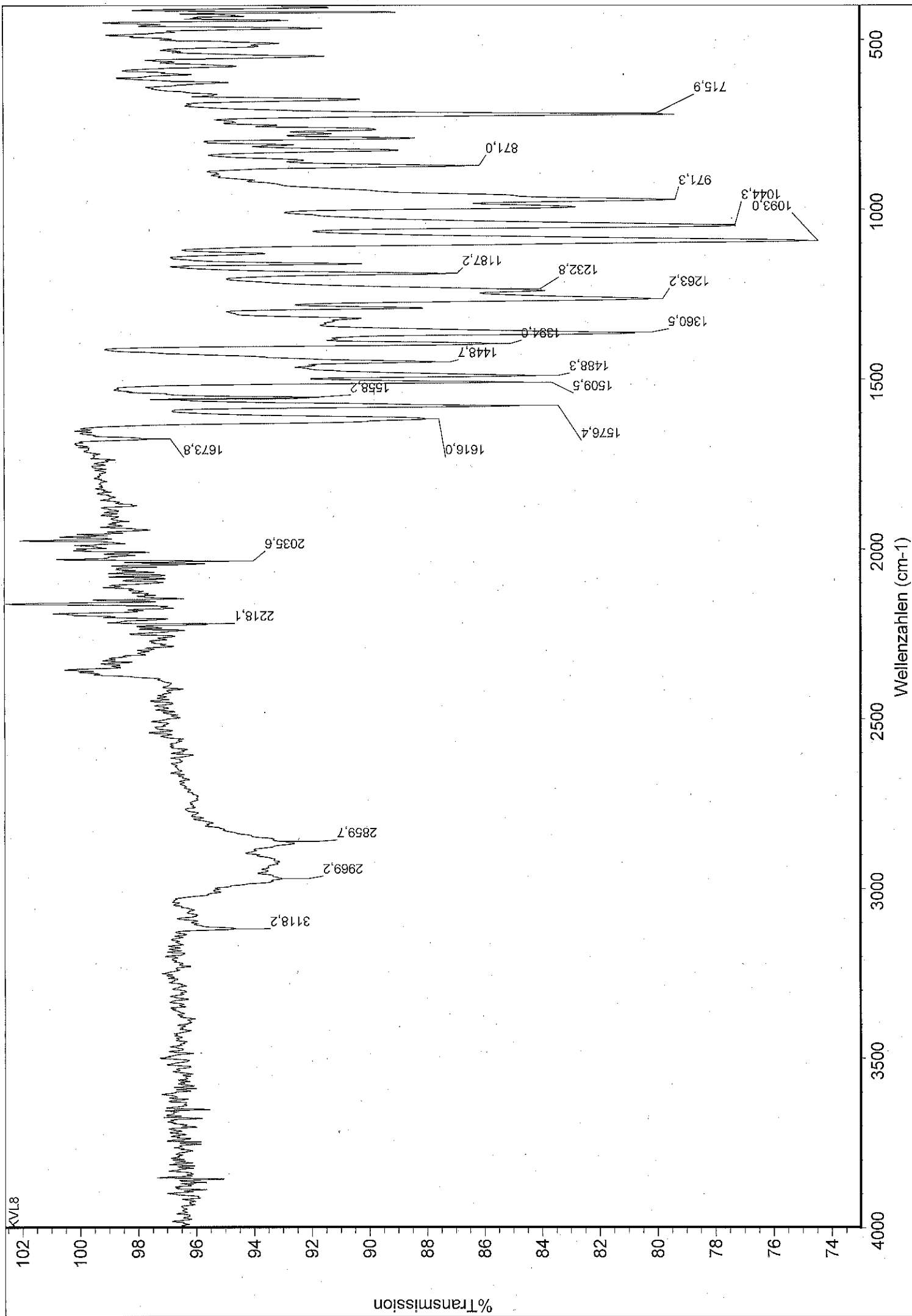
f1 (ppm)

0 50 100 150 200

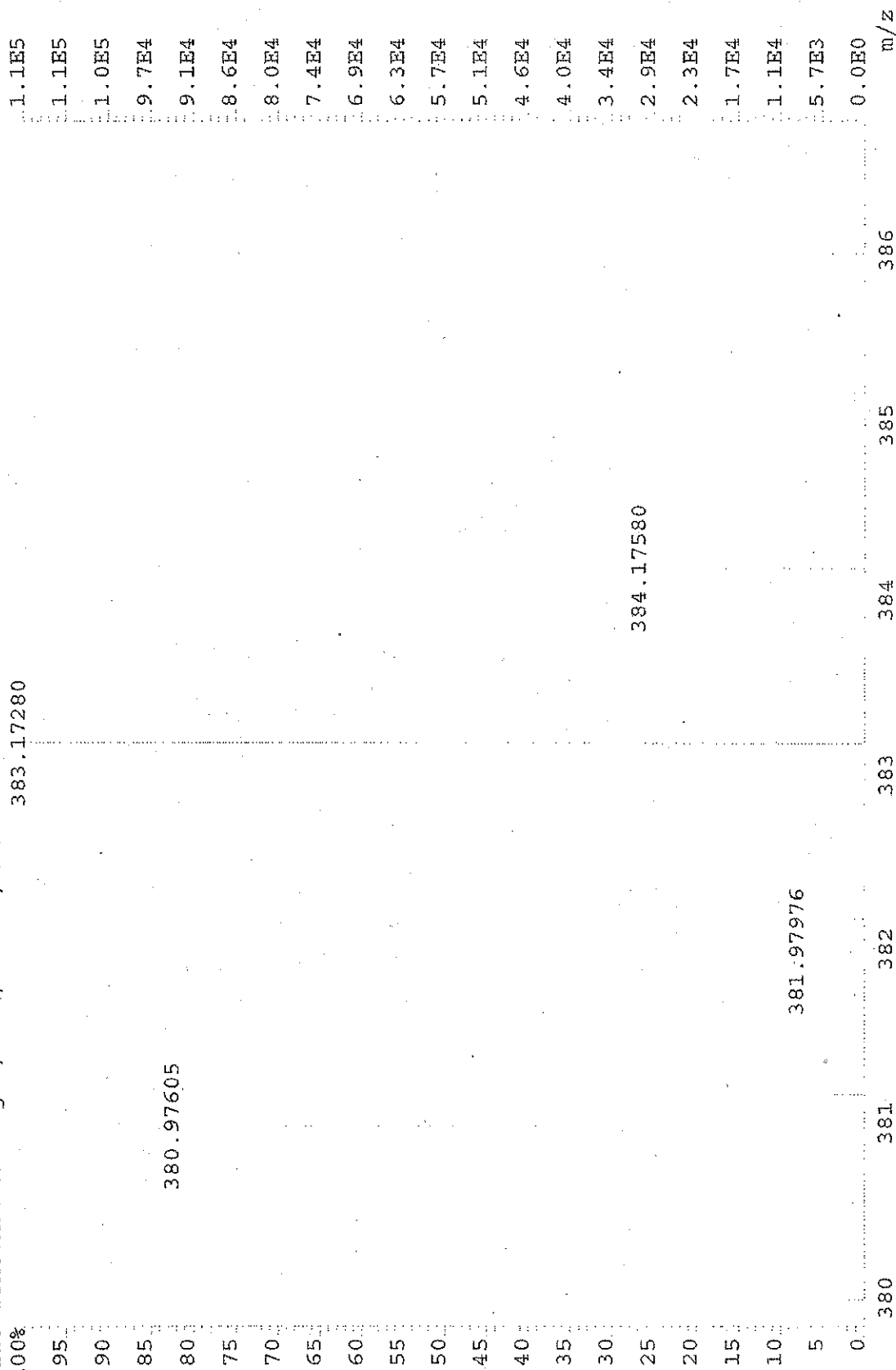
OC3\_KenmogneAr\_0810\_AKVL6.11.ser  
Ar: Kenmogne, OC3, AKVL6  
NOESYPHSW CDCI3 {C:\Bruker\TopSpin3.0} Service 53



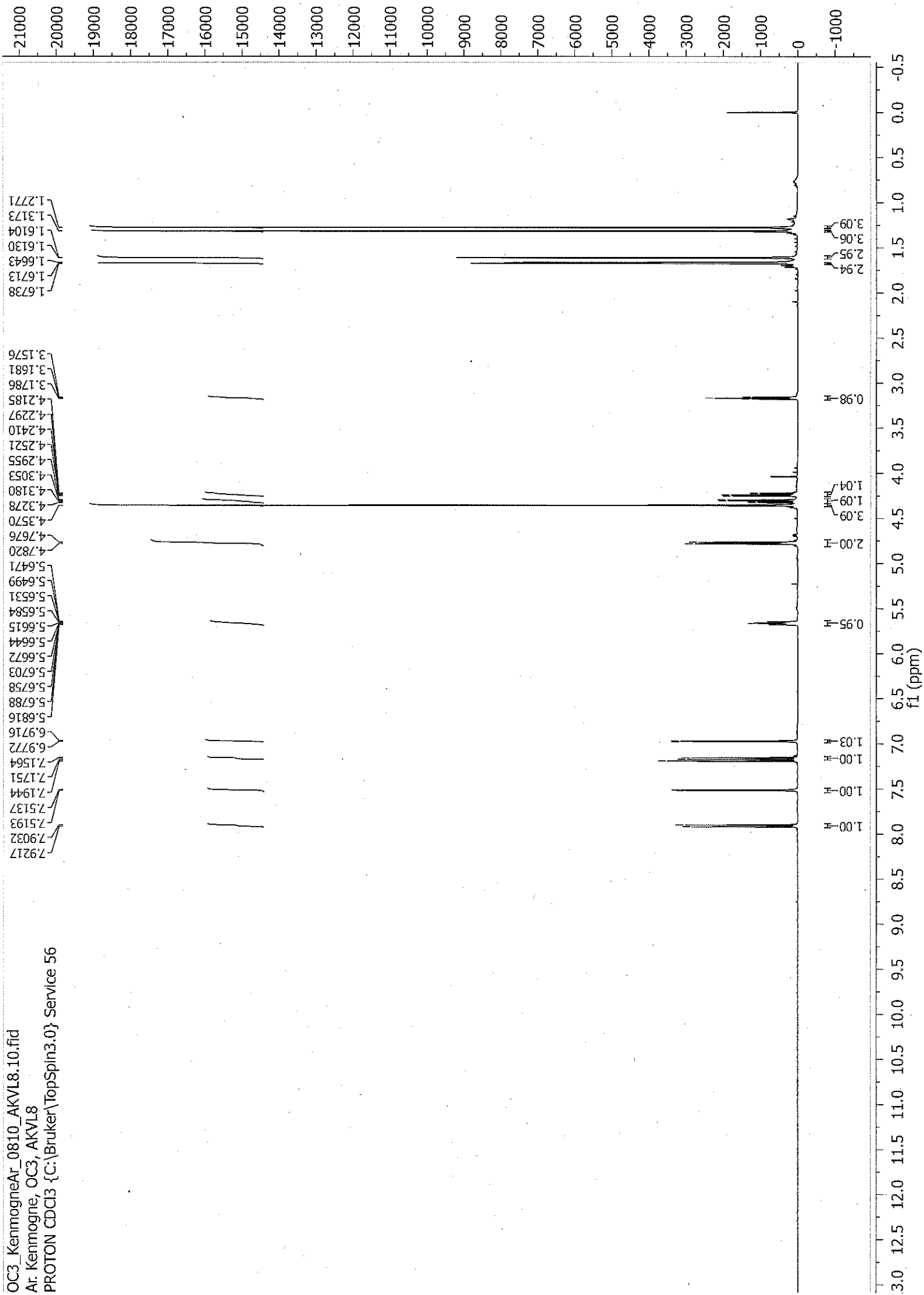
# COMPOUND 2



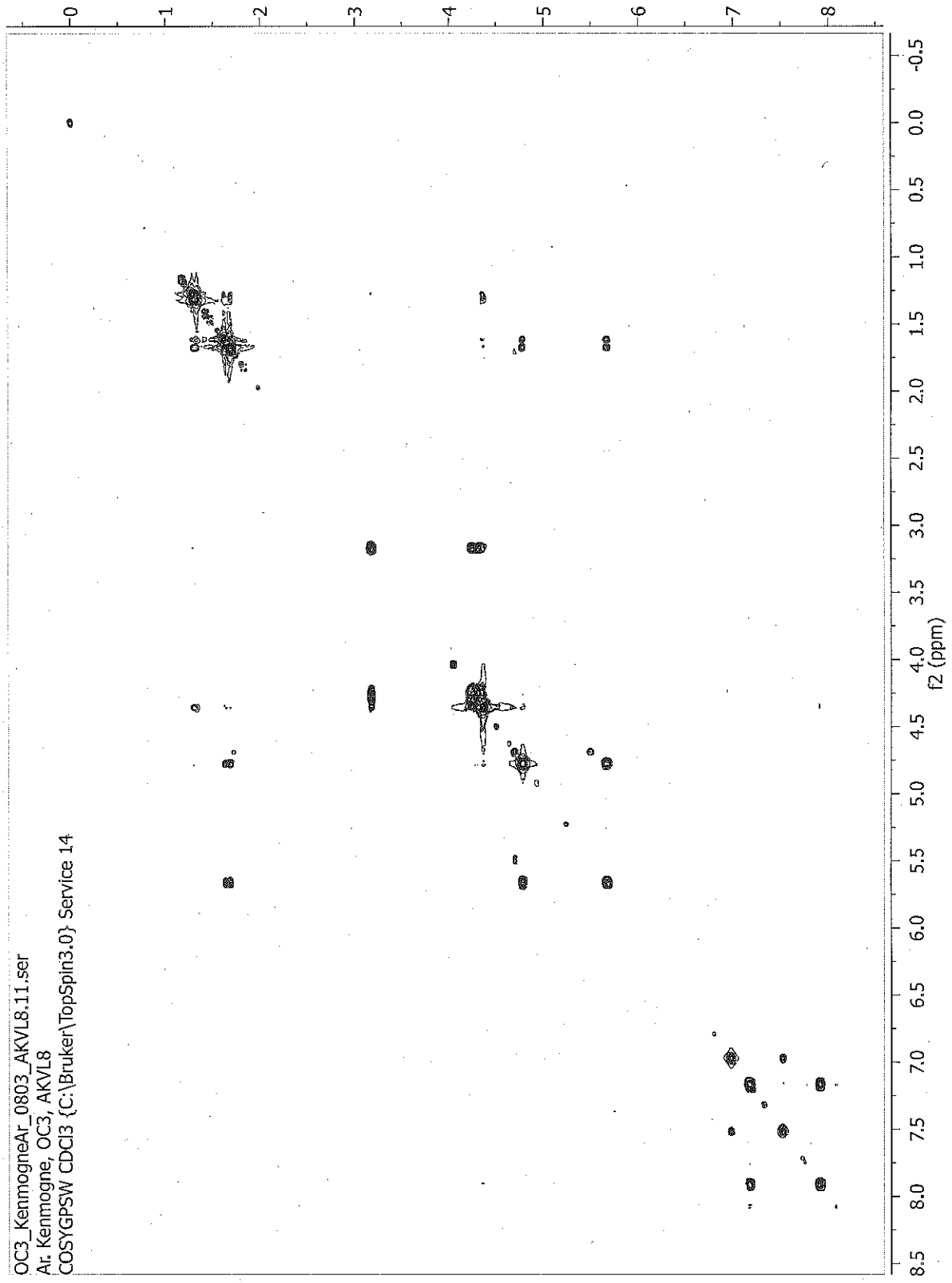
File:MFB2016\_109 Ident:48 52 SMO(1,7) PKD(7,3,7,0.50%,0.0,0.00%,F,F) SPEC(Heights, Centroid) Acq>  
 AutoSpec EI+ Voltage BpM:383 BpI:114236 TIC:359861 Flags:NORM  
 File Text:Ar. Kenmogne, OC3, AKVL8, HWP



OC3\_KenmogneAr\_0810\_AKVL8.10.fid  
Ar: Kenmogne, OC3, AKVL8  
PROTON CDCl3 {C:\Bruker\TopSpin3.0} Service 56



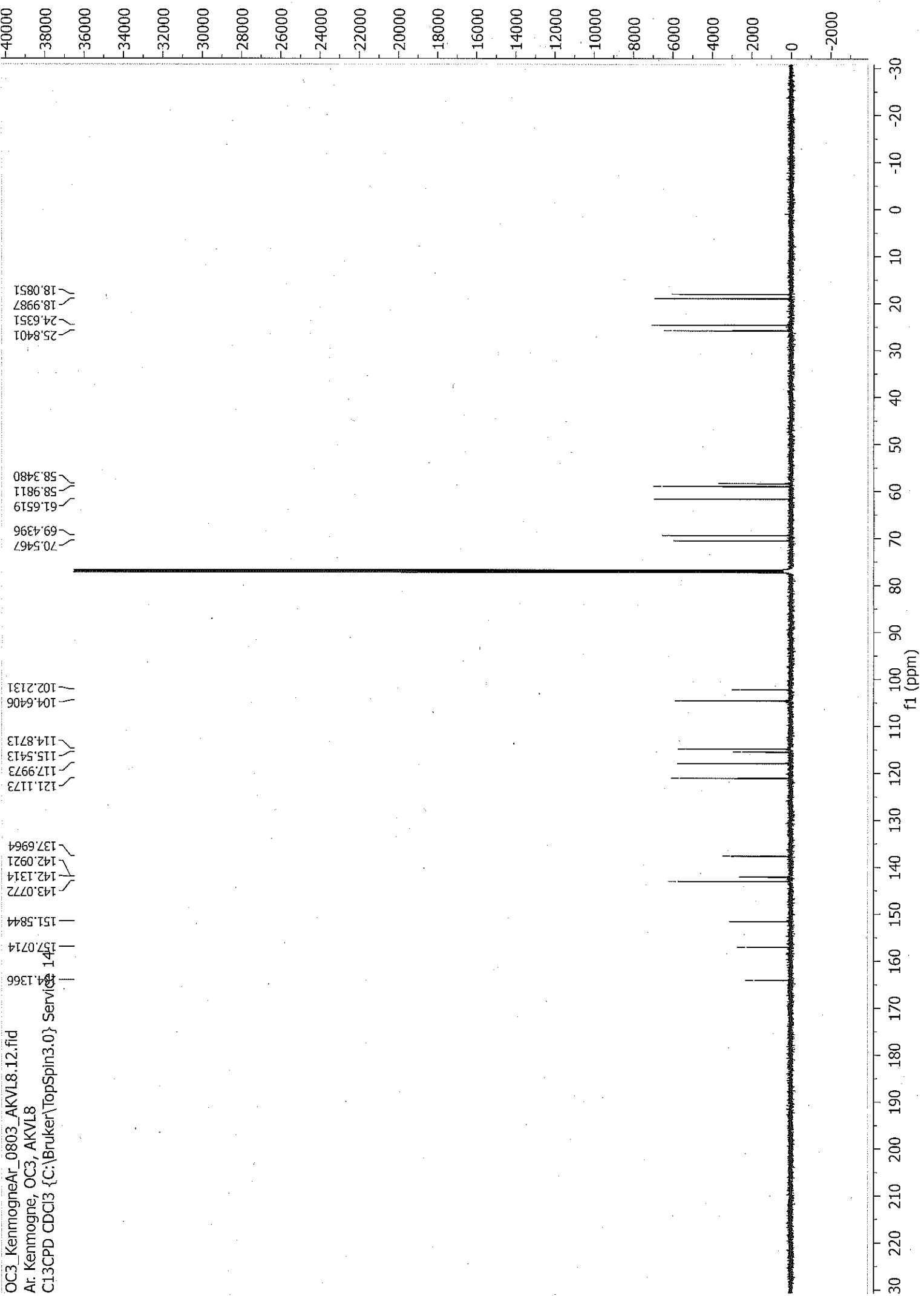
OC3\_KennogneAr\_0803\_AKVL8.11.ser  
Ar, Kennogne, OC3, AKVL8  
COSYGPSW CDCl3 {c:\Bruker\TopSpin3.0} Service 14



f1 (ppm)

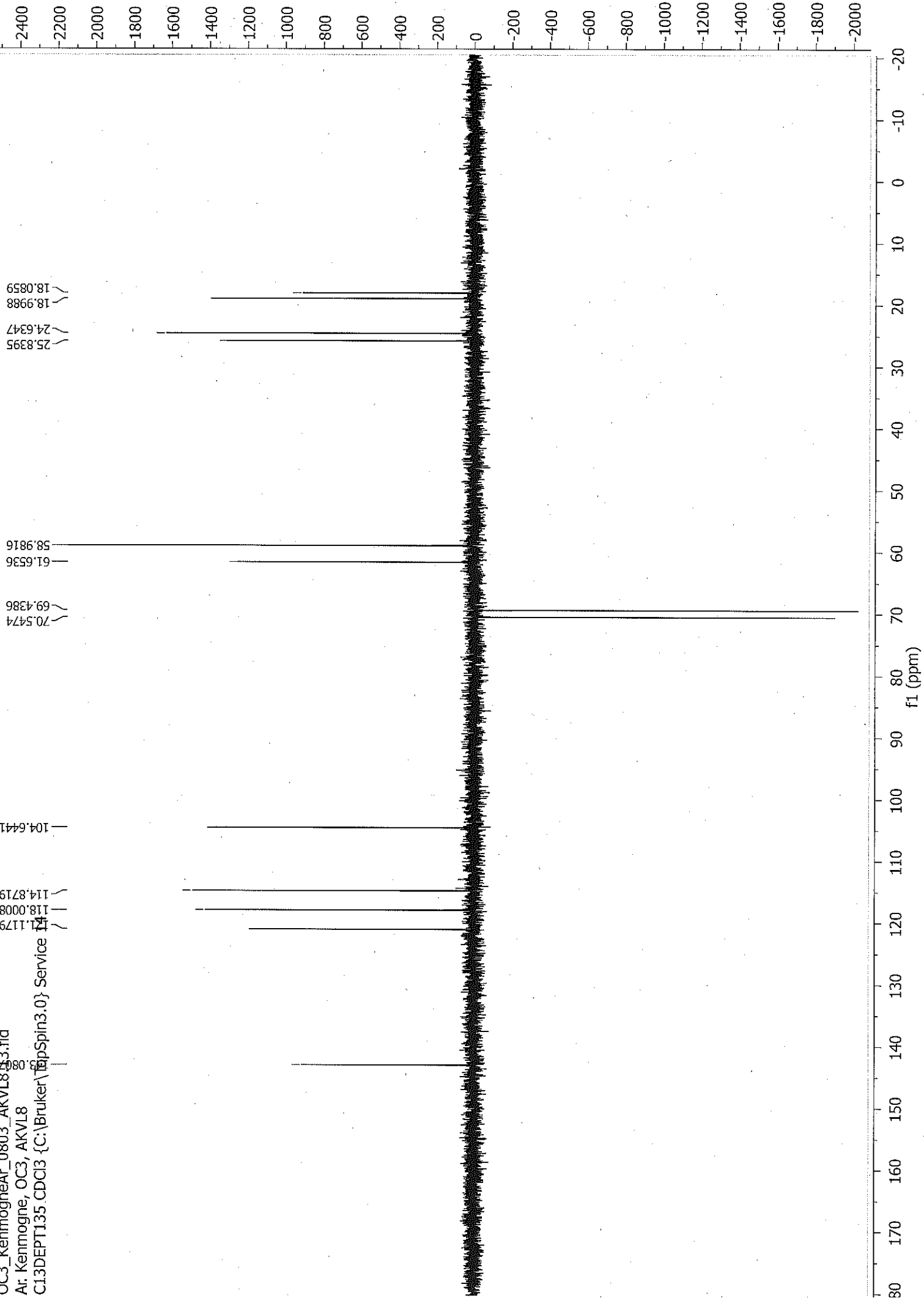
f2 (ppm)

OC3\_KenmogneAr\_0803\_AKV18.12.fid  
Ar: Kenmogne, OC3, AKV18  
C13CPD CDCl3 {C:\Bruker\TopSpin3.0} Service

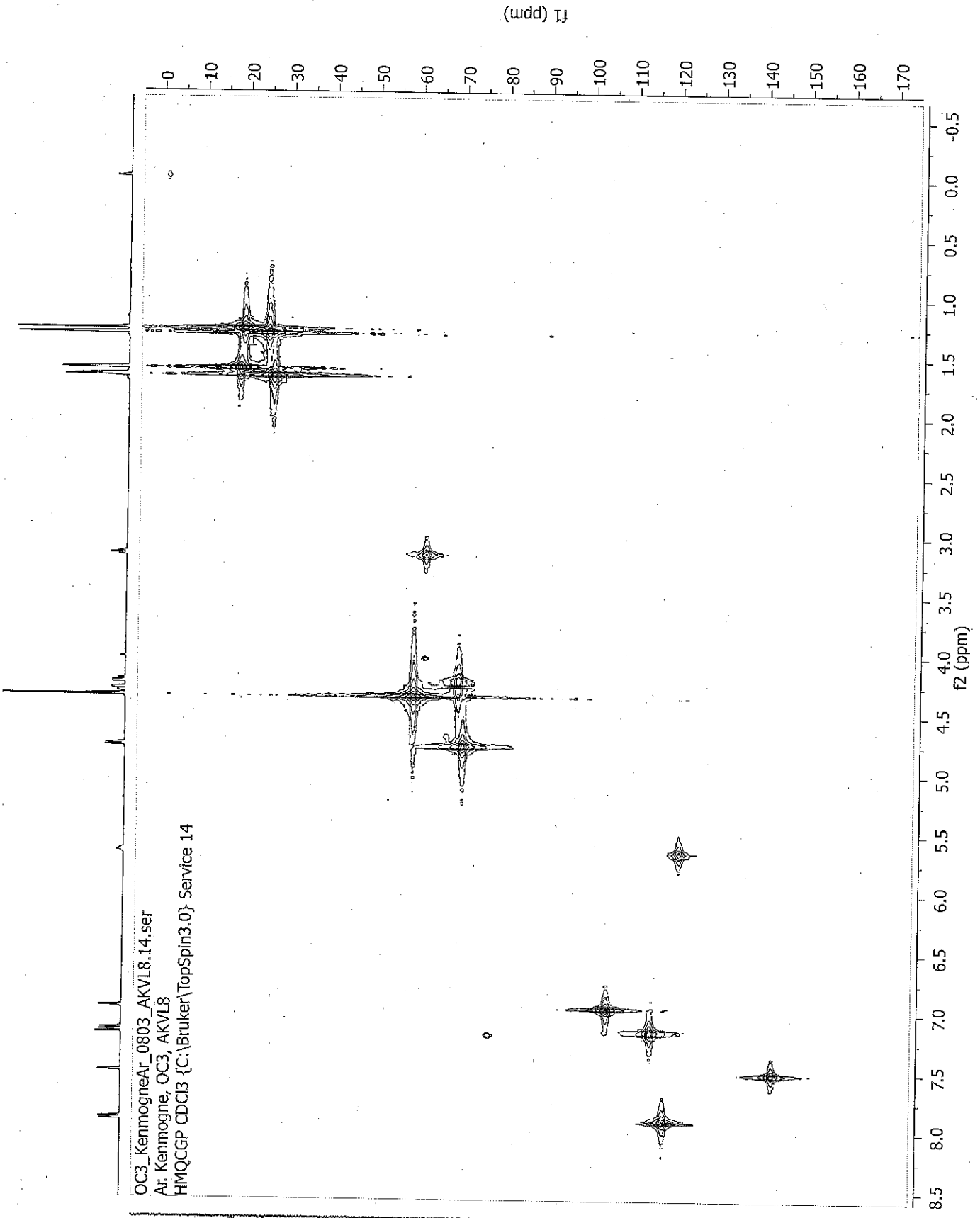




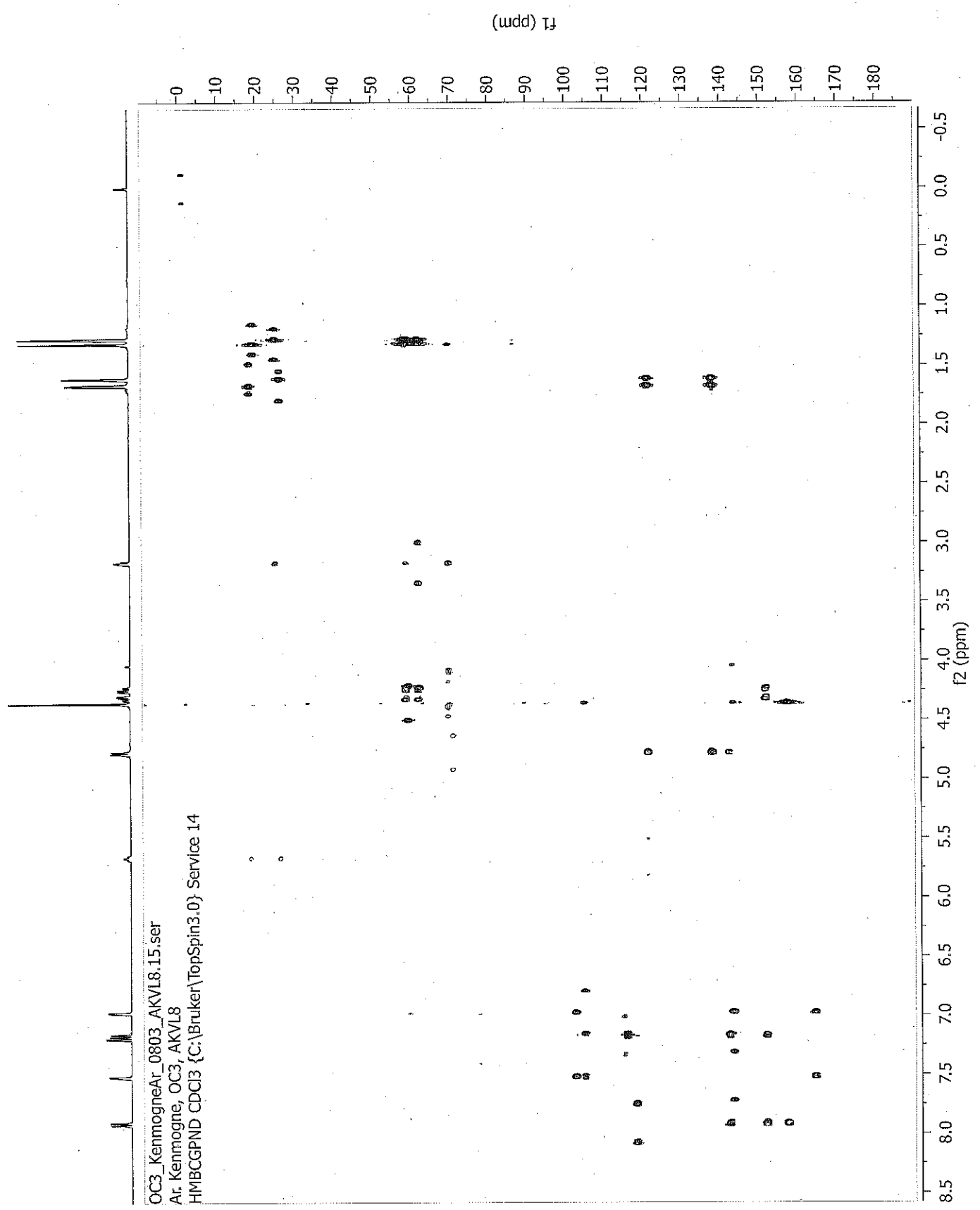
OC3\_KenmogneAr\_0803\_AKVL853.fid  
Ar: Kenmogne, OC3, AKVL8  
C13DEPT135.CDC3 {C:\Bruker\TopSpin3.0} Service 14



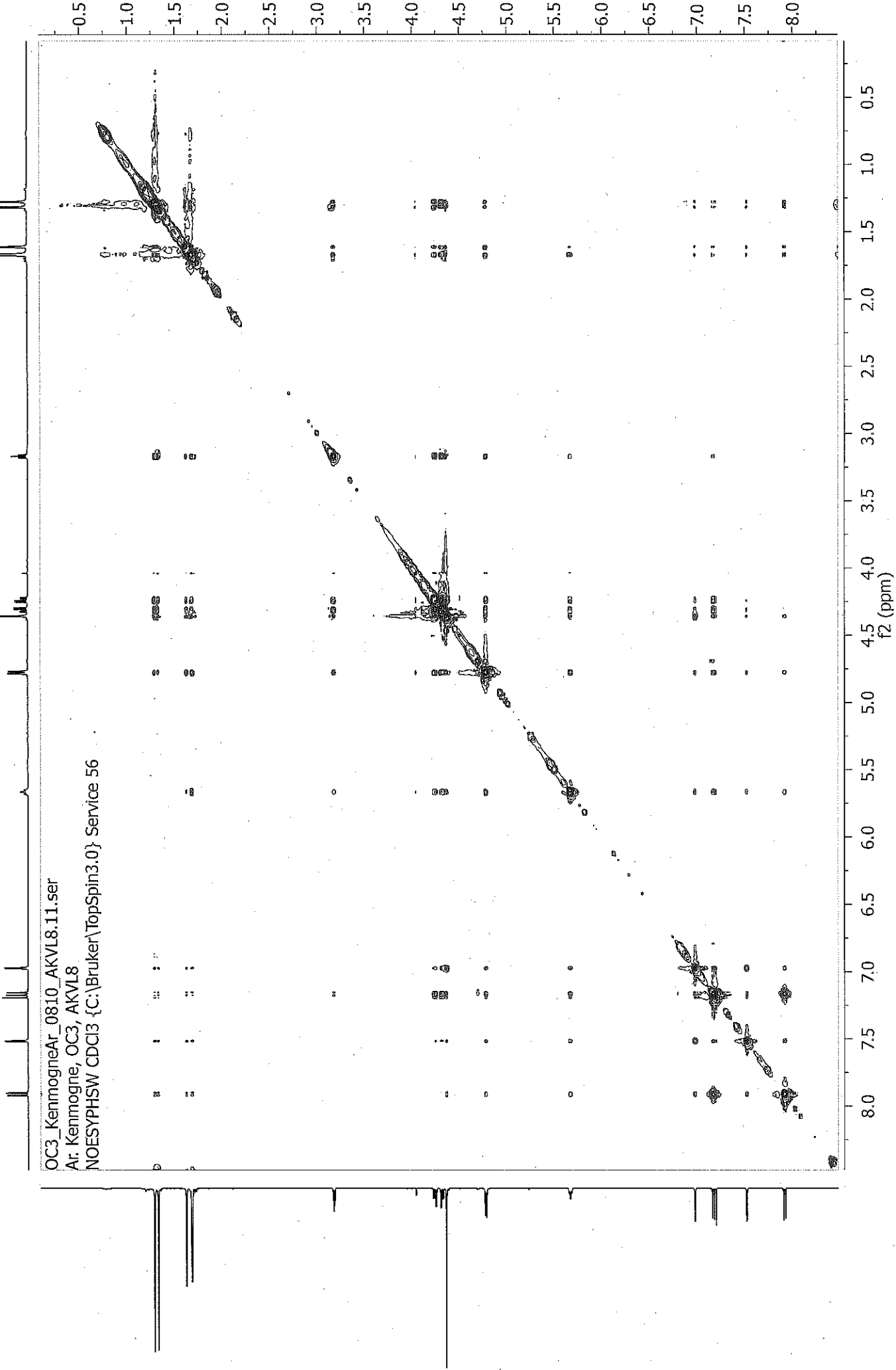
OC3\_KenmogneAr\_0803\_AKVL8.14.ser  
Ar: Kenmogne, OC3, AKVL8  
HMQCGP CDC13 {C:\Bruker\TopSpin3.0} Service 14



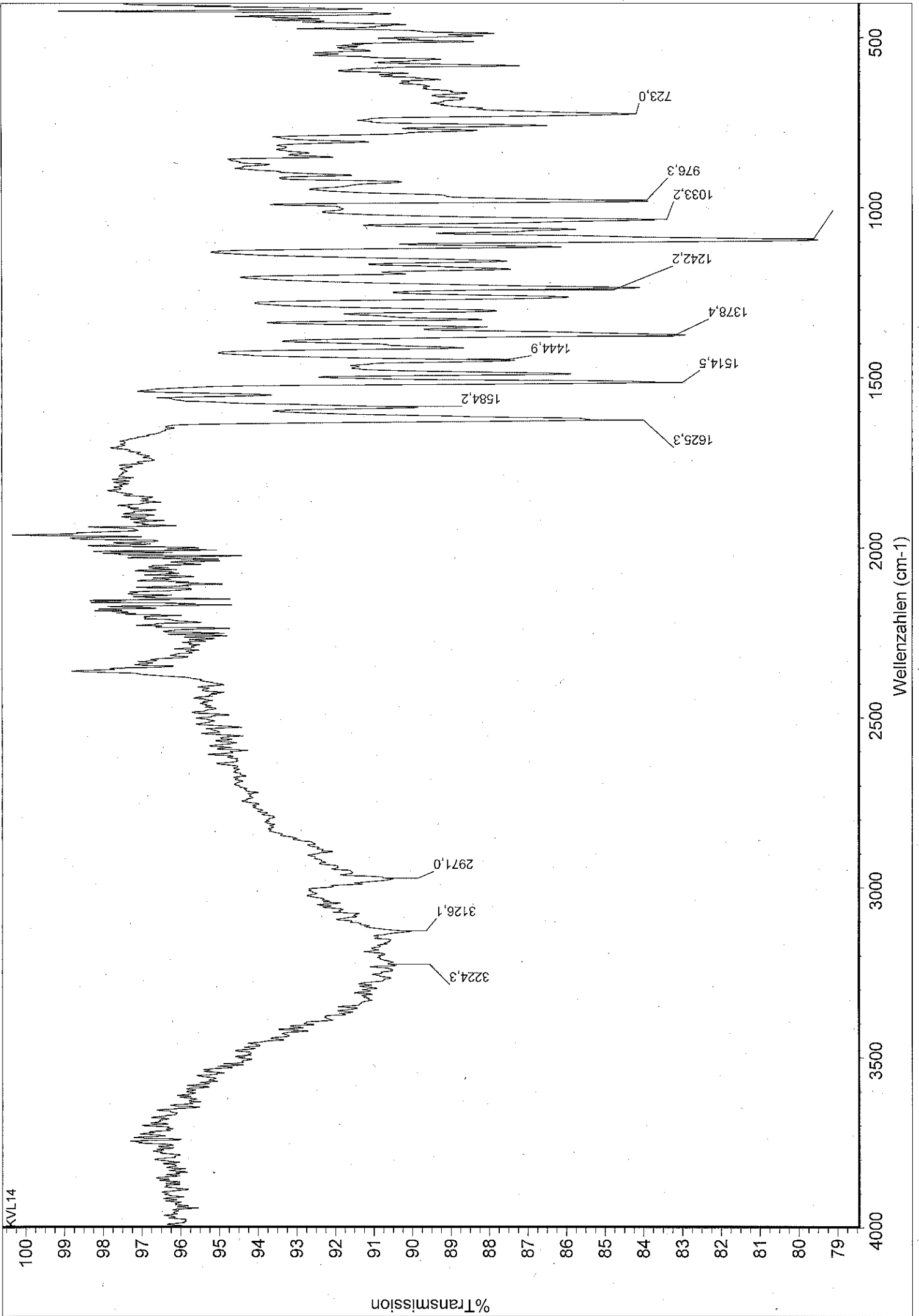
OC3\_KenmogneAr\_0803\_AKVL8.15.ser  
Ar: Kenmogne, OC3, AKVL8  
HMBCGPND CDCl3 {C:\Bruker\TopSpin3.0} Service 14



OC3\_KenmogneAr\_0810\_AKVL8.11.ser  
Ar. Kenmogne, OC3, AKVL8  
NOESYPHSW CDCI3 {C:\Bruker\TopSpin3.0} Service 56

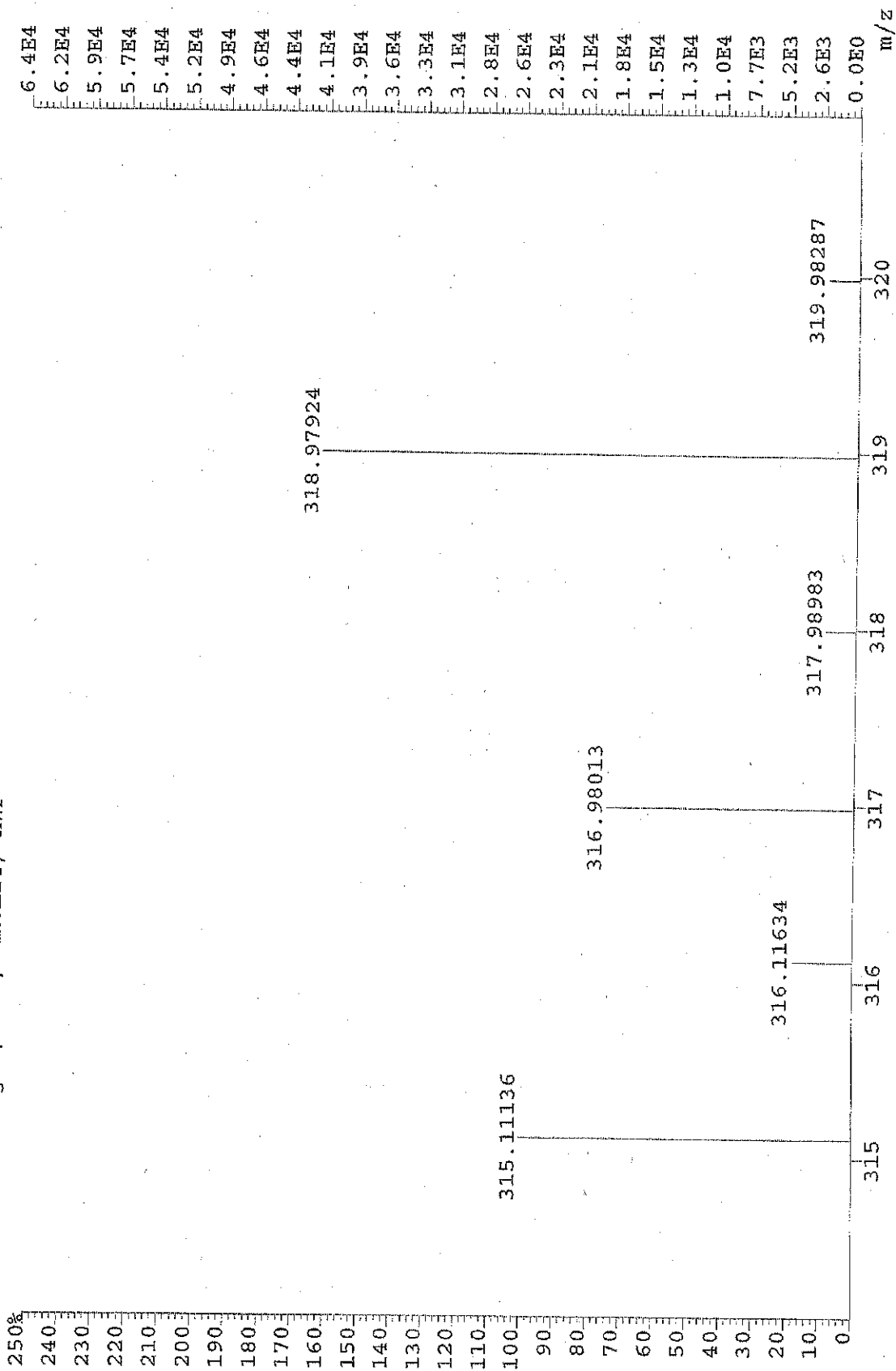


# COMPOUND 3

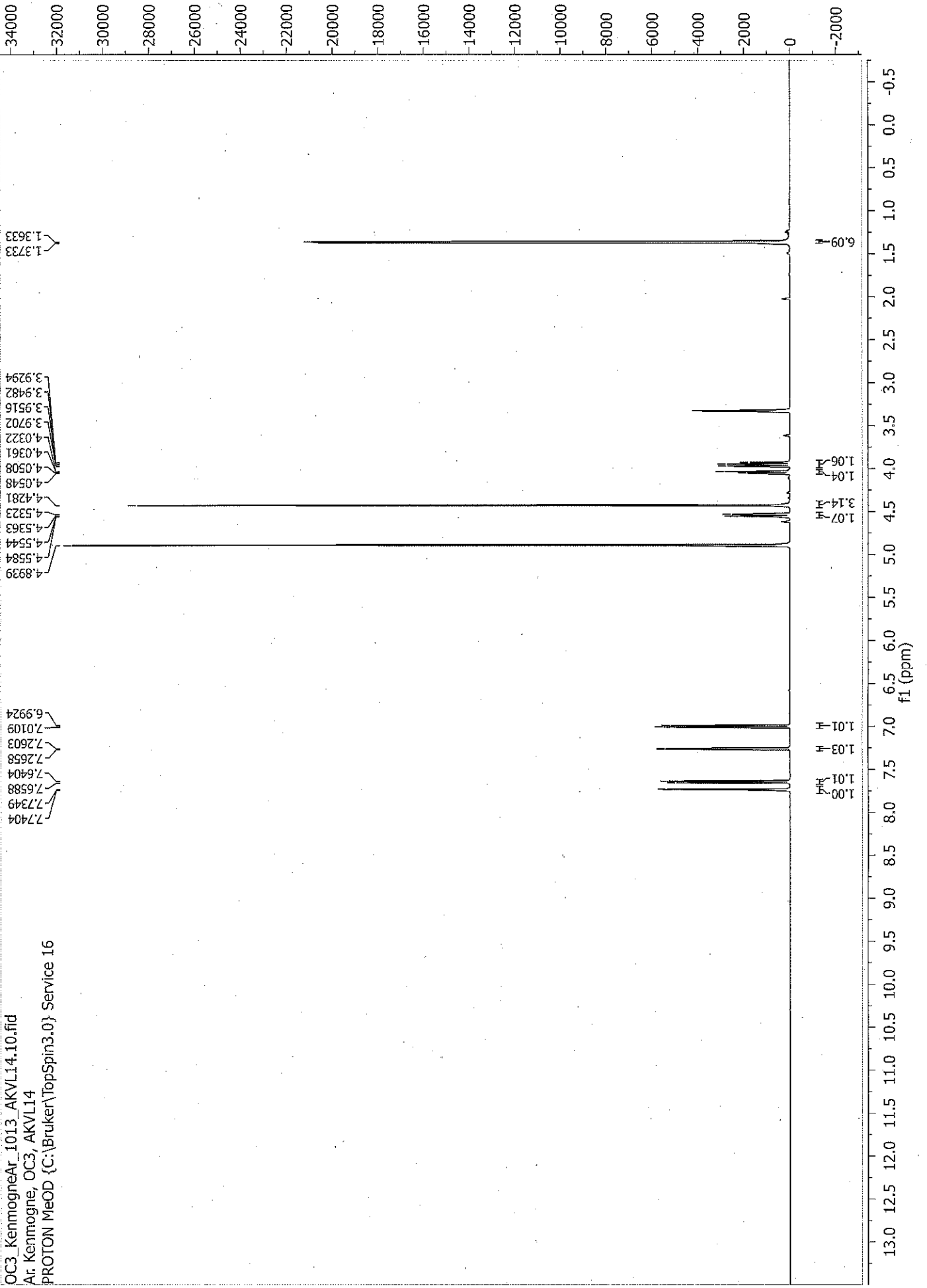


KVL14

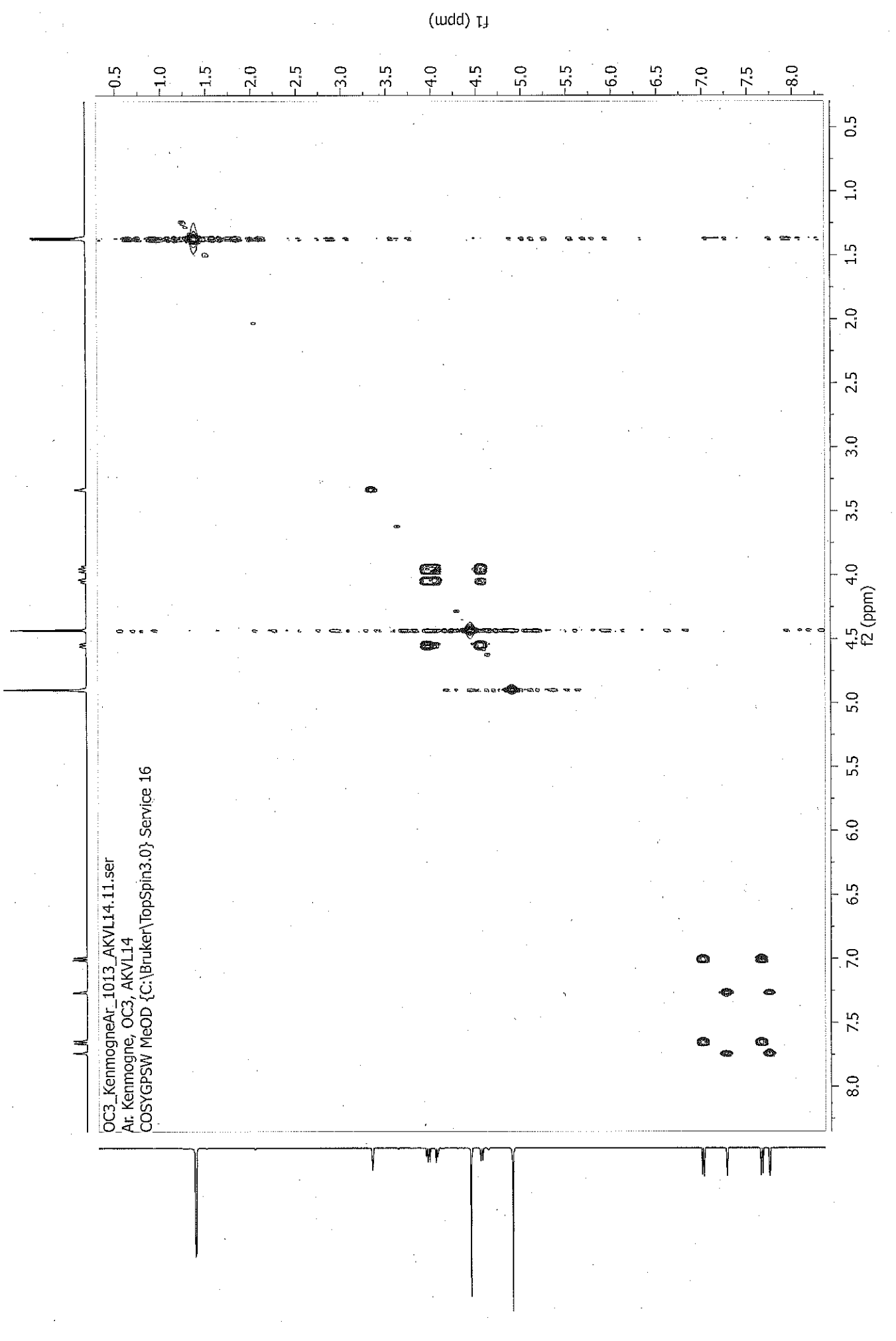
File:MFB2016\_123X Ident:40\_50 SMO(1,7) PKD(7,3,7,0.50%,0.0,0.00%,F,F) SPEC(Heights, Centroid) Ac>  
AutoSpec EI+ Voltage BpM:319 BpI:41690 TIC:159279 Flags:NORM  
File Text:Ar. Kenmogne, OC3, AKVLI14, HWP



OC3\_KenmogneAr\_1013\_AKVL14.10.fid  
Ar. Kenmogne, OC3, AKVL14  
PROTON MeOD {C:\Bruker\TopSpin3.0} Service 16

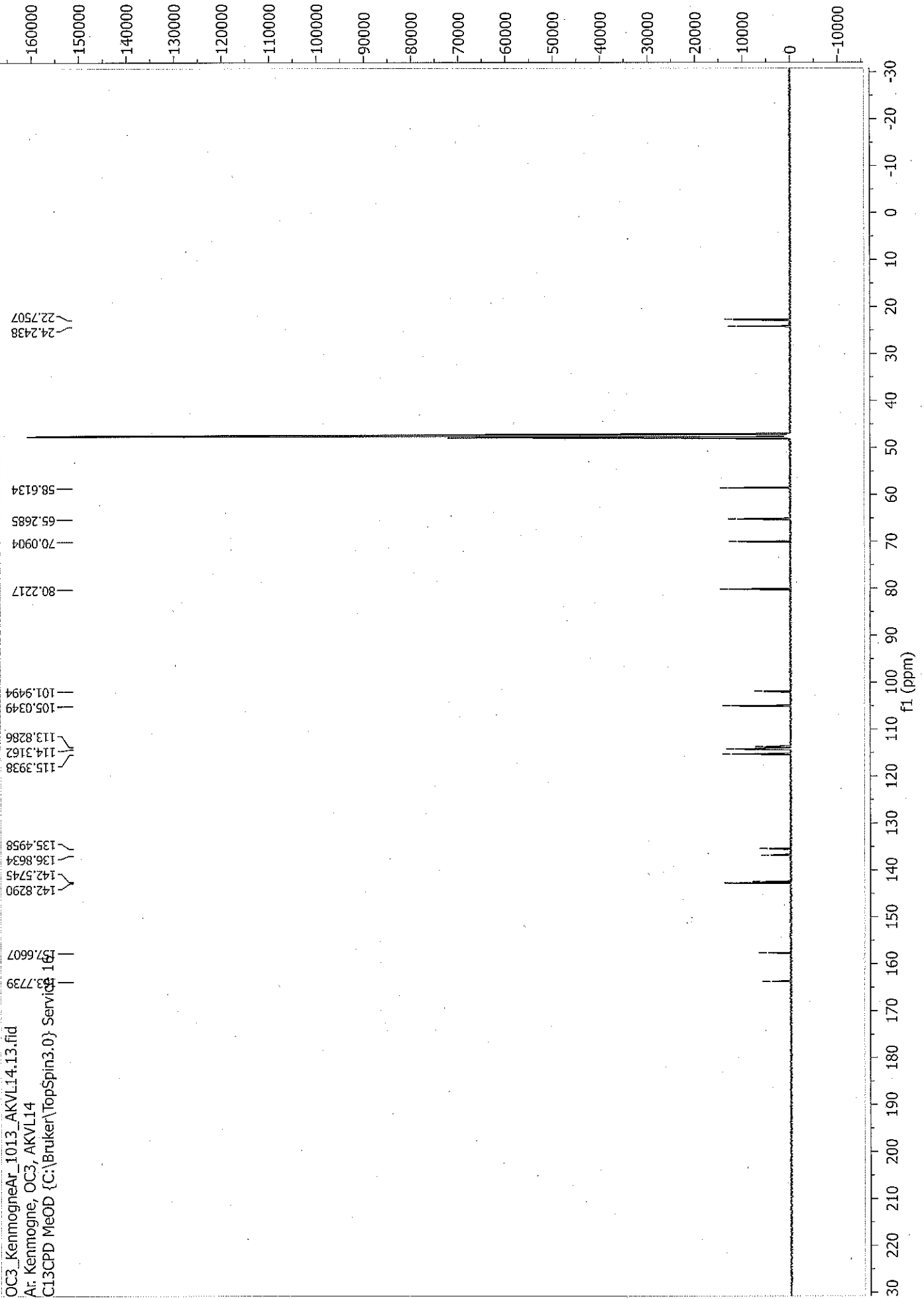


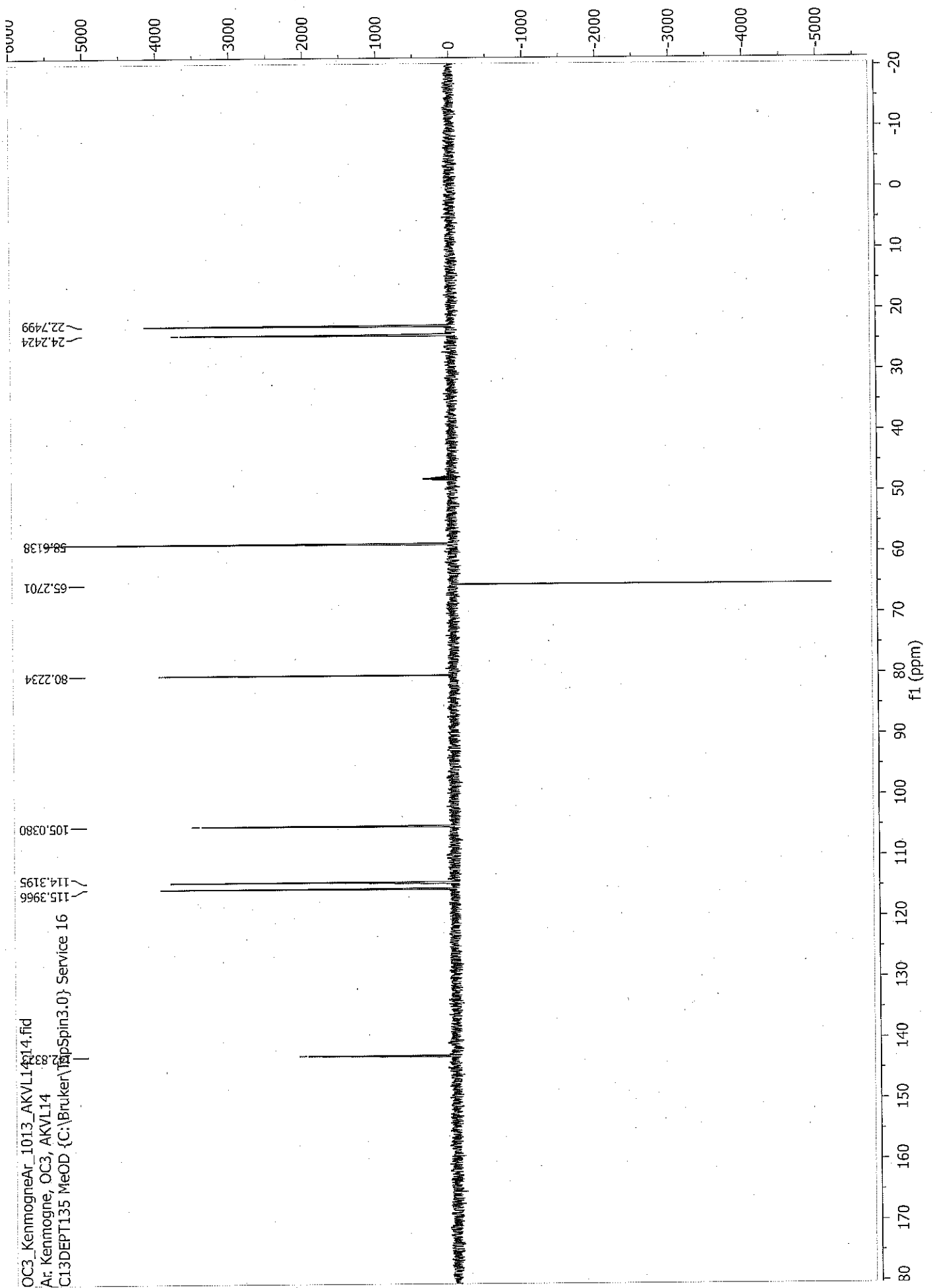




OC3\_KennogneAr\_1013\_AKVL14\_11.ser  
Ar: Kennogne, OC3, AKVL14  
COSYGPSW MeOD {C:\Bruker\TopSpin3.0} Service 16

OC3\_KenmogneAr\_1013\_AKVL14.13.fid  
Ar: Kenmogne, OC3, AKVL14  
C13CPD MeOD (C:\Bruker\TopSpin3.0) Service 16





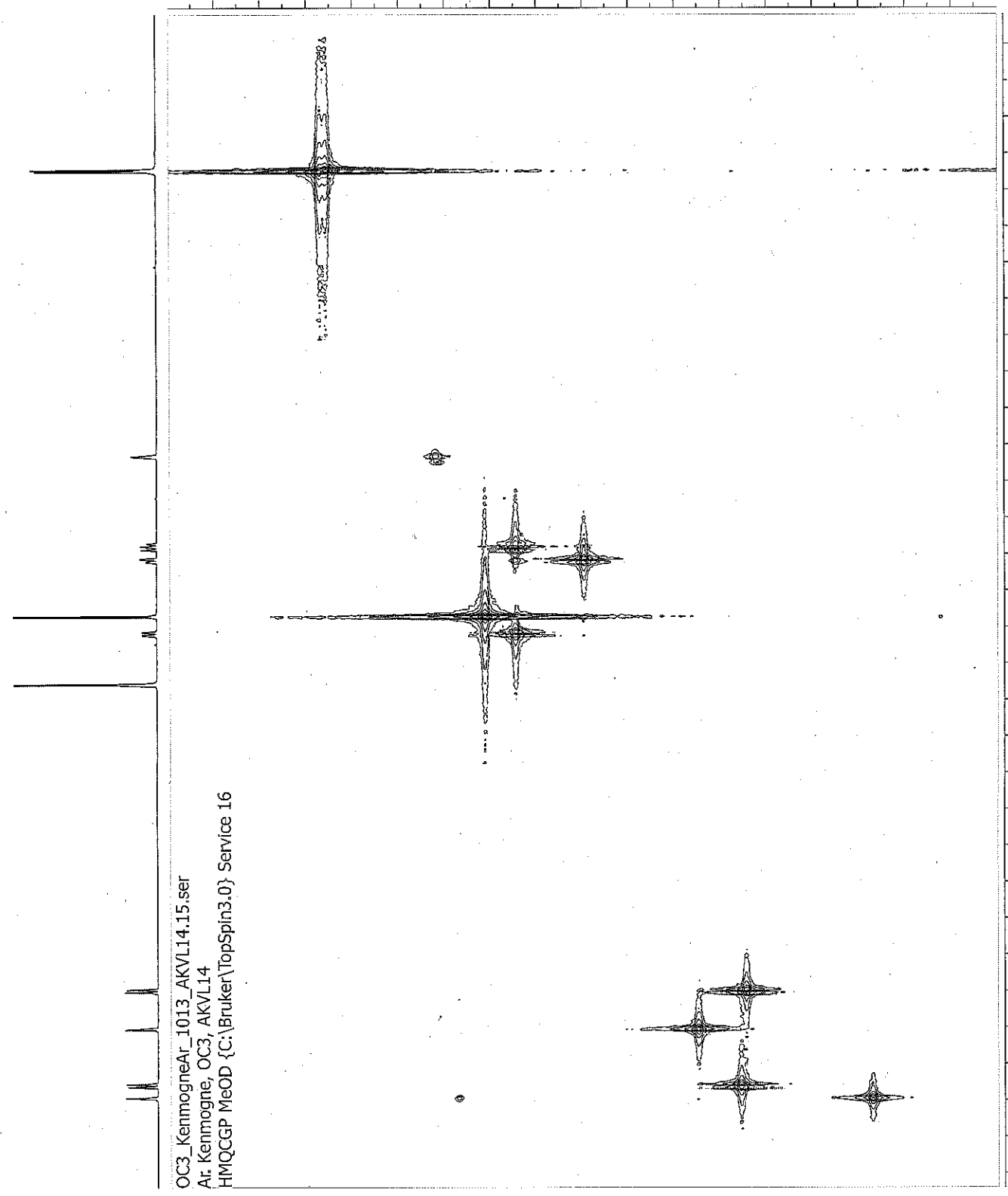
OC3\_KennogneAr\_1013\_AKVL14.15.ser  
Ar. Kennogne, OC3, AKVL14  
HMQCGP MeOD {C:\Bruker\TopSpin3.0} Service 16

F1 (ppm)

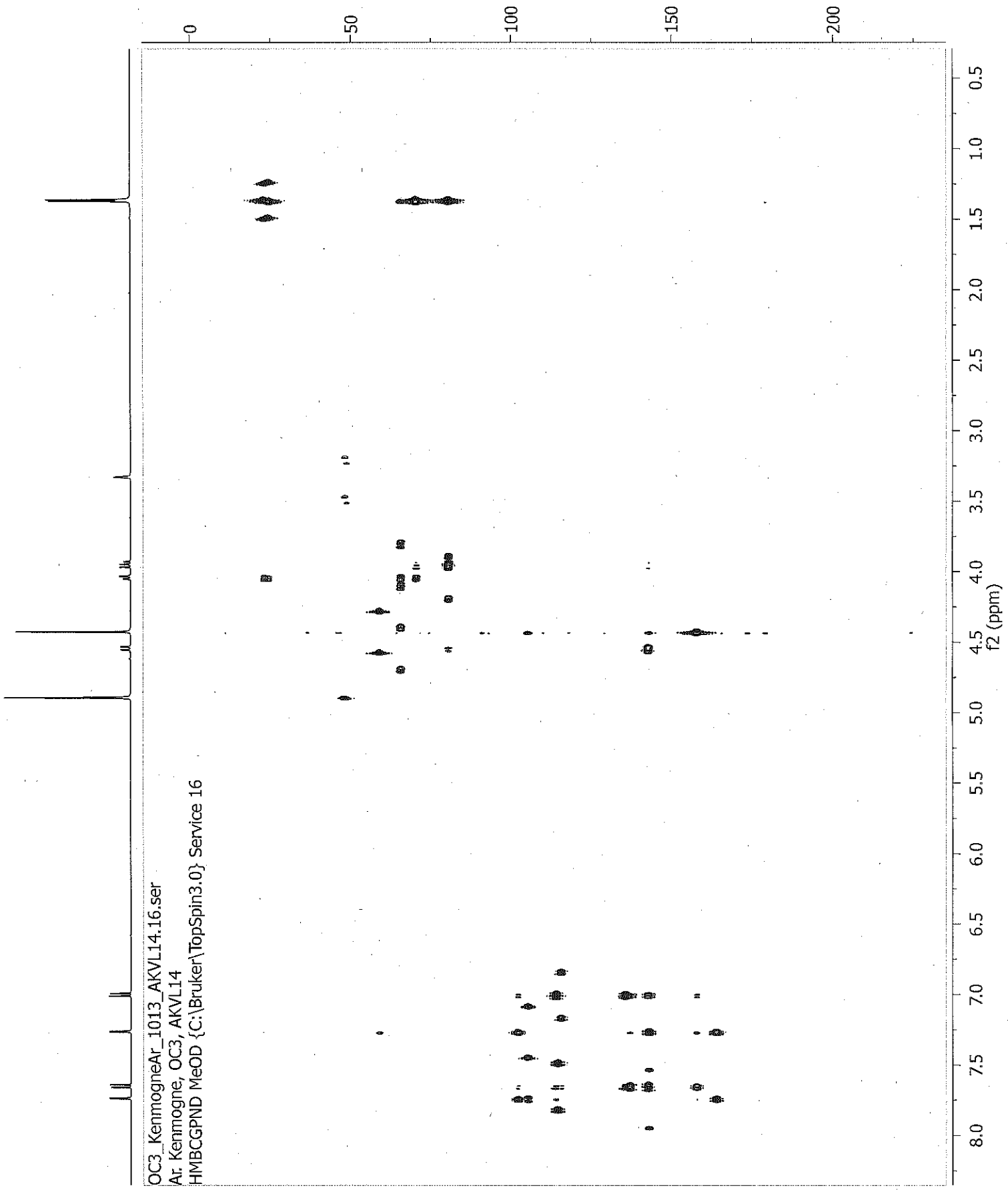
0  
-10  
-20  
30  
-40  
-50  
-60  
-70  
80  
90  
-100  
-110  
-120  
-130  
-140  
-150  
-160

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

