Anhang II

G NMR-Spektren – Teil A

H IR- und Massen-Spektren – Teil A

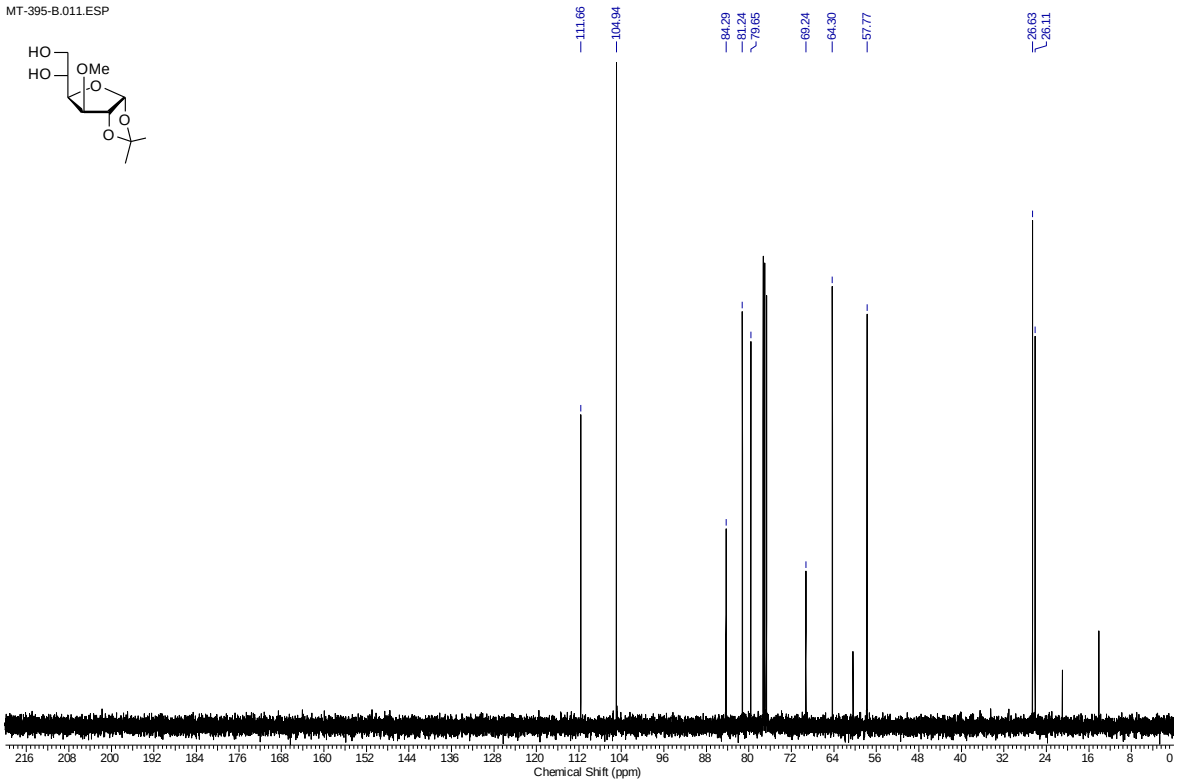
I Kristalldaten – Teil A

J NMR-Spektren – Teil B

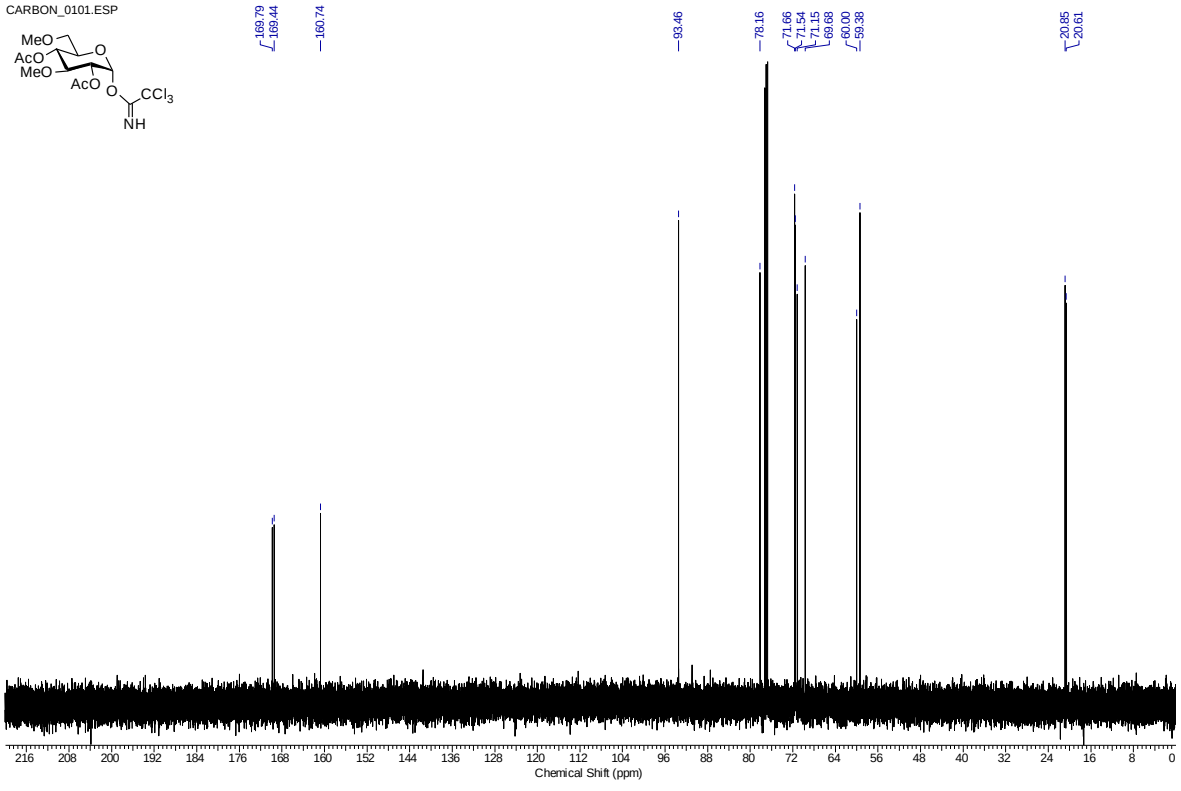
K IR- und Massen-Spektren – Teil B

G NMR-Spektren – Teil A

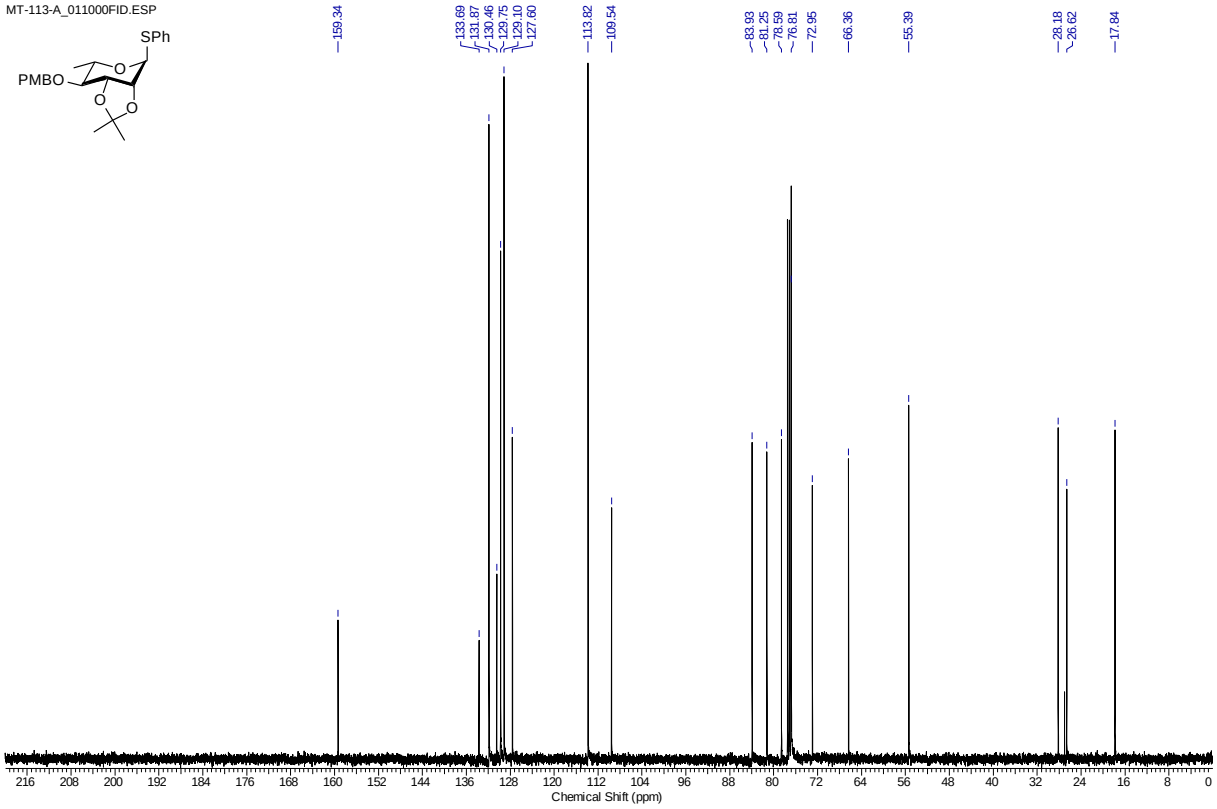
Verbindung **72**



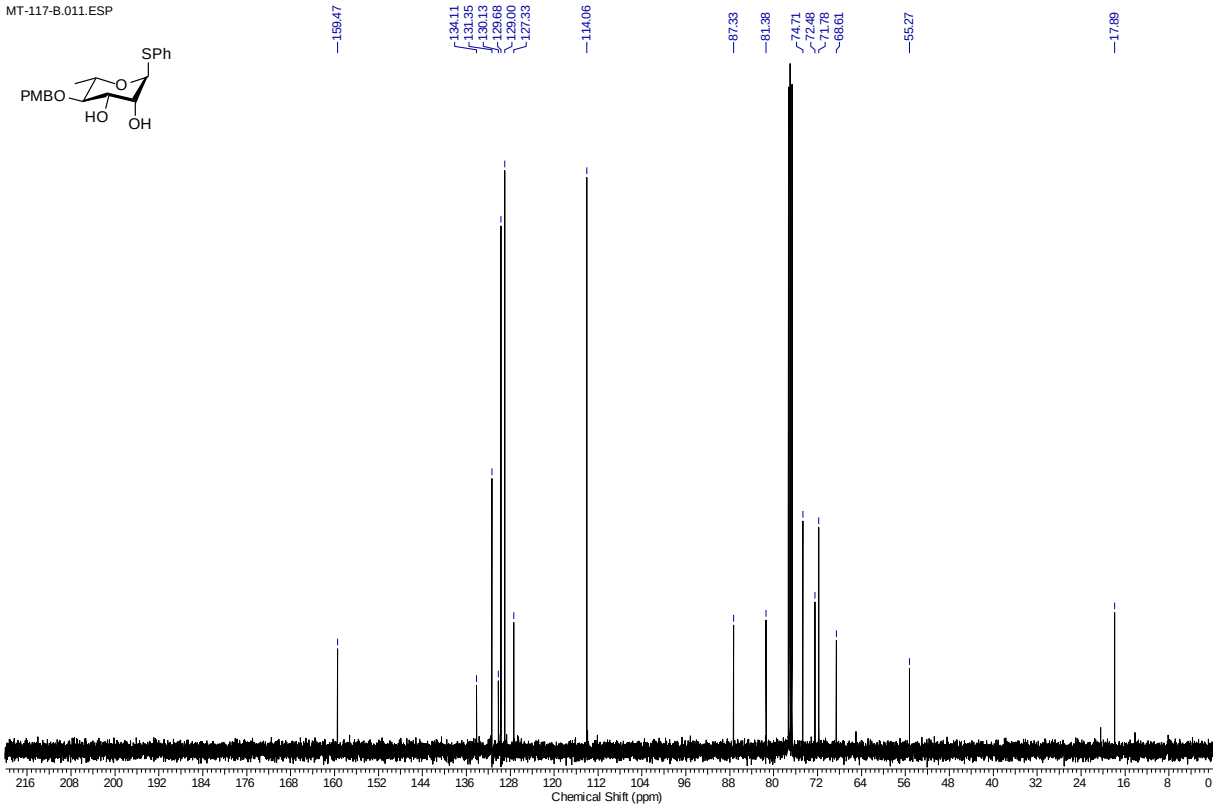
Verbindung **37**



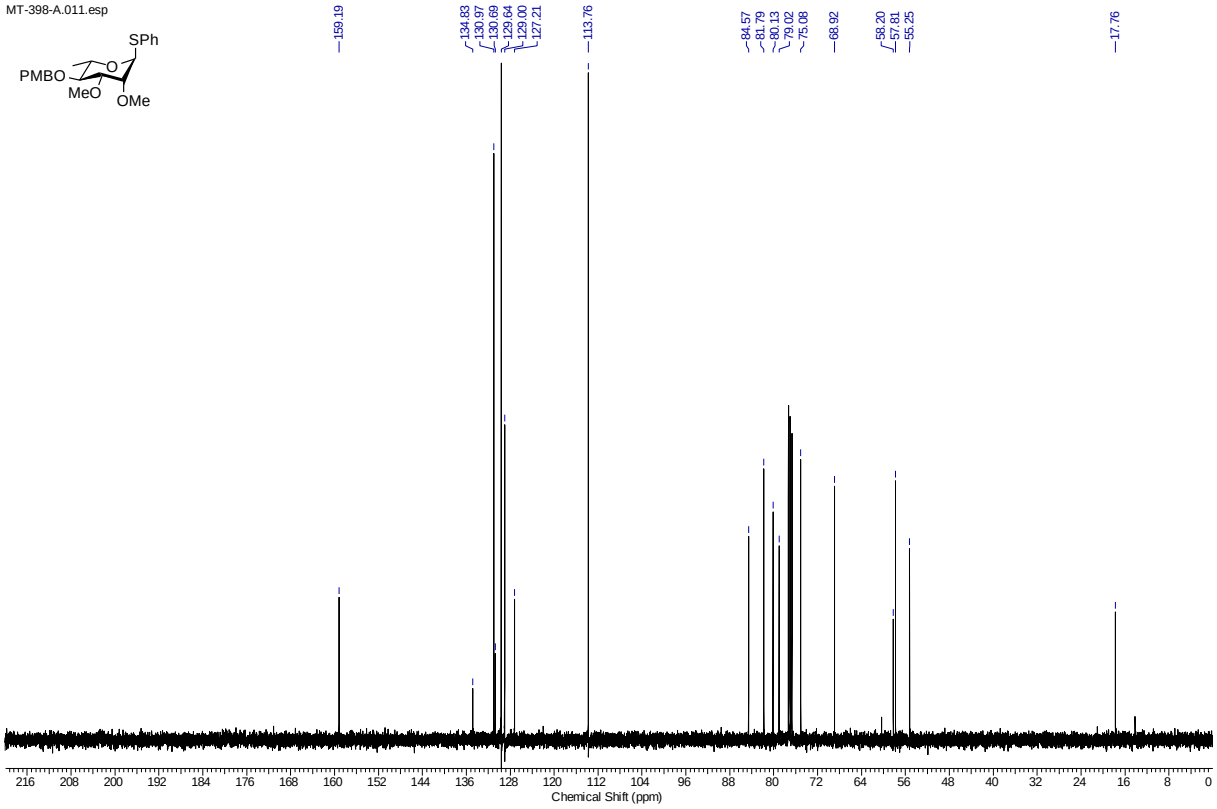
Verbindung **102**



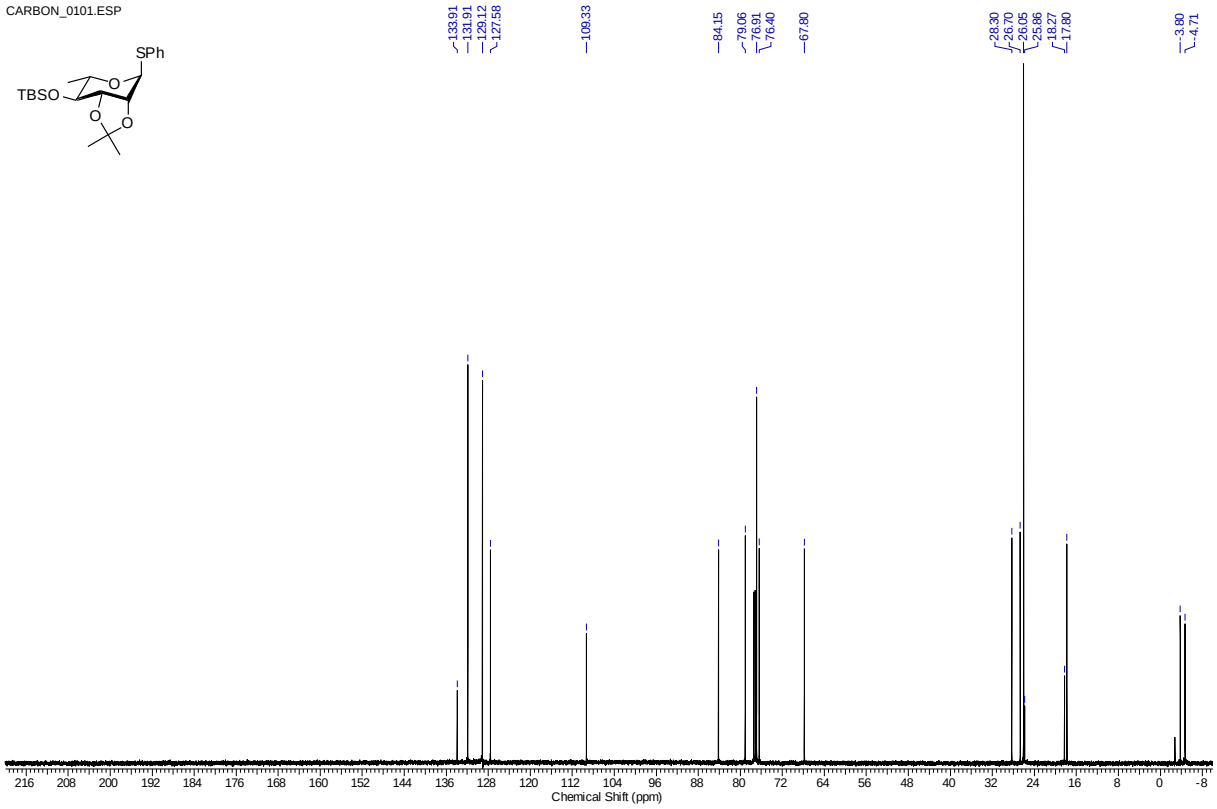
Verbindung **61**



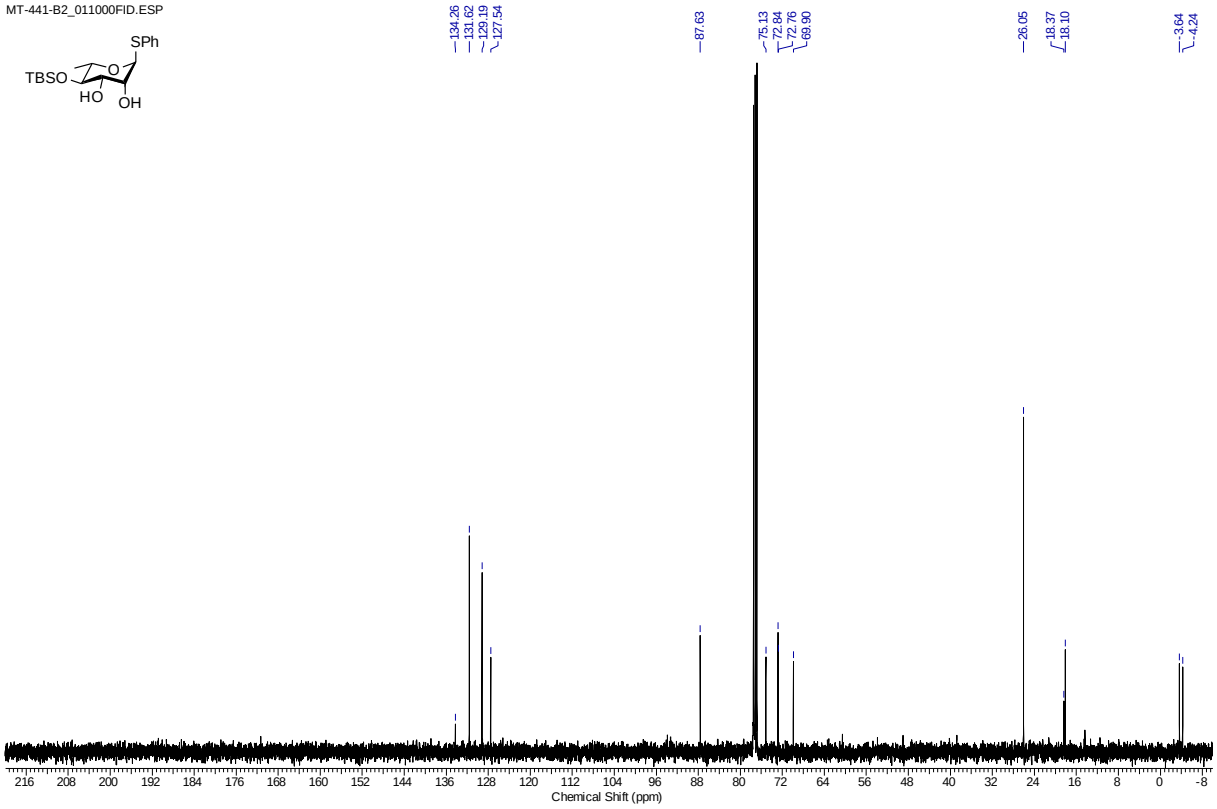
Verbindung **33**



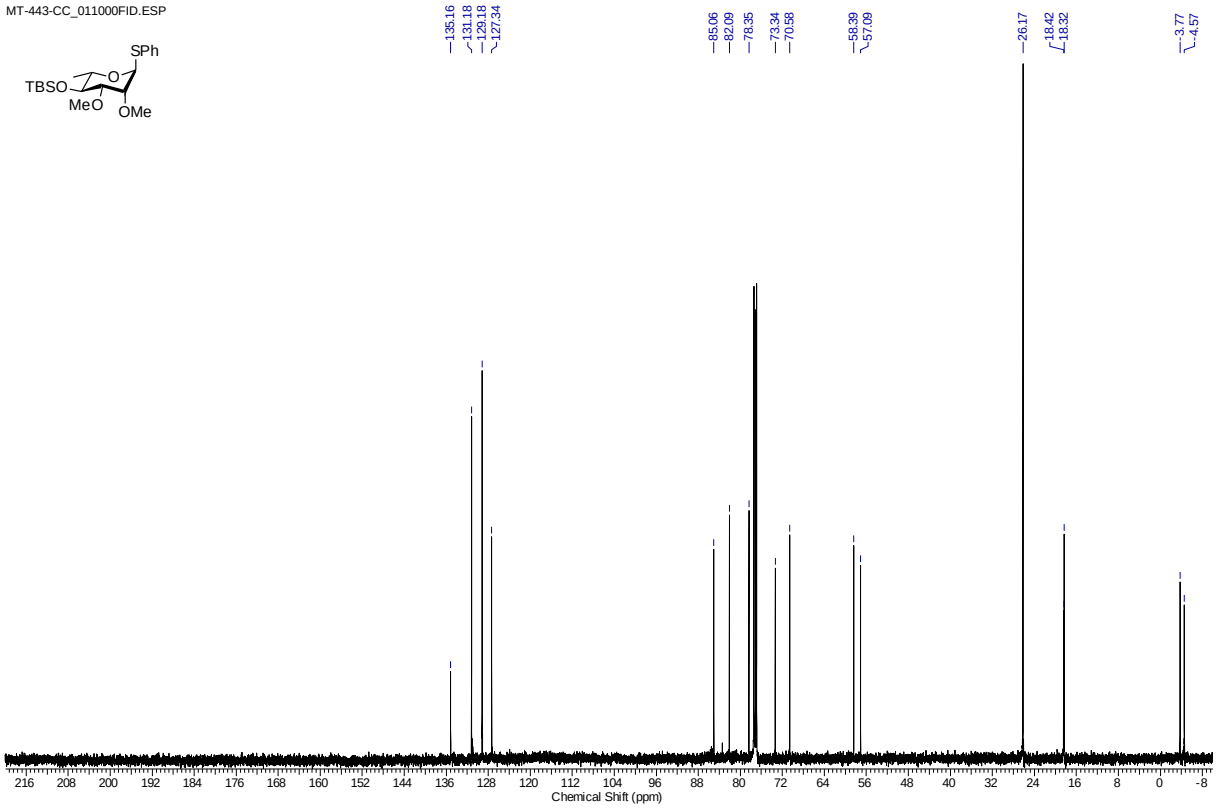
Verbindung **68**



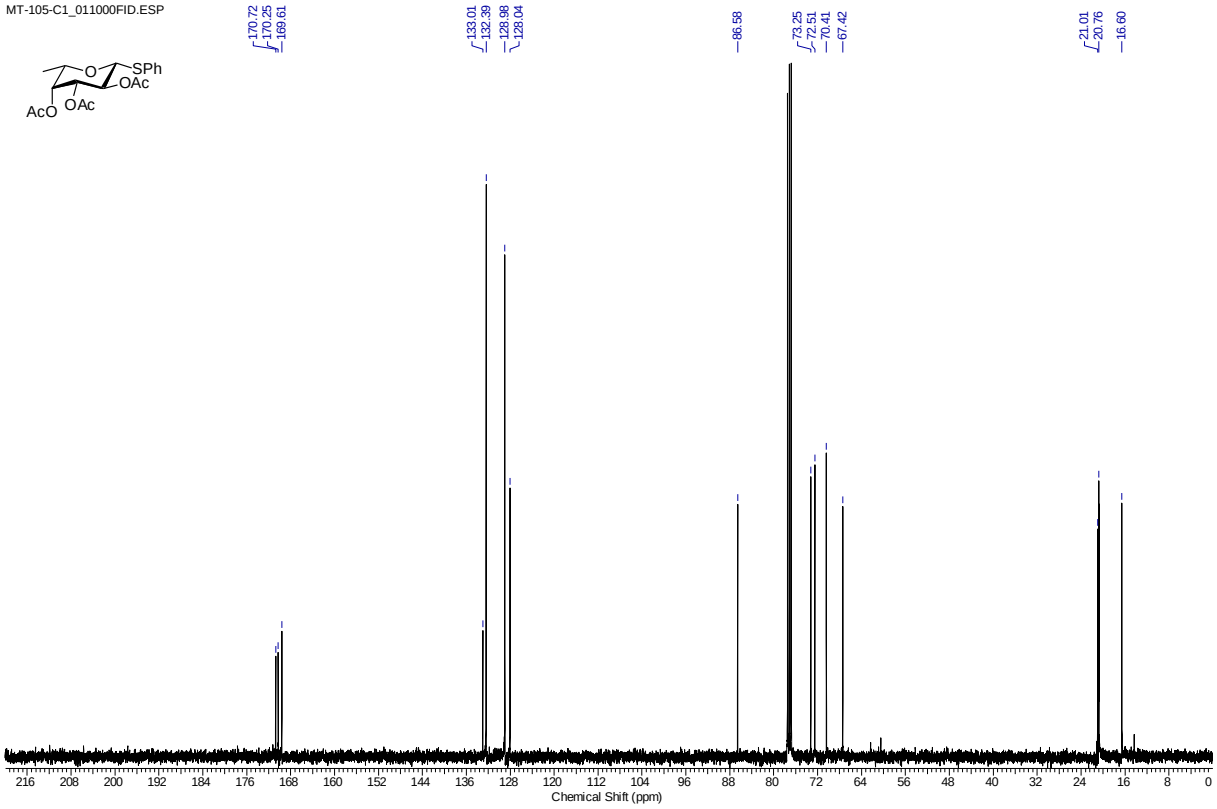
Verbindung **69**



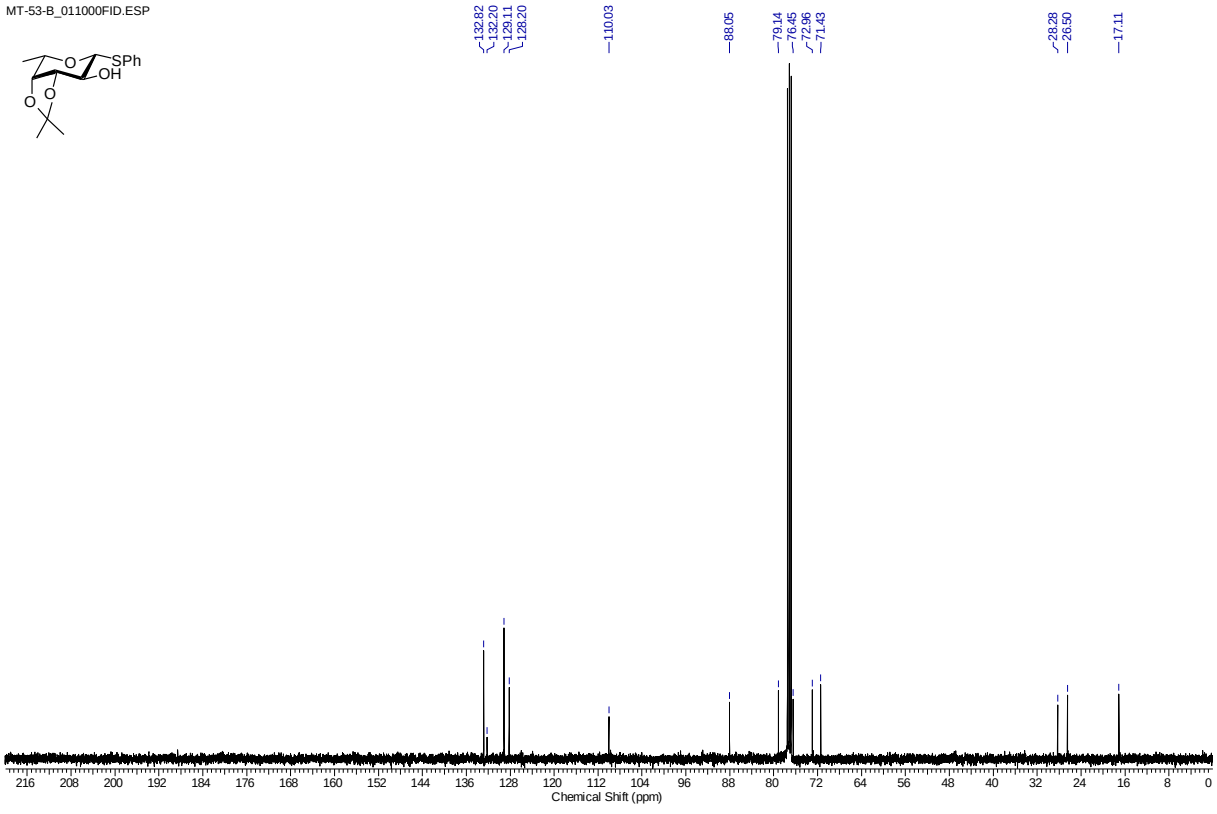
Verbindung **70**



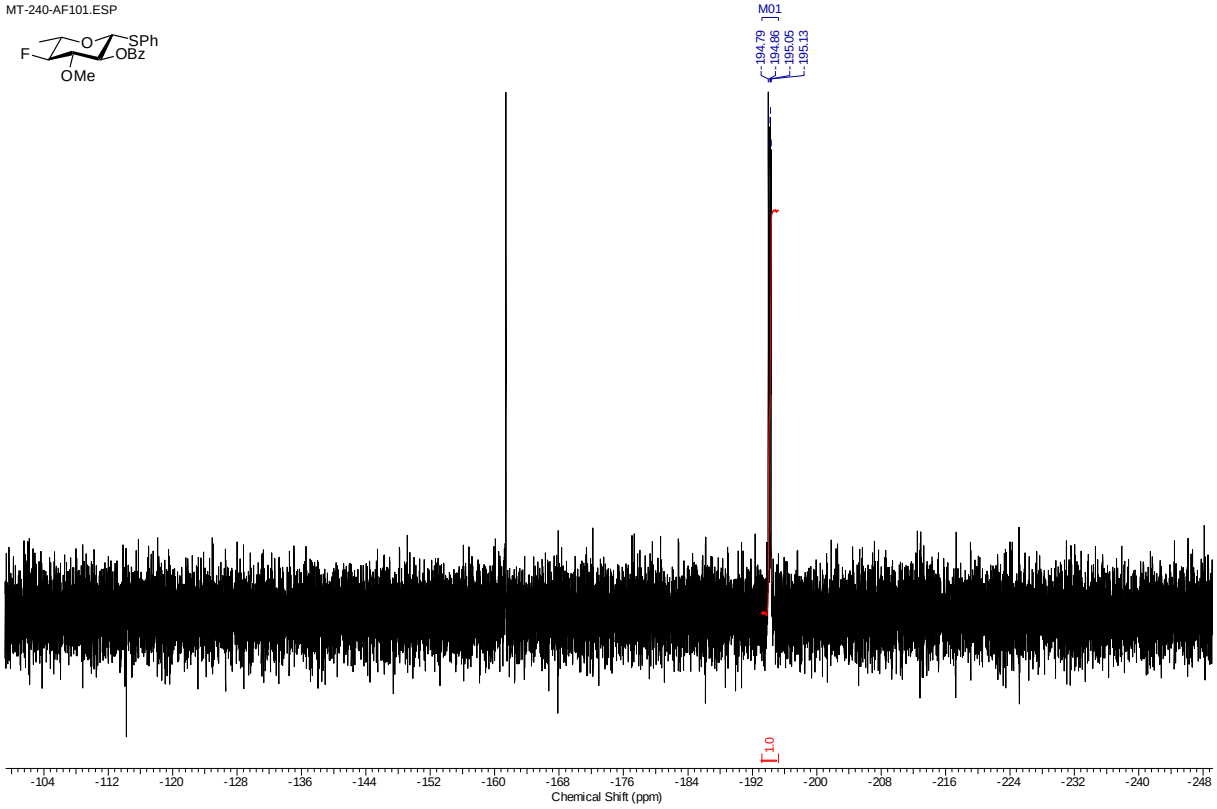
Verbindung β-**43**



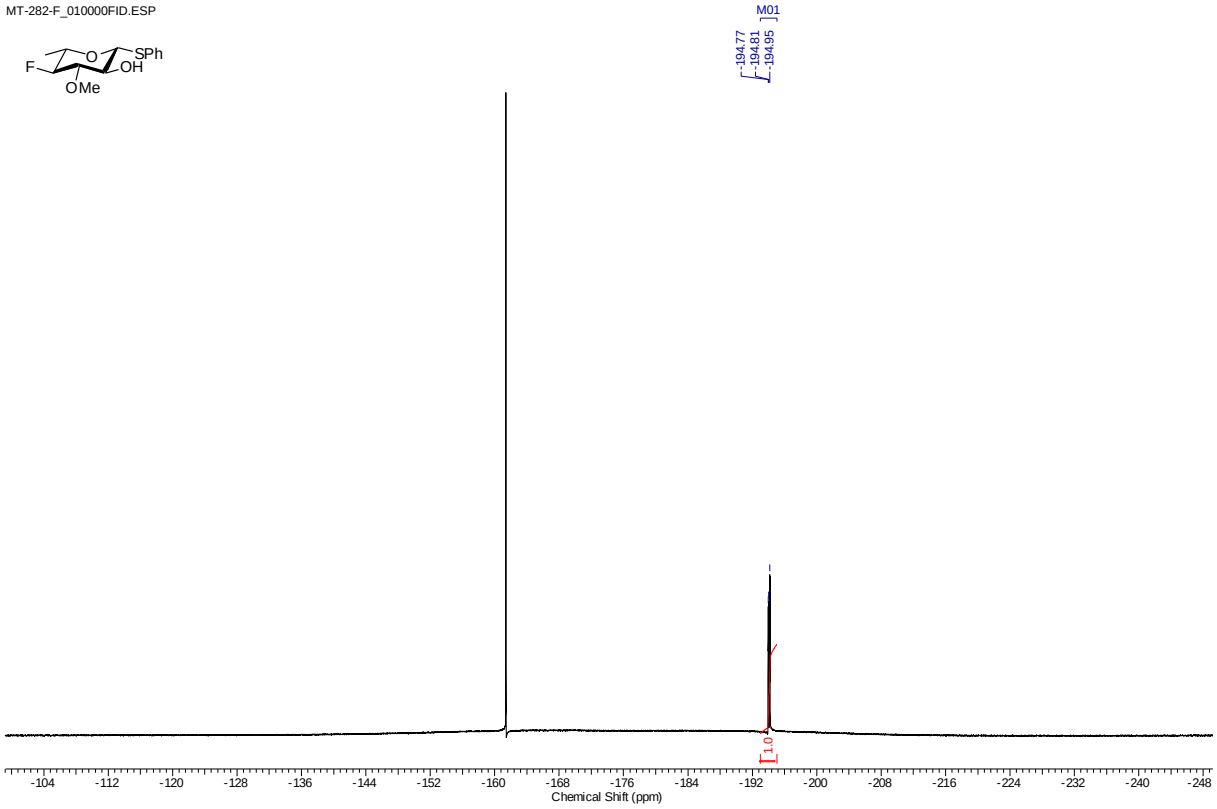
Verbindung **44**



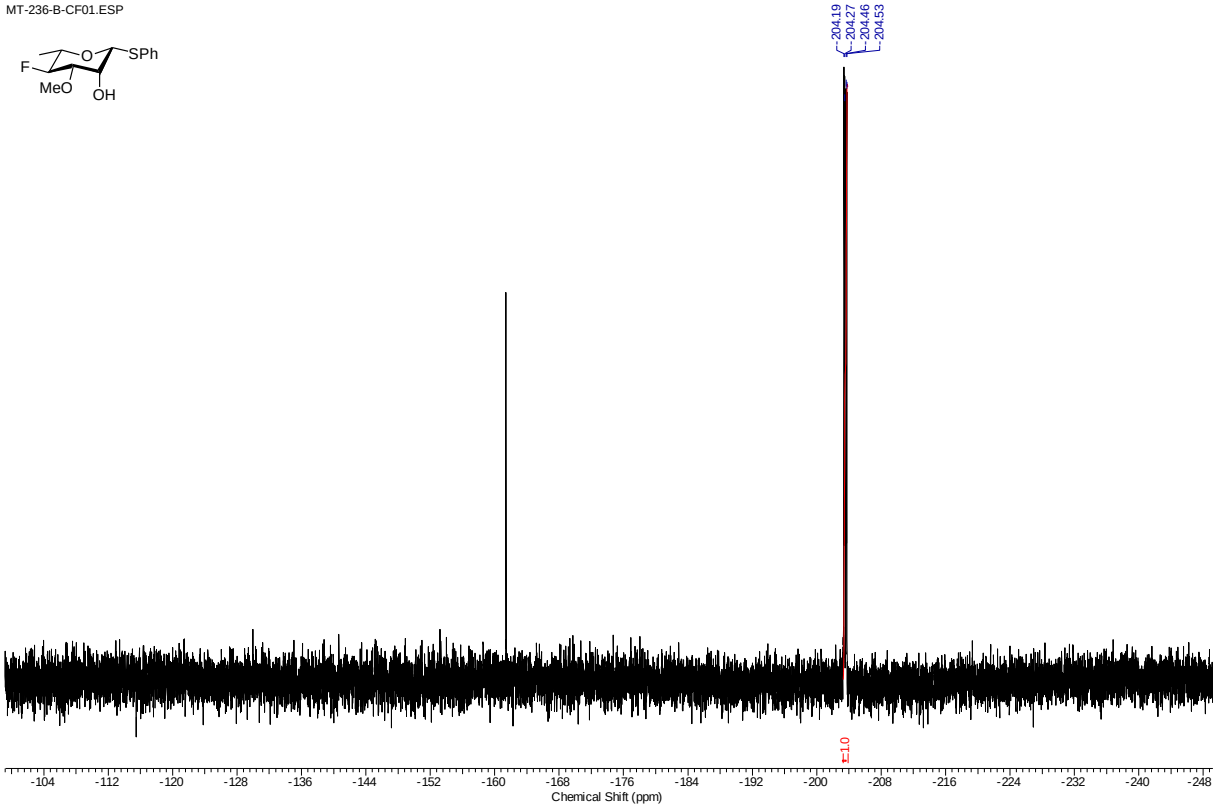
Verbindung **47** – ^{19}F-NMR-Spektrum



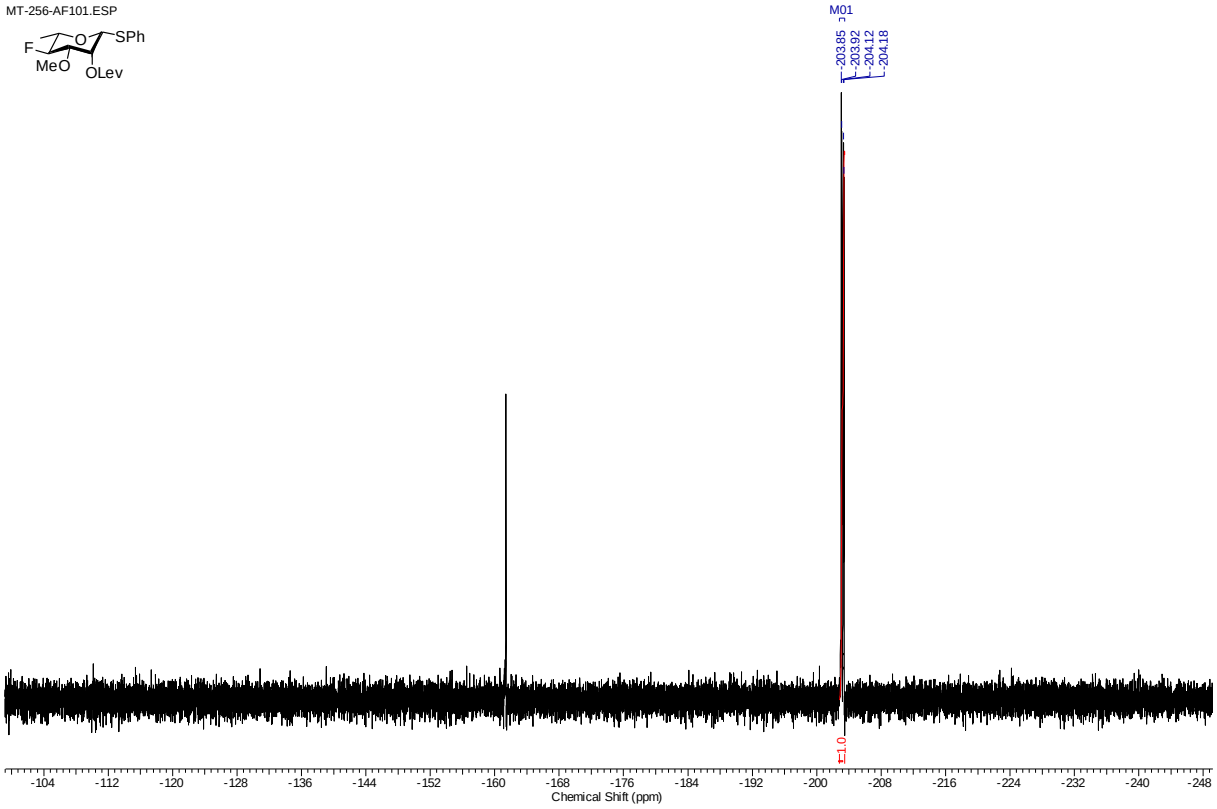
Verbindung **48** – ^{19}F-NMR-Spektrum



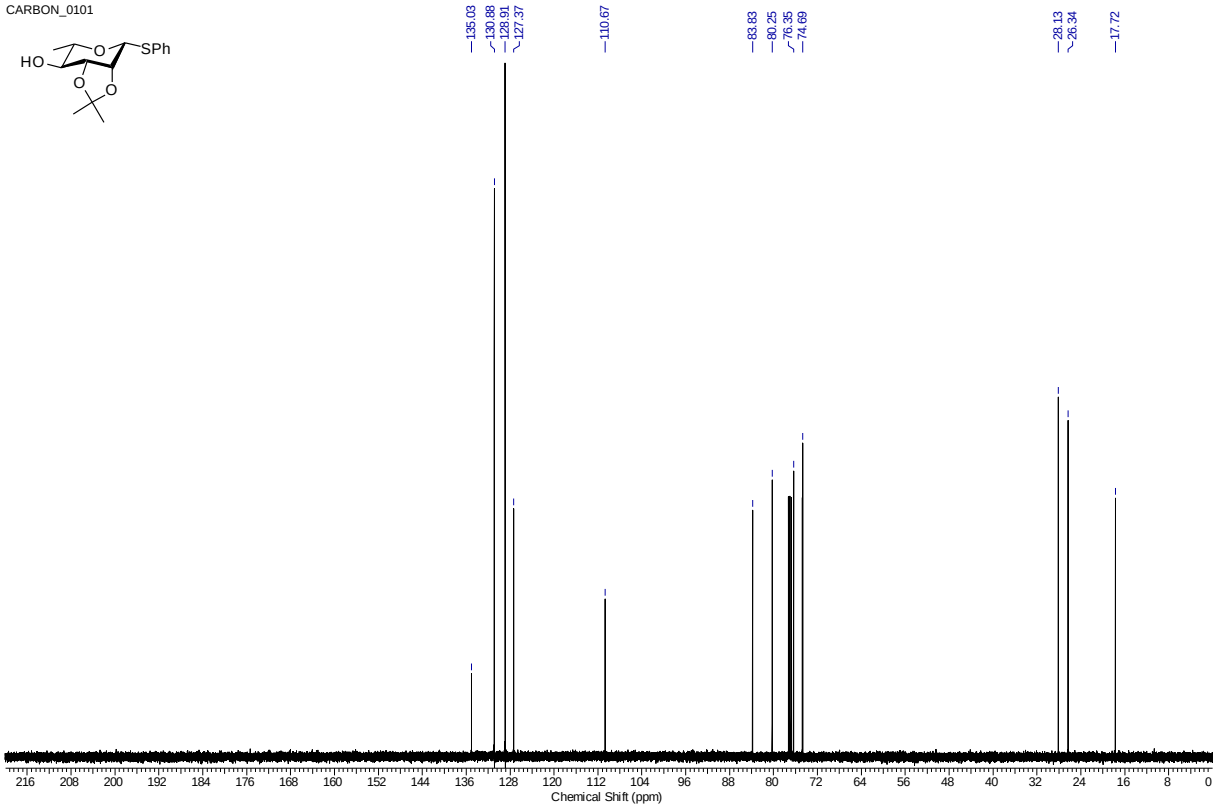
Verbindung **50** – ^{19}F-NMR-Spektrum



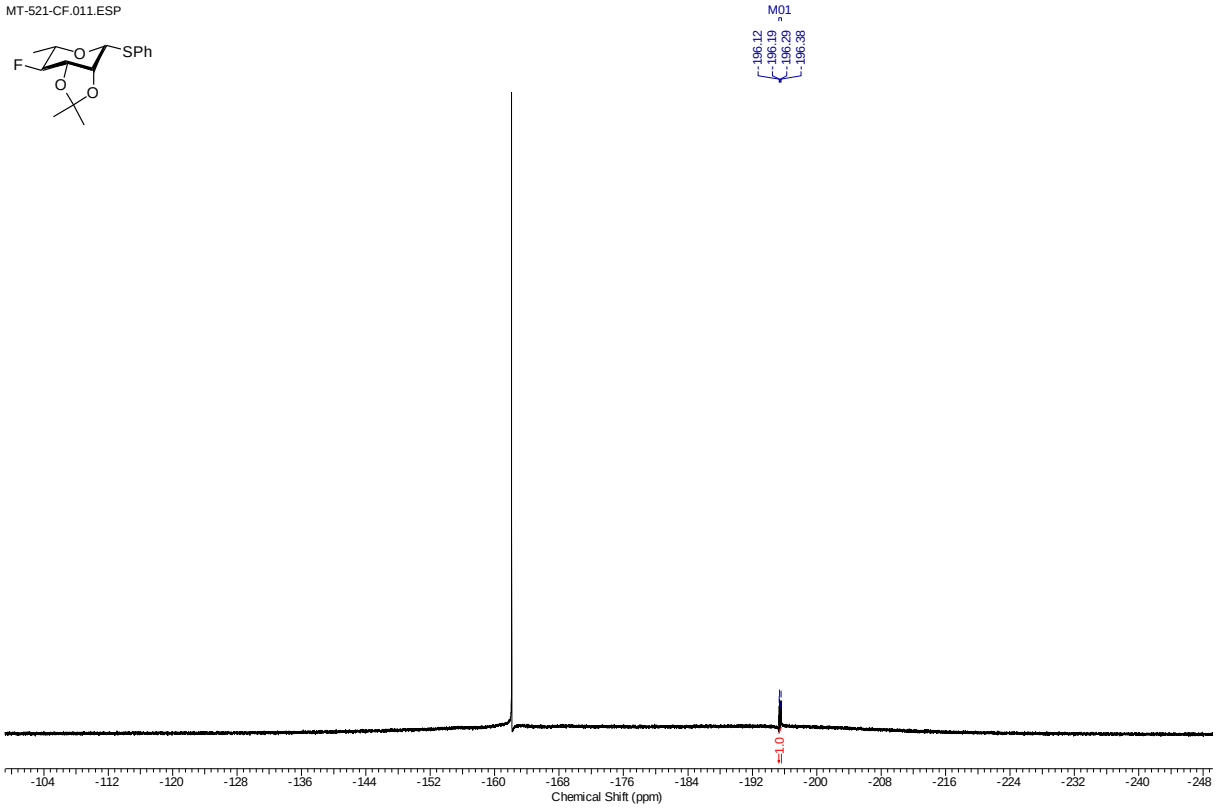
Verbindung **32** – ^{19}F-NMR-Spektrum



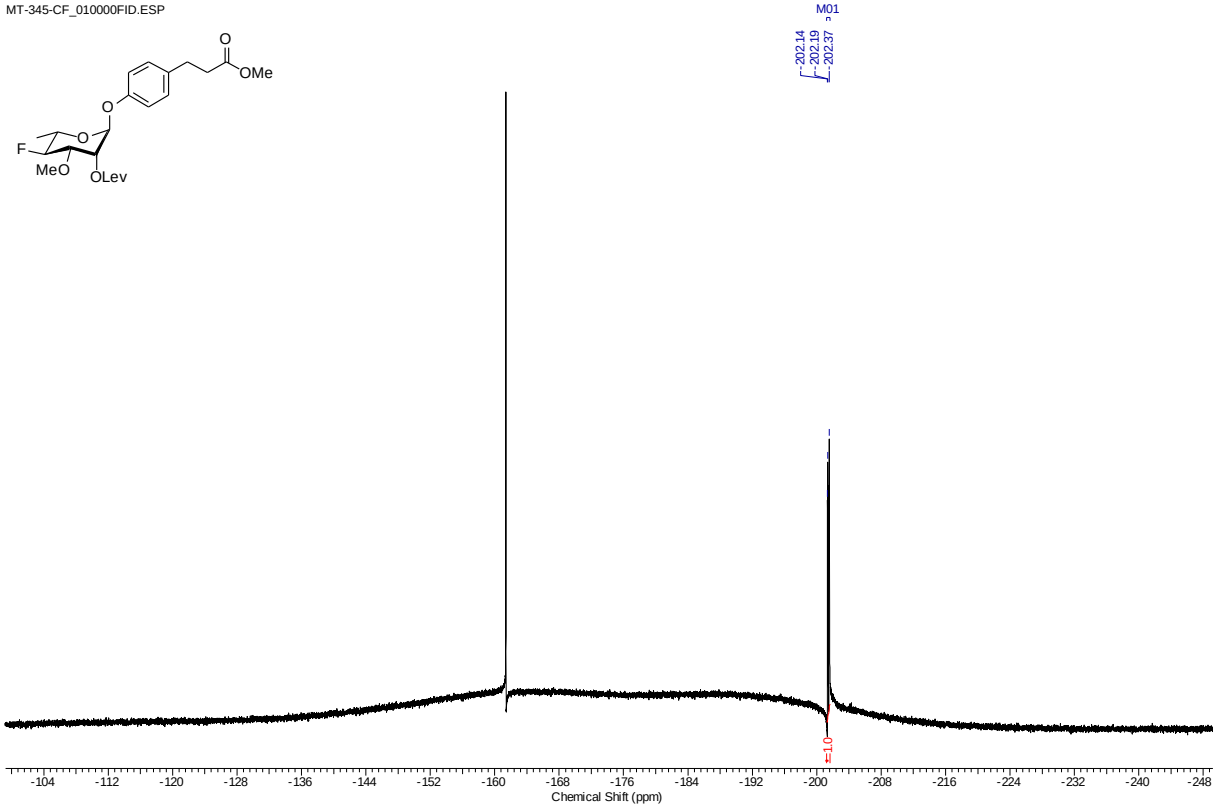
Verbindung β-**39**



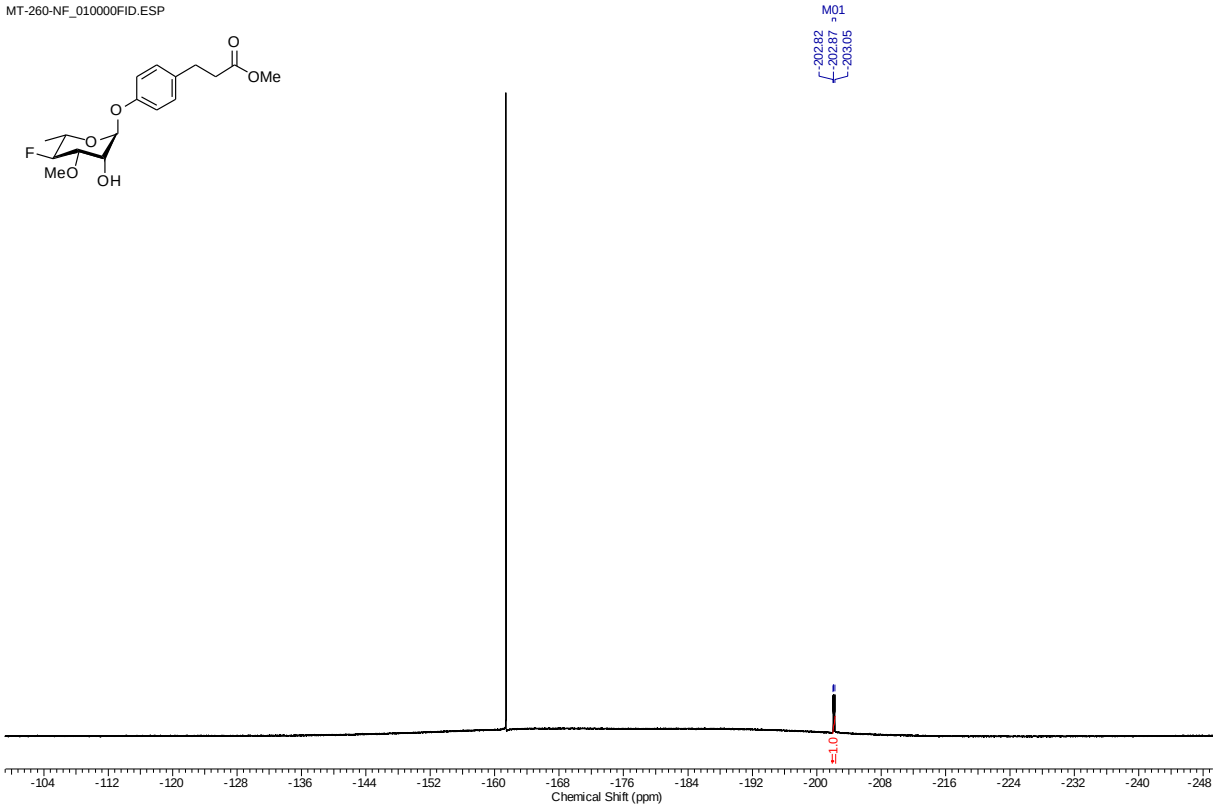
Verbindung **59** – ^{19}F-NMR-Spektrum



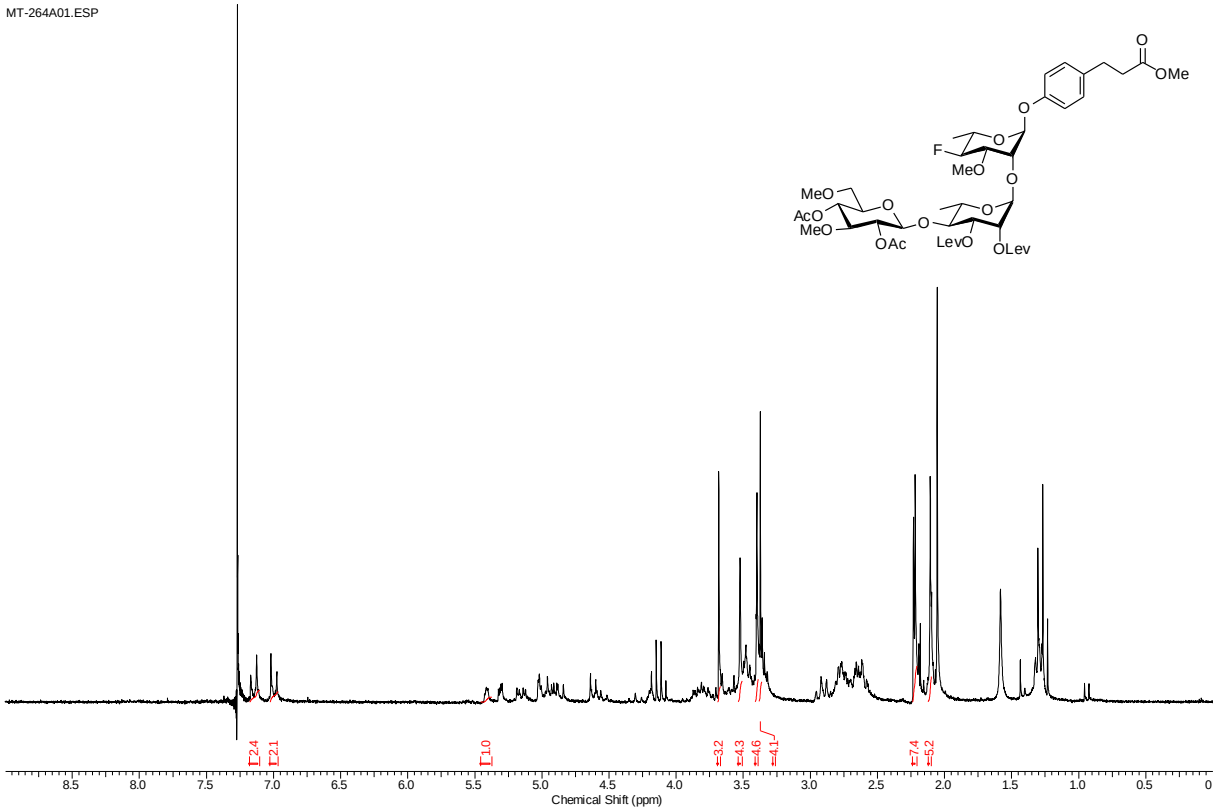
Verbindung **77** – ^{19}F-NMR-Spektrum



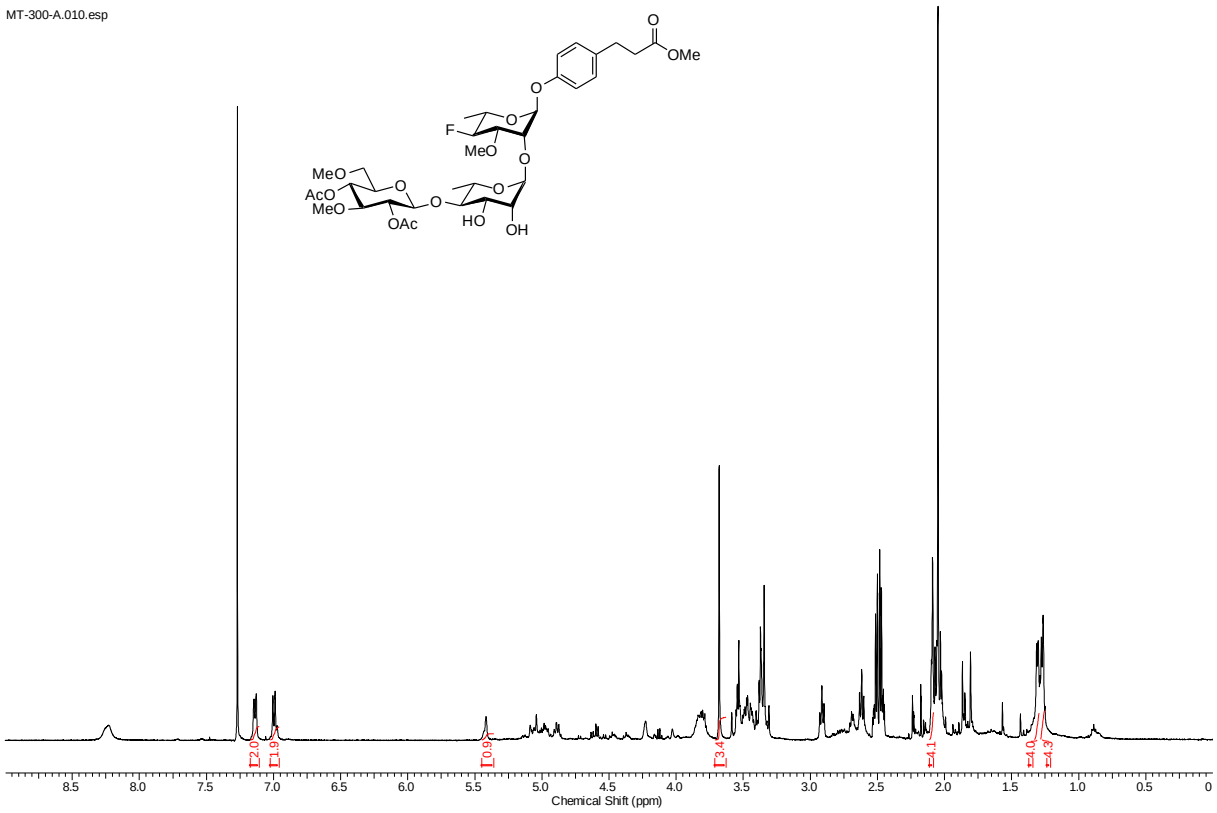
Verbindung **78** – ^{19}F-NMR-Spektrum



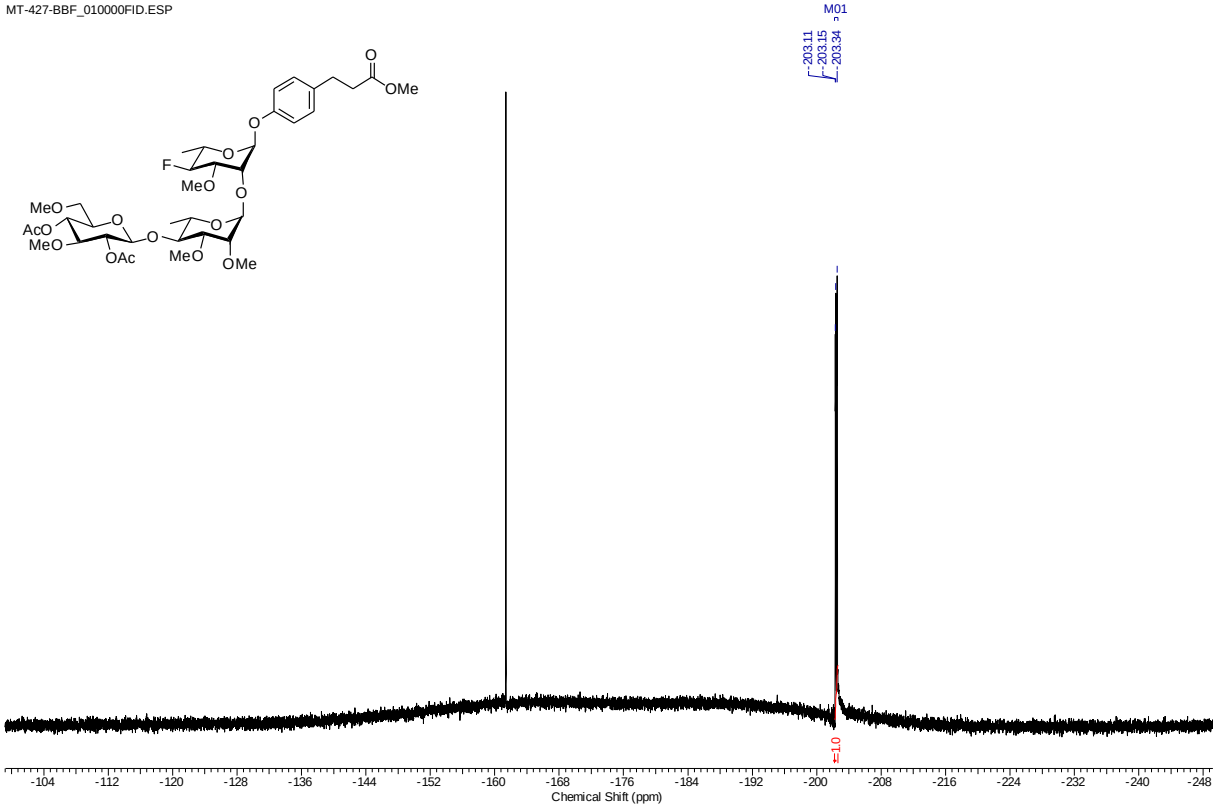
Verbindung **88** – verunreinigtes ^{1}H-NMR-Spektrum



Verbindung **89** – verunreinigtes ^{1}H-NMR-Spektrum

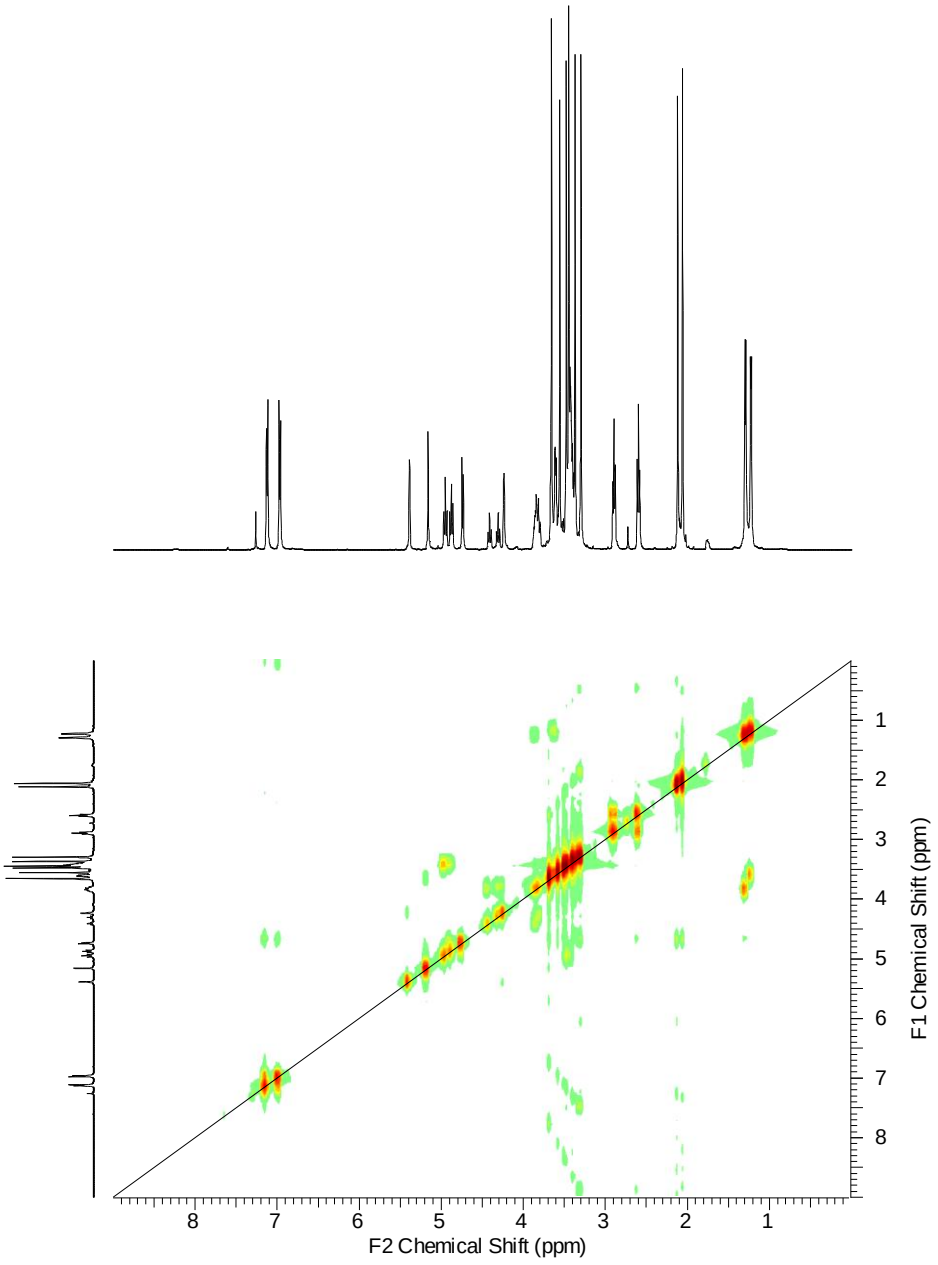


Verbindung **90** – ^{19}F-NMR-Spektrum



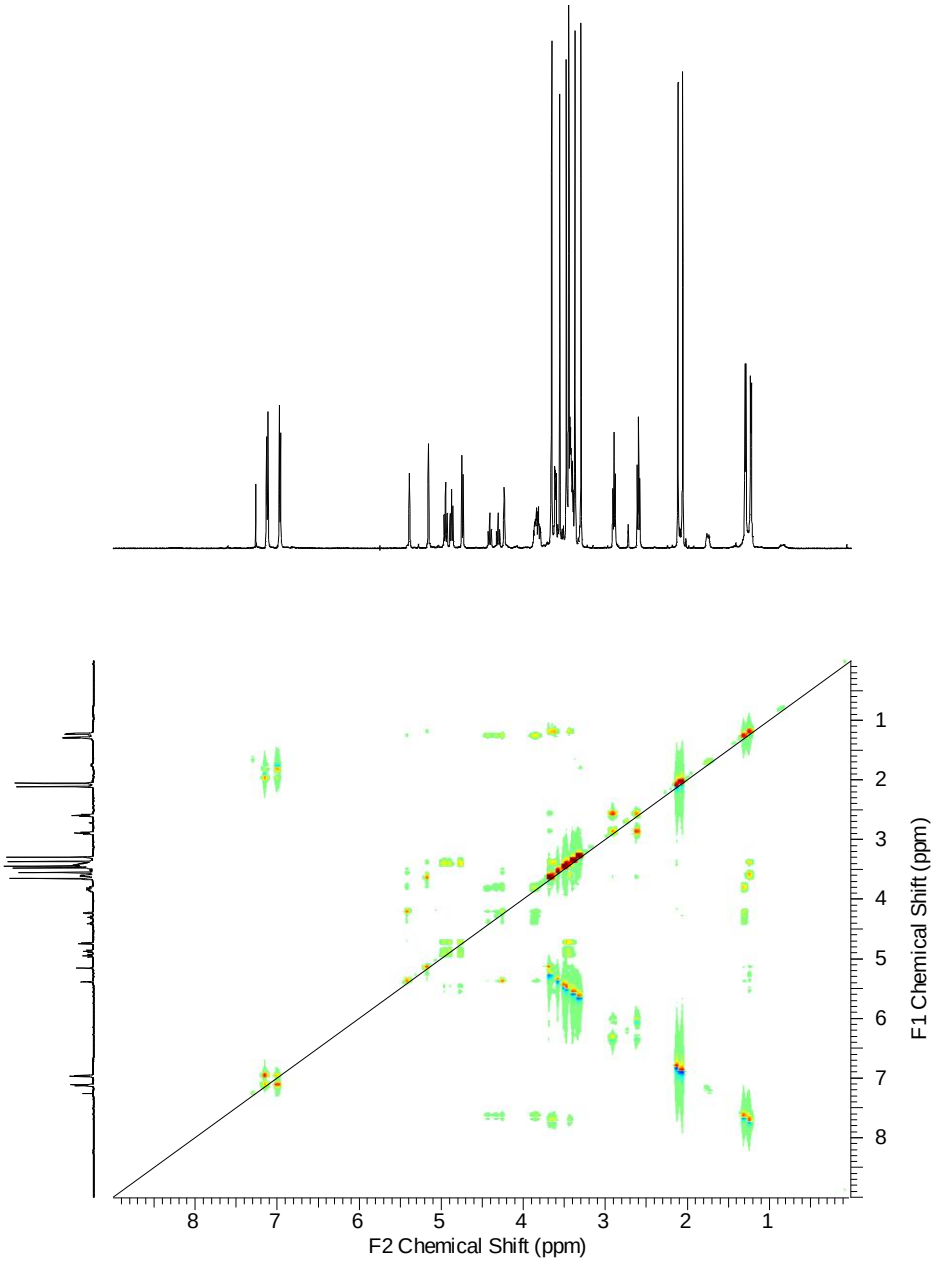
Verbindung **90** – ^{1}H-^{1}H-COSY-NMR-Spektrum

MT-427-BBCO.011.000.SER.ESP



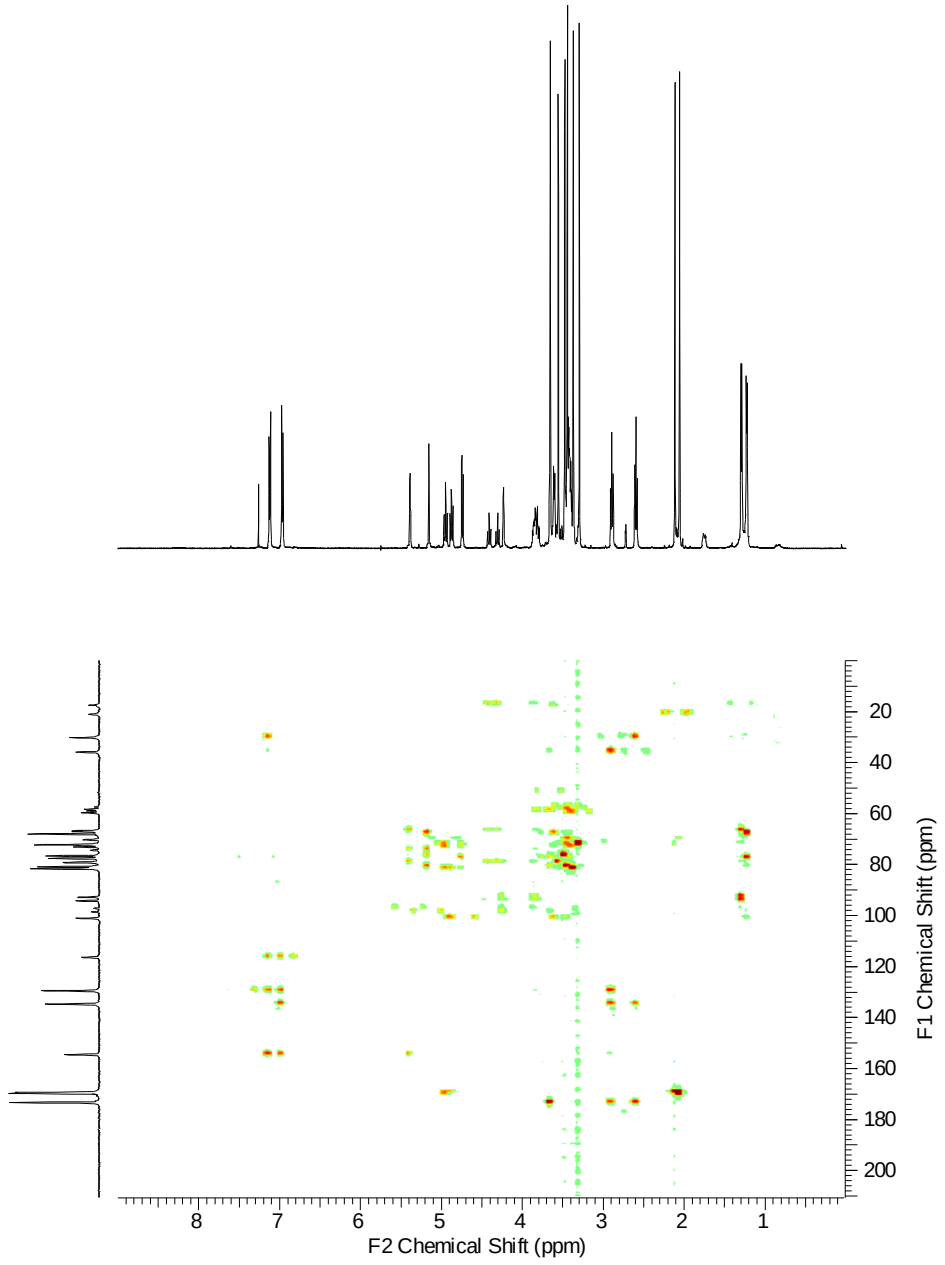
Verbindung **90** – ^{1}H-^{1}H-TOCSY-NMR-Spektrum

MT-427-BB1.012 TOCSY.ESP



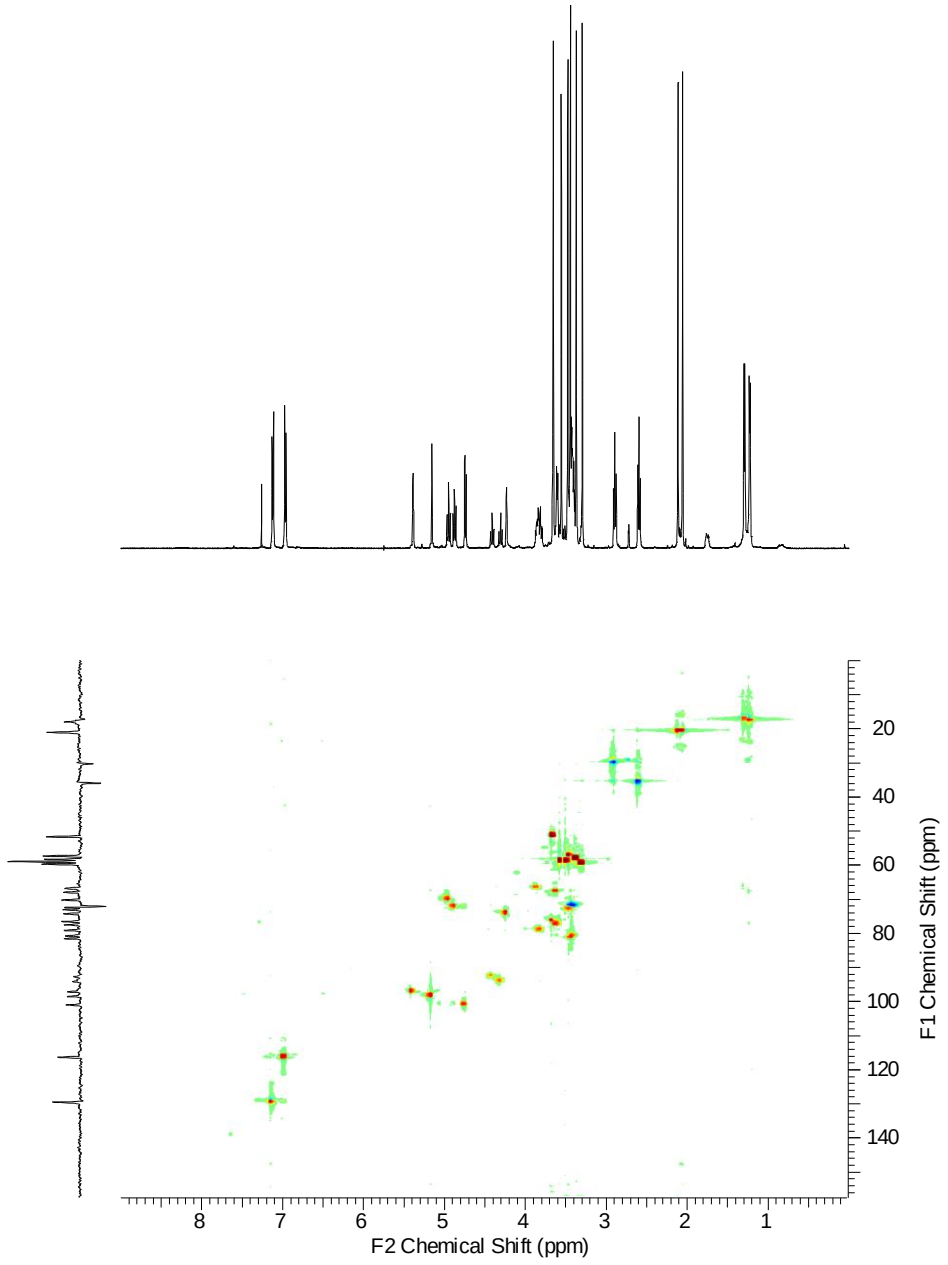
Verbindung **90** – ^{1}H-^{13}C-HMBC-NMR-Spektrum

MT-427-BB1.014.ESP

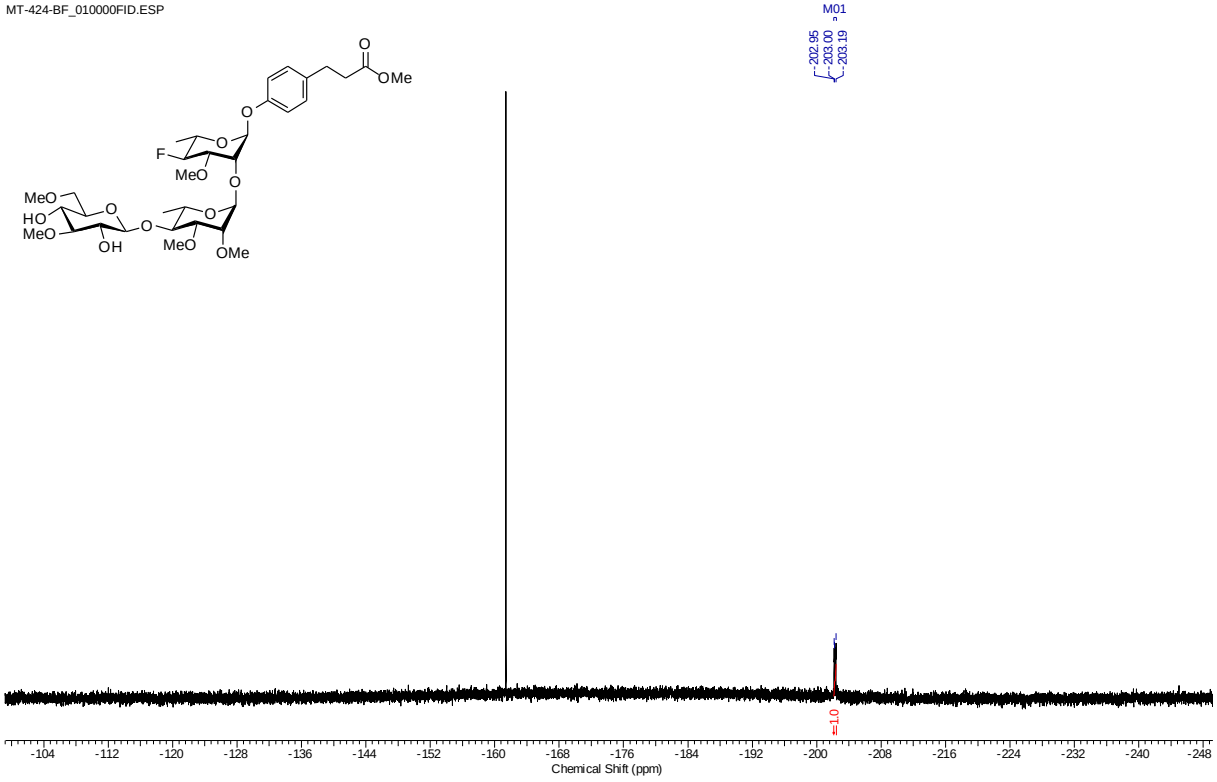


Verbindung **90** – ^{1}H-^{13}C-HSQC-DEPT-NMR-Spektrum

MT-427-BB1.015.ESP

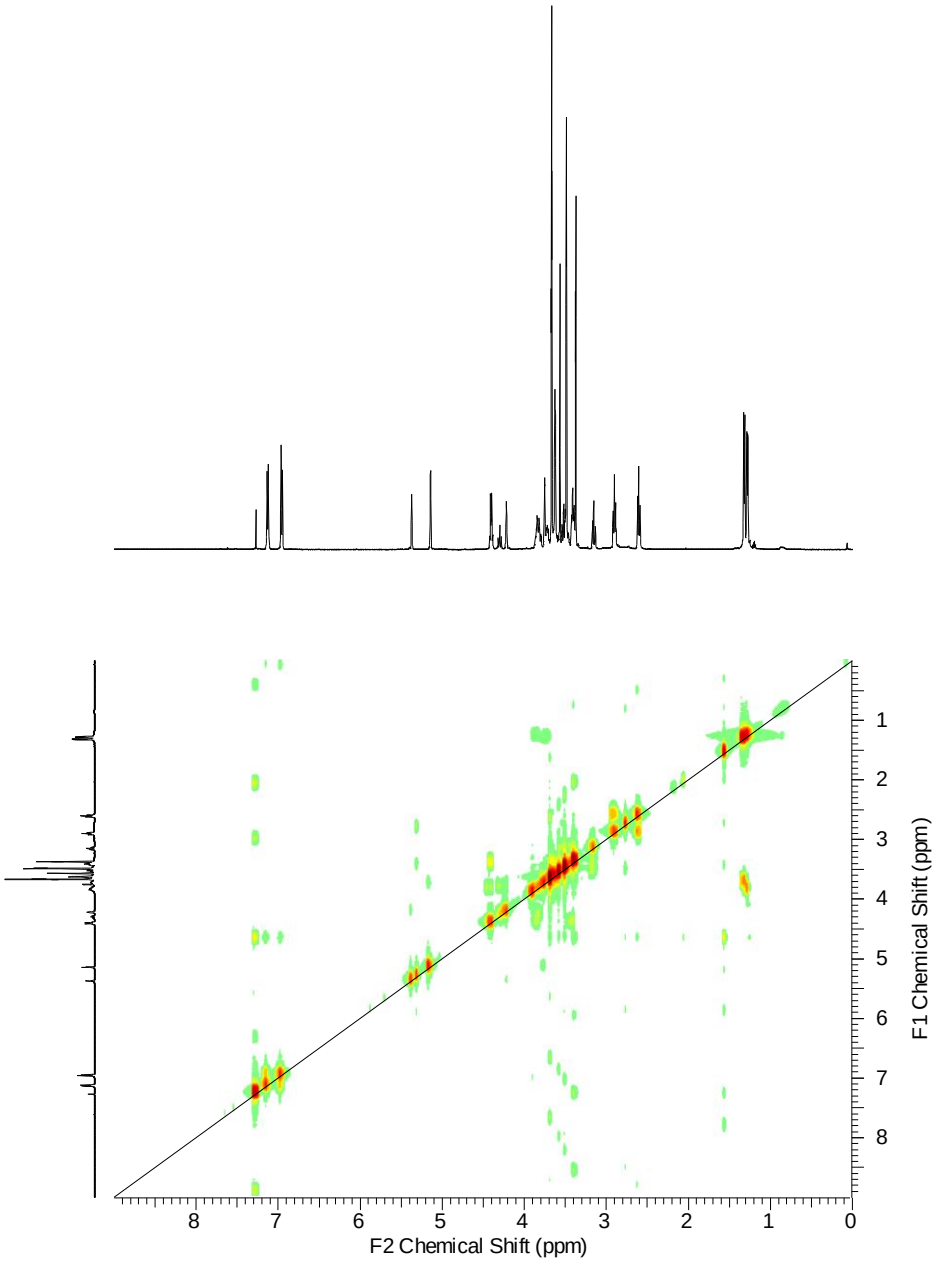


Verbindung **28** – ^{19}F-NMR-Spektrum



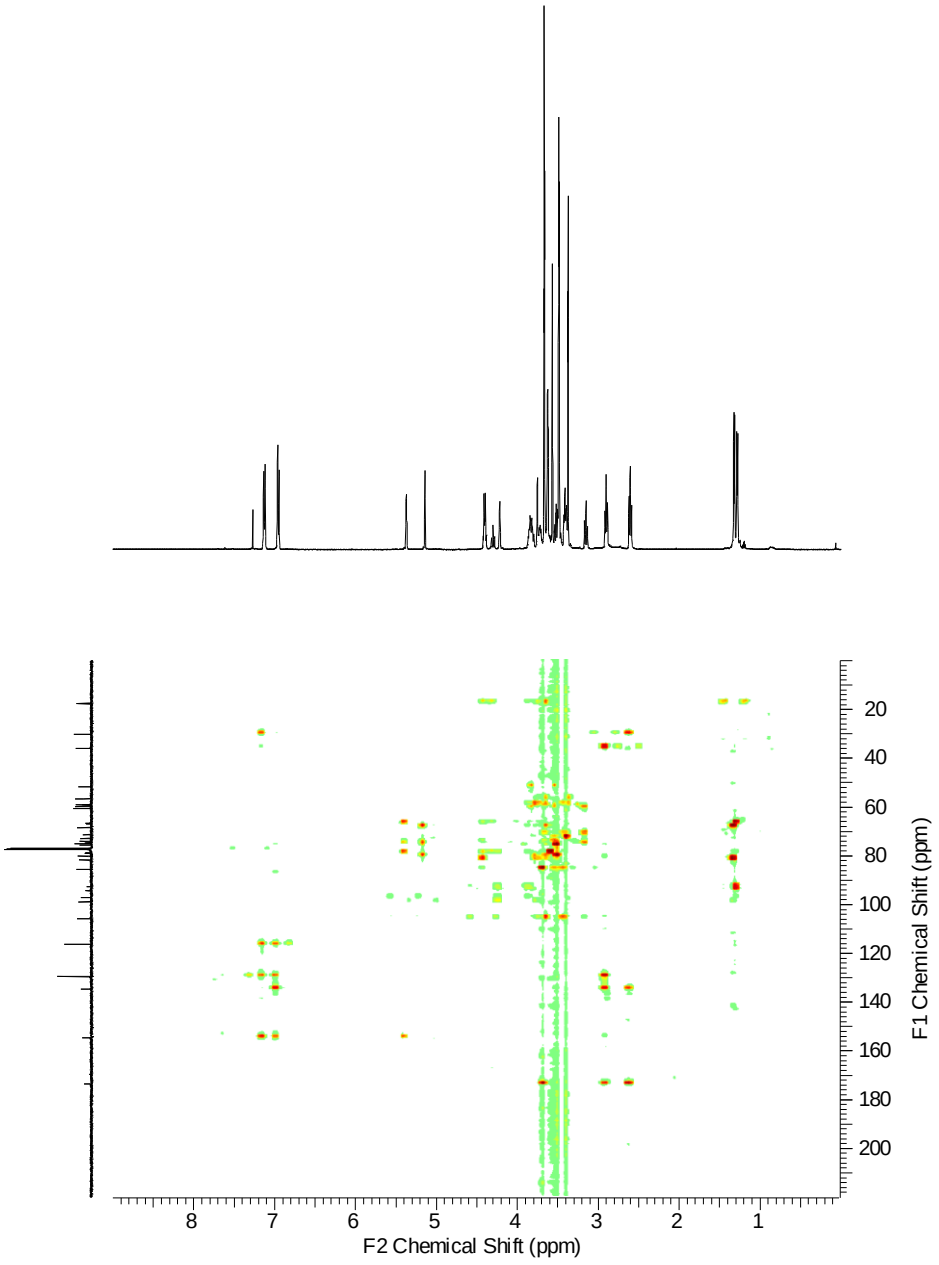
Verbindung **28** – ^{1}H-^{1}H-COSY-NMR-Spektrum

MT-433-COSY.011.esp



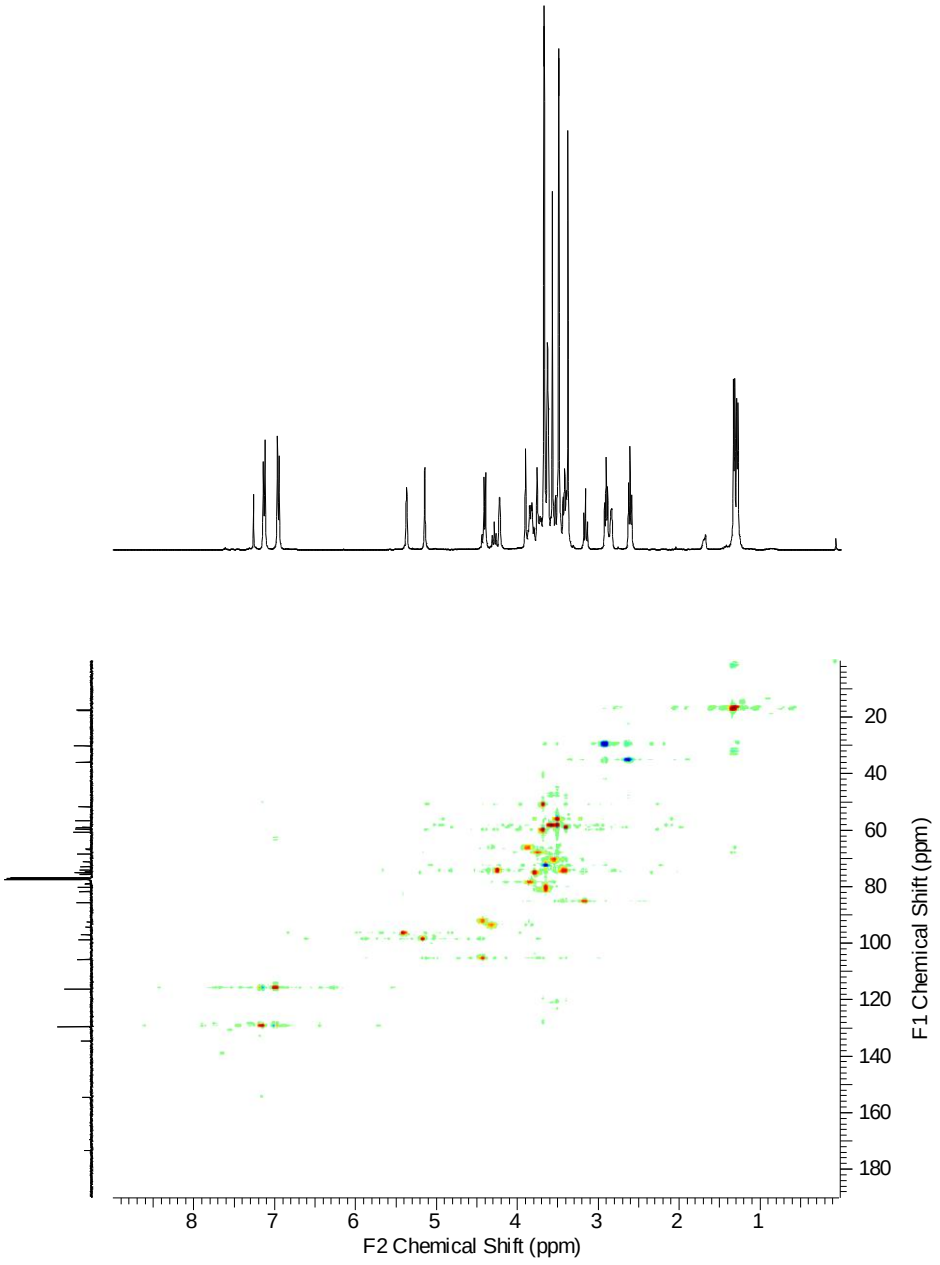
Verbindung **28** – ^{1}H-^{13}C-HMBC-NMR-Spektrum

GHMBCAD_0101.FID.esp

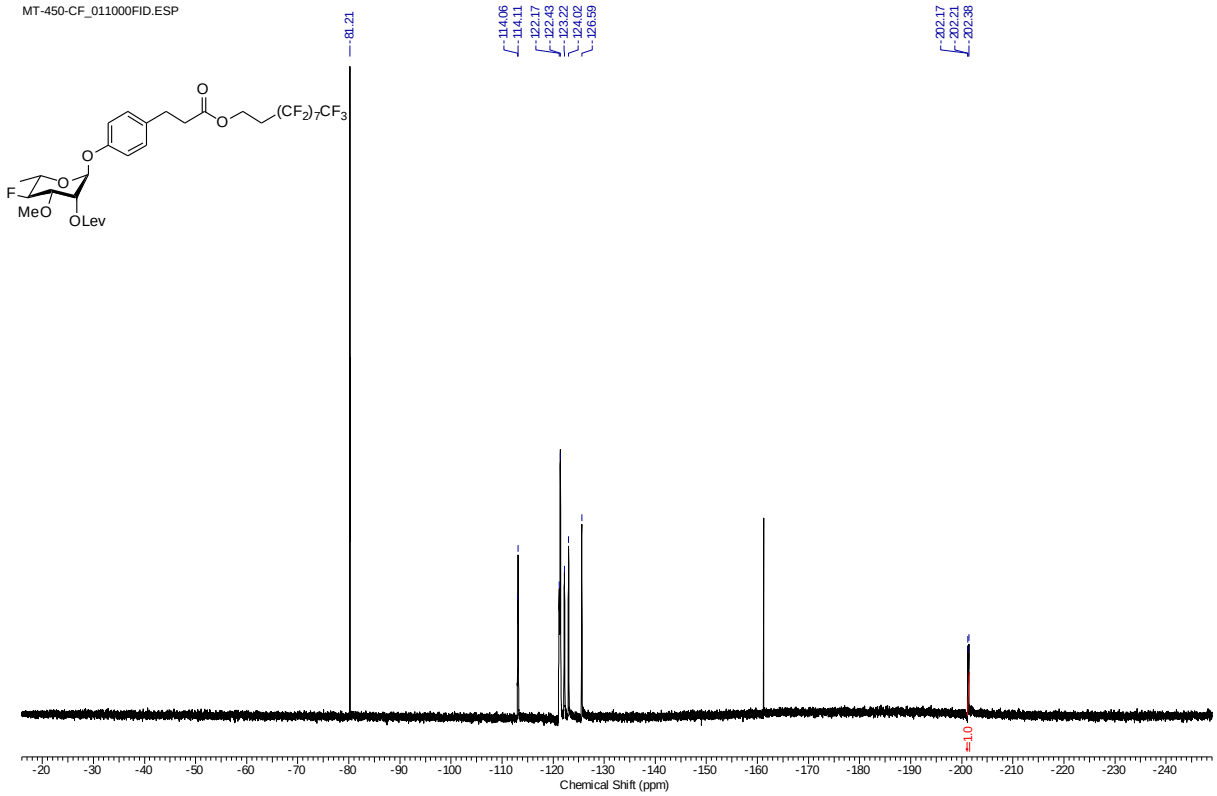


Verbindung **28** – ^{1}H-^{13}C-HSQC-DEPT-NMR-Spektrum

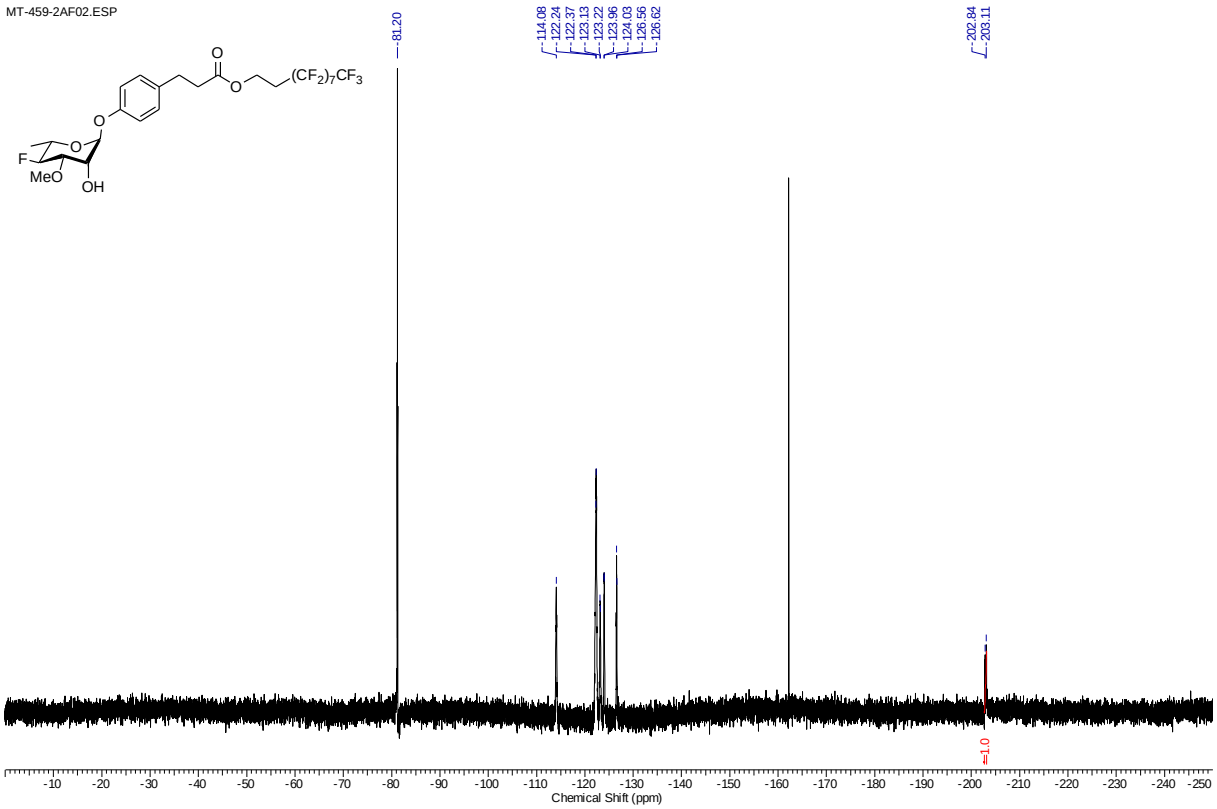
GHSQCAD_0101.FID.esp



Verbindung **98** – ^{19}F-NMR-Spektrum

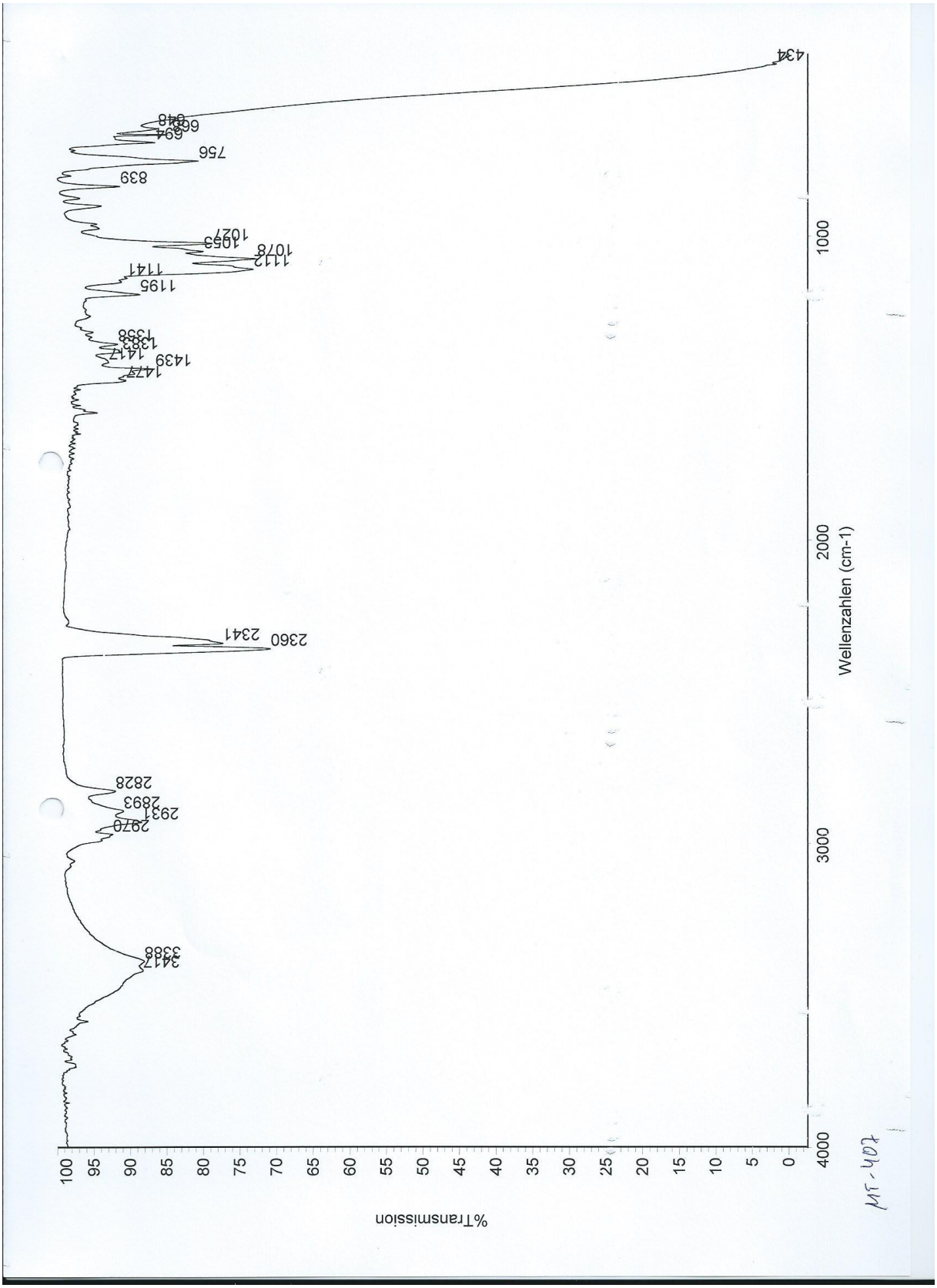


Verbindung **99** – ^{19}F-NMR-Spektrum

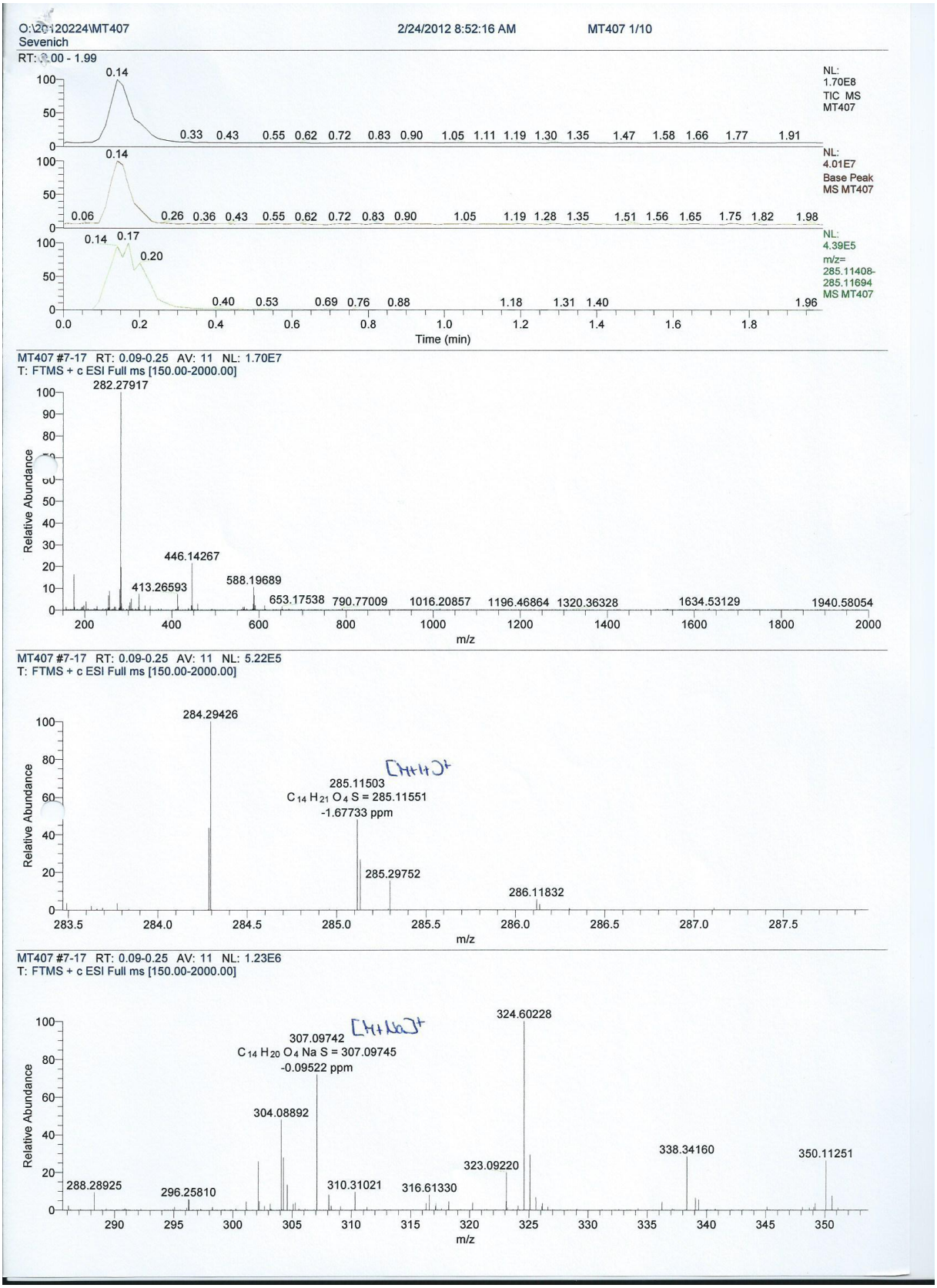


H IR- und Massen-Spektren – Teil A

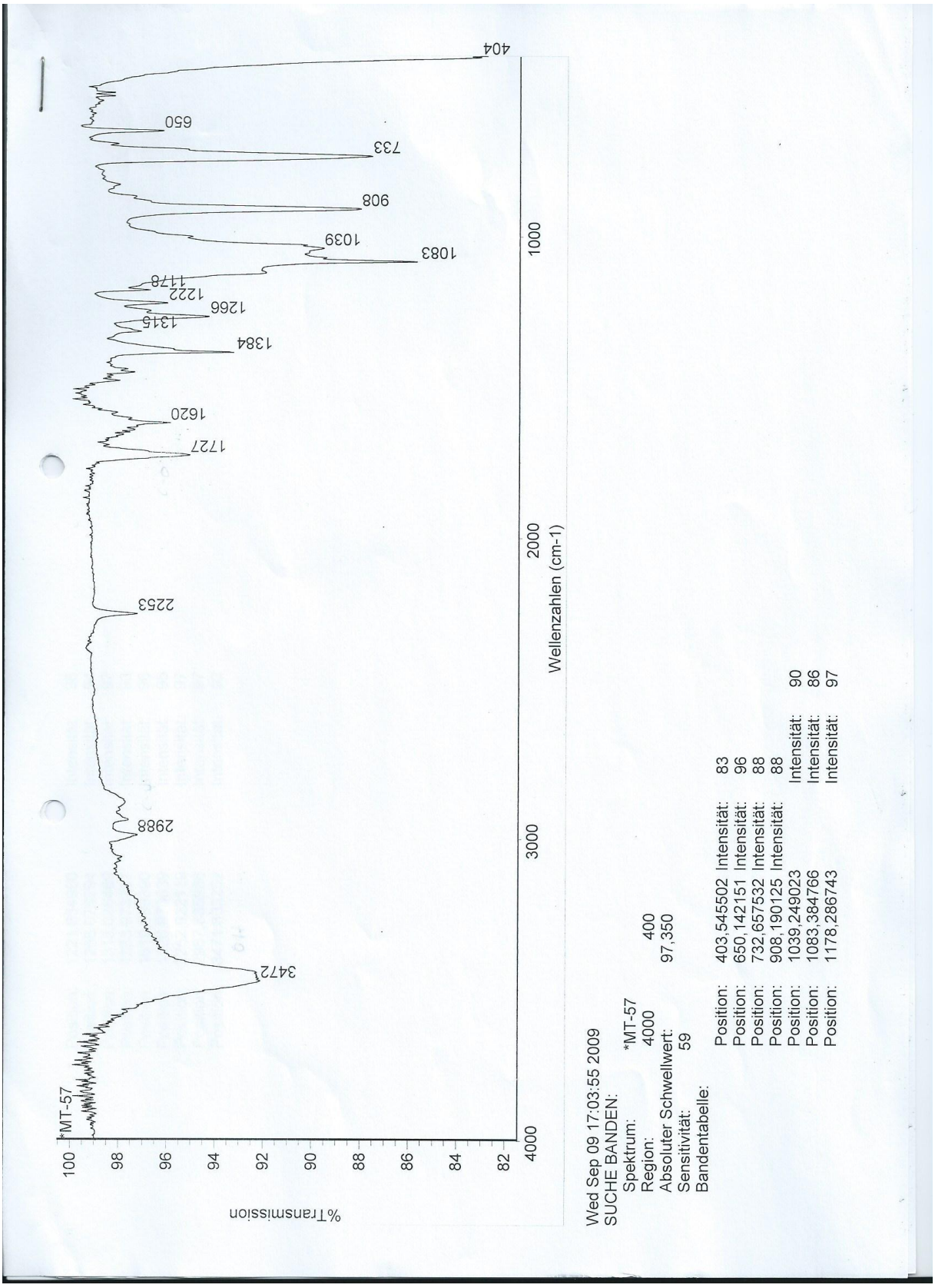
Verbindung **66** – IR



Verbindung **66** – Massenspektrum



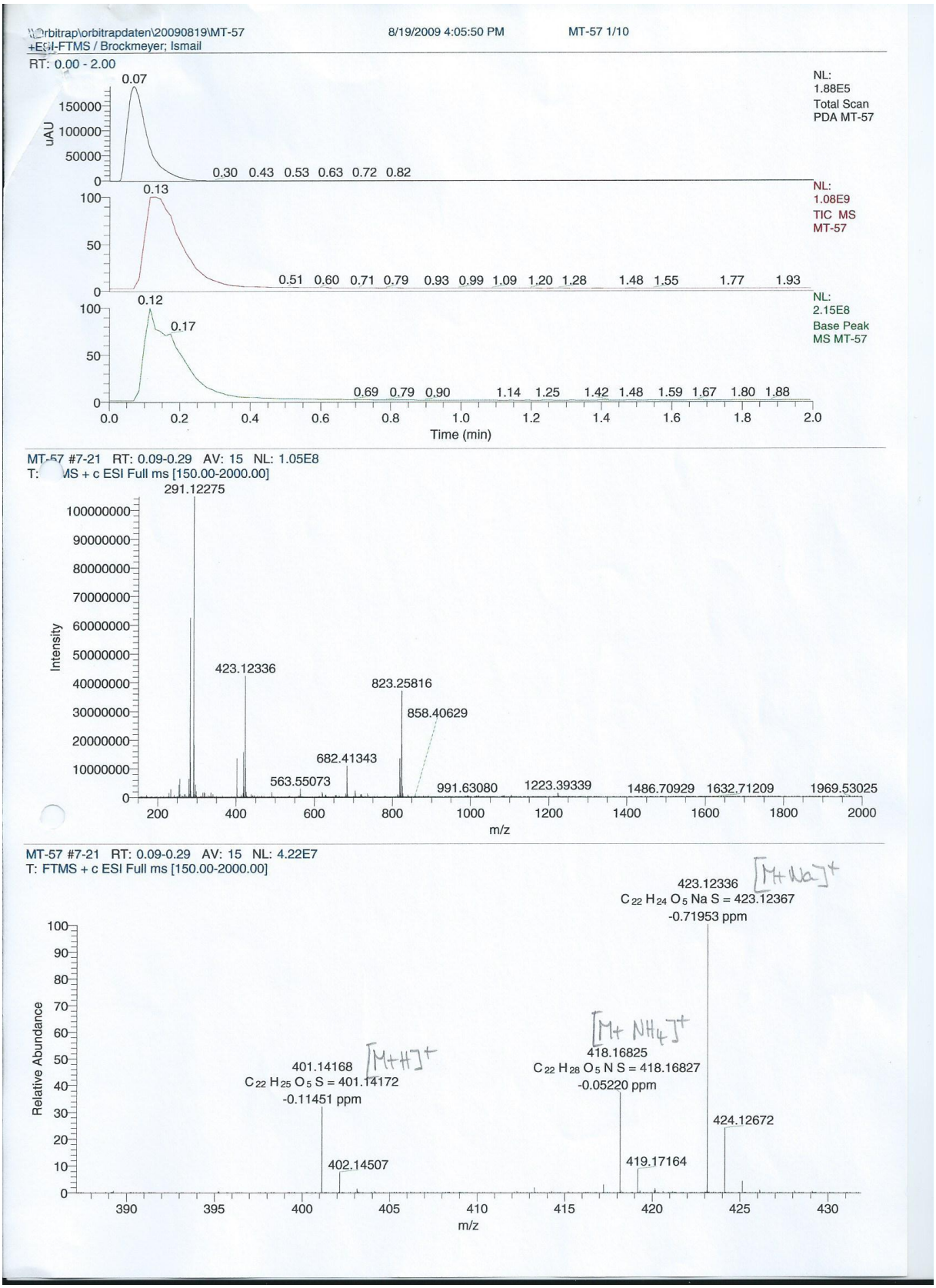
Verbindung **103** – IR



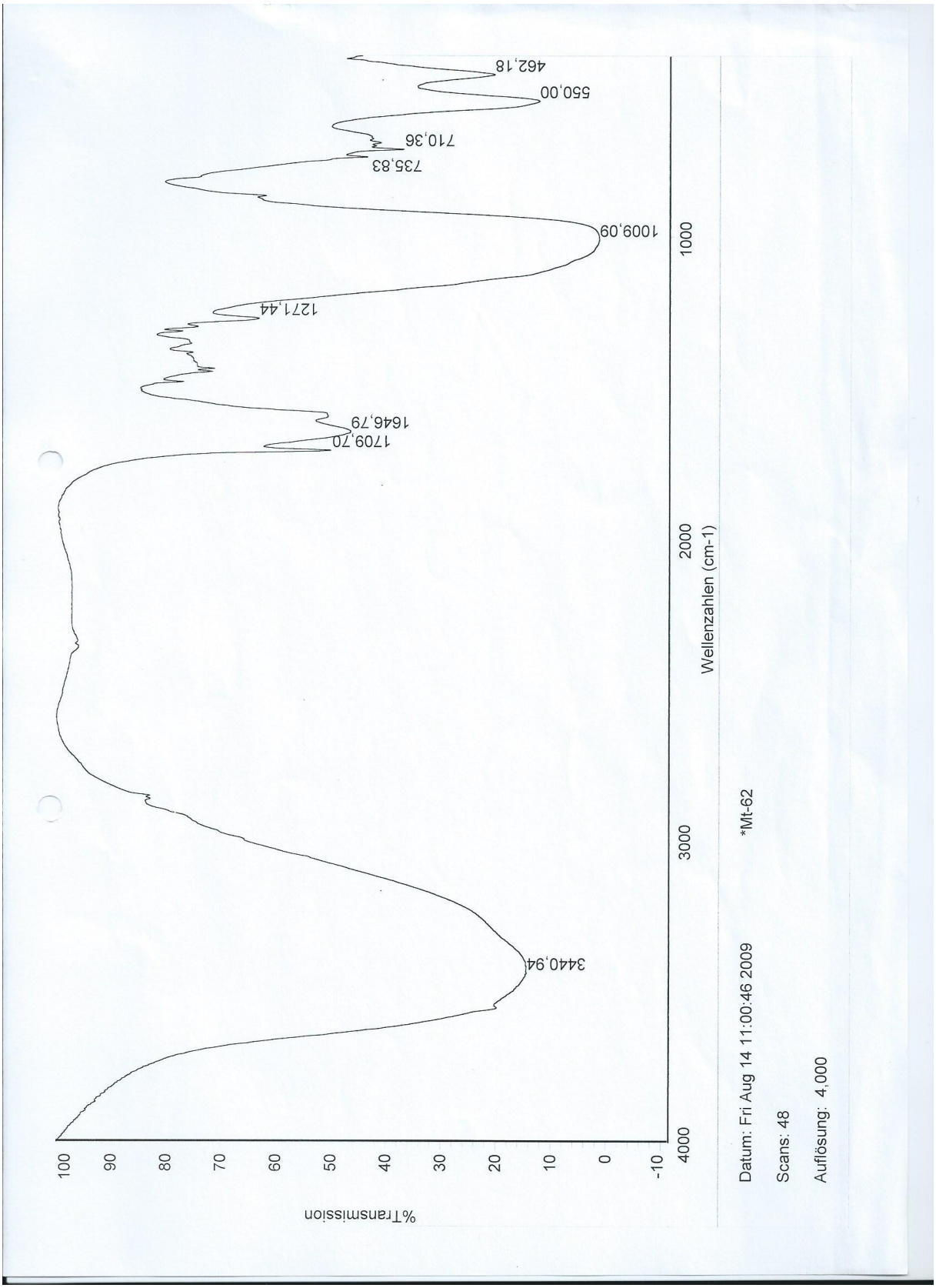
Wed Sep 09 17:03:55 2009
SUCHE BANDEN:

Spektrum:	*MT-57		
Region:	4000	400	
Absoluter Schwellwert:		97,350	
Sensitivität:		59	
Bandentabelle:			
	Position:	403,545502	Intensität: 83
	Position:	650,142151	Intensität: 96
	Position:	732,657532	Intensität: 88
	Position:	908,190125	Intensität: 88
	Position:	1039,249023	Intensität: 90
	Position:	1083,384766	Intensität: 86
	Position:	1178,286743	Intensität: 97

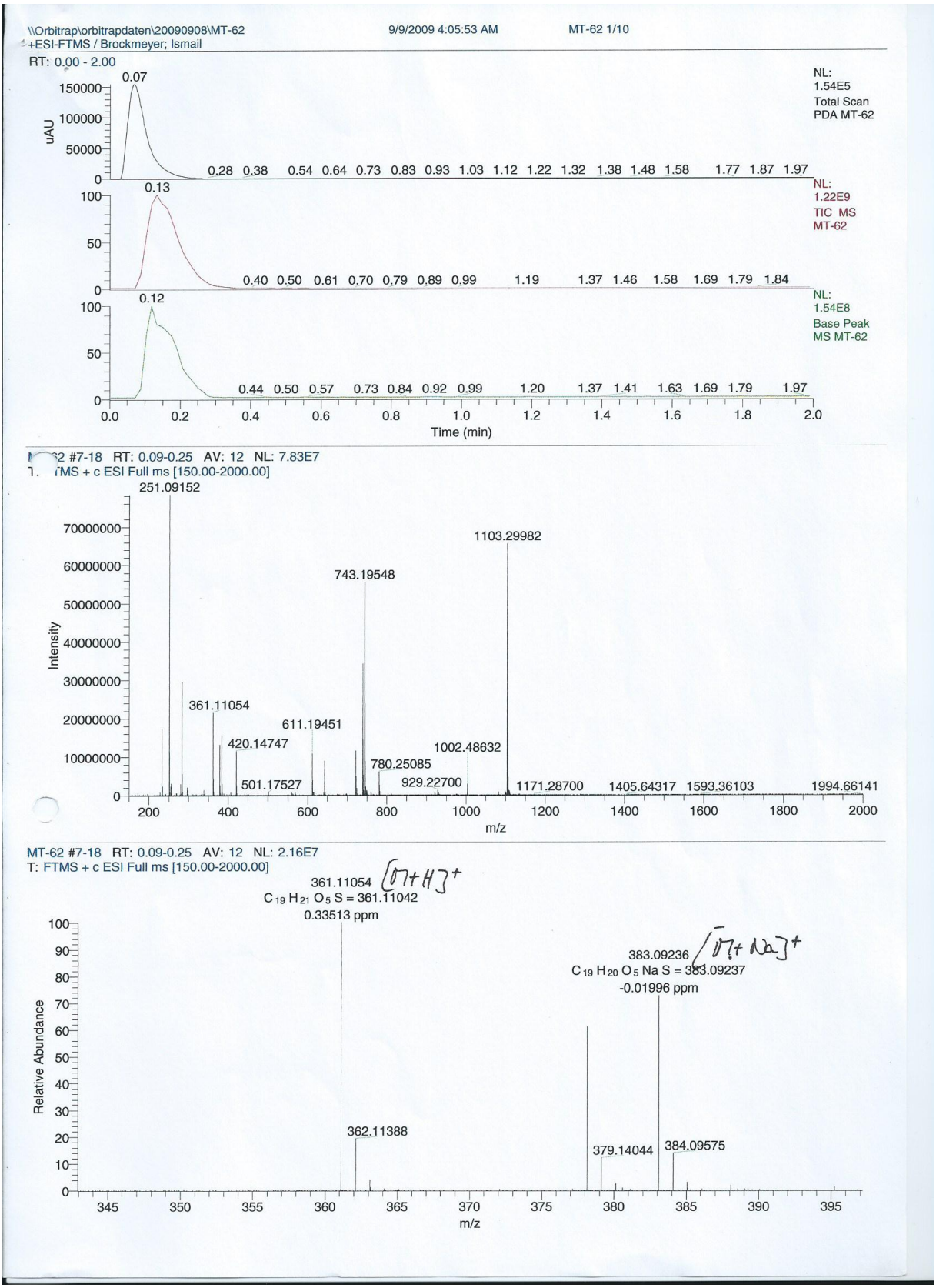
Verbindung **103** – Massenspektrum



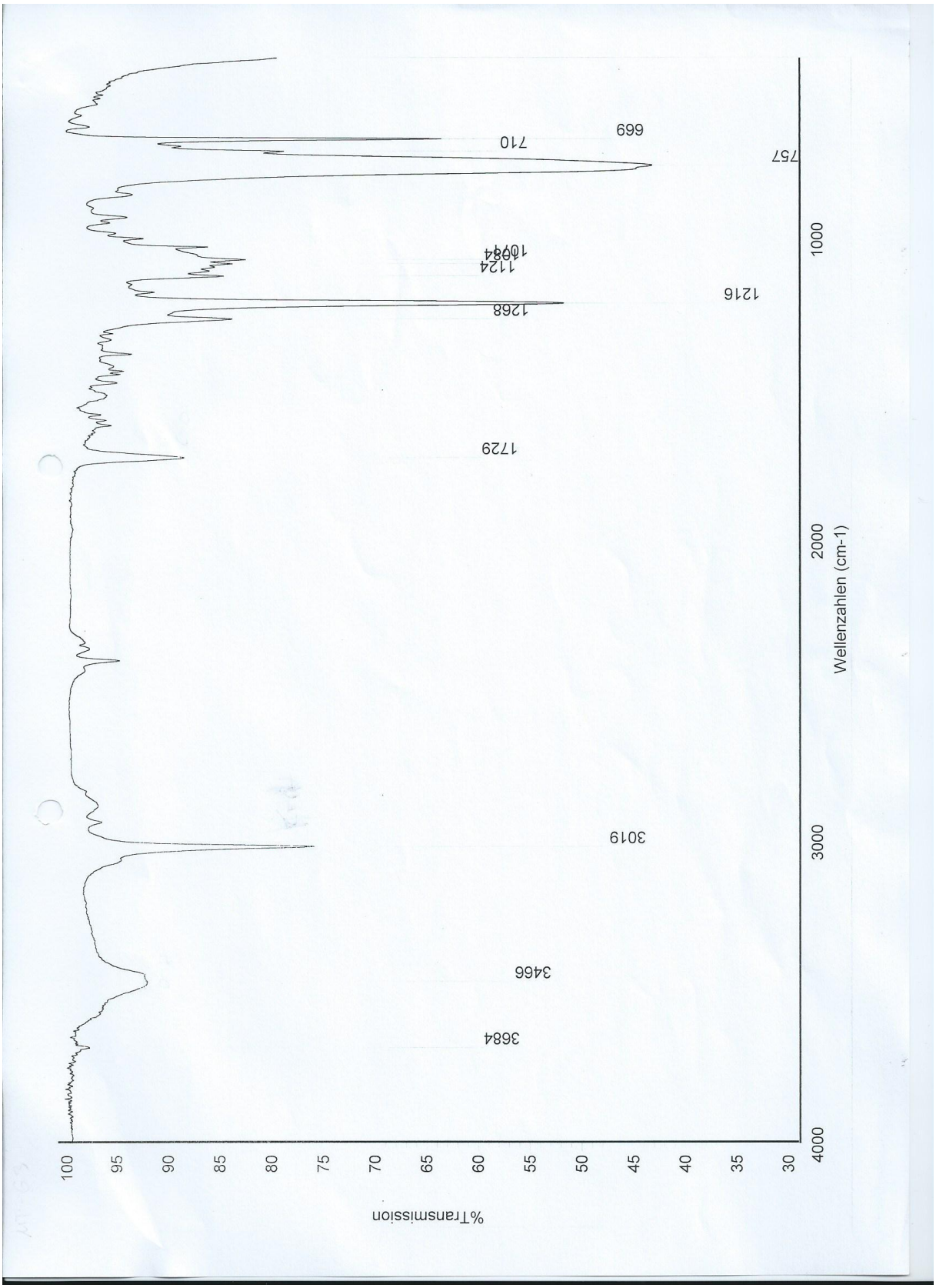
Verbindung **45**– IR



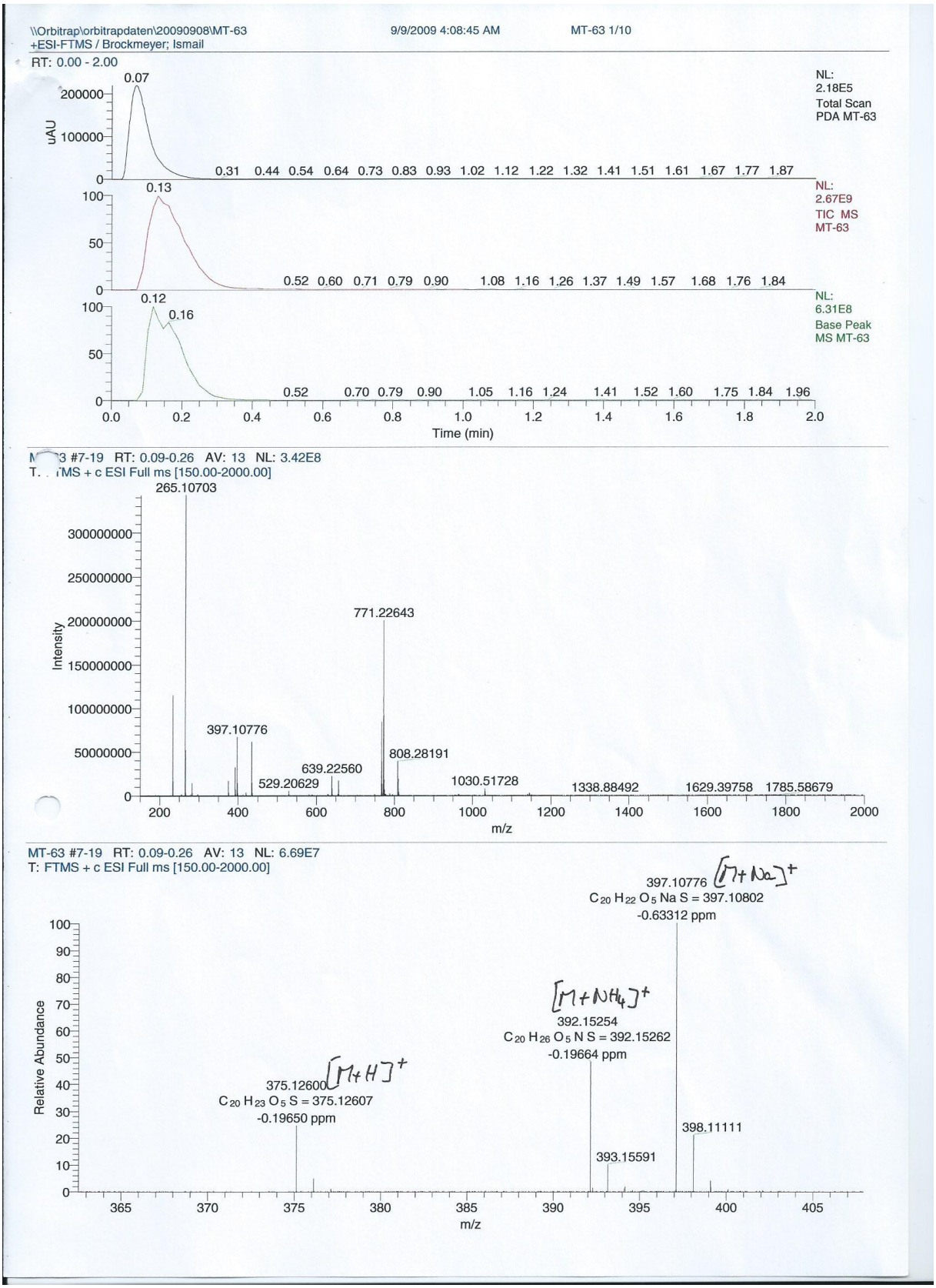
Verbindung **45** – Massenspektrum



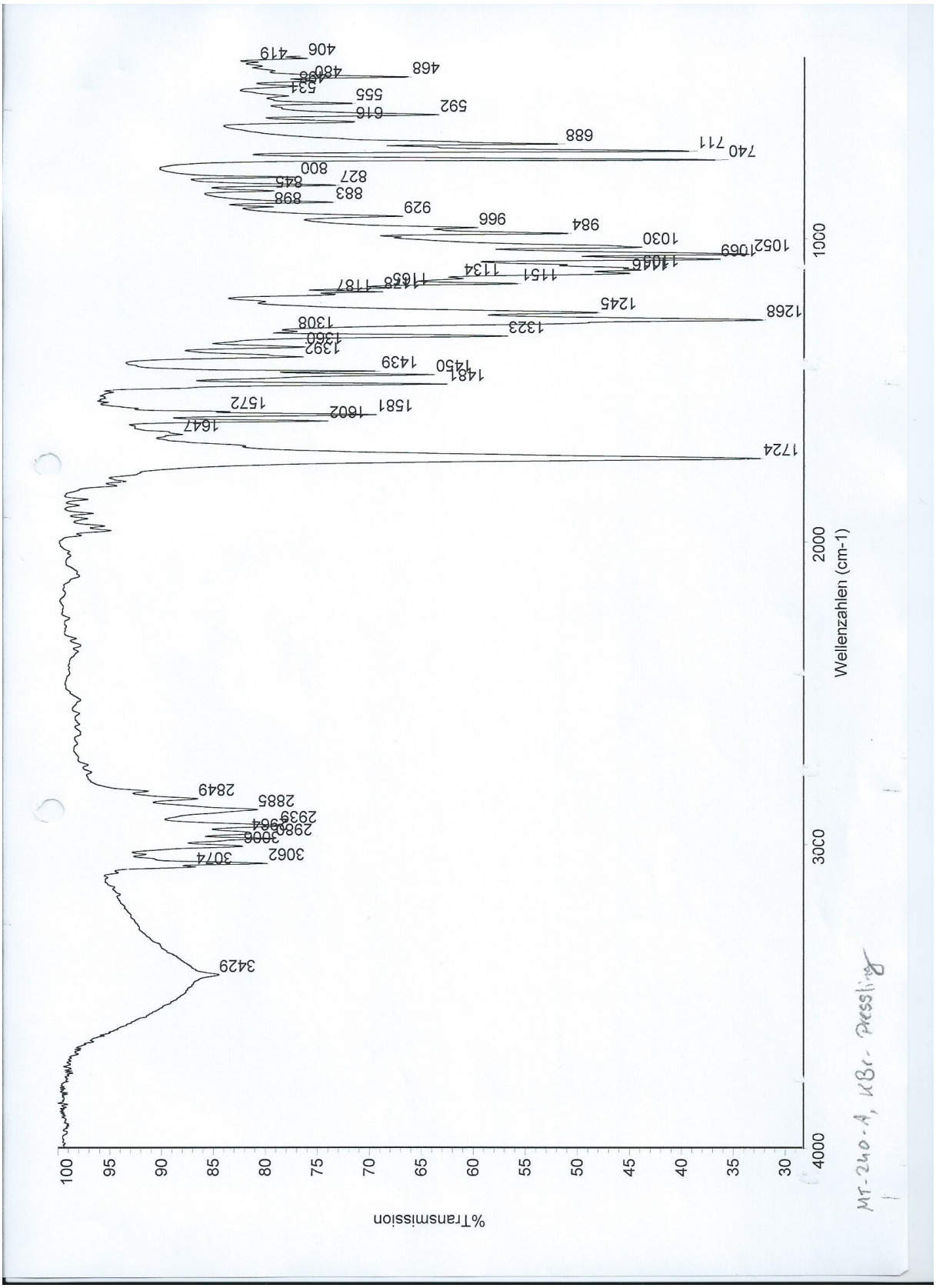
Verbindung **46** – IR



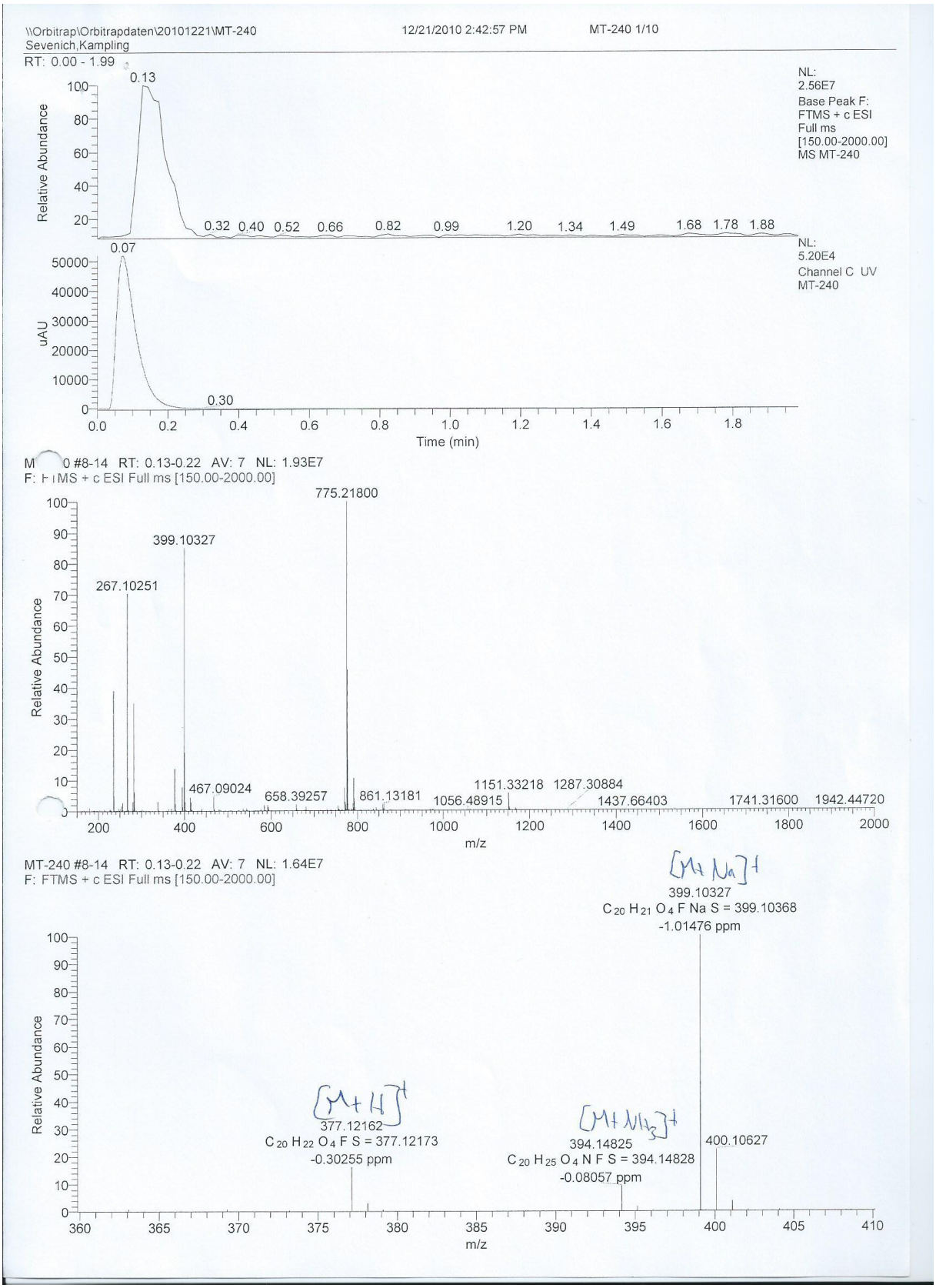
Verbindung **46** – Massenspektrum



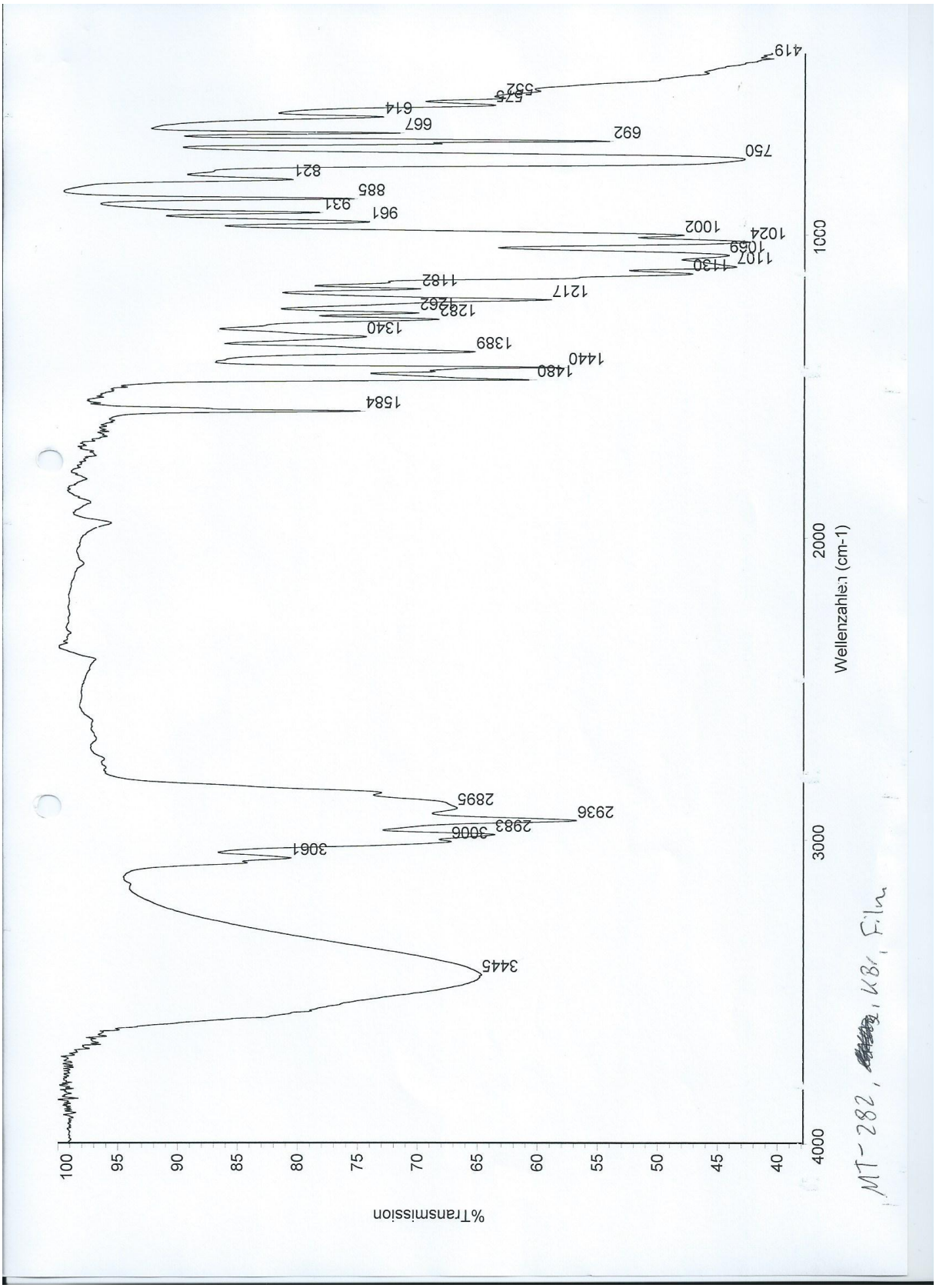
Verbindung **47** – IR



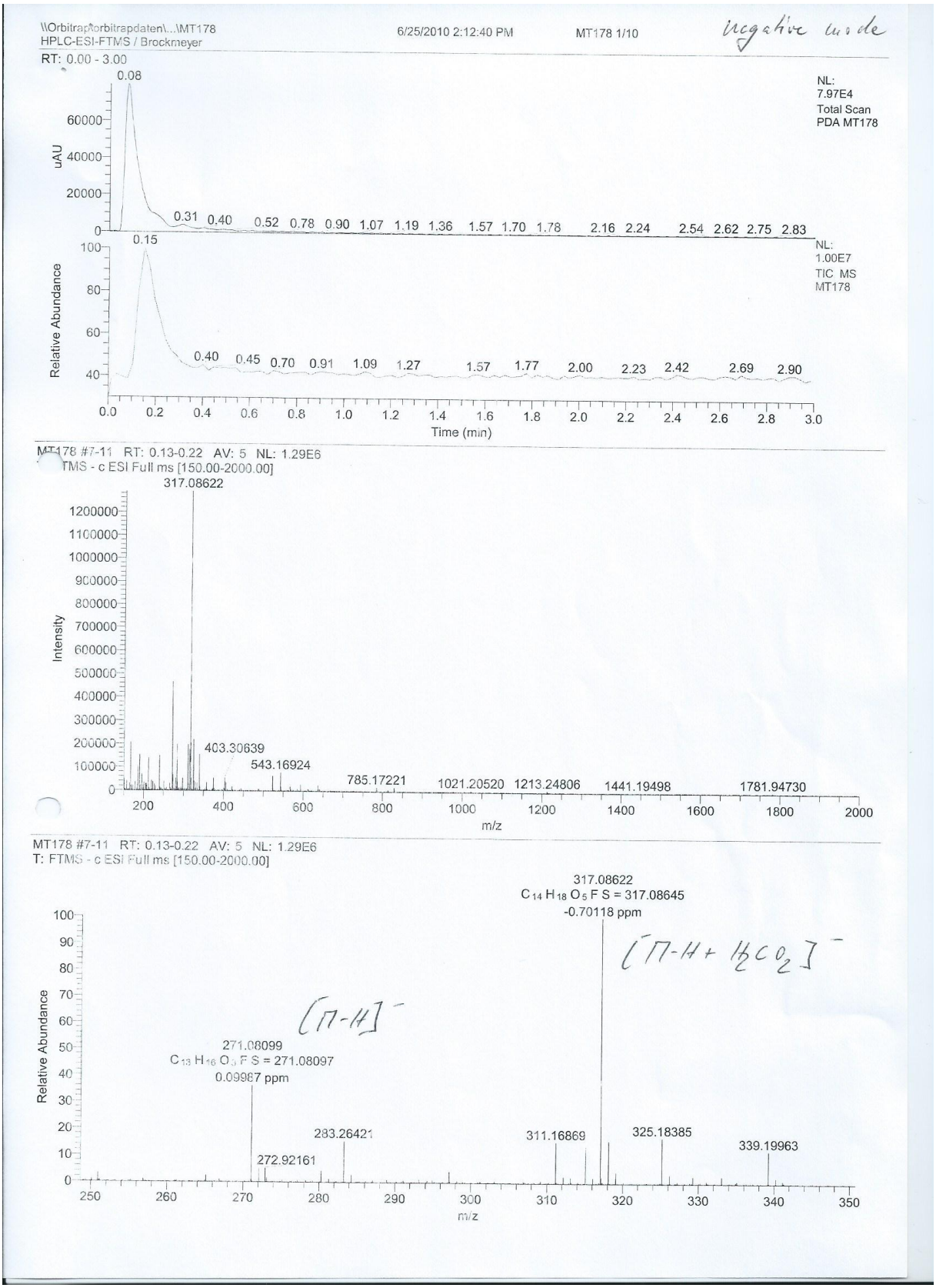
Verbindung **47** – Massenspektrum



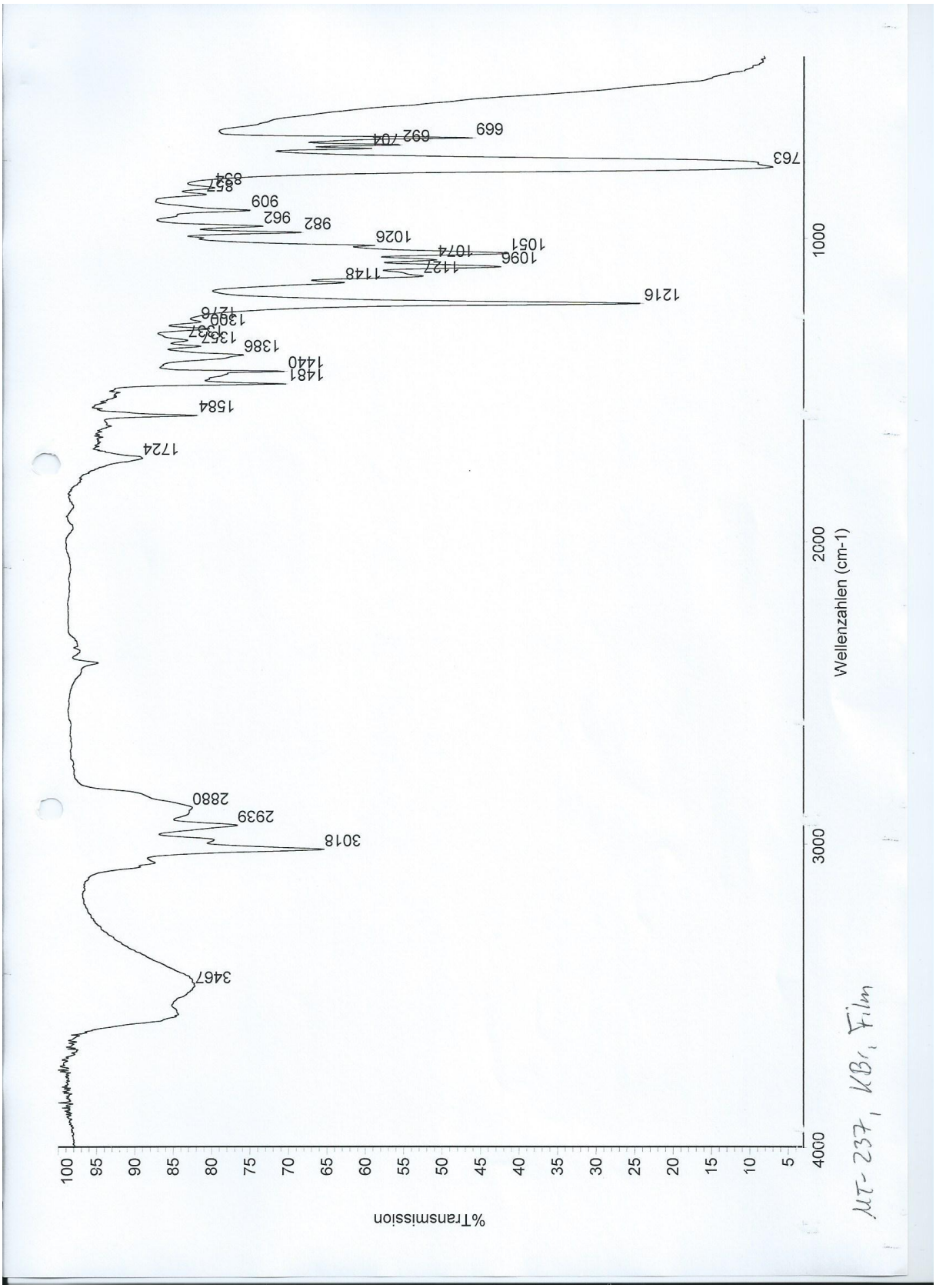
Verbindung **48** – IR



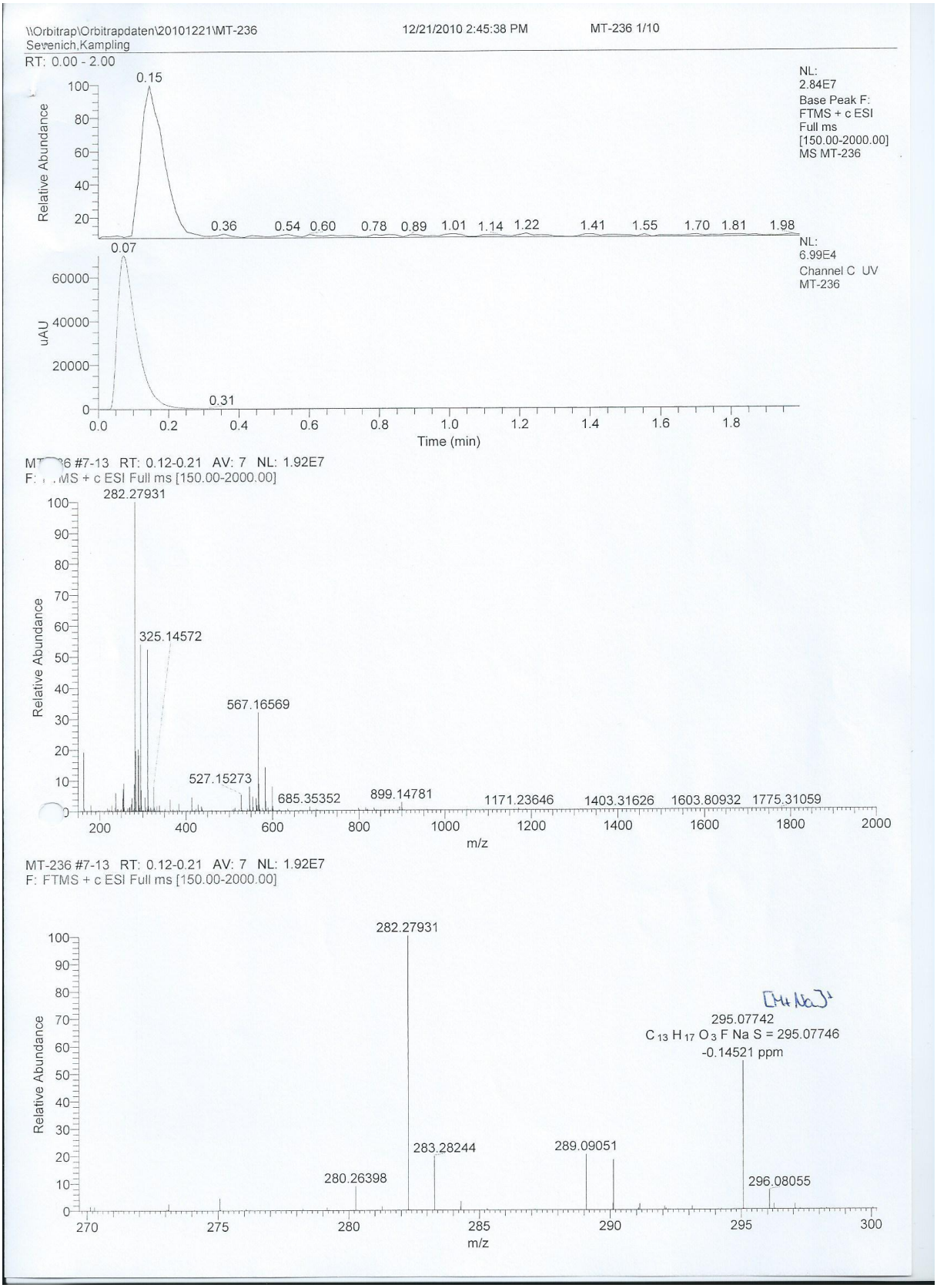
Verbindung **48** – Massenspektrum



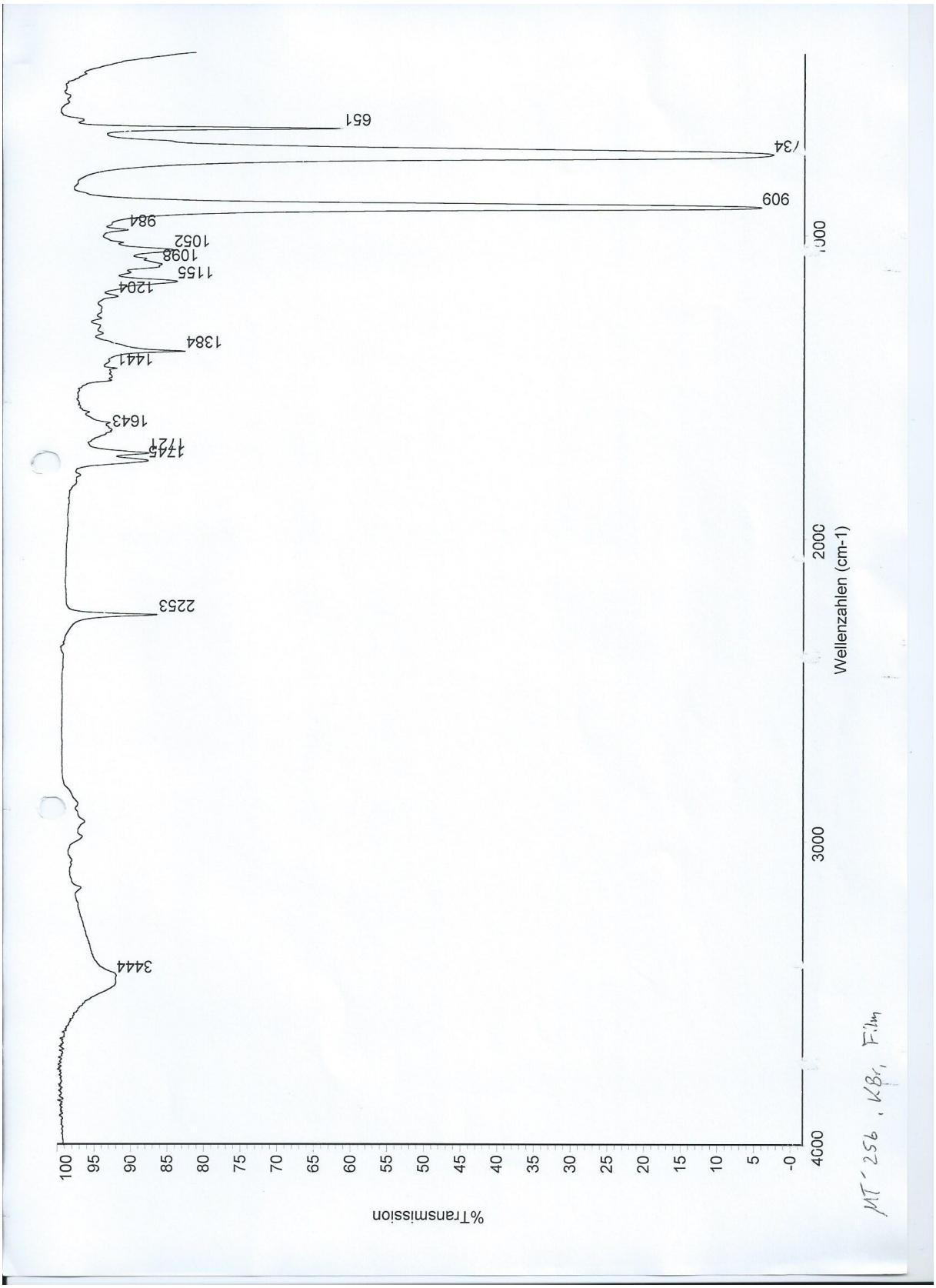
Verbindung **50** – IR



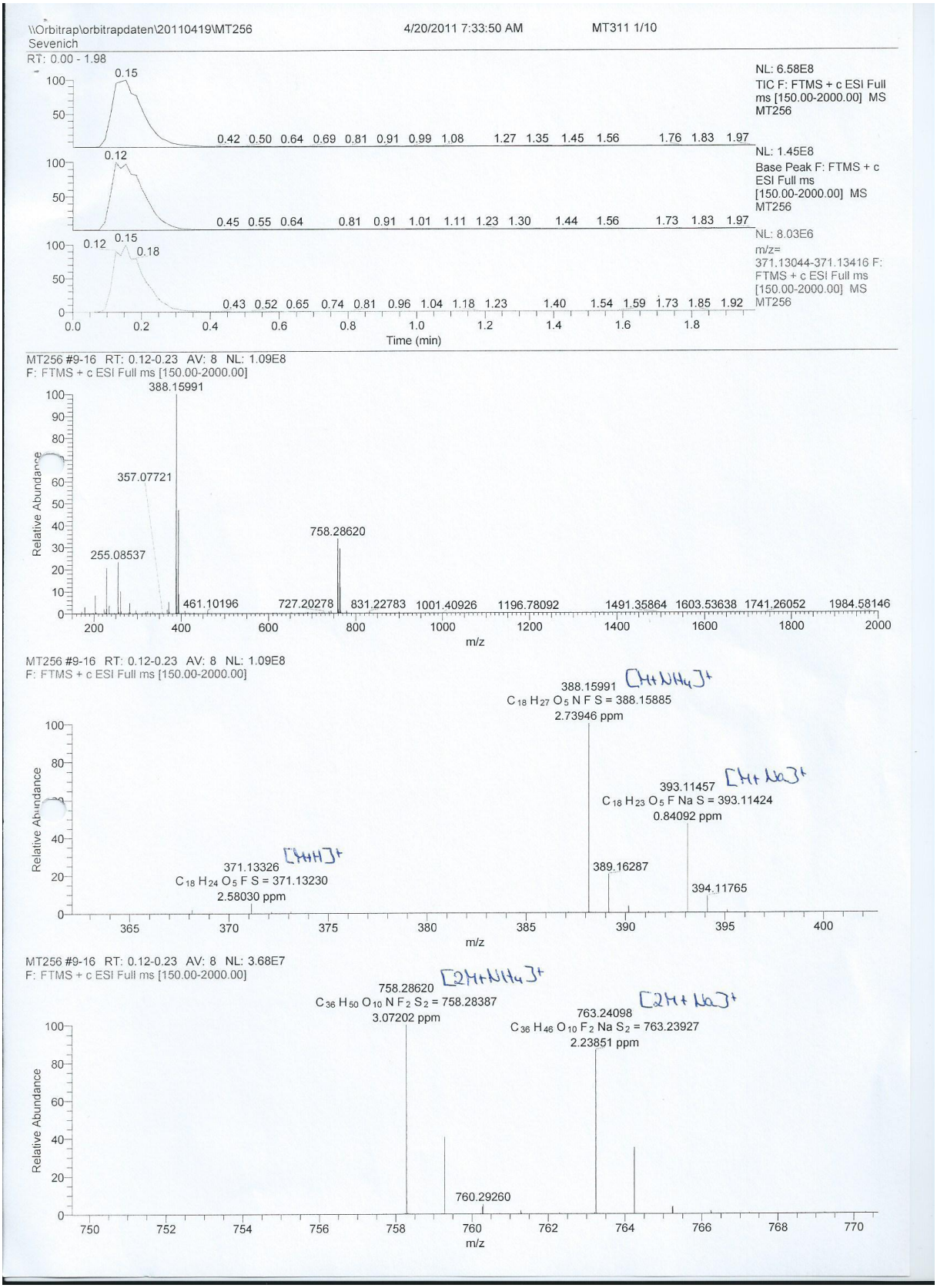
Verbindung **50** – Massenspektrum



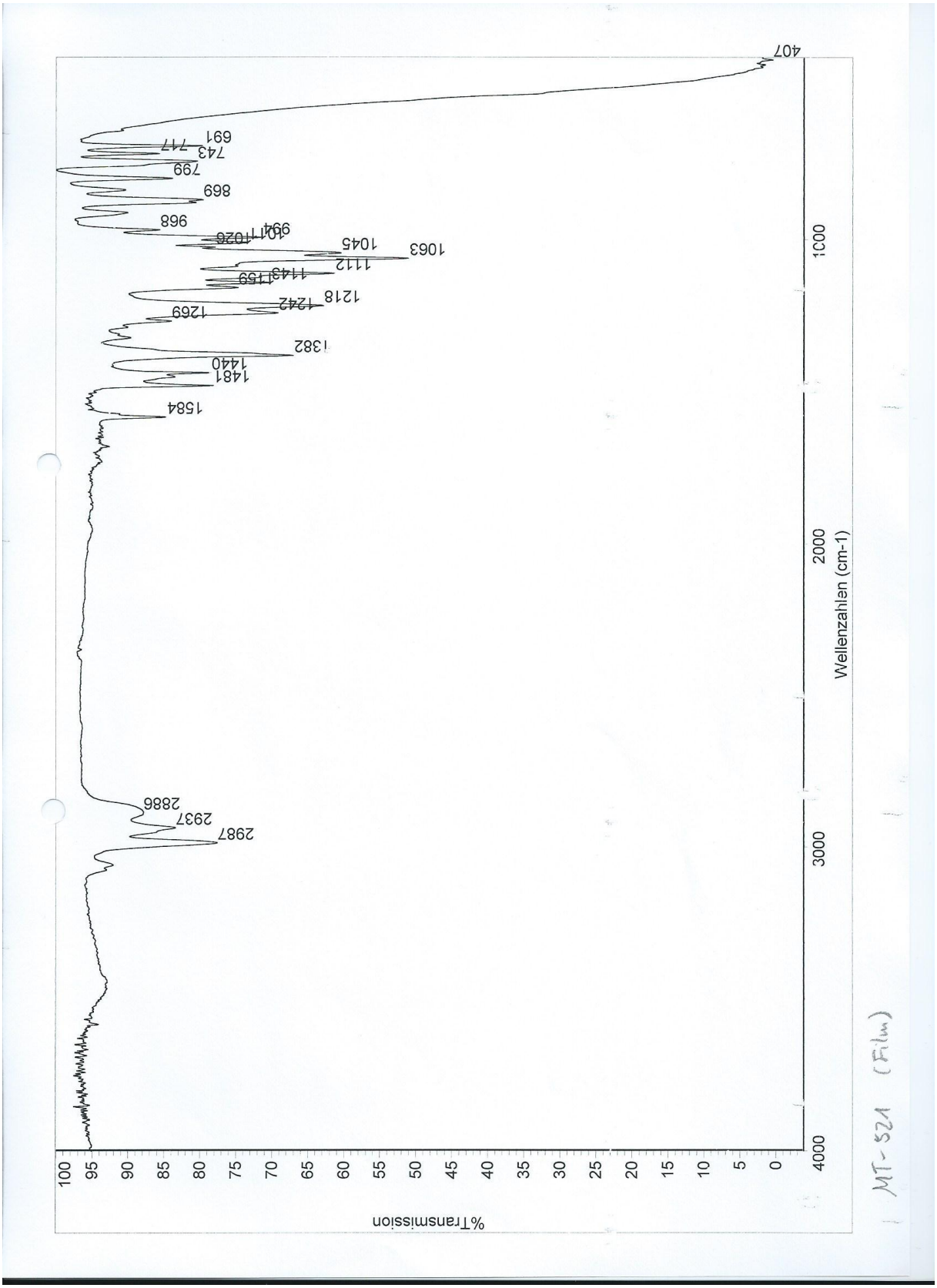
Verbindung **32** – IR



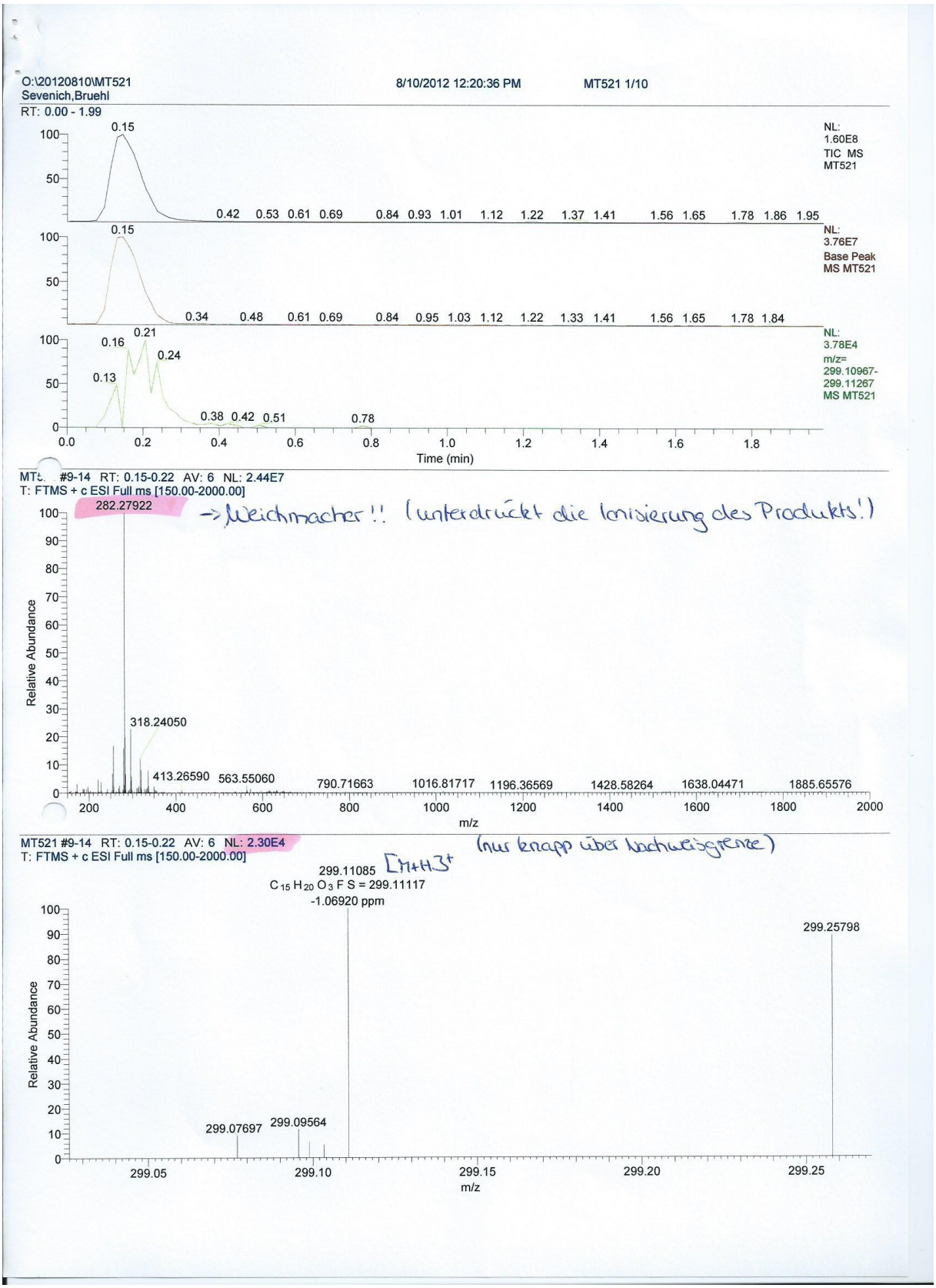
Verbindung **32** – Massenspektrum



Verbindung **59** – IR



Verbindung **59** – Massenspektrum

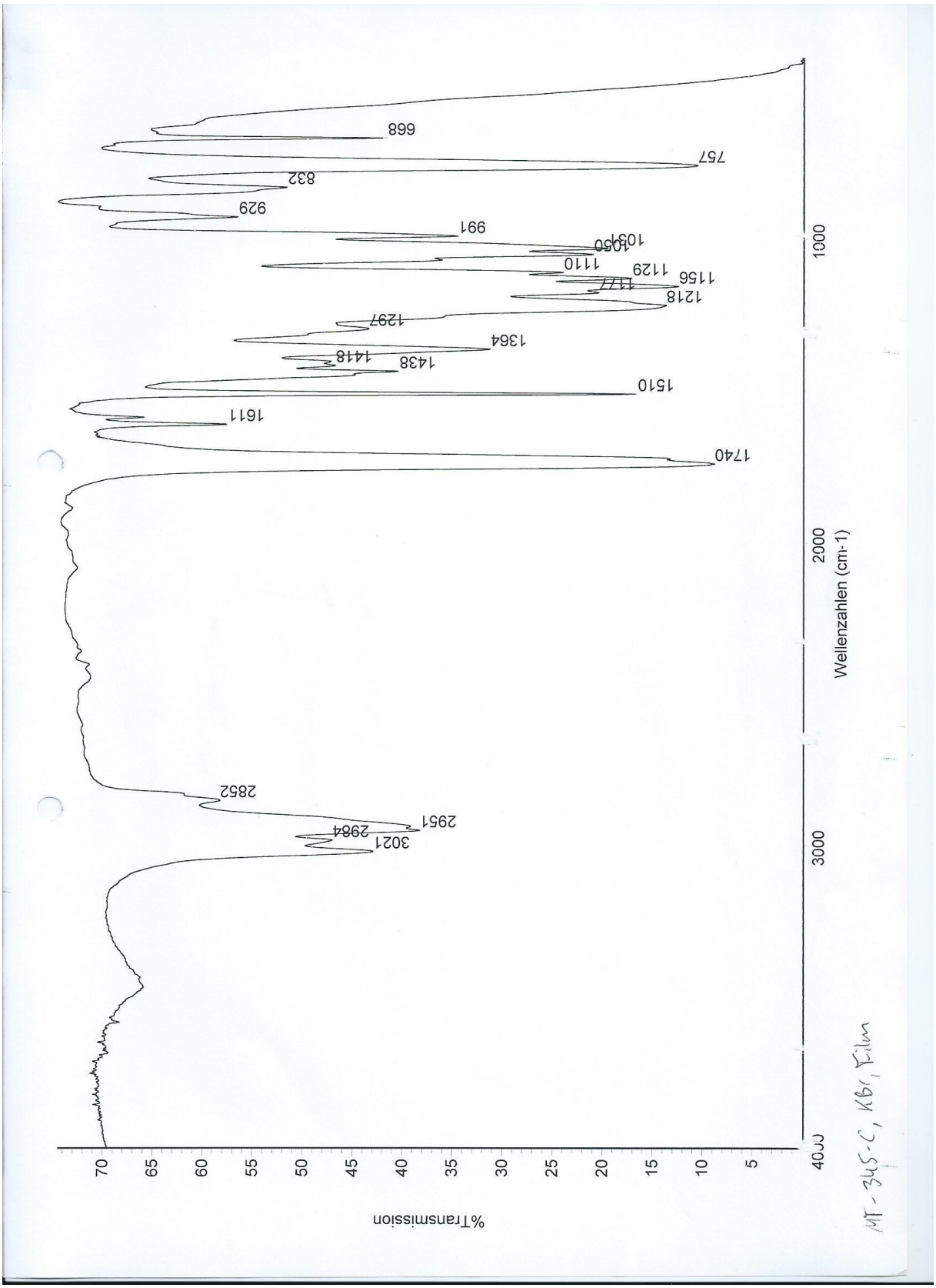


-> Weichmacher!! (unterdrückt die Ionisierung des Produkts!)

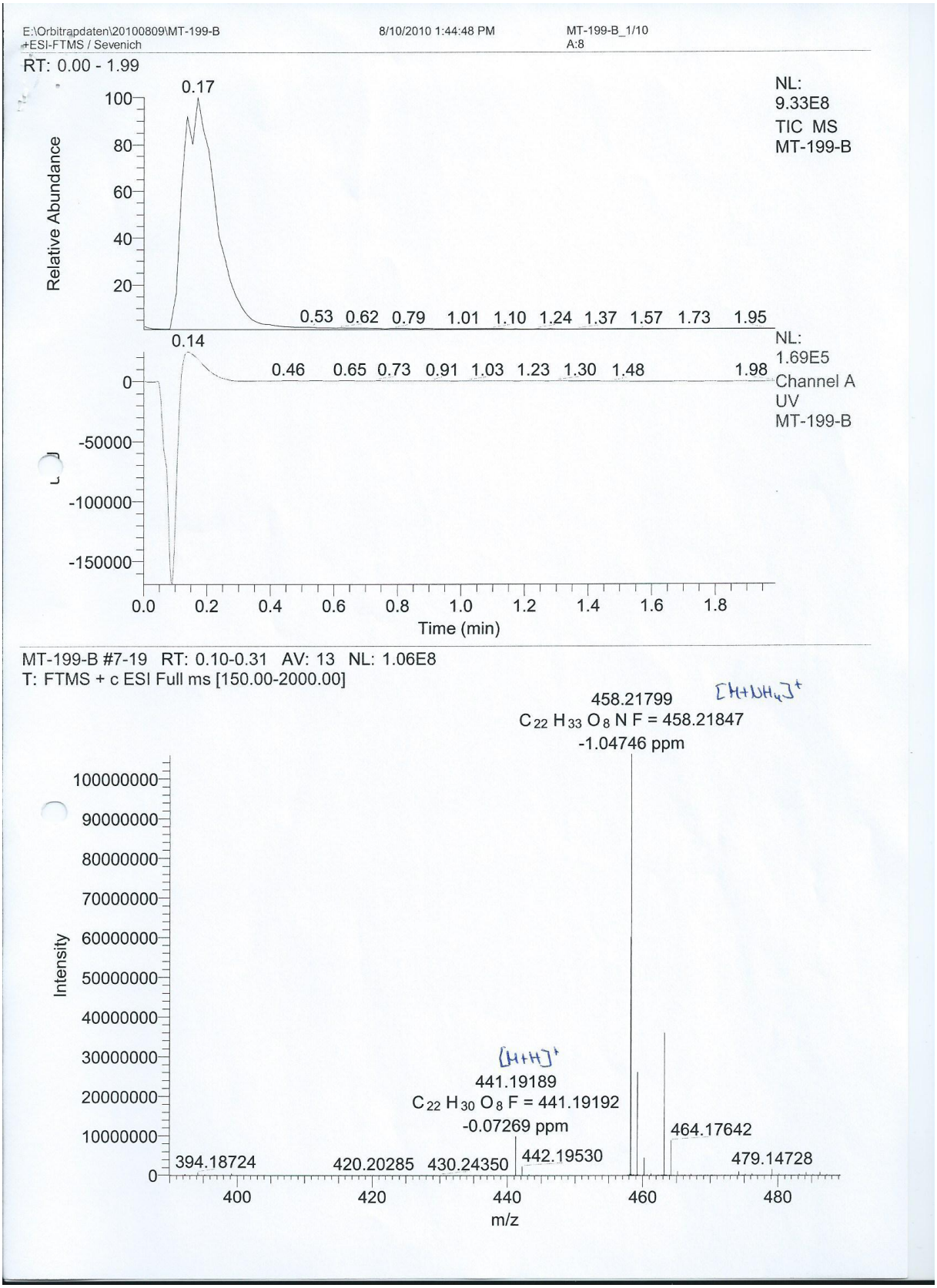
(nur knapp über Nachweisgrenze)

$[M+H]^+$

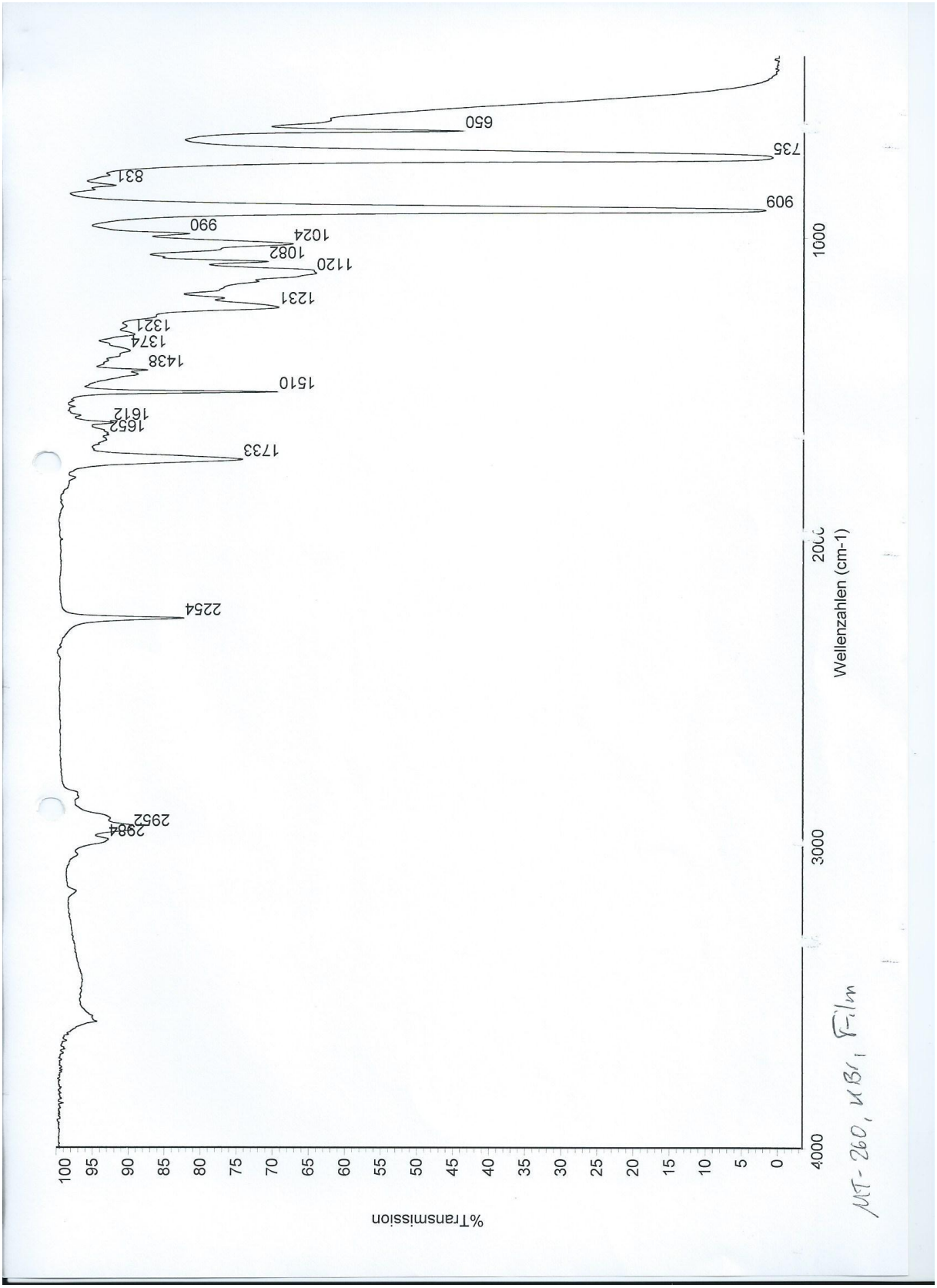
Verbindung **77** – IR



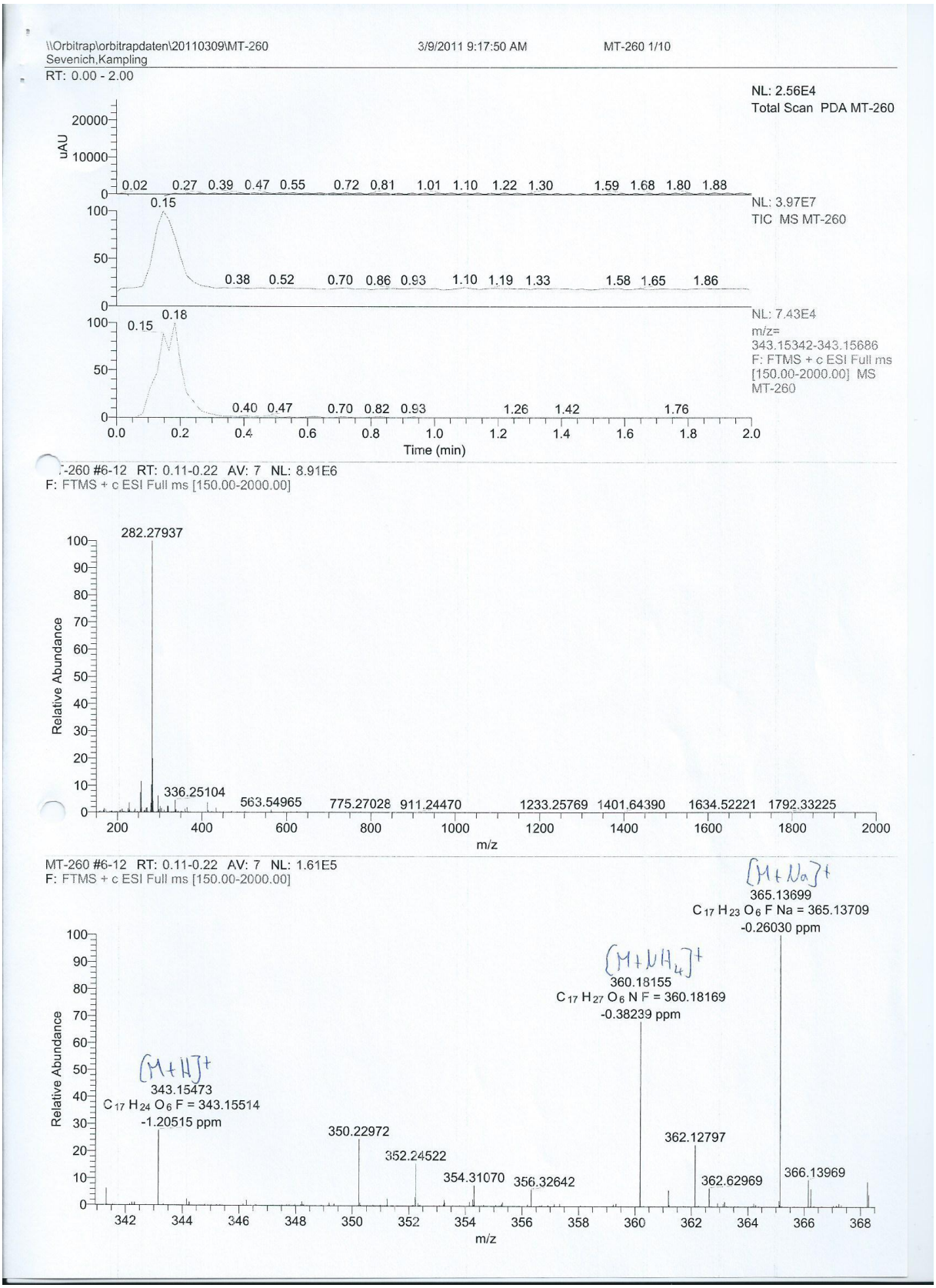
Verbindung **77** – Massenspektrum



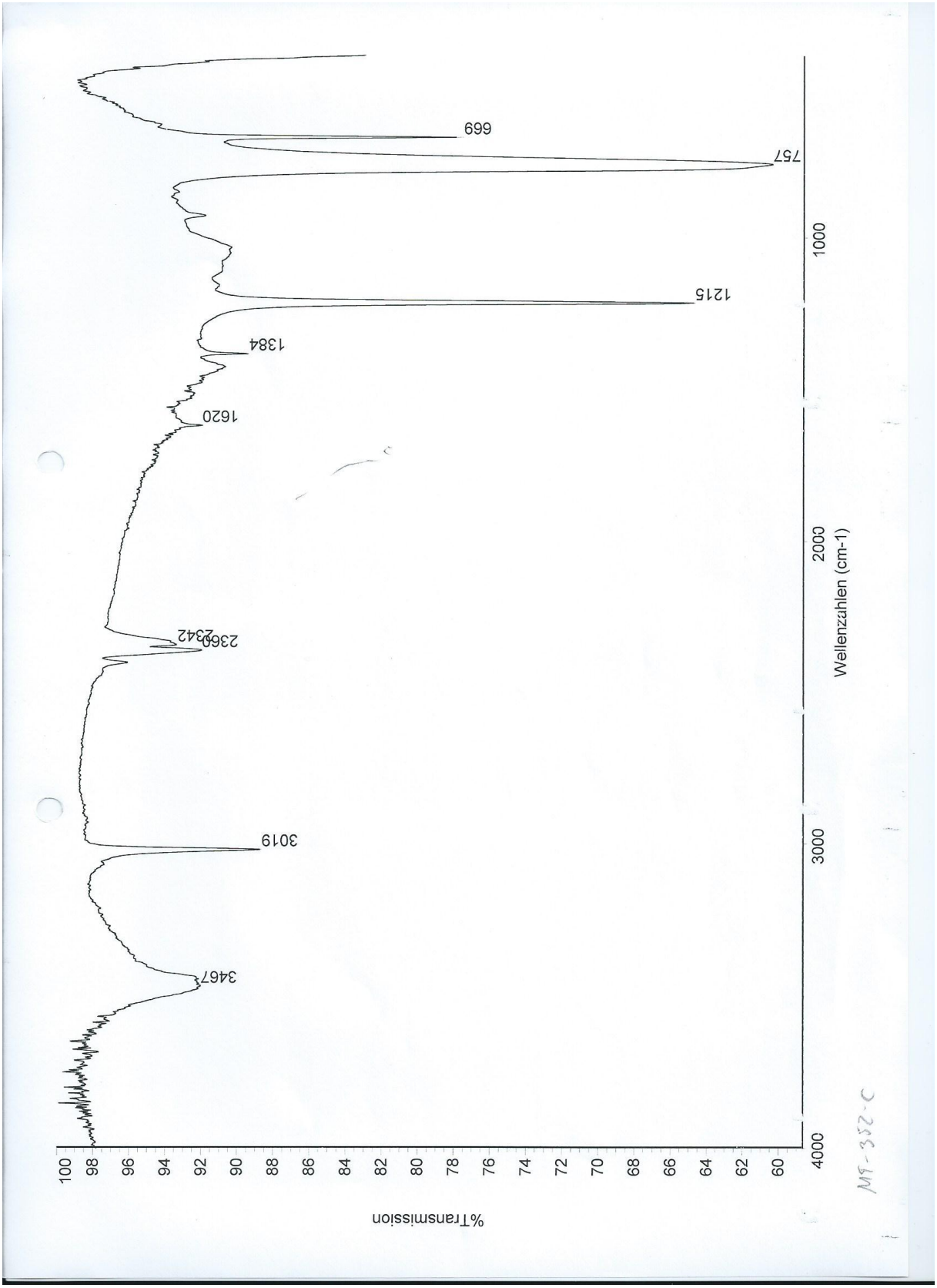
Verbindung **78** – IR



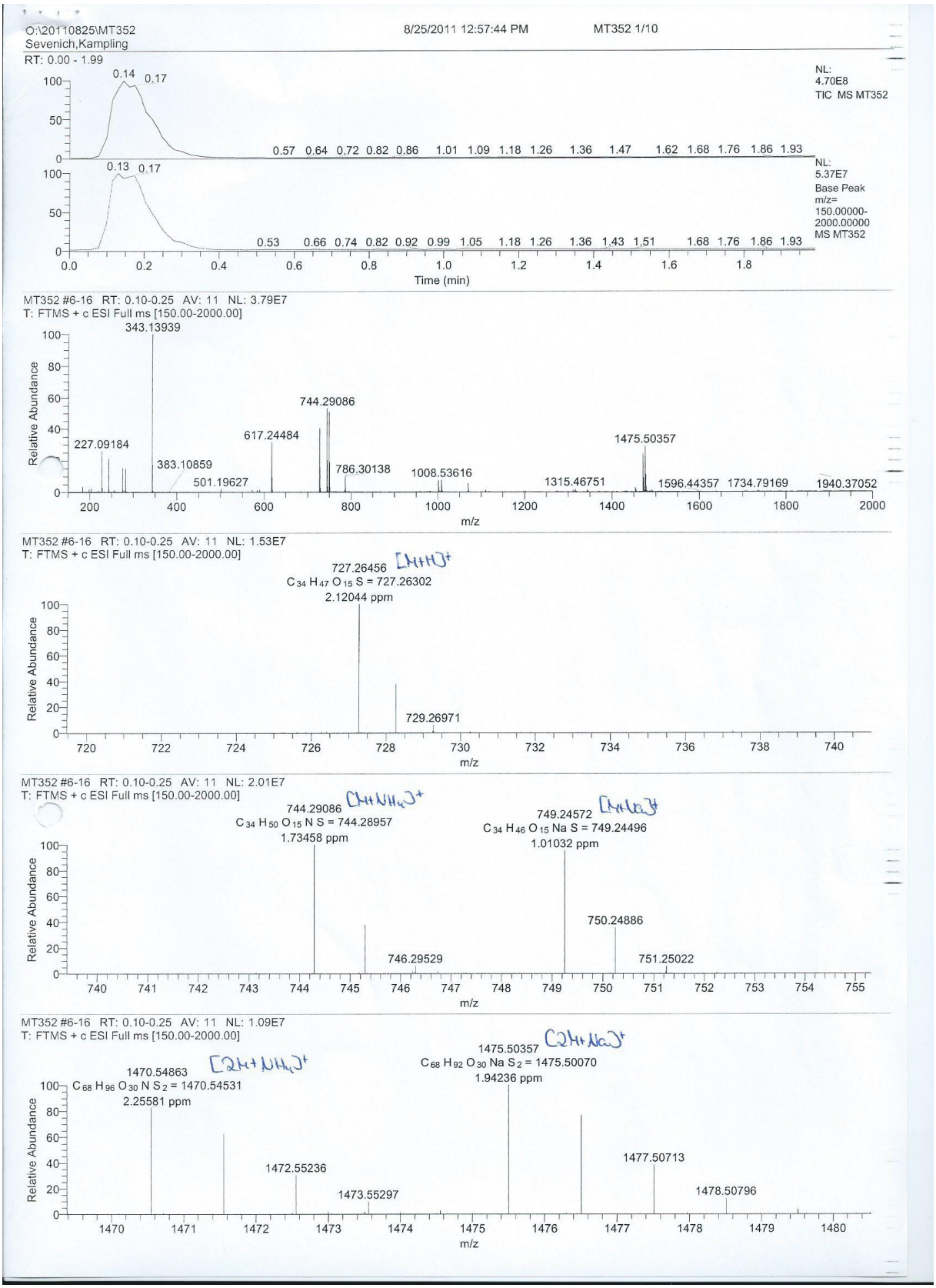
Verbindung **78**– Massenspektrum



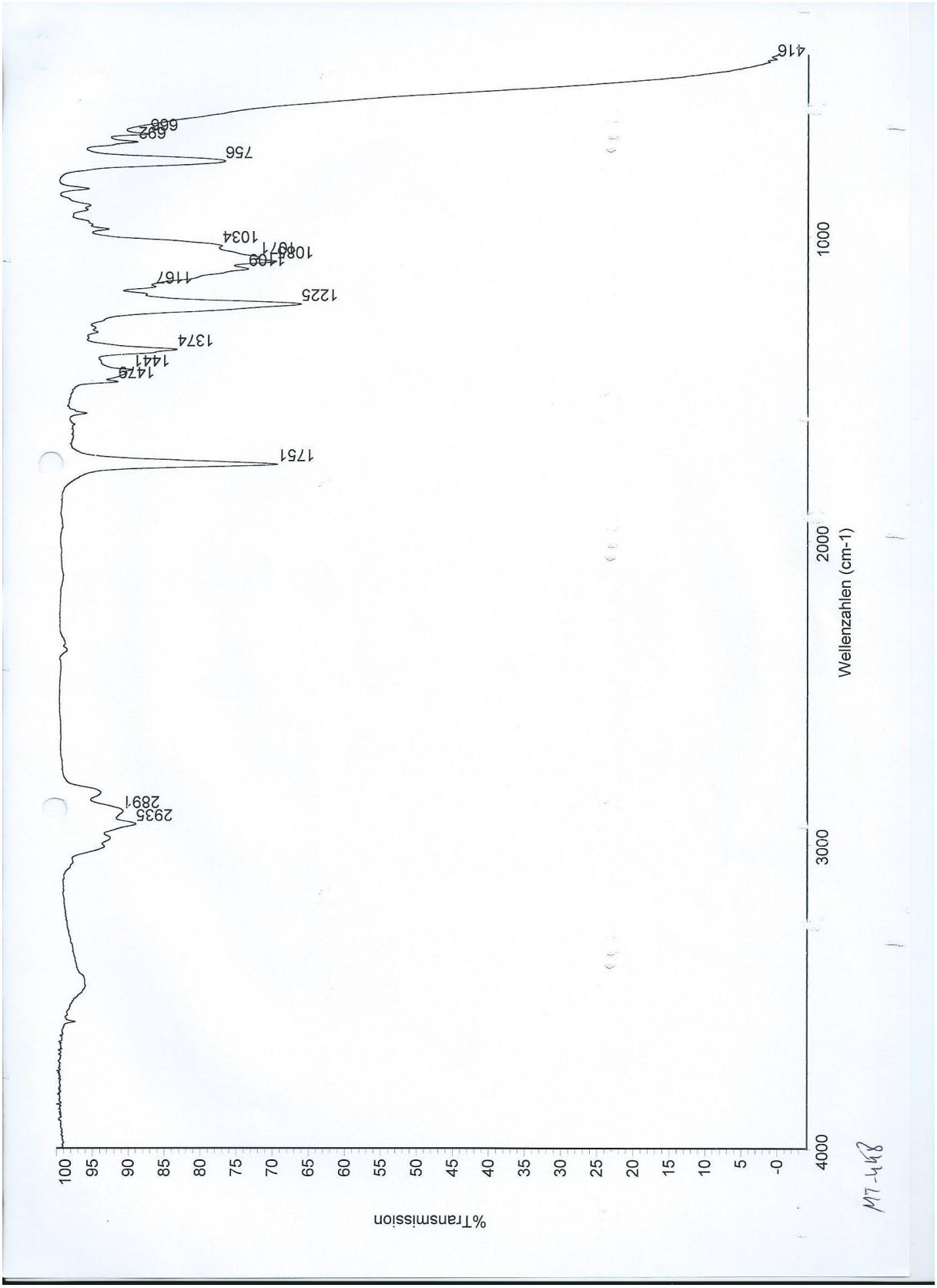
Verbindung **91** – IR



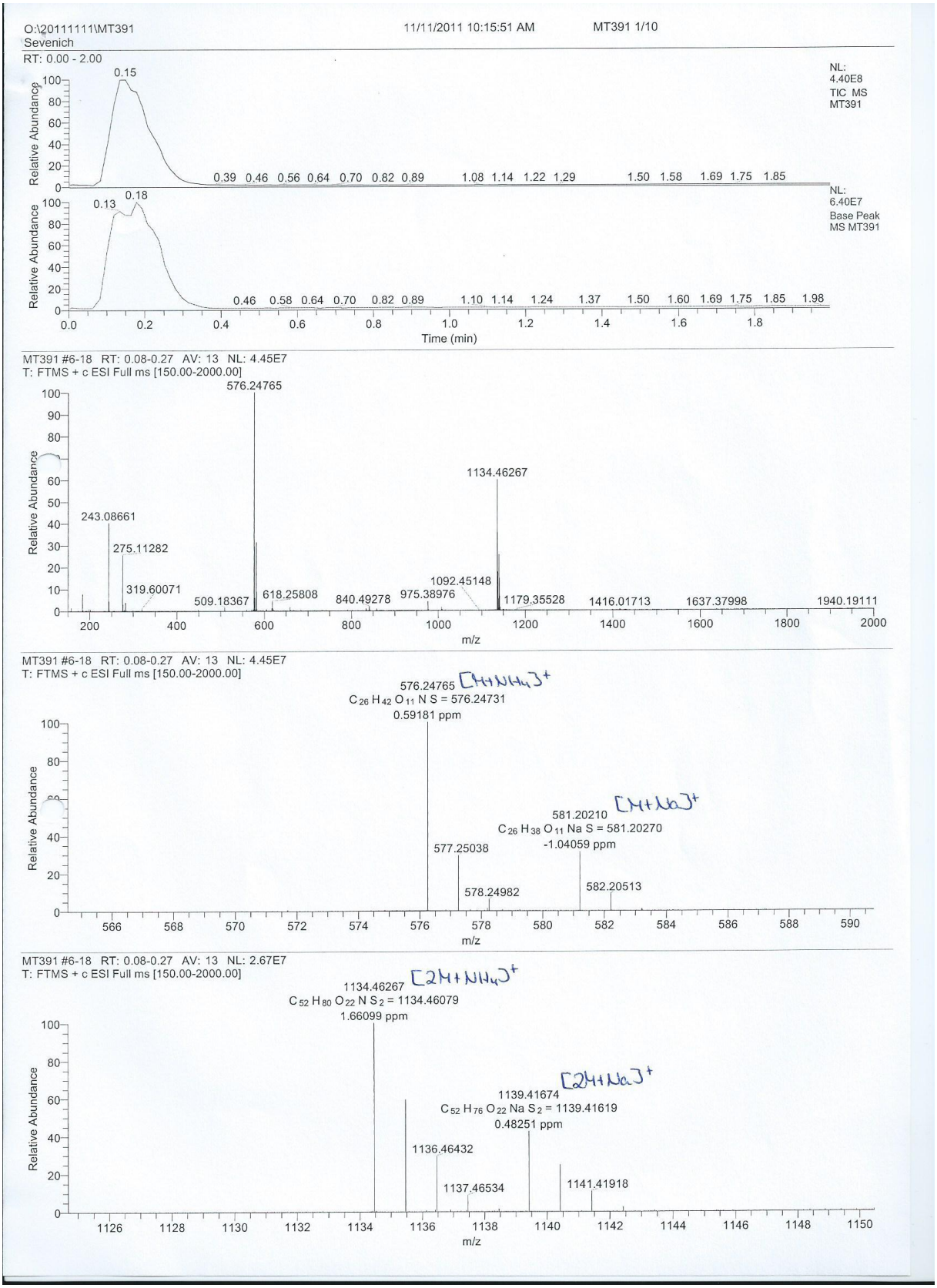
Verbindung **91** – Massenspektrum



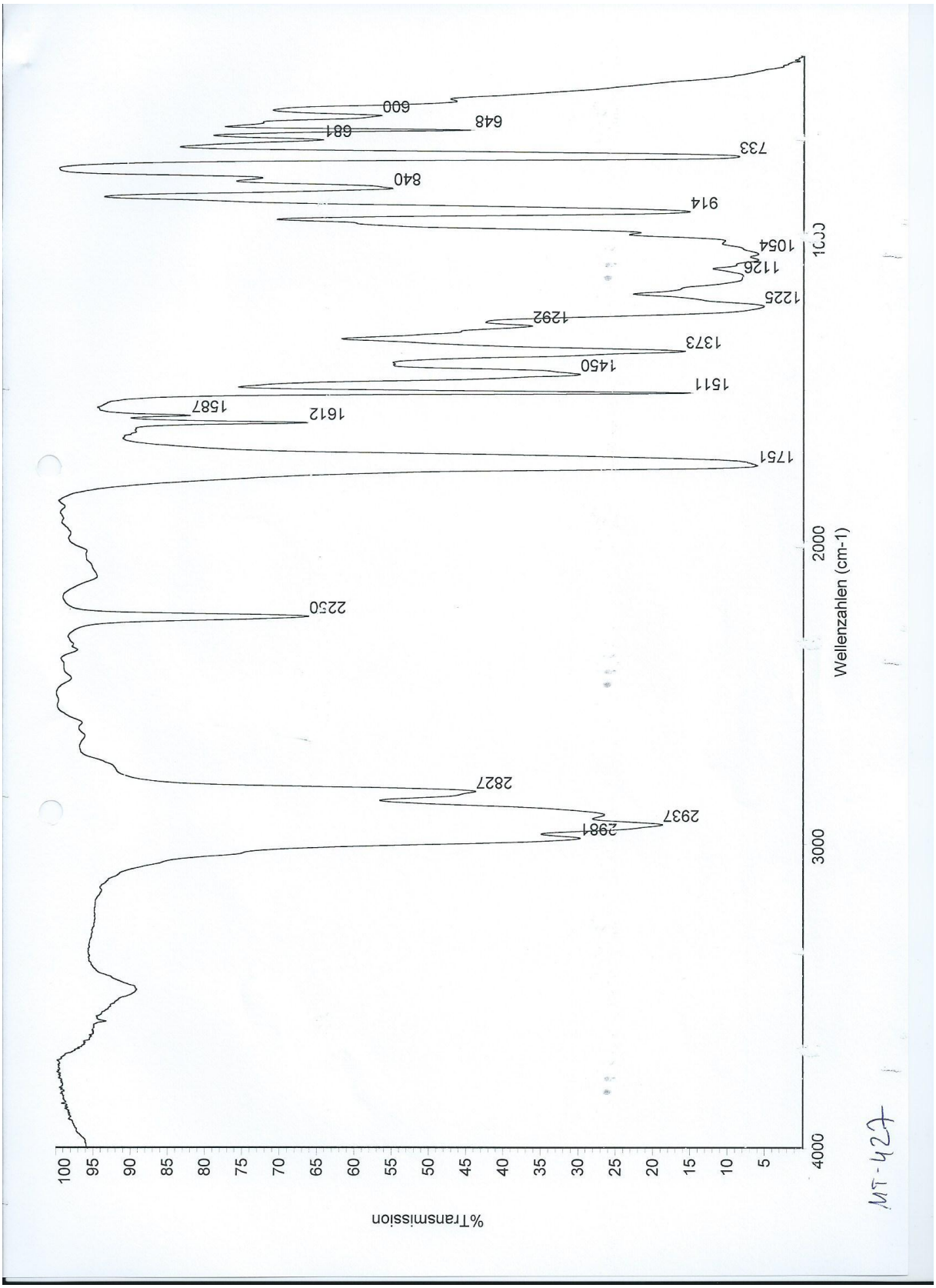
Verbindung **92** – IR



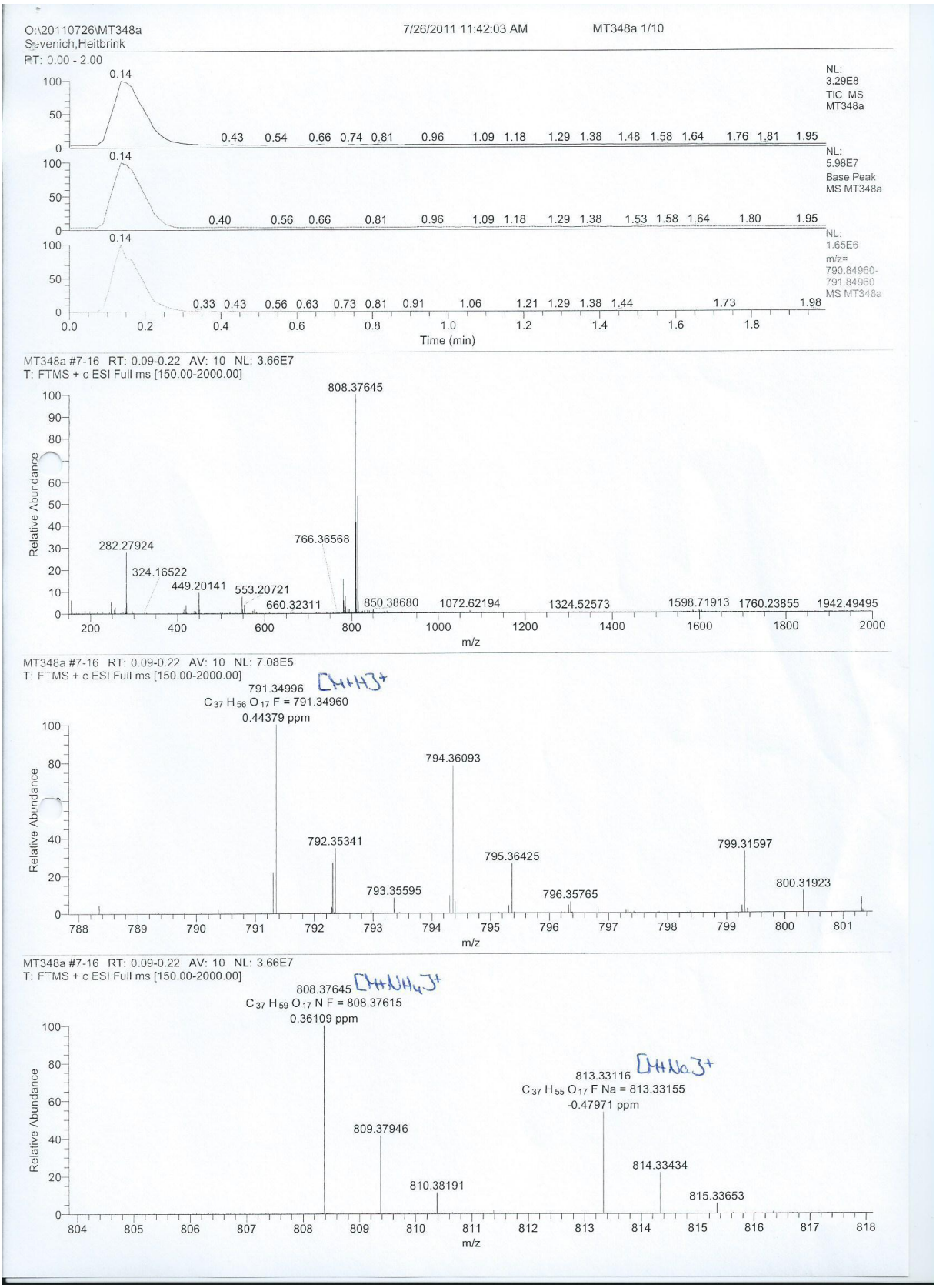
Verbindung **92** – Massenspektrum



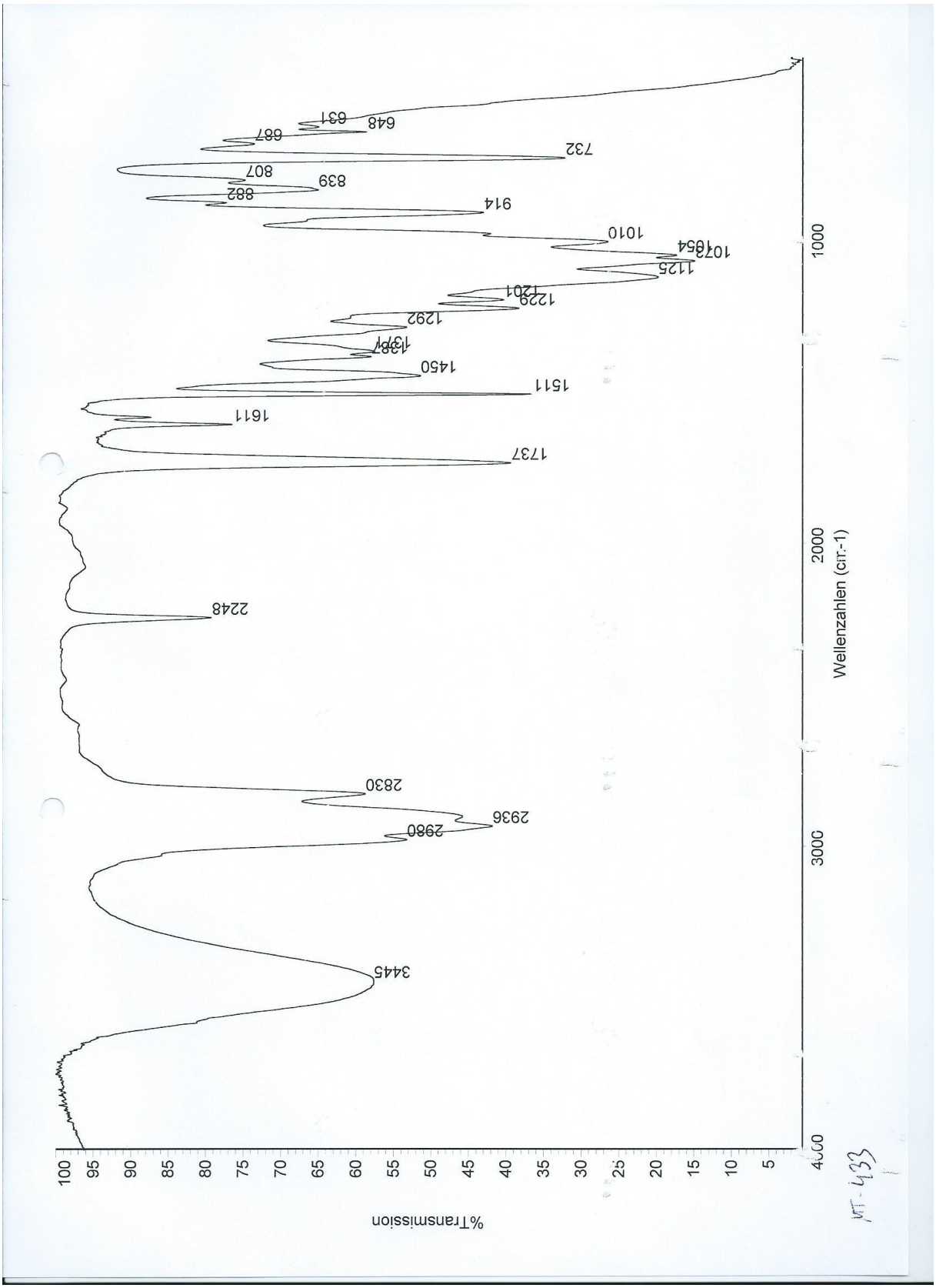
Verbindung **90** – IR



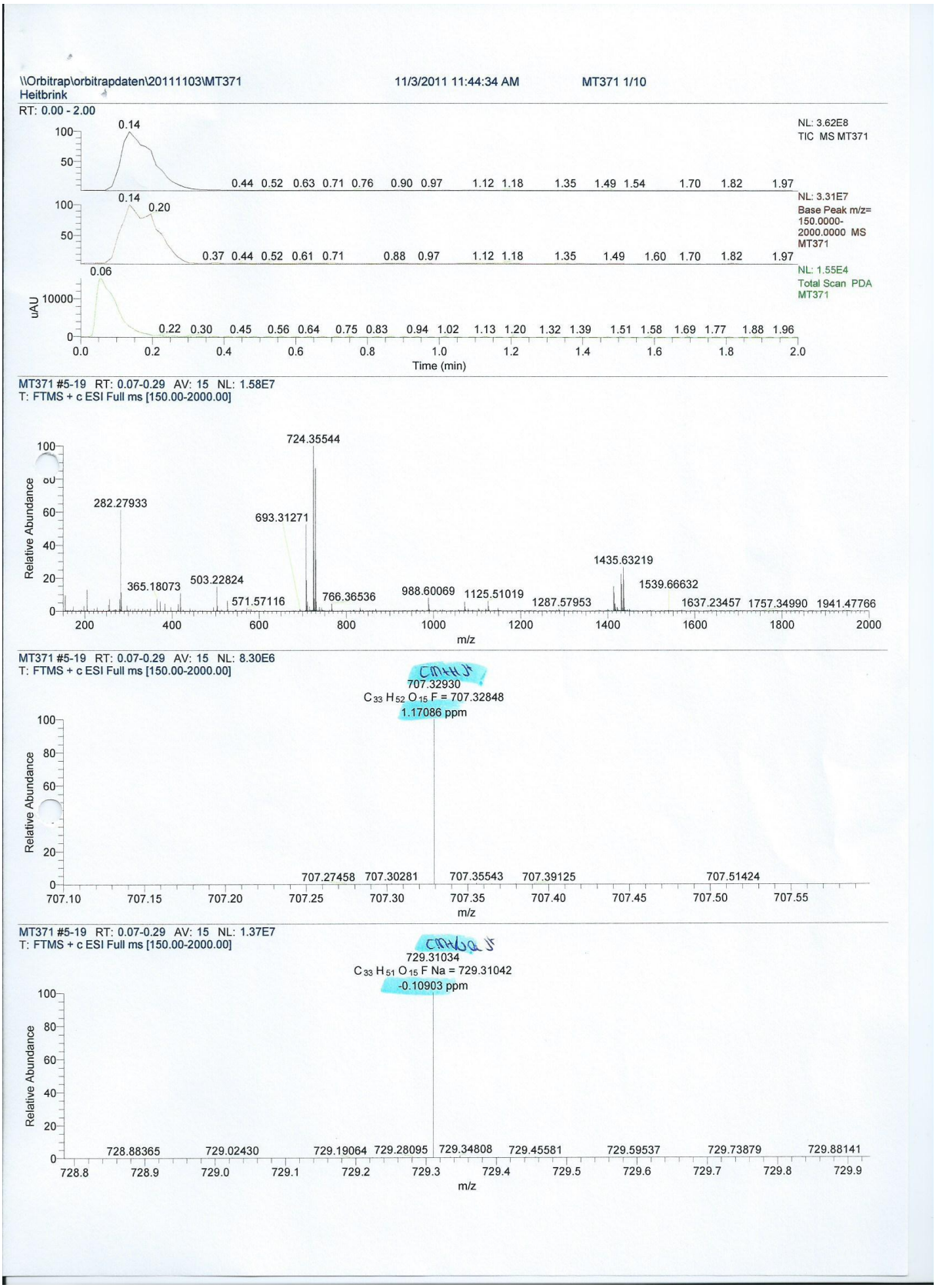
Verbindung **90** – Massenspektrum



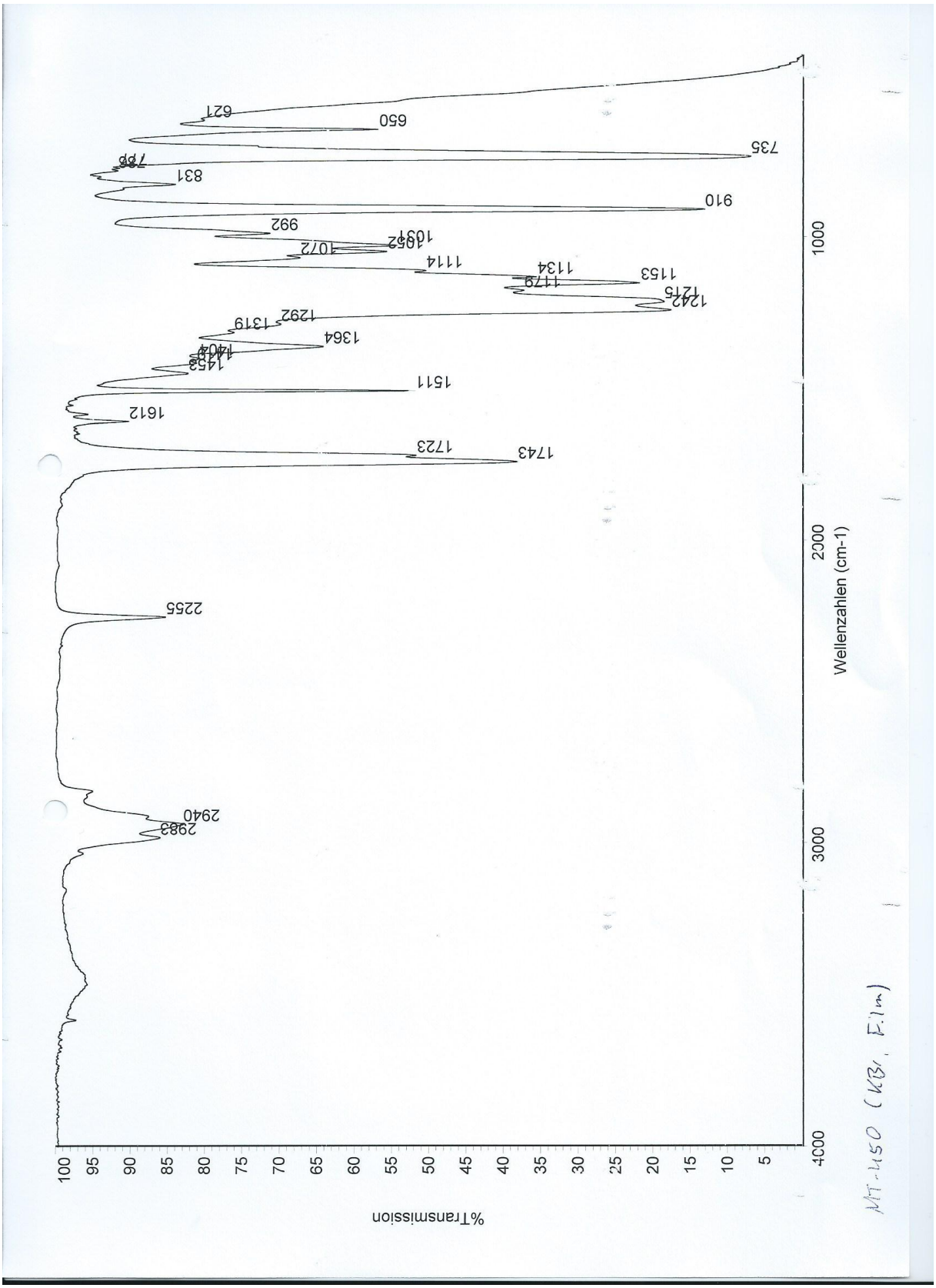
Verbindung **28** – IR



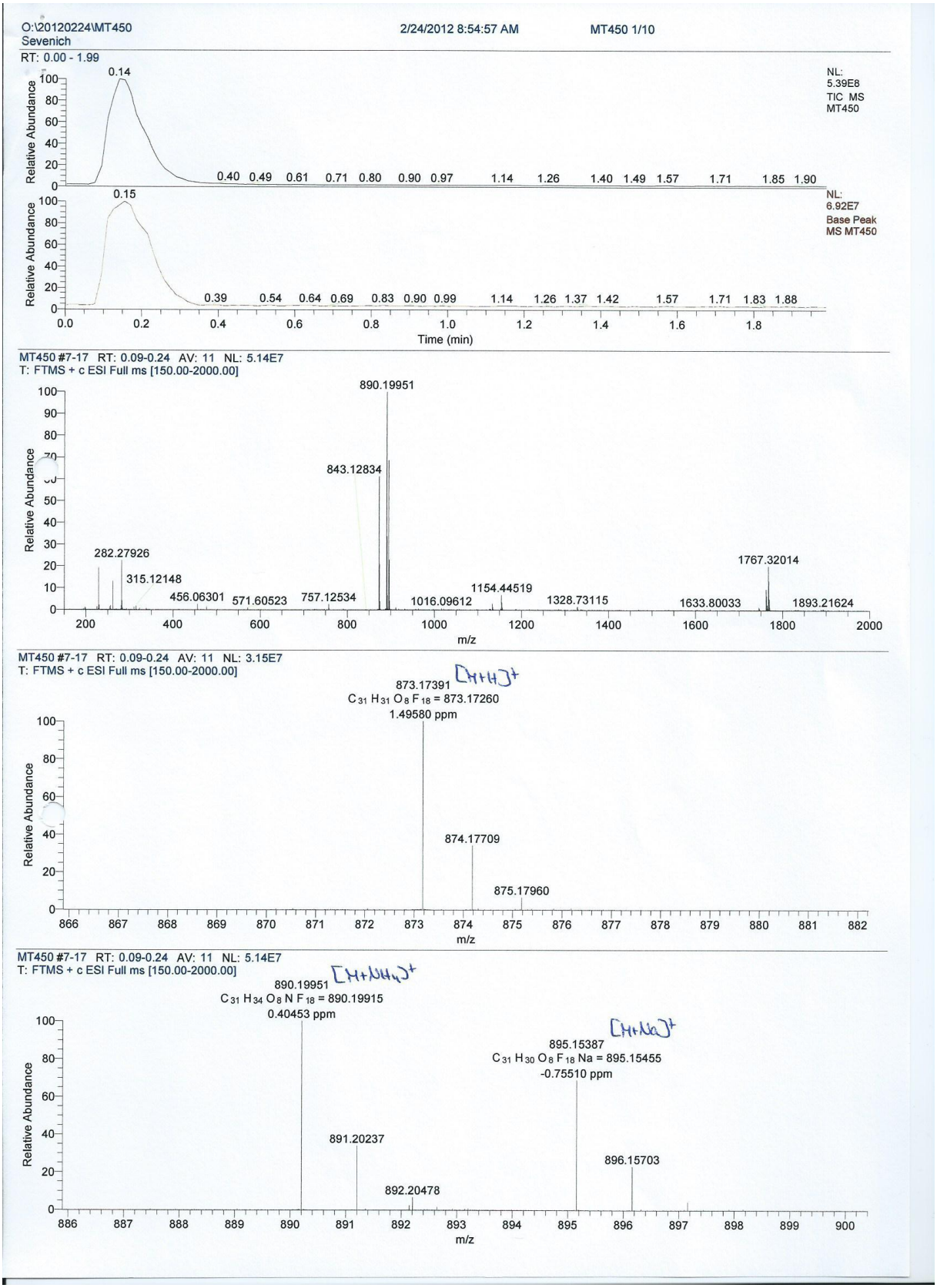
Verbindung **28** – Massenspektrum



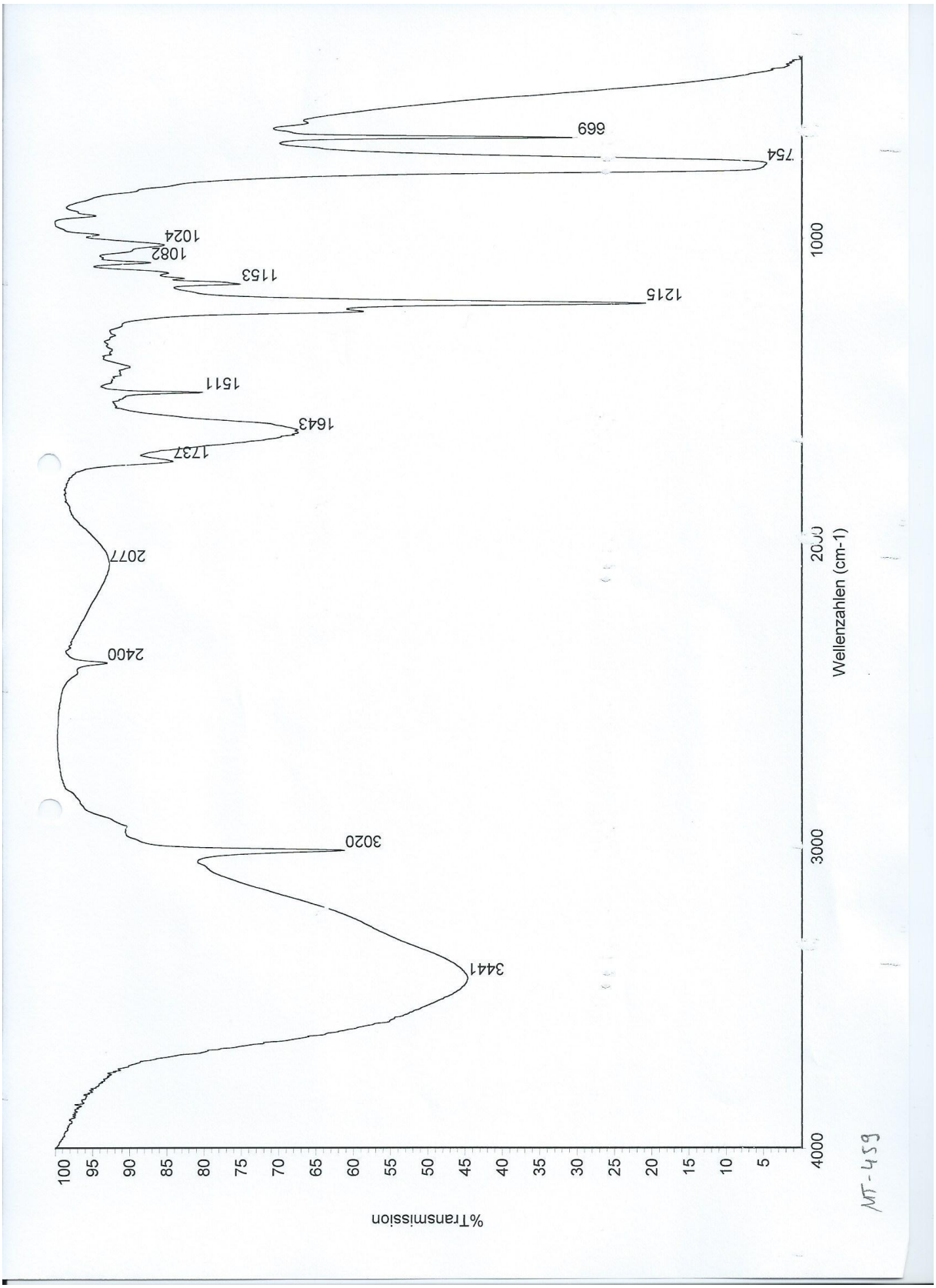
Verbindung **98** – IR



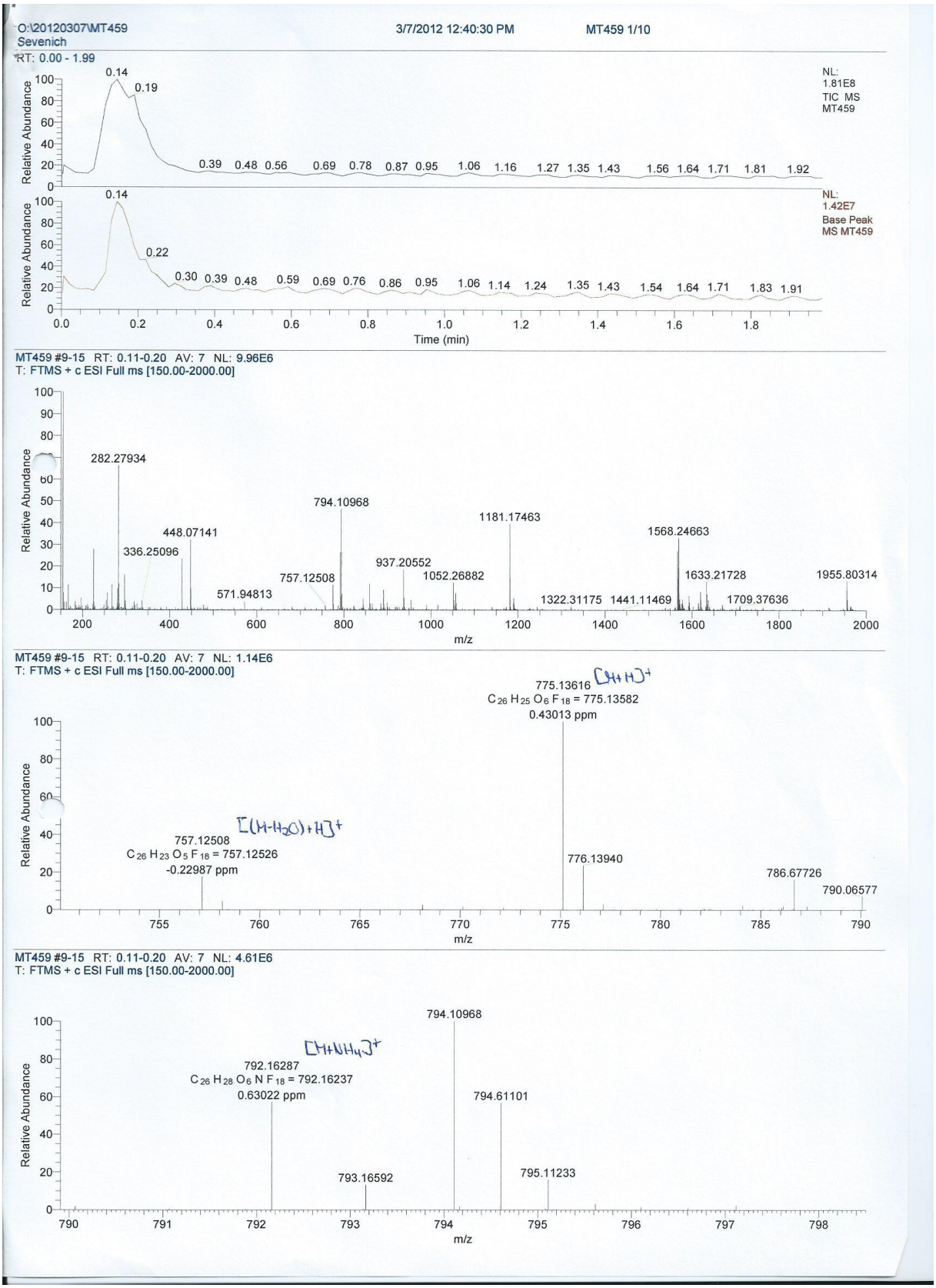
Verbindung **98** – Massenspektrum



Verbindung **99** – IR



Verbindung **99** – Massenspektrum



I Kristalldaten – Teil A (Verbindung 90)

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for a2012.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
F(1)	3838(2)	1142(1)	219(1)	62(1)
C(1)	14275(4)	827(2)	7572(2)	59(1)
O(1)	13859(2)	251(1)	6844(2)	56(1)
C(2)	14469(3)	270(2)	5864(2)	41(1)
O(2)	15345(3)	735(1)	5621(2)	70(1)
C(3)	14128(3)	-346(2)	5138(3)	54(1)
C(4)	12488(3)	-594(2)	5045(3)	56(1)
C(5)	11283(3)	-129(1)	4404(2)	35(1)
C(6)	9714(3)	-341(1)	4355(2)	31(1)
C(6')	11646(3)	489(1)	3895(2)	38(1)
C(7)	8554(3)	55(1)	3826(2)	28(1)
C(7')	10496(3)	891(1)	3345(2)	31(1)
C(8)	8952(3)	673(1)	3320(2)	25(1)
O(3)	7855(2)	1099(1)	2754(1)	28(1)
C(9)	6351(3)	1171(1)	3210(2)	26(1)
O(6)	5343(2)	607(1)	2919(1)	32(1)
C(10)	5692(3)	1869(1)	2804(2)	24(1)
O(4)	4358(2)	2024(1)	3447(1)	24(1)
C(11)	5186(3)	1842(1)	1569(2)	32(1)
O(5)	4447(2)	2489(1)	1303(1)	40(1)
C(12)	4541(4)	2684(2)	170(2)	53(1)
C(13)	4148(3)	1216(2)	1360(2)	39(1)
C(14)	4972(3)	552(1)	1754(2)	40(1)
C(15)	3985(4)	-104(2)	1578(3)	65(1)
C(16)	4287(3)	2733(1)	3768(2)	22(1)
O(10)	5193(2)	2867(1)	4755(1)	24(1)
C(17)	2572(3)	2943(1)	3866(2)	23(1)
O(7)	2505(2)	3681(1)	3952(1)	29(1)
C(18)	2526(3)	4028(1)	2912(2)	46(1)
C(19)	1882(3)	2644(1)	4909(2)	22(1)
O(8)	331(2)	2896(1)	5052(1)	25(1)
C(20)	-850(3)	2559(1)	4377(2)	36(1)
C(21)	2928(3)	2846(1)	5906(2)	21(1)
O(9)	2414(2)	2513(1)	6895(1)	25(1)
C(22)	4583(3)	2576(1)	5747(2)	25(1)
C(23)	5754(3)	2772(2)	6676(2)	37(1)
C(24)	1210(3)	2846(1)	7434(2)	27(1)
O(17)	1869(2)	3400(1)	8104(1)	28(1)
C(25)	471(3)	2301(1)	8163(2)	26(1)
O(11)	-351(2)	1832(1)	7419(1)	33(1)
C(26)	-23(3)	1141(2)	7480(2)	42(1)
O(12)	770(3)	882(1)	8216(2)	62(1)
C(27)	-720(4)	777(2)	6504(2)	66(1)
C(28)	-706(3)	2621(1)	8932(2)	28(1)
O(13)	-1331(2)	2134(1)	9679(1)	35(1)
C(29)	-206(3)	1793(1)	10420(2)	41(1)
C(30)	-34(3)	3279(1)	9482(2)	28(1)
O(14)	-1322(2)	3651(1)	9964(1)	36(1)
C(31)	-1484(4)	3588(2)	11066(2)	44(1)

O(15)	-644(3)	3234(1)	11657(2)	58(1)
C(32)	-2814(4)	4031(2)	11423(2)	65(1)
C(33)	630(3)	3765(1)	8624(2)	31(1)
C(34)	1221(3)	4451(1)	9085(2)	38(1)
O(16)	2326(2)	4337(1)	9977(1)	44(1)
C(35)	2572(4)	4954(2)	10616(2)	56(1)

Table 3. Bond lengths [A] and angles [deg] for a2012.

F(1)-C(13)	1.401(3)
C(1)-O(1)	1.443(3)
C(1)-H(1A)	0.9800
C(1)-H(1B)	0.9800
C(1)-H(1C)	0.9800
O(1)-C(2)	1.315(3)
C(2)-O(2)	1.202(3)
C(2)-C(3)	1.489(4)
C(3)-C(4)	1.467(4)
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
C(4)-C(5)	1.537(4)
C(4)-H(4A)	0.9900
C(4)-H(4B)	0.9900
C(5)-C(6')	1.371(3)
C(5)-C(6)	1.388(3)
C(6)-C(7)	1.373(3)
C(6)-H(6A)	0.9500
C(6')-C(7')	1.387(3)
C(6')-H(6'A)	0.9500
C(7)-C(8)	1.379(3)
C(7)-H(7A)	0.9500
C(7')-C(8)	1.372(3)
C(7')-H(7'A)	0.9500
C(8)-O(3)	1.391(3)
O(3)-C(9)	1.417(3)
C(9)-O(6)	1.409(3)
C(9)-C(10)	1.518(3)
C(9)-H(9A)	1.0000
O(6)-C(14)	1.434(3)
C(10)-O(4)	1.432(2)
C(10)-C(11)	1.536(3)
C(10)-H(10A)	1.0000
O(4)-C(16)	1.410(3)
C(11)-O(5)	1.416(3)
C(11)-C(13)	1.499(4)
C(11)-H(11A)	1.0000
O(5)-C(12)	1.426(3)
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(13)-C(14)	1.513(4)
C(13)-H(13A)	1.0000
C(14)-C(15)	1.515(4)
C(14)-H(14A)	1.0000
C(15)-H(15A)	0.9800
C(15)-H(15B)	0.9800
C(15)-H(15C)	0.9800

C(16)-O(10)	1.414(2)
C(16)-C(17)	1.516(3)
C(16)-H(16A)	1.0000
O(10)-C(22)	1.440(3)
C(17)-O(7)	1.415(3)
C(17)-C(19)	1.526(3)
C(17)-H(17A)	1.0000
O(7)-C(18)	1.423(3)
C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
C(19)-O(8)	1.417(3)
C(19)-C(21)	1.513(3)
C(19)-H(19A)	1.0000
O(8)-C(20)	1.416(3)
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800
C(21)-O(9)	1.440(2)
C(21)-C(22)	1.514(3)
C(21)-H(21A)	1.0000
O(9)-C(24)	1.389(3)
C(22)-C(23)	1.512(3)
C(22)-H(22A)	1.0000
C(23)-H(23A)	0.9800
C(23)-H(23B)	0.9800
C(23)-H(23C)	0.9800
C(24)-O(17)	1.431(3)
C(24)-C(25)	1.518(3)
C(24)-H(24A)	1.0000
O(17)-C(33)	1.429(3)
C(25)-O(11)	1.428(3)
C(25)-C(28)	1.521(3)
C(25)-H(25A)	1.0000
O(11)-C(26)	1.350(3)
C(26)-O(12)	1.198(3)
C(26)-C(27)	1.471(4)
C(27)-H(27A)	0.9800
C(27)-H(27B)	0.9800
C(27)-H(27C)	0.9800
C(28)-O(13)	1.416(3)
C(28)-C(30)	1.521(3)
C(28)-H(28A)	1.0000
O(13)-C(29)	1.435(3)
C(29)-H(29A)	0.9800
C(29)-H(29B)	0.9800
C(29)-H(29C)	0.9800
C(30)-O(14)	1.447(3)
C(30)-C(33)	1.520(3)
C(30)-H(30A)	1.0000
O(14)-C(31)	1.352(3)
C(31)-O(15)	1.195(3)
C(31)-C(32)	1.487(4)
C(32)-H(32A)	0.9800
C(32)-H(32B)	0.9800
C(32)-H(32C)	0.9800
C(33)-C(34)	1.501(3)
C(33)-H(33A)	1.0000
C(34)-O(16)	1.413(3)
C(34)-H(34A)	0.9900
C(34)-H(34B)	0.9900
O(16)-C(35)	1.421(3)
C(35)-H(35A)	0.9800

C(35)-H(35B)	0.9800
C(35)-H(35C)	0.9800
O(1)-C(1)-H(1A)	109.5
O(1)-C(1)-H(1B)	109.5
H(1A)-C(1)-H(1B)	109.5
O(1)-C(1)-H(1C)	109.5
H(1A)-C(1)-H(1C)	109.5
H(1B)-C(1)-H(1C)	109.5
C(2)-O(1)-C(1)	115.7(2)
O(2)-C(2)-O(1)	120.9(3)
O(2)-C(2)-C(3)	123.0(3)
O(1)-C(2)-C(3)	115.9(3)
C(4)-C(3)-C(2)	117.3(3)
C(4)-C(3)-H(3A)	108.0
C(2)-C(3)-H(3A)	108.0
C(4)-C(3)-H(3B)	108.0
C(2)-C(3)-H(3B)	108.0
H(3A)-C(3)-H(3B)	107.2
C(3)-C(4)-C(5)	117.1(2)
C(3)-C(4)-H(4A)	108.0
C(5)-C(4)-H(4A)	108.0
C(3)-C(4)-H(4B)	108.0
C(5)-C(4)-H(4B)	108.0
H(4A)-C(4)-H(4B)	107.3
C(6')-C(5)-C(6)	117.7(2)
C(6')-C(5)-C(4)	124.6(2)
C(6)-C(5)-C(4)	117.7(2)
C(7)-C(6)-C(5)	121.5(2)
C(7)-C(6)-H(6A)	119.2
C(5)-C(6)-H(6A)	119.2
C(5)-C(6')-C(7')	121.7(2)
C(5)-C(6')-H(6'A)	119.2
C(7')-C(6')-H(6'A)	119.2
C(6)-C(7)-C(8)	119.6(2)
C(6)-C(7)-H(7A)	120.2
C(8)-C(7)-H(7A)	120.2
C(8)-C(7')-C(6')	119.3(2)
C(8)-C(7')-H(7'A)	120.3
C(6')-C(7')-H(7'A)	120.3
C(7')-C(8)-C(7)	120.2(2)
C(7')-C(8)-O(3)	116.6(2)
C(7)-C(8)-O(3)	123.2(2)
C(8)-O(3)-C(9)	117.25(17)
O(6)-C(9)-O(3)	111.91(18)
O(6)-C(9)-C(10)	112.40(17)
O(3)-C(9)-C(10)	106.45(18)
O(6)-C(9)-H(9A)	108.7
O(3)-C(9)-H(9A)	108.7
C(10)-C(9)-H(9A)	108.7
C(9)-O(6)-C(14)	113.85(18)
O(4)-C(10)-C(9)	107.04(17)
O(4)-C(10)-C(11)	110.07(17)
C(9)-C(10)-C(11)	111.57(18)
O(4)-C(10)-H(10A)	109.4
C(9)-C(10)-H(10A)	109.4
C(11)-C(10)-H(10A)	109.4
C(16)-O(4)-C(10)	113.15(17)
O(5)-C(11)-C(13)	114.14(19)
O(5)-C(11)-C(10)	107.03(18)
C(13)-C(11)-C(10)	109.0(2)
O(5)-C(11)-H(11A)	108.8
C(13)-C(11)-H(11A)	108.8

C(10)-C(11)-H(11A)	108.8
C(11)-O(5)-C(12)	113.8(2)
O(5)-C(12)-H(12A)	109.5
O(5)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
O(5)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
F(1)-C(13)-C(11)	109.1(2)
F(1)-C(13)-C(14)	106.84(19)
C(11)-C(13)-C(14)	110.9(2)
F(1)-C(13)-H(13A)	110.0
C(11)-C(13)-H(13A)	110.0
C(14)-C(13)-H(13A)	110.0
O(6)-C(14)-C(13)	108.98(19)
O(6)-C(14)-C(15)	107.0(2)
C(13)-C(14)-C(15)	113.9(2)
O(6)-C(14)-H(14A)	109.0
C(13)-C(14)-H(14A)	109.0
C(15)-C(14)-H(14A)	109.0
C(14)-C(15)-H(15A)	109.5
C(14)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(14)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
O(4)-C(16)-O(10)	112.29(17)
O(4)-C(16)-C(17)	109.20(18)
O(10)-C(16)-C(17)	111.78(17)
O(4)-C(16)-H(16A)	107.8
O(10)-C(16)-H(16A)	107.8
C(17)-C(16)-H(16A)	107.8
C(16)-O(10)-C(22)	115.61(16)
O(7)-C(17)-C(16)	108.15(18)
O(7)-C(17)-C(19)	107.00(18)
C(16)-C(17)-C(19)	111.70(18)
O(7)-C(17)-H(17A)	110.0
C(16)-C(17)-H(17A)	110.0
C(19)-C(17)-H(17A)	110.0
C(17)-O(7)-C(18)	113.34(18)
O(7)-C(18)-H(18A)	109.5
O(7)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
O(7)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
O(8)-C(19)-C(21)	109.18(17)
O(8)-C(19)-C(17)	111.47(17)
C(21)-C(19)-C(17)	109.40(18)
O(8)-C(19)-H(19A)	108.9
C(21)-C(19)-H(19A)	108.9
C(17)-C(19)-H(19A)	108.9
C(20)-O(8)-C(19)	114.18(17)
O(8)-C(20)-H(20A)	109.5
O(8)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
O(8)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
O(9)-C(21)-C(19)	111.21(17)
O(9)-C(21)-C(22)	105.72(16)
C(19)-C(21)-C(22)	108.86(17)
O(9)-C(21)-H(21A)	110.3

C(19)-C(21)-H(21A)	110.3
C(22)-C(21)-H(21A)	110.3
C(24)-O(9)-C(21)	116.32(16)
O(10)-C(22)-C(23)	106.01(18)
O(10)-C(22)-C(21)	110.07(17)
C(23)-C(22)-C(21)	113.62(19)
O(10)-C(22)-H(22A)	109.0
C(23)-C(22)-H(22A)	109.0
C(21)-C(22)-H(22A)	109.0
C(22)-C(23)-H(23A)	109.5
C(22)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
C(22)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
O(9)-C(24)-O(17)	109.22(18)
O(9)-C(24)-C(25)	106.83(18)
O(17)-C(24)-C(25)	109.72(17)
O(9)-C(24)-H(24A)	110.3
O(17)-C(24)-H(24A)	110.3
C(25)-C(24)-H(24A)	110.3
C(33)-O(17)-C(24)	109.55(17)
O(11)-C(25)-C(24)	105.35(17)
O(11)-C(25)-C(28)	108.84(19)
C(24)-C(25)-C(28)	112.27(19)
O(11)-C(25)-H(25A)	110.1
C(24)-C(25)-H(25A)	110.1
C(28)-C(25)-H(25A)	110.1
C(26)-O(11)-C(25)	119.0(2)
O(12)-C(26)-O(11)	123.5(3)
O(12)-C(26)-C(27)	126.3(3)
O(11)-C(26)-C(27)	110.1(3)
C(26)-C(27)-H(27A)	109.5
C(26)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
C(26)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
O(13)-C(28)-C(30)	113.91(17)
O(13)-C(28)-C(25)	113.67(19)
C(30)-C(28)-C(25)	110.91(19)
O(13)-C(28)-H(28A)	105.9
C(30)-C(28)-H(28A)	105.9
C(25)-C(28)-H(28A)	105.9
C(28)-O(13)-C(29)	116.12(18)
O(13)-C(29)-H(29A)	109.5
O(13)-C(29)-H(29B)	109.5
H(29A)-C(29)-H(29B)	109.5
O(13)-C(29)-H(29C)	109.5
H(29A)-C(29)-H(29C)	109.5
H(29B)-C(29)-H(29C)	109.5
O(14)-C(30)-C(33)	106.53(19)
O(14)-C(30)-C(28)	108.00(18)
C(33)-C(30)-C(28)	110.35(18)
O(14)-C(30)-H(30A)	110.6
C(33)-C(30)-H(30A)	110.6
C(28)-C(30)-H(30A)	110.6
C(31)-O(14)-C(30)	117.8(2)
O(15)-C(31)-O(14)	123.8(3)
O(15)-C(31)-C(32)	125.9(3)
O(14)-C(31)-C(32)	110.3(3)
C(31)-C(32)-H(32A)	109.5
C(31)-C(32)-H(32B)	109.5

H(32A)-C(32)-H(32B)	109.5
C(31)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
O(17)-C(33)-C(34)	110.5(2)
O(17)-C(33)-C(30)	107.77(18)
C(34)-C(33)-C(30)	114.0(2)
O(17)-C(33)-H(33A)	108.2
C(34)-C(33)-H(33A)	108.2
C(30)-C(33)-H(33A)	108.2
O(16)-C(34)-C(33)	110.3(2)
O(16)-C(34)-H(34A)	109.6
C(33)-C(34)-H(34A)	109.6
O(16)-C(34)-H(34B)	109.6
C(33)-C(34)-H(34B)	109.6
H(34A)-C(34)-H(34B)	108.1
C(34)-O(16)-C(35)	111.3(2)
O(16)-C(35)-H(35A)	109.5
O(16)-C(35)-H(35B)	109.5
H(35A)-C(35)-H(35B)	109.5
O(16)-C(35)-H(35C)	109.5
H(35A)-C(35)-H(35C)	109.5
H(35B)-C(35)-H(35C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for a2012.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
F(1)	61(1)	93(1)	30(1)	-20(1)	-16(1)	6(1)
C(1)	82(3)	64(2)	30(2)	-2(2)	8(2)	18(2)
O(1)	65(2)	41(1)	65(1)	9(1)	29(1)	0(1)
C(2)	41(2)	33(2)	49(2)	4(2)	-8(2)	6(2)
O(2)	99(2)	59(2)	54(1)	1(1)	23(1)	-11(1)
C(3)	43(2)	44(2)	74(2)	2(2)	-9(2)	11(2)
C(4)	36(2)	34(2)	97(2)	2(2)	-2(2)	8(1)
C(5)	36(2)	21(1)	47(2)	-3(1)	-3(1)	5(1)
C(6)	34(2)	20(1)	39(1)	-2(1)	1(1)	-2(1)
C(6')	17(1)	39(2)	58(2)	-5(1)	3(1)	2(1)
C(7)	20(1)	29(2)	33(1)	-5(1)	3(1)	-4(1)
C(7')	26(2)	27(1)	40(1)	2(1)	8(1)	2(1)
C(8)	22(1)	29(1)	24(1)	-4(1)	5(1)	4(1)
O(3)	20(1)	36(1)	27(1)	3(1)	5(1)	5(1)
C(9)	18(1)	34(1)	26(1)	-6(1)	2(1)	-1(1)
O(6)	24(1)	34(1)	37(1)	-8(1)	0(1)	-2(1)
C(10)	18(1)	34(1)	21(1)	-2(1)	5(1)	1(1)
O(4)	21(1)	27(1)	26(1)	-6(1)	9(1)	-1(1)
C(11)	23(1)	50(2)	24(1)	-1(1)	3(1)	14(1)
O(5)	39(1)	57(1)	25(1)	9(1)	3(1)	19(1)
C(12)	50(2)	77(2)	30(2)	17(2)	-3(1)	13(2)
C(13)	28(2)	64(2)	23(1)	-15(1)	-4(1)	5(2)
C(14)	35(2)	52(2)	33(2)	-20(1)	-1(1)	-1(1)

C(15)	64(2)	60(2)	71(2)	-34(2)	-1(2)	-15(2)
C(16)	24(1)	27(2)	16(1)	-2(1)	4(1)	1(1)
O(10)	17(1)	34(1)	22(1)	-2(1)	2(1)	-4(1)
C(17)	19(1)	29(1)	21(1)	-2(1)	0(1)	2(1)
O(7)	34(1)	27(1)	27(1)	5(1)	9(1)	6(1)
C(18)	55(2)	40(2)	42(2)	11(1)	4(1)	6(1)
C(19)	16(1)	26(1)	24(1)	-2(1)	4(1)	2(1)
O(8)	16(1)	35(1)	24(1)	-6(1)	1(1)	1(1)
C(20)	20(1)	52(2)	35(1)	-7(1)	-3(1)	0(1)
C(21)	21(1)	21(1)	20(1)	-2(1)	4(1)	-1(1)
O(9)	23(1)	31(1)	21(1)	3(1)	8(1)	4(1)
C(22)	22(1)	32(1)	23(1)	-1(1)	4(1)	-2(1)
C(23)	24(1)	63(2)	25(1)	-3(1)	-2(1)	-3(1)
C(24)	28(1)	32(1)	21(1)	0(1)	2(1)	0(1)
O(17)	29(1)	32(1)	24(1)	-2(1)	7(1)	0(1)
C(25)	25(1)	31(1)	20(1)	-2(1)	2(1)	-3(1)
O(11)	31(1)	39(1)	30(1)	-9(1)	6(1)	-9(1)
C(26)	46(2)	41(2)	42(2)	-8(2)	18(1)	-10(2)
O(12)	78(2)	38(1)	69(1)	-1(1)	6(1)	2(1)
C(27)	90(3)	55(2)	55(2)	-21(2)	22(2)	-30(2)
C(28)	22(1)	40(2)	22(1)	2(1)	3(1)	3(1)
O(13)	30(1)	45(1)	29(1)	6(1)	11(1)	-1(1)
C(29)	49(2)	43(2)	32(1)	11(1)	9(1)	3(1)
C(30)	23(1)	38(2)	23(1)	-4(1)	5(1)	5(1)
O(14)	37(1)	43(1)	28(1)	-6(1)	12(1)	9(1)
C(31)	52(2)	51(2)	30(2)	-14(1)	17(1)	-7(2)
O(15)	70(2)	80(2)	25(1)	0(1)	4(1)	13(1)
C(32)	81(3)	64(2)	52(2)	-12(2)	40(2)	13(2)
C(33)	31(2)	35(2)	27(1)	0(1)	4(1)	7(1)
C(34)	50(2)	37(2)	28(1)	-1(1)	4(1)	0(1)
O(16)	55(1)	37(1)	41(1)	-11(1)	-1(1)	-5(1)
C(35)	93(3)	45(2)	30(2)	-4(1)	7(2)	-21(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for a2012.

	x	y	z	U(eq)
H(1A)	13929	724	8317	88
H(1B)	13754	1255	7295	88
H(1C)	15423	894	7598	88
H(3A)	14459	-229	4386	64
H(3B)	14800	-739	5412	64
H(4A)	12116	-660	5802	67
H(4B)	12483	-1060	4686	67
H(6A)	9436	-769	4694	37
H(6'A)	12713	644	3920	45
H(7A)	7485	-97	3810	33
H(7'A)	10776	1314	2989	37
H(9A)	6495	1189	4034	31
H(10A)	6513	2240	2928	29
H(11A)	6150	1793	1128	39
H(12A)	4039	3142	50	79
H(12B)	3996	2334	-300	79
H(12C)	5653	2711	-18	79
H(13A)	3134	1274	1743	46

H(14A)	5977	499	1358	48
H(15A)	4593	-512	1843	98
H(15B)	3706	-159	788	98
H(15C)	3018	-64	1989	98
H(16A)	4733	3021	3167	27
H(17A)	1933	2783	3197	28
H(18A)	2596	4535	3031	68
H(18B)	1554	3919	2476	68
H(18C)	3443	3870	2514	68
H(19A)	1849	2122	4851	26
H(20A)	-1890	2746	4543	54
H(20B)	-825	2055	4523	54
H(20C)	-651	2644	3596	54
H(21A)	2942	3367	6000	25
H(22A)	4547	2054	5678	30
H(23A)	6797	2584	6521	56
H(23B)	5406	2577	7373	56
H(23C)	5817	3283	6735	56
H(24A)	403	3035	6883	32
H(25A)	1314	2044	8603	31
H(27A)	-559	271	6589	100
H(27B)	-210	939	5840	100
H(27C)	-1855	877	6434	100
H(28A)	-1622	2779	8444	33
H(29A)	-766	1540	10989	62
H(29B)	495	2144	10773	62
H(29C)	422	1461	10005	62
H(30A)	798	3156	10063	33
H(32A)	-3122	3881	12157	97
H(32B)	-3716	3981	10892	97
H(32C)	-2478	4522	11454	97
H(33A)	-227	3864	8049	37
H(34A)	1727	4720	8498	46
H(34B)	321	4728	9341	46
H(35A)	3406	4871	11189	84
H(35B)	1590	5081	10966	84
H(35C)	2888	5337	10135	84

Table 6. Torsion angles [deg] for a2012.

C(1)-O(1)-C(2)-O(2)	1.7(4)
C(1)-O(1)-C(2)-C(3)	176.2(2)
O(2)-C(2)-C(3)-C(4)	-139.0(3)
O(1)-C(2)-C(3)-C(4)	46.7(4)
C(2)-C(3)-C(4)-C(5)	70.6(4)
C(3)-C(4)-C(5)-C(6')	1.7(4)
C(3)-C(4)-C(5)-C(6)	-177.0(3)
C(6')-C(5)-C(6)-C(7)	-0.7(4)
C(4)-C(5)-C(6)-C(7)	178.1(2)
C(6)-C(5)-C(6')-C(7')	-0.2(4)
C(4)-C(5)-C(6')-C(7')	-178.9(3)
C(5)-C(6)-C(7)-C(8)	0.8(4)
C(5)-C(6')-C(7')-C(8)	0.9(4)
C(6')-C(7')-C(8)-C(7)	-0.7(3)
C(6')-C(7')-C(8)-O(3)	-180.0(2)
C(6)-C(7)-C(8)-C(7')	-0.1(3)
C(6)-C(7)-C(8)-O(3)	179.1(2)
C(7')-C(8)-O(3)-C(9)	-142.3(2)

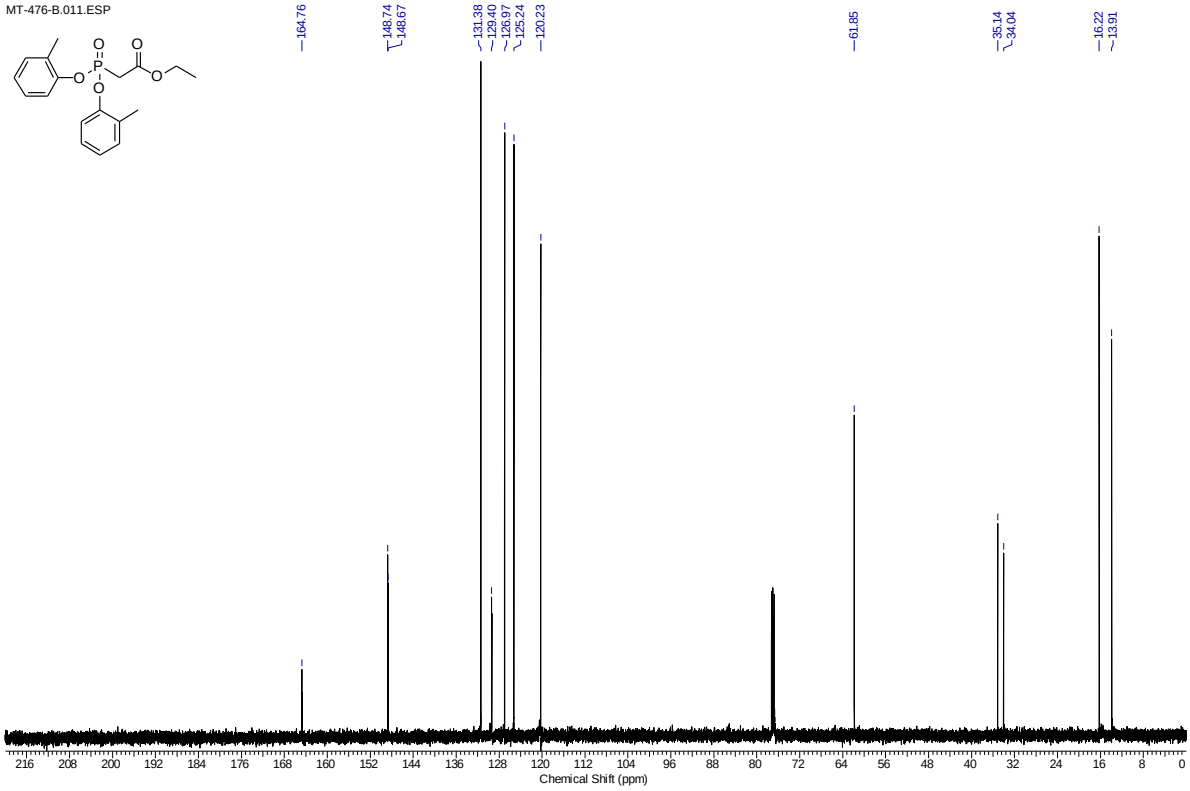
C(7)-C(8)-O(3)-C(9)	38.5(3)
C(8)-O(3)-C(9)-O(6)	-82.2(2)
C(8)-O(3)-C(9)-C(10)	154.62(17)
O(3)-C(9)-O(6)-C(14)	-63.4(2)
C(10)-C(9)-O(6)-C(14)	56.3(2)
O(6)-C(9)-C(10)-O(4)	70.0(2)
O(3)-C(9)-C(10)-O(4)	-167.11(16)
O(6)-C(9)-C(10)-C(11)	-50.4(3)
O(3)-C(9)-C(10)-C(11)	72.4(2)
C(9)-C(10)-O(4)-C(16)	138.45(17)
C(11)-C(10)-O(4)-C(16)	-100.1(2)
O(4)-C(10)-C(11)-O(5)	55.5(2)
C(9)-C(10)-C(11)-O(5)	174.16(18)
O(4)-C(10)-C(11)-C(13)	-68.4(2)
C(9)-C(10)-C(11)-C(13)	50.2(3)
C(13)-C(11)-O(5)-C(12)	-85.9(3)
C(10)-C(11)-O(5)-C(12)	153.4(2)
O(5)-C(11)-C(13)-F(1)	67.3(3)
C(10)-C(11)-C(13)-F(1)	-173.06(18)
O(5)-C(11)-C(13)-C(14)	-175.2(2)
C(10)-C(11)-C(13)-C(14)	-55.6(3)
C(9)-O(6)-C(14)-C(13)	-60.4(3)
C(9)-O(6)-C(14)-C(15)	176.1(2)
F(1)-C(13)-C(14)-O(6)	178.9(2)
C(11)-C(13)-C(14)-O(6)	60.1(3)
F(1)-C(13)-C(14)-C(15)	-61.7(3)
C(11)-C(13)-C(14)-C(15)	179.5(2)
C(10)-O(4)-C(16)-O(10)	-85.7(2)
C(10)-O(4)-C(16)-C(17)	149.75(17)
O(4)-C(16)-O(10)-C(22)	-70.1(2)
C(17)-C(16)-O(10)-C(22)	53.0(2)
O(4)-C(16)-C(17)-O(7)	-167.63(16)
O(10)-C(16)-C(17)-O(7)	67.5(2)
O(4)-C(16)-C(17)-C(19)	74.9(2)
O(10)-C(16)-C(17)-C(19)	-50.0(2)
C(16)-C(17)-O(7)-C(18)	82.1(2)
C(19)-C(17)-O(7)-C(18)	-157.41(19)
O(7)-C(17)-C(19)-O(8)	56.2(2)
C(16)-C(17)-C(19)-O(8)	174.40(17)
O(7)-C(17)-C(19)-C(21)	-64.6(2)
C(16)-C(17)-C(19)-C(21)	53.5(2)
C(21)-C(19)-O(8)-C(20)	-160.63(18)
C(17)-C(19)-O(8)-C(20)	78.4(2)
O(8)-C(19)-C(21)-O(9)	64.0(2)
C(17)-C(19)-C(21)-O(9)	-173.81(17)
O(8)-C(19)-C(21)-C(22)	-179.96(17)
C(17)-C(19)-C(21)-C(22)	-57.7(2)
C(19)-C(21)-O(9)-C(24)	-84.2(2)
C(22)-C(21)-O(9)-C(24)	157.83(18)
C(16)-O(10)-C(22)-C(23)	178.75(19)
C(16)-O(10)-C(22)-C(21)	-58.0(2)
O(9)-C(21)-C(22)-O(10)	178.56(16)
C(19)-C(21)-C(22)-O(10)	59.0(2)
O(9)-C(21)-C(22)-C(23)	-62.7(2)
C(19)-C(21)-C(22)-C(23)	177.71(19)
C(21)-O(9)-C(24)-O(17)	-81.4(2)
C(21)-O(9)-C(24)-C(25)	159.96(17)
O(9)-C(24)-O(17)-C(33)	177.50(17)
C(25)-C(24)-O(17)-C(33)	-65.7(2)
O(9)-C(24)-C(25)-O(11)	-70.2(2)
O(17)-C(24)-C(25)-O(11)	171.53(17)
O(9)-C(24)-C(25)-C(28)	171.50(18)

O(17)-C(24)-C(25)-C(28)	53.2(2)
C(24)-C(25)-O(11)-C(26)	125.1(2)
C(28)-C(25)-O(11)-C(26)	-114.3(2)
C(25)-O(11)-C(26)-O(12)	10.0(4)
C(25)-O(11)-C(26)-C(27)	-167.6(2)
O(11)-C(25)-C(28)-O(13)	68.1(2)
C(24)-C(25)-C(28)-O(13)	-175.66(17)
O(11)-C(25)-C(28)-C(30)	-162.00(18)
C(24)-C(25)-C(28)-C(30)	-45.8(2)
C(30)-C(28)-O(13)-C(29)	-68.5(3)
C(25)-C(28)-O(13)-C(29)	59.9(2)
O(13)-C(28)-C(30)-O(14)	-64.8(2)
C(25)-C(28)-C(30)-O(14)	165.49(18)
O(13)-C(28)-C(30)-C(33)	179.17(18)
C(25)-C(28)-C(30)-C(33)	49.4(3)
C(33)-C(30)-O(14)-C(31)	-140.4(2)
C(28)-C(30)-O(14)-C(31)	101.1(2)
C(30)-O(14)-C(31)-O(15)	-1.4(4)
C(30)-O(14)-C(31)-C(32)	177.3(2)
C(24)-O(17)-C(33)-C(34)	-165.27(18)
C(24)-O(17)-C(33)-C(30)	69.6(2)
O(14)-C(30)-C(33)-O(17)	-177.89(16)
C(28)-C(30)-C(33)-O(17)	-60.9(2)
O(14)-C(30)-C(33)-C(34)	59.1(2)
C(28)-C(30)-C(33)-C(34)	176.1(2)
O(17)-C(33)-C(34)-O(16)	-67.6(3)
C(30)-C(33)-C(34)-O(16)	53.9(3)
C(33)-C(34)-O(16)-C(35)	-163.8(2)

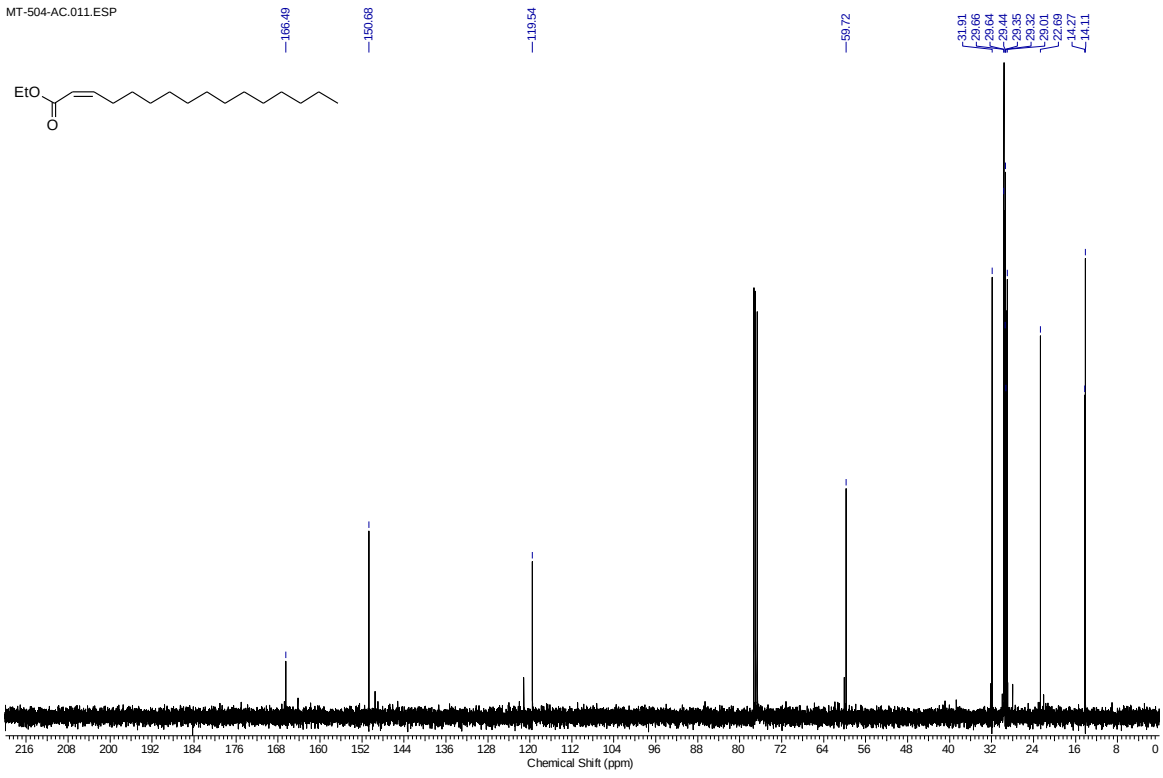
Symmetry transformations used to generate equivalent atoms:

J NMR-Spektren – Teil B

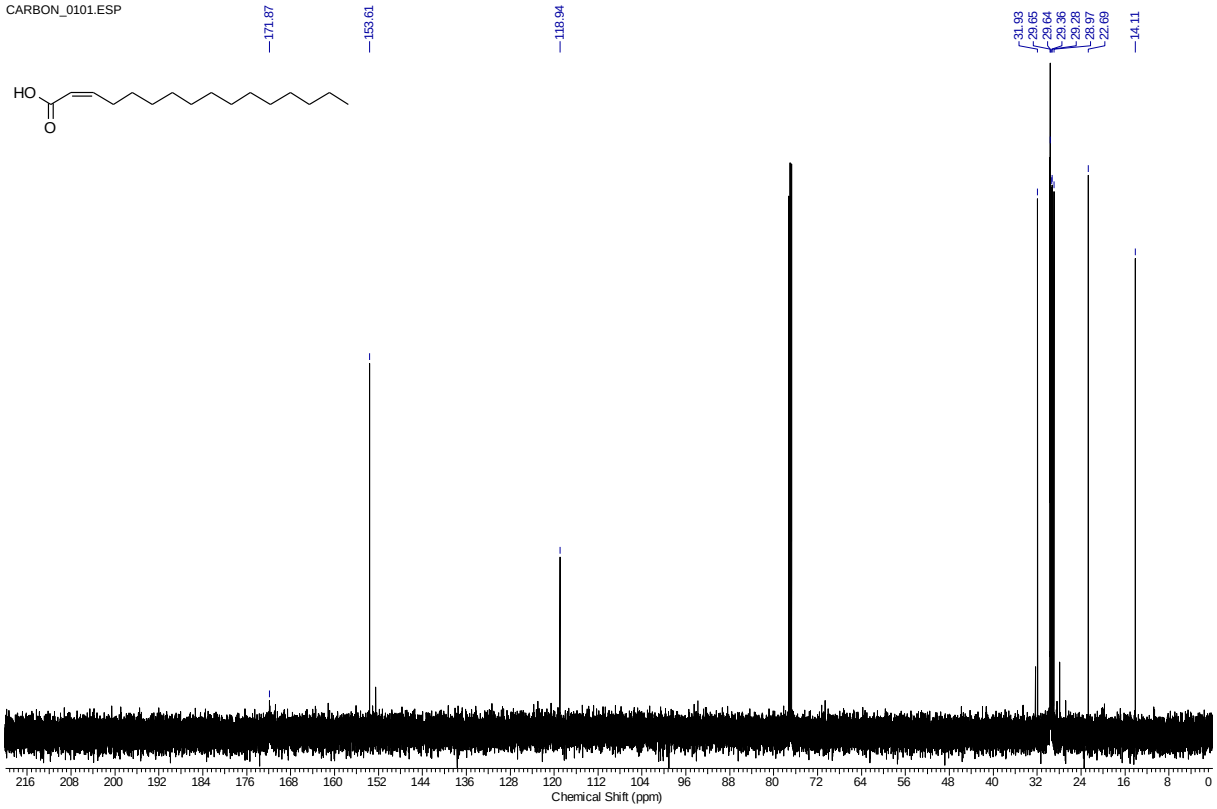
Verbindung **113**



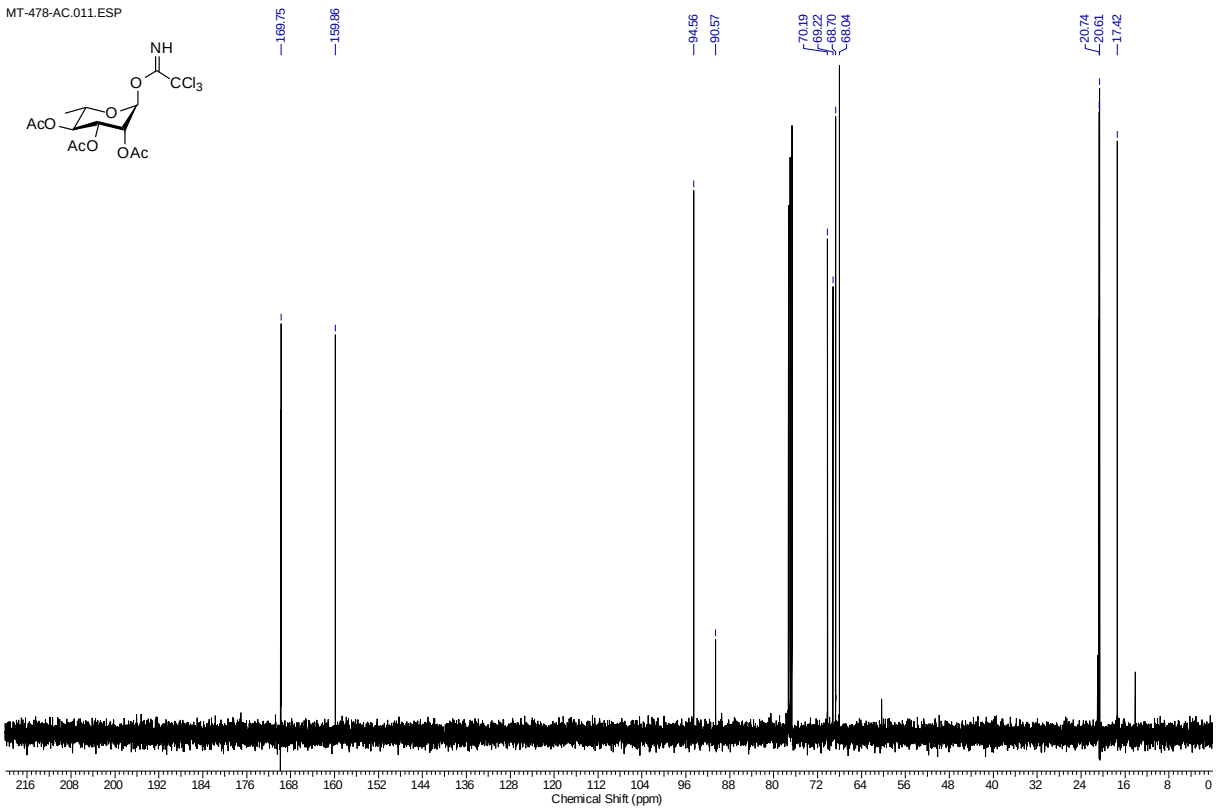
Verbindung **114**



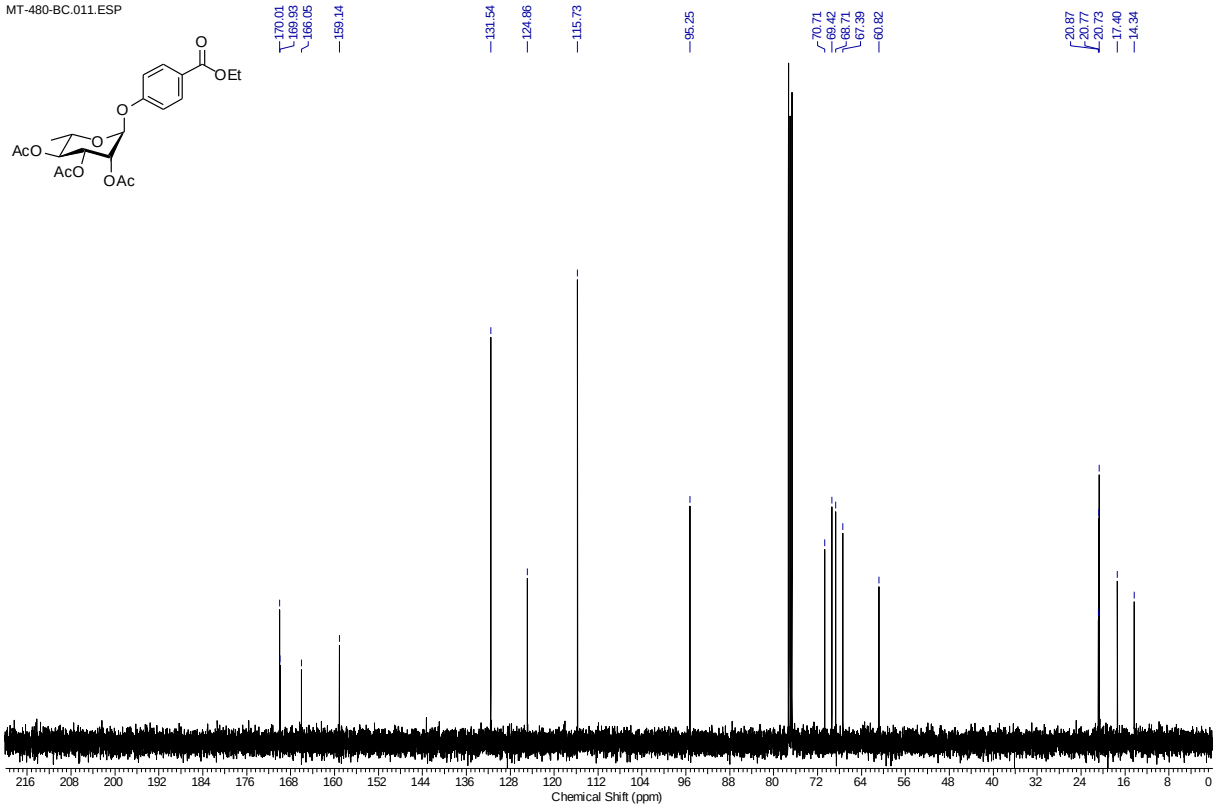
Verbindung **115**



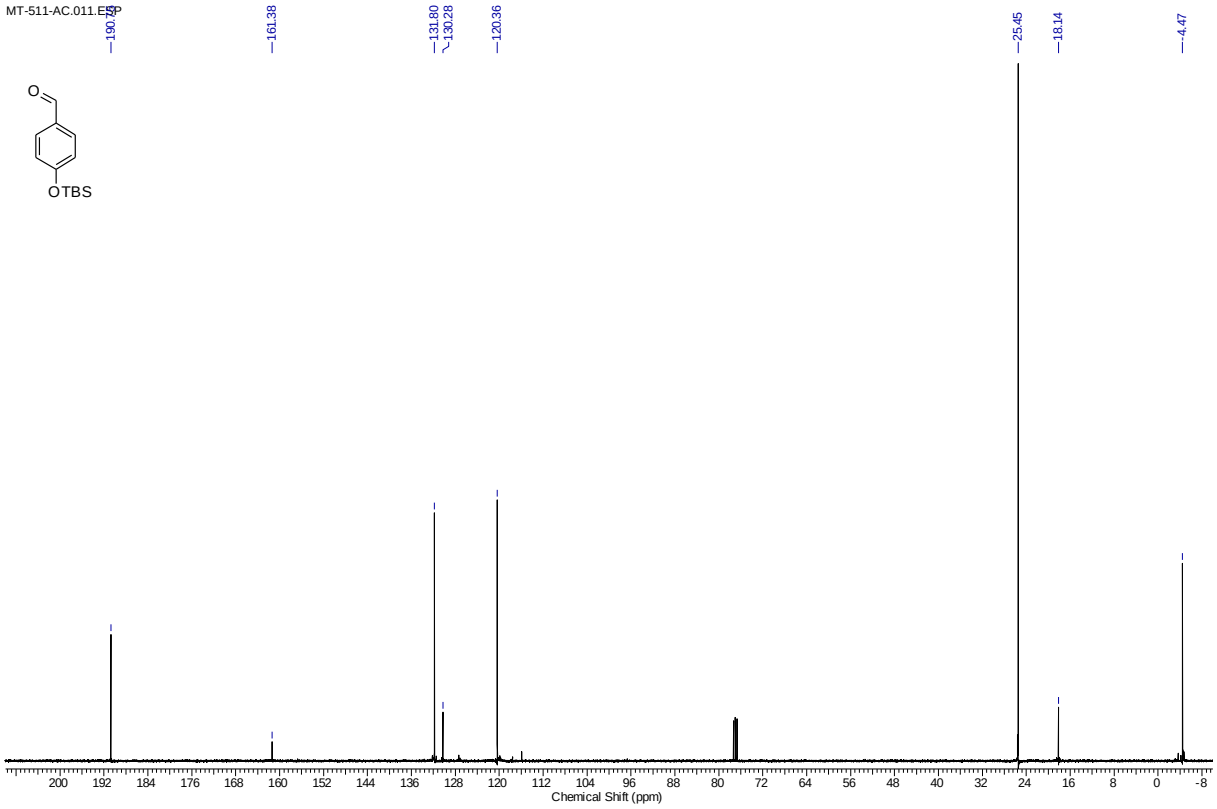
Verbindung **121**



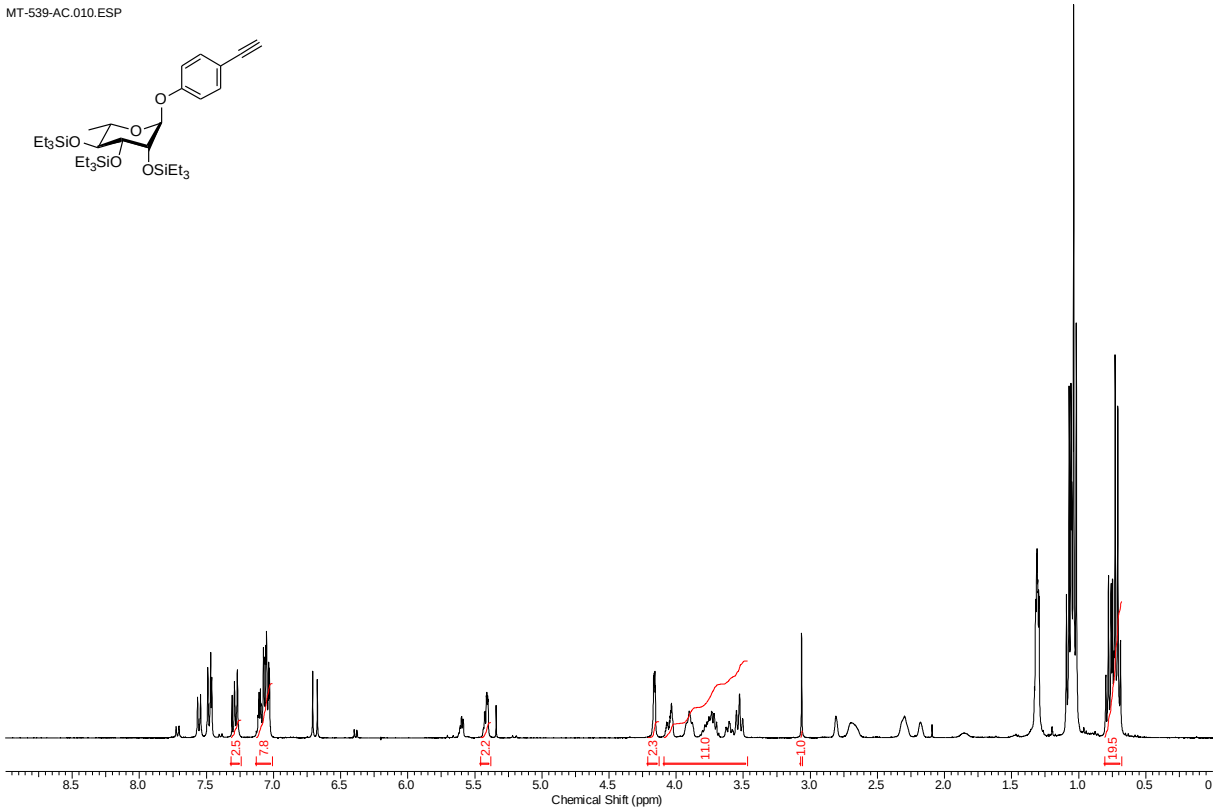
Verbindung **122**



Verbindung **135**

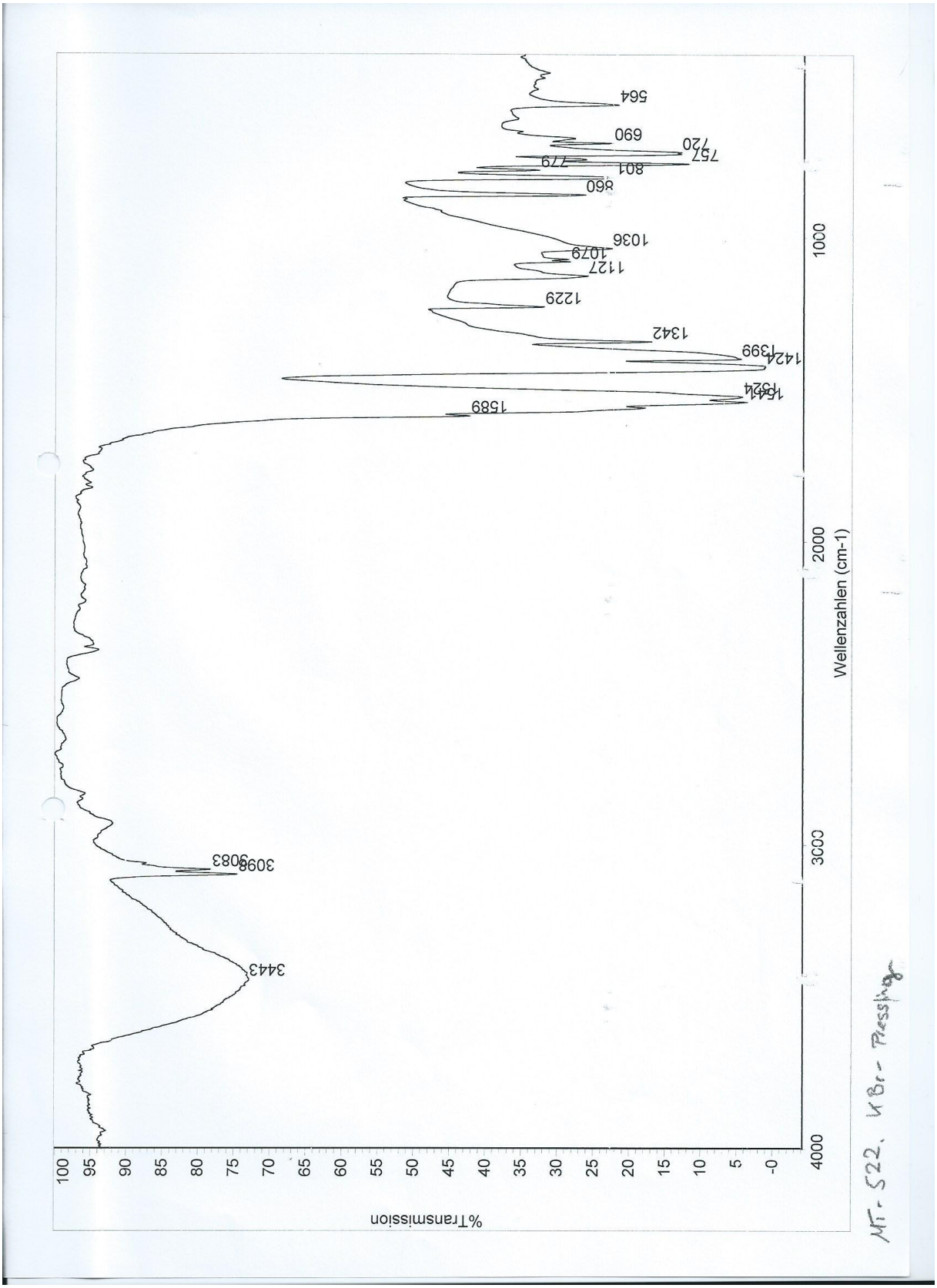


Verbindung **154** (^{1}H-NMR, verunreinigt)



K IR- und Massen-Spektren – Teil B

Verbindung **10**7 – IR



Verbindung **107** – Massenspektrum