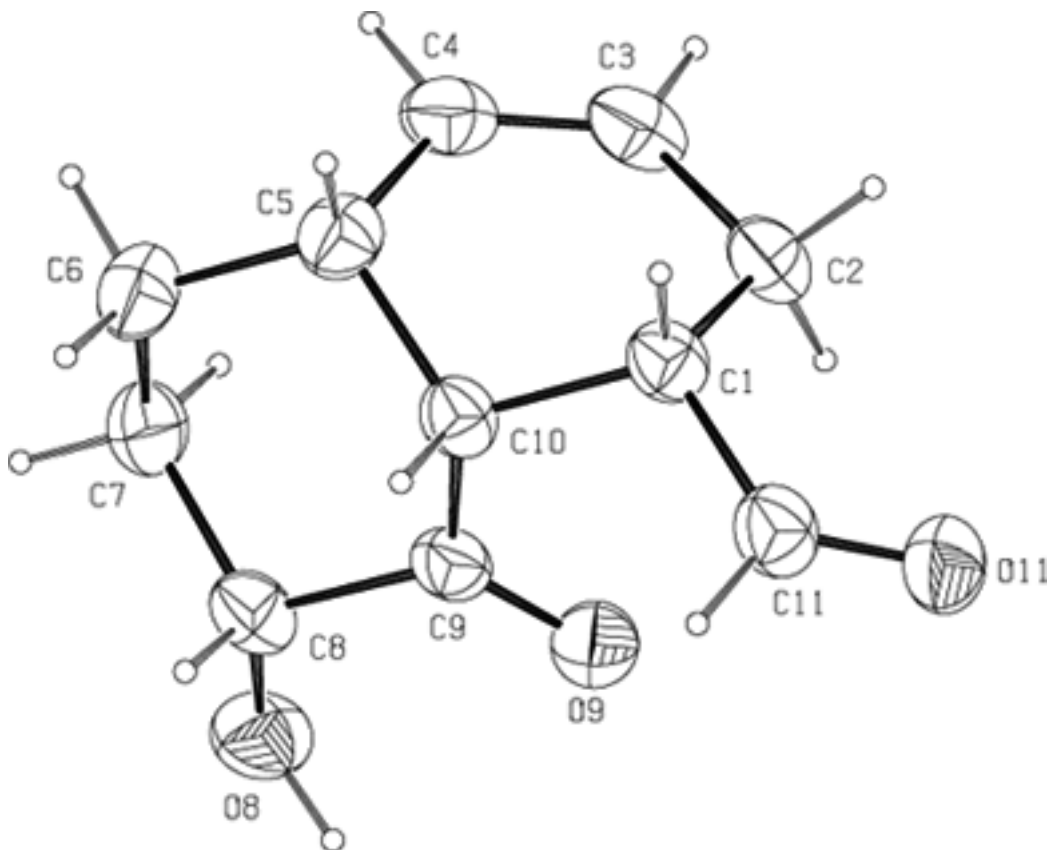


Anhang

Kristallstrukturdaten

Strukturdaten von 9-Hydroxy-10-oxobicyclo[4.4.0]dec-4-en-2-carbaldehyd (100)



Summenformel	C ₁₁ H ₁₄ O ₃
Formelgewicht	194.22
Kristallform und -farbe	farblose Nadeln
Kristallgröße (mm)	0.40×0.15×0.15
Kristallsystem	monoklin
Raumgruppe	P21/c
a (Å)	12.6156
b (Å)	5.1770
c (Å)	15.2218

α (°)	90
β (°)	103.036
γ (°)	90
Volumen (Å ³)	968.53
Z	4
$d_{\text{calc.}}$ (g/cm ³)	1.332
Absorptionskoeffizient (mm ⁻¹)	0.789
Temperatur (K)	213
Scanbereich (°)	5.96 – 64.86
gesammelte Reflexe	4589
unabhängige Reflexe	1640 ($R_{\text{int}} = 3.15\%$)
Absorptionskorrektur	Psi-Scan
F(000)	416
Verfeinerungsmethode	Vollmatrix, F^2
Goodness of fit	1.027
R (gemessene Daten)	$R_F = 3.92\%$, $R_W(F^2) = 11.01\%$
R (Gesamtdaten)	$R_F = 4.46\%$, $R_W(F^2) = 11.70\%$

Tabelle 1: Atomkoordinaten ($\times 10^4$) und äquivalente isotrope Temperaturfaktoren U_{eq} ($\text{Å}^2 \times 10^3$)

	X	Y	Z	U_{eq}
O ₈	2632(1)	1450(3)	7046(1)	48(1)
O ₉	1241(1)	-26(2)	8067(1)	44(1)
O ₁₁	-469(1)	-3180(3)	9049(1)	47(1)
C ₁	1465(1)	-3857(3)	9358(1)	33(1)
C ₂	1635(1)	-1615(4)	10022(1)	38(1)
C ₃	2811(1)	-902(4)	10330(1)	41(1)
C ₄	3600(1)	-1911(4)	9998(1)	41(1)
C ₅	3432(1)	-3850(3)	9243(1)	36(1)
C ₆	4214(1)	-3426(4)	8617(1)	42(1)
C ₇	3985(1)	-919(4)	8094(1)	41(1)
C ₈	2829(1)	-906(3)	7518(1)	37(1)
C ₉	2029(1)	-1408(3)	8106(1)	32(1)
C ₁₀	2240(1)	-3760(3)	8710(1)	31(1)
C ₁₁	311(1)	-415(3)	8845(1)	40(1)

Tabelle 2: Wasserstoffkoordinaten ($\times 10^4$) und isotrope Auslenkungsparameter U_{eq} ($\text{Å}^2 \times 10^3$)

	X	Y	Z	U_{eq}
H ₁	1623(14)	-547(4)	9693(11)	43(5)
H _{2A}	1363(14)	-207(4)	10528(12)	44(5)
H _{2B}	1199(16)	-11(4)	9728(13)	52(5)
H ₃	2985(15)	34(4)	10804(13)	52(5)
H ₄	4355(16)	-147(4)	10249(12)	51(5)
H ₅	3557(14)	-555(4)	9500(11)	41(4)
H _{6A}	4139(15)	-490(4)	8180(12)	46(5)
H _{6B}	4952(16)	-338(4)	8977(12)	52(5)
H _{7A}	4483(15)	-65(4)	7704(12)	46(5)
H _{7B}	4070(15)	61(4)	8526(12)	47(5)
H ₈	2750(13)	-239(4)	7111(11)	38(4)
H ₁₀	2098(14)	-520(4)	8301(11)	39(4)
H ₁₁	206(17)	-526(4)	8282(14)	65(6)
H ₈	1920(2)	145(5)	6741(15)	74(7)

Tabelle 3: Anisotrope Auslenkungsparameter U_{xx} ($\text{Å}^2 \times 10^3$)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O ₈	46(1)	57(1)	40(1)	16(1)	9(1)	-6(1)
O ₉	41(1)	53(1)	39(1)	9(1)	11(1)	8(1)
O ₁₁	36(1)	62(1)	46(1)	-4(1)	15(1)	-2(1)
C ₁	36(1)	33(1)	32(1)	2(1)	10(1)	-4(1)
C ₂	44(1)	45(1)	29(1)	-2(1)	14(1)	5(1)
C ₃	51(1)	45(1)	27(1)	-2(1)	8(1)	-13(1)
C ₄	38(1)	49(1)	32(1)	4(1)	2(1)	-9(1)
C ₅	35(1)	35(1)	40(1)	7(1)	9(1)	1(1)
C ₆	33(1)	45(1)	50(1)	3(1)	13(1)	3(1)
C ₇	36(1)	47(1)	42(1)	4(1)	16(1)	-3(1)
C ₈	43(1)	40(1)	30(1)	2(1)	12(1)	-4(1)
C ₉	32(1)	40(1)	25(1)	-3(1)	5(1)	-4(1)
C ₁₀	34(1)	32(1)	30(1)	-4(1)	9(1)	-3(1)
C ₁₁	38(1)	45(1)	39(1)	-3(1)	13(1)	-7(1)

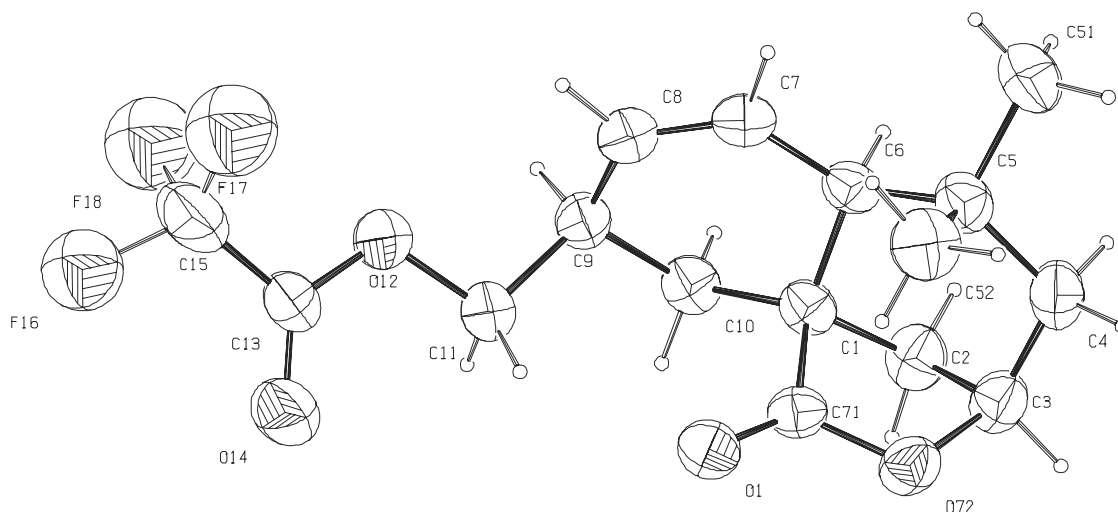
Tabelle 4: Bindungslängen in Å

O ₈	C ₈	1.409
O ₉	C ₉	1.216
O ₁₁	C ₁	1.206
C ₁	C ₁₁	1.496
C ₁	C ₂	1.523
C ₁	C ₁₀	1.537
C ₂	C ₃	1.497
C ₃	C ₄	1.321
C ₄	C ₅	1.504
C ₅	C ₆	1.534
C ₅	C ₁₀	1.540
C ₆	C ₇	1.517
C ₇	C ₈	1.522
C ₈	C ₉	1.516
C ₉	C ₁₀	1.513

Tabelle 5: Bindungswinkel in °

C ₁₁	C ₁	C ₂	113.46
C ₁₁	C ₁	C ₁₀	110.71
C ₂	C ₁	C ₁₀	112.74
C ₃	C ₂	C ₁	112.14
C ₄	C ₃	C ₂	124.14
C ₃	C ₄	C ₅	124.56
C ₄	C ₅	C ₆	112.31
C ₄	C ₅	C ₁₀	109.60
C ₆	C ₅	C ₁₀	110.88
C ₇	C ₆	C ₅	112.07
C ₆	C ₇	C ₈	110.52
O ₈	C ₈	C ₉	112.62
O ₈	C ₈	C ₇	109.49
C ₉	C ₈	C ₇	109.78
O ₉	C ₉	C ₁₀	122.24
O ₉	C ₉	C ₈	121.11
C ₁₀	C ₉	C ₈	116.61
C ₉	C ₁₀	C ₁	111.47
C ₉	C ₁₀	C ₅	111.21
C ₁	C ₁₀	C ₅	110.31
O ₁₁	C ₁	C ₁	125.35

Strukturdaten von (7,7-Dimethyl-11-oxo-10-oxatricyclo[7.2.1.0^{1,6}]dodec-4-en-3-yl)methyltrifluoroacetat (171)



Summenformel	$C_{16}H_{19}F_3O_4$
Formelgewicht	332.31
Kristallform und -farbe	farblose Plättchen
Kristallgröße (mm)	0.40×0.30×0.20
Kristallsystem	monoklin
Raumgruppe	$P2_1/c$
a (Å)	19.583
b (Å)	10.354
c (Å)	12.252
α (°)	90
β (°)	40.333
γ (°)	90
Volumen (Å ³)	1608.0
Z	4
$d_{\text{calc.}}$ (g/cm ³)	1.373
Absorptionskoeffizient (mm ⁻¹)	1.035
Temperatur (K)	213
Scanbereich (°)	5.52 – 65.03
gesammelte Reflexe	6165
unabhängige Reflexe	2737 ($R_{\text{int}} = 4.05\%$)

Absorptionskorrektur	N
F(000)	696
Verfeinerungsmethode	Vollmatrix, F^2
Goodness of fit	2.117
R (gemessene Daten)	$R_F = 7.84\%$, $R_W(F^2) = 27.04\%$
R (Gesamtdaten)	$R_F = 8.90\%$, $R_W(F^2) = 28.13\%$

Tabelle 6: Atomkoordinaten ($\times 10^4$) und äquivalente isotrope Temperaturfaktoren U_{eq} ($\text{Å}^2 \times 10^3$)

	X	Y	Z	U_{eq}
O ₇₂	0.0111(2)	0.2655(2)	0.4939(3)	46(1)
C ₁	0.1238(2)	0.1535(3)	0.4756(3)	37(1)
C ₂	0.0280(3)	0.2057(4)	0.6547(4)	47(1)
C ₃	0.0027(3)	0.3210(3)	0.6140(4)	46(1)
C ₄	0.0822(3)	0.4274(3)	0.5326(5)	50(1)
C ₅	0.1974(3)	0.3886(3)	0.3661(4)	45(1)
C ₅₁	0.2696(4)	0.4799(4)	0.3423(7)	67(1)
C ₅₂	0.2217(3)	0.4072(4)	0.2141(5)	57(1)
C ₆	0.2169(2)	0.2474(3)	0.3812(4)	38(1)
C ₇	0.3190(2)	0.1913(3)	0.2150(4)	45(1)
C ₈	0.3357(2)	0.0675(3)	0.1783(4)	46(1)
C ₉	0.2566(2)	-0.0378(3)	0.2973(4)	41(1)
C ₁₀	0.1539(3)	0.0162(3)	0.4711(4)	40(1)
O ₁₂	0.3368(2)	-0.1820(3)	0.0733(3)	59(1)
O ₁	0.1016(2)	0.1057(2)	0.3065(3)	47(1)
C ₇₁	0.0817(2)	0.1672(3)	0.4110(3)	37(1)
C ₁₁	0.2369(3)	-0.1211(4)	0.2230(5)	48(1)
C ₁₃	0.3378(3)	-0.2532(3)	-0.0161(5)	52(1)
O ₁₄	0.2638(2)	-0.2765(3)	0.0159(4)	68(1)
C ₁₅	0.4465(4)	-0.3035(6)	-0.1735(7)	96(1)
F ₁₆	0.4436(4)	-0.4154(5)	-0.2217(7)	82(1)
F ₁₇	0.5186(5)	-0.2174(7)	-0.2622(8)	104(2)
F ₁₈	0.4744(5)	-0.3836(7)	-0.0999(9)	107(2)

Tabelle 7: Wasserstoffkoordinaten ($\times 10^4$) und isotrope Auslenkungsparameter U_{eq} ($\text{Å}^2 \times 10^3$)

	X	Y	Z	U_{eq}
H ₂₁	480(3)	2300(4)	7080(5)	48(9)
H ₂₂	-370(3)	1430(4)	7290(5)	52(10)
H ₃₁	-710(3)	3540(4)	7090(5)	58(10)
H ₄₁	840(3)	4540(4)	6120(5)	54(10)
H ₄₂	560(3)	5070(4)	5270(5)	57(10)
H ₅₁₁	3390(3)	4560(4)	2460(5)	54(10)
H ₅₁₂	2620(4)	4660(5)	4320(6)	83(15)
H ₅₁₃	2440(4)	5680(6)	3540(6)	90(16)
H _{52A}	2069	4948	2117	85
H _{52B}	1786	3496	2243	85
H _{52C}	2948	3887	1117	85
H ₆₁	378(3)	2530(4)	1380(5)	47(10)
H ₆₂	225(2)	2560(3)	4530(4)	37(8)
H ₈	406(3)	370(3)	690(4)	38(8)
H ₉	288(2)	-1000(3)	3160(4)	39(9)
H ₁₀	162(3)	150(4)	5400(6)	67(13)
H ₁₀₁	960(3)	-420(4)	5230(5)	62(11)
H ₁₁	2060(3)	-700(4)	1900(5)	68(12)
H ₁₂	1870(4)	-1790(5)	2970(6)	67(13)

Tabelle 8: Anisotrope Auslenkungsparameter U_{xx} ($\text{Å}^2 \times 10^3$)

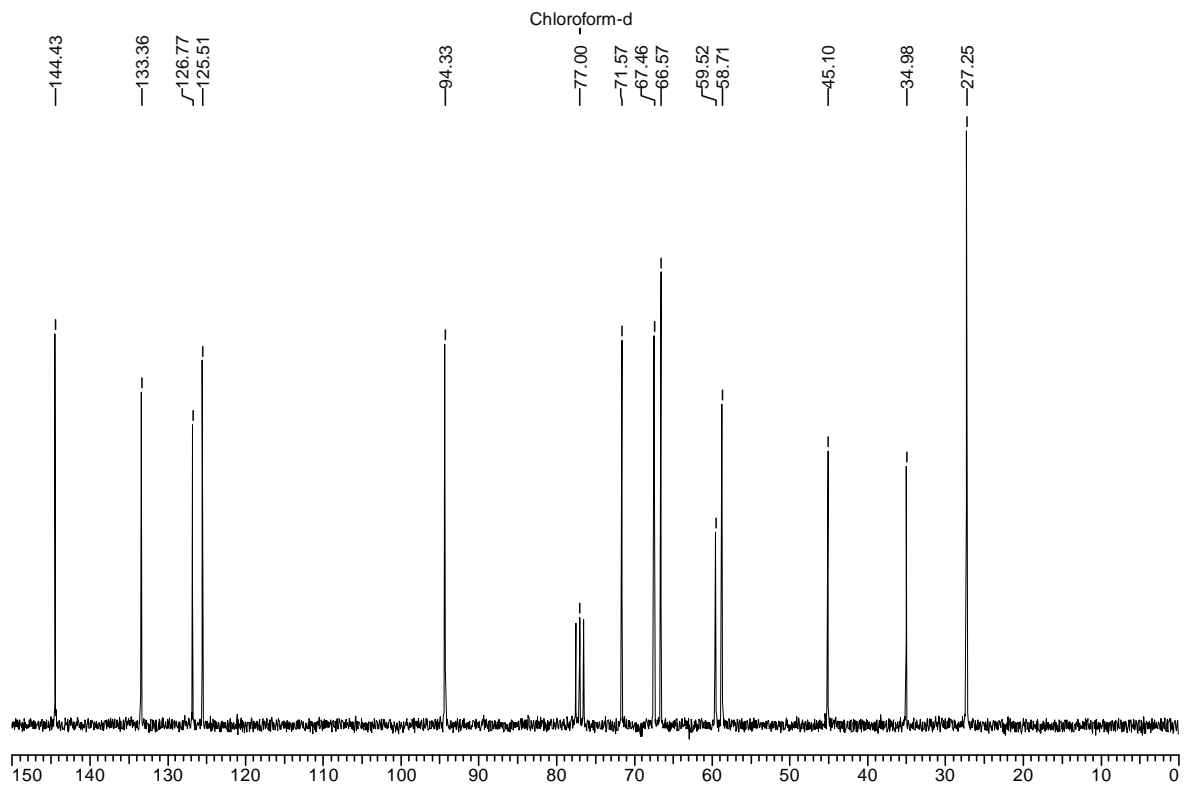
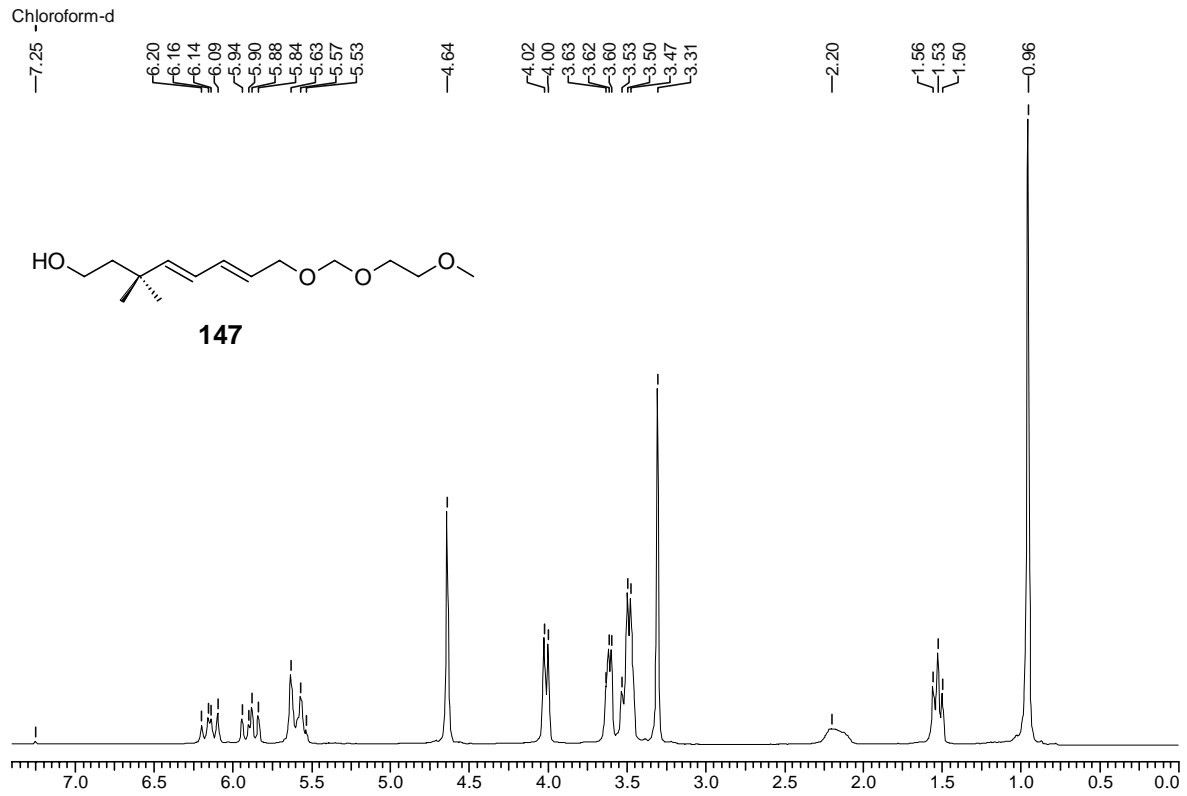
	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O ₇₂	45(1)	53(1)	47(1)	-5(1)	-38(1)	9(1)
C ₁	44(2)	39(2)	37(2)	2(1)	-34(2)	-2(1)
C ₂	50(2)	53(2)	38(2)	-3(1)	-34(2)	4(2)
C ₃	45(2)	52(2)	43(2)	-9(1)	-34(2)	11(1)
C ₄	60(2)	41(2)	55(2)	-10(1)	-45(2)	10(2)
C ₅	52(2)	37(2)	54(2)	1(1)	-42(2)	-2(1)
C ₅₁	74(3)	43(2)	92(3)	-5(2)	-66(3)	-4(2)
C ₅₂	64(2)	49(2)	58(2)	12(2)	-47(2)	-5(2)
C ₆	43(2)	42(2)	42(2)	0(1)	-36(1)	-2(1)
C ₇	36(2)	50(2)	45(2)	4(1)	-30(1)	5(1)
C ₈	38(2)	50(2)	47(2)	-3(1)	-32(2)	2(1)
C ₉	48(2)	38(2)	50(2)	-3(1)	-41(2)	5(1)
C ₁₀	48(2)	40(2)	41(2)	3(1)	-37(1)	-1(1)
O ₁₂	49(1)	65(2)	63(2)	-25(1)	-42(1)	12(1)
O ₁	54(1)	55(2)	51(1)	-6(1)	-46(1)	5(1)
C ₇₁	37(1)	44(2)	38(2)	2(1)	-30(1)	-1(1)
C ₁₁	45(2)	45(2)	52(2)	-12(2)	-37(2)	5(1)
C ₁₃	50(2)	46(2)	56(2)	-9(2)	-40(2)	-3(1)
O ₁₄	61(2)	78(2)	65(2)	-20(1)	-48(1)	1(1)
C ₁₅	66(3)	105(4)	92(3)	-45(3)	-53(3)	-2(3)

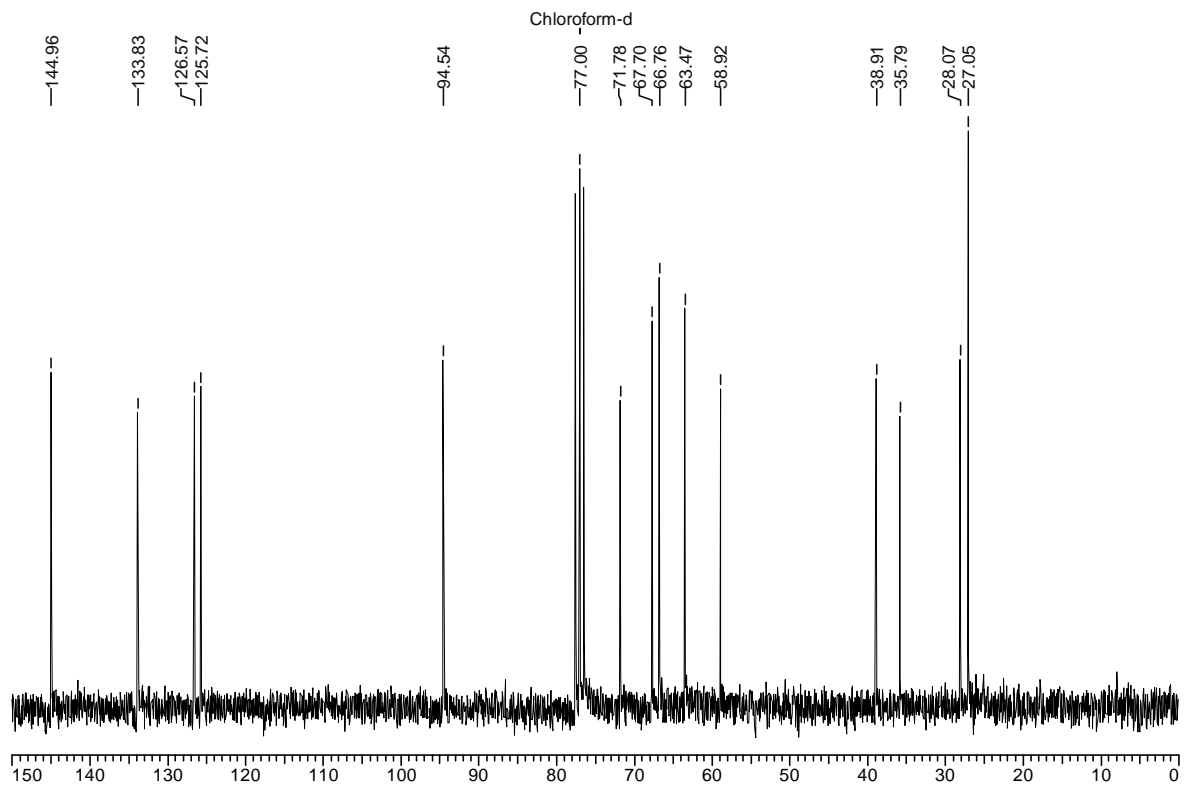
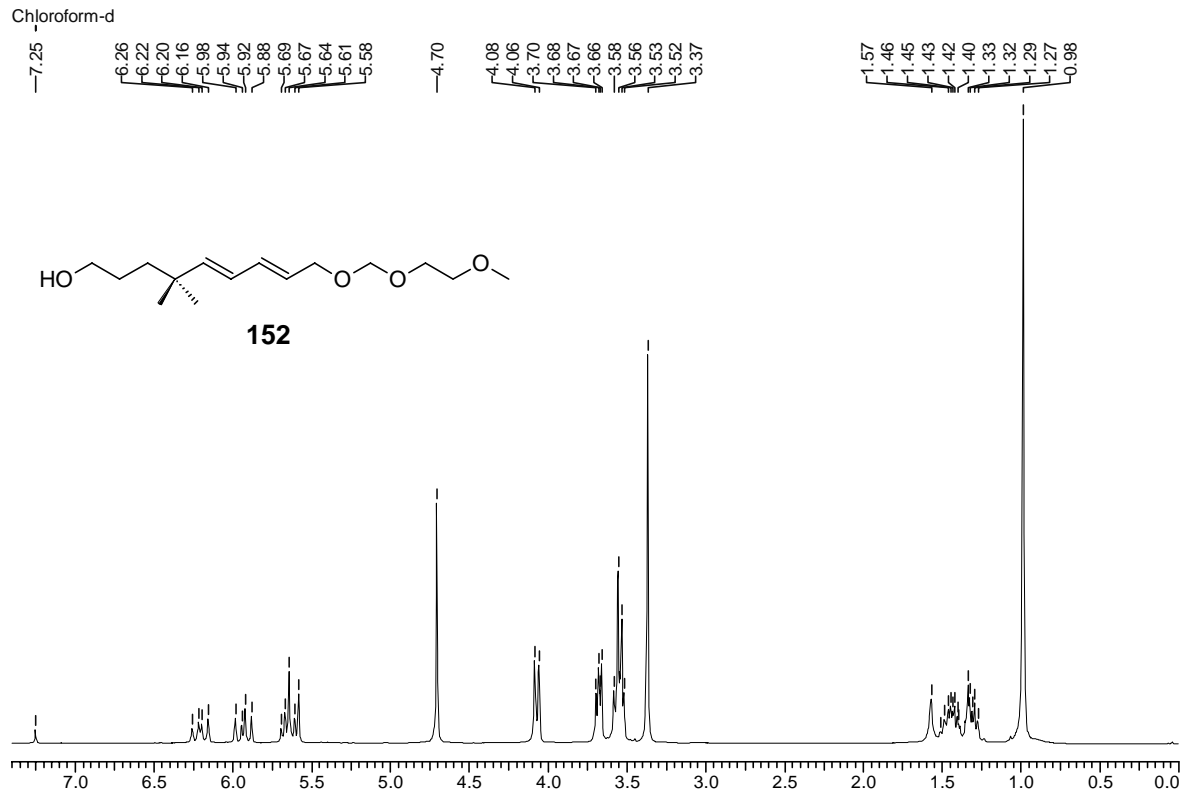
Tabelle 9: Bindungslängen in Å

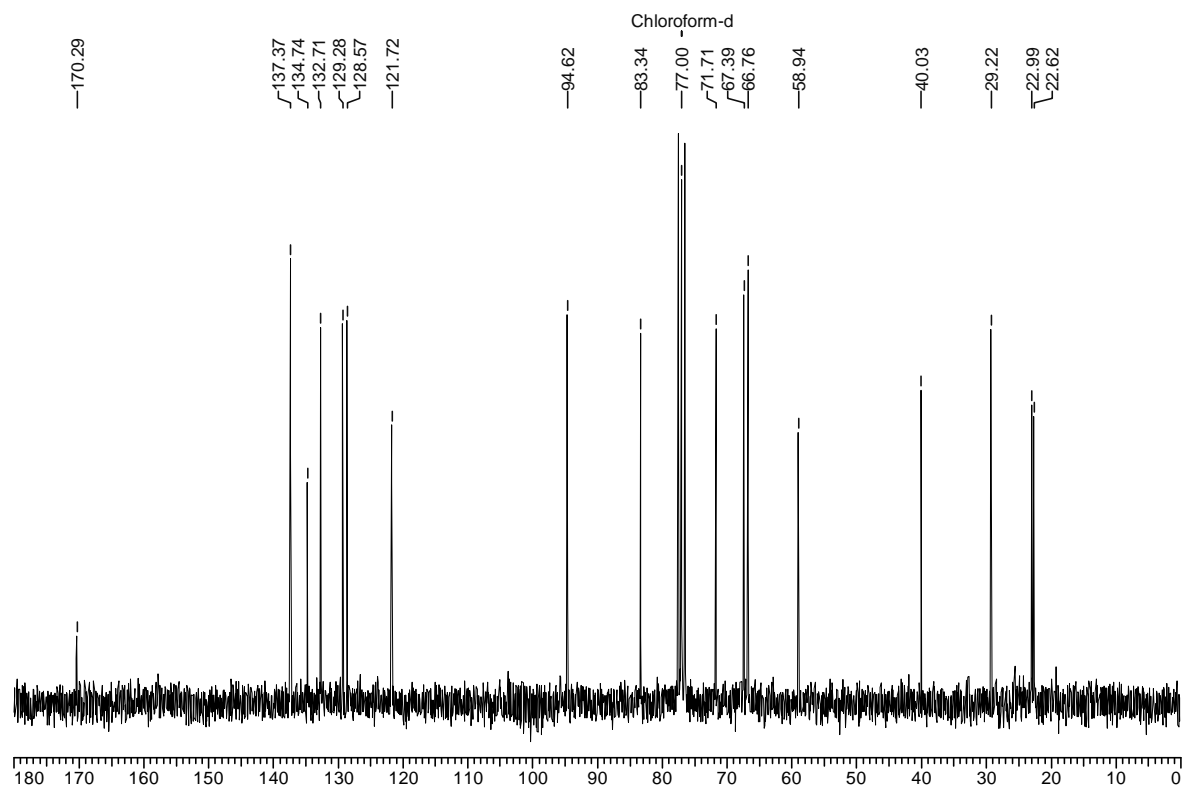
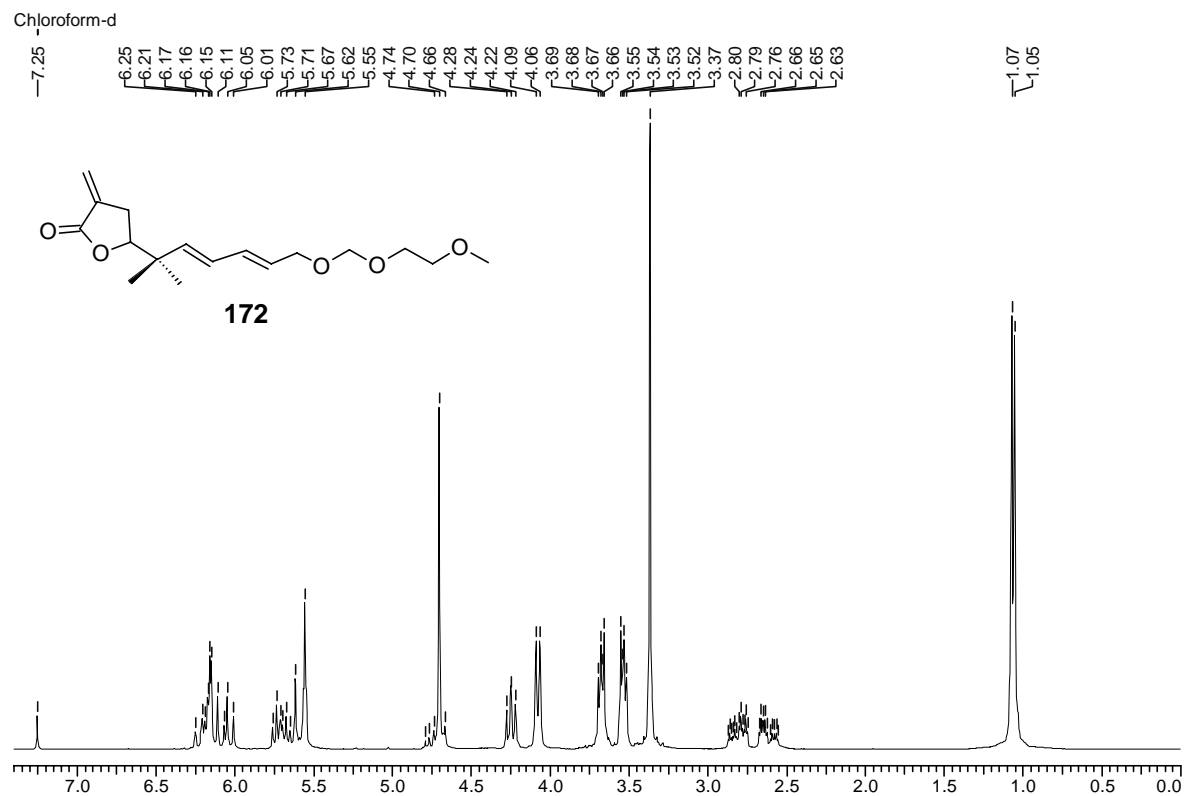
O ₇₂	C ₇₁	1.356
O ₇₂	C ₃	1.467
C ₁	C ₇₁	1.522
C ₁	C ₁₀	1.525
C ₁	C ₂	1.533
C ₁	C ₆	1.547
C ₂	C ₃	1.515
C ₃	C ₄	1.505
C ₄	C ₅	1.548
C ₅	C ₅₁	1.533
C ₅	C ₅₂	1.542
C ₅	C ₆	1.558
C ₆	C ₇	1.508
C ₇	C ₈	1.314
C ₈	C ₉	1.507
C ₉	C ₁₁	1.503
C ₉	C ₁₀	1.537
O ₁₂	C ₁₃	1.309
O ₁₂	C ₁₁	1.456
O ₁	C ₇₁	1.198
C ₁₃	O ₁₄	1.202
C ₁₃	C ₁₅	1.504
C ₁₅	F ₁₆	1.321
C ₁₅	F ₁₇	1.276
C ₁₅	F ₁₈	1.598

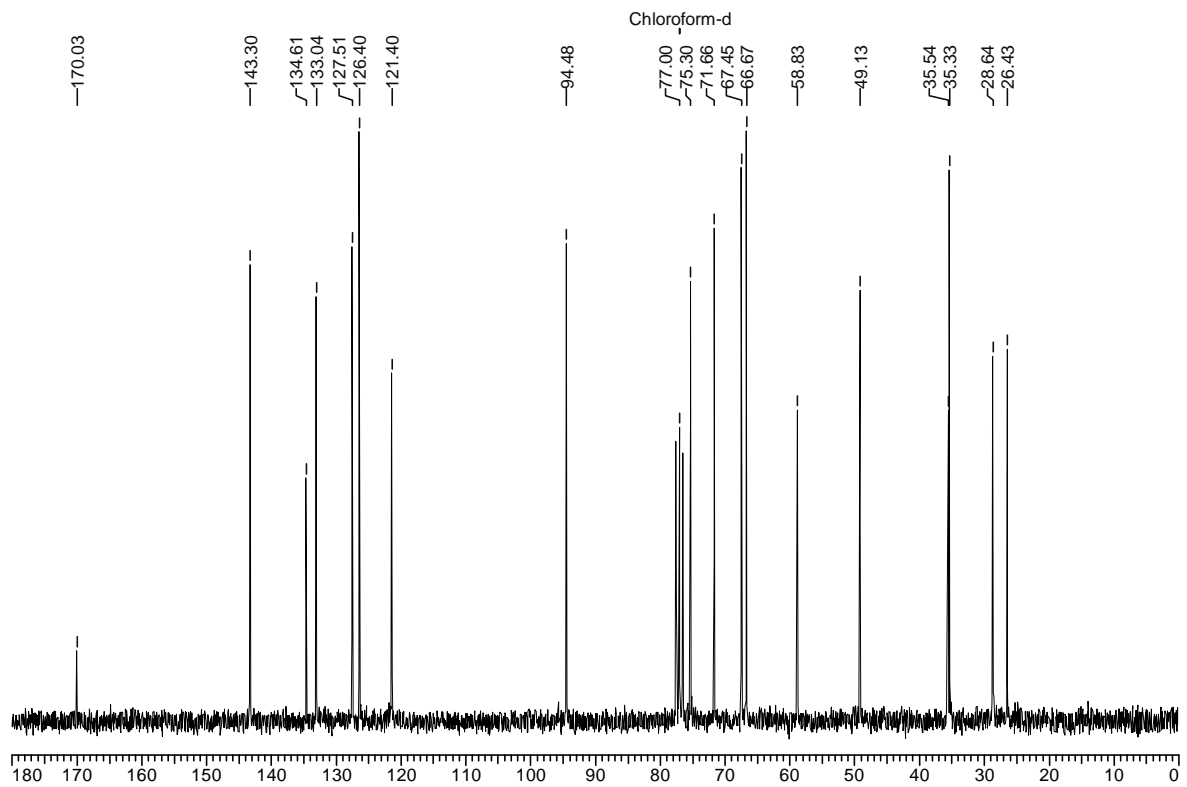
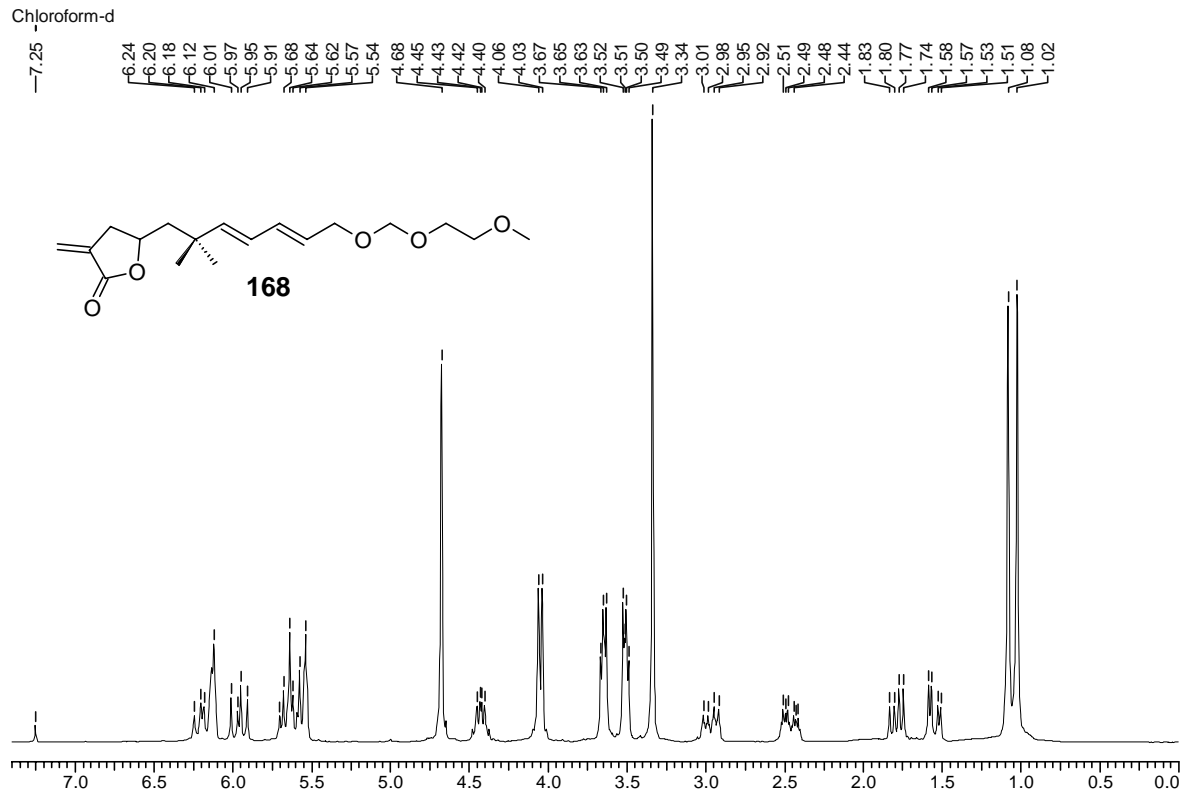
Tabelle 10: Bindungswinkel in °

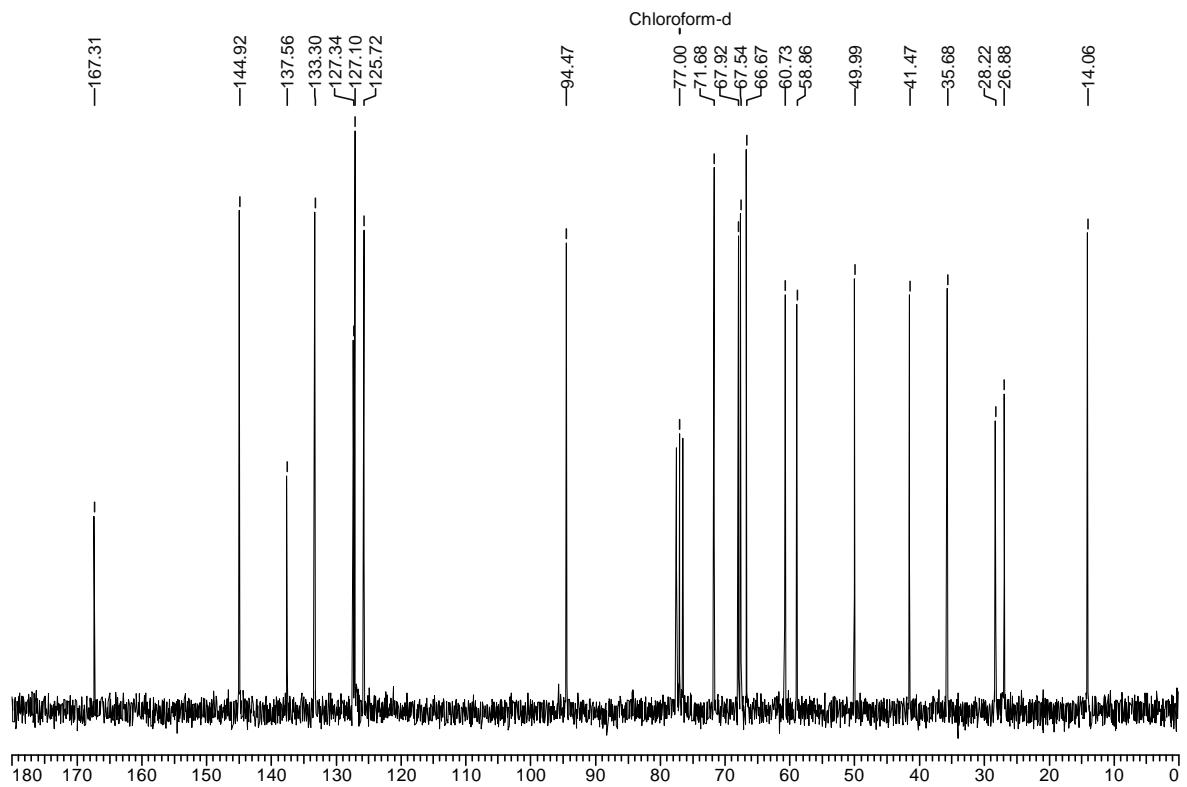
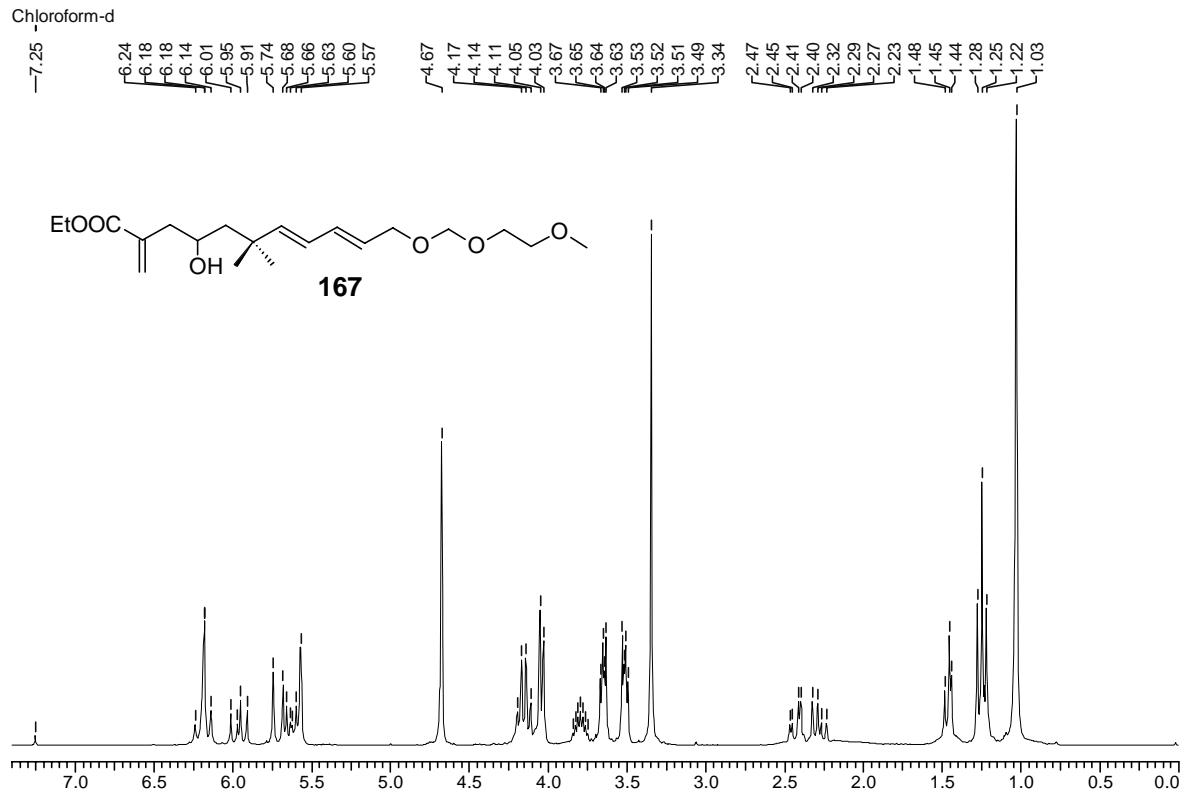
C ₇₁	O ₇₂	C ₃	108.4
C ₇₁	C ₁	C ₁₀	114.6
C ₇₁	C ₁	C ₂	98.9
C ₁₀	C ₁	C ₂	113.4
C ₇₁	C ₁	C ₆	110.5
C ₁₀	C ₁	C ₆	110.8
C ₂	C ₁	C ₆	107.9
C ₃	C ₂	C ₁	99.0
O ₇₂	C ₃	C ₄	110.7
O ₇₂	C ₃	C ₂	101.9
C ₄	C ₃	C ₂	111.3
C ₃	C ₄	C ₅	114.6
C ₅₁	C ₅	C ₅₂	107.6
C ₅₁	C ₅	C ₄	107.3
C ₅₂	C ₅	C ₄	110.9
C ₅₁	C ₅	C ₆	109.1
C ₅₂	C ₅	C ₆	112.5
C ₄	C ₅	C ₆	109.2
C ₇	C ₆	C ₁	111.2
C ₇	C ₆	C ₅	113.2
C ₁	C ₆	C ₅	115.0
C ₈	C ₇	C ₆	124.4
C ₇	C ₈	C ₉	124.8
C ₁₁	C ₉	C ₈	112.2
C ₁₁	C ₉	C ₁₀	112.2
C ₈	C ₉	C ₁₀	111.8
C ₁	C ₁₀	C ₉	116.8
C ₁₃	O ₁₂	C ₁₁	116.5
O ₁	C ₇₁	O ₇₂	121.0
O ₁	C ₇₁	C ₁	129.9
O ₇₂	C ₇₁	C ₁	109.1
O ₁₂	C ₁₁	C ₉	107.0
O ₁₄	C ₁₃	O ₁₂	126.5
O ₁₄	C ₁₃	C ₁₅	121.6
O ₁₂	C ₁₃	C ₁₅	111.8
F ₁₇	C ₁₅	F ₁₆	128.9
F ₁₇	C ₁₅	C ₁₃	114.6
F ₁₆	C ₁₅	C ₁₃	112.0
F ₁₇	C ₁₅	F ₁₈	102.2
F ₁₆	C ₁₅	F ₁₈	86.9
C ₁₃	C ₁₅	F ₁₈	102.4

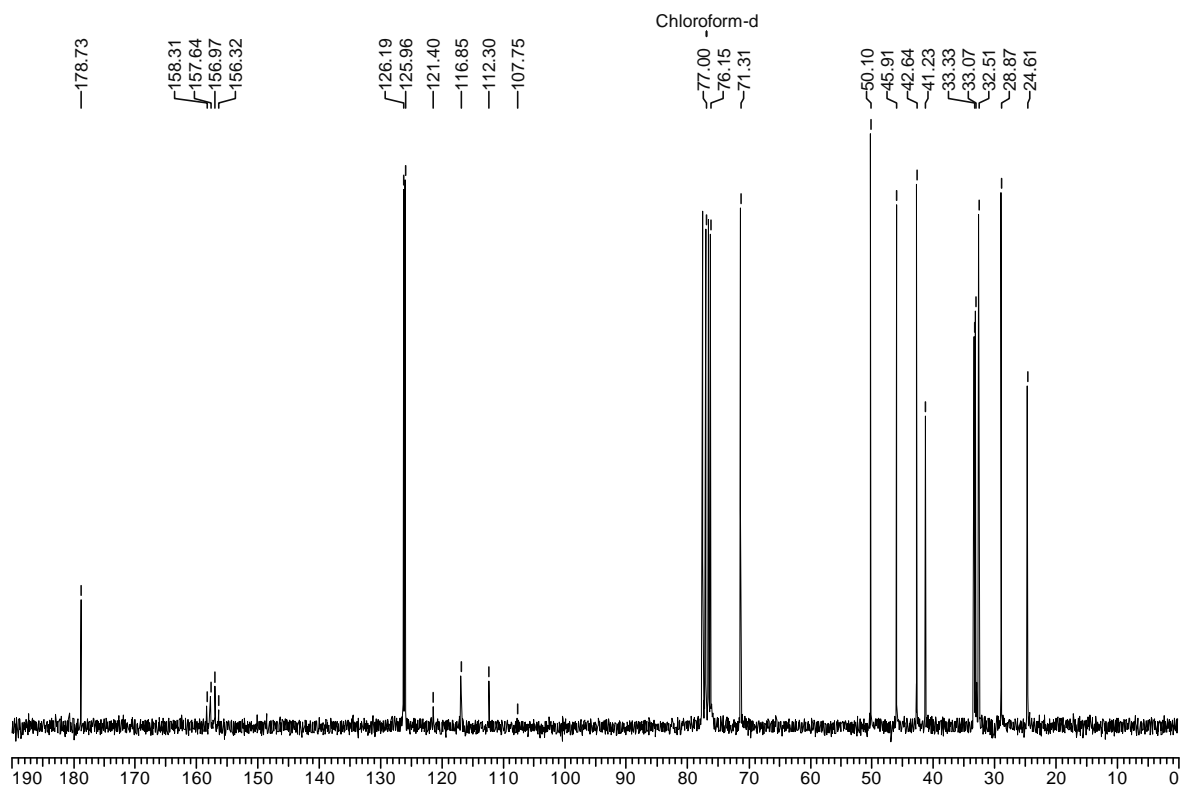
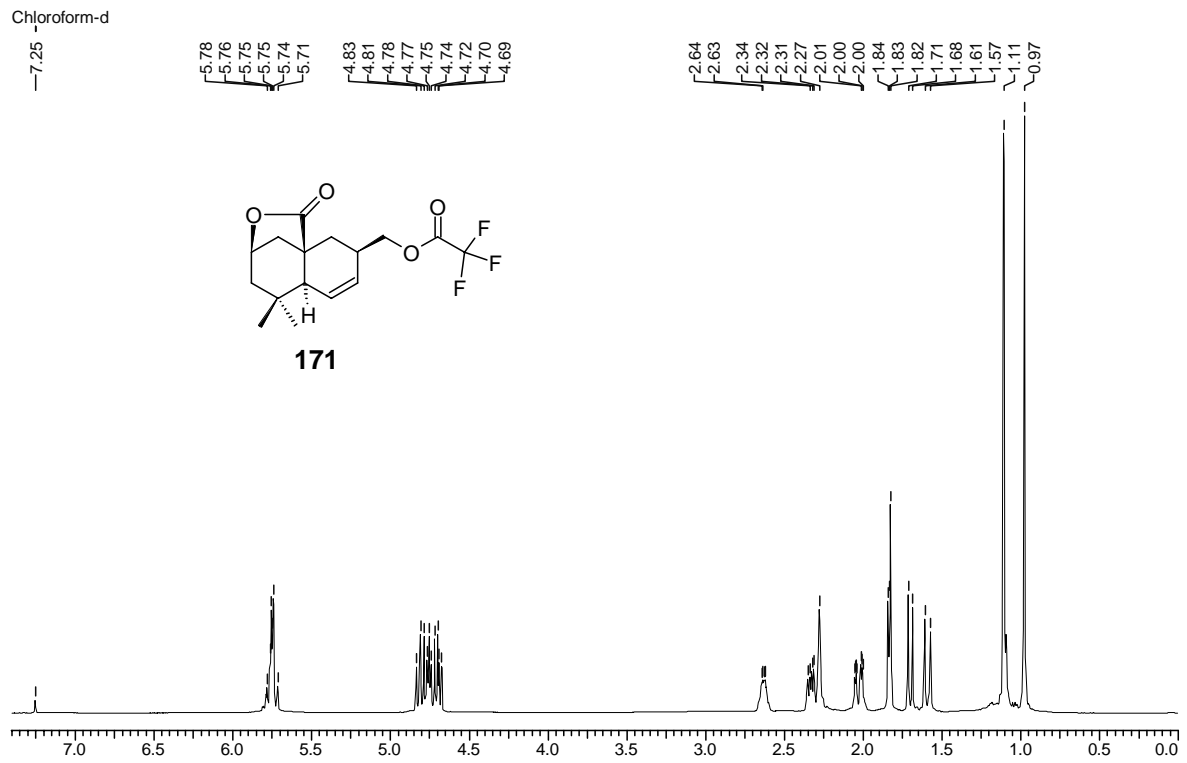


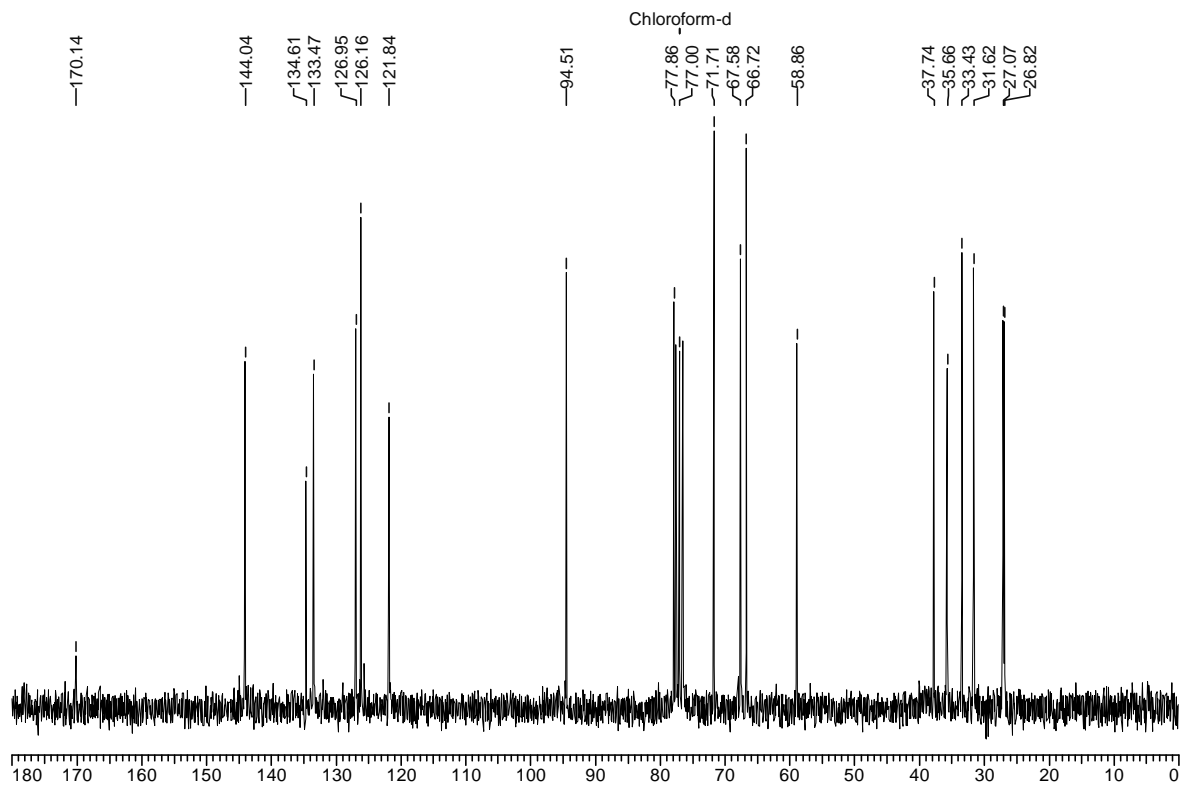
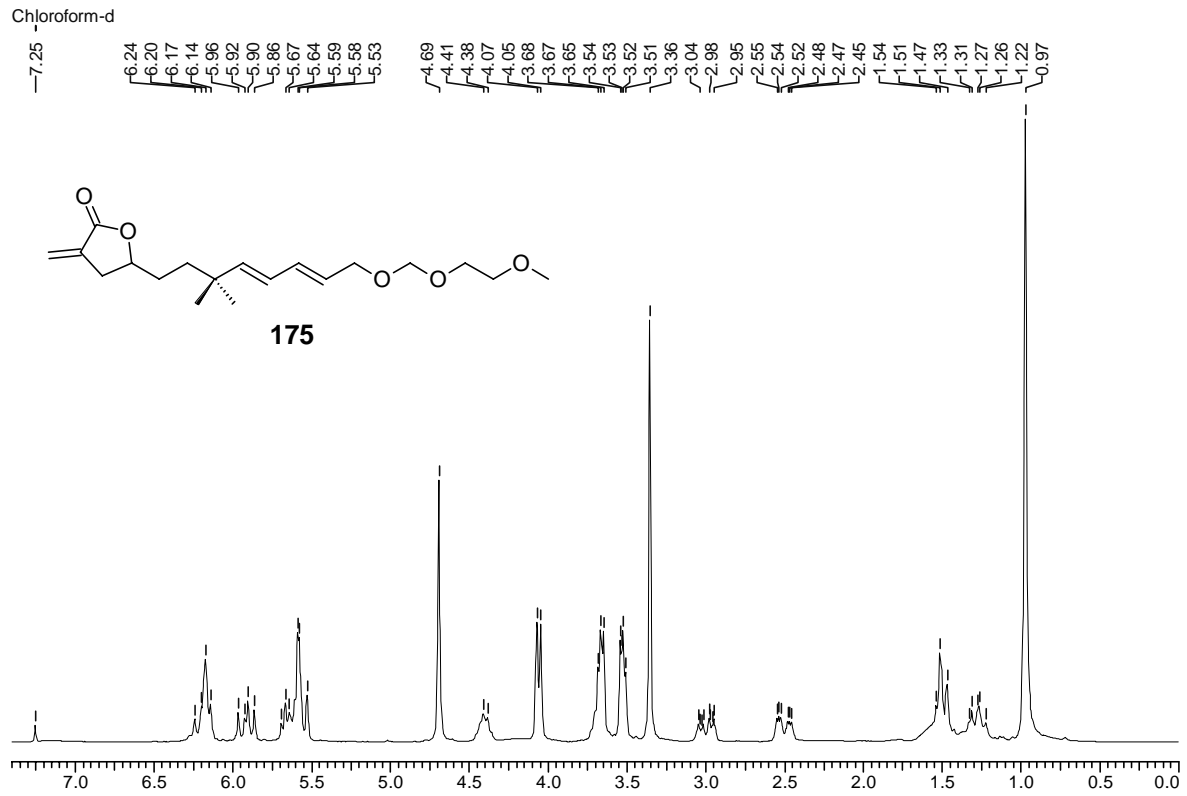


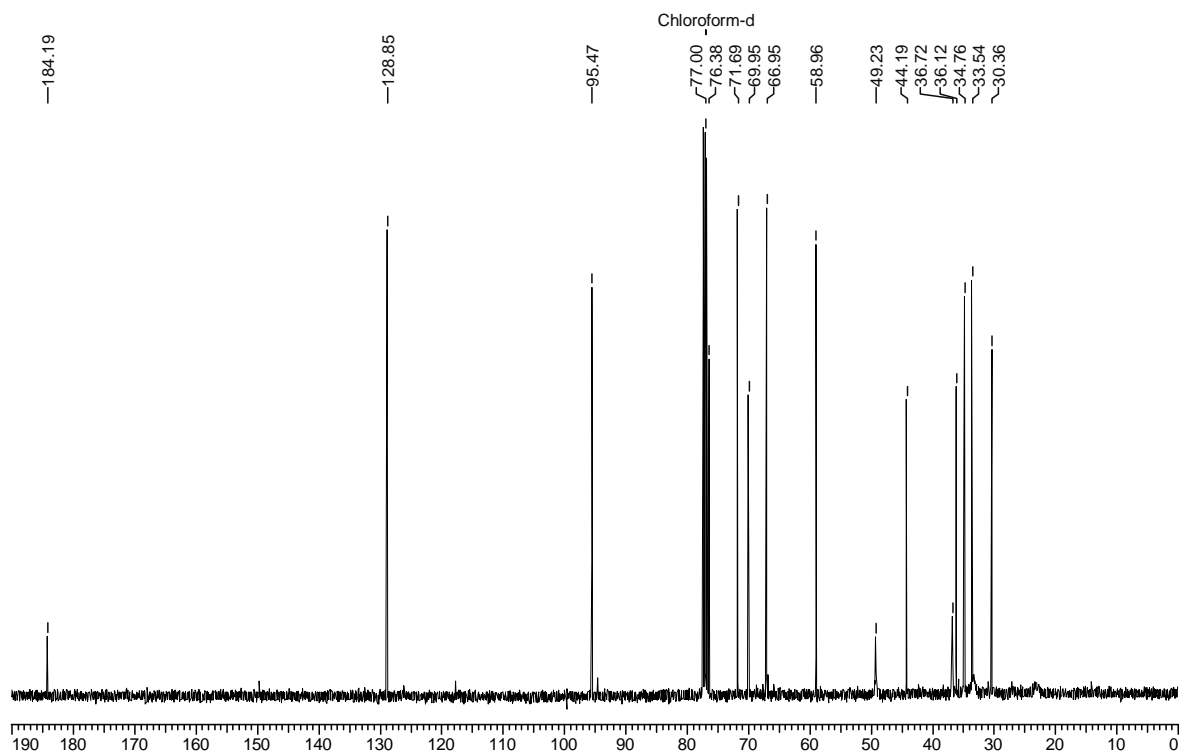
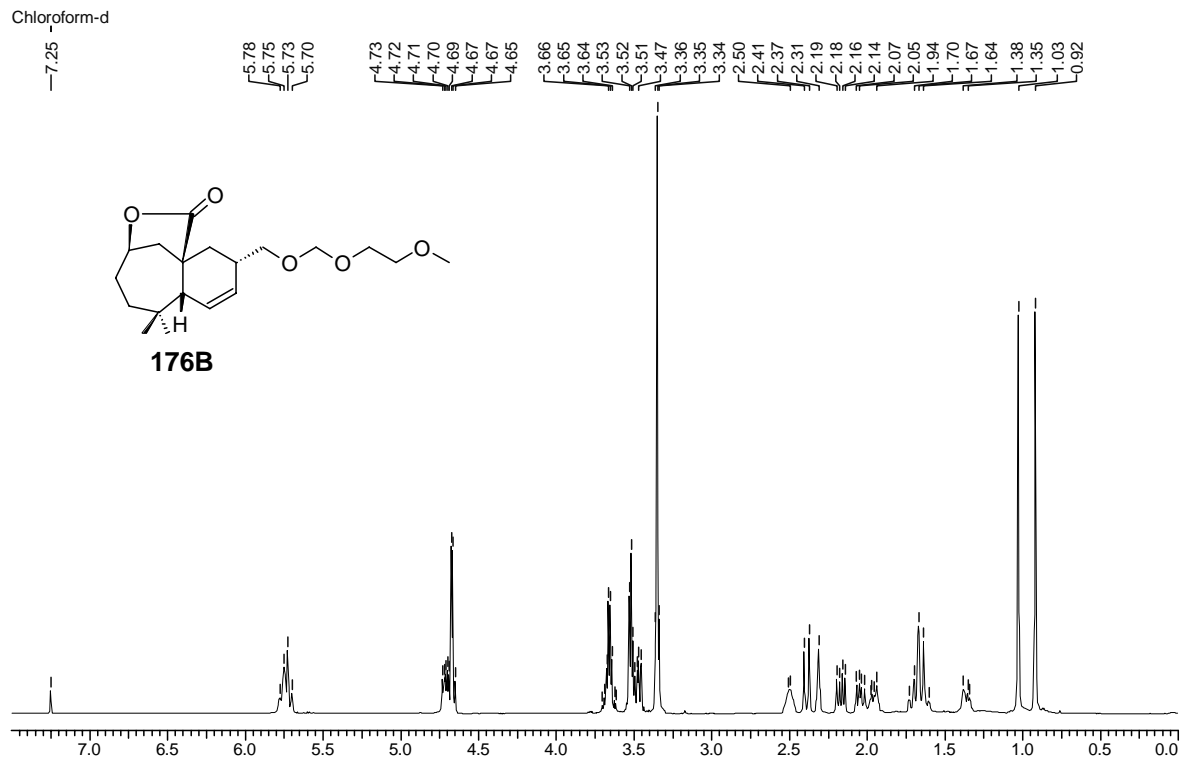


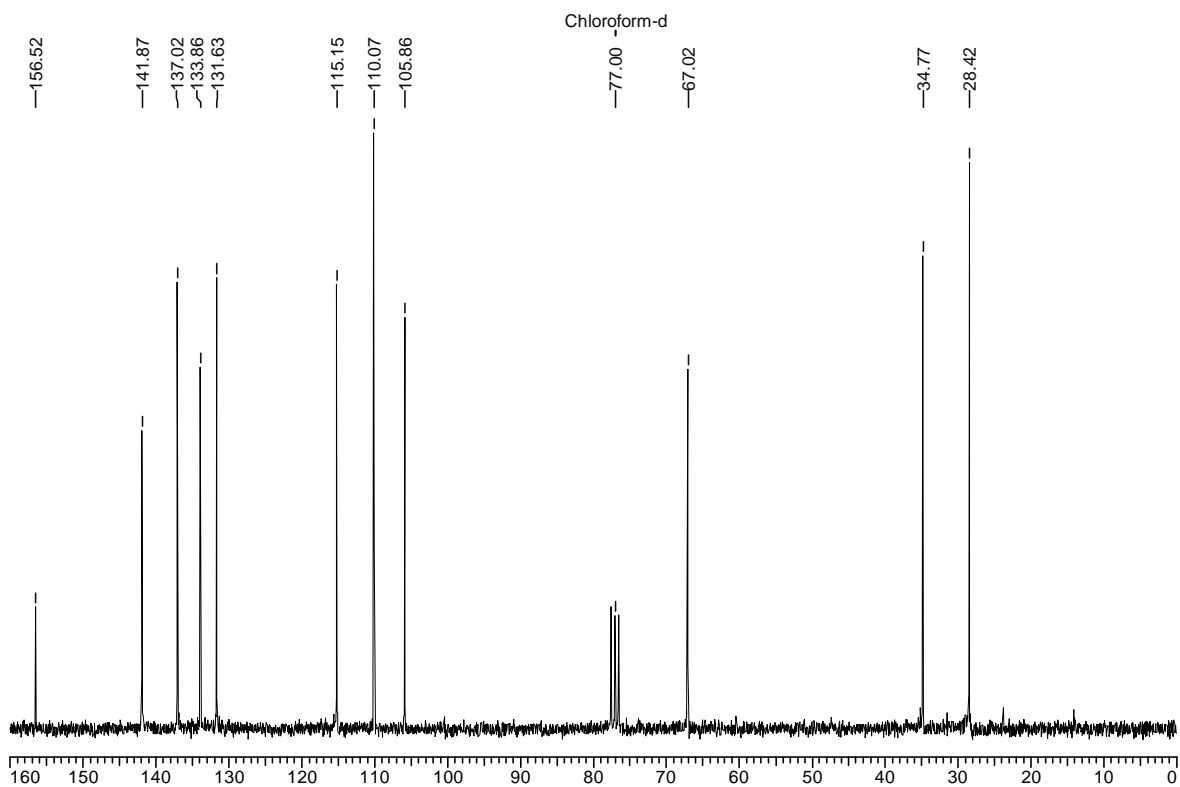
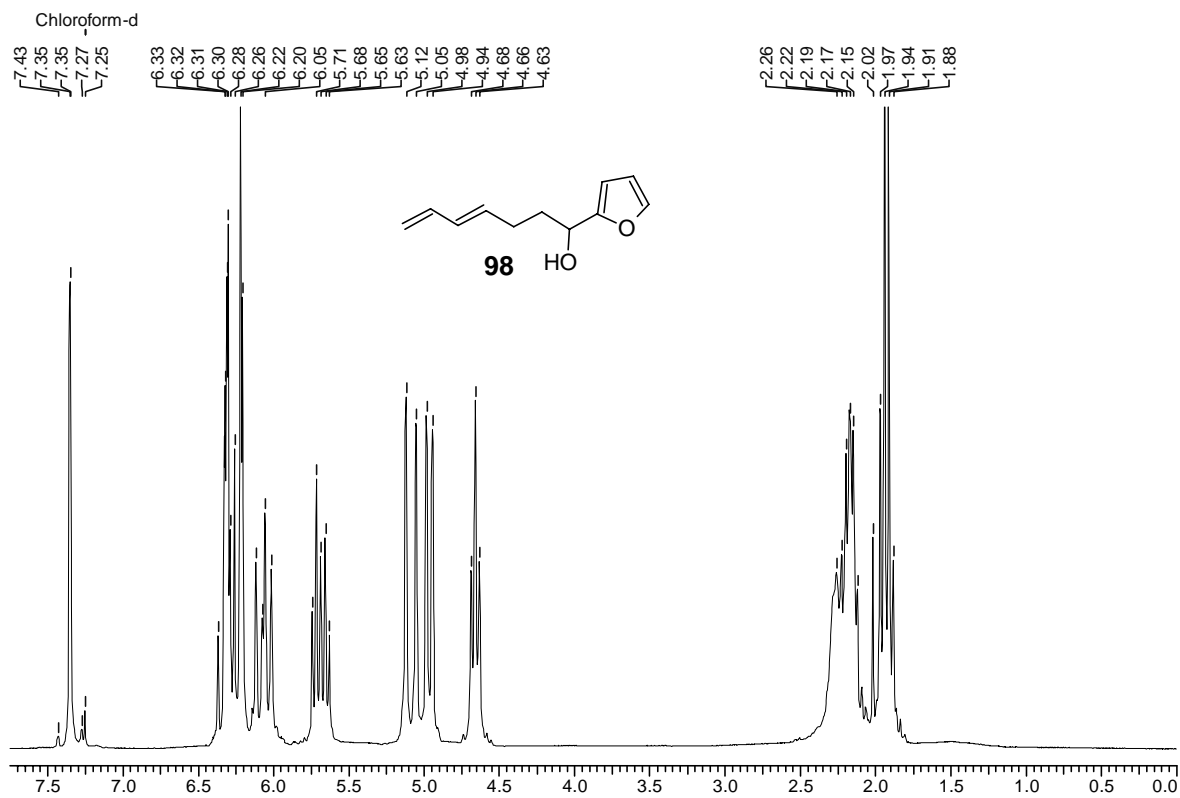


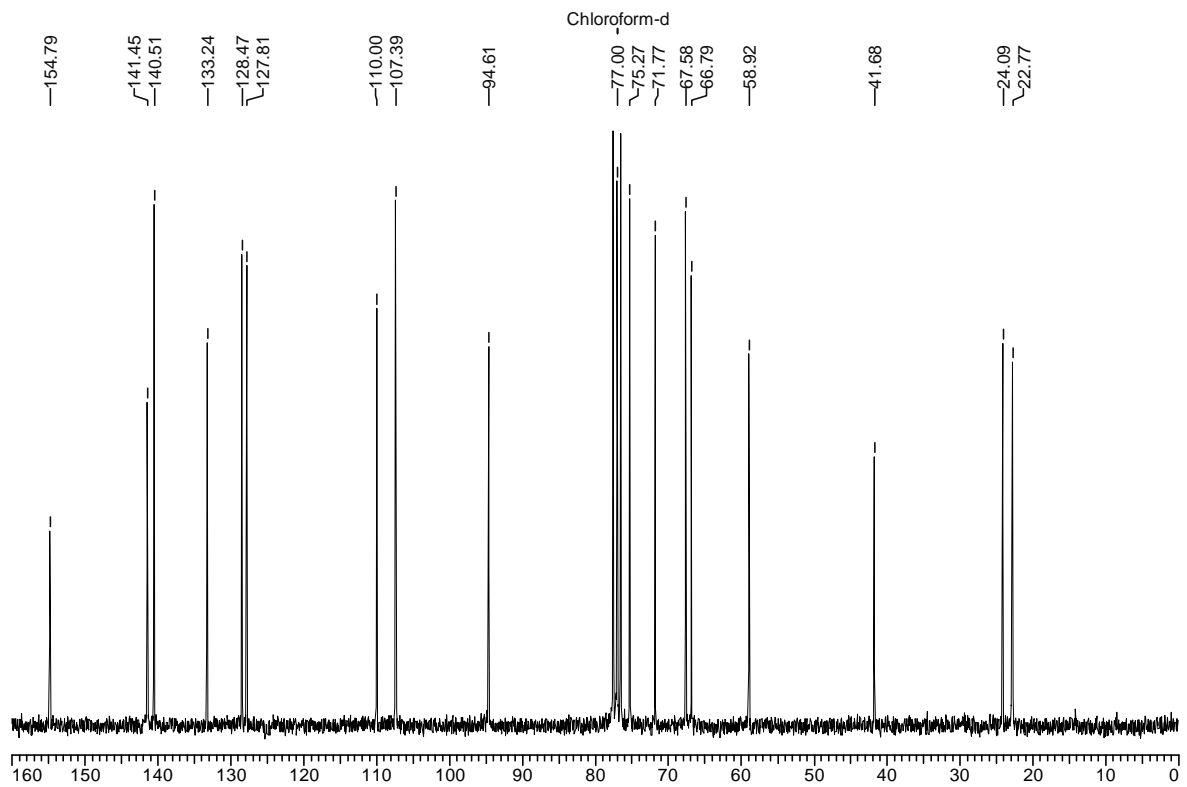
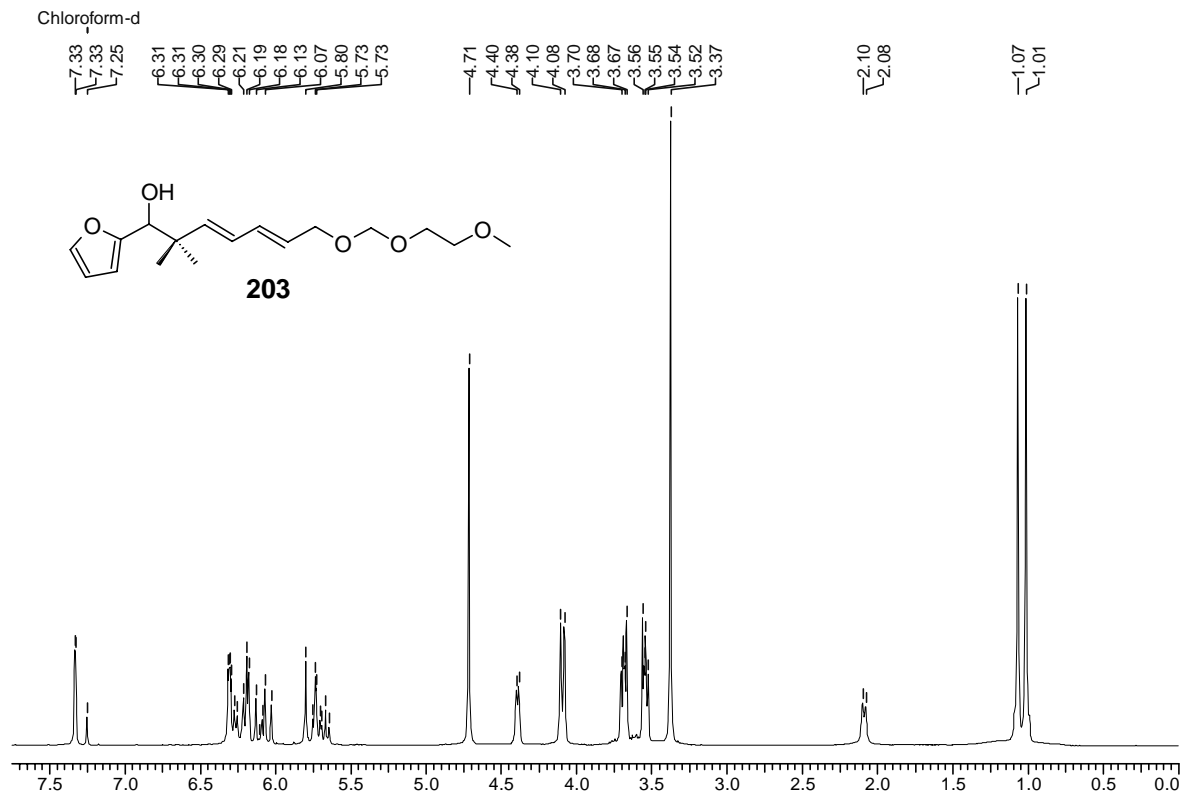


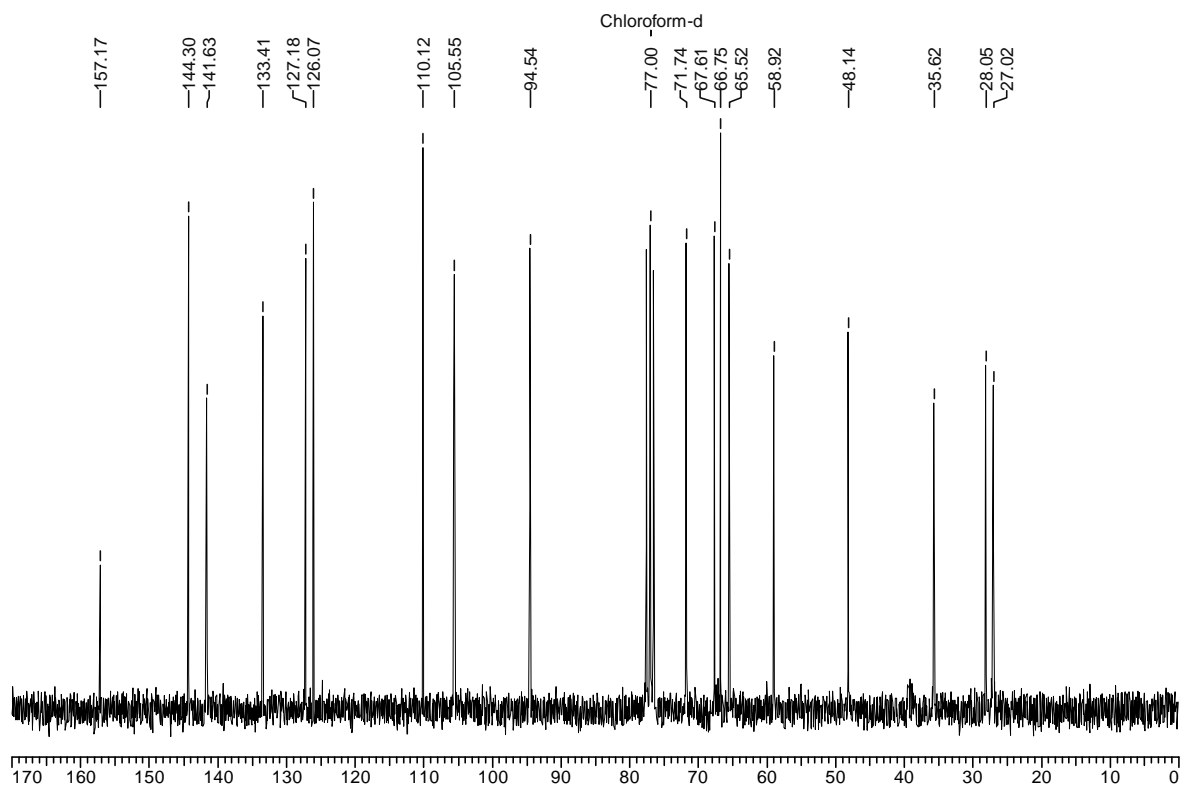
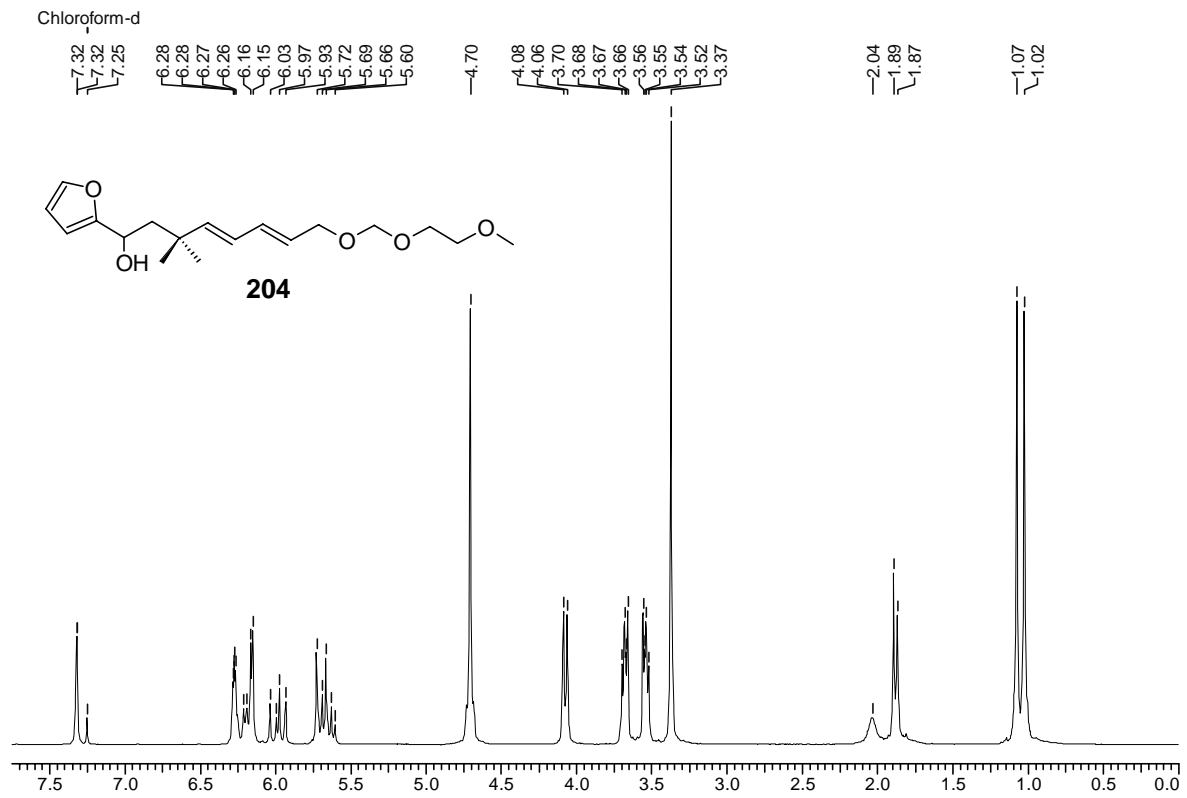


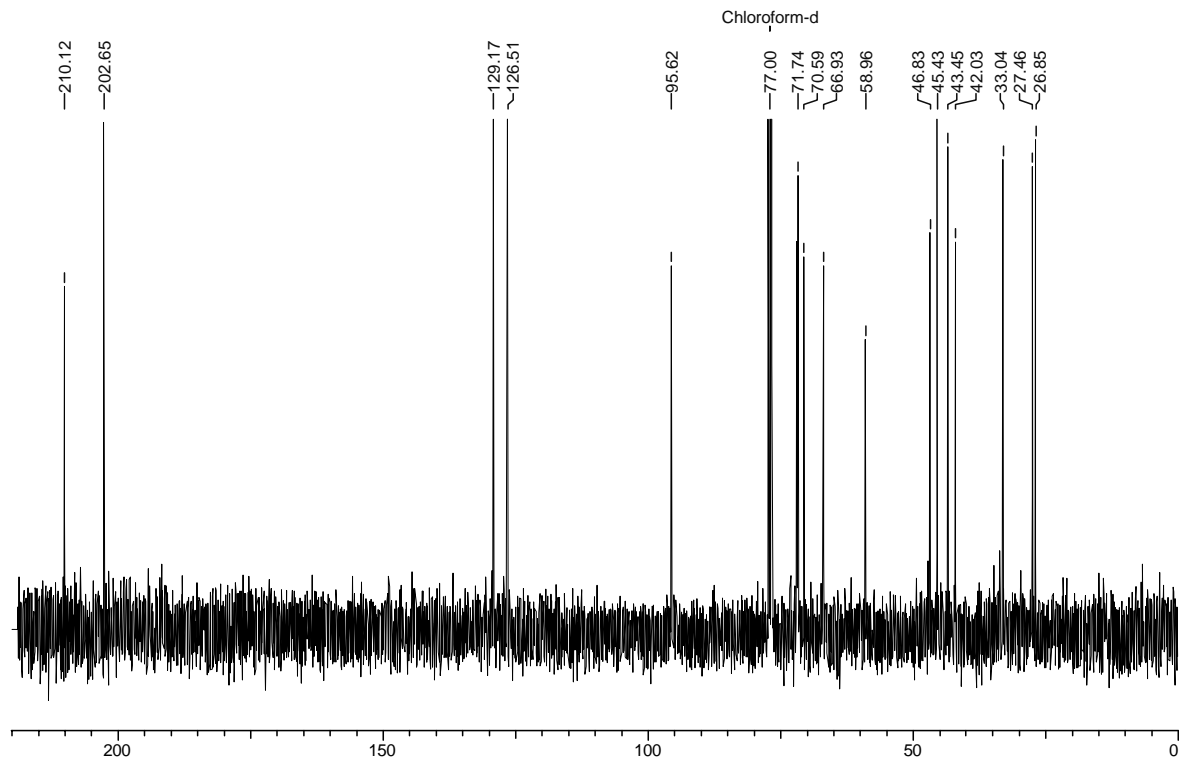
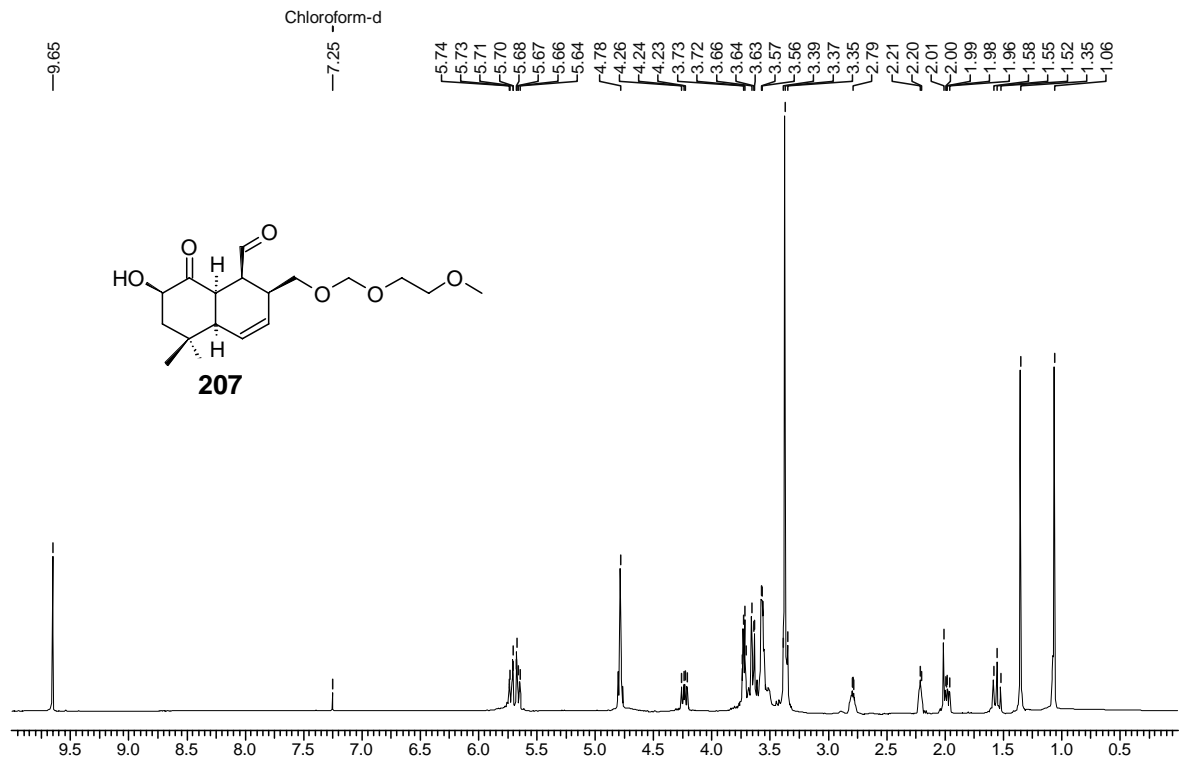












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