BEILSTEIN JOURNAL OF ORGANIC CHEMISTRY

Supporting Information

for

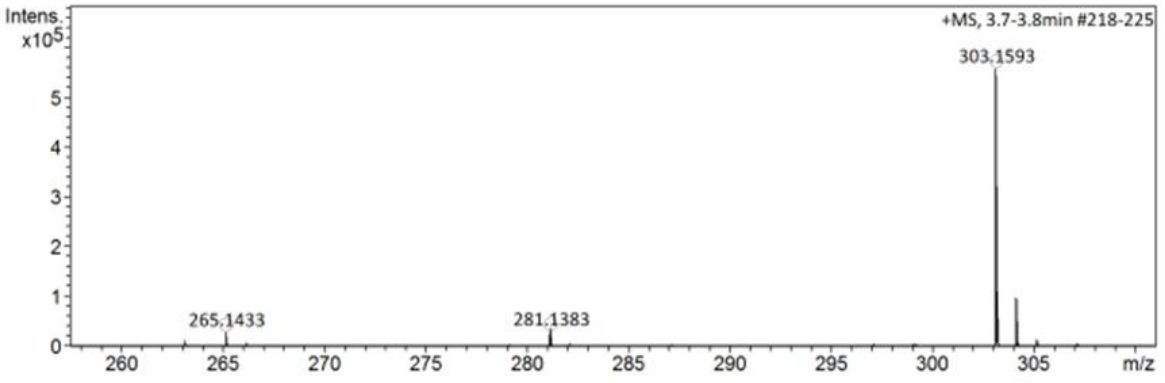
Melifoliox B, a novel phloroglucin derivative isolated from *Melicope barbigera* (Rutaceae) and synthesis of new oxidation products from melifoliones A and B

Horst Weber, Kim-Thao Tran-Cong, Bernhard Mayer, Guido J. Reiss, Iryna S. Konovalova, Marc S. Appelhans, Kenneth R. Wood and Claus M. Passreiter

Beilstein J. Org. Chem. **2026,** *22,* 535–546. doi:10.3762/bjoc.22.39

Copies of the HRESIMS, ^{1}H and ^{13}C NMR spectra

Table of content



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule
265.1433	1	C15H21O4	265.1434	0.4	6.7	1	100.00	5.5	even	ok
	2	C16H17N4	265.1448	5.5	9.0	2	47.00	10.5	even	ok
281.1383	1	C15H21O5	281.1384	0.3	6.6	1	100.00	5.5	even	ok
	2	C16H17N4O	281.1397	5.1	20.4	2	37.71	10.5	even	ok
303.1593	1	C18H23O4	303.1591	-0.8	13.2	1	100.00	7.5	even	ok

Figure S1. HRESIMS of compound **1+2**.

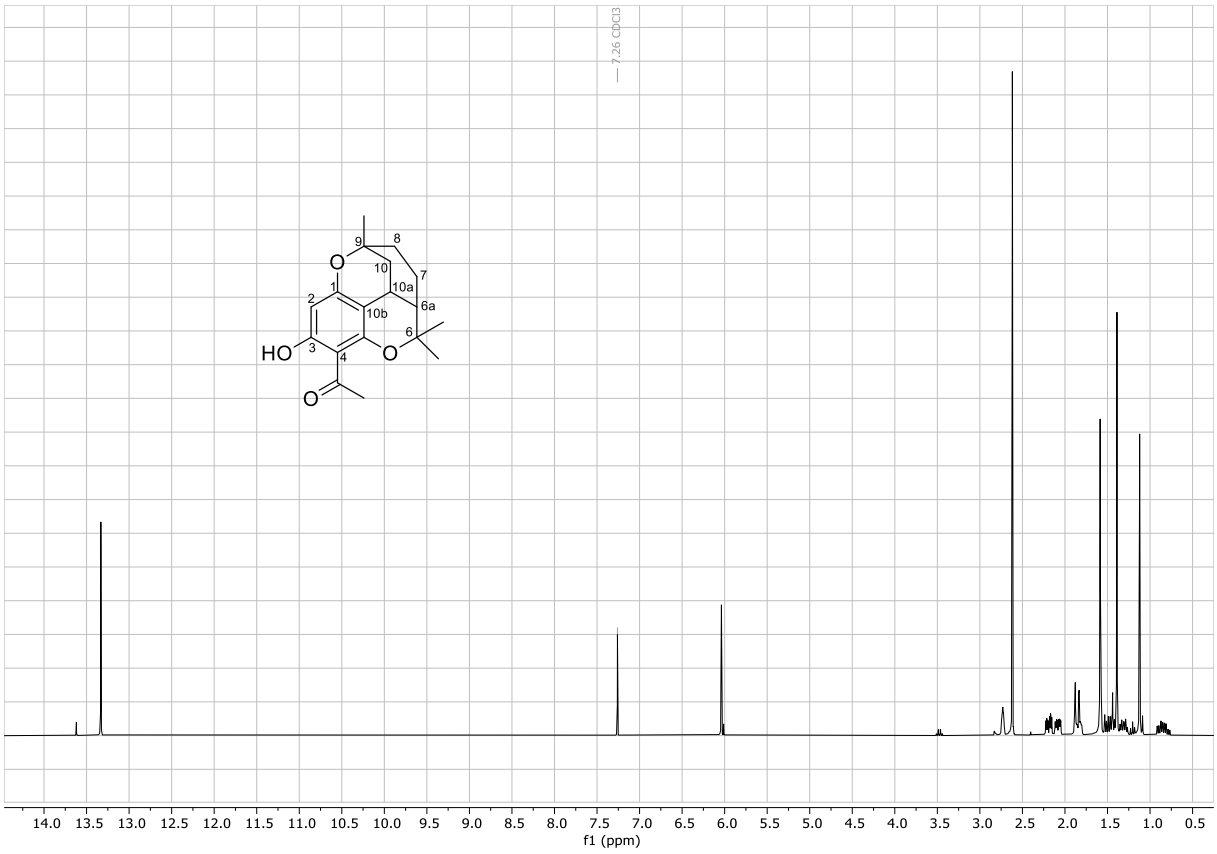


Figure S2. ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of compound **1.**

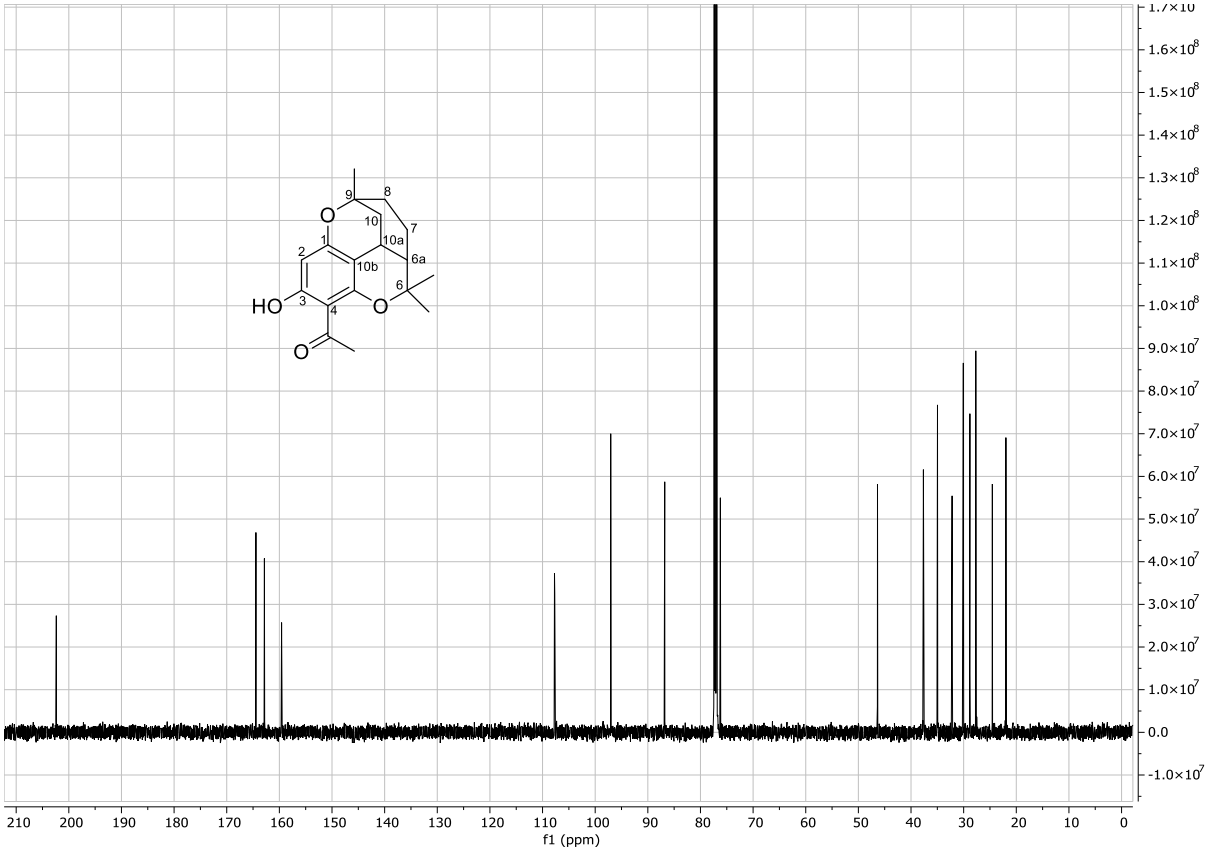


Figure S3. ^{13}C NMR (150 MHz, $CDCl_3$) spectrum of compound **1.**

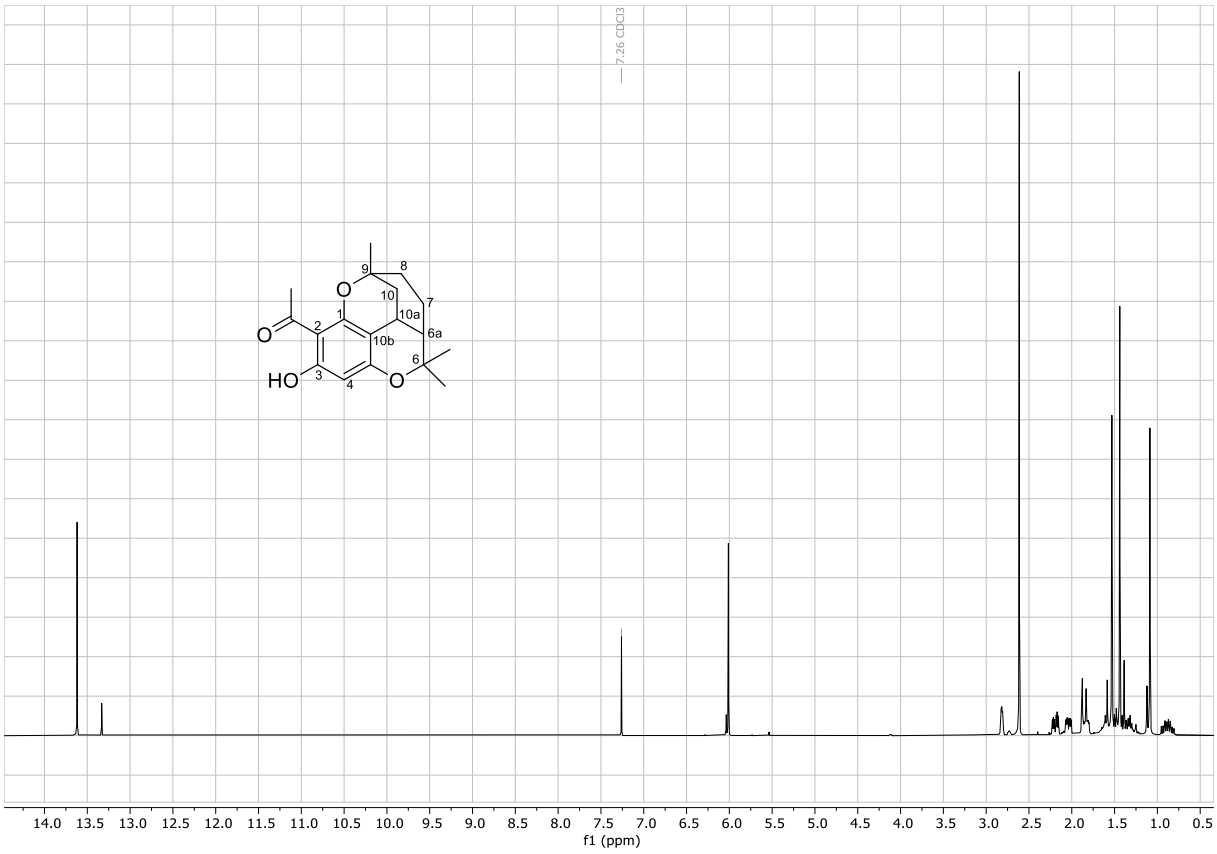


Figure S4. ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of compound **2.**

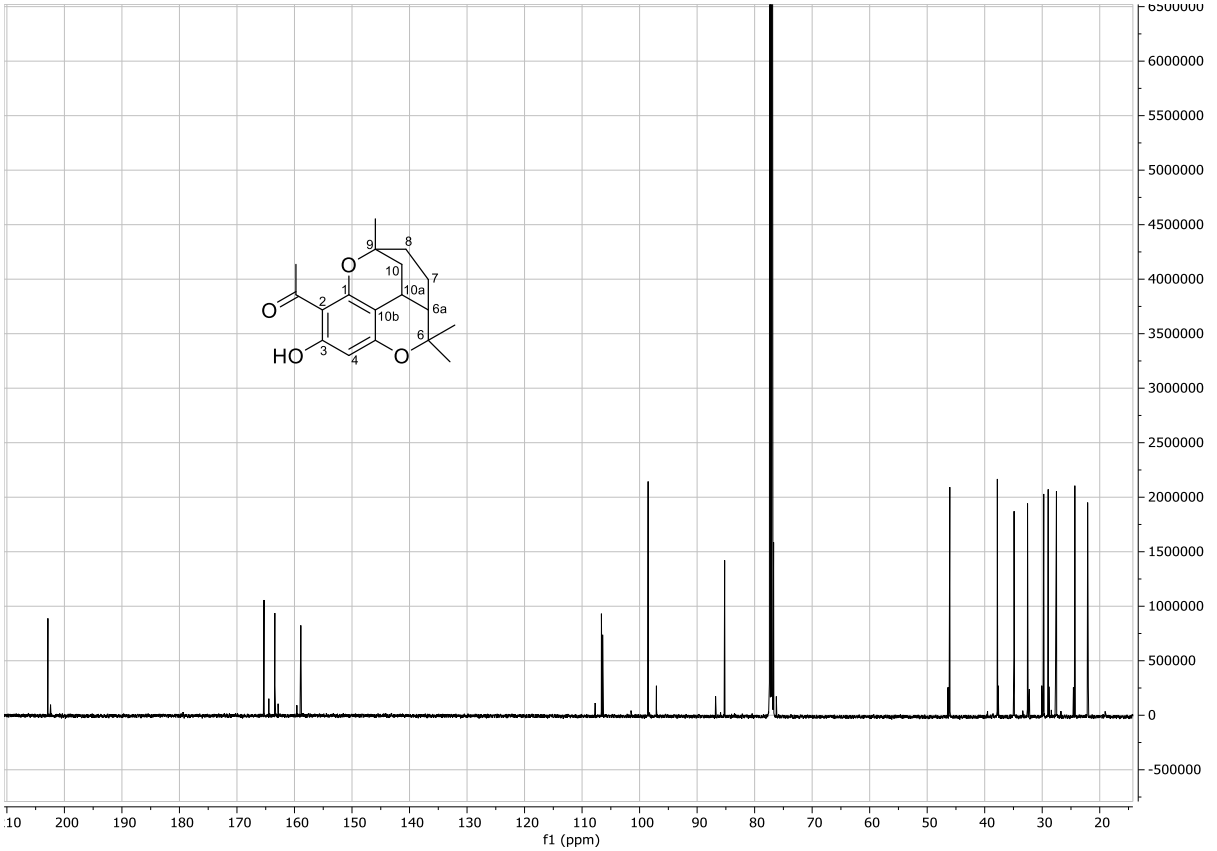
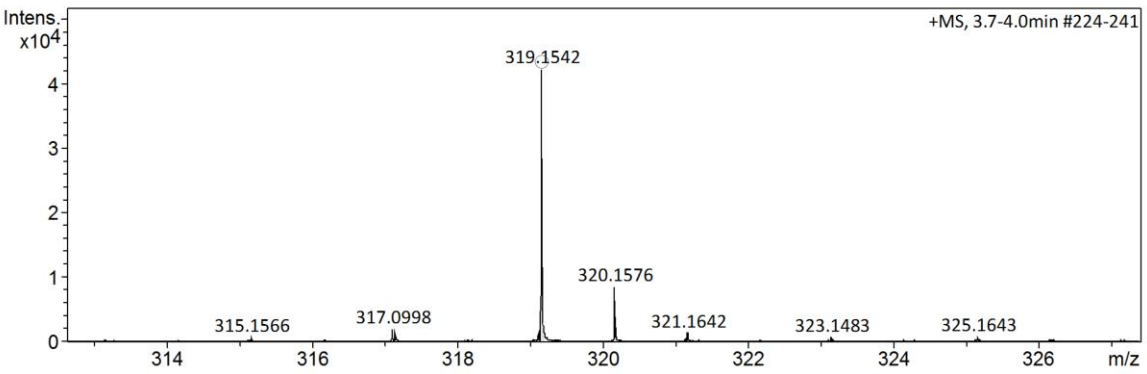


Figure S5. ^{13}C NMR (150 MHz, $CDCl_3$) spectrum of compound **2.**



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¯ Conf	N-Rule
319.1542	1	C18H23O5	319.1540	-0.6	0.8	1	100.00	7.5	even	ok
	2	C19H19N4O	319.1553	3.6	13.0	2	49.11	12.5	even	ok

Figure S6. HRESIMS of compound **4**.

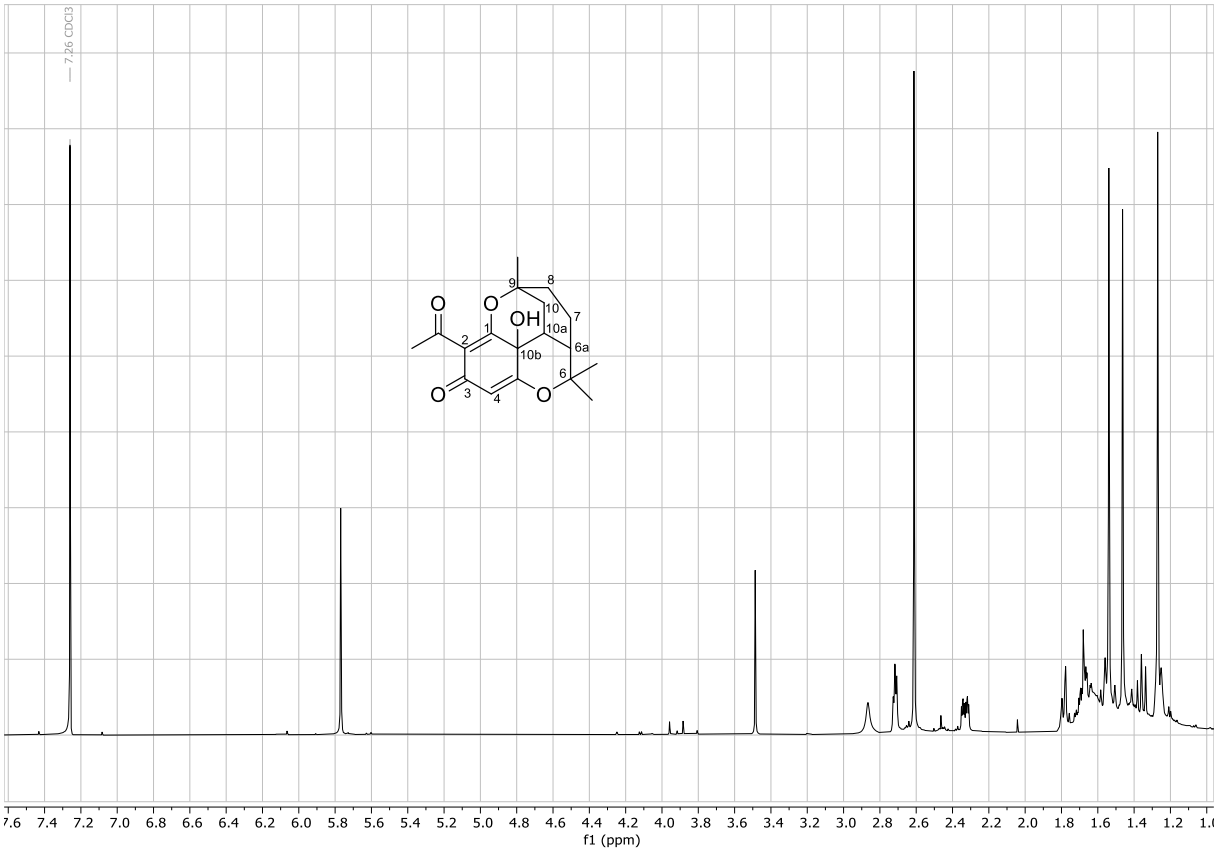


Figure S7. ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of compound **4.**

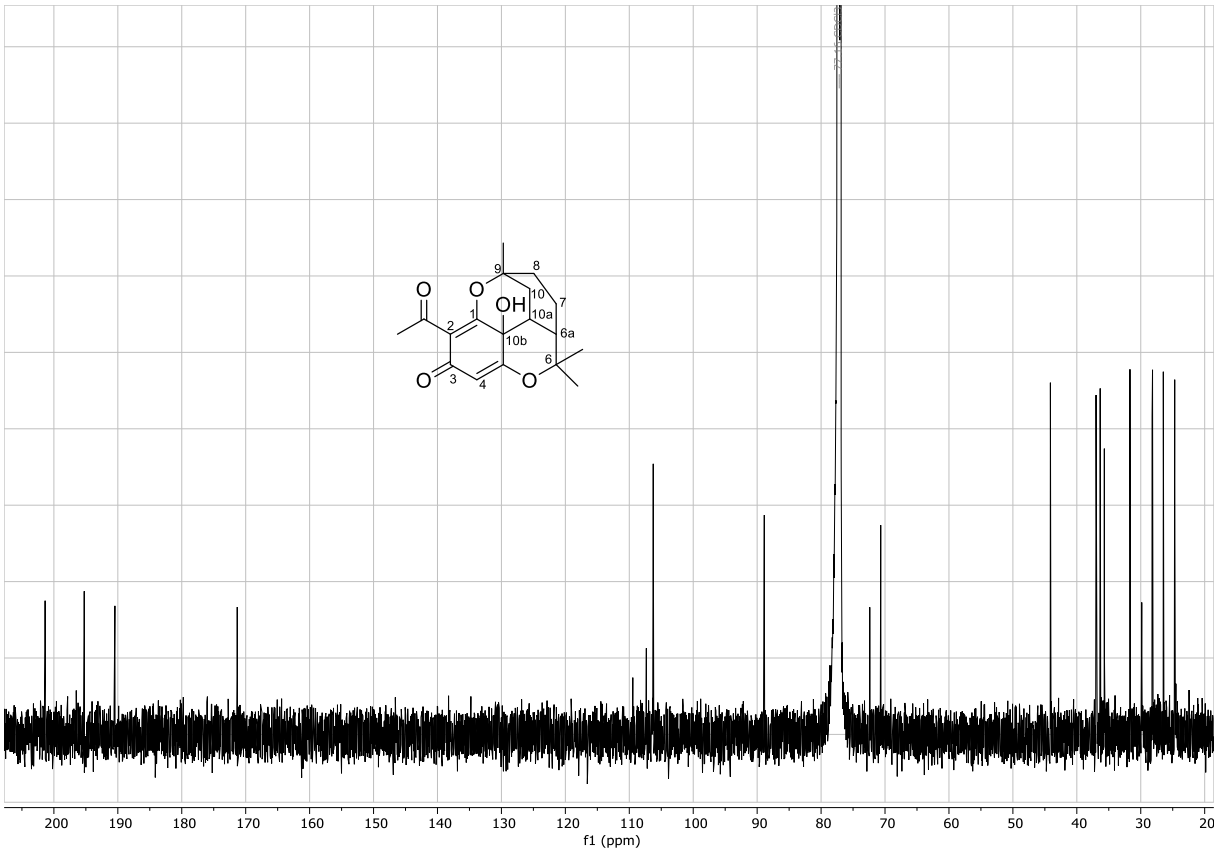
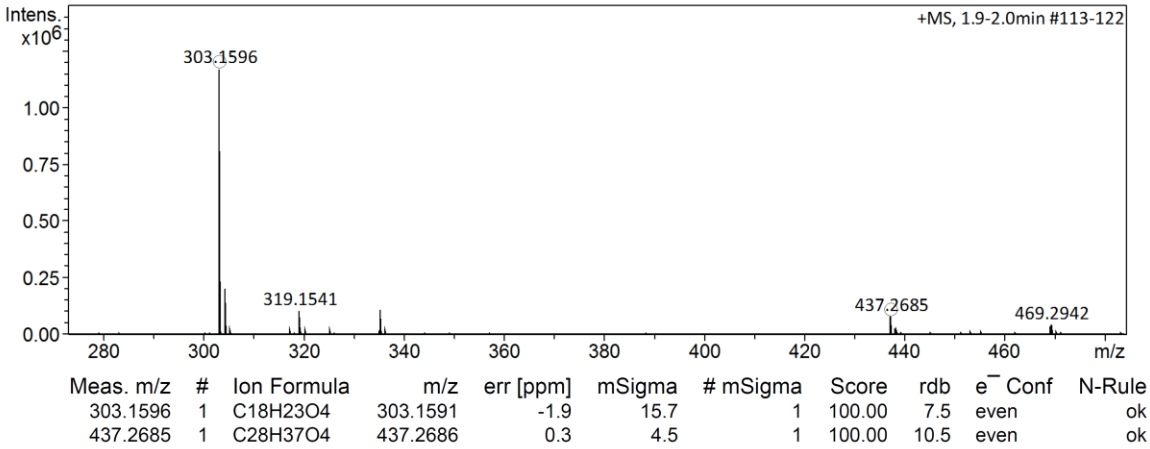
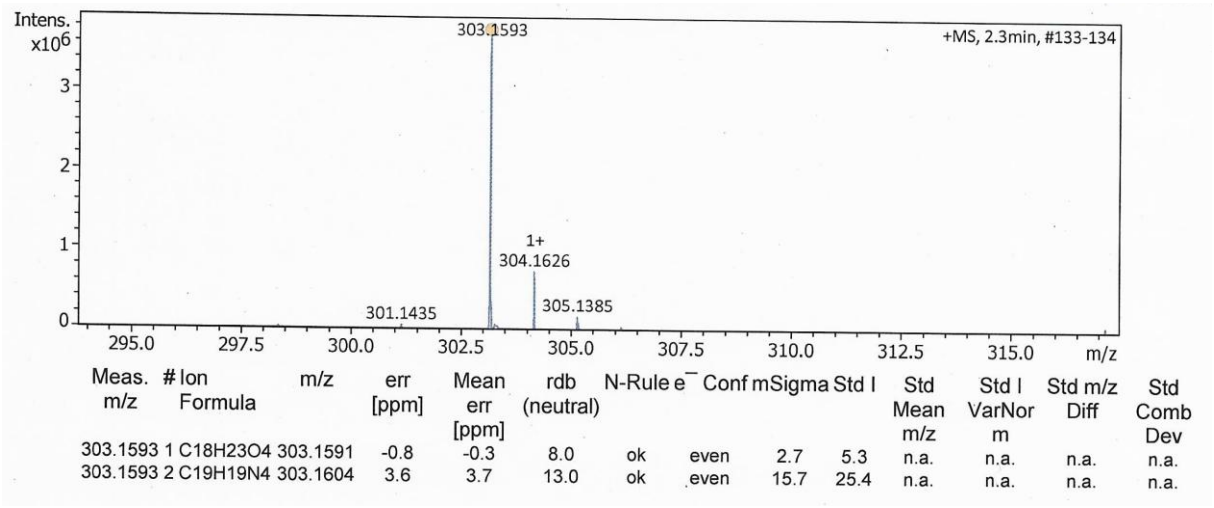


Figure S8. ^{13}C NMR (150 MHz, $CDCl_3$) spectrum of compound **4.**



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¯ Conf	N-Rule
303.1596	1	C18H23O4	303.1591	-1.9	15.7	1	100.00	7.5	even	ok
437.2685	1	C28H37O4	437.2686	0.3	4.5	1	100.00	10.5	even	ok

Figure S9. HRESIMS of compound **5.**



Meas. m/z	#	Ion Formula	m/z	err [ppm]	Mean err [ppm]	rdb	N-Rule	e⁻ Conf	mSigma	Std I	Std Mean m/z	Std I VarNorm	Std m/z Diff	Std Comb Dev
303.1593	1	C18H23O4	303.1591	-0.8	-0.3	8.0	ok	even	2.7	5.3	n.a.	n.a.	n.a.	n.a.
303.1593	2	C19H19N4	303.1604	3.6	3.7	13.0	ok	even	15.7	25.4	n.a.	n.a.	n.a.	n.a.

Figure S10. HRESIMS of compound **6**.

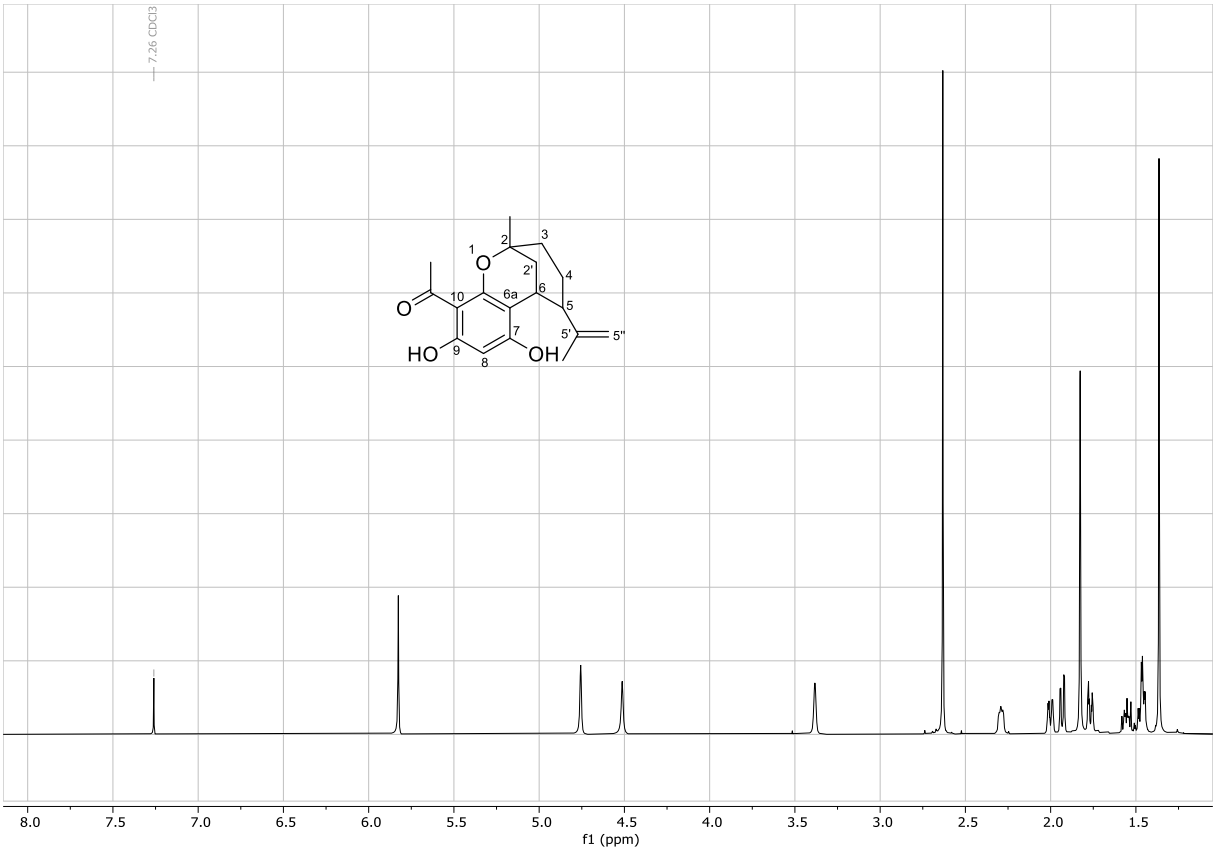


Figure S11. ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of compound **6.**

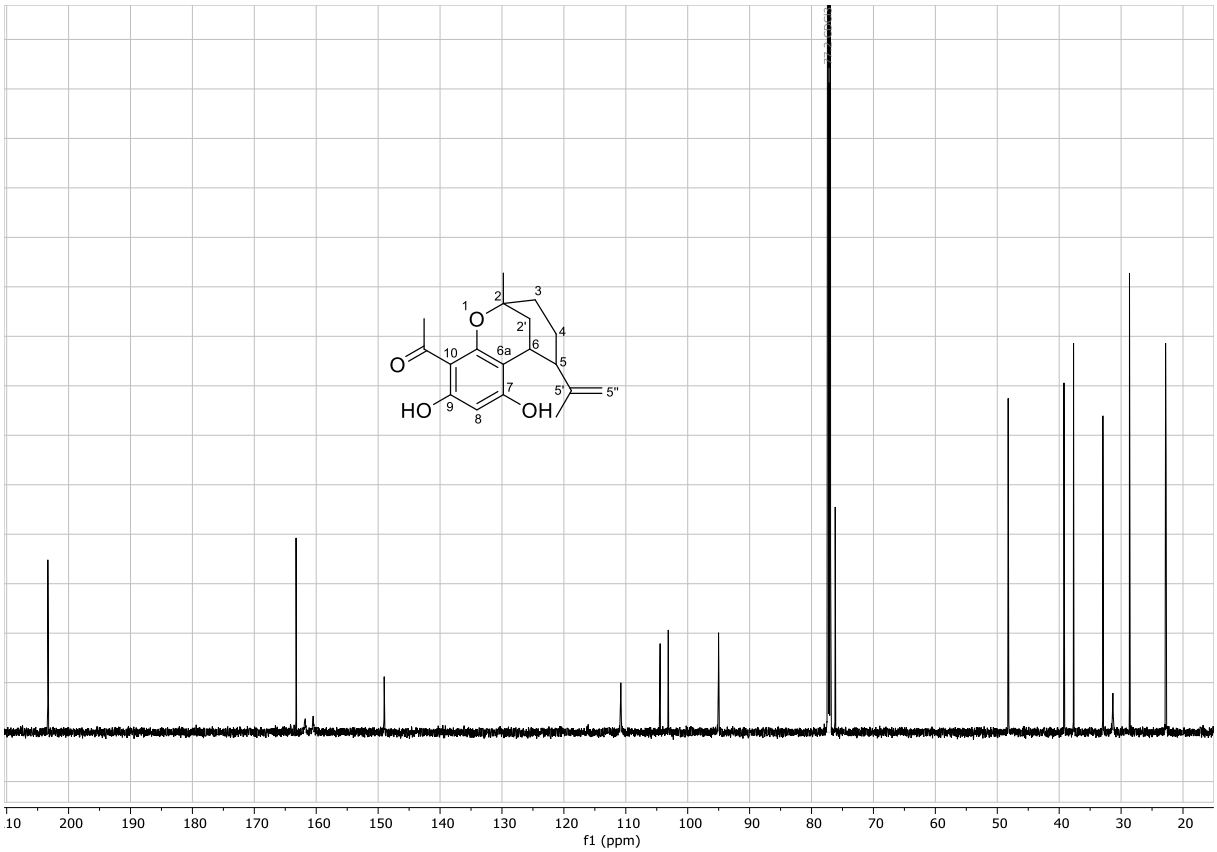
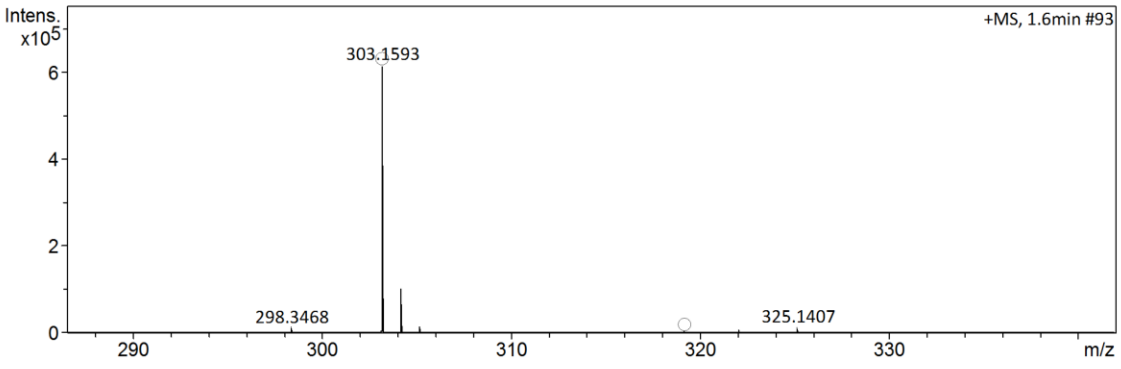


Figure S12. ^{13}C NMR (150 MHz, $CDCl_3$) spectrum of compound **6.**



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¯ Conf	N-Rule
303.1593	1	C18H23O4	303.1591	-0.8	18.4	1	100.00	7.5	even	ok
	2	C17H20N4Na	303.1580	-4.3	19.2	2	55.70	9.5	even	ok
	3	C19H19N4	303.1604	3.6	31.6	3	47.68	12.5	even	ok
319.1537	1	C19H19N4O	319.1553	5.1	15.0	1	55.73	12.5	even	ok
	2	C17H20N4NaO	319.1529	-2.4	19.3	2	86.19	9.5	even	ok
	3	C18H23O5	319.1540	0.9	23.2	3	100.00	7.5	even	ok

Figure S13. HRESIMS of compound **7**.

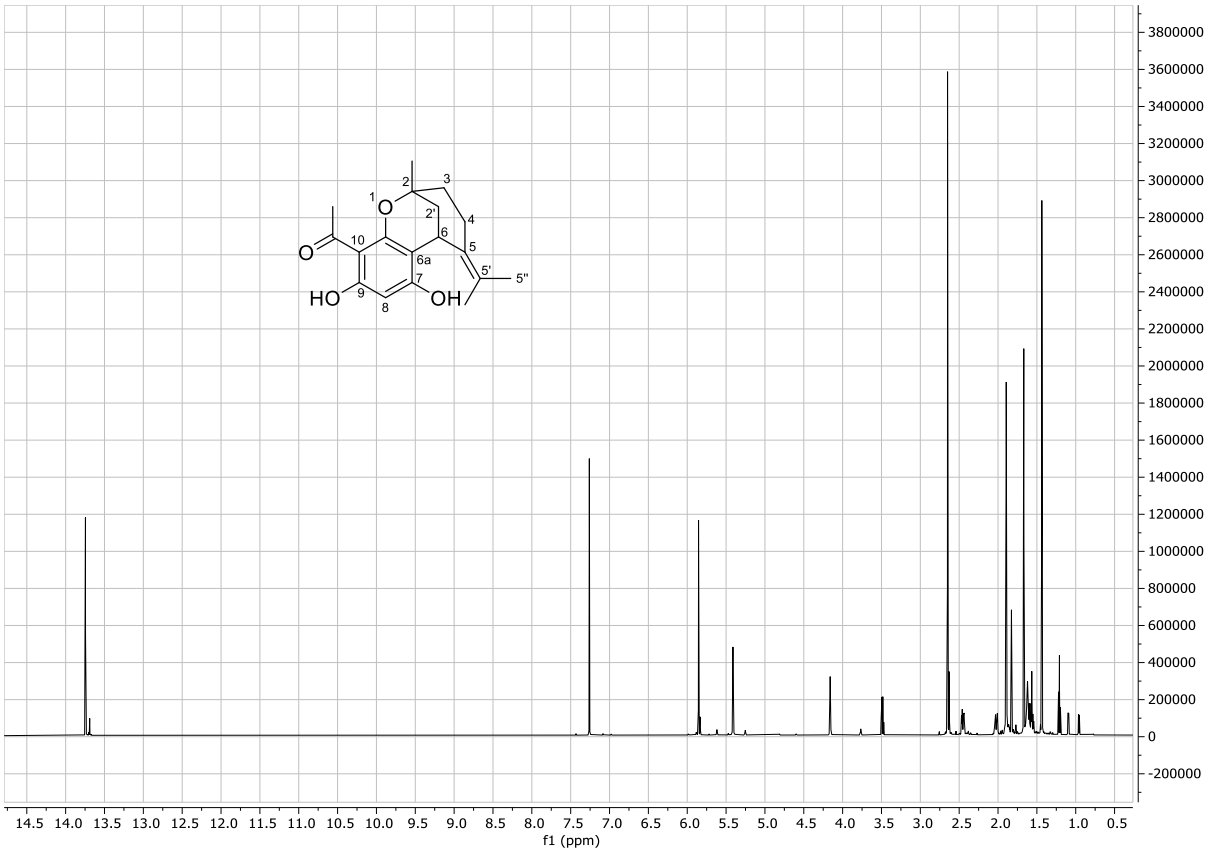


Figure S14. ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of compound **7.**

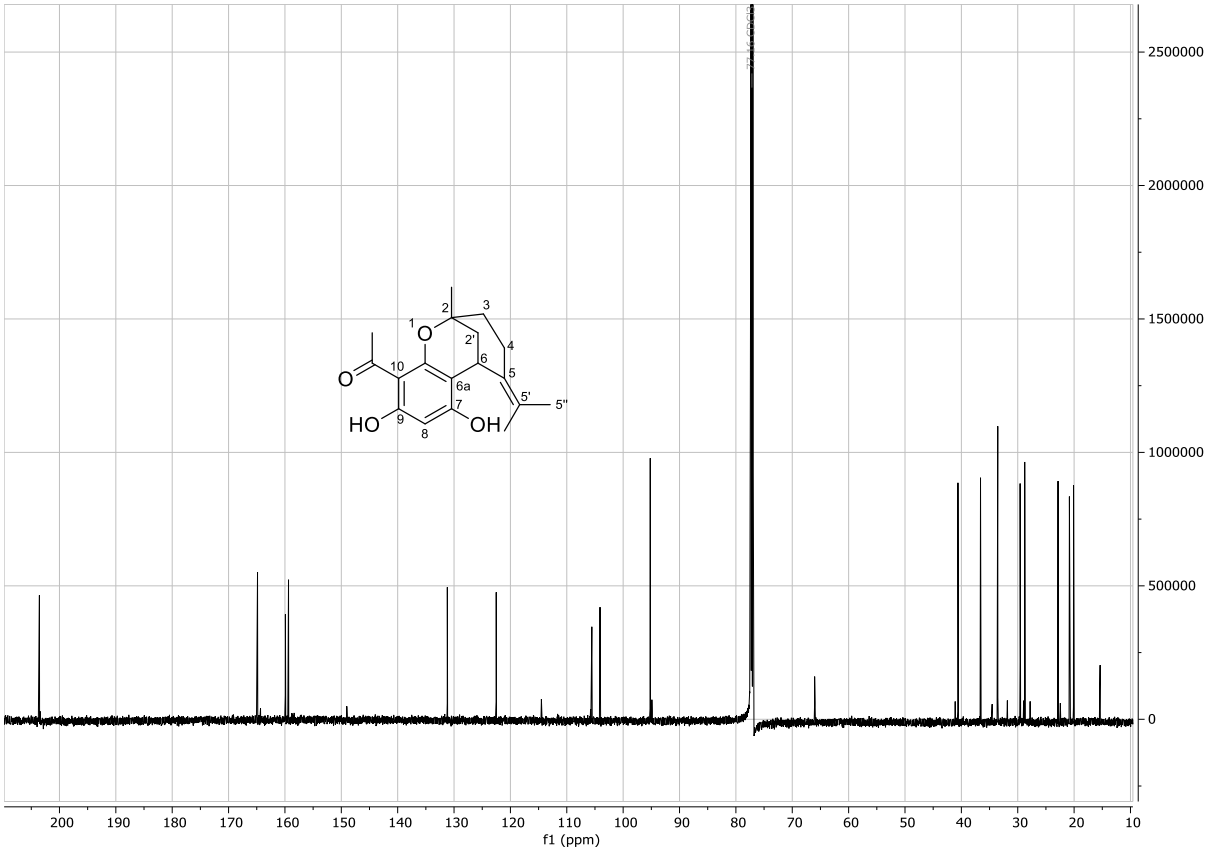
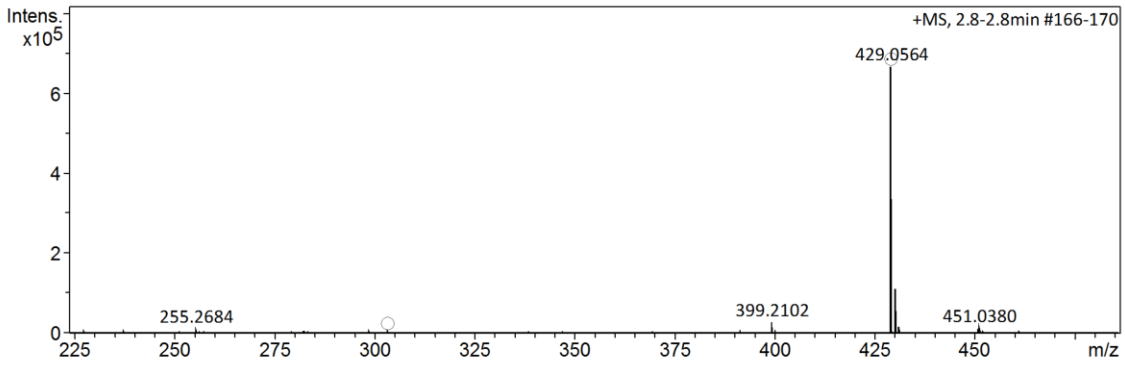


Figure S15. ^{13}C NMR (150 MHz, $CDCl_3$) spectrum of compound **7.**



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¯ Conf	N-Rule
303.1591	1	C18H23O4	303.1591	-0.1	15.6	1	100.00	7.5	even	ok
	2	C19H19N4	303.1604	4.4	19.6	2	47.19	12.5	even	ok
429.0564	1	C18H22IO4	429.0557	-1.6	17.9	1	100.00	7.5	even	ok
	2	C19H18IN4	429.0571	1.5	31.2	2	74.15	12.5	even	ok
	3	C19H13N2O10	429.0565	0.2	31.3	3	97.57	14.5	even	ok
	4	C17HN16	429.0565	0.1	43.1	4	71.73	25.5	even	ok

Figure S16. HRESIMS of compound **8+9**.

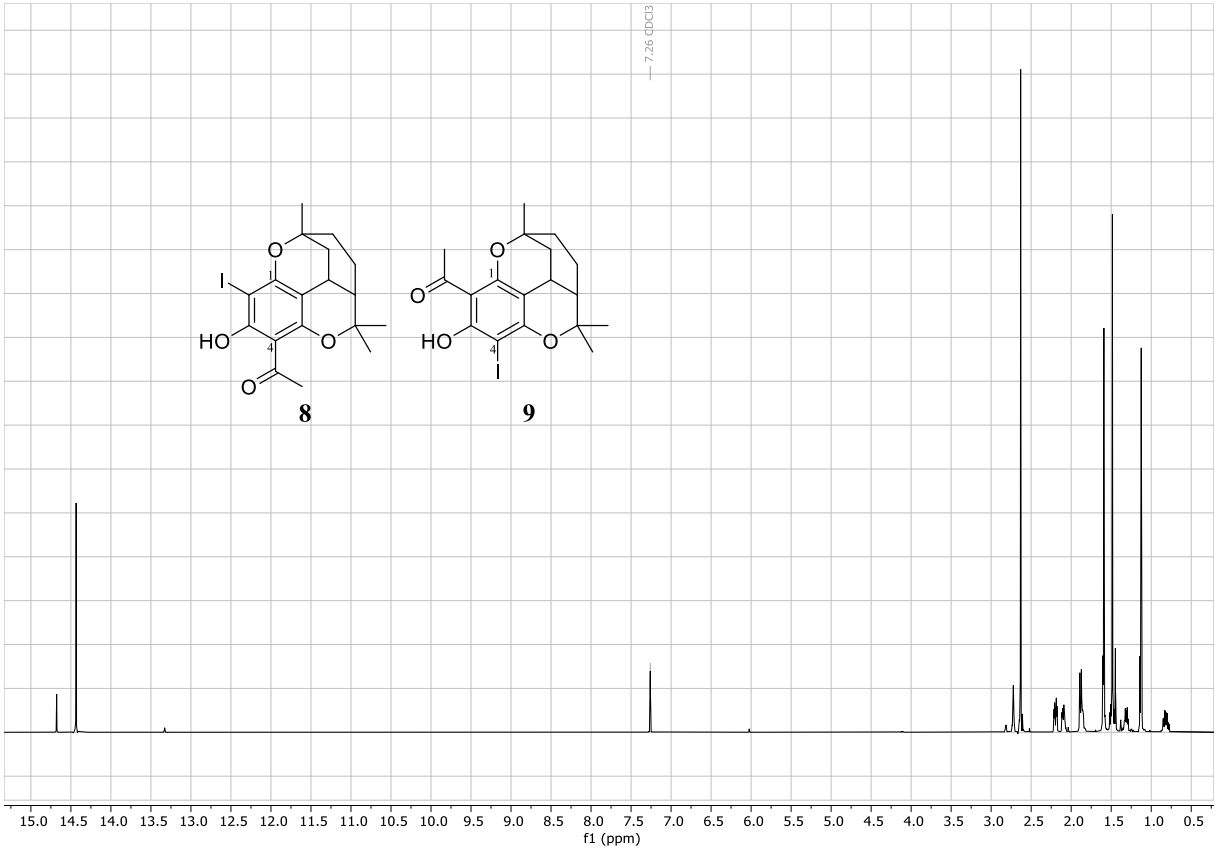


Figure S17. ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of compound **8+9.**

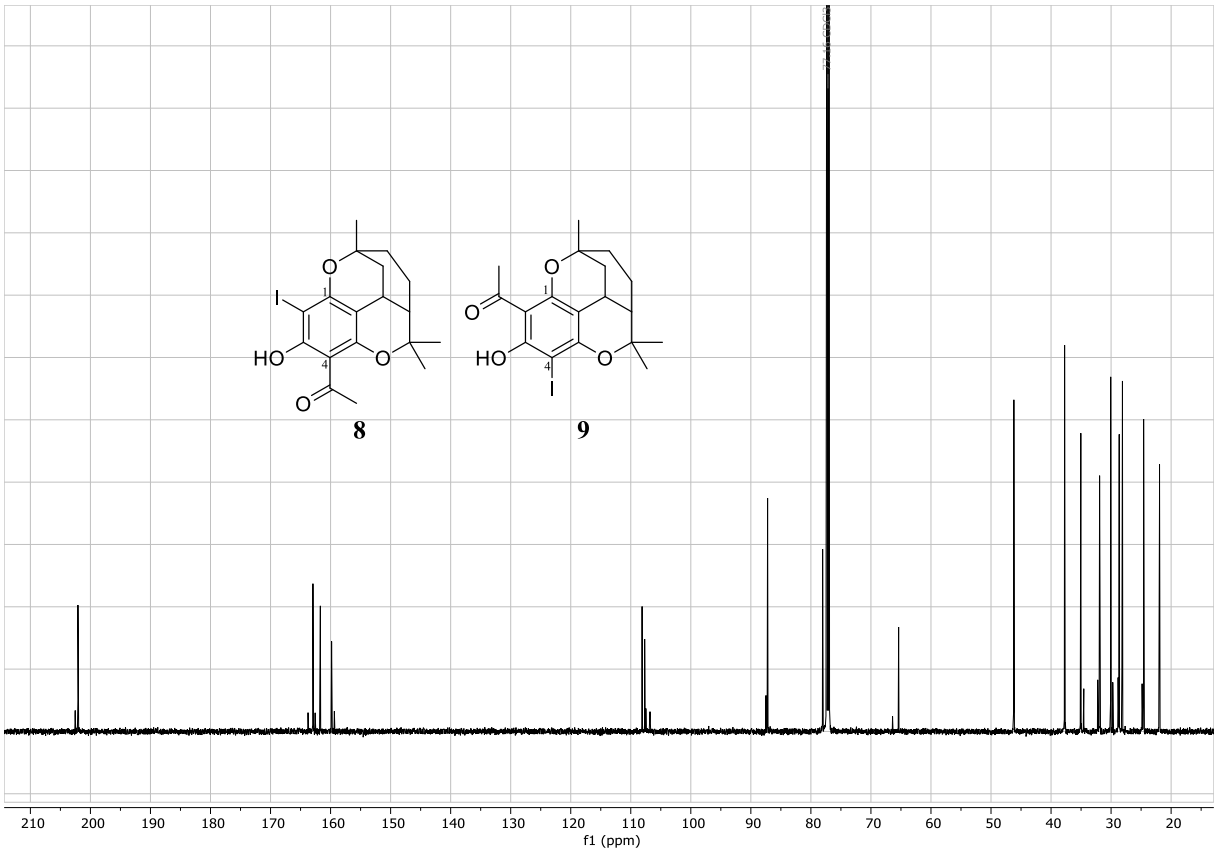
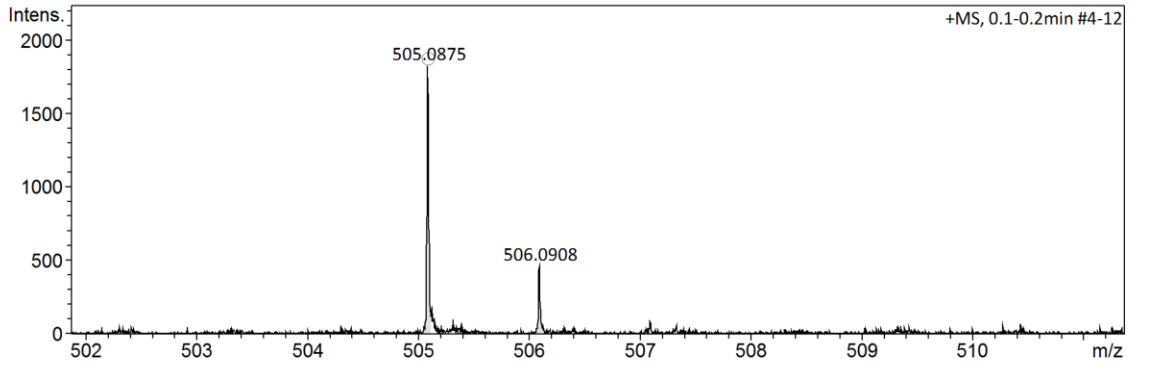


Figure S18. ^{13}C NMR (150 MHz, $CDCl_3$) spectrum of compound **8+9.**



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¯ Conf	N-Rule
505.0875	1	C24H26IO4	505.0870	-0.9	25.3	1	87.70	11.5	even	ok
	2	C25H22IN4	505.0884	1.8	31.4	2	59.59	16.5	even	ok
	3	C22H9N12O4	505.0864	-2.1	33.6	3	52.17	24.5	even	ok
	4	C25H17N2O10	505.0878	0.6	34.2	4	100.00	18.5	even	ok
	5	C23H5N16	505.0878	0.6	42.4	5	60.48	29.5	even	ok

Figure S19. HRESIMS of compound **10**.

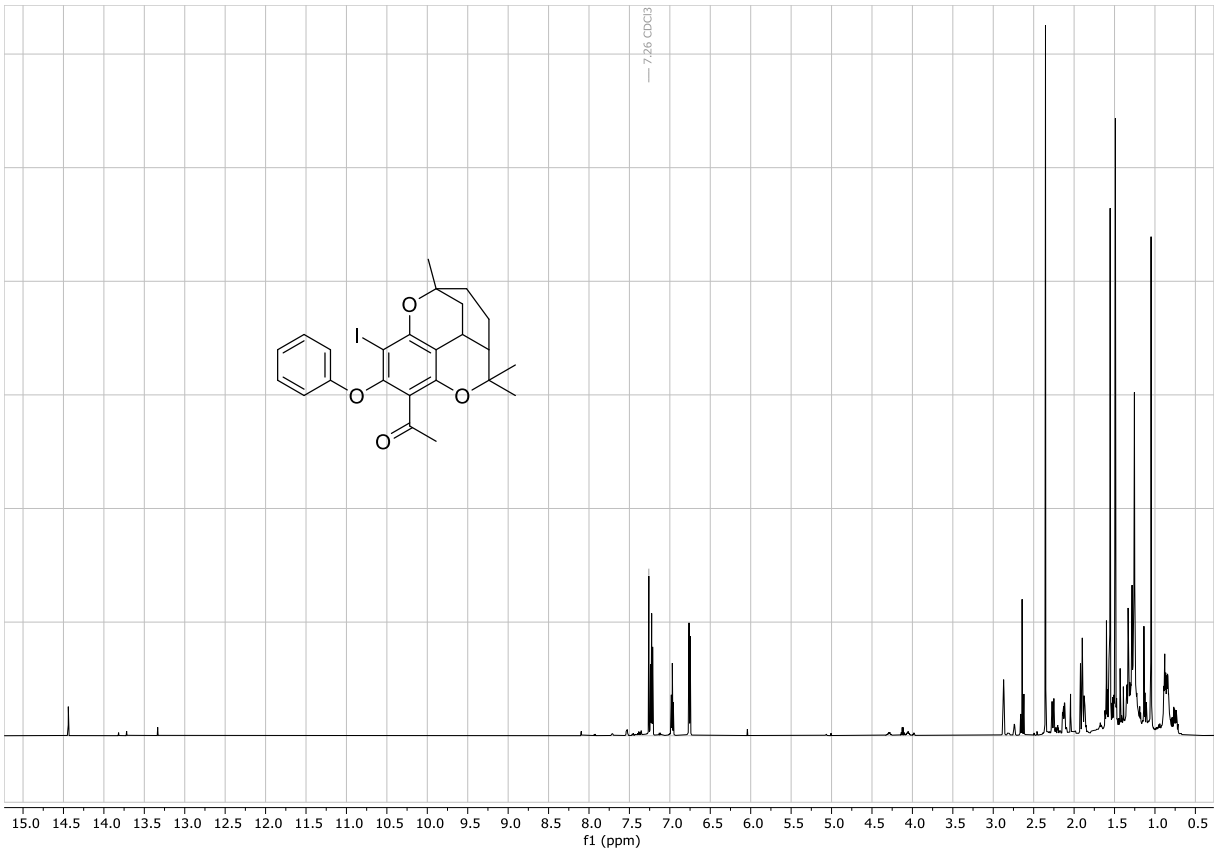
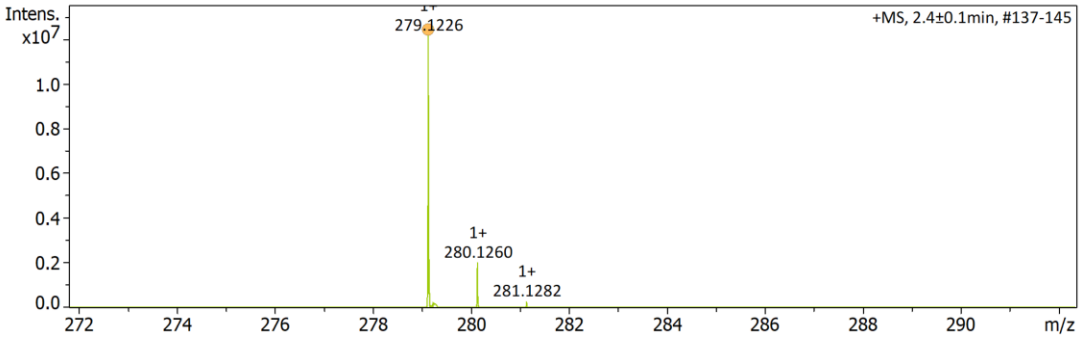


Figure S20. ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of compound **10.**



Meas. m/z	#	Ion Formula	m/z	err [ppm]	Mean err [ppm]	rdb (neutral)	N-Rule	e⁻ Conf	mSigma	Std I	Std Mean m/z	Std I VarNorm	Std m/z Diff	Std Comb Dev
279.1226	1	C15H19O5	279.1227	0.2	0.3	7.0	ok	even	1.3	2.8	n.a.	n.a.	n.a.	n.a.
279.1226	2	C16H15N4O	279.1240	5.0	4.6	12.0	ok	even	14.1	23.6	n.a.	n.a.	n.a.	n.a.

Figure S21. HRESIMS of compound **11**.

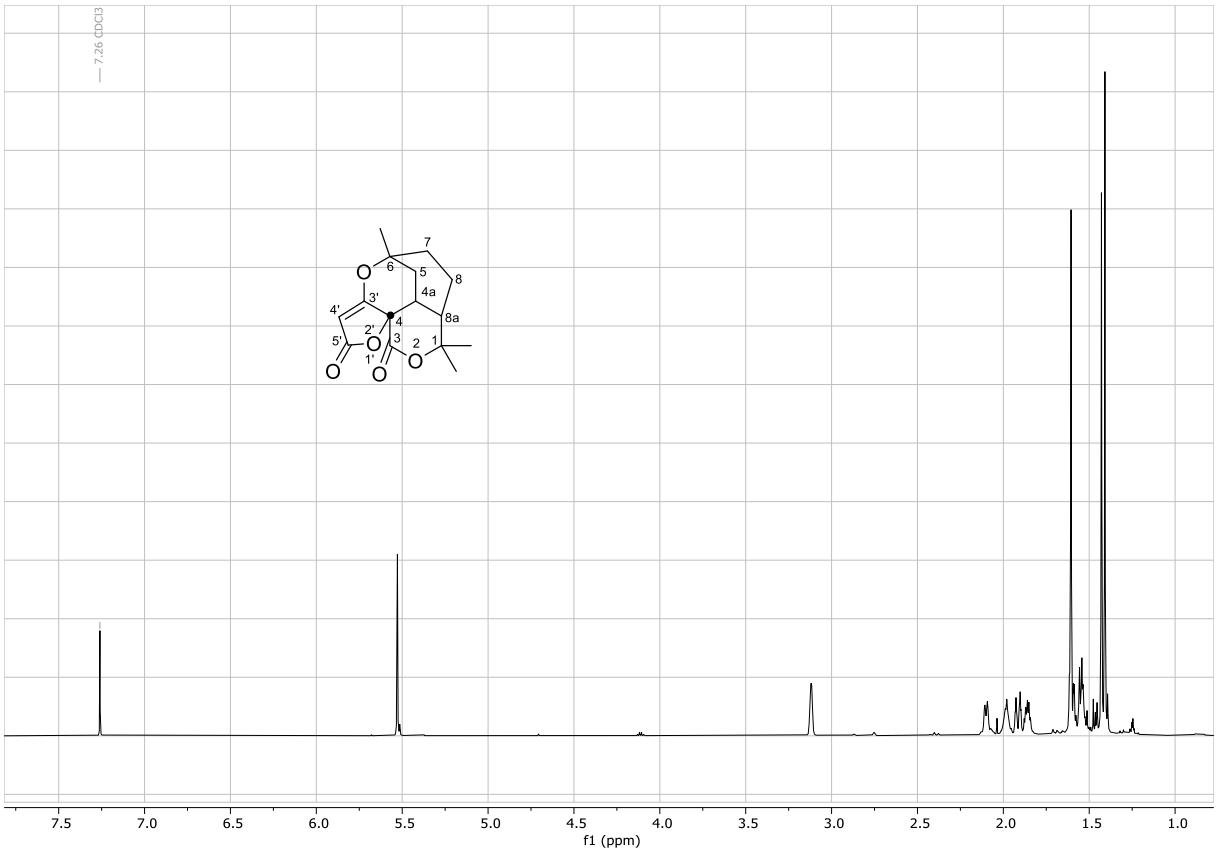


Figure S22. ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of compound **11.**

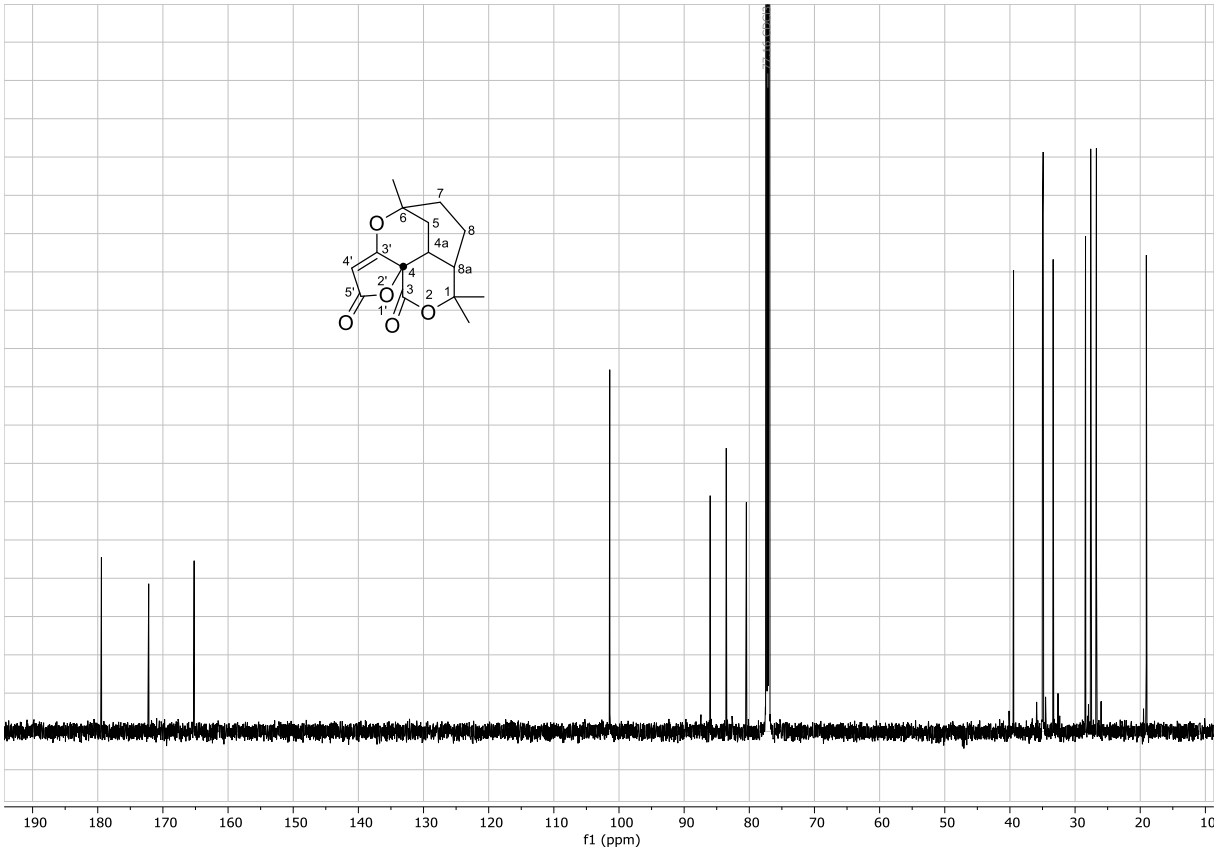


Figure S23. ^{13}C NMR (150 MHz, $CDCl_3$) spectrum of compound **11.**

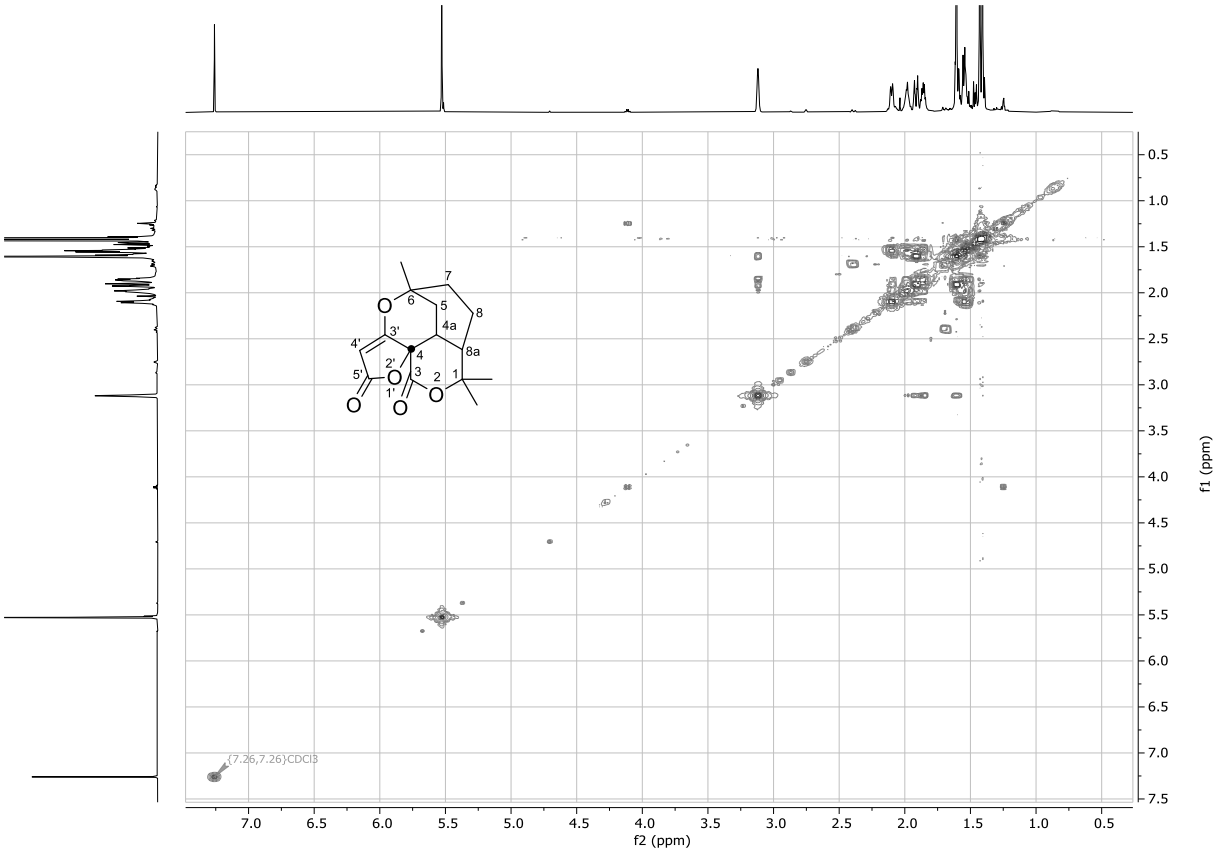


Figure S24. 2D-COSY-spectrum of compound **11.**

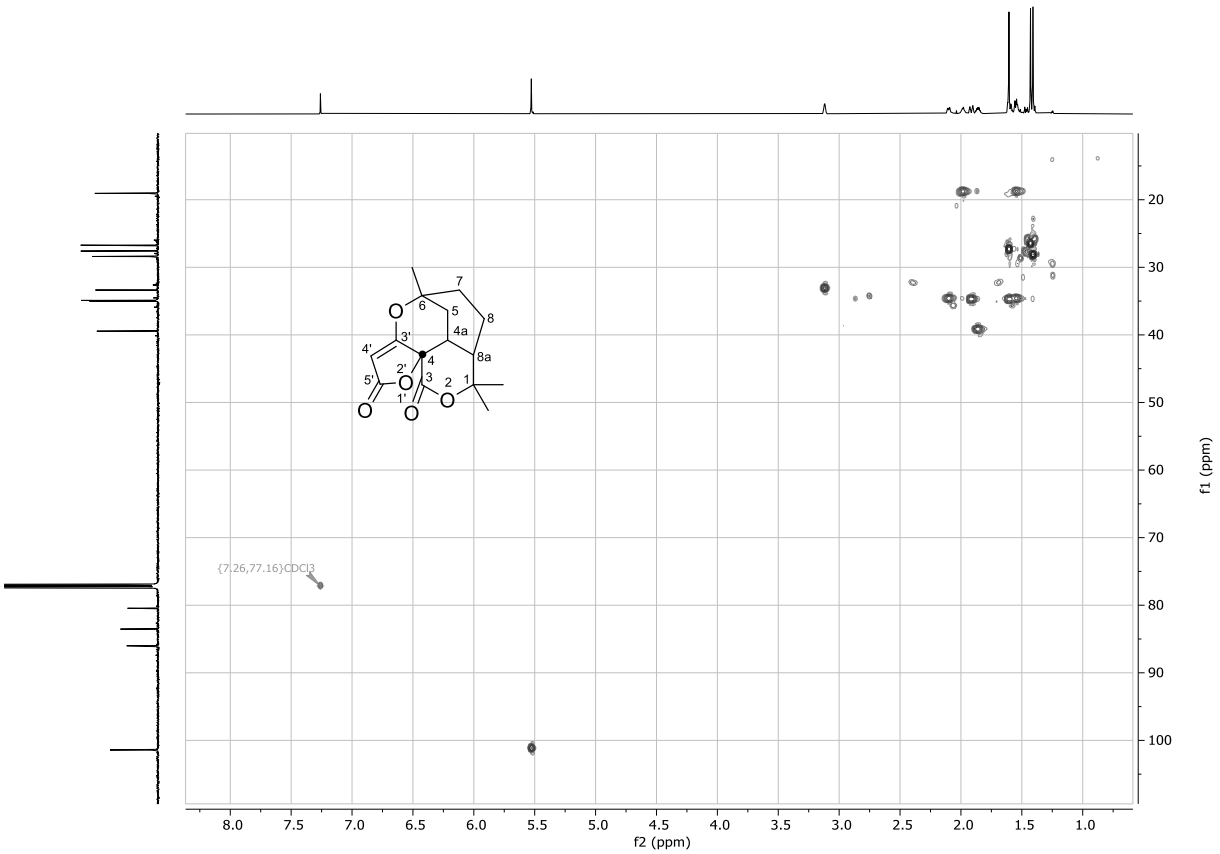


Figure S25. 2D-HSQC-spectrum of compound **11.**

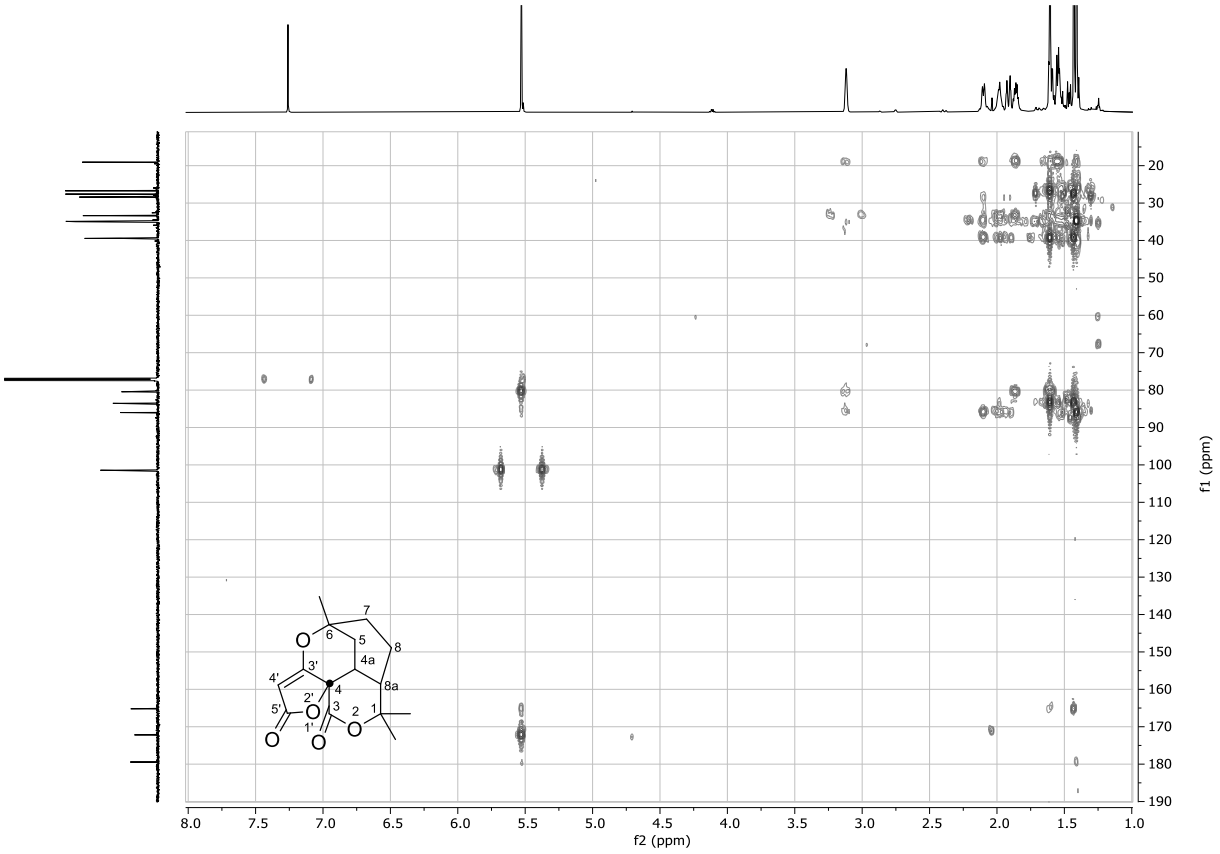


Figure S26. 2D-HMBC-spectrum of compound **11.**