Supplementary data for the article:

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Supplementary material

Integration of dry-column flash chromatography with NMR and FTIR metabolomics to reveal cytotoxic metabolites from *Amphoricarpos autariatus*

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Table S1: The results of cytotoxic activity test

Extract	HeLa mean*	SD	A549 mean	SD
I1	194.33	8.03	>200	/
I2	8.91	0.55	58.22	8.93
I3	27.55	5.80	43.64	3.02
I4	13.15	2.69	21.17	2.28
I5	8.49	0.87	34.77	10.28
I6	8.94	0.09	62.61	10.76
I7	15.68	3.58	71.46	1.87
I8	200.00	/	200.00	0.00
I9	14.98	1.99	29.20	6.43
I10	14.82	0.44	18.42	5.07
I11	20.95	2.64	32.14	6.13
I12	34.70	6.90	52.98	10.40
I13	>200	/	>200	/
II1	9.15	0.65	24.16	3.77
II2	8.34	0.99	18.13	4.69
II3	16.95	6.52	42.63	6.12
II4	137.35	2.50	128.90	1.37
II5	9.55	1.50	46.96	4.81
II6	11.49	4.08	50.16	4.58
II7	134.32	10.27	>200	/
II8	8.95	1.69	22.35	0.58
II9	10.84	3.93	28.45	8.32
II10	13.20	3.47	22.05	0.16
II11	32.46	1.92	61.46	1.75
II12	72.13	9.33	121.62	2.98
II13	>200	/	>200	/
III1	14.39	6.09	16.32	3.71
III2	38.72	1.65	41.26	1.11
III3	23.75	4.74	19.66	2.69
III4	21.36	0.27	16.40	5.25
III5	26.63	6.09	17.42	5.09
III6	24.32	5.90	24.93	5.07
III7	10.77	1.32	15.57	3.43
III8	47.13	3.20	69.91	3.44
III9	134.03	9.65	>200	/
III10	13.01	0.86	21.50	2.26
III11	19.27	5.19	22.36	3.34
III12	22.03	6.39	21.09	2.94
III13	146.71	3.34	>200	/
IV1	20.94	1.00	47.26	2.93

IV2	50.40	4.96	69.84	9.78
IV3	130.80	3.87	137.59	4.79
IV4	21.92	1.55	43.55	1.10
IV5	21.25	6.21	14.46	5.15
IV6	19.10	6.36	17.02	3.34
IV7	19.25	4.70	44.55	3.45
IV8	30.63	3.82	73.44	1.46
IV9	23.40	0.20	27.23	4.15
IV10	19.62	1.45	41.80	5.11
IV11	40.03	2.08	84.36	8.64
IV12	96.79	9.87	>200	/
IV13	22.11	8.01	38.50	10.97

*All experiments were done in triplicates, and the data are presented as mean ± standard deviation (SD) of the results obtained in three independent experiments.

Table S2. Important variables of NMR based OPLS models

Variable (ppm)	VIPpred HeLa cells	P(corr) HeLa cells	VIPpred A549 cells	P(corr) A549 cells
2.00	4.7	-0.78	4.7	-0.77
1.96	3.6	-0.68	3.7	-0.69
5.00	2.8	-0.68	2.9	-0.68
2.32	2.6	-0.67	2.6	-0.65
2.16	2.6	-0.84	2.6	-0.81
4.04	2.3	-0.73	2.3	-0.77
4.00	2.3	-0.71	2.3	-0.69
2.88	2.3	-0.71	2.3	-0.69
6.00	2.3	-0.62	2.4	-0.63
2.44	2.3	-0.71	2.3	-0.77
2.20	2.3	-0.74	2.2	-0.69
5.36	2.2	-0.61	2.3	-0.61
2.84	2.2	-0.67	2.2	-0.67
5.60	2.1	-0.58	2.2	-0.58
4.96	2.0	-0.61	2.0	-0.61
3.96	1.9	-0.67	2.0	-0.68
4.20	1.9	-0.67	1.9	-0.65
2.28	1.7	-0.70	1.6	-0.66
1.68	1.7	-0.63	1.8	-0.66
3.84	1.6	-0.57	1.7	-0.57
4.24	1.6	-0.66	1.6	-0.63
2.12	1.6	-0.62	1.6	-0.64
3.88	1.5	-0.64	1.5	-0.62
2.36	1.5	-0.52	1.5	-0.52

Table S3. Important variables of FTIR based OPLS models

Variable (cm⁻¹)	VIPpred HeLa cells	P(corr) HeLa cells	VIPpred A549 cells	P(corr) A549 cells
1242	3.6	-0.87	3.7	-0.87
1234	3.5	-0.85	3.6	-0.85
1728	3.5	-0.93	3.4	-0.93
1736	3.4	-0.93	3.4	-0.93
1250	3.3	-0.92	3.3	-0.92
1720	3.2	-0.95	3.2	-0.95
1227	3.1	-0.85	3.2	-0.85
1743	3.0	-0.94	2.9	-0.94
1713	2.9	-0.96	2.7	-0.96
1767	2.8	-0.94	2.7	-0.94
1759	2.8	-0.94	2.6	-0.94
1257	2.7	-0.96	2.7	-0.96
1751	2.7	-0.97	2.5	-0.97
1219	2.5	-0.86	2.6	-0.86
1705	2.5	-0.93	2.3	-0.93
1774	2.4	-0.93	2.3	-0.93
1265	2.2	-0.96	2.1	-0.96
1211	2.1	-0.88	2.2	-0.88
1149	2.0	-0.92	2.0	-0.92
1142	2.0	-0.90	2.0	-0.90
1697	2.0	-0.88	1.9	-0.88
910	2.0	-0.85	1.9	-0.85
1134	1.8	-0.92	1.7	-0.92
1203	1.8	-0.86	1.9	-0.86
903	1.8	-0.84	1.7	-0.84
1273	1.8	-0.96	1.7	-0.96
1157	1.8	-0.83	1.8	-0.83
949	1.7	-0.82	-	-
1689	1.6	-0.85	1.5	-0.85
918	1.6	-0.79	1.5	-0.79
1196	1.6	-0.8	1.6	-0.80
941	1.6	-0.79	-	-
933	1.6	-0.81	-	-
1782	1.5	-0.88	1.5	-0.88
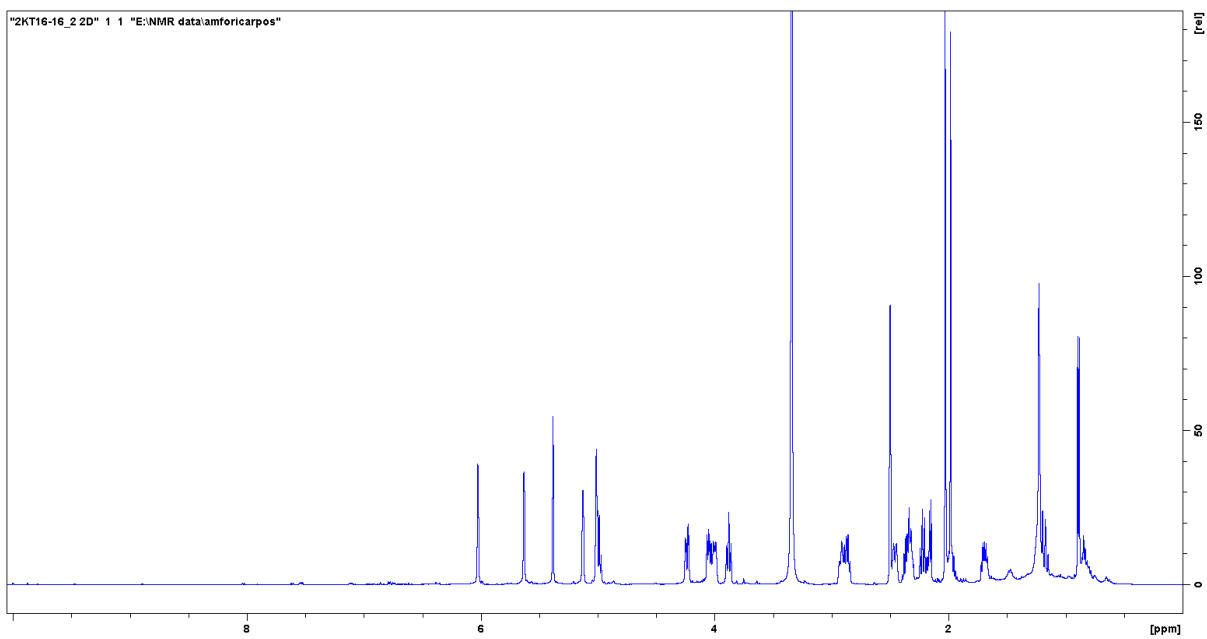
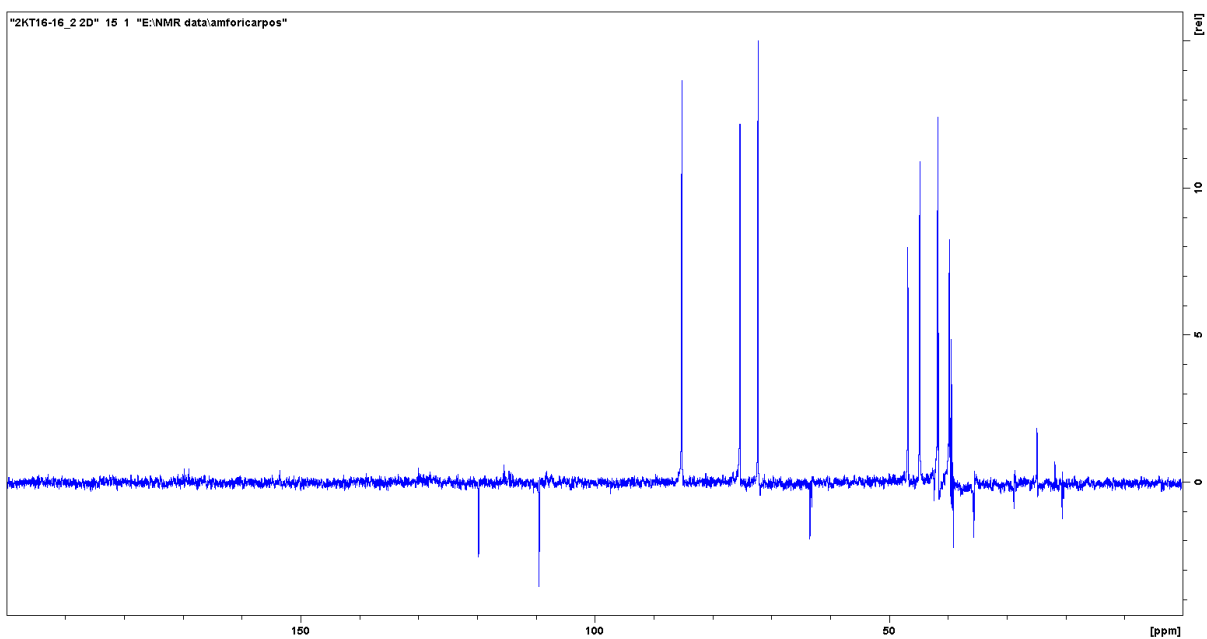Figure S1. ^{1}H NMR spectrum of fraction reach in sesquiterpene γ-lactones

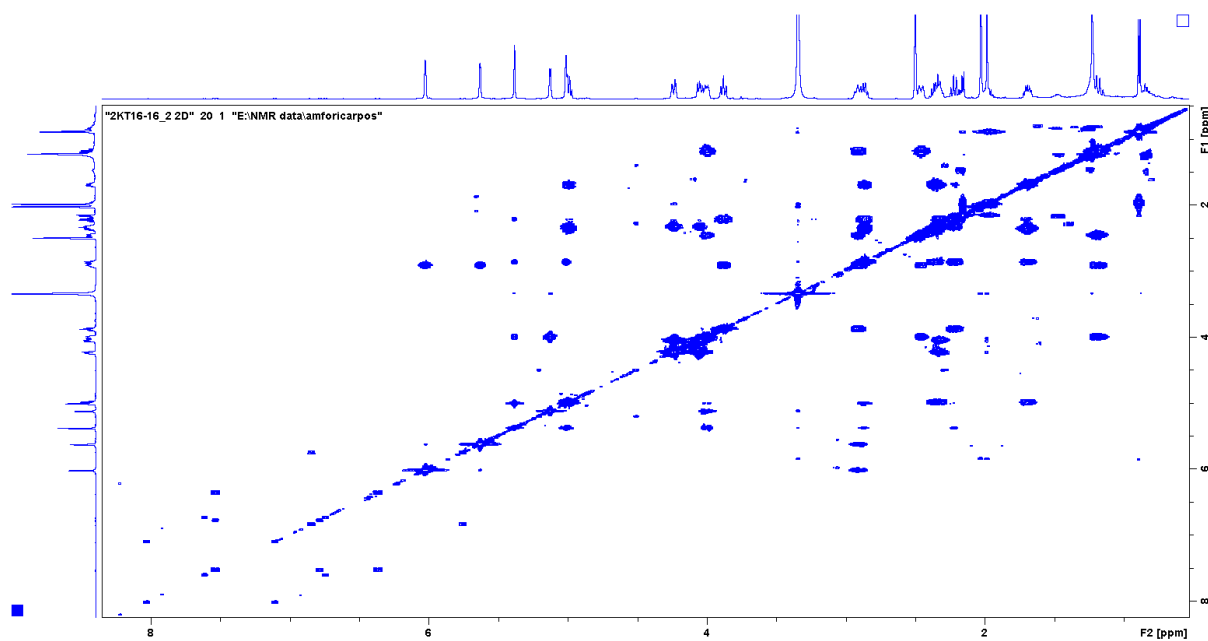Figure S2. DEPT spectrum of fraction reach in sesquiterpene γ-lactones

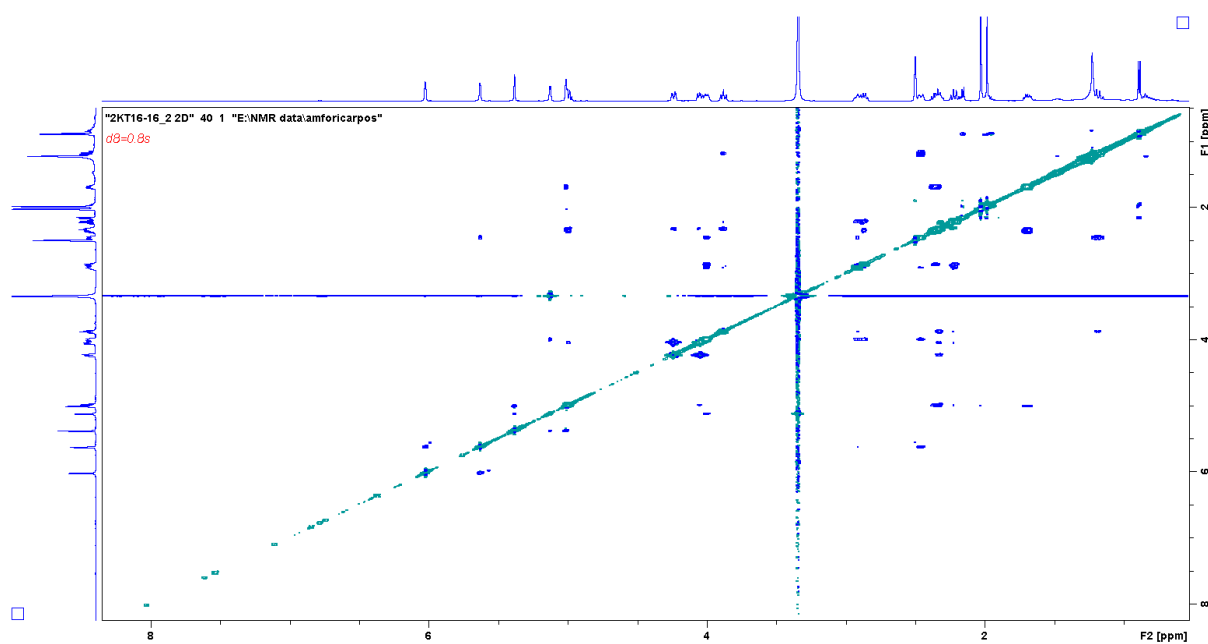Figure S3. COSY spectrum of fraction reach in sesquiterpene γ-lactones

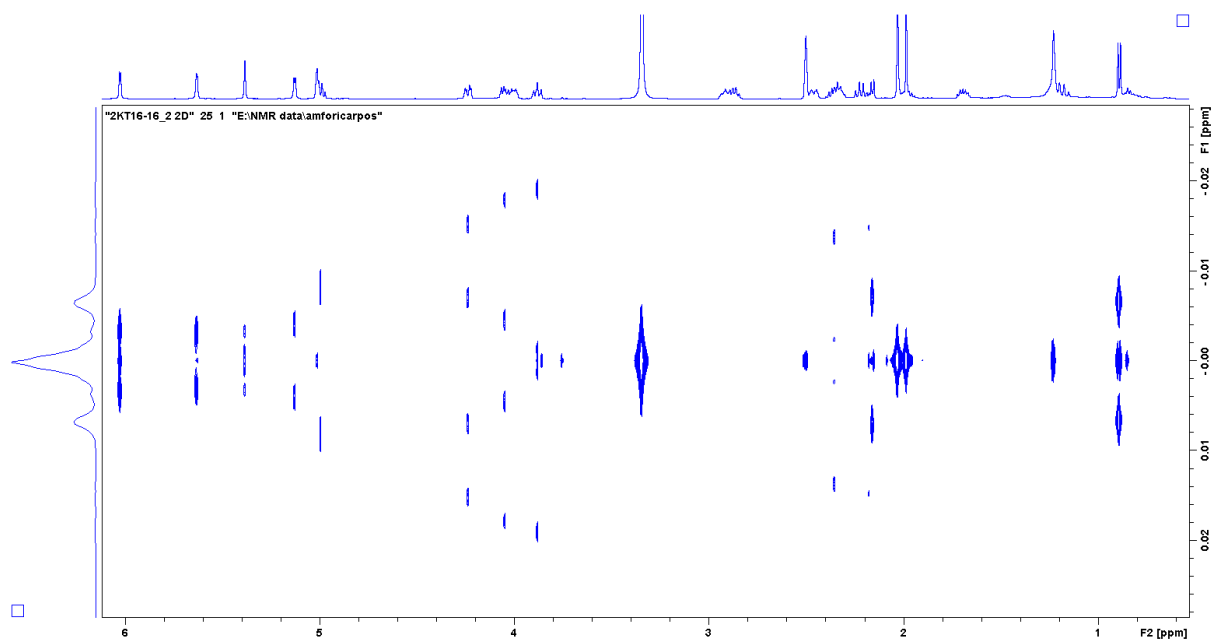Figure S4. NOESY spectrum of fraction reach in sesquiterpene γ-lactones

Figure S5. H,H J-resolved spectrum of fraction reach in sesquiterpene γ-lactones

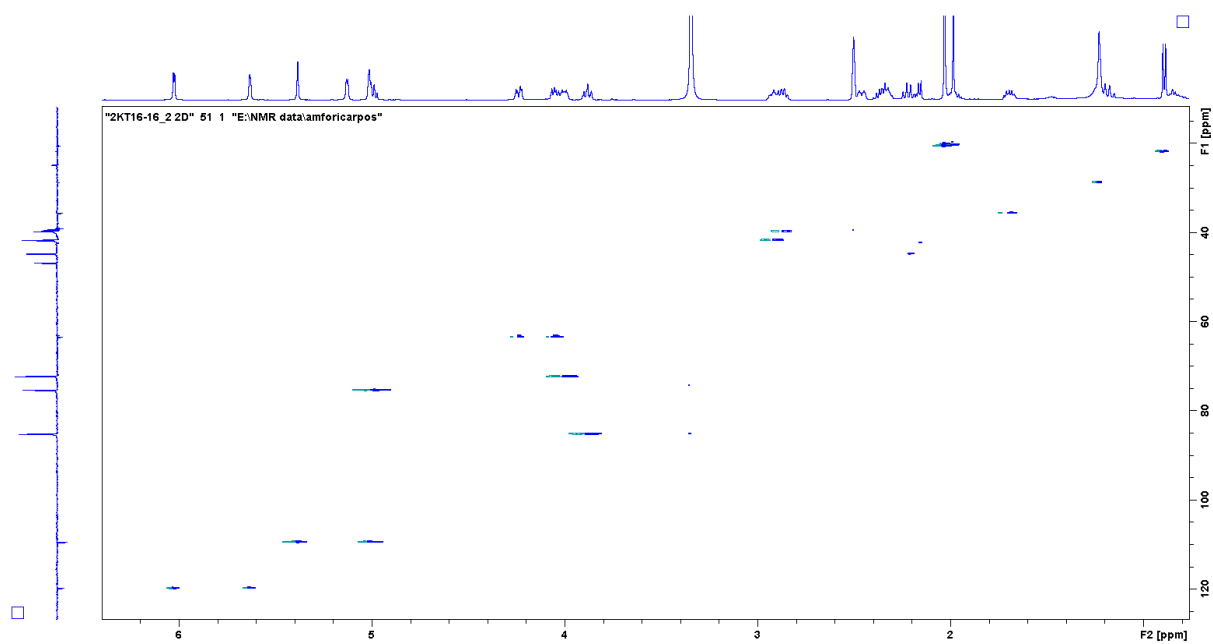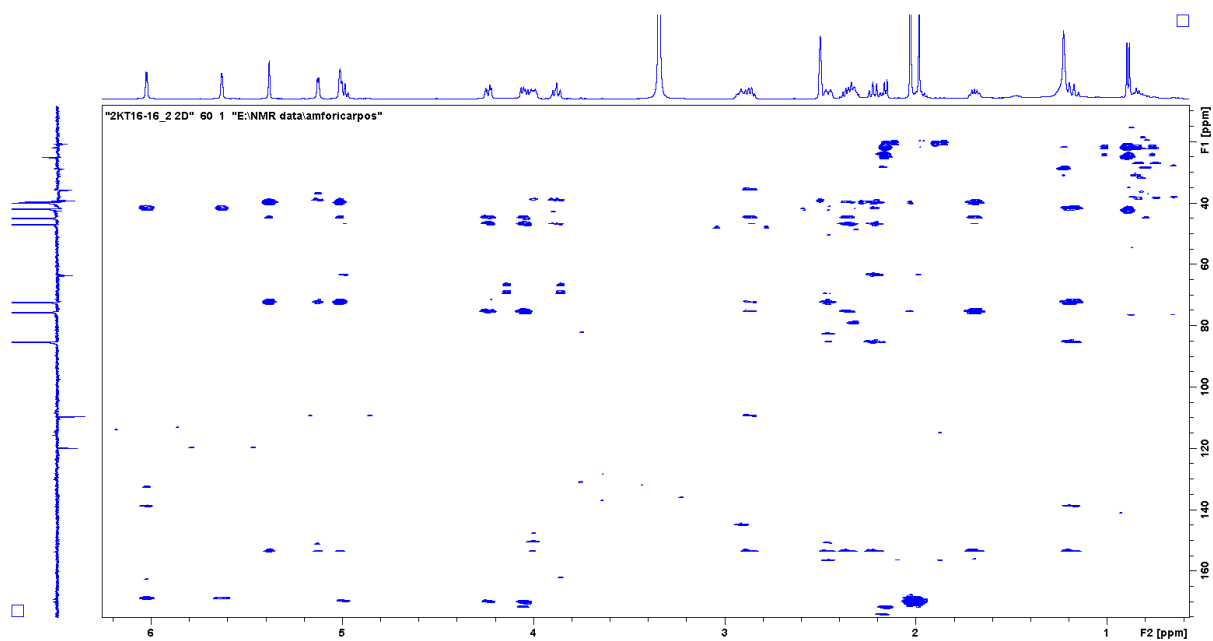Figure S6. HSQC spectrum of fraction reach in sesquiterpene γ-lactones

Figure S7. HMBC spectrum of fraction reach in sesquiterpene γ-lactones
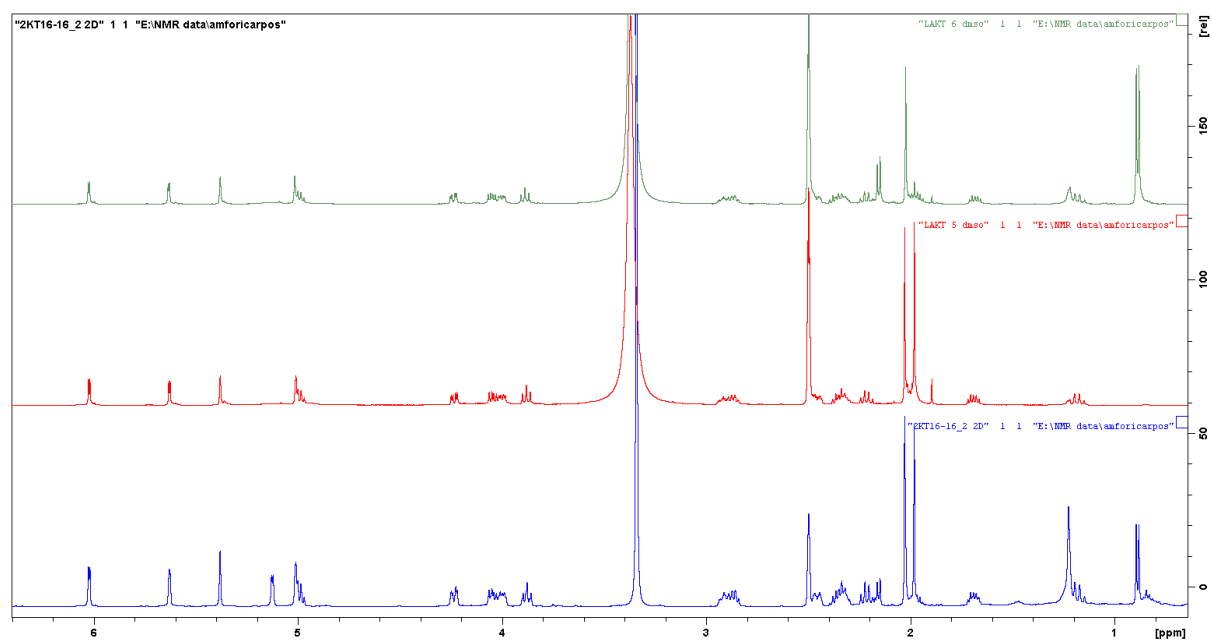

Figure S8. ¹H NMR spectrum of fraction reach in sesquiterpene γ-lactones (blue), compound **1** (green), and compound **2** (red)
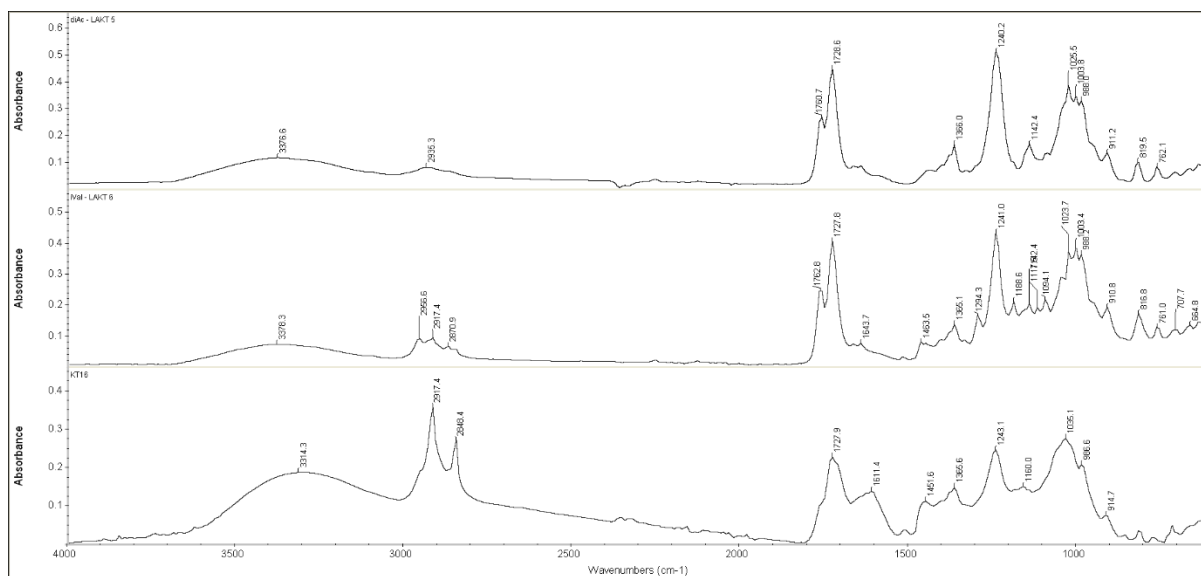
Figure S9. FTIRR spectrum of fraction reach in sesquiterpene γ-lactones (down), compound **1** (middle), and compound **2** (up)