Electronic Supplementary Material (ESI) for Analyst.

SUPPLEMENTARY MATERIALS

Raman spectroscopy as tool for tracking cyclopropane fatty acids in genetically engineered *Saccharomyces cerevisiae*

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Table S1. Band position and assignment in the theoretically calculated Raman spectra of *cis*-9,10-methyleneoctadecanoic acid, using different combinations of length of side chains, basic sets and functionals. The band used for scaling in each spectrum is highlighted in light grey and the scaling factor for each spectrum is highlighted in orange.

Functional	Basis set	Ethyl			Butyl		
		Theoretical Wavenumber (cm^{-1})			Theoretical Wavenumber (cm^{-1})		
		Raman (cm^{-1})	Intensity	Assignment	Raman (cm^{-1})	Intensity	Assignment
wB97XD	cc-pVDZ	589.19	4.5656	γ(-COOH)	593.04	3.4314	γ(-COOH)
		626.73	2.3479	α(-COO) + δ(-COH)	628.74	2.886	γ(-COOH) + α(-COO)
		725.66	2.567	γ(-COOH) + ρ(-CH2(ethyl)	730.44	1.8791	γ(-COOH) + ρ(-CH2(butyl))
		762.4	4.1035	ρ(-CH2(ethyl)) + ω(-CH2(ring)) + ρ(-C-C-C- (ring))	783.1	5.3038	γ(-COOH) + ρ(-CH2(butyl)) + ω(-CH2(ring)) + δ(-CH(ring)) + τ(-CH2 (butyl))
		788.2	1.0699	ρ(-CH2(ethyl)) + τ(-CH2(ring))	828.49	5.15	ρ(-CH2(butyl)) + α(-C-C-C- (ring)) + τ(-CH2(ring))
		823	6.7405	ρ(-CH2(ethyl)) + ρ(-CH2(ring)) + δ(-CH(ring))	880.82	3.9963	ρ(-CH2(butyl)) + τ(-CH2(ring)) + ω(-CH(ring))
		861.74	6.1143	vs(-C-C-O) + τ(-CH2(ring)) + δ(-CH(ring)) + vass(-C-C-C-)	912.47	3.6228	ρ(-CH2 (ring)) + τ(CH2 (butyl))
		897.87	2.6001	τ(-CH2(ethyl)) + ρ(-CH2 (ring)) + ρ(H-C-C-H (ring))	924.43	5.7959	δ(-COH) + ρ(-CH2(butyl)) + τ(-CH2(butyl)) + τ(-CH2(ring)) + δ(-CH(ring))
		908.28	6.8929	vs(-COO) + τ(-CH2(ring)) + α(H-C-C-H (ring))	961.9	10.3272	α(-C-C-C- (ring)) + ω(-CH2(butyl))
		950.44	8.8181	vs(-COO) + α(-C-C-C-) + τ(-CH2(ethyl)) + ρ(-CH3) + ω(-CH2(ethyl) + α(-C-C-C- (ring))	1075.24	3.9951	vs(-C-C-C-) + ω(-CH2 (butyl)) + ω(-CH2 (ring)) + ω(H-C-C-H (ring))
		965.42	7.5527	ρ(-CH2) + τ(-CH2 (ring))	1083.94	6.4244	vass(-C-C- (butyl)) + ω(-CH2(ring))
		1019.14	2.4452	ω(-CH2(ring)) + δ(-CH(ring)) + α(H-C-C-H (ring, ethyl)) + ρ(-CH3)	1095.17	10.662	ω(-CH2(butyl)) + τ(-CH2(ring)) + δ(-CH(ring)) + vass(-CH2(butyl))
		1033.9	1.4906	ω(-CH2(ring)) + ω(-CH2(ethyl)) + ω(H-C-C-H(ring))	1134.83	11.3164	τ(-CH2(butyl)) + τ(-CH2(ring)) + ω(H-C-C-H (ring))
		1052.28	1.3821	ω(-CH2(ring)) + α(H-C-C-H (ring, ethyl	1147.15	4.8086	τ(-CH2(butyl)) + ω(H-C-C-H (ring))
		1078.42	8.7501	vass(-C-C-C-) + τ(-CH2(ring)) + δ(-CH(ring)	1226.28	20.3851	δ(-COH) + ρ(-CH2(butyl)) + α(-CH2(ring)) + α(H-C-C-H (ring))
		1106.77	1.8724	α(H-C-C-H (ring)) + τ(-CH2(ethyl)) + τ(-CH2(ring))	1249.65	4.0139	δ(-COH) + ρ(-CH2(butyl)) + τ(-CH2(ring)) + τ(-CH2(butyl))
		1120.37	3.5269	α(H-C-C-H (ring)) + τ(-CH2(ethyl)) + τ(-CH2(ring))	1277.63	5.7097	τ(-CH2(butyl)) + ω(-CH2(butyl)) + ω(-CH(ring))
		1138.13	2.613	α(-C-C-H (ring)) + ρ(-CH2(ethyl)) + τ(-CH2(ring))	1328.52	20.6676	τ(-CH2(butyl))
		1206.21	1.4255	ρ(-CH2(ring)) + ω(-CH (ring)) + vass(-C-C-C-)	1405.59	2.2334	τ(-CH2 (butyl)) + ω(-CH2 (butyl)) + α(-CH2 (ring))
		1217.06	4.2574	δ(-COH) + τ(-CH2(ethyl)) + ρ(-CH2(ethyl)) + ρ(-C-C-H (ring))	1434.5	4.5	α(-CH2 (ring)) + ω(-CH2 (butyl)) + α(H-C-C-H (ring))

Functional	Basis set	Ethyl			Butyl		
		Theoretical Wavenumber (cm^{-1})			Theoretical Wavenumber (cm^{-1})		
		Raman (cm^{-1})	Intensity	Assignment	Raman (cm^{-1})	Intensity	Assignment
		1228.48	16.9717	vs(-C-C-C- (ring)) + τ(-CH2(ring)) + α(H-C-C-H (ring))	1472.25	25.172	α(-CH2(butyl)) + α(-CH3)
		1247.15	4.8065	δ(-COH) + τ(-CH2(ethyl)) +τ(-CH2(ring))	1516.78	12.5005	α(-CH2(ring)) + vs(-C-C-C-(ring))
		1292.44	2.7922	ω(-CH2(ethyl)) + τ(-CH2(ring)) + ω(-CH (ring)) + τ(-CH2 (ethyl))	3028.34	177.596	vs(-CH2(butyl))
		1317.94	8.9215	τ(-CH2(ethyl)) + τ(-CH2(ring))	3043.76	182.6362	vs(-CH3(butyl))
		1328.4	4.7735	ρ(H-C-C-H (ring, ethyl)	3058.77	157.4713	vass(-CH2(butyl))
		1361.88	2.3049	ω(-CH2(ethyl)	3065.01	53.7627	vs(-CH2(butyl))
		1396.33	2.0617	α(-COH) + ω(-CH2(ethyl)) + ω(H-C-C-H (ring))	3089.38	24.6143	vass(-CH2(butyl))
		1432.39	5.4502	α(-CH2(ring))	3107.31	45.608	vass(-CH2(butyl))
		1455.67	12.8005	α(-CH2(ethyl))	3135.24	42.5471	vass(-CH3) + vs(-CH2(ring)) + δ(-CH(ring))
		1469.34	19.3327	α(-CH2(ethyl)) + α(-CH2(ring)) + α(-CH3)	3142.8	155.7186	vs(-CH2(ring)) + ν(-CH(ring))
		1477.97	5.7917	α(-CH2(ethyl))	3231.23	48.1213	vass(-CH2(ring))
		1517.34	12.7175	vs(-C-C-C- (ring)) + α(-CH2(ring)) + δ(-CH(ring))	3800.63	128.5	ν(-OH)
		1882.83	6.9764	ν(C=O) + α(-COH) + τ(-CH2(ethyl))	SCALING FACTOR	0.939782191	
		3046.79	162.5392	vs(-CH3) + vs(-CH2(ethyl))			
		3068.89	39.0607	vs(-CH2(ethyl))			
		3082.11	96.3816	vass(-CH3) + vass(-CH2(ethyl))			
		3105.47	79.9938	vass(-CH2(ethyl)) + ν(-CH(ring))			
		3136.71	99.3456	vass(-CH3)			
		3144.12	90.9367	vass(-CH2(ethyl)) + ν(-CH(ring)) + vs(-CH2(ring))			
		3231.25	50.5085	vass(-CH2(ring))			
		3800.48	123.663	ν(-OH)			
		SCALING FACTOR	0.93409129				
	aug-cc-pVDZ	596.73	1.7143	γ(-COOH)	599.08	1.2506	γ(-COOH)
		626.38	1.2625	γ(-COOH) + α(-COO)	630.78	1.2531	γ(-COOH) + α(-COO)

Functional	Basis set	Ethyl			Butyl		
		Theoretical Wavenumber (cm^{-1})			Theoretical Wavenumber (cm^{-1})		
		Raman (cm^{-1})	Intensity	Assignment	Raman (cm^{-1})	Intensity	Assignment
		745.23	3.6559	ρ(-CH2) + ρ(-C-C-C-) + γ(-COOH)	762.38	4.2555	ρ(-C-C-C-) + γ(-COOH)
		763.3	3.7594	ρ(-CH2 (ethyl)) + ω(-COH)	773.42	3.7797	ρ(-CH2(butyl)) + τ(-CH2(butyl)) +α(-C-C-C- (ring))
		818.97	5.6014	ρ(-CH2(ethyl)) + ρ(-CH2(ring))	825.23	3.9401	ρ(-CH2(butyl)) +τ(-CH2(butyl)) + ρ(-CH2(ring)) + α(-C-C-C-(ring))
		858.85	4.0416	vs(-O-C-C-) + τ(-CH2(ring)) + α(H-C-C-H(ring))	877.95	1.954	ρ(-CH2(butyl)) + τ(-CH2 (ring)) + α(H-C-C-H (ring))
		895.28	2.5179	ρ(-CH2(ring)) + ρ(H-C-C-H (ring)) + τ(-CH2(ethyl))	910.76	8.8352	vs(-COO) + ρ(-CH2(butyl)) + ρ(-CH2(ring)) + α(-C-C-C- (ring))
		909.85	8.4364	vs(-C-C-O) + τ(-CH2(ring)) + α(H-C-C-H (ring))	921.86	2.787	ρ(-CH2 (butyl)) + τ(-CH2 (butyl)) + α(-C-C-C- (ring))
		946.36	6.0068	vs(-COO) + ω(-CH2(ethyl)) + α(-C-C-C- (ring))	957.54	6.904	α(-C-C-C- (ring)) + ω(-CH2(butyl))
		962.82	4.723	α(-C-C-C- (ring)) + ρ(-CH2(ethyl))	1028.89	1.1162	τ(-CH2 (butyl)) + α(-C-C-C- (ring)) + ω(-CH2(ring)) + ω(-CH (ring))
		1016.32	1.6788	vs(-C-C-C- (ring)) + τ(-CH2(ethyl)) + vs(-C-C-C-(ethyl, ring))	1046.89	3.0882	vass(-C-C-(ring)) + ω(-CH2(ring))
		1031.18	1.9613	ω(-CH2(ring)) + ω(H-C-C-H (ring)) + vs(-C-C-C- (ethyl, ring))	1070.12	4.4119	τ(-CH2(butyl)) + ρ(-CH2(ring)) + ω(H-C-C-H (ring))
		1047.05	3.4118	ω(-CH2(ring))	1082.08	4.9613	vass(-C-C-C(butyl))
		1067.88	12.6149	τ(H-C-C-H (ring)) + vass(-C-C-C- (ethyl))	1091.04	9.3555	vass(-C-C-C-(butyl))
		1102.02	2.1276	τ(-CH2(ring)) + α(H-C-C-H (ring)) + τ(-CH2(ethyl))	1102.02	9.7095	ν(-C-C-C- (butyl)) + τ(-CH2(ring)) + ω(-CH(ring))
		1117.34	5.9982	τ(-CH2(ethyl)) + ρ(-CH2(ring))	1126.91	11.6793	τ(-CH2(butyl)) + ω(H-C-C-H (ring))
		1136.08	2.3629	α(-COH) + τ(-CH2(ethyl)) + τ(-CH2(ring)) + ω(H-C-C-H (ring))	1144.61	7.3543	τ(-CH2(butyl)) + vs(-C-C-C- (butyl)) + ρ(H-C-C-H (ring)) + ω(-CH2(butyl))
		1228.25	20.068	δ(-COH) + vs(-C-C-C- (ring)) + α(H-C-C-H (ring)) + τ(-CH2(ethyl))	1226.03	17.4839	ρ(-COH) + α(H-C-C-H (ring)) + vs(-C-C-C- (ring))
		1247.48	3.736	δ(-COH) + τ(-CH2(ethyl)) +ρ(-CH2(ring))	1248.69	3.8315	τ(-CH2 (butyl)) + ω(-CH2 (butyl)) + α(H-C-C-H (ring)) + τ(-CH2 (ring))
		1290.67	1.6819	τ(-CH2(ring)) + ω(-CH (ring)) + τ(-CH2(ring))	1276.75	2.9531	δ(-COH) + τ(-CH2(butyl))
		1313.06	4.2475	δ(-COH) + τ(-CH2(ethyl)) + τ(-CH2(ring)) + δ(-CH(ring))	1294.29	1.6641	ω(-CH2(butyl)) + ω(-CH (ring)) + δ(-COH)
		1326.81	1.6932	τ(-CH2(ethyl)) + ω(H-C-C-H (ring))	1324.95	5.4819	τ(-CH2(butyl))
		1354.05	3.1705	ω(-CH2(ethyl)) + ω(-C-H (ring))	1408.88	2.4142	ω(-CH2 (butyl)) + ω(-CH (ring)) + α(-CH2 (ring))
		1396.21	3.4731	α(-COH) + ω(-CH2(ethyl))+ ω(-CH(ring))	1442.66	4.3967	α(-CH2(ring)) + α(H-C-C-H (ring))
		1441.63	5.422	α(-CH2(ethyl)) + α(-CH2(ring)) + α(H-C-C-H (ring))	1473.96	27.2866	α(-CH2(butyl)) + α(-CH2(ring))

Functional	Basis set	Ethyl			Butyl		
		Theoretical Wavenumber (cm^{-1})			Theoretical Wavenumber (cm^{-1})		
		Raman (cm^{-1})	Intensity	Assignment	Raman (cm^{-1})	Intensity	Assignment
		1472.96	8.0436	α(-CH2(ethyl))	1517.72	13.3833	α(-CH2(ring)) + vs(-C-C-C- (ring))
		1518.05	13.3123	v(-C-C-C- (ring)) + α(-CH2(ring)) + δ(-CH(ring))	1844.12	16.6225	v(C=O) + α(-COH) + τ(-CH2(ethyl))
		1843.41	17.1462	v(C=O) + α(-COH) + τ(-CH2(ethyl))	3029.13	140.7988	vs(-CH2(butyl))
		3043.39	263.9167	vs(-CH2(ethyl)) + vs(-CH3)	3040.94	253.4047	vs(-CH3)
		3051.93	125.2432	vs(-CH2(ethyl))	3057.02	131.2962	vass(-CH2(butyl))
		3082.37	81.8897	vass(-CH3) + vass(-CH2(ethyl))	3064.72	109.7682	vass(-CH2(butyl))
		3100.99	62.5775	vass(-CH2(ethyl)) + v(-CH(ring))	3084.28	56.6679	vass(-CH2(butyl)) + vs(-CH2(butyl))
		3129.65	79.2444	vass(-CH3) + vass(-CH2(ethyl))	3105.31	23.9724	vass(-CH2(butyl))
		3138.79	56.0535	vs(-CH2(ring) + v(-CH (ring))	3127.8	98.3032	v(-CH3)
		3148.87	156.6131	vs(-CH2(ethyl)) + v(-CH(ring))	3147.95	175.9082	vs(-CH2(ring)) + v(-CH(ring))
		3232.1	44.1849	vass(-CH2(ethyl))	3230.87	42.6271	vass(-CH2(ring)) + v(-CH(ring))
		3828.31	108.7194	v(-OH)	3828.77	112.7502	v(-OH)
		SCALING FACTOR	0.935134833		SCALING FACTOR	0.939537095	
M06-2X	cc-pVDZ	585.88	4.7152	γ(-COOH)	586.45	3.767	γ(-COOH)
		625.69	2.1367	γ(-COOH) + α(-COO)	626.78	2.5408	γ(-COOH) + α(-COO)
		718.35	2.47	γ(-COOH) + ρ(-CH2(ethyl))	720.23	1.6915	γ(-COOH) + ρ(-CH2(butyl))
		764.55	2.5088	ρ(-CH2(ethyl)) + ω(-CH2(ring))	779.79	2.9847	ρ(-CH2(butyl)) + τ(-CH2(ring)) + τ(-CH2(butyl))
		821.11	7.7815	ρ(-CH2(ethyl)) + τ(-CH2(ring)) + δ(-CH(ring))	833.75	6.7483	τ(-CH2(butyl)) + ρ(-C-C-C- (ring)) + ρ(-CH2(butyl))
		863.39	5.909	vs(-C-C-O) + τ(-CH2(ring)) + τ(-CH2(ethyl)) + ω(-CH (ring))	875.32	3.6071	ρ(-CH2(butyl)) + τ(-CH2(ring)) + α(H-C-C-H (ring))
		888.82	3.1565	ρ(-CH2(ethyl)) + τ(-CH2(ethyl)) + ρ(-CH2(ring)) + ρ(H-C-C-H (ring))	907.91	3.0312	ρ(-CH2(ring)) + ρ(-CH2 (butyl)) + vs(-C-C-O-)
		910.53	6.2592	vs(-C-C-O) + τ(-CH2(ring)) + α(H-C-C-H (ring))	921.15	7.0976	ρ(-CH2(butyl)) + τ(-CH2(butyl)) + τ(-CH2(ring)) + δ(-CH(ring))
		950.41	5.7795	τ(-CH2(ring)) + τ(-CH2(ethyl)) + ω(-CH (ring))	944.64	3.3727	τ(-CH2(butyl)) + ρ(-C-C-C-(ring))
		976.87	8.182	α(-C-C-C- (ring)) + ρ(-CH2(ethyl))	974.72	9.5596	α(-C-C-C- (ring)) + α(-C-C-C- (ring, butyl))
		1018.81	2.4065	ω(-CH2 (ring)) + ω(-CH (ring)) + τ(-CH2(ethyl))	1069.07	2.071	ω(-CH2 (butyl)) + ρ(-CH2(ring)) + ω(H-C-C-H (ring))

Functional	Basis set	Ethyl			Butyl		
		Theoretical Wavenumber (cm^{-1})			Theoretical Wavenumber (cm^{-1})		
		Raman (cm^{-1})	Intensity	Assignment	Raman (cm^{-1})	Intensity	Assignment
		1080.78	8.571	τ(-CH2(ethyl)) + τ(-CH2(ring)) + δ(-CH(ring)) + vass(-C-C-C-)	1084.52	6.0568	vass(-C-C-C- (butyl)) + τ(-CH2(ring)) + α(H-C-C-H (ring))
		1113.73	4.2913	τ(-CH2(ethyl)) + τ(-CH2(ring)) + α(H-C-C-H (ring))	1095.05	9.1696	τ(-CH2(ring)) + α(H-C-C-H (ring)) + vass(-C-C-C-(butyl))
		1133.68	3.2175	ρ(-CH2(ethyl)) + τ(-CH2(ethyl)) +ω(H-C-C-H (ring))	1112.01	3.4197	ρ(-CH2 (ring)) + ρ(H-C-C-H (ring)) + vass(-C-C-C- (butyl, ring))
		1212.35	3.8319	δ(-COH) + τ(-CH2(ethyl)) + ρ(-CH2(ring)) + α(H-C-C-H (ring))	1131	11.7461	τ(-CH2(butyl)) + α(-C-C-C- (ring)) + δ(-CH(ring))
		1228.2	17.7471	δ(-COH) + τ(-CH2(ethyl)) + τ(-CH2(ring)) + α(H-C-C-H(ring))	1144.14	6.2076	τ(-CH2(butyl)) + ω(-CH(ring)) + ω(-CH2(butyl))
		1248.48	3.807	δ(-COH) + τ(-CH2(ethyl))	1224.77	18.1052	τ(-CH2(butyl)) + ρ(-CH2(butyl)) + α(-CH2(ring)) + vs(-C-C-C-(ring))
		1281.14	2.8401	τ(-CH2 (ethyl)) + τ(-CH2 (ring)) + ω(-CH (ring))	1245.82	3.956	α(-COH) + vass(-O-C-C-) + τ(-CH2(butyl)) + τ(-CH2(ring)) + ω(-CH (ring))
		1307.85	9.2933	τ(-CH2(ethyl)) + τ(-CH2(ring)) + δ(-CH(ring))	1267.68	6.3262	δ(-COH) + τ(-CH2(butyl)) + ρ(-CH2(butyl)) + τ(-CH2(ring)) + ω(-CH2(butyl)) + ω(-CH (ring))
		1351.23	2.4718	ω(-CH2 (ethyl)) + ω(-CH (ring)) + α(-CH2(ring))	1315.3	20.377	τ(-CH2(butyl))
		1422.1	5.06	α(-CH2 (ring)) + ω(-CH2 (ethyl))	1397	2.2093	ω(-CH2(butyl)) + α(-CH2 (ring))
		1443.33	13.1987	α(-CH2(ethyl))	1423.96	4.5357	α(-CH2(ring)) + ω(-CH2(butyl)) + ω(-CH (ring))
		1460.88	19.5208	α(-CH2(ethyl)) + vs(-C-C-C- (ring)) + α(-CH2(ring))	1459	21.6703	vs(-C-C-C- (ring)) + α(-CH2(ring)) + ω(-CH (ring))
		1470.46	16.0968	α(-CH3)	1472.79	14.3098	α(-CH2(butyl)) + α(-CH3)
		1522.05	12.9312	α(-CH2(ring)) + vs(-C-C-C-(ring))	1521.36	12.5989	α(-CH2(ring)) + vs(-C-C-C-(ring))
		1904.45	7.7864	ν(C=O) + α(-COH) + τ(-CH2(ethyl))	1904.38	7.5641	ν(C=O) + α(-COH) + τ(-CH2(ethyl))
		3060.17	269.957	vs(-CH2(ethyl)) + vs(-CH3)	3036.49	208.3453	vs(-CH2(butyl))
		3089.88	105.1511	vass(-CH2(ethyl)) + vass(-CH3)	3057.14	136.847	vs(-CH2(butyl))
		3111.21	84.3875	vass(-CH2(ethyl))	3064.53	164.9593	vass(-CH2(butyl))
		3152.19	149.8719	vass(-CH2(ethyl)) + vs(-CH2(ring)) + ν(-CH(ring))	3070.83	130.1758	vass(-CH2(butyl))
		3239.45	53.2957	vass(-CH2(ring))	3095.84	31.0422	vass(-CH2(butyl))
		3782.89	121.073	ν(-OH)	3114.24	51.2442	vass(-CH2(butyl))
		SCALING FACTOR	0.930007156		3142.95	120.7271	ν(-CH3)
					3150	168.4671	vs(-CH2(ring)) + ν(-CH(ring))

Functional	Basis set	Ethyl			Butyl		
		Theoretical Wavenumber (cm^{-1})			Theoretical Wavenumber (cm^{-1})		
		Raman (cm^{-1})	Intensity	Assignment	Raman (cm^{-1})	Intensity	Assignment
					3237.92	50.4399	vass(-CH2(ring))
					3785.39	125.6187	ν(-OH)
					SCALING FACTOR	0.937259797	
	aug-cc-pVDZ	591.91	1.8192	γ(-COOH)	590.82	1.319	γ(-COOH)
		620.77	1.1878	γ(-COOH) + α(-COO)	620.15	1.237	γ(-COOH) + α(-COO)
		739.63	4.1026	γ(-COOH) + ρ(-CH2(ethyl))	754.51	3.5695	γ(-COOH) + ρ(-CH2(butyl))
		758.02	1.3269	α(-C-C-C- (ring)) + ρ(-CH2(ethyl))	769.5	2.5494	τ(-CH2 (butyl)) + ρ(-CH2 (butyl)) + ρ(-C-C-C- (ring))
		772.21	1.0031	ρ(-CH2(ethyl)) + τ(-CH2 (ring)) + ω(-CH (ring))	830.9	4.8707	α(-C-C-C- (ring)) + ρ(-CH2(butyl))
		818.53	6.6936	ρ(-CH2(ethyl)) + τ(-CH2(ring)) + δ(-CH(ring)) + α(-C-C-C- (ring))	869.69	1.064	τ(-CH2 (ring)) + ω(-CH (ring)) + ρ(-CH2 (butyl)) +
		861.28	3.6811	vs(-C-C-O-) + τ(-CH2(ring)) + τ(-CH2(ethyl)) + ω(-CH (ring))	909.82	10.0107	vs(-C-C-O) + τ(-CH2(butyl)) + τ(-CH2(ring)) + ρ(-CH3)
		886.15	2.9925	ρ(-CH2(ethyl)) + τ(-CH2(ethyl)) + ρ(-CH2(ring)) + ρ(H-C-C-H (ring))	919.9	2.9026	ρ(-CH2 (butyl)) + τ(-CH2 (butyl)) + τ(-CH2(ring)) + α(H-C-C-H (ring))
		911.41	7.0368	vs(-C-C-O) + τ(-CH2(ring)) + α(H-C-C-H (ring))	944.31	3.4635	τ(-CH2 (butyl)) + ρ(-CH2 (butyl)) + ρ(-C-C-C- (ring))
		947.42	4.8069	vs(-C-C-O) + τ(-CH2(ring)) + τ(-CH2(ethyl)) + ω(-CH (ring))	970.82	6.9362	α(-C-C-C- (ring)) + ω(-CH2(butyl))
		973.05	6.7812	ρ(-CH2(ethyl)) + α(-C-C-C- (ring))	1024.44	0.77	ω(-CH2 (ring)) + ω(-CH (ring)) + τ(-CH2 (butyl))
		1039.3	2.6983	ω(-CH2 (ring)) + ω(-CH (ring)) + ω(-CH2(ethyl))	1037.96	1.1679	vass(-C-C-C- (butyl)) + ω(-CH2 (ring)) + ω(-CH (ring))
		1069.74	12.7101	τ(-CH2(ring)) + δ(-CH(ring)) + vass(-C-C-C-)	1050.18	3.5128	vass(-C-C-C- (butyl))
		1093.9	1.4505	τ(-CH2(ethyl)) + ρ(-CH2(ring))	1064.69	2.4653	ω(-CH2 (butyl)) + ρ(-CH2 (ring)) + ρ(H-C-C-H (ring))
		1110.73	7.5841	τ(-CH2(ethyl)) + τ(-CH2(ring)) + α(H-C-C-H (ring))	1083.22	4.5204	vass(-C-C-C- (butyl)) + ω(-CH (ring))
		1131.34	2.7991	ρ(-CH2(ethyl)) + τ(-CH2(ethyl)) +ω(H-C-C-H (ring))	1091.45	1.0815	τ(-CH2 (ring)) + vass(-C-C-C- (butyl))
		1228.59	19.7083	vs(-C-C-C-) + τ(-CH2(ring)) + α(H-C-C-H (ring)) + τ(-CH2(ethyl))	1104.03	17.1359	vs(-C-C-C- (butyl)) + ω(-CH (ring))
		1243.44	2.8818	τ(-CH2 (ring)) + ω(-CH2 (ethyl)) + ρ(-COH)	1123.87	11.3234	τ(-CH2(butyl)) + ω(-CH (ring))
		1250.64	2.2487	δ(-COH) + ω(-CH2(ethyl))	1141.75	9.2098	vs(-C-C-C- (butyl)) + τ(-CH2 (butyl)) + α(-C-C-C- (ring))
		1281.08	1.9264	ω(-CH (ring)) + τ(-CH2 (ethyl))	1199.92	1.4104	ρ(-CH2(butyl)) + ω(-CH (ring)) + ω(-CH2(butyl))

Functional	Basis set	Ethyl			Butyl		
		Theoretical Wavenumber (cm^{-1})			Theoretical Wavenumber (cm^{-1})		
		Raman (cm^{-1})	Intensity	Assignment	Raman (cm^{-1})	Intensity	Assignment
		1304.46	4.3358	τ(-CH2(ethyl)) + τ(-CH2(ring)) + δ(-CH(ring))	1226.84	15.9591	α(-CH2 (ring)) + τ(-CH2 (butyl)) + α(H-C-C-H (ring))
		1344.18	3.4007	ω(-CH2(ethyl)) + α(-CH2(ring)) + δ(-CH(ring)) + α(-COH)	1242.52	8.167	ρ(-COH) + τ(-CH2 (butyl)) + τ(-CH2 (butyl)) + α(H-C-C-H (ring))
		1389.98	2.4369	α(-COH) + α(-CH2(ethyl)) + α(-CH2(ring)) + ω(-CH3)	1268.9	2.7699	δ(-COH) + τ(-CH2(butyl)) + ρ(-CH2(butyl)) + τ(-CH2(ring)) + ω(-CH2(butyl))
		1436.41	5.6878	α(-CH2(ethyl)) + α(-CH2(ring) + α(H-C-C-H(ring))	1281.9	2.0443	ω(-CH2 (butyl)) + α(H-C-C-H (ring))
		1458.44	8.6226	α(-CH2(ethyl))	1313.12	5.5122	τ(-CH2 (butyl))
		1465.75	8.7749	α(-CH3) + α(-CH2(ethyl))	1396.43	3.4201	ω(-CH2 (butyl)) + α(-CH2 (ring)) + α(H-C-C-H (ring))
		1474.16	5.2024	α(-CH3)	1436.51	4.8579	α(-CH2 (ring)) + vs(-C-C-C- (ring)) + α(-CH2 (butyl))
		1521.86	14.8475	α(-CH2(ring)) + vs(-C-C-C-(ring))	1464.5	24.602	α(-CH2(butyl))
		1867.11	17.1562	ν(C=O) + α(-COH) + τ(-CH2(ethyl))	1521.03	14.3208	α(-CH2 (ring)) + vs(-C-C-C- (ring)) + α(H-C-C-H (ring))
		3059.53	147.4468	vs(-CH3)	1866.01	16.6873	ν(C=O) + α(-COH) + τ(-CH2(butyl))
		3093.96	90.4507	vass(-CH2(ethyl)) + vass(-CH3)	3039.26	225.3399	vs(-CH2(butyl))
		3111.76	65.332	vass(-CH2(ethyl))	3056.78	150.3069	vs(-CH2(butyl)) + vs(-CH3)
		3141.76	99.8112	vass(-CH3)	3068.07	139.4147	vass(-CH2 (butyl))
		3160.52	155.8493	vass(-CH2(ethyl)) + vs(-CH2(ring)) + ν(-CH(ring))	3095.93	69.8328	vs(-CH2(butyl))
		3246.86	47.8349	vass(-CH2(ring))	3114.41	25.9871	vass(-CH2(butyl))
		3816.41	107.3022	ν(-OH)	3139.34	108.8872	vass(-CH3)
		SCALING FACTOR	0.930201698		3159.14	201.567	vs(-CH2(ring)) + ν(-CH(ring))
					3244.48	45.297	vass(-CH2(ring))
					3816.11	111.2333	ν(-OH)
					SCALING FACTOR	0.936405572	

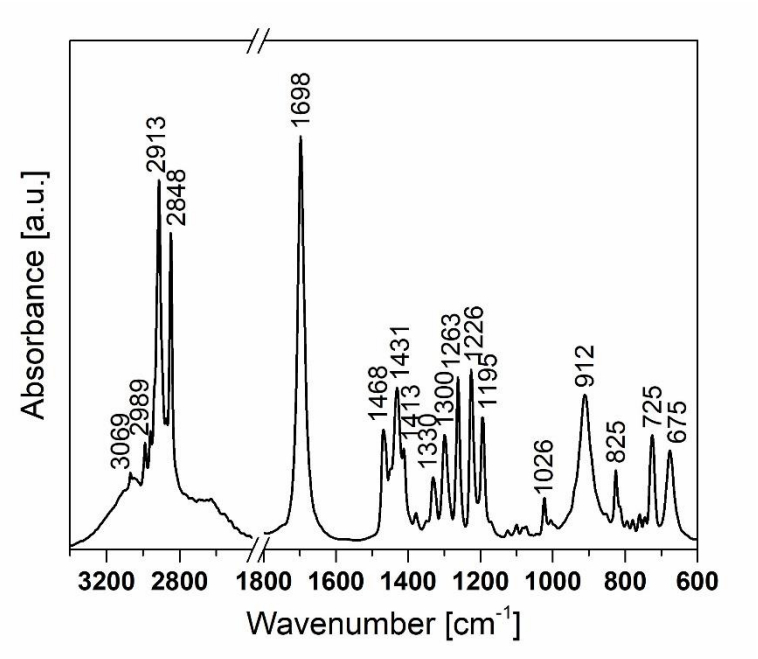

Figure S1. ATR-FTIR spectrum of the CFA standard (*cis*-9,10-methyleneoctadecanoic acid (CycC19)) with marked band positions.

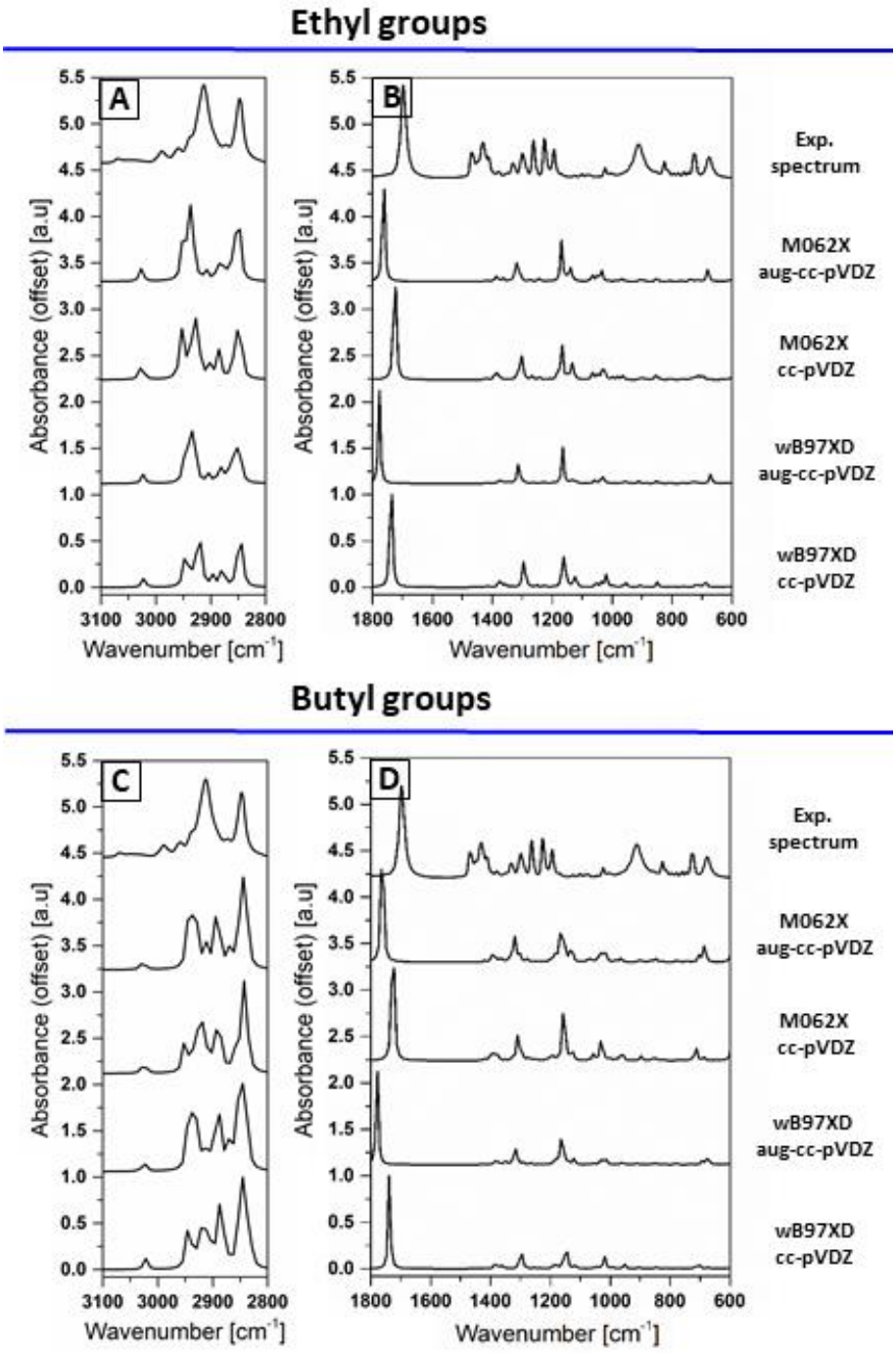

Figure S2. A comparison of the experimental ATR-FTIR spectrum of CFA standard with calculated IR spectra using various length of side chains: (**A**, **B**) ethyl and (**C**, **D**) butyl groups. For each length of side chains spectra were calculated using combinations of functionals: M06-2X, wB97XD and basic sets: cc-pVDZ, aug-cc-pVDZ, as marked on the right side of spectra. Spectra are presented in spectral ranges: (**A**, **C**) 3100 – 2800 cm^{-1} and (**B**, **D**) 1800 – 600 cm^{-1}. The scaling factors for each calculated spectrum are given in Supplementary Materials, Table S2. All spectra in (A, C) were normalized to 1 in the range 3100 -2800 cm^{-1}. All spectra in (B, D) were normalised to 1 in the range 1800 – 600 cm^{-1}.

Table S2. Band position and assignment in the theoretically calculated ATR-FTIR spectra of *cis*-9,10-methyleneoctadecanoic acid, using different combinations of length of side chains, basic sets and functionals. The band used for scaling in each spectrum is highlighted in light grey and the scaling factor for each spectrum is highlighted in orange.

Functional	Basis set	Ethyl			Butyl		
		Theoretical Wavenumber (cm^{-1})			Theoretical Wavenumber (cm^{-1})		
		IR (cm^{-1})	Intensity	Assignment	IR (cm^{-1})	Intensity	Assignment
wB97XD	cc-pVDZ	589.19	53.2784	γ(-COOH)	593.04	51.6178	γ(-COOH)
		626.73	65.62	γ(-COOH) + α(-COO)	628.74	67.9427	γ(-COOH) + α(-COO)
		725.66	41.5133	γ(-COOH) + ρ(-CH2(ethyl)	730.44	40.673	γ(-COOH) + ρ(-CH2(butyl))
		788.2	10.0407	ρ(-CH2) + τ(-CH2 (ring))	749.71	11.2401	ρ(-CH2(butyl))
		908.28	11.858	vs(-C-C-O) + τ(-CH2(ring)) + α(H-C-C-H (ring))	828.49	5.1566	ρ(-CH2(butyl)) + α(-C-C-C- (ring)) + τ(-CH2(ring))
		965.42	7.5227	ρ(-CH2) + τ(-CH2 (ring))	904.85	6.1701	vs(-C-C-O) + ρ(-CH2(ring))
		1033.9	9.1491	ω(-CH2(ring)) + ω(-CH2(ethyl)) + ω(H-C-C-H(ring))	924.43	2.8065	τ(-CH2(butyl)) + ρ(-CH2(butyl)) + τ(-CH2(ring))
		1106.77	19.777	α(H-C-C-H (ring)) + τ(-CH2(ethyl)) + τ(-CH2(ring))	961.9	6.0458	α(-C-C-C- (ring)) + ω(-CH2(butyl))
		1120.37	13.2446	α(H-C-C-H (ring)) + τ(-CH2(ethyl)) + τ(-CH2(ring))	1027.81	6.8145	τ(-CH2(butyl)) + ω(-CH2(ring)) + ω(-CH (ring))
		1138.13	20.0366	α(-C-C-H (ring)) + ρ(-CH2(ethyl)) + τ(-CH2(ring))	1049.26	3.8461	ω(-CH2(ring))
		1217.06	34.5956	δ(-COH) + τ(-CH2(ethyl)) + ρ(-CH2(ethyl)) + ρ(-C-C-H (ring))	1083.94	14.696	vass(-C-C- (butyl)) + ω(-CH2(ring))
		1247.15	111.5994	δ(-COH) + τ(-CH2(ethyl)) +τ(-CH2(ring))	1097.82	30.7353	τ(-CH2(butyl)) + τ(-CH2(ring))
		1328.4	7.3429	ρ(H-C-C-H (ring, ethyl)	1134.83	7.5333	τ(-CH2(butyl)) + τ(-CH2(ring)) + ω(H-C-C-H (ring))
		1361.88	5.05	ω(-CH2(ethyl)	1147.15	4.0593	τ(-CH2(butyl)) + ω(H-C-C-H (ring))
		1396.33	24.9744	α(-COH) + ω(-CH2(ethyl)) + ω(H-C-C-H (ring))	1206.33	33.7072	ρ(-COH) + τ(-CH2(butyl)) +ρ(-CH2(butyl)) + τ(-CH2(ring)) + ω(-C-H (ring))
		1406.19	42.0823	α(-COH) + ω(-CH3)	1233.26	33.0586	δ(-COH) + ω(-CH2(butyl)) +τ(-CH2(butyl)) + ρ(-CH2(ring)) + ρ(H-C-C-H (ring))
		1412.36	25.297	α(-COH) + ω(-CH2(ethyl)) + α(-CH2(ring))	1242.63	70.1082	ω(-CH2(butyl)) + α(-COH)
		1432.39	2.0404	α(-CH2(ring)) + α(-C-C-H (ring))	1263.97	12.0534	δ(-COH) + ω(-CH2(butyl)) + ω(H-C-C-H (ring))
		1455.67	8.587	α(-CH2(ethyl))	1277.63	8.7411	τ(-CH2(butyl)) + ω(-CH2(butyl)) + ω(-CH(ring))
		1477.62	8.2001	α(-CH3)	1365.89	8.4521	α(-COH) + ω(-CH2(butyl)) + δ(-CH(ring))

Functional	Basis set	Ethyl			Butyl		
		Theoretical Wavenumber (cm^{-1})			Theoretical Wavenumber (cm^{-1})		
		IR (cm^{-1})	Intensity	Assignment	IR (cm^{-1})	Intensity	Assignment
		1882.73	353.795	ν(C=O) + α(-COH) + τ(-CH2(ethyl))	1390.44	12.7833	α(-COH) + ω(-CH2(butyl)) + α(-CH2(ring)) + ω(H-C-C-H (ring))
		3040.21	35.3464	νs(-CH2(ethyl))	1411.14	38.6131	α(-COH) + ω(-CH2(butyl)) + δ(-CH(ring))
		3046.79	27.3126	νs(-CH3) + νs(-CH2(ethyl))	1456.95	10.3466	α(-CH2(butyl))
		3136.71	34.4759	νass(-CH3) + νass(-CH2(ethyl))	1479.96	7.2514	α(-CH3)
		3149.58	36.8001	νass(-CH2(ethyl) + ν(-CH(ring))	1489.2	7.5028	α(-CH2(butyl))
		3231.25	10.9901	νass(-CH2(ring))	1881.01	347.6157	ν(C=O) + α(-COH) + τ(-CH2(butyl))
		3800.48	80.3813	ν(-OH)	3036.65	78.7837	νs(-CH3) + νs(-CH2(butyl))
		SCALING FACTOR	0.936537279		3089.38	63.0143	νass(-CH3) + νass(-CH2(butyl))
					3125.68	47.6656	νass(-CH3) + νass(-CH2(butyl))
					3135.24	36.6548	νass(-CH3) + νs(-CH2(butyl)) + ν(-CH2(ring))
					3145.54	32.3427	ν(-CH(ring))
					3231.23	12.3742	νass(-CH2(ring))
					3800.63	80.9905	ν(-OH)
					SCALING FACTOR	0.937635223	
	aug-cc-pVDZ	596.73	63.7292	γ(-COOH)	599.08	57.8357	γ(-COOH)
		626.38	69.3445	γ(-COOH) + α(-COO)	630.78	73.4059	γ(-COOH) + α(-COO)
		745.23	13.3142	ρ(-CH2) + ρ(-C-C-C-) + γ(-COOH)	762.38	31.0397	ρ(-C-C-C-) + γ(-COOH)
		763.3	14.7572	ρ(-CH2 (ethyl)) + ω(-COH)	910.76	4.8018	νs(-C-C-O) + ρ(-CH2(ring)) + ω(-CH2(butyl))
		781.63	6.0197	ρ(-CH2(ethyl)) + τ(-CH2(ring))	957.54	8.1779	α(-C-C-C- (ring)) + ω(-CH2(butyl))
		909.85	15.8449	νs(-C-C-O) + τ(-CH2(ring)) + α(H-C-C-H (ring))	1023.34	11.6104	τ(-CH2(butyl)) + νs(-C-C-C- (butyl, ring)) + ω(-CH2(ring))
		962.82	7.234	α(-C-C-C- (ring)) + ρ(-CH2(ethyl))	1070.12	6.0733	τ(-CH2 (butyl)) + ω(-CH2(ring)) + ω(H-C-C-H (ring))
		1031.18	9.2902	ω(-CH2(ring)) + ω(-CH2(ethyl)) + ω(H-C-C-H(ring))	1098.48	51.1369	ρ(-COH) + τ(-CH2(butyl)) + ρ(-CH2(ring))
		1047.05	6.7059	ω(-CH2(ring))	1126.91	14.772	τ(-CH2(butyl)) + ω(H-C-C-H (ring))

Functional	Basis set	Ethyl			Butyl		
		Theoretical Wavenumber (cm^{-1})			Theoretical Wavenumber (cm^{-1})		
		IR (cm^{-1})	Intensity	Assignment	IR (cm^{-1})	Intensity	Assignment
		1067.88	6.6895	τ(H-C-C-H (ring)) + vass(-C-C-C- (ethyl))	1204.91	21.6323	ρ(-CH2(butyl)) + τ(-CH2(ring)) + ω(-CH (ring))
		1097.05	35.5219	ρ(-COH) + τ(-CH2(ethyl)) + ρ(-CH2(ring))	1235.29	92.2637	δ(-COH) + ω(-CH2(butyl)
		1117.34	15.2285	τ(-CH2(ethyl)) + ρ(-CH2(ring))	1276.75	14.672	δ(-COH) + τ(-CH2(butyl))
		1136.08	19.5905	α(-COH) + τ(-CH2(ethyl)) + τ(-CH2(ring)) + ω(H-C-C-H (ring))	1359.03	7.5185	ω(-CH2(butyl)) + ω(-CH (ring)) + α(-COH)
		1212.13	42.341	δ(-COH) + τ(-CH2(ethyl)) + τ(-CH2(ring))	1384.13	13.196	α(-COH) + ω(-CH2(butyl)) + α(H-C-C-H (ring))
		1247.48	90.5494	δ(-COH) + τ(-CH2(ethyl)) +ρ(-CH2(ring))	1396.19	65.1871	α(-COH) + ω(-CH2(butyl)) + ω(-CH (ring))
		1260.47	18.5188	δ(-COH) + ω(-CH2(ethyl)) + ω(-C-H (ring))	1468.49	11.8409	α(-CH2(butyl))
		1290.67	1.3773	ω(-CH2(ethyl)) + τ(-CH2(ring)) + τ(-CH2(ethyl))	1481.08	7.9592	α(-CH3)
		1326.81	6.0138	τ(-CH2(ethyl)) + ω(H-C-C-H (ring))	1491.96	13.6855	α(-CH2(butyl))
		1354.05	8.0805	ω(-CH2(ethyl)) + ω(-C-H (ring))	1844.12	372.4437	ν(C=O) + α(-COH) + τ(-CH2(butyl))
		1388.28	57.9513	α(-COH)+ τ(-CH2(ethyl) + ω(-CH(ring))	3038.63	80.9691	vs(-CH3) + vs(-CH2(butyl))
		1396.21	23.7076	α(-COH) + ω(-CH2(ethyl))+ ω(-CH(ring))	3052.49	30.8586	vs(-CH2(butyl))
		1468.4	6.9945	α(-CH2(ethyl))	3088.89	56.4046	vass(-CH3) + vass(-CH2(butyl))
		1483.92	14.8575	α(-CH2(ethyl))	3105.31	39.8738	vass(-CH2(butyl))
		1843.41	380.9819	ν(C=O) + α(-COH) + τ(-CH2(ethyl))	3119.1	60.0423	vass(-CH3) + vass(-CH2(butyl))
		3041.64	43.4321	vs(-CH3) + vs(-CH2(ethyl))	3127.8	41.4733	vass(-CH3)
		3082.37	14.0301	vass(-CH3) + vass(-CH2(ethyl))	3150.99	32.6728	ν(-CH(ring))
		3129.65	39.4178	vass(-CH3) + vass(-CH2(ethyl))	3230.87	15.9274	vass(-CH2(ring))
		3155.6	28.8659	vass(-CH2(ethyl) + ν(-CH(ring))	3828.77	77.7509	ν(-OH)
		3232.1	13.7274	vass(-CH2(ring))	SCALING FACTOR	0.937024251	
		3828.31	77.2783	ν(-OH)			
		SCALING FACTOR	0.936096974				
M06-2X	**cc-pVDZ**	585.88	54.008	γ(-COOH)	586.45	55.8901	γ(-COOH)
		626.69	65.6301	γ(-COOH) + α(-COO)	626.78	66.5047	γ(-COOH) + α(-COO)

Functional	Basis set	Ethyl			Butyl		
		Theoretical Wavenumber (cm^{-1})			Theoretical Wavenumber (cm^{-1})		
		IR (cm^{-1})	Intensity	Assignment	IR (cm^{-1})	Intensity	Assignment
		718.35	42.6179	γ(-COOH) + ρ(-CH2(ethyl))	720.23	36.1121	γ(-COOH) + ρ(-CH2(butyl))
		780.02	11.6458	ρ(-CH2(ethyl)) + τ(-CH2(ring))	740.1	13.4172	ρ(-CH2(butyl))
		910.53	10.7298	vs(-C-C-O) + τ(-CH2(ring)) + α(H-C-C-H (ring))	833.75	5.9748	τ(-CH2(butyl)) + α(-C-C-C- (ring)) + ρ(-CH2(butyl))
		976.87	8.6217	α(-C-C-C- (ring)) + ρ(-CH2(ethyl))	907.91	4.3416	vs(-C-C-O) + τ(-CH2(butyl)) + ρ(-CH2(ring))
		1026.86	8.6262	ω(-CH2(ring)) + ω(-CH2(ethyl)) + ω(H-C-C-H(ring))	974.72	4.7532	α(-C-C-C- (ring)) + ω(-CH2(butyl))
		1102.43	26.2195	τ(-CH2(ethyl)) + ρ(-CH2(ring))	1027.85	5.8017	ω(-CH2(ring)) + τ(-CH2(butyl)) + ω(-CH (ring))
		1113.73	13.4252	τ(-CH2(ethyl)) + τ(-CH2(ring)) + α(H-C-C-H (ring))	1084.52	16.9595	τ(-CH2(butyl)) + vass(-C-C-C- (butyl)) + τ(-CH2(ring)) + α(H-C-C-H (ring))
		1133.68	16.5012	ρ(-CH2(ethyl)) + τ(-CH2(ethyl)) +ω(H-C-C-H (ring))	1097.81	21.0193	ρ(-COH) + vass(-C-C- (butyl)) + τ(-CH2(ring)) + α(H-C-C-H (ring))
		1212.35	19.8392	δ(-COH) + τ(-CH2(ethyl)) + ρ(-CH2(ring)) + α(H-C-C-H (ring))	1131	4.6931	τ(-CH2(butyl)) + ρ(H-C-C-H (ring))
		1248.48	134.8336	δ(-COH) + τ(-CH2(ethyl))	1200.9	19.9588	δ(-COH)) + τ(-CH2(butyl)) + τ(-CH2(ring)) + α(H-C-C-H (ring))
		1316.49	6.768	τ(-CH2(ethyl)) + ω(H-C-C-H (ring))	1221.69	8.7772	ω(-CH2(butyl)) + ρ(H-C-C-H (ring))
		1388.18	8.0457	α(-COH) + ω(-CH2(ethyl)) + ω(H-C-C-H (ring))	1236.99	39.304	δ(-COH) + ω(-CH2(butyl)) + ρ(-CH2(ring)) + τ(-CH2(butyl))
		1407.94	82.2086	α(-COH) + ω(-CH2(ethyl))+ ω(-CH(ring)) + α(-CH2(ring))	1245.82	75.5447	α(-COH) + vass(-O-C-C-) + τ(-CH2(butyl)) + τ(-CH2(ring)) + ω(-CH (ring))
		1443.33	10.7463	α(-CH2(ethyl))	1267.68	25.3533	δ(-COH) + τ(-CH2(butyl)) + ρ(-CH2(butyl)) + τ(-CH2(ring)) + ω(-CH2(butyl)) + ω(-CH (ring))
		1467.85	8.678	α(-CH2(ethyl)) + α(-CH2(ring))	1410.65	60.6087	α(-COH) + vass(-O-C-C-) + τ(-CH2(butyl)) + ω(-CH2(butyl))+ α(-CH2(ring))
		1904.45	375.8479	ν(C=O) + α(-COH) + τ(-CH2(ethyl))	1445.45	12.2097	α(-CH2(butyl))
		3051.26	27.6972	vs(-CH3) + vs(-CH2(ethyl))	1480.63	8.3493	α(-CH2(butyl)) + α(-CH2(ring))
		3060.17	15.2555	vs(-CH3) + vs(-CH2(ethyl))	1904.38	369.6616	ν(C=O) + α(-COH) + τ(-CH2(butyl))
		3146.15	31.5145	vass(-CH3) + vass(-CH2(ethyl))	3047.91	61.7076	vs(-CH2(butyl))
		3157.28	27.6363	vass(-CH3) + vass(-CH2(ethyl))	3056.98	30.1311	vs(-CH3)
		3239.45	8.3971	vass(-CH2(ring))	3073.09	18.1185	vs(-CH2(butyl))
		3782.9	93.6337	ν(-OH)	3095.84	58.6963	vass(-CH3) + vass(-CH2(butyl))

Functional	Basis set	Ethyl			Butyl		
		Theoretical Wavenumber (cm^{-1})			Theoretical Wavenumber (cm^{-1})		
		IR (cm^{-1})	Intensity	Assignment	IR (cm^{-1})	Intensity	Assignment
		SCALING FACTOR	0.933145651		3114.24	26.0717	vass(-CH2(butyl))
					3133.82	43.3852	vass(-CH3) + vass(-CH2(butyl))
					3142.95	31.743	vass(-CH3)
					3152.95	25.5331	v(-CH(ring))
					3237.92	9.5577	vass(-CH2(ring))
					3785.39	94.4516	v(-OH)
					SCALING FACTOR	0.934171285	
	aug-cc-pVDZ	591.91	73.2967	γ(-COOH)	590.82	76.6254	γ(-COOH)
		620.77	62.3724	γ(-COOH) + α(-COO)	620.15	60.6644	γ(-COOH) + α(-COO)
		739.63	20.4423	γ(-COOH) + ρ(-CH2(ethyl))	754.51	23.752	γ(-COOH) + ρ(-CH2(butyl))
		772.21	9.6556	ρ(-CH2(ethyl)) + τ(-CH2(ring))	909.83	6.0156	vs(-C-C-O) + τ(-CH2(butyl)) + τ(-CH2(ring)) + ρ(-CH3)
		911.41	14.2785	vs(-C-C-O) + τ(-CH2(ring)) + α(H-C-C-H (ring))	970.82	9.1392	α(-C-C-C- (ring)) + ω(-CH2(butyl))
		973.05	7.3581	ρ(-CH2(ethyl)) + α(-C-C-C- (ring))	1021.01	12.638	ρ(-CH2(butyl)) + τ(-CH2(butyl)) + ω(-CH2(ring)) + ω(-CH (ring))
		1025.97	12.9501	ω(-CH2(ring)) + ω(-CH2(ethyl)) + ω(H-C-C-H(ring))	1093.9	45.9454	α(-COH) + τ(-CH2(butyl)) + ρ(-CH2(ring))+ ω(-CH (ring))
		1093.9	28.5284	τ(-CH2(ethyl)) + ρ(-CH2(ring))	1123.87	9.5484	τ(-CH2(butyl)) + ω(-CH (ring))
		1110.73	14.1046	τ(-CH2(ethyl)) + τ(-CH2(ring)) + α(H-C-C-H (ring))	1199.92	9.9629	ρ(-CH2(butyl)) + ω(-CH (ring)) + ω(-CH2(butyl))
		1131.34	15.8306	ρ(-CH2(ethyl)) + τ(-CH2(ethyl)) +ω(H-C-C-H (ring))	1231.78	116.1563	δ(-COH) + ρ(-CH2(butyl))+ τ(-CH2(butyl))
		1209.23	28.3859	δ(-COH) + τ(-CH2(ethyl)) + ρ(-CH2(ethyl)) +ω(-CH(ring))	1268.9	25.3122	δ(-COH) + τ(-CH2(butyl)) + ρ(-CH2(butyl)) + τ(-CH2(ring)) + ω(-CH2(butyl))
		1250.64	87.0344	δ(-COH) + ω(-CH2(ethyl))	1347.92	5.2391	ω(-CH2(buty)) + ω(-CH (ring))
		1316.76	6.0717	τ(-CH2(ethyl)) + ω(H-C-C-H (ring))	1393.9	67.1766	α(-COH) + ω(-CH2(butyl)) + δ(-CH(ring))
		1344.18	5.5888	α(-COH) + ω(-CH2(ethyl)) + ω(-CH(ring))	1459.3	13.7628	α(-CH2(butyl))
		1389.98	54.3981	α(-COH) + α(-CH2(ethyl)) + α(-CH2(ring)) + ω(-CH3)	1476.21	8.2121	α(-CH3)
		1458.44	8.7057	α(-CH2(ethyl))	1485.97	17.2566	α(-CH2(butyl))

Functional	Basis set	Ethyl			Butyl		
		Theoretical Wavenumber (cm^{-1})			Theoretical Wavenumber (cm^{-1})		
		IR (cm^{-1})	Intensity	Assignment	IR (cm^{-1})	Intensity	Assignment
		1477.74	14.4667	α(-CH2(ethyl)) + α(-CH2(ring))	1866.01	391.6054	ν(C=O) + α(-COH) + τ(-CH2(butyl))
		1867.11	402.0688	ν(C=O) + α(-COH) + τ(-CH2(ethyl))	3056.78	47.3878	νs(-CH3) + νs(-CH2(butyl))
		3059.53	31.2542	νs(-CH3)	3099.88	50.1134	νass(-CH3) + νass(-CH2(butyl))
		3093.96	11.746	νass(-CH3) + νass(-CH2(ethyl))	3114.41	34.5346	νass(-CH2(butyl))
		3111.76	9.9836	νass(-CH2(ethyl)) + ν(-CH (ring))	3130.23	51.3975	νass(-CH3) + νass(-CH2(butyl))
		3135.63	31.4895	νass(-CH3) + νass(-CH2(ethyl))	3139.34	35.8143	νass(-CH3)
		3141.76	33.884	νass(-CH3) + νass(-CH2(ethyl))	3162.01	24.5095	ν(-CH(ring))
		3166.68	26.122	νass(-CH2(ethyl) + ν(-CH(ring))	3244.48	10.7667	νass(-CH2(ring))
		3246.86	8.926	νass(-CH2(ring))	3816.11	83.1051	ν(-OH)
		3816.51	92.8748	ν(-OH)	SCALING FACTOR	0.931460557	
		SCALING FACTOR	0.930623331				

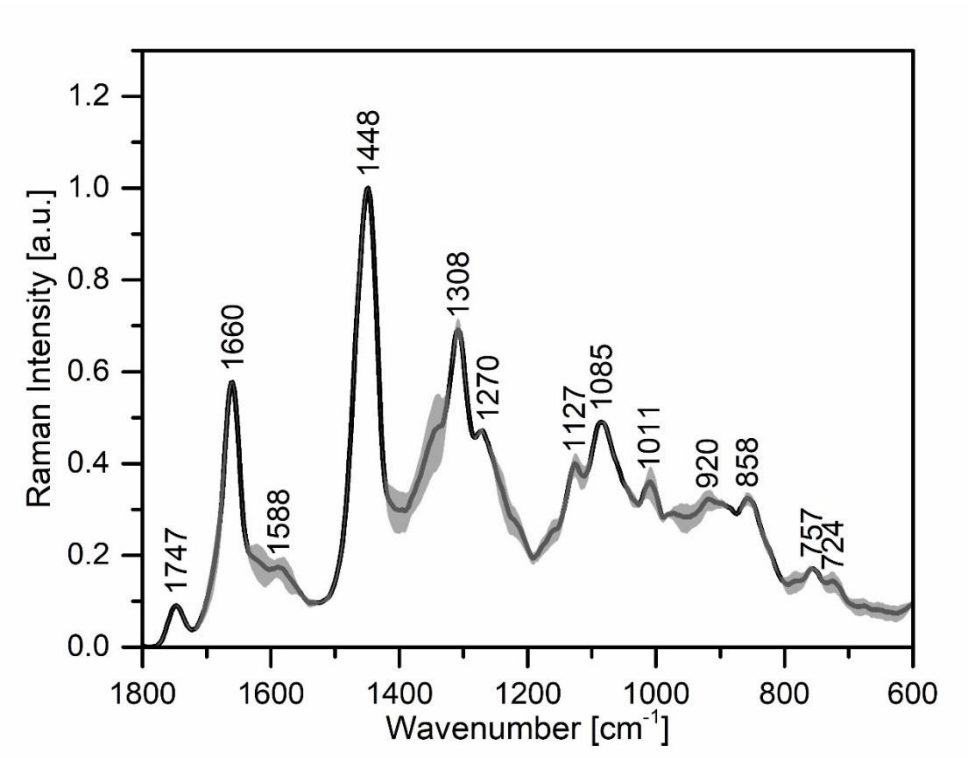

Figure S3. The average Raman spectrum (1800 – 600 cm^{-1}) of LBs from the control cell line (**black line**) together with standard deviation (grey background), with marked band positions.

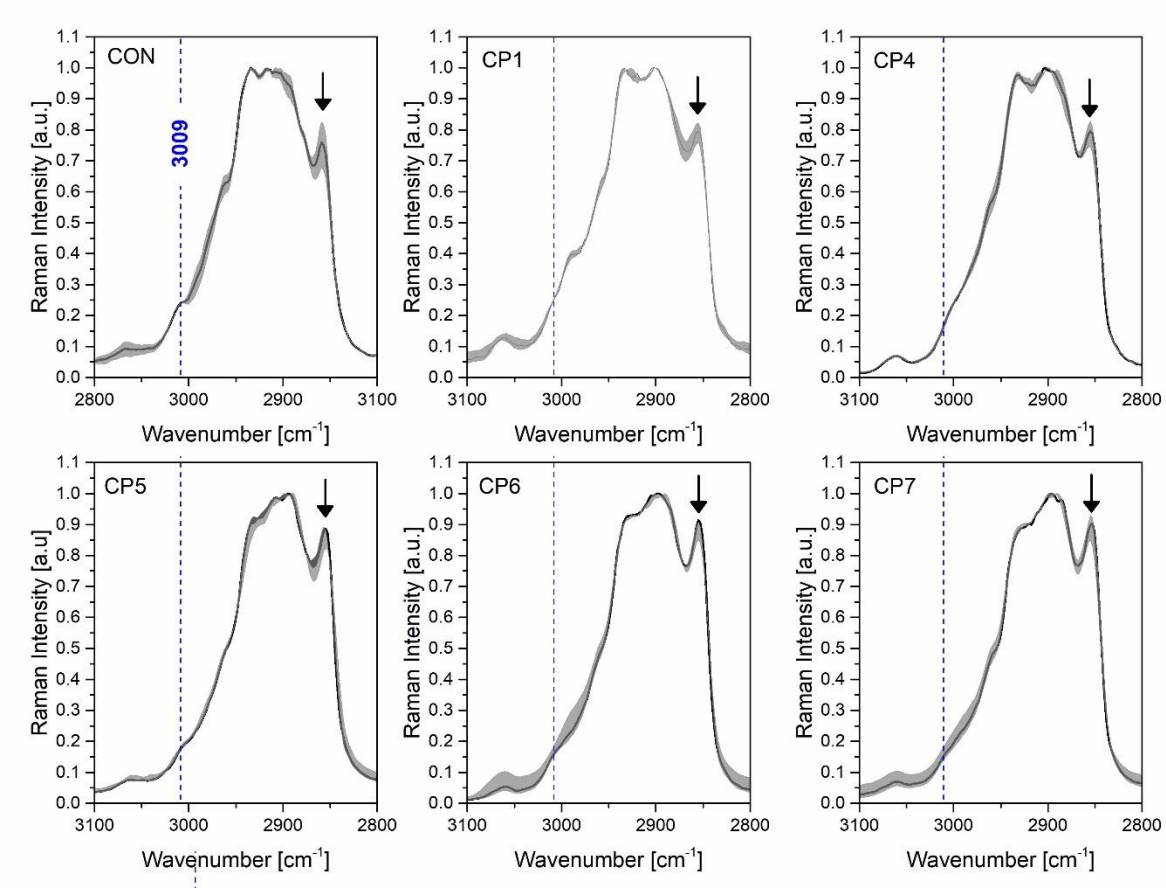

Figure S4. Average Raman spectra (in the range 3100 – 2800 cm^{-1}) of LBs from each cell line (**black line**, in each panel) together with standard deviation (grey background, in each panel). Each spectrum was obtained by averaging all average spectra of LBs originating from the selected cell line (more details are given in the 'Materials and Methods' section). The **black arrow** marks the position of the band originating from $\nu(CH_2)$, located at 2855 cm^{-1}. All spectra were normalized. **Blue dashed line** marks the position of the band located at 3009 cm^{-1} (ν(=C-H)), characteristic for UFAs.

Table S3. Lipid content in the studied cell line obtained *via* GC.

Strain	TCFAs(mg/g DCW)*†	TFAs (mg/g DCW)†	TUFAs(%DCW)**	TSFAs(%DCW)***
CON	0.0	21.3	64.32%	35.68%
CP1	6.7	19.4	24.05%	30.60%
CP4	11.5	35.9	24.41%	34.69%
CP5	11.9	56.1	28.91%	29.89%
CP6	18.3	90.3	19.12%	37.46%
CP7	10.6	70.3	19.35%	31.14%

TFAs – Total Fatty Acids; DCW – Dry Cell Weight; TUFAs – Total Unsaturated Fatty Acids,
TSFAs – Total Saturated Fatty Acids, TCFAs – Total Cyclopropane Fatty Acids
* includes: CycC17, CycC19; ** includes: C16:1, C18:1; ***includes: C16:0, C18:0
†TFAs and TCFAs based on TAG and PL

Table S4. Lipid content of the TAG and PL fractions (Bligh Dyer extraction procedure) obtained *via* GC.

Strain	TAG fraction		PL fraction	
	TAGs (%DCW)	CFAs (%TAGs)	PLs (%DCW)	CAFs (%PLs)
CON	0.6%	0.0%	1.5%	0.0%
CP1	0.7%	42.4%	1.2%	29.9%
CP4	2.2%	27.9%	1.4%	38.4%
CP5	4.3%	17.2%	1.3%	34.4%
CP6	7.4%	16.1%	1.6%	40.0%
CP7	6.2%	12.5%	0.8%	34.2%

TAGs – Triacylglycerols; DCW – Dry Cell Weight; PLs – Phospholipids