Supporting Information

DIRECT LACTONIZATION OF ALKENOLS VIA OSMIUM TETROXIDE-MEDIATED OXIDATIVE CLEAVAGE

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General: All commercially available starting materials were obtained from Aldrich and used without further purification. ^1H and ^{13}C NMR spectra were recorded on either a 300 or 500 MHz NMR spectrometer (VARIAN INOVA) using either CDCl_3 or DMSO-d_6 as solvents. Gas chromatographic analyses were performed using an HP 6890 GC system equipped with an AltechSE-54 capillary column (30m x 320 μm x 0.25 μm). Analytical and prep TLC was performed using pre-coated silica gel 60 F₂₅₄ plates and visualized using either UV light, *p*-anisaldehyde or potassium permanganate stain. Column chromatography utilized Silicycle 40-60 μm silica gel. As a general note, Oxone or purified Oxone ($\text{KHSO}_5 \cdot \text{H}_2\text{O}$) can be used interchangeably for oxidations described in this manuscript without any substantial observable difference.

Experimental:

General Procedure for the Oxidative Cyclization Yielding Water-Soluble Products:

A 0.1 M solution of the appropriate alkenol was prepared in dimethylformamide that had been dried over calcium sulfate. Oxone (4.0 equiv) was added in one portion, followed by 1.0 mol% of OsO₄ as a 0.2 M solution in *t*BuOH or dichloromethane. An internal standard could be added either prior to or immediately following reaction to determine the in-pot yield. Both 1,2,3,4-tetramethylbenzene and dodecane were used in this capacity. The reaction was stirred at room temperature, and progress monitored by either TLC or GC. In a few cases, the reactions were also performed in deuterated DMF and the NMR was compared to that of an authentic sample of the lactone in deuterated DMF prior to isolation using benzene as an internal standard. Compounds **13a** and **14a** are known compounds and had spectral properties in accord with the literature data, as well as with authentic samples obtained from Aldrich (**7a-9a**).¹⁻³ In some cases, the water-soluble products could be isolated by diluting the final reaction mixture with ethyl acetate, filtering off the resulting solids, and concentrating the reaction mixture under vacuum at rt for several hours. The resulting residue could then be chromatographed. This approach was successful for higher-boiling lactones, but the lower-boiling lactones were removed along with the DMF under high vacuum.

General Procedure for the Oxidative Cyclization Yielding Water-Insoluble Products:

A 0.1 M solution of the appropriate alkenol was prepared in dimethylformamide that had been dried over calcium sulfate. Oxone (4.0 equiv) was added in one portion, followed by 1.0 mol% of OsO₄ as a 0.2 M solution in *t*BuOH or dichloromethane. The reaction was stirred at room

temperature, and progress monitored by either TLC or GC. After completion of the reaction, an equal volume of water was added and the solution was saturated with NaCl. It was then extracted with 3x portions of ethyl acetate. The combined organics were washed 1x with NaHCO₃, dried over Na₂SO₄ and evaporated under reduced pressure. The resultant lactones could be purified by column chromatography using 1:1 petroleum ether/diethyl ether. Compounds **6**, **10a**, and **15a-19a** are known and had NMR spectra in accord with the literature data.⁴⁻¹⁰

6; ¹H NMR (500 MHz, CDCl₃) δ 7.99 (d, 1H), 7.65 (m, 2H), 7.61 (d, 1H), 7.53 (m, 2H), 7.45 (m, 2H), 5.02 (d, 2H); ¹³C NMR (500 MHz, DMF-d₇) δ 170.3, 139.3, 137.4, 136.1, 133.4, 132.0, 131.4, 130.7, 129.4, 129.4, 129.3, 129.1, 69.2. **10a**; ¹H NMR (500 MHz, CDCl₃) δ 3.99 (m, 1H), 2.65 (dd, 1H), 2.51 (t, 1H), 2.09 (m, 1H), 0.94-1.97 (several m, 12H); ¹³C NMR (500 MHz, CDCl₃) δ 175.7, 82.2, 42.0, 37.9, 35.2, 33.4, 32.9, 24.8, 24.4, 22.5. **15a**; ¹H NMR (500 MHz, CDCl₃) δ 2.5 (m, 2H), 2.1 (m, 2H), 1.9 (m, 2H), 1.8 (m, 2H), 1.6 (m, 4H); ¹³C NMR (500 MHz, CDCl₃) δ 176.6, 94.8, 38.3, 32.4, 29.7, 23.6. **16a**; ¹H NMR (500 MHz, CDCl₃) δ 3.7 (m, 1H), 2.5 (dd, 1H), 2.2 (m, 2H), 1.9 (m, 3H), 1.8 (m, 1H), 1.5 (m, 1H), 1.2-1.4 (m, 3H); ¹³C NMR (500 MHz, CDCl₃) δ 176.4, 85.1, 44.8, 35.8, 30.2, 28.3, 25.3, 24.0. **17a**; ¹H NMR (500 MHz, CDCl₃) δ 7.9 (d, 1H), 7.7 (t, 1H), 7.5 (d, 1H), 7.5 (t, 1H), 5.3 (s, 2H); ¹³C NMR (500 MHz, CDCl₃) δ 171.1, 146.5, 135.9, 134.0, 129.0, 125.7, 122.1, 69.6. **19a**; ¹H NMR (500 MHz, CDCl₃) δ 7.39 (d, 1H), 7.23 (m, 2H), 7.16 (d, 1H), 5.53 (dd, 1H), 2.75 (m, 1H), 2.60 (m, 1H), 2.34 (s, 3H), 2.09-2.16 (m, 2H), 2.02 (m, 2H); ¹³C NMR (500 MHz, CDCl₃) δ 171.6, 137.6, 134.1, 130.5, 128.0, 126.3, 125.6, 78.9, 29.5, 29.1, 18.9, 18.8.

Oxidative Cyclization of **12**.

Oxidation of compound **12**¹¹ proceeds best if the oxidative cleavage of the olefinic bond is performed with the addition of NaHCO₃.¹² Compound **12** (0.1 g, 0.79 mmol, 1.0 equiv) was placed in dry DMF (10 mL). Purified Oxone (0.77 g, 4.74 mmol, 6.0 equiv), NaHCO₃ (0.50 g, 4.74 mmol, 6.0 equiv), and OsO₄ (0.01 equiv) were added and the reaction heated to 40° C overnight. The reaction was diluted with an equal volume of water, saturated with NaCl and extracted 3x with diethyl ether. The combined organics were washed with brine, dried over Na₂SO₄, and concentrated under reduced pressure. The resulting residue was not purified, but analyzed by NMR to give a 45% yield of **12a**.¹³ ¹H NMR (500 MHz, CDCl₃) δ 4.5 (t, 2H), 2.8 (t, 2H), 2.4 (m, 2H), 2.3 (m, 2H), 1.9 (m, 2H), 1.8 (m, 2H); ¹³C NMR (500 MHz, CDCl₃) δ 210.7, 174.6, 60.5, 42.1, 41.4, 34.9, 24.5, 23.6.

Preparation of Substrates for the Oxidative Cyclizations:

tert-Butyl-dimethyl-(2'-vinyl-2-biphenylmethanol)-silane (**5**).¹⁴ The 2,2'-biphenylmethanol (5.0 g 23.4 mmol, 1.0 equiv) was combined with *tert*-butyldimethylsilyl chloride (4.2 g, 28.1 mmol, 1.2 equiv) and imidazole (1.9 g, 28.1 mmol, 1.2 equiv) in DMF (25 mL). The solution was allowed to stir at rt overnight and then quenched by addition of an equal volume of water. The solution was extracted 3x with diethyl ether and after standard workup, the residue was purified via column chromatography to yield the mono-protected diol in 63% yield. The mono-alcohol (5.0 g, 15.2 mmol, 1.0 equiv) was placed in dichloromethane and treated with NMO (2.7 g, 22.8 mmol, 1.5 equiv) and 5 mol% TPAP and stirred at rt for 1 h. The mixture was diluted with dichloromethane and washed 3x with water, 1x with brine and 1x with saturated copper sulfate solution. An emulsion ensued which was passed through a pad of Celite. The organics were separated, dried over Na₂SO₄, and concentrated under reduced pressure. The aldehyde was purified by passing it through a plug of silica eluted with 9:1 hexanes/ethyl acetate to obtain the product in 89% yield as a pale green, pungent liquid. Triphenylphosphonium bromide (4.0 g, 11.0 mmol, 1.2 equiv) was placed in dry THF, cooled to 0° C, and treated with *n*BuLi (12.0 mmol, 12 mL of a 1 M solution, 1.3 equiv). The mixture was stirred for 10 min, then a solution of the aldehyde (3.0 g, 9.2 mmol, 1.0 equiv) in THF was added dropwise to the ylide. The reaction was stirred overnight at rt and diluted with diethyl ether. The solution was washed with 2x water and 1x brine, dried over Na₂SO₄, and concentrated under reduced pressure. The residue was purified by column chromatography (99:1 hexanes/ethyl acetate) to give **5** in 78% yield as a clear liquid. ¹H NMR (500 MHz, CDCl₃) δ 7.67 (m, 2H), 7.42 (t, 1H), 7.37 (m, 2H), 7.31 (t, 1H), 7.17 (d, 1H), 7.13 (d, 1H), 6.35 (dd, 1H), 5.68 (dd, 1H), 5.12 (dd, 1H), 4.44 (d, 2H), 0.91 (s, 9H), -0.01 (2 s, 6H); δ ¹³C NMR (500 MHz, CDCl₃) 139.4, 139.3, 138.5, 136.9, 135.1, 129.9, 129.6, 127.6, 127.5, 127.4, 126.5, 124.8, 114.6, 62.9, 25.9, 18.3, -5.4.

2-Pent-4-enyl-cyclohexanol (10).¹⁵ 5-Bromo-1-pentene (1 g, 6.7 mmol, 2.6 equiv) in dry diethyl ether (1 mL) was added dropwise to Mg metal (0.16 g, 6.5 mmol, 2.5 equiv) over 15 minutes. After refluxing commenced, additional diethyl ether was added to bring the total volume to 10 mL. After addition of the alkene was complete, the mixture was allowed to reflux for 1 h. The reaction was then cooled in an ice bath and cyclohexene oxide (0.25 g in 5 mL of ether, 2.6 mmol, 1.0 equiv) was added dropwise over 5 minutes. The reaction was allowed to warm to rt, stirred for 3 h, and quenched with saturated ammonium chloride. The layers were separated and the aqueous layer was extracted 3x with diethyl ether. The combined organics were washed with water and brine, dried over Na₂SO₄, and concentrated under reduced pressure. The residue was purified by column chromatography (hexane/ethyl acetate gradient) to yield **10** in 70% yield. ¹H NMR (500 MHz, CDCl₃) δ 5.8 (m, 1H), 4.9 (m, 2H), 3.2 (m, 1H), 0.8-2.1 (overlapping m, 15H); ¹³C NMR (500 MHz, CDCl₃) δ 139.1, 114.3, 74.7, 45.0, 35.7, 34.2, 31.7, 30.1, 25.9, 25.5, 24.9.

2-(2-Allyl-phenoxy)-ethanol (11): 2-Allyl phenol (2.0 g, 14.9 mmol, 1.0 equiv) was combined with 2-bromoethanol (2.0 g, 16.4 mmol, 1.1 equiv) and NaOH (0.9 g, 22.4 mmol, 1.5 equiv) in a

50/50 mixture of dioxane/water (30 mL). The mixture was heated to reflux for 4 h and worked up by extraction with diethyl ether. The residue was purified by column chromatography (3:1 hexanes/ethyl acetate) to give **11** in 46% yield as a thick, light yellow oil. ^1H NMR (500 MHz, CDCl_3) δ 7.20 (m, 2H), 6.95 (t, 1H), 6.87 (d, 1H), 6.02 (m, 1H), 5.06 (m, 2H), 4.10 (t, 2H), 3.96 (t, 2H), 3.44 (d, 2H), 2.35 (bs, 1H); ^{13}C NMR (500 MHz, CDCl_3) δ 156.3, 137.5, 130.2, 128.4, 127.5, 121.1, 115.1, 111.2, 69.2, 61.4, 34.7.

*2-Cyclohex-1-en-1-ylethanol (12):*¹¹ Compound **12** was prepared according to the method of Crotti with the exception that 2.2 equiv of DIBAL in THF was used as the reducing agent in place of LAH. ^1H NMR (500 MHz, CDCl_3) δ 5.5 (bs, 1H), 3.6 (t, 2H), 2.2 (t, 2H), 2.0 (m, 2H), 1.9 (m, 2H), 1.6 (m, 2H), 1.5 (m, 3H); ^{13}C NMR (500 MHz, CDCl_3) δ 134.0, 124.2, 60.2, 41.1, 28.0, 25.2, 22.8, 22.3.

*2,2-Dimethyl-pent-4-en-1-ol (13):*¹⁶ 2,2-Dimethyl-4-pentenal (1.0 g, 8.9 mmol, 1.0 equiv) was placed in methanol (10 mL) and cooled to 0° C in an ice bath. Sodium borohydride (0.68 g, 17.9 mmol, 2.0 equiv) was added in portions over 15 minutes and the reaction allowed to warm slowly to rt and stirred for 1 h. A small amount of water was added to the reaction mixture and the methanol was removed under reduced pressure. The remaining water was extracted with

three portions of diethyl ether and the organics combined and washed with brine, dried over Na_2SO_4 , and evaporated under reduced pressure to yield the title compound in 92% yield as a clear liquid. This material could be used without further purification.

2-Methyl-hex-5-en-2-ol (14):¹⁷ The 5-hexen-2-one (1.0 g, 10.2 mmol, 1.0 equiv) was placed in diethyl ether and cooled to 0° C in an ice bath. Methyl magnesium iodide (10.2 mmol, 1.0 equiv as a 1M solution in diethyl ether) was added dropwise over 15 minutes and the solution was allowed to warm slowly to rt and stirred for 1 h. After standard work-up, the residue was purified via column chromatography (95:5 hexanes/ethyl acetate) to give **14** in 91% yield as a clear liquid. ^1H NMR (500 MHz, CDCl_3) δ 5.8 (m, 1H), 5.0 (m, 2H), 2.1 (m, 2H), 1.5 (t, 2H), 1.2 (s, 6H); ^{13}C NMR (500 MHz, CDCl_3) δ 139.0, 114.4, 70.9, 42.7, 29.2, 28.7.

2-Allyl-cyclohex-1-ol (15):¹⁹ Allyl magnesium bromide (30.6 mL, 30.6 mmol, 3.0 equiv as a 1 M solution in diethyl ether) was added to dry diethyl ether (25 mL). Cyclohexene oxide (1.0 g, 10.2 mmol, 1.0 equiv) was added dropwise over 15 minutes and the reaction was refluxed for 3 h and then cooled. Saturated ammonium chloride was added and the reaction was diluted with diethyl ether, washed 3x with water and 1x with brine. The combined organics were dried over Na_2SO_4 and concentrated under reduced pressure. The residue was purified via column chromatography (3:1 hexanes/ethyl acetate) to give **15** in 96% yield as a light yellow oil. ^1H

NMR (500 MHz, CDCl_3) δ 5.8 (m, 1H), 5.0 (dd, 1H), 4.9 (dd, 1H), 3.2 (m, 1H), 2.4 (m, 1H), 1.9 (m, 2H), 1.5-1.8 (m, 4H), 1.0-1.3 (several m, 4H), 0.9 (m, 1H); ^{13}C NMR (500 MHz, CDCl_3) δ 137.4, 115.9, 74.6, 44.9, 37.4, 35.5, 30.3, 25.5, 24.9.

1-But-3-enyl-cyclopentanol (16):¹⁸ The Grignard reagent of 4-bromo-1-butene (2.8 g, 17.9 mmol, 1.5 equiv) was prepared in a similar manner as for compound **10**, cooled in an ice bath and a solution of cyclopentanone (1.0 g, 11.9 mmol, 1.0 equiv) in diethyl ether was added dropwise over 15 minutes. The reaction was allowed to warm to rt and stirred until it was complete as evidenced by GC analysis. Standard workup and purification by column chromatography (3:1 hexanes/ethyl acetate) gave **16** in 73% yield as a clear liquid. ^1H NMR (500 MHz, CDCl_3) δ 5.9 (m, 1H), 5.0 (d of t, 1H), 4.9 (dd, 1H), 2.2 (m, 2H), 1.8 (m, 1H), 1.4-1.7 (several m, 9H), 1.3 (br s, 1H); ^{13}C NMR (500 MHz, CDCl_3) δ 139.3, 114.3, 82.5, 40.5, 39.8, 29.3, 23.8.

tert-Butyl-dimethyl-(2-vinyl-benzyloxy)-silane (17):²⁰ The same procedure outlined below for compound **5** was followed to yield the mono-protected alcohol in 45% yield, the aldehyde in 81% yield, and the alkene in 68% yield. ^1H NMR (500 MHz, CDCl_3) δ 7.5 (d, 1H), 7.4 (d, 1H),

7.2 (m, 2H), 6.9 (dd, 1H), 5.6 (dd, 1H), 5.3 (dd, 1H), 4.8 (s, 2H), 0.9 (s, 9H), 0.08 (s, 6H); ^{13}C NMR (500 MHz, CDCl_3) δ 138.1, 135.8, 134.0, 127.7, 127.2, 126.9, 125.5, 115.8, 63.1, 25.9, 18.4, -5.3.

Procedure for oxidative cyclization of:

Compound **25** (1.0 g, 0.39 mmol, 1.0 equiv) was placed in dry acetonitrile (10 mL) and soluble Oxone ($n\text{Bu}_4\text{NHSO}_5$, 0.6 g, 1.7 mmol, 4.4 equiv) was added, followed by 2.5 mol% of OsO_4 as a 0.2 M solution in CH_2Cl_2 . The reaction was refluxed overnight, after which the solvent was removed under reduced pressure. The residue was picked up with Et_2O and stirred vigorously until the gummy brown residue was transformed into a brown powder. The solid was filtered and washed with Et_2O . The solvent from the filtrate was removed under reduced pressure to yield a brown oil, which was purified by silica flash chromatography using 1:1 petroleum ether/ Et_2O to give the desired lactone in 64% yield. ^1H NMR (500 MHz, CDCl_3) δ 3.6 (d, 1H), 3.4 (d, 1H), 2.4 (m, 2H), 1.5-2.0 (m, 4H), 1.3 (s, 3H), 0.8 (s, 9H), 0.0-0.01 (2 s, 6H); ^{13}C NMR (500 MHz, CDCl_3) δ 171.3, 83.7, 69.0, 29.7, 29.1, 25.7, 24.4, 18.1, 16.7, -5.6, -5.7.

Oxidative lactonization of 4 -> 6 in an NMR tube (observation of the hemiacetal intermediate):

Deprotection of **4** (100 mg, 0.305 mmol) with TBAF (0.915 mmol, 3.0 equiv, 1 M in THF) proceed smoothly to deliver the hydroxy-aldehyde in quantitative yield. Upon routine work-up the product was purified by flash column chromatography. After thorough drying of the purified residue, the material was picked up in ⁷d-DMF (0.75 mL) and its NMR was recorded. As can be seen in the following page, the hydroxy-aldehyde **4a** exists mainly in its hemiacetal form **4b**. This is evident by the small aldehydic signal at 9.75 ppm and the presence of the anomeric proton signal at 5.7 ppm. Addition of KHSO₅•H₂O (2.0 equiv) to the NMR tube resulted in the clean conversion of the **4a/4b** mixture to the expected lactone product **6** (selected spectra taken over 6 h are shown in the following pages).

References:

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INDEX	FREQUENCY	PPM	HEIGHT
1	17595.028	139.962	19.4
2	17432.007	138.665	21.8
3	16300.449	129.664	69.1
4	16277.434	129.481	67.7
5	16102.906	128.093	65.9
6	16047.287	127.651	63.3
7	9711.519	77.252	95.4
8	9678.915	76.992	101.2
9	9647.270	76.741	103.6
10	7906.780	62.896	71.0

4

O=Cc1ccccc1-c2ccccc2COCc3ccccc3

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INDEX	FREQUENCY	PPM	HEIGHT
1	17523.107	139.390	17.9
2	17513.518	139.314	22.0
3	17409.952	138.490	15.8
4	17083.909	135.896	18.6
5	16979.384	135.065	39.8
6	16823.076	133.822	6.4
7	16803.897	133.669	5.4
8	16325.382	129.863	46.6
9	16298.531	129.649	44.7
10	16176.745	128.680	7.0
11	16154.689	128.505	7.5
12	16147.018	128.444	6.4
13	16040.574	127.597	42.5
14	16033.862	127.544	48.6
15	16016.601	127.406	44.4
16	15901.527	126.491	72.0
17	15688.641	124.798	42.7
18	14402.692	114.568	35.6
19	9711.520	77.252	51.5
20	9679.874	77.000	50.4
21	9647.270	76.741	49.0
22	7905.821	62.888	47.3
23	3259.720	25.930	150.5
24	2304.608	18.332	18.9
25	-685.391	-5.452	45.5

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INDEX	FREQUENCY	PPM	HEIGHT
1	12847.181	170.245	17.2
2	10485.739	138.952	33.4
3	10356.180	137.235	29.3
4	10172.493	134.801	48.4
5	10003.201	132.558	99.9
6	9955.408	131.924	117.0
7	9857.519	130.627	35.0
8	9818.939	130.116	106.6
9	9708.381	128.651	142.1
10	9699.744	128.536	165.5
11	9690.531	128.414	110.0
12	5842.319	77.420	127.4
13	5810.649	77.000	128.2
14	5778.403	76.573	131.4
15	5219.281	69.163	120.2

7a

INDEX	FREQUENCY	PPM	HEIGHT
1	13438.371	178.079	9.7
2	5864.917	77.719	16.2
3	5831.678	77.279	17.8
4	5800.453	76.865	18.7
5	5190.064	68.776	137.6
6	2112.939	28.000	85.4
7	1688.890	22.380	55.9

INDEX	FREQUENCY	PPM	HEIGHT
1	12928.831	171.327	37.8
2	5843.888	77.440	41.1
3	5811.657	77.013	42.6
4	5779.425	76.586	40.6
5	5235.514	69.379	100.2
6	4813.480	63.786	14.3
7	2532.076	33.554	18.7
8	2244.005	29.736	94.5
9	2108.027	27.935	18.0
10	1675.920	22.209	117.7
11	1606.420	21.288	17.9
12	1433.175	18.992	76.0

INDEX	FREQUENCY	PPM	HEIGHT
1	13289.424	176.105	29.3
2	5841.875	77.414	24.3
3	5809.643	76.987	24.8
4	5777.411	76.560	23.7
5	5214.363	69.098	113.5
6	2589.489	34.315	110.9
7	2191.629	29.042	123.3
8	2164.433	28.682	126.7
9	1713.188	22.702	101.6

INDEX	FREQUENCY	PPM	HEIGHT
1	10495.333	139.079	32.0
2	8624.884	114.293	75.0
3	5842.881	77.427	85.4
4	5810.649	77.000	86.1
5	5779.425	76.586	81.8
6	5635.389	74.678	64.5
7	3398.304	45.033	68.2
8	2694.241	35.703	79.2
9	2578.409	34.168	81.9
10	2391.062	31.685	83.3
11	2270.192	30.084	88.4
12	1953.918	25.892	84.6
13	1926.723	25.532	86.8
14	1876.361	24.865	89.3

INDEX	FREQUENCY	PPM	HEIGHT
1	22083.862	175.669	11.4
2	10330.041	82.172	45.9
3	9711.519	77.252	285.0
4	9679.874	77.000	304.7
5	9648.229	76.748	299.7
6	5279.263	41.995	41.2
7	4769.103	37.937	64.0
8	4421.964	35.175	57.8
9	4200.447	33.413	57.0
10	4140.033	32.933	52.2
11	3910.845	31.109	9.1
12	3753.578	29.858	9.0
13	3334.517	26.525	10.2
14	3164.784	25.175	11.2
15	3112.042	24.755	57.3
16	3069.848	24.420	45.7
17	2823.398	22.459	48.3

INDEX	FREQUENCY	PPM	HEIGHT
1	16850.885	134.043	28.6
2	15608.089	124.157	57.2
3	9712.479	77.259	85.6
4	9679.874	77.000	87.1
5	9648.229	76.748	87.1
6	7564.436	60.172	79.6
7	5168.026	41.110	96.3
8	3532.471	28.020	83.3
9	3170.538	25.221	95.2
10	2869.428	22.825	79.3
11	2806.138	22.322	87.2

INDEX	FREQUENCY	PPM	HEIGHT
1	26493.104	210.743	17.0
2	21947.692	174.586	25.3
3	9711.530	77.252	157.4
4	9679.874	77.000	160.1
5	9647.270	76.741	151.5
6	7539.917	60.455	135.2
7	5296.525	42.132	121.2
8	5198.712	41.354	124.9
9	4388.401	34.908	162.6
10	3074.643	24.458	145.0
11	2972.994	23.649	150.6

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INDEX	FREQUENCY	PPM	HEIGHT
1	17502.970	139.230	58.0
2	14362.416	114.248	85.5
3	10358.810	82.401	45.0
4	9712.479	77.259	98.4
5	9679.875	77.000	94.9
6	9648.229	76.748	99.9
7	5092.269	40.507	66.8
8	4991.579	39.706	205.3
9	3674.944	29.233	86.0
10	2982.584	23.725	178.1

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INDEX	FREQUENCY	PPM	HEIGHT
1	22204.691	176.630	21.4
2	11922.854	94.842	27.7
3	9711.520	77.252	55.6
4	9679.875	77.000	55.5
5	9647.271	76.741	53.3
6	4818.969	38.333	99.4
7	4070.031	32.376	28.5
8	3731.523	29.683	27.5
9	2972.036	23.642	100.0

INDEX	FREQUENCY	PPM	HEIGHT
1	17278.576	137.445	86.8
2	14572.425	115.919	113.2
3	9710.561	77.244	113.3
4	9678.916	76.992	116.0
5	9646.311	76.733	106.4
6	9372.052	74.551	84.1
7	5643.664	44.893	104.5
8	4701.018	37.395	106.9
9	4468.953	35.549	143.8
10	3813.033	30.331	134.1
11	3203.142	25.480	157.6
12	3125.467	24.862	152.8

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INDEX	FREQUENCY	PPM	HEIGHT
1	22177.839	176.417	16.3
2	10698.277	85.101	95.6
3	9711.520	77.252	141.5
4	9679.874	77.000	145.5
5	9647.270	76.741	139.1
6	5628.320	44.771	102.6
7	4505.393	35.839	101.3
8	3794.813	30.186	114.2
9	3560.829	28.325	110.3
10	3180.127	25.297	119.2
11	3021.901	24.038	120.1

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INDEX	FREQUENCY	PPM	HEIGHT
1	17363.922	138.124	14.9
2	17072.402	135.805	13.7
3	16848.008	134.020	34.9
4	16048.246	127.658	41.9
5	15989.750	127.193	44.2
6	15959.063	126.949	49.6
7	15777.822	125.507	42.5
8	14553.246	115.766	41.0
9	9711.519	77.252	208.8
10	9679.874	77.000	208.7
11	9647.270	76.741	200.4
12	7936.507	63.132	51.0
13	3260.678	25.938	144.5
14	2311.320	18.386	13.9
15	-663.335	-5.277	64.1

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INDEX	FREQUENCY	PPM	HEIGHT
1	21499.863	171.024	10.8
2	18417.806	146.507	30.7
3	17074.320	135.820	11.2
4	16922.806	134.615	9.8
5	16841.296	133.967	129.4
6	16451.963	130.870	11.1
7	16217.980	129.008	126.2
8	15808.509	125.751	143.6
9	15790.289	125.606	10.4
10	15344.378	122.059	94.5
11	9711.520	77.252	128.3
12	9679.874	77.000	130.8
13	9647.270	76.741	127.8
14	9227.251	73.400	9.8
15	8749.695	69.601	141.4

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INDEX	FREQUENCY	PPM	HEIGHT
1	12945.954	171.554	28.1
2	10383.529	137.598	29.0
3	10121.646	134.127	29.0
4	9846.669	130.483	88.7
5	9660.329	128.014	97.6
6	9533.417	126.332	87.5
7	9477.011	125.585	74.3
8	5954.685	78.909	75.8
9	5842.881	77.427	74.7
10	5810.649	77.000	73.0
11	5779.425	76.586	77.1
12	2222.852	29.456	83.3
13	2199.686	29.149	92.9
14	1427.131	18.912	53.4
15	1417.059	18.778	88.2

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CC(C(=O)O)CCC(C1=CC=CC=C1)C(=O)Si(C)(C)C(C)(C)C

INDEX	FREQUENCY	PPM	HEIGHT
1	17440.638	138.734	36.3
2	14394.061	114.500	49.5
3	9712.478	77.259	55.8
4	9679.874	77.000	63.2
5	9648.229	76.748	61.7
6	9080.532	72.232	31.4
7	8818.739	70.150	46.0
8	4785.405	38.066	51.3
9	4311.685	34.298	50.3
10	3250.130	25.854	136.7
11	2905.868	23.115	45.8
12	2903.950	23.100	51.0
13	-692.104	-5.505	36.7
14	-690.186	-5.490	38.2

INDEX	FREQUENCY	PPM	HEIGHT
1	12927.557	171.324	14.8
2	6312.912	83.663	32.5
3	5842.237	77.425	36.9
4	5810.171	77.000	36.5
5	5778.106	76.575	37.5
6	5205.508	68.987	24.3
7	2244.035	29.739	46.7
8	2194.791	29.087	46.8
9	1939.413	25.702	148.5
10	1837.491	24.352	56.2
11	1365.670	18.099	19.2
12	1256.877	16.657	42.2
13	-420.833	-5.577	36.6
14	-426.559	-5.653	30.0

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