Chiral Lewis Acid-Catalyze Asymmetric Baylis-Hillman Reaction

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Supporting Information

An effective chiral Lewis acid catalyzed asymmetric Baylis-Hillman reaction has been developed. Good to high enantioselectivities can be obtained using 3 mol% of catalyst. Novel camphor-derived dimerized ligands were prepared from the condensation of (+)-ketopinic acid with the corresponding diamines and hydrazine under acidic conditions. When α -naphthyl acrylate was used as a Michael acceptor, the reaction completes within 20 min with high stereoselectivity and reasonable chemical yields.

CH1675

Space Group and Cell Dimensions Tetragonal, P 43212
a 7.8028(13) c 40.282(4)
Volume 2452.5(5) Å³

Empirical formula : C₂₆ H₃₈ N₂ O₄

Cell dimensions were obtained from 25 reflections with 2Theta angle in the range 18.86 - 24.82 degrees.

Crystal dimensions : 0.45 X 0.40 X 0.35 mm

FW = 442.59 Z = 4 F(000) = 960.56

Dcalc 1.199Mg.m-3, mu 0.08mm-1, lambda 0.70930A, 2Theta(max) 51.8

The intensity data were collected on a Nonius diffractometer, using the theta/2theta scan mode.

The h,k,l ranges used during structure solution and refinement are :--
Hmin,max -9 9; Kmin,max -6 6; Lmin,max -48 49

No. of reflections measured	5242
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No. of unique reflections	2424
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No. of reflections with $I_{net} > 2.0\sigma(I_{net})$	1705
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Merging R-value on intensities 0.030

Absorption corrections were made.

The minimum and maximum transmission factors are 0.909190 and 0.979513.

Details of the last least squares cycle

35 atoms, 146 parameters Full-matrix on Fo Unit wts

The residuals are as follows :-

Significant reflections: 1084 Rf 0.059, Rw 0.051

All reflections: 1529 Rf 0.088, Rw 0.067

Included reflections: 1507 Rf 0.084, Rw 0.063 GoF 1.0379

where $R_f = \text{Sum}(F_o - F_c) / \text{Sum}(F_o)$,

$$Rw = \text{Sqrt}[\text{Sum}(w(Fo-Fc)**2)/\text{Sum}(wFo**2)] \text{ and}$$
$$\text{GoF} = \text{Sqrt}[\text{Sum}(w(\text{Fo}-\text{Fc})^2)/(\text{No. of reflns} - \text{No. of params.})]$$

The maximum shift/sigma ratio was 0.000.

In the last D-map, the deepest hole was $-0.290e/A^{**3}$, and the highest peak $0.340e/A^{**3}$.

Secondary ext. coeff. 0.6732microns sigma 0.0756

DISANG -- The NRCVAX Distance and Angle Program

The Space Group is P 43 21 2 NonCentrosymmetric
 The Equivalent Positions are:

1) x y z	2) 1/2-y 1/2+x 3/4+z
3) -x -y 1/2+z	4) 1/2+y 1/2-x 1/4+z
5) 1/2-x 1/2+y 3/4-z	6) y x -z
7) 1/2+x 1/2-y 1/4-z	8) -y -x 1/2-z

The Lattice is Primitive. There are no Centring Vectors

CH1675

20-Jun-2001

The following Atoms are from the CD File

* Indicates that there are Symmetry Equivalents of an atom.

Name	x	y	z	
O1	0.17276(64)	0.79310(49)	0.04980(10)	
O2	-0.02967(70)	0.65805(48)	0.07627(10)	
N	0.14067(50)	1.11051(45)	0.03580(8)	
C1	0.02740(91)	0.78932(68)	0.06635(13)	
C2	-0.05576(68)	0.96168(58)	0.07321(10)	
C3	0.00179(60)	1.11203(53)	0.05212(10)	
C4	-0.13163(62)	1.25040(57)	0.05584(11)	
C5	-0.25450(64)	1.16681(67)	0.08028(10)	
C6	-0.16528(77)	1.16328(73)	0.11401(11)	
C7	-0.02679(72)	1.02089(65)	0.10964(10)	
C8	-0.25462(71)	0.97584(72)	0.06960(10)	
C9	-0.36014(87)	0.86164(88)	0.09247(14)	
C10	-0.31538(71)	0.94219(71)	0.03408(12)	
C11	0.19462(61)	1.26351(59)	0.01752(9)	*
C12	0.34284(72)	1.34884(70)	0.03639(11)	
C13	0.42803(74)	1.49081(70)	0.01647(13)	*
Ho1	0.18808(0)	0.89971(0)	0.03673(0)	
H4a	-0.07477(0)	1.37167(0)	0.06587(0)	
H4b	-0.19342(0)	1.28758(0)	0.03236(0)	
H5	-0.38296(0)	1.22691(0)	0.08099(0)	
H6a	-0.25585(0)	1.13027(0)	0.13454(0)	
H6b	-0.10753(0)	1.28598(0)	0.12107(0)	
H7a	0.10163(0)	1.07215(0)	0.11431(0)	
H7b	-0.04593(0)	0.91682(0)	0.12825(0)	
H9a	-0.34518(0)	0.72227(0)	0.08891(0)	
H9b	-0.49529(0)	0.88834(0)	0.09493(0)	
H9c	-0.30342(0)	0.88581(0)	0.11784(0)	
H10a	-0.44814(0)	0.98135(0)	0.03109(0)	
H10b	-0.30512(0)	0.80697(0)	0.02819(0)	

H10c	-0.23127(0)	1.01871(0)	0.01760(0)
H11	0.28743(0)	1.18760(0)	0.00327(0)
H12a	0.29589(0)	1.38970(0)	0.05985(0)
H12b	0.44022(0)	1.24692(0)	0.04061(0)
H13a	0.33055(0)	1.59369(0)	0.01248(0)
H13b	0.52980(0)	1.54984(0)	0.03132(0)

There are Symmetry Equivalent atoms.
The Bond and Angle Tables may need editing.

The following Atoms are the Symmetry Equivalents

Name	x	y	z			
C11a	0.26351	1.19462	-0.01752	-1.000+y	1.000+x	-z
C13a	0.49081	1.42803	-0.01647	-1.000+y	1.000+x	-z
CH1675						

20-Jun-2001

O1-C1	1.316(8)	C5-C6	1.527(7)
O2-C1	1.186(7)	C5-C8	1.551(8)
N-C3	1.268(6)	C6-C7	1.560(8)
N-C11	1.464(6)	C8-C9	1.523(8)
C1-C2	1.519(7)	C8-C10	1.530(7)
C2-C3	1.516(6)	C11-C11a	1.603(8)
C2-C7	1.555(6)	C11-C12	1.536(7)
C2-C8	1.562(8)	C12-C13	1.521(8)
C3-C4	1.507(6)	C13-C13a	1.497(10)
C4-C5	1.521(7)		

C3-N-C11	119.9(4)	C4-C5-C8	103.5(4)
O1-C1-O2	120.9(6)	C6-C5-C8	103.3(4)
O1-C1-C2	116.1(5)	C5-C6-C7	103.2(4)
O2-C1-C2	122.9(6)	C2-C7-C6	102.6(4)
C1-C2-C3	117.2(4)	C2-C8-C5	92.4(4)
C1-C2-C7	111.9(4)	C2-C8-C9	116.1(5)
C1-C2-C8	118.0(4)	C2-C8-C10	112.5(4)
C3-C2-C7	104.8(4)	C5-C8-C9	113.2(4)
C3-C2-C8	100.8(4)	C5-C8-C10	115.1(4)
C7-C2-C8	102.2(4)	C9-C8-C10	107.3(4)
N-C3-C2	122.4(4)	N-C11-C11a	105.4(3)
N-C3-C4	130.4(4)	N-C11-C12	108.7(4)
C2-C3-C4	107.1(4)	C11a-C11-C12	109.2(4)
C3-C4-C5	101.1(4)	C11-C12-C13	112.6(4)
C4-C5-C6	107.2(4)	C12-C13-C13a	111.9(4)

CH1674

Space Group and Cell Dimensions Monoclinic, C 2
 a 11.414(3) b 7.580(4) c 21.887(3)
 beta 99.919(18)
 Volume 1865.4(12)Å³

Empirical formula : C₂₀ H₂₈ N₂ O₄

Cell dimensions were obtained from 25 reflections with 2Theta angle in the range 17.88 - 26.60 degrees.

Crystal dimensions : 0.25 X 0.15 X 0.08 mm

FW = 360.45 Z = 4 F(000) = 776.48

Dcalc 1.283Mg.m⁻³, mu 0.09mm⁻¹, lambda 0.70930Å, 2Theta(max) 49.8

The intensity data were collected on a Nonius diffractometer, using the theta/2theta scan mode.

The h,k,l ranges used during structure solution and refinement are :--

Hmin,max -13 13; Kmin,max 0 8; Lmin,max 0 25

No. of reflections measured 1812

No. of unique reflections 1765

No. of reflections with I_{net} > 2.0sigma(I_{net}) 1142

Merging R-value on intensities 0.010

Absorption corrections were made.

The minimum and maximum transmission factors are 0.924394 and 0.977313.

Details of the last least squares cycle

54 atoms, 235 parameters Full-matrix on Fo Unit wts

The residuals are as follows :--

Significant reflections: 1142 R_f 0.044, R_w 0.042

All reflections: 1765 R_f 0.088, R_w 0.079

Included reflections: 1744 R_f 0.083, R_w 0.073 GoF 0.8396

where R_f = Sum(Fo-Fc)/Sum(Fo),

R_w = Sqrt[Sum(w(Fo-Fc)²)/Sum(wFo²)] and

GoF = Sqrt[Sum(w(Fo-Fc)²)/(No. of reflns - No. of params.)]

The maximum shift/sigma ratio was 0.000.

In the last D-map, the deepest hole was -0.150e/Å³,
 and the highest peak 0.130e/Å³.

Secondary ext. coeff. 0.2651microns sigma 0.0307

DISANG -- The NRCVAX Distance and Angle Program

The Space Group is C 2 NonCentrosymmetric

The Equivalent Positions are:

1) x y z 2) -x y -z

The Lattice is C-centred. The Centring Vectors are:

1) 0, 0, 0 2) 1/2, 1/2, 0

CH1674

21-Jun-2001

The following Atoms are from the CD File

* Indicates that-there are Symmetry Equivalents of an atom.

Name	x	y	z
O1	0.31593(48)	0.07331(0)	0.38580(25)
O2	0.16826(50)	0.08850(91)	0.30983(27)
O3	-0.29850(43)	-0.56186(78)	0.11346(22)
O4	-0.15736(48)	-0.57532(91)	0.19384(22)
N1	0.06362(37)	-0.19814(90)	0.26455(19)
N2	-0.02336(39)	-0.30165(96)	0.22666(19)
C1	0.24193(61)	-0.00099(101)	0.35070(29)
C2	0.22960(48)	-0.20024(97)	0.35094(25)
C3	0.33782(49)	-0.29530(108)	0.33000(26)
C4	0.33038(53)	-0.48404(108)	0.35441(27)
C5	0.21895(54)	-0.48038(99)	0.38460(24)
C6	0.11188(50)	-0.47051(96)	0.33151(25)
C7	0.12380(43)	-0.28366(97)	0.30924(22)
C8	0.22382(50)	-0.29360(99)	0.41343(23)
C9	0.33303(57)	-0.26393(112)	0.46433(26)
C10	0.11347(58)	-0.24438(110)	0.44105(28)
C11	-0.21636(58)	-0.49198(110)	0.14566(26)
C12	-0.17277(46)	-0.31014(96)	0.13170(22)
C13	-0.11130(52)	-0.31007(113)	0.07383(25)
C14	-0.11354(54)	-0.11422(113)	0.05343(25)
C15	-0.17092(55)	-0.02465(104)	0.10248(25)
C16	-0.07752(52)	-0.02992(109)	0.16326(25)
C17	-0.08280(46)	-0.21913(95)	0.18112(23)
C18	-0.26526(47)	-0.15919(98)	0.11535(24)
C19	-0.36218(49)	-0.19489(110)	0.05867(26)
C20	-0.32523(50)	-0.10798(116)	0.17037(28)
Ho2	0.10984(0)	0.03085(0)	0.27753(0)
Ho4	-0.09301(0)	-0.51579(0)	0.21953(0)
H3a	0.42151(0)	-0.23126(0)	0.34964(0)
H3b	0.33080(0)	-0.29070(0)	0.27907(0)
H4a	0.41097(0)	-0.52128(0)	0.38608(0)

(Disang)

H4b	0.32122(0)	-0.58114(0)	0.31527(0)
H5	0.21612(0)	-0.58850(0)	0.41703(0)
H6a	0.02997(0)	-0.49521(0)	0.34786(0)
H6b	0.12054(0)	-0.56600(0)	0.29495(0)
H9a	0.36560(0)	-0.12894(0)	0.46478(0)
H9b	0.40446(0)	-0.35277(0)	0.45908(0)
H9c	0.30526(0)	-0.29002(0)	0.50944(0)
H10a	0.03554(0)	-0.29382(0)	0.41243(0)
H10b	0.10900(0)	-0.10373(0)	0.44612(0)
H10c	0.12159(0)	-0.30458(0)	0.48746(0)
H13a	-0.15833(0)	-0.39199(0)	0.03606(0)
H13b	-0.01982(0)	-0.35736(0)	0.08436(0)
H14a	-0.16449(0)	-0.10165(0)	0.00642(0)
H14b	-0.02344(0)	-0.06910(0)	0.05249(0)
H15	-0.20542(0)	0.10402(0)	0.08750(0)
H16a	-0.10162(0)	0.05873(0)	0.19886(0)
H16b	0.01291(0)	0.01010(0)	0.15673(0)
H19a	-0.32392(0)	-0.25809(0)	0.02175(0)
H19b	-0.40403(0)	-0.07309(0)	0.04090(0)
H19c	-0.43459(0)	-0.28331(0)	0.06748(0)
H20a	-0.26822(0)	-0.14379(0)	0.21262(0)
H20b	-0.40711(0)	-0.19327(0)	0.16685(0)
H20c	-0.35580(0)	0.02344(0)	0.17383(0)

CH1674

21-Jun-2001

O1-C1	1.182(8)	C6-C7	1.512(10)
O2-C1	1.307(9)	C8-C9	1.539(8)
O3-C11	1.195(8)	C8-C10	1.534(9)
O4-C11	1.311(8)	C11-C12	1.514(11)
N1-N2	1.416(7)	C12-C13	1.550(8)
N1-C7	1.272(7)	C12-C17	1.522(8)
N2-C17	1.270(8)	C12-C18	1.556(9)
C1-C2	1.517(11)	C13-C14	1.549(12)
C2-C3	1.565(9)	C14-C15	1.511(10)
C2-C7	1.520(8)	C15-C16	1.556(8)
C2-C8	1.551(8)	C15-C18	1.544(10)
C3-C4	1.535(11)	C16-C17	1.491(11)
C4-C5	1.531(9)	C18-C19	1.537(8)
C5-C6	1.536(8)	C18-C20	1.534(8)
C5-C8	1.547(10)		

N2-N1-C7	113.5(6)	C9-C8-C10	107.3(5)
N1-N2-C17	114.4(6)	O3-C11-O4	120.2(7)
O1-C1-O2	120.1(7)	O3-C11-C12	122.4(6)
O1-C1-C2	121.9(6)	O4-C11-C12	117.4(6)
O2-C1-C2	118.0(6)	C11-C12-C13	112.1(6)

(Disang)

C1-C2-C3	112.3(5)	C11-C12-C17	118.3(5)
C1-C2-C7	118.5(5)	C11-C12-C18	118.8(5)
C1-C2-C8	118.4(5)	C13-C12-C17	103.6(5)
C3-C2-C7	102.6(5)	C13-C12-C18	101.3(5)
C3-C2-C8	101.8(5)	C17-C12-C18	100.3(5)
C7-C2-C8	100.9(5)	C12-C13-C14	104.4(5)
C2-C3-C4	103.5(5)	C13-C14-C15	102.3(5)
C3-C4-C5	103.5(6)	C14-C15-C16	106.2(5)
C4-C5-C6	106.6(4)	C14-C15-C18	103.5(6)
C4-C5-C8	102.6(5)	C16-C15-C18	102.9(5)
C6-C5-C8	103.4(5)	C15-C16-C17	101.3(5)
C5-C6-C7	100.7(5)	N2-C17-C12	122.6(7)
N1-C7-C2	121.2(6)	N2-C17-C16	129.8(6)
N1-C7-C6	131.2(6)	C12-C17-C16	107.6(5)
C2-C7-C6	107.6(5)	C12-C18-C15	93.5(5)
C2-C8-C5	93.6(4)	C12-C18-C19	114.9(6)
C2-C8-C9	114.8(5)	C12-C18-C20	112.5(5)
C2-C8-C10	113.5(5)	C15-C18-C19	113.4(5)
C5-C8-C9	113.4(6)	C15-C18-C20	113.3(6)
C5-C8-C10	114.1(6)	C19-C18-C20	108.8(5)

INDEX	FREQUENCY (PPM)	HEIGHT	INDEX	FREQUENCY (PPM)	HEIGHT
1	7.260	0.5	40	1.060	0.3
2	7.256	0.2	41	0.872	12.1
3	3.715	0.4			
4	3.659	2.5			
5	3.640	2.5			
6	3.589	0.4			
7	2.586	0.6			
8	2.568	0.5			
9	2.495	0.9			
10	2.478	0.9			
11	2.453	0.4			
12	2.409	0.7			
13	2.392	0.9			
14	2.350	0.5			
15	2.331	0.7			
16	2.145	0.4			
17	2.127	0.4			
18	2.108	0.4			
19	2.087	0.6			
20	2.059	2.6			
21	2.041	1.5			
22	2.018	2.1			
23	1.970	1.6			
24	1.676	0.4			
25	1.639	0.7			
26	1.619	1.0			
27	1.602	0.4			
28	1.575	0.6			
29	1.555	0.6			
30	1.426	0.7			
31	1.404	0.5			
32	1.381	0.6			
33	1.368	0.8			
34	1.349	0.6			
35	1.321	0.4			
36	1.300	0.2			
37	1.252	12.3			
38	1.187	0.2			
39	1.155	0.3

INDEX	FREQUENCY (PPM)	HEIGHT
1	185.086	1.8
2	173.206	1.4
3	77.637	2.4
4	77.000	2.5
5	76.363	2.5
6	60.675	1.2
7	50.783	2.9
8	50.297	2.2
9	43.864	3.1
10	35.398	2.8
11	31.620	2.6
12	27.842	2.9
13	20.074	3.1
14	19.847	2.8

INDEX	FREQUENCY (PPM)	HEIGHT
1	7.260	0.4
2	5.262	5.5
3	5.254	1.1
4	4.078	0.4
5	4.042	0.4
6	3.449	0.6
7	3.429	0.5
8	3.402	0.6
9	2.572	0.4
10	2.498	0.4
11	2.481	0.6
12	2.461	0.5
13	2.359	0.8
14	2.317	0.5
15	2.111	1.9
16	2.065	0.4
17	2.043	0.5
18	2.022	1.7
19	1.996	1.1
20	1.986	2.4
21	1.979	1.7
22	1.810	0.5
23	1.770	0.5
24	1.728	0.4
25	1.665	0.7
26	1.468	0.5
27	1.428	0.8
28	1.411	1.0
29	1.385	0.7
30	1.367	2.5
31	1.327	0.8
32	1.311	0.6
33	1.235	0.6
34	1.217	10.0
35	1.199	1.3
36	1.164	0.5
37	0.858	9.4

INDEX	FREQUENCY (PPM)	HEIGHT
1	183.341	3.0
2	173.131	2.7
3	77.637	2.3
4	77.000	2.4
5	76.363	2.3
6	64.377	4.0
7	60.189	3.0
8	50.373	3.2
9	43.682	4.4
10	34.988	3.8
11	31.772	3.7
12	30.543	3.4
13	27.842	3.7
14	23.761	3.5
15	20.044	4.5
16	19.573	4.5

INDEX	FREQUENCY (PPM)	HEIGHT	INDEX	FREQUENCY (PPM)	HEIGHT
1	7.260	0.5	40	1.249	0.6
2	3.447	0.6	41	1.227	12.2
3	3.431	0.6	42	0.825	10.8
4	3.405	0.6			
5	2.648	0.3			
6	2.633	0.5			
7	2.611	0.4			
8	2.560	0.4			
9	2.543	0.7			
10	2.524	0.5			
11	2.414	0.3			
12	2.372	0.5			
13	2.353	0.7			
14	2.316	0.4			
15	2.293	0.5			
16	2.114	0.3			
17	2.098	0.3			
18	2.077	0.3			
19	2.055	0.5			
20	2.036	0.6			
21	2.013	2.3			
22	1.981	1.6			
23	1.924	1.6			
24	1.844	0.5			
25	1.811	0.5			
26	1.653	0.3			
27	1.602	1.0			
28	1.567	0.9			
29	1.547	1.0			
30	1.528	0.6			
31	1.503	0.8			
32	1.482	0.7			
33	1.457	0.4			
34	1.403	0.9			
35	1.370	0.4			
36	1.329	0.7			
37	1.306	0.6			
38	1.283	0.5			
39	1.269	0.6

INDEX	FREQUENCY (PPM)	HEIGHT
1	183.235	2.3
2	173.100	1.8
3	77.637	2.5
4	77.000	2.6
5	76.363	2.5
6	64.331	3.8
7	60.553	2.4
8	49.311	2.9
9	43.925	3.1
10	34.928	3.0
11	32.409	2.9
12	31.074	3.1
13	27.903	3.1
14	23.852	3.1
15	20.165	3.4
16	20.059	3.7

INDEX	FREQUENCY (PPM)	HEIGHT	INDEX	FREQUENCY (PPM)	HEIGHT
1	7.291	0.6	40	1.308	16.0
2	2.858	0.4	41	1.006	15.6
3	2.842	0.7	42	0.000	0.3
4	2.822	0.5			
5	2.765	0.7			
6	2.747	1.1			
7	2.727	0.8			
8	2.635	0.3			
9	2.612	0.5			
10	2.586	0.3			
11	2.568	0.7			
12	2.550	0.9			
13	2.511	0.6			
14	2.487	0.7			
15	2.343	3.2			
16	2.249	2.3			
17	2.222	0.5			
18	2.204	0.5			
19	2.183	0.4			
20	2.161	0.7			
21	2.143	0.8			
22	2.124	0.6			
23	2.104	1.8			
24	2.083	2.3			
25	2.063	0.9			
26	1.905	0.4			
27	1.896	0.5			
28	1.860	0.9			
29	1.840	1.1			
30	1.821	0.6			
31	1.795	0.7			
32	1.774	0.6			
33	1.496	0.7			
34	1.473	0.7			
35	1.448	0.7			
36	1.434	0.8			
37	1.415	0.7			
38	1.388	0.5			
39	1.368	0.3

INDEX	FREQUENCY (PPM)	HEIGHT
1	181.536	0.6
2	171.978	1.0
3	77.637	1.0
4	77.000	1.0
5	76.363	1.0
6	61.009	1.5
7	51.647	1.7
8	44.061	2.7
9	35.595	2.4
10	31.544	1.9
11	27.615	2.1
12	19.998	2.6
13	19.831	2.3

INDEX	FREQUENCY (PPM)	HEIGHT
1	7.282	5.3
2	7.279	4.6
3	7.271	1.7
4	7.248	1.8
5	7.246	1.5
6	7.237	6.9
7	6.865	7.3
8	6.855	2.0
9	6.832	1.8
10	6.821	5.7
11	6.301	4.1
12	6.296	6.0
13	6.293	2.9
14	6.291	3.3
15	5.861	3.3
16	5.854	6.1
17	5.848	3.5
18	5.501	1.6
19	5.477	1.7
20	3.764	36.2
21	3.687	1.1
22	3.678	39.8
23	3.674	1.5
24	3.152	3.3
25	3.127	3.0

INDEX	FREQUENCY (PPM)	HEIGHT
1	166.728	1.2
2	159.172	1.9
3	142.255	2.1
4	133.516	2.6
5	127.887	14.2
6	125.323	5.3
7	113.717	13.4
8	77.637	1.9
9	77.000	1.9
10	76.363	1.8
11	72.433	6.5
12	55.061	6.3
13	51.708	5.1

INDEX	FREQUENCY (PPM)	HEIGHT
1	164.695	1.7
2	150.342	2.1
3	141.891	2.8
4	141.193	3.0
5	129.344	15.4
6	128.449	15.4
7	127.918	7.1
8	127.205	5.8
9	126.719	13.4
10	125.885	7.7
11	121.394	13.1
12	77.637	1.8
13	77.000	1.9
14	76.363	1.8
15	72.767	6.9

INDEX	FREQUENCY (PPM)	HEIGHT
1	166.425	1.0
2	143.606	1.4
3	135.655	1.2
4	128.600	8.4
5	128.312	4.8
6	128.085	8.4
7	124.413	3.9
8	77.637	2.2
9	77.000	2.2
10	76.363	2.2
11	66.880	4.4
12	66.471	4.2
13	22.001	4.0

INDEX	FREQUENCY (PPM)	HEIGHT
1	166.364	1.1
2	142.301	1.8
3	135.655	1.4
4	128.555	8.3
5	128.251	5.2
6	128.024	8.0
7	125.293	3.7
8	77.637	1.9
9	77.000	1.9
10	76.363	1.9
11	72.661	4.3
12	66.395	3.8
13	28.965	5.1
14	9.878	4.6

INDEX	FREQUENCY (PPM)	HEIGHT
1	7.388	1.2
2	7.365	3.5
3	7.355	3.4
4	7.349	3.5
5	7.333	3.7
6	7.321	1.7
7	7.301	0.5
8	7.281	1.4
9	7.262	1.2
10	7.258	1.1
11	7.243	0.7
12	7.232	0.5
13	6.416	1.8
14	5.916	0.7
15	5.911	1.3
16	5.906	1.3
17	5.901	0.9
18	5.592	1.7
19	5.152	4.6
20	2.948	0.3

INDEX	FREQUENCY (PPM)	HEIGHT
1	166.060	1.1
2	142.073	1.0
3	141.315	0.9
4	135.504	1.1
5	128.494	8.4
6	128.403	10.3
7	128.206	4.8
8	128.009	7.1
9	127.796	5.5
10	126.674	6.1
11	126.218	3.2
12	77.637	1.3
13	77.000	1.3
14	76.363	1.4
15	72.995	3.0
16	66.501	4.4

INDEX	FREQUENCY (PPM)	HEIGHT	INDEX	FREQUENCY (PPM)	HEIGHT
1	7.430	0.1	40	4.335	0.1
2	7.395	0.1	41	4.154	0.1
3	7.373	0.6	42	3.910	0.1
4	7.363	0.4	43	3.797	20.5
5	7.355	1.9	44	3.679	0.2
6	7.346	1.8	45	3.434	0.1
7	7.331	3.9	46	2.700	0.2
8	7.319	5.8	47	2.043	0.1
9	7.301	4.5	48	1.283	0.2
10	7.290	1.3	49	1.265	0.1
11	7.273	2.9			
12	7.271	3.0			
13	7.259	5.6			
14	7.257	6.3			
15	7.242	1.0			
16	7.235	1.3			
17	7.225	0.9			
18	7.209	0.1			
19	6.901	0.5			
20	6.886	4.5			
21	6.875	1.3			
22	6.852	1.1			
23	6.842	3.8			
24	6.827	0.3			
25	6.393	1.9			
26	6.388	3.3			
27	5.911	1.7			
28	5.909	1.6			
29	5.904	3.3			
30	5.899	2.0			
31	5.875	0.1			
32	5.546	2.7			
33	5.256	0.1			
34	5.227	0.1			
35	5.207	0.4			
36	5.145	5.1			
37	5.141	5.5			
38	5.076	0.2			
39	4.668	0.2

INDEX	FREQUENCY (PPM)	HEIGHT
1	166.151	0.8
2	159.309	1.1
3	142.316	1.6
4	135.595	0.9
5	133.516	1.6
6	128.509	5.6
7	128.221	3.9
8	128.009	8.9
9	125.763	2.7
10	113.838	6.8
11	77.637	2.3
12	77.000	2.3
13	76.363	2.2
14	72.615	3.5
15	66.471	3.3
16	55.152	3.2

INDEX	FREQUENCY (PPM)	HEIGHT
1	8.136	3.7
2	8.126	1.7
3	8.102	1.2
4	8.092	4.6
5	8.080	1.3
6	7.532	3.7
7	7.522	1.7
8	7.498	0.9
9	7.490	3.1
10	7.476	1.0
11	7.340	2.1
12	7.329	1.7
13	7.320	4.0
14	7.314	2.4
15	7.306	7.1
16	7.296	2.2
17	7.292	2.4
18	7.268	2.6
19	7.252	1.9
20	7.249	2.0
21	7.240	1.1
22	7.232	1.2
23	7.218	1.0
24	6.440	3.7
25	5.940	1.9
26	5.935	3.1
27	5.931	2.5
28	5.634	2.8
29	5.133	7.9
30	3.315	1.0

INDEX	FREQUENCY (PPM)	HEIGHT
1	165.605	2.3
2	148.673	4.1
3	147.308	1.7
4	141.163	3.3
5	135.109	2.4
6	128.509	15.2
7	128.403	8.9
8	128.100	13.4
9	127.371	16.0
10	127.220	5.6
11	123.457	14.4
12	77.652	2.0
13	77.000	2.0
14	76.363	2.0
15	72.221	7.2
16	66.774	7.3