

Table S1. Organoleptic parameters of Samples “Aa”

Flavors	Colors	Declared Ingredients	Samples	Lots	Expiration Date
Ananas	Yellow	Carbonated water, sugar, aromas, natural fruit extracts, citric acid, sodium benzoate.	S1	21059 E2	03/01/22 at 11:22 AM
			S2	21060B2	03/01/22 at 11:48 AM
			S3	21101 E1	04/12/22 at 10:48 AM
Cola	Black	Carbonated water, sugar, aroma, natural fruit extracts, citric acid, sodium benzoate.	S1	21177H	06/27/22 at 8:05 AM
			S2	21107B1	04/18/22 at 1:53 PM
			S3	21107 E1	04/18/22 at 12:12 PM
Grenadine	Red	Carbonated water, sugar, aromas, natural fruit extracts, citric acid, sodium benzoate.	S1	120354C2	12/19/21 at 6:30 PM
			S2	21173B1	06/23/22 at 02:17 AM
			S3	20336B1	12/02/21 at 2:42 PM
Orange	Orange	Carbonated water, sugar, aromas, natural fruit extracts, citric acid, sodium benzoate.	S1	21170F2	06/20/22 at 4:29 AM
			S2	21006A2	01/06/22 at 6:21 PM
			S3	21170F2	06/20/22 at 4:29 AM

*S1, S2, S3 = *Samples 1, 2, 3, respectively*

Table S2. Organoleptic Characteristics of Samples “Bb”

Flavors	Colors	Declared Ingredients	Samples	Lots	Expiration Date
Ananas	Yellow	Carbonated water, fruit extracts, sugar, E202, E330, E951.	S1	168	06/27/22 at 3:06 PM
			S2	168	06/27/22 at 3:06 PM
			S3	168	06/27/22 at 3:06 PM
Cola	Black	Carbonated water, fruit extracts, sugar, E202, E330, E951.	S1	82	04/04/22 at 12:01 AM
			S2	182	07/09/22 at 7:17 AM
			S3	182	07/09/22 at 7:17 AM
Grenadine	Red	Carbonated water, fruit extracts, sugar, E202, E330, E951.	S1	86	04/07/22 at 8:48 AM
			S2	122	05/27/22 at 7:34 AM
			S3	122	05/27/22 at 7:35 AM
Orange	Orange	Carbonated water, fruit extracts, sugar, E202, E330, E951.	S1	ND	02/07/2022
			S2	180	02/07/22 at 01:24 AM
			S3	180	07/07/22 at 01:24 AM

*S1, S2, S3 = *Samples 1, 2, 3, respectively*

*ND = ***Not Declared***

Table S3. Organoleptic Characteristics of Samples “Cc”

Flavors	Colors	Declared Ingredients	Samples	Lots	Expiration Date
Grenadine	Red	Carbonated water, sugar, citric acid, natural grenadine flavor, authorized coloring, preservative (sodium benzoate, potassium sorbate)	S1	B330	10/21/21 at 1:15 AM
			S2	B330	10/21/21 at 01:21 AM
Orange	Orange	Carbonated water, sugar, citric acid, natural grenadine flavor, authorized coloring, preservative (sodium benzoate, potassium sorbate).	S1	B331	10/22/21 at 2:45 AM
			S2	B333	10/22/21 at 4:53 PM

*S1, S2= Samples 1, 2, respectively

Table S4. Organoleptic Characteristics of Samples “Dd”

Flavors	Colors	Declared Ingredients	Samples	Lots	Expiration Date
Ananas	Yellow	Carbonated water, sugar, citric acid, natural pineapple flavor, authorized coloring, ascorbic acid, preservative (sodium benzoate and potassium sorbate)	S1	1247	07/05/22 at 13:19
			S2	B131	02/20/22 at 8:34 PM
			S3	474	03/04/22 at 8:43 PM
Cola	Black	Carbonated water, sugar, phosphoric acid, natural cola flavor, caffeine, authorized coloring, preservative (sodium benzoate)	S1	617	04/01/22 at 4:53 PM
			S2	452	05/02/22 at 12:35 PM
			S3	159	01/23/22 at 9:10 PM
Grenadine	Red	Carbonated water, sugar, citric acid, natural grenadine flavor, authorized coloring, preservative (sodium benzoate, potassium sorbate)	S1	371	02/20/22 at 6:48 PM
			S2	1042	06/02/22 at 02:20 AM
			S3	1013	06/29/22 at 6:24 PM
Orange	Orange	Carbonated water, sugar, citric acid, natural orange flavor,	S1	408	02/25/22 at 02:16 AM
			S2	B457	06/29/22 at 4:45 PM

		authorized coloring, preservative (sodium benzoate)	S3	1103	06/16/22 at 7:07 PM
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*S1, S2, S3 = *Samples 1, 2, 3, respectively*

Table S5. Organoleptic Characteristics of samples “Ee”

Flavors	Colors	Declared Ingredients	Samples	Lots	Expiration Date
Ananas	Yello	Carbonated water, sugar, aroma, acid regulator (citric acid), authorized coloring, preservative (sodium benzoate).	S1	ND	07/09/22 at 09:43 AM
			S2	ND	07/09/22 at 09:43 AM
			S3	ND	03/04/22 at 7:17 AM
Cola	Black	Carbonated water, sugar, caffeine, aroma, acid regulator (citric acid), authorized coloring, preservative (sodium benzoate).	S1	ND	07/11/22 at 8:21 AM
			S2	ND	02/28/22 at 1:10 PM
			S3	ND	06/26/22 at 03:44 AM
Energy	Yellow lemon	Carbonated water, sugar, aroma, acid regulator (citric acid), preservative (sodium benzoate), vitamin B5 (2.3mg/100mL), vitamin B6 (2mg/100mL), taurine (0.003%), and authorized coloring.	S1	ND	07/05/22 at 06:25 AM
			S2	ND	02/08/22 at 04:14 AM
			S3	ND	03/22/22 at 05:25 AM
Grena line	Red	Carbonated water, sugar, aroma, acid regulator (citric acid),	S1	ND	07/08/22 at 5:30 PM
			S2	ND	02/25/22 at 10:18 PM

		authorized coloring, preservative (sodium benzoate).	S3	ND	04/12/22 at 11:01 AM
Lime	Colorless	Carbonated water, sugar, aroma, acid regulator (citric acid), authorized coloring, preservative (sodium benzoate).	S1	ND	07/06/22 at 02:13 AM
			S2	ND	03/03/22 at 2:01 PM
			S3	ND	04/15/22 at 03:08 AM
Orange	Orange	Carbonated water, sugar, aroma, acid regulator (citric acid), authorized coloring, preservative (sodium benzoate).	S1	ND	04/10/22 at 5:51 PM
			S2	ND	07/09/22 at 05:10 AM
			S3	ND	03/02/22 at 09:24 AM
Tangawisi (Ginger flavor)	Beige	Carbonated water, sugar, aroma, acid regulator (citric acid), authorized coloring, preservative (sodium benzoate).	S1	ND	03/01/22 at 08:21 PM
			S2	ND	03/28/22 at 5:09 PM
			S3	ND	04/04/22 at 07:37 PM

*S1, S2, S3 = *Samples 1, 2, 3, respectively*

*ND = ***Not Declared***

Table S6. Organoleptic Characteristics of samples “Ff”

Flavors	Colors	Declared Ingredients	Samples	Lots	Expiration Date
Cola	Black	ND	S1	ND	06/18/2022
			S2	ND	06/18/2022
			S3	ND	06/18/2022
Grenadine	Red	ND	S1	ND	06/27/2022
			S2	ND	05/22
			S3	ND	06/17/2022
Mango	Yellow	ND	S1	ND	06/09/2022
			S2	ND	06/09/2022
			S3	ND	06/09/2022
Orange	Orange	ND	S1	ND	06/18/2022
			S2	ND	06/18/2022
			S3	ND	06/18/2022

*S1, S2, S3 = *Samples 1, 2, 3, respectively*

*ND = *Not Declared*

Table S7. Organoleptic Characteristics of Samples “Gg”

Flavors	Colors	Declared Ingredients	Samples	Lots	Expiration Date
Tangawisi (Ginger flavor)	Beige	Purified water, sugar, citric acid, stabilizers, preservatives, vitamin C, sweetener, color, natural and artificial flavor.	S1	B/J-21	07/30/22 at 01:47 PM
			S2	B/J-21	07/30/22 at 01:47 PM
			S3	BN: 054-21	03/26/22 at 9:39 PM

*S1, S2, S3 = Samples 1, 2, 3, respectively

Table S8. Organoleptic Characteristics of Samples “Hh”

Flavors	Colors	Declared Ingredients	Samples	Lots	Expiration Date
Energy	Yellow	Water, sugar, taurine (0.4%), citric acid, glucuronolactone, inositol, stabilizers, preservatives, vitamin C, sweetener, color, natural and artificial flavor.	S1	BN: 059	02/06/22 at 01:54 AM
			S2	BN: 060	02/06/22 at 11:46 PM
			S3	B/J-07	06/30/22 at 11:23 AM

*S1, S2, S3 = *Samples 1, 2, 3*, respectively

Table S9. Organoleptic Characteristics of Samples “Ii”

Flavors	Colors	Declared Ingredients	Samples	Lots	Expiration Date
Coffee	Black	Carbonated water, sugar, aroma, acidifier (phosphoric acid), authorized coloring, and the preservative (sodium benzoate and potassium sorbate).	S1	1413C21	03/13/22 at 02:12 AM
			S2	0706L20	12/06/21 at 03:22 AM
			S3	1412C21	03/12/22 at 6:26 PM
Cola	Black	Carbonated water, sugar, aroma, acidifier (phosphoric acid), caffeine, authorized color (caramel E-150D), and a preservative (sodium benzoate).	S1	0806G21	07/06/22 at 9:01 PM
			S2	0504G21	07/04/22 at 03:35 AM
			S3	3101F21	06/01/22 at 05:31 AM
Grenadine	Red	Carbonated water, sugar, aroma, acidifier (citric acid), authorized coloring (E-122), and a preservative (sodium benzoate).	S1	46B17D21	02/17/22 at 2:31 PM
			S2	46B17D21	02/17/22 at 7:15 PM
			S3	46B17D21	02/17/22 at 2:31 PM
Orange	Orange	Carbonated water, sugar, aroma, acidifier (citric acid), authorized coloring, and a preservative (sodium benzoate)	S1	0505 E21	05/05/22 at 7:42 AM
			S2	1309G21	07/09/22 at 12:48 AM
			S3	1309G21	07/09/22 at 12:48 AM
Tropical	Yellow	Carbonated water, sugar, aroma, acidifier (citric acid), authorized coloring, and a preservative (sodium benzoate).	S1	0503F21	06/03/22 at 10:51 PM
			S2	0803N20	12/03/22 at 10:07 PM
			S3	1812G21	07/12/22 at 07:53 PM

*S1, S2, S3 = Samples 1, 2, 3, respectively

Table S10. Organoleptic Characteristics of Samples “Jj”

Flavors	Colors	Declared Ingredients	Samples	Lots	Expiration Date
Ananas	Yello	Carbonated water, sugar, citric acid, pineapple extract, sodium benzoate, color.	S1	C: 0619	05/14/22 at 7:03 AM
			S2	C: 0529	04/20/22 at 01:45 AM
			S3	C: 0310	03/03/22 at 03:50 AM
Cola	Black	Carbonated water, sugar, cola base, sodium benzoate, phosphoric acid, caffeine, color.	S1	C: 0799	_ / 07/22 at 05:34 AM
			S2	C: 0314	03/03/23 at 4:30 PM
			S3	C: 0618	05/13/22 at 9:16 PM
Energy	Yellow Lemon	Water, sugar, citric acid acidifier (E330), carbon dioxide, acidity regulator (trisodium citrate (E331)), sweetener, flavor, glucuronolactone, taurine, preservative (sodium benzoate (E211)) maltodextrin, caffeine, niacin, coloring tartrazine (E102), pantothenic acid, vitamin B6, vitamin B12.	S1	C: 0747	06/20/22 at 7:33 AM
			S2	C: 0796	07/03/22 at 11:34 AM
			S3	C: 0246	02/19/22 at 5:20 PM

Grenadine	Red	Carbonated water, sugar, citric acid, aroma, sodium benzoate, color.	S1	C: 0511	04/15/22 at 01:57 AM
			S2	C: 0699	06/06/22 at 10:11 PM
			S3	C: 0348	03/09/22 at 15:34 AM
Banana-flavored milk	Butter Yellow	Water, sugar, sweetener, stabilizers, partially skimmed milk, citric acid, emulsifier, preservatives, betacarotene color, banana flavor.	S1	Z: 1924	04/04/22 at 10 AM
			S2	Z: 0838	12/23/21 at 7:50 AM
			S3	Z: 0614	11/24/22 at 9:55 AM
Mango	Mango Orange	Water, sugar, citric acid, stabilizers, preservatives, vitamin C antioxidants, sweetener, flavor, beta-carotene.	S1	Z: 0712	12/09/21 at 01:11 AM
			S2	Z: 1049	ND
			S3	Z: 1373	02/05/22 at 6:11 PM
Maracuja	Tollens maracuja	Carbonated water, sugar, citric acid, maracuja extract, sodium benzoate, color.	S1	C: 0743	06/18/22 at 11:45 PM
			S2	C: 0610	05/11/22 at 9:02 PM
			S3	C: 0316	03/04/22 at 01:03 AM
Orange	Orange	Carbonated water, sugar, citric acid, orange extract, sodium benzoate, color.	S1	C: 0791	07/02/22 at 12:42 AM
			S2	C: 0847	11/17/21 at 8:25 AM
			S3	C: 0344	03/08/22 at 11:09 PM

*S1, S2, S3 = Samples 1, 2, 3, respectively

*ND = **Not Declared**

Table S11. pH values recorded for all samples

Brands	Flavors	pH values with measurement temperature (T in °C)							
		S1		S2		S3		Averages	
		pH	T°C	pH	T°C	pH	T°C	pH	T°C
Aa	Ananas	2.86	25.1	2.85	24.9	2.86	24.9	2.86	24.97
	Cola	2.33	25	2.31	24.9	2.29	24.9	2.31	24.93
	Grenadine	2.74	25	2.76	24.9	2.74	25	2.75	24.97
	Orange	2.63	25	2.64	25	2.62	24.9	2.63	24.97
Bb	Ananas	3.12	25.2	3.12	25.1	3.12	25	3.12	25.10
	Cola	2.25	25.2	2.22	25.1	2.22	25.2	2.23	25.17
	Grenadine	2.84	25.1	2.84	24.9	2.84	24.9	2.84	24.97
	Orange	2.79	24.9	2.76	25	2.76	24.9	2.77	24.93
Cc	Grenadine	2.88	25.1	2.87	25.1	-	-	2.88	25.10
	Orange	2.6	25.1	2.61	25.1	-	-	2.61	25.10
Dd	Ananas	2.71	25	2.7	25	2.68	25	2.70	25.00
	Cola	2.59	25.1	2.61	24.9	2.6	25	2.60	25.00

	Grenadine	2.93	25.1	2.88	25	2.87	25	2.8 9	25.0 3
	Orange	2.63	25.1	2.63	24. 9	2.64	24.9	2.6 3	24.9 7
Ee	Ananas	2.85	24.7	2.85	24. 6	2.94	24.8	2.8 8	24.7 0
	Cola	2.69	24.8	2.64	24. 6	2.67	24.7	2.6 7	24.7 0
	Energy	2.49	24.7	2.47	24. 6	2.49	24.6	2.4 8	24.6 3
	Grenadine	2.8	24.6	2.8	24. 6	2.78	24.6	2.7 9	24.6 0
	Lime	2.78	24.9	2.83	24. 8	2.81	24.8	2.8 1	24.8 3
	Orange	2.79	24.8	2.81	24. 7	2.79	24.6	2.8 0	24.7 0
	Tangawisi (Ginger flavor)	3.26	24.8	3.18	24. 7	3.16	24.6	3.2 0	24.7 0
Ff	Cola	2.39	25.2	2.38	25	2.38	25.2	2.3 8	25.1 3
	Grenadine	2.69	25.1	2.68	25	2.69	25.1	2.6 9	25.0 7
	Mango	2.72	25.1	2.71	25. 1	2.71	25.2	2.7 1	25.1 3
	Orange	2.74	25.1	2.75	25	2.76	25.2	2.7 5	25.1 0
Gg	Tangawisi	3.39	25.1	3.38	25. 1	3.36	25.4	3.3 8	25.2 0
Hh	Energy	2.67	25.1	2.64	25	2.68	25.2	2.6 6	25.1 0

Ii	Coffee	2.28	24.7	2.31	24. 6	2.27	24.8	2.2 9	24.7 0
	Cola	2.2	24.6	2.19	24. 5	2.19	24.7	2.1 9	24.6 0
	Grenadine	2.71	24.9	2.72	24. 8	2.7	24.9	2.7 1	24.8 7
	Orange	2.54	24.8	2.52	24. 7	2.51	24.7	2.5 2	24.7 3
	Tropical	2.63	24.8	2.65	24. 7	2.64	24.7	2.6 4	24.7 3
Jj	Ananas	2.57	24.9	2.57	24. 9	2.56	24.9	2.5 7	24.9 0
	Cola	2.43	24.9	2.44	25. 1	2.39	25	2.4 2	25.0 0
	Energy	3.86	24.9	3.82	25	3.7	25	3.7 9	24.9 7
	Grenadine	2.85	25	2.86	25. 1	2.84	25	2.8 5	25.0 3
	Banana	4.28	24.9	3.86	24. 9	3.75	24.8	3.9 6	24.8 7
	Mango	2.97	24.9	3	24. 8	2.99	24.8	2.9 9	24.8 3
	Maracuja	2.67	25	2.65	25	2.63	24.9	2.6 5	24.9 7
	Orange	2.92	25	2.88	25. 1	2.86	25	2.8 9	25.0 3

*S1, S2, S3 = Samples 1, 2, 3, respectively

Table S12. Volumes of NaOH after titration of the different samples.

Brands	Flavor	Volumes of NaOH (0.1N) used (mL)			
		S1	S2	S3	Averages
Aa	Ananas	3.7	3.8	4.3	3.93
	Cola	5.5	4.4	4.5	4.80
	Grenadine	3.6	5	3.6	4.07
	Orange	6.1	4.8	5.8	5.57
Bb	Ananas	5.1	3.6	3.6	4.10
	Cola	3.5	3.1	3.2	3.27
	Grenadine	5.3	6.7	6	6.00
	Orange	3.8	3.6	3.8	3.73
Cc	Grenadine	3.4	3.7	—	3.55
	Orange	4.3	4.3	—	4.30
Dd	Ananas	5.3	5	5.1	5.13
	Cola	3.7	3.5	3.3	3.50
	Grenadine	5	4	4.2	4.40
	Orange	4.8	5.5	5	5.10
Ee	Ananas	5.5	5.1	4.6	5.07
	Cola	4.2	5.3	5.5	5.00
	Energy	8.1	7.9	7.9	7.97
	Grenadine	5.8	4.6	4.8	5.07
	Lime	4.5	4.4	5.1	4.67
	Orange	5.1	7	4.9	5.67
	Tangawisi (Ginger flavor)	3.3	3.7	3.8	3.60
Ff	Cola	3.1	3	3	3.03

	Grenadine	7.3	6	7.5	6.93
	Mangue	5.4	6.1	5.8	5.77
	Orange	5.1	5.4	5	5.17
Gg	Tangawisi (Ginger flavor)	2.7	2.8	2.9	2.80
Hh	Energy	6.9	7.2	7.1	7.07
Ii	Café	6.4	7.2	6.6	6.73
	Cola	3.8	3.7	4.6	4.03
	Grenadine	5.6	4.4	4.6	4.87
	Orange	6.5	5.9	6.5	6.30
	Tropical	7.9	4.2	7.4	6.50
Jj	Ananas	6	5.5	5.5	5.67
	Cola	4.6	4.2	3.4	4.07
	Energy	8.6	8.8	8.1	8.50
	Grenadine	4	3.9	4	3.97
	Lait aromatisé banane	2.8	3.5	3.6	3.30
	Mangue	5	4.8	5	4.93
	Maracuja	7	4.9	5.3	5.73
	Orange	5	4.2	4.8	4.67

*S1, S2, S3 = *Samples 1, 2, 3*, respectively

Table S13. Values of titratable acidity of the different samples

Brands	Flavor	Amounts of free acid (g/L)			
		S1	S2	S3	Averages
Aa	Ananas	2.368	2.432	2.752	2.517
	Cola	3.52	2.816	2.88	3.072
	Grenadine	2.304	3.2	2.304	2.603
	Orange	3.904	3.072	3.712	3.563
Bb	Ananas	3.264	2.304	2.304	2.624
	Cola	2.24	1.984	2.048	2.091
	Grenadine	3.392	4.288	3.84	3.840
	Orange	2.432	2.304	2.432	2.389
Cc	Grenadine	2.176	2.368	—	2.272
	Orange	2.752	2.752	—	2.752
Dd	Ananas	3.392	3.2	3.264	3.285
	Cola	2.368	2.24	2.112	2.240
	Grenadine	3.2	2.56	2.688	2.816
	Orange	3.072	3.52	3.2	3.264
Ee	Ananas	3.52	3.264	2.944	3.243
	Cola	2.688	3.392	3.52	3.200
	Energy	5.184	5.056	5.056	5.099
	Grenadine	3.712	2.944	3.072	3.243
	Lime	2.88	2.816	3.264	2.987
	Orange	3.264	4.48	3.136	3.627
	Tangawisi (Ginger flavor)	2.112	2.368	2.432	2.304
Ff	Cola	1.984	1.92	1.92	1.941
	Grenadine	4.672	3.84	4.8	4.437
	Mangue	3.456	3.904	3.712	3.691
	Orange	3.264	3.456	3.2	3.307
Gg	Tangawisi (Ginger flavor)	1.728	1.792	1.856	1.792

Hh	Energy	4.416	4.608	4.544	4.523
Ii	Café	4.096	4.608	4.224	4.309
	Cola	2.432	2.368	2.944	2.581
	Grenadine	3.584	2.816	2.944	3.115
	Orange	4.16	3.776	4.16	4.032
	Tropical	5.056	2.688	4.736	4.160
Jj	Ananas	3.84	3.52	3.52	3.627
	Cola	2.944	2.688	2.176	2.603
	Energy	5.504	5.632	5.184	5.440
	Grenadine	2.56	2.496	2.56	2.539
	Lait aromatisé banane	1.792	2.24	2.304	2.112
	Mango	3.2	3.072	3.2	3.157
	Maracuja (Passion fruit)	4.48	3.136	3.392	3.669
	Orange	3.2	2.688	3.072	2.987

*S1, S2, S3 = *Samples 1, 2, 3*, respectively

Table S14. Quantity of sugar (glucose) and corresponding ° Brix for reference solutions

Quantities of sugar (glucose) in grams (g) dissolved in 100mL of water (Q) and Brix Degree (°B) values							
Q1	°B1	Q2	°B2	Q3	°B3	Average Q	Average °B
1	1	1	1	1	1	1	1
5	5	5	5.2	5	5.1	5	5.1
10	9.5	10	10	10	10	10	9.83
15	14.9	15	15.1	15	14.9	15	14.97
20	19.6	20	19.9	20	20.2	20	19.9

Table S15. Identity information could be retrieved from the molecular formula data.

Initial identifier	NMR Identifier (Title+ Barcode)	¹³ C-NMR Fingerprint features	M+H and M-H observed in LC-HR-MS (main peaks in LC are marked bold)
Maltina2	DT_A1 5001183916	¹³ C NMR (H ₂ O+D ₂ O, 176 MHz) δ 180.0, 177.6, 177.0 , 100.1, 100.1, 100.0, 100.0, 99.8, 99.7, 99.6, 99.5, 98.6, 98.5, 98.5, 97.8, 95.9, 92.0, 81.2, 77.3, 77.2, 77.1, 77.0, 77.0, 77.0, 76.9, 76.9, 76.8, 76.3, 76.2, 74.5, 74.3, 73.5, 73.5, 73.4, 73.4, 73.3, 73.2, 73.2, 73.1, 73.1, 73.0, 72.9, 72.9, 72.7, 72.7, 73.0, 72.5, 72.2, 72.2, 72.0, 72.0, 71.9, 71.9, 71.7, 71.6, 71.3, 71.2, 71.5, 71.2, 71.1, 71.0, 71.0, 71.5, 70.9, 70.5, 70.3, 70.3, 70.2, 69.9, 69.9, 69.7, 69.7, 69.6, 69.5, 69.4, 69.4, 69.3, 68.0, 67.2, 66.7, 63.8, 63.3, 63.1, 63.1, 63.1, 62.9, 62.7, 62.6, 62.5, 61.7, 60.9, 60.8, 60.7, 60.7, 60.6, 60.5, 60.5, 60.4, 60.4, 59.3, 57.7, 57.7, 57.5, 53.3, 43.7, 39.5, 37.8, 29.4, 28.9, 20.7, 19.6, 18.1, 17.7, 17.2, 17.1, 17.0, 16.9, 16.8, 16.8, 14.1, 13.3	305.1338 (BCP: Butyl cyclohexyl phthalate); 399.3219
AmC2	DT_A2 5001183938	¹³ C NMR (H ₂ O+D ₂ O_salt, 176 MHz) δ 104.5, 101.5, 98.1, 96.0, 92.1, 82.1, 81.3, 80.7, 76.1, 75.9, 75.9, 75.8, 75.5, 74.5, 74.3, 72.9, 71.6, 71.4, 70.6, 69.8, 69.7, 69.7, 69.3, 67.7, 64.0, 63.4, 63.0, 62.8, 62.4, 61.2, 60.8, 60.7	277.0326 (DBP: Dibutyl phthalate or DIBP: Diisobutyl phthalate); 281.1128; 281.1128; 195.0874 (caffeine) and 261.0876 ; 295.1285;

Coca2	DT_A3 5001183965	¹³ C NMR (H2O+D2O, 176 MHz) δ 177.1, 176.8, 174.7, 104.5, 101.5, 98.1, 96.1, 96.0, 95.8, 92.1, 82.1, 81.3, 80.7, 76.1, 76.1, 75.9, 75.9, 75.8, 75.8, 75.5, 74.5, 74.4, 74.4, 74.3, 74.1, 72.9, 72.2, 72.2, 71.6, 71.4, 71.3, 71.0, 70.6, 70.4, 70.2, 69.8, 69.7, 69.7, 69.6, 69.4, 69.4, 69.3, 67.7, 67.1, 64.0, 63.4, 63.1, 63.1, 63.0, 62.7, 62.5, 62.6, 61.2, 60.9, 60.8, 60.7, 57.5, 38.7, 28.9, 17.7, 17.0, 16.9, 16.8	195.0874 (Caffeine); 289.0705; 289.0706; 289.0702
ZnCf 3	DT_A4 5001183909	¹³ C NMR (H2O+D2O, 176 MHz) Shift 213.5, 129.6, 129.2, 128.7, 104.5, 101.5, 98.2, 98.1, 98.1, 98.0, 96.0, 92.3, 92.1, 92.0, 82.1, 81.3, 80.7, 76.1, 76.0, 75.9, 75.9, 75.8, 75.6, 75.5, 75.1, 74.6, 74.5, 74.4, 74.3, 74.3, 74.1, 72.9, 71.7, 71.7, 71.6, 71.5, 71.4, 70.5, 70.3, 69.9, 69.8, 69.7, 69.7, 69.6, 69.3, 69.2, 69.1, 69.3, 68.0, 69.5, 67.8, 67.7, 67.5, 66.7, 66.1, 65.3, 64.1, 64.0, 63.8, 63.4, 63.0, 62.9, 62.8, 62.7, 62.5, 62.4, 61.2, 61.0, 61.0, 60.9, 60.8, 60.7, 60.5, 55.9, 18.0	277.0326 (DBP or DIBP); 281.1130; 179.0551 (Propyl-Paraben?); 163.0978; 281.1132; 281.1131; 195.0878 (DMP) and/or 261.0877 (Neothramycin?); 153.0547 (Methylparaben or Vanillin); 153.0547 (Methylparaben or Vanillin); 187.0967 (Azelaic acid)
CC2	DT_A5 5001183969	¹³ C NMR (H2O+D2O, 176 MHz) Shift 213.5, 147.5, 142.2, 133.6, 129.6, 129.2, 128.7, 117.5, 104.5, 101.5, 98.2, 98.1, 98.1, 98.0, 96.9, 96.1, 96.0, 95.8, 92.3, 92.1, 92.0, 82.1, 81.3, 81.3, 80.6, 80.7, 76.5, 76.2, 76.1, 76.0, 75.9, 75.9, 75.8, 75.6, 75.5, 75.3, 75.1, 74.9, 74.6, 74.5, 74.4, 74.3, 74.3, 74.1, 73.0, 72.8, 72.7, 72.4, 72.9, 71.7, 71.6, 71.5, 71.4, 71.3, 71.1, 70.5, 70.3,	277.0327 (DBP or DIBP); 195.0878 (Caffeine and/or DMP, Butyl-paraben) and/or 179.0551 (Glucose); 319.0502 and 187.0965

		70.0, 69.9, 69.8, 69.7, 69.7, 69.6, 69.5, 69.4, 69.3, 69.1, 67.8, 67.8, 67.7, 67.5, 66.1, 65.3, 64.1, 64.0, 63.8, 63.5, 63.2, 63.4, 63.0, 62.9, 62.8, 62.6, 62.4, 62.3, 61.2, 60.9, 60.8, 60.7, 60.5, 60.2, 18.1	
Jg01	DT_A6 5001183999	¹³ C NMR (H ₂ O+D ₂ O, 176 MHz) Shift 177.5, 176.8, 176.2, 173.9, 173.6, 104.5, 101.5, 98.1, 96.0, 92.1, 82.1, 81.5, 81.3, 80.7, 79.7, 76.1, 76.0, 75.9, 75.9, 75.8, 75.5, 74.5, 74.3, 74.1, 73.5, 73.1, 72.9, 72.7, 72.6, 72.6, 72.2, 71.6, 71.4, 70.9, 70.7, 70.6, 70.3, 69.8, 69.7, 69.7, 69.5, 69.3, 69.3, 69.2, 68.0, 67.7, 67.0, 66.7, 64.0, 63.3, 63.0, 62.8, 62.7, 62.6, 62.4, 61.2, 60.8, 60.7, 60.0, 57.5, 43.5, 28.9, 27.3, 20.5, 18.0, 16.9, 8.4	203.0525, 195.0500; 144.1019, 205.0707, 191.0187, 195.0500; 191.0185; 191.0187, 143.0340, 219.0862; 154.9903, 179.0552 (Glucose), 495.0425, 191.0189, 225.0612; 154.9902, 179.0550, 195.0500, 219.0504; 154.9901, 181.0497; 231.1130, 179.0551, 191.0188, 195.0501; 595.1650, 157.0494, 233.0661; 471.2013, 668.2912, 649.2499; 581.1856, 611.1957 (main); 533.2379, 730.3277; 711.2865; 595.2015 and 639.1924
TopOrange 2	DT_A7 5001183964	¹³ C NMR (H ₂ O+D ₂ O, 176 MHz) δ 177.5, 176.2, 173.9, 173.7, 147.6, 142.2, 129.2, 117.5, 104.5, 103.6, 101.5, 98.1, 98.1, 96.0, 92.2, 82.1, 81.5, 81.4, 81.3, 80.7, 79.7, 76.5, 76.1, 76.1, 75.9, 75.9, 75.8, 75.5, 75.1, 74.5, 74.3, 74.1, 74.1, 73.5, 73.1, 72.9, 72.7, 72.7, 72.6, 72.6, 72.4, 71.7, 71.6, 71.5, 71.4, 71.1, 71.1, 70.9, 70.8, 70.6, 70.3, 69.8, 69.7, 69.7, 69.3, 69.3, 69.4, 69.4, 67.8, 67.8, 67.7, 67.5, 67.1, 66.1, 65.3, 64.1, 64.0, 63.8, 63.5, 63.4, 63.2, 63.0, 62.9, 62.8, 62.7, 62.6, 62.4, 62.4, 61.4, 61.2, 60.8, 60.7, 60.2, 60.0, 43.5, 20.5, 19.0, 18.0	203.0525, 365.1051, 195.0500; 195.0500; 210.0608, 342.1392, 191.0186; 281.1132 (Oleic acid?); 163.0977; 281.1130, 181.9906, 279.0981; 281.1128, 181.9906; 180.1018, 191.0187, 191.0187; 163.0977 (D-cymarose?); 281.1130, 181.9906; 180.1018, 191.0187, 195.0500; 263.1025; 163.0977, 202.9963; 295.1288; 294.0967, 294.0968

Sprite3	DT_B1 5001183959	¹³ C NMR (H ₂ O+D ₂ O, 176 MHz) δ 177.5, 176.9, 176.2, 173.9, 173.7, 133.7, 129.6, 128.7, 104.5, 103.6, 101.5, 98.1, 98.1, 96.1, 96.0, 92.1, 92.1, 82.1, 81.5, 81.4, 81.3, 80.7, 79.7, 76.5, 76.1, 76.1, 75.9, 75.9, 75.8, 75.5, 75.1, 74.5, 74.3, 74.3, 74.1, 73.6, 73.1, 72.9, 72.7, 72.7, 72.6, 72.6, 72.4, 71.7, 71.6, 71.5, 71.4, 71.1, 70.9, 70.8, 70.6, 70.3, 69.8, 69.7, 69.7, 69.3, 69.4, 69.4, 68.0, 67.8, 67.7, 67.1, 66.7, 66.1, 65.3, 64.1, 64.0, 63.4, 63.2, 63.0, 62.9, 62.8, 62.7, 62.4, 62.4, 61.4, 61.2, 60.9, 60.8, 60.8, 60.7, 60.2, 60.0, 43.5, 18.0	203.0526, 365.1053, 195.0502; 215.0161, 191.0187; 143.0338, 191.0187; 163.0977; 163.0977 (D-cymarose?) and 187.0966
Energy Malt3	DT_B2 5001183958	¹³ C NMR (H ₂ O+D ₂ O, 176 MHz) δ 177.4, 177.2, 176.8, 173.9, 143.5, 133.7, 129.6, 128.7, 99.8, 99.6, 99.6, 99.5, 96.0, 92.1, 92.0, 91.9, 77.0, 76.9, 76.8, 76.8, 76.3, 76.2, 76.0, 75.9, 75.9, 75.8, 75.8, 74.5, 74.5, 74.4, 74.3, 74.1, 73.5, 73.4, 73.4, 73.3, 73.3, 73.0, 73.0, 72.9, 72.8, 72.7, 72.7, 72.2, 72.2, 72.0, 71.9, 71.8, 71.6, 71.4, 71.4, 72.7, 70.5, 70.3, 69.9, 69.7, 69.7, 69.6, 69.4, 68.0, 67.2, 66.7, 62.7, 62.6, 62.5, 60.9, 60.8, 60.7, 60.7, 60.6, 60.5, 60.5, 57.5, 47.5, 43.5, 38.8, 35.6, 33.5, 29.9, 28.9, 28.0, 26.4, 20.5, 18.0, 17.7, 16.9, 16.8	203.0525, 365.1053; 191.0188; 195.0876 (caffeine or DMP), 191.0189; 195.0878 (DMP), 187.0967; 195.0878 (Butyl- paraben) and 187.0967

AmA1	DT_B3 5001183955	¹³ C NMR (H ₂ O+D ₂ O, 176 MHz) δ 177.4, 176.9, 176.8, 176.2, 173.9, 173.7, 147.6, 142.2, 129.6, 129.2, 128.7, 117.5, 104.5, 103.6, 101.5, 98.2, 98.1, 98.1, 98.0, 96.1, 96.0, 95.8, 92.1, 92.1, 92.0, 82.1, 81.5, 81.4, 81.3, 81.2, 80.8, 80.7, 80.5, 79.7, 76.6, 76.5, 76.1, 75.9, 75.9, 75.8, 75.5, 75.5, 75.1, 74.5, 74.3, 74.3, 74.1, 74.0, 73.9, 73.1, 72.9, 72.7, 72.7, 72.6, 72.5, 72.4, 72.3, 71.7, 71.6, 71.4, 71.4, 71.2, 71.1, 71.0, 71.0, 71.1, 70.9, 70.8, 70.6, 70.3, 69.8, 69.7, 69.7, 69.6, 69.4, 69.3, 67.8, 67.8, 67.7, 67.5, 67.0, 66.1, 65.3, 64.1, 64.0, 63.4, 63.0, 62.8, 62.7, 62.9, 62.6, 62.6, 62.4, 62.4, 62.3, 62.3, 61.5, 61.4, 61.2, 61.2, 60.9, 60.8, 60.7, 60.5, 60.3, 60.2, 60.1, 60.0, 57.5, 43.5, 33.0, 25.0, 24.6, 20.5, 18.0, 16.9	203.0524, 365.1048, 195.0499; 195.0500; 210.0608, 360.1495, 191.0187; 166.0862, 191.0188; 281.1128, 181.9905, 279.0981; 281.1132, 181.9906; 180.1017, 191.0187, 195.0500; 263.1023; 295.1282 ; 295.1283; 187.0964 (main); 163.0977
XXL Energy 2	DT_B4 5001184001	¹³ C NMR (H ₂ O+D ₂ O, 176 MHz) δ 177.5, 173.9, 166.4, 147.6, 143.6, 142.2, 133.7, 129.6, 129.2, 128.7, 126.7, 117.5, 104.5, 103.6, 101.5, 98.1, 98.1, 96.1, 95.9, 96.0, 92.2, 82.1, 81.4, 81.3, 80.7, 76.5, 76.4, 76.5, 76.4, 76.1, 76.1, 76.0, 75.9, 75.8, 75.8, 75.5, 75.1, 74.5, 74.4, 74.3, 74.1, 74.1, 73.7, 73.6, 73.3, 73.6, 73.3, 72.9, 72.7, 72.4, 72.2, 71.6, 71.5, 71.5, 71.1, 70.7, 70.7, 70.6, 70.5, 70.3, 70.3, 70.1, 69.8, 69.7, 69.7, 70.1, 69.6, 69.4, 69.3, 69.9, 68.0, 67.8, 67.8, 67.7, 67.5, 67.3, 67.2, 66.7, 66.1, 65.3, 64.8,	203.0524, 365.1049, 179.0550, 341.1085; 170.0810, 191.0187; 191.0187; 220.1178, 161.9855; 281.1128; 180.1019; 195.0878 (caffeine) , 261.0880 ; 295.1285; 195.0878 (DMP) and 187.0966

		64.1, 64.0, 63.0, 63.4, 62.8, 62.6, 62.5, 62.4, 61.6, 61.4, 61.3, 61.3, 61.2, 60.9, 60.8, 60.7, 60.2, 43.5, 43.4, 33.5, 29.9, 28.0, 24.4, 19.0, 18.0	
Am03	DT_B5 5001183911	¹³ C NMR (H ₂ O+D ₂ O, 176 MHz) δ 177.8, 174.1, 147.5, 142.2, 129.2, 117.6, 104.5, 103.6, 101.5, 98.2, 98.1, 98.1, 98.0, 96.1, 96.0, 95.8, 92.3, 92.3, 92.1, 92.1, 82.1, 81.4, 81.3, 80.8, 80.7, 76.5, 76.1, 76.0, 75.9, 75.9, 75.8, 75.8, 75.6, 75.5, 75.1, 74.6, 74.5, 74.4, 74.4, 74.3, 74.1, 73.6, 72.9, 72.7, 72.6, 72.4, 71.7, 71.6, 71.5, 71.4, 71.3, 71.1, 70.6, 70.5, 70.3, 69.9, 69.8, 69.7, 69.7, 69.4, 69.4, 69.3, 69.2, 69.6, 67.8, 67.7, 69.6, 66.1, 65.3, 64.1, 64.0, 63.8, 63.4, 63.2, 63.0, 62.9, 62.8, 62.6, 62.4, 62.4, 62.3, 61.4, 61.2, 60.9, 60.8, 60.7, 60.5, 60.2, 43.5, 18.0	203.0524, 365.1048, 179.0551, 341.1086, 387.1142, 683.2252; 195.0499; 365.1057, 179.0551, 215.0321, 341.1085, 377.0852; 191.0188; 281.1131, 191.0189; 166.0863, 179.0551, 191.0188, 210.9993; 281.1131, 279.0987; 281.1132 , 181.9908; 180.1019, 179.0551, 191.0188, 210.9993; 263.1025, 261.0879; 163.0977, 202.9963; 295.1285 ; 295.1285; 187.0968; 187.0968 (main: Azelaic acid : ozonolysis product from Oleic acid)
Fanta Plastique	DT_B6 5001183912	¹³ C NMR (H ₂ O+D ₂ O, 176 MHz) Shift 213.6, 177.7, 177.3, 175.0, 174.0, 166.7, 104.5, 102.5, 101.5, 98.1, 98.1, 96.1, 96.0, 95.8, 92.1, 82.1, 81.3, 81.2, 80.7, 80.5, 76.5, 76.1, 76.0, 75.9, 75.9, 75.8, 75.4, 75.5, 74.6, 74.5, 74.4, 74.3, 74.3, 74.1, 73.6, 72.9, 74.1, 72.4, 71.7, 71.7, 71.6, 71.5, 71.4, 71.1, 70.5, 70.3, 69.9, 69.8, 69.7, 69.7, 69.6, 69.4, 69.3, 69.2, 69.5, 67.8, 67.7, 67.5, 67.4, 66.1, 65.3, 64.1, 64.0, 63.8, 63.4, 63.2, 63.0, 62.9, 62.8,	203.0524, 179.0549; 203.0525, 325.1127, 133.0129, 215.0319; 210.0606, 325.1125, 191.0185; 242.9825, 179.0551, 191.0188; 163.0976; 163.0978; 163.0977 (D-cymarose?) and 202.9961 ; 187.0966

		62.6, 62.5, 62.4, 62.3, 61.4, 61.2, 60.9, 60.8, 60.7, 60.5, 60.2, 57.5, 43.5, 38.9, 16.9	
Fanta verre	DT_B7 5001183940	¹³ C NMR (H ₂ O+D ₂ O, 176 MHz) δ 177.5, 177.1, 176.9, 176.2, 174.8, 173.9, 173.7, 147.6, 142.2, 129.2, 117.5, 104.5, 103.6, 101.5, 98.2, 98.1, 98.1, 98.0, 96.1, 96.0, 95.8, 92.1, 92.1, 82.1, 81.5, 81.4, 81.3, 81.2, 80.7, 80.5, 79.7, 76.5, 76.1, 76.0, 75.9, 75.9, 75.8, 75.8, 75.5, 75.1, 74.6, 74.5, 74.3, 74.3, 74.1, 73.5, 73.1, 72.9, 72.7, 72.6, 72.6, 72.5, 72.4, 72.3, 71.7, 71.7, 71.6, 71.4, 71.2, 71.1, 71.1, 70.9, 70.8, 70.6, 70.3, 69.8, 69.7, 69.7, 69.6, 69.5, 69.5, 69.4, 69.3, 67.8, 67.7, 67.2, 67.0, 66.1, 65.3, 64.1, 64.0, 63.8, 63.4, 63.2, 63.0, 62.9, 62.8, 62.7, 62.7, 62.6, 63.5, 62.4, 62.4, 62.3, 61.4, 61.3, 61.2, 60.9, 60.8, 60.7, 60.6, 60.5, 60.2, 60.0, 57.5, 43.5, 38.8, 18.1, 16.9	203.0525, 365.1053, 195.0501; 204.0864, 325.1123 342.1388, 191.0186; 204.0865, 225.0968, 360.1497, 179.0551, 191.0188; 204.0866, 179.0550; 163.0977, 161.9854; 163.0977 (D-cymarose?) , 344.2277, 409.0157, 202.9962; 319.0501, 202.9962 and 187.0966
CG1	DT_C1 5001183961	¹³ C NMR (H ₂ O+D ₂ O, 176 MHz) δ 177.9, 174.2, 147.5, 142.1, 133.6, 129.6, 129.2, 128.7, 117.6, 104.5, 103.6, 101.5, 100.9, 98.3, 98.1, 98.1, 96.0, 92.2, 92.2, 92.0, 82.1, 81.5, 81.4, 81.3, 80.7, 76.5, 76.1, 76.1, 75.9, 75.9, 75.8, 75.6, 75.5, 75.1, 74.6, 74.5, 74.5, 74.3, 74.3, 74.1, 73.7, 72.9, 72.7, 72.6, 72.4, 72.2, 71.7, 71.7, 71.6, 71.5, 71.4, 71.1, 70.6, 70.5, 70.3, 70.0, 69.9, 69.8, 69.7, 69.7, 69.6, 69.4, 69.4,	365.1053, 203.0523, 341.1084, 387.1140, 179.0550, 191.0187; 281.1130, 191.0188, 181.0444; 161.9856; 281.1130, 261.0880; 180.1015, 191.0188; 263.1024; 295.1283; 295.1285; 319.0497, 187.0965; 459.0307 and 228.0041;

		69.3, 69.2, 68.0, 67.8, 67.5, 67.7, 66.7, 66.1, 65.3, 64.1, 64.0, 63.8, 63.4, 63.0, 62.9, 62.8, 62.6, 62.4, 62.4, 61.4, 61.3, 61.2, 61.0, 60.8, 60.7, 60.3, 60.2, 43.6, 21.8, 18.0, 16.9	
Top rouge3	DT_C2 5006953684	¹³ C NMR (H ₂ O+D ₂ O, 176 MHz) δ 177.6, 176.8, 173.9, 147.6, 142.2, 129.2, 117.5, 104.5, 103.6, 101.5, 98.1, 98.1, 96.0, 92.2, 82.1, 81.4, 81.3, 80.8, 80.7, 76.5, 76.1, 76.1, 76.0, 75.9, 75.8, 75.5, 75.1, 74.5, 74.4, 74.4, 74.3, 74.1, 74.1, 73.6, 72.9, 72.8, 72.7, 72.4, 72.2, 71.6, 71.5, 71.4, 71.1, 70.6, 70.5, 70.3, 69.9, 69.8, 69.7, 69.7, 69.6, 69.4, 69.4, 69.3, 69.2, 69.2, 68.0, 67.8, 67.7, 67.2, 66.7, 66.1, 65.3, 64.1, 64.0, 63.5, 63.2, 63.0, 63.4, 62.8, 62.6, 62.5, 62.4, 62.4, 61.4, 61.2, 60.9, 60.8, 60.7, 60.5, 60.2, 57.5, 43.5, 38.8, 28.9, 20.5, 18.0, 16.9	210.0608, 437.9727, 191.0188; 281.1130, 191.0189; 161.9855; 281.1131, 261.0880; 180.1018; 263.1022; 295.1284; 295.1287; 153.0547, 165.0547 (Ethyl-paraben); 319.0503, 187.0967, 228.0043, 263.0923; 459.0313 and 228.0043; 228.0043
VitalO 2	DT_C3 5001183966	¹³ C NMR (H ₂ O+D ₂ O, 176 MHz) δ 213.6, 177.7, 176.4, 174.0, 173.7, 133.6, 129.6, 128.7, 104.5, 103.6, 101.5, 98.1, 98.1, 96.1, 96.0, 95.8, 92.1, 82.1, 81.5, 81.3, 81.3, 81.2, 81.2, 80.8, 80.7, 80.5, 79.7, 76.5, 76.1, 76.0, 75.9, 75.9, 75.8, 75.5, 75.1, 74.6, 74.5, 74.4, 74.3, 74.1, 74.1, 73.6, 73.1, 72.9, 72.7, 72.6, 72.4, 72.2, 71.8, 71.7, 71.7, 71.6, 71.5, 71.4, 71.3, 71.2, 71.1, 70.9, 70.8, 70.6, 70.3, 69.8, 69.7, 69.7, 69.6, 69.4, 69.2, 69.1, 69.3, 67.8,	203.0523, 365.1049, 195.0500, 341.1082, 387.1138; 204.0865, 195.0500; 210.0607, 191.0186; 163.0976 (D-cymarose?), 179.0549, 191.0186, 195.0500; 163.0977, 191.0189, 167.0339, 179.0551 and 195.0551;

		67.8, 67.7, 67.5, 67.0, 66.1, 65.3, 64.1, 64.0, 63.8, 63.4, 63.0, 62.9, 62.8, 62.7, 62.6, 62.6, 62.4, 62.4, 61.4, 61.3, 61.2, 61.0, 60.9, 60.8, 60.7, 60.5, 60.2, 60.0, 57.5, 43.5, 20.5, 16.9	
JgC1	DT_A6b_3m m 3002297494	13C NMR (H2O+D2O, 176 MHz) Shift 176.9, 176.7, 175.9, 173.7, 142.1, 142.0, 114.6, 104.4, 101.5, 98.1, 98.0, 96.8, 96.7, 95.9, 92.8, 92.8, 92.1, 83.2, 82.0, 81.5, 81.3, 81.2, 80.7, 79.7, 78.3, 76.1, 75.9, 75.8, 75.4, 74.5, 74.2, 74.0, 74.0, 73.4, 73.3, 73.1, 73.0, 72.8, 72.6, 72.4, 72.1, 71.6, 71.5, 71.5, 71.4, 71.3, 71.1, 70.7, 70.3, 69.7, 69.7, 69.6, 69.5, 69.3, 69.2, 70.9, 70.9, 67.6, 67.0, 66.6, 65.8, 65.0, 64.9, 64.4, 63.9, 63.8, 63.7, 63.3, 63.3, 62.9, 62.7, 62.7, 62.6, 62.5, 62.4, 61.9, 61.1, 60.8, 60.6, 60.0, 57.5, 24.9, 20.4, 19.3, 18.2, 18.0, 16.8	205.0684, 219.0474, 195.0502; 157.0133, 195.0503; 143.0339, 221.0661 (DEP) ; 143.340, 195.0502; 181.0498; 141.0546, 195.0503; 2+J2004.0662; 611.1965;