| Brand | Sample ¹ | Caffeine (mg/L) | Acesulfame -K (mg/L) | Aspartame ² (mg/L) | Cyclamate (mg/L) | Benzoate (mg/L) | E 150D (g/L) | HMF (mg/L) | Vanillin (mg/L) |
|------------------|---------------------|--------------------|-------------------------|----------------------------------|---------------------|--------------------|--------------------|---------------|--------------------|
| Brand 1 | Sample 1 G | 98 | ND | ND | ND | ND | 2.14 | 4.9 | ND |
| | Sample 2 G | 96 | ND | ND | ND | ND | 2.05 | 3.9 | ND |
| | Sample 3 F | 95 | ND | ND | ND | ND | 2.68 | 4.9 | ND |
| | Sample 4 F | 106 | ND | ND | ND | ND | 1.95 | 5.8 | ND |
| | Sample 5 F | 105 | ND | ND | ND | ND | 2.05 | 5.8 | ND |
| | Sample 6 F | 101 | ND | ND | ND | ND | 2.09 | 5.8 | ND |
| | Sample 7 F | 103 | ND | ND | ND | ND | 1.86 | 5.8 | ND |
| | Sample 8 F | 96 | ND | ND | ND | ND | 2.55 | 4.9 | ND |
| | Sample 9 F | 105 | ND | ND | ND | ND | 1.91 | 4.9 | ND |
| | Sample 10 G | 100 | ND | ND | ND | ND | 2.05 | 3.9 | ND |
| | Sample 11 G | 100 | ND | ND | ND | ND | 2.05 | 3.9 | ND |
| | Sample 12 G | 100 | ND | ND | ND | ND | 2.18 | 3.9 | ND |
| | Sample 13 G | 99 | ND | ND | ND | ND | 2.00 | 3.9 | ND |
| | Sample 14 G | 103 | ND | ND | ND | ND | 3.05 | 3.9 | ND |
| | Sample 15 G | 104 | ND | ND | ND | ND | 2.27 | 2.9 | ND |
| | Sample 16 G | 104 | ND | ND | ND | ND | 2.09 | 4.9 | ND |
| | Sample 17 G | 99 | ND | ND | ND | ND | 2.14 | 3.9 | ND |
| Brand 1 light | Sample 1 F | 125 | 158 | 243 | ND | ND | 2.32 | 3.9 | ND |
| | Sample 2 F | 124 | 158 | 249 | ND | ND | 1.64 | 3.9 | ND |
| | Sample 3 F | 124 | 160 | 249 | ND | ND | 1.68 | 3.9 | ND |
| | Sample 4 F | 126 | 160 | 255 | ND | ND | 1.68 | 3.9 | ND |
| | Sample 5 F | 125 | 160 | 255 | ND | ND | 1.73 | 3.9 | ND |
| | Sample 6 F | 125 | 156 | 249 | ND | ND | 1.68 | 3.9 | ND |
| | Sample 7 G | 130 | 156 | 146 | 254 | ND | 2.00 | 3.9 | ND |
| | Sample 8 G | 125 | 154 | 143 | 254 | ND | 1.86 | 3.9 | ND |
| | Sample 9 G | 129 | 153 | 153 | 254 | ND | 2.23 | 2.9 | ND |
| | Sample 10 G | 133 | 153 | 146 | 260 | ND | 2.00 | 3.9 | ND |
| | Sample 11 G | 121 | 156 | 156 | 244 | ND | 2.91 | 1.0 | ND |
| Brand 1 zero | Sample 1 F | 98 | 44 | 430 | ND | ND | 1.82 | 3.9 | ND |
| | Sample 2 F | 96 | 41 | 423 | ND | ND | 1.86 | 2.9 | ND |
| | Sample 3 F | 98 | 43 | 419 | ND | ND | 1.95 | 2.9 | ND |
| | Sample 4 F | 96 | 44 | 416 | ND | ND | 1.91 | 2.9 | ND |
| | Sample 5 F | 96 | 44 | 427 | ND | ND | 1.95 | 2.9 | ND |
| | Sample 6 F | 94 | 41 | 434 | ND | ND | 1.95 | 2.9 | ND |
| | Sample 7 F | 99 | 41 | Overlap | 250 | ND | 2.09 | 2.9 | ND |
| | Sample 8 G | 100 | 164 | Overlap | 247 | ND | 3.00 | ND | ND |

Supporting information: Results of the quantitative determination of substances by NMR

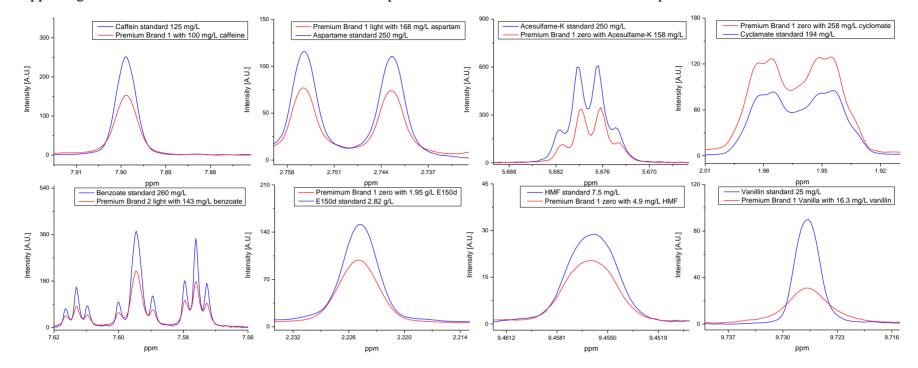
| | 1 | Sample 9 G | 94 | 150 | Overlap | 247 | ND | 1.55 | 3.9 | ND |
|---|----------|-------------|-----|-----|---------|-----|-----|------|-----|------|
| | | - | | | | | | | | |
| | | - | | | | | | | | |
| Sample 13 G 98 148 Overlap Interferenc e ND 2.14 3.9 ND Brand 1 without caffeine Sample 1 F ND ND ND ND ND ND 1.82 3.9 ND Brand 1 light without caffeine Sample 1 F ND 166 255 ND ND 1.82 2.9 ND Sample 3 F ND 166 255 ND ND 1.86 2.9 ND Sample 3 F ND 166 237 ND ND 1.99 3.9 ND Brand 1 Sample 5 F ND 156 237 ND ND 1.99 1.03 Brand 1 Sample 2 G 103 ND ND ND ND 1.99 1.01 1.73 Brand 2 Sample 3 G 113 ND ND ND ND ND 1.99 ND Sample 4 G 108 ND ND ND ND ND <t< td=""><td></td><td>*</td><td></td><td></td><td>-</td><td></td><td></td><td></td><td></td><td></td></t<> | | * | | | - | | | | | |
| Sample 13 G 98 148 Overlap c ND 2.14 3.9 ND Brand 1 without caffeine Sample 1 F ND ND ND ND ND ND ND 1.82 3.9 ND Brand 1 without caffeine Sample 1 F ND 170 224 ND ND 1.82 2.9 ND Sample 3 F ND 166 255 ND ND 1.82 2.9 ND Sample 3 F ND 156 237 ND ND 1.99 3.9 ND Sample 5 F ND 156 237 ND ND 1.99 2.9 ND Brand 1 Sample 1 G 105 ND ND ND ND 1.99 1.9 16.3 Sample 2 G 103 ND ND ND ND ND 1.41 1.0 17.3 Brand 2 Sample 1 F 108 ND ND ND ND | | ^ | | | | | | | | |
| winout caffeine Sample 1 F ND ND ND ND ND 1.82 3.9 ND Brand 1 light winout caffeine Sample 1 F ND 170 224 ND ND 1.82 2.9 ND Sample 3 F ND 166 255 ND ND 1.86 2.9 ND Sample 3 F ND 168 231 ND ND 1.90 3.9 ND Sample 5 F ND 156 237 ND ND 1.99 2.9 ND Brand 1 Sample 1 G 105 ND ND ND ND 1.99 2.9 ND Wanilla Sample 2 G 103 ND ND ND ND 1.99 ND ND Sample 2 G 104 ND ND ND ND ND 1.45 1.9 ND Sample 3 G 113 ND ND ND ND 1.45 1.9 ND | | Sample 13 G | 98 | 148 | Overlap | | ND | 2.14 | 3.9 | ND |
| $ \begin{array}{ c c c c c c c c c c c c c c c c c c c$ | | G 1 1 F | | | ND | | ND | 1.02 | 2.0 | |
| Brand 1 without caffeine Sample 1 F ND 170 224 ND ND 1.82 2.9 ND Sample 2 F ND 166 255 ND ND 1.82 2.9 ND Sample 3 F ND 166 255 ND ND 1.86 2.9 ND Sample 5 F ND 156 237 ND ND 1.99 3.9 ND Sample 5 F ND 156 237 ND ND 1.99 2.9 ND Brand 1 Sample 1 G 105 ND ND ND ND 1.99 1.9 16.3 Sample 2 G 103 ND ND ND ND 1.12 1.9 ND Sample 3 G 113 ND ND ND ND ND 1.45 1.9 ND Sample 4 G 108 ND ND ND ND 1.41 1.9 ND Sample 4 G 11 | | Sample 1 F | ND | ND | ND | ND | ND | 1.82 | 3.9 | ND |
| | | | | | | | | | | |
| without caffeine Sample 1 F ND 170 224 ND ND 1.82 2.93 ND sample 2 F ND 166 255 ND ND 1.82 2.93 ND Sample 3 F ND 166 237 ND ND 1.99 3.9 ND Sample 5 F ND 156 237 ND ND 1.99 2.9 ND Brand 1 Sample 1 G 105 ND ND ND ND 1.99 2.9 ND Brand 2 Sample 1 F 108 ND ND ND ND 1.27 1.9 ND Sample 2 G 103 ND ND ND ND ND 1.27 1.9 ND Sample 3 G 113 ND ND ND ND ND 1.45 1.9 ND Sample 5 G 111 ND ND ND ND ND 1.45 1.9 ND < | | Complete E | ND | 170 | 224 | ND | ND | 1.02 | 2.0 | ND |
| | without | Sample 1 F | ND | 170 | 224 | ND | ND | 1.82 | 2.9 | ND |
| | caffeine | | | | | | | | | |
| | | - | | | | | | | | |
| $ \begin{array}{ c c c c c c c c c c c c c c c c c c c$ | | - | | | | | | | | |
| Brand 1 Vanilla Sample 1 G 105 ND ND ND ND ND 2.91 1.9 16.3 Brand 2 Sample 2 G 103 ND ND ND ND ND 3.14 1.0 17.3 Brand 2 Sample 2 G 104 ND ND ND ND 1.27 1.9 ND Sample 3 G 113 ND ND ND ND ND 1.45 1.9 ND Sample 4 G 108 ND ND ND ND ND 1.45 1.9 ND Sample 5 G 111 ND ND ND ND ND 1.45 1.9 ND Sample 6 G 113 ND ND ND ND ND 1.68 2.9 ND Sample 9 G 111 ND ND ND ND 1.86 2.9 ND Sample 1 G 125 93 Overlap ND 1.43 | | - | | | | | | | | |
| Vanilla Sample 1 G 105 ND ND ND ND ND 2.91 1.9 16.3 Brand 2 Sample 2 G 103 ND ND ND ND ND 3.14 1.0 17.3 Brand 2 Sample 1 F 108 ND ND ND ND ND 1.27 1.9 ND Sample 3 G 113 ND ND ND ND ND 1.45 1.9 ND Sample 5 G 111 ND ND ND ND ND 1.45 1.9 ND Sample 6 G 113 ND ND ND ND 1.45 1.9 ND Sample 6 G 113 ND ND ND ND 1.68 2.9 ND Sample 8 G 113 ND ND ND ND 1.23 2.9 ND Sample 1 G 113 ND ND ND ND 1.31 ND <td></td> <td>Sample 5 F</td> <td>ND</td> <td>156</td> <td>237</td> <td>ND</td> <td>ND</td> <td>1.99</td> <td>2.9</td> <td>ND</td> | | Sample 5 F | ND | 156 | 237 | ND | ND | 1.99 | 2.9 | ND |
| Brand 2 Sample 1 F 108 ND ND ND ND ND 1.27 1.9 ND Sample 2 G 104 ND 1.68 1.9 ND Sample 3.0 Sample 3.0 Sample 3.0 Sample 3.0 Sample 3.0 Sample 3.0 <td></td> <td>-</td> <td></td> <td>ND</td> <td>ND</td> <td>ND</td> <td>ND</td> <td>2.91</td> <td>1.9</td> <td>16.3</td> | | - | | ND | ND | ND | ND | 2.91 | 1.9 | 16.3 |
| Sample 2 G 104 ND ND ND ND ND 1.82 1.9 ND Sample 3 G 113 ND ND ND ND ND 1.45 1.9 ND Sample 4 G 108 ND ND ND ND ND 1.45 1.9 ND Sample 5 G 111 ND ND ND ND ND 1.41 1.9 ND Sample 6 G 113 ND ND ND ND ND 1.68 2.9 ND Sample 7 G 113 ND ND ND ND ND 1.68 2.9 ND Sample 9 G 111 ND ND ND ND 1.68 2.9 ND Sample 10 G 113 ND ND ND ND 1.68 1.9 ND Sample 10 G 113 ND ND ND 143 1.32 1.9 ND S | | Sample 2 G | 103 | ND | ND | ND | ND | 3.14 | 1.0 | 17.3 |
| Sample 3 G 113 ND ND ND ND ND 1.45 1.9 ND Sample 4 G 108 ND ND ND ND ND ND 1.45 1.9 ND Sample 5 G 111 ND ND ND ND ND 1.41 1.9 ND Sample 6 G 113 ND ND ND ND ND 1.68 2.9 ND Sample 7 G 113 ND ND ND ND ND 1.68 1.9 ND Sample 9 G 111 ND ND ND ND ND 1.68 1.9 ND Sample 10 G 113 ND ND ND ND 1.68 2.9 ND Brand 2 G 113 ND ND ND 1.45 1.32 1.9 ND Sample 10 G 113 ND Overlap ND 143 1.27 1.9 < | Brand 2 | Sample 1 F | 108 | ND | ND | ND | ND | 1.27 | 1.9 | ND |
| Sample 4 G108NDNDNDND1.451.9NDSample 5 G111NDNDNDNDND1.411.9NDSample 6 G113NDNDNDNDND1.682.9NDSample 7 G113NDNDNDND1.682.9NDSample 8 G113NDNDNDND1.681.9NDSample 9 G111NDNDNDND1.682.9NDSample 10 G113NDNDNDND1.682.9NDBrand 2 lightSample 1 G12593OverlapNDND1.501.9NDBrand 2 lightSample 3 G12993OverlapND1431.321.9NDSample 3 G12693OverlapND1431.271.9NDSample 4 G13093OverlapND1431.271.9NDSample 5 G12696OverlapND1441.9NDSample 6 G13193OverlapND1481.271.9NDSample 7 G13193OverlapND1481.271.9NDSample 7 G13193OverlapND1481.271.9NDSample 8 G13996OverlapND1481.271.9ND <t< td=""><td></td><td>Sample 2 G</td><td>104</td><td>ND</td><td>ND</td><td>ND</td><td>ND</td><td>1.82</td><td>1.9</td><td>ND</td></t<> | | Sample 2 G | 104 | ND | ND | ND | ND | 1.82 | 1.9 | ND |
| Sample 5 G111NDNDNDND1.411.9NDSample 6 G113NDNDNDNDND1.682.9NDSample 7 G113NDNDNDND1.232.9NDSample 8 G113NDNDNDND1.681.9NDSample 9 G111NDNDNDND1.682.9NDSample 10 G113NDNDNDND1.682.9NDBrand 2Sample 1 G12593OverlapND1431.321.9NDSample 2 G12394OverlapND1431.321.9NDSample 3 G12993OverlapND1431.271.9NDSample 5 G12698OverlapND1431.271.9NDSample 5 G12698OverlapND1451.271.9NDSample 6 G12696OverlapND1481.271.9NDSample 7 G13193OverlapND1481.271.9NDSample 8 G13996OverlapND1491.141.9NDSample 7 G13193OverlapND1491.221.9NDBrand 2 zeroSample 1 F13041601NDND2.361.9NDS | | Sample 3 G | 113 | ND | ND | ND | ND | 1.45 | 1.9 | ND |
| Sample 6 G113NDNDNDND1.682.9NDSample 7 G113NDNDNDNDND1.232.9NDSample 8 G113NDNDNDNDND1.681.9NDSample 9 G111NDNDNDND1.682.9NDSample 10 G113NDNDNDND1.682.9NDBrand 2Sample 1 G12593OverlapND1431.321.9NDSample 2 G12394OverlapND1431.321.9NDSample 3 G12993OverlapND1431.271.9NDSample 4 G13093OverlapND1451.271.9NDSample 5 G12698OverlapND1451.271.9NDSample 6 G12696OverlapND1481.271.9NDSample 7 G13193OverlapND1481.271.9NDSample 8 G13996OverlapND1481.221.9NDBrand 2 zeroSample 1 F13041601NDND2.361.9NDBrand 3 discountSample 1 F116NDNDNDND2.321.9NDSample 3 F119NDNDNDNDND2 | | Sample 4 G | 108 | ND | ND | ND | ND | 1.45 | 1.9 | ND |
| Sample 7 G 113 ND ND ND ND 1.23 2.9 ND Sample 8 G 113 ND ND ND ND ND 1.68 1.9 ND Sample 9 G 111 ND ND ND ND ND 1.86 2.9 ND Brand 2 Sample 10 G 113 ND ND ND ND 1.43 1.32 1.9 ND Brand 2 Sample 2 G 123 94 Overlap ND 143 1.32 1.9 ND Sample 3 G 129 93 Overlap ND 143 1.27 1.9 ND Sample 4 G 130 93 Overlap ND 145 1.27 1.9 ND Sample 5 G 126 96 Overlap ND 145 1.27 1.9 ND Sample 6 G 126 96 Overlap ND 148 1.27 1.9 ND | | Sample 5 G | 111 | ND | ND | ND | ND | 1.41 | 1.9 | ND |
| Sample 8 G 113 ND ND ND ND ND 1.68 1.9 ND Sample 9 G 111 ND ND ND ND ND ND 1.86 2.9 ND Brand 2 light Sample 1 G 125 93 Overlap ND 143 1.32 1.9 ND Sample 3 G 129 93 Overlap ND 143 1.32 1.9 ND Sample 3 G 129 93 Overlap ND 143 1.27 1.9 ND Sample 4 G 130 93 Overlap ND 145 1.27 1.9 ND Sample 5 G 126 98 Overlap ND 145 1.27 1.9 ND Sample 6 G 126 96 Overlap ND 149 1.14 1.9 ND Sample 7 G 131 93 Overlap ND 149 1.22 1.9 ND | | Sample 6 G | 113 | ND | ND | ND | ND | 1.68 | 2.9 | ND |
| Sample 9 G 111 ND ND ND ND ND ND 1.86 2.9 ND Brand 2 light Sample 10 G 113 ND ND ND ND ND 1.50 1.9 ND Brand 2 light Sample 1 G 125 93 Overlap ND 143 1.32 1.9 ND Sample 3 G 129 93 Overlap ND 143 1.32 1.9 ND Sample 3 G 129 93 Overlap ND 143 1.27 1.9 ND Sample 4 G 130 93 Overlap ND 145 1.27 1.9 ND Sample 5 G 126 98 Overlap ND 149 1.14 1.9 ND Sample 6 G 126 96 Overlap ND 148 1.27 1.9 ND Sample 7 G 131 93 Overlap ND 148 1.27 1.9 <t< td=""><td></td><td>Sample 7 G</td><td>113</td><td>ND</td><td>ND</td><td>ND</td><td>ND</td><td>1.23</td><td>2.9</td><td>ND</td></t<> | | Sample 7 G | 113 | ND | ND | ND | ND | 1.23 | 2.9 | ND |
| Sample 10 G 113 ND ND ND ND 1.50 1.9 ND Brand 2 light Sample 1 G 125 93 Overlap ND 143 1.32 1.9 ND Sample 2 G 123 94 Overlap ND 145 1.32 1.9 ND Sample 3 G 129 93 Overlap ND 143 1.27 1.9 ND Sample 4 G 130 93 Overlap ND 145 1.27 1.9 ND Sample 5 G 126 98 Overlap ND 145 1.27 1.9 ND Sample 6 G 126 96 Overlap ND 149 1.14 1.9 ND Sample 7 G 131 93 Overlap ND 148 1.27 1.9 ND Sample 7 G 131 93 Overlap ND 148 1.27 1.9 ND Brand 2 Sample 8 G | | Sample 8 G | 113 | ND | ND | ND | ND | 1.68 | 1.9 | ND |
| Brand 2 light Sample 1 G 125 93 Overlap ND 143 1.32 1.9 ND Sample 2 G 123 94 Overlap ND 145 1.32 1.9 ND Sample 3 G 129 93 Overlap ND 145 1.32 1.9 ND Sample 4 G 130 93 Overlap ND 145 1.27 1.9 ND Sample 5 G 126 98 Overlap ND 145 1.27 1.9 ND Sample 6 G 126 98 Overlap ND 145 1.27 1.9 ND Sample 6 G 126 96 Overlap ND 148 1.27 1.9 ND Sample 7 G 131 93 Overlap ND 148 1.27 1.9 ND Sample 8 G 139 96 Overlap ND 149 1.32 1.9 ND Brand 2 Sample 1 F <td></td> <td>Sample 9 G</td> <td>111</td> <td>ND</td> <td>ND</td> <td>ND</td> <td>ND</td> <td>1.86</td> <td>2.9</td> <td>ND</td> | | Sample 9 G | 111 | ND | ND | ND | ND | 1.86 | 2.9 | ND |
| light Sample 1 G 125 93 Overlap ND 143 1.32 1.9 ND Sample 2 G 123 94 Overlap ND 145 1.32 1.9 ND Sample 3 G 129 93 Overlap ND 143 1.27 1.9 ND Sample 4 G 130 93 Overlap ND 145 1.27 1.9 ND Sample 5 G 126 98 Overlap ND 145 1.27 1.9 ND Sample 6 G 126 98 Overlap ND 149 1.14 1.9 ND Sample 6 G 126 96 Overlap ND 148 1.27 1.9 ND Sample 7 G 131 93 Overlap ND 148 1.27 1.9 ND Sample 8 G 139 96 Overlap ND 149 1.32 1.9 ND Brand 2 Sample 1 F | | Sample 10 G | 113 | ND | ND | ND | ND | 1.50 | 1.9 | ND |
| Sample 2 G 123 94 Overlap ND 145 1.32 1.9 ND Sample 3 G 129 93 Overlap ND 143 1.27 1.9 ND Sample 4 G 130 93 Overlap ND 145 1.27 1.9 ND Sample 5 G 126 98 Overlap ND 151 1.32 1.9 ND Sample 6 G 126 96 Overlap ND 149 1.14 1.9 ND Sample 6 G 126 96 Overlap ND 148 1.27 1.9 ND Sample 7 G 131 93 Overlap ND 148 1.27 1.9 ND Sample 7 G 131 93 Overlap ND 148 1.27 1.9 ND Sample 8 G 139 96 Overlap ND 149 1.32 1.9 ND Brand 2 Sample 1 F 130 | | Sample 1 G | 125 | 93 | Overlap | ND | 143 | 1.32 | 1.9 | ND |
| Sample 4 G 130 93 Overlap ND 145 1.27 1.9 ND Sample 5 G 126 98 Overlap ND 151 1.32 1.9 ND Sample 6 G 126 96 Overlap ND 149 1.14 1.9 ND Sample 6 G 126 96 Overlap ND 149 1.14 1.9 ND Sample 7 G 131 93 Overlap ND 148 1.27 1.9 ND Sample 8 G 139 96 Overlap ND 149 1.32 1.9 ND Brand 2 zero Sample 1 F 130 41 601 ND ND 2.23 1.9 ND Brand 3 discount Sample 2 F 116 ND ND ND ND 2.36 1.9 ND Sample 3 F 119 ND ND ND ND ND 2.32 1.9 ND Sam | C | Sample 2 G | 123 | 94 | Overlap | ND | 145 | 1.32 | 1.9 | ND |
| $ \begin{array}{c ccccccccccccccccccccccccccccccccccc$ | | Sample 3 G | 129 | 93 | Overlap | ND | 143 | 1.27 | 1.9 | ND |
| Sample 6 G 126 96 Overlap ND 149 1.14 1.9 ND Sample 7 G 131 93 Overlap ND 148 1.27 1.9 ND Sample 8 G 139 96 Overlap ND 149 1.32 1.9 ND Brand 2 zero Sample 1 F 130 41 601 ND ND 2.23 1.9 ND Brand 3 discount Sample 1 F 116 ND ND ND ND 2.36 1.9 ND Brand 3 discount Sample 2 F 114 ND ND ND ND 2.36 1.9 ND Sample 3 F 119 ND ND ND ND 1.82 1.9 ND Sample 3 F 119 ND ND ND ND 2.32 1.9 ND Sample 4 F 124 ND ND ND ND 2.14 1.9 ND | | Sample 4 G | 130 | 93 | Overlap | ND | 145 | 1.27 | 1.9 | ND |
| Sample 7 G 131 93 Overlap ND 148 1.27 1.9 ND Sample 8 G 139 96 Overlap ND 149 1.32 1.9 ND Brand 2 zero Sample 1 F 130 41 601 ND ND 2.23 1.9 ND Brand 3 discount Sample 1 F 116 ND ND ND ND 2.36 1.9 ND Brand 3 discount Sample 2 F 114 ND ND ND ND 2.36 1.9 ND Sample 3 F 119 ND ND ND ND 1.82 1.9 ND Sample 4 F 124 ND ND ND ND ND 2.32 1.9 ND | | Sample 5 G | 126 | 98 | Overlap | ND | 151 | 1.32 | 1.9 | ND |
| Sample 8 G 139 96 Overlap ND 149 1.32 1.9 ND Brand 2 zero Sample 1 F 130 41 601 ND ND 2.23 1.9 ND Brand 3 discount Sample 1 F 116 ND ND ND 2.23 1.9 ND Brand 3 discount Sample 2 F 116 ND ND ND ND 2.36 1.9 ND Sample 2 F 114 ND ND ND ND 1.82 1.9 ND Sample 3 F 119 ND ND ND ND 2.32 1.9 ND Sample 4 F 124 ND ND ND ND 2.32 1.9 ND | | Sample 6 G | 126 | 96 | Overlap | ND | 149 | 1.14 | 1.9 | ND |
| Brand 2 zero Sample 1 F 130 41 601 ND ND 2.23 1.9 ND Brand 3 discount Sample 1 F 116 ND ND ND ND 2.36 1.9 ND Brand 3 discount Sample 1 F 116 ND ND ND ND 2.36 1.9 ND Sample 2 F 114 ND ND ND ND 1.82 1.9 ND Sample 3 F 119 ND ND ND ND 2.32 1.9 ND Sample 4 F 124 ND ND ND ND 2.32 1.9 ND | | Sample 7 G | 131 | 93 | Overlap | ND | 148 | 1.27 | 1.9 | ND |
| zero Sample 1 F 130 41 601 ND ND 2.23 1.9 ND Brand 3 discount Sample 1 F 116 ND ND ND ND 2.36 1.9 ND Brand 3 discount Sample 2 F 114 ND ND ND ND 2.36 1.9 ND Sample 2 F 114 ND ND ND ND 1.82 1.9 ND Sample 3 F 119 ND ND ND ND ND 2.32 1.9 ND Sample 4 F 124 ND ND ND ND ND 2.14 1.9 ND | | Sample 8 G | 139 | 96 | Overlap | ND | 149 | 1.32 | 1.9 | ND |
| discount Sample 1 F 116 ND ND ND ND 2.36 1.9 ND Sample 2 F 114 ND ND ND ND 1.82 1.9 ND Sample 3 F 119 ND ND ND ND 2.32 1.9 ND Sample 4 F 124 ND ND ND ND 2.14 1.9 ND | | Sample 1 F | 130 | 41 | 601 | ND | ND | 2.23 | 1.9 | ND |
| Sample 2 F 114 ND ND ND ND 1.82 1.9 ND Sample 3 F 119 ND ND ND ND 2.32 1.9 ND Sample 4 F 124 ND ND ND ND 2.14 1.9 ND | Brand 3 | Sample 1 F | 116 | ND | ND | ND | ND | 2.36 | 1.9 | ND |
| Sample 3 F 119 ND ND ND ND 2.32 1.9 ND Sample 4 F 124 ND ND ND ND 2.14 1.9 ND | | Sample 2 F | 114 | ND | ND | ND | ND | 1.82 | 1.9 | ND |
| Sample 4 F124NDNDNDND2.141.9ND | | - | 119 | ND | ND | ND | ND | | 1.9 | ND |
| | | - | 124 | ND | ND | ND | ND | 2.14 | 1.9 | ND |
| | | Sample 5 F | 136 | ND | ND | ND | ND | 1.95 | 1.9 | ND |

| | Sample 6 F | 115 | ND | ND | ND | ND | 2.59 | 1.9 | ND |
|------------------------------|------------|-----|-----|---------|-----|-----|------|-----|----|
| | Sample 7 F | 115 | ND | ND | ND | ND | 2.64 | 1.9 | ND |
| Brand 4 discount | Sample 1 G | 69 | ND | ND | ND | ND | 2.50 | 1.9 | ND |
| | Sample 2 G | 71 | ND | ND | ND | ND | 2.18 | 1.0 | ND |
| | Sample 3 G | 71 | ND | ND | ND | ND | 2.18 | 1.9 | ND |
| | Sample 4 G | 73 | ND | ND | ND | ND | 2.23 | 1.0 | ND |
| | Sample 5 G | 74 | ND | ND | ND | ND | 2.27 | 1.0 | ND |
| Brand 4 | - | | | | | | | | |
| discount zero | Sample 1 G | 63 | 104 | 168 | 278 | ND | 1.55 | 2.9 | ND |
| | Sample 2 G | 61 | 88 | 137 | 230 | ND | 1.55 | 1.0 | ND |
| | Sample 3 G | 63 | 96 | 115 | 225 | ND | 1.45 | 1.0 | ND |
| | Sample 4 G | 61 | 89 | 134 | 228 | ND | 1.50 | 1.0 | ND |
| | Sample 5 G | 65 | 91 | 137 | 231 | ND | 1.59 | 1.0 | ND |
| Brand 5 discount | Sample 1 F | 86 | ND | ND | ND | ND | 1.27 | 4.9 | ND |
| | Sample 2 F | 86 | ND | ND | ND | ND | 1.32 | 3.9 | ND |
| | Sample 3 F | 84 | ND | ND | ND | ND | 1.50 | 4.9 | ND |
| | Sample 4 F | 91 | ND | ND | ND | ND | 1.18 | 5.8 | ND |
| | Sample 5 F | 88 | ND | ND | ND | ND | 1.23 | 4.9 | ND |
| | Sample 6 F | 86 | ND | ND | ND | ND | 1.45 | 3.9 | ND |
| Brand 5 discount zero | Sample 1 F | 81 | 109 | 388 | ND | 117 | 1.41 | 3.9 | ND |
| | Sample 2 F | 78 | 108 | 373 | ND | 115 | 1.41 | 3.9 | ND |
| | Sample 3 F | 81 | 105 | 386 | ND | 116 | 1.41 | 3.9 | ND |
| | Sample 4 F | 80 | 115 | 349 | ND | 120 | 1.27 | 3.9 | ND |
| | Sample 5 F | 65 | 106 | 330 | ND | 116 | 1.18 | 3.9 | ND |
| | Sample 6 F | 80 | 108 | 375 | ND | 116 | 1.41 | 3.9 | ND |
| Brand 6 discount | Sample 1 G | 104 | ND | ND | ND | ND | 4.05 | ND | ND |
| | Sample 2 G | 98 | ND | ND | ND | ND | 3.86 | ND | ND |
| | Sample 3 G | 101 | ND | ND | ND | ND | 3.95 | ND | ND |
| | Sample 4 G | 100 | ND | ND | ND | ND | 3.50 | ND | ND |
| | Sample 5 G | 96 | ND | ND | ND | ND | 3.95 | ND | ND |
| | Sample 6 G | 105 | ND | ND | ND | ND | 4.14 | ND | ND |
| | Sample 7 G | 95 | ND | ND | ND | ND | 2.14 | 1.9 | ND |
| | Sample 8 G | 94 | ND | ND | ND | ND | 3.68 | ND | ND |
| Brand 6 discount light | Sample 1 G | 89 | 150 | Overlap | 264 | ND | 2.73 | 1.0 | ND |
| | Sample 2 G | 88 | 139 | Overlap | 251 | ND | 2.73 | ND | ND |
| | Sample 3 G | 91 | 156 | Overlap | 249 | ND | 2.64 | ND | ND |
| | Sample 4 G | 86 | 144 | Overlap | 260 | ND | 2.73 | ND | ND |
| | Sample 5 G | 81 | 135 | Overlap | 247 | ND | 2.59 | 1.9 | ND |
| Brand 6 | Sample 1 G | 95 | 154 | Overlap | 276 | ND | 1.50 | 1.9 | ND |

| discount | | | | | | | | | |
|-------------------------------|------------|-----|-----|---------|-----|----|------|-----|----|
| zero | | | | | | | | | |
| | Sample 2 G | 106 | 158 | Overlap | 271 | ND | 1.82 | 1.0 | ND |
| | Sample 3 G | 103 | 160 | Overlap | 265 | ND | 2.64 | ND | ND |
| | Sample 4 G | 104 | 158 | Overlap | 266 | ND | 1.91 | 1.0 | ND |
| | Sample 5 G | 104 | 154 | Overlap | 264 | ND | 1.91 | 1.0 | ND |
| Brand 6 discount strong | Sample 1 G | 235 | ND | ND | ND | ND | 2.59 | 3.9 | ND |
| Brand 7 discount | Sample 1 G | 96 | ND | ND | ND | ND | 4.09 | ND | ND |
| | Sample 2 G | 93 | ND | ND | ND | ND | 4.23 | ND | ND |
| | Sample 3 G | 91 | ND | ND | ND | ND | 4.14 | ND | ND |
| | Sample 4 G | 95 | ND | ND | ND | ND | 4.23 | ND | ND |
| | Sample 5 G | 100 | ND | ND | ND | ND | 4.14 | ND | ND |
| Brand 7 discount light | Sample 1 G | 84 | 130 | Overlap | 222 | ND | 3.27 | ND | ND |
| _ | Sample 2 G | 83 | 139 | Overlap | 244 | ND | 3.32 | 1.0 | ND |
| | Sample 3 G | 80 | 139 | Overlap | 246 | ND | 3.05 | 1.0 | ND |
| | Sample 4 G | 81 | 133 | Overlap | 231 | ND | 3.09 | 1.0 | ND |
| | Sample 5 G | 81 | 143 | Overlap | 216 | ND | 2.91 | ND | ND |
| Brand 8 strong | Sample 1 G | 243 | ND | ND | ND | ND | 2.95 | 7.8 | ND |
| Brand 9 strong | Sample 1 G | 252 | ND | ND | ND | ND | 1.73 | 2.9 | ND |

 1 G and F means that the samples were produced in Germany and France, respectively

 2 For the brand 1 light, brand 1 light without caffeine and brand 4 discount zero (containing small amount of citric acid), the doublet between 2.73 and 2.76 ppm was integrated while for the brand 1 zero, brand 2 zero and brand 5 discount zero, the multiplet between 3.03 and 3.11 ppm was integrated



1 Supporting information: NMR resonances of selected compounds in standard solutions and cola samples