

Supplementary Fig 1. D'Ippolito et al. 2019



Supplementary Fig 2. D'Ippolito et al. 2019

Supplemental Table 1: Additional Mass Sepctrometry Infomration for Identified Protamines. The lower portion contain protamines identified in low abundance. Amino acid is brackets do not have a corresponding fragment ion to confirm sequence.

| Protein Name | NCBI Accession Number | Sequence | Modifications | M+H | Observed m/z | Precursor Charge | HCD MS ³ Taken? | Notes |
|----------------------|-----------------------------|---|--|--------------------|----------------------|---------------------|-------------------------------|---|
| PL-1 (MpPRM) | BAU71552 | RRRRRKSRRRRRRRRRRRKGSRSPRRR* | Di-aminopropanelation (C- terminus) | 3955.51 | 495.3208 | 8 | No | |
| PL-1 (MpPRM) | BAU71552 | RRRRRKSRRRRRRRRRRKGSRSPRR* | Di-aminopropanelation (C- terminus) | 3799.41 | 543.6367 | 7 | No | |
| PL-1 (MpPRM) | BAU71552 | RRRRRRHHKKGKKKGRRRRRKRRRGRR* | Di-aminopropanelation (C- terminus) | 3942.56 | 438.9591 | 9 | Yes | |
| PL-1 (MpPRM) | BAU71552 | RRRRRRRRRRRRRRRRRRRRRRRRRRRRR | Di-aminopropanelation (C- terminus) | 3313.16 | 553.0345 | 6 | No | |
| PL-3 | PTQ32223 | RRRRRRHGRKGKKPKRHRRRRRRRRRRGRRKAHRGRKKKRGGRRKGKRRHRRRRR* | Di-aminopropanelation (C- terminus) | 7466.75 | 575.2967 | 13 | No | |
| PL-2 | PTQ35141 | RSTSRSRSRGRRRRRRRRRRRRRRRRRRRRRRRRRRR | Di-aminopropanelation (C- terminus) | 4082.51 | 584.0801 | 7 | No | |
| | | | | | | | | |
| | | | | | | | | |
| PL-1 (MpPRM) | BAU71552 | RRRRRRKSRRRRRRRRRR[SKGSH]SPRR* | Di-aminopropanelation (C- terminus) | 3780.36 | 540.9152 | 7 | No | |
| PL-1 (MpPRM) | BAU71552 | RRRRRRKSRRRR[RRTVDRRRRRRRRRR] | | 4139.33 | 690.7283 | 6 | | Very poor C-terminal coverage limits the deduction of sequence. The residues within the brackets are unknown |
| PL-1 (MpPRM) PL-3 | BAU71552 PTQ32223 | RRRRRKSRRRRRRRRRKSKGSRSPRRHSSR RRRRRRHGRKGKKPKRHRRRRRRRRRRRRRRKAHRGRKKKRGGRRKGKRHRRRRR[GKSH] | | 4366.65 7819.01 | 546.7151 602.4605 | 8 13 | | and may contain different amino acids |

Annotated ETD MS² Spectra

This document contains the spectra obtained from the analysis of *Marchantia polymorpha* protamines. Each observed protamine in this document contains a page with the spectrum on a single axis, multiple pages for the manual annotation, and a page containing theoretical fragment masses.

Table of Contents

| <u>Pages</u> | <u>Sequence</u> |
|--------------|--|
| 2-6 | RRRRRRKSRRRRRRRRRRSKGSRSPRRR* |
| 7-12 | RRRRRRKSRRRRRRRRRRSKGSRSPRR* |
| 13-16 | RRRRRRRHHKKGKKKGRRRRRRKRRRGRR* |
| 17-22 | RRRRRRRRRRRRRRRRRRRRRRRRRRRRRRRRRRRRRR |
| 23-30 | RRRRRRHGRKGKKPKRHRRRRRRRRRRRGRRKAHRGRKKKRGGRRKGKRRHRRRR* |
| 31-35 | RSTSRSRSRGRRRRRRRRRRRRRRRRRRRRRRRRRRRRR |
| 36-38 | RRRRRRKSRRRRRRRRRRR[SKGSH]SPRR* |
| 39-41 | RRRRRRKSRRRR[RRTVDRRRRRRRRRR] |
| 42-45 | RRRRRRKSRRRRRRRRRRSKGSRSPRRRHSSR |
| 46-51 | RRRRRRHGRKGKKPKRHRRRRRRRRRRRRRRRRRKAHRGRKKKRGGRRKGKRRHRRRRR[GKSH |

021519_0p2perYellowTube_Gradient_DD_Heat15 #2679-3590 RT: 11.45-13.86 AV: 11 NL: 1.19E5 T: FTMS + p NSI d Full ms2 495.4470@etd6.66 [120.0000-2000.0000]



021519_0p2perYellowTube_Gradient_DD_H...



021519_0p2perYellowTube_Gradient_DD_Heat15 #2680-3590 RT: 11.45-13.86 AV: 11 NL: 5.25E4 T: FTMS + p NSI d Full ms2 495.4470@etd6.66 [120.0000-2000.0000]



02/15/19 13:37:41



| | | | | | | | | | | | P | | | |
|------------|------------|--------------|------------|-------------|-------------|----|-------------|----|-------------|-------------|------------|------------|------------|------------|
| +6 c ions | +5 c ions | +4 c ions | +3 c ions | +2 c ions | +1 c ions | | Sequence | | +1 z ions | +2 z ions | +3 z ions | +4 z ions | +5 z ions | +6 z ions |
| 29.8619 | 35.6328 | 44.2892 | 58.7165 | 87.5711 | 174.1349 J | 1 | R | 28 | 3955.5063 | 1978.2568 | 1319.1736 | 989.6320 | 791.9071 | 660.0905 |
| 55.8787 | 66.8530 | 83.3145 | 110.7502 | 165.6217 | 330.2360 V | 2 | R | 27 | 3783.3865 | 1892.1969 | 1261.8003 | 946.6021 🗸 | 757.4831 | 631.4038 |
| 81.8956 | 98.0733 | 122.3397 | 162.7839 | 243.6722 | 486.3372 J | 3 | R | 26 | 3627.2854 | 1814.1463 | 1209.7666 | 907.5768 🗸 | 726.2629 V | 605.3870 🗸 |
| 107.9124 | 129.2935 | 161.3650 | 214.8176 | 321.7228 | 642.4383 🗸 | 4 | R | 25 | 3471.1843 | 1736.0958 | 1157.7329 | 868.5515 | 695.0427 | 579.3701 . |
| 133.9293 | 160.5137 | 200.3903 | 266.8513 | 399.7733 🗸 | 798.5394 | 5 | R | 24 | 3315.0832 | 1658.0452 | 1105.6992 | 829.5262 🗸 | 663.8225 V | 553.3533 |
| 159.9461 | 191.7339 | 239,4156 | 318.8850 | 477.8239 V | 954.6405 🗸 | 6 | R | 23 | 3158.9821 | 1579.9947 | 1053.6655 | 790.5010 🗸 | 632.6022 V | 527.3364 |
| 181.2953 | 217.3529 | 271.4393 | 361.5833 | 541.8714 / | 1082.7355 ~ | 7 | к | 22 | 3002.8809 | 1501.9441 | 1001.6318 | 751.4757 | 601.3820 | 501.3196 |
| 195.8006 | 234.7593 | 293,1973 | 390.5940 / | 585.3874 J | 1169.7675 | 8 | S | 21 | 2874.7860 | 1437.8966 | 958.9335 V | 719.4520 | 575.7630 | 479.9704 |
| 221.8175 | 265.9795 | 332.2226 | 442.6277 | 663.4379 | 1325.8686 | 9 | R | 20 | 2787.7539 | 1394.3806 | 929.9228 | 697.6939 V | 558.3566 | 465.4651 |
| 247.8343 | 297.1998 | 371.2479 | 494.6614 | 741.4885 | 1481.9697 | 10 | R | 19 | 2631.6528 | 1316.3301 | 877.8891 | 658.6687 | 527.1364 | 439.4482 |
| 273.8512 | 328.4200 | 410.2732 | 546.6951 , | 819.5390 | 1638.0708 | 11 | R | 18 | 2475.5517 | 1238.2795 | 825.8554 | 619.6434 | 495.9162 | 413.4314 |
| 299.8681 | 359.6402 | 449.2984 | 598.7288 V | 897.5896 | 1794,1719 | 12 | R | 17 | 2319.4506 | 1160.2289 | 773.8217 | 580.6181 | 464.6959 | 387,4145 |
| 325.8849 | 390.8604 | 488.3237 | 650.7625 | 975.6402 🗸 | 1950.2730 | 13 | IR | 16 | 2163.3495 | 1082.1784 | 721.7880 | 541.5928V, | 433.4757 | 361.3976 |
| 351,9018 | 422.0807 | 527.3490 J | 702.7962 | 1053.6907 🗸 | 2106.3741 | 14 | R | 15 | 2007.2484 | 1004.1278 | 669.7543 🗸 | 502.5676 | 402.2555 | 335.3808 |
| 377.9186 | 453.3009 | 566.3743 V | 754.8299 | 1131.7413 | 2262.4753 | 15 | R | 14 | 1851.1473 | 926.0773 🗸 | 617.7206 🗸 | 463.5423 🗸 | 371.0353 | 309.3639 |
| 403.9355 | 484.5211 , | 605.3995 V | 806.8636 🗸 | 1209.7918 | 2418.5764 | 16 | R | 13 | 1695.0462 | 848.0267 V, | 565.6869 🗸 | 424.5170 | 339.8151 | 283.3471 |
| 429.9523 | 515.7413 V | 644.4248 | 858.8973 🗸 | 1287.8424 | 2574.6775 | 17 | R | 12 | 1538.9451 | 769.9762 | 513.6532 V | 385.4917 | 308.5948 | 257,3302 |
| 455.9692 | 546.9615 🗸 | 683.4501 | 910.9310 🗸 | 1365.8929 | 2730.7786 | 18 | R | 11 | 1382.8439 | 691.9256 | 461.6195 🗸 | 346.4664 | 277.3746 | 231.3134 |
| 470.4745 | 564.3679 J | 705.2081 1. | 939.9417 | 4409.4089 | 2817.8106 | 19 | S | 10 | 1226.7428 🗸 | 613.8751 🗸 | 409.5858 | 307.4412 | 246.1544 | 205.2965 |
| 491.8237 | 589.9869 | 737.2319 ~ / | 982.6400 🗸 | 1473.4564 | 2945.9056 | 20 | к | 9 | 1139.7108 | 570.3590 1/ | 380.5751 | 285.6832 | 228.7480 | 190.7912 |
| 501.3272 | 601.3912 ^ | 751.4872 | 1001.6472 | 1501.9672 | 3002.9270 | 21 | G | 8 | 1011.6158 | 506.3116 🗸 | 337.8768 | 253.6594 | 203.1290 | 169.4420 |
| 515.8326 / | 618.7976 🗸 | 773.2452 | 1030.6579 | 1545.4832 | 3089.9591 | 22 | S | 7 | 954.5944 V | 477.8008 1/ | 318.8696 | 239.4041 | 191.7247 | 159.9385 |
| 541.8494 | 650.0179 J | 812.2705 🗸 | 1082.6916 | 1623.5337 | 3246.0602 | 23 | R | 6 | 867.5624 | 434.2848 | 289.8590 | 217.6460 | 174.3183 | 145.4331 |
| 556.3548 | 667.4243 | 834:0285 | 1111.7023 | 1667-0497 | 3333.0922 | 24 | S | 5 | 711,4612 🗸 | 356.2343 🗸 | 237.8253 | 178.6208 | 143.0981 | 119.4163 |
| 572.5302 | 686.8348 🗸 | 858.2917 | 1144.0532 | 1715.5761 | 3430.1450 | 25 | P | 4 | 624.4292 | 312.7182 | 208.8146 | 156.8628 | 125.6917 | 104.9109 |
| 598.5471 J | 718.0550 | 897.3170 | 1196.0869 | 1793.6267 | 3586.2461 | 26 | R | 3 | 527.3764 | 264.1919 | 176.4637 | 132.5996 | 106.2811 | 88.7355 |
| 624.5639 | 749.2753 | 936.3423 | 1248.1206 | 1871.6772 | 3742.3472 | 27 | R | 2 | 371.2753 V | 186.1413 | 124.4300 | 93.5743 | 75.0609 | 62.7186 |
| 660,0905 | 791.9071 | 989.6320 | 1319.1736 | 1978.2568 | 3955.5063 | 28 | R | 1 | 215.1742 🗸 | 108.0908 | 72.3963 | 54.5490 | 43.8407 | 36.7018 |
| | | | | | | 1 | (cterm + 56 | | 1 | | 1 | | | 4 |

021519_0p2perYellowTube_Gradient_DD_Heat15 #2877-4040 RT: 12.14-15.39 AV: 16 NL: 1.04E5 T: FTMS + p NSI d Full ms2 543.9236@etd8.70 [120.0000-2000.0000]



021519_0p2perYellowTube_Gradient_DD_H... 0-10-30-70-100 in 0-10-20-30-35 02/15/19 13:37:41

AV; ~0.2% Yellow Tube





021519_0p2perYellowTube_Gradient_DD_H...





| | | | | | | | Soguonea | | +1 7 ions | +2 z ions | +3 z ions | +4 z ions | +5 z ions | +6 z ions |
|------------|------------|------------|------------|-------------|-------------|---------|-------------|----|------------|-------------|-------------|------------|-----------|-----------|
| +6 c ions | +5 c ions | +4 c ions | +3 c ions | +2 c ions | +1 C IONS | | Sequence | 27 | 3799 4052 | 1900 2062 | 1267,1399 | 950,6068 | 760.6869 | 634.0736 |
| 29.8619 | 35.6328 | 44.2892 | 58.7165 | 87.5711 | 174.1349 | <u></u> | ۲ - | 27 | 3627 2854 | 1814 1463 | 1209.7666 V | 907.5768 V | 726.2629 | 605.3870 |
| 55.8787 | 66.8530 | 83.3145 | 110.7502 | 165.6217 | 330.2360 | 2 1 | <u> </u> | 20 | 3474 1943 | 1736 0958 | 1157 7329 | 868 5515 | 695.0427 | 579.3701 |
| 81.8956 | 98.0733 | 122.3397 | 162.7839 | 243.6722 | 486.3372 | 3 | к | 25 | 34/1.1043 | 1659 0452" | 1105 6992 | 829 5262 | 663 8225 | 553,3533 |
| 107.9124 | 129.2935 | 161.3650 | 214.8176 | 321.7228 | 642.4383 🗸 | 4 | R | 24 | 3315.0632 | 1030.0432 | 1052 6655 | 790 5010 | 632 6022 | 527 3364 |
| 133,9293 | 160.5137 | 200.3903 | 266.8513 | 399.7733 🗸 | 798.5394 🏒 | 5 | R | 23 | 3158.9821 | 15/9.994/0 | 1053.0055 + | 751 4757 1 | 601 3820 | 501 3196 |
| 159 9461 | 191,7339 | 239.4156 | 318.8850 | 477.8239 🗸 | 954.6405 | 6 | R | 22 | 3002.8809 | 1501.9441 | 1001.0310 | 740 4504 | 570 1618 | 475 3027 |
| 181 2953 | 217.3529 | 271,4393 | 361.5833 | 541.8714 🗸 | 1082.7355 | 7 | к | 21 | 2846,7798 | 1423.8936 | 949.5961 V | 712.4504 V | 570.1010 | 452 0535 |
| 195 8006 | 234 7593 | 293,1973 | 390,5940 | 585.3874 🗸 | 1169.7675 🗸 | 8 | s | 20 | 2718.6849 | 1359.8461 | 906.8998 | 680.4267 | 544.5420 | 430 4492 |
| 221 8175 | 265 9795 | 332,2226 | 442.6277 | 663.4379 🗸 | 1325.8686 V | 9 | R | 19 | 2631.6528 | 1316.3301 V | 877.8891 | 658.668/ V | 527,1304 | 412 4214 |
| 247 8343 | 207 1998 | 371 2479 | 494.6614 | 741.4885 . | 1481.9697 🗸 | 10 | R | 18 | 2475.5517 | 1238.2795 V | 825.8554 | 619.6434 V | 495.9162 | 413.4314 |
| 247.0540 | 228 4200 | 410 2732 | 546 6951 | 819.5390 | 1638,0708 | 11 | R | 17 | 2319.4506 | 1160.2289 | 773.8217 V | 580.6181 V | 464.6959 | 367.4145 |
| 200 8681 | 359 6402 | 449,2984 | 508.7288 V | 897.5896 V | 1794.1719 | 12 | R | 16 | 2163.3495 | 1082.1784 | 721.7880 V | 541.5928 | 433.4757 | 301.3970 |
| 225.0001 | 390 8604 | 488 3237 | 650.7625 | 975.6402 V | 1950.2730 | 13 | R | 15 | 2007.2484 | 1004.1278 | 669.7543 V | 502.5676 V | 402.2555 | 333.3000 |
| 251 0018 | 422 0807 | 527 3490 | 702 7962 | 1053.6907 V | 2106.3741 | 14 | R | 14 | 1851.1473 | 926.0773 | 617.7206 V | 463.5423 | 3/1.0353 | 309.3039 |
| 277.0186 | 452 2000 | 566 3743 J | 754 8299 | 1131 7413 | 2262.4753 | 15 | R | 13 | 1695.0462 | 848.0267 | 565.6869 🗸 | 424.5170 | 339.8151 | 283.34/1 |
| 377.9100 | 404 5011 | 605 2005 | 806 8636 V | 1209 7918 | 2418.5764 | 16 | R | 12 | 1538.9451 | 769.9762 🗸 | 513.6532 🗸 | 385.4917 | 308.5948 | 257.3302 |
| 403.9355 | 404.JZ11 | 644 4248 | 858 8973 | 1287 8424 | 2574.6775 | 17 | R | 11 | 1382.8439 | 691.9256 J | 461.6195 | 346.4664 | 277.3746 | 231.3134 |
| 429.9523 | 515.7415 | 682 4501 | 910 9310 | 1365 8929W | 2730 7786 | 18 | R | 10 | 1226.7428 | 613.8751 🗸 | 409.5858 🗸 | 307.4412 | 246.1544 | 205.2965 |
| 455.9092 | 540.9015 | 705 2081 | 030 0417 | 1409 4089 | 2817 8106 | 19 | S | 9 | 1070.6417 | 535.8245 🗸 | 357.5521 | 268.4159 | 214.9342 | 179.2797 |
| 4/0.4/45 | 504.3079 | 703.2001 9 | 092 54004 | 1473 4564 | 2945 9056 | 20 | к | 8 | 983.6097 🖌 | 492.3085 🗸 | 328.5414 | 246.6579 | 197.5278 | 164.7743 |
| 491.8237 | 589.9809 | 754 4070 0 | 1001 64723 | 1501 06727 | 3002 9270 | 21 | G | 7 | 855.5147 | 428.2610 1 | 285.8431 | 214.6341 | 171.9088 | 143.4252 |
| 501.3272 | 601.3912 | 770 245200 | 1020 6579 | 4545 4832 | 3089 9591 | 22 | s | 6 | 798.4933 | 399.7503 | 266.8359 | 200.3788 | 160.5045 | 133.9216 |
| 515.8326 | 618.7976 | 113.2452 | 1030.0579 | 1043.4032 | 2246.0602 | 23 | 8 | 5 | 711.4612 | 356.2343 V | 237.8253 | 178.6208 | 143.0981 | 119.4163 |
| 541.8494 | 650.0179 | 812.2705 • | 1082.0910 | 1023.5337 | 3240.0002 | 20 | 9 | 4 | 555,3601 V | 278.1837 | 185.7916 | 139.5955 | 111.8778 | 93.3994 |
| 556.3548~~ | 667.4243 | 004:0285 | 1444 0500 | 4745 5764 | 2420 1450 | 25 | P | 3 | 468-3281 | 234.6677 | 156.7809 | 417,8375 | 94.4714 | -78.8941 |
| 572.5302 | 686.8348 V | 858.2917 ¥ | 1144.0532 | 4700 0007 | 0596 0461 | 20 | p | 2 | 371.2753 V | 186,1413 | 124.4300 | 93.5743 | 75.0609 | 62.7186 |
| 598.5471 | 718.0550 V | 897.3170 V | 1196.0869 | 1/93.6267 | 0700.2401 | 20 | <u> </u> | 1 | 215 1742 V | 108.0908 | 72.3963 | 54.5490 | 43.8407 | 36.7018 |
| 634.0736 | 760.6869 | 950.6068 | 1267.1399 | 1900.2062 | 3199.4052 | 21 | (ctorr + 56 | -+ | 1 | 1 | | | | |

56.074





021519_0p2perYellowTube_Rinse_DD_Heat15 #1357-2260 RT: 5.66-8.00 AV: 13 NL: 1.29E4 T: FTMS + p NSI sid=40.00 d Full ms2 439.0706@etd5.26 [120.0000-2000.0000]



| +7 c ions | +6 c ions | +5 c ions | +4 c ions | +3 c ions | +2 c ions | +1 c ions | 2 0 | | Sequence | | | +1 z ions | +2 z ions | +3 z ions | +4 z ions | +5 z ions | +6 z ions | +7 z ions |
|------------|------------|------------|------------|-----------------------|------------|------------|-------|---|-------------|------|----------|------------|------------|------------|-------------|------------|------------|------------|
| 25.7398 | 29.8619 | 35.6328 | 44.2892 | 58.7165 | 87.5711 | 174.1349 | 1 | | R | 28 | | 3942.5627 | 1971.7850 | 1314.8591 | 986,3961 | 789.3184 | 657.9332 | 564.0866 |
| 48.0400 | 55.8787 | 66.8530 | 83.3145 | 110.7502 | 165.6217 | 330.2360 | 2 🗸 | | R | 27 | / | 3770.4429 | 1885.7251 | 1257.4858 | 943.3662 | 754.8944 | 629.2465 | 539.4981 🗸 |
| 70.3401 | 81.8956 | 98.0733 | 122.3397 | 162.7839 | 243.6722 | 486.3372 | 3 4 | | R | 26 | × | 3614.3418 | 1807.6745 | 1205.4521 | 904.3409 | 723.6742 🗸 | 603.2297 🗸 | 517.1979 🏑 |
| 92.6403 | 107.9124 | 129.2935 | 161.3650 | 214.8176 | 321.7228 | 642.4383 🗸 | 4 | | R | 25 | S. | 3458.2407 | 1729.6240 | 1153.4184 | 865.3156 | 692.4540 🗸 | 577.2128 | 494.8978 🗸 |
| 114.9404 | 133.9293 | 160.5137 | 200.3903 | 266.8513 | 399.7733 🗸 | 798.5394 🗸 | 5 🖋 | ĺ | R | 24 | ¥' | 3302.1396 | 1651.5734 | 1101.3847 | 826.2903 | 661.2337 🎸 | 551.1960 🗸 | 472.5976 🖌 |
| 137.2406 | 159.9461 | 191.7339 | 239.4156 | 318.8850 | 477.8239 | 954.6405 | 6 🖌 | | R | 23 | tí 🗌 | 3146.0384 | 1573.5229 | 1049.3510 | 787.2651 🗸 | 630.0135 | 525.1791 🗸 | 450.2974 |
| 159.5408 | 185.9630 | 222.9541 | 278.4409 | 370.9187 🎝 | 555.8744 🗸 | 1110.7416 | 7 🕩 | | R | 22 | ¥ | 2989.9373 | 1495.4723 | 997.3173 | 748.2398 🗸 | 598.7933 🗸 | 499.1623 🗸 | 427.9973 |
| 179.1206 | 208.8061 | 250.3659 | 312.7056 | 416.6050 🎝 | 624.4039 🗸 | 1247.8005 | 8 🗸 | | н | 21 | 2, | 2833.8362 | 1417.4217 | 945.2836 | 709.2145 🗸 | 567.5731 🗸 | 473.1454 | 405.6971 |
| 198.7004 | 231.6493 | 277.7777 | 346.9703 | 462.2913 - | 692.9334 🗸 | 1384.8594 | 9 👻 | | н | 20 | 3 | 2696.7773 | 1348.8923 | 899.5973 | 674.9498 🗸 | 540.1613 | 450.3023 | 386.1173 |
| 216.9997 | 252.9985 | 303.3967 | 378.9941 | 504.9896 w | 756.9808 | 1512.9544 | 10 👐 | | к | 19 | ~ | 2559.7184 | 1280.3628 | 853.9110 | 640.6851 vy | 512.7495 | 427.4591 | 366.5374 |
| 235.2990 | 274.3476 | 329.0157 | 411.0178 | 547.6880 | 821.0283 🗸 | 1641.0494 | 11 🗸 | | к | 18 | 4 | 2431.6234 | 1216.3154 | 811.2127 | 608.6613 🗸 | 487.1305 | 406.1100 | 348.2382 |
| 243.4449 | 283.8512 | 340.4200 | 425.2732 🗸 | 566.6951 🤳 | 849.5390 | 1698.0708 | 12 🗸 | | G | 17 🛰 | 1 | 2303.5285 | 1152.2679 | 768.5143 💜 | 576.6376 | 461.5115 | 384,7608 | 329.9389 |
| 261.7442 | 305.2004 | 366.0390 | 457.2969 🗸 | 609.3934 🗸 | 913.5865 | 1826.1658 | 13 🖌 | 1 | к | 16 | ¥ | 2246.5070 | 1123.7571 | 749.5072 | 562.3822 | 450.1072 | 375.2572 | 321.7930 |
| 280.0435 | 326.5495 | 391.6580 | 489.3206 | 652.0918 | 977.6340 | 1954.2607 | 14 🗸 | | к | 15 | <u>~</u> | 2118.4120 | 1059,7097 | 706.8089 🗸 | 530.3585 4 | 424.4882 | 353.9081 | 303.4937 |
| 298.3428 | 347.8987 | 417.2770 | 521.3444 🖌 | 694.7901 / | 1041.6815 | 2082.3557 | 15 🖋 | | к | 14 | r | 1990.3171 | 995.6622 | 664.1105 🗸 | 498.3347 🗸 | 398.8692 | 332.5589 | 285.1944 |
| 306.4887 | 357.4023 | 428.6813 | 535.5997 🗸 | 713.7972 🗸 | 1070.1922 | 2139.3772 | 16 🗸 | | G | 13 | V | 1862.2221 | 931.6147 | 621.4122 🗸 | 466.3110 🗸 | 373.2502 | 311.2097 | 266.8951 |
| 328.7888 | 383.4191 | 459.9015 1 | 574.6250 V | 765.8309 🖌 | 1148.2428 | 2295.4783 | 17 🗸 | | R | 12 | V. | 1805.2007 | 903.1040 | 602.4051 🗸 | 452.0556 🗸 | 361.8460 | 301.7062 | 258.7492 |
| 351.0890 | 409.4360 | 491.1217 🗸 | 613.6503 🗸 | 817.8646 🗸 | 1226.2933 | 2451.5794 | 18 🖌 | | R | 11 | V | 1649.0995 | 825.0534 🖌 | 550.3714 4 | 413.0303 | 330.6257 | 275.6893 | 236.4490 |
| 373.3892 | 435.4528 | 522.3419 V | 652.6756 | 869.8984 | 1304.3439 | 2607.6805 | 19 ¥ | | R | 10 | V | 1492.9984 | 747.0029 🗸 | 498.3377 🗸 | 374.0051 | 299,4055 | 249.6725 | 214.1489 |
| 395.6893 | 461.4697 🗸 | 553.5621 | 691.7009 🗸 | 921.9321 | 1382.3944 | 2763.7816 | 20 * | | R | 9 | Υ | 1336.8973 | 668.9523 🎝 | 446.3040 🗸 | 334.9798 | 268.1853 | 223.6556 | 191.8487 |
| 417,9895 | 487.4865 🗸 | 584.7824 | 730.7261 🗸 | 973.9658 | 1460.4450 | 2919.8827 | 21 ¥, | | R | 8 | 5 | 1180.7962 | 590.9017 🗸 | 394.2703 🗸 | 295.9545 | 236.9651 | 197.6388 | 169.5486 |
| 436.2888 | 508.8357 | 610.4014 🗸 | 762.7499 | 1016.6641 | 1524.4925 | 3047,9777 | 22 * | | ĸ | 7 | 8 | 1024.6951 | 512.8512 | 342.2366 | 256.9292 | 205.7448 | 171.6219 | 147.2484 |
| 458,5889 | 534.8525 🗸 | 641.6216 🗸 | 801.7752 | 1068,6978 | 1602.5430 | 3204.0788 | 23 4 | | R | 6 | ٤. | 896.6001 | 448.8037 V | 299.5382 | 224.9055 | 180.1258 | 150.2728 | 128.9491 |
| 480.8891 - | 560.8694 N | 672.8418 🗸 | 840.8004 | 1120.7315 | 1680.5936 | 3360,1799 | 24 7 | | R | 5 | 2 | 740.4990 🗸 | 370.7532 | 247.5045 | 185.8802 | 148.9056 | 124.2559 | 106.6490 |
| 503.1892 | 586.8862 | 704.0620 ^ | 879.8257 | 1172.7652 | 1758.6441 | 3516.2810 | 25 * | | R | 4 | ä | 584.3979 🗸 | 292.7026 V | 195.4708 | 146.8549 | 117.6854 | 98.2390 | 84.3488 |
| 511.3352 | 596.3898 | 715.4663 4 | 894.0811 | 1191.7723 | 1787.1549 | 3573.3025 | 26 % | | G | 3 | 8, | 428.2968 | 214.6520 | 143.4371 | 107.8297 | 86.4652 | 72.2222 | 62.0486 |
| 533.6353 V | 622.4067 | 746.6865 | 933.1064 | 1243.8060 | 1865.2054 | 3729.4036 | 27 ¥ | / | R | 2 | 5 | 371.2753 🗸 | 186.1413 | 124.4300 | 93.5743 | 75.0609 | 62.7186 | 53.9027 |
| 564.0866 | 657.9332 | 789.3184 | 986.3961 | 1314.8591 | 1971.7850 | 3942.5627 | 28 | | R | 1 | 4 | 215.1742 🗸 | 108.0908 | 72.3963 | 54.5490 | 43.8407 | 36.7018 | 31.6026 |
| | 1 | | | | | 1 | | | (cterm + 56 | 1 | | | | | | | | |

021519_0p2perYellowTube_Gradient_DD_Heat15 #2644-4489 RT: 11.35-16.61 AV: 28 NL: 1.10E5 T: FTMS + p NSI d Full ms2 553.2017@etd11.84 [120.0000-2000.0000]







021519_0p2perYellowTube_Gradient_DD_H... 0-10-30-70-100 in 0-10-20-30-35





| +5 c ions | +4 c ions | +3 c ions | +2 c ions | +1 c ions | | Sequence | | +1 z ions | +2 z ions | +3 z ions | +4 z ions | +5 z ions |
|-----------|------------|-------------|-------------|-------------|----|---------------|----|-------------|-----------------------|--------------|------------|-----------|
| 35.6328 | 44.2892 | 58.7165 | 87.5711 | 174.1349 🗸 | 1 | R | 22 | 3313.1614 | 1657.0843 | 1105.0587 | 829.0458 | 663.4381 |
| 66.8530 | 83.3145 | 110,7502 | 165.6217 | 330.2360 / | 2 | R | 21 | 3141.0416 | 1571.0244 🗸 | 1047.6854 | 786.0158 🗸 | 629.0141 |
| 98.0733 | 122.3397 | 162.7839 | 243.6722 | 486.3372 🗸 | 3 | R | 20 | 2984.9405 | 1492.9739 🗸 | 995.6517 🗸 | 746.9906 🗸 | 597.7939 |
| 129.2935 | 161.3650 | 214.8176 | 321.7228 | 642.4383 🗸 | 4 | R | 19 | 2828.8393 | 1414.9233 🗸 | 943.6180 🗸 | 707.9653 🏒 | 566.5737 |
| 160.5137 | 200.3903 | 266.8513 | 399.7733 | 798.5394 🗸 | 5 | R | 18 | 2672.7382 | 1336.8728 | 891.5843 🗸 | 668.9400 🗸 | 535.3535 |
| 191.7339 | 239.4156 | 318.8850 | 477.8239 🗸 | 954.6405 🗸 | 6 | R | 17 | 2516.6371 | 1258.8222 🗸 | 839.5506 🗸 , | 629.9147 🗸 | 504.1332 |
| 222.9541 | 278.4409 | 370.9187 | 555.8744 🗸 | 1110.7416 🗸 | 7 | R | 16 | 2360.5360 | 1180.7716 | 787.5169 🗸 | 590.8895 🗸 | 472.9130 |
| 254.1744 | 317.4661 | 422.9524 | 633.9250 V | 1266.8427 🗸 | 8 | R | 15 | 2204.4349 | 1102.7211 | 735.4832 ^ | 551.8642 | 441.6928 |
| 285.3946 | 356.4914 | 474.9861 | 711.9756 🗸 | 1422.9438 🗸 | 9 | R | 14 | 2048.3338 | 1024.6705 | 683.4494 1. | 512.8389 | 410.4726 |
| 316.6148 | 395.5167 | 527.0198 | 790.0261 🗸 | 1579.0449 🗸 | 10 | R | 13 | 1892.2327 | 946.6200 1. | 631.4157 🗸 | 473.8136 | 379.2524 |
| 347.8350 | 434.5420 | 579.0535 √ | 868.0767 🗸 | 1735.1460 | 11 | R | 12 | 1/36.1316". | 868.5694 1 | 579.3820 🗸 | 434.7884 | 348.0321 |
| 379.0553 | 473.5672 | 631.0872 🗸 | 946.1272 🗸 | 1891.2472 | 12 | R | 11 | 1580.0305 7 | 790,5189 7 | 527.3483 🗸 | 395.7631 | 316.8119 |
| 410.2755 | 512.5925 | 683.1209 🗸 | 1024.1778 🗸 | 2047.3483 | 13 | R | 10 | 1423.92937 | 712.4683 ^ | 475.3146 🗸 | 356.7378 | 285.5917 |
| 441.4957 | 551.6178 | 735.1546 | 1102.2283 🗸 | 2203.4494 | 14 | R | 9 | 1267.8282 | 634.4178 | 423.2809 | 317.7125 | 254.3715 |
| 458.9021 | 573.3758 | 764.1653 🗸 | 1145.7443 🖌 | 2290.4814 | 15 | S | 8 | 1111.7271 🗸 | 556.3672 ⁰ | 371.2472 | 278.6872 | 223.1512 |
| 490.1223 | 612.4011 | 816.1990 🗸 | 1223.7949 🗸 | 2446.5825 | 16 | R | 7 | 1024.6951 | 512.8512 🗸 | 342.2366 | 256.9292 | 205.7448 |
| 521.3425 | 651.4264 🗸 | 868.2327 🗸 | 1301.8455 🗸 | 2602.6836 | 17 | R | 6 | 868.5940 🗸 | 434.8006 🗸 | 290.2028 | 217.9040 | 174.5246 |
| 552,5628 | 690.4516 🗸 | 920.2664 V | 1379.8960 🗸 | 2758.7847 | 18 | R | 5 | 712.4929 🗸 | 356.7501 🗸 | 238.1691 | 178.8787 | 143.3044 |
| 583.7830 | 729.4769 🗸 | 972.3001 🗸 | 1457.9466 🗸 | 2914.8859 | 19 | R | 4 | 556.3918 🗸 | 278.6995 | 186.1354 | 139.8534 | 112.0842 |
| 595.1873 | 743.7323 🗸 | 991.3073 🗸 | 1486.4573 🗸 | 2971.9073 | 20 | G | 3 | 400.2907 V | 200.6490 | 134.1017 | 100.8281 | 80.8640 |
| 626.4075 | 782.7576 √ | 1043.3410 🗸 | 1564.5079 | 3128.0084 | 21 | R | 2 | 343.2692 🗸 | 172.1382 | 115.0946 | 86.5728 | 69.4597 |
| 663.4381 | 829.0458 | 1105.0587 | 1657.0843 | 3313.1614 | 22 | К | 1 | 187.1681 🗸 | 94.0877 | 63.0609 | 47.5475 | 38.2394 |
| | | | | | | (cterm + 56., | .] | | | | | |







021519_0p2perYellowTube_Gradient_DD_H... 0-10-30-70-100 in 0-10-20-30-35

021519_0p2perYellowTube_Gradient_DD_Heat15 #2930-7239 RT: 12.04-24.54 AV: 46 NL: 1.74E4 T: FTMS + p NSI d Full ms2 575.5286@etd2.52 [120.0000-2000.0000]





m/z

021519_0p2perYellowTube_Gradient_DD_Heat15 #2930-7239 RT: 12.04-24.54 AV: 46 NL: 2.69E2 T: FTMS + p NSI d Full ms2 575.5286@etd2.52 [120.0000-2000.0000]



| +11 c ions | +10 c ions | +9 c ions | +8 c ions | +7 c ions | +6 c ions | +5 c ions | +4 c ions | +3 c ions | +2 c ions | +1 c ions | 1 | Sequence |
|------------|------------|------------|------------|------------|------------|--------------|------------|------------|-----------|-----------|-------|---------------|
| 16.7462 | 18.3200 | 20.2437 | 22.6482 | 25,7398 | 29.8619 | 35.6328 | 44 2892 | 58 7165 | 87 5711 | 174 1349 | 1 7 | D |
| 30.9372 | 33.9302 | 37.5883 | 42,1609 | 48,0400 | 55 8787 | 66 8530 | 83 3145 | 110 7502 | 165 6217 | 330 2360 | 2 | |
| 45.1282 | 49.5403 | 54,9328 | 61.6735 | 70.3401 | 81 8956 | 98 0733 | 122 3397 | 162 7839 | 243 6722 | 496 2272 | 2 1 | D D |
| 59.3192 | 65.1504 | 72.2774 | 81,1862 | 92,6403 | 107 9124 | 129 2935 | 161 3650 | 214 8176 | 321 7228 | 642 4392 | J 4 | |
| 73.5102 | 80.7605 | 89.6220 | 100.6988 | 114,9404 | 133.9293 | 160.5137 | 200 3903 | 266 8513 | 399 7733 | 798 5394 | 5 | |
| 87.7012 | 96.3706 | 106.9665 | 120,2114 | 137 2406 | 159 9461 | 191 7339 | 239 4156 | 318 8850 | 477 8230 | 054 6405 | 6 3 | |
| 101.8922 | 111.9807 | 124.3111 | 139.7241 | 159,5408 | 185,9630 | 222 9541 | 278 4409 | 370 9187 | 555 8744 | 1110 7/16 | 7 3 | |
| 114.3521 | 125.6866 | 139.5399 | 156.8564 | 179,1206 | 208.8061 | 250 3659 | 312 7056 | 416 6050 | 624 4039 | 1247 8005 | 8 1 | <u>u</u> |
| 119.5359 | 131.3887 | 145.8756 | 163.9841 | 187,2665 | 218.3097 | 261,7702 | 326 9610 | 435 6122 | 652 9146 | 1304 8220 | a / | G |
| 133.7269 | 146.9989 | 163.2201 | 183,4968 | 209.5667 | 244,3266 | 292 9904 | 365 9862 | 487 6459 | 730 9652 | 1460 9231 | 10 1 | B |
| 145.3719 | 159.8084 | 177.4529 | 199.5086 | 227.8660 | 265.6757 | 318.6094 | 398.0100 | 530,3442 | 795 0127 | 1589 0181 | 11 | ĸ |
| 150.5557 | 165.5105 | 183.7886 | 206.6363 | 236.0119 | 275.1793 | 330.0137 | 412.2653 | 549.3514 | 823.5234 | 1646 0395 | 12 | G |
| 162.2007 | 178.3200 | 198.0214 | 222.6482 | 254.3112 | 296.5285 | 355.6327 | 444,2891 | 592.0497 🗸 | 887.5709 | 1774 1345 | 13 1 | ĸ |
| 173.8457 | 191.1295 | 212.2542 | 238.6600 | 272.6104 | 317-8776 | 381.2517 | 476.3128 | 634-7480 | 951-0184 | 1902 2294 | 44 | K |
| 182.6686 | 200.8348 | 223.0378 | 250.7916 | 286.4751 | 334.0531 | 400.6623 | 500.5760 | 667.0989 J | 1000.1447 | 1999,2822 | 15 | P |
| 194.3136 | 213.6443 | 237.2706 | 266.8035 | 304.7744 | 355.4023 | 426.2813 | 532.5997 / | 709.7972 🗸 | 1064.1922 | 2127.3772 | تى 16 | ĸ |
| 208.5046 | 229.2544 | 254.6152 | 286.3162 | 327.0746 | 381.4191 | 457.5015 | 571.6250 🗸 | 761.8309 V | 1142.2428 | 2283.4783 | 17 | R |
| 220.9645 | 242.9603 | 269.8439 | 303.4485 | 346.6544 | 404.2623 | 484.9133 | 605.8898 √ | 807.5172 🗸 | 1210.7722 | 2420.5372 | 18 💉 | Н |
| 235.1556 | 258.5704 | 287.1885 | 322.9612 | 368.9546 | 430.2791 | 516.1335 | 644.9150 🗸 | 859.5510 | 1288.8228 | 2576.6383 | 19 V | R |
| 249.3466 | 274.1805 | 304.5331 | 342.4738 | 391.2547 | 456.2960 | 547.3537 | 683.9403 У | 911.5847 | 1366.8733 | 2732.7394 | 20 🗸 | R |
| 263.5376 | 289.7906 | 321.8776 | 361.9864 | 413.5549 | 482.3128 | 578.5739 J | 722.9656 1 | 963.6184 | 1444.9239 | 2888.8405 | 21 🚽 | R |
| 277.7286 | 305.4007 | 339.2222 | 381.4991 | 435.8550 | 508.3297 | 609.7941 🖌 , | 761.9909 🤳 | 1015.6521 | 1522.9745 | 3044.9416 | 22 | R |
| 291.9196 | 321.0108 | 356.5668 | 401.0117 | 458.1552 | 534.3465 | 641.0144 🗸 | 801.0161 🗸 | 1067.6858 | 1601.0250 | 3201.0427 | 23 🗸 | R |
| 306.1106 | 336.6209 | 373.9113 | 420.5243 | 480.4554 | 560.3634 | 672.2346 J | 840.0414 | 1119.7195 | 1679.0756 | 3357.1439 | 24 V | R |
| 320.3016 | 352.2310 | 391.2559 | 440.0370 | 502.7555 | 586.3802 / | 703.4548 🗸 | 879.0667 | 1171.7532 | 1757.1261 | 3513.2450 | 25 👻 | R |
| 334.4926 | 367.8412 | 408.6005 | 459.5496 | 525.0557 | 612.3971 🗸 | 734.6750 🗸 | 918.0920 | 1223.7869 | 1835.1767 | 3669.3461 | 26 | R |
| 348.6836 | 383.4513 | 425.9450 | 479.0623 | 547.3558 | 638.4139 🗸 | 765.8953 🗸 | 957,1173 | 1275.8206 | 1913.2272 | 3825.4472 | 27 1 | R |
| 353.8674 | 389.1534 | 432.2808 | 486.1899 | 555.5018 | 647.9175 🗸 | 777.2996 🗸 | 971.3726 | 1294.8277 | 1941.7380 | 3882.4687 | 28 | G |
| 368.0584 | 404.7635 | 449.6253 | 505.7026 | 577.8019 | 673.9344 V | 808.5198 | 1010.3979 | 1346.8614 | 2019.7885 | 4038.5698 | 29 | R |
| 382.2494 | 420,3736 | 466.9699 | 525.2152 | 600.1021 | 699.9512 | 839.7400 | 1049.4232 | 1398.8951 | 2097.8391 | 4194.6709 | 30 | R |
| 393.8944 | 433.1831 | 481.2027 | 541.2271 | 618.4014 , | 721.3004 | 865.3590 | 1081.4469 | 1441.5935 | 2161.8866 | 4322.7658 | 31 | к |
| 400.3523 | 440.2868 | 489.0957 | 550.1067 | 628.5495 🧸 | 733.1399 | 879.5664 | 1099.2062 | 1465.2725 | 2197.4051 | 4393.8030 | 32 🖌 | A |
| 412.8122 | 453.9927 | 504.3245 | 567.2391 | 648.1294 🗸 | 755.9830 | 906.9782 | 1133.4709 | 1510.9588 | 2265.9346 | 4530.8619 | 33 🏒 | н |
| 427.0032 | 469.6028 | 521.6690 | 586.7517 | 670.4295 J | 781.9999 🗸 | 938.1984 | 1172.4962 | 1562.9925 | 2343.9851 | 4686.9630 | 34 √ | R |
| 432.1870 | 475.3050 | 528,0047 | 593.8794 | 678.5754 🗸 | 791.5035 | 949.6027 | 1186.7516 | 1581.9997 | 2372.4959 | 4743.9844 | 35 🖌 | G |
| 446.3780 | 490.9151 | 545.3493 | 613.3921 | 700.8756 | 817.5203 | 980.8229 | 1225.7768 | 1634.0334 | 2450.5464 | 4900.0856 | 36 🖌 | R |
| 458.0230 | 503.7246 | 559.5821 | 629.4039 | 719.1749 | 838.8695 | 1006.4419 | 1257.8006 | 1676.7317 | 2514.5939 | 5028.1805 | 37 🗸 | к |
| 469.6680 | 516.5341 | 5/3.8149 | 645.4158 | 131.4/42 | 860.2186 | 1032.0609 | 1289.8243 | 1719.4300 | 2578.6414 | 5156.2755 | 38 🔹 | ĸ |
| 401.3130 | 529.3436 | 588.0476 | 661.42// V | 755.7734 4 | 881.5678 | 1057.6799 | 1321.8481 | 1762.1283 | 2642.6889 | 5284.3704 | 39 V | ĸ |
| 495.5040 | 544.9537 | 605.3922 | 680.9403 | 778.0736 V | 907.5847 | 1088.9001 | 1360.8733 | 1814.1620 | 2720.7394 | 5440.4716 | 40 🗸 | R |
| 505 9716 | 550,0009 | 011.7279 | 605 1057 | 704.2654 | 917.0882 | 1100.3044 | 13/5.128/ | 1833.1692 | 2749.2501 | 5497.4930 | 41 2 | G |
| 505.6716 | 536.3360 | 018.0030 | 095.1957 V | 794.3654 | 926.5918 | 1111.7087 | 1389.3841 | 1852.1763 | 2777.7609 | 5554.5145 | 42 - | G |
| 520.0626 | 5/1.9681 | 035.4082 | 714.7083 | 816.6656 | 952.6087 | 1142.9289 | 1428.4094 | 1904.2100 | 2855.8114 | 5710.6156 | 43 * | R |
| 534.2030 | 587.5782 | 002./028 9 | 734.2210 | 838.9658 | 9/8.6255 | 11/4.1492 | 1467.4346 | 1956.2438 | 2933.8620 | 5866.7167 | 44 | R |
| 545.6966 | 600.3877 | 000.9855 | 750.2328 4 | 857.2650 | 999.9747 | 1199.7682 | 1499.4584 | 1998.9421 | 2997.9095 | 5994.8117 | 45 🗸 | ĸ |
| 551.0824 | 000.0899 | 073.3213 | 770 0704 1 | 805.4110 | 1009.4783 | 1211.1/24 | 1513./13/ | 2017.9492 | 3026.4202 | 6051.8331 | 46 | G |
| 562.7274 | 618.8994 | 687.5540 🗸 | 773.3724 J | 883.7102 | 1030.8274 | 1236.7914 | 1545.7375 | 2060.6475 | 3090,4677 | 6179.9281 | 4/ | ĸ |
| 5/6.9184 | 034.5095 | 704.8986 - | 792.8850 | 906.0104 | 1056.8443 | 1268.0117 | 1584.7628 | 2112.6813 | 3168.5182 | 6336.0292 | 48 🗸 | R |
| 591.1094 | | 722.2432 | 812.39/7 | 928.3106 | 1082.8611 | 1299.2319 | 1623.7880 | 2164.7150 | 3246.5688 | 6492.1303 | 49 | ĸ |
| 003.5693 | 003.8255 | 754 9405 | 829.5300 | 947.8904 | 1105./043 | 1326.6437 | 1658.0528 | 2210.4013 | 3315.0983 | 6629.1892 | 50 | H |
| 017.7603 / | 0/9.4356 V | 104.0165 | 049.0427 | 970.1906 | 1131./211 | 1357.8639 | 1697.0780 | 2262.4350 | 3393.1488 | 6785.2903 | 51 V | ĸ |
| 031.9513 V | | 7/2.1611 | 868.5553 | 992.4907 | 1157.7380 | 1389.0841 | 1/36.1033 | 2314.4687 | 34/1.1994 | 6941.3914 | 52 . | ĸ |
| 046.1423 V | 700.0050 | 789.5056 | 888.0679 | 1014.7909 | 1183,7548 | 1420.3043 | 1//5.1286 | 2366.5024 | 3549.2499 | 7097.4926 | 53 | ĸ |
| 000.3333 V | 747 5949 | 806.8502 | 907.5806 | 1037.0910 | 1209.7717 | 1451.5246 | 1814.1539 | 2418.5361 | 3627.3005 | 7253.5937 | 54 | ĸ |
| 0/9./114 | 141.0010 | 030.9340 | 934.2293 | 1007.5424 | 1240.2982 | 1494.1004 | 1007.4437 | 2409.309 | 3/33.8800 | 1400.1028 | 00 | K (otorm t EC |
| 1 | | | | (| | | | | | | | Norenni ± 00 |

| | | | | | | | | | · | | | | |
|-------------|-------|---|------------|------------|-------------|------------|------------|------------|------------|-------------|------------|------------|------------|
| Sequence | 1 | | +1 z ions | +2 z ions | +3 z ions | +4 z ions | +5 z ions | +6 z ions | +7 z ions | +8 z ions | +9 z ions | +10 z ions | +11 z ions |
| Dequeries | 55 | | 7466 7528 | 3733 8800 | 489.5891 1 | 867.4437 | 494.1564 | 1245.2982 | 1067.5424 | 934.2255 | 830.5346 | 747.5818 | 679.7114 |
| <u> </u> | 54 14 | ÿ | 7294 6330 | 3647 8201 | 432 2158 1 | 824,4137 | 459,7324 | 1216.6116 | 1042.9538 | 912.7105 | 811.4101 | 730.3698 | 664.0642 🗸 |
| | 53 9 | \$ | 7138 5319 | 3569 7696 | 2380 1821 1 | 785 3884 | 428.5122 | 1190.5947 | 1020.6536 | 893.1978 | 794.0656 | 714.7597 🖌 | 649.8731 |
| | 50 | 1 | 6092 4307 | 3/01 7100 | 328 1484 1 | 746 3631 | 397,2920 | 1164.5779 | 998.3535 | 873.6852 | 776.7210 | 699.1496 🗸 | 635.6821 🖌 |
| K | 52 | | 6902.4307 | 3431.7130 | 2276 1147 1 | 707 3379 | 1366 0717 | 1138 5610 | 976.0533 | 854.1726 | 759.3764 | 683.5395 | 621.4911 |
| R | 50 1 | | 6670 2295 | 2225 6170 | 2224 0810 | 668 3126 | 1334 8515 | 1112 5441 | 953,7532 | 834.6599 | 742.0319 | 667.9294 | 607.3001 🖌 |
| R | 40 | v | 6670.2265 | 3257 5673 | 2172 0473 | 629 2873 | 1303 6313 | 1086.5273 | 931,4530 | 815.1473 | 724.6873 🗸 | 652.3193 🗸 | 593.1091 |
| K | 49 | 2 | 6259 0262 | 3179 5168 | 2120 0136 | 590 2620 | 1272 4111 | 1060.5104 | 909.1529 | 795.6347 | 707.3427 🗸 | 636.7092 🗸 | 578.9181 |
| <u> </u> | 40 | 6 | 6220 9674 | 3110 9873 | 2074 3273 | 555 9973 | 1244,9993 | 1037.6673 | 889.5730 | 778.5023 | 692.1140 🗸 | 623.0033 🗸 | 566.4582 |
| <u> </u> | 4/ | 5 | 6163 0450 | 3082 4766 | 2055 3202 | 541 7419 | 1233 5950 | 1028.1637 | 881.4271 | 771.3746 🗸 | 685.7782 🗸 | 617.3011 | 561.2744 |
| к v | 40 | - | 6007 8448 | 3004 4260 | 2003 2865 | 502 7167 | 1202.3748 | 1002.1469 | 859.1269 | 751.8620 | 668.4337 | 601.6910 | 547.0834 |
| 2 | 45 | | 5879 7498 | 2940 3786 | 1960 5881 | 470,6929 | 1176.7558 | 980,7977 | 840.8276 | 735.8501 | 654.2009 | 588.8815 | 535.4384 |
| | 49 | | 5922 7284 | 2011 8678 | 1941 5810 | 1456 4376 | 1165.3515 | 971.2941 | 832.6817 | 728.7224 | 647.8652 | 583.1794 | 530.2546 |
| | 40 | <u> </u> | 5604 6334 | 2847 8203 | 1898 8827 | 1424 4138 | 1139 7325 | 949,9450 | 814.3824 🗸 | 712.7105 | 633.6324 🗸 | 570.3699 | 518.6097 |
| n | 42 | AP | CECC 5295 | 2792-7720 | 1856 1873 | 1302 3001 | 1144-1135 | 928 5958 | 796:0832 | 696:6987 | 619.3996 | 557-5604 | 506.9647 |
| P | 41 | <u></u> | 5300-0300 | 2705.7725 | 1973 9334 | 1368 1269 | 1094 7030 | 912 4203 | 782.2185 | 684,5671 | 608.6160 🗸 | 547.8551 | 498.1417 |
| ĸ | 40 | | 5409.4007 | 2133.2403 | 1781 1351 | 1336 1031 | 1069 0840 | 891 0712 | 763.9192 | 668.5552 🗸 | 594.3832 🖌 | 535.0456 | 486.4967 |
| ĸ | 39 1 | , | 5341.3907 | 20/1.1990 | 1700.1001 | 1207 0770 | 1037 8637 | 865 0543 | 741 6190 | 649.0426 V. | 577.0386 🗸 | 519.4355 | 472.3057 |
| H | 38 | ·/ | 5185.2896 | 2593.1484 | 1692 4454 | 1201.0110 | 1010 4520 | 842 2112 | 722 0392 | 631,9102 | 561,8099 | 505.7296 | 459.8458 |
| R | 3/ | v N | 15048.2307 | 2024.0190 | 1003.4151 | 1202.0131 | 070 0347 | 816 10/3 | 699 7390 | 612 3976 | 544,4653 | 490.1195 | 445.6548 |
| R | 36 | <u>v</u> | 4892.1296 | 2446.5684 | 1631.3814 | 1223.7679 | 9/9.2317 | 700 1775 | 677 1389 | 592 8849 | 527 1207 | 474,5094 | 431,4637 |
| R | 35 | <u> </u> | 4736.0285 | 2368.51/9 | 15/9.34// | 1184.7626 | 940.0115 | 790.1775 | 655 1387 | 573 3723 | 509 7762 | 458 8993 | 417.2727 |
| R | 34 | ¥. | 4579.9274 | 2290,4673 | 1527.3140 | 1145.7373 | 910.7913 | 704.1000 | 632 8386 | 553 8596 | 492 4316 | 443 2892 | 403.0817 |
| R | 33 | * | 4423.8263 | 2212.4168 | 14/5.2803 | 1106.7120 | 885.5/11 | 730.1430 | 610 5394 | 534 3470 | 475 0870 | 427 6791 | 388,8907 |
| R | 32 | * | 4267.7252 | 2134.3662 | 1423.2466 | 1067.6867 | 854.3509 | 712.1209 V | 500 2292 | 514 8344 | 457 7425 | 412 0690 | 374 6997 |
| R | 31 | \$4° | 4111.6240 | 2056.3157 | 1371.2129 | 1028.6615 | 823.1306 | 660.0022 | 565 0381 | 405 3217 | 440 3979 | 396 4588 | 360,5087 |
| R | 30 | * | 3955.5229 | 1978.2651 | 1319.1792 | 989.6362 | 791.9104 | 660,0932 | 542 6379 V | 495.5211 | 423 0533 | 380 8487 | 346.3177 |
| R | 29 | ¢. | 3799.4218 | 1900.2145 | 1267.1455 | 950.6109 | 760.6902 | 634.0704 V | 521 2279 V | 456 2065 | 405 7088 | 365 2386 | 332 1267 |
| G | 28 | ¥ | 3643.3207 | 1822.1640 | 1215.1118 | 911.5856 | 729.4700 | 500 5550 | 512 1019 | 430.2300 | 300 3731 | 359 5365 | 326 9429 |
| R | 27 | 17 | 3586.2992 | 1793.6533 | 1196,1046 | 897.3303 | /18.065/ V | 698.5559 | 400 9017 | 449.1000 | 382 0285 | 343 9264 | 312 7519 |
| R | 26 | 4 | 3430.1981 | 1715.6027 | 1144.0709 | 858.3050 | 686.8454 V | 5/2.5391 | 490.6917 | 429.0001 | 364 6839 | 328 3163 | 298 5609 |
| ĸ | 25 | ¥ | 3274.0970 | 1637.5521 | 1092.0372 | 819.2797 | 655.6252 | 546.5222 | 466,5915 | 204 1316 | 350 4511 | 315 5068 | 286 9159 |
| А | 24 | 14 | 3146.0021 | 1573.5047 | 1049.3389 | 787.2560 | 630.0062 | 525.1/31 | 450.2922 | 295 2520 | 342 5581 | 308 4030 | 280 4580 |
| н | 23 | V | 3074.9649 | 1537.9861 | 1025.6598 | 769.4967 | 615.7988 | 513.3335 V | 440.1441 | 269 1106 | 327 3204 | 294 6972 | 267 9981 |
| R | 22 | 8 | 2937.9060 | 1469.4567 | 979.9735 | 735.2320 | 588.3870 V | 490.4904 | 420.0042 | 249 6070 | 309 9848 | 279 0870 | 253 8071 |
| G | 21 | 4 | 2781.8049 | 1391.4061 | 927.9398 | 696.2067 | 557.1668 | 464.4736 | 390.2041 | 341.4793 | 303 6491 | 273 3849 | 248.6233 |
| R | 20 | वे | 2724.7835 | 1362.8954 | 908.9327 | 681.9513 • | 545.7625 ¥ | 404.9700 | 390.1102 | 321 9667 | 286 3045 | 257 7748 | 234,4323 |
| к | 19 | <u>, </u> | 2568.6823 | 1284.8448 | 856.8990 | 042.9260 | 14.0423 | 407 6040 | 349 5187 | 305 9548 | 272 0717 | 244,9653 | 222,7873 |
| K | 18 🗸 | r 3 | 2440.5874 | 1220.7973 | 814.2006 | 610.9023 V | 468.9233 | 206 2549 | 331 2104 | 289 9429 | 257 8390 | 232,1558 | 211,1423 |
| ĸ | 17 * | | 2312.4924 | 1156.7498 | //1.5023 | 5/8.8/86 V | 403.3043 | 264 0056 | 312 0202 | 273 9310 | 243 6062 | 219,3463 | 199,4973 |
| R | 16 V | | 2184.3975 | 1092.7024 | 728.8040 | 545.8548 V | 400 4051 | 220 0000 | 290 6200 | 254 4184 | 226 2616 | 203,7362 | 185.3063 |
| G | 15 V | <u> </u> | 2028,2963 | 1014.6518 | 676.7703 V | 507.8295 V | 405.4001 | 220 2952 | 290.0200 | 247 2907 | 219 9259 | 198.0340 | 180,1225 |
| G | 14 | <u> </u> | 1971.2749 | 986.1411 | 657.7631 V | 493.5/42 | 395.0608 | 329,3032 | 202.4741 | 240 1630 | 213 5902 | 192 3319 | 174,9387 |
| R | 13 🔹 | ſ, | 1914.2534 | 957.6303 | 638.7560 | 4/9.3188 V | 383.6565 | 319.8810 | 214.3202 | 240.1000 | 106 2456 | 176 7218 | 160 7477 |
| R | 12 | 3 | 1758.1523 | 879.5798 | 586.7223 🗸 | 440.2935 | 352.4363 | 293.8648 | 202.0280 | 220.0004 | 179 0010 | 161 1117 | 146 5567 |
| к | 11 | a | 1602.0512 | 801.5292 🗸 | 534.6886 🗸 | 401.2683 | 321.2161 | 267.8479 | 229.1218 | 195 1250 | 164 6693 | 148 3022 | 134 9117 |
| G | 10 | £ | 1473.9562 | 737.4818 | 491.9903 🗸 | 369.2445 | 295.5971 | 246.4988 | 211.4286 | 100.1209 | 159 2206 | 142 6000 | 129 7280 |
| К | 9 4 | 7 | 1416.9348 | 708.9710 | 472.9831 🗸 | 354.9891 | 284.1928 | 236.9952 | 203.2826 | 1/7.9982 | 100.0020 | 120 7005 | 118 0830 |
| R | 8 🗸 | | 1288.8398 | 644.9235 🗸 | 430.2848 🗸 | 322.9654 | 258.5738 | 215.6460 | 184.9834 | 161.9863 | 144.0998 | 114 1904 | 103 8020 |
| R | 7 4 | | 1132.7387 | 566.8730 | 378.2511 | 283.9401 | 227.3536 | 189.6292 | 162.6832 | 142.4/37 | 120.7552 | 09 5702 | 103.0920 |
| н | 6 V | | 976.6376 | 488.8224 | 326.2174 | 244.9149 | 196.1333 | 163.6123 | 140.3830 | 122.9611 | 109,4106 | 98.5703 | 77 2410 |
| R | 5 ¥ | , | 839.5787 | 420.2930 🗸 | 280.5311 | 210.6501 | 168.7216 | 140.7692 | 120.8032 | 105.8287 | 94.1819 | 04.0044 | 63 0500 |
| R | 4 2 | | 683.4776 | 342.2424 | 228.4974 | 171.6248 | 137.5013 | 114.7523 | 98.5030 | 86.3161 | 10.83/3 | 09.2043 | 19 8500 |
| R | 3 6 | | 527.3764 🗸 | 264.1919 | 176.4637 | 132.5996 | 106.2811 | 88.7355 | 76.2029 | 66.8034 | 59.4927 | 03.0442 | 40.0090 |
| R | 2 * | | 371.2753 | 186.1413 | 124.4300 | 93.5743 | 75.0609 | 62.7186 | 53.9027 | 47.2908 | 42.1482 | 38.0341 | 34.0000 |
| R | 1 * | i | 215.1742 | 108.0908 | 72.3963 | 54.5490 | 43.8407 | 36.7018 | 31.6026 | 27.7781 | 24.8036 | 22.4240 | 20.4770 |
| (cterm + 56 | | | 1 | 1 | | | | | | 1 | 1 | | |

02/15/19 13:37:41

AV; ~0.2% Yellow Tube

021519_0p2perYellowTube_Gradient_DD_Heat15 #2623-3827 RT: 11.17-14.25 AV: 8 NL: 2.93E4 T: FTMS + p NSI d Full ms2 584.3674@etd8.70 [120.0000-2000.0000]







233.0468

z=?

240

252+

356.7505

z=2

360

230

350

m/z





| +5 c ions | +4 c ions | +3 c ions | +2 c ions | +1 c ions | | Sequence | | | +1 z ions | +2 z ions | +3 z ions | +4 z ions | +5 z ions |
|------------|------------|-------------|-------------|-------------|------------|-------------|-----|-------------------|------------|------------|------------|------------|------------|
| 35.6328 | 44.2892 | 58.7165 | 87.5711 | 174.1349 | 1 🗸 | R | 30 | | 4082.5081 | 2041.7577 | 1361.5076 | 1021.3825 | 817.3074 |
| 53.0392 | 66.0472 | 87.7272 | 131.0871 | 261.1670 🗸 | 2 🗸 | S | 29 | v | 3910.3883 | 1955.6978 | 1304.1343 | 978.3525 | 782.8835 🗸 |
| 73.2487 | 91.3091 | 121.4097 | 181.6110 | 362.2146 | 3 🖌 | Т | 28 | 7 | 3823.3563 | 1912.1818 | 1275.1236 | 956.5945 🗸 | 765.4771 🗸 |
| 90.6552 | 113.0671 | 150.4204 | 225.1270 | 449.2467 V | 4 🗸 | S | 27 | 1 | 3722.3086 | 1861.6579 | 1241.4410 | 931.3326 🗸 | 745.2675 |
| 121.8754 | 152.0924 | 202.4541 | 303.1775 | 605.3478 🗸 | 5 🖌 | R | 26 | 1 | 3635.2766 | 1818.1419 | 1212.4304 | 909.5746 | 727.8611 |
| 139.2818 | 173.8504 | 231.4648 | 346.6935 | 692.3798 | 6 | S | 25 | V | 3479.1754 | 1740.0914 | 1160.3967 | 870.5493 🗸 | 696.6409 🗸 |
| 170.5020 | 212.8757 | 283.4985 | 424.7441 | 848.4809 🗸 | 7 🥡 | R | 24 | · . | 3392.1434 | 1696.5753 | 1131.3860 | 848,7913 | 679.2345 🗸 |
| 187.9084 | 234.6337 | 312.5092 | 468.2601 | 935.5130 🗸 | 8 V | S | 23 | 5 | 3236.0423 | 1618.5248 | 1079.3523 | 809.7660 🗸 | 648.0143 🗸 |
| 219.1286 | 273.6590 | 364.5429 | 546.3107 🏒 | 1091.6141 🗸 | 9 V | R | 22 | and a | 3149.0103 | 1575.0088 | 1050.3416 | 788.0080 🗸 | 630.6079 🗸 |
| 230.5329 | 287.9143 | 383.5500 | 574.8214 | 1148.6355 | 10 V | G | 21 | ~ | 2992.9092 | 1496.9582 | 998.3079 4 | 748.9827 🗸 | 599.3877 |
| 261.7531 | 326.9396 | 435.5837 | 652.8720 🗸 | 1304.7366 | 11 🖌 | R | 20 | V | 2935.8877 | 1468.4475 | 979.3007 V | 734.7274 | 587.9834 |
| 292.9734 | 365.9649 | 487.6174 | 730.9225 🗸 | 1460.8378 | 12 🖌 / | R | 19 | / | 2779.7866 | 1390.3969 | 927.2670 🗸 | 695.7021 V | 556.7631 |
| 324.1936 | 404.9902 | 539.6511 | 808.9731 | 1616.9389 | 13 | R | 18 | 4 | 2623.6855 | 1312.3464 | 875.2333 🗸 | 656.6768 🗸 | 525.5429 |
| 355.4138 | 444.0155 | 591.6848 | 887.0236 V | 1773.0400 | 14 🚽 | R | 17 | v | 2467.5844 | 1234.2958 | 823.1996 🗸 | 617.6515 | 494.3227 |
| 386.6340 | 483.0407 | 643.7185 🗸 | 965.0742 | 1929.1411 | 15 Ý | R | 16 | V | 2311.4833 | 1156.2453 | 771.1659 🗸 | 578.6263 V | 463.1025 |
| 417.8543 | 522.0660 | 695.7522 🗸 | 1043.1247 🗸 | 2085.2422 | 16 🖌 | R | 15 | Ý | 2155.3821 | 1078.1947 | 719.1322 | 539.6010 | 431.8822 |
| 449.0745 | 561.0913 | 747.7860 🗸 | 1121.1753 | 2241.3433 | 17 🗸 | R | 14 | ~ | 1999.2810 | 1000.1442 | 667.0985 🗸 | 500.5757 | 400.6620 |
| 476.4863 | 595,3560 | 793.4723 🗸 | 1189.7047 🗸 | 2378.4022 | 18 ∮ | н | 13 | 1 | 1843.1799 | 922.0936 🛩 | 615.0648 🗸 | 461.5504 | 369.4418 |
| 507.7065 | 634.3813 | 845.5060 🗸 | 1267.7553 | 2534.5033 | 19 ¥ | R | 12 | \mathcal{N}_{i} | 1706.1210 | 853.5641 🗸 | 569.3785 | 427.2857 | 342.0300 |
| 538.9267 | 673.4066 🗸 | 897.5397 🗸 | 1345.8059 | 2690.6044 | 20 ¥ | R | 11 | 1 | 1550.0199 | 775.5136 , | 517.3448 🗸 | 388.2604 | 310.8098 |
| 570.1469 | 712.4318 J | 949.5734 | 1423.8564 | 2846.7056 | 21 👻 | R | 10 | ι. | 1393.9188 | 697.4630 🗸 | 465.3111 | 349.2352 | 279.5896 |
| 601.3672 | 751.4571 | 1001.6071 | 1501.9070 | 3002.8067 | 22 ° | R | 9 🗸 | 1 | 1237.8177 | 619.4125 🗸 | 413.2774 | 310.2099 | 248.3694 |
| 612.7714 | 765.7125 🏒 | 1020.6142 | 1530.4177 | 3059.8281 | 23 🖌 | G | 8 ~ | J | 1081.7166 | 541.3619 | 361.2437 | 271.1846 | 217.1491 |
| 643.9917 / | 804.7378 | 1072.6479 🗸 | 1608.4683 | 3215.9292 | 24 | R | 7 🗸 | le series | 1024.6951 | 512.8512 | 342.2366 | 256.9292 | 205.7448 |
| 675.2119 🗸 | 843.7630 🗸 | 1124.6816 🖌 | 1686.5188 | 3372.0303 | 25 | R | 6 | | 868.5940 | 434.8006 🗸 | 290.2028 | 217.9040 | 174.5246 |
| 706.4321 🗸 | 882.7883 🗸 | 1176.7153 | 1764.5694 | 3528.1315 | 26 🖌 | R | 5 ⊻ | / | 712.4929 🗸 | 356.7501 🗸 | 238.1691 | 178.8787 | 143.3044 |
| 737.6523 | 921.8136 | 1228.7490 | 1842.6199 | 3684.2326 | 27 | R | 4 | U. | 556.3918 🗸 | 278.6995 | 186.1354 | 139.8534 | 112.0842 |
| 749.0566 🗸 | 936.0690 | 1247.7562 | 1871.1307 | 3741.2540 | 28 🗸 | G | 3. | · | 400.2907 | 200.6490 | 134.1017 | 100.8281 | 80.8640 |
| 780.2768 | 975.0942 | 1299.7899 | 1949.1812 | 3897.3551 | 29 - | R | 2 * | 1 | 343.2692 🗸 | 172.1382 | 115.0946 | 86.5728 | 69.4597 |
| 817.3074 | 1021.3825 | 1361.5076 | 2041.7577 | 4082.5081 | 30 | к | 1 | | 187.1681 | 94.0877 | 63.0609 | 47.5475 | 38.2394 |
| | | | | | | (cterm + 56 | | | | | | | |



RRKKKK

021519 0p2perYellowTube_Gradient_DD_H... 0-10-30-70-100 in 0-10-20-30-35

02/15/19 13:37:41

AV; ~0.2% Yellow Tube



240

360

z=2

z=5

480

5+ Zu

32

62

ሪ

600

| +6 c ions | +5 c ions | +4 c ions | +3 c ions | +2 c ions | +1 c ions | | Sequence | | +1 z ions | +2 7 1005 | +3 7 1000 | 14 7 1000 | 1.15 | 1.0 |
|-----------|------------|------------|------------|------------|------------|-----|-------------|----|-----------|------------|------------|------------|------------|------------|
| 29.8619 | 35.6328 | 44.2892 | 58.7165 | 87.5711 | 174.1349 | 1 | R | 27 | 3780 3630 | 1800 6851 | 1260 7025 | 74 2 1011S | 1750 0704 | +6 Z 10115 |
| 55.8787 | 66.8530 | 83.3145 | 110.7502 | 165.6217 | 330.2360 V | 2 | R | 26 | 3608 2432 | 1804 6252 | 1200.7920 | 945,6402 | 700.0704 | 630.8999 |
| 81.8956 | 98.0733 | 122.3397 | 162.7839 | 243.6722 | 486.3372 | 3 | R | 25 | 3452 1421 | 1706 5747 | 1151 2055 | 902.0103 | 122.4345 | 002.2133 |
| 107.9124 | 129.2935 | 161.3650 | 214.8176 | 321,7228 | 642 4383 | 4 | R | 24 | 3206 0410 | 1649 5244 | 1000 0040 | 003.7910 | 691.2342 V | 5/6.1964 |
| 133.9293 | 160.5137 | 200.3903 | 266.8513 | 399 7733 | 798 5394 | 5 | B | 27 | 3290.0410 | 1040.5241 | 1099.3518 | 824.7657 | 660.0140 | 550.1796 |
| 159.9461 | 191.7339 | 239,4156 | 318 8850 | 477 8239 J | 954 6405 | 6 | | 20 | 3139.9399 | 15/0.4/36 | 1047.3181 | 785.7404 2 | 628.7938 | 524.1627 |
| 181.2953 | 217.3529 | 271 4393 | 361 5833 | 541 8714 | 1082 7255 | 7 | K | 22 | 2903.0387 | 1492.4230 | 995.2844 | 746.7151 🗸 | 597.5736 | 498.1459 |
| 195.8006 | 234,7593 | 293 1973 | 390 5940 | 585 3874 | 1160 7675 | 0 | <u></u> | 21 | 2827.7376 | 1414.3725 | 943.2507 | 707.6899 | 566.3533 | 472.1290 |
| 221.8175 | 265,9795 | 332 2226 | 442 6277 | 663 4370 | 1335 9696 | 0 | 5 | 20 | 2699.6427 | 1350.3250 | 900.5524 | 675.6661 | 540.7344 | 450.7798 |
| 247 8343 | 297 1998 | 371 2470 | 494 6614 | 741 4005 | 1323.0000 | 9 | R | 19 | 2612.6106 | 1306.8090 | 871.5417 | 653.9081 🗸 | 523.3279 | 436.2745 |
| 273 8512 | 328 4200 | 410 2722 | 546 8054 | 741.4005 | 1401.9097 | 110 | R | 18 | 2456.5095 | 1228.7584 | 819.5080 🗸 | 614.8828 🗸 | 492.1077 | 410.2577 |
| 299 8681 | 359 6402 | 410.2732 | 540.0951 | 1019.5390 | 1638.0708 | 11 | R | 17 | 2300.4084 | 1150.7078 | 767.4743 🗸 | 575.8576 🗸 | 460.8875 | 384,2408 |
| 325 8849 | 390 8604 | 449.2904 | 598.7286 | 075 6400 | 1794.1719 | 12 | R | 16 | 2144.3073 | 1072.6573 | 715.4406 | 536.8323 | 429.6673 | 358.2239 |
| 351 9018 | 422 0807 | 527 2400 | 707 7082 | 1052 0007 | 1950.2730 | 13 | K | 15 | 1988.2062 | 994.6067 | 663.4069 | 497.8070 | 398.4471 | 332.2071 |
| 277 0186 | 422.0007 | 527.3490 | 754 0000 | 1053.6907 | 2106.3741 | 14 | R | 14 | 1832.1051 | 916.5562 | 611.3732 🗸 | 458.7817 | 367.2268 | 306.1902 |
| 403 0355 | 455.5009 | 506.3743 | 754.8299 | 1131./413 | 2262.4753 | 15 | R | 13 | 1676.0040 | 838.5056 | 559.3395 🗸 | 419.7565 | 336,0066 | 280.1734 |
| 403.9355 | 404.5211 | 605.3995 | 806.8636 | 1209.7918 | 2418.5764 | 16 | R | 12 | 1519.9029 | 760.4551 | 507.3058 🗸 | 380.7312 | 304.7864 | 254.1565 |
| 429.9523 | 515./413 | 644.4248 | 858.8973 | 1287.8424 | 2574.6775 | 17 | R | 11 | 1363.8018 | 682,4045 | 455.2721 | 341.7059 | 273.5662 | 228.1397 |
| 455.9692 | 546.9615 | 683.4501 🗸 | 910.9310 🗸 | 1365.8929 | 2730.7786 | 18 | R | 10 | 1207.7006 | 604.3540 | 403.2384 | 302,6806 | 242.3459 | 202,1228 |
| 470.4745 | 564.3679 | 705.2081 | 939.9417 | 1409.4089 | 2817.8106 | 19 | S | 9 | 1051.5995 | 526.3034 1 | 351.2047 | 263.6553 | 211.1257 | 176,1060 |
| 491.8237 | 589.9869 | 737.2319 | 982.6400 | 1473.4564 | 2945.9056 | 20 | ĸ | 8 | 964.5675 | 482.7874 | 322.1940 | 241.8973 | 193.7193 | 161.6006 |
| 501.3272 | 601.3912 | 751.4872 | 1001.6472 | 1501.9672 | 3002.9270 | 21 | G | 7 | 836.4725 | 418.7399 | 279.4957 | 209.8736 | 168,1003 | 140.2515 |
| 515.8326 | 618.7976 | 773.2452 | 1030.6579 | 1545.4832 | 3089.9591 | 22 | S | 6 | 779.4511 | 390.2292 | 260,4885 | 195.6182 | 156,6960 | 130 7479 |
| 538.6757 | 646.2094 🗸 | 807.5100 🗸 | 1076.3442 | 1614.0126 | 3227.0180 | 23 | н | 5 | 692,4190 | 346,7132 | 231,4779 | 173.8602 | 139 2896 | 116 2426 |
| 553,1811 | 663.6158 | 829.2680 | 1105.3549 | 1657:5286 | 3314.0500 | 24 | S | 4 | 555.3601 | 278,1837 | 185,7916 | 139 5955 | 111 8778 | 93 3994 |
| 569.3565 | 683.0264 🗸 | 853.5312 | 1137.7058 | 1706.0550 | 3411.1028 | 25 | Р | 3 | 468:3281 | 234,6677 | 156-7809 | 117-8975 | 94 4744 | 78 8941 |
| 595.3734 | 714.2466 🗸 | 892.5564 🗸 | 1189.7395 | 1784.1056 | 3567.2039 | 26 | R | 2 | 371 2753 | 186 1413 | 124 4300 | 93 5743 | 75.0609 | 62 7186 |
| 630.8999 | 756.8784 | 945.8462 | 1260.7925 | 1890.6851 | 3780.3630 | 27 | R | 1 | 215 1742 | 108 0908 | 72 3963 | 54 5490 | 43 8407 | 36 7019 |
| | | | | | | | (cterm + 56 | | | | | 01.01.00 | | 00.1010 |

02/15/19 13:37:41

021519_0p2perYellowTube_Gradient_DD_Heat15 #2887-3608 RT: 11.77-13.95 AV: 13 NL: 1.61E4 T: FTMS + p NSI d Full ms2 691.2317@etd11.84 [120.0000-2000.0000]





m/z

| | | | | | | | | T | | |
|------------|-----------|------------|-------------|----------------|--|-----------|-----------|------------|-------------|------------|
| +4 c ions | +3 c ions | +2 c ions | +1 c ions | | Sequence | | +1 z ions | +2 z ions | +3 z ions | +4 z ions |
| 14 2802 | 58 7165 | 87 5711 | 174.1349 \/ | 1 | R | 28 | 4139.6134 | 2070.3103 | 1380.5427 | 1035.6588 |
| 93 31/5 | 110 7502 | 165 6217 | 330,2360 | ¹ 2 | R | 27 | 3967.4936 | 1984.2504 | 1323.1694 🗸 | 992.6289 🖌 |
| 100 2207 | 162 7830 | 243 6722 | 486 3372 | /3 | R | 26 | 3811.3925 | 1906.1999 | 1271.1357 🗸 | 953.6036 🗸 |
| 161 2650 | 214 8176 | 321 7228 | 642 4383 | 4 | R | 25 | 3655.2914 | 1828.1493 | 1219.1020 🗸 | 914.5783 🗸 |
| 101.3030 | 214.0170 | 399 7733 | 798 5394 | 15 | R | 24 | 3499.1903 | 1750.0988 | 1167.0683 🗸 | 875.5530 🗸 |
| 200.3803 | 218 8950 | 477 8239 1 | 954 6405 | 6 | R | 23 | 3343.0891 | 1672.0482 | 1115.0346 🗸 | 836.5277 |
| 239.4130 | 361 5933 | 541 8714 | 1082,7355 | 7 | ĸ | 22 | 3186.9880 | 1593.9977 | 1063.0009 🕤 | 797.5025 |
| 211.4383 | 300 5040 | 585 3874 V | 11169 7675 | 8 | S | 21 | 3058.8931 | 1529.9502 | 1020.3025 🗸 | 765.4787 |
| 283.18/3 | 1390.3940 | 663 4379 V | 1325,8686 | 9 | R | 20 | 2971.8610 | 1486.4342 | 991.2919 🗸 | 743.7207 |
| 332.2220 | 404 6614 | 741 4885 | 1481 9697 | 10 | R | 19 | 2815.7599 | 1408.3836 | 939.2582 🗸 | 704.6954 |
| 3/1.24/9 | F46 6051 | 910 5300 | 1638 0708 | 11 | R | 18 | 2659.6588 | 1330.3330 | 887.2245 🗸 | 665.6702 |
| 410.2732 | 540.0931 | 013.0000 | 170/ 1710 | 12 | R | 17 | 2503.5577 | 1252.2825 | 835.1908 🗸 | 626.6449 |
| 449.2984 | 398.7288 | 075 6400 | 1050 2720 | 13 | R | 16 | 2347.4566 | 1174.23194 | 783.1570 🗸 | 587.6196 |
| 488.3237 | 650.7625 | 9/0.0402 | 2106 2744 | 14 | R R | 15 | 2191,3555 | 1096.1814 | 731.1233 | 548.5943 |
| 527.3490 | 702.7962 | 1053.6907 | 2100.3741 | 14 / | ,l \$ | 14 | 2035 2544 | 1018,1308 | 679,0896 | 509.5691 |
| 552.6109 | 736.4788 | 1104.2146 | 2207.4218 | 10 | $\left \frac{1}{\sqrt{2}} \right $ | 13 1 | 1934 2067 | 967,6070 | 645,4071 | 484.3071 |
| 577.3780 | 769.5016 | 1153.7488 | 2306.4902 | | the design of th | 10 112 | 1835 1383 | 918 0728 | 612,3843 | 459.5400 |
| 606.1348 | 807.8439 | 1211.2622 | 2421.51/2 | 17 \ | <u>ل</u> | 14 . | 1720 1112 | 860 5593 | 574 0420 | 430,7833 |
| 645.1600 · | 859.8776 | 1289.3128 | 2577.6183 | 18 | <u> </u> | 10 | 1564 0102 | 782 5088 | 522.0083 | 391,7580 |
| 684.1853 | 911.9113 | 1367.3633 | 2733.7194 | 19 | ĸ | | 1407 0001 | 704 4582 | 469 9746 | 352,7327 |
| 723.2106 | 963.9450 | 1445.4139 | 2889.8205 | 20 | | 3 | 1251 8080 | 626 4076 | 417 9409 | 313,7075 |
| 762.2359 | 1015.9787 | 1523.4645 | 3045.9216 | 21 | <u></u> | 7 | 1005 7060 | 548 3571 | 365 9071 | 274,6822 |
| 801.2611 | 1068.0124 | 1601.5150 | 3202.0227 | 22 | ĸ | | 030 6058 | 470 3065 | 313 8734 | 235 6569 |
| 840.2864 | 1120.0461 | 1679.5656 | 3358.1239 | 23 | <u> </u> | 0 | 793 5047 | 392 2560 | 261 8397 | 196 6316 |
| 879.3117 | 1172.0798 | 1757.6161 | 3514.2250 | 24 | ĸ | 0 | 103.3047 | 314 2054 | 201.0007 | 157 6063 |
| 918.3370 | 1224.1135 | 1835.6667 | 3670.3261 | 25 | R | 4 | 027.4030 | 014.2004 | 157 7702 | 118 5811 |
| 957.3623 | 1276.1472 | 1913.7172 | 3826.4272 | 26 | R | 3 | 4/1.3024 | 230.1549 | 105 7296 | 70 5558 |
| 996.3875 | 1328.1809 | 1991.7678 | 3982.5283 | 27 | R | 2 | 315.2013 | 158.1043 | 105.7300 | 19.5550 |
| 1035 6588 | 1380.5427 | 2070.3103 | 4139.6134 | 28 | R | 1 | 159.1002 | 80.0538 | 153.7049 | 40.000 |

021519_0p2perYellowTube_Gradient_DD_H... 0-10-30-70-100 in 0-10-20-30-35

02/15/19 13:37:41

021519_0p2perYellowTube_Gradient_DD_Heat15 #2617-4457 RT: 11.06-15.59 AV: 11 NL: 1.22E4 T: FTMS + p NSI d Full ms2 547.0918@etd6.66 [120.0000-2000.0000]



02/15/19 13:37:41

021519_0p2perYellowTube_Gradient_DD_Heat15 #2617-4458 RT: 11.06-15.59 AV: 11 NL: 1.22E4 T: FTMS + p NSI d Full ms2 547.0918@etd6.66 [120.0000-2000.0000]





| +7 c ions | +6 c ions | +5 c ions | +4 c ions | +3 c ions | +2 c ions | +1 c ions | | Sequence | 1 | +1 zione | +2 = jage | 12 - 1 | 1 | 1.5 | | T |
|-----------|-------------|------------|--------------|------------|-------------|-------------|------|----------|-----|------------|------------|------------|-------------|------------|-----------|-----------|
| 25.7398 | 29.8619 | 35.6328 | 44,2892 | 58 7165 | 87 5711 | 174 1349 | ti | D | 120 | 1000 0504 | 72210118 | +3 2 10hs | +4 z ions | +5 Z 1005 | +6 z ions | +7 z ions |
| 48.0400 | 55.8787 | 66.8530 | 83.3145 | 110,7502 | 165 6217 | 330 2360 \$ | 12 | D | 32 | 4300.0004 | 2183.8318 | 1456.2237 | 1092.4196 | 874.1371 | 728.6155 | 624.6714 |
| 70.3401 | 81.8956 | 98.0733 | 122 3397 | 162 7839 | 243 6722 | 486 3372 | 12 | <u> </u> | 31 | 4194.5366 | 2097.7719 | 1398.8504 | 1049.3896 | 839.7131 | 699.9288 | 600.0829 |
| 92.6403 | 107,9124 | 129 2935 | 161 3650 | 214 8176 | 321 7228 | 642 4282 1 | 1 | | 130 | 4038.4355 | 2019./214 | 1346.8167 | 1010.3643 | 808.4929 | 673.9120 | 577.7827 |
| 114,9404 | 133 9293 | 160 5137 | 200 3003 | 266 8513 | 200 7722 | 708 5204 | A | <u>к</u> | 29 | 3882.3344 | 1941,6708 | 1294.7830 | 971.3390 | 777.2727 | 647.8951 | 555.4826 |
| 137 2406 | 159 9461 | 101 7330 | 230 4156 | 210.0013 | 477 0000 - | 798.5394 1 | # 15 | <u>R</u> | 28 | 3726.2332 | 1863.6203 | 1242.7493 | 932.3138 | 746.0525 | 621.8783 | 533.1824 |
| 155 5399 | 181 2953 | 217 3529 | 271 4393 | 361 5833 | E41 9714 34 | 954.6405 | - 6 | R | 27 | 3570.1321 | 1785.5697 | 1190.7156 | 893.2885 | 714.8322 | 595.8614V | 510.8823 |
| 167 9730 | 195,8006 | 234 7593 | 203 1073 | 300 5040 | 595 3074 | 1062.7355 | 10 | ĸ | 26 | 3414.0310 | 1707,5191 | 1138.6819 | 854.2632 | 683.6120 | 569.8446 | 488.5821 |
| 190 2732 | 221 8175 | 265 9795 | 332 2226 | 442 6277 | 563.3074 | 1109.7075 | 8 | S | 25 | 3285.9361 | 1643.4717 | 1095.9835 | 822.2395 | 657.9930 🗸 | 548.4954 | 470.2828 |
| 212 5733 | 247 8343 | 207 1008 | 371 2470 | 442.0211 | 741 4005 + | 1325.8086 | 9 | 18 | 24 | 3198,9040 | 1599.9557 | 1066.9729 | 800.4815 | 640.5866 | 533.9901 | 457.8497 |
| 234 8735 | 273 8512 | 328 4200 | 410 2732 | 546 6051 | 810 5200 | 1461.9097 | 10 | R | 23 | 3042.8029 | 1521.9051 | 1014.9392 | 761.4562 | 609.3664 | 507,9732 | 435.5495 |
| 257 1737 | 299 8681 | 359 6402 | 410.27.52 | 540.0931 V | 807 5906 | 1036.0708 | 111 | R | 22 | 2886.7018 | 1443.8545 | 962.9055 | 722.4309 | 578.1462 🖌 | 481.9564 | 413.2494 |
| 279.4738 | 325 8849 | 390 8604 | 445.2304 | 650 7626 | 2097.3690 | 1794.1719 | 12 | R | 21 | 2730.6007 | 1365.8040 | 910.8717 | 683.4056 🕶 | 546.9260 | 455.9395 | 390.9492 |
| 301 7740 | 351 9018 | 422 0807 | 627 3400 | 702 7062 1 | 1053 6007 | 1950.2730 | 13 | R | 20 | 2574.4996 | 1287.7534 | 858.8380 | 644.3804 | 515.7057 | 429.9227 | 368.6490 |
| 324.0741 | 377 9186 | 453 3009 | 566 3743 | 754 8200 | 1131 7413 | 2100.3741 | 14 | R | 119 | 2418.3985 | 1209.7029 | 806.8043 | 605.3551 | 484.4855 | 403.9058 | 346.3489 |
| 346.3743 | 403 9355 | 484 5211 | 605 3995 | 806 8636 | 1200 7018 | 2202.4733 | 10 | R | 18 | 2262.2974 | 1131.6523 | 754 7706 | 566.3298 | 453.2653 | 377.8890 | 324.0487 |
| 368.6744 | 429 9523 | 515 7413 | 644 4748 | 1858 8973 | 1203.7918 | 2418.3704 | 10 | R | 1/ | 2105.1963 | 1053.6018 | 702.7369 🗸 | 527.3045 🗸 | 422.0451 | 351.8721 | 301.7486 |
| 390 9746 | 455 9692 | 546 9615 | 683 4501 104 | 010 0210 | 1267.0424 | 2374.0775 | 17 | R | 16 | 1950.0951 | 975.5512 | 1650.7032 | 488.2792 | 390.8248 | 325.8553 | 279,4484 |
| 403 4078 | 470 4745 | 564 3670 | 706 2091 | 020 0447 | 1400 4000 | 2/30.//00 | 10 | R | 15 | 1/93.9940 | 897.5007 | 598.6695 | 449.2540 | 359.6046 | 299.8384 | 257.1482 |
| 421 7070 | 401 8737 | 580 0860 | 737 2210 | 939.9417 | 1409.4069 | 2817.8106 | 19 | S | 14 | 1637.8929 | 819.4501 | 546.6358 | 410.2287 | 328.3844 | 273,8216 | 234.8481 |
| 429 8530 | 501 2272 | 601 2012 | 751 4970 | 1001 6470 | 1473.4504 | 2945.9056 | 20 | к | 13 | 1550,8609 | 775.9341 | 517.6251 | 388.4707 | 310.9780 | 259.3162 | 222.4149 |
| 442 2861 | 515 8326 | 619 7076 | 772 2452 - | 1001.0472 | 1501.9672 | 3002.9270 | 21 | G | 12 | 1422.7659 | 711.8866 | 474.9268 | 356.4469 | 285.3590 | 237.9671 | 204.1157 |
| 464 5863 | 541 8404 | 650.0170-1 | 042 2705 | 1030.0579 | 1045.4832 | 3089.9591 | 22 | IS | 11 | 1365.7445 | 683.3759 | 455.9197 | 342.1916 | 273.9547 | 228.4635 | 195.9697 |
| 77-0104 | 555 75/0/2% | 650.0179 | 812.2705 | 1082.0916 | 1623.5337 | 3246.0602 | 23 | R | 10 | 1278.7124 | 639.8599 | 426.9090 | 320.4336 | 256.5483 | 213.9581 | 183.5366 |
| 400 9844 | 570 5000 | 007.4243 | 034-0203 | 1111.7023 | 1687.0497-4 | 3333.0922 | 24 ~ | S | 9 | 1122.6113 | 561.8093 🗸 | 374.8753 | 281.4083 | 225.3281 | 187.9413 | 161.2364 |
| 612 1042 | 1572.5302 | 740.0550 | 858.2917 | 1144.0532 | 1/15.5761 | 3430.1450 | 25 | P | 8 | 1035.5793 | 518:2933 | 345.8646 | 259.6503 ~~ | 207.9247 | 173:4350 | 448.8033 |
| 513.1643 | 598.54/1 | 1/18.0550 | 897.3170 4 | 1196.0869 | 1793.6267 | 3586.2461 | 26 | R | 7 | 938.5265 | 469.7669 | 313.5137 | 235.3871 | 188.5111 | 157.2605 | 134.9386 |
| 535.4844 | 624.5639 | 749.2753 | 936.3423 | 1248.1206 | 1871.6772 | 3742.3472 | 27 | R | 6 | 782.4254 | 391.7163 | 261.4800 | 196.3618 | 157.2909 | 131.2436 | 112.6384 |
| 557.7846 | 650.5808 | 780.4955 | 975.3675 | 1300.1543 | 1949.7278 | 3898.4483 | 28 | R | 5 | 626.3243 | 313.6658 | 209,4463 | 157.3365 | 126.0707 | 105.2268 | 90.3383 |
| 577.3644 | 673.4239 | 807.9073 V | 1009.6323 | 1345.8406 | 2018.2573 | 4035.5072 | 29 | н | 4 | 470.2232 J | 235.6152 | 157.4126 | 118.3113 | 94.8505 | 79.2099 | 68.0381 |
| 589.7976 | 687.9293 | 825.3137 🗸 | 1031.3903 | 1374.8513 | 2061.7733 | 4122.5393 | 30 | S | 3 | 333.1643 | 167.0858 | 111.7263 | 84.0465 | 67.4387 | 56,3668 | 48.4583 |
| 602,2307 | 702.4346 | 842.7201 | 1053.1483 | 1403.8619 | 2105.2893 | 4209.5713 | 31 | S | 2 | 246.1323 | 123.5698 | 82.7156 | 62.2885 | 50.0323 | 41.8614 | 36.0251 |
| 624.6714 | 728.6155 | 874.1371 | 1092.4196 | 1456.2237 | 2183.8318 | 4366.6564 | 32 | R | 1 | 159 1002 | 80.0538 | 53 7049 | 40 5305 | 22 6250 | 27 2561 | 22 6020 |

021519_0p2perYellowTube_Gradient_DD_H... 0-10-30-70-100 in 0-10-20-30-35

02/15/19 13:37:41

021519_0p2perYellowTube_Gradient_DD_Heat15 #2864-5591 RT: 11.80-20.45 AV: 21 NL: 1.55E4 T: FTMS + p NSI d Full ms2 602.9250@etd2.52 [120.0000-2000.0000]



02/15/19 13:37:41

021519_0p2perYellowTube_Gradient_DD_Heat15 #2865-5592 RT: 11.80-20.45 AV: 21 NL: 1.53E3 T: FTMS + p NSI d Full ms2 602.9250@etd2.52 [120.0000-2000.0000]





z=12

650

700

749.8485

z=?

750



02/15/19 13:37:41

021519_0p2perYellowTube_Gradient_DD_Heat15 #2865-5592 RT: 11.80-20.45 AV: 21 NL: 5.99E2 T: FTMS + p NSI d Full ms2 602.9250@etd2.52 [120.0000-2000.0000]



| +11 c ions | +10 c ions | +9 c ions | +8 c ions | +7 c ions | +6 c ions | +5 c ions | +4 c ions | +3 c ione | +2 0 1000 | 14 - 1 | T | |
|------------|------------|------------|------------|-----------|-----------|------------|------------|-----------|------------|-----------|----------|-------------|
| 16.7462 | 18.3200 | 20.2437 | 22.6482 | 25.7398 | 29.8619 | 35 6328 | 44 2892 | 58 7165 | 97 5711 | +1 C IONS | | Sequence |
| 30.9372 | 33.9302 | 37.5883 | 42.1609 | 48.0400 | 55.8787 | 66 8530 | 83 3145 | 110 7502 | 165 6017 | 174.1349 | 1 | R |
| 45.1282 | 49.5403 | 54.9328 | 61.6735 | 70.3401 | 81,8956 | 98 0733 | 122 3397 | 162 7830 | 242 6722 | 486 2270 | 2 | <u>R</u> |
| 59.3192 | 65.1504 | 72.2774 | 81.1862 | 92.6403 | 107 9124 | 129 2935 | 161 3650 | 214 9176 | 243.0722 | 400.3372 | 3 | R |
| 73.5102 | 80.7605 | 89.6220 | 100.6988 | 114.9404 | 133,9293 | 160.5137 | 200 3903 | 266 8513 | 300 7732 | 709 5204 | 4 | R |
| 87.7012 | 96.3706 | 106.9665 | 120.2114 | 137.2406 | 159,9461 | 191 7339 | 239 4156 | 318 8850 | 477 9220 | 054 0405 | 0 | R |
| 101.8922 | 111.9807 | 124.3111 | 139.7241 | 159.5408 | 185.9630 | 222,9541 | 278 4409 | 370 9187 | 555 8744 | 954.6405 | 5 | R |
| 114.3521 | 125.6866 | 139.5399 | 156.8564 | 179.1206 | 208.8061 | 250,3659 | 312 7056 | 416 6050 | 624 4039 - | 1247 9005 | <u>/</u> | <u>R</u> |
| 119.5359 | 131.3887 | 145.8756 | 163.9841 | 187.2665 | 218.3097 | 261.7702 | 326 9610 | 435 6122 | 652 91/6 | 1304 9220 | 0 | H |
| 133.7269 | 146.9989 | 163.2201 | 183.4968 | 209.5667 | 244.3266 | 292,9904 | 365 9862 | 487 6459 | 730 9652 | 1460 0220 | 10 | <u> </u> |
| 145.3719 | 159.8084 | 177.4529 | 199.5086 | 227.8660 | 265.6757 | 318.6094 | 398.0100 | 530,3442 | 795.0127 | 1589 0181 | 11 | <u>K</u> |
| 150.5557 | 165.5105 | 183.7886 | 206.6363 | 236.0119 | 275.1793 | 330.0137 | 412.2653 | 549.3514 | 823 5234 | 1646 0395 | 12 | |
| 162.2007 | 178.3200 | 198.0214 | 222.6482 | 254.3112 | 296.5285 | 355.6327 | 444.2891 | 592.0497 | 887.5709 | 1774 1345 | 13 | K |
| 173.8457 | 191.1295 | 212.2542 | 238:6600 | 272.6104 | 317.8776 | 381:2517 | 476.3128 | 634 7480 | 951 6184 | 1902-2201 | 13 | K |
| 182.6686 | 200.8348 | 223.0378 | 250.7916 | 286.4751 | 334.0531 | 400.6623 | 500,5760 | 667 0989 | 1000 1447 | 1000 2822 | 15 | <u> </u> |
| 194.3136 | 213.6443 | 237.2706 | 266.8035 | 304.7744 | 355.4023 | 426.2813 | 532,5997 | 709 7972 | 1064 1922 | 2127 3772 | 16 | r |
| 208.5046 | 229.2544 | 254.6152 | 286.3162 | 327.0746 | 381.4191 | 457.5015 | 571 6250 🗸 | 761 8309 | 1142 2428 | 2783 4783 | 17 | <u>N</u> |
| 220.9645 | 242.9603 | 269.8439 | 303.4485 | 346.6544 | 404.2623 | 484 9133 | 605 8898 | 807 5172 | 1210 7722 | 2203.4703 | 10 | <u>R</u> |
| 235.1556 | 258.5704 | 287.1885 | 322.9612 | 368,9546 | 430,2791 | 516 1335 | 644 9150 | 859 5510 | 1299 9229 | 2420.0072 | 10 | <u>H</u> |
| 249.3466 | 274.1805 | 304.5331 | 342.4738 | 391.2547 | 456.2960 | 547 3537 | 683 9403 | 911 5847 | 1366 9733 | 2370.0303 | 19 | <u>K</u> |
| 263.5376 | 289.7906 | 321.8776 | 361.9864 | 413.5549 | 482 3128 | 578 5739 | 722 9656 | 063 6194 | 1444 0020 | 2/32./394 | 20 | <u>R</u> |
| 277.7286 | 305.4007 | 339.2222 | 381.4991 | 435.8550 | 508.3297 | 609 7941 | 761 9909 | 1015 6521 | 1522 0745 | 2888.8405 | 21 | <u>R</u> |
| 291.9196 | 321.0108 | 356.5668 | 401.0117 | 458,1552 | 534 3465 | 641 0144 3 | 801.0161 | 1067 6959 | 1522.9745 | 3044.9416 | 22 | <u>R</u> |
| 306.1106 | 336.6209 | 373.9113 | 420.5243 | 480 4554 | 560 3634 | 672 2346 | 840.0414 | 1110 7105 | 1601.0250 | 3201.0427 | 23 | R |
| 320.3016 | 352,2310 | 391,2559 | 440.0370 | 502 7555 | 586 3802 | 702 4549 | 870.0667 | 1119.7195 | 1679.0756 | 3357.1439 | 24 | R |
| 334.4926 | 367.8412 | 408,6005 | 459 5496 | 525.0557 | 612 3071 | 734 6750 | 019.0007 | 11/1./532 | 1/5/.1261 | 3513.2450 | 25 | R |
| 348.6836 | 383,4513 | 425 9450 | 479 0623 | 547 3558 | 638 4130 | 765 9052 | 910.0920 | 1223.7869 | 1835.1767 | 3669.3461 | 26 | 8 |
| 353.8674 | 389,1534 | 432 2808 | 486 1899 | 555 5018 | 647 0175 | 705.0955 | 957.1173 | 1275.8206 | 1913.2272 | 3825.4472 | 27 | R |
| 368.0584 | 404,7635 | 449.6253 | 505 7026 | 577 8019 | 673 0344 | 909 5109 | 9/1.3/20 | 1294.8277 | 1941.7380 | 3882.4687 | 28 | <u>G</u> |
| 382.2494 | 420.3736 | 466,9699 | 525 2152 | 600 1021 | 600 0512 | 820 7400 | 1010.3979 | 1346.8614 | 2019.7885 | 4038.5698 | 29 | <u>م</u> |
| 393.8944 | 433,1831 | 481 2027 | 541 2271 | 618 4014 | 721 2004 | 039.7400 | 1049.4232 | 1398.8951 | 2097.8391 | 4194.6709 | 30 | R |
| 400.3523 | 440,2868 | 489 0957 | 550 1067 | 628 5495 | 721.3004 | 870 5664 | 1001.4469 | 1441.5935 | 2161.8866 | 4322.7658 | 31 | <u><</u> |
| 412.8122 | 453,9927 | 504 3245 | 567 2391 | 648 1294 | 755.0930 | 006 0792 | 1122 1700 | 1465.2725 | 2197.4051 | 4393.8030 | 32 | <u>A</u> |
| 427.0032 | 469.6028 | 521 6690 | 586 7517 | 670 4295 | 781 0000 | 900.9702 | 1133.4709 | 1510.9588 | 2265.9346 | 4530.8619 | 33 | 4 |
| 432,1870 | 475 3050 | 528 0047 | 593 8794 | 678 5754 | 701.5955 | 930,1904 | 11/2.4962 | 1562.9925 | 2343.9851 | 4686.9630 | 34 | <u> </u> |
| 446 3780 | 490 9151 | 545 3493 | 613 3021 | 700.9756 | 917 5000 | 949.6027 | 1186.7516 | 1581.9997 | 2372.4959 | 4/43.9844 | 35 | Э |
| 458.0230 | 503,7246 | 559 5821 | 629 4039 V | 719 1749 | 838 8605 | 1006 4410 | 1225.7768 | 1634.0334 | 2450.5464 | 4900.0856 | 36 | २ |
| 469 6680 | 516 5341 | 573 8149 | 645 4158 | 737 4749 | 000.0090 | 1000.4419 | 1257.8006 | 16/6./31/ | 2514.5939 | 5028.1805 | 37 | <u><</u> |
| 481 3130 | 529 3436 | 588 0476 | 661 4277 | 755 7724 | 000.2100 | 1032.0609 | 1289.8243 | 1719.4300 | 2578.6414 | 5156.2755 | 38 | < |
| 495 5040 | 544 9537 | 605 2022 | 690.0402 | 730.7734 | 001.00/8 | 1057.6799 | 1321.8481 | 1762.1283 | 2642.6889 | 5284.3704 | 39 | < |
| 500 6979 | 650 6550 | 611 7070 | 000.9403 | 778.0736 | 907.5847 | 1088.9001 | 1360.8733 | 1814.1620 | 2720.7394 | 5440.4716 | 40 | २ |
| 505.9716 | 550.0009 | 619.0626 | 005 4057 | 786.2195 | 917.0882 | 1100.3044 | 1375.1287 | 1833.1692 | 2749.2501 | 5497.4930 | 41 (| 3 |
| 500.000 | 530.3580 | 018.0030 | 695.1957 | /94.3654 | 926.5918 | 1111.7087 | 1389.3841 | 1852.1763 | 2777.7609 | 5554.5145 | 42 (| 3 |
| 520.0626 | 571.9681 | 635.4082 | /14./083 | 816.6656 | 952.6087 | 1142.9289 | 1428.4094 | 1904.2100 | 2855.8114 | 5710.6156 | 43 | २ |
| 534.2535 | 567.5782 | 002.7528 | /34.2210 | 838.9658 | 978.6255 | 1174,1492 | 1467.4346 | 1956.2438 | 2933.8620 | 5866.7167 | 44 | २ |
| 543.8986 | 600.3877 | 666.9855 | /50.2328 | 857.2650 | 999.9747 | 1199.7682 | 1499.4584 | 1998.9421 | 2997.9095 | 5994.8117 | 45 I | < |
| 551.0824 | 606.0899 | 6/3.3213 | /57.3605 | 865.4110 | 1009.4783 | 1211.1724 | 1513.7137 | 2017.9492 | 3026.4202 | 6051.8331 | 46 (| 3 |
| 562.7274 | 618.8994 | 687.5540 ~ | 773.3724 | 883.7102 | 1030.8274 | 1236.7914 | 1545.7375 | 2060.6475 | 3090.4677 | 3179.9281 | 47ł | < |
| 5/6.9184 | 634.5095 | 704.8986 | 792.8850 | 906.0104 | 1056.8443 | 1268.0117 | 1584.7628 | 2112.6813 | 3168.5182 | 6336.0292 | 48 F | 3 |
| 591.1094 | 050.1196 | 122.2432 / | 812.3977 | 928.3106 | 1082.8611 | 1299.2319 | 1623.7880 | 2164.7150 | 3246.5688 | 6492.1303 | 49 F | 2 |
| 003.5693 | 003.8255 | /37.4719 | 829.5300 | 947.8904 | 1105.7043 | 1326.6437 | 1658.0528 | 2210.4013 | 3315.0983 | 629.1892 | 50 H | 1 |
| 017.7603 | 679.4356 J | 754.8165 | 849.0427 | 970.1906 | 1131.7211 | 1357.8639 | 1697.0780 | 2262.4350 | 3393.1488 | 3785.2903 | 51 F | 2 |
| 031.9513 | 695.0457 | /72.1611 | 868.5553 | 992.4907 | 1157.7380 | 1389.0841 | 1736.1033 | 2314.4687 | 3471.1994 | 941.3914 | 52 F | र |
| 646.1423 | 710.6558 / | 789.5056 | 888.0679 | 1014.7909 | 1183.7548 | 1420.3043 | 1775.1286 | 2366.5024 | 3549.2499 | 7097.4926 | 53 F | 2 |
| 660.3333 🗸 | 726.2659 J | 806.8502 | 907.5806 | 1037.0910 | 1209.7717 | 1451.5246 | 1814.1539 | 2418.5361 | 3627.3005 | 253.5937 | 54 F | ξ |
| 674.5243 | 741.8760 | 824.1948 | 927.0932 | 1059.3912 | 1235.7885 | 1482.7448 | 1853,1792 | 2470.5698 | 3705.3510 | 409.6948 | 55 F | 2 |
| 679.7081 | 747.5782 | 830.5305 | 934.2209 | 1067.5371 | 1245.2921 | 1494.1491 | 1867.4345 | 2489.5769 | 3733.8618 | 466.7162 | 56 0 | 3 |
| 691.3531 | 760.3877 | 844.7633 | 950.2328 | 1085.8364 | 1266.6413 | 1519.7681 | 1899.4583 | 2532.2753 | 3797.9092 | 7594.8112 | 57 | (|
| 699.2651 | 769.0909 | 854.4335 | 961.1118 | 1098.2696 | 1281.1466 | 1537.1745 | 1921.2163 | 2561.2859 | 3841.4253 | 681.8432 | 58 5 | 3 |
| 711.8144 | 782.8952 | 869.7716 | 978.3671 | 1117.9900 | 1304.1538 | 1564.7831 | 1955.7270 | 2607.3002 | 3910.4467 | 819.8862 | 59 H | 1 |

| Sequence | | +1 z ions | +2 z ions | +3 z ions | +4 z ions | +5 z ions | +6 7 1005 | +7 7 1005 | +9 = 1000 | 10 - 10 - 10 | 1 . 40 | <u> </u> |
|----------|-----|------------|------------|------------|------------|------------|------------|-----------|------------|--------------|------------|--------------|
| R | 59 | 7819.8862 | 3910 4467 | 2607 3002 | 1955 7270 | 1564 7921 | 1204 1520 | 1117 0000 | +6 Z IONS | +9 Z 1005 | +10 z ions | +11 z ions |
| R | 58 | 7647 7663 | 3824 3868 | 2549 9270 | 1012 6070 | 1504.763 | 1304.1538 | 1117.9900 | 978.3671 | 869.7716 | 782.8952 | 711.8144 |
| R | 57 | 7491 6652 | 3746 3363 | 2049.9270 | 1972.0970 | 1530.3591 | 12/5.46/1 | 1093.4014 | 956.8522 | 850.6472 | 765.6832 🖌 | 696.1672 |
| R | 56 | 7335 5641 | 3669 2957 | 2497.0933 | 1073.0718 | 1499.1389 | 1249.4503 | 1071.1013 | 937.3395 | 833.3026 | 750.0731 | 681.9762 🗸 |
| R | 55 | 7170 4620 | 3500.2057 | 2445.6596 | 1834.6465 | 1467.9186 | 1223.4334 | 1048.8011 | 917.8269 | 815.9580 | 734.4630 | 667.7852 🗸 , |
| R | 54 | 7022 2610 | 3590.2351 | 2393.8258 | 1795.6212 | 1436.6984 | 1197.4166 | 1026.5010 | 898.3142 | 798.6135 | 718.8528 🖌 | 653.5942 🗸 |
| R | 53 | 6967 2609 | 3512.1840 | 2341.7921 | 1756.5959 | 1405.4782 | 1171.3997 | 1004.2008 | 878.8016 | 781.2689 | 703.2427 | 639.4031 |
| | 52 | 0007.2008 | 3434.1340 | 2289.7584 | 1717.5707 | 1374.2580 | 1145.3829 | 981.9006 | 859.2890 | 763.9243 | 687.6326 🗸 | 625.2121 |
| <u> </u> | 54 | 0/11.159/ | 3356.0835 | 2237.7247 | 1678.5454 | 1343.0378 | 1119.3660 | 959.6005 | 839.7763 | 746.5798 | 672.0225 🗸 | 611.0211 |
| 0 | 51 | 6574.1008 | 3287.5540 | 2192.0384 | 1644.2806 | 1315.6260 | 1096.5229 | 940.0206 | 822.6440 | 731.3510 🜱 | 658.3166 🗸 | 598.5612 |
| R | 150 | 6517.0793 | 3259.0433 | 2173.0313 | 1630.0253 | 1304.2217 | 1087.0193 | 931.8747 | 815.5163 | 725.0153 | 652.6145 | 593.3775 |
| <u>~</u> | 49 | 6360.9782 | 3180.9927 | 2120.9976 | 1591.0000 | 1273.0015 | 1061.0024 | 909.5745 | 796.0036 | 707.6707 | 637.0044 | 579.1864 |
| <u> </u> | 48 | 6232.8832 | 3116.9452 | 2078.2993 | 1558.9763 | 1247.3825 | 1039.6533 | 891.2753 | 779.9918 | 693.4379 | 624.1949 | 567.5415 |
| n. | 47 | 6175.8617 | 3088.4345 | 2059.2921 | 1544.7209 | 1235.9782 | 1030.1497 | 883.1293 | 772.8641 | 687.1022 | 618.4927 | 562.3577 |
| <u>к</u> | 46 | 6047.7668 | 3024.3870 | 2016.5938 | 1512.6972 | 1210.3592 | 1008.8005 | 864.8301 | 756.8522 🗸 | 672.8694 | 605,6832 | 550,7127 |
| P | 45 | 5919.6718 | 2960-3396 | 1973.8955 | 1480.6734 | 1184,7402 | 987.4514 | 846.5308 | 740.8403 | 658 6367 | 592,8737 | 539 0677 |
| ĸ | 44 | 5822.6191 | 2911.8132 | 1941.5445 | 1456.4102 | 1165.3296 | 971.2759 | 832.6661 | 728,7087 | 647 8530 | 583 1685 | 530 2447 |
| R | 43 | 5694.5241 | 2847.7657 | 1898.8462 | 1424.3865 | 1139.7106 | 949.9267 | 814,3668 | 712,6969 | 633 6203 V | 570 3590 | 518 5997 |
| Н | 42 | 5538.4230 | 2769.7151 | 1846.8125 | 1385.3612 | 1108.4904 | 923,9099 | 792.0667 | 693 1842 | 616 2757 | 554 7488 | 504 4087 |
| R | 41 | 5401.3641 | 2701.1857 | 1801.1262 | 1351.0965 | 1081.0786 | 901.0667 | 772,4868 | 676 0519 | 601 0469 | 541 0430 | 191 9/88 |
| R | 40 | 5245.2630 | 2623.1351 | 1749.0925 | 1312.0712 | 1049.8584 | 875 0499 | 750 1867 | 656 5392 | 583 7024 | 525 4329 | 431.3400 |
| R | 39 | 5089.1619 | 2545,0846 | 1697.0588 | 1273 0459 | 1018 6382 | 849 0330 | 727 8865 | 637 0266 | 566 3579 | 500 9337 | 477.7576 |
| R | 38 | 4933.0607 | 2467.0340 | 1645.0251 | 1234.0206 | 987 4180 | 823 0162 | 705 5863 | 617 5140 | 540.0122 | 104 2126 | 403.3008 |
| R | 37 | 4776.9596 | 2388,9835 | 1592,9914 | 1194 9954 | 956 1977 | 796 9993 | 683 2862 | 598 0013 | 531 6696 | 494.2120 | 449.3756 |
| R | 36 | 4620.8585 | 2310,9329 | 1540,9577 | 1155 9701 | 924 9775 | 770 9825 | 660 9860 | 578 4887 | 514 3241 | 470.0020 | 430.1040 |
| R | 35 | 4464,7574 | 2232.8823 | 1488.9240 | 1116 9448 | 893 7573 | 744 9656 | 638 6850 | 558 0760 | 106 0705 | 402.9924 | 420.9938 |
| R | 34 | 4308.6563 | 2154.8318 | 1436 8903 | 1077 9195 | 862 5371 | 718 9488 | 616 3857 | 530 4634 | 430.9795 | 447.3023 | 400.0027 |
| R | 33 | 4152,5552 | 2076 7812 | 1384 8566 | 1038 8943 | 831 3160 | 602 0310 | 504 0955 | 539.4034 | 479.0349 | 431.7722 | 392.6117 |
| G | 32 | 3996,4541 | 1998 7307 | 1332 8229 | 999 8690 | 800.0966 | 666 0151 | 571 7954 | 519.9006 | 402.2904 | 416.1621 | 378.4207 |
| R | 31 | 3939,4326 | 1970 2199 | 1313 8157 | 985 6136 | 788 6023 | 657 4115 | 562 6205 | 402 2104 | 444.9458 | 400.5520 | 364.2297 |
| R | 30 | 3783.3315 | 1892 1694 | 1261 7820 | 946 5883 | 757 4721 | 631 30/6 V | 541 3393 | 433.3104 | 430.0101 | 394.0496 | 359.0459 |
| ĸ | 29 | 3627 2304 | 1814 1188 | 1209.7483 | 007 5631 | 726 2510 | 605 2779 | 541.3393 | 4/3./9/0 | 421.2000 | 379.2397 | 344.8549 |
| A | 28 | 3499 1354 | 1750 0714 | 1167.0500 | 975 5202 | 720.2319 | 594 0000 | 519.0391 | 404.2802 | 403.9210 | 363.6296 | 330.6639 |
| Н | 27 | 3428 0983 | 1714 5529 | 1142 2710 | 957 7900 | 100.0329 | 504.0200 | 500.7399 | 438.2733 | 389.6882 | 350.8201 | 319.0189 |
| R | 26 | 3201 0304 | 1646 0022 | 1007 6947 | 007.7800 | 000.4255 | 572.1891 | 490.5917 | 429.3937 | 381.7952 | 343.7164 | 312.5610 |
| è | 25 | 3134 0393 | 1567 0700 | 1097,0047 | 823.5153 | 659.0137 | 549.3460 | 4/1.0119 | 412.2613 | 366.5664 | 330.0105 | 300.1011 |
| D | 20 | 3134,9303 | 1507.9720 | 1045.6509 | 784.4900 | 627.7935 | 523.3291 | 448.7117 | 392.7487 | 349.2218 | 314.4004 | 285.9101 |
| ĸ | 24 | 3077.9100 | 1039.4021 | 1026.6438 | 770.2347 | 616.3892 • | 513.8255 | 440.5658 | 385.6210 | 342.8861 | 308.6982 | 280.7263 |
| K | 23 | 2921.0107 | 1401.4110 | 974.6101 | 731.2094 | 585.1690 | 487.8087 | 418.2656 | 366.1083 | 325.5415 | 293.0881 | 266.5353 |
| | 22 | 2793.7208 | 1397.3640 | 931.9118 | 699.1856 | 559.5500 | 466.4595 | 399.9663 | 350.0965 | 311.3088 | 280.2786 | 254.8903 |
| <u></u> | 21 | 2005.0258 | 1333.3165 | 889.2134 | 667.1619 | 533.9310 | 445.1104 | 381.6671 | 334.0846 | 297.0760 | 267.4691 | 243.2453 |
| n | 20 | 2537.5308 | 1269.2691 | 846.5151 | 635.1382 🗸 | 508.3120 | 423.7612 | 363.3678 | 318.0727 | 282.8432 | 254.6596 | 231.6003 |
| 9 | 19 | 2381.4297 | 1191.2185 | /94.4814 | 596.1129 | 477.0918 | 397.7443 | 341.0676 | 298.5601 | 265.4987 | 239.0495 | 217.4093 |
| 6 | 18 | 2324.4082 | 1162.7078 | 775.4743 | 581.8575 | 465.6875 | 388.2408 | 332.9217 | 291.4324 | 259.1629 | 233.3474 | 212.2255 |
| K I | 1/ | 2267.3868 | 1134.1970 | /56.4671 | 567.6022 | 454.2832 | 378.7372 | 324.7758 | 284.3047 | 252.8272 | 227.6452 | 207.0418 |
| K | 10 | 2111.2857 | 1056.1465 | /04.4334 🗸 | 528.5769 | 423.0630 | 352.7203 | 302.4756 | 264.7921 | 235.4827 | 212.0351 | 192.8508 |
| ĸ | 15 | 1955.1846 | 978.0959 | 652.3997 | 489.5516 | 391.8427 | 326.7035 | 280,1755 | 245.2794 | 218.1381 | 196.4250 | 178.6598 |
| G | 14 | 1827.0896 | 914.0484 | 609.7014 🗸 | 457.5279 | 366.2237 | 305.3543 | 261.8762 | 229.2676 | 203.9053 | 183.6155 | 167.0148 |
| K | 13 | 1770.0681 | 885.5377 | 590.6942 | 443.2725 | 354.8194 | 295.8508 | 253.7303 | 222.1399 | 197.5696 | 177.9134 | 161.8310 |
| R | 12 | 1641.9732 | 821.4902 | 547.9959 | 411.2488 | 329.2005 | 274.5016 | 235.4310 | 206.1280 | 183.3368 | 165.1039 | 150.1860 |
| R | 11 | 1485.8721 | 743.4397 | 495.9622 | 372.2235 | 297.9802 | 248.4847 | 213.1308 | 186.6154 | 165.9923 | 149.4938 | 135.9950 |
| Н | 10 | 1329.7710 | 665.3891 | 443.9285 | 333.1982 | 266.7600 | 222.4679 | 190.8307 | 167.1027 | 148.6477 | 133.8836 | 121.8040 |
| R | 9 | 1192.7120 | 596.8597 🗸 | 398.2422 | 298.9335 | 239.3482 | 199.6247 | 171.2508 | 149.9704 | 133.4189 | 120.1778 | 109.3441 |
| R | 8 | 1036.6109 | 518.8091 🗸 | 346.2085 | 259.9082 | 208.1280 | 173.6079 | 148.9507 | 130.4577 | 116.0743 | 104.5676 | 95.1531 |
| R | 7 | 880.5098 | 440.7585 🗸 | 294.1748 | 220.8829 | 176.9078 | 147.5910 | 126.6505 | 110.9451 | 98.7298 | 88.9575 | 80.9621 |
| R | 6 | 724.4087 | 362.7080 | 242.1411 | 181.8576 | 145.6876 | 121.5742 | 104.3503 | 91.4325 | 81.3852 | 73.3474 | 66.7710 |
| R | 5 | 568.3076 🖌 | 284.6574 | 190.1074 | 142.8324 | 114.4673 | 95.5573 | 82.0502 | 71.9198 | 64.0406 | 57.7373 | 52.5800 |
| G | 4 | 412.2065 | 206.6069 | 138.0737 | 103.8071 | 83.2471 | 69.5405 | 59.7500 | 52.4072 | 46.6961 | 42.1272 | 38.3890 |
| K | 3 | 355.1850 | 178.0961 | 119.0665 | 89.5517 | 71.8428 | 60.0369 | 51.6041 | 45.2795 | 40.3604 | 36.4251 | 33.2053 |
| S | 2 | 227.0901 | 114.0487 | 76.3682 | 57.5280 | 46.2238 | 38.6877 | 33.3048 | 29.2676 | 26.1276 | 23.6156 | 21.5603 |
| н | 1 | 140.0580 | 70.5327 | 47.3575 | 35.7700 | 28.8174 | 24.1824 | 20.8717 | 18.3886 | 16.4574 | 14.9124 | 13.6483 |