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$^1$H NMR (400 MHz, CDCl$_3$, 22 °C) δ
8.46 (d, J = 8.4 Hz, 2H),
8.26 (d, J = 8.4 Hz, 2H),
8.24 (dd, J = 7.8, 1.3 Hz, 2H),
7.87 (s, 2H),
7.61 (dd, J = 7.9, 1.3 Hz, 2H),
7.52 (td, J = 7.6, 1.4 Hz, 2H),
7.38 (td, J = 7.5, 1.4 Hz, 2H),
0.13 (s, 18H).

$^{13}$C NMR (101 MHz, CDCl$_3$, 22 °C) δ
157.68, 146.22, 143.06,
135.23, 133.46, 131.08,
129.21, 128.47, 127.90,
126.45, 124.63, 121.63,
105.10, 98.23, -0.16.
# High Resolution Mass Spectrometry Report

## Measured m/z vs. theoretical m/z

| Meas. m/z | # | Formula | Score | m/z | err [mDa] | err [ppm] | mFormula | db | Conf. | even | 1+ |
|-----------|---|---------|-------|-----|----------|----------|-----------|----|-------|------|----|
| 431.0671  | 1 | C 23 H 20 Br N 2 Si | 100.00 | 431.0574 | 0.2 | -0.2 | 7.6 | 15.5 | even | 1+ |
| 453.0395  | 1 | C 23 H 19 Br N 2 Na Si | | | | | | | | |

## Mass list

| # | m/z | l% | l |
|---|-----|----|---|
| 1 | 165.1144 | 4.4 | 3727 |
| 2 | 160.1179 | 0.5 | 417 |
| 3 | 167.0787 | 0.5 | 395 |
| 4 | 201.1025 | 0.5 | 401 |
| 5 | 205.0592 | 1.5 | 1234 |
| 6 | 217.1043 | 0.8 | 634 |
| 7 | 239.0869 | 0.8 | 664 |
| 8 | 241.0825 | 0.7 | 621 |
| 9 | 273.1050 | 0.5 | 448 |
| 10 | 279.0923 | 1.5 | 1270 |
| 11 | 280.0599 | 0.5 | 430 |
| 12 | 301.0742 | 3.4 | 2803 |
| 13 | 301.1276 | 0.8 | 727 |
| 14 | 302.1078 | 0.9 | 762 |
| 15 | 304.2615 | 0.9 | 772 |
| 16 | 315.1913 | 0.7 | 578 |
| 17 | 322.1654 | 0.5 | 449 |
| 18 | 323.1606 | 1.7 | 1434 |
| 19 | 331.0468 | 0.6 | 493 |
| 20 | 367.1072 | 0.7 | 548 |
| 21 | 393.2580 | 0.5 | 451 |
| 22 | 413.2686 | 1.7 | 1422 |
| 23 | 430.6919 | 0.6 | 491 |
| 24 | 430.9182 | 0.6 | 525 |
| 25 | 430.9428 | 0.6 | 480 |
| 26 | 430.9696 | 0.8 | 633 |
| 27 | 431.0017 | 0.5 | 444 |
| 28 | 431.0571 | 93.9 | 78815 |
| 29 | 431.2372 | 0.6 | 485 |
| 30 | 431.2474 | 0.6 | 462 |
| 31 | 431.2911 | 0.5 | 400 |
| 32 | 431.9708 | 0.5 | 418 |
| 33 | 432.0596 | 28.3 | 23763 |
| 34 | 432.2630 | 0.5 | 446 |
| 35 | 432.7568 | 0.6 | 480 |
| 36 | 432.9057 | 0.6 | 486 |
| 37 | 432.9322 | 0.8 | 697 |
| 38 | 432.9578 | 0.6 | 519 |
| 39 | 432.9897 | 0.8 | 674 |
| 40 | 433.6553 | 100.0 | 83898 |
| 41 | 433.2897 | 0.5 | 432 |
| 42 | 433.3500 | 0.5 | 456 |
| 43 | 433.3737 | 0.5 | 306 |
| 44 | 434.0580 | 29.0 | 24339 |
| 45 | 435.6570 | 0.4 | 5348 |
| 46 | 436.6587 | 1.3 | 1073 |
| 47 | 444.1894 | 2.8 | 2358 |
| 48 | 445.1017 | 1.5 | 1277 |
| 49 | 447.3438 | 0.8 | 664 |
| 50 | 453.6395 | 0.3 | 7761 |
| 51 | 453.1746 | 0.6 | 464 |
| 52 | 454.0412 | 3.0 | 2514 |
| 53 | 455.0375 | 10.9 | 9184 |
| 54 | 456.0388 | 2.5 | 2139 |
| 55 | 467.0385 | 0.6 | 447 |
| 56 | 469.0118 | 0.6 | 476 |
| 57 | 494.9770 | 0.5 | 409 |
| 58 | 525.2173 | 1.3 | 1093 |
| 59 | 526.2168 | 0.7 | 507 |
| 60 | 731.1234 | 0.6 | 475 |
| 61 | 661.1044 | 6.8 | 5685 |

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| #  | m/z  | %  |
|----|------|----|
| 62 | 852.1005 | 4.3 |
| 63 | 853.1033 | 14.8 |
| 64 | 854.1059 | 8.5 |
| 65 | 855.1037 | 9.0 |
| 66 | 856.1052 | 4.7 |
| 67 | 857.1016 | 2.0 |
| 68 | 858.1071 | 0.6 |
| 69 | 874.2357 | 1.2 |
| 70 | 875.2382 | 1.0 |
| 71 | 876.2397 | 1.3 |
| 72 | 877.2371 | 0.8 |
| 73 | 878.2382 | 0.5 |
| 74 | 883.0863 | 12.1 |
| 75 | 884.0903 | 7.4 |
| 76 | 884.9027 | 0.5 |
| 77 | 886.0854 | 28.0 |
| 78 | 888.8862 | 0.6 |
| 79 | 886.9873 | 15.7 |
| 80 | 887.0849 | 17.4 |
| 81 | 888.0865 | 8.5 |
| 82 | 889.0847 | 3.3 |
| 83 | 890.0882 | 1.1 |
| 84 | 899.0993 | 0.5 |
| 85 | 901.0560 | 0.9 |
| 86 | 902.0610 | 0.6 |
| 87 | 903.0590 | 0.6 |
| 88 | 923.0279 | 2.0 |
| 89 | 924.0287 | 1.3 |
| 90 | 925.0290 | 5.3 |
| 91 | 926.0291 | 3.2 |
| 92 | 927.0230 | 4.7 |
| 93 | 928.0244 | 2.6 |
| 94 | 929.0226 | 1.9 |
| 95 | 930.0275 | 0.8 |
| 96 | 931.0224 | 0.5 |
| 97 | 1017.1866 | 0.7 |
| 98 | 1019.1882 | 1.2 |
| 99 | 1020.1871 | 0.7 |
| 100| 1021.1833 | 0.5 |

**Acquisition Parameter**

| Source Type | ESI | Ion Polarity | Positive | Set Nebulizer | Set Dry Heater | Set Dry Gas | Set Ion Energy (MS only) |
|-------------|-----|--------------|----------|---------------|---------------|-------------|-------------------------|
| Focus       | Not active | Set Capillary | 3600 V | 0.4 Bar | 180 °C | 4.0 l/min | 4.0 eV |
| Scan Begin  | 75 m/z | Set End Plate Offset | -500 V | Set Collision Cell RF | 350.0 Vpp | | |
| Scan End    | 1700 m/z | | | | | | |
$^1$H, $^{13}$C-NMR (CD$_2$Cl$_2$, 400/101 MHz, 22 °C) and HR-ESI-MS spectra of compound (4)

$^1$H NMR (400 MHz, CD$_2$Cl$_2$, 22 °C) δ
8.50 (d, $J = 8.3$ Hz, 4H),
8.16 (d, $J = 8.4$ Hz, 4H),
8.08 (s, 4H),
7.11 (dd, $J = 7.8$, 0.8 Hz, 4H),
7.06 (dd, $J = 7.7$, 0.8 Hz, 4H),
6.72 (td, $J = 7.7$, 1.3 Hz, 4H),
6.23 (td, $J = 7.6$, 1.3 Hz, 4H),
0.05 (s, 36H).

$^{13}$C NMR (101 MHz, CD$_2$Cl$_2$, 22 °C) δ
156.91, 143.88, 141.66, 136.46,
132.95, 129.25, 129.08, 128.98,
127.85, 127.72, 127.35, 121.74,
103.54, 100.26, -0.23.
## High Resolution Mass Spectrometry Report

### Measured m/z vs. theoretical m/z

| Meas. m/z | # | Formula | Score | m/z    | err (mDa) | err (ppm) | mSigma | mDB | e<sup>-</sup> | Cont | e<sup>-</sup> | z     |
|-----------|---|---------|-------|--------|-----------|-----------|--------|-----|-------------|-------|-------------|-------|
| 967.2713  | 1 | C_62 H_48 Cu N_4 S_i_2 | 100.00 | 967.2708 | -0.5      | -0.5      | 18.0   | 425 | even        | 1    | even        |       |
| 1039.5108 | 1 | C_66 H_50 Cu N_4 S_i_3 | 100.00 | 1039.5103 | -0.4      | -0.4      | 20.2   | 425 | even        | 1    | even        |       |
| 1111.3490 | 1 | C_68 H_64 Cu N_4 S_i_4 | 100.00 | 1111.3499 | 0.8       | 0.8       | 13.4   | 425 | even        | 1    | even        |       |

### Mass list

| # | m/z  | [%] |
|---|------|-----|
| 1 | 567.1335 | 3.0 |
| 2 | 568.1360 | 1.7 |
| 3 | 569.1306 | 2.2 |
| 4 | 590.1346 | 1.2 |
| 5 | 583.1369 | 0.9 |
| 6 | 855.2908 | 1.0 |
| 7 | 895.2316 | 10.0 |
| 8 | 896.2352 | 7.1 |
| 9 | 897.2316 | 6.4 |
| 10 | 898.2333 | 3.7 |
| 11 | 899.2367 | 1.5 |
| 12 | 905.2345 | 1.0 |
| 13 | 906.3029 | 1.0 |
| 14 | 927.3315 | 4.5 |
| 15 | 928.3331 | 3.5 |
| 16 | 929.3340 | 1.7 |
| 17 | 947.3170 | 1.4 |
| 18 | 948.1497 | 0.9 |
| 19 | 957.2713 | 58.1 |
| 20 | 958.2740 | 46.5 |
| 21 | 959.1371 | 1.1 |
| 22 | 969.2718 | 45.0 |
| 23 | 970.2724 | 27.5 |
| 24 | 971.2739 | 10.6 |
| 25 | 972.2731 | 3.6 |
| 26 | 973.2713 | 1.0 |
| 27 | 977.2652 | 2.3 |
| 28 | 979.3619 | 2.0 |
| 29 | 979.3607 | 1.2 |
| 30 | 955.1215 | 1.0 |
| 31 | 995.3659 | 7.2 |
| 32 | 1000.3726 | 6.6 |
| 33 | 1001.3749 | 3.3 |
| 34 | 1002.3739 | 1.4 |
| 35 | 1019.1677 | 1.4 |
| 36 | 1020.1911 | 1.0 |
| 37 | 1022.5602 | 1.2 |
| 38 | 1024.6620 | 0.9 |
| 39 | 1025.6588 | 3.1 |
| 40 | 1026.5610 | 2.0 |
| 41 | 1027.5654 | 2.9 |
| 42 | 1028.5686 | 1.7 |
| 43 | 1029.6002 | 1.3 |
| 44 | 1030.5915 | 2.0 |
| 45 | 1030.1961 | 1.3 |
| 46 | 1031.1925 | 2.1 |
| 47 | 1032.1046 | 1.5 |
| 48 | 1033.1922 | 1.1 |
| 49 | 1039.6177 | 1.0 |
| 50 | 1040.1030 | 1.7 |
| 51 | 1039.3108 | 100.0 |
| 52 | 1039.8101 | 1.1 |
| 53 | 1039.8657 | 1.5 |
| 54 | 1040.0740 | 1.3 |
| 55 | 1040.1331 | 1.7 |
| 56 | 1040.2009 | 1.1 |
| 57 | 1040.3132 | 88.4 |
| 58 | 1040.4046 | 0.9 |
| 59 | 1040.6529 | 1.5 |
| 60 | 1040.7058 | 0.9 |
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| #  | m/z         | % | |
|----|-------------|---|---|
| 01 | 1040.0054   | 1.0| 1010|
| 02 | 1041.0291   | 1.1| 1044|
| 03 | 1041.0801   | 1.0| 1005|
| 04 | 1041.1575   | 1.0| 1015|
| 05 | 1041.3133   | 87.2| 86268|
| 06 | 1041.6008   | 1.1| 1079|
| 07 | 1042.1291   | 1.0| 1036|
| 08 | 1042.3122   | 57.1| 56553|
| 09 | 1043.1471   | 1.0| 961|
| 10 | 1043.5123   | 25.7| 25428|
| 11 | 1044.3127   | 0.7| 9572|
| 12 | 1045.3134   | 3.3| 3279|
| 13 | 1046.3158   | 0.9| 862|
| 14 | 1049.4237   | 1.1| 1138|
| 15 | 1050.4209   | 1.3| 1285|
| 16 | 1057.1586   | 1.0| 1002|
| 17 | 1071.4090   | 4.1| 4020|
| 18 | 1072.4119   | 3.5| 3440|
| 19 | 1073.4130   | 2.3| 2311|
| 20 | 1074.4132   | 1.1| 1115|
| 21 | 1095.9683   | 1.0| 956|
| 22 | 1096.0860   | 1.0| 954|
| 23 | 1097.0972   | 2.6| 2003|
| 24 | 1098.1014   | 2.0| 1985|
| 25 | 1099.0961   | 2.9| 2691|
| 26 | 1100.0978   | 2.1| 2049|
| 27 | 1101.0967   | 1.4| 1418|
| 28 | 1101.2295   | 2.0| 1984|
| 29 | 1102.2327   | 1.9| 1907|
| 30 | 1103.2300   | 2.8| 2742|
| 31 | 1104.2321   | 1.8| 1755|
| 32 | 1105.2304   | 1.3| 1330|
| 33 | 1111.3490   | 52.5| 51998|
| 34 | 1112.3513   | 48.8| 48259|
| 35 | 1113.3496   | 52.1| 51815|
| 36 | 1114.3500   | 36.0| 35660|
| 37 | 1115.3503   | 17.9| 17771|
| 38 | 1116.3507   | 7.5| 7419|
| 39 | 1117.3504   | 2.6| 2758|
| 40 | 1118.3505   | 0.9| 936|

**Acquisition Parameter**

| Source Type | ESI | Ion Polarity | Positive | Set Nebulizer | 0.4 Bar |
|-------------|-----|--------------|----------|---------------|---------|
| Focus Begin  | Not active | Set Capillary | 3600 V | Set Dry Heater | 180 °C |
| Scan End     | 1700 m/z | Set Collision Cell RF | 500 V ppp | Set Dry Gas | 4.6 l/min |
| Source Type | ESI | Ion Polarity | Positive | Set Nebulizer | 0.4 Bar |
| Focus Begin  | Not active | Set Capillary | 3600 V | Set Dry Heater | 180 °C |
| Scan End     | 1700 m/z | Set Collision Cell RF | 500 V ppp | Set Dry Gas | 4.6 l/min |
$^1$H-, $^{13}$C-NMR (CD$_2$Cl$_2$, 400/101 MHz, 22 °C) and HR-ESI-MS spectra of compound (11)

$^1$H NMR (400 MHz, CD$_2$Cl$_2$, 22 °C) $\delta$
8.53 (d, $J = 8.3$ Hz, 4H), 8.10 (d, $J = 8.4$ Hz, 4H), 8.08 (s, 4H), 7.14 (td, $J = 8.2$, 1.3 Hz, 8H), 6.79 (td, $J = 7.6$, 1.4 Hz, 4H), 6.32 (td, $J = 7.6$, 1.3 Hz, 4H), 3.05 (s, 4H).

$^{13}$C NMR (101 MHz, CD$_2$Cl$_2$, 22 °C) $\delta$
156.66, 143.94, 141.82, 136.99, 133.34, 129.32, 129.05, 129.04, 127.92, 127.66, 127.44, 120.62, 82.72, 82.29.
High Resolution Mass Spectrometry Report

## Measured m/z vs. theoretical m/z

| Mass list | # | m/z     | I% | I  |
|-----------|---|---------|----|----|
| 1         | 1 | 202.0886| 2.6| 851|
| 2         | 2 | 292.1984| 1.9| 633|
| 3         | 3 | 392.2429| 2.2| 742|
| 4         | 4 | 301.1398| 2.6| 891|
| 5         | 5 | 315.1603| 2.6| 862|
| 6         | 6 | 315.1913| 6.6| 2210|
| 7         | 7 | 316.1665| 2.0| 769|
| 8         | 8 | 317.1721| 3.4| 1133|
| 9         | 9 | 319.1657| 2.0| 665|
| 10        | 10| 321.2391| 2.2| 725|
| 11        | 11| 321.2744| 1.8| 615|
| 12        | 12| 331.1081| 1.8| 613|
| 13        | 13| 339.1768| 2.3| 760|
| 14        | 14| 353.2568| 3.8| 1277|
| 15        | 15| 365.2870| 2.1| 716|
| 16        | 16| 367.2079| 2.1| 713|
| 17        | 17| 370.1221| 100.0| 3378|
| 18        | 18| 380.1226| 29.4| 5917|
| 19        | 19| 381.1376| 31.8| 10711|
| 20        | 20| 381.2971| 3.8| 1277|
| 21        | 21| 382.1410| 10.2| 3442|
| 22        | 22| 385.0283| 2.8| 943|
| 23        | 23| 391.2266| 1.9| 691|
| 24        | 24| 301.2845| 2.6| 972|
| 25        | 25| 392.0096| 7.5| 2532|
| 26        | 26| 393.0069| 4.1| 1382|
| 27        | 27| 393.2971| 3.8| 1284|
| 28        | 28| 394.0078| 7.5| 2539|
| 29        | 29| 395.0047| 4.6| 1541|
| 30        | 30| 397.1354| 2.0| 669|
| 31        | 31| 400.0029| 3.1| 1037|
| 32        | 32| 413.1276| 2.0| 667|
| 33        | 33| 413.2654| 11.8| 3969|
| 34        | 34| 414.2085| 2.0| 975|
| 35        | 35| 418.0994| 2.0| 666|
| 36        | 36| 420.9384| 1.8| 607|
| 37        | 37| 421.3285| 2.7| 920|
| 38        | 38| 422.0380| 2.7| 904|
| 39        | 39| 431.0568| 5.8| 1942|
| 40        | 40| 432.0586| 1.9| 638|
| 41        | 41| 433.0544| 5.0| 1974|
| 42        | 42| 433.1026| 12.5| 4196|
| 43        | 43| 434.1074| 3.6| 1199|
| 44        | 44| 441.0443| 6.8| 2283|
| 45        | 45| 441.2567| 3.6| 1219|
| 46        | 46| 442.0477| 2.5| 629|
| 47        | 47| 443.0522| 15.0| 5041|
| 48        | 48| 444.0632| 5.4| 1833|
| 49        | 49| 444.1891| 8.9| 2981|
| 50        | 50| 445.0579| 6.8| 2301|
| 51        | 51| 445.1914| 3.2| 1090|
| 52        | 52| 446.0592| 1.6| 615|
| 53        | 53| 447.3438| 5.2| 1744|
| 54        | 54| 449.2950| 2.5| 841|
| 55        | 55| 453.3757| 2.2| 740|
| 56        | 56| 457.3113| 2.2| 753|
| 57        | 57| 459.3287| 3.2| 1093|
| 58        | 58| 473.3170| 2.4| 622|
| 59        | 59| 473.3410| 1.9| 843|
| 60        | 60| 477.0443| 1.9| 633|
| 61        | 61| 492.1177| 5.7| 1915|
| 62        | 62| 492.0778| 4.0| 1361|
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|  #  | m/z       | I % | I     |
|-----|-----------|-----|-------|
| 63  | 403.1222  | 1.0 | 664   |
| 64  | 403.9696  | 1.9 | 641   |
| 65  | 494.9759  | 6.9 | 2317  |
| 66  | 495.0797  | 2.5 | 828   |
| 67  | 496.0757  | 2.5 | 653   |
| 68  | 506.1113  | 7.4 | 2482  |
| 69  | 507.1135  | 3.1 | 1033  |
| 70  | 508.1093  | 4.4 | 1484  |
| 71  | 509.1138  | 1.9 | 627   |
| 72  | 511.0423  | 1.8 | 611   |
| 73  | 517.3688  | 2.0 | 672   |
| 74  | 525.2172  | 3.5 | 1179  |
| 75  | 561.3655  | 1.9 | 659   |
| 76  | 567.3381  | 3.3 | 1101  |
| 77  | 589.1368  | 2.0 | 677   |
| 78  | 649.4486  | 2.2 | 745   |
| 79  | 685.4305  | 1.6 | 601   |
| 80  | 693.4647  | 1.0 | 633   |
| 81  | 705.5813  | 2.0 | 672   |
| 82  | 819.1592  | 7.2 | 2433  |
| 83  | 820.1625  | 4.0 | 1342  |
| 84  | 821.1574  | 4.0 | 1342  |
| 85  | 822.1644  | 2.2 | 738   |
| 86  | 823.1905  | 28.0 | 9436 |
| 87  | 824.1805  | 6.0 | 6694  |
| 88  | 825.1919  | 20.0 | 6737 |
| 89  | 826.1918  | 8.7 | 2941  |
| 90  | 827.1949  | 4.0 | 1341  |
| 91  | 835.0484  | 2.3 | 790   |
| 92  | 873.1099  | 3.6 | 1215  |
| 93  | 874.1108  | 2.0 | 672   |
| 94  | 875.1096  | 5.2 | 1766  |
| 95  | 876.1131  | 2.9 | 964   |
| 96  | 877.1097  | 2.2 | 759   |
| 97  | 925.0251  | 2.3 | 773   |
| 98  | 938.1560  | 3.0 | 994   |
| 99  | 1019.1650 | 1.9 | 625   |
| 100 | 1135.2621 | 2.1 | 709   |

### Acquisition Parameter

| Source Type | ESI | Ion Polarity | Positive | Set Nebulizer | 0.4 Bar |
|-------------|-----|--------------|----------|---------------|--------|
| Focus       | Not active | Set Capillary | 3800 V | Set Dry Heater | 180 °C |
| Scan Begin  | 75 m/z | Set End Plate Offset | -500 V | Set Dry Gas | 4.0 l/min |
| Scan End    | 1750 m/z | Set Collision Cell RF | 500.0 Vpp | Set Ion Energy (M3 only) | 4.0 eV |

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$^1$H-, $^{13}$C-, HMBC-NMR (CD$_2$Cl$_2$, 400/126 MHz, 22/25 °C) and HR-ESI-MS spectra of compound (2)

$^1$H NMR (400 MHz, CD$_2$Cl$_2$, 22 °C) δ
8.42 (d, J = 8.4 Hz, 4H),
7.99 (d, J = 8.6 Hz, 6H),
7.95 (d, J = 6.7 Hz, 6H),
7.66 (dd, J = 7.7, 1.5 Hz, 4H),
7.59 (td, J = 7.7, 1.5 Hz, 4H),
7.49 (td, J = 7.5, 1.2 Hz, 4H).

$^{13}$C NMR (126 MHz, CD$_2$Cl$_2$, 22 °C) δ
157.29, 146.10, 142.13, 137.08,
131.80, 130.92, 129.23, 128.39,
126.99, 124.42, 120.87, 92.43.
# High Resolution Mass Spectrometry Report

## Measured m/z vs. theoretical m/z

| # | m/z   | l % | l | Score | m/z | err [mDa] | err [ppm] | mSigma | rdb | e^− Conf | z |
|---|-------|-----|---|-------|-----|----------|----------|--------|-----|-------|----|
| 1 | 273.1544 | 0.8 | 1130 | 1819.1599 | 1 | C 56 H 28 Cu N 4 | 100.00 | 1819.1604 | 0.5 | 0.6 | 25.1 | 44.5 | even | 1+ |

## Mass list

| # | m/z   | l % | l |
|---|-------|-----|---|
| 1 | 273.1544 | 0.8 | 1130 |
| 2 | 299.1512 | 1.2 | 1765 |
| 3 | 301.0650 | 0.6 | 265 |
| 4 | 301.1311 | 1.6 | 2257 |
| 5 | 304.2509 | 1.7 | 2356 |
| 6 | 315.1839 | 1.2 | 1685 |
| 7 | 317.1831 | 3.9 | 5438 |
| 8 | 318.1868 | 0.8 | 1138 |
| 9 | 331.1795 | 0.6 | 778 |
| 10 | 331.2008 | 1.1 | 1525 |
| 11 | 339.1470 | 1.1 | 1548 |
| 12 | 339.1705 | 0.6 | 801 |
| 13 | 353.2599 | 1.0 | 1440 |
| 14 | 360.3173 | 2.3 | 3208 |
| 15 | 361.3211 | 0.7 | 1029 |
| 16 | 379.0349 | 0.6 | 645 |
| 17 | 379.1183 | 100.0 | 138278 |
| 18 | 380.1213 | 28.6 | 39014 |
| 19 | 381.1293 | 7.1 | 9170 |
| 20 | 381.2924 | 0.8 | 1134 |
| 21 | 382.1356 | 1.9 | 2641 |
| 22 | 389.0299 | 1.9 | 2634 |
| 23 | 391.0220 | 2.1 | 2948 |
| 24 | 392.0265 | 0.8 | 1127 |
| 25 | 393.0017 | 1.6 | 2154 |
| 26 | 393.2937 | 0.8 | 1167 |
| 27 | 394.0041 | 1.2 | 1628 |
| 28 | 394.0097 | 1.6 | 2254 |
| 29 | 395.1139 | 0.9 | 1201 |
| 30 | 399.1060 | 1.1 | 1489 |
| 31 | 401.1000 | 5.8 | 8064 |
| 32 | 402.1042 | 1.8 | 2514 |
| 33 | 411.1093 | 1.2 | 1692 |
| 34 | 412.1141 | 0.6 | 852 |
| 35 | 413.1244 | 1.8 | 2532 |
| 36 | 413.2631 | 4.6 | 6351 |
| 37 | 414.1281 | 0.6 | 783 |
| 38 | 414.2567 | 1.3 | 1807 |
| 39 | 415.1095 | 1.4 | 1888 |
| 40 | 424.1091 | 1.1 | 1460 |
| 41 | 425.0064 | 0.6 | 830 |
| 42 | 427.0882 | 0.8 | 1112 |
| 43 | 431.0540 | 2.0 | 2762 |
| 44 | 432.0576 | 0.7 | 933 |
| 45 | 433.0526 | 2.2 | 3000 |
| 46 | 433.0994 | 1.4 | 1964 |
| 47 | 434.0954 | 0.8 | 1104 |
| 48 | 436.0036 | 0.6 | 897 |
| 49 | 441.0412 | 0.9 | 1265 |
| 50 | 441.2950 | 1.2 | 1720 |
| 51 | 444.1904 | 0.9 | 1203 |
| 52 | 447.3421 | 2.0 | 2632 |
| 53 | 448.3446 | 0.6 | 763 |
| 54 | 453.0375 | 1.2 | 1662 |
| 55 | 455.0357 | 1.2 | 1663 |
| 56 | 463.3171 | 1.0 | 1368 |
| 57 | 492.1171 | 0.9 | 1209 |
| 58 | 492.9770 | 1.3 | 1840 |
| 59 | 494.0700 | 1.9 | 2026 |
| 60 | 495.9796 | 0.6 | 804 |
| 61 | 496.9725 | 0.7 | 924 |
| 62 | 506.1103 | 0.6 | 875 |

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**Bruker Compass Data Analysis 4.0**

**Acquisition Date**: 22.10.2016 12:06:45

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### High Resolution Mass Spectrometry Report

| #  | m/z  | I %  | I   |
|----|------|------|-----|
| 63 | 611.0412 | 0.9 | 990 |
| 64 | 613.3391 | 1.0 | 1383 |
| 65 | 623.3231 | 2.9 | 4002 |
| 66 | 624.3264 | 0.9 | 1282 |
| 67 | 625.2170 | 0.9 | 1037 |
| 68 | 657.3652 | 1.2 | 1713 |
| 69 | 569.0097 | 0.7 | 937 |
| 70 | 571.0590 | 0.7 | 911 |
| 71 | 573.1032 | 0.7 | 947 |
| 72 | 601.3916 | 1.1 | 1562 |
| 73 | 645.4173 | 1.0 | 1322 |
| 74 | 655.4598 | 0.8 | 1122 |
| 75 | 660.4446 | 0.7 | 970 |
| 76 | 757.2382 | 8.3 | 11416 |
| 77 | 758.2409 | 5.8 | 8035 |
| 78 | 759.2409 | 2.0 | 2708 |
| 79 | 761.2339 | 0.6 | 852 |
| 80 | 771.2337 | 0.7 | 977 |
| 81 | 779.2193 | 11.5 | 15958 |
| 82 | 780.2234 | 7.2 | 9691 |
| 83 | 781.2257 | 2.4 | 3399 |
| 84 | 782.2302 | 2.1 | 948 |
| 85 | 769.2276 | 0.6 | 877 |
| 86 | 819.1599 | 5.1 | 6994 |
| 87 | 820.1625 | 3.2 | 4399 |
| 88 | 821.1602 | 2.9 | 4059 |
| 89 | 822.1637 | 1.7 | 2332 |
| 90 | 831.1523 | 0.8 | 1107 |
| 91 | 833.0415 | 0.9 | 1188 |
| 92 | 833.1529 | 0.9 | 1205 |
| 93 | 834.0465 | 0.6 | 770 |
| 94 | 835.0406 | 1.2 | 1690 |
| 95 | 850.0419 | 0.8 | 1137 |
| 96 | 857.0419 | 0.6 | 821 |
| 97 | 849.9225 | 0.9 | 1272 |
| 98 | 850.9208 | 0.9 | 1202 |
| 99 | 825.0271 | 0.8 | 1135 |
| 100 | 827.0250 | 0.8 | 1104 |

### Acquisition Parameter

| Source Type | ESI |
|-------------|-----|
| Ion Polarity | Positive |
| Set Nebulizer | 0.4 Bar |
| Focus | Not active |
| Set Capillary | 3600 V |
| Scan Begin | 75 m/z |
| Set End Plate Offset | -500 V |
| Scan End | 1700 m/z |
| Set Collision RF | 500.0 Vpp |
| Set Ion Energy ( MS only ) | 4.0 eV |
| Set Dry Heater | 180 °C |
| Set Dry Gas | 4.0 l/min |
| Acquisition Date | 22.10.2018 12:06:45 |

Bruker Compass DataAnalysis 4.0
$^1$H, $^{13}$C-NMR (CD$_2$Cl$_2$, 400/101 MHz, 22 °C) and HR-ESI-MS spectra of compound (12)

$^1$H NMR (400 MHz, CD$_2$Cl$_2$, 22 °C) δ
8.19 (d, $J = 8.6$ Hz, 2H),
7.68 (s, 2H),
7.52 (dd, $J = 7.7$, 1.7 Hz, 2H),
7.41 (dd, $J = 8.2$, 1.2 Hz, 2H),
7.31 (ddd, $J = 8.2$, 7.4, 1.8 Hz, 2H),
7.24 (d, $J = 8.6$ Hz, 2H),
7.19 (td, $J = 7.5$, 1.2 Hz, 2H),
0.91 (s, 42H).

$^{13}$C NMR (101 MHz, CD$_2$Cl$_2$, 22 °C) δ
161.96, 155.20, 144.02, 140.16,
134.29, 130.34, 126.77, 125.02,
124.53, 122.84, 117.57, 114.03,
103.10, 96.23, 18.82, 11.72.
# High Resolution Mass Spectrometry Report

## Measured m/z vs. theoretical m/z

| Meas. m/z | # | Formula | Score | Theoret. m/z | err [ppm] | err [mDa] | mSigma | nDB | eConf | Even |
|-----------|---|---------|-------|--------------|-----------|-----------|--------|-----|-------|------|
| 725.3948  | 1 | C45H57N2O2Si2 | 100.00 | 725.3983 | 0.5 | 0.7 | 13.4 | 21.5 | even | 1+ |
| 747.3773  | 1 | C45H59N2NaO2Si2 | 100.00 | 747.3773 | 1.0 | 1.4 | 8.3 | 21.5 | even | 1+ |

## Mass list

| # | m/z   | % |  |
|---|-------|---|---|
| 1 | 173.08119 | 0.5 | 746 |
| 2 | 183.08086 | 1.0 | 1551 |
| 3 | 185.1177 | 4.7 | 7050 |
| 4 | 201.1046 | 1.1 | 1625 |
| 5 | 205.0821 | 5.5 | 8271 |
| 6 | 206.0657 | 0.5 | 717 |
| 7 | 215.1278 | 0.6 | 843 |
| 8 | 217.1069 | 1.2 | 1827 |
| 9 | 239.0903 | 0.7 | 1119 |
| 10 | 245.0800 | 0.6 | 844 |
| 11 | 261.1313 | 0.6 | 782 |
| 12 | 273.1683 | 1.5 | 2303 |
| 13 | 301.1406 | 0.8 | 1245 |
| 14 | 315.1521 | 0.8 | 1162 |
| 15 | 331.2087 | 1.1 | 1050 |
| 16 | 353.2661 | 0.6 | 841 |
| 17 | 361.2964 | 0.5 | 727 |
| 18 | 393.2962 | 0.5 | 703 |
| 19 | 413.2657 | 1.2 | 1895 |
| 20 | 433.1021 | 1.3 | 1988 |
| 21 | 441.2688 | 2.1 | 3191 |
| 22 | 442.3385 | 0.7 | 1013 |
| 23 | 447.3437 | 0.8 | 1248 |
| 24 | 463.3095 | 1.1 | 1684 |
| 25 | 464.3120 | 0.5 | 713 |
| 26 | 492.1175 | 0.6 | 849 |
| 27 | 633.3675 | 0.8 | 1101 |
| 28 | 634.3710 | 0.5 | 738 |
| 29 | 724.7456 | 0.6 | 885 |
| 30 | 725.1371 | 0.6 | 952 |
| 31 | 725.1740 | 0.6 | 856 |
| 32 | 725.2070 | 0.7 | 1081 |
| 33 | 725.2605 | 1.1 | 1614 |
| 34 | 725.2848 | 100.00 | 15160 |
| 35 | 725.6000 | 0.6 | 929 |
| 36 | 725.7152 | 0.5 | 829 |
| 37 | 725.7727 | 0.5 | 701 |
| 38 | 725.8332 | 0.6 | 893 |
| 39 | 725.8701 | 0.6 | 897 |
| 40 | 726.0006 | 0.6 | 1194 |
| 41 | 726.1554 | 0.5 | 712 |
| 42 | 726.2137 | 0.6 | 970 |
| 43 | 726.2630 | 0.6 | 852 |
| 44 | 726.3666 | 0.7 | 1016 |
| 45 | 726.3974 | 58.7 | 8965 |
| 46 | 727.0201 | 0.5 | 744 |
| 47 | 727.3677 | 24.1 | 30547 |
| 48 | 728.3974 | 6.7 | 10202 |
| 49 | 729.4002 | 1.6 | 2457 |
| 50 | 730.4005 | 0.5 | 832 |
| 51 | 731.5263 | 0.6 | 800 |
| 52 | 733.5301 | 0.5 | 726 |
| 53 | 747.3762 | 218.0 | 33109 |
| 54 | 748.3793 | 13.6 | 20647 |
| 55 | 749.3790 | 5.3 | 803 |
| 56 | 750.3789 | 1.7 | 2541 |
| 57 | 763.3495 | 2.8 | 4246 |
| 58 | 764.3522 | 1.6 | 2398 |
| 59 | 765.3511 | 0.7 | 1081 |
| 60 | 767.3157 | 12.4 | 19701 |
| 61 | 788.3189 | 7.8 | 11812 |
# High Resolution Mass Spectrometry Report

| #  | m/z     | %     | Int  |
|----|---------|-------|------|
| 62 | 780.3155| 0.0   | 12077|
| 63 | 780.3167| 4.2   | 6321 |
| 64 | 781.3178| 1.7   | 2546 |
| 65 | 810.3834| 0.6   | 842  |
| 66 | 826.5141| 3.5   | 5294 |
| 67 | 827.5178| 2.2   | 3299 |
| 68 | 828.5180| 1.0   | 1529 |
| 69 | 907.5461| 0.8   | 1174 |
| 70 | 908.5451| 0.5   | 791  |
| 71 | 969.4646| 4.0   | 6113 |
| 72 | 970.4669| 3.3   | 4937 |
| 73 | 971.4647| 3.4   | 5219 |
| 74 | 972.4657| 2.1   | 3140 |
| 75 | 973.4659| 1.1   | 1981 |
| 76 | 1199.4332| 1.0 | 1458 |
| 77 | 1200.4366| 0.8 | 1154 |
| 78 | 1201.4347| 0.6 | 1144 |
| 79 | 1202.4366| 0.7 | 9816 |
| 80 | 1449.7796| 1.2 | 1747 |
| 81 | 1450.7801| 1.5 | 2305 |
| 82 | 1451.7818| 1.1 | 1686 |
| 83 | 1452.7842| 0.6 | 892  |
| 84 | 1466.8035| 0.5 | 740  |
| 85 | 1467.8049| 0.6 | 881  |
| 86 | 1471.7604| 7.0 | 10628|
| 87 | 1472.7633| 0.6 | 13071|
| 88 | 1473.7642| 5.9 | 9020 |
| 89 | 1474.7670| 3.1 | 4730 |
| 90 | 1475.7648| 1.3 | 2009 |
| 91 | 1476.7703| 0.5 | 732  |
| 92 | 1487.7342| 0.5 | 785  |
| 93 | 1488.7365| 0.7 | 999  |
| 94 | 1489.7403| 0.6 | 949  |
| 95 | 1490.7417| 0.5 | 774  |
| 96 | 1511.7025| 1.7 | 2578 |
| 97 | 1512.6991| 1.8 | 2719 |
| 98 | 1513.7007| 1.8 | 2743 |
| 99 | 1514.7021| 1.4 | 2137 |
| 100| 1515.7046| 0.9 | 1303 |

## Acquisition Parameter

| Source Type | ESI  | Ion Polarity | Positive | Nebulizer | 0.4 Bar |
|-------------|------|--------------|----------|-----------|---------|
| Focus       | Not active | Set Capillary | 3500 V | Set Dry Heater | 180 °C |
| Scan Begin  | 75 m/z  | Set End Plate Offset | -500 V | Set Dry Gas | 4.0 l/min |
| Scan End    | 1700 m/z | Set Collision Cell RF | 300.0 Vpp | Set Ion Energy (MS only) | 4.0 eV |
$^1$H-, $^{13}$C-NMR (CD$_2$Cl$_2$, 400/101 MHz, 22 °C) and HR-ESI-MS spectra of compound (13)

$^1$H NMR (400 MHz, CD$_2$Cl$_2$, 22 °C) δ
8.24 (d, $J = 8.6$ Hz, 2H),
7.72 (s, 2H),
7.58 – 7.54 (m, 2H),
7.39 – 7.31 (m, 4H),
7.27 (d, $J = 8.6$ Hz, 2H),
7.22 (ddd, $J = 7.7$, 6.4, 2.2 Hz, 2H),
3.14 (s, 2H).

$^{13}$C NMR (101 MHz, CD$_2$Cl$_2$, 22 °C) δ
162.17, 155.72, 143.98, 140.46,
134.41, 130.80, 126.85, 125.26,
124.79, 122.72, 116.18, 113.93,
82.25, 79.82.
# High Resolution Mass Spectrometry Report

## Measured m/z vs. theoretical m/z

| Meas. m/z | Formula | Score | Theo m/z | err [mDa] | err [ppm] | mSigma | rdb | e  | Conf | z |
|-----------|---------|-------|----------|-----------|-----------|--------|-----|----|------|---|
| 413.1265  | C28 H17 N2 O2 | 100.00 | 413.1265 | -0.6 | -0.8 | 10.4 | 21.5 | even | 1+ |
| 435.1902  | C28 H16 N2 Na O2 | 100.00 | 435.1904 | 0.5 | 1.1 | 0.8 | 21.0 | even | 1+ |

## Mass list

| # | m/z | Int. |
|---|-----|------|
| 1 | 165.0485 | 0.3 | 889 |
| 2 | 183.0778 | 0.4 | 149 |
| 3 | 185.1146 | 0.5 | 10814 |
| 4 | 186.1715 | 0.6 | 2144 |
| 5 | 201.0579 | 0.3 | 934 |
| 6 | 201.1014 | 0.2 | 744 |
| 7 | 205.0568 | 1.5 | 5269 |
| 8 | 215.1244 | 0.3 | 1060 |
| 9 | 215.1049 | 0.5 | 1559 |
| 10 | 239.0984 | 0.4 | 1395 |
| 11 | 241.0681 | 0.3 | 877 |
| 12 | 273.1666 | 0.5 | 1667 |
| 13 | 301.1969 | 0.3 | 1102 |
| 14 | 315.1020 | 0.2 | 750 |
| 15 | 331.2085 | 0.5 | 1620 |
| 16 | 339.1797 | 0.2 | 750 |
| 17 | 353.2654 | 0.3 | 979 |
| 18 | 367.2865 | 0.2 | 685 |
| 19 | 381.2971 | 0.2 | 732 |
| 20 | 383.1409 | 0.2 | 809 |
| 21 | 389.2529 | 0.3 | 918 |
| 22 | 391.2837 | 0.3 | 868 |
| 23 | 393.2981 | 0.3 | 1000 |
| 24 | 405.1223 | 0.3 | 940 |
| 25 | 412.9777 | 0.2 | 712 |
| 26 | 412.9968 | 0.3 | 981 |
| 27 | 413.0072 | 0.2 | 710 |
| 28 | 413.0385 | 0.4 | 1415 |
| 29 | 413.0633 | 0.3 | 1021 |
| 30 | 413.1265 | 100.00 | 345404 |
| 31 | 413.2668 | 1.0 | 3517 |
| 32 | 413.3165 | 0.4 | 1261 |
| 33 | 413.3459 | 0.3 | 1094 |
| 34 | 413.4646 | 0.2 | 851 |
| 35 | 413.5640 | 0.2 | 745 |
| 36 | 414.0509 | 0.2 | 739 |
| 37 | 414.1314 | 29.0 | 99473 |
| 38 | 414.2004 | 0.3 | 1024 |
| 39 | 415.1344 | 4.7 | 16157 |
| 40 | 416.1366 | 0.6 | 944 |
| 41 | 420.2401 | 0.3 | 1010 |
| 42 | 420.2812 | 0.2 | 753 |
| 43 | 433.1026 | 0.4 | 1382 |
| 44 | 435.1099 | 15.6 | 53462 |
| 45 | 436.1131 | 4.0 | 13910 |
| 46 | 437.1169 | 0.8 | 2768 |
| 47 | 439.1432 | 0.4 | 1449 |
| 48 | 441.2962 | 0.2 | 794 |
| 49 | 447.3436 | 0.5 | 1730 |
| 50 | 451.0937 | 4.0 | 13661 |
| 51 | 452.0683 | 1.3 | 4394 |
| 52 | 453.0832 | 0.5 | 1617 |
| 53 | 458.1859 | 0.4 | 1430 |
| 54 | 465.3660 | 0.2 | 730 |
| 55 | 475.0490 | 0.4 | 1405 |
| 56 | 477.0489 | 0.3 | 1130 |
| 57 | 486.1822 | 0.4 | 1259 |
| 58 | 514.2481 | 0.4 | 1447 |
| 59 | 596.4413 | 0.2 | 763 |
| 60 | 597.2066 | 1.1 | 3883 |

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| #  | m/z   | I %   | l   |
|----|-------|-------|-----|
| 62 | 558.2090 | 0.6   | 2041 |
| 63 | 579.1878 | 0.2   | 730  |
| 64 | 601.1641 | 0.2   | 778  |
| 65 | 605.4145 | 0.3   | 896  |
| 66 | 624.4935 | 0.2   | 719  |
| 67 | 644.4918 | 0.2   | 775  |
| 68 | 659.5051 | 0.2   | 799  |
| 69 | 689.5126 | 0.2   | 730  |
| 70 | 691.4686 | 0.2   | 739  |
| 71 | 693.4632 | 0.2   | 769  |
| 72 | 717.5446 | 0.2   | 774  |
| 73 | 732.5433 | 0.2   | 688  |
| 74 | 733.5338 | 0.2   | 784  |
| 75 | 737.4993 | 0.2   | 693  |
| 76 | 749.5230 | 0.2   | 697  |
| 77 | 820.6010 | 0.2   | 700  |
| 78 | 826.2479 | 4.5   | 15602|
| 79 | 826.2504 | 3.1   | 10508|
| 80 | 827.2540 | 1.0   | 3317 |
| 81 | 828.2564 | 0.2   | 804  |
| 82 | 842.2702 | 0.2   | 790  |
| 83 | 847.2294 | 16.0  | 57975|
| 84 | 848.2326 | 10.6  | 36952|
| 85 | 849.2355 | 3.6   | 12080|
| 86 | 849.6198 | 0.2   | 686  |
| 87 | 850.2393 | 0.7   | 25507|
| 88 | 863.2027 | 2.8   | 9417 |
| 89 | 864.2050 | 1.7   | 5762 |
| 90 | 865.2073 | 0.7   | 2491 |
| 91 | 865.6126 | 0.2   | 684  |
| 92 | 866.2087 | 0.3   | 874  |
| 93 | 867.1685 | 6.7   | 23006|
| 94 | 868.1717 | 4.4   | 15096|
| 95 | 869.1602 | 4.2   | 14530|
| 96 | 890.1712 | 2.2   | 7664 |
| 97 | 891.1729 | 0.7   | 2497 |
| 98 | 951.3062 | 0.3   | 890  |
| 99 | 992.3070 | 0.2   | 790  |
|100 |1063.7647 | 0.2   | 744  |

### Acquisition Parameter

- **Source Type**: ESI
- **Ion Polarity**: Positive
- **Set Nebulizer**: 0.4 Bar
- **Set Dry Gas**: 4.0 L/min
- **Set Ion Energy**: (MS only) 4.0 eV
- **Scan Begin**: 75 m/z
- **Scan End**: 1700 m/z
- **Set Collision Cell RF**: 350.0 Vpp
- **Set End Plate Offset**: -500 V
- **Set Capillary**: 3600 V
- **Set Dry Heater**: 180 °C

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**Bruker Compass DataAnalysis 4.0**

**Acquisition Date**: 03.12.2018 10:07:10

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$^1$H-, $^{13}$C-NMR (CD$_2$Cl$_2$, 500/126 MHz, 25 °C) and HR-ESI-MS spectra of compound (7)

$^1$H NMR (500 MHz, CD$_2$Cl$_2$, 25 °C) δ
8.23 (d, $J = 8.6$ Hz, 2H),
7.71 (s, 2H),
7.47 (ddd, $J = 7.7$, 1.7, 0.6 Hz, 2H),
7.37 – 7.29 (m, 4H),
7.27 (d, $J = 8.8$ Hz, 2H),
7.19 (ddd, $J = 7.7$, 7.1, 1.6 Hz, 2H),
-0.04 (s, 18H).

$^{13}$C NMR (126 MHz, CD$_2$Cl$_2$, 25 °C) δ
162.29, 155.67, 143.97, 140.22,
133.88, 130.54, 126.75, 125.20,
124.63, 122.93, 117.21, 114.12,
101.02, 100.10, -0.13.
High Resolution Mass Spectrometry Report

Sample Name: Thomas Brandl / BRT5G2
Comment: 10 ug/mL in MeCN, analyzed in MeCN
Instrument: maxxis 4G
Method: 22 Direct_pos_mid.m

![Mass Spectrogram](chart)

- C34H32N2O2S2H, M 557.21
- C34H32N2O2S2Na, M 575.19
- C34H32N2O2S2Na2, M 1135.39

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# High Resolution Mass Spectrometry Report

## Measured m/z vs. theoretical m/z

| Meas. m/z | # | Formula | Score | m/z  | err [mDa] | err [ppm] | nSigma | db | e~ Conf. |
|-----------|---|---------|-------|------|-----------|-----------|--------|---|----------|
| 557 2074  | 1 | C34 H33 N2 O2 Si2 | 100.00 | 557.2075 | 0.2 | 0.3 | 15.7 | 21.5 | even |
| 579 1892  | 1 | C34 H32 N2 O2 Si2 | 100.00 | 579.1895 | 0.2 | 0.4 | 17.3 | 21.5 | even |
| 1135 3887 | 1 | C68 H64 N4 Na O4 Si4 | 100.00 | 1135.3897 | 1.0 | 0.8 | 9.4  | 42.5 | even |

## Mass list

| # | m/z  | I% |
|---|------|----|
| 1 | 165.1141 | 1.4 |
| 2 | 205.0590 | 2.9 |
| 3 | 217.0331 | 1.2 |
| 4 | 481.2551 | 1.6 |
| 5 | 482.2685 | 0.9 |
| 6 | 511.1828 | 0.7 |
| 7 | 537.2347 | 0.7 |
| 8 | 557.0243 | 0.8 |
| 9 | 557.0511 | 0.8 |
| 10 | 557.2074 | 100.00 |
| 11 | 558.2097 | 46.5 |
| 12 | 560.2000 | 15.0 |
| 13 | 560.2056 | 4.5 |
| 14 | 561.2099 | 0.9 |
| 15 | 579.0813 | 1.0 |
| 16 | 579.1802 | 73.0 |
| 17 | 580.1917 | 32.9 |
| 18 | 581.1913 | 11.4 |
| 19 | 582.1919 | 2.9 |
| 20 | 583.1912 | 0.7 |
| 21 | 595.1632 | 7.9 |
| 22 | 596.1655 | 4.3 |
| 23 | 597.1645 | 1.9 |
| 24 | 613.2700 | 2.2 |
| 25 | 614.2725 | 1.1 |
| 26 | 619.1280 | 5.1 |
| 27 | 620.1312 | 2.4 |
| 28 | 621.1279 | 3.1 |
| 29 | 622.1300 | 1.6 |
| 30 | 635.2516 | 0.9 |
| 31 | 658.3281 | 1.1 |
| 32 | 658.4081 | 7.9 |
| 33 | 658.4085 | 7.0 |
| 34 | 658.4099 | 4.4 |
| 35 | 676.4113 | 2.0 |
| 36 | 677.4132 | 0.8 |
| 37 | 678.4336 | 4.6 |
| 38 | 679.4345 | 4.3 |
| 39 | 679.4357 | 2.8 |
| 40 | 683.4356 | 1.6 |
| 41 | 684.4339 | 0.8 |
| 42 | 694.8237 | 0.8 |
| 43 | 694.8083 | 0.8 |
| 44 | 695.0372 | 1.3 |
| 45 | 695.1711 | 0.8 |
| 46 | 695.1559 | 0.7 |
| 47 | 695.2305 | 0.9 |
| 48 | 695.2367 | 84.6 |
| 49 | 695.6702 | 1.0 |
| 50 | 695.7507 | 0.7 |
| 51 | 695.8048 | 0.9 |
| 52 | 695.8518 | 1.0 |
| 53 | 695.9085 | 0.7 |
| 54 | 695.9484 | 1.5 |
| 55 | 695.9990 | 1.1 |
| 56 | 696.0686 | 1.3 |
| 57 | 696.1305 | 1.0 |
| 58 | 696.2000 | 0.9 |
| 59 | 696.2642 | 1.0 |
| 60 | 696.3909 | 82.9 |
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| #  | m/z  | i %  | I   |
|----|------|------|-----|
| 61 | 1136.5546  | 0.8  | 663 |
| 62 | 1136.7120  | 0.7  | 609 |
| 63 | 1136.7926  | 0.7  | 589 |
| 64 | 1136.8513  | 0.8  | 653 |
| 65 | 1136.9536  | 0.8  | 665 |
| 66 | 1136.9963  | 0.9  | 748 |
| 67 | 1137.0405  | 0.9  | 705 |
| 68 | 1137.1048  | 1.2  | 962 |
| 69 | 1137.1530  | 0.7  | 500 |
| 70 | 1137.1879  | 0.9  | 723 |
| 71 | 1137.3819  | 50.8 | 41483|
| 72 | 1137.7360  | 0.8  | 645 |
| 73 | 1137.7818  | 0.9  | 722 |
| 74 | 1137.8290  | 0.8  | 649 |
| 75 | 1137.9021  | 0.8  | 627 |
| 76 | 1138.0566  | 1.0  | 765 |
| 77 | 1138.3923  | 22.1 | 18047|
| 78 | 1138.9565  | 0.8  | 672 |
| 79 | 1139.3923  | 8.5  | 6954|
| 80 | 1140.3222  | 2.5  | 2006|
| 81 | 1141.4116  | 1.5  | 1299|
| 82 | 1142.3358  | 0.8  | 650 |
| 83 | 1143.4556  | 0.9  | 771 |
| 84 | 1144.7480  | 0.7  | 579 |
| 85 | 1145.6966  | 0.7  | 564 |
| 86 | 1151.3617  | 9.0  | 7333|
| 87 | 1152.3845  | 9.7  | 7952|
| 88 | 1153.6363  | 6.6  | 5361|
| 89 | 1154.3637  | 3.4  | 2813|
| 90 | 1155.3083  | 1.5  | 1204|
| 91 | 1156.3669  | 0.7  | 552 |
| 92 | 1175.3271  | 4.7  | 3858|
| 93 | 1176.3321  | 4.3  | 3548|
| 94 | 1177.2262  | 4.9  | 4227|
| 95 | 1178.3305  | 3.3  | 2657|
| 96 | 1179.3305  | 1.0  | 1341|
| 97 | 1180.3260  | 0.7  | 563 |
| 98 | 1191.4500  | 1.6  | 1328|
| 99 | 1192.4530  | 1.9  | 1519|
| 100| 1193.4540  | 1.3  | 1028|

Acquisition Parameter

| Source Type | ESI | Ion Polarity | Positive | Set Nebulizer | 0.4 Bar |
|-------------|-----|--------------|----------|---------------|--------|
| Focus       | Not active | Set Capillary | 3600 V | Set Dry Heater | 180 °C |
| Scan Began  | 75 m/z | Set Collision Offset | -500 V | Set Dry Gas | 4.0 l/min |
| Scan End    | 1700 m/z | Set Collision Cell RF | 350.0 Vpp | Set Ion Energy (MS only) | 4.0 eV |

Bruker Compass DataAnalysis 4.0  Acquisition Date 03.12.2018 09:48:59  Page 3 of 3
$^1$H, $^{13}$C-NMR (CD$_2$Cl$_2$, 400/101 MHz, 22 °C) and HR-ESI-MS spectra of compound (5)

$^1$H NMR (400 MHz, CD$_2$Cl$_2$, 22 °C) δ
8.40 (d, $J = 8.7$ Hz, 4H),
7.90 (s, 4H),
7.30 (d, $J = 8.7$ Hz, 4H),
7.03 (dd, $J = 7.7$, 1.7 Hz, 4H),
6.76 (ddd, $J = 8.3$, 7.4, 1.7 Hz, 4H),
6.65 (dd, $J = 8.3$, 1.2 Hz, 4H),
6.55 (td, $J = 7.6$, 1.2 Hz, 4H),
-0.10 (s, 36H).

$^{13}$C NMR (101 MHz, CD$_2$Cl$_2$, 22 °C) δ
160.52, 154.46, 142.11, 140.84,
134.66, 130.12, 126.84, 125.46,
124.81, 120.13, 116.86, 115.71,
101.17, 100.18, -0.14.
High Resolution Mass Spectrometry Report

Sample Name: Thomas Brandt / BRT563
Comment: 10 µg/mL in MeCN, analyzed in MeCN
Instrument: maXis 4G
Method: 24 Direct_pos_high.m

+-MS, 0.24-0.34 min #1(14-20)

+-MS, 0.24-0.34 min #1(14-20)

C34H32N2O2S2H₂M⁺, M⁺, 587.21

C34H32N2O2S2Na⁺, M⁺, 579.19

C34H32N2O2S2Cu⁺, M⁺, 619.13

C68H64N4O4S4Na⁺, M⁺, 1135.39

C68H64N4O4S4Cu⁺, M⁺, 1175.33

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## High Resolution Mass Spectrometry Report

### Measured m/z vs. theoretical m/z

| #   | m/z    | Formula | Score | m/z   | err [Da] | err [ppm] | mSigma | rdp | z      | Conf |
|-----|--------|---------|-------|-------|----------|-----------|--------|-----|--------|-------|
| 1   | 381.2076 | C34H33N2O2Si2 | 100.00 | 557.2075 | -0.5 | -0.8 | 14.1 | 21.5 | even | 1+    |
| 1   | 381.2076 | C34H33N2O2Si2 | 100.00 | 579.1995 | -0.2 | -0.4 | 13.4 | 21.5 | even | 1+    |
| 1   | 381.2076 | C34H33N2O2Si2 | 100.00 | 619.1293 | 0.3  | 0.5  | 5.7  | 21.5 | even | 1+    |
| 1   | 381.2076 | C34H33N2O2Si2 | 100.00 | 1135.3897 | 0.5 | 0.5 | 15.7 | 42.5 | even | 1+    |
| 1   | 381.2076 | C34H33N2O2Si2 | 100.00 | 1175.3295 | 0.9 | 0.8 | 23.7 | 42.5 | even | 1+    |

### Mass list

| #   | m/z    | I %  | I   |
|-----|--------|------|-----|
| 1   | 381.2076 | 0.9  | 1214|
| 2   | 429.3163 | 0.8  | 1088|
| 3   | 439.1463 | 6.1  | 7609|
| 4   | 440.1475 | 2.1  | 2662|
| 5   | 443.2327 | 1.0  | 1242|
| 6   | 453.1236 | 7.7  | 9936|
| 7   | 454.1270 | 2.5  | 3246|
| 8   | 461.1263 | 2.4  | 3161|
| 9   | 462.1297 | 0.9  | 1123|
| 10  | 475.1052 | 11.4 | 14718|
| 11  | 476.1081 | 3.9  | 5077|
| 12  | 477.1087 | 0.9  | 1140|
| 13  | 491.0792 | 3.4  | 4341|
| 14  | 492.0821 | 1.3  | 1731|
| 15  | 501.0660 | 1.9  | 2465|
| 16  | 503.0647 | 1.0  | 1275|
| 17  | 515.0459 | 1.4  | 1767|
| 18  | 517.0439 | 0.9  | 1112|
| 19  | 557.2080 | 66.3 | 65729|
| 20  | 558.2107 | 30.4 | 52069|
| 21  | 559.2107 | 10.6 | 13724|
| 22  | 560.2107 | 2.9  | 3711|
| 23  | 579.1697 | 76.6 | 96061|
| 24  | 580.1021 | 35.5 | 48844|
| 25  | 581.1913 | 12.1 | 15607|
| 26  | 582.1921 | 3.3  | 4323|
| 27  | 595.1634 | 7.3  | 9382|
| 28  | 596.1659 | 3.4  | 4386|
| 29  | 597.1647 | 1.8  | 2284|
| 30  | 613.2695 | 1.2  | 1538|
| 31  | 619.1290 | 32.0 | 42191|
| 32  | 620.1316 | 15.8 | 26471|
| 33  | 621.1281 | 20.2 | 26158|
| 34  | 622.1300 | 8.6  | 11129|
| 35  | 623.1294 | 3.0  | 3920|
| 36  | 624.1322 | 0.9  | 1152|
| 37  | 693.2719 | 0.9  | 1116|
| 38  | 905.2376 | 1.2  | 1581|
| 39  | 920.2352 | 1.0  | 2500|
| 40  | 930.2368 | 1.2  | 1602|
| 41  | 939.2007 | 1.1  | 1424|
| 42  | 943.2071 | 1.0  | 1267|
| 43  | 966.3430 | 1.0  | 1269|
| 44  | 1000.3239 | 2.5 | 3216|
| 45  | 1010.3237 | 2.0 | 2575|
| 46  | 1011.3252 | 1.1 | 1373|
| 47  | 1017.3261 | 1.2 | 1524|
| 48  | 1018.3276 | 1.1 | 1371|
| 49  | 1026.3500 | 0.9 | 1200|
| 50  | 1031.3036 | 7.9 | 10174|
| 51  | 1032.3068 | 6.5 | 8413|
| 52  | 1033.3076 | 3.6 | 4600|
| 53  | 1034.3073 | 1.5 | 1877|
| 54  | 1047.2785 | 2.1 | 2720|
| 55  | 1048.2622 | 1.9 | 2465|
| 56  | 1049.2623 | 1.3 | 1630|
| 57  | 1052.2695 | 1.1 | 1412|
| 58  | 1056.2674 | 1.0 | 1326|

**Bruker Compass Data Analysis 4.0**

**Acquisition Date**: 29.11.2018 10:50:56
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| m/z   | Intensity | %   | Intensity |
|-------|-----------|-----|-----------|
| 59    | 1059.2022 | 1.1 | 1425      |
| 60    | 1063.3477 | 1.3 | 1708      |
| 61    | 1064.3404 | 1.2 | 1598      |
| 62    | 1093.2684 | 0.9 | 1120      |
| 63    | 1113.4066 | 3.3 | 4309      |
| 64    | 1144.4097 | 3.4 | 4401      |
| 65    | 1115.4084 | 1.9 | 2492      |
| 66    | 1116.4108 | 0.9 | 1176      |
| 67    | 1130.4332 | 1.2 | 1561      |
| 68    | 1131.4380 | 1.1 | 1406      |
| 69    | 1132.4309 | 0.8 | 1091      |
| 70    | 1135.0518 | 1.2 | 1495      |
| 71    | 1135.1189 | 1.2 | 1558      |
| 72    | 1135.3894 | 100.0| 129313    |
| 73    | 1135.7722 | 0.9 | 1141      |
| 74    | 1136.0442 | 0.8 | 1098      |
| 75    | 1136.1211 | 0.9 | 1114      |
| 76    | 1136.3516 | 96.2| 120697    |
| 77    | 1136.6602 | 1.1 | 1378      |
| 78    | 1137.0542 | 1.0 | 1326      |
| 79    | 1137.2542 | 0.9 | 1152      |
| 80    | 1137.3026 | 56.6| 73150     |
| 81    | 1138.0800 | 0.8 | 1069      |
| 82    | 1138.3928 | 25.5| 32921     |
| 83    | 1139.3934 | 9.5 | 12296     |
| 84    | 1140.3323 | 3.0 | 3885      |
| 85    | 1141.3342 | 1.1 | 1389      |
| 86    | 1151.3518 | 6.3 | 8175      |
| 87    | 1152.3553 | 6.0 | 7794      |
| 88    | 1153.3044 | 3.8 | 4957      |
| 89    | 1154.3665 | 2.1 | 2755      |
| 90    | 1155.3625 | 1.0 | 1235      |
| 91    | 1175.3286 | 23.9| 30889     |
| 92    | 1176.3309 | 23.0| 29776     |
| 93    | 1177.3206 | 23.3| 30072     |
| 94    | 1178.3299 | 16.4| 21248     |
| 95    | 1179.3311 | 8.5 | 11074     |
| 96    | 1180.3311 | 3.6 | 4590      |
| 97    | 1181.3332 | 1.5 | 1878      |
| 98    | 1191.4407 | 1.0 | 2445      |
| 99    | 1192.4538 | 1.9 | 2500      |
| 100   | 1193.4542 | 1.2 | 1591      |

## Acquisition Parameter

| Source Type | ESI      | Ion Polarity | Positive | Set Nebulizer | 0.4 Bar |
|-------------|----------|--------------|----------|---------------|---------|
| Focus       | Not active| Set Capillary| 3600 V   | Set Dry Heater| 180 °C  |
| Scan Begin  | 75 m/z   | Set End Plate Offset| -500 V  | Set Dry Gas   | 4.0 l/min |
| Scan End    | 2000 m/z | Set Collision Cell RF| 1000.0 Vpp| Set Ion Energy ( MS only )| 4.0 eV |

Bruker Compass DataAnalysis 4.0  Acquisition Date  29.11.2018 10:50:56  Page 3 of 3
$^{1}$H-, $^{13}$C-NMR (CD$_2$Cl$_2$, 500/126 MHz, 25 °C) and HR-ESI-MS spectra of compound (3)

$^{1}$H NMR (500 MHz, CD$_2$Cl$_2$, 25 °C) $\delta$
- 8.38 (d, $J = 8.9$ Hz, 4H),
- 7.84 (s, 4H),
- 7.60 (dd, $J = 8.2$, 7.5, 1.7 Hz, 4H),
- 7.44 (dd, $J = 7.6$, 1.7, 0.5 Hz, 4H),
- 7.35 – 7.30 (m, 8H),
- 6.96 (d, $J = 8.9$ Hz, 4H).

$^{13}$C NMR (126 MHz, CD$_2$Cl$_2$, 25 °C) $\delta$
- 162.34, 156.59, 143.05, 141.18,
- 133.27, 132.19, 127.45, 126.62,
- 125.07, 123.23, 116.68, 111.62,
- 80.54, 79.05.
# High Resolution Mass Spectrometry Report

## Measured m/z vs. theoretical m/z

| Mass List | m/z    | Int. % | Score | m/z, err [mDa] | err [ppm] | mSigma | rdb   | e-Conf | z     |
|-----------|--------|--------|-------|---------------|-----------|--------|-------|--------|-------|
| 883.1414  | 411.1123 | 4.5    | 8741  |               |           |        |       |        |       |
|           | 412.1156 | 1.3    | 2642  |               |           |        |       |        |       |
|           | 433.0347 | 1.9    | 3726  |               |           |        |       |        |       |
|           | 434.0977 | 0.5    | 1000  |               |           |        |       |        |       |
| 441.5859  | 2.3    | 4458   |       |               |           |        |       |        |       |
|           | 482.0705 | 1.2    | 2312  |               |           |        |       |        |       |
|           | 442.5706 | 1.4    | 2758  |               |           |        |       |        |       |
|           | 443.0712 | 0.7    | 1390  |               |           |        |       |        |       |
|           | 443.1933 | 0.8    | 1520  |               |           |        |       |        |       |
|           | 473.0348 | 1.5    | 2012  |               |           |        |       |        |       |
|           | 474.0902 | 0.6    | 1150  |               |           |        |       |        |       |
|           | 475.0535 | 0.6    | 1192  |               |           |        |       |        |       |
|           | 505.0605 | 0.6    | 1180  |               |           |        |       |        |       |
|           | 531.1529 | 0.5    | 1006  |               |           |        |       |        |       |
|           | 799.1363 | 0.6    | 1144  |               |           |        |       |        |       |
|           | 821.2188 | 2.6    | 5022  |               |           |        |       |        |       |
|           | 822.2214 | 2.0    | 3655  |               |           |        |       |        |       |
|           | 823.2252 | 0.0    | 1502  |               |           |        |       |        |       |
|           | 825.1913 | 0.9    | 1617  |               |           |        |       |        |       |
|           | 826.1964 | 0.5    | 992   |               |           |        |       |        |       |
|           | 827.1989 | 0.6    | 1124  |               |           |        |       |        |       |
|           | 843.2005 | 2.6    | 5114  |               |           |        |       |        |       |
|           | 844.2026 | 1.7    | 3248  |               |           |        |       |        |       |
|           | 845.2101 | 0.7    | 1404  |               |           |        |       |        |       |
|           | 869.2003 | 0.6    | 1093  |               |           |        |       |        |       |
|           | 875.2214 | 0.4    | 762   |               |           |        |       |        |       |
|           | 882.9039 | 0.5    | 900   |               |           |        |       |        |       |
|           | 883.5688 | 0.5    | 915   |               |           |        |       |        |       |
|           | 883.5691 | 0.6    | 1088  |               |           |        |       |        |       |
|           | 883.1414 | 100.0  | 196422|               |           |        |       |        |       |
|           | 883.2872 | 0.4    | 765   |               |           |        |       |        |       |
|           | 883.3329 | 0.4    | 779   |               |           |        |       |        |       |
|           | 883.5111 | 0.4    | 770   |               |           |        |       |        |       |
|           | 883.6096 | 0.4    | 765   |               |           |        |       |        |       |
|           | 883.6339 | 0.4    | 757   |               |           |        |       |        |       |
|           | 883.6780 | 0.4    | 782   |               |           |        |       |        |       |
|           | 883.9504 | 0.4    | 878   |               |           |        |       |        |       |
|           | 884.0308 | 0.5    | 884   |               |           |        |       |        |       |
|           | 884.0655 | 0.4    | 857   |               |           |        |       |        |       |
|           | 884.1442 | 60.7   | 119318|               |           |        |       |        |       |
|           | 884.6376 | 0.4    | 854   |               |           |        |       |        |       |
|           | 884.7052 | 0.4    | 851   |               |           |        |       |        |       |
|           | 885.0040 | 0.5    | 695   |               |           |        |       |        |       |
|           | 885.0095 | 0.6    | 1234  |               |           |        |       |        |       |
|           | 885.1420 | 69.7   | 17282 |               |           |        |       |        |       |
|           | 886.1343 | 29.7   | 59382 |               |           |        |       |        |       |
|           | 887.1465 | 10.2   | 20037 |               |           |        |       |        |       |
|           | 888.1518 | 2.9    | 5774  |               |           |        |       |        |       |
|           | 889.1515 | 0.6    | 1172  |               |           |        |       |        |       |
|           | 891.1964 | 2.2    | 4242  |               |           |        |       |        |       |
|           | 918.1692 | 1.5    | 2659  |               |           |        |       |        |       |
|           | 917.1863 | 1.6    | 3184  |               |           |        |       |        |       |
|           | 918.1693 | 0.8    | 1512  |               |           |        |       |        |       |
|           | 919.1757 | 0.4    | 772   |               |           |        |       |        |       |
|           | 933.1777 | 4.5    | 8614  |               |           |        |       |        |       |
|           | 934.1809 | 3.2    | 6239  |               |           |        |       |        |       |
|           | 935.1787 | 3.0    | 5620  |               |           |        |       |        |       |
|           | 936.1692 | 1.8    | 3541  |               |           |        |       |        |       |
|           | 937.1871 | 0.4    | 856   |               |           |        |       |        |       |
|           | 945.1768 | 0.6    | 1120  |               |           |        |       |        |       |
|           | 946.1798 | 0.0    | 895   |               |           |        |       |        |       |
|           | 947.1861 | 0.5    | 1064  |               |           |        |       |        |       |

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*Acquisition Date: 06.03.2019 10:17:51*  
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| #  | m/z   | I %  | I   |
|----|-------|------|-----|
| 53 | 957.1949 | 1.7  | 3250 |
| 64 | 958.1980 | 1.4  | 2629 |
| 55 | 959.1976 | 1.0  | 1987 |
| 56 | 960.1905 | 0.7  | 1396 |
| 67 | 961.2031 | 0.4  | 776  |
| 68 | 963.1737 | 0.6  | 1512 |
| 69 | 964.1903 | 0.6  | 1183 |
| 70 | 965.1992 | 0.6  | 1252 |
| 71 | 967.2100 | 1.0  | 1986 |
| 72 | 967.1988 | 0.5  | 918  |
| 73 | 963.2047 | 0.5  | 993  |
| 74 | 969.1694 | 0.9  | 1762 |
| 75 | 1000.1691 | 0.7  | 1343 |
| 76 | 1001.1010 | 2.3  | 4698 |
| 77 | 1002.1645 | 1.7  | 3348 |
| 78 | 1003.1905 | 1.5  | 2991 |
| 79 | 1004.1669 | 1.0  | 2025 |
| 80 | 1001.1664 | 0.9  | 1624 |
| 81 | 1002.1902 | 0.7  | 1313 |
| 82 | 1003.1945 | 0.6  | 1104 |
| 83 | 1034.2013 | 0.4  | 658  |
| 84 | 1041.3902 | 0.4  | 688  |
| 85 | 1049.2001 | 1.0  | 1996 |
| 86 | 1050.2078 | 0.7  | 1322 |
| 87 | 1051.2084 | 0.5  | 1054 |
| 88 | 1052.2056 | 0.6  | 898  |
| 89 | 1233.2420 | 0.9  | 1760 |
| 90 | 1234.3323 | 0.8  | 1351 |
| 91 | 1235.3330 | 0.7  | 1338 |
| 92 | 1323.2530 | 0.9  | 1612 |
| 93 | 1294.2558 | 0.9  | 1760 |
| 94 | 1295.2590 | 0.8  | 1028 |
| 95 | 1266.2613 | 0.6  | 1185 |
| 96 | 1703.3798 | 1.3  | 2509 |
| 97 | 1704.3825 | 1.5  | 2988 |
| 98 | 1705.3830 | 1.2  | 2450 |
| 99 | 1706.3855 | 1.1  | 2101 |
| 100 | 1707.3877 | 0.6  | 1262 |

Acquisition Parameter

| General   |      |      |      |      |      |
|-----------|------|------|------|------|------|
| Fore Vacuum | 2.68e+000 mBar | High Vacuum | 9.53e-008 mBar | Source Type | ESI |
| Scan Begin  | 75 mV | Scan End | 2000 mV | Ion Polarity | Positive |
| Source      |      |      |      |      |      |
| Set Nebulizer | 0.4 Bar | Set Capillary | 3600 V | Set Dry Gas | 4.0 l/min |
| Set Dry Heater | 180 °C | Set End Plate Offset | -500 V |      |      |

Quadrupole Set Ion Energy (MS only ) | 4.0 eV
Coll. Cell Collision Energy | 10.0 eV
Ion Cooler Set Ion Cooler Transfer Time | 160.0 μs
Ion Cooler Set Ion Cooler Pre Pulse Storage Time | 18.0 μs

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$^1$H, $^{13}$C-NMR (CDCl$_3$, 400/101 MHz, 22 °C) and HR-ESI-MS spectra of compound (14)

$^1$H NMR (400 MHz, CDCl$_3$, 22 °C) $\delta$
8.19 (d, $J = 8.6$ Hz, 2H),
7.68 (s, 2H),
7.40 – 7.29 (m, 8H),
7.24 – 7.17 (m, 4H).

$^{13}$C NMR (101 MHz, CDCl$_3$, 22 °C) $\delta$
162.06, 154.13, 143.69, 139.83,
129.64, 126.19, 124.55, 124.23,
121.17, 113.88.
# High Resolution Mass Spectrometry Report

Measured m/z vs. theoretical m/z

| Mass list | # | m/z   | l % | I     |
|-----------|---|-------|-----|-------|
| 1         | 1 | 123.0917 | 0.3 | 1504  |
| 2         | 2 | 137.1072 | 0.3 | 1576  |
| 3         | 3 | 136.0910 | 0.2 | 1351  |
| 4         | 4 | 139.0902 | 0.2 | 960   |
| 5         | 5 | 140.0916 | 0.3 | 1541  |
| 6         | 6 | 147.0914 | 0.4 | 1916  |
| 7         | 7 | 149.0232 | 0.3 | 1581  |
| 8         | 8 | 163.1025 | 0.2 | 1221  |
| 9         | 9 | 163.1327 | 0.6 | 393   |
| 10        | 10| 169.0467 | 0.2 | 1023  |
| 11        | 11| 173.0764 | 0.4 | 2893  |
| 12        | 12| 183.0777 | 0.4 | 2007  |
| 13        | 13| 183.0968 | 0.2 | 1131  |
| 14        | 14| 185.1147 | 5.2 | 27002 |
| 15        | 15| 186.1182 | 0.4 | 2376  |
| 16        | 16| 187.0782 | 0.2 | 1280  |
| 17        | 17| 201.1033 | 0.7 | 3532  |
| 18        | 18| 205.0568 | 0.4 | 1929  |
| 19        | 19| 211.0037 | 0.2 | 1251  |
| 20        | 20| 215.1254 | 0.2 | 1007  |
| 21        | 21| 217.1044 | 0.7 | 3886  |
| 22        | 22| 219.0476 | 0.2 | 1348  |
| 23        | 23| 225.1064 | 0.2 | 1068  |
| 24        | 24| 241.0294 | 0.2 | 1227  |
| 25        | 25| 251.1613 | 0.3 | 1564  |
| 26        | 26| 261.1299 | 0.3 | 1350  |
| 27        | 27| 265.1763 | 0.2 | 1128  |
| 28        | 28| 267.1569 | 0.4 | 1936  |
| 29        | 29| 273.1671 | 0.3 | 1375  |
| 30        | 30| 273.1945 | 0.3 | 1633  |
| 31        | 31| 279.2284 | 0.2 | 1117  |
| 32        | 32| 283.1012 | 0.2 | 1073  |
| 33        | 33| 281.1932 | 0.2 | 1233  |
| 34        | 34| 293.2065 | 0.3 | 1466  |
| 35        | 35| 303.1779 | 0.8 | 4367  |
| 36        | 36| 304.2067 | 0.2 | 1162  |
| 37        | 37| 305.2086 | 0.3 | 1659  |
| 38        | 38| 309.2048 | 0.2 | 1032  |
| 39        | 39| 315.1025 | 0.3 | 1813  |
| 40        | 40| 319.2244 | 0.3 | 1565  |
| 41        | 41| 321.2035 | 0.2 | 1071  |
| 42        | 42| 331.2065 | 0.3 | 1443  |
| 43        | 43| 339.1764 | 0.2 | 968   |
| 44        | 44| 363.1453 | 0.3 | 1788  |
| 45        | 45| 353.2660 | 0.9 | 4674  |
| 46        | 46| 354.2696 | 0.2 | 1078  |
| 47        | 47| 363.1490 | 0.5 | 2722  |
| 48        | 48| 365.0978 | 0.3 | 1564  |
| 49        | 49| 365.1289 | 100.0 | 541132 |
| 50        | 50| 365.2760 | 0.2 | 1202  |
| 51        | 51| 365.3164 | 0.3 | 1513  |
| 52        | 52| 365.3497 | 0.2 | 1224  |
| 53        | 53| 365.3859 | 0.2 | 1103  |
| 54        | 54| 365.4053 | 0.2 | 1141  |
| 55        | 55| 365.4422 | 0.2 | 1102  |
| 56        | 56| 365.4964 | 0.2 | 1288  |
| 57        | 57| 360.1318 | 25.1 | 135939 |
| 58        | 58| 367.1345 | 3.5 | 18969  |
| 59        | 59| 365.1349 | 0.4 | 2200  |
| 60        | 60| 381.2076 | 0.7 | 3064  |
| 61        | 61| 382.3012 | 0.2 | 1328  |
| 62        | 62| 360.2926 | 0.2 | 1026  |

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| #  | m/z     | I % | I     |
|----|---------|-----|-------|
| 63 | 587.1102| 4.7 | 25256 |
| 64 | 388.1132| 1.4 | 7551  |
| 65 | 389.1100| 0.2 | 1185  |
| 66 | 391.2646| 0.2 | 1211  |
| 67 | 393.2692| 0.2 | 1160  |
| 68 | 403.0037| 0.3 | 1649  |
| 69 | 413.2696| 0.7 | 3684  |
| 70 | 414.2691| 0.2 | 569   |
| 71 | 427.0496| 0.9 | 4613  |
| 72 | 427.2086| 0.6 | 4277  |
| 73 | 428.0536| 0.2 | 1228  |
| 74 | 428.2116| 0.2 | 1164  |
| 75 | 429.0484| 0.4 | 2302  |
| 76 | 429.3179| 0.3 | 1588  |
| 77 | 433.1033| 0.3 | 1647  |
| 78 | 441.3275| 0.2 | 1315  |
| 79 | 447.3449| 0.3 | 1807  |
| 80 | 449.3748| 0.2 | 1027  |
| 81 | 473.3436| 0.3 | 1781  |
| 82 | 487.3062| 0.2 | 1043  |
| 83 | 512.4154| 0.2 | 1003  |
| 84 | 517.3703| 0.2 | 1269  |
| 85 | 556.4406| 0.2 | 1047  |
| 86 | 561.3981| 0.2 | 1319  |
| 87 | 700.6294| 0.2 | 1098  |
| 88 | 705.5813| 0.4 | 2082  |
| 89 | 729.2485| 1.3 | 6950  |
| 90 | 730.2529| 0.7 | 3703  |
| 91 | 731.2530| 0.2 | 1153  |
| 92 | 735.2591| 0.2 | 1220  |
| 93 | 751.2313| 3.6 | 19695 |
| 94 | 752.2341| 2.1 | 11427 |
| 95 | 753.2376| 0.6 | 3224  |
| 96 | 791.1712| 6.1 | 32004 |
| 97 | 792.1749| 3.2 | 17222 |
| 98 | 793.1706| 3.2 | 17290 |
| 99 | 794.1727| 1.6 | 6607  |
| 100| 795.1748| 0.4 | 2187  |

#### Acquisition Parameter

| Parameter                  | Value        |
|----------------------------|--------------|
| General Fore Vacuum        | 2.79e+000 mBar |
| General Scan Begin         | 75 m/z       |
| General Source Nebulizer   | 0.4 Bar      |
| General Source Dry Heater  | 180 °C       |
| Quadropole Set Ion Energy (M3 only) | 4.0 eV |
| Collision Cell Energy      | 8.0 eV       |
| Ion Cooler Transfer Time   | 55.0 μs      |
| Source Capillary           | 3600 V       |
| Source End Plate Offset    | -500 V       |
| Source Ion Cooler          | 350.0 Vpp    |
| Source Ion Cooler Pro Pulse Storage Time | 7.0 μs |
$^1$H-, $^{13}$C-NMR (CD$_2$Cl$_2$, 400/101 MHz, 22 °C) and HR-ESI-MS spectra of compound (15)

$^1$H NMR (400 MHz, CD$_2$Cl$_2$, 22 °C) δ
8.43 (d, $J = 8.7$ Hz, 4H),
7.91 (s, 4H),
7.29 (d, $J = 8.7$ Hz, 4H),
6.94 – 6.87 (m, 8H),
6.77 – 6.69 (m, 4H),
6.66 – 6.59 (m, 8H).

$^{13}$C NMR (101 MHz, CD$_2$Cl$_2$, 22 °C) δ
160.31, 153.69, 141.95, 140.47,
129.47, 126.20, 124.78, 124.55,
118.90, 115.06.
## Measured m/z vs. theoretical m/z

| Mass | m/z | % | I | Score | m/z | err [mDa] | err [ppm] | mSigma | ndx | Conf | z |
|------|-----|---|---|-------|-----|---------|----------|--------|-----|------|---|
| 791.1724 | 1 | C_{46}H_{52}CuN_{4}O_{4} | 100.00 | 791.1714 | -1.0 | -1.3 | 16.7 | 34.5 | even | 1+ |

### Mass list

| # | m/z | % | I |
|---|-----|---|---|
| 1 | 315.1930 | 0.5 | 2049 |
| 2 | 353.2681 | 1.4 | 5707 |
| 3 | 365.1287 | 39.1 | 154740 |
| 4 | 366.1319 | 9.8 | 36636 |
| 5 | 367.1345 | 1.4 | 5465 |
| 6 | 368.2977 | 2.3 | 6968 |
| 7 | 369.3007 | 0.6 | 2232 |
| 8 | 369.3053 | 0.4 | 1746 |
| 9 | 387.1105 | 19.9 | 78768 |
| 10 | 388.1138 | 5.0 | 16878 |
| 11 | 389.1168 | 0.8 | 3186 |
| 12 | 390.2680 | 0.7 | 9733 |
| 13 | 403.0845 | 4.3 | 17186 |
| 14 | 404.0875 | 1.1 | 4445 |
| 15 | 407.3151 | 0.6 | 1603 |
| 16 | 413.2663 | 3.4 | 13633 |
| 17 | 414.2696 | 0.9 | 3665 |
| 18 | 421.3294 | 0.8 | 3086 |
| 19 | 429.2408 | 0.6 | 2677 |
| 20 | 429.3199 | 0.7 | 2788 |
| 21 | 435.3444 | 0.5 | 2111 |
| 22 | 441.2691 | 0.9 | 3541 |
| 23 | 447.3449 | 2.6 | 10301 |
| 24 | 448.3490 | 0.7 | 2704 |
| 25 | 449.3512 | 0.9 | 3716 |
| 26 | 463.3169 | 0.5 | 1872 |
| 27 | 463.3759 | 0.5 | 2066 |
| 28 | 469.3268 | 0.7 | 2812 |
| 29 | 472.3448 | 0.6 | 3038 |
| 30 | 487.3611 | 0.5 | 1700 |
| 31 | 517.3720 | 0.8 | 3123 |
| 32 | 523.3249 | 0.6 | 2339 |
| 33 | 524.3277 | 0.6 | 2324 |
| 34 | 531.3863 | 0.6 | 2247 |
| 35 | 533.3456 | 0.6 | 2186 |
| 36 | 561.3970 | 1.0 | 3903 |
| 37 | 575.4131 | 0.6 | 2470 |
| 38 | 577.3722 | 0.8 | 3086 |
| 39 | 577.4806 | 0.9 | 1010 |
| 40 | 591.3877 | 0.5 | 2028 |
| 41 | 591.4595 | 0.5 | 2032 |
| 42 | 605.4225 | 0.9 | 3493 |
| 43 | 619.4332 | 0.6 | 2332 |
| 44 | 621.3962 | 0.8 | 3046 |
| 45 | 635.4130 | 0.5 | 1919 |
| 46 | 646.4511 | 0.8 | 3201 |
| 47 | 663.4638 | 0.8 | 3264 |
| 48 | 665.4242 | 0.6 | 3187 |
| 49 | 677.4659 | 0.5 | 1526 |
| 50 | 679.4382 | 0.7 | 2947 |
| 51 | 685.4359 | 1.4 | 5547 |
| 52 | 686.4395 | 0.7 | 2738 |
| 53 | 691.4094 | 0.6 | 2258 |
| 54 | 693.4728 | 0.7 | 2742 |
| 55 | 700.6277 | 1.0 | 4012 |
| 56 | 701.5998 | 0.6 | 1076 |
| 57 | 705.5267 | 0.6 | 2427 |
| 58 | 705.5831 | 16.9 | 66977 |
| 59 | 706.5681 | 0.4 | 33333 |
| 60 | 707.4889 | 0.6 | 2480 |
| 61 | 707.5870 | 2.4 | 9530 |
| 62 | 708.5869 | 0.7 | 2783 |

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**Acquisition Date:** 10.05.2019 12:54:56
| #  | m/z   | I [%] | I [a.u.] |
|----|-------|-------|----------|
| 63 | 709.4992 | 0.5 | 2013 |
| 64 | 719.5428 | 0.7 | 2975 |
| 65 | 721.5014 | 0.5 | 2021 |
| 66 | 721.5689 | 3.1 | 12162 |
| 67 | 722.5690 | 1.5 | 5763 |
| 68 | 723.5699 | 0.4 | 1758 |
| 69 | 723.5628 | 0.7 | 2797 |
| 70 | 729.2487 | 0.7 | 2759 |
| 71 | 733.5587 | 0.6 | 2417 |
| 72 | 737.5996 | 0.6 | 2429 |
| 73 | 747.5723 | 0.4 | 1771 |
| 74 | 751.5112 | 9.3 | 3694 |
| 75 | 751.5103 | 0.5 | 1919 |
| 76 | 752.2346 | 4.8 | 18762 |
| 77 | 753.2374 | 1.4 | 5681 |
| 78 | 767.2048 | 0.9 | 3697 |
| 79 | 768.2073 | 0.5 | 2160 |
| 80 | 769.2141 | 0.7 | 2622 |
| 81 | 790.2404 | 0.5 | 2028 |
| 82 | 791.1724 | 100.0 | 395546 |
| 83 | 791.5837 | 0.5 | 1889 |
| 84 | 792.1753 | 53.1 | 210033 |
| 85 | 793.1722 | 55.5 | 219700 |
| 86 | 794.1739 | 24.8 | 97946 |
| 87 | 795.1764 | 0.6 | 26029 |
| 88 | 796.2416 | 0.5 | 2004 |
| 89 | 796.1791 | 1.4 | 5482 |
| 90 | 1049.5577 | 0.8 | 3333 |
| 91 | 1050.5595 | 0.7 | 2703 |
| 92 | 1069.7020 | 1.0 | 3930 |
| 93 | 1070.7081 | 0.8 | 3092 |
| 94 | 1095.6582 | 0.7 | 2586 |
| 95 | 1096.6612 | 0.4 | 1772 |
| 96 | 1129.9375 | 0.5 | 2171 |
| 97 | 1338.1772 | 2.0 | 7907 |
| 98 | 1339.1815 | 1.8 | 6925 |
| 99 | 1390.1827 | 1.0 | 3967 |
| 100 | 1391.1852 | 0.5 | 1965 |

**Acquisition Parameter**

| General  | Fore Vacuum  | 2.86e+000 mBar | High Vacuum  | 1.02e-007 mBar | Source Type | ESI |
|----------|--------------|-----------------|--------------|-----------------|-------------|-----|
| Scan Begin | 75 m/z | Scan End | 2000 m/z | Ion Polarity | Positive |
| Source | Set Nebulizer | 0.4 Bar | Set Capillary | 3500 V | Set Dry Gas |
| Set Dry Heater | 100 °C | Set End Plate Offset | -500 V |
| Quadrupole Set Ion Energy (MS only) | 4.0 eV |
| Collision Cell | Collision Energy | 10.0 eV | Set Collision Cell RF | 1000.0 Vpp |
| Ion Cooler | Set Ion Cooler Transfer Time | 160.0 µs | Set Ion Cooler Pre Pulse Storage Time | 18.0 µs |
$^{1}$H, $^{13}$C, COSY-, NOESY-, HMQC-, HMBC-NMR (CD$_2$Cl$_2$, 500/126 MHz, 22 °C) and HR-ESI-MS spectra and full assignment of compound (1)

$^1$H NMR (500 MHz, CD$_2$Cl$_2$, 25 °C) δ
8.37 (d, $J = 8.9$ Hz, 4H),
7.84 (s, 4H),
7.28 (ddd, $J = 7.9, 5.7, 3.4$ Hz, 4H),
7.24 – 7.16 (m, 8H),
7.11 (d, $J = 7.8$ Hz, 3H),
7.03 (d, $J = 8.8$ Hz, 4H),
2.24 (ddd, $J = 14.4, 10.3, 4.7$ Hz, 4H),
2.11 – 2.01 (m, 4H),
1.54 – 1.44 (m, 4H),
1.16 (ddd, $J = 9.4, 6.6, 4.3$ Hz, 4H).

$^{13}$C NMR (126 MHz, CD$_2$Cl$_2$, 25 °C) δ
162.37, 151.43, 142.94, 141.12,
135.75, 131.55, 128.48, 127.41,
126.33, 124.91, 122.62, 112.12,
29.92, 29.16.
## Measured m/z vs. theoretical m/z

| Mass list | # | m/z    | l%  | l  |
|-----------|---|--------|-----|----|
| 1         | 1 | 282.2779| 3.0 | 489|
| 2         | 2 | 293.2442| 2.5 | 416|
| 3         | 3 | 299.1614| 4.1 | 602|
| 4         | 4 | 301.1367| 3.0 | 484|
| 5         | 5 | 304.2602| 3.8 | 823|
| 6         | 6 | 305.2051| 10.6| 1735|
| 7         | 7 | 310.2375| 15.6| 2540|
| 8         | 8 | 312.1847| 4.6 | 750|
| 9         | 9 | 315.1929| 100.0| 16305|
| 10        | 10| 316.1958| 16.9| 2762|
| 11        | 11| 320.1810| 3.2 | 526|
| 12        | 12| 321.2709| 4.4 | 722|
| 13        | 13| 325.2002| 2.4 | 390|
| 14        | 14| 331.1660| 5.7 | 929|
| 15        | 15| 331.1878| 33.9| 5518|
| 16        | 16| 331.2162| 2.3 | 371|
| 17        | 17| 332.1910| 6.6 | 1074|
| 18        | 18| 341.1613| 3.2 | 520|
| 19        | 19| 347.1833| 15.1| 2456|
| 20        | 20| 348.1890| 3.9 | 631|
| 21        | 21| 353.2684| 28.3| 4607|
| 22        | 22| 354.2659| 5.0 | 813|
| 23        | 23| 355.2152| 3.6 | 587|
| 24        | 24| 356.2106| 2.8 | 464|
| 25        | 25| 375.2145| 6.9 | 1103|
| 26        | 26| 381.2678| 23.2| 3758|
| 27        | 27| 382.2697| 5.0 | 822|
| 28        | 28| 413.2669| 2.7 | 430|
| 29        | 29| 419.2416| 13.4| 2182|
| 30        | 30| 420.2445| 4.9 | 795|
| 31        | 31| 427.2851| 2.2 | 382|
| 32        | 32| 445.3209| 2.9 | 471|
| 33        | 33| 467.3176| 27.9| 4952|
| 34        | 34| 468.3190| 7.9 | 1293|
| 35        | 35| 483.3108| 2.6 | 428|
| 36        | 36| 551.3660| 2.3 | 382|
| 37        | 37| 623.3079| 3.6 | 858|
| 38        | 38| 645.4000| 5.5 | 896|
| 39        | 39| 645.4725| 4.9 | 799|
| 40        | 40| 645.4730| 2.4 | 391|
| 41        | 41| 647.4553| 2.3 | 378|
| 42        | 42| 663.4545| 20.2| 3296|
| 43        | 43| 664.4603| 6.3 | 1020|
| 44        | 44| 673.5031| 3.0 | 497|
| 45        | 45| 674.4981| 2.5 | 404|
| 46        | 46| 679.4167| 7.8 | 1284|
| 47        | 47| 680.4218| 3.3 | 541|
| 48        | 48| 680.4807| 16.8| 2740|
| 49        | 49| 681.4847| 8.7 | 1420|
| 50        | 50| 682.4866| 2.3 | 382|
| 51        | 51| 683.5414| 3.3 | 546|
| 52        | 52| 685.4343| 19.0| 3104|
| 53        | 53| 686.4835| 7.8 | 1296|
| 54        | 54| 687.4360| 3.0 | 497|
| 55        | 55| 699.4990| 3.4 | 557|
| 56        | 56| 751.4683| 2.8 | 482|
| 57        | 57| 705.5511| 3.7 | 606|
| 58        | 58| 706.5668| 2.5 | 400|
| 59        | 59| 711.5730| 4.0 | 640|
| 60        | 60| 712.5755| 2.7 | 444|
| 61        | 61| 733.6013| 3.5 | 564|
| 62        | 62| 745.5031| 2.4 | 396|

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| #  | m/z  | I % | I   |
|----|------|-----|-----|
| 63 | 764.5721 | 3.1 | 508 |
| 64 | 647.5663 | 2.2 | 362 |
| 65 | 697.5478 | 7.3 | 1196 |
| 66 | 866.5410 | 5.2 | 841 |
| 67 | 995.5653 | 68.1 | 11108 |
| 68 | 602.5665 | 30.7 | 6307 |
| 69 | 901.5660 | 36.7 | 5684 |
| 70 | 922.5675 | 18.5 | 3014 |
| 71 | 953.5718 | 5.1 | 830 |
| 72 | 639.5683 | 2.6 | 422 |
| 73 | 944.7277 | 3.7 | 600 |
| 74 | 951.7299 | 2.6 | 417 |
| 75 | 958.7353 | 3.2 | 517 |
| 76 | 967.7112 | 2.4 | 308 |
| 77 | 972.8618 | 3.0 | 488 |
| 78 | 977.6410 | 20.2 | 3290 |
| 79 | 978.6423 | 11.1 | 1903 |
| 80 | 979.6429 | 4.6 | 738 |
| 81 | 993.6344 | 5.6 | 941 |
| 82 | 994.6399 | 3.5 | 564 |
| 83 | 1015.7156 | 6.5 | 1062 |
| 84 | 1016.7143 | 4.0 | 657 |
| 85 | 1045.7435 | 5.1 | 826 |
| 86 | 1044.7455 | 5.3 | 857 |
| 87 | 1129.7621 | 9.7 | 1574 |
| 88 | 1130.7632 | 7.7 | 1250 |
| 89 | 1131.7732 | 3.4 | 582 |
| 90 | 1325.9913 | 4.6 | 753 |
| 91 | 1326.9963 | 3.3 | 543 |
| 92 | 1342.9348 | 7.6 | 1241 |
| 93 | 1343.9264 | 5.1 | 838 |
| 94 | 1344.9284 | 3.6 | 566 |
| 95 | 1347.9418 | 2.4 | 362 |
| 96 | 1348.9412 | 14.6 | 2420 |
| 97 | 1349.9419 | 7.4 | 1200 |
| 98 | 1350.9415 | 3.9 | 634 |
| 99 | 1356.0272 | 2.3 | 379 |

### Acquisition Parameter

| Feature                  | Value                  |
|--------------------------|------------------------|
| Fore Vacuum              | 2.68e+000 mBar         |
| Scan Begin               | 75 m/z                 |
| Set Neulitser            | 0.4 Bar                |
| Set Dry Heater           | 180 °C                 |
| Ion Energy (MS only)     | 4.0 eV                 |
| Collision Energy         | 8.0 eV                 |
| Set Ion Cooler Transfer Time | 80.0 µs               |
| Set Collision Cell RF    | 500.0 Vpp              |
| Set Ion Cooler Pre Pulse Storage Time | 18.0 µs               |
Computational investigations

Figure SI1: DFT-optimized structure (left) and calculated frontier orbitals HOMO (middle) and LUMO (right) of reference complex 15.

Figure SI2: Space-filling representations of the optimized excited state geometries of the macrocyclic complex 1 (left) and the reference complex 15 (right).
Crystal data for 11

Single crystals were grown by vapor diffusion technique using dichloromethane as solvent and diethyl ether as anti-solvent. Solid state structure in the manuscript are displayed with rotation ellipsoids at 50% probability. Hydrogen atoms, solvent molecules and the PF$_6$ counter ions were omitted for clarity. Color code: N: blue, Cu: yellow, C: gray for one and purple for the other ligand for clarity.

Formula C$_{56}$H$_{32}$Cu$_1$F$_6$N$_4$P$_1$, M = 969.40, F(000) = 988, brown block, size 0.23 x 0.28 x 0.31 mm$^3$, triclinic, space group P -1 , Z = 2, a = 8.8141(10) Å, b = 14.6956(16) Å, c = 16.8143(19) Å, α = 95.110(3)°, β = 95.863(3)°, γ = 90.880(3)°, V = 2157.3(4) Å$^3$, D$_{calc}$ = 1.492 Mg*m$^{-3}$. The crystal was measured on a Bruker Kappa Apex2 diffractometer at 130(2)K using graphite-monochromated Cu K$_\alpha$-radiation with $\lambda$ = 1.54178 Å, $\Theta_{max}$ = 70.376°. Minimal/maximal transmission 0.91/1.00, $\mu$ = 1.677 mm$^{-1}$. The Apex2 suite has been used for data collection and integration. From a total of 21167 reflections, 7807 were independent (merging $r$ = 0.041). From these, 7806 were considered as observed (I>2.0σ(I)) and were used to refine 613 parameters. The structure was solved by other methods using the program Superflip. Least-squares refinement against Fsqd was carried out on all non-hydrogen atoms using the program CRYSTALS. R = 0.0371 (observed data), wR = 0.0910 (all data), GOF = 0.9995. Minimal/maximal residual electron density = -0.28/0.38 e Å$^{-3}$. Chebychev polynomial weights were used to complete the refinement. Plots were produced using CAMERON. Crystallographic data (excluding structure factors) for the structure in this paper have been deposited with the Cambridge Crystallographic Data Center, the deposition number is (1948428). Copies of the data can be obtained, free of charge, on application to the CCDC, 12 Union Road, Cambridge CB2 1EZ, UK [fax: +44-1223-336033 or e-mail: deposit@ccdc.cam.ac.uk].
Photostability investigations

A very similar strategy as in our recent investigation on acridinium dyes was used to compare the photostabilities of 1 and 15.[1]

We irradiated diluted and deoxygenated solutions of both complexes, and monitored their UV-Vis spectra over two hours of photoirradiation. The cuvettes were irradiated in the sample chamber of the spectrophotometer (see Figure SI4) with a 455 nm LED from Thorlabs (M455L3-C1, 500 mW optical output). Our cuvette holder permits LED irradiation of the whole detection volume. For recording the absorption spectra after the desired irradiation times, the LED was blocked for 2 minutes.

The absorptions of both irradiated solutions at the LED peak wavelength (455 nm) were standardized to 0.10, which ensures that almost the same amount of light is absorbed while sample heating is avoided. Concentrations of ~36 μM for 1 and ~211 μM for 15 were required for these standardized conditions.

The UV-Vis data displayed in figure 6 of the main paper show good photostability for 1 under our test conditions. A significant decrease of the MLCT absorption band is expected to occur upon photodecomposition, but all spectra are virtually identical; the maximum relative absorption variation is with less than 0.5% within the accuracy of the analysis.

The situation is completely different for 15. Our photostability assay revealed a constant decrease of the MLCT band, which amounts to 7% after 2 hours of photoirradiation (compare, lower part of figure 6a and figure 6b). Assuming that the decomposition products do not absorb at the detection wavelength allows us to set a lower limit for the concentration change caused by photodecomposition: 14.8 μM (211 μM x 0.07). To be able to make a relative stability statement, we assume a maximum absolute concentration change for 1 under identical irradiation conditions of 0.4 μM, corresponding to an experimental error of up to 1% hiding the alteration of the observed MLCT band (36 μM x 0.01). Taking the widely differing starting concentration of both complexes into account[2] the actual photodecomposition of 15 is thus significantly faster (compared to that of 1) than the absorption spectra in figure 6 suggest. Hence, the analysis presented in this section revealed the photodegradation of 1 (macrocycle) to be slower than that of 15 by a factor of at least ~37.

In order to identify the photodecomposition product, we irradiated complex 15 in an NMR tube. The peaks in acetonitrile-d₃ are rather broad, which is the reason why we performed this experiment in deuterated dichloromethane. In the NMR spectrum recorded after irradiation with a blue high-power LED at 440 nm (from Kessil), which was very recently purchased and has a much higher output than the 455 nm LED used for the investigations presented in figure 3 of the main paper, we observed noticeable photodecomposition after 3h of irradiation, but we could not detect the release of the free ligand (Figure SI3). The photodecomposition products could not be identified.

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1 C. Fischer, C. Kerzig, B. Zilate, O. S. Wenger, C. Sparr, ACS Catal. 2019, DOI 10.1021/acscatal.9b03606.
2 C. Kerzig, X. Guo, O. S. Wenger, J. Am. Chem. Soc., 2019, 141, 2122-2127.
Figure SI3: NMR investigations of the photodecomposition of the reference complex 15 upon irradiation with an LED at 440 nm. The NMR spectra in deuterated dichloromethane of the free ligand (top), the complex (middle) and the decomposition product after irradiation for 3 hours (bottom) are illustrated. It can be seen that the decomposition product is not the free ligand.
Figure S14: Instrumental setup for the photostability investigations.

Table S1: UV-Vis data of complex 1 after 0, 60 and 120 minutes photoirradiation.

| Wavelength [nm] | Absorption before irradiation | Absorption after 60 min irradiation | Absorption after 120 min irradiation |
|-----------------|-------------------------------|-------------------------------------|---------------------------------------|
| 750             | 6.33E-04                      | 5.59E-04                            | 6.62E-04                              |
| 749             | 6.76E-04                      | 5.29E-04                            | 6.31E-04                              |
| 748             | 7.24E-04                      | 6.53E-04                            | 7.36E-04                              |
| 747             | 5.84E-04                      | 5.49E-04                            | 6.76E-04                              |
| 746             | 6.35E-04                      | 6.58E-04                            | 7.66E-04                              |
| 745             | 7.26E-04                      | 7.03E-04                            | 6.47E-04                              |
| 744             | 5.78E-04                      | 6.04E-04                            | 6.13E-04                              |
| 743             | 6.72E-04                      | 6.15E-04                            | 7.78E-04                              |
| 742             | 6.47E-04                      | 5.66E-04                            | 7.55E-04                              |
| 741             | 6.68E-04                      | 5.83E-04                            | 6.42E-04                              |
| 740             | 6.54E-04                      | 6.20E-04                            | 6.64E-04                              |
| 739             | 6.58E-04                      | 6.30E-04                            | 6.84E-04                              |
| 738             | 7.14E-04                      | 7.67E-04                            | 7.11E-04                              |
| 737             | 5.85E-04                      | 7.25E-04                            | 6.35E-04                              |
| 736             | 6.58E-04                      | 6.54E-04                            | 6.13E-04                              |
| 735             | 5.59E-04                      | 5.11E-04                            | 5.92E-04                              |
|    |       |       |       |
|----|-------|-------|-------|
| 734| 6.16E-04 | 6.23E-04 | 6.62E-04 |
| 733| 6.20E-04 | 6.77E-04 | 6.65E-04 |
| 732| 5.75E-04 | 6.27E-04 | 6.60E-04 |
| 731| 6.79E-04 | 6.74E-04 | 6.88E-04 |
| 730| 6.21E-04 | 4.94E-04 | 5.71E-04 |
| 729| 5.85E-04 | 7.07E-04 | 7.45E-04 |
| 728| 5.72E-04 | 5.99E-04 | 6.07E-04 |
| 727| 7.09E-04 | 6.27E-04 | 6.59E-04 |
| 726| 5.00E-04 | 5.13E-04 | 5.03E-04 |
| 725| 5.82E-04 | 5.72E-04 | 5.82E-04 |
| 724| 5.93E-04 | 5.45E-04 | 4.75E-04 |
| 723| 6.36E-04 | 5.57E-04 | 5.31E-04 |
| 722| 6.61E-04 | 5.26E-04 | 5.59E-04 |
| 721| 6.27E-04 | 5.44E-04 | 4.87E-04 |
| 720| 5.71E-04 | 4.99E-04 | 4.84E-04 |
| 719| 4.90E-04 | 5.00E-04 | 4.97E-04 |
| 718| 5.25E-04 | 5.28E-04 | 5.37E-04 |
| 717| 5.53E-04 | 5.02E-04 | 4.14E-04 |
| 716| 4.85E-04 | 4.86E-04 | 5.26E-04 |
| 715| 5.62E-04 | 5.41E-04 | 4.40E-04 |
| 714| 5.30E-04 | 5.43E-04 | 4.96E-04 |
| 713| 5.70E-04 | 4.52E-04 | 4.62E-04 |
| 712| 4.49E-04 | 4.78E-04 | 4.05E-04 |
| 711| 5.06E-04 | 3.82E-04 | 4.28E-04 |
| 710| 4.61E-04 | 4.62E-04 | 4.56E-04 |
| 709| 4.46E-04 | 3.90E-04 | 3.67E-04 |
| 708| 5.10E-04 | 4.04E-04 | 3.89E-04 |
| 707| 4.37E-04 | 4.50E-04 | 3.47E-04 |
| 706| 4.35E-04 | 4.40E-04 | 3.42E-04 |
| 705| 4.12E-04 | 3.92E-04 | 3.50E-04 |
| 704| 4.70E-04 | 4.08E-04 | 3.78E-04 |
| 703| 4.24E-04 | 3.42E-04 | 4.04E-04 |
| 702| 4.98E-04 | 3.99E-04 | 3.85E-04 |
| 701| 4.35E-04 | 4.06E-04 | 3.89E-04 |
| 700| 3.83E-04 | 3.67E-04 | 2.96E-04 |
| 699| 4.24E-04 | 4.11E-04 | 3.34E-04 |
| 698| 4.03E-04 | 4.28E-04 | 4.14E-04 |
| 697| 4.31E-04 | 3.85E-04 | 3.86E-04 |
| 696| 4.35E-04 | 3.79E-04 | 3.14E-04 |
| 695| 3.22E-04 | 3.25E-04 | 3.14E-04 |
| 694| 3.78E-04 | 3.81E-04 | 3.02E-04 |
| 693| 3.71E-04 | 3.53E-04 | 3.03E-04 |
| 692| 4.12E-04 | 3.88E-04 | 3.37E-04 |
| 691| 3.78E-04 | 3.49E-04 | 3.32E-04 |
| 690| 4.33E-04 | 3.58E-04 | 3.90E-04 |
| 689| 3.91E-04 | 3.64E-04 | 3.64E-04 |
| 688| 3.27E-04 | 3.74E-04 | 3.08E-04 |
|   |     |     |     |
|---|-----|-----|-----|
| 687| 3.62E-04 | 3.11E-04 | 2.97E-04 |
| 686| 4.00E-04 | 3.42E-04 | 3.43E-04 |
| 685| 3.78E-04 | 3.11E-04 | 2.89E-04 |
| 684| 3.96E-04 | 3.10E-04 | 2.89E-04 |
| 683| 3.40E-04 | 3.45E-04 | 3.09E-04 |
| 682| 3.55E-04 | 2.87E-04 | 3.23E-04 |
| 681| 3.54E-04 | 3.30E-04 | 3.06E-04 |
| 680| 3.18E-04 | 2.88E-04 | 2.42E-04 |
| 679| 3.85E-04 | 3.47E-04 | 2.81E-04 |
| 678| 4.30E-04 | 3.26E-04 | 2.74E-04 |
| 677| 4.16E-04 | 2.76E-04 | 2.69E-04 |
| 676| 3.68E-04 | 3.22E-04 | 2.63E-04 |
| 675| 2.79E-04 | 2.84E-04 | 2.51E-04 |
| 674| 3.45E-04 | 3.22E-04 | 2.59E-04 |
| 673| 3.84E-04 | 3.50E-04 | 3.25E-04 |
| 672| 3.81E-04 | 3.24E-04 | 3.10E-04 |
| 671| 3.84E-04 | 3.24E-04 | 3.21E-04 |
| 670| 3.28E-04 | 3.11E-04 | 2.60E-04 |
| 669| 3.73E-04 | 3.64E-04 | 2.78E-04 |
| 668| 3.48E-04 | 3.35E-04 | 2.73E-04 |
| 667| 3.87E-04 | 3.44E-04 | 2.95E-04 |
| 666| 3.19E-04 | 2.96E-04 | 3.39E-04 |
| 665| 3.48E-04 | 3.42E-04 | 2.64E-04 |
| 664| 3.57E-04 | 3.42E-04 | 3.34E-04 |
| 663| 3.25E-04 | 2.79E-04 | 2.71E-04 |
| 662| 4.09E-04 | 3.56E-04 | 3.38E-04 |
| 661| 4.85E-04 | 4.87E-04 | 4.75E-04 |
| 660| 3.23E-04 | 3.63E-04 | 2.90E-04 |
| 659| 3.23E-04 | 2.45E-04 | 2.10E-04 |
| 658| 4.07E-04 | 4.08E-04 | 3.51E-04 |
| 657| 4.85E-04 | 4.37E-04 | 3.81E-04 |
| 656| 3.51E-04 | 3.00E-04 | 2.53E-04 |
| 655| 2.99E-04 | 2.76E-04 | 2.86E-04 |
| 654| 3.95E-04 | 3.67E-04 | 3.32E-04 |
| 653| 4.16E-04 | 3.94E-04 | 3.49E-04 |
| 652| 3.84E-04 | 3.32E-04 | 3.11E-04 |
| 651| 4.17E-04 | 3.95E-04 | 3.71E-04 |
| 650| 3.92E-04 | 3.86E-04 | 3.64E-04 |
| 649| 4.28E-04 | 3.86E-04 | 3.60E-04 |
| 648| 4.42E-04 | 3.57E-04 | 3.54E-04 |
| 647| 4.29E-04 | 3.82E-04 | 3.53E-04 |
| 646| 4.43E-04 | 3.75E-04 | 3.82E-04 |
| 645| 4.38E-04 | 3.58E-04 | 3.43E-04 |
| 644| 4.70E-04 | 4.55E-04 | 3.95E-04 |
| 643| 4.81E-04 | 4.40E-04 | 4.24E-04 |
| 642| 4.72E-04 | 4.47E-04 | 4.13E-04 |
| 641| 5.33E-04 | 4.85E-04 | 4.56E-04 |
|     |        |        |        |
|-----|--------|--------|--------|
| 640 | 5.23E-04 | 4.66E-04 | 4.76E-04 |
| 639 | 5.35E-04 | 4.80E-04 | 4.79E-04 |
| 638 | 5.45E-04 | 5.10E-04 | 4.59E-04 |
| 637 | 6.02E-04 | 5.40E-04 | 5.24E-04 |
| 636 | 5.97E-04 | 5.29E-04 | 5.28E-04 |
| 635 | 6.67E-04 | 5.84E-04 | 6.26E-04 |
| 634 | 6.37E-04 | 5.89E-04 | 5.98E-04 |
| 633 | 6.50E-04 | 6.13E-04 | 5.73E-04 |
| 632 | 6.92E-04 | 6.81E-04 | 6.49E-04 |
| 631 | 6.87E-04 | 6.49E-04 | 6.36E-04 |
| 630 | 7.36E-04 | 7.43E-04 | 7.14E-04 |
| 629 | 7.87E-04 | 7.31E-04 | 7.35E-04 |
| 628 | 8.85E-04 | 7.98E-04 | 7.99E-04 |
| 627 | 8.88E-04 | 8.73E-04 | 8.22E-04 |
| 626 | 8.81E-04 | 8.24E-04 | 8.17E-04 |
| 625 | 9.12E-04 | 8.83E-04 | 8.60E-04 |
| 624 | 9.66E-04 | 9.25E-04 | 8.84E-04 |
| 623 | 0.00103  | 0.00101  | 9.63E-04 |
| 622 | 0.00106  | 0.00103  | 0.00105  |
| 621 | 0.00111  | 0.00107  | 0.00106  |
| 620 | 0.00115  | 0.00111  | 0.00108  |
| 619 | 0.00123  | 0.00119  | 0.00119  |
| 618 | 0.00131  | 0.00125  | 0.00122  |
| 617 | 0.00142  | 0.00133  | 0.00129  |
| 616 | 0.00157  | 0.0014  | 0.00143  |
| 615 | 0.00159  | 0.00147  | 0.00148  |
| 614 | 0.0016  | 0.00149  | 0.0015  |
| 613 | 0.00163  | 0.00155  | 0.00149  |
| 612 | 0.00175  | 0.00167  | 0.00169  |
| 611 | 0.0019  | 0.00179  | 0.00176  |
| 610 | 0.00197  | 0.00187  | 0.00188  |
| 609 | 0.0021  | 0.00191  | 0.00188  |
| 608 | 0.0021  | 0.00204  | 0.00201  |
| 607 | 0.00216  | 0.00214  | 0.00212  |
| 606 | 0.00227  | 0.00224  | 0.00221  |
| 605 | 0.00236  | 0.00232  | 0.00231  |
| 604 | 0.00249  | 0.00246  | 0.00245  |
| 603 | 0.00263  | 0.00253  | 0.00258  |
| 602 | 0.00274  | 0.00265  | 0.00267  |
| 601 | 0.00282  | 0.00283  | 0.00277  |
| 600 | 0.00294  | 0.00289  | 0.00287  |
| 599 | 0.0031  | 0.00299  | 0.00305  |
| 598 | 0.00326  | 0.00322  | 0.00323  |
| 597 | 0.0034  | 0.00337  | 0.00337  |
| 596 | 0.00349  | 0.00342  | 0.00344  |
| 595 | 0.00366  | 0.00359  | 0.00364  |
| 594 | 0.00382  | 0.00376  | 0.0038  |
| 593 | 0.00399 | 0.00397 | 0.00396 |
| 592 | 0.00414 | 0.00408 | 0.00407 |
| 591 | 0.00432 | 0.00424 | 0.00427 |
| 590 | 0.00449 | 0.00446 | 0.00447 |
| 589 | 0.00465 | 0.00462 | 0.00466 |
| 588 | 0.00486 | 0.00482 | 0.00481 |
| 587 | 0.00506 | 0.00501 | 0.00503 |
| 586 | 0.00528 | 0.00519 | 0.0052 |
| 585 | 0.00543 | 0.00535 | 0.0054 |
| 584 | 0.00567 | 0.00558 | 0.00565 |
| 583 | 0.00592 | 0.00582 | 0.00586 |
| 582 | 0.00604 | 0.00604 | 0.00605 |
| 581 | 0.00627 | 0.00628 | 0.00622 |
| 580 | 0.00656 | 0.00651 | 0.00651 |
| 579 | 0.00668 | 0.00674 | 0.00678 |
| 578 | 0.00701 | 0.00695 | 0.00706 |
| 577 | 0.00729 | 0.0072 | 0.00728 |
| 576 | 0.00756 | 0.0075 | 0.00756 |
| 575 | 0.00778 | 0.00775 | 0.00777 |
| 574 | 0.00811 | 0.00803 | 0.00813 |
| 573 | 0.00835 | 0.00829 | 0.00837 |
| 572 | 0.00867 | 0.00853 | 0.00863 |
| 571 | 0.00886 | 0.00878 | 0.00886 |
| 570 | 0.0091 | 0.00907 | 0.00914 |
| 569 | 0.00943 | 0.00939 | 0.00945 |
| 568 | 0.00975 | 0.00969 | 0.00977 |
| 567 | 0.01008 | 0.01002 | 0.01008 |
| 566 | 0.01042 | 0.01028 | 0.01037 |
| 565 | 0.01063 | 0.01062 | 0.01072 |
| 564 | 0.01101 | 0.01094 | 0.011 |
| 563 | 0.01129 | 0.01121 | 0.01134 |
| 562 | 0.01168 | 0.01164 | 0.01175 |
| 561 | 0.01201 | 0.01193 | 0.01202 |
| 560 | 0.01233 | 0.01227 | 0.01234 |
| 559 | 0.01267 | 0.01258 | 0.01271 |
| 558 | 0.01298 | 0.01286 | 0.01302 |
| 557 | 0.01337 | 0.01331 | 0.01342 |
| 556 | 0.01364 | 0.01361 | 0.01373 |
| 555 | 0.01405 | 0.01397 | 0.01408 |
| 554 | 0.01444 | 0.01432 | 0.01441 |
| 553 | 0.01479 | 0.0147 | 0.01485 |
| 552 | 0.01512 | 0.01498 | 0.01519 |
| 551 | 0.01544 | 0.01537 | 0.01552 |
| 550 | 0.01583 | 0.01579 | 0.01595 |
| 549 | 0.01616 | 0.01606 | 0.01624 |
| 548 | 0.01651 | 0.01646 | 0.01662 |
| 547 | 0.01693 | 0.01683 | 0.01697 |
| 546 | 0.01727 | 0.01712 | 0.0173  |
|-----|---------|---------|---------|
| 545 | 0.01772 | 0.01761 | 0.01781 |
| 544 | 0.01802 | 0.01795 | 0.01814 |
| 543 | 0.01838 | 0.01829 | 0.0184  |
| 542 | 0.01879 | 0.01876 | 0.0189  |
| 541 | 0.01918 | 0.01912 | 0.01933 |
| 540 | 0.01952 | 0.01941 | 0.01959 |
| 539 | 0.01987 | 0.0198  | 0.02002 |
| 538 | 0.02026 | 0.02023 | 0.02042 |
| 537 | 0.0207  | 0.02062 | 0.02079 |
| 536 | 0.02107 | 0.02099 | 0.02117 |
| 535 | 0.02143 | 0.02133 | 0.0215  |
| 534 | 0.02186 | 0.02172 | 0.02195 |
| 533 | 0.02223 | 0.0221  | 0.02234 |
| 532 | 0.02255 | 0.02253 | 0.02275 |
| 531 | 0.02299 | 0.02289 | 0.02316 |
| 530 | 0.02342 | 0.02328 | 0.02352 |
| 529 | 0.02376 | 0.02369 | 0.02395 |
| 528 | 0.02425 | 0.02412 | 0.02437 |
| 527 | 0.02469 | 0.02448 | 0.02481 |
| 526 | 0.02504 | 0.02496 | 0.02518 |
| 525 | 0.02553 | 0.02536 | 0.02562 |
| 524 | 0.02591 | 0.02586 | 0.02613 |
| 523 | 0.02637 | 0.0263  | 0.02656 |
| 522 | 0.02684 | 0.02678 | 0.02703 |
| 521 | 0.02729 | 0.0272  | 0.02747 |
| 520 | 0.0278  | 0.02769 | 0.02802 |
| 519 | 0.02831 | 0.0282  | 0.02854 |
| 518 | 0.02885 | 0.02875 | 0.02905 |
| 517 | 0.02935 | 0.02936 | 0.02965 |
| 516 | 0.02999 | 0.02982 | 0.03019 |
| 515 | 0.03052 | 0.03038 | 0.03074 |
| 514 | 0.03116 | 0.03105 | 0.0314  |
| 513 | 0.0318  | 0.03168 | 0.03207 |
| 512 | 0.0325  | 0.03239 | 0.03275 |
| 511 | 0.03322 | 0.03311 | 0.03351 |
| 510 | 0.03404 | 0.0339  | 0.03428 |
| 509 | 0.03476 | 0.03463 | 0.03505 |
| 508 | 0.03559 | 0.03549 | 0.03588 |
| 507 | 0.03647 | 0.03641 | 0.03682 |
| 506 | 0.03744 | 0.03735 | 0.03774 |
| 505 | 0.03851 | 0.03838 | 0.03882 |
| 504 | 0.03953 | 0.03943 | 0.03983 |
| 503 | 0.04062 | 0.04048 | 0.04097 |
| 502 | 0.04181 | 0.04169 | 0.04217 |
| 501 | 0.04301 | 0.0429  | 0.04336 |
| 500 | 0.04432 | 0.04422 | 0.04474 |
|   |   |   |   |
|---|---|---|---|
|499| 0.04568 | 0.04555 | 0.04608 |
|498| 0.04715 | 0.04701 | 0.0475  |
|497| 0.04867 | 0.04845 | 0.04906 |
|496| 0.05009 | 0.04991 | 0.05055 |
|495| 0.0517  | 0.05152 | 0.05215 |
|494| 0.05334 | 0.0532  | 0.05384 |
|493| 0.05503 | 0.0549  | 0.0555  |
|492| 0.05675 | 0.05662 | 0.05723 |
|491| 0.05848 | 0.05831 | 0.05894 |
|490| 0.06024 | 0.06007 | 0.06077 |
|489| 0.06201 | 0.06182 | 0.06255 |
|488| 0.06383 | 0.06361 | 0.06438 |
|487| 0.06562 | 0.06547 | 0.06618 |
|486| 0.06738 | 0.06723 | 0.06794 |
|485| 0.06912 | 0.069    | 0.06973 |
|484| 0.07088 | 0.07065 | 0.07142 |
|483| 0.07259 | 0.07234 | 0.07319 |
|482| 0.07416 | 0.07395 | 0.07477 |
|481| 0.0758  | 0.0756  | 0.07639 |
|480| 0.07741 | 0.07717 | 0.07801 |
|479| 0.07895 | 0.07865 | 0.07951 |
|478| 0.08029 | 0.08003 | 0.08092 |
|477| 0.08165 | 0.08142 | 0.08232 |
|476| 0.08291 | 0.08266 | 0.08364 |
|475| 0.08419 | 0.08394 | 0.08487 |
|474| 0.0853  | 0.08512 | 0.086   |
|473| 0.08642 | 0.08617 | 0.08708 |
|472| 0.08746 | 0.08715 | 0.08808 |
|471| 0.08843 | 0.0881  | 0.08902 |
|470| 0.08931 | 0.08905 | 0.08995 |
|469| 0.09014 | 0.08987 | 0.09083 |
|468| 0.09096 | 0.09068 | 0.09165 |
|467| 0.09167 | 0.09137 | 0.09229 |
|466| 0.09227 | 0.09199 | 0.09299 |
|465| 0.09291 | 0.0926  | 0.09358 |
|464| 0.09346 | 0.09316 | 0.09415 |
|463| 0.09396 | 0.09374 | 0.09469 |
|462| 0.09447 | 0.09422 | 0.0952  |
|461| 0.09493 | 0.09465 | 0.09563 |
|460| 0.09532 | 0.09502 | 0.09595 |
|459| 0.09564 | 0.09533 | 0.09634 |
|458| 0.09596 | 0.09566 | 0.09666 |
|457| 0.09619 | 0.09591 | 0.09695 |
|456| 0.09639 | 0.09618 | 0.09719 |
|455| 0.09665 | 0.09634 | 0.09724 |
|454| 0.09671 | 0.09644 | 0.09736 |
|453| 0.09685 | 0.09655 | 0.09754 |
|   |        |        |        |
|---|--------|--------|--------|
| 452| 0.09687| 0.09656| 0.09761|
| 451| 0.09684| 0.09652| 0.09755|
| 450| 0.09682| 0.09653| 0.09745|
| 449| 0.09669| 0.09644| 0.09736|
| 448| 0.0965  | 0.0962  | 0.09724|
| 447| 0.0963  | 0.09591 | 0.09685|
| 446| 0.09594 | 0.09561 | 0.09658|
| 445| 0.09562 | 0.09536 | 0.09637|
| 444| 0.0953  | 0.09503 | 0.09602|
| 443| 0.09481 | 0.09454 | 0.09549|
| 442| 0.09437 | 0.09408 | 0.09499|
| 441| 0.09381 | 0.09351 | 0.09447|
| 440| 0.09327 | 0.09299 | 0.09391|
| 439| 0.09265 | 0.09235 | 0.0933 |
| 438| 0.09203 | 0.09172 | 0.09261|
| 437| 0.09136 | 0.09108 | 0.09198|
| 436| 0.09056 | 0.09029 | 0.0912 |
| 435| 0.08984 | 0.08954 | 0.0904 |
| 434| 0.08903 | 0.08877 | 0.08965|
| 433| 0.08828 | 0.08795 | 0.08887|
| 432| 0.08743 | 0.08718 | 0.08806|
| 431| 0.08661 | 0.08635 | 0.08719|
| 430| 0.08576 | 0.08555 | 0.08635|
| 429| 0.08498 | 0.0847  | 0.08551|
| 428| 0.08414 | 0.08385 | 0.08473|
| 427| 0.08323 | 0.08292 | 0.08381|
| 426| 0.08236 | 0.08213 | 0.08292|
| 425| 0.08153 | 0.08126 | 0.08209|
| 424| 0.08073 | 0.08048 | 0.08126|
| 423| 0.07987 | 0.07958 | 0.08035|
| 422| 0.07896 | 0.07866 | 0.07948|
| 421| 0.07813 | 0.07785 | 0.07867|
| 420| 0.07727 | 0.07701 | 0.07778|
| 419| 0.07642 | 0.07615 | 0.07695|
| 418| 0.07554 | 0.07533 | 0.07599|
| 417| 0.07473 | 0.07449 | 0.07517|
| 416| 0.07379 | 0.07355 | 0.0743 |
| 415| 0.07304 | 0.07276 | 0.07351|
| 414| 0.07217 | 0.07195 | 0.0727 |
| 413| 0.07145 | 0.07117 | 0.0719 |
| 412| 0.07056 | 0.07038 | 0.0711 |
| 411| 0.06991 | 0.06966 | 0.07029|
| 410| 0.06912 | 0.06886 | 0.0696 |
| 409| 0.06839 | 0.06813 | 0.06885|
| 408| 0.06776 | 0.0675  | 0.06816|
| 407| 0.06712 | 0.06687 | 0.0675 |
| 406| 0.06654 | 0.06629 | 0.06693|
| x  | y1   | y2   | y3   |
|----|------|------|------|
| 359 | 0.08226 | 0.08144 | 0.08175 |
| 360 | 0.08122 | 0.08037 | 0.0807 |
| 361 | 0.08031 | 0.07956 | 0.07988 |
| 362 | 0.07941 | 0.07876 | 0.07893 |
| 363 | 0.0787 | 0.07811 | 0.07837 |
| 364 | 0.07781 | 0.07737 | 0.0777 |
| 365 | 0.07718 | 0.07645 | 0.07697 |
| 366 | 0.07651 | 0.07589 | 0.07621 |
| 367 | 0.07586 | 0.07524 | 0.07555 |
| 368 | 0.07498 | 0.07428 | 0.07474 |
| 369 | 0.07396 | 0.07346 | 0.07383 |
| 370 | 0.07302 | 0.07257 | 0.07298 |
| 371 | 0.07195 | 0.07148 | 0.07195 |
| 372 | 0.07102 | 0.07042 | 0.07093 |
| 373 | 0.07002 | 0.06948 | 0.06997 |
| 374 | 0.06911 | 0.06866 | 0.06911 |
| 375 | 0.06813 | 0.06785 | 0.06829 |
| 376 | 0.06724 | 0.06687 | 0.06744 |
| 377 | 0.06641 | 0.06611 | 0.06666 |
| 378 | 0.06564 | 0.06529 | 0.06586 |
| 379 | 0.06498 | 0.06467 | 0.06512 |
| 380 | 0.06441 | 0.06415 | 0.06458 |
| 381 | 0.0638 | 0.06359 | 0.06413 |
| 382 | 0.06331 | 0.06308 | 0.06358 |
| 383 | 0.06291 | 0.06263 | 0.06318 |
| 384 | 0.06247 | 0.06216 | 0.06271 |
| 385 | 0.0622 | 0.06189 | 0.06238 |
| 386 | 0.06196 | 0.06166 | 0.06223 |
| 387 | 0.0619 | 0.06159 | 0.06214 |
| 388 | 0.06158 | 0.0614 | 0.06194 |
| 389 | 0.06152 | 0.06128 | 0.06187 |
| 390 | 0.06152 | 0.06125 | 0.06182 |
| 391 | 0.06151 | 0.0612 | 0.06175 |
| 392 | 0.06156 | 0.06132 | 0.06192 |
| 393 | 0.06174 | 0.0615 | 0.06206 |
| 394 | 0.06181 | 0.06161 | 0.06216 |
| 395 | 0.06204 | 0.06177 | 0.06237 |
| 396 | 0.06221 | 0.06195 | 0.06261 |
| 397 | 0.06242 | 0.0622 | 0.06276 |
| 398 | 0.06281 | 0.06259 | 0.0632 |
| 399 | 0.06316 | 0.06291 | 0.06348 |
| 400 | 0.06347 | 0.06331 | 0.06387 |
| 401 | 0.06394 | 0.06366 | 0.0643 |
| 402 | 0.06436 | 0.06408 | 0.06471 |
| 403 | 0.06486 | 0.06457 | 0.06516 |
| 404 | 0.06533 | 0.06513 | 0.06573 |
| 405 | 0.06586 | 0.0657 | 0.06626 |
|   |      |      |      |
|---|------|------|------|
| 358| 0.08347 | 0.08258 | 0.08287 |
| 357| 0.08506 | 0.08417 | 0.08541 |
| 356| 0.08674 | 0.08587 | 0.08594 |
| 355| 0.08867 | 0.08764 | 0.0878  |
| 354| 0.09083 | 0.08975 | 0.08984 |
| 353| 0.09315 | 0.09197 | 0.09209 |
| 352| 0.09559 | 0.09443 | 0.09447 |
| 351| 0.09814 | 0.09689 | 0.09685 |
| 350| 0.10071 | 0.09946 | 0.09936 |
| 349| 0.10359 | 0.1012  | 0.10194 |
| 348| 0.10744 | 0.1046  | 0.10426 |
| 347| 0.10883 | 0.1067  | 0.10656 |
| 346| 0.11021 | 0.10878 | 0.10931 |
| 345| 0.11373 | 0.11188 | 0.11247 |
| 344| 0.11738 | 0.11487 | 0.11531 |
| 343| 0.11944 | 0.11729 | 0.11746 |
| 342| 0.1218  | 0.12037 | 0.1201  |
| 341| 0.12598 | 0.12467 | 0.12426 |
| 340| 0.13084 | 0.12859 | 0.12858 |
| 339| 0.13405 | 0.13207 | 0.13205 |
| 338| 0.13919 | 0.13683 | 0.1367  |
| 337| 0.14394 | 0.14173 | 0.1414  |
| 336| 0.1492  | 0.14682 | 0.14667 |
| 335| 0.15459 | 0.15224 | 0.15186 |
| 334| 0.16028 | 0.15754 | 0.15701 |
| 333| 0.16569 | 0.16265 | 0.16224 |
| 332| 0.17182 | 0.16883 | 0.16836 |
| 331| 0.17836 | 0.17502 | 0.17444 |
| 330| 0.1849  | 0.18166 | 0.18096 |
| 329| 0.19266 | 0.18944 | 0.18833 |
| 328| 0.20173 | 0.19821 | 0.19715 |
| 327| 0.21216 | 0.20819 | 0.20707 |
| 326| 0.22395 | 0.2195  | 0.218   |
| 325| 0.23741 | 0.23268 | 0.23074 |
| 324| 0.25276 | 0.24746 | 0.24531 |
| 323| 0.26925 | 0.26382 | 0.26167 |
| 322| 0.28807 | 0.28255 | 0.27991 |
| 321| 0.30916 | 0.30276 | 0.30019 |
| 320| 0.33309 | 0.32647 | 0.32393 |
| 319| 0.36031 | 0.35345 | 0.35132 |
| 318| 0.39279 | 0.38589 | 0.38353 |
| 317| 0.4316  | 0.42468 | 0.42288 |
| 316| 0.47902 | 0.47175 | 0.47058 |
| 315| 0.53697 | 0.52946 | 0.52851 |
| 314| 0.6067  | 0.59838 | 0.59828 |
| 313| 0.68603 | 0.67765 | 0.67827 |
| 312| 0.77648 | 0.76732 | 0.76825 |
|     |     |     |     |
|-----|-----|-----|-----|
| 311 | 0.86148 | 0.86054 | 0.8617 |
| 310 | 0.95007 | 0.94943 | 0.95072 |
| 309 | 1.02648 | 1.02538 | 1.02726 |
| 308 | 1.08354 | 1.08141 | 1.08384 |
| 307 | 1.12394 | 1.11994 | 1.1221 |
| 306 | 1.15238 | 1.14587 | 1.14819 |
| 305 | 1.17554 | 1.16728 | 1.16979 |
| 304 | 1.19657 | 1.1898 | 1.19288 |
| 303 | 1.22313 | 1.21601 | 1.21863 |
| 302 | 1.24686 | 1.2421 | 1.2446 |
| 301 | 1.27096 | 1.26477 | 1.26785 |
| 300 | 1.29058 | 1.28439 | 1.28679 |
| 299 | 1.30673 | 1.30069 | 1.3046 |
| 298 | 1.32021 | 1.31574 | 1.3188 |
| 297 | 1.33493 | 1.32963 | 1.33246 |
| 296 | 1.3473 | 1.34104 | 1.34448 |
| 295 | 1.35634 | 1.3498 | 1.35315 |
| 294 | 1.36165 | 1.35486 | 1.35761 |
| 293 | 1.36179 | 1.35728 | 1.36022 |
| 292 | 1.36118 | 1.3578 | 1.3602 |
| 291 | 1.35954 | 1.35581 | 1.35719 |
| 290 | 1.3547 | 1.35245 | 1.35316 |
| 289 | 1.34628 | 1.34597 | 1.34728 |
| 288 | 1.3341 | 1.33421 | 1.33642 |
| 287 | 1.31783 | 1.31747 | 1.31928 |
| 286 | 1.29546 | 1.29562 | 1.29702 |
| 285 | 1.27041 | 1.26962 | 1.27091 |
| 284 | 1.2424 | 1.24063 | 1.24179 |
| 283 | 1.21205 | 1.21019 | 1.21039 |
| 282 | 1.18096 | 1.17957 | 1.18027 |
| 281 | 1.15168 | 1.15098 | 1.15091 |
| 280 | 1.12444 | 1.12346 | 1.12322 |
| 279 | 1.10147 | 1.09917 | 1.09844 |
| 278 | 1.0806 | 1.07811 | 1.07701 |
| 277 | 1.06222 | 1.05928 | 1.05827 |
| 276 | 1.04609 | 1.04332 | 1.04211 |
| 275 | 1.03157 | 1.02873 | 1.02705 |
| 274 | 1.01597 | 1.01328 | 1.01235 |
| 273 | 0.99903 | 0.99593 | 0.99489 |
| 272 | 0.97914 | 0.97618 | 0.97541 |
| 271 | 0.95839 | 0.95503 | 0.95383 |
| 270 | 0.93693 | 0.93407 | 0.93299 |
| 269 | 0.91772 | 0.91488 | 0.91381 |
| 268 | 0.89978 | 0.89685 | 0.89588 |
| 267 | 0.87974 | 0.87754 | 0.87679 |
| 266 | 0.85739 | 0.855 | 0.85452 |
| 265 | 0.83186 | 0.82973 | 0.82908 |
|   |       |       |       |
|---|-------|-------|-------|
| 264 | 0.80335 | 0.80159 | 0.80102 |
| 263 | 0.77469 | 0.77269 | 0.77233 |
| 262 | 0.74579 | 0.74431 | 0.74425 |
| 261 | 0.71923 | 0.71755 | 0.71775 |
| 260 | 0.69569 | 0.6942  | 0.69418 |
| 259 | 0.67498 | 0.67381 | 0.67371 |
| 258 | 0.65779 | 0.6563  | 0.65642 |
| 257 | 0.64301 | 0.6418  | 0.64172 |
| 256 | 0.63125 | 0.63012 | 0.6305  |
| 255 | 0.62205 | 0.62136 | 0.62178 |
| 254 | 0.61546 | 0.61489 | 0.61517 |
| 253 | 0.61213 | 0.61141 | 0.61211 |
| 252 | 0.61298 | 0.61233 | 0.61295 |
| 251 | 0.61874 | 0.61823 | 0.61892 |
| 250 | 0.63086 | 0.63019 | 0.63126 |
| 249 | 0.64968 | 0.64961 | 0.65081 |
| 248 | 0.67707 | 0.67698 | 0.67808 |
| 247 | 0.71134 | 0.71123 | 0.71216 |
| 246 | 0.75339 | 0.75337 | 0.75449 |
| 245 | 0.80236 | 0.80188 | 0.80316 |
| 244 | 0.85707 | 0.85676 | 0.85813 |
| 243 | 0.91799 | 0.91749 | 0.91864 |
| 242 | 0.98516 | 0.98497 | 0.98585 |
| 241 | 1.05992 | 1.05911 | 1.06043 |
| 240 | 1.14299 | 1.14202 | 1.14322 |
| 239 | 1.23217 | 1.23129 | 1.23304 |
| 238 | 1.32933 | 1.32824 | 1.3304  |
| 237 | 1.42941 | 1.42755 | 1.43006 |
| 236 | 1.52687 | 1.52621 | 1.52861 |
| 235 | 1.61908 | 1.61839 | 1.62113 |
| 234 | 1.69758 | 1.69674 | 1.69948 |
| 233 | 1.763   | 1.76168 | 1.76307 |
| 232 | 1.8127  | 1.81108 | 1.81344 |
| 231 | 1.85413 | 1.85151 | 1.85323 |
| 230 | 1.88722 | 1.88527 | 1.88626 |
| 229 | 1.9132  | 1.90806 | 1.90978 |
| 228 | 1.92876 | 1.92429 | 1.92649 |
| 227 | 1.93466 | 1.93215 | 1.93214 |
| 226 | 1.92874 | 1.92382 | 1.92362 |
| 225 | 1.91333 | 1.91152 | 1.91068 |
| 224 | 1.89315 | 1.88967 | 1.88913 |
| 223 | 1.87229 | 1.86766 | 1.87079 |
| 222 | 1.85887 | 1.85374 | 1.85572 |
| 221 | 1.85661 | 1.85132 | 1.85058 |
| 220 | 1.86876 | 1.86386 | 1.86684 |
| Wavelength [nm] | Absorption before irradiation | Absorption after 6 min irradiation | Absorption after 25 min irradiation | Absorption after 60 min irradiation | Absorption after 120 min irradiation |
|----------------|-------------------------------|-----------------------------------|-----------------------------------|-----------------------------------|-----------------------------------|
| 750            | 1.81E-03                      | 2.06E-03                          | 2.41E-03                          | 0.00246                           | 0.00219                           |
| 749            | 1.68E-03                      | 2.03E-03                          | 2.30E-03                          | 0.00237                           | 0.00207                           |
| 748            | 1.76E-03                      | 2.09E-03                          | 2.35E-03                          | 0.0023                           | 0.00214                           |
| 747            | 1.83E-03                      | 2.17E-03                          | 2.34E-03                          | 0.00235                           | 0.00215                           |
| 746            | 1.82E-03                      | 2.13E-03                          | 2.37E-03                          | 0.00232                           | 0.00212                           |
| 745            | 1.82E-03                      | 2.18E-03                          | 2.40E-03                          | 0.00238                           | 0.00209                           |
| 744            | 1.78E-03                      | 2.20E-03                          | 2.37E-03                          | 0.00238                           | 0.00217                           |
| 743            | 1.69E-03                      | 2.12E-03                          | 2.34E-03                          | 0.00229                           | 0.00212                           |
| 742            | 1.71E-03                      | 2.11E-03                          | 2.26E-03                          | 0.0023                           | 0.00207                           |
| 741            | 1.86E-03                      | 2.16E-03                          | 2.43E-03                          | 0.00228                           | 0.00207                           |
| 740            | 1.77E-03                      | 2.16E-03                          | 2.34E-03                          | 0.00227                           | 0.00212                           |
| 739            | 1.70E-03                      | 2.00E-03                          | 2.17E-03                          | 0.00225                           | 0.00195                           |
| 738            | 1.61E-03                      | 2.00E-03                          | 2.28E-03                          | 0.00226                           | 0.00204                           |
| 737            | 1.77E-03                      | 2.17E-03                          | 2.36E-03                          | 0.00239                           | 0.00216                           |
| 736            | 1.73E-03                      | 2.06E-03                          | 2.38E-03                          | 0.00229                           | 0.00207                           |
| 735            | 1.66E-03                      | 2.10E-03                          | 2.22E-03                          | 0.00222                           | 0.00199                           |
| 734            | 1.64E-03                      | 2.02E-03                          | 2.24E-03                          | 0.00226                           | 0.00201                           |
| 733            | 1.68E-03                      | 2.08E-03                          | 2.28E-03                          | 0.00224                           | 0.00205                           |
| 732            | 1.74E-03                      | 2.09E-03                          | 2.32E-03                          | 0.00234                           | 0.00208                           |
| 731            | 1.69E-03                      | 2.12E-03                          | 2.33E-03                          | 0.00231                           | 0.00212                           |
| 730            | 1.79E-03                      | 2.10E-03                          | 2.30E-03                          | 0.00228                           | 0.00209                           |
| 729            | 1.70E-03                      | 2.07E-03                          | 2.21E-03                          | 0.00222                           | 0.00205                           |
| 728            | 1.76E-03                      | 2.04E-03                          | 2.19E-03                          | 0.00228                           | 0.00197                           |
| 727            | 1.74E-03                      | 1.97E-03                          | 2.30E-03                          | 0.00226                           | 0.00194                           |
| 726            | 1.64E-03                      | 2.03E-03                          | 2.25E-03                          | 0.00227                           | 0.00194                           |
| 725            | 1.73E-03                      | 2.07E-03                          | 2.24E-03                          | 0.00229                           | 0.00208                           |
| 724            | 1.62E-03                      | 2.02E-03                          | 2.25E-03                          | 0.0022                           | 0.002 |
| 723            | 1.65E-03                      | 1.97E-03                          | 2.17E-03                          | 0.00221                           | 0.00192                           |
| 722            | 1.64E-03                      | 2.00E-03                          | 2.18E-03                          | 0.00216                           | 0.00199                           |
| 721            | 1.67E-03                      | 1.99E-03                          | 2.18E-03                          | 0.00228                           | 0.00199                           |
| 720            | 1.68E-03                      | 2.05E-03                          | 2.19E-03                          | 0.00226                           | 0.00204                           |
| 719            | 1.65E-03                      | 1.92E-03                          | 2.24E-03                          | 0.00214                           | 0.00201                           |
| 718            | 1.68E-03                      | 1.98E-03                          | 2.17E-03                          | 0.00211                           | 0.00191                           |
| 717            | 1.70E-03                      | 2.07E-03                          | 2.28E-03                          | 0.00227                           | 0.00207                           |
| 716            | 1.60E-03                      | 1.99E-03                          | 2.09E-03                          | 0.00211                           | 0.00191                           |
| 715            | 1.68E-03                      | 2.05E-03                          | 2.16E-03                          | 0.00218                           | 0.00197                           |
| 714            | 1.63E-03                      | 1.91E-03                          | 2.15E-03                          | 0.00213                           | 0.00189                           |
| 713            | 1.60E-03                      | 1.98E-03                          | 2.18E-03                          | 0.00223                           | 0.00193                           |
| 712            | 1.56E-03                      | 1.98E-03                          | 2.14E-03                          | 0.00217                           | 0.00193                           |
| 711            | 1.62E-03                      | 2.03E-03                          | 2.17E-03                          | 0.00217                           | 0.00192                           |
| 710            | 1.65E-03                      | 1.98E-03                          | 2.10E-03                          | 0.00205                           | 0.00186                           |
| 709            | 1.60E-03                      | 1.96E-03                          | 2.10E-03                          | 0.00224                           | 0.00193                           |
| 708            | 1.65E-03                      | 1.93E-03                          | 2.10E-03                          | 0.00217                           | 0.00184                           |
| 707            | 1.51E-03                      | 1.92E-03                          | 2.12E-03                          | 0.00205                           | 0.00177                           |
|     | 6.9E-03 | 1.99E-03 | 2.16E-03 | 0.00218 | 0.00172 |
|-----|---------|----------|----------|----------|----------|
| 658 | 1.65E-03 | 1.97E-03 | 2.16E-03 | 0.00211 | 0.00176 |
| 657 | 1.70E-03 | 1.98E-03 | 2.17E-03 | 0.00206 | 0.00178 |
| 656 | 1.71E-03 | 2.06E-03 | 2.21E-03 | 0.00214 | 0.0018 |
| 655 | 1.80E-03 | 2.05E-03 | 2.21E-03 | 0.00218 | 0.00179 |
| 654 | 1.76E-03 | 2.10E-03 | 2.24E-03 | 0.00217 | 0.00181 |
| 653 | 1.80E-03 | 2.10E-03 | 2.26E-03 | 0.0022 | 0.00186 |
| 652 | 1.82E-03 | 2.13E-03 | 2.25E-03 | 0.00222 | 0.00184 |
| 651 | 1.85E-03 | 2.18E-03 | 2.31E-03 | 0.00224 | 0.00185 |
| 650 | 1.91E-03 | 2.23E-03 | 2.38E-03 | 0.00232 | 0.00198 |
| 649 | 1.93E-03 | 2.25E-03 | 2.40E-03 | 0.00231 | 0.00192 |
| 648 | 1.97E-03 | 2.25E-03 | 2.39E-03 | 0.00235 | 0.00192 |
| 647 | 2.07E-03 | 2.37E-03 | 2.47E-03 | 0.00243 | 0.00203 |
| 646 | 2.06E-03 | 2.30E-03 | 2.47E-03 | 0.00244 | 0.00206 |
| 645 | 2.07E-03 | 2.40E-03 | 2.53E-03 | 0.00245 | 0.00213 |
| 644 | 2.09E-03 | 2.40E-03 | 2.57E-03 | 0.00251 | 0.00212 |
| 643 | 2.19E-03 | 2.47E-03 | 2.63E-03 | 0.0025 | 0.00214 |
| 642 | 2.23E-03 | 2.52E-03 | 2.65E-03 | 0.00259 | 0.00219 |
| 641 | 2.27E-03 | 2.54E-03 | 2.67E-03 | 0.00264 | 0.00222 |
| 640 | 2.33E-03 | 2.64E-03 | 2.79E-03 | 0.00271 | 0.00231 |
| 639 | 2.41E-03 | 2.69E-03 | 2.86E-03 | 0.00279 | 0.00237 |
| 638 | 2.44E-03 | 2.75E-03 | 2.89E-03 | 0.00276 | 0.00236 |
| 637 | 2.51E-03 | 2.82E-03 | 2.95E-03 | 0.00289 | 0.00245 |
| 636 | 2.63E-03 | 2.88E-03 | 2.99E-03 | 0.00293 | 0.00252 |
| 635 | 2.69E-03 | 2.92E-03 | 3.09E-03 | 0.00303 | 0.00263 |
| 634 | 2.76E-03 | 3.06E-03 | 3.20E-03 | 0.00312 | 0.0027 |
| 633 | 2.83E-03 | 3.10E-03 | 3.26E-03 | 0.00318 | 0.00277 |
| 632 | 2.86E-03 | 3.18E-03 | 3.32E-03 | 0.00318 | 0.00281 |
| 631 | 2.99E-03 | 3.26E-03 | 3.39E-03 | 0.0033 | 0.00287 |
| 630 | 3.10E-03 | 3.37E-03 | 3.47E-03 | 0.00339 | 0.00298 |
| 629 | 3.21E-03 | 3.48E-03 | 3.58E-03 | 0.00353 | 0.00304 |
| 628 | 3.27E-03 | 3.56E-03 | 3.60E-03 | 0.00356 | 0.00311 |
| 627 | 3.40E-03 | 3.65E-03 | 3.77E-03 | 0.00368 | 0.00316 |
| 626 | 3.50E-03 | 3.69E-03 | 3.85E-03 | 0.00378 | 0.00329 |
| 625 | 3.60E-03 | 3.89E-03 | 3.97E-03 | 0.00383 | 0.00345 |
| 624 | 3.78E-03 | 4.02E-03 | 4.10E-03 | 0.00405 | 0.00356 |
| 623 | 0.00384 | 0.00412 | 4.21E-03 | 0.00411 | 0.00369 |
| 622 | 0.004 | 0.0043 | 0.00432 | 0.00421 | 0.00374 |
| 621 | 0.00419 | 0.00436 | 0.0045 | 0.00429 | 0.00385 |
| 620 | 0.00419 | 0.00451 | 0.00461 | 0.00439 | 0.00391 |
| 619 | 0.00444 | 0.00464 | 0.00469 | 0.00459 | 0.00407 |
| 618 | 0.00457 | 0.0048 | 0.00488 | 0.00474 | 0.00417 |
| 617 | 0.0048 | 0.00498 | 0.00509 | 0.00497 | 0.0044 |
| 616 | 0.00498 | 0.00512 | 0.0052 | 0.00507 | 0.00452 |
| 615 | 0.00513 | 0.0053 | 0.00538 | 0.00524 | 0.00474 |
| 614 | 0.00523 | 0.00544 | 0.00554 | 0.00536 | 0.00482 |
| 613 | 0.00546 | 0.0057 | 0.00576 | 0.00558 | 0.00505 |
|    |      |      |      |      |      |
|----|------|------|------|------|------|
| 612| 0.00567 | 0.00584 | 0.00591 | 0.00576 | 0.00523 |
| 611| 0.00587 | 0.00607 | 0.0061  | 0.00595 | 0.00537 |
| 610| 0.00613 | 0.00626 | 0.00635 | 0.00622 | 0.0056  |
| 609| 0.00626 | 0.00641 | 0.00645 | 0.00631 | 0.00574 |
| 608| 0.00653 | 0.00666 | 0.00674 | 0.00655 | 0.00598 |
| 607| 0.00673 | 0.00669 | 0.00693 | 0.00677 | 0.00624 |
| 606| 0.00698 | 0.00712 | 0.00714 | 0.00699 | 0.00647 |
| 605| 0.00722 | 0.00735 | 0.00736 | 0.00719 | 0.00664 |
| 604| 0.00751 | 0.00763 | 0.00764 | 0.00746 | 0.0069  |
| 603| 0.00778 | 0.00786 | 0.00788 | 0.00772 | 0.00715 |
| 602| 0.00801 | 0.00813 | 0.00813 | 0.00792 | 0.00739 |
| 601| 0.00839 | 0.00885 | 0.00846 | 0.00825 | 0.00775 |
| 600| 0.00865 | 0.00876 | 0.00872 | 0.00854 | 0.00793 |
| 599| 0.00895 | 0.009  | 0.00896 | 0.00879 | 0.0082  |
| 598| 0.00924 | 0.00931 | 0.00921 | 0.00904 | 0.0085  |
| 597| 0.00954 | 0.00961 | 0.00957 | 0.00934 | 0.00879 |
| 596| 0.00988 | 0.00993 | 0.00992 | 0.00966 | 0.00913 |
| 595| 0.01018 | 0.01024 | 0.01019 | 0.00997 | 0.00943 |
| 594| 0.01052 | 0.01057 | 0.01049 | 0.01026 | 0.00973 |
| 593| 0.01094 | 0.01095 | 0.01084 | 0.01063 | 0.01005 |
| 592| 0.01125 | 0.01129 | 0.01115 | 0.01095 | 0.01039 |
| 591| 0.01163 | 0.01163 | 0.01154 | 0.01128 | 0.01069 |
| 590| 0.01199 | 0.01195 | 0.01187 | 0.01164 | 0.01105 |
| 589| 0.0123  | 0.01229 | 0.01216 | 0.01188 | 0.01132 |
| 588| 0.01273 | 0.0127  | 0.01254 | 0.01229 | 0.01173 |
| 587| 0.0131  | 0.01305 | 0.01291 | 0.01264 | 0.01206 |
| 586| 0.01357 | 0.01345 | 0.01332 | 0.01304 | 0.01242 |
| 585| 0.01393 | 0.01389 | 0.01372 | 0.01346 | 0.01283 |
| 584| 0.01439 | 0.01426 | 0.01415 | 0.01383 | 0.01321 |
| 583| 0.01479 | 0.01471 | 0.01445 | 0.01416 | 0.01354 |
| 582| 0.01518 | 0.0151  | 0.0149  | 0.01455 | 0.01397 |
| 581| 0.01568 | 0.01556 | 0.01529 | 0.01504 | 0.01442 |
| 580| 0.01616 | 0.01592 | 0.01567 | 0.01542 | 0.01477 |
| 579| 0.01656 | 0.01636 | 0.0162  | 0.01587 | 0.01519 |
| 578| 0.01698 | 0.01685 | 0.01661 | 0.0162  | 0.01558 |
| 577| 0.0175  | 0.01735 | 0.01711 | 0.01668 | 0.01605 |
| 576| 0.01794 | 0.01775 | 0.01746 | 0.01706 | 0.01642 |
| 575| 0.01843 | 0.01824 | 0.01795 | 0.01758 | 0.01695 |
| 574| 0.01891 | 0.01872 | 0.0184  | 0.018   | 0.01734 |
| 573| 0.01944 | 0.0192  | 0.01889 | 0.01853 | 0.01783 |
| 572| 0.01986 | 0.0196  | 0.01924 | 0.01888 | 0.01819 |
| 571| 0.0204  | 0.02012 | 0.01979 | 0.01937 | 0.01871 |
| 570| 0.02083 | 0.02061 | 0.02024 | 0.0199  | 0.01919 |
| 569| 0.02138 | 0.02108 | 0.02075 | 0.02037 | 0.01964 |
| 568| 0.02185 | 0.0215  | 0.02116 | 0.02083 | 0.02008 |
| 567| 0.0224  | 0.02211 | 0.02162 | 0.02126 | 0.02053 |
| 566| 0.02286 | 0.02254 | 0.02201 | 0.02167 | 0.02094 |
|   |       |       |       |       |       |       |
|---|-------|-------|-------|-------|-------|-------|
| 565| 0.02337 | 0.02302 | 0.02255 | 0.02213 | 0.02141 |
| 564| 0.02381 | 0.02345 | 0.02297 | 0.02252 | 0.02178 |
| 563| 0.02439 | 0.02401 | 0.02351 | 0.02304 | 0.02236 |
| 562| 0.02489 | 0.02451 | 0.02396 | 0.02356 | 0.0228 |
| 561| 0.02538 | 0.02497 | 0.02444 | 0.02401 | 0.02324 |
| 560| 0.02587 | 0.02554 | 0.02491 | 0.02451 | 0.02374 |
| 559| 0.02641 | 0.0262 | 0.02574 | 0.02496 | 0.02419 |
| 558| 0.02683 | 0.02647 | 0.02594 | 0.02541 | 0.02462 |
| 557| 0.02739 | 0.02696 | 0.02635 | 0.02587 | 0.02516 |
| 556| 0.02788 | 0.02742 | 0.02678 | 0.02632 | 0.02559 |
| 555| 0.02837 | 0.02792 | 0.0273 | 0.02679 | 0.02608 |
| 554| 0.02887 | 0.0284 | 0.02775 | 0.02727 | 0.0265 |
| 553| 0.02941 | 0.02887 | 0.02825 | 0.02774 | 0.02697 |
| 552| 0.02984 | 0.02934 | 0.02874 | 0.0282 | 0.02743 |
| 551| 0.03032 | 0.02979 | 0.02917 | 0.02865 | 0.02785 |
| 550| 0.03081 | 0.03032 | 0.02967 | 0.02914 | 0.02836 |
| 549| 0.03128 | 0.03075 | 0.03005 | 0.02956 | 0.02874 |
| 548| 0.03177 | 0.03121 | 0.03048 | 0.03003 | 0.02923 |
| 547| 0.03222 | 0.03162 | 0.03095 | 0.03043 | 0.0296 |
| 546| 0.03263 | 0.03202 | 0.03133 | 0.03082 | 0.03001 |
| 545| 0.03308 | 0.03253 | 0.03181 | 0.03128 | 0.03046 |
| 544| 0.03353 | 0.03291 | 0.0322 | 0.0317 | 0.03084 |
| 543| 0.034 | 0.03342 | 0.03264 | 0.03218 | 0.03128 |
| 542| 0.03441 | 0.03377 | 0.03301 | 0.03249 | 0.03168 |
| 541| 0.03487 | 0.03424 | 0.03354 | 0.03298 | 0.03213 |
| 540| 0.03524 | 0.03463 | 0.03388 | 0.03335 | 0.03247 |
| 539| 0.03565 | 0.03508 | 0.03432 | 0.03376 | 0.03287 |
| 538| 0.03603 | 0.03543 | 0.03462 | 0.03408 | 0.03326 |
| 537| 0.03649 | 0.03586 | 0.03506 | 0.03448 | 0.03365 |
| 536| 0.03679 | 0.03615 | 0.03541 | 0.03489 | 0.03398 |
| 535| 0.03723 | 0.03658 | 0.03591 | 0.03531 | 0.03443 |
| 534| 0.03761 | 0.03699 | 0.03631 | 0.03572 | 0.03487 |
| 533| 0.03801 | 0.03733 | 0.03666 | 0.03609 | 0.03519 |
| 532| 0.0384 | 0.03771 | 0.03703 | 0.03646 | 0.03555 |
| 531| 0.0387 | 0.03804 | 0.03737 | 0.03678 | 0.03587 |
| 530| 0.03919 | 0.03846 | 0.03772 | 0.03718 | 0.03625 |
| 529| 0.03948 | 0.03879 | 0.03804 | 0.03749 | 0.0366 |
| 528| 0.03983 | 0.03909 | 0.0384 | 0.03784 | 0.03689 |
| 527| 0.04018 | 0.03946 | 0.03878 | 0.03817 | 0.03726 |
| 526| 0.04048 | 0.03981 | 0.03911 | 0.03851 | 0.03759 |
| 525| 0.04084 | 0.04017 | 0.03944 | 0.03882 | 0.03786 |
| 524| 0.04123 | 0.04053 | 0.03975 | 0.0392 | 0.03813 |
| 523| 0.04153 | 0.04081 | 0.04008 | 0.03947 | 0.03847 |
| 522| 0.04191 | 0.04116 | 0.04045 | 0.03979 | 0.03879 |
| 521| 0.04219 | 0.04146 | 0.04077 | 0.04003 | 0.03906 |
| 520| 0.04243 | 0.04178 | 0.041 | 0.0403 | 0.03934 |
| 519| 0.04288 | 0.04214 | 0.04133 | 0.04069 | 0.03974 |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 518 | 0.04318 | 0.04249 | 0.04159 | 0.04101 | 0.04003 |
| 517 | 0.04351 | 0.04275 | 0.04187 | 0.04131 | 0.04035 |
| 516 | 0.04381 | 0.04308 | 0.0423 | 0.04164 | 0.04068 |
| 515 | 0.04419 | 0.04345 | 0.04274 | 0.04204 | 0.04109 |
| 514 | 0.04451 | 0.04378 | 0.04301 | 0.0424 | 0.04142 |
| 513 | 0.04491 | 0.04419 | 0.04344 | 0.04276 | 0.04179 |
| 512 | 0.04531 | 0.04453 | 0.04376 | 0.04314 | 0.04212 |
| 511 | 0.04569 | 0.04491 | 0.04412 | 0.04352 | 0.04249 |
| 510 | 0.04608 | 0.04534 | 0.04458 | 0.04391 | 0.04291 |
| 509 | 0.04648 | 0.0447 | 0.04492 | 0.04428 | 0.04326 |
| 508 | 0.04687 | 0.04614 | 0.04542 | 0.0447 | 0.0437 |
| 507 | 0.0473 | 0.04654 | 0.04576 | 0.04509 | 0.04408 |
| 506 | 0.04777 | 0.04704 | 0.0462 | 0.04556 | 0.04451 |
| 505 | 0.0483 | 0.04752 | 0.04671 | 0.0461 | 0.045 |
| 504 | 0.04879 | 0.04795 | 0.04721 | 0.04652 | 0.04546 |
| 503 | 0.04933 | 0.04852 | 0.04779 | 0.04705 | 0.04598 |
| 502 | 0.0498 | 0.04907 | 0.04828 | 0.04754 | 0.04648 |
| 501 | 0.05043 | 0.04965 | 0.04887 | 0.0481 | 0.04702 |
| 500 | 0.05101 | 0.05026 | 0.04943 | 0.0487 | 0.04761 |
| 499 | 0.05169 | 0.05092 | 0.05006 | 0.04931 | 0.0482 |
| 498 | 0.05244 | 0.0516 | 0.05076 | 0.04999 | 0.04887 |
| 497 | 0.05316 | 0.0523 | 0.05146 | 0.05077 | 0.04959 |
| 496 | 0.05393 | 0.05304 | 0.05221 | 0.05139 | 0.0503 |
| 495 | 0.05466 | 0.0538 | 0.05296 | 0.05216 | 0.05102 |
| 494 | 0.05549 | 0.05462 | 0.0537 | 0.0529 | 0.05183 |
| 493 | 0.05641 | 0.0555 | 0.05459 | 0.05381 | 0.05261 |
| 492 | 0.05735 | 0.05641 | 0.05549 | 0.05471 | 0.05348 |
| 491 | 0.05828 | 0.05733 | 0.0564 | 0.05555 | 0.05435 |
| 490 | 0.05926 | 0.05832 | 0.05736 | 0.05653 | 0.05528 |
| 489 | 0.06029 | 0.05936 | 0.05836 | 0.05748 | 0.05625 |
| 488 | 0.06133 | 0.06036 | 0.05932 | 0.05849 | 0.05722 |
| 487 | 0.06247 | 0.06145 | 0.06047 | 0.05958 | 0.05831 |
| 486 | 0.06361 | 0.06255 | 0.06154 | 0.06062 | 0.05931 |
| 485 | 0.06483 | 0.06378 | 0.06274 | 0.06176 | 0.06046 |
| 484 | 0.06601 | 0.06495 | 0.06384 | 0.0629 | 0.06161 |
| 483 | 0.06722 | 0.06613 | 0.06501 | 0.06409 | 0.06271 |
| 482 | 0.06848 | 0.06736 | 0.0662 | 0.06522 | 0.06387 |
| 481 | 0.0698 | 0.06865 | 0.06744 | 0.06643 | 0.06505 |
| 480 | 0.07103 | 0.06988 | 0.06861 | 0.06764 | 0.0662 |
| 479 | 0.07244 | 0.07124 | 0.06993 | 0.06891 | 0.06749 |
| 478 | 0.07372 | 0.07245 | 0.07124 | 0.07009 | 0.06864 |
| 477 | 0.075 | 0.07374 | 0.07244 | 0.0714 | 0.06988 |
| 476 | 0.07637 | 0.07512 | 0.07376 | 0.07264 | 0.0714 |
| 475 | 0.07765 | 0.07636 | 0.07492 | 0.07388 | 0.07238 |
| 474 | 0.0791 | 0.07773 | 0.07632 | 0.07517 | 0.0736 |
| 473 | 0.08041 | 0.07901 | 0.07756 | 0.07641 | 0.07483 |
| 472 | 0.0818 | 0.08036 | 0.07892 | 0.07771 | 0.07612 |
| 471 | 0.0831 | 0.08163 | 0.08017 | 0.07891 | 0.07729 |
| 470 | 0.08442 | 0.08293 | 0.08137 | 0.08015 | 0.07857 |
| 469 | 0.08583 | 0.08432 | 0.0827 | 0.08145 | 0.07977 |
| 468 | 0.08716 | 0.0856 | 0.08395 | 0.08275 | 0.08103 |
| 467 | 0.08849 | 0.08686 | 0.08527 | 0.08393 | 0.08226 |
| 466 | 0.08978 | 0.08816 | 0.08651 | 0.08517 | 0.08344 |
| 465 | 0.09104 | 0.08938 | 0.08773 | 0.08636 | 0.08465 |
| 464 | 0.09237 | 0.09068 | 0.08896 | 0.08759 | 0.0859 |
| 463 | 0.09364 | 0.09193 | 0.09014 | 0.08878 | 0.08702 |
| 462 | 0.09494 | 0.0932 | 0.09139 | 0.08999 | 0.08826 |
| 461 | 0.0963 | 0.09447 | 0.09269 | 0.09123 | 0.08942 |
| 460 | 0.09749 | 0.09566 | 0.09388 | 0.0924 | 0.09057 |
| 459 | 0.0987 | 0.09679 | 0.09495 | 0.09345 | 0.09167 |
| 458 | 0.09998 | 0.09807 | 0.09604 | 0.09457 | 0.09274 |
| 457 | 0.10124 | 0.09935 | 0.09735 | 0.09576 | 0.09392 |
| 456 | 0.1024 | 0.10048 | 0.09854 | 0.09695 | 0.09501 |
| 455 | 0.10364 | 0.10174 | 0.09978 | 0.09821 | 0.09627 |
| 454 | 0.10483 | 0.10283 | 0.10089 | 0.09928 | 0.09735 |
| 453 | 0.10596 | 0.10396 | 0.10196 | 0.10031 | 0.09842 |
| 452 | 0.10709 | 0.10508 | 0.10302 | 0.10137 | 0.0995 |
| 451 | 0.10826 | 0.10625 | 0.10416 | 0.1025 | 0.10057 |
| 450 | 0.10931 | 0.10714 | 0.10506 | 0.10344 | 0.1015 |
| 449 | 0.11029 | 0.1082 | 0.10603 | 0.10439 | 0.1024 |
| 448 | 0.11143 | 0.10936 | 0.10713 | 0.10536 | 0.10338 |
| 447 | 0.11242 | 0.11024 | 0.10817 | 0.10643 | 0.10431 |
| 446 | 0.11336 | 0.11122 | 0.10907 | 0.10738 | 0.10532 |
| 445 | 0.1143 | 0.1122 | 0.10995 | 0.10822 | 0.10624 |
| 444 | 0.11513 | 0.113 | 0.11081 | 0.10906 | 0.10704 |
| 443 | 0.11603 | 0.11385 | 0.11155 | 0.1099 | 0.10784 |
| 442 | 0.11682 | 0.11461 | 0.1123 | 0.11051 | 0.10848 |
| 441 | 0.11744 | 0.11525 | 0.11297 | 0.11119 | 0.10904 |
| 440 | 0.11815 | 0.11586 | 0.11366 | 0.11185 | 0.10978 |
| 439 | 0.11864 | 0.11644 | 0.1142 | 0.11239 | 0.11034 |
| 438 | 0.11912 | 0.11695 | 0.11461 | 0.11287 | 0.11076 |
| 437 | 0.11961 | 0.11732 | 0.11498 | 0.11323 | 0.11114 |
| 436 | 0.11992 | 0.11765 | 0.1154 | 0.11356 | 0.11136 |
| 435 | 0.12019 | 0.11793 | 0.11565 | 0.11386 | 0.11167 |
| 434 | 0.12034 | 0.11809 | 0.11584 | 0.11405 | 0.11199 |
| 433 | 0.12041 | 0.11819 | 0.11595 | 0.11406 | 0.11193 |
| 432 | 0.12044 | 0.11825 | 0.11594 | 0.1141 | 0.11204 |
| 431 | 0.12042 | 0.11819 | 0.11591 | 0.11415 | 0.11209 |
| 430 | 0.12025 | 0.11793 | 0.11573 | 0.11394 | 0.1118 |
| 429 | 0.12001 | 0.11782 | 0.11561 | 0.11374 | 0.11157 |
| 428 | 0.11969 | 0.11758 | 0.11531 | 0.11355 | 0.11144 |
| 427 | 0.11936 | 0.11726 | 0.11502 | 0.1133 | 0.11122 |
| 426 | 0.11899 | 0.11693 | 0.1147 | 0.11283 | 0.11079 |
| 425 | 0.11859 | 0.11646 | 0.11432 | 0.11252 | 0.11046 |
|   | 377 | 0.12015 | 0.11897 | 0.11768 | 0.11652 | 0.11495 |
|---|-----|---------|---------|---------|---------|---------|
| 376 | 0.1214 | 0.1202 | 0.11904 | 0.11792 | 0.11623 |
| 375 | 0.12269 | 0.12154 | 0.12049 | 0.11932 | 0.11774 |
| 374 | 0.12399 | 0.12291 | 0.12187 | 0.12072 | 0.11921 |
| 373 | 0.12542 | 0.12445 | 0.1232 | 0.12219 | 0.12072 |
| 372 | 0.12696 | 0.1259 | 0.1248 | 0.12371 | 0.12229 |
| 371 | 0.12858 | 0.12764 | 0.12641 | 0.12546 | 0.12405 |
| 370 | 0.13021 | 0.12917 | 0.12807 | 0.12711 | 0.12584 |
| 369 | 0.13193 | 0.13087 | 0.12984 | 0.12899 | 0.12769 |
| 368 | 0.13369 | 0.13261 | 0.13156 | 0.13063 | 0.12949 |
| 367 | 0.13546 | 0.13454 | 0.13347 | 0.13261 | 0.13149 |
| 366 | 0.13743 | 0.13638 | 0.13542 | 0.13473 | 0.13358 |
| 365 | 0.13967 | 0.13861 | 0.13765 | 0.13686 | 0.13584 |
| 364 | 0.14214 | 0.14111 | 0.14014 | 0.13946 | 0.13852 |
| 363 | 0.14503 | 0.14403 | 0.14309 | 0.14246 | 0.14154 |
| 362 | 0.14818 | 0.14718 | 0.1464 | 0.14576 | 0.14495 |
| 361 | 0.15203 | 0.15104 | 0.1503 | 0.14955 | 0.14886 |
| 360 | 0.15628 | 0.15542 | 0.15461 | 0.1539 | 0.15334 |
| 359 | 0.16099 | 0.16012 | 0.15926 | 0.15886 | 0.15824 |
| 358 | 0.16589 | 0.16499 | 0.16403 | 0.16373 | 0.16323 |
| 357 | 0.17078 | 0.1698 | 0.16916 | 0.16866 | 0.16826 |
| 356 | 0.17543 | 0.17448 | 0.17383 | 0.17345 | 0.17321 |
| 355 | 0.17972 | 0.17876 | 0.17805 | 0.17776 | 0.17757 |
| 354 | 0.18418 | 0.18331 | 0.1825 | 0.18242 | 0.18232 |
| 353 | 0.18875 | 0.18789 | 0.18724 | 0.18717 | 0.18727 |
| 352 | 0.19397 | 0.19312 | 0.19249 | 0.1924 | 0.19257 |
| 351 | 0.19989 | 0.19905 | 0.19838 | 0.19837 | 0.19867 |
| 350 | 0.20635 | 0.20544 | 0.20488 | 0.20488 | 0.20534 |
| 349 | 0.21243 | 0.21143 | 0.21038 | 0.21121 | 0.21065 |
| 348 | 0.22289 | 0.22206 | 0.22172 | 0.22125 | 0.2212 |
| 347 | 0.23163 | 0.23085 | 0.23145 | 0.23024 | 0.23081 |
| 346 | 0.2408 | 0.24003 | 0.23954 | 0.23918 | 0.23981 |
| 345 | 0.25233 | 0.25155 | 0.25026 | 0.24994 | 0.2507 |
| 344 | 0.26572 | 0.26447 | 0.26405 | 0.26339 | 0.26412 |
| 343 | 0.27934 | 0.27839 | 0.27827 | 0.27811 | 0.27844 |
| 342 | 0.29231 | 0.29121 | 0.29094 | 0.29132 | 0.29174 |
| 341 | 0.30596 | 0.30452 | 0.30449 | 0.30427 | 0.30478 |
| 340 | 0.31792 | 0.31683 | 0.3162 | 0.3154 | 0.3166 |
| 339 | 0.32761 | 0.32693 | 0.32609 | 0.3262 | 0.32686 |
| 338 | 0.33604 | 0.33519 | 0.33474 | 0.33434 | 0.33557 |
| 337 | 0.3436 | 0.3428 | 0.34189 | 0.34204 | 0.34366 |
| 336 | 0.35214 | 0.351 | 0.35037 | 0.35088 | 0.35266 |
| 335 | 0.36153 | 0.3603 | 0.35996 | 0.36049 | 0.36257 |
| 334 | 0.37235 | 0.3714 | 0.37127 | 0.37175 | 0.37417 |
| 333 | 0.385 | 0.38369 | 0.38378 | 0.38462 | 0.38703 |
| 332 | 0.39982 | 0.39874 | 0.39869 | 0.39936 | 0.40276 |
| 331 | 0.41673 | 0.41574 | 0.41546 | 0.41655 | 0.42031 |
| 330 | 0.43737 | 0.43582 | 0.43586 | 0.43751 | 0.44152 |
| 329 | 0.46032 | 0.45898 | 0.4596  | 0.46151 | 0.46601 |
| 328 | 0.48837 | 0.48732 | 0.48775 | 0.4897  | 0.49514 |
| 327 | 0.51967 | 0.51841 | 0.51924 | 0.52104 | 0.52741 |
| 326 | 0.55335 | 0.55154 | 0.55265 | 0.55538 | 0.56248 |
| 325 | 0.58926 | 0.5876  | 0.58881 | 0.59146 | 0.59995 |
| 324 | 0.62565 | 0.62405 | 0.62514 | 0.62857 | 0.63744 |
| 323 | 0.66319 | 0.66156 | 0.66255 | 0.66653 | 0.67712 |
| 322 | 0.70313 | 0.70072 | 0.70236 | 0.70647 | 0.71785 |
| 321 | 0.74602 | 0.74365 | 0.74462 | 0.74919 | 0.76143 |
| 320 | 0.79398 | 0.79141 | 0.79214 | 0.79645 | 0.80961 |
| 319 | 0.84946 | 0.84629 | 0.8463  | 0.8514  | 0.86444 |
| 318 | 0.91309 | 0.90928 | 0.90927 | 0.91364 | 0.92661 |
| 317 | 0.98757 | 0.98365 | 0.98201 | 0.98693 | 0.99936 |
| 316 | 1.07609 | 1.07144 | 1.0696  | 1.07249 | 1.08541 |
| 315 | 1.17975 | 1.17414 | 1.1702  | 1.17422 | 1.18591 |
| 314 | 1.29995 | 1.29227 | 1.28836 | 1.29049 | 1.30247 |
| 313 | 1.43373 | 1.42489 | 1.41976 | 1.42206 | 1.43417 |
| 312 | 1.5827  | 1.57071 | 1.56378 | 1.56637 | 1.57971 |
| 311 | 1.73744 | 1.7273  | 1.71635 | 1.71668 | 1.72724 |
| 310 | 1.89905 | 1.88121 | 1.87578 | 1.87334 | 1.8895 |
| 309 | 2.0535  | 2.03759 | 2.02746 | 2.02897 | 2.04127 |
| 308 | 2.21389 | 2.20209 | 2.18667 | 2.185   | 2.19527 |
| 307 | 2.37129 | 2.35535 | 2.34051 | 2.3317  | 2.35284 |
| 306 | 2.52929 | 2.5264  | 2.50353 | 2.49823 | 2.5056 |
| 305 | 2.68721 | 2.68288 | 2.64673 | 2.62738 | 2.65 |
| 304 | 2.8505  | 2.81505 | 2.79199 | 2.76109 | 2.799 |
| 303 | 2.97916 | 2.93146 | 2.93625 | 2.8622  | 2.88129 |
| 302 | 3.03997 | 3.02976 | 3.01712 | 2.92828 | 2.91943 |
| 301 | 3.12881 | 3.05553 | 3.07882 | 2.98752 | 2.93646 |
| 300 | 3.14512 | 3.12629 | 3.07804 | 3.03773 | 3.02039 |
| 299 | 3.12222 | 3.14133 | 3.11773 | 3.05718 | 3.04773 |
| 298 | 3.17349 | 3.19632 | 3.13876 | 3.08438 | 3.05854 |
| 297 | 3.20052 | 3.17376 | 3.13311 | 3.02062 | 3.04721 |
| 296 | 3.21625 | 3.22382 | 3.18469 | 3.11392 | 3.07324 |
| 295 | 3.21179 | 3.21788 | 3.19007 | 3.10458 | 3.10956 |
| 294 | 3.30109 | 3.31584 | 3.19788 | 3.07795 | 3.15469 |
| 293 | 3.23109 | 3.27259 | 3.22791 | 3.14459 | 3.14165 |
| 292 | 3.25181 | 3.20104 | 3.23438 | 3.18793 | 3.16276 |
| 291 | 3.334   | 3.26699 | 3.21558 | 3.19881 | 3.14092 |
| 290 | 3.35061 | 3.2814  | 3.29038 | 3.17687 | 3.16709 |
| 289 | 3.34431 | 3.31882 | 3.26682 | 3.18641 | 3.20726 |
| 288 | 3.29072 | 3.30237 | 3.29689 | 3.21367 | 3.21452 |
| 287 | 3.3442  | 3.36022 | 3.3705  | 3.21635 | 3.20981 |
| 286 | 3.3833  | 3.45496 | 3.35672 | 3.21393 | 3.25933 |
| 285 | 3.33541 | 3.57932 | 3.31657 | 3.24959 | 3.21796 |
| 284 | 3.36973 | 3.50518 | 3.30564 | 3.22345 | 3.20144 |
|    |       |       |       |       |
|----|-------|-------|-------|-------|
| 283| 3.30735| 4.6392| 3.24665| 3.194 |
| 282| 3.27843| 3.62403| 3.29523| 3.19789 |
| 281| 3.31897| 3.41942| 3.24833| 3.19554 |
| 280| 3.29248| 3.52668| 3.20829| 3.18674 |
| 279| 3.26373| 3.51869| 3.2423 | 3.1659 |
| 278| 3.21195| 3.37145| 3.24151| 3.17219 |
| 277| 3.21475| 3.27774| 3.18377| 3.12686 |
| 276| 3.25324| 3.22804| 3.20214| 3.13909 |
| 275| 3.21014| 3.22419| 3.16077| 3.13918 |
| 274| 3.1709 | 3.18502| 3.11233| 3.12686 |
| 273| 3.14035| 3.21491| 3.124  | 3.10622 |
| 272| 3.1112 | 3.1647 | 3.11233| 3.11803 |
| 271| 3.08902| 3.05044| 3.07128| 3.05061 |
| 270| 3.11185| 3.04282| 3.06208| 3.04337 |
| 269| 3.05613| 3.10975| 3.02599| 3.01792 |
| 268| 3.02012| 3.00604| 2.99591| 2.98297 |
| 267| 2.95774| 2.98152| 2.93627| 2.94316 |
| 266| 2.91829| 2.92294| 2.90131| 2.88947 |
| 265| 2.87837| 2.89838| 2.87096| 2.84674 |
| 264| 2.82836| 2.81608| 2.82417| 2.81802 |
| 263| 2.77554| 2.7313 | 2.78867| 2.77767 |
| 262| 2.73918| 2.69563| 2.71683| 2.71627 |
| 261| 2.6807 | 2.65089| 2.66484| 2.65561 |
| 260| 2.61891| 2.59303| 2.61352| 2.59517 |
| 259| 2.55633| 2.54233| 2.5552 | 2.55702 |
| 258| 2.50674| 2.50384| 2.50266| 2.49665 |
| 257| 2.46088| 2.4659 | 2.45748| 2.45527 |
| 256| 2.43245| 2.4269 | 2.43009| 2.42318 |
| 255| 2.42224| 2.41159| 2.41342| 2.40725 |
| 254| 2.42142| 2.41955| 2.42048| 2.41395 |
| 253| 2.43765| 2.44104| 2.44133| 2.43151 |
| 252| 2.48725| 2.48388| 2.4793 | 2.47302 |
| 251| 2.53968| 2.55175| 2.53638| 2.52709 |
| 250| 2.61999| 2.63545| 2.61655| 2.60284 |
| 249| 2.71655| 2.73331| 2.70779| 2.70355 |
| 248| 2.83606| 2.8537 | 2.83391| 2.8187 |
| 247| 2.98292| 3.00913| 2.96047| 2.94712 |
| 246| 3.13577| 3.21536| 3.13552| 3.09126 |
| 245| 3.2817 | 3.4343 | 3.27616| 3.21405 |
| 244| 3.43073| 3.59488| 3.35661| 3.32828 |
| 243| 3.48731| 3.72126| 3.48735| 3.37472 |
| 242| 3.56927| 3.73018| 3.56101| 3.46279 |
| 241| 3.63481| 4.17702| 3.57772| 3.47142 |
| 240| 3.65077| 3.95821| 3.64564| 3.49378 |
| 239| 3.72959| 3.95401| 3.60581| 3.54487 |
| 238| 3.69096| 3.67707| 3.554  | 3.55191 |
| 237| 3.6727 | 3.63635| 3.67595| 3.562 |

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|    | SI   | AI   | SI-AI | SI   | AI  |
|----|------|------|-------|------|-----|
| 236| 3.68275 | 3.66374 | 3.57358 | 3.55622 | 3.52526 |
| 235| 3.6392 | 3.76789 | 3.57046 | 3.5416 | 3.49835 |
| 234| 3.64212 | 3.65816 | 3.55262 | 3.53397 | 3.50245 |
| 233| 3.62529 | 3.66562 | 3.5918 | 3.48042 | 3.46854 |
| 232| 3.65775 | 3.61407 | 3.57447 | 3.51077 | 3.53543 |
| 231| 3.59879 | 3.46724 | 3.55259 | 3.49939 | 3.45765 |
| 230| 3.67739 | 3.52781 | 3.60564 | 3.49652 | 3.53628 |
| 229| 3.63603 | 3.52275 | 3.59006 | 3.52117 | 3.47702 |
| 228| 3.60925 | 3.66613 | 3.5603 | 3.41461 | 3.47867 |
| 227| 3.55174 | 3.65488 | 3.5788 | 3.50431 | 3.49178 |
| 226| 3.64724 | 3.68299 | 3.53808 | 3.53167 | 3.4533 |
| 225| 3.64914 | 3.50055 | 3.52065 | 3.43466 | 3.50253 |
| 224| 3.64229 | 3.49292 | 3.55342 | 3.43767 | 3.44659 |
| 223| 3.54244 | 3.63704 | 3.53928 | 3.49207 | 3.45375 |
| 222| 3.54817 | 3.59049 | 3.47952 | 3.42542 | 3.44556 |
| 221| 3.58572 | 3.65803 | 3.48654 | 3.44533 | 3.36517 |
| 220| 3.54737 | 3.62303 | 3.48656 | 3.45621 | 3.38905 |
Electrochemical investigations

Cyclic voltammetry (CV) and square wave voltammetry (SWV) experiments were performed with an AutoLab PGSTAT302 potentiostat-galvanostat controlled by resident NOVA 2.1.3 software.

A spectroelectrochemical cuvette from ALS Japan was used as electrochemical cell to scope with the very limited amount of available material. Two platinum wires served as working and auxiliary electrode respectively, and a silver/silver chloride electrode served as reference.

The measurements were conducted in HPLC grade acetonitrile (CH$_3$CN) and tetrabutyl-ammonium hexafluorophosphate (Bu$_4$NPF$_6$) was used as supporting electrolyte at a concentration of 0.1 M. All recorded potentials are given relative to Ag/AgCl/3M KCl. In all the experiments, the scan rate was 100 mV/s for CV and the pulse frequency was 15 Hz for SWV.

For all complexes (1, 2, 3, 4, 5 and 15) no redox signals at negative potentials were recorded, indicating that the ligand-centered reduction steps occur outside of the potential window accessible with our set-up and skills (-1.5 to 1.5 V). And indeed, the reduction of copper(I) diimine complexes is reported in literature between -1.5 and -1.7 V vs. SCE, corresponding to values between -1.532 and -1.732 V vs. Ag/AgCl/3M KCl.

The recorded voltamograms of the complexes 1, 2, 3, 4, 5 and 15 are displayed in figure SI5 and the extracted redox values are listed in table SI3. Due to the limited stability and/or isolation properties of the complexes 2-5, the redox studies were performed with the best available sample quality. However, the appearance of additional oxidation waves in 5 and even more pronounced in 2, is most likely rather due to impurities than due to intrinsic redox features of the parent complexes.

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3Armaroli, Chem. Soc. Rev., 2001, 30, 113-124.
Figure SI5: CV (black lines) and SWV (red lines) voltamogramms recorded in 0.1M n-Bu4NPF6/CH3CN at 25 °C. Potentials are given relative to Ag/AgCl/3M KCl.

Table SI3: Electrochemical data for complexes 1-5 and 15. The measurements are performed in 0.1M n-Bu4NPF6/CH3CN at 25 °C (WE: Pt wire; RE: Ag/AgCl/3M KCl; CE: Pt wire). a) The appearance of two oxidation signals is most likely due to the quick decomposition of the complex and not a redox feature of the parent macrocyclized complex 2l.

| Complex | E_{1/2} (V vs. Ag/AgCl/3M KCl) |
|---------|---------------------------------|
| 15      | 1.00                            |
| 4       | 1.00                            |
| 2       | 0.68, 0.93\(^a\)               |
| 5       | 0.70                            |
| 3       | 0.76                            |
| 1       | 1.01                            |