| | | | | | |
|---|---|---|---|---|---|
| 765 | 0.904 | 0.403 | 0.015 | 1.28 | C60 0.97; F20 1.01; C59 1.40; F19 1.74; C61 2.34; C58 2.71; |
| 766 | 0.936 | 0.509 | 0.827 | 1.28 | F7 2.40; F19 2.48; |
| 767 | 0.618 | 0.202 | 0.275 | 1.28 | F11 1.21; C41 2.23; C42 2.28; C38 2.39; F14 2.58; F15 2.63; C40 3.04; C43 3.06; |
| 768 | 0.647 | 0.266 | 0.816 | 1.28 | F11 1.26; C38 2.33; C37 2.48; C44 2.57; C43 2.81; C36 3.08; C46 3.09; C42 3.14; N5 3.18; |
| 769 | 0.985 | 0.651 | 0.386 | 1.28 | F17 1.63; F18 2.65; C57 2.69; F9 2.91; C58 3.10; |
| 770 | 0.571 | 0.095 | 0.514 | 1.28 | F12 1.44; F1 1.92; C35 1.94; C39 2.30; C36 2.89; C34 2.92; C38 3.02; F11 3.12; C40 3.15; |
| 771 | 0.656 | 0.605 | 0.048 | 1.28 | C11 1.02; C12 1.17; C4 1.43; N2 1.65; N1 1.91; Pd1 2.44; C10 2.49; C13 2.58; C3 2.82; |
| 772 | 0.297 | 0.309 | 0.701 | 1.28 | N3 1.23; C19 1.71; C22 1.99; Pd1 2.03; N2 2.36; C20 2.55; C16 2.63; C15 2.63; C21 2.66; |
| 773 | 0.249 | 0.809 | 0.106 | 1.28 | Pd2 1.52; N6 1.96; C65 2.19; N7 2.32; C45 2.55; C64 2.64; N8 2.74; N5 2.77; C48 2.78; |
| 774 | 0.134 | 0.845 | 0.955 | 1.28 | C53 1.17; C52 1.44; C54 1.95; N7 2.20; C55 2.44; C49 2.50; C56 2.79; C51 2.80; F16 2.84; |
| 775 | 0.384 | 0.126 | 0.954 | 1.28 | C18 0.67; C16 1.93; C17 2.51; C19 2.81; C8 2.93; C15 3.07; F4 3.12; C20 3.16; C9 3.16; |
| 776 | 0.666 | 0.118 | 0.490 | 1.28 | C66 2.17; C34 2.27; F11 2.41; C35 2.90; C65 2.94; C38 3.09; N5 3.15; N8 3.17; |
| 777 | 0.104 | 0.862 | 0.921 | 1.28 | C53 1.00; C54 1.98; C52 2.02; F17 2.57; C57 2.61; F16 2.62; C56 2.64; C51 2.85; C49 2.94; |
| 778 | 0.829 | 0.519 | 0.973 | 1.28 | F7 2.04; F20 2.28; C1 2.46; C24 2.65; C33 2.90; C2 2.98; |
| 779 | 0.875 | 0.687 | 0.274 | 1.28 | C31 1.51; C30 2.00; F9 2.17; C26 2.34; C28 2.58; C32 2.62; C29 2.63; C23 2.92; C25 2.96; |
| 780 | 0.658 | 0.474 | 0.048 | 1.28 | C34 1.68; C4 2.31; C35 2.32; C11 2.48; N1 2.58; F1 2.75; C12 2.81; N5 2.95; N2 3.05; |
| 781 | 0.335 | 0.470 | 0.133 | 1.27 | C3 1.00; C4 1.28; C11 2.05; C2 2.09; N1 2.39; C10 2.39; C1 2.70; C5 2.89; F1 2.92; |
| 782 | 0.860 | 0.391 | 0.286 | 1.27 | C55 0.86; C62 1.39; C54 1.54; N7 1.94; C61 2.19; C53 2.53; C63 2.53; C52 2.64; C60 2.92; |
| 783 | 0.496 | 0.125 | 0.021 | 1.27 | F3 1.32; C7 2.17; F14 2.32; C41 2.35; F4 2.59; C8 2.72; C40 2.76; F2 2.86; C42 2.97; |
| 784 | 0.032 | 0.581 | 0.467 | 1.27 | C53 2.50; F17 2.54; C54 2.63; |
| 785 | 0.422 | 0.988 | 0.500 | 1.27 | F1 1.20; C5 2.09; C35 2.33; C10 2.60; C11 2.60; C12 2.67; C13 2.73; F12 2.83; C34 3.05; |
| 786 | 0.289 | 0.581 | 0.160 | 1.27 | C47 2.26; C46 2.46; C2 2.58; C3 2.80; C65 2.91; C66 3.14; C1 3.20; |
| 787 | 0.369 | 0.518 | 0.816 | 1.27 | C35 1.30; C34 1.36; C36 2.34; N5 2.36; N2 2.47; C12 2.62; C37 2.76; C15 2.78; C13 3.04; |
| 788 | 0.662 | 0.734 | 0.922 | 1.27 | F5 1.76; C20 1.76; C19 2.14; C21 2.58; C16 2.86; C11 2.88; C9 2.89; C18 2.93; N3 2.97; |
| 789 | 0.915 | 0.408 | 0.263 | 1.27 | C54 1.95; C61 2.14; C60 2.31; C55 2.38; C62 2.53; F20 2.68; C56 2.88; C53 3.11; C59 3.12; |
| 790 | 0.775 | 0.533 | 0.842 | 1.27 | C2 1.30; C1 1.86; C3 2.64; F6 2.96; F7 3.02; N1 3.12; C51 3.14; |
| 791 | 0.240 | 0.518 | 0.190 | 1.27 | C2 1.65; C47 2.41; C1 2.44; C3 2.69; C51 2.87; C48 2.94; |
| 792 | 0.350 | 0.285 | 0.933 | 1.27 | C20 2.16; C12 2.22; N2 2.44; C11 2.55; F5 2.79; C18 2.96; C13 2.97; C4 3.09; C19 3.11; |
| 793 | 0.227 | 0.814 | 0.149 | 1.27 | Pd2 1.45; N7 1.74; N8 2.16; C55 2.46; N6 2.55; C65 2.69; C63 2.73; C52 2.81; C64 2.81; |
| 794 | 0.211 | 0.932 | 0.184 | 1.27 | N7 1.45; Pd2 1.61; C55 2.27; C52 2.36; N8 2.42; C33 2.42; C62 2.82; C63 2.90; N6 2.92; |
| 795 | 0.283 | 0.025 | 0.507 | 1.27 | N1 1.05; C1 1.22; C4 1.57; C2 1.76; C3 1.97; C11 2.80; Pd1 2.86; |
| 796 | 0.415 | 0.882 | 0.046 | 1.27 | C42 1.64; C43 1.69; F15 2.03; F3 2.21; C44 2.22; C36 2.25; C37 2.47; C41 2.62; C38 2.63; |
| 797 | 0.171 | 0.911 | 0.935 | 1.27 | C52 0.81; C49 0.82; C51 1.74; C53 1.85; C48 2.00; N7 2.03; C50 2.14; N6 2.82; C54 2.94; |
| 798 | 0.053 | 0.671 | 0.758 | 1.27 | C56 1.69; C61 1.95; C57 1.95; C60 2.33; C58 2.35; C59 2.51; F16 2.57; C54 2.74; F17 2.91; |
| 799 | 0.242 | 0.954 | 0.355 | 1.27 | N8 2.04; C33 2.34; Pd2 2.56; C66 2.66; C63 2.68; C1 2.73; N1 2.76; N4 2.90; C34 3.09; |
| 800 | 0.557 | 0.293 | 0.584 | 1.27 | C41 0.62; C40 0.95; C42 1.46; C39 1.76; F14 1.90; C43 2.14; F13 2.16; C38 2.22; F15 2.65; |
| 801 | 0.124 | 0.599 | 0.641 | 1.27 | C54 0.87; C55 1.15; C53 1.70; N7 1.95; C52 2.14; C62 2.19; C61 2.80; C32 3.01; |
| 802 | 0.017 | 0.040 | 0.371 | 1.27 | F8 1.92; F19 2.57; |
| 803 | 0.664 | 0.787 | 0.970 | 1.27 | C20 1.20; C19 1.35; C16 1.97; C18 2.06; C21 2.45; F5 2.51; N3 2.53; C15 2.87; C22 3.05; |
| 804 | 0.729 | 0.333 | 0.669 | 1.27 | C46 0.66; C47 0.98; C45 1.74; C48 1.91; N6 2.24; C44 2.96; C66 3.17; |
| 805 | 0.620 | 0.641 | 0.298 | 1.27 | C15 0.54; C14 1.31; C16 1.49; N2 1.75; C18 2.22; C13 2.31; C19 2.44; C12 2.52; C17 2.74; |
| 806 | 0.838 | 0.516 | 0.219 | 1.27 | C33 0.78; C32 1.00; N4 2.09; C31 2.23; C30 2.66; F20 3.05; |
| 807 | 0.563 | 0.248 | 0.720 | 1.27 | C41 1.56; C40 1.61; F13 1.97; F14 1.98; F11 2.41; C39 2.56; C42 2.61; C36 2.73; C38 2.74; |
| 808 | 0.992 | 0.698 | 0.574 | 1.26 | F18 1.74; C58 2.77; F9 2.78; F17 3.12; C26 3.16; |
| 809 | 0.658 | 0.855 | 0.561 | 1.26 | C12 1.38; C11 1.51; N2 1.67; C4 1.93; N1 2.23; Pd1 2.44; C13 2.64; C10 2.80; C15 2.83; |
| 810 | 0.884 | 0.447 | 0.701 | 1.26 | C51 1.37; C53 2.33; C49 2.35; C52 2.61; C50 3.09; F19 3.16; |
| 811 | 0.850 | 0.614 | 0.935 | 1.26 | C24 0.80; F7 1.21; C23 1.51; C25 1.94; F6 2.13; C28 2.68; F8 2.82; C26 2.94; C27 3.16; |
| 812 | 0.984 | 0.281 | 0.768 | 1.26 | F17 1.21; C57 1.71; C56 2.32; F16 2.50; F9 2.53; F18 2.61; C58 2.77; F19 3.15; |

```
957 0.994 0.077 0.174  1.20      F17  2.17; F8   3.15;
958 0.026 0.269 0.644  1.20      F17  1.80; F18  1.85; F9   2.04; C57  2.27; C58  2.30;
959 0.820 0.796 0.611  1.20      C27  2.10; C28  2.27; C26  2.46; C21  2.52; C30  2.57; C23  2.70; F10  2.80; C25  2.87; N4   2.91;
960 0.729 0.085 0.828  1.20      Pd2  0.85; N5   1.56; N6   1.94; C34  2.50; N8   2.52; N7   2.61; C37  2.64; C45  2.87; C48  3.03;
961 0.335 0.200 0.621  1.20      F5   1.61; C20  2.38; C4   2.48; C11  2.53; C9   2.53; C3   2.73; C19  2.76; C10  2.84; C21  2.85;
962 0.197 0.220 0.113  1.20      C29  0.52; C28  1.22; C22  1.41; C30  1.83; C23  2.04; F6   2.36; C21  2.38; C27  2.41; N3   2.68;
963 0.762 0.844 0.441  1.20      C1   1.89; C21  2.19; C2   2.28; N1   2.44; F6   2.48; C23  2.58; C22  2.78; C3   2.92; C28  2.93;
964 0.180 0.093 0.585  1.20      F7   1.71; C24  1.74; C23  1.94; F6   2.04; C1   2.38; C2   2.67; C25  2.84; C28  3.10;
965 0.514 0.579 0.795  1.20      C6   1.17; C7   1.54; C5   1.73; F2   2.10; C8   2.16; C10  2.43; F3   2.49; C9   2.53; F1   2.76;
966 0.571 0.160 0.633  1.20      C36  1.83; C39  1.83; C35  1.92; C40  1.94; F12  2.05; F13  2.24; C38  2.74; C41  2.88; C37  2.94;
967 0.382 0.641 0.065  1.20      F11  1.42; C38  2.05; F12  2.24; C39  2.39; F1   2.56; C35  2.92; C34  3.03;
968 0.820 0.845 0.074  1.20      F10  1.40; C27  2.10; C29  2.22; C28  2.36; C22  2.41; F6   2.49; C21  2.72; C50  2.74; C30  2.96;
969 0.687 0.042 0.183  1.20      C46  2.26; C47  2.42; F15  2.51; C3   2.61; C45  2.65; C2   2.81; C48  2.91; C17  3.03; N6   3.04;
970 0.463 0.718 0.690  1.20      F13  2.19; C38  2.39; C39  2.47; F4   2.50; F14  2.66; C40  2.68; F3   2.75; C8   2.80; C36  2.80;
971 0.846 0.378 0.057  1.20      F20  1.26; C60  1.58; C61  1.82; C62  1.88; C63  1.93; C64  2.17; C59  2.85; C55  3.04; N8   3.08;
972 0.360 0.359 0.304  1.20      C9   2.15; F5   2.22; C18  2.30; C3   2.43; C10  2.66; C8   2.72; C4   3.14;
973 0.475 0.512 0.505  1.20      F3   1.85; F2   2.38; F2   2.54; F3   2.59; C7   2.68; C7   2.84; C6   2.86; C6   2.90; F15  3.07;
974 0.597 0.783 0.641  1.20      C13  2.00; F4   2.07; C14  2.16; C12  2.31; F5   2.43; C15  2.51; N2   2.60; C8   2.91; C9   3.06;
975 0.954 0.729 0.578  1.20      F9   1.76; C26  1.90; F18  1.98; C27  2.52; C25  2.67; F10  2.88; F8   3.14;
976 0.681 0.640 0.059  1.20      N1   1.67; C4   1.71; C11  1.83; N2   1.94; C12  1.95; Pd1  2.05; C20  2.80; C1   2.83; C3   2.94;
977 0.270 0.107 0.109  1.20      N3   0.85; C19  1.68; C22  1.95; Pd1  1.98; C16  2.47; C17  2.55; N4   2.56; C29  2.74; C20  2.74;
978 0.076 0.028 0.905  1.20 void C53  2.85; F10  3.14;
979 0.072 0.830 0.528  1.20      C59  0.65; C58  1.44; F19  1.45; C60  1.63; F18  2.32; F16  2.44; C57  2.46; F20  2.55; C61  2.61;
980 0.635 0.236 0.892  1.20      F11  1.11; C38  1.47; C43  1.69; C44  1.73; C37  2.08; C36  2.72; C45  2.78; C39  2.81; C42  3.06;
981 0.326 0.776 0.550  1.19      F11  1.67; C66  2.14; C65  2.19; C38  2.28; C44  2.32; C43  2.49; C45  2.67; C37  3.03;
982 0.757 0.996 0.204  1.19      C2   2.15; C50  2.34; C48  2.40; C47  2.49; C49  2.54; C51  2.73; C3   2.95;
983 0.820 0.060 0.513  1.19      F20  1.62; C63  2.60; C60  2.72; C64  2.81; C62  2.93; C33  2.98; C1   3.04;
984 0.252 0.459 0.577  1.19      C50  1.95; N3   2.22; C17  2.60; N4   2.62; Pd1  2.64; C19  2.86; C22  2.99; N6   3.05; C49  3.11;
985 0.016 0.312 0.871  1.19      F18  1.78; F8   2.10; F9   2.11; F17  2.35; C26  2.52; C25  2.55; F19  2.70; C58  2.81; C59  3.17;
986 0.054 0.501 0.817  1.19      F8   2.28; F20  2.86; C32  2.96; C60  3.08;
987 0.062 0.658 0.284  1.19      F17  1.38; F16  1.76; C57  1.93; C56  2.10; F19  2.63; C53  2.77;
988 0.656 0.655 0.590  1.19      C18  1.55; C20  2.09; C16  2.12; C19  2.19; C17  2.73;
989 0.845 0.972 0.635  1.19      C33  1.42; C32  1.47; F20  2.51; N4   2.56; C31  2.60; C30  3.08; C1   3.12; F7   3.16; F8   3.17;
990 0.522 0.845 0.953  1.19      F3   2.09; F14  2.30; F4   2.35; C41  2.48; F13  2.59; C40  2.60; C7   2.64; C18  2.69; C8   2.80;
991 0.100 0.019 0.702  1.19      F7   1.73; C51  2.43; C24  2.94; F19  3.03;
992 0.956 0.749 0.415  1.19      F18  1.56; F9   2.46; C58  2.51; F17  2.68; C26  2.89; C25  2.93; C57  2.95;
993 0.201 0.169 0.786  1.19      F6   0.87; C23  2.18; F10  2.57; C21  2.90; C24  3.10; C28  3.11;
994 0.748 0.485 0.346  1.19      Pd2  2.01; C50  2.55; N6   2.58; N4   2.62; Pd1  2.71; N5   2.71; C33  2.79; N7   2.80; C17  3.14;
995 0.053 0.033 0.527  1.19      F8   2.00; F7   2.33; F19  2.65; C25  2.79; C24  2.94; F20  3.13;
996 0.724 0.098 0.453  1.19      C66  1.97; C65  2.14; N8   2.65; C64  2.86; C2   3.06; C1   3.09; C63  3.10; C47  3.12;
997 0.556 0.809 0.920  1.19      C18  2.00; F13  2.46; F4   2.60; C14  2.68; F5   2.81; F14  2.96; C40  3.10; C16  3.11; C15  3.16;
998 0.086 0.395 0.409  1.19      F10  1.85; C27  2.76;
999 0.907 0.686 0.222  1.19      F9   1.20; C26  1.53; C25  2.12; C31  2.25; F8   2.34; C27  2.61; C32  2.98; C30  3.09; F10  3.19;
*** 0.967 0.836 0.077  1.19      F18  2.55; F9   2.68; C26  2.98; F10  3.03; C27  3.18;
*** 0.944 0.860 0.671  1.19      F8   1.08; C25  1.77; F9   1.88; C26  2.06; F17  2.89; C24  3.09; C31  3.15;
*** 0.150 0.839 0.362  1.19      C62  0.85; C61  1.08; C63  1.47; C60  1.82; C64  2.13; C55  2.16; F20  2.17; C56  2.35; N8   2.77;
*** 0.530 0.284 0.776  1.19      F14  1.41; C41  2.03; F13  2.17; F12  2.31; C40  2.40; C39  2.53; C38  2.72; F11  2.76; F4   2.77;
*** 0.631 0.059-0.007  1.19      F15  1.88; C44  2.05; C17  2.16; C37  2.40; C42  2.46; C45  2.51; C43  2.51; C36  2.77;
```