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formula         calc_mw         m_z         day         height         location           C16 H10 N2 O2         262.07435         263.08161         1 bottom         half           C16 H10 N2 O2         262.07434         263.08161         1 bottom         half           C16 H10 N2 O2         262.07434         263.08162         1 bottom         quarter           C16 H10 N2 O2         262.07434         263.08162         1 bottom         quarter           C16 H10 N2 O2         262.07434         263.08162         1 top         quarter           C16 H10 N2 O2         262.07434         263.08162         1 bottom         quarter           C16 H10 N2 O2         262.07434         263.08162         1 bottom         quarter           C16 H10 N2 O2         262.07434         263.08162         1 bottom         quarter           C16 H10 N2 O2         262.07434         263.08162         1 top         half           C16 H10 N2 O2         262.07434         263.08162         1 top         puarter           C16 H10 N2 O2         262.07434         263.08162         1 bottom         half           C16 H10 N2 O2         262.07434         263.08162         2 bottom         half           C16 H10 N2 O2
C16 H10 N2 O2         262.07435         263.08161         1 middle half           C16 H10 N2 O2         262.07434         263.08162         1 bottom half           C16 H10 N2 O2         262.07434         263.08162         1 bottom quarter           C16 H10 N2 O2         262.07434         263.08162         1 middle half           C16 H10 N2 O2         262.07434         263.08162         1 top quarter           C16 H10 N2 O2         262.07434         263.08162         29 middle half           C16 H10 N2 O2         262.07434         263.08162         1 bottom quarter           C16 H10 N2 O2         262.07434         263.08162         1 bottom quarter           C16 H10 N2 O2         262.07434         263.08162         1 bottom quarter           C16 H10 N2 O2         262.07434         263.08162         1 top half           C16 H10 N2 O2         262.07434         263.08162         1 top half           C16 H10 N2 O2         262.07434         263.08162         1 bottom half           C16 H10 N2 O2         262.07434         263.08162         4 bottom half           C16 H10 N2 O2         262.07434         263.08162         8 bottom half           C16 H10 N2 O2         262.07434         263.08162         25 bottom half
C16 H10 N2 O2         262.07434         263.08162         1 bottom         quarter           C16 H10 N2 O2         262.07434         263.08162         1 middle         half           C16 H10 N2 O2         262.07434         263.08162         1 top         quarter           C16 H10 N2 O2         262.07434         263.08162         29 middle         half           C16 H10 N2 O2         262.07434         263.08162         1 bottom         quarter           C16 H10 N2 O2         262.07434         263.08162         1 top         half           C16 H10 N2 O2         262.07434         263.08162         1 top         half           C16 H10 N2 O2         262.07434         263.08162         1 top         quarter           C16 H10 N2 O2         262.07434         263.08162         4 bottom         half           C16 H10 N2 O2         262.07434         263.08162         4 bottom         half           C16 H10 N2 O2         262.07434         263.08162         15 bottom         half           C16 H10 N2 O2         262.07434         263.08162         25 bottom         half           C16 H10 N2 O2         262.07434         263.08162         29 bottom         quarter           C16 H10 N2 O2         262.07434
C16 H10 N2 O2         262.07434         263.08162         1 middle         half           C16 H10 N2 O2         262.07434         263.08162         1 top         quarter           C16 H10 N2 O2         262.07434         263.08162         29 middle         half           C16 H10 N2 O2         262.07434         263.08162         1 bottom         quarter           C16 H10 N2 O2         262.07434         263.08162         1 top         half           C16 H10 N2 O2         262.07434         263.08162         1 top         half           C16 H10 N2 O2         262.07434         263.08162         1 top         quarter           C16 H10 N2 O2         262.07434         263.08162         4 bottom         half           C16 H10 N2 O2         262.07434         263.08162         4 bottom         half           C16 H10 N2 O2         262.07434         263.08162         15 bottom         half           C16 H10 N2 O2         262.07434         263.08162         25 bottom         half           C16 H10 N2 O2         262.07434         263.08162         29 bottom         quarter           C16 H10 N2 O2         262.07434         263.08162         29 bottom         half           C16 H10 N2 O2         262.07431 </td
C16 H10 N2 O2         262.07434         263.08162         1 top         quarter           C16 H10 N2 O2         262.07434         263.08162         29 middle         half           C16 H10 N2 O2         262.07434         263.08162         1 bottom         quarter           C16 H10 N2 O2         262.07434         263.08162         1 middle         quarter           C16 H10 N2 O2         262.07434         263.08162         1 top         half           C16 H10 N2 O2         262.07434         263.08162         1 top         quarter           C16 H10 N2 O2         262.07434         263.08162         4 bottom         half           C16 H10 N2 O2         262.07434         263.08162         8 bottom         half           C16 H10 N2 O2         262.07434         263.08162         18 bottom         half           C16 H10 N2 O2         262.07434         263.08162         29 bottom         half           C16 H10 N2 O2         262.07434         263.08162         29 bottom         half           C16 H10 N2 O2         262.07434         263.08162         29 bottom         quarter           C16 H10 N2 O2         262.07434         263.08162         29 bottom         half           C16 H10 N2 O2         262.
C16 H10 N2 O2         262.07434         263.08162         29 middle         half           C16 H10 N2 O2         262.07434         263.08162         1 bottom         quarter           C16 H10 N2 O2         262.07434         263.08162         1 middle         quarter           C16 H10 N2 O2         262.07434         263.08162         1 top         half           C16 H10 N2 O2         262.07434         263.08162         1 top         quarter           C16 H10 N2 O2         262.07434         263.08162         4 bottom         half           C16 H10 N2 O2         262.07434         263.08162         8 bottom         half           C16 H10 N2 O2         262.07434         263.08162         15 bottom         half           C16 H10 N2 O2         262.07434         263.08162         15 bottom         half           C16 H10 N2 O2         262.07434         263.08162         29 bottom         quarter           C16 H10 N2 O2         262.07434         263.08162         29 bottom         quarter           C16 H10 N2 O2         262.07434         263.08162         29 bottom         quarter           C16 H10 N2 O2         262.07431         263.08162         29 top         half           C16 H10 N2 O2
C16 H10 N2 O2         262.07434         263.08162         1 bottom         quarter           C16 H10 N2 O2         262.07434         263.08162         1 middle         quarter           C16 H10 N2 O2         262.07434         263.08162         1 top         half           C16 H10 N2 O2         262.07434         263.08162         1 top         quarter           C16 H10 N2 O2         262.07434         263.08162         4 bottom         half           C16 H10 N2 O2         262.07434         263.08162         8 bottom         half           C16 H10 N2 O2         262.07434         263.08162         15 bottom         half           C16 H10 N2 O2         262.07434         263.08162         15 bottom         half           C16 H10 N2 O2         262.07434         263.08162         25 bottom         half           C16 H10 N2 O2         262.07434         263.08162         29 bottom         quarter           C16 H10 N2 O2         262.07434         263.08162         29 bottom         half           C16 H10 N2 O2         262.07431         263.08162         29 top         half           C16 H10 N2 O2         262.07431         263.08159         1 middle         half           C16 H10 N2 O3         262.074
C16 H10 N2 O2         262.07434         263.08162         1 middle         quarter           C16 H10 N2 O2         262.07434         263.08162         1 top         half           C16 H10 N2 O2         262.07434         263.08162         1 top         quarter           C16 H10 N2 O2         262.07434         263.08162         4 bottom         half           C16 H10 N2 O2         262.07434         263.08162         8 bottom         half           C16 H10 N2 O2         262.07434         263.08162         15 bottom         half           C16 H10 N2 O2         262.07434         263.08162         15 bottom         half           C16 H10 N2 O2         262.07434         263.08162         25 bottom         half           C16 H10 N2 O2         262.07434         263.08162         29 bottom         quarter           C16 H10 N2 O2         262.07434         263.08162         29 bottom         half           C16 H10 N2 O2         262.07434         263.08162         29 top         half           C16 H10 N2 O2         262.07431         263.08159         1 middle         half           C16 H10 N2 O2         262.07431         263.08159         1 bottom         half           C16 H10 N2 O3         262.07431<
C16 H10 N2 O2         262.07434         263.08162         1 top         half           C16 H10 N2 O2         262.07434         263.08162         1 top         quarter           C16 H10 N2 O2         262.07434         263.08162         4 bottom         half           C16 H10 N2 O2         262.07434         263.08162         8 bottom         half           C16 H10 N2 O2         262.07434         263.08162         15 bottom         half           C16 H10 N2 O2         262.07434         263.08162         18 bottom         half           C16 H10 N2 O2         262.07434         263.08162         29 bottom         half           C16 H10 N2 O2         262.07434         263.08162         29 bottom         quarter           C16 H10 N2 O2         262.07434         263.08162         29 middle         half           C16 H10 N2 O2         262.07434         263.08162         29 top         half           C16 H10 N2 O2         262.07431         263.08159         1 middle         half           C16 H10 N2 O2         262.07431         263.08159         8 bottom         half           C16 H10 N2 O2         262.07431         263.08159         8 bottom         half           C6 H13 N O4         163.08448
C16 H10 N2 O2         262.07434         263.08162         1 top         quarter           C16 H10 N2 O2         262.07434         263.08162         4 bottom         half           C16 H10 N2 O2         262.07434         263.08162         8 bottom         half           C16 H10 N2 O2         262.07434         263.08162         15 bottom         half           C16 H10 N2 O2         262.07434         263.08162         25 bottom         half           C16 H10 N2 O2         262.07434         263.08162         29 bottom         quarter           C16 H10 N2 O2         262.07434         263.08162         29 bottom         quarter           C16 H10 N2 O2         262.07434         263.08162         29 bottom         quarter           C16 H10 N2 O2         262.07434         263.08162         29 top         half           C16 H10 N2 O2         262.07431         263.08159         1 middle         half           C16 H10 N2 O2         262.07431         263.08159         1 top         half           C6 H13 N O4         163.08448         164.09175         1 top         half           C6 H13 N O4         163.08448         164.09175         20 bottom         half           C6 H13 N O4         163.08448
C16 H10 N2 O2         262.07434         263.08162         4 bottom         half           C16 H10 N2 O2         262.07434         263.08162         8 bottom         half           C16 H10 N2 O2         262.07434         263.08162         15 bottom         half           C16 H10 N2 O2         262.07434         263.08162         18 bottom         half           C16 H10 N2 O2         262.07434         263.08162         25 bottom         half           C16 H10 N2 O2         262.07434         263.08162         29 bottom         quarter           C16 H10 N2 O2         262.07434         263.08162         29 middle         half           C16 H10 N2 O2         262.07434         263.08162         29 top         half           C16 H10 N2 O2         262.07434         263.08162         29 top         half           C16 H10 N2 O2         262.07431         263.08159         1 middle         half           C6 H13 N O4         163.08448         164.09175         1 top         half           C6 H13 N O4         163.08448         164.09175         1 bottom         half           C6 H13 N O4         163.08448         164.09175         29 bottom         quarter           C6 H13 N O4         163.08448
C16 H10 N2 O2         262.07434         263.08162         8 bottom         half           C16 H10 N2 O2         262.07434         263.08162         15 bottom         half           C16 H10 N2 O2         262.07434         263.08162         18 bottom         half           C16 H10 N2 O2         262.07434         263.08162         25 bottom         half           C16 H10 N2 O2         262.07434         263.08162         29 bottom         quarter           C16 H10 N2 O2         262.07434         263.08162         29 middle         half           C16 H10 N2 O2         262.07434         263.08162         29 top         half           C16 H10 N2 O2         262.07431         263.08159         1 middle         half           C16 H10 N2 O2         262.07431         263.08159         8 bottom         half           C16 H10 N2 O2         262.07431         263.08159         8 bottom         half           C6 H13 N O4         163.08448         164.09175         1 top         half           C6 H13 N O4         163.08448         164.09175         4 bottom         half           C6 H13 N O4         163.08448         164.09175         29 bottom         quarter           C6 H13 N O4         163.08448
C16 H10 N2 O2         262.07434         263.08162         15 bottom         half           C16 H10 N2 O2         262.07434         263.08162         18 bottom         half           C16 H10 N2 O2         262.07434         263.08162         25 bottom         half           C16 H10 N2 O2         262.07434         263.08162         29 bottom         quarter           C16 H10 N2 O2         262.07434         263.08162         29 middle         half           C16 H10 N2 O2         262.07434         263.08159         1 middle         half           C16 H10 N2 O2         262.07431         263.08159         1 middle         half           C16 H10 N2 O2         262.07431         263.08159         8 bottom         half           C6 H13 N O4         163.08448         164.09175         1 top         half           C6 H13 N O4         163.08448         164.09175         4 bottom         half           C6 H13 N O4         163.08448         164.09175         22 bottom         half           C6 H13 N O4         163.08448         164.09175         29 bottom         quarter           C6 H13 N O4         163.08448         164.09175         29 bottom         half           C6 H13 N O4         163.08448
C16 H10 N2 O2         262.07434         263.08162         18 bottom         half           C16 H10 N2 O2         262.07434         263.08162         25 bottom         half           C16 H10 N2 O2         262.07434         263.08162         29 bottom         quarter           C16 H10 N2 O2         262.07434         263.08162         29 middle         half           C16 H10 N2 O2         262.07434         263.08162         29 top         half           C16 H10 N2 O2         262.07431         263.08159         1 middle         half           C16 H10 N2 O2         262.07431         263.08159         8 bottom         half           C6 H13 N O4         163.08448         164.09175         1 top         half           C6 H13 N O4         163.08448         164.09175         4 bottom         half           C6 H13 N O4         163.08448         164.09175         22 bottom         half           C6 H13 N O4         163.08448         164.09175         29 bottom         quarter           C6 H13 N O4         163.08448         164.09175         29 bottom         paidle           C6 H13 N O4         163.08448         164.09175         29 bottom         paidle           C6 H13 N O4         163.08448
C16 H10 N2 O2         262.07434         263.08162         25 bottom         half           C16 H10 N2 O2         262.07434         263.08162         29 bottom         quarter           C16 H10 N2 O2         262.07434         263.08162         29 middle         half           C16 H10 N2 O2         262.07434         263.08162         29 top         half           C16 H10 N2 O2         262.07431         263.08159         1 middle         half           C16 H10 N2 O2         262.07431         263.08159         8 bottom         half           C6 H13 N O4         163.08448         164.09175         1 top         half           C6 H13 N O4         163.08448         164.09175         4 bottom         half           C6 H13 N O4         163.08448         164.09175         22 bottom         half           C6 H13 N O4         163.08448         164.09175         29 bottom         quarter           C6 H13 N O4         163.08448         164.09175         29 bottom         half           C6 H13 N O4         163.08448         164.09175         29 top         quarter           C6 H13 N O4         163.08448         164.09175         29 top         quarter           C6 H13 N O4         163.08448
C16 H10 N2 O2         262.07434         263.08162         29 bottom         quarter           C16 H10 N2 O2         262.07434         263.08162         29 middle         half           C16 H10 N2 O2         262.07434         263.08162         29 top         half           C16 H10 N2 O2         262.07431         263.08159         1 middle         half           C16 H10 N2 O2         262.07431         263.08159         8 bottom         half           C6 H13 N O4         163.08448         164.09175         1 top         half           C6 H13 N O4         163.08448         164.09175         4 bottom         half           C6 H13 N O4         163.08448         164.09175         22 bottom         half           C6 H13 N O4         163.08448         164.09175         29 bottom         quarter           C6 H13 N O4         163.08448         164.09175         29 bottom         quarter           C6 H13 N O4         163.08448         164.09175         29 bottom         half           C6 H13 N O4         163.08448         164.09175         29 top         quarter           C6 H13 N O4         163.08448         164.09175         29 top         quarter           C22 H30 F3 N5 O8         549.207
C16 H10 N2 O2         262.07434         263.08162         29 middle         half           C16 H10 N2 O2         262.07434         263.08162         29 top         half           C16 H10 N2 O2         262.07431         263.08159         1 middle         half           C16 H10 N2 O2         262.07431         263.08159         8 bottom         half           C6 H13 N O4         163.08448         164.09175         1 top         half           C6 H13 N O4         163.08448         164.09175         4 bottom         half           C6 H13 N O4         163.08448         164.09175         11 bottom         half           C6 H13 N O4         163.08448         164.09175         29 bottom         quarter           C6 H13 N O4         163.08448         164.09175         29 bottom         quarter           C6 H13 N O4         163.08448         164.09175         29 bottom         quarter           C6 H13 N O4         163.08448         164.09175         29 bottom         half           C6 H13 N O4         163.08448         164.09175         29 bottom         half           C22 H30 F3 N5 O8         549.207         550.21431         29 top         quarter           C22 H30 F3 N5 O8         549.207
C16 H10 N2 O2         262.07434         263.08162         29 top         half           C16 H10 N2 O2         262.07431         263.08159         1 middle         half           C16 H10 N2 O2         262.07431         263.08159         8 bottom         half           C6 H13 N O4         163.08448         164.09175         1 top         half           C6 H13 N O4         163.08448         164.09175         4 bottom         half           C6 H13 N O4         163.08448         164.09175         22 bottom         half           C6 H13 N O4         163.08448         164.09175         29 bottom         quarter           C6 H13 N O4         163.08448         164.09175         29 middle         half           C6 H13 N O4         163.08448         164.09175         29 top         quarter           C6 H13 N O4         163.08448         164.09175         29 top         quarter           C6 H13 N O4         163.08448         164.09175         29 top         quarter           C22 H30 F3 N5 O8         549.207         550.21431         18 bottom         half           C22 H30 F3 N5 O8         549.207         550.21431         29 bottom         half           C22 H30 F3 N5 O8         549.207
C16 H10 N2 O2         262.07431         263.08159         1 middle         half           C16 H10 N2 O2         262.07431         263.08159         8 bottom         half           C6 H13 N O4         163.08448         164.09175         1 top         half           C6 H13 N O4         163.08448         164.09175         4 bottom         half           C6 H13 N O4         163.08448         164.09175         11 bottom         half           C6 H13 N O4         163.08448         164.09175         22 bottom         quarter           C6 H13 N O4         163.08448         164.09175         29 bottom         quarter           C6 H13 N O4         163.08448         164.09175         29 top         quarter           C6 H13 N O4         163.08448         164.09175         29 top         quarter           C6 H13 N O4         163.08448         164.09175         29 top         quarter           C22 H30 F3 N5 O8         549.207         550.21431         18 bottom         half           C22 H30 F3 N5 O8         549.207         550.21431         29 bottom         half           C22 H30 F3 N5 O8         549.207         550.21431         29 top         half           C22 H30 F3 N5 O8         549.207
C16 H10 N2 O2         262.07431         263.08159         8 bottom         half           C6 H13 N O4         163.08448         164.09175         1 top         half           C6 H13 N O4         163.08448         164.09175         4 bottom         half           C6 H13 N O4         163.08448         164.09175         22 bottom         half           C6 H13 N O4         163.08448         164.09175         29 bottom         quarter           C6 H13 N O4         163.08448         164.09175         29 middle         half           C6 H13 N O4         163.08448         164.09175         29 top         quarter           C6 H13 N O4         163.08448         164.09175         29 top         quarter           C6 H13 N O4         163.08448         164.09175         29 top         quarter           C22 H30 F3 N5 O8         549.207         550.21431         18 bottom         half           C22 H30 F3 N5 O8         549.207         550.21431         29 bottom         half           C22 H30 F3 N5 O8         549.207         550.21431         29 top         half           C22 H30 F3 N5 O8         549.207         550.21431         29 top         half           C22 H30 F3 N5 O8         549.207
C6 H13 N O4         163.08448         164.09175         1 top         half           C6 H13 N O4         163.08448         164.09175         4 bottom         half           C6 H13 N O4         163.08448         164.09175         11 bottom         half           C6 H13 N O4         163.08448         164.09175         22 bottom         half           C6 H13 N O4         163.08448         164.09175         29 bottom         quarter           C6 H13 N O4         163.08448         164.09175         29 middle         half           C6 H13 N O4         163.08448         164.09175         29 top         quarter           C22 H30 F3 N5 O8         549.207         550.21431         18 bottom         half           C22 H30 F3 N5 O8         549.207         550.21431         22 bottom         half           C22 H30 F3 N5 O8         549.207         550.21431         29 bottom         half           C22 H30 F3 N5 O8         549.207         550.21431         29 top         half           C22 H30 F3 N5 O8         549.207         550.21431         29 top         half           C22 H30 F3 N5 O8         549.207         550.21431         29 top         half           C22 H30 F3 N5 O8         549.207
C6 H13 N O4         163.08448         164.09175         4 bottom         half           C6 H13 N O4         163.08448         164.09175         11 bottom         half           C6 H13 N O4         163.08448         164.09175         22 bottom         half           C6 H13 N O4         163.08448         164.09175         29 bottom         quarter           C6 H13 N O4         163.08448         164.09175         29 middle         half           C6 H13 N O4         163.08448         164.09175         29 top         quarter           C22 H30 F3 N5 O8         549.207         550.21431         18 bottom         half           C22 H30 F3 N5 O8         549.207         550.21431         22 bottom         half           C22 H30 F3 N5 O8         549.207         550.21431         29 middle         half           C22 H30 F3 N5 O8         549.207         550.21431         29 top         half           C22 H30 F3 N5 O8         549.207         550.21431         29 top         quarter           C22 H30 F3 N5 O8         549.207         550.21431         29 top         quarter           C22 H30 F3 N5 O8         549.207         550.21431         29 top         quarter           C22 H26 N6 O2         406.21206
C6 H13 N O4         163.08448         164.09175         11 bottom         half           C6 H13 N O4         163.08448         164.09175         22 bottom         half           C6 H13 N O4         163.08448         164.09175         29 bottom         quarter           C6 H13 N O4         163.08448         164.09175         29 middle         half           C6 H13 N O4         163.08448         164.09175         29 top         quarter           C22 H30 F3 N5 O8         549.207         550.21431         18 bottom         half           C22 H30 F3 N5 O8         549.207         550.21431         22 bottom         half           C22 H30 F3 N5 O8         549.207         550.21431         29 bottom         half           C22 H30 F3 N5 O8         549.207         550.21431         29 middle         half           C22 H30 F3 N5 O8         549.207         550.21431         29 top         quarter           C22 H30 F3 N5 O8         549.207         550.21431         29 top         quarter           C22 H30 F3 N5 O8         549.207         550.21431         29 top         quarter           C22 H30 F3 N5 O8         549.207         550.21431         29 top         quarter           C22 H30 N6 O2         40
C6 H13 N O4         163.08448         164.09175         22 bottom         half           C6 H13 N O4         163.08448         164.09175         29 bottom         quarter           C6 H13 N O4         163.08448         164.09175         29 middle         half           C6 H13 N O4         163.08448         164.09175         29 top         quarter           C22 H30 F3 N5 O8         549.207         550.21431         18 bottom         half           C22 H30 F3 N5 O8         549.207         550.21431         29 bottom         half           C22 H30 F3 N5 O8         549.207         550.21431         29 middle         half           C22 H30 F3 N5 O8         549.207         550.21431         29 top         half           C22 H30 F3 N5 O8         549.207         550.21431         29 top         quarter           C22 H30 F3 N5 O8         549.207         550.21431         29 top         quarter           C22 H30 F3 N5 O8         549.207         550.21431         29 top         quarter           C22 H30 F3 N5 O8         549.207         550.21431         29 top         parter           C22 H30 F3 N5 O8         406.21206         407.21934         1 middle         half           C22 H26 N6 O2         40
C6 H13 N O4         163.08448         164.09175         29 bottom         quarter           C6 H13 N O4         163.08448         164.09175         29 middle         half           C6 H13 N O4         163.08448         164.09175         29 top         quarter           C22 H30 F3 N5 O8         549.207         550.21431         18 bottom         half           C22 H30 F3 N5 O8         549.207         550.21431         22 bottom         half           C22 H30 F3 N5 O8         549.207         550.21431         29 bottom         half           C22 H30 F3 N5 O8         549.207         550.21431         29 middle         half           C22 H30 F3 N5 O8         549.207         550.21431         29 top         half           C22 H30 F3 N5 O8         549.207         550.21431         29 top         quarter           C22 H30 F3 N5 O8         549.207         550.21431         29 top         half           C22 H26 N6 O2         406.21206         407.21934         1 middle         half           C22 H26 N6 O2         406.21206         407.21934         4 bottom         half           C22 H26 N6 O2         406.21206         407.21934         15 bottom         half
C6 H13 N O4         163.08448         164.09175         29 middle         half           C6 H13 N O4         163.08448         164.09175         29 top         quarter           C22 H30 F3 N5 O8         549.207         550.21431         18 bottom         half           C22 H30 F3 N5 O8         549.207         550.21431         22 bottom         half           C22 H30 F3 N5 O8         549.207         550.21431         29 bottom         half           C22 H30 F3 N5 O8         549.207         550.21431         29 middle         half           C22 H30 F3 N5 O8         549.207         550.21431         29 top         half           C22 H30 F3 N5 O8         549.207         550.21431         29 top         quarter           C22 H30 F3 N5 O8         549.207         550.21431         29 top         quarter           C22 H30 F3 N5 O8         549.207         550.21431         29 top         half           C22 H30 F3 N5 O8         406.21206         407.21934         1 middle         half           C22 H26 N6 O2         406.21206         407.21934         4 bottom         half           C22 H26 N6 O2         406.21206         407.21934         15 bottom         half
C6 H13 N O4         163.08448         164.09175         29 top         quarter           C22 H30 F3 N5 O8         549.207         550.21431         18 bottom         half           C22 H30 F3 N5 O8         549.207         550.21431         22 bottom         half           C22 H30 F3 N5 O8         549.207         550.21431         29 bottom         half           C22 H30 F3 N5 O8         549.207         550.21431         29 middle         half           C22 H30 F3 N5 O8         549.207         550.21431         29 top         quarter           C22 H30 F3 N5 O8         549.207         550.21431         29 top         quarter           C22 H26 N6 O2         406.21206         407.21934         1 middle         half           C22 H26 N6 O2         406.21206         407.21934         4 bottom         half           C22 H26 N6 O2         406.21206         407.21934         15 bottom         half
C22 H30 F3 N5 O8         549.207         550.21431         18 bottom         half           C22 H30 F3 N5 O8         549.207         550.21431         22 bottom         half           C22 H30 F3 N5 O8         549.207         550.21431         29 bottom         half           C22 H30 F3 N5 O8         549.207         550.21431         29 middle         half           C22 H30 F3 N5 O8         549.207         550.21431         29 top         half           C22 H30 F3 N5 O8         549.207         550.21431         29 top         quarter           C22 H30 F3 N5 O8         549.207         550.21431         29 top         half           C22 H30 F3 N5 O8         406.21206         407.21934         1 middle         half           C22 H26 N6 O2         406.21206         407.21934         4 bottom         half           C22 H26 N6 O2         406.21206         407.21934         15 bottom         half
C22 H30 F3 N5 O8         549.207         550.21431         22 bottom         half           C22 H30 F3 N5 O8         549.207         550.21431         29 bottom         half           C22 H30 F3 N5 O8         549.207         550.21431         29 middle         half           C22 H30 F3 N5 O8         549.207         550.21431         29 top         half           C22 H30 F3 N5 O8         549.207         550.21431         29 top         quarter           C22 H26 N6 O2         406.21206         407.21934         1 middle         half           C22 H26 N6 O2         406.21206         407.21934         4 bottom         half           C22 H26 N6 O2         406.21206         407.21934         15 bottom         half
C22 H30 F3 N5 O8       549.207       550.21431       29 bottom       half         C22 H30 F3 N5 O8       549.207       550.21431       29 middle       half         C22 H30 F3 N5 O8       549.207       550.21431       29 top       half         C22 H30 F3 N5 O8       549.207       550.21431       29 top       quarter         C22 H26 N6 O2       406.21206       407.21934       1 middle       half         C22 H26 N6 O2       406.21206       407.21934       4 bottom       half         C22 H26 N6 O2       406.21206       407.21934       15 bottom       half
C22 H30 F3 N5 O8       549.207       550.21431       29 middle       half         C22 H30 F3 N5 O8       549.207       550.21431       29 top       half         C22 H30 F3 N5 O8       549.207       550.21431       29 top       quarter         C22 H26 N6 O2       406.21206       407.21934       1 middle       half         C22 H26 N6 O2       406.21206       407.21934       4 bottom       half         C22 H26 N6 O2       406.21206       407.21934       15 bottom       half
C22 H30 F3 N5 O8       549.207       550.21431       29 top       half         C22 H30 F3 N5 O8       549.207       550.21431       29 top       quarter         C22 H26 N6 O2       406.21206       407.21934       1 middle       half         C22 H26 N6 O2       406.21206       407.21934       4 bottom       half         C22 H26 N6 O2       406.21206       407.21934       15 bottom       half
C22 H30 F3 N5 O8       549.207       550.21431       29 top       quarter         C22 H26 N6 O2       406.21206       407.21934       1 middle       half         C22 H26 N6 O2       406.21206       407.21934       4 bottom       half         C22 H26 N6 O2       406.21206       407.21934       15 bottom       half
C22 H26 N6 O2       406.21206       407.21934       1 middle       half         C22 H26 N6 O2       406.21206       407.21934       4 bottom       half         C22 H26 N6 O2       406.21206       407.21934       15 bottom       half
C22 H26 N6 O2       406.21206       407.21934       4 bottom       half         C22 H26 N6 O2       406.21206       407.21934       15 bottom       half
C22 H26 N6 O2 406.21206 407.21934 15 bottom half
000 LI00 NO 00 400 04000 407 04004 00 haware half
C22 H26 N6 O2 406.21206 407.21934 29 bottom half
C13 H22 O7 290.13678 291.14405 4 bottom half
C13 H22 O7 290.13678 291.14405 11 bottom half
C25 H36 O5 416.25607 434.29006 18 bottom half
C25 H36 O5 416.25626 417.26353 29 bottom quarter
C24 H23 N3 O3 401.1733 402.18058 11 bottom half
C24 H23 N3 O3 401.1733 402.18058 29 middle quarter
C9 H7 N O 145.05282 146.0601 1 bottom half
C9 H7 N O 145.05282 146.0601 1 bottom quarter
C9 H7 N O 145.05282 146.0601 1 middle half
C9 H7 N O 145.05282 146.0601 1 middle quarter
C9 H7 N O 145.05282 146.0601 1 top half

C9 H7 N O	145.05282	146.0601	1 top	quarter
C9 H7 N O	145.05282	146.0601	4 bottom	half
C9 H7 N O	145.05282	146.0601	8 bottom	half
C9 H7 N O	145.05282	146.0601	11 bottom	half
C9 H7 N O	145.05282	146.0601	15 bottom	half
C9 H7 N O	145.05282	146.0601	18 bottom	half
C9 H7 N O	145.05282	146.0601	22 bottom	half
C9 H7 N O	145.05282	146.0601	25 bottom	half
C9 H7 N O	145.05282	146.0601	29 bottom	half
C9 H7 N O	145.05282	146.0601	29 bottom	quarter
C9 H7 N O	145.05282	146.0601	29 middle	half
C9 H7 N O	145.05282	146.0601	29 middle	quarter
C9 H7 N O	145.05282	146.0601	29 top	half
C9 H7 N O	145.05282	146.0601	29 top	quarter
C9 H7 N O	145.05283	146.06011	1 bottom	half
C9 H7 N O	145.05283	146.06011	1 bottom	quarter
C9 H7 N O	145.05283	146.06011	1 middle	half
C9 H7 N O	145.05283	146.06011	1 middle	quarter
C9 H7 N O	145.05283	146.06011	1 top	half
C9 H7 N O	145.05283	146.06011	1 top	quarter
C9 H7 N O	145.05283	146.06011	4 bottom	half
C9 H7 N O	145.05283	146.06011	8 bottom	half
C9 H7 N O	145.05283	146.06011	11 bottom	half
C9 H7 N O	145.05283	146.06011	15 bottom	half
C9 H7 N O	145.05283	146.06011	18 bottom	half
C9 H7 N O	145.05283	146.06011	22 bottom	half
C9 H7 N O	145.05283	146.06011	25 bottom	half
C9 H7 N O	145.05283	146.06011	29 bottom	half
C9 H7 N O	145.05283	146.06011	29 middle	half
C9 H7 N O	145.05283	146.06011	29 top	half
C9 H7 N O	145.05283	146.06011	29 top	quarter
C9 H7 N O	145.05283	146.06011	1 bottom	quarter
C9 H7 N O	145.05283	146.06011	1 middle	half
C9 H7 N O	145.05283	146.06011	1 middle	quarter
C9 H7 N O	145.05283	146.06011	1 top	half
C9 H7 N O	145.05283	146.06011	1 top	quarter
C9 H7 N O	145.05283	146.06011	4 bottom	half
C9 H7 N O	145.05283	146.06011	25 bottom	half
C9 H7 N O	145.05283	146.06011	29 bottom	half
C9 H7 N O	145.05283	146.06011	29 middle	half
C9 H7 N O	145.05283	146.06011	29 top	half
C9 H7 N O	145.05283	146.06011	29 top	quarter
C9 H7 N O	145.05282	146.0601	1 top	half
C9 H7 N O	145.05282	146.0601	1 top	quarter
C9 H7 N O	145.05282	146.0601	29 bottom	half
C9 H7 N O	145.05282	146.0601	29 middle	half
C9 H7 N O	145.05282	146.0601	29 middle	quarter
C9 H7 N O	145.05282	146.0601	29 top	half
C9 H7 N O	145.05282	146.0601	29 top	quarter
C9 H7 N O	145.05282	146.06009	29 top	quarter

C9 H7 N O	145.05283	146.06011	1 bottom	quarter
C9 H7 N O	145.05283	146.06011	4 bottom	half
C9 H7 N O	145.05283	146.06011	8 bottom	half
C9 H7 N O	145.05283	146.06011	29 middle	half
C9 H7 N O	145.05283	146.06011	29 top	half
C9 H7 N O	145.05284	146.06012	1 bottom	quarter
C9 H7 N O	145.05284	146.06012	1 middle	quarter
C9 H7 N O	145.05284	146.06012	11 bottom	half
C9 H7 N O	145.05284	146.06012	18 bottom	half
C9 H7 N O	145.05284	146.06012	29 bottom	half
C9 H7 N O	145.05284	146.06012	29 middle	half
C9 H7 N O	145.05284	146.06012	29 top	quarter
C8 H11 N5 O3	225.08727	226.09454	29 bottom	quarter
C16 H18 N2	238.14707	239.15434	29 middle	quarter
C5 H13 N2 O4 P	196.06128	197.06856	1 bottom	quarter
C5 H13 N2 O4 P	196.06128	197.06856	1 middle	half
C5 H13 N2 O4 P	196.06128	197.06856	1 top	half
C5 H13 N2 O4 P	196.06128	197.06856	1 top	quarter
C5 H13 N2 O4 P	196.06128	197.06856	8 bottom	half
C5 H13 N2 O4 P	196.06128	197.06856	11 bottom	half
C5 H13 N2 O4 P	196.06128	197.06856	15 bottom	half
C5 H13 N2 O4 P	196.06128	197.06856	18 bottom	half
C5 H13 N2 O4 P	196.06128	197.06856	29 bottom	half
C5 H13 N2 O4 P	196.06128	197.06856	29 top	half
C21 H38 N4 O8	474.26743	492.30124	29 middle	quarter
C21 H23 N3 O7	429.15228	430.15956	29 top	half
C14 H19 N O4	265.13151	266.13879	29 middle	half
C14 H19 N O4	265.13151	266.13878	29 top	half
C20 H34 O4	338.24577	361.23502	8 bottom	half
C22 H44 N6 O10	552.31458	553.32185	1 bottom	quarter
C22 H44 N6 O10	552.31458	553.32185	8 bottom	half
C22 H44 N6 O10	552.31458	553.32185	11 bottom	half
C22 H44 N6 O10	552.31458	553.32185	18 bottom	half
C22 H44 N6 O10	552.31458	553.32185	29 bottom	half
C17 H35 N5 O6	405.26031	406.26759	25 bottom	half
C17 H35 N5 O6	405.26031	406.26759	29 bottom	quarter
C17 H35 N5 O6	405.26031	406.26759	29 top	quarter
C10 H12 O4	196.07357	197.08084	4 bottom	half
C10 H12 O4	196.07357	197.08084	8 bottom	half
C10 H12 O4	196.07357	197.08084	29 bottom	half
C10 H12 O4	196.07357	197.08084	29 middle	half
C10 H12 O4	196.07357	197.08085	29 top	quarter
C10 H12 O4	196.07359	197.08086	1 middle	quarter
C10 H12 O4	196.07359	197.08086	8 bottom	half
C10 H12 O4	196.07359	197.08086	15 bottom	half
C10 H12 O4	196.07359	197.08086	25 bottom	half
C10 H12 O4	196.07359	197.08086	29 bottom	half
C10 H12 O4	196.07359	197.08086	29 middle	half
C10 H12 O4	196.07359	197.08086	29 middle	quarter
C10 H12 O4	196.07359	197.08086	29 top	quarter

C10 H12 O4	196.07357	197.08084	25 bottom	half
C10 H12 O4	196.07359	197.08087	29 middle	half
C10 H12 O4	196.07359	197.08086	25 bottom	half
C10 H12 O4	196.0736	197.08087	4 bottom	half
C10 H12 O4	196.0736	197.08087	29 middle	half
C10 H12 O4	196.0736	197.08087	29 top	half
C10 H12 O4	196.07356	197.08084	29 bottom	quarter
C10 H12 O4	196.07361	197.08088	1 middle	quarter
C6 H9 N3 O2	155.06951	156.07679	4 bottom	half
C6 H9 N3 O2	155.06951	156.07679	29 top	quarter
C16 H24 N2 O4	308.1738	309.18105	4 bottom	half
C16 H24 N2 O4	308.1738	309.181	29 middle	half
C16 H24 N2 O4	308.17378	309.18106	1 bottom	quarter
C16 H24 N2 O4	308.17378	309.18106	1 top	quarter
C16 H24 N2 O4	308.17378	309.18106	15 bottom	half
C16 H24 N2 O4	308.17378	309.18106	18 bottom	half
C16 H24 N2 O4	308.17378	309.18106	29 bottom	half
C16 H24 O4	280.16761	281.17489	1 middle	half
C16 H24 O4	280.16761	281.17489	1 middle	quarter
C16 H24 O4	280.16761	281.17489	25 bottom	half
C16 H24 O4	280.16761	281.17489	29 bottom	half
C16 H24 O4	280.16747	281.17475	1 middle	quarter
C16 H24 O4	280.16759	281.17487	25 bottom	half
C12 H11 N3 O2	229.08522	230.0925	1 bottom	half
C12 H11 N3 O2	229.08522	230.0925	1 bottom	quarter
C12 H11 N3 O2	229.08522	230.0925	1 middle	half
C12 H11 N3 O2	229.08522	230.0925	1 middle	quarter
C12 H11 N3 O2	229.08522	230.0925	1 top	half
C12 H11 N3 O2	229.08522	230.0925	1 top	quarter
C12 H11 N3 O2	229.08522	230.0925	4 bottom	half
C12 H11 N3 O2	229.08522	230.0925	8 bottom	half
C12 H11 N3 O2	229.08522	230.0925	11 bottom	half
C12 H11 N3 O2	229.08522	230.0925	15 bottom	half
C12 H11 N3 O2	229.08522	230.0925	18 bottom	half
C12 H11 N3 O2	229.08522	230.0925	25 bottom	half
C12 H11 N3 O2	229.08522	230.0925	29 bottom	half
C12 H11 N3 O2	229.08522	230.0925	29 bottom	quarter
C12 H11 N3 O2	229.08522	230.0925	29 middle	half
C12 H11 N3 O2	229.08522	230.0925	29 middle	quarter
C12 H11 N3 O2	229.08523	230.0925	1 bottom	quarter
C12 H11 N3 O2	229.08523	230.0925	1 middle	half
C12 H11 N3 O2	229.08523	230.0925	1 middle	quarter
C12 H11 N3 O2	229.08523	230.0925	1 top	half
C12 H11 N3 O2	229.08523	230.0925	1 top	quarter
C12 H11 N3 O2	229.08523	230.0925	4 bottom	half
C12 H11 N3 O2	229.08523	230.0925	8 bottom	half
C12 H11 N3 O2	229.08523	230.0925	11 bottom	half
C12 H11 N3 O2	229.08523	230.0925	15 bottom	half
C12 H11 N3 O2	229.08523	230.0925	18 bottom	half
C12 H11 N3 O2	229.08523	230.0925	22 bottom	half

C12 H11 N3 O2	229.08523	230.0925	29 bottom	half
C12 H11 N3 O2	229.08523	230.0925	29 bottom	quarter
C12 H11 N3 O2	229.08523	230.0925	29 middle	quarter
C12 H11 N3 O2	229.08524	230.09252	29 middle	half
C12 H11 N3 O2	229.08524	230.09252	29 middle	quarter
C21 H26 Cl2 O	364.13744	365.14472	4 bottom	half
C13 H19 Cl2 N O2	291.07918	292.08646	1 bottom	half
C13 H19 Cl2 N O2	291.07918	292.08646	1 bottom	quarter
C13 H19 Cl2 N O2	291.07918	292.08646	1 middle	quarter
C13 H19 Cl2 N O2	291.07918	292.08646	1 top	half
C13 H19 Cl2 N O2	291.07918	292.08646	1 top	quarter
C13 H19 Cl2 N O2	291.07918	292.08646	4 bottom	half
C13 H19 Cl2 N O2	291.07918	292.08646	8 bottom	half
C13 H19 Cl2 N O2	291.07918	292.08646	11 bottom	half
C13 H19 Cl2 N O2	291.07918	292.08646	15 bottom	half
C13 H19 Cl2 N O2	291.07918	292.08646	18 bottom	half
C10 H13 N5 O3	251.10228	269.13606	1 bottom	half
C10 H13 N5 O3	251.10228	269.13606	1 bottom	quarter
C10 H13 N5 O3	251.10228	269.13606	1 middle	half
C10 H13 N5 O3	251.10228	269.13606	1 middle	quarter
C10 H13 N5 O3	251.10228	269.13606	1 top	quarter
C10 H13 N5 O3	251.10228	269.13606	4 bottom	half
C10 H13 N5 O3	251.10228	269.13606	8 bottom	half
C10 H13 N5 O3	251.10228	269.13606	15 bottom	half
C10 H13 N5 O3	251.10196	252.10919	1 middle	quarter
C10 H13 N5 O3	251.10196	252.10919	18 bottom	half
C10 H13 N5 O3	251.10196	252.10919	29 middle	quarter
C10 H13 N5 O3	251.10196	252.10919	29 top	half
C10 H13 N5 O3	251.10193	252.10921	4 bottom	half
C19 H20 O3	296.14143	297.14871	1 bottom	half
C19 H20 O3	296.14143	297.14871	1 bottom	quarter
C19 H20 O3	296.14143	297.14871	1 middle	half
C19 H20 O3	296.14143	297.14871	1 middle	quarter
C19 H20 O3	296.14143	297.14871	1 top	half
C19 H20 O3	296.14143	297.14871	1 top	quarter
C19 H20 O3	296.14143	297.14871	4 bottom	half
C19 H20 O3	296.14143	297.14871	8 bottom	half
C19 H20 O3	296.14143	297.14871	11 bottom	half
C19 H20 O3	296.14143	297.14871	15 bottom	half
C19 H20 O3	296.14143	297.14871	18 bottom	half
C19 H20 O3	296.14143	297.14871	25 bottom	half
C19 H20 O3	296.14143	297.14871	29 bottom	half
C19 H20 O3	296.14143	297.14871	29 middle	half
C19 H20 O3	296.14143	297.14871	29 top	half
C19 H20 O3	296.14143	297.14871	29 top	quarter
C19 H20 O3	296.14142	297.14869	22 bottom	half
C19 H20 O3	296.14142	297.14869	29 middle	quarter
C19 H20 O3	296.14143	297.14871	29 bottom	quarter
C15 H23 N O4	281.16309	282.17036	29 top	quarter
C6 H10 N6 O	182.09194	183.09921	1 bottom	half
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C6 H10 N6 O	182.09194	183.09921	1 bottom	quarter
C6 H10 N6 O	182.09194	183.09921	1 middle	half
C6 H10 N6 O	182.09194	183.09921	1 middle	quarter
C6 H10 N6 O	182.09194	183.09921	1 top	half
C6 H10 N6 O	182.09194	183.09921	1 top	quarter
C6 H10 N6 O	182.09194	183.09921	4 bottom	half
C6 H10 N6 O	182.09194	183.09921	8 bottom	half
C6 H10 N6 O	182.09194	183.09921	11 bottom	half
C6 H10 N6 O	182.09194	183.09921	15 bottom	half
C6 H10 N6 O	182.09194	183.09921	18 bottom	half
C6 H10 N6 O	182.09194	183.09921	22 bottom	half
C6 H10 N6 O	182.09194	183.09921	25 bottom	half
C6 H10 N6 O	182.09194	183.09921	29 bottom	half
C6 H10 N6 O	182.09194	183.09921	29 bottom	quarter
C6 H10 N6 O	182.09194	183.09921	29 middle	half
C6 H10 N6 O	182.09194	183.09921	29 middle	quarter
C6 H10 N6 O	182.09194	183.09921	29 top	half
C6 H10 N6 O	182.09194	183.09921	29 top	quarter
C21 H20 O9	416.11068	439.09989	1 bottom	half
C21 H20 O9	416.11068	439.09989	1 bottom	quarter
C21 H20 O9	416.11068	439.09989	1 middle	half
C21 H20 O9	416.11068	439.09989	1 middle	quarter
C21 H20 O9	416.11068	439.09989	1 top	half
C21 H20 O9	416.11068	439.09989	1 top	quarter
C21 H20 O9	416.11068	439.09989	4 bottom	half
C21 H20 O9	416.11068	439.09989	8 bottom	half
C21 H20 O9	416.11068	439.09989	11 bottom	half
C21 H20 O9	416.11068	439.09989	15 bottom	half
C21 H20 O9	416.11068	439.09989	18 bottom	half
C21 H20 O9	416.11068	439.09989	22 bottom	half
C21 H20 O9	416.11068	439.09989	25 bottom	half
C21 H20 O9	416.11068	439.09989	29 bottom	half
C21 H20 O9	416.11068	439.09989	29 bottom	quarter
C21 H20 O9	416.11068	439.09989	29 middle	half
C21 H20 O9	416.11068	439.09989	29 middle	quarter
C21 H20 O9	416.11068	439.09989	29 top	half
C21 H20 O9	416.11068	439.09989	29 top	quarter
C21 H20 O9	416.11066	417.11797	29 middle	quarter
C15 H15 N3 O	253.12159	254.12887	22 bottom	half
C15 H15 N3 O	253.12159	254.12887	29 bottom	half
C15 H15 N3 O	253.12159	254.12887	29 middle	half
C15 H15 N3 O	253.12159	254.12887	29 middle	quarter
C15 H15 N3 O	253.12159	254.12887	29 top	quarter
C15 H15 N3 O	253.12162	254.1289	18 bottom	half
C14 H15 CI N2 O2	278.08239	279.08967	1 bottom	half
C14 H15 CI N2 O2	278.08239	279.08967	1 bottom	quarter
C14 H15 CI N2 O2	278.08239	279.08967	1 middle	half
C14 H15 CI N2 O2	278.08239	279.08967	1 top	half
C14 H15 CI N2 O2	278.08239	279.08967	1 top	quarter
C14 H15 CI N2 O2	278.08239	279.08967	4 bottom	half

C14 H15 CI N2 O2	278.08239	279.08967	8 bottom	half
C14 H15 CI N2 O2	278.08239	279.08967	11 bottom	half
C14 H15 CI N2 O2	278.08239	279.08967	15 bottom	half
C14 H15 CI N2 O2	278.08239	279.08967	18 bottom	half
C14 H15 CI N2 O2	278.08239	279.08967	22 bottom	half
C14 H15 CI N2 O2	278.08239	279.08967	29 bottom	half
C14 H15 CI N2 O2	278.08239	279.08967	29 middle	half
C14 H15 CI N2 O2	278.08239	279.08967	29 top	half
C17 H18 F3 N3 O3	369.12999	370.13727	1 top	half
C22 H28 F2 O5	410.19174	411.19902	1 top	quarter
C8 H8 O5	184.03722	185.0445	1 middle	quarter
C15 H32 N4 O5	348.23881	349.24628	1 bottom	half
C10 H13 N O2	179.09466	180.10194	15 bottom	half
C10 H13 N O2	179.09466	180.10194	29 middle	quarter
C10 H13 N O2	179.09466	180.10194	1 bottom	half
C10 H13 N O2	179.09466	180.10194	1 middle	half
C10 H13 N O2	179.09465	180.10193	29 top	half
C10 H13 N O2	179.09465	180.10193	29 top	quarter
C10 H14 O4	198.08923	199.0965	4 bottom	half
C10 H14 O4	198.08923	199.0965	29 top	half
C10 H14 O4	198.08927	199.09653	1 top	half
C29 H38 N8 O8	626.28168	644.31551	1 bottom	quarter
C29 H38 N8 O8	626.28168	644.31551	1 middle	half
C29 H38 N8 O8	626.28168	644.31551	1 middle	quarter
C29 H38 N8 O8	626.28168	644.31551	1 top	quarter
C29 H38 N8 O8	626.28168	644.31551	4 bottom	half
C29 H38 N8 O8	626.28168	644.31551	15 bottom	half
C29 H38 N8 O8	626.28168	644.31551	18 bottom	half
C29 H38 N8 O8	626.28168	644.31551	29 bottom	half
C29 H38 N8 O8	626.28168	644.31551	29 middle	quarter
C18 H18 O2	266.13084	267.13813	29 middle	quarter
C27 H21 N3 O5	467.14949	468.15677	1 bottom	quarter
C16 H12 O6	300.06348	301.07076	1 middle	quarter
C16 H12 O6	300.06348	301.07076	29 top	quarter
C16 H12 O6	300.0636	301.07088	4 bottom	half
C16 H12 O6	300.0636	301.07088	29 bottom	half
C16 H12 O6	300.0636	301.07088	29 middle	quarter
C16 H12 O6	300.0636	301.07088	29 top	half
C16 H12 O6	300.0636	301.07088	29 top	quarter
C40 H67 N O14	785.45563	786.46291	29 bottom	half
C40 H67 N O14	785.45563	786.46291	29 top	half
C23 H34 O5	390.24048	391.24761	1 top	quarter
C23 H34 O5	390.24048	391.24761	15 bottom	half
C31 H44 O7	528.30639	529.31366	1 middle	half
C16 H18 O3	258.12572	259.133	25 bottom	half
C18 H23 CI N2 O2	334.14566	335.15294	15 bottom	half
C18 H23 CI N2 O2	334.14566	335.15294	29 bottom	half
C18 H23 CI N2 O2	334.14481	335.15209	29 middle	half
C15 H20 N6 O5	364.14935	365.15663	1 bottom	quarter
C15 H20 N6 O5	364.14935	365.15663	1 middle	half

C15 H20 N6 O5	364.14935	365.15663	1 top	half
C15 H20 N6 O5	364.14935	365.15663	4 bottom	half
C15 H20 N6 O5	364.14935	365.15663	8 bottom	half
C15 H20 N6 O5	364.14935	365.15663	11 bottom	half
C15 H20 N6 O5	364.14935	365.15663	15 bottom	half
C15 H20 N6 O5	364.14935	365.15663	18 bottom	half
C15 H20 N6 O5	364.14935	365.15663	29 bottom	half
C15 H20 N6 O5	364.14935	365.15663	29 middle	half
C15 H20 N6 O5	364.14935	365.15663	29 middle	quarter
C15 H20 N6 O5	364.14935	365.15663	29 top	quarter
C7 H15 N O4	177.10012	178.1074	4 bottom	half
C29 H38 N4 O10	602.25741	620.29129	1 bottom	half
C29 H38 N4 O10	602.25741	620.29129	1 bottom	quarter
C29 H38 N4 O10	602.25741	620.29129	1 top	half
C29 H38 N4 O10	602.25741	620.29129	4 bottom	half
C29 H38 N4 O10	602.25741	620.29129	8 bottom	half
C29 H38 N4 O10	602.25741	620.29129	11 bottom	half
C29 H38 N4 O10	602.25741	620.29129	15 bottom	half
C29 H38 N4 O10	602.25741	620.29129	18 bottom	half
C29 H38 N4 O10	602.25741	620.29129	29 top	half
C16 H14 O6	302.07925	303.08653	25 bottom	half
C16 H14 O6	302.07925	303.08653	29 bottom	half
C16 H14 O6	302.07923	303.08651	4 bottom	half
C16 H14 O6	302.07923	303.08651	15 bottom	half
C19 H18 N6 O6	426.12926	427.13653	11 bottom	half
C19 H18 N6 O6	426.12926	427.13653	15 bottom	half
C19 H18 N6 O6	426.12905	427.13633	1 bottom	half
C19 H18 N6 O6	426.12905	427.13633	1 bottom	quarter
C19 H18 N6 O6	426.12905	427.13633	1 middle	half
C19 H18 N6 O6	426.12905	427.13633	1 top	half
C19 H18 N6 O6	426.12905	427.13633	1 top	quarter
C19 H18 N6 O6	426.12905	427.13633	11 bottom	half
C19 H18 N6 O6	426.12905	427.13633	15 bottom	half
C19 H18 N6 O6	426.1291	427.13638	1 top	half
C19 H18 N6 O6	426.1291	427.13638	4 bottom	half
C19 H18 N6 O6	426.12906	427.13634	15 bottom	half
C17 H31 CI N2 O5 S	410.16472	411.172	1 bottom	half
C17 H31 CI N2 O5 S	410.16472	411.172	1 bottom	quarter
C17 H31 CI N2 O5 S	410.16472	411.172	1 middle	half
C17 H31 CI N2 O5 S	410.16472	411.172	1 middle	quarter
C17 H31 CI N2 O5 S	410.16472	411.172	1 top	half
C17 H31 CI N2 O5 S	410.16472	411.172	1 top	quarter
C17 H31 CI N2 O5 S	410.16472	411.172	8 bottom	half
C17 H31 CI N2 O5 S	410.16472	411.172	11 bottom	half
C17 H31 CI N2 O5 S	410.16472	411.172	15 bottom	half
C17 H31 CI N2 O5 S	410.16472	411.172	18 bottom	half
C17 H31 CI N2 O5 S	410.16472	411.172	22 bottom	half
C17 H31 CI N2 O5 S	410.16472	411.172	25 bottom	half
C17 H31 CI N2 O5 S	410.16472	411.172	29 bottom	half
C17 H31 CI N2 O5 S	410.16472	411.172	29 bottom	quarter

C17 H31 CI N2 O5 S	410.16472	411.172	29 middle	half
C17 H31 CI N2 O5 S	410.16472	411.172	29 middle	quarter
C17 H31 CI N2 O5 S	410.16472	411.172	29 top	half
C17 H31 CI N2 O5 S	410.16472	411.172	29 top	quarter
C17 H31 CI N2 O5 S	410.16474	411.17202	1 middle	half
C17 H31 CI N2 O5 S	410.16474	411.17202	1 middle	quarter
C17 H31 CI N2 O5 S	410.16474	411.17202	1 top	half
C17 H31 CI N2 O5 S	410.16474	411.17202	1 top	quarter
C17 H31 CI N2 O5 S	410.16474	411.17202	18 bottom	half
C17 H31 CI N2 O5 S	410.16474	411.17202	22 bottom	half
C17 H31 CI N2 O5 S	410.16474	411.17202	29 bottom	half
C17 H31 CI N2 O5 S	410.16474	411.17202	29 bottom	quarter
C17 H31 CI N2 O5 S	410.16474	411.17202	29 middle	half
C17 H31 CI N2 O5 S	410.16474	411.17202	29 top	quarter
C17 H31 CI N2 O5 S	410.16475	411.17203	1 bottom	quarter
C17 H31 CI N2 O5 S	410.16475	411.17203	1 middle	quarter
C17 H31 CI N2 O5 S	410.16475	411.17203	1 top	quarter
C17 H31 CI N2 O5 S	410.16475	411.17203	8 bottom	half
C17 H31 CI N2 O5 S	410.16475	411.17203	11 bottom	half
C17 H31 CI N2 O5 S	410.16475	411.17203	15 bottom	half
C17 H31 CI N2 O5 S	410.16475	411.17203	22 bottom	half
C17 H31 CI N2 O5 S	410.16475	411.17203	29 bottom	half
C17 H31 CI N2 O5 S	410.16475	411.17203	29 bottom	quarter
C17 H31 CI N2 O5 S	410.16475	411.17203	29 top	quarter
C17 H31 CI N2 O5 S	410.16482	411.1721	29 bottom	quarter
C17 H31 CI N2 O5 S	410.16409	411.17134	29 top	quarter
C14 H16 N4 O3	288.1224	289.12969	1 bottom	half
C14 H16 N4 O3	288.1224	289.12969	1 bottom	quarter
C14 H16 N4 O3	288.1224	289.12969	1 middle	half
C14 H16 N4 O3	288.1224	289.12969	1 top	half
C14 H16 N4 O3	288.1224	289.12969	1 top	quarter
C14 H16 N4 O3	288.1224	289.12969	4 bottom	half
C14 H16 N4 O3	288.1224	289.12969	8 bottom	half
C14 H16 N4 O3	288.1224	289.12969	11 bottom	half
C14 H16 N4 O3	288.1224	289.12969	15 bottom	half
C14 H16 N4 O3	288.1224	289.12969	18 bottom	half
C14 H16 N4 O3	288.1224	289.12969	22 bottom	half
C14 H16 N4 O3	288.1224	289.12969	29 middle	quarter
C14 H16 N4 O3	288.1224	289.12969	29 top	half
C14 H16 N4 O3	288.1224	289.12969	29 top	quarter
C22 H34 O5	378.2415	379.24878	29 top	half
C8 H6 N2 O2	162.04299	163.05024	29 top	half
C8 H6 N2 O2	162.04299	163.05024	29 top	quarter
C8 H6 N2 O2	162.04296	163.05023	29 top	half
C8 H6 N2 O2	162.04296	163.05023	29 top	quarter
C8 H6 N2 O2	162.04296	163.05024	1 bottom	quarter
C8 H6 N2 O2	162.04296	163.05024	1 top	quarter
C8 H6 N2 O2	162.04296	163.05024	4 bottom	half
C8 H6 N2 O2	162.04296	163.05024	29 top	half
C17 H20 F6 N2 O3	414.13787	415.14514	8 bottom	half

C17 H20 F6 N2 O3	414.13787	415.14514	11 bottom	half
C17 H20 F6 N2 O3	414.13787	415.14514	15 bottom	half
C17 H20 F6 N2 O3	414.13787	415.14514	18 bottom	half
C17 H20 F6 N2 O3	414.13787	415.14514	22 bottom	half
C17 H20 F6 N2 O3	414.13787	415.14514	29 bottom	half
C17 H20 F6 N2 O3	414.13787	415.14514	29 middle	quarter
C17 H20 F6 N2 O3	414.13787	415.14514	29 top	half
C17 H20 F6 N2 O3	414.13787	415.14514	29 top	quarter
C13 H18 N4 O5	310.12654	333.11574	18 bottom	half
C22 H21 Cl3 N4 O	462.07979	463.08707	1 middle	quarter
C22 H21 Cl3 N4 O	462.07979	463.08707	22 bottom	half
C22 H21 Cl3 N4 O	462.07979	463.08707	29 bottom	half
C29 H40 O9	532.26516	533.27243	29 middle	half
C29 H40 O9	532.26469	533.27197	29 middle	half
C17 H14 N2 O3	294.10063	295.10791	1 bottom	half
C17 H14 N2 O3	294.10063	295.10791	18 bottom	half
C27 H30 N4 O3	458.23154	459.23882	25 bottom	half
C19 H37 N5 O7	447.26771	448.27498	29 middle	half
C19 H37 N5 O7	447.26771	448.27498	29 middle	quarter
C27 H40 O8	492.27357	493.28079	1 bottom	half
C27 H40 O8	492.27357	493.28079	1 bottom	quarter
C27 H40 O8	492.27357	493.28079	1 middle	half
C27 H40 O8	492.27357	493.28079	1 middle	quarter
C27 H40 O8	492.27357	493.28079	1 top	half
C27 H40 O8	492.27357	493.28079	1 top	quarter
C27 H40 O8	492.27357	493.28079	4 bottom	half
C27 H40 O8	492.27357	493.28079	8 bottom	half
C27 H40 O8	492.27357	493.28079	11 bottom	half
C27 H40 O8	492.27357	493.28079	15 bottom	half
C27 H40 O8	492.27357	493.28079	18 bottom	half
C27 H40 O8	492.27357	493.28079	22 bottom	half
C27 H40 O8	492.27357	493.28079	25 bottom	half
C27 H40 O8	492.27357	493.28079	29 bottom	half
C27 H40 O8	492.27357	493.28079	29 middle	quarter
C27 H40 O8	492.27357	493.28079	29 top	half
C27 H40 O8	492.27357	493.28079	29 top	quarter
C27 H40 O8	492.27346	515.26266	29 bottom	quarter
C22 H41 N O7	431.28823	432.29551	29 middle	quarter
C10 H12 N4 O5 S	300.05235	301.05963	4 bottom	half
C10 H12 N4 O5 S	300.05235	301.05963	25 bottom	half
C10 H12 N4 O5 S	300.05235	301.05963	29 middle	half
C10 H12 N4 O5 S	300.05235	301.05963	29 top	half
C10 H7 N3 S	201.03608	202.04336	1 bottom	half
C10 H7 N3 S	201.03608	202.04336	1 bottom	quarter
C10 H7 N3 S	201.03608	202.04336	1 middle	half
C10 H7 N3 S	201.03608	202.04336	1 middle	quarter
C10 H7 N3 S	201.03608	202.04336	1 top	half
C10 H7 N3 S	201.03608	202.04336	1 top	quarter
C10 H7 N3 S	201.03608	202.04336	4 bottom	half
C10 H7 N3 S	201.03608	202.04336	8 bottom	half

C10 H7 N3 S	201.03608	202.04336	11 bottom	half
C10 H7 N3 S	201.03608	202.04336	15 bottom	half
C10 H7 N3 S	201.03608	202.04336	18 bottom	half
C10 H7 N3 S	201.03608	202.04336	22 bottom	half
C10 H7 N3 S	201.03608	202.04336	25 bottom	half
C10 H7 N3 S	201.03608	202.04336	29 bottom	half
C10 H7 N3 S	201.03608	202.04336	29 bottom	quarter
C10 H7 N3 S	201.03608	202.04336	29 middle	half
C10 H7 N3 S	201.03608	202.04336	29 middle	quarter
C10 H7 N3 S	201.03608	202.04336	29 top	half
C10 H7 N3 S	201.03608	202.04336	29 top	quarter
C10 H14 O	150.10452	168.13834	29 top	quarter
C10 H14 O	150.10451	151.11179	1 bottom	quarter
C10 H14 O	150.10451	151.11179	1 middle	quarter
C10 H14 O	150.10451	151.11179	1 top	half
C10 H14 O	150.10451	151.11179	1 top	quarter
C10 H14 O	150.10451	151.11179	8 bottom	half
C10 H14 O	150.10451	151.11179	25 bottom	half
C10 H14 O	150.10452	151.11179	1 bottom	quarter
C10 H14 O	150.10452	151.11179	29 bottom	quarter
C10 H14 O	150.10451	151.11179	29 bottom	quarter
C10 H14 O	150.10451	151.11179	1 top	quarter
C10 H14 O	150.10451	151.11179	25 bottom	half
C12 H13 N5 O4	291.09692	314.08617	4 bottom	half
C17 H30 N2 O7	374.20714	375.21441	25 bottom	half
C17 H30 N2 O7	374.20696	375.21423	11 bottom	half
C17 H30 N2 O7	374.20696	375.21423	29 middle	quarter
C10 H11 N O2	177.07902	178.08629	11 bottom	half
C10 H11 N O2	177.07902	178.08629	15 bottom	half
C10 H11 N O2	177.07901	178.08629	1 bottom	quarter
C10 H11 N O2	177.07901	178.08629	11 bottom	half
C10 H11 N O2	177.07901	178.08629	18 bottom	half
C10 H11 N O2	177.07901	178.08629	1 middle	quarter
C19 H23 N O3	313.16799	314.17527	1 top	quarter
C19 H23 N O3	313.16799	314.17527	25 bottom	half
C19 H23 N O3	313.16786	314.17513	29 top	half
C19 H23 N O3	313.1679	314.17519	8 bottom	half
C18 H26 O	258.19848	259.20576	1 bottom	half
C18 H26 O	258.19848	259.20576	1 bottom	quarter
C18 H26 O	258.19848	259.20576	1 middle	half
C18 H26 O	258.19848	259.20576	1 middle	quarter
C18 H26 O	258.19848	259.20576	1 top	half
C18 H26 O	258.19848	259.20576	1 top	quarter
C18 H26 O	258.19848	259.20576	4 bottom	half
C18 H26 O	258.19848	259.20576	8 bottom	half
C18 H26 O	258.19848	259.20576	11 bottom	half
C18 H26 O	258.19848	259.20576	15 bottom	half
C18 H26 O	258.19848	259.20576	18 bottom	half
C18 H26 O	258.19848	259.20576	22 bottom	half
C18 H26 O	258.19848	259.20576	25 bottom	half

C18 H26 O	258.19848	259.20576	29 bottom	half
C18 H26 O	258.19848	259.20576	29 bottom	quarter
C18 H26 O	258.19848	259.20576	29 middle	half
C18 H26 O	258.19848	259.20576	29 middle	quarter
C18 H26 O	258.19848	259.20576	29 top	half
C18 H26 O	258.19848	259.20576	29 top	quarter
C18 H26 O	258.19846	259.20576	1 bottom	quarter
C18 H26 O	258.19846	259.20576	1 middle	quarter
C18 H26 O	258.19846	259.20576	1 top	half
C18 H26 O	258.19846	259.20576	1 top	quarter
C18 H26 O	258.19846	259.20576	8 bottom	half
C18 H26 O	258.19846	259.20576	11 bottom	half
C18 H26 O	258.19846	259.20576	29 bottom	half
C18 H26 O	258.19846	259.20576	29 bottom	quarter
C18 H26 O	258.19846	259.20576	29 top	quarter

maan	otal r		
	std r		e 05545 6777
2680179.844	135079.5668	2	95515.6777
1064649.468	22567.26252	2	15957.46436
1000572.728	93324.00098	2	65990.03394
1723174.313	10479.96167	2	7410.451965
387931.7657	12780.22232	2	9036.981864
323393.8597	1787.44065	2	1263.911404
649162.8633	6594.065178	2	4662.708203
723129.94	97011.44114	2	68597.44788
488100.0893	22746.53576	2	16084.22969
840348.0313	40369.84687	2	28545.79247
534006.5592	1399.81853	2	989.8211748
770471.8473	19574.50528	2	13841.26543
621287.6042	5740.837152	2	4059.38488
731796.7679	128689.8539	2	90997.46839
565111.0726	97818.13686	2	69167.86789
646976.6809	92227.47204	2	65214.67089
628483.6773	49505.43911	2	35005.6317
556786.7351	126238.0092	2	89263.75236
559479.1658	20867.7616	2	14755.73574
199811.4251	1604.1523	2	1134.306969
179074.8281	23436.30579	2	16571.97075
181922.9337	35219.17716	2	24903.719
156837.7475	27617.05484	2	19528.20676
254278.9248	63166.24338	2	44665.27903
1009715.159	37676.12591	2	26641.04412
295569.6326	16848.5686	2	11913.73711
1059180.732	227894.5745	2	161145.799
308686.569	41428.19497	2	29294.15759
128054.6305	1713.783933	2	1211.82824
240296.1213	22065.92492	2	15602.96514
367023.1405	22419.46591	2	15852.95637
830997.0501	10914.95883	2	7718.041408
916094.2086	41119.46262	2	29075.85086
957762.8007	49890.29204	2	35277.76382
2266001.766	118725.0597	2	83951.29478
2277812.299	207506.9953	2	146729.6035
3286547.258	17889.80163	2	12650.00005
2280837.211	192001.7498	2	135765.7393
182058.6212	7200.211571	2	5091.318428
138665.5401	12640.7226	2	8938.340673
459606.0282	101159.651	2	71530.67519
316280.0571	31920.02341	2	22570.86501
246041.4903	18316.08204	2	12951.42582
879186.8114	96143.18993	2	67983.50156
53859647.19	1565239.945	2	1106791.779
	694779.8796	2	491283.5643
44956036.51		2	
43842176.35	976789.0978		690694.1949
84533838.26	1309870.431	2	926218.2645
60096826.87	992057.7278		701490.7467

49611869.46	1315176.302	2	929970.0816
34219567.04	340688.1638	2	240902.9109
26647772.38	1189347.805	2	840995.8981
35750258.95	377125.3163	2	266667.8685
26723820.19	714421.7624	2	505172.4728
34349608.22	198669.8541	2	140480.801
15251590.7	129010.6188	2	91224.28341
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