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1 #Display of program name and author
2 print("Ka solvation in a one-compartment oral model")
3 print("by @David MALNOË")
4
5 #Import of the module to calculate logarithms (math.log), exponentials (math.exp) and powers (math.pow)
6 import math
7
8 #Initiation of the variable allowing to return to the beginning of the program
9 continue = True
10
11 #As long as the 'continue' variable is considered true, the program returns to this point after calculating the ka and MAT
12 while continue:
13     while continue:
14         print("_____")
15         print("\nChoice of pharmacokinetic model:")
16         print("    1. Monocompartmental model, single oral administration: analytical approach")
17         print("    2. Monocompartmental model, single oral administration: iterative approach")
18         print("    3. One-compartment model, repeated oral administration: iterative approach")
19         print("    4. Leave \n")
20     #Choice of the appropriate pharmacokinetic model
21     choice = input("Choice ? ")
22     print("_____ \n")
23
24 #Ka solvation for a monocompartmental model, with single oral administration according an analytical approach
25 if choice == "1" :
26
27     #User input of known variables: as long as the variables are not a floating point number, the program stops and displays 'Enter a number'
28     test_var = 0
29     while test_var == 0 :
30         print("Please fill in the following parameters using . as decimal separator:")
31         half_life= input("t1/2 (h) = ")
32         tmax = input("tmax (h) = ")
33         try:
34             float(half_life)
35             float(tmax)
36             test_var = 1
37             break
38         except ValueError:
39             print("\nEnter a nombre\n")
40
41 # Conversion of variables into floating point number (float), definition and calculation of the intermediate variables necessary afterwards,
initiation of Lambert's W function

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42 ka = float(1)
43 half_life= float(half_life)
44 tmax = float (tmax)
45 t = float(0)
46 n = int(0)
47 ke = math.log(2)/half_life
48 X = ke * tmax
49 Z = (-X)/(math.exp(X))
50 W = float(1)
51
52 #Solving ka via Lambert's W function in its main branch
53 if X >= 1 :
54
55     #Loop for estimating W according to the Halley method for 100 iterations
56     while n < 100 :
57         n=n+1
58         W = W-((W*math.exp(W)-Z)/((math.exp(W)*(W+1))-(((W+2)*(W*math.exp(W)-Z))/(2*W+2))))
59
60     #Calculation of ka and MAT, display of results
61     ka = W/(-tmax)
62     mat = 1/ka
63     print("\n_____ \n")
64     print("Estimation of ka using the main branch W0 of Lambert's function by Halley's method:\n")
65     print("ka = ",ka," h^-1")
66     print("mat = ",mat," h")
67
68 # Solving ka via Lambert's W function in its alternative branch
69 else :
70
71     #Estimation of W by algorithmic approach (a, b, c and d are intermediate variables making it easier to express W)
72     alpha = float(0.3205)
73     a = math.log(-Z)
74     b = math.pow(-(1+a)/2),0.5)
75     c = math.pow((1+alpha*b),(-1))
76     d = math.pow(alpha,(-1))
77     W = a - (2*d*(1-c))
78
79     #Calculation of ka and MAT, display of results
80     ka = W/(-tmax)
81     mat = 1/ka
82     print("_____ \n")
83     print("Estimation of ka using the alternative branch W-1 of Lambert's function by logarithmic approach:\n")
84     print("ka = ",ka," h^-1")

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85         print("mat = ",mat," h")
86
87     #If user input is not ok, OK, o, O, yes, y, YES, Y, then continue becomes false and exits loop, else returns to beginning of loop
88     print("\n_____")
89     suite = input("Do you want to continue (yes/no) ?")
90     if suite not in ("ok","OK","o","O","yes","y","YES","Y"):
91         continue = False
92         fin = input("Thank you: press enter to exit")
93
94 #Resolution of ka for a monocompartmental model, with single oral administration according to an iterative approach
95     elif choice == "2" :
96
97     # User input of known variables: as long as the variables are not a floating point number, the program stops and displays 'Enter a number'
98     test_var = 0
99     while test_var == 0 :
100         print("Please fill in the following parameters using . as decimal separator:")
101         half_life= input("t1/2 (h) = ")
102         tmax = input("tmax (h) = ")
103         ka = input("Estimate ka (if unknown, enter 1) :")
104         try:
105             float(half_life)
106             float(tmax)
107             float(ka)
108             test_var = 1
109             break
110         except ValueError:
111             print("\nEnter a nombre\n")
112
113     # Conversion of variables into floating point number (float), definition and initiation of t (estimate of tmax) and n (counter of
    the number of iterations), calculation of ke
114     half_life=
115     float(half_life)
116     tmax = float(tmax)
117     ka = float(ka)
118     t = float(0)
119     n = int(0)
120     ke =
121     math.log(2)/half_life
122
123     # Loop calculating t until t is close to tmax true
124     while t < (0.9999999 * tmax) or t > (1.00000001 * tmax) :
125         n=n+1

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125     # If t > tmax then ka is too small, and a new value of ka is assigned
126     if t > tmax:
127         ka = ka+(ka/8)
128
129     # If t < tmax then ka is too large, and a new value of ka is assigned
130     else:
131         ka = ka-(ka/8)
132
133     # Calculation of t with the new value of ka
134     t = (math.log(ka/ke))/(ka-ke)
135
136 #Calculation of MAT from the approximate value of ka and display of the results
137 mat = 1/ka
138 print("\n_____ \n")
139 print("Estimation of ka by iteration:\n")
140 print("iteration = ",n)
141 print("ka = ",ka," h^-1")
142 print("mat = ",mat," h")
143
144 #If user input is not ok, OK, o, 0, yes, y, YES, Y, then continue becomes false and exits loop, else returns to beginning of loop
145 print("\n_____ \n")
146 suite = input("Do you want to continue (yes/no) ? ")
147 if suite not in ("ok","OK","o","0","yes","y","YES","Y"):
148     continue = False
149     fin = input("Thank you: press enter to exit")
150
151 # Resolution of ka for a monocompartmental model, with repeated oral administration according to an iterative approach
152 elif choice == "3" :
153
154     # User input of known variables: as long as the variables are not a floating point number, the program stops and displays 'Enter a number'
155     test_var = 0
156     while test_var == 0 :
157         print("Please fill in the following parameters using . as decimal separator decimal :")
158         half_life= input("t1/2 (h) = ")
159         tmax = input("tmax (h) = ")
160         tau = input("tau (h) = ")
161         ka = input("Estimate ka (if unknown, enter 1):")
162         try:
163             float(half_life)
164             float(tmax)
165             float(tau)

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166         float(ka)
167         test_var = 1
168         break
169     except ValueError:
170         print("\nEnter a nombre \n")
171
172 # Conversion of variables into floating point number (float), definition and initiation of t (estimate of tmax) and n (counter of the
number of iteration), calculation of ke
173     half_life= float(half_life)
174     tmax = float(tmax)
175     tau = float(tau)
176     ka = float(ka)
177     t = float(0)
178     n = int(0)
179     ke = math.log(2)/half_life
180
181 #Loop calculating t until t is close to tmax true
182     while t < (0.9999999 * tmax) or t > (1.00000001 * tmax) :
183         n=n+1
184
185     #If t > tmax then ka is too small, and a new value of ka is assigned
186     if t > tmax:
187         ka = ka+(ka/8)
188
189     # If t < tmax then ka is too large, and a new value of ka is assigned
190     else:
191         ka = ka-(ka/8)
192
193     #Calculate t with the new valu of ka (a, b, A and B are intermediate variables to facilitate the expression of t)
194     a = -ke * tau
195     b = -ka * tau
196     A = ka * (1-math.exp(a))
197     B = ke * (1-math.exp(b))
198     t = (math.log(A/B))/(ka-ke)
199
200 #Calculation of MAT from the approximate value of ka and display of the results
201     mat = 1/ka
202     print("_____ \n")
203     print("Estimation of ka by iteration:\n")
204     print("iteration = ",n)
205     print("ka = ",ka," h^-1")
206     print("mat = ",mat," h")
207

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208 # If user input is not ok, OK, o, O, yes, y, YES, Y, then continue becomes false and exits loop, else returns to beginning of loop
209 print("\n_____ \n")
210 suite = input("Do you want to continue (yes/no) ? ")
211 if suite not in ("ok", "OK", "o", "O", "yes", "y", "YES", "Y"):
212     continue = False
213     fin = input("Thank you: press enter to exit ")
214
215 #Choice de quitter le programme
216 elif choice == "4" :
217     continue = False
218     fin = input("Thank you: press enter to exit")
219
220 # Returns 'Error' if the model choice entry is not compliant (different from 1, 2, 3 or 4)
221 else:
222     print("Error : entry is not valid.")
223
224 # If user input is not ok, OK, o, O, yes, y, YES, Y, then continue becomes false and exits loop, else returns to beginning of loop
225 print("\n_____ \n")
226 suite = input("Do you want to continue (yes/no) ? ")
227 if suite not in ("ok", "OK", "o", "O", "yes", "y", "YES", "Y"):
228     continue = False
229     fin = input("Thank you: press enter to exit")
230
231 #End of the programm
232 print("\n_____ \n")

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