Bioinformation Volume 5

open access

www.bioinformation.net Issue 4 **Hypothesis**

Supplementary material:

Genetic algorithm methodology to optimize the objection function that is [RA]t, carried out 200 iterations of optimization. Results are as follows:
Optimization:
Maximize [RA]t

Method: Genetic algorithm
Generations = 200
Iterations = 200
Simulations = 2048
Time = 31 s
Speed = 66.0323 simulation/s

Best solution:
[RA]t = 0.00632031
[3C4HPLA]i = 0.025

Table 1: Metabolites and their initial concentrations (in mM)

Metabolites	Initial Concentration in mM (Approx)
L-Phenylalanine (L-Phe)	1.394000e-002
t- Cinnamic acid (t-CA)	1.250000e-002
4- Coumaric acid (4CouA)	1.385000e-002
4-Coumaroyl- CoA (4CouCoA)	1.538000e-002
L-tyrosine (L-Tyr)	1.519000e-002
4-Hydroxyphenylpyruvic acid (4HPA)	1.527000e-002
4-Hydroxyphenyllactic acid (4HPLA)	1.538000e-002
4-Coumaroyl-4'-hydroxyphenyllactic acid (4C4HPLA)	1.542000e-002
Caffeoyl-4'hydroxyphenyllactic acid (3C4HPLA)	1.526000e-002
Caffeoyl-3'-4'hydroxyphenyllactic acid (3'C4HPLA)	1.526000e-002
Rosmarinic acid (RA)	0.0

Table 2: Results of integration (after 5.00e+002 s)

[L		Phe]	initial = 1.394000e	002 mM, final = 5.714014e 152 mM
[t		CA]	initial = 1.250000e	002 mM, final = 4.960081e 151 mM
[4CouA]	initial = 1.385000e	002 mM, final = 7.150533e	149 mM	
[CAH]	initial = 1.000000e	002 mM, final = 1.000000e	002 mM	
[4CL]	initial = 1.000000e	002 mM, final = 1.000000e	002 mM	
[4CouCoA]	initial = 1.538000e	005 mM, final = 3.342895e	004 mM	
[LTyr]	initial = 1.519000e	002 mM, final = 2.373387e	141 mM	
[TAT]	initial = 1.000000e	002 mM, final = 1.000000e	002 mM	
[4HPA]	initial = 1.527000e	002 mM, final = 1.595839e	138 mM	
[HPPR]	initial = 1.000000e	002 mM, final = 1.000000e	002 mM	
[4HPLA]	initial = 1.538000e	002 mM, final = 5.868909e	003 mM	
[4C4HPLA]	initial = 1.542000e	002 mM, final = 1.535336e	006 mM	
[RA]	**initial = 0.000000e+000 mM, final = 4.047119e**	**002 mM**		
[3C4HPLA]	initial = 1.526000e	002 mM, final = 2.483589e	003 mM	
[3`C4HPLA]	initial = 1.526000e	002 mM, final = 2.483589e	003 mM	
[RAS]	initial = 1.000000e	002 mM, final = 1.000000e	002 mM	
[P450]	initial = 1.000000e	002 mM, final = 1.000000e	002 mM	
[PAL]	initial = 1.000000e	002 mM, final = 1.000000e	002 mM	

Table 3: Change in the concentration of the metabolites with time.

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Real time	[4HPLA]t	[3C4HPLA]t	[RA]t	J(R9)
1.60E-0	**1.54E-02**	**1.53E-02**	**0.00E+00**	**2.33E-04**
3.10E-02	3.80E-02	2.17E-02	4.39E-03	4.69E-04
1.00E+01	2.94E-02	2.17E-02	9.18E-03	4.72E-04
2.00E+01	2.38E-02	2.02E-02	1.36E-02	4.07E-04
3.00E+01	2.02E-02	1.83E-02	1.73E-02	3.36E-04
4.00E+01	1.77E-02	1.66E-02	2.04E-02	2.75E-04
5.00E+01	1.58E-02	1.50E-02	2.29E-02	2.26E-04
6.00E+01	1.44E-02	1.37E-02	2.49E-02	1.88E-04
7.00E+01	1.32E-02	1.26E-02	2.67E-02	1.58E-04
8.00E+01	1.23E-02	1.16E-02	2.81E-02	1.34E-04
9.00E+01	1.16E-02	1.07E-02	2.94E-02	1.15E-04
1.00E+02	1.09E-02	9.98E-03	3.04E-02	9.97E-05
1.10E+02	1.04E-02	9.33E-03	3.14E-02	8.70E-05
1.20E+02	9.91E-03	8.75E-03	3.22E-02	7.65E-05
1.30E+02	9.51E-03	8.23E-03	3.29E-02	6.78E-05
1.40E+02	9.15E-03	7.77E-03	3.35E-02	6.04E-05
1.50E+02	8.84E-03	7.36E-03	3.41E-02	5.41E-05
1.60E+02	8.57E-03	6.98E-03	3.46E-02	4.87E-05
1.70E+02	8.32E-03	6.64E-03	3.51E-02	4.41E-05
1.80E+02	8.10E-03	6.33E-03	3.55E-02	4.01E-05
1.90E+02	7.90E-03	6.05E-03	3.59E-02	3.66E-05
2.00E+02	7.73E-03	5.79E-03	3.62E-02	3.35E-05
2.10E+02	7.56E-03	5.55E-03	3.66E-02	3.08E-05
2.20E+02	7.42E-03	5.33E-03	3.68E-02	2.84E-05
2.30E+02	7.28E-03	5.12E-03	3.71E-02	2.62E-05
2.40E+02	7.16E-03	4.93E-03	3.74E-02	2.43E-05
2.50E+02	7.05E-03	4.75E-03	3.76E-02	2.26E-05
2.60E+02	6.95E-03	4.59E-03	3.78E-02	2.10E-05
2.70E+02	6.85E-03	4.43E-03	3.80E-02	1.96E-05
2.80E+02	6.77E-03	4.28E-03	3.82E-02	1.83E-05
2.90E+02	6.69E-03	4.15E-03	3.84E-02	1.72E-05
3.00E+02	6.61E-03	4.02E-03	3.86E-02	1.61E-05
3.10E+02	6.54E-03	3.89E-03	3.87E-02	1.52E-05
3.20E+02	6.48E-03	3.78E-03	3.89E-02	1.43E-05
3.30E+02	6.42E-03	3.67E-03	3.90E-02	1.35E-05
3.40E+02	6.37E-03	3.57E-03	3.91E-02	1.27E-05
3.50E+02	6.32E-03	3.47E-03	3.93E-02	1.20E-05
3.60E+02	6.27E-03	3.38E-03	3.94E-02	1.14E-05
3.70E+02	6.22E-03	3.29E-03	3.95E-02	1.08E-05
3.80E+02	6.18E-03	3.20E-03	3.96E-02	1.03E-05
3.90E+02	6.14E-03	3.12E-03	3.97E-02	9.75E-06
4.00E+02	6.11E-03	3.05E-03	3.98E-02	9.27E-06
4.10E+02	6.07E-03	2.97E-03	3.99E-02	8.83E-06
4.20E+02	6.04E-03	2.90E-03	4.00E-02	8.42E-06
4.30E+02	6.01E-03	2.83E-03	4.00E-02	8.03E-06
4.40E+02	5.98E-03	2.77E-03	4.01E-02	7.67E-06
4.50E+02	5.96E-03	2.71E-03	4.02E-02	7.33E-06
4.60E+02	5.93E-03	2.65E-03	4.03E-02	7.01E-06
4.70E+02	5.91E-03	2.59E-03	4.03E-02	6.71E-06
4.80E+02	5.89E-03	2.54E-03	4.04E-02	6.43E-06
4.90E+02	**5.87E-03**	**2.48E-03**	**4.05E-02**	**6.17E-06**