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R E S E A R C H A R T I C L E

A Spreadsheet Program for One Compartment IV Bolus Administration

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A B S T R A C T

Pharmacokinetics softwares plays a crucial role in the pharmaceutical field. Improvements in the quantitative analysis of drugs in biological tissues, such as plasma, and the increasing sophistication of computers and softwares along with access to the internet have greatly accelerated the development of pharmacokinetics. Pharmacokinetic softwares now allow for the rapid solution of complicated pharmacokinetic equations and rapid modelling of pharmacokinetic process. Apart from, using pharmacokinetic softwares are the tedious process for freshers in pharmaceutical companies. Proper tuitorials would be needed for this. This is one of the problem faced by the pharmaceutical firms. The use of simple spreadsheets, provide the solution for this. In this work, the simple spreadsheet was used to create a one compartment IV bolus administration using standard spreadsheet commands the technique is shown to be applicable to the full range of advanced pharmacokinetic simulations. The technique is very simple to use and is always in the complete control of the modeller.

A R T I C L E I N F O

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C O N T E N T S

1. Introduction

Software used for data analysis such as statistical and pharmacokinetic calculations should be validated with respect to the accuracy, quality, integrity, and security of the data. One approach for determining the accuracy of the data analysis is to compare the results obtained from two different software packages using the same set of data.[1] For general computation, many programs, such as electronic spreadsheets, are very adaptable to calculation and pharmacokinetic curve plotting. Electronic spreadsheet software programs such as Microsoft Excel are easy to use. Data are entered in columns(referred to alphabetically as A, B, C,..) and rows (referred to numerically as 1,2,3..). Data

are generally displayed on screen and can be selected by moving the arrow keys followed by pressing the Return or Enter key.[2]

2. Materials and Methods

Microsoft excel was used here, and basic knowledge of pharmacokinetics was needed.

Method development

The use of simple spreadsheets is described to create simulations of complex pharmacokinetic phenomena. The basics of spreadsheets are first described and are developed to demonstrate classical pharmacokinetics without the use of differential or integral calculus. Using standard spreadsheet commands, the technique is shown to be applicable to the full range of advanced pharmacokinetic simulations. Demonstrations of the effect of a variety of physiological eventualities are included to show the versatility of the technique. The technique is very simple to use and is always in the complete control of the modeller.[3]

Basic knowledge of pharmacokinetics was needed to creating excel sheet software for this model. This work showing how to create a simple worksheet for one compartment IV bolus administration. Table 1 illustrates the equations placed in the cells of a spreadsheet to simulate the one compartment IV bolus administration.

3. Results and Discussion

The following is a brief description of the formulae in each of these initial cells. Column A contains time of drug release in hour and corresponding plasma drug concentration (µg/ml) can be enter in column B .Click 1st cell of column C and enter the equation[=LOG10(B3)] will gives the corresponding log plasma drug concentration. Experienced users of spreadsheets will recognise that remainder of the cells in column C will shows the results for next concentrations in log through simple dragging. Column D gives the sum of the values in cells of the column C ,[=SUM(B2:B3)].Same dragging towards down the column gives all the summation values from (B3:B4) to (B12:B13). Column E contains the value t2-t1, indicates the difference in time in hours. Column F titled as 1/2(C1+C2)(t2-t1) is the equation for determination of AUC_0^{t*} theoretically. On column A and row 15 enter the dose of particular drug. Table 2 shows various pharmacokinetic parameters such as intercept C0, slope, Elimination rate constant (kE), Elimination half-life(t1/2), Volume of distribution(Vd), Clearance(Cl), AUC(0-t*), AUC(t*-α), AUC(0-α) and their equation for excel spreadsheet.

Plotting of graphs –time vs plasma drug concentration

Select column A, & B that includes the datas time, plasma drug concentration. Select X-Y scatter in all chart types produces curved lines with equations. It was shown in fig 3 and 4.

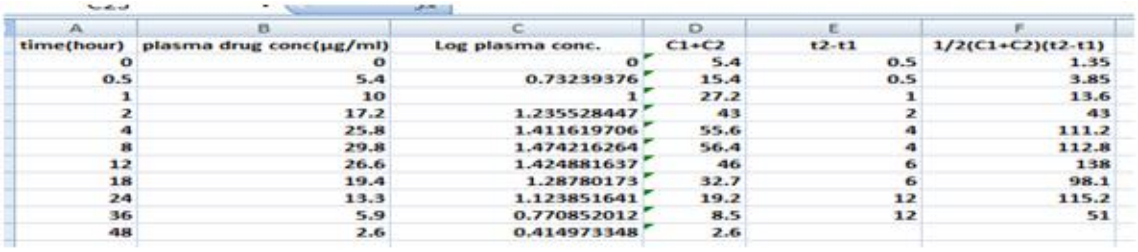
Plotting of graphs –time vs log plasma drug concentration: Select column A, & C that includes the datas time, log plasma drug concentration. Select X-Y scatter in all chart types produces curved lines with equations. It shown in fig 5 and 6.

4. Conclusion

This work shows the very complex pharmacokinetic models can be constructed using only standard spreadsheet packages. By knowing the basic knowledge of pharmacokinetic principles we can easily construct the excel sheet for one compartment IV bolus administration. By using the spreadsheet skills we can construct next level compartments in pharmacokinetics.

Table 1: Spreadsheet results for Simulation of one compartment IV bolus administration following an initial dose X_0-300mg

Time(hour)	plasma drug conc(µg/ml)	Log plasma conc.	C1+C2	t2-t1	1/2(C1+C2)(t2-t1)
0	0	0	5.4	0.5	1.35
0.5	5.4	0.73239376	15.4	0.5	3.85
1	10	1	27.2	1	13.6
2	17.2	1.235528447	43	2	43
4	25.8	1.411619706	55.6	4	111.2
8	29.8	1.474216264	56.4	4	112.8
12	26.6	1.424881637	46	6	138
18	19.4	1.28780173	32.7	6	98.1
24	13.3	1.123851641	19.2	12	115.2
36	5.9	0.770852012	8.5	12	51
48	2.6	0.414973348	2.6		



A	B	C	D	E	F
time(hour)	plasma drug conc(µg/ml)	Log plasma conc.	C1+C2	t2-t1	1/2(C1+C2)(t2-t1)
0	0	0	5.4	0.5	1.35
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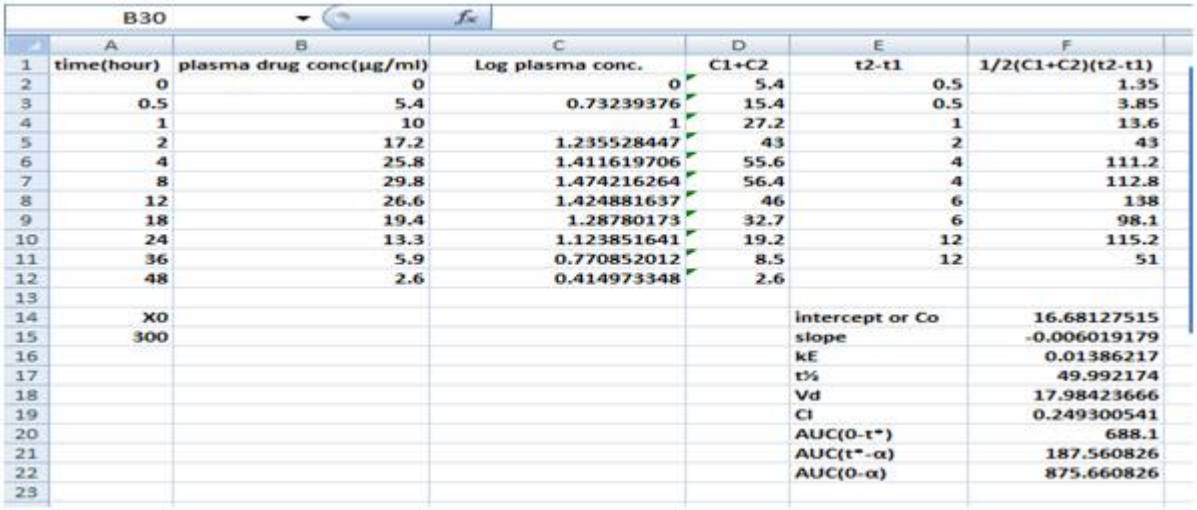
48	2.6	0.414973348	2.6		

Figure 1: Screen capture of the Spreadsheet results for Simulation of one compartment IV



	A	B	C	D	E	F
1	time(hour)	plasma drug conc(µg/ml)	Log plasma conc.	C1+C2	t2-t1	1/2(C1+C2)(t2-t1)
2	0	0	0	5.4	0.5	1.35
3	0.5	5.4	0.73239376	15.4	0.5	3.85
4	1	10	1	27.2	1	13.6
5	2	17.2	1.235528447	43	2	43
6	4	25.8	1.411619706	55.6	4	111.2
7	8	29.8	1.474216264	56.4	4	112.8
8	12	26.6	1.424881637	46	6	138
9	18	19.4	1.28780173	32.7	6	98.1
10	24	13.3	1.123851641	19.2	12	115.2
11	36	5.9	0.770852012	8.5	12	51
12	48	2.6	0.414973348	2.6		
13						
14	X0				intercept or Co	16.68127515
15	300				slope	-0.006019179
16					kE	0.01386217
17					t½	49.992174
18					Vd	17.98423666
19					Cl	0.249300541
20					AUC(0-t*)	688.1
21					AUC(t*-α)	187.560826
22					AUC(0-α)	875.660826
23						

Figure 2: Screen capture of total results of one compartment IV bolus administration

Table 2: Various Pharmacokinetic Parameters and their equation for excel spreadsheet

Sl.No.	Pharmacokinetic Parameters	Equation For Excel Spread Sheet
1	Intercept or Co	=INTERCEPT(B2:B12,A2:A12)
2	Slope	=SLOPE(C2:C12,A2:A12)
3	kE (per hour)	=2.303*-F15
4	t½ (hr)	=(0.693/F16)
5	Vd (L)	=A15/F14
6	Cl (L/hr)	=(F16*F18)
7	AUC(0-t*) (µg hr/ml)	=SUM(F2:F11)
8	AUC(t*-α) (µg hr/ml)	=(B12/F16)
9	AUC(0-α) (µg hr/ml)	=SUM(F20:F21)

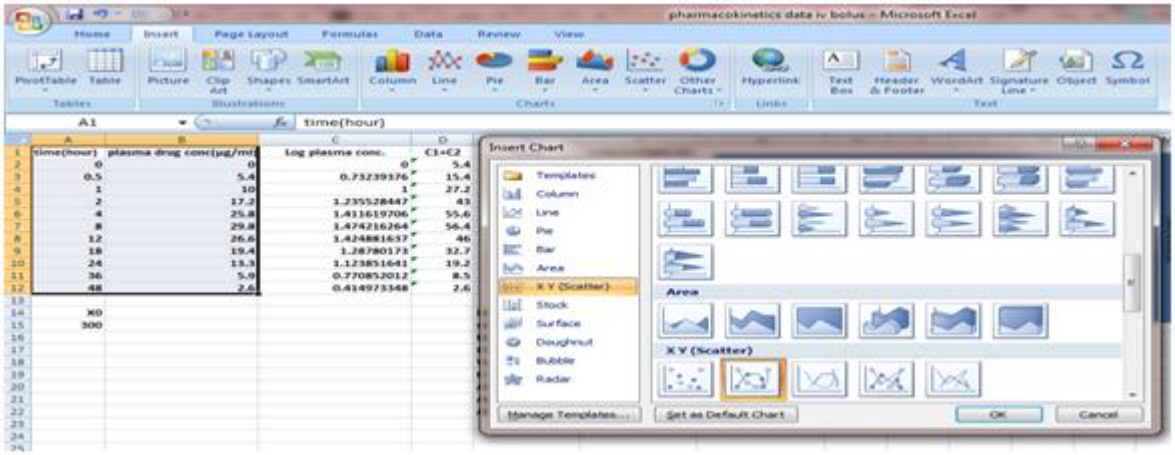


Figure 3: Screen capture of the making graph of time vs plasma drug concentration

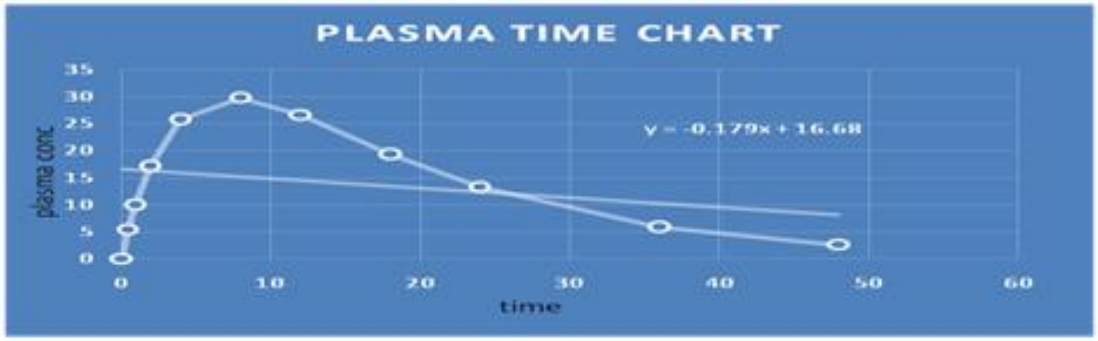


Figure 4: Graph of time vs plasma drug concentration

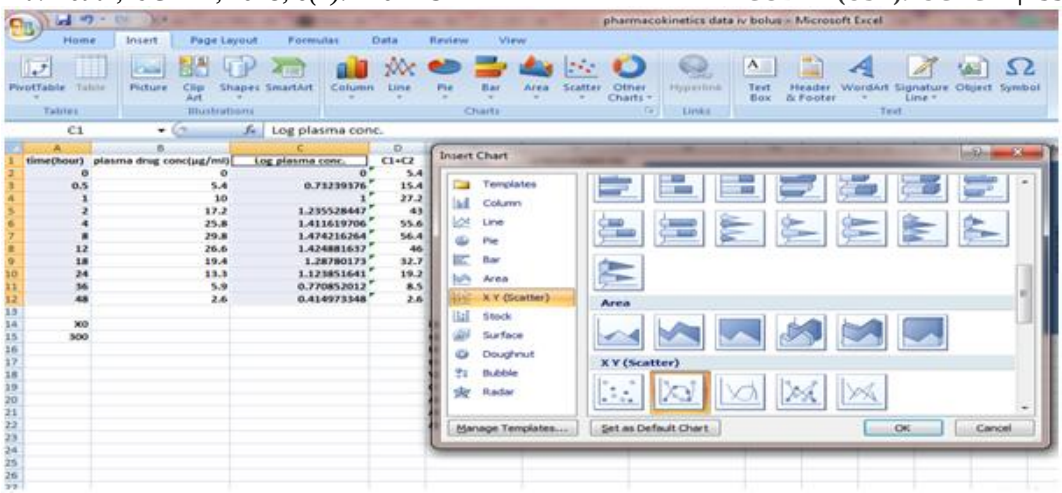


Figure 5: Screen capture of the making graph of time vs log plasma drug concentration

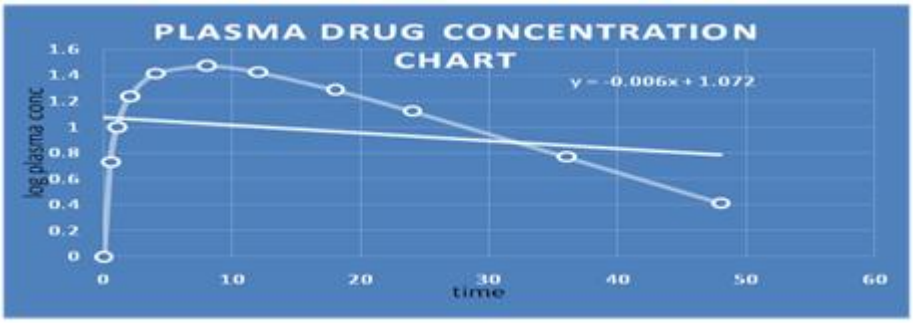


Figure 6: Graph of time vs log plasma drug concentration

5. References

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