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NEURAL NETWORK : AN INSTRUMENT TO STUDY FLOW AND PACKING PROPERTIES OF PHARMACEUTICAL POWDERS.

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Data mining is an emerging area of new research efforts with the purpose of finding new knowledge from databases where dimension, complexity or amount of data is prohibitively large for human observation alone. Data mining is an interactive process requiring that the intuition and background knowledge of humans are coupled with the computational efficiency of modern computer technology and tools, such as artificial neural networks. One of the most famous neural networks algorithms is self-organising maps (SOM) (1-3). Powder flow is involved in many processes of pharmaceutical formulation; frequently glidants are employed in order to improve the flow properties of powders. In the present study five brands of microcrystalline cellulose (Ph101, Vivapur, Ph 301, Emcocel and Prosolv), three brands of Crospovidone (XL, XL-10 and INF) and pregelatinized Starch were mixed with 2% w/w of Aerosil 200, Aerosil R972 (two different kinds of colloidal silicon dioxide) or Mg stearate, to obtain 27 distinct mixtures. Flow rate, bulk and tapped density of mixtures were measured and tablets were prepared. Kawakita equation parameters and tablets weight variation were also studied. In order to have a better insight into material and operator variables involved in powder flow, self-organizing maps (SOMs) were fitted to the data, and possible correlations were investigated using correlation ellipse matrices and SOM component planes. It was found that Aerosil 200 and Aerosil R972 have a better glidant action than Mg Stearate. Use of neural networks revealed the presence of three clusters with distinct flow behaviour. Finally, correlation between flow rate and the $1/b$ parameter of the Kawakita equation, as well as the tablet weight, and corresponding coefficient of variation were found.

References

1. Antikainen O.K., Rantanen J.T., Yliruusi J.K., 2000. Use of the Kohonen self-organising map to predict the flowability of powders. *STP Pharm. Sci.* 10, 349-354.
2. Kohonen T., Self-Organizing maps, *Springer series in information sciences* vol. 30, Springer, Berlin, Heidelberg (1995).
3. Vesanto J., 1999. SOM-based data visualization methods. *Intelligent Data Analysis*, 3, 111-126.