P-779 - THE CORRELATION BETWEEN THE PREDICTION OF THE THEORETICAL EFFICIENCY THROUGH MOLECULAR MODELING AND CLINICAL EFFECTIVENESS IN SSRI ANTIDEPRESSANTS

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Aim: Our study has sought to correlate the QSAR analysis (quantitative structure-activity relationship) of SSRIs (Selective serotonin reuptake inhibitors) and their receptorial affinity with a serie of clinical cases of depression treated with SSRIs.
Materials and method: Through molecular modeling and analysis of quantitative structure-activity relationship (QSAR), we analyzed and compared the activity of serotonergic antidepressants - escitalopram, sertraline, fluoxetine, fluvoxamine, paroxetine and we have performed their hierarchy based on their theoretical antidepressant effectiveness.
Were constituted five lots of 50 patients with depression in order to determine the clinical efficacy of these antidepressants. Each of these groups received treatment with one of the five antidepressants. The initial distribution of patients was made based the severity of untreated depression, in each group being included in equal proportions of patients with severe, medium and middle depression. The Hamilton Depression Scale and Beck Depression Inventory were applied to the patients before the start of antidepressant treatment, at 2 weeks and 2 months after treatment.
Results: The theoretical ranking aquired from molecular modeling and QSAR analysis was, in the order of increasing effectiveness of antidepressants, paroxetine, fluvoxamine, fluoxetine, sertraline, escitalopram, while the practice ranking has been: fluvoxamine, fluoxetine, sertraline, paroxetine and escitalopram.
Conclusion: Our clinical study has not fully confirmed the theoretical prediction, so that we consider the improvement of theoretical models of molecular simulation, including exploring the interaction of antidepressants with ions (sodium, potassium, magnesium, calcium).

https://doi.org/10.1016/S0924-9338(12)74946-5 Published online by Cambridge University Press