FEDERATION OF EUROPEAN BIOCHEMICAL SOCIETIES CONGRESS 2013

MECHANISMS IN BIOLOGY

ST. PETERSBURG
JULY 6-11, 2013

38th FEBS CONGRESS
RUSSIA | SAINT PETERSBURG 2013

FEBS

structed two hypothesis of TP distribution on set of coding sequences and simulated corresponding artificial datasets. We explored modeling sets of two types: the first one where all sequences TP were obtained from one TP pattern (*Perf*) and the second one where conversely TP of all sequences were independent and random (*Rand*). We found that triplet periodicity more similar inside genome than between genomes and that TP distribution inside genome corresponds to hypothesis which imply common TP pattern for majority of sequences inside a genome (*Perf*). Additionally we performed gene classification based on triplet periodicity matrixes. This classification showed that triplet periodicity allows to identify genome to which a given gene belongs with more than 85% accuracy for the most cases. Our results suggest that there is some process inside genomes that formed and maintained special TP type of genes inside one genome. Without such process it is hard to explain how TP could persist in the context of mutation process even if all genes inside genome initially had the same TP type. In practice genome-specificity of TP could be useful for pathological genome identification in medicine and homogeneity of TP inside genome – for prediction of horizontally transferred genes.

SW06.W29–10
In silico methods as a prominent tool for predicting the potential biological activity of dietary flavones

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In the last few years, special attention has been paid to flavones – which are comprised in the flavonoids′ family and present in the daily diet – due to their high antioxidant activity. The recognition of such properties led to the development of enriched foodstuff – the so-called nutraceuticals – which are sold without any kind of regulation, even though it is well known that every antioxidant would act as a pro-oxidant agent at high concentrations [1]. Thus, the overconsumption of this kind of compounds constitutes a problem for human health. Concomitantly with the difficulty of separating and characterising each one of these agents – either from foodstuff or from the blended extracts – urges for the development of simple and reliable methods for determining, in a reliable and simple way, the properties of this type of phytochemicals.

Hence, the present study reports the improvement of Density Functional Theory (DFT) *in Silico* methodologies, capable of yielding relevant parameters such as the enthalpy of formation of the radical species (BDE) of these antioxidants [1]. Apart from the evaluation of the free radical scavenging ability of the compounds included in the training set, these methods allowed to accurately predict antioxidant activities in the light of the molecule′s structural features (establishing SAR′s).

The widely used B3LYP functional, coupled to distinct Gaussian basis sets, was applied for the BDEs prediction, while the DPPH standard assay was applied concomitantly for the assessment of radical scavenging properties. Additionally, a pure DFT method (VSXC), and additional basis sets and core potentials, were used for the calculation of other properties (spin density, pKa, ionization potentials). From the 18 tested compounds, 3 – fisetin, luteolin and quercetin – have shown to act as effective antiradicals, due to their lower BDE values [1].

Reference

1. Dias M M, Machado N F L, Marques M P M (2011) Dietary chromones as antioxidant agents—the structural variable. Food Funt 2, 595–602.

SW06.W29–11
Molecular dynamics simulation approach for DNA duplex thermal stability prediction

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Due to significant progress in development of computer software and hardware the *in silico* research became a useful tool to study biopolymers properties. Development of derivatives and analogues of nucleic acids remain laborious, costly and time-consuming. The using of computer simulations may allow precalculate physico-chemical properties of new derivatives before chemical synthesis. The aim of this work is to study a molecular dynamics (MD) simulation approach for nucleic acid thermal stability calculation.

Using Amber 11 software (UCSF, USA) we simulated single and double stranded oligodeoxyribonucleotides. The enthalpies of DNA duplex formation were calculated as a difference of the total internal energy of double- and single-stranded states which were averaged from 10 ns MD trajectory. Computations were performed on NVIDIA GTX580/Intel i7-2600 hardware and resources of Siberian supercomputer center (ICMMG SB RAS). The use of GPU has speeded up the modeling in implicit solvent up to 60 times and up to 30 times in explicit solvent in comparison with the one node of CPU.

To determine optimal parameter set of modeling we have used Dickerson-Drew dodecamer (DDD) 5'-CGCGAATTCGCG-3' with well characterized secondary structure and thermal stability. We have varied force field, temperature, heating protocol, and ion concentration in implicit and explicit solvent, solvent shell radius and compared averaged double stranded DNA structures with those experimentally obtained. We have determined the optimal parameters of modeling in implicit and explicit solvent. It was shown that the experimental and obtained via the MD simulation conformations of duplexes structures are close to each other. Also the difference of experimental and calculated via the MD simulations enthalpies differ <15% whereas the experimental accuracy is about 10%.

To verify the MD predictive ability we have collected database of experimentally determined thermodynamic parameters (enthalpy and entropy) of hybridization of more than 300 oligodeoxyribonucleotides. The length of oligonucleotides varies from 4 up to 16 base pair (aver. 9 bp), GC-content 0–100% (aver. 57%). The total energy of oligonucleotide or duplex was averaged over 10 000 snapshots of 10 ns trajectories simulated with optimal parameter set. We have observed high correlation between the values of hybridization enthalpies obtained experimentally and calculated using MD in implicit and explicit solvent. The best prediction of thermodynamic parameters was obtained in explicit solvent after analysis of 10 ns MD trajectories using Molecular Mechanics Poisson Boltzmann Surface Area (MMPBSA) calculations at 300K.

The RMSD and average error values of calculated and experimental enthalpies were <12 and 15%, respectively. The results obtained show that MD modeling allows one to calculate enthalpy of matched DNA duplexes with surprisingly good accuracy.

It is known that experimental enthalpies and entropies of DNA duplex formation are in a very good linear correlation ($R^2 > 0.99$). Based on this this dependence we have calculated entropy and free Gibbs energy of complexation. The average error of Gibbs energy prediction was 13%. Using these values we calculate DNA duplex melting temperatures. The average error of melting temperature calculation using molecular dynamics simulation was 4.6 °C. The results obtained is unexpectedly very