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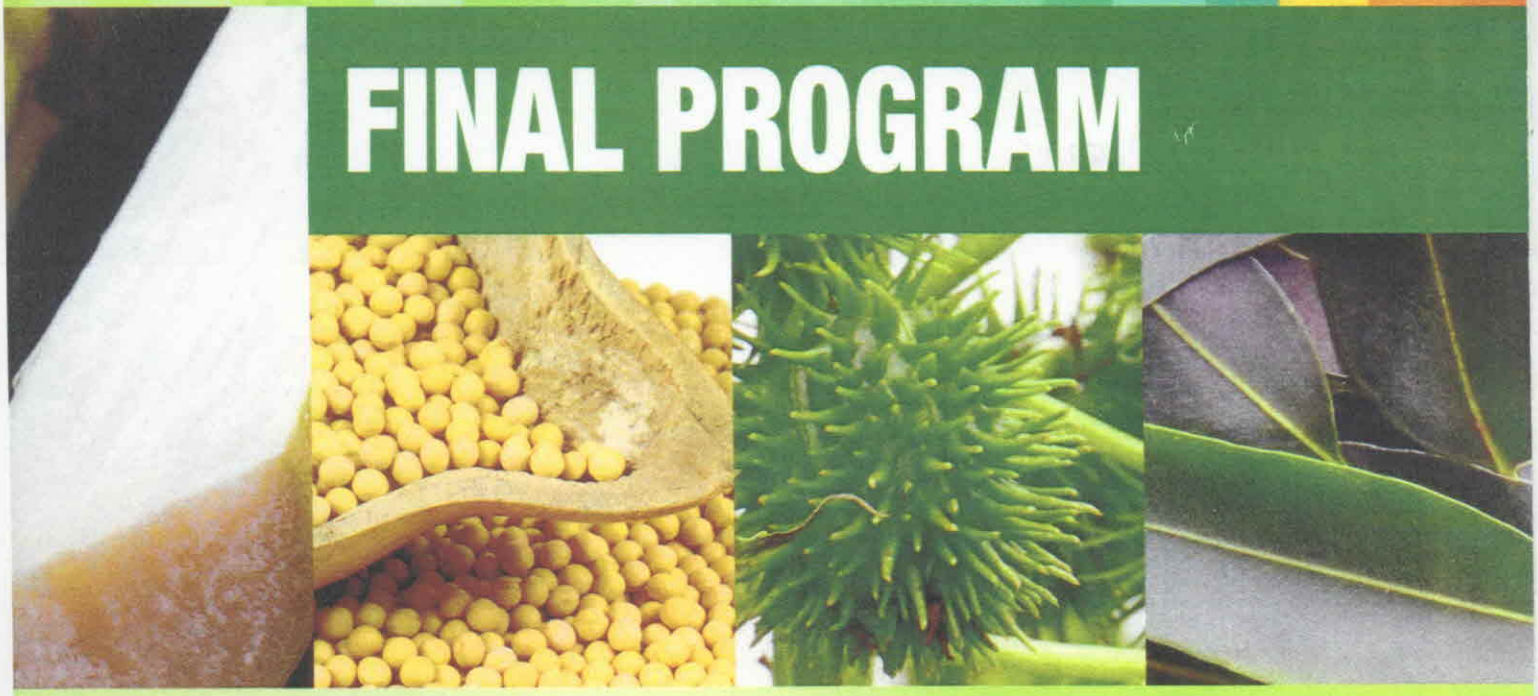
FINAL PROGRAM



University). In a simulation that uses the MD computational technique, the motion of the particles composing any system can be determined, since the potential interaction between these particles and the equations governing their motion are known. Aiming to discover structural properties that confer the hyperthermostability to RmLam, two other enzymes structurally very similar were also studied: the laminarinases from Nocardiopsis sp., thermophilic, and from Phanerochaete chrysosporium, mesophilic. The interaction potentials were computed according to the CHARMM27 force field. Several simulations of these enzymes' dynamics were performed in aqueous isotonic solution at 25 °C and at 90 °C, and all simulations were run at atmospheric pressure. To examine the mobility of different regions of the enzymes, we computed the average RMSF (root mean square fluctuation) of -carbons on amino acids relative to their average positions in the simulations. As a result, it is emphasized that the residues in the catalytic tunnel of thermophilic enzymes display, at high temperature, mobility values very close to the ones observed for the mesophilic enzyme at room temperature, which indicates the correspondence between the states in which the enzymatic activity is optimized. The three enzymes have almost the same percentage of nonpolar residues, but the hyperthermophilic enzyme has a larger quantity of charged residues. It was found that, in RmLam, these residues are arranged to form large salt clusters around the catalytic tunnel, like a beam that stabilizes the three dimensional structure. The salt bridges on the remainder enzymes occur in smaller quantities and are distant from each other. Specifically in the mesophilic enzyme it was found that salt bridges occur between the layers of beta-sheets, 'contaminating' the hydrophobic core. In this region there is a water intake when the temperature is increased, which, it is suggested, is one factor that contributes to the inactivation of this enzyme at high temperature.

glycosil hydrolase, hyperthermophilic enzyme, laminarinase, molecular dynamics,

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Towards Higher Yield In Vegetable Oil Production: Profit From Biodiversity

Felix L P2, Pereira Cabral, S1, Pinho R S1, Vizzotto L3, Colnago L A3, Harand W1

1. CETENE, Centro de Tecnologias Estratégicas do Nordeste, Av. Prof. Luiz Freire, 01. Cidade Universitária - CEP: 50.740-540 - Recife - PE2. UFPB, Universidade Federal da Paraíba, Campus III, CEP: 58.397-000 - Areia - PB - Brasil3. EMBRAPA, Empresa Brasil

Abstract: Brazilian legislation requires substitution of 5% of mineral diesel with biodiesel. The rapid launch of the Brazilian biodiesel program favored already existing raw materials for biodiesel production, provoking a dominance of soybean, which is responsible for 80% of biodiesel production. Although abundantly available, this source comprises several problems, for example low oil yield per hectare and geographic limitation. To guarantee international competitiveness and long

term progress of the Brazilian biodiesel program, the promotion of new oil crops is mandatory. However, the lack of domesticated oil crops contrasts with an overwhelming natural biodiversity. To identify and test criteria to narrow Brazilian biodiversity down to promising groups of species for future vegetable oil production, two strategies were applied: A phylogenetic approach, evaluating a database (Aitzetmüller et al., 2003) for plant families with high numbers of species with high seed oil content, and a life-form approach, derived from Levin (1974). Plant material, collected in various regions of north-eastern Brazil in 2008 and 2009, was analysed for oil content by soxhlet extraction and, in case of individual seeds, by low-resolution nuclear magnetic resonance. The database analysis yielded nine families with 15 or more registered species with a seed oil content higher than 50% (Lauraceae, Euphorbiaceae, Cucurbitaceae, Arecaceae, Sapotaceae, Sapindaceae, Meliaceae, Myristicaceae, Malvaceae). For oil content analysis, 23 species from 11 families were collected following either the phylogenetic or the life-form approach. 16 of those had oil contents higher than 20%, thus considered promising. 13 belonged to families classified promising by the phylogenetic approach, whereas twelve are tropical trees, indicated as promising by life-form analysis. Highest oil contents were found in palm kernels (Attalea oleifera 66%, Syagrus cearensis 67% and S. coronata 68%), followed by samples from the families Malvaceae (Pachira aquatica 47%, Bombacopsis retusa 44% and B. glabra 30%) and Sterculiaceae (Sterculia foetida 39%). For three species, inter-individual variation was determined. In Azadirachta indica (Meliaceae), the maximum exceeded the mean by 35% (n=10), in Ouratea sp. (Ochnaceae), by 24% (n=5), and in Manihot glaziovii (Euphorbiaceae), by 13% (n=5). Variation within seeds of the same individual was in the order of 5% to 12% (S. cearensis 5%, Acrocomia intumescens 6%, Moringa oleifera 10%, S. foetida: 10%, P. aquatica 12% (n=10 in all cases). Both strategies yielded a considerable number of promising species for vegetable oil production. The phylogenetic approach, however, favours species-rich families, which rules out promising samples from smaller families. Oil contents detected in the seeds were up to four times higher than that of soybeans. Both inter- and intra-individual variation of the species indicate high potential for increase of oil yield in domestication processes.

alternative oilseed crops, bio prospecting, vegetable oil, biodiesel,

Area: Plant breeding and bioenergy

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Identification Of DNA Polymorphisms Associated To Cell Wall Degradability In Alfalfa

Dube, M.-P., Duceppe, M.-O., Castonguay, Y., Michaud, R., Bertrand, A.

1. AAC, Agriculture and Agri-Food Canada, 2560, Hochelaga blvd, Quebec city, QC, G1V 2J3, Canada