

ORIGIN OF THE DISCRIMINATORY MECHANISM OF PROTEINOUS AMINOACIDS FROM THE NON-PROTEINOUS AMINOACIDS BY THE PROTEIN SYNTHESIZING MACHINERY.

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Out of the about two hundred biologically available aminoacids (Mooz, 1976; Hunt, 1985) only twenty are used by the present day protein synthesizing machinery. Though they are not commonly found in the protein main chains the non-proteinous aminoacids play vital roles in living systems (by even being present in natural polypeptides due to post-translational modifications etc.,). Moreover they are invariably produced in prebiotic synthesis type of experiments (Miller, 1953; Harada and Fox 1964; Ring et al., 1972, Barak and Bar-Nun, 1975; Schlesinger and Miller, 1983). Studies on Martian atmosphere Thule group cherts, carbonaceous chondrites and gaseous mixtures of lunar samples etc., also reveal the presence of non-proteinous aminoacids (Kvenvolden, 1974, Kotra et al., 1982, Hatori et al., 1984; Yuasa et al., 1984). In spite of the above facts why only twenty aminoacids are being coded by the present day protein synthesizing machinery and whether the discriminatory mechanism of proteinous and non-proteinous aminoacids originated along with the origin of very protein synthesizing machinery are critical questions which are yet to be fully understood. Certain explanations for the occurrence of only twenty coded aminoacids have been put forward (Rohlfing and Saunders, 1978; Weber and Miller, 1981).

In order to understand these questions we reviewed certain experimental studies aimed at understanding the origin of the genetic code which were done after such a

review by Lacey and Mullins(1983). In summary these experimental studies do not give any clear mechanism for the origin of the genetic code. So as a logical next step, we explored the various theoretical models for the origin of the genetic code, which involve various forms of adaptor molecules(Hopfield, 1978; Tyagi, 1981; Kuhn and Waser, 1981; Balasubramanian, 1980; Ishigami et al., 1984). The primitive tRNA(PIT) model proposed by our lab seemed to possess quite interesting features(Balasubramanian, 1985) including an explanation for the origin of the discriminatory mechanism of proteinous and non-proteinous aminoacids by the protein synthesizing machinery(Balasubramanian and Raghunathan 1985). We carried out elaborate computer-graphics(Rafi and Balasubramanian, unpublished results) aided conformational energy studies on the interaction of proteinous aminoacids Alanine, Valine, Leucine and Threonine and their close non proteinous analogs Beta-Alanine, Nor-Valine, Nor-Leucine and allothreonine.

The results of these studies show whereas the proteinous analogs fit well in the cleft of their cognate PITs, their non-proteinous counterparts do not snugly fit in the cleft because of either or more of the following reasons.

- 1) Development of unrelievable short-contacts between the aminoacid side-chains and the primitive tRNA atoms.
 - 2) Breakage of the specific hydrogen bonds that hold the aminoacids in the PIT.
 - 3) Considerations of close packedness.
- Complete results of these studies are reported in the paper. The partial charges for these non-proteinous aminoacids which were necessary for our calculations were also calculated by us and reported in this paper.

Finally our results some-what support the hardware interpretation of the evolution of the genetic code proposal (Angelica Soto and Jose Toha, 1985) rather than the co-evolution theory (Wong, 1981).

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