

Supplementary Materials

Effect of Point Mutations on Structural and Allergenic Properties of the Lentil Allergen Len c 3

Daria N. Melnikova ^{1,2,*}, Ekaterina I. Finkina ¹, Ivan V. Bogdanov ¹, Anastasia A. Ignatova ¹, Natalia S. Matveevskaya ³, Andrey A. Tagaev ¹ and Tatiana V. Ovchinnikova ^{1,2}

¹ M.M. Shemyakin & Yu.A. Ovchinnikov Institute of Bioorganic Chemistry, The Russian Academy of Sciences, Miklukho-Maklaya Str., 16/10, 117997 Moscow, Russia; finkina@mail.ru (E.I.F.); contraton@mail.ru (I.V.B.); aignatova_83@mail.ru (A.A.I.); andazitag@yandex.ru (A.A.T.); ovch@ibch.ru (T.V.O.)

² Phystech School of Biological and Medical Physics, Moscow Institute of Physics and Technology (State University), 141701 Dolgoprudny, Russia

³ G.N. Gabrichhevsky Research Institute for Epidemiology and Microbiology, Admiral Makarov St., 10, 125212 Moscow, Russia; matveevskaya@mail.ru

* Correspondence: d_n_m@mail.ru; Tel.: +7-495-335-42-00

Table S1. List of mutagenizing primers.

| Mutation | Mutagenizing primer sequences (5'-3') |
|----------|--|
| sT41A | ACGCCTGATCGTCAGGCTGCCTG |
| ansT41A | GCAGCCTGACGATCAGGCGTTGCAGCAAGAACCT |
| sY80A | AAGATCAGTACCAACCACCAACTG |
| ansY80A | TTGGTGCTGGTACTGATCTTGCAGGAATGTTGACACCACATT |

Table S2. Secondary structure evaluation (%) predicted from Far-UV CD spectra.

| Sample | α -helix, % | β -sheet, % | β -turn, % | random, % | NRMSD* |
|------------|--------------------|-------------------|------------------|-----------|--------|
| Len c 3 | 28.4 | 19.1 | 22.1 | 30.3 | 0.01 |
| T41A | 29.3 | 18.1 | 22.3 | 30.1 | 0.02 |
| R45A | 29.2 | 18.6 | 21.8 | 30.5 | 0.01 |
| Y80A | 29.1 | 19.1 | 21.5 | 30.3 | 0.02 |
| T41A/ Y80A | 29.2 | 18.4 | 22.2 | 30.2 | 0.02 |
| R45A/ Y80A | 29.0 | 18.2 | 21.1 | 31.7 | 0.01 |

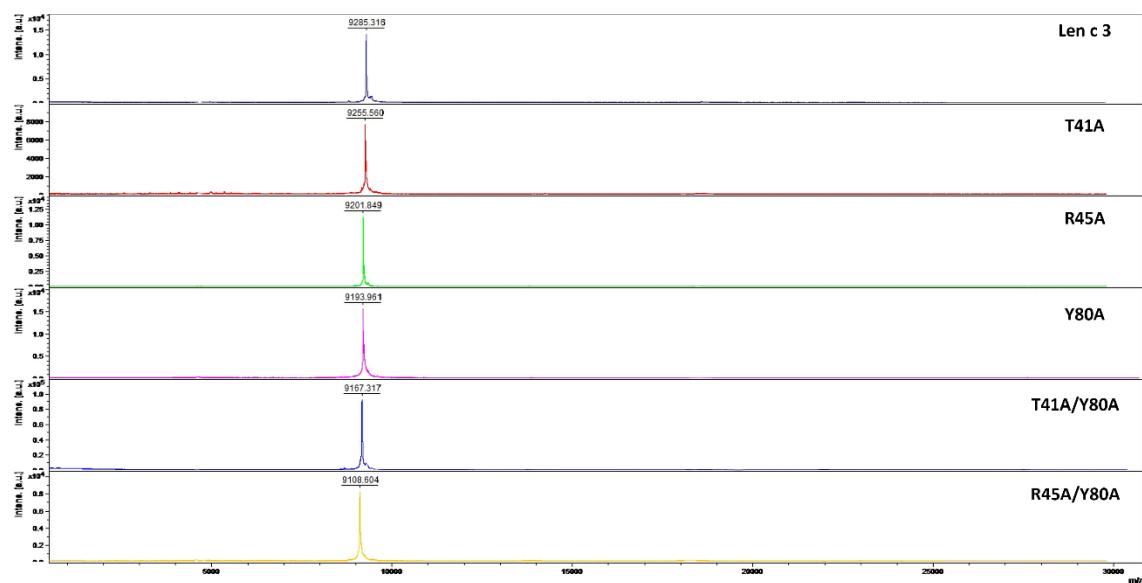


Figure S1. MALDI mass spectra of the Len c 3 and its mutant analogues.