Electronic Supplementary Material (ESI) for Natural Product Reports.

SUPPLEMENTAL MATERIAL

STRUCTURE-FUNCTION-RELATIONSHIP OF TERPENOID GLYCOSYLTRANSFERASES FROM PLANTS

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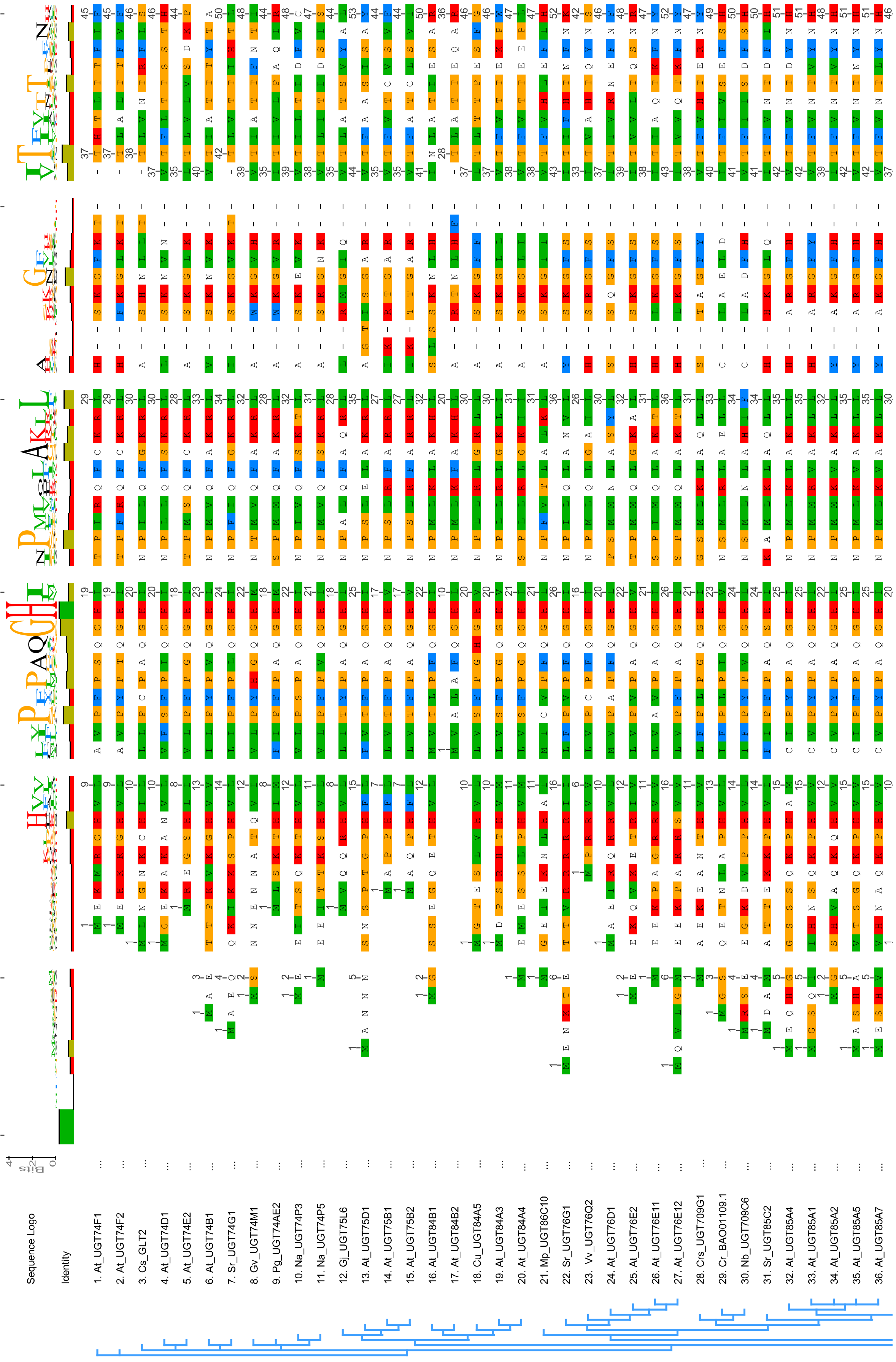
[2]Chair of Food Chemistry, Institute of Nutritional and Food Sciences, University of Bonn, Endenicher Allee 19C, 53115 Bonn, Germany
[3]State Key Laboratory of Tea Plant Biology and Utilization and International Joint Laboratory on Tea Chemistry and Health Effects, Anhui Agricultural University, Hefei, Anhui 230036, People's Republic of China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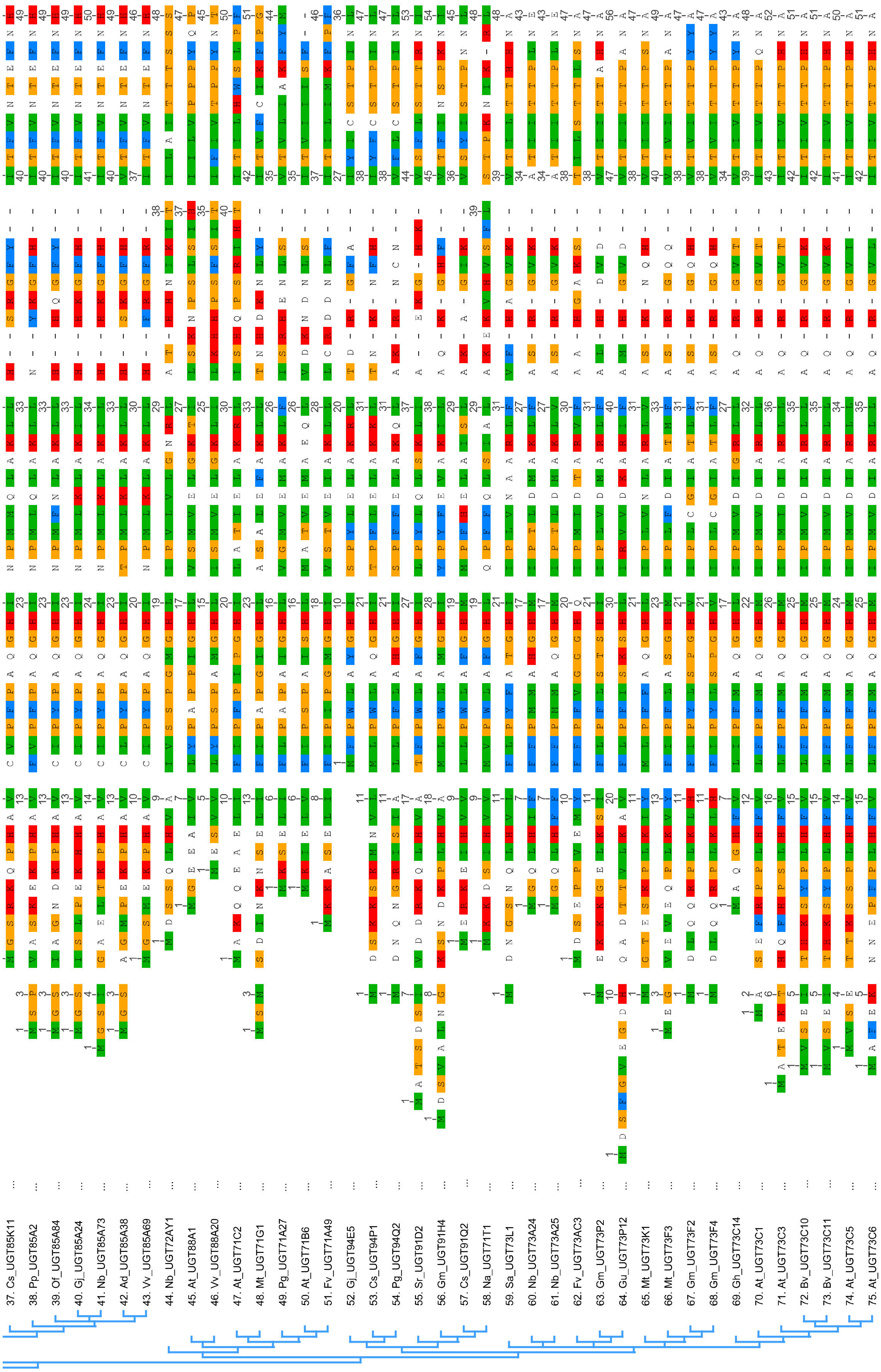
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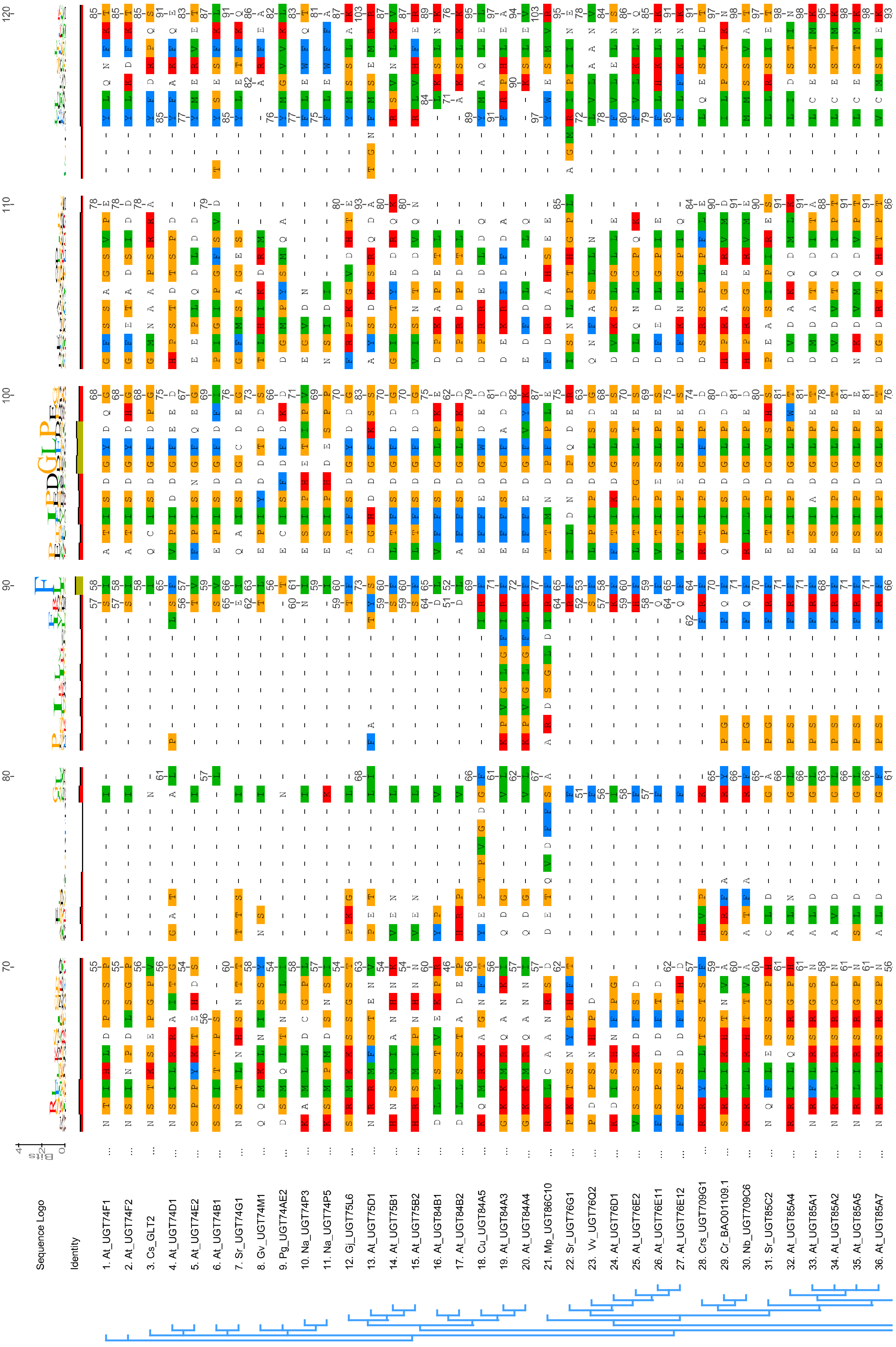
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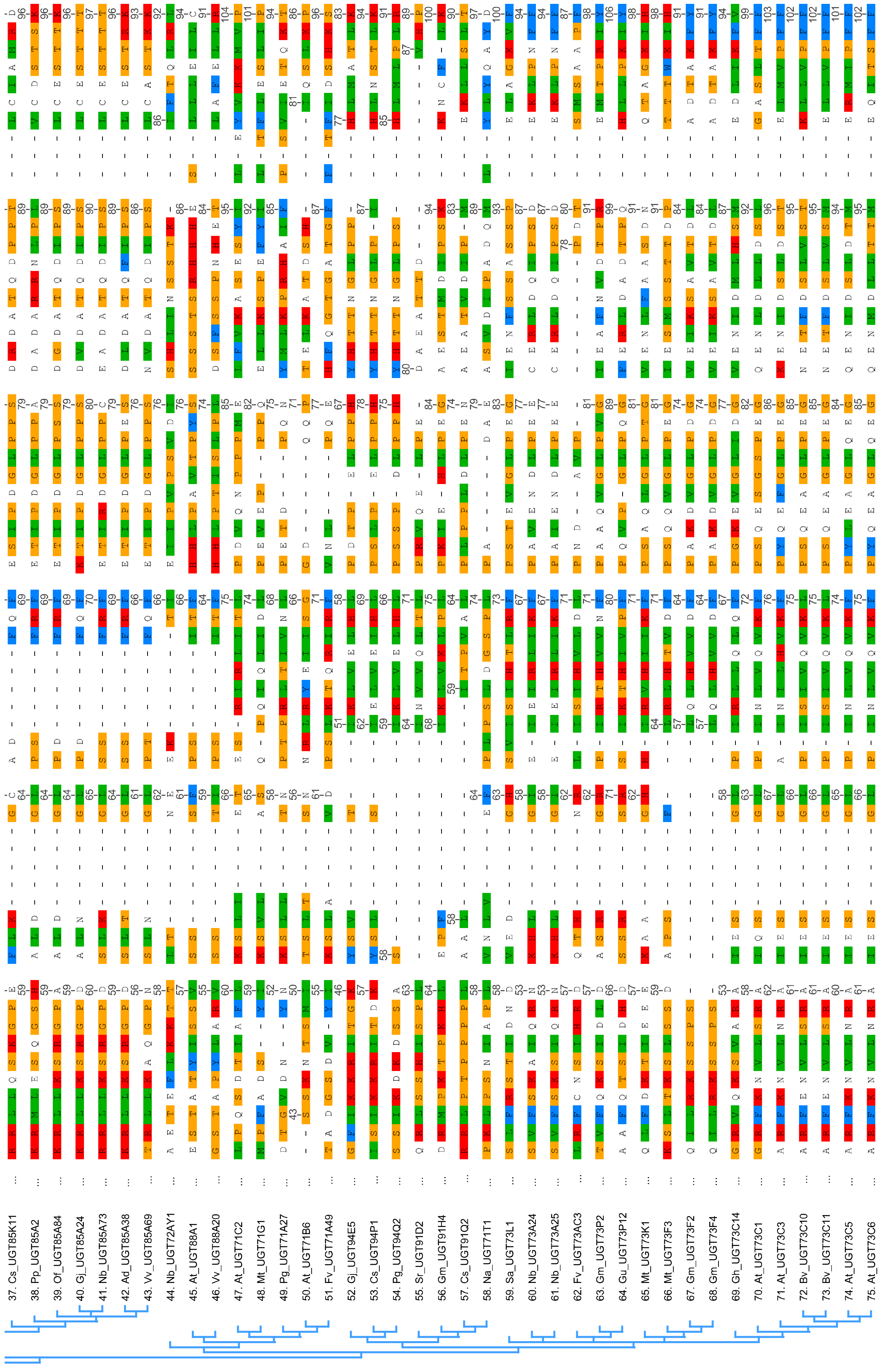
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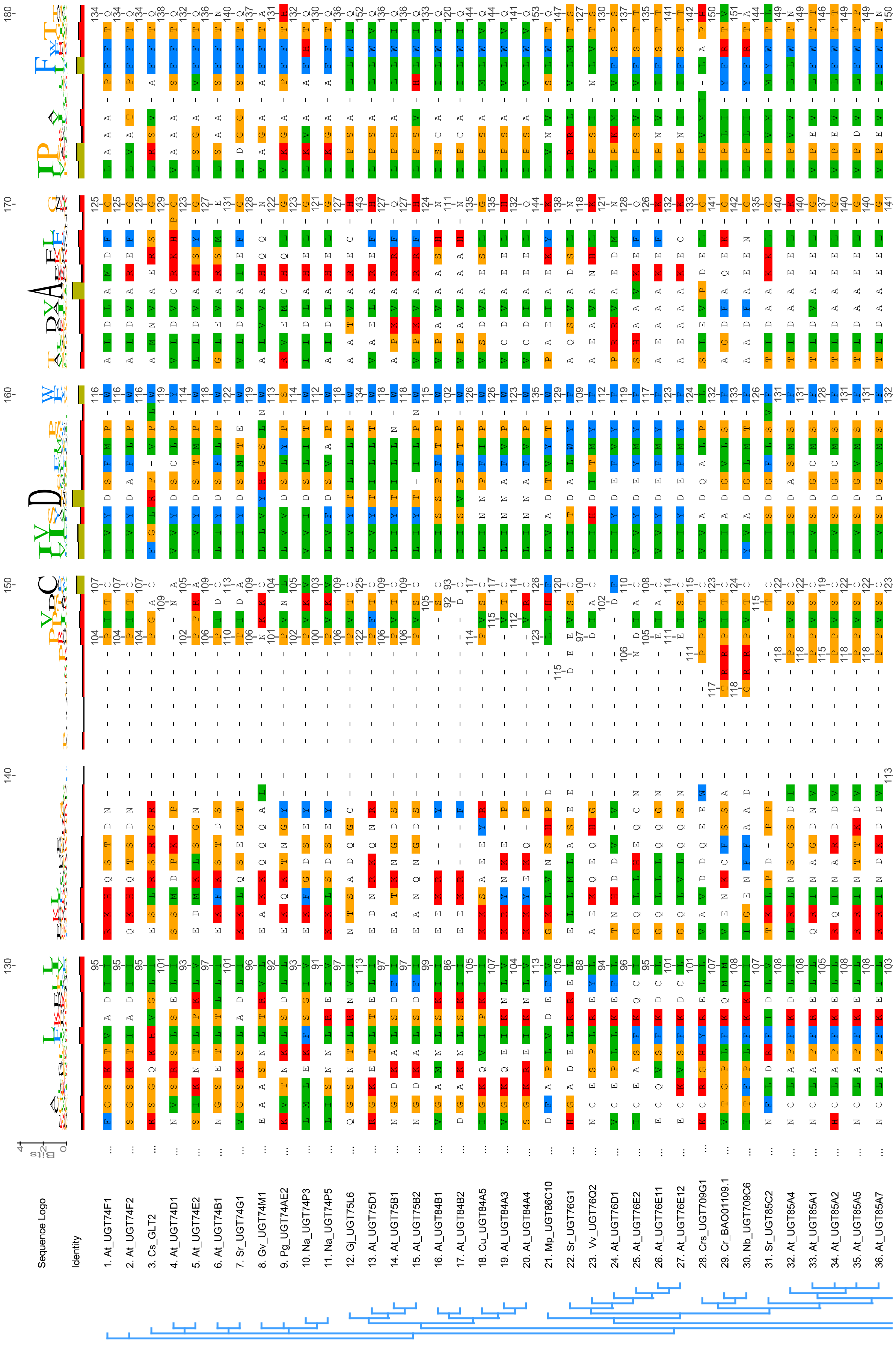
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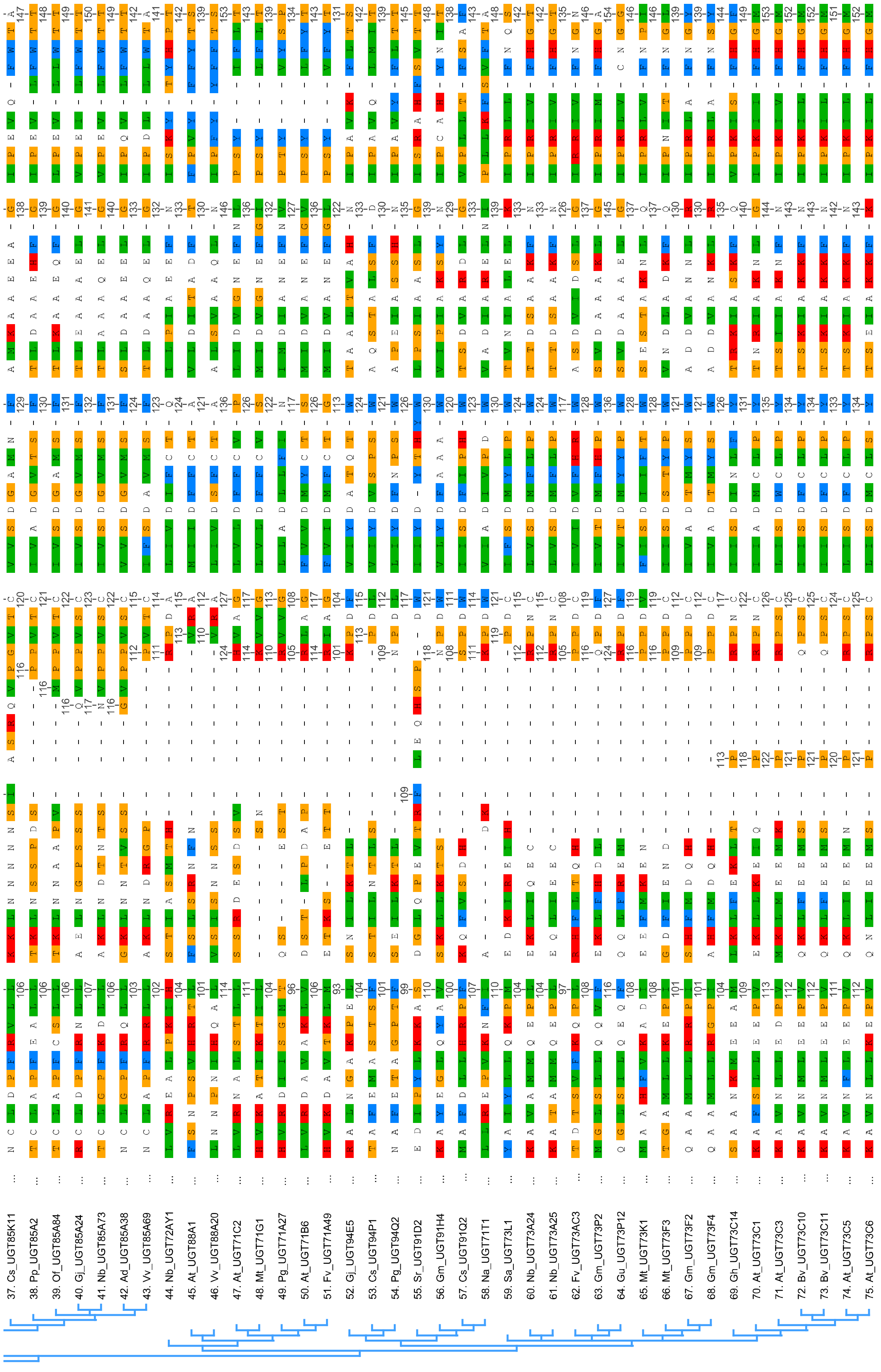
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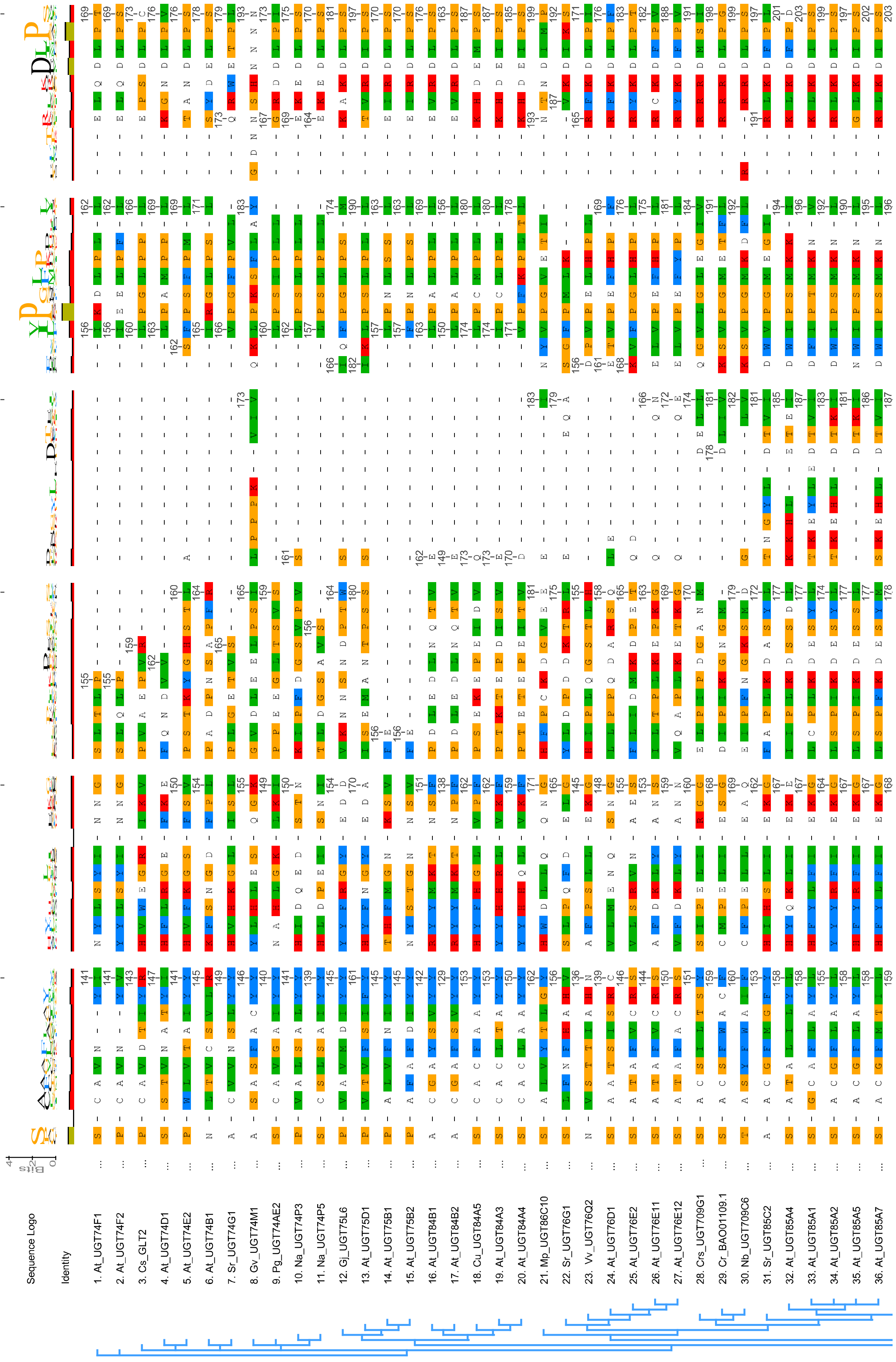
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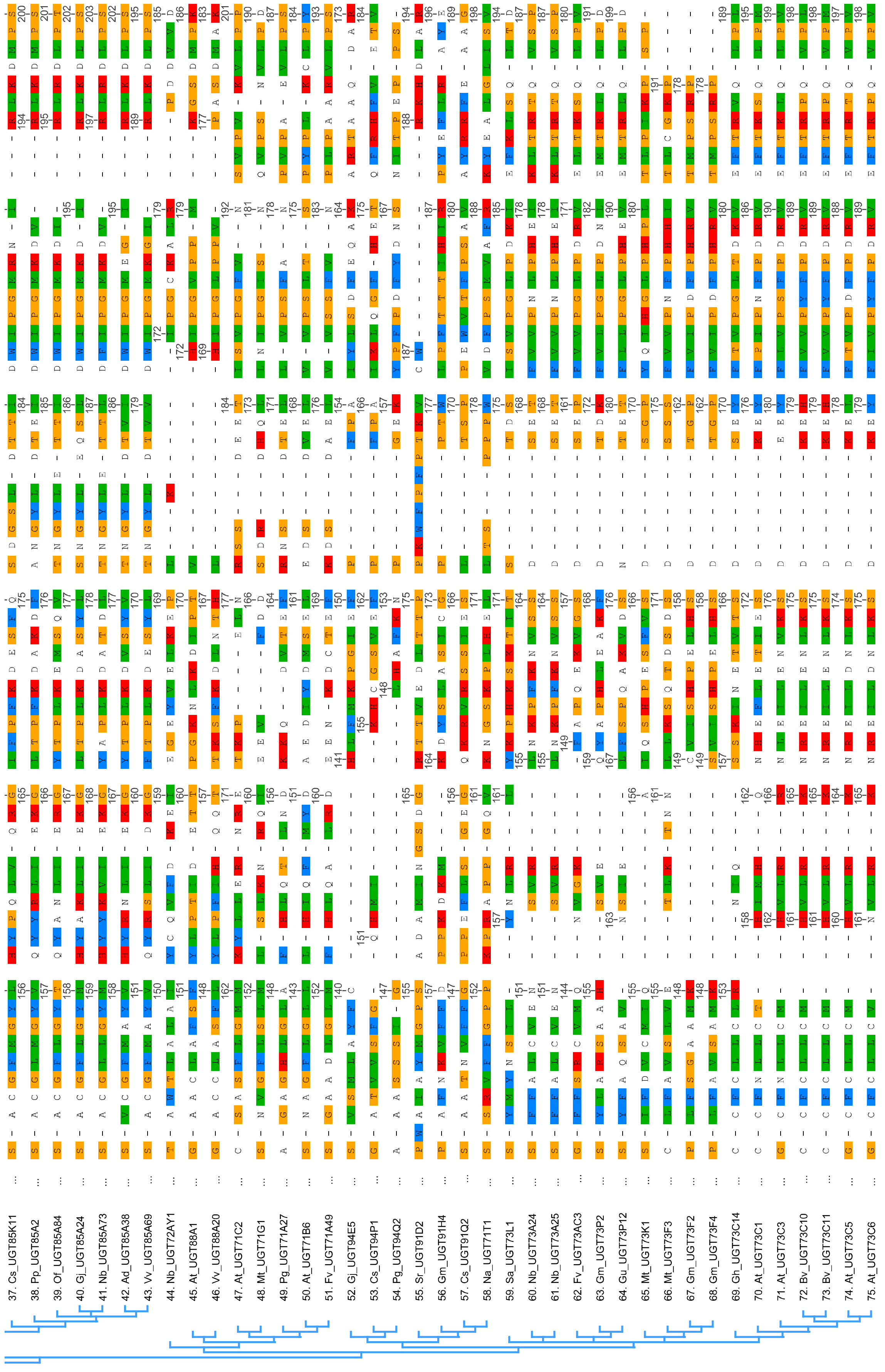
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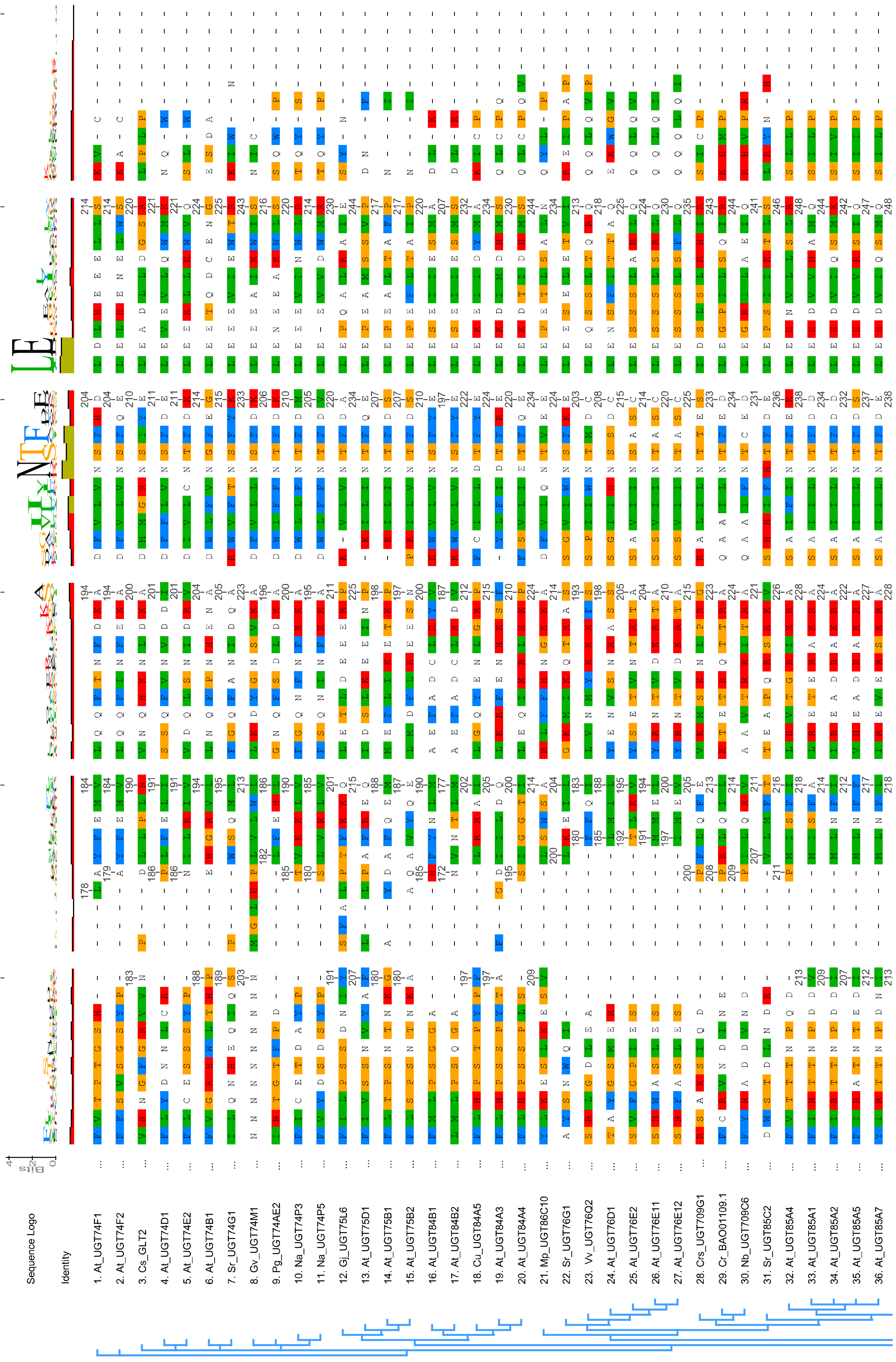
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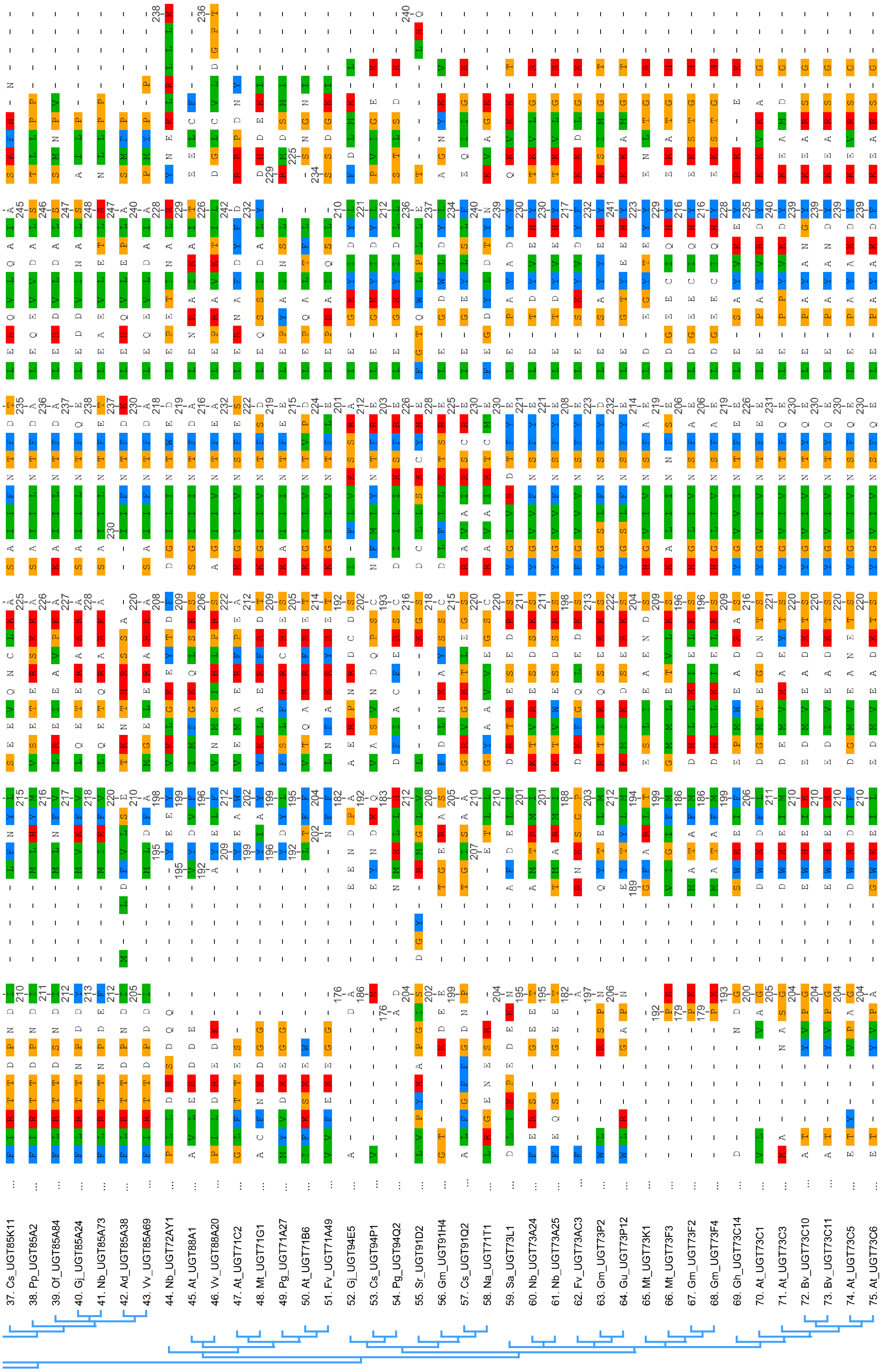
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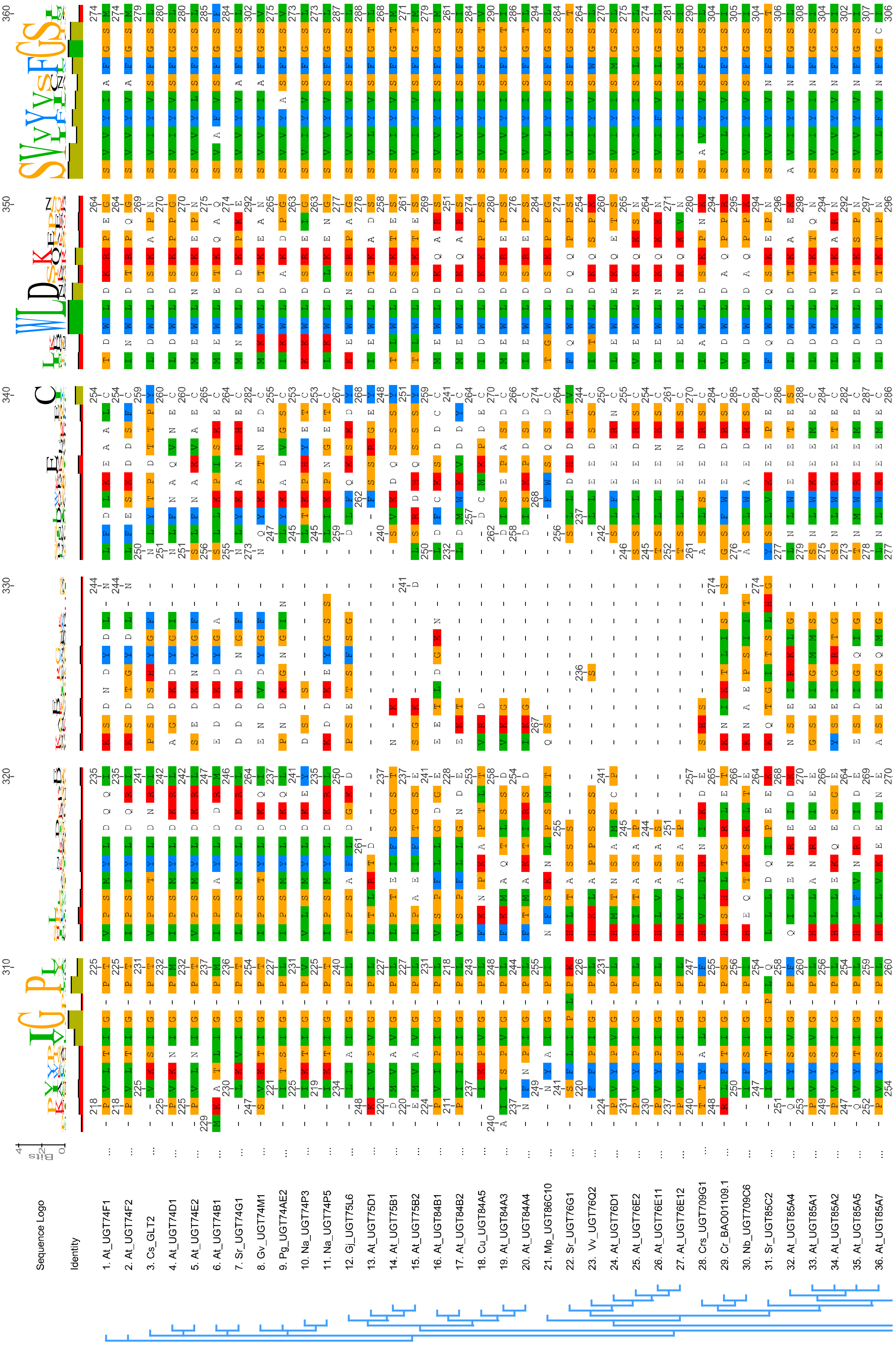
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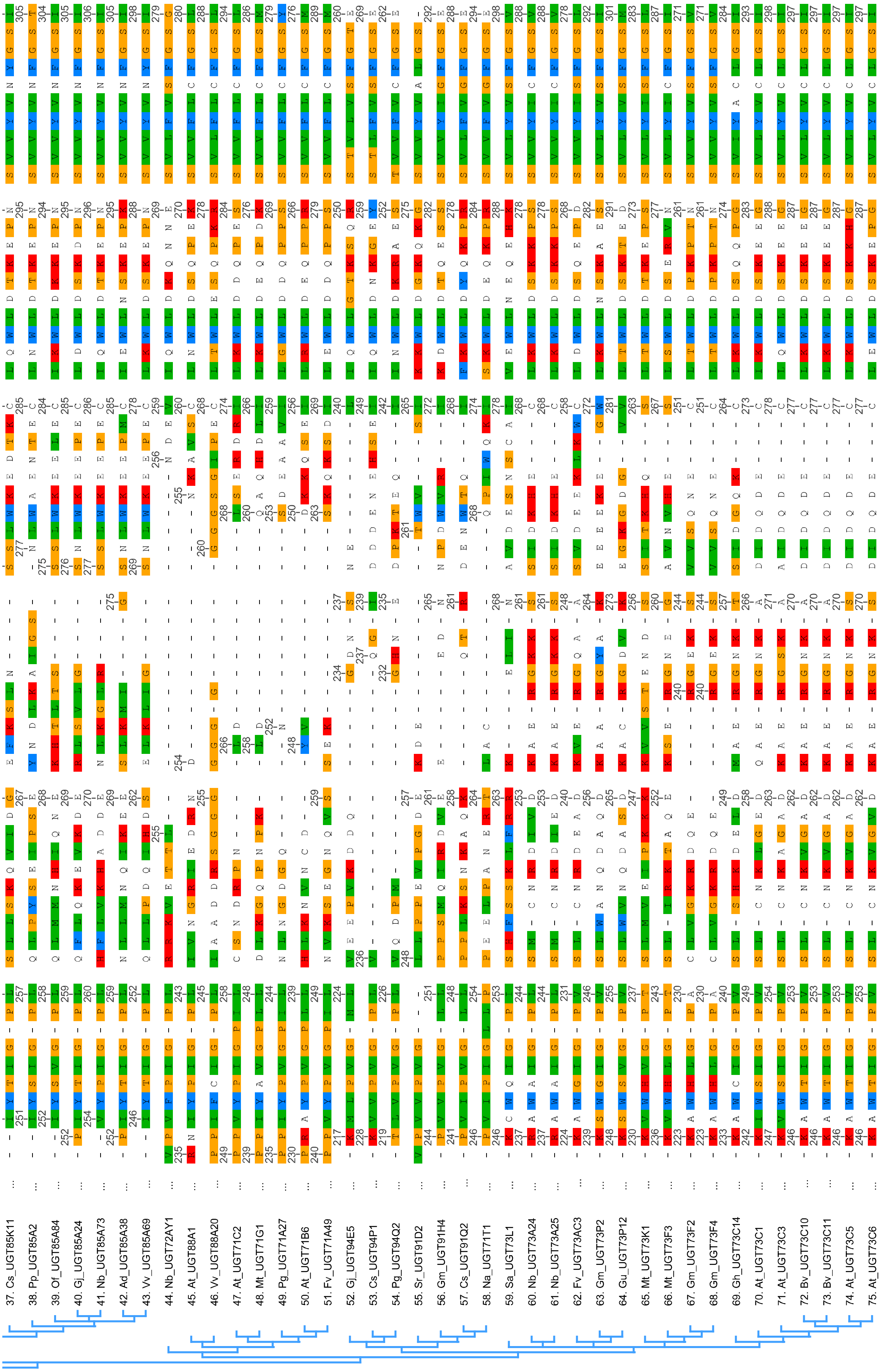
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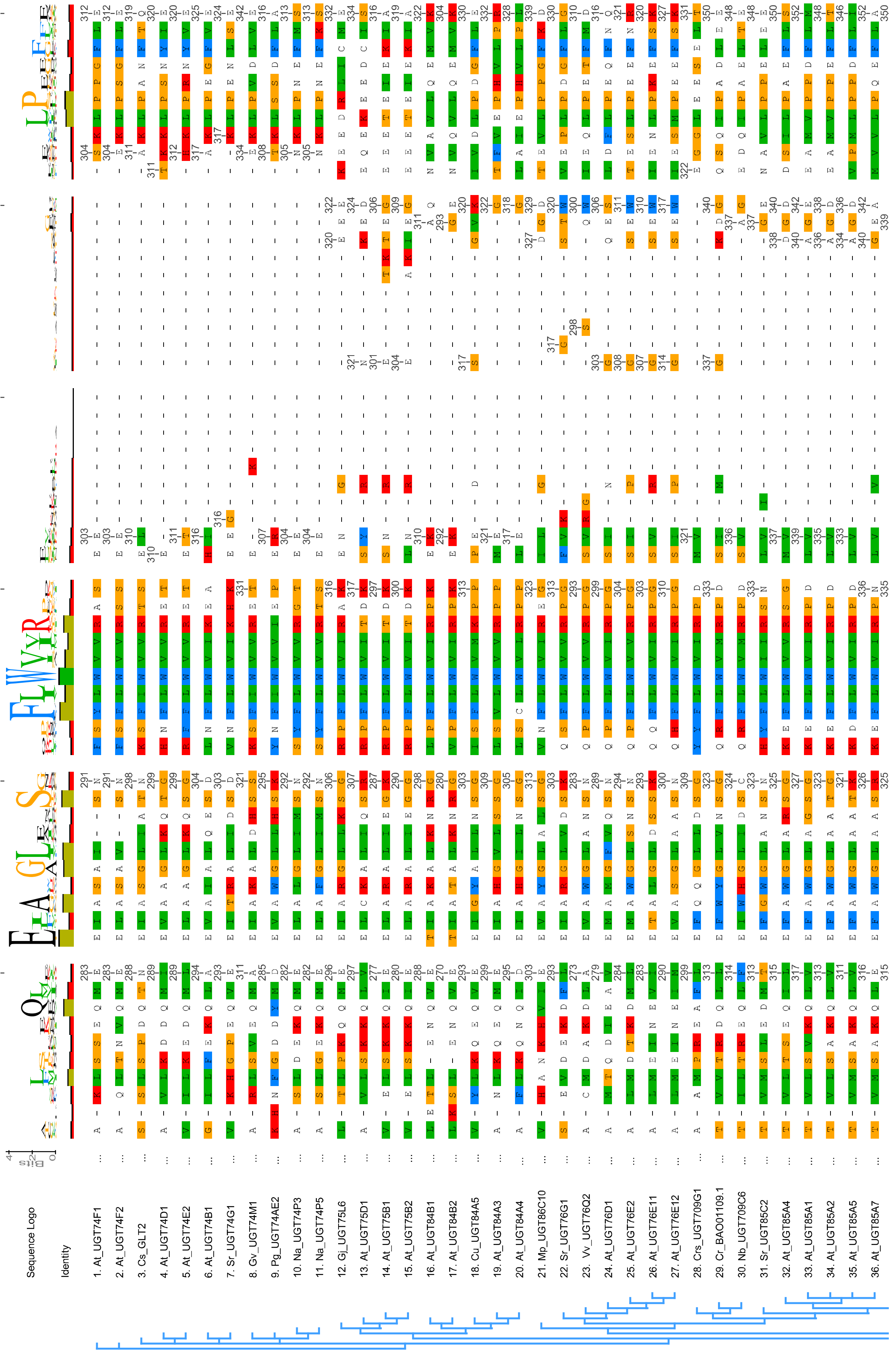
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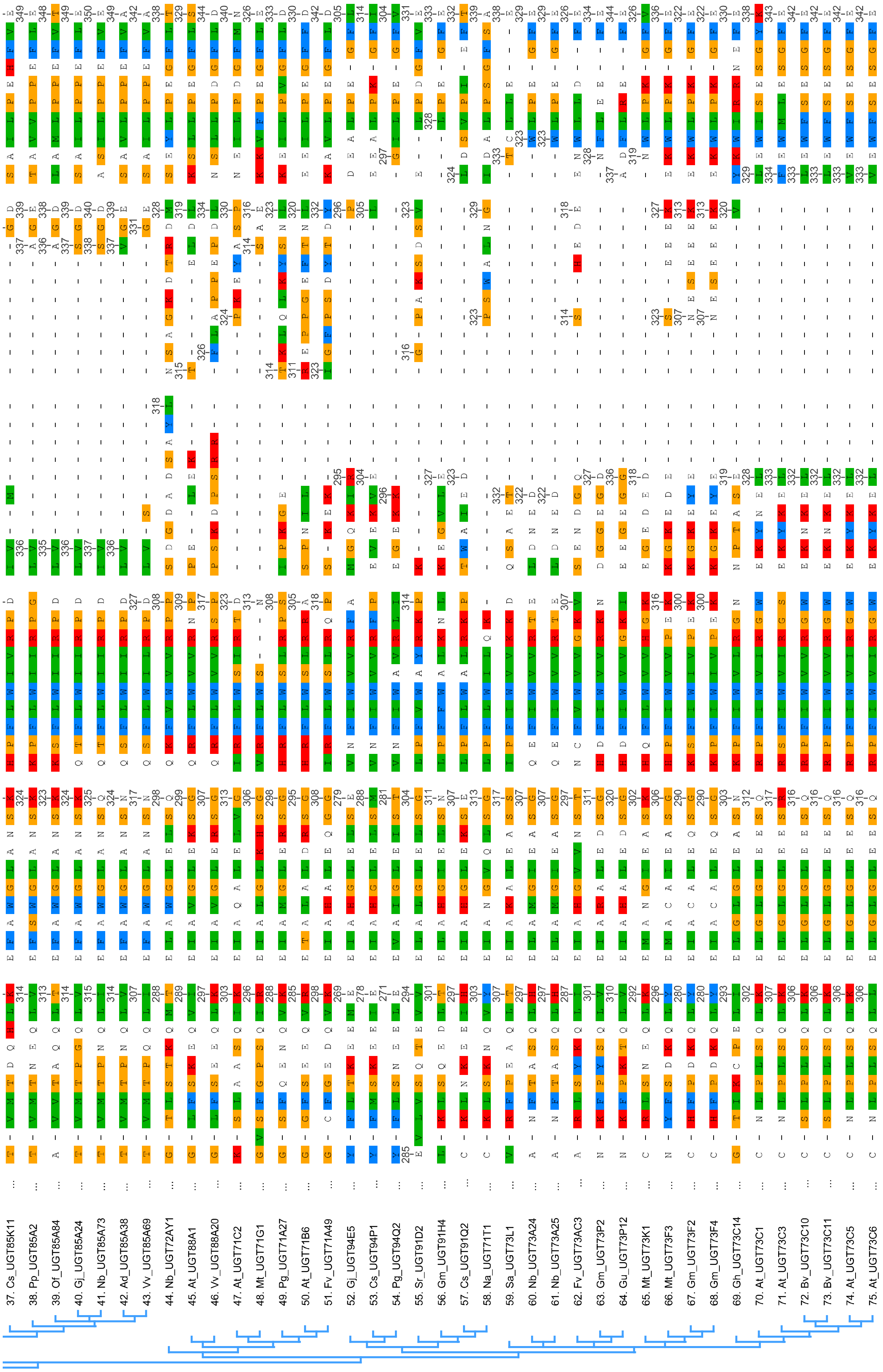
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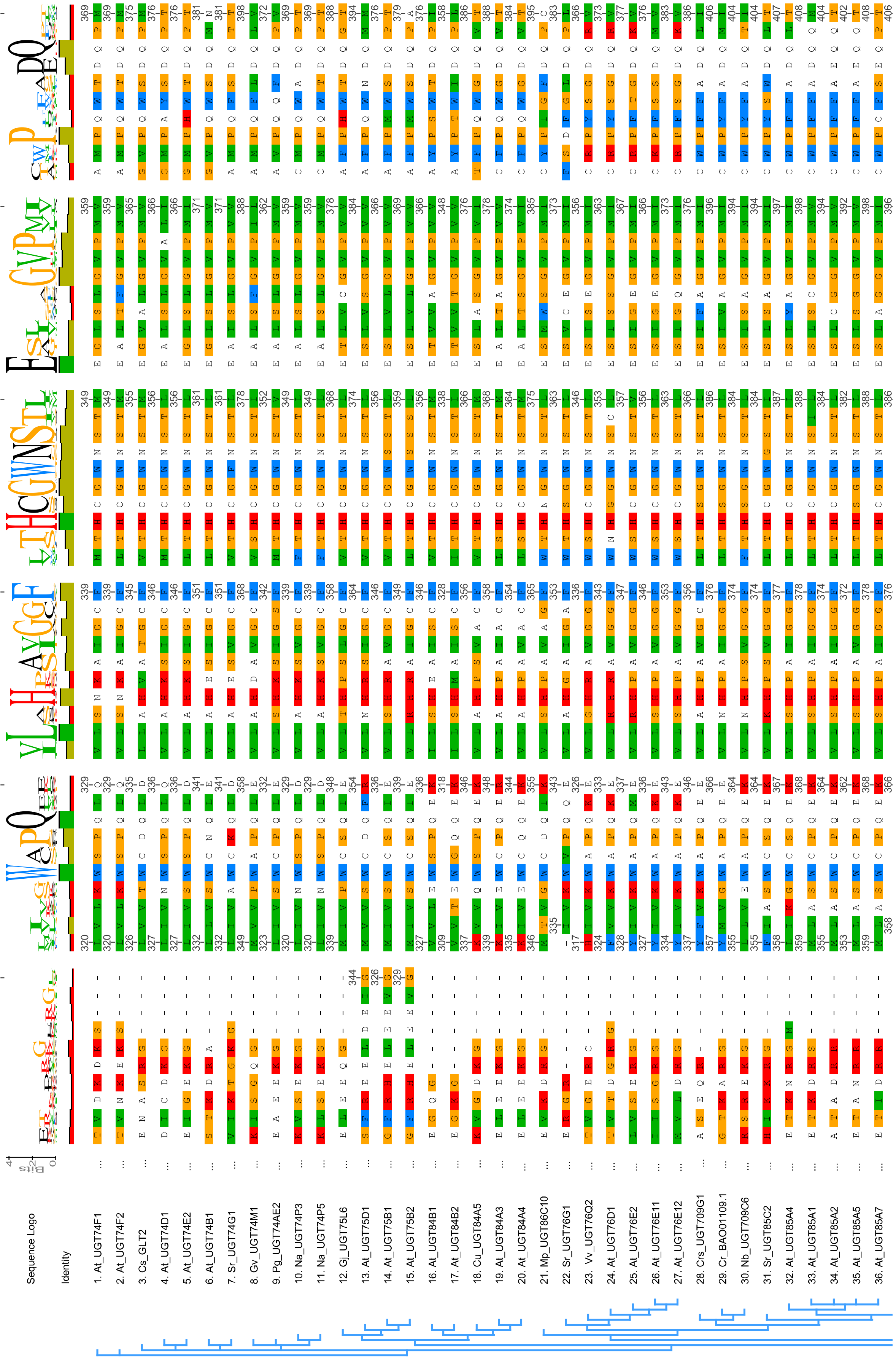
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26. At_UGT76E11
27. At_UGT76E12
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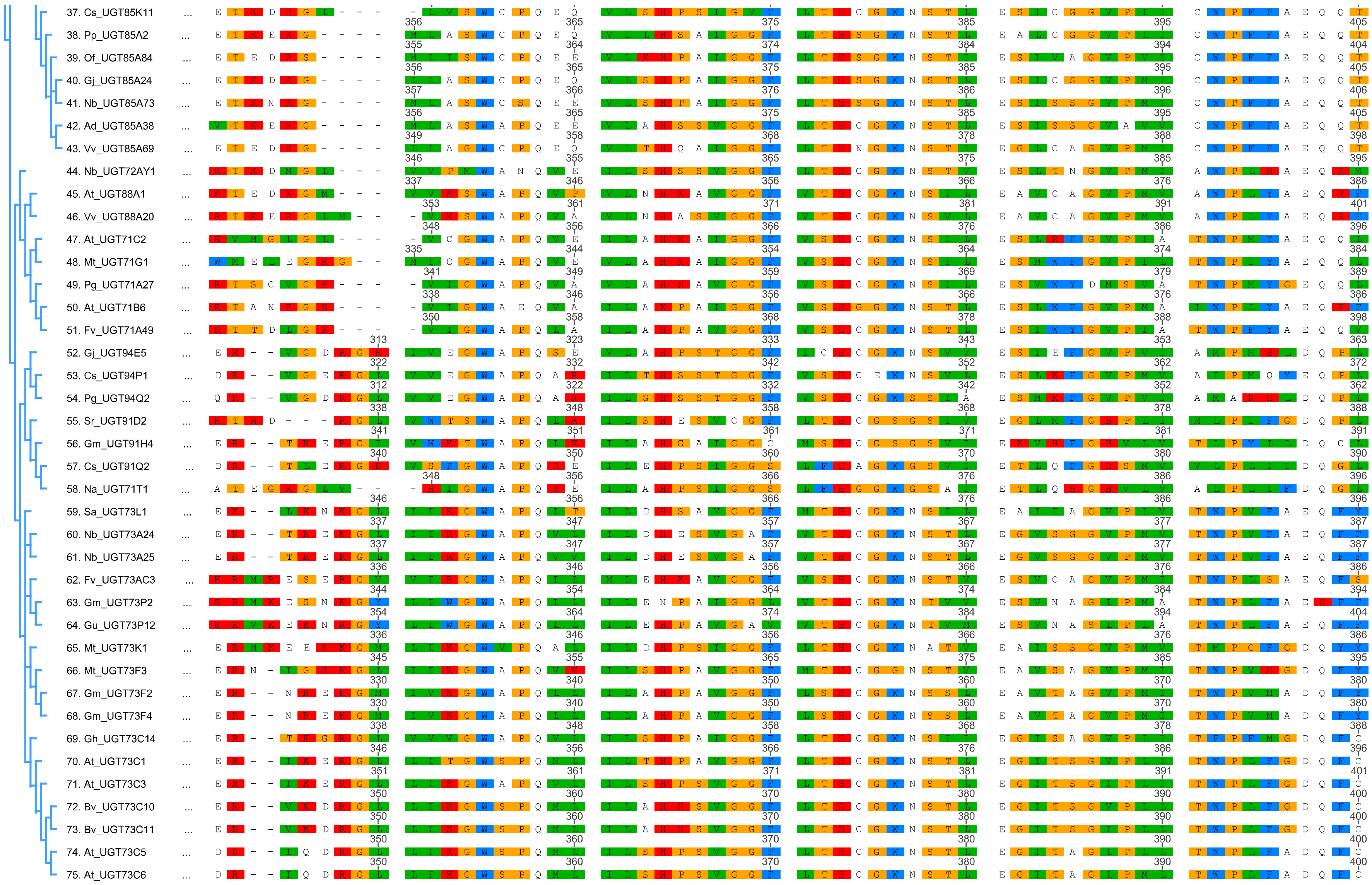
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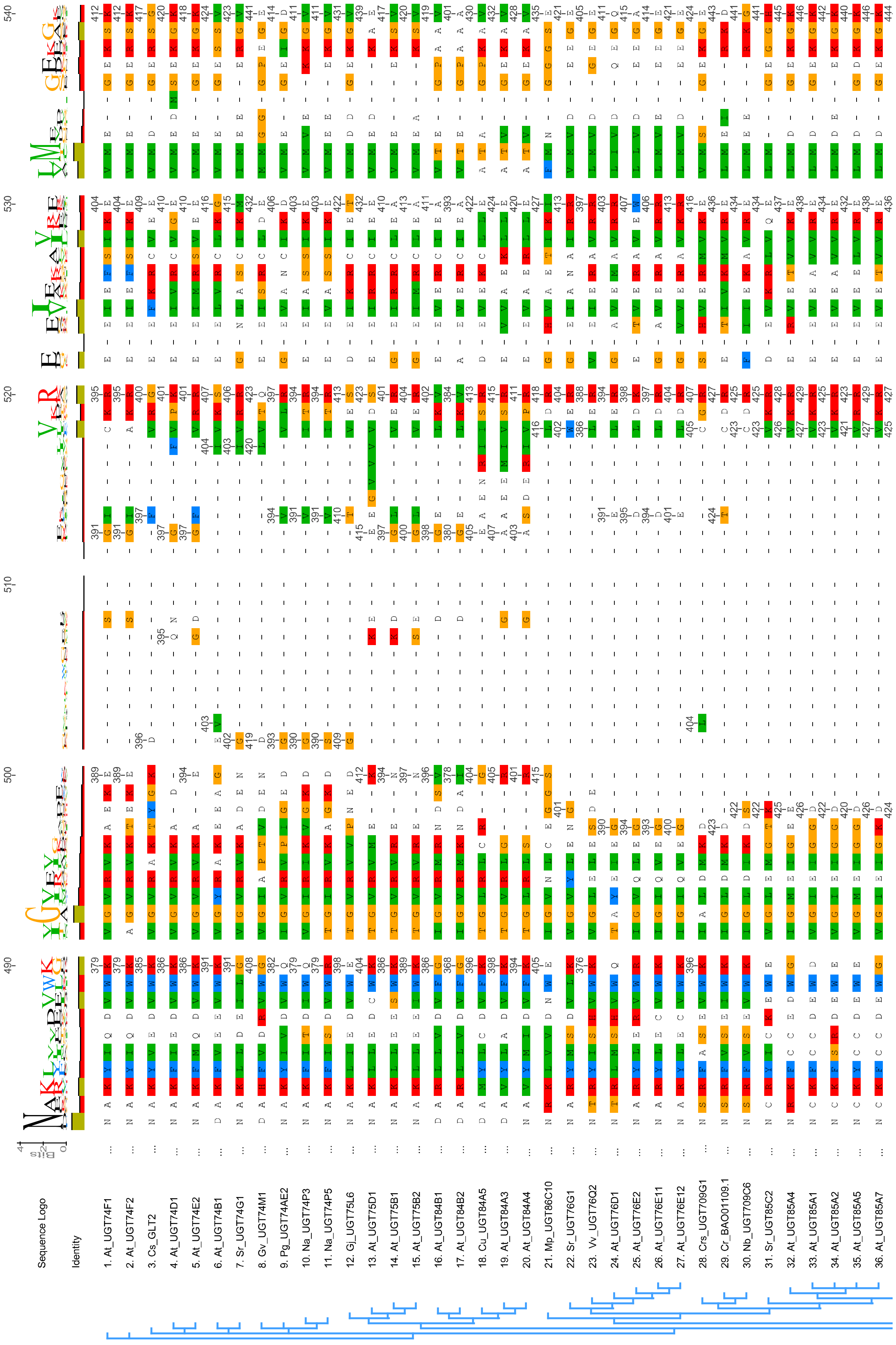
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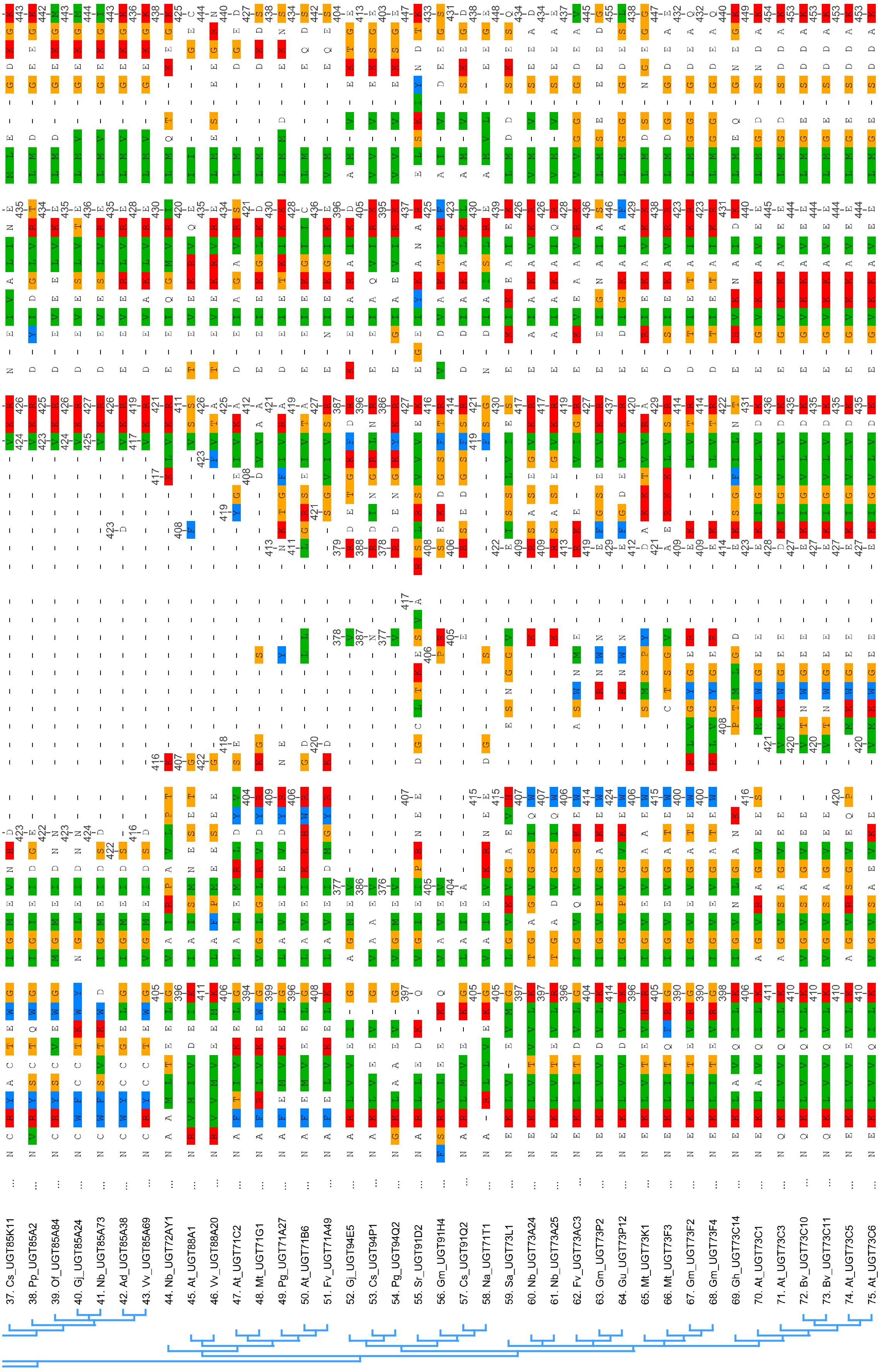
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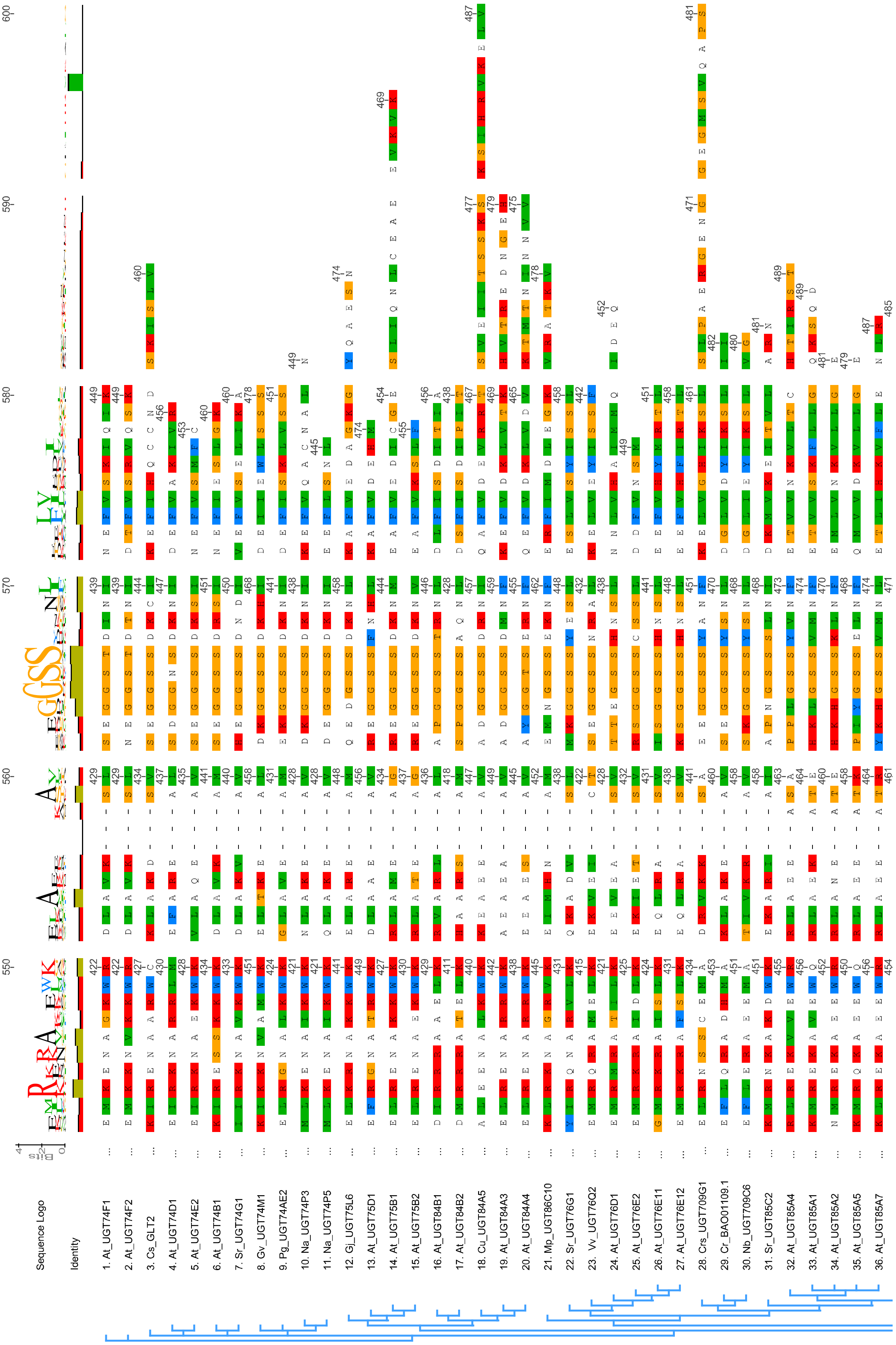
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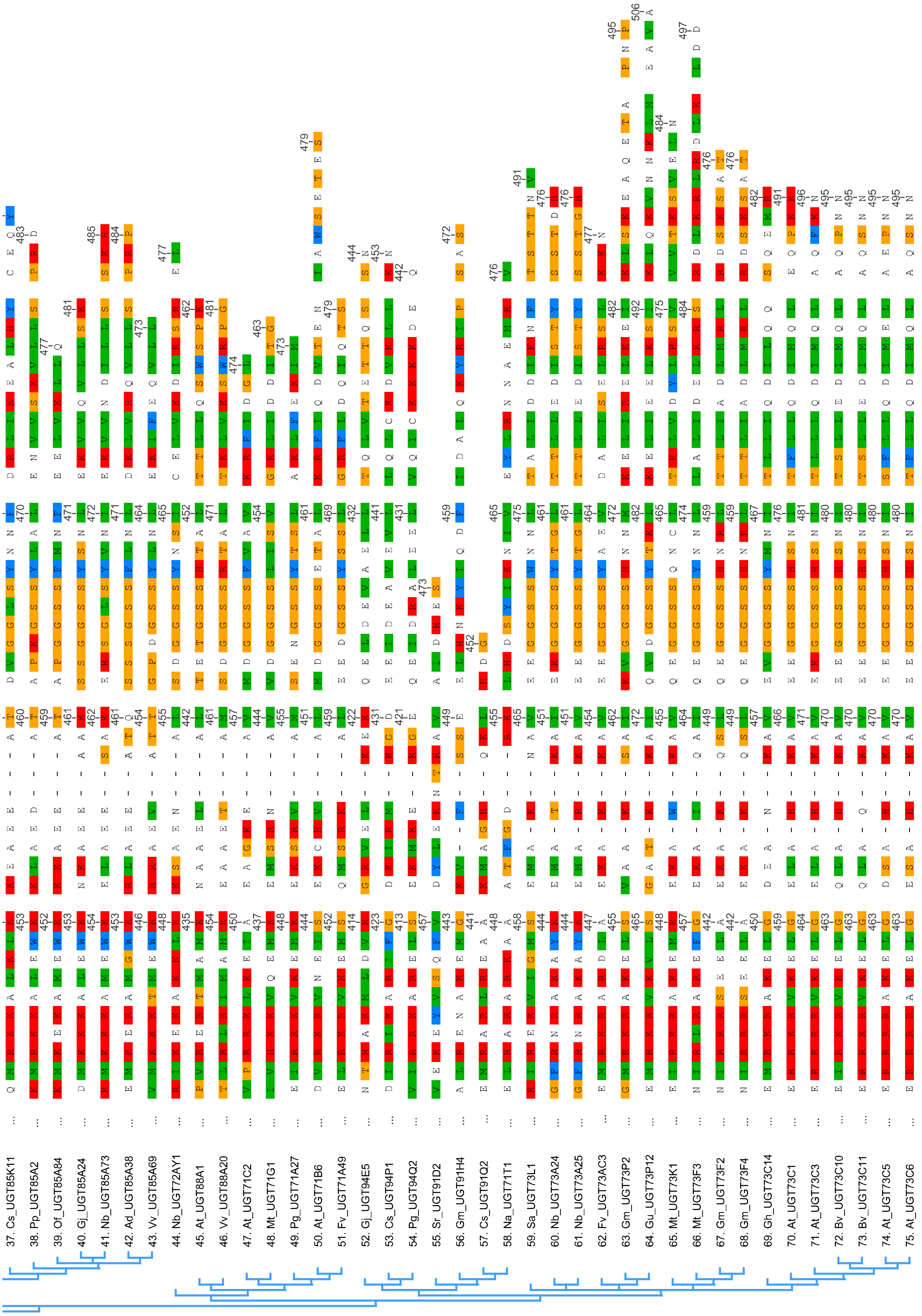
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45. At_UGT88A1
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48. Mt_UGT71G1
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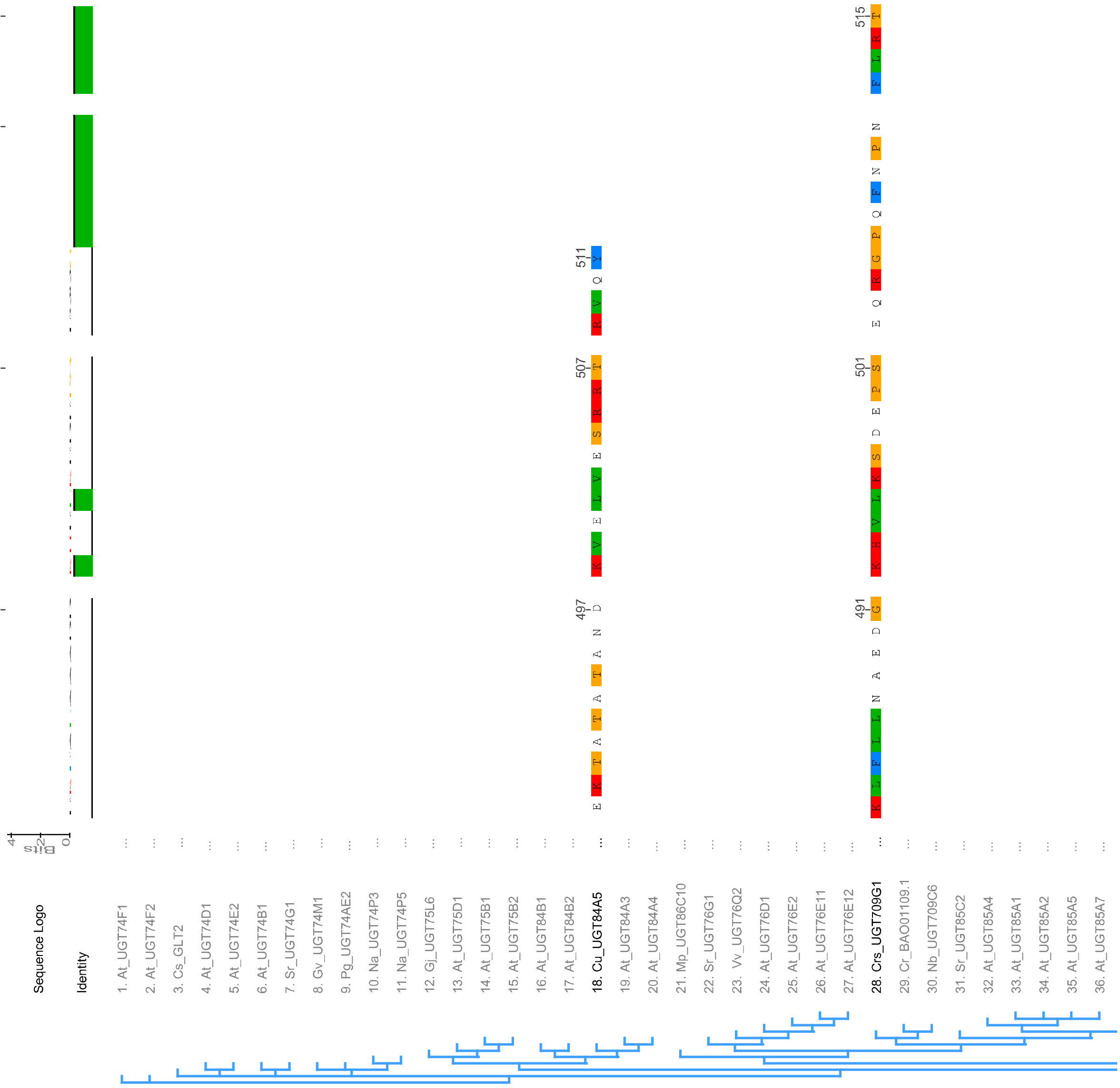

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8. Gv_UGT74M1
9. Pg_UGT74AE2
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19. At_UGT84A3
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23. Vv_UGT76Q2
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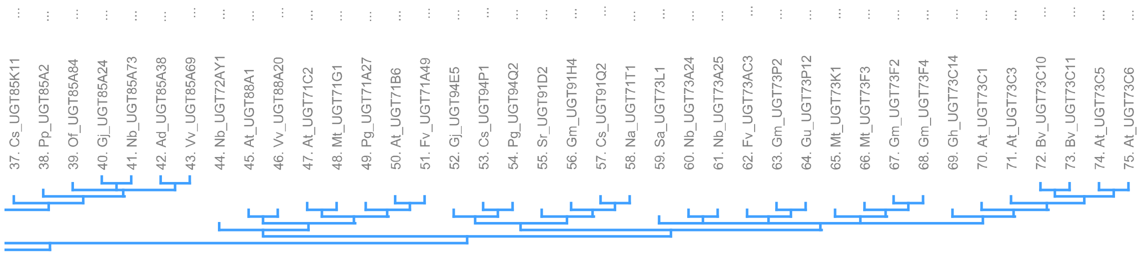
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Supplemental Figure S1. Amino acid sequence alignment of functionally characterized terpenoid glycosyltransferases. The numbers at the top show the position numbers of the entire sequence alignment. The sequences were aligned with Geneious 5.6.7 using the Geneious alignment tool with default values. The accession numbers of the sequences are as follows.

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At_UGT73C1_sp|Q9ZQ99|U73C1_ARATH UDP-glycosyltransferase 73C1 [Arabidopsis thaliana]
At_UGT73C3_sp|Q9ZQ96|U73C3_ARATH UDP-glycosyltransferase 73C3 [Arabidopsis thaliana]
At_UGT73C5_sp|Q9ZQ94|U73C5_ARATH_1 UDP-glycosyltransferase 73C5 [Arabidopsis thaliana]
At_UGT73C6_sp|Q9ZQ95|U73C6_ARATH UDP-glycosyltransferase 73C6 [Arabidopsis thaliana]
At_UGT74B1_sp|O48676|U74B1_ARATH UDP-glycosyltransferase 74B1 [Arabidopsis thaliana]
At_UGT74D1_sp|Q9SKC5|U74D1_ARATH UDP-glycosyltransferase 74D1 [Arabidopsis thaliana]
At_UGT74E2_sp|Q9SYK9|U74E2_ARATH UDP-glycosyltransferase 74E2 [Arabidopsis thaliana]
At_UGT74F1_sp|O22820|U74F1_ARATH Flavonol 7-O-beta-glucosyltransferase UGT74F1 [Arabidopsis thaliana]
At_UGT74F2_sp|O22822|U74F2_ARATH UDP-glycosyltransferase 74F2 [Arabidopsis thaliana]
At_UGT75B1_sp|Q9LR44|U75B1_ARATH UDP-glycosyltransferase 75B1 [Arabidopsis thaliana]
At_UGT75B2_sp|Q9ZVY5|U75B2_ARATH UDP-glycosyltransferase 75B2 [Arabidopsis thaliana]
At_UGT75D1_sp|O23406|U75D1_ARATH UDP-glycosyltransferase 75D1 [Arabidopsis thaliana]
At_UGT76D1_sp|O48715|U76D1_ARATH UDP-glycosyltransferase 76D1 [Arabidopsis thaliana]
At_UGT76E11_sp|Q9SNB1|U76E11_ARATH UDP-glycosyltransferase 76E11 [Arabidopsis thaliana]
At_UGT76E12_sp|Q94AB5|U76E12_ARATH Flavonol 3-O-glucosyltransferase UGT76E12 [Arabidopsis thaliana]
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Fv_UGT73AC3_XP_004304020.1 PREDICTED: abscisate beta-glucosyltransferase-like [Fragaria vesca subsp. vesca]
Gh_UGT73C14_NP_001314468.1 abscisic acid GT UDP-glycosyltransferase 73C6-like [Gossypium hirsutum]
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Gj_UGT85A24_sp|F8WKW1|UGT2_GARJA 7-deoxyloganetin glucosyltransferase [Gardenia jasminoides]
Gj_UGT94E5_sp|F8WKW8|UGT9_GARJA Beta-D-glucosyl crocetin beta-1,6-glucosyltransferase [Gardenia jasminoides]
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Gm_UGT73F4_BAM29363.1 UDP-glucosyltransferase UGT73F4 [Glycine max]
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Pp_UGT85A2_XP_007227474.1 Linalool GT 7-deoxyloganetin glucosyltransferase [Prunus persica]
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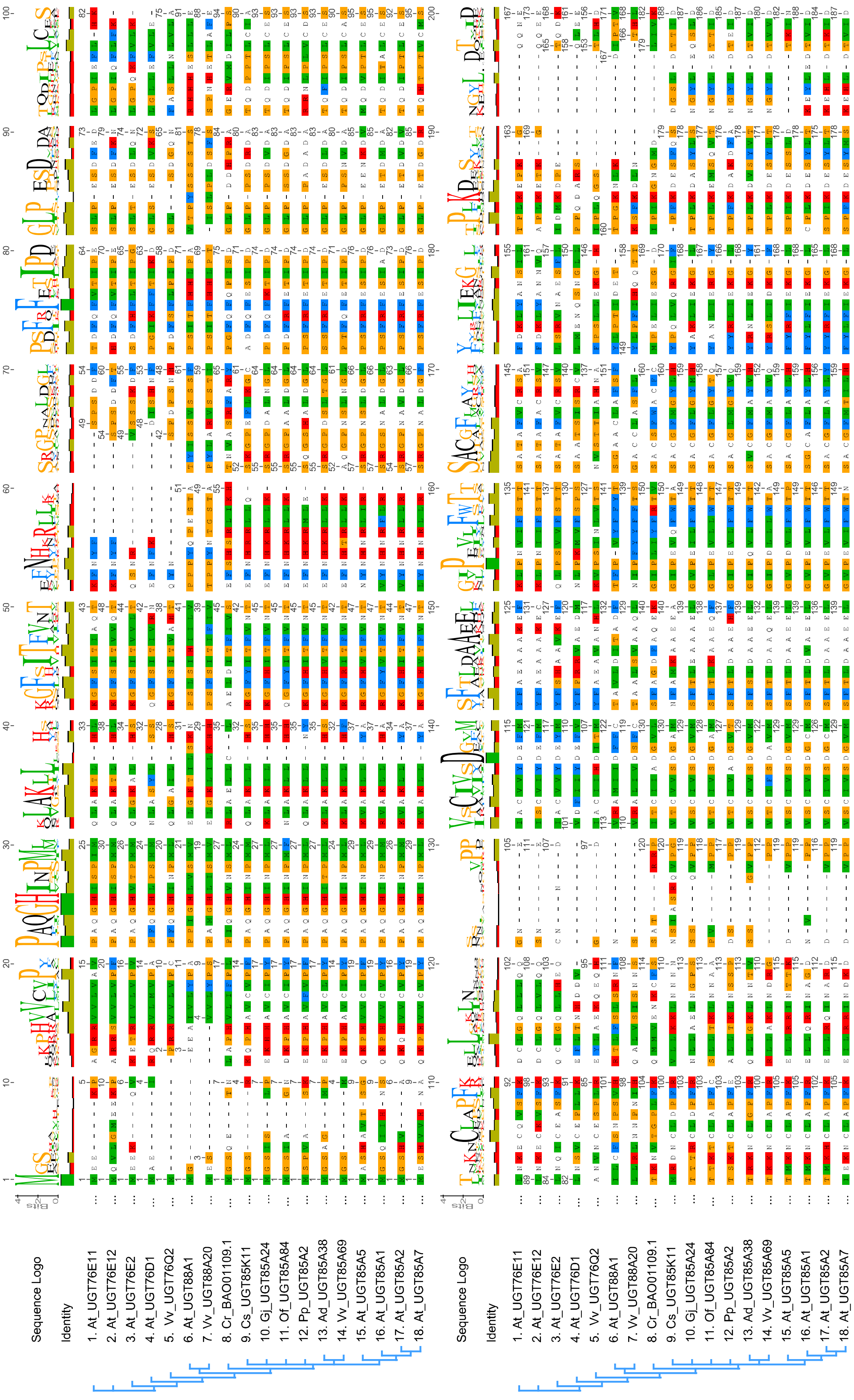
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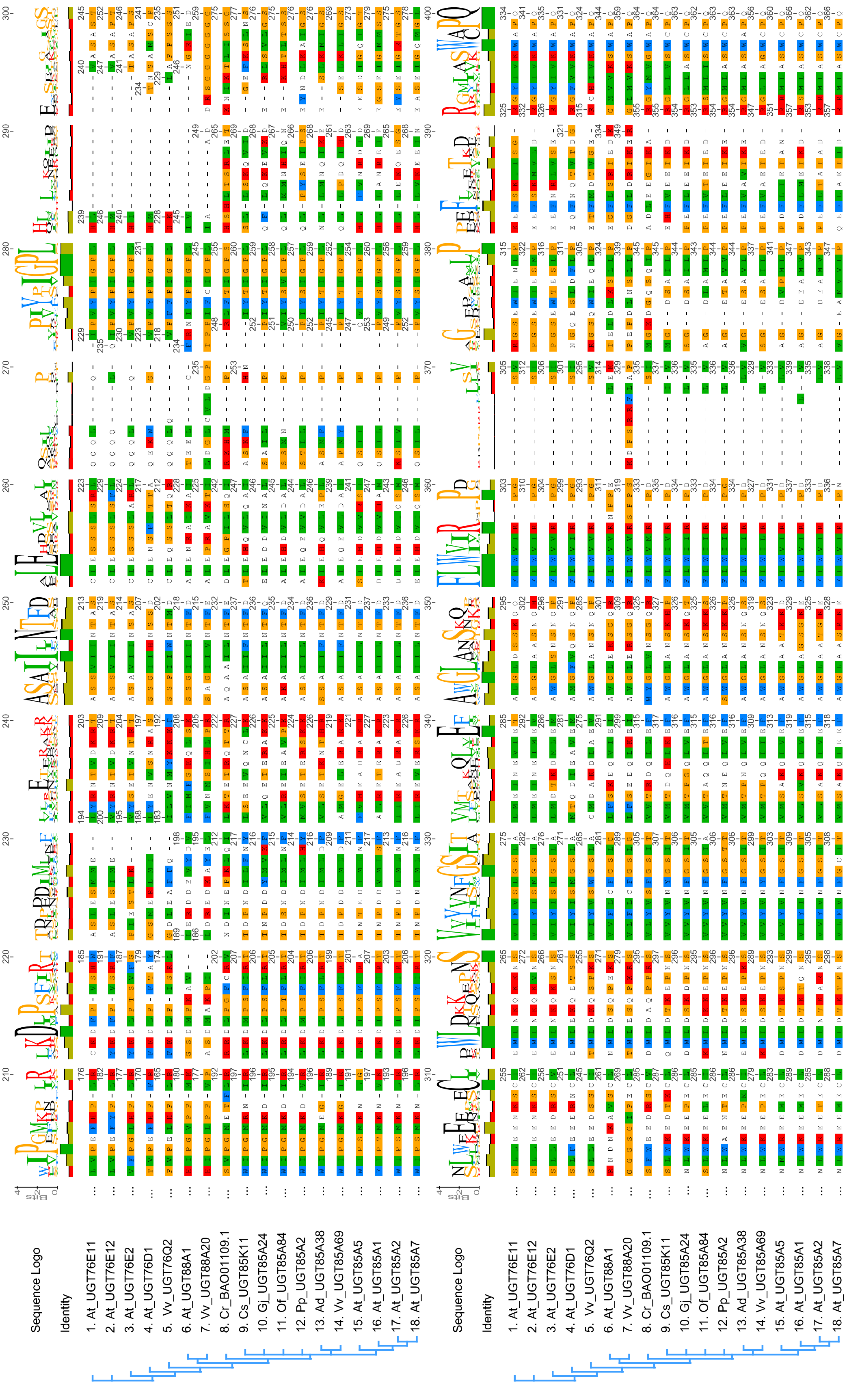
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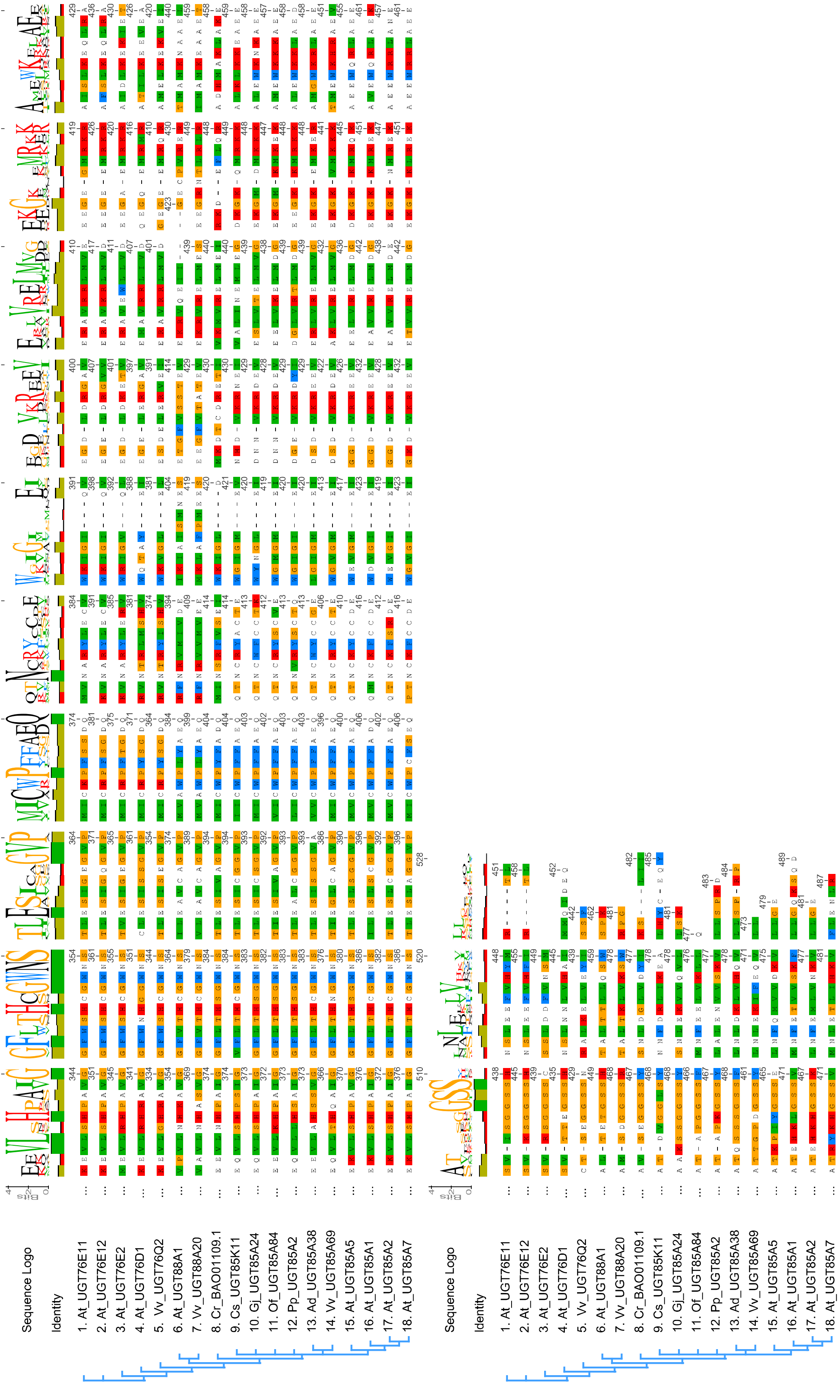
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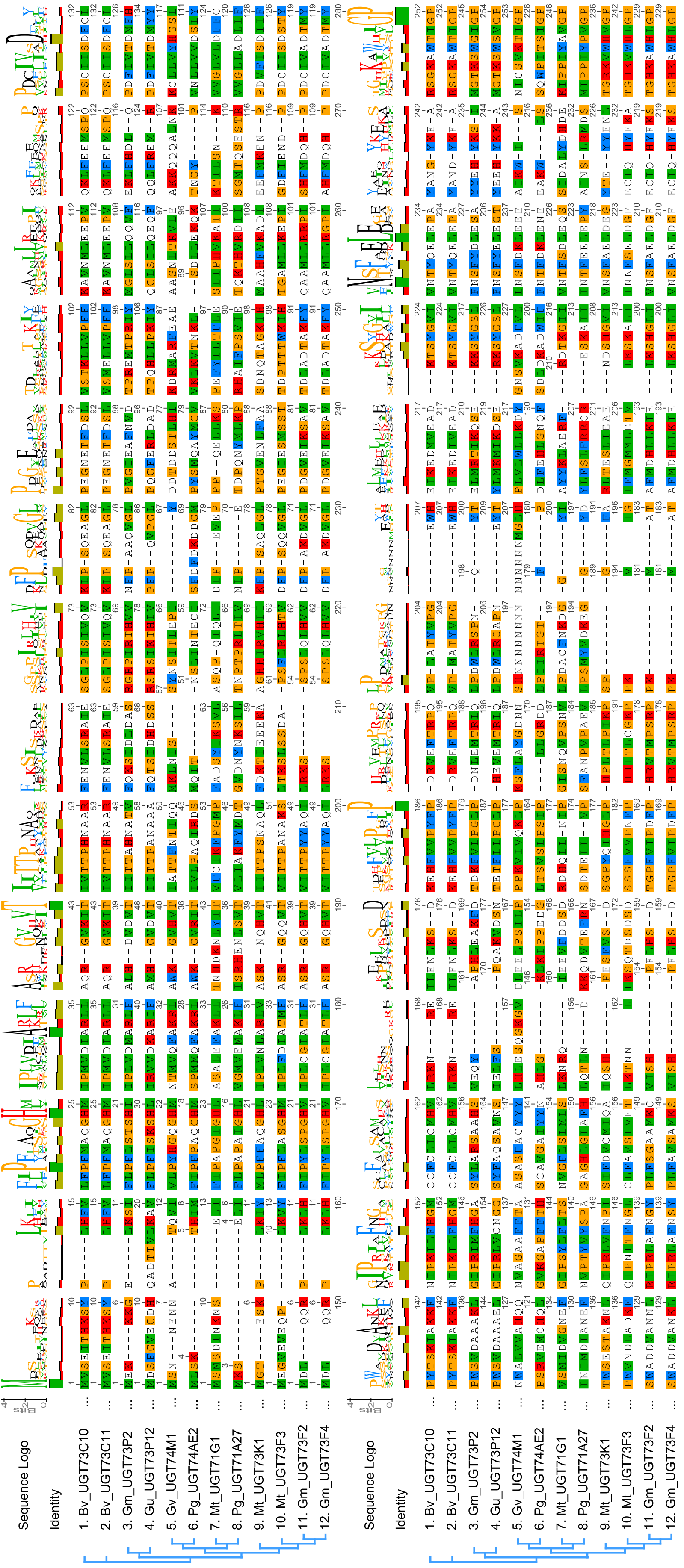
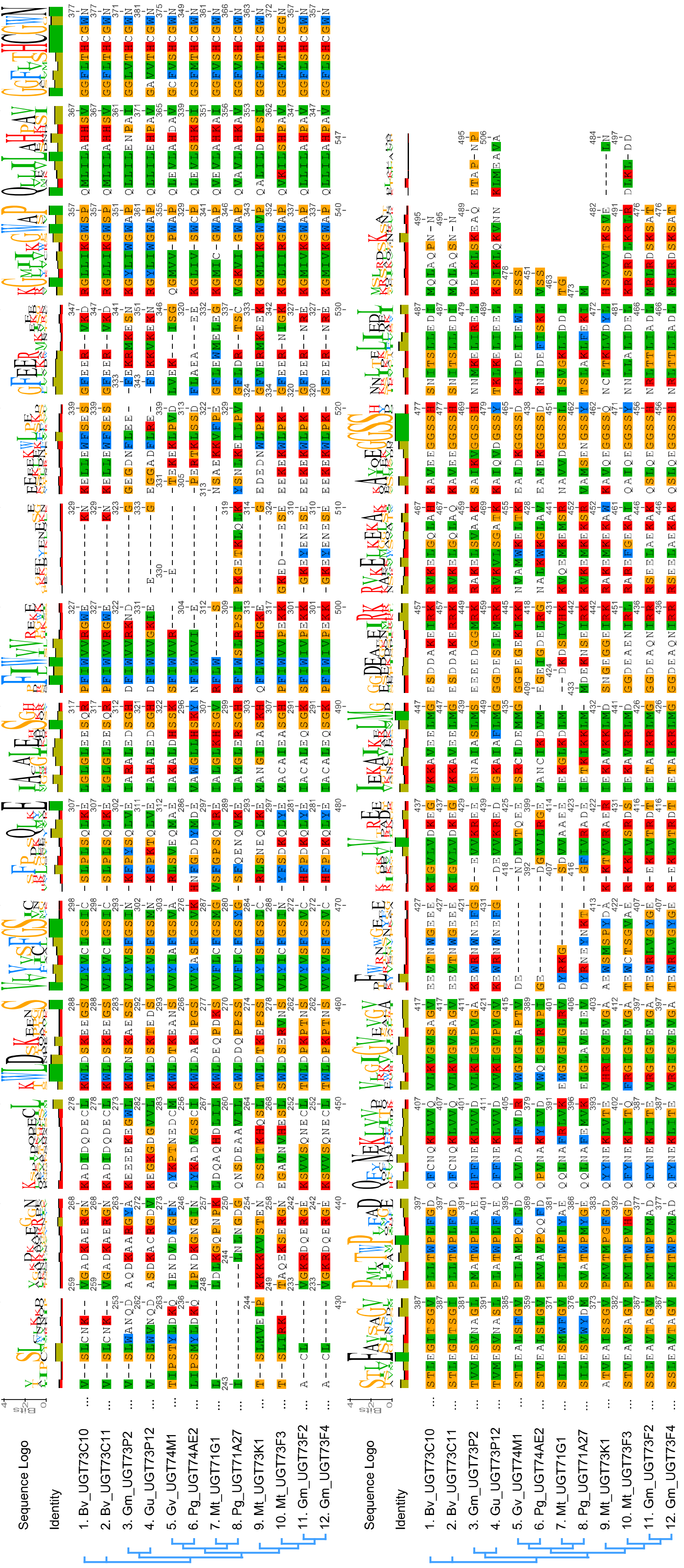
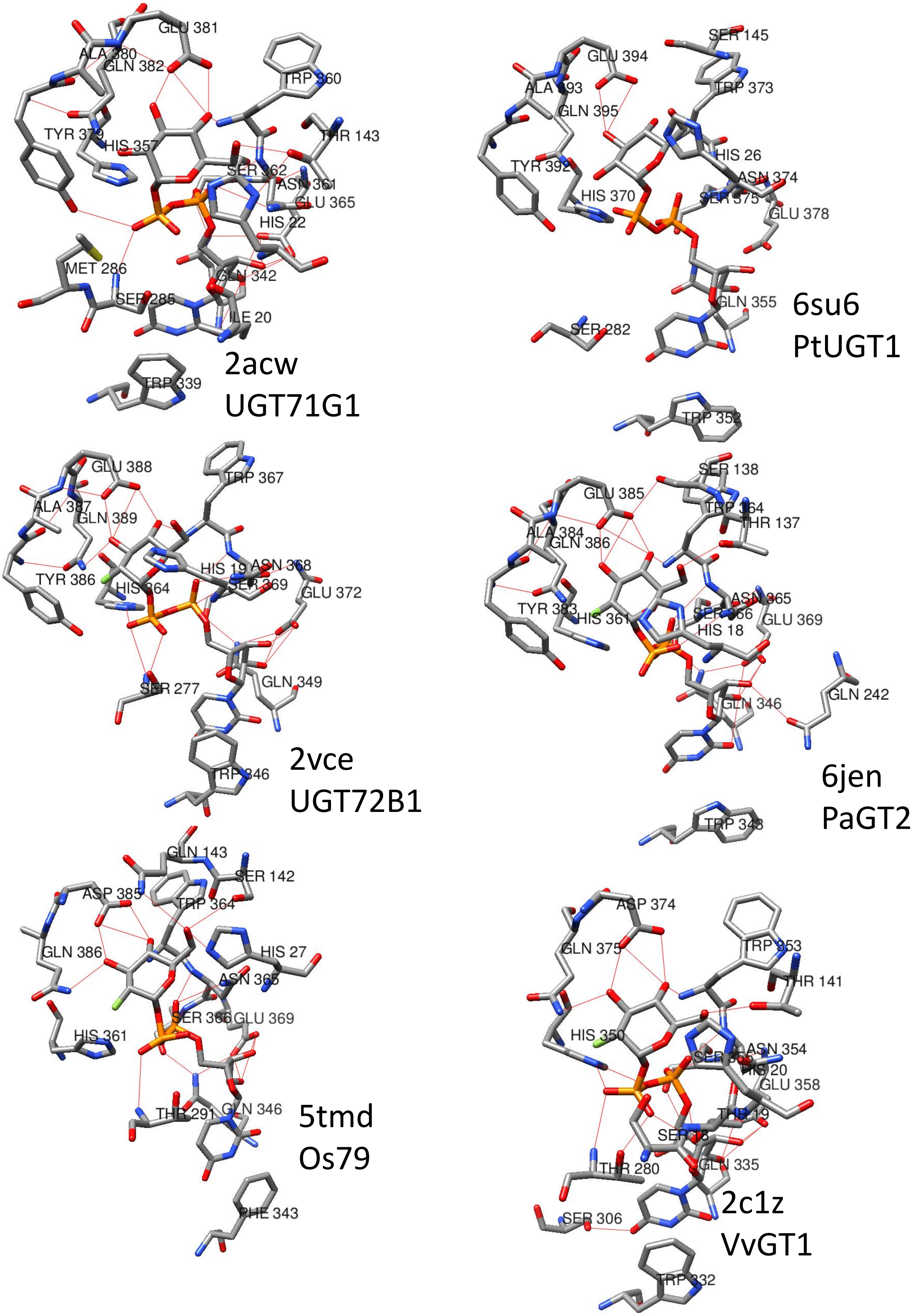
5. Vv_UGT76Q2
6. At_UGT88A1
7. Vv_UGT88A20
8. Cr_BAO01109.1
9. Cs_UGT85K11
10. Gj_UGT85A24
11. Of_UGT85A84
12. Pp_UGT85A2
13. Ad_UGT85A38
14. Vv_UGT85A69
15. At_UGT85A5
16. At_UGT85A1
17. At_UGT85A2
18. At_UGT85A7
Bits
410
420
430
440
450
460
470
480
490
500

Supplemental Figure S2. Amino acid sequence alignment of functionally characterized monoterpenoid glycosyltransferases. The sequences were aligned with Geneious 5.6.7 using the Geneious alignment tool with default values. The accession numbers of the sequences are shown in the legend of Supplemental Figure S1.


Sequence Logo
Identity
1. Bv_UGT73C10
2. Bv_UGT73C11
3. Gm_UGT73P2
4. Gu_UGT73P12
5. Gv_UGT74M1
6. Pg_UGT74AE2
7. Mt_UGT71G1
8. Pg_UGT71A27
9. Mt_UGT73K1
10. Mt_UGT73F3
11. Gm_UGT73F2
12. Gm_UGT73F4
Bits


Sequence Logo
Identity
1. Bv_UGT73C10
2. Bv_UGT73C11
3. Gm_UGT73P2
4. Gu_UGT73P12
5. Gv_UGT74M1
6. Pg_UGT74AE2
7. Mt_UGT71G1
8. Pg_UGT71A27
9. Mt_UGT73K1
10. Mt_UGT73F3
11. Gm_UGT73F2
12. Gm_UGT73F4
Bits

Supplemental Figure S3. Amino acid sequence alignment of functionally characterized triterpenoid glycosyltransferases. The sequences were aligned with Geneious 5.6.7 using the Geneious alignment tool with default values. The accession numbers of the sequences are shown in the legend of Supplemental Figure S1.



Supplemental Figure S4. Sugar donor binding site in UGT71G1, PtUGT1, UGT72B1, PaGT, Os79, and VvGT1. Amino acids in the vicinity of 5 Å are shown. Images were generated with UCSF Chimera 1.15.