

## Using machine learning model explanations to identify proteins related to severity of meibomian gland dysfunction

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**Table A.1.** Fold changes in relative protein quantifications for the proteins detected as most important by the ML models, listed in alphabetical order. level: MGD level, NA: not available.

Protein (accession number)	Fold changes (level 2: level 3: level 4)
40S ribosomal protein SA (P08865)	1.00 : 0.91 : 1.48
60S acidic ribosomal protein P0 (P05388)	1.00 : 0.96 : 0.95
60S ribosomal protein L38 (P63173)	1.00 : 1.71 : 1.40
Adenylate kinase isoenzyme 1 (P00568)	1.00 : 0.82 : 0.78
Adenylyl cyclase-associated protein 1 (Q01518)	1.00 : 1.18 : 1.03
ADH7 (P40394)	1.00 : 1.14 : 0.84
Alpha-centractin (P61163)	1.00 : 1.11 : 0.97
Cathepsin D (P07339)	1.00 : 1.22 : 1.27
Corticosteroid-binding globulin (P08185)	1.00 : 2.83 : 1.88
CYFIP-related Rac1 interactor B (Q9NUQ9)	1.00 : 0.91 : 0.95
Dynactin subunit 2 (Q13561)	1.00 : 1.27 : 0.70
Endoplasmic reticulum resident protein 29 (P30040)	1.00 : 1.38 : 1.06
Eukaryotic translation initiation factor 6 (P56537)	1.00 : 1.00 : 0.85
Glutathione peroxidase 1 (P07203)	1.00 : 1.11 : 0.96
Golgi membrane protein 1 (Q8NBJ4)	1.00 : 2.75 : 1.57
Heterogeneous nuclear ribonucleoprotein M (P52272)	1.00 : 1.36 : 0.72
IGA2 (P0DOX2)	1.00 : 1.28 : 1.83
IGG1 (Q95M34)	NA
IGKV2-24 (A0A0C4DH68)	1.00 : 0.76 : 1.11
IGLV6-57 (P01721)	1.00 : 1.96 : 2.13
IGLV8-61 (A0A075B610)	1.00 : 0.82 : 1.13
Immunoglobulin heavy constant gamma 4 (P01861)	1.00 : 0.71 : 1.57
Immunoglobulin heavy variable 3-74 (A0A0B4J1X5)	1.00 : 1.03 : 1.23
Lactoylglutathione lyase (Q04760)	1.00 : 1.06 : 1.21
Lysozyme C (P61626)	1.00 : 0.89 : 0.70
Malate dehydrogenase, cytoplasmic (P40925)	1.00 : 1.00 : 0.92
Mannose-1-phosphate guanyltransferase alpha (Q96IJ6)	1.00 : 2.36 : 2.32
Methanethiol oxidase (Q13228)	1.00 : 1.26 : 1.03
Mitogen-activated protein kinase 1 (P28482)	1.00 : 0.97 : 0.93
Peptidyl-prolyl cis-trans isomerase B (P23284)	1.00 : 0.97 : 0.83
Phosphatidylinositol 5-phosphate 4-kinase type-2 gamma (Q8TBX8)	1.00 : 1.44 : 1.18
Phospholipid transfer protein (P55058)	1.00 : 1.33 : 0.96
Polymeric immunoglobulin receptor (P01833)	1.00 : 1.09 : 1.37
Prostaglandin reductase 1 (Q14914)	1.00 : 0.88 : 0.71
Protein NDRG1 (Q92597)	1.00 : 1.25 : 0.82
Protein S100-A8 (P05109)	1.00 : 2.08 : 2.86
PRP4 (Q16378)	1.00 : 0.78 : 0.59
Psoriasin (P31151)	1.00 : 0.87 : 2.44
Serotransferrin (P02787)	1.00 : 1.32 : 1.02
SH2 domain-containing protein 4A (Q9H788)	NA
Tissue alpha-L-fucosidase (P04066)	1.00 : 1.00 : 1.00
Ubiquitin-conjugating enzyme E2 variant 1 (Q13404)	1.00 : 0.88 : 0.99
UDP-glucose 4-epimerase (Q14376)	1.00 : 1.92 : 1.04
X-ray repair cross-complementing protein 5 (P13010)	1.00 : 1.47 : 1.16

**Table A.2.** Fold changes in relative quantifications for the proteins found to be significantly altered between patients with MGD levels 2, 3 and 4, respectively using the PEAKS X Pro software. The protein ranking is based on significance value: Higher values receive higher ranks. level: MGD level.

Rank	Protein (accession number)	Fold changes (level 2: level 3: level 4)
1	S-methyl-5'-thioadenosine phosphorylase (Q13126)	1.00 : 2.38 : 1.21
2	60S ribosomal protein L6 (Q02878)	1.00 : 2.02 : 1.86
3	Mannose-1-phosphate guanyltransferase alpha (Q96IJ6)	1.00 : 2.09 : 1.78
4	Programmed cell death protein 10 (Q9BUL8)	1.00 : 1.60 : 2.29
5	Eukaryotic peptide chain release factor GTP-binding subunit ERF3A (P15170)	1.00 : 1.62 : 2.00
6	Proteasome subunit alpha type-7 (O14818)	1.00 : 1.82 : 2.07
7	V-type proton ATPase catalytic subunit A (P38606)	1.00 : 2.62 : 1.63
8	Complement C1q subcomponent subunit B (P02746)	1.00 : 2.01 : 1.70
9	60S ribosomal protein L13 (P26373)	1.00 : 2.44 : 1.25
10	Thymidine phosphorylase (P19971)	1.00 : 2.48 : 2.53
11	Protein Niban 2 (Q96TA1)	1.00 : 1.85 : 2.68
12	T-complex protein 1 subunit eta (Q99832)	1.00 : 2.33 : 1.18
13	GMP reductase 2 (Q9P2T1)	1.00 : 2.62 : 1.78