# HW 1: Medical Imaging Systems

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# Q1

## a

I found the nitric oxide synthase heme domain at 1.65 Å resolution in Bos taurus found via X-ray crystallography on rcsb.org. The catelog ID is 1D0C. The amino acid sequence of chain B is as follows:

SRAPAPATPHAPDHSPAPNSPTLTRPPEGPKFPRVKNWELGSITYDTLCAQSQQDGPCT
PRRCLGSLVLPRKLQTRPSPGPPPAEQLLSQARDFINQYYSSIKRSGSQAHEERLQEVEAEVAS
TGTYHLRESELVFGAKQAWRNAPRCVGRIQWGKLQVFDARDCSSAQEMFTYICNHIKYATN
RGNLRSAITVFPQRAPGRGDFRIWNSQLVRYAGYRQQDGSVRGDPANVEITELCIQHGWTPG
NGRFDVLPLLLQAPDEAPELFVLPPELVLEVPLEHPTLEWFAALGLRWYALPAVSNMLLEIGG
LEFSAAPFSGWYMSTEIGTRNLCDPHRYNILEDVAVCMDLDTRTTSSLWKDKAAVEINLAVL
HSFQLAKVTIVDHHAATVSFMKHLDNEQKARGGCPADWAWIVPPISGSLTPVFHQEMVNYIL
SPAFRYQPDPW

## b

With the search criteria Thrombin, and homo sapiens I found that the thee most recent structures available are 6GBW, 6FJT, and 6EVV as of 9/3/19.

# Q2

## a

Position g in the structure has the highest proportion of amino acids that are charged at 4/5. The first of those is an arginine. It is at the amino terminal end which implies a pKa near 9.04. Even if this were a non terminal amino acid it would have a pKa of 12.48. Thus this amino acid will be positively charged. The two are lysines which have a side chain pKa of 10.79, resulting in a positive charge. The next is a glutamic acid which has a side chain pKa of 4.25, resulting in a negative charge at neutral pH. The last amino acid in this position is a leucene which does not ionize as a side chain and thus will have a neutral charge.

**b**