PON1 multiple Sequences

PON1 Wild

MAKLIALTLLGMGLALFRNHQSSYQTRLNALREVQPVELPNCNLVKGIETGSEDLEILPNGLAFISSGLK
YPGIKSFNPNSPGKILLMDLNEEDPTVLELGITGSKFDVSSFNPHGISTFTDEDNAMYLLVVNHPDAKST
VELFKFQEEEKSLLHLKTIRHKLLPNLNDIVAVGPEHFYGTNDHYFLDPYLQSWEMYLGLAWSYVVYYS
PSEVRVVAEGFDFANGINISPDGKYVYIAELLAHKIHVYEKHANWTLTPLKSLDFNTLVDNISVDPETG
DLWVGCHPNGMKIFFYDSENPPASEVLRIQNILTEEPKVTQVYAENGTVLQGSTVASVYKGKLLIGTVF
HKALYCEL

L55M

MAKLIALTLLGMGLALFRNHQSSYQTRLNALREVQPVELPNCNLVKGIETGSED**M**EILPNGLAFISSGL
KYPGIKSFNPNSPGKILLMDLNEEDPTVLELGITGSKFDVSSFNPHGISTFTDEDNAMYLLVVNHPDAKS
TVELFKFQEEEKSLLHLKTIRHKLLPNLNDIVAVGPEHFYGTNDHYFLDPYLQSWEMYLGLAWSYVVY
YSPSEVRVVAEGFDFANGINISPDGKYVYIAELLAHKIHVYEKHANWTLTPLKSLDFNTLVDNISVDPET
GDLWVGCHPNGMKIFFYDSENPPASEVLRIQNILTEEPKVTQVYAENGTVLQGSTVASVYKGKLLIGTV
FHKALYCEL

Q192R

MAKLIALTLLGMGLALFRNHQSSYQTRLNALREVQPVELPNCNLVKGIETGSEDLEILPNGLAFISSGLK
YPGIKSFNPNSPGKILLMDLNEEDPTVLELGITGSKFDVSSFNPHGISTFTDEDNAMYLLVVNHPDAKST
VELFKFQEEEKSLLHLKTIRHKLLPNLNDIVAVGPEHFYGTNDHYFLDPYL**R**SWEMYLGLAWSYVVYYS
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DLWVGCHPNGMKIFFYDSENPPASEVLRIQNILTEEPKVTQVYAENGTVLQGSTVASVYKGKLLIGTVF
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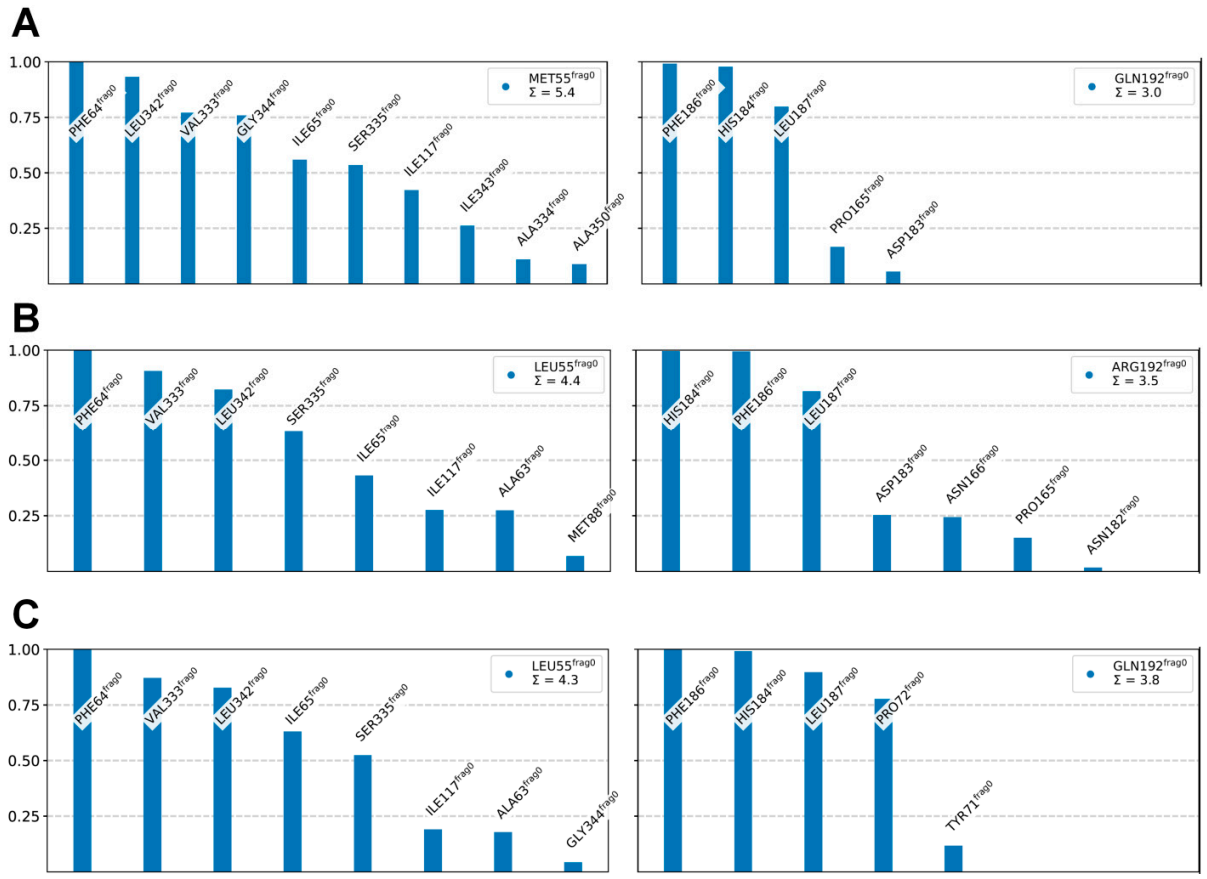
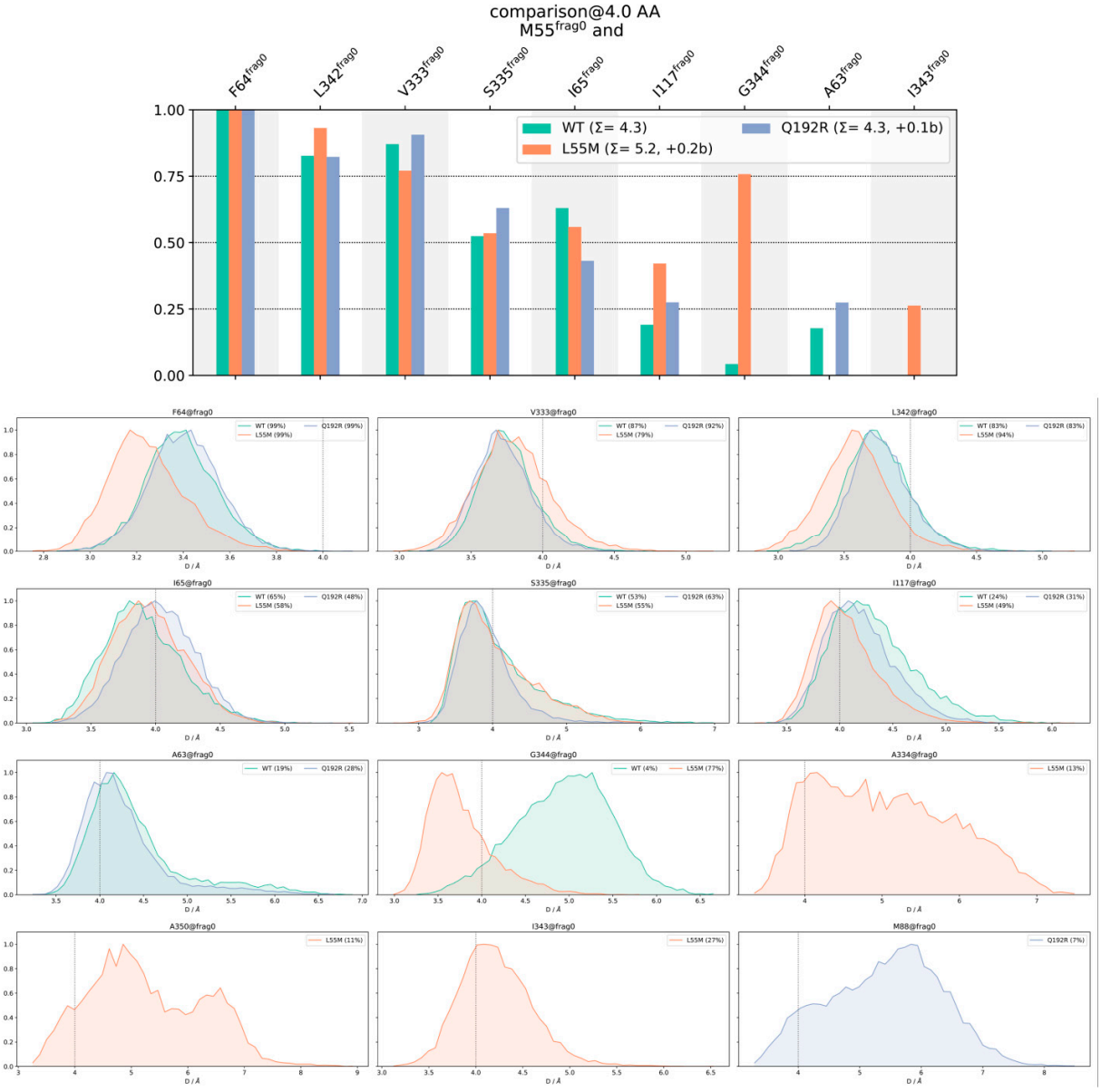
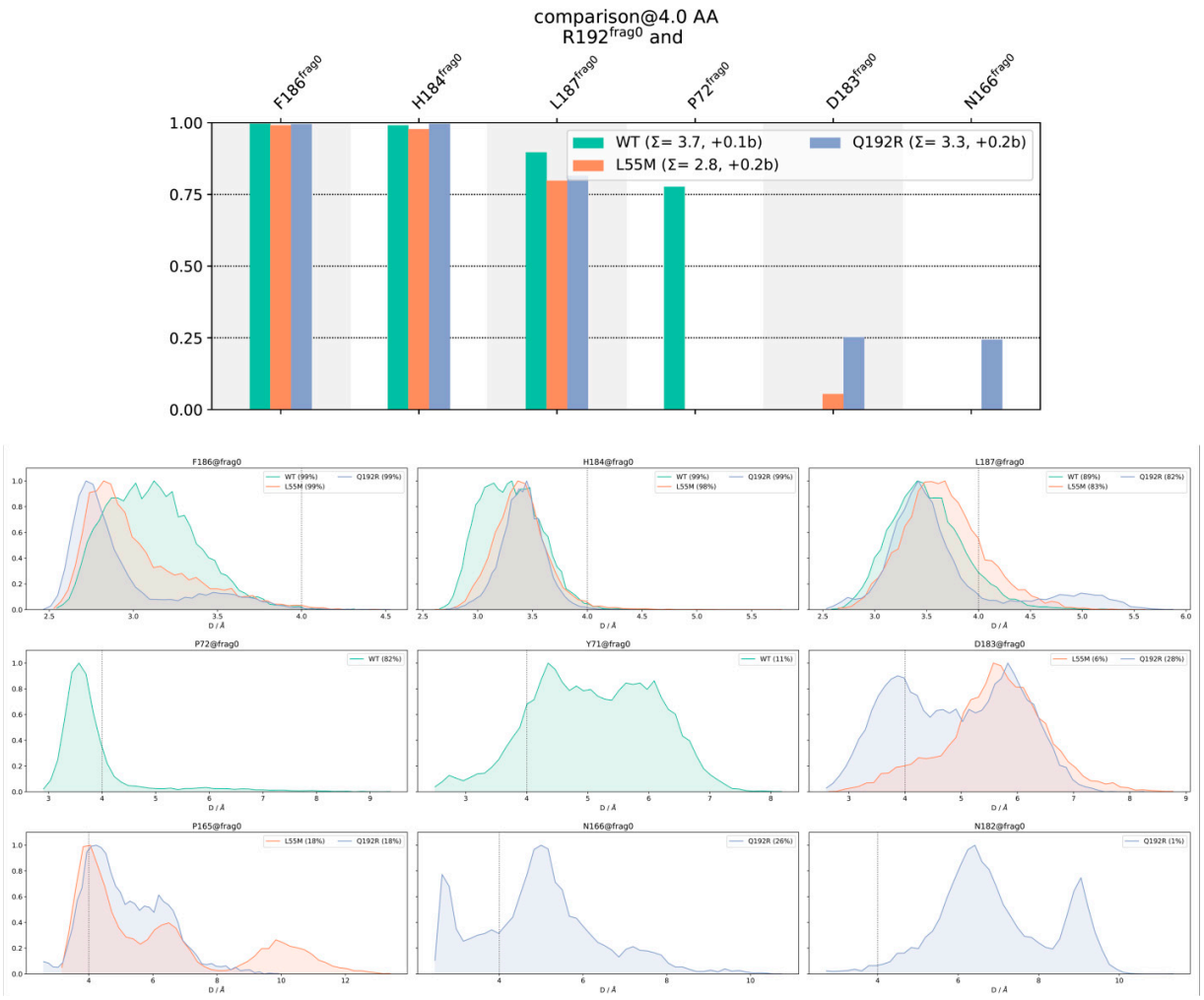
Figures S1. Contact frequency analysis. A) Leu55Met, B) Gln192Arg, and C) wild-type.



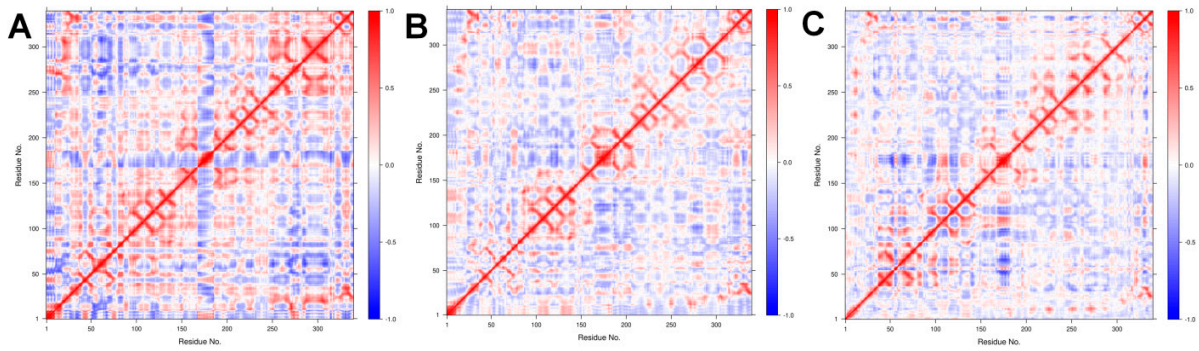
Figures S2. Contact frequency analysis for Leu55Met PON1 for Met55 mutation. The top panel plot shows the comparison in contact frequency between three variants of PON1, while the other panels show the distance independent contact frequency distribution comparison for Met55 mutation.



Figures S3. Contact frequency analysis for Gln192Arg PON1. The top panel plot shows the comparison in contact frequency between three variants of PON1 for Arg192 mutation, while the other panels show the distance independent contact frequency distribution comparison for Arg192 mutation.



Figures S4. DCCM analysis. A) Leu55Met, B) Gln192Arg, and C) wild-type PON1



Figures S5. The PON1 wild-type docking with endogenous lactones: A) Dihydrocoumarin, B) 2-Hydroxy-gamma-butyrolactone C) Alpha-Angelica lactone, and D) Gamma-nonalactone. Leu55Met interacts with E) Dihydrocoumarin, F) 2-Hydroxy-gamma-butyrolactone G) Alpha-Angelica lactone, and H) Gam-ma-nonalactone. Gln192Arg interacts with I) Dihydrocoumarin, J) 2-Hydroxy-gamma-butyrolactone K) Alpha-Angelica lactone, and L) Gamma-non alac-tone.

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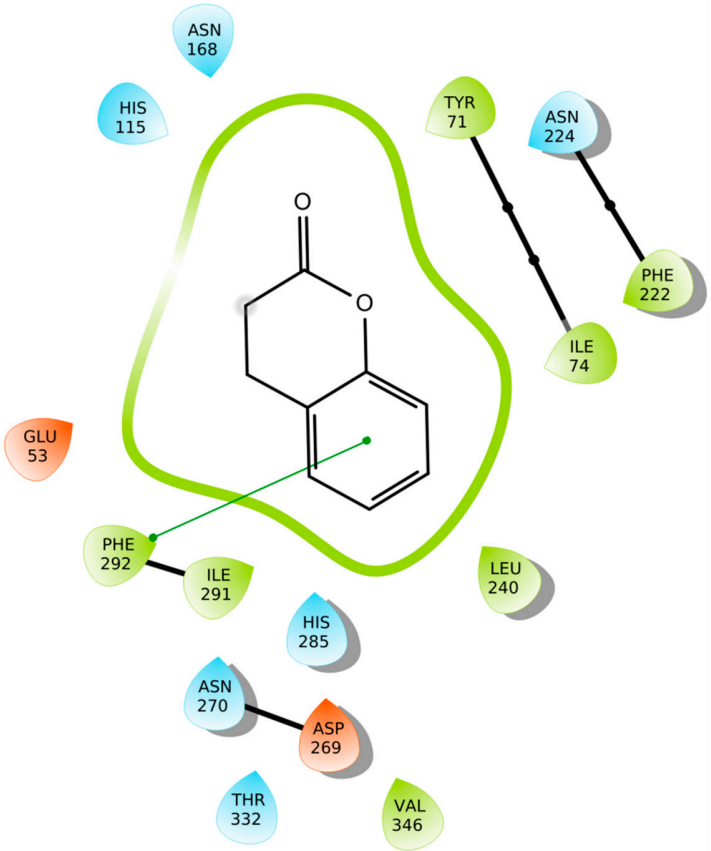

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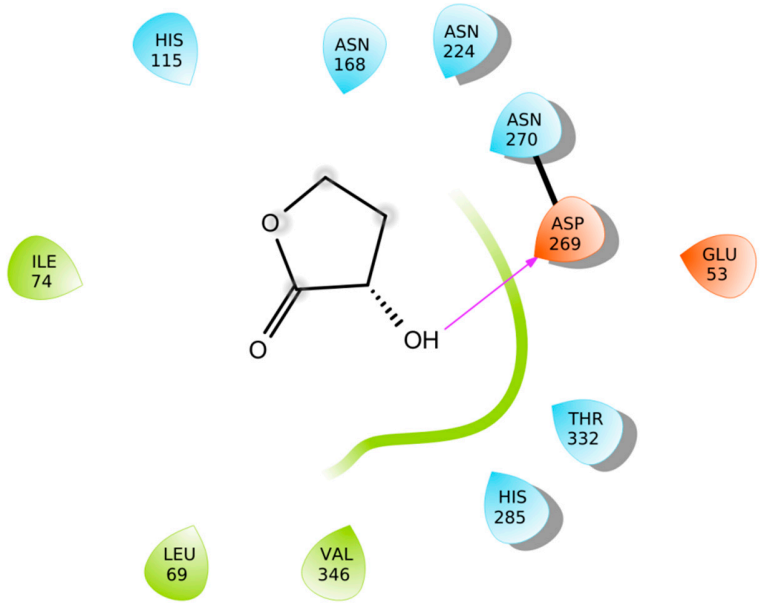
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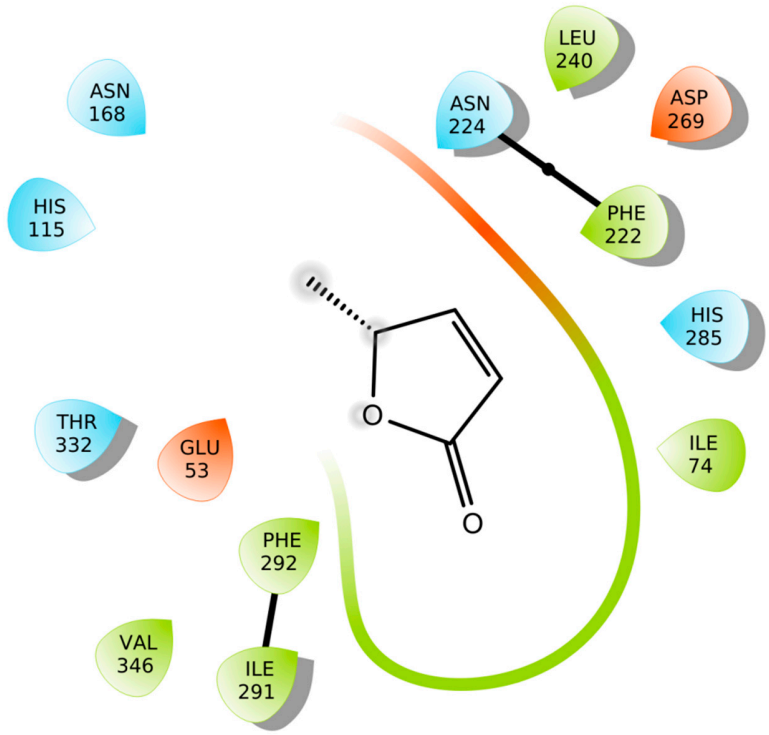
VAL 346

C)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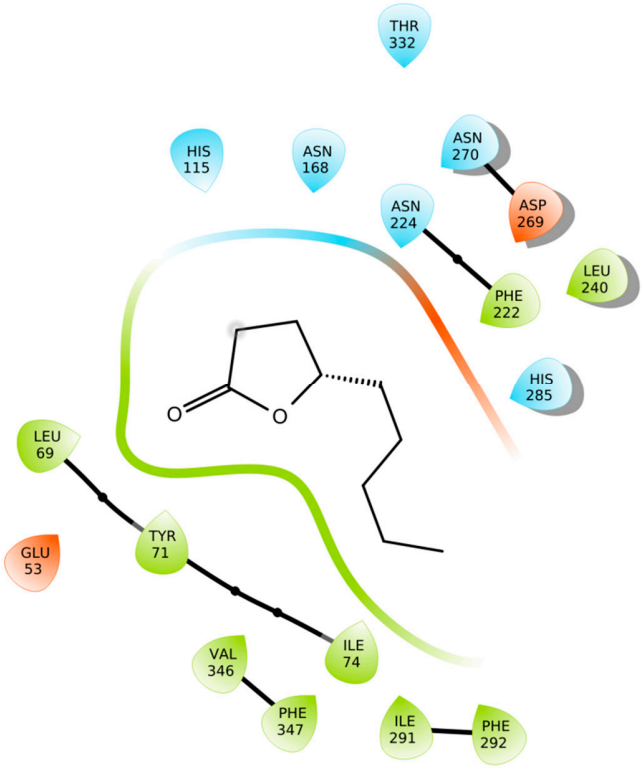
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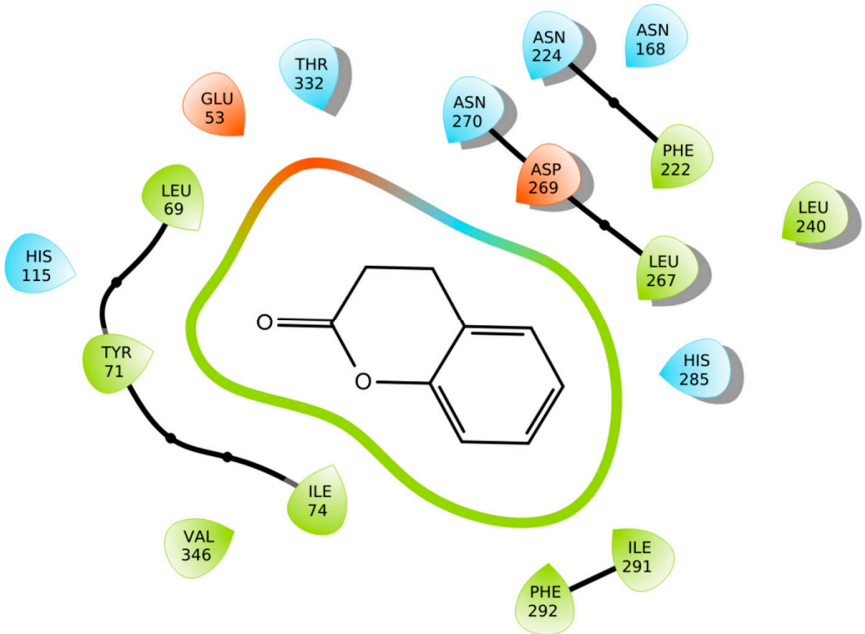
O

E)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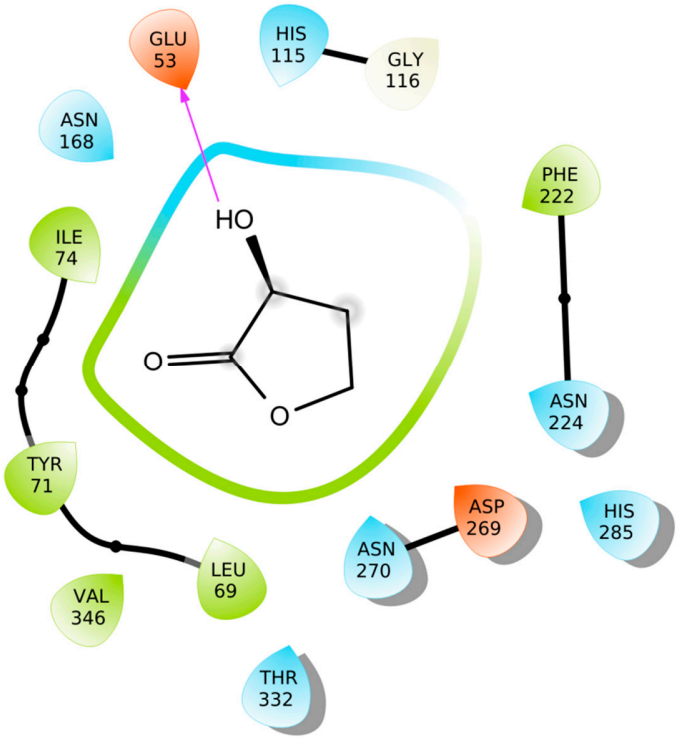
O
O

F)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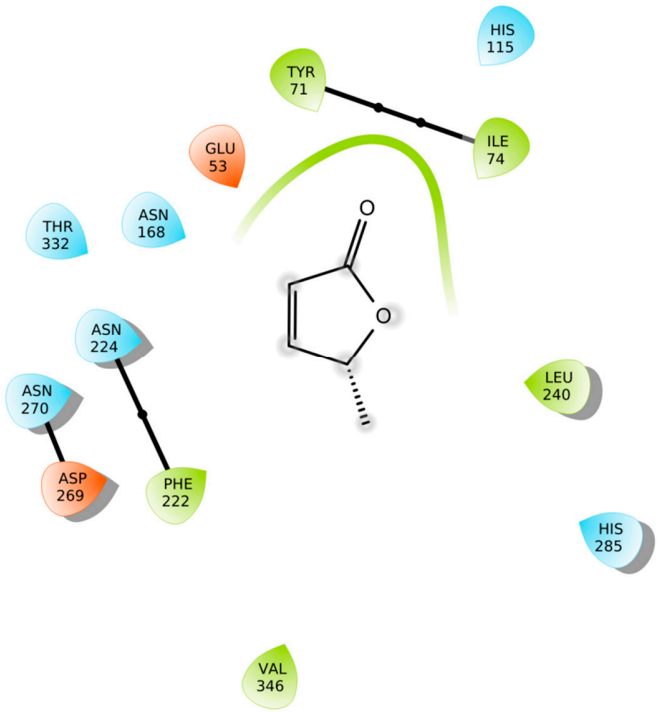
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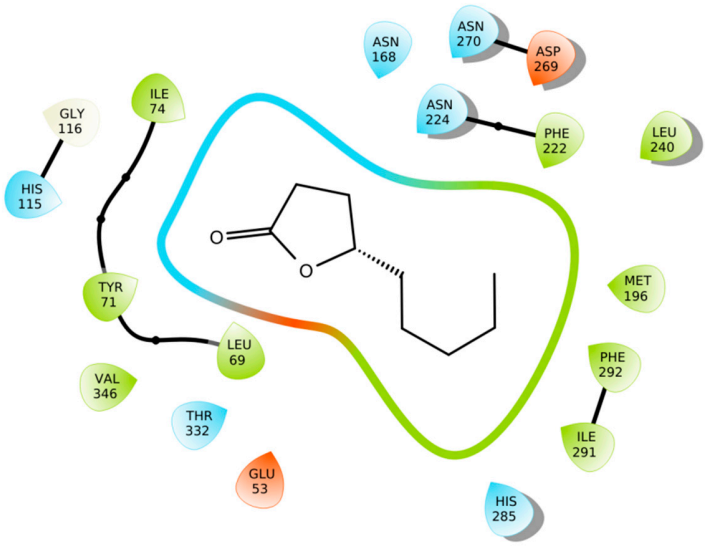
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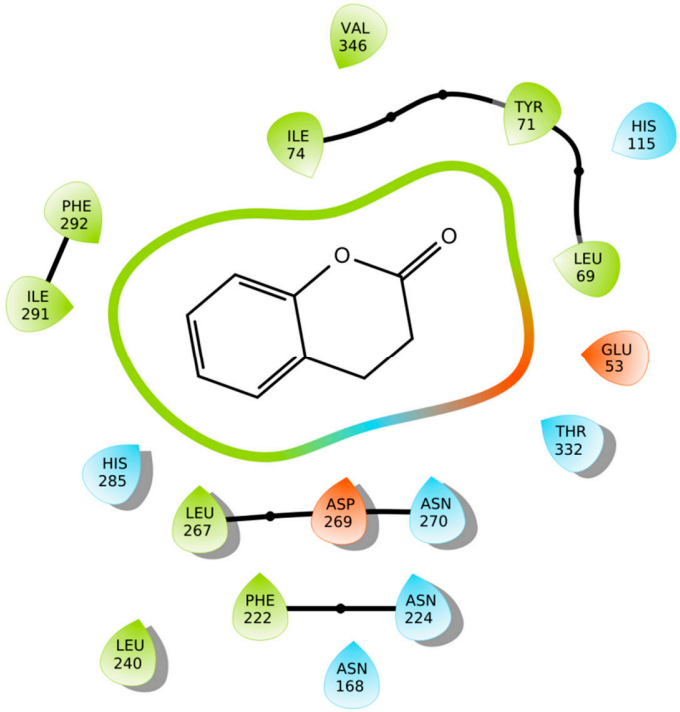
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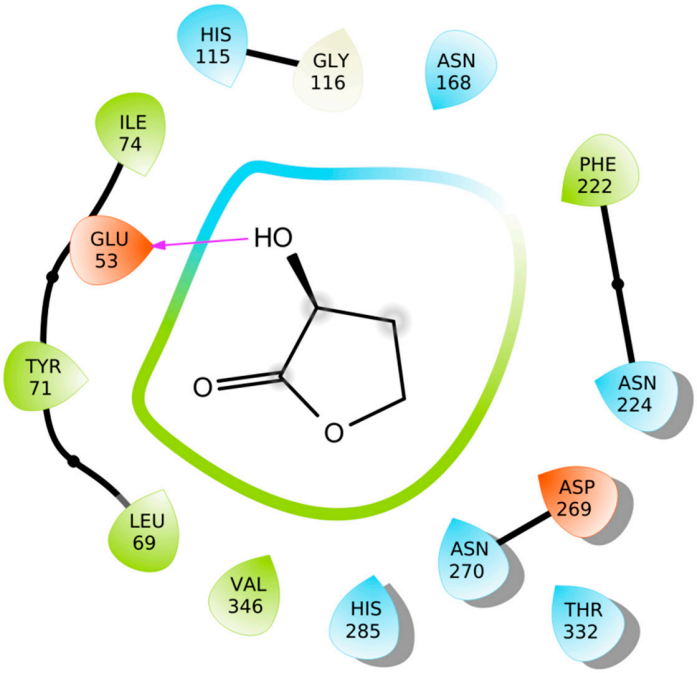
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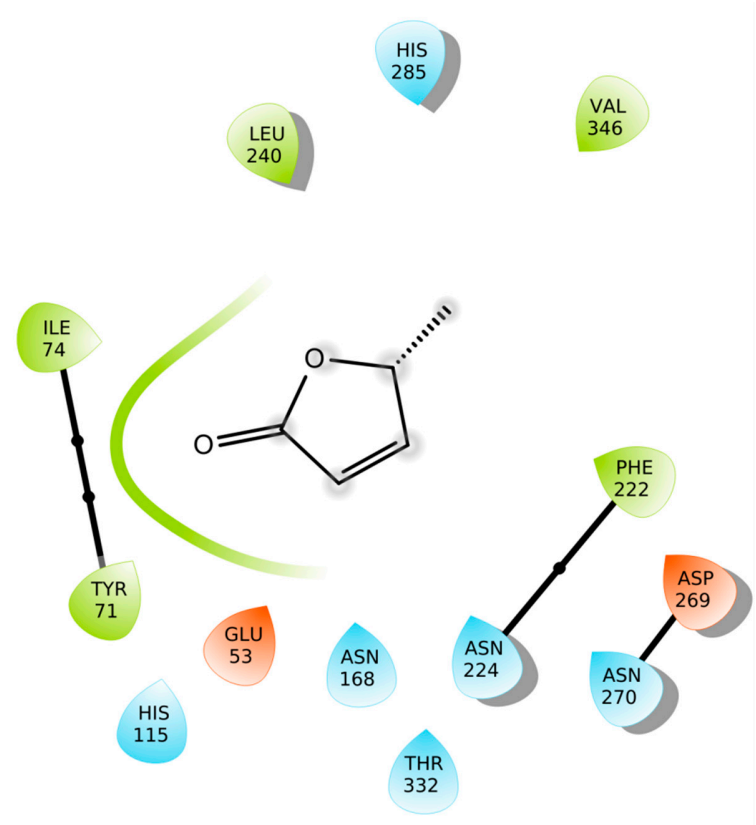
K)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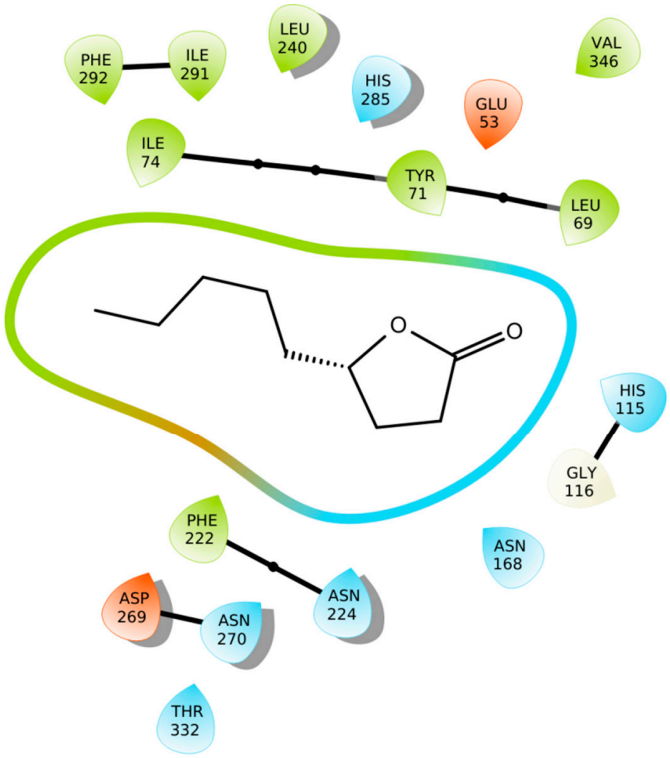
L)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ASN 168
ASP 269
ASN 270
ASN 224
THR 332

Figures S6. The interaction of PON1 wild-type with synthetic molecules: A) (2S,3R)-3-amino-2-hydroxyheptonicacid, B) arachidonic acid, C) 4-hydroxy docosahexaenoic acid, D) dihydropyran, E) mevalonic acid,and F) 2-Hydroxyvaleric acid. Leu55Met docked with G) (2S,3R)-3-amino-2-hydroxyheptonicacid, H) arachidonic acid, I) 4-hydroxy docosahexaenoic acid, J) dihydropyran, K) mevalonic acid, and L) 2-Hydroxyvaleric acid. Gln192Arg docked with M)(2S,3R)-3-amino-2-hydroxyheptonicacid, N) arachidonic acid, O) 4-hydroxy docosahexaenoic acid, P) dihydropyran, Q) mevalonic acid, and R) 2-Hydroxyvaleric acid.

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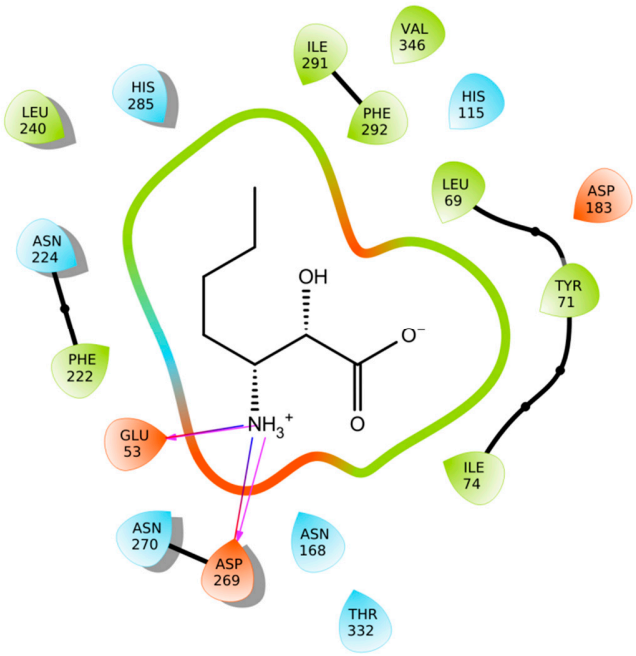

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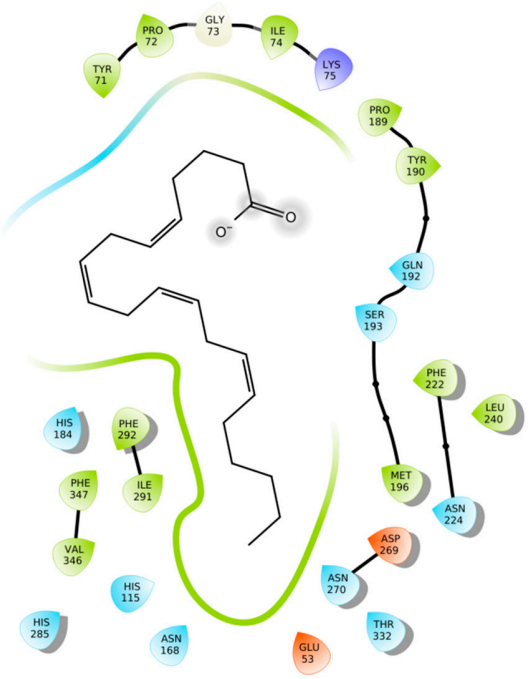
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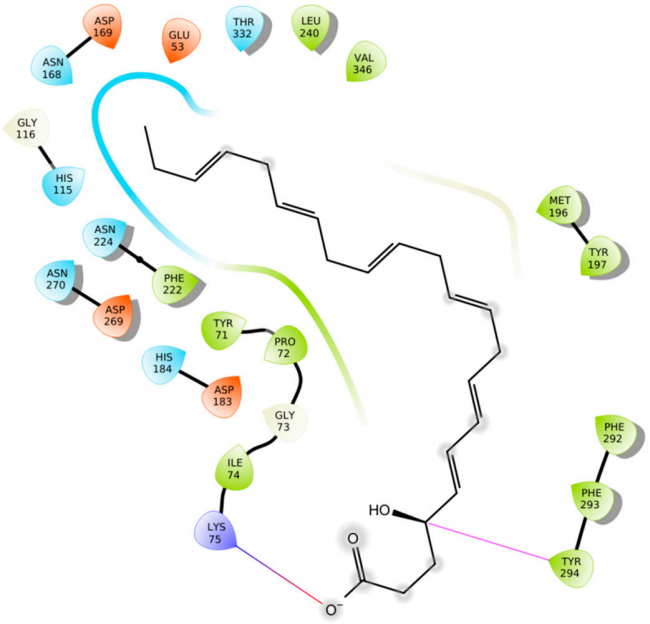
O⁻
O

C)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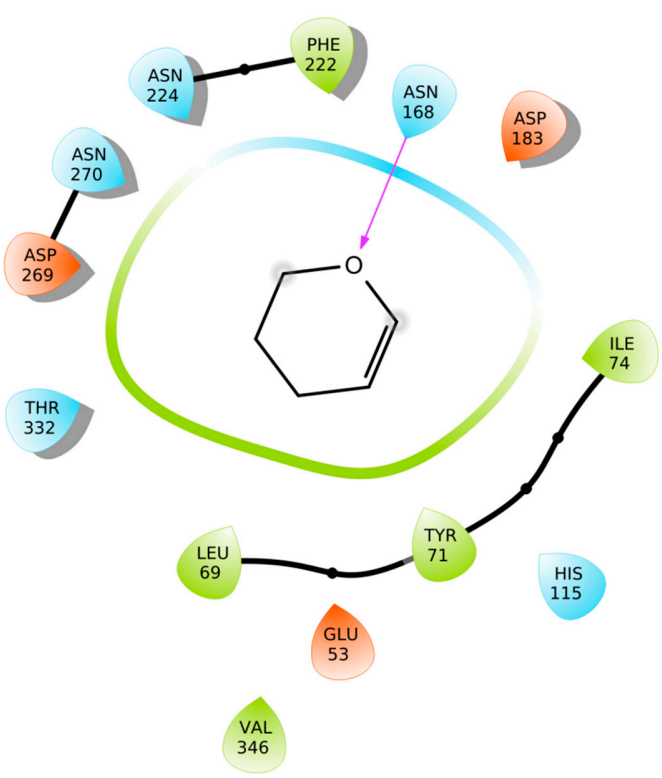
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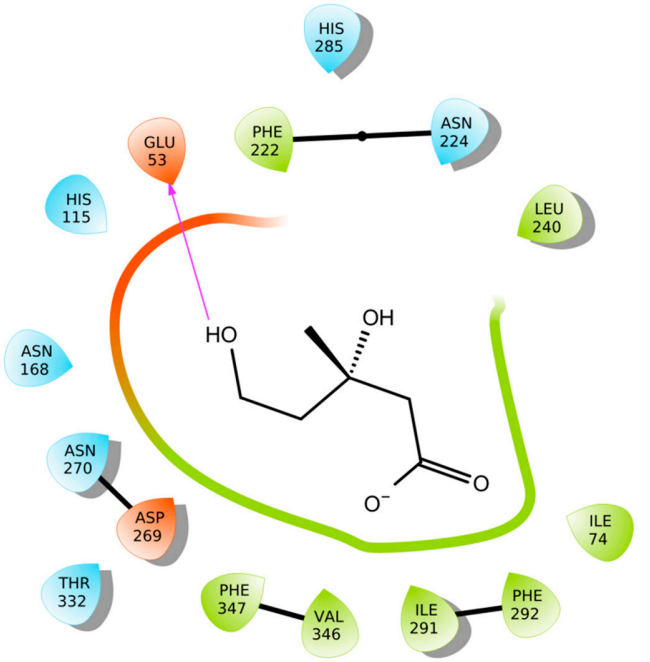
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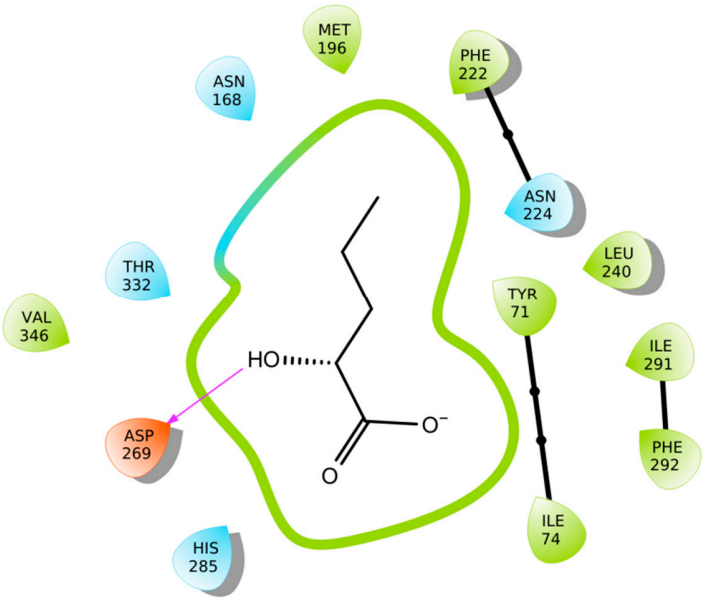
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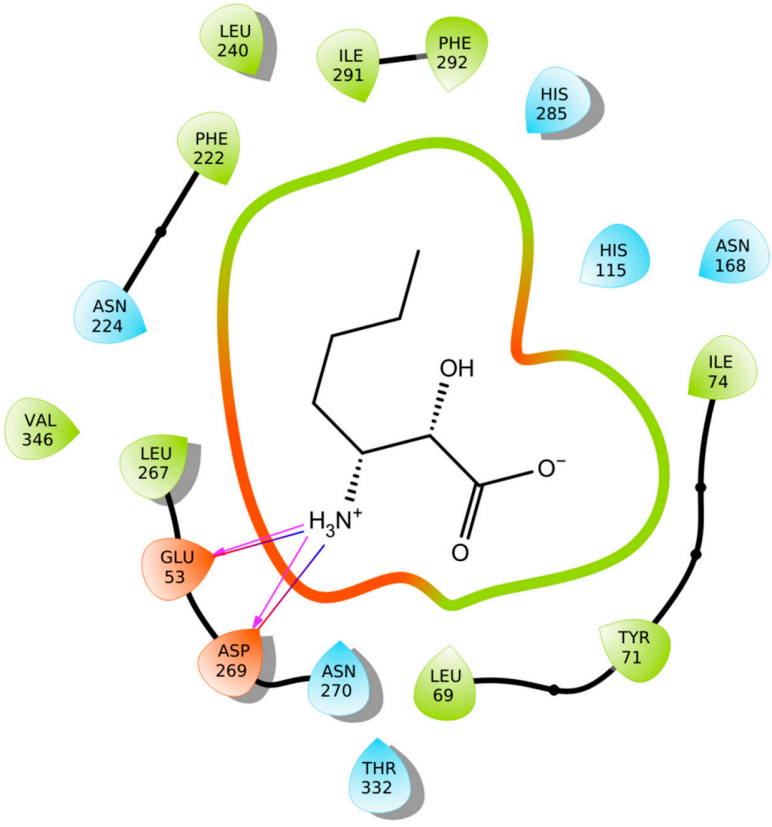
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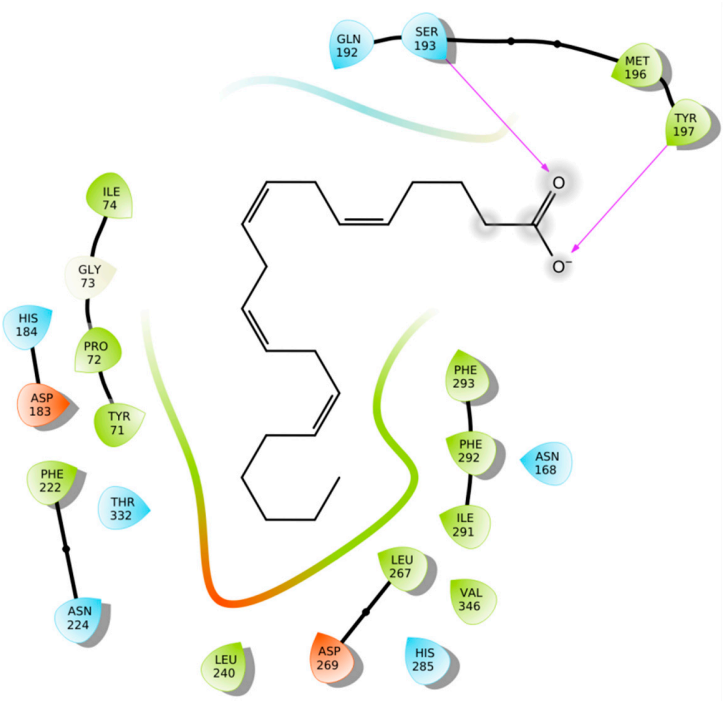
H)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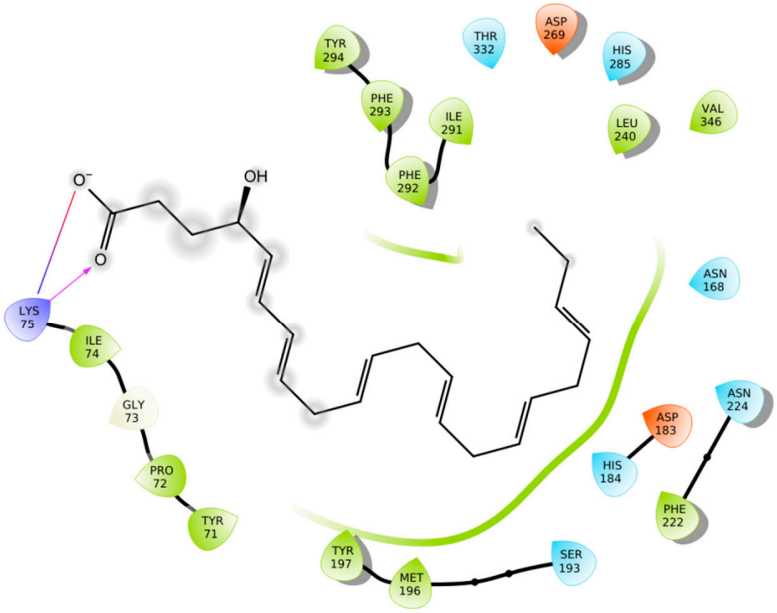
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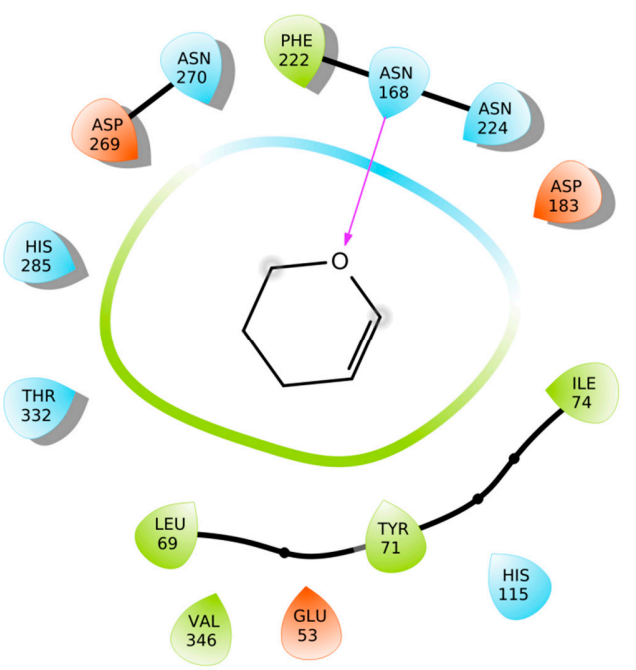
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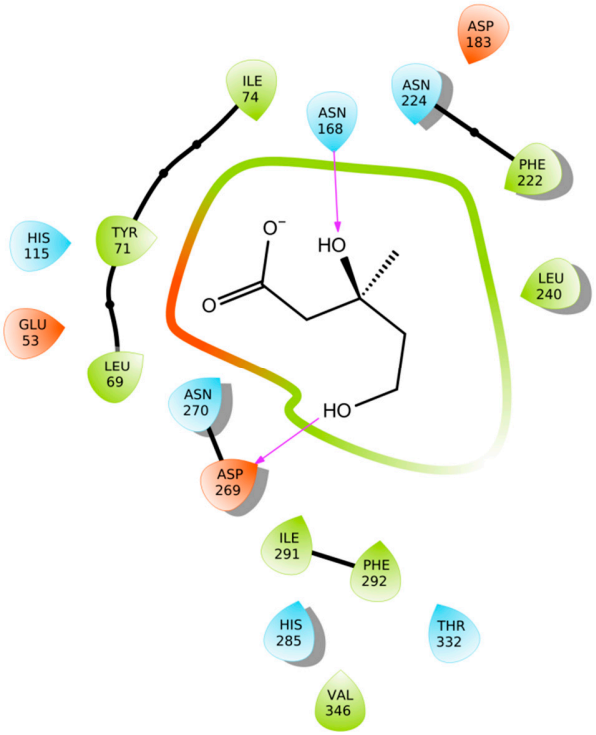
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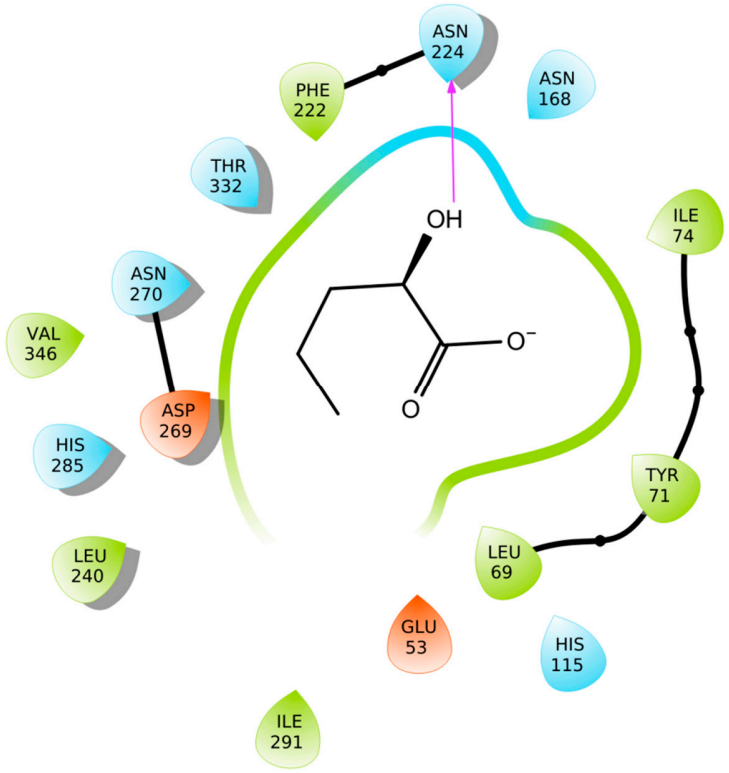
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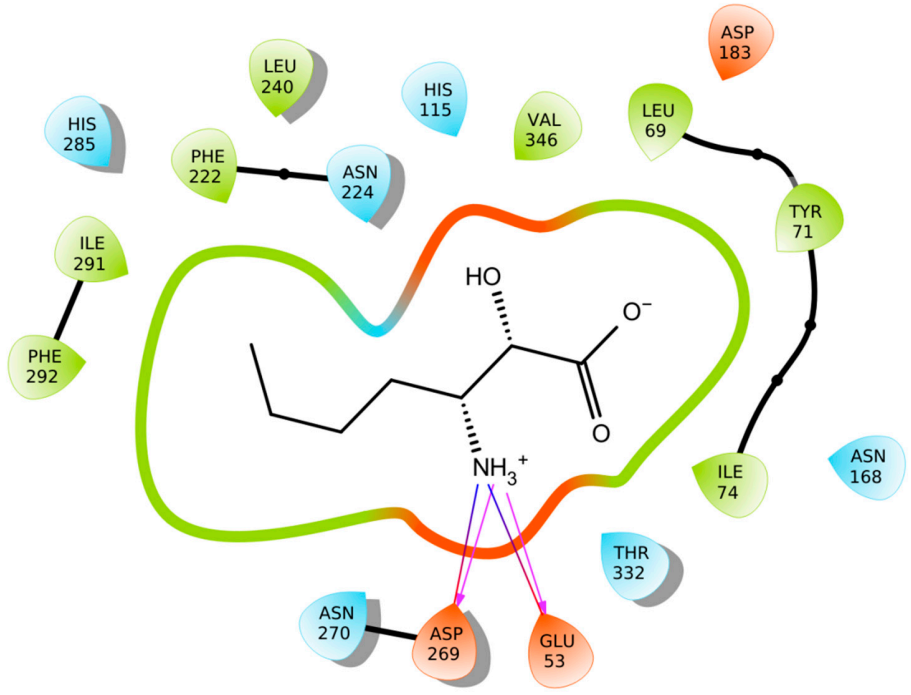
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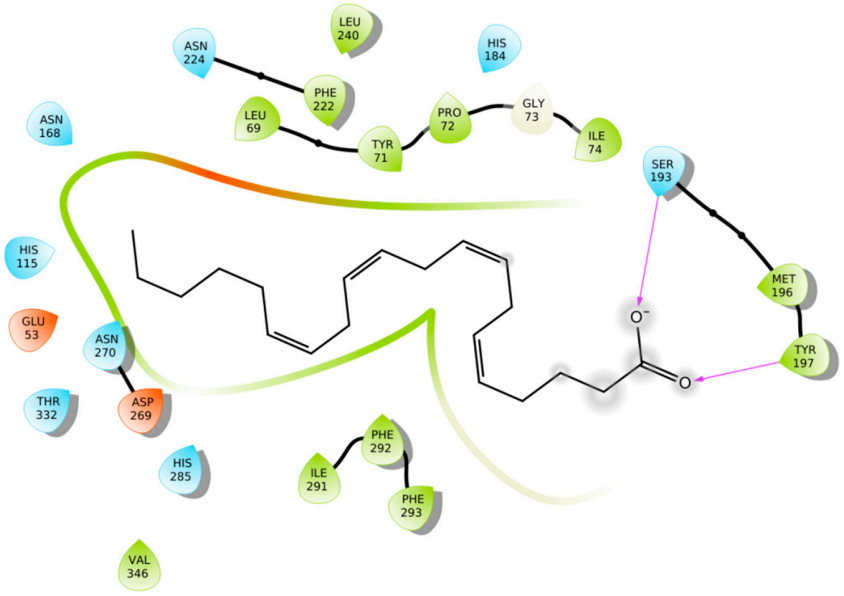
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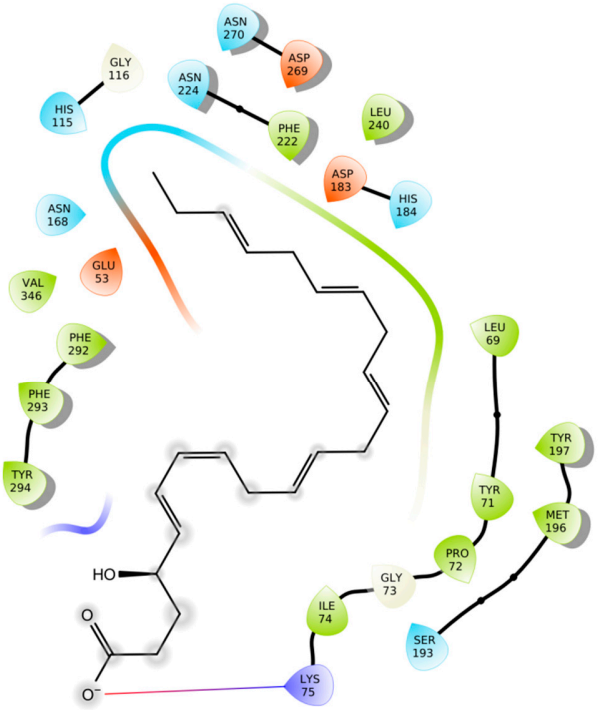
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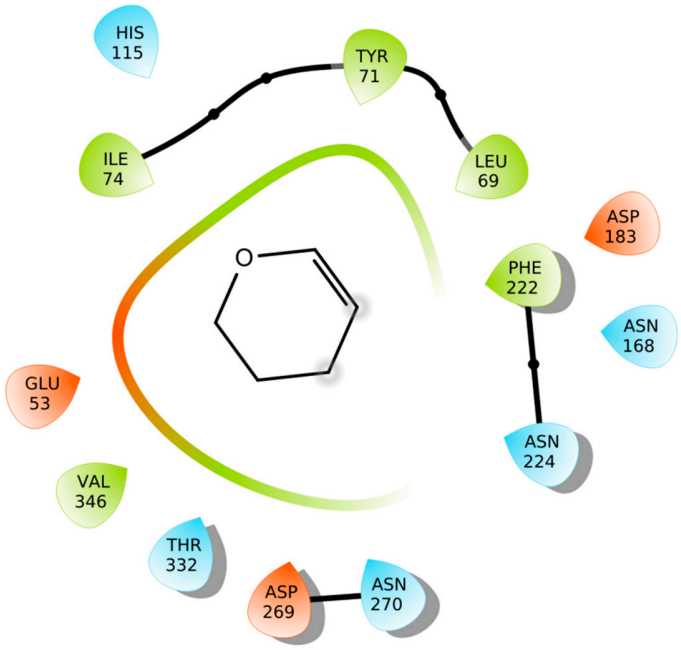
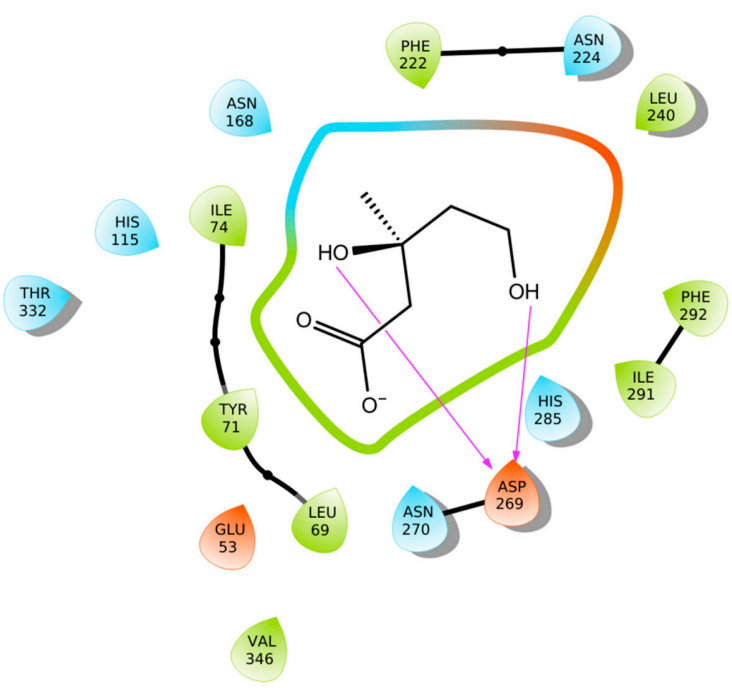
O⁻
LYS 75

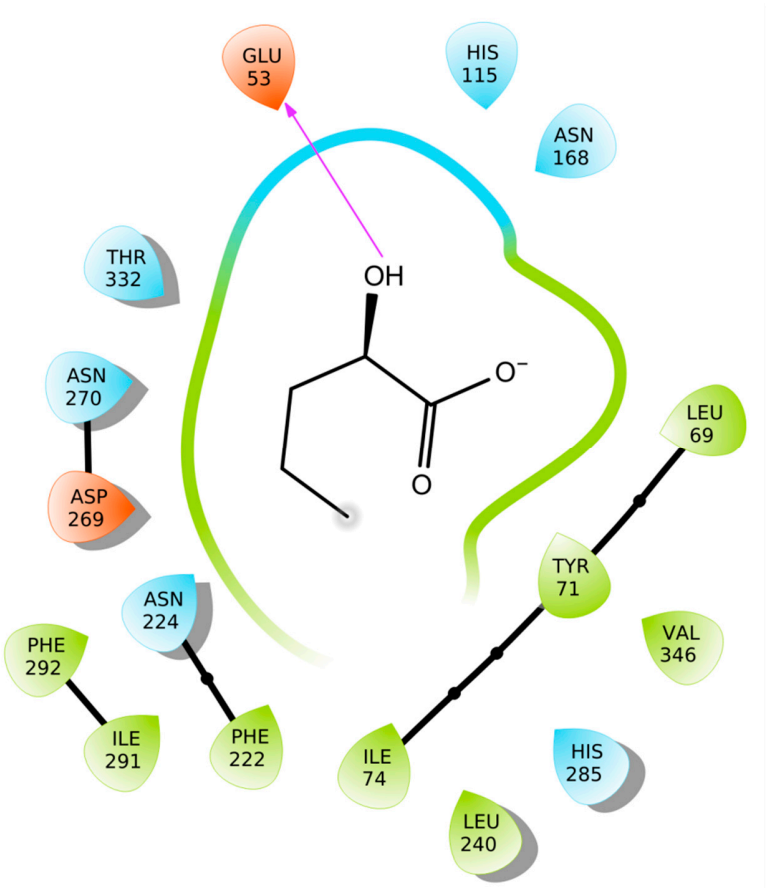
P)


HIS 115
TYR 71
ILE 74
LEU 69
ASP 183
PHE 222
ASN 168
O
GLU 53
ASN 224
VAL 346
THR 332
ASP 269
ASN 270

Q)


PHE 222
ASN 224
ASN 168
LEU 240
HIS 115
ILE 74
HO
OH
THR 332
O
PHE 292
ILE 291
O⁻
TYR 71
HIS 285
ASP 269
ASN 270
LEU 69
GLU 53
VAL 346

R)


GLU
53
HIS
115
ASN
168
THR
332
OH
O⁻
ASN
270
LEU
69
ASP
269
TYR
71
ASN
224
VAL
346
PHE
292
ILE
291
PHE
222
ILE
74
HIS
285
LEU
240
O