**S3 Table.** Prominent binding site and their residues identification of predicted (SDH) and retrieved (GAPDH, HK 2, LDH, PDH, PGK and IDH 1) protein models by MetaPocket 2.0 server and reported binding site residues from PDB X-ray crystal structures.

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| --- | --- | --- |
| **Protein Name** | **Predicted prominent binding site residues** | **Reported binding site residues** |
| **GAPDH** | **Binding site : 1**  Thr153, Thr177, His179, Thr211, Ala232, Arg234, Ala213, Ala209, Ser210, Ser151, Cys152, Asn316, Tyr314, Arg197, Pro208, Gly212, Thr182, Ile181, Thr237, Ala238, Asn239, Glu317, Thr52, Ser51, Arg13, Thr154, Ile14, Asp50, Asp198, Ile207, Gln185, Thr187, Ala202, Leu203, Pro124, Ala216, Ala183, Thr184, Lys186, Lys215, Lys219 , Met130, Ala150, Tyr320, Leu195, Trp196, Ala123, Ser122, Arg16, Tyr49, Val188, Ser125, Tyr45, Met46, Lys194, Ser192, Ala126, Gly15, Phe47, Gly12, Ser98, Gly100, Thr103, Gly199, Thr99, Glu97, Tyr42, Gly193, Pro191, Phe11, Ile121, Ile38, Val101, Gly10, Asp35, Thr104, Lys107, Phe37, Asn34, Pro36, Asn9, Phe102, Glu79, Arg80, Pro82, Ile85, Asp81  **Binding site : 2**  Asn24, Ser288, Thr290, Phe318, His57, His53, Arg20, Lys55, Phe56, Gly58, Phe23, Asn70, Ala21, Ser25, Asn322, Leu17, Ser321, Gly54, Gly319  **Binding site : 3**  Glu138, Lys139, Val135, Asn136, His137, Gly134, Pro269, Lys162, Asp166, Glu223, His165, Ile221, Val220, Pro222, Lys219, Pro129, Phe131, Leu144, Met130 | Asn9, Gly10, Phe11, Gly12, Arg13, Ile14, Asn34, Asp35, Pro36, Phe37, Ile38, Arg80, Ser98, Thr99, Gly100, Phe102, Ser122, Ala123, Cys152, Asp315 |
| **HK 2** | **Binding site : 1**  Arg69, Val248, Glu249, Cys813, Asp814, Met242, Phe67, Thr161, Ile817, Lys162, Leu463, Glu252, Thr812, Leu163, Asp164, Arg470, His467, Val68, Val459, Ile818, Ile203, Ala460, Asp815, Ala464, Ser70,Arg769, Gly253, Arg254, Gln466, Val456, Leu766, Leu767, Phe768, Gly765, Met215, Arg462, Thr71, Asp73, Met455, Glu821, Leu474, Glu76, Pro72, Gln471, Val825, Gln478, Leu797, Gly250, Met247, Val822,Phe761, Thr66, Asp465, Gly770, Tyr461, Val207, Thr75  **Binding site : 2**  Thr88, Ser415, Lys419, Asn89, Glu335, Lys337, Thr232, Gly299, Met300, Gly231, Thr336, Ser340, Val416, Met302, His420, Gly303, Glu304, Gly332, Phe334, Tyr301, Glu280, Met283, Gly284, Arg307, Thr331,Leu308, Ile281, Ser285,Leu286, Lys295, Arg120, Met119, Gly174, Gly87, Phe175, Gly86, Lys173, Ile114, Asp341, Glu116, Phe90, Tyr112, Ala113, Ile111, Leu85, Asp282, Pro157, Thr172, Asn235, Glu260,Gln291, Glu294, Ser234, Gly262, Phe156, Ser155, Asn287, Asn208, Asn258, Gly233, Trp171, Phe154, Asp209, Ile229, Asn330, Arg333, Gly414, Asp84, Ser449, Thr213, Asp413, Pro115, Gly448, Gly450, Lys418,Arg91, Asp447, Ser445, Leu93, Glu446, Met107, Asn109  **Binding site : 3**  Thr88,Gly231,Thr232, Gly414, Ser415, Gly87, Lys173, Asp209, Ile229, Gly233, Ser234, Gly86, Arg91, Asp413, Lys418, Lys419, Arg444, Asn89, Asp84, Gly448, Ser449, Thr213, Leu85, Phe90, Ser155, Phe156, Pro157, Thr172, Asn208, Asn235, Glu260, Gln291, Glu294, Gly262, Asp447, Glu446, Leu93, ASN109, Met107, Gly450, Ser445  **Binding site : 4**  Arg539, Asn557, Glu894, Asp895, Met555, Gly896, Asp532, Leu541, Ser897, Gly898, Asp861, Lys866, Gly534, Gly535, Thr536, Asn537, Thr863, Asp657, Ile677, Gly679, Thr680, Gly862, Phe538, Ser603, Lys621, Gly681, Ser682, Asn683, Glu708, Gly710, Gln739, Glu742, Asn656, Thr620, Ser893, Thr661, Ile559, Phe604, Phe602, Pro605, Asn706 | Glu46, Lys49, Ala59, Ala60, Val61, Asp84, Gly87, Thr88, Asn89, Thr153, Phe154, Ser155, Phe156, Pro157, Cys158, Thr172, Lys173, Asn208, Asp209, Thr210, Ile229, Gly131, Thr232, Ser234, Asn235, Met242, Ile245, Val248, Gly250, Glu260, Gly262, Asp267, Gln291, Glu294, Asp413, Gly414, Ser415, Pro421, His422, Ala424, Lys425, Gly448, Ser449, Ala458, Arg470, Arg489, Asp532, Gly535, Thr536, Ser603, Phe604 , Pro605, Thr620, Lys621, Asn656, Asp657, Ile677, Gly679, Thr680, Ser682, Asn683, Glu708, Thr723, Glu724, Gln739, Glu742, Asp861, Gly862, Thr863, Gly896, Ser897 |
| **LDH** | **Binding site : 1**  Tyr83, Phe119, Ile120, Gln123, Lys81, Asp82, Val53, Val51, Asp52, Val116, Ala96, Val26, Gly97, Gly27, Val98, Leu54, Thr95, Gly29, Arg99, Ser137, Asn138, Val28, Val136, Leu109, Lys57, Gly32, Gln100, Val31, Gln30, Val140, Ser161, His193, Ile252, Gly162, Arg106, Thr248, Tyr247, Leu165, Ile242, Ala238, Gly246, Arg169, Asn249, Asp166, Trp250, Ala251, Ser255, Asn115, Asn164, Leu259  **Binding site : 2**  Val241, Lys245, Trp250, Thr248, Asn249, Ala251, Leu254,Arg169, Tyr172, Ala168, Pro182, Leu165, Ser255, Asn164, Arg171, Ser183, His181, Trp188, Ile270, His271, Pro272, Asp258, Arg269, Ser167, Gly187, Lys42,Ala257, Glu261, Ile252, Ser38, His186, Ser237, Ala238, Met233, Val234, Leu173, Glu240, Tyr239, Glu236, Leu244  **Binding site : 3**  Val198, Ala199, Trp201, Asp311, Glu312, Gln315, His231, Gly219, Lys228, Ser197, Gln212, Lys309, Met218, Thr220, Lys318, Pro216, Asp195, Ser196, Val235, Lys232, Asp310, Val200, Ser202, Asp221 | Gly29, Gln30, Val31, Asp52, Val53, Leu54, Thr95, Ala96, Gly97, Val98, Arg99, Gln100, Arg106, Asn108, Val136, Ser137, Asn138, Ser161, Leu165, Arg169, His193, Ala238, Thr248, Ile252 |
| **SDH** | **Binding site : 1**  Gly17, Ser45, His46, Thr203, Gly52, Gly53, Phe120, Arg287, Arg398, Ala401, Gln51, His243, Leu253, Thr255, Glu256, Ala50, Thr143, Leu404, His354, Ser403, Ala49, Tyr355, Thr47, Glu387, Thr214, Leu407, Gly386, Gly204, Gly18, Gly205, Ser219, Ala19, Ala202, Cys385, Gly20, Thr218, Cys252, Thr333, Ala16, Gly15, Leu40, Lys39, Thr38, Ala216, Thr220, Arg44, Val14, Val37, Asp222, Gly221, Tyr166, Ala168, Phe167, Met226, Ala183, Asp406, Phe337, Gly329, Glu332, Val48, Ile330, Asp141, Arg142, His145, Pro328, Ser215, Gly207, Gly400, Asn356  **Binding site : 2**  Gly205, Arg208, His217, Thr218, Ser219, Thr220, Gly221, Leu518, Lys39, Thr203, Asp222, Gly204, Tyr206, Gly207, Thr209, Tyr210, Val240, Asn356, Ser215, His354, Glu387, His46, Val353, Tyr355, Gln241, Ser45, Gly17, Gly18, Thr47, Ala202, Leu40, Gly15, Ala16, Thr38, Ala216  **Binding site : 3**  Phe167, Ala168, Leu169, Asp222, Arg229, Asn517, Leu513, Asp170, Ser439, Asn442, Gln516, Leu443, Met226, Lys445, Val579, Tyr490, Leu520, Leu493, Glu438, Gly580, Leu171, Leu172, Met173, Gly436, Leu446, Lys494, Leu496, Gly491, Thr581, Ala449, Ala230, Ile182, Thr228, Ala435, Glu174, Lys432, Ile431, Glu437, Asn434, Met441, Gly582, Thr498, His495, Gly451, Asp450, Phe448 |  |
| **PDH** | **Binding site: 1**  Thr87, Ala88, Gln141, Leu164, Tyr165, Gly166, Glu194, Val138, Asp167, Gly168, Ala169, Asn196, Tyr198, Gly199, Gln68, Gly139, Tyr89, Phe94, Cys71, Cys72, Ile137, Arg90, Met200, Cys65, Ala91, Arg259, Gly93, His263, Leu64, His92, Gly201, His63, Phe61, Ser264, Ser266, Met124, Gly136, Asn195, Asn135  **Binding site: 2**  Lys118, Gly119, Lys120, Pro330, Glu334, Tyr337, His338, Val360, Pro331, Leu332, Leu335, Cys116, Ala117, Lys113, Gly115, Glu329, Glu333, Gly121, His125, Tyr127, Gly336, Ile339, Val348, Arg349, Phe357, Gly350, Ala351, Tyr340, Ser341, Ser361, Ser342  **Binding site: 3**  Ala326, Pro328, Arg112, Asp327, Glu329, Thr110, Lys56, Ile57, Arg59, Ile58, Leu109, Gly111, Gly119, Lys120, Gly121, Gly122, Phe61, Ser123, Met124, His125, Glu108, Gly60, Lys118, Pro330, Cys62, Leu335, Ala117, Glu334, Pro331, Leu332, Glu333, Phe35 | Tyr89, Arg90, Gly136, Val138, Lys153, Gly166, Asp167, Gly168, Ala169, Trp185, Leu187, Asn196, Tyr198, Gly199, His263 |
| **PGK** | **Binding site : 1**  Lys30, Asn31, Glu294, Trp345, Asn295, Asp293, Glu344, Met29, Val342, Asn32, Phe292, Thr35, Gln33, Asp74, Lys75, Pro28, Asp375, Gly341, Phe343, Gly313, Leu314, Asp315, Val340, Gly238, Phe242, Cys316, Pro80, Pro339, Pro73, Gly239, Leu257, Met312, Ser256, Thr378, Ser77, Tyr76, Ala215, Thr255, Glu79, Val27, Leu64, Gly214, Gly338, Met72, Thr376, Gly213, Gly374, Asn26, Gly65, Lys216, Arg66, Arg39, Asn337, Gly373, Lys220, Gly396, Val217, Gly397, His63, Arg123, Asp24, Gly167, Thr168, His170, Arg171, Asp219, Asp68, Glu129, His173, Lys131, Ala132, Gly130, Glu128, Lys382, Phe286, Ala241, Pro283, Tyr324, Leu223, Glu401, Ala218, Gln222, Lys406, Met240, Leu212, Asp259, Phe258,  **Binding site : 2**  Lys41, Pro45, Lys192, Ala42, Leu189, Ser46, Asp164, Phe188, Glu386, Val389, Ser390, His391, Val392, Asp387, Gln38, Asn36, Ala377, Ala381, Thr394, Glu193, Tyr196, Asn37, Arg39  **Binding site : 3**  Ala215, Phe292, Val342, Glu344, Gly214, Gly238, Gly239, Leu314, Pro339, Val340, Gly341, Asp375, Phe343, Gly313, Asp315, Thr255, Ser256, Leu257, Met312, Phe242, Pro283, Phe286, Cys316, Ala241, Tyr324 | Asp24, Asn26, Arg39, His63, Arg66, Arg123, Gly167, Thr168, Arg171, Gly214, Ala215, Lys216, Asp219, Lys220, Gly238, Gly239, Phe242, Leu257, Gly313, Leu314, Asn337, Pro339, Gly341, Val342, Glu344, Gly373, Gly374, Asp375, Thr376, Gly396, Gly397 |
| **IDH 1** | **Binding site : 1**  Arg100, Tyr272, His132, His133, Asn271, Asp273, Gly274, Asp275, Ala134, Tyr135,Val107, Arg109, Gln277, Val276, Ser293, Glu306, Ala307, Ala308, Lys72, Cys73, Ala74, Thr75, Asn96, His309, Ser94, Thr77, Gly310, Thr311, Gln283, Leu288, Thr19, Trp23, Ser332, Ala335, Ile22, Phe108, Ile130, Asp279, Glu110, Met291, Ala282, Val281, Trp267, Gly136, Gly97, Asn101, Asp137, Ile76, Tyr139, Thr98,  **Binding site : 2**  Ala111, Tyr285, Gly286, Ser287, Met291, Val281, Ala282, Pro118, Met290, Leu120, Arg119, Ile112, Trp124, Ile117, Ile113, Cys379, Leu376, Asp279, Ile130, Cys114, Ile128, Arg109, Glu110, Pro127, Lys126, Trp267, Ala258, Met259, Val255, Phe265, Met254, Ile251, Ser278, Ser280, His132, Asp273, Gly274, Asp275, Cys269, Asn271, Leu288, Gln283, Gly284, Gly289, Gln277, Val276, Tyr272, Asn116, Lys115, Val121, Ser210, Ala256, Asp252,  **Binding site : 3**  Phe108, Glu110, Ile129, Thr292, Val294, Arg338, Lys203, Ser293, Met199, Val296, Val303, Ser202, Ala341, Glu360, His342, Lys345, Gln198, Gly300, Ser195, Thr302, Thr337, Ala356, Asn357, Ala353, Cys297, Phe354, Arg109, Ile112, Ile113, Cys114, Pro127, Phe334, Ile364, Ala111, Ile128, Ala305, Gly339, Ile130, Leu295, Lys115, Glu368, Arg119, Val125, Glu361, Lys126, Trp205, Glu365, Trp124, Ala358, Asp299, Gly264, Leu346, Pro298, Gly204, Leu201, Ala344, Glu306, Ala307, Ala335, Asn348, Asn349, Lys350 | Lys72, Ala74, Thr75, Ile76, Thr77, Arg82, Asn96, Trp128, Ile130, Met254, Ala258, Trp267, Gln277, Asp279, Val281, Ala282, Gly289, Met291, His309, Gly310, Thr311, Val312, Thr313, Arg314, His315, Asn328 |