**Supporting Information**

**REINDEER: A Protein-Ligand Feature Generator Software for Machine Learning Algorithms**

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Table S1- PDBIDs of train, validation, and test sets.

|  |  |
| --- | --- |
| Set | PDBIDs |
| Train | 10gs, 184l, 185l, 186l, 187l, 188l, 1a1e, 1a28, 1a4r, 1a4w, 1a69, 1a94, 1a99, 1a9m, 1a9q, 1aaq, 1add, 1adl, 1ado, 1afk, 1afl, 1ai4, 1ai7, 1aid, 1aj7, 1ajn, 1ajp, 1ajv, 1ajx, 1alw, 1amw, 1apv, 1atl, 1atr, 1avn, 1ax0, 1azm, 1b05, 1b0h, 1b1h, 1b2h, 1b32, 1b38, 1b3f, 1b3g, 1b3h, 1b3l, 1b40, 1b46, 1b4h, 1b4z, 1b51, 1b52, 1b55, 1b57, 1b58, 1b5h, 1b5i, 1b5j, 1b6h, 1b6j, 1b6l, 1b7h, 1b8n, 1b8o, 1b8y, 1b9j, 1bai, 1bcd, 1bdq, 1bgq, 1bhf, 1bhx, 1bju, 1bm7, 1bma, 1bn1, 1bn3, 1bnn, 1bnq, 1bnt, 1bnv, 1bnw, 1bp0, 1br6, 1bty, 1bv7, 1bv9, 1bwa, 1bwb, 1bxo, 1bxq, 1bzj, 1bzy, 1c1r, 1c1u, 1c1v, 1c4u, 1c5c, 1c5n, 1c5o, 1c5p, 1c5q, 1c5s, 1c5t, 1c5x, 1c5y, 1c70, 1c83, 1c84, 1c86, 1c87, 1c88, 1cbx, 1ceb, 1cet, 1cgl, 1ciz, 1cnw, 1cnx, 1cny, 1cps, 1ctt, 1ctu, 1d09, 1d2e, 1d3d, 1d3p, 1d4h, 1d4i, 1d4j, 1d4k, 1d4l, 1d4p, 1d6v, 1d6w, 1d7i, 1d7j, 1d9i, 1dar, 1df8, 1dgm, 1dhi, 1dhj, 1dif, 1dmp, 1dqn, 1drj, 1drk, 1drv, 1dud, 1duv, 1dy4, 1dzk, 1e1v, 1e2k, 1e2l, 1e3g, 1e3v, 1e4h, 1e5j, 1e6q, 1e6s, 1eb2, 1ebw, 1ec0, 1ec1, 1ec2, 1ec3, 1ec9, 1ecq, 1ecv, 1efy, 1egh, 1ejn, 1ela, 1elb, 1elc, 1eld, 1ele, 1elr, 1enu, 1eoc, 1epo, 1ew8, 1ew9, 1ex8, 1ez9, 1ezq, 1f0r, 1f0s, 1f0t, 1f0u, 1f3e, 1f4e, 1f4f, 1f4g, 1f4x, 1f57, 1f5k, 1f5l, 1f73, 1f74, 1f8b, 1f8c, 1f8d, 1f8e, 1fao, 1fch, 1fcx, 1fcy, 1fh7, 1fh9, 1fhd, 1fiv, 1fjs, 1fkb, 1fkf, 1fkg, 1fkh, 1fkw, 1fl3, 1flr, 1fm9, 1fo0, 1fpc, 1fq5, 1ftm, 1fv0, 1fzj, 1fzk, 1fzm, 1fzo, 1fzq, 1g1d, 1g2l, 1g2o, 1g30, 1g32, 1g35, 1g36, 1g3d, 1g3e, 1g45, 1g46, 1g48, 1g4o, 1g52, 1g53, 1g54, 1g74, 1g7f, 1g7g, 1g7q, 1g7v, 1g85, 1g98, 1gai, 1gar, 1gfy, 1ghv, 1ghw, 1ghy, 1ghz, 1gi1, 1gi4, 1gi7, 1gj6, 1gjc, 1gnm, 1gnn, 1gno, 1grp, 1gwv, 1gx8, 1gyx, 1gyy, 1h0a, 1h1s, 1h2k, 1h2t, 1h46, 1h4w, 1h5v, 1h6h, 1hbv, 1hdq, 1hee, 1hfs, 1hi3, 1hi4, 1hi5, 1hih, 1hii, 1hk4, 1hlk, 1hmr, 1hms, 1hmt, 1hn4, 1hos, 1hp5, 1hpo, 1hps, 1hpv, 1hpx, 1hsh, 1hsl, 1hvh, 1hvi, 1hvj, 1hvk, 1hvl, 1hvr, 1hvs, 1hwr, 1hxb, 1hxw, 1hyo, 1i1e, 1i2s, 1i37, 1i5r, 1i7z, 1i9n, 1i9p, 1ie9, 1if7, 1if8, 1igb, 1igj, 1ii5, 1iih, 1iiq, 1ik4, 1ikt, 1ivp, 1iy7, 1izh, 1izi, 1j01, 1j14, 1j16, 1j17, 1j36, 1j37, 1j4r, 1jak, 1jaq, 1jcx, 1jet, 1jeu, 1jev, 1jgl, 1jlr, 1jmf, 1jmg, 1jn4, 1jq8, 1jqy, 1jsv, 1jvu, 1jyq, 1jys, 1jzs, 1k1j, 1k1l, 1k1n, 1k1o, 1k1y, 1k21, 1k22, 1k27, 1k4g, 1k4h, 1k6c, 1k6p, 1k6t, 1k6v, 1k9s, 1kav, 1kc7, 1kdk, 1kel, 1kjr, 1km3, 1kmy, 1koj, 1kpm, 1ksn, 1kug, 1kui, 1kuk, 1kv1, 1kv5, 1kzk, 1kzn, 1l83, 1laf, 1lag, 1lah, 1lan, 1lbf, 1lbk, 1lcp, 1lee, 1lf2, 1lgt, 1lgw, 1lhu, 1li2, 1li3, 1li6, 1lke, 1lkk, 1lkl, 1lnm, 1loq, 1lpk, 1lpz, 1lrh, 1lst, 1lvu, 1lyb, 1lyx, 1lzq, 1m0b, 1m0n, 1m0q, 1m1b, 1m2p, 1m2q, 1m2r, 1m2x, 1m48, 1m5w, 1m7d, 1m7i, 1m7y, 1m83, 1mes, 1met, 1mfa, 1mfd, 1mfi, 1mh5, 1mjj, 1mmq, 1mmr, 1moq, 1mq5, 1mrn, 1mrs, 1msm, 1msn, 1mtr, 1mu6, 1mue, 1my4, 1n0s, 1n1m, 1n3i, 1n4h, 1n4k, 1n51, 1ndv, 1ndw, 1ndy, 1nf8, 1nfu, 1nfw, 1nfx, 1nfy, 1nh0, 1nhu, 1nhz, 1nja, 1njc, 1njd, 1nje, 1njs, 1nl9, 1nli, 1nm6, 1nny, 1no6, 1np0, 1nq7, 1nt1, 1nvr, 1nvs, 1nw4, 1nw7, 1nwl, 1nz7, 1o0f, 1o0m, 1o0n, 1o1s, 1o2j, 1o2n, 1o2o, 1o2q, 1o2r, 1o2w, 1o2z, 1o30, 1o33, 1o35, 1o36, 1o38, 1o3d, 1o3i, 1o3j, 1o3l, 1o5a, 1o5c, 1o5e, 1o5g, 1o5r, 1o7o, 1oar, 1oau, 1oba, 1ocq, 1od8, 1odi, 1odj, 1oe8, 1ogd, 1ogg, 1ogx, 1ogz, 1ohr, 1oif, 1okl, 1olu, 1olx, 1om1, 1ony, 1onz, 1ork, 1os0, 1os5, 1oss, 1owe, 1oxr, 1oz0, 1p19, 1p1o, 1p57, 1pa9, 1pb8, 1pb9, 1pbq, 1pdz, 1pgp, 1phw, 1pkx, 1pme, 1pot, 1ppc, 1pph, 1ppi, 1ppk, 1ppl, 1ppm, 1pr5, 1pro, 1pvn, 1px4, 1pxo, 1pxp, 1pyn, 1pz5, 1pzi, 1pzp, 1q1g, 1q54, 1q5k, 1q72, 1q7a, 1q84, 1q8w, 1q91, 1qan, 1qaw, 1qb1, 1qb6, 1qb9, 1qbn, 1qbo, 1qbq, 1qbr, 1qbs, 1qbt, 1qbu, 1qf0, 1qf2, 1qft, 1qhc, 1qin, 1qji, 1qk3, 1qk4, 1qka, 1qkb, 1ql9, 1qxk, 1qxl, 1qy1, 1qy2, 1qyg, 1r0p, 1r1h, 1r1j, 1r9l, 1rbp, 1rd4, 1rjk, 1rmz, 1rnm, 1rnt, 1ro6, 1rp7, 1rpf, 1rpj, 1rql, 1rr6, 1rtf, 1s39, 1s5z, 1s89, 1sbg, 1sdu, 1sdv, 1sgu, 1sh9, 1siv, 1sl3, 1sld, 1sqo, 1sqt, 1sr7, 1srg, 1ssq, 1stc, 1str, 1sv3, 1sw2, 1swg, 1swr, 1syh, 1szd, 1t32, 1t4v, 1t5f, 1t7d, 1t7j, 1ta6, 1tcx, 1td7, 1thz, 1tjp, 1tkb, 1tlp, 1tmn, 1tng, 1tnh, 1tni, 1tom, 1tpw, 1trd, 1tsy, 1ttm, 1tx7, 1txr, 1u0g, 1u33, 1u71, 1ua4, 1ucn, 1ugx, 1uho, 1ui0, 1uj5, 1uml, 1uou, 1ur9, 1usi, 1usk, 1usn, 1utj, 1utl, 1utm, 1utn, 1uv6, 1uvt, 1uw6, 1uwf, 1uwt, 1uwu, 1uz1, 1uz4, 1uz8, 1v0k, 1v0l, 1v11, 1v16, 1v2j, 1v2k, 1v2l, 1v2n, 1v2o, 1v2r, 1v2s, 1v2t, 1v2u, 1v2w, 1v48, 1v7a, 1vfn, 1vyf, 1vyg, 1vzq, 1w0z, 1w11, 1w13, 1w3j, 1w3k, 1w3l, 1w4p, 1w4q, 1w5v, 1w5w, 1w5x, 1w5y, 1w7g, 1w96, 1w9u, 1w9v, 1wc1, 1wcq, 1wdn, 1wht, 1wm1, 1ws1, 1ws4, 1wuq, 1wur, 1wvj, 1x1z, 1x38, 1x39, 1x8d, 1x8j, 1x8r, 1x8t, 1xap, 1xbo, 1xd0, 1xff, 1xgi, 1xh4, 1xh5, 1xh9, 1xhy, 1xjd, 1xk5, 1xk9, 1xow, 1xpz, 1xq0, 1xr9, 1xt8, 1xug, 1xws, 1y0l, 1y20, 1y3n, 1y3p, 1y3v, 1y3x, 1y6q, 1yc4, 1yda, 1ydb, 1ydk, 1yds, 1yei, 1yej, 1yet, 1yfz, 1yp9, 1ypg, 1ypj, 1yq7, 1yqj, 1yqy, 1yvm, 1z1h, 1z4o, 1z6s, 1z71, 1z9y, 1zc9, 1zdp, 1zea, 1zfq, 1zge, 1zgi, 1zhy, 1zoe, 1zog, 1zoh, 1zp8, 1zpa, 1zs0, 1zvx, 2a14, 2a4m, 2a5b, 2a5c, 2a5s, 2a8g, 2aac, 2afw, 2afx, 2aj8, 2am4, 2amt, 2ans, 2aoc, 2aod, 2aoe, 2aog, 2aqu, 2arm, 2avm, 2avo, 2avq, 2avs, 2ax9, 2ayr, 2azr, 2b07, 2b1g, 2b4l, 2b7d, 2b9a, 2baj, 2bak, 2bal, 2bes, 2bet, 2bfq, 2bfr, 2bmk, 2bo4, 2boh, 2boj, 2bok, 2bpy, 2bq7, 2bqv, 2bt9, 2buv, 2bvd, 2bvr, 2bvs, 2byr, 2bys, 2bz6, 2bza, 2c1p, 2c3l, 2c80, 2c92, 2c94, 2c97, 2ca8, 2cbj, 2cbu, 2cbz, 2cc7, 2ccb, 2ccc, 2ce9, 2cej, 2cen, 2ceq, 2cer, 2ces, 2cex, 2cf8, 2cf9, 2cgf, 2cht, 2cle, 2clh, 2cli, 2clk, 2cn0, 2csn, 2ctc, 2d0k, 2d1n, 2d1o, 2d3u, 2d3z, 2doo, 2drc, 2dri, 2dw7, 2e1w, 2e27, 2e2p, 2e2r, 2e7f, 2e91, 2e92, 2e94, 2e9u, 2epn, 2erz, 2euk, 2ewa, 2ewb, 2ews, 2exm, 2ez7, 2f1g, 2f2h, 2f34, 2f35, 2f6t, 2f7i, 2f7o, 2f7p, 2f80, 2f81, 2f8g, 2f94, 2f9k, 2fdp, 2fgu, 2fgv, 2fle, 2flr, 2fpz, 2fqo, 2fqt, 2fqw, 2fqx, 2fqy, 2fu8, 2fw6, 2fx6, 2fxu, 2fxv, 2fzc, 2fzg, 2fzk, 2g5u, 2gh9, 2gj5, 2gkl, 2gl0, 2glp, 2gss, 2gst, 2gsu, 2gv6, 2gvj, 2gvv, 2gyi, 2gz2, 2h15, 2h21, 2h3e, 2h4g, 2h4k, 2h4n, 2h6t, 2ha2, 2ha3, 2ha6, 2hah, 2haw, 2hb3, 2hhn, 2hjb, 2hkf, 2hl4, 2hmu, 2hmv, 2hnc, 2hnx, 2hoc, 2hu6, 2hxm, 2hzl, 2hzy, 2i0a, 2i19, 2i2c, 2i3h, 2i3i, 2i4d, 2i4j, 2i4u, 2i4v, 2i4w, 2i4x, 2i4z, 2i6b, 2i80, 2idw, 2ihj, 2ihq, 2isw, 2iuz, 2izl, 2j27, 2j2u, 2j34, 2j47, 2j4i, 2j62, 2j75, 2j77, 2j79, 2j7b, 2j7d, 2j7e, 2j7f, 2j7g, 2j94, 2j95, 2jdm, 2jdp, 2jds, 2jdu, 2jew, 2jf4, 2jfz, 2jg0, 2jgs, 2jh0, 2jh5, 2jh6, 2jiw, 2jke, 2jkh, 2jkp, 2jxr, 2mas, 2nmx, 2nmz, 2nn1, 2nn7, 2nnd, 2nsj, 2nsl, 2nt7, 2nta, 2o4j, 2o4k, 2o4l, 2o4n, 2o4r, 2o4z, 2o8h, 2oag, 2oax, 2oc2, 2ogy, 2oi0, 2oi2, 2oiq, 2ojg, 2ojj, 2olb, 2ole, 2on6, 2ot1, 2ovv, 2ovy, 2oxd, 2oxn, 2oxx, 2oym, 2p09, 2p2a, 2p3b, 2p3c, 2p3i, 2p4j, 2p4s, 2p53, 2p7a, 2p7g, 2p7z, 2p95, 2pbw, 2pcp, 2pgz, 2pk5, 2pk6, 2pou, 2pov, 2pow, 2pq9, 2pqb, 2pqc, 2pql, 2pqz, 2psu, 2ptz, 2pu1, 2pu2, 2pvh, 2pvj, 2pvk, 2pvl, 2pvm, 2pvu, 2pwc, 2pwd, 2pwg, 2pwr, 2py4, 2pym, 2pyn, 2pyy, 2q1q, 2q2a, 2q38, 2q54, 2q55, 2q5k, 2q63, 2q64, 2q6f, 2q7q, 2q88, 2q89, 2q8h, 2q8m, 2q8z, 2qbs, 2qbw, 2qci, 2qd6, 2qd7, 2qd8, 2qdt, 2qg0, 2qg2, 2qhz, 2qi0, 2qi1, 2qi3, 2qi4, 2qi5, 2qi6, 2qi7, 2qmg, 2qnn, 2qnp, 2qpq, 2qpu, 2qrk, 2qrl, 2qta, 2qtg, 2qtn, 2qtt, 2qu6, 2qw1, 2qwb, 2qwc, 2qwd, 2qwe, 2qwf, 2qzr, 2r0h, 2r0z, 2r1y, 2r23, 2r2m, 2r2w, 2r38, 2r3t, 2r3w, 2r43, 2r58, 2r59, 2r5a, 2r5p, 2r75, 2r9x, 2ra0, 2ra6, 2rcb, 2rd6, 2reg, 2ri9, 2rin, 2rio, 2rka, 2rkd, 2rke, 2rkf, 2rkg, 2rkm, 2sim, 2std, 2tmn, 2tpi, 2usn, 2uwd, 2uwl, 2uwo, 2uwp, 2uxi, 2uxz, 2uy0, 2uy3, 2uy4, 2uy5, 2uyn, 2uyq, 2uz9, 2v2c, 2v2h, 2v2q, 2v2v, 2v3d, 2v3u, 2v54, 2v57, 2v58, 2v59, 2v77, 2v88, 2v8w, 2v95, 2vba, 2vc9, 2ves, 2vfk, 2vh0, 2vhj, 2vj8, 2vjx, 2vk2, 2vk6, 2vl4, 2vmc, 2vmd, 2vmf, 2vnp, 2vnt, 2vo4, 2vo5, 2vot, 2vpe, 2vpn, 2vpo, 2vqt, 2vrj, 2vsl, 2vt3, 2vuk, 2vvc, 2vvs, 2vvu, 2vvv, 2vw1, 2vw2, 2vwc, 2vwl, 2vwm, 2vwn, 2vwo, 2vxn, 2vyt, 2vzr, 2w08, 2w26, 2w47, 2w5g, 2w67, 2w8j, 2w8w, 2w8y, 2w9h, 2wb5, 2wc3, 2we3, 2web, 2wec, 2wed, 2weh, 2wej, 2weo, 2weq, 2wf5, 2wgj, 2whp, 2wjg, 2wk6, 2wkz, 2wl0, 2wly, 2wlz, 2wm0, 2wnj, 2wos, 2wq5, 2wr8, 2wvz, 2wyg, 2wyj, 2wzf, 2wzm, 2x09, 2x0y, 2x2r, 2x4z, 2x6x, 2x7t, 2x7u, 2x8z, 2x91, 2x95, 2x96, 2xab, 2xb7, 2xbp, 2xbw, 2xbx, 2xc0, 2xc4, 2xd9, 2xda, 2xde, 2xdk, 2xdx, 2xef, 2xeg, 2xei, 2xej, 2xg9, 2xhm, 2xht, 2xib, 2xj1, 2xj2, 2xjg, 2xjj, 2xjx, 2xm1, 2xm2, 2xmy, 2xn3, 2xn5, 2xog, 2xpk, 2xxr, 2xxt, 2xxx, 2xyd, 2xye, 2xyf, 2xyt, 2y5f, 2y5g, 2y7i, 2y7z, 2y80, 2y81, 2y82, 2ya6, 2ya8, 2yay, 2yaz, 2yb0, 2ydt, 2ydw, 2yek, 2yel, 2yfa, 2yfx, 2ygf, 2yhw, 2yi0, 2yix, 2yk1, 2ylc, 2yme, 2ypi, 2ypo, 2yxj, 2yz3, 2z1w, 2z4o, 2z94, 2za0, 2za5, 2zc9, 2zcs, 2zdk, 2zdl, 2zdm, 2zdn, 2zfp, 2zfs, 2zft, 2zgx, 2zjw, 2zkj, 2zmm, 2zn7, 2zq0, 2zq2, 2zwz, 2zx6, 2zx7, 2zx8, 2zxd, 2zxg, 2zym, 2zz1, 2zz2, 3a1c, 3a1d, 3a1e, 3a2o, 3a5y, 3a6t, 3a9i, 3aaq, 3aas, 3aau, 3acl, 3acx, 3agl, 3ahn, 3ai8, 3aid, 3alt, 3ao2, 3ao5, 3ap4, 3aqt, 3arw, 3arx, 3axz, 3b24, 3b25, 3b26, 3b2q, 3b3c, 3b3s, 3b3w, 3b3x, 3b4f, 3b4p, 3b50, 3b66, 3b67, 3b7i, 3b7j, 3b7r, 3b7u, 3b92, 3bbb, 3bbf, 3be9, 3bex, 3bft, 3bfu, 3bgb, 3bgq, 3bkk, 3bkl, 3bl0, 3bl1, 3bpc, 3bqc, 3bra, 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3fwv, 3fzn, 3fzy, 3g0e, 3g0i, 3g19, 3g1d, 3g1v, 3g2y, 3g30, 3g32, 3g34, 3g35, 3g3r, 3g5k, 3ga5, 3gba, 3gbe, 3gc4, 3gcp, 3gcs, 3gcu, 3gdt, 3ggu, 3gi4, 3gi5, 3gi6, 3gjw, 3gk1, 3gkz, 3gm0, 3gqz, 3gs6, 3gsm, 3gss, 3gst, 3gt9, 3gta, 3gtc, 3gvb, 3gvu, 3gx0, 3gy2, 3gy3, 3gy7, 3h30, 3h5b, 3h78, 3h89, 3h8b, 3hb4, 3hcm, 3hek, 3hf8, 3hfb, 3hig, 3hit, 3hk1, 3hkn, 3hkq, 3hkt, 3hku, 3hkw, 3hky, 3hl5, 3hl7, 3hl8, 3hll, 3hmo, 3hmp, 3hp9, 3hs4, 3hu3, 3hub, 3huc, 3hv8, 3hvi, 3hww, 3hzk, 3hzm, 3hzv, 3i25, 3i3b, 3i4b, 3i4y, 3i51, 3i5z, 3i60, 3i6o, 3i73, 3i7e, 3i9g, 3iae, 3ibl, 3ibn, 3ibu, 3ies, 3igp, 3ijh, 3ikd, 3ikg, 3imc, 3ime, 3iob, 3ioc, 3iod, 3ioe, 3iof, 3iog, 3ip5, 3ip6, 3ip8, 3ip9, 3iph, 3ipq, 3iqu, 3isj, 3iss, 3iub, 3iue, 3ivc, 3ivx, 3iw5, 3iw6, 3iww, 3jdw, 3jrs, 3jrx, 3juk, 3juo, 3jup, 3jy0, 3jyr, 3jzh, 3jzj, 3k00, 3k02, 3k1j, 3k2f, 3k37, 3k4d, 3k4q, 3k5x, 3k8c, 3k8o, 3k8q, 3k97, 3k99, 3kdb, 3kdc, 3kdd, 3kdm, 3kek, 3kgq, 3kgt, 3kgu, 3kiv, 3kjd, 3kku, 3kmc, 3kmx, 3kmy, 3kqr, 3kr4, 3kv2, 3kyq, 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5flq, 5fls, 5flt, 5fnc, 5fnd, 5fnf, 5fng, 5fnr, 5fns, 5fnt, 5fnu, 5fog, 5fol, 5fot, 5fou, 5fov, 5fox, 5fpk, 5fs5, 5fsc, 5fsn, 5fso, 5fsx, 5fsy, 5ftg, 5fto, 5fyx, 5g17, 5g1a, 5g1z, 5g2b, 5g2g, 5g46, 5g4m, 5g4n, 5g4o, 5g57, 5g5f, 5g5v, 5g5z, 5g60, 5g61, 5gj9, 5gja, 5gmh, 5gmn, 5gof, 5gs9, 5gsa, 5h1t, 5h1u, 5h1v, 5h5f, 5h85, 5h8e, 5h9r, 5ha1, 5hbn, 5hbs, 5hct, 5hcv, 5hcy, 5his, 5hjq, 5hrv, 5hrw, 5hrx, 5htl, 5hu9, 5hva, 5hvs, 5hvt, 5hwu, 5hwv, 5hz5, 5hz6, 5hz8, 5hz9, 5i1q, 5i29, 5i2e, 5i2f, 5i3a, 5i3v, 5i3w, 5i3x, 5i3y, 5i7x, 5i7y, 5i80, 5i88, 5i8g, 5i9x, 5i9y, 5i9z, 5ia0, 5ia1, 5ia2, 5ia3, 5ia4, 5ia5, 5ie1, 5igm, 5ih9, 5ihh, 5ii2, 5ijr, 5ikb, 5ime, 5ioz, 5ipc, 5ipj, 5irr, 5isz, 5ito, 5itp, 5ivc, 5ive, 5ivv, 5ivy, 5iwg, 5izf, 5izj, 5j0d, 5j1r, 5j1x, 5j20, 5j27, 5j2x, 5j3l, 5j41, 5j64, 5j6a, 5j6l, 5j6m, 5j6n, 5j7q, 5j82, 5j86, 5j8m, 5j8u, 5j8z, 5j9x, 5ja0, 5jfp, 5jfu, 5jg1, 5jgi, 5jgq, 5jhb, 5jhk, 5ji8, 5jox, 5jq5, 5js3, 5jsg, 5jsj, 5jsq, 5jss, 5jt9, 5jvi, 5jxn, 5jxq, 5jy3, 5jzi, 5k03, 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5nwe, 5nwi, 5nxg, 5nxi, 5nxo, 5nxp, 5nxw, 5ny1, 5ny3, 5nya, 5nyh, 5nz4, 5nze, 5nzf, 5nzn, 5o07, 5o1d, 5o1f, 5o1h, 5o4f, 5o58, 5o5a, 5o87, 5o9o, 5o9p, 5o9q, 5o9r, 5o9y, 5oa2, 5oa6, 5oaj, 5obg, 5od1, 5odx, 5oei, 5ogb, 5oh3, 5oh4, 5oh7, 5oh9, 5oha, 5oht, 5ohy, 5oku, 5om2, 5om3, 5om7, 5op4, 5oq8, 5oqu, 5org, 5orh, 5orj, 5ork, 5orv, 5orw, 5os2, 5os4, 5os5, 5os7, 5ose, 5osl, 5oss, 5ost, 5ot8, 5ot9, 5ota, 5otc, 5otr, 5otz, 5ouh, 5ov8, 5ovc, 5ovp, 5ovr, 5ovv, 5ovx, 5owl, 5oxk, 5qa8, 5qay, 5qqp, 5qtt, 5std, 5sxm, 5sym, 5sz0, 5sz1, 5sz2, 5sz4, 5sz5, 5sz6, 5sz7, 5t19, 5t7s, 5t8o, 5t8p, 5t9u, 5t9w, 5t9z, 5ta2, 5ta4, 5tbe, 5tcj, 5tcy, 5tef, 5tfx, 5th4, 5ti0, 5tkj, 5tkk, 5tmp, 5tp0, 5tpx, 5tt3, 5ttw, 5tuo, 5tuz, 5txy, 5ty9, 5u0d, 5u0e, 5u0g, 5u0w, 5u0y, 5u0z, 5u11, 5u12, 5u13, 5u14, 5u28, 5u49, 5u4b, 5u4d, 5u6j, 5u8c, 5uc4, 5ucj, 5ueu, 5uez, 5uf0, 5ufc, 5uff, 5ufp, 5ufs, 5uk8, 5ula, 5uln, 5ulp, 5ult, 5umx, 5umy, 5uov, 5upe, 5upf, 5upj, 5upz, 5ut6, 5uxf, 5v0n, 5v79, 5v7a, 5v82, 5var, 5vb5, 5vb6, 5vb7, 5vc3, 5vc4, 5vcv, 5vcw, 5vcy, 5vd0, 5vd1, 5vd2, 5vd3, 5vgy, 5vi6, 5vih, 5vij, 5vja, 5vkc, 5vl2, 5vm0, 5vo1, 5vp9, 5vr8, 5vsf, 5vsj, 5vyy, 5w2s, 5w44, 5wa5, 5wa8, 5wa9, 5wal, 5wbm, 5wbo, 5wcm, 5we9, 5wex, 5wgp, 5wij, 5win, 5wl0, 5wlo, 5wp5, 5wqc, 5wxh, 5wyx, 5wyz, 5x54, 5x62, 5x74, 5xg5, 5xo7, 5xpi, 5xsr, 5xva, 5xvg, 5y12, 5y13, 5y8y, 5y94, 5ya5, 5yas, 5yfs, 5yft, 5yh8, 5yhe, 5yhg, 5yj8, 5yjm, 5yl2, 5ymx, 5yum, 5yyf, 5yz2, 5z5f, 5z66, 5z7b, 5z7j, 5z99, 5za7, 5za8, 5za9, 5zae, 5zaf, 5zag, 5zaj, 5zc5, 5zdb, 5zg0, 5zg1, 5zhl, 5zkc, 5znc, 5zni, 5zo8, 5zvw, 5zw6, 5zyg, 5zyl, 5zym, 6a87, 6abx, 6ajr, 6ajv, 6ajy, 6ajz, 6aox, 6aqs, 6arm, 6arn, 6aro, 6as8, 6ayi, 6ayo, 6ayq, 6ayr, 6ays, 6ayt, 6b1k, 6b4d, 6b4l, 6b4n, 6b4u, 6b59, 6b5q, 6b7a, 6b7b, 6b96, 6b97, 6b98, 6bbx, 6bdy, 6bhv, 6bm5, 6bm6, 6bs3, 6bs4, 6c0s, 6c2r, 6c7q, 6c7w, 6c7x, 6c85, 6c9s, 6c9v, 6cbf, 6cbg, 6cdj, 6cdl, 6cdo, 6cdp, 6ce6, 6ced, 6cfc, 6chp, 6cjr, 6cjs, 6cjv, 6ckr, 6cks, 6ckw, 6cn5, 6cpa, 6cpw, 6csp, 6csq, 6csr, 6css, 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| Validation | 1a4k, 1ai5, 1ajq, 1amk, 1b6k, 1bjv, 1bn4, 1bnu, 1bxr, 1c3x, 1d4y, 1det, 1dl7, 1e1x, 1ebz, 1erb, 1fcz, 1fd0, 1fh8, 1fki, 1fkn, 1ft7, 1gaf, 1gvw, 1gvx, 1jao, 1k1m, 1kyv, 1l8g, 1m0o, 1m4h, 1mai, 1mrw, 1mrx, 1mu8, 1n46, 1n5r, 1ndz, 1nw5, 1o2h, 1o86, 1ols, 1oyq, 1pfu, 1q65, 1qbv, 1ql7, 1s19, 1sb1, 1sdt, 1sln, 1t31, 1tq4, 1u1w, 1upf, 1v1j, 1v1m, 1wn6, 1xka, 1xkk, 1y1z, 1ydd, 1ype, 1zsf, 2b1i, 2bpv, 2brm, 2cgr, 2evl, 2fmb, 2g94, 2gv7, 2gzl, 2h6b, 2hs1, 2iko, 2j4g, 2jjb, 2o0u, 2oxy, 2p16, 2p3a, 2psv, 2pv1, 2qbu, 2qhy, 2qm9, 2rcn, 2rfh, 2v25, 2vb8, 2vh6, 2wc4, 2wky, 2wor, 2wuf, 2wyf, 2wzs, 2x97, 2xp7, 2y7x, 2y8c, 2ya7, 2yi7, 3aho, 3bgc, 3bgs, 3bxf, 3c56, 3ccz, 3cdb, 3cyx, 3d51, 3d6p, 3d8w, 3dp9, 3dx3, 3e5u, 3eeb, 3ejp, 3ekx, 3exh, 3f17, 3f68, 3ffp, 3fql, 3fx6, 3h1x, 3hvj, 3ibi, 3ifl, 3ipu, 3lxe, 3mhw, 3nuj, 3nyx, 3ok9, 3p3t, 3p58, 3pcn, 3pgu, 3pn4, 3qox, 3rz0, 3rz7, 3s45, 3sug, 3sus, 3tfp, 3uil, 3upv, 3zcl, 3zns, 4abb, 4bb9, 4cfl, 4czs, 4dmw, 4dv8, 4e7r, 4elf, 4erf, 4ezx, 4ffs, 4fm7, 4g0z, 4g95, 4gql, 4ido, 4igt, 4io3, 4jfm, 4jsa, 4k4j, 4l50, 4llk, 4lov, 4m0e, 4m14, 4mrg, 4n6g, 4o61, 4oc0, 4pg9, 4phu, 4pmm, 4pow, 4q19, 4q7w, 4q8y, 4qdk, 4qgi, 4qsv, 4rlu, 4ruz, 4sga, 4u5o, 4uof, 4w9o, 4wk1, 4wov, 4x48, 4x5q, 4x6o, 4xu2, 4yk0, 4yyt, 4zx3, 5aa9, 5afv, 5am6, 5d48, 5dh5, 5dus, 5e8f, 5eek, 5efh, 5eqp, 5er2, 5evb, 5f61, 5f9b, 5fe7, 5fut, 5g45, 5h8g, 5hi7, 5htz, 5ix0, 5iyy, 5j7w, 5jop, 5k8s, 5kly, 5kr1, 5l4i, 5llh, 5lud, 5m5d, 5m7u, 5mkr, 5mrm, 5n99, 5ngz, 5njz, 5nk8, 5nkd, 5nw7, 5o2d, 5oh2, 5oot, 5op5, 5os8, 5qal, 5sz3, 5tb6, 5tbm, 5twj, 5tya, 5u0f, 5ufr, 5uoo, 5uv2, 5vcz, 5vh0, 5voj, 5w1e, 5wmg, 5wuk, 5xmx, 5yqx, 5zg3, 6cq1, 6d1b, 6dar, 6det, 6e6m, 6e7r, 6f90, 6fe0, 6ftw, 6fv4, 6g24, 6gj8, 6gji, 6hhr, 6i5g, 6ibk, 6ior, 6jao, 6jaq, 6mj4, 6mlj, 6mm2, 6n5x, 6pid, 6qge, 6r1a, 6t1j, 2rk8 |
| Test | 1a30, 1bcu, 1bzc, 1c5z, 1e66, 1eby, 1g2k, 1gpk, 1gpn, 1h22, 1h23, 1k1i, 1lpg, 1mq6, 1nc1, 1nc3, 1nvq, 1o0h, 1o3f, 1o5b, 1owh, 1oyt, 1p1n, 1p1q, 1ps3, 1pxn, 1q8t, 1q8u, 1qf1, 1qkt, 1r5y, 1s38, 1sqa, 1syi, 1u1b, 1uto, 1vso, 1w4o, 1y6r, 1yc1, 1ydr, 1ydt, 1z6e, 1z95, 1z9g, 2al5, 2br1, 2brb, 2c3i, 2cbv, 2cet, 2fvd, 2fxs, 2hb1, 2iwx, 2j78, 2j7h, 2p15, 2p4y, 2pog, 2qbp, 2qbq, 2qbr, 2qe4, 2qnq, 2r9w, 2v00, 2v7a, 2vkm, 2vvn, 2vw5, 2w4x, 2w66, 2wbg, 2wca, 2weg, 2wer, 2wn9, 2wnc, 2wtv, 2wvt, 2x00, 2xb8, 2xbv, 2xdl, 2xii, 2xj7, 2xnb, 2xys, 2y5h, 2yfe, 2yge, 2yki, 2ymd, 2zb1, 2zcq, 2zcr, 2zda, 2zy1, 3acw, 3ag9, 3ao4, 3arp, 3arq, 3aru, 3arv, 3ary, 3b1m, 3b27, 3b5r, 3b65, 3b68, 3bgz, 3bv9, 3cj4, 3coy, 3coz, 3d4z, 3d6q, 3dd0, 3dx1, 3dx2, 3dxg, 3e5a, 3e92, 3e93, 3ebp, 3ehy, 3ejr, 3f3a, 3f3c, 3f3d, 3f3e, 3fcq, 3fur, 3fv1, 3fv2, 3g0w, 3g2n, 3g2z, 3g31, 3gbb, 3gc5, 3ge7, 3gnw, 3gr2, 3gv9, 3gy4, 3ivg, 3jvr, 3jvs, 3jya, 3k5v, 3kgp, 3kr8, 3kwa, 3l7b, 3lka, 3mss, 3myg, 3n76, 3n7a, 3n86, 3nq9, 3nw9, 3nx7, 3o9i, 3oe4, 3oe5, 3ozs, 3ozt, 3p5o, 3prs, 3pww, 3pxf, 3pyy, 3qgy, 3qqs, 3r88, 3rlr, 3rr4, 3rsx, 3ryj, 3syr, 3tsk, 3twp, 3u5j, 3u8k, 3u8n, 3u9q, 3udh, 3ueu, 3uev, 3uew, 3uex, 3ui7, 3uo4, 3up2, 3uri, 3utu, 3uuo, 3wtj, 3wz8, 3zdg, 3zso, 3zsx, 3zt2, 4abg, 4agn, 4agp, 4agq, 4bkt, 4cig, 4ciw, 4cr9, 4cra, 4crc, 4ddh, 4ddk, 4de1, 4de2, 4de3, 4djv, 4dld, 4dli, 4e5w, 4e6q, 4ea2, 4eky, 4eo8, 4eor, 4f09, 4f2w, 4f3c, 4f9w, 4gfm, 4gid, 4gkm, 4gr0, 4hge, 4ih5, 4ih7, 4ivb, 4ivc, 4ivd, 4j21, 4j28, 4j3l, 4jfs, 4jia, 4jsz, 4jxs, 4k18, 4k77, 4kz6, 4kzq, 4kzu, 4llx, 4lzs, 4m0y, 4m0z, 4mgd, 4mme, 4ogj, 4owm, 4pcs, 4qac, 4qd6, 4rfm, 4tmn, 4twp, 4ty7, 4u4s, 4w9c, 4w9h, 4w9i, 4w9l, 4wiv, 4x6p, 5a7b, 5aba, 5c28, 5c2h, 5dwr, 5tmn |

Table S2- The interested hyperparameters of the XGB algorithm and their ranges for fine-tuning by the Optuna package. For the meaning of each hyperparameter, refer to the XGBoost website at https://xgboost.readthedocs.io/. The Optimize column designates which hyperparameters should be optimized. The rest of the hyperparameters are set to their default values of the XGBoost package.

|  |  |  |
| --- | --- | --- |
| Hyperparameter | Suggested Value | Optimize |
| objective | reg:squarederror | False |
| verbosity | 0 | False |
| device | cuda | False |
| tree\_method | hist | False |
| n\_estimators | 100-20000 | True |
| learning\_rate | 0.001-0.1 | True |
| max\_depth | 1-10 | True |
| subsample | 0.05-1.0 | True |
| colsample\_bytree | 0.05-1.0 | True |
| min\_child\_weight | 1-20 | True |