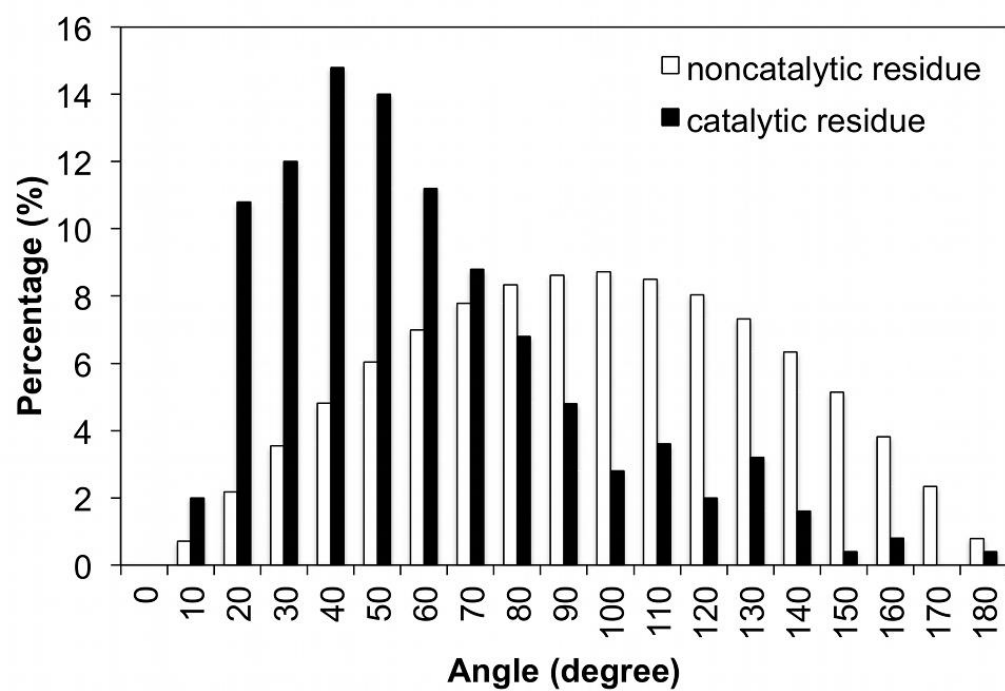
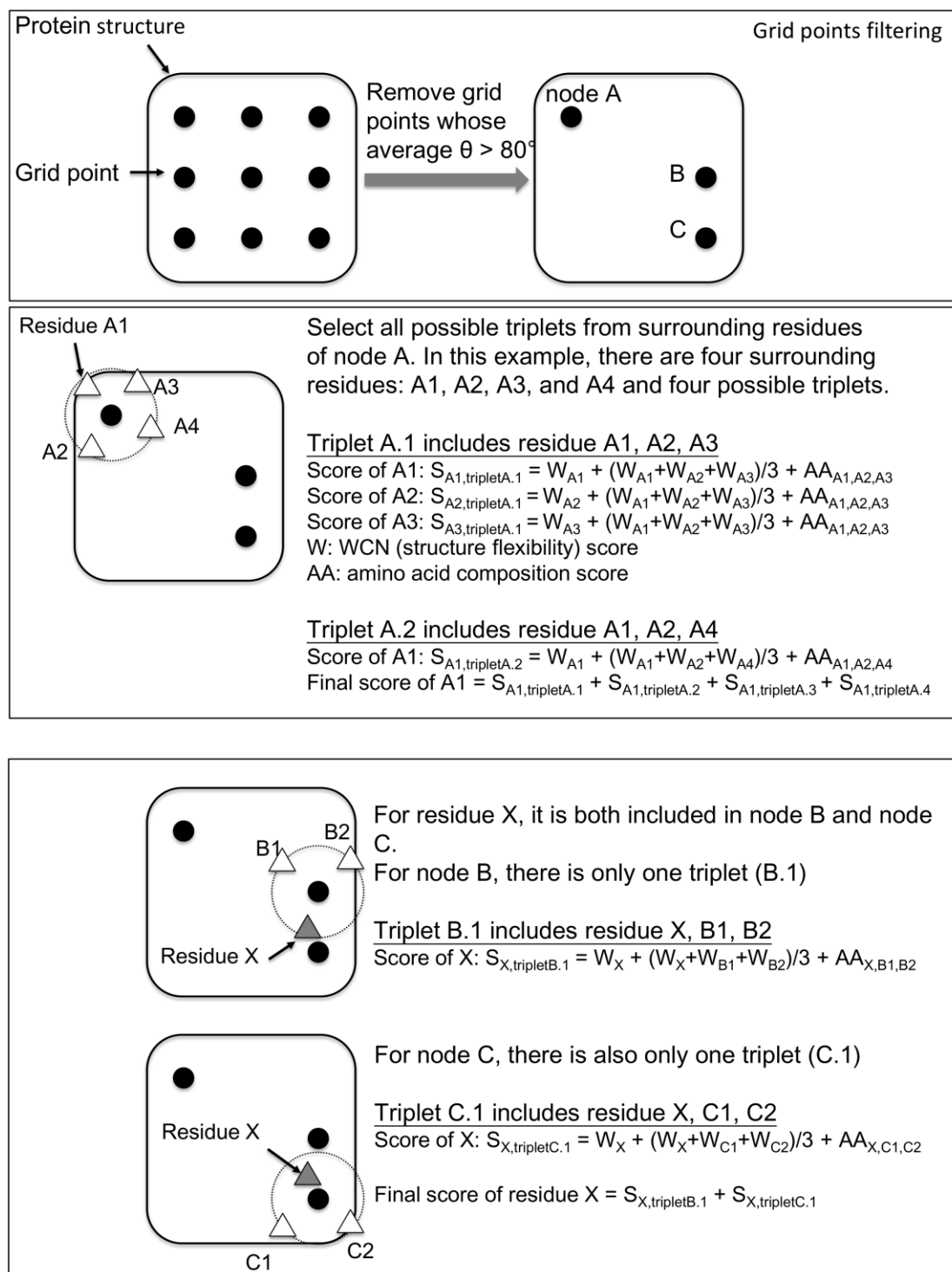


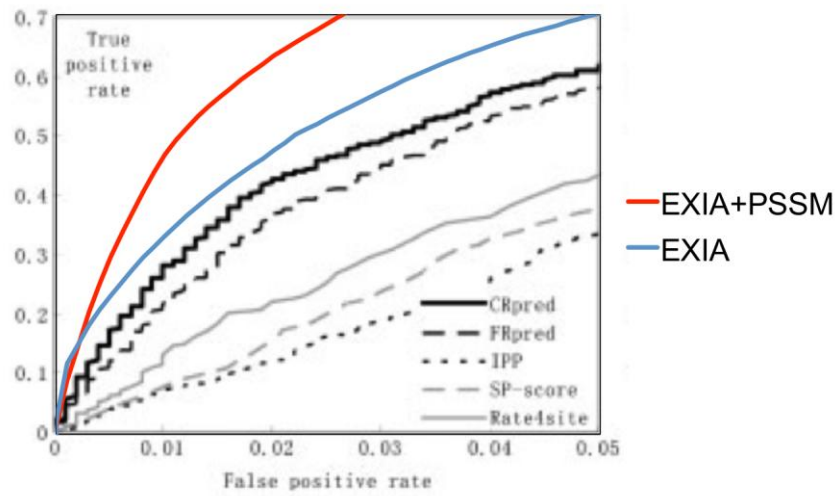
**Figure S1 Side chain orientation for catalytic and noncatalytic residues of PW79 dataset**



**Figure S2 Examples of triplet selection and score calculations**

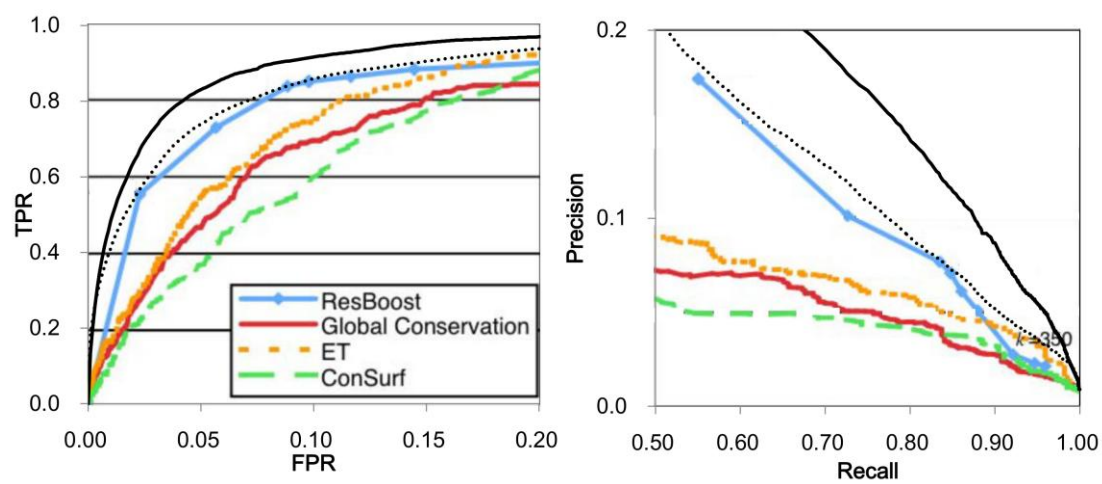


**Figure S3 Comparison of ROC curves of EXIA and CRpred**



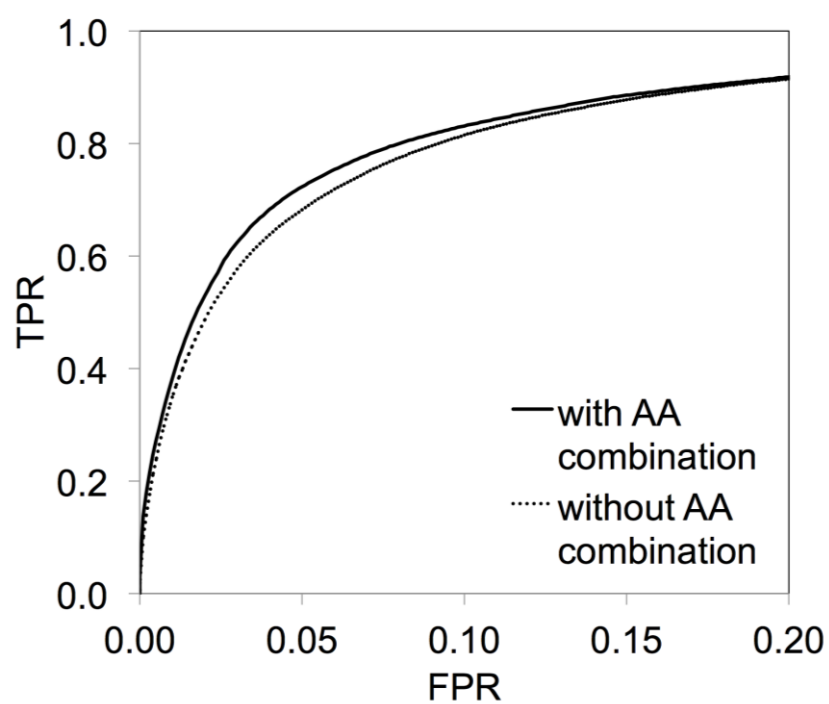
ROC curves of EXIA superimposed with that reported by CRpred.

**Figure S4 Comparison of ROC and RP curves of EXIA, ResBoost, and ConSurf**



Black solid lines: EXIA+PSSM; black dotted lines: EXIA

**Figure S5 ROC curve of prediction with and without amino acid combination feature on the EX79 dataset**



**Table S1 List of PDB IDs and chain for 55 pairs of structures of the L55 dataset**

<b>PDB IDs and Chain of L55 Dataset</b>			
<b>Unbounded structure</b>	<b>Bounded Structure</b>	<b>Unbounded structure</b>	<b>Bounded Structure</b>
1a4s_a	1bpw_a	1kra_c	1krb_c
1a4y_b	4aoh_a	1l6p_a	3pfu_a
1a6d_a	1a6e_a	1l7d_a	1f8g_a
1ab4_a	2y3p_a	1lci_a	1ba3_a
1akm_a	1duv_a	1lxa_a	2qiv_x
1ako_a	2voa_a	1m53_a	2pwg_a
1aug_a	3ro0_a	1mla_a	2g2o_a
1auo_a	1aur_a	1pgs_a	1pnf_a
1b65_a	3n2w_a	1pjb_a	1say_a
1b6b_a	1cjw_a	1pma_b	1yar_h
1b73_a	1b74_a	1qfn_a	1grx_a
1bml_a	1l4d_a	1smn_a	1g8t_a
1bo1_a	2ybx_a	1tyf_a	1yg6_a
1brm_a	1gl3_a	1uch_a	1xd3_a
1bwp_a	1wab_a	1uok_a	4aie_a
1c4z_a	ld5f_a	1vie_a	1vif_a
1cd5_a	1fs5_a	1zym_a	3eze_a
1cz1_a	1eqc_a	2alr_a	3cv7_a
1db3_a	1t2a_a	2eng_a	3eng_a
1dco_a	1dch_a	2fok_a	1fok_a
1di1_a	1dgp_a	2plc_a	1aod_a
1esc_a	1esd_a	2pth_a	3vjr_a
1eug_a	3eug_a	1jfl_a	2dx7_a
1f2v_a	1i1h_a	1k30_a	1iuq_a
1fcq_a	1fcv_a	1k32_a	1n6e_a
1fug_a	1rg9_ab	1kas_a	1b3n_a
1g24_a	2a9k_b	1kfu_l	3bow_a
1geq_a	1wdw_a		

**Table S2**  
**List of PDB IDs and chains of EX79 dataset**

12asA  
13pkA  
1a05AB  
1a0iA  
1a41A  
1a4yB  
1a6dA  
1a79A  
1a8hA  
1a8qA  
1aa6A  
1ab4A  
1adnA  
1af7A  
1afrA  
1ak0A  
1akoA  
1alkA  
1am2A  
1apyB  
1aq0A  
1astA  
1augA  
1auiA  
1aukA  
1auoA  
1avqA  
1ax4A  
1b04A  
1b5qA  
1b5tA  
1b65A  
1b66B  
1b66A  
1b6gA  
1b73A  
1b9hA  
1bcrA  
1bd0AB  
1bd3A  
1bf2A  
1bfdA  
1bg0A

1bg6A  
1bhgA  
1bjpA  
1bmlA  
1bmtA  
1bo1A  
1bobA  
1booA  
1bouB  
1bqcA  
1brwA  
1bs0A  
1bwdA  
1bwpA  
1c17A  
1c3cAB  
1c3jA  
1c4xA  
1c4zA  
1cb8A  
1cc1LS  
1cf2O  
1cfrA  
1cg2A  
1chkA  
1chkB  
1chmA  
1cjwA  
1cjyA  
1cl1A  
1cmxA  
1coyA  
1cqqA  
1cs1AC  
1cvrA  
1cz1A  
1d0sA  
1d1qA  
1d2tA  
1d3gA  
1d4aA  
1d4cA  
1d5rA  
1d8cA  
1d8hA  
1dciA



1dekA  
1dgsA  
1dhpA  
1di1A  
1diiA  
1dinA  
1dkiA  
1dl2A  
1dl5A  
1dliA  
1dmuA  
1do8A  
1dpgA  
1dqaAB  
1dtwAB  
1dw9AF  
1dxmA  
1e0cA  
1e19A  
1e1aA  
1e2tA  
1e5qA  
1e7lAB  
1eb6A  
1ebfA  
1ecfA  
1ecmAB  
1eejA  
1eg7A  
1ehkAB  
1ehyA  
1ei5A  
1eq2A  
1escA  
1et0A  
1eu1A  
1eugA  
1eulA  
1f2dA  
1f2vA  
1f6dA  
1f75A  
1f7lA  
1f7uA  
1f8mA  
1f8rA

1fa0A  
1fcqA  
1fftF  
1fghA  
1fgjAB  
1fobA  
1fohA  
1fr2B  
1froA  
1fugA  
1fuiA  
1g0dA  
1g24A  
1g72A  
1g8fA  
1g8pA  
1g99A  
1ga8A  
1gdhA  
1gdoB  
1geqA  
1getAB  
1gogA  
1goxA  
1gp1A  
1gpjA  
1gq8A  
1gsaA  
1gt7A  
1gtpA  
1gtxA  
1h3iA  
1h4gA  
1h54A  
1hdhA  
1hfeM  
1hfsA  
1hr6B  
1hrkA  
1hv9B  
1hzdA  
1hzfA  
1i19A  
1i1iP  
1i6pA  
1i78A

1i7dA  
1i7qAB  
1i8dA  
1i8tB  
1ig8A  
1im5A  
1inpA  
1itxA  
1iu4A  
1ivhA  
1j09A  
1j79A  
1jchA  
1jflA  
1jh6A  
1jhfA  
1jkmA  
1jm6A  
1jmsA  
1jnrAB  
1jofA  
1jqnA  
1k0wA  
1k30A  
1k32A  
1k4tA  
1k82A  
1kdgA  
1kfuL  
1kl7A  
1knyA  
1kwsA  
1kyqA  
1kzhA  
1kzlA  
1l0oA  
1l1dA  
1l1lA  
1l6pA  
1l7dA  
1l9fA  
1l9xA  
1lamA  
1lbuA  
1lcbA  
1lciA

1ldmA  
1lmlA  
1ltqA  
1lucA  
1m53A  
1m6kA  
1masA  
1mekA  
1mhlAC  
1mhyD  
1mkaAB  
1mppA  
1mpxA  
1mt5A  
1mucA  
1mugA  
1nbfA  
1nf9A  
1ni4AD  
1nidA  
1nsjA  
1nvmA  
1nvtA  
1nw9B  
1nwwA  
1nzyA  
1o04A  
1o8aA  
1o98A  
1oacA  
1oe8A  
1ofdA  
1ofgA  
1otgA  
1p3dA  
1pbgA  
1pgsA  
1piiA  
1pknA  
1pmaB  
1pmiA  
1ps1A  
1psdA  
1pvdA  
1pyaA  
1pyaF

1pyaAEF  
1pymA  
1qamA  
1qazA  
1qbaA  
1qd1A  
1qd6CD  
1qdlAB  
1qe3A  
1qf6A  
1qfmA  
1qfnA  
1qgnA  
1qh5A  
1qhoA  
1qi9A  
1qj4A  
1qmhA  
1qprAB  
1qq5A  
1qtnA  
1qumA  
1r51A  
1ra2A  
1rblA  
1reqA  
1rhsA  
1rptA  
1rtuA  
1slmA  
1smlA  
1soxA  
1tdjA  
1thtA  
1tmlA  
1tyfA  
1uagA  
1uaqA  
1uasA  
1uchA  
1uroA  
1ushA  
1vaoA  
1vieA  
1vncA  
1xyzA

1ytwA  
1zioA  
1zymA  
2abkA  
2admA  
2ahjAB  
2aprA  
2ayhA  
2bmiA  
2dorA  
2ebnA  
2engA  
2fokA  
2gsaA  
2hdhA  
2nacA  
2nlrA  
2oatA  
2pdaA  
2pgdA  
2phkA  
2piaA  
2pthA  
2sqcA  
2thiA  
2tpsA  
3claA  
3csmA  
3mddA  
3pcaM  
4kbpA  
5coxA  
5enlA  
5fitA  
7odcA  
8tlnE  
9papA