

# KRAKEN ID 00000015

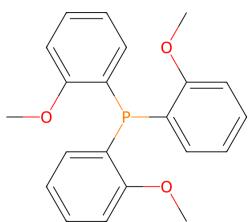


Table 1. Properties that exceed 1% relative difference

property	old	new	abs_diff	rel_diff (%)	squared_diff
vbur_ovtot_min_vbur_min_conf	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_vbur_min_conf	0.0	0.0	0.0	inf	0.0
vbur_ovtot_min_min	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_min	0.0	0.0	0.0	inf	0.0
vbur_near_vtot_delta	4.908	2.586	2.322	47.304	5.39
spindens_P_ra_boltz	0.021	0.024	0.003	16.909	0.0
vbur_vtot_delta	1.186	1.308	0.122	10.315	0.015
vbur_ovbur_min_max	0.041	0.038	0.003	7.692	0.0
vbur_ovbur_min_delta	0.041	0.038	0.003	7.692	0.0
vbur_ovbur_min_boltz	0.036	0.034	0.003	7.086	0.0
vbur_ovtot_min_max	0.219	0.213	0.006	2.926	0.0
vbur_ovtot_min_delta	0.219	0.213	0.006	2.926	0.0
E_reduction_boltz	0.025	0.026	0.001	2.9	0.0
somo_ra_boltz	0.068	0.07	0.002	2.776	0.0
vbur_ovtot_min_boltz	0.194	0.19	0.004	2.288	0.0
vbur_max_delta_qvbur_min	2.924	2.965	0.041	1.395	0.002
vbur_far_vbur_boltz	1.278	1.293	0.016	1.236	0.0
vbur_far_vbur_min	0.362	0.358	0.004	1.156	0.0
fukui_p_boltz	0.041	0.041	0.0	1.128	0.0

# KRAKEN ID 00000030

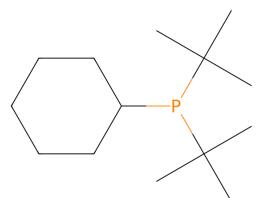


Table 1. Properties that exceed 1% relative difference

property	old	new	abs_diff	rel_diff (%)	squared_diff
vbur_far_vbur_boltz	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_max	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_vbur_min_conf	0.0	0.0	0.0	inf	0.0
vbur_far_vtot_vbur_min_conf	0.0	0.0	0.0	inf	0.0
vbur_far_vbur_vbur_min_conf	0.0	0.0	0.0	inf	0.0
vbur_overt_min_min	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_min	0.0	0.0	0.0	inf	0.0
vbur_far_vtot_min	0.0	0.0	0.0	inf	0.0
vbur_far_vbur_min	0.0	0.0	0.0	inf	0.0
vbur_overt_min_max	0.0	0.0	0.0	inf	0.0
vbur_far_vtot_max	0.0	0.0	0.0	inf	0.0
vbur_far_vtot_boltz	0.0	0.0	0.0	inf	0.0
vbur_far_vbur_max	0.0	0.0	0.0	inf	0.0
vbur_overt_min_delta	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_delta	0.0	0.0	0.0	inf	0.0
vbur_far_vtot_delta	0.0	0.0	0.0	inf	0.0
vbur_far_vbur_delta	0.0	0.0	0.0	inf	0.0
vbur_overt_min_boltz	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_boltz	0.0	0.0	0.0	inf	0.0
vbur_overt_min_vbur_min_conf	0.0	0.0	0.0	inf	0.0
vbur_vtot_delta	0.889	0.862	0.027	3.025	0.001

# KRAKEN ID 00000062

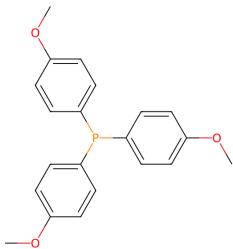


Table 1. Properties that exceed 1% relative difference

property	old	new	abs_diff	rel_diff (%)	squared_diff
vbur_ovtot_min_vbur_min_conf	0.0	0.0	0.0	inf	0.0
vbur_ovtot_min_min	0.0	0.0	0.0	inf	0.0
vbur_far_vtot_max	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_max	0.0	0.0	0.0	inf	0.0
vbur_ovtot_min_max	0.0	0.0	0.0	inf	0.0
vbur_ovtot_min_delta	0.0	0.0	0.0	inf	0.0
vbur_far_vbur_min	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_delta	0.0	0.0	0.0	inf	0.0
vbur_far_vtot_min	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_min	0.0	0.0	0.0	inf	0.0
vbur_far_vbur_max	0.0	0.0	0.0	inf	0.0
vbur_far_vbur_delta	0.0	0.0	0.0	inf	0.0
vbur_far_vtot_delta	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_boltz	0.0	0.0	0.0	inf	0.0
vbur_far_vbur_boltz	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_vbur_min_conf	0.0	0.0	0.0	inf	0.0
vbur_ovtot_min_boltz	0.0	0.0	0.0	inf	0.0
vbur_far_vbur_vbur_min_conf	0.0	0.0	0.0	inf	0.0
vbur_far_vtot_vbur_min_conf	0.0	0.0	0.0	inf	0.0
vbur_far_vtot_boltz	0.0	0.0	0.0	inf	0.0
pyr_P_delta	0.0	0.001	0.0	46.224	0.0
pyr_alpha_delta	0.055	0.08	0.025	46.084	0.001
qpoletens_yy_boltz	1.067	1.468	0.4	37.518	0.16
vbur_qvbur_min_delta	0.077	0.098	0.021	27.027	0.0
vbur_vtot_delta	0.146	0.123	0.023	15.522	0.001
vbur_near_vbur_delta	0.15	0.128	0.022	14.685	0.0

vbur_vbur_delta	0.15	0.128	0.022	14.685	0.0
vbur_max_delta_qvbur_delta	0.224	0.255	0.031	14.019	0.001
vbur_near_vtot_delta	1.325	1.223	0.101	7.652	0.01
sterimol_burB5_delta	0.017	0.018	0.001	7.249	0.0
dipolemoment_boltz	2.635	2.5	0.135	5.138	0.018
vbur_qvbur_max_delta	0.177	0.169	0.007	4.142	0.0
vbur_ovbur_max_delta	0.177	0.169	0.007	4.142	0.0
vbur_max_delta_qvtot_delta	10.708	10.368	0.339	3.17	0.115
qpoletens_xx_min	0.531	0.516	0.015	2.749	0.0
qpoletens_xx_vbur_min_conf	0.531	0.516	0.015	2.749	0.0
vbur_max_delta_qvbur_min	1.313	1.279	0.033	2.55	0.001
qpoletens_xx_boltz	8.897	8.674	0.223	2.509	0.05
vbur_qvtot_min_delta	10.071	9.82	0.251	2.496	0.063
qpole_amp_vbur_min_conf	1.225	1.196	0.029	2.383	0.001
qpole_amp_min	1.225	1.196	0.029	2.383	0.001
qpoletens_zz_vbur_min_conf	-0.999	-0.976	0.024	2.375	0.001
qpoletens_zz_max	-0.999	-0.976	0.024	2.375	0.001
sterimol_burL_delta	0.042	0.041	0.001	2.01	0.0
qpoletens_yy_vbur_min_conf	0.469	0.459	0.009	1.951	0.0
qpoletens_zz_boltz	-9.964	-10.141	0.177	1.778	0.031
qpoletens_yy_max	6.814	6.932	0.119	1.742	0.014
vbur_max_delta_qvbur_boltz	1.439	1.415	0.024	1.689	0.001
qpoletens_yy_delta	8.385	8.504	0.119	1.414	0.014
vbur_ovtot_max_delta	0.885	0.898	0.012	1.397	0.0
vbur_qvtot_max_delta	0.885	0.898	0.012	1.397	0.0
vbur_max_delta_qvbur_vbur_min_conf	1.313	1.329	0.017	1.275	0.0

# KRAKEN ID 00000068

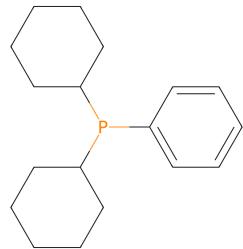


Table 1. Properties that exceed 1% relative difference

property	old	new	abs_diff	rel_diff (%)	squared_diff
vbur_ovtot_min_vbur_min_conf	0.0	0.0	0.0	inf	0.0
vbur_ovtot_min_min	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_max	0.0	0.0	0.0	inf	0.0
vbur_ovtot_min_max	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_delta	0.0	0.0	0.0	inf	0.0
vbur_far_vtot_min	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_min	0.0	0.0	0.0	inf	0.0
vbur_far_vbur_min	0.0	0.0	0.0	inf	0.0
vbur_far_vbur_vbur_min_conf	0.0	0.0	0.0	inf	0.0
vbur_far_vtot_vbur_min_conf	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_vbur_min_conf	0.0	0.0	0.0	inf	0.0
vbur_ovtot_min_boltz	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_boltz	0.0	0.0	0.0	inf	0.0
vbur_ovtot_min_delta	0.0	0.0	0.0	inf	0.0
vbur_qvbur_min_delta	2.8	4.96	2.16	77.139	4.665
sterimol_L_delta	0.202	0.353	0.151	74.895	0.023
vbur_vbur_delta	17.642	29.166	11.524	65.319	132.797
vbur_near_vbur_delta	12.555	20.257	7.702	61.346	59.321
sterimol_burL_delta	0.217	0.331	0.115	52.868	0.013
vbur_far_vtot_max	10.156	15.152	4.996	49.189	24.958
vbur_far_vtot_delta	10.156	15.152	4.996	49.189	24.958
vbur_far_vbur_max	6.291	8.909	2.618	41.613	6.853
vbur_far_vbur_delta	6.291	8.909	2.618	41.613	6.853
vbur_near_vtot_delta	14.28	18.809	4.529	31.714	20.51
dipolemoment_delta	0.228	0.279	0.051	22.364	0.003
vbur_qvtot_max_delta	7.411	9.065	1.654	22.322	2.737

vbur_ovtot_max_delta	8.502	10.27	1.768	20.791	3.125
vbur_vbur_max	69.443	80.962	11.52	16.589	132.701
vbur_qvbur_min_max	12.813	14.882	2.069	16.146	4.28
sterimol_B5_delta	0.485	0.551	0.066	13.608	0.004
qpoletens_yy_min	-0.641	-0.725	0.084	13.126	0.007
vbur_far_vtot_boltz	0.827	0.929	0.102	12.324	0.01
vbur_near_vbur_max	64.356	72.053	7.698	11.961	59.257
vbur_far_vbur_boltz	0.404	0.451	0.047	11.61	0.002
qpoletens_zz_max	-2.446	-2.176	0.27	11.041	0.073
vbur_max_delta_qvbur_delta	12.552	11.346	1.206	9.608	1.454
vbur_max_delta_qvbur_max	15.58	14.143	1.437	9.224	2.065
vbur_vtot_delta	0.895	0.816	0.079	8.834	0.006
vbur_max_delta_qvtot_delta	29.315	31.818	2.503	8.539	6.267
vbur_max_delta_qvbur_min	3.028	2.797	0.231	7.634	0.053
qpoletens_yy_delta	2.957	3.176	0.219	7.406	0.048
vbur_qvtot_min_delta	26.491	28.349	1.858	7.015	3.453
qpole_amp_min	3.966	3.696	0.27	6.802	0.073
qpoletens_yy_max	2.316	2.451	0.135	5.823	0.018
qpoletens_zz_delta	3.8	4.008	0.208	5.462	0.043
vbur_max_delta_qvtot_max	55.604	58.116	2.512	4.518	6.311
qpole_amp_delta	3.769	3.932	0.163	4.313	0.026
sterimol_B1_delta	1.154	1.108	0.045	3.93	0.002
qpoletens_xx_min	2.829	2.724	0.105	3.711	0.011
dipolemoment_min	1.176	1.136	0.04	3.395	0.002
vbur_qvbur_max_delta	13.062	13.388	0.325	2.49	0.106
qpoletens_xx_max	3.93	3.834	0.096	2.447	0.009
pyr_alpha_delta	9.064	9.258	0.193	2.131	0.037
vbur_qvtot_min_max	63.917	65.259	1.342	2.1	1.802
sterimol_burL_min	7.182	7.065	0.117	1.63	0.014
sterimol_L_min	7.659	7.537	0.122	1.597	0.015
vbur_near_vtot_min	304.256	299.606	4.65	1.528	21.623
sterimol_burB5_delta	0.451	0.444	0.006	1.433	0.0
qpole_amp_max	7.735	7.628	0.107	1.386	0.011
vbur_qvtot_min_min	37.426	36.91	0.516	1.379	0.266
vbur_qvtot_max_max	100.829	102.188	1.359	1.348	1.848

vbur_ovtot_max_max	100.829	102.188	1.359	1.348	1.848
sterimol_B1_min	3.44	3.484	0.044	1.285	0.002
sterimol_burB1_min	3.44	3.484	0.044	1.285	0.002
sterimol_burB1_max	4.481	4.537	0.057	1.263	0.003
pyr_alpha_min	15.795	15.601	0.194	1.228	0.038
sterimol_burB1_delta	1.041	1.053	0.012	1.187	0.0
vbur_qvbur_max_max	27.897	28.208	0.311	1.113	0.096
sterimol_B5_min	6.325	6.258	0.067	1.056	0.004
qpoletens_zz_min	-6.246	-6.184	0.062	1.001	0.004

# KRAKEN ID 00000069

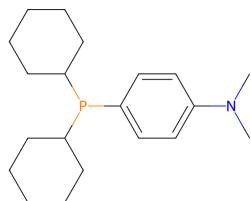


Table 1. Properties that exceed 1% relative difference

property	old	new	abs_diff	rel_diff (%)	squared_diff
vbur_ovtot_min_vbur_min_conf	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_min	0.0	0.0	0.0	inf	0.0
vbur_ovtot_min_delta	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_delta	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_max	0.0	0.0	0.0	inf	0.0
vbur_far_vbur_min	0.0	0.0	0.0	inf	0.0
vbur_far_vtot_min	0.0	0.0	0.0	inf	0.0
vbur_ovtot_min_max	0.0	0.0	0.0	inf	0.0
vbur_ovtot_min_min	0.0	0.0	0.0	inf	0.0
vbur_far_vbur_vbur_min_conf	0.0	0.0	0.0	inf	0.0
vbur_far_vtot_vbur_min_conf	0.0	0.0	0.0	inf	0.0
vbur_ovtot_min_boltz	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_boltz	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_vbur_min_conf	0.0	0.0	0.0	inf	0.0
vbur_qvbur_min_delta	2.841	5.019	2.179	76.694	4.746
vbur_vbur_delta	17.403	28.775	11.372	65.346	129.325
vbur_near_vbur_delta	12.43	20.34	7.91	63.64	62.571
vbur_near_vtot_delta	11.555	18.865	7.31	63.267	53.44
vbur_far_vbur_delta	6.001	8.435	2.434	40.554	5.923
vbur_far_vbur_max	6.001	8.435	2.434	40.554	5.923
vbur_far_vtot_max	10.234	14.314	4.08	39.866	16.646
vbur_far_vtot_delta	10.234	14.314	4.08	39.866	16.646
vbur_vtot_delta	0.982	0.687	0.295	30.067	0.087
sterimol_burL_delta	0.438	0.344	0.095	21.628	0.009
qpoletens_xx_delta	1.211	1.45	0.24	19.789	0.057
vbur_qvbur_min_max	12.756	14.934	2.179	17.079	4.746

vbur_vbur_max	69.29	80.662	11.372	16.412	129.325
vbur_near_vbur_max	64.317	72.227	7.91	12.299	62.571
sterimol_burB5_delta	0.456	0.407	0.049	10.685	0.002
qpole_amp_delta	1.924	2.115	0.191	9.927	0.036
sterimol_burB1_delta	0.693	0.629	0.065	9.317	0.004
vbur_far_vbur_boltz	0.446	0.406	0.04	8.991	0.002
vbur_qvtot_min_delta	23.677	21.556	2.121	8.958	4.499
pyr_alpha_delta	9.415	10.081	0.666	7.075	0.444
vbur_qvtot_min_min	41.19	44.071	2.88	6.993	8.297
vbur_far_vtot_boltz	0.927	0.864	0.063	6.803	0.004
pyr_P_delta	0.075	0.079	0.004	5.852	0.0
pyr_alpha_min	16.452	15.782	0.67	4.071	0.449
sterimol_L_delta	0.751	0.732	0.02	2.599	0.0
qpolelens_xx_min	10.816	10.58	0.236	2.179	0.056
vbur_max_delta_qvbur_boltz	4.195	4.106	0.089	2.112	0.008
vbur_max_delta_qvbur_min	3.017	3.079	0.062	2.045	0.004
vbur_near_vtot_min	354.963	347.754	7.209	2.031	51.969
sterimol_burL_min	6.906	7.027	0.122	1.763	0.015
vbur_qvbur_max_delta	12.673	12.874	0.201	1.585	0.04
sterimol_burB1_max	4.47	4.406	0.065	1.447	0.004
qpole_amp_min	13.657	13.465	0.192	1.406	0.037
dipolemoment_delta	0.809	0.799	0.01	1.297	0.0
vbur_qvtot_min_max	64.867	65.627	0.759	1.171	0.577

# KRAKEN ID 00000079

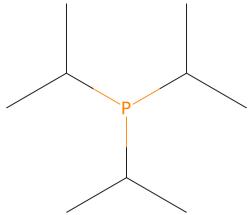


Table 1. Properties that exceed 1% relative difference

property	old	new	abs_diff	rel_diff (%)	squared_diff
vbur_ovtot_min_delta	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_delta	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_vbur_min_conf	0.0	0.0	0.0	inf	0.0
vbur_far_vtot_vbur_min_conf	0.0	0.0	0.0	inf	0.0
vbur_far_vbur_vbur_min_conf	0.0	0.0	0.0	inf	0.0
vbur_ovtot_min_min	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_min	0.0	0.0	0.0	inf	0.0
vbur_far_vtot_min	0.0	0.0	0.0	inf	0.0
vbur_far_vbur_min	0.0	0.0	0.0	inf	0.0
vbur_ovtot_min_max	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_max	0.0	0.0	0.0	inf	0.0
vbur_far_vtot_max	0.0	0.0	0.0	inf	0.0
vbur_far_vbur_max	0.0	0.0	0.0	inf	0.0
vbur_ovtot_min_vbur_min_conf	0.0	0.0	0.0	inf	0.0
vbur_far_vtot_delta	0.0	0.0	0.0	inf	0.0
vbur_far_vbur_delta	0.0	0.0	0.0	inf	0.0
vbur_ovtot_min_boltz	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_boltz	0.0	0.0	0.0	inf	0.0
vbur_far_vtot_boltz	0.0	0.0	0.0	inf	0.0
vbur_far_vbur_boltz	0.0	0.0	0.0	inf	0.0
vbur_near_vtot_delta	1.813	2.394	0.581	32.015	0.337
vbur_vtot_delta	1.617	1.675	0.058	3.588	0.003
spindens_P_ra_boltz	0.061	0.059	0.002	3.124	0.0
qpoletens_yy_boltz	0.901	0.878	0.024	2.631	0.001
fukui_p_boltz	0.049	0.048	0.001	1.878	0.0
vbur_max_delta_qvbur_boltz	3.835	3.879	0.043	1.134	0.002

qpoletens_zz_boltz	-2.365	-2.339	0.027	1.129	0.001
qpole_amp_boltz	2.94	2.909	0.031	1.044	0.001

# KRAKEN ID 00000084

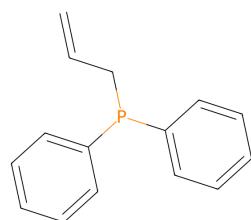


Table 1. Properties that exceed 1% relative difference

property	old	new	abs_diff	rel_diff (%)	squared_diff
vbur_ovtot_min_vbur_min_conf	0.0	0.0	0.0	inf	0.0
vbur_far_vbur_vbur_min_conf	0.0	0.0	0.0	inf	0.0
vbur_far_vtot_min	0.0	0.0	0.0	inf	0.0
vbur_far_vbur_min	0.0	0.0	0.0	inf	0.0
vbur_ovtot_min_max	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_max	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_boltz	0.0	0.0	0.0	inf	0.0
vbur_far_vtot_vbur_min_conf	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_min	0.0	0.0	0.0	inf	0.0
vbur_ovtot_min_min	0.0	0.0	0.0	inf	0.0
vbur_ovtot_min_delta	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_delta	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_vbur_min_conf	0.0	0.0	0.0	inf	0.0
vbur_ovtot_min_boltz	0.0	0.0	0.0	inf	0.0
vbur_near_vtot_delta	2.645	3.288	0.643	24.299	0.413
vbur_qvtot_min_delta	12.5	13.745	1.244	9.954	1.548
vbur_max_delta_qvtot_delta	18.13	19.834	1.703	9.395	2.901
vbur_qvtot_min_min	29.433	28.192	1.24	4.214	1.538
vbur_vtot_delta	1.282	1.333	0.051	3.949	0.003
vbur_max_delta_qvtot_max	60.113	61.816	1.703	2.833	2.899
vbur_far_vbur_max	0.501	0.493	0.008	1.67	0.0
vbur_far_vbur_delta	0.501	0.493	0.008	1.67	0.0
vbur_far_vbur_boltz	0.021	0.02	0.0	1.525	0.0

# KRAKEN ID 00000104

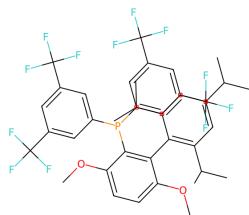


Table 1. Properties that exceed 1% relative difference

property	old	new	abs_diff	rel_diff (%)	squared_diff
vbur_ovtot_min_min	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_min	0.0	0.0	0.0	inf	0.0
vbur_ovtot_min_vbur_min_conf	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_vbur_min_conf	0.0	0.0	0.0	inf	0.0
qpoletens_yy_vbur_min_conf	-0.245	0.528	0.773	315.647	0.598
vbur_far_vbur_vbur_min_conf	0.866	2.661	1.795	207.246	3.221
vbur_max_delta_qvbur_vbur_min_conf	7.012	10.837	3.825	54.55	14.63
vbur_far_vtot_vbur_min_conf	13.512	16.737	3.226	23.873	10.404
vbur_ovbur_min_boltz	0.1	0.077	0.024	23.674	0.001
sterimol_B5_delta	1.526	1.869	0.343	22.498	0.118
qpoletens_yy_boltz	-0.409	-0.49	0.081	19.672	0.006
vbur_qvbur_max_vbur_min_conf	19.35	22.241	2.891	14.94	8.357
vbur_vtot_delta	6.568	5.656	0.912	13.892	0.833
sterimol_B5_vbur_min_conf	9.176	7.991	1.185	12.913	1.404
pyr_P_delta	0.055	0.048	0.007	12.884	0.0
pyr_alpha_delta	6.057	5.335	0.721	11.91	0.52
qpoletens_yy_min	-3.784	-3.341	0.443	11.709	0.196
vbur_qvtot_min_delta	33.538	29.85	3.688	10.997	13.602
vbur_far_vbur_min	0.866	0.955	0.089	10.266	0.008
qpoletens_yy_delta	5.102	4.672	0.43	8.427	0.185
qpoletens_zz_vbur_min_conf	-14.71	-15.69	0.98	6.664	0.961
sterimol_L_vbur_min_conf	9.579	10.168	0.589	6.151	0.347
sterimol_burL_delta	1.26	1.188	0.072	5.721	0.005
vbur_ovbur_max_vbur_min_conf	18.729	19.781	1.052	5.618	1.107
vbur_qvtot_max_delta	34.621	36.52	1.899	5.486	3.608
vbur_qvbur_min_vbur_min_conf	11.915	11.288	0.626	5.258	0.392

sterimol_B1_delta	0.589	0.619	0.03	5.133	0.001
vbur_max_delta_qvtot_vbur_min_conf	142.698	149.056	6.358	4.455	40.421
qpole_amp_vbur_min_conf	20.978	21.825	0.847	4.038	0.717
sterimol_B5_max	9.289	9.643	0.354	3.81	0.125
qpoletens_zz_delta	3.999	4.148	0.15	3.742	0.022
dipolemoment_vbur_min_conf	6.722	6.963	0.241	3.58	0.058
vbur_vbur_delta	58.139	56.159	1.98	3.405	3.92
vbur_vbur_min	60.286	62.301	2.015	3.343	4.062
vbur_vbur_vbur_min_conf	60.286	62.301	2.015	3.343	4.062
qpoletens_zz_max	-12.096	-11.721	0.374	3.095	0.14
pyr_alpha_max	25.291	24.548	0.743	2.938	0.552
sterimol_burL_vbur_min_conf	8.319	8.087	0.232	2.791	0.054
vbur_max_delta_qvtot_delta	80.364	82.571	2.207	2.747	4.872
qpoletens_zz_boltz	-13.717	-13.349	0.368	2.681	0.135
somo_ra_boltz	0.012	0.011	0.0	2.627	0.0
sterimol_burB5_vbur_min_conf	7.3	7.486	0.187	2.558	0.035
vbur_far_vtot_min	10.952	10.672	0.279	2.551	0.078
sterimol_burB5_delta	0.78	0.761	0.019	2.485	0.0
qpole_amp_boltz	19.697	19.237	0.46	2.335	0.211
qpoletens_xx_boltz	14.126	13.839	0.287	2.033	0.083
sterimol_burB5_boltz	7.239	7.117	0.123	1.695	0.015
sterimol_burB1_vbur_min_conf	5.104	5.022	0.081	1.594	0.007
vbur_ovtot_max_min	179.936	177.154	2.782	1.546	7.738
vbur_qvtot_min_min	109.055	110.671	1.616	1.481	2.61
vbur_qvtot_min_max	142.594	140.521	2.073	1.453	4.295
qpoletens_zz_min	-16.094	-15.87	0.225	1.396	0.051
qpoletens_xx_vbur_min_conf	14.955	15.162	0.207	1.385	0.043
vbur_ovtot_max_delta	104.584	105.87	1.286	1.23	1.654
vbur_far_vtot_boltz	148.043	149.812	1.77	1.195	3.131
vbur_max_delta_qvtot_max	169.79	171.68	1.891	1.113	3.574
vbur_near_vtot_delta	141.301	142.821	1.521	1.076	2.312

# KRAKEN ID 00000116

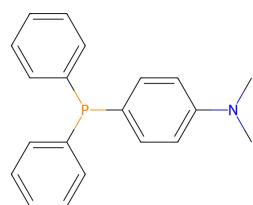


Table 1. Properties that exceed 1% relative difference

property	old	new	abs_diff	rel_diff (%)	squared_diff
vbur_far_vbur_boltz	0.0	0.0	0.0	inf	0.0
vbur_ovbur_max_delta	0.0	0.0	0.0	inf	0.0
vbur_ovtot_max_delta	0.0	0.0	0.0	inf	0.0
vbur_ovtot_min_delta	0.0	0.0	0.0	inf	0.0
vbur_qvbur_max_delta	0.0	0.0	0.0	inf	0.0
vbur_qvbur_min_delta	0.0	0.0	0.0	inf	0.0
vbur_qvtot_max_delta	0.0	0.0	0.0	inf	0.0
vbur_qvtot_min_delta	0.0	0.0	0.0	inf	0.0
vbur_vbur_delta	0.0	0.0	0.0	inf	0.0
vbur_vtot_delta	0.0	0.0	0.0	inf	0.0
vbur_far_vbur_max	0.0	0.0	0.0	inf	0.0
vbur_far_vtot_max	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_max	0.0	0.0	0.0	inf	0.0
vbur_ovtot_min_max	0.0	0.0	0.0	inf	0.0
vbur_far_vbur_min	0.0	0.0	0.0	inf	0.0
vbur_far_vtot_min	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_min	0.0	0.0	0.0	inf	0.0
vbur_ovtot_min_min	0.0	0.0	0.0	inf	0.0
vbur_far_vbur_vbur_min_conf	0.0	0.0	0.0	inf	0.0
vbur_far_vtot_vbur_min_conf	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_vbur_min_conf	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_delta	0.0	0.0	0.0	inf	0.0
vbur_near_vtot_delta	0.0	0.0	0.0	inf	0.0
vbur_far_vtot_boltz	0.0	0.0	0.0	inf	0.0
vbur_near_vbur_delta	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_boltz	0.0	0.0	0.0	inf	0.0

vbur_ovtot_min_boltz	0.0	0.0	0.0	inf	0.0
dipolemoment_delta	0.0	0.0	0.0	inf	0.0
pyr_P_delta	0.0	0.0	0.0	inf	0.0
pyr_alpha_delta	0.0	0.0	0.0	inf	0.0
qpole_amp_delta	0.0	0.0	0.0	inf	0.0
qpoletens_xx_delta	0.0	0.0	0.0	inf	0.0
qpoletens_yy_delta	0.0	0.0	0.0	inf	0.0
qpoletens_zz_delta	0.0	0.0	0.0	inf	0.0
sterimol_B1_delta	0.0	0.0	0.0	inf	0.0
sterimol_B5_delta	0.0	0.0	0.0	inf	0.0
sterimol_L_delta	0.0	0.0	0.0	inf	0.0
sterimol_burB1_delta	0.0	0.0	0.0	inf	0.0
sterimol_burB5_delta	0.0	0.0	0.0	inf	0.0
sterimol_burL_delta	0.0	0.0	0.0	inf	0.0
vbur_far_vbur_delta	0.0	0.0	0.0	inf	0.0
vbur_far_vtot_delta	0.0	0.0	0.0	inf	0.0
vbur_max_delta_qvbur_delta	0.0	0.0	0.0	inf	0.0
vbur_max_delta_qvtot_delta	0.0	0.0	0.0	inf	0.0
vbur_ovtot_min_vbur_min_conf	0.0	0.0	0.0	inf	0.0

# KRAKEN ID 00000130

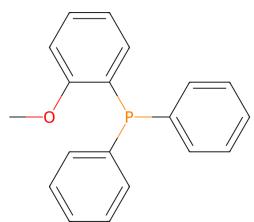


Table 1. Properties that exceed 1% relative difference

property	old	new	abs_diff	rel_diff (%)	squared_diff
vbur_ovbur_min_max	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_boltz	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_vbur_min_conf	0.0	0.0	0.0	inf	0.0
vbur_far_vtot_vbur_min_conf	0.0	0.0	0.0	inf	0.0
vbur_far_vbur_vbur_min_conf	0.0	0.0	0.0	inf	0.0
vbur_overt_min_min	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_min	0.0	0.0	0.0	inf	0.0
vbur_far_vtot_min	0.0	0.0	0.0	inf	0.0
vbur_far_vbur_min	0.0	0.0	0.0	inf	0.0
vbur_overt_min_max	0.0	0.0	0.0	inf	0.0
vbur_overt_min_vbur_min_conf	0.0	0.0	0.0	inf	0.0
vbur_overt_min_delta	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_delta	0.0	0.0	0.0	inf	0.0
vbur_overt_min_boltz	0.0	0.0	0.0	inf	0.0
vbur_near_vtot_delta	0.816	1.34	0.524	64.23	0.275
vbur_vtot_delta	0.928	0.909	0.019	2.085	0.0
vbur_far_vbur_max	0.172	0.175	0.003	1.829	0.0
vbur_far_vbur_delta	0.172	0.175	0.003	1.829	0.0
vbur_far_vbur_boltz	0.156	0.159	0.003	1.758	0.0
vmin_r_boltz	1.833	1.859	0.025	1.388	0.001
qpoletens_yy_max	-0.326	-0.322	0.003	1.022	0.0
qpoletens_yy_vbur_min_conf	-0.326	-0.322	0.003	1.022	0.0

# KRAKEN ID 00000139

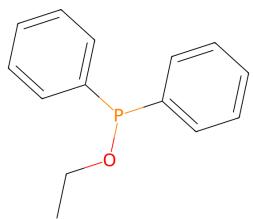


Table 1. Properties that exceed 1% relative difference

property	old	new	abs_diff	rel_diff (%)	squared_diff
vbur_ovbur_min_max	0.0	0.0	0.0	inf	0.0
vbur_overtot_min_max	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_vbur_min_conf	0.0	0.0	0.0	inf	0.0
vbur_far_vtot_vbur_min_conf	0.0	0.0	0.0	inf	0.0
vbur_far_vbur_vbur_min_conf	0.0	0.0	0.0	inf	0.0
vbur_overtot_min_min	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_min	0.0	0.0	0.0	inf	0.0
vbur_far_vtot_min	0.0	0.0	0.0	inf	0.0
vbur_far_vbur_min	0.0	0.0	0.0	inf	0.0
vbur_overtot_min_vbur_min_conf	0.0	0.0	0.0	inf	0.0
vbur_overtot_min_delta	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_delta	0.0	0.0	0.0	inf	0.0
vbur_overtot_min_boltz	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_boltz	0.0	0.0	0.0	inf	0.0
vbur_near_vtot_delta	2.605	3.044	0.438	16.829	0.192
vbur_far_vtot_boltz	0.798	0.772	0.026	3.287	0.001
vbur_far_vbur_boltz	0.477	0.462	0.015	3.165	0.0
vbur_vtot_delta	1.371	1.413	0.042	3.077	0.002
nmrtens_sxx_P_boltz	-14.658	-14.9	0.241	1.647	0.058

# KRAKEN ID 00000148

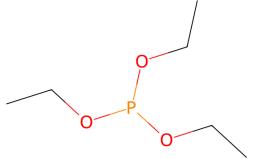


Table 1. Properties that exceed 1% relative difference

property	old	new	abs_diff	rel_diff (%)	squared_diff
vbur_ovtot_min_vbur_min_conf	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_min	0.0	0.0	0.0	inf	0.0
vbur_ovtot_min_delta	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_delta	0.0	0.0	0.0	inf	0.0
vbur_ovtot_min_max	0.0	0.0	0.0	inf	0.0
vbur_ovtot_min_boltz	0.0	0.0	0.0	inf	0.0
vbur_far_vbur_min	0.0	0.0	0.0	inf	0.0
vbur_far_vtot_min	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_boltz	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_max	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_vbur_min_conf	0.0	0.0	0.0	inf	0.0
vbur_far_vtot_vbur_min_conf	0.0	0.0	0.0	inf	0.0
vbur_ovtot_min_min	0.0	0.0	0.0	inf	0.0
vbur_far_vbur_vbur_min_conf	0.0	0.0	0.0	inf	0.0
vbur_far_vbur_boltz	0.014	0.023	0.01	69.214	0.0
vbur_far_vtot_boltz	0.018	0.024	0.006	30.134	0.0
vbur_near_vtot_delta	2.502	3.016	0.514	20.531	0.264
dipolemoment_min	0.577	0.682	0.104	18.06	0.011
dipolemoment_delta	1.246	1.058	0.188	15.118	0.036
qpoletens_xx_boltz	3.138	2.871	0.267	8.505	0.071
qpoletens_yy_boltz	1.411	1.506	0.095	6.753	0.009
vbur_max_delta_qvtot_boltz	27.392	25.684	1.707	6.233	2.915
dipolemoment_boltz	1.485	1.568	0.083	5.585	0.007
vbur_vtot_delta	0.535	0.565	0.029	5.472	0.001
qpoletens_zz_delta	1.636	1.546	0.089	5.458	0.008
vbur_max_delta_qvtot_delta	21.966	20.832	1.134	5.161	1.285

qpole_amp_boltz	5.741	5.459	0.282	4.91	0.079
dipolemoment_max	1.824	1.74	0.084	4.614	0.007
vbur_qvtot_min_boltz	27.072	28.165	1.093	4.037	1.195
qpoletens_zz_boltz	-4.549	-4.378	0.172	3.772	0.029
qpoletens_yy_min	-0.039	-0.04	0.001	3.246	0.0
vbur_max_delta_qvtot_max	36.704	35.568	1.137	3.096	1.292
vbur_near_vbur_delta	5.377	5.512	0.135	2.509	0.018
vbur_vbur_delta	5.587	5.714	0.127	2.265	0.016
vbur_far_vbur_delta	0.21	0.206	0.004	1.99	0.0
vbur_far_vbur_max	0.21	0.206	0.004	1.99	0.0
nbo_bds_occ_max_boltz	0.094	0.092	0.002	1.901	0.0
fukui_p_boltz	0.318	0.324	0.006	1.853	0.0
vbur_max_delta_qvbur_boltz	4.764	4.848	0.084	1.773	0.007
nmrtens_sxx_P_boltz	23.177	22.78	0.398	1.716	0.158
qpoletens_zz_min	-5.728	-5.638	0.09	1.57	0.008
spindens_P_ra_boltz	0.428	0.434	0.007	1.557	0.0
fmo_e_lumo_boltz	0.023	0.024	0.0	1.459	0.0
sterimol_burB5_delta	0.384	0.379	0.005	1.352	0.0
sterimol_B5_delta	0.384	0.379	0.005	1.352	0.0
sterimol_burB1_boltz	3.223	3.266	0.044	1.35	0.002
sterimol_B1_boltz	3.223	3.266	0.044	1.35	0.002
E_solv_elstat_boltz	-4.286	-4.234	0.053	1.23	0.003

# KRAKEN ID 00000217

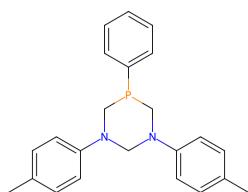


Table 1. Properties that exceed 1% relative difference

property	old	new	abs_diff	rel_diff (%)	squared_diff
vbur_ovtot_min_vbur_min_conf	0.0	0.0	0.0	inf	0.0
vbur_far_vtot_min	0.0	0.0	0.0	inf	0.0
vbur_ovtot_min_delta	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_boltz	0.0	0.0	0.0	inf	0.0
vbur_ovtot_min_boltz	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_delta	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_max	0.0	0.0	0.0	inf	0.0
vbur_ovtot_min_max	0.0	0.0	0.0	inf	0.0
vbur_far_vbur_min	0.0	0.0	0.0	inf	0.0
vbur_far_vtot_vbur_min_conf	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_min	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_vbur_min_conf	0.0	0.0	0.0	inf	0.0
vbur_ovtot_min_min	0.0	0.0	0.0	inf	0.0
vbur_far_vbur_vbur_min_conf	0.0	0.0	0.0	inf	0.0
vbur_far_vbur_boltz	0.523	0.996	0.472	90.265	0.223
vbur_far_vtot_boltz	6.445	12.135	5.69	88.283	32.374
pyr_P_delta	0.079	0.035	0.044	55.292	0.002
vbur_max_delta_qvtot_min	52.369	80.452	28.083	53.624	788.645
vbur_max_delta_qvbur_min	2.6	1.314	1.286	49.477	1.655
pyr_alpha_delta	11.479	5.938	5.542	48.274	30.709
vbur_qvtot_min_delta	41.326	24.499	16.826	40.716	283.125
dipolemoment_delta	0.903	1.232	0.329	36.46	0.108
qpoletens_zz_delta	7.948	10.312	2.364	29.741	5.588
vbur_qvtot_min_max	67.683	50.857	16.826	24.86	283.116
pyr_alpha_max	22.94	17.398	5.542	24.159	30.716
dipolemoment_max	1.463	1.792	0.329	22.513	0.108

vbur_max_delta_qvtot_delta	126.148	97.819	28.329	22.457	802.558
qpole_amp_delta	9.555	11.577	2.022	21.158	4.087
sterimol_B1_delta	1.654	1.99	0.335	20.277	0.113
qpoletens_yy_max	5.315	6.339	1.024	19.271	1.049
qpoletens_zz_min	-12.377	-14.669	2.292	18.514	5.251
vbur_qvtot_max_delta	80.19	66.935	13.256	16.53	175.71
qpoletens_yy_delta	8.156	9.18	1.024	12.56	1.049
qpole_amp_max	16.027	18.021	1.994	12.44	3.975
vbur_ovbur_max_delta	7.906	8.85	0.944	11.946	0.892
vbur_max_delta_qvbur_delta	10.14	11.336	1.195	11.79	1.429
vbur_qvtot_max_min	128.235	139.863	11.627	9.067	135.197
vbur_max_delta_qvbur_boltz	4.796	5.223	0.427	8.909	0.183
qpoletens_xx_boltz	6.061	6.592	0.531	8.759	0.282
dipolemoment_boltz	0.805	0.875	0.07	8.676	0.005
vbur_ovbur_max_min	12.368	11.384	0.984	7.958	0.969
vbur_qvbur_max_min	12.368	11.384	0.984	7.958	0.969
sterimol_B1_max	4.499	4.835	0.336	7.465	0.113
sterimol_B5_delta	3.158	2.922	0.236	7.461	0.056
vbur_qvbur_max_delta	12.106	12.996	0.89	7.352	0.792
qpoletens_yy_boltz	2.099	1.958	0.142	6.754	0.02
spindens_P_ra_boltz	0.053	0.057	0.003	6.545	0.0
sterimol_burB1_delta	1.203	1.28	0.077	6.424	0.006
vbur_max_delta_qvtot_boltz	101.501	107.712	6.211	6.119	38.579
vbur_ovtot_max_min	128.235	135.751	7.515	5.861	56.483
vbur_ovtot_max_max	176.87	186.525	9.655	5.459	93.228
pyr_P_min	0.891	0.935	0.044	4.921	0.002
qpoletens_zz_boltz	-8.161	-8.55	0.389	4.768	0.151
qpole_amp_boltz	10.611	11.115	0.503	4.745	0.253
nmrten_szz_P_boltz	416.363	434.995	18.632	4.475	347.147
vbur_vtot_delta	2.628	2.744	0.117	4.435	0.014
vbur_ovtot_max_delta	48.634	50.774	2.14	4.4	4.579
vbur_vbur_boltz	44.975	46.766	1.79	3.981	3.206
vbur_qvbur_max_boltz	14.67	15.249	0.579	3.947	0.335
vbur_ratio_vbur_vtot_boltz	0.111	0.115	0.004	3.946	0.0
sterimol_B5_min	6.712	6.977	0.265	3.945	0.07

vbur_qvtot_max_boltz	149.662	155.215	5.553	3.71	30.832
efgtens_yy_P_boltz	-0.613	-0.595	0.019	3.071	0.0
vbur_near_vtot_delta	80.911	83.354	2.443	3.019	5.967
vbur_near_vbur_boltz	44.452	45.77	1.318	2.965	1.738
vbur_far_vtot_max	80.981	78.869	2.111	2.607	4.457
vbur_far_vtot_delta	80.981	78.869	2.111	2.607	4.457
sterimol_L_delta	5.449	5.579	0.13	2.387	0.017
sterimol_L_boltz	10.321	10.088	0.232	2.253	0.054
nbo_bds_occ_avg_boltz	0.044	0.045	0.001	2.093	0.0
fukui_p_boltz	0.054	0.055	0.001	2.067	0.0
vbur_ovbur_max_boltz	14.339	14.623	0.284	1.979	0.081
vmin_vmin_boltz	-0.046	-0.046	0.001	1.928	0.0
sterimol_burB1_max	4.048	4.125	0.078	1.919	0.006
vbur_qvbur_min_boltz	9.555	9.738	0.183	1.918	0.034
fmo_e_lumo_boltz	-0.023	-0.024	0.0	1.766	0.0
vbur_qvbur_min_delta	2.354	2.394	0.04	1.688	0.002
qpoletens_zz_max	-4.429	-4.357	0.072	1.632	0.005
nmrten_sxx_P_boltz	269.184	264.8	4.384	1.629	19.22
vbur_near_vtot_boltz	397.23	390.81	6.42	1.616	41.219
sterimol_burB5_boltz	6.167	6.261	0.095	1.533	0.009
sterimol_B1_boltz	3.438	3.387	0.051	1.475	0.003
pyr_alpha_boltz	15.226	15.008	0.218	1.429	0.047
sterimol_B5_boltz	8.188	8.074	0.115	1.398	0.013
efgtens_xx_P_boltz	-0.758	-0.768	0.011	1.391	0.0
sterimol_burB1_boltz	3.401	3.355	0.047	1.377	0.002
E_solv_elstat_boltz	-9.929	-10.063	0.134	1.352	0.018
vbur_qvtot_min_boltz	42.633	42.062	0.571	1.34	0.326
nbo_bds_occ_max_boltz	0.06	0.061	0.001	1.301	0.0
nmr_P_boltz	327.608	331.835	4.227	1.29	17.868
sterimol_L_max	11.803	11.933	0.13	1.102	0.017
nbo_P_ra_boltz	0.667	0.66	0.007	1.063	0.0

# KRAKEN ID 00000251

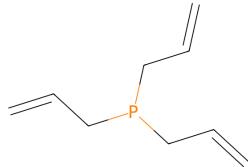


Table 1. Properties that exceed 1% relative difference

property	old	new	abs_diff	rel_diff (%)	squared_diff
vbur_ovtot_min_min	0.0	0.0	0.0	inf	0.0
vbur_far_vbur_min	0.0	0.0	0.0	inf	0.0
vbur_far_vtot_min	0.0	0.0	0.0	inf	0.0
vbur_far_vtot_vbur_min_conf	0.0	0.0	0.0	inf	0.0
vbur_ovtot_min_vbur_min_conf	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_min	0.0	0.0	0.0	inf	0.0
vbur_far_vbur_vbur_min_conf	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_vbur_min_conf	0.0	0.0	0.0	inf	0.0
qpoletens_xx_vbur_min_conf	1.069	0.254	0.815	76.25	0.665
qpole_amp_vbur_min_conf	1.683	0.618	1.065	63.277	1.135
qpoletens_zz_vbur_min_conf	-1.282	-0.505	0.778	60.643	0.605
vbur_far_vtot_max	1.625	2.292	0.666	40.981	0.444
vbur_far_vtot_delta	1.625	2.292	0.666	40.981	0.444
vbur_far_vbur_boltz	0.007	0.004	0.003	40.884	0.0
vbur_max_delta_qvtot_vbur_min_conf	19.346	11.47	7.876	40.713	62.037
vbur_far_vtot_boltz	0.01	0.006	0.004	38.295	0.0
vbur_max_delta_qvtot_min	15.215	11.47	3.745	24.613	14.023
vbur_qvtot_min_vbur_min_conf	35.291	43.955	8.663	24.548	75.051
qpoletens_yy_vbur_min_conf	0.213	0.251	0.038	17.687	0.001
vbur_max_delta_qvbur_min	0.982	0.823	0.159	16.187	0.025
vbur_max_delta_qvbur_vbur_min_conf	0.982	0.823	0.159	16.187	0.025
dipolemoment_vbur_min_conf	0.592	0.501	0.091	15.328	0.008
vbur_far_vbur_delta	1.381	1.583	0.203	14.697	0.041
vbur_far_vbur_max	1.381	1.583	0.203	14.697	0.041
sterimol_B5_delta	0.926	1.053	0.127	13.714	0.016
sterimol_burB5_delta	0.926	1.053	0.127	13.714	0.016

vbur_ovbur_min_boltz	0.0	0.0	0.0	13.193	0.0
vbur_overt_min_boltz	0.0	0.0	0.0	13.191	0.0
dipolemoment_min	0.576	0.501	0.075	13.015	0.006
vbur_max_delta_qvbur_delta	8.995	10.095	1.1	12.233	1.211
qpoletens_yy_boltz	-0.169	-0.188	0.02	11.722	0.0
vbur_max_delta_qvtot_delta	32.119	35.867	3.748	11.668	14.046
sterimol_burL_vbur_min_conf	7.621	6.841	0.78	10.229	0.608
vbur_qvtot_min_delta	19.647	21.65	2.004	10.198	4.014
qpoletens_yy_min	-0.7	-0.769	0.069	9.868	0.005
vbur_qvbur_max_delta	9.302	10.182	0.88	9.456	0.774
vbur_max_delta_qvbur_max	9.977	10.918	0.941	9.435	0.886
sterimol_L_vbur_min_conf	7.922	7.256	0.666	8.408	0.444
dipolemoment_delta	1.085	1.16	0.075	6.92	0.006
vbur_near_vtot_delta	5.424	5.779	0.355	6.554	0.126
fukui_p_boltz	0.071	0.067	0.005	6.342	0.0
spindens_P_ra_boltz	0.093	0.087	0.006	6.171	0.0
qpoletens_zz_boltz	-0.677	-0.637	0.04	5.89	0.002
vbur_vtot_delta	1.93	1.826	0.104	5.406	0.011
vbur_ovbur_max_delta	8.166	8.599	0.433	5.302	0.187
vbur_qvtot_min_max	41.95	43.955	2.004	4.778	4.018
qpoletens_xx_delta	2.897	3.033	0.136	4.707	0.019
qpole_amp_boltz	1.153	1.103	0.051	4.391	0.003
qpoletens_xx_max	3.139	3.275	0.136	4.332	0.018
vbur_qvbur_max_max	20.126	20.9	0.774	3.846	0.599
qpoletens_yy_delta	2.445	2.514	0.069	2.818	0.005
sterimol_burB5_vbur_min_conf	4.901	4.777	0.124	2.53	0.015
sterimol_burB5_min	4.901	4.777	0.124	2.53	0.015
sterimol_B5_min	4.901	4.777	0.124	2.53	0.015
sterimol_B5_vbur_min_conf	4.901	4.777	0.124	2.53	0.015
qpoletens_xx_boltz	0.846	0.826	0.02	2.377	0.0
pyr_alpha_vbur_min_conf	21.257	21.76	0.503	2.368	0.253
vbur_overt_max_delta	17.372	17.752	0.38	2.186	0.144
vbur_qvtot_max_delta	17.372	17.752	0.38	2.186	0.144
sterimol_B1_vbur_min_conf	3.289	3.358	0.069	2.113	0.005
sterimol_burB1_vbur_min_conf	3.289	3.358	0.069	2.113	0.005

dipolemoment_boltz	0.839	0.823	0.016	1.87	0.0
vbur_ovbur_max_max	18.99	19.318	0.327	1.724	0.107
vbur_ovtot_max_vbur_min_conf	56.393	55.425	0.969	1.718	0.939
vbur_qvtot_max_vbur_min_conf	56.393	55.425	0.969	1.718	0.939
vbur_qvtot_max_min	56.312	55.425	0.887	1.575	0.787
vbur_ovtot_max_min	56.312	55.425	0.887	1.575	0.787
sterimol_burB1_delta	0.895	0.882	0.013	1.43	0.0
sterimol_B1_delta	0.895	0.882	0.013	1.43	0.0
vbur_max_delta_qvbur_boltz	2.968	2.926	0.042	1.418	0.002
pyr_P_delta	0.067	0.066	0.001	1.374	0.0
vbur_qvbur_min_delta	4.951	4.894	0.058	1.162	0.003

# KRAKEN ID 00000280

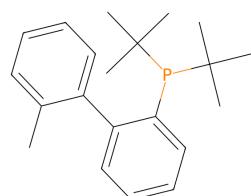


Table 1. Properties that exceed 1% relative difference

property	old	new	abs_diff	rel_diff (%)	squared_diff
vbur_ovtot_min_vbur_min_conf	0.0	0.0	0.0	inf	0.0
vbur_ovtot_min_delta	0.0	0.0	0.0	inf	0.0
vbur_ovtot_min_max	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_max	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_min	0.0	0.0	0.0	inf	0.0
vbur_ovtot_min_min	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_boltz	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_vbur_min_conf	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_delta	0.0	0.0	0.0	inf	0.0
vbur_ovtot_min_boltz	0.0	0.0	0.0	inf	0.0
sterimol_burL_delta	0.185	1.151	0.966	522.543	0.933
dipolemoment_delta	0.074	0.211	0.137	184.136	0.019
vbur_qvtot_min_delta	2.072	5.087	3.015	145.489	9.09
sterimol_B1_delta	0.074	0.156	0.081	109.465	0.007
sterimol_burB1_delta	0.074	0.156	0.081	109.465	0.007
vbur_vtot_delta	0.568	1.046	0.479	84.303	0.229
vbur_far_vtot_min	0.383	0.096	0.288	75.069	0.083
pyr_alpha_delta	7.197	10.584	3.386	47.051	11.467
pyr_P_delta	0.076	0.111	0.035	45.935	0.001
vbur_max_delta_qvbur_min	6.304	3.57	2.734	43.371	7.475
vbur_far_vbur_min	0.375	0.223	0.153	40.669	0.023
vbur_ovbur_max_delta	2.345	3.206	0.861	36.708	0.741
sterimol_B5_delta	0.339	0.429	0.09	26.577	0.008
sterimol_L_delta	2.118	2.654	0.536	25.294	0.287
qpoletens_xx_delta	0.809	0.965	0.155	19.194	0.024
vbur_max_delta_qvbur_delta	18.728	21.463	2.735	14.604	7.48

sterimol_burL_max	7.291	8.257	0.966	13.248	0.933
dipolemoment_max	1.209	1.344	0.136	11.226	0.018
pyr_alpha_max	33.218	36.623	3.405	10.251	11.595
vbur_qvbur_max_min	20.295	19.055	1.239	6.107	1.536
qpoletens_xx_max	2.74	2.898	0.158	5.752	0.025
vbur_qvbur_max_delta	21.706	22.944	1.238	5.705	1.534
sterimol_L_max	9.657	10.193	0.536	5.551	0.287
vbur_qvtot_min_max	57.196	60.21	3.014	5.269	9.083
pyr_P_min	0.788	0.753	0.035	4.453	0.001
vbur_ovbur_max_min	19.916	19.055	0.861	4.322	0.741
qpoletens_yy_boltz	0.56	0.577	0.016	2.905	0.0
qpoletens_yy_min	0.232	0.238	0.006	2.57	0.0
sterimol_B1_min	3.916	3.835	0.081	2.078	0.007
sterimol_burB1_min	3.916	3.835	0.081	2.078	0.007
sterimol_B5_max	6.706	6.796	0.09	1.346	0.008

# KRAKEN ID 00000327



Table 1. Properties that exceed 1% relative difference

property	old	new	abs_diff	rel_diff (%)	squared_diff
vbur_ovtot_min_vbur_min_conf	0.0	0.0	0.0	inf	0.0
vbur_far_vbur_vbur_min_conf	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_min	0.0	0.0	0.0	inf	0.0
vbur_far_vbur_min	0.0	0.0	0.0	inf	0.0
vbur_ovtot_min_min	0.0	0.0	0.0	inf	0.0
vbur_far_vtot_min	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_vbur_min_conf	0.0	0.0	0.0	inf	0.0
vbur_ovtot_min_boltz	0.0	0.006	0.006	2435.301	0.0
vbur_ovbur_min_max	2.088	0.074	2.013	96.443	4.054
vbur_ovbur_min_delta	2.088	0.074	2.013	96.443	4.054
vbur_ovtot_min_delta	2.238	0.682	1.556	69.526	2.421
vbur_ovtot_min_max	2.238	0.682	1.556	69.526	2.421
sterimol_L_delta	4.016	6.646	2.63	65.507	6.919
vbur_qvtot_min_delta	45.529	64.686	19.157	42.077	366.993
qpoletens_yy_max	4.113	5.656	1.543	37.508	2.38
qpoletens_yy_delta	6.023	8.222	2.2	36.523	4.839
qpoletens_yy_min	-1.91	-2.567	0.657	34.402	0.432
sterimol_L_max	10.786	13.416	2.63	24.387	6.919
vbur_ovbur_min_boltz	0.0	0.0	0.0	23.048	0.0
vbur_max_delta_qvtot_min	138.341	106.706	31.636	22.868	1000.82
vbur_qvtot_min_max	90.693	109.227	18.534	20.436	343.522
qpoletens_xx_delta	5.224	6.214	0.99	18.955	0.981
qpole_amp_delta	4.358	5.149	0.791	18.155	0.626
vbur_qvtot_max_delta	95.215	79.359	15.856	16.653	251.425
vbur_far_vbur_max	51.01	42.561	8.449	16.563	71.383
vbur_far_vbur_delta	51.01	42.561	8.449	16.563	71.383

sterimol_burB1_delta	1.059	1.217	0.158	14.894	0.025
vbur_vtot_delta	3.141	3.591	0.45	14.33	0.203
sterimol_burB5_delta	1.38	1.574	0.194	14.069	0.038
vbur_max_delta_qvtot_delta	118.403	131.096	12.693	10.72	161.114
sterimol_B1_delta	1.065	1.172	0.107	10.019	0.011
vbur_near_vbur_delta	21.623	23.74	2.117	9.79	4.481
vbur_qvtot_max_max	324.415	295.292	29.123	8.977	848.163
pyr_alpha_delta	8.093	8.804	0.712	8.793	0.506
dipolemoment_min	1.839	1.991	0.152	8.28	0.023
qpoletens_xx_min	9.263	8.544	0.718	7.755	0.516
pyr_P_delta	0.063	0.067	0.005	7.394	0.0
vbur_max_delta_qvtot_max	256.744	237.802	18.943	7.378	358.825
vbur_near_vtot_delta	180.185	191.605	11.42	6.338	130.414
vbur_qvtot_max_min	229.2	215.933	13.267	5.788	176.009
vbur_far_vtot_max	183.677	192.062	8.385	4.565	70.314
vbur_far_vtot_delta	183.677	192.062	8.385	4.565	70.314
sterimol_burB1_min	3.851	3.693	0.158	4.101	0.025
qpoletens_zz_delta	4.724	4.915	0.191	4.044	0.036
sterimol_burL_delta	1.401	1.452	0.051	3.645	0.003
pyr_alpha_min	15.841	15.323	0.518	3.269	0.268
vbur_ovtot_max_min	133.987	138.365	4.378	3.268	19.168
dipolemoment_max	3.852	3.962	0.11	2.862	0.012
vbur_qvbur_max_delta	28.981	28.16	0.821	2.833	0.674
vbur_far_vtot_vbur_min_conf	9.994	9.713	0.281	2.812	0.079
vbur_near_vbur_max	75.714	77.834	2.12	2.8	4.495
spindens_P_ra_boltz	0.003	0.003	0.0	2.587	0.0
vbur_max_delta_qvbur_min	2.535	2.475	0.061	2.393	0.004
qpole_amp_max	21.139	21.627	0.488	2.308	0.238
vbur_ovtot_max_delta	145.656	142.298	3.357	2.305	11.272
fukui_m_boltz	0.174	0.178	0.004	2.204	0.0
dipolemoment_delta	2.012	1.97	0.042	2.09	0.002
vbur_vbur_delta	63.506	64.805	1.299	2.045	1.687
sterimol_burB5_min	6.524	6.393	0.131	2.001	0.017
vbur_qvbur_max_max	44.637	43.758	0.88	1.971	0.774
qpoletens_xx_max	14.487	14.759	0.272	1.877	0.074

qpole_amp_min	16.781	16.478	0.303	1.808	0.092
spindens_P_rc_boltz	0.238	0.242	0.004	1.747	0.0
sterimol_B1_min	3.927	3.866	0.061	1.56	0.004
vbur_near_vtot_min	432.22	425.778	6.441	1.49	41.491
vbur_qvtot_min_min	45.165	44.542	0.623	1.379	0.388
E_reduction_boltz	-0.01	-0.01	0.0	1.375	0.0
vbur_qvbur_min_boltz	12.476	12.64	0.164	1.315	0.027
vbur_qvbur_min_delta	5.489	5.559	0.07	1.277	0.005
qpoletens_yy_boltz	2.832	2.864	0.032	1.132	0.001
qpoletens_zz_min	-16.299	-16.481	0.181	1.112	0.033
vbur_vbur_max	117.597	118.899	1.302	1.107	1.696
sterimol_B5_delta	3.184	3.149	0.035	1.107	0.001
vbur_qvtot_min_boltz	60.2	60.805	0.606	1.006	0.367

# KRAKEN ID 00000329

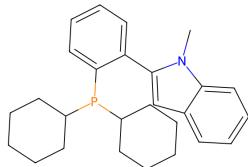


Table 1. Properties that exceed 1% relative difference

property	old	new	abs_diff	rel_diff (%)	squared_diff
vbur_far_vtot_vbur_min_conf	0.0	0.0	0.0	inf	0.0
vbur_far_vbur_vbur_min_conf	0.0	0.0	0.0	inf	0.0
vbur_ovtot_min_min	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_min	0.0	0.0	0.0	inf	0.0
vbur_far_vtot_min	0.0	0.0	0.0	inf	0.0
vbur_ovtot_min_vbur_min_conf	0.0	0.0	0.0	inf	0.0
vbur_far_vbur_min	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_vbur_min_conf	0.0	0.0	0.0	inf	0.0
qpoletens_yy_vbur_min_conf	1.788	0.073	1.716	95.932	2.943
vbur_max_delta_qvbur_vbur_min_conf	3.082	5.92	2.838	92.06	8.052
vbur_ovtot_min_boltz	0.342	0.054	0.288	84.248	0.083
vbur_ovbur_min_boltz	0.136	0.022	0.115	84.221	0.013
vbur_vtot_delta	1.24	2.254	1.015	81.836	1.029
vbur_max_delta_qvtot_vbur_min_conf	76.071	129.08	53.01	69.685	2810.028
vbur_qvtot_max_delta	53.872	83.788	29.916	55.532	894.971
dipolemoment_vbur_min_conf	1.714	2.578	0.864	50.421	0.747
qpoletens_zz_vbur_min_conf	-8.843	-4.911	3.933	44.471	15.466
qpole_amp_vbur_min_conf	11.453	6.894	4.559	39.809	20.788
vbur_ovbur_min_max	0.816	0.548	0.268	32.821	0.072
vbur_ovbur_min_delta	0.816	0.548	0.268	32.821	0.072
qpoletens_xx_vbur_min_conf	7.055	4.838	2.217	31.427	4.916
dipolemoment_delta	1.735	2.276	0.541	31.186	0.293
fukui_m_boltz	0.152	0.107	0.045	29.881	0.002
vbur_max_delta_qvtot_min	57.831	42.106	15.725	27.191	247.275
vbur_far_vbur_boltz	22.335	28.342	6.007	26.894	36.083
spindens_P_rc_boltz	0.213	0.163	0.05	23.428	0.003

vbur_qvtot_min_vbur_min_conf	75.177	58.17	17.007	22.622	289.232
vbur_far_vtot_boltz	80.382	97.281	16.899	21.023	285.572
dipolemoment_min	1.656	1.333	0.324	19.534	0.105
qpoletens_xx_min	2.712	2.185	0.527	19.435	0.278
vbur_max_delta_qvbur_boltz	21.105	25.098	3.993	18.921	15.946
vbur_max_delta_qvtot_delta	87.529	103.253	15.724	17.965	247.255
qpoletens_xx_boltz	4.581	3.763	0.819	17.872	0.67
qpoletens_yy_max	2.159	2.541	0.382	17.7	0.146
pyr_P_delta	0.073	0.085	0.012	16.792	0.0
qpole_amp_boltz	7.236	6.054	1.182	16.335	1.397
vbur_qvbur_max_boltz	35.756	41.592	5.836	16.321	34.054
qpoletens_zz_boltz	-5.472	-4.625	0.846	15.469	0.716
E_reduction_boltz	0.008	0.009	0.001	14.515	0.0
vbur_near_vbur_delta	19.23	22.015	2.785	14.484	7.758
vbur_ovtot_min_delta	1.011	0.869	0.143	14.106	0.02
vbur_ovtot_min_max	1.011	0.869	0.143	14.106	0.02
vbur_qvtot_max_min	154.164	132.462	21.702	14.077	470.987
pyr_alpha_delta	9.508	10.837	1.329	13.979	1.767
spindens_P_ra_boltz	0.015	0.013	0.002	13.425	0.0
qpoletens_yy_delta	2.933	3.315	0.382	13.032	0.146
vbur_qvtot_min_min	50.297	44.074	6.223	12.373	38.73
pyr_alpha_vbur_min_conf	21.012	23.415	2.403	11.435	5.773
dipolemoment_boltz	2.832	3.154	0.322	11.361	0.104
vbur_qvbur_min_vbur_min_conf	12.649	11.227	1.422	11.245	2.023
qpole_amp_min	4.065	3.619	0.446	10.966	0.199
sterimol_B5_vbur_min_conf	6.768	7.493	0.725	10.717	0.526
vbur_ovtot_max_boltz	127.961	114.271	13.69	10.699	187.416
vbur_qvtot_max_vbur_min_conf	170.157	187.25	17.093	10.045	292.17
vbur_ovtot_max_vbur_min_conf	170.157	187.25	17.093	10.045	292.17
sterimol_burB1_delta	0.84	0.92	0.081	9.602	0.007
vbur_vbur_delta	53.85	59.015	5.165	9.591	26.674
sterimol_L_delta	4.229	4.631	0.402	9.498	0.161
fukui_p_boltz	0.021	0.019	0.002	9.147	0.0
sterimol_burL_vbur_min_conf	8.225	7.478	0.747	9.081	0.558
sterimol_B1_vbur_min_conf	4.715	4.379	0.336	7.123	0.113

vbur_far_vbur_delta	34.639	37.0	2.361	6.815	5.572
vbur_far_vbur_max	34.639	37.0	2.361	6.815	5.572
vbur_qvtot_min_max	91.96	85.872	6.088	6.621	37.07
qpoletens_zz_max	-3.013	-2.815	0.198	6.557	0.039
dipolemoment_max	3.392	3.609	0.218	6.416	0.047
qpole_amp_max	11.755	11.054	0.701	5.96	0.491
vbur_qvbur_max_vbur_min_conf	16.256	17.147	0.89	5.475	0.792
vbur_ovbur_max_vbur_min_conf	16.256	17.147	0.89	5.475	0.792
pyr_alpha_max	24.764	26.093	1.329	5.365	1.765
sterimol_B5_boltz	7.38	6.987	0.393	5.319	0.154
qpoletens_xx_max	7.714	7.31	0.403	5.23	0.163
vbur_max_delta_qvtot_boltz	114.561	108.686	5.875	5.128	34.513
sterimol_burB5_boltz	7.1	6.743	0.356	5.019	0.127
vbur_qvbur_min_boltz	13.652	12.977	0.675	4.947	0.456
vbur_vbur_boltz	92.142	96.621	4.48	4.862	20.067
vbur_ratio_vbur_vtot_boltz	0.202	0.212	0.01	4.822	0.0
vbur_near_vtot_boltz	372.208	355.55	16.658	4.475	277.488
qpoletens_zz_min	-8.954	-8.563	0.391	4.368	0.153
vbur_ovbur_max_boltz	21.3	22.204	0.904	4.244	0.817
sterimol_burB1_vbur_min_conf	4.571	4.379	0.191	4.189	0.037
nbo_bds_occ_avg_boltz	0.037	0.035	0.002	4.171	0.0
nbo_P_rc_boltz	0.934	0.897	0.037	4.001	0.001
vbur_qvtot_max_max	208.036	216.249	8.214	3.948	67.467
vbur_qvtot_min_boltz	64.839	62.291	2.548	3.93	6.493
vbur_near_vtot_delta	115.282	119.589	4.307	3.736	18.55
vbur_max_delta_qvbur_delta	24.83	25.745	0.915	3.686	0.838
sterimol_L_boltz	8.054	7.769	0.285	3.538	0.081
sterimol_L_max	11.545	11.95	0.405	3.505	0.164
vbur_ovtot_max_delta	77.82	80.517	2.697	3.466	7.275
vbur_max_delta_qvbur_max	27.103	28.019	0.916	3.381	0.839
qpole_amp_delta	7.69	7.435	0.255	3.314	0.065
qpoletens_zz_delta	5.941	5.748	0.194	3.257	0.037
vbur_vbur_max	111.819	115.434	3.616	3.234	13.073
sterimol_L_vbur_min_conf	10.846	10.496	0.35	3.227	0.122
qpoletens_yy_boltz	0.89	0.863	0.028	3.106	0.001

fmo_e_lumo_boltz	-0.035	-0.034	0.001	2.939	0.0
nmrtens_szz_P_boltz	339.029	329.358	9.671	2.853	93.53
vbur_near_vbur_min	57.968	56.419	1.549	2.672	2.399
vbur_near_vbur_vbur_min_conf	57.968	56.419	1.549	2.672	2.399
vbur_vbur_vbur_min_conf	57.968	56.419	1.549	2.672	2.399
vbur_vbur_min	57.968	56.419	1.549	2.672	2.399
vbur_far_vtot_max	111.866	114.636	2.77	2.477	7.675
vbur_far_vtot_delta	111.866	114.636	2.77	2.477	7.675
qpoletens_xx_delta	5.002	5.126	0.124	2.471	0.015
somo_ra_boltz	0.051	0.052	0.001	2.462	0.0
pyr_P_vbur_min_conf	0.91	0.888	0.022	2.419	0.0
vbur_near_vbur_boltz	69.806	68.279	1.527	2.188	2.333
sterimol_burB1_max	4.571	4.652	0.082	1.784	0.007
vbur_near_vbur_max	77.198	78.434	1.236	1.601	1.528
fmo_omega_boltz	0.042	0.042	0.001	1.482	0.0
vbur_ovtot_max_max	189.817	192.513	2.696	1.42	7.268
pyr_P_min	0.877	0.865	0.012	1.398	0.0
E_solv_cds_boltz	-11.451	-11.604	0.154	1.341	0.024
surface_area_boltz	439.106	444.982	5.877	1.338	34.536
nbo_P_ra_boltz	0.761	0.771	0.01	1.307	0.0
pyr_alpha_boltz	18.975	18.739	0.236	1.242	0.056
efgtens_xx_P_boltz	-0.87	-0.859	0.01	1.192	0.0
sphericity_boltz	0.735	0.726	0.009	1.182	0.0
sterimol_burL_boltz	7.392	7.305	0.087	1.177	0.008
vbur_near_vtot_min	340.654	336.717	3.937	1.156	15.497
vbur_qvbur_min_delta	6.794	6.717	0.077	1.139	0.006
nmr_P_boltz	302.949	299.599	3.35	1.106	11.221
Pint_P_min_boltz	13.089	12.947	0.142	1.082	0.02
nbo_P_boltz	0.782	0.79	0.008	1.027	0.0

# KRAKEN ID 00000338

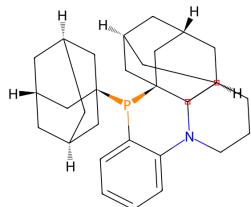


Table 1. Properties that exceed 1% relative difference

property	old	new	abs_diff	rel_diff (%)	squared_diff
vbur_ovbur_min_min	0.0	0.0	0.0	inf	0.0
vbur_overtot_min_min	0.0	0.0	0.0	inf	0.0
vbur_overtot_min_vbur_min_conf	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_vbur_min_conf	0.0	0.0	0.0	inf	0.0
qpoletens_yy_vbur_min_conf	0.044	-0.555	0.599	1376.235	0.359
qpoletens_yy_max	0.044	-0.437	0.48	1103.676	0.231
sterimol_B5_delta	0.057	0.198	0.141	246.582	0.02
sterimol_burL_delta	0.246	0.812	0.566	229.526	0.32
pyr_P_delta	0.067	0.134	0.067	100.25	0.005
pyr_alpha_delta	6.747	12.709	5.962	88.355	35.54
vbur_far_vtot_vbur_min_conf	1.665	0.318	1.347	80.911	1.815
qpoletens_zz_delta	0.814	1.328	0.514	63.227	0.265
vbur_far_vtot_min	0.32	0.157	0.163	50.947	0.027
sterimol_burB1_delta	0.549	0.774	0.225	40.919	0.051
vbur_far_vbur_vbur_min_conf	0.355	0.218	0.137	38.643	0.019
sterimol_burB5_delta	0.517	0.68	0.163	31.537	0.027
vbur_max_delta_qvtot_delta	23.951	30.64	6.689	27.927	44.743
vbur_far_vbur_min	0.217	0.158	0.059	27.053	0.003
qpoletens_yy_delta	1.78	1.3	0.48	26.984	0.231
vbur_max_delta_qvbur_vbur_min_conf	6.302	4.714	1.588	25.195	2.521
vbur_qvbur_min_delta	1.634	1.233	0.401	24.52	0.16
vbur_max_delta_qvbur_min	4.714	3.708	1.006	21.345	1.012
vbur_ovbur_max_delta	2.983	3.604	0.621	20.827	0.386
vbur_max_delta_qvtot_vbur_min_conf	55.697	66.713	11.016	19.779	121.361
qpoletens_zz_vbur_min_conf	-3.663	-2.96	0.704	19.211	0.495
qpole_amp_delta	2.271	2.687	0.416	18.314	0.173

pyr_alpha_max	32.802	38.767	5.965	18.184	35.58
vbur_near_vbur_delta	6.727	5.557	1.17	17.397	1.37
qpoletens_zz_max	-2.959	-2.517	0.442	14.951	0.196
dipolemoment_delta	1.913	2.16	0.247	12.901	0.061
dipolemoment_max	2.021	2.267	0.247	12.218	0.061
vbur_max_delta_qvtot_min	55.697	49.016	6.681	11.995	44.636
sterimol_B1_delta	0.615	0.688	0.073	11.948	0.005
qpoletens_xx_delta	1.994	2.221	0.227	11.368	0.051
qpole_amp_vbur_min_conf	5.15	4.628	0.522	10.132	0.272
vbur_vtot_delta	1.286	1.403	0.117	9.137	0.014
vbur_qvtot_min_delta	8.124	8.865	0.742	9.13	0.55
qpole_amp_min	4.628	4.212	0.417	9.0	0.174
pyr_P_min	0.796	0.729	0.067	8.45	0.005
sterimol_burL_max	7.431	7.996	0.566	7.613	0.32
vbur_qvtot_max_delta	19.44	20.775	1.334	6.865	1.781
qpoletens_xx_min	3.515	3.288	0.227	6.463	0.052
sterimol_burB5_vbur_min_conf	6.771	6.36	0.411	6.069	0.169
sterimol_L_delta	2.912	3.078	0.166	5.715	0.028
sterimol_B1_vbur_min_conf	5.038	4.756	0.282	5.591	0.079
vbur_qvtot_max_vbur_min_conf	155.142	163.32	8.178	5.271	66.876
vbur_ovtot_max_vbur_min_conf	155.142	163.007	7.865	5.07	61.859
vbur_max_delta_qvbur_delta	20.45	21.456	1.006	4.92	1.012
vbur_qvbur_max_vbur_min_conf	20.475	19.491	0.983	4.802	0.967
sterimol_burB1_max	4.886	5.111	0.225	4.604	0.051
sterimol_L_vbur_min_conf	10.103	10.53	0.426	4.221	0.182
vbur_ovbur_max_vbur_min_conf	20.118	19.272	0.846	4.206	0.716
vbur_qvbur_max_min	19.491	18.73	0.761	3.906	0.58
dipolemoment_vbur_min_conf	2.021	1.947	0.074	3.647	0.005
vbur_qvtot_min_vbur_min_conf	93.497	96.607	3.11	3.326	9.669
vbur_ovbur_max_min	19.272	18.651	0.621	3.224	0.386
vbur_qvbur_max_delta	24.211	24.973	0.762	3.149	0.581
qpoletens_xx_vbur_min_conf	3.62	3.515	0.105	2.898	0.011
vbur_qvbur_min_vbur_min_conf	14.173	14.575	0.402	2.834	0.161
vbur_qvbur_min_min	14.173	14.575	0.402	2.834	0.161
vbur_vbur_delta	39.636	38.604	1.031	2.602	1.064

sterimol_burB1_vbur_min_conf	4.812	4.716	0.096	1.986	0.009
sterimol_B5_max	6.869	7.005	0.136	1.981	0.019
sterimol_burB5_max	6.869	7.005	0.136	1.981	0.019
qpoletens_zz_min	-3.773	-3.845	0.072	1.907	0.005
vbur_near_vbur_vbur_min_conf	65.966	67.138	1.171	1.776	1.372
vbur_near_vbur_min	65.966	67.138	1.171	1.776	1.372
vbur_far_vtot_delta	64.146	65.193	1.047	1.632	1.095
sterimol_L_max	10.53	10.696	0.166	1.58	0.028
vbur_vbur_min	66.321	67.355	1.034	1.56	1.07
vbur_vbur_vbur_min_conf	66.321	67.355	1.034	1.56	1.07
sterimol_B1_max	5.038	5.111	0.073	1.445	0.005
pyr_alpha_vbur_min_conf	32.358	32.805	0.447	1.382	0.2
vbur_far_vtot_max	64.466	65.35	0.884	1.371	0.781

# KRAKEN ID 00000340

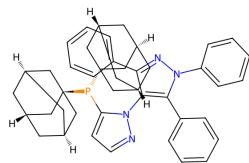


Table 1. Properties that exceed 1% relative difference

property	old	new	abs_diff	rel_diff (%)	squared_diff
vbur_ovbur_min_boltz	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_delta	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_vbur_min_conf	0.0	0.0	0.0	inf	0.0
vbur_overtot_min_min	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_min	0.0	0.0	0.0	inf	0.0
vbur_overtot_min_max	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_max	0.0	0.0	0.0	inf	0.0
vbur_overtot_min_boltz	0.0	0.0	0.0	inf	0.0
vbur_overtot_min_delta	0.0	0.0	0.0	inf	0.0
vbur_overtot_min_vbur_min_conf	0.0	0.0	0.0	inf	0.0
vbur_qvbur_min_delta	0.183	0.664	0.481	262.857	0.231
vbur_qvtot_min_delta	0.417	1.367	0.951	228.287	0.904
pyr_alpha_delta	0.718	1.442	0.724	100.76	0.524
pyr_P_delta	0.006	0.012	0.006	90.735	0.0
dipolemoment_delta	0.392	0.523	0.131	33.504	0.017
vbur_max_delta_qvbur_delta	1.867	2.369	0.502	26.891	0.252
vbur_near_vbur_delta	1.432	1.63	0.198	13.806	0.039
sterimol_burB1_delta	0.036	0.04	0.004	10.181	0.0
sterimol_burL_delta	0.075	0.079	0.004	4.855	0.0
dipolemoment_min	2.936	2.804	0.131	4.471	0.017
vbur_qvbur_min_max	14.995	15.477	0.482	3.215	0.232
sterimol_B1_delta	0.031	0.032	0.001	3.07	0.0
pyr_alpha_max	25.628	26.351	0.723	2.822	0.523
vbur_max_delta_qvbur_max	22.171	22.672	0.501	2.26	0.251
vbur_qvtot_min_max	91.26	92.218	0.958	1.05	0.918

# KRAKEN ID 00000351

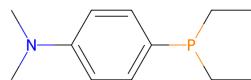


Table 1. Properties that exceed 1% relative difference

property	old	new	abs_diff	rel_diff (%)	squared_diff
vbur_ovtot_min_vbur_min_conf	0.0	0.0	0.0	inf	0.0
vbur_far_vtot_vbur_min_conf	0.0	0.0	0.0	inf	0.0
vbur_far_vtot_min	0.0	0.0	0.0	inf	0.0
vbur_far_vbur_min	0.0	0.0	0.0	inf	0.0
vbur_ovtot_min_max	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_max	0.0	0.0	0.0	inf	0.0
vbur_far_vtot_max	0.0	0.0	0.0	inf	0.0
vbur_far_vbur_max	0.0	0.0	0.0	inf	0.0
vbur_far_vbur_vbur_min_conf	0.0	0.0	0.0	inf	0.0
vbur_ovtot_min_delta	0.0	0.0	0.0	inf	0.0
vbur_ovtot_min_min	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_delta	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_vbur_min_conf	0.0	0.0	0.0	inf	0.0
vbur_far_vtot_delta	0.0	0.0	0.0	inf	0.0
vbur_far_vbur_delta	0.0	0.0	0.0	inf	0.0
vbur_ovtot_min_boltz	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_boltz	0.0	0.0	0.0	inf	0.0
vbur_far_vtot_boltz	0.0	0.0	0.0	inf	0.0
vbur_far_vbur_boltz	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_min	0.0	0.0	0.0	inf	0.0
sterimol_B5_delta	0.086	0.061	0.025	28.804	0.001
qpoletens_xx_delta	0.703	0.544	0.159	22.667	0.025
spindens_P_rc_boltz	0.005	0.006	0.001	11.689	0.0
qpoletens_xx_max	8.522	8.362	0.16	1.873	0.025
fukui_m_boltz	0.027	0.027	0.0	1.723	0.0
vbur_ovbur_max_delta	2.195	2.166	0.029	1.334	0.001

vbur_qvbur_max_delta	2.195	2.166	0.029	1.334	0.001
vbur_near_vtot_delta	4.118	4.066	0.051	1.244	0.003
vbur_vtot_delta	1.186	1.199	0.013	1.11	0.0

# KRAKEN ID 00000401

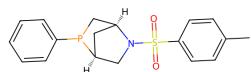


Table 1. Properties that exceed 1% relative difference

property	old	new	abs_diff	rel_diff (%)	squared_diff
vbur_ovbur_min_min	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_vbur_min_conf	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_boltz	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_delta	0.0	0.0	0.0	inf	0.0
vbur_far_vbur_vbur_min_conf	0.0	0.0	0.0	inf	0.0
vbur_overtot_min_delta	0.0	0.0	0.0	inf	0.0
vbur_far_vtot_vbur_min_conf	0.0	0.0	0.0	inf	0.0
vbur_overtot_min_min	0.0	0.0	0.0	inf	0.0
vbur_far_vbur_min	0.0	0.0	0.0	inf	0.0
vbur_overtot_min_boltz	0.0	0.0	0.0	inf	0.0
vbur_overtot_min_max	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_max	0.0	0.0	0.0	inf	0.0
vbur_far_vtot_min	0.0	0.0	0.0	inf	0.0
vbur_overtot_min_vbur_min_conf	0.0	0.0	0.0	inf	0.0
pyr_P_delta	0.001	0.03	0.028	2042.102	0.001
pyr_alpha_delta	0.255	4.559	4.304	1687.913	18.525
sterimol_burL_delta	0.026	0.364	0.339	1317.888	0.115
vbur_vtot_delta	0.479	2.126	1.646	343.544	2.711
vbur_qvtot_min_delta	6.571	27.225	20.653	314.29	426.562
vbur_qvtot_max_delta	24.099	94.382	70.283	291.641	4939.654
vbur_max_delta_qvtot_delta	33.027	121.056	88.029	266.536	7749.156
qpoletens_yy_vbur_min_conf	0.67	2.287	1.618	241.586	2.617
qpoletens_yy_boltz	0.739	2.429	1.69	228.726	2.856
qpoletens_xx_delta	7.738	14.408	6.67	86.202	44.493
vbur_qvbur_min_delta	0.382	0.692	0.311	81.37	0.096
sterimol_burB1_delta	0.216	0.377	0.161	74.289	0.026

sterimol_B1_delta	0.232	0.395	0.163	69.996	0.026
vbur_max_delta_qvtot_min	147.733	59.708	88.025	59.584	7748.47
sterimol_L_delta	4.249	6.724	2.475	58.251	6.126
vbur_qvtot_min_max	35.632	56.285	20.653	57.963	426.561
qpole_amp_delta	11.031	17.336	6.305	57.162	39.757
vbur_qvtot_min_vbur_min_conf	30.558	47.5	16.941	55.439	287.012
qpoletens_xx_min	13.612	6.942	6.67	49.001	44.491
qpoletens_yy_max	4.536	6.725	2.188	48.242	4.789
vbur_far_vbur_boltz	3.407	1.772	1.636	48.001	2.675
vbur_far_vtot_boltz	23.551	12.291	11.26	47.81	126.78
sterimol_burB5_delta	1.101	1.535	0.434	39.373	0.188
vbur_qvtot_max_min	185.722	115.443	70.279	37.841	4939.11
fukui_p_boltz	0.023	0.031	0.008	35.831	0.0
pyr_alpha_max	12.703	17.008	4.305	33.89	18.534
dipolemoment_vbur_min_conf	7.144	4.725	2.42	33.867	5.854
qpole_amp_min	19.741	13.435	6.306	31.942	39.764
vbur_ovtot_max_delta	70.985	91.922	20.937	29.495	438.359
vbur_max_delta_qvtot_vbur_min_conf	176.81	126.173	50.637	28.639	2564.105
vbur_max_delta_qvbur_vbur_min_conf	2.396	3.063	0.667	27.848	0.445
vbur_qvtot_min_boltz	32.56	41.577	9.016	27.692	81.296
E_reduction_boltz	0.004	0.004	0.001	23.189	0.0
sterimol_L_max	11.193	13.669	2.475	22.113	6.126
pyr_alpha_vbur_min_conf	12.47	15.223	2.753	22.076	7.578
vbur_max_delta_qvtot_boltz	166.14	134.645	31.495	18.957	991.91
pyr_alpha_boltz	12.579	14.961	2.382	18.936	5.673
qpoletens_yy_delta	13.456	15.644	2.187	16.254	4.784
nbo_bds_occ_max_boltz	0.033	0.038	0.005	16.228	0.0
vbur_ovtot_max_vbur_min_conf	207.368	174.876	32.493	15.669	1055.763
vbur_qvtot_max_vbur_min_conf	207.368	174.876	32.493	15.669	1055.763
vbur_ovtot_max_min	136.383	115.443	20.939	15.353	438.45
qpoletens_zz_vbur_min_conf	-14.282	-16.248	1.966	13.767	3.866
vbur_near_vbur_delta	7.25	8.223	0.973	13.416	0.946
sterimol_B5_vbur_min_conf	7.613	6.614	0.999	13.119	0.997
dipolemoment_boltz	6.029	5.341	0.688	11.412	0.473
vbur_qvtot_max_boltz	199.513	178.615	20.898	10.474	436.714

sterimol_burB5_vbur_min_conf	6.819	6.146	0.672	9.862	0.452
nbo_bds_occ_avg_boltz	0.03	0.033	0.003	9.173	0.0
qpole_amp_vbur_min_conf	19.741	21.544	1.803	9.131	3.249
sterimol_L_boltz	8.789	9.539	0.749	8.526	0.562
qpoletens_zz_boltz	-16.461	-17.719	1.258	7.642	1.582
nmrtens_sxx_P_boltz	234.607	250.518	15.911	6.782	253.15
sterimol_burB5_boltz	6.926	6.46	0.466	6.727	0.217
sterimol_burB5_min	6.58	6.146	0.434	6.592	0.188
vbur_ovtot_max_boltz	180.463	168.652	11.81	6.545	139.486
vbur_ovbur_max_vbur_min_conf	12.122	12.904	0.782	6.454	0.612
vbur_qvbur_max_vbur_min_conf	12.122	12.904	0.782	6.454	0.612
vbur_max_delta_qvbur_boltz	7.48	7.042	0.439	5.866	0.193
fukui_m_boltz	0.326	0.344	0.018	5.485	0.0
efgtens_xx_P_boltz	-0.703	-0.74	0.037	5.311	0.001
vbur_ovbur_max_boltz	14.47	15.231	0.761	5.257	0.579
sterimol_B1_min	3.164	3.0	0.164	5.185	0.027
sterimol_burB1_min	3.164	3.0	0.164	5.185	0.027
nmrtens_syy_P_boltz	311.088	295.205	15.883	5.106	252.267
sterimol_burL_max	6.966	7.305	0.339	4.861	0.115
sterimol_B5_boltz	8.064	7.675	0.389	4.821	0.151
vbur_vbur_boltz	50.062	47.772	2.29	4.574	5.244
somo_ra_boltz	0.047	0.049	0.002	4.451	0.0
vbur_ratio_vbur_vtot_boltz	0.139	0.133	0.006	4.406	0.0
sterimol_burL_vbur_min_conf	6.948	7.24	0.293	4.21	0.086
vbur_qvbur_max_boltz	17.544	16.844	0.7	3.988	0.489
vbur_near_vtot_delta	64.874	62.324	2.55	3.931	6.503
spindens_P_rc_boltz	0.435	0.452	0.017	3.924	0.0
vbur_vbur_delta	17.095	17.718	0.622	3.64	0.387
vbur_far_vbur_delta	9.845	9.495	0.35	3.559	0.123
vbur_far_vbur_max	9.845	9.495	0.35	3.559	0.123
sterimol_burB1_boltz	3.271	3.16	0.11	3.376	0.012
E_solv_elstat_boltz	-11.472	-11.085	0.387	3.375	0.15
vbur_qvbur_min_min	9.68	9.364	0.316	3.263	0.1
E_solv_total_boltz	-17.889	-17.307	0.582	3.253	0.339
sphericity_boltz	0.754	0.778	0.024	3.213	0.001

surface_area_boltz	355.761	344.678	11.083	3.115	122.824
vbur_near_vtot_boltz	335.852	346.229	10.377	3.09	107.674
E_solv_cds_boltz	-6.417	-6.222	0.195	3.036	0.038
pyr_P_min	0.962	0.934	0.028	2.953	0.001
sterimol_B5_delta	4.434	4.564	0.129	2.916	0.017
sterimol_L_vbur_min_conf	11.193	11.505	0.312	2.787	0.097
sterimol_burL_boltz	6.948	7.141	0.193	2.781	0.037
qpoletens_xx_boltz	15.722	15.29	0.432	2.748	0.187
qpole_amp_boltz	23.274	23.885	0.611	2.624	0.373
qpoletens_xx_vbur_min_conf	13.612	13.961	0.349	2.56	0.121
vbur_near_vbur_min	43.753	42.687	1.067	2.438	1.138
vbur_vbur_min	43.753	42.687	1.067	2.438	1.138
vbur_near_vbur_vbur_min_conf	43.753	42.687	1.067	2.438	1.138
vbur_vbur_vbur_min_conf	43.753	42.687	1.067	2.438	1.138
spindens_P_ra_boltz	0.014	0.014	0.0	2.41	0.0
nbo_lp_P_percent_s_boltz	55.78	54.47	1.31	2.349	1.716
vbur_max_delta_qvbur_delta	13.828	13.507	0.321	2.322	0.103
efg_amp_P_boltz	1.686	1.725	0.039	2.295	0.001
qpoletens_zz_max	-11.078	-10.827	0.251	2.264	0.063
qpoletens_zz_delta	11.068	11.318	0.25	2.259	0.062
efgtens_zz_P_boltz	1.376	1.407	0.031	2.245	0.001
vbur_qvbur_max_delta	14.718	14.396	0.322	2.189	0.104
nbo_P_ra_boltz	0.724	0.709	0.015	2.015	0.0
vbur_max_delta_qvbur_max	16.224	15.902	0.322	1.986	0.104
vbur_near_vtot_vbur_min_conf	360.561	353.536	7.026	1.949	49.358
sterimol_B5_min	6.737	6.608	0.129	1.919	0.017
pyr_P_vbur_min_conf	0.964	0.947	0.017	1.744	0.0
vmin_vmin_boltz	-0.044	-0.044	0.001	1.693	0.0
nbo_lp_P_e_boltz	-0.341	-0.335	0.006	1.665	0.0
vbur_qvbur_min_boltz	9.851	9.688	0.163	1.653	0.027
pyr_P_boltz	0.963	0.948	0.015	1.607	0.0
vbur_ovbur_max_delta	5.842	5.755	0.088	1.504	0.008
vbur_near_vbur_boltz	46.655	46.001	0.654	1.403	0.428
sterimol_B1_boltz	3.282	3.239	0.043	1.323	0.002
somo_rc_boltz	-0.371	-0.376	0.005	1.266	0.0

sterimol_burB1_vbur_min_conf	3.164	3.124	0.039	1.247	0.002
sterimol_B1_vbur_min_conf	3.164	3.124	0.039	1.247	0.002
Pint_P_int_boltz	19.782	20.025	0.243	1.226	0.059
fmo_e_lumo_boltz	-0.044	-0.044	0.001	1.205	0.0
vbur_qvbur_max_max	26.84	26.518	0.322	1.2	0.104
Pint_P_min_boltz	12.611	12.758	0.147	1.167	0.022
nbo_P_rc_boltz	1.072	1.084	0.011	1.064	0.0
Pint_dP_boltz	4.055	4.096	0.041	1.017	0.002

# KRAKEN ID 00000449

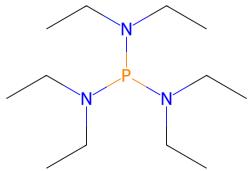


Table 1. Properties that exceed 1% relative difference

property	old	new	abs_diff	rel_diff (%)	squared_diff
vbur_ovtot_min_vbur_min_conf	0.0	0.0	0.0	inf	0.0
vbur_far_vtot_min	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_vbur_min_conf	0.0	0.0	0.0	inf	0.0
vbur_far_vbur_min	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_min	0.0	0.0	0.0	inf	0.0
vbur_ovtot_min_min	0.0	0.0	0.0	inf	0.0
vbur_ovtot_min_max	0.021	0.951	0.929	4353.44	0.864
vbur_ovtot_min_delta	0.021	0.951	0.929	4353.44	0.864
vbur_ovbur_min_max	0.022	0.528	0.506	2304.762	0.256
vbur_ovbur_min_delta	0.022	0.528	0.506	2304.762	0.256
vbur_ovtot_min_boltz	0.0	0.0	0.0	116.234	0.0
vbur_far_vbur_vbur_min_conf	0.001	0.0	0.001	100.0	0.0
vbur_far_vbur_max	7.688	13.854	6.166	80.193	38.015
vbur_far_vbur_delta	7.688	13.854	6.166	80.193	38.015
qpoletens_zz_delta	0.865	1.557	0.693	80.109	0.48
vbur_far_vtot_max	9.931	17.763	7.832	78.859	61.334
vbur_far_vtot_delta	9.931	17.763	7.832	78.859	61.334
vbur_near_vtot_delta	12.166	19.144	6.978	57.36	48.699
qpoletens_yy_max	1.047	1.627	0.58	55.425	0.336
vbur_far_vtot_vbur_min_conf	0.002	0.001	0.001	49.998	0.0
qpoletens_yy_min	-0.62	-0.314	0.307	49.446	0.094
vbur_vtot_delta	2.337	3.371	1.034	44.241	1.069
vbur_vbur_delta	22.101	31.53	9.429	42.662	88.903
vbur_qvbur_min_delta	5.113	7.269	2.156	42.156	4.647
qpole_amp_delta	1.292	1.676	0.383	29.656	0.147
dipolemoment_delta	0.534	0.686	0.152	28.448	0.023

vbur_far_vbur_boltz	0.271	0.196	0.075	27.66	0.006
qpoletens_zz_min	-2.593	-3.286	0.693	26.715	0.48
sterimol_B5_delta	0.47	0.585	0.115	24.437	0.013
sterimol_burB5_delta	0.47	0.585	0.115	24.437	0.013
vbur_near_vbur_delta	14.414	17.676	3.262	22.633	10.642
vbur_ovbur_min_boltz	0.0	0.0	0.0	21.381	0.0
dipolemoment_min	0.721	0.569	0.152	21.087	0.023
vbur_max_delta_qvbur_delta	10.527	8.619	1.908	18.122	3.639
qpoletens_yy_delta	1.667	1.94	0.273	16.402	0.075
vbur_far_vtot_boltz	0.433	0.366	0.067	15.395	0.004
vbur_max_delta_qvbur_max	13.945	12.034	1.911	13.703	3.651
vbur_qvbur_min_max	16.096	18.27	2.173	13.502	4.724
vbur_vbur_max	79.677	89.085	9.408	11.808	88.509
qpole_amp_max	3.641	4.024	0.383	10.523	0.147
qpoletens_yy_boltz	0.721	0.792	0.071	9.793	0.005
vbur_qvtot_max_delta	7.596	6.86	0.736	9.693	0.542
vbur_ovbur_max_delta	3.793	4.125	0.332	8.74	0.11
vbur_ovtot_max_delta	10.912	11.617	0.705	6.46	0.497
vbur_qvbur_max_delta	10.71	11.387	0.677	6.318	0.458
sterimol_burB1_delta	0.926	0.974	0.048	5.187	0.002
sterimol_B1_delta	0.959	1.007	0.048	5.058	0.002
vbur_near_vbur_max	71.989	75.231	3.242	4.504	10.513
qpoletens_xx_boltz	1.442	1.378	0.064	4.463	0.004
vbur_max_delta_qvtot_delta	21.314	22.06	0.747	3.503	0.557
vbur_qvtot_min_delta	16.941	17.452	0.511	3.015	0.261
vbur_ovbur_max_min	17.626	17.141	0.484	2.747	0.235
vbur_qvbur_max_min	17.626	17.141	0.484	2.747	0.235
vbur_near_vtot_min	286.999	279.729	7.27	2.533	52.853
vbur_max_delta_qvtot_boltz	23.256	22.731	0.525	2.258	0.276
qpoletens_xx_delta	1.645	1.681	0.036	2.177	0.001
sterimol_B5_min	5.343	5.228	0.115	2.154	0.013
sterimol_burB5_min	5.343	5.228	0.115	2.154	0.013
sterimol_L_delta	0.625	0.613	0.012	1.969	0.0
vbur_max_delta_qvtot_max	41.164	41.9	0.736	1.788	0.541
sterimol_B1_min	3.576	3.528	0.048	1.354	0.002

sterimol_burB1_min	3.576	3.528	0.048	1.354	0.002
dipolemoment_boltz	0.956	0.968	0.013	1.321	0.0
pyr_P_delta	0.046	0.045	0.001	1.287	0.0
qpoletens_xx_max	2.828	2.864	0.036	1.264	0.001
nmrten_syy_P_boltz	122.164	120.683	1.481	1.212	2.192
vbur_qvtot_min_min	48.102	47.594	0.508	1.057	0.258
pyr_alpha_min	18.918	18.718	0.199	1.053	0.04
vbur_qvbur_max_boltz	18.277	18.088	0.189	1.032	0.036

# KRAKEN ID 00000458

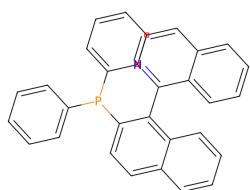


Table 1. Properties that exceed 1% relative difference

property	old	new	abs_diff	rel_diff (%)	squared_diff
vbur_ovbur_min_boltz	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_delta	0.0	0.0	0.0	inf	0.0
vbur_ovtot_min_max	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_max	0.0	0.0	0.0	inf	0.0
vbur_ovtot_min_boltz	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_min	0.0	0.0	0.0	inf	0.0
vbur_ovtot_min_min	0.0	0.0	0.0	inf	0.0
vbur_far_vbur_vbur_min_conf	0.0	0.0	0.0	inf	0.0
vbur_ovtot_min_delta	0.0	0.0	0.0	inf	0.0
vbur_far_vbur_min	0.0	0.0	0.0	inf	0.0
vbur_far_vtot_vbur_min_conf	0.0	0.0	0.0	inf	0.0
vbur_far_vtot_min	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_vbur_min_conf	0.0	0.0	0.0	inf	0.0
vbur_ovtot_min_vbur_min_conf	0.0	0.0	0.0	inf	0.0
vbur_qvtot_min_delta	7.104	25.966	18.862	265.529	355.774
qpoletens_yy_vbur_min_conf	2.537	-1.919	4.456	175.62	19.858
sterimol_B1_delta	0.28	0.568	0.287	102.399	0.082
sterimol_L_delta	1.982	3.344	1.361	68.682	1.853
sterimol_burB1_delta	0.314	0.527	0.213	67.945	0.045
qpoletens_xx_vbur_min_conf	6.278	9.852	3.574	56.935	12.774
vbur_max_delta_qvtot_delta	54.469	80.891	26.422	48.509	698.143
vbur_max_delta_qvbur_vbur_min_conf	3.463	4.805	1.342	38.75	1.801
vbur_qvtot_max_delta	55.862	73.139	17.276	30.927	298.472
vbur_qvtot_min_vbur_min_conf	64.068	82.93	18.862	29.441	355.782
vbur_qvtot_min_max	64.068	82.93	18.862	29.441	355.782
sterimol_burL_delta	0.98	1.243	0.264	26.914	0.07

pyr_P_delta	0.05	0.063	0.013	25.44	0.0
vbur_max_delta_qvtot_vbur_min_conf	104.755	78.307	26.447	25.247	699.464
vbur_max_delta_qvtot_min	104.755	78.307	26.447	25.247	699.464
pyr_alpha_delta	6.195	7.498	1.303	21.038	1.699
sterimol_B5_delta	0.22	0.26	0.039	17.851	0.002
qpole_amp_vbur_min_conf	11.115	12.793	1.678	15.096	2.816
sterimol_L_max	9.269	10.63	1.361	14.687	1.853
sterimol_L_vbur_min_conf	9.269	10.63	1.361	14.687	1.853
qpoletens_zz_vbur_min_conf	-8.815	-7.933	0.882	10.007	0.778
vbur_ovtot_max_vbur_min_conf	178.531	161.237	17.294	9.687	299.095
vbur_qvtot_max_min	178.531	161.237	17.294	9.687	299.095
vbur_qvtot_max_vbur_min_conf	178.531	161.237	17.294	9.687	299.095
vbur_near_vbur_delta	8.775	9.568	0.793	9.035	0.629
sterimol_burB1_vbur_min_conf	4.215	4.563	0.349	8.275	0.122
sterimol_B1_vbur_min_conf	4.301	4.638	0.338	7.852	0.114
sterimol_B1_max	4.351	4.638	0.287	6.599	0.082
dipolemoment_vbur_min_conf	2.871	3.05	0.179	6.235	0.032
vbur_qvbur_min_vbur_min_conf	11.947	11.239	0.708	5.927	0.501
pyr_alpha_max	24.063	25.367	1.304	5.418	1.7
pyr_alpha_vbur_min_conf	24.063	25.367	1.304	5.418	1.7
vbur_ovtot_max_delta	43.154	45.432	2.278	5.278	5.188
sterimol_burB1_max	4.349	4.563	0.214	4.925	0.046
sterimol_burL_max	7.959	8.223	0.264	3.312	0.069
sterimol_burL_vbur_min_conf	7.959	8.223	0.264	3.312	0.069
vbur_vbur_delta	35.756	36.558	0.801	2.241	0.642
sterimol_burB5_delta	1.001	1.018	0.017	1.712	0.0
vbur_near_vbur_min	54.501	53.712	0.789	1.447	0.622
vbur_near_vbur_vbur_min_conf	54.501	53.712	0.789	1.447	0.622
vbur_vbur_vbur_min_conf	54.501	53.712	0.789	1.447	0.622
vbur_vbur_min	54.501	53.712	0.789	1.447	0.622
pyr_P_vbur_min_conf	0.883	0.871	0.013	1.443	0.0
pyr_P_min	0.883	0.871	0.013	1.443	0.0
vbur_ovtot_max_min	163.512	161.237	2.275	1.391	5.176
vbur_ovbur_max_delta	5.849	5.909	0.061	1.037	0.004

# KRAKEN ID 00000487



Table 1. Properties that exceed 1% relative difference

property	old	new	abs_diff	rel_diff (%)	squared_diff
vbur_ovtot_min_vbur_min_conf	0.0	0.0	0.0	inf	0.0
vbur_ovtot_min_max	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_max	0.0	0.0	0.0	inf	0.0
vbur_far_vbur_delta	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_delta	0.0	0.0	0.0	inf	0.0
vbur_ovtot_min_delta	0.0	0.0	0.0	inf	0.0
vbur_far_vtot_min	0.0	0.0	0.0	inf	0.0
vbur_ovtot_min_boltz	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_boltz	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_min	0.0	0.0	0.0	inf	0.0
vbur_far_vbur_boltz	0.0	0.0	0.0	inf	0.0
vbur_ovtot_min_min	0.0	0.0	0.0	inf	0.0
vbur_far_vbur_vbur_min_conf	0.0	0.0	0.0	inf	0.0
vbur_far_vbur_max	0.0	0.0	0.0	inf	0.0
vbur_far_vtot_vbur_min_conf	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_vbur_min_conf	0.0	0.0	0.0	inf	0.0
vbur_far_vbur_min	0.0	0.0	0.0	inf	0.0
vbur_far_vtot_boltz	5.96	4.068	1.892	31.749	3.581
vbur_qvtot_max_delta	97.756	128.777	31.021	31.733	962.306
vbur_near_vtot_delta	46.973	60.645	13.672	29.105	186.911
qpoletens_yy_boltz	1.186	0.87	0.315	26.594	0.099
vbur_ovtot_max_delta	110.842	136.6	25.757	23.238	663.434
vbur_max_delta_qvtot_delta	107.462	131.742	24.279	22.593	589.488
vbur_vtot_delta	3.719	2.917	0.802	21.562	0.643
pyr_alpha_delta	1.469	1.785	0.316	21.535	0.1
pyr_P_delta	0.01	0.012	0.002	21.198	0.0

vbur_far_vtot_max	41.918	50.652	8.733	20.834	76.268
vbur_far_vtot_delta	41.918	50.652	8.733	20.834	76.268
qpoletens_xx_min	6.374	5.181	1.194	18.726	1.425
sterimol_burL_delta	0.373	0.434	0.061	16.401	0.004
qpoletens_xx_delta	9.885	11.327	1.442	14.593	2.081
sterimol_L_delta	4.349	4.922	0.573	13.174	0.328
vbur_ovbur_max_delta	0.87	0.768	0.102	11.779	0.011
vbur_qvbur_max_delta	0.87	0.768	0.102	11.779	0.011
qpole_amp_delta	17.417	15.459	1.958	11.241	3.833
sterimol_burB1_delta	0.363	0.333	0.03	8.255	0.001
vbur_max_delta_qvtot_max	329.992	356.426	26.434	8.011	698.76
dipolemoment_boltz	2.53	2.378	0.152	6.012	0.023
qpoletens_zz_delta	16.288	15.358	0.93	5.712	0.866
qpole_amp_min	10.205	10.784	0.579	5.669	0.335
vbur_max_delta_qvbur_boltz	1.824	1.726	0.098	5.368	0.01
vbur_qvtot_max_max	404.608	425.648	21.04	5.2	442.662
vbur_ovtot_max_max	404.608	425.648	21.04	5.2	442.662
dipolemoment_min	0.649	0.682	0.033	5.073	0.001
vbur_max_delta_qvbur_min	1.427	1.354	0.072	5.059	0.005
qpole_amp_max	27.623	26.243	1.379	4.994	1.903
qpoletens_yy_max	6.1	6.395	0.295	4.839	0.087
vbur_max_delta_qvbur_max	4.101	3.911	0.19	4.642	0.036
qpoletens_zz_min	-21.68	-20.691	0.989	4.56	0.977
vbur_max_delta_qvbur_delta	2.674	2.556	0.118	4.419	0.014
vbur_qvtot_min_delta	32.04	30.716	1.324	4.133	1.754
spindens_P_ra_boltz	0.03	0.031	0.001	3.481	0.0
qpoletens_yy_delta	10.041	10.379	0.338	3.362	0.114
vbur_qvtot_max_min	306.852	296.871	9.982	3.253	99.631
dipolemoment_delta	3.67	3.555	0.115	3.14	0.013
sterimol_L_max	12.959	13.332	0.373	2.88	0.139
qpoletens_xx_boltz	12.172	12.518	0.345	2.837	0.119
sterimol_burB5_delta	1.335	1.37	0.035	2.65	0.001
sterimol_L_min	8.609	8.41	0.2	2.319	0.04
vbur_vbur_delta	1.373	1.343	0.03	2.209	0.001
vbur_near_vbur_delta	1.373	1.343	0.03	2.209	0.001

dipolemoment_max	4.319	4.237	0.082	1.906	0.007
vbur_near_vtot_min	711.208	698.043	13.164	1.851	173.301
pyr_alpha_min	16.522	16.237	0.285	1.725	0.081
vbur_ovtot_max_min	293.766	289.048	4.718	1.606	22.256
vbur_qvbur_min_delta	1.213	1.232	0.019	1.552	0.0
qpoletens_xx_max	16.259	16.508	0.249	1.531	0.062
vbur_qvtot_min_max	88.264	86.967	1.296	1.469	1.681
fukui_p_boltz	0.042	0.043	0.001	1.455	0.0
qpole_amp_boltz	18.491	18.751	0.26	1.405	0.067
sterimol_B1_delta	1.623	1.601	0.023	1.391	0.001
sterimol_B1_boltz	5.072	5.132	0.059	1.168	0.004
qpoletens_zz_max	-5.391	-5.333	0.058	1.08	0.003
qpoletens_yy_min	-3.941	-3.984	0.042	1.077	0.002

# KRAKEN ID 00000640

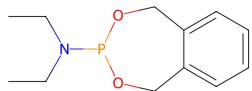


Table 1. Properties that exceed 1% relative difference

property	old	new	abs_diff	rel_diff (%)	squared_diff
vbur_ovtot_min_vbur_min_conf	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_min	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_vbur_min_conf	0.0	0.0	0.0	inf	0.0
vbur_far_vtot_vbur_min_conf	0.0	0.0	0.0	inf	0.0
vbur_far_vbur_vbur_min_conf	0.0	0.0	0.0	inf	0.0
vbur_far_vbur_min	0.0	0.0	0.0	inf	0.0
vbur_ovtot_min_min	0.0	0.0	0.0	inf	0.0
vbur_far_vtot_min	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_boltz	0.0	0.0	0.0	301.947	0.0
vbur_ovbur_min_max	0.006	0.017	0.01	166.667	0.0
vbur_ovbur_min_delta	0.006	0.017	0.01	166.667	0.0
vbur_ovtot_min_boltz	0.0	0.0	0.0	144.735	0.0
vbur_ovtot_min_delta	0.032	0.041	0.009	27.592	0.0
vbur_ovtot_min_max	0.032	0.041	0.009	27.592	0.0
nmrtens_sxx_P_boltz	-6.239	-7.931	1.692	27.129	2.864
vbur_far_vtot_boltz	0.4	0.363	0.037	9.347	0.001
pyr_alpha_delta	6.525	7.076	0.551	8.444	0.304
vbur_qvtot_max_delta	19.706	18.104	1.603	8.132	2.568
vbur_max_delta_qvtot_delta	38.093	35.085	3.009	7.898	9.051
vbur_max_delta_qvbur_delta	10.887	11.655	0.768	7.052	0.589
vbur_far_vbur_boltz	0.154	0.144	0.01	6.615	0.0
vbur_qvtot_min_delta	21.495	20.149	1.346	6.26	1.811
vbur_max_delta_qvtot_min	50.259	53.245	2.986	5.941	8.915
vbur_max_delta_qvbur_max	13.549	14.316	0.768	5.666	0.589
qpoletens_xx_delta	2.304	2.424	0.12	5.207	0.014
pyr_P_delta	0.049	0.052	0.002	5.014	0.0

vbur_far_vbur_delta	7.611	7.99	0.379	4.975	0.143
vbur_far_vbur_max	7.611	7.99	0.379	4.975	0.143
pyr_alpha_min	12.316	11.759	0.557	4.521	0.31
dipolemoment_delta	2.372	2.288	0.083	3.52	0.007
vbur_qvbur_max_delta	11.353	11.748	0.394	3.473	0.155
qpoletens_yy_boltz	-0.7	-0.724	0.024	3.436	0.001
vbur_near_vtot_delta	31.763	32.761	0.999	3.144	0.997
vbur_ovtot_max_delta	25.136	24.358	0.778	3.097	0.606
vbur_qvtot_min_max	44.25	42.901	1.349	3.048	1.82
vbur_far_vtot_delta	26.353	27.135	0.782	2.967	0.612
vbur_far_vtot_max	26.353	27.135	0.782	2.967	0.612
dipolemoment_max	2.837	2.753	0.084	2.965	0.007
vbur_vtot_delta	1.277	1.314	0.038	2.941	0.001
qpoletens_xx_min	4.36	4.24	0.12	2.762	0.015
sterimol_B5_delta	0.511	0.524	0.013	2.639	0.0
qpoletens_yy_max	2.33	2.278	0.052	2.217	0.003
dipolemoment_boltz	0.911	0.892	0.019	2.115	0.0
vbur_qvtot_max_min	94.541	96.146	1.606	1.698	2.578
vbur_vbur_delta	26.131	26.566	0.435	1.665	0.189
vbur_qvbur_max_max	24.06	24.454	0.394	1.639	0.155
qpoletens_yy_delta	3.506	3.455	0.052	1.472	0.003
spindens_P_rc_boltz	0.035	0.035	0.0	1.352	0.0
qpoletens_zz_boltz	-4.318	-4.262	0.055	1.278	0.003
vbur_qvtot_min_boltz	32.012	31.624	0.388	1.213	0.151
sterimol_L_delta	1.608	1.625	0.017	1.072	0.0

# KRAKEN ID 00000644



Table 1. Properties that exceed 1% relative difference

property	old	new	abs_diff	rel_diff (%)	squared_diff
vbur_ovtot_min_vbur_min_conf	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_delta	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_boltz	0.0	0.0	0.0	inf	0.0
vbur_ovtot_min_boltz	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_vbur_min_conf	0.0	0.0	0.0	inf	0.0
vbur_far_vtot_vbur_min_conf	0.0	0.0	0.0	inf	0.0
vbur_far_vbur_vbur_min_conf	0.0	0.0	0.0	inf	0.0
vbur_ovtot_min_min	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_min	0.0	0.0	0.0	inf	0.0
vbur_far_vtot_min	0.0	0.0	0.0	inf	0.0
vbur_far_vbur_min	0.0	0.0	0.0	inf	0.0
vbur_ovtot_min_max	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_max	0.0	0.0	0.0	inf	0.0
vbur_ovtot_min_delta	0.0	0.0	0.0	inf	0.0
vbur_far_vbur_boltz	0.0	0.0	0.0	99.748	0.0
vbur_far_vbur_max	1.776	0.018	1.758	98.999	3.091
vbur_far_vbur_delta	1.776	0.018	1.758	98.999	3.091
vbur_far_vtot_boltz	0.003	0.0	0.002	90.291	0.0
vbur_far_vtot_delta	8.615	1.066	7.549	87.628	56.994
vbur_far_vtot_max	8.615	1.066	7.549	87.628	56.994
vbur_near_vtot_delta	10.952	3.726	7.226	65.979	52.215
vbur_qvbur_max_delta	10.127	6.476	3.651	36.053	13.332
vbur_qvbur_min_delta	0.553	0.37	0.183	33.081	0.034
vbur_max_delta_qvbur_delta	9.955	6.754	3.2	32.15	10.243
vbur_max_delta_qvbur_max	11.031	7.834	3.197	28.985	10.223
qpoletens_zz_delta	5.437	4.031	1.406	25.856	1.976

vbur_ovbur_max_delta	8.352	6.458	1.893	22.668	3.584
vbur_vtot_delta	1.237	0.981	0.256	20.682	0.065
vbur_ovtot_max_delta	31.236	25.353	5.883	18.834	34.611
vbur_qvbur_max_max	20.351	16.703	3.648	17.926	13.309
vbur_qvtot_max_delta	31.236	26.079	5.157	16.509	26.591
qpoletens_zz_min	-8.779	-7.373	1.406	16.012	1.976
sterimol_burL_delta	1.414	1.197	0.216	15.312	0.047
dipolemoment_min	1.703	1.959	0.256	15.015	0.065
dipolemoment_delta	2.28	2.024	0.256	11.225	0.066
sterimol_burB1_delta	0.616	0.552	0.064	10.398	0.004
sterimol_B1_delta	0.624	0.56	0.064	10.258	0.004
vbur_ovbur_max_max	18.575	16.685	1.89	10.175	3.572
vbur_ovtot_max_max	111.218	105.339	5.879	5.286	34.564
vbur_qvtot_max_max	111.218	106.065	5.153	4.633	26.551
vbur_vbur_delta	10.889	10.415	0.474	4.351	0.224
vbur_near_vtot_min	229.439	236.544	7.105	3.097	50.485
sterimol_burL_max	8.088	7.871	0.217	2.678	0.047
sterimol_burB1_min	2.634	2.698	0.064	2.43	0.004
sterimol_B1_min	2.634	2.698	0.064	2.43	0.004
vbur_qvbur_min_max	9.32	9.138	0.182	1.953	0.033

# KRAKEN ID 00000648

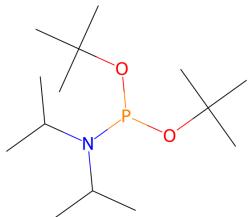


Table 1. Properties that exceed 1% relative difference

property	old	new	abs_diff	rel_diff (%)	squared_diff
vbur_ovtot_min_vbur_min_conf	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_vbur_min_conf	0.0	0.0	0.0	inf	0.0
vbur_ovtot_min_min	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_min	0.0	0.0	0.0	inf	0.0
qpoletens_yy_min	0.22	-0.143	0.364	165.13	0.132
qpoletens_yy_delta	0.876	1.24	0.364	41.524	0.132
sterimol_L_delta	0.247	0.28	0.033	13.522	0.001
vbur_near_vtot_delta	11.421	10.555	0.866	7.581	0.75
sterimol_burL_delta	0.297	0.319	0.021	7.216	0.0
vbur_qvtot_min_delta	12.758	13.511	0.753	5.903	0.567
vbur_vtot_delta	1.642	1.729	0.087	5.314	0.008
vbur_near_vbur_delta	18.032	18.542	0.509	2.825	0.259
vbur_qvtot_max_delta	16.071	16.474	0.403	2.507	0.162
vbur_ovbur_max_delta	1.665	1.705	0.04	2.387	0.002
vbur_qvbur_min_delta	8.86	9.044	0.184	2.078	0.034
vbur_far_vtot_min	1.694	1.724	0.03	1.784	0.001
vbur_far_vtot_vbur_min_conf	1.694	1.724	0.03	1.784	0.001
vbur_max_delta_qvtot_min	23.51	23.096	0.414	1.761	0.171
vbur_qvbur_min_min	10.405	10.223	0.182	1.749	0.033
sterimol_burB5_delta	0.082	0.084	0.001	1.686	0.0
sterimol_B5_delta	0.082	0.084	0.001	1.686	0.0
vbur_max_delta_qvtot_delta	27.411	27.825	0.415	1.512	0.172
vbur_far_vtot_boltz	6.665	6.573	0.091	1.371	0.008
fukui_p_boltz	0.002	0.002	0.0	1.2	0.0
vbur_ovtot_max_delta	21.164	21.392	0.227	1.074	0.052

# KRAKEN ID 00000650

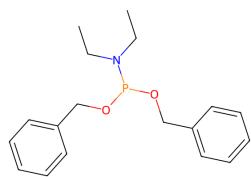


Table 1. Properties that exceed 1% relative difference

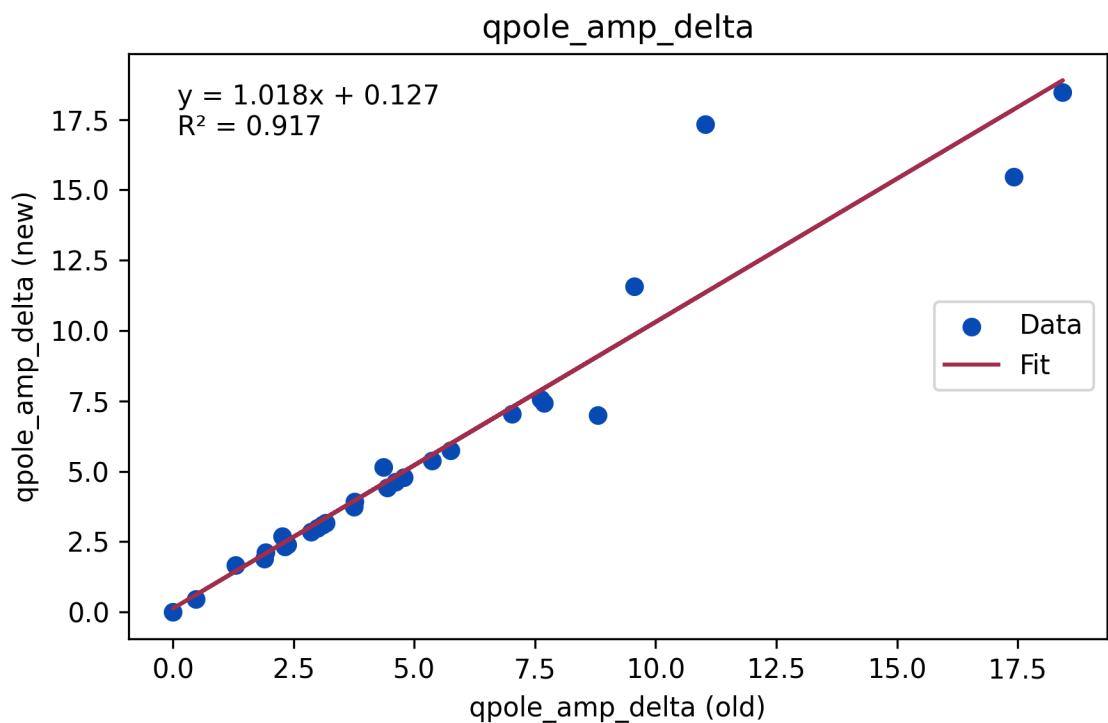
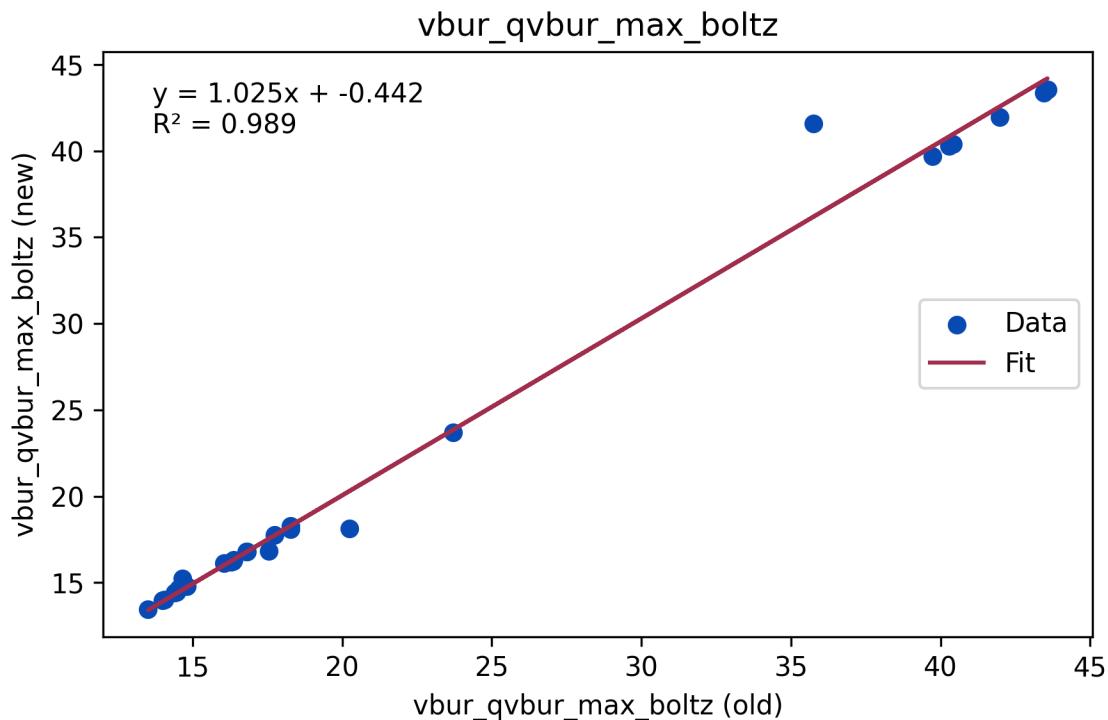
property	old	new	abs_diff	rel_diff (%)	squared_diff
vbur_ovtot_min_min	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_vbur_min_conf	0.0	0.0	0.0	inf	0.0
vbur_ovbur_min_min	0.0	0.0	0.0	inf	0.0
vbur_far_vbur_vbur_min_conf	0.0	0.0	0.0	inf	0.0
vbur_far_vtot_min	0.0	0.0	0.0	inf	0.0
vbur_far_vbur_min	0.0	0.0	0.0	inf	0.0
vbur_far_vtot_vbur_min_conf	0.0	0.0	0.0	inf	0.0
vbur_ovtot_min_vbur_min_conf	0.0	0.0	0.0	inf	0.0
nmrtens_sxx_P_boltz	-0.962	-2.082	1.12	116.401	1.255
vbur_ovtot_min_boltz	0.002	0.001	0.002	77.951	0.0
vbur_ovbur_min_boltz	0.001	0.0	0.001	75.118	0.0
qpoletens_yy_vbur_min_conf	-1.436	-0.419	1.017	70.845	1.035
spindens_P_rc_boltz	0.052	0.023	0.029	55.837	0.001
vbur_far_vbur_boltz	3.265	1.459	1.806	55.32	3.262
vbur_far_vtot_boltz	15.176	6.805	8.371	55.158	70.07
qpoletens_yy_boltz	0.217	0.105	0.113	51.749	0.013
qpoletens_xx_vbur_min_conf	9.033	4.471	4.562	50.506	20.814
qpole_amp_vbur_min_conf	11.89	6.049	5.842	49.13	34.125
qpoletens_zz_vbur_min_conf	-7.597	-4.052	3.545	46.662	12.567
qpoletens_zz_max	-2.49	-1.454	1.036	41.599	1.073
vbur_max_delta_qvbur_vbur_min_conf	3.983	5.5	1.518	38.104	2.303
sterimol_B1_delta	1.354	1.855	0.502	37.071	0.252
sterimol_burB1_delta	1.354	1.843	0.489	36.116	0.239
vbur_max_delta_qvbur_min	3.983	5.268	1.285	32.274	1.652
fukui_m_boltz	0.083	0.057	0.026	31.472	0.001
dipolemoment_vbur_min_conf	1.294	1.678	0.384	29.675	0.147

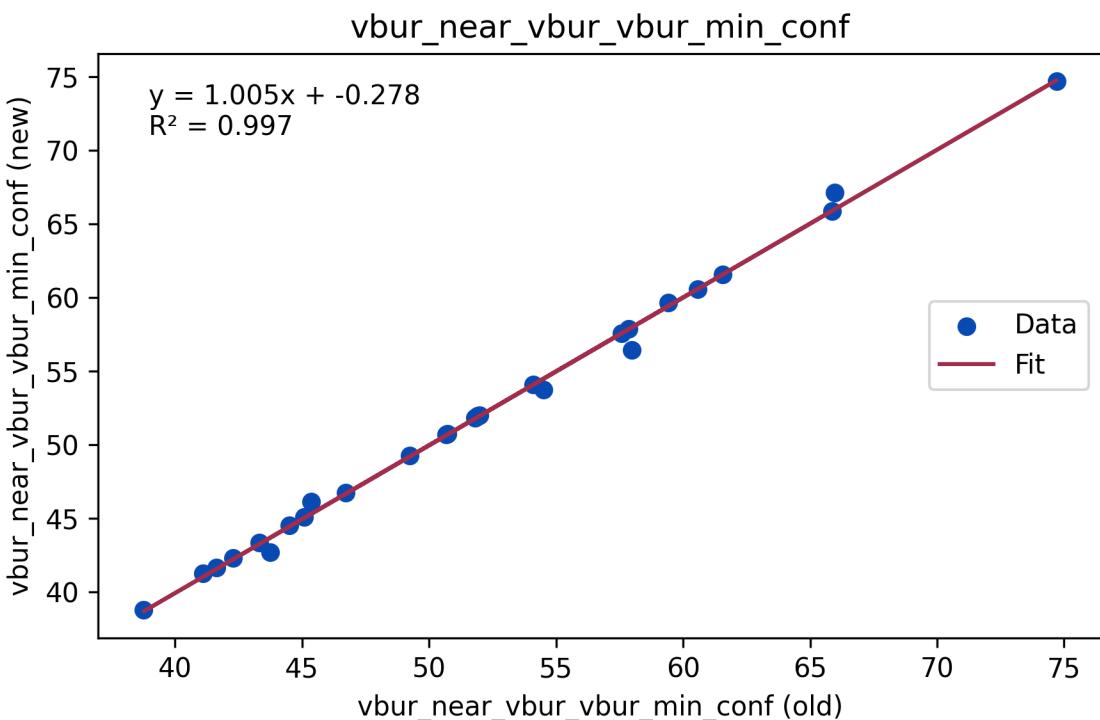
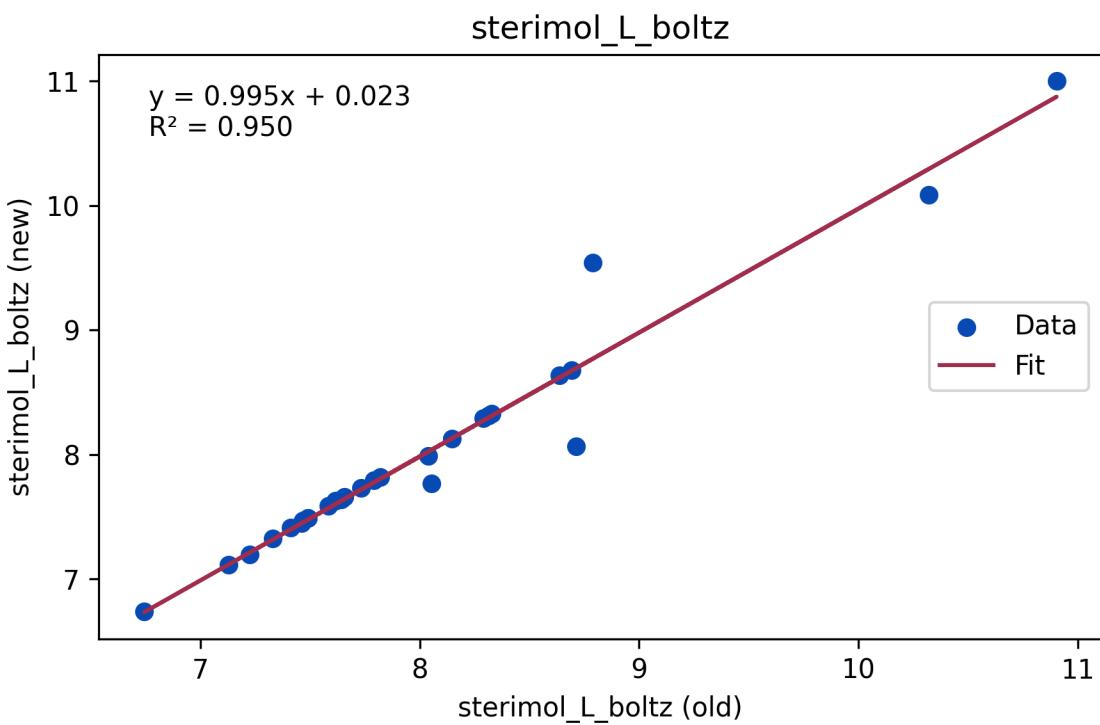
qpoletens_xx_delta	7.072	5.233	1.84	26.011	3.384
qpoletens_xx_max	9.261	7.027	2.235	24.129	4.994
spindens_P_ra_boltz	0.058	0.045	0.013	22.049	0.0
vbur_max_delta_qvtot_vbur_min_conf	131.873	103.434	28.439	21.565	808.769
qpole_amp_delta	8.804	6.99	1.814	20.606	3.291
vbur_max_delta_qvbur_boltz	9.221	7.378	1.843	19.988	3.397
vbur_qvtot_min_boltz	38.086	45.055	6.969	18.298	48.566
qpoletens_xx_min	2.189	1.794	0.395	18.05	0.156
qpole_amp_max	12.208	10.054	2.154	17.646	4.64
fukui_p_boltz	0.043	0.036	0.007	15.97	0.0
vbur_ovbur_max_delta	8.672	7.35	1.322	15.245	1.748
vbur_qvtot_min_delta	46.855	40.036	6.819	14.553	46.493
vbur_qvtot_min_vbur_min_conf	45.759	52.105	6.346	13.868	40.272
dipolemoment_min	0.847	0.736	0.111	13.057	0.012
vbur_qvtot_min_max	66.62	58.466	8.154	12.24	66.494
vbur_qvtot_max_vbur_min_conf	179.476	158.336	21.139	11.778	446.871
vbur_ovtot_max_vbur_min_conf	179.476	158.336	21.139	11.778	446.871
vbur_max_delta_qvtot_boltz	100.754	89.754	11.0	10.918	121.006
sterimol_burB1_boltz	3.481	3.855	0.374	10.755	0.14
qpoletens_zz_delta	5.665	6.267	0.602	10.624	0.362
sterimol_B1_max	4.01	4.435	0.425	10.609	0.181
vbur_qvbur_max_boltz	20.235	18.114	2.121	10.48	4.497
sterimol_burB1_max	4.01	4.422	0.412	10.287	0.17
dipolemoment_boltz	1.262	1.391	0.128	10.171	0.016
sterimol_L_vbur_min_conf	8.936	9.835	0.899	10.061	0.808
qpole_amp_min	3.403	3.063	0.34	9.989	0.116
vbur_qvbur_max_min	13.39	14.712	1.322	9.873	1.748
vbur_ovbur_max_min	13.39	14.712	1.322	9.873	1.748
vbur_ovbur_max_vbur_min_conf	13.39	14.712	1.322	9.873	1.748
vbur_qvbur_max_vbur_min_conf	13.39	14.712	1.322	9.873	1.748
sterimol_B1_boltz	3.567	3.908	0.341	9.561	0.116
pyr_alpha_delta	8.192	7.532	0.66	8.056	0.436
vbur_max_delta_qvbur_delta	17.104	15.82	1.283	7.503	1.647
sterimol_L_boltz	8.712	8.068	0.645	7.401	0.416
sterimol_burB1_vbur_min_conf	3.636	3.901	0.265	7.284	0.07

vbur_ratio_vbur_vtot_boltz	0.162	0.151	0.011	6.941	0.0
vbur_vbur_boltz	58.593	54.529	4.065	6.937	16.521
vbur_qvtot_min_min	19.765	18.43	1.336	6.758	1.784
sterimol_L_delta	4.748	4.431	0.317	6.672	0.1
nmrtens_syy_P_boltz	72.811	77.636	4.826	6.628	23.287
vbur_qvbur_max_delta	20.619	19.306	1.313	6.366	1.723
qpoletens_zz_boltz	-5.794	-5.439	0.355	6.134	0.126
pyr_P_delta	0.059	0.056	0.003	5.748	0.0
qpoletens_yy_min	-1.98	-2.092	0.112	5.678	0.013
pyr_alpha_vbur_min_conf	17.422	18.391	0.969	5.562	0.939
vbur_qvtot_max_boltz	148.636	140.39	8.247	5.548	68.008
qpoletens_zz_min	-8.155	-7.721	0.434	5.322	0.188
vbur_ovtot_max_delta	97.776	92.868	4.907	5.019	24.083
dipolemoment_max	2.583	2.458	0.126	4.858	0.016
vbur_ovbur_max_boltz	17.919	17.1	0.818	4.568	0.67
qpoletens_xx_boltz	5.577	5.334	0.243	4.356	0.059
sterimol_B1_vbur_min_conf	3.746	3.901	0.155	4.136	0.024
vbur_near_vbur_boltz	55.328	53.07	2.258	4.082	5.1
vbur_max_delta_qvtot_min	64.619	61.993	2.626	4.063	6.894
qpole_amp_boltz	8.118	7.796	0.322	3.966	0.104
sterimol_burL_vbur_min_conf	7.618	7.317	0.302	3.959	0.091
nbo_bds_occ_max_boltz	0.104	0.1	0.003	3.344	0.0
pyr_alpha_max	20.36	19.699	0.661	3.247	0.437
sterimol_L_max	10.656	10.339	0.317	2.973	0.1
vbur_ovtot_max_boltz	141.244	137.1	4.144	2.934	17.175
Pint_dP_boltz	3.981	3.866	0.115	2.893	0.013
sterimol_B1_min	2.656	2.58	0.076	2.877	0.006
sterimol_burB1_min	2.656	2.58	0.076	2.877	0.006
vbur_max_delta_qvtot_delta	93.609	96.231	2.621	2.8	6.872
sterimol_B5_boltz	8.04	8.262	0.222	2.76	0.049
vbur_ovtot_max_max	184.361	179.454	4.907	2.662	24.078
qpoletens_yy_delta	4.344	4.459	0.115	2.639	0.013
E_solv_cds_boltz	-7.334	-7.517	0.183	2.502	0.034
vmin_vmin_boltz	-0.041	-0.04	0.001	2.498	0.0
vbur_near_vbur_delta	29.373	28.644	0.729	2.482	0.531

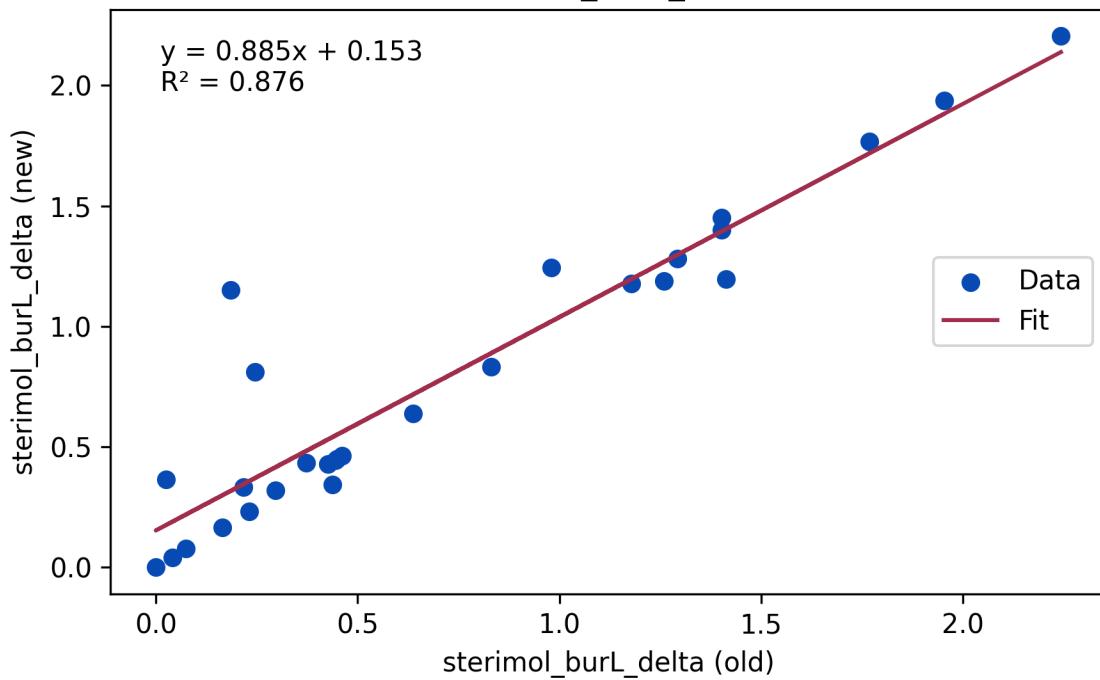
sterimol_burL_boltz	7.361	7.19	0.171	2.323	0.029
vbur_near_vtot_boltz	344.559	352.546	7.987	2.318	63.784
vbur_qvbur_min_vbur_min_conf	9.407	9.211	0.196	2.079	0.038
E_solv_total_boltz	-14.979	-15.264	0.285	1.905	0.081
fmo_e_lumo_boltz	-0.016	-0.016	0.0	1.889	0.0
sterimol_burL_delta	2.243	2.204	0.039	1.719	0.001
nbo_P_rc_boltz	1.525	1.499	0.026	1.678	0.001
vbur_near_vbur_min	45.348	46.105	0.756	1.668	0.572
vbur_near_vbur_vbur_min_conf	45.348	46.105	0.756	1.668	0.572
vbur_vbur_min	45.348	46.105	0.756	1.668	0.572
vbur_vbur_vbur_min_conf	45.348	46.105	0.756	1.668	0.572
fmo_eta_boltz	0.225	0.229	0.003	1.499	0.0
sterimol_B5_vbur_min_conf	7.911	8.025	0.114	1.447	0.013
nbo_bds_occ_avg_boltz	0.086	0.084	0.001	1.343	0.0
E_solv_elstat_boltz	-7.645	-7.747	0.102	1.333	0.01
somo_ra_boltz	0.073	0.072	0.001	1.304	0.0
vbur_vtot_delta	3.156	3.196	0.041	1.288	0.002
fmo_e_homo_boltz	-0.242	-0.245	0.003	1.271	0.0
surface_area_boltz	369.108	373.678	4.57	1.238	20.888
vbur_vbur_delta	56.338	55.646	0.691	1.227	0.478
sterimol_burB5_vbur_min_conf	6.58	6.507	0.073	1.112	0.005
sterimol_burB5_boltz	6.87	6.796	0.074	1.082	0.006
sphericity_boltz	0.74	0.732	0.008	1.081	0.0
fmo_mu_boltz	-0.129	-0.13	0.001	1.072	0.0
vbur_qvbur_min_delta	7.297	7.374	0.076	1.046	0.006
Pint_P_min_boltz	12.209	12.332	0.123	1.009	0.015

## Linear regressions for all properties with at least 1% difference in any tested monophosphine

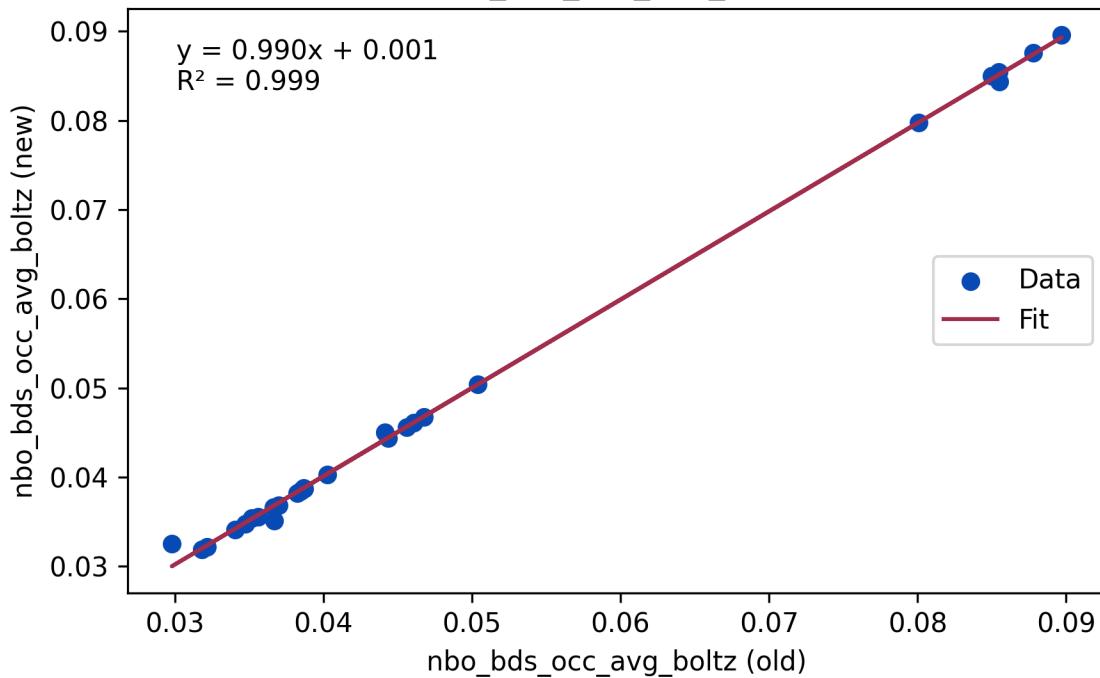




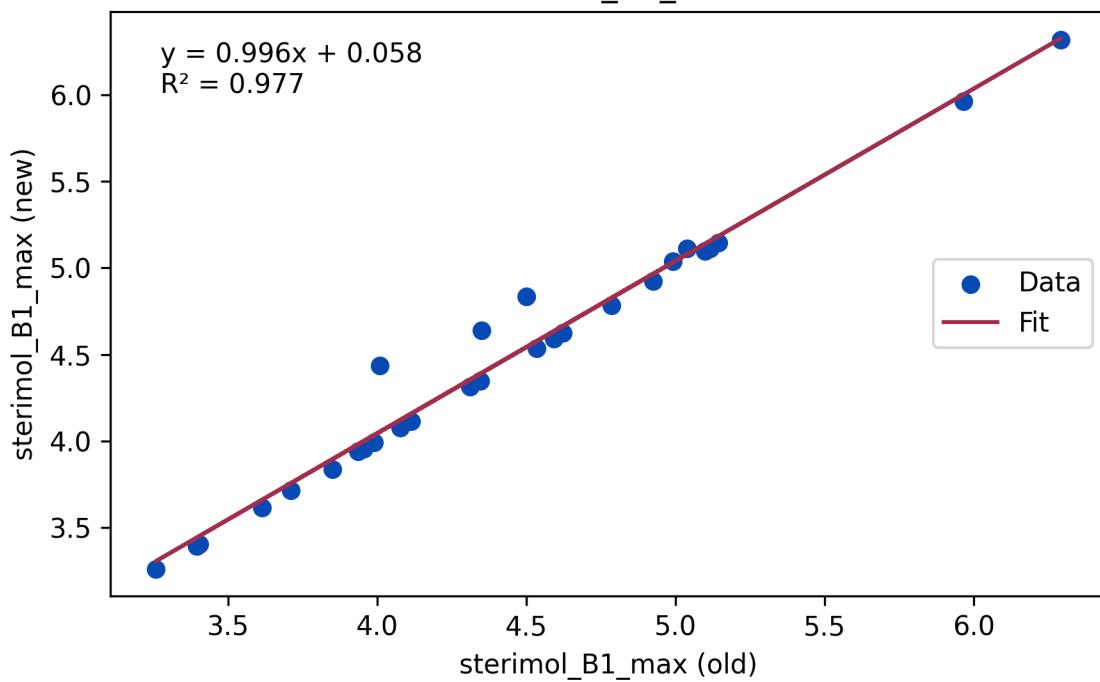
sterimol\_burL\_delta



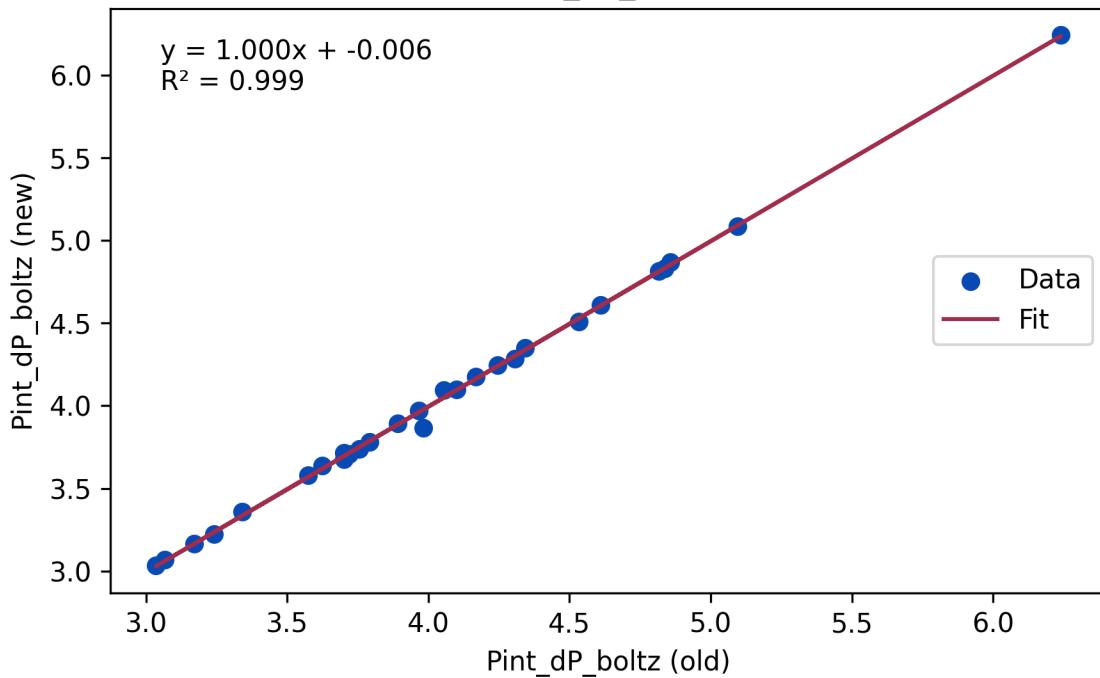
nbo\_bds\_occ\_avg\_boltz

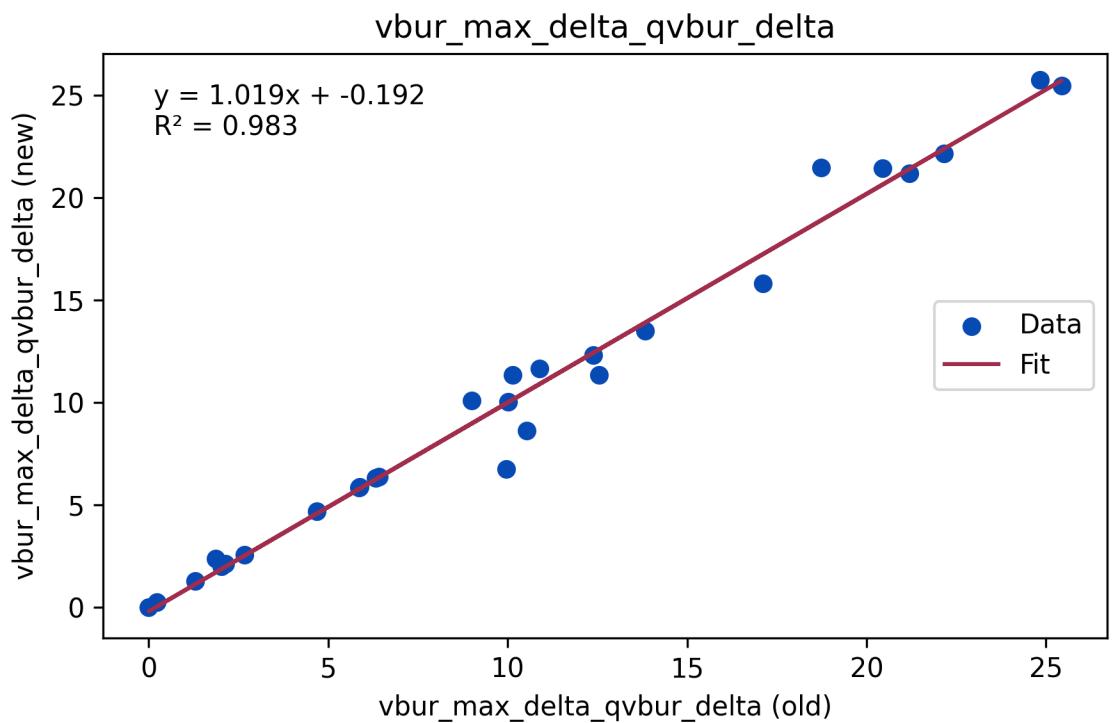
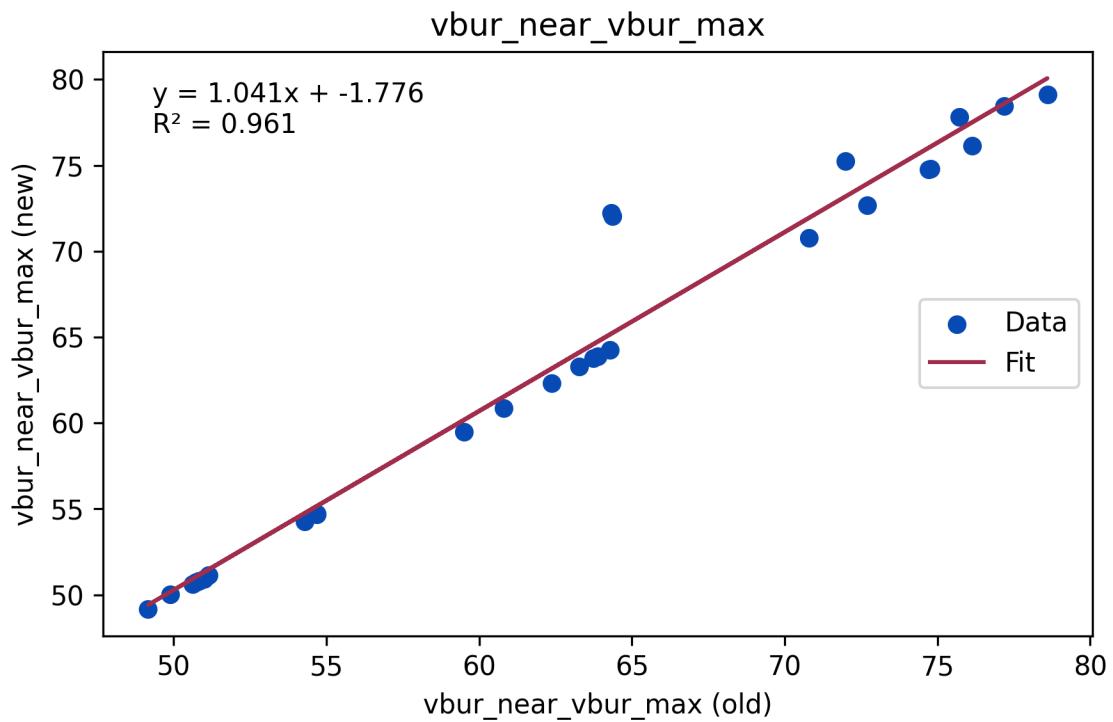


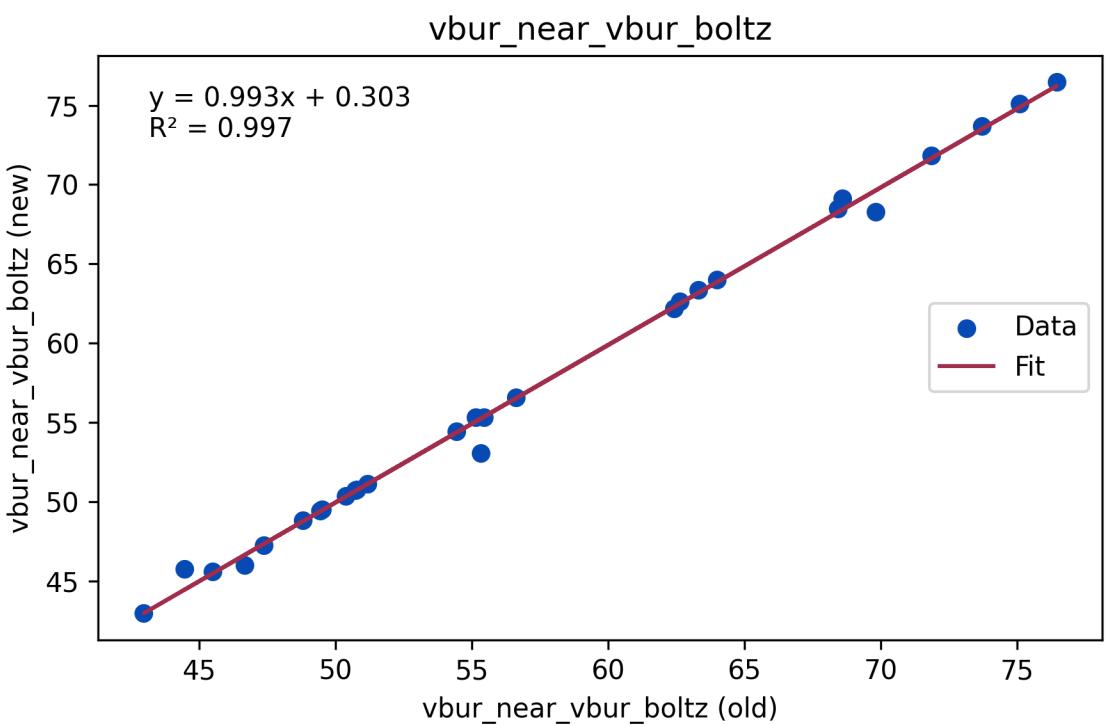
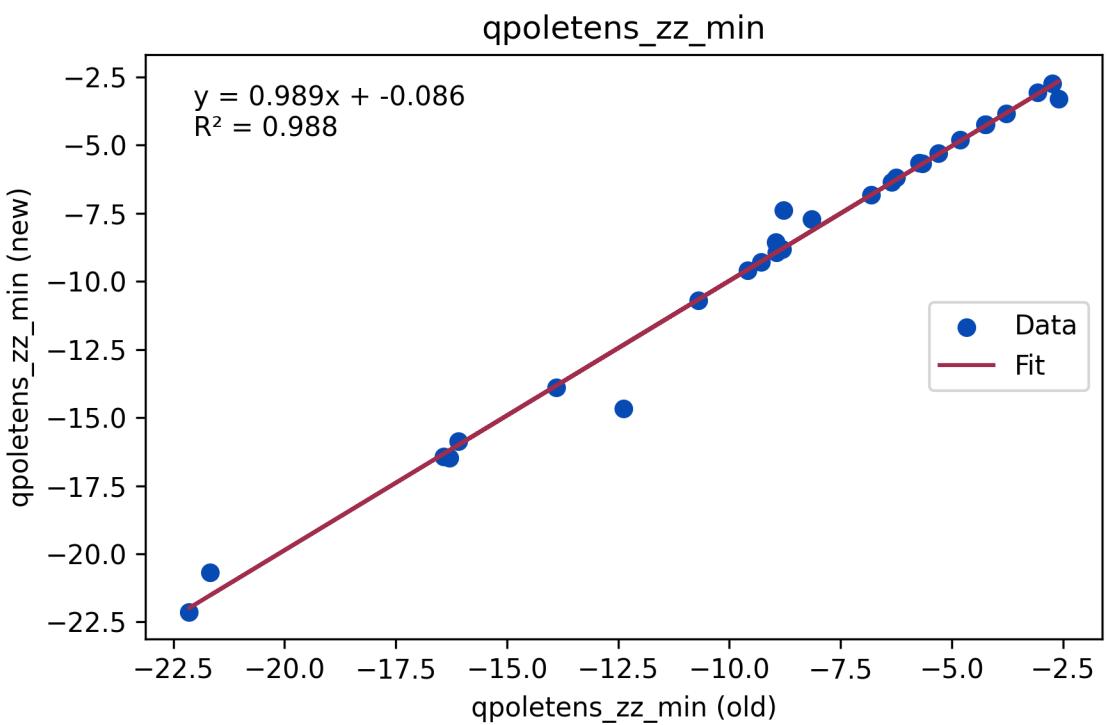
sterimol\_B1\_max



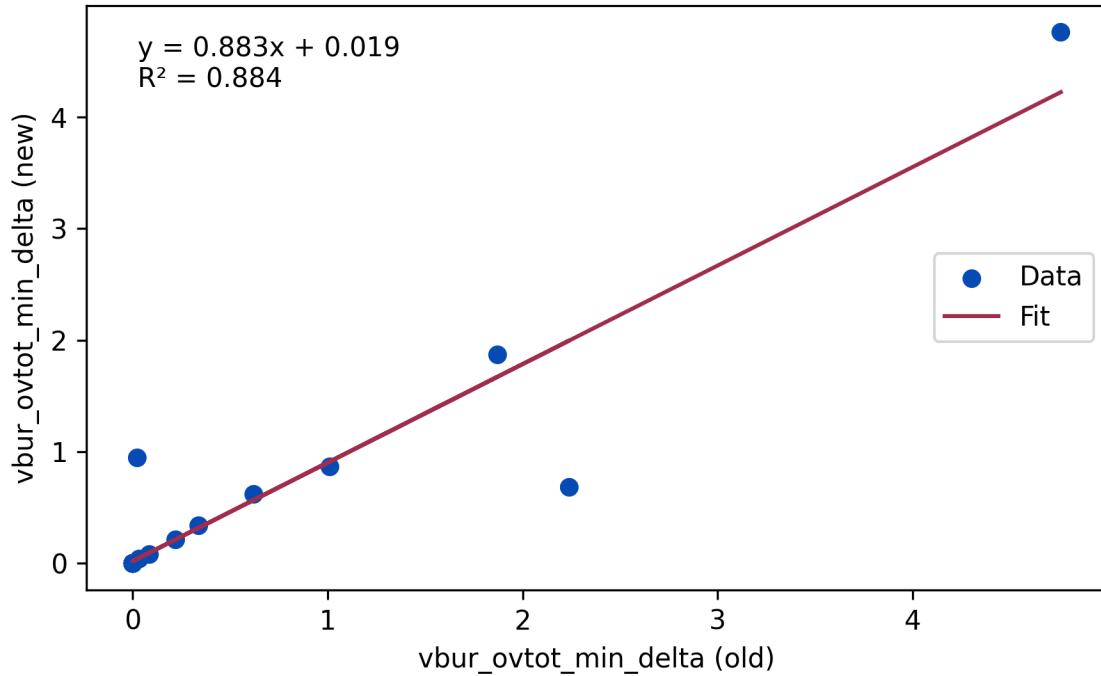
Pint\_dP\_boltz



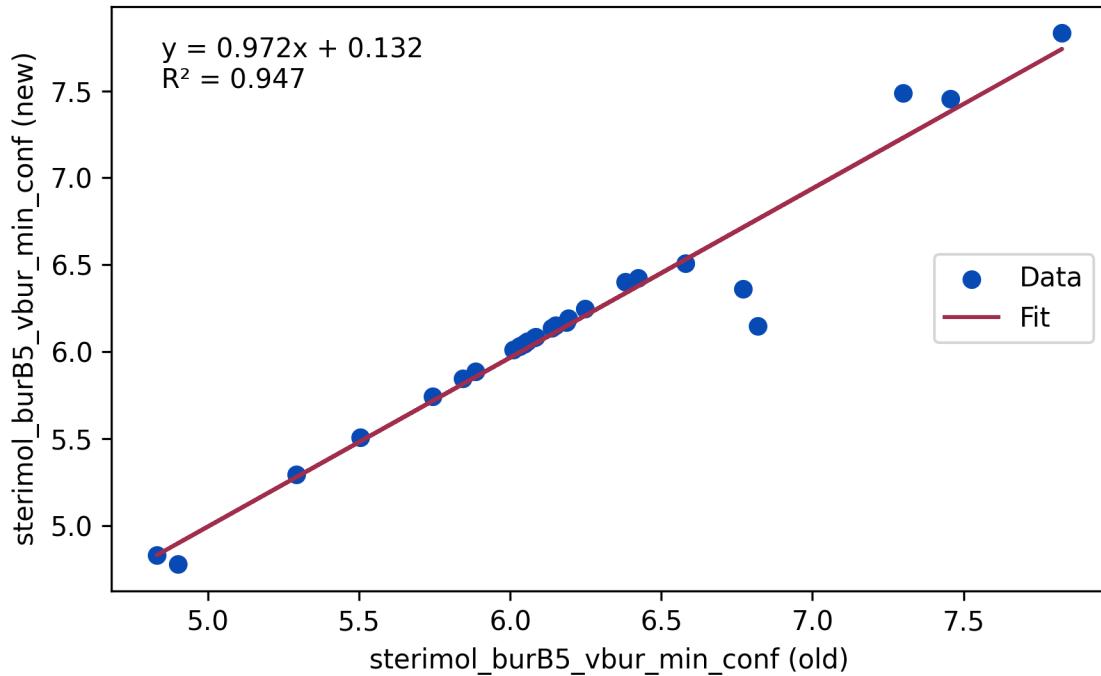


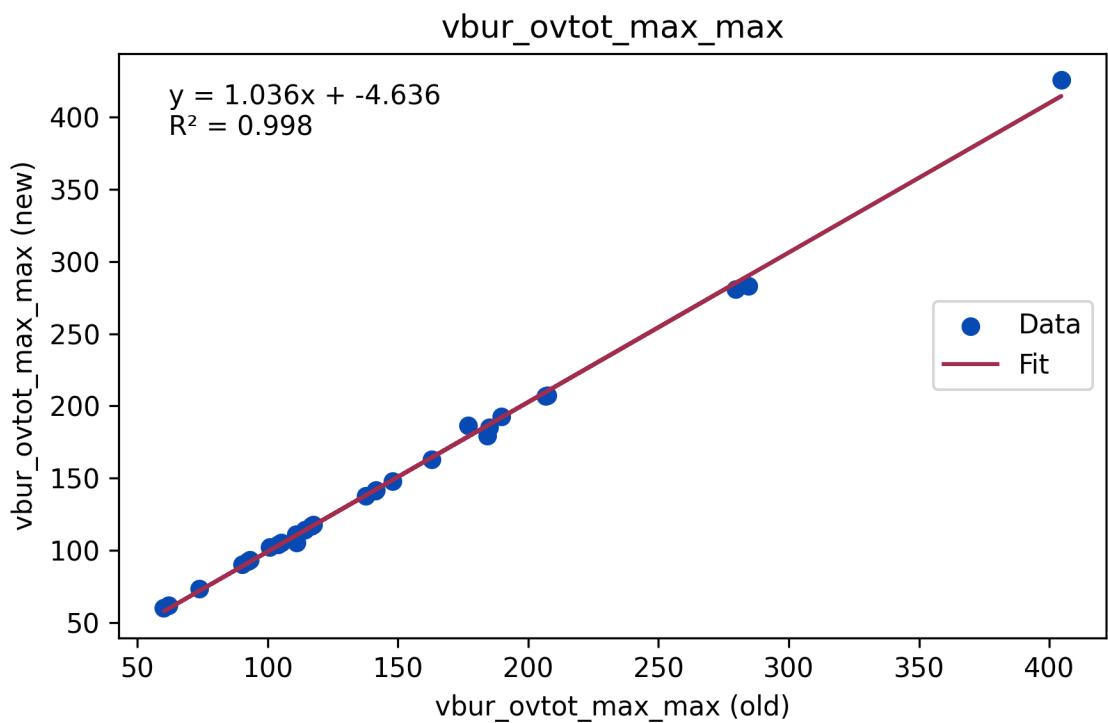
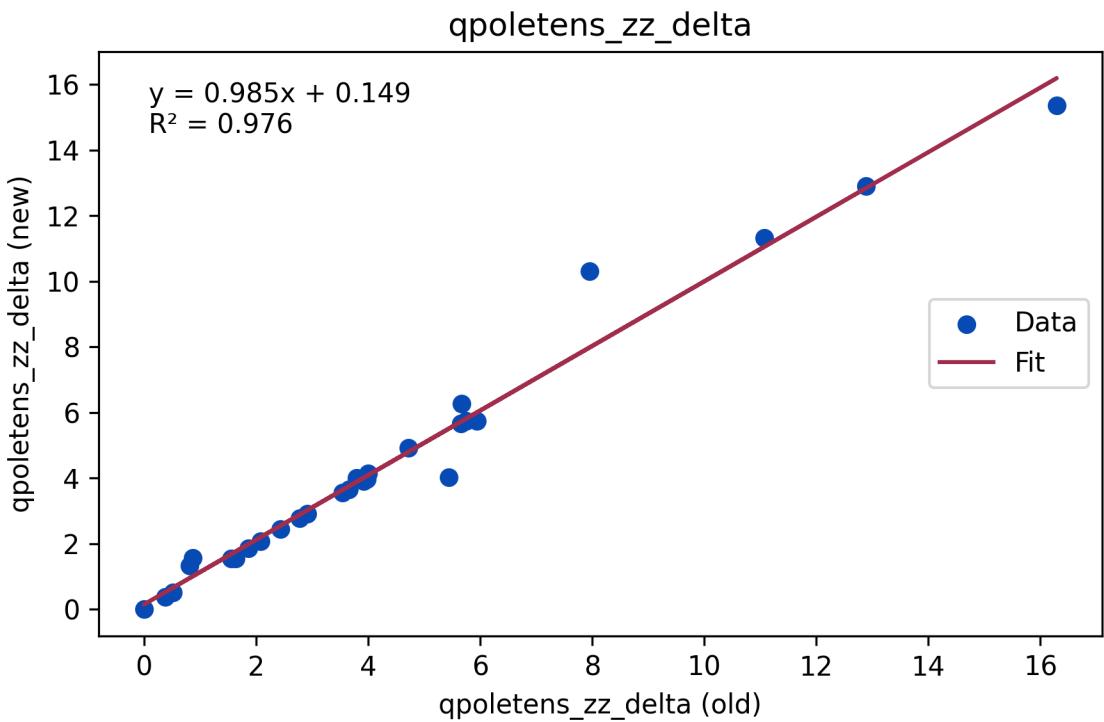


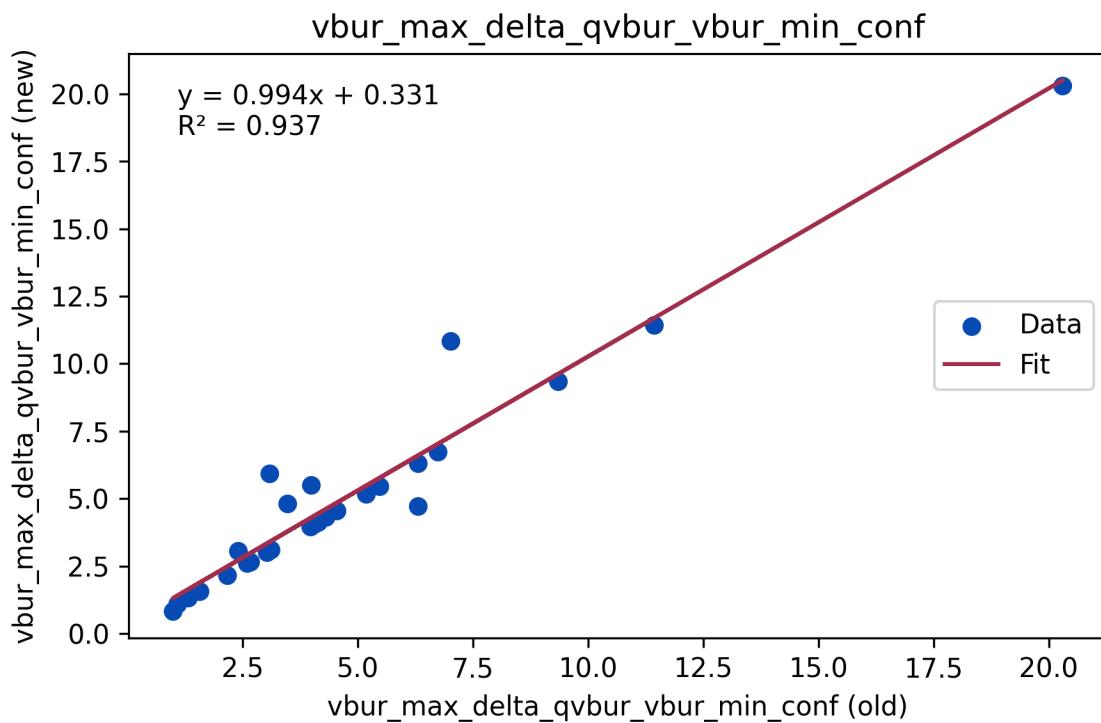
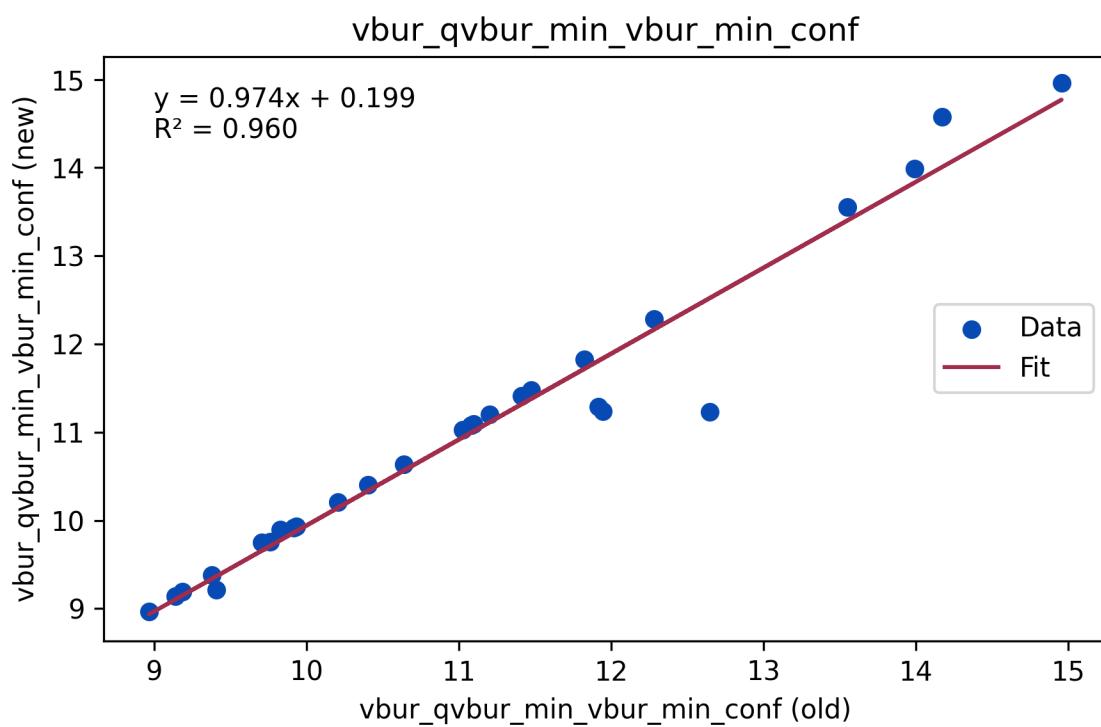
vbur\_ovtot\_min\_delta

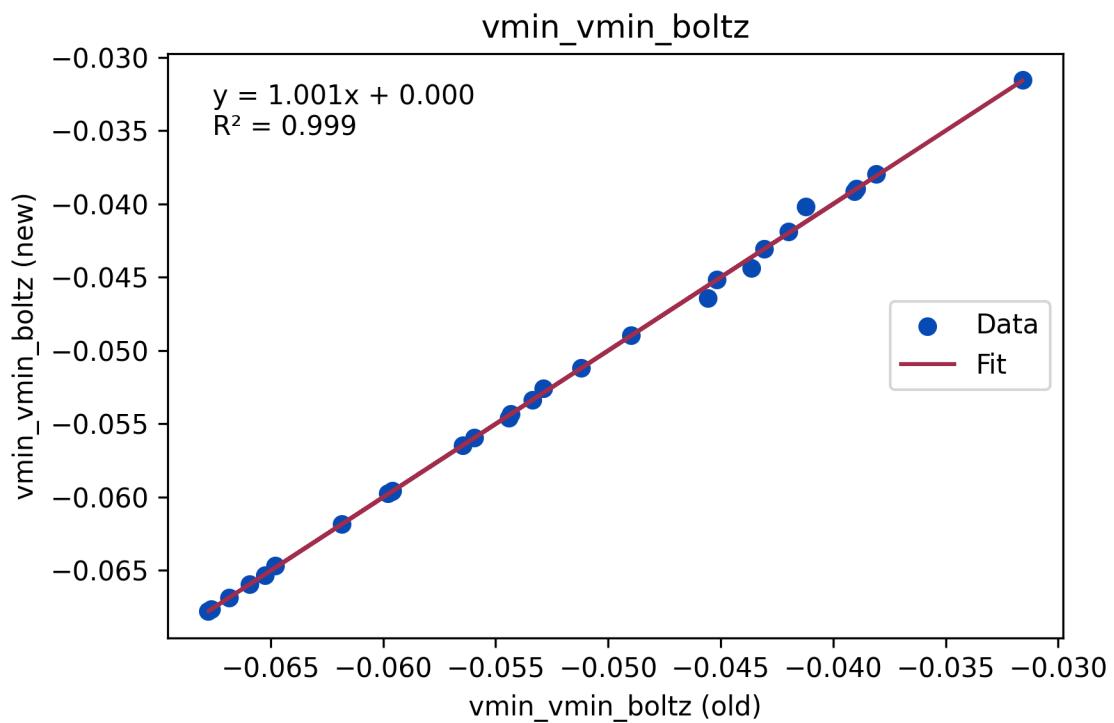
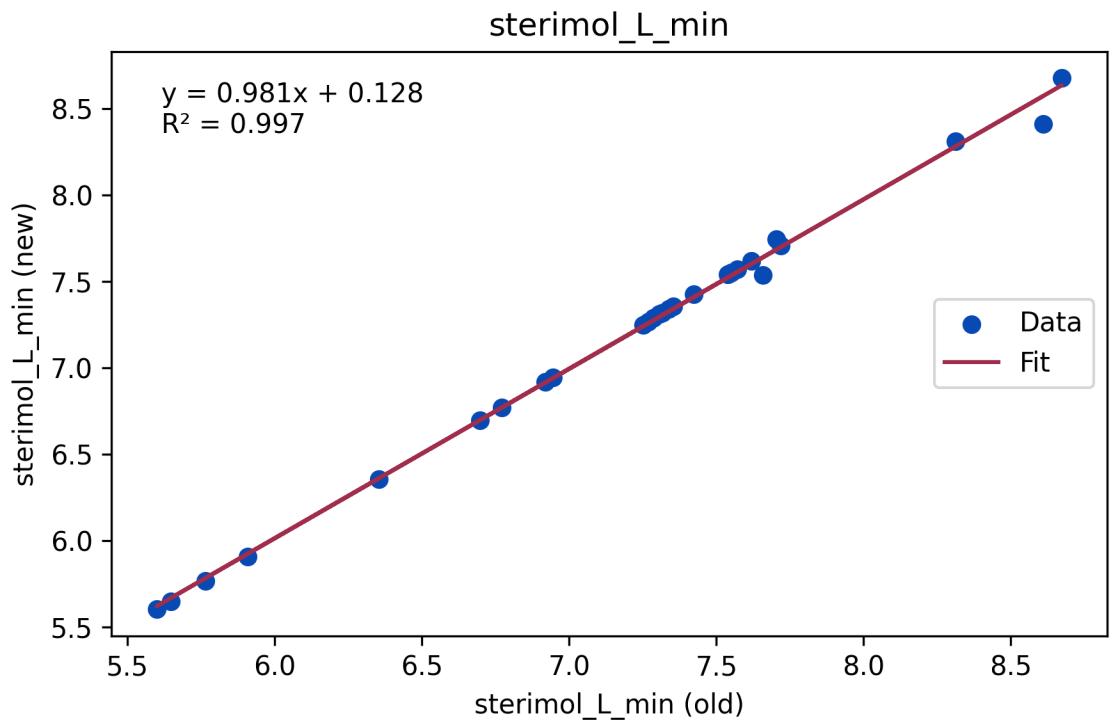


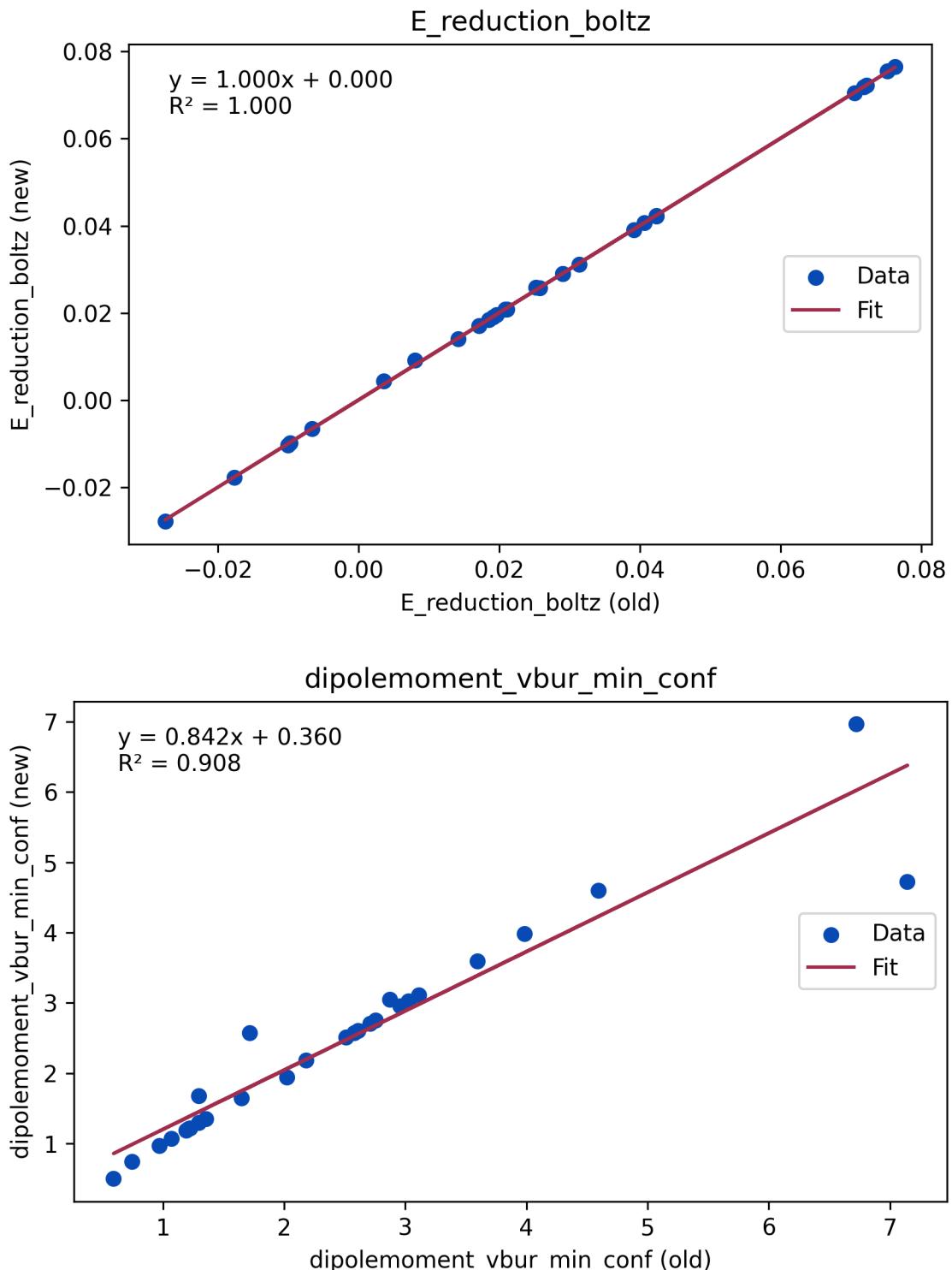
sterimol\_burB5\_vbur\_min\_conf

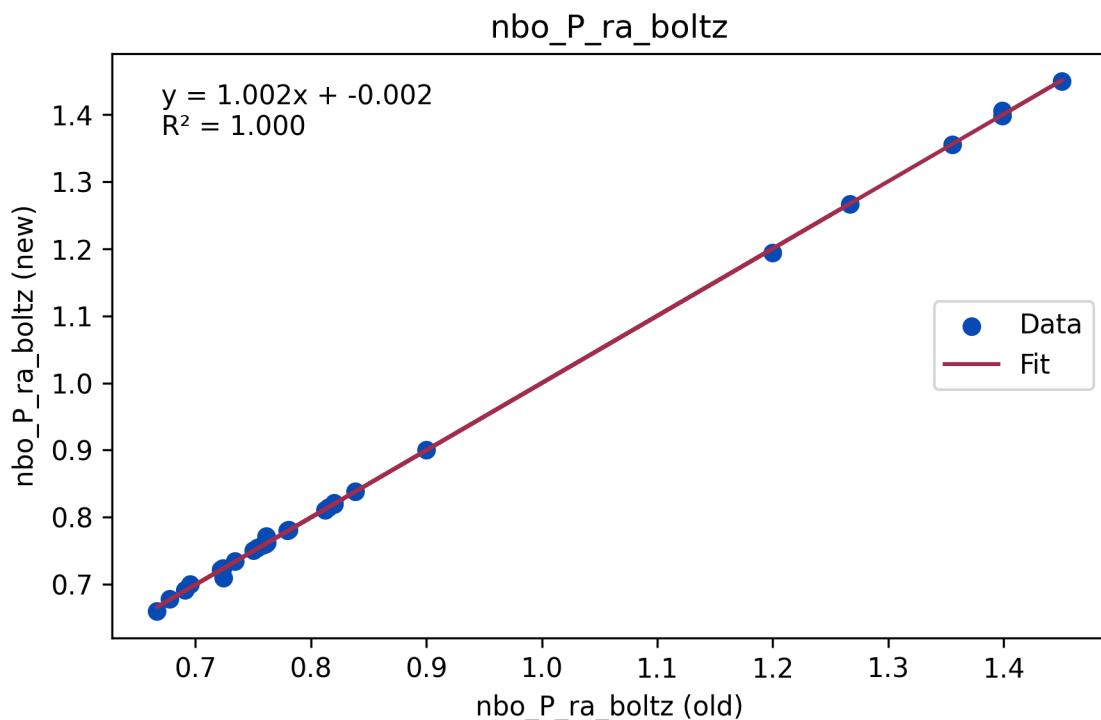
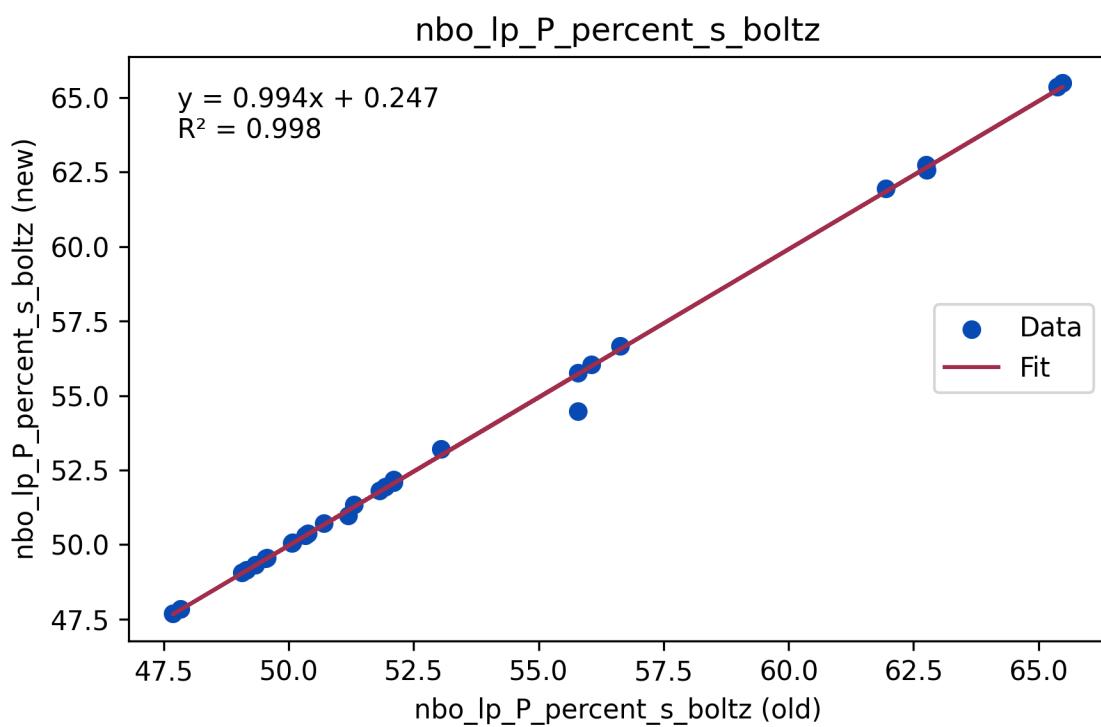


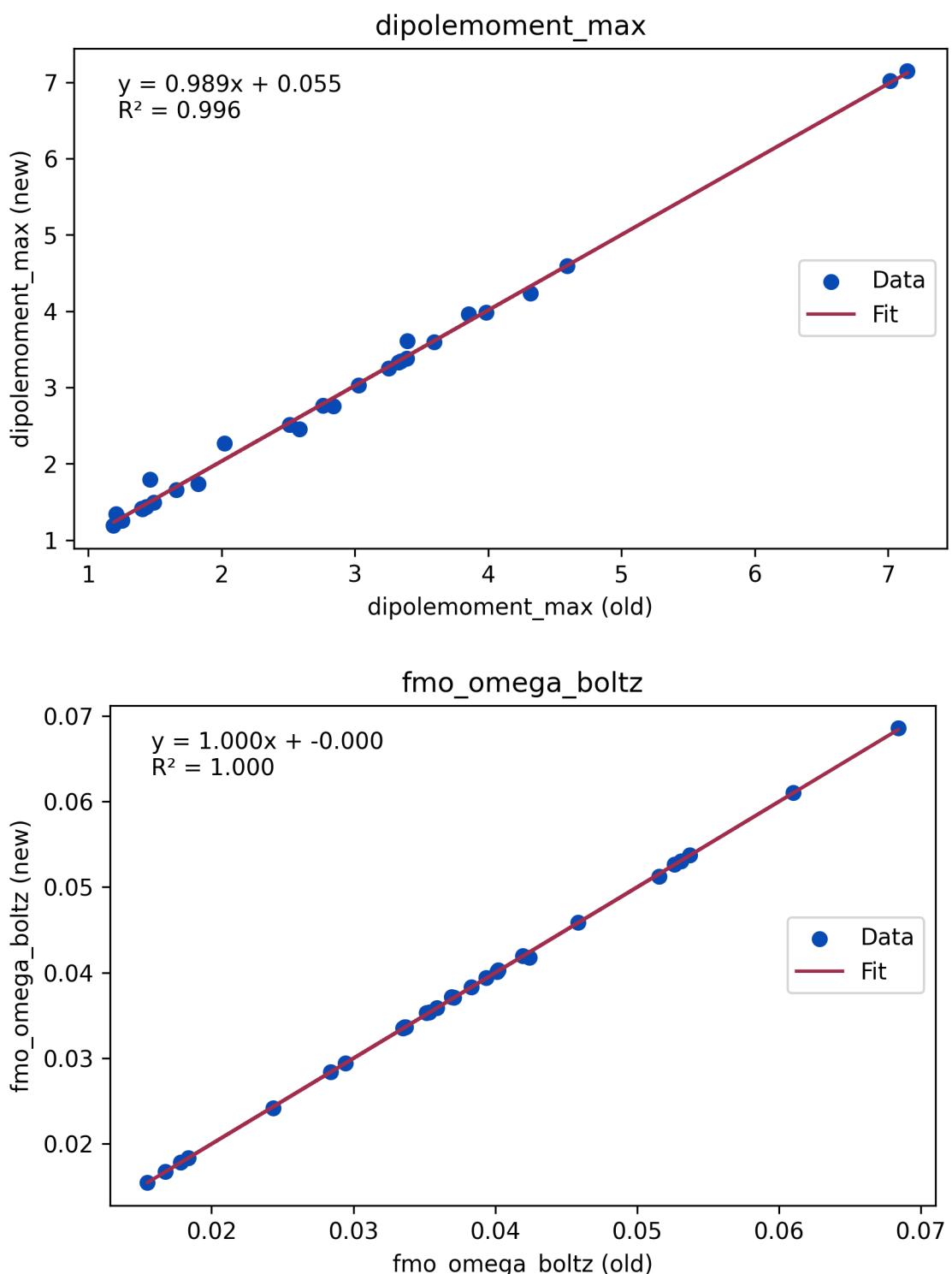


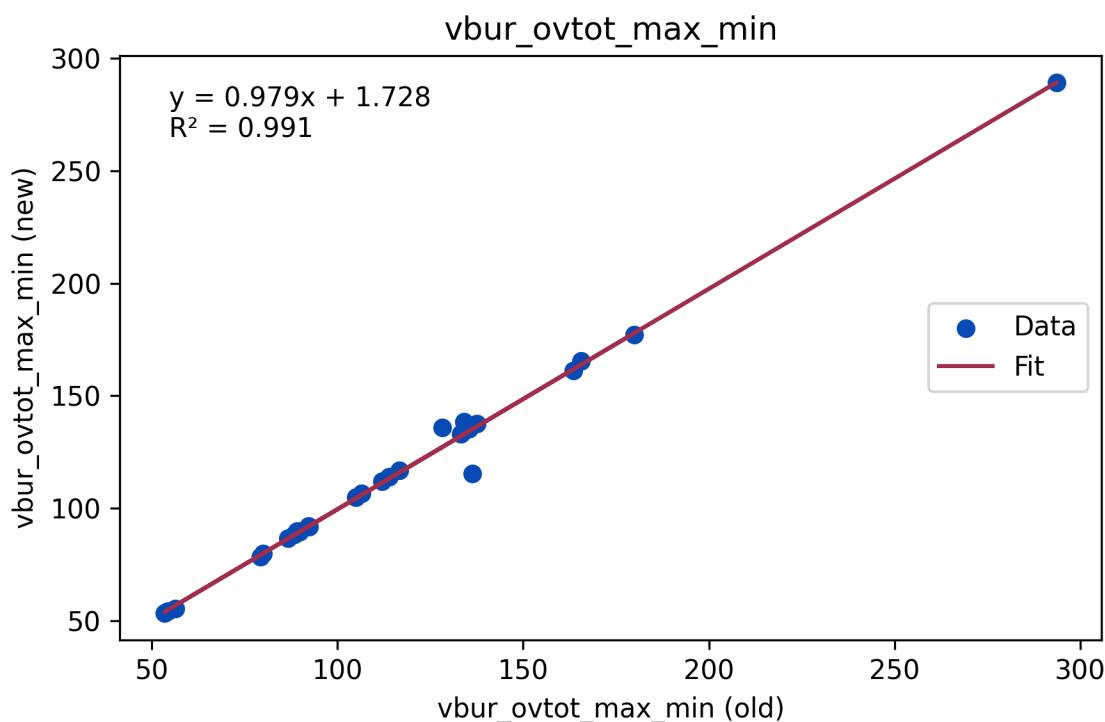
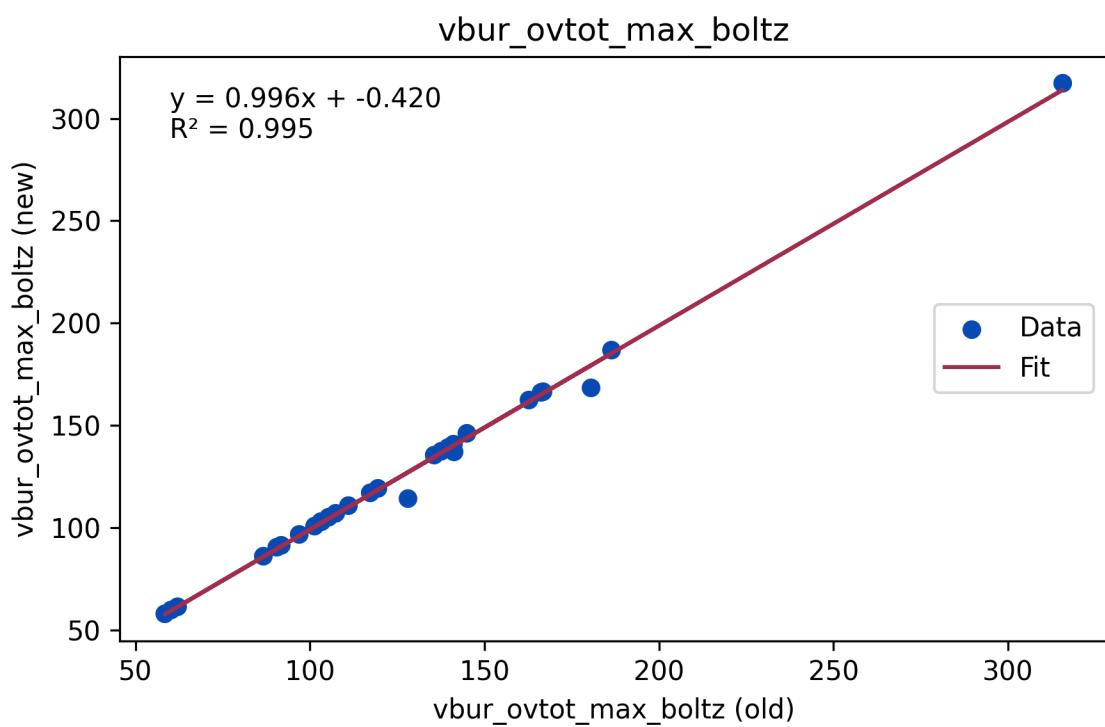


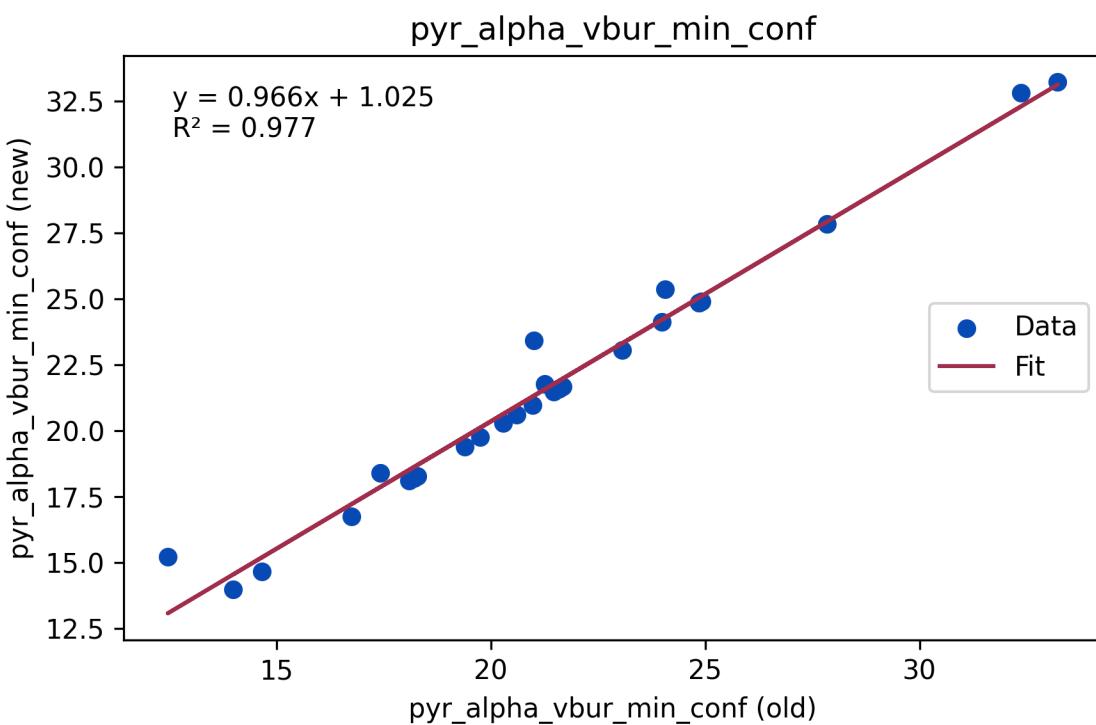
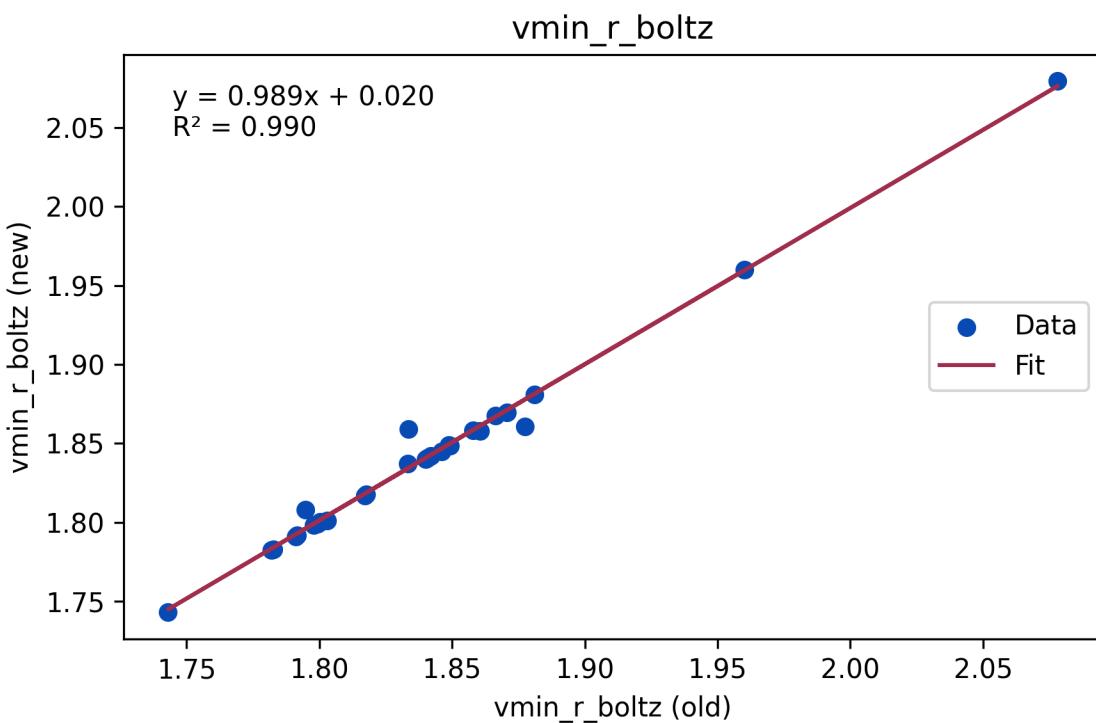


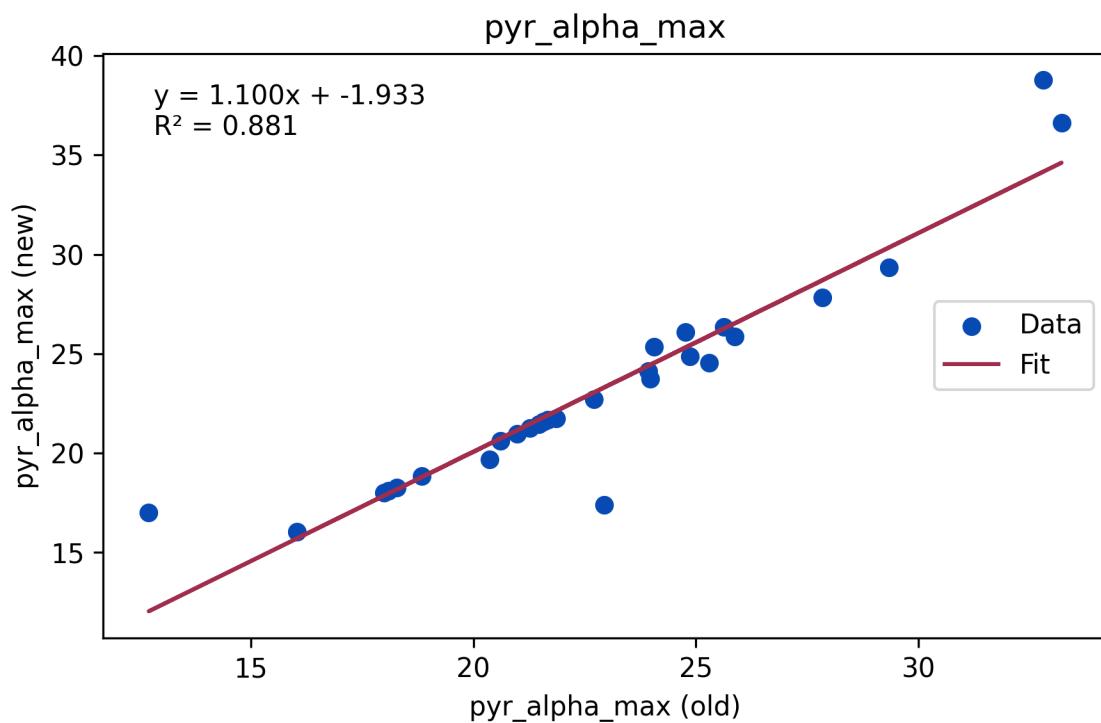
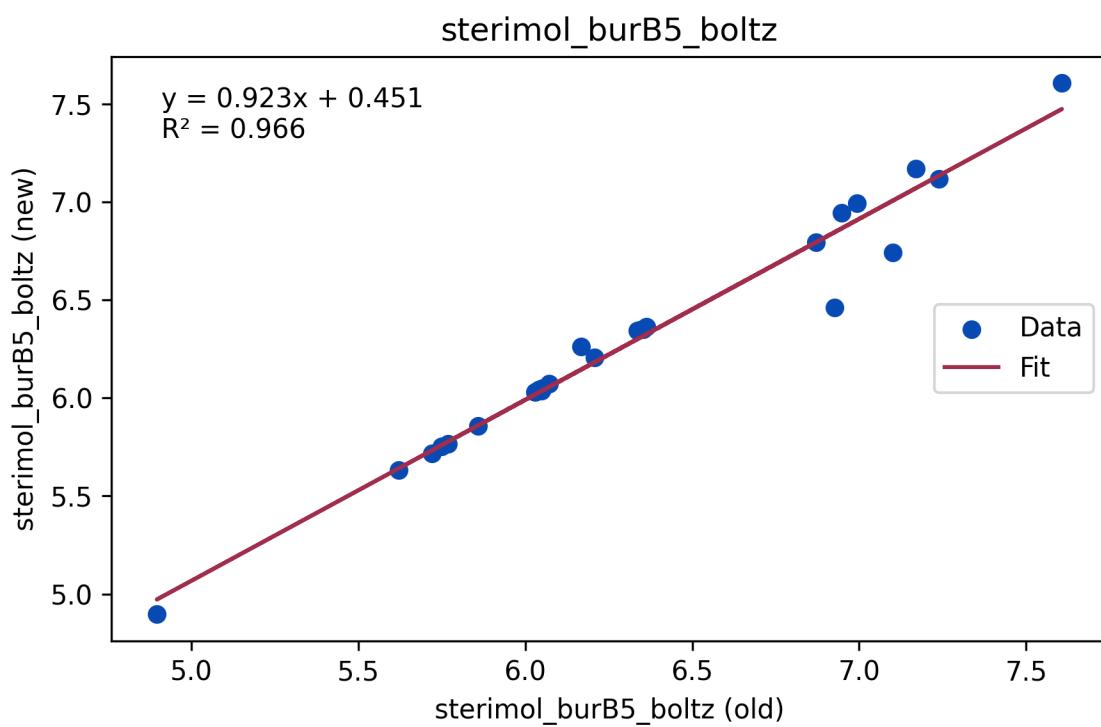


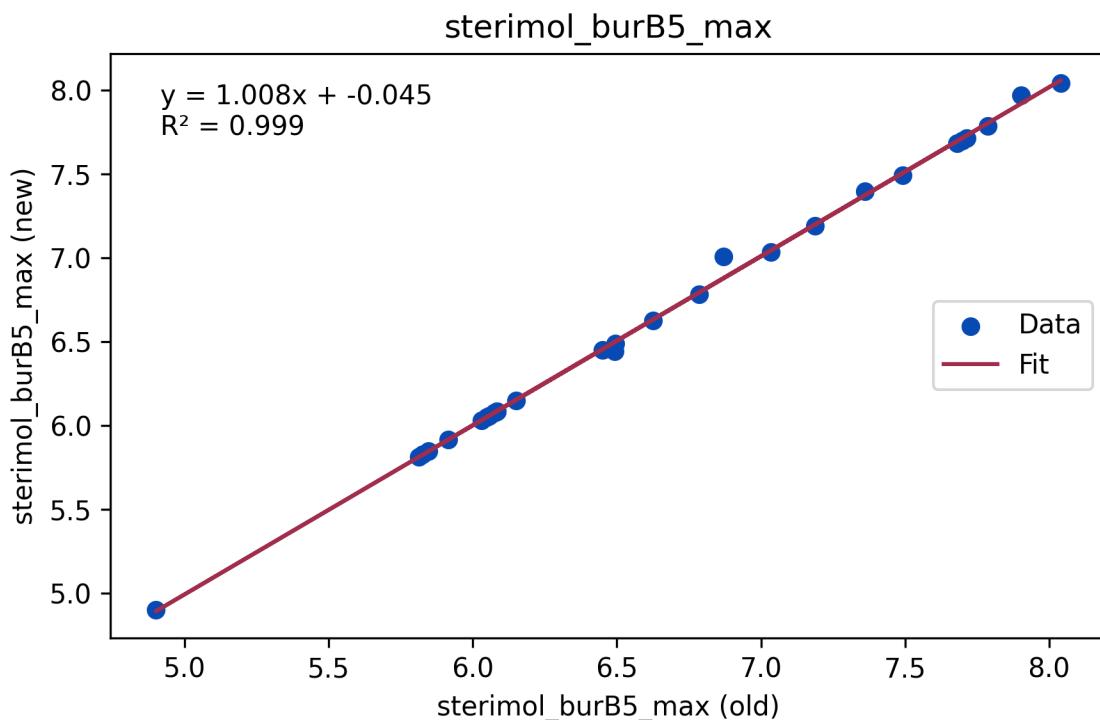
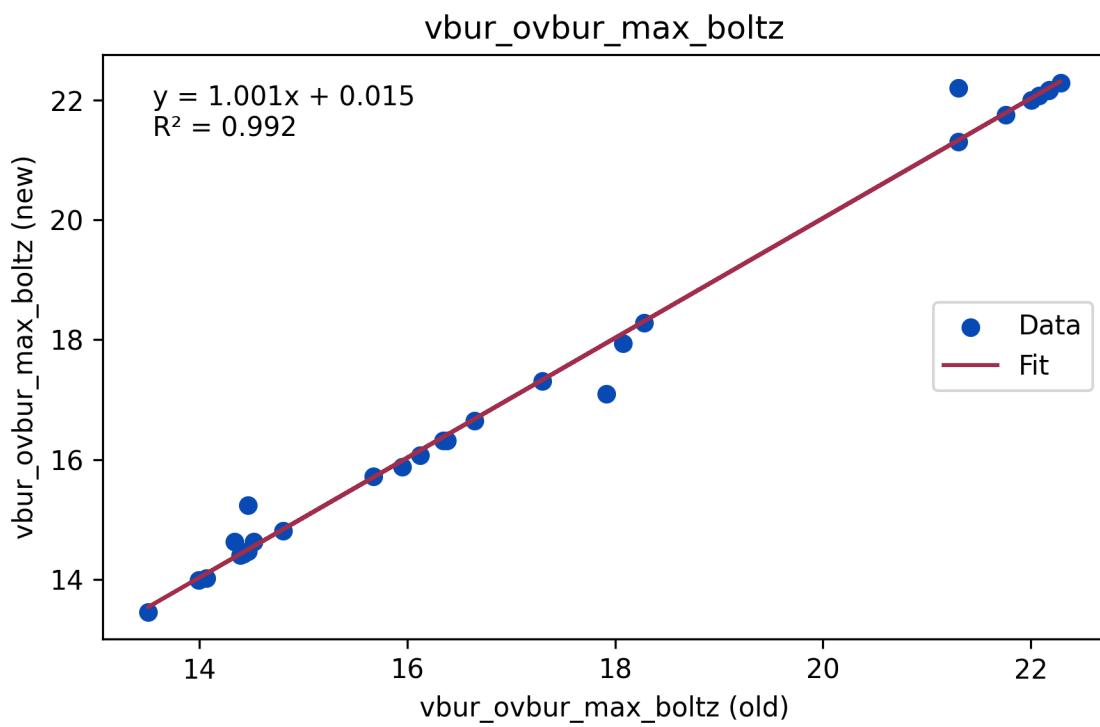




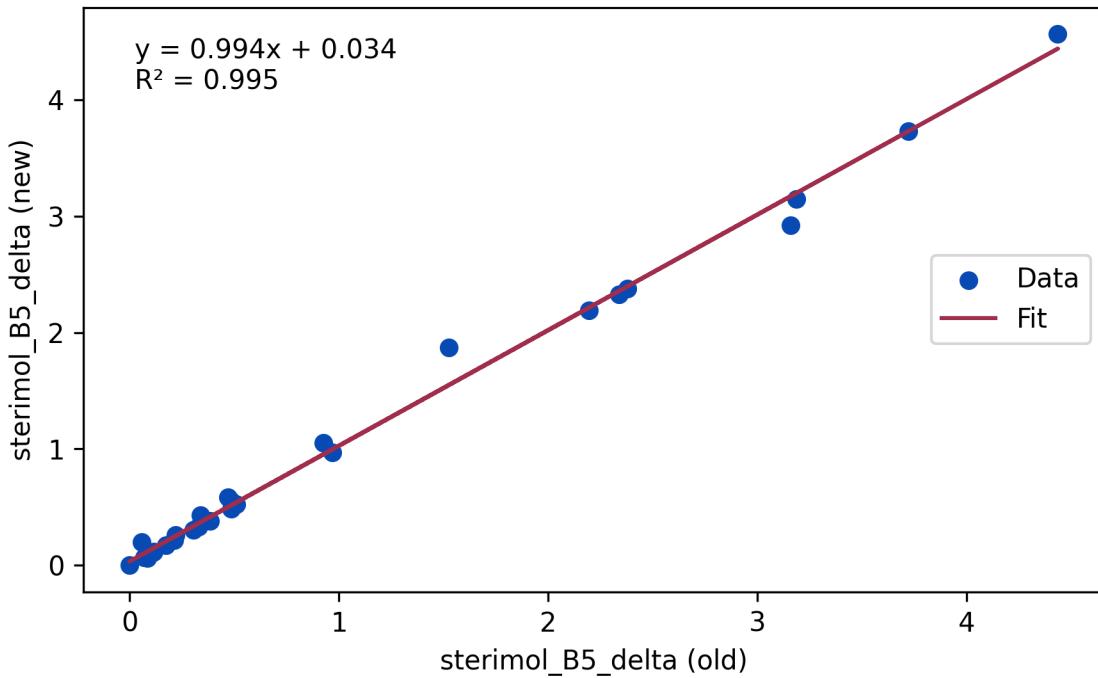




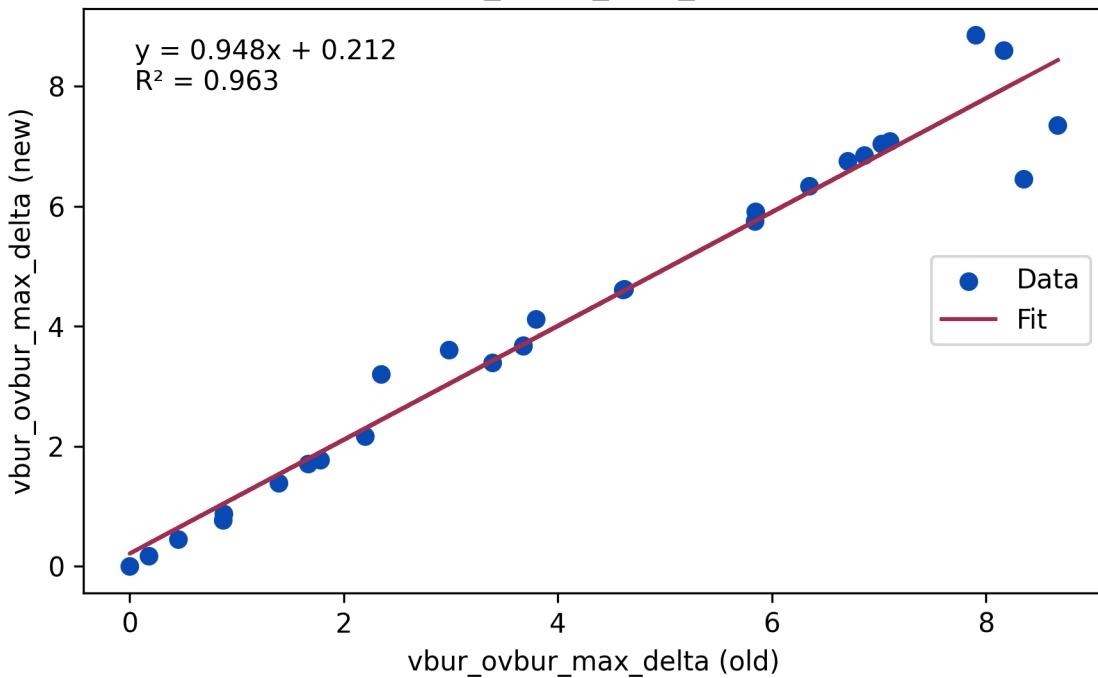


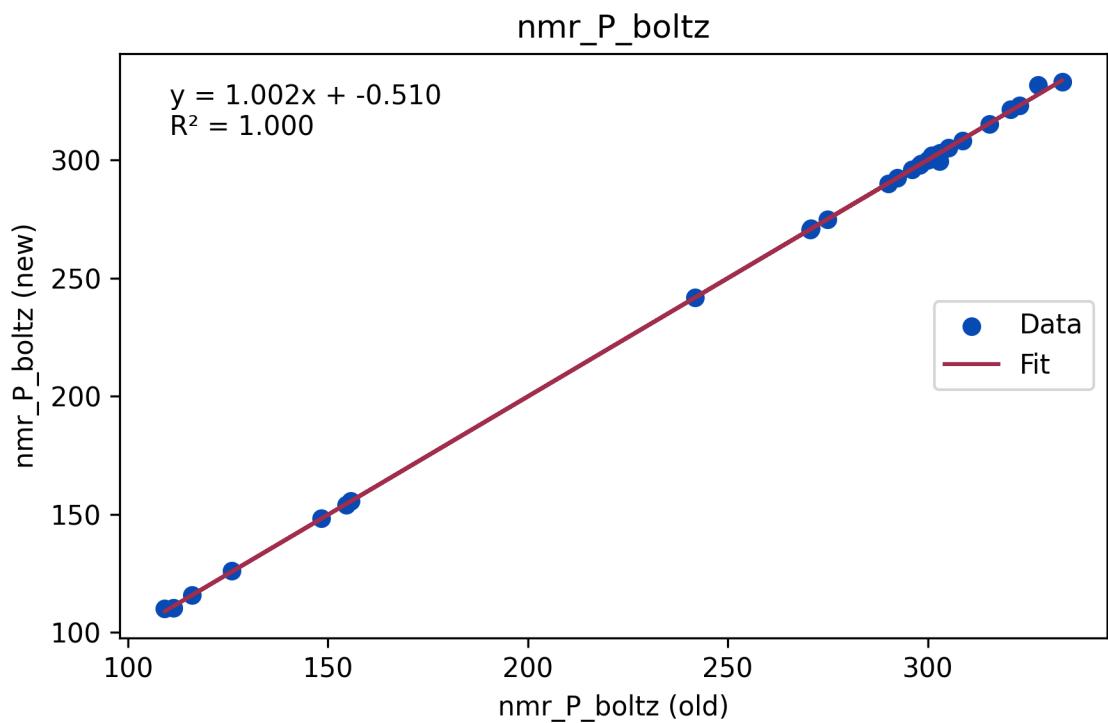
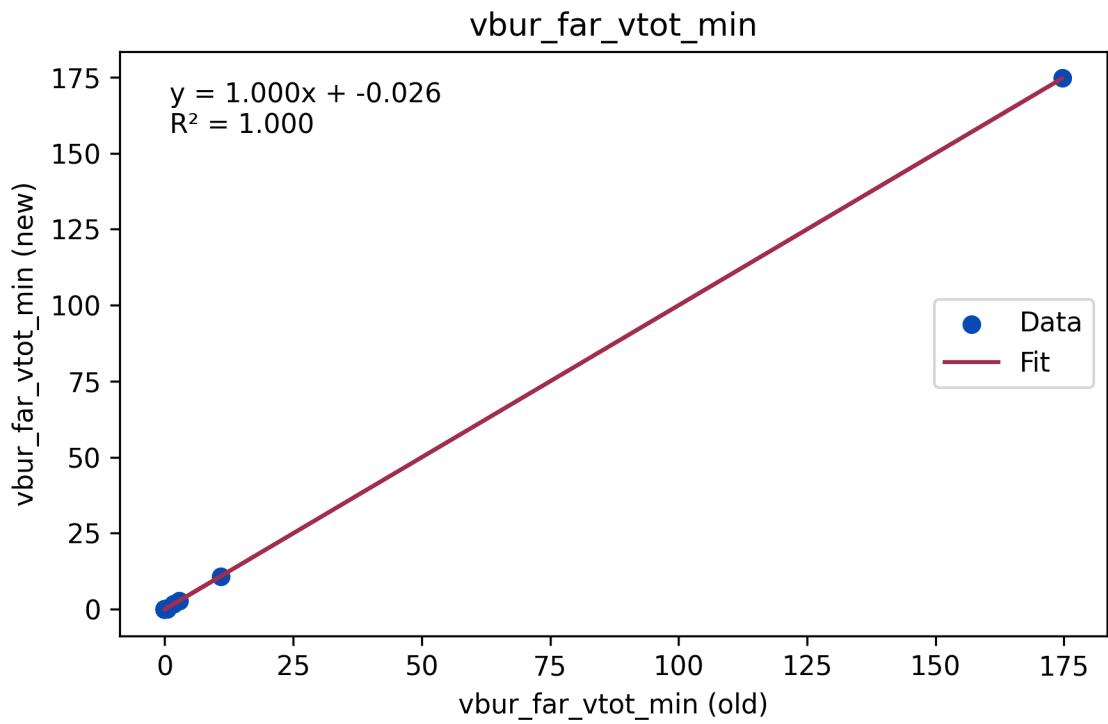


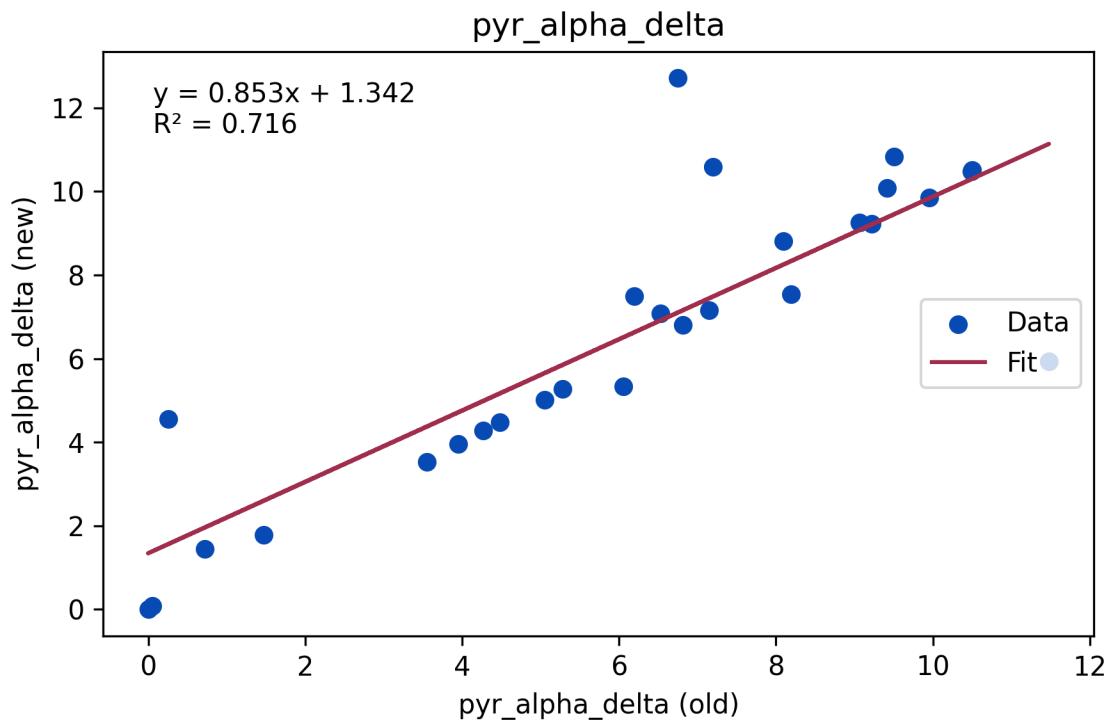
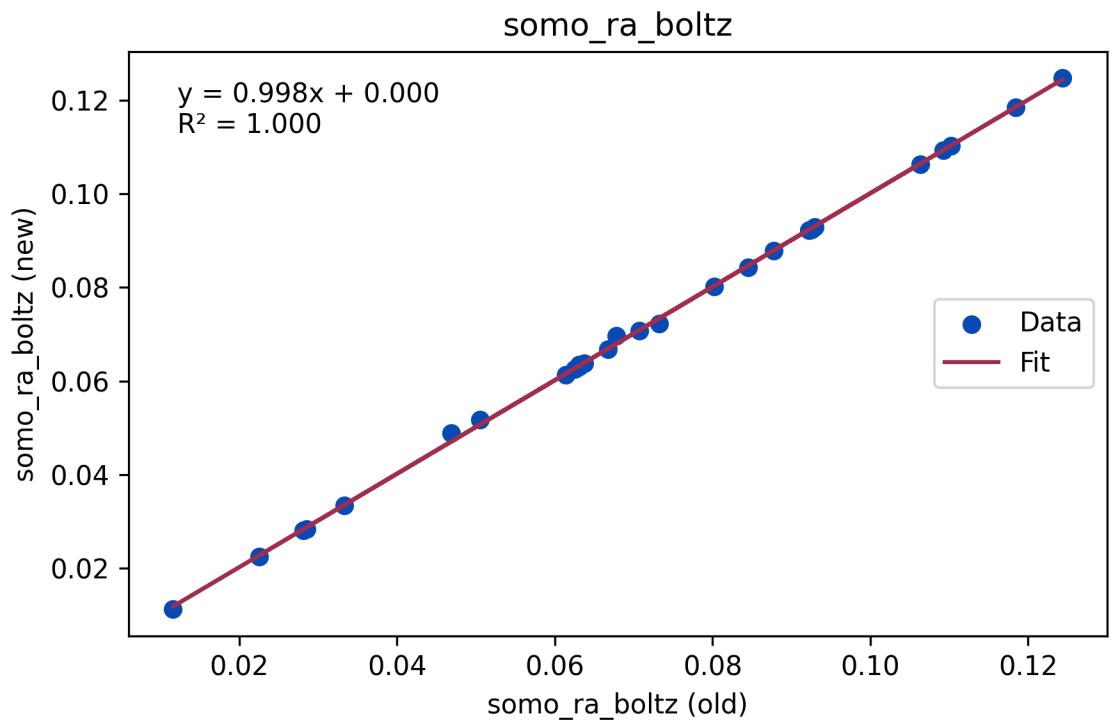
sterimol\_B5\_delta

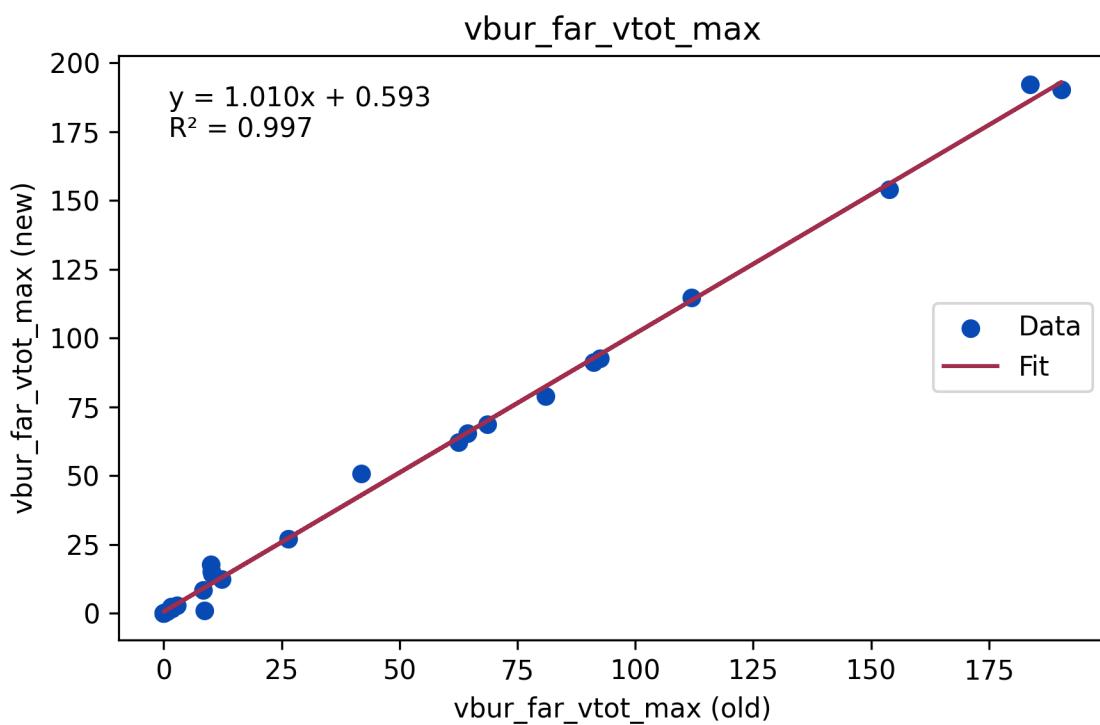
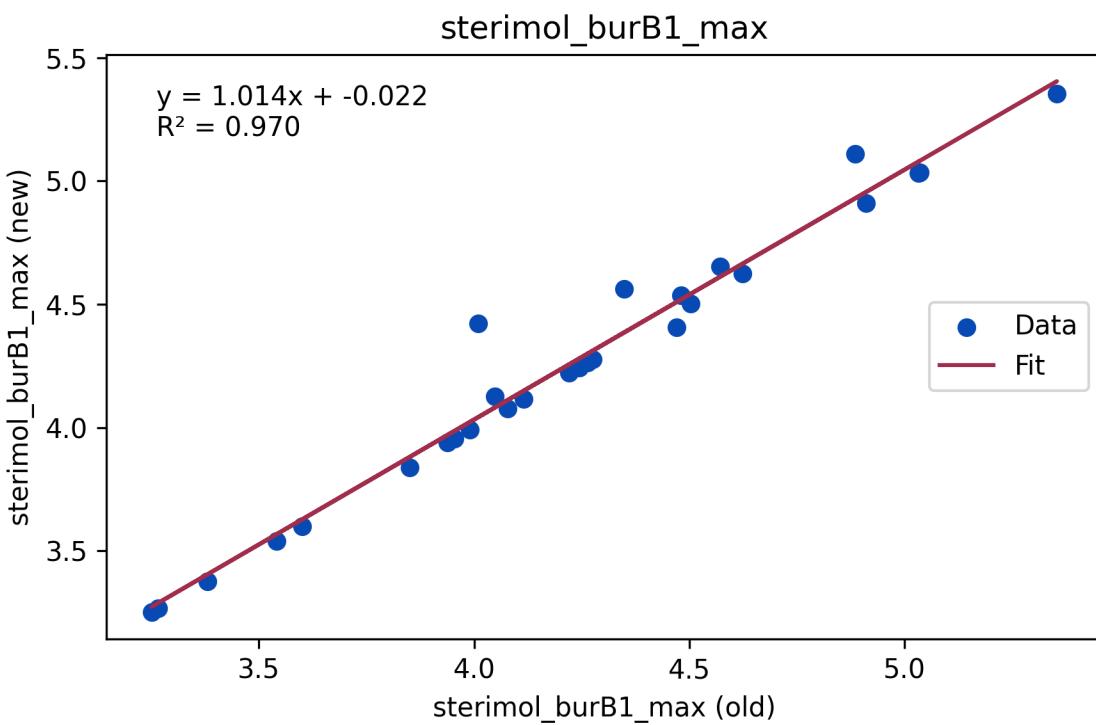


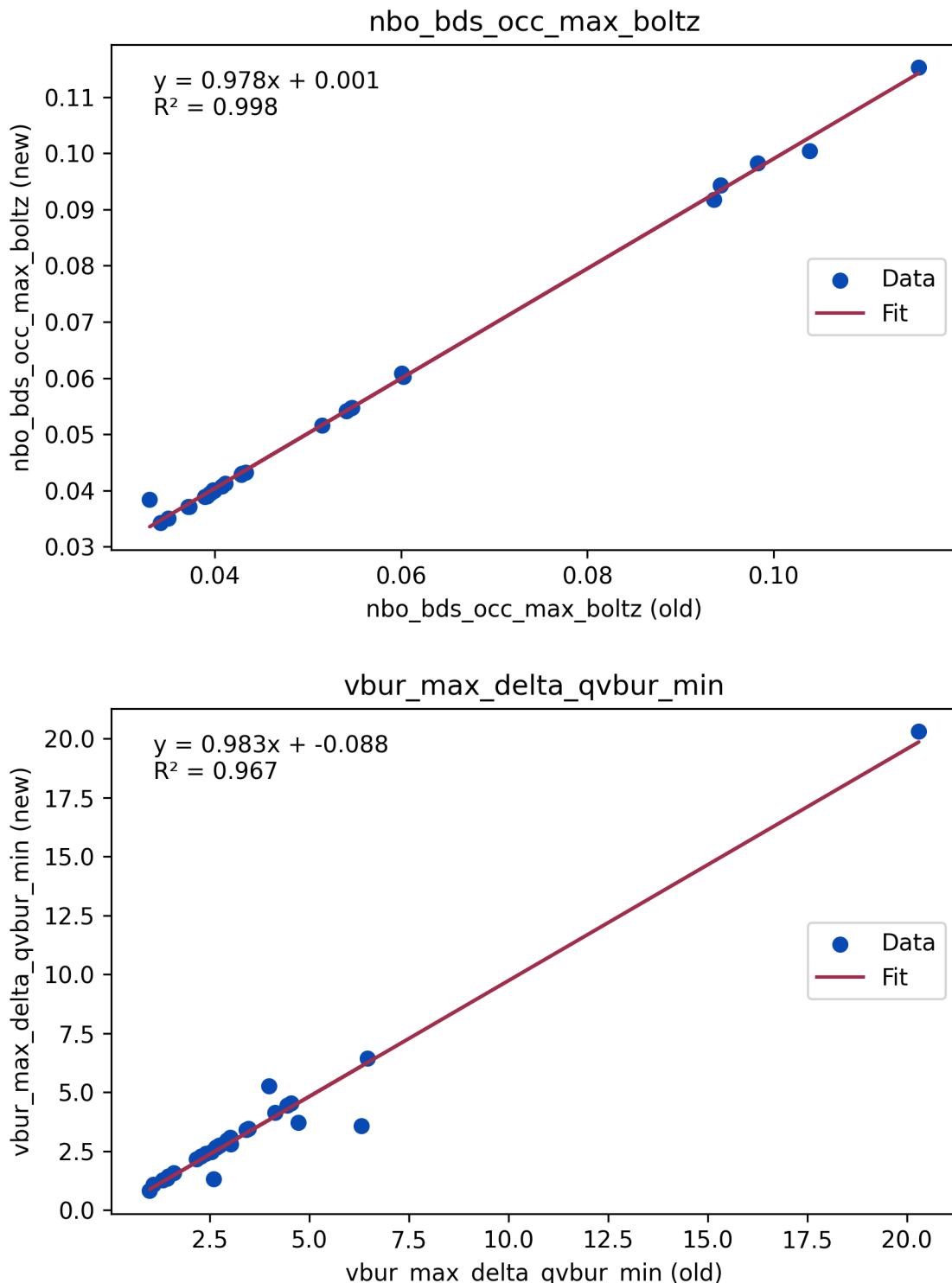
vbur\_ovbur\_max\_delta

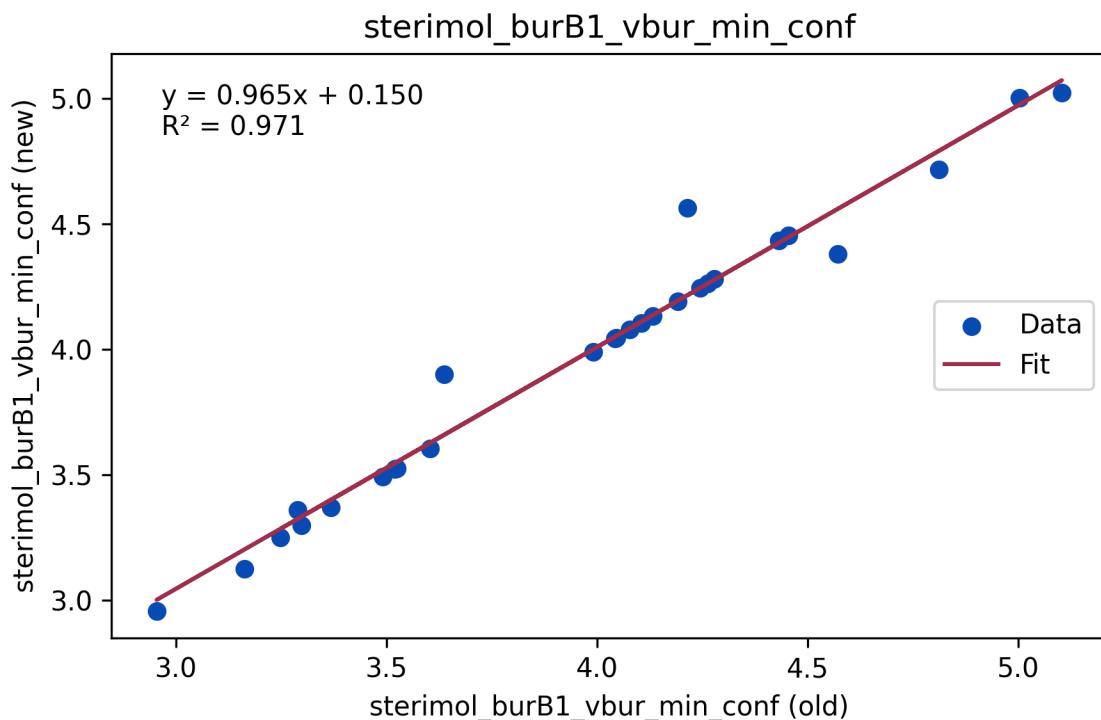
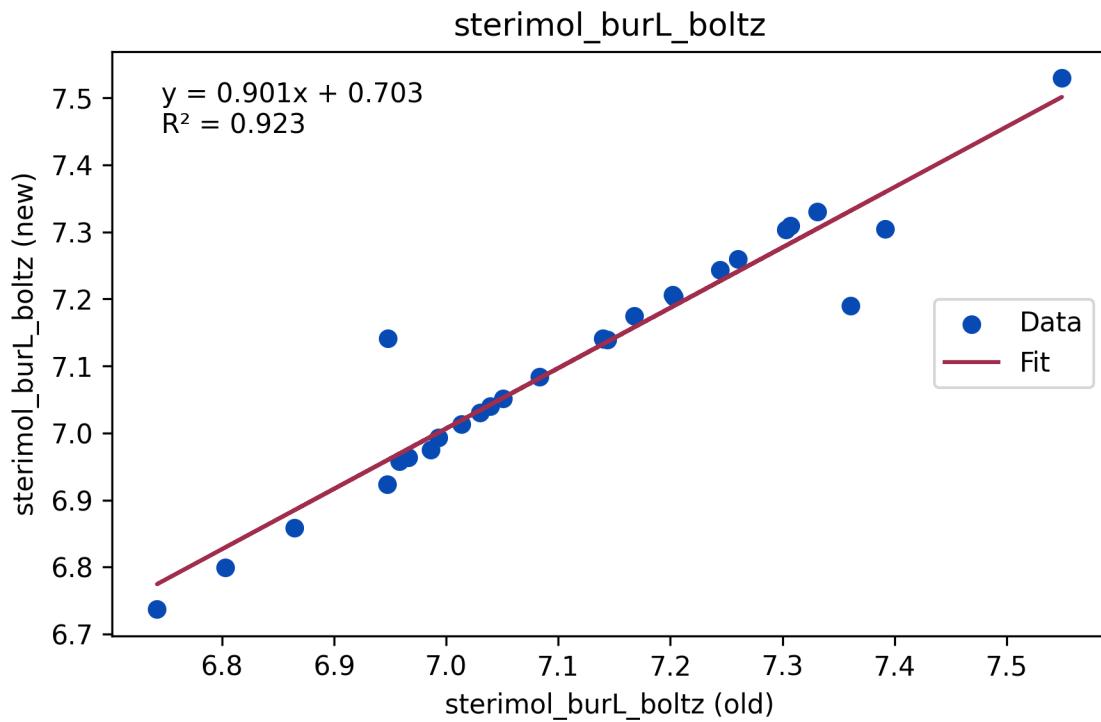


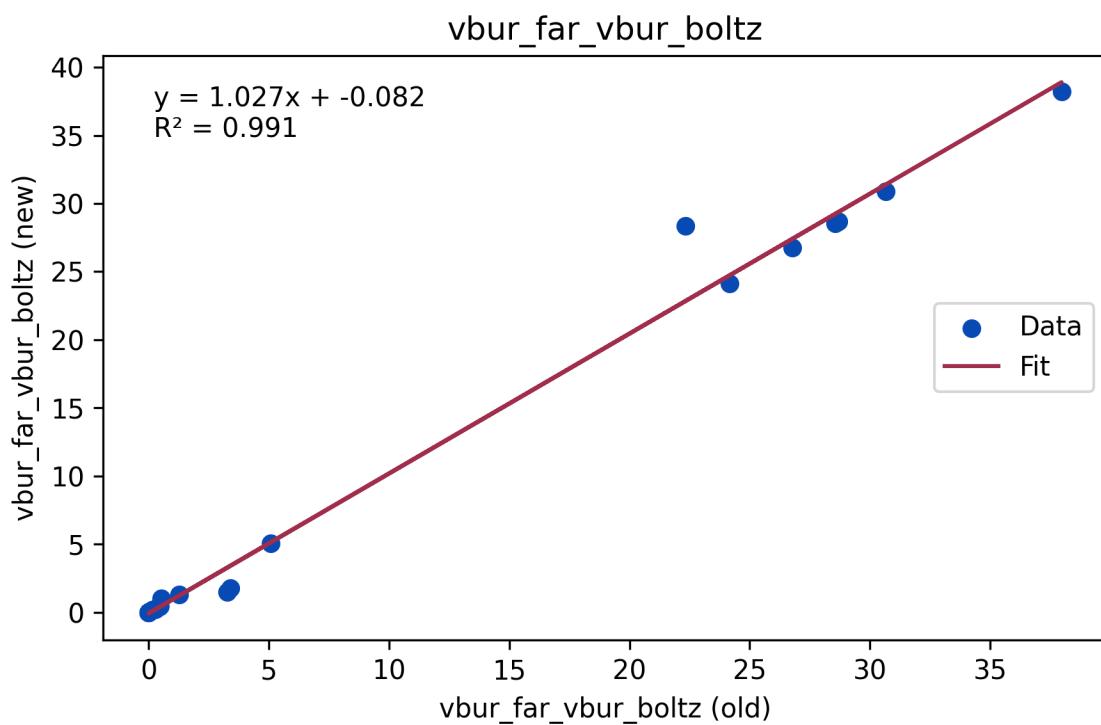
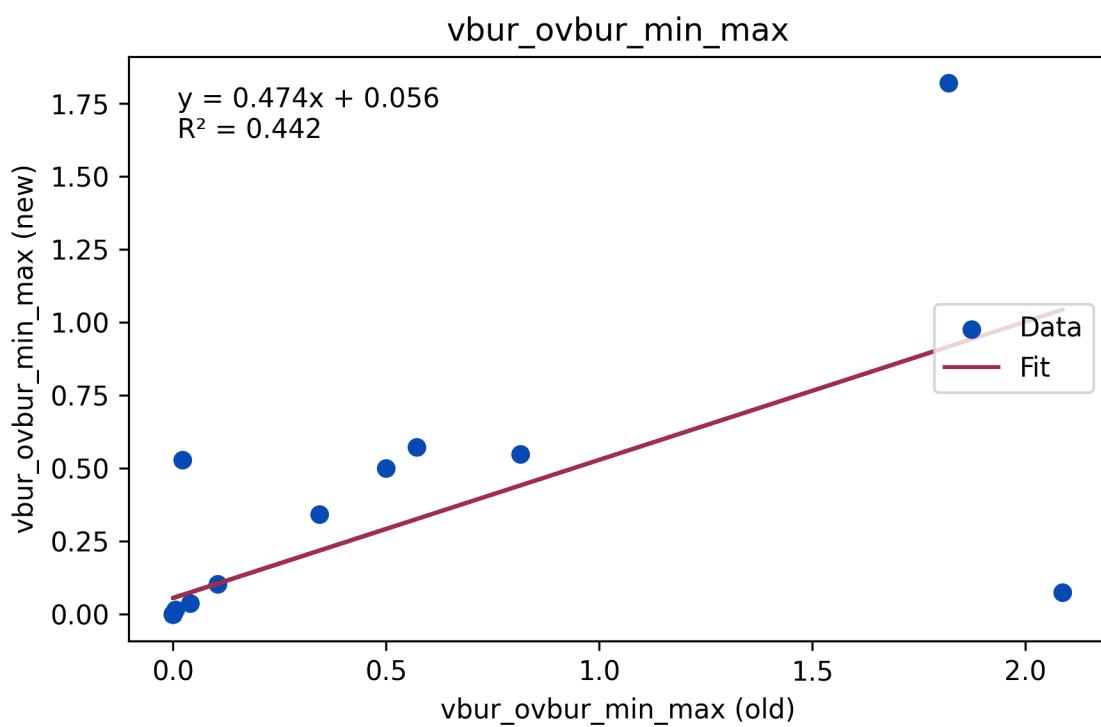


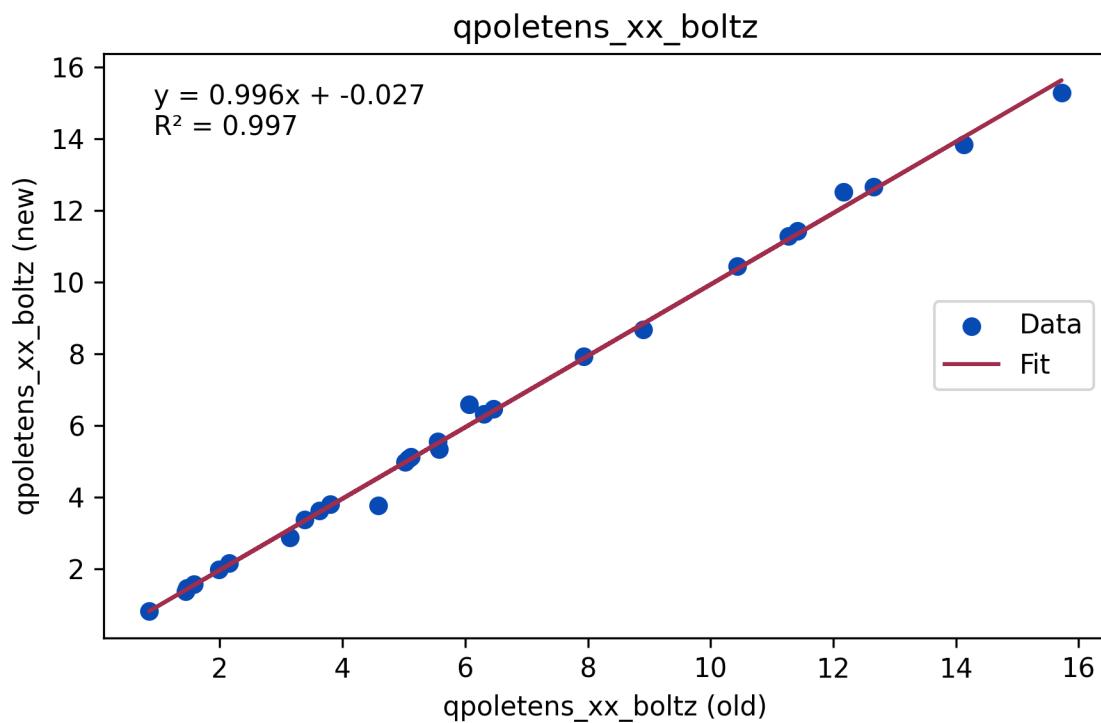
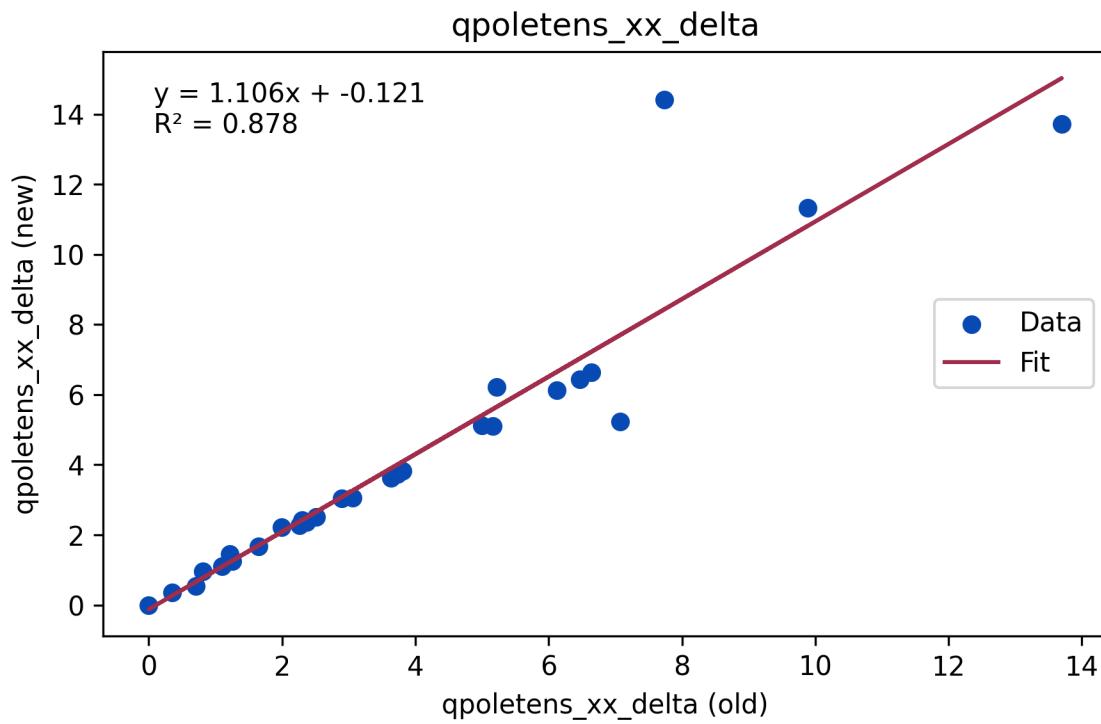


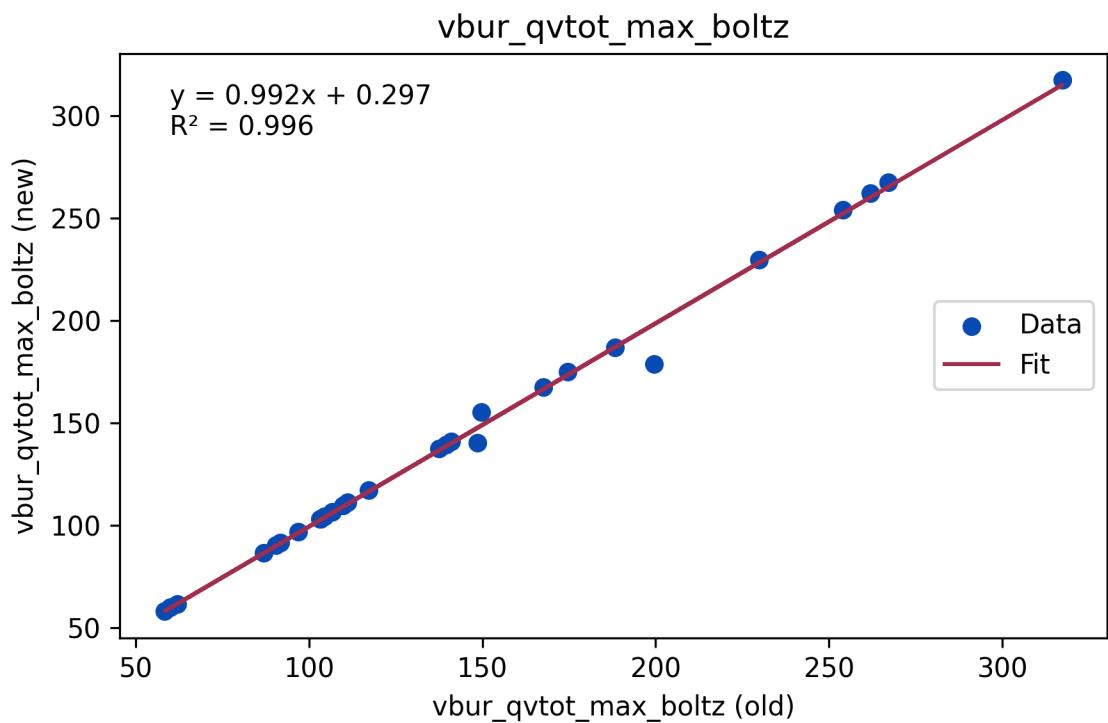
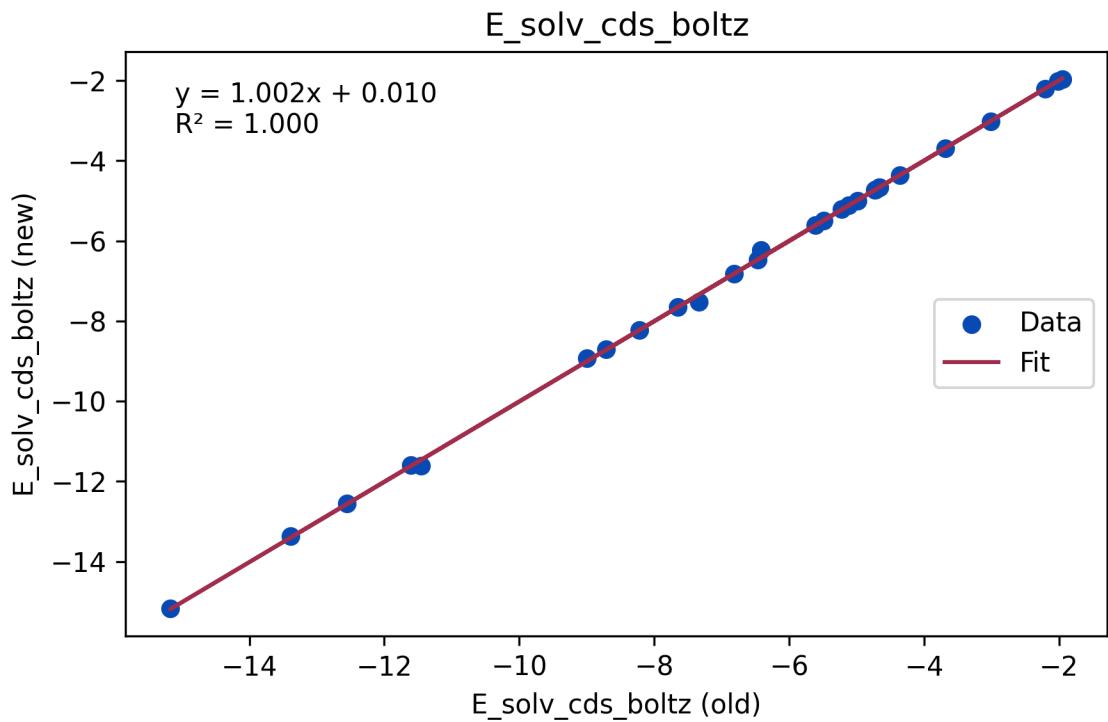




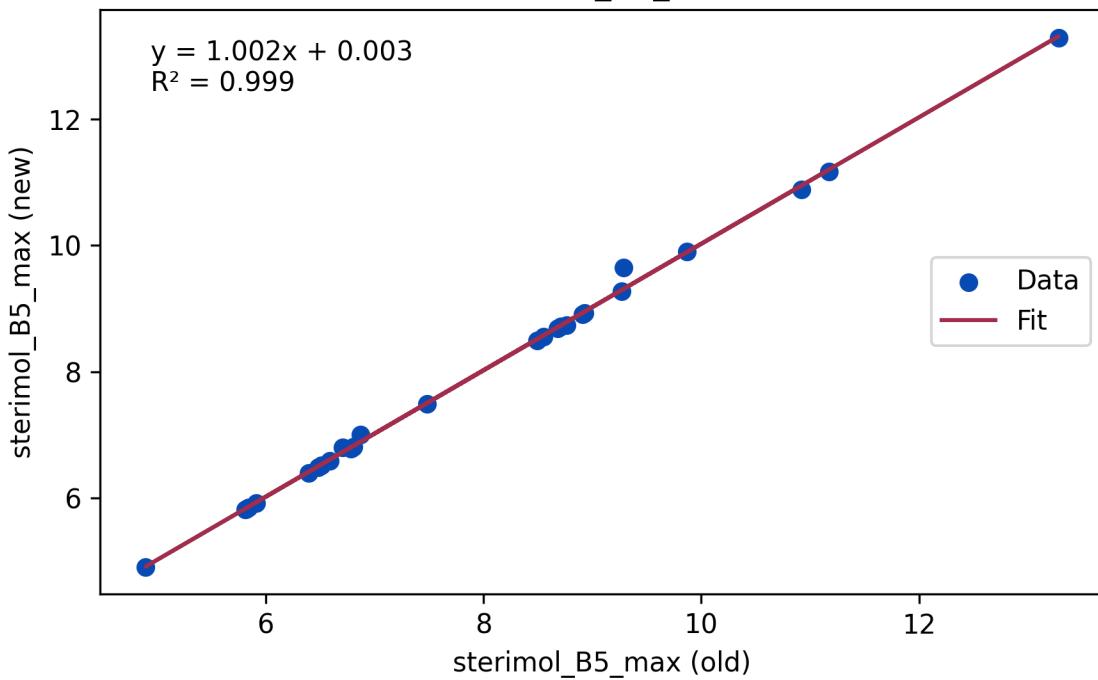




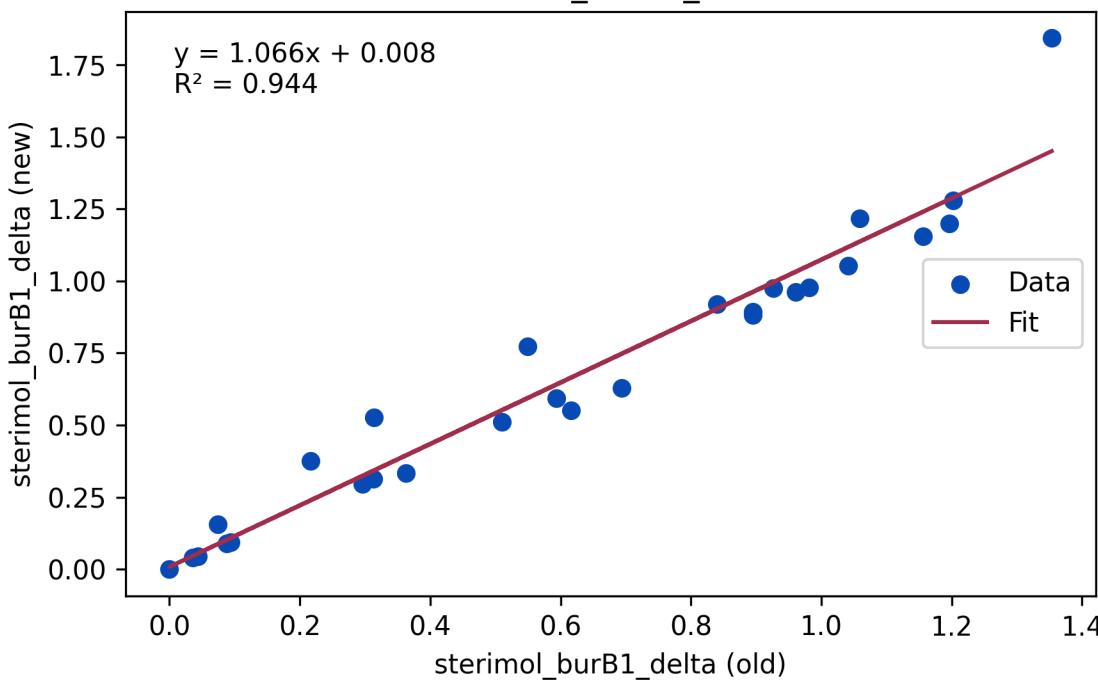


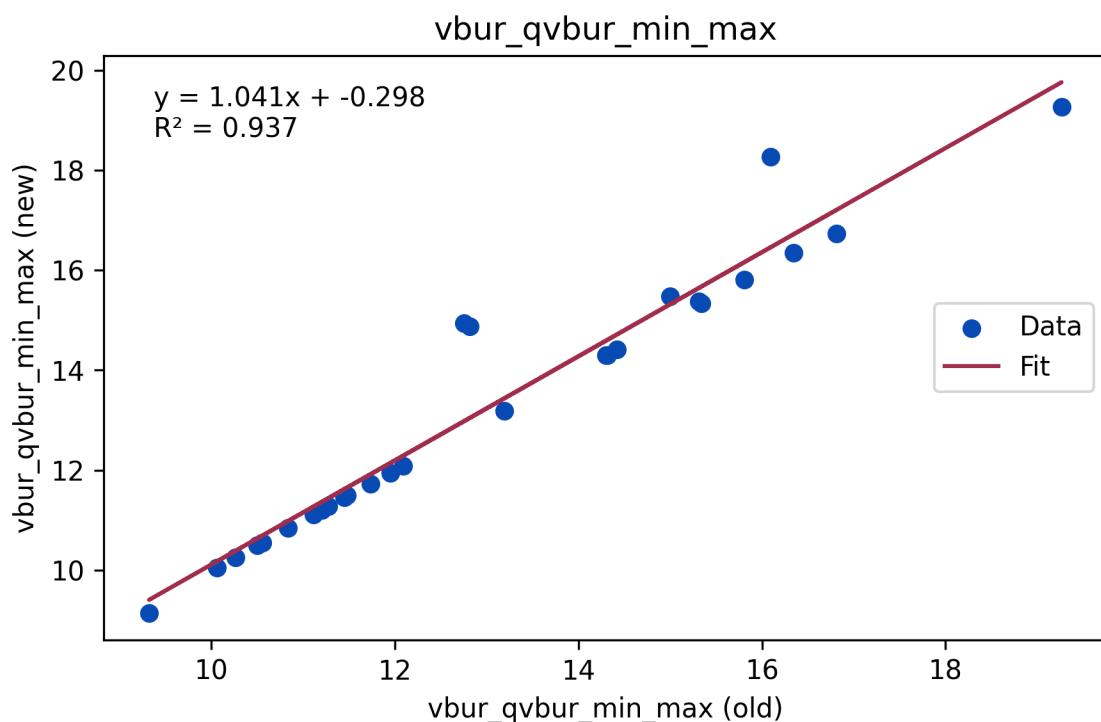
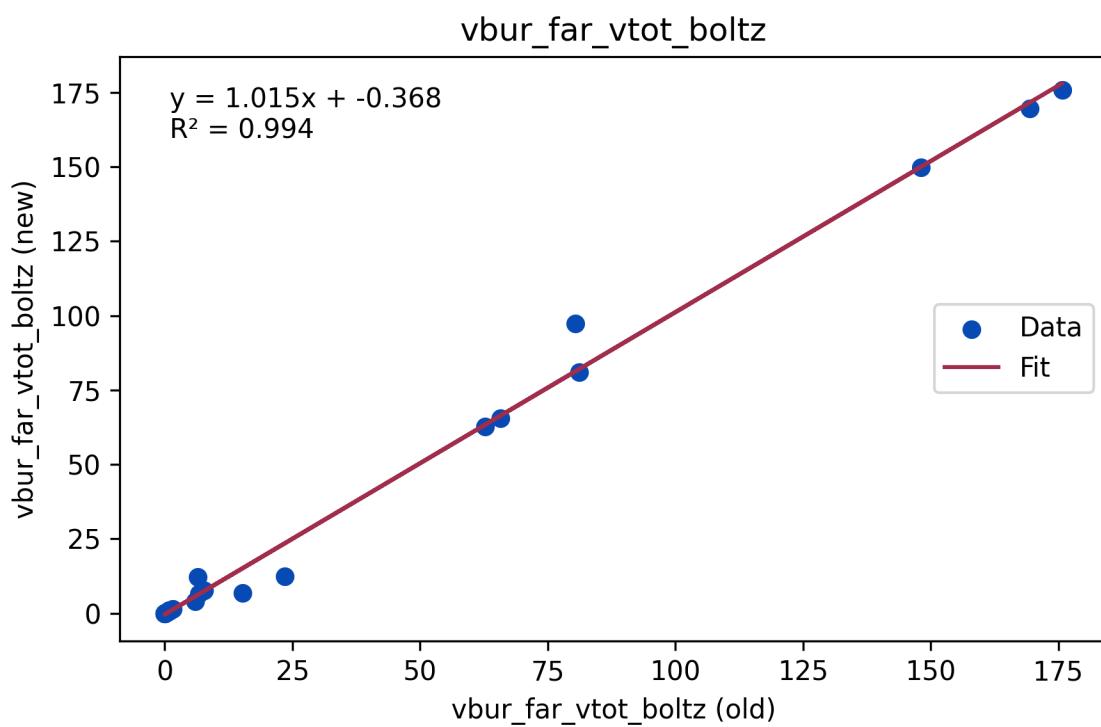


sterimol\_B5\_max

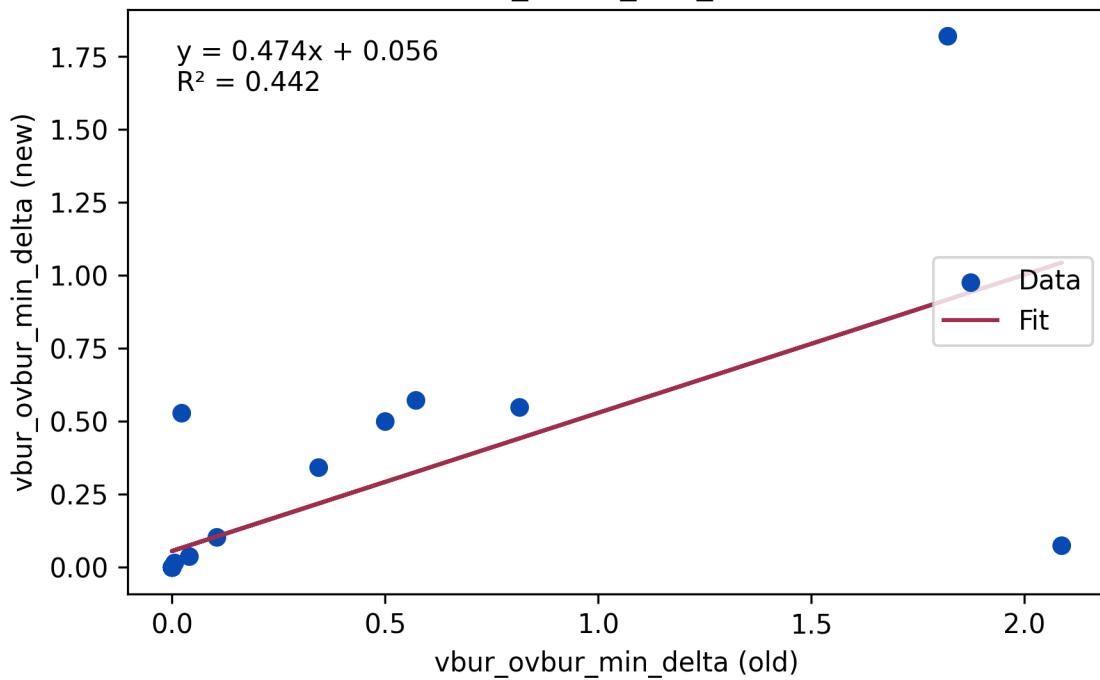


sterimol\_burB1\_delta

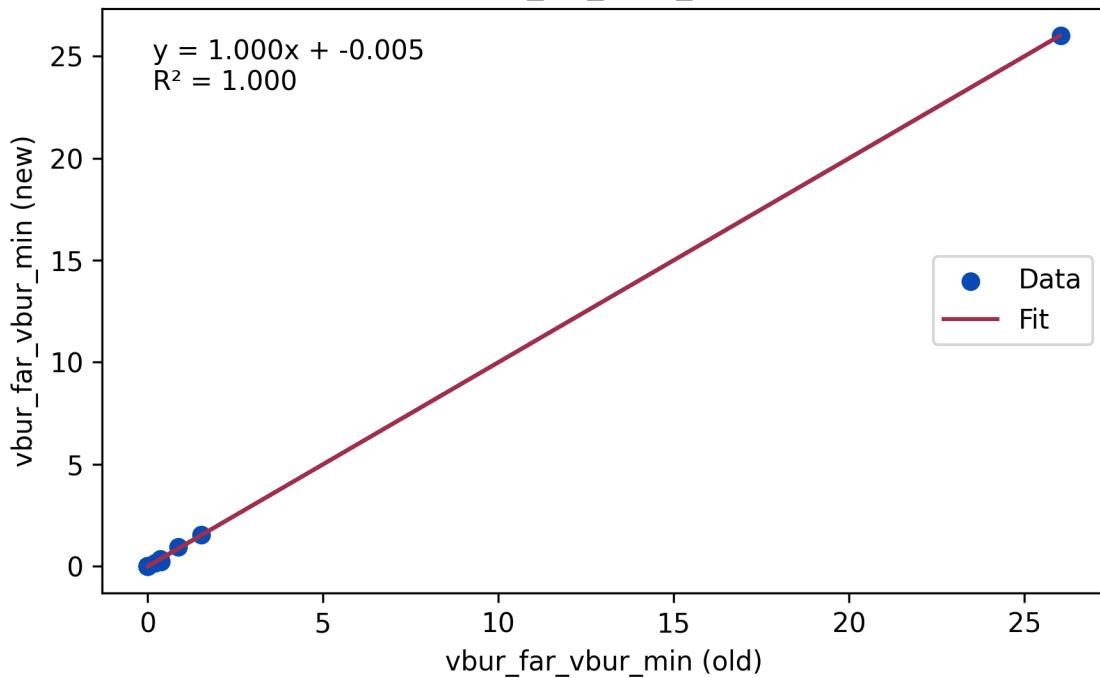




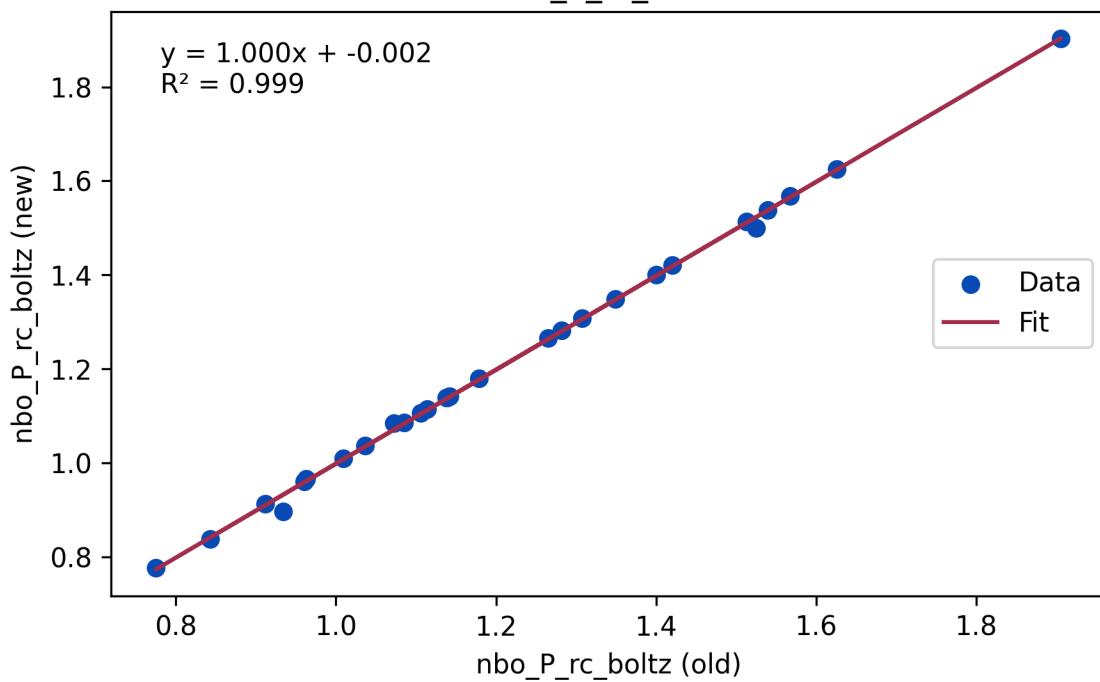
vbur\_ovbur\_min\_delta



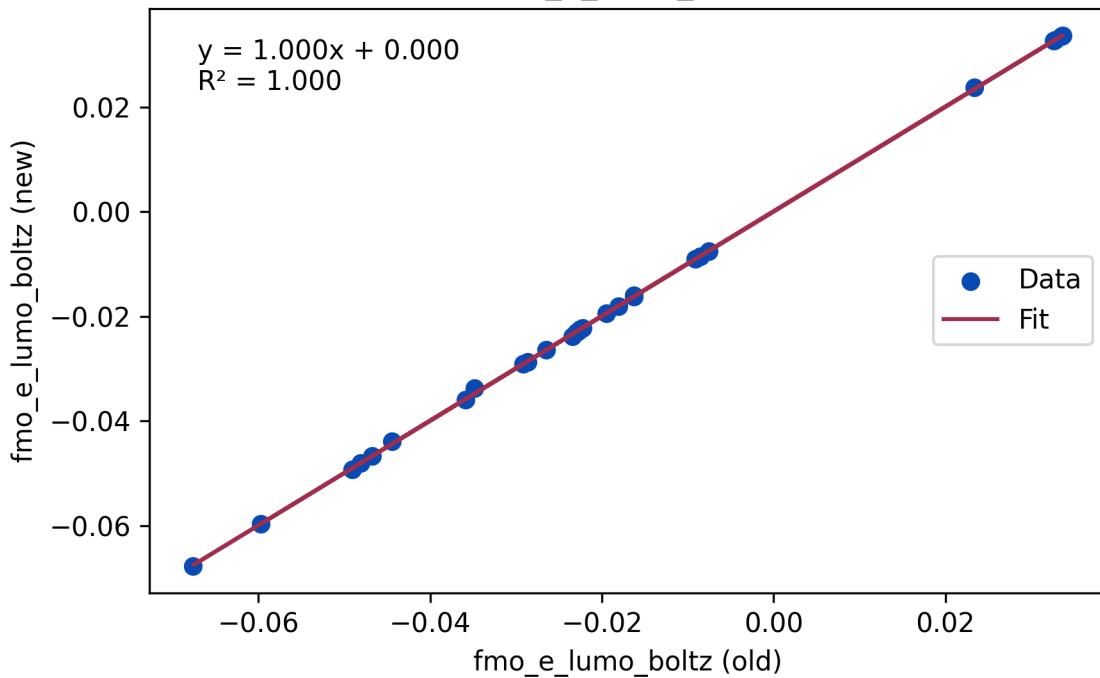
vbur\_far\_vbur\_min

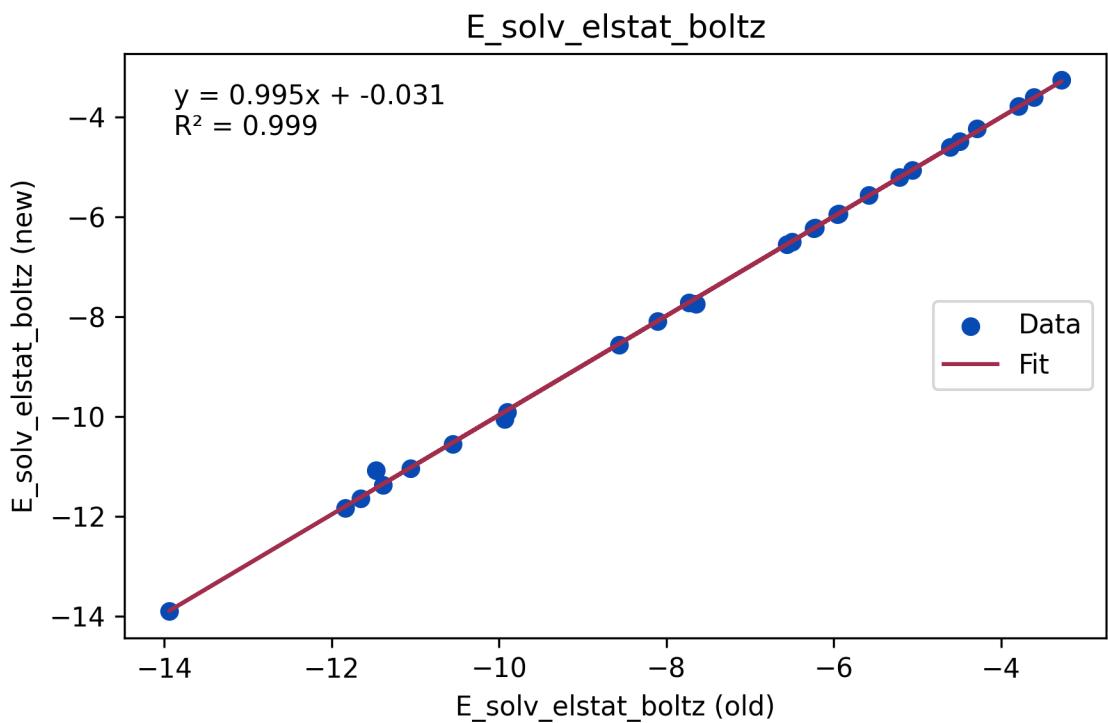
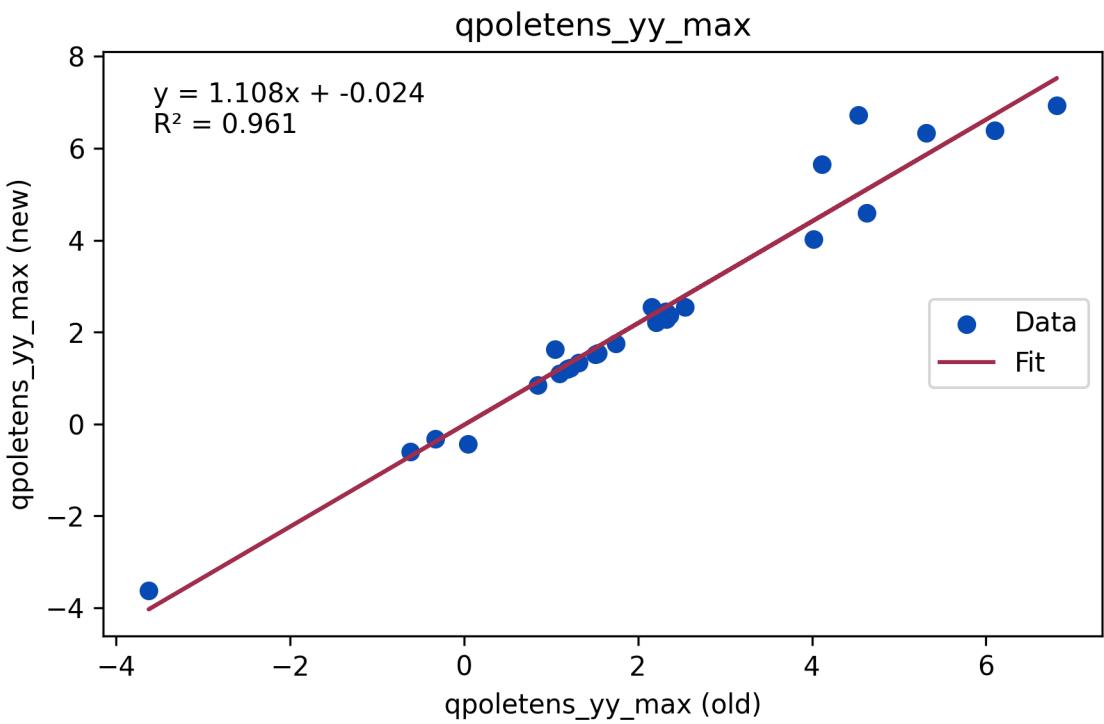


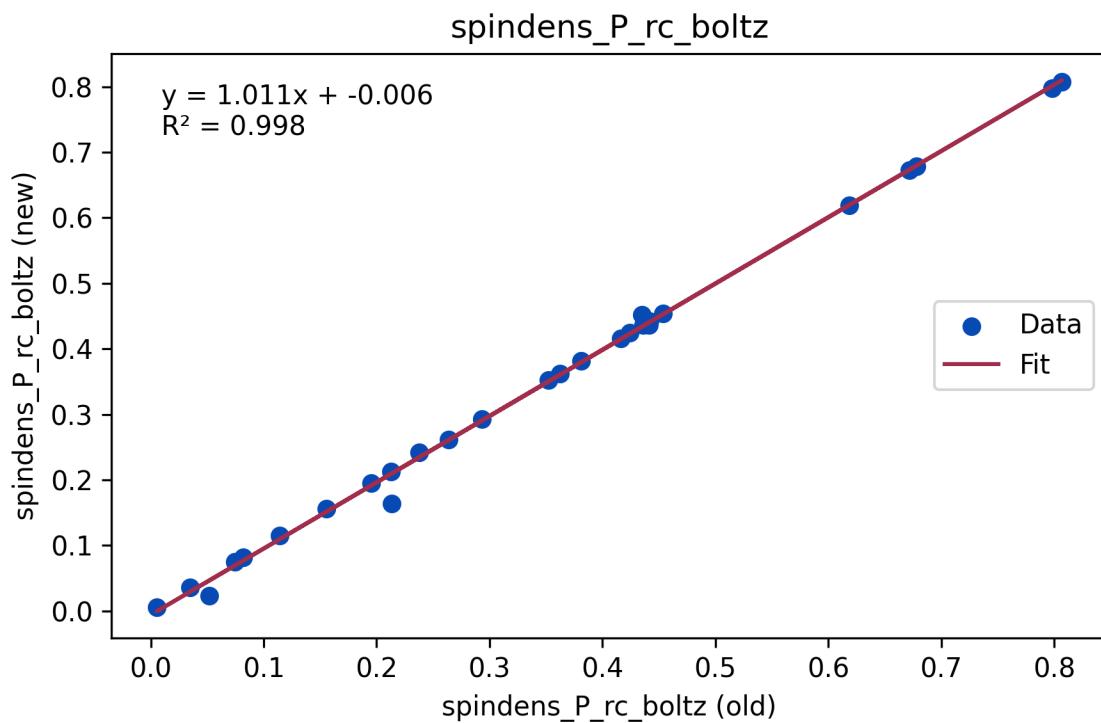
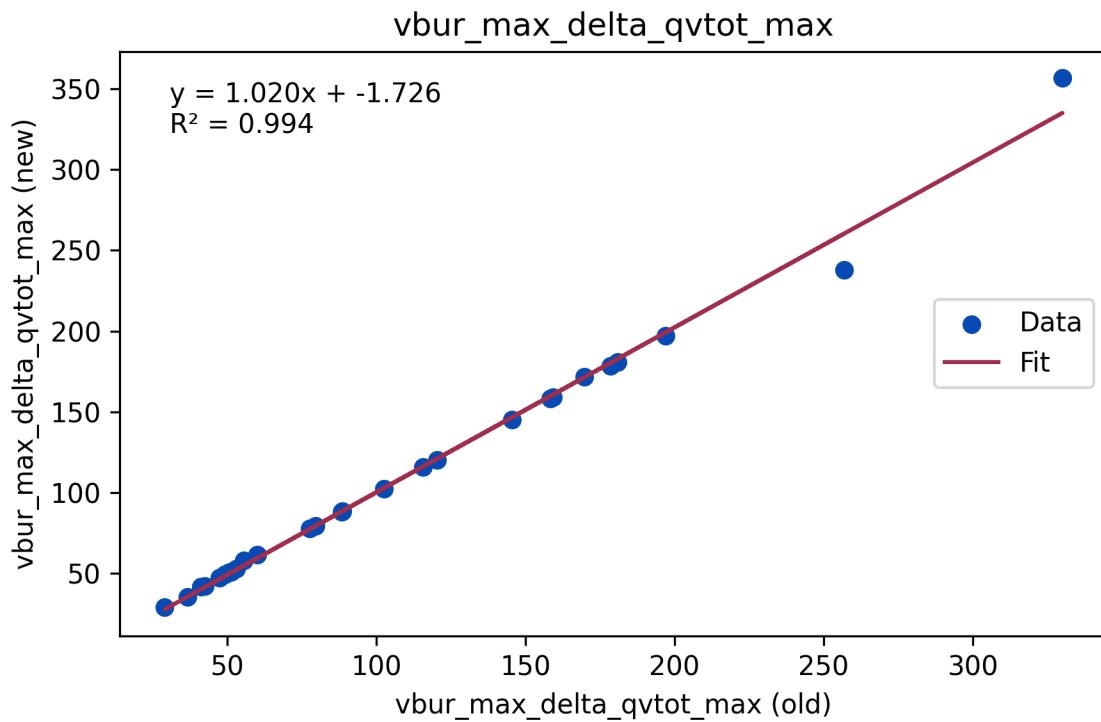
nbo\_P\_rc\_boltz

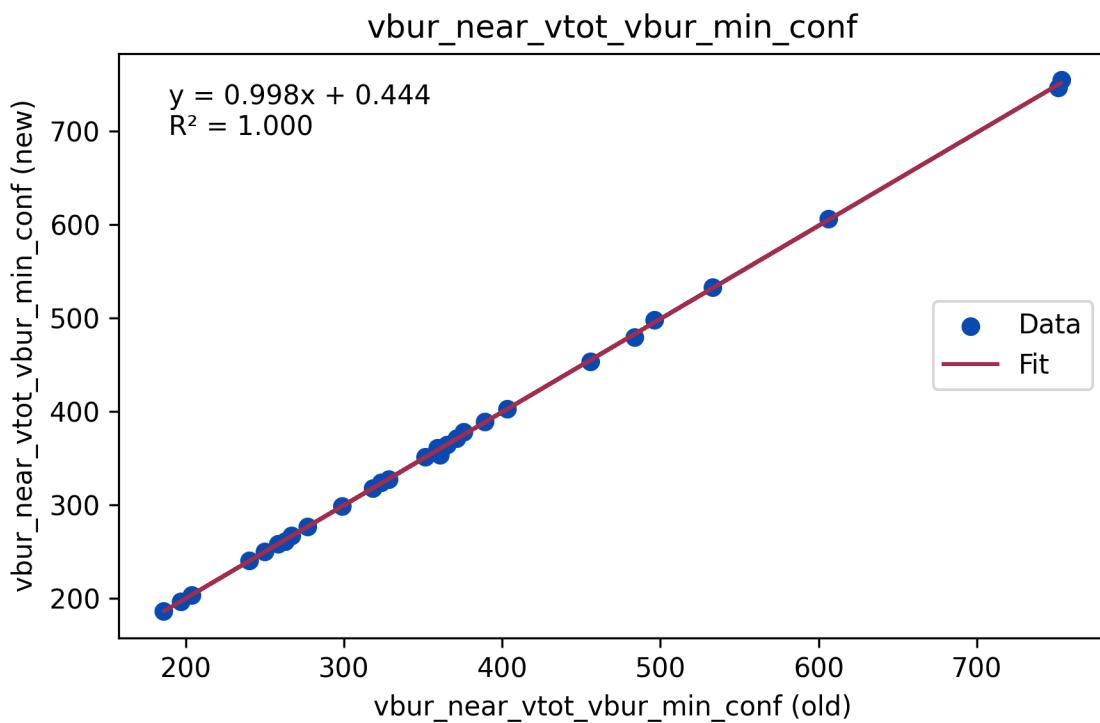
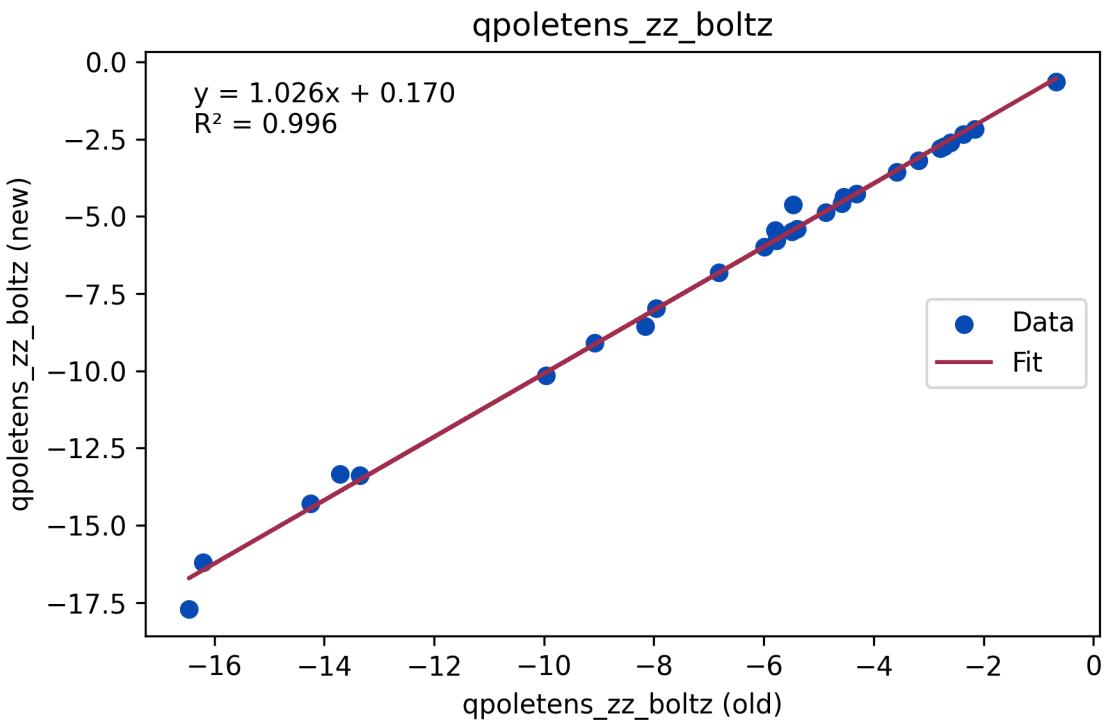


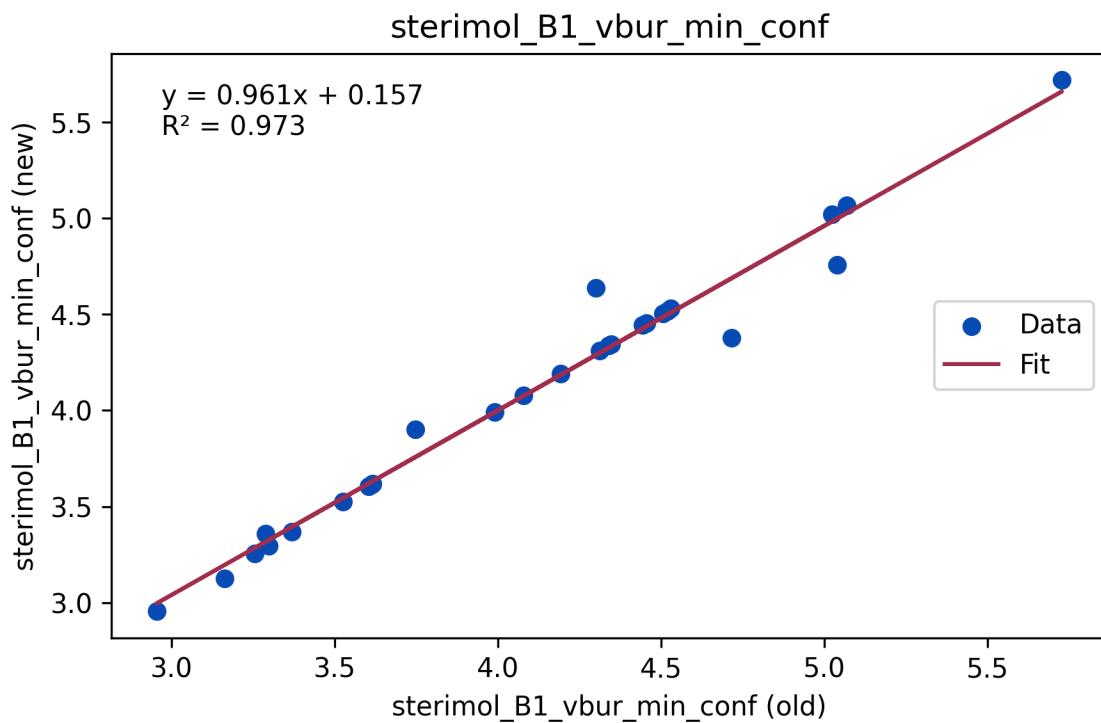
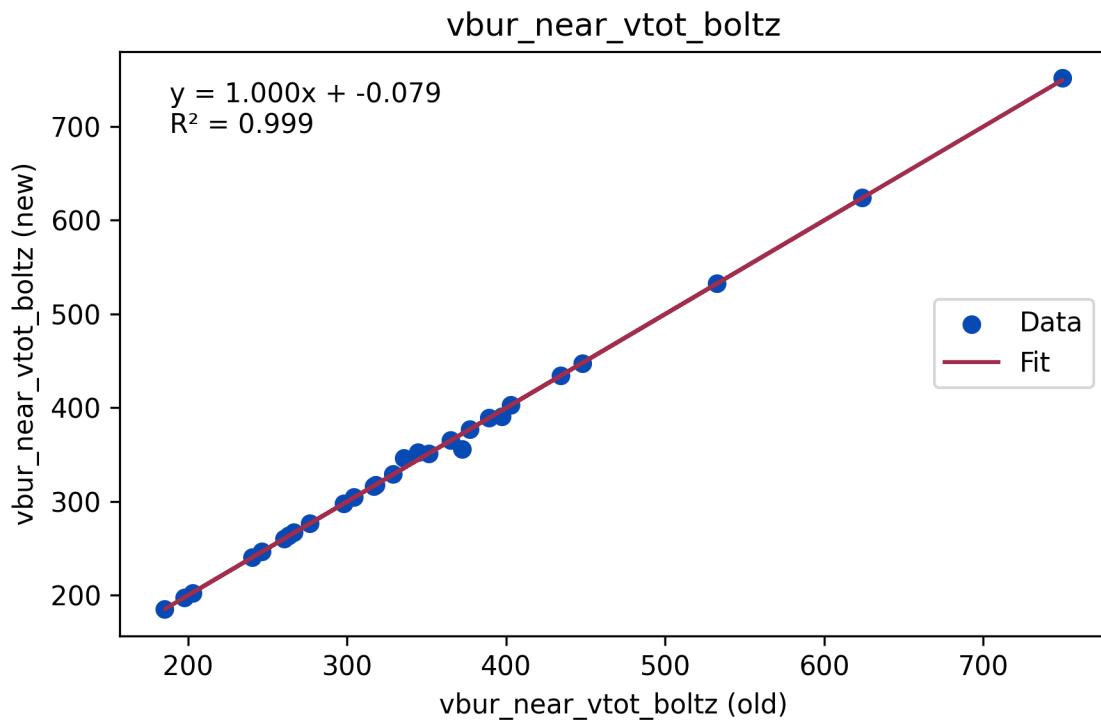
fmo\_e\_lumo\_boltz



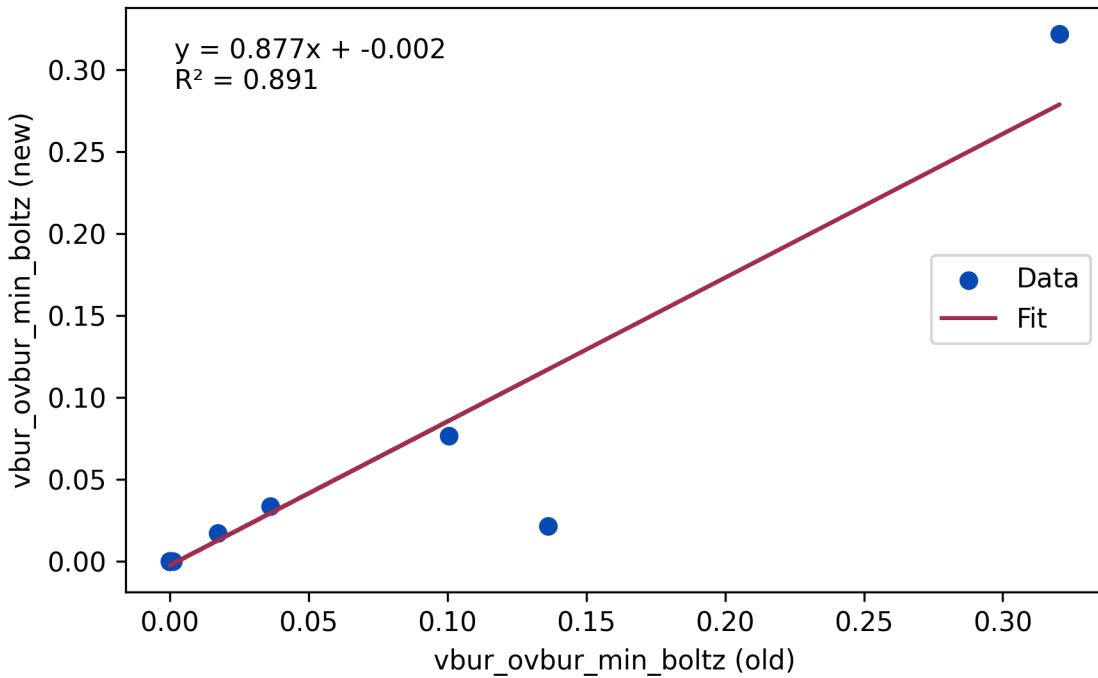




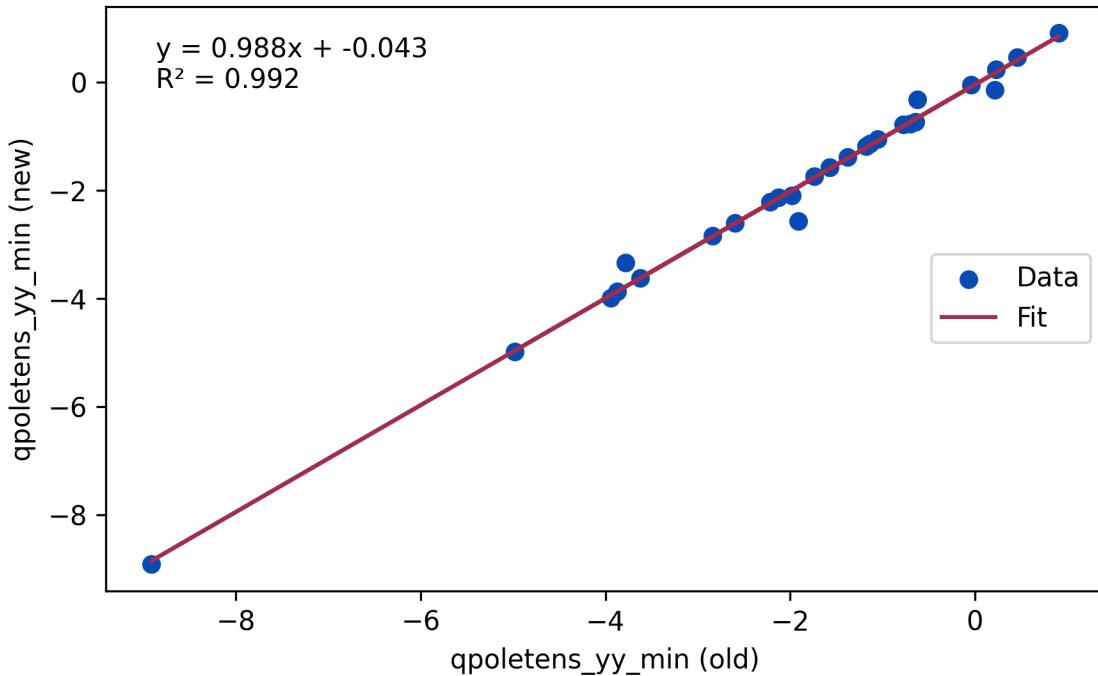


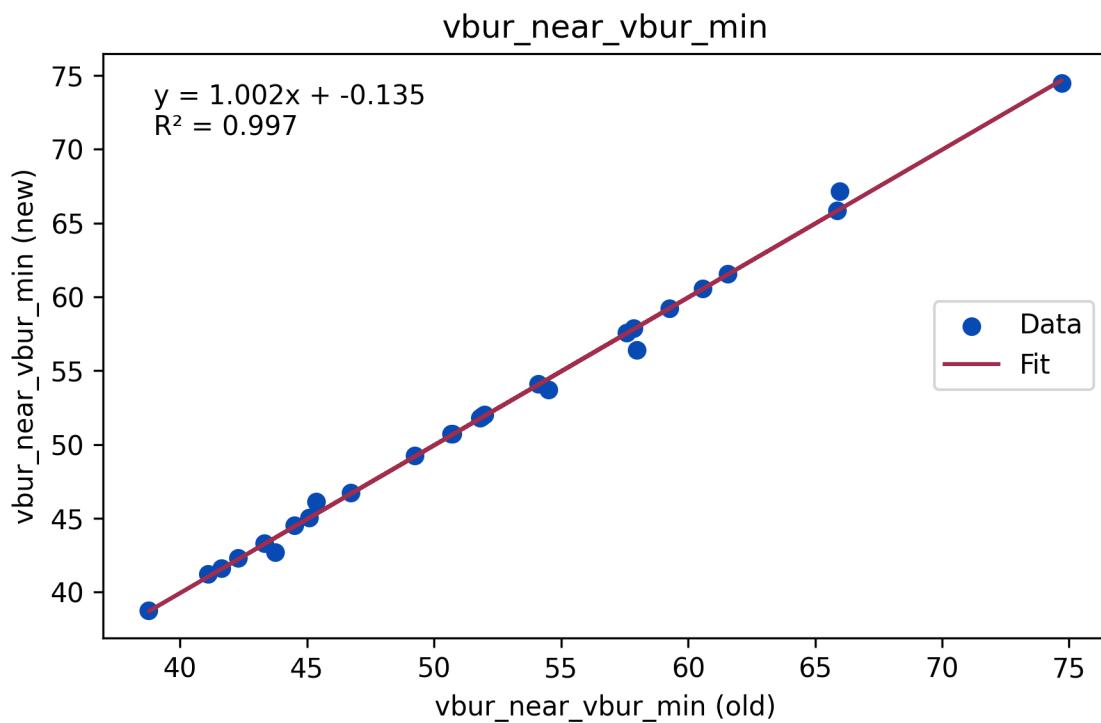
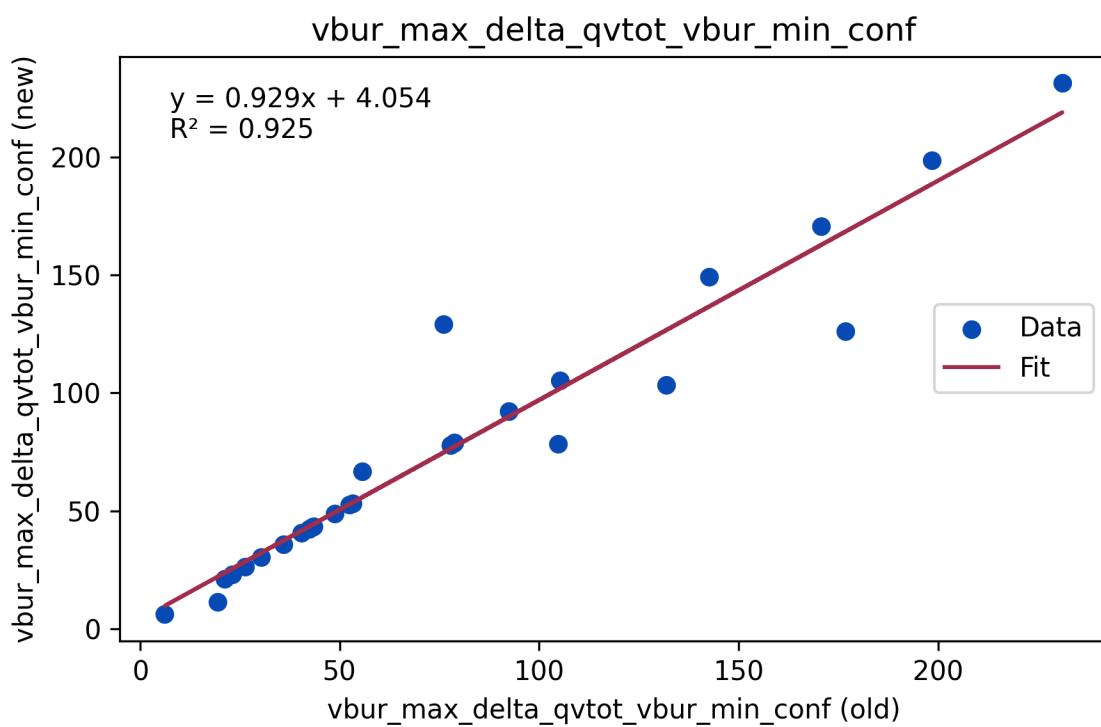


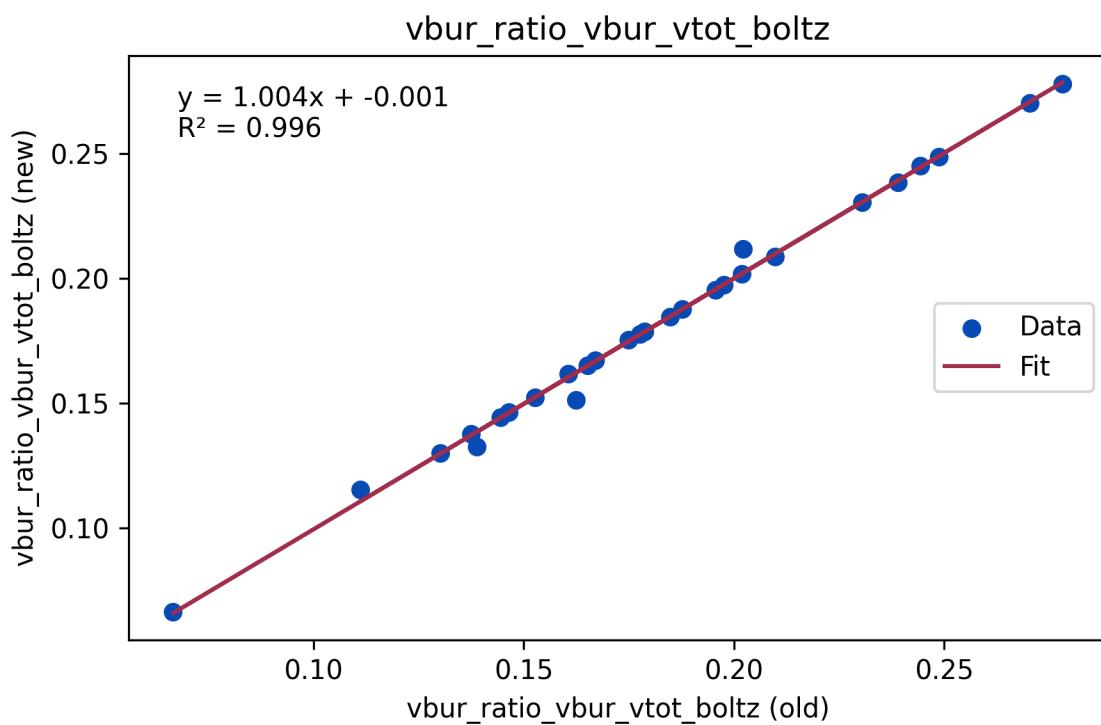
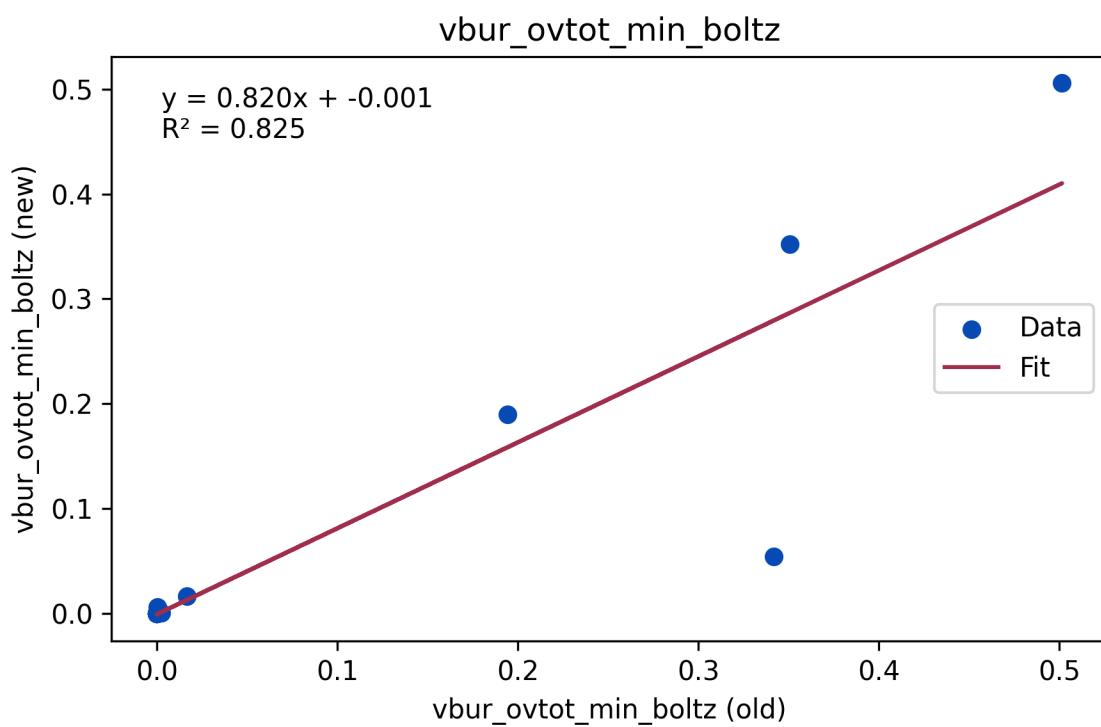
vbur\_ovbur\_min\_boltz

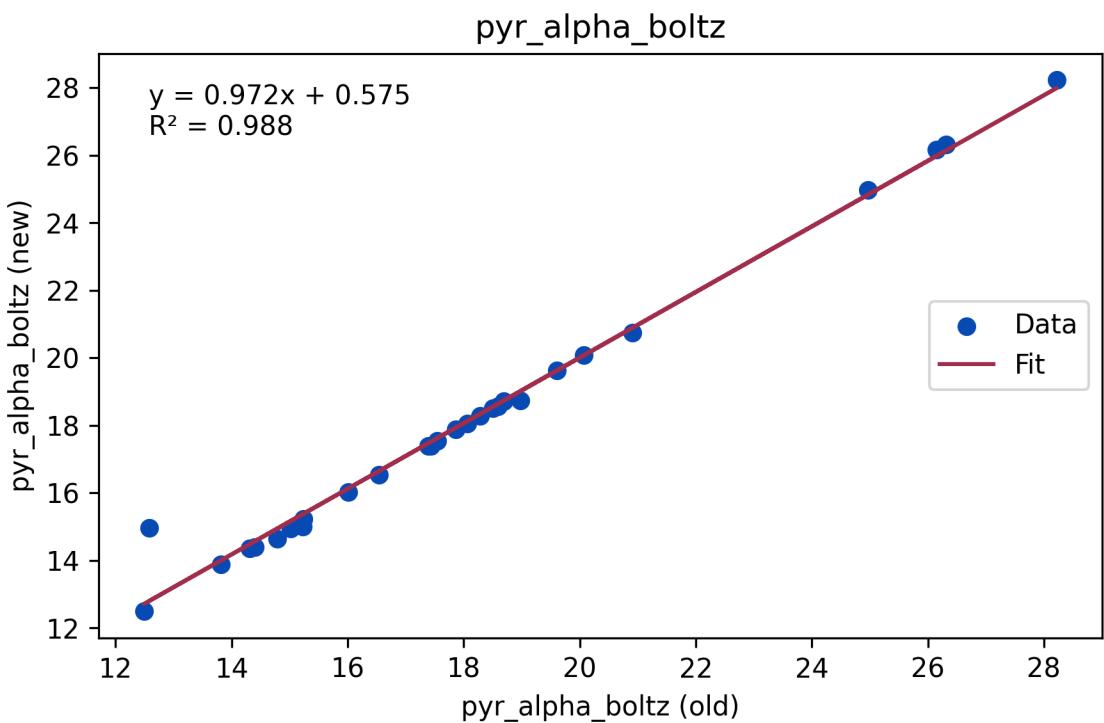
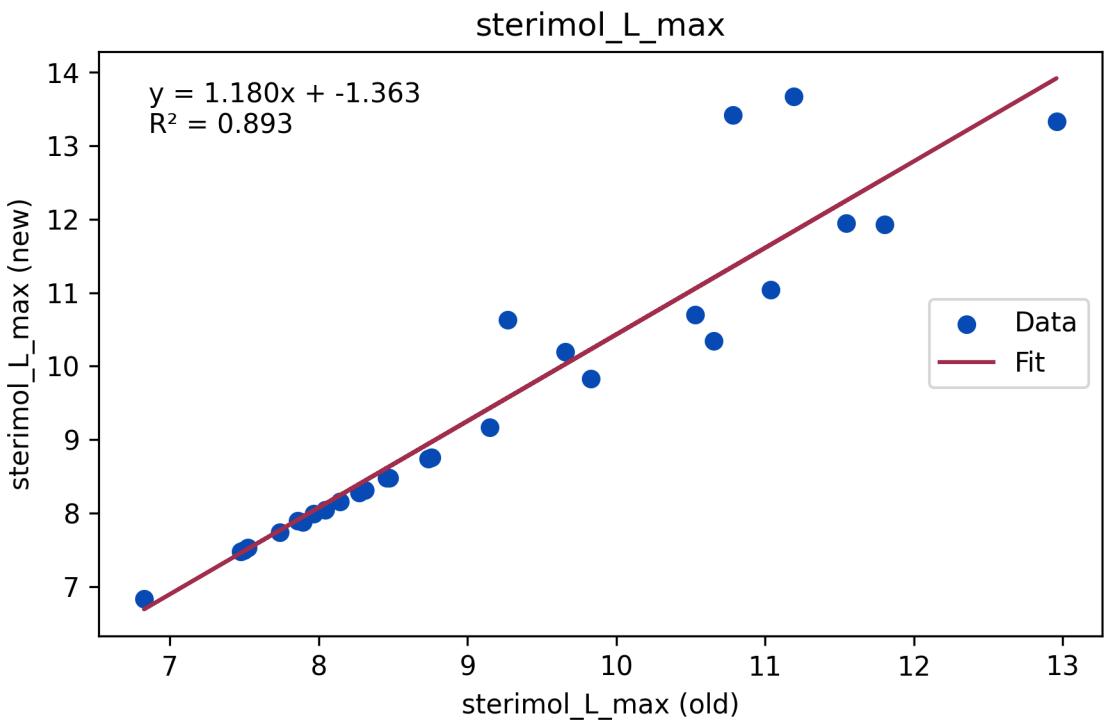


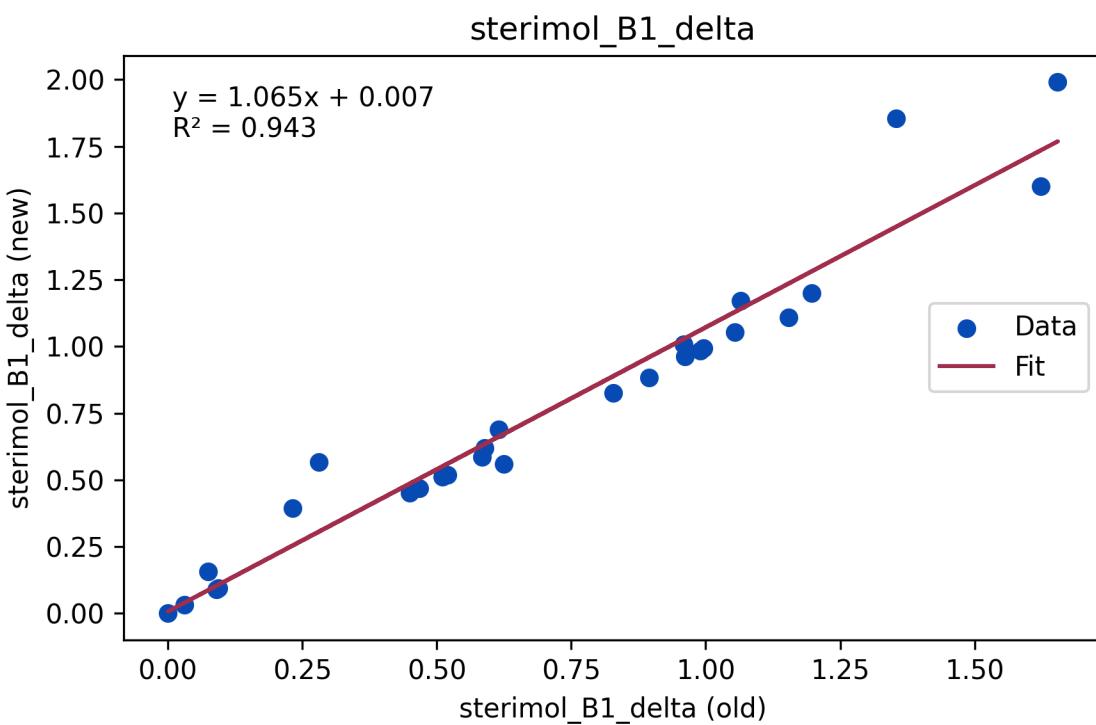
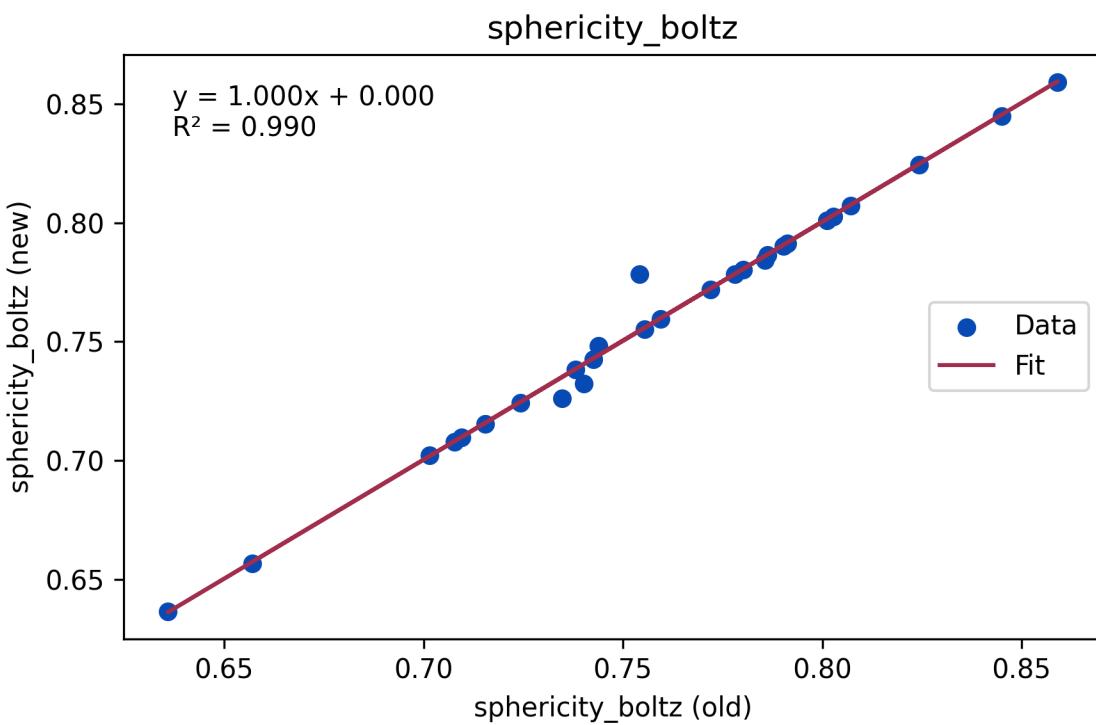
qpoletens\_yy\_min

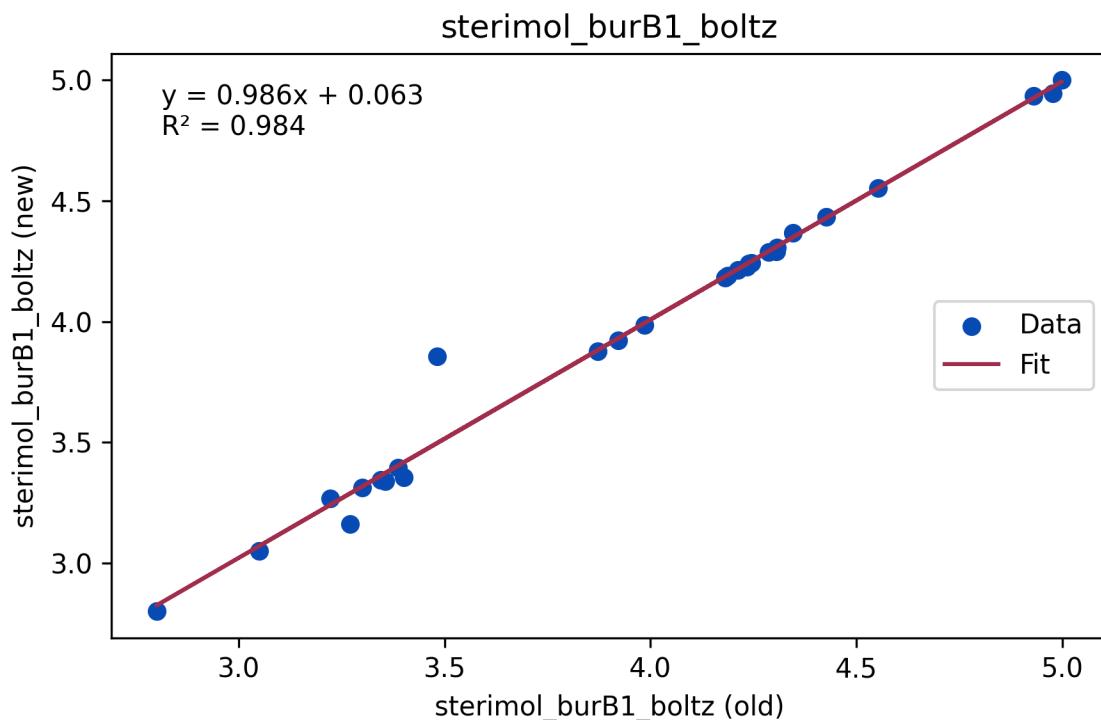
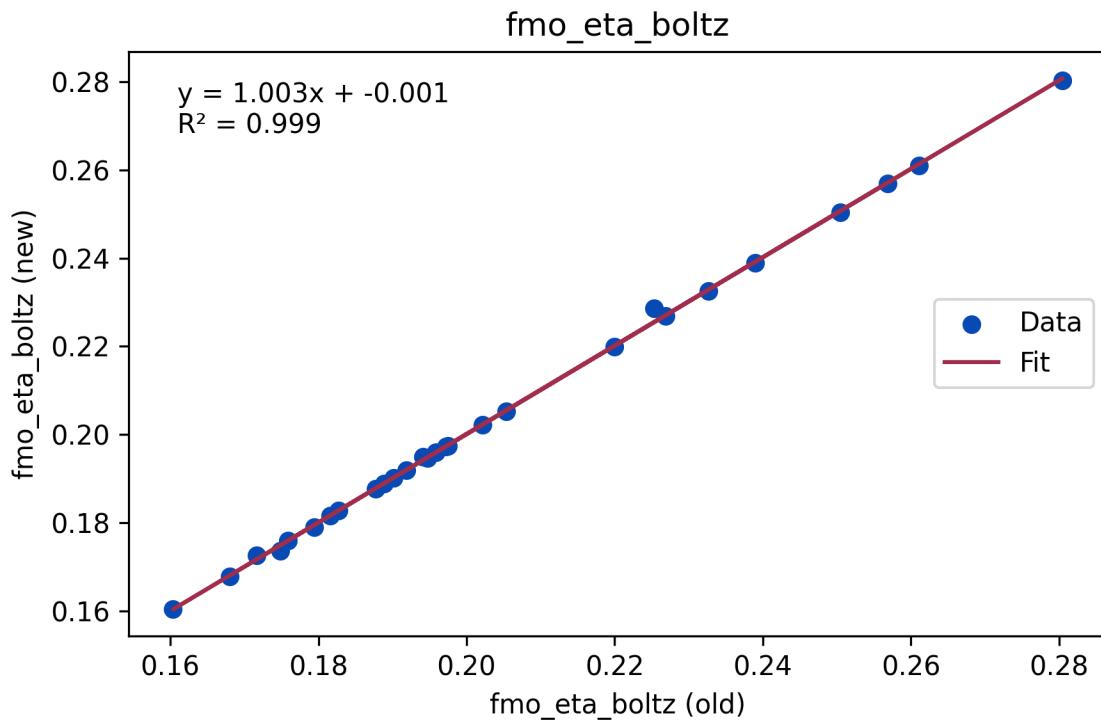


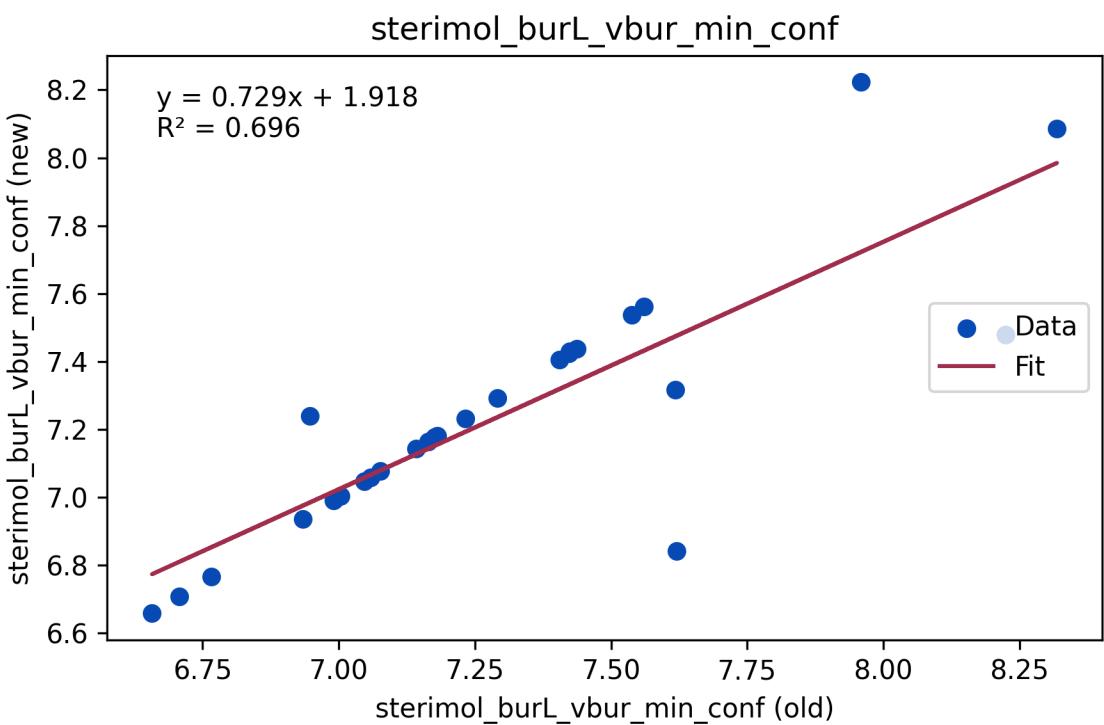
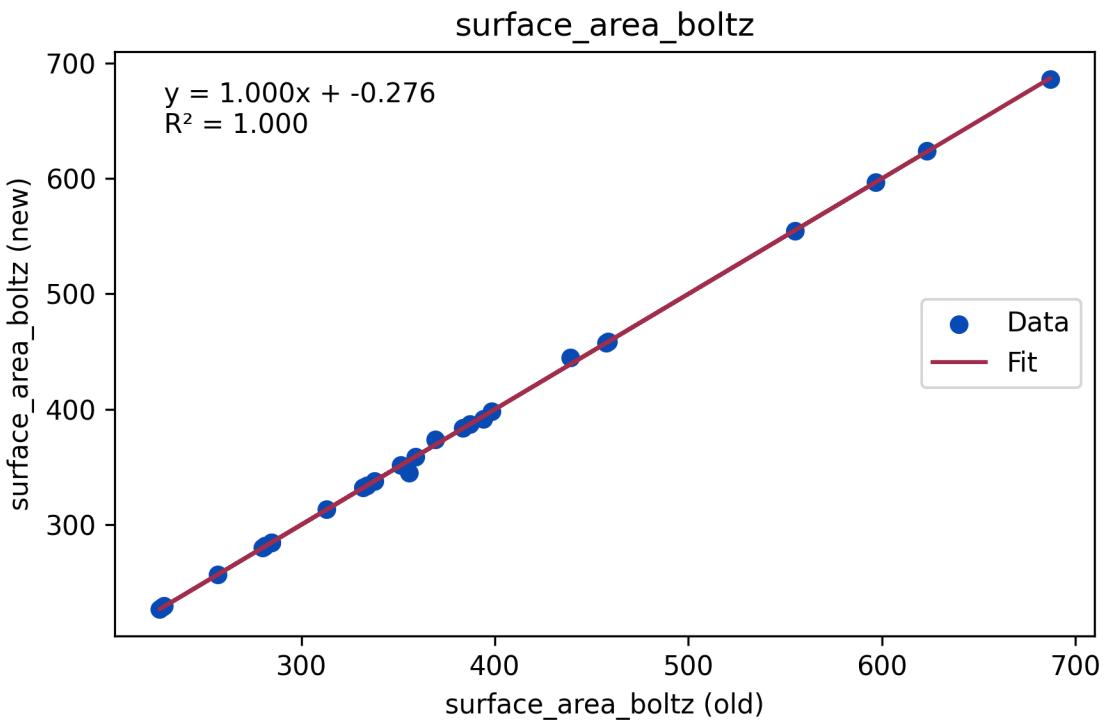


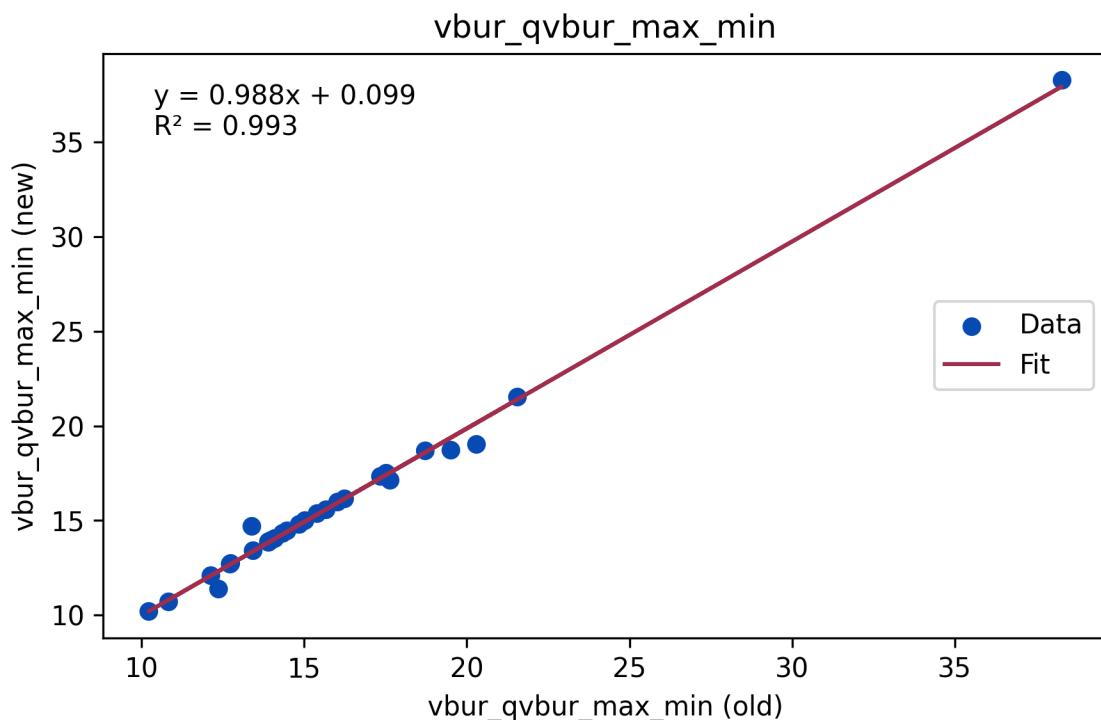
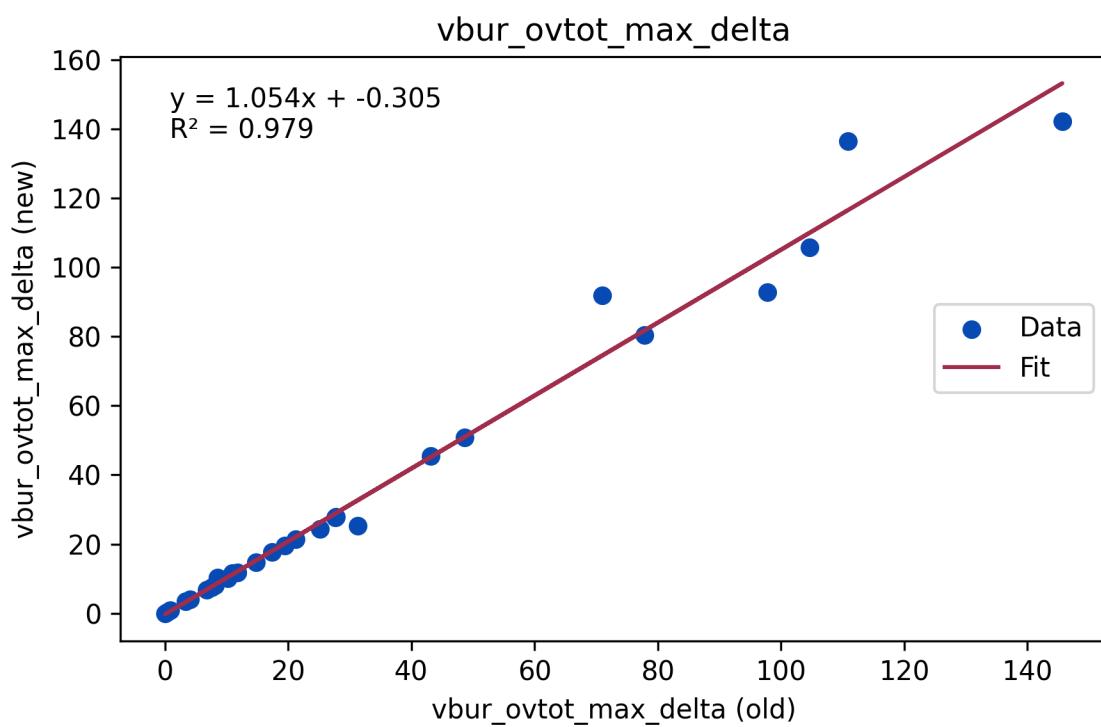


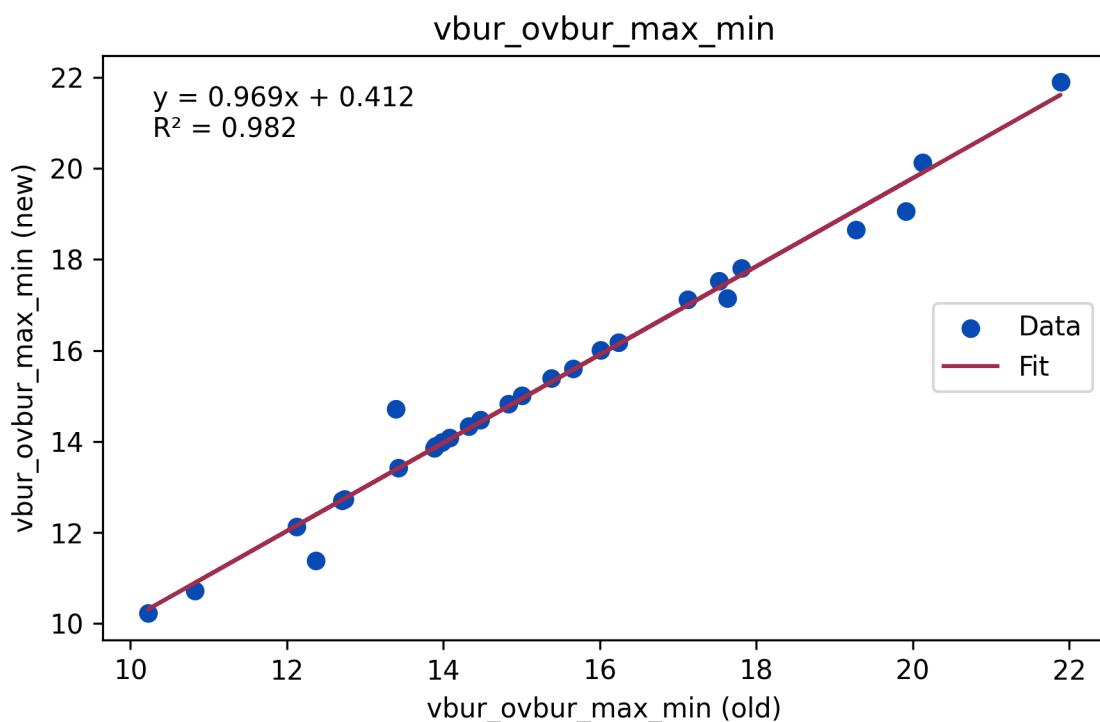
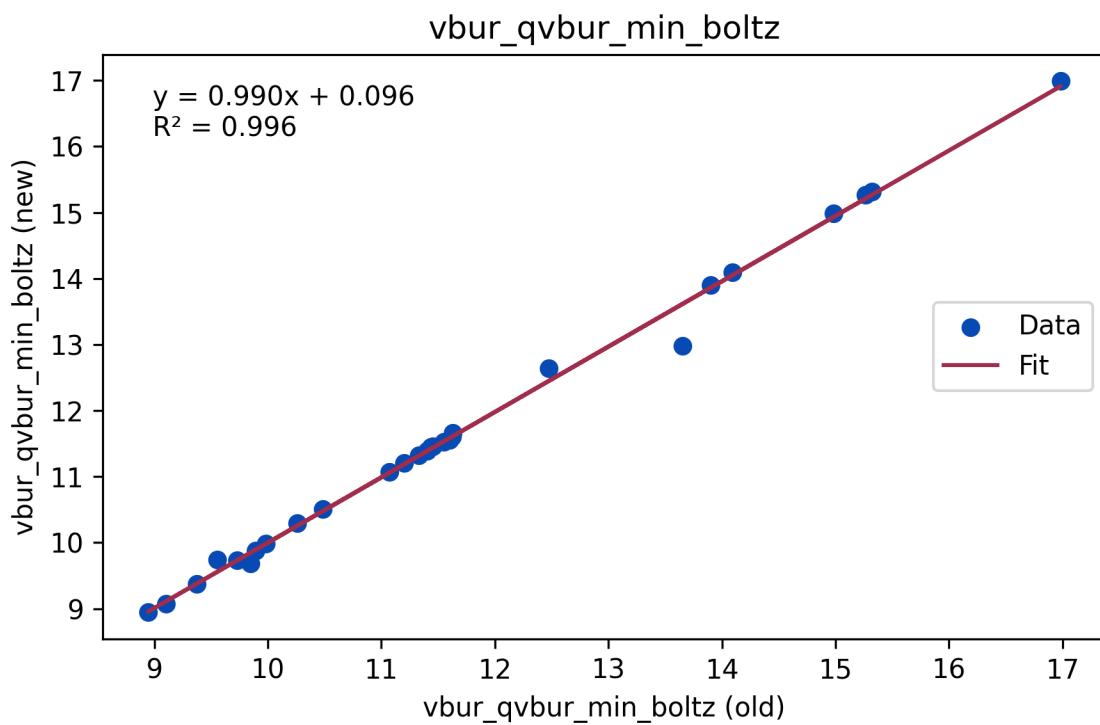


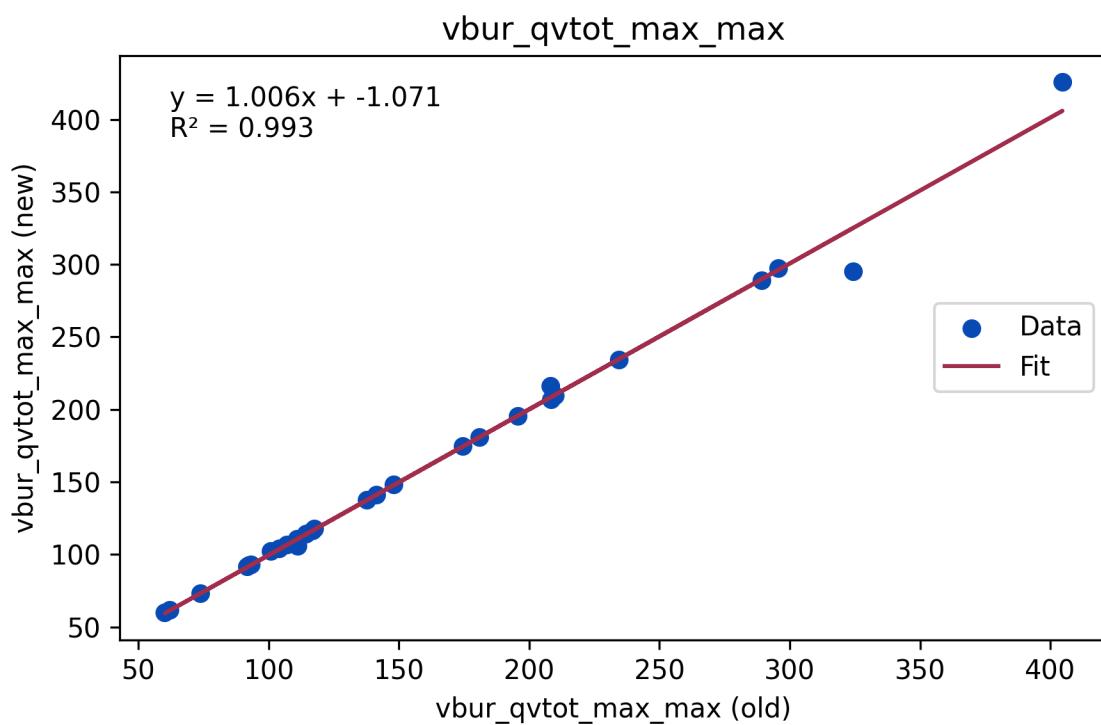
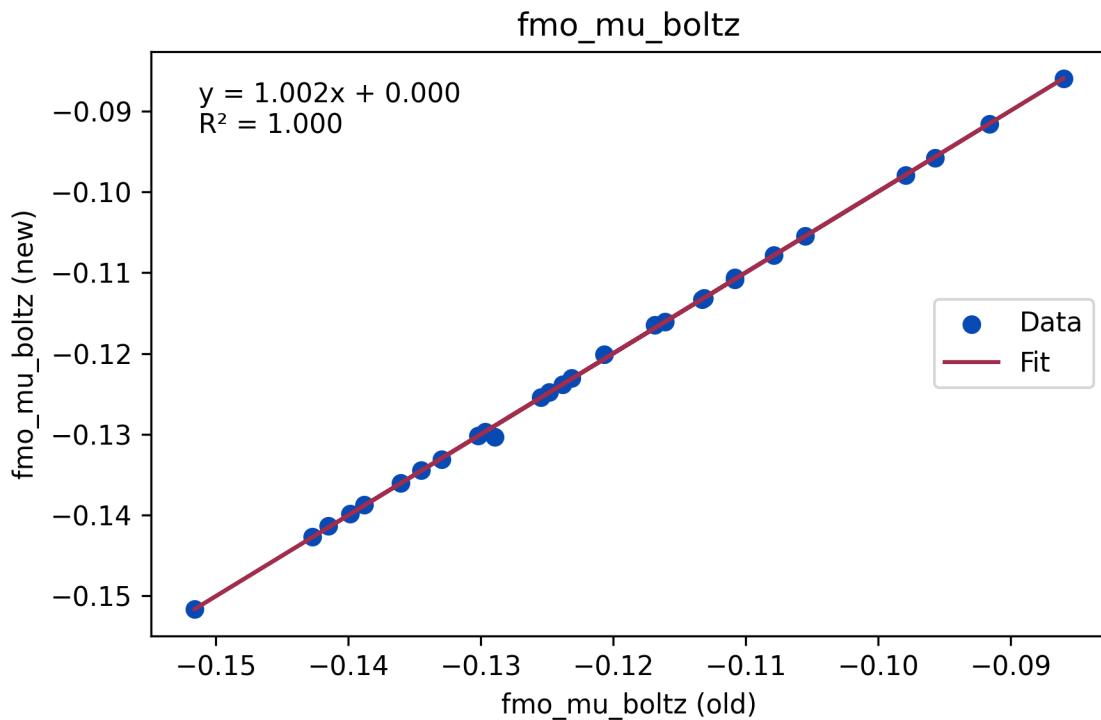


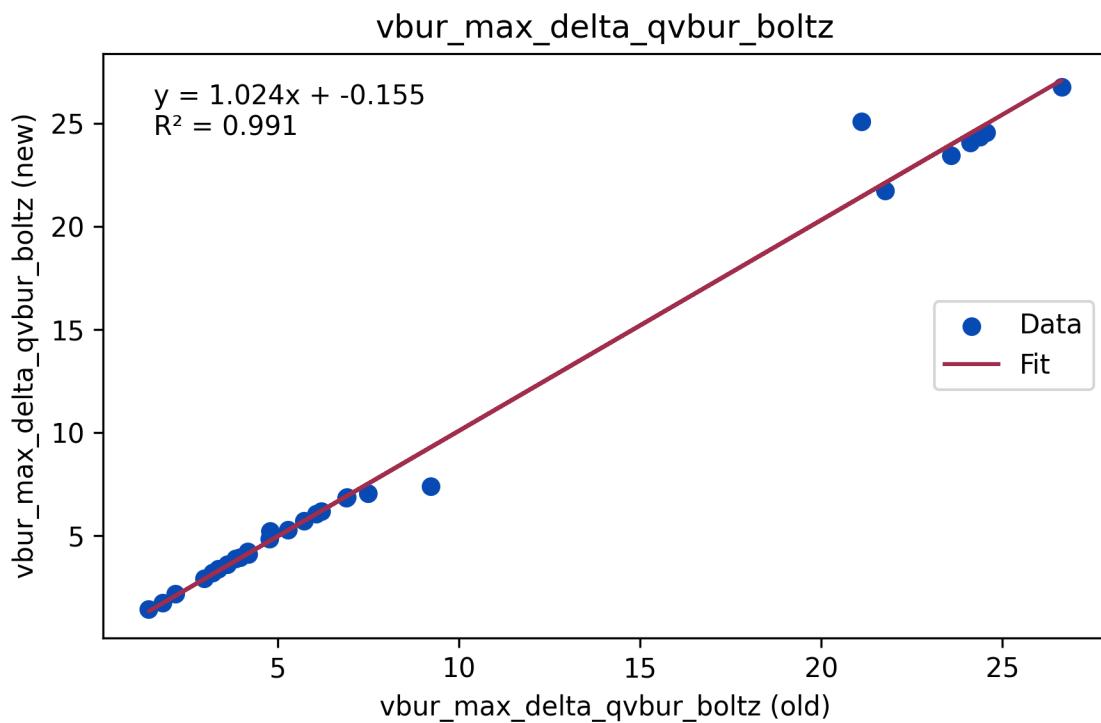
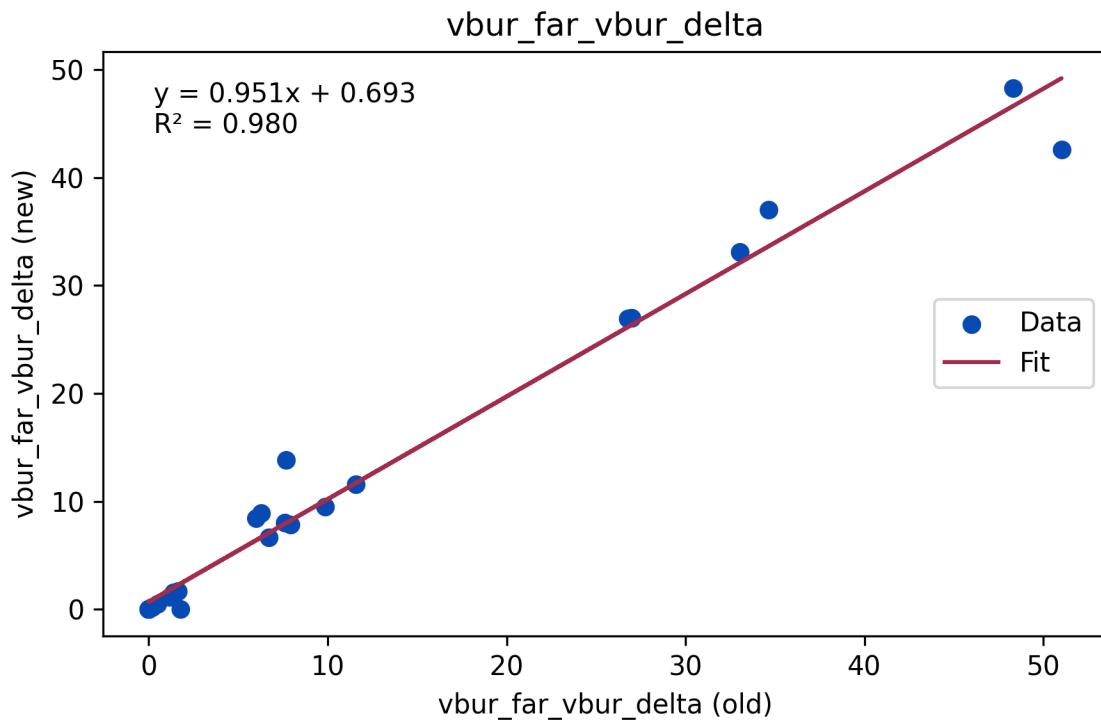


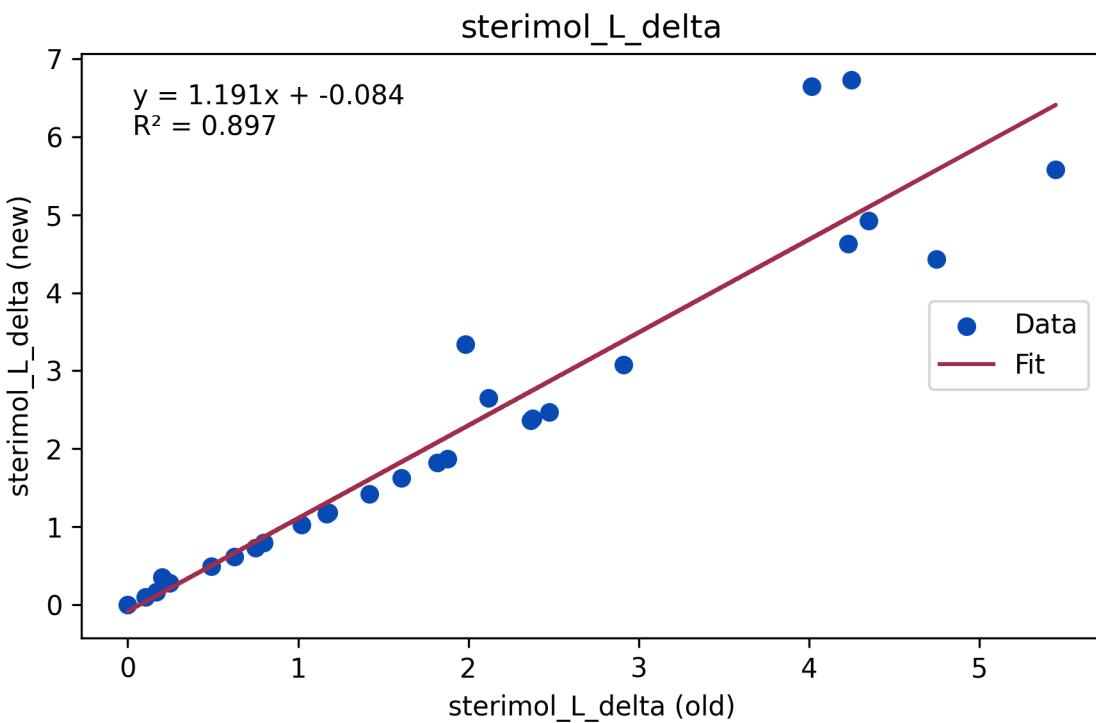
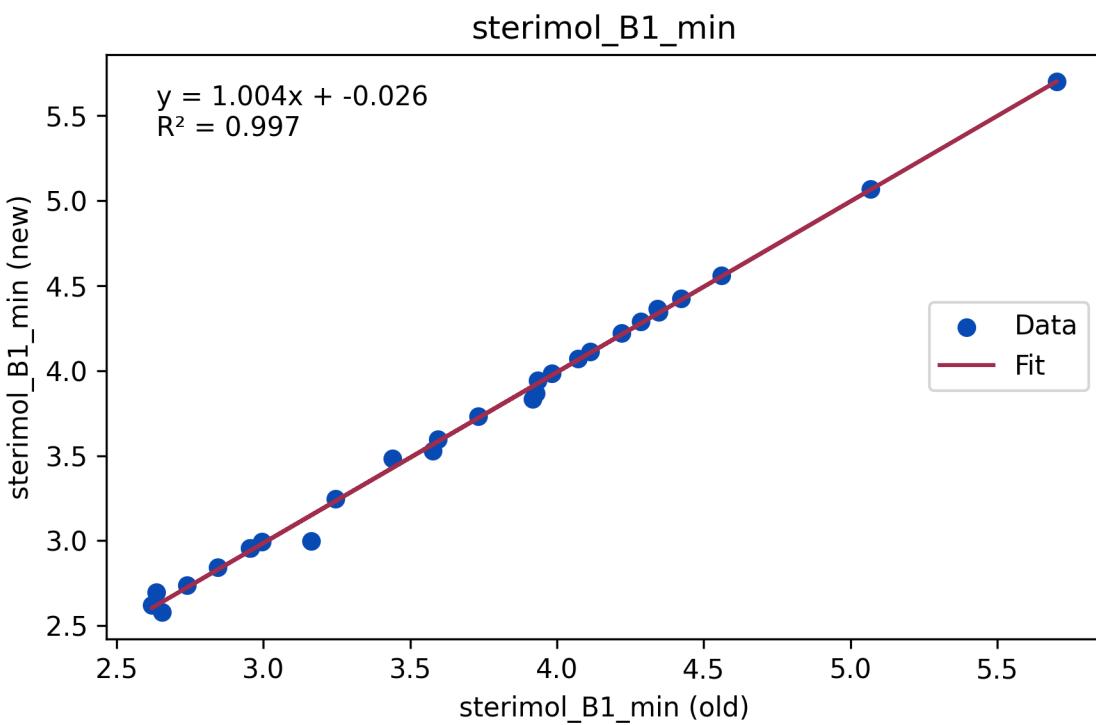


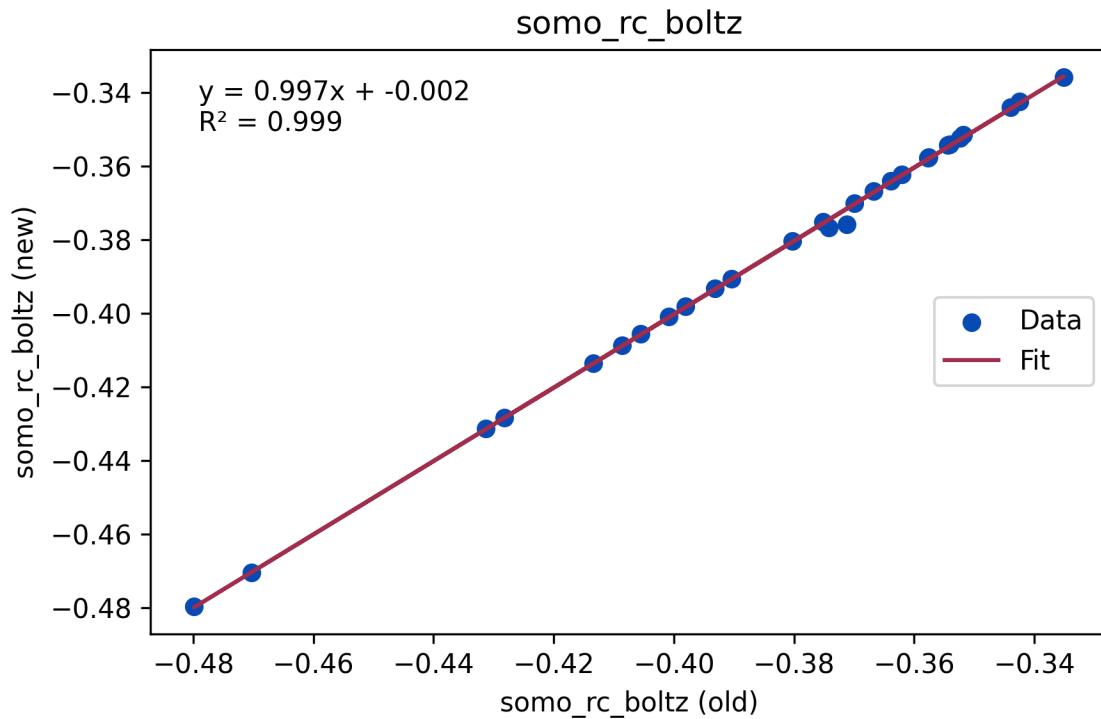
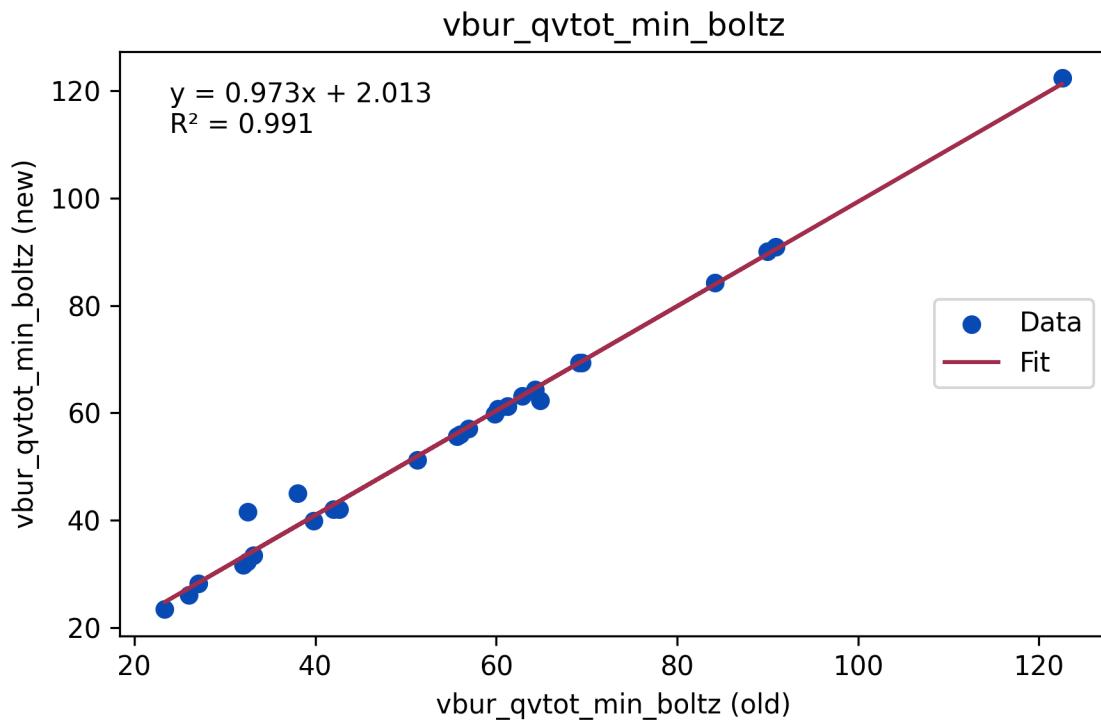


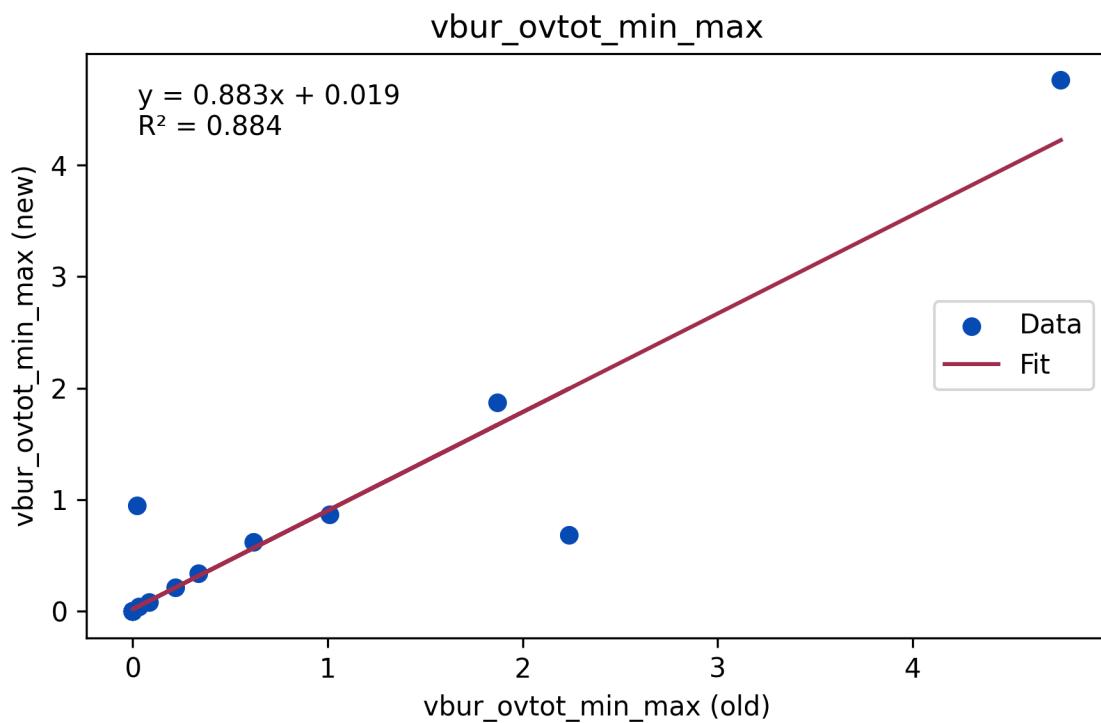
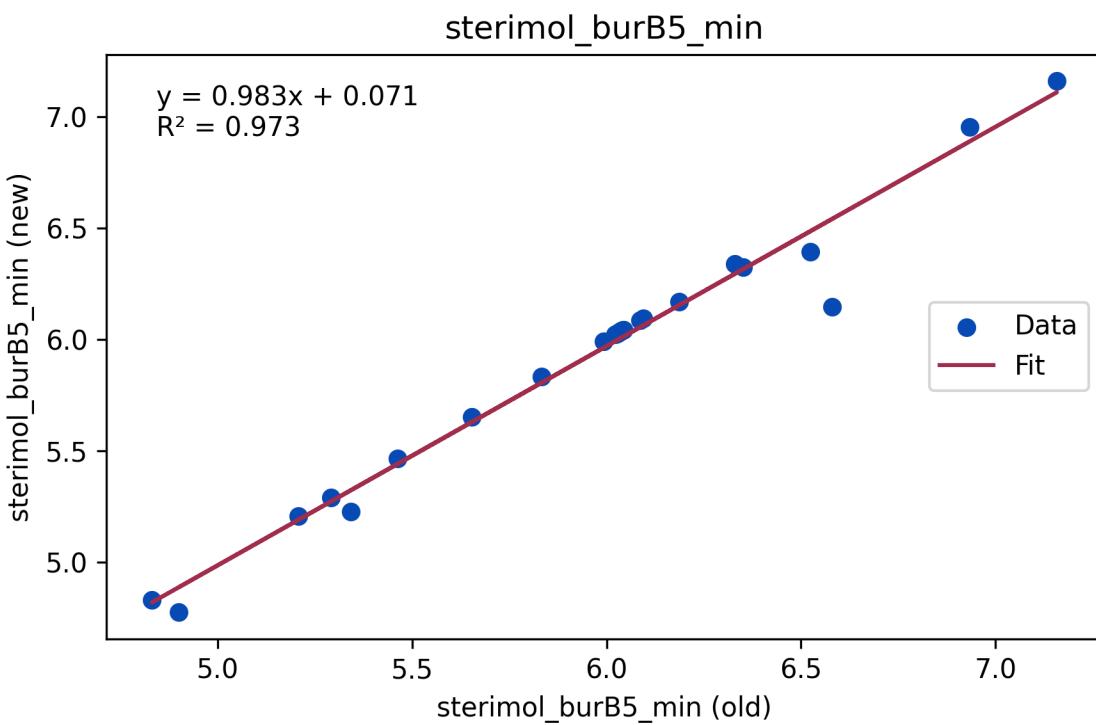


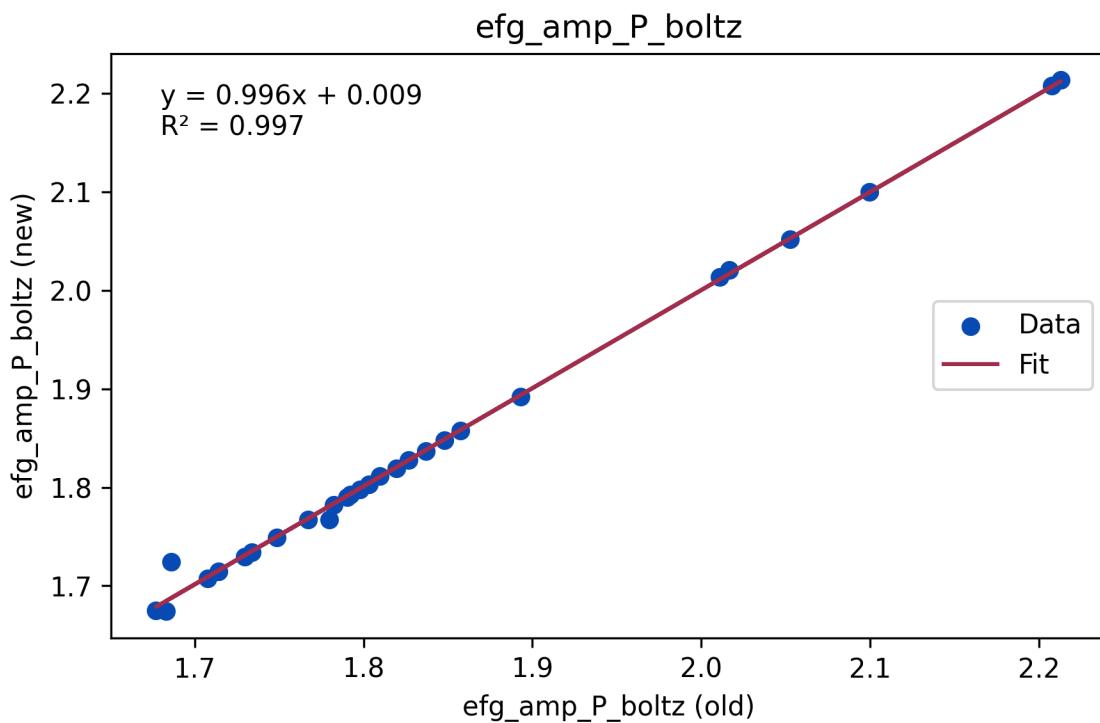
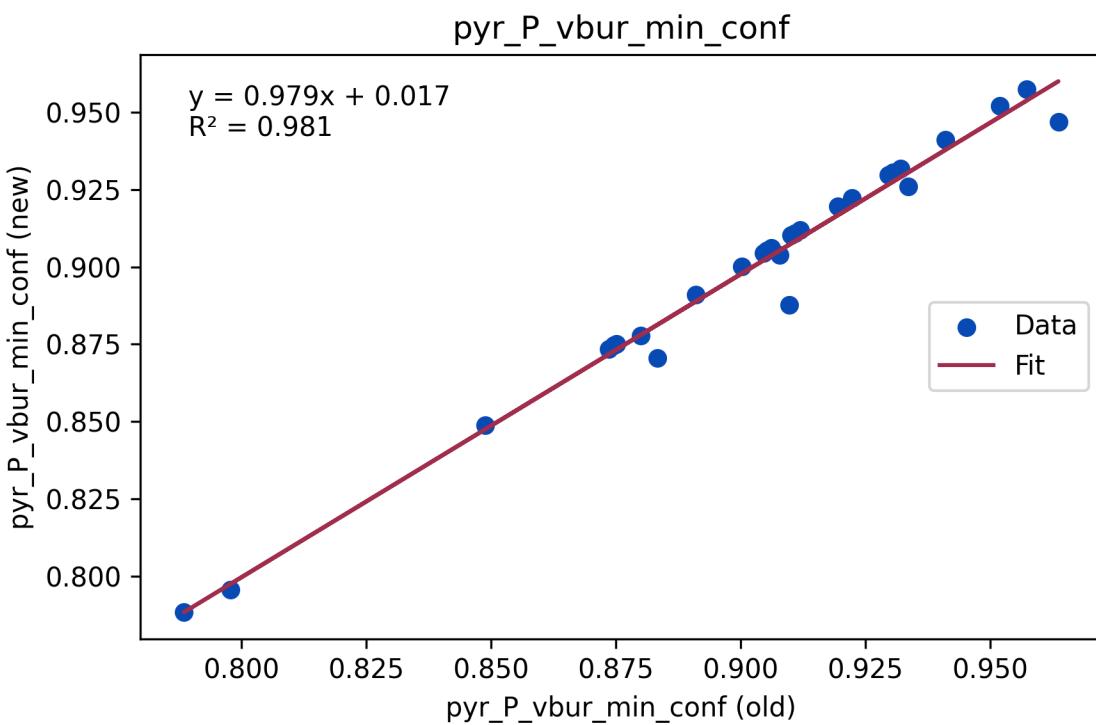




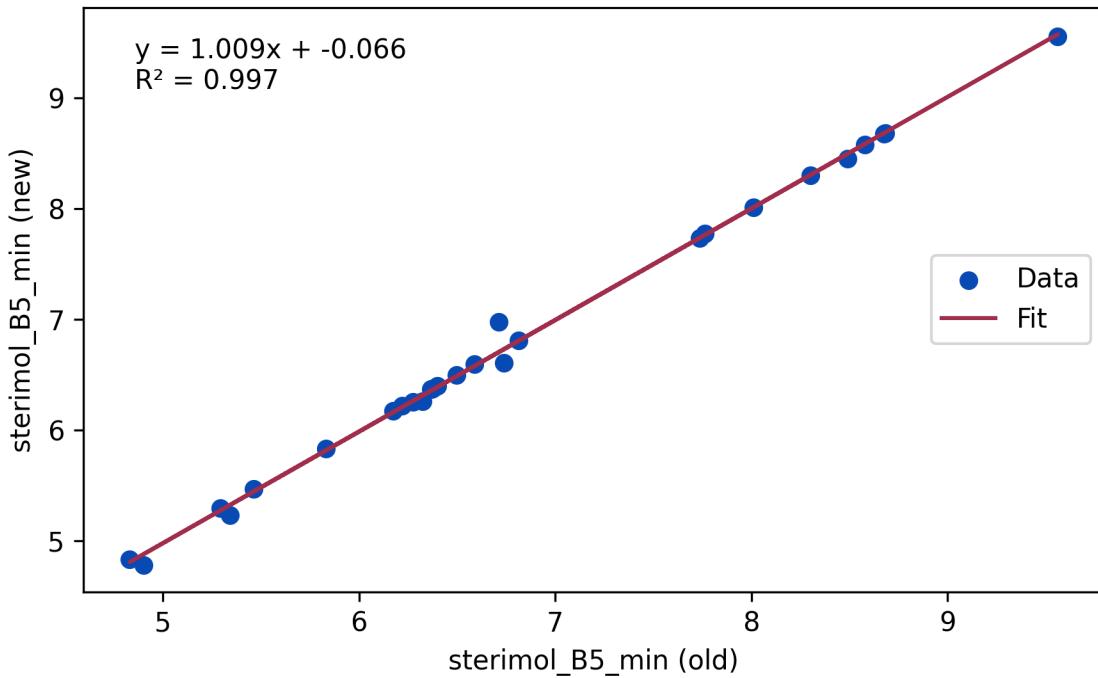




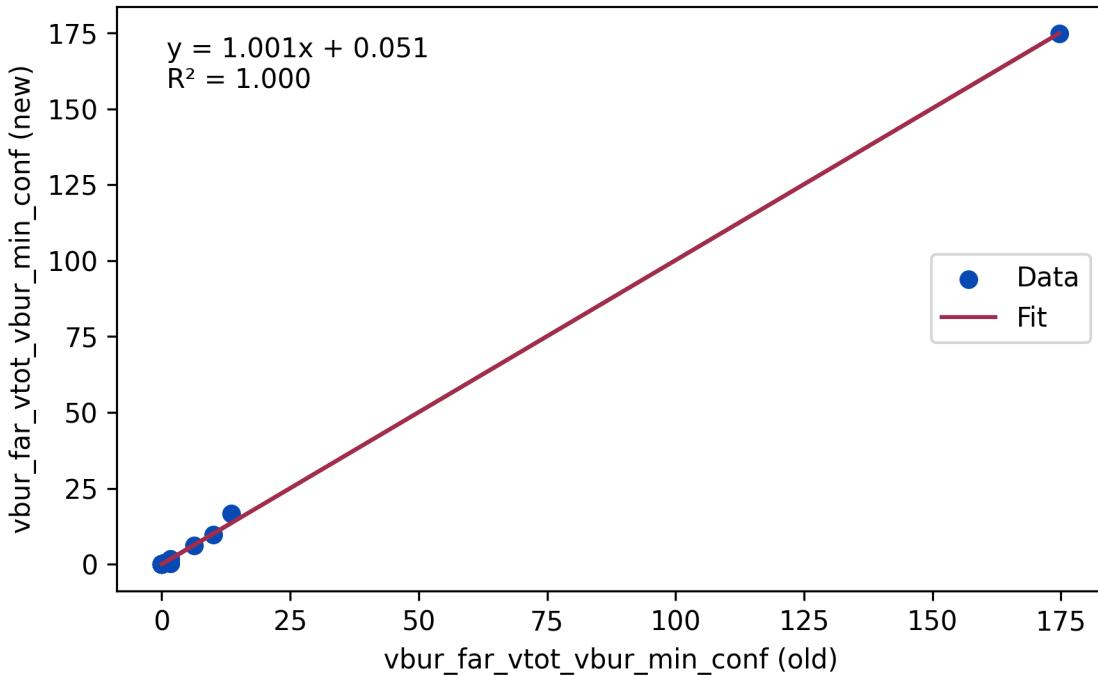


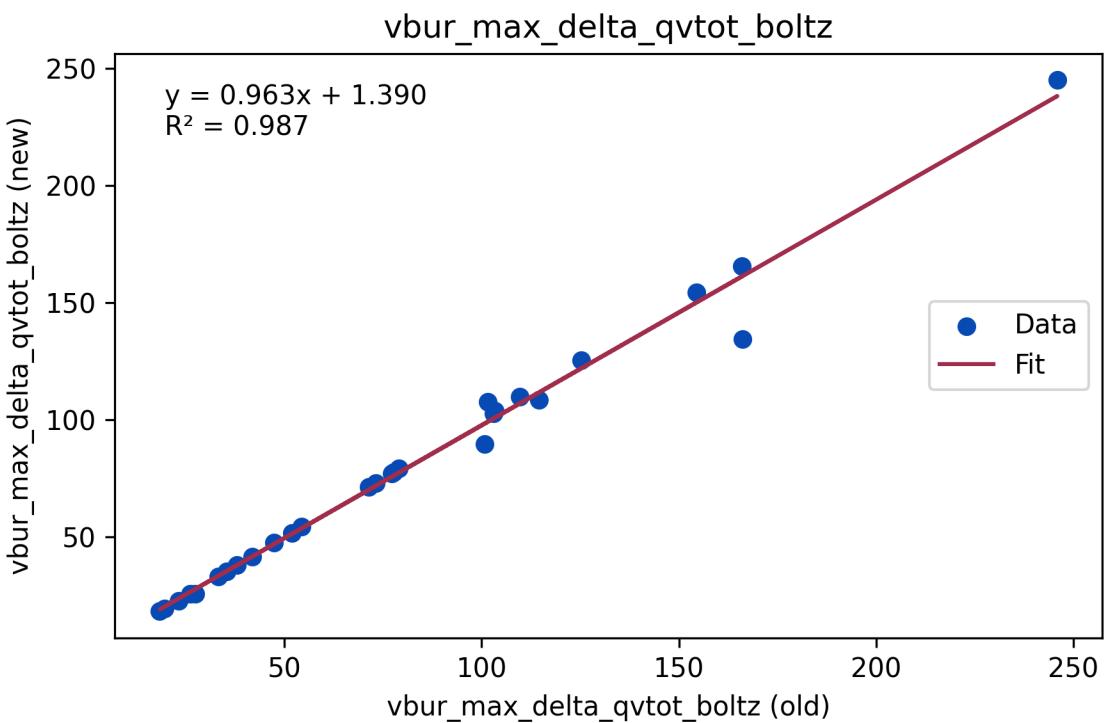
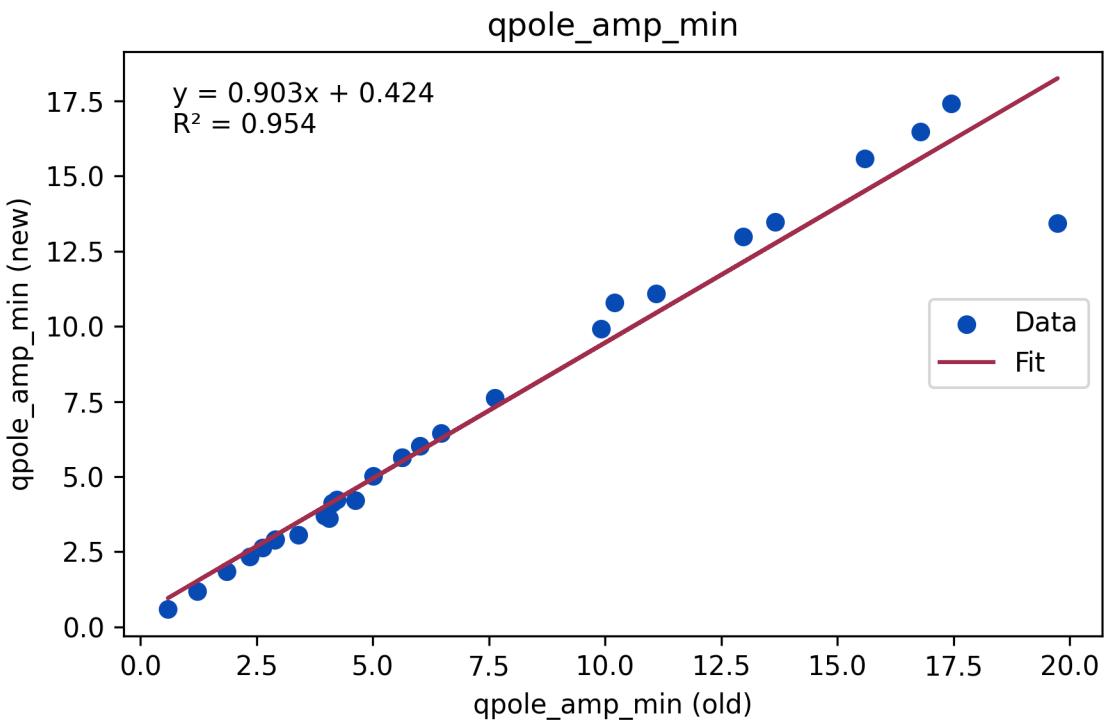


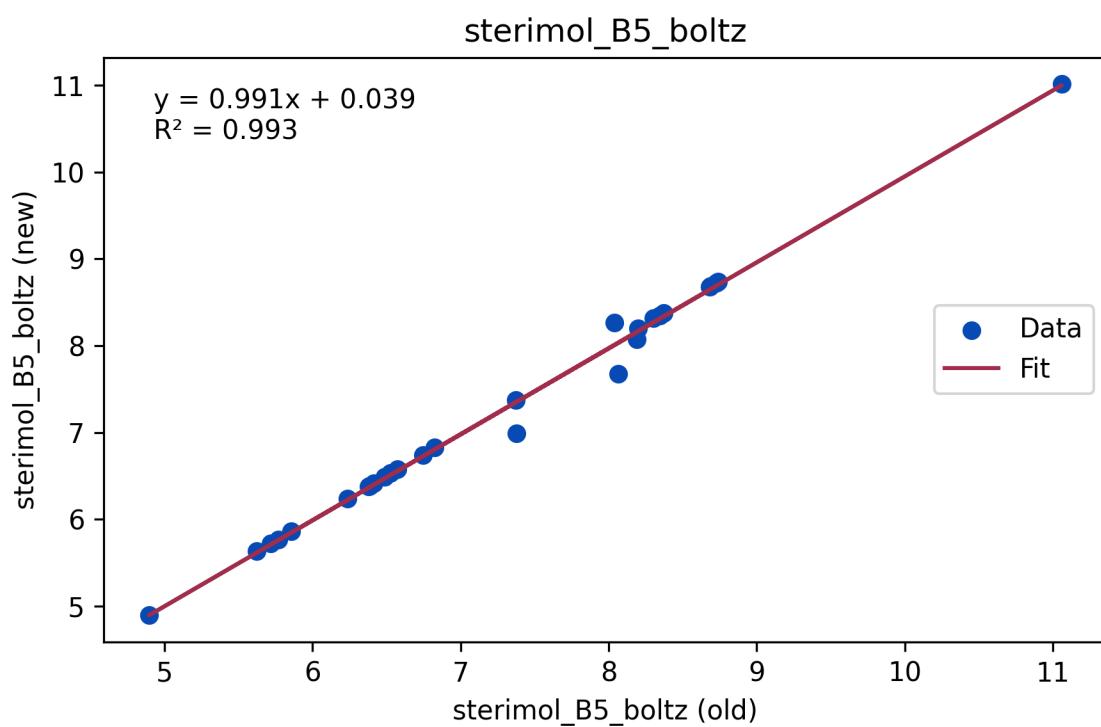
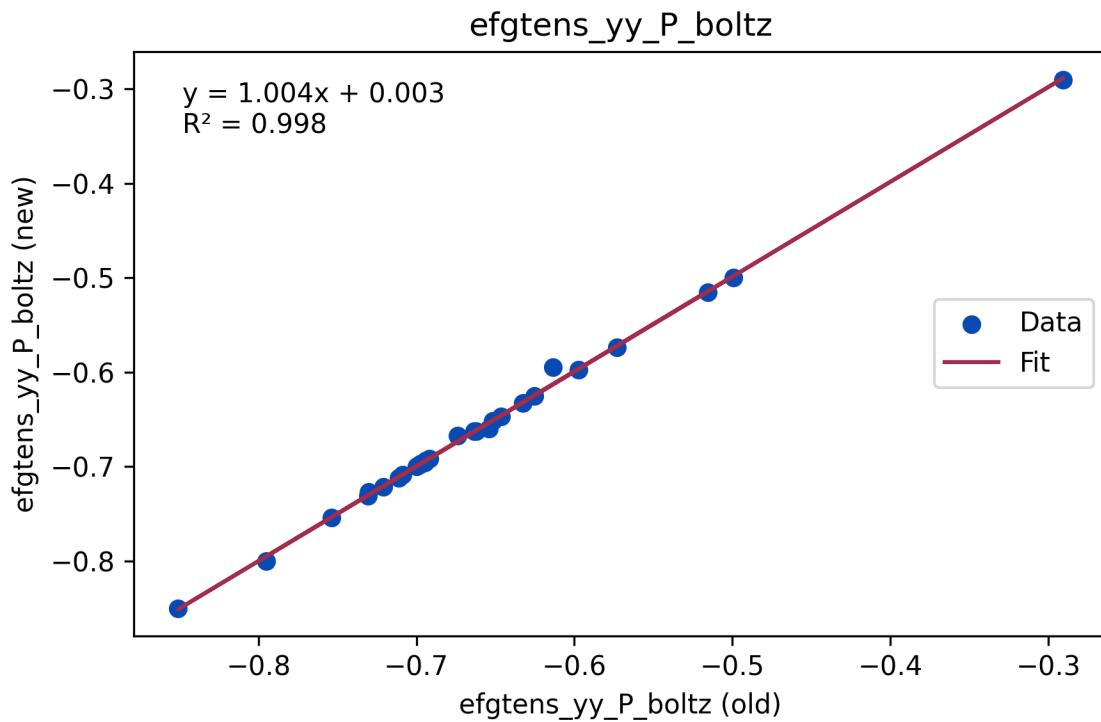
sterimol\_B5\_min

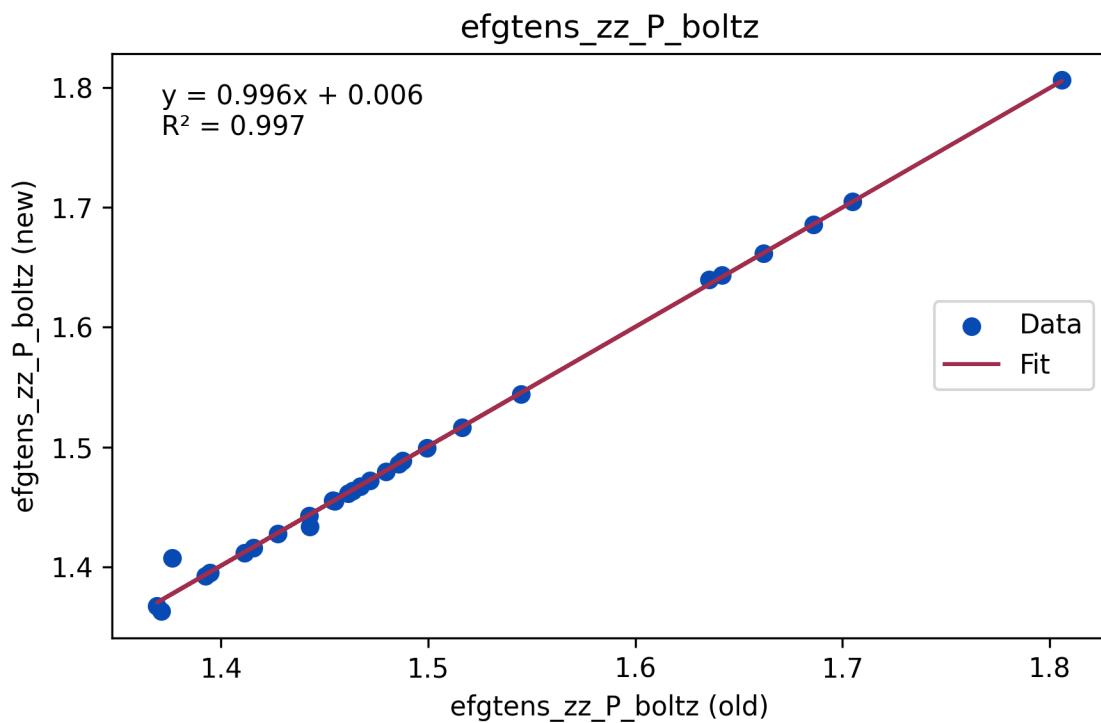
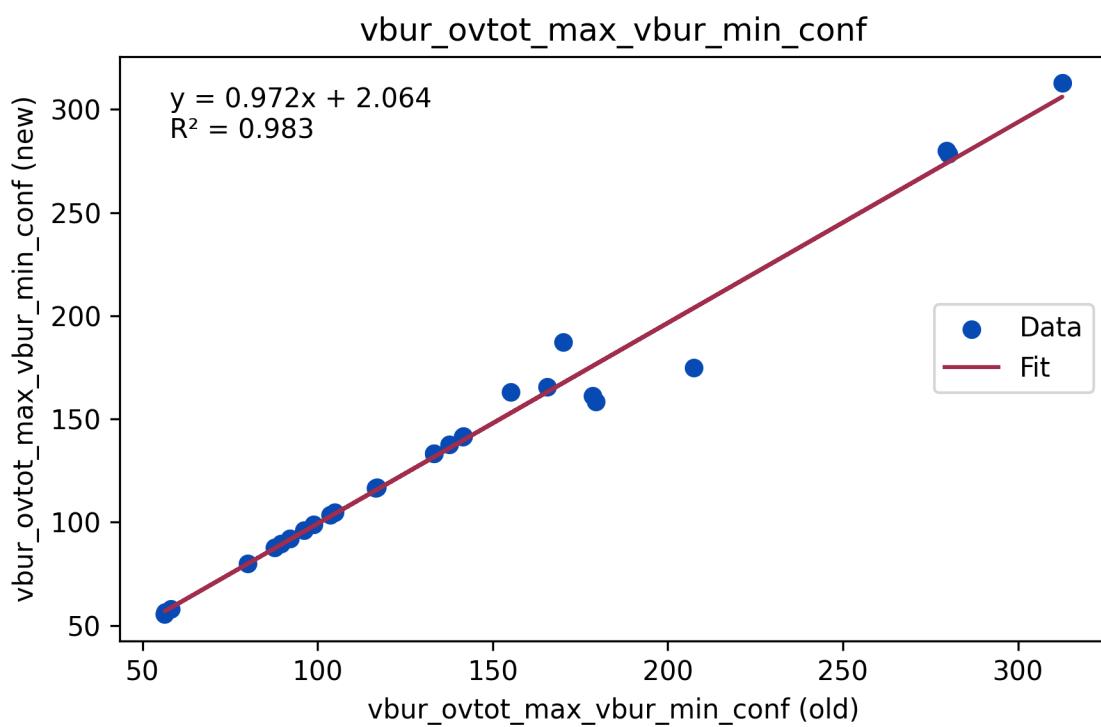


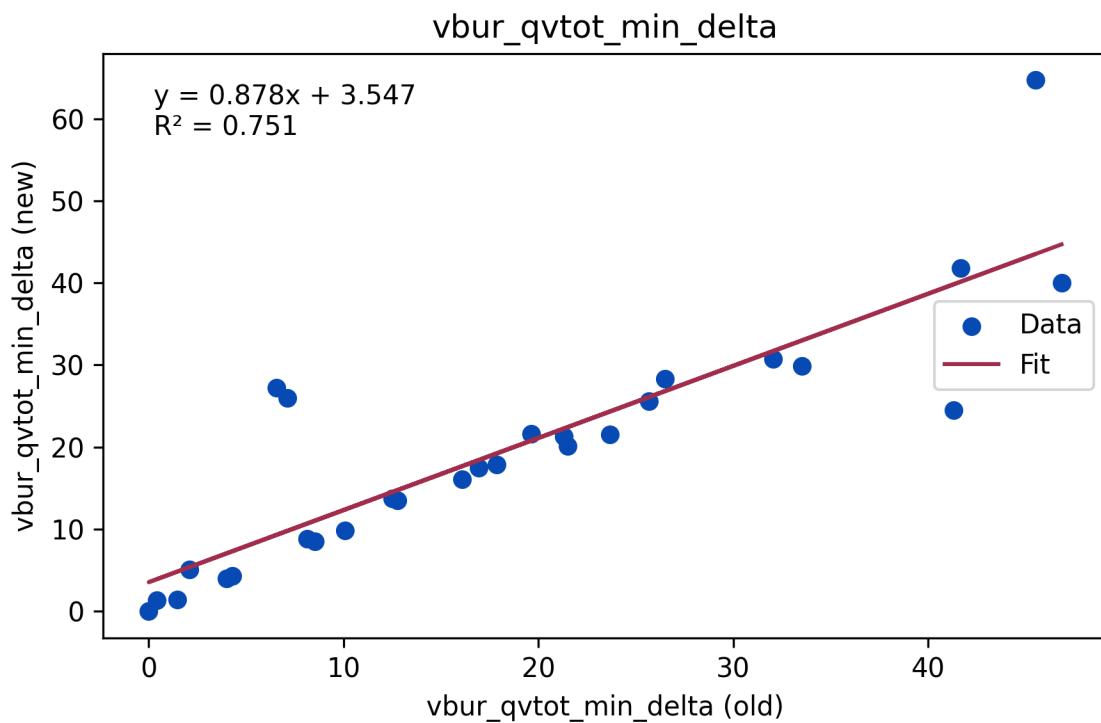
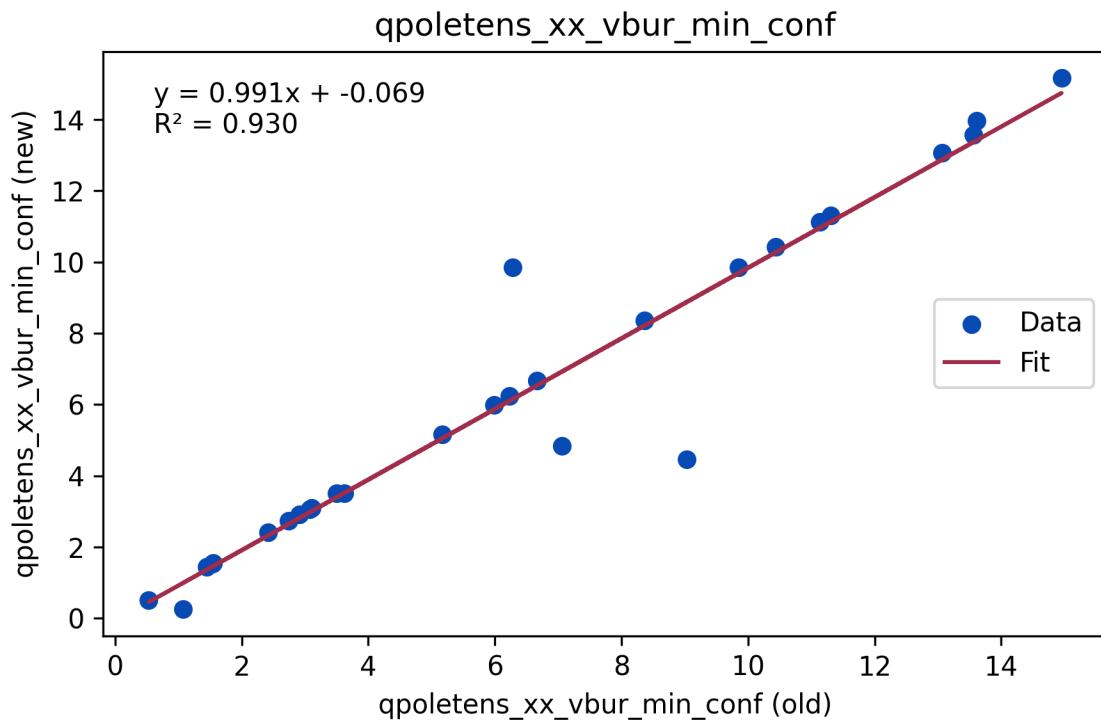
vbur\_far\_vtot\_vbur\_min\_conf

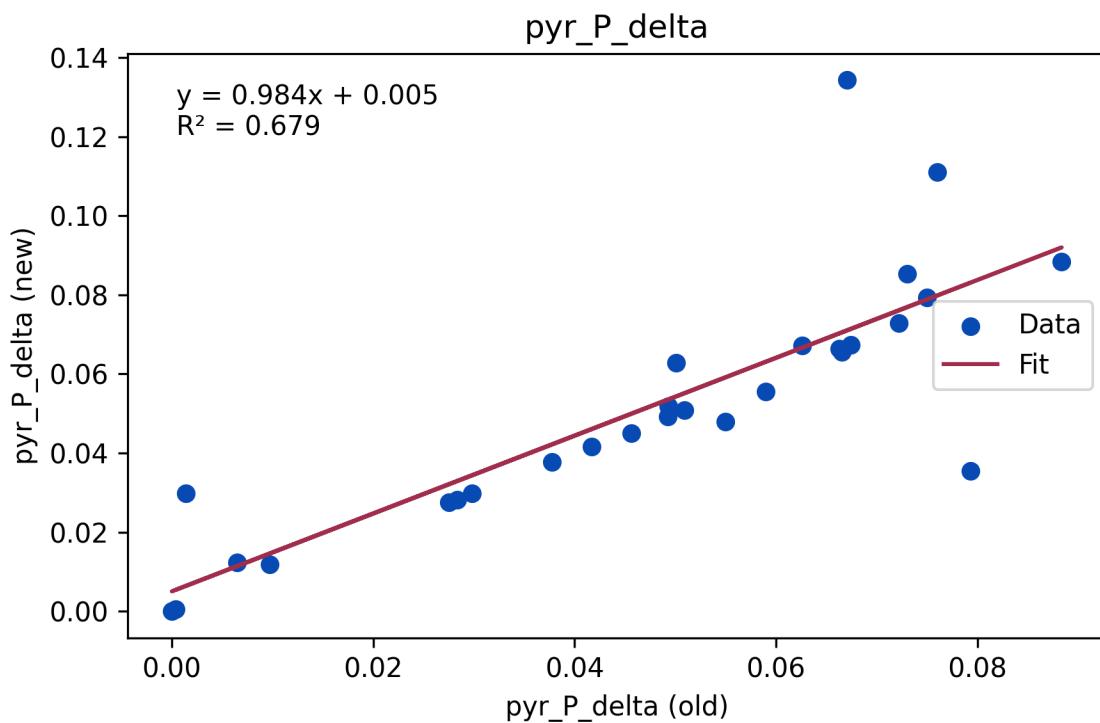
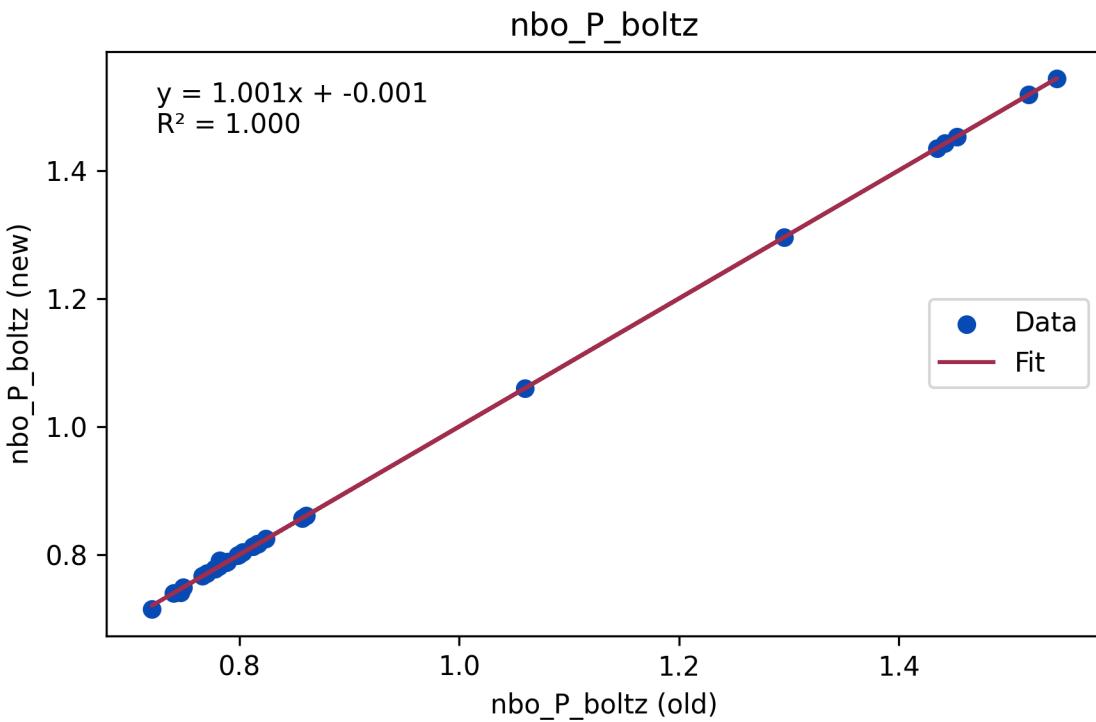


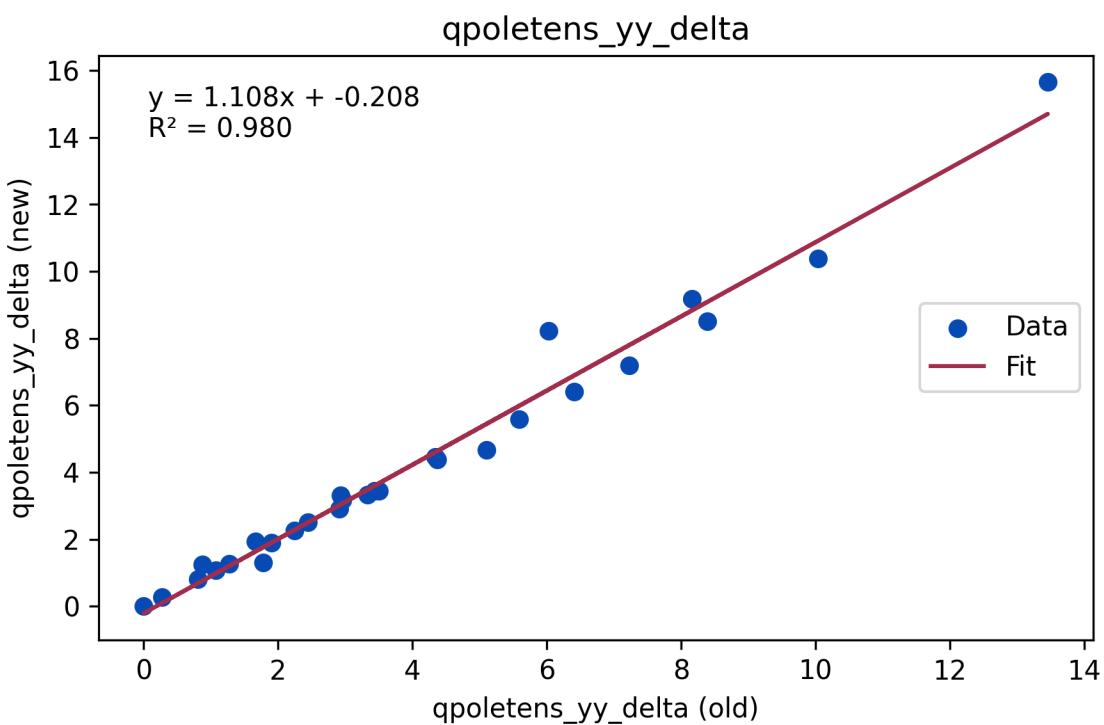
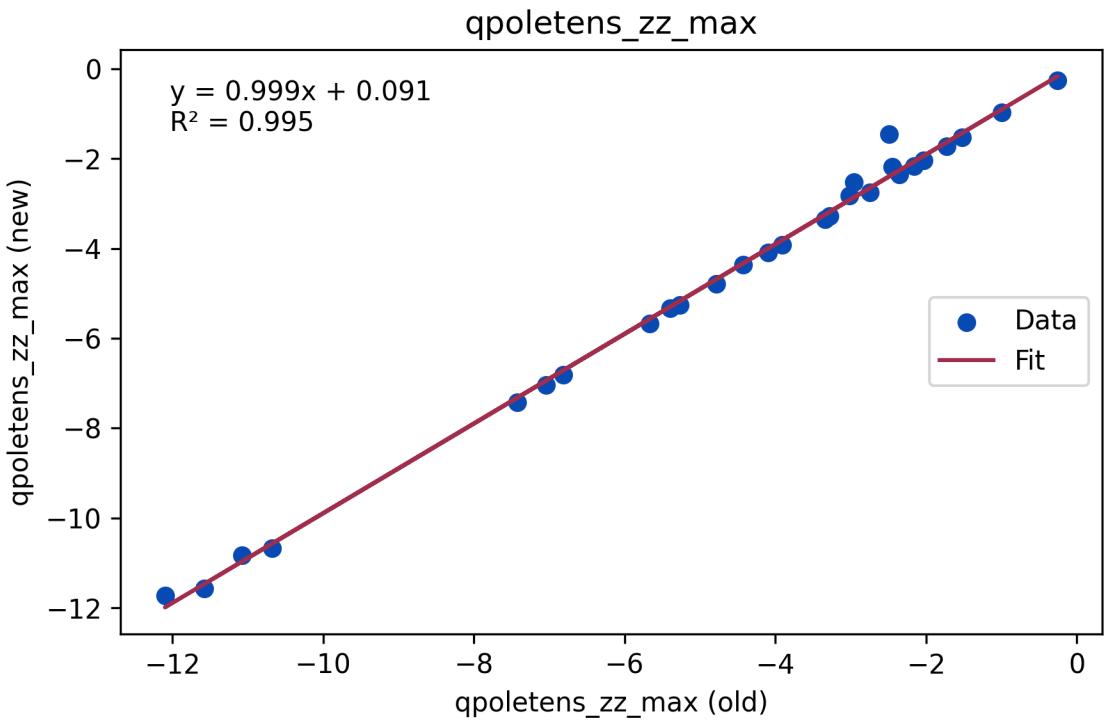


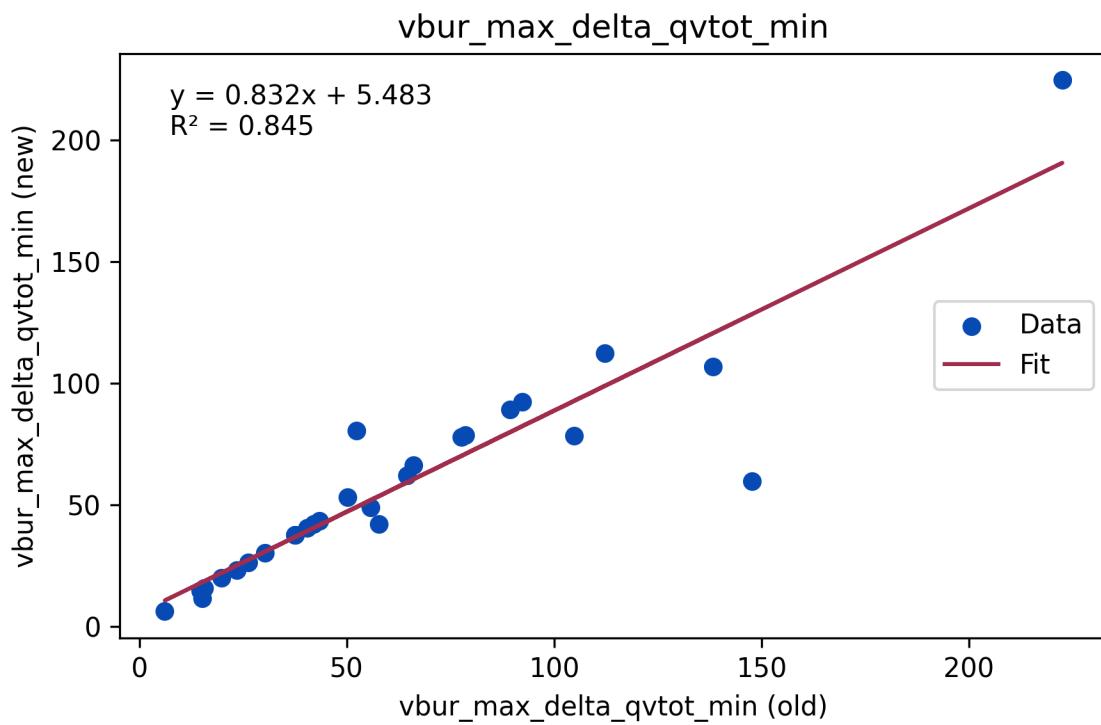
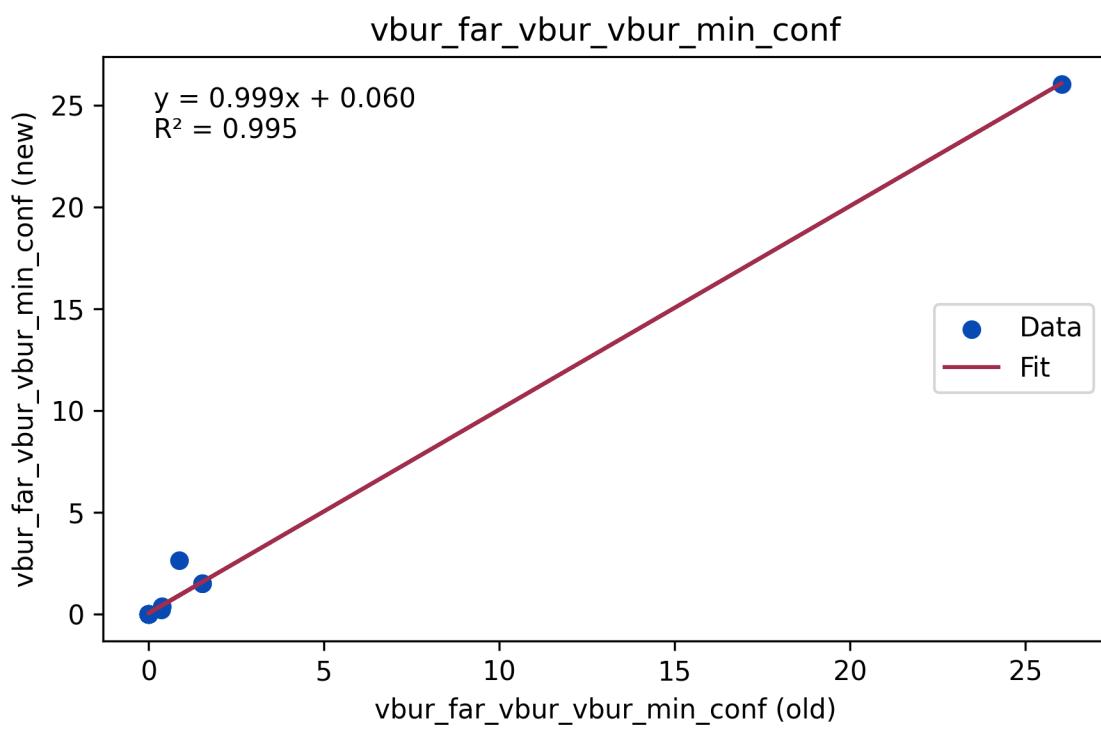


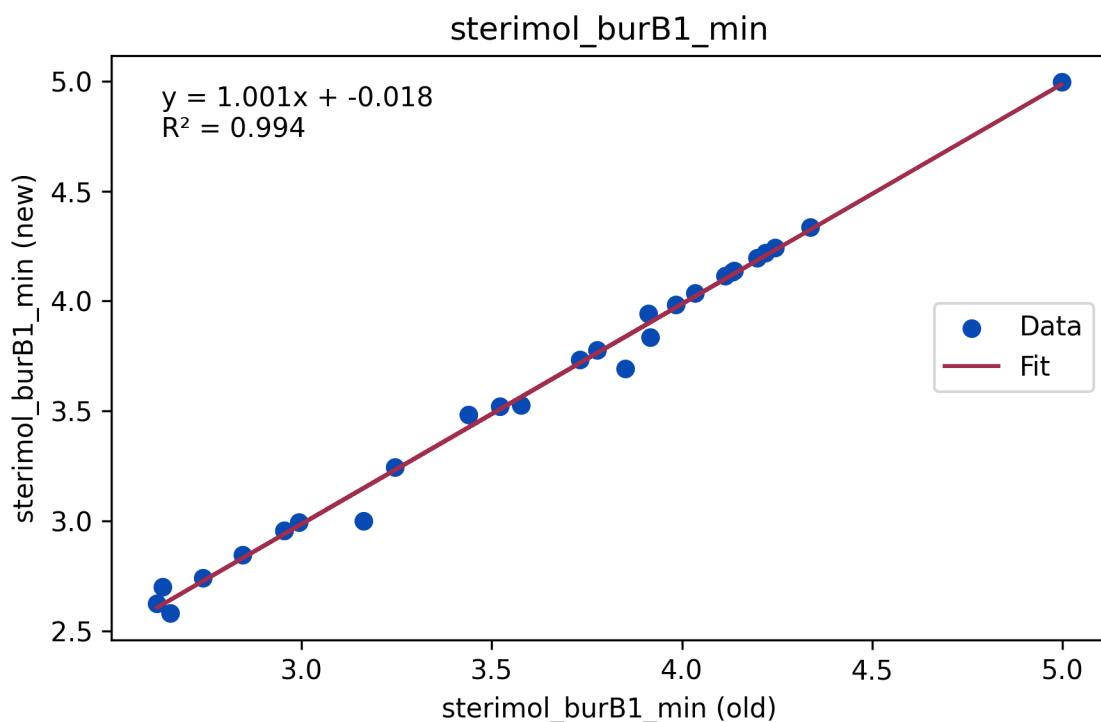
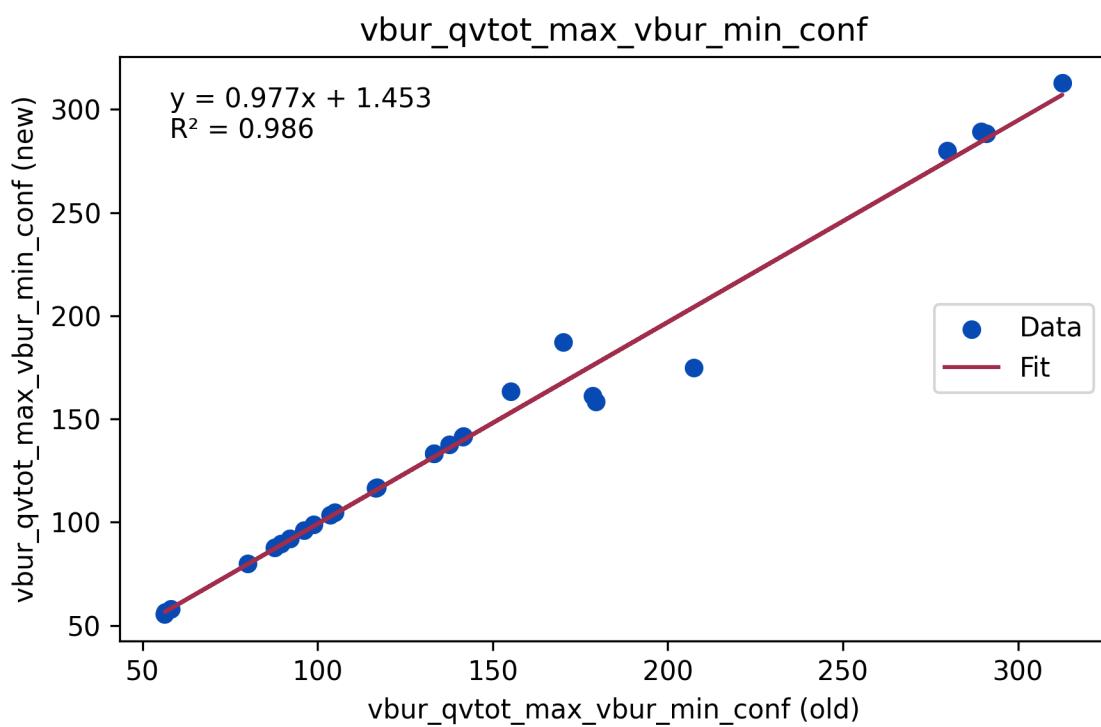


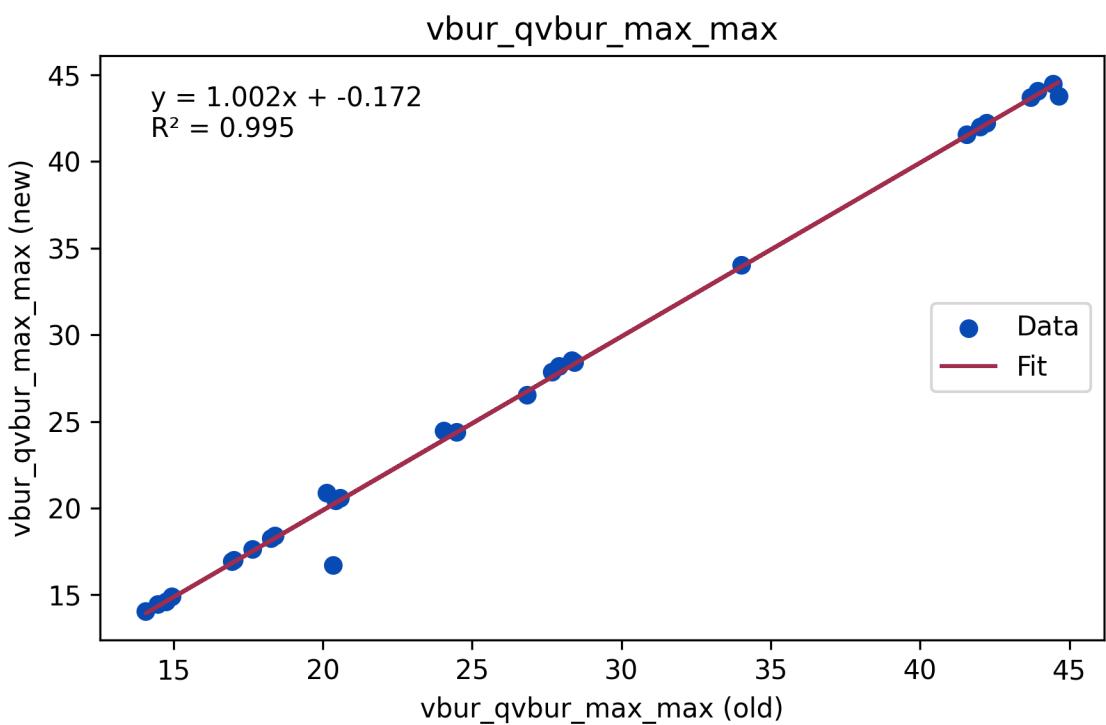
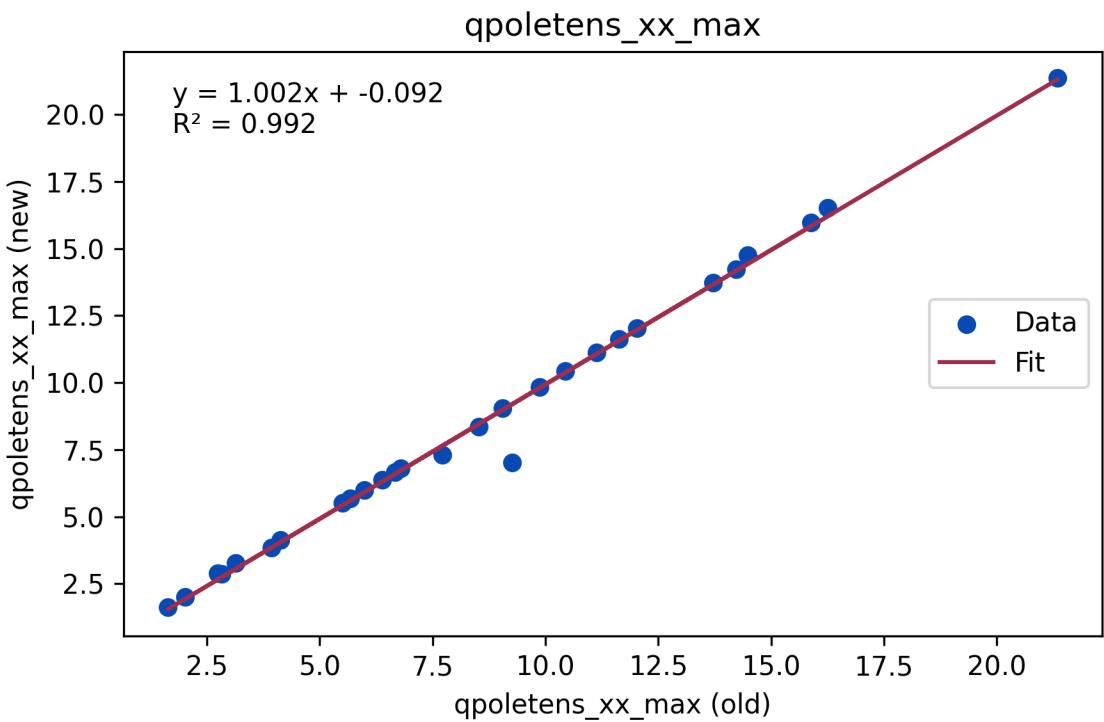


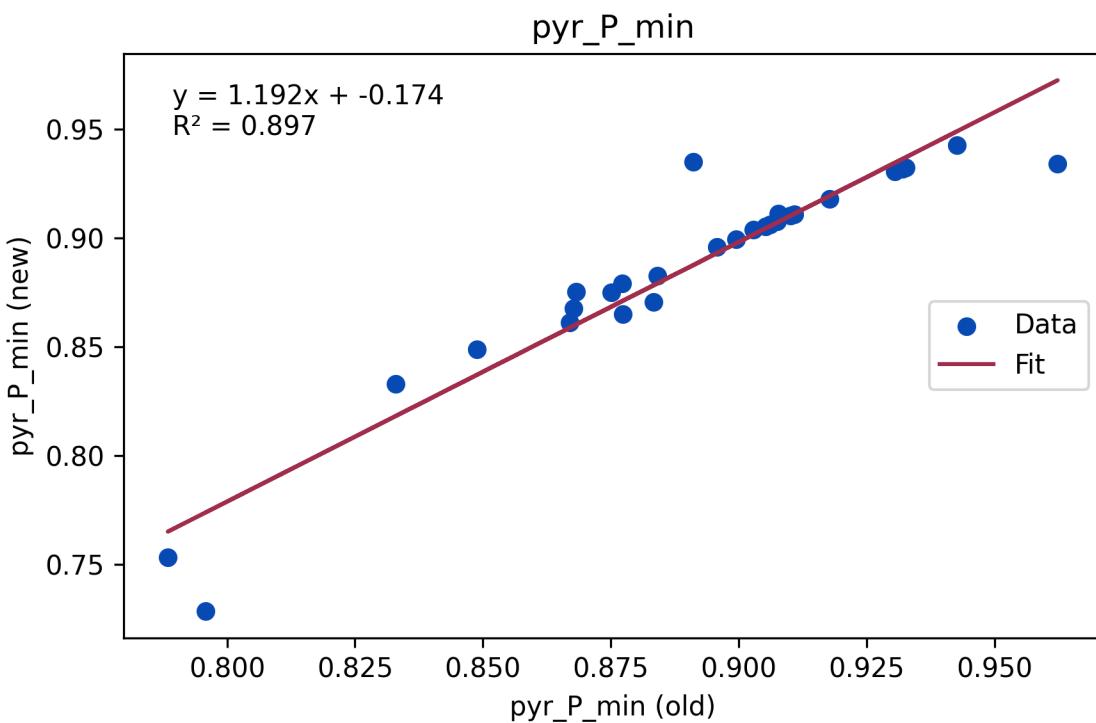
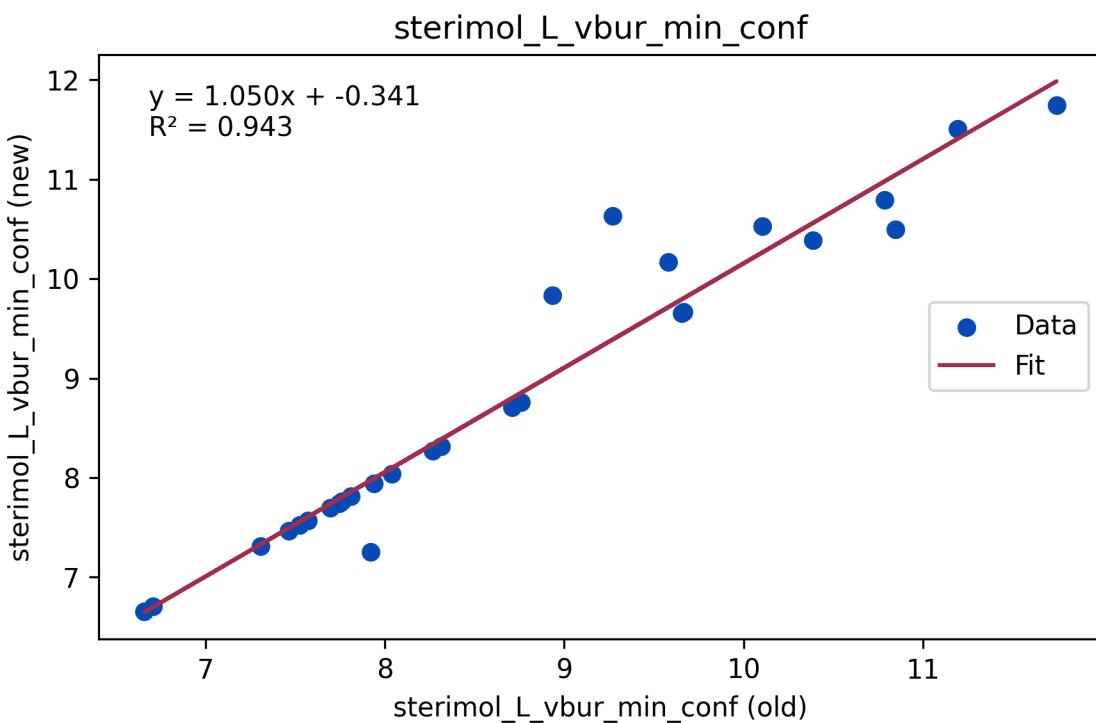


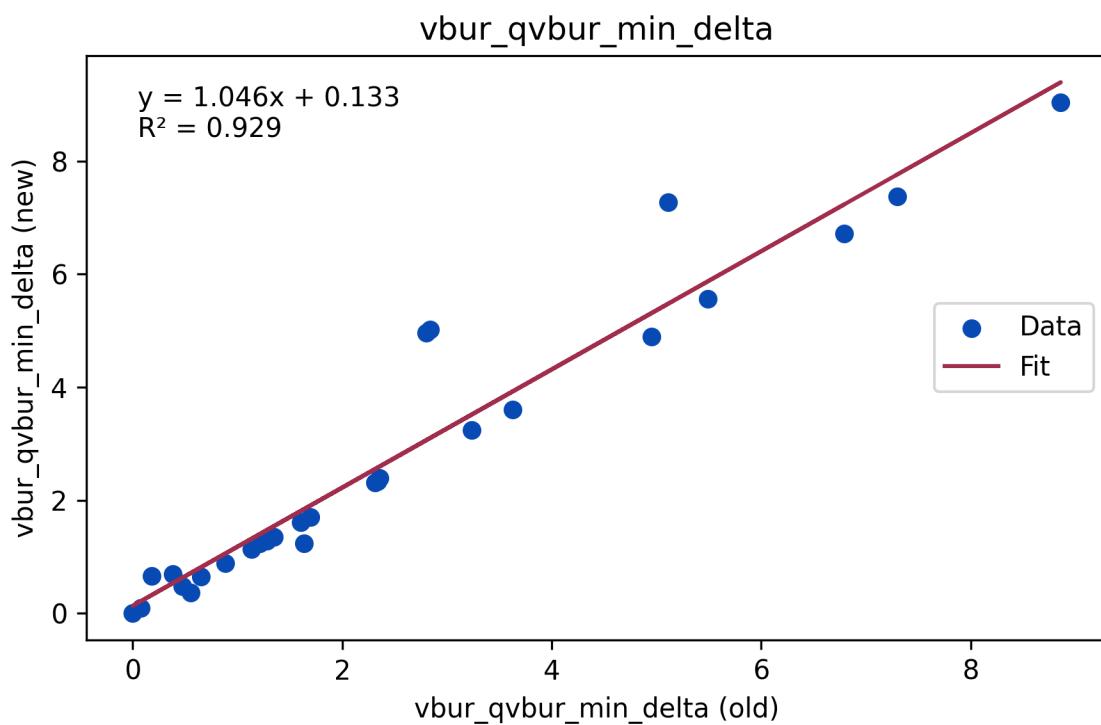
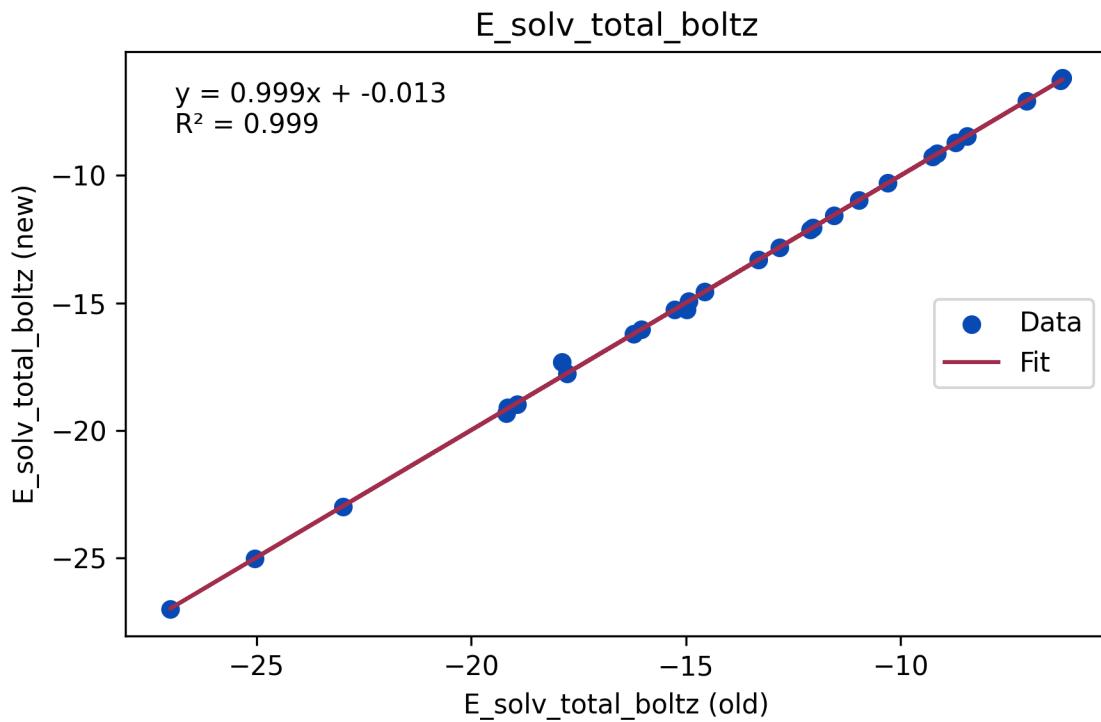


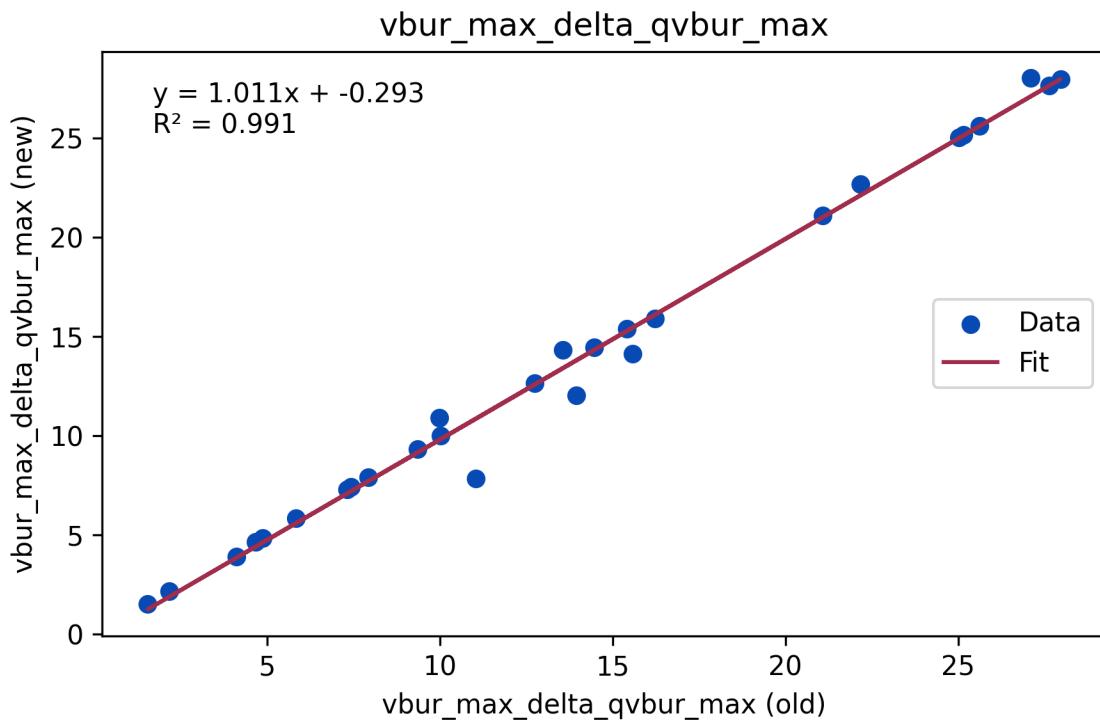
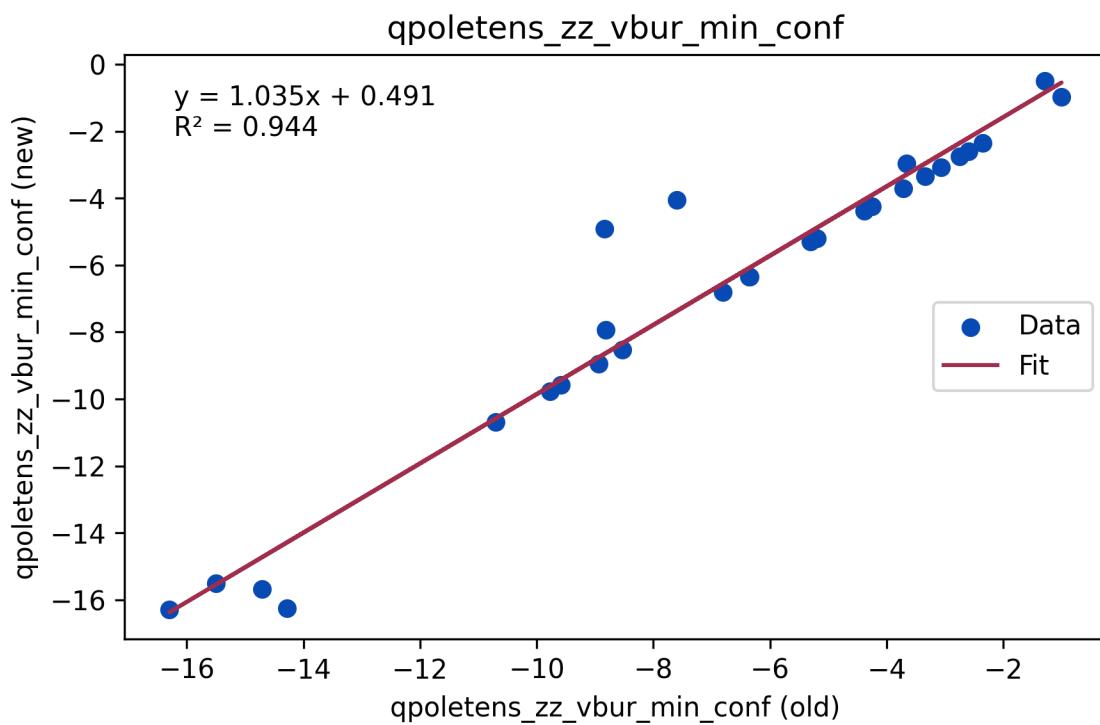




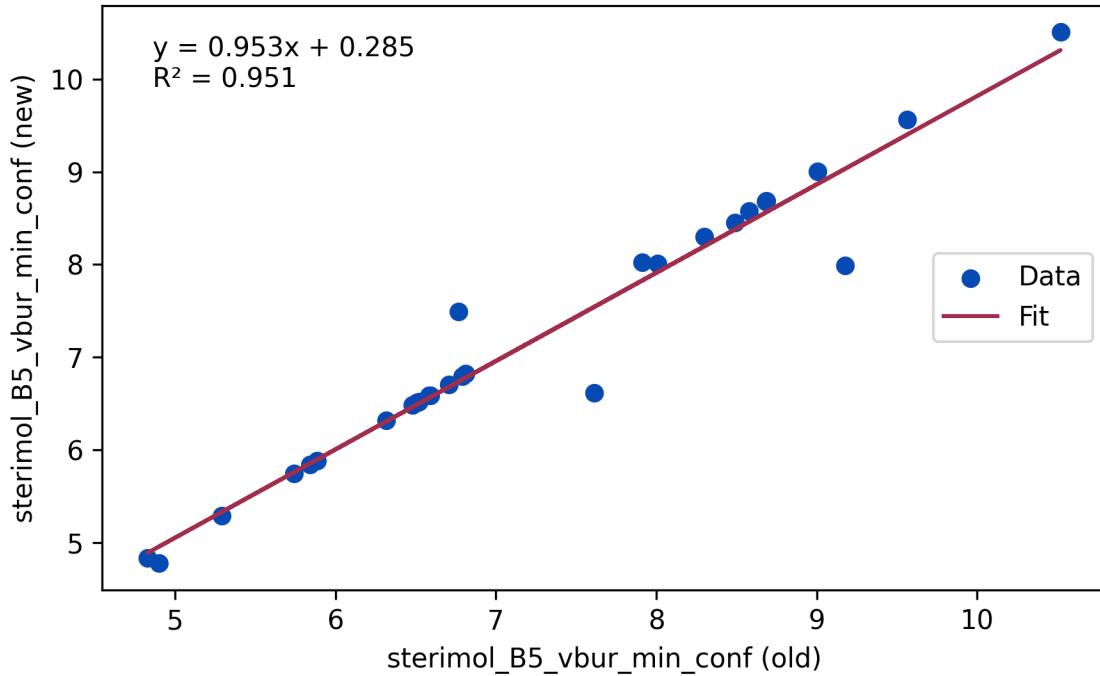




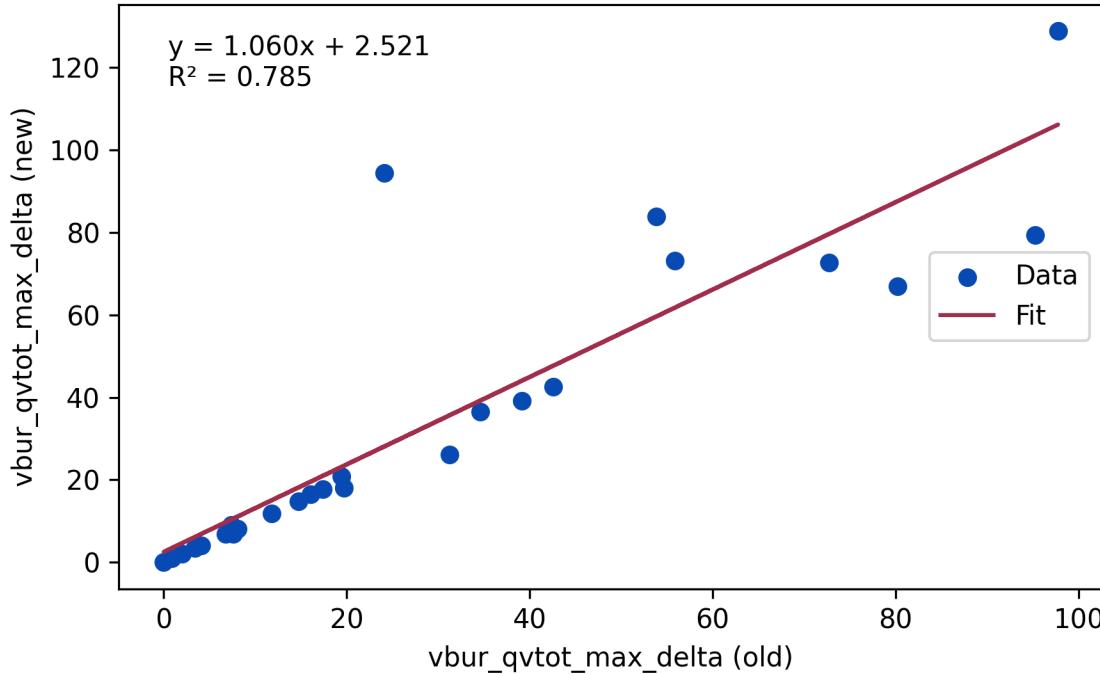


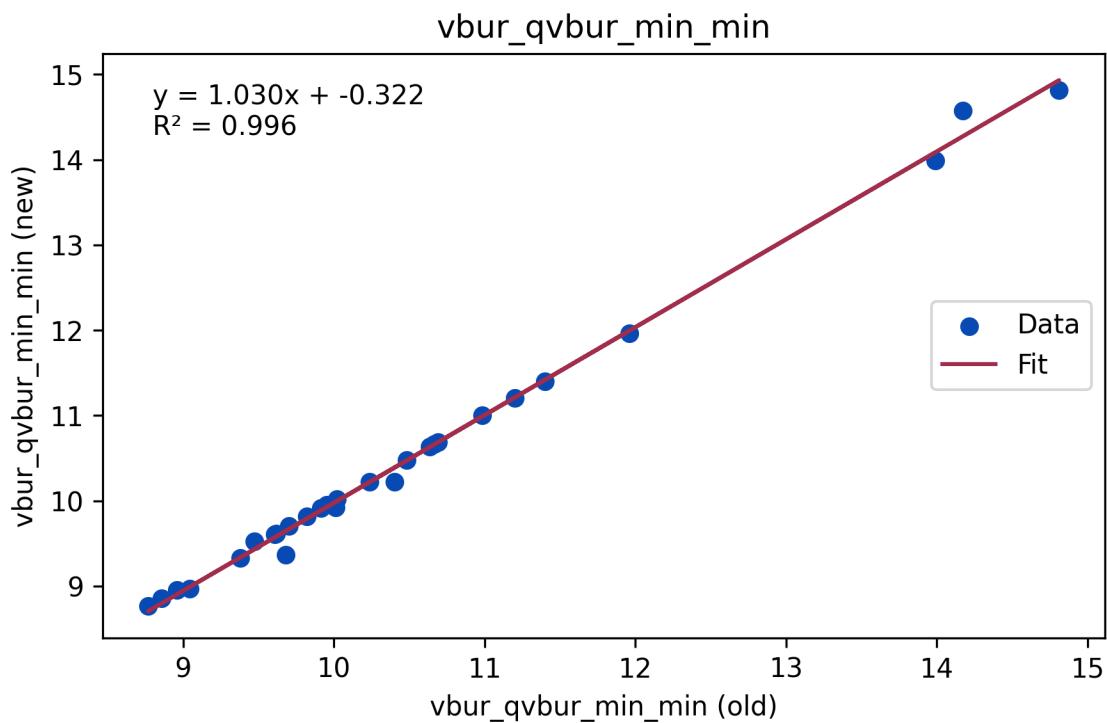
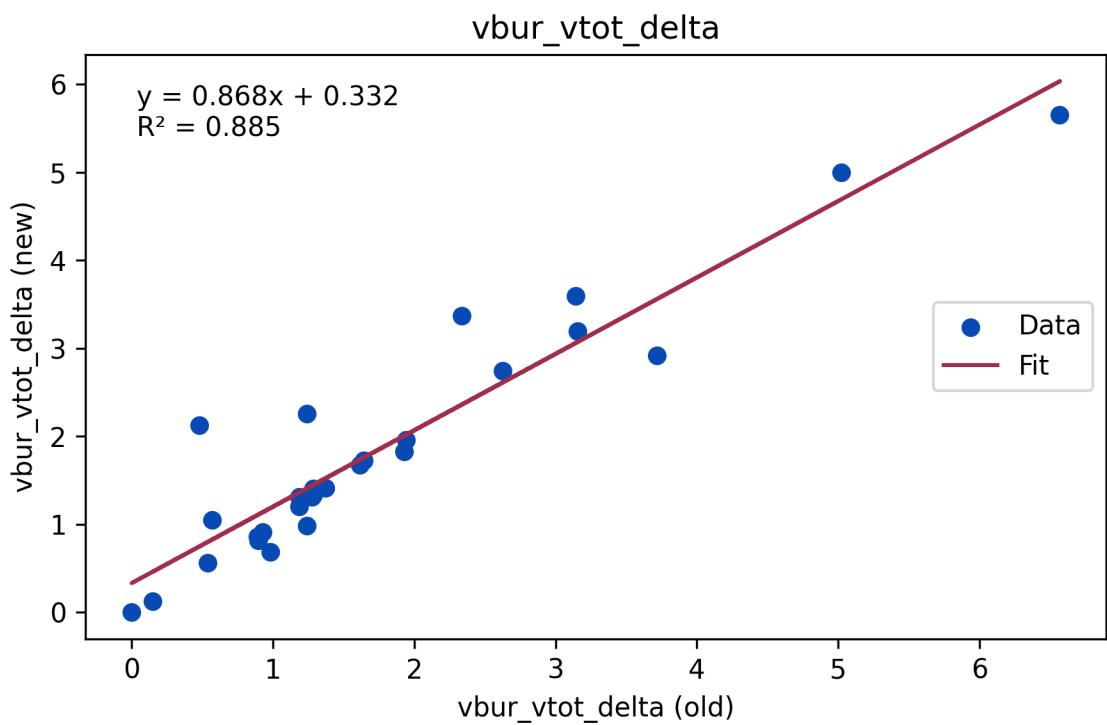


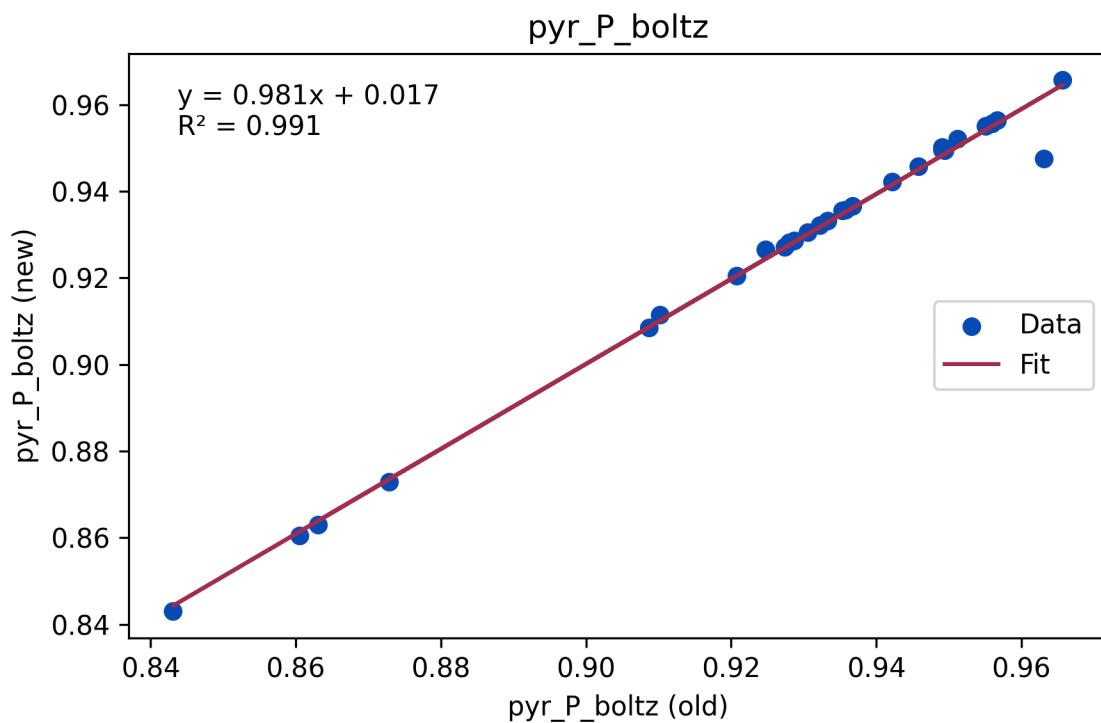
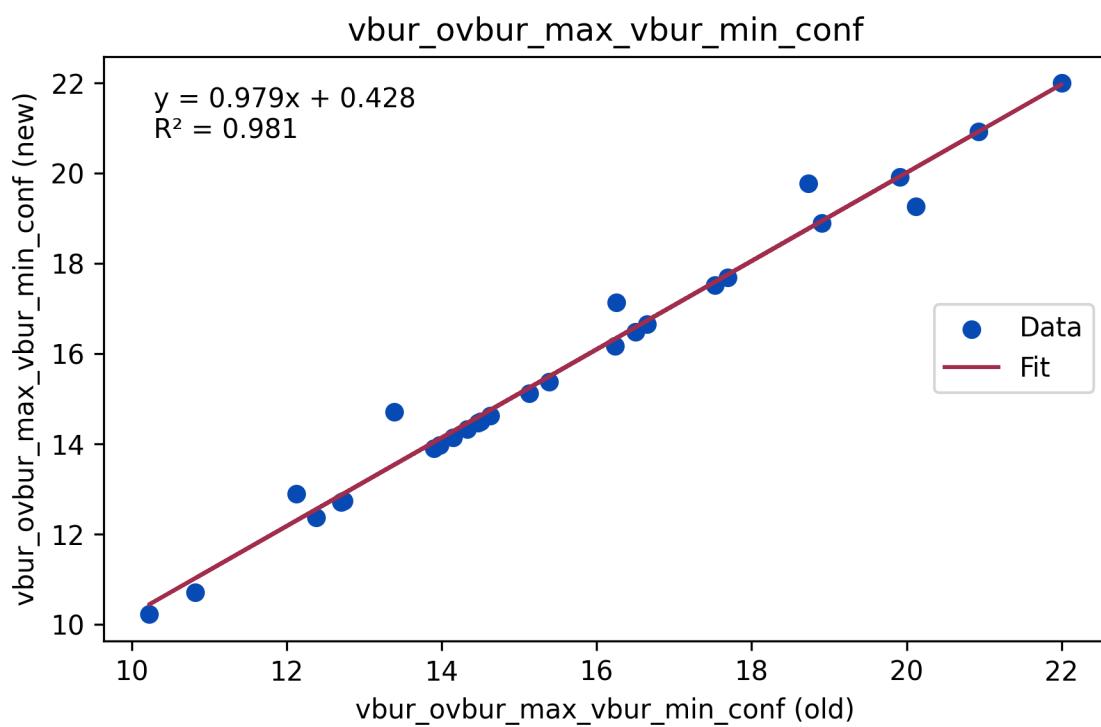
sterimol\_B5\_vbur\_min\_conf

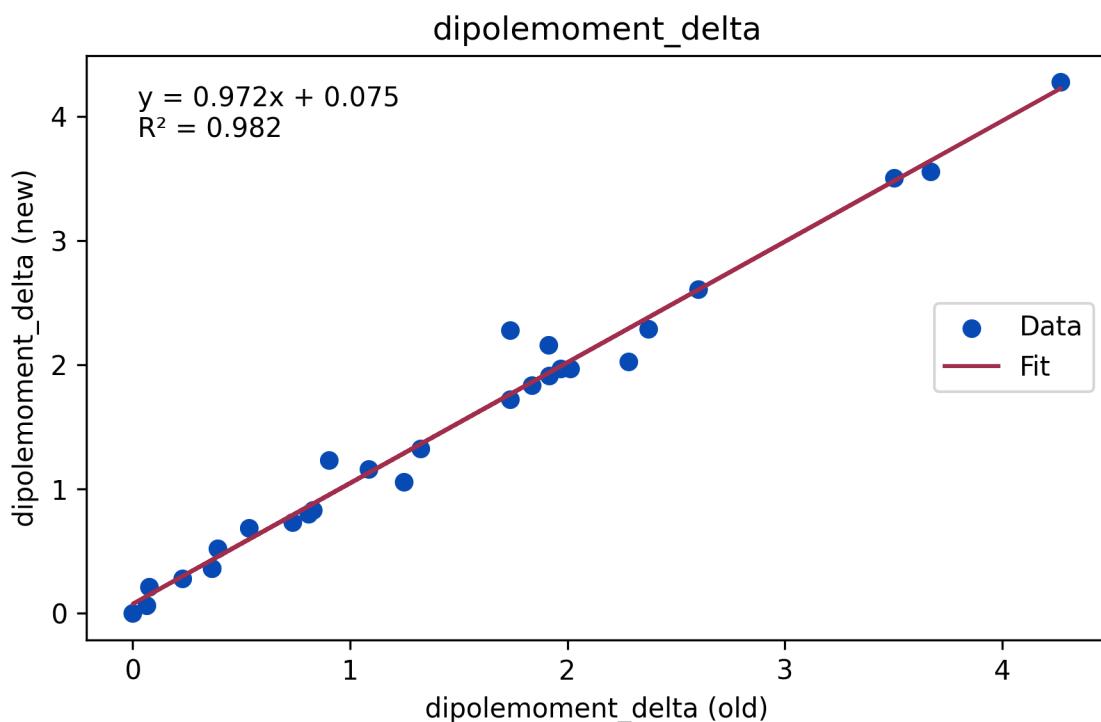
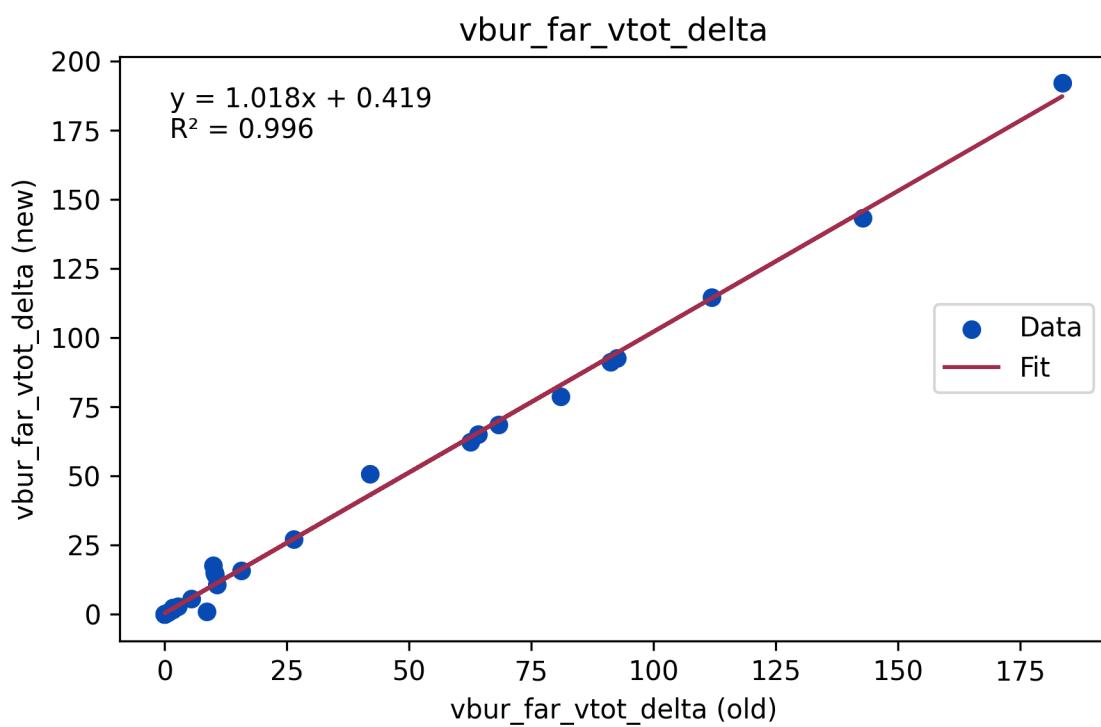


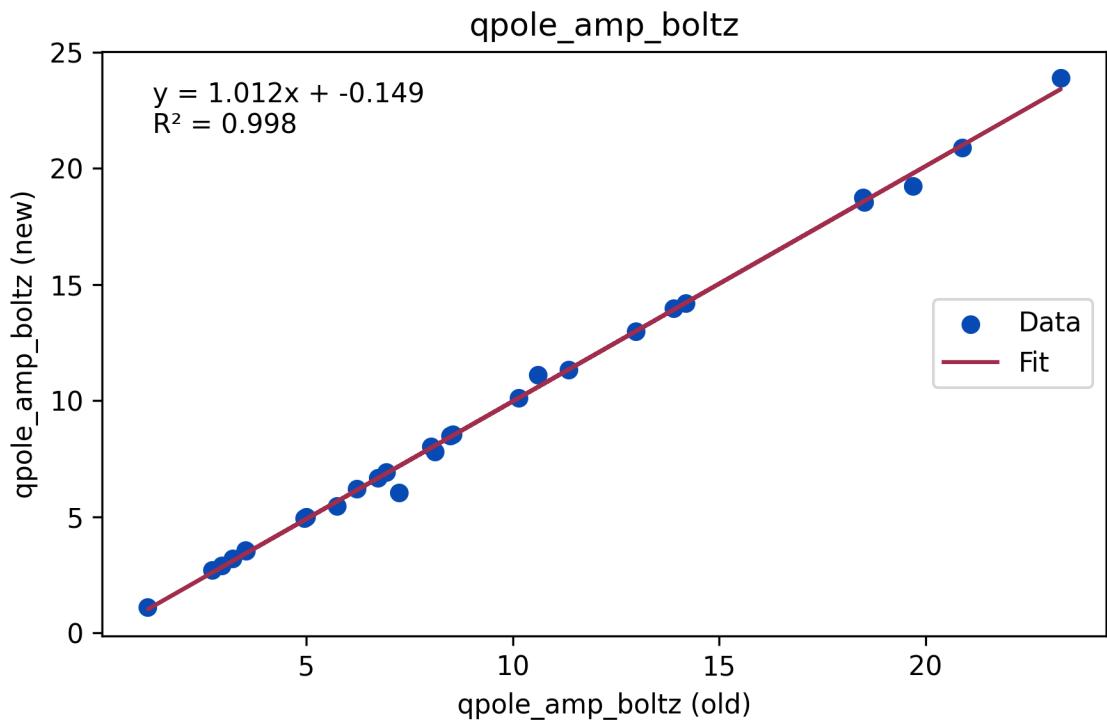
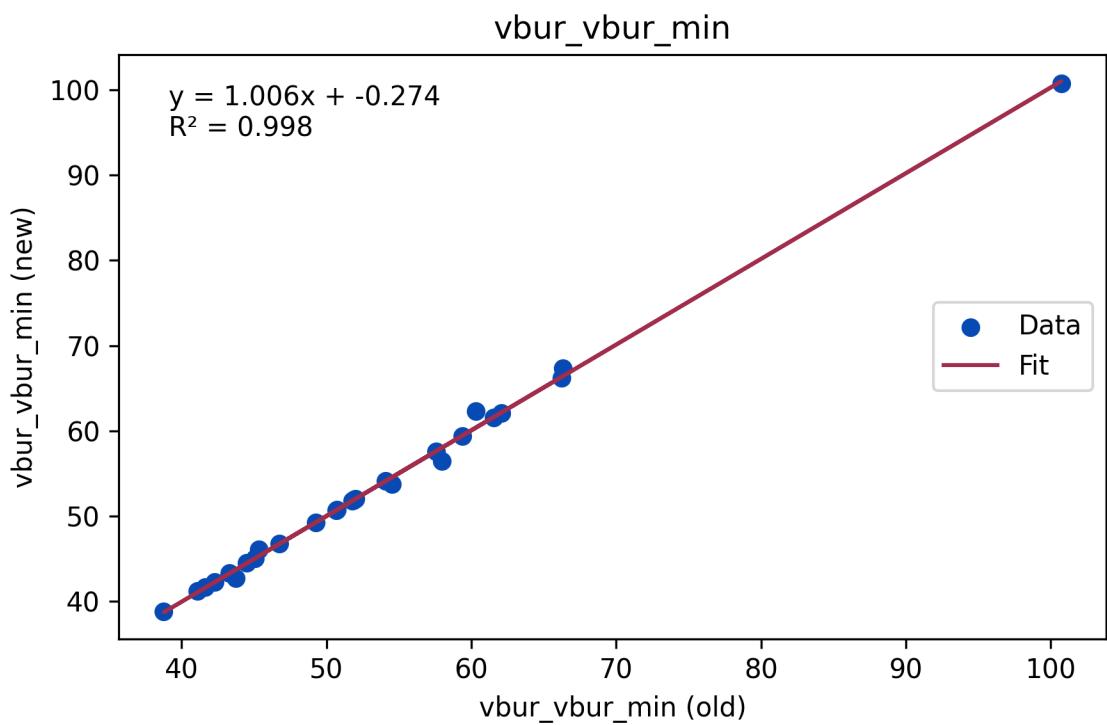
vbur\_qvtot\_max\_delta

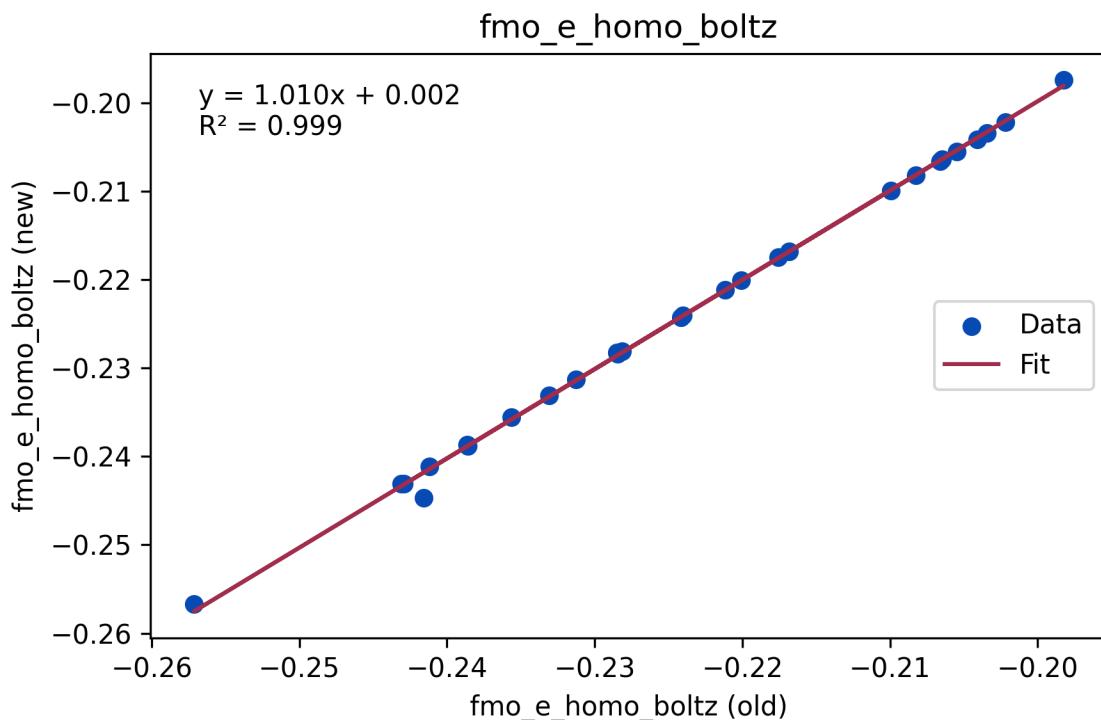
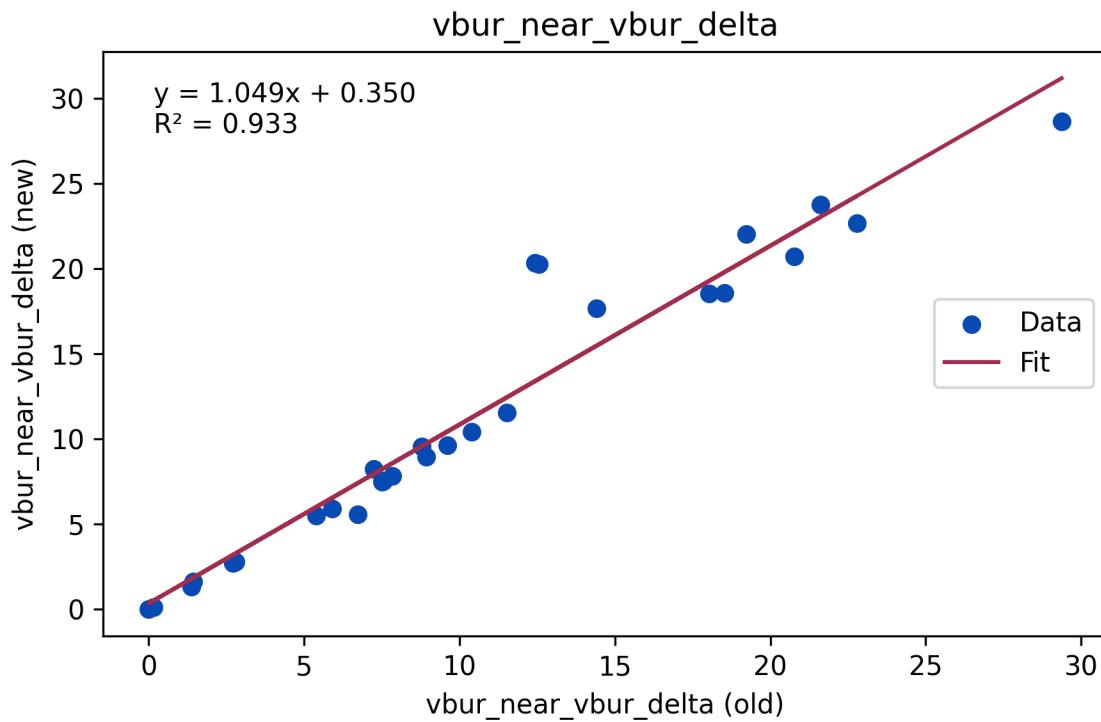


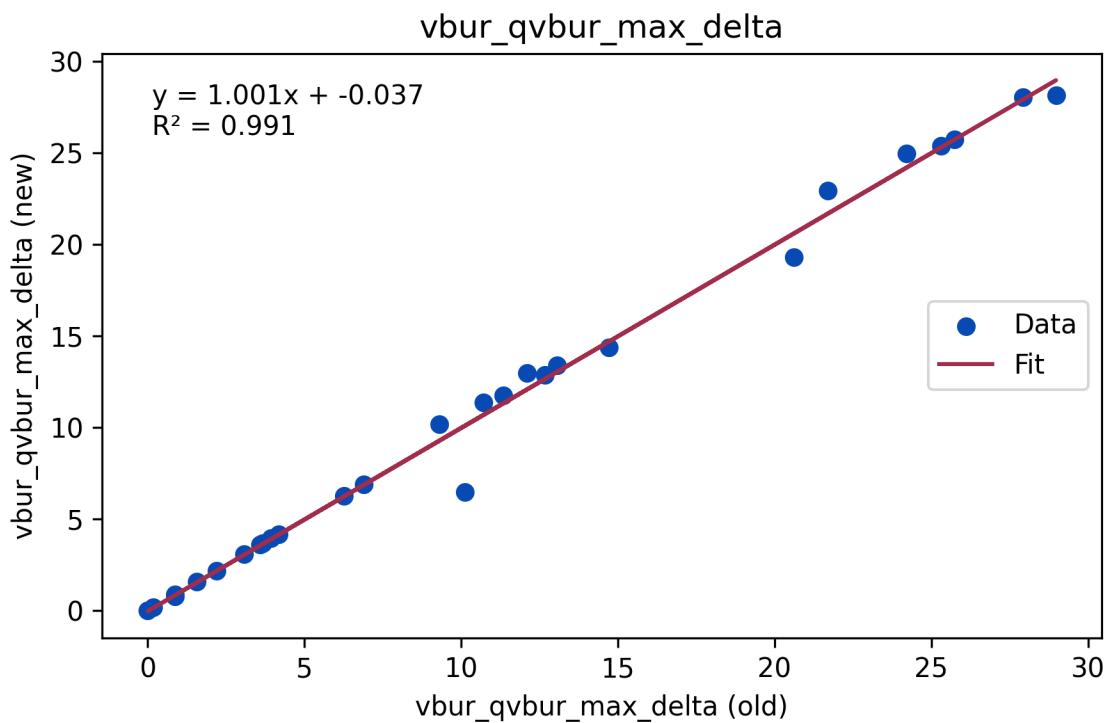
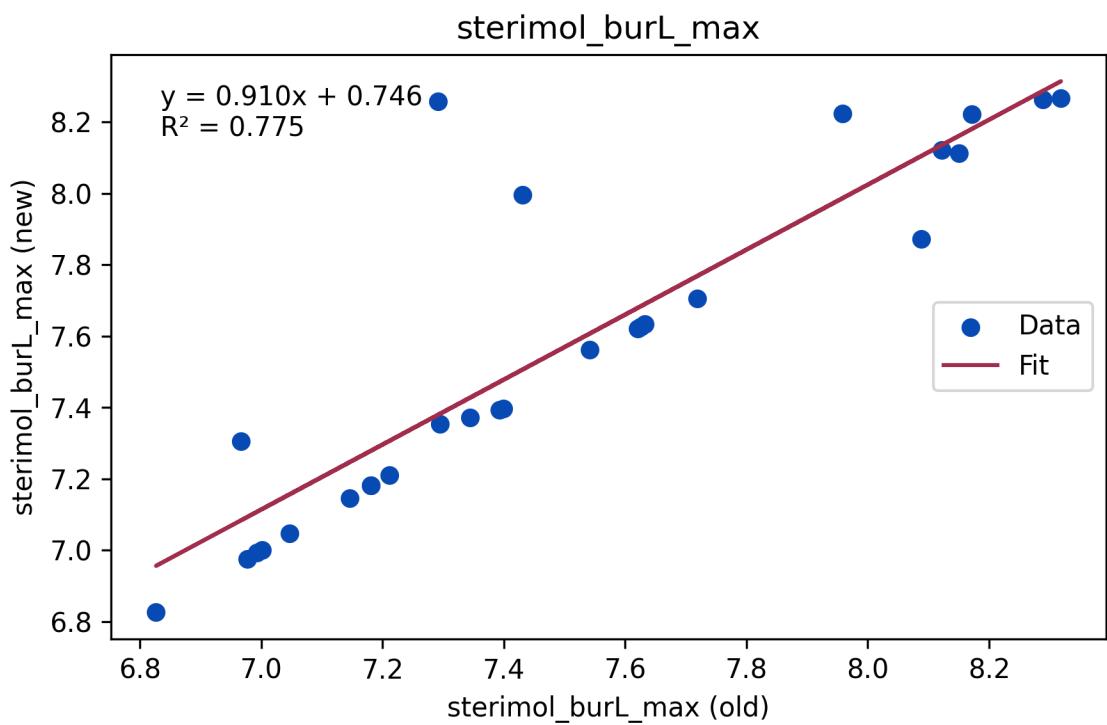


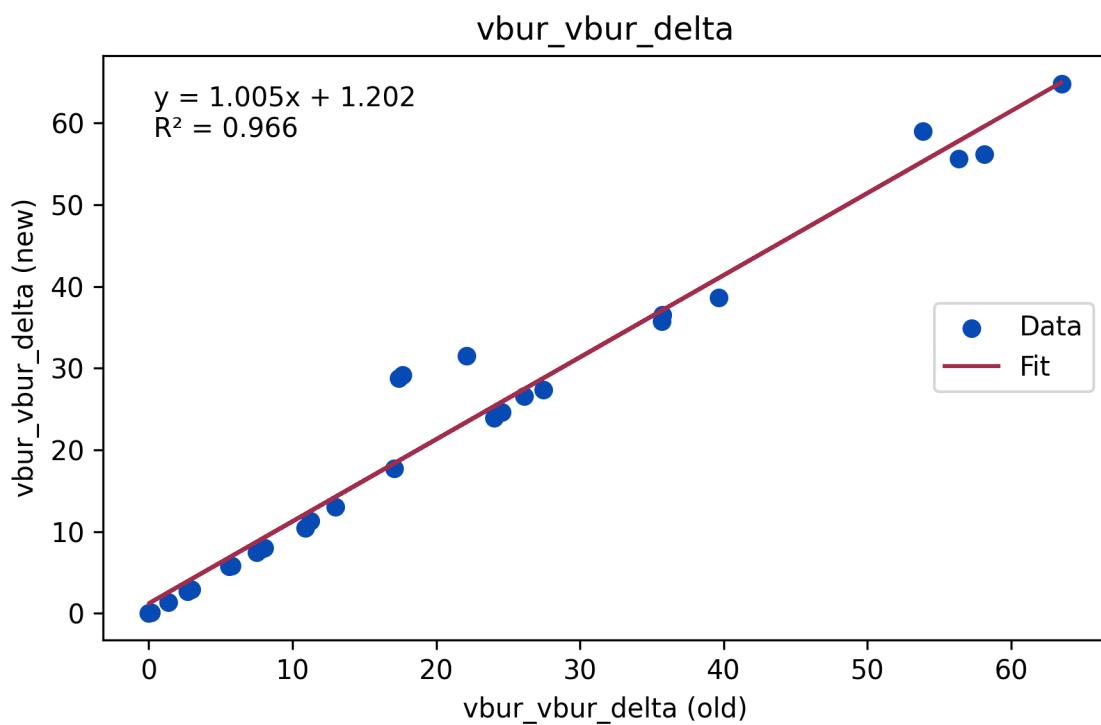
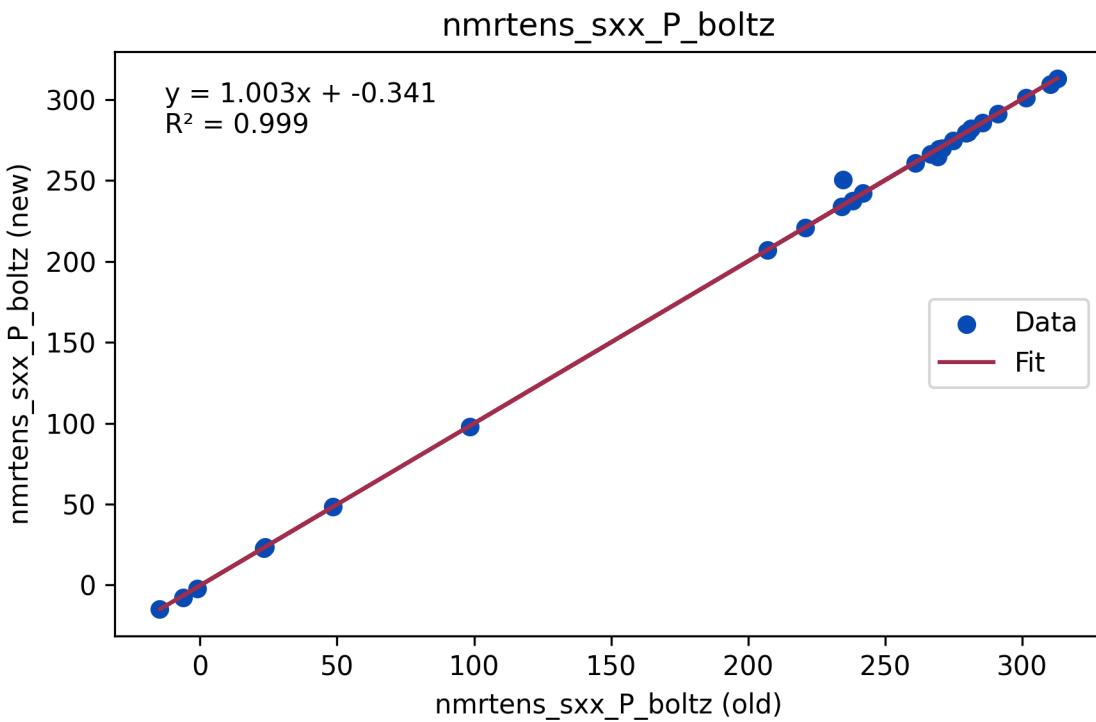


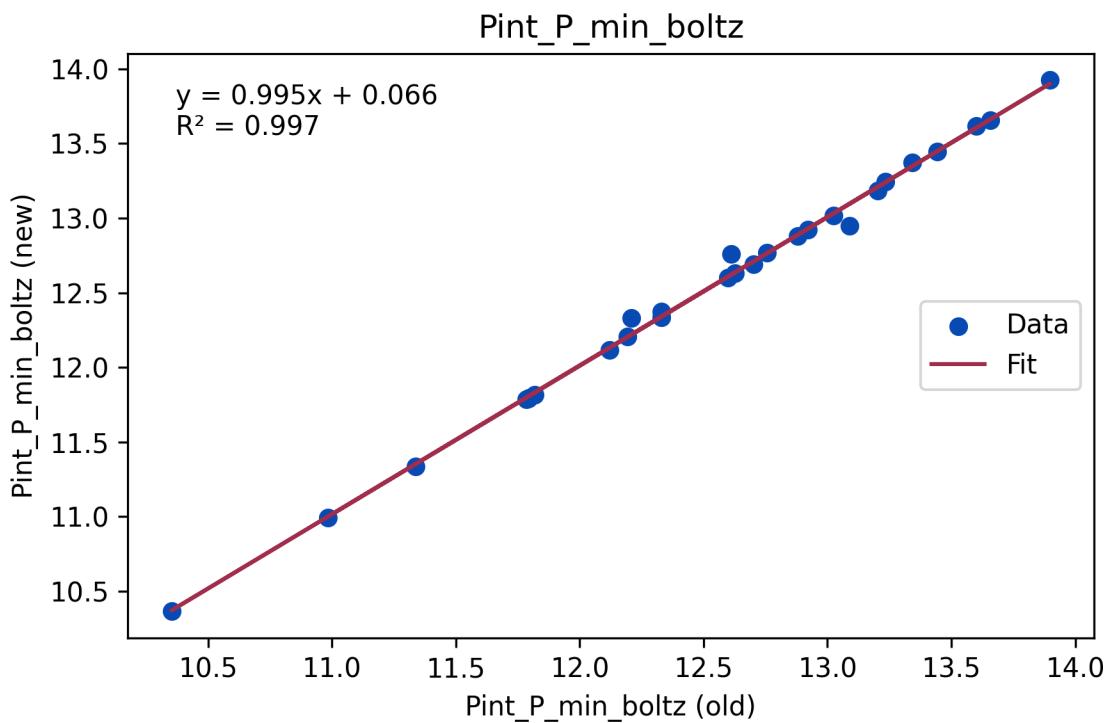
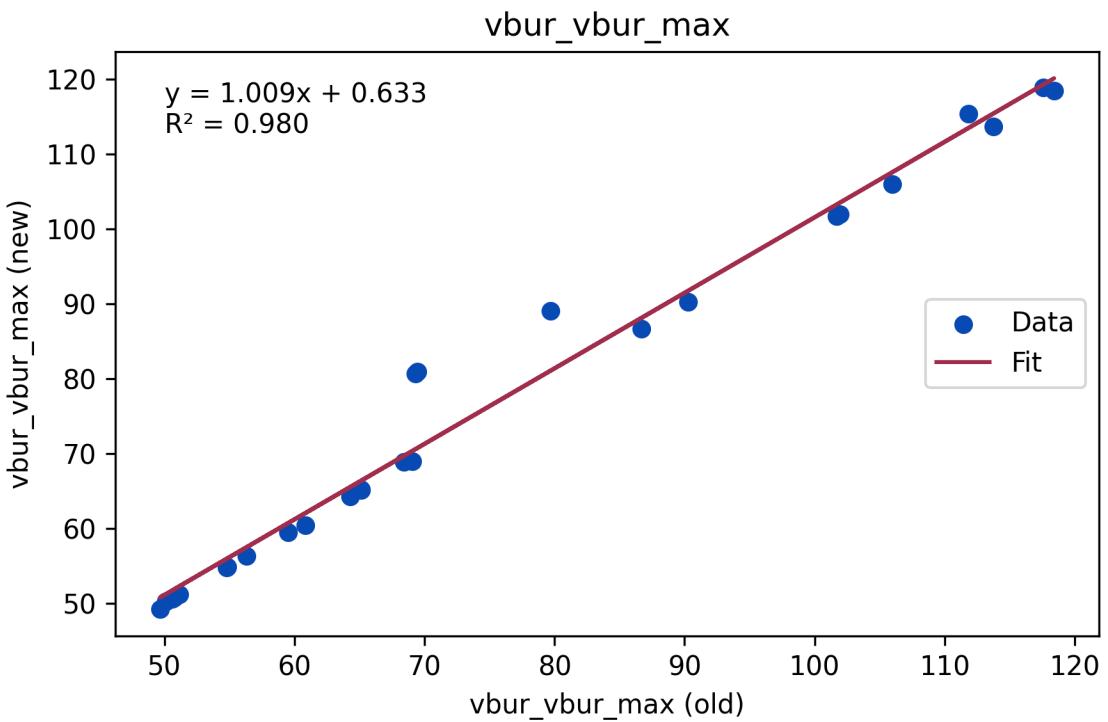




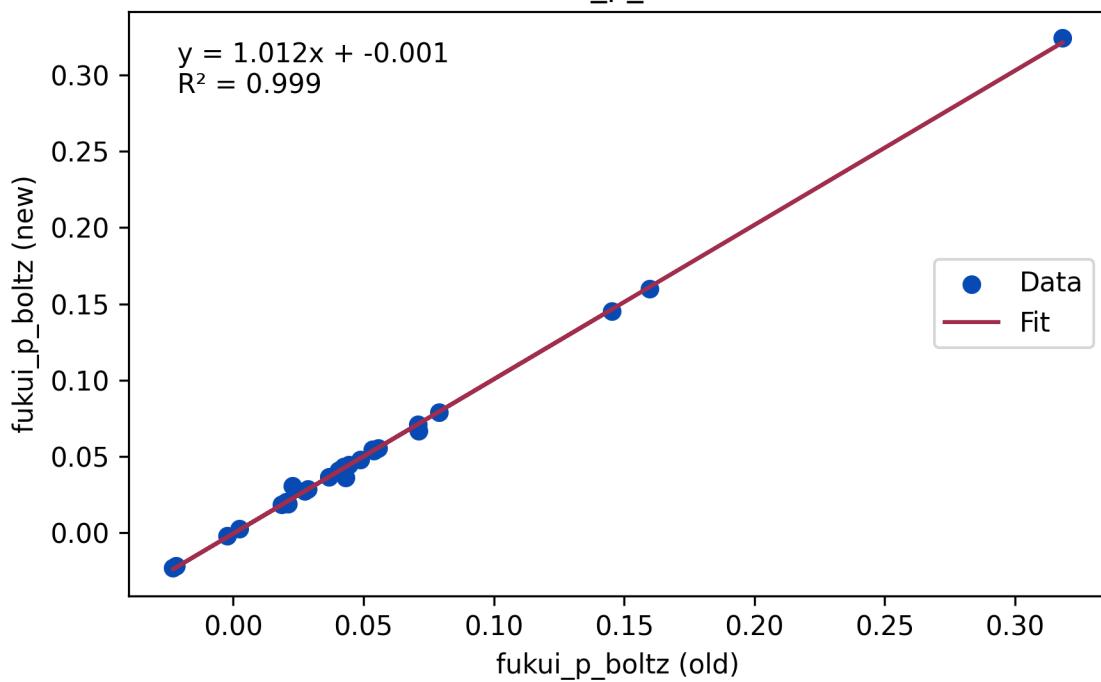




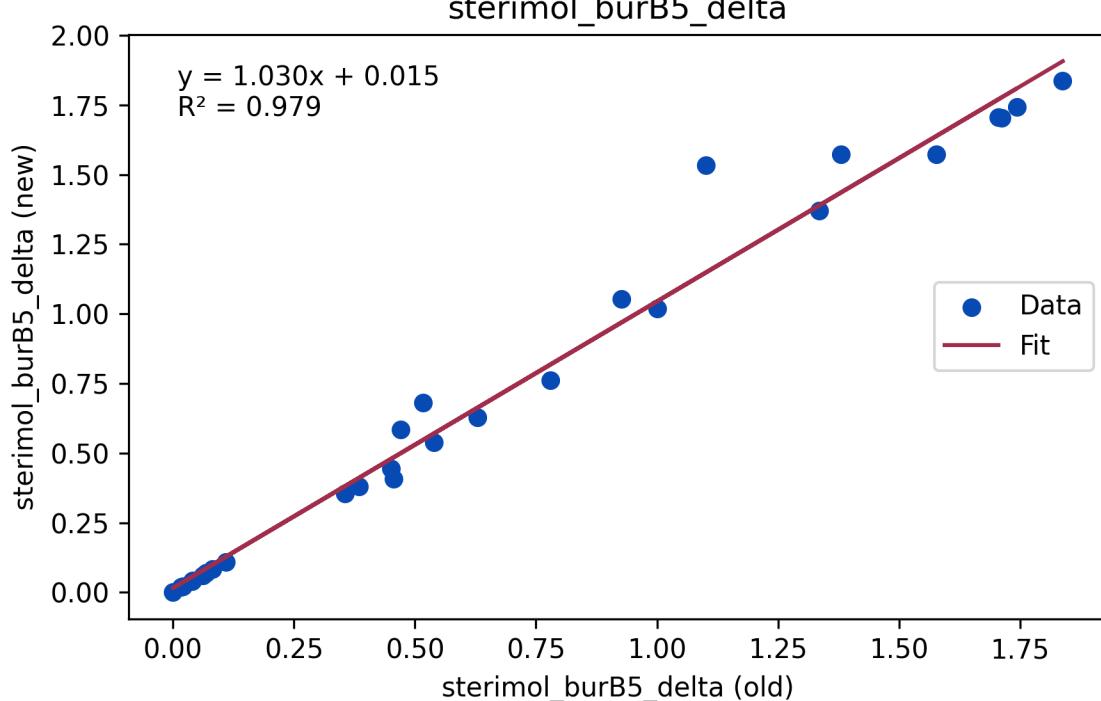




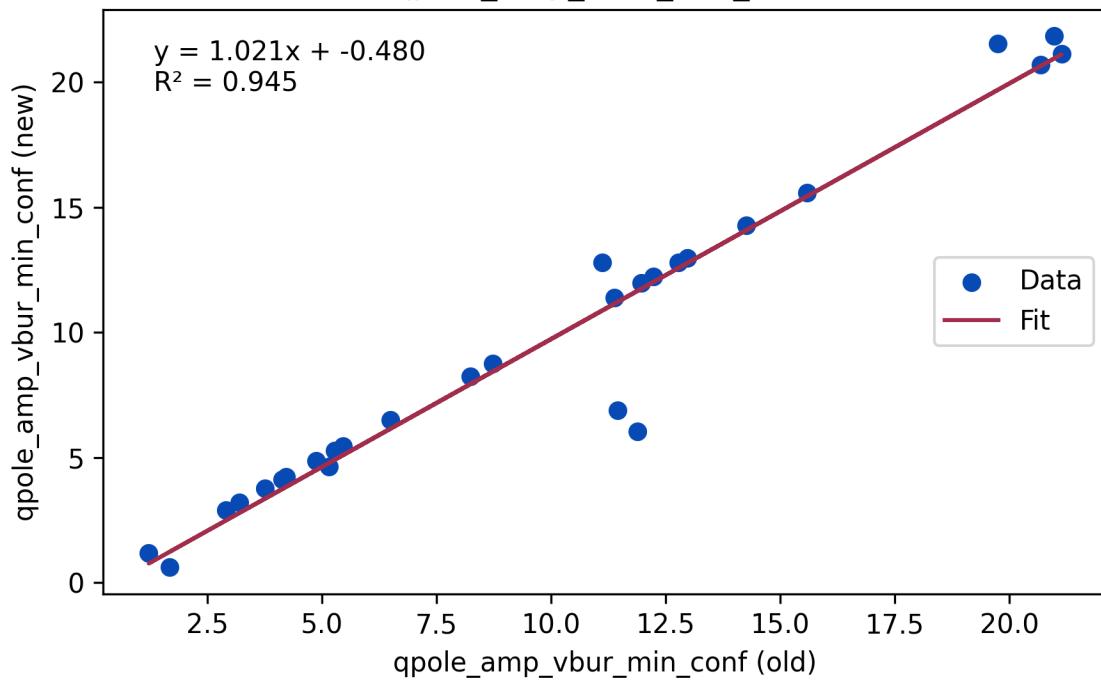
fukui\_p\_boltz



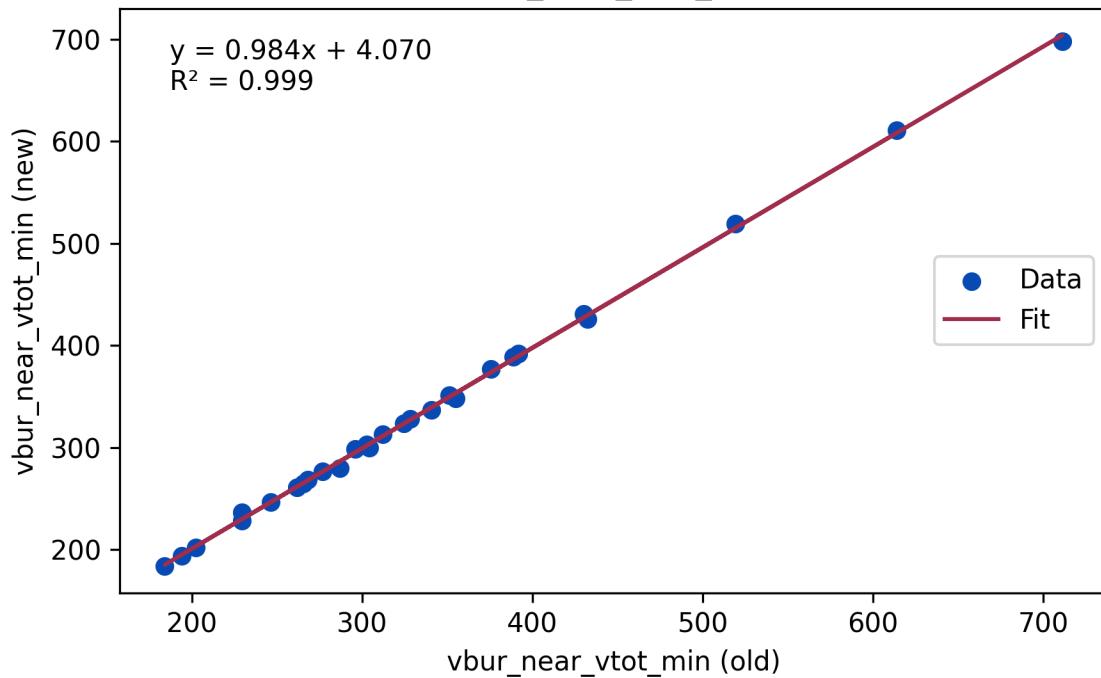
sterimol\_burB5\_delta

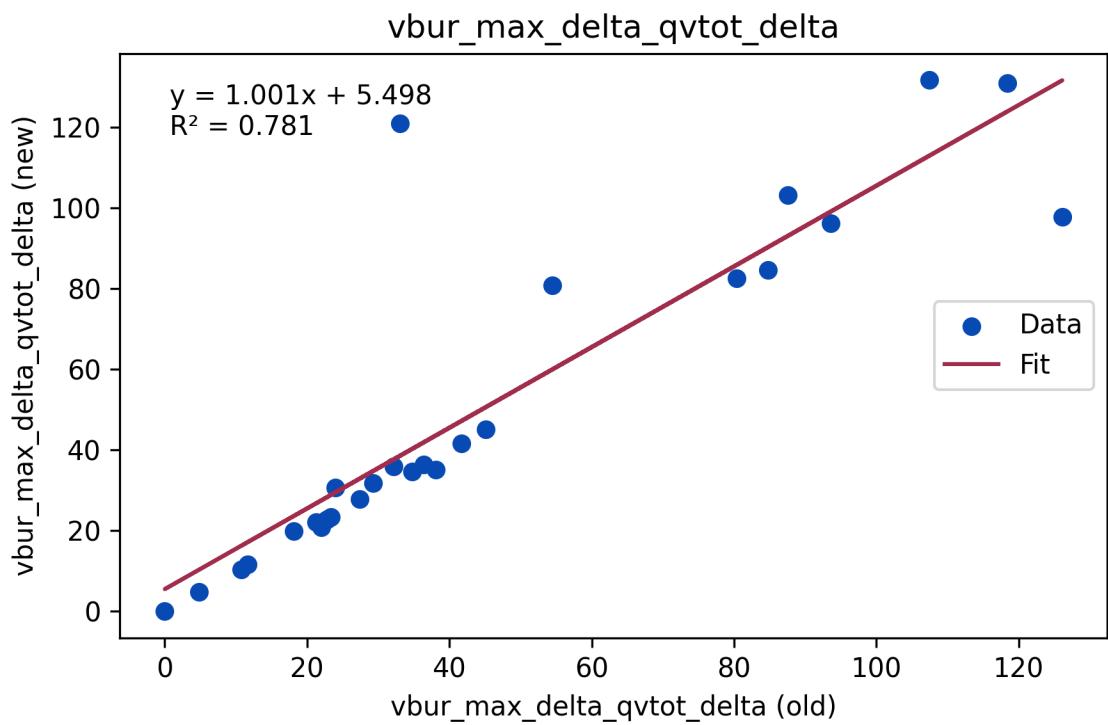
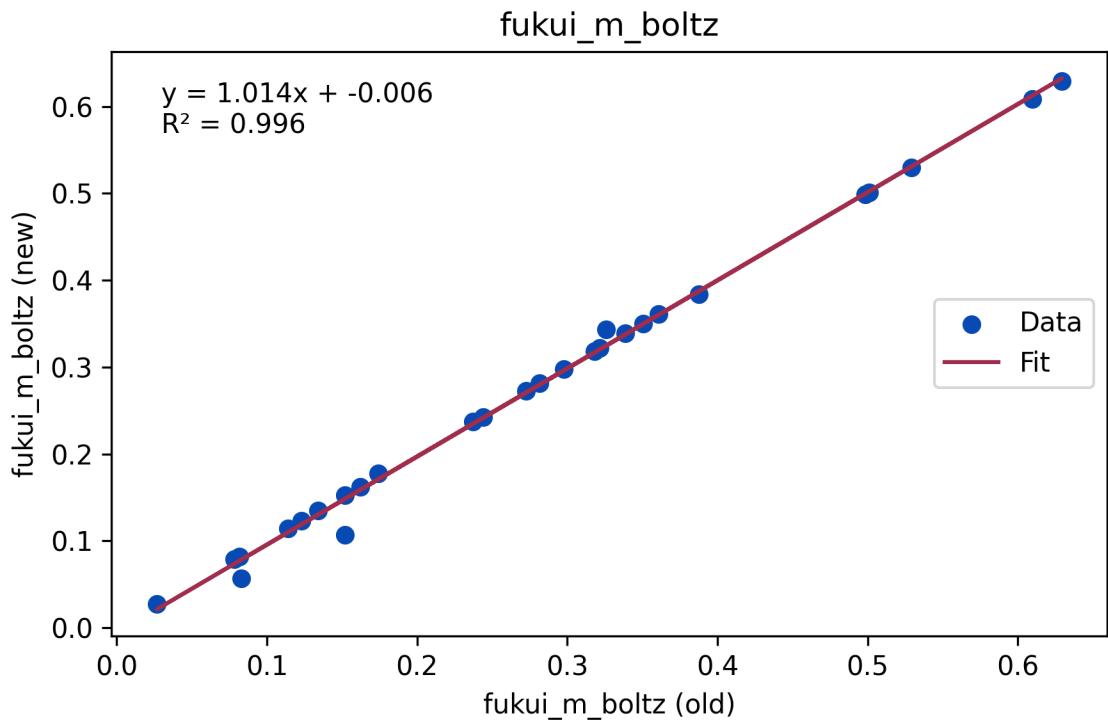


qpole\_amp\_vbur\_min\_conf

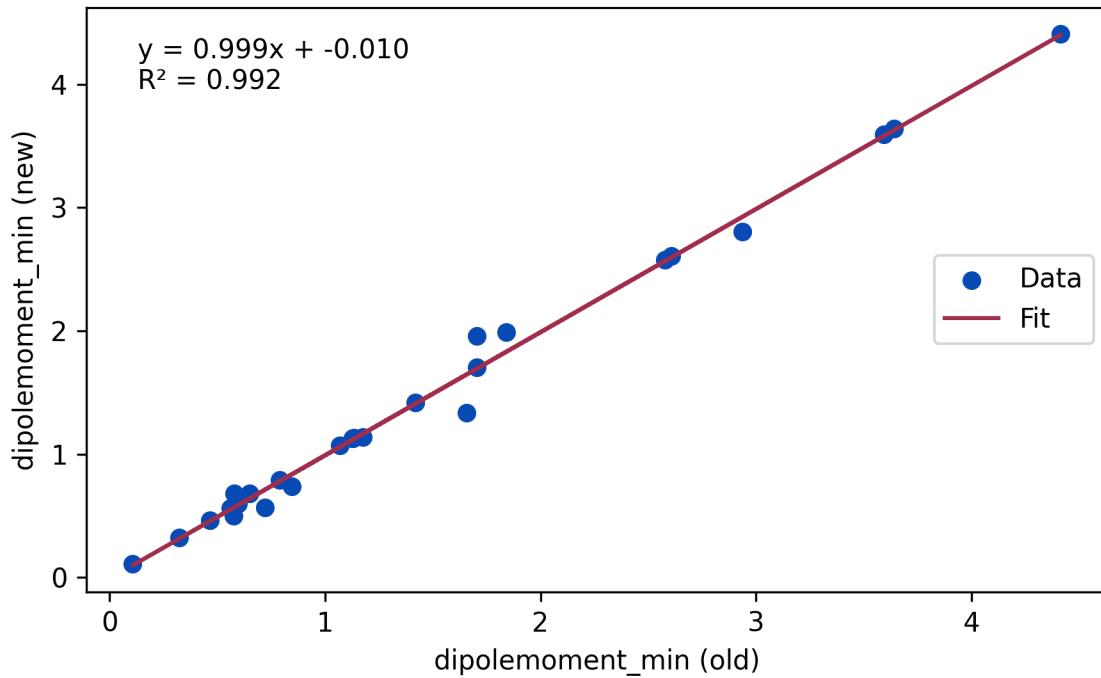


vbur\_near\_vtot\_min

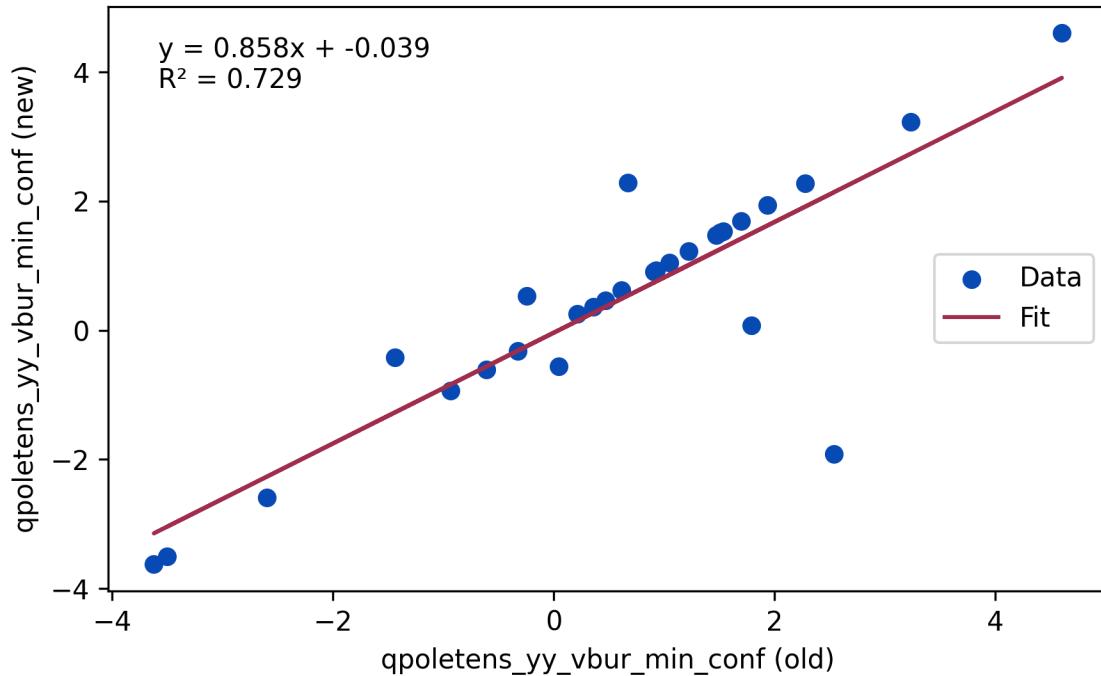


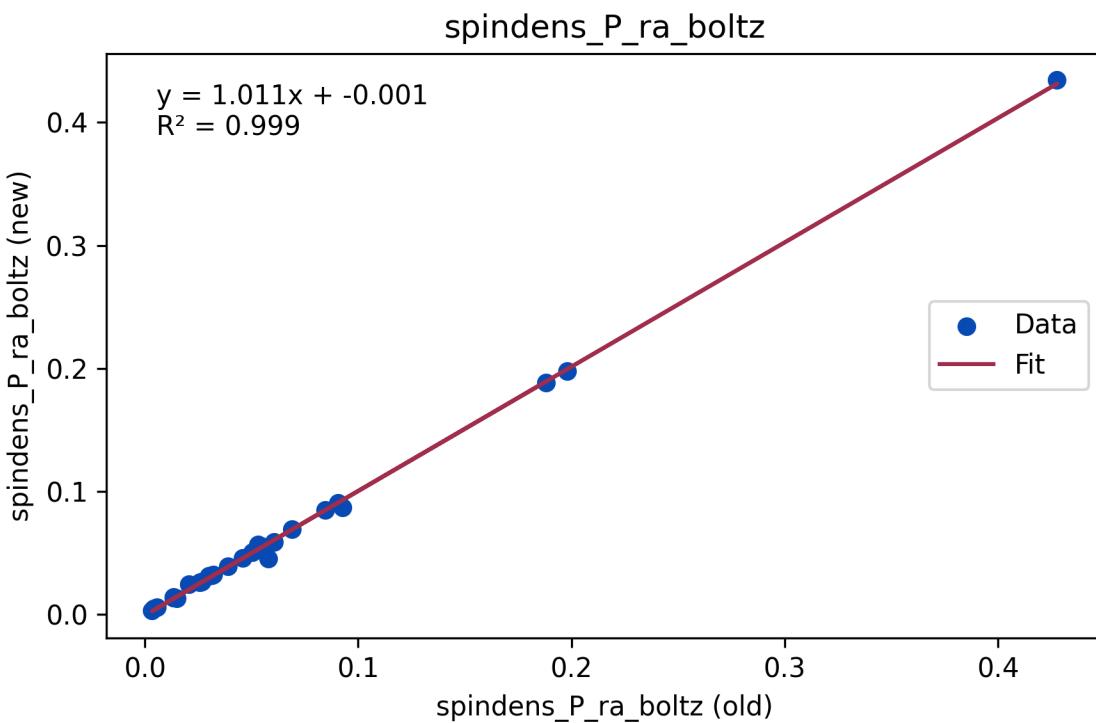
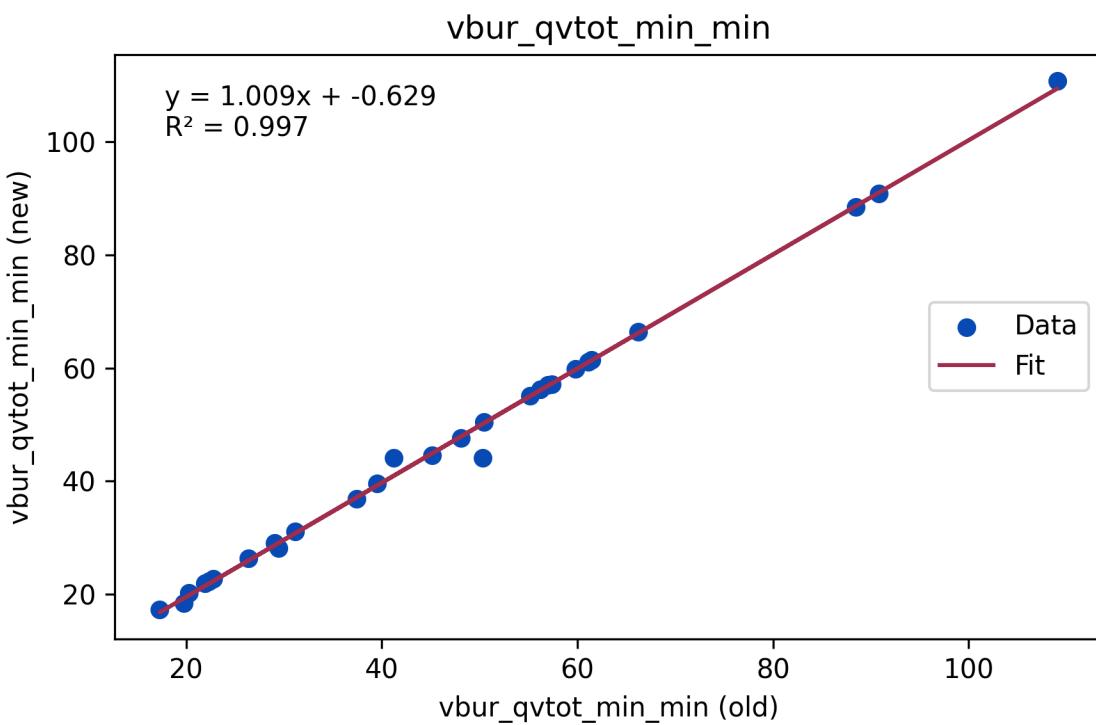


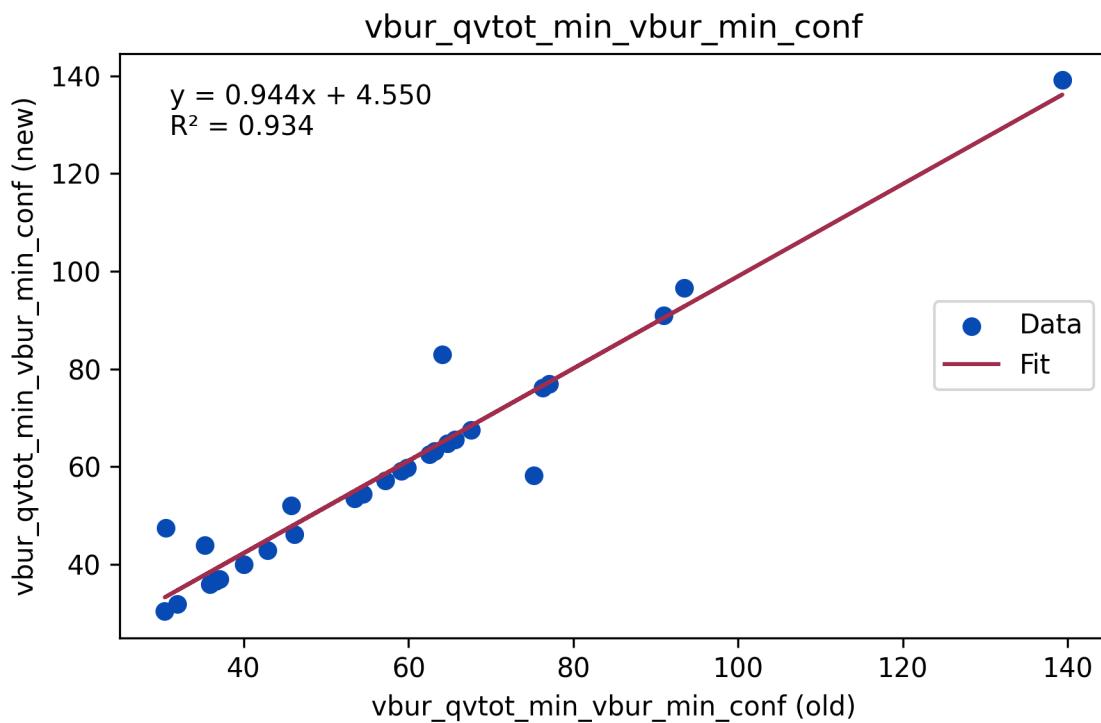
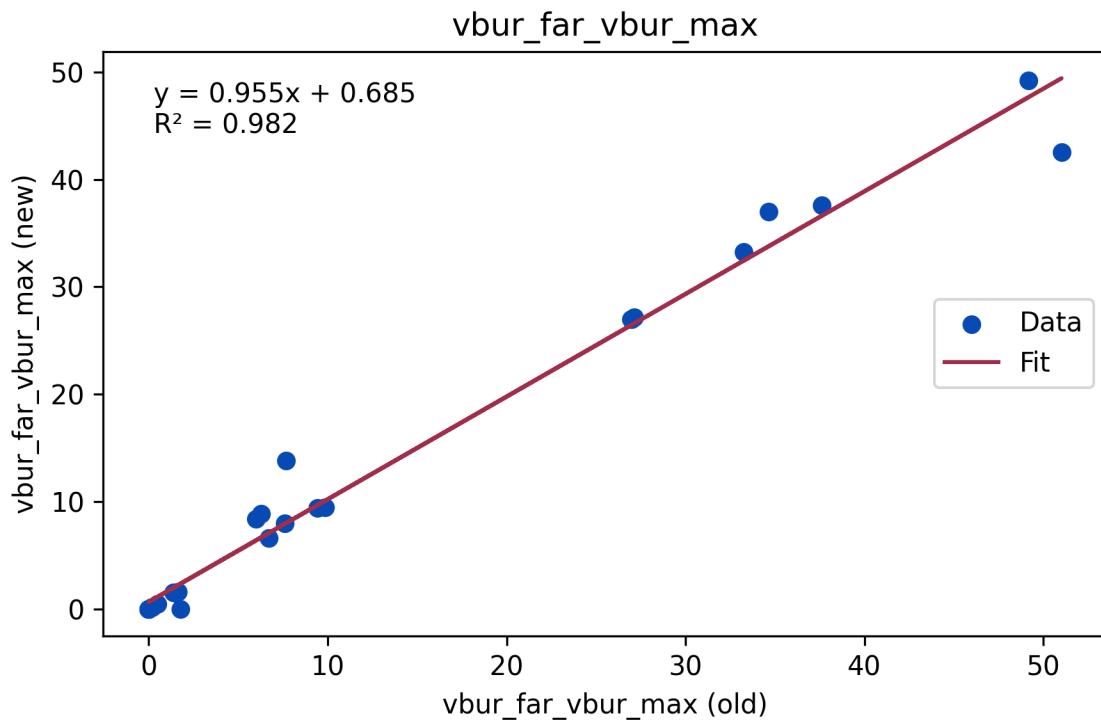
dipolemoment\_min

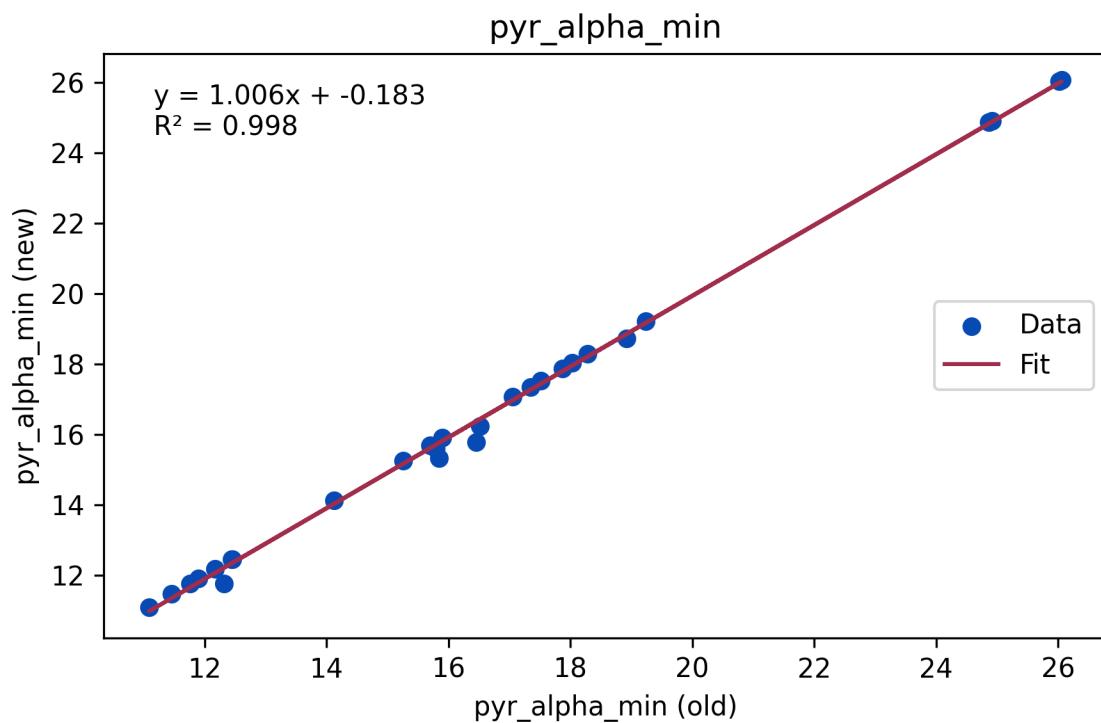
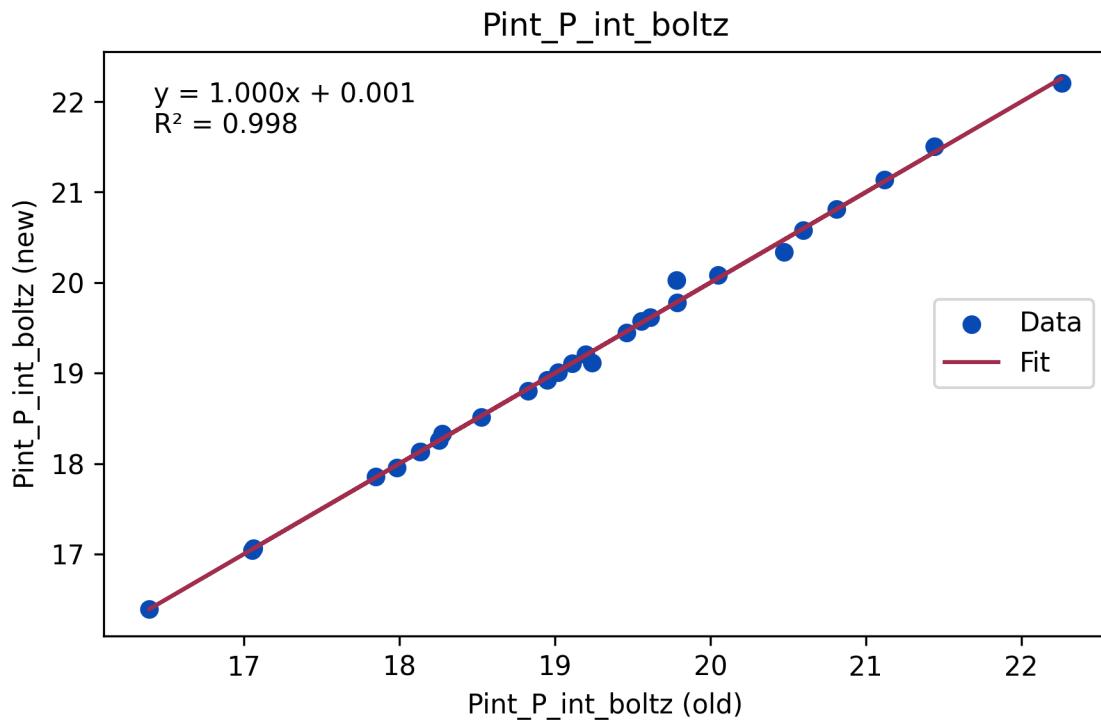


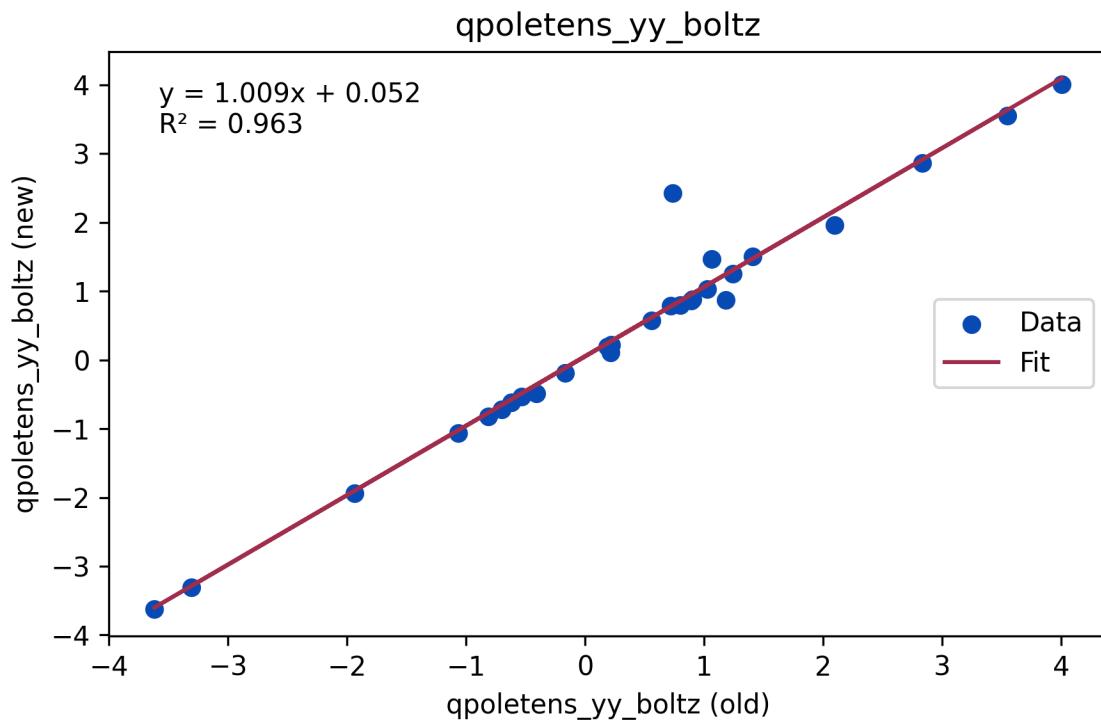
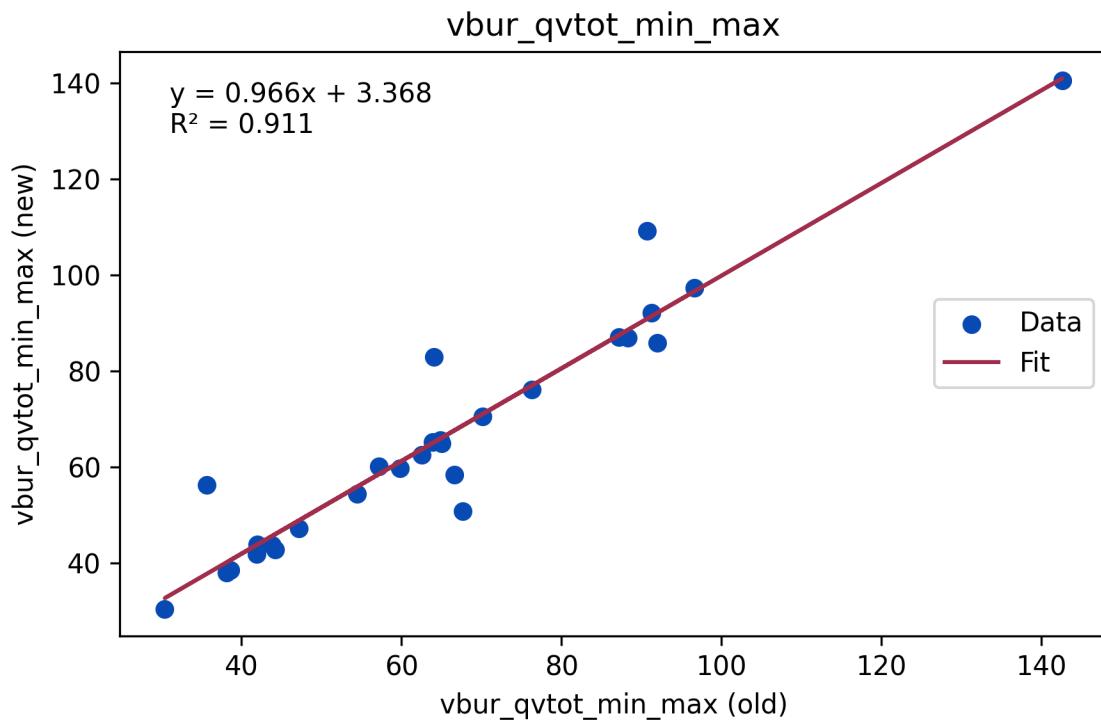
qpoletens\_yy\_vbur\_min\_conf

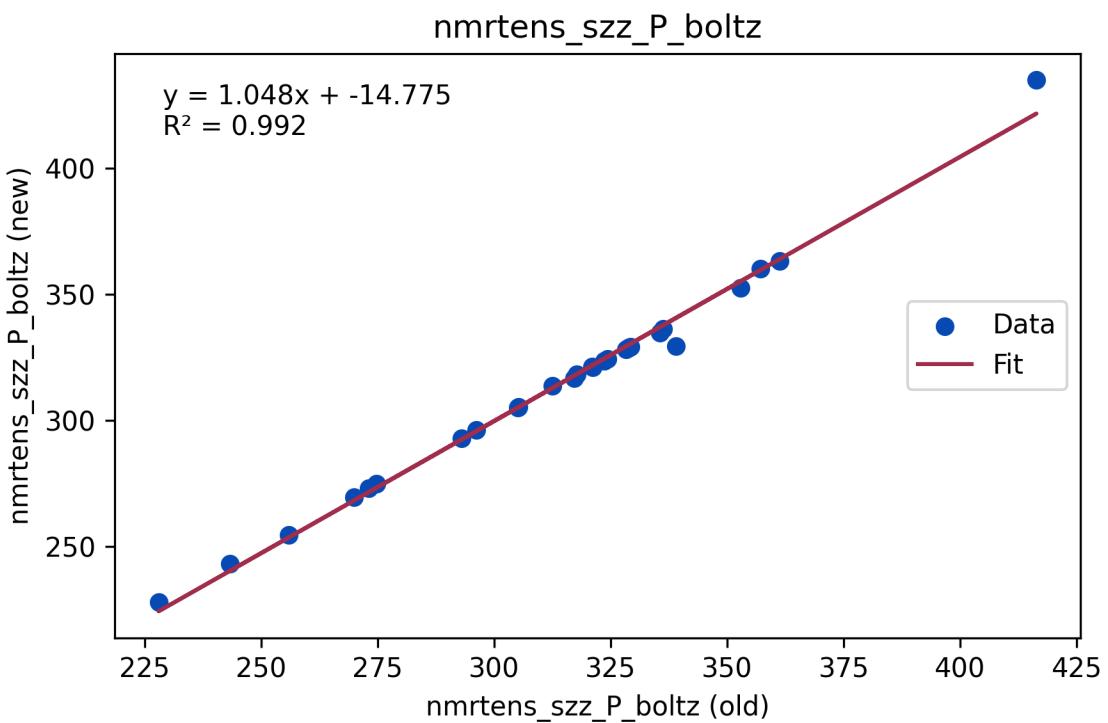
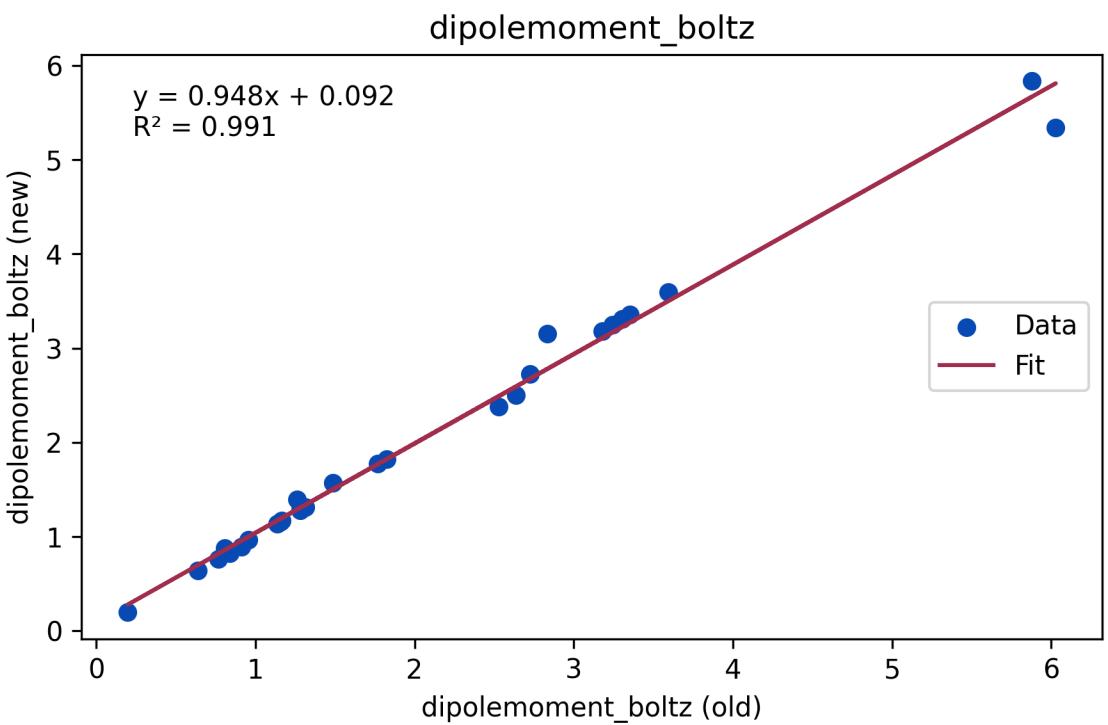


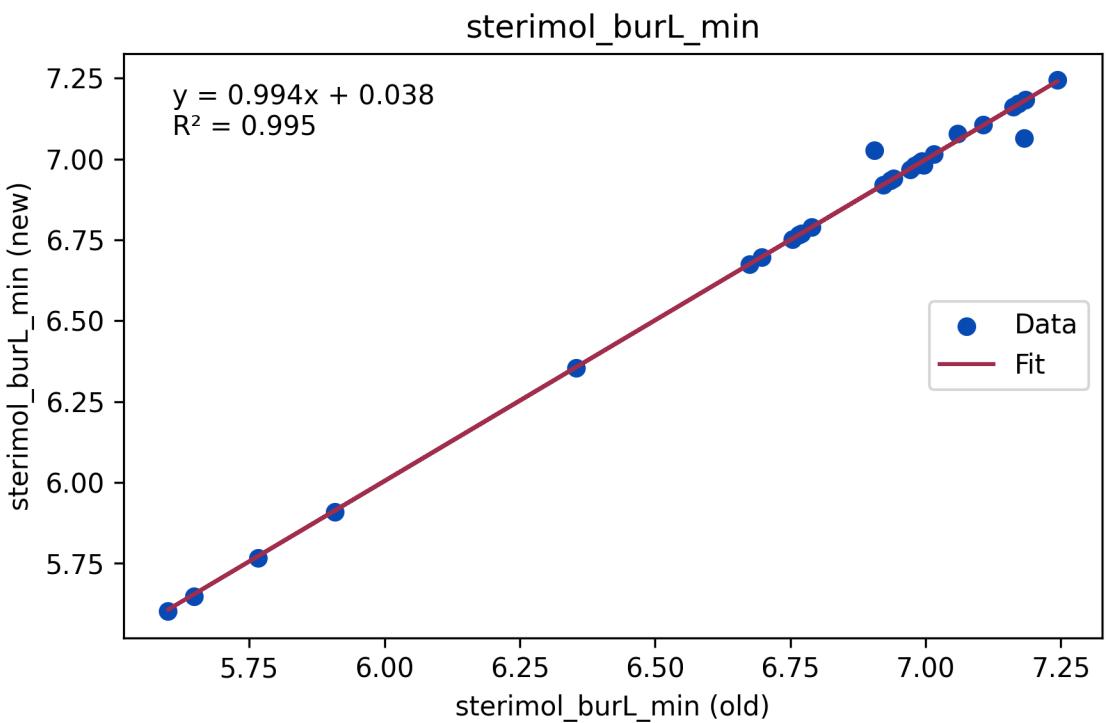
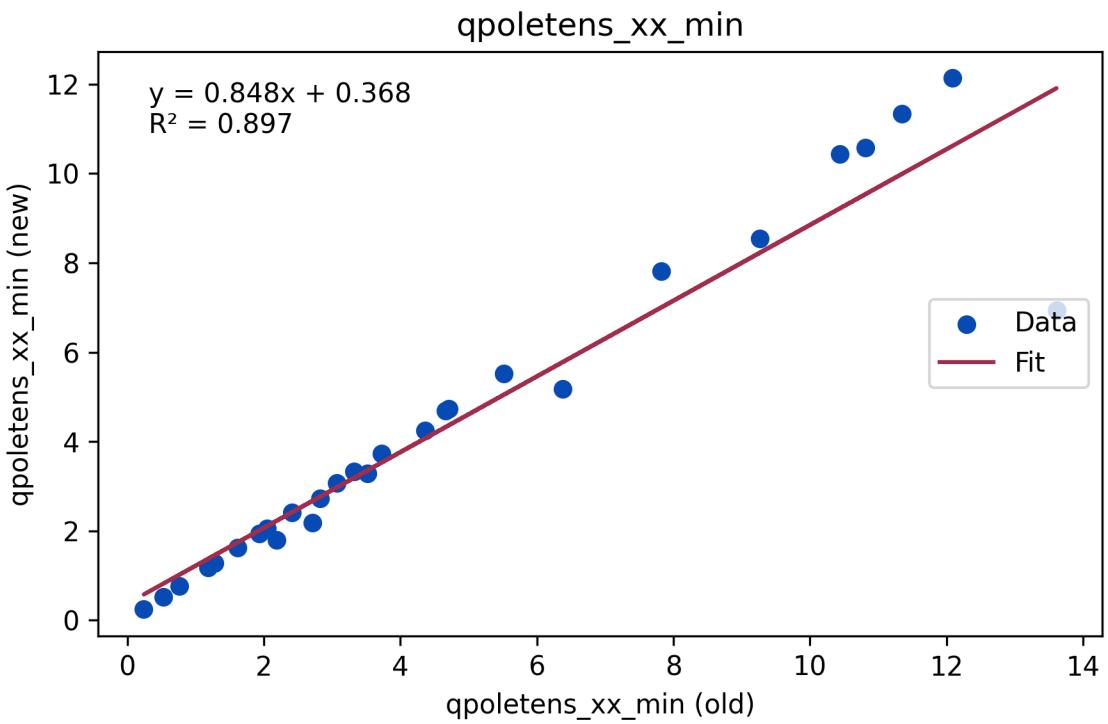


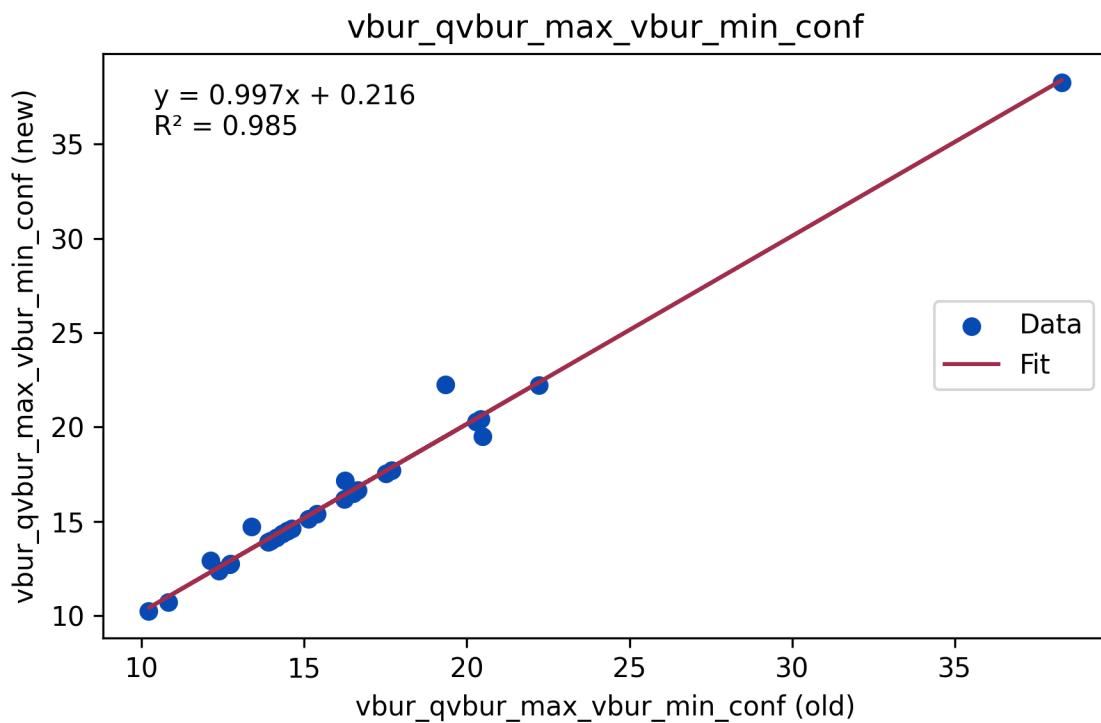
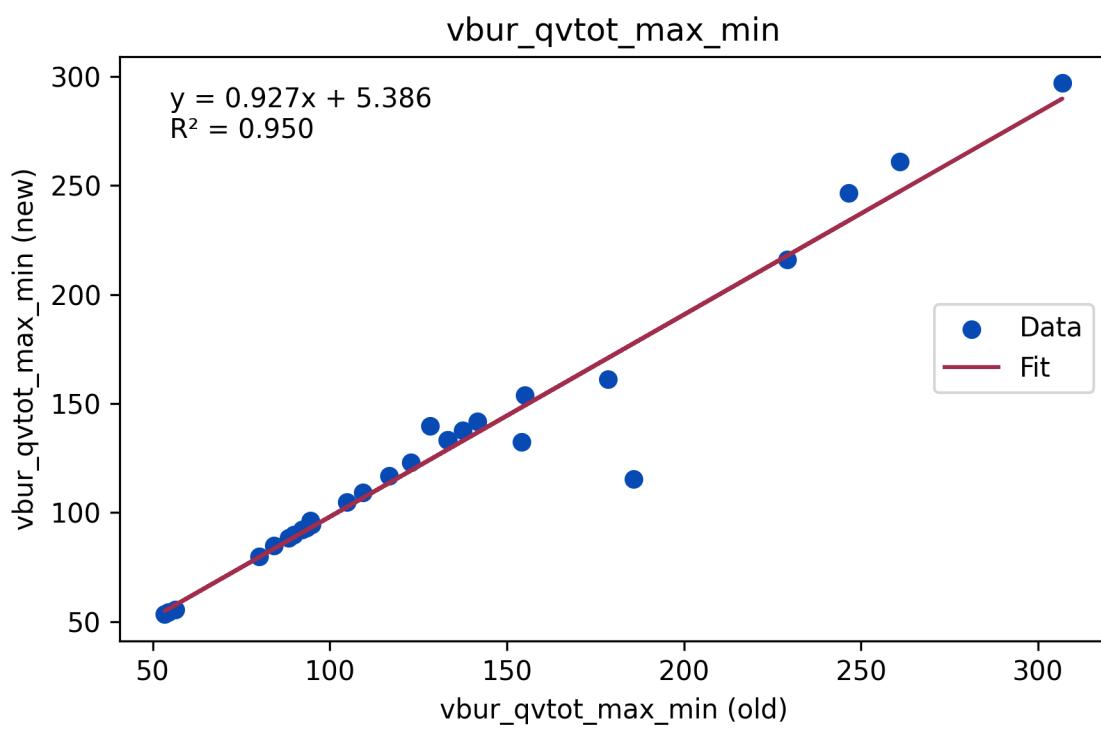


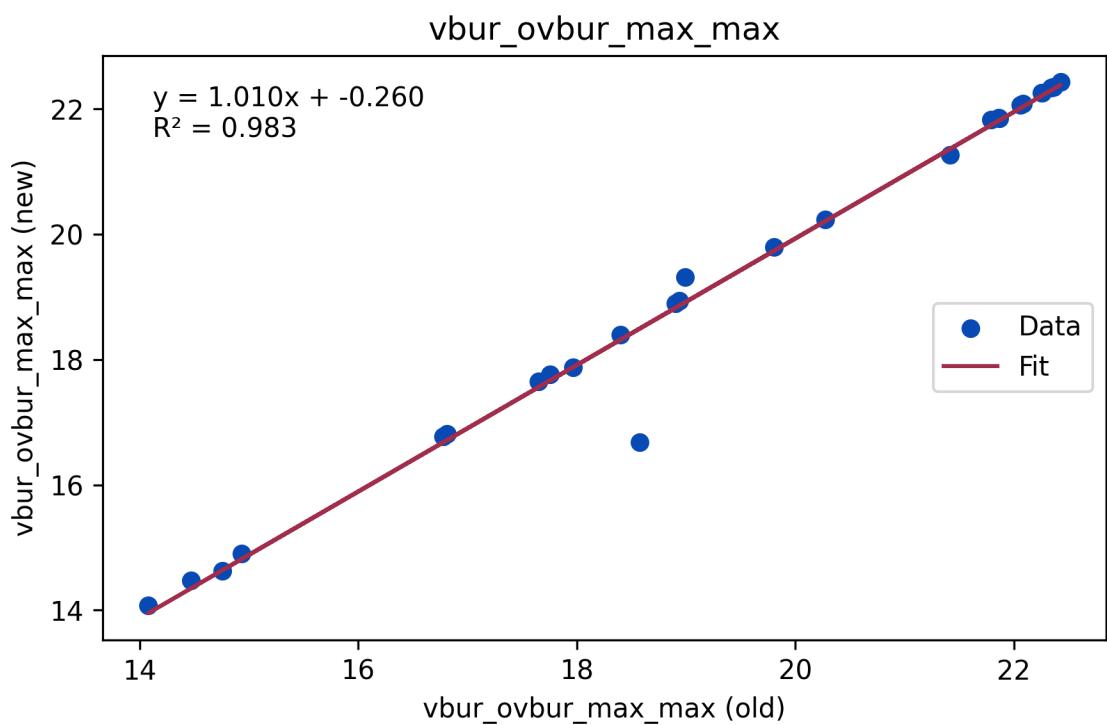
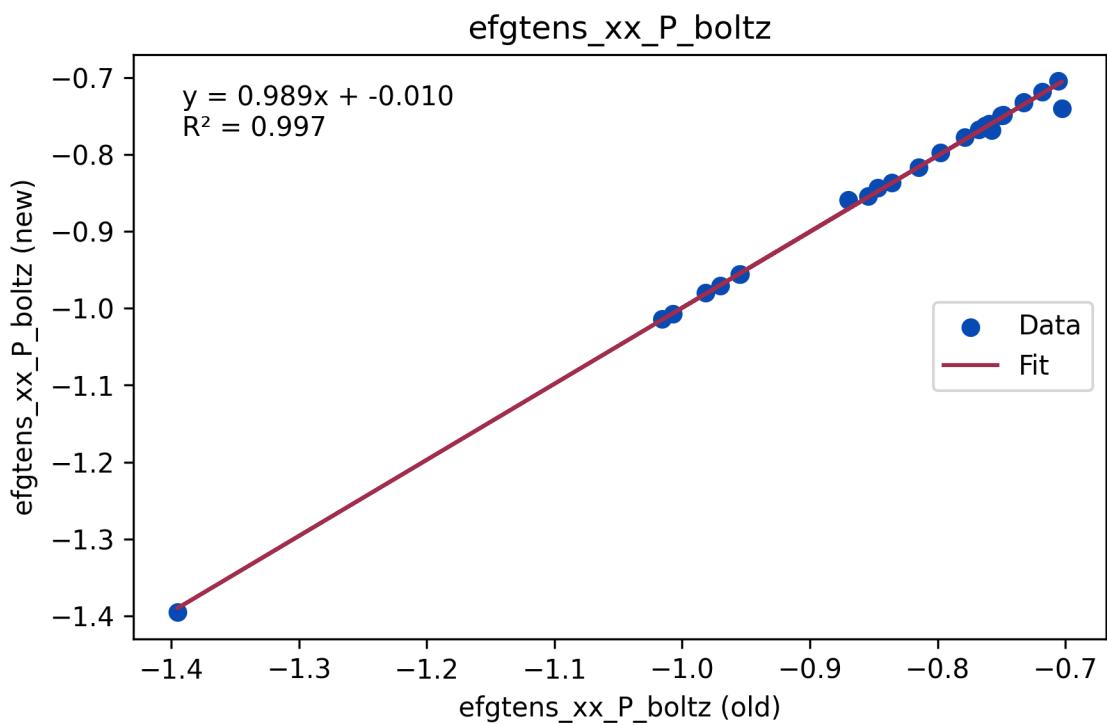




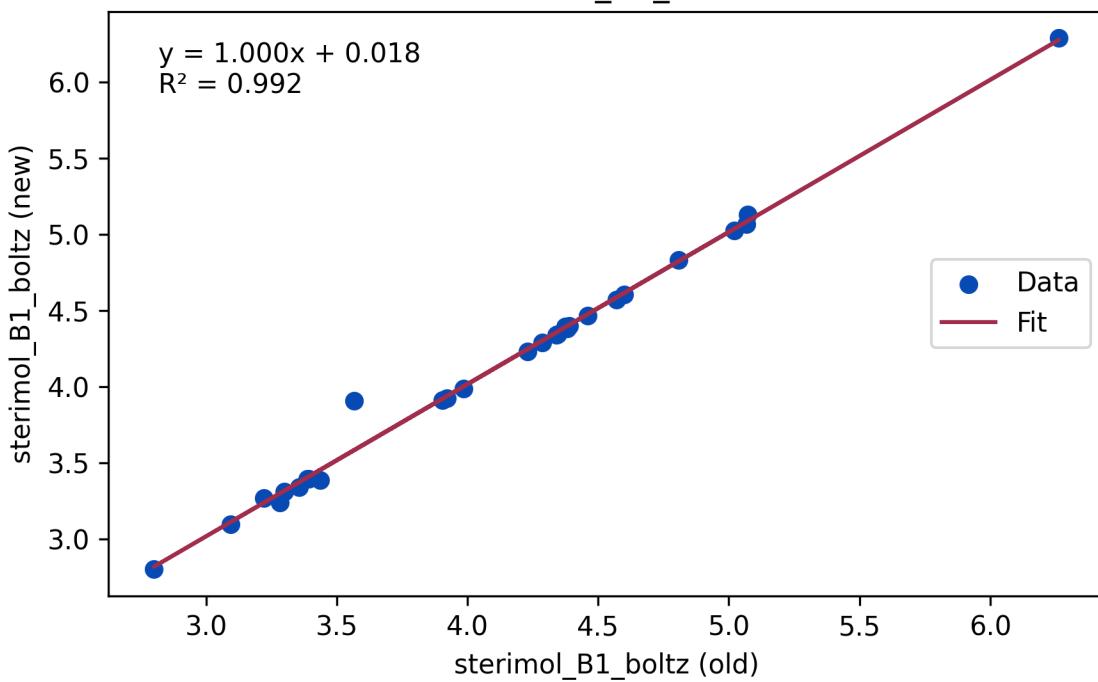








sterimol\_B1\_boltz



vbur\_near\_vtot\_delta

