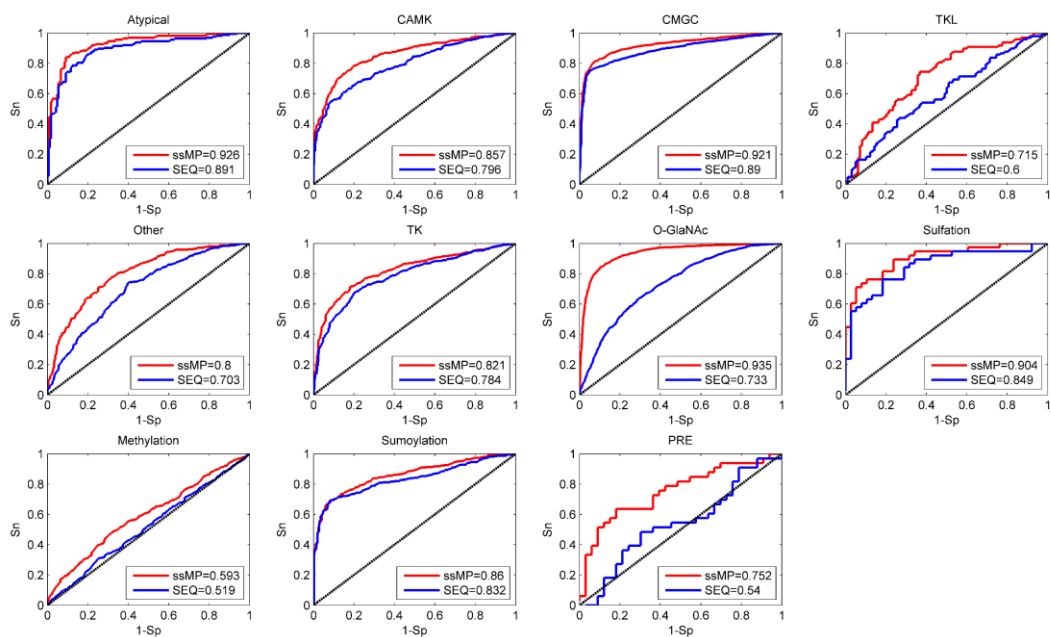
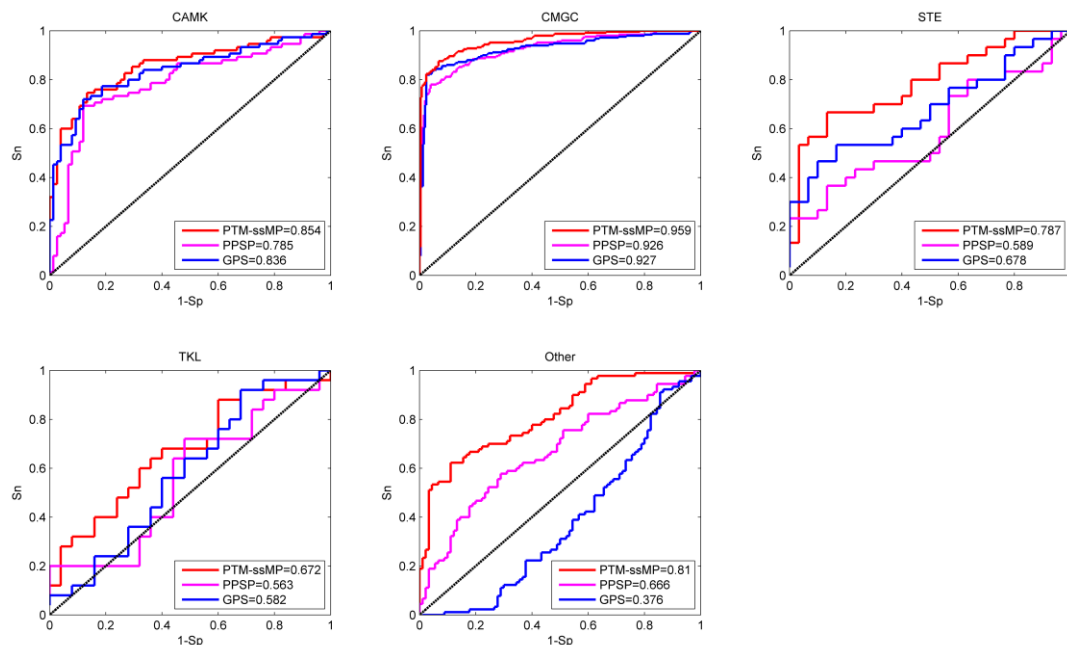


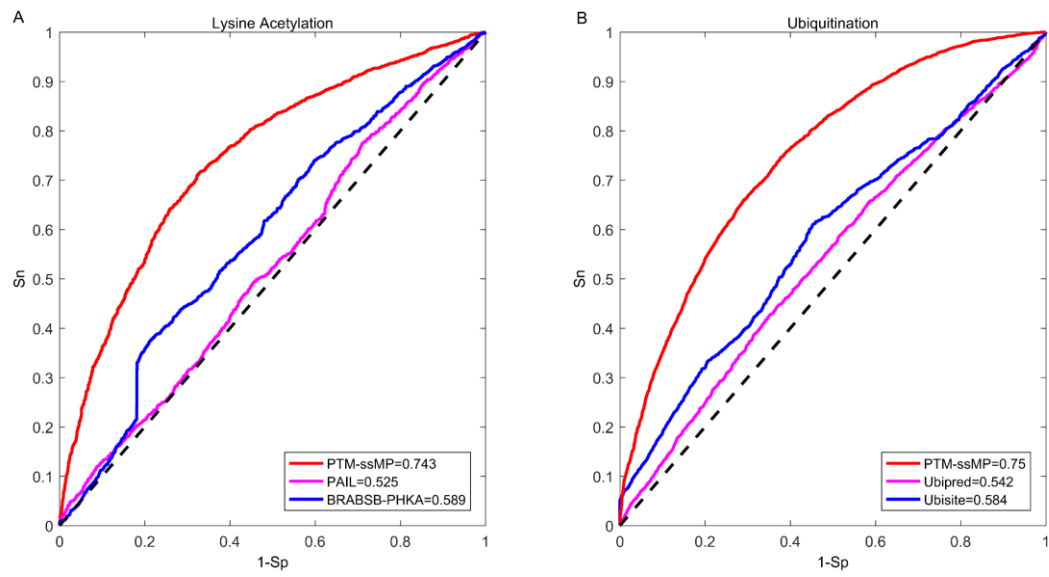
**Figure S1.** ROC curves of different PTMs: lysine acetylation, ubiquitination, phosphorylation AGC group, phosphorylation CK1 group, phosphorylation STE group and O-GlcNAc. The solid lines represent the predictive model constructed with ssMP, and the dotted lines represent the performance of the proposed method with only local sequences. SEQ and ssMP represent sequence and site-specific modification profile, respectively.



**Figure S2.** Performance of phosphorylation ROC curves in kinase group CAMK, CMGC, STE, TKL and Other with different methods. The red lines represent the performance of PTM-ssMP, and the blue and purple lines show the GPS, PPSP respectively.



**Figure S3.** Performance of phosphorylation ROC curves in kinase group CAMK, CMGC, STE, Other and TKL with different methods. The red lines represent the performance of PTM-ssMP, the blue and purple lines represent the GPS, PPSP respectively.



**Figure S4.** Performance of ROC curves for lysine acetylation and ubiquitination with different methods. In Figure S4A, the red lines represent the performance of PTM-ssMP, and the blue and purple lines show the BRABSB-PHKA, PAIL respectively. In Figure S4B, the red lines represent the performance of PTM-ssMP, and the blue and purple lines show the Ubsite, Ubipred respectively.

**Table S1.** Distribution of positive and negative sample numbers in non-redundant datasets (with a threshold of 40% identity by CD-HIT)

Attribute	AGC	Atypical	CAMK	CK1	CMGC	STE	TKL	TK	Other
protein	502	97	256	213	554	97	35	273	176
Positive	1025	204	436	543	1299	184	123	672	401
Negative	14661	5336	9436	5816	19330	2482	923	1137	6391

Attribute	Ubi	Ace	Meth	Sumo	O-GalNAc	O-GlcNAc	Sulfation	Prot
protein	5563	3857	433	255	458	129	24	31
Positive	28243	11067	644	465	1858	255	58	43
Negative	92154	94090	16303	9262	17129	12717	73	1303

Ubi, ubiquitination; Ace, lysine acetylation; Meth, methylation; Sumo, sumoylation; O-GalNAc, O-N-acetylgalactosamine; O-GlcNAc, O-N-acetylglucosamine; Prot, proteolytic cleavage

**Table S2.** Distribution of positive and negative sample numbers in benchmark datasets

Attribute	AGC	Atypical	CAMK	CK1	CMGC	STE	TKL	TK	Other
Positive	825	164	361	443	1049	154	25	125	90
Negative	825	164	361	443	1049	154	25	125	90

Attribute	Ubi	Ace	Meth	Sumo	O-GalNAc	O-GlcNAc	Sulfation	Prot
Positive	5000	2000	100	100	350	50	20	10
Negative	5000	2000	100	100	350	50	20	10

Ubi, ubiquitination; Ace, lysine acetylation; Meth, methylation; Sumo, sumoylation; O-GalNAc, O-N-acetylgalactosamine; O-GlcNAc, O-N-acetylglucosamine; Prot, proteolytic cleavage

**Table S3.** Distribution of positive and negative sample numbers in independent test datasets

Attribute	AGC	Atypical	CAMK	CK1	CMGC	STE	TKL	TK	Other
Positive	200	40	75	100	250	30	25	125	90
Negative	200	40	75	100	250	30	25	125	90

Attribute	Ubi	Ace	Meth	Sumo	O-GalNAc	O-GlcNAc	Sulfation	Prot
Positive	5000	2000	100	100	350	50	20	10
Negative	5000	2000	100	100	350	50	20	10

Ubi, ubiquitination; Ace, lysine acetylation; Meth, methylation; Sumo, sumoylation; O-GalNAc, O-N-acetylgalactosamine; O-GlcNAc, O-N-acetylglucosamine; Prot, proteolytic cleavage

**Table S4:** AUC values comparison of ssMP and local sequences of the other PTM and kinase groups

PTM	method	AUC	PTM	method	AUC
Phosphorylation (Atypical)	SEQ	0.899±2.02e-5	sulfation	SEQ	0.845±5.87e-4
	ssMP	<b>0.927</b> ±1.31e-5		ssMP	<b>0.898</b> ±3.60e-4
Phosphorylation (CAMK)	SEQ	0.813±8.67e-5	O-GalNAc	SEQ	0.716±8.82e-5
	ssMP	<b>0.859</b> ±3.86e-5		ssMP	<b>0.928</b> ±2.11e-5
Phosphorylation (CMGC)	SEQ	0.900±2.18e-5	Proteolytic cleavage	SEQ	0.592±4.20e-3
	ssMP	<b>0.932</b> ±1.70e-5		ssMP	<b>0.777</b> ±2.32e-4
Phosphorylation (Other)	SEQ	0.699±3.15e-4	methylation	SEQ	0.549±2.08e-4
	ssMP	<b>0.791</b> ±3.33e-4		ssMP	<b>0.598</b> ±2.23e-4
Phosphorylation (TKL)	SEQ	0.597±9.47e-4	sumoylation	SEQ	0.822±2.00e-5
	ssMP	<b>0.718</b> ±6.58e-4		ssMP	<b>0.850</b> ±1.83e-5
Phosphorylation (TK)	SEQ	0.784±9.13e-5	_____	_____	_____
	ssMP	<b>0.814</b> ±5.68e-5	_____	_____	_____

**Table S5:** performance comparison of ssMP and local sequences at high stringency level (Sp=95.0%)

PTM	Feature	Acc	Sn	Pre	F-score	MCC
Lysine Acetylation	SEQ	0.541±6.01e-6	0.133±2.64e-5	0.726±5.66e-5	0.224±5.91e-5	0.144±4.96e-5
	ssMP	0.586±8.47e-6	0.223±3.39e-5	0.817±1.51e-5	0.350±5.68e-5	0.252±3.58e-5
Ubiquitination	SEQ	0.526±3.26e-6	0.103±1.31e-5	0.672±5.93e-5	0.178±3.25e-5	0.099±3.26e-5
	ssMP	0.588±3.03e-6	0.227±1.21e-5	0.819±5.25e-6	0.355±2.02e-5	0.256±1.37e-5
Methylation	SEQ	0.506±1.37e-4	0.061±5.50e-4	0.524±1.89e-2	0.108±1.66e-3	0.019±3.22e-3
	ssMP	0.515±3.20e-4	0.079±1.28e-3	0.573±3.03e-2	0.138±3.62e-3	0.051±5.99e-3
Sumoylation	SEQ	0.720±1.62e-3	0.489±6.49e-3	0.907±2.09e-4	0.633±5.18e-3	0.495±4.61e-3
	ssMP	0.720±1.75e-3	0.489±7.01e-3	0.906±2.71e-4	0.632±5.87e-3	0.495±5.05e-3
Phosphorylation (AGC)	SEQ	0.706±1.49e-5	0.461±5.98e-4	0.903±2.47e-5	0.610±5.26e-4	0.472±4.31e-4
	ssMP	0.743±1.34e-4	0.536±5.36e-4	0.915±1.18e-5	0.675±3.80e-4	0.534±3.71e-4
Phosphorylation (Atypical)	SEQ	0.796±1.35e-3	0.641±5.23e-3	0.929±6.21e-5	0.757±2.90e-3	0.624±3.70e-3
	ssMP	0.819±9.42e-4	0.686±3.77e-3	0.933±3.40e-5	0.789±1.89e-3	0.661±2.72e-3
Phosphorylation (CAMK)	SEQ	0.704±5.18e-4	0.458±2.07e-3	0.901±9.46e-5	0.606±1.86e-3	0.468±1.51e-3
	ssMP	0.738±5.98e-4	0.525±2.39e-3	0.913±6.09e-5	0.666±1.77e-3	0.525±1.67e-3
Phosphorylation (CK1)	SEQ	0.742±4.76e-4	0.534±1.90e-3	0.914±4.17e-5	0.673±1.34e-3	0.533±1.32e-3
	ssMP	0.791±2.19e-4	0.631±8.78e-4	0.927±1.04e-5	0.750±4.89e-4	0.613±6.15e-4
Phosphorylation (CMGC)	SEQ	0.852±2.11e-5	0.754±8.44e-5	0.938±5.02e-7	0.836±3.53e-5	0.718±6.43e-5
	ssMP	0.867±5.40e-5	0.783±2.16e-4	0.940±1.15e-6	0.854±8.58e-5	0.744±1.69e-4
Phosphorylation (STE)	SEQ	0.597±9.55e-4	0.245±3.82e-3	0.819±1.22e-3	0.375±5.63e-3	0.269±3.90e-3
	ssMP	0.667±8.01e-4	0.385±3.21e-3	0.879±2.94e-4	0.534±3.46e-3	0.402±2.55e-3
Phosphorylation (TKL)	SEQ	0.530±3.98e-4	0.110±1.59e-3	0.667±5.75e-3	0.188±3.73e-3	0.104±3.53e-3
	ssMP	0.560±9.42e-4	0.170±3.77e-3	0.749±7.33e-3	0.275±7.69e-3	0.183±6.41e-3
Phosphorylation (Other)	SEQ	0.569±2.28e-4	0.188±9.13e-4	0.788±6.74e-4	0.303±1.68e-3	0.212±1.20e-3
	ssMP	0.634±4.28e-4	0.318±1.71e-3	0.863±2.20e-4	0.463±2.09e-3	0.345±1.45e-3
Phosphorylation (TK)	SEQ	0.647±1.53e-4	0.344±6.12e-4	0.874±7.01e-5	0.493±7.7.37e-4	0.370±5.09e-5
	ssMP	0.680±2.11e-4	0.408±8.45e-4	0.892±4.61e-5	0.560±8.16e-4	0.427±6.26e-4
O-GlcNAc	SEQ	0.624±4.03e-4	0.298±1.61e-3	0.857±3.15e-4	0.441±2.22e-3	0.328±1.49e-3
	ssMP	0.671±8.07e-4	0.391±3.23e-3	0.887±1.79e-4	0.541±3.12e-3	0.412±2.40e-3
O-GalNAc	SEQ	0.562±5.44e-5	0.174±2.18e-4	0.777±2.27e-4	0.285±4.31e-4	0.197±3.19e-4
	ssMP	0.821±1.77e-4	0.691±7.10e-4	0.933±6.39e-6	0.794±3.53e-4	0.664±5.10e-4
Proteolytic Cleavage	SEQ	0.521±3.68e-3	0.103±1.47e-2	0.451±9.40e-2	0.161±3.03e-2	0.030±3.42e-2
	ssMP	0.694±4.68e-3	0.448±1.87e-2	0.871±1.70e-3	0.584±1.75e-2	0.442±1.48e-2
Sulfation	SEQ	0.708±5.20e-3	0.468±2.07e-2	0.885±3.79e-3	0.603±2.30e-2	0.468±1.83e-2
	ssMP	0.776±6.43e-3	0.605±2.57e-2	0.913±1.20e-3	0.718±1.97e-2	0.587±1.96e-2

**Table S6:** Performance comparison of site-specific modification profiles and local sequences at medium stringency level (Sp=90.0%)

PTM	Feature	Acc	Sn	Pre	F-score	MCC
Lysine Acetylation	SEQ	0.563±1.85e-5	0.227±7.40e-5	0.694±6.53e-5	0.342±1.57e-4	0.172±9.66e-5
	ssMP	0.621±2.63e-5	0.342±1.05e-4	0.774±2.71e-5	0.474±1.70e-4	0.292±9.82e-5
Ubiquitination	SEQ	0.550±4.30e-6	0.201±1.72e-5	0.667±2.11e-5	0.308±2.92e-5	0.141±2.51e-5
	ssMP	0.627±3.56e-6	0.354±1.42e-5	0.780±3.41e-6	0.487±1.55e-5	0.303±1.31e-5
Methylation	SEQ	0.511±5.81e-5	0.122±3.23e-4	0.548±9.65e-4	0.199±5.05e-4	0.035±5.40e-4
	ssMP	0.529±1.75e-4	0.157±6.99e-4	0.609±1.55e-3	0.249±1.34e-3	0.085±1.26e-3
Sumoylation	SEQ	0.766±4.90e-4	0.630±1.96e-3	0.864±7.81e-5	0.728±1.12e-3	0.522±1.51e-3
	ssMP	0.766±2.08e-4	0.651±8.32e-4	0.868±2.51e-5	0.744±4.24e-4	0.571±6.46e-4
Phosphorylation (AGC)	SEQ	0.737±6.31e-5	0.573±2.52e-4	0.852±1.24e-5	0.685±1.57e-4	0.502±1.93e-4
	ssMP	0.775±1.56e-4	0.650±6.24e-4	0.867±1.90e-5	0.743±3.17e-4	0.569±4.76e-4
Phosphorylation (Atypical)	SEQ	0.836±5.94e-4	0.770±2.38e-3	0.887±4.05e-5	0.824±9.44e-4	0.678±2.01e-3
	ssMP	0.859±1.32e-4	0.816±5.27e-4	0.893±7.21e-6	0.853±1.89e-4	0.721±4.68e-4
Phosphorylation (CAMK)	SEQ	0.724±1.65e-4	0.547±6.62e-4	0.846±3.81e-5	0.664±4.37e-4	0.478±5.09e-4
	ssMP	0.768±2.04e-4	0.635±8.16e-4	0.864±2.85e-5	0.732±4.93e-4	0.555±6.31e-4
Phosphorylation (CK1)	SEQ	0.767±2.94e-4	0.634±1.18e-3	0.864±4.21e-5	0.731±6.42e-4	0.555±9.08e-4
	ssMP	0.814±2.13e-4	0.728±8.53e-4	0.880±1.83e-5	0.797±3.72e-4	0.639±6.93e-4
Phosphorylation (CMGC)	SEQ	0.848±1.07e-5	0.796±4.26e-5	0.888±6.81e-7	0.839±1.62e-5	0.699±3.68e-5
	ssMP	0.875±2.47e-5	0.850±9.86e-5	0.895±1.23e-6	0.872±3.33e-5	0.751±9.11e-5
Phosphorylation (STE)	SEQ	0.6181.48e-3±	0.333±5.93e-3	0.7662.21e-3±	0.462±7.11e-3	0.284±5.99e-3
	ssMP	0.702±1.20e-3	0.501±4.80e-3	8.835±3.41e-4	0.624±3.44e-3	0.440±3.74e-3
Phosphorylation (TKL)	SEQ	0.540±4.61e-4	0.182±1.85e-3	0.632±3.51e-3	0.281±3.32e-3	0.111±3.08e-3
	ssMP	0.596±5.54e-4	0.294±2.22e-3	0.739±9.77e-4	0.419±2.84e-3	0.239±2.35e-3
Phosphorylation (Other)	SEQ	0.601±2.31e-4	0.301±9.24e-4	0.750±3.65e-4	0.429±1.16e-3	0.251±9.55e-4
	ssMP	0.678±4.12e-4	0.456±1.65e-3	0.820±1.76e-4	0.586±1.36e-3	0.398±1.33e-3
Phosphorylation (TK)	SEQ	0.687±1.37e-4	0.475±5.50e-4	0.825±5.05e-5	0.603±4.31e-4	0.414±4.36e-4
	ssMP	0.725±1.78e-4	0.551±7.13e-4	0.846±4.11e-5	0.667±4.68e-4	0.481±5.49e-4
O-GlcNAc	SEQ	0.675±5.67e-4	0.448±2.27e-3	0.820±2.84e-4	0.578±2.00e-3	0.393±1.87e-3
	ssMP	0.731±6.59e-4	0.560±2.64e-3	0.851±1.26e-4	0.675±1.63e-3	0.493±2.02e-3
O-GalNAc	SEQ	0.599±1.19e-4	0.299±4.76e-4	0.748±2.00e-4	0.427±6.10e-4	0.249±5.00e-4
	ssMP	0.861±6.79e-5	0.821±2.72e-4	0.891±3.85e-6	0.855±9.73e-5	0.724±2.42e-4
Proteolytic Cleavage	SEQ	0.558±5.24e-3	0.206±2.10e-2	0.597±6.38e-2	0.299±3.56e-2	0.130±3.70e-2
	ssMP	0.706±2.51e-3	0.503±1.00e-2	0.842±9.90e-4	0.626±8.18e-3	0.450±8.07e-3
Sulfation	SEQ	0.742±1.12e-3	0.589±4.49e-3	0.847±2.28e-4	0.694±2.70e-3	0.509±3.51e-3
	ssMP	0.793±1.58e-3	0.692±6.32e-3	0.867±1.92e-4	0.768±3.06e-3	0.600±5.07e-3

**Table S7:** Performance comparison of PTM-ssMP and GPS, PPSP at high stringency level (Sp=95.0%)

PTM	method	Acc	Sn	Pre	F-score	MCC
AGC	PTM-ssMP	<b>0.788</b>	<b>0.625</b>	<b>0.926</b>	<b>0.746</b>	<b>0.608</b>
	GPS	0.550	0.150	0.750	0.250	0.167
	PPSP	0.703	0.455	0.901	0.605	0.466
Atypical	PTM-ssMP	<b>0.788</b>	<b>0.625</b>	<b>0.926</b>	<b>0.746</b>	<b>0.608</b>
	GPS	0.688	0.450	0.857	0.590	0.426
	PPSP	0.663	0.375	0.882	0.526	0.397
CAMK	PTM-ssMP	<b>0.773</b>	<b>0.600</b>	<b>0.914</b>	<b>0.726</b>	<b>0.583</b>
	GPS	0.740	0.533	0.909	0.672	0.527
	PPSP	0.560	0.173	0.765	0.283	0.189
CK1	PTM-ssMP	<b>0.775</b>	<b>0.600</b>	<b>0.923</b>	<b>0.727</b>	<b>0.587</b>
	GPS	0.565	0.180	0.783	0.293	0.204
	PPSP	0.725	0.500	0.909	0.645	0.504
CMGC	PTM-ssMP	<b>0.896</b>	<b>0.840</b>	<b>0.946</b>	<b>0.890</b>	<b>0.797</b>
	GPS	0.894	0.836	0.946	0.888	0.793
	PPSP	0.866	0.780	0.942	0.853	0.743
STE	PTM-ssMP	<b>0.733</b>	<b>0.533</b>	<b>0.889</b>	<b>0.667</b>	<b>0.509</b>
	GPS	0.617	0.300	0.818	0.439	0.302
	PPSP	0.583	0.233	0.778	0.359	0.233
TKL	PTM-ssMP	<b>0.540</b>	<b>0.120</b>	<b>0.750</b>	<b>0.207</b>	<b>0.147</b>
	GPS	0.520	0.120	0.600	0.200	0.067
	PPSP	0.580	0.200	0.833	0.323	0.246
Other	PTM-ssMP	<b>0.739</b>	<b>0.533</b>	<b>0.906</b>	<b>0.671</b>	<b>0.524</b>
	GPS	0.472	0	0	0	-0.169
	PPSP	0.567	0.189	0.773	0.304	0.204
TK	PTM-ssMP	<b>0.628</b>	<b>0.304</b>	<b>0.864</b>	<b>0.450</b>	<b>0.336</b>
	GPS	0.596	0.240	0.833	0.373	0.273
	PPSP	0.624	0.296	0.861	0.441	0.329



**Table S8:** Performance comparison of PTM-ssMP and GPS, PPSP at medium stringency level (Sp=90.0%)

PTM	method	Acc	Sn	Pre	F-score	MCC
AGC	<b>PTM-ssMP</b>	<b>0.793</b>	<b>0.685</b>	<b>0.873</b>	<b>0.768</b>	<b>0.599</b>
	GPS	0.558	0.215	0.683	0.327	0.158
	PPSP	0.763	0.625	0.862	0.725	0.546
Atypical	<b>PTM-ssMP</b>	<b>0.838</b>	<b>0.775</b>	<b>0.886</b>	<b>0.827</b>	<b>0.680</b>
	GPS	0.738	0.575	0.852	0.687	0.502
	PPSP	0.688	0.475	0.826	0.603	0.414
CAMK	<b>PTM-ssMP</b>	<b>0.773</b>	<b>0.640</b>	<b>0.873</b>	<b>0.739</b>	<b>0.567</b>
	GPS	0.740	0.573	0.860	0.688	0.509
	PPSP	0.707	0.507	0.844	0.633	0.451
CK1	<b>PTM-ssMP</b>	<b>0.820</b>	<b>0.740</b>	<b>0.881</b>	<b>0.804</b>	<b>0.648</b>
	GPS	0.575	0.250	0.714	0.370	0.197
	PPSP	0.765	0.630	0.863	0.728	0.550
CMGC	<b>PTM-ssMP</b>	<b>0.894</b>	<b>0.888</b>	<b>0.899</b>	<b>0.893</b>	<b>0.788</b>
	GPS	0.880	0.860	0.896	0.878	0.761
	PPSP	0.856	0.812	0.890	0.849	0.715
STE	<b>PTM-ssMP</b>	<b>0.733</b>	<b>0.567</b>	<b>0.850</b>	<b>0.680</b>	<b>0.495</b>
	GPS	0.650	0.400	0.800	0.533	0.346
	PPSP	0.567	0.233	0.700	0.350	0.179
TKL	<b>PTM-ssMP</b>	<b>0.600</b>	<b>0.280</b>	<b>0.778</b>	<b>0.412</b>	<b>0.260</b>
	GPS	0.520	0.120	0.600	0.200	0.067
	PPSP	0.560	0.200	0.714	0.313	0.173
Other	<b>PTM-ssMP</b>	<b>0.722</b>	<b>0.544</b>	<b>0.845</b>	<b>0.662</b>	<b>0.476</b>
	GPS	0.456	0.011	0.100	0.020	-0.194
	PPSP	0.567	0.233	0.700	0.350	0.179
TK	<b>PTM-ssMP</b>	<b>0.732</b>	<b>0.560</b>	<b>0.854</b>	<b>0.676</b>	<b>0.494</b>
	GPS	0.612	0.320	0.769	0.452	0.276
	PPSP	0.660	0.416	0.813	0.550	0.367