

Description

TableS1. Summary of baseline and clinicopathologic features for all 31 MiniPDX models corresponding to 22 CRC cases.

TableS2. The details of the fraction combinations in proteome or phosphoproteome.

TableS3. The detail of DIA isolation windows with variable width for proteome were determined by DDA searching results from MaxQuant.

TableS4. The detail of DIA isolation windows with variable width for phosphoproteome were determined by DDA searching results from MaxQuant.

TableS5. Structural information of the proteome and phosphoproteome hybrid spectral library. CT, primary tumor tissues; CN, remote normal tissues; CP, para-carcinoma tissues; LM, liver metastatic tissues.

TableS6. Number of peptides precursor and protein group for randomly selected 32 proteomic DIA runs.

TableS7. The situation of phosphopeptide precursor and phosphoprotein group for randomly selected 32 phosphoproteomic DIA runs.

TableS1. Summary of baseline and clinicopathologic features for all 31 MiniPDX models corresponding to 22 CRC cases.

Characteristics	Training set	Validation set	<i>P</i> value
n	9	13	
Tissue = Rectum (%)	4(44.4)	9(69.2)	0.471
Gender = male (%)	6(66.7)	6(46.2)	0.607
Age (mean (SD))	60.89(13.99)	60.85(14.94)	0.995
Stage (%)			0.002
II	0	5(38.5)	
III	0	5(38.5)	
IV	9(100.00)	3(23.1)	
M (%)			0.002
M	9(100.00)	3(23.1)	
noM	0	10(76.9)	
Hitopathologic type-adenocarcinoma			
Moderately differentiated	7(77.8)	11(84.6)	
Poorly-moderately differentiated	2(22.2)	2(15.4)	
CEA (mean (SD))	62.27(106.58)	4.01(3.43)	0.140
CA19.9 (mean (SD))	159.46(393.46)	32.83(38.16)	0.364
Calcium.nodus = 1 (%)	4(44.4)	4(30.8)	0.838
Intravascular.tumor.thrombus = 1 (%)	4(44.4)	4(30.8)	0.838
Neurological.invasion = 1 (%)	4(44.4)	2(15.4)	0.309
Invasion.in.turn (mean (SD))	0.74(0.28)	0.82(0.19)	0.445

TableS2. The details of the fraction combinations in proteome or phosphoproteome.
The combination of 96 offline fractions by a concatenation scheme in proteome.

Proteome	Fraction No.	Fraction No.	Fraction No.	Fraction No.
Combined fraction 1	1	31	61	91
Combined fraction 2	2	32	62	92
Combined fraction 3	3	33	63	93
Combined fraction 4	4	34	64	94
Combined fraction 5	5	35	65	95
Combined fraction 6	6	36	66	96
Combined fraction 7	7	37	67	
Combined fraction 8	8	38	68	
Combined fraction 9	9	39	69	
Combined fraction 10	10	40	70	
Combined fraction 11	11	41	71	
Combined fraction 12	12	42	72	
Combined fraction 13	13	43	73	
Combined fraction 14	14	44	74	
Combined fraction 15	15	45	75	
Combined fraction 16	16	46	76	
Combined fraction 17	17	47	77	
Combined fraction 18	18	48	78	
Combined fraction 19	19	49	79	
Combined fraction 20	20	50	80	
Combined fraction 21	21	51	81	
Combined fraction 22	22	52	82	
Combined fraction 23	23	53	83	
Combined fraction 24	24	54	84	
Combined fraction 25	25	55	85	
Combined fraction 26	26	56	86	
Combined fraction 27	27	57	87	
Combined fraction 28	28	58	88	
Combined fraction 29	29	59	89	
Combined fraction 30	30	60	90	

The combination of 42 offline fractions by a concatenation scheme in phosphoproteome.

Phosphoproteome	Fraction No.	Fraction No.	Fraction No.
Combined fraction 1	1	21	41
Combined fraction 2	2	22	42
Combined fraction 3	3	23	
Combined fraction 4	4	24	
Combined fraction 5	5	25	
Combined fraction 6	6	26	
Combined fraction 7	7	27	
Combined fraction 8	8	28	
Combined fraction 9	9	29	
Combined fraction 10	10	30	
Combined fraction 11	11	31	
Combined fraction 12	12	32	
Combined fraction 13	13	33	
Combined fraction 14	14	34	
Combined fraction 15	15	35	
Combined fraction 16	16	36	
Combined fraction 17	17	37	
Combined fraction 18	18	38	
Combined fraction 19	19	39	
Combined fraction 20	20	40	

TableS3. The detail of DIA isolation windows with variable width for proteome were determined by DDA searching results from MaxQuant.

The distribution of peptide precursors in test DDA MS runs.

m/z	Peptide Precursor	Peptide Precursor % in total	Windows No	Isolation Window (m/z)
300-400	2654	5.54%		
400-500	7483	15.62%	10	29
500-600	9200	19.20%		
600-700	8263	17.25%		
700-800	6725	14.04%	11	28
800-900	4966	10.37%		
900-1000	3521	7.35%		
1000-1100	2361	4.93%	5	55
1100-1200	1389	2.90%		
1200-1300	750	1.57%		
1300-1400	411	0.86%	1	300
1400-1500	187	0.39%		
total	47910		27	

27 variable DIA windows for proteome DIA MS runs.

m/z (center)	t start (min)	t stop (min)	Isolation Window (m/z)	Window: left	Window: right
314.5	0	75	29	300	329
343.5	0	75	29	329	358
372.5	0	75	29	358	387
401.5	0	75	29	387	416
430.5	0	75	29	416	445
459.5	0	75	29	445	474
488.5	0	75	29	474	503
517.5	0	75	29	503	532
546.5	0	75	29	532	561
575.5	0	75	29	561	590
604	0	75	28	590	618
632	0	75	28	618	646
660	0	75	28	646	674
688	0	75	28	674	702
716	0	75	28	702	730
744	0	75	28	730	758
772	0	75	28	758	786
800	0	75	28	786	814
828	0	75	28	814	842
856	0	75	28	842	870
884	0	75	28	870	898
925.5	0	75	55	898	953
980.5	0	75	55	953	1008
1035.5	0	75	55	1008	1063
1090.5	0	75	55	1063	1118
1145.5	0	75	55	1118	1173
1323	0	75	300	1173	1473

TableS4. The detail of DIA isolation windows with variable width for phosphoproteome were determined by DDA searching results from MaxQuant.
The distribution of phosphopeptide precursors in test DDA MS runs.

m/z	Peptide Precursor	Phosphopeptide Precursor	Phospho %	Phosphopeptide Precursor % in total	Windows No	Isolation Window (m/z)
300-400	484	314	64.9%	1.3%		
400-500	2550	2010	78.8%	8.4%	2	46
500-600	3802	3218	84.6%	13.4%	4	24
600-700	3802	3324	87.4%	13.8%		
700-800	3637	3245	89.2%	13.5%	16	19
800-900	3956	3620	91.5%	15.1%		
900-1000	3263	3006	92.1%	12.5%	10	21
1000-1100	2533	2333	92.1%	9.7%		
1100-1200	1535	1427	93.0%	5.9%	2	99
1200-1300	944	880	93.2%	3.7%		
1300-1400	467	435	93.1%	1.8%		
1400-1500	237	223	94.1%	0.9%		
Total	27210	24035	88.3%		34	
400~1300 % in total	95.6%	96.0%				

34 variable DIA windows for phosphoproteome DIA MS runs

m/z (center)	t start (min)	t stop (min)	Isolation Window (m/z)	Window: left	Window: right
423	0	75	46	400	446
469	0	75	46	446	492
504	0	75	24	492	516
528	0	75	24	516	540
552	0	75	24	540	564
576	0	75	24	564	588
597.5	0	75	19	588	607
616.5	0	75	19	607	626
635.5	0	75	19	626	645
654.5	0	75	19	645	664
673.5	0	75	19	664	683
692.5	0	75	19	683	702
711.5	0	75	19	702	721
730.5	0	75	19	721	740
749.5	0	75	19	740	759
768.5	0	75	19	759	778
787.5	0	75	19	778	797
806.5	0	75	19	797	816
825.5	0	75	19	816	835
844.5	0	75	19	835	854
863.5	0	75	19	854	873
882.5	0	75	19	873	892
902.5	0	75	21	892	913
923.5	0	75	21	913	934
944.5	0	75	21	934	955
965.5	0	75	21	955	976
986.5	0	75	21	976	997
1007.5	0	75	21	997	1018
1028.5	0	75	21	1018	1039
1049.5	0	75	21	1039	1060
1070.5	0	75	21	1060	1081
1091.5	0	75	21	1081	1102
1151.5	0	75	99	1102	1201
1250.5	0	75	99	1201	1300

TableS5. Structural information of the proteome and phosphoproteome hybrid spectral library.

Proteome libraries

MS run No. for proteome libraries	DirectDIA library	Project-specific library	Sum
Cell line sample*	8	16 ^{&}	8
CN tissue sample	174	31	205
CP tissue sample	172	29	201
CT tissue sample	173	32	205
LM tissue sample	37	23	60
Mixed sample of four tissue types	/	4	4
Mixed sample of four tissue types (offline fraction)	/	30	30
Total MS run No.	564	149	713

Spectral library for proteome	DirectDIA library	Project-specific library	Hybird library	Pan Human Library [#]
Peptide Precursors	66,451	161,671	179,382	210,921
Protein Groups	4,931	11,126	11,510	12,567

Phosphoproteome libraries

MS run No. for phosphoproteome libraries	DirectDIA library	Project-specific library	Sum
Cell line sample*	8	8	16
CN tissue sample	139	33	172
CP tissue sample	139	19	158
CT tissue sample	195	28	223
LM tissue sample	38	15	53
Mixed sample of four tissue types	/	/	0
Mixed sample of four tissue types (offline fraction)	/	20	20
Total MS run No.	519	123	642

Spectral library for phosphoproteome	DirectDIA library	Project-specific library	Hybird library
Phosphopeptide Precursors	60,152	84,637	116,121
Phosphoprotein Groups	3,951	9,770	9,977

*Cell line sample: a total of 8 colorectal cell lines were used in library generation, including CCD 841 CoN, Caco2, colo205, HCT116, HT29, LOVO, SW48, and SW620.

[&]Two technical replicates were performed for each cell line sample

[#]Pan Human Library: a generic large-scale human assay library generated by ETH (Rosenberger *et al.* 2014)

TableS6. Number of peptides precursor and protein group for randomly selected 32 proteomic DIA runs.

Peptide precursor No. for randomly selected 32 protein DIA runs.

Name	Precursors_Pa n Human Library	Precursors_dir ectDIA	Precursors_dir ectDIA library	Precursors_Pr oject-specific library	Precursors_Hy brid library
Protein_CN_1	26157	49434	49170	64306	61823
Protein_CN_2	21042	42052	47017	54761	45943
Protein_CN_3	19186	35088	47508	65173	36134
Protein_CN_4	22867	45967	38093	40034	48233
Protein_CN_5	21267	40715	38567	46971	41745
Protein_CN_6	24269	44813	30804	32362	54235
Protein_CN_7	23341	43062	35313	39259	49439
Protein_CN_8	24446	44164	36278	44346	52874
Protein_CP_1	33608	54413	35323	37296	71941
Protein_CP_2	20916	41546	36151	37001	43263
Protein_CP_3	17487	40081	39659	43858	41778
Protein_CP_4	19243	38423	38516	44397	38022
Protein_CP_5	23548	46793	34404	33643	50548
Protein_CP_6	25378	45509	36170	38416	56494
Protein_CP_7	23727	42212	41300	44940	49858
Protein_CP_8	27016	50233	37899	45551	61848
Protein_CT_1	26802	44595	37273	50723	50680
Protein_CT_2	23204	42010	38953	52189	48986
Protein_CT_3	18988	39118	30824	39329	41452
Protein_CT_4	24318	44747	35366	46557	49661
Protein_CT_5	23271	42826	35253	45485	49042
Protein_CT_6	19158	38906	40959	58608	43376
Protein_CT_7	30344	48475	31235	40329	62836
Protein_CT_8	36397	52620	37372	47279	74024
Protein_LM_1	36472	53531	43448	56436	71538
Protein_LM_2	22719	39469	46176	68752	43263
Protein_LM_3	24722	47516	37467	49052	53634
Protein_LM_4	23694	41625	32531	45066	48242
Protein_LM_5	19484	35737	32979	37905	41847
Protein_LM_6	25133	40129	35578	46473	51215
Protein_LM_7	28976	48198	44718	53557	60922
Protein_LM_8	36061	51222	47017	64229	70901
mean	24789	44226	38416	47321	52056
median	23711	43613	37420	45518	49760
mean recovery rate	11.75%	/	57.81%	29.27%	29.02%
median recovery rate	11.24%	/	56.31%	28.15%	27.74%

Protein group No. for randomly selected 32 protein DIA runs.

Name	PGs_Pan Human Library	PGs_directDIA	PGs_directDIA library	PGs_Project- specific library	PGs_Hybrid library
Protein_CN_1	3709	4760	4336	5739	5325
Protein_CN_2	3249	4273	4175	5267	4544
Protein_CN_3	3205	4128	4262	5757	4430
Protein_CN_4	3657	4595	3697	4374	4884
Protein_CN_5	3361	4320	4035	5018	4457
Protein_CN_6	3662	4588	3542	4256	5256
Protein_CN_7	3569	4489	3718	4513	5025
Protein_CN_8	3706	4554	4014	5356	5254
Protein_CP_1	4107	4956	3757	4471	5779
Protein_CP_2	3378	4396	3781	4456	4615
Protein_CP_3	3243	4343	3879	4884	4662
Protein_CP_4	3183	4139	3911	5023	4358
Protein_CP_5	3697	4661	3641	4200	5088
Protein_CP_6	3726	4603	3763	4543	5442
Protein_CP_7	3626	4522	4067	4973	5226
Protein_CP_8	3838	4823	4027	5098	5543
Protein_CT_1	3794	4568	3842	5202	5001
Protein_CT_2	3780	4686	3915	5351	5423
Protein_CT_3	3344	4256	3600	4894	4581
Protein_CT_4	3762	4585	3757	5100	5107
Protein_CT_5	3660	4593	3779	5144	5053
Protein_CT_6	3371	4410	4062	5534	5011
Protein_CT_7	3964	4821	3642	4946	5600
Protein_CT_8	4162	4978	3827	5155	5901
Protein_LM_1	4157	4982	4105	5464	5832
Protein_LM_2	3549	4417	4230	5876	5021
Protein_LM_3	3740	4816	3939	5414	5490
Protein_LM_4	3628	4563	3666	5166	5192
Protein_LM_5	2906	3822	3410	4360	4414
Protein_LM_6	3604	4409	3798	5195	5264
Protein_LM_7	3549	4464	3943	4948	5123
Protein_LM_8	3998	4793	4181	5602	5625
mean	3621	4541	3884	5040	5110
median	3659	4566	3861	5099	5115
mean recovery rate	28.82%	/	78.78%	45.30%	44.40%
median recovery rate	29.11%	/	78.29%	45.83%	44.44%

