

Supplementary Table 1 Active ingredients information

No.	Molecule ID	Molecule Name	OB (%)	DL
1	MOL0028 79	Diop	43.59	0.39
2	MOL0004 49	Stigmasterol	43.83	0.76
3	MOL0003 58	beta-sitosterol	36.91	0.75
4	MOL0036 48	Inermin	65.83	0.54
5	MOL0004 22	kaempferol	41.88	0.24
6	MOL0044 92	Chrysanthemaxanthin	38.72	0.58
7	MOL0053 08	Aposiopoline	66.65	0.22
8	MOL0053 14	Celabenzine	101.88	0.49
9	MOL0053 17	Deoxyharringtonine	39.27	0.81
10	MOL0053 18	Dianthramine	40.45	0.2
11	MOL0053 20	arachidonate	45.57	0.2
12	MOL0053 21	Frutinone A	65.9	0.34
13	MOL0053 44	ginsenoside rh2	36.32	0.56
14	MOL0053 48	Ginsenoside-Rh4_qt	31.11	0.78

15	MOL0053 56	Girinimbin	61.22	0.31
16	MOL0053 57	Gomisin B	31.99	0.83
17	MOL0053 60	malkangunin	57.71	0.63
18	MOL0053 76	Panaxadiol	33.09	0.79
19	MOL0053 84	suchilactone	57.52	0.56
20	MOL0053 99	alexandrin_qt	36.91	0.75
21	MOL0054 01	ginsenoside Rg5_qt	39.56	0.79
22	MOL0007 87	Fumarine	59.26	0.83
23	MOL0002 73	(2R)-2-[(3S,5R,10S,13R,14R,16R,17R)-3,16-dihydroxy-4,4,10,13,14-pentamethyl-2,3,5,6,12,15,16,17-octahydro-1H-cyclopenta[a]phenanthren-17-yl]-6-methylhept-5-enoic acid	30.93	0.81
24	MOL0002 75	trametenolic acid	38.71	0.8
25	MOL0002 76	7,9(11)-dehydropachymic acid	35.11	0.81
26	MOL0002 79	Cerevisterol	37.96	0.77
27	MOL0002 80	(2R)-2-[(3S,5R,10S,13R,14R,16R,17R)-3,16-dihydroxy-4,4,10,13,14-pentamethyl-2,3,5,6,12,15,16,17-octahydro-1H-cyclopenta[a]ph	31.07	0.82

		enanthren-17-yl]-5-isopropyl-hex-5-enoic acid		
28	MOL0002 82	ergosta-7,22E-dien-3beta-ol	43.51	0.72
29	MOL0002 83	Ergosterol peroxide	40.36	0.81
30	MOL0002 85	(2R)-2-[(5R,10S,13R,14R,16R,17R)-16-hydroxy-3-keto-4,4,10,13,14-pentamethyl-1,2,5,6,12,15,16,17-octahydrocyclopenta[a]phenanthren-17-yl]-5-isopropyl-hex-5-enoic acid	38.26	0.82
31	MOL0002 87	3beta-Hydroxy-24-methylene-8-lanostene-21-oic acid	38.7	0.81
32	MOL0002 89	pachymic acid	33.63	0.81
33	MOL0002 90	Poricoic acid A	30.61	0.76
34	MOL0002 91	Poricoic acid B	30.52	0.75
35	MOL0002 92	poricoic acid C	38.15	0.75
36	MOL0002 96	hederagenin	36.91	0.75
37	MOL0003 00	dehydroeburicoic acid	44.17	0.83
38	MOL0000 72	8β-ethoxy atractylenolide III	35.95	0.21
39	MOL0000 49	3β-acetoxyatractylone	54.07	0.22
40	MOL0000 20	12-senecioid-2E,8E,10E-atractylentriol	62.4	0.22

41	MOL0000 22	14-acetyl-12-senecieryl-2E,8Z,10E-atractylol	63.37	0.3
42	MOL0000 21	14-acetyl-12-senecieryl-2E,8E,10E-atractylol	60.31	0.31
43	MOL0000 28	α -Amyrin	39.51	0.76
44	MOL0000 33	(3S,8S,9S,10R,13R,14S,17R)-10,13-dimethyl-17-[(2R,5S)-5-propan-2-yl]octan-2-yl]-2,3,4,7,8,9,11,12,14,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthren-3-ol	36.23	0.78
45	MOL0003 59	stigmasterol	36.91	0.75
46	MOL0043 28	naringenin	59.29	0.21
47	MOL0051 00	5,7-dihydroxy-2-(3-hydroxy-4-methoxyphenyl)chroman-4-one	47.74	0.27
48	MOL0058 15	Citromitin	86.9	0.51
49	MOL0058 28	nobiletin	61.67	0.52
50	MOL0048 06	euchrenone	30.29	0.57
51	MOL0048 64	5,7-dihydroxy-3-(4-methoxyphenyl)-8-(3-methylbut-2-enyl)chromone	30.49	0.41
52	MOL0049 85	icos-5-enoic acid	30.7	0.2
53	MOL0049 96	gadelaidic acid	30.7	0.2
54	MOL0048 05	(2S)-2-[4-hydroxy-3-(3-methylbut-2-enyl)phenyl]-8,8-dimethyl-2,3-dihydropyrano[2,	31.79	0.72

3-f]chromen-4-one				
55	MOL0048 14	Isotrifoliol	31.94	0.42
56	MOL0048 33	Phaseolinisoflavan	32.01	0.45
57	MOL0049 88	Kanzonol F	32.47	0.89
58	MOL0017 92	DFV	32.76	0.18
59	MOL0048 60	licorice glycoside E	32.89	0.27
60	MOL0048 82	Licocoumarone	33.21	0.36
61	MOL0049 05	3,22-Dihydroxy-11-oxo-delta(12)-oleanene -27-alpha-methoxycarbonyl-29-oic acid	34.32	0.55
62	MOL0049 35	Sigmoidin-B	34.88	0.41
63	MOL0049 78	2-[(3R)-8,8-dimethyl-3,4-dihydro-2H-pyran- no[6,5-f]chromen-3-yl]-5-methoxyphenol	36.21	0.52
64	MOL0049 45	(2S)-7-hydroxy-2-(4-hydroxyphenyl)-8-(3- methylbut-2-enyl)chroman-4-one	36.57	0.32
65	MOL0049 17	glycyroside	37.25	0.79
66	MOL0049 57	HMO	38.37	0.21
67	MOL0049 91	7-Acetoxy-2-methylisoflavone	38.92	0.26
68	MOL0048 84	Licoisoflavone B	38.93	0.55
69	MOL0049	6-prenylated eriodictyol	39.22	0.41

	89			
70	MOL0048 15	(E)-1-(2,4-dihydroxyphenyl)-3-(2,2-dimethylchromen-6-yl)prop-2-en-1-one	39.62	0.35
71	MOL0049 80	Inflacoumarin A	39.71	0.33
72	MOL0004 97	licochalcone a	40.79	0.29
73	MOL0049 24	(-)-Medicocarpin	40.99	0.95
74	MOL0050 13	18 α -hydroxyglycyrrhetic acid	41.16	0.71
75	MOL0050 08	Glycyrrhiza flavonol A	41.28	0.6
76	MOL0048 83	Licoisoflavone	41.61	0.42
77	MOL0038 96	7-Methoxy-2-methyl isoflavone	42.56	0.2
78	MOL0049 15	Eurycarpin A	43.28	0.37
79	MOL0049 66	3'-Hydroxy-4'-O-Methylglabridin	43.71	0.57
80	MOL0048 66	2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-6-(3-methylbut-2-enyl)chromone	44.15	0.41
81	MOL0049 48	Isoglycyrol	44.7	0.84
82	MOL0048 28	Glepidotin A	44.72	0.35
83	MOL0049 49	Isolicoflavonol	45.17	0.42
84	MOL0048	Glyasperin C	45.56	0.4

	11			
85	MOL0049 74	3'-Methoxyglabridin	46.16	0.57
86	MOL0049 11	Glabrene	46.27	0.44
87	MOL0048 98	(E)-3-[3,4-dihydroxy-5-(3-methylbut-2-enyl)phenyl]-1-(2,4-dihydroxyphenyl)prop-2-en-1-one	46.27	0.31
88	MOL0000 98	quercetin	46.43	0.28
89	MOL0049 61	Quercetin der.	46.45	0.33
90	MOL0004 17	Calycosin	47.75	0.24
91	MOL0049 13	1,3-dihydroxy-9-methoxy-6-benzofurano[3,2-c]chromenone	48.14	0.43
92	MOL0048 27	Semilicoisoflavone B	48.78	0.55
93	MOL0048 57	Gancaonin B	48.79	0.45
94	MOL0025 65	Medicarpin	49.22	0.34
95	MOL0048 48	licochalcone G	49.25	0.32
96	MOL0003 54	isorhamnetin	49.6	0.31
97	MOL0050 16	Odoratin	49.95	0.3
98	MOL0050 01	Gancaonin H	50.1	0.78

99	MOL0048 20	kanzonols W	50.48	0.52
100	MOL0002 39	Jaranol	50.83	0.29
101	MOL0048 56	Gancaonin A	51.08	0.4
102	MOL0036 56	Lupiwighteone	51.64	0.37
103	MOL0048 85	licoisoflavanone	52.47	0.54
104	MOL0049 12	Glabrone	52.51	0.5
105	MOL0048 79	Glycyrin	52.61	0.47
106	MOL0049 10	Glabranin	52.9	0.31
107	MOL0049 08	Glabridin	53.25	0.47
108	MOL0049 93	8-prenylated eriodictyol	53.79	0.4
109	MOL0050 20	dehydroglyasperins C	53.82	0.37
110	MOL0050 18	Xambioona	54.85	0.87
111	MOL0002 11	Mairin	55.38	0.78
112	MOL0050 12	Licoagroisoflavone	57.28	0.49
113	MOL0048 38	8-(6-hydroxy-2-benzofuranyl)-2,2-dimethyl-5-chromenol	58.44	0.38

114	MOL0050 03	Licoagrocarpin	58.81	0.58
115	MOL0048 49	3-(2,4-dihydroxyphenyl)-8-(1,1-dimethylprop-2-enyl)-7-hydroxy-5-methoxy-coumarin	59.62	0.43
116	MOL0048 24	(2S)-6-(2,4-dihydroxyphenyl)-2-(2-hydroxypropan-2-yl)-4-methoxy-2,3-dihydrofuro[3,2-g]chromen-7-one	60.25	0.63
117	MOL0050 00	Gancaonin G	60.44	0.39
118	MOL0049 07	Glyzaglabrin	61.07	0.35
119	MOL0048 35	Glypallichalcone	61.6	0.19
120	MOL0049 14	1,3-dihydroxy-8,9-dimethoxy-6-benzofurano[3,2-c]chromenone	62.9	0.53
121	MOL0048 55	Licoricone	63.58	0.47
122	MOL0048 29	Glepidotin B	64.46	0.34
123	MOL0048 08	glyasperin B	65.22	0.44
124	MOL0049 03	liquiritin	65.69	0.74
125	MOL0048 63	3-(3,4-dihydroxyphenyl)-5,7-dihydroxy-8-(3-methylbut-2-enyl)chromone	66.37	0.41
126	MOL0003 92	formononetin	69.67	0.21
127	MOL0049 59	1-Methoxyphaseollidin	69.98	0.64

128	MOL0049 41	(2R)-7-hydroxy-2-(4-hydroxyphenyl)chro man-4-one	71.12	0.18
129	MOL0050 07	Glyasperins M	72.67	0.59
130	MOL0005 00	Vestitol	74.66	0.21
131	MOL0014 84	Inermine	75.18	0.54
132	MOL0048 10	glyasperin F	75.84	0.54
133	MOL0048 41	Licochalcone B	76.76	0.19
134	MOL0050 17	Phaseol	78.77	0.58
135	MOL0048 91	shinpterocarpin	80.3	0.73
136	MOL0049 04	licopyranocoumarin	80.36	0.65
137	MOL0049 90	7,2',4'-trihydroxy — 5-methoxy-3 — arylcoumarin	83.71	0.27
138	MOL0023 11	Glycyrol	90.78	0.67

Supplementary Table 2 Common targets information

Number	Target name	Number	Target name	Number	Target name
1	ADH1C	20	CXCL2	39	MMP9
2	ADRA2A	21	CYP19A1	40	MPO
3	AKR1B1	22	CYP1B1	41	NOS2
4	AKR1C1	23	DUOX2	42	NR1I2
5	AKR1C3	24	E2F1	43	NR3C2
6	BIRC5	25	EGFR	44	OLR1
7	CA2	26	EPHB2	45	PCOLCE
8	CCL2	27	GJA1	46	PDE3A
9	CCNA2	28	GSTM2	47	PLAU
10	CDK1	29	HMOX1	48	PTGER3
11	CDKN2A	30	HTR2A	49	SELE
12	CHRM1	31	ICAM1	50	SERPINE1
13	CHRM2	32	IFNG	51	SPP1
14	CHRM3	33	IGF2	52	TGFB1
15	CHRNA7	34	IGFBP3	53	TIMP1
16	CLDN4	35	IL1A	54	TOP2A
17	COL1A1	36	IL6	55	VCAM1
18	COL3A1	37	MAOA		
19	CXCL10	38	MMP2		

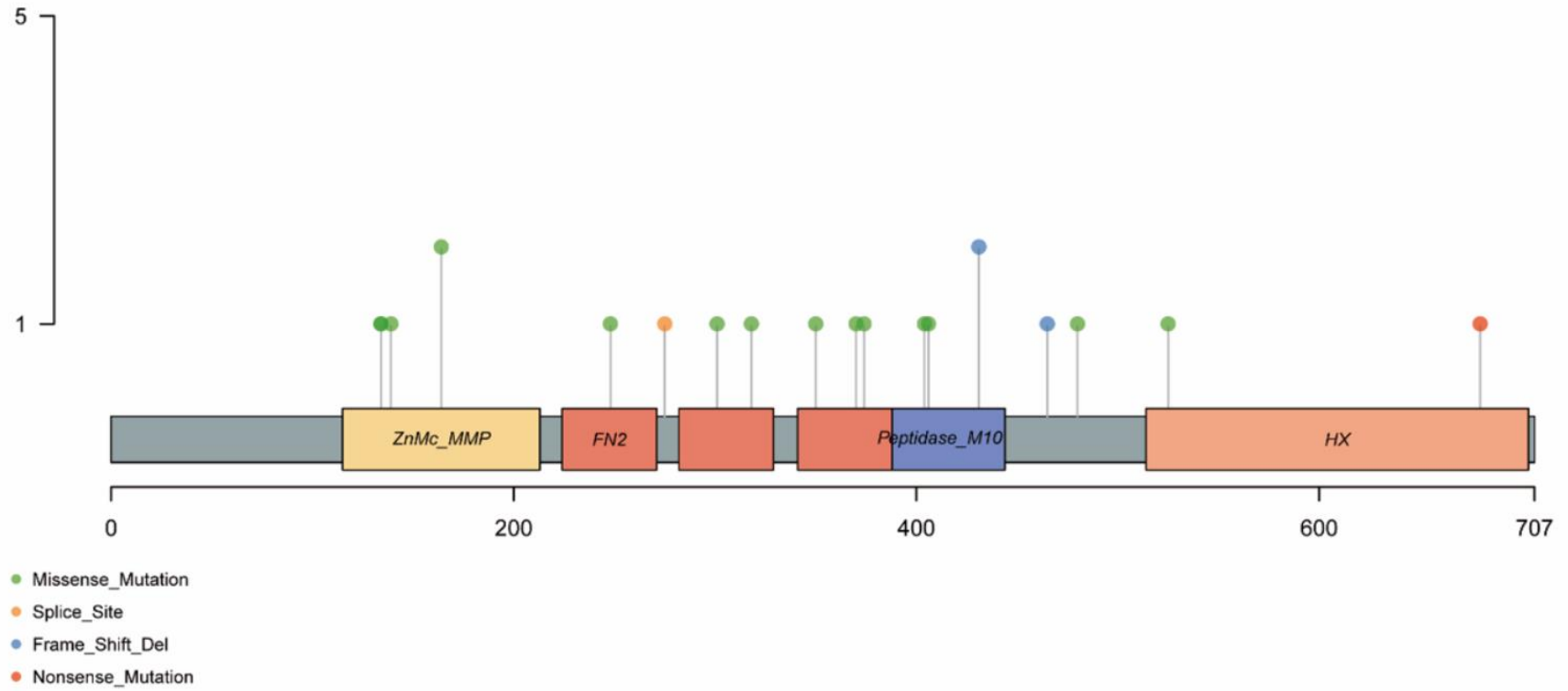
Supplementary Table 3 Immunohistochemical antibody and patient information

Gene	Antibody	Gender	Age	Organ	Sampling site	Patient ID
IL6-Normal	CAB023406	Female	56	Stomach, (T-62350)	upper Normal tissue NOS (M-00100)	2130
IL6-Cancer	CAB023406	Female	73	Stomach (T-63000)	Adenocarcinoma (M-81403)	NOS 2557
MMP2-Normal	CAB002788	Female	56	Stomach, (T-62350)	upper Normal tissue NOS (M-00100)	2130
MMP2-Cancer	CAB002788	Male	62	Stomach (T-63000)	Adenocarcinoma (M-81403)	NOS 2105
MMP9-Normal	CAB068199	Female	57	Stomach (T-63000)	Normal tissue NOS (M-00100)	1467
MMP9-Cancer	CAB068199	Female	71	Stomach, (T-63700)	lower Adenocarcinoma (M-81403)	NOS 1061
EGFR-Normal	HPA001200	Male	76	Stomach, (T-62350)	upper Normal tissue NOS (M-00100)	2066
EGFR-Cancer	HPA001200	Female	50	Stomach, (T-62350)	upper Adenocarcinoma (M-81403)	NOS 664
TGFB1-Normal	CAB000361	Female	56	Stomach,	upper Normal tissue NOS (M-00100)	2130

TGFB1-Cancer	CAB000361	Female	50	(T-62350) Stomach, (T-62350)	upper	Adenocarcinoma (M-81403)	NOS	664
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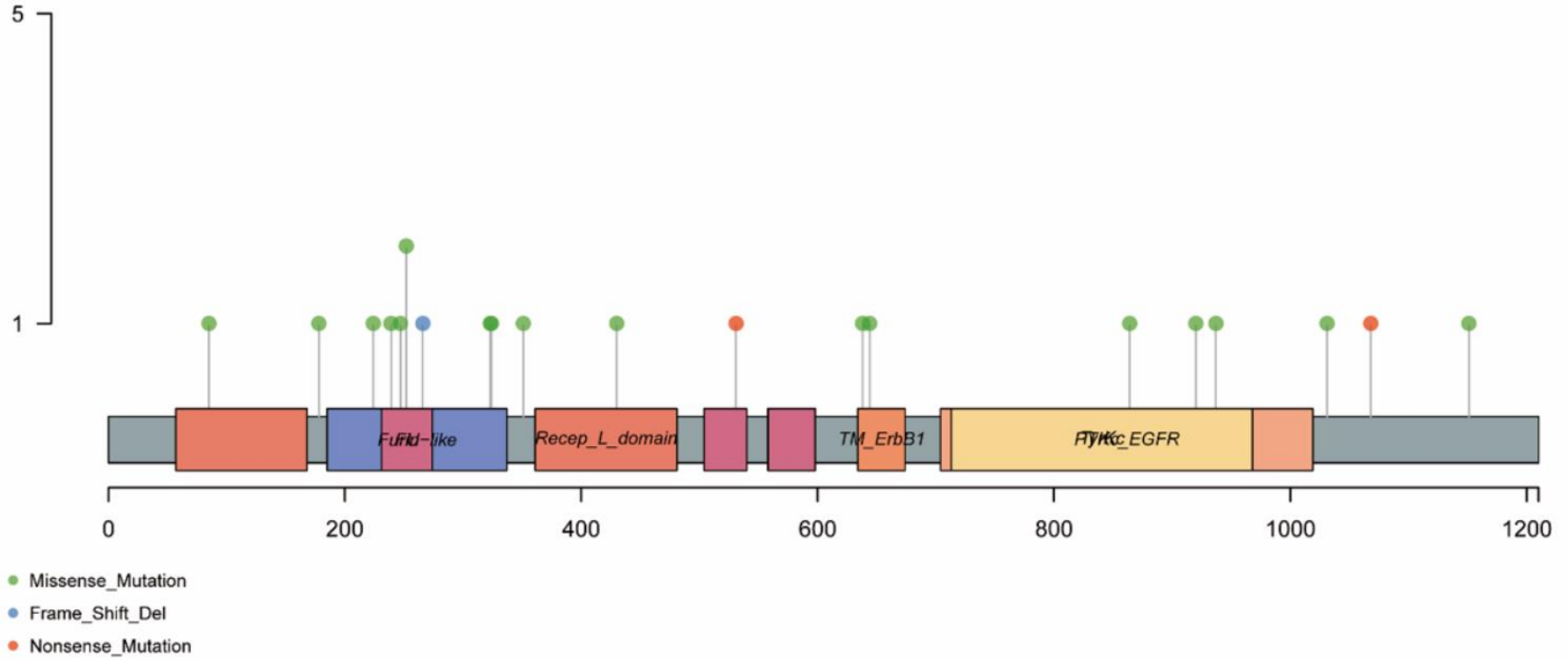
A

MMP9 : [Somatic Mutation Rate: 3.87%]
NM_004994

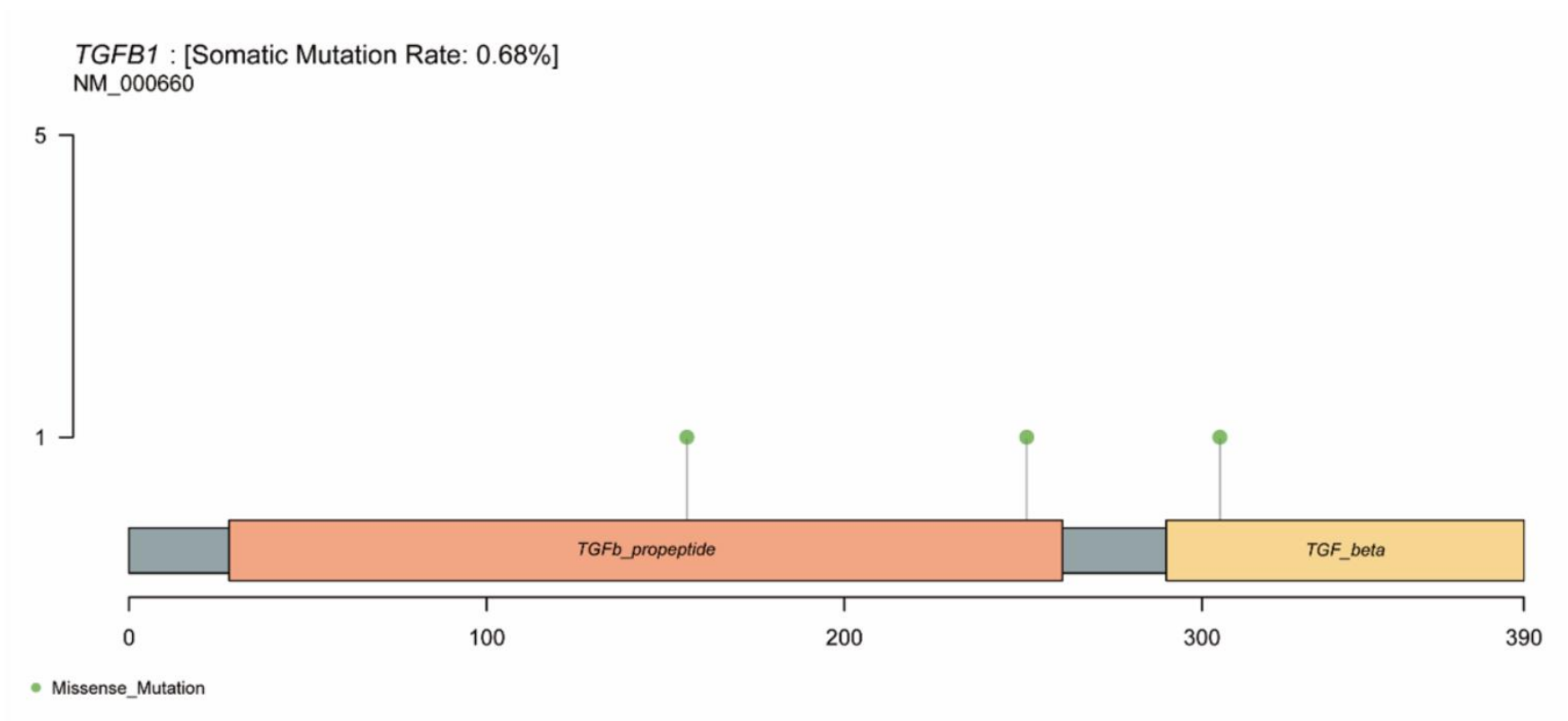


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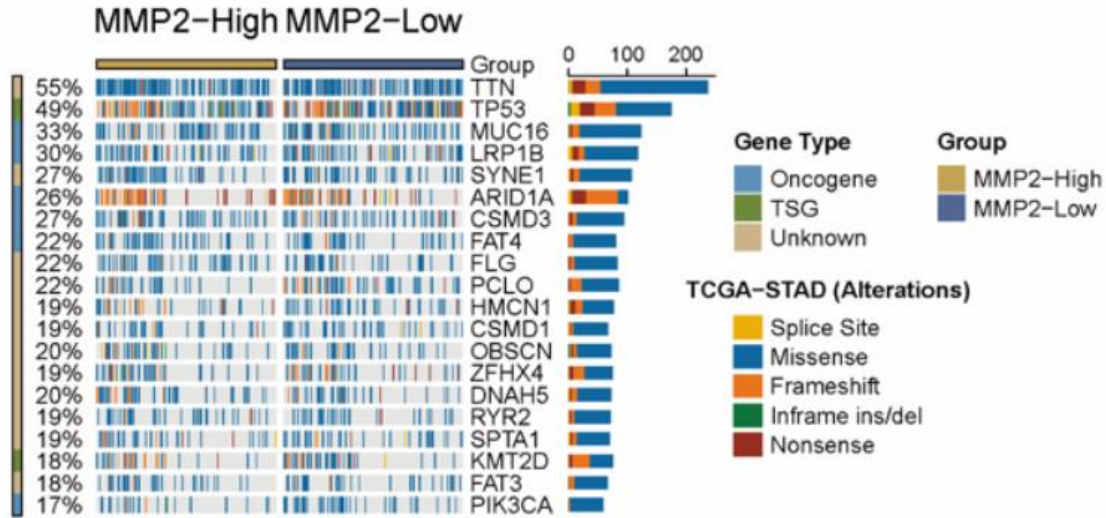
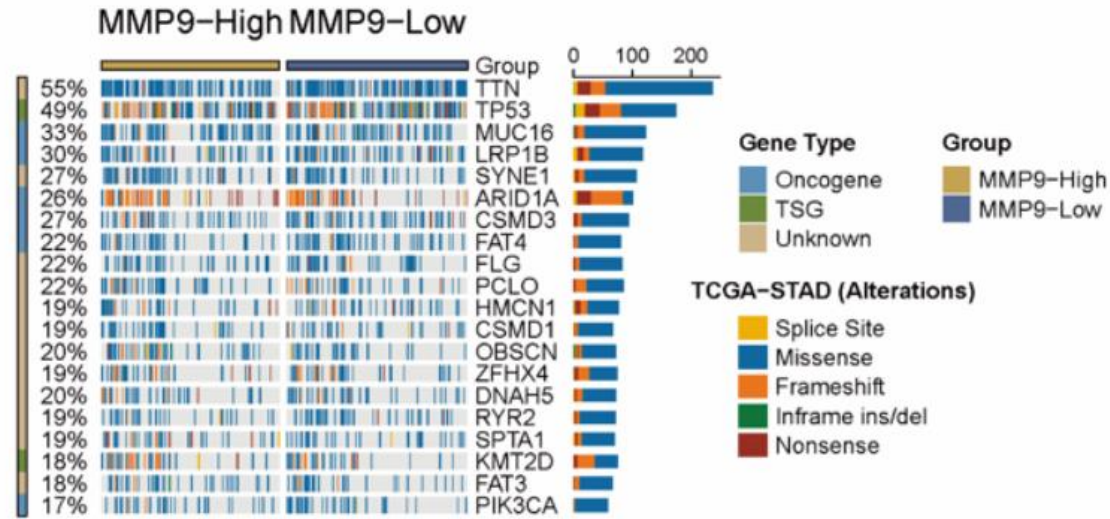
EGFR : [Somatic Mutation Rate: 4.78%]
NM_005228

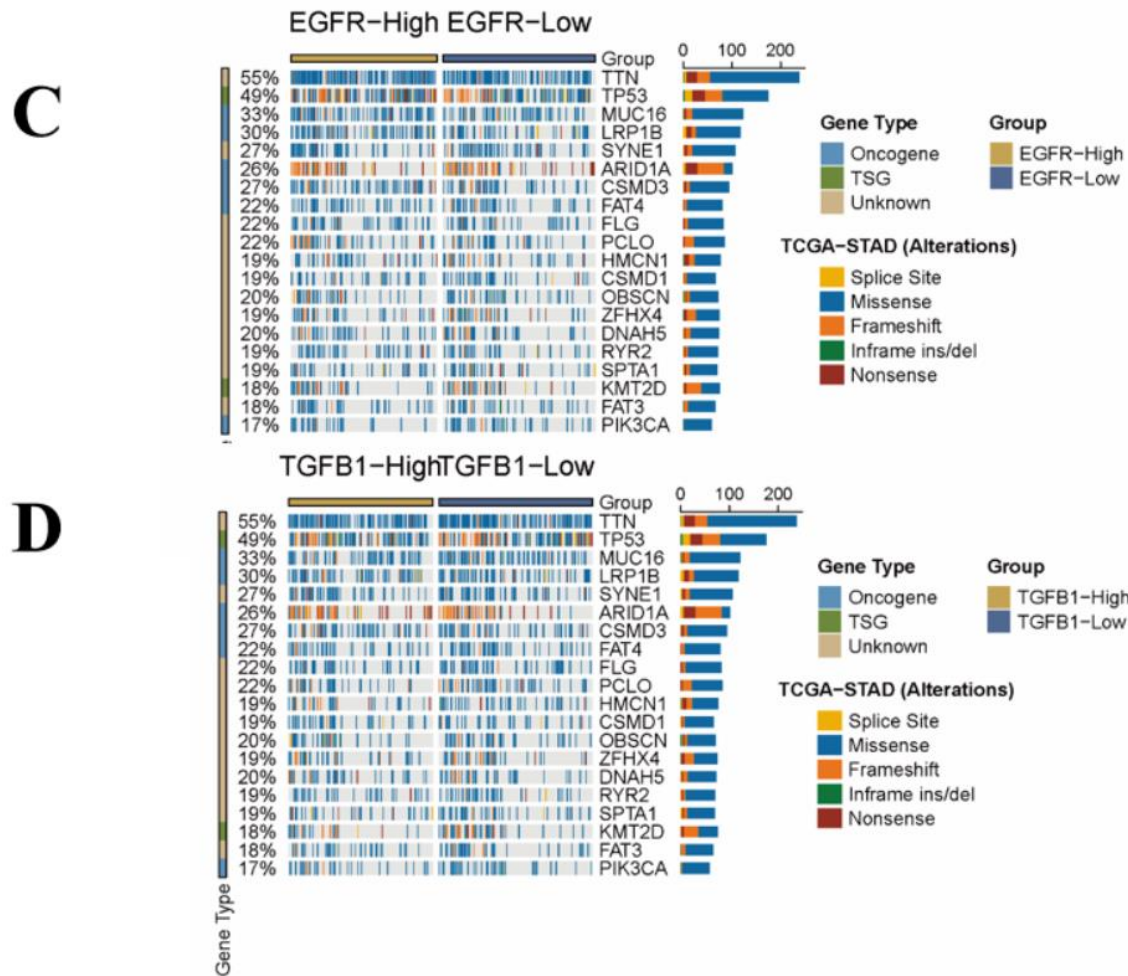


C



Supplementary Figure 1 Single nucleotide site mutations (SNVs) mutation sites and types of hub genes. A: *MMP9*; B: *EGFR*; C: *TGFB1*.

A**B**



Supplementary Figure 2 Mutational associations of driver genes with the hub genes. A: *MMP2*; B: *MMP9*; C: *EGFR*; D: *TGFB1*.