

Table S1

case number	IDH status	mutation type	m/z	signal/noise	intensity	TIC	I/TIC	concentration [mM]		diameter [mm]	diagnosis	WHO grade	comments
								mean	stdev				
1	wildtype	n.d.	147,028	4	2016	28546798	7,06E-05	0,205	0,01	0,8	Schwannoma	I	
2	wildtype	n.d.	147,032	2	1186	68980951	1,72E-05	0,199	0,01	0,5	Schwannoma	I	
3	wildtype	IDH1/2 WT	147,044	5	2545	38324126	6,64E-05	0,199	0,06	5,0	PA	I	
4	wildtype	n.d.	147,040	6	3091	60155586	5,14E-05	0,127	0,01	0,7	Schwannoma	I	
5	wildtype	n.d.	147,040	5	2860	65314306	4,38E-05	0,071	0,03	0,6	Schwannoma	I	
6	wildtype	n.d.	147,031	4	2386	65452931	3,65E-05	0,073	0,00	0,7	Schwannoma	I	
7	wildtype	n.d.	147,025	5	2913	47863525	6,09E-05	0,137	0,02	0,4	Schwannoma	I	
8	wildtype	n.d.	147,250	7	3828	47380043	8,08E-05	0,092	0,01	0,5	Schwannoma	I	
9	wildtype	n.d.	147,051	5	3806	60897595	6,25E-05	0,123	0,02	0,7	Schwannoma	I	
10	wildtype	IDH1/2 WT	147,027	n.a	943	63507992	1,48E-05	-0,124	0,09	4,0	CNS-tissue	n.d.	post removal of brain metastasis of NSCLC
11	wildtype	IDH1/2 WT	147,053	n.a	3822	77954962	4,90E-05	0,050	0,07	4,0	GBM, IDH-wildtype	IV	
12	wildtype	IDH1/2 WT	147,039	8	5382	58334631	9,23E-05	0,093	0,02	3,0	GBM, IDH-wildtype	IV	
13	wildtype	IDH1/2 WT	147,044	6	3028	58895052	5,14E-05	-0,014	0,13	5,0	GBM, IDH-wildtype	IV	recurrent
14	wildtype	IDH1/2 WT	147,035	2	1577	55349373	2,85E-05	0,005	0,06	5,0	GBM, IDH-wildtype	IV	
15	wildtype	IDH1/2 WT	147,040	6	3964	78153046	5,07E-05	0,302	0,07	5,0	GBM, IDH-wildtype	IV	
16	wildtype	IDH1/2 WT	147,037	6	4260	60980504	6,99E-05	0,152	0,13	5,0	GBM, IDH-wildtype	IV	
17	wildtype	IDH1/2 WT	147,037	4	2431	55031200	4,42E-05	0,189	0,13	10,0	GBM, IDH-wildtype	IV	
18	wildtype	n.d.	147,042	3	1563	52592945	2,97E-05	0,179	0,01	0,5	Schwannoma	I	
19	wildtype	n.d.	147,044	4	2034	53058169	3,83E-05	0,219	0,03	0,5	Schwannoma	I	
20	wildtype	IDH1/2 WT	147,040	4	1928	55785640	3,46E-05	0,205	0,02	0,8	GBM, IDH-wildtype	IV	recurrent
21	wildtype	n.d.	147,049	6	4806	103763061	4,63E-05	0,138	0,01	1,5	Schwannoma	I	
22	wildtype	IDH1/2 WT	147,048	2	2233	81158333	2,75E-05	0,196	0,02	0,6	GBM, IDH-wildtype	IV	
23	wildtype	IDH1/2 WT	147,039	n.a	558	91891355	6,07E-06	0,381	0,02	0,5	GBM, IDH-wildtype	IV	
24	wildtype	n.d.	147,047	5	4811	60624503	7,94E-05	0,186	0,01	8,0	mamma carcinoma	n.d.	brain metastasis
25	wildtype	IDH1/2 WT	147,051	6	6963	79431637	8,77E-05	0,166	0,01	4,0	Ganglioglioma	I	
26	wildtype	IDH1/2 WT	147,044	3	1947	49104572	3,97E-05	-0,032	0,12	3,0	GBM, IDH-wildtype	IV	
27	wildtype	n.d.	147,028	4	1791	25277191	7,09E-05	0,245	0,01	1,0	Schwannoma	I	
28	wildtype	n.d.	147,028	4	2144	32752104	6,55E-05	0,133	0,01	0,8	Schwannoma	I	
IDH WT	wildtype	IDH1/2 WT	n.a	n.a	n.a	n.a	n.a	n.a	n.a	3,0	CNS-tissue with reactive changes	n.d.	post removal of brain metastasis of NSCLC; used as IDH WT test tissue
29	mutant	IDH1 R132C	147,022	36	40512	135854699	2,98E-04	1,835	0,05	3,0	DA, IDH-mutant	II	
30	mutant	IDH1 R132S	147,022	15	12114	43109658	2,81E-04	1,861	0,08	3,0	GBM, IDH-mutant	IV	
31	mutant	IDH1 R132H	147,030	20	18201	66766186	2,73E-04	0,929	0,03	5,0	DA, IDH-mutant	II	
32	mutant	IDH1 R132H	147,024	155	114446	81108146	1,41E-03	8,248	0,09	7,0	O, IDH-mutant	II	
33	mutant	IDH1 R132H	147,025	27	23149	51931875	4,46E-04	2,483	0,05	4,0	DA, IDH-mutant	II	
34	mutant	IDH2 R172S	147,045	105	100791	82013716	1,23E-03	10,888	0,07	2,0	AA, IDH-mutant	III	
35	mutant	IDH2 R172K	147,026	176	108533	62437245	1,74E-03	10,327	0,28	4,0	O, IDH-mutant	II	
36	mutant	IDH1 R132H	147,019	96	63516	55198583	1,15E-03	6,030	0,01	3,5	AO, IDH-mutant	III	
37	mutant	IDH1 R132G	147,033	73	49540	77233864	6,41E-04	5,916	0,01	3,5	DA, IDH-mutant	II	
38	mutant	IDH1 R132H	147,052	59	37592	74163194	5,07E-04	6,085	0,48	2,5	DA, IDH-mutant	II	
39	mutant	IDH1 R132H	147,035	37	31468	82834763	3,80E-04	0,836	0,04	4,0	DA, IDH-mutant	II	
40	mutant	IDH1 R132H	147,023	40	30460	97772018	3,12E-04	1,700	0,10	3,5	DA, IDH-mutant	II	
41	mutant	IDH1 R132H	147,043	20	15069	77395588	1,95E-04	0,822	0,03	3,0	AA, IDH-mutant	III	
42	mutant	IDH1 R132H	147,025	25	20651	77395588	2,67E-04	2,076	0,11	4,0	O, IDH-mutant	II	
43	mutant	IDH1 R132H	147,042	42	21363	47273930	4,52E-04	5,625	0,10	4,0	AA, IDH-mutant	III	
44	mutant	IDH1 R132H	147,012	78	44614	40859217	1,09E-03	8,211	0,07	6,0	DA, IDH-mutant	II	
45	mutant	IDH1 R132H	147,017	34	19733	44756867	4,41E-04	3,956	0,00	3,0	AA, IDH-mutant	III	
46	mutant	IDH1 R132H	147,011	136	95951	47218496	2,03E-03	6,513	0,06	6,0	DA, IDH-mutant	II	
47	mutant	IDH2 R172K	147,017	244	160500	39765170	4,04E-03	7,718	0,03	3,5	DA, IDH-mutant	II	
48	mutant	IDH2 R172M	147,017	212	80931	16499557	4,91E-03	7,067	0,10	3,5	O, IDH-mutant	II	
49	mutant	IDH1 R132H	147,029	39	18018	53399393	3,37E-04	3,781	0,03	3,0	DA, IDH-mutant	II	
50	mutant	IDH1 R132H	147,021	34	23379	70721892	3,31E-04	5,263	0,20	2,0	AO, IDH-mutant	III	
51	mutant	IDH1 R132H	147,035	31	22517	72943304	3,09E-04	5,129	0,01	3,0	O, IDH-mutant	II	
52	mutant	IDH1 R132H	147,024	29	18186	39943127	4,55E-04	1,502	0,08	5,0	AO, IDH-mutant	III	
53	mutant	IDH1 R132H	147,035	21	12071	45173193	2,67E-04	0,839	0,07	2,0	O, IDH-mutant	II	
54	mutant	IDH1 R132H	147,043	41	52076	10454407	4,98E-03	2,974	0,15	3,0	O, IDH-mutant	II	
IDH mutant	mutant	IDH1 R132H	n.a	n.a	n.a	n.a	n.a	n.a	n.a	4,0	DA, IDH-mutant	II	used as IDH mutant test tissue