SELF-ORGANIZING MAP CLASSIFICATION MODEL FOR THE PREDICTION OF MEK1 INHIBITORS

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SUPPORTING INFORMATION

Table S1

Description of the MEK1 inhibitors used for training and testing of the SOM model

Name	SMILES	BMF ID	IC50 (nM)	Training/ Test
CHEMBL151430	c1c([nH+]c([nH]1)N)C2CCNC(=O)c3c2c(c([nH]3)Br)Br	21	6	training
CHEMBL1614701	Cn1cnc2c1cc(c(c2F)Nc3ccc(cc3Cl)Br)C(=O)NOCCO	28	80	test
CHEMBL1668411	CC1CC=CC(=O)C(C(CC=Cc2cc(cc(c2C(=O)O1)[O-])OC)O)O	30	620	training
CHEMBL1956073	CC(c1ccccc1)C(C(=O)Nc2ccc(cc2F)I)N3C(=O)C(NC3=O)c4ccc(cc4)OCC(CO)O	15	32	training
CHEMBL199749	Cn1cc(c(cc1=O)Nc2ccc(cc2F)Br)C(=O)NOCCO	4	100	test
CHEMBL199774	Cn1cc(c(c(c1=O)Cl)Nc2ccc(cc2F)Br)C(=O)NOCCO	4	85	training
CHEMBL199860	Cc1c(c(cn(c1=O)C)C(=O)NOCCO)Nc2ccc(cc2F)Br	4	230	training
CHEMBL201156	Cn1cc(c(c(c1=O)F)Nc2ccc(cc2F)Br)C(=O)NOC	4	940	training
CHEMBL201379	Cn1cc(c(c(c1=O)Cl)Nc2ccc(cc2F)Br)C(=O)NOCC3CC3	10	740	test
CHEMBL201417	Cn1cc(c(cc1=O)Nc2ccc(cc2F)Br)C(=O)NOCC3CC3	10	44	test
CHEMBL201426	CCONC(=O)c1cn(c(=O)c(c1Nc2ccc(cc2F)Br)F)C	4	44	training
CHEMBL201629	Cn1cc(c(c(c1=O)F)Nc2ccc(cc2F)Br)C(=O)NOCC3CC3	10	86	test
CHEMBL201630	Cc1c(c(cn(c1=O)C)C(=O)NOCC2CC2)Nc3ccc(cc3F)Br	10	420	test
CHEMBL201691	CNC(=O)c1cn(c(=O)c(c1Nc2ccc(cc2F)Br)F)C	4	53	training
CHEMBL203138	CCONC(=O)c1cn(c(=O)c(c1Nc2ccc(cc2F)Br)C)C	4	110	training
CHEMBL203258	Cn1cc(c(c(c1=O)F)Nc2ccc(cc2F)Br)C(=O)NO	4	240	training
CHEMBL203417	Cn1cc(c(c(c1=O)F)Nc2ccc(cc2F)Br)C(=O)[O-]	4	60	training
CHEMBL209502	Cc1ccc(c(c1)C)Nc2c(c(ns2)O)C(=[NH2+])NCC3CCCCC3	6	137	training
CHEMBL209845	c1cc(c(cc1Cl)Nc2c(c(ns2)O)C#N)Cl	3	48	training
CHEMBL209868	CC(C)[NH+]=C(c1c(nsc1Nc2ccc(cc2)I)O)N	3	23	training
CHEMBL2103875	Cc1c2c(c(n(c1=O)C)Nc3ccc(cc3F)I)c(=O)n(c(=O)n2c4cccc(c4)NC(=O)C)C5CC5	23	15	training
CHEMBL211201	Cc1cc(ccc1Nc2c(c(ns2)O)C(=[NH+]C(C)CO)N)I	3	25	training
CHEMBL211359	Cc1cc(ccc1Nc2c(c(ns2)O)C(=[NH+]C(C)C)N)I	3	2	training
CHEMBL212110	c1cc(ccc1Nc2c(c(ns2)O)C(=[NH+]CC3CCCCC3)N)Br	6	207	training
CHEMBL212214	c1cc(cc(c1)Br)Nc2c(c(ns2)O)C#N	3	660	test
CHEMBL212305	c1cc(c(cc1Nc2c(c(ns2)O)C#N)C(F)(F)F)Cl	3	800	test
CHEMBL212474	c1c(cc(cc1Cl)Cl)Nc2c(c(ns2)O)C#N	3	253	training
CHEMBL212480	Cc1ccc(cc1)Nc2c(c(ns2)O)C(=[NH2+])NCC3CCCCC3	6	85	training

CHEMBL213167	CC(CO)[NH+]=C(c1c(nsc1Nc2ccc(cc2Cl)I)O)N	3	34	training
CHEMBL213168	CC(CO)[NH+]=C(c1c(nsc1Nc2ccc(cc2Cl)C(F)(F)F)O)N	3	44	training
CHEMBL213563	c1cc(ccc1Nc2c(c(ns2)O)C(=[NH+]CC3CCCCC3)N)Cl	6	37	training
CHEMBL213651	CC(C)[NH+]=C(c1c(nsc1Nc2cccc(c2Cl)Cl)O)N	3	30	training
CHEMBL213992	CC(C)[NH+]=C(c1c(nsc1Nc2ccc(cc2Cl)I)O)N	3	94.33	training
CHEMBL214032	CC(CO)[NH+]=C(c1c(nsc1Nc2ccc(cc2)Oc3cccc(c3Cl)Cl)O)N	1	30	training
CHEMBL214425	CC(CO)[NH+]=C(c1c(nsc1Nc2ccc(cc2)Oc3cc(ccc3Cl)F)O)N	1	8	training
CHEMBL214587	c1cc(ccc1Nc2c(c(ns2)O)C(=NCC[NH+]3CCOCC3)N)Oc4cc(ccc4Cl)Cl	9	13	training
CHEMBL214613	CC(CO)[NH+]=C(c1c(nsc1Nc2ccc(cc2)Oc3cccc(c3F)F)O)N	1	450	test
CHEMBL214614	CC(CO)[NH+]=C(c1c(nsc1Nc2ccc(c(c2)Cl)Oc3cccc(c3Cl)Cl)O)N	1	14	test
CHEMBL214636	c1cc(ccc1Nc2c(c(ns2)O)C(=[NH+]CCC[NH+]3CCOCC3)N)Oc4cc(ccc4Cl)Cl	20	96	training
CHEMBL214683	c1cc(ccc1Nc2c(c(ns2)O)C(=NCCN3CC[NH2+]CC3)N)Oc4cc(ccc4Cl)Cl	9	16	training
CHEMBL214734	CC(CO)[NH+]=C(c1c(nsc1Nc2ccc(cc2)Oc3cc(cc(c3)Cl)Cl)O)N	1	9.3	test
CHEMBL214816	CC(CO)[NH+]=C(c1c(nsc1Nc2ccc(cc2)Oc3ccc(cc3Cl)Cl)O)N	1	38	training
CHEMBL214901	c1cc(ccc1Nc2c(c(ns2)O)C(=N[NH+]3CCOCC3)N)Oc4cc(ccc4Cl)Cl	12	22	test
CHEMBL214977	CN1CC[NH+](CC1)CCN=C(c2c(nsc2Nc3ccc(cc3)Oc4cc(ccc4Cl)Cl)O)N	9	26	training
CHEMBL215011	CC(CO)[NH+]=C(c1c(nsc1Nc2ccc(cc2)Oc3cc(cc(c3)F)F)O)N	1	350	training
CHEMBL215012	CC(CO)[NH+]=C(c1c(nsc1Nc2ccc(cc2)Oc3ccc(cc3Cl)F)O)N	1	68	training
CHEMBL215038	CC(CO)[NH+]=C(c1c(nsc1Nc2ccc(cc2)Oc3cc(cc(c3Cl)F)F)O)N	1	500	training
CHEMBL215193	CC(CO)[NH+]=C(c1c(nsc1Nc2ccc(cc2)Oc3cc(ccc3Cl)Cl)O)N	1	670	training
CHEMBL216201	CC(C)C(CO)[NH+]=C(c1c(nsc1Nc2ccc(cc2)Oc3cc(ccc3Cl)Cl)O)N	1	500	training
CHEMBL216325	c1cc(ccc1Nc2c(c(ns2)O)C(=[NH+]C(CO)CO)N)Oc3cc(ccc3Cl)Cl	1	790	training
CHEMBL216449	c1cc(ccc1Nc2c(c(ns2)O)C(=[NH+]CC3CCCO3)N)Oc4cc(ccc4Cl)Cl	26	21	test
CHEMBL216500	CC(C)[NH+]=C(c1c(nsc1Nc2ccc(c(c2)Cl)I)O)N	3	100	training
CHEMBL216832	c1cc(ccc1Nc2c(c(ns2)O)C(=NCC[NH+]3CCNC(=O)C3)N)Oc4cc(ccc4Cl)Cl	9	182	training
CHEMBL216833	c1cc(ccc1Nc2c(c(ns2)O)C(=[NH+]CCO)N)Oc3cc(ccc3Cl)Cl	1	410	training
CHEMBL217117	CC(CO)[NH+]=C(c1c(nsc1Nc2ccc(cc2)S(=O)(=O)c3ccccc3)O)N	1	34	training
CHEMBL217126	CC(CO)[NH+]=C(c1c(nsc1Nc2ccc(c(c2)Cl)Oc3cccc(c3Cl)C(F)(F)F)O)N	1	46	training
CHEMBL217130	CC(CO)[NH+]=C(c1c(nsc1Nc2ccc(cc2)C(=O)c3ccccc3)O)N	1	107	training
CHEMBL217310	CC(CO)[NH+]=C(c1c(nsc1Nc2ccc(cc2)Cc3ccccc3)O)N	1	40	training
CHEMBL217355	CC(CO)[NH+]=C(c1c(nsc1Nc2ccc(cc2)Oc3cc(ccc3Cl)C(F)(F)F)O)N	1	145	test
CHEMBL217414	CC(CO)[NH+]=C(c1c(nsc1Nc2ccc(c(c2)F)Oc3cccc(c3Cl)C(F)(F)F)O)N	1	26	training
CHEMBL217415	CC(CO)[NH+]=C(c1c(nsc1Nc2ccc(cc2)Oc3cc(ccc3F)C(F)(F)F)O)N	1	250	training
CHEMBL217416	Cc1cc(ccc1Oc2cc(ccc2Cl)F)Nc3c(c(ns3)O)C(=[NH+]C(C)CO)N	1	28	training
CHEMBL217832	CC(CO)[NH+]=C(c1c(nsc1Nc2ccc(cc2)Oc3cccc(c3F)C(F)(F)F)O)N	1	45	training
CHEMBL217833	CC(CO)[NH+]=C(c1c(nsc1Nc2ccc(cc2)Oc3cccc(c3Cl)C(F)(F)F)O)N	1	298	training
CHEMBL2335185	c1cc(c(cc1Cl)F)Nc2c(ccc(c2F)F)C(=O)NOCCO	4	110	training
CHEMBL2335186	c1cc(c(cc1Br)F)Nc2c(ccc(c2F)F)C(=O)NOCCO	4	38	training
CHEMBL2375372	CS(=O)(=O)Nc1cccc(c1)Oc2cc(cc(c2C(=O)N)Nc3ccc(cc3F)I)F	5	220	training
CHEMBL2376660	c1cc2c(cc1Oc3cc(cc(c3C(=O)N)Nc4ccc(cc4F)I)F)[nH]c(=O)o2	18	46	training
CHEMBL2376661	CCS(=O)(=O)Nc1cccc(c1)Oc2cc(cc(c2C(=O)N)Nc3ccc(cc3F)I)F	5	42	training
CHEMBL2376662	CC(C)S(=O)(=O)Nc1cccc(c1)Oc2cc(cc(c2C(=O)N)Nc3ccc(cc3F)I)F	5	75	training
CHEMBL2376663	CN(C)S(=O)(=O)Nc1cccc(c1)Oc2cc(cc(c2C(=O)N)Nc3ccc(cc3F)I)F	5	80	training
CHEMBL2376664	c1cc(cc(c1)Oc2cc(cc(c2C(=O)N)Nc3ccc(cc3F)I)F)NS(=O)(=O)N4CCCC4	25	21	test
CHEMBL2376665	CNS(=O)(=O)Nc1cccc(c1)Oc2cc(cc(c2C(=O)N)Nc3ccc(cc3F)I)F	5	40	training

CHEMBL2376666	c1cc(cc(c1)Oc2cc(cc(c2C(=O)N)Nc3ccc(cc3F)I)F)NS(=O)(=O)N	5	20	training
CHEMBL2376667	c1cc(cc(c1)Oc2cc(cc(c2C(=O)N)Nc3ccc(cc3F)I)F)CS(=O)(=O)N	5	27	test
CHEMBL2376669	COc1cc(cc(c1C(=O)N)Nc2ccc(cc2F)I)F	4	64	training
CHEMBL2376674	c1cnn(c1)CC(CCOc2cc(cc(c2C(=O)N)Nc3ccc(cc3F)I)F)O	19	58	training
CHEMBL2376675	c1cc(c(cc1I)F)Nc2cc(cc(c2C(=O)N)OCCC(Cn3ccnc3)O)F	19	540	training
CHEMBL2376676	c1cc(c(cc1I)F)Nc2cc(cc(c2C(=O)N)OCC3CCC[NH2+]3)F	8	62	test
CHEMBL2376677	C[NH+]1CCCC1COc2cc(cc(c2C(=O)N)Nc3ccc(cc3F)I)F	8	430	test
CHEMBL2376678	CCS(=O)(=O)N1CCCC1COc2cc(cc(c2C(=O)N)Nc3ccc(cc3F)I)F	8	500	test
CHEMBL2376679	CN(C)S(=O)(=O)N1CCCC1COc2cc(cc(c2C(=O)N)Nc3ccc(cc3F)I)F	8	650	test
CHEMBL2376680	c1cc(c(cc1I)F)Nc2cc(cc(c2C(=O)N)OCC3CCCN3S(=O)(=O)N)F	8	800	test
CHEMBL2376681	c1ccc(cc1)Oc2cc(cc(c2C(=O)N)Nc3ccc(cc3F)I)F	5	147	training
CHEMBL2376682	c1cc(cnc1)Oc2cc(cc(c2C(=O)N)Nc3ccc(cc3F)I)F	5	58	training
CHEMBL2376683	c1cc2cn[nH]c2cc1Oc3cc(cc(c3C(=O)N)Nc4ccc(cc4F)I)F	18	150	training
CHEMBL2376684	CC(=O)Nc1cccc(c1)Oc2cc(cc(c2C(=O)N)Nc3ccc(cc3F)I)F	5	20	training
CHEMBL2376685	CC(=O)Nc1ccc(cc1)Oc2cc(cc(c2C(=O)N)Nc3ccc(cc3F)I)F	5	64	training
CHEMBL2376686	CC(C)C(=O)Nc1cccc(c1)Oc2cc(cc(c2C(=O)N)Nc3ccc(cc3F)I)F	5	32	training
CHEMBL2396994	CCC(=O)c1csc(n1)NC(=O)C(C(C)c2ccccc2)N3C(=O)C(NC3=O)c4ccc(cc4)OCCO	24	18	test
CHEMBL2396995	CC(CO)COc1ccc(cc1)C2C(=O)N(C(=O)N2)C(C(=O)Nc3ccc(cc3F)I)C(C)c4ccccc4	15	74	training
CHEMBL244488	c1cc(c(cc1I)F)Nc2c(ccc(c2F)F)C(=O)NOCCO	4	66	training
CHEMBL245884	CC1CNC(=O)c2c1c3cc(ccc3[nH]2)C(=O)Nc4nc(cs4)C(=O)NCC[NH+](C)C	11	510	training
CHEMBL246089	CC1CNC(=O)c2c1c3cc(ccc3[nH]2)C(=O)Nc4nc(cs4)C(=O)NCC(=O)N	11	3.4	training
CHEMBL253116	CC(CO)NC(=[NH2+])c1c(nsc1Nc2ccc(cc2)Nc3ccccc3)O	1	56	training
CHEMBL263039	c1cc(ccc1Nc2c(c(ns2)O)C(=[NH+]CCC(CO)O)N)Oc3cc(ccc3Cl)Cl	1	750	training
CHEMBL265478	CC(CO)[NH+]=C(c1c(nsc1Nc2ccc(cc2)Oc3cccc(c3)C(F)(F)F)O)N	1	160	training
CHEMBL269696	CC(CO)[NH+]=C(c1c(nsc1Nc2ccc(c(c2)Cl)Oc3cc(ccc3Cl)F)O)N	1	7	training
CHEMBL30551	COc1cc2c(cc1OCCC[NH+]3CCOCC3)ncc(c2Nc4ccc(cc4)CCc5ccccc5)C#N	29	539	training
CHEMBL30763	COc1cc2c(cc1OC)ncc(c2Nc3cccc(c3)Oc4ccccc4)C#N	22	7.7	test
CHEMBL3086065	Cc1c2cc(c(cc2oc(=O)c1Cc3cccc(c3)NS(=O)(=O)NC)OC(=O)N(C)C)Cl	2	2	training
CHEMBL3092176	Cc1c2ccc(cc2oc(=O)c1Cc3cccc(c3F)NS(=O)(=O)NC)Oc4nccs4	17	67	test
CHEMBL3092178	Cc1c2cc(c(cc2oc(=O)c1Cc3cccc(c3)NS(=O)(=O)NC)OC(=O)N(C)C)I	2	46.25	training
CHEMBL3092179	Cc1cc2c(c(c(=O)oc2cc1OC(=O)N(C)C)Cc3cccc(c3)NS(=O)(=O)NC)C	2	30	test
CHEMBL3092180	Cc1c2cc(c(cc2oc(=O)c1Cc3cccc(c3)NS(=O)(=O)NC)OC(=O)N(C)C)C#C	2	45	training
CHEMBL3092181	Cc1c2cc(c(cc2oc(=O)c1Cc3cccc(c3)NS(=O)(=O)NC)OC(=O)N(C)C)C#N	2	18	training
CHEMBL3092182	Cc1c2ccc(cc2oc(=O)c1Cc3cccc(c3)NS(=O)(=O)N)OC(=O)N(C)C	2	43	test
CHEMBL3092183	Cc1c2ccc(cc2oc(=O)c1Cc3cc(ccc3F)NS(=O)(=O)N)OC(=O)N(C)C	2	124	training
CHEMBL3092184	Cc1c2ccc(cc2oc(=O)c1Cc3ccc(c(c3)NS(=O)(=O)N)F)OC(=O)N(C)C	2	39	training
CHEMBL3092185	Cc1c2ccc(cc2oc(=O)c1Cc3cccc(c3F)NS(=O)(=O)N)OC(=O)N(C)C	2	33	training
CHEMBL3092186	Cc1c2cc(c(cc2oc(=O)c1Cc3cccc(c3)NS(=O)(=O)N)OC(=O)N(C)C)F	2	6.8	training
CHEMBL3092187	Cc1c2ccc(c(c2oc(=O)c1Cc3cccc(c3)NS(=O)(=O)N)F)OC(=O)N(C)C	2	40	training
CHEMBL3092188	CN(C)C(=O)Oc1ccc2c(c1)oc(=O)c(c2CF)Cc3cccc(c3)NS(=O)(=O)N	2	118	training
CHEMBL3092189	Cc1c2ccc(cc2oc(=O)c1Cc3cccc(c3)NS(=O)(=O)NC)OC(=O)N(C)C	2	82	training
CHEMBL3092191	Cc1c2ccc(cc2oc(=O)c1Cc3cccc(c3F)NS(=O)(=O)NC)OC(=O)N(C)C	2	15	training
CHEMBL3092192	Cc1c2cc(c(cc2oc(=O)c1Cc3cccc(c3)NS(=O)(=O)NC)OC(=O)N(C)C)F	2	30	training
CHEMBL3092193	CNS(=O)(=O)Nc1cccc(c1)Cc2c(c3ccc(cc3oc2=O)OC(=O)N(C)C)CF	2	690	training
CHEMBL3092194	Cc1c2ccc(cc2oc(=O)c1Cc3cccc(c3)NS(=O)(=O)NC)Oc4ncccn4	13	21	training

CHEMBL3092195	Cc1c2ccc(cc2oc(=O)c1Cc3cccc(c3F)NS(=O)(=O)NC)Oc4ncccn4	13	36	training
CHEMBL3092196	Cc1c2ccc(cc2oc(=O)c1Cc3cccc(c3)NS(=O)(=O)NC)Oc4nccs4	17	120	test
CHEMBL31733	COc1cc2c(cc1OC)ncc(c2Nc3ccc(cc3)Oc4ccccc4)C#N	7	52	training
CHEMBL318804	Cn1ccnc1Sc2ccc(cc2Cl)Nc3c4cc(c(cc4ncc3C#N)OCCC[NH+]5CCOCC5)OC	16	73	training
CHEMBL330388	COc1cccc2c1c(c(cn2)C#N)Nc3ccc(cc3)Oc4ccccc4	7	60	training
CHEMBL371693	Cn1cc(c(c(c1=O)F)Nc2ccc(cc2F)Br)C(=O)N	4	810	training
CHEMBL372600	Cn1cc(c(c(c1=O)F)Nc2ccc(cc2F)Br)C(=O)NOCCO	4	97	test
CHEMBL375609	CC(CO)[NH+]=C(c1c(nsc1Nc2cccc(c2Cl)Cl)O)N	3	7	training
CHEMBL377592	COC(=O)c1ccc(cc1)Nc2c(c(ns2)O)C(=[NH2+])NCC3CCCCC3	6	30	training
CHEMBL377783	CC(C)[NH+]=C(c1c(nsc1Nc2ccc(cc2Cl)C(F)(F)F)O)N	3	26	training
CHEMBL378014	c1cc(cc(c1)Cl)Nc2c(c(ns2)O)C(=[NH+]CC3CCCCC3)N	6	744	training
CHEMBL378688	COc1cc(ccc1Nc2c(c(ns2)O)C(=[NH2+])NCC3CCCCC3)[N+](=O)[O-]	6	35	training
CHEMBL378719	c1cc(cc(c1)Br)Nc2c(c(ns2)O)C(=[NH+]CC3CCCCC3)N	6	34	training
CHEMBL378833	c1c(cc(cc1Cl)Cl)Nc2c(c(ns2)O)C(=[NH+]CC3CCCCC3)N	6	200	training
CHEMBL380328	c1cc(c(cc1Cl)Cl)Nc2c(c(ns2)O)C(=[NH+]CC3CCCCC3)N	6	44	test
CHEMBL383858	CN1CC[NH+](CC1)N=C(c2c(nsc2Nc3ccc(cc3)Oc4cc(ccc4Cl)Cl)O)N	12	14	test
CHEMBL384012	c1cc(ccc1Nc2c(c(ns2)O)C(=[NH+]CC(CO)O)N)Oc3cc(ccc3Cl)Cl	1	57	training
CHEMBL384784	CC(CO)[NH+]=C(c1c(nsc1Nc2ccc(c(c2)Cl)Oc3ccc(cc3Cl)F)O)N	1	410	training
CHEMBL385059	CCC(CO)[NH+]=C(c1c(nsc1Nc2ccc(cc2)Oc3cc(ccc3Cl)Cl)O)N	1	140	training
CHEMBL385203	CC(CO)[NH+]=C(c1c(nsc1Nc2ccc(cc2)Oc3cccc(c3F)Cl)O)N	1	105	training
CHEMBL385446	CC(CO)[NH+]=C(c1c(nsc1Nc2ccc(c(c2)F)Oc3cc(ccc3Cl)Cl)O)N	1	29.5	training
CHEMBL385820	c1cc(c(cc1Cl)Cl)Nc2c(c(ns2)O)C#N	3	5	training
CHEMBL385905	CC(C[NH+]=C(c1c(nsc1Nc2ccc(cc2)Oc3cc(ccc3Cl)Cl)O)N)O	1	225	training
CHEMBL386230	CC(CO)[NH+]=C(c1c(nsc1Nc2ccc(cc2)Sc3ccccc3)O)N	1	68	training
CHEMBL386457	CN1CC[NH+](CC1)CCC[NH+]=C(c2c(nsc2Nc3ccc(cc3)Oc4cc(ccc4Cl)Cl)O)N	20	1000	training
CHEMBL386469	c1cc(ccc1Nc2c(c(ns2)O)C(=[NH+]OCC(CO)O)N)Oc3cc(ccc3Cl)Cl	1	25	training
CHEMBL397332	CC1CNC(=O)c2c1c3cc(ccc3[nH]2)C(=O)Nc4nc(cs4)C(=O)N	11	73	training
CHEMBL413636	CC(CO)[NH+]=C(c1c(nsc1Nc2ccc(cc2)Oc3cccc(c3)N(C)C)O)N	1	185	training
CHEMBL414139	COc1cc2c(cc1OCCC[NH+]3CCOCC3)ncc(c2Nc4ccc(cc4)Oc5ccccc5)C#N	14	54	training
CHEMBL424897	Cc1cc(ccc1Nc2c(c(ns2)O)C(=[NH+]C(C)CO)N)Oc3ccc(cc3Cl)F	1	35	training
CHEMBL425065	c1cc(ccc1Nc2c(c(ns2)O)C#N)Cl	3	29	training
CHEMBL425980	CC(CO)[NH+]=C(c1c(nsc1Nc2ccc(cc2)Oc3cc(cc(c3)F)C(F)(F)F)O)N	1	680	training
CHEMBL426840	Cc1c(c(cn(c1=O)C)C(=O)NOC)Nc2ccc(cc2F)Br	4	59	training
CHEMBL437331	CC(CO)[NH+]=C(c1c(nsc1Nc2ccc(cc2)Oc3cccccc3)O)N	1	125	training
CHEMBL489058	CCN1CC[NH+](CC1)CCC=Cc2ccc3c(c2)ncc(c3Nc4ccc(c(c4)Cl)Sc5nccn5C)C#N	16	99	training
CHEMBL94965	c1ccc(cc1)Oc2ccc(cc2)Nc3c4ccc(cc4ncc3C#N)OCCC[NH+]5CCOCC5	14	28	training
CHEMBL95002	COc1cc2c(cc1OCC[NH+]3CCOCC3)ncc(c2Nc4ccc(cc4)Oc5ccccc5)C#N	27	76	test
CHEMBL97463	COc1cc2c(c(c1)OC)c(c(cn2)C#N)Nc3ccc(cc3)Oc4ccccc4	7	280	training
CHEMBL97714	COc1ccc2c(c1)c(c(cn2)C#N)Nc3ccc(cc3)Oc4ccccc4	7	58	training
CHEMBL98130	c1ccc(cc1)Oc2ccc(cc2)Nc3c4ccccc4ncc3C#N	7	120	test
CHEMBL98131	COc1ccc2c(c1)ncc(c2Nc3ccc(cc3)Oc4ccccc4)C#N	7	26	training

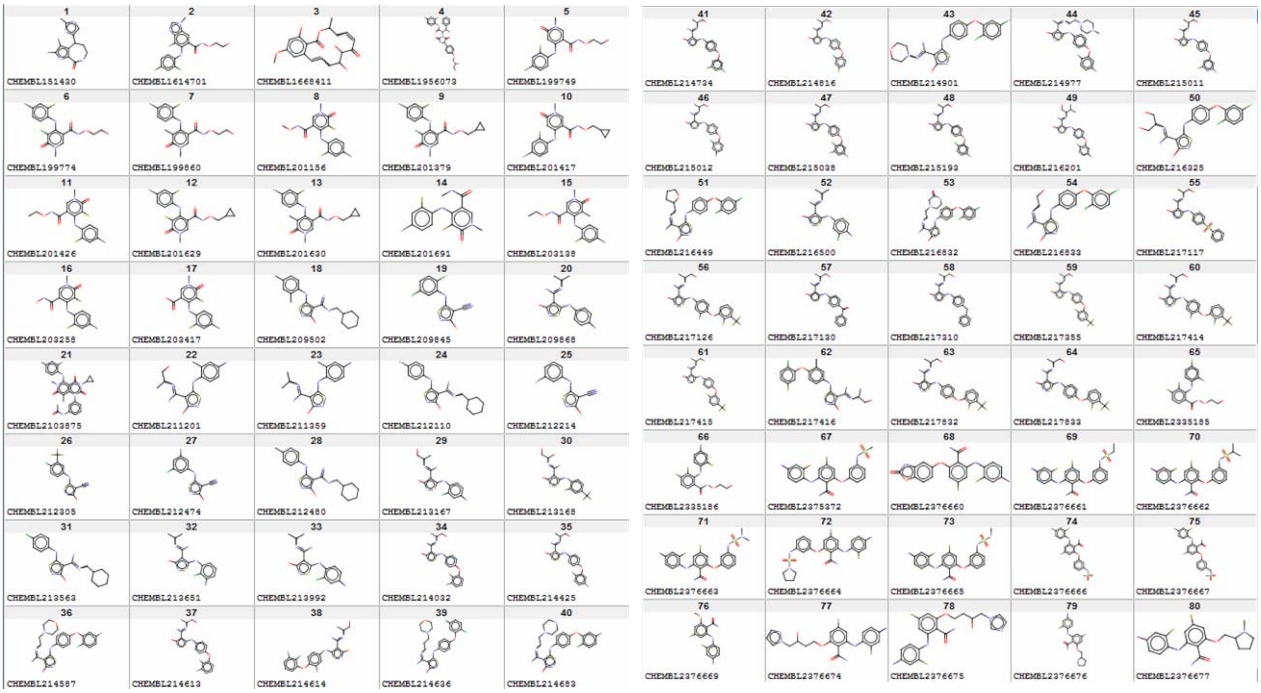

Fig. S2 Chemical representation of the MEK inhibitors 1 to 80

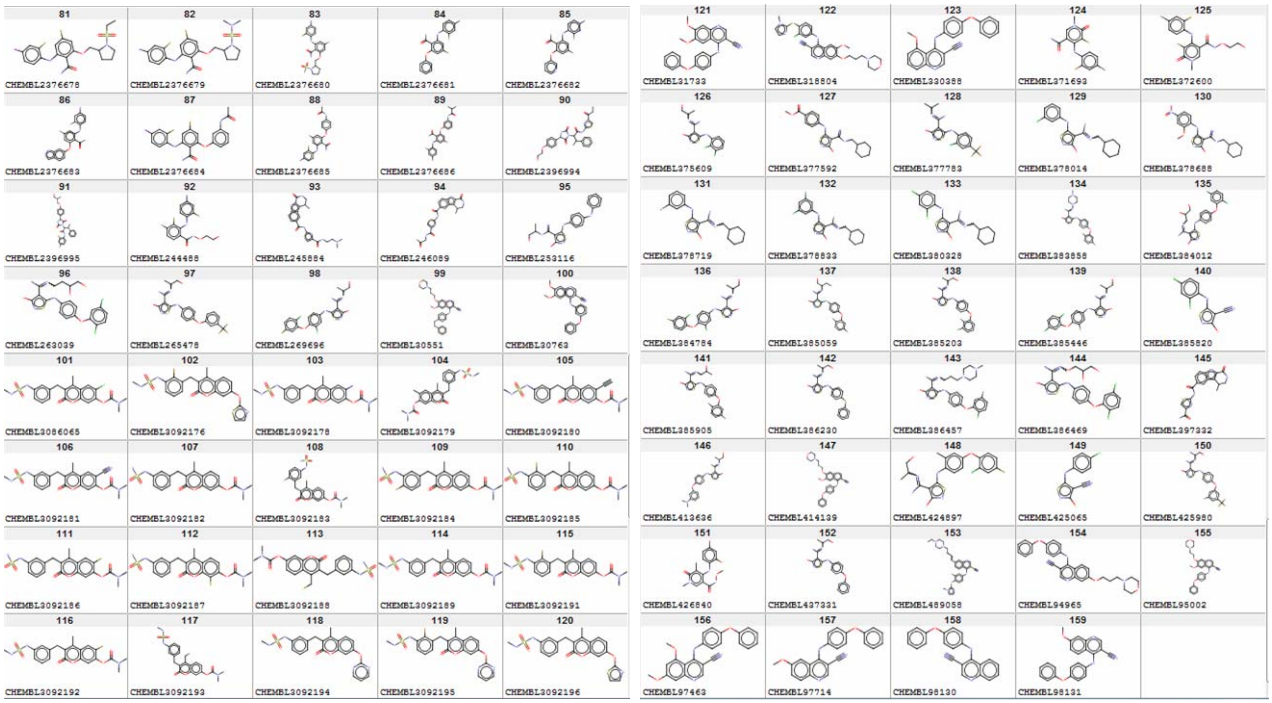

Fig. S2 Chemical representation of the MEK inhibitors 81 to 159