

#	Sequence	CEST Contrast Value (±4 ppm)	Epoch	#	Sequence	CEST Contrast Value (±4 ppm)	Epoch	#	Sequence	CEST Contrast Value (±4 ppm)	Epoch	#	Sequence	CEST Contrast Value (±4 ppm)	Epoch
1	KKKKKKKKKK	12.3	1	47	QIFKTRKIKNS	7.61	2	89	QRRRDRLWD	2.25684	6	133	UQLWRPCKAS	19.332	TEST
2	SSSSSSSSSS	17	1	46	SNHSMGIGLE	3.96	2	90	RRHEDLELE	15.1934	6	134	QCAGWVWRGR	23.0585	TEST
3	KRRRHHHHHH	17.2	1	42	PNNSTPTNSM	5.29	2	91	VNRLDRLHL	21.8229	7	135	RRCKRQWVGLA	9.31314	TEST
4	KKCKKGGGKGG	10.8	1	48	VNSDPSGQHRD	4.15	2	92	LHSSWLKVDHLL	18.17873	7	136	GLHRAAMQCC	2.70676	TEST
5	SSSSSSSSSS	13.2	1	49	LSNRHRRDQAG	7.69	2	93	VNNSVPCVN	8.10188	7	137	QRKRAMPPVY	12.6569	TEST
6	KKCKKGGGKGG	11.8	1	50	QIATVENSAMSG	3.63	2	94	GNKKNWRVYKNE	14.71331	7	138	NPLKAGQCQIQ	18.1656	TEST
7	SSSSSSSSSS	18	1	51	QIHTVENSARNS	4.69	2	95	RLLKSPQCGD	29.8647	7	139	AGCCQHRGVMN	14.6937	TEST
8	KKCKKGGGKGG	12.1	1	52	KDRGSKPKRVC	8.67	3	96	LSNRKRLKRT	49.8796	7	140	NQTESVRYRM	3.68273	TEST
9	RRRRRRRRRR	22	1	53	GRRGAIWKDKV	12.75	3	97	NWRDCLSLVFN	3.17673	7	141	NVVQRHHTS	28.0341	TEST
10	SSSSSSSSSS	12.8	1	54	CCVWNPWRRTB	18.46	3	98	KMRKLGCPVK	47.8888	7	142	VNKVSCPVCN	8.10024	TEST
11	RRRRRRRRRR	17.2	1	55	KYVYRKGSSKA	27.88	3	99	NHRSKCNNSNV	8.82446	7	143	GRHWVWVAA	6.0831	TEST
12	RRRRRRRRRR	5.5	1	60	RKMPLRWTRK	17.14	3	100	VSLQWELGPNK	15.76919	7	144	NNKQVVAVM	6.40218	TEST
13	RRRRRRRRRR	18.1	1	57	GNPRKVSFPG	8.89	3	101	VSEFVHVSYS	7.71894	8	145	VETWSMNSVA	0	TEST
14	RFTFTFTFTT	16.5	1	58	VNLFMRLNEM	4.53	3	102	PSWVYRRTM	18.27371	8	146	NSCVNANVQ	0	TEST
15	RFTFTFTFTT	18.9	1	59	GPMPNKAAMKLC	5.81	3	103	PGVNSDLEEV	11.18031	8	147	HAVNVVNVGH	0	TEST
16	FTFTFTFTTT	6.5	1	60	KVRYWAPRL	8.21	3	104	VVNLGKSSNKG	28.8256	8	148	CNDRGKNSNV	0	TEST
17	TKTKTKTKTK	14.1	1	61	KCOMIKMPTDQ	9.35	3	105	VGSKSNLEMR	26.2286	8	149	VPSQVKGSK	4.9926	TEST
18	DTDTDTDTDT	2.2	1	62	NWQMKVTRTBE	16.24	4	106	TSNKKRMTAK	29.8349	8	150	PVRRVVGQHP	18.6468	TEST
19	FTFTFTFTFT	1.7	1	63	HGRWRRRTD	15.49	4	107	EVNRYVSSS	5.70766	8	151	VFTFTQKSK	20.4713	TEST
20	TKTKTKTKTK	12.6	1	64	RRMVNRTRFMW	15.01	4	108	EPSNLPKGMNEK	24.6024	8	152	MAMADAAAPNA	6.96546	TEST
21	DTDTDTDTDT	4	1	65	WVSTCFRTLS	17.1	4	109	RLVNSGDRLEN	12.26758	8	153	MKVAAMAPQC	18.6169	TEST
22	FTFTFTFTFT	4.4	1	66	VWVWKPGRDPM	6.28	4	110	RSTGVAVNM	0	8	154	PVYVYVQCPD	4.33159	TEST
23	TKTKTKTKTK	13.8	1	67	HRVHLTKGRT	16.08	4	111	RPPHLNVVRVG	6.48029	TEST	155	KVLWRPAPGQ	13.0793	TEST
24	DTDTDTDTDT	4	1	68	WRHTSTSNL	14.49	4	112	KVWVPRRRL	14.62146	TEST	156	VSVVAGVWET	14.3656	TEST
25	FTFTFTFTTT	4	1	69	KPVHGCASRTKR	16.19014	4	113	RVLSNKKQTVR	28.5674	TEST	157	AKKVAQANVCK	17.82153	TEST
26	FTTKTKTKTK	13.8	1	70	KKRLWVWVHG	12.0156	5	114	VNKVSSPCVN	8.516833	TEST	158	VAVVAKAHVCTM	4.20168	TEST
27	DTFTFTFTTT	7.2	1	71	RRRHWVWQVW	13.5662	5	115	EVNRYVSSS	2.96102	TEST				
28	FTFTFTFTTT	5.9	1	72	WFLGRHLKKKD	19.0715	5	116	RLPKRVQZNVK	30.61573	TEST				
29	ISDSDSISDSDS	2.5	1	73	CHLADLRKUGLR	10.1388	5	117	GLGNQHVVLGV	4.52619	TEST				
30	SSSSSSSSSS	7	1	74	KMVTWFGKAKW	24.1149	5	118	KVRLVAFPSN	5.19056	TEST				
31	SSSSSSSSSS	9.1	1	75	QRHSHRIGLWL	7.54669	5	119	HVVSPVSSWGC	3.36282	TEST				
32	KKCKKGGGKGG	11.9	1	76	LELALGRDPMGW	20.2477	5	120	HHSPCVSW	12.80188	TEST				
33	KKCKKGGGKGG	9.9	1	77	QGVWYKAKRGM	11.8626	5	121	DKRGRQKQAWG	31.1841	TEST				
34	KKCKKGGGKGG	11.3	1	78	MWYKGRHKKMK	11.2326	5	122	RRHGWVWEGPW	20.0466	TEST				
35	KKCKKGGGKGG	9.3	1	79	LEHFTKWRKNS	11.5626	5	123	RRHGWVWEGPW	4.36828	TEST				
36	MPPRRSSRPVRRRR	19	1	80	DKVCKQQRKWH	12.5172	5	124	PRGWVPHH	11.6599	TEST				
37	DNVNYVYKLE	0	1	81	WVYLGKQKWT	31.2653	6	125	KMVDVYKAKAW	14.09143	TEST				
38	VYVWVWVWQ	0	1	82	FRQLEKIKW	20.7927	6	126	ARNKBDIMRW	20.01464	TEST				
39	NVNVWVGLVLA	0	1	83	SFGSKKRD	8.63029	6	127	NAPWVWVWVW	8.89852	TEST				
40	NYNVWVGLVLA	0.81	1	84	SSQPRRWVW	19.8206	6	128	VQRGRLSRRS	28.2809	TEST				
41	NENQWVWVWQ	0	1	85	LRRLGLVER	3.07419	6	129	LSQPRKRAVW	12.6838	TEST				
42	NGVLYNVVVE	0	1	86	KEVWVWVW	13.4267	6	130	RRVWVWVW	13.9899	TEST				
43	NSNMVWVWQ	14.06	2	87	KKRLKGRNS	29.2892	6	131	MALLQRLAHS	4.29221	TEST				
44	RTVLRNRRTQ	8.00	2	88	HDDKNKESDD	7.47947	6	132	RPCRWAGRAK	16.6629	TEST				

Table 1: All the available data in the dataset used for all the epochs of POET including the mock test data and the discovered protein sequences. All the data points with epoch N and less than N were used to evolve models and predict the data points marked as $N + 1$.