

Implementation, planning and saving of calibrations

Code 1. Convenience class BaseAsymmetricLogisticT.

```
1 class BaseAsymmetricLogisticT(BaseModelT):
2     def __init__(
3         self, *,
4         independent_key:str, dependent_key:str,
5         scale_degree:int=0,
6         theta_names: Optional[Tuple[str]]=None,
7     ):
8         """ Template for a model with asymmetric logistic trend (mu)
9             and polynomial scale (as a function of mu).
10
11         Parameters
12         -----
13         independent_key : str
14             name of the independent variable
15         dependent_key : str
16             name of the dependent variable
17         scale_degree : optional, int
18             degree of the polynomial model
19             describing the scale as a function of mu
20         theta_names : optional, tuple of str
21             may be used to set the names of the model parameters
22         """
23         self.scale_degree = scale_degree
24         if theta_names is None:
25             theta_names = tuple("L,L,U,I,x,S,c".split(",") + tuple(
26                 f"scale_{d}"
27                 for d in range(scale_degree + 1)
28             ) + ("df",))
29         super().__init__(independent_key, dependent_key, theta_names=theta_names)
```

Code 2. Human-readable pipetting instructions for the serial dilution of biomass for the calibration experiment.

```
1 Serial dilution plan (0.00102 to 1.00) from at least 12232.0 L stock and 54368.0 µL diluent:
2 Prepare column 1 with [2000. 1727. 1491. 1287. 1111. 959.] µL from stock and fill up to 2000 µL
3 Prepare column 2 with [538. 465. 401. 346. 299. 258.] µL from stock and fill up to 1300 µL
4 Prepare column 3 with [223. 192. 166. 143. 124. 107.] µL from stock and fill up to 1300 µL
5 Prepare column 4 with [92. 80. 69. 59. 51. 44.] µL from stock and fill up to 1300 µL
6 Prepare column 5 with [39. 39. 39. 39. 39. 39.] µL from column 1 and fill up to 1300 µL (1 serial dilutions)
7 Prepare column 6 with [39. 39. 39. 39. 39. 39.] µL from column 2 and fill up to 1300 µL (1 serial dilutions)
8 Prepare column 7 with [39. 39. 39. 39. 39. 39.] µL from column 3 and fill up to 1300 µL (1 serial dilutions)
9 Prepare column 8 with [39. 39. 39. 39. 39. 39.] µL from column 4 and fill up to 1300 µL (1 serial dilutions)
```

Code 3. JSON file containing stored model properties.

```
1 {
2   "calibr8_version": "6.0.0",
3   "model_type": "models.LogisticGlucoseCalibrationModelV1",
4   "theta_names": [
5     "L_L", "L_U", "I_x", "S", "c", "scale_0", "scale_1", "df"
6   ],
7   "theta_bounds": [
8     [-Infinity, 0.3],
9     [2, 5],
10    [-50, 50],
11    [0, 20],
12    [-3, 3],
13    [0, 0.1],
14    [0, 0.06],
15    [1, 20]
16  ],
17  "theta_guess": [0.1, 2.8, 1.2, 10, 1, 0.08, 0.01, 3],
18  "theta_fitted": [
19    -8.812, 2.765, 8.246, 0.0839,
20    2.69, 0.000374, 0.0154, 3.007
21  ],
22  "theta_timestamp": "2021-02-15T14:27:11Z",
23  "independent_key": "glc",
24  "dependent_key": "A365",
25  "cal_independent": [
26    50.0,
27    27.94736842105263,
28    ...,
29    0.05030330952033825
30  ],
31  "cal_dependent": [
32    2.6449,
33    2.2389,
34    ...,
35    0.1166
36  ]
37 }
```