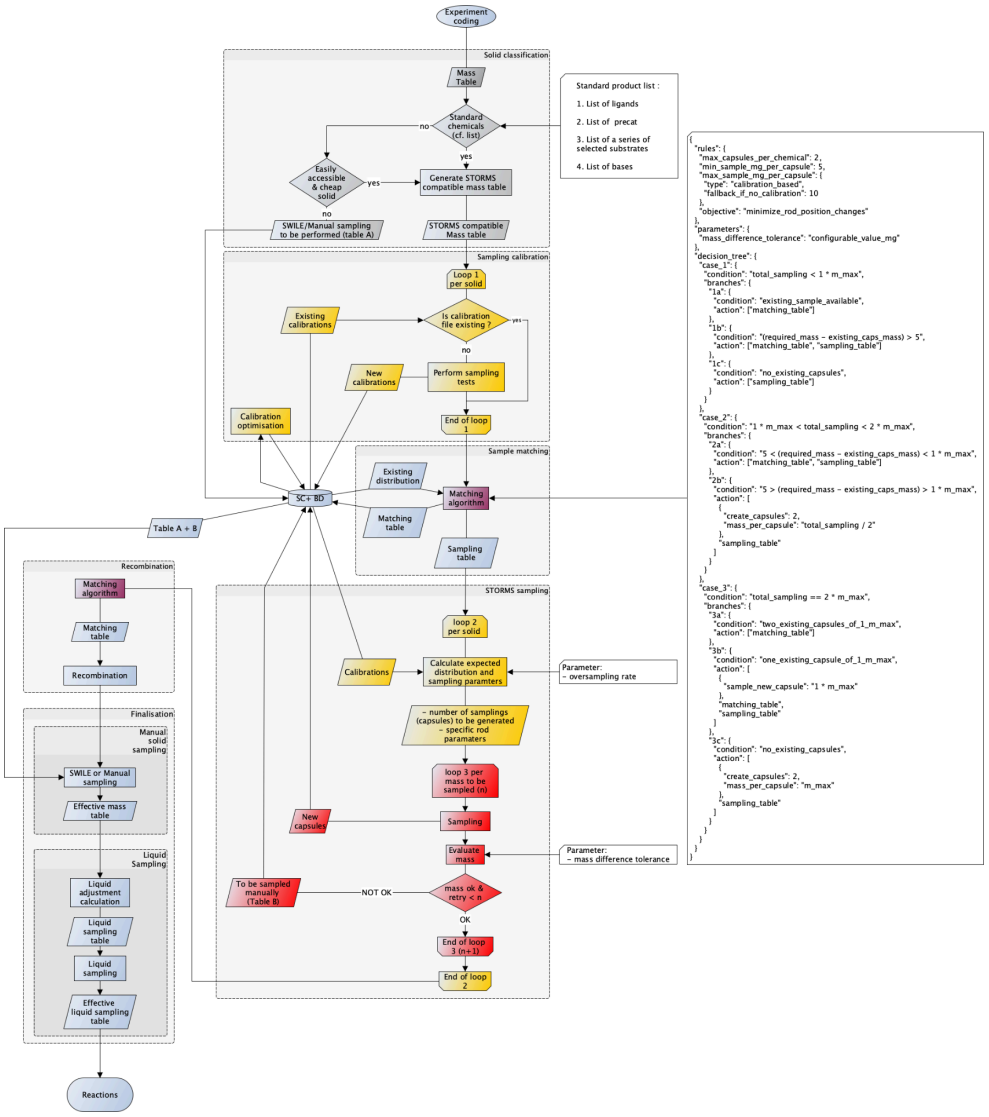
Supplementary material for

High-throughput solid microsampling through stochastic robotic automation

Adam Lisowski, Henryk Żołnowski, Keyan Villat, Alec Schmidt, Edy Mariano, Jean-Charles Cousty, Jérôme Guérin, Ashley Stark, Frédéric Vasserot, Achim Ammon, David Gueller, Florian de Nanteuil, Jean-Jacques Schwartz, Mathias Cherbuin, Marc Kunze, Giuseppe Costanzo, Pascal Miéville*

*pascal.mieville@epfl.ch
codes available at www.github.com/*swisscatplus/DC_Sampler*

S1 - Global STORMS workflow as deployed at EPFL Swiss Cat+ West Hub



S2 - Rule-based decision algorithm containing- decision rules and parameters for the *Matching algorithm* as set at EPFL Swiss Cat+ West Hub

```
MASS MATCHING DECISION LOGIC

INPUT DEFINITIONS
- required_mass_mg
  Total target mass required for the chemical, expressed in mg.

- existing_sample_available
  Boolean variable indicating whether reusable sample material is available.

- existing_match_within_tolerance
   Boolean variable indicating whether at least one valid combination of existing capsules already matches the
required mass within mass_difference_tolerance_mg.

- best_existing_match_mass_mg
  Mass in mg of the best reusable combination selected from existing capsules, with the constraint:
  best_existing_match_mass_mg < required_mass_mg

- existing_capsule_count
  Total number of reusable capsules currently available for the chemical.

- existing_capsules_of_m_max_count
  Number of reusable capsules currently available with mass exactly equal to m_max_mg.

- m_max_mg
  Maximum allowable mass per capsule, expressed in mg.

- mass_difference_tolerance_mg
  Acceptable tolerance on the mass difference, expressed in mg.

DERIVED VALUES
- small_sampling_threshold_mg = 5
- min_capsule_mass_mg = 3
- max_capsules_per_chemical = 2
- max_total_mass_mg = 2 * m_max_mg
- no_existing_capsules = (existing_capsule_count = 0)
- one_existing_capsule_of_m_max = (existing_capsules_of_m_max_count = 1)
- two_existing_capsules_of_m_max = (existing_capsules_of_m_max_count >= 2)
- best_existing_match_difference_mg = ABS(required_mass_mg - best_existing_match_mass_mg)
- residual_mass_to_sample_mg = required_mass_mg - best_existing_match_mass_mg
- required_capsule_count =
    IF required_mass_mg <= m_max_mg THEN 1
    ELSE 2

RULES
- all masses are expressed in mg
- maximum capsules per chemical = 2
- minimum sample mass per capsule = 3 mg
- maximum sample mass per capsule = calibration-based m_max_mg
- if no calibration exists, use 10 mg as m_max_mg
- reuse existing capsules whenever possible before creating new capsules
- objective = minimize rod position changes
- existing_match_within_tolerance = true means at least one valid combination of existing capsules satisfies:
  ABS(combination_mass_mg - required_mass_mg) <= mass_difference_tolerance_mg
- best_existing_match_mass_mg must always satisfy:
  best_existing_match_mass_mg < required_mass_mg
- residual_mass_to_sample_mg must always satisfy:
  residual_mass_to_sample_mg > 0
- if residual_mass_to_sample_mg > 0, a sampling_table must always be returned
- small_sampling_threshold_mg only determines whether the missing mass is sampled as a small adjustment or as a
standard new capsule decision branch
- no branch may return matching_table alone if residual_mass_to_sample_mg > 0

OUTPUT DEFINITIONS
- matching_table
   Table containing the selected existing capsules or reusable sample combinations used to satisfy all or part
of the required mass.

- sampling_table
  Table containing the quantities in mg that must be newly sampled to complete the required mass combination.

- create_capsules
  Number of new capsules that must be created.

- mass_per_capsule_mg
```

```
  Target mass in mg for each newly created capsule when multiple capsules of equal mass are created.

- sample_new_capsule_mg
  Target mass in mg for one newly created capsule when exactly one specific capsule mass must be sampled.

FUNCTIONAL LOGIC

IF required_mass_mg <= 0 THEN
  RETURN error
END IF
IF required_mass_mg > max_total_mass_mg THEN
  RETURN error
END IF
IF existing_match_within_tolerance = true THEN
  RETURN {
    matching_table,
    sampling_table: null,
    create_capsules: 0,
    mass_per_capsule_mg: null,
    sample_new_capsule_mg: null
  }
END IF
IF required_mass_mg <= m_max_mg THEN
  IF no_existing_capsules = true THEN
    RETURN {
      matching_table: null,
      sampling_table,
      create_capsules: 1,
      mass_per_capsule_mg: required_mass_mg,
      sample_new_capsule_mg: required_mass_mg
    }
  END IF
  IF existing_sample_available = true THEN
    IF residual_mass_to_sample_mg <= small_sampling_threshold_mg THEN
      RETURN {
        matching_table,
        sampling_table,
        create_capsules: 1,
        mass_per_capsule_mg: residual_mass_to_sample_mg,
        sample_new_capsule_mg: residual_mass_to_sample_mg
      }
    END IF
    IF residual_mass_to_sample_mg > small_sampling_threshold_mg THEN
      RETURN {
        matching_table,
        sampling_table,
        create_capsules: 1,
        mass_per_capsule_mg: residual_mass_to_sample_mg,
        sample_new_capsule_mg: residual_mass_to_sample_mg
      }
    END IF
  END IF
END IF
IF m_max_mg < required_mass_mg AND required_mass_mg < 2 * m_max_mg THEN
  IF no_existing_capsules = true THEN
    RETURN {
      matching_table: null,
      sampling_table,
      create_capsules: 2,
      mass_per_capsule_mg: required_mass_mg / 2,
      sample_new_capsule_mg: null
    }
  END IF
  IF residual_mass_to_sample_mg < m_max_mg THEN
    RETURN {
      matching_table,
      sampling_table,
      create_capsules: 1,
      mass_per_capsule_mg: residual_mass_to_sample_mg,
      sample_new_capsule_mg: residual_mass_to_sample_mg
    }
  END IF
  IF residual_mass_to_sample_mg >= m_max_mg THEN
    RETURN {
      matching_table,
      sampling_table,
      create_capsules: 2,
      mass_per_capsule_mg: required_mass_mg / 2,
      sample_new_capsule_mg: null
    }
  END IF
END IF
IF required_mass_mg = 2 * m_max_mg THEN
  IF two_existing_capsules_of_m_max = true THEN
    RETURN {
      matching_table,
      sampling_table: null,
      create_capsules: 0,
```

```
      mass_per_capsule_mg: null,
      sample_new_capsule_mg: null
    }
  END IF

  IF one_existing_capsule_of_m_max = true THEN
    RETURN {
      matching_table,
      sampling_table,
      create_capsules: 1,
      mass_per_capsule_mg: m_max_mg,
      sample_new_capsule_mg: m_max_mg
    }
  END IF
  IF no_existing_capsules = true THEN
    RETURN {
      matching_table: null,
      sampling_table,
      create_capsules: 2,
      mass_per_capsule_mg: m_max_mg,
      sample_new_capsule_mg: null
    }
  END IF
  RETURN {
    matching_table,
    sampling_table,
    create_capsules: 2,
    mass_per_capsule_mg: m_max_mg,
    sample_new_capsule_mg: null
  }
END IF
```

S3 - Validation data for 1mm rod - masses from 0.1 to 1 mg

Rod height (mm)	1	2	3	4	5
Granulac 70	0.34	0.42	0.56	0.36	0.47
Granulac 200	0.35	0.57	0.56	0.54	0.62
Srbolac 400	0.34	0.64	0.74	0.90	0.90
Tablettose 70	0.43	0.53	0.35	0.72	0.64
Flowlac 100	0.27	0.52	0.79	0.89	1.16
Spherolac 100	0.30	0.68	0.82	0.75	0.99
Inhalac 70	0.30	0.54	0.70	0.61	0.39
Inhalac 230	0.40	0.65	0.73	0.79	0.93
Inhalac 500	0.31	0.37	0.35	0.43	0.35
Bicarbonate Na	0.66	1.04	1.02	1.33	1.07

S4 - Validation data for 2mm rod - masses from 1 to 10 mg

product_name	Rod height (mm)	mass (mg)
Bicarbonate Dec	1	0.80
Bicarbonate Dec	2	3.91
Bicarbonate Dec	3	5.18
Bicarbonate Dec	4	7.41
Bicarbonate Dec	5	9.95
Bicarbonate Dec	6	11.64
Bicarbonate Dec	7	14.29
Bicarbonate Dec	8	14.01
Bicarbonate Dec	9	12.94
FlowLac 100	1	0.83
FlowLac 100	1	3.15
FlowLac 100	2	1.89
FlowLac 100	2	5.50
FlowLac 100	3	3.10
FlowLac 100	3	7.52
FlowLac 100	4	4.39
FlowLac 100	4	9.28
FlowLac 100	5	5.93
FlowLac 100	5	11.45
FlowLac 100	6	7.03
FlowLac 100	6	13.66
FlowLac 100	7	8.27
FlowLac 100	7	15.40
FlowLac 100	8	9.45
FlowLac 100	8	15.95
FlowLac 100	9	10.80
FlowLac 100	9	15.77
FlowLac 100	9	8.47
GranuLac 200	1	0.98
GranuLac 200	2	2.69
GranuLac 200	3	4.22
GranuLac 200	4	5.70
GranuLac 200	5	7.13

GranuLac 200	6	7.67
GranuLac 200	7	8.53
GranuLac 200	8	8.59
GranuLac 200	9	9.15
GranuLac 70	1	1.02
GranuLac 70	2	2.85
GranuLac 70	3	4.32
GranuLac 70	4	5.99
GranuLac 70	5	7.85
GranuLac 70	6	8.83
GranuLac 70	7	10.50
GranuLac 70	8	11.17
GranuLac 70	9	11.33
InhaLac 230	1	0.89
InhaLac 230	2	2.47
InhaLac 230	3	3.74
InhaLac 230	4	5.26
InhaLac 230	5	7.24
InhaLac 230	6	8.47
InhaLac 230	7	10.13
InhaLac 230	8	11.19
InhaLac 230	9	13.12
InhaLac 500	1	0.01
InhaLac 500	2	0.02
InhaLac 500	3	0.05
InhaLac 500	4	2.32
InhaLac 500	5	2.70
InhaLac 500	6	2.41
InhaLac 500	7	4.35
InhaLac 500	8	2.34
InhaLac 500	9	3.39
InhaLac 70	1	1.14
InhaLac 70	1	2.72
InhaLac 70	1	2.65
InhaLac 70	1	1.63
InhaLac 70	1	1.2
InhaLac 70	1	1.81
InhaLac 70	1	1.97
InhaLac 70	1	1.72
InhaLac 70	1	2.29

InhaLac 70	1	1.52
InhaLac 70	2	2.58
InhaLac 70	2	3.45
InhaLac 70	2	3.06
InhaLac 70	2	3.07
InhaLac 70	2	3.44
InhaLac 70	2	3.53
InhaLac 70	2	3.48
InhaLac 70	2	3.22
InhaLac 70	2	2.86
InhaLac 70	2	3.12
InhaLac 70	3	3.49
InhaLac 70	3	4.36
InhaLac 70	3	4.99
InhaLac 70	3	4.28
InhaLac 70	3	4.43
InhaLac 70	3	4.91
InhaLac 70	3	4.51
InhaLac 70	3	4.13
InhaLac 70	3	4.11
InhaLac 70	3	4.38
InhaLac 70	4	4.7
InhaLac 70	4	5.42
InhaLac 70	4	5.72
InhaLac 70	4	5.56
InhaLac 70	4	5.83
InhaLac 70	4	5.58
InhaLac 70	4	5.28
InhaLac 70	4	6.36
InhaLac 70	4	6.29
InhaLac 70	4	5.31
InhaLac 70	5	5.95
InhaLac 70	5	7.64
InhaLac 70	5	6.66
InhaLac 70	5	6.43
InhaLac 70	5	6.33
InhaLac 70	5	7.24
InhaLac 70	5	6.73
InhaLac 70	5	7.38
InhaLac 70	5	7.26

InhaLac 70	6	7.03
InhaLac 70	6	8.08
InhaLac 70	6	7.89
InhaLac 70	6	8.19
InhaLac 70	6	7.54
InhaLac 70	6	8.27
InhaLac 70	6	8.27
InhaLac 70	6	8.12
InhaLac 70	6	8.68
InhaLac 70	7	8.36
InhaLac 70	7	8.86
InhaLac 70	7	9.2
InhaLac 70	7	8.98
InhaLac 70	7	9.55
InhaLac 70	7	9.29
InhaLac 70	7	9.39
InhaLac 70	7	8.08
InhaLac 70	7	8.76
InhaLac 70	7	8.53
InhaLac 70	8	8.72
InhaLac 70	8	9.9
InhaLac 70	8	10.06
InhaLac 70	8	9.63
InhaLac 70	8	9.92
InhaLac 70	8	9.81
InhaLac 70	8	9.79
InhaLac 70	8	9.13
InhaLac 70	8	8.89
InhaLac 70	8	8.02
InhaLac 70	9	9.65
InhaLac 70	9	10.56
InhaLac 70	9	10.43
InhaLac 70	9	10.07
InhaLac 70	9	9.79
InhaLac 70	9	9.65
InhaLac 70	9	9.09
InhaLac 70	9	9.08
InhaLac 70	9	8.97
InhaLac 70	9	8.47
SorboLac 400	1	0.98

SorboLac 400	2	2.59
SorboLac 400	3	4.09
SorboLac 400	4	5.50
SorboLac 400	5	6.34
SorboLac 400	6	6.37
SorboLac 400	7	6.51
SorboLac 400	8	6.45
SorboLac 400	9	9.35
SpheroLac 100	1	1.96
SpheroLac 100	1	0.93
SpheroLac 100	1	2.18
SpheroLac 100	1	1.44
SpheroLac 100	1	2.01
SpheroLac 100	2	3.23
SpheroLac 100	2	2.29
SpheroLac 100	2	3.09
SpheroLac 100	2	3.54
SpheroLac 100	2	3.01
SpheroLac 100	3	4.66
SpheroLac 100	3	3.79
SpheroLac 100	3	4.35
SpheroLac 100	3	5.02
SpheroLac 100	3	4.53
SpheroLac 100	4	6.44
SpheroLac 100	4	5.33
SpheroLac 100	4	6.04
SpheroLac 100	4	5.89
SpheroLac 100	4	6.12
SpheroLac 100	5	7.96
SpheroLac 100	5	6.94
SpheroLac 100	5	7.67
SpheroLac 100	5	7.96
SpheroLac 100	6	9.07
SpheroLac 100	6	8.20
SpheroLac 100	6	0.01
SpheroLac 100	6	8.59
SpheroLac 100	6	8.95
SpheroLac 100	7	9.63
SpheroLac 100	7	9.87
SpheroLac 100	7	10.47

SpheroLac 100	7	10.55
SpheroLac 100	7	10.33
SpheroLac 100	8	9.58
SpheroLac 100	8	10.95
SpheroLac 100	8	11.52
SpheroLac 100	8	11.43
SpheroLac 100	8	11.61
SpheroLac 100	9	9.52
SpheroLac 100	9	12.25
SpheroLac 100	9	12.13
SpheroLac 100	9	12.66
SpheroLac 100	9	12.58
Tablettose 70	1	1.17
Tablettose 70	2	2.44
Tablettose 70	3	3.42
Tablettose 70	4	4.54
Tablettose 70	5	5.70
Tablettose 70	6	6.81
Tablettose 70	7	7.87
Tablettose 70	8	9.04