# Fitting drug response curves with sigmoid function

In [1]:

```
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
from scipy.optimize import curve_fit
from sklearn.metrics import r2_score
from tqdm import tqdm
import warnings
warnings.filterwarnings("ignore")
import os, sys
sys.path.insert(1, os.path.relpath("../functions"))
from fitting import *
from filtering import *

_FOLDER = "../data/"
_FOLDER_2 = "../figures/"
_FOLDER_3 = "../results/"
SAVE_FIGURES = False
```

# Fitting data

In [2]:

```
drug_curves = pd.read_csv(_FOLDER+"normalised_dose_response_data.csv")

conc_columns= ["fd_num_"+str(i) for i in range(10)]
response_norm = ['norm_cells_'+str(i) for i in range(10)]
```

# Comparison of fitting models

In [3]:

```
functions = [
             "fsigmoid",
             "sigmoid_2_param",
             "sigmoid_3_param",
             "sigmoid_4_param",
             "logistic_4_param",
            "ll4_4_param",
            "ll4R_4_param",
            "logLogist_3_param"]
```

## Which function gives the best fitting?

In [4]:

```
%%time
df_123_04 = filtering_sigmoid_curves(drug_curves, filtering_scenario=[1,2,3], ₩
                        response_columns = response_norm, ₩
                        first_points_lower_limit = 0.8, last_points_upper_limit = 0.4)

compare_fitting_functions(df_123_04, functions, conc_columns, response_norm)
```

```
Original dataset: (225384, 44)

  0%|          | 0/2776 [00:00<?, ?it/s]

1st filtration (Ensure that all the response are less than 1): Filtered datase
t: (63325, 44)
2d filtration (Ensure that first and last points form plateus): Filtered datas
et: (6321, 46)
3d stage filtration (Specified location of the plateus): Filtered dataset: (27
76, 46)
(2776, 46)

 fsigmoid

100%|██████████| 2776/2776 [00:04<00:00, 561.98it/s]
  2%|▏         | 44/2776 [00:00<00:06, 438.64it/s]

<function fsigmoid at 0x7ffe7f2cc9d8>
```

In [5]:

```
%%time
df_123_02 = filtering_sigmoid_curves(drug_curves, filtering_scenario=[1,2,3], ₩
                        response_columns = response_norm, ₩
                        first_points_lower_limit = 0.8, last_points_upper_limit = 0.2)

compare_fitting_functions(df_123_02, functions, conc_columns, response_norm)
```

```
Original dataset: (225384, 44)

  3%|▌          | 69/2152 [00:00<00:03, 687.63it/s]

1st filtration (Ensure that all the response are less than 1): Filtered dataset:
(63325, 44)
2d filtration (Ensure that first and last points form plateus): Filtered dataset:
(6321, 46)
3d stage filtration (Specified location of the plateus): Filtered dataset: (2152,
46)
(2152, 46)

100%|██████████| 2152/2152 [00:03<00:00, 666.72it/s]
  3%|▌          | 74/2152 [00:00<00:02, 734.64it/s]

<function fsigmoid at 0x7f86253c7598>

100%|██████████| 2152/2152 [00:03<00:00, 713.55it/s]
  2%|▏          | 50/2152 [00:00<00:04, 491.54it/s]

<function sigmoid_2_param at 0x7f86253c7510>

100%|██████████| 2152/2152 [00:04<00:00, 442.53it/s]
  2%|▏          | 43/2152 [00:00<00:04, 429.58it/s]

<function sigmoid_3_param at 0x7f86253c7620>

100%|██████████| 2152/2152 [00:05<00:00, 384.74it/s]
  2%|▏          | 42/2152 [00:00<00:05, 417.61it/s]

<function sigmoid_4_param at 0x7f86253c76a8>

100%|██████████| 2152/2152 [00:05<00:00, 373.62it/s]
  2%|▏          | 35/2152 [00:00<00:06, 343.92it/s]

<function logistic_4_param at 0x7f86253c7840>

100%|██████████| 2152/2152 [00:06<00:00, 307.90it/s]
  2%|▏          | 36/2152 [00:00<00:05, 355.00it/s]

<function ll4_4_param at 0x7f86253c7730>

100%|██████████| 2152/2152 [00:06<00:00, 316.71it/s]
  1%|▏          | 32/2152 [00:00<00:06, 312.69it/s]

<function ll4R_4_param at 0x7f86253c77b8>

100%|██████████| 2152/2152 [00:06<00:00, 336.80it/s]

<function logLogist_3_param at 0x7f86253c78c8>
```

| | best_fitting_count | min | max | r2>0 | r2>0.8 | r2>0.9 |
|---|---|---|---|---|---|---|
| **fsigmoid** | 0.0 | 4.602484e-01 | 0.999899 | 2152.0 | 2135.0 | 2074.0 |
| **sigmoid_2_param** | 0.0 | 4.602485e-01 | 0.999899 | 2152.0 | 2135.0 | 2074.0 |
| **sigmoid_3_param** | 3.0 | 5.922767e-01 | 0.999926 | 2152.0 | 2139.0 | 2118.0 |
| **sigmoid_4_param** | 899.0 | -4.195295e-07 | 0.999981 | 2133.0 | 2105.0 | 2094.0 |
| **logistic_4_param** | 218.0 | 6.016469e-01 | 0.999981 | 2152.0 | 2141.0 | 2126.0 |
| **ll4_4_param** | 195.0 | 6.016469e-01 | 0.999981 | 2152.0 | 2141.0 | 2127.0 |
| **ll4R_4_param** | 204.0 | 9.126042e-08 | 0.999981 | 2152.0 | 2139.0 | 2122.0 |
| **logLogist_3_param** | 633.0 | 4.998448e-01 | 0.999978 | 2152.0 | 2140.0 | 2122.0 |

Examples of bad fitting with sigmoid_4_param (r2<0.61): 39

| | COSMIC_ID | DRUG_ID | fsigmoid_r2 | sigmoid_2_param_r2 | sigmoid_3_param_r2 | sigm |
|---|---|---|---|---|---|---|
| **570** | 910851 | 170 | 0.991346 | 0.991346 | 0.995994 | |
| **2311** | 1290724 | 268 | 0.948049 | 0.948049 | 0.985379 | |
| **3576** | 907064 | 180 | 0.988098 | 0.988098 | 0.996652 | |
| **138632** | 949174 | 272 | 0.728071 | 0.728071 | 0.878181 | |
| **7905** | 910549 | 272 | 0.589601 | 0.589601 | 0.592277 | |

CPU times: user 42.6 s, sys: 1.77 s, total: 44.4 s
Wall time: 43.7 s

In [6]:

```
%%time
df_1234_04 = filtering_sigmoid_curves(drug_curves, filtering_scenario=[1,2,3,4], ₩
                        response_columns = response_norm, ₩
                        first_points_lower_limit = 0.8,
                        last_points_upper_limit = 0.4,
                        middle_points_limit = -0.2)

compare_fitting_functions(df_1234_04, functions, conc_columns, response_norm)
```

```
Original dataset: (225384, 44)

  3%|▌          | 72/2719 [00:00<00:03, 716.16it/s]

1st filtration (Ensure that all the response are less than 1): Filtered dataset:
(63325, 44)
2d filtration (Ensure that first and last points form plateus): Filtered dataset:
(6321, 46)
3d stage filtration (Specified location of the plateus): Filtered dataset: (2776,
46)
4th stage filtration (Cut off high ancedent points): Filtered dataset: (2719, 46)
(2719, 46)

100%|██████████| 2719/2719 [00:04<00:00, 667.08it/s]
  2%|▏          | 67/2719 [00:00<00:03, 666.17it/s]

<function fsigmoid at 0x7f86253c7598>

100%|██████████| 2719/2719 [00:03<00:00, 711.69it/s]
  2%|▏          | 53/2719 [00:00<00:05, 523.88it/s]

<function sigmoid_2_param at 0x7f86253c7510>

100%|██████████| 2719/2719 [00:05<00:00, 455.70it/s]
  2%|▏          | 43/2719 [00:00<00:06, 428.95it/s]

<function sigmoid_3_param at 0x7f86253c7620>

100%|██████████| 2719/2719 [00:07<00:00, 384.77it/s]
  2%|▏          | 42/2719 [00:00<00:06, 411.53it/s]

<function sigmoid_4_param at 0x7f86253c76a8>

100%|██████████| 2719/2719 [00:07<00:00, 375.27it/s]
  1%|          | 32/2719 [00:00<00:08, 313.67it/s]

<function logistic_4_param at 0x7f86253c7840>

100%|██████████| 2719/2719 [00:08<00:00, 309.68it/s]
  1%|          | 33/2719 [00:00<00:08, 324.88it/s]

<function ll4_4_param at 0x7f86253c7730>

100%|██████████| 2719/2719 [00:08<00:00, 320.17it/s]
  1%|▏          | 36/2719 [00:00<00:07, 353.97it/s]

<function ll4R_4_param at 0x7f86253c77b8>

100%|██████████| 2719/2719 [00:08<00:00, 337.15it/s]

<function logLogist_3_param at 0x7f86253c78c8>
```

| | best_fitting_count | min | max | r2>0 | r2>0.8 | r2>0.9 |
|---|---|---|---|---|---|---|
| **fsigmoid** | 0.0 | 4.503432e-01 | 0.999899 | 2719.0 | 2671.0 | 2456.0 |
| **sigmoid_2_param** | 0.0 | 4.503431e-01 | 0.999899 | 2719.0 | 2671.0 | 2456.0 |
| **sigmoid_3_param** | 2.0 | 8.127070e-01 | 0.999926 | 2719.0 | 2719.0 | 2681.0 |
| **sigmoid_4_param** | 1109.0 | -4.195295e-07 | 0.999981 | 2699.0 | 2680.0 | 2675.0 |
| **logistic_4_param** | 292.0 | 8.453735e-01 | 0.999981 | 2719.0 | 2719.0 | 2712.0 |
| **ll4_4_param** | 257.0 | 8.453634e-01 | 0.999981 | 2719.0 | 2719.0 | 2712.0 |
| **ll4R_4_param** | 269.0 | 9.126042e-08 | 0.999981 | 2719.0 | 2717.0 | 2708.0 |
| **logLogist_3_param** | 790.0 | 8.272879e-01 | 0.999978 | 2719.0 | 2719.0 | 2707.0 |

Examples of bad fitting with sigmoid_4_param (r2<0.61): 39

| | COSMIC_ID | DRUG_ID | fsigmoid_r2 | sigmoid_2_param_r2 | sigmoid_3_param_r2 | sigm |
|---|---|---|---|---|---|---|
| **155787** | 1287706 | 1014 | 0.882047 | 0.882047 | 0.983959 | |
| **570** | 910851 | 170 | 0.991346 | 0.991346 | 0.995994 | |
| **74484** | 724878 | 268 | 0.982274 | 0.982274 | 0.993826 | |
| **82744** | 907172 | 344 | 0.998927 | 0.998927 | 0.999046 | |
| **107980** | 909706 | 182 | 0.971662 | 0.971662 | 0.988824 | |

CPU times: user 53.3 s, sys: 2.19 s, total: 55.5 s
Wall time: 54.6 s

In [7]:

```
%%time
df_1234_02 = filtering_sigmoid_curves(drug_curves, filtering_scenario=[1,2,3,4], ₩
                        response_columns = response_norm, ₩
                        first_points_lower_limit = 0.8,
                        last_points_upper_limit = 0.2,
                        middle_points_limit = -0.2)

compare_fitting_functions(df_1234_02, functions, conc_columns, response_norm)
```

```
Original dataset: (225384, 44)

  3%|▌          | 64/2108 [00:00<00:03, 632.32it/s]

1st filtration (Ensure that all the response are less than 1): Filtered dataset:
(63325, 44)
2d filtration (Ensure that first and last points form plateus): Filtered dataset:
(6321, 46)
3d stage filtration (Specified location of the plateus): Filtered dataset: (2152,
46)
4th stage filtration (Cut off high ancedent points): Filtered dataset: (2108, 46)
(2108, 46)

100%|██████████| 2108/2108 [00:03<00:00, 655.88it/s]
  4%|▌          | 76/2108 [00:00<00:02, 758.43it/s]

<function fsigmoid at 0x7f86253c7598>

100%|██████████| 2108/2108 [00:02<00:00, 711.63it/s]
  2%|▏          | 49/2108 [00:00<00:04, 488.64it/s]

<function sigmoid_2_param at 0x7f86253c7510>

100%|██████████| 2108/2108 [00:04<00:00, 457.72it/s]
  2%|▏          | 43/2108 [00:00<00:04, 427.33it/s]

<function sigmoid_3_param at 0x7f86253c7620>

100%|██████████| 2108/2108 [00:05<00:00, 374.09it/s]
  2%|▏          | 37/2108 [00:00<00:05, 362.11it/s]

<function sigmoid_4_param at 0x7f86253c76a8>

100%|██████████| 2108/2108 [00:05<00:00, 377.98it/s]
  1%|▏          | 31/2108 [00:00<00:06, 305.66it/s]

<function logistic_4_param at 0x7f86253c7840>

100%|██████████| 2108/2108 [00:06<00:00, 311.18it/s]
  2%|▏          | 32/2108 [00:00<00:06, 314.78it/s]

<function ll4_4_param at 0x7f86253c7730>

100%|██████████| 2108/2108 [00:06<00:00, 305.93it/s]
  2%|▏          | 34/2108 [00:00<00:06, 338.80it/s]

<function ll4R_4_param at 0x7f86253c77b8>

100%|██████████| 2108/2108 [00:06<00:00, 342.47it/s]

<function logLogist_3_param at 0x7f86253c78c8>
```

| | best_fitting_count | min | max | r2>0 | r2>0.8 | r2>0.9 |
|---|---|---|---|---|---|---|
| **fsigmoid** | 0.0 | 7.768212e-01 | 0.999899 | 2108.0 | 2105.0 | 2058.0 |
| **sigmoid_2_param** | 0.0 | 7.768212e-01 | 0.999899 | 2108.0 | 2105.0 | 2058.0 |
| **sigmoid_3_param** | 2.0 | 8.127070e-01 | 0.999926 | 2108.0 | 2108.0 | 2098.0 |
| **sigmoid_4_param** | 886.0 | -4.195295e-07 | 0.999981 | 2090.0 | 2073.0 | 2070.0 |
| **logistic_4_param** | 213.0 | 8.453735e-01 | 0.999981 | 2108.0 | 2108.0 | 2103.0 |
| **ll4_4_param** | 189.0 | 8.453634e-01 | 0.999981 | 2108.0 | 2108.0 | 2103.0 |
| **ll4R_4_param** | 195.0 | 9.126042e-08 | 0.999981 | 2108.0 | 2106.0 | 2099.0 |
| **logLogist_3_param** | 623.0 | 8.272879e-01 | 0.999978 | 2108.0 | 2108.0 | 2100.0 |

Examples of bad fitting with sigmoid_4_param (r2<0.61): 35

| | COSMIC_ID | DRUG_ID | fsigmoid_r2 | sigmoid_2_param_r2 | sigmoid_3_param_r2 | sigm |
|---|---|---|---|---|---|---|
| **155787** | 1287706 | 1014 | 0.882047 | 0.882047 | 0.983959 | |
| **570** | 910851 | 170 | 0.991346 | 0.991346 | 0.995994 | |
| **74484** | 724878 | 268 | 0.982274 | 0.982274 | 0.993826 | |
| **82744** | 907172 | 344 | 0.998927 | 0.998927 | 0.999046 | |
| **107980** | 909706 | 182 | 0.971662 | 0.971662 | 0.988824 | |

CPU times: user 41.8 s, sys: 1.76 s, total: 43.6 s
Wall time: 42.9 s

In [8]:

```
%%time
df_134_04 = filtering_sigmoid_curves(drug_curves, filtering_scenario=[1,3,4], ₩
                        response_columns = response_norm, ₩
                        first_points_lower_limit = 0.8, last_points_upper_limit = 0.4,
                        middle_points_limit =-0.2)

compare_fitting_functions(df_134_04, functions, conc_columns, response_norm)
```

```
Original dataset: (225384, 44)

  0%|          | 62/18415 [00:00<00:30, 610.48it/s]

1st filtration (Ensure that all the response are less than 1): Filtered dataset:
(63325, 44)
3d stage filtration (Specified location of the plateus): Filtered dataset: (1903
7, 44)
4th stage filtration (Cut off high ancedent points): Filtered dataset: (18415, 4
4)
(18415, 44)

100%|██████████| 18415/18415 [00:32<00:00, 570.94it/s]
  0%|          | 68/18415 [00:00<00:27, 675.74it/s]

<function fsigmoid at 0x7f86253c7598>

100%|██████████| 18415/18415 [00:26<00:00, 701.68it/s]
  0%|          | 41/18415 [00:00<00:45, 403.85it/s]

<function sigmoid_2_param at 0x7f86253c7510>

100%|██████████| 18415/18415 [00:39<00:00, 465.47it/s]
  0%|          | 15/18415 [00:00<02:14, 136.67it/s]

<function sigmoid_3_param at 0x7f86253c7620>

100%|██████████| 18415/18415 [01:21<00:00, 225.60it/s]
  0%|          | 32/18415 [00:00<00:58, 313.19it/s]

<function sigmoid_4_param at 0x7f86253c76a8>

100%|██████████| 18415/18415 [00:56<00:00, 328.81it/s]
  0%|          | 23/18415 [00:00<01:20, 228.15it/s]

<function logistic_4_param at 0x7f86253c7840>

100%|██████████| 18415/18415 [01:11<00:00, 259.17it/s]
  0%|          | 25/18415 [00:00<01:14, 247.52it/s]

<function ll4_4_param at 0x7f86253c7730>

100%|██████████| 18415/18415 [01:08<00:00, 268.64it/s]
  0%|          | 20/18415 [00:00<01:32, 199.85it/s]

<function ll4R_4_param at 0x7f86253c77b8>

100%|██████████| 18415/18415 [01:00<00:00, 305.08it/s]

<function logLogist_3_param at 0x7f86253c78c8>
```

| | best_fitting_count | min | max | r2>0 | r2>0.8 | r2>0.9 |
|---|---|---|---|---|---|---|
| **fsigmoid** | 1.0 | 2.755202e-01 | 0.999938 | 18415.0 | 17174.0 | 14274.0 |
| **sigmoid_2_param** | 1.0 | 2.755201e-01 | 0.999938 | 18415.0 | 17172.0 | 14271.0 |
| **sigmoid_3_param** | 90.0 | -2.047581e-04 | 0.999998 | 18414.0 | 18219.0 | 16928.0 |
| **sigmoid_4_param** | 5843.0 | -7.220099e-06 | 0.999981 | 17333.0 | 16350.0 | 15635.0 |
| **logistic_4_param** | 1733.0 | 0.000000e+00 | 0.999981 | 18414.0 | 18270.0 | 17399.0 |
| **ll4_4_param** | 1603.0 | 0.000000e+00 | 0.999981 | 18413.0 | 18268.0 | 17396.0 |
| **ll4R_4_param** | 1488.0 | -5.176513e-07 | 0.999981 | 18411.0 | 18262.0 | 17384.0 |
| **logLogist_3_param** | 7656.0 | 6.058932e-01 | 0.999996 | 18415.0 | 18372.0 | 17906.0 |

Examples of bad fitting with sigmoid_4_param (r2<0.61): 1941

| | COSMIC_ID | DRUG_ID | fsigmoid_r2 | sigmoid_2_param_r2 | sigmoid_3_param_r2 | sigm |
|---|---|---|---|---|---|---|
| **131092** | 909726 | 252 | 0.896614 | 0.896614 | 0.931205 | |
| **131122** | 753584 | 222 | 0.974394 | 0.974394 | 0.984243 | |
| **72** | 908449 | 273 | 0.989093 | 0.989093 | 0.994160 | |
| **65611** | 688010 | 134 | 0.921392 | 0.921392 | 0.940102 | |
| **65620** | 1330996 | 235 | 0.943544 | 0.943544 | 0.968856 | |

CPU times: user 7min 7s, sys: 19 s, total: 7min 26s
Wall time: 7min 17s

In [9]:

```
%%time
df_134_02 = filtering_sigmoid_curves(drug_curves, filtering_scenario=[1,3,4], ₩
                        response_columns = response_norm, ₩
                        first_points_lower_limit = 0.8,
                        last_points_upper_limit = 0.2,
                        middle_points_limit = -0.2)

compare_fitting_functions(df_134_02, functions, conc_columns, response_norm)
```

```
Original dataset: (225384, 44)

  1%|          | 63/11997 [00:00<00:19, 627.27it/s]

1st filtration (Ensure that all the response are less than 1): Filtered dataset:
(63325, 44)
3d stage filtration (Specified location of the plateus): Filtered dataset: (1235
5, 44)
4th stage filtration (Cut off high ancedent points): Filtered dataset: (11997, 4
4)
(11997, 44)

100%|██████████| 11997/11997 [00:18<00:00, 638.87it/s]
  1%|          | 68/11997 [00:00<00:17, 676.23it/s]

<function fsigmoid at 0x7f86253c7598>

100%|██████████| 11997/11997 [00:17<00:00, 702.34it/s]
  0%|          | 45/11997 [00:00<00:26, 443.95it/s]

<function sigmoid_2_param at 0x7f86253c7510>

100%|██████████| 11997/11997 [00:25<00:00, 461.67it/s]
  0%|          | 25/11997 [00:00<00:48, 244.99it/s]

<function sigmoid_3_param at 0x7f86253c7620>

100%|██████████| 11997/11997 [00:49<00:00, 243.46it/s]
  0%|          | 37/11997 [00:00<00:32, 363.75it/s]

<function sigmoid_4_param at 0x7f86253c76a8>

100%|██████████| 11997/11997 [00:36<00:00, 326.06it/s]
  0%|          | 21/11997 [00:00<00:57, 206.97it/s]

<function logistic_4_param at 0x7f86253c7840>

100%|██████████| 11997/11997 [00:46<00:00, 259.96it/s]
  0%|          | 26/11997 [00:00<00:46, 255.63it/s]

<function ll4_4_param at 0x7f86253c7730>

100%|██████████| 11997/11997 [00:47<00:00, 251.97it/s]
  0%|          | 26/11997 [00:00<00:46, 256.27it/s]

<function ll4R_4_param at 0x7f86253c77b8>

100%|██████████| 11997/11997 [00:41<00:00, 286.68it/s]

<function logLogist_3_param at 0x7f86253c78c8>
```

| | best_fitting_count | min | max | r2>0 | r2>0.8 | r2>0.9 |
|---|---|---|---|---|---|---|
| **fsigmoid** | 0.0 | 2.788415e-01 | 0.999938 | 11997.0 | 11520.0 | 10282.0 |
| **sigmoid_2_param** | 1.0 | 2.788415e-01 | 0.999938 | 11997.0 | 11520.0 | 10282.0 |
| **sigmoid_3_param** | 61.0 | -2.047581e-04 | 0.999998 | 11996.0 | 11927.0 | 11378.0 |
| **sigmoid_4_param** | 4271.0 | -4.170810e-06 | 0.999981 | 11358.0 | 10828.0 | 10556.0 |
| **logistic_4_param** | 1109.0 | 5.782919e-01 | 0.999981 | 11997.0 | 11958.0 | 11603.0 |
| **ll4_4_param** | 1031.0 | 0.000000e+00 | 0.999981 | 11996.0 | 11957.0 | 11601.0 |
| **ll4R_4_param** | 931.0 | -5.176513e-07 | 0.999981 | 11994.0 | 11951.0 | 11592.0 |
| **logLogist_3_param** | 4593.0 | 7.085231e-01 | 0.999996 | 11997.0 | 11989.0 | 11840.0 |

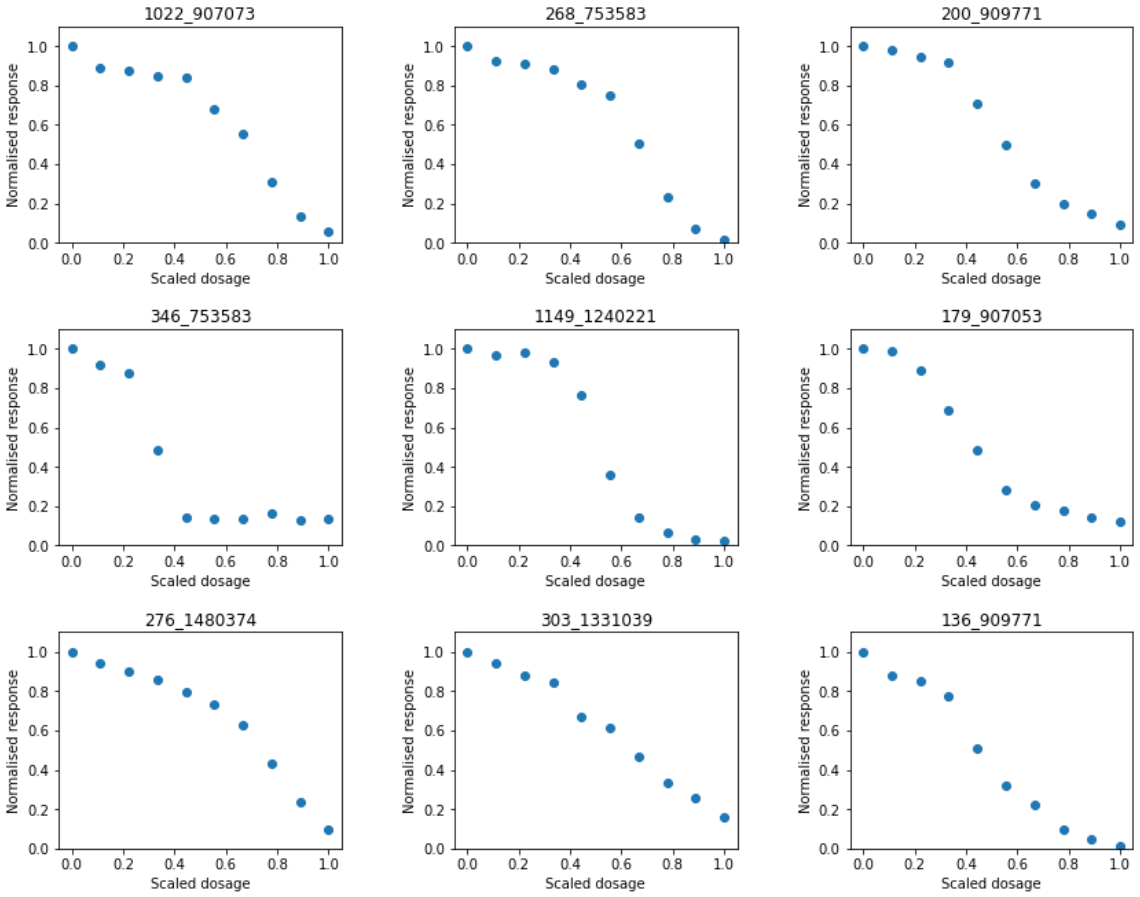
Examples of bad fitting with sigmoid_4_param (r2<0.61): 1136

| | COSMIC_ID | DRUG_ID | fsigmoid_r2 | sigmoid_2_param_r2 | sigmoid_3_param_r2 | sigm |
|---|---|---|---|---|---|---|
| **131092** | 909726 | 252 | 0.896614 | 0.896614 | 0.931205 | |
| **98368** | 908443 | 225 | 0.797873 | 0.797873 | 0.904829 | |
| **72** | 908449 | 273 | 0.989093 | 0.989093 | 0.994160 | |
| **65639** | 907053 | 257 | 0.819013 | 0.819013 | 0.931013 | |
| **65655** | 1290801 | 346 | 0.969306 | 0.969306 | 0.970429 | |

CPU times: user 4min 35s, sys: 12 s, total: 4min 47s
Wall time: 4min 44s

In [10]:

```
new_df = df_134_02[df_134_02["sigmoid_4_param_r2"]>0.9]
show_response_curves(new_df, plots_in_row=3, plots_in_column=3, ₩
                     x_columns=conc_columns, y_columns=response_norm, indexes=new_df.index[:9])
```



## What if don't use any filtering

In [11]:

```
%%time
compare_fitting_functions(drug_curves, functions, conc_columns, response_norm)
```

```
  0%|          | 0/225384 [00:00<?, ?it/s]
(225384, 44)
100%|██████████| 225384/225384 [06:30<00:00, 577.46it/s]
<function fsigmoid at 0x7f86253c7598>
100%|██████████| 225384/225384 [05:41<00:00, 660.18it/s]
<function sigmoid_2_param at 0x7f86253c7510>
100%|██████████| 225384/225384 [09:26<00:00, 397.85it/s]
<function sigmoid_3_param at 0x7f86253c7620>
100%|██████████| 225384/225384 [1:02:44<00:00, 59.88it/s]
<function sigmoid_4_param at 0x7f86253c76a8>
100%|██████████| 225384/225384 [3:21:50<00:00, 18.61it/s]
<function logistic_4_param at 0x7f86253c7840>
100%|██████████| 225384/225384 [33:00<00:00, 113.79it/s]
<function ll4_4_param at 0x7f86253c7730>
100%|██████████| 225384/225384 [1:31:08<00:00, 41.22it/s]
<function ll4R_4_param at 0x7f86253c77b8>
100%|██████████| 225384/225384 [38:13<00:00, 98.25it/s]
<function logLogist_3_param at 0x7f86253c78c8>
```

| | best_fitting_count | min | max | r2>0 | r2>0.8 | r2>0.9 |
|---|---|---|---|---|---|---|
| **fsigmoid** | 34024.0 | -794.650193 | 0.999988 | 154078.0 | 78135.0 | 53108.0 |
| **sigmoid_2_param** | 372.0 | -8.680730 | 0.999988 | 147301.0 | 78052.0 | 53016.0 |
| **sigmoid_3_param** | 10074.0 | -4.204919 | 0.999998 | 189861.0 | 94438.0 | 70277.0 |
| **sigmoid_4_param** | 30058.0 | -0.051301 | 0.999981 | 168543.0 | 81792.0 | 65700.0 |
| **logistic_4_param** | 31543.0 | -0.030124 | 0.999999 | 182648.0 | 101579.0 | 78979.0 |
| **ll4_4_param** | 31552.0 | -0.046189 | 1.000000 | 182050.0 | 101237.0 | 78843.0 |
| **ll4R_4_param** | 33135.0 | -0.716794 | 0.999998 | 183161.0 | 100964.0 | 78654.0 |
| **logLogist_3_param** | 54626.0 | -7.161534 | 1.000000 | 167680.0 | 94818.0 | 75034.0 |

```
Examples of bad fitting with sigmoid_4_param (r2<0.61): 127328
```

| | COSMIC_ID | DRUG_ID | fsigmoid_r2 | sigmoid_2_param_r2 | sigmoid_3_param_r2 | sigmoid_4_ |
|---|---|---|---|---|---|---|
| **0** | 1290922 | 332 | -0.356727 | -0.356736 | 0.019575 | 2.1 |
| **1** | 1290922 | 257 | 0.816939 | 0.816947 | 0.878794 | -4.0 |
| **4** | 1290922 | 192 | -0.362288 | -0.362288 | 0.215762 | 2.1 |
| **7** | 1290922 | 306 | 0.717135 | 0.717145 | 0.774391 | -4.5 |
| **9** | 1290922 | 277 | 0.542245 | 0.542245 | 0.147251 | -4.9 |

CPU times: user 1h 57min, sys: 7min, total: 2h 4min
Wall time: 7h 28min 42s

## df_123_04 was used in the MSc project

In [12]:

```
df = df_123_04.copy()
```

In [ ]:

```

```