Filtering

In [1]:

```
import pandas as pd
import numpy as np
import os
import gc
import matplotlib.pyplot as plt
import time

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

from functions.filtering import *
from functions.plotting import *
```

Original data

In [2]:

```
_FOLDER = "C:/Users/junny/GitRepos/DrugProfiles_2/database/"

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

if "Unnamed: 0" in drug_curves:
    drug_curves.drop("Unnamed: 0", axis=1, inplace =True)

col_to_drop = ["per_slope_change_"+str(i) for i in range(8)]+₩
            ["slope_" + str(i) for i in range(9)]
drug_curves.drop(col_to_drop, axis=1, inplace=True)

conc_columns= ["fd_num_"+str(i) for i in range(10)]
response_norm = ['norm_cells_'+str(i) for i in range(10)]
CCL_names = dict(zip(drug_curves["COSMIC_ID"], drug_curves["CELL_LINE_NAME"]))
df= pd.read_csv(_FOLDER+'Drug_Features.csv')
drug_names = dict(zip(df["Drug ID"].values, df["Drug Name"].values))
del df
drug_curves["drug_name"] = drug_curves["DRUG_ID"].map(drug_names)
drug_curves["CCL_name"] = drug_curves["COSMIC_ID"].map(CCL_names)
drug_curves.shape
```

Out[2]:

```
(225384, 28)
```

Filtering 1: 4 stage filtering

```
# Description of filtering_sigmoid_curves:
"""
    filtering_scenario = [1,2,3,4]
    1. Ensure that all the response are less than 1
    2. Ensure that first and last points form plateus
    the minimal number of points are specified in the function arguments
    by default, two points for both lpateus are considered
    tolerance =0.05 values to ensure the points form a plateu
    first_columns_to_compare = [1, 2]  - first two columns for plateu
    last_columns_to_compare = [-1, -2] - last two columns for plateu

    3. Specify location of the plateus - first_points_lower_limit and last_points_upper_limit

    4. Cutting off ambiqueos data:
    Among all "middle" datapoints a subsequent point should not be higher than antecedent by
0.2
"""
```

In [3]:

```
%%time
# difference between middle points 0.2
df_filt_1234 = 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)
df_filt_1234.to_csv(_FOLDER_3+"filt_1234_02.csv", index=False)
```

```
Original dataset: (225384, 28)
1st filtration (Ensure that all the response are less than 1): Filtered dataset:
(63325, 28)
2d filtration (Ensure that first and last points form plateus): Filtered dataset:
(6321, 30)
3d stage filtration (Specified location of the plateus): Filtered dataset: (2152,
30)
4th stage filtration (Cut off high ancedent points): Filtered dataset: (2108, 30)
CPU times: total: 781 ms
Wall time: 780 ms
```

Bad data after filtering 1

In [4]:

```
high_resp_data = find_high_responses(df_filt_1234, response_norm)

if high_resp_data.shape[0]==0:
    print("No high response data")
else:
    print("Responses above 1:", high_resp_data.shape[0])
    df = high_resp_data
    show_response_curves(df, plots_in_row=3, plots_in_column=3, ₩
                    x_columns=conc_columns, y_columns=response_norm, indexes=df.index[:9],
                   drug_dict = drug_names, CCL_dict = CCL_names, upper_limit=1)
```

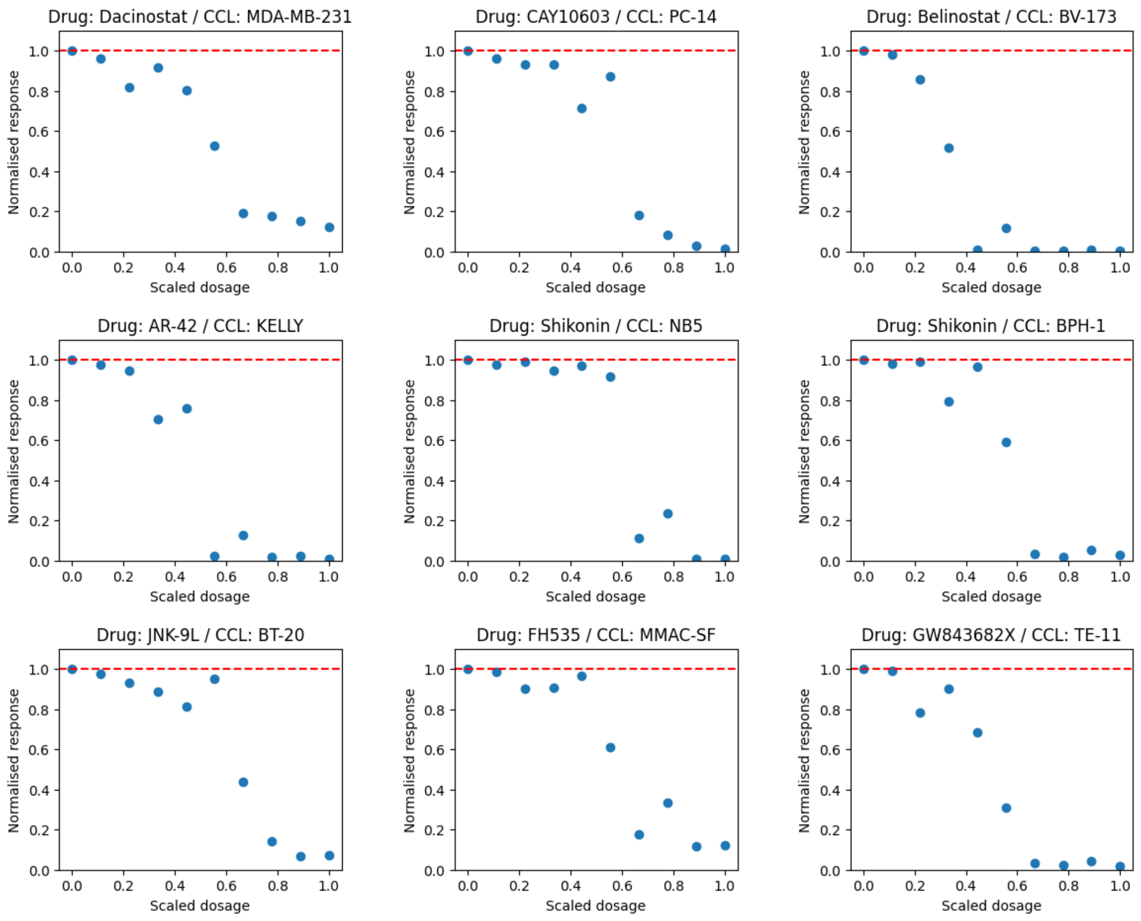
```
No high response data
```

In [5]:

```
ascend_data = find_ascending_data(df_filt_1234, response_norm, middle_points_limit=-0.1)
print("Ascending points:", ascend_data.shape[0])

df = ascend_data
show_response_curves(df, plots_in_row=3, plots_in_column=3, ₩
                     x_columns=conc_columns, y_columns=response_norm, indexes=df.index[:9],
                    drug_dict = drug_names, CCL_dict = CCL_names, upper_limit=1)
```

```
Ascending points: 71
```



Filtering 2: auc>0.7 and spearman_r<0

```
# description of auc_filtration
"""
    1. Remove all the curves where the normalised response value is greater than one at zero
dosage.
    2. Leave only those curves with an Area Under the Curve (AUC) >0.7.
    3. Compute the Spearman correlation coefficient between the normalised response
    and the scaled dosage (so the x-axis and the y-axis).
    4. Further remove the curves for which the Spearman correlation coefficient is zero or
positive.
    5. Cut off samples with last response above 0.2
"""
```

In [6]:

```
%%time
df_filt_auc = auc_filtration(drug_curves, conc_columns, response_norm,
                             auc_limit=0.7, final_response_limit=0.2)
df_filt_auc.to_csv(_FOLDER_3+"filt_auc_02.csv", index=False)
```

```
100%|████████████████████████████████████████████████████████████████████| 2
25384/225384 [15:27<00:00, 243.06it/s]

CPU times: total: 15min 29s
Wall time: 15min 27s
```

In [7]:

```
df_filt_auc.shape
```

Out[7]:

```
(14084, 31)
```

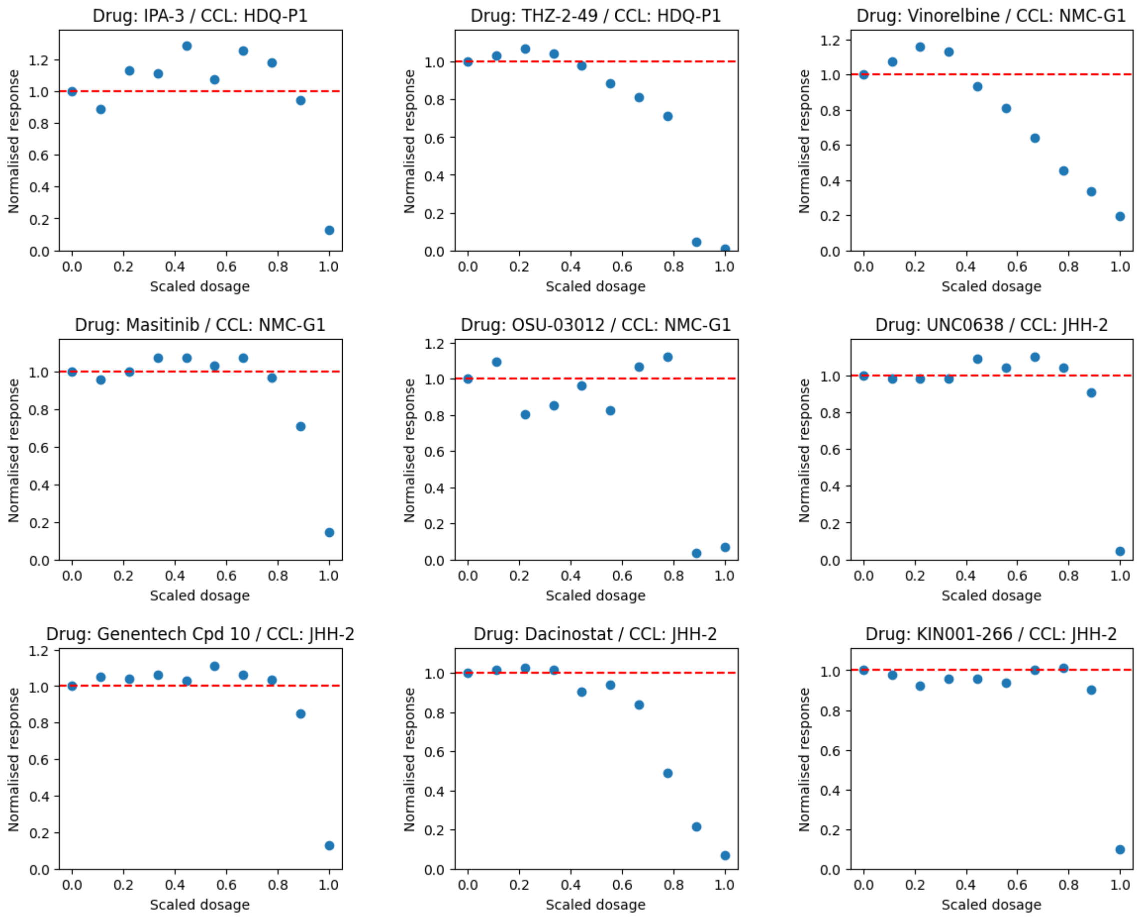
Bad data left after filtering 2

In [8]:

```
high_resp_data = find_high_responses(df_filt_auc, response_norm)
print("Responses above 1:", high_resp_data.shape[0])

df = high_resp_data
show_response_curves(df, plots_in_row=3, plots_in_column=3, ₩
                     x_columns=conc_columns, y_columns=response_norm, indexes=df.index[:9],
                    drug_dict = drug_names, CCL_dict = CCL_names, upper_limit=1)
```

```
Responses above 1: 8404
```

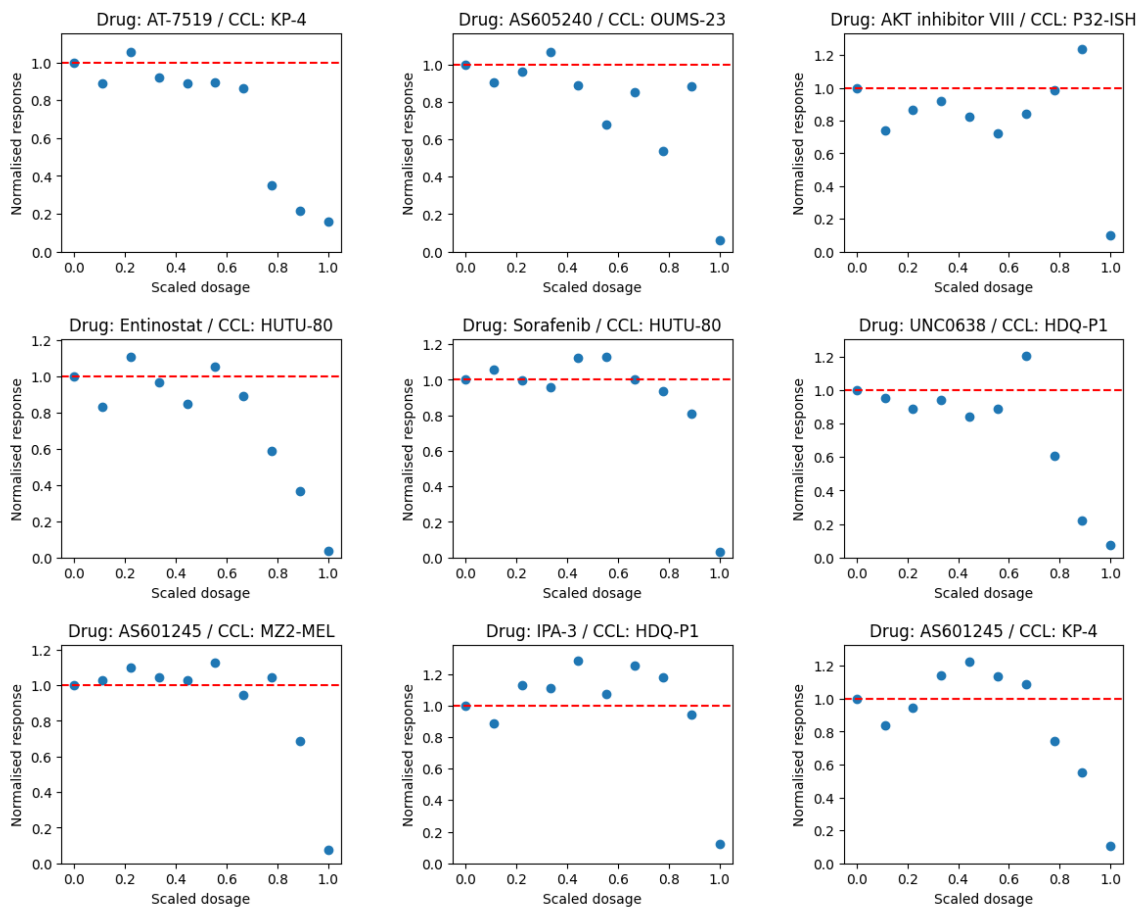


In [9]:

```
ascend_data = find_ascending_data(df_filt_auc, response_norm, middle_points_limit=-0.1)
print("Ascending points:", ascend_data.shape[0])

df = ascend_data
show_response_curves(df, plots_in_row=3, plots_in_column=3, ₩
                   x_columns=conc_columns, y_columns=response_norm, indexes=df.index[:9],
                  drug_dict = drug_names, CCL_dict = CCL_names, upper_limit=1)
```

```
Ascending points: 4797
```



Filtering 3: direct fitting

In [10]:

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

In [11]:

```
%%time
df_no_filt = compare_fitting_functions(drug_curves, functions, conc_columns, response_norm,
                                        save_file_name = _FOLDER_3 +"fit_no_filt.csv")
```

```
(225384, 28)

 fsigmoid

100%|██████████████████████████████████████████████████████████████████████| 2
25384/225384 [04:30<00:00, 832.34it/s]

<function fsigmoid at 0x000002305FA5CCC0>

 sigmoid_2_param

100%|█████████████████████████████████████████████████████████████████████| 22
5384/225384 [03:16<00:00, 1149.18it/s]

<function sigmoid_2_param at 0x000002305FA5CC20>

 sigmoid_3_param

100%|██████████████████████████████████████████████████████████████████████| 2
25384/225384 [07:30<00:00, 500.28it/s]

<function sigmoid_3_param at 0x000002305FA5CD60>

 sigmoid_4_param

100%|██████████████████████████████████████████████████████████████████████| 2
25384/225384 [34:06<00:00, 110.15it/s]

<function sigmoid_4_param at 0x000002305FA5CE00>

 logistic_4_param

 13%|██████████                                                              |
30092/225384 [07:29<37:00, 87.97it/s]IOPub message rate exceeded.
The notebook server will temporarily stop sending output
to the client in order to avoid crashing it.
To change this limit, set the config variable
`--NotebookApp.iopub_msg_rate_limit`.

Current values:
NotebookApp.iopub_msg_rate_limit=1000.0 (msgs/sec)
NotebookApp.rate_limit_window=3.0 (secs)

100%|███████████████████████████████████████████████████████████████████████|
225384/225384 [37:54<00:00, 99.09it/s]

<function ll4R_4_param at 0x000002305FA5CF40>

 logLogist_3_param

100%|██████████████████████████████████████████████████████████████████████| 2
25384/225384 [32:20<00:00, 116.14it/s]

<function logLogist_3_param at 0x000002305FA5D080>
```

	best_fitting_count	min	max	r2>0	r2>0.8	r2>0.9	r2>
fsigmoid	33900.0	-8.680730	0.999988	154649.0	78118.0	53091.0	530
sigmoid_2_param	197.0	-8.680730	0.999988	151367.0	78100.0	53063.0	530
sigmoid_3_param	19932.0	-0.000003	0.999998	189138.0	95607.0	70557.0	705
sigmoid_4_param	27310.0	-0.000007	0.999981	119614.0	65659.0	53846.0	538
logistic_4_param	27747.0	-0.607641	0.999997	163685.0	94899.0	73125.0	731
ll4_4_param	27365.0	-2.963147	1.000000	163747.0	94635.0	73134.0	731
ll4R_4_param	39514.0	-0.831922	0.999998	159464.0	88618.0	67848.0	678
logLogist_3_param	49419.0	-177.845334	1.000000	144487.0	91132.0	72883.0	728

```
Examples of bad fitting with sigmoid_4_param (r2<0.61): 146021
```

	COSMIC_ID	DRUG_ID	fsigmoid_r2	sigmoid_2_param_r2	sigmoid_3_param_r2	sigmoid_4_
0	1290922	332	-0.356726	-0.356726	0.037388	0.0
4	1290922	192	-0.362288	-0.362288	0.216033	0.0
6	1290922	310	0.752543	0.752543	0.922580	3.1
7	1290922	306	0.717145	0.717145	0.774391	2.5
8	1290922	225	0.769099	0.769099	0.806332	0.0

```
CPU times: total: 2h 55min 8s
Wall time: 2h 59min 50s
```

In [ ]: