# Using controlSBML

## Preliminaries

In [1]:
```
import controlSBML.control_sbml as ctl
import pandas as pd
```

In [2]:
```
ctlsb = ctl.ControlSBML("https://www.ebi.ac.uk/biomodels/model/download/BIOMD
```

In [3]:
```
# Print the first few lines of the antimony representation of this model
print(ctlsb.antimony[:380])
```

```
// Created by libAntimony v2.12.0
function Constant_flux__irreversible(v)
  v;
end

Constant_flux__irreversible is "Constant flux (irreversible)"

function Henri_Michaelis_Menten__irreversible(substrate, Km, V)
  V*substrate/(Km + substrate);
end

Henri_Michaelis_Menten__irreversible is "Henri-Michaelis-Menten (irreversibl
e)"

function HMM_Mod(V, s, m, Km)
  V*s*m/(Km + s);
end
```

In [4]:
```
ctlsb.species_names
```

Out[4]:
```
['IR',
 'pIR',
 'IRS',
 'pIRS',
 'iIRS',
 'Akt',
 'pAkt',
 'mTORC1',
 'pmTORC1',
 'mTORC2',
 'pmTORC2',
 'imTORC2',
 'mTORC1_DEPTOR',
 'mTORC2_DEPTOR',
 'DEPTOR',
 'pDEPTOR']
```

In [5]:
```
ctlsb.jacobian
```

Out[5]:

| | IR | pIR | IRS | pIRS | iIRS | Akt | pAkt | mTORC1 | pmTORC1 |
|---|---|---|---|---|---|---|---|---|---|
| **IR** | -0.004518 | 0.028571 | 0.0 | 0.000000 | 0.00 | 0.0 | 0.000000 | 0.00 | 0.000000 |
| **pIR** | 0.004518 | -0.028571 | 0.0 | 0.000000 | 0.00 | 0.0 | 0.000000 | 0.00 | 0.000000 |
| **IRS** | 0.000000 | -0.066667 | 0.0 | 0.020000 | 0.02 | 0.0 | 0.000000 | 0.00 | -0.066667 |
| **pIRS** | 0.000000 | 0.066667 | 0.0 | -0.020000 | 0.00 | 0.0 | 0.000000 | 0.00 | 0.000000 |
| **iIRS** | 0.000000 | 0.000000 | 0.0 | 0.000000 | -0.02 | 0.0 | 0.000000 | 0.00 | 0.066667 |
| **Akt** | 0.000000 | 0.000000 | 0.0 | -0.046729 | 0.00 | 0.0 | 0.058824 | 0.00 | 0.000000 |
| **pAkt** | 0.000000 | 0.000000 | 0.0 | 0.046729 | 0.00 | 0.0 | -0.058824 | 0.00 | 0.000000 |
| **mTORC1** | 0.000000 | 0.000000 | 0.0 | 0.000000 | 0.00 | 0.0 | -0.099206 | -0.35 | 5.999848 |
| **pmTORC1** | 0.000000 | 0.000000 | 0.0 | 0.000000 | 0.00 | 0.0 | 0.099206 | 0.00 | -5.999848 |
| **mTORC2** | 0.000000 | -0.166667 | 0.0 | 0.000000 | 0.00 | 0.0 | 0.000000 | 0.00 | 0.000000 |
| **pmTORC2** | 0.000000 | 0.166667 | 0.0 | 0.000000 | 0.00 | 0.0 | 0.000000 | 0.00 | 0.000000 |
| **imTORC2** | 0.000000 | 0.000000 | 0.0 | 0.000000 | 0.00 | 0.0 | 0.000000 | 0.00 | 0.000000 |
| **mTORC1_DEPTOR** | 0.000000 | 0.000000 | 0.0 | 0.000000 | 0.00 | 0.0 | 0.000000 | 0.35 | 0.000000 |
| **mTORC2_DEPTOR** | 0.000000 | 0.000000 | 0.0 | 0.000000 | 0.00 | 0.0 | 0.000000 | 0.00 | 0.000000 |
| **DEPTOR** | 0.000000 | 0.000000 | 0.0 | 0.000000 | 0.00 | 0.0 | 0.000000 | -0.35 | -0.291667 |
| **pDEPTOR** | 0.000000 | 0.000000 | 0.0 | 0.000000 | 0.00 | 0.0 | 0.000000 | 0.00 | 0.291667 |

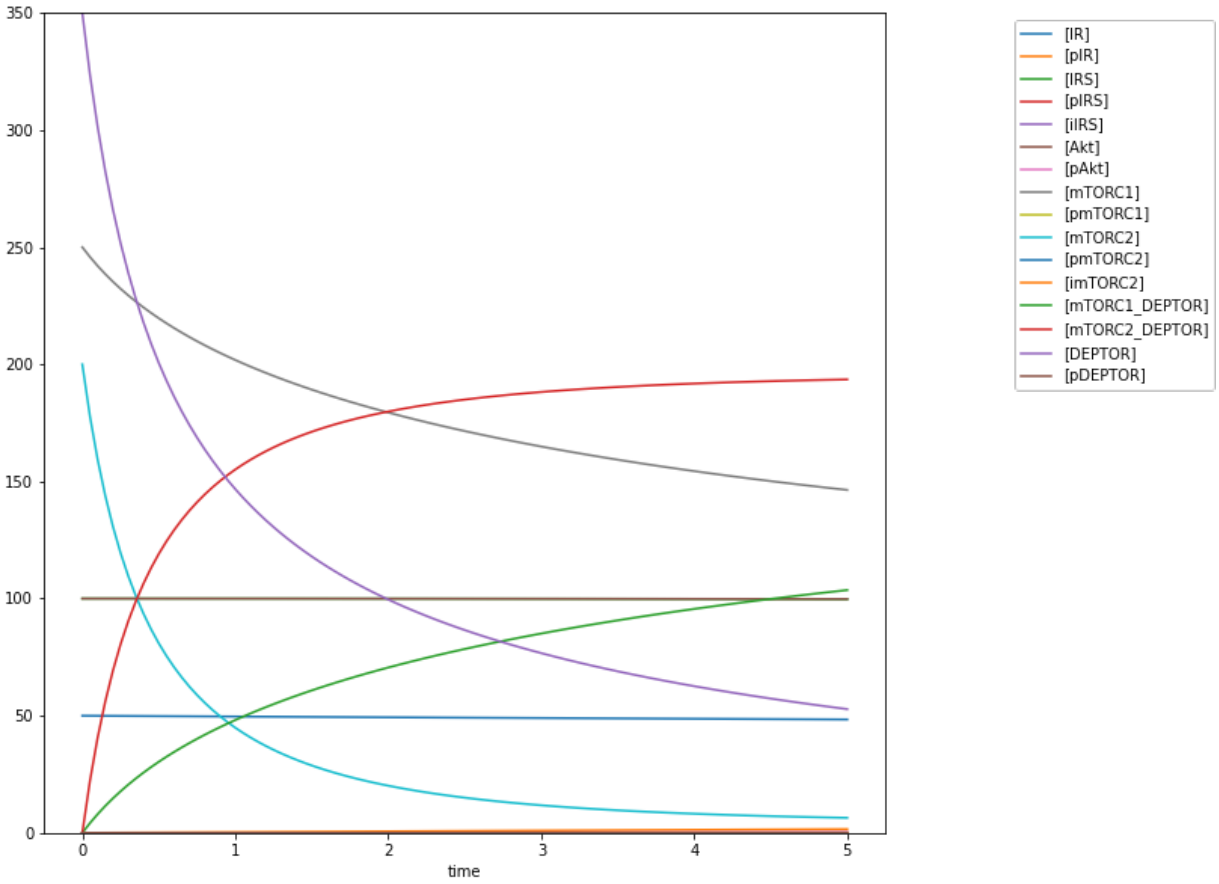
In [6]:
```
# Create a state space representation of the model using the Jacobian at time
ctlsb.setTime(1)
sys = ctlsb.makeStateSpace()
pd.DataFrame(sys.A)
```

Out[6]:

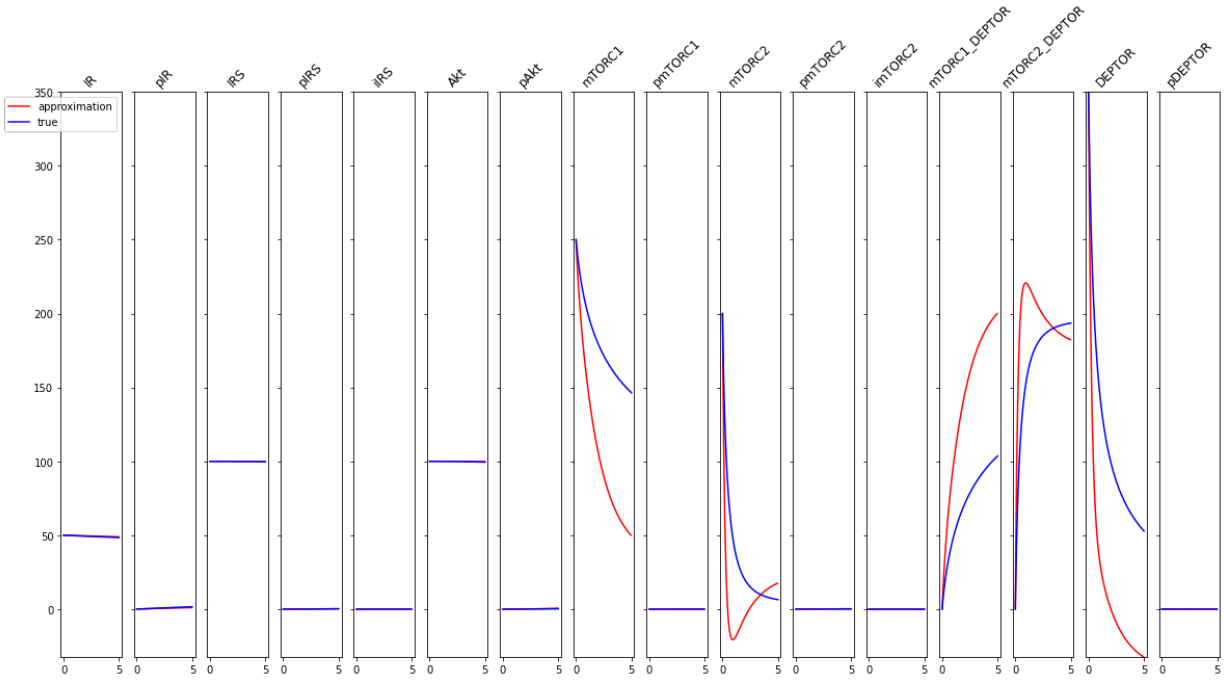
| | 0 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | |
|---|---|---|---|---|---|---|---|---|---|
| **0** | -0.00454 | 0.028026 | 0.000000e+00 | 0.000000 | 0.00 | 0.000000 | 0.000000 | 0.000000e+00 | 0.0000 |
| **1** | 0.00454 | -0.028026 | 0.000000e+00 | 0.000000 | 0.00 | 0.000000 | 0.000000 | 0.000000e+00 | 0.0000 |
| **2** | 0.00000 | -0.066664 | -7.541108e-05 | 0.019991 | 0.02 | 0.000000 | 0.000000 | 0.000000e+00 | -0.0666 |
| **3** | 0.00000 | 0.066664 | 7.539203e-05 | -0.019991 | 0.00 | 0.000000 | 0.000000 | 0.000000e+00 | 0.0000 |
| **4** | 0.00000 | 0.000000 | 1.904712e-08 | 0.000000 | -0.02 | 0.000000 | 0.000000 | 0.000000e+00 | 0.0666 |
| **5** | 0.00000 | 0.000000 | 0.000000e+00 | -0.046729 | 0.00 | -0.000008 | 0.058797 | 0.000000e+00 | 0.0000 |
| **6** | 0.00000 | 0.000000 | 0.000000e+00 | 0.046729 | 0.00 | 0.000008 | -0.058797 | 0.000000e+00 | 0.0000 |
| **7** | 0.00000 | 0.000000 | 0.000000e+00 | 0.000000 | 0.00 | 0.000000 | -0.099019 | -1.467335e-01 | 5.9989 |
| **8** | 0.00000 | 0.000000 | 0.000000e+00 | 0.000000 | 0.00 | 0.000000 | 0.099019 | 3.691504e-08 | -5.9989 |
| **9** | 0.00000 | -0.065718 | 0.000000e+00 | 0.000000 | 0.00 | 0.000000 | 0.000000 | 0.000000e+00 | 0.0000 |
| **10** | 0.00000 | 0.065718 | 0.000000e+00 | 0.000000 | 0.00 | 0.000000 | 0.000000 | 0.000000e+00 | 0.0000 |
| **11** | 0.00000 | 0.000000 | 0.000000e+00 | 0.000000 | 0.00 | 0.000000 | 0.000000 | 0.000000e+00 | 0.0000 |

| | 0 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | |
|---|---|---|---|---|---|---|---|---|---|
| **12** | 0.00000 | 0.000000 | 0.000000e+00 | 0.000000 | 0.00 | 0.000000 | 0.000000 | 1.467334e-01 | 0.0000 |
| **13** | 0.00000 | 0.000000 | 0.000000e+00 | 0.000000 | 0.00 | 0.000000 | 0.000000 | 0.000000e+00 | 0.0000 |
| **14** | 0.00000 | 0.000000 | 0.000000e+00 | 0.000000 | 0.00 | 0.000000 | 0.000000 | -1.467334e-01 | -0.1222 |

In [7]:
```
# Plot roadrunner simulation, with better placement of the legend.
ctlsb.plotTrueModel()
```




In [8]:
```
# Compare the linear approximation using the Jacobian at time 0 with the true
ctlsb.setTime(1)
ctlsb.plotLinearApproximation(figsize=(20, 10))
```


IR
pIR
IRS
pIRS
iIRS
Akt
pAkt
mTORC1
pmTORC1
rmTORC2
pmTORC2
imTORC2
mTORC1_DEPTOR
mTORC2_DEPTOR
DEPTOR
pDEPTOR
approximation
true
350
300
250
200
150
100
50
0
0
5