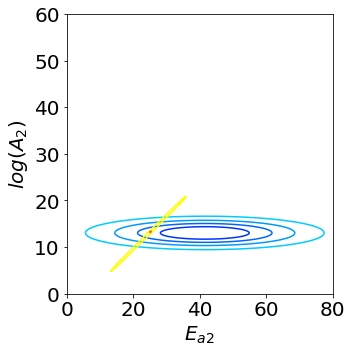
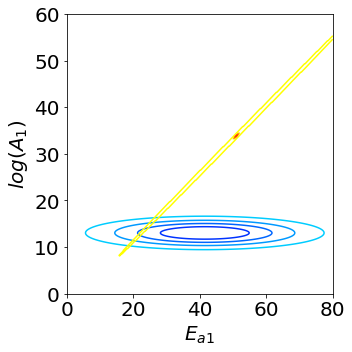
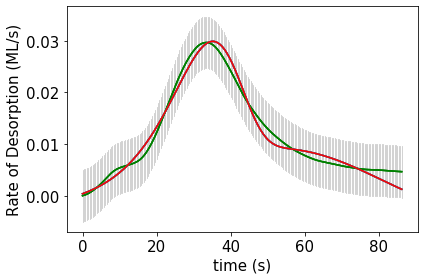
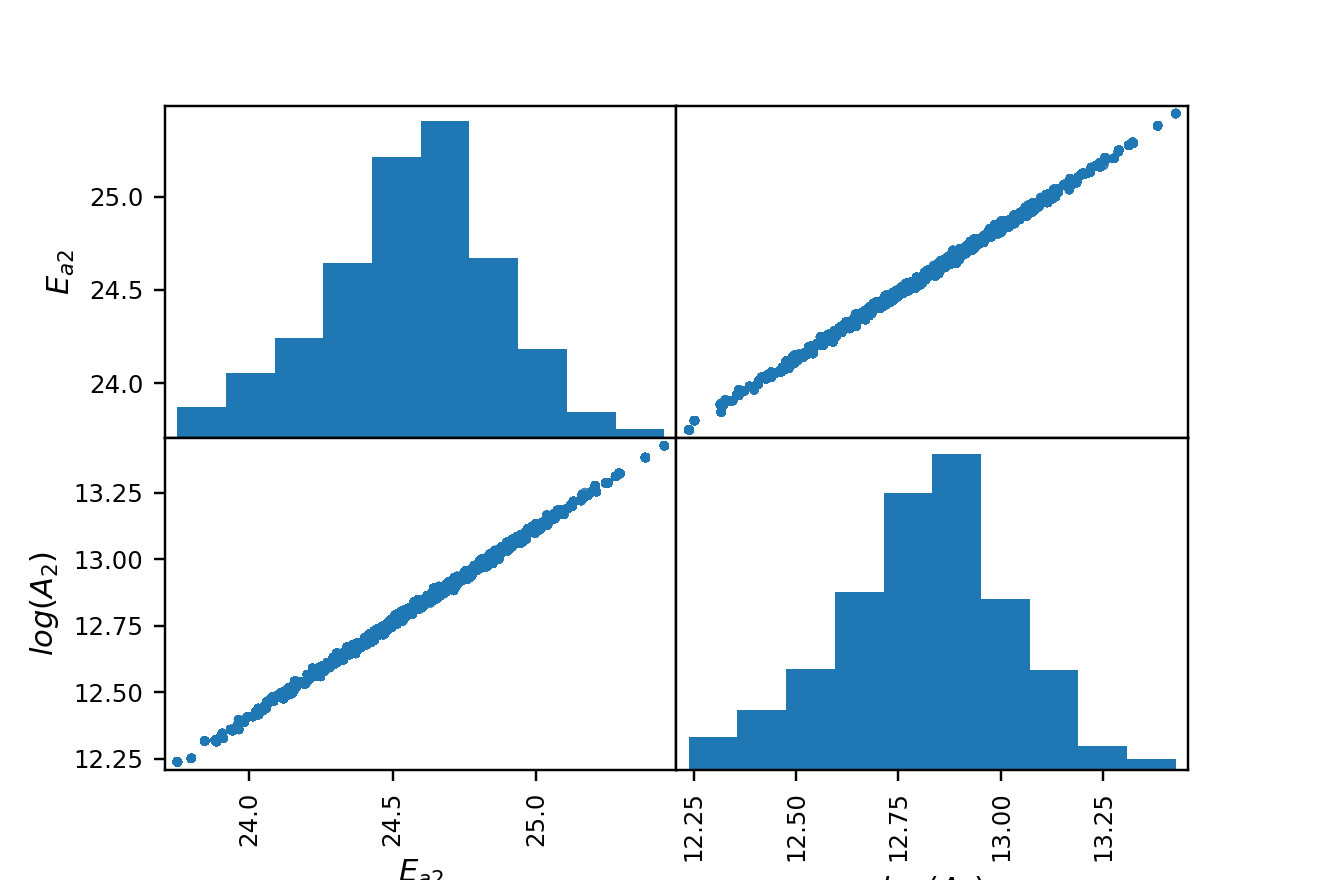
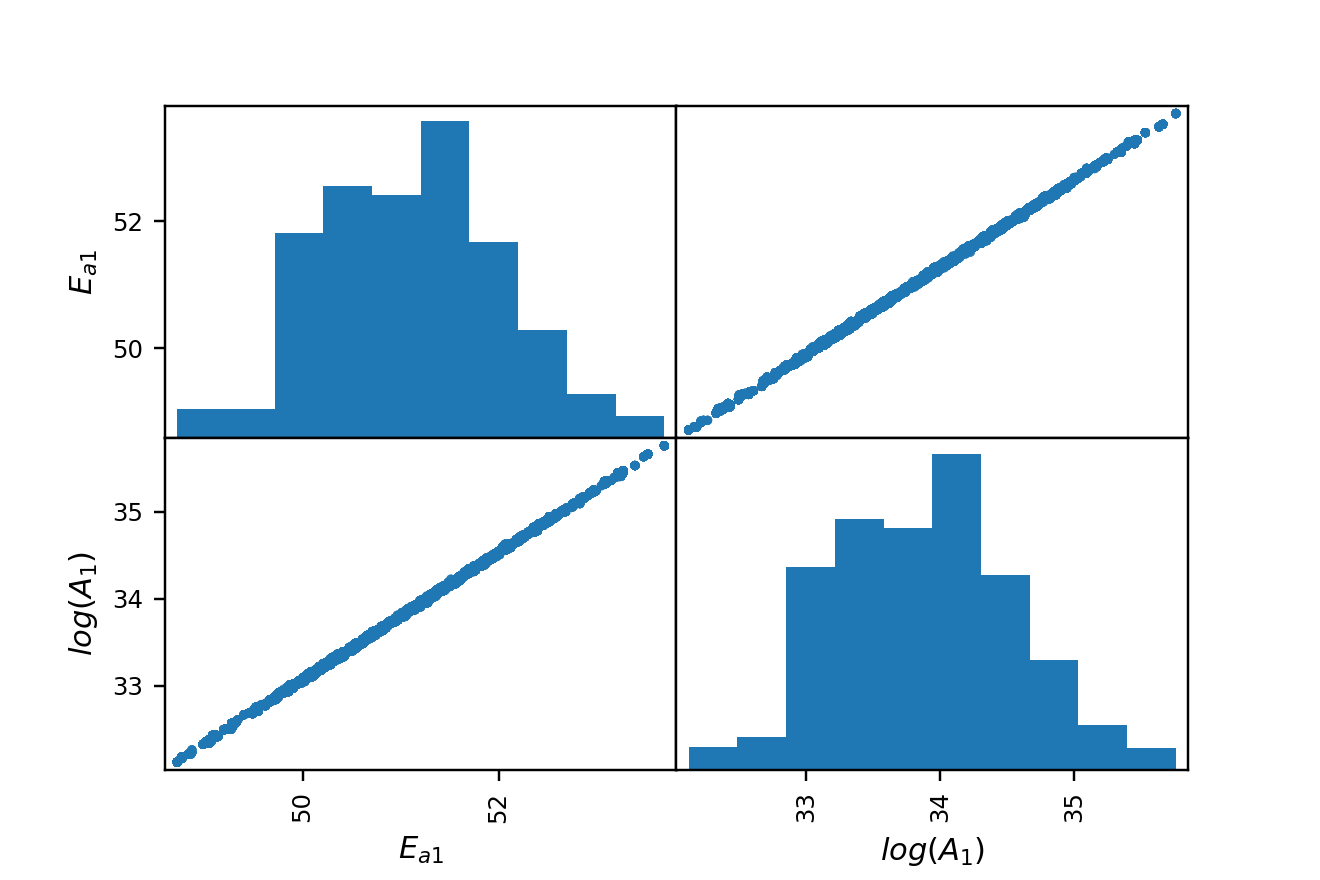
Name of Runfile: runfile\_Example19a\_CPE\_grid\_opt 243 points

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Parameter Name** | **Initial Value** | **Uncertainty** | **Final Value** | **Uncertainty** |
| Scaling | 1.0 | 0.10 | 1.31421932e+00 |  |
| Offset | 0.0 | 0.005 | 2.35426700e-03 |  |
| Site2Ratio | 0.50 | 0.50/3 | 5.83002034e-01 |  |
| Ea\_1 | 41.5 | 20 | 5.13330577e+01 |  |
| Ea\_2 | 41.5 | 20 | 2.45940382e+01 |  |
| log\_A1 | 13.0 | 2 | 3.40421731e+01 |  |
| log\_A2 | 13.0 | 2 | 1.28288185e+01 |  |
| gamma1 | 0.1 | 0.1 | 7.02821337e-08 |  |
| gamma2 | 0.1 | 0.1 | 1.72447219e+00 |  |
| logP |  | N/A | 699.3353304927623 | N/A |

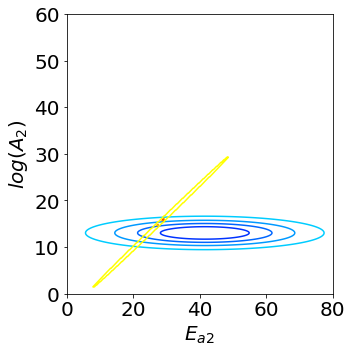
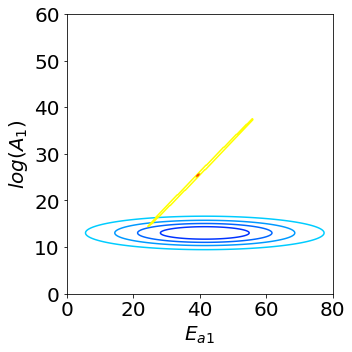
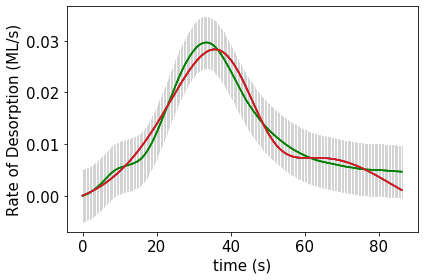
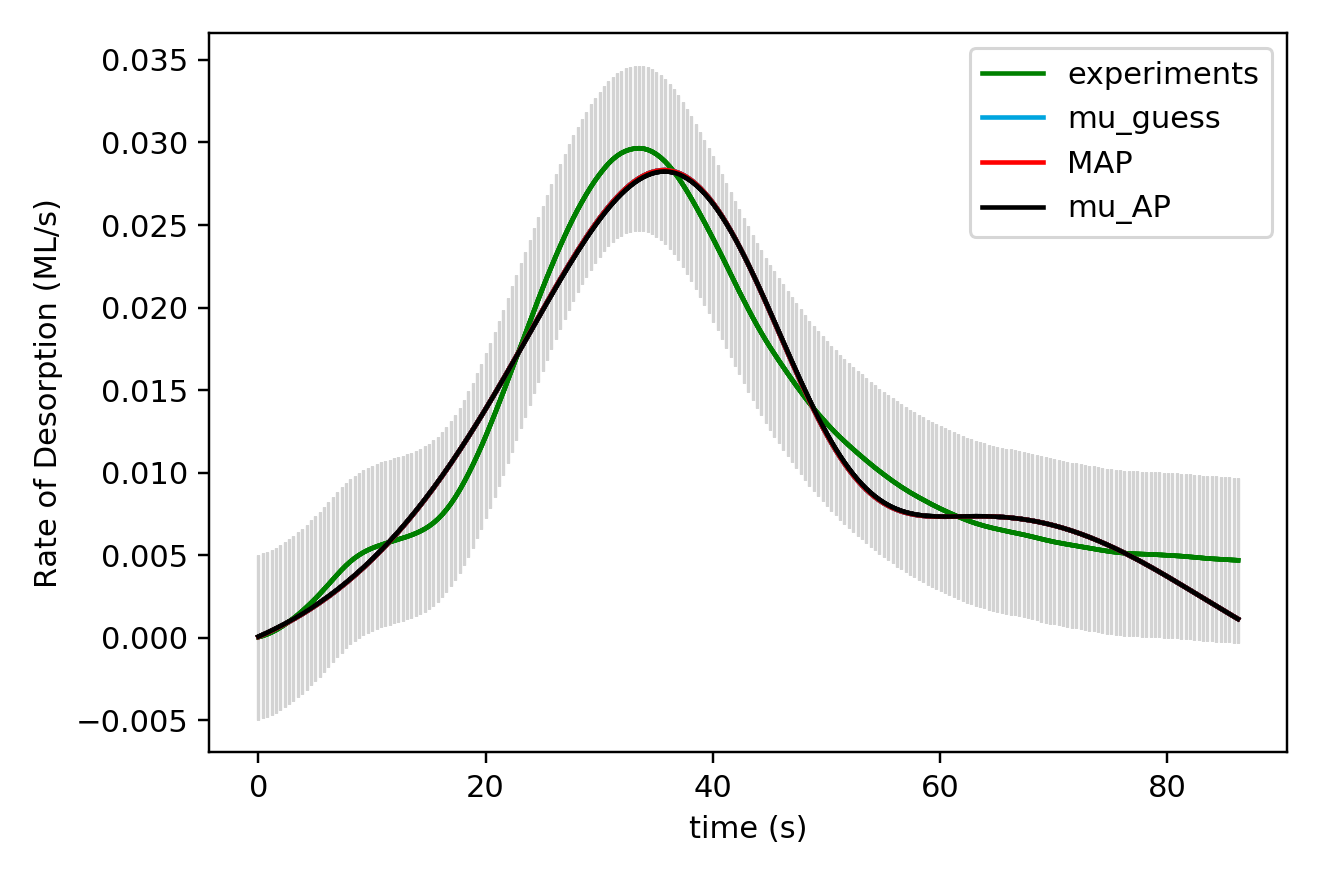


Final results from doOptimizeNegLogP: [1.31421932e+00 2.35426700e-03 5.83002034e-01 5.13330577e+01 2.45940382e+01 3.40421731e+01 1.28288185e+01 7.02821337e-08 1.72447219e+00] final logP: 699.3353304927623

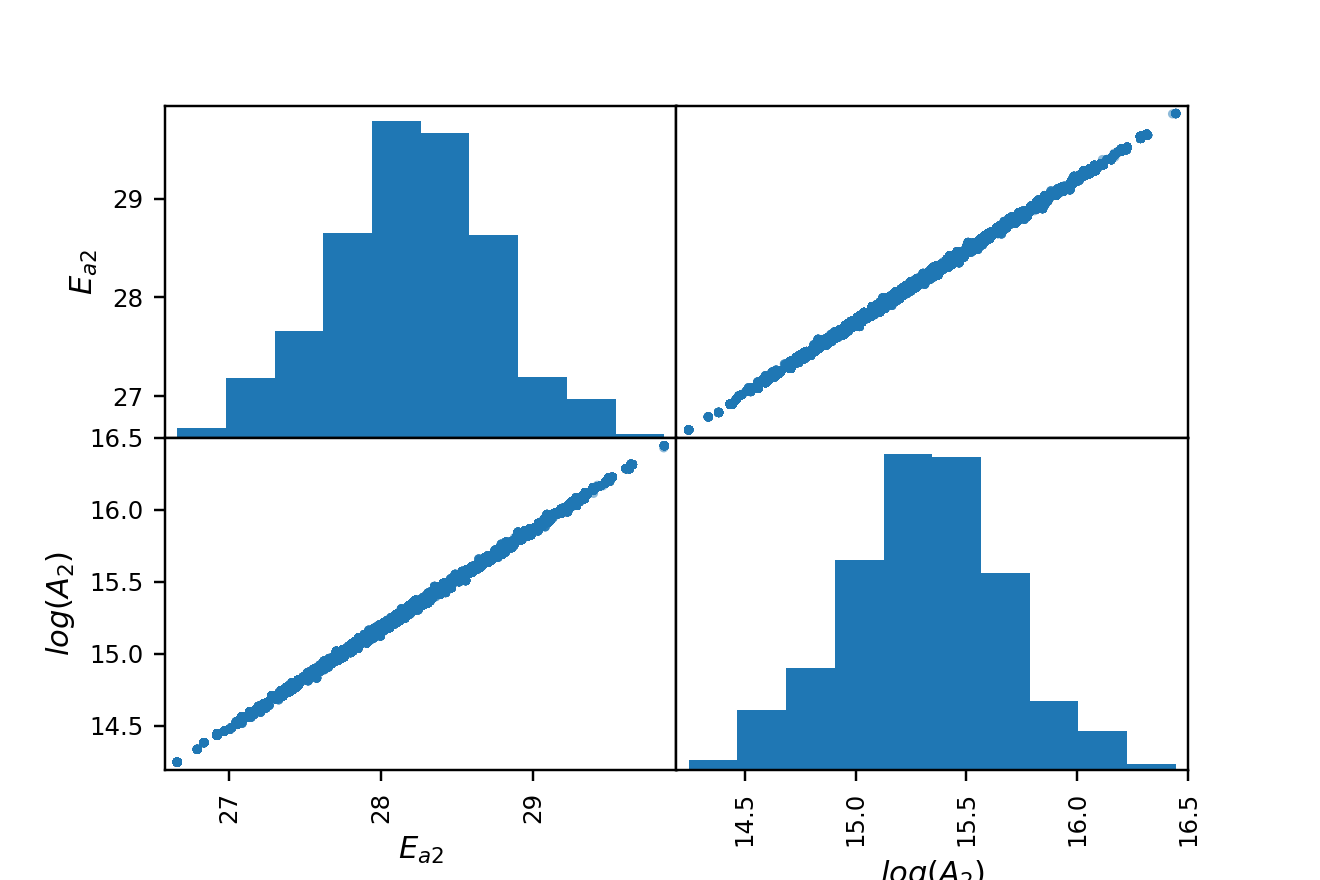
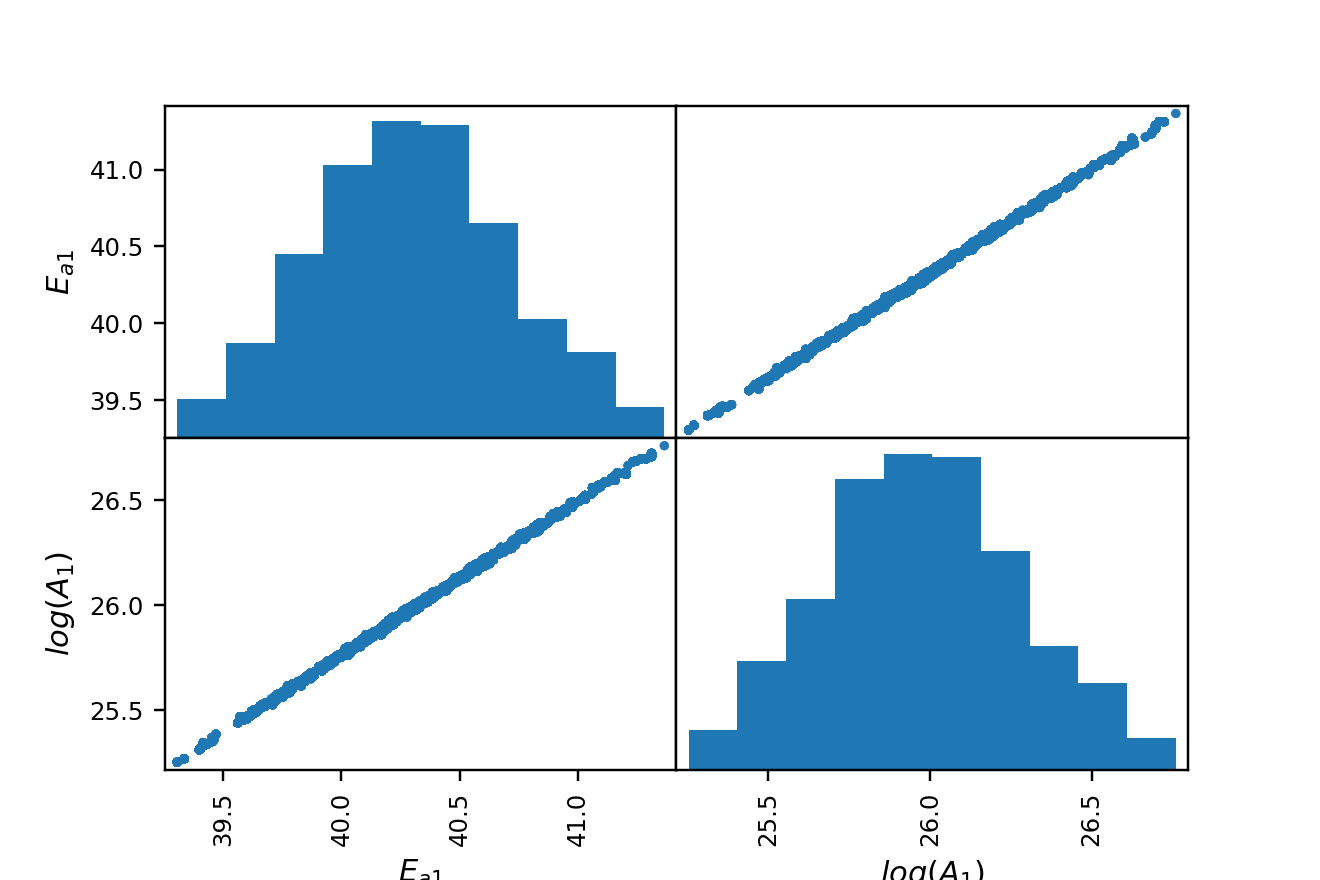


Name of Runfile: runfile\_Example19a\_BPE\_grid\_opt 243 points

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Parameter Name** | **Initial Value** | **Uncertainty** | **Final Value** | **Uncertainty** |
| Scaling | 1.0 | 0.10 | 1.30780046e+00 |  |
| Offset | 0.0 | 0.005 | 2.38753805e-03 |  |
| Site2Ratio | 0.50 | 0.50/3 | 3.96167260e-01 |  |
| Ea\_1 | 41.5 | 20 | 4.04366288e+01 |  |
| Ea\_2 | 41.5 | 20 | 2.82381353e+01 |  |
| log\_A1 | 13.0 | 2 | 2.60829373e+01 |  |
| log\_A2 | 13.0 | 2 | 1.53386412e+01 |  |
| gamma1 | 0.1 | 0.1 | 9.88872337e-08 |  |
| gamma2 | 0.1 | 0.1 | 9.63298973e-02 |  |
| logP |  | N/A | 656.1518643147978 | N/A |

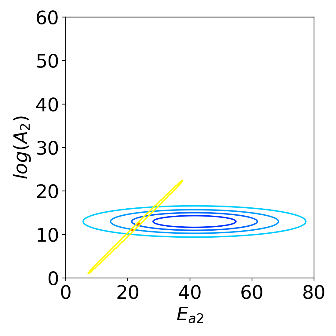
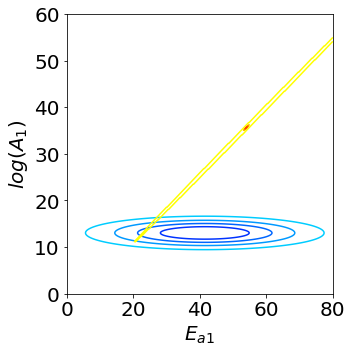
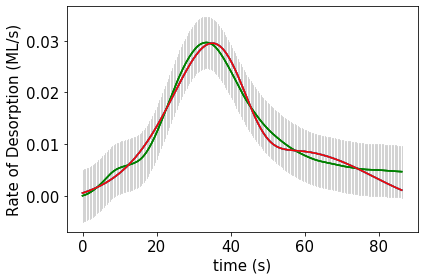


Final results from doOptimizeNegLogP: [1.30780046e+00 2.38753805e-03 3.96167260e-01 4.04366288e+01 2.82381353e+01 2.60829373e+01 1.53386412e+01 9.88872337e-08 9.63298973e-02] final logP: 656.1518643147978



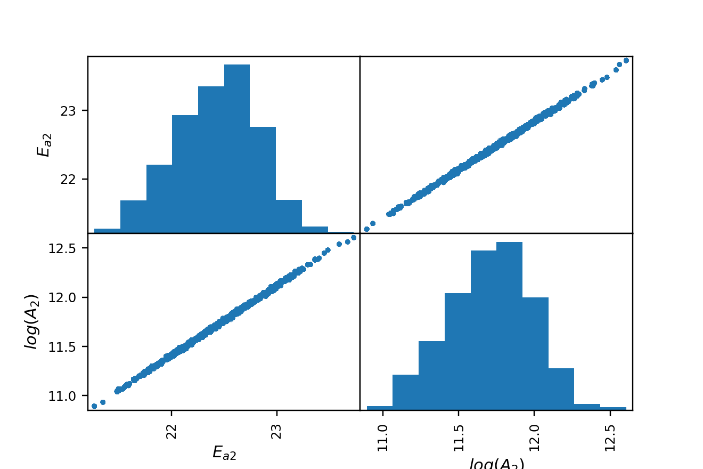
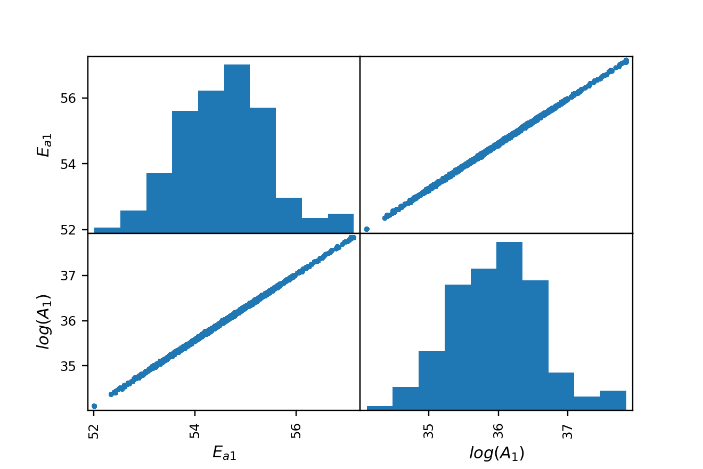
Name of Runfile: 20a\_CPE\_grid\_opt 243 points

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Parameter Name** | **Initial Value** | **Uncertainty** | **Final Value** | **Uncertainty** |
| Scaling | 1.0 | 0.10 |  |  |
| Offset | 0.0 | 0.005 |  |  |
| Site2Ratio | 0.50 | 0.50/3 |  |  |
| Ea\_1 | 41.5 | 20 |  |  |
| Ea\_2 | 41.5 | 20 |  |  |
| log\_A1 | 13.0 | 2 |  |  |
| log\_A2 | 13.0 | 2 |  |  |
| gamma1 | 0.1 | 0.1 |  |  |
| gamma2 | 0.1 | 0.1 |  |  |
| logP |  | N/A |  |  |



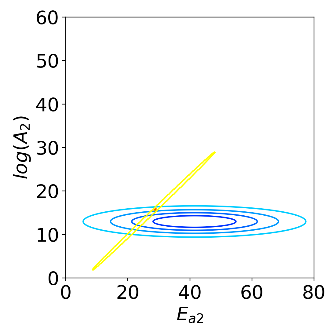
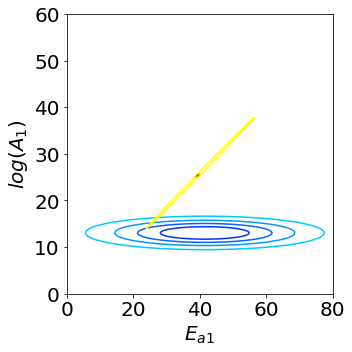
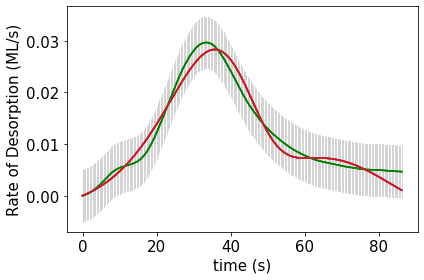
Final results from doOptimizeNegLogP: [1.21355547e+00 1.74845211e-03 5.06714710e-01 5.46160957e+01 2.24663731e+01 3.60124850e+01 1.17382693e+01 7.30286649e-01

2.26749171e-05] final logP: 699.3022446923912



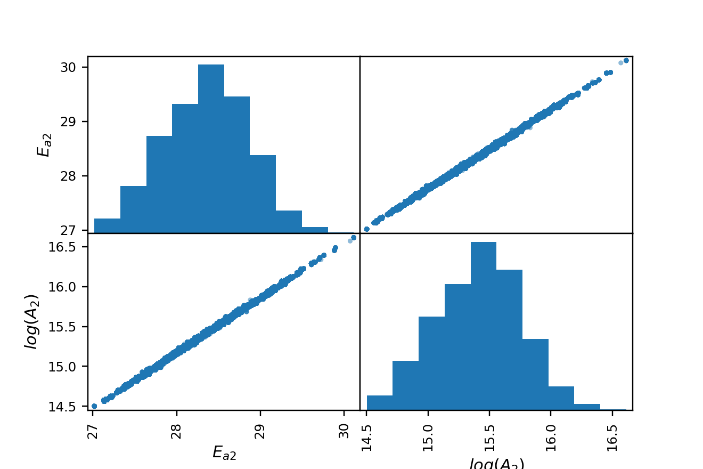
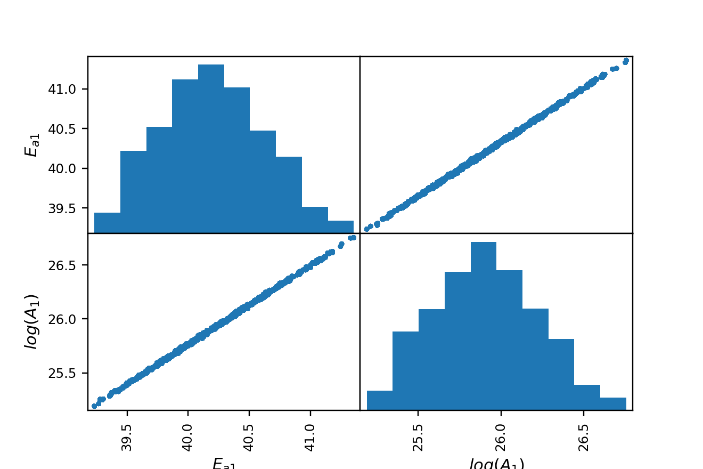
Name of Runfile: 20a\_BPE\_grid\_opt 243 points

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Parameter Name** | **Initial Value** | **Uncertainty** | **Final Value** | **Uncertainty** |
| Scaling | 1.0 | 0.10 |  |  |
| Offset | 0.0 | 0.005 |  |  |
| Site2Ratio | 0.50 | 0.50/3 |  |  |
| Ea\_1 | 41.5 | 20 |  |  |
| Ea\_2 | 41.5 | 20 |  |  |
| log\_A1 | 13.0 | 2 |  |  |
| log\_A2 | 13.0 | 2 |  |  |
| gamma1 | 0.1 | 0.1 |  |  |
| gamma2 | 0.1 | 0.1 |  |  |
| logP |  | N/A |  |  |



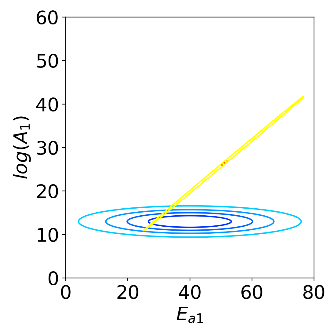
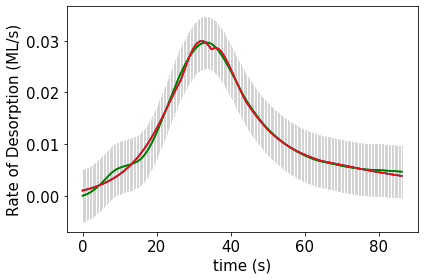
Final results from doOptimizeNegLogP: [1.31127639e+00 2.41324344e-03 6.04122702e-01 2.84225571e+01 4.03158778e+01 1.54584948e+01 2.59928937e+01 8.29500179e-02 9.48684766e-09] final logP: 656.0563026370578 Reverse site order:

Final results from doOptimizeNegLogP: [1.31127639e+00 2.41324344e-03 0.395877298 4.03158778e+01 2.84225571e+01 2.59928937e+01 1.54584948e+01 9.48684766e-09 8.29500179e-02] final logP: 656.0563026370578

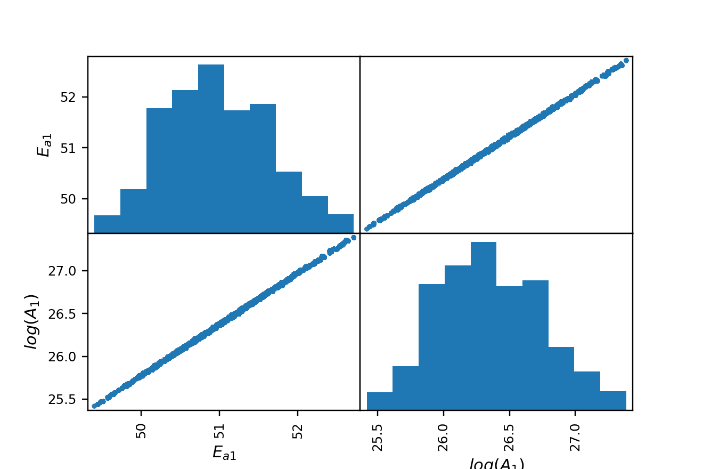


Name of Runfile: 21a\_CPE\_grid\_mcmc 243 points

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Parameter Name** | **Initial Value** | **Uncertainty** | **Final Value** | **Uncertainty** |
| Scaling | 1 | .1 | 1.17368386e+00 |  |
| Offset | 0 | .005 | 5.47779012e-04 |  |
| Ea\_1 | 40 | 20 | 5.10933629e+01 |  |
| Log\_A1 | 13 | 2 | 2.64261595e+01 |  |
| gamma\_1 | 0.1 | 0.3 | -3.63005846e-01 |  |
| gamma\_mod1 | 0 | 0.1 | 1.02209077e+00 |  |
| gamma\_mod2 | 0 | 0.1 | -1.65337855e-01 |  |
| gamma\_mod3 | 0 | 0.1 | -1.05166295e-01 |  |
| gamma\_mod4 | 0 | 0.1 | -9.10023180e-02 |  |
| gamma\_mod5 | 0 | 0.1 | -6.68286021e-02 |  |
| gamma\_mod6 | 0 | 0.1 | -5.32330378e-02 |  |
| logP |  |  | 703.6255581383327 |  |

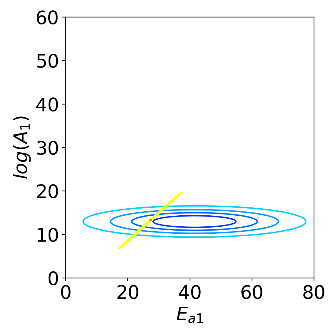
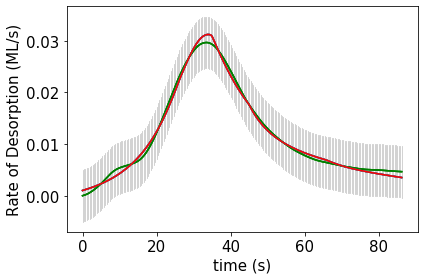


Final results from doOptimizeNegLogP: [ 1.17368386e+00 5.47779012e-04 5.10933629e+01 2.64261595e+01 -3.63005846e-01 1.02209077e+00 -1.65337855e-01 -1.05166295e-01 -9.10023180e-02 -6.68286021e-02 -5.32330378e-02] final logP: 703.6255581383327



Name of Runfile: 21a\_BPE\_grid\_mcmc 243 points

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Parameter Name** | **Initial Value** | **Uncertainty** | **Final Value** | **Uncertainty** |
| Scaling | 1 | .1 | 1.28851541e+00 |  |
| Offset | 0 | .005 | 1.76289404e-03 |  |
| Ea\_1 | 40 | 20 | 2.72954925e+01 |  |
| Log\_A1 | 13 | 2 | 1.32623534e+01 |  |
| gamma\_1 | 0.1 | 0.3 | 1.23034376e-01 |  |
| gamma\_mod1 | 0 | 0.1 | 2.95334492e-02 |  |
| gamma\_mod2 | 0 | 0.1 | 1.30795864e-01 |  |
| gamma\_mod3 | 0 | 0.1 | 6.19306330e-03 |  |
| gamma\_mod4 | 0 | 0.1 | -4.35789424e-02 |  |
| gamma\_mod5 | 0 | 0.1 | -7.13674248e-02 |  |
| gamma\_mod6 | 0 | 0.1 | -7.81026579e-02 |  |
| logP |  |  | 704.9080568893369 |  |



Final results from doOptimizeNegLogP: [ 1.28851541e+00 1.76289404e-03 2.72954925e+01 1.32623534e+01 1.23034376e-01 2.95334492e-02 1.30795864e-01 6.19306330e-03 -4.35789424e-02 -7.13674248e-02 -7.81026579e-02] final logP: 704.9080568893369

