Name of Runfile: runfile\_Example19a\_CPE\_grid 1361367 points

|  |  |  |  |
| --- | --- | --- | --- |
| **Parameter Name** | **Initial Value** | **Uncertainty** | **Final Value** |
| Scaling | 1.0 | 0.10 | 1.20211634e+00 |
| Offset | 0.0 | 0.005 | 1.70181657e-03 |
| Site2Ratio | 0.50 | 0.50/3 | 4.94458588e-01 |
| Ea\_1 | 41.5 | 20 | 2.36031461e+01 |
| Ea\_2 | 41.5 | 20 | 5.18978020e+01 |
| log\_A1 | 13.0 | 2 | 1.25026762e+01 |
| log\_A2 | 13.0 | 2 | 3.43682980e+01 |
| gamma1 | 0.1 | 0.1 | 1.81157414e-01 |
| gamma2 | 0.1 | 0.1 | 3.71989231e-01 |
| logP |  | N/A | 699.008579223728 |

Final results from doOptimizeNegLogP: [1.20211634e+00 1.70181657e-03 4.94458588e-01 2.36031461e+01 5.18978020e+01 1.25026762e+01 3.43682980e+01 1.81157414e-01 3.71989231e-01] final logP: 699.008579223728

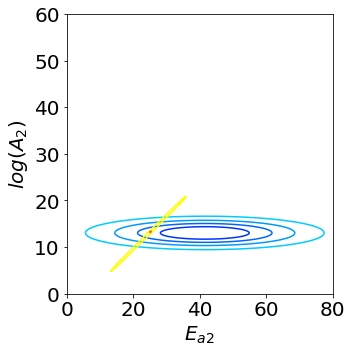
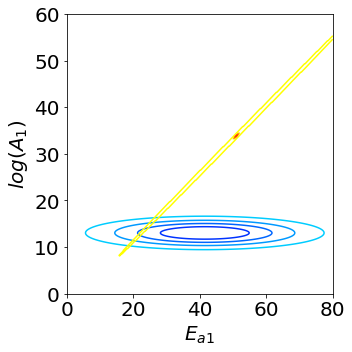
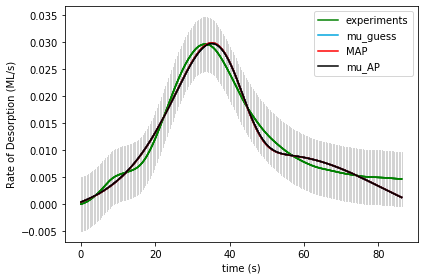
Name of Runfile: runfile\_Example19a\_BPE\_grid 1361367 points

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Parameter Name** | **Initial Value** | **Uncertainty** | **Final Value** | **Uncertainty** |
| Scaling | 1.0 | 0.10 | 1.97263453e+00 |  |
| Offset | 0.0 | 0.005 | 3.50013685e-03 |  |
| Site2Ratio | 0.50 | 0.50/3 | 5.50608444e-01 |  |
| Ea\_1 | 41.5 | 20 | 2.55827249e+01 |  |
| Ea\_2 | 41.5 | 20 | 3.23192191e+01 |  |
| log\_A1 | 13.0 | 2 | 1.23522015e+01 |  |
| log\_A2 | 13.0 | 2 | 1.99750895e+01 |  |
| gamma1 | 0.1 | 0.1 | 9.54750144e-01 |  |
| gamma2 | 0.1 | 0.1 | 3.63390509e-01 |  |
| logP |  | N/A | 558.9918553187981 | N/A |

Final results from doOptimizeNegLogP: [1.97263453e+00 3.50013685e-03 5.50608444e-01 2.55827249e+01 3.23192191e+01 1.23522015e+01 1.99750895e+01 9.54750144e-01 3.63390509e-01] final logP: 558.9918553187981

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

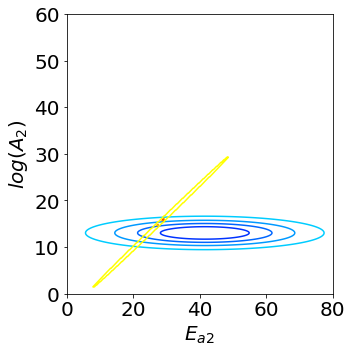
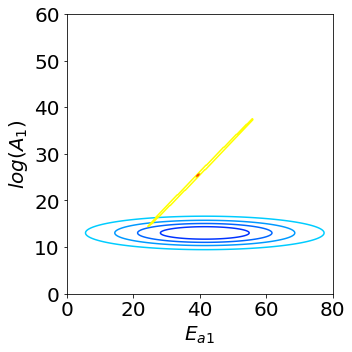
|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Parameter Name** | **Initial Value** | **Uncertainty** | **Final Value** | **Uncertainty** |
| Scaling | 1.0 | 0.10 | 1.31421932e+00 |  |
| Offset | 0.0 | 0.005 | 2.35426700e-03 |  |
| Site2Ratio | 0.50 | 0.50/3 | 5.83002034e-01 |  |
| Ea\_1 | 41.5 | 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: 19a\_CPE\_grid\_mcmc 243 points

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Parameter Name** | **Initial Value** | **Uncertainty** | **Final Value** | **Uncertainty** |
| Scaling | 1.0 | 0.10 | 1.76790946e+00 |  |
| Offset | 0.0 | 0.005 | 5.49443957e-03 |  |
| Site2Ratio | 0.50 | 0.50/3 | 4.52973126e-01 |  |
| Ea\_1 | 41.5 | 20 | 2.48833920e+01 |  |
| Ea\_2 | 41.5 | 20 | 2.62763349e+01 |  |
| log\_A1 | 13.0 | 2 | 1.47619158e+01 |  |
| log\_A2 | 13.0 | 2 | 1.44338901e+01 |  |
| gamma1 | 0.1 | 0.1 | 1.44211740e-02 |  |
| gamma2 | 0.1 | 0.1 | 1.26259207e-10 |  |
| logP |  | N/A | 482.93725416456704 | N/A |

Final results from doOptimizeNegLogP: [1.76790946e+00 5.49443957e-03 4.52973126e-01 2.48833920e+01 2.62763349e+01 1.47619158e+01 1.44338901e+01 1.44211740e-02 1.26259207e-10] final logP: 482.93725416456704

Name of Runfile: 19a\_BPE\_grid\_mcmc 243 points

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Parameter Name** | **Initial Value** | **Uncertainty** | **Final Value** | **Uncertainty** |
| Scaling | 1.0 | 0.10 | 1.32117883e+00 |  |
| Offset | 0.0 | 0.005 | 3.61785840e-03 |  |
| Site2Ratio | 0.50 | 0.50/3 | 1.22430317e-04 |  |
| Ea\_1 | 41.5 | 20 | 2.60743217e+01 |  |
| Ea\_2 | 41.5 | 20 | 2.46383070e+01 |  |
| log\_A1 | 13.0 | 2 | 1.51326537e+01 |  |
| log\_A2 | 13.0 | 2 | 1.47230472e+01 |  |
| gamma1 | 0.1 | 0.1 | 4.55066303e-07 |  |
| gamma2 | 0.1 | 0.1 | 1.17964962e-01 |  |
| logP |  | N/A | 325.7457657638958 |  |

Final results from doOptimizeNegLogP: [1.32117883e+00 3.61785840e-03 1.22430317e-04 2.60743217e+01 2.46383070e+01 1.51326537e+01 1.47230472e+01 4.55066303e-07 1.17964962e-01] final logP: 325.7457657638958

Name of Runfile: runfile\_Example19a\_CPE\_grid\_fine 1361367 points

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Parameter Name** | **Initial Value** | **Uncertainty** | **Final Value** | **Uncertainty** |
| Scaling | 1.0 | 0.10 | 1.97414341e+00 |  |
| Offset | 0.0 | 0.005 | 3.97844007e-03 |  |
| Site2Ratio | 0.50 | 0.50/3 | 4.58532911e-01 |  |
| Ea\_1 | 41.5 | 20 | 2.96667546e+01 |  |
| Ea\_2 | 41.5 | 20 | 1.89905007e+01 |  |
| log\_A1 | 13.0 | 2 | 1.81043133e+01 |  |
| log\_A2 | 13.0 | 2 | 8.32550743e+00 |  |
| gamma1 | 0.1 | 0.1 | 1.22172150e-12 |  |
| gamma2 | 0.1 | 0.1 | 4.38660989e-01 |  |
| logP |  | N/A | 640.1080542544692 | N/A |

Final results from doOptimizeNegLogP: [1.97414341e+00 3.97844007e-03 4.58532911e-01 2.96667546e+01 1.89905007e+01 1.81043133e+01 8.32550743e+00 1.22172150e-12 4.38660989e-01] final logP: 640.1080542544692

Name of Runfile: runfile\_Example19a\_BPE\_grid\_fine 1361367 points

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Parameter Name** | **Initial Value** | **Uncertainty** | **Final Value** | **Uncertainty** |
| Scaling | 1.0 | 0.10 | 1.27833531e+00 |  |
| Offset | 0.0 | 0.005 | 2.13793051e-03 |  |
| Site2Ratio | 0.50 | 0.50/3 | 2.90554984e-01 |  |
| Ea\_1 | 41.5 | 20 | 3.67789955e+01 |  |
| Ea\_2 | 41.5 | 20 | 3.04767217e+01 |  |
| log\_A1 | 13.0 | 2 | 2.32578508e+01 |  |
| log\_A2 | 13.0 | 2 | 1.64995600e+01 |  |
| gamma1 | 0.1 | 0.1 | 9.14278150e-11 |  |
| gamma2 | 0.1 | 0.1 | 1.31620425e-04 |  |
| logP |  | N/A | 629.5435677195965 | N/A |

Final results from doOptimizeNegLogP: [1.27833531e+00 2.13793051e-03 2.90554984e-01 3.67789955e+01 3.04767217e+01 2.32578508e+01 1.64995600e+01 9.14278150e-11 1.31620425e-04] final logP: 629.5435677195965

Name of Runfile: 20a\_CPE\_grid 1361367 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: [1.74369653e+00 3.85583260e-03 4.65236701e-01 3.43843984e+01

2.33926769e+01 2.16637499e+01 1.16939088e+01 2.98832055e-02

2.03512673e-01] final logP: 678.3232828162805

Name of Runfile: 20a\_BPE\_grid 1361367 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: [1.33331902e+00 2.48941682e-03 4.20779351e-01 4.07668743e+01

2.65069502e+01 2.62995915e+01 1.41588821e+01 3.99282063e-02

1.61157410e-01] final logP: 655.0895815045784

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: 20a\_CPE\_grid\_mcmc 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: [1.39603735e+00 2.77496348e-03 4.21606751e-01 3.92761524e+01

2.79373537e+01 2.52280353e+01 1.49492243e+01 7.35775644e-12

5.44236063e-01] final logP: 691.3112594737023

Name of Runfile: 20a\_BPE\_grid\_mcmc 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: [ 9.19069198e-01 -3.00044520e-04 7.83364640e-03 3.86757896e+01

7.43913674e+01 2.42817823e+01 1.27653110e+01 1.04810967e-01

5.18390652e-11] final logP: 398.73287031833854

Name of Runfile: runfile\_Example20a\_CPE\_grid\_fine 1361367 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 |  | N/A |

Final results from doOptimizeNegLogP: [3.05906353e+00 5.28243686e-03 1.81917087e-01 9.18307078e+00

5.43232363e+01 2.10504512e+00 3.55820328e+01 1.36765638e-11

9.55367229e-01] final logP: 696.5447975227618

Name of Runfile: runfile\_Example20a\_BPE\_grid\_fine 1361367 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 |  | N/A |

Final results from doOptimizeNegLogP: [1.44166046e+00 3.12549995e-03 6.18297644e-01 2.95532737e+01

3.63750480e+01 1.60531654e+01 2.31080860e+01 1.58537754e-01

9.98379497e-15] final logP: 651.4471609533417

Name of Runfile: 21a\_CPE\_grid 59535 points

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Parameter Name** | **Initial Value** | **Uncertainty** | **Final Value** | **Uncertainty** |
| Scaling | 1 | .1 | 1.05002437e+00 |  |
| Offset | 0 | .005 | 3.14064264e-04 |  |
| Ea\_1 | 40 | 20 | 4.20937447e+01 |  |
| Log\_A1 | 13 | 2 | 2.47895534e+01 |  |
| gamma\_1 | 0.1 | 0.3 | -5.68254307e-01 |  |
| gamma\_mod1 | 0 | 0.1 | 6.57744612e-03 |  |
| gamma\_mod2 | 0 | 0.1 | 6.69010130e-01 |  |
| gamma\_mod3 | 0 | 0.1 | 1.67294858e-02 |  |
| gamma\_mod4 | 0 | 0.1 | -1.10890142e-02 |  |
| gamma\_mod5 | 0 | 0.1 | -2.55082426e-02 |  |
| gamma\_mod6 | 0 | 0.1 | -3.33941904e-02 |  |
| logP |  |  | 700.9710577216481 |  |

Final results from doOptimizeNegLogP: [ 1.05002437e+00 3.14064264e-04 4.20937447e+01 2.47895534e+01 -5.68254307e-01 6.57744612e-03 6.69010130e-01 1.67294858e-02 -1.10890142e-02 -2.55082426e-02 -3.33941904e-02] final logP: 700.9710577216481

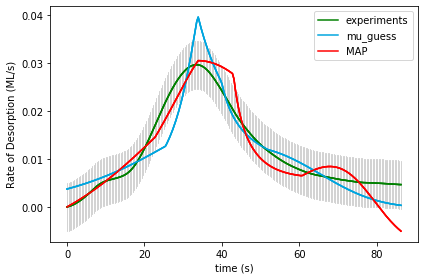
Name of Runfile: 21a\_BPE\_grid 59535 points

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Parameter Name** | **Initial Value** | **Uncertainty** | **Final Value** | **Uncertainty** |
| Scaling | 1 | .1 | 1.08814515e+00 |  |
| Offset | 0 | .005 | 6.52138337e-04 |  |
| Ea\_1 | 40 | 20 | 3.32080624e+01 |  |
| Log\_A1 | 13 | 2 | 1.82085466e+01 |  |
| gamma\_1 | 0.1 | 0.3 | 1.38466271e-01 |  |
| gamma\_mod1 | 0 | 0.1 | -9.02361398e-03 |  |
| gamma\_mod2 | 0 | 0.1 | 5.75061231e-02 |  |
| gamma\_mod3 | 0 | 0.1 | 2.15891832e-02 |  |
| gamma\_mod4 | 0 | 0.1 | -5.49028647e-02 |  |
| gamma\_mod5 | 0 | 0.1 | -3.33494600e-02 |  |
| gamma\_mod6 | 0 | 0.1 | -6.10868941e-02 |  |
| logP |  |  | 704.7922967800008 |  |

Final results from doOptimizeNegLogP: [ 1.08814515e+00 6.52138337e-04 3.32080624e+01 1.82085466e+01 1.38466271e-01 -9.02361398e-03 5.75061231e-02 2.15891832e-02 -5.49028647e-02 -3.33494600e-02 -6.10868941e-02] final logP: 704.7922967800008

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

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Parameter Name** | **Initial Value** | **Uncertainty** | **Final Value** | **Uncertainty** |
| Scaling | 1 | .1 | 1.74310440e+00 |  |
| Offset | 0 | .005 | 8.70006487e-03 |  |
| Ea\_1 | 40 | 20 | 2.12956141e+01 |  |
| Log\_A1 | 13 | 2 | 1.15946417e+01 |  |
| gamma\_1 | 0.1 | 0.3 | -3.33467082e-01 |  |
| gamma\_mod1 | 0 | 0.1 | 6.45219070e-02 |  |
| gamma\_mod2 | 0 | 0.1 | -6.28761998e-04 |  |
| gamma\_mod3 | 0 | 0.1 | 2.92399668e-01 |  |
| gamma\_mod4 | 0 | 0.1 | -9.66804716e-04 |  |
| gamma\_mod5 | 0 | 0.1 | -3.00598938e-02 |  |
| gamma\_mod6 | 0 | 0.1 | -5.79978529e-04 |  |
| logP |  |  | 670.6817343596232 |  |



Final results from doOptimizeNegLogP: [ 1.74310440e+00 8.70006487e-03 2.12956141e+01 1.15946417e+01 -3.33467082e-01 6.45219070e-02 -6.28761998e-04 2.92399668e-01 -9.66804716e-04 -3.00598938e-02 -5.79978529e-04] final logP: 670.6817343596232

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

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Parameter Name** | **Initial Value** | **Uncertainty** | **Final Value** | **Uncertainty** |
| Scaling | 1 | .1 | 1.48136991e+00 |  |
| Offset | 0 | .005 | 5.48386499e-03 |  |
| Ea\_1 | 40 | 20 | 3.20125763e+01 |  |
| Log\_A1 | 13 | 2 | 1.79458995e+01 |  |
| gamma\_1 | 0.1 | 0.3 | -5.97845694e-03 |  |
| gamma\_mod1 | 0 | 0.1 | 2.23405217e-02 |  |
| gamma\_mod2 | 0 | 0.1 | 8.39623308e-04 |  |
| gamma\_mod3 | 0 | 0.1 | 1.07252420e-01 |  |
| gamma\_mod4 | 0 | 0.1 | -7.13506696e-03 |  |
| gamma\_mod5 | 0 | 0.1 | -4.36261524e-02 |  |
| gamma\_mod6 | 0 | 0.1 | -9.07648741e-03 |  |
| logP |  |  | 684.9517448596014 |  |

Final results from doOptimizeNegLogP: [ 1.48136991e+00 5.48386499e-03 3.20125763e+01 1.79458995e+01 -5.97845694e-03 2.23405217e-02 8.39623308e-04 1.07252420e-01 -7.13506696e-03 -4.36261524e-02 -9.07648741e-03] final logP: 684.9517448596014

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

Name of Runfile: 21a\_CPE\_grid\_fine 68921 points

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Parameter Name** | **Initial Value** | **Uncertainty** | **Final Value** | **Uncertainty** |
| Scaling | 1 | .1 | 1.09381058e+00 |  |
| Offset | 0 | .005 | 6.73190201e-04 |  |
| Ea\_1 | 40 | 20 | 1.31911362e+01 |  |
| Log\_A1 | 13 | 2 | 5.45884675e+00 |  |
| gamma\_1 | 0.1 | 0.3 | 1.24854029e-01 |  |
| gamma\_mod1 | 0 | 0.1 | 6.54942654e-02 |  |
| gamma\_mod2 | 0 | 0.1 | -2.38717141e-02 |  |
| gamma\_mod3 | 0 | 0.1 | 4.08477869e-02 |  |
| gamma\_mod4 | 0 | 0.1 | -8.67038797e-02 |  |
| gamma\_mod5 | 0 | 0.1 | -2.72010983e-02 |  |
| gamma\_mod6 | 0 | 0.1 | -2.12582515e-01 |  |
| logP |  |  | 691.9697917259778 |  |

Final results from doOptimizeNegLogP: [ 1.09381058e+00 6.73190201e-04 1.31911362e+01 5.45884675e+00 1.24854029e-01 6.54942654e-02 -2.38717141e-02 4.08477869e-02 -8.67038797e-02 -2.72010983e-02 -2.12582515e-01] final logP: 691.9697917259778

Name of Runfile: 21a\_BPE\_grid\_fine 68921 points

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Parameter Name** | **Initial Value** | **Uncertainty** | **Final Value** | **Uncertainty** |
| Scaling | 1 | .1 | 1.19305713e+00 |  |
| Offset | 0 | .005 | 1.84248295e-03 |  |
| Ea\_1 | 40 | 20 | 2.95005588e+01 |  |
| Log\_A1 | 13 | 2 | 1.59850817e+01 |  |
| gamma\_1 | 0.1 | 0.3 | 4.70530765e-02 |  |
| gamma\_mod1 | 0 | 0.1 | 8.51632551e-02 |  |
| gamma\_mod2 | 0 | 0.1 | -2.98911408e-02 |  |
| gamma\_mod3 | 0 | 0.1 | 7.92878478e-02 |  |
| gamma\_mod4 | 0 | 0.1 | -3.83877710e-02 |  |
| gamma\_mod5 | 0 | 0.1 | -4.34671363e-02 |  |
| gamma\_mod6 | 0 | 0.1 | -5.12406172e-02 |  |
| logP |  |  | 705.0732574304127 |  |

Final results from doOptimizeNegLogP: [ 1.19305713e+00 1.84248295e-03 2.95005588e+01 1.59850817e+01 4.70530765e-02 8.51632551e-02 -2.98911408e-02 7.92878478e-02 -3.83877710e-02 -4.34671363e-02 -5.12406172e-02] final logP: 705.0732574304127

Name of Runfile: 21a\_CPE\_grid\_fine\_10kJ 68921 points

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Parameter Name** | **Initial Value** | **Uncertainty** | **Final Value** | **Uncertainty** |
| Scaling | 1 | .1 | 1.09381058e+00 |  |
| Offset | 0 | .005 | 6.73190201e-04 |  |
| Ea\_1 | 40 | 10 | 1.31911362e+01 |  |
| Log\_A1 | 13 | 2 | 5.45884675e+00 |  |
| gamma\_1 | 0.1 | 0.3 | 1.24854029e-01 |  |
| gamma\_mod1 | 0 | 0.1 | 6.54942654e-02 |  |
| gamma\_mod2 | 0 | 0.1 | -2.38717141e-02 |  |
| gamma\_mod3 | 0 | 0.1 | 4.08477869e-02 |  |
| gamma\_mod4 | 0 | 0.1 | -8.67038797e-02 |  |
| gamma\_mod5 | 0 | 0.1 | -2.72010983e-02 |  |
| gamma\_mod6 | 0 | 0.1 | -2.12582515e-01 |  |
| logP |  |  | 691.9697917259778 |  |

[ 1.09381058e+00 6.73190201e-04 1.31911362e+01 5.45884675e+00 1.24854029e-01 6.54942654e-02 -2.38717141e-02 4.08477869e-02 -8.67038797e-02 -2.72010983e-02 -2.12582515e-01] final logP: 691.9697917259778

Name of Runfile: 21a\_BPE\_grid\_fine\_10kJ 68921 points

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Parameter Name** | **Initial Value** | **Uncertainty** | **Final Value** | **Uncertainty** |
| Scaling | 1 | .1 | 1.15084888e+00 |  |
| Offset | 0 | .005 | 1.38423323e-03 |  |
| Ea\_1 | 40 | 10 | 2.77981561e+01 |  |
| Log\_A1 | 13 | 2 | 1.48508723e+01 |  |
| gamma\_1 | 0.1 | 0.3 | 4.28302638e-02 |  |
| gamma\_mod1 | 0 | 0.1 | 1.69463014e-01 |  |
| gamma\_mod2 | 0 | 0.1 | -8.81116778e-02 |  |
| gamma\_mod3 | 0 | 0.1 | 6.94850027e-02 |  |
| gamma\_mod4 | 0 | 0.1 | -4.96440744e-02 |  |
| gamma\_mod5 | 0 | 0.1 | -3.96318339e-02 |  |
| gamma\_mod6 | 0 | 0.1 | -6.54816054e-02 |  |
| logP |  |  | 704.5773825977183 |  |

Final results from doOptimizeNegLogP: [ 1.15084888e+00 1.38423323e-03 2.77981561e+01 1.48508723e+01 4.28302638e-02 1.69463014e-01 -8.81116778e-02 6.94850027e-02 -4.96440744e-02 -3.96318339e-02 -6.54816054e-02] final logP: 704.5773825977183