Supplemental Materials for Character Angle Effects on Dissociated Dislocation Core Energy in Aluminum:

Accuracy of molecular dynamics vs. molecular statics

Fig. 1, which is taken from reference [1], shows that when the same bond order potential was used to simulate a dislocation-containing aluminum system that is large enough (say 129600 atoms), the molecular statics (MS) total energies obtained from 10 random number seeds vary on the same order of the total snapshot energies from a molecular dynamics (MD) simulation. This demonstrates that MS has difficulty achieving high accuracy.

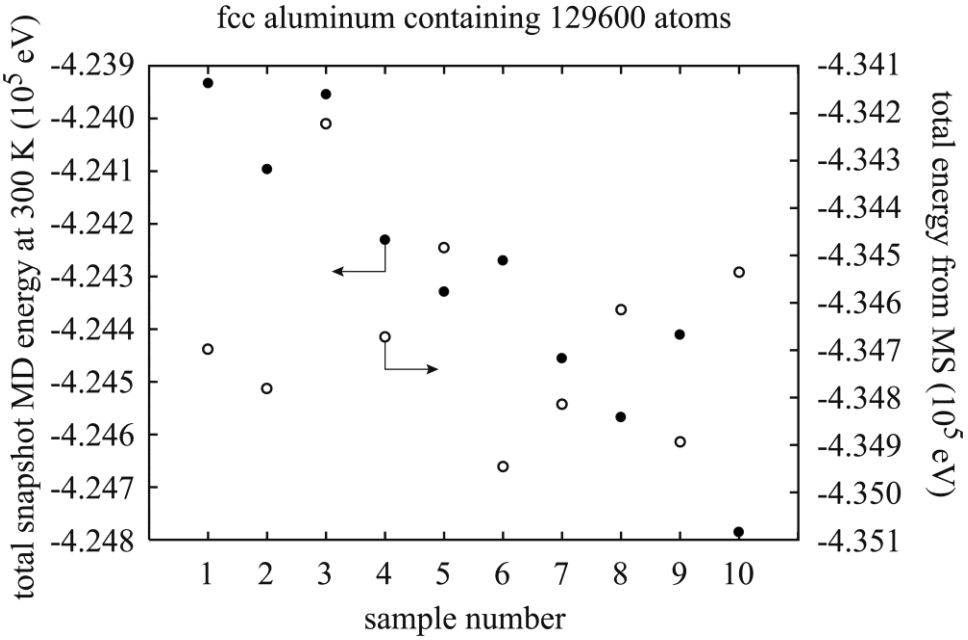
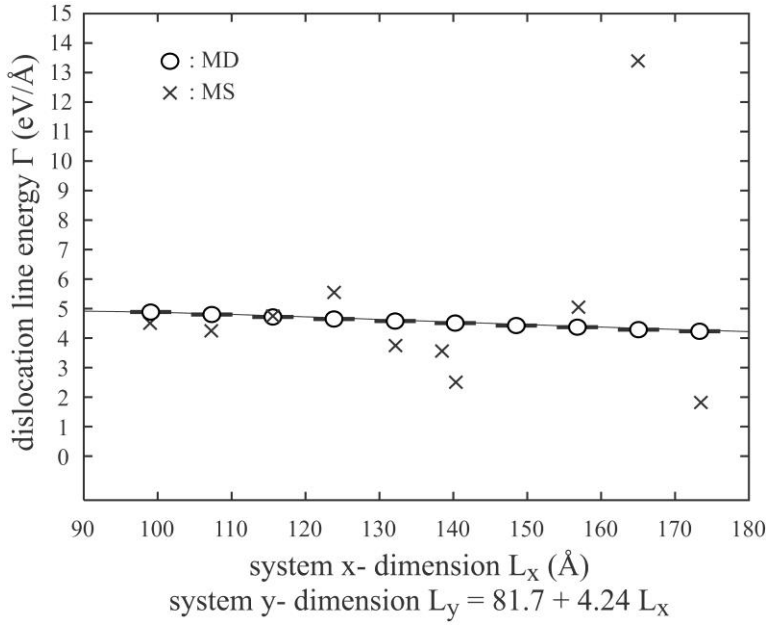


Fig. 1. Comparison of total energies of a 129600 atom, dislocation containing aluminum system obtained from 10 snapshots of MD configurations and 10 MS simulations with different random number seeds.

Fig. 2, which is taken from reference [2], compares directly MS and time-averaged MD results of edge dislocation energy in CdS. This figure shows that MS results are reasonable when system dimension L_x is below 130 Å but are essentially meaningless when the dimension is above 130 Å (especially the data point near 165 Å). Time-averaged MD results, however, are near "error-free" for the entire dimension range shown in the figure.



In the following, we attach raw figures of our dislocation energies as functions of lateral and vertical dislocation spacings at various character angles, as well as other derived figures (see the main paper for details).

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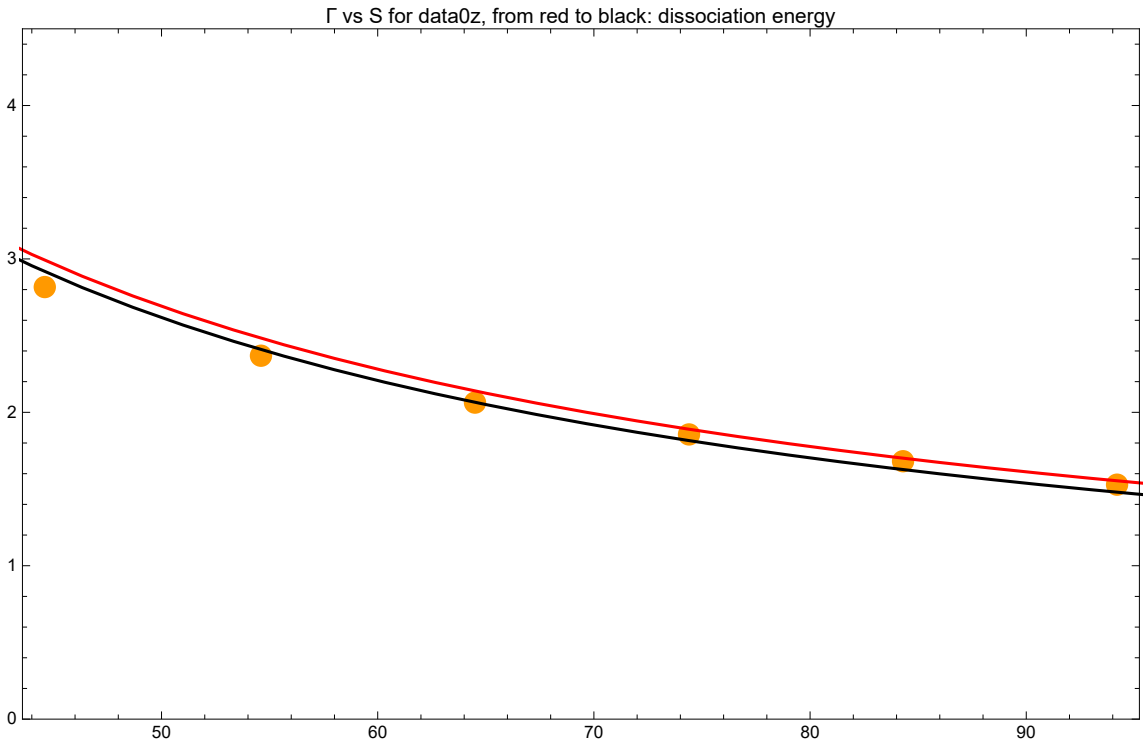
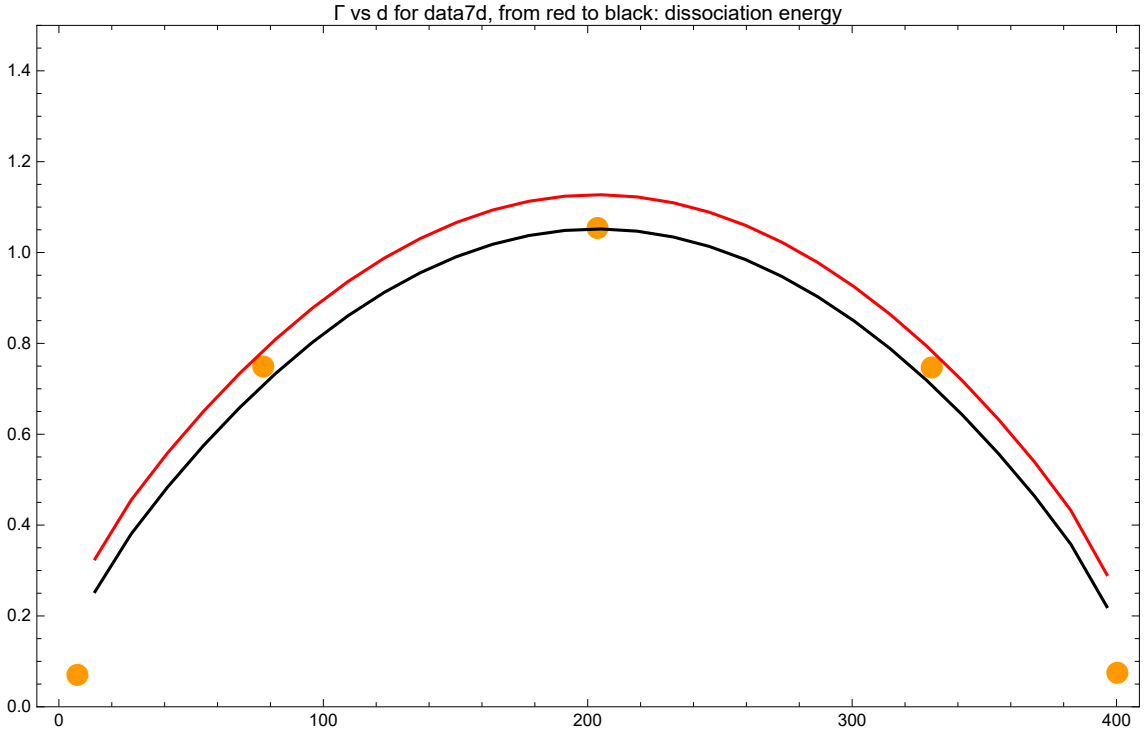
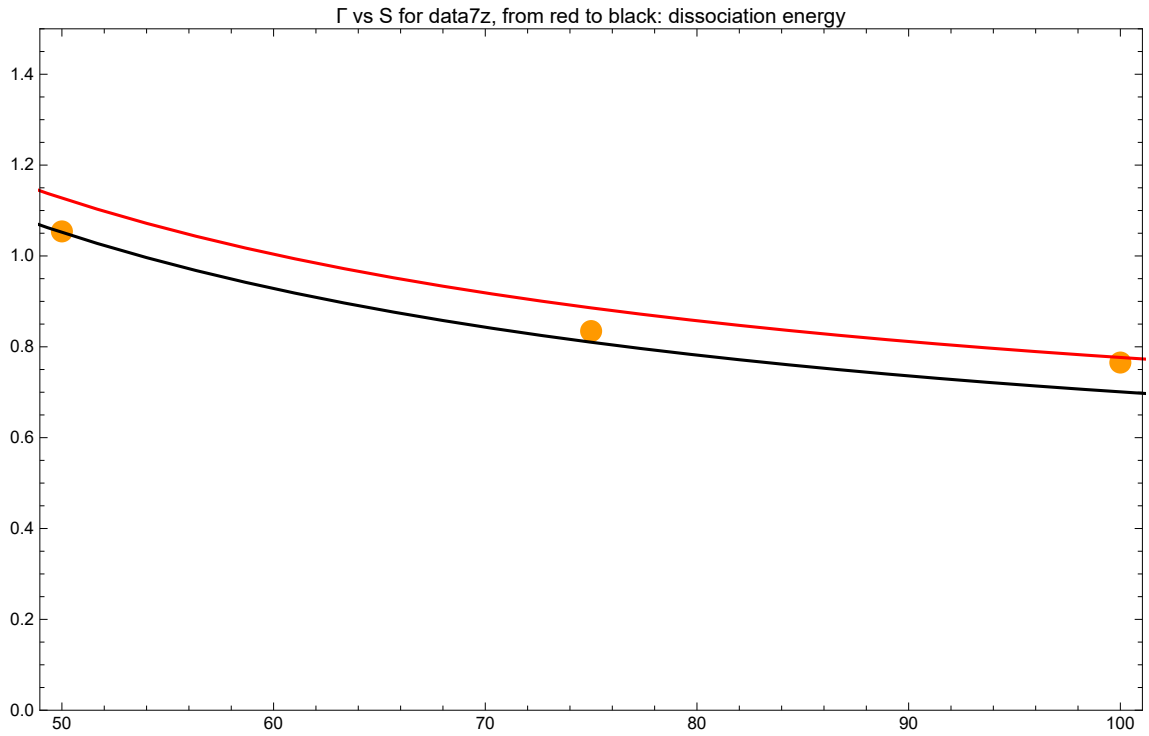
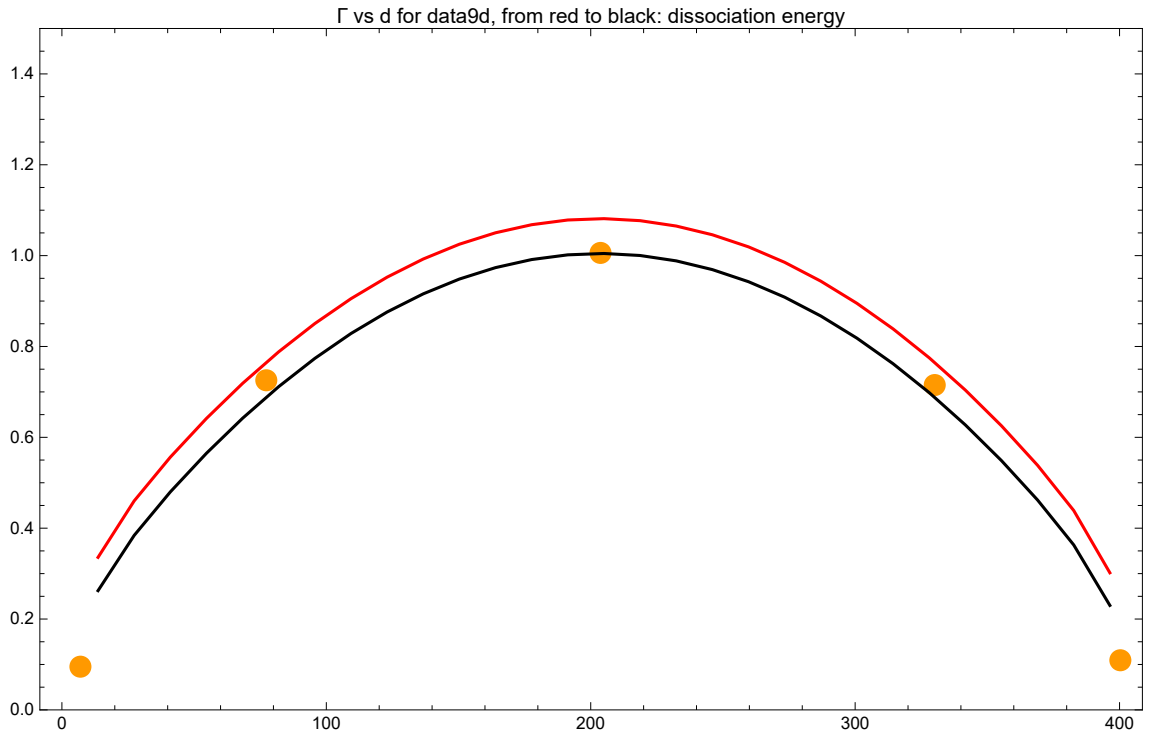
1 X. W. Zhou, and S. M. Foiles, Ed. J. P. Hessling, *Uncertainty Quantification and Model Calibration* (INTECH, Rijeka, Croatia, 2017).

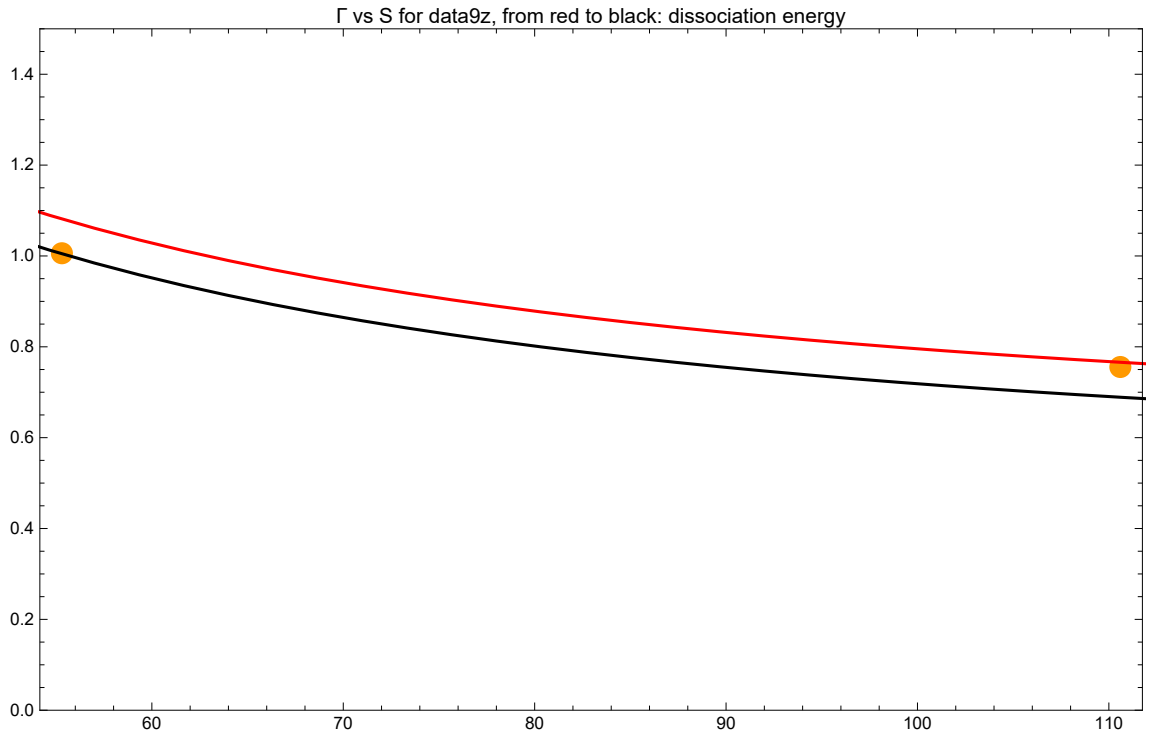
2 X. W. Zhou, D. K. Ward, J. A. Zimmerman, J. L. Cruz-Campa, D. Zubia, J. E. Martin, F. van Swol, An Atomistically Validated Continuum Model for Strain Relaxation and Misfit Dislocation Formation, J. Mech. Phys. Sol. 91 (2016) 265-277.

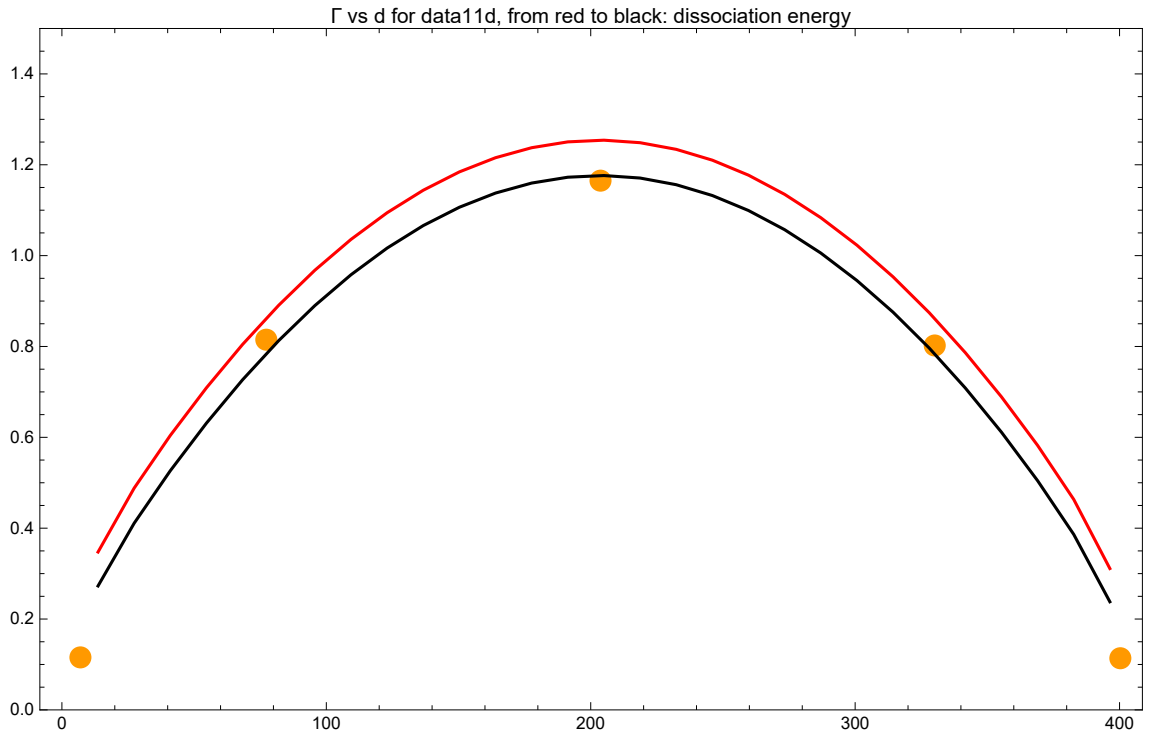

Γ vs S for data0z, from red to black: dissociation energy
4
3
2
1
0
50
60
70
80
90

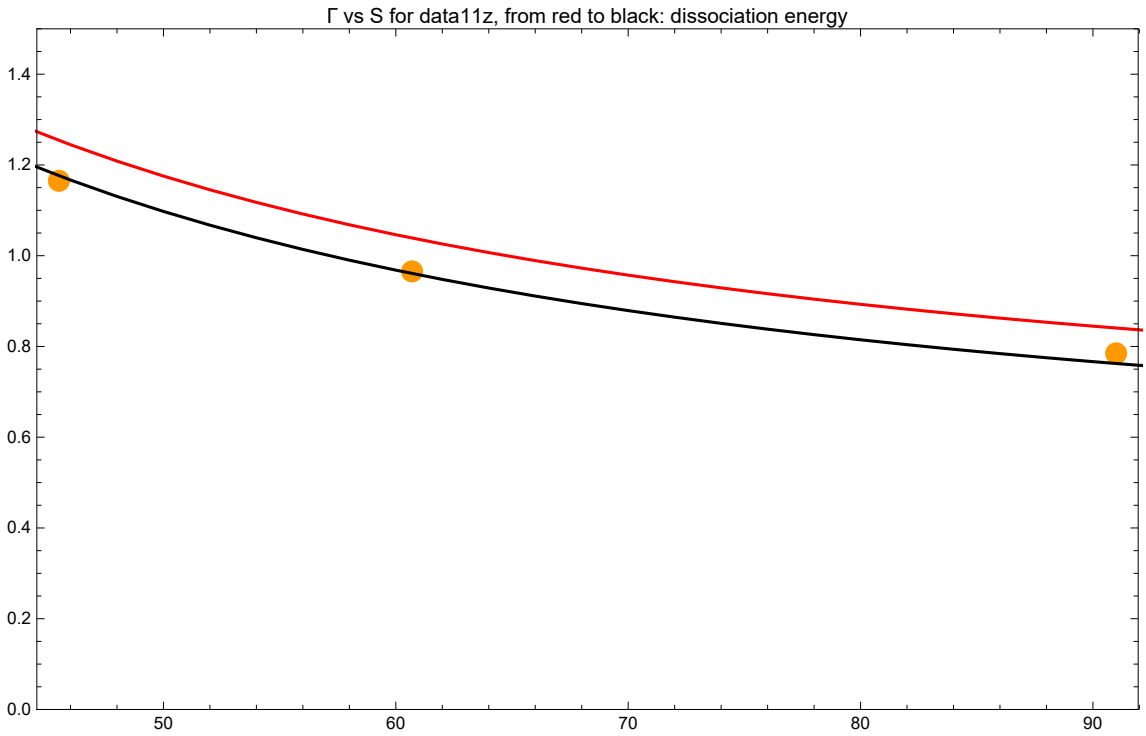

Γ vs d for data7d, from red to black: dissociation energy
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
0
100
200
300
400

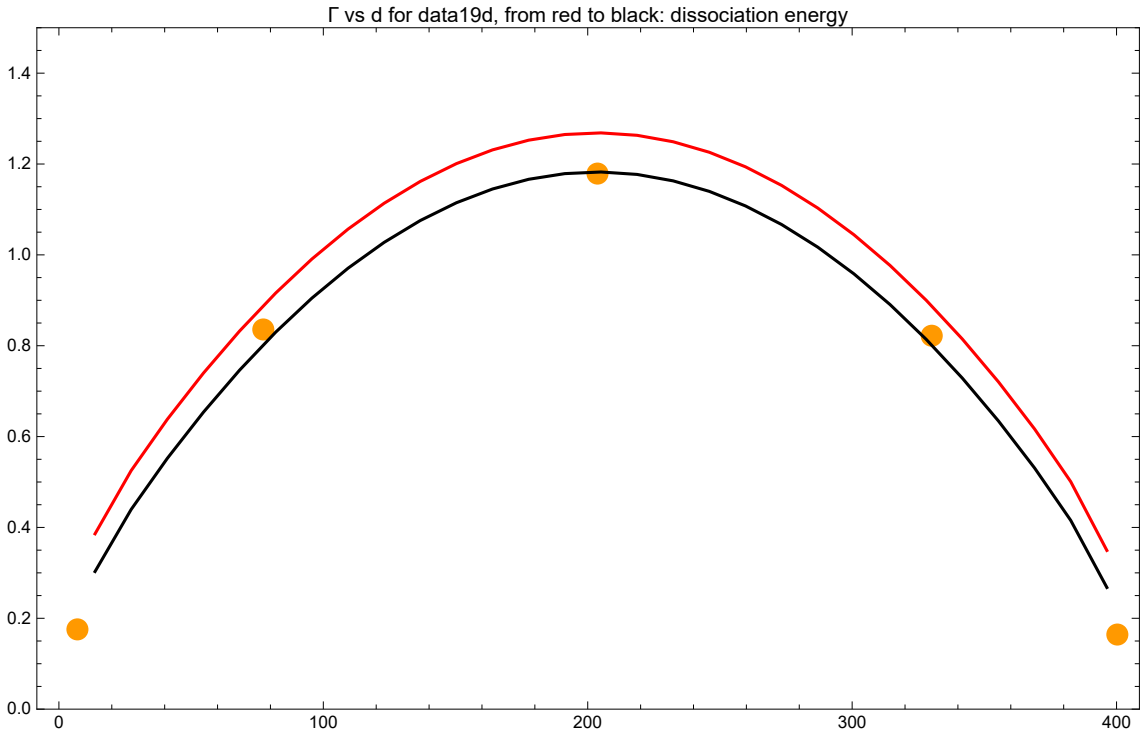

Γ vs S for data7z, from red to black: dissociation energy
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
50
60
70
80
90
100

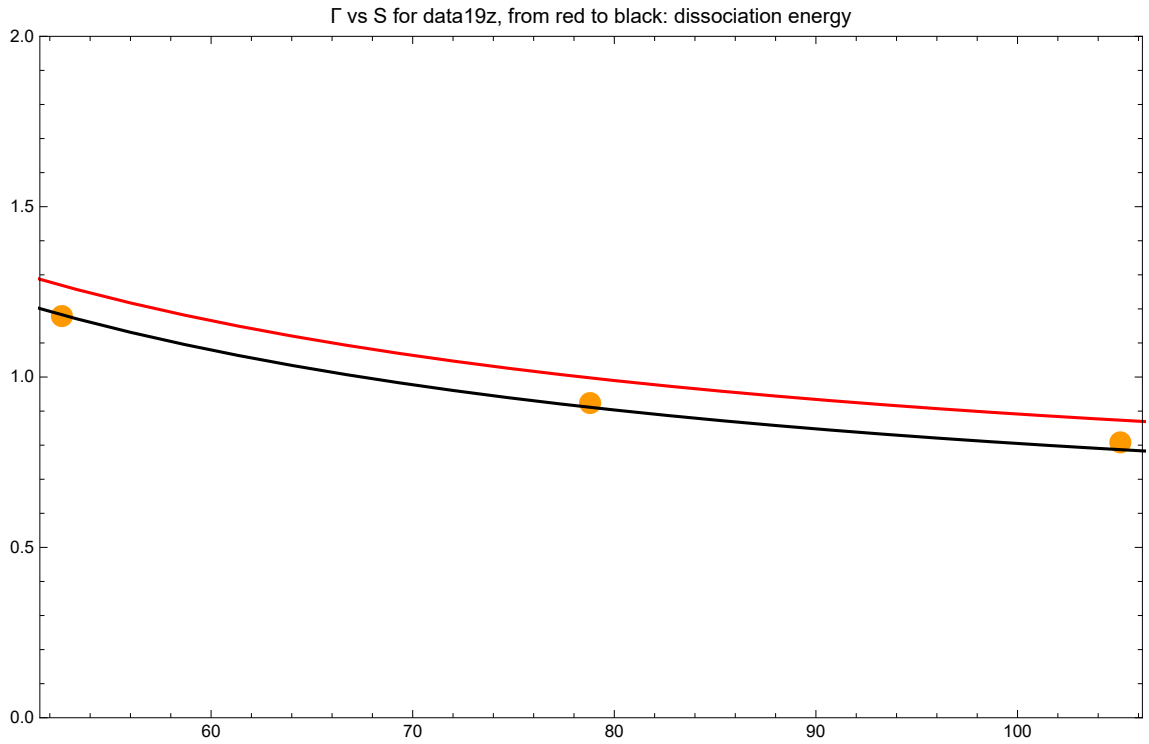

Γ vs d for data9d, from red to black: dissociation energy
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
0
100
200
300
400

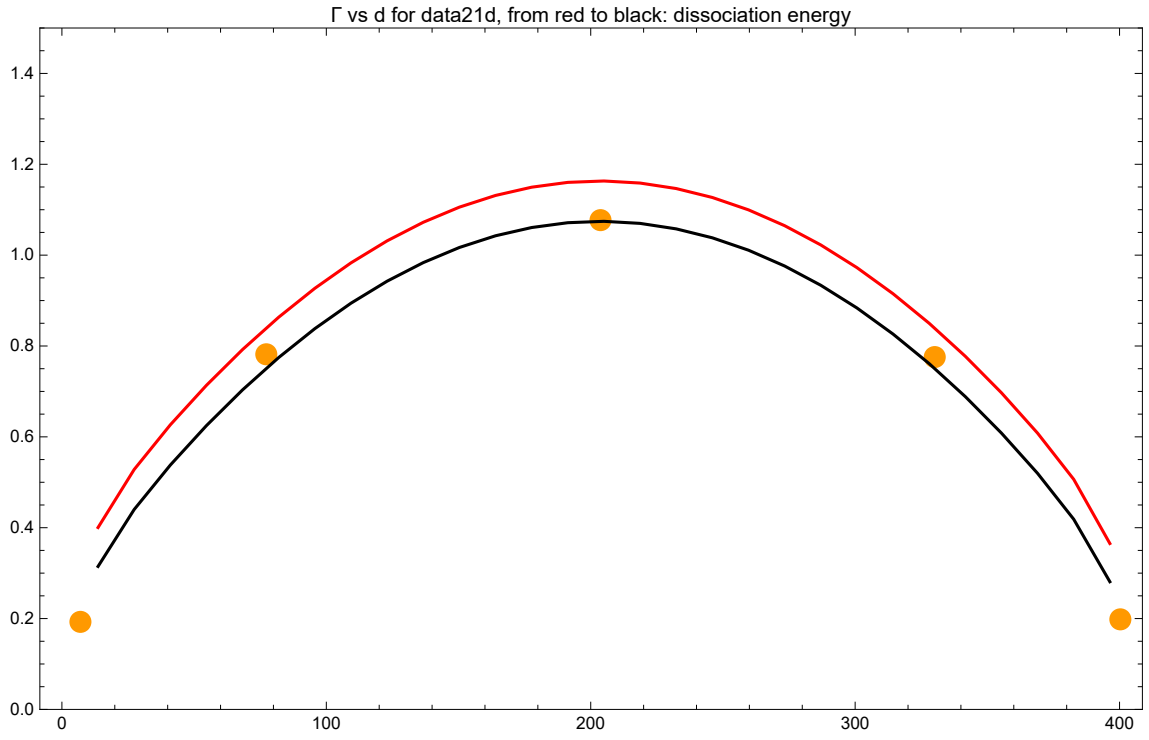

Γ vs S for data9z, from red to black: dissociation energy
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
60
70
80
90
100
110

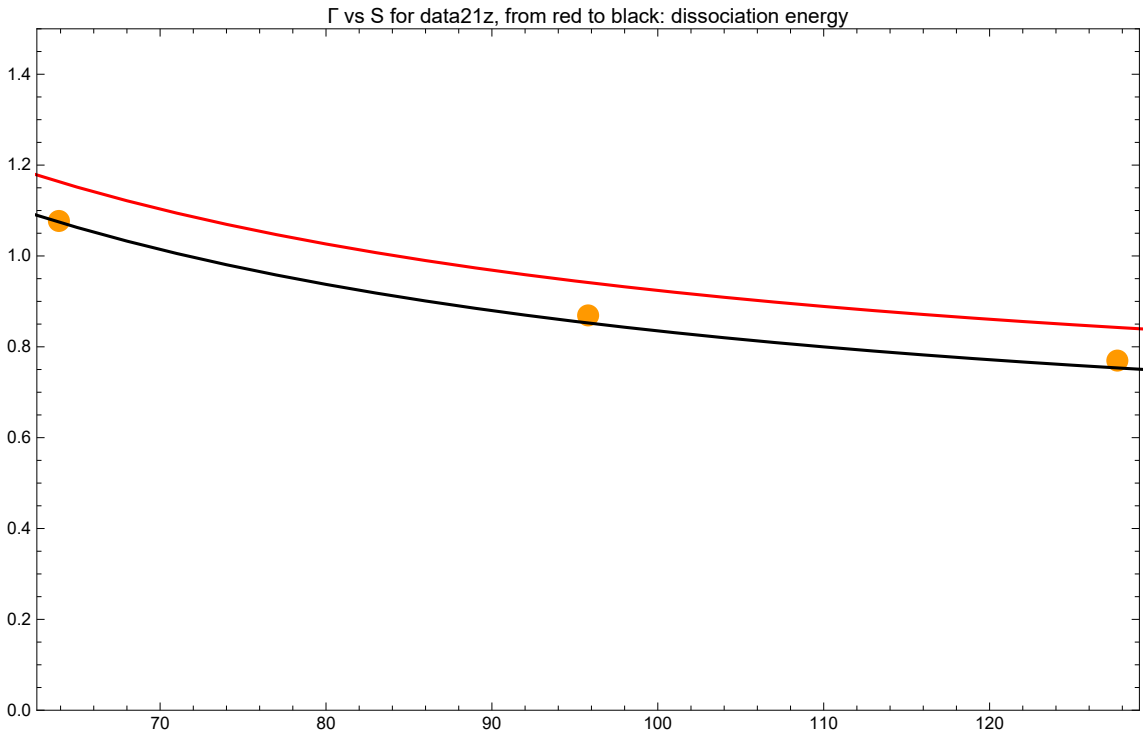

Γ vs d for data11d, from red to black: dissociation energy
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
0
100
200
300
400

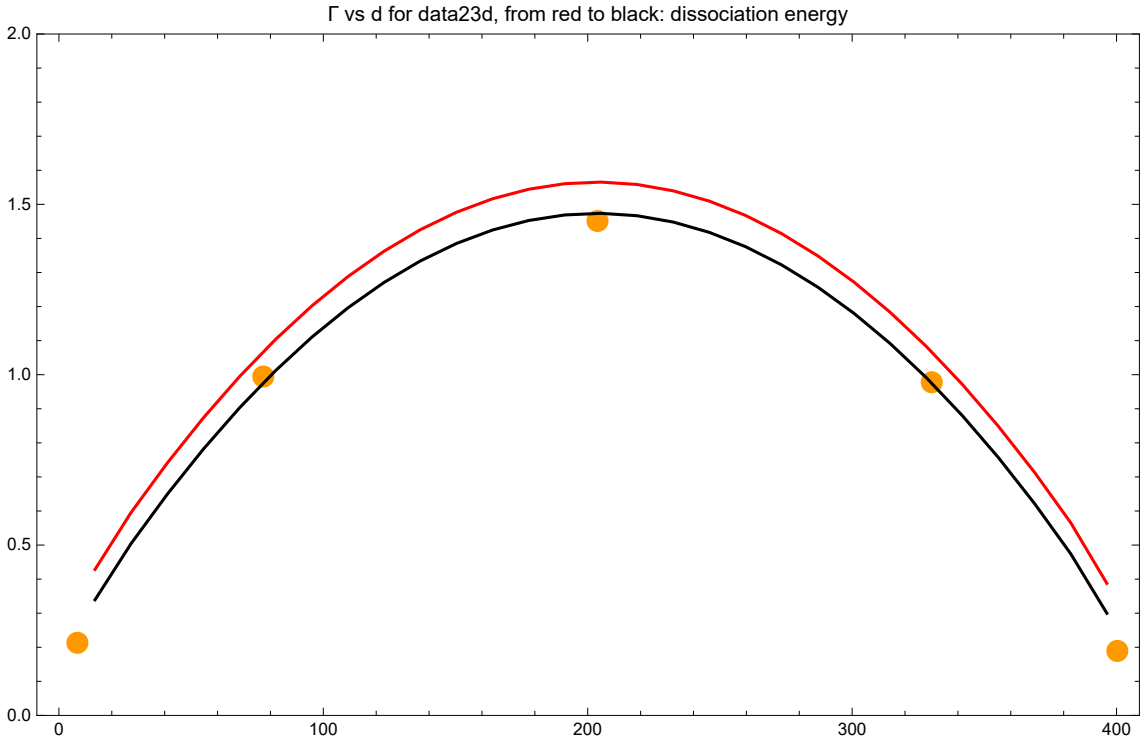

Γ vs S for data11z, from red to black: dissociation energy
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
50
60
70
80
90

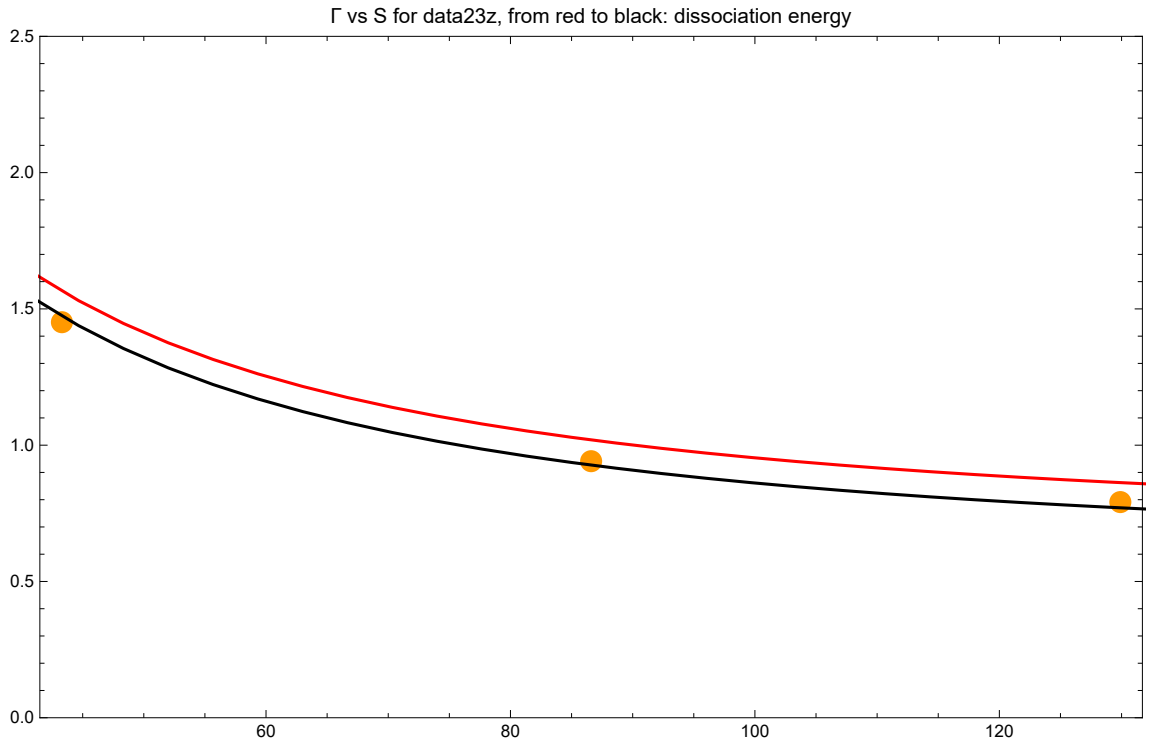

Γ vs d for data19d, from red to black: dissociation energy
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
0
100
200
300
400

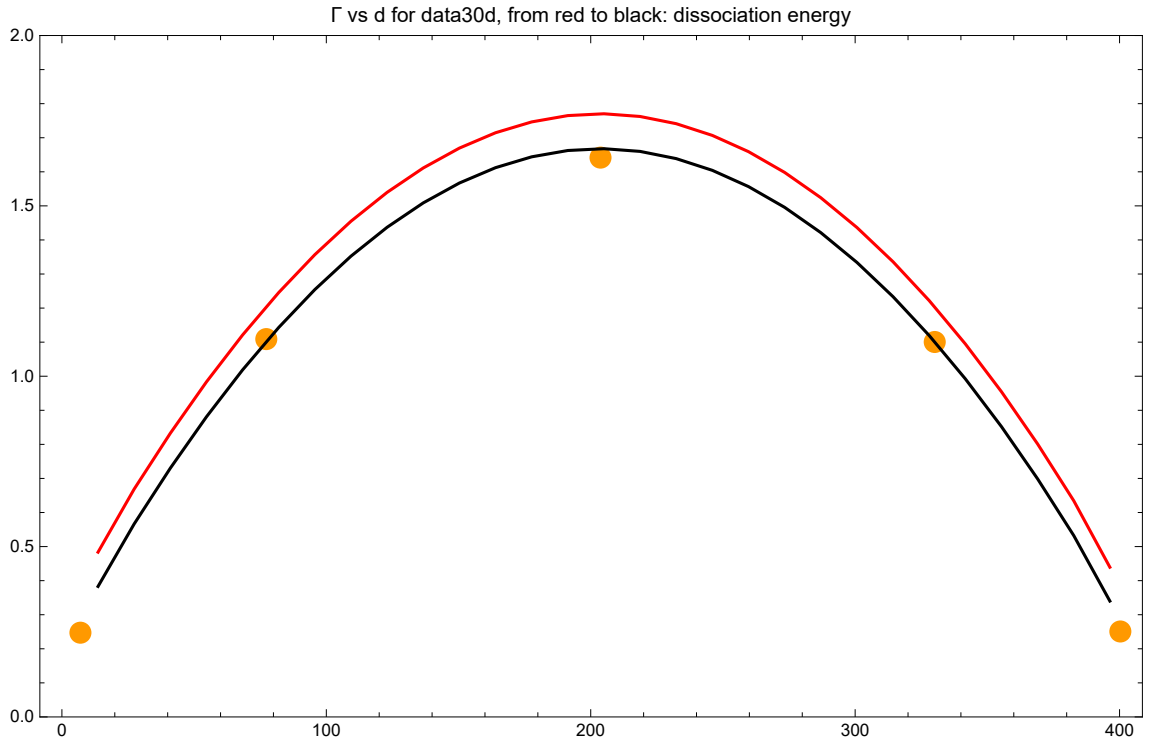

Γ vs S for data19z, from red to black: dissociation energy
2.0
1.5
1.0
0.5
0.0
60
70
80
90
100

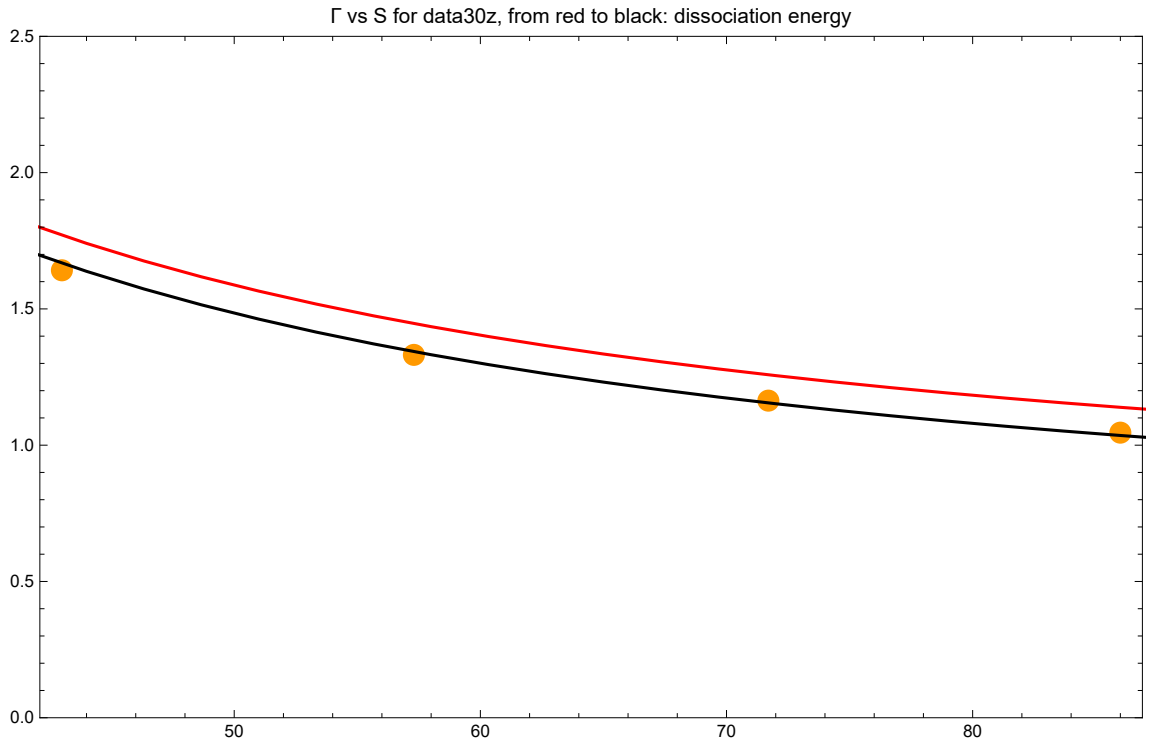

Γ vs d for data21d, from red to black: dissociation energy
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
0
100
200
300
400

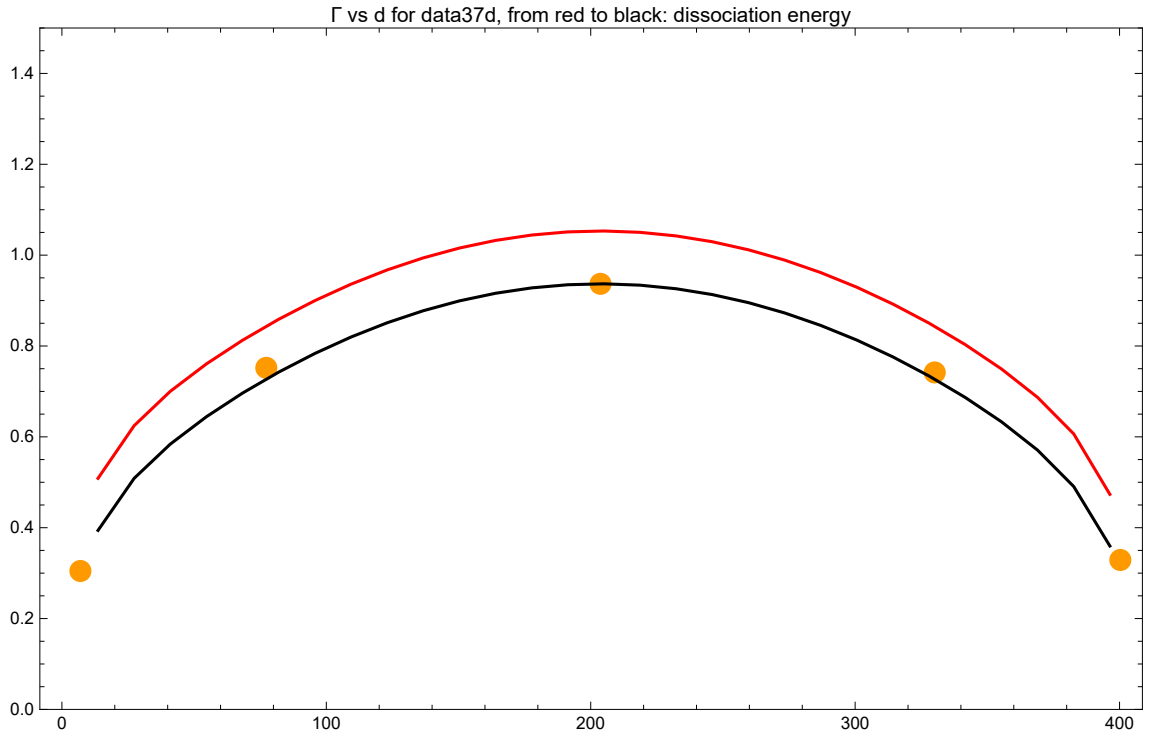

Γ vs S for data21z, from red to black: dissociation energy
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
70
80
90
100
110
120

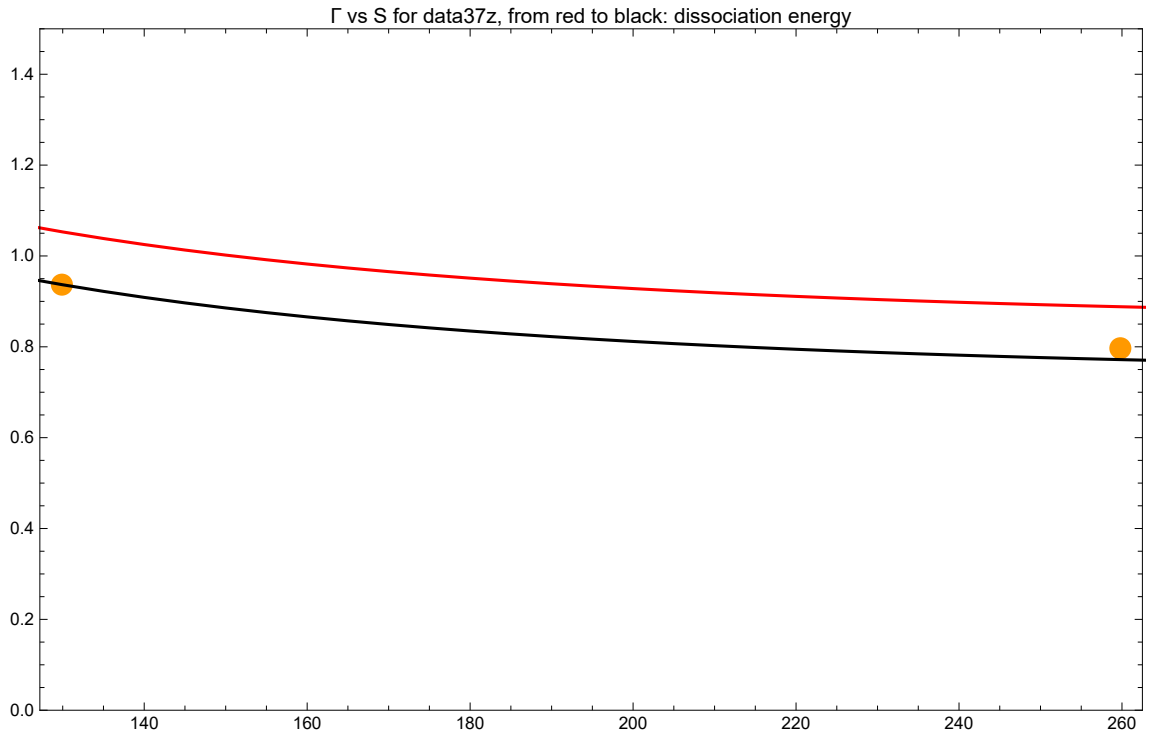

Γ vs d for data23d, from red to black: dissociation energy
2.0
1.5
1.0
0.5
0.0
0
100
200
300
400

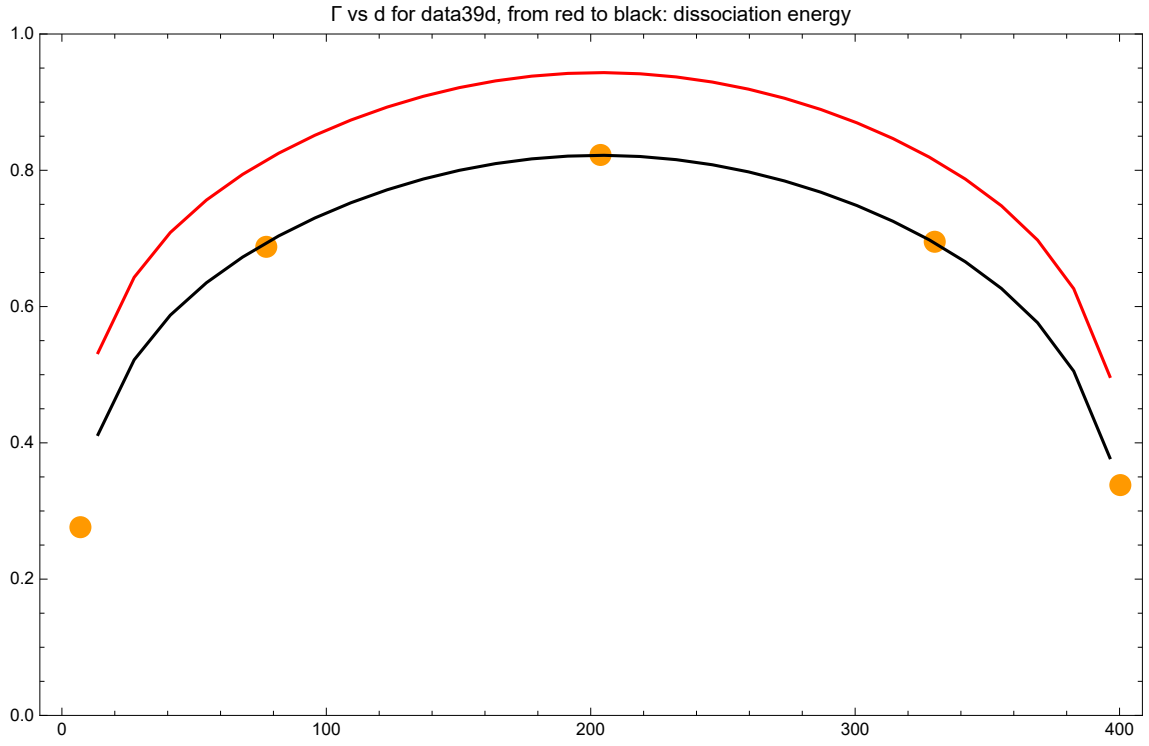

Γ vs S for data23z, from red to black: dissociation energy
2.5
2.0
1.5
1.0
0.5
0.0
60
80
100
120

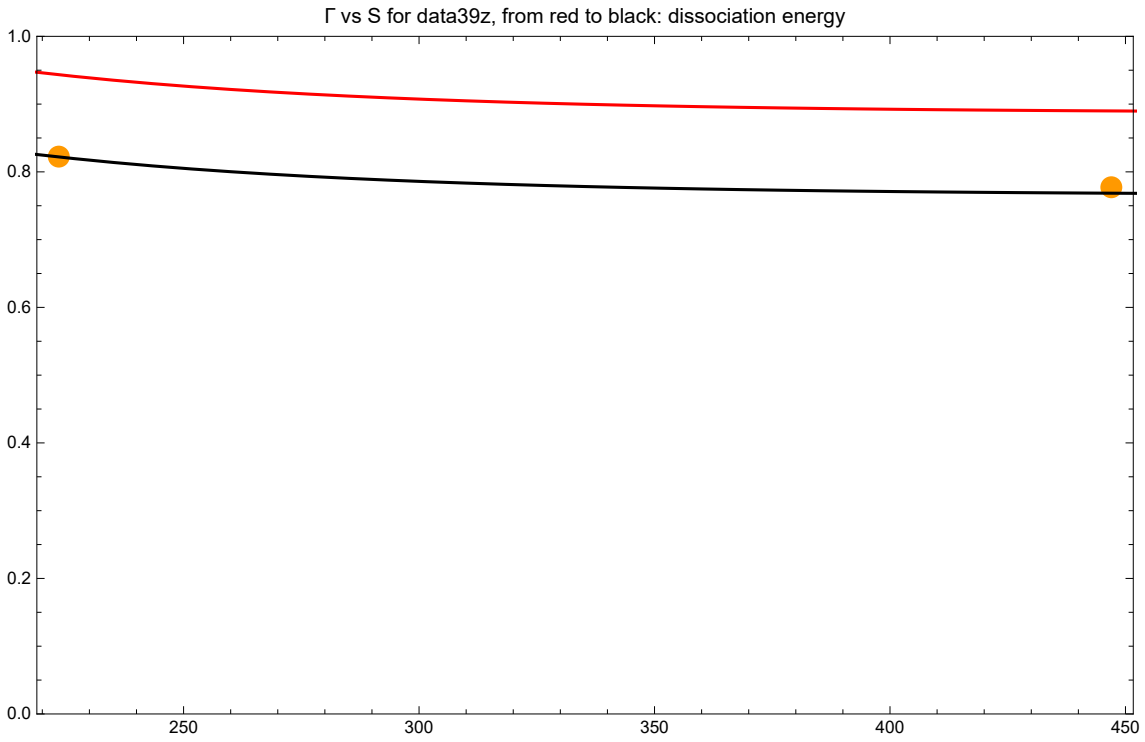

Γ vs d for data30d, from red to black: dissociation energy
2.0
1.5
1.0
0.5
0.0
0
100
200
300
400

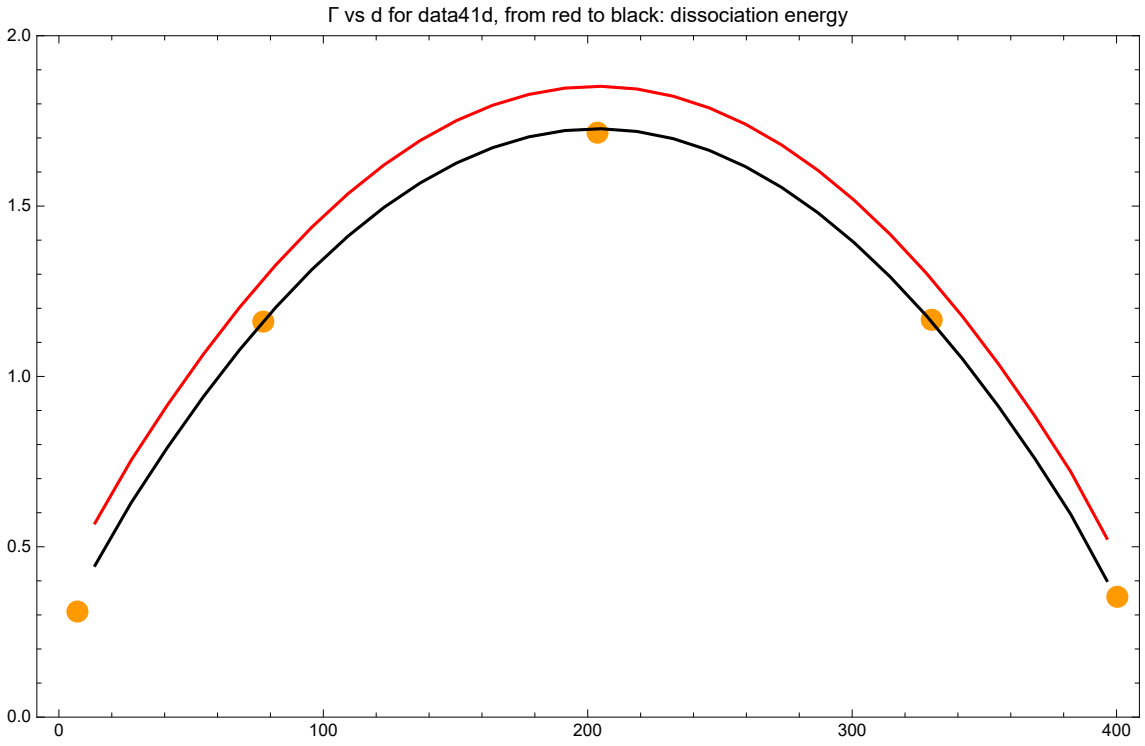

Γ vs S for data30z, from red to black: dissociation energy
2.5
2.0
1.5
1.0
0.5
0.0
50
60
70
80

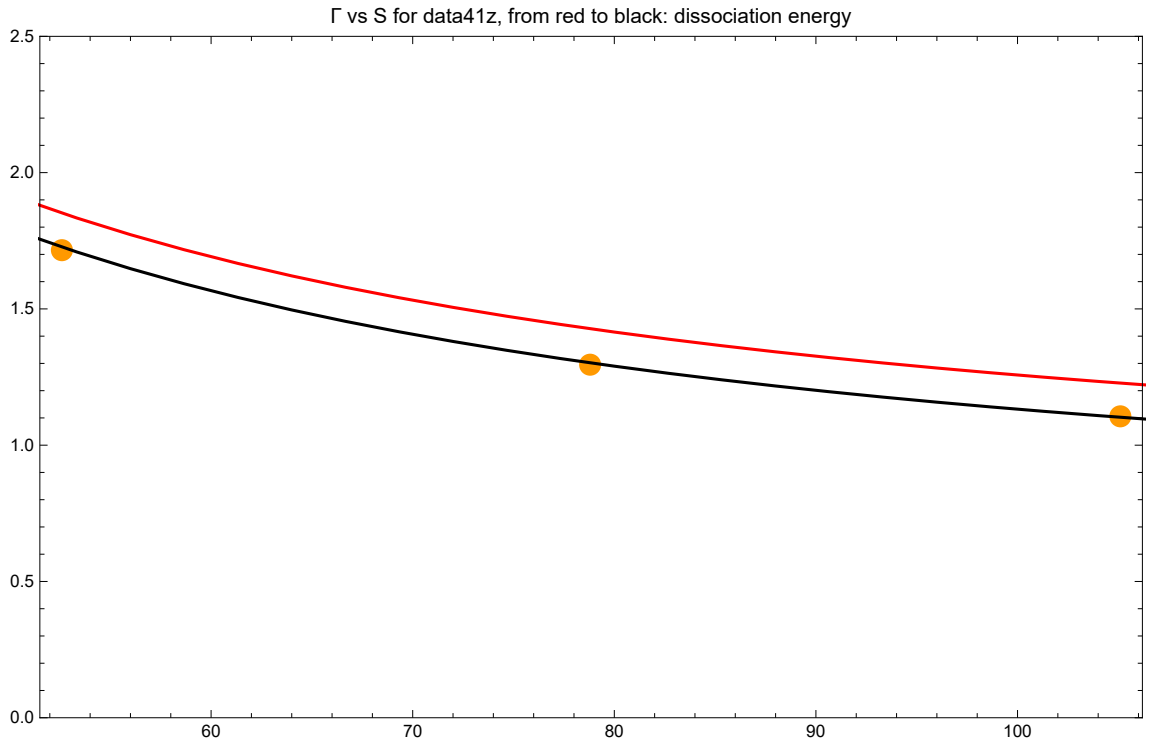

Γ vs d for data37d, from red to black: dissociation energy
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
0
100
200
300
400

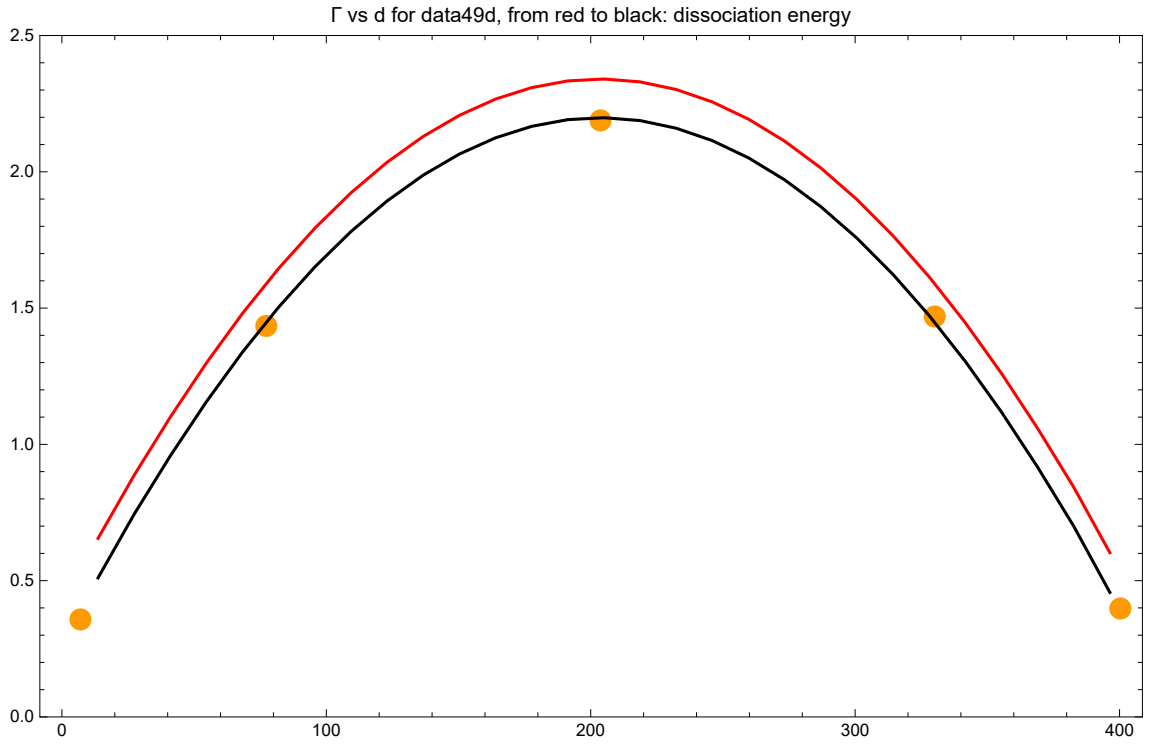

Γ vs S for data37z, from red to black: dissociation energy
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
140
160
180
200
220
240
260

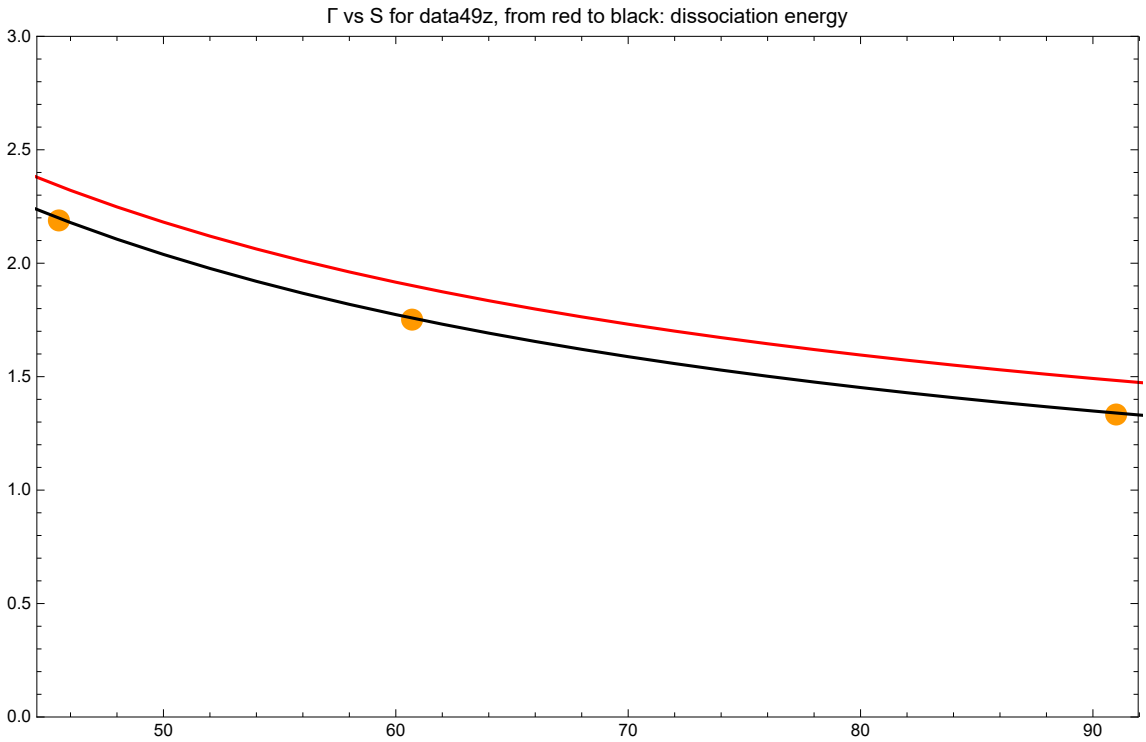

Γ vs d for data39d, from red to black: dissociation energy
1.0
0.8
0.6
0.4
0.2
0.0
0
100
200
300
400

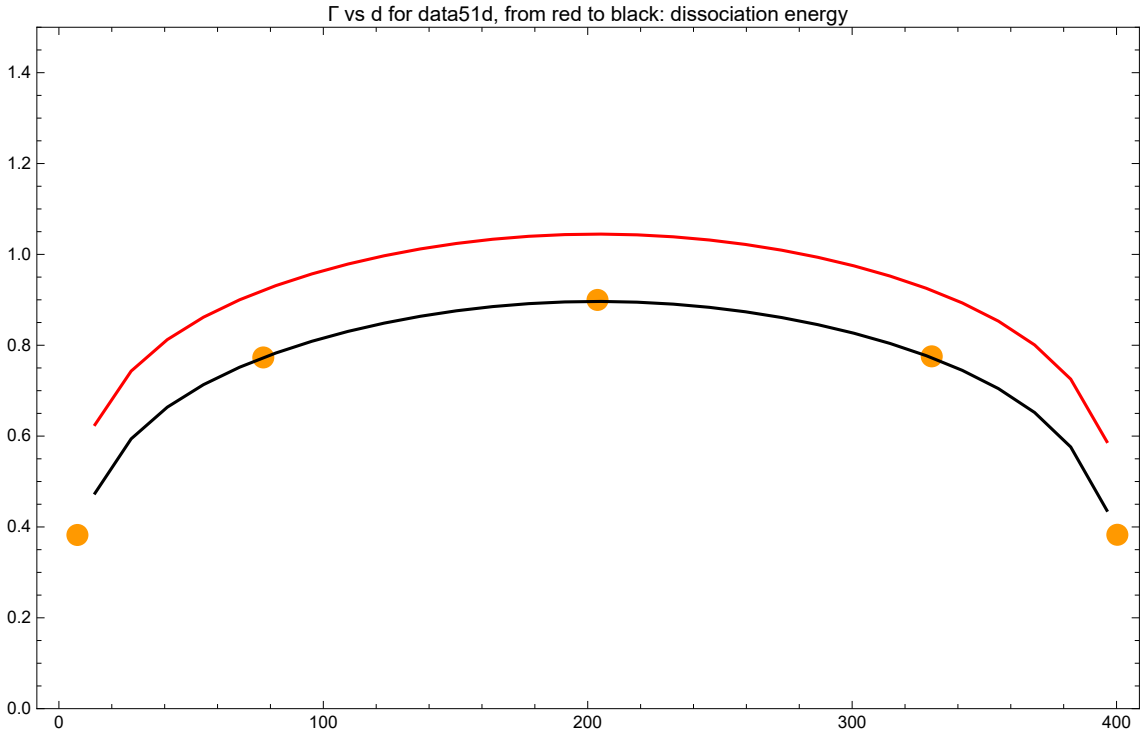

Γ vs S for data39z, from red to black: dissociation energy
1.0
0.8
0.6
0.4
0.2
0.0
250
300
350
400
450

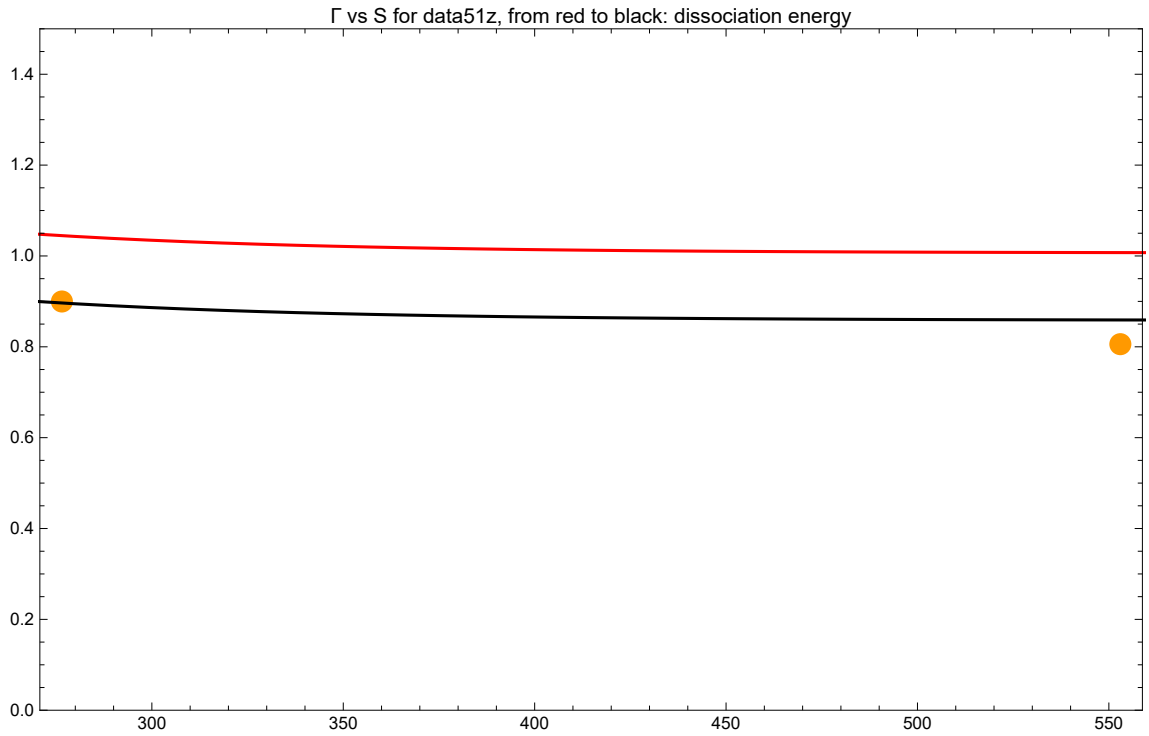

Γ vs d for data41d, from red to black: dissociation energy
2.0
1.5
1.0
0.5
0.0
0
100
200
300
400

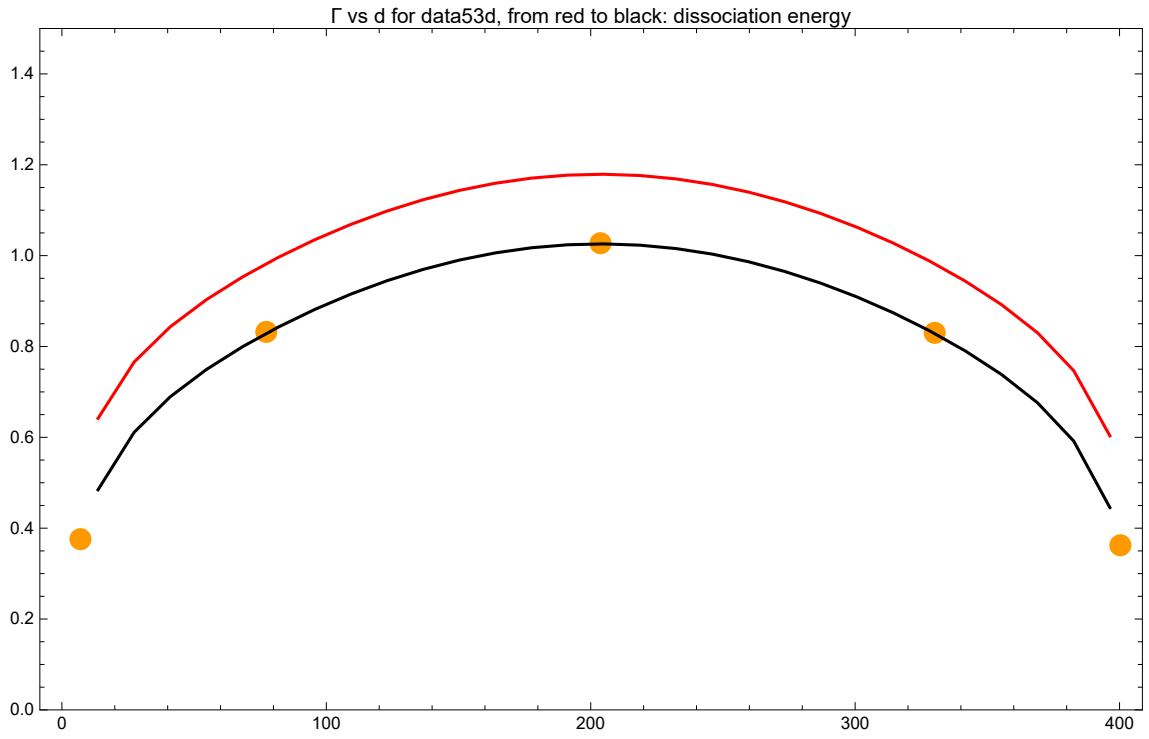

Γ vs S for data41z, from red to black: dissociation energy
2.5
2.0
1.5
1.0
0.5
0.0
60
70
80
90
100

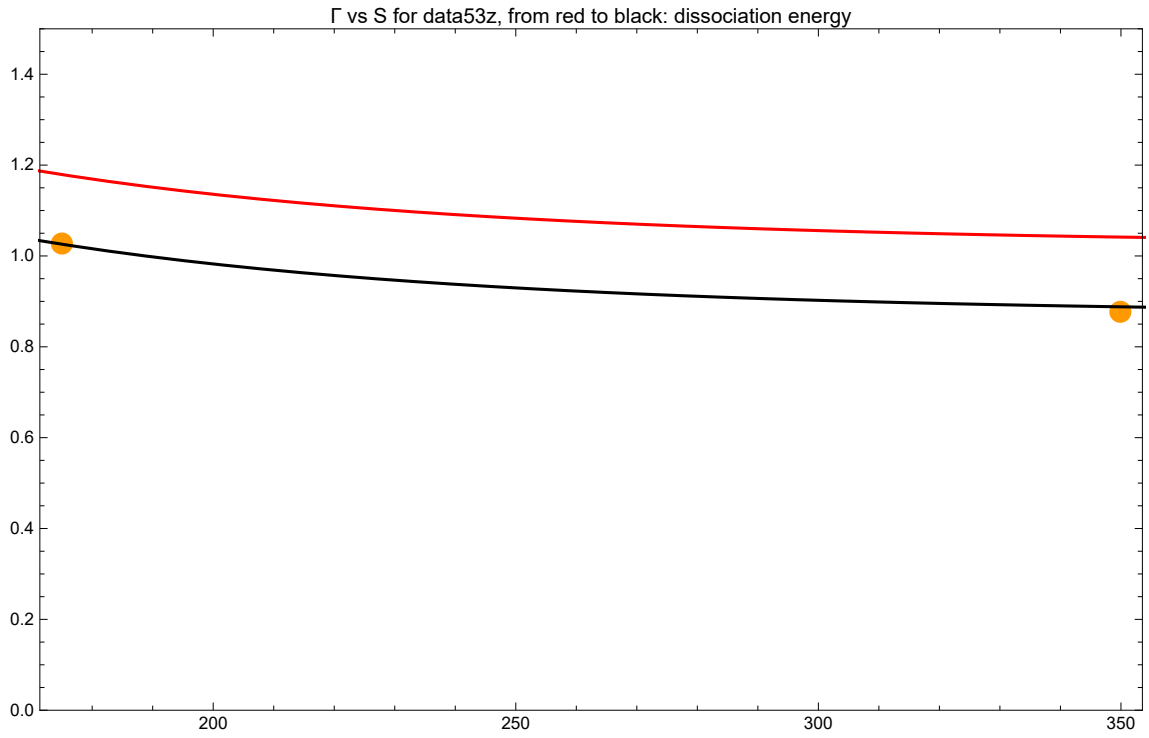

Γ vs d for data49d, from red to black: dissociation energy
2.5
2.0
1.5
1.0
0.5
0.0
0
100
200
300
400

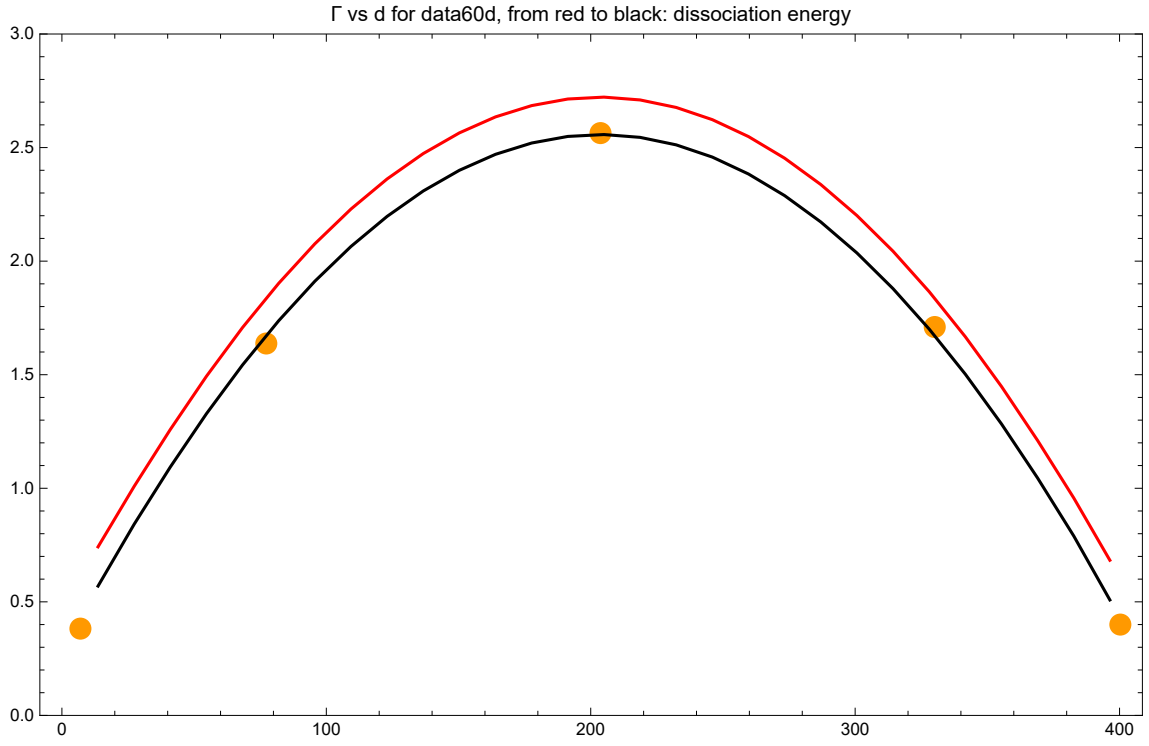

Γ vs S for data49z, from red to black: dissociation energy
3.0
2.5
2.0
1.5
1.0
0.5
0.0
50
60
70
80
90

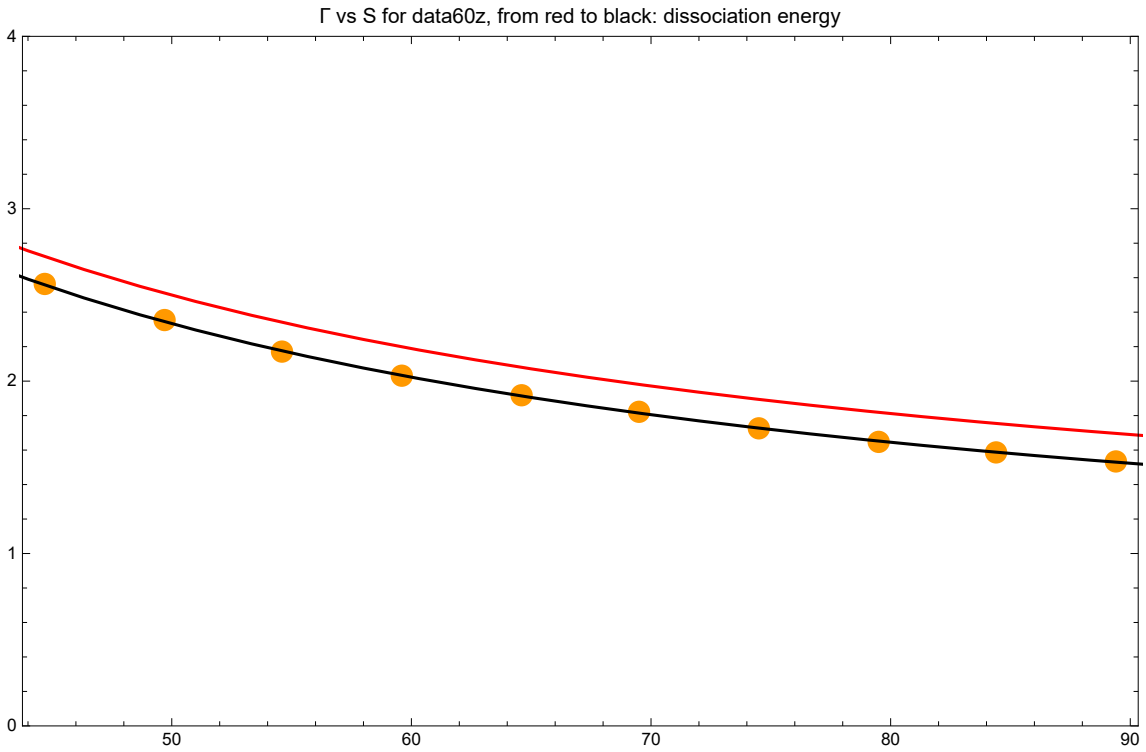

Γ vs d for data51d, from red to black: dissociation energy
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
0
100
200
300
400

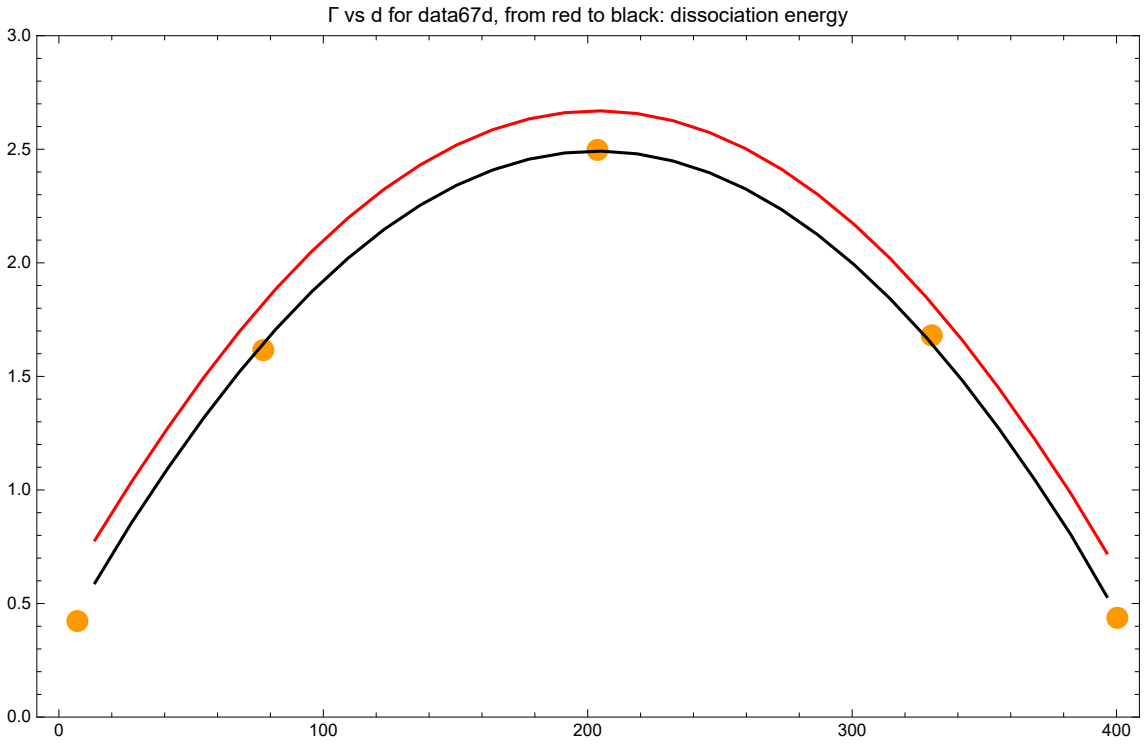

Γ vs S for data51z, from red to black: dissociation energy
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
300
350
400
450
500
550

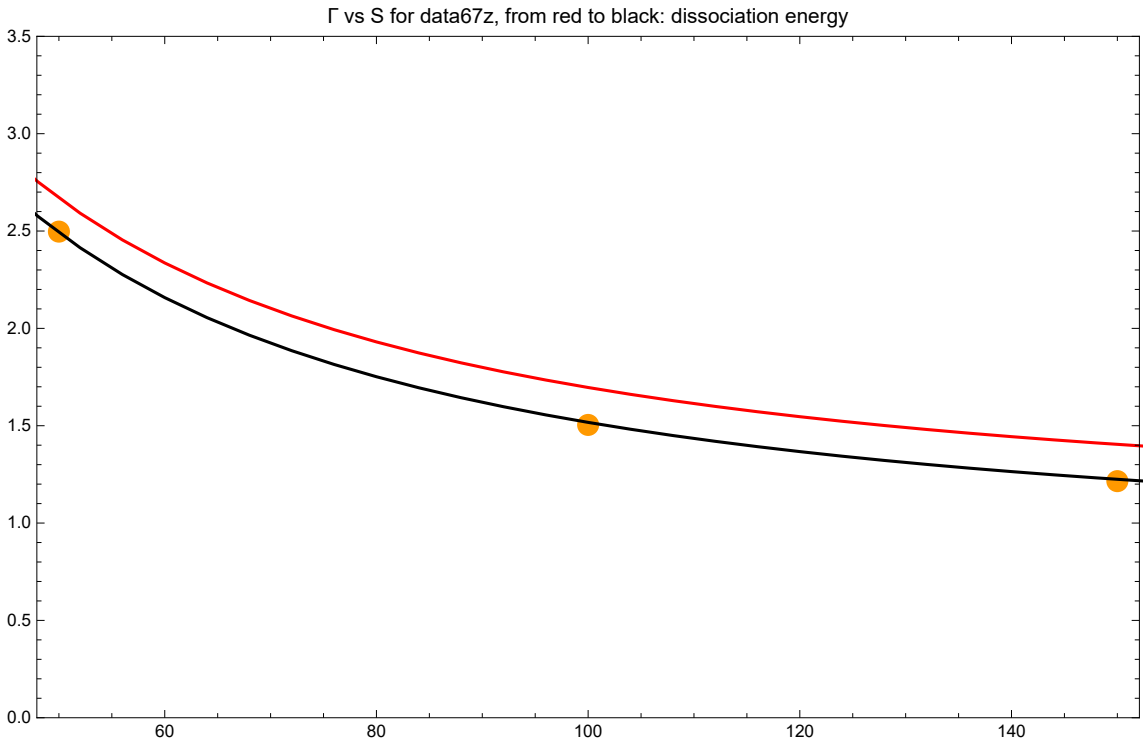

Γ vs d for data53d, from red to black: dissociation energy
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
0
100
200
300
400

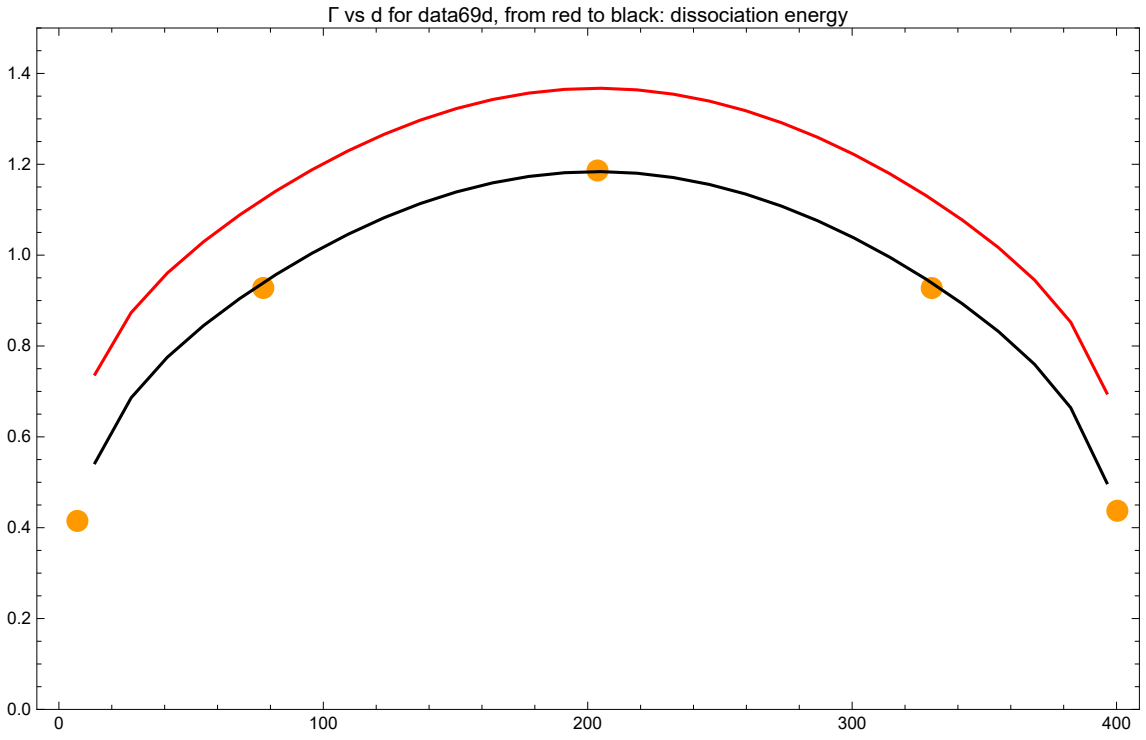

Γ vs S for data53z, from red to black: dissociation energy
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
200
250
300
350

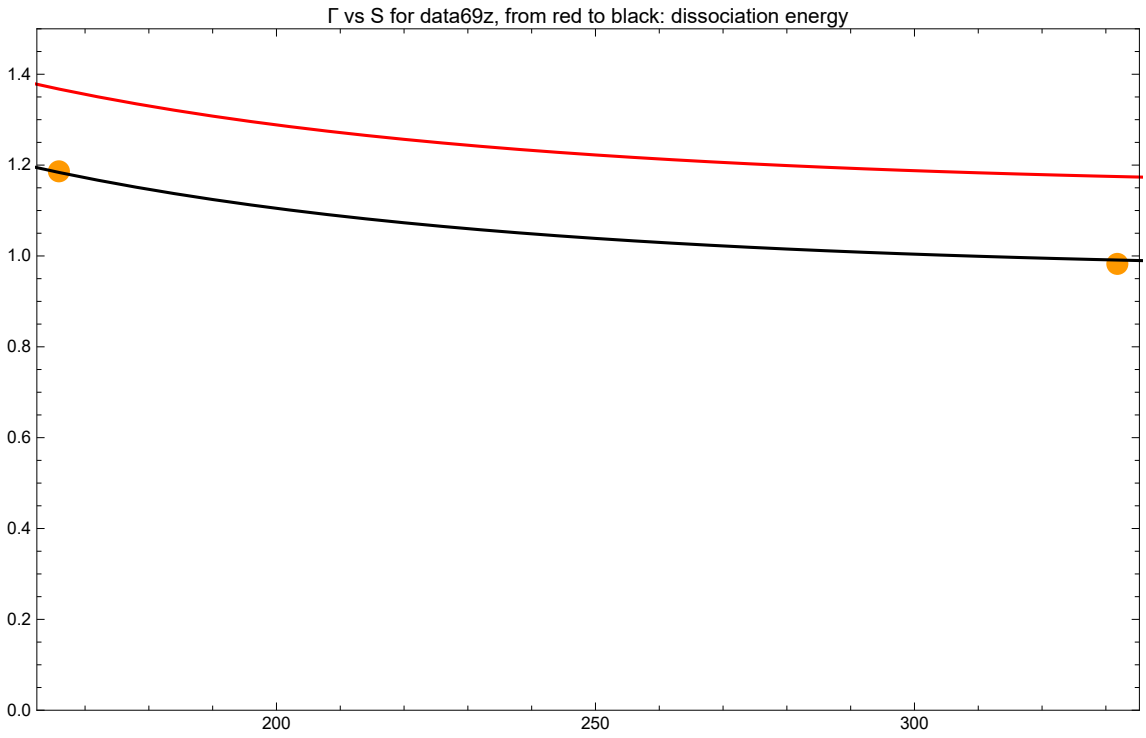

Γ vs d for data60d, from red to black: dissociation energy
3.0
2.5
2.0
1.5
1.0
0.5
0.0
0
100
200
300
400

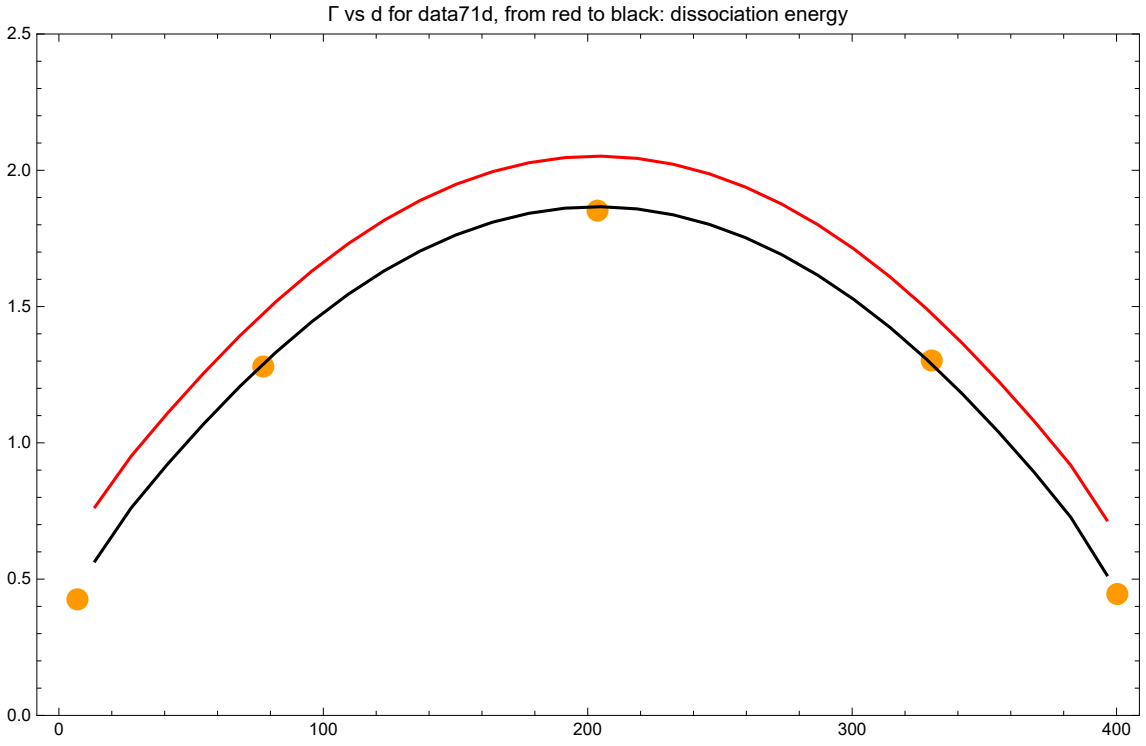

Γ vs S for data60z, from red to black: dissociation energy
4
3
2
1
0
50
60
70
80
90

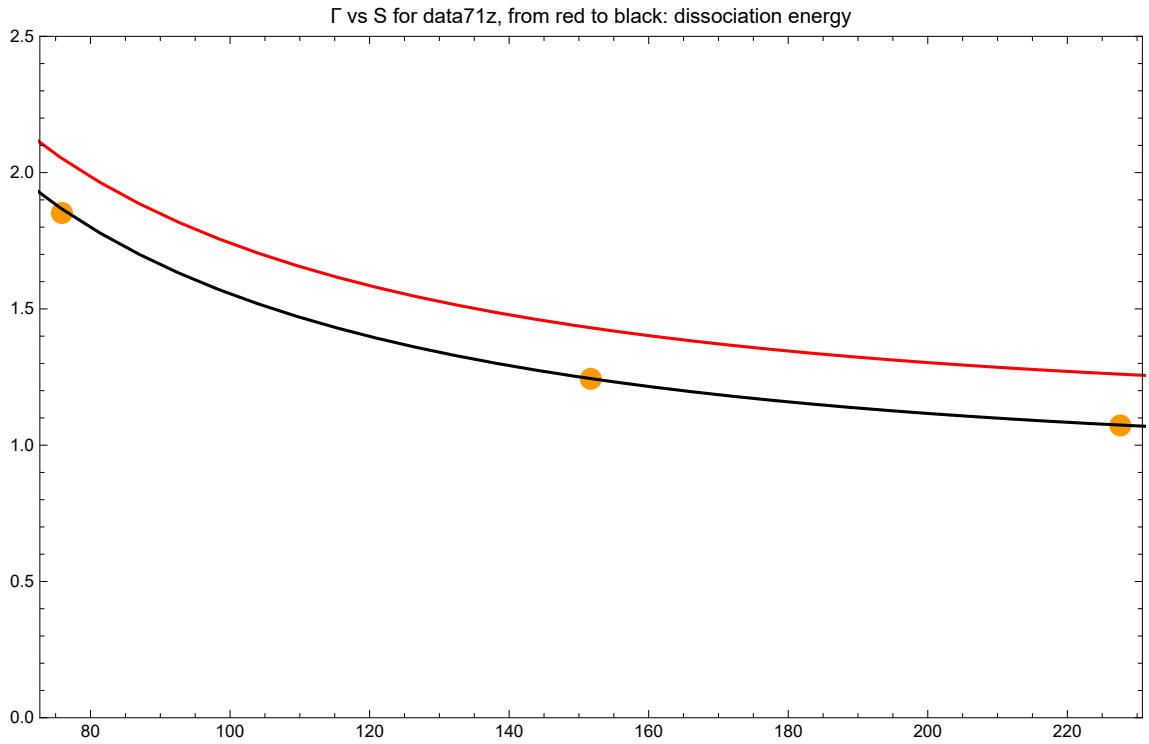

Γ vs d for data67d, from red to black: dissociation energy
3.0
2.5
2.0
1.5
1.0
0.5
0.0
0
100
200
300
400

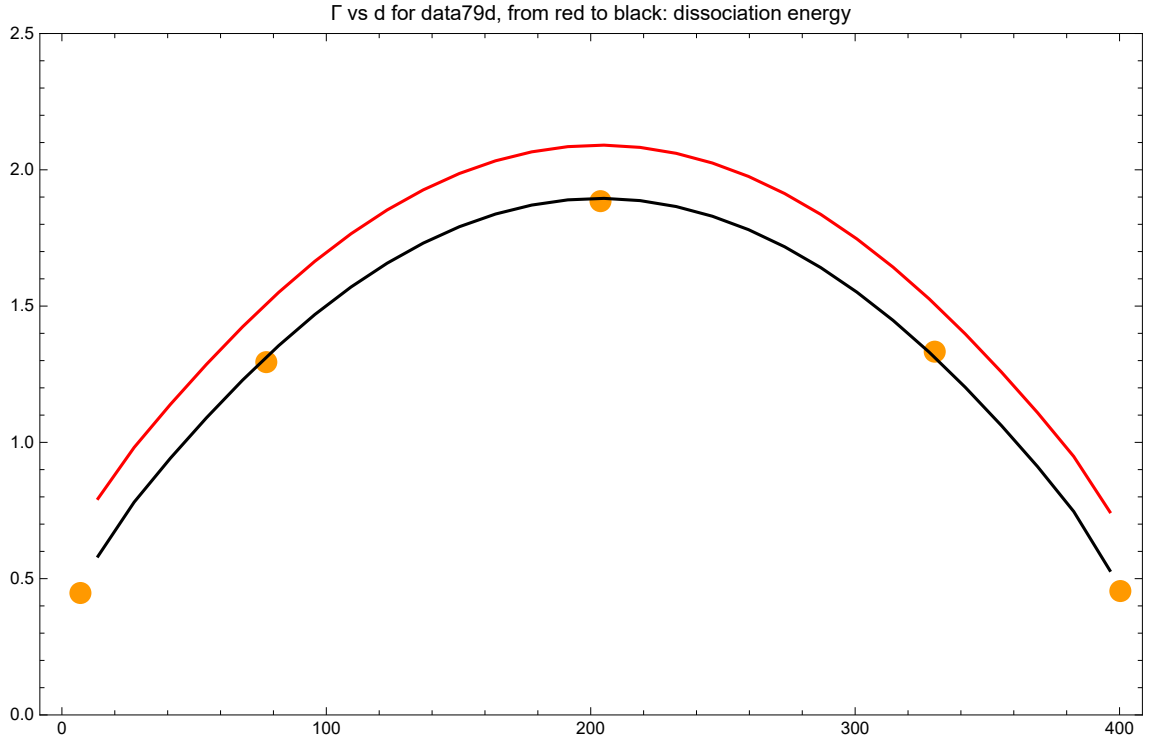

Γ vs S for data67z, from red to black: dissociation energy
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
60
80
100
120
140

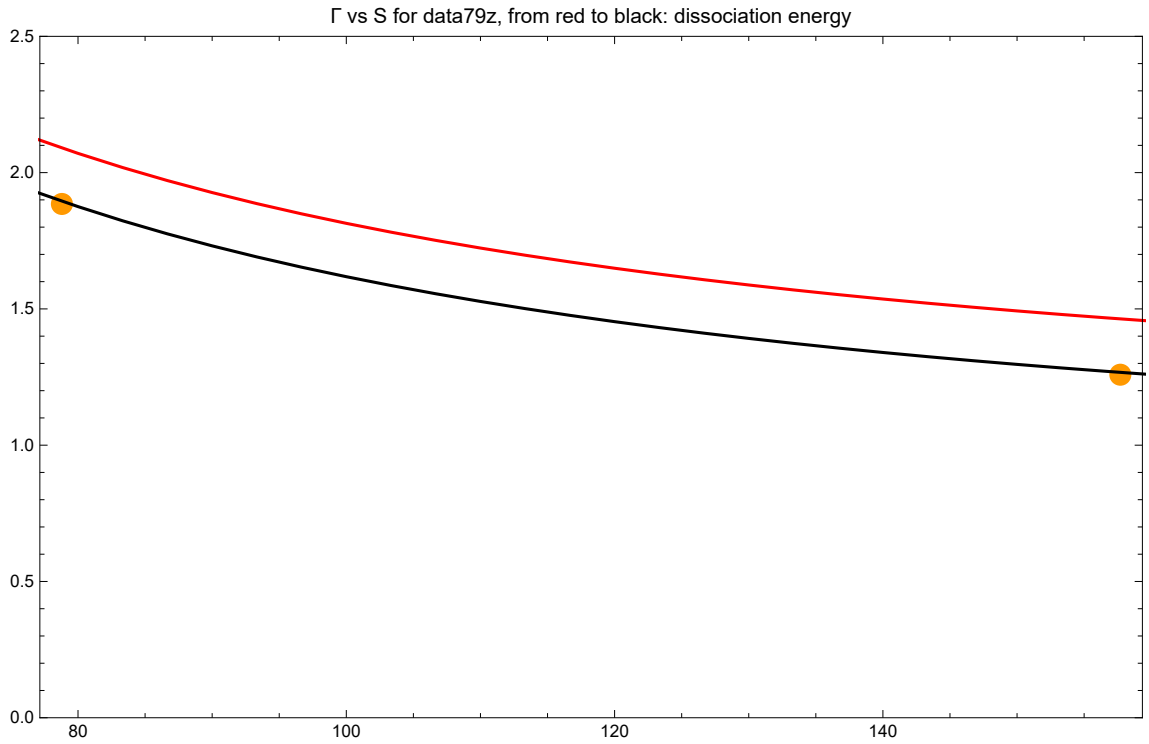

Γ vs d for data69d, from red to black: dissociation energy
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
0
100
200
300
400

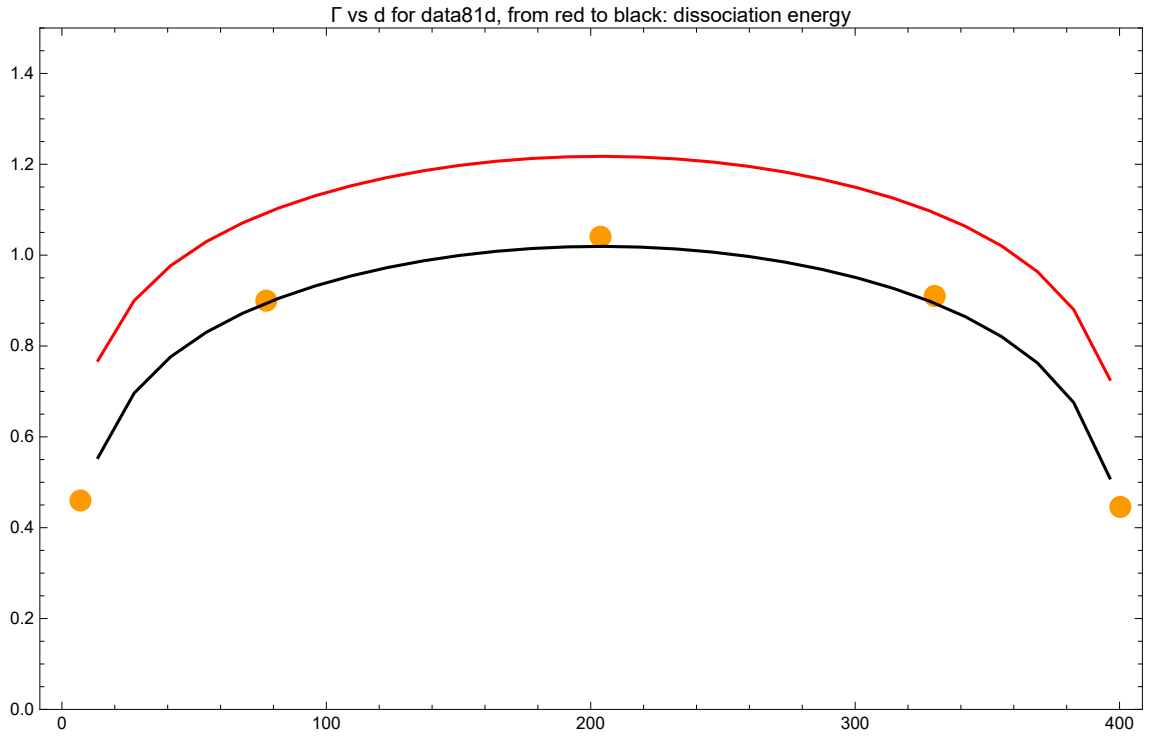

Γ vs S for data69z, from red to black: dissociation energy
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
200
250
300

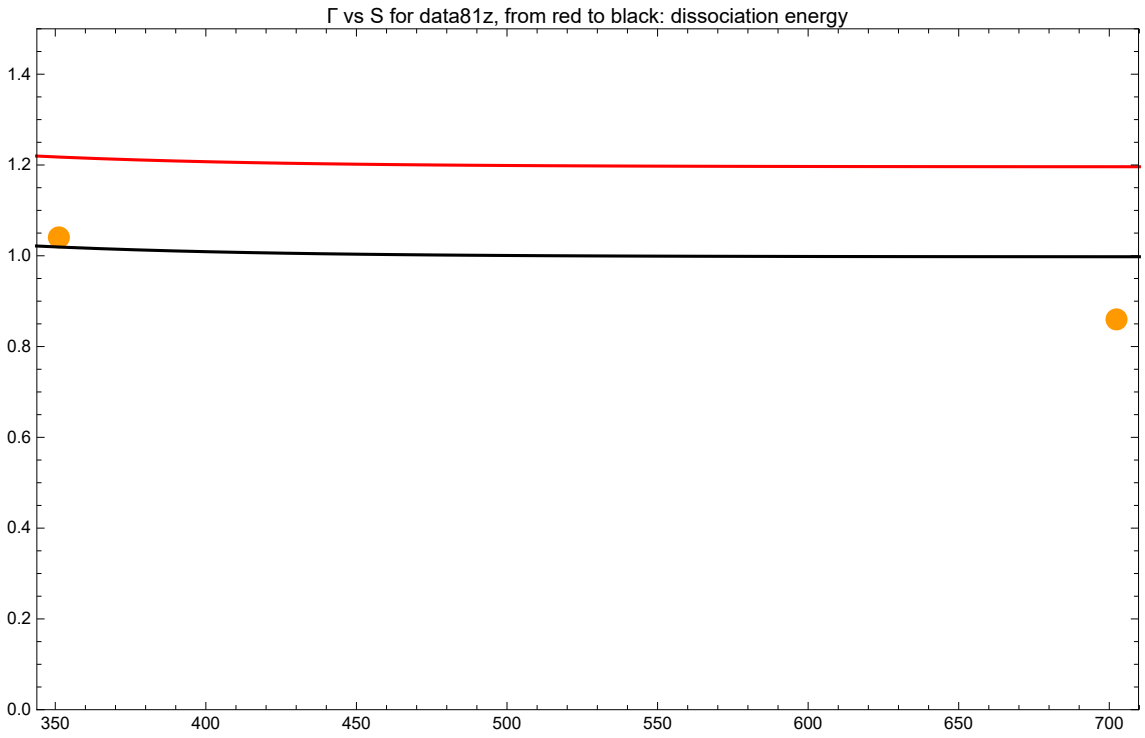

Γ vs d for data71d, from red to black: dissociation energy
2.5
2.0
1.5
1.0
0.5
0.0
0
100
200
300
400

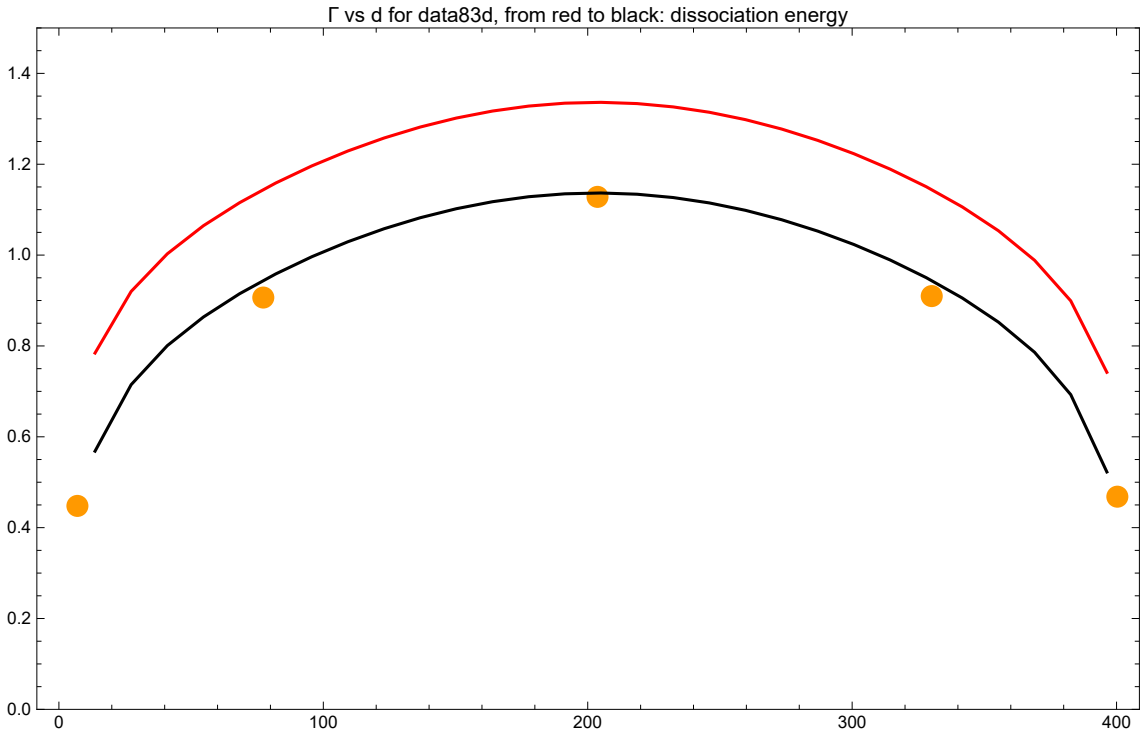

Γ vs S for data71z, from red to black: dissociation energy
2.5
2.0
1.5
1.0
0.5
0.0
80
100
120
140
160
180
200
220

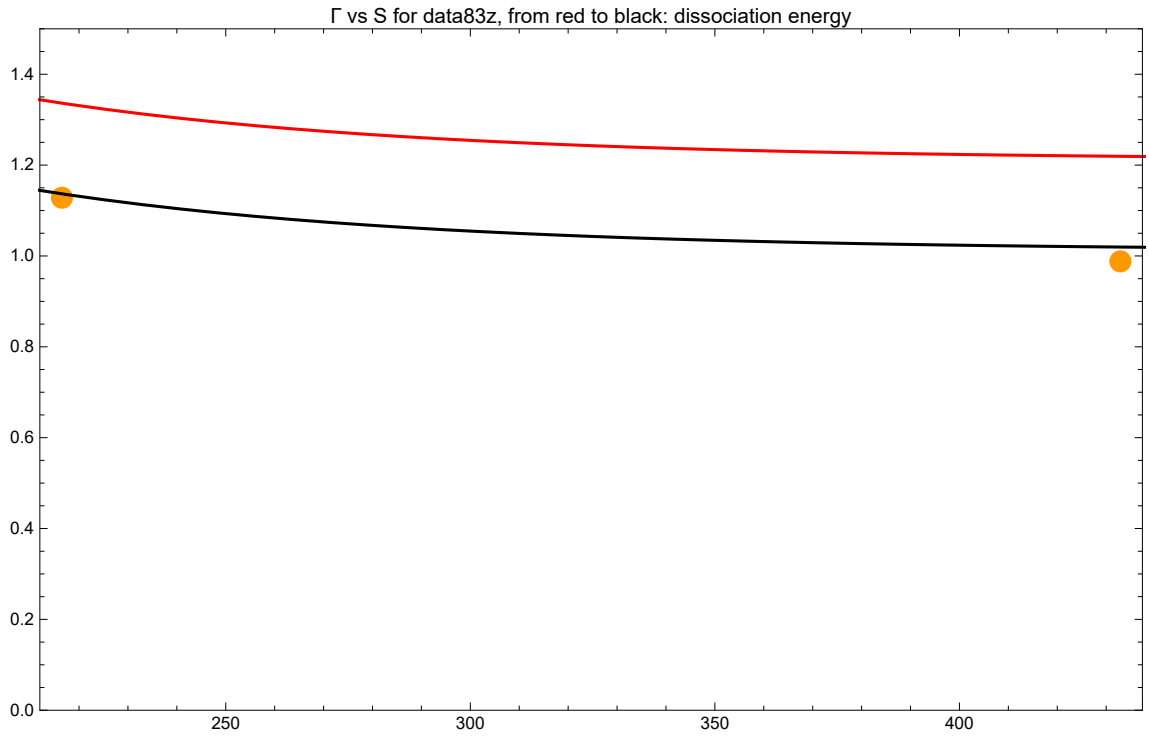

Γ vs d for data79d, from red to black: dissociation energy
2.5
2.0
1.5
1.0
0.5
0.0
0
100
200
300
400

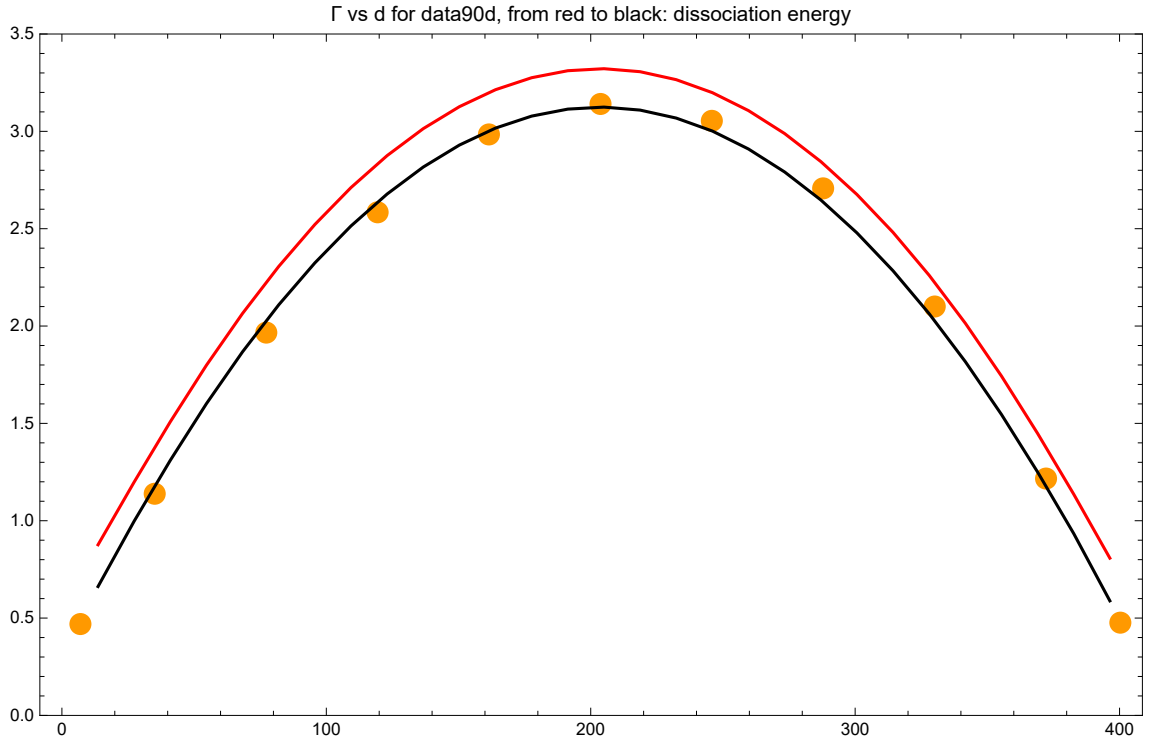

Γ vs S for data79z, from red to black: dissociation energy
2.5
2.0
1.5
1.0
0.5
0.0
80
100
120
140

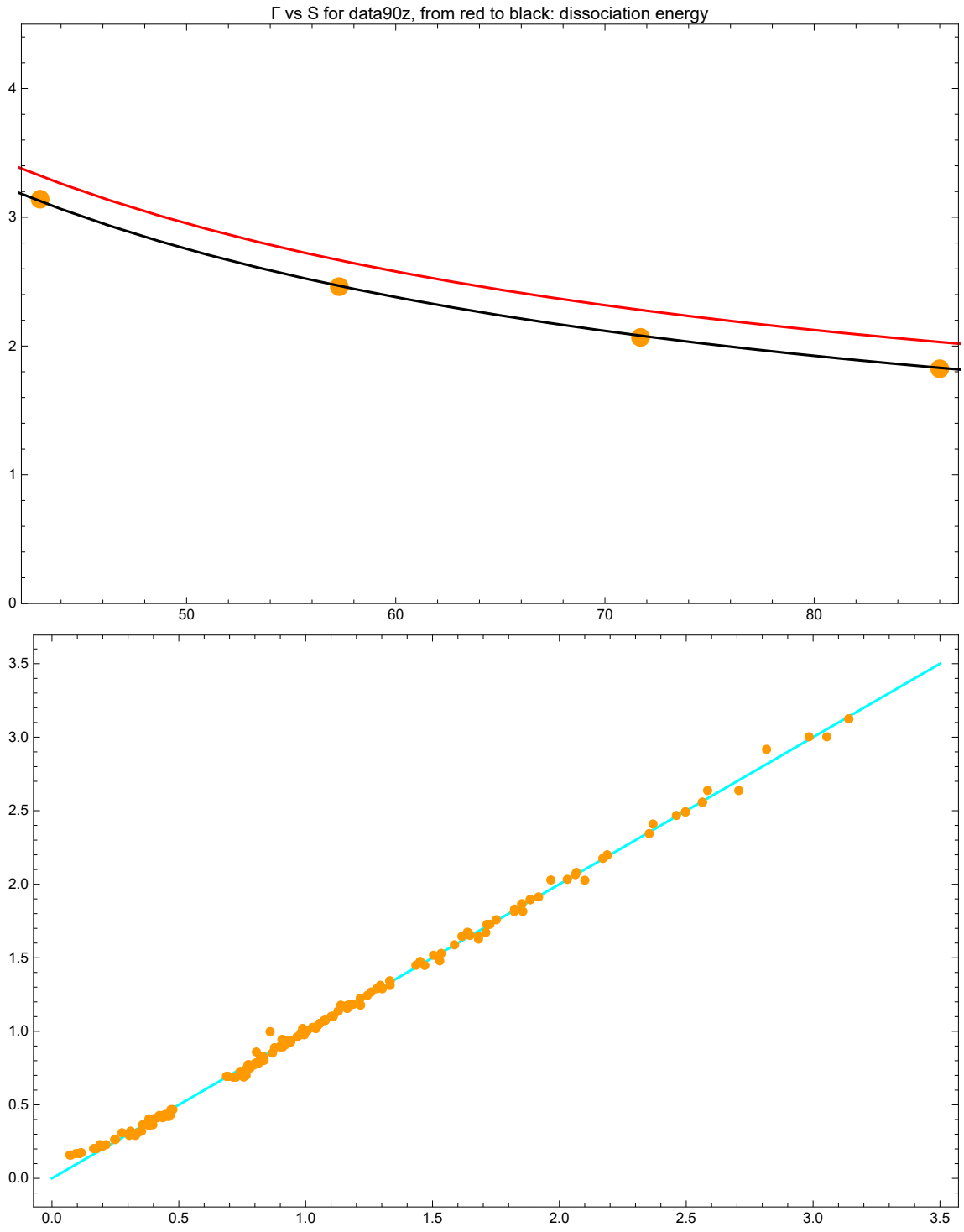

Γ vs d for data81d, from red to black: dissociation energy
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
0
100
200
300
400


Γ vs S for data81z, from red to black: dissociation energy
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
350
400
450
500
550
600
650
700


Γ vs d for data83d, from red to black: dissociation energy
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
0
100
200
300
400


Γ vs S for data83z, from red to black: dissociation energy
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
250
300
350
400

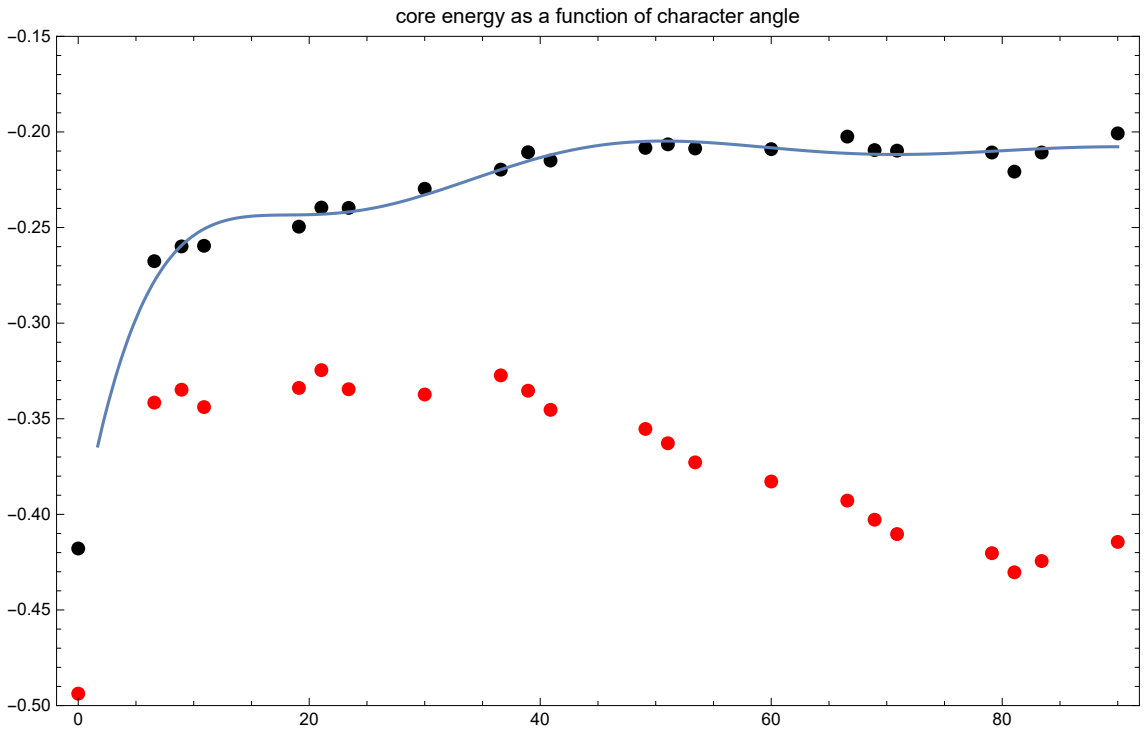

Γ vs d for data90d, from red to black: dissociation energy
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
0
100
200
300
400



total number of points tested: 180

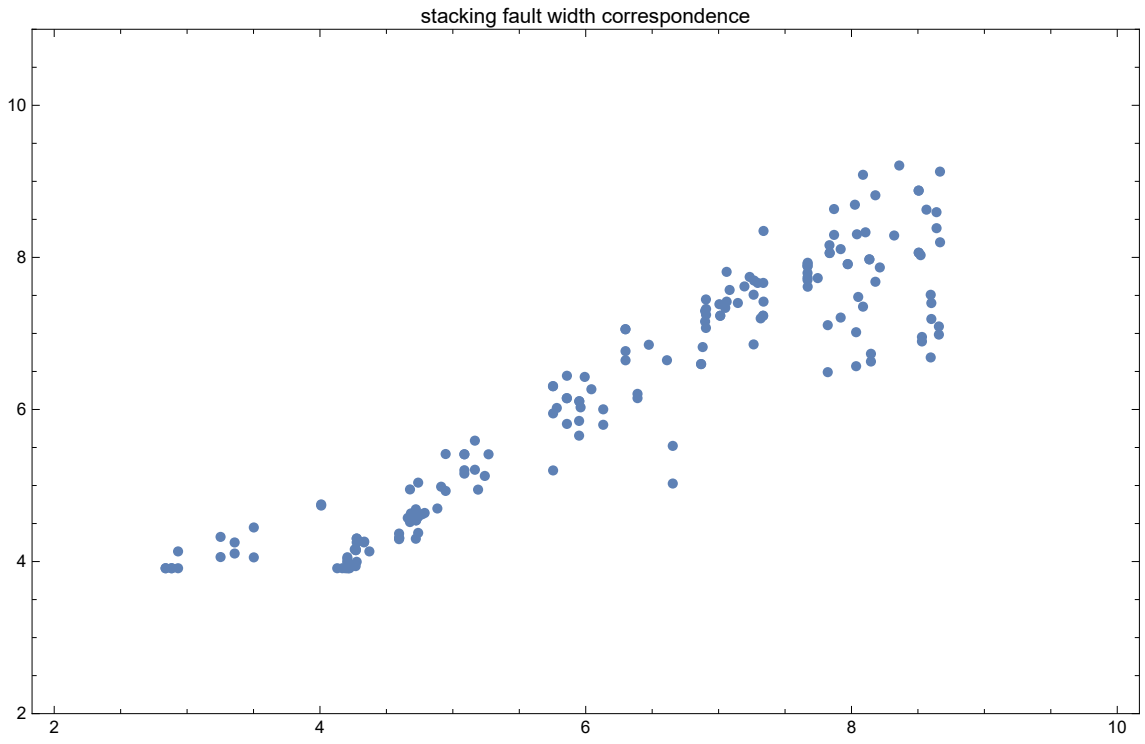
core energy function parameters:

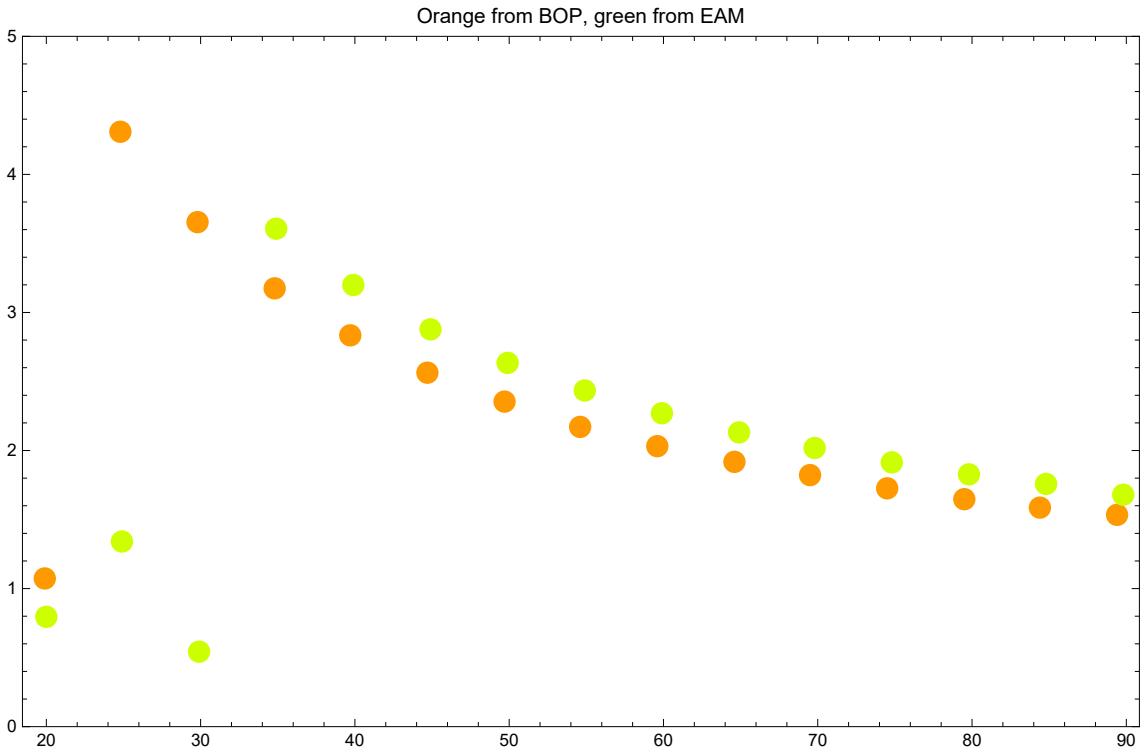
{c1 → −0.415641, c2 → 1.98852, c3 → −8.70465, c4 → 17.7093, c5 → −16.3861, c6 → 5.60079}



stacking fault width function parameters: {aa → 3.91222, bb → 0.891902}

Out[167]=




Orange from BOP, green from EAM
5
4
3
2
1
0
20
30
40
50
60
70
80
90