Supplementary material for "**Protein imperfections: separating intrinsic from extrinsic variation of torsion angles**" by Glenn L. Butterfoss, Jane S. Richardson and Jan Hermans.

Computed energy and torque for each of 47 methionine residues in the database for which the C^γ-S^δ torsion angle, χ_3 lies within 30° of the canonical value for a skewed conformation (120° or -120°).   These have been sorted into 6 sets according to the criteria given in the following table. See also legend of Figure 8 of the accompanying paper.

Set	Distance from eclipsed	Sign of torque	Distance from energy minimum	Number of instances
1	> 10°	Correct		22
2	> 10°	Wrong	≤ 5°	8
3	> 10°	Wrong	> 5 °	4
4	< 10°		≤ 5°	9
5	< 10°		> 5° but ≤ 10°	1
6	< 10°		> 10°	3

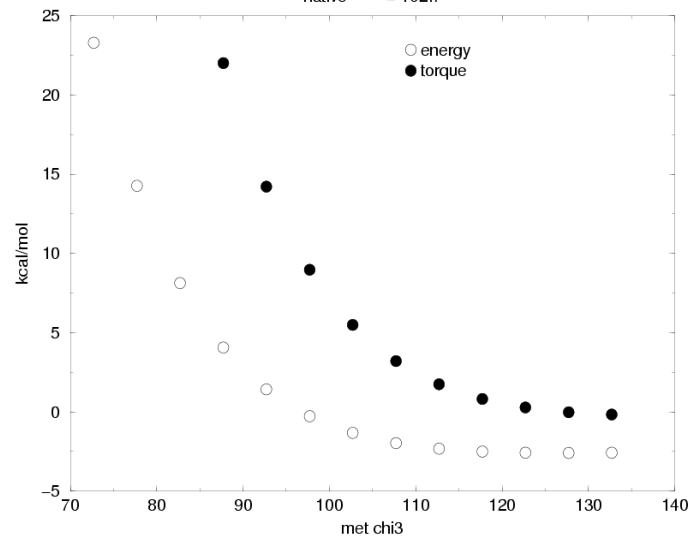# Set 1 = Native > 10° from eclipsed, correct torque, # 1-4 of 22
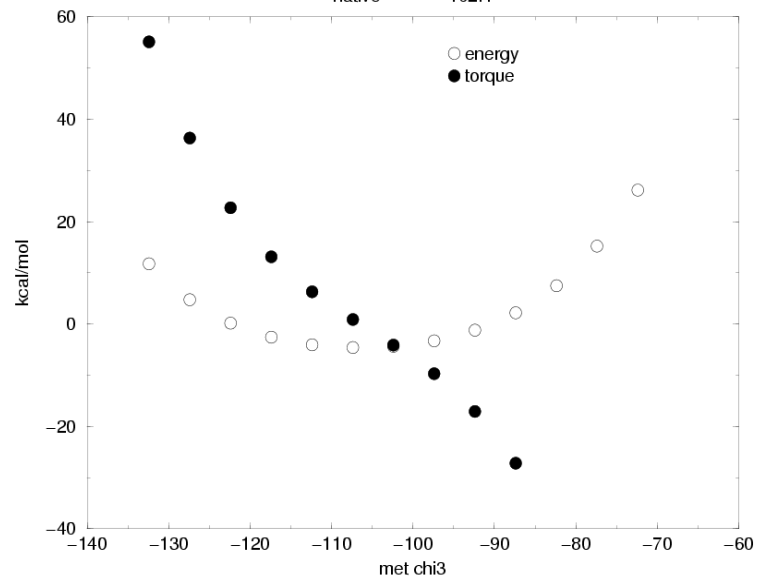

1eco Met 35

native = 97.2
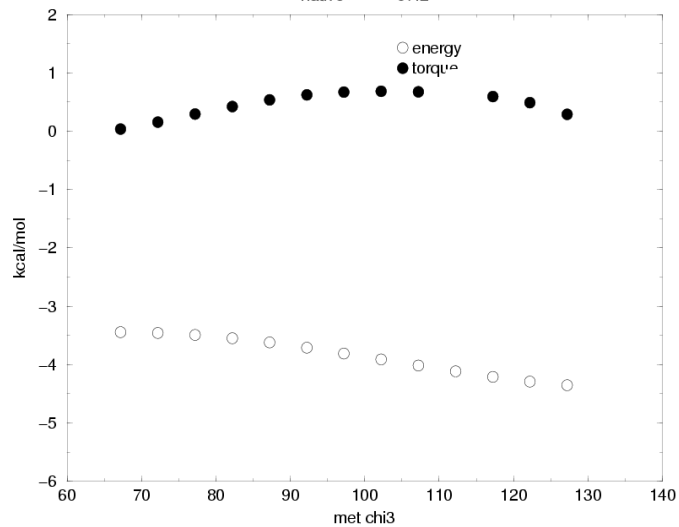
1lam Met 270

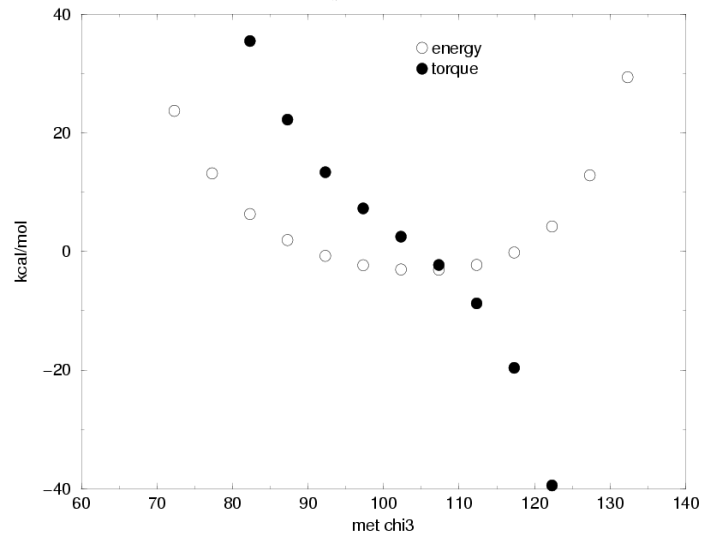native = 102.7

1a41 Met 282

native = 97.8
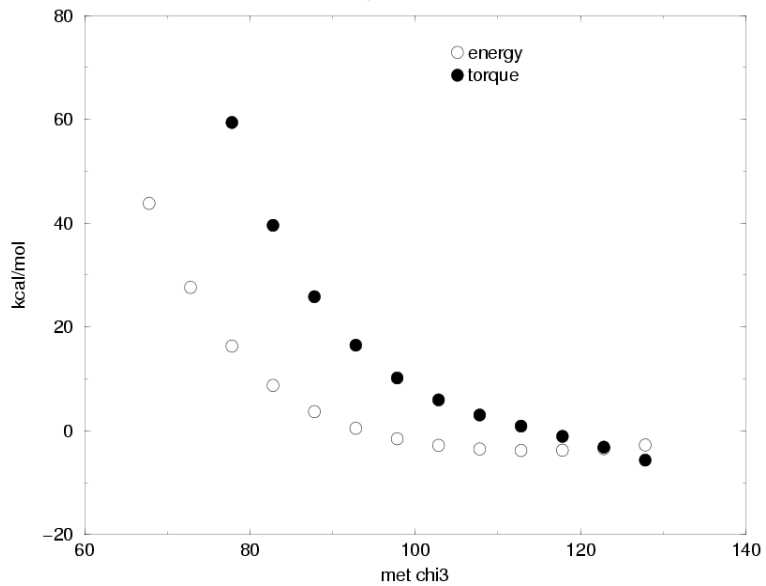
1bi5 Met 158

native = −102.4

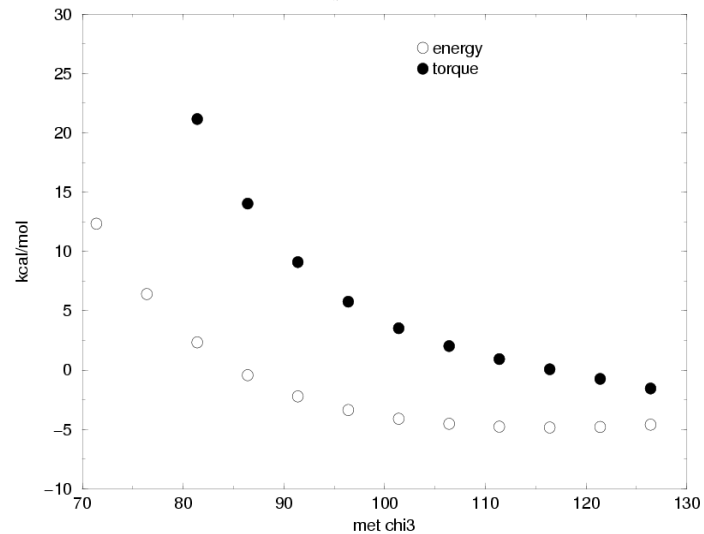# Set 1 = Native > 10° from eclipsed, correct torque, # 5-8 of 22
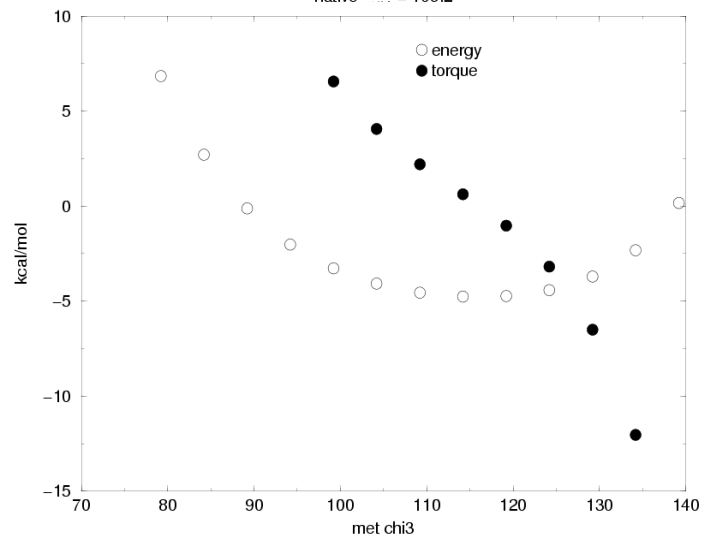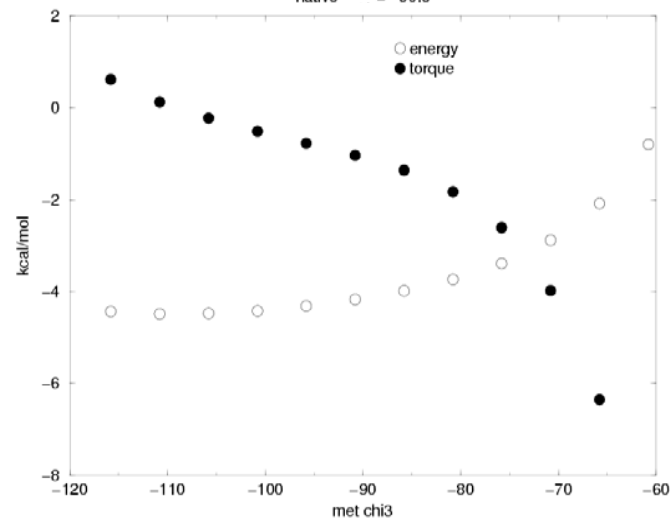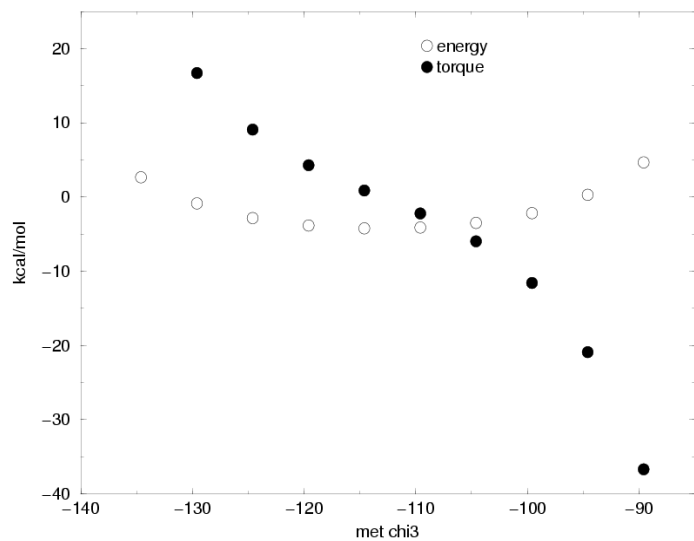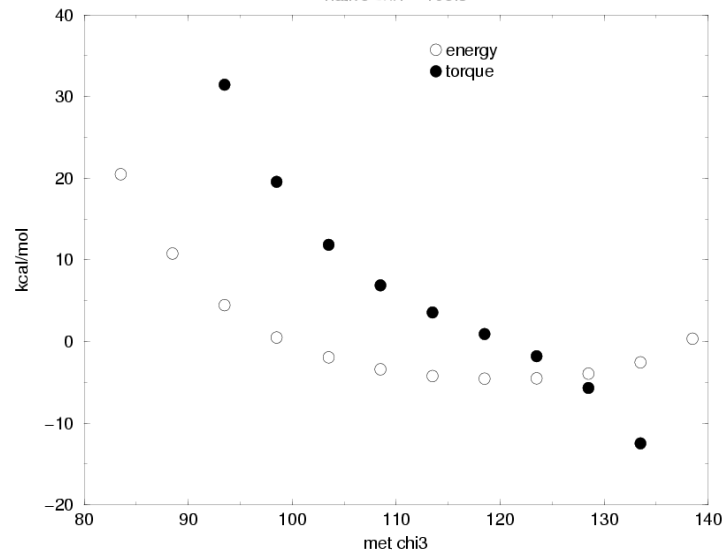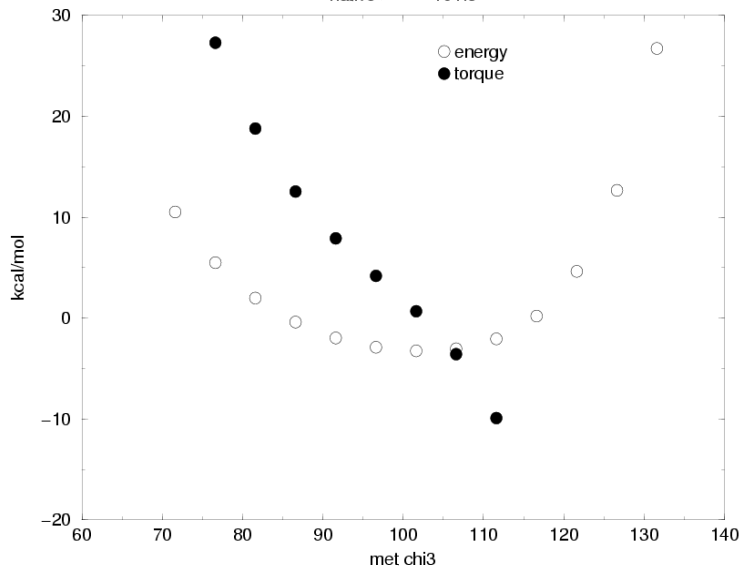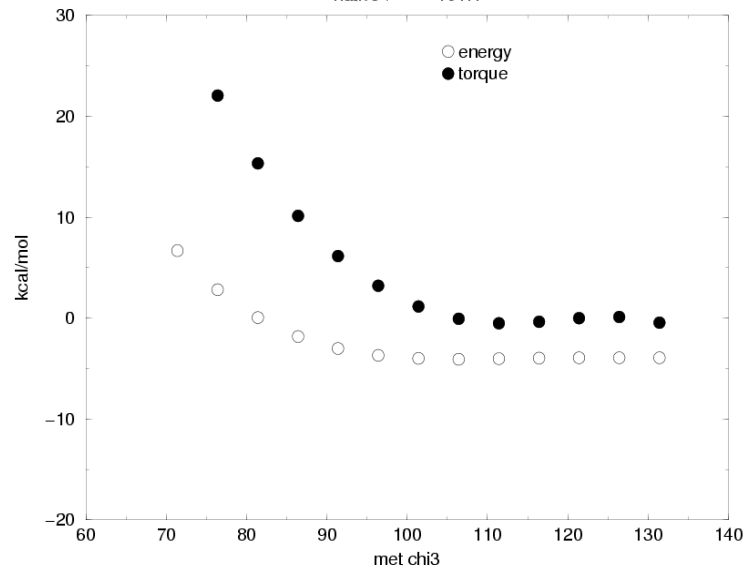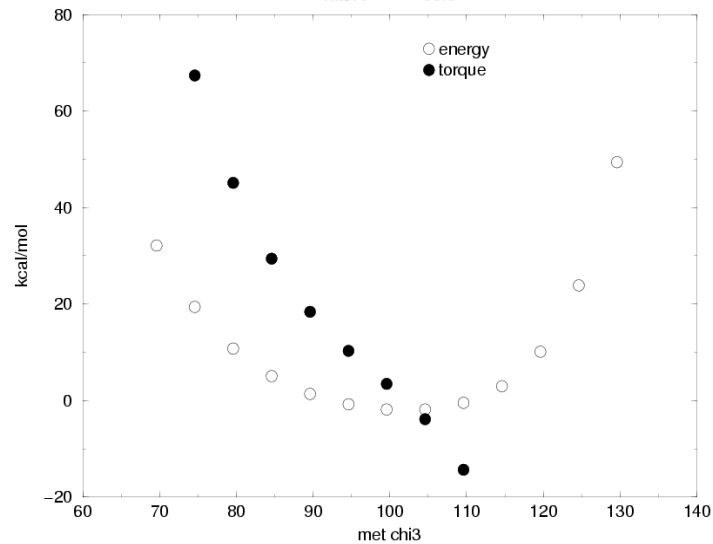
1bf6 Met 40

native = 102.3

1cip Met 53

native = 101.4

1ayl Met 218

native = 101.6

1bf6 Met 54

native = 101.4

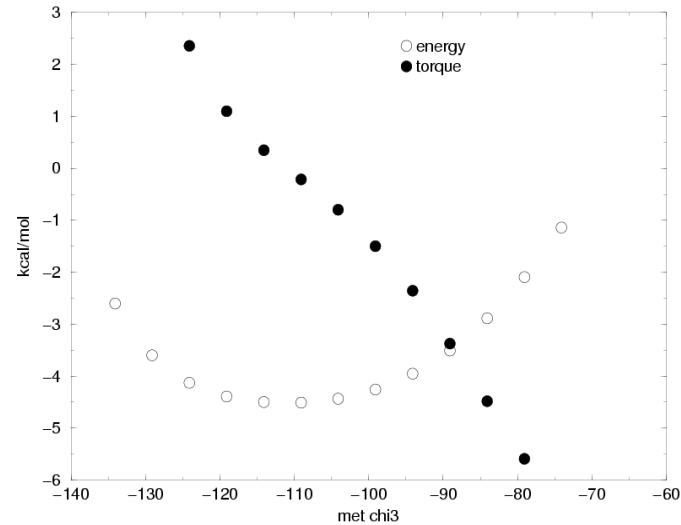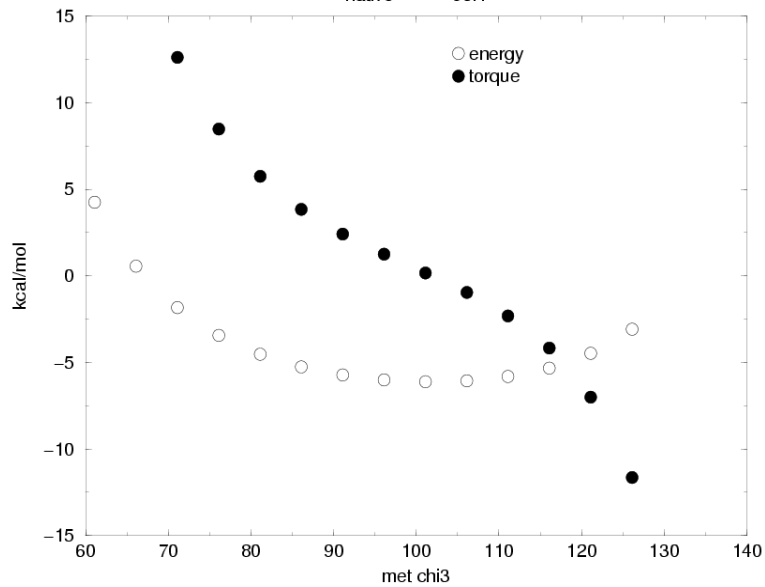Set 1 = Native > 10° from eclipsed, correct torque, # 13-16 of 22

16pk Met 341
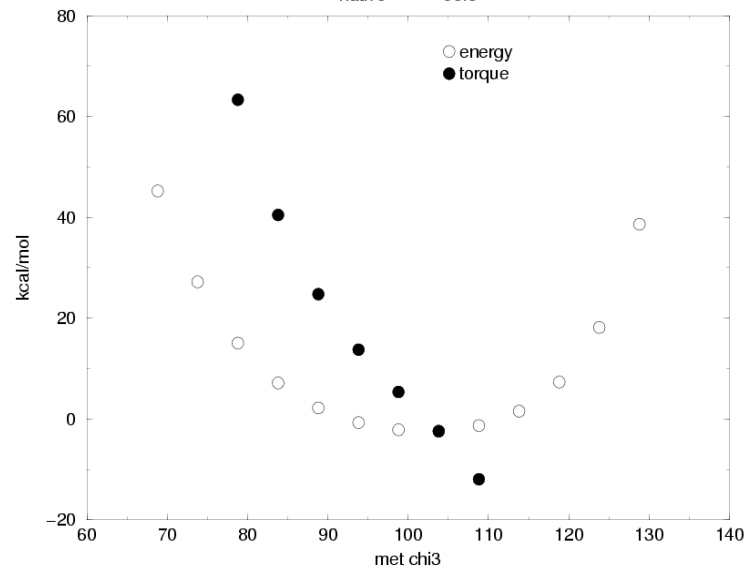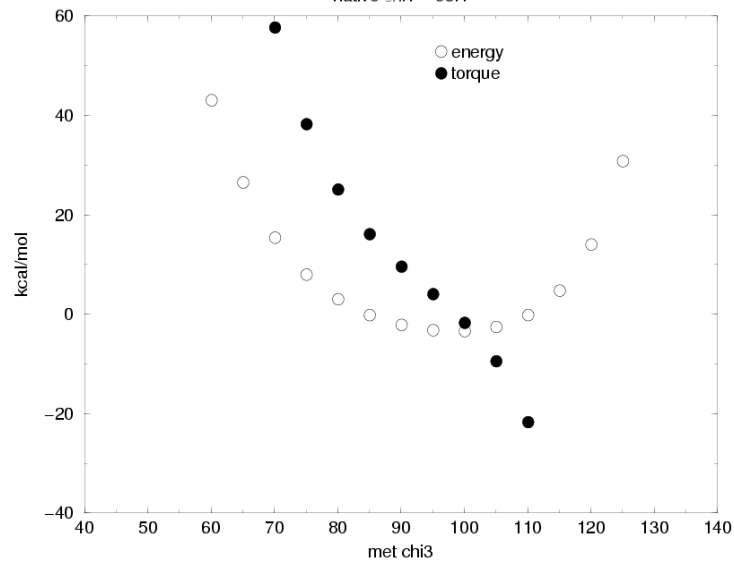
1fmb Met 80
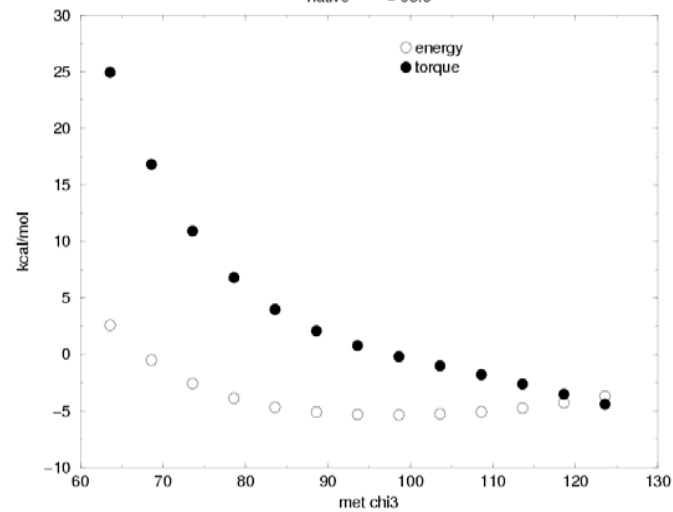
1bu7 Met 145
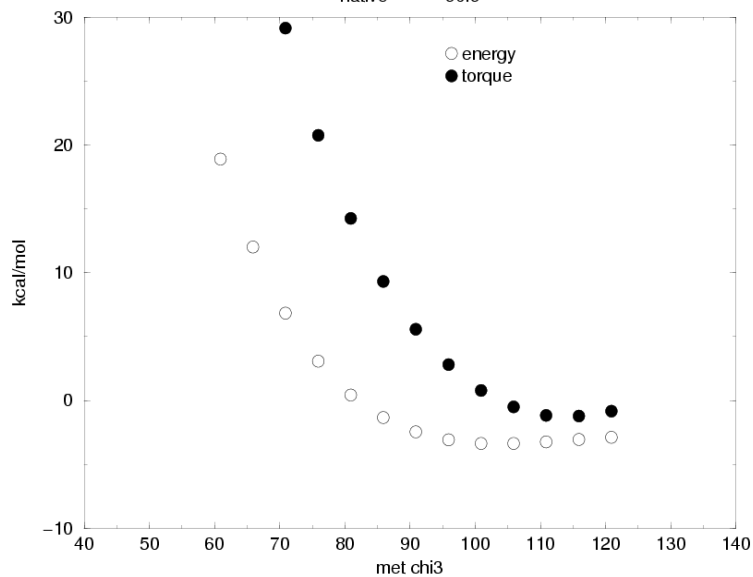
1ezm Met 102
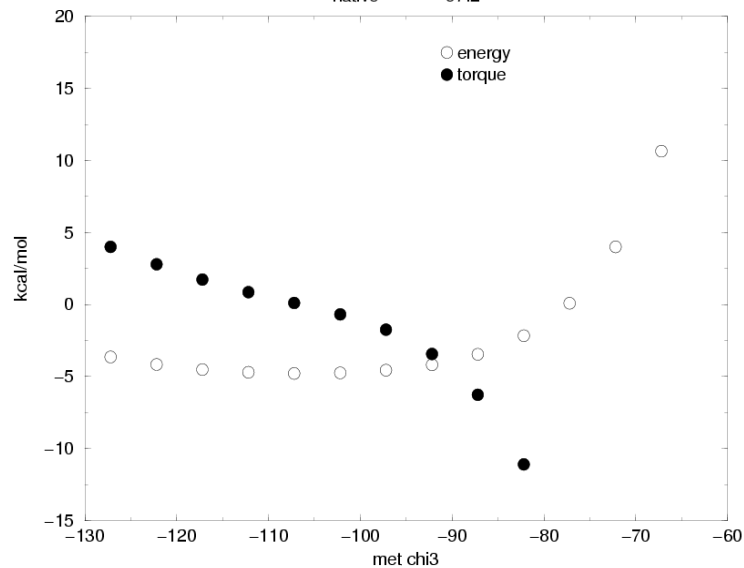
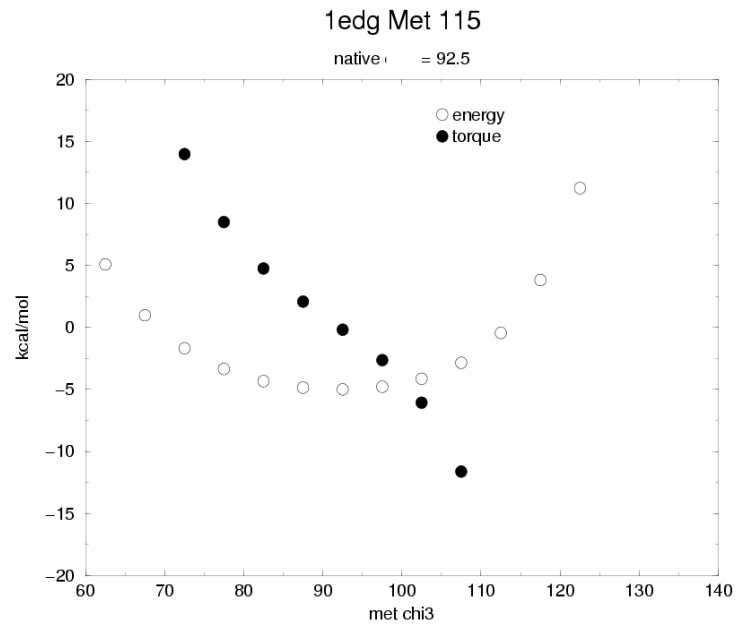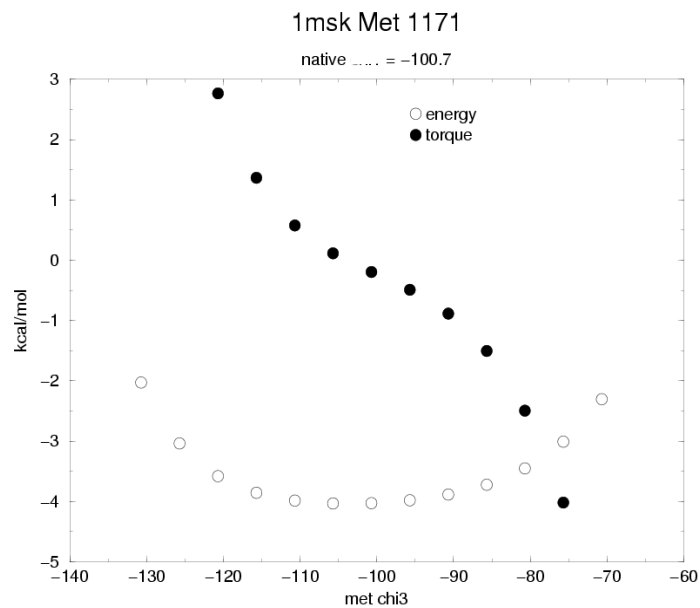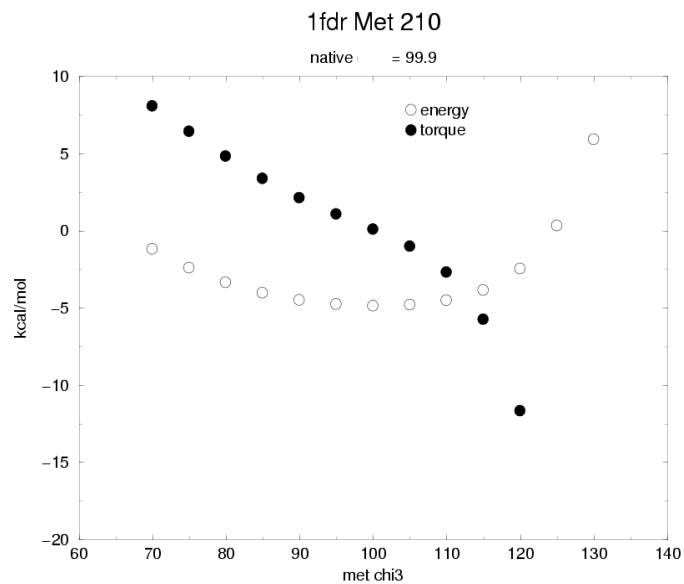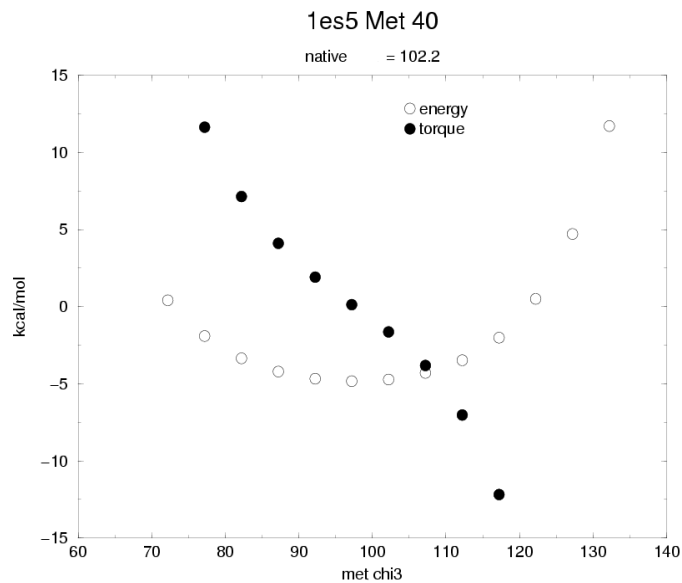Set 1 = Native > 10° from eclipsed, correct torque, # 21 and 22 of 22
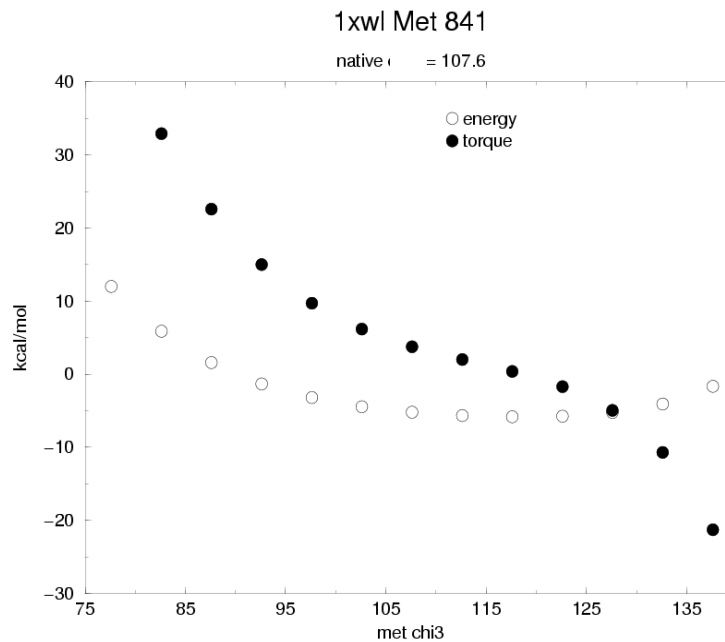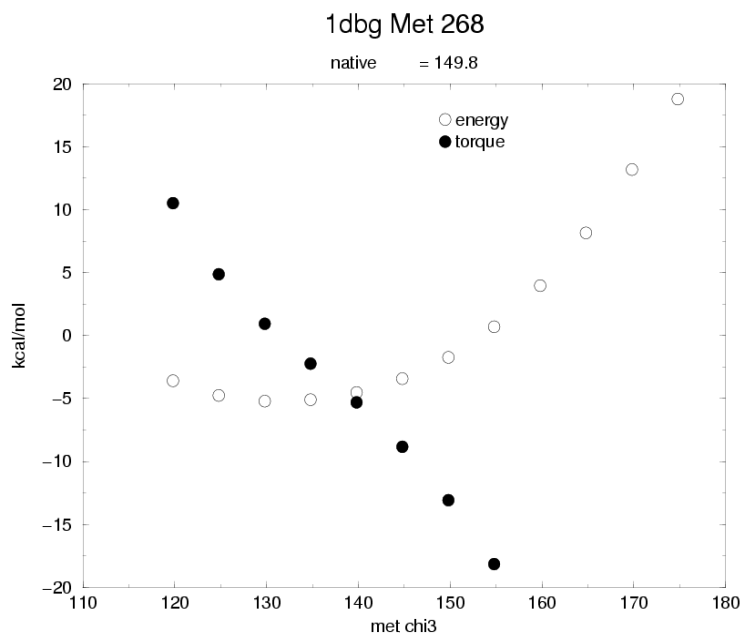
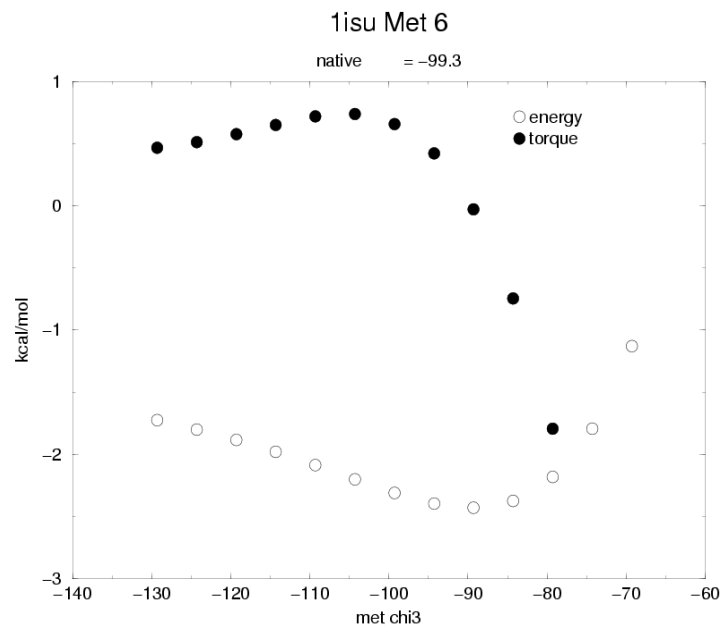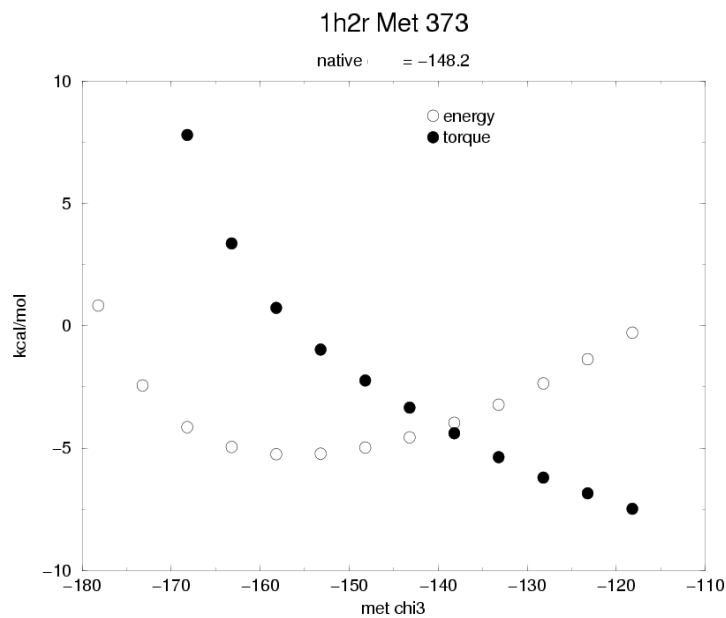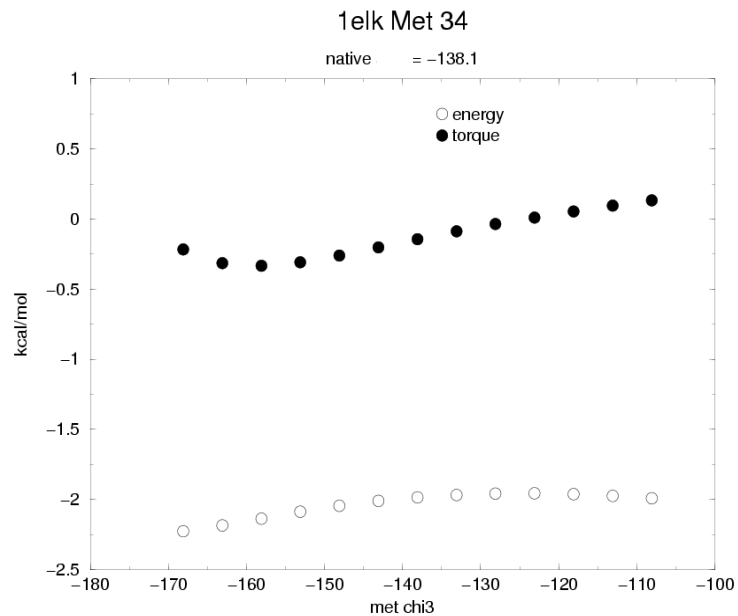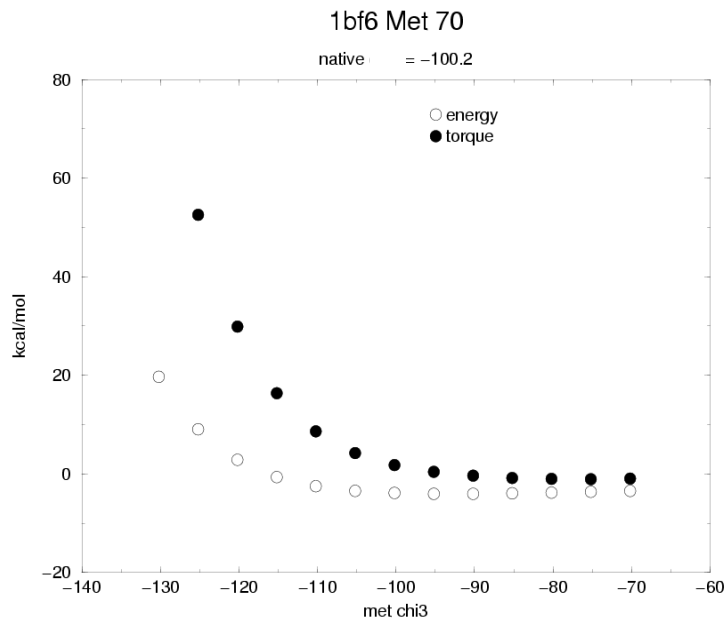Set 2 = Native > 10° from eclipsed, wrong torque and native <= 5 ° away from local energy minimum, # 1-4 of 8
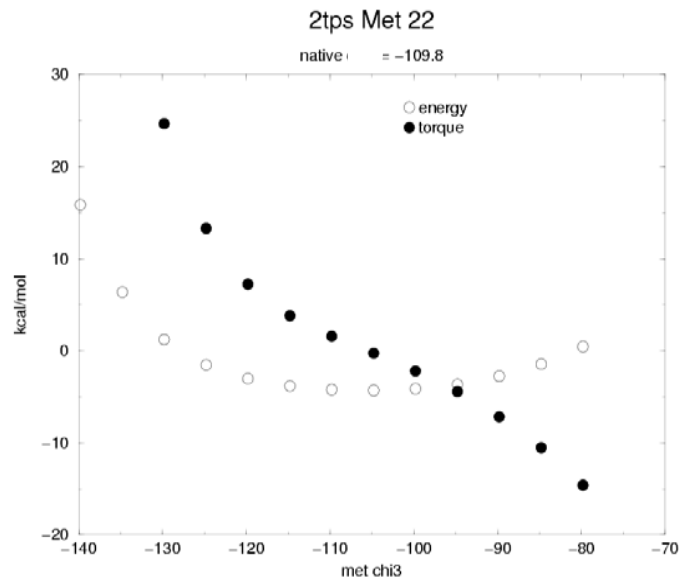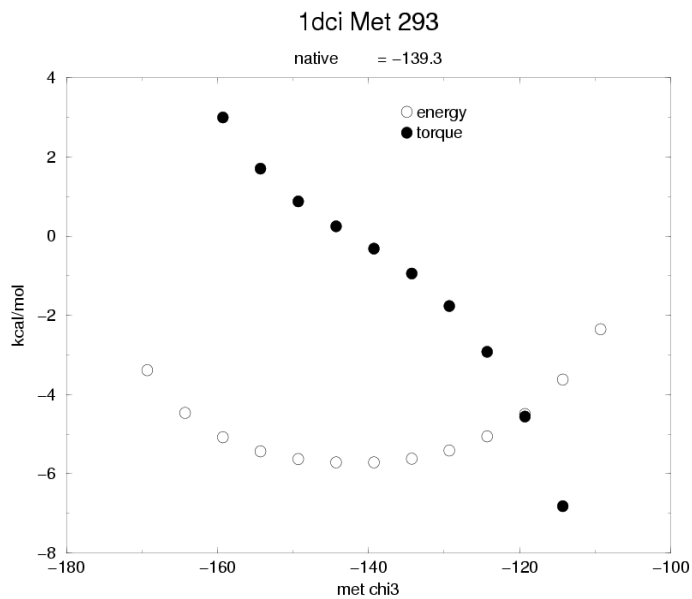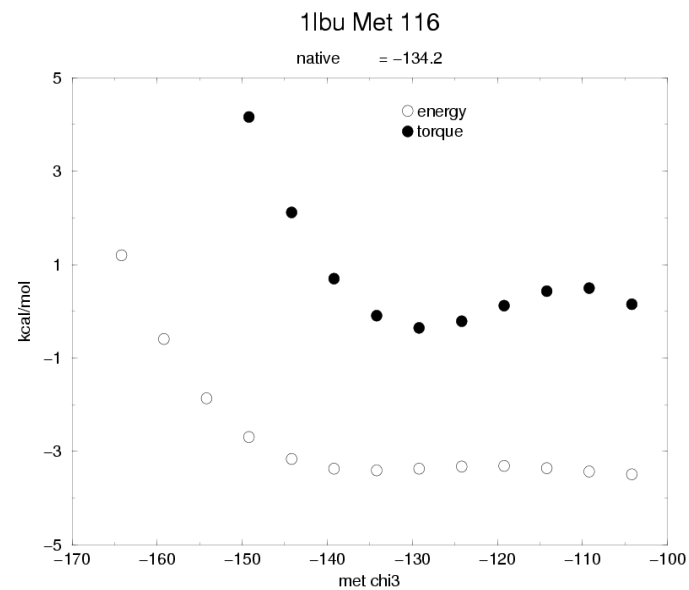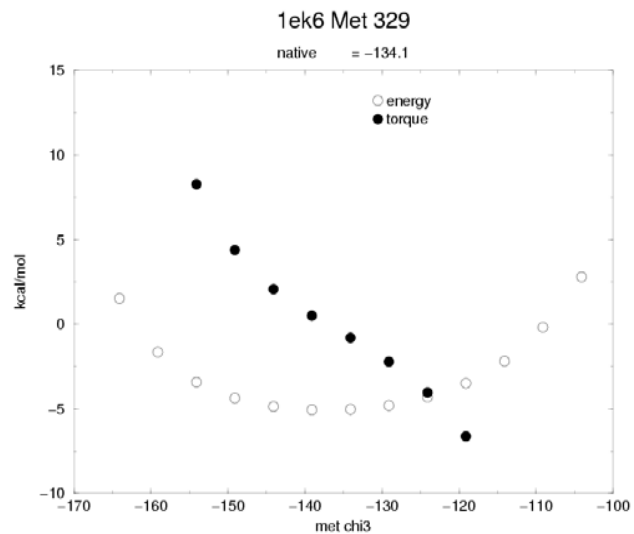
Set 2 = Native > 10° from eclipsed, wrong torque and native <= 5 ° away from local energy minimum, # 5-8 of 8
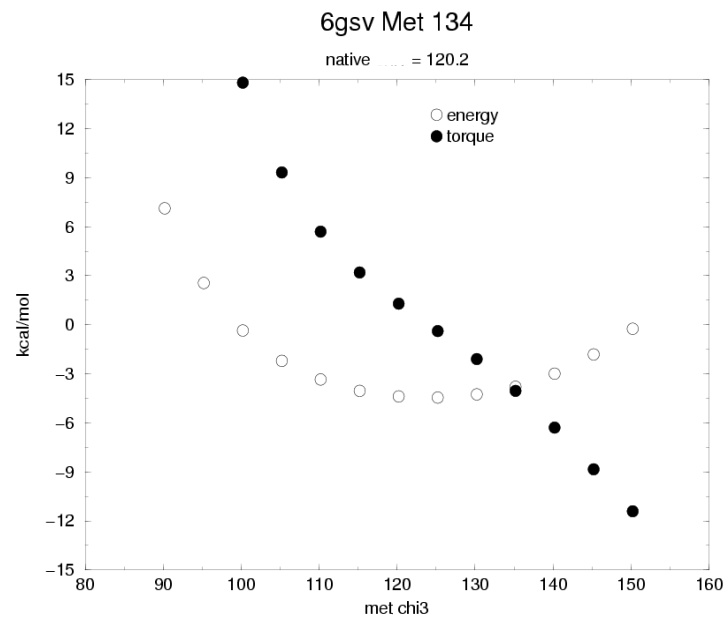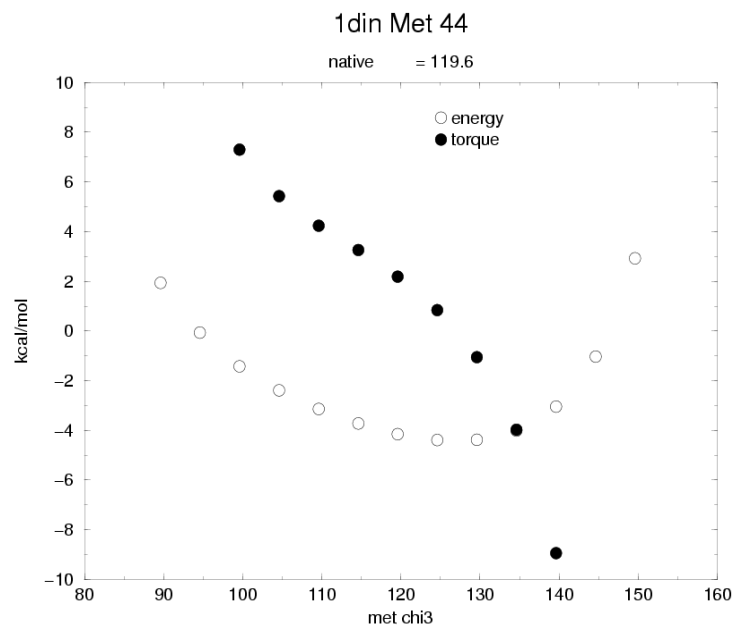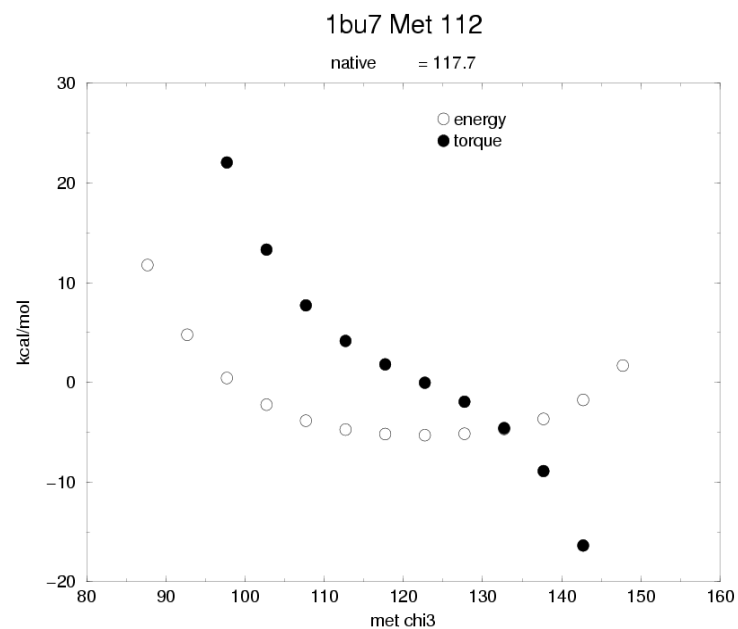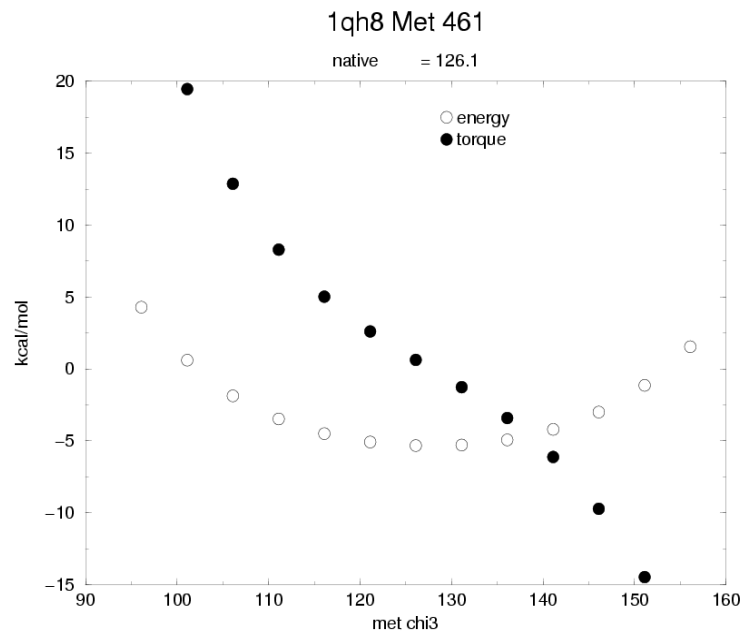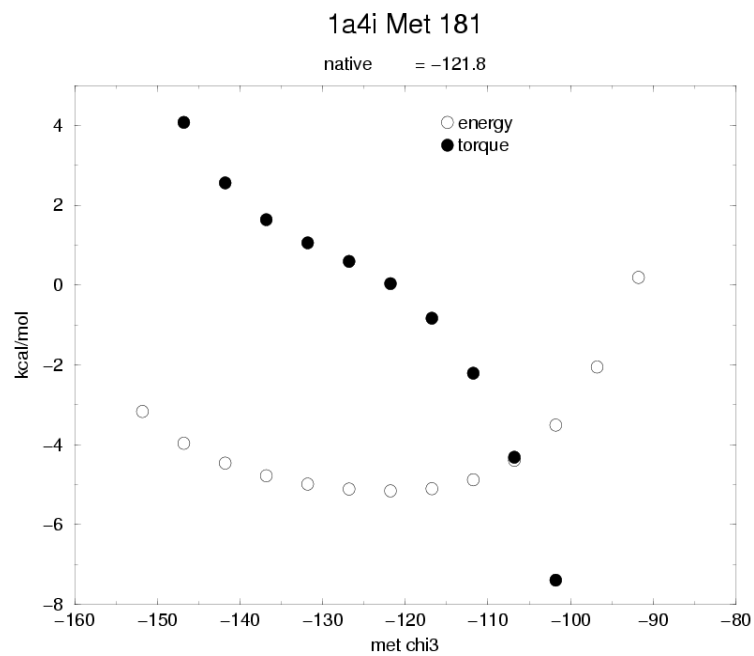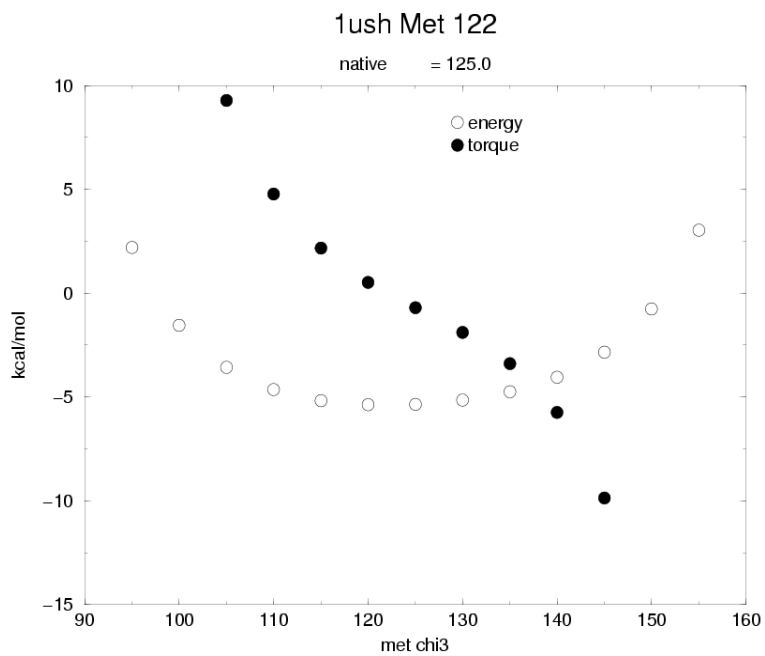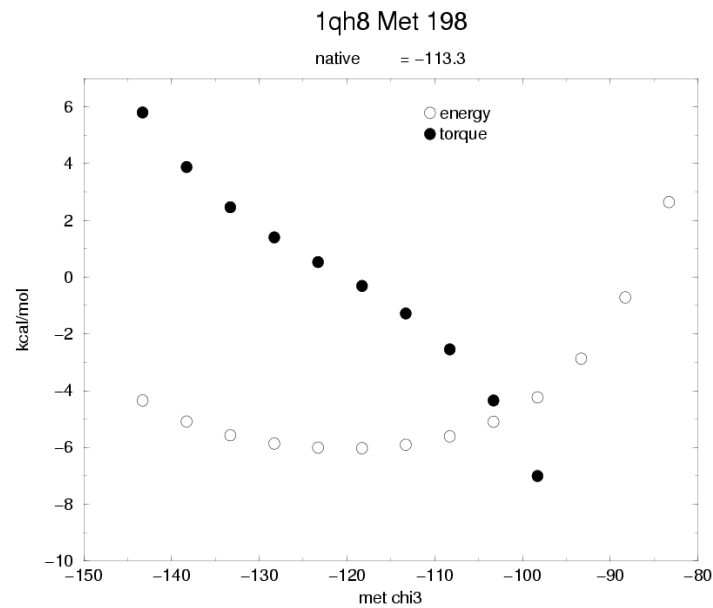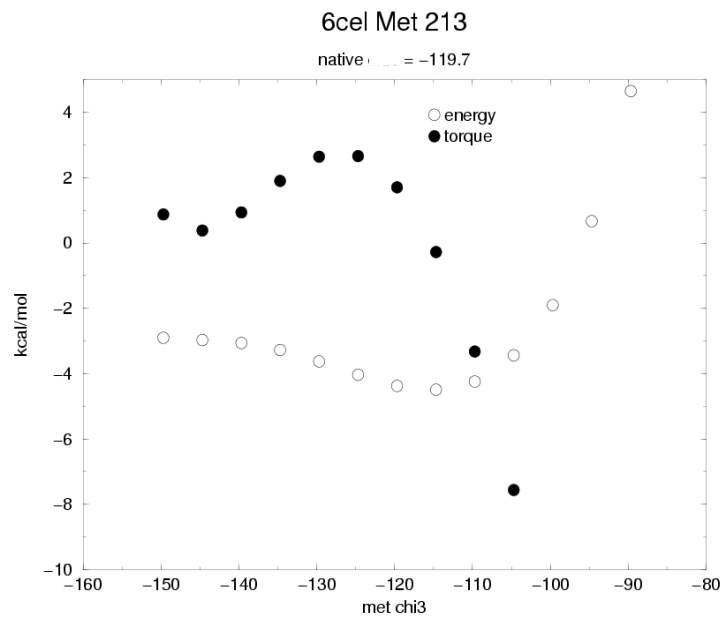
Set 3 = Native > 10° from eclipsed, wrong torque and native > 5 ° away from local energy minimum, # 1-4 of 4

1qh8 Met 461
native = 126.1

1bu7 Met 112
native = 117.7

1din Met 44
native = 119.6

6gsv Met 134
native = 120.2

6cel Met 213

native   = −119.7

1qh8 Met 198

native   = −113.3

1ush Met 122

native   = 125.0

1a4i Met 181

native   = −121.8

1gci Met 119

native   = 110.8

Set 5 = Native within 10° of eclipsed and native >5 ° but <= 10 ° away from local energy minimum , # 1 of 1

1lam Met 364

native   = −122.2

○ energy
● torque

kcal/mol

met chi3
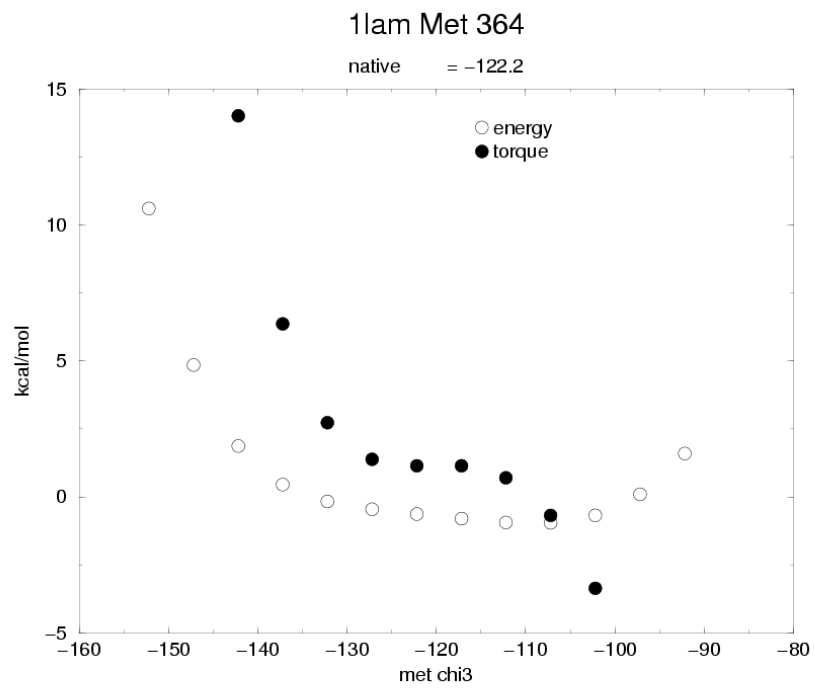
Set 6 = Native within 10° of eclipsed and native > 10 ° away from local energy minimum , # 1-3 of 3

1bf6 Met 199

1cnz Met 259

1ute Met 245