## Appendix B. Schrodinger Graphs

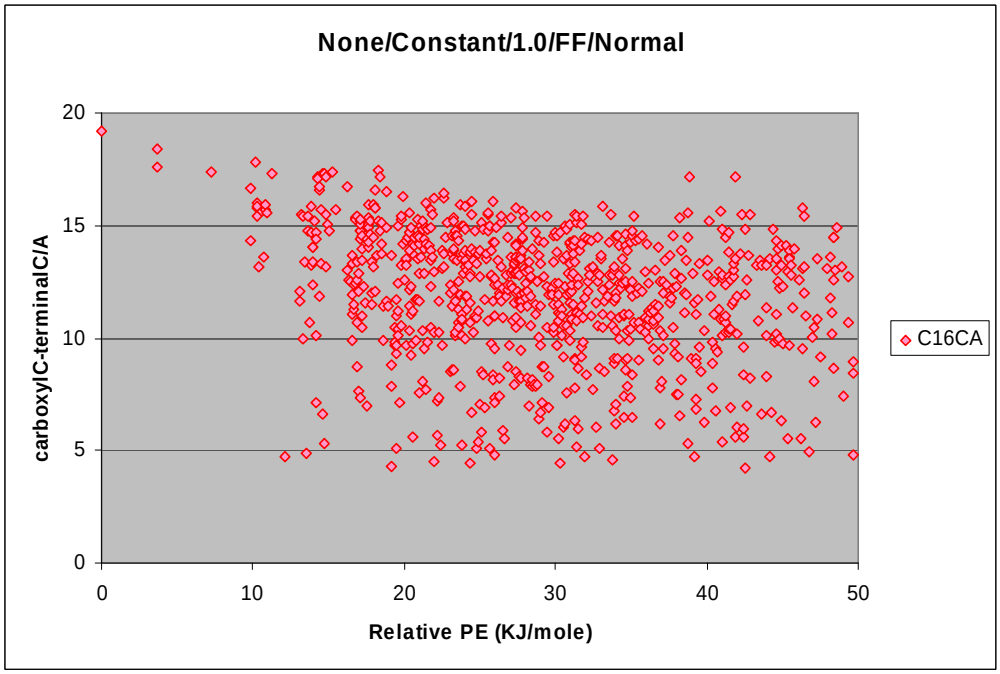


Figure 1: Plot of relative potential energy against distance – hexadecanoic acid (CA16csMiv1).

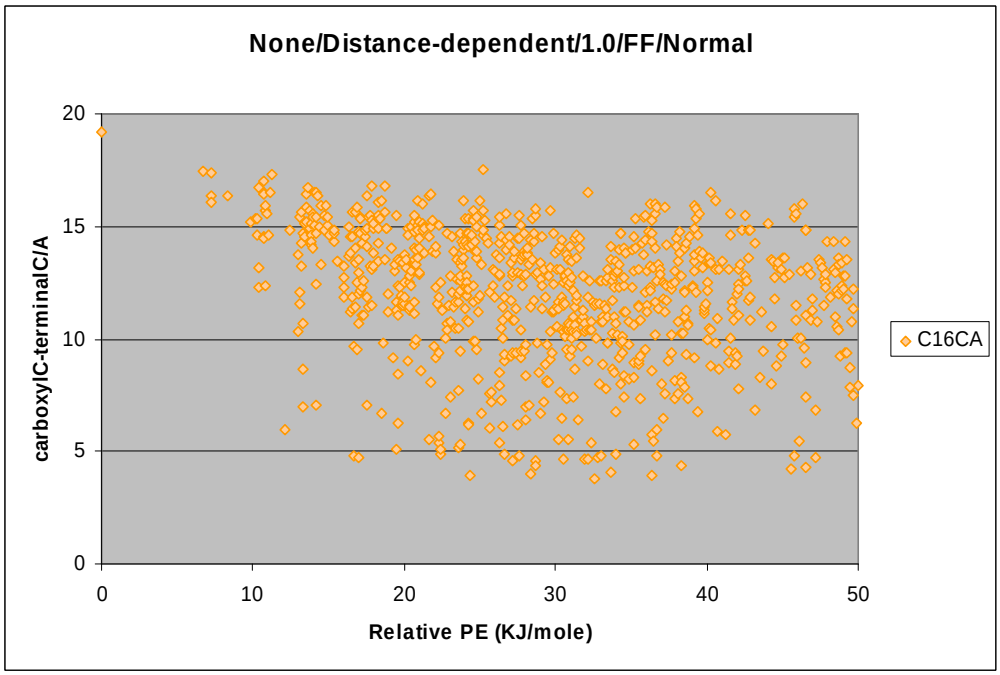


Figure 2: Plot of relative potential energy against distance – hexadecanoic acid (CA16csMiv2).

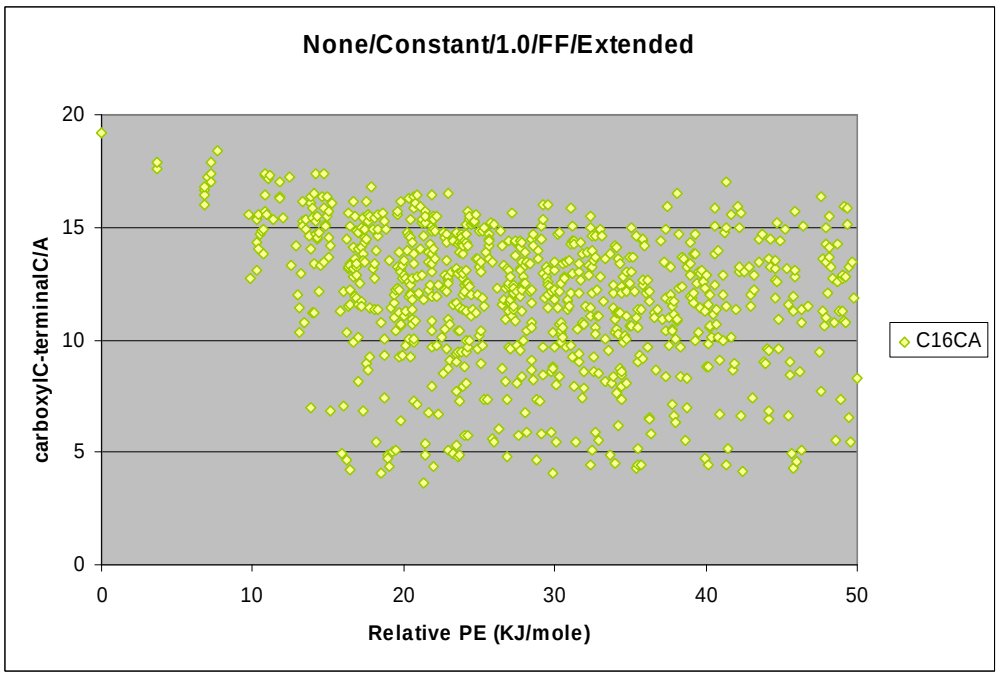


Figure 3: Plot of relative potential energy against distance – hexadecanoic acid (CA16csMiv3).

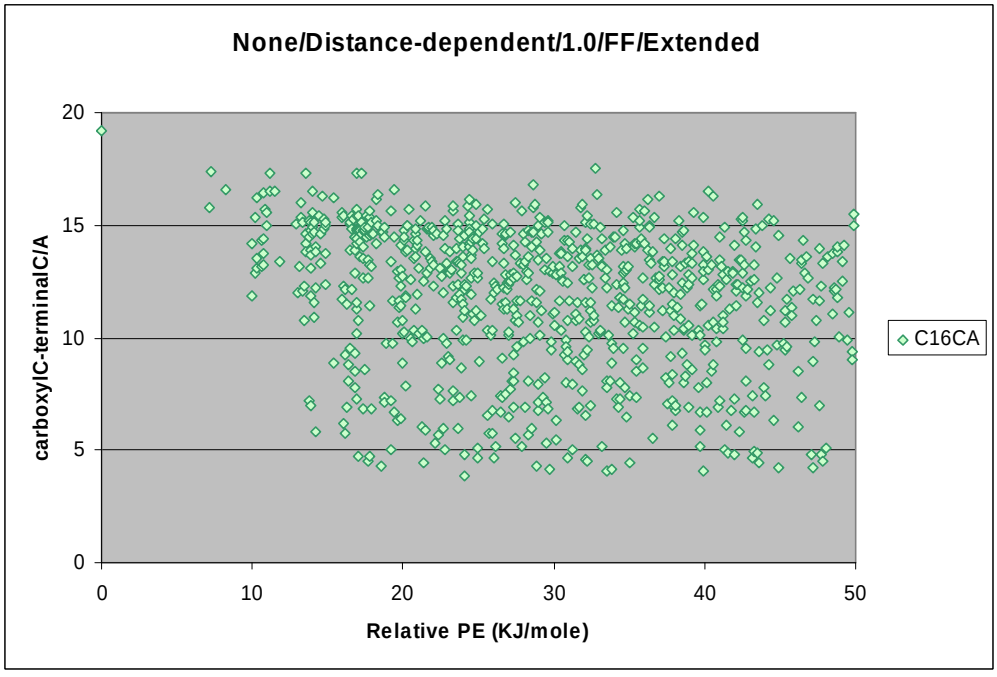


Figure 4: Plot of relative potential energy against distance – hexadecanoic acid (CA16csMiv4).

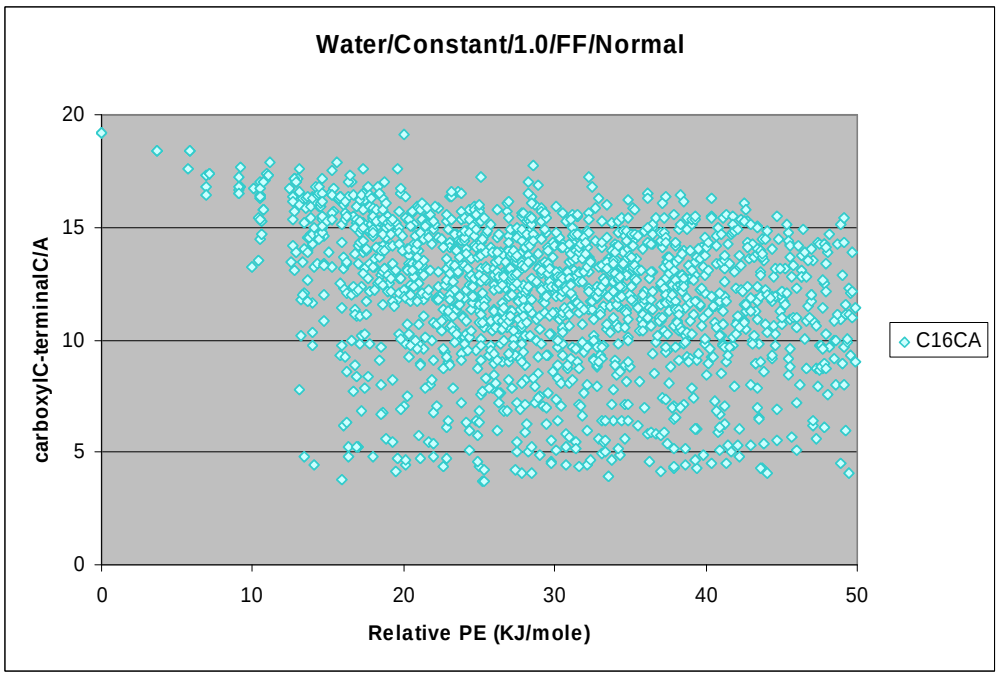


Figure 5: Plot of relative potential energy against distance – hexadecanoic acid (CA16csMsm1).

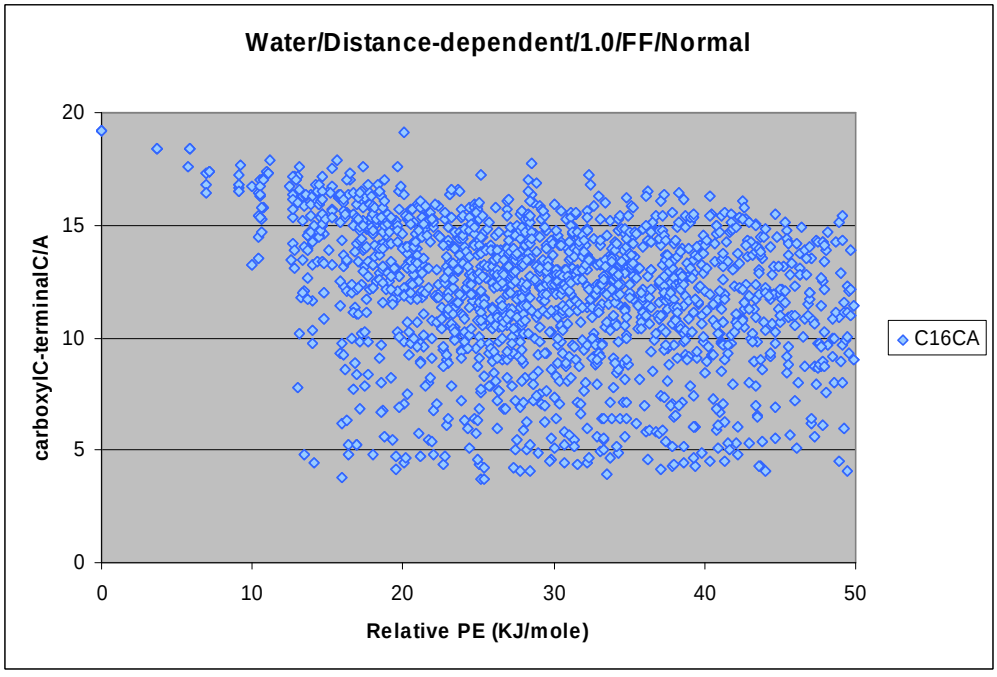


Figure 6: Plot of relative potential energy against distance – hexadecanoic acid (CA16csMsm2).

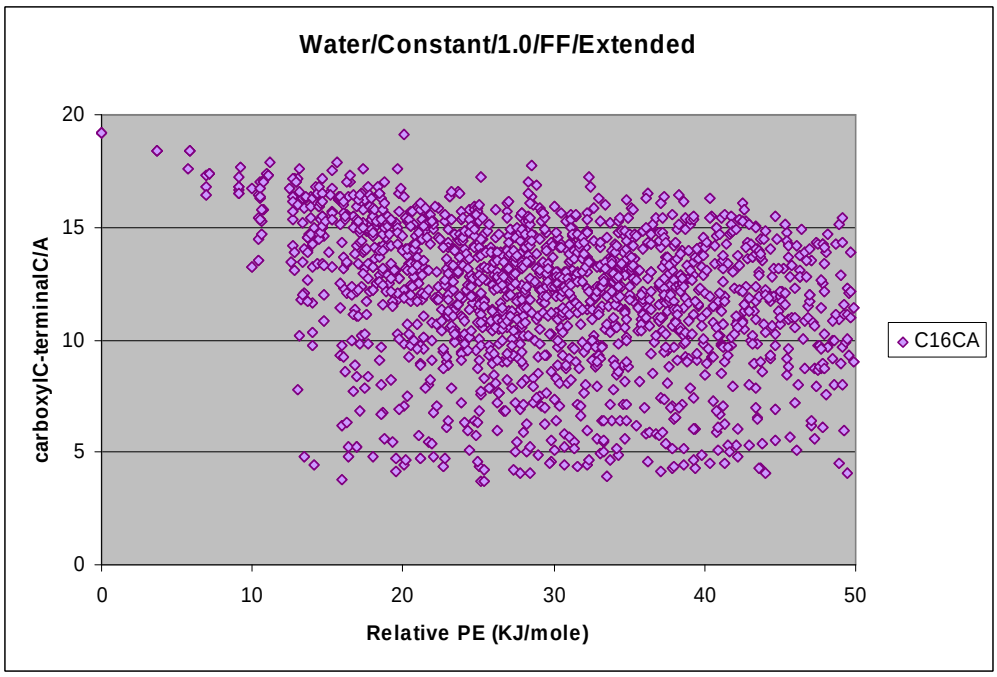


Figure 7: Plot of relative potential energy against distance – hexadecanoic acid (CA16csMsm3).

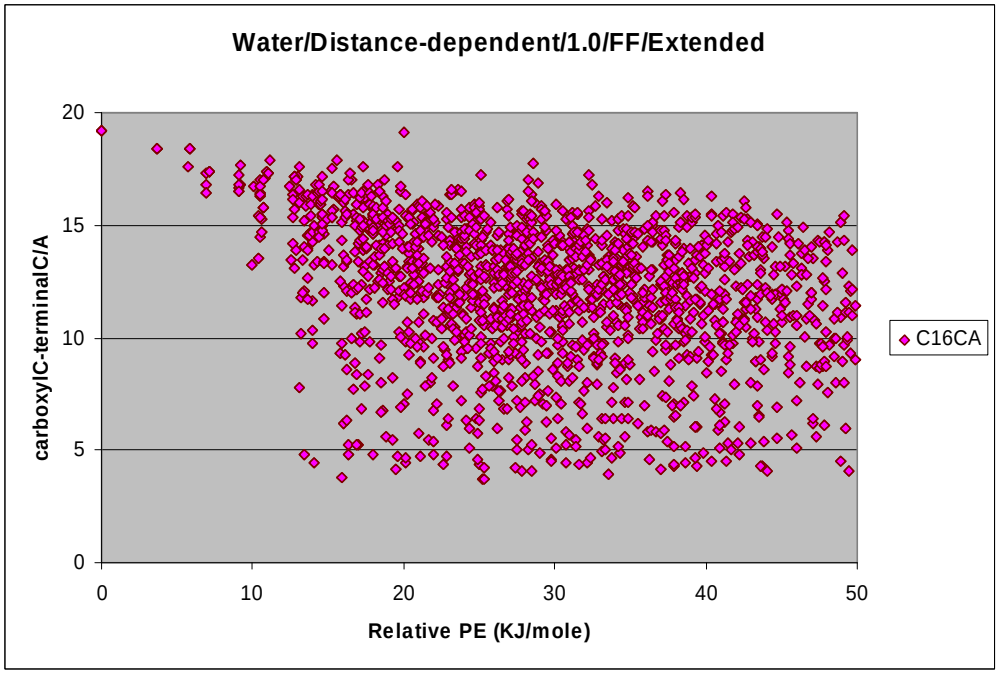


Figure 8: Plot of relative potential energy against distance – hexadecanoic acid (CA16csMsm4).

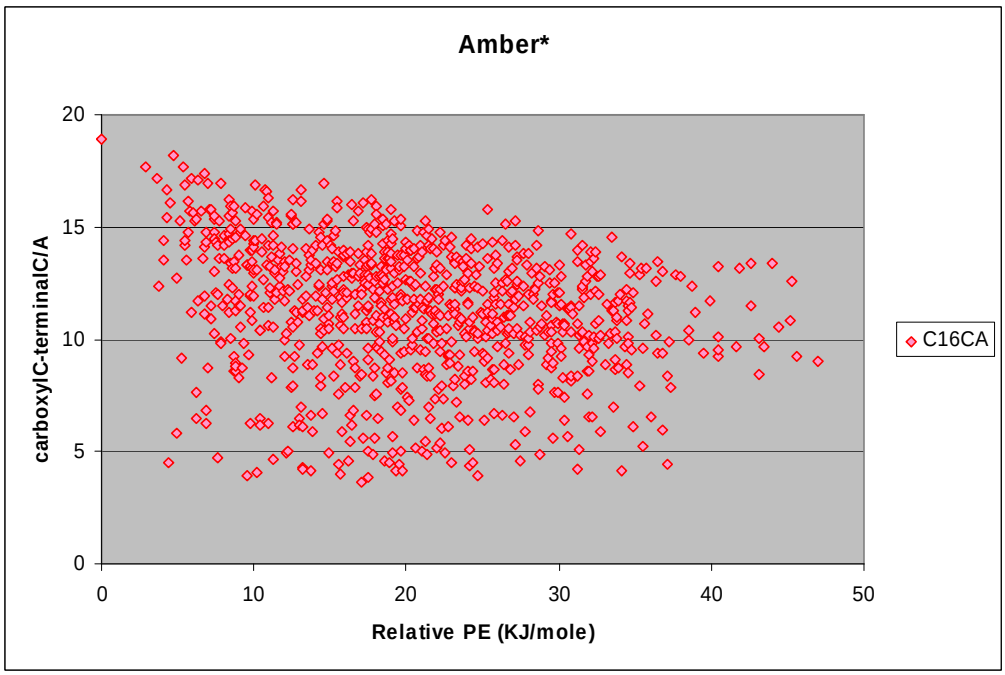


Figure 9: Plot of relative potential energy against distance – hexadecanoic acid/Amber.

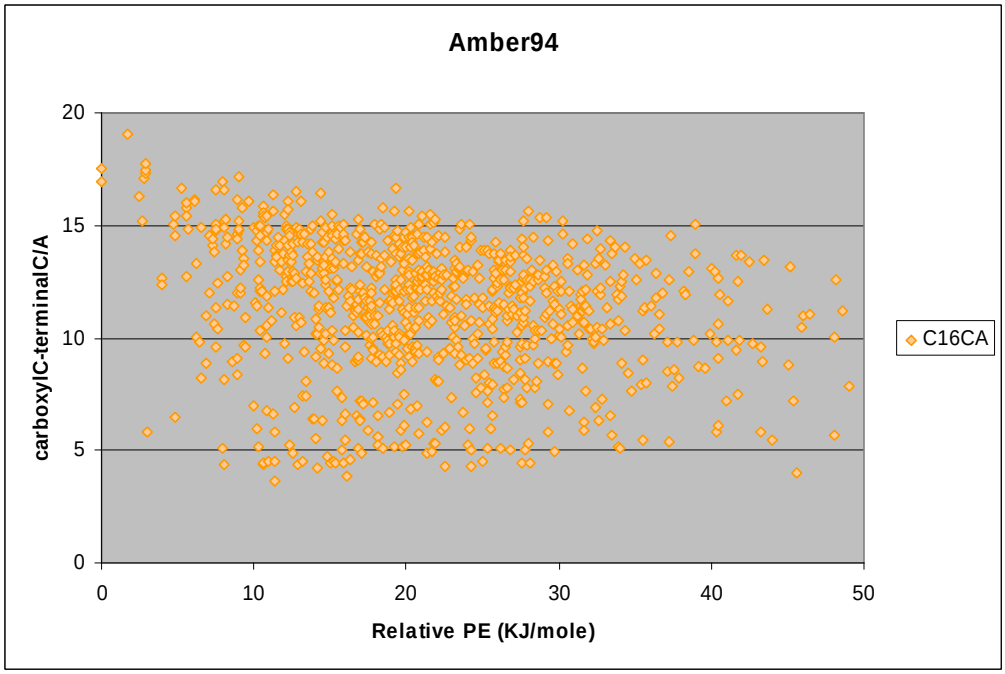


Figure 10: Plot of relative potential energy against distance – hexadecanoic acid/Amber94.

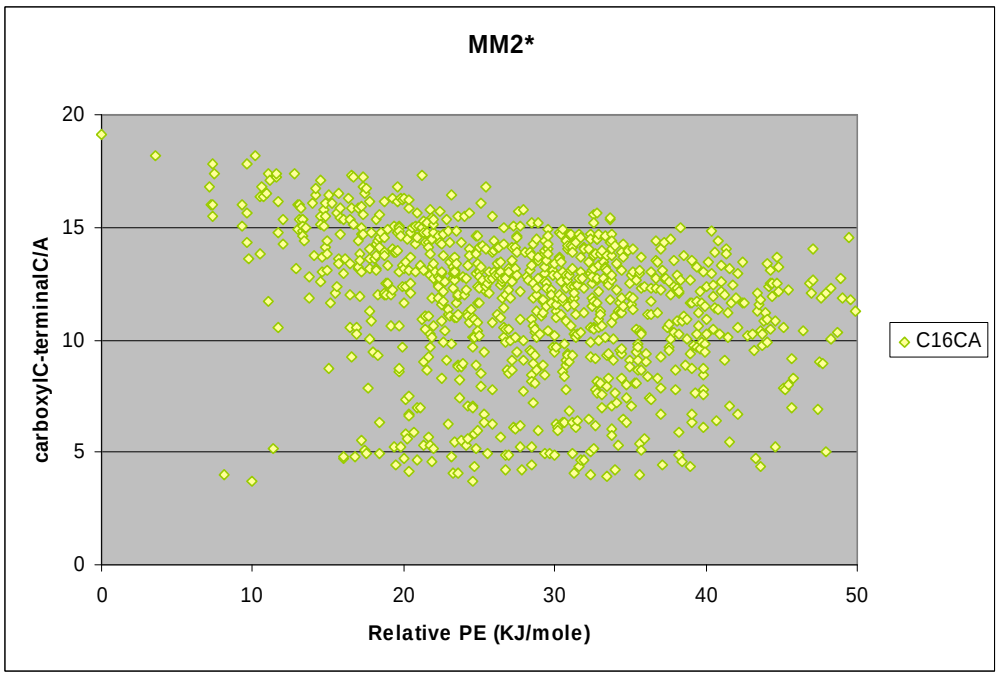


Figure 11: Plot of relative potential energy against distance – hexadecanoic acid/MM2.

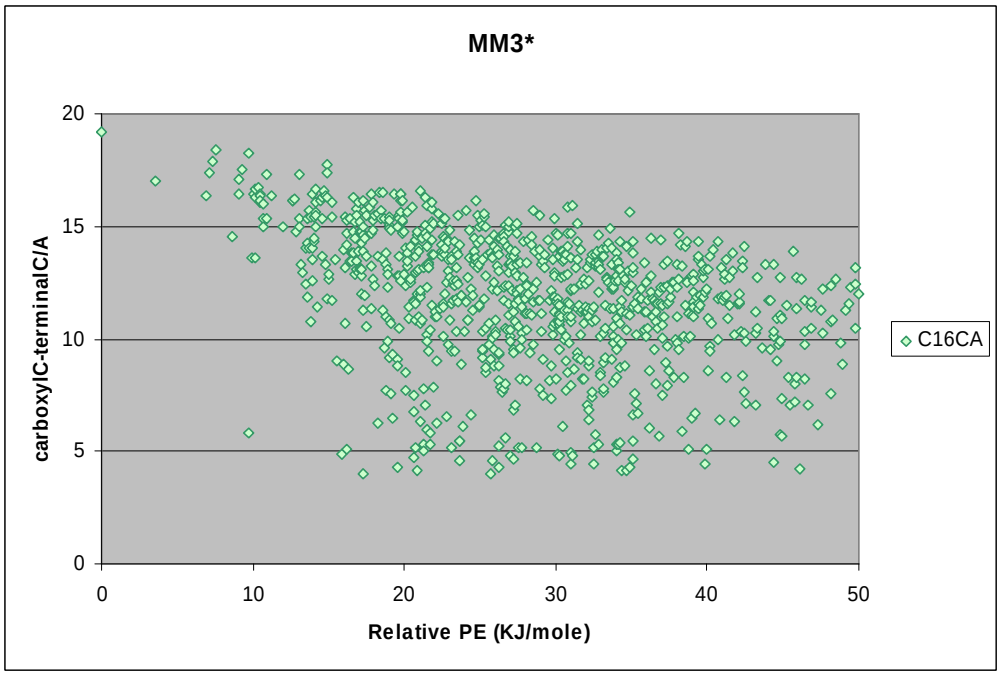


Figure 12: Plot of relative potential energy against distance – hexadecanoic acid/MM3.

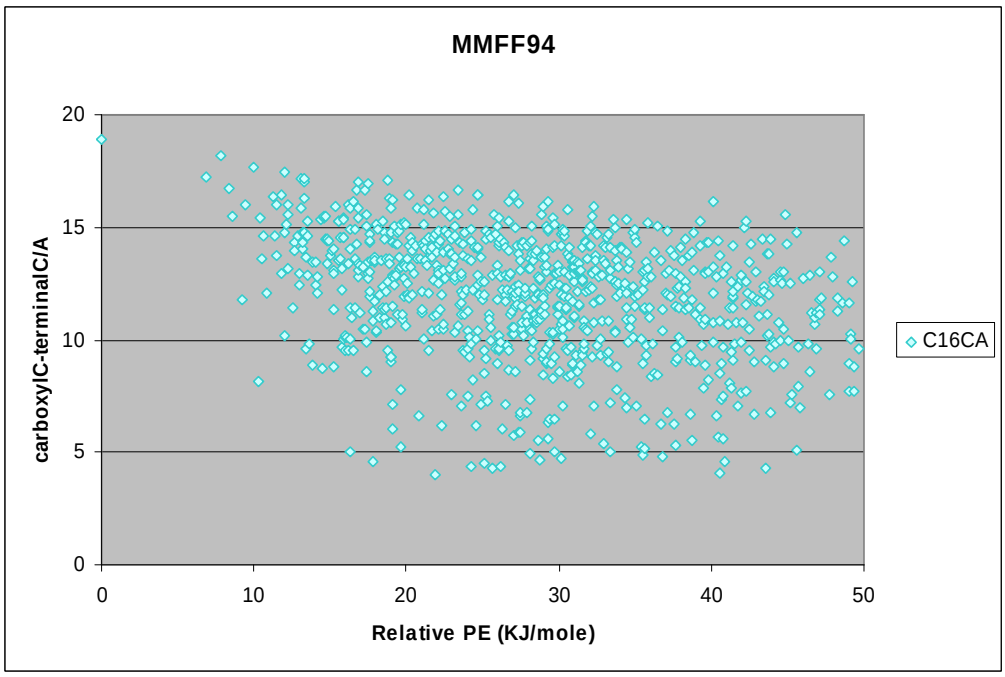


Figure 13: Plot of relative potential energy against distance – hexadecanoic acid/MMFF.

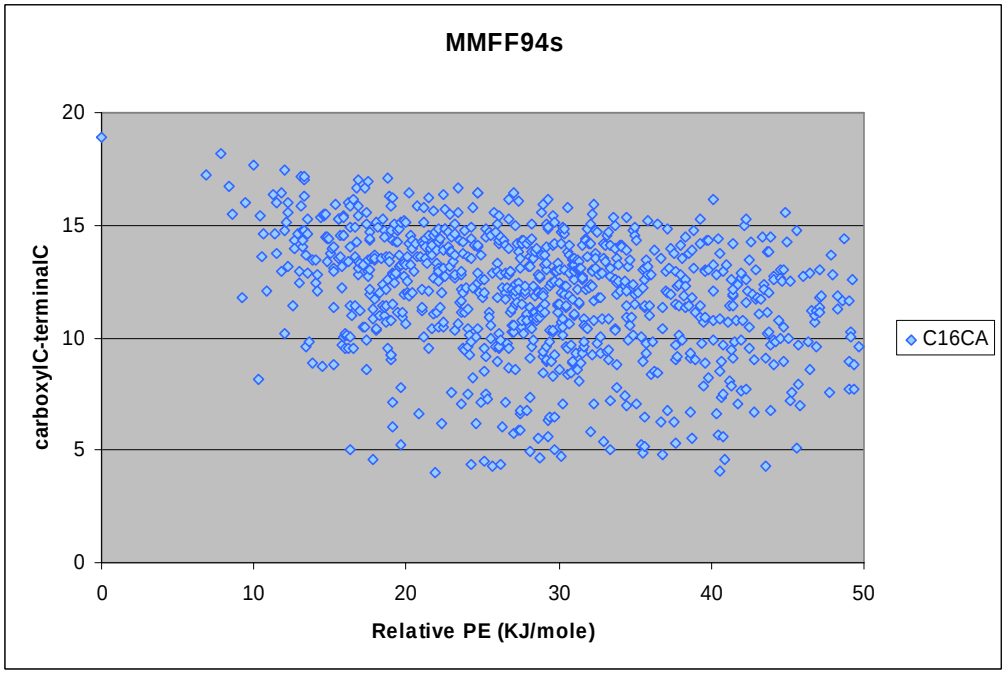


Figure 14: Plot of relative potential energy against distance – hexadecanoic acid/MMFFS.

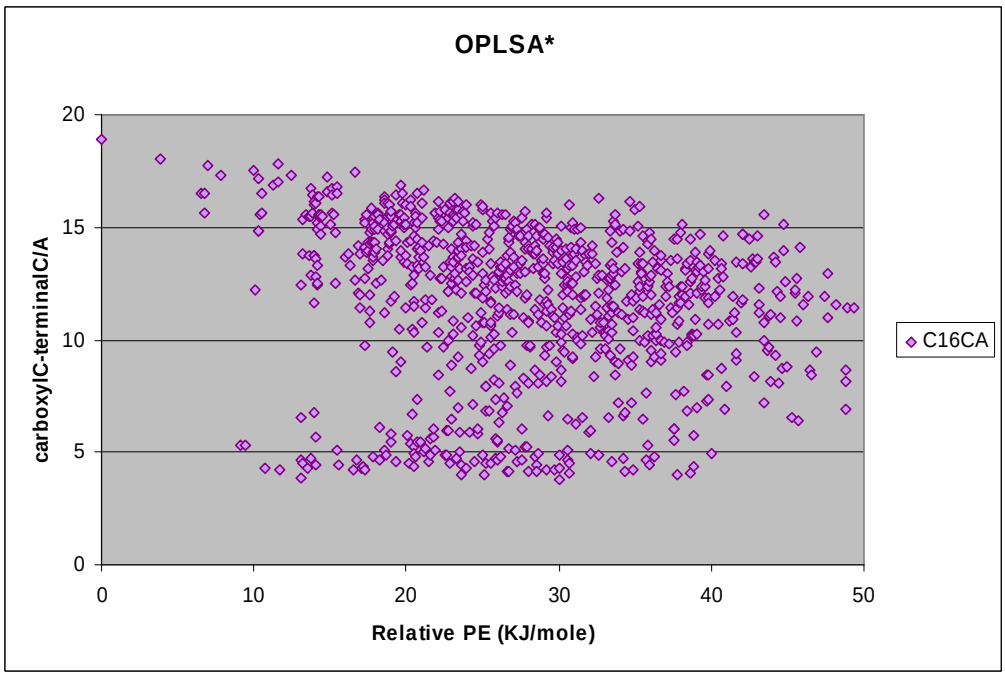


Figure 15: Plot of relative potential energy against distance – hexadecanoic acid/OPLS-1999.

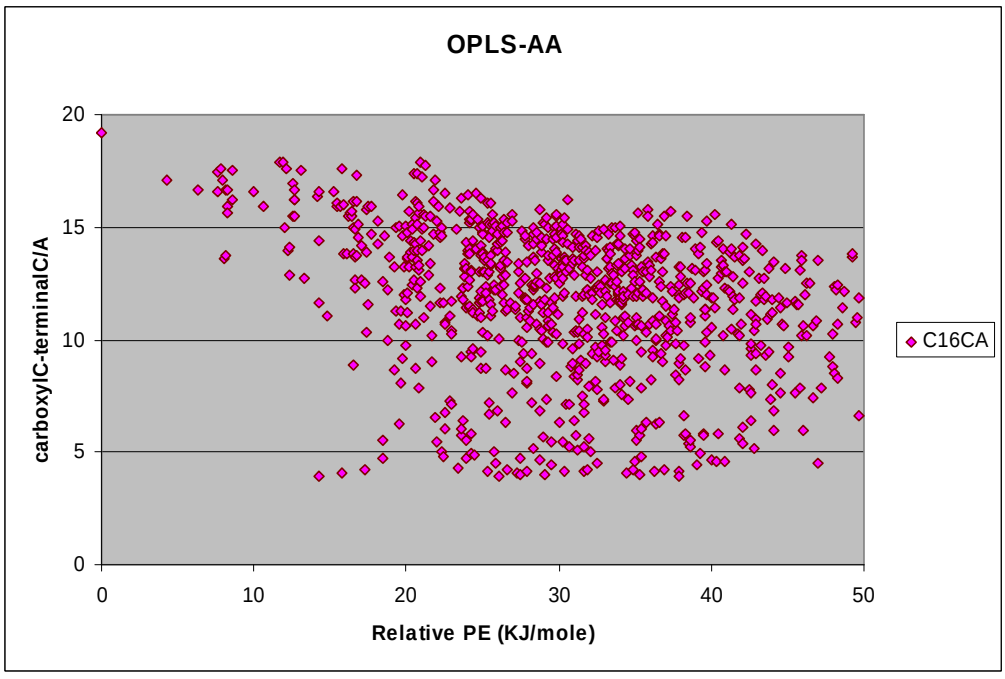


Figure 16: Plot of relative potential energy against distance – hexadecanoic acid/OPLS-2001.

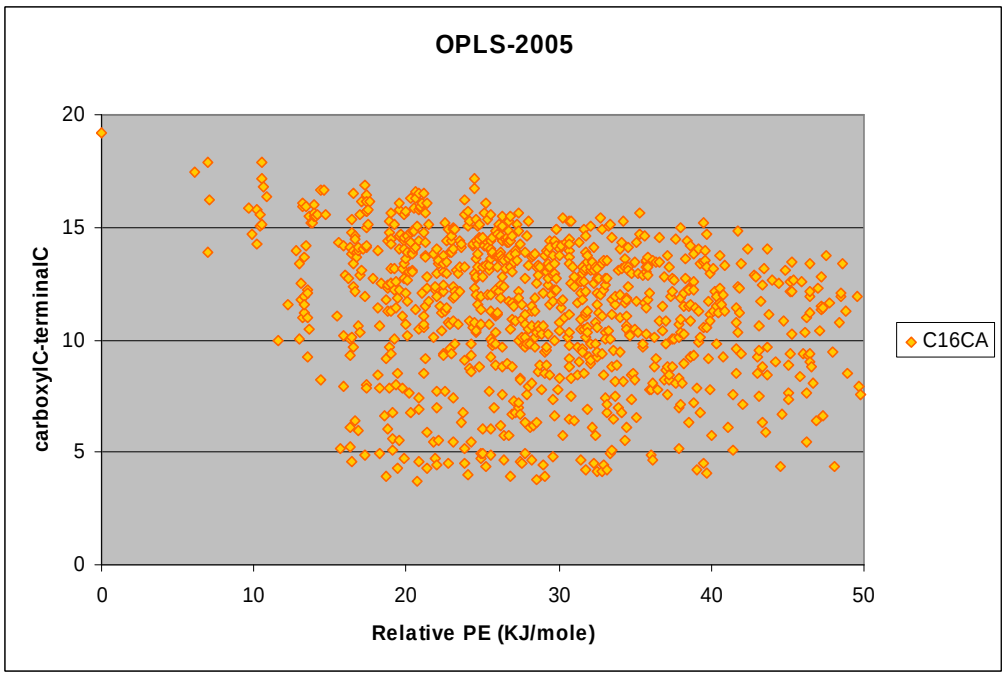


Figure 17: Plot of relative potential energy against distance – hexadecanoic acid/OPLS-2005.

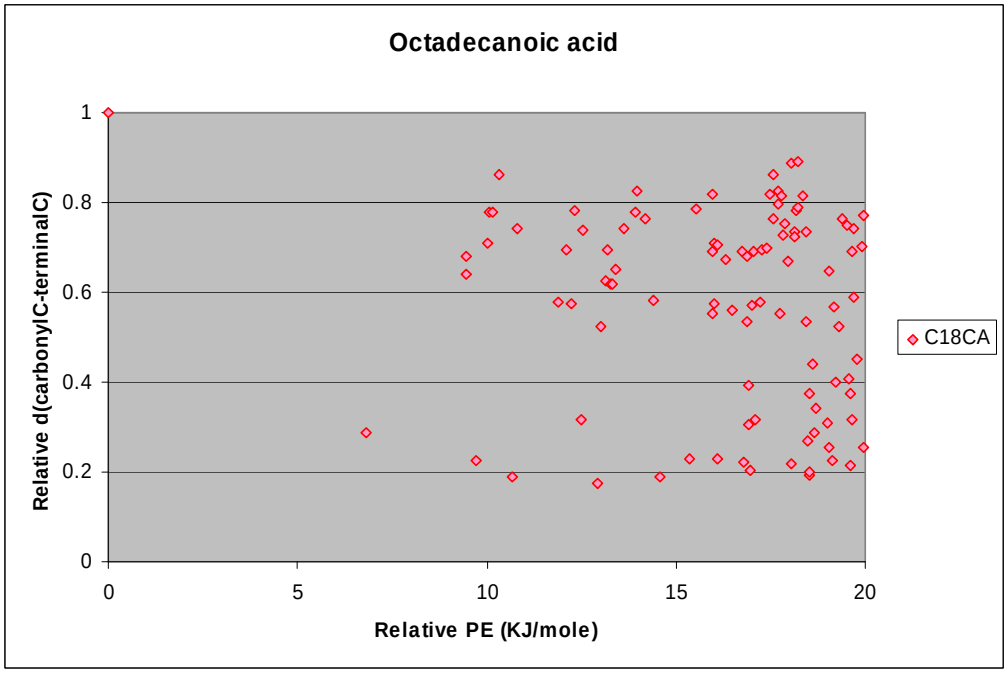


Figure 18: Octadecanoic acid - Monte Carlo search with MM3 minimisation in GB/SA water.

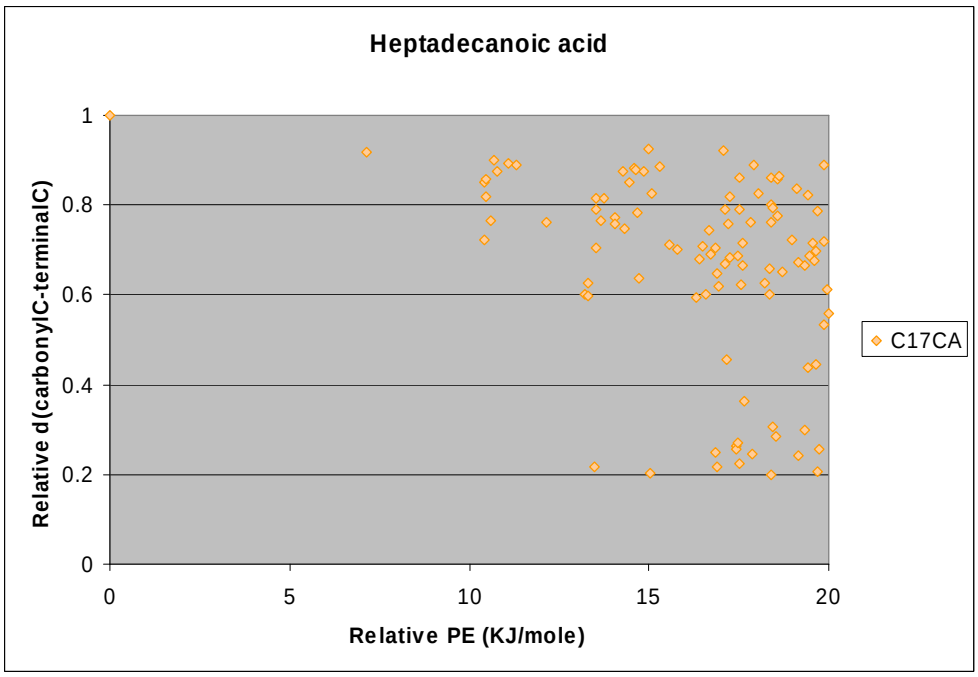


Figure 19: Heptadecanoic acid - Monte Carlo search with MM3 minimisation in GB/SA water.

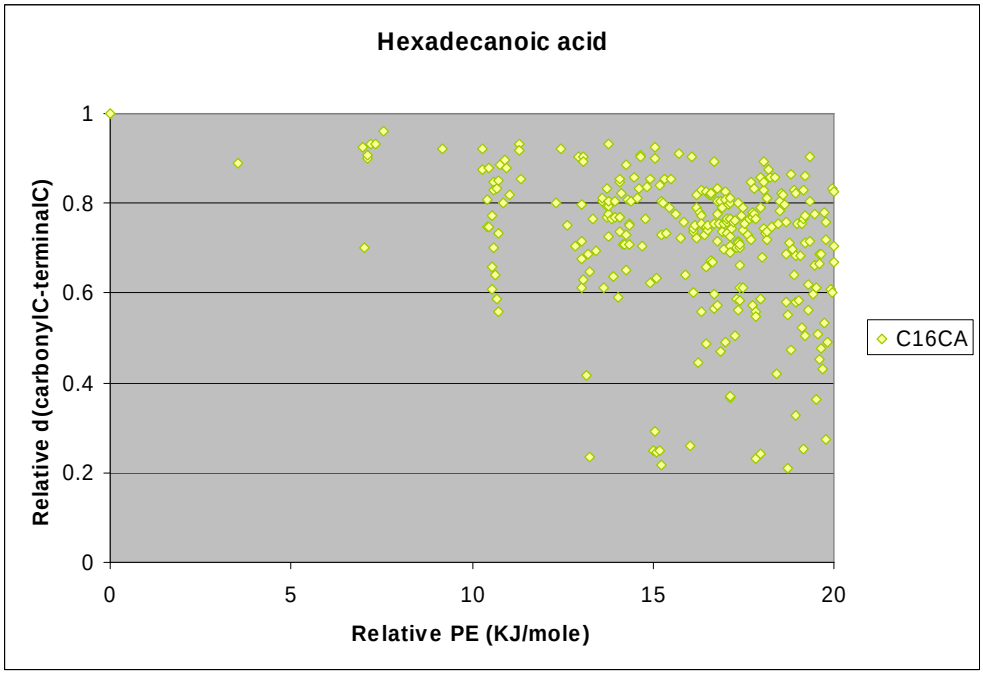


Figure 20: Hexadecanoic acid - Monte Carlo search with MM3 minimisation in GB/SA water.

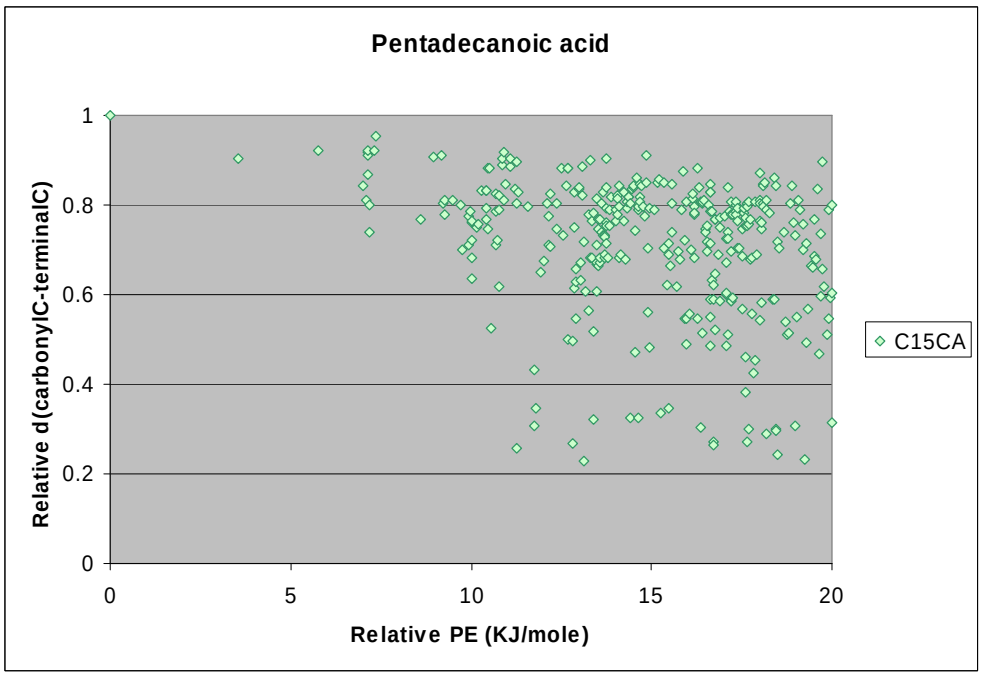


Figure 21: Pentadecanoic acid - Monte Carlo search with MM3 minimisation in GB/SA water.

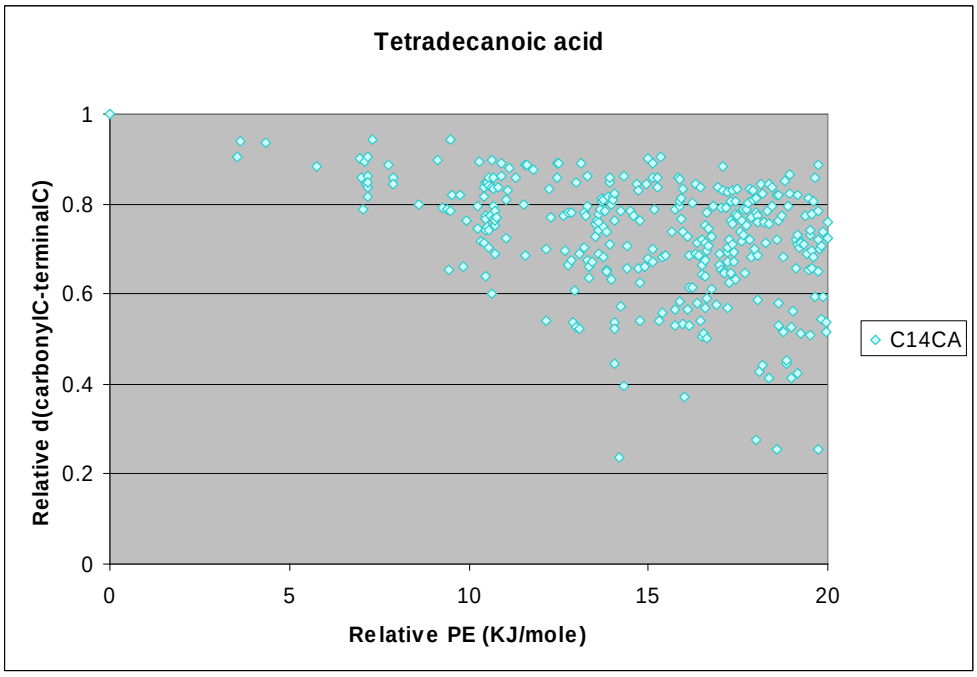


Figure 22: Tetradecanoic acid - Monte Carlo search with MM3 minimisation in GB/SA water.

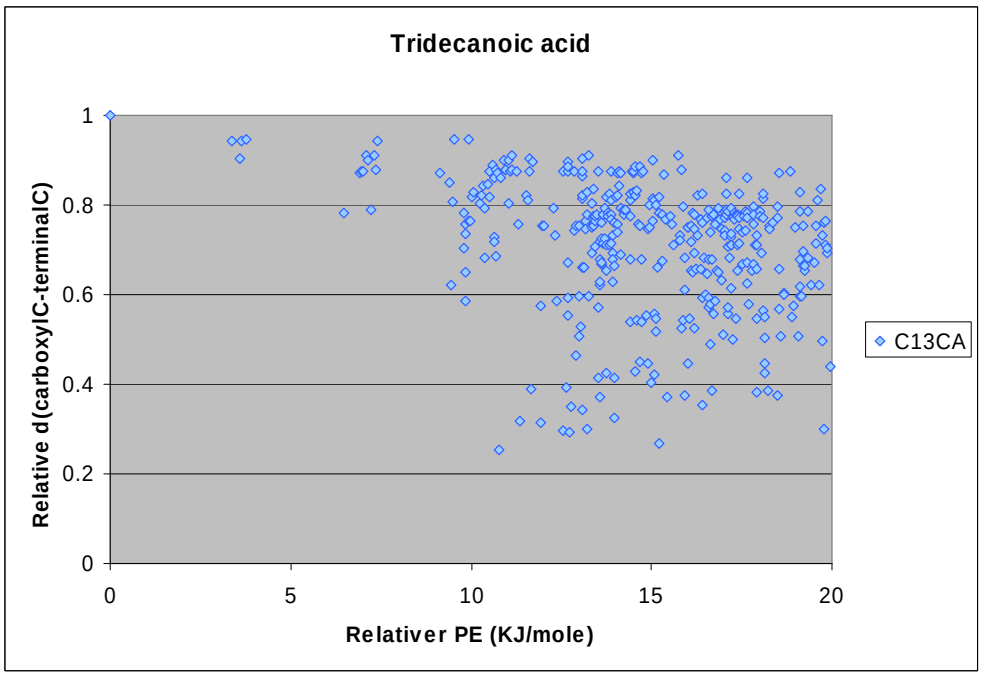


Figure 23: Tridecanoic acid - Monte Carlo search with MM3 minimisation in GB/SA water.

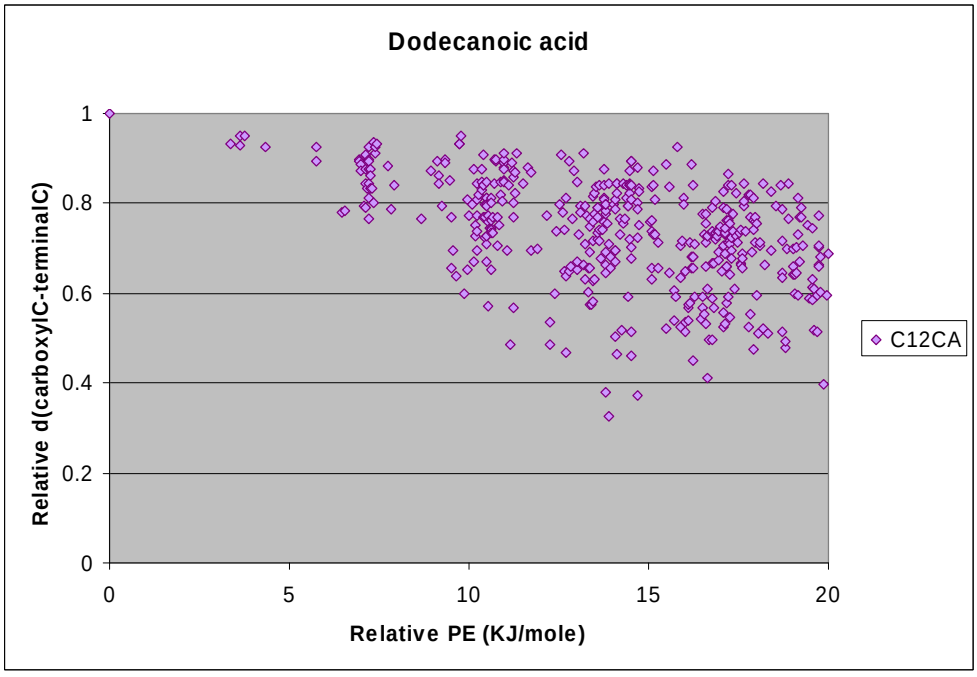


Figure 24: Dodecanoic acid - Monte Carlo search with MM3 minimisation in GB/SA water.

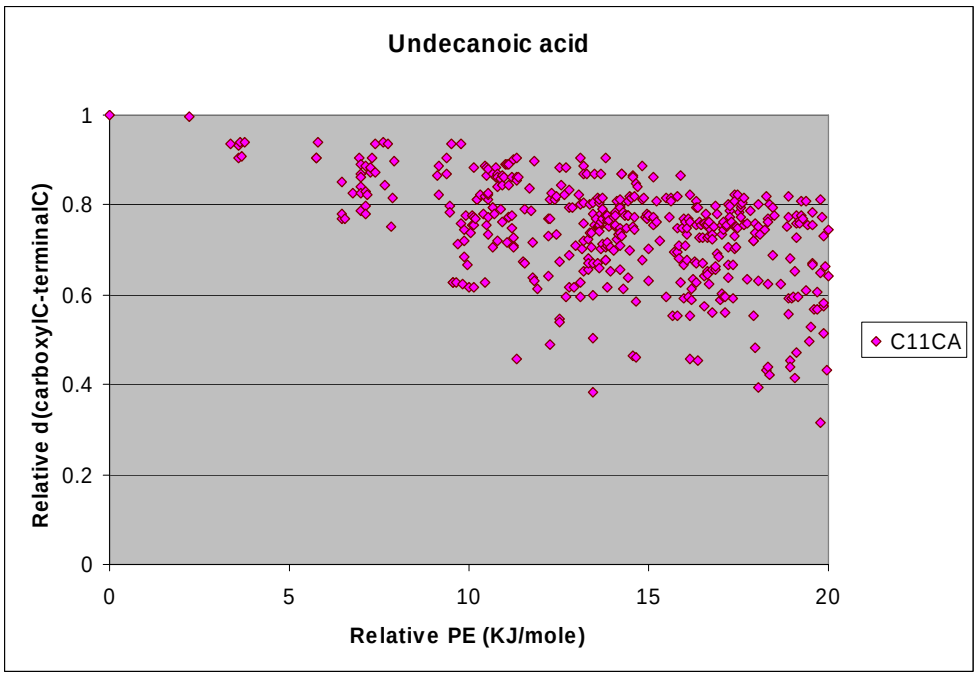


Figure 25: Undecanoic acid - Monte Carlo search with MM3 minimisation in GB/SA water.

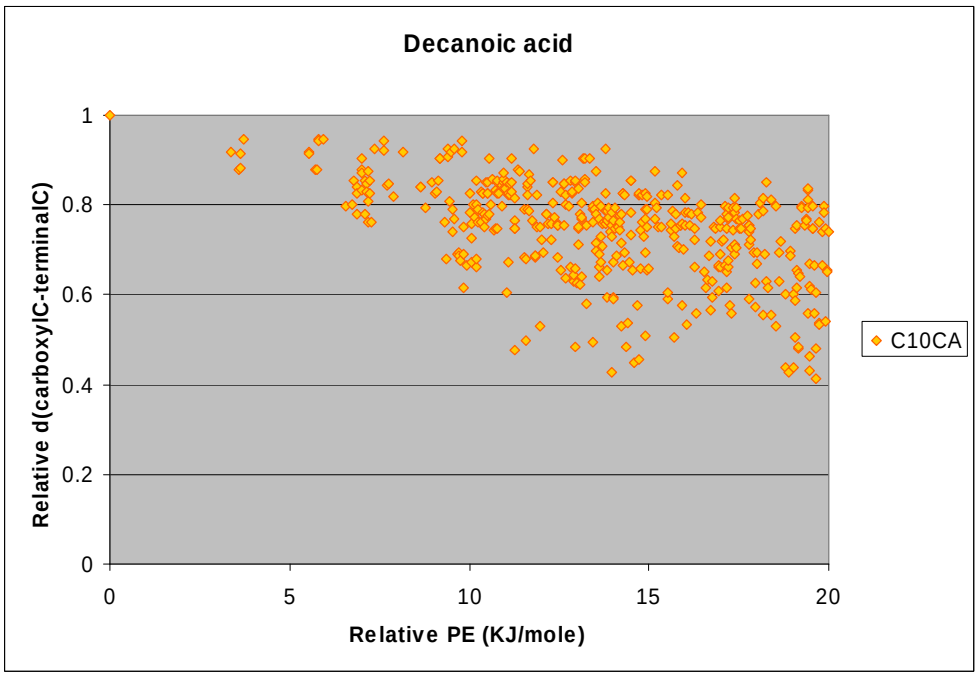


Figure 26: Decanoic acid - Monte Carlo search with MM3 minimisation in GB/SA water.

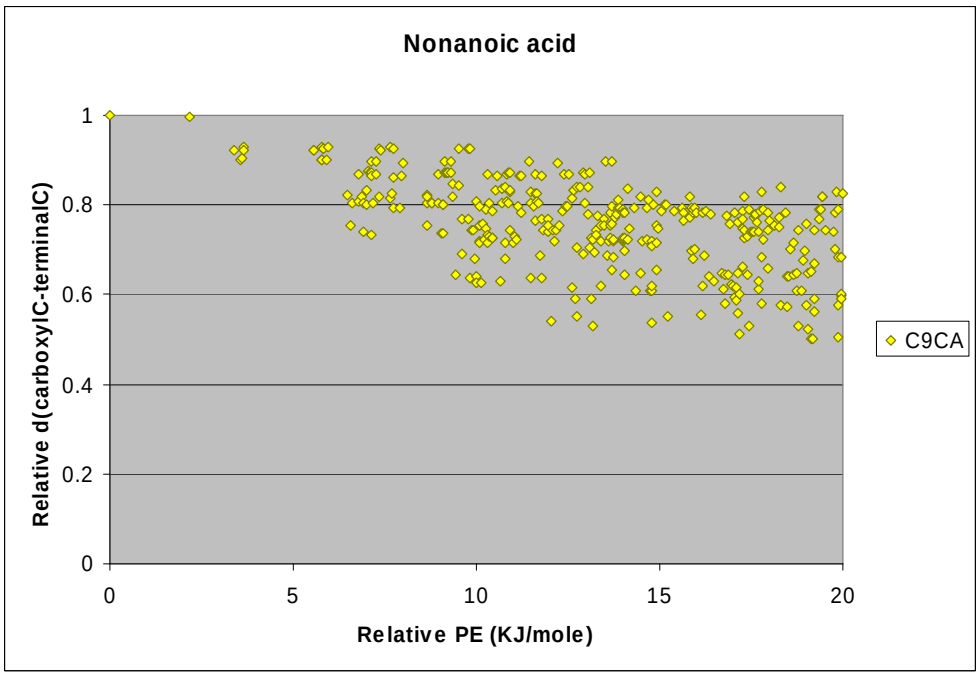


Figure 27: Nonanoic acid - Monte Carlo search with MM3 minimisation in GB/SA water.

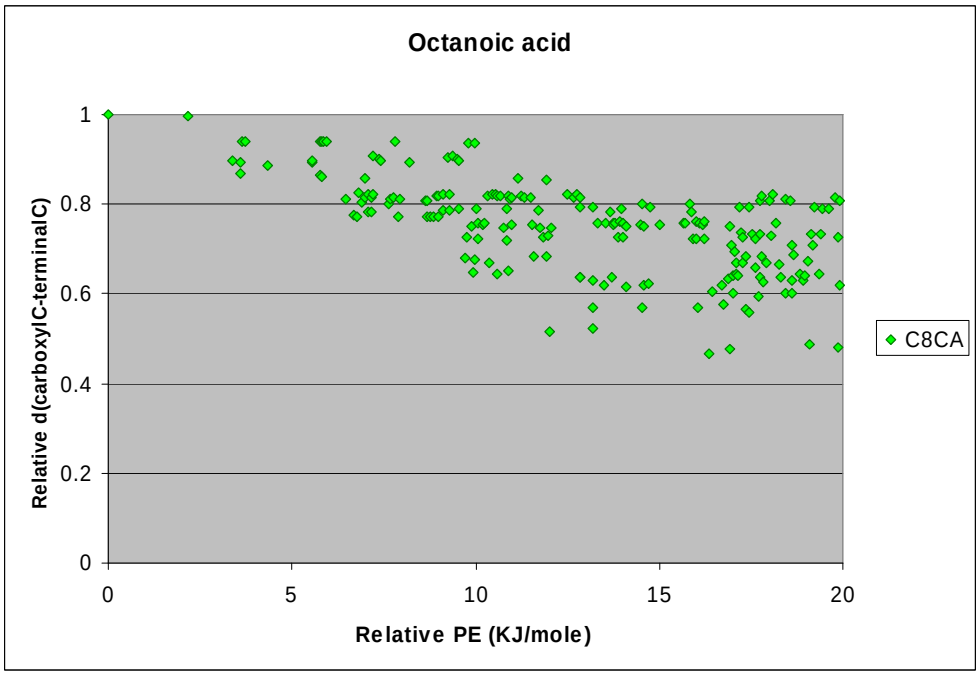


Figure 28: Octanoic acid - Monte Carlo search with MM3 minimisation in GB/SA water.

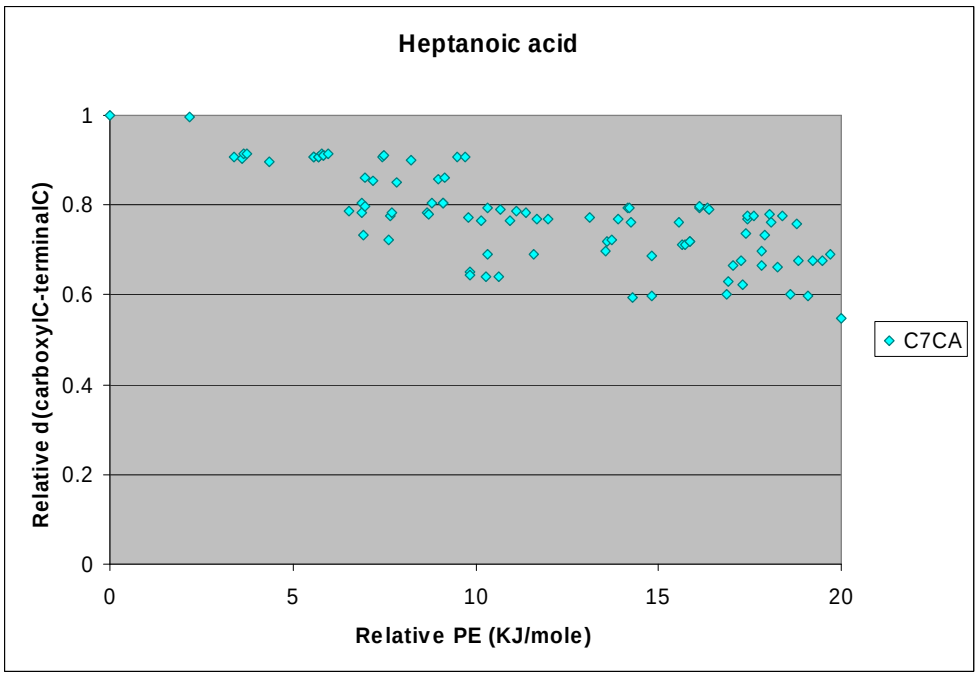


Figure 29: Heptanoic acid - Monte Carlo search with MM3 minimisation in GB/SA water.

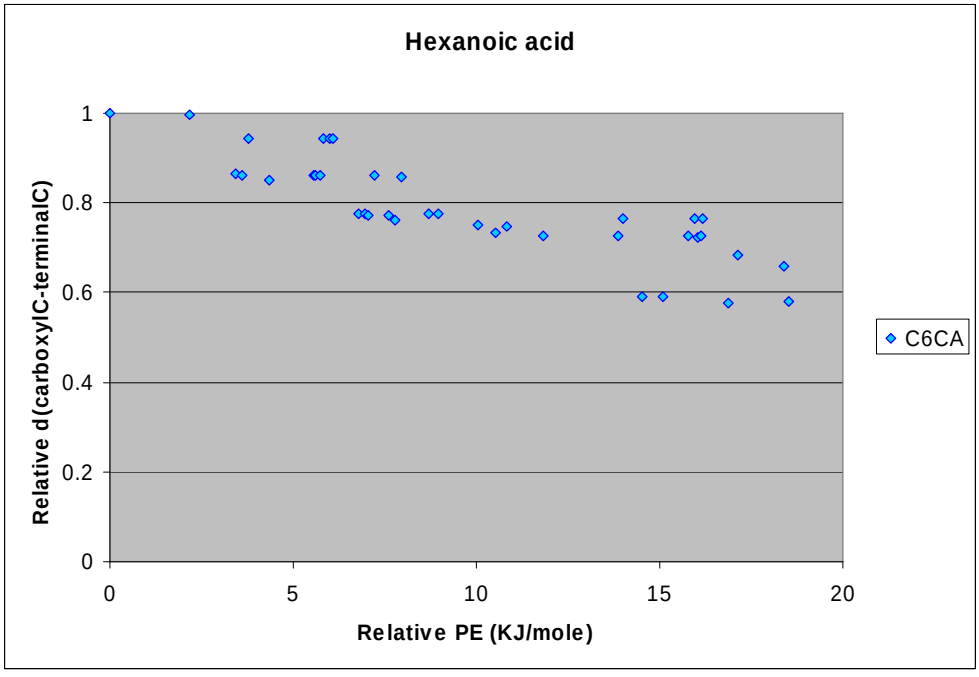


Figure 30: Hexanoic acid - Monte Carlo search with MM3 minimisation in GB/SA water.

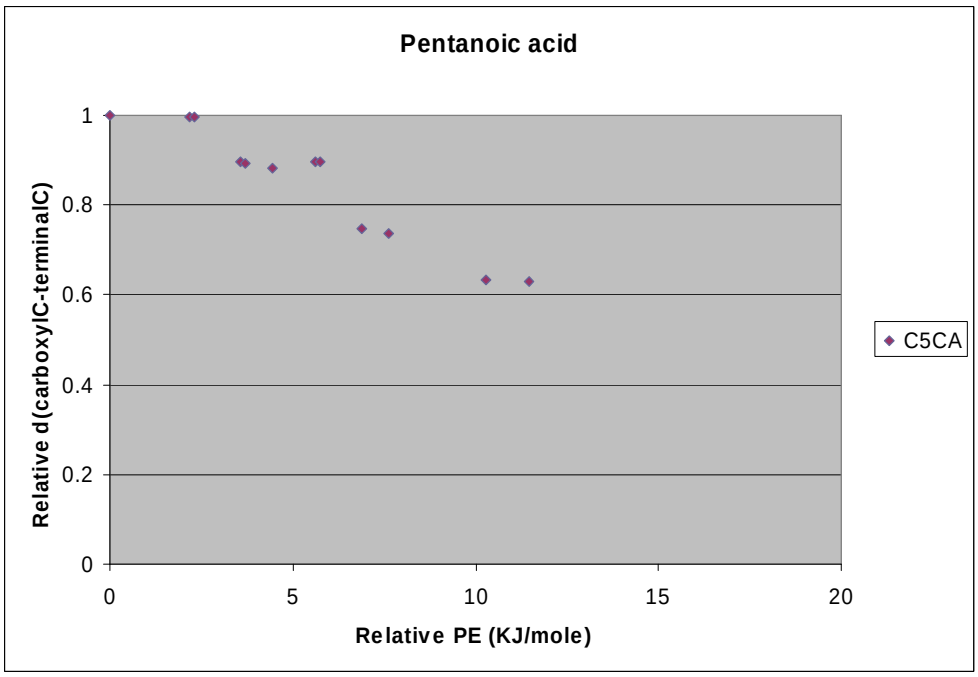


Figure 31: Pentanoic acid - Monte Carlo search with MM3 minimisation in GB/SA water.

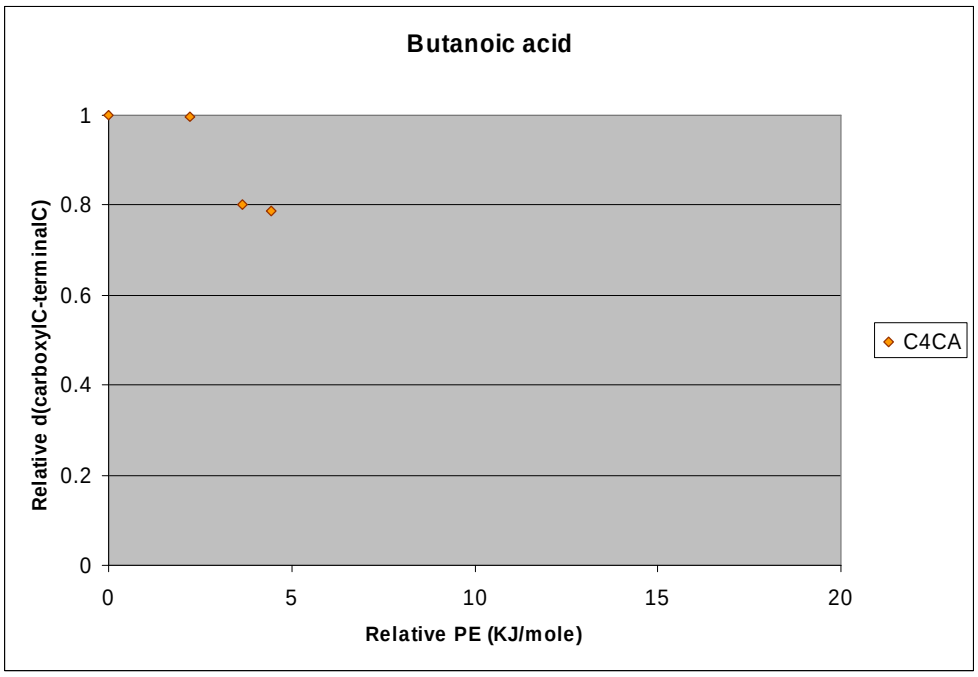


Figure 32: Butanoic acid - Monte Carlo search with MM3 minimisation in GB/SA water.

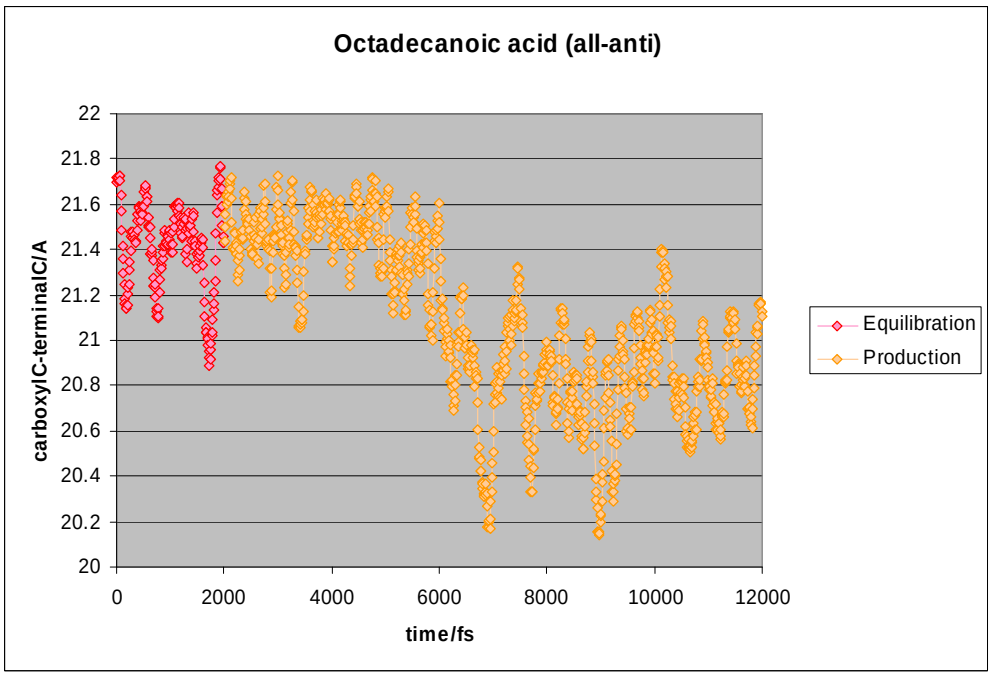


Figure 33: MD trajectory distance monitor plot for octadecanoic acid (all-anti conformer).

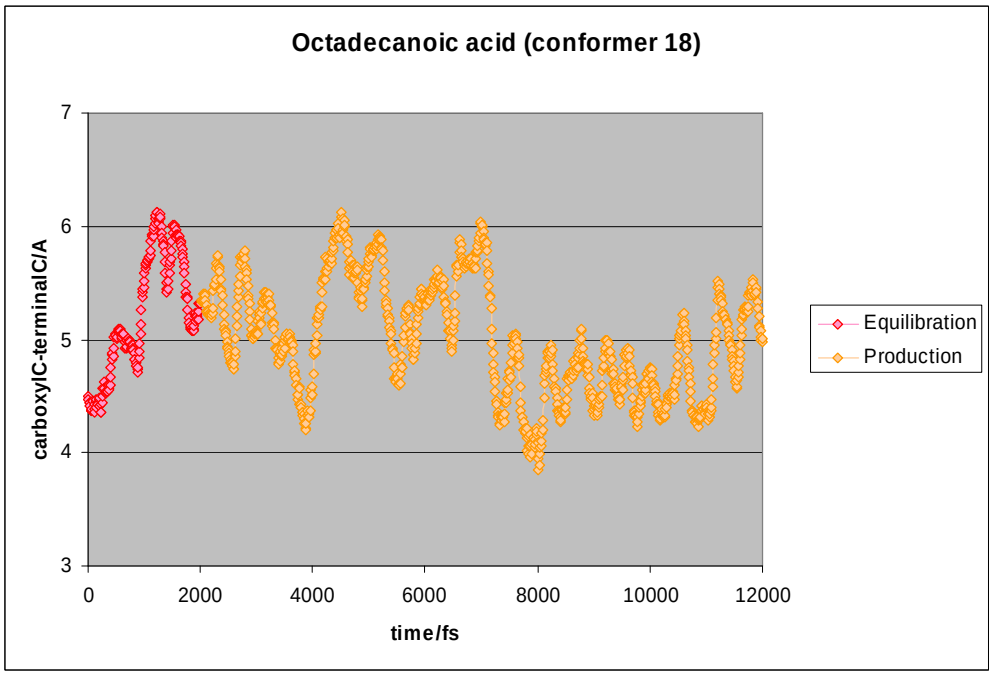


Figure 34: MD trajectory distance monitor plot for octadecanoic acid (conformer 18).

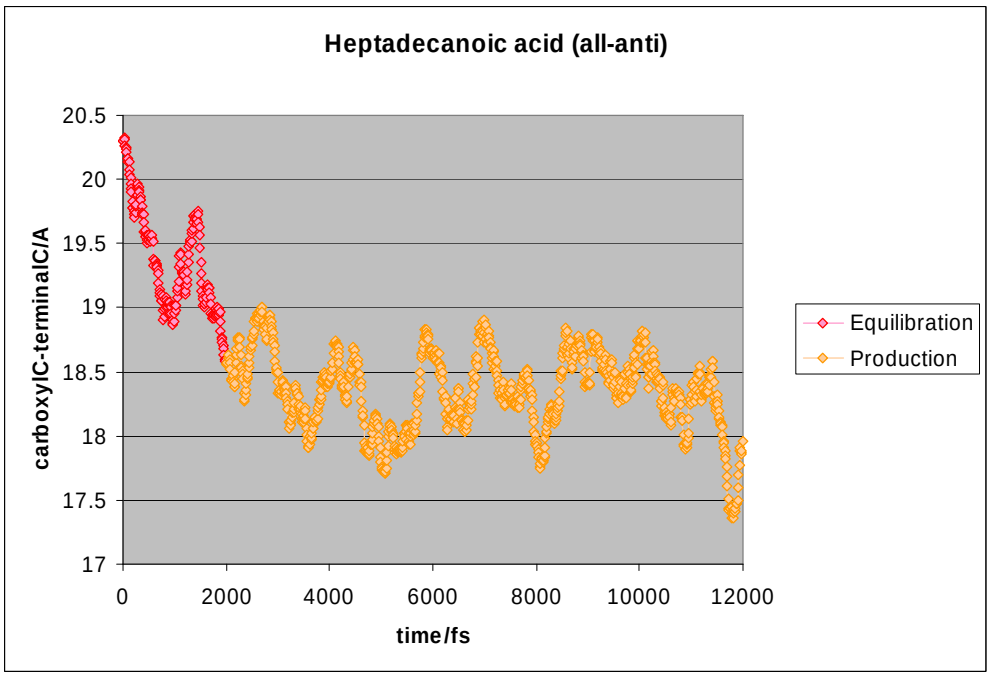


Figure 35: MD trajectory distance monitor plot for heptadecanoic acid (all-anti conformer).

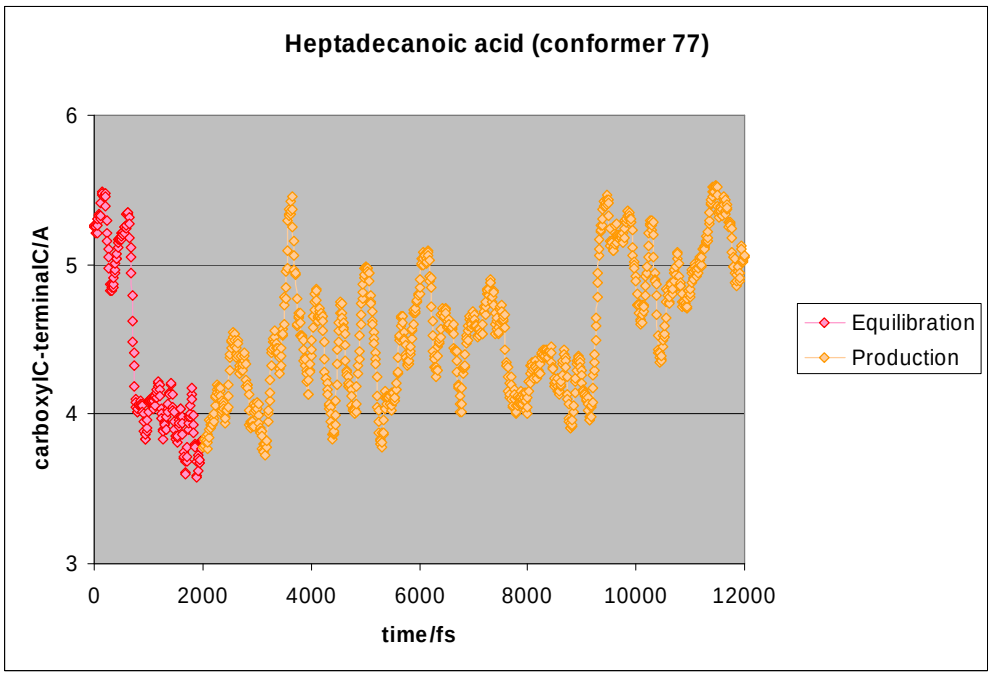


Figure 36: MD trajectory distance monitor plot for heptadecanoic acid (conformer 77).

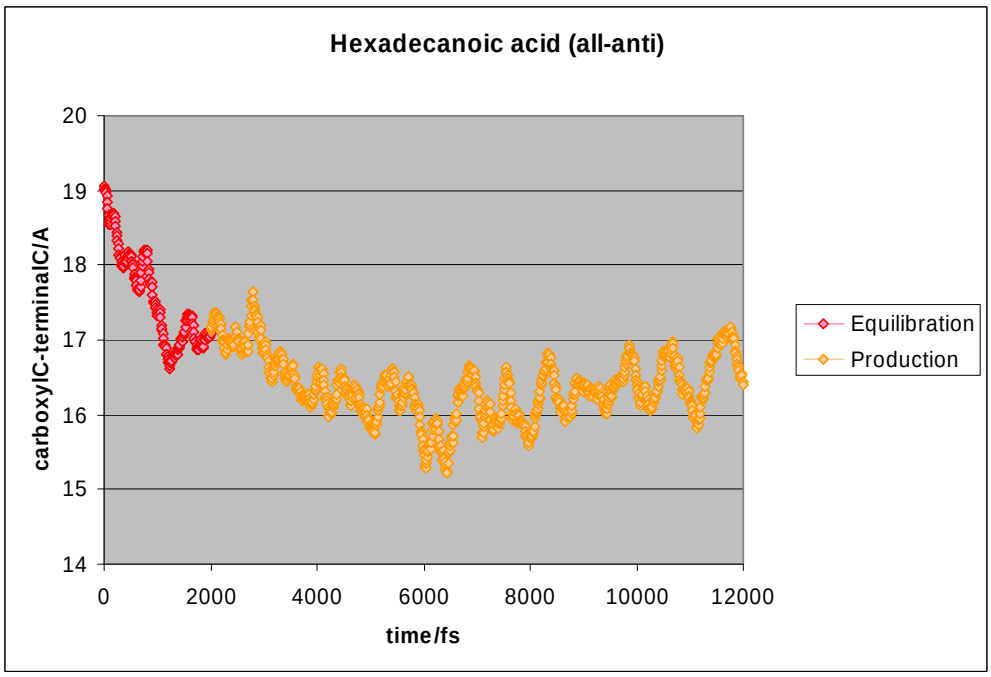


Figure 37: MD trajectory distance monitor plot for hexadecanoic acid (all-anti conformer).

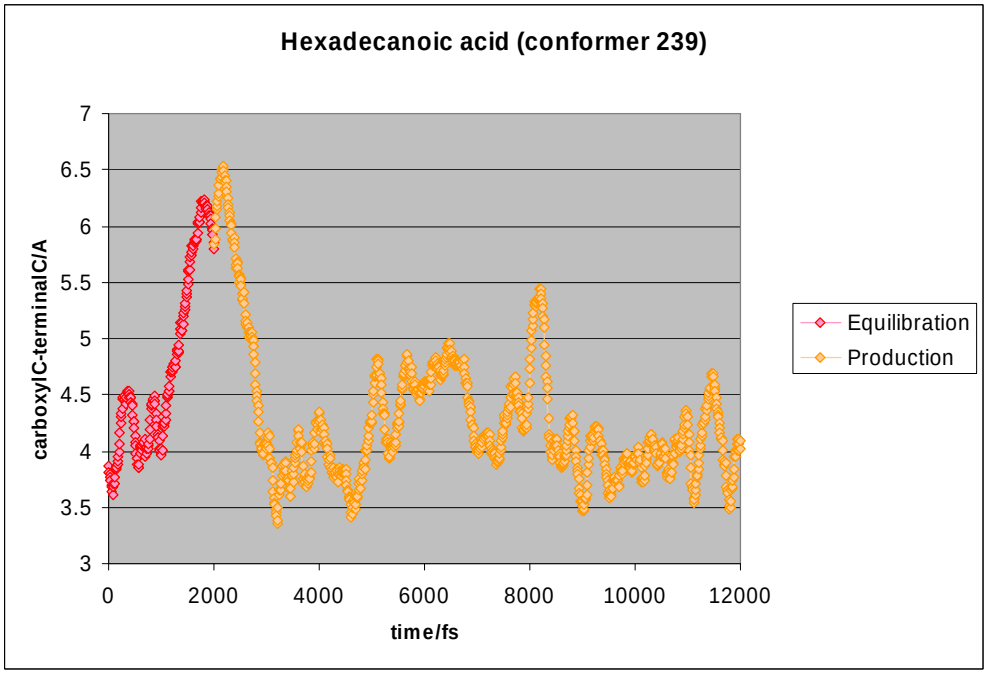


Figure 38: MD trajectory distance monitor plot for hexadecanoic acid (conformer 239).

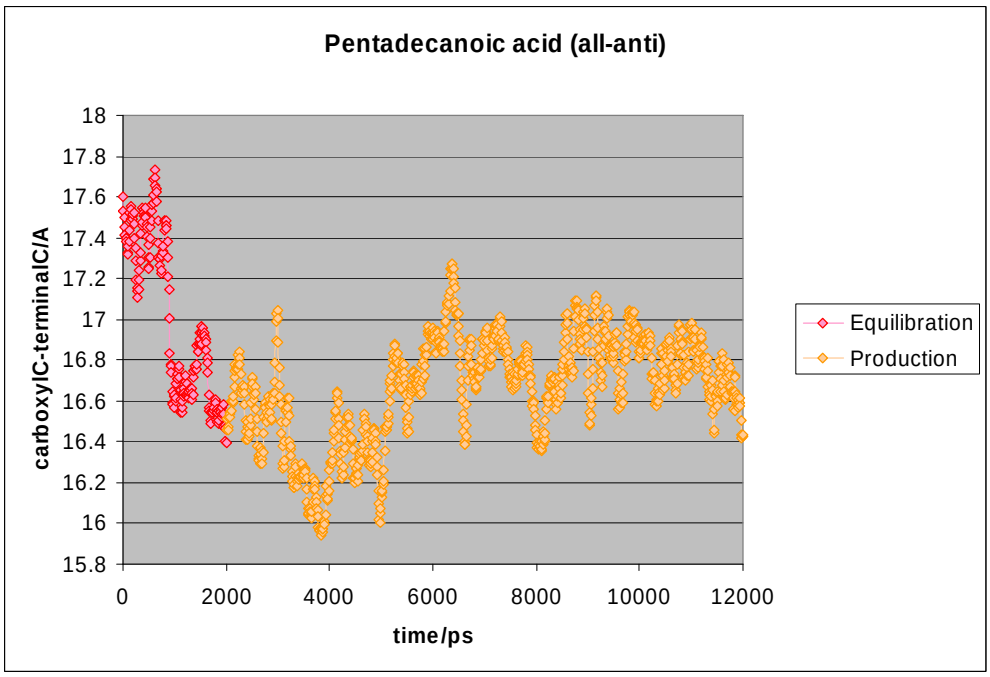


Figure 39: MD trajectory distance monitor plot for pentadecanoic acid (all-anti conformer).

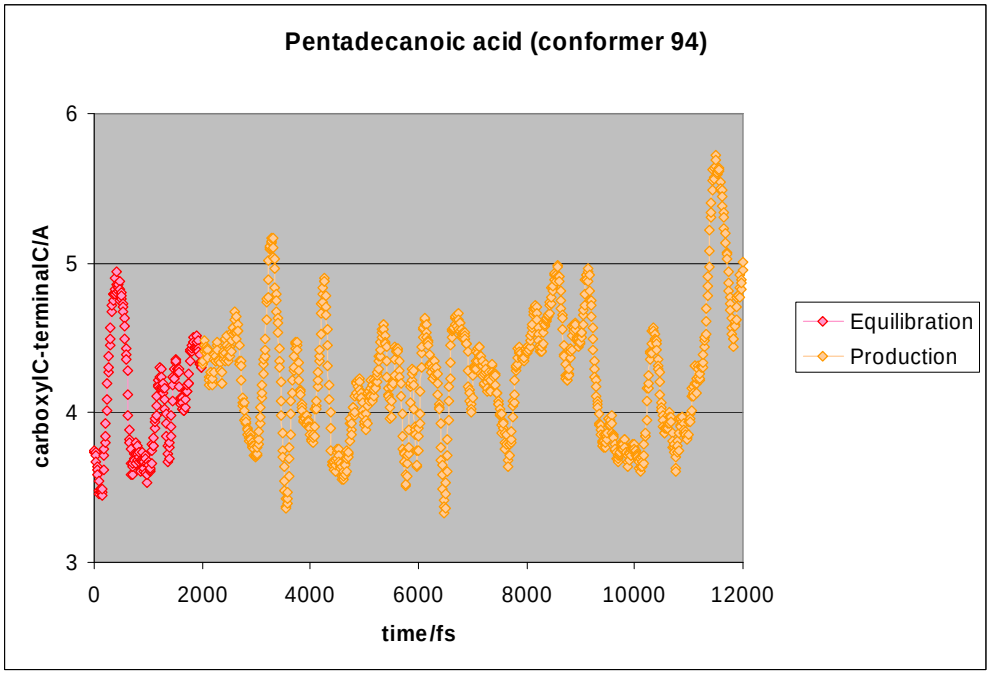


Figure 40: MD trajectory distance monitor plot for pentadecanoic acid (conformer 94).

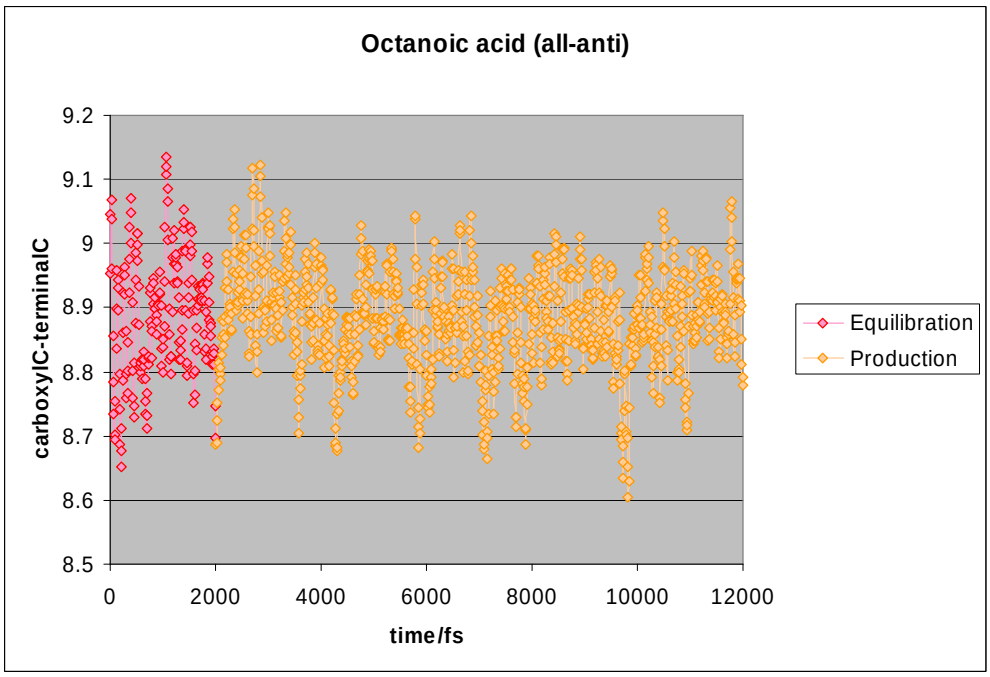


Figure 41: MD trajectory distance monitor plot for octanoic acid (all-anti conformer).

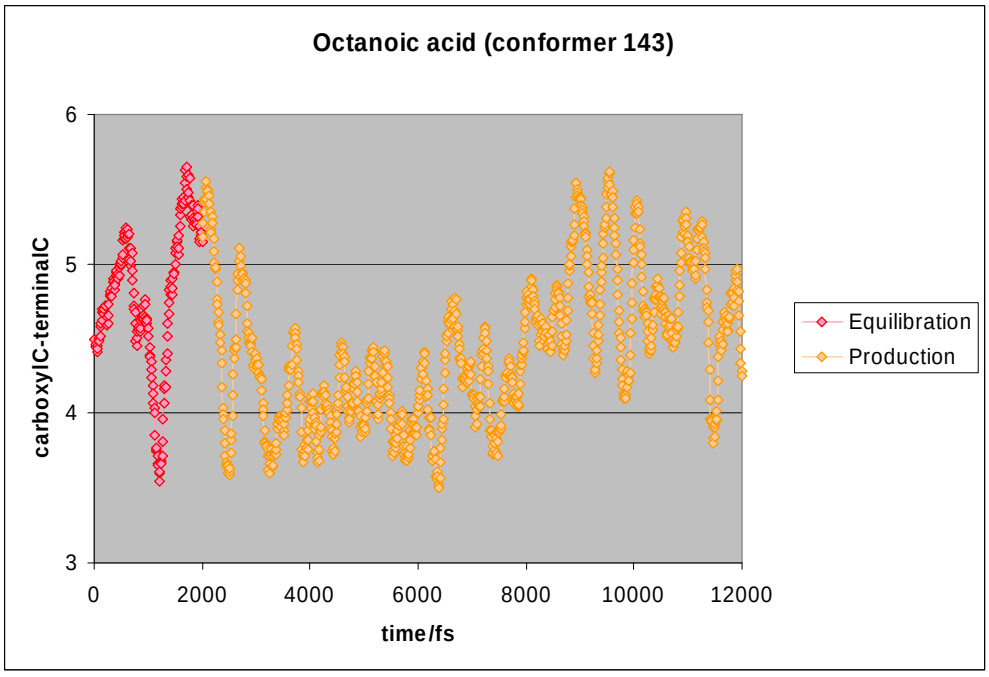


Figure 42: MD trajectory distance monitor plot for octanoic acid (conformer 143).

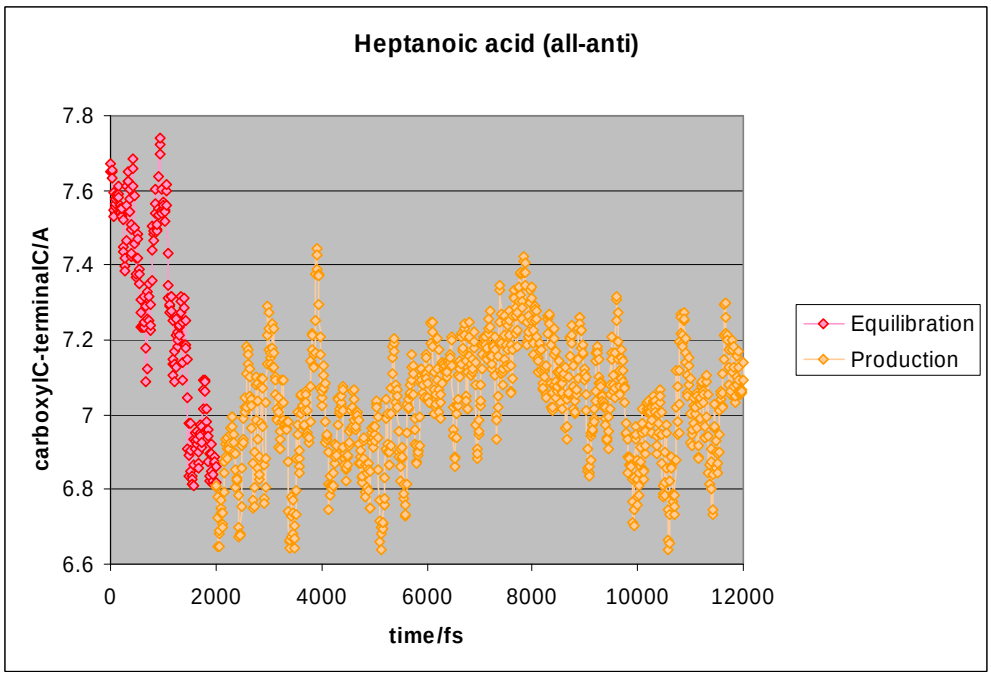


Figure 43: MD trajectory distance monitor plot for heptanoic acid (all-anti conformer).

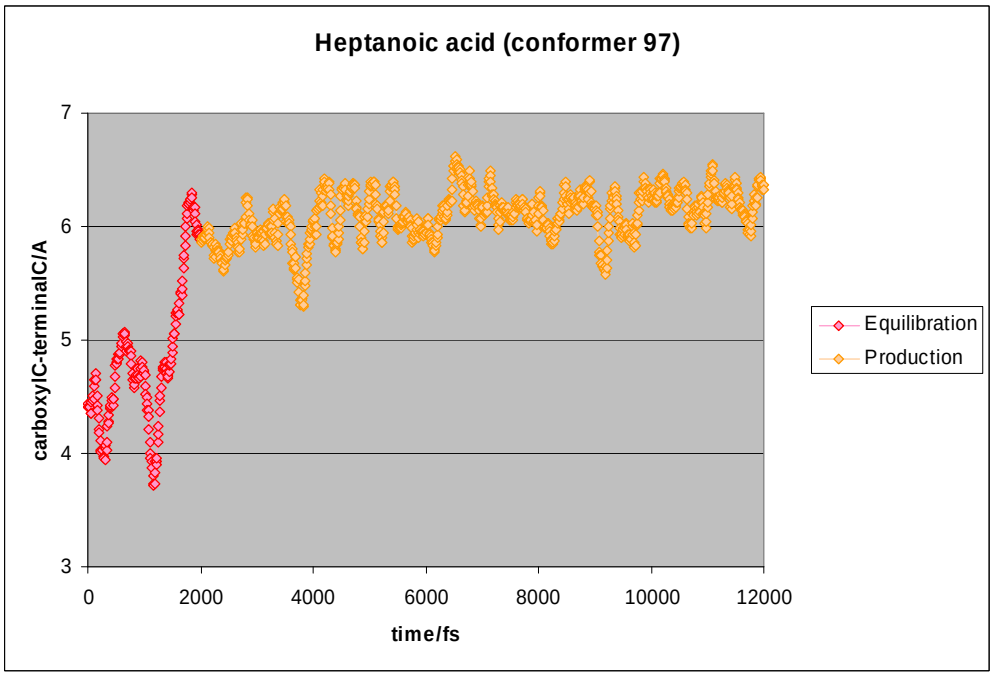


Figure 44: MD trajectory distance monitor plot for heptanoic acid (conformer 97).

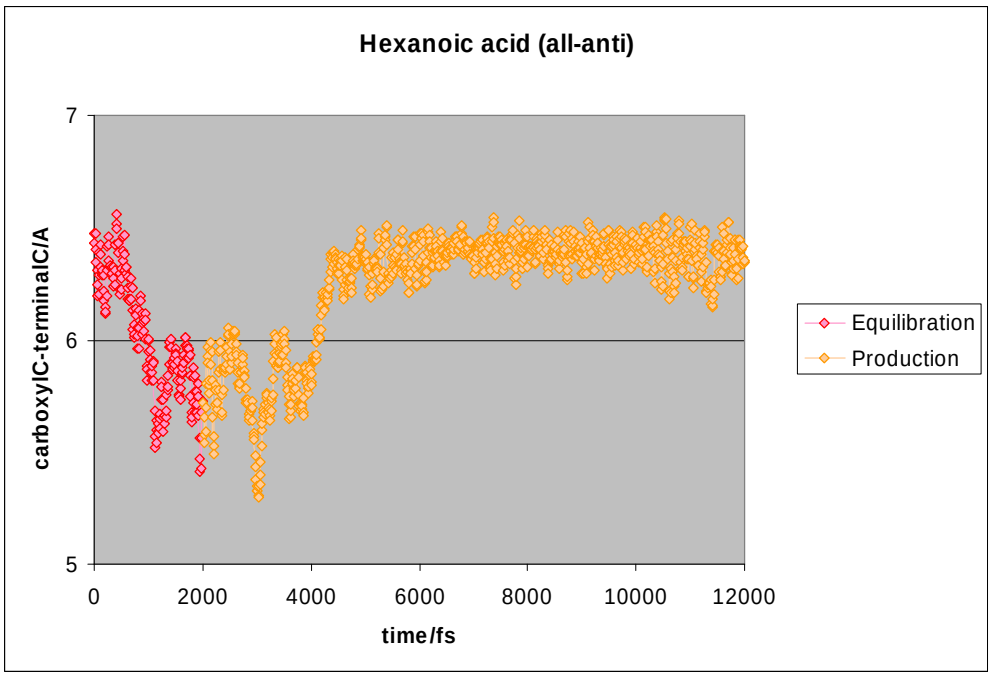


Figure 45: MD trajectory distance monitor plot for hexanoic acid (all-anti conformer).

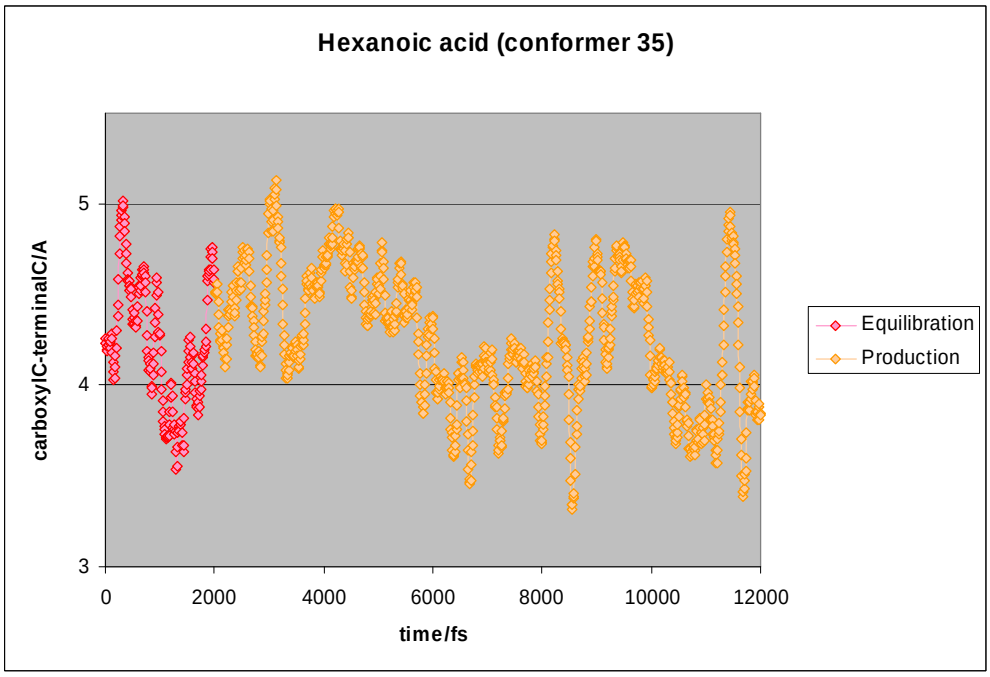


Figure 46: MD trajectory distance monitor plot for hexanoic acid (conformer 35).

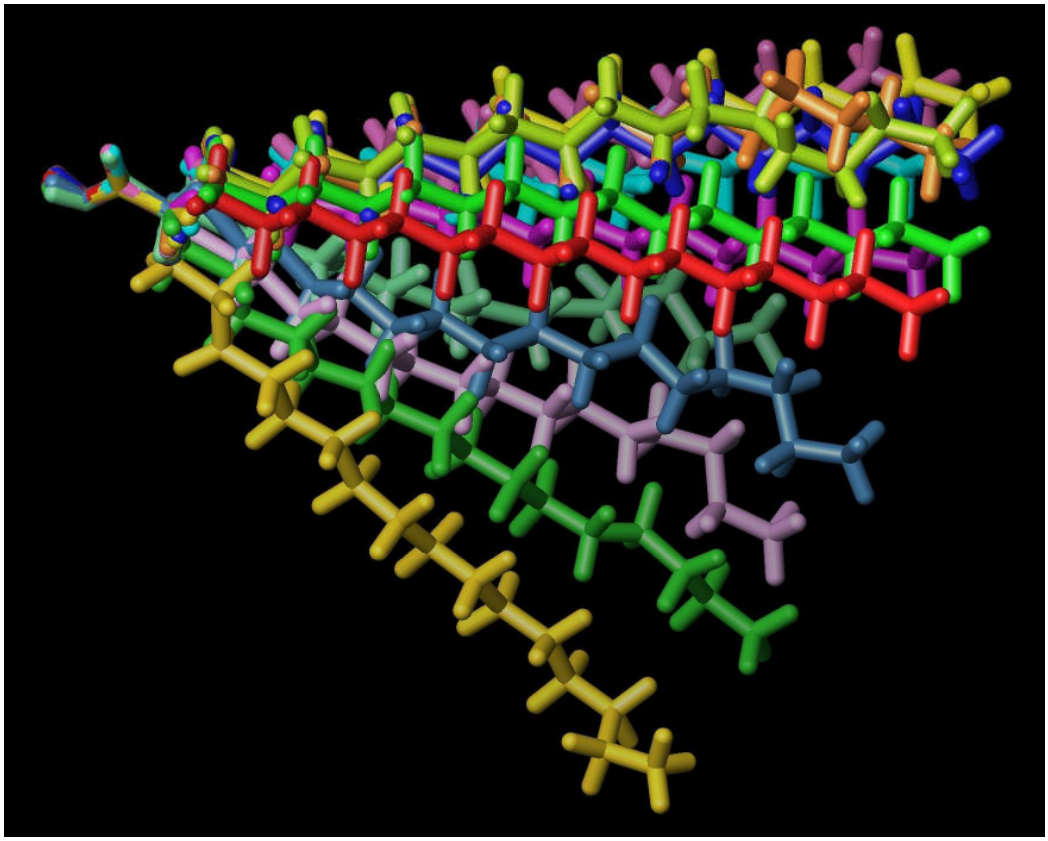

Figure 47:  Octadecanoic acid (all-anti) MD – superposition of structure snapshots taken at 1ps intervals.

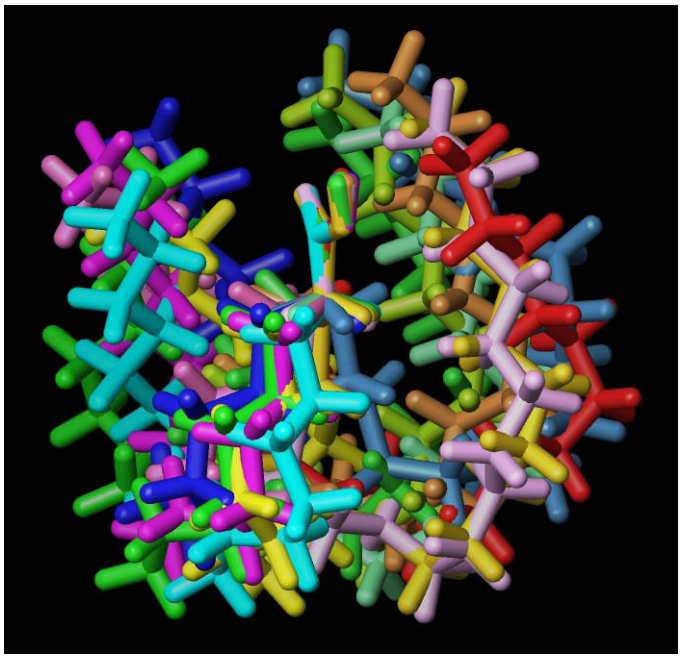

Figure 48: Octadecanoic acid (conformer 18) MD – superposition of structure snapshots taken at 1ps intervals.

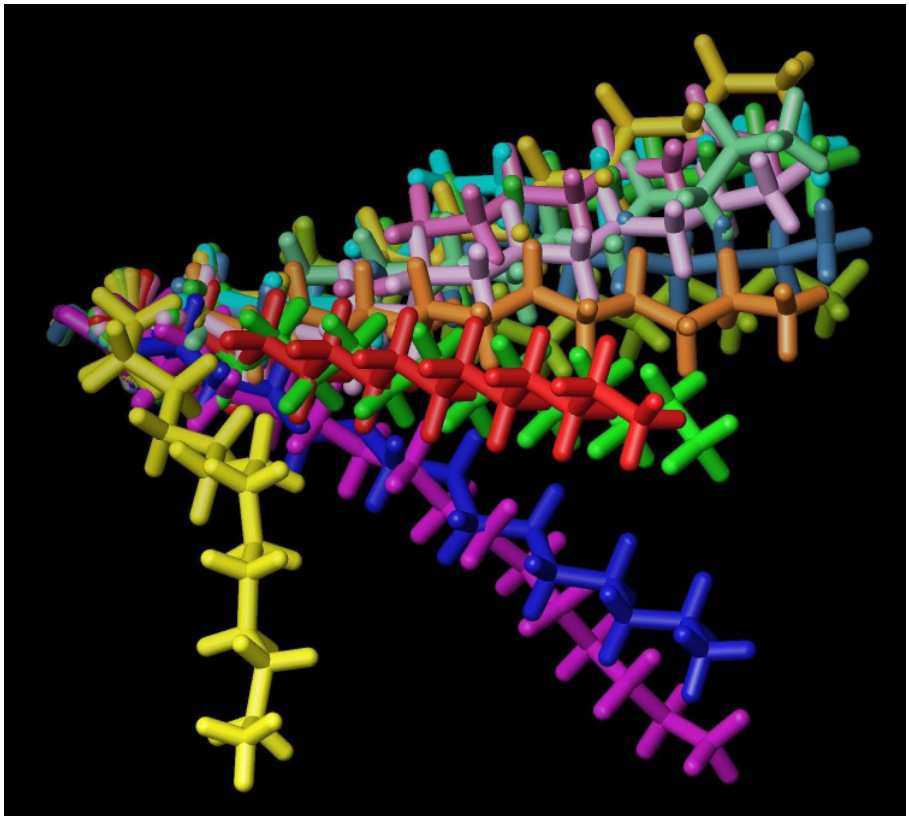

Figure 49:  Heptadecanoic acid (all-anti) MD – superposition of structure snapshots taken at 1ps intervals.

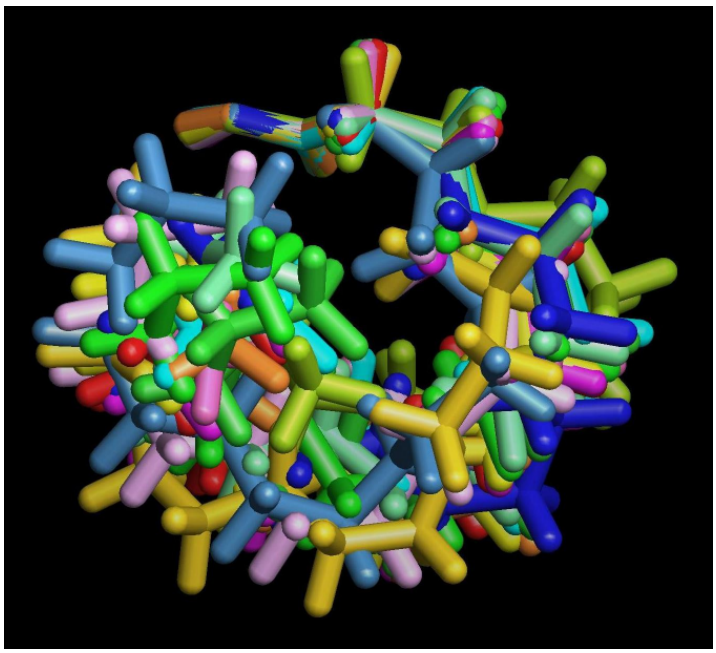

Figure 50:  Heptadecanoic acid (conformer 77) MD – superposition of structure snapshots taken at 1ps intervals.

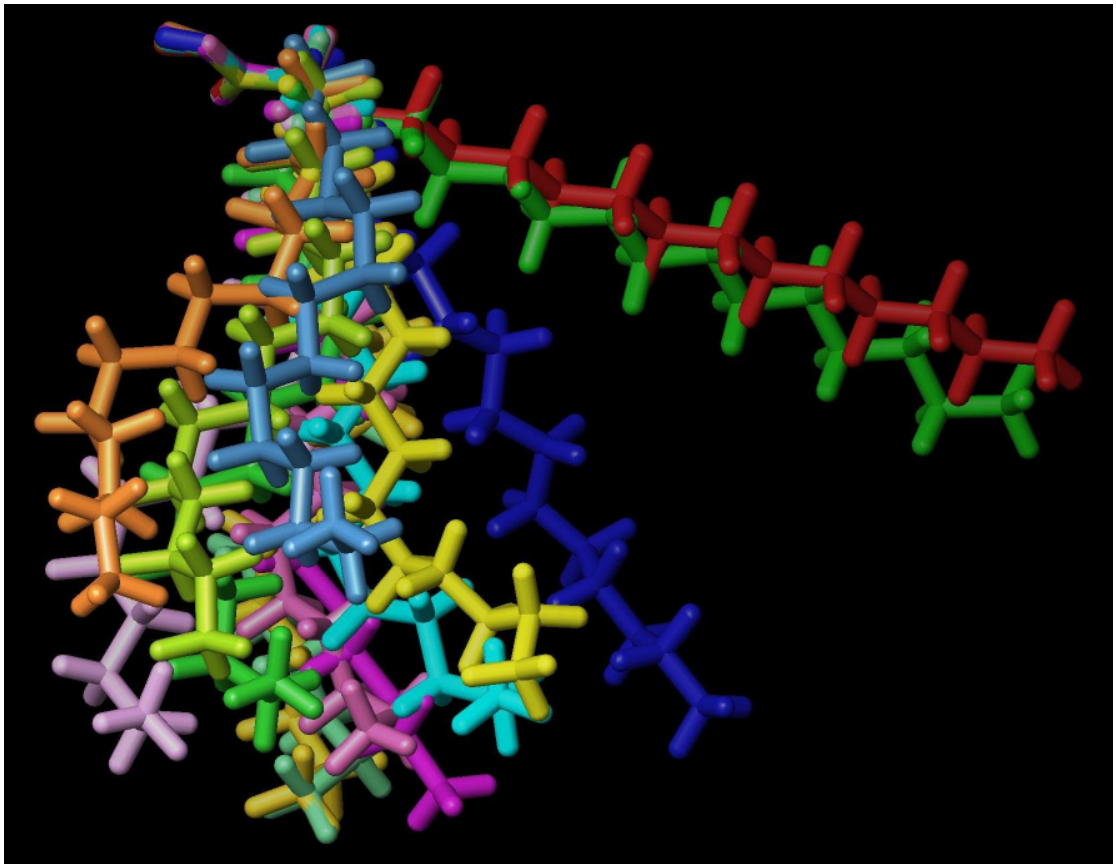

Figure 51:  Hexadecanoic acid (all-anti) MD – superposition of structure snapshots taken at 1ps intervals.

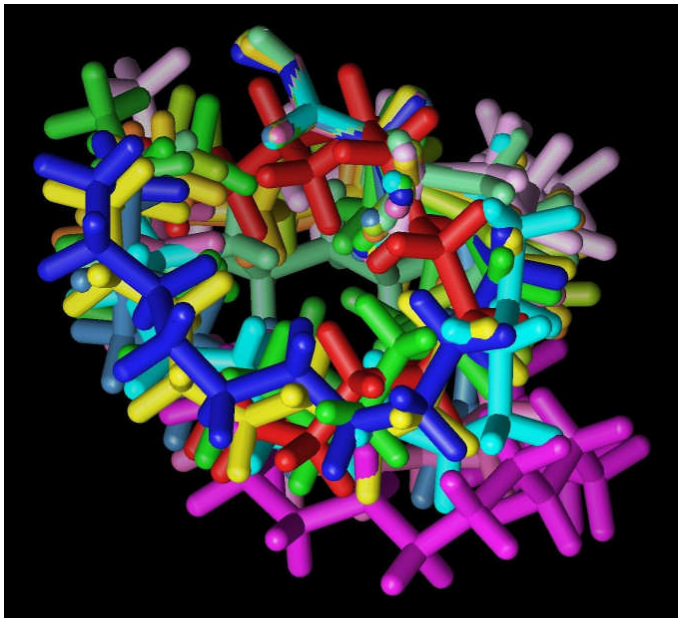

Figure 52:  Hexadecanoic acid (conformer 239) MD – superposition of structure snapshots taken at 1ps intervals.

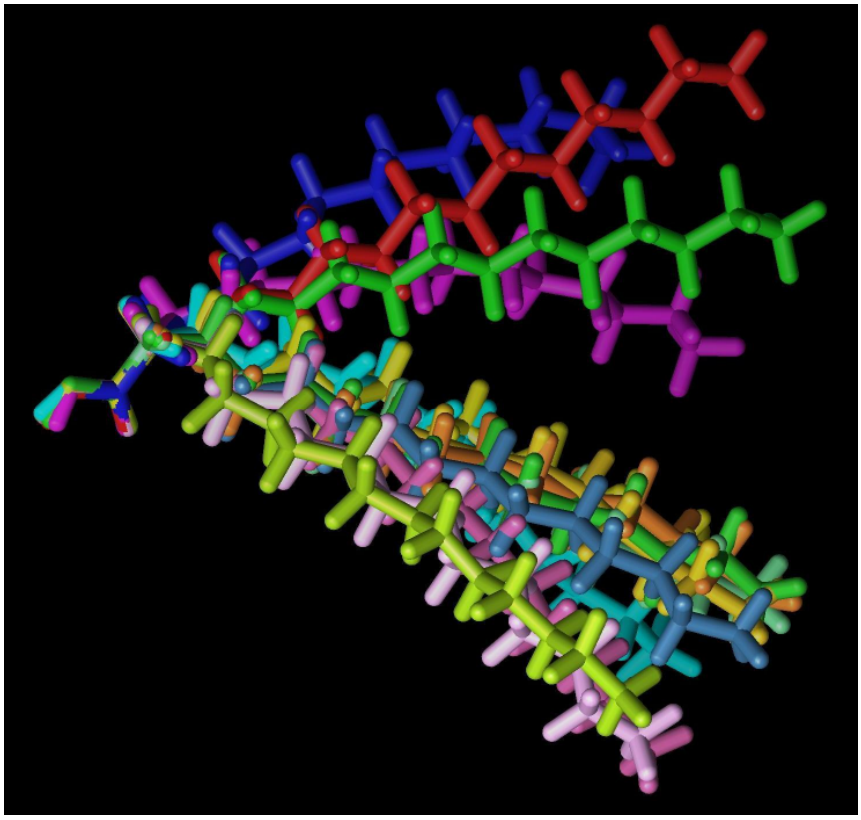

Figure 53:  Pentadecanoic acid (all-anti) MD – superposition of structure snapshots taken at 1ps intervals.

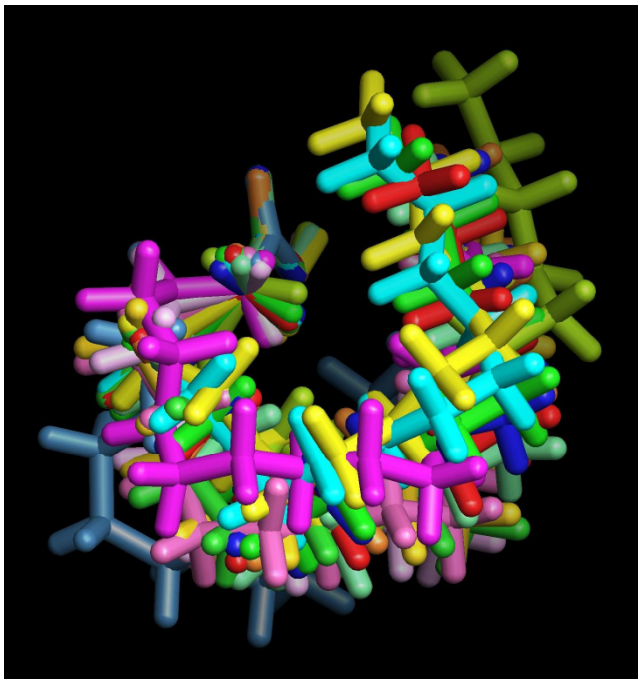

Figure 54:  Pentadecanoic acid (conformer 94) MD – superposition of structure snapshots taken at 1ps intervals.

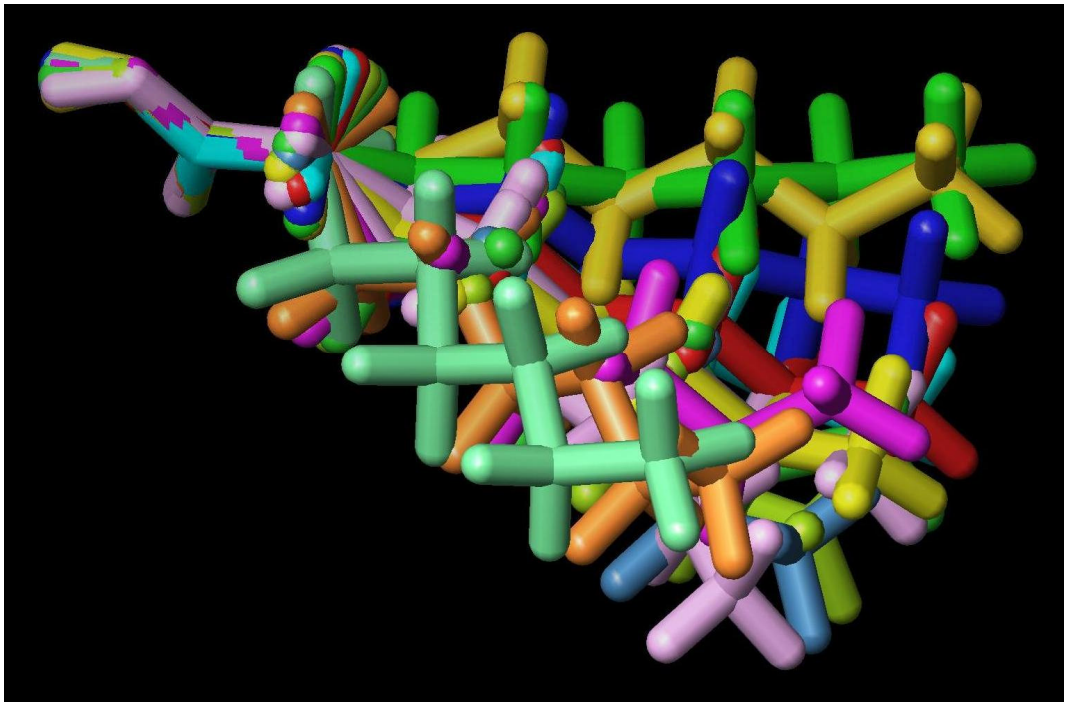

Figure 55:  Octanoic acid (all-anti) MD – superposition of structure snapshots taken at 1ps intervals.

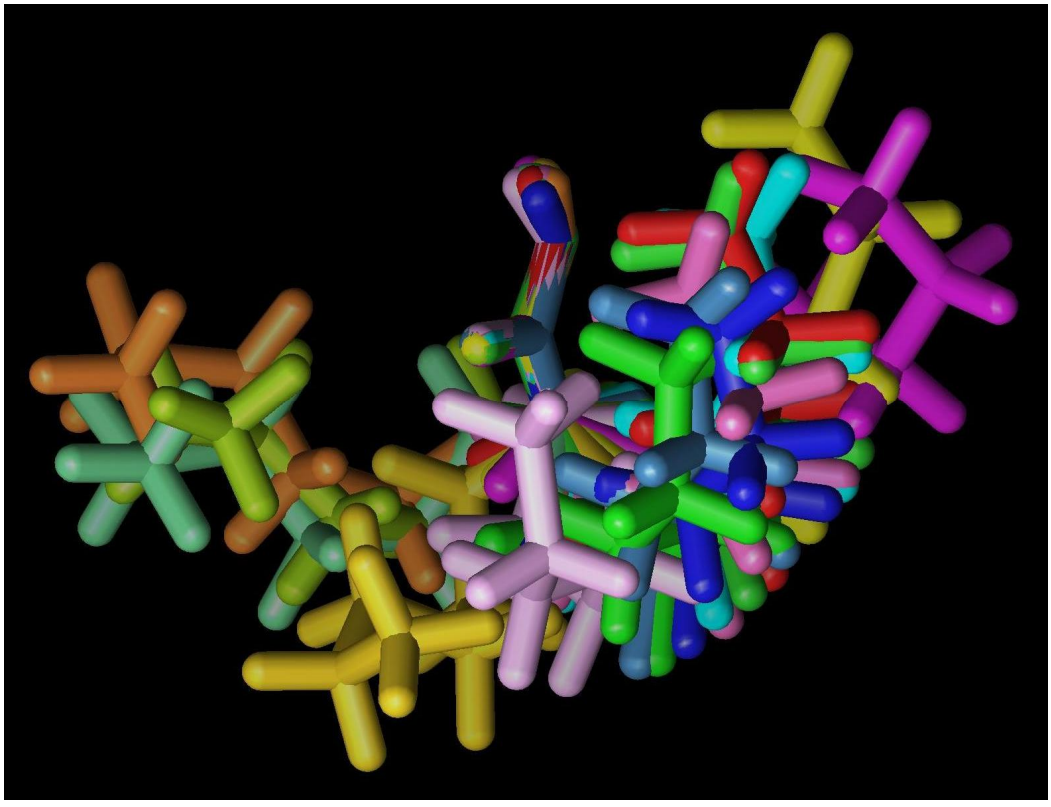

Figure  56:  Octanoic acid (conformer 143) MD – superposition of structure snapshots taken at 1ps intervals.

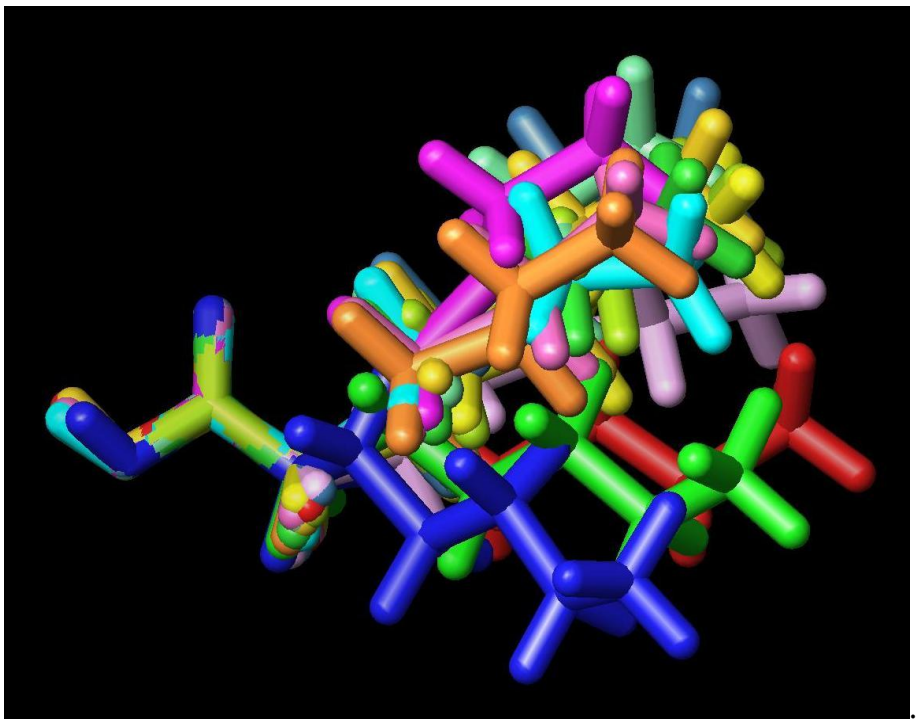

Figure 57:  Heptanoic acid (all-anti) MD – superposition of structure snapshots taken at 1ps intervals.

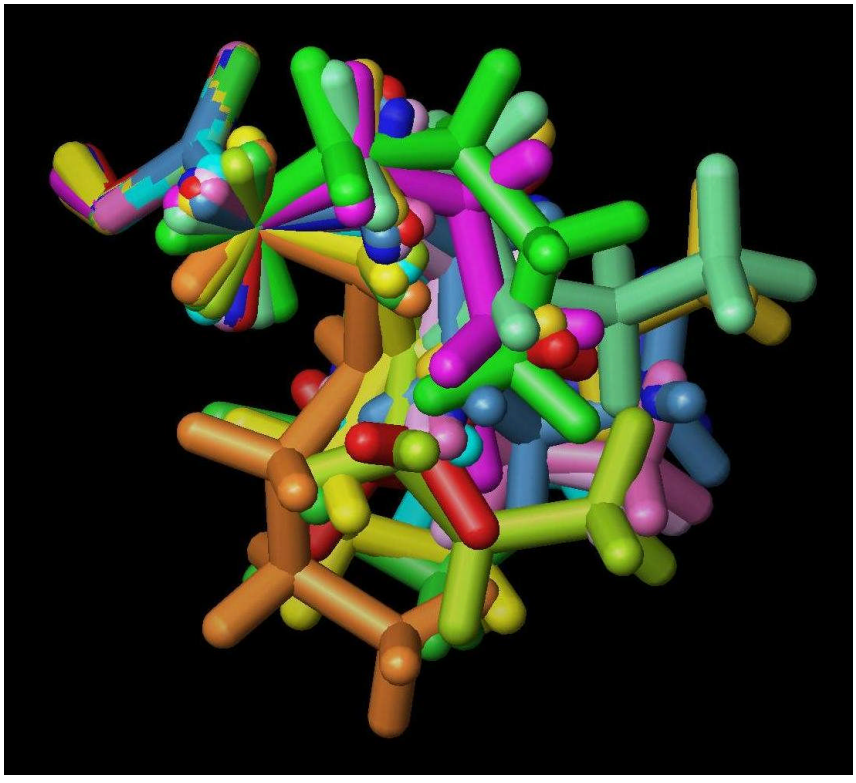

Figure 58:  Heptanoic acid (conformer 97) MD – superposition of structure snapshots taken at 1ps intervals.

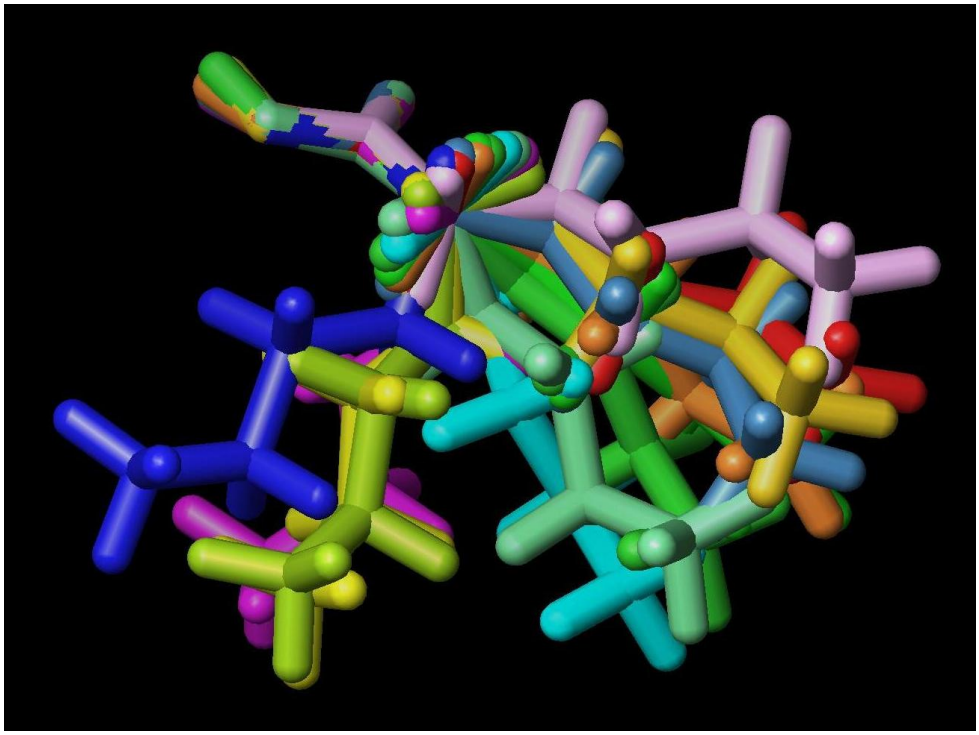

Figure 59:  Hexanoic acid (all-anti) MD – superposition of structure snapshots taken at 1ps intervals.

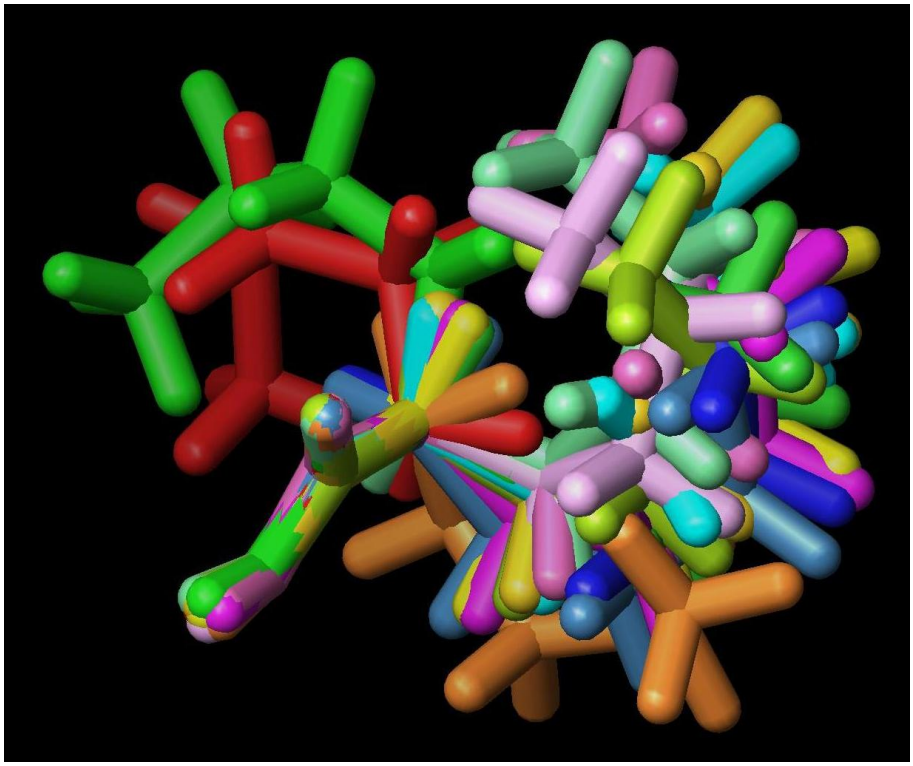

Figure 60: Hexadecanoic acid (conformer 35) MD – superposition of structure snapshots taken at 1ps intervals.

| **Table X.** Legend for figures 47 to 60 | | |
|---|---|---|
| **Atom Colour** | **Simulation Step** | **Time (cumulative)/ps** |
| Red | Soak | -- |
| Green | Post-minimization | -- |
| Blue | Equilibration MD | 1 (1) |
| Magenta | Equilibration MD | 2 (2) |
| Yellow | Production MD | 1 (3) |
| Cyan | Production MD | 2 (4) |
| Pink | Production MD | 3 (5) |
| Lime green | Production MD | 4 (6) |
| Steel blue | Production MD | 5 (7) |
| Plum | Production MD | 6 (8) |
| Gold | Production MD | 7 (9) |
| Aquamarine | Production MD | 8 (10) |
| Orange | Production MD | 9 (11) |
| Yellow-green | Production MD | 10 (12) |