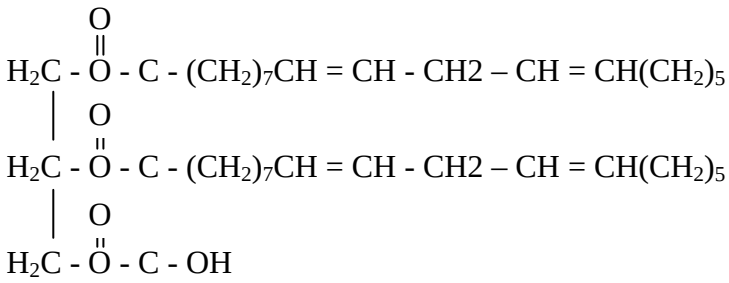
APPENDIX

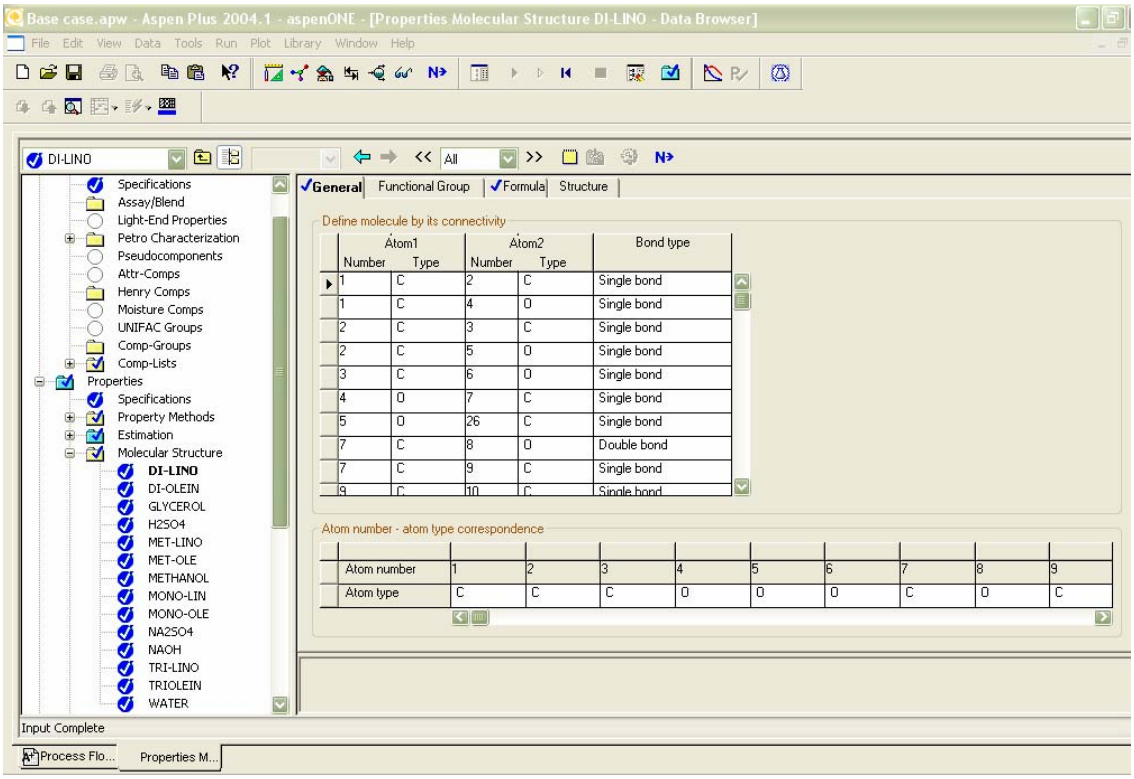
APPENDIX A

Define molecular

There are two techniques for adding the chemical structure used to calculate the properties. The first technique is importing the structure in the mol file form. This structure is drawn by molecular programming such as GAUSSIAN 03. The second technique is directly defining molecular in the ASPEN PLUS program. For example, the structure of di-linoleic showing in the Figure 44, this structure is defined in the part of molecular structure shown in the Figure 45. The properties estimations by adding structure from two techniques are similar.



Appendix Figure A1 The structure of di-linoleic



Appendix Figure A2 The defining structure of di-linoleic