# Energy-Directed Tree Search: An Efficient Systematic Algorithm for Finding the Lowest Energy Conformation of Molecules

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SUPPORTING INFORMATION

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**Table S1.** Performance of the EDTS algorithm for $S=C(CH_3)$-$SCH(COOCH_3)CH_2$-$CH(COOCH_3)$-$CH_3$ (structure **1**) for various values of EC1, EC2 and NMAX.[a]

| NMAX | EC1 | EC2 | Lowest conf | Nalg |
|---|---|---|---|---|
| **5** | **3.0** | 3.0 | Conf1 | 8 % |
| | | **4.0** | **Conf1** | **8 %** |
| | | 5.0 | Conf1 | 8 % |
| | 4.0 | 3.0 | Conf1 | 8 % |
| | | 4.0 | Conf1 | 8 % |
| | | 5.0 | Conf1 | 8 % |
| | 5.0 | 3.0 | Conf1 | 8 % |
| | | 4.0 | Conf1 | 8 % |
| | | 5.0 | Conf1 | 8 % |
| 8 | 3.0 | 3.0 | Conf1 | 8 % |
| | | 4.0 | Conf1 | 8 % |
| | | 5.0 | Conf1 | 8 % |
| | 4.0 | 3.0 | Conf1 | 8 % |
| | | 4.0 | Conf1 | 8 % |
| | | 5.0 | Conf1 | 8 % |
| | 5.0 | 3.0 | Conf1 | 8 % |
| | | 4.0 | Conf1 | 8 % |
| | | 5.0 | Conf1 | 8 % |

[a]In this table, conf 1 is the global minimum. Nalg is the number of conformers optimised during the search and the number in parentheses is the percentage of the full conformation space that this corresponds to. All structure numbers refer to Figure 3. The optimal values are shown in bold.

**Table S2.** Performance of the EDTS algorithm for $CH_3$-CH($COOCH_3$)-S-C•($CH_3$)-S-$CH_2CN$ (structure **3**) for various values of EC1, EC2 and NMAX.[a]

| NMAX | EC2 | EC1 | Lowest conf | Nalg |
|---|---|---|---|---|
| **5** | **3.0** | 3.0 | Conf 2 | 32 % |
| | | **4.0** | **Conf 1** | **38 %** |
| | | 5.0 | Conf 1 | 38 % |
| | 4.0 | 3.0 | Conf 2 | 32 % |
| | | 4.0 | Conf 2 | 32 % |
| | | 5.0 | Conf 2 | 32 % |
| | 5.0 | 3.0 | Conf 2 | 32 % |
| | | 4.0 | Conf 2 | 32 % |
| | | 5.0 | Conf 2 | 32 % |
| 8 | 3.0 | 3.0 | Conf 2 | 32 % |
| | | 4.0 | Conf 1 | 44 % |
| | | 5.0 | Conf 1 | 44 % |
| | 4.0 | 3.0 | Conf 1 | 50 % |
| | | 4.0 | Conf 1 | 50 % |
| | | 5.0 | Conf 1 | 50 % |
| | 5.0 | 3.0 | Conf 1 | 50 % |
| | | 4.0 | Conf 1 | 50 % |
| | | 5.0 | Conf 1 | 50 % |

[a]In this table, conf 1 is the global minimum and conf 2 is the second lowest conformation which lies 2.7 kJ $mol^{-1}$ above the global minimum. Nalg is the number of conformers optimised during the search and the number in parentheses is the percentage of the full conformation space that this corresponds to. All structure numbers refer to Figure 3. The optimal values are shown in bold.

**Table S3.** Performance of the EDTS algorithm for $CH_3$-$CH(COOCH_3)$-$CH_2$-$C•H(COOCH_3)$ (structure **4**) for various values of EC1, EC2 and NMAX.[a]

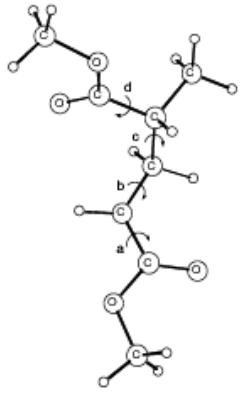
| NMAX | EC1 | EC2 | Lowest conf | Nalg |
|---|---|---|---|---|
| **5** | **3.0** | 3.0 | Conf 1 | 58 % |
| | | **4.0** | **Conf 1** | **58 %** |
| | | 5.0 | Conf 1 | 58 % |
| | 4.0 | 3.0 | Conf 1 | 58 % |
| | | 4.0 | Conf 1 | 58 % |
| | | 5.0 | Conf 1 | 58 % |
| | 5.0 | 3.0 | Conf 1 | 58 % |
| | | 4.0 | Conf 1 | 58 % |
| | | 5.0 | Conf 1 | 58 % |
| 8 | 3.0 | 3.0 | Conf 1 | 69 % |
| | | 4.0 | Conf 1 | 69 % |
| | | 5.0 | Conf 1 | 69 % |
| | 4.0 | 3.0 | Conf 1 | 69 % |
| | | 4.0 | Conf 1 | 69 % |
| | | 5.0 | Conf 1 | 69 % |
| | 5.0 | 3.0 | Conf 1 | 69 % |
| | | 4.0 | Conf 1 | 69 % |
| | | 5.0 | Conf 1 | 69 % |

[a]In this table, conf 1 is the global minimum. Nalg is the number of conformers optimised during the search and the number in parentheses is the percentage of the full conformation space that this corresponds to. All structure numbers refer to Figure 3. The optimal values are shown in bold.

**Appendix S1. Two fully worked examples of the EDTS algorithm.**

**Example 1.** $CH_3$-CH($COOCH_3$)-$CH_2$-C•H($COOCH_3$): a case of $E_1$-$E_2$ ≤ EC1, *i.e.* the leading conformation is not found and the algorithm follows the YES arm on the flowchart in Figure 1.

**Step 1.** Having decided which rotations to include in a full search of the conformational space, the next step in the algorithm is to perform a linear search of this conformational space. In this initial scan we do not update values of the torsional angles after each rotation. Rather, we generate starting structures having all possible values for rotation *a*, but with bonds *b*–*c* unchanged, we generate starting structures having all possible values for rotation *b*, but with bonds *a* and *c* unchanged, and then all rotations of bond *c* with *a*–*b* unchanged. This allows us to establish which rotations have the largest effect on the conformational energy. In the case of $CH_3$-CH($COOCH_3$)-$CH_2$-C•H($COOCH_3$) we have 4 bonds, around which we would like to perform rotations (see structure below).




Rotations ***a*** and ***d*** are two-fold (the resolution is 180°, $g_i = 1$), whereas rotations ***b*** and ***c*** are three-fold (the resolution is 120°, $g_i = 2$). These rotations form a set of individual rotations: ***a2***, ***b2***, ***b3***, ***c2***, ***c3*** and ***d2***. These give us 6 new conformations in addition to the starting one: {*a1****b2****c1d1*}, {*a1****b3****c1d1*}, {***a2****b1c1d1*}, {*a1b1****c2****d1*}, {*a1b1****c3****d1*} and {*a1b1c1****d2***}. The ranked optimized conformations according to their total energies are given below.

| Conformations | Energy, a.u. | ΔE, kJ mol$^{-1}$ |
|---|---|---|
| *a1**b2**c1d1* | $E_1$ = -613.547298 | 0.00 |
| *a1**b3**c1d1* | $E_2$ = -613.547157 | 0.37 |
| ***a2**b1c1d1* | $E_3$ = -613.546887 | 1.08 |
| *a1b1**c2**d1* | $E_4$ = -613.546832 | 1.22 |
| *a1b1**c3**d1* | $E_5$ = -613.546830 | 1.23 |
| *a1b1c1d1* **starting conformation** | $E_6$ = -613.546471 | 2.17 |
| *a1b1c1**d2*** | $E_7$ = -613.545285 | 5.28 |

The order of the individual rotations in accord with their energies is ***b2***, ***b3***, ***a2, c2***, ***c3*** and ***d2***. The difference between $E_1$ and $E_2$ is just 0.37 kJ mol$^{-1}$ showing that there is no leading conformation ($E_1$-$E_2$ ≤ EC1 = 3 kJ mol$^{-1}$).

**Step 2.** As no leading conformation was found, a full conformation search on the half of the conformation space needs to be performed. Given that there are 6 individual rotations, we need to perform a full conformational search on three first rotations, i.e. ***b2***, ***b3*** and ***a2***. All possible combinations of these rotations give us four conformations in total, only two of them being new.

| Conformations | Energy, a.u. | ΔE, kJ mol$^{-1}$ |
|---|---|---|
| ***a2b3**c1d1* | -613.547837 | **0.00** |
| ***a2b2**c1d1* | -613.547357 | **1.26** |
| *a1**b2**c1d1* | -613.547298 | **1.41** |
| *a1**b3**c1d1* | -613.547157 | **1.79** |

These four conformations are close in energy, the largest difference being about 1.8 kJ mol$^{-1}$. For the next step we need to pick NMAX conformations (NMAX is set to 5). Moreover, these conformations should satisfy the second tolerance level, i.e. the species

should be within EC2 (4 kJ $mol^{-1}$) of the lowest energy structure. All four conformations {***a2b3****c1d1*}, {***a2b2****c1d1*}, {*a1****b2****c1d1*} and {*a1****b3****c1d1*} satisfy this criterion.

**Step 3.** Linear searches are performed for the rest of the rotations.

• The first rotation out of the three rotations left (***c2***, ***c3*** and ***d2***) is ***c2***. Performing this rotation on the four conformations from Step 2 gives us additional 4 conformations, whose energies are summarized in Table below.

| Conformations | Energy, a.u. | ΔE, kJ $mol^{-1}$ |
|---|---|---|
| *a1****b2c2****d1* | -613.548451 | **0.00** |
| ***a2b3****c1d1* | -613.547837 | **1.61** |
| ***a2b3c2****d1* | -613.547837 | **1.61** |
| ***a2b2****c1d1* | -613.547357 | **2.87** |
| *a1****b2****c1d1* | -613.547298 | **3.03** |
| *a1****b3c2****d1* | -613.547167 | 3.37 |
| *a1****b3****c1d1* | -613.547157 | 3.40 |
| ***a2b2c2****d1* | -613.546371 | 5.46 |

Using the second tolerance level EC2, we pick only first 5 (NMAX) conformations with energies within 4 kJ $mol^{-1}$ from the starting conformation to continue the linear search. This leaves us with first 5 conformations: {*a1****b2c2****d1*}, {***a2b3****c1d1*}, {***a2b3c2****d1*}, {***a2b2****c1d1*} and {*a1****b2****c1d1*}.

• The second rotation out of the three rotations left (***c2***, ***c3*** and ***d2***) is ***c3***. This rotation is performed on the chosen conformations producing 3 more new conformations, whose energies are summarized in Table below. The reason that we don't end up having 5 new conformations is because some conformations repeat twice. For example, after perform the ***c3*** rotation both selected conformations, {*a1****b2c2****d1*} and {*a1****b2****c1d1*}, give rise to the same conformation {*a1****b2c3****d1*}.

| Conformations | Energy, a.u. | ΔE, kJ mol$^{-1}$ |
|---|---|---|
| *a1**b2c2**d1* | -613.548451 | 0.00 |
| *a1**b2c3**d1* | -613.548433 | 0.05 |
| ***a2b3**c1d1* | -613.547837 | 1.61 |
| ***a2b3c2**d1* | -613.547837 | 1.61 |
| ***a2b2**c1d1* | -613.547357 | 2.87 |
| *a1**b2**c1d1* | -613.547298 | 3.03 |
| ***a2b2c3**d1* | -613.546514 | 5.09 |
| ***a2b3c3**d1* | -613.545412 | 7.98 |

Even though the first 6 conformations satisfy the tolerance level EC2, only the first 5 (NMAX) conformations are selected for the next step.

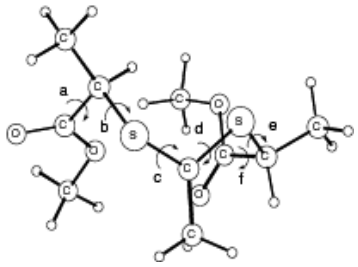
• The last rotation out of the three rotations left (***c2***, ***c3*** and ***d2***) is ***d2***. This rotation is performed on the chosen conformations producing 5 more new conformations, whose energies are summarized in Table below.

| Conformations | Energy, a.u. | ΔE, kJ mol$^{-1}$ |
|---|---|---|
| *a1**b2c2**d1* | -613.548451 | 0.00 |
| *a1**b2c3**d1* | -613.548433 | 0.05 |
| ***a2b3**c1d1* | -613.547837 | 1.61 |
| ***a2b3c2**d1* | -613.547837 | 1.61 |
| ***a2b2**c2d1* | -613.547357 | 2.87 |
| *a1**b2c3d2* | -613.546689 | 4.63 |
| *a1**b2c2d2* | -613.545765 | 7.05 |
| ***a2b3**c1**d2* | -613.545746 | 7.10 |
| ***a2b2**c1**d2* | -613.544306 | 10.88 |
| ***a2b3c2d2*** | -613.543936 | 11.85 |

After having ranked the energies of the ten conformations, the lowest energy structure {*a1**b2c2**d1*} is assigned as the global minimum.

**Example 2.** $CH_3$-CH($COOCH_3$)-S-C•($CH_3$)-S-CH($COOCH_3$)-$CH_3$: a case of $E_1$-$E_2$ > EC1, *i.e.* the leading conformation is found and the algorithm follows the NO arm on the flowchart in Figure 1.

**Step 1.** Having decided which rotations to include in a full search of the conformational space, the next step in the algorithm is to perform a linear search of this conformational space. In this initial scan we do not update values of the torsional angles after each rotation. Rather, we generate starting structures having all possible values for rotation *a*, but with bonds *b*–*c* unchanged, we generate starting structures having all possible values for rotation *b*, but with bonds *a* and *c* unchanged, and then all rotations of bond *c* with *a*–*b* unchanged. This allows us to establish which rotations have the largest effect on the conformational energy. In the case of $CH_3$-CH($COOCH_3$)-S-C•($CH_3$)-S-CH($COOCH_3$)-$CH_3$ we have 6 bonds, around which we would like to perform rotations (see structure below).




Rotations ***a, c, d*** and ***f*** are two-fold (the resolution is 180°, $g_i = 1$), whereas rotations ***b*** and ***e*** are three-fold (the resolution is 120°, $g_i = 2$). These rotations form a set of individual rotations: ***a2***, ***b2***, ***b3***, ***c2***, ***d2, e2, e3*** and ***f2***. These give us 8 new conformations in addition to the starting one: {***a2***b1c1d1e1f1}, {a1***b2***c1d1e1f1}, {a1***b3***c1d1e1f1}, {a1b1***c2***d1e1f1}, {a1b1c1***d2***e1f1}, {a1b1c1d1***e2***f1}, {a1b1c1d1***e3***f1} and {a1b1c1d1e1***f2***}. The ranked optimized conformations according to their total energies are given below.

| Conformations | Energy, a.u. | ΔE, kJ mol$^{-1}$ |
|---|---|---|
| *a1b1**c2**d1e1f1* | $E_1$ = -1488.545624 | 0.00 |
| *a1b1c1**d2**e1f1* | $E_2$ = -1488.544353 | 3.34 |
| *a1b1c1d1**e3**f1* | $E_3$ = -1488.544231 | 3.66 |
| *a1**b2**c1d1e1f1* | $E_4$ = -1488.544230 | 3.66 |
| *a1b1c1d1e1**f2*** | $E_5$ = -1488.543960 | 4.37 |
| *a1**b3**c1d1e1f1* | $E_6$ = -1488.543814 | 4.75 |
| *a1b1c1d1**e2**f1* | $E_7$ = -1488.543272 | 6.17 |
| *a1b1c1d1e1f1* **starting conformation** | $E_8$ = -1488.543251 | 6.23 |
| ***a2**b1c1d1e1f1* | $E_9$ = -1488.542907 | 7.13 |

The order of the 8 individual rotations in accord with their energies is ***c2***, ***d2, e3, b2, f2, b3, e2*** and ***a2***. The difference between $E_1$ and $E_2$ is over 3 kJ mol$^{-1}$ showing that there is a leading conformation {*a1b1**c2**d1e1f1*} ($E_1$-$E_2$ > EC1 = 3 kJ mol$^{-1}$).

**Step 2.** The linear searches are performed for all the rotations with accord to their rank, with the starting conformation {*a1b1**c2**d1e1f1*}.

• The first rotation to be performed is ***d2***. This rotation is performed on the chosen conformation giving one new conformation {*a1b1**c2d2**e1f1*}. The energies of these conformations are given below.

| Conformations | Energy, a.u. | ΔE, kJ mol$^{-1}$ |
|---|---|---|
| *a1b1**c2d2**e1f1* | -1488.546502 | **0.00** |
| *a1b1**c2**d1e1f1* | -1488.545624 | **2.31** |

Both conformations satisfy the tolerance level EC2 and are chosen for the next linear search.

• The second rotation to be performed is ***e3***. This rotation is performed on the chosen conformations producing 2 more new conformations, whose energies are summarized in Table below.

| Conformations | Energy, a.u. | ΔE, kJ mol$^{-1}$ |
|---|---|---|
| *a1b1**c2d2**e1f1* | -1488.546502 | **0.00** |
| *a1b1**c2**d1e1f1* | -1488.545624 | **2.31** |
| *a1b1**c2d2e3**f1* | -1488.544958 | **4.00** |
| *a1b1**c2**d1**e3**f1* | -1488.542142 | 11.45 |

Only first 3 conformations satisfy the tolerance level EC2 and are chosen for the lext linear search.

• The second rotation to be performed is ***b2***. This rotation is performed on the chosen conformations producing 3 more new conformations, whose energies are summarized in Table below.

| Conformations | Energy, a.u. | ΔE, kJ mol$^{-1}$ |
|---|---|---|
| *a1**b2c2d2**e1f1* | -1488.546977 | **0.00** |
| *a1**b2c2**d1e1f1* | -1488.546742 | **0.61** |
| *a1b1**c2d2**e1f1* | -1488.546502 | **1.24** |
| *a1b1**c2**d1e1f1* | -1488.545624 | **3.55** |
| *a1b1**c2d2e3**f1* | -1488.544958 | 5.30 |
| *a1**b2c2d2e3**f1* | -1488.544879 | 5.51 |

Only first 4 conformations satisfy the tolerance level EC2 and are chosen for the next linear search.

• The third rotation to be performed is ***f2***. This rotation is performed on the chosen conformations producing 4 more new conformations, whose energies are summarized in Table below.

| Conformations | Energy, a.u. | ΔE, kJ mol$^{-1}$ |
|---|---|---|
| *a1**b2c2**d1e1**f2*** | -1488.547505 | **0.00** |
| *a1**b2c2**d1e1f1* | -1488.546977 | **1.39** |
| *a1**b2c2d2**e1f1* | -1488.546742 | **2.00** |
| *a1b1**c2d2**e1f1* | -1488.546502 | **2.63** |
| *a1b1**c2**d1e1**f2*** | -1488.546499 | **2.64** |
| *a1b1**c2d2**e1**f2*** | -1488.546444 | 2.79 |
| *a1**b2c2d2**e1**f2*** | -1488.546332 | 3.08 |
| *a1b1**c2**d1e1f1* | -1488.545624 | 4.94 |

First 5 (NMAX) conformations are chosen for the next linear search.

• The fourth rotation to be performed is ***b3***. This rotation is performed on the chosen conformations producing 3 new conformations, whose energies are summarized in Table below. Two conformations {*a1**b2c2**d1e1**f2***} and {*a1b1**c2**d1e1**f2***} give rise to one new conformation {*a1**b3c2**d1e1**f2***}; two other conformations {*a1**b2c2d2**e1f1*} and {*a1b1**c2d2**e1f1*} also give rise to only one new conformation {*a1**b3c2d2**e1f1*}.

| Conformations | Energy, a.u. | ΔE, kJ mol$^{-1}$ |
|---|---|---|
| *a1**b3c2**d1e1**f2*** | -1488.549281 | **0.00** |
| *a1**b3c2**d1e1f1* | -1488.547803 | **3.88** |
| *a1**b2c2**d1e1**f2*** | -1488.547505 | 4.66 |
| *a1**b2c2**d1e1f1* | -1488.546977 | 6.05 |
| *a1**b2c2d2**e1f1* | -1488.546742 | 6.66 |
| *a1b1**c2d2**e1f1* | -1488.546502 | 7.29 |
| *a1b1**c2**d1e1**f2*** | -1488.546499 | 7.30 |
| *a1**b3c2d2**e1f1* | -1488.546490 | 7.33 |

Only first 2 conformations satisfy the tolerance level EC2 and are chosen for the next linear search.

• The fifth rotation to be performed is ***e2***. This rotation is performed on the chosen conformations producing 2 new conformations, whose energies are summarized in Table below.

| Conformations | Energy, a.u. | ΔE, kJ mol$^{-1}$ |
|---|---|---|
| *a1**b3c2**d1e1**f2*** | -1488.549281 | **0.00** |
| *a1**b3c2**d1e1f1* | -1488.547803 | **3.88** |
| *a1**b3c2**d1**e2f2*** | -1488.545646 | 9.54 |
| *a1**b3c2**d1**e2**f1* | -1488.542477 | 17.86 |

Only first 2 conformations satisfy the tolerance level EC2 and are chosen for the next linear search.

• The last rotation to be performed is ***a2***. This rotation is performed on the chosen conformations producing 2 new conformations, whose energies are summarized in Table below.

| Conformations | Energy, a.u. | ΔE, kJ mol$^{-1}$ |
|---|---|---|
| ***a2b3c2**d1e1f1* | -1488.549560 | 0.00 |
| *a1**b3c2**d1e1**f2*** | -1488.549281 | 0.73 |
| *a1**b3c2**d1e1f1* | -1488.547803 | 4.61 |
| ***a2b3c2**d1e1**f2*** | -1488.545187 | 11.48 |

After having ranked the energies of the 4 conformations, the lowest energy structure {***a2b3c2**d1e1f1*} is assigned as the global minimum.

**Appendix S2. The efficiency (the fraction of the full conformational space explored) of the EDTS algorithm in the "worst-case scenario"**

The worst-case scenario includes following the left-hand side of the flowchart on Figure 1. The algorithm can be divided into three steps:

1) A linear search of the conformations generated for all individual rotations (see box 2 in the flowchart, Fig. 1)

$$N_{tot}^{step1} = \sum_{i=1}^{N} g_i$$

where N is the total number of rotatable bonds and $g_i$ is the degeneracy of the rotation. In this context $g_i$ shows how many individual conformations can be generated by rotating around the $i^{th}$ bond. For three-fold rotations (the resolution of 120°), the degeneracy is 2, whereas for two-fold rotations (the resolution of 180°) the degeneracy is 1. Assuming that we use the resolution of 120° for all the bonds, then $N_{tot}^{step1}$ is just 2N.

2) No leading conformation is found and a full conformational search is performed on the lower half of the conformation space.

The half of the conformational search is equivalent to $\frac{2N}{2} = N$. In this case the total number of conformations to be optimised is as follows:

$$N_{tot}^{step2} = \sum_{n=2}^{N} \frac{N!}{(N-n)!\ n!} = 2^N - 1 - N$$

3) The linear search on the upper half of the rotations (which is $\frac{2N}{2} = N$) is performed:

$$N_{tot}^{step3} = NMAX \cdot N$$

In the end the total number of the conformations to be optimised is:

$$N_{tot} = 2N + 2^N - 1 - N + NMAX \cdot N = 2^N + N(NMAX + 1) - 1$$

Basically, with N increasing $N_{tot}$ is approaching $2^N$ and with respect to the full conformational space the efficiency of the algorithm is proportional to $\left(\frac{2}{3}\right)^N \cdot 100\%$. In Table below the efficiency (in %) of the algorithm versus the number of rotatable bonds is presented. $N_{tot}(EDTS)$ was calculated using the formula $N_{tot}(EDTS) = 2^N + N(NMAX + 2) - 1$, with NMAX equal 5 and all the bonds were considered three-fold (*i.e.* the full conformation space consisting of $3^N$ conformations).

| N | $N_{tot}(full\ \ search)$ | $N_{tot}(EDTS)$ | Efficiency, % |
|---|---|---|---|
| 4 | 81 | 43 | 48.1 |
| 5 | 243 | 66 | 25.1 |
| 6 | 729 | 105 | 13.6 |
| 7 | 2187 | 176 | 7.7 |
| 8 | 6561 | 311 | 4.6 |
| 9 | 19683 | 574 | 2.9 |
| 10 | 59049 | 1093 | 1.8 |
| 11 | 177147 | 2124 | 1.2 |
| 12 | 531441 | 4179 | 0.8 |
| 13 | 1594323 | 8282 | 0.5 |
| 14 | 4782969 | 16481 | 0.3 |
| 15 | 14348907 | 32872 | 0.2 |
| 16 | 4.3E+07 | 6.6E+04 | 0.2 |
| 17 | 1.3E+08 | 1.3E+05 | 0.1 |
| 18 | 3.9E+08 | 2.6E+05 | 6.8E-02 |
| 19 | 1.2E+09 | 5.2E+05 | 4.5E-02 |
| 20 | 3.5E+09 | 1.0E+06 | 3.0E-02 |

**Appendix S3. B3-LYP/6-31G(d) optimised geometries in the form of Gaussian archive entries for all species in the test set-1, both in their starting conformations and final global minimum conformations.**

**S=C($CH_3$)-SCH(COO$CH_3$)$CH_2$-CH(COO$CH_3$)-$CH_3$ (structure 1)**

**Starting conformation**


1\1\GINC-SC59\FOpt\RB3LYP\6-31G(d)\C10H16O4S2\MLC501\20-May-2004\0\\#
B3LYP/6-31G* OPT=(MAXCYC=300,Z-MATRIX) MAXDISK=402653184\\RAFT_Z=CH3_R
=MAdim-a1b1c1d1e1f1-6dub3\\0,1\C,1.812684433,-3.3676047164,-0.69575879
6\C,1.87086631,-2.0045542545,-0.0388311406\S,3.2725125843,-1.348973081
9,0.521523014\S,0.2764608591,-1.2659812456,-0.0080252244\C,0.574072381
2,0.3884242217,0.7151962079\C,-0.6687212236,0.9491057814,1.4512272965\
C,-1.9772640011,1.2103264946,0.6624791737\C,-2.7578835757,-0.090945402
1,0.458330357\O,-2.8983906676,-0.9353230847,1.3186597157\O,-3.31662861
58,-0.1807475883,-0.7651937589\C,-4.0964253281,-1.3655777399,-1.000867
7579\H,-4.9217673056,-1.4293762682,-0.286967325\H,-4.4732311906,-1.268
4357758,-2.0192990613\H,-3.4720421996,-2.2572610702,-0.9035045567\H,-2
.610647334,1.7671749618,1.3700692944\C,-1.8212667208,2.0712632131,-0.5
977592199\H,-1.2713531329,1.5509038409,-1.3858103448\H,-1.2837105087,2
.9942618837,-0.3537016069\H,-2.7990263086,2.3440672207,-1.0030848128\H
,-0.3457325264,1.8971912734,1.8933030446\H,-0.9055137893,0.2692069603,
2.2743347706\H,1.3509566371,0.236074278,1.4738878169\C,1.196051936,1.3
436375952,-0.3122608651\O,1.3833711062,1.1249994565,-1.4856799727\O,1.
5364151935,2.4975566103,0.3011295828\C,2.1791393851,3.4729245512,-0.54
01034704\H,3.1017716621,3.063430607,-0.9583245257\H,1.5160461375,3.769
0486735,-1.3571452519\H,2.3933958921,4.3215814434,0.1097559397\H,0.824
0288271,-3.8324644622,-0.6108401304\H,2.0414062154,-3.2549776857,-1.76
29562228\H,2.5661861217,-4.0250382562,-0.256916908\\Version=DEC-AXP-OS
F/1-G03RevB.03\State=1-A\HF=-1487.9806137\RMSD=7.174e-09\RMSF=1.732e-0
5\Dipole=-0.8651022,0.6949288,-0.3084766\PG=C01 [X(C10H16O4S2)]\\@


**Global minimum**


1\1\GINC-LC70\FOpt\RB3LYP\6-31G(d)\C10H16O4S2\MLC501\30-Jun-2004\0\\#
B3LYP/6-31G* OPT=(MAXCYC=300) MAXDISK=402653184\\RAFT_Z=CH3_R=MAdim-a1
b1c1d1e2f1-6dub3\\0,1\C,4.5452402159,0.3120435334,-1.2636792233\C,3.30
43742391,-0.1672049766,-0.536774526\S,3.3534780065,-1.3499208234,0.606
1984124\S,1.893710073,0.7363336885,-1.0746154145\C,0.5057399016,0.0937
492596,-0.035898979\C,-0.2015318889,-1.0775076891,-0.7421431683\C,-1.3
480856341,-1.7510541862,0.0666191199\C,-2.5752438414,-0.8467568082,0.1
300840723\O,-2.954177408,-0.242100793,1.1132109046\O,-3.1889368944,-0.
7819082079,-1.0678722549\C,-4.2712928576,0.1610267692,-1.1609186684\H,
-3.8947196891,1.1734740486,-0.9960678033\H,-4.6619473281,0.0568686855,
-2.1735142203\H,-5.0447659623,-0.0675539991,-0.42336088\H,-1.643239988
6,-2.6224039325,-0.5313424501\C,-0.9291835165,-2.2099560402,1.46722051
72\H,-0.7567314388,-1.3569513496,2.128936286\H,-0.012023175,-2.8058445
455,1.4168312815\H,-1.7138119034,-2.8213195946,1.9241368076\H,0.556120
6671,-1.8409391877,-0.9464757911\H,-0.5953206632,-0.7299740777,-1.7016
327619\H,0.9595738181,-0.2224893584,0.9051651427\C,-0.4197825199,1.283
2785949,0.1958240266\O,-1.1051507969,1.7868647814,-0.6707675016\O,-0.3
791393763,1.6874835094,1.4721185741\C,-1.3050783961,2.736022778,1.8208
370286\H,-1.1460138772,3.6119465077,1.1875167261\H,-2.3271655826,2.370
0495072,1.7020725124\H,-1.0967447357,2.9687360567,2.8649505079\H,5.176
5234825,-0.5418649668,-1.5211388401\H,4.3134716474,0.8808214235,-2.170

6295215\H,5.1200870488,0.9602772137,-0.5913139383\\Version=x86-Linux-G
03RevB.03\State=1-A\HF=-1487.9887623\RMSD=4.176e-09\RMSF=6.933e-06\Dip
ole=-0.1266152,0.334882,-0.4080501\PG=C01 [X(C10H16O4S2)]\\@

**$CH_3$-CH($COOCH_3$)-S-C•($CH_3$)-S-CH($COOCH_3$)-$CH_3$ (structure 2)**

**Starting conformation**

1\1\GINC-LC60\FOpt\UB3LYP\6-31G(d)\C10H17O4S2(2)\MLC501\01-Apr-2004\1\
\# B3LYP/6-31G* OPT=(MAXCYC=300,Z-MATRIX) MAXDISK=268435456\\RRAD_R=MA
_R=MA-a1b1c1d1e1f1-6dub3\\0,2\S\C,1,B1\S,2,B2,1,A1\C,2,B3,1,A2,3,D1,0\
C,1,B4,2,A3,3,D2,0\C,5,B5,1,A4,2,D3,0\C,5,B6,1,A5,6,D4,0\H,5,B7,1,A6,6
,D5,0\O,7,B8,5,A7,1,D6,0\O,7,B9,5,A8,9,D7,0\C,10,B10,7,A9,5,D8,0\H,11,
B11,10,A10,7,D9,0\H,11,B12,10,A11,12,D10,0\H,11,B13,10,A12,12,D11,0\H,
6,B14,5,A13,1,D12,0\H,6,B15,5,A14,15,D13,0\H,6,B16,5,A15,15,D14,0\H,4,
B17,2,A16,1,D15,0\H,4,B18,2,A17,18,D16,0\H,4,B19,2,A18,18,D17,0\C,3,B2
0,2,A19,1,D18,0\C,21,B21,3,A20,2,D19,0\C,21,B22,3,A21,22,D20,0\H,21,B2
3,3,A22,22,D21,0\O,23,B24,21,A23,3,D22,0\O,23,B25,21,A24,25,D23,0\C,26
,B26,23,A25,21,D24,0\H,27,B27,26,A26,23,D25,0\H,27,B28,26,A27,28,D26,0
\H,27,B29,26,A28,28,D27,0\H,22,B30,21,A29,3,D28,0\H,22,B31,21,A30,31,D
29,0\H,22,B32,21,A31,31,D30,0\\B1=1.750943\B2=1.75764545\B3=1.50143172
\B4=1.87960197\B5=1.52601082\B6=1.5207978\B7=1.09202121\B8=1.21155842\
B9=1.34908769\B10=1.43825664\B11=1.0901862\B12=1.09315578\B13=1.093071
98\B14=1.0923956\B15=1.09727392\B16=1.09410026\B17=1.10255834\B18=1.09
395722\B19=1.09651985\B20=1.87894482\B21=1.52767778\B22=1.51985104\B23
=1.09180162\B24=1.21099198\B25=1.35269305\B26=1.43865533\B27=1.0930363
6\B28=1.09289829\B29=1.09019954\B30=1.09307165\B31=1.09298739\B32=1.09
638525\A1=114.18731613\A2=121.93450416\A3=103.29220145\A4=111.75094842
\A5=105.6922179\A6=106.72558864\A7=124.79687224\A8=111.20668708\A9=115
.24314044\A10=105.51108934\A11=110.5073798\A12=110.44034126\A13=110.31
031501\A14=110.30807135\A15=110.52018949\A16=111.91135672\A17=111.5000
7373\A18=110.68837664\A19=104.42606937\A20=109.49795234\A21=108.338820
9\A22=106.08298038\A23=124.86887511\A24=111.48559243\A25=115.30545778\
A26=110.39926561\A27=110.46269427\A28=105.53123906\A29=110.73597542\A3
0=110.36126542\A31=110.11382268\D1=-169.93548789\D2=122.15146655\D3=-7
7.13177183\D4=-122.07754328\D5=122.76297094\D6=86.70875774\D7=-179.319
67425\D8=177.57044963\D9=-179.82444426\D10=-119.67818675\D11=119.61947
334\D12=-63.87460955\D13=-119.65842801\D14=120.58941292\D15=78.8823311
5\D16=119.00694571\D17=-119.85408587\D18=134.81806074\D19=-128.4428870
6\D20=-121.81282921\D21=120.47352592\D22=91.15474205\D23=-179.28032665
\D24=176.79965371\D25=-60.3723108\D26=120.70095326\D27=-119.63857607\D
28=-61.00942172\D29=120.85459915\D30=-118.96503808\\Version=x86-Linux-
G03RevB.03\State=2-A\HF=-1488.5432506\S2=0.756473\S2-1=0.\S2A=0.75003\
RMSD=8.899e-09\RMSF=5.649e-05\Dipole=-1.6853833,0.1199487,0.7126631\PG
=C01 [X(C10H17O4S2)]\\@

**Global minimum**

1\1\GINC-LC95\FOpt\UB3LYP\6-31G(d)\C10H17O4S2(2)\MLC501\13-Apr-2004\1\
\# B3LYP/6-31G* OPT=(MAXCYC=300,Z-MATRIX) MAXDISK=268435456\\RRAD_R=MA
_R=MA-a2b3c2d1e1f1-6dub3\\0,2\S\C,1,B1\S,2,B2,1,A1\C,2,B3,1,A2,3,D1,0\
C,1,B4,2,A3,3,D2,0\C,5,B5,1,A4,2,D3,0\C,5,B6,1,A5,6,D4,0\H,5,B7,1,A6,6
,D5,0\O,7,B8,5,A7,1,D6,0\O,7,B9,5,A8,9,D7,0\C,10,B10,7,A9,5,D8,0\H,11,
B11,10,A10,7,D9,0\H,11,B12,10,A11,12,D10,0\H,11,B13,10,A12,12,D11,0\H,
6,B14,5,A13,1,D12,0\H,6,B15,5,A14,15,D13,0\H,6,B16,5,A15,15,D14,0\H,4,
B17,2,A16,1,D15,0\H,4,B18,2,A17,18,D16,0\H,4,B19,2,A18,18,D17,0\C,3,B2
0,2,A19,1,D18,0\C,21,B21,3,A20,2,D19,0\C,21,B22,3,A21,22,D20,0\H,21,B2
3,3,A22,22,D21,0\O,23,B24,21,A23,3,D22,0\O,23,B25,21,A24,25,D23,0\C,26

,B26,23,A25,21,D24,0\H,27,B27,26,A26,23,D25,0\H,27,B28,26,A27,28,D26,0
\H,27,B29,26,A28,28,D27,0\H,22,B30,21,A29,3,D28,0\H,22,B31,21,A30,31,D
29,0\H,22,B32,21,A31,31,D30,0\\B1=1.75853936\B2=1.74840433\B3=1.501563
43\B4=1.86276629\B5=1.53306408\B6=1.5216228\B7=1.09135972\B8=1.2146144
9\B9=1.34467307\B10=1.43815597\B11=1.09030837\B12=1.09241579\B13=1.092
69654\B14=1.09294157\B15=1.09562542\B16=1.09389723\B17=1.09912953\B18=
1.09355129\B19=1.09932909\B20=1.88901509\B21=1.52464512\B22=1.51589195
\B23=1.0925883\B24=1.21237138\B25=1.3525762\B26=1.43946612\B27=1.09312
029\B28=1.09357288\B29=1.08906834\B30=1.09347526\B31=1.09338593\B32=1.
09547455\A1=116.05846865\A2=122.04714541\A3=105.03113235\A4=107.483322
47\A5=110.76129486\A6=108.01265417\A7=123.90003104\A8=111.95918717\A9=
115.93372173\A10=105.46653152\A11=109.74497473\A12=110.62384824\A13=11
1.24302939\A14=109.93883364\A15=110.26125407\A16=111.62061356\A17=110.
15658659\A18=111.24656322\A19=104.8418079\A20=108.3046961\A21=107.8719
1971\A22=105.87364046\A23=125.32946057\A24=110.8294117\A25=115.8208220
6\A26=110.23006271\A27=110.4631726\A28=104.98014265\A29=110.91169528\A
30=110.54033204\A31=109.92946539\D1=-172.0568561\D2=207.39229882\D3=-1
67.54667617\D4=-124.50262813\D5=119.14743898\D6=-105.74992215\D7=-179.
69013681\D8=182.69210947\D9=-173.59295244\D10=-119.18264457\D11=119.74
929268\D12=-60.5146371\D13=-119.71071204\D14=120.92390781\D15=49.01033
438\D16=120.22688925\D17=-120.22453833\D18=67.50787247\D19=-160.438438
37\D20=-121.71687426\D21=120.42593203\D22=96.33635142\D23=-178.5102921
9\D24=173.5538817\D25=-56.91796285\D26=120.38943863\D27=-119.4597016\D
28=-61.56990693\D29=121.29715164\D30=-118.68428231\\Version=x86-Linux-
G03RevB.03\State=2-A\HF=-1488.5495599\S2=0.756381\S2-1=0.\S2A=0.750031
\RMSD=4.089e-09\RMSF=7.159e-05\Dipole=-0.7503745,0.5497008,-1.1562442\
PG=C01 [X(C10H17O4S2)]\\@

**$CH_3$-CH($COOCH_3$)-S-C•($CH_3$)-S-$CH_2CN$ (structure 3)**

**Starting conformation**

1\1\GINC-SC29\FOpt\UB3LYP\6-31G(d)\C8H12N1O2S2(2)\MLC501\02-Apr-2004\1
\\# B3LYP/6-31G* OPT=(MAXCYC=300,Z-MATRIX) MAXDISK=268435456\\RRAD_R=M
A_R=CH2CN-a1b1c1d1e1-6dub3\\0,2\S\C,1,B1\S,2,B2,1,A1\C,2,B3,1,A2,3,D1,
0\C,1,B4,2,A3,3,D2,0\C,3,B5,2,A4,1,D3,0\C,5,B6,1,A5,2,D4,0\H,5,B7,1,A6
,7,D5,0\H,5,B8,1,A7,7,D6,0\C,6,B9,3,A8,2,D7,0\C,6,B10,3,A9,10,D8,0\H,6
,B11,3,A10,10,D9,0\O,11,B12,6,A11,3,D10,0\O,11,B13,6,A12,13,D11,0\C,14
,B14,11,A13,6,D12,0\H,15,B15,14,A14,11,D13,0\H,15,B16,14,A15,16,D14,0\
H,15,B17,14,A16,16,D15,0\H,10,B18,6,A17,3,D16,0\H,10,B19,6,A18,19,D17,
0\H,10,B20,6,A19,19,D18,0\H,4,B21,2,A20,1,D19,0\H,4,B22,2,A21,22,D20,0
\H,4,B23,2,A22,22,D21,0\X,7,1.,5,90.,1,D22,0\N,7,B24,25,A23,5,180.,0\\
B1=1.75810194\B2=1.76577809\B3=1.50461246\B4=1.85989688\B5=1.87271656\
B6=1.45719125\B7=1.09362801\B8=1.0940896\B9=1.52637854\B10=1.52346759\
B11=1.0917791\B12=1.21133982\B13=1.34648985\B14=1.43988795\B15=1.08994
138\B16=1.09289169\B17=1.09292517\B18=1.09267515\B19=1.09402789\B20=1.
09698472\B21=1.09519807\B22=1.09530209\B23=1.10128026\B24=1.16077065\A
1=117.78261121\A2=115.72700528\A3=101.96174464\A4=102.20391939\A5=109.
6680215\A6=108.79570216\A7=109.2201706\A8=112.27330812\A9=105.32877998
\A10=106.92906672\A11=124.42640339\A12=111.25053125\A13=115.29511682\A
14=105.46741371\A15=110.34784345\A16=110.42922642\A17=110.38973697\A18
=110.35648257\A19=110.22340756\A20=111.29937536\A21=110.83370109\A22=1
11.86538677\A23=89.51419382\D1=155.36155057\D2=54.89558595\D3=-142.530
87404\D4=-172.85123279\D5=120.77103949\D6=-120.5014285\D7=78.50900043\
D8=121.82803471\D9=-122.97350403\D10=-83.29208562\D11=179.48680704\D12
=-177.78994246\D13=-179.95997767\D14=-119.6044616\D15=119.68757153\D16
=63.51103904\D17=-121.04721427\D18=119.52106398\D19=167.21967009\D20=-
120.49013722\D21=119.21345007\D22=-30.60943356\\Version=DEC-AXP-OSF/1-
G03RevB.03\State=2-A\HF=-1313.5913308\S2=0.755841\S2-1=0.\S2A=0.750025

\RMSD=9.255e-09\RMSF=5.831e-05\Dipole=-0.8759447,0.0322234,2.2993476\P
G=C01 [X(C8H12N1O2S2)]\\@

**Global minimum**

1\1\GINC-SC102\FOpt\UB3LYP\6-31G(d)\C8H12N1O2S2(2)\MLC501\01-May-2004\
1\\# B3LYP/6-31G* OPT=(MAXCYC=300,Z-MATRIX) MAXDISK=402653184 GEOM=CHE
CK GUESS=READ\\RRAD_R=MA_R=CH2CN-a3b2c1d2e2-6dub3\\0,2\S\C,1,B1\S,2,B2
,1,A1\C,2,B3,1,A2,3,D1,0\C,1,B4,2,A3,3,D2,0\C,3,B5,2,A4,1,D3,0\C,5,B6,
1,A5,2,D4,0\H,5,B7,1,A6,7,D5,0\H,5,B8,1,A7,7,D6,0\C,6,B9,3,A8,2,D7,0\C
,6,B10,3,A9,10,D8,0\H,6,B11,3,A10,10,D9,0\O,11,B12,6,A11,3,D10,0\O,11,
B13,6,A12,13,D11,0\C,14,B14,11,A13,6,D12,0\H,15,B15,14,A14,11,D13,0\H,
15,B16,14,A15,16,D14,0\H,15,B17,14,A16,16,D15,0\H,10,B18,6,A17,3,D16,0
\H,10,B19,6,A18,19,D17,0\H,10,B20,6,A19,19,D18,0\H,4,B21,2,A20,1,D19,0
\H,4,B22,2,A21,22,D20,0\H,4,B23,2,A22,22,D21,0\X,7,1.,5,90.,1,D22,0\N,
7,B24,25,A23,5,180.,0\\B1=1.75935056\B2=1.75286213\B3=1.50359279\B4=1.
86845908\B5=1.86699106\B6=1.45783174\B7=1.09509931\B8=1.09431427\B9=1.
52861381\B10=1.51862298\B11=1.09238701\B12=1.21692013\B13=1.34370785\B
14=1.43944576\B15=1.08991938\B16=1.09280757\B17=1.09288472\B18=1.09308
311\B19=1.09362883\B20=1.09528939\B21=1.09619271\B22=1.10076057\B23=1.
09441358\B24=1.16166629\A1=120.53303749\A2=121.61440739\A3=103.1157478
1\A4=105.16516264\A5=114.06472916\A6=104.89740468\A7=107.86607789\A8=1
08.72596154\A9=107.81958191\A10=106.05110753\A11=124.02975098\A12=112.
5403427\A13=115.64732854\A14=105.42660489\A15=110.48045093\A16=110.292
61437\A17=111.63166473\A18=110.04574991\A19=109.95783386\A20=111.38285
36\A21=111.20583578\A22=110.98808012\A23=89.28611496\D1=172.90707229\D
2=117.23434881\D3=-45.96839444\D4=-287.05503299\D5=120.05683547\D6=-12
3.89934982\D7=159.83464859\D8=125.74735887\D9=-119.75913451\D10=86.955
30844\D11=181.5583837\D12=-183.1614275\D13=-180.25515638\D14=-119.6858
4478\D15=119.5516788\D16=58.9754022\D17=-120.97016445\D18=119.61368879
\D19=207.5119804\D20=-119.28893835\D21=121.38632708\D22=-410.92108159\
\Version=DEC-AXP-OSF/1-G03RevB.03\State=2-A\HF=-1313.5980317\S2=0.7562
71\S2-1=0.\S2A=0.750029\RMSD=5.666e-09\RMSF=5.318e-05\Dipole=1.8261481
,-0.6219673,0.5397314\PG=C01 [X(C8H12N1O2S2)]\\@

**$CH_3$-CH($COOCH_3$)-$CH_2$-C•H($COOCH_3$) (structure 4)**

**Starting conformation**

1\1\GINC-SC82\FOpt\UB3LYP\6-31G(d)\C8H13O4(2)\MLC501\18-Mar-2004\1\\#
B3LYP/6-31G* OPT=(MAXCYC=300,Z-MATRIX) MAXDISK=402653184\\MA_dim-a1b1c
1d1-6dub3\\0,2\C\O,1,B1\C,2,B2,1,A1\O,3,B3,2,A2,1,D1,0\C,3,B4,2,A3,4,D
2,0\C,5,B5,3,A4,2,D3,0\H,5,B6,3,A5,6,D4,0\C,6,B7,5,A6,3,D5,0\C,8,B8,6,
A7,5,D6,0\O,9,B9,8,A8,6,D7,0\O,9,B10,8,A9,10,D8,0\C,11,B11,9,A10,8,D9,
0\H,1,B12,2,A11,3,D10,0\H,1,B13,2,A12,13,D11,0\H,1,B14,2,A13,13,D12,0\
H,6,B15,5,A14,8,D13,0\H,6,B16,5,A15,8,D14,0\H,8,B17,6,A16,9,D15,0\C,8,
B18,6,A17,9,D16,0\H,19,B19,8,A18,6,D17,0\H,19,B20,8,A19,20,D18,0\H,19,
B21,8,A20,20,D19,0\H,12,B22,11,A21,9,D20,0\H,12,B23,11,A22,23,D21,0\H,
12,B24,11,A23,23,D22,0\\B1=1.43329743\B2=1.36076599\B3=1.22491788\B4=1
.45101654\B5=1.48883617\B6=1.08517198\B7=1.56734875\B8=1.5238883\B9=1.
21265281\B10=1.35209741\B11=1.43675235\B12=1.09063549\B13=1.09388107\B
14=1.09400297\B15=1.09659387\B16=1.09513518\B17=1.09634655\B18=1.52998
893\B19=1.09488498\B20=1.09483228\B21=1.09394181\B22=1.0903291\B23=1.0
933148\B24=1.09338461\A1=114.99229302\A2=123.22972756\A3=111.96795415\
A4=120.3815099\A5=118.12517666\A6=113.06825141\A7=108.96561303\A8=125.
45428976\A9=111.25098454\A10=115.49702213\A11=105.63013724\A12=110.748
41665\A13=110.73183106\A14=109.78760441\A15=109.32701557\A16=106.29075
361\A17=113.02807757\A18=110.56224061\A19=110.95496629\A20=110.8961762

2\A21=105.54903459\A22=110.53141652\A23=110.63443788\D1=0.12226803\D2=
179.74914092\D3=-179.94067793\D4=177.48524223\D5=78.11421726\D6=-176.8
6024911\D7=-113.47470345\D8=179.29164518\D9=-179.08394413\D10=179.5319
3987\D11=-119.70460982\D12=119.66473233\D13=121.59462499\D14=-119.4218
7366\D15=115.28154063\D16=-123.32101466\D17=-60.39013055\D18=120.61321
003\D19=-120.16834567\D20=179.65931546\D21=119.6079875\D22=-119.724608
06\\Version=DEC-AXP-OSF/1-G03RevB.03\State=2-A\HF=-613.5464708\S2=0.75
6407\S2-1=0.\S2A=0.750027\RMSD=4.818e-09\RMSF=3.394e-05\Dipole=-0.3647
728,-0.340167,-0.2746599\PG=C01 [X(C8H13O4)]\\@

**Global minimum**

1\1\GINC-SC49\FOpt\UB3LYP\6-31G(d)\C8H13O4(2)\MLC501\29-Apr-2004\1\\#
B3LYP/6-31G* OPT=(MAXCYC=300,Z-MATRIX) MAXDISK=402653184 GEOM=CHECK GU
ESS=READ\\MA_dim-a1b1c1d1-6dub3\\0,2\C\O,1,B1\C,2,B2,1,A1\O,3,B3,2,A2,
1,D1,0\C,3,B4,2,A3,4,D2,0\C,5,B5,3,A4,2,D3,0\H,5,B6,3,A5,6,D4,0\C,6,B7
,5,A6,3,D5,0\C,8,B8,6,A7,5,D6,0\O,9,B9,8,A8,6,D7,0\O,9,B10,8,A9,10,D8,
0\C,11,B11,9,A10,8,D9,0\H,1,B12,2,A11,3,D10,0\H,1,B13,2,A12,13,D11,0\H
,1,B14,2,A13,13,D12,0\H,6,B15,5,A14,8,D13,0\H,6,B16,5,A15,8,D14,0\H,8,
B17,6,A16,9,D15,0\C,8,B18,6,A17,9,D16,0\H,19,B19,8,A18,6,D17,0\H,19,B2
0,8,A19,20,D18,0\H,19,B21,8,A20,20,D19,0\H,12,B22,11,A21,9,D20,0\H,12,
B23,11,A22,23,D21,0\H,12,B24,11,A23,23,D22,0\\B1=1.43215648\B2=1.36213
814\B3=1.22552789\B4=1.44965597\B5=1.48808727\B6=1.08459979\B7=1.54970
192\B8=1.52318039\B9=1.21364679\B10=1.35133874\B11=1.43774884\B12=1.09
079268\B13=1.09411131\B14=1.09410839\B15=1.09412117\B16=1.09860779\B17
=1.09638314\B18=1.54243964\B19=1.09483985\B20=1.09614224\B21=1.0938573
1\B22=1.09031039\B23=1.09326478\B24=1.09314528\A1=115.07421848\A2=123.
01013515\A3=111.72639223\A4=121.07376518\A5=118.70668596\A6=113.981298
68\A7=111.01460985\A8=125.65367944\A9=111.05444086\A10=115.50451619\A1
1=105.64756498\A12=110.80652137\A13=110.79360158\A14=108.99203585\A15=
109.2401226\A16=109.3482094\A17=111.15330401\A18=110.09022621\A19=110.
82467448\A20=110.89000898\A21=105.54986883\A22=110.58998859\A23=110.52
30262\D1=-0.3767865\D2=179.9971432\D3=-179.95826763\D4=181.17307182\D5
=250.80821724\D6=-63.11112908\D7=-18.39470682\D8=181.46715167\D9=-182.
1546828\D10=180.06846671\D11=-119.68805427\D12=119.6664507\D13=121.198
96656\D14=-120.27868541\D15=118.39667216\D16=-122.20119908\D17=-59.070
66858\D18=119.54075166\D19=-119.96052666\D20=179.74036187\D21=119.6682
8691\D22=-119.63463745\\Version=DEC-AXP-OSF/1-G03RevB.03\State=2-A\HF=
-613.5484511\S2=0.756635\S2-1=0.\S2A=0.750028\RMSD=5.782e-09\RMSF=2.68
0e-05\Dipole=-0.180574,-0.6554378,0.3929149\PG=C01 [X(C8H13O4)]\\@

**$P(CH_3)_2(CH_2)_4P{\bullet}CH_3$ (structure 5)**

**Starting conformation**

1\1\GINC-LC5\FOpt\UB3LYP\6-31G(d)\C7H17P2(2)\MLC501\27-Jan-2005\0\\# B
3LYP/6-31G* OPT MAXDISK=402653184\\PMe2-4CPMe-a1b1c1d1e1-6drb3\\0,2\H,
-1.5946812678,-1.8238835915,-3.7111008078\C,-1.8201340006,-1.893058752
2,-2.6390029068\P,-0.2953590349,-2.3345448931,-1.6527627595\H,-2.25035
91419,-0.9344801862,-2.3236187341\H,-2.5793942788,-2.6678470663,-2.495
8251102\C,0.8483058767,-0.9481936013,-2.2037366145\C,0.4832666412,0.51
75695569,-1.8715350203\H,0.9480294444,-1.0428007735,-3.2953197885\H,1.
83794859,-1.1755524575,-1.7859420524\C,0.6720957776,0.9475655643,-0.40
30238107\H,1.1262946973,1.1576824746,-2.4921797036\H,-0.5458780556,0.7
332113478,-2.1894666624\C,-0.3934751291,0.4257108136,0.5712539455\H,0.
6721943941,2.0448942006,-0.3776067268\H,1.6716418431,0.6350642235,-0.0
7174874\P,-0.3187655635,0.9257990378,2.3834456726\H,-1.3913647525,0.72
80295086,0.2221505823\H,-0.4058744319,-0.6727763223,0.5771956313\C,-0.

1131024491,2.7799103327,2.2684954454\C,1.4297503946,0.444701279,2.8342
765245\H,1.622360342,0.7473064329,3.8693614686\H,1.532540468,-0.644922
5367,2.7857766329\H,2.1944642685,0.8993119866,2.1941547171\H,-0.000536
2608,3.1825089192,3.2811477511\H,0.7517528921,3.0961585011,1.674408053
9\H,-1.0175124418,3.2240520119,1.8380044135\\Version=x86-Linux-G03RevB
.03\State=2-A\HF=-959.6596427\S2=0.753991\S2-1=0.\S2A=0.750006\RMSD=7.
778e-09\RMSF=1.609e-06\Dipole=0.3107694,0.6767127,-0.6733323\PG=C01 [X
(C7H17P2)]\\@

**Global minimum**

1\1\GINC-SC8\FOpt\UB3LYP\6-31G(d)\C7H17P2(2)\MLC501\29-Jan-2005\0\\# B
3LYP/6-31G* OPT MAXDISK=268435456\\PMe2-4CPMe-a3b3c3d1e3-6drb3\\0,2\H,
-3.8177744643,-3.4153351557,-0.9273822713\C,-4.0545647094,-3.170340275
1,0.1159425807\P,-2.505607414,-2.8149007539,1.0987736089\H,-4.73125406
29,-2.3062227191,0.1119367389\H,-4.5849644113,-4.0198791547,0.55660393
78\C,-1.8673095703,-1.3647250803,0.0950157419\C,-0.5533681599,-0.78887
74803,0.6427575373\H,-2.6416654999,-0.5830706609,0.0711793716\H,-1.732
3114611,-1.6904247194,-0.9476759965\C,-0.0283746391,0.396710816,-0.181
647651\H,-0.6992988009,-0.4691100237,1.6839697173\H,0.2096761881,-1.57
92464182,0.6714115287\C,1.2825650821,0.976649473,0.3698656214\H,-0.792
1093631,1.186190113,-0.2113367117\H,0.1157438716,0.0718474248,-1.22189
00875\P,1.8879245184,2.4862174775,-0.5670708053\H,1.1299781495,1.29526
82241,1.4105029501\H,2.0647431721,0.2033414039,0.3875069095\C,2.603195
4019,1.6668948402,-2.0865861647\C,3.4720785041,2.7956973498,0.37268885
69\H,4.0525205831,3.5731868184,-0.1357524817\H,3.2375601952,3.16180930
22,1.3780778227\H,4.095022108,1.89704872,0.4629903107\H,3.1591252946,2
.4084411738,-2.6706800828\H,3.2783319259,0.8372866117,-1.8408531678\H,
1.7965885532,1.2870603466,-2.722369677\\Version=DEC-AXP-OSF/1-G03RevB.
03\State=2-A\HF=-959.6662164\S2=0.754007\S2-1=0.\S2A=0.750006\RMSD=9.0
88e-09\RMSF=2.435e-06\Dipole=0.1215788,-0.108081,-0.41212\PG=C01 [X(C7
H17P2)]\\@

**TS[$CH_3CH(COOCH_2CH_3)CH_2CH(COOCH_2CH_3)\bullet + CH_2{=}CHCOOCH_2CH_3$] (structure 6)**

**Starting conformation**

1\1\GINC-LC5\FTS\UB3LYP\6-31G(d)\C15H25O6(2)\MLC501\03-Dec-2004\0\\# B
3LYP/6-31G* OPT=(TS,CALCFC,NOEIGENTEST,MAXCYC=300) MAXDISK=402653184\\
EAdim_TS-a1b1c1-6dub3\\0,2\C,-0.0856397469,-1.338200389,-0.027069278\C
,-0.0856730363,-1.3380251939,1.3398002099\C,1.1811813093,-1.337907011,
2.0891871799\O,2.2947359806,-1.4004002845,1.5928718989\O,0.9601835897,
-1.2714140439,3.4224855629\C,2.1402445889,-1.2398681343,4.25378339\H,0
.8472310851,-1.5204618554,-0.5509728975\H,-1.0045475388,-1.486699948,-
0.5838666464\H,-1.0041842102,-1.2817299274,1.9159822587\C,-0.026307536
4,0.8415880791,-0.7575748741\H,-0.0846545059,0.5136094586,-1.791807247
6\C,-1.1817532537,1.5917683395,-0.166067335\C,1.3155263551,1.167790008
7,-0.2550545388\O,1.532508045,1.7758610491,0.781514916\O,2.2858608999,
0.6851445329,-1.0657810202\C,3.6408634729,0.8386245391,-0.5809006988\H
,-1.0142551542,1.7060939551,0.9099943076\C,-2.5937355893,1.0053345183,
-0.4056290528\H,-1.1710213711,2.6138069727,-0.5816948367\C,-3.66561570
92,1.9057356331,0.226627509\C,-2.8517151537,0.8660621958,-1.8998889772
\H,-2.6438920671,0.008105188,0.0420398094\H,-4.6625380085,1.4622074577
,0.1307501357\H,-3.4593162871,2.0518647398,1.2921756139\H,-3.682569490
8,2.8829151494,-0.2648260246\O,-3.1159954331,1.7845625862,-2.645941990
5\O,-2.7233831657,-0.4173457403,-2.3155958014\C,-2.9256979827,-0.64775
80551,-3.7325231065\C,-2.750606553,-2.1329222568,-3.9857126306\H,-2.20
40483902,-0.045016562,-4.2929468991\H,-3.9271620811,-0.2983473994,-4.0

01959077\H,-2.9041390133,-2.3476918917,-5.0488281646\H,-1.7433864304,-
2.4633877434,-3.7117365209\H,-3.4746769583,-2.7172100711,-3.4088718942
\C,4.561600797,0.1930140681,-1.5990287636\H,3.7096294941,0.3582526236,
0.3983482494\H,3.8508005068,1.9063201511,-0.4571999981\H,5.6028719123,
0.2943410361,-1.2736180149\H,4.3373040403,-0.8733334221,-1.7035284947\
H,4.4600576609,0.6674446177,-2.5808666009\C,1.6798621548,-1.1645212546
,5.6974787564\H,2.7460003464,-0.3733557302,3.9692111851\H,2.7355520107
,-2.1379932234,4.0578834632\H,2.5489199385,-1.1360301224,6.3638675621\
H,1.0834673025,-0.2630091177,5.8704036167\H,1.0720731772,-2.0362496541
,5.9610718516\\Version=x86-Linux-G03RevB.03\State=2-A\HF=-1037.9665761
\S2=0.777947\S2-1=0.\S2A=0.750231\RMSD=9.306e-09\RMSF=2.600e-06\Dipole
=-0.4040511,-0.9185492,-0.0843034\PG=C01 [X(C15H25O6)]\\@

**Global minimum**

1\1\GINC-LC83\FTS\UB3LYP\6-31G(d)\C15H25O6(2)\MLC501\04-Jan-2005\0\\#
B3LYP/6-31G* OPT=(TS,CALCFC,NOEIGENTEST,MAXCYC=300) MAXDISK=402653184\
\EAdim_TS-a1b2c1d2-6dub3\\0,2\C,-1.4332964898,0.7601268772,2.4422861472
\C,-2.0458200391,-0.3627117041,1.9620953849\C,-2.8880535435,-0.2999455134,0.7563399174\O,-3.1497614288,0.714961385,0.1307144289\O,-3.356440015,-1.5249223762,0.424360384\C,-4.1779193939,-1.5833580922,-0.7614191824\H,-1.7194288802,1.7292422637,2.0464093087\H,-0.9362282585,0.7410242609,3.4069157118\H,-1.8886125176,-1.3392552809,2.4090480267\C,0.6179265285,0.9744892588,1.4330755083\H,0.828718463,1.90239808,1.959034027\C,1.3789915664,-0.2543233629,1.8275213892\C,0.1442653713,1.1136656166,0.0489089415\O,0.0906366003,0.1935369414,-0.755581672\O,-0.2660646408,2.37140167,-0.2130052752\C,-0.8494745671,2.5869970682,-1.5192011464\H,1.2626158798,-0.4327184966,2.9042882385\C,2.9123991297,-0.1643317918,1.5461979577\H,0.9734954662,-1.1202744443,1.2953091206\C,3.642781851,-1.3842377729,2.1259814083\C,3.1459153421,0.018952297,0.0513232576\H,3.2960405469,0.7501962819,2.0116115307\H,4.7200471755,-1.3264091621,1.9361118068\H,3.4940538194,-1.4347488465,3.2106927034\H,3.2713724408,-2.3122184671,1.6820665772\O,3.3532607469,1.0913746608,-0.478489226\O,3.0460541306,-1.1445075864,-0.6177838485\C,3.0574327709,-1.0491091793,-2.0624191812\C,2.8764660979,-2.4520956338,-2.6094606694\H,4.0044649414,-0.6004919385,-2.3790711915\H,2.2437900878,-0.3834458908,-2.3624089378\H,2.8772578926,-2.4264271097,-3.704802957\H,3.686210019,-3.1118210272,-2.280217599\H,1.9245214518,-2.8764746283,-2.2753861579\C,-1.2898729526,4.0370524037,-1.5827723349\H,-1.6889526,1.89729888,-1.6373350569\H,-0.0972256621,2.3527233015,-2.2796689485\H,-1.7317315785,4.2477666103,-2.5630033984\H,-2.0414107364,4.2470100537,-0.8150928969\H,-0.4414607478,4.7131750145,-1.434479542\C,-4.5964574767,-3.0286602836,-0.9559606426\H,-3.5969396046,-1.2054650851,-1.6090728958\H,-5.0387933103,-0.9195304258,-0.6288799822\H,-5.2231347926,-3.1173191063,-1.8501430508\H,-3.7217782766,-3.6746124454,-1.0825938382\H,-5.1700795351,-3.3894410743,-0.096029459\\Version=x86-Linux-G03RevB.03\State=2-A\HF=-1037.9670775\S2=0.777812\S2-1=0.\S2A=0.750229\RMSD=8.483e-09\RMSF=1.127e-06\Dipole=-0.2619806,-0.7332023,0.4919168\PG=C01 [X(C15H25O6)]\\@

**TS[$CH_3CH(COOCH_3)CH_2CH(COOCH_3)$• + $CH_2$=$CHCOOCH_3$] (structure 7)**

**Starting conformation**

1\1\GINC-LC114\FTS\UB3LYP\6-31G(d)\C12H19O6(2)\MLC501\15-Dec-2004\0\\#
B3LYP/6-31G* OPT=(TS,CALCFC,NOEIGENTEST,MAXCYC=300) MAXDISK=402653184
\\MAdim_TS-a1b1c1d1-6dub3\\0,2\C,0.,0.,0.\C,0.0445657693,-1.274949654,
-0.4913501789\C,-0.887932737,-1.7034146855,-1.5456130683\O,-1.7882811005,-1.0258476105,-2.0133451335\O,-0.6309353267,-2.9739486871,-1.9383349603\C,-1.4743430399,-3.4706294278,-2.9870166237\H,-1.139261391,-4.491379097,-3.1743972923\H,-0.8421021076,0.633014066,-0.2607903695\H,0.579

0259791,0.280194606,0.8733807808\H,0.7940045414,-1.9913200861,-0.16908
32192\H,-2.5229542597,-3.4611342263,-2.6765417077\H,-1.364992154,-2.85
88124022,-3.8866704918\C,1.3587194902,1.3274832597,-1.2957985398\H,1.1
730030449,2.1811049385,-0.6496596014\C,2.7348424485,0.7337782129,-1.33
81113014\C,0.5572367419,1.2599191541,-2.5248434704\O,0.796804321,0.521
2198392,-3.4665414354\O,-0.5058340655,2.0983512005,-2.475626622\C,-1.4
217591433,1.9871187361,-3.5786792745\H,-2.1921209831,2.7364637527,-3.3
920044077\H,2.7026580648,-0.1902256648,-1.9245406826\C,3.4165946289,0.
4532728232,0.0227134755\H,3.3855664027,1.4250932237,-1.8999369003\H,-1
.8539156048,0.9843466844,-3.6000985394\H,-0.9111241787,2.1897776394,-4
.5239695249\C,4.8324627721,-0.1040914387,-0.1888456602\C,3.4837654754,
1.7331421618,0.843520345\H,2.8154456802,-0.2738822314,0.5766975874\H,5
.2991473401,-0.3744861732,0.764450879\H,4.7979296737,-1.0003994232,-0.
8170317529\H,5.4672696627,0.6416689302,-0.676455468\O,4.2498158828,2.6
5030038,0.6419850549\O,2.5539871212,1.7469381783,1.8310684986\C,2.5335
840995,2.9363616189,2.6422550482\H,1.7405976612,2.7780418422,3.3734034
503\H,3.4963376608,3.073629892,3.1408809984\H,2.323326055,3.8163658134
,2.0288970297\\Version=x86-Linux-G03RevB.03\State=2-A\HF=-920.0095154\
S2=0.778036\S2-1=0.\S2A=0.750233\RMSD=5.411e-09\RMSF=3.271e-06\Dipole=
-0.4573063,-0.796047,-0.0889792\Polar=156.9615891,-8.1534492,134.29661
99,16.3456948,-11.5309102,167.1749049\PG=C01 [X(C12H19O6)]\\@

**Global minimum**

1\1\GINC-LC121\FTS\UB3LYP\6-31G(d)\C12H19O6(2)\MLC501\15-Dec-2004\0\\#
B3LYP/6-31G* OPT=(TS,CALCFC,NOEIGENTEST,MAXCYC=300) MAXDISK=402653184
\\MAdim_TS-a1b2c2d2-6dub3\\0,2\C,-0.4753889437,-2.2219021415,-0.005245
3829\C,-0.567849465,-2.3079320372,1.3558118404\C,0.6283463391,-2.55756
41346,2.1741968959\O,1.7540484924,-2.751660905,1.7449050894\O,0.325204
9155,-2.5579681182,3.4944878679\C,1.436634929,-2.7679719793,4.37596058
39\H,1.0196960795,-2.7491641791,5.3835292125\H,0.4451931525,-2.5270514
854,-0.4926148062\H,-1.3720955256,-2.1819028408,-0.6151492915\H,-1.502
2045835,-2.1347072439,1.8801565522\H,1.9129940268,-3.731718985,4.17504
27571\H,2.177753107,-1.973385259,4.2524547011\C,-0.0651831681,-0.04709
33523,-0.5751018833\H,-0.0578471659,-0.3037001473,-1.6292260434\C,-1.2
343276709,0.7270650201,-0.0427719264\C,1.2383826786,0.0879047641,0.085
1792911\O,1.413399246,0.5787638896,1.1907411144\O,2.2356604843,-0.4324
839985,-0.670089457\C,3.524461895,-0.4777134461,-0.0353666744\H,4.2016
933829,-0.8914073268,-0.7837819418\H,-2.1529104337,0.144371887,-0.1744
123545\C,-1.4529756261,2.1059780655,-0.7175300647\H,-1.0852006361,0.89
04959465,1.0287530666\H,3.4802913726,-1.123482705,0.8442695194\H,3.844
8181625,0.5257387855,0.2583496161\C,-0.2180349918,3.026903761,-0.66121
22402\C,-1.9568449415,1.9398059098,-2.1467622612\H,-2.2641859776,2.608
6496817,-0.1715096988\H,-0.4670058537,4.030003763,-1.0165171768\H,0.15
17123671,3.0931139673,0.3661604481\H,0.5970061948,2.6387067609,-1.2819
354981\O,-2.0883566508,0.8864303717,-2.7367601031\O,-2.2626795244,3.13
46599823,-2.6991074873\C,-2.7477743817,3.0862810711,-4.0513618073\H,-2
.9359121341,4.1230862767,-4.3315000291\H,-2.0004460249,2.6386636355,-4
.7117874682\H,-3.6682451315,2.4991906894,-4.1084759851\\Version=x86-Li
nux-G03RevB.03\State=2-A\HF=-920.0101389\S2=0.777779\S2-1=0.\S2A=0.750
232\RMSD=7.468e-09\RMSF=4.032e-06\Dipole=-0.5555045,0.5425765,-0.25951
84\PG=C01 [X(C12H19O6)]\\@

**$CH_3O$-C(=O)-$CH_2$-SC•($OC_2H_5$)-$SCH_3$ (structure 8)**

**Starting conformation**

1\1\GINC-SC53\FOpt\UHF\6-31G(d)\C7H13O3S2(2)\MLC501\30-Apr-2003\0\\#P
HF/6-31G* OPT=TIGHT FREQ MAXDISK=131072000\\RRAD(Z=Oet,R=VA) a1b1c1d1e

1f1\\0,2\S,1.2728779393,0.653954648,-1.3733763784\C,1.031215222,0.7454
960031,0.3770358391\S,2.5038986753,0.8636793096,1.3555546731\C,2.93038
3908,-0.8937573426,1.5662364063\C,-0.4199219569,0.7134234469,-1.989163
4418\O,-0.0214458514,0.0469603568,0.8570873022\C,-0.7393009275,0.64415
22267,1.9325363052\O,-1.0118643251,-0.566033558,-2.0172480395\C,-2.187
2769825,-0.7516357082,-1.4228481472\O,-2.8351178134,0.118471879,-0.938
3241405\C,-2.5758757084,-2.2029637715,-1.4543144338\H,-1.0162712815,1.
3912435553,-1.4060398884\H,-0.3537957453,1.0660506176,-3.0074970796\H,
2.1089208812,-1.4314494311,2.0170678768\H,3.7876347386,-0.9298055218,2
.2257176043\H,3.1892890073,-1.3438893125,0.6182014584\H,-1.8747150175,
-2.768905875,-0.85139147\H,-2.5209539144,-2.5814909253,-2.467648992\H,
-3.5759930478,-2.3194843245,-1.0641467236\C,-1.7140487726,-0.379382504
8,2.4747160089\H,-1.2600360053,1.518244189,1.5600109947\H,-0.041153074
6,0.9587590977,2.6973511938\H,-2.2595761453,0.0424318389,3.312851868\H
,-2.4276998992,-0.6680722385,1.7141165405\H,-1.187701103,-1.2629585123
,2.8192417042\\Version=DEC-AXP-OSF/1-G98RevA.11.3\HF=-1292.2138899\S2=
0.767095\S2-1=0.\S2A=0.750239\RMSD=3.125e-09\RMSF=3.016e-08\Dipole=-0.
2107101,-0.7708179,0.2222467\PG=C01 [X(C7H13O3S2)]\\@

**Global minimum**

1\1\GINC-SC103\FOpt\UHF\6-31G(d)\C7H13O3S2(2)\MLC501\01-May-2003\0\\#P
HF/6-31G* OPT=TIGHT FREQ MAXDISK=131072000\\RAFT(Z=Oet,R=VA) a1b1c1d3
e2f1\\0,2\S,0.7977889948,-1.0211898928,-1.1555418443\C,0.755124444,-0.
3879745486,0.5005922794\S,2.3128296538,-0.3361719558,1.3450880384\C,2.
3913617119,-2.0118970451,2.0531145927\C,-0.86920653,-0.6719211727,-1.7
581606445\O,-0.358387466,-0.7007550831,1.1920672997\C,-0.7854293423,0.
2277033141,2.1838377616\O,-0.9604421108,0.5318857775,-2.4919169643\C,-
1.2772513629,1.6547740544,-1.8546562032\O,-1.5361028996,1.7062810375,-
0.6964594645\C,-1.2670703432,2.8291846021,-2.7922570069\H,-1.110537072
2,-1.4511417965,-2.4621219147\H,-1.5615321586,-0.6765686339,-0.9357628
175\H,1.5245876583,-2.2059539787,2.6683788468\H,3.2819970228,-2.049979
6208,2.6667189912\H,2.4625936871,-2.7579969528,1.2741281858\H,-1.91980
855,2.634991117,-3.6348750517\H,-0.263992117,2.9710487038,-3.178008414
3\H,-1.5888146889,3.7153766518,-2.2661194588\C,-2.1686960072,-0.192192
6462,2.6334295297\H,-0.7986847115,1.2193798081,1.7559203289\H,-0.08503
17364,0.2123246783,3.0100713731\H,-2.5202274452,0.4710418444,3.4173692
172\H,-2.8670447841,-0.1448282687,1.8061857543\H,-2.1569390924,-1.2052
571779,3.0204470348\\Version=DEC-AXP-OSF/1-G98RevA.11.3\HF=-1292.21519
75\S2=0.767081\S2-1=0.\S2A=0.750239\RMSD=8.445e-09\RMSF=3.346e-08\Dipo
le=-0.5851001,-0.0898349,-0.0851187\PG=C01 [X(C7H13O3S2)]\\@

**$CH_3O$-C(=O)-$CH_2$-SC•($OC(CH_3)_3$)-$SCH_3$ (structure 9)**

**Starting conformation**

1\1\GINC-AC47\FOpt\UHF\6-31G(d)\C9H17O3S2(2)\EXI501\23-Aug-2006\0\\#P
gfinput HF/6-31G* opt maxdisk=1342177280\\opt\\0,2\C,0.,0.,0.\S,0.,0.,
1.820055\C,1.7369329564,0.,2.1732485878\O,2.533363722,1.005209711,1.76
09675136\C,2.5536345611,2.2924424729,2.424988452\C,1.51435282,3.212406
8053,1.7860405149\S,2.4781230655,-1.6163108179,2.1605547689\C,4.223117
5906,-1.2527535882,2.3711488032\O,4.8234536922,-0.990005474,1.11851867
54\C,6.0086874504,-0.3911676659,1.1251649725\C,6.506320102,-0.15570670
96,-0.2736962546\C,3.958539786,2.819022152,2.1474237712\C,2.3180778898
,2.1462453632,3.9263175267\O,6.5858617816,-0.0880702985,2.1192078324\H
,4.3640231176,-0.4197634074,3.0349774847\H,4.6766956296,-2.1319048502,
2.8052561205\H,0.5127673913,0.8717235361,-0.380081689\H,-1.0357658252,
0.0281174536,-0.3126537588\H,0.4653036718,-0.8975850943,-0.3821545659\
H,5.7974752945,0.4630565723,-0.8112943469\H,6.5821298485,-1.1007592225
,-0.7986614972\H,7.4712117581,0.3275343548,-0.2379024288\H,4.074285629

8,3.8181048185,2.5538739282\H,4.7115536169,2.1793691716,2.5917072291\H
,4.1364941953,2.8637574277,1.0786496135\H,2.4458266029,3.1109096567,4.
405579817\H,1.3171469689,1.7951979854,4.1459989616\H,3.0293129008,1.45
64465944,4.3674344443\H,1.6140847402,4.2158861621,2.1875617484\H,1.667
9678468,3.2615755813,0.7134823296\H,0.5062270081,2.8702131107,1.975511
6735\\Version=IA64L-G03RevD.01\State=2-A\HF=-1370.282809\S2=0.766902\S
2-1=0.\S2A=0.750231\RMSD=6.000e-09\RMSF=8.821e-07\Thermal=0.\Dipole=0.
1264246,0.4477161,0.8831198\PG=C01 [X(C9H17O3S2)]\\@

**Global minimum**

1\1\GINC-AC1\FOpt\UHF\6-31G(d)\C9H17O3S2(2)\EXI501\23-Aug-2006\0\\#P g
finput HF/6-31G* opt maxdisk=1342177280\\opt\\0,2\C,0.,0.,0.\S,0.,0.,1
.819218\C,1.7447612219,0.,2.1472227776\O,2.4595272839,1.0298141043,1.6
466167253\C,2.9251781405,2.092945293,2.5063730506\C,1.7389199501,2.850
752005,3.0979260419\S,2.6960849242,-1.5067343392,2.1416772657\C,1.7335
348776,-2.5653260096,3.2375674665\O,1.8436004281,-2.2051498339,4.59734
60735\C,2.8420310446,-2.7320207252,5.3088281605\C,2.8353072933,-2.2097
210982,6.7181659565\C,3.7203439773,2.9846537142,1.560415575\C,3.823003
5648,1.5328110939,3.6068883433\O,3.6186545387,-3.5136360477,4.87029783
24\H,0.6873781832,-2.4940484542,2.9960398072\H,2.0900964016,-3.5699807
171,3.0852269263\H,0.5324371557,0.8626279431,-0.372652799\H,-1.0344290
839,0.0498138637,-0.3140950459\H,0.4481285396,-0.9060423031,-0.3837073
412\H,1.8699218816,-2.3923815083,7.1748857008\H,2.9975232901,-1.137903
6513,6.7078979433\H,3.6152589767,-2.694273799,7.2860777944\H,4.1292275
707,3.8357016234,2.094600073\H,4.5382079239,2.4293608798,1.1161901911\
H,3.0844330958,3.3515373809,0.7628159763\H,4.2286898009,2.3473598458,4
.1981535628\H,3.2707849622,0.8787070089,4.2717521178\H,4.6466533418,0.
9704025874,3.1840257483\H,2.0951822702,3.7060964827,3.6630673136\H,1.0
810544431,3.2059133438,2.3137936378\H,1.1602161985,2.2254097197,3.7674
220844\\Version=IA64L-G03RevD.01\State=2-A\HF=-1370.2854298\S2=0.76721
9\S2-1=0.\S2A=0.750239\RMSD=6.045e-09\RMSF=9.066e-07\Thermal=0.\Dipole
=0.5652566,-0.2152264,0.8445164\PG=C01 [X(C9H17O3S2)]\\@

**$P(CH_3)_2(CH_2)_3P{\bullet}CH_3$ (structure 10)**

**Starting conformation**

1\1\GINC-LC146\FOpt\UB3LYP\6-31G(d)\C6H15P2(2)\MLC501\25-Jan-2005\0\\#
B3LYP/6-31G* OPT MAXDISK=402653184\\Me2P-3CPMe-a1b1c1d1-6drb3\\0,2\H,
-2.6863434734,-0.9003781925,0.4781322877\C,-2.8640138659,-0.7942567215
,1.5555348435\P,-1.2716433838,-0.5566073031,2.5056358297\H,-3.36336354
75,-1.7024737871,1.9063935984\H,-3.5454987984,0.0537145693,1.701587935
6\C,-0.7422598732,1.1077386032,1.8094560909\C,-0.3642503511,1.15121117
01,0.3129972066\H,0.1145190846,1.4396893656,2.4099788952\H,-1.55403348
45,1.825313995,1.9988334547\C,0.8677616402,0.3041297468,-0.0393355957\
H,-0.1719482809,2.1965178619,0.0347971632\H,-1.223928607,0.8320870339,
-0.2904038839\P,1.4021210262,0.4815816404,-1.8292678671\H,1.7184036342
,0.6291420779,0.575889263\H,0.6920110065,-0.7542523172,0.2017902873\C,
2.8322800779,-0.7191496438,-1.8244264421\C,0.1188712812,-0.5889772644,
-2.665728401\H,3.6609354275,-0.300533099,-1.2431273628\H,3.1883445219,
-0.867505142,-2.8496230029\H,2.5655172321,-1.6955614626,-1.4014553574\
H,-0.8548662299,-0.0880817708,-2.6501084237\H,0.3959669828,-0.73219832
21,-3.7158317981\H,0.0167864408,-1.5742712115,-2.193358709\\Version=x8
6-Linux-G03RevB.03\State=2-A\HF=-920.3506376\S2=0.753984\S2-1=0.\S2A=0
.750006\RMSD=7.419e-09\RMSF=2.729e-06\Dipole=-0.2843139,-0.1148219,-0.
2702577\PG=C01 [X(C6H15P2)]\\@

**Global minimum**

1\1\GINC-LC143\FOpt\UB3LYP\6-31G(d)\C6H15P2(2)\MLC501\27-Jan-2005\0\\#
 B3LYP/6-31G* OPT MAXDISK=402653184\\Me2P-3CPMe-a3b3c1d3-6drb3\\0,2\H,
-3.2098042506,-2.9143763995,-1.6014413908\C,-3.5214892919,-2.770111660
1,-0.5590107499\P,-2.056746953,-2.4152191952,0.5454899553\H,-4.0259152
633,-3.6806787869,-0.2219714253\H,-4.2464908333,-1.9464233616,-0.53672
59396\C,-1.446050442,-0.854952963,-0.2999346948\C,-0.2021555935,-0.257
2702529,0.3761253213\H,-2.2613026813,-0.1157608475,-0.3121761866\H,-1.
2297672856,-1.0871884914,-1.3538051519\C,0.3047183032,1.0104755041,-0.
3291816743\H,0.5931085073,-1.0143143105,0.3972926072\H,-0.4300160084,-
0.024859681,1.4245466254\P,1.7783793705,1.8033456339,0.5235934817\H,0.
5493653376,0.7902405388,-1.3790322769\H,-0.4939976235,1.7652627226,-0.
3419337214\C,3.134348937,0.6350103574,-0.0116948431\C,2.0941000039,3.1
939317408,-0.682866315\H,3.0350059089,-0.3202443731,0.5141188367\H,4.1
066158159,1.0595371138,0.261431499\H,3.126739712,0.4448081651,-1.09255
14002\H,1.2903105271,3.9344750439,-0.6090753501\H,3.0320406966,3.69668
14616,-0.4232753728\H,2.1587896774,2.8484482677,-1.7222751713\\Version
=x86-Linux-G03RevB.03\State=2-A\HF=-920.3522732\S2=0.75401\S2-1=0.\S2A
=0.750006\RMSD=3.449e-09\RMSF=4.116e-06\Dipole=-0.1518408,0.195648,-0.
9720945\PG=C01 [X(C6H15P2)]\\@

**$P(CH_3)_2(CH_2)_4P^-(CH_3)$ (structure 11)**

**Starting conformation**

1\1\GINC-SC84\FOpt\RB3LYP\6-31+G(d)\C7H17P2(1-)\MLC501\05-Feb-2005\0\\
# B3LYP/6-31+G* OPT MAXDISK=402653184\\PMe2-4CPMe--a1b1c1d1e1-6+drb3\\
-1,1\H,0.,0.,0.\C,-1.0802184736,0.2093766277,-0.098691158\P,-1.7187329
067,1.4087162885,1.241553576\H,-1.2522470174,0.5438376187,-1.136139188
6\H,-1.6088565222,-0.7476760834,0.0199004913\C,-0.4846447357,2.8218220
378,0.9041617921\C,-0.5729813582,3.6338267625,-0.4136455293\H,0.551146
1077,2.4388415123,0.9767584176\H,-0.6017184919,3.5277318613,1.74344453
64\C,-1.9122921061,4.3735528609,-0.6516067619\H,0.2434652853,4.3799936
387,-0.4200264323\H,-0.3710608002,2.9684695646,-1.2671985351\C,-2.9147
021566,3.55679109,-1.4816292196\H,-1.7155083799,5.3327464013,-1.153596
8409\H,-2.3529446366,4.6097219373,0.3271477616\P,-4.6462930169,4.21193
74203,-1.7531589502\H,-2.4969147615,3.3561402905,-2.4802040748\H,-3.04
15808658,2.5828771996,-0.9820743185\C,-4.360072983,6.0247262514,-2.144
5692928\C,-5.2548765128,4.3748905418,0.006675824\H,-6.3013903927,4.705
3517057,0.0058879823\H,-5.1956415289,3.3937367975,0.4910826976\H,-4.66
32975462,5.0791727488,0.604163179\H,-5.329894931,6.5324551997,-2.22459
6891\H,-3.7588283734,6.5389679018,-1.3843665012\H,-3.8532066595,6.1197
260843,-3.1129018958\\Version=DEC-AXP-OSF/1-G03RevB.03\State=1-A\HF=-9
59.7002302\RMSD=2.419e-09\RMSF=5.613e-06\Dipole=-0.0084479,3.3373783,1
.7365874\PG=C01 [X(C7H17P2)]\\@

**Global minimum**

1\1\GINC-SC15\FOpt\RB3LYP\6-31+G(d)\C7H17P2(1-)\MLC501\12-Feb-2005\0\\
# B3LYP/6-31+G* OPT MAXDISK=268435456\\PMe2-4CPMe--a2b2c3d1e2-6+drb3\\
-1,1\H,-3.2027245282,0.3127432701,2.082797818\C,-3.9358041872,0.541019
7171,1.2922258187\P,-3.1767702728,0.7954177214,-0.4435424792\H,-4.6976
555412,-0.2586458409,1.3095410113\H,-4.4381807932,1.4753159978,1.58306
30881\C,-2.4921339701,-0.9727564687,-0.6535704208\C,-1.1722030382,-1.3
144639203,0.0804788248\H,-2.3415748322,-1.1399960535,-1.7331447322\H,-
3.2599152067,-1.7026273253,-0.3402990216\C,0.0493479618,-0.6049755282,
-0.5207784708\H,-1.2675334206,-1.0290729869,1.1391233394\H,-0.99157603
83,-2.4071813348,0.0654158565\C,1.3323548206,-0.7846757396,0.306031203
6\H,-0.2069658333,0.4596571192,-0.6036640308\H,0.2158510354,-0.9780024

7,-1.5440627271\P,2.8532194541,-0.0245417369,-0.4786028642\H,1.1899910
711,-0.3620185507,1.3130409589\H,1.5498928456,-1.8558149736,0.43844787
\C,4.0740328536,-0.2611605086,0.9237853681\C,2.4879458419,1.7919631184
,-0.240885259\H,3.3711420633,2.3844783484,-0.5105400324\H,1.6644319989
,2.0927403783,-0.8966873091\H,2.2016296511,2.0286639755,0.7926231059\H
,5.0071738783,0.2708146178,0.7007412614\H,3.6836556994,0.1023491063,1.
8845716131\H,4.3143785371,-1.326247064,1.027489693\\Version=DEC-AXP-OS
F/1-G03RevB.03\State=1-A\HF=-959.7044582\RMSD=4.606e-09\RMSF=4.190e-06
\Dipole=4.6757914,-1.1302574,1.1690995\PG=C01 [X(C7H17P2)]\\@

**S=C(Ph)-SCH(Ph)-$CH_2$-CH(Ph)-$CH_2$-C$(CH_3)_2$Ph (structure 12)**

**Starting conformation**

1\1\GINC-AC1\FOpt\RB3LYP\6-31G(d)\C27H27N1S2\EXI501\23-Aug-2006\0\\#P
gfinput B3LYP/6-31G(d) INT(grid=ultrafine) opt maxdisk=1342177280\\opt
\\0,1\C,-0.0000644825,0.0000834907,-0.0000438069\C,0.000000841,0.00024
55206,1.4080403026\C,1.2312942853,0.0004840464,2.0896306856\C,2.428851
583,-0.0169270886,1.3827801387\C,2.4206882626,-0.0146488866,-0.0153758
948\C,1.2057925163,0.0018924405,-0.7006507033\C,-1.2681160519,0.019129
3919,2.1896139193\S,-1.4416684983,0.9273988104,3.5626815788\S,-2.45378
74903,-1.0606243913,1.4627420797\C,-4.130193869,-0.9171623792,2.298749
4981\C,-4.2122477567,-1.7135064422,3.591737284\C,-4.0702806423,-1.1330
67528,4.8595998864\C,-4.1790200939,-1.9124713412,6.0128504506\C,-4.428
5547084,-3.281765862,5.9217880065\C,-4.5723196435,-3.871398646,4.66447
07437\C,-4.4675764482,-3.091545863,3.514428514\C,-4.728074215,0.500489
5389,2.368410947\C,-4.748191387,1.3326497553,1.05624772\C,-5.626735514
1,0.6757589347,-0.0356887272\C,-5.4051705658,1.1154758206,-1.517042774
5\C,-5.7925111578,2.5888501903,-1.7852652346\C,-5.1513535358,2.7625642
155,1.4066820873\C,-4.1906835788,3.7834663881,1.4066778814\C,-4.527816
3616,5.0901573287,1.7647811874\C,-5.8366601543,5.3996608213,2.13607101
96\C,-6.8020278028,4.3911700253,2.1513458721\C,-6.4606640347,3.0867956
49,1.792162919\C,-6.2460497119,0.1935204876,-2.4345076073\C,-3.9810197
769,0.9306488407,-1.8670120613\N,-2.8627783625,0.7826522999,-2.1441915
749\H,-3.7189594815,1.366485252,0.6805782971\H,-6.6892894053,0.8320371
493,0.1892924359\H,-5.4677493529,-0.4081218175,-0.0108649349\H,-5.7556
577576,0.3817772424,2.7403527939\H,-4.1929020213,1.0843421201,3.118358
6143\H,-5.1749184391,3.2864167306,-1.2175179697\H,-4.5835438203,-3.559
2819415,2.5387104585\H,-4.7710099031,-4.9363881931,4.5782708921\H,-4.5
119573138,-3.8846483199,6.8220916256\H,-4.0642841823,-1.4433192954,6.9
864107106\H,-3.8597490931,-0.0744463444,4.9503255634\H,-3.1662747308,3
.5504097961,1.1257191731\H,-3.7651925108,5.8643808672,1.7543475903\H,-
6.102139252,6.4159495207,2.4143987702\H,-7.8234378444,4.6189258391,2.4
455007022\H,-7.2264599945,2.3148241776,1.8185279427\H,-5.9733973262,-0
.8583075878,-2.3020120633\H,-7.3081472738,0.3094282908,-2.1914699997\H
,-6.1045927237,0.4547485859,-3.4878288698\H,-6.8374555548,2.7485854038
,-1.4988972769\H,-5.6868589354,2.8194415932,-2.8504706548\H,1.23104862
11,0.0041659259,3.1744230157\H,3.3715178002,-0.0318810464,1.9230757562
\H,3.357938973,-0.020081691,-0.5655907364\H,1.1886258411,0.0245884111,
-1.7865830013\H,-0.9342184294,0.0454213577,-0.550969488\H,-4.691405236
2,-1.4907413855,1.5514432478\\Version=IA64L-G03RevD.01\State=1-A\HF=-1
896.2498879\RMSD=8.436e-09\RMSF=1.255e-06\Thermal=0.\Dipole=-1.5030276
,-0.1217073,-0.2792084\PG=C01 [X(C27H27N1S2)]\\@

**Global minimum**

1\1\GINC-AC1\FOpt\RB3LYP\6-31G(d)\C27H27N1S2\EXI501\15-Jan-2006\0\\#P
gfinput B3LYP/6-31G(d) INT(grid=ultrafine) opt maxdisk=536870912\\opt\
\0,1\S,-0.2921730838,0.0423992429,-0.0082419923\C,0.0229190832,0.03958
74437,1.6167486925\S,1.5886020761,-0.1051856697,2.4067935493\C,-1.0697

912519,0.1378501295,2.6278301275\C,3.0048882389,-0.0426978386,1.168956
9654\C,3.3191944087,-1.4216139109,0.6133460374\H,3.7923059151,0.192490
5826,1.8958191892\C,2.930001555,1.1421083148,0.1738206627\H,2.23623033
4,1.892399161,0.5630348984\H,2.5157597718,0.8160342354,-0.7828866337\C
,4.3019816526,1.8471793164,-0.0447525637\H,4.7054718064,2.0499465687,0
.9565433761\C,4.0698186998,3.1993351545,-0.7122106711\C,5.319236119,0.
9469704075,-0.7984593297\H,5.2849599576,1.1577791574,-1.8737162724\H,5
.0361389432,-0.1023470207,-0.6833111257\C,6.8095100914,1.0678234601,-0
.3587942284\C,7.387603625,2.4811268386,-0.5963581293\C,7.6481557795,0.
0230000735,-1.1328620643\N,6.9264477127,0.4913615799,2.2155402675\C,6.
8921927662,0.749187684,1.08284506\C,3.6731600147,3.2983562571,-2.05417
25306\C,3.4211614991,4.5394122694,-2.6395951673\C,3.5594828446,5.71069
87502,-1.8924413397\C,3.9460506711,5.6283584767,-0.5545216128\C,4.1944
038267,4.3837407566,0.02705707\C,2.6670109578,-1.9563771234,-0.5081602
257\C,2.9926576573,-3.2294627133,-0.9771289151\C,3.9743771919,-3.98977
89947,-0.3390650753\C,4.6318657146,-3.4668242202,0.7754214679\C,4.3055
187893,-2.1949680074,1.2468523877\C,-0.9200503037,0.8758972557,3.81690
38502\C,-1.9657621545,0.9601584274,4.7347403782\C,-3.17022878,0.299757
7752,4.4910075618\C,-3.3289473168,-0.4384394011,3.3149261206\C,-2.2941
117174,-0.5130210998,2.3883526193\H,4.4906628684,4.3301556791,1.072807
1775\H,6.8449204029,3.2456663817,-0.0359299988\H,4.8337840291,-1.79046
15654,2.1068839562\H,5.4012725877,-4.045662124,1.2793999573\H,4.225795
3402,-4.9804829092,-0.7083943407\H,2.473450433,-3.6283618229,-1.844714
6765\H,1.8909711941,-1.3816485923,-1.0013487678\H,4.0549496008,6.53211
79152,0.0393899077\H,3.365217315,6.6775168918,-2.3487651313\H,3.113607
6845,4.5906021451,-3.6808627229\H,3.5507238985,2.397396711,-2.65085056
55\H,7.2741530851,-0.9909399834,-0.9601211113\H,7.5915754082,0.2349882
484,-2.2062667539\H,8.69949498,0.0604393152,-0.8302686663\H,7.31508761
3,2.727317121,-1.6611471856\H,8.4416732661,2.5209844837,-0.3027118567\
H,-2.4145711842,-1.0814758967,1.4725973021\H,-4.2627904614,-0.95821920
14,3.1192360162\H,-3.9823741441,0.3621369569,5.210266686\H,-1.83841170
57,1.5488903715,5.6389396595\H,0.0044650572,1.4105974911,4.0070798765\
\Version=IA64L-G03RevD.01\State=1-A\HF=-1896.2479806\RMSD=3.912e-09\RM
SF=1.798e-06\Thermal=0.\Dipole=0.209248,0.3443612,-0.7287586\PG=C01 [X
(C27H27N1S2)]\\@

**$CN(CH_3)_2S$-C•(Ph)-SCH(Ph)-$CH_2$-CH(Ph)-$CH_2$-$C(CH_3)_2CN$ (structure 13)**

**Starting conformation**

1\1\GINC-AC4\FOpt\UB3LYP\6-31G(d)\C31H33N2S2(2)\EXI501\23-Aug-2006\0\\
#P gfinput B3LYP/6-31G(d) INT(grid=ultrafine) opt maxdisk=1342177280\\
opt\\0,2\C,-0.0003311419,-0.0002534958,-0.0000676164\C,-0.0001986238,-
0.0001474024,1.4190647744\C,1.2607406994,-0.0001265162,2.0686023176\C,
2.4452817293,-0.0148451355,1.3415212279\C,2.4214488329,-0.0297767226,-
0.0565495193\C,1.1884737784,-0.0193587098,-0.7186023293\C,-1.236395604
6,0.0080810366,2.1790323001\S,-2.6551251454,0.8477503468,1.5464105652\
C,-4.0252399292,-0.4415240869,1.2771773631\C,-4.3637943714,-1.12839497
62,2.529155524\N,-4.6767341943,-1.6928970402,3.4951450594\S,-1.3501765
243,-0.4156389184,3.8815701169\C,-0.5140597254,-2.0840985228,4.1342481
008\C,-0.8095913685,-2.4464579751,5.5787924002\C,0.2383227375,-2.55453
42585,6.5029125845\C,-0.0126597579,-2.9058008709,7.8306028257\C,-1.320
0807499,-3.1459507457,8.2545037139\C,-2.3734544937,-3.0285803808,7.344
6262826\C,-2.1244640404,-2.679689598,6.0168018393\C,-0.9743657611,-3.1
486826007,3.1183806756\C,-0.241427298,-4.4993370476,3.3187478745\C,-0.
7253157565,-5.6329782112,2.3759278568\C,-2.1819936611,-6.1787765868,2.
5138539276\C,-2.2595150458,-7.5341054639,1.7625905666\C,1.2750854476,-
4.3809320561,3.1728122264\C,2.1201298094,-4.8520701323,4.1875351946\C,

3.5088996914,-4.7954080299,4.0552538664\C,4.0801261424,-4.263204988,2.
8987429723\C,3.2515545552,-3.7885187733,1.8802990318\C,1.8640484647,-3
.8486824875,2.0161027811\C,-2.6013302446,-6.3834396977,3.9867746464\C,
-3.145625831,-5.2778610558,1.8497123978\N,-3.9204337192,-4.620281065,1
.2873670052\C,-5.2392978323,0.3924192271,0.8178081928\C,-3.6029241616,
-1.4574325822,0.2050495636\H,-0.0669478634,-6.4923106707,2.5551811014\
H,-0.5613378015,-5.3402376364,1.3312015503\H,0.5612573095,-1.931916629
3,4.0214211034\H,-0.9487846962,0.0110013582,-0.5255715792\H,1.15511791
7,-0.0253336009,-1.8050865514\H,3.3488757276,-0.0378662104,-0.62243250
57\H,3.3949089897,-0.00146926,1.86975877\H,1.2947108534,0.0565032854,3
.1515140488\H,-2.0554389485,-3.2894657833,3.2087456234\H,-0.7931777282
,-2.7750178748,2.1040913279\H,-0.4335045018,-4.8246960946,4.3474074196
\H,-2.9570758628,-2.5641260554,5.3270812389\H,-3.3962041244,-3.2001972
869,7.6694641765\H,-1.5184667392,-3.4162259734,9.2883302535\H,0.813326
1252,-2.9867602947,8.5324908274\H,1.2588037928,-2.3690976555,6.1768919
224\H,1.683113945,-5.2639960165,5.0944506669\H,4.1426279401,-5.1658519
688,4.8570274863\H,5.1606917107,-4.2164129216,2.7925971576\H,3.6828423
039,-3.3647095046,0.9774142203\H,1.2389150251,-3.4677917521,1.21271095
64\H,-3.5874624404,-6.855181008,4.041932626\H,-1.8785249,-7.0410470967
,4.4829722722\H,-2.6464437826,-5.4415041142,4.5394970467\H,-3.28111086
61,-7.9265464557,1.7666380163\H,-1.9364328852,-7.4279415879,0.72202137
6\H,-1.6060554218,-8.2620690412,2.2555969032\H,-6.0816891308,-0.274193
8007,0.6062450059\H,-5.5454179257,1.1090542248,1.5847189685\H,-4.98850
12541,0.937772831,-0.0975911985\H,-4.3780360211,-2.218017098,0.0715512
799\H,-3.4376974853,-0.9336956005,-0.7417869095\H,-2.6843260691,-1.974
2837305,0.4909688488\\Version=IA64L-G03RevD.01\State=2-A\HF=-2106.9999
643\S2=0.767796\S2-1=0.\S2A=0.750248\RMSD=4.564e-09\RMSF=1.011e-06\The
rmal=0.\Dipole=1.4233517,-1.3006602,-0.4548975\PG=C01 [X(C31H33N2S2)]\
\@

**Global minimum**

1\1\GINC-AC5\FOpt\UB3LYP\6-31G(d)\C31H33N2S2(2)\EXI501\23-Jan-2006\0\\
#P gfinput B3LYP/6-31G(d) INT(grid=ultrafine) opt maxdisk=671088640\\o
pt\\0,2\S,-0.0434518204,0.1838911464,0.3038936472\C,0.2695470027,0.094
0990081,2.0357870979\S,1.8794794276,-0.3113828257,2.6378397223\C,-0.81
55164123,0.3268823798,2.9700801709\C,2.2481666097,-2.0939260978,2.0831
090691\N,3.1639206922,-2.1009197871,-0.3821718235\C,1.0134352115,-2.99
66573536,2.2116011677\C,3.3914708931,-2.5532067846,3.011460382\C,2.738
5643574,-2.0835763462,0.6991511282\C,1.3789219914,1.1725926621,-0.4324
447692\C,1.1677476584,1.1284737547,-1.9347724019\H,2.2919938249,0.6274
345803,-0.1867645139\C,1.4311940591,2.5793346261,0.1844382774\H,0.4816
054246,3.0926228492,0.0105023189\H,1.535958499,2.4775672067,1.27117796
11\C,2.5989894231,3.4501555272,-0.3507980676\C,3.9587979509,2.85250805
2,-0.0039094703\H,2.5257030958,3.4644971342,-1.4436916615\C,2.49050756
97,4.9130219423,0.1703951332\H,3.4991806869,5.3316971194,0.2656619202\
H,2.0627941482,4.9104320277,1.1812313266\C,1.7000327219,5.942988191,-0
.6934981111\C,2.3611939965,6.1488023466,-2.0774466126\C,1.6634890262,7
.293515861,0.0643449987\N,-0.801260506,5.1975554959,-1.0810997694\C,0.
3033710979,5.5115048085,-0.9043104371\C,0.2039994708,1.929094157,-2.56
86530047\C,0.0316528065,1.868097162,-3.9521789912\C,0.8124568531,1.003
8006156,-4.722002538\C,1.7651357252,0.1960461296,-4.0988363177\C,1.940
1207208,0.2552993842,-2.7155655542\C,4.804805237,2.3710334203,-1.01133
82238\C,6.0565981703,1.8330432668,-0.7050719079\C,6.4869907708,1.77102
48216,0.6201636248\C,5.6542562564,2.2462634013,1.6355691887\C,4.403072
3289,2.7789941973,1.3255241083\C,-0.7520860545,-0.1152345642,4.3196970
075\C,-1.8007951361,0.1078441825,5.201784953\C,-2.9557472646,0.7774374
213,4.783389194\C,-3.0399206911,1.2266832919,3.4614677119\C,-1.9960689
58,1.0122373479,2.5711277859\H,0.1328072679,-0.6401376064,4.6609527022

\H,-1.7201169429,-0.2485007404,6.2256182873\H,-3.7741176515,0.9494614429,5.4768164005\H,-3.9248655412,1.7594210446,3.1233590756\H,-2.0710182
1,1.3872116389,1.5568629363\H,-0.4138160604,2.6085167786,-1.988979385\
H,-0.7167857719,2.4976681008,-4.4261654668\H,0.6763135515,0.9578232093
,-5.7994679595\H,2.3727118668,-0.486135996,-4.6878052494\H,2.669333715
,-0.3893240217,-2.2325118066\H,4.4755389374,2.4098324292,-2.0470488454
\H,6.6931898597,1.4619027801,-1.5039799005\H,7.4613293351,1.3542865135
,0.8610496716\H,5.9783481445,2.2016497047,2.6722732759\H,3.7665803215,
3.1413902117,2.129332803\H,1.8338196249,6.9216467345,-2.6454503254\H,3
.3996313643,6.4695448511,-1.9390484268\H,2.3581066974,5.2327994589,-2.
6739603161\H,1.1182027825,8.0505146275,-0.5079530789\H,1.1806553725,7.
1868021608,1.0407723532\H,2.6872437319,7.6504485646,0.2216815953\H,3.7
236985423,-3.5560394558,2.72190459\H,4.2498799681,-1.8775026028,2.9514
027293\H,3.0365644335,-2.5833212482,4.0456326976\H,1.2743646818,-4.021
712108,1.923923823\H,0.6656463453,-2.9997800054,3.2486136011\H,0.20091
11689,-2.6540032598,1.5673619972\\Version=IA64L-G03RevD.01\State=2-A\H
F=-2107.0036689\S2=0.770348\S2-1=0.\S2A=0.750319\RMSD=7.488e-09\RMSF=7
.633e-07\Thermal=0.\Dipole=1.00757,0.4559075,1.130196\PG=C01 [X(C31H33
N2S2)]\\@

**C•H(Ph)-$CH_2$-CH(Ph)-$CH_2$-$CH(CH_3)$Ph (structure 14)**

**Starting conformation**

1\1\GINC-AC22\FOpt\UB3LYP\6-31G(d)\C24H25(2)\EXI501\23-Aug-2006\0\\#P
gfinput B3LYP/6-31G(d) INT(grid=ultrafine) opt maxdisk=1342177280\\opt
\\0,2\C,0.,0.,0.\C,0.,0.,1.401401\C,1.2395978557,0.,2.0600074256\C,2.4
36265693,-0.0024604427,1.3429667531\C,2.4189353638,-0.0040778079,-0.05
35077793\C,1.1950191358,-0.002382069,-0.7228365262\C,-1.3115147864,0.0
180110905,2.176242627\C,-1.4596510239,-1.1863809952,3.1325078149\C,-1.
4653062369,-2.5741418797,2.4514256514\C,-1.4438456405,-3.6935098856,3.
5109922553\C,-1.4949547176,1.3530097781,2.9685044312\C,-1.4849736105,2
.5818472834,2.1136821927\C,-2.6184442709,3.2244267372,1.5594214239\C,-
3.956738638,2.7754117856,1.7645255843\C,-5.0330477868,3.4456893656,1.2
008981019\C,-4.8336255212,4.5863545731,0.4121900753\C,-3.5281205971,5.
0487819512,0.1918767451\C,-2.4461702151,4.386375181,0.7484966712\C,-2.
6285196504,-2.7510704722,1.4824027041\C,-2.3932154589,-3.0066872527,0.
1249187321\C,-3.4494427827,-3.1881871112,-0.770756923\C,-4.7681778657,
-3.1160962044,-0.3221453361\C,-5.0198738382,-2.8618600945,1.027898819\
C,-3.9610875222,-2.6823934294,1.9180472314\H,-2.4315659057,1.280794984
2,3.535392096\H,-0.5114690163,2.9895800253,1.8504673795\H,-1.436723532
,4.7508262129,0.5724246858\H,-3.3618902889,5.9319585708,-0.4199707333\
H,-5.6813487542,5.1060136438,-0.0252953895\H,-6.0416152498,3.078029331
4,1.3734301313\H,-4.1389926431,1.8903744469,2.3664011926\H,-2.12769097
66,-0.03202446,1.4453195606\H,-0.646410886,-1.1668780952,3.8712679931\
H,-2.38920466,-1.0634237578,3.7058587113\H,-0.5398185716,-2.6571476253
,1.8677320681\H,-0.9496934353,0.001935929,-0.5293103521\H,1.1672663493
,-0.0015769852,-1.8096049247\H,3.3507488184,-0.0060276248,-0.612843365
2\H,3.3838387937,-0.0025221127,1.8759386515\H,1.274222579,0.003805194,
3.1471575267\H,-1.3680081058,-3.0611169889,-0.2340322682\H,-3.23954300
27,-3.3855793039,-1.8190161637\H,-5.5926681302,-3.2562107181,-1.016163
6744\H,-6.0436163777,-2.8046661713,1.3893920898\H,-4.1770960426,-2.490
1627591,2.9665786177\H,-1.419354134,-4.6812328699,3.0381662563\H,-2.33
16189384,-3.6544295147,4.1535653179\H,-0.5612070784,-3.6012961004,4.15
51762042\H,-0.6900799973,1.4255430178,3.713326943\\Version=IA64L-G03Re
vD.01\State=2-A\HF=-929.5847525\S2=0.780606\S2-1=0.\S2A=0.750642\RMSD=
5.559e-10\RMSF=4.056e-06\Thermal=0.\Dipole=-0.1515576,0.0644165,-0.047
2376\PG=C01 [X(C24H25)]\\@

**Global minimum**

1\1\GINC-AC8\FOpt\UB3LYP\6-31G(d)\C24H25(2)\EXI501\23-Aug-2006\0\\#P g
finput B3LYP/6-31G(d) INT(grid=ultrafine) opt maxdisk=1342177280\\opt\
\0,2\C,0.,0.,0.\C,0.,0.,1.403728\C,1.2376717222,0.,2.0609233192\C,2.43
7250631,-0.0007505921,1.3453200392\C,2.4202588141,-0.0005719894,-0.049
4244497\C,1.1948571376,0.0001286326,-0.7197568291\C,-1.3004896587,-0.0
19878554,2.1987383679\C,-2.0777078953,-1.3302661795,1.9640767377\C,-2.
2012702642,1.2009519238,1.9046251497\C,-1.5830859872,2.5722955121,2.25
13736413\C,-1.2870797657,2.7334321112,3.7363153644\C,0.0144432369,3.01
00983855,4.176815853\C,0.2974885747,3.1836051172,5.533301919\C,-0.7224
186589,3.0838947255,6.4797938432\C,-2.024915441,2.8091924366,6.0574447
908\C,-2.3018746527,2.6364280324,4.7012282932\C,-2.4842599659,3.739389
1874,1.7396521886\C,-2.5914170883,3.7966165944,0.2484371943\C,-3.76636
20873,3.7756879505,-0.5404848069\C,-3.6583221326,3.8518396777,-1.96276
48616\C,-4.778148804,3.8357737658,-2.7778694977\C,-6.0613204546,3.7434
310662,-2.2197142526\C,-6.198620725,3.6682426991,-0.8272446173\C,-5.08
41617566,3.6838375101,-0.0012298138\H,-3.4698704415,3.6683583722,2.212
9243013\H,-2.0407544447,4.6788260786,2.1056424574\H,-0.6274249112,2.64
97269105,1.7165021411\H,-2.4759431836,1.2038077212,0.841799998\H,-3.14
2693394,1.0770299457,2.458083642\H,-1.0316045752,0.0163004026,3.262295
0323\H,-1.6458237256,3.8686121654,-0.2892035849\H,-2.6669584138,3.9246
575819,-2.4042271237\H,-4.6591724284,3.8955800797,-3.8568514656\H,-6.9
391739838,3.7311979658,-2.8593639478\H,-7.1896598196,3.5973842675,-0.3
856879399\H,-5.2209956488,3.6257787092,1.0739198144\H,0.8163108525,3.0
85996309,3.4459349809\H,1.3158922026,3.3964078548,5.848636507\H,-0.506
0208425,3.2182623063,7.5362941469\H,-2.828076242,2.7295721909,6.785795
6607\H,-3.3226537427,2.423885765,4.3920907263\H,-0.9441493902,-0.00197
28583,-0.5396270121\H,1.1690142618,-0.0008263857,-1.8066692277\H,3.351
4023632,-0.0012686023,-0.6099298531\H,3.3840098551,-0.0017874691,1.879
7719683\H,1.2600535803,0.0024041003,3.1483873584\H,-2.4020990955,-1.42
12658502,0.9205854683\H,-1.4574113745,-2.2024993074,2.1971356732\H,-2.
9728370555,-1.368904861,2.5963740921\\Version=IA64L-G03RevD.01\State=2
-A\HF=-929.5850677\S2=0.781086\S2-1=0.\S2A=0.750664\RMSD=1.621e-09\RMS
F=3.912e-06\Thermal=0.\Dipole=-0.0643906,-0.0516207,0.0236321\PG=C01 [
X(C24H25)]\\@

**Appendix S4. AM1 optimised geometries in the form of Gaussian archive entries for all species in the test set-2, both in their starting conformations and final global minimum conformations.**

**$(CH_3)_2C(CN)(CH_2C(CH_3)COOCH_3)_2SC•(Ph)SC(CH_3)_2CN$ (structure 15)**

**Starting conformation**


1\1\GINC-AC12\FOpt\UAM1\ZDO\C25H33N2O4S2(2)\CYL509\21-Nov-2006\0\\#T O
PT AM1\\AIBNMMA2-DB-AIBN\\0,2\C,0.9833467317,2.3388961389,1.1393371454
\C,0.8557562806,1.6289307924,2.4861800614\C,2.2448791157,1.8631022128,
0.4435237443\O,2.4170014377,1.5516958345,-0.737907613\O,3.3314108737,1
.81763092,1.2758464733\C,4.5610659323,1.3711406504,0.7014481155\H,4.43
78184174,0.3435070634,0.2830145459\H,4.8792970592,2.0775121544,-0.1028
504058\H,5.2730341837,1.3814183279,1.563006323\H,1.1766112674,0.557543
9019,2.417487268\H,-0.2014646745,1.6774967223,2.8457458236\H,1.5232634
413,2.113115894,3.2412890124\C,-0.2350920479,2.119221868,0.241977635\C
,-0.8923813306,0.7360425489,0.1248404164\H,-1.0336023017,2.8273182778,
0.6039405504\H,0.0644068332,2.4465729215,-0.7943414155\C,-2.1365640726
,0.7205508787,0.9866557939\C,-1.2563346498,0.4988861078,-1.3302963788\
O,-2.288290422,1.1744205938,2.1238743241\O,-3.2287716403,0.1503636667,
0.3875179413\C,-4.4257142527,0.0899564283,1.1659630573\H,-5.1613787701
,-0.3930571471,0.4764776969\H,-4.2536734773,-0.5274420692,2.0801593113
\H,-4.7473384637,1.1198171679,1.4530382883\H,-0.3352733517,0.502517356
2,-1.9636189172\H,-1.9462638003,1.3026593326,-1.687197393\H,-1.7766668
05,-0.4837642282,-1.4499187241\C,1.1317587706,3.8404338508,1.457153939
5\C,1.1781502523,4.8761863225,0.3268518447\C,-0.1274021177,5.038366565
7,-0.3071950321\C,1.5558363118,6.2203884755,0.9650857039\H,2.593013686
9,6.1607027283,1.3729222564\H,1.5167119632,7.0343414714,0.2025906937\H
,0.8533702505,6.4706091477,1.7950323659\H,2.088960586,3.9529563612,2.0
391443479\H,0.2815067672,4.1159936368,2.1389911931\C,2.2152377233,4.53
67906497,-0.7373528314\H,2.4407332413,5.4374904024,-1.3574563595\H,3.1
579094375,4.1906153507,-0.2467152969\H,1.8478624876,3.7250342139,-1.41
19334853\S,0.1999576002,-0.5709325057,0.7489625557\C,-0.0668055713,-1.
9894621029,-0.1313059939\C,0.783766025,-2.4285877298,-1.1797900914\S,-
1.2782371365,-2.6705706482,0.7097916255\C,0.8635573571,-3.7941920015,-
1.5471783589\C,1.701854997,-4.2107759601,-2.5792515211\C,2.4881271798,
-3.2823387833,-3.2708492272\C,2.4403276616,-1.931505552,-2.9068680441\
C,1.6088453056,-1.5062557221,-1.8732577306\H,0.276271269,-4.5400660589
,-0.9923513878\H,1.7491893942,-5.2770769863,-2.8451288247\H,3.14432549
62,-3.6130566109,-4.0877483867\H,3.0663910442,-1.1977471396,-3.4358446
865\H,1.6032948101,-0.4431129634,-1.5759587466\C,-2.3305675906,-3.8686
011445,-0.1216801439\C,-3.6527322582,-3.679497574,0.6143738695\C,-1.83
50779591,-5.2103453555,0.0971833438\C,-2.5149604927,-3.5870941408,-1.5
994095778\N,-1.4587364692,-6.2942666583,0.2883782334\H,-4.4314233772,-
4.3536109611,0.182301683\H,-3.5369452542,-3.9163391629,1.6999939018\H,
-3.9934437675,-2.6183111726,0.5084100705\H,-3.2374092104,-4.3148296326
,-2.0436796838\H,-2.9193026258,-2.5542960335,-1.7386215357\H,-1.544129
9728,-3.67065598,-2.1467836893\N,-1.1537276738,5.2136783032,-0.8247997
667\\Version=IA64L-G03RevC.02\State=2-A\HF=-0.1465373\S2=0.\S2-1=0.\S2
A=0.\RMSD=0.000e+00\RMSF=4.742e-06\Dipole=0.2861291,0.8962543,-0.11434
42\PG=C01 [X(C25H33N2O4S2)]\\@


**Global minimum**


1\1\GINC-AC57\FOpt\UAM1\ZDO\C25H33N2O4S2(2)\CYL509\21-Nov-2006\0\\#T O

PT AM1\\AIBNMMA2-DB-AIBN\\0,2\C,0.279381931,-0.1558739355,3.1694062007
\C,-0.4761401784,-0.7492883627,4.3559908303\C,1.6648061835,-0.77106303
28,3.1129184972\O,2.7562584378,-0.2189636467,2.9635548773\O,1.65329148
56,-2.1362428793,3.2291884282\C,2.9233392732,-2.7907667569,3.199482794
4\H,3.4098579345,-2.6217758159,2.2086031581\H,3.5745544514,-2.40091057
24,4.0183631418\H,2.6678142446,-3.8677909657,3.3537358297\H,-0.5838943
573,-1.8542034874,4.2259690006\H,-1.4920406505,-0.2912596343,4.4251309
549\H,0.0746884323,-0.5631221582,5.3081657058\C,-0.5047985477,-0.57353
51085,1.909904193\C,-0.0684783864,-0.0428507953,0.5463196887\H,-0.4691
937046,-1.6999264367,1.8646199376\H,-1.5754045775,-0.2612631594,2.0697
363657\C,-0.5243443644,1.3790558914,0.3545999524\C,1.404924577,-0.2025
398749,0.2701281553\O,-1.5352337712,1.9245107644,0.8072843891\O,0.3122
193567,2.1329141603,-0.4209607829\C,-0.0997134471,3.4752571576,-0.6897
444533\H,0.7102866786,3.8678394909,-1.3527042142\H,-1.0897356491,3.475
5251452,-1.2055117736\H,-0.1641858628,4.0501366634,0.2650658794\H,1.74
56934243,-1.2242835445,0.5709530708\H,2.0006104968,0.5542919431,0.8409
016667\H,1.6139719473,-0.049568011,-0.8184402774\C,0.3706498213,1.3670
83981,3.2455979041\C,0.8014579548,2.0400613611,4.5568635154\C,1.769703
6038,1.2540087162,5.3124969788\C,1.4551558515,3.3815192696,4.201840458
\H,0.7460311533,3.9905297637,3.5921187108\H,1.7075272469,3.9445209843,
5.131667598\H,2.39080525,3.2172393201,3.6158352388\H,-0.6447452966,1.7
78430026,2.9840705737\H,1.0838877405,1.69183955,2.436259816\C,-0.41017
53295,2.3235048036,5.4451684452\H,-0.0886993453,2.8514746491,6.3751373
989\H,-1.1322048499,2.9750564231,4.8964333369\H,-0.926932368,1.3783142
659,5.7334775425\S,-1.066363927,-1.1352575953,-0.518585285\C,-0.850866
4018,-0.8061987951,-2.1424919324\C,0.3339085758,-0.9336649452,-2.91762
38624\S,-2.391815481,-0.4035964498,-2.5164673611\C,0.5477218354,-0.143
3936488,-4.0708067017\C,1.7118660347,-0.2850864424,-4.8245212152\C,2.6
871070934,-1.2166487667,-4.4519502692\C,2.4929499672,-2.0033178025,-3.
3107410509\C,1.3358581111,-1.8634325563,-2.5472159609\H,-0.2058810813,
0.6031795222,-4.362087267\H,1.8639278,0.3431753633,-5.7146472516\H,3.6
023220663,-1.3275834765,-5.0501828969\H,3.2575936332,-2.7359238516,-3.
0134963037\H,1.1867883173,-2.4799939764,-1.6473553462\C,-2.9241978089,
-0.8142382774,-4.1867813086\C,-2.2533254304,-2.044411999,-4.7634940434
\C,-2.7088750204,0.3364912025,-5.0393452391\C,-4.4175324656,-1.0572534
079,-4.0112318704\N,-2.5573254092,1.2621503908,-5.7270483352\H,-2.6711
219134,-2.2721122354,-5.7746480479\H,-1.1509010621,-1.8833352008,-4.85
98249608\H,-2.4336615136,-2.9232794091,-4.0981146214\H,-4.9018593724,-
1.2029760094,-5.0074400072\H,-4.5814178495,-1.9751987759,-3.3962680357
\H,-4.9013652223,-0.1875218644,-3.5028530189\N,2.5534925113,0.66411900
32,5.9366223217\\Version=IA64L-G03RevC.02\State=2-A\HF=-0.1540458\S2=0
.\S2-1=0.\S2A=0.\RMSD=0.000e+00\RMSF=3.137e-06\Dipole=-0.7276417,-0.71
74964,-0.481941\PG=C01 [X(C25H33N2O4S2)]\\@

**$H(CH_2C(CH_3)COOCH_3)_3SC•(Ph)SC(CH_3)_3$ (structure 16)**

**Starting conformation**

1\1\GINC-AC47\FOpt\UAM1\ZDO\C26H39O6S2(2)\CYL509\21-Nov-2006\0\\#T OPT
 AM1\\HMMA3-DB-tBu\\0,2\C,1.2050883618,1.827682506,1.062887399\C,1.445
2641715,1.1415816974,2.4066356982\C,2.1334721402,1.2388515744,0.018135
964\O,1.9199477969,1.0017828143,-1.1743960095\O,3.3907025879,0.9791868
597,0.496037753\C,4.3093552166,0.3770161984,-0.4173340065\H,3.87818525
83,-0.5704366911,-0.827368894\H,4.5325799628,1.0878649127,-1.248972802
3\H,5.2137005006,0.1802415347,0.2090127246\H,1.5711740016,0.0356091805
,2.28568505\H,0.5850173373,1.337162283,3.0931831782\H,2.3859781646,1.5
271758606,2.871016691\C,-0.2493017962,1.7144219893,0.6056671295\C,-0.9

913254138,0.3685790974,0.6535004555\H,-0.8412755028,2.4422052423,1.232
4552625\H,-0.2806102006,2.0879510904,-0.458690502\C,-1.8883753246,0.36
60633947,1.8716209871\C,-1.80803328,0.238725329,-0.6193928188\O,-1.602
5289656,0.6574415347,3.0359630682\O,-3.1880522081,0.0202369865,1.61329
36085\C,-4.0708422281,-0.0250397881,2.7361843926\H,-5.0474805116,-0.33
32871385,2.288624129\H,-3.7052577275,-0.7739035142,3.4789741832\H,-4.1
361833579,0.9839237174,3.2098127304\H,-1.1310171948,0.2095414586,-1.50
78716345\H,-2.5010267692,1.1100353885,-0.718354051\H,-2.4252153105,-0.
6966757149,-0.5955077669\C,1.5721988645,3.3112507567,1.2710431115\C,1.
2788556064,4.3475105019,0.1813467921\C,-0.2113343845,4.6156607162,0.11
74112655\C,1.9308636117,5.664160356,0.6192570786\O,-0.9674075492,4.898
7270418,1.0506930816\O,-0.747950214,4.5616664746,-1.1400510504\C,-2.14
57975626,4.8340462049,-1.2535963061\H,-2.3362735986,4.7794604247,-2.35
35940575\H,-2.7268145454,4.0589853791,-0.6978573975\H,-2.3741176326,5.
8483731832,-0.8471121319\H,3.0378414843,5.5345243939,0.6722204166\H,1.
6992569941,6.4707220077,-0.1166166311\H,1.5484714784,5.9704379095,1.62
25097493\H,2.6787929251,3.3460694057,1.4707069103\H,1.0403923418,3.650
8769499,2.2035701493\C,1.8365234223,3.9554175677,-1.1744910964\H,1.834
9559832,4.8374758442,-1.8594056736\H,2.882813773,3.5815886732,-1.06063
23138\H,1.218325579,3.1517815788,-1.645566365\S,0.1615024229,-1.005185
8162,0.8630462225\C,-0.2542030934,-2.3664793382,0.0215596183\C,0.87993
77547,-3.0192677648,-0.5843979075\S,-1.7691901133,-2.9885836836,0.1194
434918\C,1.1489273877,-4.37985557,-0.3185563339\C,2.2635431868,-5.0032
369154,-0.8783717145\C,3.1283893311,-4.2875950916,-1.7127213926\C,2.87
50526794,-2.9382332593,-1.9788322318\C,1.7655667703,-2.3042813845,-1.4
197064028\H,0.4773592462,-4.9413235464,0.3490178251\H,2.4650991174,-6.
0613920732,-0.6571349718\H,4.0045043769,-4.7829040379,-2.1540108674\H,
3.5523391162,-2.3700422848,-2.6331669326\H,1.5781871966,-1.2361141235,
-1.6233577166\C,-2.2635669243,-3.801583344,-1.4142053706\C,-1.78361553
77,-3.0519106569,-2.6347091119\C,-3.7760093826,-3.7365724064,-1.306865
1229\C,-1.8060257532,-5.2414194148,-1.4574374607\H,-4.2404904957,-4.23
65523579,-2.1916592091\H,-4.1256793547,-4.2573471905,-0.3819373743\H,-
4.1221781796,-2.6745244624,-1.2763147199\H,-2.1608662144,-3.5492827326
,-3.5616789597\H,-2.1550424671,-1.9977182321,-2.6202195076\H,-0.665673
4827,-3.0358015872,-2.6697638734\H,-2.3243771547,-5.7819188395,-2.2877
93652\H,-0.704290737,-5.299983571,-1.6361842304\H,-2.0434398824,-5.757
7777511,-0.495971492\\Version=IA64L-G03RevC.02\State=2-A\HF=-0.3905652
\S2=0.\S2-1=0.\S2A=0.\RMSD=0.000e+00\RMSF=2.133e-06\Dipole=-0.0347958,
-0.2638616,-1.0697131\PG=C01 [X(C26H39O6S2)]\\@

**Global minimum**

1\1\GINC-AC9\FOpt\UAM1\ZDO\C26H39O6S2(2)\CYL509\17-Nov-2006\0\\#T OPT
AM1\\HMMA3-DB-tBu\\0,2\C,1.7124206338,1.8659112812,0.8315142422\C,0.87
12581231,1.6682263616,2.0904335214\C,3.0904828981,1.2812808474,1.07283
26611\O,3.7512622354,0.5046740725,0.3801455787\O,3.6574670782,1.714944
5072,2.2443630732\C,4.9701362263,1.2350434691,2.5373014751\H,4.9661332
466,0.1202793871,2.5973157928\H,5.6812266811,1.5730953511,1.7452240233
\H,5.2062630669,1.698515211,3.5265508963\H,0.8396456015,0.5912584101,2
.383813115\H,-0.1741832826,2.0214332818,1.9050298471\H,1.307879932,2.2
516321408,2.9377258166\C,1.0547802549,1.2462837295,-0.3996905111\C,0.4
690129206,-0.1669198722,-0.3263838811\H,0.218050031,1.9336009757,-0.72
01525744\H,1.818514512,1.2460226566,-1.2303725352\C,0.0799997414,-0.53
76350935,-1.7418565397\C,1.4238349742,-1.1942625222,0.2318432899\O,-0.
1837600155,0.2164769188,-2.6820105353\O,0.0442972771,-1.8848718141,-1.
9861232193\C,-0.3292111833,-2.2844202271,-3.3060648421\H,-0.3231545659
,-3.4009616435,-3.2518309704\H,-1.3441061631,-1.8906069457,-3.55353019
47\H,0.4189697886,-1.9054792345,-4.0429015889\H,1.7344385776,-0.920461
4365,1.2687409224\H,2.3431775598,-1.2507861537,-0.4038573334\H,0.93752

30996,-2.2020725931,0.2525202789\C,1.8524643663,3.3890665429,0.6395740
12\C,2.523919724,3.9338321187,-0.625186379\C,1.5696448704,3.7922615684
,-1.7951614032\C,2.7396039756,5.436498124,-0.4208553585\O,0.4031503197
,4.1912144008,-1.8542130212\O,2.0984453262,3.1789847061,-2.894158134\C
,1.2112831358,2.9630997341,-3.9964053223\H,1.8729126005,2.5183670042,-
4.779518677\H,0.4028208246,2.253958806,-3.6889681446\H,0.7738254174,3.
9333360111,-4.3322907071\H,3.4431354432,5.6037078458,0.4288699634\H,3.
1760840241,5.8900773402,-1.3425520567\H,1.7676801535,5.9388259538,-0.1
979109742\H,2.4321115034,3.7777779801,1.5216893795\H,0.8171828297,3.82
78155746,0.6851703714\C,3.8644146876,3.2805328867,-0.9059295647\H,4.42
00751967,3.862765374,-1.680006797\H,4.4716881993,3.2433527063,0.031553
1827\H,3.7308545357,2.2387057542,-1.2888280832\S,-1.0270591806,0.01303
27783,0.6752526775\C,-1.9335968994,-1.3865513537,0.6616718457\C,-1.515
1828115,-2.6349761001,1.2505210525\S,-3.339118012,-0.9815448783,-0.029
435055\C,-1.4976257387,-2.7897245864,2.648510658\C,-1.0890734497,-3.99
51603186,3.2191828998\C,-0.6884821405,-5.0582917819,2.4069838551\C,-0.
6916858064,-4.9097921254,1.0184051086\C,-1.0997768617,-3.7073850793,0.
4407374226\H,-1.8050093702,-1.9511704446,3.290739804\H,-1.0811395824,-
4.1062686828,4.3132537102\H,-0.3672341589,-6.0072499347,2.8594475889\H
,-0.3662771861,-5.7409909051,0.3760830041\H,-1.0762245956,-3.580676150
6,-0.6538407149\C,-4.6816660831,-2.1235359508,0.3053592561\C,-5.867273
9362,-1.4089220581,-0.3167287527\C,-4.90284517,-2.314713935,1.78835322
24\C,-4.4584347573,-3.455192926,-0.3747109657\H,-5.7765659236,-2.98995
96391,1.961698169\H,-3.999829022,-2.7745319567,2.2617674406\H,-5.10993
6024,-1.3357037114,2.2846613431\H,-6.7876589129,-2.0314715716,-0.19877
8761\H,-6.03998408,-0.4242764355,0.1823439026\H,-5.6948005183,-1.23606
95793,-1.4072236761\H,-5.3384330395,-4.1237896649,-0.2069665405\H,-4.3
256131403,-3.3168207265,-1.4750823848\H,-3.5485161118,-3.9576854866,0.
0377962505\\Version=IA64L-G03RevC.02\State=2-A\HF=-0.3989199\S2=0.\S2-
1=0.\S2A=0.\RMSD=0.000e+00\RMSF=8.247e-06\Dipole=-0.0198087,-0.747683,
0.6693894\PG=C01 [X(C26H39O6S2)]\\@

**his-arg (structure 17)**

**Starting conformation**

1\1\GINC-AC16\FOpt\RAM1\ZDO\C12H21N7O2\CYL509\21-Nov-2006\0\\#T OPT AM
1\\his-arg\\0,1\N,-2.3600378618,-2.2148057142,-4.8304940296\C,-2.48666
79893,-1.7411598441,-3.5274269162\C,-1.1956524748,-1.7944112249,-2.959
2095496\N,-0.2863599333,-2.2945105819,-3.9058536926\C,-1.0095333213,-2
.5386495288,-5.0164713975\C,-0.7994354775,-1.3719362031,-1.6000816578\
C,-1.7022008054,-1.9911234859,-0.5188917848\C,-0.9236925159,-1.9889388
317,0.8214132612\N,-0.5676611984,-0.7569923322,1.346226996\C,0.2668101
367,-0.6420096871,2.518324926\C,1.6022882041,0.0781486128,2.2746704461
\C,1.4315789146,1.5090000023,1.8117128716\C,2.7962159685,2.1950502565,
1.7545710343\N,2.7471368262,3.6301715217,1.5508578118\C,2.0927091294,4
.0628476886,0.3245148996\N,2.9444252886,4.3577496582,-0.7903199573\N,-
3.004123719,-1.3766684538,-0.4335886836\O,-0.6930765037,-3.0515198658,
1.4252120533\C,-0.4603727396,0.0341679116,3.6799930676\O,0.0941549517,
0.2120254616,4.763484506\N,0.7984666641,4.1815407626,0.199904546\H,-3.
5640254402,-1.8231697231,0.2648176695\H,-2.9425356099,-0.3965882682,-0
.2444767206\H,-1.861444903,-3.0846686755,-0.7712599327\H,0.2589205886,
-1.690260704,-1.3922015257\H,-0.8317735167,-0.2493760708,-1.5467041187
\H,-3.4382617716,-1.4234742068,-3.1035572164\H,-3.0858360798,-2.312087
8357,-5.4880307451\H,-0.6188940731,-2.9378550457,-5.9576008813\H,-1.51
62607981,0.3368529564,3.5062654545\H,-0.5945307601,0.0322288407,0.7436
955577\H,0.5118188677,-1.6957003997,2.8738018539\H,2.2035871248,-0.496
0003721,1.522617436\H,2.1629799775,0.0602281909,3.2484845265\H,0.75236

88644,2.0535516684,2.5199637799\H,0.9614835902,1.5320855121,0.79407046
79\H,3.3156371835,2.0396063144,2.7453322337\H,3.4127742206,1.677934783
7,0.9613596414\H,3.6717397381,4.0114469424,1.6331225522\H,0.2606291427
,3.8729052611,0.9807463268\H,2.4488216076,4.7043671946,-1.5865890978\H
,3.708969822,4.9526208508,-0.5492758741\\Version=IA64L-G03RevC.02\Stat
e=1-A\HF=-0.0077073\RMSD=0.000e+00\RMSF=2.481e-06\Dipole=-0.4366256,0.
9660907,-1.4348481\PG=C01 [X(C12H21N7O2)]\\@

**Global minimum**

1\1\GINC-AC18\FOpt\RAM1\ZDO\C12H21N7O2\CYL509\17-Nov-2006\0\\# OPT AM1
\\his-arg\\0,1\N,-2.1218535567,-1.618741034,-0.020589402\C,-1.47259602
,-2.0131168787,1.1448477569\C,-0.1681082569,-2.403350802,0.7626780974\
N,-0.0218525796,-2.2480254083,-0.6219349845\C,-1.2045236762,-1.7660661
338,-1.064631696\C,0.8739711198,-2.9242021012,1.6705113284\C,2.2368088
293,-2.2326717093,1.4703470739\C,2.0149068827,-0.7112870638,1.66255946
25\N,1.8326944844,0.0611520737,0.5332714768\C,1.3804413972,1.429465116
7,0.6179277647\C,1.4132806316,2.1594699746,-0.7314793707\C,0.681442219
1,1.4500424153,-1.8527326974\C,-0.2371498663,2.3929416174,-2.636918869
5\N,-1.5046523754,2.7060444662,-2.0176149749\C,-2.4674569105,1.6292711
596,-1.8908554367\N,-2.7256180803,0.8795483229,-3.0837833452\N,3.24423
68019,-2.7673560032,2.3596037327\O,2.0370783207,-0.1998826395,2.802418
0544\C,0.0130044986,1.5692352834,1.287231518\O,-0.8275274335,2.3937428
244,0.9230606563\N,-3.1146971704,1.305127153,-0.7975584371\H,4.1202996
943,-2.3076808921,2.2058571728\H,2.9742935559,-2.6405369268,3.31686990
36\H,2.5875107453,-2.4376492832,0.4147812694\H,0.5325838259,-2.7859399
255,2.7316147084\H,1.0074131807,-4.0264200728,1.4903691139\H,-1.953440
9964,-2.001307265,2.1208572046\H,-3.0278789671,-1.2287073466,-0.084935
5197\H,-1.4463688288,-1.5138180273,-2.1041479336\H,-0.1576367816,0.902
0801288,2.1624458447\H,1.7141963225,-0.3936411697,-0.343797781\H,2.090
0501644,1.9713768129,1.3246002403\H,2.4845247807,2.3142941756,-1.02703
86062\H,0.9673646743,3.1757650303,-0.5546361715\H,0.0674399224,0.59313
16009,-1.4630649311\H,1.4284243832,1.016301927,-2.5682142197\H,0.29241
37208,3.3772853694,-2.7937282922\H,-0.4163826347,1.9456355421,-3.65434
67958\H,-1.3647098034,3.1653015714,-1.132403089\H,-2.8419250896,1.7912
62053,0.0296987201\H,-3.6046764114,0.4039315173,-3.0565001136\H,-2.631
830312,1.4258214396,-3.9147784608\\Version=IA64L-G03RevC.02\State=1-A\
HF=-0.0207869\RMSD=0.000e+00\RMSF=5.772e-06\Dipole=-0.3848574,0.476058
3,-1.0100687\PG=C01 [X(C12H21N7O2)]\\@

**thr-lys (structure 18)**

**Starting conformation**

1\1\GINC-AC3\FOpt\RAM1\ZDO\C10H21N3O3\CYL509\21-Nov-2006\0\\# OPT AM1\
\thr-lys\\0,1\C,-0.3082470239,-1.5871433605,-4.0847401067\C,-0.3780479
667,-1.1181044392,-2.6458468671\O,0.2608311519,0.1367851736,-2.4673982
381\C,-1.8466827653,-1.0818443791,-2.1483472033\C,-1.8464048435,-1.129
429247,-0.6005022975\N,-1.2384869306,-0.0749310424,0.0564289783\C,-1.0
351806432,-0.0906080736,1.4865365521\C,0.4246661316,-0.3094670747,1.91
80181633\C,1.3836358655,0.6998243338,1.3252977109\C,2.7440825264,0.598
0803123,1.9824321955\C,3.7160970313,1.5834931913,1.3350037282\N,5.0211
987055,1.5869788225,1.9512440555\N,-2.605809703,0.0091221496,-2.706307
162\O,-2.4316140498,-2.0496287694,-0.0005235849\C,-1.5427568291,1.1920
910093,2.1436536017\O,-1.6842977835,1.2690745695,3.362797415\H,-3.5697
214423,-0.0603558517,-2.4467681069\H,-2.2413080126,0.8944671381,-2.414
2889613\H,-2.3380633757,-2.0465191633,-2.4819132995\H,0.2029309557,-1.
8171798012,-1.9769481862\H,0.0162593494,0.7018918695,-3.2108756872\H,-
0.6961375786,-2.6301983057,-4.1660303129\H,0.7517048357,-1.567142389,-

4.4360191365\H,-0.9182326383,-0.9266409698,-4.7470505267\H,-1.77723111
18,2.0465957715,1.4717917706\H,-0.5961829607,0.4795314225,-0.469534306
\H,-1.6473857619,-0.9467316537,1.9165140307\H,0.7419303513,-1.34501152
23,1.6284991646\H,0.4512176437,-0.2471293331,3.0393077725\H,0.97518149
78,1.7359043808,1.4662346792\H,1.4930461495,0.53063329,0.2204005082\H,
2.6533391545,0.8162398617,3.0788577568\H,3.1330521504,-0.4488266087,1.
8798280412\H,3.2967240041,2.6256706098,1.4360109684\H,3.7607349807,1.3
525531548,0.2279798453\H,5.3895723498,0.6598184821,2.0238737849\H,5.65
39315088,2.1530386839,1.4225314982\\Version=IA64L-G03RevC.02\State=1-A
\HF=-0.2428176\RMSD=0.000e+00\RMSF=1.776e-06\Dipole=0.716241,0.2709137
,-1.9643438\PG=C01 [X(C10H21N3O3)]\\@

**Global minimum**

1\1\GINC-AC8\FOpt\RAM1\ZDO\C10H21N3O3\CYL509\23-Nov-2006\0\\#T OPT AM1
\\thr-lys\\0,1\C,1.7736819446,0.1071481036,-3.8538654088\C,0.860379047
,-0.0762820252,-2.6590539315\O,-0.3514634944,-0.7229549244,-3.01254800
16\C,1.5915804769,-0.8298987257,-1.5174220083\C,0.8611340269,-0.537045
1362,-0.1833564803\N,-0.4475012629,-0.9464983954,-0.0839679208\C,-1.24
06155813,-0.7364900819,1.1014483549\C,-2.0936483633,0.5481344025,1.085
3624781\C,-1.2557175078,1.803385112,1.1965908435\C,-0.7825082842,2.063
0740793,2.6106518559\C,0.3772646019,3.061403394,2.6529255425\N,1.66153
07505,2.6011076226,2.1925573869\N,1.77515337,-2.2324071867,-1.79255312
64\O,1.4713152947,0.003026522,0.7626341774\C,-2.1898627709,-1.89592926
51,1.3856395444\O,-2.4727294983,-2.7834551047,0.5841208864\H,2.3253037
342,-2.666278905,-1.0784271819\H,0.897850365,-2.7071467587,-1.87874134
59\H,2.6185633697,-0.3645123853,-1.4091182\H,0.528308092,0.9264090419,
-2.2611760031\H,-0.1380137414,-1.4455957356,-3.6161399776\H,2.65271140
45,0.7335062572,-3.5711527811\H,1.2170244798,0.6157960096,-4.677722076
\H,2.1425325128,-0.8790432783,-4.2258432731\H,-2.6263539289,-1.8638090
611,2.4091043012\H,-0.9347109635,-1.2174719812,-0.911187184\H,-0.52264
41532,-0.6707631486,1.9787748096\H,-2.8125229491,0.5024539889,1.945558
575\H,-2.696684918,0.5837248495,0.1404120762\H,-1.8668297524,2.6788478
852,0.8487499745\H,-0.3738128772,1.725036261,0.5061128012\H,-1.6313136
98,2.4730250667,3.2176003333\H,-0.4640242227,1.1022425038,3.0941705589
\H,0.5034888788,3.3983787651,3.7217096804\H,0.0933650099,3.9649968615,
2.0422773171\H,1.951569724,1.7882836417,2.7032885896\H,1.6248096774,2.
3485747513,1.2223133881\\Version=IA64L-G03RevC.02\State=1-A\HF=-0.2489
228\RMSD=0.000e+00\RMSF=2.080e-06\Dipole=-0.6093029,-0.2722975,-0.3349
492\PG=C01 [X(C10H21N3O3)]\\@

**Oleocanthal (structure 19)**

**Starting conformation**

1\1\GINC-AC31\FOpt\RAM1\ZDO\C17H20O5\CYL509\21-Nov-2006\0\\#T OPT AM1\
\Oleocanthal\\0,1\C,-2.2725091942,0.0582548624,4.1611359576\C,-2.25378
58511,0.1099537738,5.5529643999\C,-1.0311252182,0.2824225961,6.2156200
993\C,0.1682137855,0.4046208402,5.4928572403\C,0.1271947717,0.35128011
,4.1052266238\C,-1.0881081095,0.1763505934,3.4277876294\C,-1.110268512
8,0.1331543903,1.9422349504\C,-0.579820687,-1.1967235171,1.4300446314\
O,-0.6702656843,-1.2542144936,-0.0006364671\C,0.315493804,-0.653732137
9,-0.7300228044\O,1.230839195,-0.0779127632,-0.1357453397\O,-0.9298581
564,0.3423551188,7.5864946795\C,0.1179672312,-0.8280898744,-2.20615381
87\C,0.8742039235,0.2255200815,-3.014632027\C,2.1021215725,-0.36212165
22,-3.69826936\C,3.1231220854,-0.8530936304,-2.7144367406\O,4.00000109
95,-1.6586743843,-3.0290136075\C,-0.0174900092,0.8920592656,-4.0150882
854\C,-0.6576815557,0.287267067,-5.0333624178\C,-0.6303922874,-1.14030
77917,-5.390033192\C,-0.1776951899,2.3528571838,-3.840529976\O,-0.8851
97144,3.0505011228,-4.5718641354\H,1.0599331381,0.4496819085,3.5275630
719\H,1.1156072608,0.5415951677,6.0325542011\H,-3.2315189981,-0.074553

8532,3.6373937582\H,-3.1873538394,0.0178379245,6.1250773734\H,-1.82044
49372,0.2532086927,7.955637311\H,-0.4708527247,0.9589019582,1.52623911
47\H,-2.1531160246,0.2883926439,1.5582592211\H,0.4803117728,-1.3570182
212,1.7569436594\H,-1.2275035602,-2.0537260085,1.7568253108\H,-0.98188
90553,-0.7845626074,-2.4280722314\H,0.4745667706,-1.8621952777,-2.4646
627515\H,0.3881554001,2.801390277,-2.9920286902\H,1.8069726075,-1.1941
380242,-4.3909600789\H,2.5883030485,0.432830427,-4.3276464535\H,3.0426
134174,-0.4391764531,-1.682366966\H,-1.2780599848,0.917592792,-5.70419
2652\H,1.2479851694,1.0118699394,-2.2892346913\H,0.0862246491,-1.29967
88356,-6.2373725796\H,-1.6448071538,-1.4717337231,-5.7283378411\H,-0.3
159247884,-1.7909884942,-4.5375565866\\Version=IA64L-G03RevC.02\State=
1-A\HF=-0.2868452\RMSD=0.000e+00\RMSF=2.567e-06\Dipole=-1.2843595,-0.5
951423,0.0346198\PG=C01 [X(C17H20O5)]\\@

**Global minimum**

1\1\GINC-AC55\FOpt\RAM1\ZDO\C17H20O5\CYL509\17-Nov-2006\0\\#T OPT AM1\
\Oleocanthal\\0,1\C,0.2078263062,-3.9932897833,1.4344343607\C,0.329290
2524,-5.3760581082,1.5364456862\C,1.5529294147,-5.9281462239,1.9411488
816\C,2.6491971982,-5.1035657193,2.2430162037\C,2.50685037,-3.72474371
18,2.1338218129\C,1.2915772294,-3.1579485234,1.7292665226\C,1.14304383
74,-1.6827214556,1.6251541755\C,1.1575292641,-1.2360710876,0.171340313
4\O,1.0588589802,0.1910438506,0.0852770964\C,-0.182206784,0.7576775599
,0.1793700636\O,-1.1569089051,0.0174394787,0.333745254\O,1.7517347289,
-7.2843161614,2.0656673705\C,-0.1387159673,2.2520471043,0.0902912144\C
,-0.9260468555,2.7707718719,-1.111855914\C,-2.4241766928,2.6267116346,
-0.875766342\C,-3.2447256044,2.6027864582,-2.1240457892\O,-2.792415129
9,2.4706902555,-3.2628784559\C,-0.5429702393,4.1941157157,-1.38118751\
C,-0.0266366424,4.6020366364,-2.5575367677\C,0.222218601,3.7426367526,
-3.7278446527\C,-0.7396741957,5.1936546651,-0.3142606844\O,-1.21803724
62,4.9501975925,0.7967806947\H,3.3614511209,-3.0726085649,2.371404888\
H,3.5984082457,-5.5568187274,2.5604981565\H,-0.750313864,-3.5500912154
,1.1205009905\H,-0.5242517867,-6.0280589605,1.3045220787\H,0.922823281
8,-7.7289617435,1.8366327628\H,1.9679234726,-1.1629282527,2.1803954778
\H,0.1701929816,-1.362277765,2.0885581949\H,2.1453688046,-1.4519161914
,-0.3165373016\H,0.3226555244,-1.7169184746,-0.4017164446\H,0.92959125
65,2.5872439146,0.0144681859\H,-0.5735969797,2.6711681648,1.0390811157
\H,-0.4195157175,6.229898152,-0.5785155687\H,-2.6195699892,1.655650579
2,-0.3348050065\H,-2.7864877134,3.45605365,-0.2099252236\H,-4.34233124
1,2.6952892337,-1.9507950959\H,0.2363395633,5.66807762,-2.6928014976\H
,-0.6568837053,2.1422985875,-2.0111836596\H,0.9863349133,2.9601788626,
-3.4872272806\H,0.5964577217,4.3436734083,-4.5923303714\H,-0.722312266
,3.2212448833,-4.0397095242\\Version=IA64L-G03RevC.02\State=1-A\HF=-0.
2895742\RMSD=0.000e+00\RMSF=1.159e-06\Dipole=0.2157221,0.6218076,-0.53
77472\PG=C01 [X(C17H20O5)]\\@

**Pantothenic acid (structure 20)**

**Starting conformation**

1\1\GINC-AC4\FOpt\RAM1\ZDO\C9H17N1O5\CYL509\30-Oct-2006\0\\# OPT AM1\\
pantothenicAcid\\0,1\H,-1.094380355,-2.0016855382,-0.3975534652\O,-1.0
460295955,-1.6459364156,0.4999796795\C,0.3328972176,-1.5629614205,0.82
89921713\H,0.9093368684,-1.1305316709,-0.0331075097\C,0.4993023547,-0.
6839680735,2.075408966\C,1.9883394497,-0.4457820299,2.2889123768\C,-0.
0760625986,-1.4079592978,3.2843134016\C,-0.2048620473,0.6788949512,1.9
269731818\O,-1.5978938506,0.6203927609,2.1359033358\H,-1.9442586003,-0
.1732228088,1.7048943131\C,0.1454127949,1.3504986115,0.5864583612\N,-0
.6889116093,1.1449578913,-0.4908097029\C,-0.4878508395,1.7917406998,-1

.7534415619\C,-0.8097662265,0.9182761264,-2.9689642085\C,-0.0192153191
,-0.3483495629,-2.973290838\O,0.9247871462,-0.4166635168,-3.9496343072
\H,1.4029980083,-1.2607287873,-3.8908144596\O,1.1511844683,2.084067594
9,0.4959103629\O,-0.1191929067,-1.3322978049,-2.2304226762\H,-0.583859
8502,1.5101073692,-3.8954946695\H,-1.897695485,0.641159663,-2.97953357
07\H,-1.1569025805,2.7009150106,-1.8145817192\H,0.58193612,2.148254752
4,-1.8178756662\H,-1.4209853299,0.4775736889,-0.4105804644\H,0.1662141
074,1.3779413139,2.7356356833\H,0.7194453488,-2.5957391042,1.045236134
6\H,2.5407296128,-1.4153511216,2.2653183698\H,2.1595842137,0.037373129
4,3.2808415765\H,2.3945697429,0.2253015263,1.492386091\H,0.5408911113,
-2.3077023313,3.5198670265\H,-1.122720259,-1.7362639159,3.0733944944\H
,-0.0845322169,-0.730947389,4.171573495\\Version=IA64L-G03RevC.02\Stat
e=1-A\HF=-0.4101298\RMSD=0.000e+00\RMSF=1.298e-05\Dipole=-0.2190463,-0
.7939001,-1.1263219\PG=C01 [X(C9H17N1O5)]\\@

**Global minimum**

1\1\GINC-AC54\FOpt\RAM1\ZDO\C9H17N1O5\CYL509\01-Nov-2006\0\\# OPT AM1\
\pantothenicAcid\\0,1\H,1.3348456819,-0.7813781713,-1.3662519106\O,1.9
618827134,-0.7607264631,-0.6295534952\C,2.4788095664,0.551036517,-0.53
87212994\H,2.7805770127,0.9274279261,-1.5520194392\C,1.493838931,1.545
2170202,0.0957296433\C,0.3350080167,1.801186589,-0.8522286903\C,2.2537
843818,2.8506630709,0.3142837795\C,0.9810924225,1.061328147,1.47083092
91\O,1.8917412906,0.2233090768,2.1436277634\H,2.04857927,-0.5661073586
,1.6070781352\C,-0.4258486579,0.4438004449,1.3906864745\N,-0.555377088
3,-0.8819036231,1.0163461934\C,-1.8446260473,-1.495467817,0.8933094262
\C,-2.6050004603,-1.1918513768,-0.4025931268\C,-1.846746284,-1.6186987
208,-1.6137747812\O,-2.5802463628,-2.3332207272,-2.50988254\H,-2.03197
90204,-2.5648000504,-3.2781358811\O,-1.4195830374,1.1216347624,1.72243
9942\O,-0.6664330431,-1.4048378761,-1.9191953356\H,-2.7883772036,-0.08
5248599,-0.485989295\H,-3.5979687641,-1.712511959,-0.3714939531\H,-1.7
070607292,-2.6103131806,0.9836666197\H,-2.4928316317,-1.1390530181,1.7
467840052\H,0.1932129874,-1.2998767697,0.5068006295\H,0.8806264588,1.9
527439617,2.1636836792\H,3.3931858085,0.4528900437,0.1095414658\H,0.69
59970809,2.3423078443,-1.7600811935\H,-0.4453453192,2.4249623702,-0.35
11355683\H,-0.1312599135,0.838102861,-1.1791188835\H,2.7270321999,3.18
66699516,-0.6392596945\H,3.0514436151,2.706189671,1.0823042786\H,1.556
198384,3.6487664098,0.6645788467\\Version=IA64L-G03RevC.02\State=1-A\H
F=-0.4122313\RMSD=0.000e+00\RMSF=1.143e-05\Dipole=-0.1392524,-0.343294
9,-1.2297536\PG=C01 [X(C9H17N1O5)]\\@

**Taxol (structure 21)**

**Starting conformation**

1\1\GINC-AC36\FOpt\RAM1\ZDO\C31H38O11\CYL509\21-Nov-2006\0\\# OPT AM1\
\taxol\\0,1\C,-3.7266580465,3.8902017879,-4.0339769891\C,-3.3896931511
,3.3540931267,-2.7931391847\C,-2.2964198447,2.4820566418,-2.68653687\C
,-1.5471521159,2.1488496252,-3.8219270926\C,-1.8934623091,2.690108823,
-5.0590980736\C,-2.9795641665,3.5595577668,-5.1655685951\C,-1.96358369
88,1.9443248872,-1.3601791609\O,-2.5904964587,2.0788562338,-0.30632835
99\O,-0.8205396158,1.1762309671,-1.3462012808\C,-0.2311906193,0.843718
513,-0.0741656365\C,1.1862263524,1.5142630662,-0.133052671\C,1.8682300
366,1.5551939813,1.2670027037\C,2.1705489702,0.1149180024,1.5901466154
\C,2.9355742746,-0.5895087366,0.723970207\C,3.2593105817,0.024255579,-
0.6147327992\C,2.096716096,0.8531177042,-1.1758988957\C,1.5257903155,-
0.5531123762,2.7645756378\O,1.9908858346,0.1085666599,3.943993632\C,1.
9871333955,-0.5726001933,5.1445591389\O,2.4208656038,0.1327703868,6.05
54963085\O,0.9694323899,2.8774188912,-0.4932663894\C,1.0002131104,2.27

42727106,2.2879142039\C,3.1821976806,2.3526779927,1.181253552\C,3.4380
571594,-1.960345945,0.9637938462\O,3.6425105869,-0.9597569826,-1.56260
80704\C,-0.0040263804,-0.5080490279,2.710381038\O,-0.6220744131,-0.135
2406279,3.7122854291\C,-0.7859115878,-1.0900169286,1.5202814028\C,-0.2
439843475,-0.6810728805,0.1388095761\C,-0.8969367981,-1.4741429564,-0.
9993295536\C,-1.4908240276,-2.9003826144,-0.6903826453\C,-1.5530805348
,-3.3936709419,0.729532608\C,-0.61310368,-2.6277465732,1.6472227831\C,
-2.2487908852,-0.6982342997,1.6997602953\C,-2.3351793281,-1.1224243455
,-1.4794321598\O,-2.8017010127,-2.4647412809,-1.1727389717\O,0.1124863
567,-1.5398529312,-2.0011921319\C,-0.2281419284,-1.6307374384,-3.34776
98808\O,0.2524297196,-0.7141700393,-4.0098832823\O,-0.7657805742,-3.05
66077783,2.9887867902\C,-0.942645716,-2.8319387332,-3.8535499917\C,1.5
256885069,-1.9825699531,5.2470966098\H,0.8320242801,-1.0308458435,0.10
05702516\H,1.8052672368,-1.6484702578,2.7999022945\H,-0.8125347609,1.3
502319114,0.7479725205\H,4.1846383972,0.6651111443,-0.5119071202\H,1.4
695788628,0.2097041107,-1.8540901142\H,2.542197478,1.6575358159,-1.821
7801981\H,0.6315949582,2.8813542122,-1.3991925761\H,-1.0942332865,-3.6
842002629,-1.3816027216\H,-2.6084642346,-3.3240362012,1.1088635198\H,-
1.2697652338,-4.4796626705,0.7658335761\H,0.4575171559,-2.8970711205,1
.4042021826\H,-2.8710548001,-0.3675725507,-0.861393167\H,-2.441653136,
-0.9069275993,-2.5649399539\H,-2.3895600676,0.3979629141,1.528513408\H
,-2.904796925,-1.2557000719,0.9898617205\H,-2.5853303702,-0.9274275593
,2.7415246112\H,4.3123270233,-2.1762267974,0.2974977329\H,2.6402416496
,-2.7142800296,0.7422121265\H,3.7690458847,-2.0903343567,2.0239173144\
H,2.8608080074,-1.4932715102,-1.7583466144\H,-1.649543077,-2.799120140
7,3.2832838012\H,0.8294658147,3.3242353738,1.9422720597\H,1.5198653378
,2.2885182104,3.2786404316\H,0.0038514413,1.7984149111,2.4330143868\H,
4.047856072,1.7300205923,1.5106912978\H,3.3626870286,2.7082884928,0.13
84259896\H,3.1402412893,3.2540307615,1.8402298524\H,-0.3268579934,-3.7
407456397,-3.6378783064\H,-1.0887441001,-2.7432707391,-4.9583140286\H,
-1.9392243647,-2.9460396368,-3.3575280782\H,0.5331949067,-2.1131301799
,4.7441710879\H,2.2726275828,-2.6627674618,4.7688579838\H,1.4259845394
,-2.2594027078,6.3256570666\H,-3.9704888106,3.6082297398,-1.891350501\
H,-0.690032126,1.4567869731,-3.7355106051\H,-1.3046858184,2.429288877,
-5.9514208098\H,-3.2475824421,3.9865235966,-6.1440495181\H,-4.58263461
66,4.5761401261,-4.1189204008\\Version=IA64L-G03RevC.02\State=1-A\HF=-
0.598797\RMSD=0.000e+00\RMSF=3.892e-06\Dipole=-1.283702,-1.9676516,-2.
6022313\PG=C01 [X(C31H38O11)]\\@

**Global minimum**

1\1\GINC-AC58\FOpt\RAM1\ZDO\C31H38O11\CYL509\02-Nov-2006\0\\# OPT AM1\
\taxol\\0,1\C,-3.6635498228,3.8826217049,-4.3686084716\C,-3.1674780649
,3.6562275279,-3.0861901764\C,-2.4251935813,2.4966075597,-2.8237441556
\C,-2.1811047353,1.5695770081,-3.8447849552\C,-2.6817738705,1.80494230
49,-5.1240659972\C,-3.4214099681,2.9589465002,-5.3861024012\C,-1.91075
93994,2.2865643628,-1.4623674982\O,-2.0846498678,2.9970234585,-0.46656
88549\O,-1.1811260537,1.1325828887,-1.3253966067\C,-0.5478845752,0.872
2260523,-0.0566412557\C,0.8372457126,1.6011383162,-0.1089953959\C,1.55
74869725,1.6074248417,1.2725252839\C,1.9850844944,0.1815562044,1.50209
54577\C,2.7805148938,-0.404798381,0.5771880585\C,3.0137794761,0.318713
2367,-0.7221322818\C,1.7422112832,1.0272380768,-1.2101328669\C,1.43074
77142,-0.605594463,2.6434802782\O,1.8936161097,-0.0627531539,3.8928845
019\C,2.8487148579,-0.7538355933,4.590819253\O,3.3252340559,-1.7801913
616,4.1034085139\O,0.5782040415,2.9399290356,-0.5274559319\C,0.6733256
437,2.189946638,2.3661638432\C,2.7994013783,2.5150952505,1.2027613895\
C,3.3837107295,-1.7481905341,0.7166940242\O,3.4817513954,-0.5412181368
,-1.7514321077\C,-0.0935306524,-0.5764472618,2.6984795272\O,-0.6590826
262,-0.2338311734,3.7404155007\C,-0.9275086146,-1.1323584837,1.5310122

015\C,-0.5019556973,-0.6579056962,0.1254760541\C,-1.2566518473,-1.4128
697319,-0.9694505254\C,-1.8033553102,-2.8583849262,-0.6830500903\C,-1.
7088577279,-3.4205787645,0.7092727761\C,-0.6981022712,-2.6704782978,1.
5639394463\C,-2.3837005684,-0.8024333833,1.8422371278\C,-2.7438110902,
-1.0641938421,-1.3132303115\O,-3.1629090785,-2.4179820998,-0.996093738
7\O,-0.5627695041,-1.3446879207,-2.2200946307\C,0.5798679377,-2.063277
6608,-2.4257943059\O,1.0547857636,-2.728603717,-1.5008831911\O,-0.7000
106272,-3.1677877611,2.8883153005\C,1.1148035118,-1.895669905,-3.80726
07471\C,3.1719911718,-0.1062795028,5.8925636307\H,0.576676526,-0.97723
47872,-0.0033447162\H,1.7233882892,-1.6981231937,2.5690012736\H,-1.173
8526436,1.3385724581,0.7546109511\H,3.8529378763,1.0657570306,-0.60423
4608\H,1.1425438145,0.3145636905,-1.8374447928\H,2.0532738307,1.869568
4936,-1.8859102151\H,0.0225762088,3.3555177618,0.1467291504\H,-1.47157
02521,-3.5926190118,-1.4571767864\H,-2.7211045839,-3.4014939642,1.1958
007016\H,-1.3918162733,-4.4967402516,0.6606272251\H,0.3475039055,-2.89
30837593,1.192603277\H,-3.226796241,-0.3214617812,-0.6453499986\H,-2.9
210599503,-0.8401873494,-2.3881373098\H,-2.5530648629,0.3002706426,1.8
03258286\H,-3.0793067264,-1.3047164115,1.1302277558\H,-2.639749738,-1.
1469335355,2.875865985\H,4.3264846471,-1.8144297333,0.1164405054\H,2.6
714805527,-2.5286970741,0.338806637\H,3.6357114439,-1.9768463646,1.784
1634337\H,2.9434633005,-1.3451074515,-1.7321165776\H,-1.5607600934,-2.
9679324048,3.2788076856\H,0.5439611184,3.289096553,2.2036458153\H,1.15
4782164,2.031504812,3.3633639867\H,-0.3434004605,1.7358844124,2.403778
2715\H,3.7354014605,1.9299533343,1.3679092052\H,2.8564152318,3.0236419
331,0.2094262091\H,2.759874557,3.3070465071,1.98989481\H,1.4311947307,
-2.8925648433,-4.1998792225\H,2.004584138,-1.2157204676,-3.7634632784\
H,0.3458558478,-1.4490137955,-4.482426826\H,2.6364280044,0.86787749,5.
9993546338\H,2.8607073617,-0.792264665,6.7186626976\H,4.2750931117,0.0
615688025,5.9496788976\H,-3.3498529306,4.3783105033,-2.2736882505\H,-1
.5936797118,0.6605639148,-3.6266130306\H,-2.4920519779,1.0786582813,-5
.9280128303\H,-3.8142447614,3.1413661985,-6.3978599354\H,-4.2459236658
,4.792432612,-4.576730554\\Version=IA64L-G03RevC.02\State=1-A\HF=-0.62
28053\RMSD=0.000e+00\RMSF=1.712e-06\Dipole=-0.3643897,0.3940234,-1.312
7794\PG=C01 [X(C31H38O11)]\\@

**Viagra (structure 22)**

**Starting conformation**

1\1\GINC-AC31\FOpt\RAM1\ZDO\C22H30N6O4S1\CYL509\21-Nov-2006\0\\# OPT A
M1\\viagra\\0,1\N,-1.645983391,0.6291345194,-4.8941963697\C,-1.8121880
874,0.290606575,-3.5525740085\C,-0.5484578398,0.4981471894,-2.90538667
\C,0.322955864,0.9704789795,-3.9683179367\N,-0.3902511971,1.0249541364
,-5.1343216429\C,-2.9636832347,-0.1744252544,-2.7910227154\N,-2.672201
6581,-0.4163171916,-1.4383425703\C,-1.4022992519,-0.1740760736,-0.8851
831607\N,-0.3428257257,0.264352371,-1.563098204\C,-1.2422360738,-0.472
57111,0.5630802631\C,-2.1401117277,0.0206198006,1.5403208802\C,-1.9250
6713,-0.2706832279,2.8976049486\C,-0.8289514468,-1.0352590298,3.272812
8252\C,0.0741751699,-1.5287121152,2.3236224442\C,-0.1522980458,-1.2408
46374,0.9737055112\S,1.3837563196,-2.4907609962,2.7980218579\O,1.57823
14805,-3.4777837555,1.8084565487\O,-3.1840038384,0.7759742767,1.070664
9905\C,-4.0947630204,1.3496975532,2.0181655129\C,-5.1247683607,0.34730
88268,2.4762162138\O,-4.1136119739,-0.3654324715,-3.2295754566\C,1.758
4391064,1.3007170972,-3.8226138982\C,2.1662068924,2.5917356119,-4.5051
427455\C,1.5738351966,3.8066457926,-3.8393363842\C,-2.6796420386,0.554
9345774,-5.9026351475\N,2.6400156846,-1.4645073722,2.8014950467\C,3.00
24493941,-0.6668705848,3.9447073114\C,3.1588926509,0.834694452,3.62217
11855\N,4.0014654617,1.0794811321,2.4608803043\C,3.618621145,0.2787213

986,1.3064832913\C,3.4586618492,-1.2196093457,1.6410107793\C,4.1084385
147,2.4857404612,2.1443255511\O,1.1268473401,-2.9377937855,4.114284237
5\H,3.9794688556,-1.0494970263,4.3606312669\H,2.2137218185,-0.77934506
1,4.7423143435\H,3.6491385664,1.3250580134,4.5091890875\H,2.1331915858
,1.2907659136,3.4986582109\H,4.4388338468,0.3711148326,0.5407502241\H,
2.6624007649,0.6522466477,0.8360255046\H,3.0023424067,-1.7353790656,0.
7478836913\H,4.481771397,-1.6617938833,1.8180385405\H,3.1305158877,2.9
504538418,1.8388329211\H,4.4960255754,3.0292758126,3.04534946\H,4.8402
787333,2.6104713912,1.3038507111\H,-0.6709190068,-1.274911434,4.341289
6812\H,-2.6192918708,0.0955232201,3.6674128396\H,0.5448272671,-1.64305
75144,0.2138764674\H,-4.5736643037,2.1693721535,1.4115424243\H,-3.5362
336923,1.8033058533,2.8765994077\H,-5.8580727711,0.8513539659,3.150621
392\H,-4.6473456052,-0.497238119,3.0288387034\H,-5.6735522053,-0.07511
15791,1.5998453186\H,-3.4221141609,-0.6625591399,-0.8286016774\H,-2.37
77288067,-0.1725529545,-6.7027216307\H,-2.8327906941,1.5666466388,-6.3
64396408\H,-3.6295453905,0.2103119334,-5.4108408497\H,2.3616848146,0.4
532648729,-4.252180828\H,1.9967642508,1.3647583305,-2.7265270823\H,1.8
633577459,2.5663822103,-5.5847343572\H,3.2868468434,2.6631105179,-4.47
769653\H,1.8987352588,4.7345957191,-4.3689649347\H,1.9026444865,3.8742
018952,-2.7740283754\H,0.4581118459,3.7600394733,-3.858850066\\Version
=IA64L-G03RevC.02\State=1-A\HF=-0.0393671\RMSD=0.000e+00\RMSF=3.161e-0
6\Dipole=-0.9474696,2.1404943,0.7712647\PG=C01 [X(C22H30N6O4S1)]\\@

**Global minimum**

1\1\GINC-AC20\FOpt\RAM1\ZDO\C22H30N6O4S1\CYL509\21-Nov-2006\0\\# OPT A
M1\\viagra\\0,1\N,-2.3911223931,-0.2360766025,-4.3078218267\C,-2.37210
85966,-0.2319222241,-2.9139750857\C,-1.0070127599,-0.0486702526,-2.512
4046829\C,-0.2760864132,0.0457790895,-3.7638050737\N,-1.1582965023,-0.
0745463904,-4.802572482\C,-3.4241292233,-0.3527933405,-1.9133143905\N,
-2.9428803717,-0.3104298045,-0.5935282151\C,-1.5845953284,-0.112722322
9,-0.2925752834\N,-0.611458618,0.0115927761,-1.1947682227\C,-1.2104203
677,-0.0726900883,1.1461013129\C,-1.8946736724,0.7278419383,2.09110874
18\C,-1.4475120754,0.7773166472,3.4220673417\C,-0.3332231516,0.0416459
648,3.8028752823\C,0.3542694682,-0.7646436898,2.8870259157\C,-0.105981
9026,-0.8147262081,1.5680736991\S,1.6912933749,-1.6794098147,3.3873972
27\O,1.4277470795,-3.0380296309,3.1146780889\O,-2.9844948347,1.4202570
906,1.6297085219\C,-3.6309211543,2.3099153339,2.558838963\C,-4.7338052
83,2.9840794218,1.7770907263\O,-4.6423412925,-0.4885065958,-2.13309732
36\C,1.185885007,0.2294285283,-3.901941688\C,1.5366286312,1.5235093031
,-4.6120386126\C,3.0297701254,1.7247183239,-4.6562709249\C,-3.57562154
69,-0.4050070221,-5.1200468681\N,2.8945517569,-1.1569352546,2.43429136
44\C,3.6106077622,0.0709821536,2.6684223557\C,3.6529221062,1.001271071
4,1.4366940003\N,4.0733066954,0.3162571463,0.2225525021\C,3.3412561037
,-0.9211724159,-0.0104201149\C,3.2988992091,-1.8387715777,1.2300001502
\C,4.0563250999,1.1845894166,-0.9338081203\O,1.9474847517,-1.340927290
7,4.7351476235\H,4.6694886614,-0.1769445701,2.9702004059\H,3.124633900
8,0.6280915606,3.5189670419\H,4.4051857908,1.8118971808,1.647819814\H,
2.6428060664,1.4904609958,1.3133618762\H,3.8735960386,-1.4812336052,-0
.8294239136\H,2.28405497,-0.7229323097,-0.3578161552\H,2.5843884359,-2
.6859736837,1.0207573878\H,4.3264955144,-2.2770972958,1.3901319114\H,3
.0224883317,1.5185152576,-1.2279693027\H,4.677692871,2.0918004519,-0.7
150384392\H,4.5107851322,0.6349608506,-1.7998391555\H,0.0202857858,0.0
88605232,4.8508265702\H,-1.9687966599,1.3943080352,4.1676624724\H,0.42
16788428,-1.4561409244,0.8372103703\H,-2.8830449575,3.0543794972,2.938
1542069\H,-4.0415670076,1.7097530996,3.4127921208\H,-5.2778417962,3.68
65891298,2.4525786575\H,-5.4521664194,2.2280549924,1.378753375\H,-4.31
14611757,3.555368531,0.9159934672\H,-3.6055534432,-0.3079846499,0.1524
085417\H,-3.4767924031,-1.3309484992,-5.7472373425\H,-3.7036458436,0.4

837008577,-5.7938557674\H,-4.4626516727,-0.4987648995,-4.4363861569\H,
1.620642388,-0.6382249296,-4.4696385382\H,1.6457406281,0.2270583932,-2
.8758945756\H,1.0551149284,2.3852281809,-4.0792821533\H,1.1247352877,1
.5047888987,-5.6551504241\H,3.2749141273,2.6895812105,-5.1619557686\H,
3.5237340063,0.8959342816,-5.2189050793\H,3.455663845,1.7485957845,-3.
6223340705\\Version=IA64L-G03RevC.02\State=1-A\HF=-0.0412795\RMSD=0.00
0e+00\RMSF=6.702e-06\Dipole=-0.819324,2.0524331,-0.2323274\PG=C01 [X(C
22H30N6O4S1)]\\@

**Figure S1.** Global Minimum Energy Conformations of the Species in the Test Set-1.

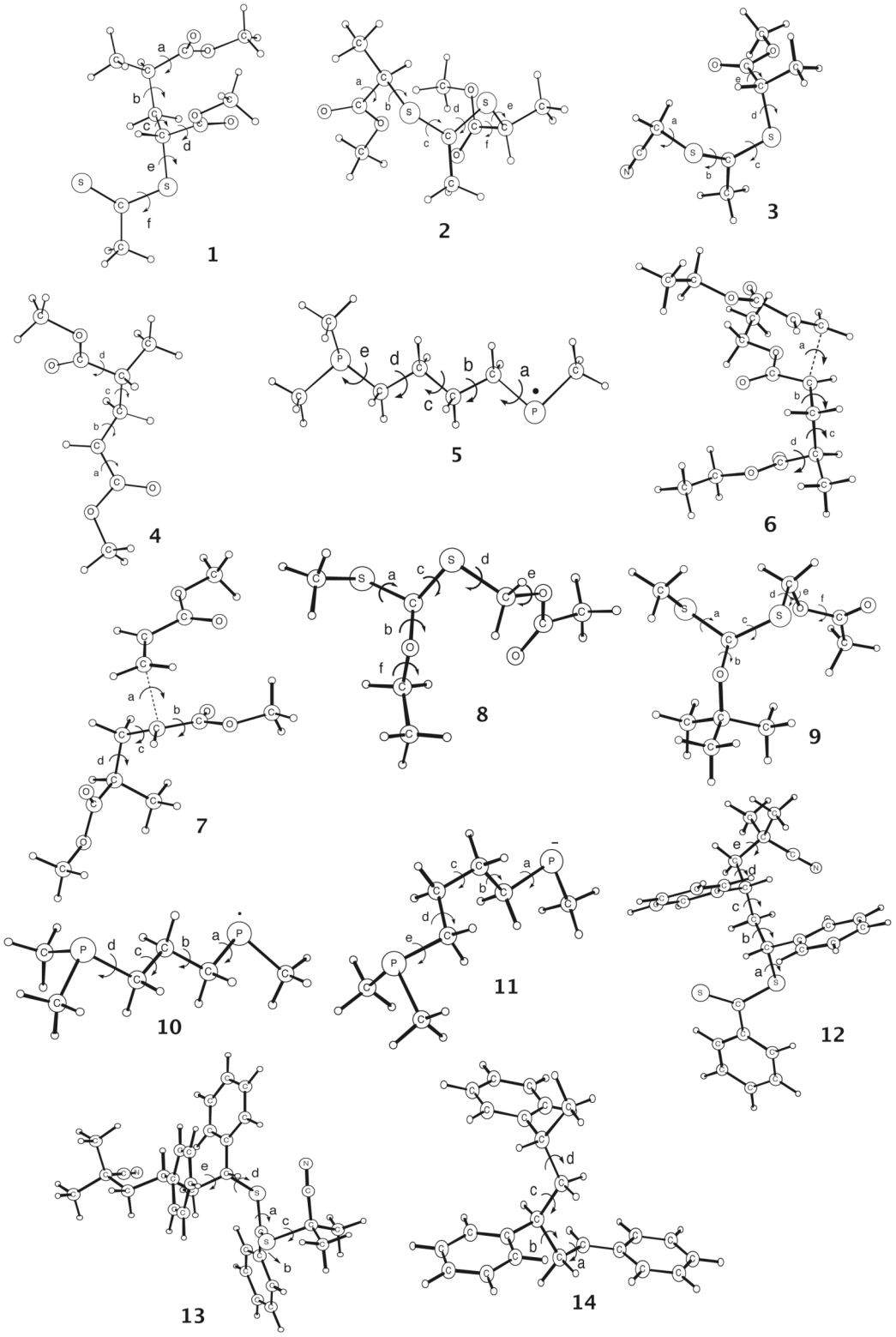


**Figure S2.** Global Minimum Energy Conformations of the Species in the Test Set-2.