Supporting Information for

A permutation approach to the assignment of the configuration to diastereomeric tetrads by comparison of experimental and ab initio calculated differences in NMR data

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Plots of NMR spectra for new compounds, HSQC experiments for tetrad 1, supporting tables, complete reference 16, synthetic references for compounds 1–4, presentation of manual workflow and Python code for automated processing

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**S1. Supporting references**

Synthesis of **1a**:

Boratyński, P. J.; Kowalczyk, R. *J. Org. Chem.* **2016**, *81*, 8029-8034.

Synthesis of **2a** and **2c**:

Boratyński, P. J.; Turowska-Tyrk, I.; Skarżewski, J. *Org. Lett.* **2008**, *10*, 385–388.

Synthesis **2d** and **3a-d** including NMR calculation for tetrad **3**.

Boratyński, P. J.; Turowska-Tyrk, I.; Skarżewski, J. *Tetrahedron: Asymmetry* **2012**, *23*, 876-883.

Synthesis and NMR calculation of **4a-d**:

Boratyński, P. J.; Skarżewski, J. *J. Org. Chem.* **2013**, *78*, 4473-4482.

Complete Gaussian reference, Reference 16 from main text

Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr., Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. *Gaussian 09, E.01*, Gaussian, Inc.: Wallingford, CT, 2009.
S2. Manual workflow example

Here the approach is exemplified by conducting the entire process manually and stepwise on the example of three signals assigned to three atoms (C-6, C-7, and C-8) for diastereomeric tetrad 1. For automatic processing, a simple computer program can be implemented, for example see Section S6.

Part A. Initial data

Interpretation of $^{13}$C NMR data for four diastereomers 1a-1d. Assignment of chemical shifts to particular atoms.

Molecular models of diastereomers 1 of specified configurations (SS, SR, RR, RS) are made, their geometries are optimized. Populations of individual conformers are evaluated based on their energy. Calculation of GIAO isotropic shieldings, e.g. at B3LYP/6-31G(d,p) level of theory or higher.

For corresponding atoms, four individual shifts (or shieldings) are averaged. Then individual shifts are expressed as deviations from this average.

| atom | 1a | 1b | 1c | 1d | average | 85,9S | 85,9R | 8R,9R | 8R,9S |
|------|----|----|----|----|---------|------|------|------|------|
| C-6  | 141.8 | 144.6 | 136.3 | 136.3 | 140.5 | -4.3 | -4.1 | 4.2 | 4.2 |
| C-7  | 157.3 | 160.0 | 158.2 | 160.7 | 159.0 | 1.8 | -1.0 | 0.8 | -1.6 |
| C-8  | 126.4 | 127.1 | 126.2 | 126.8 | 126.6 | 0.2 | -0.4 | 0.4 | -0.2 |

GIAO calculation

Negative sign of deviation is used for shieldings.
Part B. Processing

24 differently ordered non-repeating assignments of four configurations to four compounds, corresponding to permutations of experimental and DFT data

And corresponding data are set together for all atoms and all isomers

Selected comparison measure (cf. Table 1 in main text) is calculated to rank all the 24 permutations. In the example below: aggregate overlap

1. IF signs of Δ exp and Δ DFT match add lower value from |Δ exp| and |Δ DFT|
2. Repeat for next item

Finally the permutations are sorted according to their scores, the highest ranking permutation reflects the assignment predicted by computation
S3. Peripheral discussion

Alternative number of stereocenters (N) and diastereomers

N = 1: For one varying stereocenter there are can be two diastereomers. The number of permutations \( P_2 = 2! = 2 \) reduces the approach to the method by Goodman and Smith of comparing two isomers (CP3), and offers no advantage.

N = 3: For three varying stereocenters and eight possible diastereomers the number of permutations increases significantly \( P_8 = 8! = 40320 \). The method could easily be applied by using the algorithm run by a computer, however both experimental and DFT computed data have to be obtained with very high precision and accuracy which is often unattainable for some compounds.

N = 4: For four varying centers and sixteen diastereomers the number of permutation becomes very large \( P_{16} = 16! = 2 \times 10^{13} \) to the point of unfeasibility.

Alternative definition of midpoint.

Referencing the data instead of averages of chemical shifts and isotropic shieldings can be done using alternatively the corresponding median values. This approach was considered, because the midpoint is unaffected by the extreme values. However, for the studied compounds 1–7 no advantage of using the median was noted, the correct permutations received slightly worse scores, and separation between two highest rating permutations did not improve. In case of assignments of four possible configurations to three compounds the application of the median had a noticeably lower success ratio.

S4. Supporting Tables

Table S1. Percentage of correctly identified configuration by highest ranking permutation for sets of three diastereomers of compounds 1–7. This is an expanded version of Table 4 from the main text

|          | \(^{13}\)C NMR data |          | \(^{1}\)H NMR data |
|----------|----------------------|----------|----------------------|
|          | 1        | 2        | 3        | 4        | 5        | 6        | 7        | 1        | 2        | 3        | 4        | 5        | 6        | 7        |
| CP1      | 75%      | 100%     | 100%     | 100%     | 100%     | 100%     | 80%      | 50%      | 0%       | 100%     | 75%      | 25%      | 25%      |
| CP2      | 75%      | 75%      | 100%     | 100%     | 50%      | 75%      | 75%      | 75%      | 50%      | 100%     | 100%     | 100%     | 50%      | 25%      |
| CP3      | 75%      | 100%     | 100%     | 100%     | 100%     | 75%      | 75%      | 75%      | 25%      | 100%     | 100%     | 25%      | 25%      |
| OL\(^c\) | 100%     | 100%     | 100%     | 100%     | 100%     | 100%     | 50%      | 75%      | 100%     | 25%      | 100%     | 100%     | 75%      | 50%      | 50%      |
| RMS      | 100%     | 100%     | 100%     | 100%     | 100%     | 100%     | 100%     | 100%     | 25%      | 100%     | 100%     | 100%     | 100%     | 25%      | 25%      |
| R\(^b\)  | 100%     | 100%     | 100%     | 100%     | 100%     | 100%     | 100%     | 100%     | 25%      | 100%     | 100%     | 25%      | 100%     | 25%      |
| MAE      | 100%     | 100%     | 100%     | 100%     | 100%     | 75%      | 100%     | 100%     | 25%      | 100%     | 100%     | 100%     | 100%     | 50%      | 25%      |

\(^a\) Aggregate overlap, \(^b\) Pearson correlation coefficient, \(^c\) Average for compound tetrad. Cases when some of the measures did not point to the correct assignment were highlighted in yellow or orange. Each entry corresponds to four tests, where one experimental data was taken out.
### S4.1. Tables of experimental NMR shifts and GIAO shieldings

**Table S2.** Assignment of $^{13}$C and $^1$H NMR signals for tetrad 1, and calculated isotropic shieldings at the GIAO/PW1PW91/6-311+G(2d,p) level of theory

| Atom label | Experimental chemical shift $\delta$ (ppm) | DFT isotropic shielding, $\sigma$ (ppm) |
|------------|-------------------------------------------|----------------------------------------|
|            | 1a       | 1b       | 1c       | 1d       | 8S,9S | 8S,9R | 8R,9R | 8R,9S |
| $^{13}$C    |          |          |          |          |       |       |       |       |
| C-2        | 56.21    | 55.84    | 47.22    | 49.25    | 127.66| 128.15| 137.03| 136.81|
| C-3        | 39.26    | 39.46    | 39.01    | 39.76    | 141.24| 140.86| 140.61| 140.65|
| C-4        | 27.79    | 27.21    | 27.61    | 27.52    | 153.46| 154.39| 153.55| 154.31|
| C-5        | 27.77    | 27.74    | 26.47    | 26.43    | 156.78| 156.55| 158.32| 158.15|
| C-6        | 41.19    | 41.47    | 49.41    | 48.27    | 144.78| 144.59| 136.28| 136.32|
| C-7        | 27.65    | 25.20    | 26.19    | 24.70    | 157.25| 160.04| 158.20| 160.66|
| C-8        | 58.21    | 57.39    | 58.28    | 57.48    | 126.40| 127.07| 126.25| 126.85|
| C-9        | 60.67    | 61.39    | 59.60    | 60.83    | 122.83| 122.15| 123.95| 122.51|
| C-10       | 141.44   | 141.67   | 140.24   | 140.02   | 34.99 | 35.10 | 37.04 | 36.77 |
| C-11       | 114.97   | 114.91   | 115.02   | 115.30   | 68.84 | 69.08 | 68.83 | 68.65 |
| C-2'       | 147.46   | 147.60   | 147.38   | 147.59   | 35.11 | 34.91 | 35.02 | 35.18 |
| C-3'       | 119.45   | 119.93   | 119.52   | 119.69   | 63.26 | 61.57 | 62.89 | 61.97 |
| C-4'       | 139.30   | 139.64   | 139.72   | 140.06   | 41.57 | 40.89 | 41.19 | 40.63 |
| C-5'       | 100.89   | 100.41   | 100.50   | 100.48   | 83.58 | 83.51 | 83.35 | 84.27 |
| C-6'       | 158.83   | 158.55   | 158.72   | 158.54   | 22.43 | 22.89 | 22.52 | 22.89 |
| C-7'       | 122.53   | 122.20   | 122.50   | 122.21   | 59.43 | 60.34 | 59.69 | 60.31 |
| C-8'       | 134.04   | 132.07   | 132.08   | 132.08   | 49.91 | 49.65 | 49.67 | 49.80 |
| C-9'       | 128.33   | 128.00   | 128.12   | 128.07   | 53.23 | 54.53 | 53.56 | 54.10 |
| C-10'      | 145.20   | 145.13   | 145.03   | 145.12   | 37.09 | 36.93 | 36.87 | 37.21 |
| OCH$_3$    | 55.96    | 56.02    | 55.77    | 55.85    | 131.09| 131.28| 131.05| 131.35|
| C-4''      | 139.26   | 134.58   | 133.81   | 134.44   | 48.66 | 48.10 | 48.61 | 48.18 |
| C-5''      | 122.12   | 122.25   | 122.50   | 122.46   | 59.92 | 58.51 | 59.71 | 58.42 |
| $^1$H      |          |          |          |          |       |       |       |       |
| H-2a       | 2.778    | 2.899    | 3.073    | 2.715    | 29.263| 29.042| 28.641| 29.141|
| H-2s       | 3.214    | 3.168    | 2.990    | 2.891    | 28.639| 28.604| 29.012| 29.119|
| H-3        | 2.340    | 2.324    | 2.298    | 2.288    | 29.459| 29.484| 29.493| 29.539|
| H-4        | 1.787    | 1.870    | 1.758    | 1.807    | 30.244| 30.178| 30.223| 30.166|
| H-5n       | 1.627    | 1.564    | 1.642    | 1.651    | 30.245| 30.314| 30.223| 30.232|
| H-5x       | 1.627    | 1.771    | 1.642    | 1.651    | 30.218| 30.067| 30.185| 30.159|
| H-6n       | 2.751    | 2.653    | 2.902    | 2.885    | 29.235| 29.299| 28.985| 28.987|
| H-6x       | 3.462    | 3.899    | 3.984    | 3.070    | 28.240| 28.892| 28.951| 28.778|
| H-7n       | 1.937    | 1.182    | 1.436    | 1.685    | 29.726| 30.187| 30.413| 29.873|
| Atom label | Experimental chemical shift $\delta$ (ppm) | DFT isotropic shielding, $\sigma$ (ppm) |
|------------|------------------------------------------|--------------------------------------|
|            | 2a | 2b | 2c | 2d | 8S,9S | 8S,9R | 8R,9R | 8R,9S |
| $^{13}$C   |    |    |    |    |       |       |       |       |
| C-2        | 56.55 | 56.18 | 47.55 | 47.63 | 133.77 | 134.05 | 142.43 | 142.92 |
| C-3        | 39.58 | 39.76 | 39.78 | 39.80 | 146.46 | 146.57 | 145.87 | 146.04 |
| C-4        | 28.08 | 28.02 | 28.02 | 28.15 | 159.43 | 159.72 | 159.66 | 159.59 |
| C-5        | 28.08 | 28.14 | 26.66 | 26.58 | 160.80 | 161.38 | 162.63 | 162.41 |
| C-6        | 40.92 | 41.03 | 49.58 | 49.33 | 149.18 | 149.82 | 141.03 | 141.25 |
| C-7        | 28.81 | 27.86 | 27.74 | 27.15 | 160.63 | 161.92 | 161.55 | 162.77 |
| C-8        | 59.48 | 58.26 | 58.99 | 58.08 | 129.30 | 130.49 | 129.34 | 131.29 |
| C-9        | 49.47 | 50.18 | 48.11 | 49.33 | 139.57 | 138.10 | 140.60 | 139.30 |
| C-10       | 142.03 | 142.12 | 140.90 | 140.83 | 54.30  | 54.70  | 56.27  | 56.11  |
| C-11       | 114.28 | 114.71 | 114.44 | 114.67 | 82.15  | 82.23  | 81.77  | 81.71  |
| OCH$_3$    | 55.48 | 55.47 | 55.45 | 55.54 | 138.74 | 138.73 | 138.74 | 139.05 |
| C-2'       | 147.61 | 147.81 | 147.55 | 147.82 | 50.31  | 50.45  | 50.32  | 50.40  |
| C-3'       | 119.75 | 119.70 | 120.06 | 119.46 | 75.03  | 73.39  | 75.34  | 74.31  |
| C-4'       | 146.76 | 146.93 | 147.16 | 147.20 | 48.77  | 49.90  | 49.04  | 49.22  |
| C-5'       | 102.09 | 102.01 | 101.71 | 102.17 | 93.68  | 93.91  | 93.84  | 93.69  |
| C-6'       | 157.72 | 157.45 | 157.83 | 157.53 | 39.55  | 40.06  | 39.49  | 40.07  |
| C-7'       | 120.92 | 120.53 | 121.28 | 121.47 | 74.91  | 75.68  | 74.88  | 75.63  |
| C-8'       | 131.91 | 131.87 | 131.88 | 131.83 | 63.90  | 63.98  | 63.90  | 64.00  |
| C-9'       | 128.79 | 128.44 | 128.79 | 128.67 | 65.90  | 66.31  | 65.79  | 66.17  |
| C-10'      | 144.77 | 144.86 | 144.80 | 144.89 | 51.29  | 51.41  | 51.31  | 51.32  |
| C-ipso     | 142.16 | 140.71 | 142.32 | 140.73 | 52.68  | 54.14  | 52.59  | 54.25  |

**Table S3.** Assignment of $^{13}$C NMR signals for tetrad 2, and calculated isotropic shieldings at the GIAO/B3LYP/6-31G(d,p) level of theory.
| Atom label | Experimental chemical shift $\delta$ (ppm) | DFT isotropic shielding, $\sigma$ (ppm) |
|------------|------------------------------------------|----------------------------------------|
|            | $3a$ | $3b$ | $3c$ | $3d$ | $8S,9S$ | $8S,9R$ | $8R,9R$ | $8R,9S$ |
| C-2        | 57.5 | 57.6 | 48.8 | 49.5 | 127.22 | 126.87 | 135.10 | 134.91 |
| C-3        | 39.8 | 39.9 | 39.6 | 39.8 | 140.73 | 140.36 | 141.06 | 140.25 |
| C-4        | 28.4 | 28.3 | 29.4 | 29.1 | 153.18 | 153.25 | 152.56 | 152.42 |
| C-5        | 27.5 | 27.8 | 26.4 | 26.2 | 157.63 | 157.50 | 157.78 | 158.64 |
| C-6        | 43.1 | 43.6 | 50.8 | 50.8 | 143.02 | 141.56 | 134.35 | 135.29 |
| C-7        | 25.3 | 25.1 | 24.4 | 23.8 | 158.99 | 160.24 | 159.73 | 161.35 |
| C-8        | 62.8 | 61.1 | 63.1 | 61.4 | 120.68 | 124.68 | 119.89 | 124.50 |
| C-9        | 78.9 | 79.7 | 78.4 | 79.3 | 103.37 | 101.10 | 103.37 | 99.96  |
| C-10       | 141.9| 142.2| 139.1| 139.7| 35.07  | 34.37  | 37.43  | 35.64  |
| C-11       | 115  | 114.7| 114.6| 114.4| 68.39  | 69.79  | 68.66  | 70.09  |
| C-2'       | 147.1| 147.4| 144  | 147.4| 35.65  | 35.06  | 35.56  | 35.03  |
| C-3'       | 117.6| 120.4| 117.5| 120.5| 66.23  | 61.51  | 65.70  | 61.37  |
| C-4'       | 150  | 149.4| 149.8| 149.7| 28.63  | 29.16  | 28.85  | 29.57  |
| C-5'       | 106.3| 104.8| 106.3| 105.1| 77.09  | 80.02  | 77.48  | 80.31  |
| C-6'       | 156.8| 156.5| 156.7| 156.4| 24.76  | 24.45  | 24.47  | 24.74  |
| C-7'       | 121.5| 121.3| 121.5| 121.1| 61.36  | 61.43  | 61.36  | 61.57  |
| C-8'       | 131.2| 131.5| 131  | 131.4| 50.63  | 49.76  | 50.65  | 49.66  |
| C-9'       | 128.8| 126.9| 127.5| 127.1| 54.55  | 55.93  | 54.67  | 56.29  |
| C-10'      | 146.1| 145.3| 146.8| 145.3| 35.70  | 36.41  | 35.87  | 36.81  |
| OCH3       | 55.4 | 55.3 | 55.3 | 55.3 | 131.85 | 132.06 | 131.88 | 132.04 |
| C-ortho    | 143.9| 145.7| 146.1| 145.5| 35.40  | 31.84  | 35.67  | 32.62  |
| C-meta     | 127.7| 126.9| 127.5| 127.2| 53.71  | 53.22  | 54.05  | 53.23  |
| C-meta     | 127.6| 128.5| 127.7| 128.6| 55.58  | 53.81  | 55.63  | 53.76  |

**Table S4.** Assignment of $^{13}$C and $^1$H NMR signals for tetrad 3, and calculated isotropic shieldings at the GIAO/PW1PW91/6-311+G(2d,p) level of theory.
| Atom label | Experimental chemical shift δ (ppm) | DFT isotropic shielding, σ (ppm) |
|------------|-------------------------------------|----------------------------------|
|            | 4a  | 4b  | 4c  | 4d  | 8S,9S | 8S,9R | 8R,9R | 8R,9S |
| C-2        | 56.1| 57.4| 49  | 49.1| 134.26| 133.52| 141.51| 141.21|
| C-3        | 39.4| 39.8| 40.1| 39.7| 146.62| 145.96| 146.27| 146.02|
| C-4        | 27.7| 27.8| 28.3| 28.3| 159.41| 159.38| 158.97| 159.14|
| C-5        | 27.4| 27.8| 26.6| 26.4| 161.58| 161.31| 162.58| 162.89|
| C-6        | 42.4| 42.7| 49.4| 50.3| 148.12| 147.70| 141.24| 140.41|
| C-7        | 20.2| 24  | 20.1| 20.9| 168.32| 163.98| 168.73| 165.13|
| C-8        | 57.5| 56.1| 57.6| 55.5| 131.30| 134.72| 131.41| 134.87|
| C-9        | 59.1| 62.8| 59.2| 63.2| 130.45| 125.81| 130.07| 125.91|
| C-10       | 142.1|141.8|140.7|140.3| 54.40  | 54.69  | 54.58  | 55.85  |
| C-11       | 114.5|114.4|114.1|114.5| 82.06  | 82.09  | 81.82  | 81.84  |
| C-2'       | 147.7|147.4|147.7|147.4| 50.08  | 49.89  | 50.07  | 49.91  |
| C-3'       | 119.9|120.2|120.3|120  | 75.61  | 75.32  | 75.49  | 75.38  |
| C-4'       | 144.1|143.7|144.6|143.7| 49.17  | 51.16  | 49.18  | 51.12  |
| C-5'       | 102.2|102.1|102.4|102.0| 94.20  | 93.99  | 94.30  | 93.94  |
| C-6'       | 157.5|158 |157.5|157.9| 39.58  | 39.20  | 39.63  | 39.31  |
| C-7'       | 120.5|121.8|120.4|121.7| 74.49  | 74.46  | 74.82  | 74.47  |
| C-8'       | 131.9|131.8|132 |131.8| 63.65  | 63.69  | 63.69  | 63.71  |
| C-9'       | 126.7|126.8|126.7|126.8| 68.07  | 68.09  | 68.07  | 68.09  |
| C-10'      | 144.7|144.5|144.1|144.4| 51.84  | 51.90  | 51.87  | 51.88  |
### Tables with all permutations and their scores

**Table S6a.** Complete list of permutations with scores for comparison of experimental and calculated $^{13}$C NMR data for compound tetrad 1

| Permutation | $^{13}$C data score |
|-------------|---------------------|
| Perm. 1a    | Perm. 1b | Perm. 1c | Perm. 1d | CP1  | CP2  | CP3  | overlap | RMS  | correl | MAE  |
| 8S,9S       | 8S,9R    | 8R,9R    | 8R,9S    | 0.951 | 0.740 | 0.739 | 48.05   | 0.640 | 0.892  | 0.378 |
| 8S,9S       | 8S,9R    | 8R,9S    | 8R,9R    | 0.905 | 0.700 | 0.694 | 43.59   | 0.758 | 0.849  | 0.479 |
| 8S,9R       | 8S,9S    | 8R,9R    | 8R,9S    | 0.902 | 0.720 | 0.705 | 42.51   | 0.764 | 0.846  | 0.503 |
| 8S,9R       | 8S,9S    | 8R,9S    | 8R,9R    | 0.855 | 0.640 | 0.600 | 38.05   | 0.864 | 0.802  | 0.605 |
| 8S,9S       | 8R,9S    | 8R,9R    | 8S,9R    | 0.180 | 0.237 | 0.101 | 30.47   | 1.766 | 0.169  | 0.777 |
| 8S,9S       | 8R,9R    | 8R,9S    | 8S,9R    | 0.120 | 0.210 | 0.053 | 26.60   | 1.824 | 0.113  | 0.865 |
| 8S,9R       | 8R,9S    | 8R,9R    | 8S,9S    | 0.098 | 0.226 | 0.059 | 25.45   | 1.846 | 0.092  | 0.891 |
| 8R,9S       | 8S,9R    | 8R,9R    | 8S,9R    | 0.085 | 0.124 | -0.001 | 24.53  | 1.857 | 0.080  | 0.912 |
| 8R,9R       | 8S,9S    | 8R,9R    | 8S,9R    | 0.077 | 0.133 | -0.007 | 25.41  | 1.866 | 0.072  | 0.892 |
| Permutation | 1a     | 1b     | 1c     | 1d     | CP1   | CP2   | CP3   | overlap | RMS   | correl | MAE   |
|------------|--------|--------|--------|--------|-------|-------|-------|---------|-------|--------|-------|
| 8R,9S      | 8S,9R  | 8R,9R  | 8S,9S  | 0.052  | 0.134 | -0.009 | 25.04 | 1.888   | 0.049 | 0.900  |
| 8R,9R      | 8S,9R  | 8S,9S  | 8S,9S  | 0.044  | 0.143 | -0.015 | 25.93 | 1.897   | 0.041 | 0.880  |
| 8S,9R      | 8R,9R  | 8R,9S  | 8S,9S  | -0.036 | -0.134 | -0.199 | 24.14 | 1.969   | -0.034 | 0.921  |
| 8S,9S      | 8R,9R  | 8S,9S  | 8R,9R  | -0.049 | -0.120 | -0.201 | 24.72 | 1.981   | -0.046 | 0.908  |
| 8R,9R      | 8R,9S  | 8S,9S  | 8R,9R  | -0.080 | -0.143 | -0.209 | 22.50 | 2.008   | -0.075 | 0.958  |
| 8R,9S      | 8S,9S  | 8R,9S  | 8R,9S  | -0.087 | -0.187 | -0.238 | 27.44 | 2.014   | -0.082 | 0.846  |
| 8R,9R      | 8R,9S  | 8S,9S  | 8R,9R  | -0.093 | -0.198 | -0.262 | 23.54 | 2.019   | -0.087 | 0.934  |
| 8R,9S      | 8R,9R  | 8S,9S  | 8R,9R  | -0.093 | -0.130 | -0.122 | 23.08 | 2.019   | -0.087 | 0.945  |
| 8R,9S      | 8S,9S  | 8S,9S  | 8R,9S  | -0.125 | -0.236 | -0.277 | 22.09 | 2.047   | -0.117 | 0.967  |
| 8R,9S      | 8S,9S  | 8S,9R  | 8R,9R  | -0.130 | -0.246 | -0.301 | 18.20 | 2.051   | -0.122 | 1.056  |
| 8R,9S      | 8R,9S  | 8S,9S  | 8S,9R  | -0.859 | -0.691 | -0.876 | 9.86  | 2.601   | -0.806 | 1.245  |
| 8R,9S      | 8R,9S  | 8S,9S  | 8R,9S  | -0.897 | -0.691 | -0.908 | 6.48  | 2.627   | -0.841 | 1.322  |
| 8R,9S      | 8R,9R  | 8S,9S  | 8S,9R  | -0.910 | -0.726 | -0.918 | 5.10  | 2.635   | -0.854 | 1.354  |
| 8R,9S      | 8S,9R  | 8S,9R  | 8S,9S  | -0.948 | -0.727 | -0.949 | 1.72  | 2.661   | -0.889 | 1.430  |

**Table S6b.** Complete list of permutations with scores for comparison of experimental and calculated $^1$H NMR data for compound tetrad 1
Table S7. Complete list of permutations with scores for comparison of experimental and calculated $^{13}$C NMR data for compound tetrads 2

| Permutation | $^{13}$C data score |
|-------------|---------------------|
|             | CP1  | CP2  | CP3  | overlap | RMS  | correl | MAE  |
| 8R,9R       | 8S,9R| 8R,9R| 8R,9S|         |      |        |      |
| 8S,9S       | 0.995| 0.938| 0.935| 52.82   | 0.330| 0.969  | 0.226|
| 8S,9R       | 0.950| 0.901| 0.894| 47.55   | 0.512| 0.925  | 0.336|
| 8S,9S       | 0.948| 0.891| 0.884| 46.58   | 0.519| 0.923  | 0.356|
| 8S,9S       | 0.903| 0.854| 0.843| 41.31   | 0.650| 0.879  | 0.466|
| 8S,9S       | 0.057| 0.081| 0.035| 31.99   | 1.813| 0.055  | 0.660|
| 8R,9R       | 0.037| 0.003| -0.014|31.11 | 1.831| 0.036  | 0.678|
| 8S,9R       | 0.028| 0.046| -0.002|27.97 | 1.839| 0.027  | 0.744|
| 8S,9S       | 0.018| 0.031| -0.007|26.37 | 1.849| 0.017  | 0.777|
| 8S,9R       | 0.015| 0.001| -0.025|25.63 | 1.852| 0.014  | 0.774|
| 8R,9R       | 0.011| -0.001| -0.028|26.93 | 1.855| 0.011  | 0.766|
| 8S,9R       | 0.009| 0.014| -0.025|26.88 | 1.857| 0.009  | 0.767|
| 8S,9S       | 0.001| -0.005| -0.032|27.40 | 1.865| 0.001  | 0.756|
| 8R,9S       | -0.002| -0.002| -0.033|28.18 | 1.867| -0.002 | 0.739|
| 8S,9S       | -0.005| 0.007| -0.032|27.75 | 1.870| -0.005 | 0.748|
| 8S,9S       | -0.007| -0.014| -0.046|24.72 | 1.872| -0.007 | 0.812|
| 8S,9S       | -0.011| -0.003| -0.040|22.35 | 1.875| -0.011 | 0.861|
| 8R,9S       | -0.021| -0.015| -0.051|25.97 | 1.884| -0.020 | 0.786|
| 8R,9S       | -0.021| -0.034| -0.060|27.09 | 1.884| -0.021 | 0.762|
| 8R,9S       | -0.025| -0.051| -0.072|25.74 | 1.887| -0.024 | 0.790|
| 8R,9S       | -0.083| -0.089| -0.118|21.72 | 1.939| -0.081 | 0.874|
| 8R,9S       | -0.901| -0.854| -0.914|10.28 | 2.556| -0.878 | 1.112|
| 8R,9S       | -0.954| -0.904| -0.961|5.92  | 2.590| -0.929 | 1.203|
| 8R,9S       | -0.997| -0.945| -1.001|2.76  | 2.618| -0.971 | 1.269|

Data is sorted according to Pearson correlation coefficient (correl); permutation corresponding to correct assignment is highlighted in green, scores corresponding to best match of the data (highest CP1, CP2, CP3, aggregate overlap, correlation; and lowest RMS deviation and MAE) are highlighted in blue.

Table S8a. Complete list of permutations with scores for comparison of experimental and calculated $^{13}$C NMR data for compound tetrad 3

| Permutation | $^{13}$C data score |
|-------------|---------------------|
|             | CP1  | CP2  | CP3  | overlap | RMS  | correl | MAE  |

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| 3a     | 3b     | 3c     | 3d     | CP1   | CP2    | CP3   | overlap | RMS   | correl | MAE  |
|--------|--------|--------|--------|-------|--------|-------|---------|-------|--------|------|
| 8S,9R  | 8S,9R  | 8R,9R  | 8R,9S  | 0.986 | 0.806  | 0.797 | 62.86   | 0.703 | 0.881  | 0.522|
| 8S,9R  | 8S,9R  | 8R,9R  | 8R,9R  | 0.780 | 0.707  | 0.641 | 50.74   | 1.104 | 0.697  | 0.775|
| 8S,9R  | 8S,9S  | 8R,9R  | 8R,9S  | 0.747 | 0.697  | 0.612 | 49.75   | 1.157 | 0.667  | 0.795|
| 8S,9S  | 8R,9S  | 8R,9R  | 8R,9R  | 0.541 | 0.599  | 0.456 | 37.63   | 1.437 | 0.483  | 1.048|
| 8R,9R  | 8S,9S  | 8R,9R  | 8R,9S  | 0.295 | 0.135  | 0.108 | 44.98   | 1.711 | 0.264  | 0.895|
| 8R,9R  | 8S,9R  | 8S,9S  | 8R,9S  | 0.141 | 0.055  | -0.001| 44.09   | 1.863 | 0.126  | 0.913|
| 8S,9S  | 8R,9R  | 8S,9S  | 8R,9R  | 0.072 | -0.015 | -0.076| 34.25   | 1.928 | 0.064  | 1.118|
| 8R,9S  | 8S,9S  | 8R,9R  | 8R,9S  | 0.038 | 0.015  | -0.086| 30.96   | 1.959 | 0.034  | 1.187|
| 8R,9R  | 8R,9R  | 8R,9R  | 8R,9S  | 0.029 | 0.046  | -0.070| 32.95   | 1.967 | 0.025  | 1.145|
| 8S,9S  | 8R,9R  | 8R,9S  | 8R,9S  | 0.015 | 0.039  | -0.083| 32.68   | 1.979 | 0.014  | 1.151|
| 8R,9S  | 8R,9S  | 8R,9R  | 8R,9S  | 0.010 | 0.035  | -0.079| 32.03   | 1.983 | 0.009  | 1.165|
| 8R,9S  | 8R,9S  | 8S,9S  | 8R,9R  | 0.001 | -0.010 | -0.116| 32.09   | 1.992 | 0.001  | 1.163|
| 8R,9R  | 8R,9R  | 8S,9S  | 8R,9S  | -0.002| -0.013 | -0.111| 34.07   | 1.994 | -0.002 | 1.122|
| 8R,9S  | 8S,9S  | 8R,9R  | 8R,9R  | -0.009| -0.007 | -0.119| 31.76   | 2.000 | -0.008 | 1.170|
| 8R,9S  | 8S,9S  | 8R,9R  | 8R,9R  | -0.017| -0.021 | -0.125| 31.17   | 2.008 | -0.016 | 1.183|
| 8R,9S  | 8S,9S  | 8R,9S  | 8R,9R  | -0.027| -0.059 | -0.146| 33.15   | 2.016 | -0.024 | 1.141|
| 8R,9R  | 8S,9S  | 8R,9S  | 8S,9S  | -0.036| 0.012  | -0.111| 32.83   | 2.024 | -0.033 | 1.148|
| 8R,9R  | 8R,9R  | 8S,9S  | 8R,9S  | -0.074| -0.008 | -0.151| 31.91   | 2.056 | -0.066 | 1.167|
| 8R,9S  | 8S,9S  | 8R,9R  | 8R,9R  | -0.185| -0.135 | -0.271| 20.23   | 2.150 | -0.166 | 1.410|
| 8R,9R  | 8R,9S  | 8S,9S  | 8R,9R  | -0.251| -0.050 | -0.261| 20.64   | 2.204 | -0.225 | 1.402|
| 8R,9R  | 8R,9S  | 8S,9S  | 8R,9R  | -0.549| -0.616 | -0.690| 26.22   | 2.430 | -0.491 | 1.286|
| 8R,9R  | 8R,9S  | 8S,9R  | 8S,9S  | -0.745| -0.710 | -0.828| 16.35   | 2.568 | -0.665 | 1.491|
| 8R,9S  | 8R,9R  | 8S,9S  | 8R,9R  | -0.782| -0.689 | -0.849| 13.11   | 2.594 | -0.699 | 1.559|
| 8R,9S  | 8R,9R  | 8R,9R  | 8S,9S  | -0.978| -0.783 | -0.987| 3.24    | 2.723 | -0.873 | 1.764|

### Table S8b. Complete list of permutations with scores for comparison of experimental and calculated $^1$H NMR data for compound tetrad 3
Table S9a. Complete list of permutations with scores for comparison of experimental and calculated $^{13}$C NMR data for compound tetrad 4

| Permutation | $^{13}$C data score |
|-------------|---------------------|
|              | CP1     | CP2     | CP3     | overlap | RMS     | correl  | MAE    |
| 8S,9R 8S,9S | 0.006   | 0.059   | -0.274  | 5.90    | 0.357   | 0.004   | 0.237  |
| 8R,9R 8S,9S | -0.099  | -0.113  | -0.369  | 4.20    | 0.368   | -0.064  | 0.274  |
| 8S,9S 8R,9R | -0.102  | 0.019   | -0.320  | 5.20    | 0.368   | -0.065  | 0.252  |
| 8S,9S 8R,9R | -0.111  | 0.080   | -0.277  | 5.12    | 0.369   | -0.071  | 0.254  |
| 8R,9R 8S,9S | -0.139  | -0.038  | -0.369  | 4.20    | 0.372   | -0.089  | 0.274  |
| 8R,9R 8S,9S | -0.186  | -0.111  | -0.419  | 4.18    | 0.377   | -0.119  | 0.275  |
| 8S,9R 8S,9S | -0.248  | -0.096  | -0.458  | 4.59    | 0.383   | -0.159  | 0.266  |
| 8S,9R 8S,9S | -0.257  | -0.035  | -0.416  | 4.51    | 0.384   | -0.165  | 0.267  |
| 8R,9R 8S,9S | -0.371  | -0.158  | -0.538  | 3.63    | 0.395   | -0.238  | 0.287  |
| 8S,9R 8S,9S | -0.545  | -0.321  | -0.735  | 3.03    | 0.411   | -0.351  | 0.299  |
| 8R,9R 8S,9S | -0.642  | -0.259  | -0.743  | 2.93    | 0.420   | -0.412  | 0.302  |
| 8R,9R 8S,9S | -0.643  | -0.285  | -0.732  | 1.73    | 0.420   | -0.413  | 0.328  |
| 8R,9R 8S,9S | -1.089  | -0.493  | -1.098  | 0.56    | 0.458   | -0.700  | 0.353  |

Data is sorted according to Pearson correlation coefficient (correl), permutation corresponding to correct assignment is highlighted in green, scores corresponding to best match of the data (highest CP1, CP2, CP3, aggregate overlap, correlation; and lowest RMS deviation and MAE) are highlighted in blue.
Table S9b. Complete list of permutations with scores for comparison of experimental and calculated $^1$H NMR data for compound tetrad 4

| Permutation | $^1$H data score |
|-------------|------------------|
|             | CP1 | CP2 | CP3 | overlap | RMS  | correl | MAE  |
| 8S,9R       | 1.528 | 0.655 | 0.654 | 6.59 | 0.089 | 0.952 | 0.056 |
| 8S,9R       | 0.836 | 0.366 | 0.233 | 4.95 | 0.169 | 0.521 | 0.093 |
| 8S,9R       | 0.799 | 0.320 | 0.197 | 4.68 | 0.173 | 0.498 | 0.099 |
| 8S,9R       | 0.596 | 0.210 | 0.005 | 4.85 | 0.190 | 0.371 | 0.096 |
| 8S,9R       | 0.593 | 0.314 | 0.076 | 4.06 | 0.190 | 0.370 | 0.114 |
| 8S,9R       | 0.168 | 0.029 | -0.309 | 3.57 | 0.221 | 0.105 | 0.125 |
| 8S,9R       | 0.107 | 0.031 | -0.224 | 3.04 | 0.225 | 0.067 | 0.137 |
| 8S,9R       | 0.076 | 0.066 | -0.299 | 3.49 | 0.227 | 0.047 | 0.127 |
| 8S,9R       | 0.067 | 0.010 | -0.312 | 2.89 | 0.228 | 0.042 | 0.140 |
| 8S,9R       | 0.064 | 0.004 | -0.356 | 3.33 | 0.228 | 0.040 | 0.130 |
| 8S,9R       | 0.006 | 0.118 | -0.299 | 2.93 | 0.232 | 0.004 | 0.139 |
| 8S,9R       | 0.001 | -0.042 | -0.384 | 3.13 | 0.232 | 0.000 | 0.135 |
| 8S,9R       | -0.003 | -0.116 | -0.426 | 3.29 | 0.232 | -0.002 | 0.131 |
| 8S,9R       | -0.035 | -0.002 | -0.377 | 2.82 | 0.234 | -0.022 | 0.142 |
| 8S,9R       | -0.042 | -0.089 | -0.402 | 2.81 | 0.235 | -0.026 | 0.142 |
| 8S,9R       | -0.070 | -0.079 | -0.424 | 3.13 | 0.237 | -0.044 | 0.135 |
| 8S,9R       | -0.104 | -0.134 | -0.429 | 2.62 | 0.239 | -0.065 | 0.146 |
| 8S,9R       | -0.127 | 0.035 | -0.368 | 2.74 | 0.240 | -0.079 | 0.144 |
| 8S,9R       | -0.339 | -0.130 | -0.572 | 2.32 | 0.253 | -0.211 | 0.153 |
| 8S,9R       | -0.520 | -0.186 | -0.688 | 1.77 | 0.264 | -0.324 | 0.166 |
| 8S,9R       | -0.670 | -0.405 | -0.855 | 1.58 | 0.272 | -0.417 | 0.170 |
| 8S,9R       | -0.802 | -0.389 | -0.933 | 1.35 | 0.279 | -0.500 | 0.175 |
| 8S,9R       | -0.833 | -0.364 | -0.958 | 1.27 | 0.281 | -0.519 | 0.177 |
| 8S,9R       | -1.297 | -0.622 | -1.318 | 0.31 | 0.305 | -0.808 | 0.199 |

Data is sorted according to Pearson correlation coefficient (correl), permutation corresponding to correct assignment is highlighted in green, scores corresponding to best match of the data (highest CP1, CP2, CP3, aggregate overlap, correlation; and lowest RMS deviation and MAE) are highlighted in blue.

Table S10a. Complete list of permutations with scores for comparison of experimental and calculated $^{13}$C NMR data for compound tetrad 5

| Permutation | $^{13}$C data score |
|-------------|-------------------|

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Table S10b. Complete list of permutations with scores for comparison of experimental and calculated $^1$H NMR data for compound tetrad 5

| Permutation | $^1$H data score |
|-------------|-------------------|
|             | CP1   | CP2   | CP3   | overlap | RMS | correl | MAE |
| 1S,3R 1R,3R 1S,3S 1R,3S | 1.260 | 0.657 | 0.654 | 1.61 | 0.116 | 0.827 | 0.081 |
| 1S,3R 1S,3S 1R,3R 1R,3S | 0.927 | 0.524 | 0.476 | 1.24 | 0.157 | 0.608 | 0.118 |
| 1R,3R 1S,3R 1S,3S 1S,3R | 0.822 | 0.313 | 0.303 | 1.16 | 0.168 | 0.539 | 0.126 |
| 1R,3R 1S,3R 1S,3S 1R,3S | 0.621 | 0.187 | 0.081 | 0.95 | 0.187 | 0.408 | 0.148 |
| 1S,3R 1R,3S 1S,3S 1R,3R | 0.530 | 0.293 | 0.117 | 0.96 | 0.195 | 0.347 | 0.146 |
| 1R,3S 1S,3S 1R,3R 1S,3R | 0.489 | 0.180 | 0.125 | 0.79 | 0.199 | 0.321 | 0.163 |
| 1R,3S 1S,3S 1R,3S 1R,3S | 0.407 | 0.027 | -0.106 | 0.73 | 0.205 | 0.267 | 0.170 |
| 1R,3R 1R,3S 1S,3S 1S,3R | 0.306 | 0.109 | -0.047 | 0.73 | 0.214 | 0.201 | 0.169 |
| 1R,3R 1S,3S 1S,3R 1R,3S | 0.196 | -0.102 | -0.182 | 0.65 | 0.222 | 0.128 | 0.177 |
| 1S,3S 1S,3S 1R,3S 1R,3R | 0.108 | -0.003 | -0.177 | 0.85 | 0.229 | 0.071 | 0.157 |
| 1R,3S 1S,3S 1S,3R 1R,3R | -0.018 | -0.262 | -0.370 | 0.43 | 0.238 | -0.012 | 0.199 |
| 1S,3R 1R,3S 1R,3R 1S,3S | -0.068 | 0.276 | -0.176 | 0.80 | 0.241 | -0.045 | 0.162 |
Data is sorted according to Pearson correlation coefficient (correl), permutation corresponding to correct assignment is highlighted in blue.

| Permutation | CP1 | CP2 | CP3 | overlap | RMS | correl | MAE |
|-------------|-----|-----|-----|---------|-----|--------|-----|
| 1R,3R 1S,3S | -0.116 | -0.187 | -0.341 | 0.62 | 0.245 | -0.076 | 0.180 |
| 1S,3S 1R,3R | -0.130 | 0.049 | -0.334 | 0.61 | 0.246 | -0.085 | 0.181 |
| 1S,3S 1R,3R | -0.157 | 0.114 | -0.292 | 1.05 | 0.247 | -0.103 | 0.137 |
| 1R,3R 1R,3R | -0.190 | 0.011 | -0.399 | 0.56 | 0.250 | -0.125 | 0.186 |
| 1S,3S 1R,3R | -0.223 | -0.107 | -0.419 | 0.68 | 0.252 | -0.146 | 0.174 |
| 1R,3S 1R,3R | -0.283 | -0.145 | -0.484 | 0.64 | 0.256 | -0.186 | 0.179 |
| 1R,3R 1R,3R | -0.446 | -0.029 | -0.462 | 0.39 | 0.266 | -0.292 | 0.203 |
| 1S,3S 1R,3R | -0.535 | -0.191 | -0.578 | 0.64 | 0.272 | -0.351 | 0.178 |
| 1R,3R 1R,3S | -0.796 | -0.355 | -0.865 | 0.39 | 0.288 | -0.522 | 0.203 |
| 1R,3R 1R,3R | -0.799 | -0.349 | -0.834 | 0.21 | 0.288 | -0.524 | 0.221 |
| 1S,3S 1R,3S | -0.950 | -0.477 | -0.987 | 0.21 | 0.296 | -0.623 | 0.221 |
| 1S,3S 1R,3R | -0.953 | -0.471 | -0.956 | 0.03 | 0.297 | -0.625 | 0.239 |

Table S11a. Complete list of permutations with scores for comparison of experimental and calculated $^{13}$C NMR data for compound tetrad 6
Data is sorted according to Pearson correlation coefficient (correl), permutation corresponding to correct assignment is calculated.

### Table S11b.
Complete list of permutations with scores for comparison of experimental and calculated $^1$H NMR data for compound tetrad 6

| Permutation | $^1$H data score |
|-------------|------------------|
|             | CP1  | CP2  | CP3  | overlap | RMS   | correl | MAE   |
| 6a          | 6b   | 6c   | 6d   |        |       |        |       |
| 2R,4R       | 2S,4R| 2S,4S| 2R,4S| 1.817  | 0.435 | 0.303  | 1.32  | 0.131 | 0.713 | 0.096 |
| 2R,4S       | 2S,4R| 2S,4S| 2R,4R| 1.508  | 0.417 | 0.196  | 1.20  | 0.141 | 0.591 | 0.102 |
| 2R,4R       | 2S,4R| 2R,4S| 2S,4S| 1.432  | 0.327 | 0.080  | 1.22  | 0.143 | 0.561 | 0.101 |
| 2R,4S       | 2R,4R| 2S,4S| 2R,4R| 1.090  | 0.371 | 0.048  | 1.16  | 0.153 | 0.428 | 0.104 |
| 2R,4R       | 2R,4R| 2S,4S| 2R,4S| 1.001  | 0.353 | -0.030 | 1.11  | 0.156 | 0.393 | 0.107 |
| 2R,4S       | 2R,4R| 2R,4S| 2R,4R| 0.841  | 0.287 | -0.196 | 0.95  | 0.160 | 0.330 | 0.115 |
| 2R,4S       | 2R,4R| 2R,4S| 2S,4S| 0.615  | 0.245 | -0.252 | 1.01  | 0.166 | 0.241 | 0.112 |
| 2R,4S       | 2R,4R| 2R,4S| 2S,4R| 0.604  | 0.178 | -0.360 | 0.91  | 0.167 | 0.237 | 0.117 |
| 2R,4S       | 2R,4R| 2R,4S| 2S,4R| 0.423  | 0.241 | -0.344 | 0.91  | 0.171 | 0.166 | 0.117 |
| 2R,4S       | 2R,4R| 2S,4R| 2S,4S| 0.390  | 0.233 | -0.381 | 0.98  | 0.172 | 0.153 | 0.113 |
| 2R,4S       | 2S,4R| 2R,4R| 2R,4S| 0.322  | 0.157 | -0.530 | 0.76  | 0.174 | 0.126 | 0.124 |
| 2R,4S       | 2R,4S| 2S,4S| 2S,4S| 0.108  | 0.212 | -0.550 | 0.83  | 0.179 | 0.042 | 0.121 |
| 2R,4S       | 2R,4S| 2S,4S| 2S,4S| -0.075 | -0.210| -0.890 | 0.86  | 0.184 | -0.029| 0.119 |
| 2R,4S       | 2S,4S| 2R,4S| 2R,4R| -0.238 | -0.130| -0.965 | 0.88  | 0.188 | -0.093| 0.118 |
| 2R,4S       | 2R,4S| 2S,4S| 2R,4R| -0.474 | -0.246| -1.074 | 0.69  | 0.193 | -0.186| 0.128 |
| 2R,4S       | 2S,4S| 2S,4R| 2R,4S| -0.553 | -0.159| -1.171 | 0.80  | 0.195 | -0.217| 0.122 |
| 2R,4S       | 2S,4S| 2S,4R| 2R,4R| -0.637 | -0.166| -1.150 | 0.71  | 0.197 | -0.250| 0.127 |
| 2R,4S       | 2S,4S| 2S,4R| 2S,4S| -0.775 | -0.347| -1.318 | 0.68  | 0.200 | -0.304| 0.128 |
| 2R,4S       | 2S,4S| 2S,4R| 2R,4R| -0.862 | -0.178| -1.279 | 0.68  | 0.202 | -0.338| 0.128 |
| 2R,4S       | 2S,4S| 2R,4R| 2R,4R| -1.066 | -0.279| -1.406 | 0.57  | 0.206 | -0.418| 0.134 |
| 2R,4S       | 2S,4S| 2R,4R| 2R,4S| -1.156 | -0.297| -1.483 | 0.52  | 0.208 | -0.453| 0.136 |
| 2S,4S       | 2R,4S| 2S,4S| 2R,4R| -1.366 | -0.387| -1.595 | 0.41  | 0.213 | -0.536| 0.142 |
| 2S,4S       | 2R,4S| 2R,4R| 2S,4S| -1.378 | -0.485| -1.630 | 0.40  | 0.213 | -0.540| 0.142 |
| 2S,4S       | 2R,4S| 2R,4R| 2S,4R| -1.571 | -0.488| -1.722 | 0.30  | 0.217 | -0.616| 0.147 |

Data is sorted according to Pearson correlation coefficient (correl), permutation corresponding to correct assignment is highlighted in green, scores corresponding to best match of the data (highest CP1, CP2, CP3, aggregate overlap, correlation; and lowest RMS deviation and MAE) are highlighted in blue.

### Table S12a.
Complete list of permutations with scores for comparison of experimental and calculated $^{13}$C NMR data for compound tetrad 7

| Permutation | $^{13}$C data score |
|-------------|---------------------|
|             | CP1    | CP2    | CP3    | overlap | RMS   | correl | MAE   |
| 7a          | 7b     | 7c     | 7d     |        |       |        |       |
|             |        |        |        |        |       |        |       |
| 2R,4S       | 2S,4S  | 2R,4S  | 2R,4R  | -0.519 | -0.402| -0.670| 7.39  | 2.322 | -0.397| 1.790 |
| 2S,4R       | 2R,4S  | 2R,4R  | 2S,4S  | -0.579 | -0.429| -0.732| 7.88  | 2.359 | -0.444| 1.766 |
| 2S,4S       | 2R,4S  | 2R,4R  | 2S,4R  | -0.779 | -0.451| -0.836| 6.07  | 2.478 | -0.597| 1.856 |

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Table S12b. Complete list of permutations with scores for comparison of experimental and calculated $^1$H NMR data for compound tetrad 7

| Permutation | $^1$H data score |
|-------------|------------------|
| 7a 7b 7c 7d | CP1  CP2  CP3  overlap  RMS  correl  MAE |
| 3R,5R 3R,5S 3S,5S 3S,5R | 0.698 0.435 0.365 0.98 0.058 0.469 0.042 |
| 3R,5R 3R,5S 3S,5S 3S,5R | 0.608 0.120 0.101 0.99 0.061 0.409 0.041 |
| 3S,5S 3R,5S 3S,5R 3R,5R | 0.371 0.196 0.125 0.78 0.068 0.249 0.049 |
| 3S,5R 3R,5R 3S,5S 3R,5S | 0.364 0.395 0.168 0.84 0.068 0.244 0.047 |
| 3S,5R 3S,5S 3R,5S 3R,5R | 0.268 0.181 -0.003 0.77 0.070 0.180 0.050 |
| 3S,5S 3R,5R 3S,5S 3S,5R | 0.225 0.157 -0.034 0.76 0.071 0.151 0.050 |
| 3R,5R 3S,5S 3S,5R 3S,5S | 0.215 -0.047 -0.163 0.79 0.072 0.144 0.049 |
| 3R,5S 3S,5S 3R,5S 3S,5R | 0.178 -0.134 -0.267 0.78 0.073 0.120 0.050 |
| 3S,5S 3R,5S 3R,5R 3S,5S | 0.173 0.178 -0.039 0.73 0.073 0.116 0.051 |
| 3S,5R 3R,5R 3R,5S 3S,5S | 0.158 0.228 -0.058 0.76 0.073 0.106 0.050 |
| 3S,5R 3R,5S 3S,5S 3R,5S | 0.106 0.250 -0.063 0.73 0.074 0.071 0.051 |
| 3R,5R 3S,5R 3S,5S 3R,5S | 0.057 -0.109 -0.254 0.62 0.076 0.039 0.056 |
|     | 3S,5S | 3R,5R | 3S,5R | 3R,5S | 0.036 | 0.156 | -0.072 | 0.63  | 0.076 | 0.025 | 0.055 |
|-----|-------|-------|-------|-------|-------|-------|--------|-------|-------|-------|-------|
| 3S,5S | 0.008 | -0.032 | -0.193 | 0.53  | 0.077 | 0.006 | 0.059  |
| 3R,5S | 0.076 | 0.025  | 0.055  | 0.056 |
| 3R,5R | 3S,5S | 3S,5R | 3R,5S | 3R,5S | -0.119 | 0.163 | -0.205 | 0.59  | 0.080 | -0.080 | 0.057 |
| 3R,5R | 3S,5S | 3R,5S | 3S,5S | 3S,5S | -0.321 | -0.306 | -0.534 | 0.47  | 0.084 | -0.216 | 0.061 |
| 3S,5S | 3S,5R | 3R,5R | 3R,5S | 3R,5S | -0.378 | -0.050 | -0.395 | 0.35  | 0.086 | -0.254 | 0.066 |
| 3R,5S | 3S,5S | 3S,5R | 3S,5R | 3R,5R | -0.389 | -0.332 | -0.584 | 0.51  | 0.086 | -0.261 | 0.060 |
| 3R,5S | 3S,5R | 3S,5R | 3S,5S | 3S,5S | -0.498 | -0.284 | -0.639 | 0.50  | 0.088 | -0.335 | 0.060 |
| 3R,5S | 3S,5S | 3S,5R | 3S,5R | 3S,5R | -0.587 | -0.349 | -0.748 | 0.46  | 0.090 | -0.394 | 0.062 |
| 3R,5S | 3S,5R | 3R,5R | 3S,5S | 3S,5S | -0.913 | -0.491 | -0.962 | 0.22  | 0.096 | -0.613 | 0.071 |

Data is sorted according to Pearson correlation coefficient (correl), permutation corresponding to correct assignment is highlighted in green, scores corresponding to best match of the data (highest CP1, CP2, CP3, aggregate overlap, correlation; and lowest RMS deviation and MAE) are highlighted in blue.
Figure S1. $^1$H and $^{13}$C NMR spectra for 9R-(4-trimethylsilyl-1,2,3-triazol-1-yl)-9-deoxyquinidine. Sample contains approx. 10 %mol of tBuOH ($^1$H NMR: 1.24 ppm (s))
Figure S2. $^1$H and $^{13}$C NMR spectra for 1b
Figure S3. $^1$H and $^{13}$C NMR spectra for 1c
Figure S4. $^1$H and $^{13}$C NMR spectra for 1d
Figure S5. $^1$H and $^{13}$C NMR spectra for 2b. Trace contamination with 2a is visible.
S5. Plots of $^1$H, $^{13}$C HSQC experiments for tetrad 1.
S7. Computer program (python) for quick calculation of permutations and their scores

Prerequisites: python 2.7, open source libraries: openpyxl, numpy. Excel file (Book1.xlsx) arranged as in the example below.

Program code (filename: code.py, intended for Public-domain):
```python
# Required libraries: numpy - for calculations and openpyxl - for handling excel files
# Use python code.py [filename] [-1 (for shieldings)], otherwise program
# will take Book1.xlsx
from openpyxl import Workbook
from openpyxl import load_workbook
from itertools import permutations
from operator import itemgetter
from statistics import mean
import sys
import numpy

def comparison_measure(x, y, z):
    # main comparison routine returns a/b from input lists
    # x[] - experimental list, y[] - dft list;
    # comparison_measure: z=0 sum product, z = 1 CP1, z = 2 CP2, Z = 3 CP3,
    # Z = 4 overlap, Z = 5 RMS deviation, Z = 6 correlation coefficient, Z = 7 MAE
    a = 0
    b = 0
    if (z == 6):
        a = numpy.corrcoef(x, y)[0, 1]
        b = 1
    elif (z == 0):
        for i in range (min(len(x),len(y))):
            a += x[i]*y[i]
            b = 1
    elif (z == 1):
        for i in range (min(len(x),len(y))):
            b += x[i]*x[i]
        a += x[i]*y[i]
    elif (z == 2):
        for i in range (min(len(x),len(y))):
            if (x[i]<>0 and y[i]<>0):
                if (abs(y[i]/x[i])<>1):
                    a += x[i]*x[i]*y[i]/y[i]
                else:
```

1C Data

1H Data

1D Data

1E Data

1F Data

1G Data

1H Data

1I Data

1J Data

Column A:

keyword H

indicates change from 13C to 1H data

Cell F1:

keyword shieldings

indicates type of DFT data

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elif (z == 3):
    # for overlap
    for i in range(min(len(x),len(y))):
        if (x[i]>0 and y[i]<0):
            a += x[i]*x[i]/y[i]
            b += y[i]
        else:
            a += x[i]*y[i]
elif (z == 4):
    # for overlap
    for i in range(min(len(x),len(y))):
        if (x[i]*y[i]>0):
            # if signs are equal
            a += min (abs(x[i]), abs(y[i]))
        count report min absolute value
        b = 1

e1f (z == 5):
    for i in range(min(len(x),len(y))):
        b = 1
        a += (x[i]-y[i])*(x[i]-y[i])
        a = a**.5
        b = b**.5
else:
    return a/b

shf = 1

if len(sys.argv)<2:
    excelfilename=sys.argv[1]
else:
    excelfilename=sys.argv[1]
if len(sys.argv)>2:
    if sys.argv[2]==-1:
        shf=1
        excelfile = load_workbook(excelfilename, data_only=True)
        sheet = excelfile.active
        split_row=0
        if sheet.cell(row=1, column=6).value=='shieldings':
            # cell F1 keyword "shieldings"
            shf=1
        for row in range (2, sheet.max_row+1):
            xtab,otab,xabs,yabs=[0], [0], 0, 0
            for col in range (1,6):
                if (sheet.cell(row=row, column=col).value == None):
                    break
                xtab.append(float(sheet.cell(row=row, column=col+1).value))
                otab.append(float(sheet.cell(row=row, column=col+6).value))
                sheet.cell(row=row, column=12).value=mean(xtab)
                sheet.cell(row=row, column=13).value=mean(otab)
        for col in range (1,5):
            sheet.cell(row=row, column=14+col).value=
            sheet.cell(row=row, column=14+col).value=mean(sheet.cell(row=row, column=12).value)
            sheet.cell(row=row, column=14+col).value=
            sheet.cell(row=row, column=15).value=mean(sheet.cell(row=row, column=13).value)*shf
            sheet.cell(row=1, column=12).value="avg exper"
            sheet.cell(row=1, column=13).value="avg dft"
            sheet.cell(row=1, column=15).value="dev exper"
            sheet.cell(row=1, column=20).value="dev dft"
            sheet.append ("H","experiment",",",",",",",","dft")
        xc,xh,yh=[0], [0], [0], [0], [0]
        if (x[i]<0 and y[i]<0):
            a += x[i]*x[i]/y[i]
            b += y[i]
            a += x[i]*y[i]
            else:
                a += x[i]*y[i]

elif (z == 4):
    # for overlap
    for i in range(min(len(x),len(y))):
        if (x[i]*y[i]>0):
            # if signs are equal
            a += min (abs(x[i]), abs(y[i]))
        count report min absolute value
        b = 1

e1f (z == 5):
    for i in range(min(len(x),len(y))):
        b = 1
        a += (x[i]-y[i])*(x[i]-y[i])
        a = a**.5
        b = b**.5
else:
    return a/b

shf = 1

if len(sys.argv)<2:
    excelfilename=sys.argv[1]
else:
    excelfilename=sys.argv[1]
if len(sys.argv)>2:
    if sys.argv[2]==-1:
        shf=1
        excelfile = load_workbook(excelfilename, data_only=True)
        sheet = excelfile.active
        split_row=0
        if sheet.cell(row=1, column=6).value=='shieldings':
            # cell F1 keyword "shieldings"
            shf=1
        for row in range (2, sheet.max_row+1):
            xtab,otab,xabs,yabs=[0], [0], 0, 0
            for col in range (1,6):
                if (sheet.cell(row=row, column=col).value == None):
                    break
                xtab.append(float(sheet.cell(row=row, column=col+1).value))
                otab.append(float(sheet.cell(row=row, column=col+6).value))
                sheet.cell(row=row, column=12).value=mean(xtab)
                sheet.cell(row=row, column=13).value=mean(otab)
        for col in range (1,5):
            sheet.cell(row=row, column=14+col).value=
            sheet.cell(row=row, column=14+col).value=mean(sheet.cell(row=row, column=12).value)
            sheet.cell(row=row, column=14+col).value=
            sheet.cell(row=row, column=15).value=mean(sheet.cell(row=row, column=13).value)*shf
            sheet.cell(row=1, column=12).value="avg exper"
            sheet.cell(row=1, column=13).value="avg dft"
            sheet.cell(row=1, column=15).value="dev exper"
            sheet.cell(row=1, column=20).value="dev dft"
            sheet.append ("H","experiment",",",",",",",","dft")
        xc,xh,yh=[0], [0], [0], [0], [0]
        if (x[i]<0 and y[i]<0):
            a += x[i]*x[i]/y[i]
            b += y[i]
            a += x[i]*y[i]
            else:
                a += x[i]*y[i]
```python
sheet.cell(row=k, column=19+i).value == None):
    continue
x.append(sheet.cell(row=k, column=14+i).value)
y.append(sheet.cell(row=k, column=19+i).value)
x.append(x)
y.append(y)
x,y=[[],[]]
for k in range(split_row,sheet.max_row):
    if (sheet.cell(row=k, column=14+i).value == None or \
        sheet.cell(row=k, column=19+i).value == None):
        continue
    x.append(sheet.cell(row=k, column=14+i).value)
y.append(sheet.cell(row=k, column=19+i).value)
xh.append(x)
yh.append(y)
permu=[] #create permutation indexed list permu
permu = list(permutations("1234")) #create permutation list
for i in range (0, len(permu)):
    x=[] #create permutation list
    for j in range (0,4):
        k.append(int(permu[i][j])) #create permutation list
        permu[i]=k
for i in range (len(permu)):
    x,y=[],[[]]
    for j in range (4):
        for t in range (len(xc[j])):
            x.append(xc[j][t])
y.append(yc[permu[i][j]-1][t])
    for met in range(5):
        permu[i].append(comparison_measure(x,y,met))
for i in range (len(permu)):
    x,y=[],[[]]
    for j in range (4):
        for t in range (len(xc[j])):
            x.append(xh[j][t])
y.append(yh[permu[i][j]-1][t])
    for met in range(5):
        permu[i].append(comparison_measure(x,y,met))
permu = sorted(permu, key=itemgetter(10), reverse = True)
name_of_operation=["product", "CP1", "CP2", "CP3", "overlap", "RMS", "correl", "MAE","H_product", "H_CP1", "H_CP2", "H_CP3", "H_overlap", "H_RMS", "H_correl", "H_MAE",]
resultsheet=excelfile.create_sheet("Result")
resultsheet.sheet_properties.tabColor = "00FFFF"
for j in range (len(name_of_operation)):
    resultsheet.cell(row=1, column=j+1).value=sheet.cell(row=1, column=2+j).value
for j in range (len(name_of_operation)):
    resultsheet.cell(row=1, column=j+5).value=name_of_operation[j]
for i in range (len(permu)):
    for j in range (len(permu[i])):
        if j<1:
            resultsheet.cell(row=i+2, column=j+1).value=sheet.cell(row=1, column=6+permu[i][j]).value
        else:
            resultsheet.cell(row=i+2, column=j+1).value=permu[i][j]
excelfile.save(excelfilename.replace(".xlsx","-result.xlsx"))
```
S8. Cartesian coordinates for gas phase optimized geometries of tetrads 1–3

1a-conformer 1 [mPW1PW91/6-311+G(2d,p)]

| atom | X     | Y     | Z     |
|------|-------|-------|-------|
| C    | -0.13643 | 0.853889 | -0.411364 |
| C    | 0.925017 | 0.886628 | 0.684104 |
| C    | 0.725448 | 1.657693 | 1.806586 |
| C    | 1.691079 | 1.681519 | 2.829064 |
| N    | 2.811200 | 0.996361 | 2.789955 |
| C    | 3.042206 | 0.230229 | 1.694486 |
| C    | 4.257371 | -0.503390 | 1.651683 |
| C    | 4.568814 | -1.293910 | 0.586546 |
| C    | 3.672450 | -1.395171 | -0.506665 |
| C    | 2.483438 | -0.793089 | -0.503063 |
| C    | 2.131658 | 0.130757 | 0.595652 |
| N    | 2.811200 | 0.996361 | 2.789955 |
| C    | 3.271322 | -2.369005 | -2.654078 |
| C    | 1.425654 | 0.122413 | 0.025513 |
| C    | -2.012964 | -1.079446 | -2.018652 |
| C    | -2.037849 | -2.469298 | -1.316643 |
| C    | -2.762415 | -2.227701 | 0.182367 |
| C    | -1.180027 | -1.266723 | 0.680998 |
| C    | -3.699218 | -1.685975 | 0.343222 |
| C    | -3.703283 | -0.290297 | -0.520164 |
| N    | -2.381852 | 0.005190 | -1.093178 |
| C    | -4.083762 | -1.362909 | 1.770158 |
| C    | -5.088174 | -1.965912 | 2.397211 |
| H    | 0.267854 | 0.353916 | -1.287627 |
| H    | -0.164086 | 2.267224 | 1.900433 |
| H    | 1.524426 | 2.292344 | 3.710132 |
| H    | 4.925873 | -0.407953 | 2.497785 |
| H    | 5.493682 | -1.855366 | 0.545364 |
| H    | 1.814615 | -0.798125 | -1.343888 |
| H    | 2.303409 | -2.805194 | -2.388543 |
| H    | 3.803775 | -3.048927 | -3.315210 |
| H    | 3.115374 | -1.413790 | -3.164912 |
| H    | -1.904741 | 0.779238 | 0.752437 |
| H    | -1.026037 | -0.867884 | -2.435437 |
| H    | -2.711004 | -1.049593 | -2.857461 |
| H    | -1.095154 | -3.002021 | -1.465108 |
| H    | -2.830000 | -3.101765 | -1.728153 |
| H    | -2.227793 | -3.168501 | 0.733980 |
| H    | -0.284087 | -1.676881 | 0.407272 |
| H    | -1.182806 | -1.183204 | 1.768667 |
| H    | -4.486730 | -2.317876 | -0.879457 |
| H    | -4.17907 | -0.381841 | -1.340704 |
| H    | -4.012282 | 0.566425 | 0.881421 |
| H    | -3.502618 | -0.622386 | 2.316234 |
| H    | -5.706781 | -2.795606 | 1.898635 |
| H    | -5.339820 | -1.741497 | 3.428980 |
| N    | -0.462521 | 2.297574 | -0.883198 |
| C    | -0.020774 | 2.826642 | -2.001113 |
| C    | -0.594598 | 4.072213 | -1.954817 |
| H    | 0.636301 | 2.351952 | -2.708819 |
| H    | -0.516400 | 4.891227 | -2.649655 |
| N    | -1.266629 | 3.027822 | -0.180541 |
| N    | -1.347506 | 4.156804 | -0.827772 |

Energies in solvent (SMD)

|                  | SCF | Sum of electronic and zero-point Energies | Sum of electronic and thermal Energies | Sum of electronic and thermal Enthalpies | Sum of electronic and thermal Free Energies |
|------------------|-----|------------------------------------------|----------------------------------------|------------------------------------------|---------------------------------------------|
|                  |     | -1202.3757735                           | -1201.930975                           | -1201.907832                             | -1201.983488                               |

Number of imaginary frequencies: 0
### Energies in solvent (SMD)

| Energy Type                        | Value             |
|-----------------------------------|-------------------|
| SCF                               | \(-1202.37770714\) |
| Sum of electronic and zero-point  | \(-1201.932427\) |
| Energies                          |                   |
| Sum of electronic and thermal     | \(-1201.909437\) |
| Enthalpies                         |                   |
| Sum of electronic and thermal     | \(-1201.984540\) |
| Free Energies                     |                   |
| Number of imaginary frequencies   | 0                 |

---

**Conformer 2 [mPW1PW91/6-311+G(2d,p)]**

| Atom | X      | Y      | Z      |
|------|--------|--------|--------|
| C    | 0.127840 | 0.212899 | 0.209910 |
| C    | -0.755780 | 1.010111 | 0.441003 |
| C    | -0.291963 | 2.146307 | 1.061591 |
| C    | -1.142117 | 3.255253 | 1.246539 |
| N    | -2.392442 | 3.286969 | 0.851093 |
| C    | -2.889886 | 2.178843 | 0.243412 |
| C    | -4.244710 | 2.207786 | \(-0.178857\) |
| C    | -4.817547 | 1.125237 | \(-0.777223\) |
| C    | -4.061792 | 0.956697 | 0.805934 |
| C    | -7.402560 | -1.072737 | \(-1.566364\) |
| C    | -4.073130 | -2.309718 | \(-1.781333\) |
| C    | 1.646316  | 0.064721 | 0.248036 |
| C    | 2.351993  | \(-1.821764\) | -1.138553 |
| C    | 2.864102  | \(-0.870648\) | -2.260739 |
| C    | 3.399174  | 0.445184  | \(-1.601708\) |
| C    | 2.093672  | 1.050006  | \(-0.876453\) |
| C    | 4.484184  | 0.116943  | \(-0.598756\) |
| C    | 3.831471  | \(-0.853499\) | 0.473815 |
| N    | 2.429662  | \(-1.818557\) | 0.187613 |
| C    | 5.080678  | 1.327086  | 0.819655 |
| C    | 6.352514  | 1.684333  | \(-0.125090\) |
| H    | -0.112217 | \(-0.618429\) | \(-0.773034\) |
| H    | 0.728791  | 2.221761  | 1.410793 |
| H    | -0.760595 | 4.147225  | 1.735845 |
| H    | -4.804609 | 3.117334  | \(-0.002391\) |
| H    | -5.852011 | 1.134535  | \(-1.097135\) |
| H    | -2.184323 | \(-1.033353\) | \(-0.742101\) |
| H    | -3.234982 | \(-2.183814\) | \(-2.472521\) |
| H    | -4.810828 | \(-2.975945\) | \(-2.221848\) |
| H    | -3.708689 | \(-2.731332\) | \(-0.841488\) |
| H    | 1.881860  | 0.495972  | 1.224541 |
| H    | 1.327118  | \(-2.145916\) | \(-1.315360\) |
| H    | 2.953716  | \(-2.730916\) | \(-1.087583\) |
| H    | 2.077517  | \(-0.669148\) | \(-2.993589\) |
| H    | 3.698225  | \(-1.320573\) | \(-2.805589\) |
| H    | 3.676453  | 1.144655  | \(-2.355343\) |
| H    | 1.298169  | 1.210585  | \(-1.601727\) |
| H    | 2.329813  | 2.032734  | \(-0.464885\) |
| H    | 5.227072  | \(-0.414095\) | \(-1.154636\) |
| H    | 4.399117  | \(-1.785183\) | 0.514002 |
| H    | 3.881399  | \(-0.465387\) | 1.469374 |
| H    | 4.438760  | 1.944739  | 0.646086 |
| H    | 7.840118  | 1.182851  | \(-0.731027\) |
| H    | 6.753431  | 2.568239  | 0.356418 |
| N    | -0.244351 | \(-1.293699\) | 1.130511 |
| C    | -0.257439 | \(-1.317991\) | 2.480811 |
| C    | -0.653196 | \(-2.593874\) | 2.796841 |
| H    | -0.006952 | \(-0.463986\) | 3.084949 |
| H    | -0.799999 | \(-3.046549\) | 3.762933 |
| N    | -0.613550 | \(-2.493689\) | 0.635674 |
| N    | -0.863369 | \(-3.279933\) | 1.643141 |
Energies in solvent (SMD)

\[
\text{SCF} = -1202.37403101
\]

Sum of electronic and zero-point Energies = -1201.928856

Sum of electronic and thermal Energies = -1201.905837

Sum of electronic and thermal Enthalpies = -1201.904893

Sum of electronic and thermal Free Energies = -1201.980948

Number of imaginary frequencies: 0
1b - conformer 1 [mPW1PW91/6-311+G(2d,p)]

|  |  |  |  |
|-----|-----|-----|-----|
| C   | -0.136787 | -0.898596 | 1.063386 |
| C   | 1.072882 | -1.391897 | 0.276761 |
| C   | 1.290871 | -2.749988 | 0.242832 |
| C   | 2.361587 | -3.289775 | -0.493575 |
| N   | 3.288150 | -2.556240 | -1.175882 |
| C   | 3.037973 | -1.208658 | -1.151228 |
| C   | 3.965248 | -0.420787 | -1.881772 |
| C   | 3.878723 | 0.939289 | -1.894747 |
| C   | 2.851859 | 1.591319 | -1.167390 |
| C   | 1.922946 | 0.863378 | -0.458768 |
| C   | 1.986679 | -0.554992 | -0.432617 |
| O   | 2.884508 | 2.947955 | -1.235035 |
| C   | 1.912398 | 3.685183 | -0.498928 |
| C   | -1.258684 | -0.244716 | 0.217812 |
| C   | -2.379007 | -2.276249 | -0.565471 |
| C   | -3.726474 | -1.888519 | 0.893664 |
| C   | -3.764515 | -0.357335 | 0.222063 |
| C   | -2.537514 | 0.081872 | 1.041932 |
| C   | -3.722975 | 0.241123 | -1.210152 |
| C   | -2.391559 | -0.273901 | -1.871735 |
| N   | -1.588675 | -1.086218 | -0.946760 |
| C   | -3.839625 | 1.735826 | -1.242502 |
| C   | -4.833598 | 2.411524 | -1.809362 |
| H   | -0.566965 | -1.779164 | 1.544557 |
| H   | 0.629659 | -3.425318 | 0.774371 |
| H   | 2.513864 | -4.365443 | -0.516059 |
| H   | 4.745361 | -0.942117 | -2.742169 |
| H   | 4.585704 | 1.548623 | -2.443828 |
| H   | 1.162088 | 1.373731 | 0.108024 |
| H   | 0.901634 | 3.472376 | -0.858460 |
| H   | 2.145061 | 4.733607 | -0.676040 |
| H   | 1.976247 | 3.464041 | 0.569477 |
| H   | -0.857946 | 0.680622 | -0.193607 |
| H   | -1.769923 | -2.896836 | 0.101865 |
| H   | -2.824051 | -2.846062 | -1.472055 |
| H   | -3.827653 | -2.347807 | 1.081094 |
| H   | -4.568819 | -2.239718 | -0.508388 |
| H   | -4.681089 | -0.038680 | 0.722506 |
| H   | -2.548310 | -0.456471 | 1.996099 |
| H   | -2.579565 | 1.141416 | 1.289891 |
| H   | -4.575972 | -0.169147 | -1.759466 |
| H   | -2.615402 | -0.881515 | -2.750929 |
| H   | -1.778769 | 0.564753 | -2.208935 |
| H   | -3.834021 | 2.295999 | -0.771275 |
| H   | -5.659147 | 1.983853 | -2.298269 |
| H   | -4.859105 | 3.494673 | -1.806092 |
| N   | 0.241158 | -0.018427 | 2.187614 |
| C   | 0.815592 | -0.387880 | 3.355916 |
| C   | 0.998444 | 0.786091 | 4.843226 |
| H   | 1.050016 | -1.411840 | 3.589545 |
| H   | 1.411229 | 0.954408 | 5.020066 |
| N   | 0.872388 | 1.319720 | 2.155870 |
| N   | 0.523568 | 1.806457 | 3.277136 |

**Energies in solvent (SMD)**

|  |  |
|---|---|
| SCF | -1202.37463188 |
| Sum of electronic and zero-point Energies | -1201.929464 |
| Sum of electronic and thermal Energies | -1201.906468 |
| Sum of electronic and thermal Enthalpies | -1201.905523 |
| Sum of electronic and thermal Free Energies | -1201.981352 |

Number of imaginary frequencies: 0
1b - conformer 2 [mPW1PW91/6-311+G(2d,p)]

C  -0.139418  0.216002  -0.135754
C   0.787779  -0.946680  -0.467126
C   0.345745  -2.074182  -0.135754
C   2.513781  -3.184563  -1.085886
C   2.985398  -2.006227  -0.441736
C   4.360102  -1.985267  -0.088300
C   2.762882  -0.228159  -0.109088
C   2.168939  -0.881931  -0.182638
N   2.513781  -3.104563  -1.085886
C   2.985398  -2.006227  -0.441736
C   4.360102  -1.985267  -0.088300
C   4.906631  -0.910978  0.548415
C   4.102368    0.213071    0.866265
C   2.762882    0.228159    0.548428
C   2.168939  -0.881931  -0.109088
O   4.764193  1.226919  1.481456
C   4.037475  2.407181  1.810741
C  -1.659155  -0.071965  -0.182638
C  -1.950714  -0.823441  2.128583
C  -2.915373  -0.351511  2.457800
C  -3.618395  -0.781082  1.154928
C  -4.435701  -1.425954  0.633267
C  -3.409181  -1.598935  0.383356
N  -2.08952  -1.196327  0.696690
C  -5.259959  -0.117913  -0.580796
C  -5.86481  -0.171818  -0.638063
H   0.104685    0.582528    0.861784
H  -0.693826  -2.193334  -1.384420
H   0.879688  -4.007797  -1.922296
H   4.955821  -2.851728  -0.346015
H   5.954739  -0.883775    0.819134
H   2.168683    1.100005    0.773035
H   3.607749    2.870695    0.919243
H   4.759849    3.082318    2.263499
H   3.248403    2.190759    2.527841
H  -1.895437  -0.399795  -1.199060
H  -0.917751  -0.572648    2.364668
H  -2.194388  -1.715528    2.700486
H  -2.368575    1.197264    2.882441
H  -3.658691    0.046612    3.199608
H  -4.276393    1.625997    1.340322
H  -1.907417    1.978447    0.586581
H  -2.954854    1.607729  -0.761095
H  -5.121810  -0.721332    1.432494
H  -3.662986  -2.457341    0.994919
H  -3.444192  -1.912183  -0.660315
H  -4.713756    0.155687  -1.482055
H  -7.181852  -0.444850    0.227486
H  -7.125816    0.054578  -1.550045
N  -0.163639    1.365593  -1.004859
C   0.195075    1.440446  -2.354578
C   0.584739    2.751716  -2.618505
H   0.823587    0.590234  -2.991100
H   0.636197    3.247899  -3.565285
N   0.444064    2.570928  -0.462035
N   0.650065    3.408371  -1.437924

---

**Energies in solvent (SMD)**

```
SCF = -1202.37742888
Sum of electronic and zero-point Energies= -1201.932469
Sum of electronic and thermal Energies= -1201.909423
Sum of electronic and thermal Enthalpies= -1201.908479
Sum of electronic and thermal Free Energies= -1201.984658
Number of imaginary frequencies: 0
```
1b - conformer 3 [mPW1PW91/6-311+G(2d,p)]

| Atom | x         | y         | z         |
|------|-----------|-----------|-----------|
| C    | 0.151152  | 0.718440  | -0.441897 |
| C    | -0.899844 | 0.843554  | 0.655181  |
| C    | -0.649021 | 1.652825  | 1.739375  |
| C    | -1.601924 | 1.776624  | 2.765415  |
| N    | -2.768435 | 1.157377  | 2.761913  |
| C    | -3.846269 | 0.364365  | 1.699027  |
| C    | -4.306372 | -0.290135 | 1.690127  |
| C    | -4.678271 | -1.093232 | 0.654195  |
| C    | -3.801061 | -1.287351 | -0.441689 |
| C    | -2.569610 | -0.675468 | 0.599800  |
| C    | -2.152392 | -1.287351 | -0.441689 |
| O    | -4.289574 | -2.195785 | -1.415496 |
| C    | -3.484109 | -2.359791 | -2.558400 |
| C    | 1.475812  | 0.086642  | 0.046719  |
| C    | 1.016626  | -2.278710 | -0.360066 |
| C    | 2.258018  | -2.461826 | -1.282457 |
| C    | 3.274615  | -1.367986 | 0.654228  |
| C    | 3.735459  | -1.617561 | 1.019052  |
| C    | 4.781684  | -0.653461 | 1.372814  |
| C    | 6.018480  | -0.986604 | 1.372814  |
| H    | -0.235730 | 0.115310  | -1.260067 |
| H    | 0.276133  | 2.210512  | 1.806464  |
| H    | -1.392099 | 2.414843  | 3.619080  |
| H    | -4.959784 | -0.122526 | 2.536793  |
| H    | -5.638023 | -1.594195 | 0.638126  |
| H    | -1.916776 | -0.838891 | -1.312546 |
| H    | -3.266325 | -1.436383 | -3.101800 |
| H    | -4.865095 | -3.042773 | -3.190574 |
| H    | -2.546454 | -2.851256 | -2.278496 |
| H    | 1.839732  | 0.725961  | 0.850828  |
| H    | 0.130423  | -2.019466 | -0.940140 |
| H    | 0.775431  | -3.202594 | 0.169028  |
| H    | 1.978263  | -2.377137 | -2.336438 |
| H    | 2.709291  | -3.451797 | -1.149546 |
| H    | 4.138822  | -1.411432 | -1.584479 |
| H    | 2.132051  | 0.067689  | -2.855356 |
| H    | 3.278840  | 0.825336  | -0.965050 |
| H    | 4.169829  | -2.621344 | 0.581007  |
| H    | 2.270074  | -2.564707 | 1.891903  |
| H    | 2.544356  | -0.865865 | 2.245269  |
| H    | 4.48240  | 0.391964  | 1.086332  |
| H    | 6.363325  | -2.015115 | 1.331716  |
| H    | 6.738286  | -0.245733 | 1.716685  |
| N    | 0.428595  | 2.030561  | -1.858196 |
| C    | -0.172567 | 2.597458  | -2.121965 |
| C    | 0.396317  | 3.842367  | -2.217644 |
| H    | -0.928340 | 2.099380  | -2.699377 |
| H    | 0.215841  | 4.627224  | -2.932587 |
| N    | 1.318351  | 2.885843  | -0.506468 |
| N    | 1.302420  | 3.979894  | -1.214864 |
1c - conformer 1 [mPW1PW91/6-311+G(2d,p)]

Energies in solvent (SMD)

|SCF| -1202.37640527 |
|---|---|
|Sum of electronic and zero-point Energies| -1201.931598 |
|Sum of electronic and thermal Energies| -1201.908547 |
|Sum of electronic and thermal Enthalpies| -1201.907603 |
|Sum of electronic and thermal Free Energies| -1201.983615 |

Number of imaginary frequencies: 0
### Energies in solvent (SMD)

| Term                                      | Value            |
|-------------------------------------------|------------------|
| SCF                                       | -1202.37785436   |
| Sum of electronic and zero-point Energies | -1201.932744     |
| Sum of electronic and thermal Energies    | -1201.909740     |
| Sum of electronic and thermal Enthalpies  | -1201.908795     |
| Sum of electronic and thermal Free Energies | -1201.984868 |
Energies in solvent (SMD)

\[
\text{SCF} = -1202.37483053
\]

Sum of electronic and zero-point Energies = -1201.929744

Sum of electronic and thermal Energies = -1201.906718

Sum of electronic and thermal Enthalpies = -1201.905774

Sum of electronic and thermal Free Energies = -1201.981822

Number of imaginary frequencies: 0
1d - conformer 1 [mPW1PW91/6-311+G(2d,p)]

| Atom | X          | Y          | Z          |
|------|------------|------------|------------|
| C    | 0.230097   | 0.918341   | 0.344773   |
| C    | -1.184043  | 1.061087   | -0.379872  |
| C    | -1.332275  | 2.172087   | -1.158210  |
| C    | -2.551176  | 2.318507   | -1.843653  |
| N    | -3.526570  | 1.440536   | -1.789924  |
| C    | -3.338880  | 0.338890   | -1.020560  |
| C    | -4.399982  | -0.602218  | -0.954345  |
| C    | -4.297749  | -1.730431  | -0.197334  |
| C    | -3.115624  | -1.982278  | 0.542653   |
| C    | -2.063178  | -1.097955  | 0.501899   |
| C    | -2.140462  | 0.087777   | -0.280656  |
| C    | -1.997704  | -3.477996  | 2.037444   |
| C    | 1.423792   | 0.726661   | -0.621036  |
| C    | 2.116707   | -0.326564  | -2.639774  |
| C    | 3.587284   | -0.081659  | -2.183774  |
| C    | 3.669850   | -0.374149  | -0.673498  |
| C    | 2.088738   | 0.658449   | 0.879937   |
| C    | 3.101157   | -1.798741  | -0.447780  |
| C    | 1.569524   | -1.693544  | -0.759665  |
| N    | 1.221956   | -0.460535  | -1.474474  |
| C    | 3.366963   | -2.365705  | 0.913045   |
| C    | 4.003932   | -3.567617  | 1.156560   |
| C    | 0.194265   | 0.068732   | 1.022841   |
| H    | -0.582834  | 2.949378   | -1.238780  |
| H    | -2.719510  | 3.198455   | -2.458076  |
| H    | 5.293004   | -0.386125  | -1.526847  |
| H    | -1.169407  | -1.312818  | 1.065685   |
| H    | -1.11184   | -3.603102  | 1.408571   |
| H    | -2.346755  | -4.424186  | 2.518754   |
| H    | -1.80068   | -2.721564  | 2.803544   |
| H    | 1.413174   | 1.586863   | -1.290919  |
| H    | 1.752476   | 0.491122   | -3.264299  |
| H    | 2.032379   | -1.243139  | -3.227466  |
| H    | 3.889526   | 0.951006   | -2.378290  |
| H    | 4.278057   | -0.725306  | -2.734440  |
| H    | 4.704740   | -0.325738  | -0.329652  |
| H    | 3.284035   | 1.640016   | 0.869408   |
| H    | 2.709365   | 0.376452   | 1.132487   |
| H    | 3.579632   | -2.464563  | -1.178994  |
| H    | 1.244763   | -2.547986  | -1.363691  |
| H    | 0.995419   | -1.743399  | 0.167301   |
| H    | 2.992348   | -1.792642  | 1.759867   |
| H    | 4.397930   | -4.120711  | 0.352921   |
| H    | 4.157968   | -3.867381  | 2.166645   |
| N    | 0.479843   | 2.075685   | 1.219790   |
| C    | 0.163073   | 2.216838   | 2.528082   |
| C    | 0.544279   | 3.496703   | 2.839528   |
| H    | -0.294117  | 1.430085   | 3.103642   |
| H    | 0.488245   | 4.024131   | 3.776223   |
| N    | 1.022571   | 3.215758   | 0.745441   |
| N    | 1.085494   | 4.073834   | 1.725709   |

**Energies in solvent (SMD)**

| Description                        | Value             |
|------------------------------------|-------------------|
| SCF                                | -1202.3764241     |
| Sum of electronic and zero-point   | -1201.931236      |
| Energies                           | -1201.908229      |
| Sum of electronic and thermal      | -1201.907285      |
| Enthalpies                         | -1201.907285      |
| Sum of electronic and thermal Free | -1201.983282      |
| Energies                           | -1201.983282      |
| Number of imaginary frequencies:   | 0                 |
### Energies in solvent (SMD)

| Source                          | Value             |
|---------------------------------|-------------------|
| SCF                             | -1202.37786413    |
| Sum of electronic and zero-point Energies | -1201.932886    |
| Sum of electronic and thermal Energies | -1201.909877    |
| Sum of electronic and thermal Enthalpies | -1201.908933    |
| Sum of electronic and thermal Free Energies | -1201.984886    |
| Number of imaginary frequencies: | 0                |

**1d - conformer 2 [mPW1PW91/6-311+G(2d,p)]**

| Atoms | X    | Y    | Z    |
|-------|------|------|------|
| C     | 0.256544 | 0.153640 | 0.492778 |
| C     | -0.823486 | 1.180425 | 0.177998 |
| C     | -0.633468 | 2.528043 | 0.367224 |
| C     | -1.668272 | 3.437980 | 0.874044 |
| N     | -2.842224 | 3.082168 | -0.393003 |
| C     | -3.964211 | 1.758831 | -0.595952 |
| C     | -4.331266 | 1.369153 | -1.104515 |
| C     | -4.628762 | 0.057048 | -1.323895 |
| C     | -2.426708 | -0.611205 | -0.531325 |
| C     | -2.090405 | 0.749463 | -0.321657 |
| O     | -4.087581 | -2.215932 | -1.286108 |
| C     | -3.192084 | -3.289351 | -1.018728 |
| C     | 1.700477  | 0.686211  | 0.650944  |
| C     | 3.358770  | 2.179342  | -0.198395 |
| C     | 4.460351  | 1.289351  | -1.314808 |
| C     | 4.003948  | -0.205309 | 0.196868  |
| C     | 2.719604  | -0.437605 | 1.013444  |
| C     | 3.512902  | -1.837306 | -1.717835 |
| C     | 4.247561  | -2.488184 | -2.613892 |
| H     | 0.258447  | 0.598423  | 0.296294  |
| H     | 0.313228  | 2.915989  | 0.714055  |
| H     | -1.505918 | 4.501260  | 0.228021  |
| H     | -5.050700 | 2.152486  | -1.308768 |
| H     | -5.593151 | 0.250080  | -1.708839 |
| H     | -1.714754 | -0.387901 | 0.319774  |
| H     | -2.293065 | -3.219773 | -1.629866 |
| H     | -3.734988 | -4.198141 | -1.259709 |
| H     | -2.906511 | -3.308127 | 0.843993  |
| H     | 1.689950  | 1.420483  | 1.461185  |
| H     | 3.080485  | 2.964171  | 0.509402  |
| H     | 3.707810  | 2.676712  | -1.105665 |
| H     | 4.609989  | 1.451277  | 1.459478  |
| H     | 5.426298  | 1.421651  | -0.899233 |
| H     | 4.782543  | -0.897967 | 0.521722  |
| H     | 2.945025  | -0.419349 | 2.082187  |
| H     | 2.307643  | -1.426660 | 0.806559  |
| H     | 4.586031  | -0.032738 | -1.866354 |
| H     | 2.683592  | 1.081627  | -2.544877 |
| H     | 1.683857  | -0.127021 | 1.863247  |
| H     | 2.688189  | -2.364604 | -1.241817 |
| H     | 5.078801  | -2.010553 | -3.123032 |
| H     | 4.045297  | -3.520874 | -2.871545 |
| N     | -0.113935 | -0.612925 | 1.694406  |
| C     | -0.438585 | -0.173218 | 2.931284  |
| C     | -0.657292 | -1.318542 | 3.656071  |
| H     | -0.587131 | 0.871875  | 3.180550  |
| H     | -0.944654 | -1.432391 | 4.687724  |
| N     | -0.134008 | -1.963552 | 1.656914  |
| N     | -0.462653 | -2.389538 | 2.842983  |
1d - conformer 3 [mPW1PW91/6-311+G(2d,p)]

Energies in solvent (SMD)

SCF = -1202.37512148

Sum of electronic and zero-point Energies = -1201.930141

Sum of electronic and thermal Energies = -1201.907122

Sum of electronic and thermal Enthalpies = -1201.906178

Sum of electronic and thermal Free Energies = -1201.982132

Number of imaginary frequencies: 0
2a - conformer 1 [B3LYP/6-31G(d,p)]

| Atom | X  | Y  | Z   |
|------|----|----|-----|
| C    | -0.266105 | 2.278815 | -0.331469 |
| C    | 0.682419  | 2.390532  | -1.132513 |
| H    | 1.466980  | 2.346963  | -1.608768 |
| C    | 0.644345  | 4.311577  | -1.319764 |
| H    | 1.391155  | 4.792855  | -1.945518 |
| C    | -0.351225 | 5.071860  | -0.705004 |
| H    | -0.37197 | 6.147749  | -0.848998 |
| C    | -1.303984 | 4.435990  | 0.931178  |
| H    | -2.089501 | 5.016256  | 0.567039  |
| C    | -1.263659 | 3.052781  | 0.274325  |
| H    | -2.031289 | 2.576856  | 0.873779  |
| C    | -0.131146 | 0.768382  | -0.128523 |
| H    | 0.217992  | 0.364852  | -1.081811 |
| C    | 0.936561  | 0.463444  | 0.929330  |
| C    | 0.779735  | 0.946803  | 2.215308  |
| H    | -0.075267 | 1.564958  | 2.467256  |
| C    | 1.737376  | 0.663823  | 3.211888  |
| H    | 1.593319  | 1.053477  | 4.219133  |
| N    | 2.825579  | -0.048843 | 3.003872  |
| C    | 3.013851  | -0.530656 | 1.746212  |
| C    | 4.201008  | -1.294620 | 1.517400  |
| H    | 4.865519  | -1.443701 | 2.361719  |
| H    | 4.482480  | -1.815249 | 0.283771  |
| C    | 5.378739  | -2.397565 | 0.897707  |
| C    | 3.588684  | -1.594878 | -0.798973 |
| C    | 2.432793  | -0.860653 | -0.618423 |
| H    | 1.765332  | -0.698861 | -1.453212 |
| C    | 2.112368  | -0.308750 | 0.657091  |
| C    | 3.980275  | -2.159574 | -1.977082 |
| C    | 3.151083  | -1.986232 | -3.114796 |
| H    | 2.154808  | -2.419805 | -2.957917 |
| H    | 3.646994  | -2.510769 | -3.932670 |
| H    | 3.042840  | -0.926020 | -3.377399 |
| C    | -1.448362 | 0.025444  | 0.220038  |
| H    | -1.776125 | 0.383796  | 1.202277  |
| C    | -2.335583 | -0.207144 | -2.045611 |
| H    | -1.441217 | 0.244169  | -2.484300 |
| H    | -3.176646 | 0.107961  | -2.671880 |
| C    | -2.228015 | -1.763315 | -1.990693 |
| H    | -1.259162 | -2.106171 | -2.373696 |
| H    | -2.999209 | -2.234315 | -2.611382 |
| C    | -2.380747 | -2.197981 | -0.519745 |
| C    | -2.312664 | -3.287086 | -0.434858 |
| C    | -1.264602 | -1.527415 | 0.298363  |
| H    | -0.296789 | -1.832949 | -0.114538 |
| H    | -1.273551 | -1.868941 | 1.337867  |
| C    | -3.788297 | -1.734746 | -0.829637 |
| H    | -4.532192 | -2.160841 | -0.715594 |
| C    | -3.804490 | -0.165583 | -0.157850 |
| H    | -4.626400 | 0.155392  | -0.806625 |
| H    | -3.972963 | 0.296532  | 0.821632  |
| N    | -2.550061 | 0.367361  | -0.706479 |
| C    | -4.130049 | -2.201362 | 1.358138  |
| H    | -3.504232 | -1.817407 | 2.165465  |
| C    | -5.135414 | -3.022232 | 1.665412  |
| C    | -5.794127 | -3.427527 | 0.906626  |
| H    | -5.338852 | -3.320057 | 2.689680  |

Energies in solvent (SMD)

SCF = -1192.38180481

Sum of electronic and zero-point Energies= -1191.895611

Sum of electronic and thermal Energies= -1191.871940

Sum of electronic and thermal Enthalpies= -1191.870996

Sum of electronic and thermal Free Energies= -1191.950792

Number of imaginary frequencies: 1 (-7 cm⁻¹)

Frequencies in vacuum

Number of imaginary frequencies: 0
| Atom | X    | Y    | Z    |
|------|------|------|------|
| C    | 0.628422 | 2.032271 | -0.410046 |
| C    | 1.706631  | 2.587630  | -1.055224 |
| H    | 2.003856  | 2.158418  | -2.058149 |
| C    | 2.429382  | 3.668211  | -0.599988 |
| H    | 3.257144  | 4.075470  | -1.151454 |
| C    | 2.664822  | 4.220557  | 0.648711 |
| H    | 5.061454  | 1.846456  | 3.668419  |
| H    | 0.984345  | 3.684419  | 1.339337 |
| C    | 0.866684  | 4.112711  | 2.292722 |
| C    | 0.264916  | 2.605335  | 0.818280 |
| H    | -0.601972 | 2.234196  | 1.349089 |
| C    | -0.011211 | 0.839993  | -1.047960 |
| C    | -0.540602 | 1.216688  | -1.983059 |
| C    | -0.865636 | -0.257851 | -1.485799 |
| C    | 0.931999  | -0.603790 | -2.822765 |
| H    | 0.320917  | -0.079399 | -3.552497 |
| H    | 0.993231  | -0.363379 | 3.502665 |
| C    | 1.777139  | -1.647484 | -3.260697 |
| H    | 1.809732  | -1.904806 | -4.318812 |
| N    | 2.540826  | -2.356283 | -2.455572 |
| C    | 2.511972  | -2.032968 | -1.131610 |
| C    | 3.351013  | -2.790914 | -0.261452 |
| H    | 3.942102  | -3.584090 | -0.706637 |
| C    | 3.407968  | -2.521111 | 1.679408 |
| H    | 4.044462  | -3.087445 | 1.751200 |
| C    | 2.632317  | -1.461722 | 1.622827 |
| C    | 1.800627  | -0.711535 | 0.813731 |
| H    | 1.242786  | -0.079399 | -3.552497 |
| C    | 1.712374  | -0.980740 | -0.581590 |
| O    | 2.795781  | -1.269391 | 2.961996 |
| C    | 2.075956  | -0.210166 | 3.578216 |
| H    | 2.331282  | 0.760866  | 3.135888 |
| H    | 2.376104  | -0.219697 | 4.628999 |
| H    | 0.993231  | -0.363379 | 3.502665 |
| C    | -1.296517 | 0.233206  | -0.237639 |
| H    | -0.902747 | -0.082745 | 0.734004 |
| C    | -3.154383 | 1.577587  | -1.105935 |
| H    | -2.509510 | 2.024111  | -1.860146 |
| H    | -3.856211 | 2.362182  | -0.804448 |
| C    | -3.907070 | 0.332674  | -1.669342 |
| H    | -3.661638 | 0.169652  | -2.725150 |
| H    | -4.993362 | 0.468600  | -1.612329 |
| C    | -3.477911 | -0.892138 | -0.837924 |
| H    | -3.946971 | -1.801157 | -1.228249 |
| C    | -1.943058 | -1.009530 | -0.931920 |
| H    | -1.663145 | -1.058949 | -1.989761 |
| H    | -1.581980 | -1.938088 | -0.479399 |
| C    | -3.935523 | -0.662849 | 0.629856 |
| H    | -5.021991 | -0.507745 | 0.616271 |
| C    | -3.232113 | 0.663855  | 1.105358 |
| H    | -3.980531 | 1.419662  | 1.366568 |
| H    | -2.636754 | 0.479112  | 2.007066 |
| N    | -2.347161 | 1.232743  | 0.677770 |
| C    | -3.651036 | -1.824659 | 1.540835 |
| H    | -2.599945 | -2.077380 | 1.688485 |
| C    | -4.576626 | -2.541033 | 2.176094 |
| H    | -5.637828 | -2.331322 | 2.067709 |
| H    | -4.310972 | -3.371692 | 2.827026 |
The document contains a table and some text. Here is the representation of the content in a plain text format:

### Energies in solvent (SMD)

| Term                                | Value           |
|-------------------------------------|-----------------|
| SCF                                 | -1192.38253744  |
| Sum of electronic and zero-point Energies= | -1191.896613    |
| Sum of electronic and thermal Energies= | -1191.871975    |
| Sum of electronic and thermal Enthalpies= | -1191.871031    |
| Sum of electronic and thermal Free Energies= | -1191.955438    |
| Number of imaginary frequencies:    | 0               |

The table includes atomic coordinates for the molecule, with columns for carbon (C), hydrogen (H), oxygen (O), and nitrogen (N) atoms. The coordinates are given in angstroms (Å) with x, y, and z components.
2b - conformer 1 [B3LYP/6-31G(d,p)]

|       |   x    |   y    |   z    |
|-------|-------|-------|-------|
|       |   0.147498 | 1.632802 | -0.574126 |
| C     | 0.402927  | 2.688043  | 0.311329  |
| C     | 0.488189  | 2.498337  | 1.382215  |
| C     | 0.647830  | 3.980328  | -0.157361 |
| H     | 0.843324  | 4.782147  | 0.549098  |
| C     | 0.624348  | 4.239132  | -1.527438 |
| H     | 0.835010  | 5.242216  | -1.896200 |
| C     | 0.392720  | 3.196275  | -2.421641 |
| H     | 0.392851  | 3.385089  | -3.491360 |
| C     | 0.150042  | 3.196275  | -2.421641 |
| H     | 0.082459  | 0.223111  | 1.015466  |
| C     | 0.762130  | 2.540329  | -0.719683 |
| C     | 0.334059  | -1.623188 | -1.758372 |
| H     | -0.693502 | -1.595151 | -2.089178 |
| C     | 1.221334  | -2.540329 | -2.355837 |
| H     | 0.862334  | -3.172846 | -3.167883 |
| N     | 2.478520  | -2.701496 | -1.996652 |
| C     | 2.936296  | -1.916879 | -0.981569 |
| C     | 4.292636  | -2.084915 | -0.584038 |
| H     | 4.874930  | -2.833888 | -1.110199 |
| C     | 4.837184  | -1.328547 | 0.418587  |
| H     | 5.870322  | -1.445381 | 0.728601  |
| C     | 4.044660  | -0.351378 | 1.687964  |
| C     | 2.722320  | -0.163141 | 0.726820  |
| H     | 2.135428  | 0.598182  | 1.219381  |
| C     | 2.129938  | -0.942578 | 0.307439  |
| O     | 4.702165  | 0.349026  | 2.048105  |
| C     | 3.990253  | 1.361318  | 2.741093  |
| H     | 3.631589  | 2.141646  | 2.657796  |
| H     | 4.696547  | 1.797044  | 3.449162  |
| C     | 3.135109  | 0.947582  | 3.291602  |
| C     | -1.674218 | -0.072037 | -0.178171 |
| H     | -1.942007 | 0.036309  | -1.235805 |
| C     | -1.859118 | -1.722875 | 1.614692  |
| H     | -0.801980 | -1.618031 | 1.874430  |
| H     | -2.115958 | -2.773038 | 1.788185  |
| C     | -2.757654 | -0.775580 | 2.468978  |
| H     | -2.151574 | -0.154193 | 3.139158  |
| H     | -3.444120 | -1.348495 | 3.103191  |
| C     | -3.551254 | 0.125636  | 1.501574  |
| H     | -4.196493 | 0.899895  | 2.062387  |
| C     | -2.540014 | 0.929115  | 0.658709  |
| H     | -1.914523 | 1.523545  | 1.333480  |
| H     | -3.847193 | 1.646809  | 0.006638  |
| C     | -4.426538 | -0.787854 | 0.597809  |
| H     | -5.042116 | -1.411493 | 1.258582  |
| C     | -3.424988 | -1.706698 | -0.196773 |
| H     | -3.651457 | -2.762801 | -0.815992 |
| H     | -3.526437 | -1.538611 | -1.275182 |
| N     | -2.023498 | -1.465822 | 0.173884  |
| C     | -5.354635 | -0.030882 | -0.318420 |
| H     | -4.882224 | 0.608164  | -1.058080 |
| C     | -6.686249 | -0.099113 | 0.276974  |
| H     | -7.206737 | -0.726645 | 0.443846  |
| H     | -7.306158 | 0.466785  | -0.965973 |

**Energies in solvent (SMD)**

|                      |       |
|----------------------|-------|
| SCF                  | -1192.38311966 |
| Sum of electronic and zero-point Energies= | -1191.896829 |
| Sum of electronic and thermal Energies=   | -1191.872367 |
| Sum of electronic and thermal Enthalpies=  | -1191.871423 |
| Sum of electronic and thermal Free Energies= | -1191.953213 |

Number of imaginary frequencies: 0
2c - conformer 1 [B3LYP/6-31G(d,p)]

|     |          |          |          |
|-----|----------|----------|----------|
| C   | -0.866526| 2.070947 | 0.755787 |
| C   | -0.171573| 2.467730 | 1.907169 |
| H   | 0.623414 | 1.833842 | 2.293045 |
| C   | -0.473914| 3.662133 | 2.559251 |
| H   | 0.079937 | 3.945726 | 3.449743 |
| C   | -1.485298| 4.488991 | 2.865818 |
| H   | -1.726446| 5.419857 | 2.573337 |
| C   | -2.187584| 4.195684 | 0.926390 |
| H   | -2.982973| 4.735774 | 0.539319 |
| C   | -1.882701| 2.620725 | -0.594707|
| H   | -2.459313| 2.620725 | 2.293045 |
| H   | -1.485298| 3.662133 | 2.559251 |

Energies in solvent (SMD)

|                           |          |
|---------------------------|----------|
| SCF                       | -1192.38192999 |
| Sum of electronic and zero-point Energies | -1191.895873 |
| Sum of electronic and thermal Energies | -1191.872260 |
| Sum of electronic and thermal Enthalpies | -1191.871316 |
| Sum of electronic and thermal Free Energies | -1191.950242 |
| Number of imaginary frequencies: | 1 (-20 cm⁻¹) |

Frequencies in vacuum

|                           |          |
|---------------------------|----------|
| Number of imaginary frequencies: | 0 |

S47
2c - conformer 2 [B3LYP/6-31G(d,p)]

|        |        |        |
|--------|--------|--------|
| C      | 0.114562 | 1.854656 | -0.817191 |
| C      | 0.058010 | 2.365973 | 1.285069  |
| H      | -0.251174| 1.713722 | 2.108771  |
| C      | 0.356585 | 3.700600 | 1.559884  |
| H      | 0.299488 | 4.074526 | 2.569467  |
| C      | 0.739296 | 4.552879 | 0.511358  |
| H      | 0.979511 | 5.592391 | 0.714485  |
| C      | 0.796336 | 4.056761 | -0.791045 |
| H      | 1.090920 | 4.794957 | -1.607995 |
| C      | 0.495140 | 2.719354 | -1.858782 |
| H      | 0.571736 | 2.342565 | -2.066384 |
| C      | -0.244491| 0.391801 | -0.293413 |
| H      | -0.223070| -0.131417| 0.669221  |
| C      | 0.803456 | -0.281757| -1.178804 |
| C      | 0.629663 | -0.451229| -2.539617 |
| H      | -0.276058| -0.119099| -3.033841 |
| C      | 1.628035 | -1.076138| -3.321673 |
| H      | 1.466192 | -1.282520| -4.391652 |
| N      | 2.762861 | -1.536375| -2.838353 |
| C      | 2.978971 | -1.372671| -1.502686 |
| C      | 2.080309 | -1.856176| -0.973201 |
| H      | 4.892465 | -2.336751| -1.664384 |
| C      | 4.514042 | -1.710997| 0.353278  |
| H      | 5.450005 | -2.070143| 0.768110  |
| C      | 3.597978 | -1.063895| 1.226085  |
| C      | 2.388562 | -0.593149| 0.752178  |
| H      | 1.710260 | -0.078233| 1.416951  |
| C      | 2.043513 | -0.740603| -0.620579 |
| O      | 4.024162 | -0.959635| 2.516531  |
| C      | 3.180018 | -0.302648| 3.449905  |
| H      | 2.222823 | -0.827426| 3.565463  |
| H      | 3.714439 | -0.315666| 4.400676  |
| H      | 2.985314 | 0.736131 | 3.155243  |
| C      | -1.695857| 0.249566 | -0.832769 |
| H      | -1.747573| 0.810952 | -1.773027 |
| C      | -2.973137| 0.092607 | 1.242000  |
| H      | -2.034079| -0.146218| 1.750543  |
| H      | -3.559499| 0.695914 | 1.943169  |
| C      | -3.740457| -1.227240| 0.877995  |
| H      | -4.805118| -1.181141| 1.114499  |
| C      | -3.616252| -1.378320| -0.664163 |
| H      | -4.004476| -2.348132| -0.978094 |
| C      | -2.139554| -1.225828| -1.890405 |
| H      | -1.506277| -1.927313| -0.534620 |
| H      | -2.027822| -1.490516| -2.146356 |
| C      | -4.430988| -0.232099| -1.307331 |
| H      | -5.501334| -0.370961| -1.117007 |
| C      | -3.922364| 1.113687 | -0.700090 |
| H      | -4.662575| 1.541873 | -0.815447 |
| H      | -3.739662| 1.859637 | -1.488019 |
| N      | -2.674536| 0.915842 | 0.859026  |
| H      | -4.296584| -0.248201| -2.395573 |
| C      | -3.241165| -2.412296| 1.656266  |
| C      | -3.975257| -3.139908| 2.498654  |
| H      | -2.189927| -2.670692| 1.522062  |
| H      | -3.556232| -3.981339| 3.042402  |
| H      | -5.026029| -2.921242| 2.675088  |

**Energies in solvent (SMD)**

|        |        |
|--------|--------|
| SCF    | -1192.38305994 |
| Sum of electronic and zero-point Energies | -1191.896593 |
| Sum of electronic and thermal Energies | -1191.872186 |
| Sum of electronic and thermal Enthalpies | -1191.871242 |
| Sum of electronic and thermal Free Energies | -1191.952513 |
| Number of imaginary frequencies: | 0 |
2d - conformer 1 [B3LYP/6-31G(d,p)]

C  0.146283  1.527018  -0.974424
C  0.172896  2.661873  -0.151957
H  -0.068045  2.561395   0.904021
C  0.508365  3.917560  -0.664731
H  0.514703  4.781808  -0.066676
C  0.808632  4.069960  -2.817209
H  1.066262  5.036938  -2.419851
C  0.789749  2.938912  -2.847835
H  1.035654  3.037937  -3.901252
C  0.464367  1.685459  -2.339835
H  0.474753  0.817207  -2.982826
C  -0.249814  0.156800  -0.412882
H  -0.255546  0.253471   0.679217
C  0.787084  -0.908082  -0.770187
C  0.584339  -1.833107  -1.775484
H  -0.349897  -1.866751  -2.321477
C  1.582753  -2.780280  -2.092834
H  1.400374  -3.495451  -2.896667
N  2.742970  -2.867616  -1.475352
C  2.978724  -1.973093  -0.475351
C  4.228070  -2.060940   0.207026
H  4.912025  -2.839821  -0.119324
C  4.558351  -1.195299  1.210942
H  5.499962  -1.250926  1.732730
C  3.630460  -0.183689  1.597485
C  2.405713  -0.069147   0.969030
H  1.722846   0.717640  1.254278
C  2.043632  -0.961619  -0.879712
O  4.070356   0.624753  2.604744
C  3.228219   1.673394  3.840085
H  2.995937   2.374937  2.226477
H  3.763858   2.195615  3.828640
H  2.277428   1.284910  3.447153
C  -1.704684  -0.188496  -0.840696
H  -1.711754  -0.253293  -1.934872
C  -2.498023  -1.481803  1.866160
H  -1.645624  -1.090800  1.630228
H  -2.659604  -2.589448  1.411978
C  -3.781181  -0.615797  1.335552
H  -4.638835  -1.283884  1.488278
C  -4.038959   0.183628  0.826213
H  -4.836965   0.915260  0.188858
C  -2.743507   0.896760  -0.414998
H  -2.357880  1.515214   0.402414
H  -2.947207   1.582803  -1.243612
C  -4.444563  -0.828302  -1.065384
H  -5.419056  -1.272814  -0.833253
C  -3.332219  -1.919950  -1.133115
H  -3.687333  -2.871539  -0.723184
H  -3.028825  -2.112261  -2.168522
N  -2.141918  -1.519543  -0.361057
H  -4.558320  -0.312981  -2.927413
C  -3.649071   0.236436  2.556523
C  -4.436240   0.160273  3.639818
H  -2.830334   0.957821  2.569532
H  -4.286642   0.797866  4.506855
H  -5.261883  -0.545786  3.692325
### Energies in solvent (SMD)

| SCF                  | -1267.605955 |
|----------------------|--------------|
| Sum of electronic and zero-point Energies | -1267.115934 |
| Sum of electronic and thermal Energies | -1267.090569 |
| Sum of electronic and thermal Enthalpies | -1267.089625 |
| Sum of electronic and thermal Free Energies | -1267.169544 |

Number of imaginary frequencies: 0

---

### Conformer 1 [mPW1PW91/6-311+G(2d,p)]

| C       | 0.259217 | 0.344363 | -1.313185 |
|---------|----------|----------|-----------|
| C       | -0.758041| -0.814178| -1.274837 |
| C       | -0.738113| -1.735455| -2.299774 |
| C       | -1.667595| -2.791460| -2.339716 |
| N       | -2.689055| -2.969080| -1.443975 |
| C       | -2.669593| -2.081842| -0.417051 |
| C       | -3.686340| -2.278702| 0.558669  |
| C       | -3.819663| -1.451329| 1.626085  |
| C       | -2.983962| -0.376832| 1.793981  |
| C       | -1.985645| -0.148220| 0.876620  |
| O       | -3.113149| 0.371266 | 2.913557  |
| C       | -2.265968| 1.491828 | 3.141976  |
| C       | 1.577069 | 0.114903 | -0.485802 |
| C       | 1.189390 | -1.369866| 1.445688  |
| C       | 2.345106 | -2.339569| 1.077438  |
| C       | 3.304172 | -1.583279| 0.988366  |
| C       | 2.476032 | -1.082199| 1.012943  |
| C       | 3.949788 | -0.441538| 0.979536  |
| N       | 1.460855 | 0.012927| 0.988366  |
| C       | 4.950790 | 0.375472| 0.217100  |
| C       | 6.242923 | 0.468215| 3.141976  |
| O       | 0.727527 | 0.395868| -2.687879 |
| H       | -0.023565| -1.636933| -3.102755 |
| H       | -1.629157| -3.506306| -3.157463 |
| H       | -4.357511| -3.114578| 0.399805  |
| H       | -4.585624| -1.594465| 2.368724  |
| H       | 1.202265 | 0.650683| 1.035099  |
| H       | -1.222924| 1.182362| 3.255608  |
| H       | -2.615482| 1.943176| 4.067736  |
| H       | -2.341325| 2.215806| 2.326607  |
| H       | 2.121177 | 1.047653| -0.654532 |
| H       | 0.253134 | -1.783921| 1.012943  |
| H       | 1.037134 | -1.326129| 2.526181  |
| H       | 1.954319 | -3.227511| 0.574270  |
| H       | 2.874763 | -2.684169| 1.970295  |
| H       | 4.086026 | -2.248221| -0.224632 |
| H       | 1.878522 | -1.838492| -1.451295 |
| H       | 3.112883 | -0.661752| -1.833015 |
| H       | 4.477975 | -0.906762| 1.817936  |
| H       | 2.709170 | 0.320755 | 2.633824  |
| H       | 2.924352 | 1.479886 | 1.331057  |
| H       | 4.576197 | 0.937962 | -0.636342 |
| H       | 6.671778 | -0.067156| 1.355439  |
| H       | 6.918911 | 1.079979 | -0.871368 |
| C       | 0.409354 | 1.706145 | 1.033378  |
| C       | -1.525615| 2.043636 | -1.828624 |
| C       | 0.887099 | 2.659606 | 0.163448  |
| C       | -2.126916| 3.289454 | -1.716599 |
| H       | -1.924066| 1.319329 | 2.528372  |
| C       | -0.515779| 3.911314 | -0.850828 |
| H       | 0.926386 | 2.425417 | 0.474555  |
| C       | -1.623181| 4.231965 | 0.823849  |
| H       | -2.992003| 3.524323 | -2.325422 |
| H       | -0.113935| 4.634556 | 0.658198  |
| H       | -2.091140| 5.285180 | -0.733816 |
| H       | 1.813170 | 1.299797 | -2.861038 |
3a - conformer 2 [mPW1PW91/6-311+G(2d,p)]

| Atom | X      | Y      | Z      |
|------|--------|--------|--------|
| C    | 0.174748 | 1.231091 | -0.829705 |
| C    | -1.187951 | 0.659379 | -1.317280 |
| C    | -1.659684 | 1.077455 | -2.548062 |
| C    | -2.844243 | 0.545659 | -3.828211 |
| N    | -3.578371 | -0.371949 | -2.498442 |
| C    | -3.155541 | -0.796333 | -1.269077 |
| C    | -3.958795 | -1.771125 | -0.619764 |
| C    | -3.649265 | -2.230500 | 0.624569 |
| C    | -2.568416 | -1.727387 | 1.296260 |
| C    | -1.691348 | -0.799126 | 0.691465 |
| C    | -1.980559 | -0.307918 | -0.614440 |
| O    | -2.328354 | -2.232300 | 2.548948 |
| C    | -1.239627 | -1.755441 | 3.326719 |
| C    | 1.158586  | -0.097973 | -0.507120 |
| C    | 3.407774  | 0.611923  | -1.338073 |
| C    | 4.143170  | 0.119339  | -0.856152 |
| C    | 3.198474  | -0.851274 | 0.666399 |
| C    | 1.856292  | -0.115085 | 0.896934 |
| C    | 3.043728  | -2.107153 | -0.237982 |
| C    | 2.531366  | -1.597395 | -1.635291 |
| N    | 2.171644  | -0.169882 | -1.585520 |
| C    | 2.164252  | -3.173170 | 0.348290 |
| C    | 2.582123  | -4.372036 | 0.740751 |
| O    | 0.763484  | 1.965829  | -1.897845 |
| H    | -1.106332 | 1.817183  | -3.100024 |
| H    | -3.196084 | 0.891214  | -4.053229 |
| H    | -4.833941 | -2.124068 | -1.150192 |
| H    | -4.262251 | -2.965690 | 1.130841 |
| H    | -0.846066 | -0.403586 | 1.229578 |
| H    | -0.281036 | -2.016525 | 2.868776 |
| H    | -1.322834 | -2.251429 | 4.291307 |
| H    | -1.295262 | -0.672224 | 3.467470 |
| H    | 0.530234  | -0.891016 | -0.607494 |
| H    | 3.135007  | 1.661668  | -1.250569 |
| H    | 4.039114  | 0.513730  | -2.216423 |
| H    | 4.393231  | 0.960492  | 0.595340 |
| H    | 5.082131  | -0.381055 | -0.308398 |
| H    | 3.613781  | -1.148420 | 1.631326 |
| H    | 2.055589  | 0.861255  | 1.313227 |
| H    | 1.221073  | -0.649615 | 1.577701 |
| H    | 4.042150  | -2.537469 | -0.361722 |
| H    | 3.307339  | -1.725216 | -2.394668 |
| H    | 1.661418  | -2.166989 | -1.961712 |
| H    | 1.105042  | -2.939422 | 0.439649 |
| H    | 3.624487  | -4.664498 | 0.661294 |
| H    | 1.898721  | -5.105701 | 1.151327 |
| C    | 0.013777  | 2.253205  | 0.308312 |
| C    | -1.166324 | 2.424056  | 1.831976 |
| C    | 1.083681  | 3.198826  | 0.598017 |
| C    | -1.263587 | 3.388039  | 2.034183 |
| H    | -2.834910 | 1.821475  | 0.811827 |
| C    | 0.991095  | 4.070395  | 1.594771 |
| H    | 1.990051  | 3.040117  | 0.812619 |
| C    | -0.184849 | 4.210419  | 2.326322 |
| H    | -2.216041 | 3.499916  | 2.575057 |
| H    | 1.835958  | 4.719782  | 1.792998 |
| H    | -0.261822 | 4.962881  | 3.102223 |
| H    | 1.241264  | 1.295736  | -2.424085 |

**Energies in solvent (SMD)**

- SCF = -1267.60510711
- Sum of electronic and thermal Energies = -1267.114524
- Sum of electronic and thermal Energies = -1267.089528
- Sum of electronic and thermal Energies = -1267.168329
- Number of imaginary frequencies: 0
### 3b - conformer 1 [mPW1PW91/6-311+G(2d,p)]

|   | X         | Y         | Z         |
|---|-----------|-----------|-----------|
| C | -0.097119 | 1.084338  | -0.946738 |
| C | 0.828762  | -0.113359 | -1.508663 |
| C | 0.864117  | -0.338224 | -2.856849 |
| C | 1.643343  | -1.381280 | -3.393639 |
| N | 2.364640  | -2.203490 | -2.668681 |
| C | 2.364775  | -2.084525 | -1.322245 |
| C | 3.155899  | -2.886101 | -0.539681 |
| C | 3.235257  | -2.753268 | 0.814293  |
| C | 2.524083  | -1.714315 | 1.462876  |
| C | 1.738663  | -0.845418 | 0.740837  |
| C | 1.624612  | -0.966928 | -0.672015 |
| O | 2.700174  | -1.664692 | 2.812192  |
| C | 2.041963  | -0.637654 | 3.542011  |
| C | -1.278381 | 0.291372  | -0.208549 |
| C | -3.272188 | 1.727683  | -0.517326 |
| C | -4.072949 | 0.599936  | -1.229799 |
| C | -3.501804 | -0.749235 | -0.766126 |
| C | -1.999908 | -0.763423 | -1.101762 |
| C | -3.740697 | -0.870152 | 0.762794  |
| C | -3.009288 | 0.356294  | 1.420366  |
| N | -2.286111 | 1.172316  | 0.432363  |
| C | -3.301311 | -2.181577 | 1.341796  |
| C | -4.102321 | -3.063597 | 1.930938  |
| O | -0.681662 | 1.723545  | -2.052363 |
| H | 0.277019  | 0.280909  | -3.519579 |
| H | 1.655994  | -1.541365 | -4.468558 |
| H | 3.697293  | -3.663898 | -1.063062 |
| H | 3.840422  | -3.413070 | 1.417632  |
| H | 1.238693  | -0.041345 | 1.246088  |
| H | 2.354791  | 0.353841  | 3.202959  |
| H | 2.333994  | -0.777192 | 4.580505  |
| H | 0.954696  | -0.725627 | 3.455404  |
| H | -0.811738 | -0.240037 | 0.621238  |
| H | -2.747239 | 2.350231  | -1.234335 |
| H | -3.936675 | 2.374731  | 0.860205  |
| H | -3.978153 | 0.687273  | -2.315163 |
| H | -5.139075 | 0.661324  | -0.992861 |
| H | -4.004001 | -1.572721 | -1.278343 |
| H | -1.880385 | -0.524537 | -2.159619 |
| H | -1.565388 | -1.753507 | -0.951621 |
| H | -4.817245 | -0.776449 | 0.935678  |
| H | -3.733486 | 1.000317  | 1.924315  |
| H | -2.299466 | 0.016648  | 2.179254  |
| H | -2.238966 | -2.410499 | 1.276951  |
| H | -5.168973 | -2.886273 | 2.827403  |
| H | -3.722863 | -3.993986 | 2.336417  |
| C | 0.726439  | 2.019177  | -0.128767 |
| C | 0.285926  | 2.689230  | 1.858718  |
| C | 1.962014  | 2.428039  | -0.648719 |
| C | 1.864128  | 3.565154  | 1.707254  |
| H | -0.681269 | 2.335432  | 1.454431  |
| C | 2.731869  | 3.391177  | -0.007567 |
| H | 2.339755  | 1.973484  | -1.557273 |
| C | 2.286843  | 3.962356  | 1.179830  |
| H | 0.702172  | 4.008100  | 2.628169  |
| H | 3.685346  | 3.684319  | -0.430928 |
| H | 2.887071  | 4.708682  | 1.668756  |
| H | -0.136985 | 2.499646  | -2.225907 |

#### Energies in solvent (SMD)

| SCF = | -1267.6096191 |
|-------|----------------|
| Sum of electronic and zero-point Energies= | -1267.119875 |
| Sum of electronic and thermal Energies= | -1267.094466 |
| Sum of electronic and thermal Enthalpies= | -1267.093522 |
| Sum of electronic and thermal Free Energies= | -1267.173866 |

Number of imaginary frequencies: 0
3b - conformer 2 [mPW1PW91/6-311+G(2d,p)]

|   |   |   |   |   |   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
|   |   |   |   |   |   |   |   |   |   |   |   |   |
| C | -0.259472 | 0.800208 | -0.380773 |
| C | 0.827292 | 0.675863 | 0.728690 |
| C | 0.479881 | 1.192840 | 1.968887 |
| C | 1.338451 | 1.009386 | 3.065577 |
| N | 2.517551 | 0.516742 | 3.014310 |
| C | 2.907145 | 0.081436 | 1.821354 |
| C | 4.185864 | -0.616182 | 1.784258 |
| C | 4.672129 | -1.173405 | 0.641139 |
| C | 3.891066 | -1.139788 | -0.539291 |
| C | 2.648729 | -0.552816 | -0.558576 |
| C | 2.108575 | 0.041795 | 0.627276 |
| O | 4.479200 | -1.725618 | -1.621740 |
| C | 3.772149 | -1.726350 | -2.853625 |
| C | -1.360587 | -0.251597 | -0.056666 |
| C | -2.237337 | -1.187522 | -2.207729 |
| C | -1.998735 | -2.597883 | -1.831937 |
| C | -1.924038 | -2.682476 | -0.300537 |
| C | -0.836827 | -1.695487 | 0.168735 |
| C | -3.321357 | -2.298639 | 0.257257 |
| C | -3.642195 | -0.861256 | -0.300354 |
| N | -2.495337 | -0.274011 | -1.013027 |
| C | -3.420002 | -2.378597 | 1.751804 |
| C | -4.232959 | -3.190253 | 2.420025 |
| O | 0.328516 | 0.530821 | -1.671037 |
| H | -0.463552 | 1.766252 | 2.891917 |
| H | 1.035481 | 1.565934 | 4.022859 |
| H | 4.755410 | -0.625212 | 2.704752 |
| H | 5.646273 | -1.645060 | 0.605544 |
| H | 2.079065 | -0.520866 | -1.454806 |
| H | 2.827767 | -2.272334 | -2.769283 |
| H | 4.419959 | -2.229322 | -3.568482 |
| H | 3.579401 | -0.707182 | -3.196198 |
| H | -1.793108 | 0.888888 | 0.886218 |
| H | -1.379345 | -0.708402 | -2.739999 |
| H | -3.104167 | -1.000335 | -2.863344 |
| H | -1.067118 | -2.962508 | -2.272395 |
| H | -2.083341 | -3.235628 | -2.209185 |
| H | -1.671460 | -3.696300 | 0.816353 |
| H | 0.072706 | -1.873111 | -0.407224 |
| H | -0.579644 | -1.851267 | 1.217374 |
| H | -4.844080 | -3.006645 | -0.158419 |
| H | -4.485493 | -0.984847 | -0.993186 |
| H | -3.932751 | -0.193258 | 0.514442 |
| H | -2.777999 | -1.708327 | 2.320349 |
| H | -4.897906 | -3.877522 | 1.906236 |
| H | -4.263455 | -3.198916 | 3.503025 |
| C | -0.755712 | 2.256262 | -0.416943 |
| C | -2.053143 | 2.648985 | -0.891264 |
| C | 0.157106 | 3.245448 | -0.805417 |
| C | -2.427067 | 3.990231 | -0.149251 |
| H | -2.792791 | 1.914601 | 0.188631 |
| C | -0.215591 | 4.581137 | -0.869568 |
| H | 1.173774 | 2.962960 | -1.859200 |
| C | -1.513641 | 4.960466 | -0.539314 |
| H | -3.442131 | 4.270964 | 0.106363 |
| H | 0.510749 | 5.327552 | -1.168976 |
| H | -1.807649 | 6.062330 | -0.585091 |
| H | -0.186557 | 1.029993 | -2.314820 |

### Energies in solvent (SMD)

**SCF =** -1267.60699133

**Sum of electronic and zero-point Energies** = -1267.117158

**Sum of electronic and thermal Energies** = -1267.091805

**Sum of electronic and thermal Enthalpies** = -1267.090861

**Sum of electronic and thermal Free Energies** = -1267.171387

**Number of imaginary frequencies:** 0
### Energies in solvent (SMD)

| Term                                      | Value       |
|-------------------------------------------|-------------|
| SCF                                       | -1267.61548151 |
| Sum of electronic and zero-point Energies | -1267.124704 |
| Sum of electronic and thermal Energies    | -1267.09869 |
| Sum of electronic and thermal Enthalpies  | -1267.09825 |
| Sum of electronic and thermal Free Energies | -1267.177890 |
3c - conformer 2 [mPW1PW91/6-311+G(2d,p)]

**Energies in solvent (SMD)**

| SCF | -1267.606455 |
| Sum of electronic and zero-point Energies | -1267.115897 |
| Sum of electronic and thermal Energies | -1267.09054 |
| Sum of electronic and thermal Enthalpies | -1267.09001 |
| Sum of electronic and thermal Free Energies | -1267.169545 |

Number of imaginary frequencies: 0
3d - conformer 1 [mPW1PW91/6-311+G(2d,p)]

Energies in solvent (SMD)

SCF = -1267.61045435

Sum of electronic and zero-point Energies= -1267.120661

Sum of electronic and thermal Energies= -1267.095303

Sum of electronic and thermal Enthalpies= -1267.094359

Sum of electronic and thermal Free Energies= -1267.174507

Number of imaginary frequencies: 0
3d - conformer 2 [mPW1PW91/6-311+G(2d,p)]

C  -0.608379  -0.728490  -0.261253  
C  0.615266  -1.186394  0.572033  
C  0.344527  -2.072686  1.594986  
C  1.353169  -2.521497  2.460853  
N  2.688166  -2.151144  2.361450  
C  2.924584  -1.285877  1.365806  
C  4.287471  -0.896389  1.272976  
C  4.713324  -0.025653  0.316951  
C  3.782372  0.507246  -0.607334  
C  2.454030  0.159229  -0.555411  
N  4.322271  1.365320  -1.519931  
C  3.465509  1.931283  -2.501179  
C  -1.419661  0.276349  0.618856  
C  -3.558143  1.238137  1.008930  
C  -2.855907  2.130248  2.076489  
C  -1.528279  2.624631  1.471052  
C  -0.587905  1.419290  1.257647  
C  -1.867508  3.265714  0.101319  
C  -2.284348  2.075600  -0.823776  
N  -2.680736  0.854006  -0.856872  
C  -0.759986  4.080560  -0.492465  
C  -0.845763  5.367192  -0.814983  
O  -0.172889  -0.090118  -1.475390  
H  -0.658081  -2.455845  1.735015  
H  1.107779  -3.218148  3.257420  
H  4.971638  -1.321526  1.996152  
H  5.750838  0.274677  0.239389  
H  1.758220  0.557795  -1.269591  
H  3.002581  1.156324  -3.118978  
H  4.098680  2.562083  -3.121503  
H  2.682606  2.541276  -2.840738  
H  -1.815338  -0.329327  1.436694  
H  -3.972343  0.334441  1.463278  
H  -4.389604  1.766866  0.537470  
H  -2.661962  1.565374  2.992924  
H  -3.489701  2.976748  2.352889  
H  -1.857744  3.360940  2.125149  
H  -0.161152  1.093603  2.208053  
H  0.258500  1.763066  0.619488  
H  -2.725134  3.930888  0.246183  
H  -3.168375  2.344691  -1.418129  
H  -1.477278  1.851116  -1.515912  
H  0.176460  3.558588  -0.679490  
H  -1.757465  5.934168  -0.654700  
H  -0.009186  5.981422  -1.249479  
C  -1.412154  -1.974910  -0.686609  
C  -0.785784  -2.876976  -1.557889  
C  -2.712427  -2.255551  -0.278442  
C  -1.448341  -4.028646  -1.995721  
H  0.225124  -2.679471  -1.887148  
C  -3.368130  -3.405692  -0.705943  
H  -3.238696  -1.574217  0.380415  
C  -2.737724  -4.291473  -1.569227  
H  -0.933842  -4.705127  -2.665424  
H  -4.379894  -3.601875  -0.370227  
H  -3.249823  -5.184445  -1.907423  
H  -0.916788  -0.149580  -2.893565

**Energies in solvent (SMD)**

SCF = -1267.60817842

Sum of electronic and zero-point Energies= -1267.118010

Sum of electronic and thermal Energies= -1267.092762

Sum of electronic and thermal Enthalpies= -1267.091818

Sum of electronic and thermal Free Energies= -1267.171997

Number of imaginary frequencies: 0