Supporting Information

for

Nomimicins B–D, new tetronate-class polyketides from a marine-derived actinomycete of the genus Actinomadura

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Copies of UV, IR, and NMR spectra for 1–4 as well as Cartesian coordinates and energies of the most stable conformers of 4a–d
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Table S1. NOESY and ROESY correlations of nomimicin B (1).

| atom no. | δ_H, mult (J in Hz)^a | NOESY^a | ROESY^a |
|----------|------------------------|----------|----------|
| 5        | 1.66^b                 | 6b, 7, 9, 10 | 6b, 7, 9, 10 |
| 6ax      | 1.34, ddd (12.0, 12.0, 12.0) | 6b, 10, 25, | 6b, 10, 25, 26 |
| 6eq      | 2.41, brd (12.0)       | 5, 6a, 7  | 5, 6a, 7  |
| 7        | 3.74, dd (12.0, 4.3)   | 5, 6a, 9  | 5, 6a, 9  |
| 9        | 3.21, d (11.2)         | 5, 7      | 5, 7      |
| 10       | 2.02^b                 | 6a, 11, 25 | 6a, 11, 25, 26 |
| 11       | 5.85, d (10.1)         | 9, 10, 12 | 9, 10, 12 |
| 12       | 5.61, ddd (10.0, 5.3, 2.6) | 11, 13, 14b | 11, 13, 14b |
| 13       | 2.81, m                | 12, 15, 25 | 12, 15, 23 |
| 14a      | 1.80^b                 | 15, 16    | 15, 16    |
| 14b      | 1.98^b                 | 12, 15, 16 | 12, 13, 15, 16 |
| 15       | 5.49, dd (14.7, 11.5)  | 13, 14a, 14b, 16, 17b | 13, 14a, 14b, 16, 17b |
| 16       | 5.12, dd (14.8, 11.3)  | 14a, 15, 17a, 17b, 27 | 14a, 14b, 15 17b, 27 |
| 17a      | 1.95^b                 | 27, 17b, 19 | 27, 17b, 19 |
| 17b      | 2.32^b                 | 15, 16, 17a, 19 | 17a, 19, 16, 15 |
| 19       | 5.00, s                | 17a, 17b, 27, 28 | 27, 28, 17a, 17b |
| 21       | 2.00^b                 | 22b, 30   | 22b, 30   |
| 22a      | 1.78^b                 | 30        | 30        |
| 22b      | 2.34^b                 | 21, 27, 29b | 21, 27, 29b |
| 25       | 1.60, s                | 10, 13    | 10, 13    |
| 26       | 3.99, s                |           | 6b, 10    |
| 27       | 1.24, s                |           |           | 16, 17b, 19, 22b |
| 28       | 1.75, s                | 19, 22a, 29b, 30 | 19 |
| 29a      | 1.58^d                 | 30        | 22b, 30   |
| 29b      | 1.72^b                 | 21        | 21, 22b   |
| 30       | 0.93, t (7.4)          | 21, 22a, 29a, 29b | 21, 22a, 29a, 29b |

^aRecorded at 500 MHz. ^bOverlapping signals.
Table S2. NOESY and ROESY correlations of nomimicin C (2).

| atom no. | δ_H, mult (J in Hz)^a | NOESYa | ROESYa |
|----------|------------------------|--------|--------|
| 5        | 1.68^b                 | 6b, 7, 9| 6b, 7, 9|
| 6ax      | 1.20, ddd (11.9, 11.9, 11.9) | 6b, 10, 25| 6b, 10, 25|
| 6eq      | 2.35^b                 | 5, 6a, 7| 5, 6a, 7|
| 7        | 3.62, dd (11.8, 4.2)   | 5, 6a, 6b, 9| 5, 6a, 6b, 9|
| 9        | 3.11, d (11.0)         | 5, 7, 10| 5, 7, 10|
| 10       | 1.85^b                 | 6a, 9, 11, 25, 26| 6a, 9, 11, 25, 26|
| 11       | 5.84, d (10.0)         | 9, 10, 12| 9, 10, 12|
| 12       | 5.60, ddd (10.0, 5.1, 2.5) | 11, 13, 14b| 11, 13, 14b|
| 13       | 2.79, m                | 12, 14a, 14b, 15, 25| 12, 14a, 14b, 15, 25|
| 14a      | 1.80^b                 | 13, 16| 13, 16|
| 14b      | 1.98^b                 | 12, 13, 15, 16| 12, 13, 15, 16|
| 15       | 5.48, dd (14.5, 11.9)  | 13, 14b, 16, 17b| 13, 14b, 16, 17b|
| 16       | 5.12, dd (14.8, 11.6)  | 14a, 14b, 15, 17b, 27| 14a, 14b, 17b, 27|
| 17a      | 1.95^b                 | 16, 19, 17b, 27| 16, 19, 17b, 27|
| 17b      | 2.32^b                 | 15, 19, 17a, 27| 15, 16, 17b, 19, 27|
| 19       | 5.01, s                | 17b, 21, 27, 28| 17b, 21, 27, 28|
| 21       | 2.01^b                 | 22b, 28, 30| 22b, 28, 30|
| 22a      | 1.79^b                 | 30| 30|
| 22b      | 2.34^b                 | 21, 22a, 27, 29b| 21, 22a, 27, 29b|
| 25       | 1.59, s                | 6b, 10, 13| 6b, 10, 13|
| 26       | 1.15, s                | 10| 10|
| 27       | 1.25, s                | 16, 17b, 19, 22b| 16, 7b, 19, 22b|
| 28       | 1.75, s                | 19, 21, 30| 19, 21, 30|
| 29a      | 1.62^b                 | 30| 30|
| 29b      | 1.75^b                 | 21, 22b, 30| 21, 22b, 30|
| 30       | 0.93, t (7.4)          | 21, 22a, 28, 29a, 29b| 21, 22a, 28, 29a, 29b|

^aRecorded at 500 MHz. ^bOverlapping signals.
Table S3. ROESY and NOESY correlations of nomimicin D (3).

| Atom no. | $\delta_H$, mult ($J$ in Hz)$^a$ | NOESY$^a$ | ROESY$^a$ |
|----------|---------------------------------|-----------|-----------|
| 5        | 1.72$^b$                        | 7         | 7, 9      |
| 6ax      | 1.14, ddd (11.7, 11.7, 11.7)    | 6eq, 10, 25, 26 | 6eq, 10, 25, 26 |
| 6eq      | 1.80, brd (11.7)                | 6ax, 7    | 6ax, 7    |
| 7        | 3.83, ddd (11.6, 4.5, 4.5)      | 5, 6ax, 6eq, 8 | 5, 6eq, 8, 9 |
| 8        | 2.32, m                         | 9, 26     | 7, 9, 26  |
| 9        | 3.40, dd (10.8, 4.7)            | 5, 8, 10  | 5, 6eq, 7, 8 |
| 10       | 1.94$^b$                        | 6ax, 9, 11, 25, 26 | 6ax, 11, 26, 29 |
| 11       | 5.85, d (10.2)                  | 10, 12    | 9, 10, 12 |
| 12       | 5.72, ddd (10.2, 4.8, 2.5)      | 11, 13    | 11, 13    |
| 13       | 3.32$^b$                        | 12, 14b, 15, 25 | 12, 14b, 15, 25 |
| 14a      | 1.75$^b$                        | 14b, 15   | 14b, 15, 16 |
| 14b      | 2.00$^b$                        | 13, 14a, 15 | 13, 14a, 15, 16 |
| 15       | 5.40, dt (15.0, 7.2)            | 13, 14a, 14b, 17 | 14a, 14b, 17 |
| 16       | 5.26, dt (15.2, 7.0)            | 17        | 14a, 14b, 17 |
| 17       | 2.63, d (6.9)                   | 15, 16, 19, 27 | 15, 16, 19, 27 |
| 19       | 5.59, s                         | 17, 27, 28 | 17, 27, 28 |
| 21       | 5.20, t (7.3)                   | 28, 29    | 28, 29    |
| 22a      | 4.66, d (1.5)                   | 22b       | 22b       |
| 22b      | 5.00, d (1.5)                   | 22a       | 22a       |
| 25       | 1.38, s                         | 6ax, 10, 13 | 6ax, 10, 13 |
| 26       | 0.92, d (6.9)                   | 6ax, 8, 10 | 6ax, 8, 10 |
| 27       | 1.69, s                         | 17, 19    | 17, 19    |
| 28       | 1.67, s                         | 19, 21    | 19, 21    |
| 29       | 2.08, q (7.5)                   | 21, 30    | 21, 30    |
| 30       | 0.98, t (7.5)                   | 29        | 29        |

$^a$Recorded at 500 MHz. $^b$Overlapping signals.
Table S4. Cartesian coordinates and energies of the most stable conformer of 4a.

|      | C          | H          | C         | O          | C          | C         | C          | O          |
|------|------------|------------|-----------|------------|------------|-----------|------------|------------|
|      | −3.503719  | −2.346714  | 2.018768  | C          | −3.645152  | −0.928348 | 2.483653   |            |
|      | −2.842684  | 0.059614   | 1.614795  | C          | −1.406663  | −0.467423 | 1.327473   |            |
|      | −1.478556  | −1.858223  | 0.592342  | C          | −2.535046  | −2.744197 | 1.197996   |            |
|      | −5.114423  | −0.482563  | 2.517646  | C          | −5.279711  | 0.929994  | 3.107325   |            |
|      | −4.385326  | 1.900074   | 2.329127  | C          | −2.928249  | 1.436913  | 2.295338   |            |
|      | −3.357511  | 0.126062   | 0.644467  | H          | −3.275366  | −0.872508 | 3.519517   |            |
|      | −5.025003  | 0.971896   | 4.615534  | O          | −5.838844  | −1.443966 | 3.275191   |            |
|      | −4.511032  | 3.183884   | 2.931226  | C          | −0.628314  | −0.610233 | 2.647818   |            |
|      | −0.659504  | 0.477094   | 0.398921  | C          | 0.661656   | 0.373915  | −0.030811  |            |
|      | −1.393789  | 1.424828   | −0.127383 | O          | 1.639477   | −0.706686 | 0.113186   |            |
|      | 2.586816   | −0.577666  | −0.849731 | C          | 2.365451   | 0.552627  | −1.719717  |            |
|      | 1.091115   | 1.157639   | −1.160964 | O          | 0.536366   | 2.160395  | −1.624592  |            |
|      | 3.524265   | 1.533137   | −1.535198 | O          | 1.725959   | −1.631641 | 0.893988   |            |
|      | −1.689680  | −1.808606  | −0.957891 | C          | −0.406444  | −1.965046 | −1.729977  |            |
|      | 0.043227   | −1.135931  | −2.672441 | C          | 1.404868   | −1.243425 | −3.302139  |            |
|      | 2.266578   | 0.047683   | −3.188329 | C          | 1.683546   | 1.118875  | −4.130266  |            |

4a ($\Delta G = 0.0$ kcal/mol)
| C | 3.662248 | -0.283699 | -3.677645 |
| C | 4.887106 | 0.905325 | -1.852568 |
| C | 5.512444 | 0.066671 | -0.711618 |
| H | -4.220916 | -3.069641 | 2.399844 |
| H | -2.480596 | -3.789269 | 0.893961 |
| H | -6.322708 | 1.233321 | 2.937115 |
| H | -2.550962 | 1.377486 | 3.22789 |
| H | -3.989715 | 0.728106 | 4.874078 |
| H | -5.672929 | 0.256624 | 5.129063 |
| H | -3.988011 | 3.806797 | 2.401920 |
| H | 0.400098 | -0.923285 | 2.472441 |
| H | -0.845789 | 1.972098 | -0.768030 |
| H | 3.499613 | 1.926940 | -0.514148 |
| H | -2.207474 | -0.885844 | -1.250439 |
| H | -0.577815 | -0.283741 | -2.958990 |
| H | 1.318885 | -1.457654 | -4.376482 |
| H | 0.619692 | 1.297559 | -3.956449 |
| H | 3.681631 | -0.872176 | -4.596844 |
| H | 5.999076 | -0.804052 | -4.700691 |
| H | 6.676972 | -1.020392 | -3.079586 |
| H | 6.565455 | -0.099793 | -0.966336 |
| H | 5.792408 | 1.755548 | 0.637118 |

| C | 4.821642 | 0.087611 | -3.125828 |
| C | 6.139258 | -0.320159 | -3.729921 |
| C | 5.437464 | 0.718326 | 0.666353 |
| H | -0.513522 | -2.347953 | 0.765753 |
| H | -5.489581 | -0.477409 | 1.481599 |
| H | -4.751292 | 1.947582 | 1.290979 |
| H | -2.335827 | 2.192927 | 1.774845 |
| H | -5.241348 | 1.967971 | 5.010081 |
| H | -6.770566 | -1.171176 | 3.284207 |
| H | -1.108293 | -1.368329 | 3.274221 |
| H | -0.614276 | 0.335119 | 3.197890 |
| H | 3.343562 | 2.379927 | -2.204942 |
| H | -2.362498 | -2.633450 | -1.225418 |
| H | 0.219027 | -2.810432 | -1.431182 |
| H | 1.944444 | -2.082350 | -2.849352 |
| H | 2.210249 | 2.072954 | -4.037394 |
| H | 1.805293 | 0.771193 | -5.161667 |
| H | 5.577214 | 1.743265 | -2.030130 |
| H | 6.791306 | 0.551283 | -3.866927 |
| H | 5.039526 | -0.920376 | -0.677361 |
| H | 6.060169 | 0.172370 | 1.382180 |
| H | 4.415026 | 0.722727 | 1.058638 |
Table S5. Cartesian coordinates and energies of the most stable conformer of 4b.

![Image of 4b molecule]

4b ($\Delta G = 0.4$ kcal/mol)

| M06-2X/def2-TZVP-SMD(MeOH)//M06-2X/6-31G(d)-SMD(MeOH): |
|-----------------|-----------------|-----------------|
| Gibbs Free Energy (a.u.) | $-1617.989748$ |

| M06-2X/def2-TZVP-SMD(MeOH): |
|-----------------|-----------------|
| Electronic energy (a.u.) | $-1618.592155$ |

| M06-2X/6-31G(d)-SMD(MeOH): |
|-----------------|-----------------|
| Zero-point correction (a.u.) | $0.663404$ |
| Thermal correction to Energy (a.u.) | $0.697073$ |
| Thermal correction to Enthalpy (a.u.) | $0.698017$ |
| Thermal correction to Gibbs Free Energy (a.u.) | $0.602407$ |

C 3.618438  -2.909456  -0.579758  C 3.596050  -2.596963  0.886760
C 2.246516  -2.007607  1.341583  C 1.744913  -0.909585  0.363405
C 1.574001  -1.515065  -1.078718  C 2.729540  -2.413072  -1.436418
C 3.919407  -3.832798  1.738119  C 4.018140  -3.495126  3.236562
C 2.724025  -2.801589  3.672159  C 2.405109  -1.579392  2.810437
H 1.506189  -2.821987  1.306460  H 4.389366  -1.859668  1.088091
C 5.268592  -2.681520  3.576455  O 5.138024  -4.385086  1.254332
O 2.861065  -2.450254  5.045375  C 2.738885  0.264248  0.324390
C 0.375484  -0.398696  0.810911  C -0.358178  0.669337  0.118117
O -0.219862  -0.956279  1.743585  C -0.133183  1.376208  -1.147617
O -1.298307  1.950198  -1.549630  C -2.383160  1.661905  -0.649570
C -1.691651  0.841546  0.399706  O -2.367565  0.368997  1.407338
C -2.894037  2.981673  -0.067781  O 0.855282  1.518871  -1.836063
C 0.236993  -2.284458  -1.351032  C -0.766837  -1.451250  -2.103366
C -2.006901  -1.178225  -1.698225  C -2.919243  -0.192170  -2.376254
C -3.499885  0.907016  -1.437439  C -4.542970  0.261648  -0.504280
|   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| C | -4.225278 | 1.915965 | -2.305660 | C | -4.198722 | 3.247720 | -2.196414 |
| C | -3.363629 | 3.958870 | -1.152301 | C | -4.980385 | 4.122875 | -3.139989 |
| C | -2.242858 | 4.779816 | -1.835195 | C | -1.211742 | 5.364777 | -0.874187 |
| H | 4.416873 | -3.553661 | -0.940213 | H | 1.602124 | -0.670138 | -1.775574 |
| H | 2.794035 | -2.675314 | -2.492315 | H | 3.106877 | -4.563318 | 1.595092 |
| H | 0.402399 | -4.448033 | 3.781395 | H | 1.896101 | -3.520285 | 3.561892 |
| H | 3.219561 | -0.852265 | 2.910908 | H | 1.498088 | -1.110394 | 3.197653 |
| H | 5.263195 | -1.689580 | 3.113726 | H | 5.350434 | -2.544297 | 4.657764 |
| H | 6.165481 | -3.203811 | 3.232878 | H | 5.332275 | -5.177042 | 1.781278 |
| H | 2.022055 | -2.053943 | 5.329490 | H | 3.690265 | -0.070811 | -0.101061 |
| H | 2.368992 | 1.081147 | -0.295383 | H | 2.929024 | 0.652284 | 1.329640 |
| H | -1.734714 | -0.221670 | 1.908174 | H | -3.727638 | 2.745672 | 0.601172 |
| H | -2.106467 | 3.424195 | 0.549511 | H | 0.479290 | -3.173280 | -1.947303 |
| H | -0.195437 | -2.653647 | -0.411959 | H | -0.396145 | -0.983866 | -3.019317 |
| H | -2.362485 | -1.633739 | -0.770359 | H | -2.383595 | 0.282214 | -3.205743 |
| H | -3.789946 | -0.705525 | -2.807762 | H | -4.919434 | 0.969573 | 0.239730 |
| H | -4.154491 | -0.614174 | 0.020779 | H | -5.393040 | -0.060747 | -1.114758 |
| H | -4.847764 | 1.463781 | -3.079838 | H | -4.013156 | 4.688077 | -0.646375 |
| H | -5.641434 | 3.529251 | -3.777741 | H | -5.590130 | 4.846452 | -2.585113 |
| H | -4.314530 | 4.701212 | -3.791520 | H | -1.737548 | 4.161791 | -2.584728 |
| H | -2.723787 | 5.600685 | -2.379436 | H | -0.568568 | 6.082041 | -1.393859 |
| H | -1.694869 | 5.890488 | -0.041819 | H | -0.563519 | 4.589250 | -0.452792 |
Table S6. Cartesian coordinates and energies of the most stable conformer of 4c.

![4c (ΔG = 3.5 kcal/mol)]

**M06-2X/def2-TZVP-SMD(MeOH)//M06-2X/6-31G(d)-SMD(MeOH):**

|                      | Gibbs Free Energy (a.u.) | Electronic energy (a.u.) | Zero-point correction (a.u.) | Thermal correction to Energy (a.u.) | Thermal correction to Enthalpy (a.u.) | Thermal correction to Gibbs Free Energy (a.u.) |
|----------------------|--------------------------|--------------------------|------------------------------|------------------------------------|--------------------------------------|-----------------------------------------------|
|                      | −1617.984871             | −1618.586628             | 0.663069                     | 0.696797                           | 0.697741                             | 0.601757                                      |

C 1.860459  -3.459310  -2.831985  C 2.192833  -1.993084  -2.859413
C 1.197889  -1.132826  -2.052228  C -0.251763  -1.602591  -2.299214
C -0.397974  -3.086560  -1.796580  C 0.682014  -3.934794  -2.429161
C 3.612081  -1.676168  -2.374454  C 3.961273  -0.191477  -2.601203
C 2.903567  0.685037  -1.919253  C 1.480742  0.340058  -2.363188
H 1.415731  -1.295168  -0.991161  H 2.161243  -1.680349  -3.914794
C 4.147735  0.154664  -4.080021  O 4.512152  -2.530782  -3.068664
O 3.221913  2.045455  -2.197232  C -0.570394  -1.573346  -3.814119
C -1.344627  -0.781702  -1.620529  C -1.334381  0.041244  -0.494802
O -2.502099  -0.999269  -2.203615  C -2.617691  0.454941  0.056409
O -2.496049  0.957098  1.285166  C -1.117345  0.929387  1.731912
C -0.347569  0.355626  0.533365  O 0.868793  0.270088  0.544045
C -0.695930  2.371282  2.000210  O -3.731874  0.363810  -0.458461
C -0.295529  -3.391619  -0.274381  C -1.229319  -2.685563  0.669919
C -0.820582  -2.195345  1.841232  C -1.643751  -1.358336  2.779778
C -1.054727  0.061423  3.016344  C 0.384052  -0.061543  3.556985
C -1.876495  0.775743  4.069110  C -2.106078  2.091865  4.110946
C -1.571302  3.060906  3.068040  C -2.897411  2.695141  5.243048
C -2.699898  3.912004  2.446892  C -2.190515  5.107404  1.644890
H  2.611150 -4.140192 -3.226940  H -1.381654 -3.435593 -2.136929
H  0.488758 -5.006254 -2.460316  H  3.665326 -1.890851 -1.295217
H  4.918040  0.003764 -2.092933  H  2.965445  0.510769 -0.835070
H  1.373687  0.533681 -3.438007  H  0.781958  1.002806 -1.841389
H  3.214072  0.091985 -4.647964  H  4.531124  1.173008 -4.184646
H  4.867138 -0.526239 -4.542819  H  5.409371 -2.331953 -2.755270
H  2.599991  2.595456 -1.694684  H  0.201758 -2.095590 -4.377998
H -1.522805 -2.061216 -4.026022  H -0.627951 -0.542631 -4.178704
H -3.234325 -0.509748 -1.722967  H  0.356037  2.356798  2.297764
H -0.745179  2.919170  1.052934  H -0.457608 -4.476815 -0.198116
H  0.735084 -3.218691  0.057057  H -2.268453 -2.554477  0.356545
H  0.222227 -2.350860  2.121294  H -2.673820 -1.276961  2.412699
H -1.692504 -1.838057  3.766809  H  0.769758  0.911027  3.873369
H  1.077931 -0.486199  2.829223  H  0.368726 -0.711604  4.439169
H -2.256280  0.143831  4.873184  H -0.924534  3.766509  3.612048
H -3.013864  1.981457  6.063707  H -2.404578  3.593578  5.632692
H -3.902115  2.996720  4.921281  H -3.333373  3.274692  1.818785
H -3.336836  4.291939  3.252575  H -3.027840  5.713157  1.283832
H -1.556937  5.749962  2.267190  H -1.604970  4.807807  0.770002
Table S7. Cartesian coordinates and energies of the most stable conformer of 4d.

![4d (ΔG = 6.6 kcal/mol)](image)

### M06-2X/def2-TZVP-SMD(MeOH)//M06-2X/6-31G(d)-SMD(MeOH):

| Parameter                        | Value (a.u.) |
|----------------------------------|--------------|
| Gibbs Free Energy                | −1617.979974|
| Electronic energy                | −1618.580947|
| Zero-point correction            | 0.662219     |
| Thermal correction to Energy     | 0.695993     |
| Thermal correction to Enthalpy   | 0.696937     |
| Thermal correction to Gibbs Free Energy | 0.600973 |

### M06-2X/def2-TZVP-SMD(MeOH):

| Parameter                        | Value (a.u.) |
|----------------------------------|--------------|
| Electronic energy                | −1618.580947|

### M06-2X/6-31G(d)-SMD(MeOH):

| Parameter                        | Value (a.u.) |
|----------------------------------|--------------|
| Zero-point correction            | 0.662219     |
| Thermal correction to Energy     | 0.695993     |
| Thermal correction to Enthalpy   | 0.696937     |
| Thermal correction to Gibbs Free Energy | 0.600973 |

| X    | Y    | Z    | X    | Y    | Z    | X    | Y    | Z    | X    | Y    | Z    | X    | Y    | Z    | X    | Y    | Z    | X    | Y    | Z    | X    | Y    | Z    |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| C    | 4.798129 | 0.356612 | −0.661757 | C    | 3.865655 | −0.611239 | −1.337749 |
| C    | 2.478207 | −0.672378 | −0.665771 | C    | 2.621313 | −0.693659 | 0.870177  |
| C    | 3.296870 | 0.647454  | 1.332342  | C    | 4.576705 | 0.857650  | 0.553923  |
| C    | 3.674606 | −0.330715 | −2.832130 | C    | 2.852422 | −1.444172 | −3.511003 |
| C    | 1.516062 | −1.602040 | −2.775862 | C    | 1.697146 | −1.840457 | −1.275720 |
| H    | 1.948008 | 0.249241  | −0.931338 | H    | 4.335913 | −1.605337 | −1.274884 |
| C    | 3.620670 | −2.762442 | −3.625970 | O    | 4.962624 | −0.206470 | −3.423002 |
| O    | 0.804306 | −2.670629 | −3.939564 | C    | 3.534305 | −1.859581 | 1.311313  |
| C    | 1.320249 | −0.869455 | 1.671112  | C    | −0.037871 | −0.515583 | 1.282252  |
| O    | 1.468333 | −1.303555 | 2.834544  | C    | −1.001361 | −0.508034 | 2.302151  |
| O    | −2.154086| 0.042689  | 2.009603  | C    | −2.081994 | 0.579029  | 0.653163  |
| C    | −0.683430| 0.158578  | 0.171270  | O    | −0.316574 | 0.384584  | −0.973036 |
| C    | −3.177513| 0.099993  | −0.157614 | O    | −0.880587 | −0.951894 | 3.507228  |
| C    | 2.526872 | 1.990994  | 1.182403  | C    | 1.173362 | 2.120588  | 1.823974  |
| C    | 0.151547 | 2.728125  | 1.218604  | C    | −1.265044| 2.772635  | 1.720726  |
| C    | −2.290452| 2.111794  | 0.754683  | C    | −2.204751| 2.786596  | −0.629176 |
| Element | X    | Y    | Z    | Element | X    | Y    | Z    |
|---------|------|------|------|---------|------|------|------|
| C       | -3.693033 | 2.329702 | 1.282666 | C       | -4.714940  | 1.480821  | 1.134440  |
| C       | -4.589757  | 0.146532  | 0.414789  | C       | -6.084489  | 1.833650  | 1.657514  |
| C       | -5.076852  | -1.025825 | 1.293403  | C       | -5.283535  | -2.323622 | 0.515721  |
| H       | 5.721491   | 0.596044  | -1.184682 | H       | 3.532826   | 0.523239  | 2.397973  |
| H       | 5.303092   | 1.534682  | 1.001980  | H       | 3.132288   | 0.622443  | -2.938194 |
| H       | 2.625469   | -1.101816 | -4.531012 | H       | 0.948354   | -0.667932 | -2.898276 |
| H       | 2.229221   | -2.786784 | -1.115883 | H       | 0.706718   | -1.942932 | -0.817550 |
| H       | 3.807702   | -3.226634 | -2.652466 | H       | 3.057212   | -3.477479 | -4.231171 |
| H       | 4.587486   | -2.598744 | -4.109578 | H       | 4.837256   | -0.014227 | -4.366424 |
| H       | -0.071990  | -2.711056 | -2.978506 | H       | 3.068909   | -2.824437 | 1.084137  |
| H       | 4.498901   | -1.813103 | 0.805816  | H       | 3.717337   | -1.820720 | 2.385965  |
| H       | 0.094087   | -1.261776 | 3.549185  | H       | -3.093032  | 0.265730  | -1.184575 |
| H       | -2.957884  | -1.172475 | -0.189347 | H       | 3.202828   | 2.748388  | 1.605874  |
| H       | 2.433893   | 2.234842  | 0.117487  | H       | 1.030825   | 1.666621  | 2.808126  |
| H       | 0.331531   | 3.174889  | 0.239878  | H       | -1.331710  | 2.305737  | 2.711026  |
| H       | -1.588853  | 3.815716  | 1.838684  | H       | -3.014094  | 2.448215  | -1.281310 |
| H       | -1.255279  | 2.601946  | -1.134733 | H       | -2.320806  | 3.867898  | -0.494541 |
| H       | -3.864129  | 3.288546  | 1.773680  | H       | -5.283593  | 0.195608  | -0.438423 |
| H       | -6.142328  | 2.894263  | 1.917785  | H       | -6.857140  | 1.618341  | 0.909306  |
| H       | -6.338219  | 1.256490  | 2.553936  | H       | -4.367923  | -1.183707 | 2.114935  |
| H       | -6.032211  | -0.749527 | 1.751485  | H       | -5.687249  | -3.103498 | 1.169287  |
| H       | -5.994464  | -2.174091 | -0.305060 | H       | -4.353556  | -2.708892 | 0.085761  |