

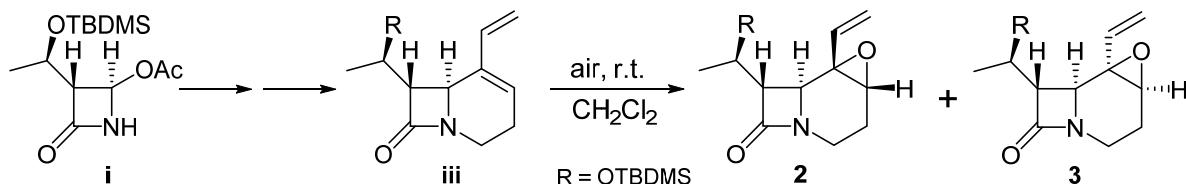
Supplementary Materials

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1. General Techniques

All solvents were dried and distilled before use. All reactions were monitored by thin-layer chromatography using aluminum-backed silica gel plates 60 F₂₅₄; visualization was accomplished with UV light and/or staining with 50% H₂SO₄. Standard flash chromatography procedures were followed using silica gel with particle size 40-63 µm. FT-IR spectra were recorded on an FT-IR spectrophotometer for films. ¹H NMR spectra were recorded at 500 or 600 MHz and ¹³C NMR at 125 and 150 MHz using CDCl₃ or C₆D₆ as solvents and TMS as internal standard and are reported as δ values (ppm) relative to residual CHCl₃ signal δ H (7.26 ppm) and CDCl₃ δ C (77.16 ppm), respectively. Mass spectra were obtained at 70 eV. Electrospray ionization (ESI) mass spectrometry (MS) experiments were performed on a mass spectrometer under normal conditions. PFK solution was used as a calibrant for HRMS measurements.

2. Synthesis of model β-lactams 2 and 3



The bicyclic diene **iii**, quite widely used as a convenient and promising substrate for further transformations aimed at obtaining new antibiotics with an enhanced or novel biological activity profile, was synthesized in a few-step synthesis according to the literature procedure.[1-3] Spectroscopic characteristics obtained in a good yield of brown-yellow oil diene **iii** were fully consistent with the literature data.[1]

Under aerobic conditions at room temperature, the diene **iii** underwent a spontaneous epoxidation to yield a mixture of two epoxides in a ratio of 17:1. The yield

of the self-epoxidation reaction accompanied by the decomposition of product **iii** was 25% after three days at room temperature. Thus, the reactivity of **iii** toward atmospheric oxygen is much smaller than its five-membered counterpart with the formation of 4-vinyl-1-azabicyclo[3.2.0]hept-3-en-7-one with a 70% yield.[4] This result is in line with the impact of internal skeletal strain on the epoxidation reaction rate descending with increasing ring size, *i.e.*, 4,5 *vs* 4,6 in this case.[5] As checked in independent experiments, autoxidation of **iii** can be inhibited by a rigorous exclusion of oxygen from the reaction mixture and by keeping it at a low temperature (refrigerator).

Adding an oxygen atom to the starting diene molecule confirmed the MS spectrum by increasing the molecular mass by 16 in **2** and **3**. Moreover, in the ¹H and ¹³C NMR spectra of both epoxides, only the resonances of vinyl protons at C5 carbon atom were visible, as well as lack of resonances originating from the diene double bond inside the six-membered ring, thus giving additional evidence for diene **iii** spontaneous epoxidation.

Oily main product **2**: ¹H NMR (600 MHz, CDCl₃): δ 0.03 (s, 3H), 0.04 (s, 3H), 0.85 (s, 9H), 1.25 (d, *J*=6.2 Hz, 3H), 2.01 (dt, *J*=15.0, 3.3 Hz, 1H), 2.12 (dddd, *J*=15.0, 11.8, 3.3 Hz, 1H), 2.83 (ddd, *J*=16.2, 11.8, 4.4 Hz, 1H), 3.14 (dd, *J*=6.2, 2.4 Hz, 1H), 3.17 (t, *J*=1.2 Hz, 1H), 3.57 (dd, *J*=13.8, 6.3 Hz, 1H), 3.76 (bs, 1H), 4.14 (dq, *J*=6.2 Hz, 1H), 5.23 (dd, *J*=10.8, 1.3 Hz, 1H), 5.48 (dd, *J*=17.1, 1.3 Hz, 1H), 5.99 (dd, *J*=17.1, 10.8 Hz, 1H). ¹³C NMR (125 MHz, CDCl₃): δ -4.84, -4.36, 17.91, 22.87, 24.95, 25.69 (3C), 33.73, 51.36, 60.21, 61.67, 61.94, 66.13, 118.07, 133.42, 169.64. IR (CHCl₃): 1744, 1642, 1472, 1256 cm⁻¹. ESI-MS m/z

$[(M+H)^+]$ 324.1996 (*calculated for* $C_{17}H_{29}NO_3Si = 324.1995$). ESI-HRMS: m/z $[(M+Na)^+]$

346.1812 (*calculated for* $C_{17}H_{29}NNaO_3Si = 346.1815$).

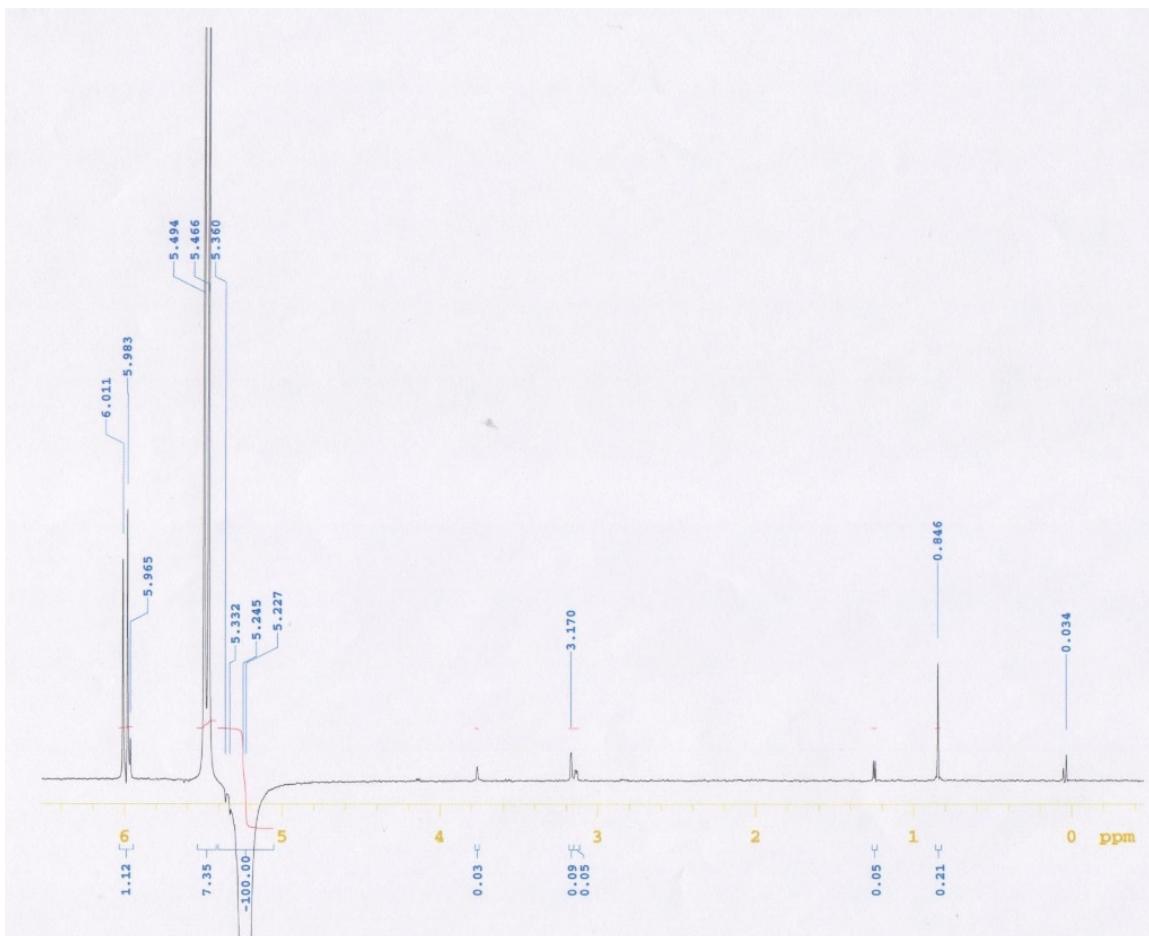
Oily minor product **3**: 1H NMR (600 MHz, $CDCl_3$): δ 0.06 (s, 3H), 0.08 (s, 3H), 0.85 (s, 9H), 1.19 (d, $J=6.3$ Hz, 3H), 1.99 (dd, $J=8.58, 5.72, 3.22$ Hz, 1H), 2.16 (ddd, $J=16.0, 8.7, 6.32, 2.0$ Hz, 1H), 2.77 (ddd, $J=13.5, 7.9, 6.3$ Hz, 1H), 3.01 (dd, $J=4.5, 1.9$ Hz, 1H), 3.14 (dd, $J=3.0, 2.1$ Hz, 1H), 3.62 (ddd, $J=13.4, 8.9, 5.7$ Hz, 1H), 3.89 (d, $J=1.9$ Hz, 1H), 4.19 (dq, $J=10.8, 6.2, 4.7, 1.7$ Hz, 1H), 5.28 (dd, $J=10.8, 1.1$ Hz, 1H), 5.48 (dd, $J=17.3, 1.1$ Hz, 1H). ^{13}C NMR (125 MHz, $CDCl_3$): δ -4.91, -4.37, 17.95, 20.13, 23.07, 25.71 (3C), 32.32, 49.30, 57.75, 59.86, 62.37, 64.83, 117.97, 133.97, 168.47. IR ($CHCl_3$): 1746, 1641, 1472, 1258 cm^{-1} . ESI-HRMS: m/z $[(M+H)^+]$ 324.1996 (*calculated for* $C_{17}H_{29}NO_3Si = 324.1995$).

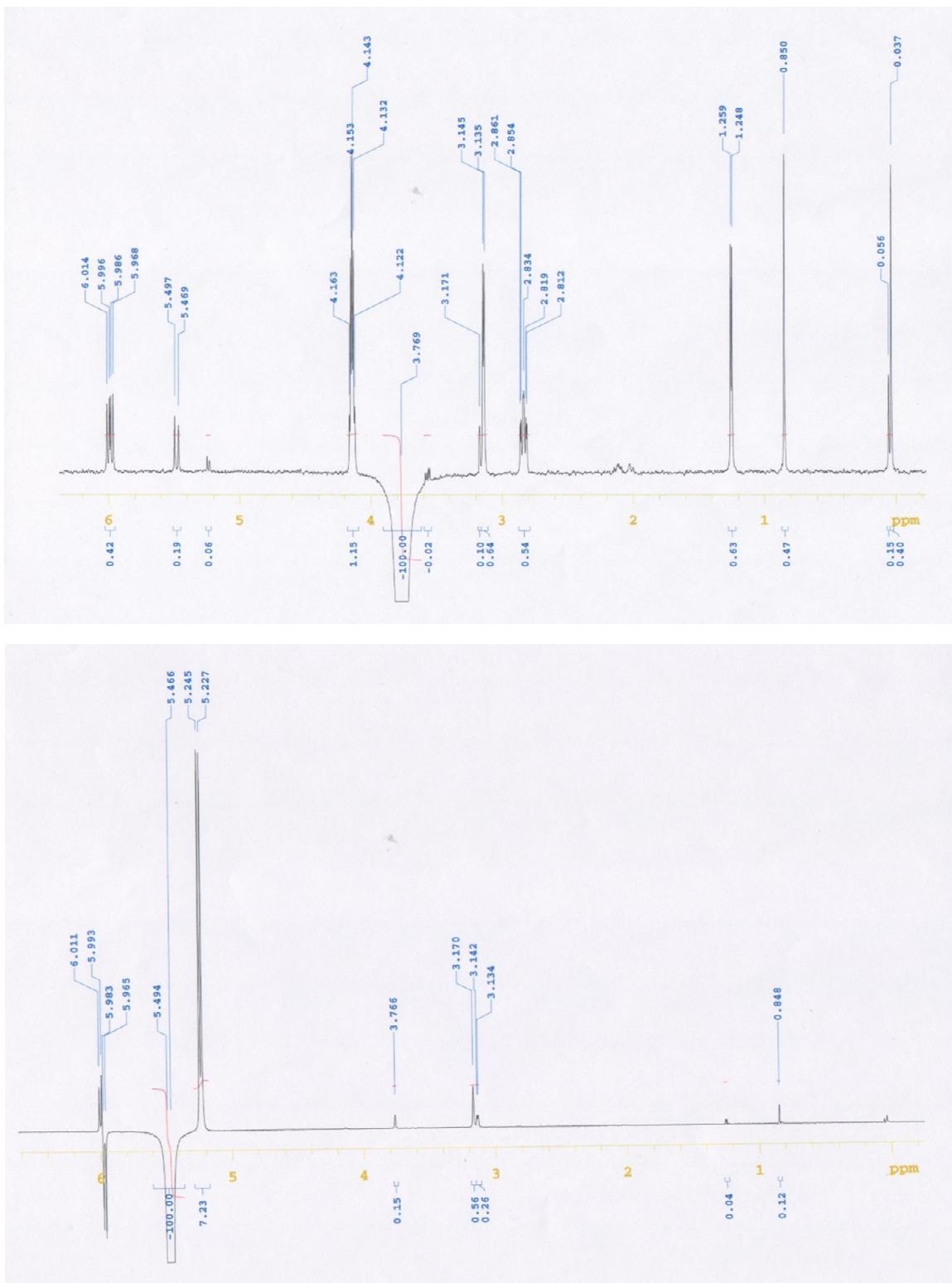
3. References

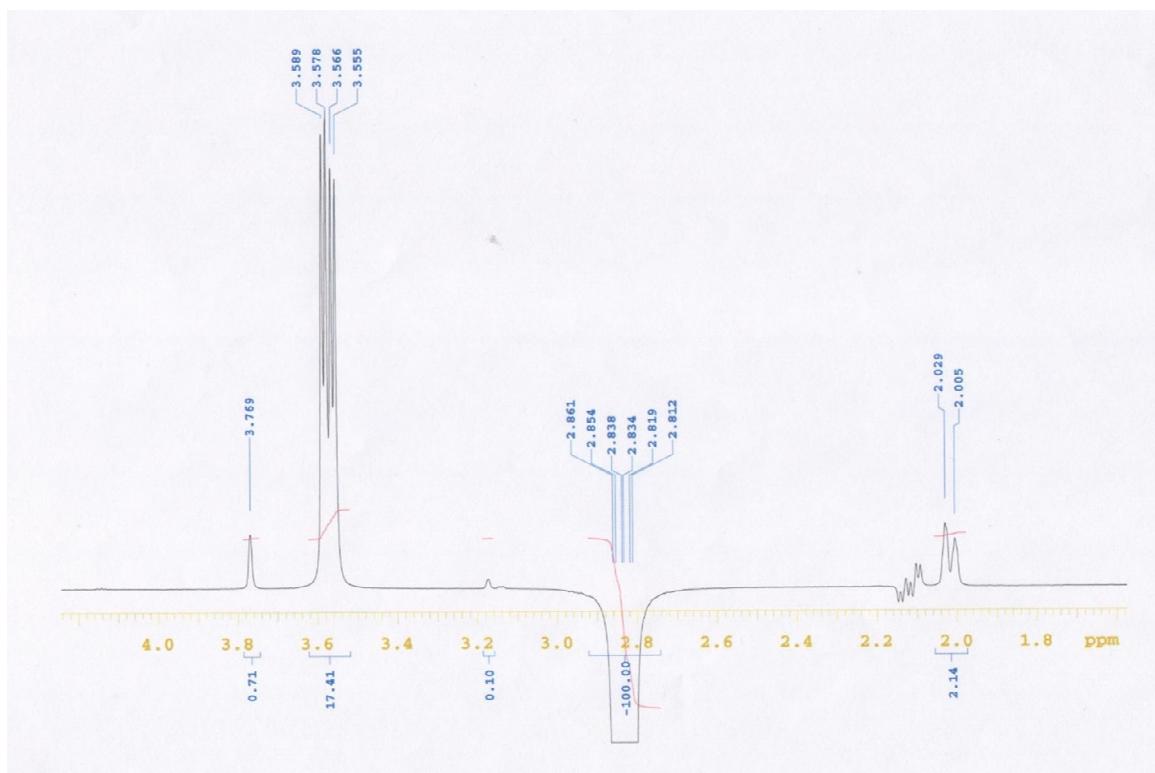
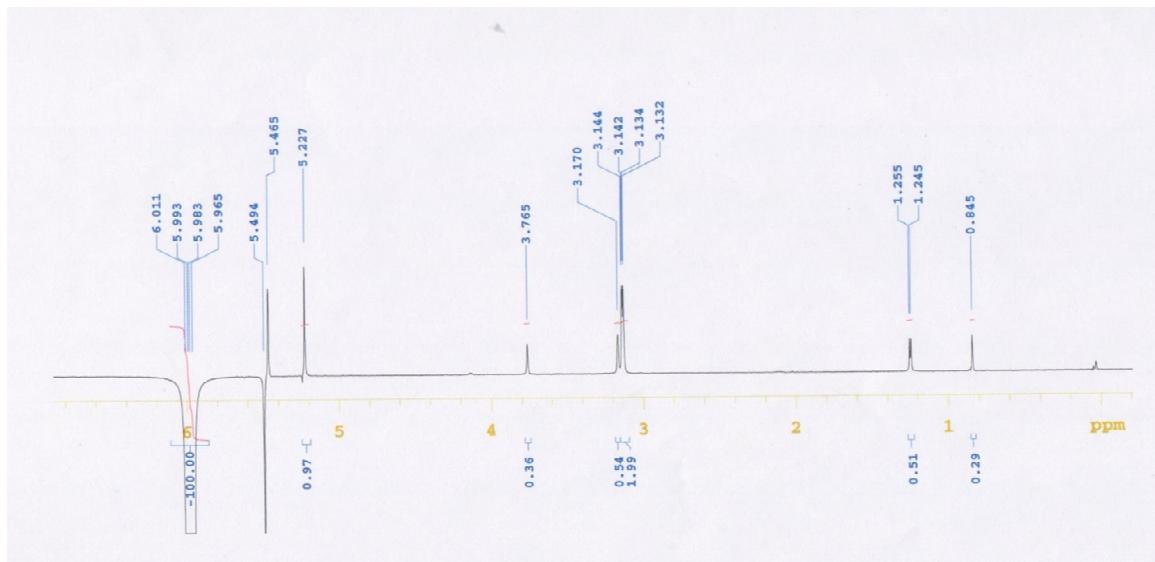
1. Desroy, N.; Robert-Peillard, F.; Toueg, J.; Hénaut, C.; Duboc, R.; Rager, M.-N.; Savignac, M.; Genet, J.-P., Synthesis of New Polycyclic β -Lactams via One-Pot Enyne Metathesis and Diels-Alder Reactions, *Synthesis*, **2004**, 16, 2665-2672.
2. Kumar, Y.; Singh, P.; Bhargava, G., Recent developments in the synthesis of condensed β -lactams, *RSC Adv.* **2016**, 6(101), 99220-99250.
3. Desroy, N.; Robert-Peillard, F.; Toueg, J.; Duboc, R.; Hénaut, C.; Rager, M.-N.; Savignac, M.; Genêt, J.-P., An Efficient Route to 4/5/6 Polycyclic β -Lactams, *Eur. J. Org. Chem.*, **2004**, 23, 4840-4849.
4. Polavarapu, P. L.; Frelek, J.; Woźnica, M., Determination of the absolute configurations using electronic and vibrational circular dichroism measurements and quantum chemical calculations, *Tetrahedron: Asymmetry*, **2011**, 22(18), 1720-1724.

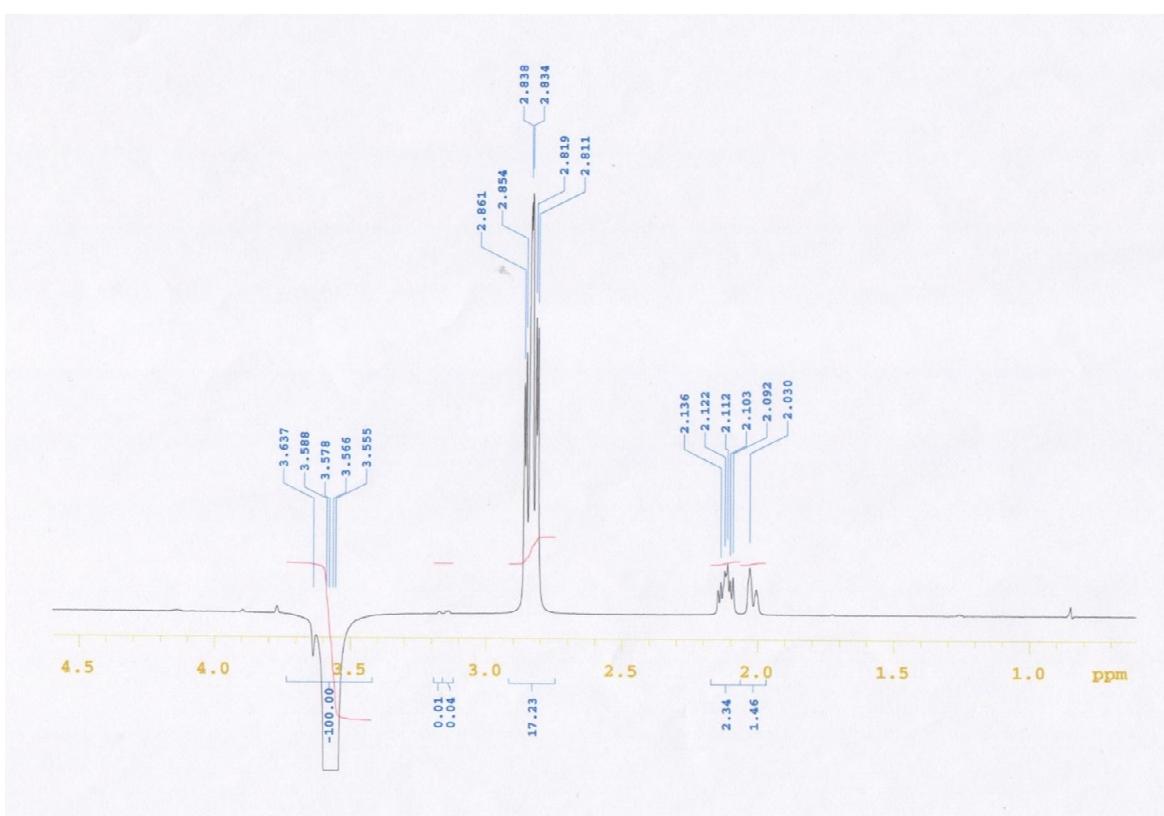
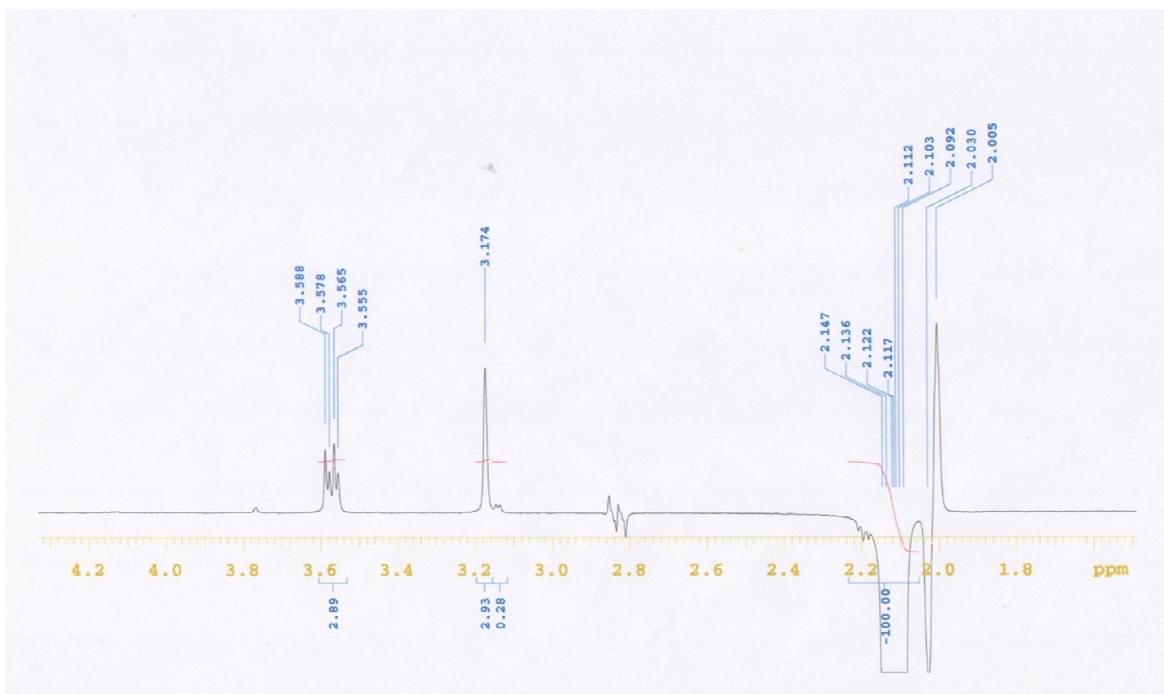
5. Bartlett, P. D.; Banavali, R., Spontaneous oxygenation of cyclic olefins. Effects of strain, *J. Org. Chem.*, **1991**, *56*(21), 6043-6050.

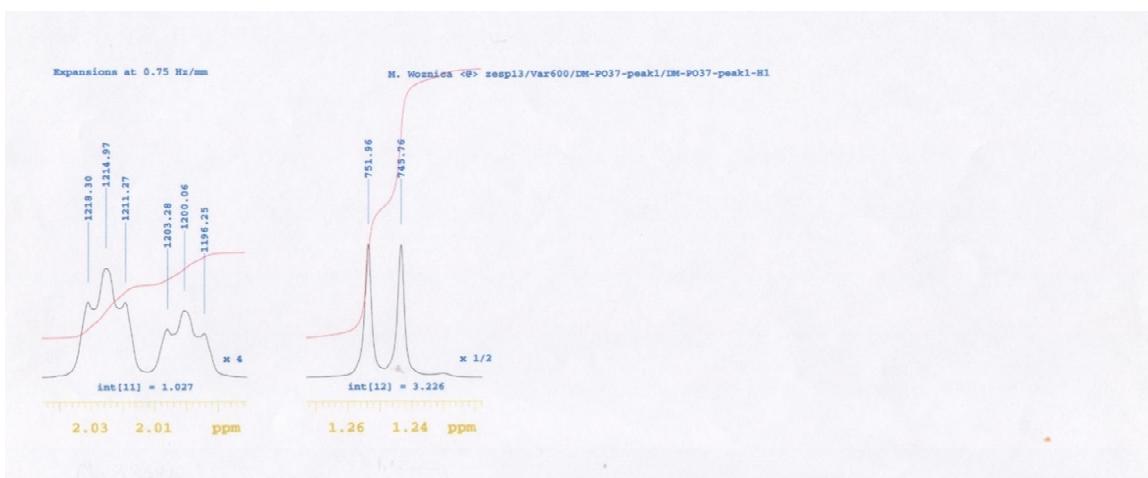
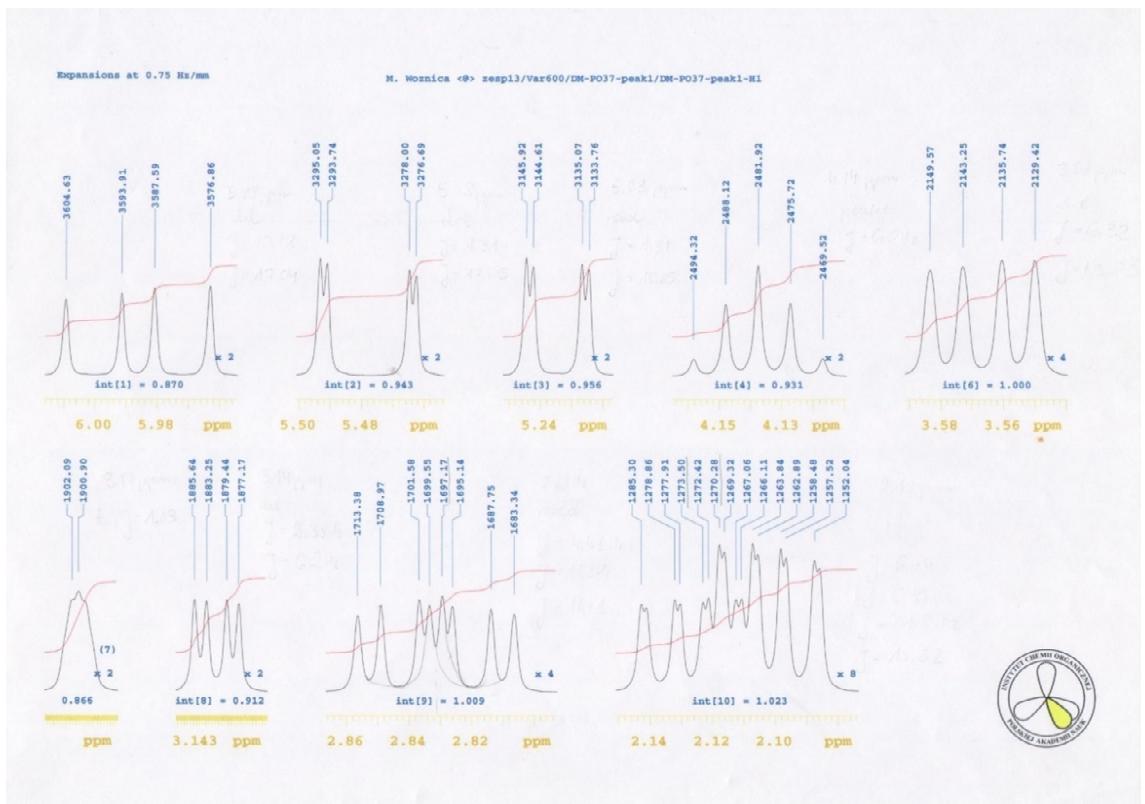
4. NMR and MS spectra of Comp. 2

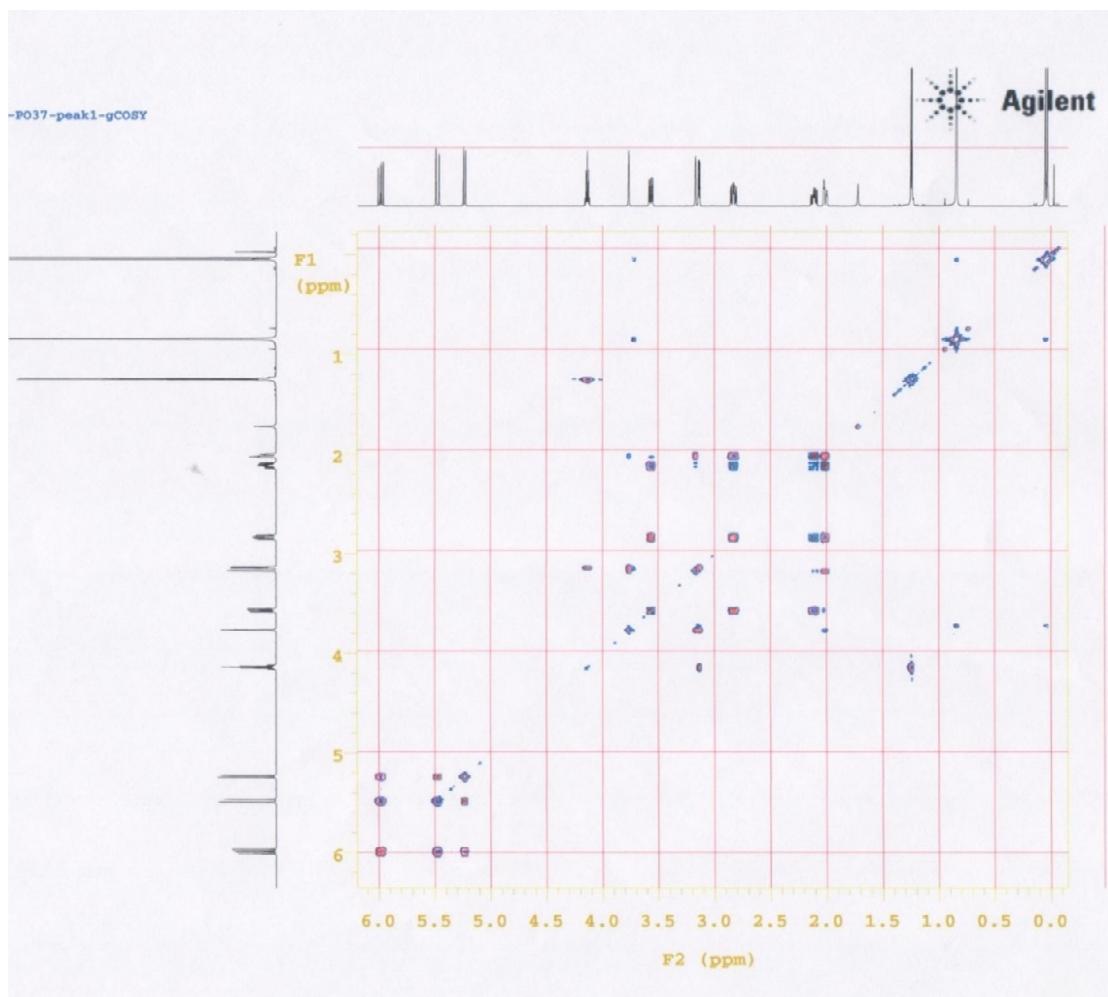
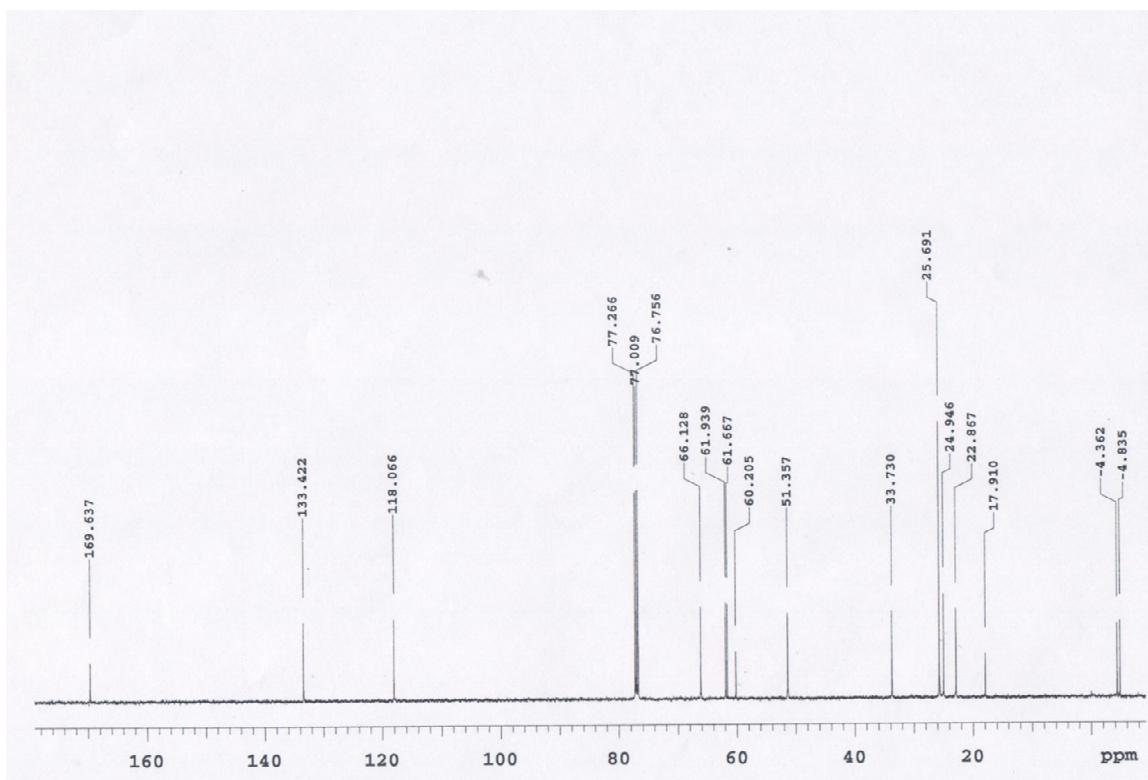


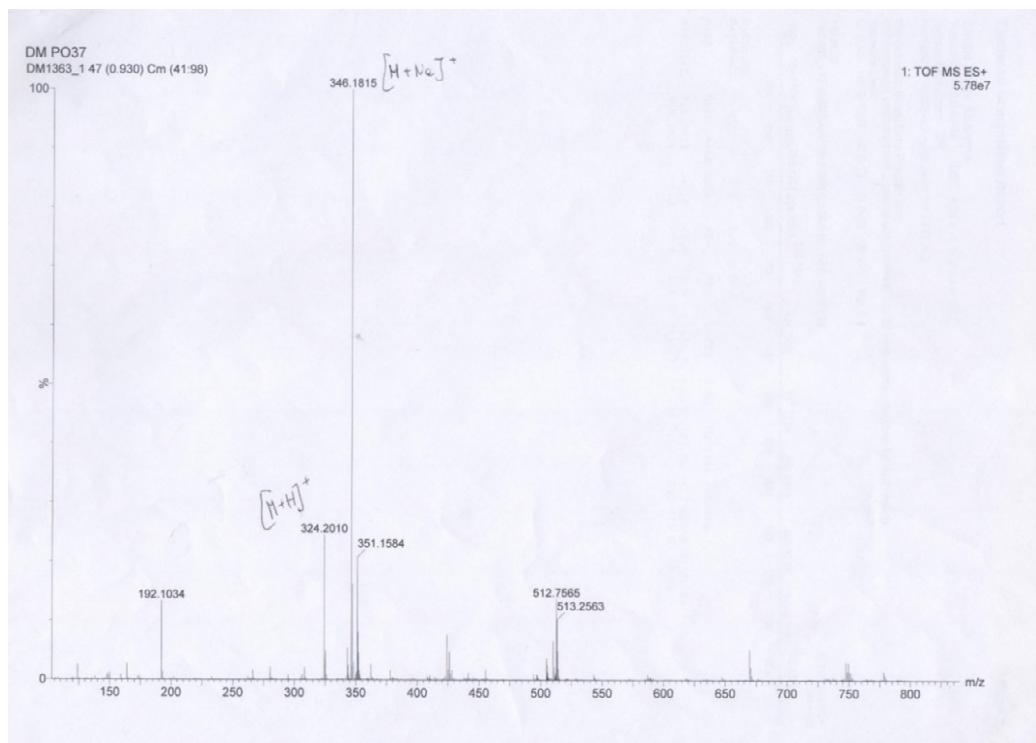
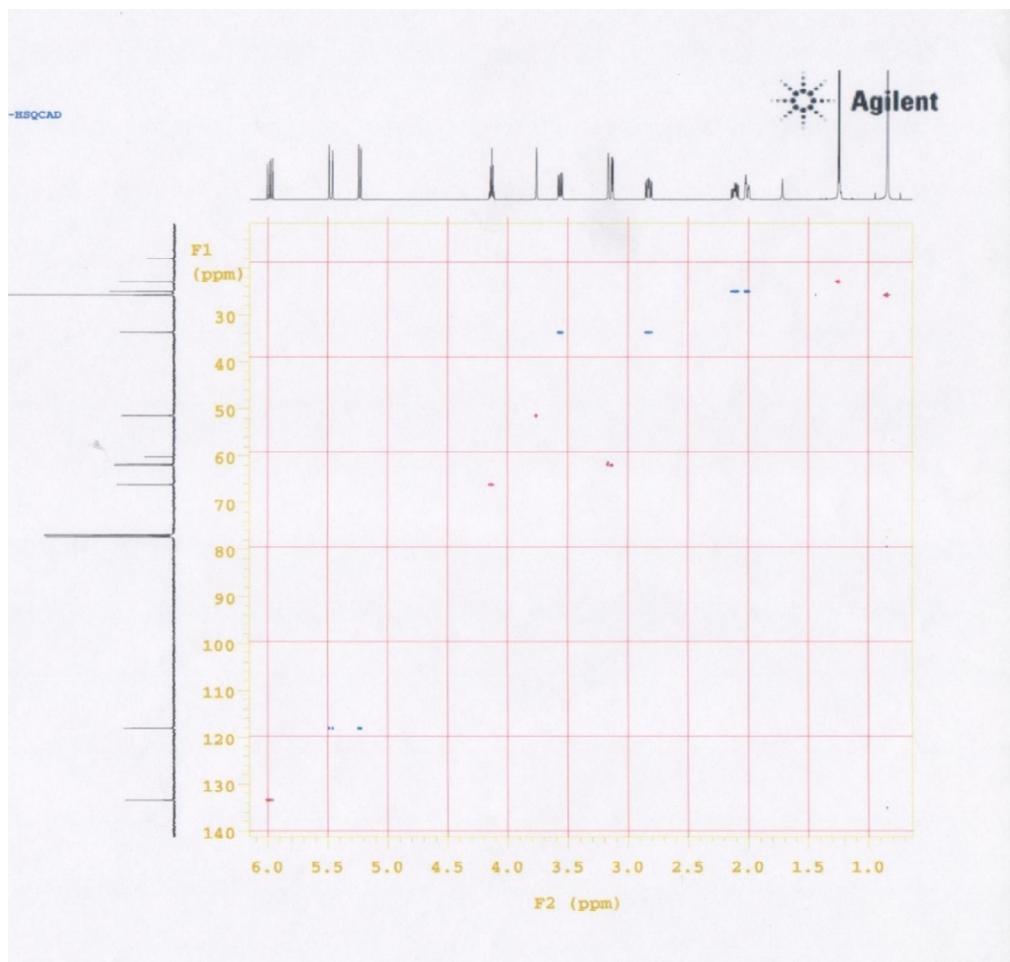




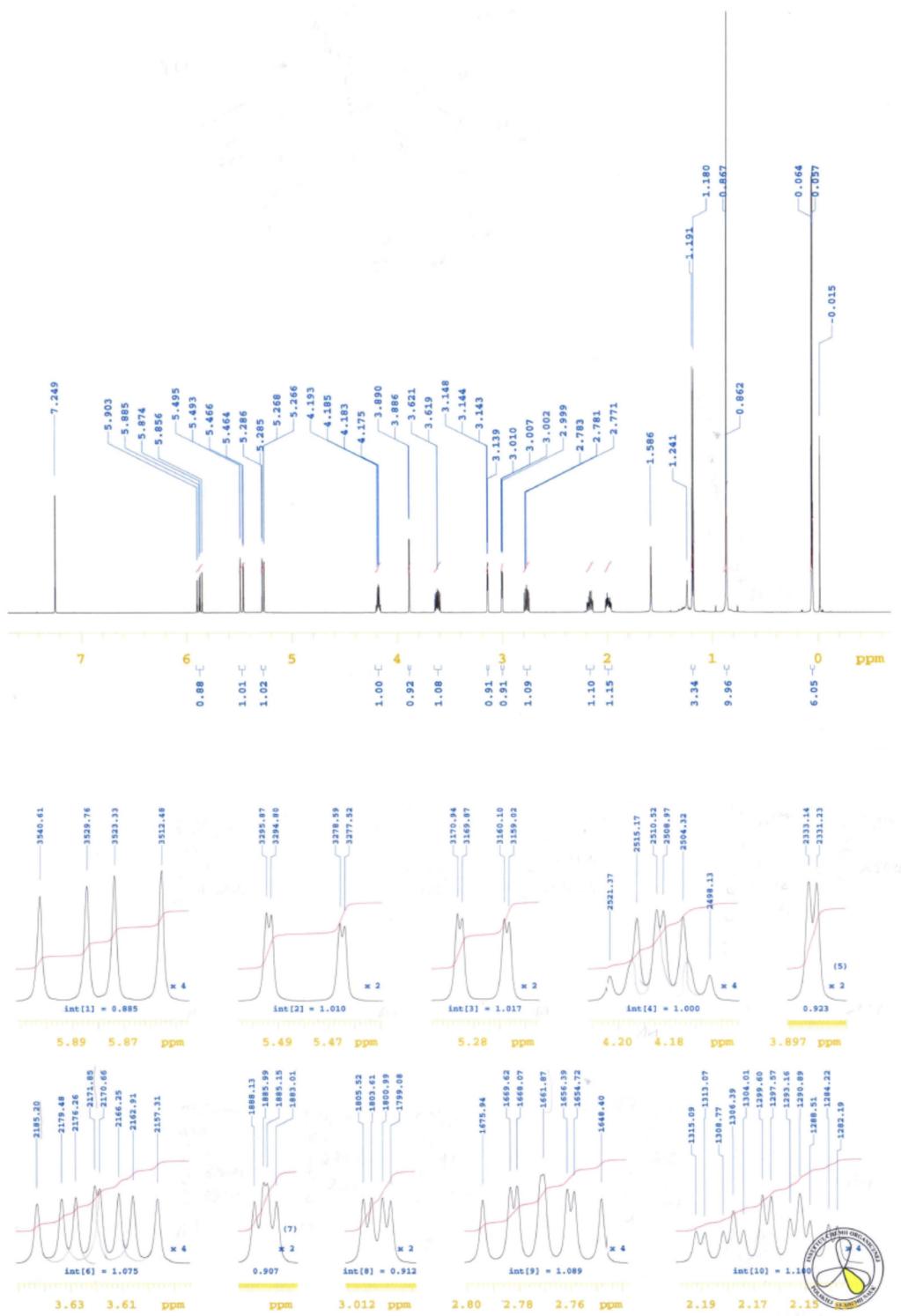


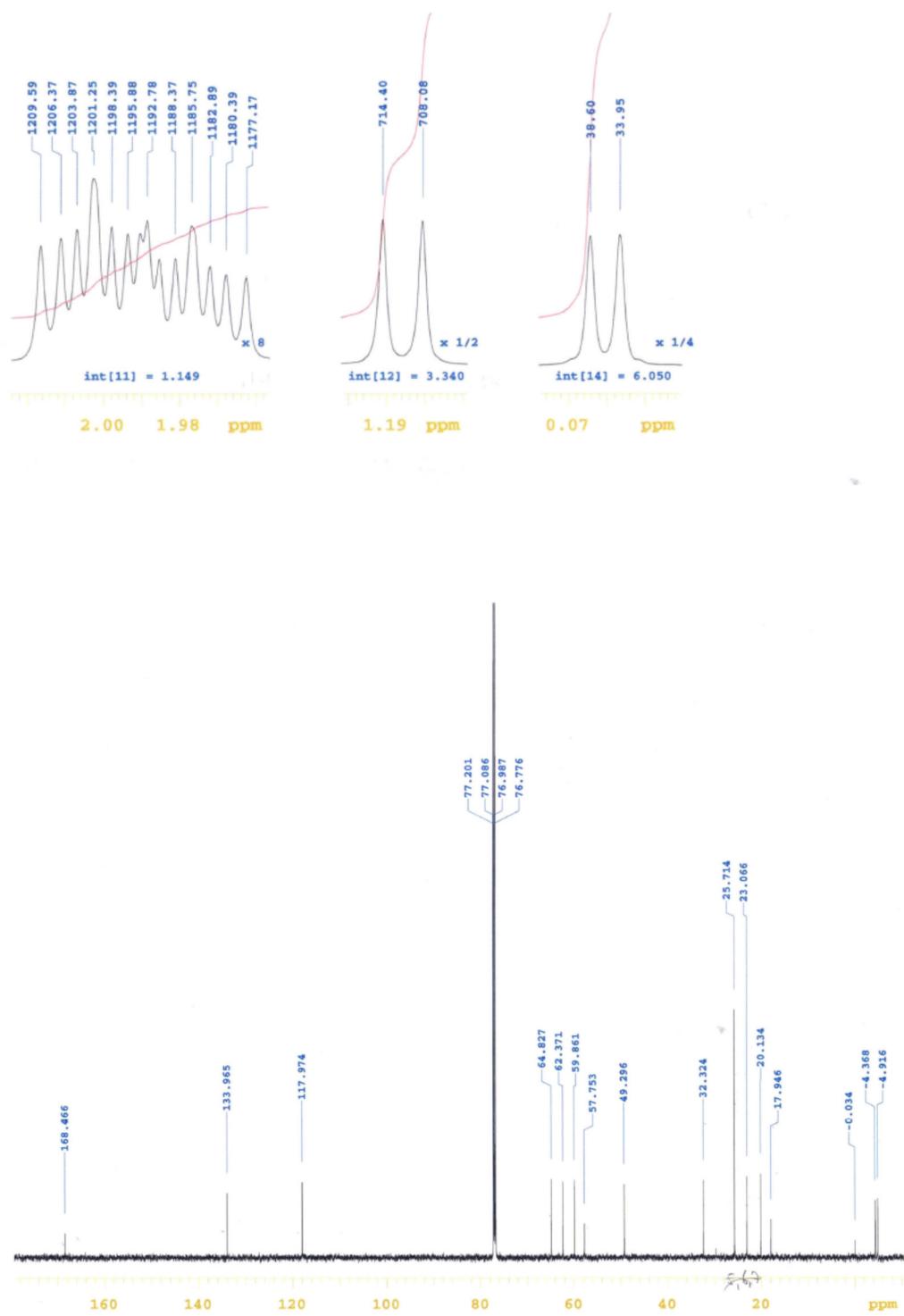




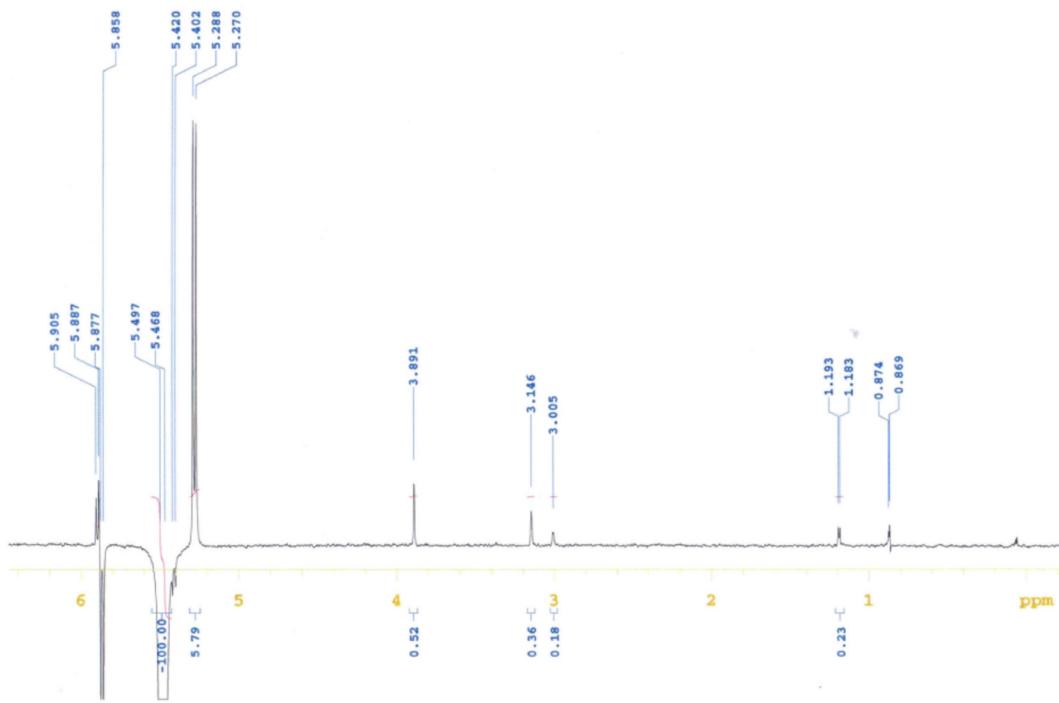
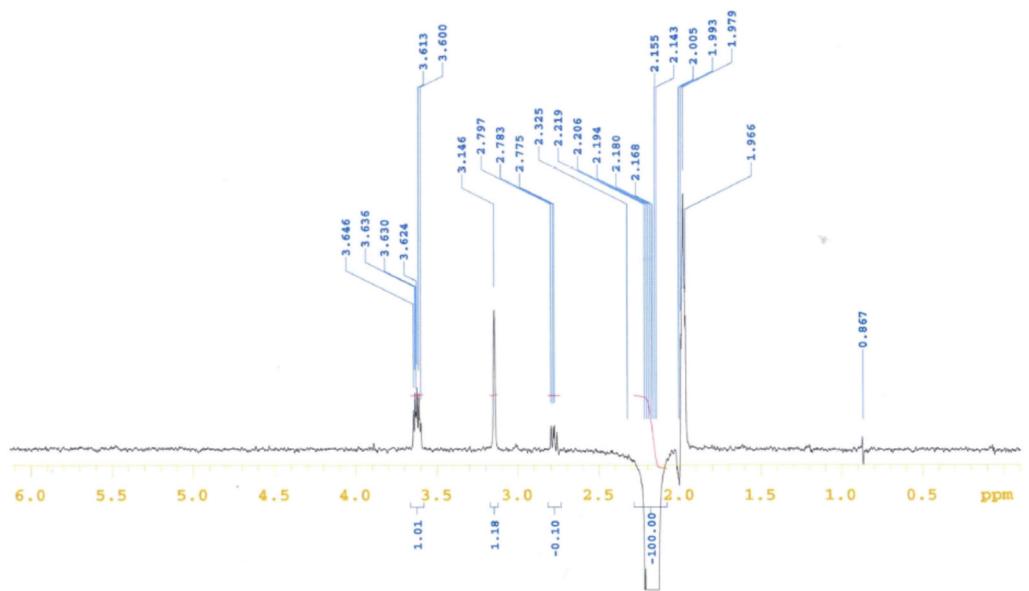


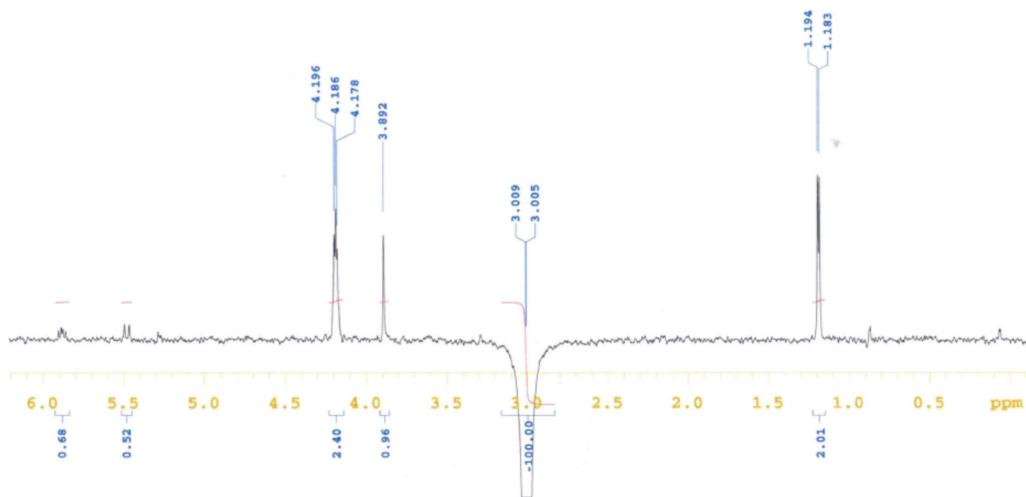
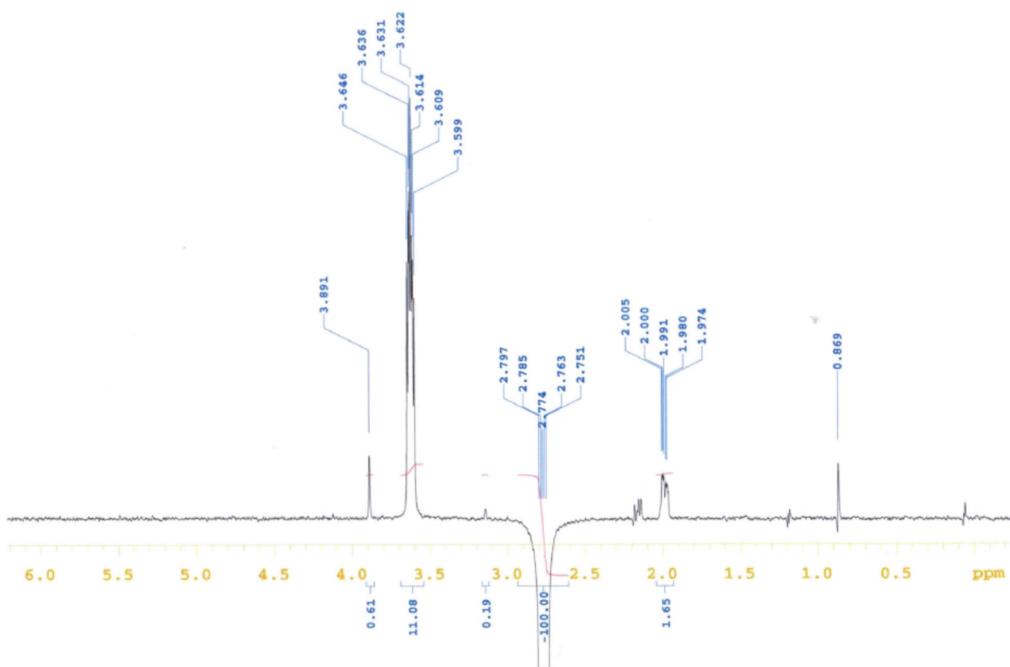
5. NMR and MS spectra of Comp. 3

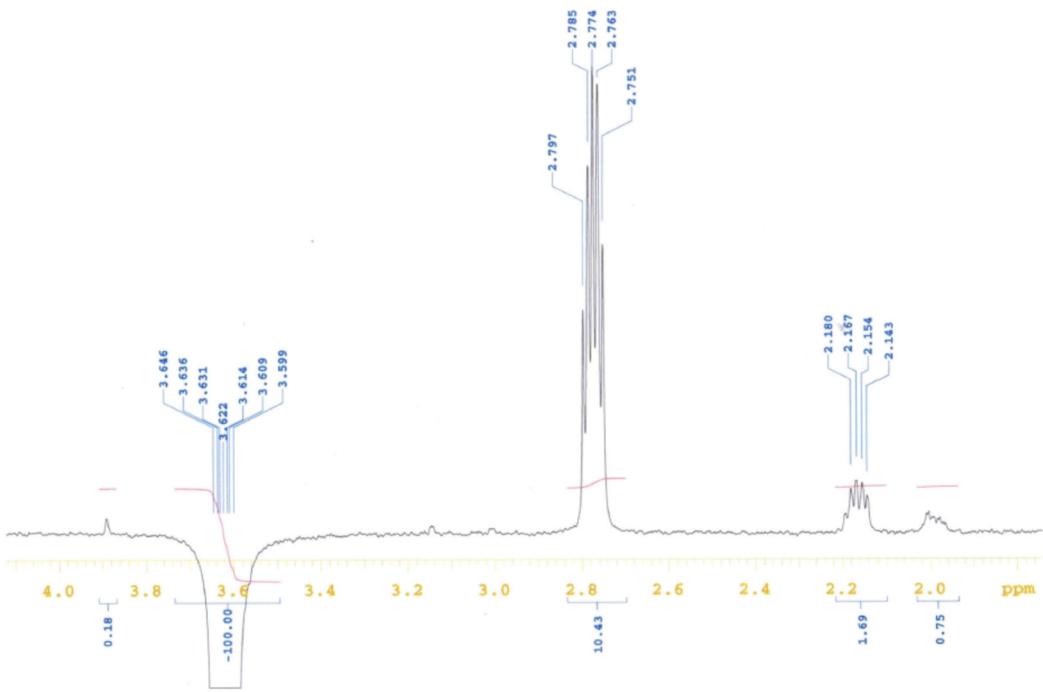
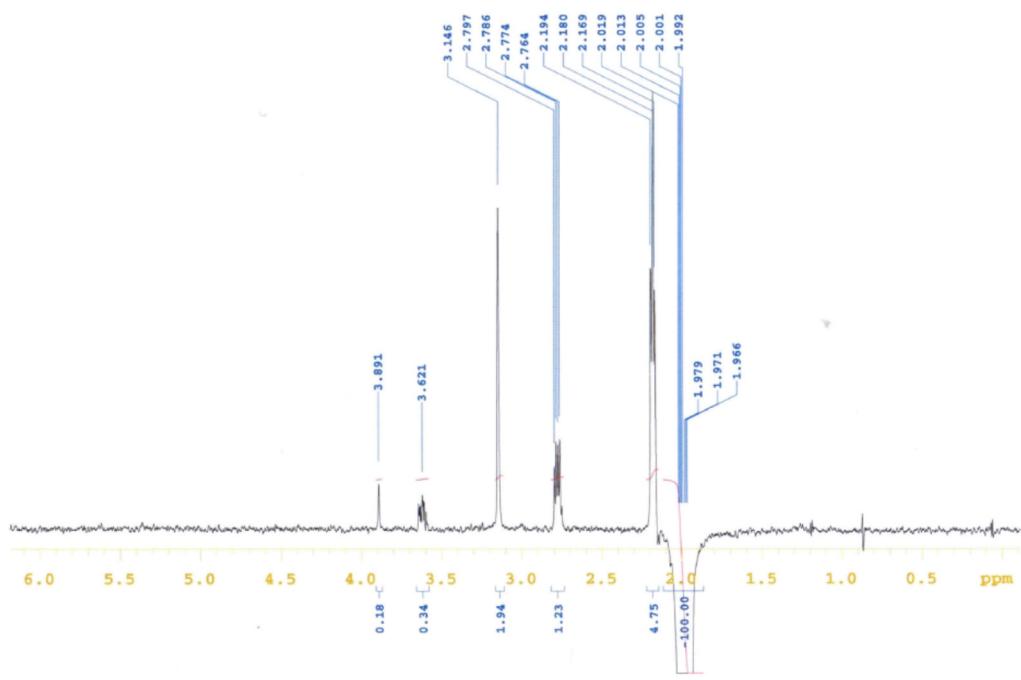






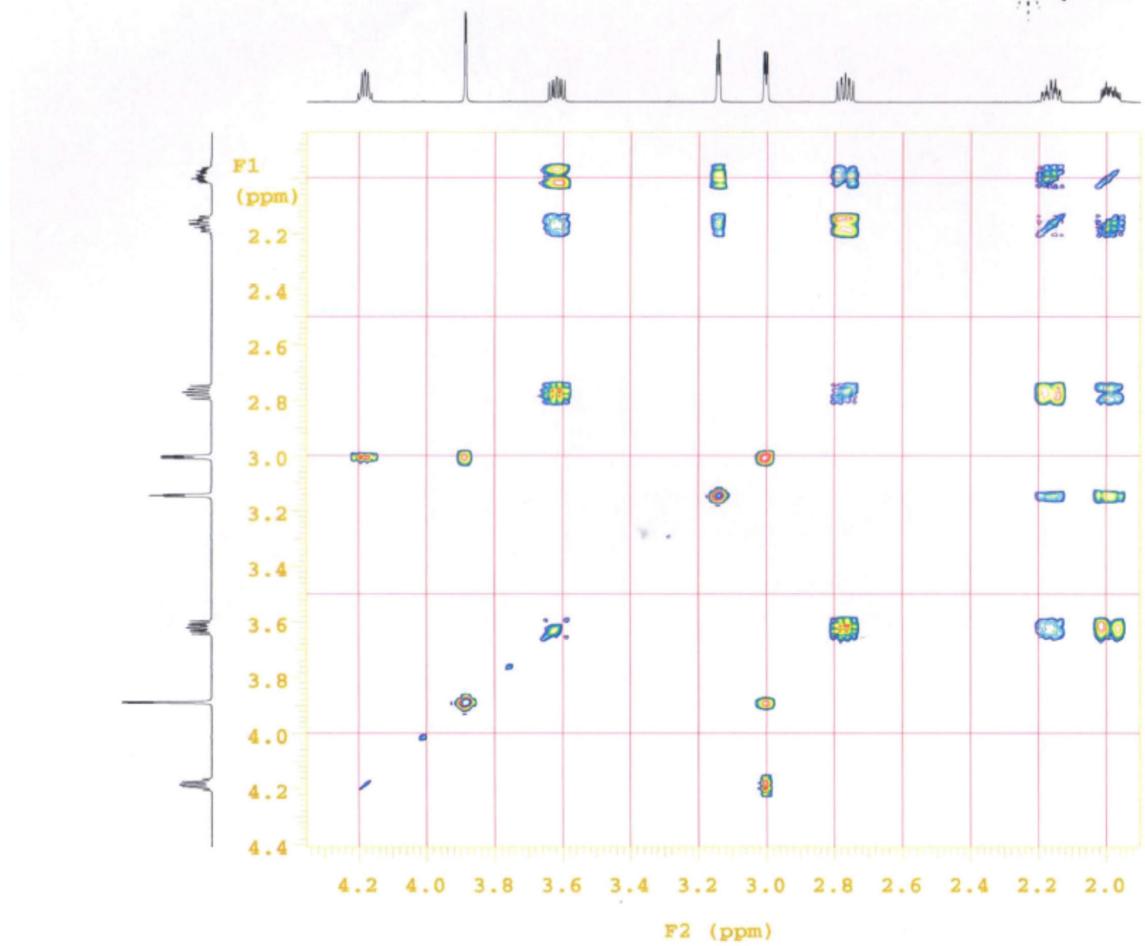






gCOSY

Agilent Technologies



H-PO37-peak2-gCOSY

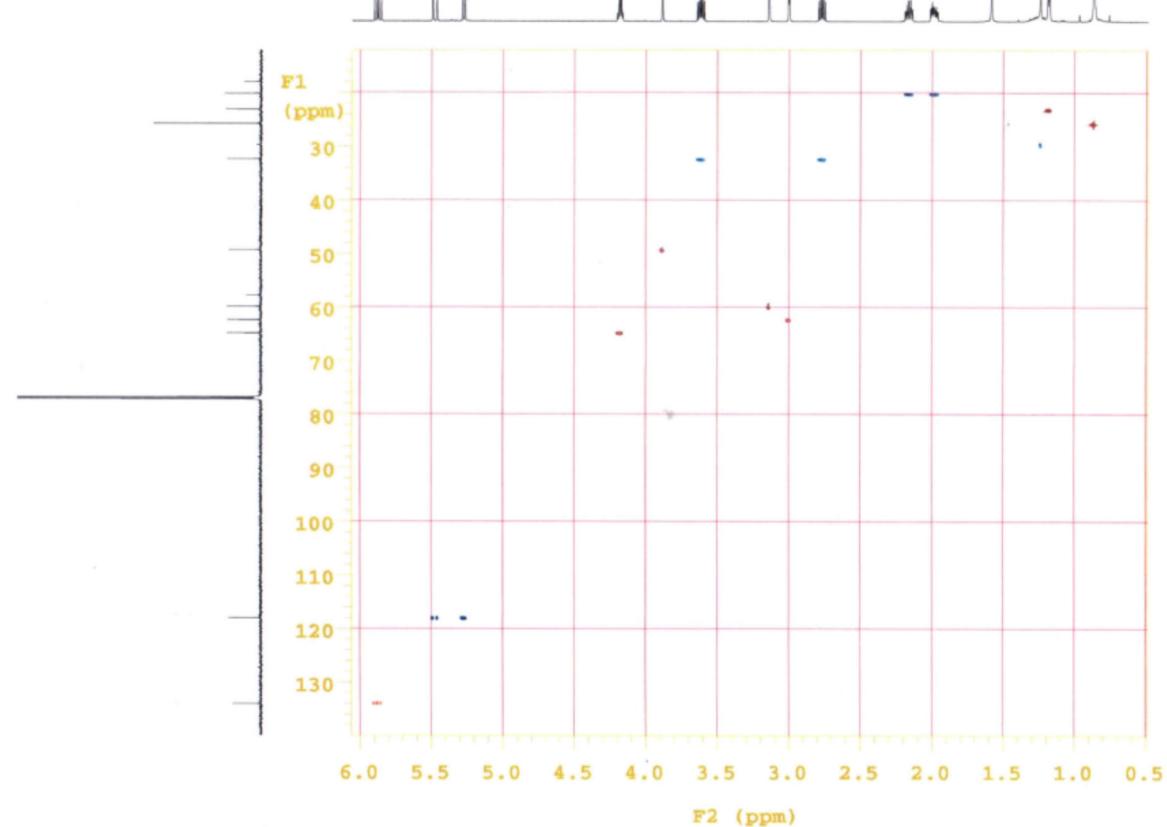
Agilent Technologies

2

F1
(ppm)

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F2 (ppm)

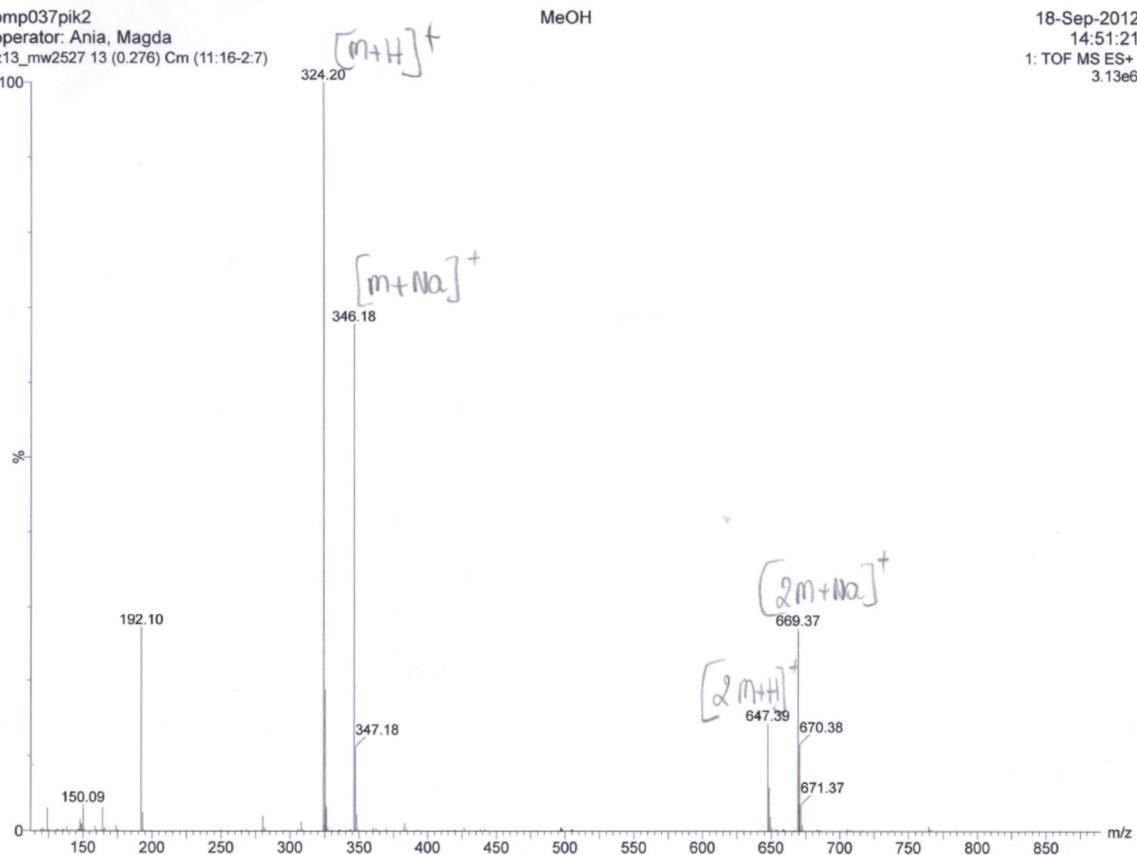
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operator: Ania, Magda
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18-Sep-2012
14:51:21
1: TOF MS ES+
3.13e6



6. Coordinates of calculated structures

Conf. 1 up a

| | | | |
|----|-----------|-----------|-----------|
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| N | 2.660426 | 0.853974 | -0.160754 |
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| C | 3.800189 | -1.270331 | 0.249980 |
| C | 3.810719 | 0.243047 | 0.469969 |
| O | 2.581557 | 3.208883 | -0.072149 |
| C | -0.431188 | 1.803997 | -0.017373 |
| C | -0.914202 | 3.234820 | -0.194195 |
| O | -1.432169 | 0.887277 | -0.419441 |
| Si | -2.378940 | -0.006109 | 0.644823 |
| C | -3.426285 | -1.124345 | -0.468136 |
| C | -3.437174 | 1.161433 | 1.659655 |
| C | -1.292307 | -1.007367 | 1.797120 |
| H | 0.624621 | 1.751949 | -1.909359 |
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| H | 4.730208 | 0.685668 | 0.075917 |
| H | 3.772901 | 0.444552 | 1.545486 |
| H | -0.170432 | 1.640719 | 1.038882 |
| H | -1.795665 | 3.415200 | 0.424734 |
| H | -0.132097 | 3.941251 | 0.095304 |
| H | -1.179341 | 3.414051 | -1.239731 |
| H | -2.807993 | 1.811382 | 2.276194 |
| H | -4.058994 | 1.796259 | 1.022414 |
| H | -4.094613 | 0.603132 | 2.333141 |
| H | -0.637347 | -0.359505 | 2.387428 |
| H | -0.661187 | -1.708616 | 1.246524 |
| H | -1.912938 | -1.574635 | 2.497845 |
| C | 3.831131 | -1.818028 | -1.148669 |
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| H | 2.344682 | -2.926565 | 0.082791 |
| H | 4.601645 | -3.083897 | 1.104498 |
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Conf. 1 up b

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| C | 1.651383 | 0.290854 | -0.697196 |
| N | 2.560430 | 1.006068 | 0.106155 |
| C | 1.798854 | -0.982061 | -1.027545 |
| C | 3.022679 | -1.678454 | -0.542398 |
| C | 3.983716 | -0.962153 | 0.387926 |
| C | 3.664915 | 0.456337 | 0.862021 |
| O | 2.048257 | 3.266056 | 0.541034 |
| C | -0.616994 | 1.480228 | -0.264910 |
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| | | | |
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| H | -4.045128 | 1.476836 | -0.721663 |
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Conf. 1 up c

| | | | |
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| H | 2.277772 | 3.173244 | -0.562977 |
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| H | 4.596167 | -1.185385 | 1.568120 |
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| | | | |
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| H | 3.017600 | -3.260569 | -1.722546 |
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Conf. 1 down a

| | | | |
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| C | 0.840546 | 1.588357 | -0.835360 |
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| C | 1.509730 | 0.236721 | -0.695637 |
| N | 2.659454 | 0.835641 | -0.144647 |
| C | 1.358578 | -1.068239 | -0.856570 |
| C | 2.448033 | -1.949098 | -0.351321 |
| C | 3.726789 | -1.336089 | 0.188002 |
| C | 3.916462 | 0.180300 | 0.141788 |
| C | 2.738727 | -1.937668 | 1.145973 |
| O | 2.672292 | 3.190018 | -0.009888 |
| C | -0.392962 | 1.830343 | 0.028126 |
| C | -0.864716 | 3.273138 | -0.059471 |
| O | -1.406619 | 0.947393 | -0.415188 |
| Si | -2.328629 | -0.011115 | 0.613704 |
| C | -1.213360 | -1.062660 | 1.692753 |
| C | -3.390535 | -1.075919 | -0.537800 |
| C | -3.377935 | 1.093596 | 1.705494 |
| H | 0.661141 | 1.900140 | -1.867329 |
| H | 0.450774 | -1.491314 | -1.264396 |
| C | 5.020427 | -2.084237 | -0.046958 |
| H | 4.320592 | 0.550224 | 1.088639 |
| H | 4.634549 | 0.423190 | -0.648631 |
| H | 2.125453 | -1.268537 | 1.740801 |
| H | 3.007939 | -2.868832 | 1.632193 |
| H | -0.123042 | 1.604284 | 1.070472 |
| H | -1.733621 | 3.426161 | 0.584114 |
| H | -1.146043 | 3.512483 | -1.088601 |
| H | -0.071383 | 3.956014 | 0.255308 |
| H | -1.817224 | -1.677892 | 2.367193 |
| H | -0.578101 | -1.721181 | 1.096078 |
| H | -0.561129 | -0.439083 | 2.311731 |

| | | | |
|---|-----------|-----------|-----------|
| H | -4.023087 | 1.745552 | 1.110162 |
| H | -4.011538 | 0.496874 | 2.368761 |
| H | -2.743668 | 1.726234 | 2.334668 |
| H | 2.562296 | -2.902728 | -0.855518 |
| H | 5.775924 | -1.790097 | 0.688883 |
| H | 5.418653 | -1.877130 | -1.044823 |
| H | 4.868022 | -3.162085 | 0.042622 |
| C | -2.489867 | -1.935868 | -1.437986 |
| H | -1.849663 | -1.315549 | -2.072225 |
| H | -1.847296 | -2.601443 | -0.852340 |
| H | -3.103474 | -2.564995 | -2.095143 |
| C | -4.278760 | -0.180670 | -1.415782 |
| H | -4.901101 | -0.798377 | -2.075674 |
| H | -4.951473 | 0.438424 | -0.813781 |
| H | -3.679978 | 0.483765 | -2.045271 |
| C | -4.282441 | -1.995862 | 0.313423 |
| H | -4.954033 | -1.424850 | 0.962596 |
| H | -4.906564 | -2.621204 | -0.336931 |
| H | -3.690962 | -2.666563 | 0.944944 |

Conf. 1 down b

| | | | |
|----|-----------|-----------|-----------|
| C | 0.813295 | 1.587212 | -0.843526 |
| C | 1.920873 | 2.189960 | 0.063337 |
| C | 1.668735 | 0.339964 | -0.757990 |
| N | 2.573290 | 0.988199 | 0.105454 |
| C | 1.788304 | -0.920184 | -1.144504 |
| C | 2.904534 | -1.711226 | -0.556059 |
| C | 3.937640 | -1.027264 | 0.319678 |
| C | 3.857352 | 0.483473 | 0.541181 |
| C | 2.915433 | -1.925521 | 0.954359 |
| O | 2.161237 | 3.265586 | 0.559355 |
| C | -0.584370 | 1.524668 | -0.229373 |
| C | -1.254604 | 2.888290 | -0.289333 |
| O | -1.343603 | 0.568442 | -0.942817 |
| Si | -2.100636 | -0.794120 | -0.306164 |
| C | -2.409714 | -1.882208 | -1.792174 |
| C | -3.735264 | -0.301433 | 0.531748 |
| C | -0.991027 | -1.651629 | 0.938146 |
| H | 0.780185 | 2.040784 | -1.837299 |
| H | 1.065925 | -1.387514 | -1.800073 |
| C | 5.364228 | -1.524775 | 0.248364 |
| H | 4.014501 | 0.728153 | 1.595613 |
| H | 4.648167 | 0.969456 | -0.040131 |
| H | 2.099538 | -1.464999 | 1.501760 |
| H | 3.250859 | -2.879935 | 1.344788 |
| H | -0.479921 | 1.218365 | 0.821050 |
| H | -2.231595 | 2.861040 | 0.196308 |
| H | -1.394595 | 3.188074 | -1.331404 |

| | | | |
|---|-----------|-----------|-----------|
| H | -0.637417 | 3.638218 | 0.212231 |
| H | -2.857825 | -2.833321 | -1.490752 |
| H | -3.084176 | -1.401281 | -2.506065 |
| H | -1.469426 | -2.100621 | -2.306242 |
| H | -0.620257 | -0.965481 | 1.704912 |
| H | -1.547554 | -2.445136 | 1.446988 |
| H | -0.126411 | -2.101314 | 0.445473 |
| H | 3.273770 | -2.533325 | -1.159744 |
| H | 5.907590 | -1.275086 | 1.165615 |
| H | 5.894334 | -1.073531 | -0.595767 |
| H | 5.392655 | -2.610001 | 0.127241 |
| C | -4.560963 | 0.597654 | -0.401255 |
| H | -4.034925 | 1.526273 | -0.639893 |
| H | -4.796090 | 0.095111 | -1.345191 |
| H | -5.512433 | 0.864464 | 0.076044 |
| C | -3.457996 | 0.444725 | 1.847477 |
| H | -4.403414 | 0.734038 | 2.323600 |
| H | -2.908360 | -0.178849 | 2.559143 |
| H | -2.880616 | 1.360929 | 1.690644 |
| C | -4.543649 | -1.572536 | 0.846444 |
| H | -3.995253 | -2.256698 | 1.502127 |
| H | -5.476785 | -1.306006 | 1.358643 |
| H | -4.812507 | -2.118772 | -0.062915 |

Conf. 1 down c

| | | | |
|----|-----------|-----------|-----------|
| C | -0.688417 | 1.770309 | 0.671764 |
| C | -1.853860 | 2.215199 | -0.253776 |
| C | -1.472439 | 0.474629 | 0.737423 |
| N | -2.426867 | 0.975494 | -0.170760 |
| C | -1.538949 | -0.727938 | 1.286571 |
| C | -2.643496 | -1.624538 | 0.845625 |
| C | -3.731207 | -1.090007 | -0.067107 |
| C | -3.709184 | 0.380226 | -0.483370 |
| C | -2.704889 | -2.035714 | -0.621240 |
| O | -2.180524 | 3.224906 | -0.831921 |
| C | 0.691455 | 1.755048 | 0.020302 |
| C | 1.223993 | 3.175651 | -0.111503 |
| O | 1.545262 | 0.954623 | 0.819034 |
| Si | 2.850085 | 0.033314 | 0.281076 |
| C | 3.878195 | 1.026715 | -0.932903 |
| C | 2.271220 | -1.585070 | -0.539978 |
| C | 3.822881 | -0.329722 | 1.833152 |
| H | -0.662777 | 2.319719 | 1.616478 |
| H | -0.798237 | -1.073560 | 1.993976 |
| C | -5.136728 | -1.614633 | 0.126543 |
| H | -3.914502 | 0.483609 | -1.552650 |
| H | -4.492523 | 0.915224 | 0.064293 |
| H | -1.929408 | -1.632605 | -1.263663 |

| | | | |
|---|-----------|-----------|-----------|
| H | -3.023411 | -3.043257 | -0.864660 |
| H | 0.590741 | 1.314987 | -0.980582 |
| H | 2.179474 | 3.185789 | -0.637076 |
| H | 1.365220 | 3.615400 | 0.879614 |
| H | 0.516006 | 3.792983 | -0.670515 |
| H | 4.773130 | 0.463642 | -1.213757 |
| H | 3.328834 | 1.256499 | -1.851029 |
| H | 4.204618 | 1.968568 | -0.483429 |
| H | 3.179873 | -0.758292 | 2.606600 |
| H | 4.626957 | -1.043423 | 1.629466 |
| H | 4.273156 | 0.584279 | 2.230171 |
| H | -2.961255 | -2.370877 | 1.565619 |
| H | -5.724672 | -1.489107 | -0.788507 |
| H | -5.646747 | -1.083075 | 0.935655 |
| H | -5.123644 | -2.678790 | 0.372724 |
| C | 1.161727 | -1.319204 | -1.569645 |
| H | 0.259552 | -0.933357 | -1.087614 |
| H | 1.474029 | -0.604513 | -2.338611 |
| H | 0.890626 | -2.252925 | -2.078979 |
| C | 1.739756 | -2.561193 | 0.521323 |
| H | 1.382653 | -3.480856 | 0.040425 |
| H | 2.515818 | -2.843339 | 1.239150 |
| H | 0.901532 | -2.134479 | 1.077135 |
| C | 3.468758 | -2.236800 | -1.254722 |
| H | 4.309549 | -2.412215 | -0.574842 |
| H | 3.171811 | -3.209727 | -1.665992 |
| H | 3.829681 | -1.625141 | -2.086820 |

Conf. 2a

| | | | |
|----|-----------|-----------|-----------|
| C | 1.160593 | 1.115798 | -0.508411 |
| C | 2.492770 | 1.831198 | -0.256916 |
| N | 2.914102 | 0.870774 | 0.615130 |
| C | 1.712660 | 0.037389 | 0.461835 |
| C | -0.159502 | 1.780227 | -0.158943 |
| O | -1.182162 | 0.835929 | -0.432246 |
| C | -0.400394 | 3.049099 | -0.959201 |
| C | 1.999244 | -1.342377 | -0.088931 |
| C | 3.401825 | -1.690193 | -0.406855 |
| C | 4.541845 | -0.714480 | -0.236306 |
| C | 4.246997 | 0.345874 | 0.829115 |
| O | 3.039407 | 2.825063 | -0.683444 |
| Si | -2.371822 | 0.348434 | 0.649695 |
| C | -3.166559 | 1.859490 | 1.421853 |
| C | -3.600710 | -0.634902 | -0.402457 |
| C | -1.600286 | -0.713211 | 1.986944 |
| C | -4.712752 | -1.190551 | 0.503184 |
| C | -4.225083 | 0.280993 | -1.467183 |
| C | -2.884231 | -1.802661 | -1.098092 |

| | | | |
|---|-----------|-----------|-----------|
| H | 1.128638 | 0.769982 | -1.546442 |
| H | 1.146618 | -0.053168 | 1.393150 |
| H | -0.145359 | 2.030239 | 0.912255 |
| H | -1.362363 | 3.485684 | -0.681795 |
| H | 0.386606 | 3.782777 | -0.768964 |
| H | -0.416600 | 2.822825 | -2.028878 |
| H | 4.719168 | -0.232272 | -1.202848 |
| H | 5.450644 | -1.264581 | 0.024238 |
| H | 4.959391 | 1.168809 | 0.769996 |
| H | 4.302010 | -0.082558 | 1.831373 |
| H | -3.954826 | 1.563487 | 2.120844 |
| H | -2.432008 | 2.443801 | 1.984639 |
| H | -3.609838 | 2.511722 | 0.664502 |
| H | -2.367284 | -1.112748 | 2.657681 |
| H | -1.050880 | -1.553722 | 1.552905 |
| H | -0.907091 | -0.127490 | 2.598797 |
| H | -5.444222 | -1.743315 | -0.099319 |
| H | -4.319548 | -1.880940 | 1.256027 |
| H | -5.252648 | -0.393238 | 1.024474 |
| H | -4.923149 | -0.290775 | -2.091755 |
| H | -4.786767 | 1.105076 | -1.016261 |
| H | -3.463493 | 0.710544 | -2.124835 |
| H | -3.602827 | -2.391379 | -1.682345 |
| H | -2.111366 | -1.444911 | -1.784253 |
| H | -2.409409 | -2.477606 | -0.379299 |
| C | 0.853750 | -2.021870 | -0.752471 |
| H | 3.551828 | -2.465634 | -1.155111 |
| O | 2.778380 | -2.160254 | 0.789382 |
| C | 0.587384 | -3.316075 | -0.623894 |
| H | 0.206167 | -1.381661 | -1.343769 |
| H | -0.266192 | -3.760469 | -1.122401 |
| H | 1.211298 | -3.960361 | -0.013390 |

Conf. 2b

| | | | |
|----|-----------|-----------|-----------|
| C | -1.036131 | -1.082044 | -0.571459 |
| C | -2.142071 | -2.048627 | -0.127784 |
| N | -2.665687 | -1.142475 | 0.745311 |
| C | -1.693715 | -0.089339 | 0.422848 |
| C | 0.433134 | -1.422499 | -0.381862 |
| O | 1.181367 | -0.306861 | -0.836576 |
| C | 0.829094 | -2.662983 | -1.165361 |
| C | -2.325125 | 1.172730 | -0.121267 |
| C | -3.798176 | 1.215019 | -0.254129 |
| C | -4.682282 | 0.038985 | 0.086982 |
| C | -4.043068 | -0.897457 | 1.117823 |
| O | -2.498693 | -3.163997 | -0.439998 |
| Si | 2.241803 | 0.674622 | 0.021313 |
| C | 1.456593 | 1.230300 | 1.630200 |

| | | | |
|---|-----------|-----------|-----------|
| C | 3.866545 | -0.250699 | 0.364997 |
| C | 2.520220 | 2.132897 | -1.110662 |
| C | 4.883652 | 0.727512 | 0.978273 |
| C | 3.633104 | -1.407171 | 1.351023 |
| C | 4.438035 | -0.809056 | -0.947782 |
| H | -1.208226 | -0.803632 | -1.616084 |
| H | -1.060063 | 0.163222 | 1.276883 |
| H | 0.615662 | -1.595226 | 0.688176 |
| H | 1.886817 | -2.885984 | -1.011862 |
| H | 0.239380 | -3.525096 | -0.845169 |
| H | 0.660629 | -2.501208 | -2.233443 |
| H | -4.884346 | -0.507277 | -0.839762 |
| H | -5.640770 | 0.408527 | 0.462669 |
| H | -4.566531 | -1.852780 | 1.157044 |
| H | -4.066426 | -0.453303 | 2.114561 |
| H | 2.167026 | 1.829838 | 2.207663 |
| H | 0.579974 | 1.853694 | 1.430819 |
| H | 1.149436 | 0.389618 | 2.259146 |
| H | 3.194875 | 2.861193 | -0.651232 |
| H | 2.955129 | 1.821394 | -2.064082 |
| H | 1.570680 | 2.635148 | -1.314382 |
| H | 5.823920 | 0.204493 | 1.193319 |
| H | 5.115928 | 1.552511 | 0.297756 |
| H | 4.524920 | 1.156381 | 1.919461 |
| H | 4.579572 | -1.923223 | 1.555868 |
| H | 3.237396 | -1.052537 | 2.307915 |
| H | 2.936867 | -2.153003 | 0.955135 |
| H | 5.375573 | -1.345500 | -0.754115 |
| H | 3.746077 | -1.507874 | -1.426373 |
| H | 4.658745 | -0.012835 | -1.666014 |
| C | -1.440329 | 2.035069 | -0.951082 |
| H | -4.199556 | 1.908318 | -0.990270 |
| O | -3.136628 | 1.858559 | 0.836213 |
| C | -1.390998 | 3.357672 | -0.845725 |
| H | -0.796835 | 1.512552 | -1.653038 |
| H | -0.728068 | 3.943910 | -1.471604 |
| H | -2.012487 | 3.887828 | -0.131845 |

Conf. 2c

| | | | |
|---|-----------|-----------|-----------|
| C | -1.132488 | -1.174621 | -0.549352 |
| C | -2.391270 | -1.889440 | -0.045646 |
| N | -2.698877 | -0.872936 | 0.809412 |
| C | -1.578495 | -0.020259 | 0.383693 |
| C | 0.227394 | -1.788377 | -0.267345 |
| O | 1.186087 | -0.787430 | -0.555676 |
| C | 0.468309 | -3.046861 | -1.086233 |
| C | -2.026373 | 1.282056 | -0.246873 |
| C | -3.479185 | 1.556501 | -0.328199 |

| | | | |
|----|-----------|-----------|-----------|
| C | -4.526935 | 0.579997 | 0.149818 |
| C | -3.992962 | -0.373607 | 1.223019 |
| O | -2.964164 | -2.926076 | -0.303295 |
| Si | 2.719067 | -0.644715 | 0.121671 |
| C | 3.975271 | -1.413331 | -1.034920 |
| C | 3.021566 | 1.215432 | 0.318663 |
| C | 2.747557 | -1.526028 | 1.775299 |
| C | 4.427347 | 1.448563 | 0.896844 |
| C | 2.912703 | 1.911891 | -1.047047 |
| C | 1.975067 | 1.811532 | 1.272921 |
| H | -1.228819 | -0.937833 | -1.612909 |
| H | -0.873389 | 0.186738 | 1.194284 |
| H | 0.269392 | -2.041611 | 0.801484 |
| H | 1.437501 | -3.485930 | -0.837542 |
| H | -0.307917 | -3.788817 | -0.882665 |
| H | 0.457316 | -2.811293 | -2.153940 |
| H | -4.871307 | 0.008081 | -0.717678 |
| H | -5.386937 | 1.134979 | 0.535163 |
| H | -4.665419 | -1.220122 | 1.362820 |
| H | -3.882518 | 0.136576 | 2.181496 |
| H | 4.988487 | -1.305515 | -0.635707 |
| H | 3.779218 | -2.481537 | -1.166023 |
| H | 3.947048 | -0.940670 | -2.020669 |
| H | 3.723310 | -1.392231 | 2.252078 |
| H | 1.984411 | -1.141065 | 2.457732 |
| H | 2.585741 | -2.601550 | 1.655268 |
| H | 4.604883 | 2.523312 | 1.027988 |
| H | 4.551482 | 0.974792 | 1.876153 |
| H | 5.210071 | 1.065719 | 0.234151 |
| H | 3.066206 | 2.992455 | -0.931024 |
| H | 3.666588 | 1.546023 | -1.751487 |
| H | 1.926474 | 1.762913 | -1.494599 |
| H | 2.147845 | 2.888122 | 1.397894 |
| H | 0.963145 | 1.684389 | 0.879842 |
| H | 2.019786 | 1.353021 | 2.265987 |
| C | -1.064228 | 1.918827 | -1.187465 |
| H | -3.797743 | 2.242499 | -1.110352 |
| O | -2.668192 | 2.170212 | 0.674033 |
| C | -0.872310 | 3.229627 | -1.273214 |
| H | -0.489220 | 1.237870 | -1.807318 |
| H | -0.154402 | 3.642352 | -1.972354 |
| H | -1.421679 | 3.919827 | -0.641632 |

Conf. 2d

| | | | |
|---|----------|-----------|-----------|
| C | 1.012259 | 1.199310 | -0.549510 |
| C | 2.138512 | 1.962509 | 0.157857 |
| N | 2.457065 | 0.890188 | 0.936816 |
| C | 1.480502 | -0.008338 | 0.303178 |

| | | | |
|----|-----------|-----------|-----------|
| C | -0.417275 | 1.684177 | -0.372839 |
| O | -1.265274 | 0.674513 | -0.892638 |
| C | -0.634609 | 3.008129 | -1.091014 |
| C | 2.125514 | -1.180030 | -0.408627 |
| C | 3.600787 | -1.301800 | -0.357739 |
| C | 4.486176 | -0.291415 | 0.331222 |
| C | 3.749007 | 0.469382 | 1.436981 |
| O | 2.629324 | 3.066928 | 0.069213 |
| Si | -2.816167 | 0.272861 | -0.372619 |
| C | -3.628596 | -0.487182 | -1.872488 |
| C | -2.723590 | -0.977509 | 1.056426 |
| C | -3.724356 | 1.815875 | 0.183747 |
| C | -4.143914 | -1.466013 | 1.392109 |
| C | -1.869185 | -2.186234 | 0.644700 |
| C | -2.118053 | -0.325181 | 2.309972 |
| H | 1.236963 | 1.087955 | -1.614255 |
| H | 0.730973 | -0.377219 | 1.007986 |
| H | -0.605595 | 1.821740 | 0.701496 |
| H | -1.649775 | 3.373643 | -0.928498 |
| H | 0.069473 | 3.758971 | -0.723933 |
| H | -0.477627 | 2.877944 | -2.165281 |
| H | 4.847539 | 0.410888 | -0.426579 |
| H | 5.360438 | -0.802041 | 0.744781 |
| H | 4.307427 | 1.353600 | 1.744626 |
| H | 3.597613 | -0.161855 | 2.314217 |
| H | -4.665020 | -0.764262 | -1.659072 |
| H | -3.634545 | 0.228584 | -2.699353 |
| H | -3.098493 | -1.384760 | -2.202917 |
| H | -4.688626 | 1.550460 | 0.627359 |
| H | -3.157360 | 2.374486 | 0.934471 |
| H | -3.917865 | 2.482326 | -0.661386 |
| H | -4.104131 | -2.194480 | 2.211663 |
| H | -4.796722 | -0.648179 | 1.713372 |
| H | -4.616750 | -1.960224 | 0.537750 |
| H | -1.818384 | -2.911461 | 1.466695 |
| H | -2.290628 | -2.702718 | -0.223641 |
| H | -0.846073 | -1.899062 | 0.390034 |
| H | -2.065937 | -1.055635 | 3.127078 |
| H | -1.101616 | 0.041195 | 2.137642 |
| H | -2.720452 | 0.519014 | 2.659633 |
| C | 1.337132 | -1.798199 | -1.510473 |
| H | 4.065898 | -1.857990 | -1.169115 |
| O | 2.766379 | -2.101385 | 0.479968 |
| C | 1.309650 | -3.103011 | -1.754895 |
| H | 0.751076 | -1.113903 | -2.116522 |
| H | 0.720196 | -3.505095 | -2.570514 |
| H | 1.871699 | -3.800564 | -1.142771 |

Conf. 2e

| | | | |
|----|-----------|-----------|-----------|
| C | 1.133608 | 0.996358 | -0.612054 |
| C | 2.430168 | 1.770556 | -0.342943 |
| N | 2.796872 | 0.923999 | 0.660944 |
| C | 1.650016 | 0.023644 | 0.478752 |
| C | -0.200187 | 1.679713 | -0.359426 |
| O | -1.208954 | 0.691911 | -0.484171 |
| C | -0.454262 | 2.813546 | -1.339506 |
| C | 2.057171 | -1.373185 | 0.057024 |
| C | 3.488593 | -1.695339 | -0.040913 |
| C | 4.570541 | -0.664570 | 0.178712 |
| C | 4.114003 | 0.490518 | 1.076163 |
| O | 2.986253 | 2.732483 | -0.827292 |
| Si | -2.440007 | 0.426187 | 0.627514 |
| C | -3.304533 | 2.046511 | 0.999033 |
| C | -3.589198 | -0.816716 | -0.218464 |
| C | -1.714650 | -0.263007 | 2.212481 |
| C | -4.731618 | -1.187952 | 0.742173 |
| C | -4.180988 | -0.196799 | -1.494340 |
| C | -2.807745 | -2.086166 | -0.592395 |
| H | 1.142013 | 0.554782 | -1.612724 |
| H | 1.011645 | -0.035586 | 1.365113 |
| H | -0.187817 | 2.086581 | 0.663234 |
| H | -1.415883 | 3.285535 | -1.126353 |
| H | 0.331736 | 3.569314 | -1.268212 |
| H | -0.475958 | 2.425560 | -2.361581 |
| H | 4.864214 | -0.277495 | -0.802315 |
| H | 5.449319 | -1.149367 | 0.612750 |
| H | 4.798583 | 1.335764 | 1.003066 |
| H | 4.067387 | 0.179329 | 2.121424 |
| H | -4.096480 | 1.900914 | 1.739997 |
| H | -2.599875 | 2.776209 | 1.410553 |
| H | -3.752335 | 2.479327 | 0.100475 |
| H | -2.501349 | -0.427216 | 2.955217 |
| H | -1.202636 | -1.214991 | 2.046663 |
| H | -0.996618 | 0.438658 | 2.648672 |
| H | -5.413556 | -1.897546 | 0.257456 |
| H | -4.358469 | -1.662833 | 1.655146 |
| H | -5.321695 | -0.312713 | 1.033378 |
| H | -4.836577 | -0.920294 | -1.995156 |
| H | -4.780485 | 0.691956 | -1.273668 |
| H | -3.398153 | 0.091069 | -2.202213 |
| H | -3.476078 | -2.811602 | -1.073084 |
| H | -1.996457 | -1.863733 | -1.291173 |
| H | -2.375966 | -2.573317 | 0.288247 |
| C | 1.015446 | -2.146976 | -0.670383 |
| H | 3.770230 | -2.524501 | -0.685832 |
| O | 2.731373 | -2.093683 | 1.107693 |

| | | | |
|---|----------|-----------|-----------|
| C | 1.151703 | -2.610478 | -1.906154 |
| H | 0.082479 | -2.290284 | -0.130480 |
| H | 0.347970 | -3.151655 | -2.393259 |
| H | 2.065014 | -2.460111 | -2.473554 |

Conf. 2f

| | | | |
|----|-----------|-----------|-----------|
| C | -1.009053 | 1.131645 | 0.482265 |
| C | -2.108204 | 1.874348 | -0.288281 |
| N | -2.380430 | 0.786311 | -1.063936 |
| C | -1.449118 | -0.098069 | -0.349762 |
| C | 0.422192 | 1.618112 | 0.315473 |
| O | 1.269751 | 0.623552 | 0.863878 |
| C | 0.622555 | 2.956920 | 1.011064 |
| C | -2.156183 | -1.227261 | 0.376067 |
| C | -3.611183 | -1.373187 | 0.209392 |
| C | -4.445666 | -0.397338 | -0.584942 |
| C | -3.631685 | 0.349513 | -1.645770 |
| O | -2.607762 | 2.977618 | -0.245817 |
| Si | 2.836426 | 0.231479 | 0.389732 |
| C | 3.618281 | -0.502616 | 1.918439 |
| C | 2.794175 | -1.036681 | -1.026667 |
| C | 3.747161 | 1.774150 | -0.162885 |
| C | 4.227976 | -1.515553 | -1.316382 |
| C | 1.940433 | -2.250586 | -0.629283 |
| C | 2.215759 | -0.404934 | -2.303536 |
| H | -1.252346 | 1.040085 | 1.544351 |
| H | -0.671358 | -0.508356 | -0.999220 |
| H | 0.623712 | 1.736431 | -0.759006 |
| H | 1.636263 | 3.327962 | 0.852557 |
| H | -0.083424 | 3.695373 | 0.622872 |
| H | 0.455130 | 2.844916 | 2.085789 |
| H | -4.878316 | 0.318322 | 0.121695 |
| H | -5.276209 | -0.930187 | -1.056102 |
| H | -4.170800 | 1.224188 | -2.009906 |
| H | -3.413014 | -0.295875 | -2.498517 |
| H | 4.663681 | -0.766998 | 1.734697 |
| H | 3.593176 | 0.221732 | 2.737395 |
| H | 3.092532 | -1.404087 | 2.245097 |
| H | 4.729890 | 1.511243 | -0.565670 |
| H | 3.202318 | 2.311405 | -0.944931 |
| H | 3.902485 | 2.458927 | 0.675411 |
| H | 4.218691 | -2.247958 | -2.133237 |
| H | 4.883810 | -0.694082 | -1.621538 |
| H | 4.678665 | -2.002120 | -0.445789 |
| H | 1.941570 | -2.994867 | -1.435257 |
| H | 2.321922 | -2.740155 | 0.272288 |
| H | 0.901175 | -1.969733 | -0.442437 |
| H | 2.192818 | -1.144935 | -3.113282 |

| | | | |
|---|-----------|-----------|-----------|
| H | 1.191037 | -0.048031 | -2.161067 |
| H | 2.818211 | 0.441709 | -2.646890 |
| C | -1.448111 | -1.788883 | 1.559767 |
| H | -4.148460 | -1.902566 | 0.992823 |
| O | -2.706549 | -2.205241 | -0.526223 |
| C | -1.917958 | -1.732772 | 2.799669 |
| H | -0.479659 | -2.241402 | 1.359714 |
| H | -1.358276 | -2.144091 | 3.632209 |
| H | -2.873934 | -1.270008 | 3.024798 |

Conf. 3a

| | | | |
|----|-----------|-----------|-----------|
| C | -1.152316 | -0.987237 | -0.688594 |
| C | -2.435277 | -1.760740 | -0.335664 |
| N | -2.727603 | -0.902772 | 0.677875 |
| C | -1.615931 | 0.002084 | 0.410341 |
| C | 0.181414 | -1.677088 | -0.456084 |
| O | 1.190135 | -0.683580 | -0.544219 |
| C | 0.435479 | -2.780170 | -1.470488 |
| C | -2.084195 | 1.365457 | -0.043993 |
| C | -3.512315 | 1.705275 | 0.170786 |
| C | -4.531098 | 0.755421 | 0.770102 |
| C | -3.932560 | -0.526153 | 1.376503 |
| O | -3.009384 | -2.739203 | -0.763791 |
| Si | 2.429004 | -0.496845 | 0.576624 |
| C | 3.308113 | -2.135602 | 0.807583 |
| C | 3.564222 | 0.821791 | -0.165186 |
| C | 1.711636 | 0.051769 | 2.219819 |
| C | 4.709645 | 1.111523 | 0.819493 |
| C | 4.150305 | 0.315224 | -1.492720 |
| C | 2.775076 | 2.115046 | -0.422938 |
| H | -1.194419 | -0.563036 | -1.694909 |
| H | -0.932990 | 0.104526 | 1.257713 |
| H | 0.167842 | -2.115317 | 0.553615 |
| H | 1.392838 | -3.265895 | -1.269527 |
| H | -0.355985 | -3.532433 | -1.425851 |
| H | 0.463225 | -2.359433 | -2.479307 |
| H | -5.235133 | 0.499401 | -0.026623 |
| H | -5.097226 | 1.284335 | 1.539454 |
| H | -4.640780 | -1.353121 | 1.326886 |
| H | -3.678558 | -0.364575 | 2.427489 |
| H | 4.110834 | -2.043846 | 1.545604 |
| H | 2.613562 | -2.899567 | 1.171247 |
| H | 3.744541 | -2.494078 | -0.128649 |
| H | 2.499465 | 0.124514 | 2.975724 |
| H | 1.227455 | 1.029358 | 2.144253 |
| H | 0.973471 | -0.668551 | 2.586505 |
| H | 5.390971 | 1.859179 | 0.394571 |
| H | 4.337969 | 1.508796 | 1.769490 |

| | | | |
|---|-----------|-----------|-----------|
| H | 5.300285 | 0.215220 | 1.035596 |
| H | 4.802630 | 1.080451 | -1.932078 |
| H | 4.751948 | -0.588328 | -1.352783 |
| H | 3.364070 | 0.088234 | -2.218747 |
| H | 3.435333 | 2.877441 | -0.855674 |
| H | 1.947731 | 1.950911 | -1.118559 |
| H | 2.358005 | 2.529634 | 0.500772 |
| C | -1.031167 | 2.412399 | -0.098635 |
| H | -3.747106 | 2.763856 | 0.252002 |
| O | -3.010090 | 1.343274 | -1.121020 |
| C | -0.912664 | 3.295024 | -1.082689 |
| H | -0.323292 | 2.408295 | 0.725920 |
| H | -0.118646 | 4.032510 | -1.078773 |
| H | -1.606377 | 3.298685 | -1.916810 |

Conf. 3b

| | | | |
|----|-----------|-----------|-----------|
| C | 1.130325 | 1.013095 | -0.689779 |
| C | 2.426423 | 1.782328 | -0.403970 |
| N | 2.793014 | 0.921188 | 0.582613 |
| C | 1.654124 | 0.019043 | 0.374666 |
| C | -0.199618 | 1.692064 | -0.411310 |
| O | -1.207192 | 0.698966 | -0.512286 |
| C | -0.477722 | 2.824966 | -1.385835 |
| C | 2.089003 | -1.349941 | -0.095388 |
| C | 3.398519 | -1.801391 | 0.398114 |
| C | 4.199221 | -0.937887 | 1.344907 |
| C | 4.128388 | 0.560056 | 1.032741 |
| O | 2.988597 | 2.749043 | -0.873453 |
| Si | -2.426148 | 0.464651 | 0.620207 |
| C | -3.311444 | 2.087711 | 0.925805 |
| C | -3.565235 | -0.831687 | -0.155048 |
| C | -1.676025 | -0.139607 | 2.228754 |
| C | -4.705276 | -1.153812 | 0.825780 |
| C | -4.158920 | -0.285342 | -1.463311 |
| C | -2.776826 | -2.115525 | -0.458515 |
| H | 1.134742 | 0.590440 | -1.698786 |
| H | 1.014637 | -0.084808 | 1.255905 |
| H | -0.167286 | 2.098807 | 0.611069 |
| H | -1.433894 | 3.297715 | -1.151131 |
| H | 0.309906 | 3.580604 | -1.333240 |
| H | -0.523057 | 2.436052 | -2.406756 |
| H | 5.246500 | -1.247369 | 1.337352 |
| H | 3.818784 | -1.135068 | 2.352422 |
| H | 4.828749 | 0.815019 | 0.232961 |
| H | 4.407358 | 1.136431 | 1.917661 |
| H | -4.098220 | 1.964540 | 1.676270 |
| H | -2.614607 | 2.843838 | 1.301228 |
| H | -3.769298 | 2.474838 | 0.011450 |

| | | | |
|---|-----------|-----------|-----------|
| H | -2.450974 | -0.256158 | 2.992552 |
| H | -1.174961 | -1.104282 | 2.108731 |
| H | -0.945194 | 0.579124 | 2.612887 |
| H | -5.384658 | -1.892692 | 0.382891 |
| H | -4.328574 | -1.575188 | 1.763345 |
| H | -5.299098 | -0.266450 | 1.068347 |
| H | -4.815673 | -1.036107 | -1.920610 |
| H | -4.757631 | 0.614909 | -1.292989 |
| H | -3.376780 | -0.038725 | -2.187263 |
| H | -3.439195 | -2.865141 | -0.909637 |
| H | -1.957090 | -1.927288 | -1.157321 |
| H | -2.353620 | -2.558437 | 0.449210 |
| C | 0.992697 | -2.295142 | -0.419405 |
| H | 3.556286 | -2.873403 | 0.485793 |
| O | 3.230834 | -1.351339 | -0.951738 |
| C | 0.982405 | -3.094058 | -1.479003 |
| H | 0.155590 | -2.286459 | 0.273366 |
| H | 0.148945 | -3.761291 | -1.666117 |
| H | 1.805131 | -3.099471 | -2.186173 |

Conf. 3c

| | | | |
|----|-----------|-----------|-----------|
| C | -1.132386 | -1.056667 | -0.578611 |
| C | -2.363578 | -1.828319 | -0.073648 |
| N | -2.637983 | -0.874087 | 0.855742 |
| C | -1.587980 | 0.039937 | 0.417566 |
| C | 0.230385 | -1.675567 | -0.317164 |
| O | 1.185428 | -0.651027 | -0.519067 |
| C | 0.487754 | -2.873228 | -1.219773 |
| C | -2.154627 | 1.312149 | -0.174930 |
| C | -3.590302 | 1.600987 | 0.061686 |
| C | -4.526675 | 0.688763 | 0.829077 |
| C | -3.828276 | -0.468563 | 1.563869 |
| O | -2.918559 | -2.868089 | -0.358685 |
| Si | 2.770319 | -0.625222 | 0.044027 |
| C | 3.915764 | -1.273033 | -1.287994 |
| C | 3.129098 | 1.194861 | 0.429914 |
| C | 2.894543 | -1.690843 | 1.580033 |
| C | 4.621118 | 1.376243 | 0.753640 |
| C | 2.762979 | 2.066930 | -0.781923 |
| C | 2.292041 | 1.633368 | 1.641806 |
| H | -1.230184 | -0.761582 | -1.626201 |
| H | -0.864726 | 0.275657 | 1.203253 |
| H | 0.262472 | -2.002907 | 0.732386 |
| H | 1.447444 | -3.338103 | -0.980988 |
| H | -0.297376 | -3.622671 | -1.091898 |
| H | 0.505392 | -2.558331 | -2.266808 |
| H | -5.249200 | 0.294619 | 0.108709 |
| H | -5.088041 | 1.285782 | 1.550517 |

| | | | |
|---|-----------|-----------|-----------|
| H | -4.489185 | -1.329948 | 1.660013 |
| H | -3.533645 | -0.157260 | 2.569539 |
| H | 4.956783 | -1.244825 | -0.951723 |
| H | 3.673082 | -2.310112 | -1.537323 |
| H | 3.838739 | -0.678290 | -2.202695 |
| H | 3.891945 | -1.601435 | 2.021427 |
| H | 2.164969 | -1.390296 | 2.337405 |
| H | 2.729393 | -2.747484 | 1.349107 |
| H | 4.824292 | 2.423102 | 1.011880 |
| H | 4.934979 | 0.761765 | 1.604272 |
| H | 5.256233 | 1.119630 | -0.099970 |
| H | 2.974220 | 3.121833 | -0.564127 |
| H | 3.341991 | 1.792585 | -1.670029 |
| H | 1.701880 | 1.981938 | -1.030085 |
| H | 2.430592 | 2.705141 | 1.831471 |
| H | 1.224812 | 1.459486 | 1.475702 |
| H | 2.580756 | 1.096390 | 2.550645 |
| C | -1.175457 | 2.405898 | -0.406083 |
| H | -3.882693 | 2.647321 | 0.015828 |
| O | -3.120436 | 1.100933 | -1.195666 |
| C | -1.127325 | 3.135908 | -1.513606 |
| H | -0.464236 | 2.576998 | 0.397487 |
| H | -0.386839 | 3.918069 | -1.634293 |
| H | -1.826360 | 2.967156 | -2.325893 |

Conf. 3d

| | | | |
|----|-----------|-----------|-----------|
| C | -1.138902 | -1.118889 | -0.586203 |
| C | -2.449180 | -1.818376 | -0.183020 |
| N | -2.777055 | -0.813138 | 0.671094 |
| C | -1.631820 | 0.025481 | 0.337010 |
| C | 0.181296 | -1.770202 | -0.210125 |
| O | 1.203123 | -0.821800 | -0.475603 |
| C | 0.438586 | -3.048021 | -0.990996 |
| C | -2.047539 | 1.322587 | -0.318754 |
| C | -3.469163 | 1.708281 | -0.250189 |
| C | -4.540598 | 0.872350 | 0.424306 |
| C | -4.007230 | -0.318453 | 1.240547 |
| O | -3.018886 | -2.844817 | -0.487170 |
| Si | 2.398128 | -0.372219 | 0.617124 |
| C | 3.247018 | -1.907937 | 1.273611 |
| C | 3.579142 | 0.719862 | -0.380939 |
| C | 1.628278 | 0.573926 | 2.040066 |
| C | 4.645712 | 1.303409 | 0.561128 |
| C | 4.268380 | -0.112899 | -1.473574 |
| C | 2.802542 | 1.869872 | -1.041136 |
| H | -1.139137 | -0.849278 | -1.645425 |
| H | -0.989666 | 0.234941 | 1.195738 |
| H | 0.152954 | -2.007736 | 0.864236 |

| | | | |
|---|-----------|-----------|-----------|
| H | 1.390255 | -3.488567 | -0.685785 |
| H | -0.357559 | -3.775398 | -0.813669 |
| H | 0.482608 | -2.831190 | -2.061787 |
| H | -5.210410 | 0.516595 | -0.363470 |
| H | -5.131861 | 1.516876 | 1.077971 |
| H | -4.732168 | -1.131816 | 1.270213 |
| H | -3.804062 | -0.012690 | 2.270399 |
| H | 4.036802 | -1.639870 | 1.982084 |
| H | 2.535540 | -2.550495 | 1.801730 |
| H | 3.696953 | -2.492138 | 0.466277 |
| H | 2.397352 | 0.885937 | 2.753346 |
| H | 1.106311 | 1.468547 | 1.687592 |
| H | 0.912393 | -0.049293 | 2.585365 |
| H | 5.354687 | 1.915280 | -0.010243 |
| H | 4.203256 | 1.944972 | 1.329551 |
| H | 5.220647 | 0.519394 | 1.065080 |
| H | 4.928197 | 0.526174 | -2.073939 |
| H | 4.882593 | -0.912547 | -1.048181 |
| H | 3.540265 | -0.569456 | -2.150865 |
| H | 3.492227 | 2.524378 | -1.588978 |
| H | 2.064709 | 1.491653 | -1.754344 |
| H | 2.276842 | 2.486385 | -0.304567 |
| C | -0.956324 | 2.320890 | -0.484951 |
| H | -3.697605 | 2.766642 | -0.345077 |
| O | -2.907720 | 1.149839 | -1.447893 |
| C | -0.894830 | 3.476621 | 0.163699 |
| H | -0.158904 | 2.022548 | -1.161411 |
| H | -0.060440 | 4.155299 | 0.024527 |
| H | -1.671538 | 3.781101 | 0.858689 |

Conf. 3e

| | | | |
|----|-----------|-----------|-----------|
| C | 1.141335 | 1.124947 | -0.610587 |
| C | 2.456027 | 1.835635 | -0.265085 |
| N | 2.846174 | 0.839683 | 0.574320 |
| C | 1.685017 | -0.011671 | 0.289388 |
| C | -0.175240 | 1.761474 | -0.199361 |
| O | -1.195245 | 0.808242 | -0.449188 |
| C | -0.461074 | 3.043841 | -0.962920 |
| C | 2.078666 | -1.313893 | -0.367320 |
| C | 3.393854 | -1.839687 | -0.003948 |
| C | 4.244390 | -1.124597 | 1.022249 |
| C | 4.189430 | 0.403260 | 0.920992 |
| O | 3.013945 | 2.854683 | -0.613873 |
| Si | -2.373237 | 0.350593 | 0.658072 |
| C | -3.184851 | 1.881651 | 1.371041 |
| C | -3.596956 | -0.690754 | -0.342742 |
| C | -1.581861 | -0.644730 | 2.034449 |
| C | -4.772509 | -1.100360 | 0.560715 |

| | | | |
|---|-----------|-----------|-----------|
| C | -4.131213 | 0.130889 | -1.526610 |
| C | -2.904464 | -1.954287 | -0.876608 |
| H | 1.111980 | 0.853716 | -1.670022 |
| H | 1.075529 | -0.224055 | 1.171624 |
| H | -0.121979 | 1.989421 | 0.876085 |
| H | -1.408052 | 3.474269 | -0.629754 |
| H | 0.333556 | 3.776245 | -0.800392 |
| H | -0.531428 | 2.835066 | -2.033911 |
| H | 5.285118 | -1.442205 | 0.931510 |
| H | 3.897600 | -1.454258 | 2.007089 |
| H | 4.865712 | 0.754727 | 0.137115 |
| H | 4.510438 | 0.850284 | 1.864501 |
| H | -3.926727 | 1.607061 | 2.126982 |
| H | -2.445309 | 2.527595 | 1.854510 |
| H | -3.688939 | 2.465445 | 0.595775 |
| H | -2.340898 | -1.016110 | 2.730128 |
| H | -1.035807 | -1.503268 | 1.632710 |
| H | -0.883074 | -0.030775 | 2.611456 |
| H | -5.486472 | -1.709242 | -0.007636 |
| H | -4.441520 | -1.696465 | 1.417340 |
| H | -5.314135 | -0.229624 | 0.943899 |
| H | -4.838142 | -0.469969 | -2.112759 |
| H | -4.660563 | 1.028790 | -1.192212 |
| H | -3.323408 | 0.444290 | -2.194018 |
| H | -3.614510 | -2.556622 | -1.457413 |
| H | -2.066002 | -1.703730 | -1.532506 |
| H | -2.522068 | -2.583142 | -0.066662 |
| C | 0.947931 | -2.175684 | -0.802206 |
| H | 3.552260 | -2.912485 | -0.076268 |
| O | 3.188854 | -1.199984 | -1.273589 |
| C | 0.653009 | -3.345611 | -0.249925 |
| H | 0.322237 | -1.763312 | -1.590027 |
| H | -0.204934 | -3.920826 | -0.579857 |
| H | 1.252259 | -3.762961 | 0.553539 |

Conf. 3f

| | | | |
|---|-----------|-----------|-----------|
| C | 1.032794 | 1.037611 | -0.642449 |
| C | 2.096995 | 1.887982 | 0.071734 |
| N | 2.347120 | 0.901639 | 0.975255 |
| C | 1.478063 | -0.081255 | 0.334201 |
| C | -0.408773 | 1.513308 | -0.554453 |
| O | -1.227028 | 0.424679 | -0.948652 |
| C | -0.628880 | 2.729247 | -1.443581 |
| C | 2.265521 | -1.225762 | -0.270551 |
| C | 3.693526 | -1.359283 | 0.109775 |
| C | 4.415205 | -0.407391 | 1.043356 |
| C | 3.488105 | 0.563075 | 1.792615 |
| O | 2.572251 | 2.993530 | -0.074258 |

| | | | |
|----|-----------|-----------|-----------|
| Si | -2.813479 | 0.091358 | -0.500680 |
| C | -3.389998 | -1.131811 | -1.788807 |
| C | -2.875754 | -0.684085 | 1.236279 |
| C | -3.849599 | 1.652628 | -0.540230 |
| C | -4.345135 | -0.948081 | 1.611469 |
| C | -2.112827 | -2.016990 | 1.245440 |
| C | -2.259572 | 0.253649 | 2.287489 |
| H | 1.301109 | 0.831394 | -1.681489 |
| H | 0.697515 | -0.462897 | 0.997162 |
| H | -0.623432 | 1.787071 | 0.487624 |
| H | -1.643880 | 3.113810 | -1.335560 |
| H | 0.072510 | 3.522685 | -1.173236 |
| H | -0.464838 | 2.461108 | -2.490879 |
| H | 5.132894 | 0.153615 | 0.438080 |
| H | 4.989768 | -0.988426 | 1.767325 |
| H | 4.011008 | 1.480414 | 2.062890 |
| H | 3.117241 | 0.103270 | 2.712261 |
| H | -4.389439 | -1.511239 | -1.557276 |
| H | -3.428795 | -0.657695 | -2.773514 |
| H | -2.708401 | -1.984785 | -1.848990 |
| H | -4.893512 | 1.418887 | -0.311160 |
| H | -3.506267 | 2.393648 | 0.187625 |
| H | -3.821529 | 2.110456 | -1.532865 |
| H | -4.397254 | -1.442318 | 2.589632 |
| H | -4.920869 | -0.020291 | 1.682661 |
| H | -4.844007 | -1.601406 | 0.888453 |
| H | -2.141950 | -2.465033 | 2.246553 |
| H | -2.544028 | -2.740152 | 0.546575 |
| H | -1.062501 | -1.878586 | 0.975822 |
| H | -2.373828 | -0.179971 | 3.289050 |
| H | -1.188918 | 0.406973 | 2.122847 |
| H | -2.742666 | 1.235864 | 2.297829 |
| C | 1.470591 | -2.411306 | -0.685705 |
| H | 4.122810 | -2.354485 | 0.023629 |
| O | 3.298275 | -0.814660 | -1.154945 |
| C | 1.597363 | -3.012312 | -1.862319 |
| H | 0.752271 | -2.773809 | 0.044489 |
| H | 0.994422 | -3.876252 | -2.116671 |
| H | 2.309692 | -2.656076 | -2.598848 |

Conf. 4a

| | | | |
|---|----------|-----------|-----------|
| C | 2.083937 | 0.500314 | -0.553014 |
| H | 1.547936 | 0.332425 | -1.493688 |
| C | 4.151455 | -0.340898 | -1.199642 |
| C | 4.178900 | -1.394836 | -0.092722 |
| C | 2.756908 | -1.811955 | 0.301435 |
| N | 1.956313 | -0.609355 | 0.380616 |
| C | 1.429384 | 0.141264 | 1.383263 |

| | | | |
|----|-----------|-----------|-----------|
| C | 1.393088 | 1.397519 | 0.496447 |
| O | 1.120561 | -0.126077 | 2.524343 |
| O | 3.425759 | 0.823683 | -0.794151 |
| H | 3.698300 | -0.751266 | -2.113516 |
| H | 5.158566 | -0.001768 | -1.438938 |
| H | 4.744214 | -2.264514 | -0.435662 |
| H | 4.693277 | -0.978115 | 0.777830 |
| H | 2.325007 | -2.478541 | -0.452158 |
| H | 2.728638 | -2.322077 | 1.264793 |
| H | 2.057932 | 2.180391 | 0.866762 |
| C | 0.016639 | 1.950181 | 0.153054 |
| O | -0.761941 | 0.894003 | -0.375044 |
| C | 0.095824 | 3.090911 | -0.850989 |
| Si | -2.287916 | 0.402039 | 0.122184 |
| C | -2.413199 | -1.392072 | -0.469023 |
| C | -2.409489 | 0.530966 | 1.986068 |
| C | -3.583333 | 1.490125 | -0.680458 |
| H | -0.426348 | 2.323102 | 1.086310 |
| H | -0.906882 | 3.458512 | -1.079521 |
| H | 0.686929 | 3.918403 | -0.450434 |
| H | 0.558197 | 2.748762 | -1.781048 |
| H | -3.316592 | 0.033127 | 2.342635 |
| H | -1.546253 | 0.063702 | 2.467872 |
| H | -2.458315 | 1.574372 | 2.311597 |
| H | -4.590539 | 1.198244 | -0.367442 |
| H | -3.434694 | 2.535003 | -0.390382 |
| H | -3.535094 | 1.431472 | -1.771487 |
| C | -1.386704 | -2.253133 | 0.284683 |
| H | -0.367470 | -1.889367 | 0.125358 |
| H | -1.577049 | -2.260798 | 1.362691 |
| H | -1.435117 | -3.291743 | -0.066931 |
| C | -2.122627 | -1.466951 | -1.976478 |
| H | -2.193863 | -2.506297 | -2.322004 |
| H | -2.837740 | -0.877304 | -2.559404 |
| H | -1.116973 | -1.104307 | -2.207821 |
| C | -3.827884 | -1.929676 | -0.198191 |
| H | -4.590371 | -1.363443 | -0.742607 |
| H | -3.900617 | -2.975479 | -0.522242 |
| H | -4.080886 | -1.898983 | 0.866772 |

Conf. 4b

| | | | |
|---|-----------|-----------|-----------|
| C | -2.213505 | 0.686050 | 0.222044 |
| H | -1.805489 | 1.065191 | 1.164705 |
| C | -4.423182 | 0.407264 | 0.894871 |
| C | -4.442857 | -1.082048 | 0.553908 |
| C | -3.041035 | -1.689854 | 0.682260 |
| N | -2.101143 | -0.761452 | 0.089447 |
| C | -1.416205 | -0.713793 | -1.084263 |

| | | | |
|----|-----------|-----------|-----------|
| C | -1.328030 | 0.819705 | -1.035361 |
| O | -1.054001 | -1.579987 | -1.850158 |
| O | -3.531739 | 1.124147 | 0.035891 |
| H | -4.123414 | 0.561822 | 1.941406 |
| H | -5.406397 | 0.853359 | 0.750513 |
| H | -5.137766 | -1.597790 | 1.220737 |
| H | -4.803844 | -1.203465 | -0.471339 |
| H | -2.779001 | -1.838382 | 1.734340 |
| H | -2.960162 | -2.649768 | 0.171169 |
| H | -1.868435 | 1.279168 | -1.865331 |
| C | 0.047157 | 1.449317 | -0.864172 |
| O | 0.645928 | 0.895861 | 0.293518 |
| C | -0.054876 | 2.963928 | -0.736976 |
| Si | 2.269482 | 0.545988 | 0.552931 |
| C | 2.659304 | -1.194967 | -0.094983 |
| C | 3.337024 | 1.823006 | -0.309015 |
| C | 2.478770 | 0.634169 | 2.406519 |
| H | 0.637120 | 1.201791 | -1.756951 |
| H | 0.936989 | 3.402769 | -0.614649 |
| H | -0.515099 | 3.394943 | -1.629719 |
| H | -0.661088 | 3.230997 | 0.133176 |
| H | 4.394213 | 1.551699 | -0.232796 |
| H | 3.092595 | 1.909508 | -1.371861 |
| H | 3.211480 | 2.807831 | 0.149742 |
| H | 3.510927 | 0.415611 | 2.695667 |
| H | 2.231764 | 1.636065 | 2.768960 |
| H | 1.826421 | -0.081673 | 2.914252 |
| C | 2.488562 | -1.243009 | -1.622123 |
| H | 1.456916 | -1.037614 | -1.921253 |
| H | 3.146286 | -0.528844 | -2.128358 |
| H | 2.741081 | -2.243841 | -1.996073 |
| C | 1.709330 | -2.214758 | 0.553727 |
| H | 1.916130 | -3.220805 | 0.166589 |
| H | 1.834079 | -2.249433 | 1.640896 |
| H | 0.662276 | -1.984772 | 0.338835 |
| C | 4.110208 | -1.562038 | 0.259965 |
| H | 4.279733 | -1.562408 | 1.341456 |
| H | 4.341915 | -2.569274 | -0.108932 |
| H | 4.830546 | -0.874357 | -0.194762 |

Conf. 4c

| | | | |
|---|----------|-----------|-----------|
| C | 2.248325 | 0.732836 | -0.299052 |
| H | 1.747976 | 0.940762 | -1.250797 |
| C | 4.449255 | 0.805352 | -1.049471 |
| C | 4.758349 | -0.616580 | -0.583490 |
| C | 3.492302 | -1.481321 | -0.594451 |
| N | 2.413039 | -0.691704 | -0.038597 |
| C | 1.763965 | -0.664084 | 1.156436 |

| | | | |
|----|-----------|-----------|-----------|
| C | 1.391352 | 0.817794 | 0.981964 |
| O | 1.590813 | -1.509647 | 2.006655 |
| O | 3.465518 | 1.422095 | -0.213966 |
| H | 4.094148 | 0.804016 | -2.090073 |
| H | 5.335082 | 1.436526 | -0.990438 |
| H | 5.517527 | -1.055072 | -1.235378 |
| H | 5.165909 | -0.573788 | 0.430526 |
| H | 3.231311 | -1.771026 | -1.617019 |
| H | 3.608891 | -2.388995 | -0.001464 |
| H | 1.861403 | 1.442716 | 1.744039 |
| C | -0.082326 | 1.169490 | 0.816561 |
| O | -0.618975 | 0.395356 | -0.239185 |
| C | -0.256698 | 2.650584 | 0.510634 |
| Si | -1.897641 | -0.694283 | -0.198012 |
| C | -3.549099 | 0.242035 | -0.277299 |
| C | -1.642453 | -1.745703 | -1.719699 |
| C | -1.810782 | -1.728171 | 1.359366 |
| H | -0.588253 | 0.933082 | 1.762326 |
| H | -1.313965 | 2.894319 | 0.391785 |
| H | 0.150665 | 3.262003 | 1.319630 |
| H | 0.260088 | 2.909363 | -0.417628 |
| H | -2.397070 | -2.535023 | -1.782666 |
| H | -1.700916 | -1.147325 | -2.633180 |
| H | -0.657702 | -2.220749 | -1.686272 |
| H | -2.642531 | -2.439147 | 1.384905 |
| H | -0.874779 | -2.290849 | 1.396950 |
| H | -1.869820 | -1.116717 | 2.264133 |
| C | -3.523874 | 1.249623 | -1.437155 |
| H | -2.728392 | 1.989795 | -1.312770 |
| H | -3.371352 | 0.754210 | -2.401514 |
| H | -4.478388 | 1.788532 | -1.491032 |
| C | -3.803999 | 0.989583 | 1.041936 |
| H | -4.744052 | 1.552491 | 0.981191 |
| H | -3.886866 | 0.300910 | 1.888173 |
| H | -3.010082 | 1.707207 | 1.271757 |
| C | -4.691988 | -0.761702 | -0.507821 |
| H | -4.747143 | -1.510921 | 0.288853 |
| H | -5.654904 | -0.235851 | -0.530002 |
| H | -4.583901 | -1.289424 | -1.460485 |

Conf. 4d

| | | | |
|---|----------|-----------|-----------|
| C | 1.820849 | -0.479450 | 0.034648 |
| H | 1.185478 | -0.850034 | 0.847307 |
| C | 3.125998 | -2.381412 | -0.262184 |
| C | 4.437898 | -1.640964 | -0.007626 |
| C | 4.218007 | -0.446829 | 0.928593 |
| N | 3.006386 | 0.226975 | 0.507613 |
| C | 2.738150 | 1.368636 | -0.184397 |

| | | | |
|----|-----------|-----------|-----------|
| C | 1.381397 | 0.820499 | -0.665031 |
| O | 3.365618 | 2.393773 | -0.332772 |
| O | 2.147804 | -1.515715 | -0.846525 |
| H | 2.728194 | -2.800733 | 0.673110 |
| H | 3.268802 | -3.196714 | -0.970156 |
| H | 5.164870 | -2.329926 | 0.428563 |
| H | 4.835154 | -1.290085 | -0.964277 |
| H | 4.096868 | -0.783344 | 1.962735 |
| H | 5.046704 | 0.261038 | 0.894364 |
| H | 1.338732 | 0.705997 | -1.750726 |
| C | 0.121453 | 1.494704 | -0.144850 |
| O | -0.970499 | 0.653548 | -0.473814 |
| C | -0.071313 | 2.877012 | -0.747658 |
| Si | -2.189822 | 0.212064 | 0.596027 |
| C | -3.363304 | -0.853330 | -0.435894 |
| C | -1.451698 | -0.754375 | 2.022151 |
| C | -3.024705 | 1.752219 | 1.257976 |
| H | 0.210269 | 1.591586 | 0.948033 |
| H | -0.974989 | 3.340636 | -0.346440 |
| H | 0.783554 | 3.518355 | -0.519190 |
| H | -0.171236 | 2.800467 | -1.833791 |
| H | -2.226936 | -1.008153 | 2.751667 |
| H | -0.989752 | -1.685619 | 1.682527 |
| H | -0.690780 | -0.166998 | 2.545617 |
| H | -3.832555 | 1.490261 | 1.948037 |
| H | -2.309958 | 2.373015 | 1.807611 |
| H | -3.447269 | 2.357001 | 0.451009 |
| C | -2.600382 | -2.053234 | -1.020177 |
| H | -1.777411 | -1.730678 | -1.664292 |
| H | -2.184222 | -2.692278 | -0.234864 |
| H | -3.277650 | -2.671487 | -1.622914 |
| C | -3.954053 | -0.020501 | -1.584799 |
| H | -4.623443 | -0.641329 | -2.193666 |
| H | -4.539203 | 0.826613 | -1.213112 |
| H | -3.171596 | 0.371162 | -2.241408 |
| C | -4.504798 | -1.364827 | 0.459080 |
| H | -5.084590 | -0.543081 | 0.891988 |
| H | -5.196235 | -1.979976 | -0.130145 |
| H | -4.132365 | -1.985150 | 1.280646 |

Conf. 4e

| | | | |
|---|----------|-----------|-----------|
| C | 1.979460 | -0.459610 | -0.032129 |
| H | 1.351596 | -1.032897 | 0.658317 |
| C | 3.693188 | -2.011944 | -0.284156 |
| C | 4.772043 | -1.046286 | 0.203271 |
| C | 4.186973 | -0.023842 | 1.184676 |
| N | 2.917368 | 0.424665 | 0.649884 |
| C | 2.489094 | 1.551112 | 0.017034 |

| | | | |
|----|-----------|-----------|-----------|
| C | 1.353785 | 0.785148 | -0.690112 |
| O | 2.889440 | 2.693875 | 0.035752 |
| O | 2.626566 | -1.312425 | -0.933030 |
| H | 3.287717 | -2.597245 | 0.553602 |
| H | 4.093909 | -2.703932 | -1.023658 |
| H | 5.573726 | -1.611033 | 0.684725 |
| H | 5.195446 | -0.526407 | -0.660734 |
| H | 4.018366 | -0.480866 | 2.164523 |
| H | 4.839908 | 0.839233 | 1.317825 |
| H | 1.478517 | 0.775158 | -1.775518 |
| C | -0.080319 | 1.141551 | -0.323992 |
| O | -0.930553 | 0.175490 | -0.917448 |
| C | -0.438691 | 2.534087 | -0.818713 |
| Si | -2.053803 | -0.819596 | -0.158044 |
| C | -3.568470 | 0.180279 | 0.407032 |
| C | -2.518553 | -2.062911 | -1.469863 |
| C | -1.264877 | -1.669479 | 1.315429 |
| H | -0.177510 | 1.111680 | 0.771071 |
| H | -1.458166 | 2.794841 | -0.529364 |
| H | 0.243620 | 3.276882 | -0.398683 |
| H | -0.368315 | 2.571511 | -1.909169 |
| H | -3.206180 | -2.813219 | -1.069010 |
| H | -3.002274 | -1.581865 | -2.324351 |
| H | -1.626270 | -2.581980 | -1.831077 |
| H | -2.019883 | -2.228646 | 1.876493 |
| H | -0.501189 | -2.381409 | 0.989513 |
| H | -0.801718 | -0.959654 | 2.007043 |
| C | -4.123987 | 1.004957 | -0.764718 |
| H | -3.385474 | 1.711794 | -1.152749 |
| H | -4.441793 | 0.365686 | -1.594563 |
| H | -4.999382 | 1.581031 | -0.439119 |
| C | -3.197524 | 1.120878 | 1.565587 |
| H | -4.081648 | 1.683646 | 1.890821 |
| H | -2.822321 | 0.568513 | 2.432757 |
| H | -2.436134 | 1.852464 | 1.279120 |
| C | -4.658899 | -0.792020 | 0.891552 |
| H | -4.320143 | -1.403963 | 1.733680 |
| H | -5.537656 | -0.228661 | 1.229707 |
| H | -4.988046 | -1.466014 | 0.094648 |

Conf. 4f

| | | | |
|---|----------|-----------|-----------|
| C | 1.698993 | -0.392504 | -0.187368 |
| H | 0.980711 | -1.001858 | 0.372202 |
| C | 3.123186 | -2.105794 | -0.848796 |
| C | 4.347963 | -1.473738 | -0.189489 |
| C | 3.941032 | -0.624858 | 1.020789 |
| N | 2.767765 | 0.139524 | 0.648767 |
| C | 2.534043 | 1.438654 | 0.315523 |

| | | | |
|----|-----------|-----------|-----------|
| C | 1.292243 | 1.056495 | -0.513795 |
| O | 3.116680 | 2.463902 | 0.590568 |
| O | 2.195571 | -1.105894 | -1.282789 |
| H | 2.618265 | -2.793104 | -0.154820 |
| H | 3.404314 | -2.664143 | -1.740659 |
| H | 5.039267 | -2.260573 | 0.120909 |
| H | 4.858044 | -0.845274 | -0.924961 |
| H | 3.694033 | -1.262559 | 1.875017 |
| H | 4.730170 | 0.063407 | 1.324927 |
| H | 1.421822 | 1.282611 | -1.574916 |
| C | -0.065155 | 1.541017 | -0.028355 |
| O | -1.045973 | 0.858394 | -0.790762 |
| C | -0.201787 | 3.047862 | -0.191103 |
| Si | -2.573382 | 0.359778 | -0.291000 |
| C | -2.456139 | -1.347236 | 0.536786 |
| C | -3.295466 | 1.611677 | 0.901953 |
| C | -3.575056 | 0.267507 | -1.863624 |
| H | -0.167037 | 1.285364 | 1.036279 |
| H | -1.171748 | 3.385465 | 0.178158 |
| H | 0.582658 | 3.565353 | 0.366514 |
| H | -0.116618 | 3.318156 | -1.247165 |
| H | -4.244886 | 1.248420 | 1.306715 |
| H | -2.627688 | 1.805232 | 1.746621 |
| H | -3.489608 | 2.562171 | 0.397155 |
| H | -4.603559 | -0.041440 | -1.655578 |
| H | -3.608354 | 1.246707 | -2.349496 |
| H | -3.142782 | -0.447637 | -2.568926 |
| C | -1.697348 | -1.250235 | 1.870498 |
| H | -0.675251 | -0.881756 | 1.742738 |
| H | -2.203331 | -0.585272 | 2.577278 |
| H | -1.629002 | -2.240113 | 2.339028 |
| C | -1.733945 | -2.331453 | -0.397454 |
| H | -1.635246 | -3.310771 | 0.087641 |
| H | -2.287754 | -2.480945 | -1.329719 |
| H | -0.730517 | -1.986417 | -0.661868 |
| C | -3.873853 | -1.876373 | 0.816433 |
| H | -4.453395 | -1.996979 | -0.103995 |
| H | -3.817337 | -2.859568 | 1.300360 |
| H | -4.434677 | -1.215384 | 1.485065 |

Conf. 5a

| | | | |
|---|----------|-----------|-----------|
| C | 2.932683 | -0.038820 | -1.573887 |
| C | 2.179748 | 1.260400 | -1.925266 |
| N | 2.021116 | 1.577425 | -0.609656 |
| C | 2.838696 | 0.472651 | -0.118258 |
| C | 1.838390 | 2.810141 | 0.131296 |
| C | 3.178606 | 3.165804 | 0.784564 |
| C | 3.832048 | 1.927308 | 1.395154 |

| | | | |
|---|-----------|-----------|-----------|
| O | 4.057149 | 0.918021 | 0.403979 |
| O | 1.832740 | 1.809619 | -2.945008 |
| C | 2.203746 | -1.336705 | -1.873085 |
| C | 2.892926 | -2.549597 | -1.276518 |
| O | 0.902754 | -1.125731 | -1.277682 |
| H | 2.311822 | -0.159308 | 0.603773 |
| C | -0.142873 | -1.887587 | -1.562455 |
| O | -0.124151 | -2.853490 | -2.282958 |
| C | -1.366954 | -1.391397 | -0.807555 |
| C | -1.443259 | -2.056694 | 0.593456 |
| C | -0.320608 | -1.675688 | 1.525711 |
| C | 0.776127 | -2.519121 | 1.704944 |
| C | 1.823734 | -2.161110 | 2.546824 |
| C | 1.791089 | -0.945948 | 3.222788 |
| C | 0.702859 | -0.095810 | 3.053392 |
| C | -0.344948 | -0.461164 | 2.215319 |
| N | -1.343330 | 0.060325 | -0.756192 |
| O | -3.530413 | 0.116871 | -0.379862 |
| C | -4.811620 | 0.678379 | 0.060410 |
| C | -5.257572 | 1.781859 | -0.892086 |
| C | -5.745262 | -0.522299 | -0.029531 |
| C | -4.695519 | 1.160543 | 1.502588 |
| C | -2.405666 | 0.835138 | -0.406950 |
| O | -2.308920 | 2.025752 | -0.170230 |
| H | 3.954317 | -0.059392 | -1.953963 |
| H | 1.491690 | 3.586269 | -0.551364 |
| H | 1.067056 | 2.651473 | 0.891186 |
| H | 3.026717 | 3.916156 | 1.563815 |
| H | 3.853163 | 3.588031 | 0.034386 |
| H | 3.205093 | 1.512654 | 2.196455 |
| H | 4.810346 | 2.165793 | 1.810158 |
| H | 2.066733 | -1.454112 | -2.950663 |
| H | 2.309570 | -3.452465 | -1.457153 |
| H | 3.872454 | -2.670523 | -1.743918 |
| H | 3.031957 | -2.424501 | -0.200695 |
| H | -2.237207 | -1.713286 | -1.377774 |
| H | -1.470302 | -3.140208 | 0.451543 |
| H | -2.404735 | -1.762002 | 1.020174 |
| H | 0.811856 | -3.467778 | 1.178113 |
| H | 2.666730 | -2.831435 | 2.672888 |
| H | 2.607989 | -0.663833 | 3.877497 |
| H | 0.666435 | 0.852665 | 3.577833 |
| H | -1.195871 | 0.203075 | 2.105516 |
| H | -0.442442 | 0.505992 | -0.654236 |
| H | -6.272620 | 2.090487 | -0.629893 |
| H | -4.600500 | 2.648259 | -0.829541 |
| H | -5.267497 | 1.413301 | -1.920945 |
| H | -6.751132 | -0.230675 | 0.280430 |

| | | | |
|---|-----------|-----------|-----------|
| H | -5.399205 | -1.326797 | 0.623672 |
| H | -5.792161 | -0.896835 | -1.054633 |
| H | -4.042833 | 2.029274 | 1.580622 |
| H | -5.688012 | 1.434418 | 1.868486 |
| H | -4.305425 | 0.361036 | 2.138130 |

Conf. 5b

| | | | |
|---|-----------|-----------|-----------|
| C | 1.422249 | -1.753645 | -0.212949 |
| C | 2.634454 | -2.428064 | -0.886614 |
| N | 3.466646 | -1.426756 | -0.491894 |
| C | 2.457284 | -0.739610 | 0.308264 |
| C | 4.887142 | -1.342334 | -0.217417 |
| C | 5.068503 | -1.375329 | 1.304131 |
| C | 4.048186 | -0.469495 | 1.990525 |
| O | 2.707206 | -0.864582 | 1.679731 |
| O | 2.819024 | -3.440709 | -1.522436 |
| C | 0.343826 | -1.237114 | -1.142852 |
| C | -0.557418 | -2.346724 | -1.650234 |
| O | -0.392846 | -0.274335 | -0.350408 |
| H | 2.319405 | 0.309824 | 0.029941 |
| C | -1.127662 | 0.627529 | -0.990890 |
| O | -1.302825 | 0.648060 | -2.184951 |
| C | -1.690383 | 1.677223 | -0.032937 |
| C | -0.974570 | 3.015739 | -0.274170 |
| C | 0.524796 | 2.936304 | -0.115810 |
| C | 1.106543 | 2.949355 | 1.153055 |
| C | 2.487715 | 2.907329 | 1.300416 |
| C | 3.308685 | 2.846945 | 0.177809 |
| C | 2.739353 | 2.815171 | -1.089959 |
| C | 1.355728 | 2.858173 | -1.233696 |
| N | -3.112304 | 1.863063 | -0.238414 |
| O | -3.483732 | -0.145580 | 0.610275 |
| C | -4.205195 | -1.389657 | 0.896470 |
| C | -4.565858 | -2.075718 | -0.415948 |
| C | -3.169056 | -2.199260 | 1.666048 |
| C | -5.424831 | -1.113329 | 1.768563 |
| C | -4.035989 | 0.877243 | -0.043746 |
| O | -5.191805 | 0.960401 | -0.411918 |
| H | 0.999965 | -2.357409 | 0.593111 |
| H | 5.393216 | -2.171934 | -0.711797 |
| H | 5.272395 | -0.406904 | -0.634029 |
| H | 6.077063 | -1.049091 | 1.568413 |
| H | 4.936711 | -2.398264 | 1.668014 |
| H | 4.196603 | 0.576268 | 1.691490 |
| H | 4.135315 | -0.533181 | 3.074348 |
| H | 0.790980 | -0.694155 | -1.980543 |
| H | -1.323032 | -1.951758 | -2.317424 |
| H | 0.045365 | -3.073255 | -2.199922 |

| | | | |
|---|-----------|-----------|-----------|
| H | -1.036721 | -2.861832 | -0.814475 |
| H | -1.510661 | 1.340952 | 0.988340 |
| H | -1.389410 | 3.739417 | 0.431977 |
| H | -1.217895 | 3.361166 | -1.283377 |
| H | 0.472309 | 3.007608 | 2.032206 |
| H | 2.923996 | 2.924990 | 2.292907 |
| H | 4.386706 | 2.819939 | 0.291176 |
| H | 3.370977 | 2.761406 | -1.969460 |
| H | 0.916535 | 2.843044 | -2.226078 |
| H | -3.409682 | 2.595131 | -0.864805 |
| H | -4.991800 | -3.059102 | -0.203068 |
| H | -5.297102 | -1.494675 | -0.977908 |
| H | -3.671356 | -2.214240 | -1.028484 |
| H | -3.574440 | -3.184504 | 1.906019 |
| H | -2.902854 | -1.695299 | 2.597986 |
| H | -2.263774 | -2.327923 | 1.069671 |
| H | -6.189324 | -0.562141 | 1.223137 |
| H | -5.845569 | -2.066125 | 2.099499 |
| H | -5.135505 | -0.542507 | 2.654594 |

Conf. 5c

| | | | |
|---|-----------|-----------|-----------|
| C | -1.425893 | -1.495782 | -0.713731 |
| C | -2.354404 | -2.724220 | -0.833336 |
| N | -3.078518 | -2.340063 | 0.252046 |
| C | -2.383803 | -1.068781 | 0.419057 |
| C | -4.444218 | -2.556443 | 0.687994 |
| C | -5.240072 | -1.279285 | 0.392598 |
| C | -4.438594 | -0.036926 | 0.776468 |
| O | -3.197074 | 0.012093 | 0.067708 |
| O | -2.443218 | -3.672070 | -1.579446 |
| C | 0.024564 | -1.782857 | -0.373441 |
| C | 0.764052 | -2.465931 | -1.505604 |
| O | 0.702447 | -0.523047 | -0.139066 |
| H | -1.957687 | -0.932870 | 1.418075 |
| C | 0.886109 | -0.106459 | 1.107682 |
| O | 0.444192 | -0.649790 | 2.092215 |
| C | 1.786995 | 1.125544 | 1.188367 |
| C | 3.161556 | 0.708779 | 1.758547 |
| C | 3.894843 | -0.291004 | 0.896287 |
| C | 3.659972 | -1.660245 | 1.042806 |
| C | 4.289608 | -2.582470 | 0.216106 |
| C | 5.167414 | -2.149375 | -0.773237 |
| C | 5.419673 | -0.790317 | -0.920328 |
| C | 4.790740 | 0.130398 | -0.087452 |
| N | 1.948092 | 1.826832 | -0.062648 |
| O | -0.116390 | 2.627879 | 0.107306 |
| C | -1.302890 | 3.408732 | -0.269925 |
| C | -1.966859 | 2.797987 | -1.498760 |

| | | | |
|---|-----------|-----------|-----------|
| C | -2.198392 | 3.255097 | 0.953206 |
| C | -0.913636 | 4.867877 | -0.477490 |
| C | 0.943823 | 2.505230 | -0.691282 |
| O | 1.048606 | 2.941035 | -1.822477 |
| H | -1.502177 | -0.836812 | -1.581716 |
| H | -4.848966 | -3.423423 | 0.165328 |
| H | -4.442252 | -2.772152 | 1.760477 |
| H | -6.181769 | -1.290013 | 0.945956 |
| H | -5.474268 | -1.230625 | -0.674507 |
| H | -4.241004 | -0.017590 | 1.857655 |
| H | -4.973162 | 0.873743 | 0.508881 |
| H | 0.086556 | -2.371685 | 0.544131 |
| H | 1.807282 | -2.626019 | -1.228072 |
| H | 0.300428 | -3.431178 | -1.717622 |
| H | 0.727478 | -1.855824 | -2.411376 |
| H | 1.316432 | 1.793947 | 1.909830 |
| H | 2.991826 | 0.294054 | 2.753720 |
| H | 3.753159 | 1.619258 | 1.875539 |
| H | 2.977663 | -2.007174 | 1.812666 |
| H | 4.095227 | -3.641437 | 0.345042 |
| H | 5.657782 | -2.868210 | -1.419749 |
| H | 6.111250 | -0.443841 | -1.680013 |
| H | 5.009937 | 1.188540 | -0.196686 |
| H | 2.669361 | 1.502876 | -0.689863 |
| H | -2.911322 | 3.317620 | -1.681373 |
| H | -1.337876 | 2.898244 | -2.382195 |
| H | -2.190186 | 1.744642 | -1.318757 |
| H | -3.130799 | 3.801954 | 0.794750 |
| H | -1.707117 | 3.656646 | 1.842737 |
| H | -2.436379 | 2.202147 | 1.115671 |
| H | -0.281895 | 4.990634 | -1.356739 |
| H | -1.820940 | 5.461306 | -0.614811 |
| H | -0.385631 | 5.249764 | 0.400132 |

Conf. 5d

| | | | |
|---|-----------|-----------|-----------|
| C | -1.037824 | -2.068797 | 0.010756 |
| C | -2.088350 | -3.142374 | 0.361633 |
| N | -3.090666 | -2.223136 | 0.369619 |
| C | -2.247671 | -1.117740 | -0.072696 |
| C | -4.520008 | -2.275498 | 0.136159 |
| C | -4.781801 | -1.711820 | -1.265021 |
| C | -3.957263 | -0.448651 | -1.503442 |
| O | -2.555476 | -0.709942 | -1.372304 |
| O | -2.074615 | -4.336310 | 0.555230 |
| C | 0.016330 | -1.777367 | 1.057738 |
| C | 1.015552 | -2.907535 | 1.209870 |
| O | 0.675162 | -0.574417 | 0.589817 |
| H | -2.257042 | -0.265970 | 0.617290 |

| | | | |
|---|-----------|-----------|-----------|
| C | 1.277378 | 0.206181 | 1.478617 |
| O | 1.330203 | -0.016302 | 2.664536 |
| C | 1.934718 | 1.428706 | 0.835673 |
| C | 3.470839 | 1.267791 | 0.839206 |
| C | 3.962305 | 0.125734 | -0.016359 |
| C | 4.074324 | -1.159996 | 0.515364 |
| C | 4.472307 | -2.227437 | -0.280049 |
| C | 4.769729 | -2.023614 | -1.623959 |
| C | 4.675639 | -0.745022 | -2.162434 |
| C | 4.277856 | 0.321513 | -1.362212 |
| N | 1.450743 | 1.721819 | -0.492541 |
| O | -0.327823 | 2.756465 | 0.352613 |
| C | -1.544944 | 3.576252 | 0.331767 |
| C | -2.728409 | 2.738754 | -0.136401 |
| C | -1.707737 | 3.963411 | 1.796263 |
| C | -1.330309 | 4.815603 | -0.530358 |
| C | 0.236699 | 2.284473 | -0.761158 |
| O | -0.228119 | 2.349099 | -1.883354 |
| H | -0.586420 | -2.240764 | -0.968770 |
| H | -4.856634 | -3.307713 | 0.235377 |
| H | -5.026168 | -1.674018 | 0.897142 |
| H | -5.842541 | -1.478913 | -1.382370 |
| H | -4.512889 | -2.457621 | -2.018283 |
| H | -4.248157 | 0.342130 | -0.798331 |
| H | -4.097940 | -0.072683 | -2.515779 |
| H | -0.452289 | -1.547364 | 2.018089 |
| H | 1.747118 | -2.673585 | 1.983662 |
| H | 0.487505 | -3.820505 | 1.493137 |
| H | 1.538205 | -3.082878 | 0.266795 |
| H | 1.690275 | 2.268322 | 1.485770 |
| H | 3.785007 | 1.125404 | 1.875076 |
| H | 3.893473 | 2.213035 | 0.492254 |
| H | 3.848434 | -1.325541 | 1.564148 |
| H | 4.550716 | -3.219584 | 0.150331 |
| H | 5.080298 | -2.855576 | -2.245756 |
| H | 4.915877 | -0.574697 | -3.205886 |
| H | 4.220716 | 1.319456 | -1.786526 |
| H | 1.812967 | 1.164613 | -1.252525 |
| H | -3.636286 | 3.345611 | -0.095299 |
| H | -2.587850 | 2.385425 | -1.157078 |
| H | -2.866407 | 1.881094 | 0.525917 |
| H | -2.611928 | 4.563564 | 1.919702 |
| H | -0.851450 | 4.549771 | 2.137261 |
| H | -1.794782 | 3.071428 | 2.420930 |
| H | -1.254489 | 4.560644 | -1.586524 |
| H | -2.176826 | 5.492757 | -0.393529 |
| H | -0.421851 | 5.339240 | -0.221819 |

Conf. 5e

| | | | |
|---|-----------|-----------|-----------|
| C | 2.612148 | 1.446114 | -0.826665 |
| C | 4.113534 | 1.628109 | -0.525585 |
| N | 4.256874 | 0.310580 | -0.217293 |
| C | 2.894735 | -0.050868 | -0.598671 |
| C | 5.366049 | -0.621303 | -0.265705 |
| C | 5.204478 | -1.470274 | -1.531420 |
| C | 3.754403 | -1.918989 | -1.699357 |
| O | 2.866940 | -0.798095 | -1.781902 |
| O | 4.893556 | 2.552580 | -0.542818 |
| C | 1.655544 | 2.136103 | 0.123938 |
| C | 1.522494 | 3.617981 | -0.168800 |
| O | 0.391212 | 1.449096 | -0.061824 |
| H | 2.337368 | -0.555943 | 0.196611 |
| C | -0.507664 | 1.521790 | 0.910984 |
| O | -0.396112 | 2.196211 | 1.906364 |
| C | -1.692954 | 0.608725 | 0.647970 |
| C | -1.663028 | -0.571427 | 1.643085 |
| C | -0.403546 | -1.398274 | 1.570825 |
| C | -0.221077 | -2.326598 | 0.543648 |
| C | 0.926214 | -3.108950 | 0.490104 |
| C | 1.911905 | -2.971454 | 1.463676 |
| C | 1.749786 | -2.036822 | 2.479852 |
| C | 0.599930 | -1.254329 | 2.529553 |
| N | -2.902634 | 1.398873 | 0.782876 |
| O | -3.986318 | -0.001511 | -0.554257 |
| C | -5.131108 | -0.629180 | -1.221813 |
| C | -5.812277 | 0.371226 | -2.148656 |
| C | -4.470245 | -1.744195 | -2.023155 |
| C | -6.085027 | -1.208087 | -0.182812 |
| C | -4.115690 | 1.030056 | 0.282006 |
| O | -5.152512 | 1.600539 | 0.565483 |
| H | 2.364861 | 1.659617 | -1.868621 |
| H | 6.300466 | -0.059569 | -0.261149 |
| H | 5.337910 | -1.249929 | 0.629297 |
| H | 5.850869 | -2.349342 | -1.478081 |
| H | 5.499428 | -0.885004 | -2.407019 |
| H | 3.449764 | -2.561534 | -0.863420 |
| H | 3.621401 | -2.474375 | -2.626817 |
| H | 1.963132 | 1.973048 | 1.160536 |
| H | 0.848021 | 4.096474 | 0.540824 |
| H | 2.505631 | 4.087359 | -0.088474 |
| H | 1.147224 | 3.771083 | -1.183499 |
| H | -1.627930 | 0.236299 | -0.372353 |
| H | -2.534155 | -1.193167 | 1.421732 |
| H | -1.790502 | -0.167236 | 2.650755 |
| H | -0.992302 | -2.447876 | -0.211167 |
| H | 1.049890 | -3.829894 | -0.310390 |

| | | | |
|---|-----------|-----------|-----------|
| H | 2.804053 | -3.586700 | 1.427382 |
| H | 2.515737 | -1.918218 | 3.237952 |
| H | 0.473401 | -0.532809 | 3.330500 |
| H | -2.940366 | 2.062873 | 1.542190 |
| H | -6.569912 | -0.149543 | -2.739470 |
| H | -6.295655 | 1.168732 | -1.585738 |
| H | -5.083781 | 0.808262 | -2.836234 |
| H | -5.229879 | -2.300563 | -2.576543 |
| H | -3.947321 | -2.435663 | -1.358232 |
| H | -3.752821 | -1.331507 | -2.736135 |
| H | -6.578484 | -0.422042 | 0.387399 |
| H | -6.848025 | -1.802231 | -0.691581 |
| H | -5.543460 | -1.863447 | 0.504274 |

Conf. 5f

| | | | |
|---|-----------|-----------|-----------|
| C | -3.083143 | -1.350548 | -0.582045 |
| C | -4.503117 | -1.687694 | -0.074028 |
| N | -4.573339 | -0.529826 | 0.637433 |
| C | -3.328298 | 0.011508 | 0.103465 |
| C | -5.674199 | 0.305664 | 1.077430 |
| C | -5.791046 | 1.482063 | 0.101979 |
| C | -4.411611 | 2.044125 | -0.232883 |
| O | -3.571535 | 1.040949 | -0.813084 |
| O | -5.279632 | -2.602301 | -0.221324 |
| C | -1.989628 | -2.250935 | -0.037057 |
| C | -2.062014 | -3.653830 | -0.605687 |
| O | -0.693420 | -1.714265 | -0.413228 |
| H | -2.620122 | 0.332388 | 0.875649 |
| C | 0.047980 | -1.113612 | 0.512374 |
| O | -0.327421 | -0.834616 | 1.624871 |
| C | 1.445938 | -0.829420 | -0.015714 |
| C | 1.416528 | 0.180138 | -1.191592 |
| C | 0.935170 | 1.546561 | -0.781678 |
| C | 1.823147 | 2.487591 | -0.256840 |
| C | 1.371614 | 3.731592 | 0.169343 |
| C | 0.020995 | 4.053686 | 0.074661 |
| C | -0.870649 | 3.126213 | -0.453557 |
| C | -0.414759 | 1.883266 | -0.878830 |
| N | 2.250176 | -0.393618 | 1.103171 |
| O | 4.121287 | -0.788550 | -0.015185 |
| C | 5.547579 | -0.686449 | -0.337347 |
| C | 6.377551 | -1.464906 | 0.677367 |
| C | 5.622593 | -1.342680 | -1.710491 |
| C | 5.951984 | 0.781477 | -0.421886 |
| C | 3.601976 | -0.286562 | 1.109779 |
| O | 4.230112 | 0.198001 | 2.034251 |
| H | -3.029480 | -1.266770 | -1.669433 |
| H | -6.582330 | -0.296775 | 1.107785 |

| | | | |
|---|-----------|-----------|-----------|
| H | -5.463105 | 0.660492 | 2.090245 |
| H | -6.408625 | 2.270471 | 0.537917 |
| H | -6.269788 | 1.148240 | -0.822806 |
| H | -3.926405 | 2.447006 | 0.667760 |
| H | -4.482252 | 2.841378 | -0.971921 |
| H | -2.035035 | -2.270610 | 1.053193 |
| H | -1.264670 | -4.271386 | -0.189488 |
| H | -3.023879 | -4.103292 | -0.352163 |
| H | -1.964273 | -3.632636 | -1.693695 |
| H | 1.836514 | -1.774465 | -0.400509 |
| H | 0.782406 | -0.234162 | -1.977991 |
| H | 2.433682 | 0.235195 | -1.582905 |
| H | 2.879428 | 2.247586 | -0.186398 |
| H | 2.075476 | 4.450903 | 0.573160 |
| H | -0.332413 | 5.024144 | 0.404727 |
| H | -1.923017 | 3.369395 | -0.542557 |
| H | -1.121845 | 1.175259 | -1.297647 |
| H | 1.768834 | -0.012237 | 1.903166 |
| H | 7.415521 | -1.499435 | 0.336955 |
| H | 6.345955 | -0.995873 | 1.659744 |
| H | 6.010617 | -2.491207 | 0.758841 |
| H | 6.652591 | -1.321965 | -2.073185 |
| H | 4.991258 | -0.809817 | -2.425414 |
| H | 5.293520 | -2.383015 | -1.657825 |
| H | 5.897464 | 1.266272 | 0.552367 |
| H | 6.979199 | 0.849224 | -0.788144 |
| H | 5.304249 | 1.312564 | -1.124631 |

Conf. 6a

| | | | |
|----|-----------|-----------|-----------|
| C | 1.106027 | 1.572823 | 0.625335 |
| C | 1.164845 | 0.332421 | 1.524324 |
| N | 1.860016 | -0.367008 | 0.602591 |
| C | 1.914388 | 0.717341 | -0.388249 |
| O | 0.757553 | 0.043511 | 2.634746 |
| C | -0.284787 | 2.022135 | 0.198439 |
| C | -0.227622 | 3.160104 | -0.810725 |
| H | 1.344704 | 0.467478 | -1.287585 |
| C | 2.459765 | -1.679604 | 0.599398 |
| C | 4.371584 | -1.108742 | -0.989685 |
| C | 4.097489 | 0.102669 | -1.475596 |
| O | -0.956228 | 0.911734 | -0.364873 |
| Si | -2.476846 | 0.322603 | 0.024985 |
| C | -2.419310 | -1.495640 | -0.501136 |
| C | -2.768996 | 0.504695 | 1.865236 |
| C | -3.777245 | 1.274983 | -0.928879 |
| C | -1.443174 | -2.260064 | 0.407023 |
| C | -1.937885 | -1.602124 | -1.956951 |
| C | -3.820698 | -2.115973 | -0.382180 |

| | | | |
|---|-----------|-----------|-----------|
| H | 1.673536 | 2.411218 | 1.037095 |
| H | -0.809622 | 2.366692 | 1.099841 |
| H | -1.237916 | 3.456738 | -1.101291 |
| H | 0.281201 | 4.029207 | -0.385593 |
| H | 0.310716 | 2.844378 | -1.708916 |
| H | 2.234260 | -2.135977 | 1.565700 |
| H | 1.992435 | -2.291245 | -0.180532 |
| H | 4.928973 | -1.797463 | -1.618964 |
| H | 4.441293 | 0.345503 | -2.477253 |
| H | -3.651493 | -0.067460 | 2.168336 |
| H | -2.943249 | 1.549042 | 2.140926 |
| H | -1.907915 | 0.140185 | 2.432275 |
| H | -4.783150 | 0.923832 | -0.678792 |
| H | -3.638604 | 1.169648 | -2.008719 |
| H | -3.725531 | 2.340274 | -0.682899 |
| H | -1.371133 | -3.307833 | 0.088302 |
| H | -1.769980 | -2.253599 | 1.451620 |
| H | -0.440257 | -1.825920 | 0.366183 |
| H | -1.909114 | -2.654448 | -2.267738 |
| H | -2.604228 | -1.073932 | -2.646964 |
| H | -0.932118 | -1.188606 | -2.074733 |
| H | -4.539970 | -1.626214 | -1.046292 |
| H | -4.210100 | -2.055771 | 0.639668 |
| H | -3.787282 | -3.177514 | -0.658059 |
| C | 3.974916 | -1.612763 | 0.378847 |
| H | 4.385460 | -2.612798 | 0.533027 |
| H | 4.404956 | -0.968029 | 1.154990 |
| C | 3.324496 | 1.169361 | -0.737009 |
| H | 3.260486 | 2.077388 | -1.341425 |
| H | 3.846033 | 1.436151 | 0.191737 |

Conf. 6b

| | | | |
|----|-----------|-----------|-----------|
| C | 1.137539 | 1.731969 | 0.473753 |
| C | 1.163415 | 0.696401 | 1.605259 |
| N | 1.894867 | -0.163534 | 0.869586 |
| C | 1.968609 | 0.688201 | -0.322553 |
| O | 0.715538 | 0.627626 | 2.735895 |
| C | -0.233816 | 2.092449 | -0.082747 |
| C | -0.131313 | 3.039944 | -1.269422 |
| H | 1.405773 | 0.260357 | -1.156545 |
| C | 2.501635 | -1.450782 | 1.125370 |
| C | 3.975883 | -1.445674 | -0.984014 |
| C | 4.190383 | -0.145914 | -1.202393 |
| O | -0.878410 | 0.898151 | -0.479613 |
| Si | -2.394506 | 0.330793 | -0.047898 |
| C | -2.272625 | -1.537532 | -0.333223 |
| C | -2.738931 | 0.744722 | 1.744603 |
| C | -3.692104 | 1.116594 | -1.146170 |

| | | | |
|---|-----------|-----------|-----------|
| C | -1.245837 | -2.134585 | 0.641855 |
| C | -1.810117 | -1.813392 | -1.772856 |
| C | -3.642915 | -2.194034 | -0.102870 |
| H | 1.702933 | 2.631924 | 0.728694 |
| H | -0.798902 | 2.581969 | 0.722148 |
| H | -1.127457 | 3.271000 | -1.653370 |
| H | 0.355156 | 3.974541 | -0.978330 |
| H | 0.449925 | 2.578556 | -2.073027 |
| H | 3.393018 | -1.328640 | 1.750714 |
| H | 1.788211 | -2.071198 | 1.675120 |
| H | 4.687535 | -2.131868 | -1.436914 |
| H | 5.067824 | 0.110473 | -1.791899 |
| H | -3.635735 | 0.221676 | 2.091078 |
| H | -2.911435 | 1.816996 | 1.877830 |
| H | -1.898340 | 0.454065 | 2.380363 |
| H | -4.694511 | 0.763298 | -0.885148 |
| H | -3.514725 | 0.889481 | -2.201216 |
| H | -3.681400 | 2.204659 | -1.027342 |
| H | -1.141233 | -3.213439 | 0.469378 |
| H | -1.543333 | -1.993090 | 1.685738 |
| H | -0.263356 | -1.674134 | 0.506350 |
| H | -1.730586 | -2.894958 | -1.942158 |
| H | -2.513876 | -1.415894 | -2.511457 |
| H | -0.829115 | -1.369486 | -1.966245 |
| H | -4.397305 | -1.816775 | -0.800798 |
| H | -4.011127 | -2.026342 | 0.914734 |
| H | -3.570751 | -3.278930 | -0.250906 |
| C | 2.876560 | -2.123982 | -0.191894 |
| H | 1.976047 | -2.231922 | -0.808769 |
| H | 3.201786 | -3.140140 | 0.041210 |
| C | 3.380909 | 1.039723 | -0.742142 |
| H | 3.333384 | 1.771448 | -1.555837 |
| H | 3.899942 | 1.539140 | 0.086477 |

Conf. 6c

| | | | |
|----|-----------|-----------|-----------|
| C | 1.147075 | 1.080444 | -0.707685 |
| C | 2.492654 | 1.658212 | -0.245431 |
| N | 2.870091 | 0.478393 | 0.293775 |
| C | 1.638374 | -0.240514 | -0.063719 |
| O | 3.047758 | 2.739402 | -0.312846 |
| C | -0.124359 | 1.682280 | -0.134023 |
| C | -0.408044 | 3.069569 | -0.685779 |
| H | 1.066951 | -0.526388 | 0.824552 |
| C | 4.096198 | 0.012408 | 0.897884 |
| C | 3.839838 | -2.430138 | 0.205518 |
| C | 2.604963 | -2.550904 | -0.283331 |
| O | -1.182042 | 0.795386 | -0.462007 |
| Si | -2.328754 | 0.208841 | 0.614361 |

| | | | |
|---|-----------|-----------|-----------|
| C | -3.362613 | -0.996281 | -0.414205 |
| C | -1.481697 | -0.666021 | 2.039877 |
| C | -3.344455 | 1.634988 | 1.278546 |
| C | -2.443167 | -2.047308 | -1.057278 |
| C | -4.113906 | -0.237905 | -1.520011 |
| C | -4.380646 | -1.700878 | 0.498198 |
| H | 1.074318 | 1.023433 | -1.797780 |
| H | -0.011526 | 1.749285 | 0.958722 |
| H | -1.324192 | 3.470820 | -0.246572 |
| H | 0.418381 | 3.747297 | -0.457521 |
| H | -0.532856 | 3.023170 | -1.771175 |
| H | 4.794538 | 0.851873 | 0.890631 |
| H | 3.907625 | -0.263067 | 1.941056 |
| H | 4.285299 | -3.294356 | 0.690902 |
| H | 2.096905 | -3.505066 | -0.174505 |
| H | -2.221649 | -0.979806 | 2.782682 |
| H | -0.770160 | -0.006720 | 2.546577 |
| H | -0.942115 | -1.556397 | 1.704822 |
| H | -4.130559 | 1.277669 | 1.950814 |
| H | -3.816567 | 2.198316 | 0.468966 |
| H | -2.711646 | 2.324617 | 1.846411 |
| H | -3.037463 | -2.758386 | -1.644993 |
| H | -1.891643 | -2.622229 | -0.306173 |
| H | -1.714910 | -1.582573 | -1.727954 |
| H | -4.696790 | -0.940597 | -2.128940 |
| H | -4.812411 | 0.496086 | -1.105995 |
| H | -3.424993 | 0.289164 | -2.186780 |
| H | -5.055833 | -0.988705 | 0.984105 |
| H | -3.889056 | -2.287835 | 1.280544 |
| H | -4.998827 | -2.389745 | -0.090902 |
| C | 4.686625 | -1.180046 | 0.136819 |
| H | 5.677409 | -1.386685 | 0.546664 |
| H | 4.829955 | -0.881264 | -0.908765 |
| C | 1.846559 | -1.441707 | -0.971907 |
| H | 0.867305 | -1.796866 | -1.301461 |
| H | 2.390303 | -1.113063 | -1.867415 |

Conf. 6d

| | | | |
|---|-----------|-----------|-----------|
| C | 1.051353 | 1.275220 | -0.585474 |
| C | 2.252977 | 1.757398 | 0.242413 |
| N | 2.652351 | 0.491135 | 0.491550 |
| C | 1.567973 | -0.149499 | -0.265550 |
| O | 2.708786 | 2.836197 | 0.573099 |
| C | -0.335718 | 1.643334 | -0.085534 |
| C | -0.618855 | 3.125495 | -0.281373 |
| H | 0.900991 | -0.717174 | 0.389501 |
| C | 3.811552 | -0.071499 | 1.144124 |
| C | 3.900706 | -2.213586 | -0.239230 |

| | | | |
|----|-----------|-----------|-----------|
| C | 2.775462 | -2.241794 | -0.954272 |
| O | -1.262701 | 0.850183 | -0.811379 |
| Si | -2.735915 | 0.241178 | -0.276873 |
| C | -2.474320 | -1.414341 | 0.621478 |
| C | -3.561599 | 1.470968 | 0.871416 |
| C | -3.734691 | -0.001799 | -1.835751 |
| C | -1.721161 | -1.199416 | 1.944590 |
| C | -1.677759 | -2.378469 | -0.271806 |
| C | -3.844116 | -2.043155 | 0.932450 |
| H | 1.147267 | 1.535542 | -1.643662 |
| H | -0.394489 | 1.405009 | 0.986486 |
| H | -1.605301 | 3.384775 | 0.107122 |
| H | 0.130669 | 3.726214 | 0.239769 |
| H | -0.586715 | 3.373149 | -1.346044 |
| H | 4.418064 | 0.766417 | 1.494011 |
| H | 3.493044 | -0.648357 | 2.018942 |
| H | 4.343739 | -3.160432 | 0.057462 |
| H | 2.346916 | -3.207184 | -1.208630 |
| H | -4.474985 | 1.042194 | 1.294649 |
| H | -3.838582 | 2.381273 | 0.332439 |
| H | -2.910912 | 1.753173 | 1.704393 |
| H | -4.734873 | -0.380483 | -1.606169 |
| H | -3.250934 | -0.711738 | -2.512373 |
| H | -3.847075 | 0.948966 | -2.364441 |
| H | -1.575579 | -2.159180 | 2.456250 |
| H | -2.274409 | -0.544127 | 2.624487 |
| H | -0.730783 | -0.760309 | 1.792479 |
| H | -1.511867 | -3.329167 | 0.250425 |
| H | -2.210841 | -2.602265 | -1.201225 |
| H | -0.699467 | -1.971632 | -0.540675 |
| H | -4.413838 | -2.251457 | 0.021610 |
| H | -4.455303 | -1.400331 | 1.574008 |
| H | -3.707149 | -2.995803 | 1.459448 |
| C | 4.624378 | -0.959803 | 0.195274 |
| H | 5.554808 | -1.230330 | 0.698660 |
| H | 4.898551 | -0.362104 | -0.682515 |
| C | 2.035455 | -1.013410 | -1.426185 |
| H | 1.164074 | -1.297128 | -2.021223 |
| H | 2.682838 | -0.406858 | -2.073002 |

Conf. 6e

| | | | |
|---|-----------|-----------|-----------|
| C | 1.114456 | 0.984396 | -0.757434 |
| C | 2.231234 | 1.789637 | -0.074489 |
| N | 2.794762 | 0.672171 | 0.432692 |
| C | 1.807640 | -0.255844 | -0.137632 |
| O | 2.535715 | 2.965322 | 0.006423 |
| C | -0.321660 | 1.261950 | -0.341357 |
| C | -0.776192 | 2.639847 | -0.794568 |

| | | | |
|----|-----------|-----------|-----------|
| H | 1.214487 | -0.738134 | 0.644075 |
| C | 4.010658 | 0.424540 | 1.171381 |
| C | 4.393929 | -1.940859 | 0.295367 |
| C | 3.286650 | -2.275724 | -0.368155 |
| O | -1.138343 | 0.262026 | -0.931276 |
| Si | -2.166959 | -0.827265 | -0.171845 |
| C | -3.713533 | 0.056953 | 0.491991 |
| C | -2.610830 | -2.043139 | -1.517056 |
| C | -1.273725 | -1.693890 | 1.230655 |
| C | -4.374091 | 0.875039 | -0.628794 |
| C | -3.347630 | 0.990111 | 1.658168 |
| C | -4.716534 | -0.994934 | 0.998150 |
| H | 1.195305 | 1.017005 | -1.847960 |
| H | -0.383184 | 1.203211 | 0.755310 |
| H | -1.800302 | 2.834126 | -0.470277 |
| H | -0.124548 | 3.411640 | -0.378222 |
| H | -0.741124 | 2.703754 | -1.885606 |
| H | 4.498467 | 1.390849 | 1.315310 |
| H | 3.762046 | 0.019567 | 2.158209 |
| H | 4.958299 | -2.731957 | 0.781726 |
| H | 2.995500 | -3.322126 | -0.392775 |
| H | -3.246560 | -2.842762 | -1.125883 |
| H | -1.705342 | -2.501731 | -1.924638 |
| H | -3.144689 | -1.556194 | -2.337657 |
| H | -1.967389 | -2.340513 | 1.776883 |
| H | -0.845209 | -0.989732 | 1.949749 |
| H | -0.467277 | -2.324035 | 0.844500 |
| H | -5.265556 | 1.388188 | -0.246426 |
| H | -4.692977 | 0.238475 | -1.460290 |
| H | -3.698627 | 1.635297 | -1.030832 |
| H | -4.249830 | 1.482004 | 2.043287 |
| H | -2.891740 | 0.442830 | 2.489181 |
| H | -2.653404 | 1.779557 | 1.355155 |
| H | -4.300835 | -1.602863 | 1.808065 |
| H | -5.037901 | -1.670369 | 0.199214 |
| H | -5.613271 | -0.498114 | 1.389349 |
| C | 4.941980 | -0.538457 | 0.426529 |
| H | 5.895339 | -0.566857 | 0.958177 |
| H | 5.143242 | -0.119945 | -0.567126 |
| C | 2.389085 | -1.294623 | -1.083380 |
| H | 1.562999 | -1.818623 | -1.570083 |
| H | 2.950561 | -0.774836 | -1.870877 |

Conf. 6f

| | | | |
|---|----------|-----------|-----------|
| C | 1.168463 | 1.167386 | -0.770535 |
| C | 2.540430 | 1.695952 | -0.324286 |
| N | 2.930284 | 0.471989 | 0.088127 |
| C | 1.681504 | -0.207412 | -0.272628 |

| | | | |
|----|-----------|-----------|-----------|
| O | 3.104971 | 2.774792 | -0.322968 |
| C | -0.069233 | 1.715384 | -0.081189 |
| C | -0.375895 | 3.145658 | -0.492624 |
| H | 1.145428 | -0.565068 | 0.611174 |
| C | 4.173447 | -0.080471 | 0.580311 |
| C | 3.500938 | -2.547401 | 0.248022 |
| C | 2.647556 | -2.495373 | -0.777393 |
| O | -1.146505 | 0.860275 | -0.429501 |
| Si | -2.229103 | 0.172947 | 0.654041 |
| C | -3.330902 | -0.927609 | -0.420323 |
| C | -1.303885 | -0.834631 | 1.936654 |
| C | -3.192651 | 1.529398 | 1.513369 |
| C | -2.460308 | -1.929109 | -1.196687 |
| C | -4.124226 | -0.067828 | -1.417176 |
| C | -4.313134 | -1.697672 | 0.478267 |
| H | 1.043243 | 1.208232 | -1.856492 |
| H | 0.101677 | 1.685634 | 1.005780 |
| H | -1.265846 | 3.506094 | 0.028246 |
| H | 0.464271 | 3.801014 | -0.249568 |
| H | -0.558212 | 3.195033 | -1.569701 |
| H | 4.895442 | -0.163565 | -0.239819 |
| H | 4.589203 | 0.601580 | 1.326434 |
| H | 3.958605 | -3.514394 | 0.442666 |
| H | 2.504503 | -3.415121 | -1.340062 |
| H | -2.002540 | -1.223349 | 2.684056 |
| H | -0.565511 | -0.224987 | 2.466789 |
| H | -0.784081 | -1.685545 | 1.487310 |
| H | -3.934497 | 1.109402 | 2.199511 |
| H | -3.714075 | 2.165751 | 0.793109 |
| H | -2.520937 | 2.163673 | 2.100767 |
| H | -3.093017 | -2.576431 | -1.817071 |
| H | -1.886147 | -2.576610 | -0.526050 |
| H | -1.754533 | -1.416865 | -1.856785 |
| H | -4.748607 | -0.708304 | -2.052993 |
| H | -4.788819 | 0.636158 | -0.906482 |
| H | -3.461138 | 0.506512 | -2.070829 |
| H | -4.955920 | -1.023090 | 1.053435 |
| H | -3.792443 | -2.351989 | 1.184684 |
| H | -4.966739 | -2.329877 | -0.135606 |
| C | 3.932971 | -1.453463 | 1.202819 |
| H | 3.205834 | -1.357051 | 2.017846 |
| H | 4.867982 | -1.764148 | 1.674088 |
| C | 1.841797 | -1.325858 | -1.280824 |
| H | 0.844171 | -1.677757 | -1.564791 |
| H | 2.299190 | -0.932351 | -2.198014 |

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| | | | |
|---|-----------|----------|-----------|
| C | -2.632855 | 0.314363 | -0.267916 |
|---|-----------|----------|-----------|

| | | | |
|---|-----------|-----------|-----------|
| C | -2.655202 | -1.184827 | 0.061345 |
| C | -1.287271 | -0.917413 | 0.712582 |
| N | -1.477667 | 0.491424 | 0.442302 |
| O | -0.212433 | -1.448470 | -0.036034 |
| C | 0.922546 | -0.673344 | -0.035949 |
| C | 0.895051 | 0.710496 | 0.164299 |
| C | -0.402605 | 1.452747 | 0.401142 |
| C | 2.124520 | -1.332112 | -0.285138 |
| C | 3.310078 | -0.616472 | -0.330903 |
| C | 3.303572 | 0.760771 | -0.118467 |
| C | 2.102367 | 1.407722 | 0.128374 |
| O | -3.317812 | 1.083052 | -0.897971 |
| H | -3.448540 | -1.495948 | 0.739162 |
| H | -2.609778 | -1.835213 | -0.811094 |
| H | -1.152307 | -1.162184 | 1.768304 |
| H | -0.599077 | 2.156436 | -0.411774 |
| H | -0.352615 | 2.023563 | 1.333021 |
| H | 2.107002 | -2.404781 | -0.438760 |
| H | 4.242145 | -1.134790 | -0.524431 |
| H | 4.228959 | 1.323662 | -0.145686 |
| H | 2.088638 | 2.481037 | 0.290971 |

Conf. 8a

| | | | |
|----|-----------|-----------|-----------|
| C | 0.179158 | 1.810886 | 0.724654 |
| C | 0.283426 | 0.588380 | 1.651438 |
| N | 1.068679 | -0.076976 | 0.745609 |
| C | 1.132135 | 1.018300 | -0.196746 |
| C | 2.007747 | -1.162812 | 0.793283 |
| C | 3.289186 | -0.682987 | 0.145937 |
| C | 3.433069 | 0.625874 | -0.328172 |
| O | 2.433162 | 1.561099 | -0.267692 |
| C | 4.378308 | -1.550102 | 0.053450 |
| C | 5.585821 | -1.133988 | -0.483242 |
| C | 5.717534 | 0.177533 | -0.937399 |
| C | 4.647445 | 1.053154 | -0.862864 |
| O | -0.142724 | 0.275000 | 2.734623 |
| H | 0.776428 | 0.767547 | -1.198003 |
| O | 1.557992 | -2.309370 | 0.105236 |
| C | -1.211016 | 2.118472 | 0.185468 |
| C | -1.188299 | 3.238992 | -0.843690 |
| H | 0.657506 | 2.695431 | 1.148705 |
| O | -1.715090 | 0.930473 | -0.390075 |
| Si | -3.228639 | 0.234727 | -0.172803 |
| C | -2.943503 | -1.608264 | -0.501329 |
| C | -3.802938 | 0.545927 | 1.581406 |
| C | -4.435120 | 0.976331 | -1.395942 |
| C | -2.134307 | -2.213454 | 0.656615 |
| C | -2.158645 | -1.787101 | -1.810739 |

| | | | |
|---|-----------|-----------|-----------|
| C | -4.294089 | -2.333767 | -0.612322 |
| H | 2.181359 | -1.399556 | 1.848368 |
| H | 4.264368 | -2.565478 | 0.416889 |
| H | 6.420100 | -1.822206 | -0.544928 |
| H | 6.657293 | 0.517663 | -1.357098 |
| H | 4.727986 | 2.073328 | -1.218900 |
| H | 0.854901 | -2.718470 | 0.617496 |
| H | -1.829653 | 2.424285 | 1.039360 |
| H | -2.198771 | 3.428701 | -1.211641 |
| H | -0.800860 | 4.160872 | -0.402782 |
| H | -0.557905 | 2.965054 | -1.694052 |
| H | -4.679282 | -0.069651 | 1.807258 |
| H | -4.086998 | 1.591415 | 1.732826 |
| H | -3.016610 | 0.296226 | 2.299609 |
| H | -4.504865 | 2.059404 | -1.255947 |
| H | -4.124037 | 0.786669 | -2.427294 |
| H | -5.436738 | 0.557033 | -1.260170 |
| H | -1.902559 | -3.265756 | 0.447427 |
| H | -2.684896 | -2.176982 | 1.601452 |
| H | -1.191015 | -1.678629 | 0.799083 |
| H | -2.002228 | -2.854504 | -2.012400 |
| H | -2.693958 | -1.365142 | -2.667820 |
| H | -1.177806 | -1.306960 | -1.755070 |
| H | -4.132594 | -3.408632 | -0.762069 |
| H | -4.898531 | -2.216765 | 0.293634 |
| H | -4.882622 | -1.968119 | -1.459537 |

Conf. 8b

| | | | |
|----|-----------|-----------|-----------|
| C | 0.189347 | 1.329370 | 1.119475 |
| C | 0.325204 | -0.128835 | 1.585265 |
| N | 1.165018 | -0.422677 | 0.542504 |
| C | 1.226585 | 0.935192 | 0.045090 |
| C | 2.156628 | -1.428896 | 0.282848 |
| C | 3.443537 | -0.719031 | -0.079781 |
| C | 3.547567 | 0.676380 | -0.059717 |
| O | 2.501671 | 1.501919 | 0.261025 |
| C | 4.575760 | -1.468428 | -0.400913 |
| C | 5.786275 | -0.857045 | -0.684307 |
| C | 5.877041 | 0.533591 | -0.645251 |
| C | 4.764098 | 1.297720 | -0.336937 |
| O | -0.101212 | -0.799581 | 2.491567 |
| H | 0.941094 | 1.044336 | -1.002331 |
| O | 1.798806 | -2.287084 | -0.777750 |
| C | -1.180261 | 1.774343 | 0.622736 |
| C | -1.143032 | 3.212502 | 0.123280 |
| H | 0.597352 | 2.030822 | 1.849096 |
| O | -1.566774 | 0.895829 | -0.416502 |
| Si | -3.109018 | 0.351740 | -0.810501 |

| | | | |
|---|-----------|-----------|-----------|
| C | -3.488280 | -1.223643 | 0.177092 |
| C | -4.366537 | 1.688997 | -0.434696 |
| C | -3.027351 | -0.006040 | -2.640915 |
| C | -3.569098 | -0.900025 | 1.677848 |
| C | -2.378269 | -2.260663 | -0.059419 |
| C | -4.832925 | -1.810811 | -0.283856 |
| H | 2.287791 | -2.004039 | 1.205714 |
| H | 4.493196 | -2.549541 | -0.420824 |
| H | 6.654381 | -1.456574 | -0.930150 |
| H | 6.818570 | 1.024986 | -0.862139 |
| H | 4.812724 | 2.379821 | -0.310730 |
| H | 1.098273 | -2.870843 | -0.474544 |
| H | -1.876945 | 1.702921 | 1.468596 |
| H | -2.129963 | 3.515576 | -0.230525 |
| H | -0.840742 | 3.890463 | 0.925336 |
| H | -0.434553 | 3.309284 | -0.704055 |
| H | -5.381880 | 1.310289 | -0.585464 |
| H | -4.229724 | 2.548426 | -1.097055 |
| H | -4.294252 | 2.040858 | 0.598603 |
| H | -2.786505 | 0.905393 | -3.195330 |
| H | -2.260437 | -0.752804 | -2.864507 |
| H | -3.985390 | -0.383117 | -3.010536 |
| H | -3.805703 | -1.809281 | 2.245532 |
| H | -4.351665 | -0.165595 | 1.894234 |
| H | -2.619703 | -0.517222 | 2.062780 |
| H | -2.575068 | -3.165388 | 0.529750 |
| H | -2.319112 | -2.558792 | -1.111109 |
| H | -1.399576 | -1.875301 | 0.238663 |
| H | -5.056704 | -2.723243 | 0.283218 |
| H | -5.661950 | -1.114413 | -0.121555 |
| H | -4.820039 | -2.079376 | -1.344948 |

Conf. 8c

| | | | |
|---|----------|-----------|-----------|
| C | 0.170405 | 1.397691 | -0.948316 |
| C | 1.333186 | 2.341759 | -0.590864 |
| N | 1.926887 | 1.373015 | 0.179756 |
| C | 0.965170 | 0.343063 | -0.155298 |
| C | 3.263742 | 1.118069 | 0.643473 |
| C | 3.629429 | -0.292094 | 0.230902 |
| C | 2.773913 | -1.080240 | -0.546543 |
| O | 1.540934 | -0.653751 | -0.968583 |
| C | 4.871921 | -0.813621 | 0.592452 |
| C | 5.266568 | -2.078091 | 0.186361 |
| C | 4.408178 | -2.844411 | -0.600608 |
| C | 3.166552 | -2.350465 | -0.964065 |
| O | 1.650437 | 3.476229 | -0.843627 |
| H | 0.480015 | -0.120167 | 0.706654 |
| O | 3.387803 | 1.227145 | 2.043282 |

| | | | |
|----|-----------|-----------|-----------|
| C | -1.211657 | 1.753878 | -0.418865 |
| C | -1.809630 | 2.940603 | -1.156824 |
| H | 0.130499 | 1.163674 | -2.014411 |
| O | -2.022496 | 0.605134 | -0.577034 |
| Si | -3.019298 | -0.030905 | 0.620736 |
| C | -3.802006 | -1.556765 | -0.175382 |
| C | -1.986718 | -0.486881 | 2.117174 |
| C | -4.292043 | 1.251447 | 1.111547 |
| C | -2.700667 | -2.509568 | -0.667964 |
| C | -4.680073 | -1.138805 | -1.365646 |
| C | -4.671469 | -2.281041 | 0.866533 |
| H | 3.923226 | 1.839555 | 0.149443 |
| H | 5.532598 | -0.204951 | 1.199758 |
| H | 6.236054 | -2.464620 | 0.476548 |
| H | 4.705463 | -3.834314 | -0.927200 |
| H | 2.481331 | -2.934456 | -1.566887 |
| H | 3.364516 | 2.158200 | 2.279537 |
| H | -1.116201 | 2.008750 | 0.647395 |
| H | -2.793867 | 3.178930 | -0.748506 |
| H | -1.167183 | 3.819121 | -1.057171 |
| H | -1.919546 | 2.704843 | -2.218662 |
| H | -2.633977 | -0.816100 | 2.935830 |
| H | -1.412279 | 0.370480 | 2.481794 |
| H | -1.287351 | -1.298065 | 1.896116 |
| H | -3.806540 | 2.132106 | 1.544054 |
| H | -4.881644 | 1.578525 | 0.250766 |
| H | -4.978391 | 0.850633 | 1.863792 |
| H | -3.151345 | -3.397358 | -1.129282 |
| H | -2.063069 | -2.854050 | 0.152454 |
| H | -2.060559 | -2.030873 | -1.414363 |
| H | -5.122315 | -2.026064 | -1.836090 |
| H | -5.502758 | -0.487327 | -1.054508 |
| H | -4.100129 | -0.610851 | -2.128306 |
| H | -5.140306 | -3.163884 | 0.414500 |
| H | -4.081373 | -2.624435 | 1.722240 |
| H | -5.475145 | -1.640977 | 1.245187 |

Conf. 8d

| | | | |
|---|----------|-----------|-----------|
| C | 0.178132 | 1.155212 | -1.010004 |
| C | 1.139256 | 2.243182 | -0.493747 |
| N | 1.833120 | 1.323979 | 0.252277 |
| C | 1.078097 | 0.183353 | -0.223128 |
| C | 3.158529 | 1.250491 | 0.804802 |
| C | 3.775906 | -0.051076 | 0.338609 |
| C | 3.116654 | -0.904381 | -0.552940 |
| O | 1.863790 | -0.646917 | -1.047445 |
| C | 5.058069 | -0.396193 | 0.767140 |
| C | 5.680146 | -1.549620 | 0.317527 |

| | | | |
|----|-----------|-----------|-----------|
| C | 5.015096 | -2.381199 | -0.582205 |
| C | 3.738578 | -2.062861 | -1.014378 |
| O | 1.279069 | 3.430797 | -0.641177 |
| H | 0.619028 | -0.411979 | 0.568170 |
| O | 3.166461 | 1.278041 | 2.213976 |
| C | -1.285817 | 1.251338 | -0.598808 |
| C | -1.962886 | 2.432365 | -1.275959 |
| H | 0.264476 | 1.004442 | -2.088443 |
| O | -1.913291 | 0.039752 | -0.973559 |
| Si | -2.759662 | -1.034975 | 0.007862 |
| C | -4.438081 | -0.303130 | 0.516808 |
| C | -2.979029 | -2.546400 | -1.063806 |
| C | -1.746217 | -1.437052 | 1.533387 |
| C | -5.204635 | 0.175113 | -0.726426 |
| C | -4.247057 | 0.874771 | 1.486672 |
| C | -5.265448 | -1.392923 | 1.222023 |
| H | 3.724569 | 2.100057 | 0.408014 |
| H | 5.567225 | 0.262406 | 1.461979 |
| H | 6.676716 | -1.799315 | 0.661045 |
| H | 5.491372 | -3.285252 | -0.943824 |
| H | 3.201410 | -2.701011 | -1.705861 |
| H | 2.975243 | 2.174534 | 2.502318 |
| H | -1.332423 | 1.384339 | 0.491843 |
| H | -3.003215 | 2.512291 | -0.956588 |
| H | -1.450102 | 3.364201 | -1.026058 |
| H | -1.943004 | 2.301220 | -2.361068 |
| H | -3.465088 | -3.351936 | -0.505829 |
| H | -2.006466 | -2.911799 | -1.405242 |
| H | -3.589454 | -2.327519 | -1.944121 |
| H | -0.864587 | -2.028557 | 1.270150 |
| H | -1.414163 | -0.539286 | 2.063143 |
| H | -2.341485 | -2.028887 | 2.235389 |
| H | -6.174717 | 0.595444 | -0.432614 |
| H | -5.400198 | -0.647074 | -1.422167 |
| H | -4.657466 | 0.949324 | -1.271265 |
| H | -5.223022 | 1.277987 | 1.784900 |
| H | -3.725074 | 0.569393 | 2.398860 |
| H | -3.682411 | 1.696605 | 1.036357 |
| H | -6.235101 | -0.983189 | 1.531375 |
| H | -5.464043 | -2.244441 | 0.563925 |
| H | -4.768574 | -1.769534 | 2.121833 |

Conf. 8e

| | | | |
|---|----------|----------|-----------|
| C | 0.035102 | 1.543326 | -0.804840 |
| C | 1.063653 | 2.436793 | -0.085149 |
| N | 1.691483 | 1.340120 | 0.450351 |
| C | 0.863143 | 0.374189 | -0.239357 |
| C | 3.004090 | 1.063796 | 0.967998 |

| | | | |
|----|-----------|-----------|-----------|
| C | 3.532806 | -0.155322 | 0.242013 |
| C | 2.821342 | -0.764209 | -0.797547 |
| O | 1.592477 | -0.325451 | -1.220443 |
| C | 4.785258 | -0.667500 | 0.581806 |
| C | 5.328335 | -1.747233 | -0.095500 |
| C | 4.612255 | -2.333096 | -1.138231 |
| C | 3.363448 | -1.846800 | -1.487154 |
| O | 1.281931 | 3.617481 | 0.013124 |
| H | 0.360831 | -0.336950 | 0.419335 |
| O | 3.001796 | 0.800750 | 2.352729 |
| C | -1.420169 | 1.655431 | -0.373044 |
| C | -2.019712 | 2.980032 | -0.822068 |
| H | 0.119819 | 1.608228 | -1.891999 |
| O | -2.104608 | 0.560161 | -0.952411 |
| Si | -3.417802 | -0.282973 | -0.317930 |
| C | -2.803192 | -1.646189 | 0.855513 |
| C | -4.552743 | 0.896815 | 0.593187 |
| C | -4.261816 | -1.020223 | -1.810368 |
| C | -2.132381 | -1.033935 | 2.096226 |
| C | -1.802409 | -2.554723 | 0.123270 |
| C | -4.000494 | -2.496746 | 1.315686 |
| H | 3.631011 | 1.935073 | 0.750554 |
| H | 5.334596 | -0.198902 | 1.390759 |
| H | 6.303121 | -2.129220 | 0.182672 |
| H | 5.026525 | -3.176986 | -1.677818 |
| H | 2.787105 | -2.294304 | -2.288084 |
| H | 2.866653 | 1.629329 | 2.820150 |
| H | -1.465907 | 1.595370 | 0.723726 |
| H | -3.054600 | 3.063613 | -0.486694 |
| H | -1.451709 | 3.816542 | -0.407454 |
| H | -1.998740 | 3.048451 | -1.912988 |
| H | -5.365196 | 0.345605 | 1.076031 |
| H | -5.001702 | 1.615308 | -0.098266 |
| H | -4.024319 | 1.456763 | 1.370368 |
| H | -4.594032 | -0.228145 | -2.487282 |
| H | -3.586745 | -1.679162 | -2.363262 |
| H | -5.139383 | -1.603280 | -1.516411 |
| H | -1.787871 | -1.828670 | 2.769642 |
| H | -2.823455 | -0.400215 | 2.660654 |
| H | -1.258971 | -0.426270 | 1.842078 |
| H | -1.416456 | -3.321222 | 0.806855 |
| H | -2.271215 | -3.071837 | -0.719754 |
| H | -0.947469 | -1.996050 | -0.267963 |
| H | -3.657080 | -3.291301 | 1.989957 |
| H | -4.740425 | -1.902687 | 1.861347 |
| H | -4.507420 | -2.978264 | 0.473752 |

Conf. 9a

| | | | |
|----|-----------|-----------|-----------|
| C | 1.238239 | -2.054303 | 0.513057 |
| C | 0.921670 | -1.056755 | 1.640226 |
| N | 0.036395 | -0.378709 | 0.840234 |
| C | 0.157160 | -1.285768 | -0.278905 |
| C | -1.082157 | 0.491047 | 1.068907 |
| C | -2.268394 | -0.092495 | 0.330618 |
| C | -2.181157 | -1.298835 | -0.371909 |
| O | -1.030814 | -2.028510 | -0.471975 |
| C | -3.493438 | 0.570281 | 0.386783 |
| C | -4.605692 | 0.030542 | -0.231659 |
| C | -4.526308 | -1.178685 | -0.915498 |
| C | -3.311603 | -1.836692 | -0.984536 |
| O | 1.271239 | -0.885518 | 2.779977 |
| H | 0.452543 | -0.808728 | -1.214897 |
| Br | -6.269779 | 0.950448 | -0.140684 |
| O | -0.868199 | 1.802959 | 0.602305 |
| C | 2.656149 | -2.018235 | -0.040418 |
| C | 2.818097 | -2.931600 | -1.246728 |
| O | 2.941343 | -0.680960 | -0.398187 |
| Si | 4.321000 | 0.187750 | 0.009806 |
| C | 3.977991 | 1.916181 | -0.676517 |
| C | 5.814134 | -0.617155 | -0.783888 |
| C | 4.527304 | 0.203784 | 1.870301 |
| C | 3.843485 | 1.852317 | -2.206340 |
| C | 2.667924 | 2.454676 | -0.078132 |
| C | 5.136675 | 2.856974 | -0.307684 |
| H | 0.923548 | -3.069939 | 0.758958 |
| H | -1.275135 | 0.497731 | 2.147007 |
| H | -3.559909 | 1.508717 | 0.923629 |
| H | -5.399640 | -1.601801 | -1.395437 |
| H | -3.220322 | -2.775081 | -1.517645 |
| H | -0.219095 | 2.226826 | 1.170598 |
| H | 3.327644 | -2.357623 | 0.760257 |
| H | 3.839114 | -2.865998 | -1.628429 |
| H | 2.612957 | -3.970814 | -0.977785 |
| H | 2.132627 | -2.634123 | -2.045008 |
| H | 5.961194 | -1.625876 | -0.384676 |
| H | 6.724229 | -0.045342 | -0.578315 |
| H | 5.696194 | -0.695970 | -1.868007 |
| H | 3.665986 | 0.662177 | 2.362378 |
| H | 4.637736 | -0.811099 | 2.264083 |
| H | 5.425069 | 0.764184 | 2.149093 |
| H | 4.768839 | 1.511229 | -2.681350 |
| H | 3.615992 | 2.848215 | -2.607152 |
| H | 3.038386 | 1.176910 | -2.510404 |
| H | 2.724905 | 2.540718 | 1.012186 |
| H | 2.455621 | 3.454653 | -0.477300 |
| H | 1.822036 | 1.806157 | -0.323248 |

| | | | |
|---|----------|----------|-----------|
| H | 5.251887 | 2.958895 | 0.776098 |
| H | 4.951539 | 3.858732 | -0.715036 |
| H | 6.090549 | 2.508576 | -0.717621 |

Conf. 9b

| | | | |
|----|-----------|-----------|-----------|
| C | -1.318065 | 1.657660 | -0.897217 |
| C | -0.357406 | 2.806443 | -0.541207 |
| N | 0.460005 | 1.950444 | 0.157780 |
| C | -0.290171 | 0.759889 | -0.184869 |
| C | 1.843920 | 1.960356 | 0.546717 |
| C | 2.464657 | 0.671064 | 0.049281 |
| C | 1.745895 | -0.245659 | -0.724245 |
| O | 0.434263 | -0.070688 | -1.065803 |
| C | 3.804466 | 0.410341 | 0.332984 |
| C | 4.410088 | -0.730878 | -0.159286 |
| C | 3.701413 | -1.635095 | -0.944365 |
| C | 2.368817 | -1.388516 | -1.220985 |
| O | -0.289753 | 3.990150 | -0.751337 |
| H | -0.631664 | 0.175580 | 0.672458 |
| Br | 6.240640 | -1.068782 | 0.239075 |
| O | 2.025439 | 2.038081 | 1.940610 |
| C | -2.718525 | 1.691095 | -0.302314 |
| C | -3.585275 | 2.754367 | -0.957448 |
| O | -3.264639 | 0.401473 | -0.493653 |
| Si | -4.140343 | -0.481424 | 0.638629 |
| C | -4.333880 | -2.188060 | -0.156123 |
| C | -5.791264 | 0.350564 | 0.937617 |
| C | -3.179231 | -0.571848 | 2.245411 |
| C | -5.035160 | -2.053033 | -1.517175 |
| C | -2.949579 | -2.825147 | -0.359219 |
| C | -5.177835 | -3.086917 | 0.763092 |
| H | -1.357115 | 1.462426 | -1.971148 |
| H | 2.314686 | 2.817889 | 0.054341 |
| H | 4.361161 | 1.114897 | 0.938622 |
| H | 4.179109 | -2.526339 | -1.330983 |
| H | 1.790086 | -2.079970 | -1.820956 |
| H | 1.830677 | 2.935003 | 2.225295 |
| H | -2.630891 | 1.911725 | 0.771623 |
| H | -4.576821 | 2.765942 | -0.500493 |
| H | -3.134452 | 3.742782 | -0.838054 |
| H | -3.694766 | 2.544981 | -2.024809 |
| H | -5.649741 | 1.336780 | 1.390787 |
| H | -6.410611 | -0.241319 | 1.618344 |
| H | -6.341589 | 0.482602 | 0.001913 |
| H | -2.209880 | -1.059891 | 2.111746 |
| H | -3.007015 | 0.422865 | 2.667075 |
| H | -3.743629 | -1.146033 | 2.986846 |
| H | -6.032099 | -1.611560 | -1.418057 |

| | | | |
|---|-----------|-----------|-----------|
| H | -5.156330 | -3.041337 | -1.978425 |
| H | -4.456212 | -1.430222 | -2.204854 |
| H | -2.432599 | -2.983024 | 0.592562 |
| H | -3.053455 | -3.804299 | -0.843487 |
| H | -2.309891 | -2.203797 | -0.992923 |
| H | -4.709748 | -3.222761 | 1.743548 |
| H | -5.292809 | -4.080695 | 0.312759 |
| H | -6.181677 | -2.679944 | 0.920967 |

Conf. 9c

| | | | |
|----|-----------|-----------|-----------|
| C | -1.200493 | 1.403823 | -0.966438 |
| C | -0.362458 | 2.562017 | -0.393009 |
| N | 0.478808 | 1.682144 | 0.244175 |
| C | -0.146604 | 0.496868 | -0.303450 |
| C | 1.830549 | 1.741613 | 0.729921 |
| C | 2.587667 | 0.586555 | 0.107688 |
| C | 1.996185 | -0.268335 | -0.827516 |
| O | 0.696183 | -0.149460 | -1.232910 |
| C | 3.926392 | 0.393834 | 0.445647 |
| C | 4.654937 | -0.619099 | -0.149667 |
| C | 4.072848 | -1.460238 | -1.092963 |
| C | 2.742250 | -1.281447 | -1.425809 |
| O | -0.381434 | 3.764939 | -0.440261 |
| H | -0.483881 | -0.221920 | 0.445078 |
| Br | 6.482043 | -0.864783 | 0.324553 |
| O | 1.918877 | 1.632741 | 2.130558 |
| C | -2.643339 | 1.271740 | -0.494937 |
| C | -3.504073 | 2.385678 | -1.069584 |
| O | -3.114356 | 0.008706 | -0.923061 |
| Si | -3.763601 | -1.229776 | 0.015946 |
| C | -5.524633 | -0.786586 | 0.575878 |
| C | -2.671653 | -1.536317 | 1.509803 |
| C | -3.766886 | -2.709141 | -1.121295 |
| C | -5.491940 | 0.341485 | 1.620082 |
| C | -6.364622 | -0.343842 | -0.632608 |
| C | -6.177037 | -2.029151 | 1.207693 |
| H | -1.146402 | 1.353802 | -2.056317 |
| H | 2.255919 | 2.693427 | 0.394546 |
| H | 4.384258 | 1.050494 | 1.175209 |
| H | 4.646137 | -2.252001 | -1.558184 |
| H | 2.260899 | -1.928491 | -2.148758 |
| H | 1.625205 | 2.460271 | 2.520865 |
| H | -2.658567 | 1.334579 | 0.602777 |
| H | -4.525705 | 2.313281 | -0.693186 |
| H | -3.100137 | 3.362809 | -0.794125 |
| H | -3.530187 | 2.310700 | -2.159871 |
| H | -1.727977 | -2.004247 | 1.215090 |
| H | -3.171649 | -2.216609 | 2.205974 |

| | | | |
|---|-----------|-----------|-----------|
| H | -2.445196 | -0.617301 | 2.058384 |
| H | -4.453938 | -2.570398 | -1.960520 |
| H | -2.764690 | -2.877678 | -1.525163 |
| H | -4.069679 | -3.611199 | -0.581731 |
| H | -4.930866 | 0.050975 | 2.513761 |
| H | -6.512496 | 0.589717 | 1.937679 |
| H | -5.043524 | 1.258549 | 1.226109 |
| H | -6.438337 | -1.134383 | -1.386175 |
| H | -7.385084 | -0.097471 | -0.313237 |
| H | -5.943953 | 0.540612 | -1.118718 |
| H | -6.259610 | -2.852748 | 0.491734 |
| H | -7.191290 | -1.786580 | 1.548694 |
| H | -5.618696 | -2.391096 | 2.077028 |

Conf. 9d

| | | | |
|----|-----------|-----------|-----------|
| C | -1.409962 | 1.723714 | -0.780798 |
| C | -0.549215 | 2.766213 | -0.040471 |
| N | 0.286169 | 1.784981 | 0.435887 |
| C | -0.362238 | 0.711043 | -0.283989 |
| C | 1.638393 | 1.739485 | 0.920866 |
| C | 2.365274 | 0.667504 | 0.134552 |
| C | 1.757973 | -0.011489 | -0.926602 |
| O | 0.463650 | 0.206417 | -1.310336 |
| C | 3.693817 | 0.382900 | 0.446168 |
| C | 4.398959 | -0.544963 | -0.297723 |
| C | 3.802814 | -1.206334 | -1.367050 |
| C | 2.480965 | -0.938161 | -1.674335 |
| O | -0.552287 | 3.961014 | 0.107009 |
| H | -0.702432 | -0.112519 | 0.346176 |
| Br | 6.212650 | -0.918758 | 0.142580 |
| O | 1.723113 | 1.428128 | 2.291209 |
| C | -2.845223 | 1.538135 | -0.307961 |
| C | -3.702207 | 2.737459 | -0.685735 |
| O | -3.326792 | 0.352017 | -0.912046 |
| Si | -4.433070 | -0.745813 | -0.273044 |
| C | -3.527252 | -2.012487 | 0.818483 |
| C | -5.187834 | -1.575865 | -1.765020 |
| C | -5.725919 | 0.167210 | 0.730371 |
| C | -2.402060 | -2.686085 | 0.016569 |
| C | -2.937304 | -1.331957 | 2.064672 |
| C | -4.524182 | -3.091726 | 1.277096 |
| H | -1.372060 | 1.847988 | -1.865286 |
| H | 2.090120 | 2.717871 | 0.726004 |
| H | 4.162347 | 0.900438 | 1.274260 |
| H | 4.359279 | -1.928777 | -1.950561 |
| H | 1.989381 | -1.446782 | -2.494535 |
| H | 1.467053 | 2.203222 | 2.798264 |
| H | -2.840237 | 1.431922 | 0.786249 |

| | | | |
|---|-----------|-----------|-----------|
| H | -4.721042 | 2.608294 | -0.317054 |
| H | -3.290301 | 3.652487 | -0.253130 |
| H | -3.734184 | 2.846968 | -1.773004 |
| H | -5.682236 | -0.837355 | -2.402175 |
| H | -5.934754 | -2.315613 | -1.462738 |
| H | -4.427774 | -2.087402 | -2.362044 |
| H | -5.275053 | 0.800119 | 1.500471 |
| H | -6.341372 | 0.801422 | 0.086317 |
| H | -6.389508 | -0.543048 | 1.232536 |
| H | -2.796739 | -3.246135 | -0.836840 |
| H | -1.854422 | -3.393139 | 0.651998 |
| H | -1.681508 | -1.960605 | -0.371417 |
| H | -3.714364 | -0.866863 | 2.679153 |
| H | -2.419830 | -2.070813 | 2.689139 |
| H | -2.207595 | -0.557391 | 1.811788 |
| H | -5.340342 | -2.670212 | 1.872398 |
| H | -4.011104 | -3.832029 | 1.903523 |
| H | -4.964543 | -3.627219 | 0.430379 |

Conf. iii-a

| | | | |
|---|-------------|-------------|-------------|
| C | 2.38719500 | -0.85831400 | 0.87760100 |
| C | 1.87612100 | -0.60661700 | -0.55394300 |
| N | 1.81684800 | 0.82135500 | -0.27679400 |
| O | 0.62117700 | -1.23688300 | -0.84686300 |
| C | -0.51739400 | -0.63804600 | -0.39471300 |
| C | -0.61094700 | 0.75525600 | -0.34843700 |
| C | 0.62749400 | 1.51547100 | -0.74637800 |
| C | -1.59557700 | -1.43891500 | -0.03797200 |
| C | -2.78252100 | -0.84124100 | 0.36661900 |
| C | -2.88756200 | 0.54418800 | 0.43371100 |
| C | -1.79756200 | 1.33355400 | 0.08312800 |
| H | 3.45695500 | -1.05933500 | 0.93005200 |
| H | 1.83500100 | -1.62630300 | 1.41769000 |
| H | 2.51343000 | -0.89316800 | -1.39224900 |
| H | 0.61926000 | 2.53127500 | -0.34336800 |
| H | 0.69324900 | 1.59866800 | -1.83711600 |
| H | -1.49104700 | -2.51613500 | -0.09023300 |
| H | -3.62743400 | -1.46341200 | 0.63976300 |
| H | -3.81136300 | 1.00651200 | 0.76112000 |
| H | -1.86929400 | 2.41590700 | 0.13731000 |
| C | 1.99498400 | 0.60391700 | 1.17403800 |
| H | 2.76152500 | 1.24469400 | 1.61465900 |
| H | 1.06698400 | 0.69136200 | 1.75291600 |

Conf. iii-b

| | | | |
|---|------------|-------------|-------------|
| C | 2.95996900 | -0.85053400 | -0.03841900 |
| C | 1.58313600 | -0.59863100 | -0.65468800 |
| N | 1.71922400 | 0.80987000 | -0.35495900 |

| | | | |
|---|-------------|-------------|-------------|
| O | 0.58546700 | -1.26393800 | 0.13102000 |
| C | -0.63059800 | -0.64663800 | 0.07589000 |
| C | -0.71889800 | 0.74261200 | -0.01868000 |
| C | 0.53702700 | 1.58144200 | -0.00501000 |
| C | -1.77583000 | -1.43487700 | 0.13816000 |
| C | -3.02466800 | -0.83404500 | 0.10204900 |
| C | -3.13300700 | 0.54921300 | -0.01619900 |
| C | -1.98332900 | 1.32331500 | -0.08155600 |
| H | 3.75557800 | -0.89776200 | -0.78072400 |
| H | 3.00700800 | -1.70596800 | 0.63247300 |
| H | 1.38924300 | -0.83644500 | -1.70553400 |
| H | 0.67548000 | 1.99153200 | 1.00405400 |
| H | 0.41619800 | 2.43671600 | -0.67939800 |
| H | -1.66420300 | -2.51002000 | 0.21385500 |
| H | -3.91690100 | -1.44777700 | 0.15335300 |
| H | -4.10825600 | 1.01963600 | -0.05972900 |
| H | -2.06183400 | 2.40283900 | -0.17265700 |
| C | 2.80053300 | 0.54528200 | 0.60626100 |
| H | 3.64640100 | 1.23316500 | 0.53562100 |
| H | 2.45697500 | 0.49366900 | 1.64839600 |