Abstract

In this work, we study the light absorption properties of a novel molecule (BTTzR) and its more extended derivatives, which hold promise as electron-donor material in organic solar cells. By employing density functional theory, we observe that the addition of two and three oligothiophene chains to the central benzene ring of the benzo[1,2-b:4,5-b’]dithiophene (BDT-T) leads to both a red-shift of the existing peaks and, interestingly, to the development of new blue-shifted features, an effect that can certainly increase the panchromaticity of the molecule in the visible spectral range.

Introduction

Together with other materials exhibiting high photovoltaic ability, such as metal-halide perovskites [1–3], semiconducting polymers [4,5], quantum dots [6,7], and carbon nanotubes [8,9], small molecules are widely studied in the solar cell research community. In these regards, atomically precise synthesis of small-molecules allows a negligible batch-to-batch variations [10], which is an important requirement for devices reproducibility and reliability. For instance, fullerene derivatives have represented the workhorse electron-acceptor materials for decades [11–13], together with poly(thiophene) derivatives as electron-donor system [14,15]. However, fullerenes suffer from two important drawbacks, such as a relatively low absorption in the visible spectrum and photo-instabilities (i.e dimerization), which limit considerably the power conversion efficiency of the related devices [16].

Therefore, recently many reports have focused on the replacement of fullerene derivatives as electron-acceptor molecule in organic solar cells [17]. For example, newly developed molecules like BPTTT-4F (also called Y6) permit to achieve a noteworthy efficiency of 16.02 % [18–20]. In addition, the research of new donor materials has been fruitful in the last years. In 2020, a novel small molecule donor, BTTzR, has been developed and an all-small-molecule solar cell employing BTTzR as donor shows a power conversion efficiency (PCE) of 13.9% [21].

Given the high interest in these promising function materials, in this work we analyse the light absorption features of BTTzR and its extended derivatives by means of density functional theory. By
increasing the length of the thiophene pendants attached to the benzo[1,2-b:4,5-b’]dithiophene (BDT-T) central unit of the molecule, we can observe a red-shift of the absorption together with the occurrence of new absorption features at higher energy. This aspect can be important to attain panchromaticity, and thus reach even higher power conversion efficiencies with these promising molecules.

Methods

The molecules have been designed with the Avogadro package [22]. We have optimized the geometries and calculated the electronic transitions, by means of the density functional theory, with the ORCA package, developed by Frank Neese and coworkers [23]. In these calculations we have used the B3LYP functional [24]. Moreover, we have employed the Ahlrichs split valence basis set [25] together with the all-electron nonrelativistic basis set SVPalls1 [26,27]. Finally, for thiese calculations we have used the Libint library [28] and the Libxc library [29,30]. The calculations have been performed on a Dell Precision Tower Workstation 7910, which mounts Dual Intel Xeon processors (10 cores, 2.35GHz) and 64 Gb of RAM memory.

Results and Discussion

In Figure 1a, we show the optimized geometry of the BTTzR molecule. The dihedral angle between the thiazolo-[5,4-d]thiazole (TTz) group and the BDT-T group along the backbone of the molecule is 14° on one side and 3° on the other side. The dihedral angle between the thiophene molecule and BDT-T is 52° on one side and 55° on the other side. These angles are in good agreement with the ones of optimized geometries reported in the literature [21].
Figure 1. a) Optimized geometry of BTTzR molecule; b) energy levels of BTTzR with the lowest four singlet excited states and the lowest four triplet excited states.

In Figure 1b, we show the energy levels of BTTzR, highlighting the ground state at -5.41 eV and the four lowest singlet excited states at -3.25 eV, -3.17 eV, -2.69 eV, and -2.36 eV, respectively. We also show the four lowest triplet excited states at -3.92 eV, -3.87 eV, -3.65 eV, and -3.43 eV, respectively.

In Figure 2a, we show the optimized geometry of BTTzRv2 (where _v2 is used to simply highlight that it is a second derivative/version of the molecule) with two thiophene molecules attached to the BDT-T unit.
Figure 2. a) Optimized geometry of BTTzRv2 molecule, with two thiophenes attached to the BDT-T unit; b) energy levels of BTTzRv2 with the lowest four singlet excited states and the lowest four triplet excited states.

In Figure 2b, we show the energy levels of BTTRv2. The ground state is at -5.36 eV and the lowest four singlet excited states are at -3.25 eV, -3.17 eV, -2.71 eV, and -2.36 eV, respectively. With respect to BTTzR, we notice a ground state higher in energy. The lowest four triplet excited states are at -3.88 eV, -3.81 eV, -3.63 eV, and – 3.40 eV, respectively.
In Figure 3a, we show the optimized geometry of BTTzRv3 in which three thiophene molecules are attached to the BDT-T unit. In Figure 3b the energy levels of the molecule are depicted with the ground state at -5.27 eV (higher with respect of BTTzR and BTTzRv2), the lowest four singlet excited states at -3.23 eV, -3.17 eV, -2.71 eV, and -2.36 eV, respectively, the lowest four triplet excited states at -3.80 eV, -3.73 eV, -3.58 eV, and -3.37 eV, respectively.
In Figure 4, we show the absorption spectra of BTTzR (solid black curve), of BTTzRv2 (dotted dashed blue curve) and of BTTzRv3 (dashed red curve) in the visible spectral range. The calculated lowest electronic transition is at lower energy with respect to the experimental one (in solution it has been reported a maximum absorption peak at 528 nm) [21] and this could be due to a discrepancy between the dihedral angles in the calculated optimized geometry and the actual dihedral angles of the molecules in solution. In the Supporting Information we report the lowest 16 electronic (singlet to singlet) transitions and the lowest 16 triplets. Here, we notice a red shift of the lowest transition from BTTzR to BTTzRv2 and BTTzRv3, due to an increased delocalization thanks to the longest thiophene chains attached to the BDT-T unit. Moreover, with BTTzR we observe two intense absorption peaks and with BTTzRv2 three intense absorption peaks. Finally, with BTTzRv3 five intense absorption peaks at 685, 595, 535, 498, and 459 nm, respectively, that span a significant range of the visible spectrum. The larger number of absorption peaks of BTTzRv3 can lead to a potential increased absorption of the Sun irradiation (the orange curve in Figure 4 displays the direct and circumsolar irradiation of the Sun, reference Air Mass 1.5 [31]), useful for the fabrication of efficient photovoltaic cells.

Conclusion

In this work, we have studied the optical properties in the visible range of the donor molecule BTTzR and of two derivatives of BTTzR in which we have increased the number of thiophene molecules attached to the BDT-T central unit. We have calculated the singlet and triplet excited states noticing
a red-shift of such levels by increasing the number of thiophene molecules. Furthermore, addition of the thiophene pendants leads to the appearance of new blue-shifted absorption features, which could lead to an increased panchromaticity and power conversion efficiencies in the related solar cells.

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### Supporting Information

#### Electronic transitions of BTTzR

| State | Energy (cm⁻¹) | Wavelength (nm) | fosc | P₂ (au²) | PX (au) | PY (au) | PZ (au) |
|-------|---------------|-----------------|------|----------|---------|---------|---------|
| 1     | 15636.7       | 639.5           | 1.477920350 | 0.15794 | 0.39145 | -0.06810 | 0.00855 |
| 2     | 16841.4       | 593.8           | 0.000148771 | 0.00002 | -0.00239 | 0.00046 | -0.00335 |
| 3     | 19169.3       | 521.7           | 0.118158338 | 0.14649 | -0.38074 | 0.03903 | -0.00286 |
| 4     | 19586.7       | 510.5           | 0.003746041 | 0.00050 | 0.01747 | -0.00375 | 0.01278 |
| 5     | 19745.5       | 506.4           | 0.189033996 | 0.02551 | -0.15151 | -0.05018 | 0.00618 |
| 6     | 20479.1       | 488.3           | 0.001839254 | 0.00026 | -0.00895 | 0.00372 | 0.00661 |
| 7     | 20837.2       | 479.9           | 0.000326065 | 0.00005 | 0.00000 | 0.00111 | 0.00672 |
| 8     | 20847.0       | 479.7           | 0.000323086 | 0.00005 | 0.00010 | 0.00151 | 0.00661 |
| 9     | 20968.3       | 476.9           | 0.015320480 | 0.00220 | -0.00449 | -0.04615 | 0.00672 |
| 10    | 22540.7       | 443.6           | 0.000874983 | 0.00013 | 0.00050 | 0.00056 | 0.01159 |
| 11    | 22775.7       | 439.1           | 0.000153792 | 0.00002 | 0.00158 | 0.00102 | 0.00452 |
| 12    | 23280.6       | 429.5           | 0.028952128 | 0.00461 | -0.06694 | -0.00978 | 0.00543 |
| 13    | 24070.7       | 415.4           | 0.01279640  | 0.00209 | -0.03382 | 0.03077 | 0.00059 |
| 14    | 24155.1       | 414.0           | 0.028952128 | 0.00461 | -0.06694 | -0.00978 | 0.00543 |
| 15    | 25124.1       | 398.0           | 0.061174498 | 0.01050 | -0.09766 | 0.03110 | -0.00055 |
| 16    | 25333.4       | 394.7           | 0.000003101 | 0.00000 | 0.00021 | 0.00011 | -0.00069 |
| 17    | 11981.2       | 834.6           | spin forbidden (mult=3) | |
| 18    | 12439.2       | 803.9           | spin forbidden (mult=3) | |
| 19    | 14194.1       | 704.5           | spin forbidden (mult=3) | |
| 20    | 15975.1       | 626.0           | spin forbidden (mult=3) | |
| 21    | 17394.4       | 574.9           | spin forbidden (mult=3) | |
| 22    | 17571.9       | 569.1           | spin forbidden (mult=3) | |
| 23    | 17997.6       | 555.6           | spin forbidden (mult=3) | |
| 24    | 19105.0       | 514.9           | spin forbidden (mult=3) | |
| 25    | 19111.4       | 523.2           | spin forbidden (mult=3) | |
| 26    | 19420.1       | 514.9           | spin forbidden (mult=3) | |
| 27    | 19885.6       | 502.9           | spin forbidden (mult=3) | |
| 28    | 20426.2       | 489.6           | spin forbidden (mult=3) | |
| 29    | 21344.0       | 468.5           | spin forbidden (mult=3) | |
| 30    | 21648.1       | 461.9           | spin forbidden (mult=3) | |
| 31    | 22325.9       | 447.9           | spin forbidden (mult=3) | |
| 32    | 22379.8       | 446.8           | spin forbidden (mult=3) | |

#### Electronic transitions of BTTzRv2

| State | Energy (cm⁻¹) | Wavelength (nm) | fosc | T₂ (au²) | TX (au) | TY (au) | TZ (au) |
|-------|---------------|-----------------|------|----------|---------|---------|---------|
| 1     | 15197.0       | 658.0           | 2.021711980 | 43.79628 | 6.61637 | 0.01638 | 0.14028 |
| 2     | 16215.0       | 616.7           | 0.0001142288 | 0.02319 | -0.03198 | -0.01493 | -0.14814 |
| 3     | 17796.4       | 561.9           | 2.135623480 | 39.50656 | 6.20020 | -1.03139 | 0.00954 |
| 4     | 18888.6       | 529.4           | 0.009513454 | 0.16583 | 0.40637 | -0.00009 | -0.02627 |
| 5     | 19294.0       | 517.3           | 0.585182800 | 9.98491 | -3.09206 | -0.58201 | -0.29207 |
| 6     | 19317.0       | 516.4           | 0.334647470 | 5.70326 | 2.34523 | 0.43517 | -0.11751 |
| 7     | 20202.4       | 495.0           | 0.188798469 | 3.07661 | 1.39238 | -1.06088 | -0.11144 |
| 8     | 20598.5       | 485.0           | 0.01422198 | 0.02273 | -0.03882 | 0.03251 | 0.14201 |
| 9     | 20833.9       | 480.0           | 0.000015203 | 0.00024 | -0.00021 | 0.00232 | 0.01532 |
| 10    | 20844.4       | 479.7           | 0.000017564 | 0.00028 | 0.00113 | 0.00339 | -0.01627 |
| 11    | 21335.9       | 468.7           | 0.127834201 | 1.97248 | 1.32198 | -0.47219 | -0.04352 |
| 12    | 21749.0       | 459.8           | 0.216770939 | 3.28123 | -1.64249 | 0.76154 | 0.05920 |
| 13    | 21979.1       | 455.0           | 0.000775872 | 0.01162 | 0.03148 | -0.01668 | -0.10174 |
| 14    | 22418.7       | 446.1           | 0.001309972 | 0.01924 | -0.12708 | 0.03627 | 0.04209 |
### Electronic transitions of BTTzRv3

| State | Energy (cm⁻¹) | Wavelength (nm) | T2 (au²) | TX (au) | TY (au) | TZ (au) |
|-------|--------------|----------------|----------|---------|--------|--------|
| 1     | 14575.0      | 686.1          | 0.958641369 | 21.65330 | 4.61040 | 0.59038 | 0.22124 |
| 2     | 15456.2      | 647.0          | 0.000546135 | 0.01163  | -0.00565 | -0.01865 | -0.10606 |
| 3     | 16801.2      | 595.2          | 2.689394058 | 52.69738 | -7.17553 | 1.09931 | -0.02526 |
| 4     | 16927.2      | 590.8          | 0.128157372 | 2.49249  | -1.56308 | 0.21671 | 0.04793  |
| 5     | 17844.4      | 560.7          | 0.101340088 | 1.87068  | 1.36645  | -0.00568 | 0.04793  |
| 6     | 18156.6      | 552.0          | 0.001088340 | 0.01978  | -0.05628 | -0.01278 | 0.12825  |
| 7     | 18677.8      | 535.4          | 0.474955273 | 8.37148  | -2.05719 | -1.99386 | -0.40489 |
| 8     | 19565.3      | 511.1          | 0.003204190 | 0.05391  | 0.01187  | -0.01572 | -0.23135 |
| 9     | 20071.7      | 498.2          | 1.175644149 | 19.28263 | -4.23088 | 1.17007 | 0.11496  |
| 10    | 20693.8      | 483.2          | 0.221034971 | 3.51639  | 1.80677  | -0.50116 | -0.02824 |
| 11    | 20834.8      | 480.0          | 0.000026763 | 0.00042  | -0.01180 | 0.00536  | 0.01597  |
| 12    | 20846.8      | 479.7          | 0.000018053 | 0.00029  | 0.00355  | 0.00334  | -0.01616 |
| 13    | 20877.7      | 479.0          | 0.002634004 | 0.04153  | -0.20215 | 0.02540  | -0.00500 |
| 14    | 21370.5      | 467.9          | 0.002071393 | 0.00416  | -0.03430 | -0.00684 | -0.05421 |
| 15    | 21783.9      | 459.1          | 0.463656807 | 7.00706  | -1.76922 | 1.93890 | 0.34289  |
| 16    | 21869.8      | 457.3          | 0.000468562 | 0.00705  | 0.02898  | -0.05660 | 0.05486  |
| 17    | 11880.7      | 841.7          | spin forbidden (mult=3) | |
| 18    | 12430.2      | 804.5          | spin forbidden (mult=3) | |
| 19    | 13670.3      | 731.5          | spin forbidden (mult=3) | |
| 20    | 15318.3      | 652.8          | spin forbidden (mult=3) | |
| 21    | 15658.5      | 638.6          | spin forbidden (mult=3) | |
| 22    | 16299.8      | 613.5          | spin forbidden (mult=3) | |
| 23    | 16330.6      | 612.3          | spin forbidden (mult=3) | |
| 24    | 16625.4      | 601.5          | spin forbidden (mult=3) | |
| 25    | 17285.8      | 578.5          | spin forbidden (mult=3) | |
| 26    | 17689.6      | 565.3          | spin forbidden (mult=3) | |
| 27    | 17861.0      | 559.9          | spin forbidden (mult=3) | |
| 28    | 18271.8      | 547.3          | spin forbidden (mult=3) | |
| 29    | 18935.2      | 528.1          | spin forbidden (mult=3) | |
| 30    | 19102.5      | 523.5          | spin forbidden (mult=3) | |
| 31    | 19110.3      | 523.3          | spin forbidden (mult=3) | |
| 32    | 19804.3      | 504.9          | spin forbidden (mult=3) | |
Optimized geometry of BTTzR

C    -1.03432534647874  1.27609255762794  -0.33137107176170
C     0.27403668772595  0.77206200386489  -0.32608693216699
C     1.37177848855338  1.73292170895384  -0.39060869321699
C    -0.100622053152298  3.12668827971284  -0.47116984855369
C    -0.30195332940943  3.63068729017538  -0.47607120928352
C    -1.34585609179201  2.67034527322190  -0.40406811597165
C    -2.76155877295254  2.8939172833210    -0.44846239467722
C    -3.51140419599594  1.74252726969653  -0.40173178899706
H    -3.20627399670976  3.88616637207674  -0.53688840705873
S     2.47658180747666  4.10197970906161  -0.4946633341710
C     2.73302651491901  1.51057521604481  -0.3354725236394
C     3.48345012070674  2.66207001601703  -0.38342137694998
H    -1.37705991716617  0.51749967780979  -0.25420438183767
C     3.59204754165998  1.60609849242000  -0.42456134161912
C     4.92313577455641  2.79856570604829  -0.34357719039001
C    -5.70365715791396  0.45699354569662  -0.63713907831342
C    -7.07914278985245  0.68337992133148  -0.59505933595959
C    -7.4201858854423    2.00813652061200  -0.34670086056222
H     5.67780001680938  0.96201889417676  -0.43537181201051
S     7.06933539885008  3.73657318036829  -0.35483545430375
H     2.03970252751061  -0.19951840752257
S     5.95988720181063  1.40369570730743  -0.15335887980506
H     5.25469930017819  -0.51896170422408  -0.83452591676586
H    -7.84224983595389  -0.10144378958953  -0.74620786759200
H     5.23277342109370  4.9520325468343   -0.56047862391774
S     7.81532135823089  4.53317424100294  -0.40813361531300
C     8.72459562279432  2.62437648308585  -0.22324737405611
C    -8.90763133930003  3.9044903257623   0.02677561461669
C     8.70091824282932  4.7564418354143  -0.07299033600227
S     10.1852541601101  2.75271573605439  -0.10440918037585
C     13.87126473401632  0.91313070060559  0.51281595639647
C     14.19834703009136  2.25051794177097  0.69889974190636
C     15.5814675867814  -2.46619948051028  0.81669061680675
C     16.34076167674582  1.2977033177516   0.72013104207710
S     15.29855445095548  0.88318239093996  0.47911564867201
H     13.45160998190886  -0.0461961058440  0.75332499090174
C     16.04046609454111  3.44668924891803  0.97205550244181
C     13.9719453400551  5.28335765956159  0.37530336922242
C     14.24730839008022  6.60427729468580  0.66409611510350
C     15.63605698324199  6.82047602446073  0.73691741177195
C     16.3924286044340  5.67098209683219  0.50498503462757
S     15.34642843071443  4.30148241102280  0.19148532598585
H     -16.09460365697263  7.7874500950370  0.95663689606141
Optimized geometry of BTTzRv2

H  -13.50023983064748  7.38588856279933  0.82077817326793
C  -17.8235698086899  5.61012361549181  0.52343316269248
C  -18.66870720109356  4.56235581538682  0.3208983991282
H  -18.33149436700356  6.55864251805709  0.73764825038354
C  -18.66870720109356  4.56235581538682  0.3208983991282
H  -18.33149436700356  6.55864251805709  0.73764825038354
C  -20.00990842292912  2.41563879435028  -0.09389620304844
S  -20.55696123194333  0.90312950857850  -0.39673961758567
N  -20.76940926611964  3.5282133420867  0.1608474781568
C  -20.14261806210255  4.75667369417538  0.40078701496481
H  -21.7844581838444  3.45835885419955  0.1753495909875
O  -20.73500944499808  5.78668309472330  0.63246849651617
C  17.76890339977175  -1.23186365743568  0.81111761805869
N  -20.76940926611964  3.5282133420867  0.1608474781568
C  -20.14261806210255  4.75667369417538  0.40078701496481
H  -21.7844581838444  3.45835885419955  0.1753495909875
O  -20.73500944499808  5.78668309472330  0.63246849651617
C  -1.07032166562176  1.3526420979801  -0.41527214705539
C  0.23502248434779  0.83850547090501  -0.44406349312342
C  1.28572235736253  1.79534924750544  -0.47837970285368
C  0.9831406657914  3.19323214760716  -0.49990195859051
C  -0.32122016307571  3.70724818909743  -0.47092811960949
C  -1.3178368637146  2.75070805141579  -0.42849934050118
C  -2.78599317417635  2.9858946001414  -0.4588558047619
S  -3.54429586996194  1.8397121635334  -0.4577795807274
H  -3.22496451489699  3.9833254670532  -0.50793140067337
S  -2.5399951998297  0.3887476662114  -0.4167579843493
C  2.45217762477451  4.15832547907478  -0.4915463964938
C  2.69973954619313  1.5616448080397  -0.44143687574345
C  3.45817490108451  2.7065367404931  -0.44861978517382
H  3.13889305772314  0.56363896126163  -0.40571294046525
C  -4.96807691085832  1.71633692812921  -0.48468860048755
C  4.89923323959686  2.83322456420278  -0.41747769009823
C  -5.74868415848190  0.58595382823325  -0.75337883540864
|   | 20.67841076958747 | 0.78439457145148 | 0.52674464093345 |
|---|-----------------|-----------------|-----------------|
| H  | 21.69251674556168 | 0.84939374294627 | 0.57921336808857 |
| S  | 20.49047865937453 | 3.43630073962386 | 0.1020488296610 |
| C  | -0.56505841419629 | 5.15908391910894 | -0.486632372752296 |
| C  | -0.04010057802059 | 6.10721431917968 | -1.343641518411719 |
| C  | -0.45881815967383 | 7.43342796579724 | -1.05547204215768 |
| C  | -1.30476144834381 | 7.52015128052422 | 0.03565334472838 |
| C  | -0.66274819639333 | 8.30225821216378 | -1.649588533111934 |
| H  | 0.60976946446892 | 5.84814929149044 | -2.18213439721599 |
| S  | -1.56995047160452 | 5.93447591863290 | 0.72198166965807 |
| C  | 0.4789784656747 | -0.61318908612903 | -0.43354886185582 |
| C  | -0.05268598746699 | -1.56623031956739 | 0.41390133235421 |
| C  | 0.36814875281050 | -2.8908410838778 | 0.12156911411580 |
| C  | 1.22260439551993 | -2.97165262983646 | -0.9633643739934 |
| H  | 0.07115492704126 | -3.76278834575594 | 0.70861591342068 |
| H  | -0.70890227366933 | -1.31233882529408 | 1.24904800523914 |
| S  | 1.49352602144833 | -1.38222029708981 | -1.63864111699218 |
| C  | 1.85337781808371 | -4.14106953370374 | -1.54940057738336 |
| C  | 2.95348025843991 | -2.10545395812027 | -2.38601407082948 |
| C  | 3.29269622101955 | -5.5413866646178 | -2.76338089556503 |
| C  | 2.45264818724999 | -6.4783023565186 | -2.21379215001197 |
| S  | 1.22753040908849 | -5.74653850916138 | -1.23744120744397 |
| H  | 4.13394551943065 | -5.79434332808951 | -3.4132145966820 |
| C  | 2.48053736076227 | -7.56259292416587 | -2.33014186000414 |
| H  | 3.51176423231136 | -3.32752259069682 | -2.70543594866620 |
| C  | -1.93115090287524 | 8.69272400433025 | 0.62010242522414 |
| C  | -3.02660801184285 | 8.76690201446271 | 1.46241975202361 |
| C  | -3.36248911240117 | 10.09975602039754 | 1.83568529423742 |
| C  | -2.52457305127911 | 11.03344235892309 | 1.27734212035293 |
| S  | -1.3054239858846 | 10.29615053426398 | 0.29778907271758 |
| H  | -3.8406407833500 | 7.88563556561956 | 1.7869006080705 |
| H  | -4.19995711822286 | 10.35639150957923 | 2.48862805197113 |
| H  | -2.55084693174215 | 12.11826351401434 | 1.38907560783680 |

Optimized geometry of BTbRv3

|   | 1.38289973744552 | -0.41005895622014 |
| C  | 0.85975120141104 | -0.45119880356502 |
| C  | 1.80959348418930 | -0.46239693987445 |
| C  | 3.2096253809953 | -0.44937868510014 |
| C  | 10.29615053426398 | 0.29778907271758 |
| C  | 2.78289122933531 | -0.38913725087179 |
| C  | 3.02909760131425 | -0.41596405233833 |
| C  | 0.8847093005729 | -0.44418904761171 |
| C  | 4.03057822041045 | -0.44043455506058 |
| C  | 0.43302922841262 | -0.43854906588389 |
| C  | 1.56448981132284 | -0.4322159985366 |
| C  | 2.70552307902761 | -0.41163068752945 |
| C  | 0.56279472479841 | -0.4238709476434 |
| C  | 1.77750215825606 | -0.47752009723443 |
| C  | 2.81840125844880 | -0.38312159639175 |
| C  | 0.65729629959240 | -0.76560426670745 |
| C  | 0.90597259312953 | -0.71625172253060 |
| C  | 2.21818753903529 | -0.38646301184907 |
| C  | 3.96760021326839 | -0.49396480175942 |
| C  | 3.71775484857169 | -0.42575923166562 |
C  -0.02770845088942      6.15158640971498    -1.21636000344986
C  -0.43735959242444      7.47267286425487    -0.89849118766896
C  -1.29310765887905      7.54004796481347     0.18824636616376
H  -0.12923070516547     8.35314109149479    -1.46671793077973
H   0.62795828906703     5.90908132100831    -2.05526360572526
S   -1.57931324550366     5.93798119173878     0.83001948402656
C   0.43320568397551     -0.59314043524264    -0.4747234887104
C  -0.11221534476294    -1.56243226688752     0.34577357582806
C   0.29882054147416    -2.88239232070578     0.02476947084979
C   1.16142624466363    -2.94553629421109     1.05674953674136
H  -0.03142074706419     -3.76499712839035     0.58730595160860
H   -1.77293241647071    -1.32355678067310     1.18176086484774
S   1.45260414749534    -1.34084043361602    -1.68977109825131
C   1.78459910035371    -4.10451552311176    -1.66177725915243
C   2.81478943876300    -4.1609456530123     2.58571824893965
C   3.16909933215915    -5.48056671201620    -2.96106056359148
C   2.41889742068727    -6.45833463218915    -2.32955911965101
S   1.25239014973643    -5.72223152953540    -1.25202025584322
H   3.95361088240239    -5.71191572691985     3.68575756821166
H   3.30836260307343    -3.26944345432521     2.97887045334752
C  -1.9129640034816     8.70130320901663     0.79233521072278
C  -2.93816445399174     8.76117746562676     1.72159128331319
S   -3.29019203653184    10.08219326803800    2.09413867011977
C  -2.54330517877773    11.0578436363049     1.45503789455114
S   -1.38284091946004    10.3174373299071     0.37382777116935
H  -3.42975010697178     7.87116960053370    2.12058535511946
H   -4.07061702810825     10.31625760590751    2.82237299875864
C  -2.60279503357969    12.50016905624032     1.58164560183237
C   -1.73147285463178    13.46323761205121    1.13625962100327
C  -2.13549738005633    14.79324931460816     1.44621942813537
C  -3.32778236902849    14.83996179599260     2.12574329880647
H  -0.80404726913526    13.21735808079875     0.61353985044391
H  -1.55939818090227    15.68188227820881     1.17830077288212
S   -3.97840066523442    13.25924027190765     2.38839396625607
H   -3.86567415360706    15.71617668627056     2.48878679677517
C   2.49734433431565    -7.90045071651930    -2.46081927947250
C   1.60617972570513    -8.86534803987005    -2.02291003365821
C   2.01187874996736    -10.19408601587136    -2.33575410217194
C   3.20713392067111    -10.23810751187573    -3.01017712737227
H   0.67630396708421    -8.62139071144277    -1.50362354162866
C   1.43467465667123    -11.08377127654508    -2.07377346274890
S   3.85908906208345    -8.65640844499774    -3.26347782651840
H   3.74680668548786    -11.11289575476165     3.37408552098615