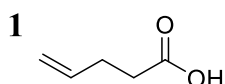


## Hatékony számítási protokoll tervezése halociklizációs reakciók leírására

### Optimált szerkezetek koordinátái

A dolgozatban szereplő, M06-2X-D3 funkcionállal gázfázisban optimált szerkezetek Descartes koordinátái. Az egyes szerkezeteket ábrái után az első sorban az atomok száma szerepel, a következőben a szerkezet neve, ezután pedig az egyes atomok *x*, *y*, *z* koordinátái következnek (angström egységben).

#### A Wang-féle reakció szerkezetei:

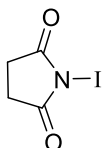


15

**1**

|   |          |          |          |
|---|----------|----------|----------|
| C | 3.22018  | 0.31316  | -0.24314 |
| H | 3.10512  | 1.38351  | -0.43596 |
| H | 4.19911  | -0.12883 | -0.43692 |
| C | 2.20499  | -0.41672 | 0.21518  |
| H | 2.35620  | -1.48786 | 0.39497  |
| C | 0.82975  | 0.11437  | 0.49635  |
| H | 0.79961  | 1.19951  | 0.32414  |
| H | 0.58046  | -0.05167 | 1.55789  |
| C | -0.23195 | -0.56995 | -0.37355 |
| H | -0.22954 | -1.65926 | -0.23874 |
| H | -0.01779 | -0.36368 | -1.43474 |
| C | -1.63569 | -0.09548 | -0.09343 |
| O | -1.71661 | 1.24580  | -0.05138 |
| H | -2.64440 | 1.46674  | 0.12398  |
| O | -2.59245 | -0.79964 | 0.06850  |

**NIS**



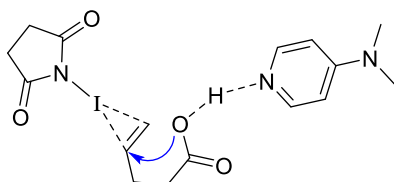
12

**NIS**

|   |         |          |          |
|---|---------|----------|----------|
| C | 1.29840 | 1.17835  | 0.00001  |
| C | 1.29837 | -1.17835 | 0.00049  |
| C | 2.76454 | -0.76447 | 0.00097  |
| C | 2.76456 | 0.76443  | -0.00078 |
| H | 3.24087 | -1.20786 | 0.88554  |
| H | 3.24256 | -1.21020 | -0.88149 |
| H | 3.24274 | 1.21016  | 0.88158  |

|   |          |          |          |
|---|----------|----------|----------|
| H | 3.24074  | 1.20779  | -0.88545 |
| N | 0.54430  | 0.00001  | 0.00014  |
| O | 0.85010  | 2.28583  | 0.00013  |
| O | 0.85004  | -2.28583 | -0.00009 |
| I | -1.49308 | 0.00001  | -0.00011 |

**W-i**



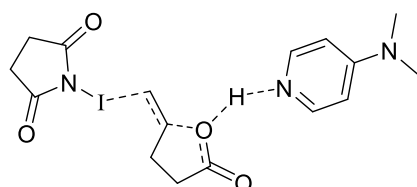
46

**W-i**

|   |          |          |          |
|---|----------|----------|----------|
| C | -1.06529 | -1.80900 | -0.36933 |
| C | 0.19321  | -2.65589 | -0.40541 |
| O | -1.00385 | -0.76219 | -1.16495 |
| C | 1.47443  | -1.81426 | -0.40657 |
| C | 1.34979  | 0.30595  | 0.93914  |
| H | 1.40001  | 0.83688  | 1.89229  |
| O | -2.02348 | -2.08955 | 0.31431  |
| H | 1.05370  | 0.87464  | 0.05296  |
| H | 2.34523  | -2.47938 | -0.51006 |
| H | 1.45707  | -1.14253 | -1.27619 |
| H | 0.14996  | -3.34241 | 0.45048  |
| H | 0.15457  | -3.26408 | -1.32318 |
| N | 6.41301  | 0.59431  | -0.03924 |
| C | 7.22563  | -0.37125 | -0.63022 |
| C | 8.61870  | 0.23287  | -0.77292 |
| C | 7.06133  | 1.79367  | 0.24909  |
| O | 6.55437  | 2.75286  | 0.75557  |
| O | 6.87466  | -1.46822 | -0.95777 |
| H | -1.87682 | -0.22630 | -1.10209 |
| C | 1.59693  | -1.00837 | 0.85512  |
| H | 1.84807  | -1.56128 | 1.76860  |
| C | -4.17878 | 0.12310  | -0.12813 |
| C | -5.40196 | 0.73460  | 0.09393  |
| C | -5.71799 | 1.93489  | -0.58505 |
| C | -4.72874 | 2.43372  | -1.46638 |
| C | -3.53948 | 1.73895  | -1.61178 |
| N | -3.25445 | 0.60725  | -0.96483 |
| H | -3.90325 | -0.80482 | 0.38088  |
| H | -6.09818 | 0.27440  | 0.79142  |
| H | -4.87791 | 3.34976  | -2.03345 |
| H | -2.77058 | 2.11805  | -2.29089 |
| C | 8.51162  | 1.64500  | -0.19897 |

|   |          |          |          |
|---|----------|----------|----------|
| H | 9.15651  | 1.82205  | 0.67209  |
| H | 8.72570  | 2.43917  | -0.92659 |
| H | 9.32627  | -0.41363 | -0.23688 |
| H | 8.89478  | 0.20340  | -1.83542 |
| N | -6.90654 | 2.57506  | -0.40189 |
| C | -7.18203 | 3.79891  | -1.12154 |
| H | -7.16480 | 3.64232  | -2.21283 |
| H | -8.17763 | 4.16249  | -0.84625 |
| H | -6.45081 | 4.58753  | -0.87854 |
| C | -7.88521 | 2.02350  | 0.50961  |
| H | -7.49140 | 1.95652  | 1.53708  |
| H | -8.76815 | 2.67113  | 0.52499  |
| H | -8.20533 | 1.01472  | 0.20102  |
| I | 4.41921  | 0.27226  | 0.37231  |

**W-i-ts**



46

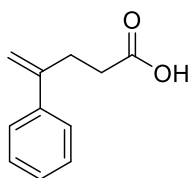
**W-i-ts**

|   |          |          |          |
|---|----------|----------|----------|
| C | -1.01346 | -2.10507 | -0.09511 |
| C | 0.30236  | -2.83210 | -0.29919 |
| O | -0.79207 | -0.85847 | 0.24225  |
| C | 1.30527  | -1.75284 | -0.69385 |
| C | 1.25554  | 0.77653  | -0.39466 |
| H | 1.02425  | 1.62616  | 0.25325  |
| O | -2.12241 | -2.58086 | -0.22556 |
| H | 1.04710  | 0.92891  | -1.45803 |
| H | 2.34801  | -2.05647 | -0.52223 |
| H | 1.20950  | -1.50227 | -1.76164 |
| H | 0.57617  | -3.29424 | 0.66329  |
| H | 0.18581  | -3.63779 | -1.03321 |
| N | 5.95696  | 0.83388  | -0.28224 |
| C | 6.71448  | -0.31344 | -0.28279 |
| C | 8.19872  | 0.07504  | -0.26952 |
| C | 6.71039  | 1.98464  | -0.26964 |
| O | 6.28620  | 3.11336  | -0.26746 |
| O | 6.29298  | -1.44424 | -0.29175 |
| H | -2.01250 | -0.05135 | 0.14184  |
| C | 1.01005  | -0.51470 | 0.12428  |
| H | 1.17912  | -0.63144 | 1.20064  |
| C | -4.09068 | -0.22300 | -0.12769 |
| C | -5.30509 | 0.39921  | -0.30322 |

|   |          |          |          |
|---|----------|----------|----------|
| C | -5.37593 | 1.81958  | -0.34459 |
| C | -4.14837 | 2.52727  | -0.19993 |
| C | -2.97812 | 1.82749  | -0.02759 |
| N | -2.96003 | 0.48773  | 0.01036  |
| H | -3.95173 | -1.30741 | -0.10132 |
| H | -6.19255 | -0.21842 | -0.41211 |
| H | -4.10854 | 3.61292  | -0.22472 |
| H | -2.01283 | 2.32501  | 0.08153  |
| C | 8.19613  | 1.59973  | -0.25863 |
| H | 8.65981  | 2.04372  | 0.63288  |
| H | 8.67639  | 2.05673  | -1.13462 |
| H | 8.66623  | -0.38069 | 0.61403  |
| H | 8.67800  | -0.36756 | -1.15348 |
| N | -6.54695 | 2.46607  | -0.51581 |
| C | -6.57623 | 3.91742  | -0.55749 |
| H | -5.96937 | 4.30729  | -1.38951 |
| H | -7.60841 | 4.25038  | -0.70207 |
| H | -6.20302 | 4.35305  | 0.38240  |
| C | -7.77760 | 1.70936  | -0.66415 |
| H | -7.97673 | 1.09047  | 0.22446  |
| H | -8.61231 | 2.40538  | -0.79066 |
| H | -7.74006 | 1.05215  | -1.54680 |
| I | 3.72762  | 0.78968  | -0.30641 |

A Borhan-féle reakció szerkezetei:

**1'**



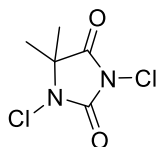
25

**1'**

|   |          |          |          |
|---|----------|----------|----------|
| H | -2.41364 | 2.07127  | -0.69722 |
| C | -2.58568 | 1.03818  | -0.39150 |
| C | -3.02399 | -1.61870 | 0.29663  |
| C | -1.50947 | 0.27472  | 0.08758  |
| C | -3.85861 | 0.48922  | -0.51200 |
| C | -4.08516 | -0.84258 | -0.16396 |
| C | -1.74883 | -1.06817 | 0.41445  |
| H | -4.67733 | 1.10231  | -0.89213 |
| H | -5.08199 | -1.27501 | -0.26114 |
| H | -0.93489 | -1.69522 | 0.77956  |
| H | -3.18651 | -2.66329 | 0.56663  |
| C | -0.15043 | 0.87266  | 0.22832  |

|   |          |          |          |
|---|----------|----------|----------|
| C | 0.00518  | 2.17676  | 0.49349  |
| H | 0.98985  | 2.63782  | 0.57548  |
| H | -0.85586 | 2.82642  | 0.65680  |
| C | 1.01500  | -0.07335 | 0.05974  |
| H | 0.99997  | -0.82409 | 0.86592  |
| H | 0.87570  | -0.65563 | -0.86535 |
| C | 2.38479  | 0.57884  | 0.04360  |
| H | 2.59108  | 1.12227  | 0.97963  |
| H | 2.47915  | 1.32342  | -0.76211 |
| C | 3.48838  | -0.43424 | -0.12886 |
| O | 4.68982  | 0.15290  | -0.23484 |
| H | 5.34542  | -0.55480 | -0.33162 |
| O | 3.34543  | -1.62483 | -0.16259 |

### DCDMH

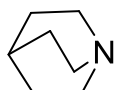


17

### DCDMH

|    |          |          |          |
|----|----------|----------|----------|
| C  | 0.25409  | -1.16592 | -0.06034 |
| N  | 1.24001  | -0.14494 | 0.00143  |
| C  | 0.72835  | 1.13956  | -0.01465 |
| C  | -0.80114 | 0.98146  | -0.00685 |
| N  | -0.92526 | -0.46531 | -0.18607 |
| O  | 1.34002  | 2.16548  | -0.01265 |
| C  | -1.42131 | 1.75238  | -1.16462 |
| C  | -1.33158 | 1.44425  | 1.35024  |
| Cl | -2.40653 | -1.25241 | 0.00191  |
| O  | 0.44336  | -2.33996 | -0.02160 |
| Cl | 2.88138  | -0.49806 | 0.01211  |
| H  | -2.51071 | 1.60661  | -1.16466 |
| H  | -1.01569 | 1.40270  | -2.12317 |
| H  | -1.19958 | 2.82139  | -1.05058 |
| H  | -2.42034 | 1.30309  | 1.39273  |
| H  | -1.09976 | 2.50882  | 1.48474  |
| H  | -0.86717 | 0.87250  | 2.16620  |

### QUI



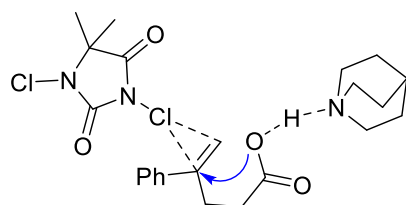
21

### QUI

|   |          |         |          |
|---|----------|---------|----------|
| C | -1.28868 | 0.00071 | -0.00008 |
|---|----------|---------|----------|

|   |          |          |          |
|---|----------|----------|----------|
| C | -0.75823 | -0.40224 | 1.38304  |
| C | 0.79684  | -0.38745 | 1.32227  |
| N | 1.27758  | -0.00047 | -0.00006 |
| C | 0.79755  | 1.33831  | -0.32588 |
| C | -0.75731 | 1.39939  | -0.34291 |
| C | -0.75850 | -0.99627 | -1.04004 |
| C | 0.79655  | -0.95196 | -0.99636 |
| H | 1.21158  | -1.37870 | 1.55894  |
| H | 1.21175  | -0.66157 | -1.97305 |
| H | 1.21401  | -1.94046 | -0.75302 |
| H | 1.21533  | 1.62156  | -1.30356 |
| H | 1.21305  | 2.03862  | 0.41408  |
| H | -1.13371 | -2.00611 | -0.81400 |
| H | -1.13582 | -0.72981 | -2.03917 |
| H | -2.38821 | 0.00125  | -0.00011 |
| H | -1.13596 | -1.40065 | 1.65161  |
| H | -1.13284 | 0.29833  | 2.14498  |
| H | -1.13440 | 2.13148  | 0.38745  |
| H | -1.13204 | 1.70902  | -1.33052 |
| H | 1.21484  | 0.31732  | 2.05657  |

### B-cl

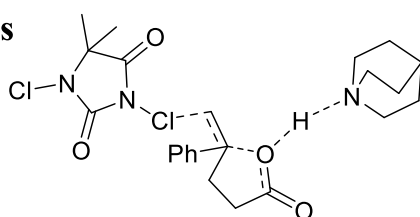


63

### B-cl

|   |          |          |          |
|---|----------|----------|----------|
| C | -2.94862 | 1.65593  | -0.52456 |
| C | -1.51899 | 2.05157  | -0.82256 |
| O | -3.24688 | 1.74308  | 0.75700  |
| C | -0.55257 | 1.15090  | -0.03838 |
| C | -0.82095 | -0.30705 | -0.32536 |
| C | -1.30891 | -1.12620 | 0.61844  |
| H | -1.50479 | -2.18086 | 0.41065  |
| O | -3.71889 | 1.25915  | -1.37199 |
| H | -1.51954 | -0.75373 | 1.62385  |
| H | 0.48630  | 1.40674  | -0.30104 |
| H | -0.67827 | 1.33660  | 1.03716  |
| H | -1.36400 | 1.95947  | -1.90497 |
| H | -1.36672 | 3.09996  | -0.52573 |
| C | -0.58050 | -0.78190 | -1.71565 |
| C | -0.12709 | -1.69919 | -4.33247 |
| C | 0.55289  | -0.36670 | -2.43103 |
| C | -1.49165 | -1.64427 | -2.34062 |

|    |          |          |          |
|----|----------|----------|----------|
| C  | -1.26610 | -2.10215 | -3.63635 |
| C  | 0.77853  | -0.82924 | -3.72603 |
| H  | 1.27660  | 0.30621  | -1.96586 |
| H  | -2.40030 | -1.93038 | -1.80806 |
| H  | -1.99094 | -2.76609 | -4.11002 |
| H  | 1.66979  | -0.50456 | -4.26566 |
| H  | 0.04860  | -2.05375 | -5.34934 |
| N  | 3.55159  | -0.39092 | 0.63371  |
| C  | 3.90963  | 0.67322  | -0.16243 |
| C  | 5.43315  | 0.81443  | -0.02809 |
| N  | 5.69647  | -0.14879 | 1.04170  |
| C  | 4.62902  | -0.95863 | 1.36486  |
| O  | 4.57944  | -1.90309 | 2.08630  |
| O  | 3.18827  | 1.34643  | -0.84374 |
| Cl | 1.96295  | -0.92396 | 0.78358  |
| Cl | 7.26879  | -0.61228 | 1.44264  |
| C  | 5.80372  | 2.23396  | 0.38102  |
| H  | 6.89300  | 2.31003  | 0.50625  |
| H  | 5.31741  | 2.50249  | 1.32813  |
| H  | 5.47985  | 2.93472  | -0.39938 |
| C  | 6.07931  | 0.40206  | -1.35099 |
| H  | 7.17325  | 0.45273  | -1.26250 |
| H  | 5.74882  | 1.08610  | -2.14347 |
| H  | 5.79158  | -0.62364 | -1.62208 |
| H  | -4.18580 | 1.35121  | 0.91535  |
| N  | -5.58239 | 0.56851  | 1.07277  |
| C  | -6.12606 | 0.50663  | 2.43401  |
| H  | -6.26567 | 1.53696  | 2.79154  |
| H  | -5.36475 | 0.04052  | 3.07647  |
| C  | -6.56271 | 1.18435  | 0.16460  |
| H  | -6.78330 | 2.18988  | 0.55249  |
| H  | -6.06629 | 1.30534  | -0.80721 |
| C  | -5.25434 | -0.78670 | 0.60024  |
| H  | -4.44463 | -1.17571 | 1.23566  |
| H  | -4.84716 | -0.67705 | -0.41455 |
| C  | -7.45743 | -0.29067 | 2.46058  |
| H  | -7.40731 | -1.11168 | 3.19097  |
| H  | -8.29613 | 0.35591  | 2.75966  |
| C  | -6.50372 | -1.70305 | 0.63934  |
| H  | -6.36688 | -2.52814 | 1.35468  |
| H  | -6.68476 | -2.15682 | -0.34606 |
| C  | -7.84646 | 0.31952  | 0.07256  |
| H  | -7.98524 | -0.06630 | -0.94843 |
| H  | -8.73943 | 0.91384  | 0.31679  |
| C  | -7.71081 | -0.85177 | 1.05457  |
| H  | -8.62571 | -1.46104 | 1.04991  |

**B-cl-ts**

63

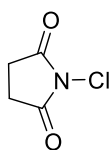
**B-cl-ts**

|    |          |          |          |
|----|----------|----------|----------|
| C  | -2.56513 | 2.00031  | -0.00932 |
| C  | -1.19820 | 2.50247  | -0.44007 |
| O  | -2.49434 | 0.88715  | 0.66260  |
| C  | -0.14940 | 1.79080  | 0.40058  |
| C  | -0.52896 | 0.33962  | 0.56022  |
| C  | -0.20943 | -0.33179 | 1.76906  |
| H  | -0.49060 | -1.38408 | 1.85280  |
| O  | -3.61203 | 2.55738  | -0.29791 |
| H  | -0.25459 | 0.25196  | 2.69078  |
| H  | 0.85703  | 1.83233  | -0.04802 |
| H  | -0.07551 | 2.24037  | 1.40104  |
| H  | -1.08983 | 2.25486  | -1.50838 |
| H  | -1.15741 | 3.59552  | -0.35783 |
| C  | -0.63113 | -0.49072 | -0.67567 |
| C  | -0.77970 | -2.10962 | -2.95340 |
| C  | 0.28089  | -0.31173 | -1.72297 |
| C  | -1.59471 | -1.50215 | -0.76680 |
| C  | -1.67734 | -2.30322 | -1.90145 |
| C  | 0.20006  | -1.12405 | -2.85478 |
| H  | 1.09354  | 0.41506  | -1.63010 |
| H  | -2.28498 | -1.64282 | 0.06773  |
| H  | -2.43459 | -3.08712 | -1.96479 |
| H  | 0.92292  | -0.98823 | -3.66017 |
| H  | -0.83646 | -2.73867 | -3.84297 |
| N  | 3.80542  | -0.21410 | 0.69638  |
| C  | 4.00654  | 0.62685  | -0.33627 |
| C  | 5.52617  | 0.74573  | -0.58981 |
| N  | 6.01191  | 0.10919  | 0.62892  |
| C  | 4.99406  | -0.61812 | 1.28180  |
| O  | 5.15852  | -1.40447 | 2.17128  |
| O  | 3.17274  | 1.20508  | -1.01367 |
| Cl | 1.82210  | -0.36715 | 1.30088  |
| Cl | 7.61146  | -0.45883 | 0.71184  |
| C  | 5.95563  | 2.20124  | -0.69099 |
| H  | 7.04305  | 2.26534  | -0.84442 |
| H  | 5.69684  | 2.73879  | 0.23098  |
| H  | 5.43966  | 2.67534  | -1.53663 |

|   |          |          |          |
|---|----------|----------|----------|
| C | 5.86541  | -0.04110 | -1.85629 |
| H | 6.94747  | -0.01185 | -2.04731 |
| H | 5.33407  | 0.40490  | -2.70791 |
| H | 5.55274  | -1.09034 | -1.75267 |
| H | -3.84183 | 0.32674  | 0.72656  |
| N | -4.88821 | -0.02593 | 0.63277  |
| C | -5.05973 | -1.36339 | 1.25459  |
| H | -4.61791 | -1.32691 | 2.25898  |
| H | -4.47508 | -2.07368 | 0.65423  |
| C | -5.77946 | 0.97247  | 1.28973  |
| H | -5.59020 | 0.89933  | 2.36944  |
| H | -5.44215 | 1.95627  | 0.94170  |
| C | -5.18755 | -0.09288 | -0.82671 |
| H | -4.37026 | -0.65571 | -1.29957 |
| H | -5.13164 | 0.94109  | -1.18945 |
| C | -6.56007 | -1.72206 | 1.27060  |
| H | -6.70027 | -2.76415 | 0.95284  |
| H | -6.96945 | -1.63514 | 2.28761  |
| C | -6.56941 | -0.74464 | -1.02527 |
| H | -6.46907 | -1.77124 | -1.40776 |
| H | -7.14717 | -0.17789 | -1.76784 |
| C | -7.24269 | 0.65088  | 0.92854  |
| H | -7.63099 | 1.38085  | 0.20360  |
| H | -7.87599 | 0.71452  | 1.82397  |
| C | -7.29778 | -0.76064 | 0.32696  |
| H | -8.33938 | -1.08192 | 0.19660  |

A Wang-cl reakció szerkezetei:

NCS



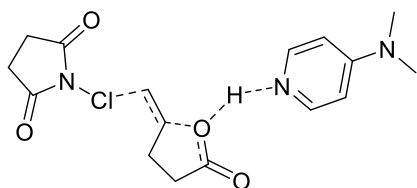
12

**NCS**

|   |          |          |          |
|---|----------|----------|----------|
| C | 0.41916  | -1.18681 | 0.00003  |
| C | 0.41915  | 1.18682  | -0.00007 |
| C | 1.88072  | 0.76578  | -0.00009 |
| C | 1.88072  | -0.76576 | 0.00020  |
| H | 2.36066  | 1.20698  | -0.88367 |
| H | 2.36080  | 1.20734  | 0.88323  |
| H | 2.36090  | -1.20732 | -0.88307 |
| H | 2.36059  | -1.20695 | 0.88383  |
| O | -0.04017 | -2.28743 | 0.00020  |
| O | -0.04020 | 2.28743  | -0.00019 |
| N | -0.32587 | 0.00000  | -0.00002 |

|    |          |          |          |
|----|----------|----------|----------|
| Cl | -2.00690 | -0.00001 | -0.00004 |
|----|----------|----------|----------|

**W-cl-ts**



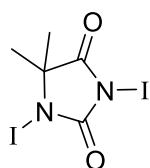
46

**W-cl-ts**

|    |          |          |          |
|----|----------|----------|----------|
| C  | -0.83671 | 2.46438  | -0.11678 |
| C  | 0.57937  | 2.97426  | 0.07206  |
| O  | -0.82261 | 1.19495  | -0.44683 |
| C  | 1.40603  | 1.75079  | 0.45052  |
| C  | 1.00007  | -0.73630 | 0.11808  |
| H  | 0.70613  | -1.55327 | -0.54456 |
| O  | -1.85592 | 3.11081  | 0.01589  |
| H  | 0.81326  | -0.89419 | 1.18345  |
| H  | 2.48553  | 1.87376  | 0.27127  |
| H  | 1.27810  | 1.50903  | 1.51712  |
| H  | 0.91047  | 3.39193  | -0.89292 |
| H  | 0.59775  | 3.78681  | 0.80759  |
| N  | 5.15681  | -0.72446 | 0.02714  |
| C  | 5.76770  | 0.49873  | 0.07501  |
| C  | 7.28691  | 0.28089  | 0.06923  |
| C  | 6.02170  | -1.79006 | -0.00919 |
| O  | 5.72623  | -2.95688 | -0.05326 |
| O  | 5.21717  | 1.57497  | 0.11401  |
| H  | -2.14744 | 0.60524  | -0.37195 |
| C  | 0.90921  | 0.58593  | -0.37367 |
| H  | 1.07720  | 0.69237  | -1.45105 |
| C  | -4.17693 | 1.11434  | -0.12837 |
| C  | -5.48243 | 0.70203  | 0.01071  |
| C  | -5.79209 | -0.68622 | 0.01193  |
| C  | -4.69854 | -1.58709 | -0.13163 |
| C  | -3.42370 | -1.09048 | -0.26590 |
| N  | -3.17919 | 0.22708  | -0.26717 |
| H  | -3.85672 | 2.16016  | -0.12483 |
| H  | -6.25531 | 1.45786  | 0.12172  |
| H  | -4.84252 | -2.66417 | -0.13588 |
| H  | -2.55388 | -1.74102 | -0.37349 |
| Cl | 3.19022  | -0.78737 | 0.03308  |
| C  | 7.45561  | -1.23545 | 0.01656  |
| H  | 7.98053  | -1.59729 | -0.87802 |
| H  | 7.97159  | -1.65894 | 0.88905  |
| H  | 7.70831  | 0.80959  | -0.79673 |

|   |          |          |          |
|---|----------|----------|----------|
| H | 7.70664  | 0.74867  | 0.97028  |
| N | -7.05917 | -1.12990 | 0.14533  |
| C | -7.33332 | -2.55571 | 0.14606  |
| H | -6.81967 | -3.06310 | 0.97756  |
| H | -8.40985 | -2.71297 | 0.26272  |
| H | -7.01782 | -3.02527 | -0.79868 |
| C | -8.14721 | -0.17976 | 0.29362  |
| H | -8.21875 | 0.48662  | -0.58000 |
| H | -9.09025 | -0.72714 | 0.38475  |
| H | -8.01924 | 0.43902  | 1.19542  |

## DIDMH

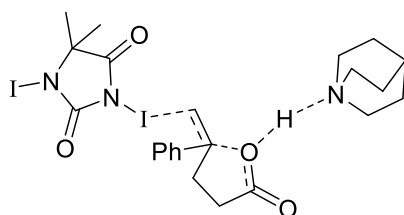


17

## DIDMH

|   |          |          |          |
|---|----------|----------|----------|
| C | 0.04835  | -0.71300 | -0.00237 |
| N | 1.16240  | 0.16716  | -0.00015 |
| C | 0.80230  | 1.49679  | 0.00061  |
| C | -0.73916 | 1.53474  | -0.00052 |
| N | -1.05224 | 0.10722  | -0.00457 |
| O | 1.52655  | 2.44994  | 0.00055  |
| C | -1.21746 | 2.24358  | -1.26482 |
| C | -1.21820 | 2.23708  | 1.26727  |
| O | 0.09799  | -1.90683 | -0.00181 |
| H | -2.31645 | 2.28273  | -1.28238 |
| H | -0.86687 | 1.71395  | -2.16136 |
| H | -0.82230 | 3.26797  | -1.27761 |
| H | -2.31717 | 2.27690  | 1.28406  |
| H | -0.82237 | 3.26112  | 1.28590  |
| H | -0.86874 | 1.70243  | 2.16130  |
| I | -2.93110 | -0.66613 | 0.00032  |
| I | 3.08566  | -0.49549 | 0.00029  |

## B-i-ts



**B-i-ts**

|   |          |          |          |
|---|----------|----------|----------|
| C | -4.13035 | 0.48796  | 2.09945  |
| C | -2.86699 | 1.03447  | 2.73251  |
| O | -3.84987 | -0.26155 | 1.06248  |
| C | -1.57143 | -1.41145 | 0.23410  |
| H | -1.81597 | -1.61402 | -0.81296 |
| O | -5.26518 | 0.72048  | 2.47074  |
| H | -1.67180 | -2.26844 | 0.90667  |
| H | -2.76392 | 2.07922  | 2.39704  |
| H | -2.96380 | 1.04684  | 3.82484  |
| N | 2.96972  | -0.27057 | 0.16105  |
| C | 3.25336  | 1.01655  | 0.47281  |
| C | 4.78266  | 1.23137  | 0.35553  |
| N | 5.19204  | -0.11989 | 0.00875  |
| C | 4.11772  | -0.99246 | -0.15216 |
| O | 4.18485  | -2.14382 | -0.49132 |
| O | 2.48210  | 1.89919  | 0.78918  |
| C | 5.34095  | 1.69307  | 1.69727  |
| H | 6.42836  | 1.84901  | 1.62863  |
| H | 5.14004  | 0.94050  | 2.47229  |
| H | 4.85841  | 2.63730  | 1.98415  |
| C | 5.05457  | 2.24624  | -0.75207 |
| H | 6.13573  | 2.42178  | -0.85820 |
| H | 4.55840  | 3.19359  | -0.50079 |
| H | 4.65906  | 1.88096  | -1.71050 |
| H | -5.14270 | -0.55280 | 0.30907  |
| N | -6.12618 | -0.62582 | -0.14066 |
| C | -6.07200 | -1.39374 | -1.41325 |
| H | -5.51173 | -2.31838 | -1.22303 |
| H | -5.49476 | -0.79090 | -2.12720 |
| C | -7.03044 | -1.29890 | 0.83858  |
| H | -6.69897 | -2.34413 | 0.90257  |
| H | -6.84770 | -0.81344 | 1.80488  |
| C | -6.59662 | 0.76855  | -0.39379 |
| H | -5.78900 | 1.29163  | -0.92458 |
| H | -6.69895 | 1.23165  | 0.59556  |
| C | -7.51170 | -1.64791 | -1.90345 |
| H | -7.57815 | -1.45639 | -2.98287 |
| H | -7.79717 | -2.69747 | -1.74198 |
| C | -7.91369 | 0.71086  | -1.19074 |
| H | -7.75150 | 1.00246  | -2.23884 |
| H | -8.63768 | 1.41913  | -0.76605 |
| C | -8.48329 | -1.17157 | 0.34222  |
| H | -9.03529 | -0.43868 | 0.94812  |

|   |          |          |          |
|---|----------|----------|----------|
| H | -9.00217 | -2.13429 | 0.44480  |
| C | -8.46014 | -0.72315 | -1.12590 |
| H | -9.46912 | -0.76703 | -1.55585 |
| C | -2.02058 | -0.15959 | 0.75324  |
| I | 0.81170  | -0.95406 | 0.16393  |
| I | 7.08349  | -0.67108 | -0.47446 |
| C | -1.73126 | 0.16754  | 2.20884  |
| H | -0.74956 | 0.65317  | 2.29006  |
| H | -1.66943 | -0.77826 | 2.76626  |
| C | -2.01184 | 1.00046  | -0.20849 |
| C | -1.08717 | 2.04296  | -0.07625 |
| C | -2.88194 | 1.00515  | -1.30487 |
| C | -1.05822 | 3.07669  | -1.01318 |
| H | -0.33432 | 2.02927  | 0.71442  |
| C | -2.85907 | 2.04072  | -2.23451 |
| H | -3.58024 | 0.17371  | -1.42014 |
| C | -1.94693 | 3.08656  | -2.08540 |
| H | -0.31522 | 3.86760  | -0.90466 |
| H | -3.54441 | 2.02846  | -3.08434 |
| H | -1.91897 | 3.89756  | -2.81449 |