

# First-principles study of electronic and optical properties in 1-dimensional oligomeric derivatives of telomestatin

## Supporting Information

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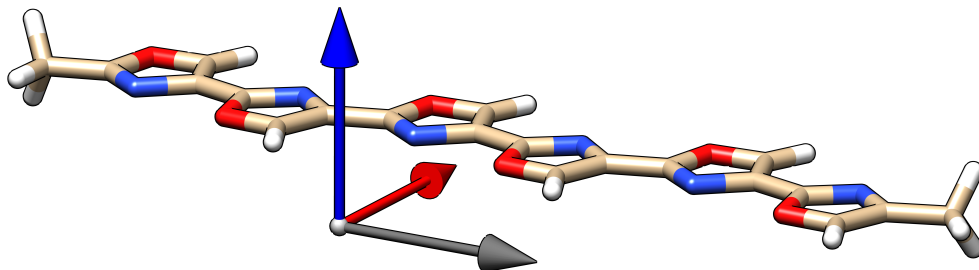


Figure S1: Geometry of 6-oxazole chain showing axes of polarisation described in the text. Axis colours: black = longitudinal, red = transverse (in plane), blue = transverse (through plane).

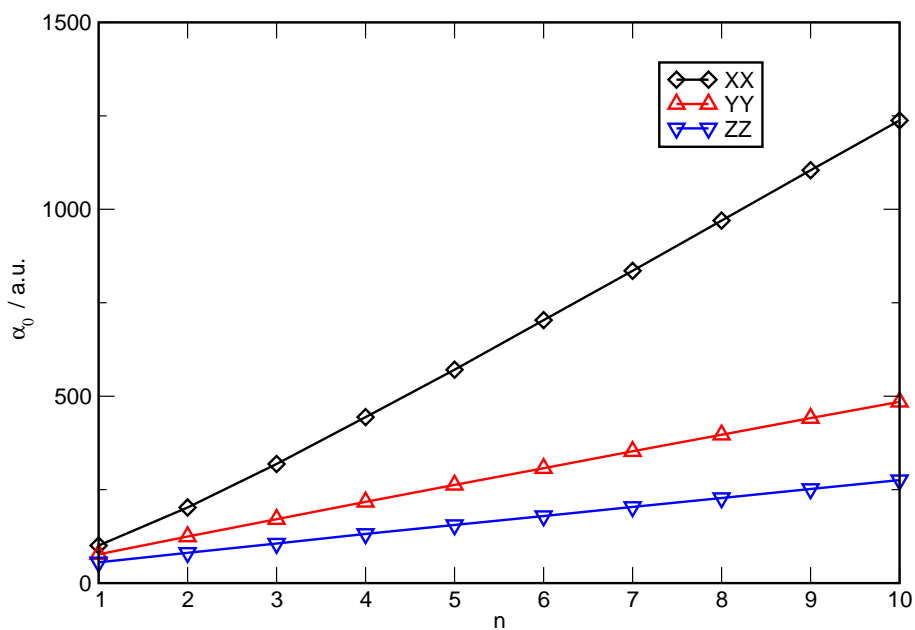


Figure S2: Anisotropy of static polarisability tensor diagonal components for polyoxazoles calculated at the ADSIC level using the Sternheimer linear response method. The largest component in all cases is XX which is aligned along the length of the oligomer chains. This component also undergoes the largest growth with chain length,  $n$ . A small deviation from linearity is seen in the XX component and  $n = 2$ , where the initial inter-ring  $\pi$ -conjugation is formed. The tensor components correspond to the axes in Figure S1 as follows: XX = black, YY = red, ZZ = blue.

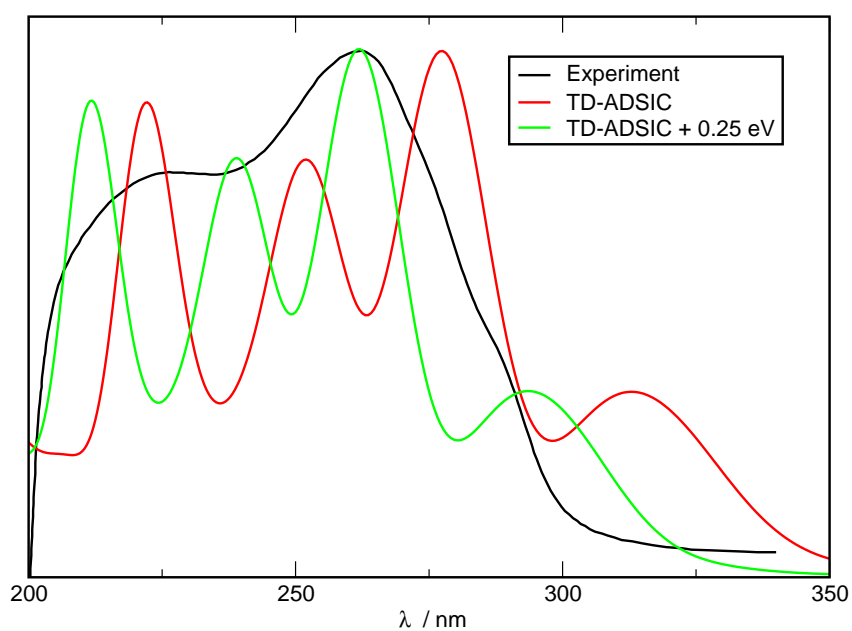


Figure S3: Comparison of telomestatin absorption spectra. The experimental UV-Vis spectrum is shown in black whilst the TD-ADSIC calculated spectrum is shown in red and the shifted spectrum in green. Both calculated spectra are normalised to the largest peak in the experimental spectrum. Applying a shift of +0.25 eV aligns the largest peak in the calculated spectrum with the experimental  $\lambda$ -max at  $\sim 260$  nm. This shift also leads to a good agreement between the smallest calculated peak with the experimentally-observed shoulder at  $\sim 290$  nm. Unfortunately, the experimental spectrum cuts off before the position of the highest energy peak in the calculated spectrum, however a small rise in intensity just before the cut-off suggests the presence of another peak in the region predicted by the calculations.

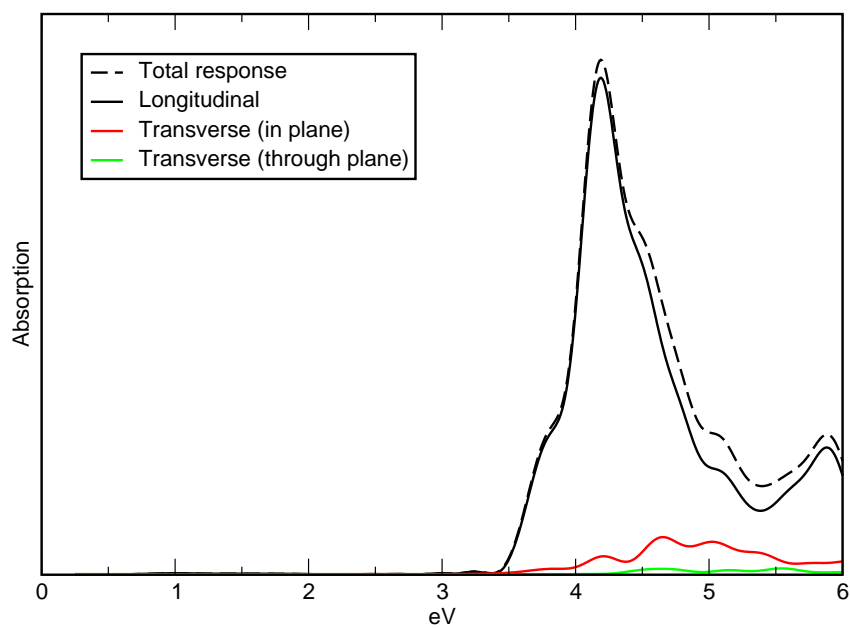


Figure S4: TD-ADSIC absorption spectrum for neutral 10-oxazole oligomer showing polarisation-dependent components of the optical response.

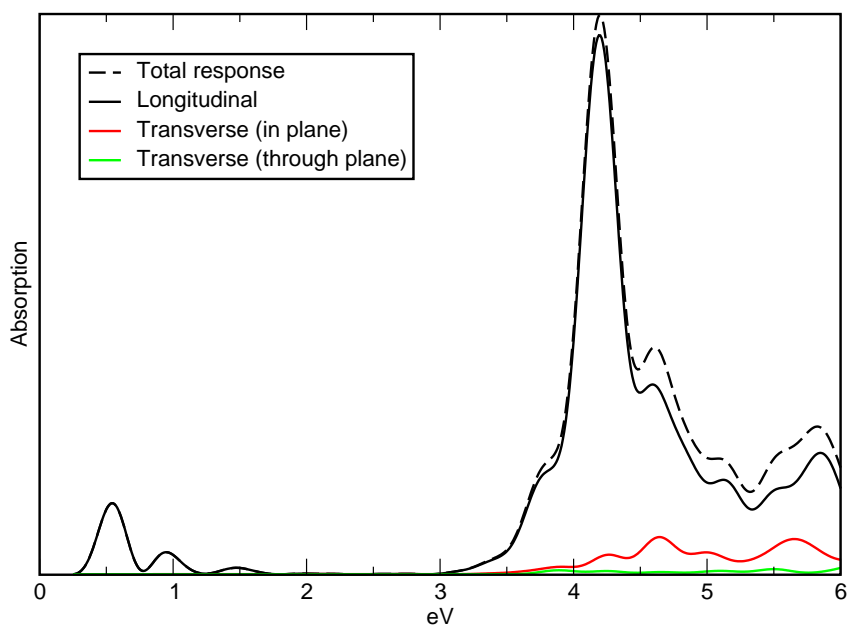


Figure S5: TD-ADSIC absorption spectrum for hole-doped 10-oxazole oligomer showing polarisation-dependent components of the optical response.

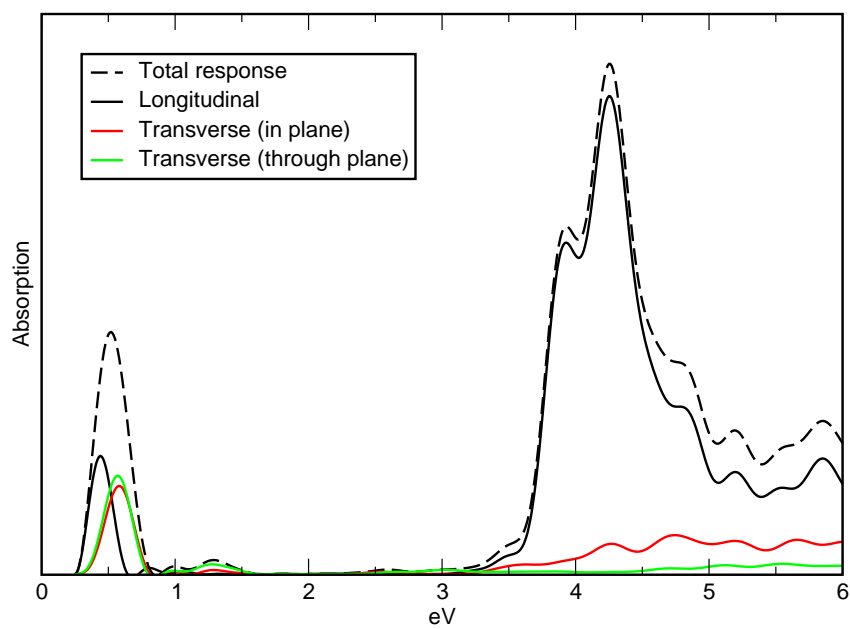


Figure S6: TD-ADSIC absorption spectrum for electron-doped 10-oxazole oligomer showing polarisation-dependent components of the optical response.

r<sup>2</sup>SCAN-D4/Def2-TZVP geometry: n = 1

14

O -0.86203916916902 1.04071254888863 -0.00000003203685  
C -0.98644328628395 -0.31235895881792 -0.00000003259320  
N 0.14810156555968 -0.93794676741674 -0.00000004065313  
C 1.11904602962912 0.05914737626193 -0.00000002595616  
C 0.49326306240801 1.26018159338049 -0.00000002241505  
C -2.35262306232974 -0.87476651641656 0.00000001113994  
C 2.57209729275495 -0.26843962885411 0.00000000985878  
H 0.81233472919550 2.28830640625055 -0.0000000444129  
H -2.28677802260184 -1.96052279451205 0.00000001475182  
H -2.90983019480505 -0.54834812416285 -0.88185217240510  
H -2.90983012458316 -0.54834811869955 0.88185223276237  
H 2.69420991010725 -1.35099005179263 -0.00000002457928  
H 3.07719492463851 0.13301790150698 0.88177441548663  
H 3.07719499489670 0.13301796891095 -0.88177432891948



r<sup>2</sup>SCAN-D4/Def2-TZVP geometry: n = 2

20

N 1.56994889625396 -1.08009629343593 -0.00000002212380  
C 0.75426846771856 -0.06430326559251 -0.00000001721412  
O 1.37542775011100 1.13893539115998 -0.00000002212847  
C 2.70775285710138 0.82937400928925 -0.00000001456781  
C 2.83653346791680 -0.52335703112706 -0.00000001496591  
C -0.68324435973796 -0.09553256848576 -0.00000001037645  
N -1.47101928443360 1.04699797067448 -0.00000001803492  
C -2.68715224792854 0.60969341180891 -0.00000001478794  
O -2.77944298311239 -0.75410333022399 -0.00000000692958  
C -1.48809005642402 -1.19180730082089 0.00000000808201  
C -3.94995707491747 1.37988071285328 0.00000000736585  
C 4.06393933300092 -1.36684034467733 0.00000001033987  
H -1.31973911502171 -2.25384156067828 0.00000001792170  
H 3.39129481295508 1.66089075045400 -0.00000000014939  
H 3.77710827420177 -2.41770143822774 -0.00000000236451  
H 4.68110124199273 -1.17927887280267 0.88174843690773  
H 4.68110129138522 -1.17927886560482 -0.88174838254434  
H -4.80426266718475 0.70517658315772 -0.00000000032261  
H -4.00162753741276 2.02285944217087 -0.88075927157764  
H -4.00162751890011 2.02285939697480 0.88075931747034

r<sup>2</sup>SCAN-D4/Def2-TZVP geometry: n = 3

26

N 3.55386374834686 0.73783479727100 -0.00000003570705  
C 4.62254094628394 -0.14089011925520 0.00000003175325  
C 4.13227896479474 -1.40829459940666 0.00000003628972  
O 2.76570194800064 -1.34585931069065 -0.00000001434142  
C 2.49396720878955 -0.01906428392457 -0.00000005920895  
C 1.11839622605784 0.40038988745712 -0.00000010434301  
N 0.05370399412521 -0.48086818275743 -0.00000011628411  
C -0.99777068133213 0.28263943336568 -0.00000012771095  
O -0.71626916244468 1.61510294166898 -0.00000013080576  
C 0.64208184039769 1.67772246435848 -0.00000011798374  
C -2.37647844602087 -0.12254314864197 -0.00000010261697  
C -2.86617671756818 -1.39067217806856 -0.00000010346465  
O -4.22550970070645 -1.30615124377421 -0.00000004099668  
C -4.49400098346069 0.03533480725814 0.00000000713223  
N -3.43509163630320 0.77595358948463 -0.00000003565260  
C 6.03257951694422 0.33832422399597 0.00000009368840  
C -5.91195865650007 0.44401263987350 0.00000013690883  
H 4.56550333882699 -2.39367065572341 0.00000007637812  
H 1.09571178507842 2.65268249411715 -0.00000010989491  
H -2.42442623724939 -2.37133446192967 -0.00000013268589  
H 6.04188848454305 1.42760294663799 0.00000005751315  
H 6.57568466945319 -0.00970474840607 -0.88176096547787  
H 6.57568455987813 -0.00970468385878 0.88176124112493  
H -5.96541722467383 1.53025674722889 0.00000018273548  
H -6.42759612359808 0.05661304887497 0.88207240978119  
H -6.42759627847553 0.05661311280726 -0.88207207613076

r<sup>2</sup>SCAN-D4/Def2-TZVP geometry: n = 4

32

C -4.71024691284153 1.17592459344588 0.00000008981705  
C -4.12774513547930 -0.05252046343965 0.00000002719444  
N -5.11620622020868 -1.02731714956805 -0.00000002841253  
C -6.22730005595164 -0.36753768618928 0.00000000247043  
O -6.05880182850710 0.99044022335559 0.00000008012298  
C -2.72298566806640 -0.35353248540246 0.00000001885284  
O -2.34243772101376 -1.66217727355460 -0.00000002160325  
C -0.98457549142435 -1.62479383149949 -0.00000000265245  
C -0.60517576418842 -0.31561541984202 0.00000002615166  
N -1.73075012035426 0.48551885726592 0.00000004930172  
C 0.73542620822491 0.20287553888368 0.00000002574130  
N 1.84619151745744 -0.47113982397055 0.00000002057582  
C 2.83425141632874 0.49503779076256 -0.00000000956356  
C 2.25376269315779 1.72863995341551 -0.00000002924034  
O 0.90551411476224 1.55397849808860 0.00000000498658  
C 4.24076051402803 0.19330631217682 -0.00000001122132  
N 5.23075096175953 1.03800909183340 -0.00000006607934  
C 6.36979619736441 0.25102387065031 -0.00000001307135  
C 5.99048987929197 -1.05214022480628 0.00000007335016  
O 4.62277854307408 -1.10685257456172 0.00000007387229  
C 7.73093517706264 0.84179318482381 -0.00000004728807  
C -7.61091058298966 -0.88000042508564 -0.00000005928210  
H 6.50850421983723 -1.99567617629154 0.00000013193405  
H 2.62551112138467 2.73768923136215 -0.00000004987393  
H -0.45908172840913 -2.56316759824758 -0.00000002665467  
H -4.34265697222420 2.18677943446319 0.00000014032402  
H 8.49541713920111 0.06416564056888 0.00000002036412  
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H 7.87611214231057 1.47306275722309 -0.88016960596934  
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H -8.15366973516806 -0.53165910581578 -0.88205717741273  
H -8.15366977449279 -0.53165923790860 0.88205708775850

r<sup>2</sup>SCAN-D4/Def2-TZVP geometry: n = 5

38

N -6.92129588989226 0.71854932676730 -0.00000002430921  
C -5.86358728266449 -0.17796899298600 -0.00000003592568  
C -6.35106907237921 -1.44765158877303 -0.00000009006239  
O -7.70935390091034 -1.36361684844476 -0.00000010804606  
C -7.98028568716748 -0.02218787426055 -0.00000006060422  
C -4.48567698728395 0.22930141034543 0.00000000967613  
N -3.43149454303182 -0.53043580036903 0.00000001612635  
C -2.37173387283738 0.35545264784542 0.00000005655944  
C -2.85097926825356 1.63150402298586 0.00000007304123  
O -4.20720010904430 1.56356529643099 0.00000005267282  
C -0.99521346549536 -0.05774735503166 0.00000007538890  
O -0.72057023905662 -1.39224284291002 0.00000008439552  
C 0.63630273065701 -1.46298491135352 0.00000009898277  
C 1.11867091427625 -0.18807627192897 0.00000009666798  
N 0.06036555332864 0.69970292726227 0.00000008749953  
C 2.49611308871203 0.22334417683629 0.00000009786959  
N 3.55043787451491 -0.53587211048078 0.00000010185667  
C 4.61143734938192 0.34964656152782 0.00000005897636  
C 4.12967763958999 1.62492914786750 0.00000003946526  
O 2.77162815375763 1.55680749780278 0.00000006929050  
C 5.98972211450656 -0.06253146062927 0.00000002503819  
N 7.04366445113928 0.70082282972211 -0.00000005814794  
C 8.11672943399474 -0.17386070848999 -0.00000005933621  
C 7.63534835677475 -1.44290405002665 0.00000003044411  
O 6.26709607540417 -1.38899084450691 0.00000007573770  
C 9.52031629007197 0.30740694340745 -0.00000014402328  
C -9.40080722034932 0.38810441092922 -0.00000005978274  
H 8.07706365893265 -2.42446780000889 0.00000006698303  
H 4.57960773101579 2.60164851278772 0.00000000427333  
H 1.08557162728273 -2.44013765864942 0.00000010846505  
H -2.39952565531752 2.60769636639291 0.00000009987710  
H -5.90860518388444 -2.42793818895751 -0.00000011410707  
H -10.04737128450045 -0.48751716732073 -0.00000011792373  
H -9.61888619977441 0.99508138670748 -0.88075690033918  
H -9.61888623090594 0.99508129035708 0.88075683984231  
H 10.22105572323432 -0.52813026146771 -0.00000012068201  
H 9.71482986830250 0.92538608118317 0.88011620773815

H 9.71482980321226 0.92538597809257 -0.88011658357831

r<sup>2</sup>SCAN-D4/Def2-TZVP geometry: n = 6

44

N -8.64038022529400 -0.93666763068027 -0.00000026370931  
C -9.72219237403156 -0.22982555582902 -0.00000044356535  
O -9.49539866518731 1.11975555993587 -0.00000046518132  
C -8.14045665435904 1.24745120966549 -0.00000026232729  
C -7.61136187520763 -0.00498098305030 -0.00000014186862  
C -6.22116080340808 -0.36678455630895 0.00000006848239  
N -5.19267313472786 0.42733669196933 0.00000018936708  
C -4.10430044652706 -0.42320625323713 0.00000034199470  
C -4.54084187482068 -1.71446930357878 0.00000030387591  
O -5.89847926106386 -1.69133795259788 0.00000014154190  
C -2.74293325792493 0.03696112724034 0.00000048118361  
O -2.51600756508696 1.38066699197831 0.00000048166131  
C -1.16319891883289 1.50043369867966 0.00000054204648  
C -0.63555089410610 0.24343533074201 0.00000058777115  
N -1.66083233423659 -0.68214737072930 0.00000056083333  
C 0.75583329559892 -0.11695181265418 0.00000060252475  
N 1.78155799825660 0.68038404639456 0.00000056354434  
C 2.87312861523882 -0.16634916977839 0.00000049566953  
C 2.43981083688756 -1.45880971201370 0.00000050695023  
O 1.08129419293338 -1.43996611672120 0.00000058924305  
C -11.12673304835332 -0.68166279244672 -0.00000064714849  
C 4.23384009637589 0.29742452624857 0.00000037687915  
N 5.31642797376383 -0.42092839358504 0.00000022251305  
C 6.34272876547894 0.50465546364944 0.00000009326703  
C 5.81233189896768 1.76066253792021 0.00000018690342  
O 4.45795244464435 1.64032004260412 0.00000036896326  
C 7.73591162711651 0.14599056200774 -0.00000011797147  
O 8.06457960532040 -1.16880148929748 -0.00000019631349  
C 9.43375883581147 -1.16968123714769 -0.00000040306815  
C 9.86570610345956 0.11705278222858 -0.00000044247356  
N 8.75948646882819 0.94961654128821 -0.00000025978300  
C 11.24957079616848 0.65233795118971 -0.00000064045880  
H -7.72954575443792 2.24150939443412 -0.00000023860697  
H -4.05714985904597 -2.67511073331908 0.00000037069374  
H -0.74906531112697 2.49301634878329 0.00000052183437  
H 2.92637431474987 -2.41794470102655 0.00000045648983  
H 6.22464397220870 2.75382769226005 0.00000014159003

H 9.91332476894505 -2.13332065328146 -0.00000049332161  
H -11.14769408587555 -1.76897128881636 -0.00000059798061  
H -11.65342846740725 -0.30954498850869 -0.88207631744621  
H -11.65342876752874 -0.30954490043841 0.88207481216175  
H 11.98204303643942 -0.15552801672914 -0.00000077129155  
H 11.42014962160462 1.27730931581864 0.88012540061392  
H 11.42014934946769 1.27730935507722 -0.88012670608350

r<sup>2</sup>SCAN-D4/Def2-TZVP geometry: n = 7

50

N -10.40773505532535 0.70288441008327 0.00000019951924  
C -9.35227770617147 -0.19618845826478 0.00000007887853  
C -9.84267136322786 -1.46484047582397 0.00000015353424  
O -11.20048894997710 -1.37740112957530 0.00000031833948  
C -11.46840164121847 -0.03536171307963 0.00000033927294  
C -7.97359852234062 0.20805818360169 -0.00000007773110  
N -6.92065625104575 -0.55328125744094 -0.00000014550940  
C -5.85981824060452 0.33119366427546 -0.00000026394613  
C -6.33684532721395 1.60814347133327 -0.00000027235408  
O -7.69271231304109 1.54213860196572 -0.00000014314391  
C -4.48417691610687 -0.08420443442037 -0.00000033343022  
O -4.21198936548103 -1.41980846033318 -0.00000026552709  
C -2.85605764341099 -1.49397114797683 -0.00000032437307  
C -2.37121940062452 -0.21995019969278 -0.00000038766267  
N -3.42688440480565 0.67066335615687 -0.00000040439803  
C -0.99364051577428 0.18958531506930 -0.00000039492677  
N 0.06133518005072 -0.56858387667479 -0.00000035765319  
C 1.11973757624485 0.31899337777072 -0.00000031155131  
C 0.63834010327759 1.59436110010007 -0.00000032917819  
O -0.71776372391050 1.52419936028317 -0.00000039589921  
C 2.49726417309570 -0.09128060580562 -0.00000022900389  
N 3.55072431308147 0.66892962180075 -0.00000013962197  
C 4.61137025971201 -0.21613775779470 -0.00000007522606  
C 4.13222191054537 -1.49237724928176 -0.00000013691614  
O 2.77522055333468 -1.42503417193940 -0.00000022217034  
C 5.98774374000030 0.19910241314528 0.00000003265133  
C -12.88800749259127 0.37797236767427 0.00000051253614  
H 4.58388848735717 -2.46841968564114 -0.00000012140787  
H 1.08825573173685 2.57125619243759 -0.00000029890203  
H -2.40914264710499 -2.47225833768035 -0.00000027620516  
H -5.88389428369049 2.58366440032909 -0.00000033659598  
H -9.40257136815744 -2.44619945534033 0.00000011673774  
H -13.53646216879878 -0.49621725012434 0.00000058455765  
H -13.10468094809223 0.98543621203146 -0.88074074147439  
H -13.10468073849739 0.98543619996584 0.88074182642216  
O 6.25918318138000 1.53348665716097 0.00000011948776  
C 7.61687557283841 1.60584181618880 0.00000018729275



C 8.10257342599037 0.33196602168435 0.00000014434056  
N 7.04429670676103 -0.55689183092988 0.00000005400996  
H 8.06379197452935 2.58393203030744 0.00000025473721  
C 9.48226616568001 -0.07560468319042 0.00000017167520  
O 9.76422178138768 -1.40127169378333 0.00000012418084  
C 11.13245289609724 -1.45055285922902 0.00000015860865  
C 11.60956346269291 -0.17984154418914 0.00000021952945  
N 10.53356058067107 0.69131220116862 0.00000022798367  
H 11.57745332079977 -2.43061665889609 0.00000013003773  
C 13.01153226129839 0.30609526757530 0.00000025284077  
H 13.71500795959184 -0.52714065527760 0.00000020810671  
H 13.20402217556738 0.92469232631217 0.88010893717518  
H 13.20402216676739 0.92469241440660 -0.88010836764772

r<sup>2</sup>SCAN-D4/Def2-TZVP geometry: n = 8

56

N -12.14038141321483 0.87148758589160 -0.00000000649833  
C -11.09853667644775 -0.04325734506218 -0.00000002356731  
C -11.60780934465495 -1.30448422959300 -0.00000012695430  
O -12.96419825888819 -1.19676398908252 -0.00000017724347  
C -13.21198660169120 0.14910585854832 -0.00000009540260  
C -9.71389652446173 0.33999605955356 0.00000005442381  
N -8.67292318646991 -0.43762723794868 0.00000004218607  
C -7.59841151971590 0.43016194030593 0.00000009652277  
C -8.05538933755844 1.71436228704411 0.00000013764582  
O -9.41224350577907 1.66956889494719 0.00000012701918  
C -6.22987349413139 -0.00784152754791 0.00000009203807  
O -5.98088492485861 -1.34788864464323 0.00000008522044  
C -4.62658733008998 -1.44564321770687 0.00000006958550  
C -4.11972153391786 -0.18019954455501 0.00000006809959  
N -5.15962092175477 0.72868692483349 0.00000008746965  
C -2.73487616403054 0.20374017693176 0.00000004803676  
N -1.69492570202463 -0.57485380429803 0.00000004109958  
C -0.61941572083611 0.29176719836247 0.00000003274476  
C -1.07552153163242 1.57632317324150 0.00000002924245  
O -2.43278233740010 1.53276402220443 0.00000003647072  
C 0.74880829778680 -0.14803673785373 0.00000003825001  
N 1.81986130985999 0.58730227104844 0.00000004178888  
C 2.85896850349242 -0.32274528600025 0.00000005772829  
C 2.35018308872560 -1.58747310761977 0.00000005587633  
O 0.99571326949555 -1.48808595202605 0.00000004870165  
C 4.24493215978206 0.05819564045757 0.00000006786963  
C -14.62525824620729 0.58351074267743 -0.00000014929232  
H 2.77893125045747 -2.57383448499560 0.00000006368386  
H -0.60659963668238 2.54426339726721 0.00000002964660  
H -4.19660831169249 -2.43149474437009 0.00000005674512  
H -7.58723713303530 2.68268628160586 0.00000018205998  
H -11.18235393875454 -2.29227894278258 -0.00000017802686  
H -15.28652059076844 -0.28103159345096 -0.00000027738883  
H -14.83292238293032 1.19412086826532 -0.88073928876141  
H -14.83292252552020 1.19412070985055 0.88073907019114  
O 4.55095529920093 1.38574349707379 0.00000006559048  
C 5.90916682306258 1.42435502206039 0.00000006230596

C 6.36128039658792 0.13834521679284 0.00000006634266  
N 5.28213263391112 -0.72411081870290 0.00000007443742  
H 6.38147310681478 2.39058641799310 0.00000006152086  
C 7.72863636120366 -0.30566415103210 0.00000005310629  
O 7.97214563180296 -1.64523587806430 0.00000008410771  
C 9.32824991083803 -1.74583312880494 0.00000005890086  
C 9.84033536325022 -0.48229944431907 0.0000000906937  
N 8.80070223745895 0.42827162261928 0.00000000283034  
H 9.75477186004899 -2.73298437469911 0.00000007774352  
C 11.22820829010076 -0.10348380000881 -0.00000003247452  
O 11.53775362749212 1.21599976607247 -0.00000011772577  
C 12.90692294983580 1.23659865274520 -0.00000017681833  
C 13.35736384297079 -0.04378225451625 -0.00000009549571  
N 12.26330265452830 -0.89219572525216 -0.0000001061158  
H 13.37242908839307 2.20710462055498 -0.00000025823307  
C 14.74884357177989 -0.55899728555961 -0.00000009274743  
H 15.46959684310744 0.25934076695892 -0.00000019199075  
H 14.92841399277800 -1.18146922703934 -0.88012019655901  
H 14.92841404588102 -1.18146905598648 0.88012011948947

r<sup>2</sup>SCAN-D4/Def2-TZVP geometry: n = 9

62

N -13.89536016105561 0.70184235245910 0.00000040193116  
C -12.84168390882190 -0.19928122910915 0.00000012321838  
C -13.33444687779317 -1.46702731086251 0.00000014485150  
O -14.69208405454845 -1.37695866491816 0.00000043037159  
C -14.95745139735222 -0.03440061305919 0.00000057734101  
C -11.46229946945809 0.20242346205881 -0.00000009813874  
N -10.41072174869730 -0.56082795416232 -0.00000027661633  
C -9.34836784098552 0.32177759763940 -0.00000035433670  
C -9.82300979453270 1.59960977208235 -0.00000025020998  
O -11.17896036593685 1.53600686555645 -0.00000007393895  
C -7.97362001821069 -0.09632556183758 -0.00000047705636  
O -7.70417253896727 -1.43255340436741 -0.00000047669157  
C -6.34850973294595 -1.50968627599067 -0.00000053379545  
C -5.86108378134036 -0.23665420821737 -0.00000055824854  
N -6.91470358701620 0.65628819463637 -0.00000052447255  
C -4.48284791228023 0.17024985038481 -0.00000056401865  
N -3.42900187994766 -0.58950500835091 -0.00000054141206  
C -2.36952515803762 0.29662664521652 -0.00000047615074  
C -2.84875803266688 1.57279600909304 -0.00000047499607  
O -4.20467607547068 1.50458491175266 -0.00000053906952  
C -0.99293718377715 -0.11607596917656 -0.00000039942630  
N 0.06236934224228 0.64152499891197 -0.00000029118288  
C 1.12035526697127 -0.24637699391796 -0.00000024368948  
C 0.63862084793579 -1.52161611487604 -0.00000033156130  
O -0.71759449435381 -1.45080820203743 -0.00000042516028  
C 2.49693927987625 0.16681350112056 -0.00000011266749  
C -16.37624418046766 0.38165204278504 0.00000092514587  
H 1.08789974888219 -2.49882091593934 -0.00000033376023  
H -2.39736549652422 2.54903688429433 -0.00000043070564  
H -5.90368686493170 -2.48893697275511 -0.00000052809887  
H -9.36829574751392 2.57431598941480 -0.00000024397953  
H -12.89619932327667 -2.44921612917061 0.00000000560283  
H -17.02628981839019 -0.49135252889018 0.00000098758960  
H -16.59175824562567 0.98955081271692 -0.88072172712112  
H -16.59175785602389 0.98955064361466 0.88072378674007  
O 2.76926094125681 1.50205606349164 -0.00000004136395  
C 4.12527575975603 1.57576603010079 0.00000002855692

C 4.61003864963340 0.30166110543571 0.00000003619573  
N 3.55387265945706 -0.58864098177645 -0.00000005410210  
H 4.57264025658590 2.55383009214648 0.00000007493926  
C 5.98869821637476 -0.10505712437406 0.00000010815843  
O 6.27008093753427 -1.43800522663786 0.00000013328989  
C 7.62734933662743 -1.50179207073503 0.00000019683737  
C 8.10320529792670 -0.22430704860972 0.00000018539951  
N 7.04017581142981 0.65795157263659 0.00000014224796  
H 8.08158940064794 -2.47663509902767 0.00000021988713  
C 9.47866467390559 0.19416629292168 0.00000019403476  
O 9.74742991287607 1.52876888405058 0.00000012437763  
C 11.10534013415884 1.60376368447693 0.00000009129942  
C 11.59347761611841 0.33071252594906 0.00000016254947  
N 10.53662733057493 -0.55997738078900 0.00000023155770  
H 11.55015647313271 2.58278404807178 0.00000002620950  
C 12.97314936974016 -0.07562281715698 0.00000017045888  
N 14.02528992007472 0.69199162355910 0.00000009571974  
C 15.10294294245386 -0.17585214216126 0.00000018089553  
C 14.62536579946932 -1.44820252739902 0.00000030017098  
O 13.25805314153351 -1.39957711616273 0.00000028625936  
H 15.06850591067477 -2.42916336832942 0.00000039793326  
C 16.50811589296758 0.31746108389502 0.00000015724334  
H 16.50672228250738 1.40676763861770 0.00000003877619  
H 17.05467074586415 -0.02521312504069 -0.88174212836776  
H 17.05467069884084 -0.02521292981991 0.88174254454920

r<sup>2</sup>SCAN-D4/Def2-TZVP geometry: n = 10

68

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C -14.58607521634641 -0.09052151456906 0.00000201311253  
C -15.08353381224118 -1.35645318826124 0.00000249035028  
O -16.44086859773979 -1.26126099034911 0.00000333314705  
C -16.70120939064107 0.08215789326742 0.00000332947393  
C -13.20510298244397 0.30561534900976 0.00000113997955  
N -12.15685534509037 -0.46208742821713 0.00000065961154  
C -11.09070200337008 0.41591210617477 0.0000004275256  
C -11.55977765998042 1.69578520601522 0.00000014787257  
O -12.91598696924751 1.63801601574064 0.00000084199738  
C -9.71811409050656 -0.00908224284746 -0.00000053137738  
O -9.45652674318569 -1.34693406294545 -0.00000053911772  
C -8.10153456494434 -1.43213765549837 -0.00000105011364  
C -7.60657963865418 -0.16198094480371 -0.00000131206692  
N -8.65477482884054 0.73728970113470 -0.00000099034504  
C -6.22547619677645 0.23491422005454 -0.00000180427755  
N -5.17806570344560 -0.53351958654178 -0.00000208107680  
C -4.11118109799730 0.34360970497011 -0.00000239331931  
C -4.57956870627464 1.62377891042162 -0.00000231278306  
O -5.93608069653610 1.56693760361058 -0.00000194866631  
C -2.73894981410621 -0.08312402734910 -0.00000267837066  
N -1.67455078131976 0.66170311503138 -0.00000283956010  
C -0.62762882882597 -0.23918901105999 -0.00000294441370  
C -1.12477373920127 -1.50854114188345 -0.00000287645804  
O -2.47964484397529 -1.42121533416813 -0.00000271149471  
C 0.75460001629609 0.15432540706179 -0.00000300184964  
C -18.11846588678813 0.50333678208262 0.00000420280742  
H -0.68732710938739 -2.49110279951723 -0.00000287682023  
H -4.12024483945630 2.59631741293795 -0.00000244860577  
H -7.66253859412192 -2.41401274988099 -0.00000113648147  
H -11.10101870737175 2.66859283241070 -0.00000015767470  
H -14.64905440533522 -2.34031765416633 0.00000236178582  
H -18.77174435164325 -0.36724527555785 0.00000472124876  
H -18.33172585016340 1.11198748015962 -0.88073732926719  
H -18.33172470572382 1.11198766857135 0.88074588141106  
O 1.04826064116733 1.48524084528630 -0.00000295327447  
C 2.40522509146993 1.53745445794345 -0.00000284498329

C 2.86945733886095 0.25575720344846 -0.00000287280393  
N 1.79940963018681 -0.61761887364402 -0.00000298861567  
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C 4.24029443634189 -0.17608714087552 -0.00000270791442  
O 4.49431937769407 -1.51493579997316 -0.00000276426154  
C 5.84915282662985 -1.60724124299395 -0.00000243393870  
C 6.35131078442956 -0.33983947009658 -0.00000219209867  
N 5.30745194028966 0.56483564019209 -0.00000240100043  
H 6.28297470818504 -2.59138072938272 -0.00000236743495  
C 7.73553812851710 0.04752772229445 -0.00000168576734  
O 8.03588951440478 1.37645316290613 -0.00000142113208  
C 9.39384521018468 1.42096668446669 -0.00000078480220  
C 9.85148875177336 0.13686906858103 -0.00000071029534  
N 8.77607832794692 -0.73025628508803 -0.00000131508872  
H 9.86178591106404 2.38931424190916 -0.00000042797446  
C 11.22070845988009 -0.30150825764230 -0.00000003144544  
N 12.28992121536133 0.43649513345502 0.00000069996036  
C 13.33297840844215 -0.47019588935883 0.00000120885223  
C 12.82571960642798 -1.73569563131255 0.00000072641180  
O 11.46944695184154 -1.64025889191466 -0.00000006405581  
H 13.25586483661730 -2.72126690802233 0.00000085426671  
C 14.71951251709365 -0.08643506538254 0.00000211113415  
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C 16.39324421161295 1.25969559349497 0.00000323856744  
C 16.84827952286400 -0.01907255071943 0.00000337330736  
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H 18.95941011190034 0.29173626844070 0.00000457687065  
H 18.42344424745573 -1.15102038369576 -0.88010899996696  
H 18.42344326901333 -1.15102051868708 0.88011733312188