

## **Supporting Information**

# **Theoretical insights into the effect of size and substitution patterns of azobenzene derivatives on the DNA G-quadruplex**

Kiana Gholamjani Moghaddam<sup>a</sup>, Goran Giudetti <sup>a</sup>, Wouter Sipma<sup>a</sup> and Shirin Faraji <sup>\*a</sup>

<sup>a</sup> *Zernike Institute for Advanced Materials, University of Groningen, Groningen, The Netherlands. Email: s.s.faraji@rug.nl*

# 1 The Cartesian geometry of critical points located on S<sub>0</sub>, S<sub>1</sub> and S<sub>2</sub> for azobenzene derivatives in trans and cis isomers

- S<sub>0</sub> optimized geometry for AZ1, AZ2 and AZ3 in trans and cis isomers

| AZ1-trans |               |               |                | AZ1-cis |               |               |               |
|-----------|---------------|---------------|----------------|---------|---------------|---------------|---------------|
| C         | -1.5132999298 | -8.4555998457 | -10.4084259173 | N       | 0.2075899954  | 0.1506806818  | 0.0356405742  |
| C         | -0.3643250616 | -8.2880571641 | -9.4489550686  | N       | 0.0985618137  | -0.2691835286 | 1.1986714571  |
| C         | 0.7899979646  | -7.5904108753 | -9.8408210579  | C       | 1.4607810233  | 0.1701307174  | -0.6657092385 |
| C         | -0.4184855903 | -8.8006833541 | -8.1507343126  | C       | 1.4671433180  | -0.3202007833 | -1.9702801358 |
| C         | 1.8538152231  | -7.4084980665 | -8.9708499182  | H       | 0.5516399313  | -0.7528217545 | -2.3773529539 |
| C         | 0.6434754676  | -8.6197534231 | -7.2672456054  | C       | 2.6339558557  | -0.2666260898 | -2.7291986867 |
| C         | 1.7840352162  | -7.9267718989 | -7.6707520124  | H       | 2.6338598477  | -0.6800263173 | -3.7404858529 |
| N         | 2.8093847039  | -7.7949864513 | -6.6953639698  | C       | 3.7967798908  | 0.3227739335  | -2.2252231278 |
| C         | 7.0249586690  | -6.7222237092 | -4.3666095600  | C       | 2.6097890617  | 0.7786354109  | -0.1501513212 |
| C         | 7.1362251218  | -6.3670890041 | -5.7135924077  | H       | 2.6024116172  | 1.1932573964  | 0.8584467692  |
| C         | 5.8108326555  | -7.2690752375 | -3.9215134183  | C       | 3.7564447264  | 0.8561534522  | -0.9302588430 |
| C         | 6.0678592516  | -6.5455133533 | -6.5885891622  | H       | 4.6474947263  | 1.3369133263  | -0.5192447922 |
| C         | 4.7420803599  | -7.4547881034 | -4.7857949900  | C       | 1.1811591824  | -0.9041192377 | 1.8970058863  |
| C         | 4.8681824708  | -7.0917674662 | -6.1329073717  | C       | 1.4315914944  | -0.4806681747 | 3.2016199237  |
| N         | 3.8451175697  | -7.2363519973 | -7.1080262859  | H       | 0.8496088365  | 0.3472178585  | 3.6100017792  |
| C         | 8.1633276570  | -6.5028842803 | -3.4049240758  | C       | 2.4239417864  | -1.1005437654 | 3.9561516187  |
| H         | -2.0315191442 | -7.4963282632 | -10.5683237491 | H       | 2.6306112800  | -0.7414421685 | 4.9671352233  |
| H         | -1.1617681992 | -8.8057314776 | -11.3907714222 | C       | 3.1458831794  | -2.1854988198 | 3.4494207945  |
| H         | 0.8491968808  | -7.1816372581 | -10.8527928997 | C       | 1.8805272930  | -1.9983213226 | 1.3790951443  |
| H         | -1.3041803602 | -9.3496314329 | -7.8231202512  | H       | 1.6693921547  | -2.3533667648 | 0.3697818126  |
| H         | 2.7499044722  | -6.8680594570 | -9.2747983877  | C       | 2.8452144178  | -2.6291270119 | 2.1553863028  |
| H         | 0.6093543116  | -9.0166178825 | -6.2513008899  | H       | 3.3838298873  | -3.4849635289 | 1.7413739793  |
| H         | 8.0721818208  | -5.9444559712 | -6.0859178194  | C       | 4.1909877484  | -2.8858486093 | 4.2788118984  |
| H         | 5.7067362573  | -7.5549466488 | -2.8717645831  | H       | 4.5196431164  | -2.2617823614 | 5.1217018824  |
| H         | 6.1453372875  | -6.2704701851 | -7.6417895406  | H       | 5.0751288659  | -3.1400354708 | 3.6755271051  |
| H         | 3.8004679733  | -7.8810481041 | -4.4402823280  | H       | 3.7956753694  | -3.8266489901 | 4.6950112417  |
| H         | 8.0065706287  | -5.5833617274 | -2.8176267897  | C       | 5.0554194149  | 0.4109118514  | -3.0488142936 |
| H         | 8.2514829250  | -7.3357540931 | -2.6918542052  | H       | 4.9530352025  | -0.1264897949 | -4.0017942220 |
| H         | -2.2521111248 | -9.1771627435 | -10.0331278658 | H       | 5.9143111375  | -0.0171004515 | -2.5092448345 |
| H         | 9.1221645221  | -6.4013405251 | -3.9324241347  | H       | 5.3031924256  | 1.4593442878  | -3.2788412625 |
| AZ2-trans |               |               |                | AZ2-cis |               |               |               |
| C         | -0.3392341716 | -8.3007313702 | -9.4761193300  | C       | 1.3569549763  | -9.3052835199 | -8.5479589147 |
| C         | 0.8009416333  | -7.5980457295 | -9.8793082484  | C       | 2.4887982578  | -8.5592934805 | -8.8765526876 |
| C         | -0.4443691717 | -8.8213940296 | -8.1848172636  | C       | 0.3920960916  | -8.7948724496 | -7.6735318261 |
| C         | 1.8583119344  | -7.4062905032 | -9.0024404233  | C       | 2.6948330415  | -7.3026617330 | -8.3185744481 |
| C         | 0.6242421043  | -8.6179518525 | -7.3048790120  | C       | 0.5880176999  | -7.5172297882 | -7.1420104760 |
| C         | 1.7654122366  | -7.9247350650 | -7.7041553256  | C       | 1.7418452481  | -6.7909087123 | -7.4334169445 |
| N         | 2.7784728340  | -7.7911394523 | -6.7125598429  | N       | 1.8151979138  | -5.4543049488 | -6.9106785361 |
| C         | 6.9783634863  | -6.7479132208 | -4.3430998288  | C       | 6.2150342416  | -7.2931327179 | -5.1738854592 |
| C         | 7.1143616658  | -6.4188279620 | -5.6943673216  | C       | 6.3293532824  | -6.0855420824 | -5.8725870122 |
| C         | 5.7487507421  | -7.2653534184 | -3.9051380841  | C       | 4.9312590009  | -7.7532911913 | -4.8614498184 |
| C         | 6.0551292569  | -6.5943245486 | -6.5810225166  | C       | 5.2022429623  | -5.3593377357 | -6.2414037556 |
| C         | 4.6889085944  | -7.4478720892 | -4.7808780530  | C       | 3.7946816005  | -7.0541525849 | -5.2544509403 |
| C         | 4.8401146377  | -7.1114326039 | -6.1322394105  | C       | 3.9287749269  | -5.8589094703 | -5.9645868211 |
| N         | 3.8285493745  | -7.2566458098 | -7.1193746244  | N       | 2.8133459822  | -5.0236002618 | -6.3124517658 |
| C         | 8.1075952356  | -6.5325540375 | -3.3698763574  | C       | 7.4418196123  | -8.0512926991 | -4.7371805514 |
| H         | 0.8570608385  | -7.1964252316 | -10.8928613064 | H       | 3.2216990994  | -8.9641370855 | -9.5766826054 |
| C         | -1.6654854648 | -9.5830213091 | -7.7370557251  | C       | -0.8322228778 | -9.5940455683 | -7.3073742380 |
| H         | 2.7566212814  | -6.8639018477 | -9.2944795331  | H       | 3.5804358270  | -6.7184828690 | -8.5696713184 |
| H         | 0.5913588898  | -9.0037209682 | -6.2832531293  | H       | -0.1593262030 | -7.0662932892 | -6.4850236731 |
| H         | 8.0624818685  | -6.0188724430 | -6.0608990736  | H       | 7.3206194249  | -5.6989403890 | -6.1212799960 |

|   |               |                |                |   |               |                |               |
|---|---------------|----------------|----------------|---|---------------|----------------|---------------|
| H | 5.6250219061  | -7.5299813452  | -2.8519824079  | H | 4.8165336399  | -8.6862317423  | -4.3046717362 |
| H | 6.1521759599  | -6.3404292426  | -7.6378558663  | H | 5.2920424145  | -4.4032064778  | -6.7599424912 |
| H | 3.7354872826  | -7.8519435893  | -4.4411665706  | H | 2.8034611025  | -7.4357498944  | -5.0079382564 |
| H | 7.9563617376  | -5.6041542355  | -2.7953068597  | H | 7.8464310457  | -7.6358248286  | -3.7998404970 |
| H | 8.1758925812  | -7.3583621978  | -2.6464916741  | H | 7.2170599456  | -9.1124659775  | -4.5588246537 |
| H | 9.0739521068  | -6.4500357200  | -3.8868861773  | H | 8.2386820092  | -7.9912206069  | -5.4928253974 |
| H | -1.1601527724 | -8.4457761908  | -10.1824603212 | H | 1.2136964522  | -10.2929813954 | -8.9920608298 |
| H | -2.4029808991 | -9.6752145104  | -8.5462592737  | H | -1.0203919354 | -10.3954088067 | -8.0354470952 |
| H | -2.1544713359 | -9.0821267319  | -6.8871247790  | H | -1.7267405463 | -8.9555011409  | -7.2635548660 |
| H | -1.3967743728 | -10.5986427445 | -7.4074016602  | H | -0.7142975367 | -10.0631811529 | -6.3172230887 |

#### AZ3-trans

|   |               |                |                |
|---|---------------|----------------|----------------|
| C | -0.4646615516 | -8.2368164384  | -9.2054193275  |
| C | 0.5040561352  | -7.2548682735  | -9.4256174236  |
| C | -0.3067155463 | -9.1906008327  | -8.1954275196  |
| C | 1.6515166328  | -7.2083800951  | -8.6443285037  |
| C | 0.8469289918  | -9.1324095361  | -7.4099280380  |
| C | 1.8213229726  | -8.1581813074  | -7.6306731915  |
| N | 2.9475239536  | -8.2142227876  | -6.7624655660  |
| C | 7.2827414795  | -7.4203582790  | -4.5626018315  |
| C | 7.2209768859  | -6.6727126617  | -5.7429851963  |
| C | 6.1645435758  | -8.1847117964  | -4.1991169395  |
| C | 6.0779013360  | -6.6871071386  | -6.5364128344  |
| C | 5.0222693662  | -8.2125165335  | -4.9873137702  |
| C | 4.9764662537  | -7.4610361988  | -6.1673119388  |
| N | 3.8609403540  | -7.4149995567  | -7.0471986856  |
| C | 8.5036825047  | -7.3646094656  | -3.6763935727  |
| H | 0.3571631779  | -6.5192103798  | -10.2186179904 |
| C | -1.3779695266 | -10.2203190532 | -7.9235103485  |
| H | 2.4228591360  | -6.4550732489  | -8.8004487565  |
| H | 1.0173531280  | -9.8543764241  | -6.6079160107  |
| H | 8.0811934755  | -6.0706046159  | -6.0455880858  |
| H | 6.1952382847  | -8.7717685077  | -3.2777164514  |
| H | 6.0200908828  | -6.1081719796  | -7.4595682014  |
| H | 4.1545331305  | -8.8111330464  | -4.7110116117  |
| H | 8.5684323629  | -8.2920101758  | -3.0856383950  |
| H | 9.4100111287  | -7.3257991208  | -4.3019645153  |
| H | -1.3615497359 | -8.2609972388  | -9.8298634824  |
| H | -1.8395816365 | -10.5306508895 | -8.8746239249  |
| H | -0.9170374956 | -11.1220419789 | -7.4902228750  |
| C | -2.4599390675 | -9.6921229503  | -6.9764300713  |
| C | 8.4812619928  | -6.1563590879  | -2.7342941646  |
| H | -2.9551547308 | -8.8061611883  | -7.4036083645  |
| H | -2.0241010174 | -9.3942424738  | -6.0100624725  |
| H | -3.2284790620 | -10.4564871538 | -6.7859547842  |
| H | 8.4494867573  | -5.2146314157  | -3.3041085239  |
| H | 9.3763082065  | -6.1384177010  | -2.0942333916  |
| H | 7.5925972647  | -6.1820904683  | -2.0847932395  |

#### AZ3-cis

|   |               |                |               |
|---|---------------|----------------|---------------|
| C | 0.5478047803  | -7.1616063232  | -7.4397840933 |
| C | 1.7392479601  | -6.5060856000  | -7.7468498843 |
| C | 0.4195340729  | -8.5409945371  | -7.6338570867 |
| C | 2.8356062750  | -7.2183010911  | -8.2219193279 |
| C | 1.5126200537  | -9.2457572678  | -8.1430370950 |
| C | 2.7203056485  | -8.5988728939  | -8.4022252737 |
| N | 3.7694722684  | -9.3852383373  | -8.9900793358 |
| C | 6.1925027280  | -7.5941034878  | -4.9082755988 |
| C | 6.8785992105  | -7.4059890320  | -6.1127862924 |
| C | 5.0501219550  | -8.4027629161  | -4.9190106803 |
| C | 6.4410061686  | -8.0059049654  | -7.2892789692 |
| C | 4.5827074035  | -8.9807559478  | -6.0939932101 |
| C | 5.2703801583  | -8.7652533622  | -7.2915755761 |
| N | 4.9203834292  | -9.4106097988  | -8.5266198898 |
| C | 6.6483540545  | -6.9152850536  | -3.6390680962 |
| H | 1.8176207506  | -5.4260315831  | -7.6095037734 |
| C | -0.8544605929 | -9.2647979054  | -7.2682178501 |
| H | 3.7728967341  | -6.7118924754  | -8.4538384134 |
| H | 1.4405374967  | -10.3184894168 | -8.3385213332 |
| H | 7.7852632759  | -6.7960473612  | -6.1262104781 |
| H | 4.5102604080  | -8.5816023396  | -3.9858088756 |
| H | 6.9957728671  | -7.8910078788  | -8.2219618020 |
| H | 3.6867809675  | -9.6020116442  | -6.0807466237 |
| H | 6.4142999999  | -7.5582009033  | -2.7755500793 |
| H | 7.7440162021  | -6.8004511818  | -3.6571417257 |
| H | -0.3027702995 | -6.5915804574  | -7.0586233096 |
| H | -1.7076225789 | -8.5750701986  | -7.3659744349 |
| H | -1.0291400656 | -10.0841792512 | -7.9835536027 |
| C | -0.8097560647 | -9.8267500046  | -5.8440447603 |
| C | 5.9931096291  | -5.5435594059  | -3.4481875319 |
| H | -0.6493102969 | -9.0221282310  | -5.1095594032 |
| H | 0.0146727280  | -10.5483487656 | -5.7314223627 |
| H | -1.7491240228 | -10.3409053748 | -5.5903036304 |
| H | 6.2331169829  | -4.8732675129  | -4.2882030727 |
| H | 6.3405974593  | -5.0665126353  | -2.5192368070 |
| H | 4.8968022537  | -5.6358448587  | -3.3983997202 |

### • S<sub>1</sub> optimized geometry for AZ1, AZ2 and AZ3 in trans and cis isomers

#### AZ1-trans

|   |               |               |                |
|---|---------------|---------------|----------------|
| C | -1.6110785807 | -7.8526404264 | -10.0576033761 |
| C | -0.3463773880 | -8.0764031275 | -9.2839674655  |
| C | 0.8143040816  | -7.3667563320 | -9.5920289971  |
| C | -0.2904176526 | -8.9870124266 | -8.2307265759  |
| C | 1.9840510625  | -7.5436820864 | -8.8829427647  |

#### AZ1-cis

|   |              |               |               |
|---|--------------|---------------|---------------|
| N | 1.8427922329 | -0.6930405467 | 0.0215026009  |
| N | 1.9356734039 | -0.3411268229 | 1.2096117390  |
| C | 2.4415531875 | -0.1018011442 | -1.0599561988 |
| C | 2.1728575358 | -0.6084526473 | -2.3342123063 |
| H | 1.5099175386 | -1.4594905443 | -2.4296385709 |

|   |               |               |                |
|---|---------------|---------------|----------------|
| C | 0.8698328461  | -9.1885849509 | -7.5101341721  |
| C | 2.0222709991  | -8.4628498360 | -7.8237386918  |
| N | 3.1610134479  | -8.6925554793 | -7.0968390320  |
| C | 6.8375248521  | -6.5350344640 | -4.4073562309  |
| C | 7.1908037949  | -6.5995515921 | -5.7544583362  |
| C | 5.5912602858  | -7.0389533565 | -4.0376355264  |
| C | 6.3424186794  | -7.1405259151 | -6.6988599672  |
| C | 4.7211291581  | -7.5777395050 | -4.9632914069  |
| C | 5.0907557666  | -7.6311401672 | -6.3150153756  |
| N | 4.2755126475  | -8.1721241705 | -7.2746253301  |
| C | 7.7558453613  | -5.9266649377 | -3.3902059026  |
| H | -2.0490746131 | -6.8749255251 | -9.8285953466  |
| H | -1.4295597622 | -7.8792741440 | -11.1359009413 |
| H | 0.8001529733  | -6.6541591051 | -10.4107935524 |
| H | -1.1770567090 | -9.5558378285 | -7.9716746892  |
| H | 2.8821893997  | -6.9924563311 | -9.1309661846  |
| H | 0.9066600548  | -9.9029108303 | -6.6969519016  |
| H | 8.1573373167  | -6.2208311678 | -6.0695984748  |
| H | 5.2935487208  | -7.0078426587 | -2.9942876048  |
| H | 6.6271532005  | -7.1935923461 | -7.7424171909  |
| H | 3.7571640046  | -7.9717674667 | -4.6674997950  |
| H | 7.4671996318  | -4.8941670747 | -3.1626101043  |
| H | 7.7344932235  | -6.4826746058 | -2.4493093789  |
| H | -2.3600033172 | -8.6120356255 | -9.8243097373  |
| H | 8.7879465143  | -5.9063065173 | -3.7466559473  |

#### AZ2-trans

|   |               |                |                |
|---|---------------|----------------|----------------|
| C | -0.4282394747 | -7.8544134466  | -9.1818939914  |
| C | 0.7269535216  | -7.1600516641  | -9.5197548845  |
| C | -0.4199281828 | -8.7786220833  | -8.1393551208  |
| C | 1.9054342474  | -7.3643446103  | -8.8326192655  |
| C | 0.7627849957  | -8.9949363436  | -7.4496931964  |
| C | 1.9247410635  | -8.2933134154  | -7.7812623385  |
| N | 3.0666279483  | -8.5566513312  | -7.0694573492  |
| C | 6.8621732648  | -6.6181987463  | -4.3782774686  |
| C | 7.1826498887  | -6.6343535488  | -5.7350699776  |
| C | 5.6113164875  | -7.1044643888  | -3.9998902293  |
| C | 6.2984286085  | -7.1119213450  | -6.6806185212  |
| C | 4.7058861706  | -7.5803646519  | -4.9258526819  |
| C | 5.0429234867  | -7.5853523264  | -6.2873293082  |
| N | 4.1919227859  | -8.0632585136  | -7.2483262142  |
| C | 7.8198170582  | -6.0781463653  | -3.3589383872  |
| H | 0.7040223238  | -6.4444681339  | -10.3342641219 |
| C | -1.6617738916 | -9.5330378255  | -7.7617414269  |
| H | 2.8142299850  | -6.8340573775  | -9.0854866594  |
| H | 0.8076826389  | -9.7108316816  | -6.6368911913  |
| H | 8.1515953445  | -6.2678936616  | -6.0571200479  |
| H | 5.3385970585  | -7.1097675259  | -2.9492980065  |
| H | 6.5572370320  | -7.1275538395  | -7.7320979641  |
| H | 3.7384521074  | -7.9608041094  | -4.6237504320  |
| H | 7.5619636353  | -5.0506211290  | -3.0782029179  |
| H | 7.8079906665  | -6.6755375766  | -2.4435815836  |
| H | 8.8429632793  | -6.0657109737  | -3.7405835017  |
| H | -1.3438678557 | -7.6789080958  | -9.7349962336  |
| H | -2.4951605071 | -9.2814800996  | -8.4199680262  |
| H | -1.9645558192 | -9.3053359453  | -6.7352555737  |
| H | -1.5007678676 | -10.6134192447 | -7.8201833787  |

#### AZ3-trans

|   |              |               |               |
|---|--------------|---------------|---------------|
| C | 2.7545286920 | -0.0289668281 | -3.4443319835 |
| H | 2.5406612674 | -0.4387320132 | -4.4256923093 |
| C | 3.6042955322 | 1.0694846687  | -3.3331626642 |
| C | 3.2961545713 | 1.0033929456  | -0.9298389324 |
| H | 3.4959710522 | 1.3977679403  | 0.0583785499  |
| C | 3.8582265597 | 1.5683356194  | -2.0553328319 |
| H | 4.5179315514 | 2.4226465784  | -1.9396118732 |
| C | 2.1700713149 | -1.1512427912 | 2.2897512490  |
| C | 2.1861591321 | -0.5787576366 | 3.5650606611  |
| H | 2.0264233007 | 0.4880721981  | 3.6613256481  |
| C | 2.4120745788 | -1.3692126898 | 4.6735630792  |
| H | 2.4296262672 | -0.9076218430 | 5.6551630047  |
| C | 2.6148977211 | -2.7437603829 | 4.5607891731  |
| C | 2.3761757440 | -2.5321947714 | 2.1579343279  |
| H | 2.3587137904 | -2.9726569336 | 1.1691510093  |
| C | 2.5925188777 | -3.3011942732 | 3.2829080709  |
| H | 2.7526515260 | -4.3683695221 | 3.1657227757  |
| C | 2.8242965723 | -3.6025617163 | 5.7717315863  |
| H | 3.1352994134 | -3.0077325968 | 6.6331050979  |
| H | 3.5881554146 | -4.3642317906 | 5.5936486659  |
| H | 1.9035274781 | -4.1273304865 | 6.0505485971  |
| C | 4.2205052334 | 1.7077772290  | -4.5418129114 |
| H | 4.0024869863 | 1.1379971894  | -5.4471219255 |
| H | 5.3080892028 | 1.7791609423  | -4.4441350861 |
| H | 3.8433689212 | 2.7250466397  | -4.6908644141 |

#### AZ2-cis

|   |               |                |                |
|---|---------------|----------------|----------------|
| C | 0.0053048458  | -8.9425671191  | -9.4186724422  |
| C | 1.2279578863  | -8.4302766433  | -9.8229065977  |
| C | -0.4122574950 | -8.8202253356  | -8.0911846749  |
| C | 2.0646423880  | -7.7918093731  | -8.9262044359  |
| C | 0.4158270953  | -8.1766246943  | -7.1903969611  |
| C | 1.6560870483  | -7.6652769096  | -7.5931649255  |
| N | 2.4279924134  | -7.0319683033  | -6.6537889202  |
| C | 6.9718807033  | -6.7895615997  | -4.4876593376  |
| C | 6.9215541594  | -5.9670375496  | -5.6154870593  |
| C | 5.8315903009  | -7.5185951193  | -4.1641420750  |
| C | 5.7840467841  | -5.8688496489  | -6.3859445980  |
| C | 4.6796799658  | -7.4437596362  | -4.9248673309  |
| C | 4.6461766920  | -6.6135038748  | -6.0517023540  |
| N | 3.5288766653  | -6.4865910297  | -6.8345513156  |
| C | 8.2150792775  | -6.8680578465  | -3.6535913058  |
| H | 1.5381052053  | -8.5326376326  | -10.8570495605 |
| C | -1.7386497495 | -9.3740063217  | -7.6596820037  |
| H | 3.0209786913  | -7.3845542332  | -9.2271767972  |
| H | 0.1232438969  | -8.0592475493  | -6.1536530441  |
| H | 7.7972298490  | -5.3882401899  | -5.8907501185  |
| H | 5.8443500207  | -8.1658289808  | -3.2932220206  |
| H | 5.7498563292  | -5.2259906027  | -7.2568836933  |
| H | 3.7960026521  | -8.0128591609  | -4.6657508101  |
| H | 8.4301083267  | -5.9098658901  | -3.1687580681  |
| H | 8.1216279319  | -7.6223681428  | -2.8699794967  |
| H | 9.0878591326  | -7.1229466123  | -4.2625975633  |
| H | -0.6356658801 | -9.4403424050  | -10.1380535188 |
| H | -2.5594220932 | -8.8946961343  | -8.2018068189  |
| H | -1.9069672760 | -9.2217571954  | -6.5921127800  |
| H | -1.8011590676 | -10.4474388661 | -7.8613400721  |

#### AZ3-cis

|   |               |                |               |   |               |                |               |
|---|---------------|----------------|---------------|---|---------------|----------------|---------------|
| C | -0.5202777677 | -7.8567564901  | -8.8322591147 | C | -0.9144772008 | -7.9578016016  | -8.9017620412 |
| C | 0.5132890753  | -6.9480391776  | -9.0081030677 | C | 0.0947018121  | -7.0179102229  | -9.0554065246 |
| C | -0.2965454598 | -9.0676630441  | -8.1750680592 | C | -0.6518330427 | -9.1888221995  | -8.2990900686 |
| C | 1.7837085896  | -7.2160003095  | -8.5364467430 | C | 1.3784465927  | -7.2745692432  | -8.6150031358 |
| C | 0.9761383137  | -9.3472704329  | -7.7087780999 | C | 0.6346110614  | -9.4566195590  | -7.8640250118 |
| C | 2.0199642328  | -8.4302815783  | -7.8773971261 | C | 1.6536616234  | -8.5088077890  | -8.0103096085 |
| N | 3.2608497777  | -8.7686662669  | -7.4049658323 | N | 2.9101548889  | -8.8370506610  | -7.5722601925 |
| C | 7.2025390678  | -7.4266343653  | -4.5650396990 | C | 6.8622703424  | -7.4960516847  | -4.7459701979 |
| C | 7.3369056808  | -6.9225550126  | -5.8590779059 | C | 6.9673445770  | -6.9500563135  | -6.0257364060 |
| C | 6.0610736665  | -8.1707332898  | -4.2722491443 | C | 5.7408293619  | -8.2724847724  | -4.4602776057 |
| C | 6.3786218262  | -7.1478869363  | -6.8248732888 | C | 5.9999510044  | -7.1660291922  | -6.9844272492 |
| C | 5.0827820450  | -8.4045695330  | -5.2179095452 | C | 4.7539415141  | -8.4980561929  | -5.3990756974 |
| C | 5.2329400698  | -7.8879148352  | -6.5127201199 | C | 4.8743011378  | -7.9390491828  | -6.6792369918 |
| N | 4.3053197479  | -8.1038862691  | -7.4965388681 | N | 3.9376452033  | -8.1450514991  | -7.6568101290 |
| C | 8.2370666876  | -7.1454471755  | -3.5118509135 | C | 7.9065513631  | -7.2254886674  | -3.6996322944 |
| H | 0.3252283973  | -6.0130071170  | -9.5242820757 | H | -0.1234375921 | -6.0672237801  | -9.5294396814 |
| C | -1.4258829873 | -10.0353292683 | -7.9465259049 | C | -1.7533927676 | -10.1927315743 | -8.0925295568 |
| H | 2.6014833865  | -6.5201730761  | -8.6708224351 | H | 2.1774657569  | -6.5544221149  | -8.7332655641 |
| H | 1.1885243800  | -10.2825972089 | -7.2038424494 | H | 0.8773021921  | -10.4067474948 | -7.4020704947 |
| H | 8.2193438769  | -6.3457390443  | -6.1162949618 | H | 7.8339126106  | -6.3473100265  | -6.2774282253 |
| H | 5.9354658049  | -8.5808365327  | -3.2750706770 | H | 5.6382075549  | -8.7151555145  | -3.4744761144 |
| H | 6.4933914579  | -6.7612522344  | -7.8299433503 | H | 6.0919699909  | -6.7468790885  | -7.9787708827 |
| H | 4.2019170943  | -8.9892489389  | -4.9853923292 | H | 3.8888637727  | -9.1081200926  | -5.1724531435 |
| H | 8.2816542298  | -7.9871430913  | -2.8135059825 | H | 7.9715567240  | -8.0827411935  | -3.0221830900 |
| H | 9.2239681578  | -7.0801863903  | -3.9810407323 | H | 8.8863481018  | -7.1355446707  | -4.1795843792 |
| H | -1.5093100868 | -7.6292925955  | -9.2146525264 | H | -1.9146813630 | -7.7387582929  | -9.2591522945 |
| H | -2.0884812963 | -10.0281128140 | -8.8177838402 | H | -2.4566088651 | -10.1334650161 | -8.9290807117 |
| H | -1.0238582016 | -11.0499963754 | -7.8702535759 | H | -1.3321575192 | -11.2024130126 | -8.1115480875 |
| C | -2.2334027878 | -9.7131799977  | -6.6938495991 | C | -2.5052060414 | -9.9805395261  | -6.7829604058 |
| C | 7.9613736205  | -5.8605029120  | -2.7366839574 | C | 7.6236575779  | -5.9631621906  | -2.8906251862 |
| H | -2.6682149500 | -8.7111565270  | -6.7534345801 | H | -2.9586200268 | -8.9856324007  | -6.7474819600 |
| H | -1.6013154970 | -9.7456403549  | -5.8016722040 | H | -1.8307143848 | -10.0660799574 | -5.9260267462 |
| H | -3.0493341902 | -10.4290387774 | -6.5585945125 | H | -3.3017252087 | -10.7206942296 | -6.6635692389 |
| H | 7.9398041070  | -4.9956206446  | -3.4062243989 | H | 7.5815657075  | -5.0830045336  | -3.5389504064 |
| H | 8.7323064267  | -5.6852552444  | -1.9804914903 | H | 8.4020014204  | -5.7950954841  | -2.1404113807 |
| H | 6.9931735040  | -5.9085861382  | -2.2297308892 | H | 6.6629321197  | -6.0367310245  | -2.3726492955 |

• S<sub>2</sub> optimized geometry for AZ1, AZ2 and AZ3 in trans and cis isomers

| AZ1-trans |               |               | AZ1-cis |              |               |
|-----------|---------------|---------------|---------|--------------|---------------|
| C         | -1.4435850937 | -8.4531294152 | N       | 1.0231458583 | -0.4368317011 |
| C         | -0.3070962798 | -8.2652300674 | N       | 1.0830645441 | -0.1873358606 |
| C         | 0.8793764707  | -7.6402104062 | C       | 1.9229926241 | -0.0214686058 |
| C         | -0.4088388740 | -8.7227843074 | C       | 1.6808271705 | -0.3570896615 |
| C         | 1.9286779837  | -7.4655254560 | H       | 0.7891962340 | -0.9240258149 |
| C         | 0.6168112178  | -8.5630396143 | C       | 2.5722237183 | 0.0257201382  |
| C         | 1.8291466301  | -7.9274519406 | H       | 2.3738951125 | -0.2482109759 |
| N         | 2.7961576529  | -7.8044410847 | C       | 3.7171603402 | 0.7600781779  |
| C         | 6.9594549685  | -6.7262240394 | C       | 3.0690697383 | 0.7227989770  |
| C         | 7.0637510582  | -6.2777233333 | H       | 3.2461994922 | 0.9998163529  |
| C         | 5.7738644179  | -7.3525320239 | C       | 3.9409921636 | 1.0994379331  |
| C         | 6.0408255964  | -6.4459359641 | H       | 4.8224367998 | 1.6770738822  |
| C         | 4.7274670949  | -7.5361410279 | C       | 1.6698095805 | -0.9816227032 |
| C         | 4.8291061290  | -7.0820106952 | C       | 1.6115367033 | -0.5679378178 |
| N         | 3.8641237674  | -7.2115590004 | H       | 1.0993103002 | 0.3574394211  |
| C         | 8.0922778351  | -6.5275977726 | C       | 2.2074858366 | -1.3272006214 |
| H         | -2.3517423011 | -7.9627068545 | H       | 2.1611553766 | -0.9882712350 |
| H         | -1.2176833929 | -8.0476544237 | C       | 2.8635917375 | -2.5210435986 |
|           |               |               |         |              | 4.1956574588  |

|   |               |               |                |   |              |               |               |
|---|---------------|---------------|----------------|---|--------------|---------------|---------------|
| H | 0.9696531374  | -7.2847710417 | -10.8402473486 | C | 2.3235399784 | -2.1823175520 | 1.8578593227  |
| H | -1.3241138648 | -9.2101860980 | -7.7734073559  | H | 2.3541136499 | -2.5115330728 | 0.8267880837  |
| H | 2.8465826087  | -6.9836277553 | -9.2496583110  | C | 2.9056555886 | -2.9278122806 | 2.8627068770  |
| H | 0.5449121243  | -8.9113536232 | -6.1852765128  | H | 3.4077910696 | -3.8552641181 | 2.6060334564  |
| H | 7.9787563236  | -5.7904175566 | -6.0396436229  | C | 3.4801491558 | -3.3590569698 | 5.2747338384  |
| H | 5.6823374200  | -7.7025109289 | -2.9664134710  | H | 3.6524288493 | -2.7768001412 | 6.1823011109  |
| H | 6.1143315575  | -6.1043096409 | -7.6305873075  | H | 4.4371335157 | -3.7801046190 | 4.9553127834  |
| H | 3.8107054399  | -8.0202008036 | -4.5602921614  | H | 2.8303635410 | -4.1999292154 | 5.5424595865  |
| H | 8.3244557486  | -5.4626862144 | -3.3143059381  | C | 4.6756567982 | 1.1899109765  | -4.0350643735 |
| H | 7.8699636083  | -6.9389690530 | -2.4493242528  | H | 4.4085553632 | 0.7642137035  | -5.0040746945 |
| H | -1.6897868331 | -9.5152530514 | -10.4884845588 | H | 5.6983928876 | 0.8788623622  | -3.8012705638 |
| H | 9.0071078482  | -7.0048168058 | -3.8054424981  | H | 4.6877308722 | 2.2797086107  | -4.1422701342 |

#### AZ2-trans

|   |               |                |                |
|---|---------------|----------------|----------------|
| C | -0.3247642702 | -8.3219134968  | -9.5226118324  |
| C | 0.8599069095  | -7.7002298769  | -9.8649382692  |
| C | -0.4680084945 | -8.7918316015  | -8.2048699978  |
| C | 1.9164206710  | -7.5269072876  | -8.9374783382  |
| C | 0.5913709559  | -8.6220871959  | -7.2625012459  |
| C | 1.8227970777  | -7.9878216758  | -7.5759685452  |
| N | 2.7450342333  | -7.8699360128  | -6.6538512102  |
| C | 6.9732476113  | -6.7335402783  | -4.3625699027  |
| C | 7.0521761104  | -6.2967929620  | -5.6857034073  |
| C | 5.7965364741  | -7.3705535117  | -3.9591011171  |
| C | 6.0034506831  | -6.4821348993  | -6.5645905380  |
| C | 4.7398413790  | -7.5636305593  | -4.8248406021  |
| C | 4.8201183515  | -7.1187128781  | -6.1579749857  |
| N | 3.8333255874  | -7.2604754585  | -7.0958329075  |
| C | 8.0985140746  | -6.5070923511  | -3.3974319871  |
| H | 1.0019863831  | -7.3266044770  | -10.8729310016 |
| C | -1.7095625511 | -9.4698499819  | -7.7555844566  |
| H | 2.8345321619  | -7.0377034310  | -9.2278924873  |
| H | 0.4669829141  | -8.9899348216  | -6.2510538994  |
| H | 7.9558644301  | -5.8037517586  | -6.0300897342  |
| H | 5.7131446318  | -7.7248271769  | -2.9357053960  |
| H | 6.0698295042  | -6.1432986514  | -7.5918471257  |
| H | 3.8342558766  | -8.0592571728  | -4.5048274960  |
| H | 7.9085404624  | -5.6368829854  | -2.7580470422  |
| H | 8.2379681902  | -7.3669191526  | -2.7361272274  |
| H | 9.0416858884  | -6.3278369578  | -3.9189929770  |
| H | -1.1239254858 | -8.4477888655  | -10.2399771147 |
| H | -2.4469298235 | -9.5518710367  | -8.5533238248  |
| H | -2.1543438426 | -8.9245138866  | -6.9151054035  |
| H | -1.4778960941 | -10.4731195987 | -7.3799899267  |

#### AZ3-trans

|   |               |               |               |
|---|---------------|---------------|---------------|
| C | -0.4231879162 | -8.3019844690 | -9.3480867129 |
| C | 0.6329896925  | -7.4424176109 | -9.5776924342 |
| C | -0.3482586675 | -9.1621115748 | -8.2369852553 |
| C | 1.7746425583  | -7.4080477222 | -8.7381731399 |
| C | 0.7981452194  | -9.1352873075 | -7.3869232733 |
| C | 1.9057742028  | -8.2699550070 | -7.5913522276 |
| N | 2.9211431135  | -8.3118875139 | -6.7655034556 |
| C | 7.2663021137  | -7.3548794517 | -4.6167173622 |
| C | 7.1289069270  | -6.5269332326 | -5.7330640251 |
| C | 6.2241609672  | -8.2404471563 | -4.3337890778 |
| C | 6.0018420546  | -6.5790273745 | -6.5278216268 |
| C | 5.0901713068  | -8.3050941211 | -5.1187801309 |

#### AZ2-cis

|   |               |                |                |
|---|---------------|----------------|----------------|
| C | 0.5373009539  | -9.2766483045  | -9.0480522331  |
| C | 1.8126063262  | -8.7901636273  | -9.2880131008  |
| C | -0.2249589146 | -8.7887919652  | -7.9835214450  |
| C | 2.3659205771  | -7.8165566792  | -8.4767344694  |
| C | 0.3203487315  | -7.8104986316  | -7.1736792428  |
| C | 1.6145852289  | -7.3248715301  | -7.4024417636  |
| N | 2.0958111606  | -6.3649713820  | -6.5431245257  |
| C | 6.7809373117  | -6.9596758962  | -4.7735416264  |
| C | 6.7033425373  | -5.8222325393  | -5.5808883987  |
| C | 5.6228555595  | -7.7088982942  | -4.5909790804  |
| C | 5.5225297811  | -5.4452120784  | -6.1804510815  |
| C | 4.4265925505  | -7.3559411723  | -5.1877967493  |
| C | 4.3665604259  | -6.2155351227  | -5.9987489442  |
| N | 3.2135692208  | -5.8181425022  | -6.6260084453  |
| C | 8.0728061246  | -7.3438970113  | -4.1178141320  |
| H | 2.3853300649  | -9.1745543531  | -10.1247866536 |
| C | -1.6066581181 | -9.3187639619  | -7.7341223494  |
| H | 3.3558014553  | -7.4194174617  | -8.6604898303  |
| H | -0.2366670026 | -7.3992155456  | -6.3402335102  |
| H | 7.5917383753  | -5.2187788805  | -5.7365085979  |
| H | 5.6558696756  | -8.5927956582  | -3.9624525045  |
| H | 5.4618970692  | -4.5608373222  | -6.8025161531  |
| H | 3.5290527170  | -7.9407854673  | -5.0308645181  |
| H | 8.3910954104  | -6.5861738520  | -3.3941272504  |
| H | 7.9832869291  | -8.2935506405  | -3.5871639639  |
| H | 8.8775408191  | -7.4438970997  | -4.8526930161  |
| H | 0.1217891872  | -10.0399133146 | -9.6970752260  |
| H | -2.2472594882 | -9.1742015605  | -8.6090355610  |
| H | -2.0782224090 | -8.8202833780  | -6.8855516840  |
| H | -1.5834655607 | -10.3922793678 | -7.5236646430  |

#### AZ3-cis

|   |               |               |               |
|---|---------------|---------------|---------------|
| C | -0.2566561286 | -7.4911943779 | -8.0583591801 |
| C | 0.8690638266  | -6.6799603173 | -8.0551670178 |
| C | -0.1347096629 | -8.8811868177 | -8.0265830774 |
| C | 2.1369135724  | -7.2270348413 | -8.0132515848 |
| C | 1.1332527150  | -9.4344052319 | -7.9923413730 |
| C | 2.2726394118  | -8.6216308607 | -7.9748113604 |
| N | 3.4992328021  | -9.2411325996 | -7.9261299941 |
| C | 6.9001006065  | -7.4378295354 | -4.6683086757 |
| C | 7.3370811563  | -7.2563827197 | -5.9811513941 |
| C | 5.6680548628  | -8.0575792568 | -4.4705760568 |
| C | 6.5795628366  | -7.6707404067 | -7.0557859981 |
| C | 4.8866812643  | -8.4753308401 | -5.5299554395 |

|   |               |                |                |   |               |                |               |
|---|---------------|----------------|----------------|---|---------------|----------------|---------------|
| C | 4.9529278228  | -7.4677487970  | -6.2409222621  | C | 5.3359928138  | -8.2770509167  | -6.8434313865 |
| N | 3.8743277454  | -7.4523441485  | -7.0846216024  | N | 4.6032149931  | -8.6615381341  | -7.9370444902 |
| C | 8.4744952322  | -7.2657367907  | -3.7270836695  | C | 7.7183922186  | -6.9505620652  | -3.5062018533 |
| H | 0.6047172227  | -6.7656535907  | -10.4245496117 | H | 0.7549015464  | -5.6022283753  | -8.0932631624 |
| C | -1.4679409537 | -10.0856948515 | -7.8994929322  | C | -1.3560866059 | -9.7594054060  | -7.9969393697 |
| H | 2.5894600847  | -6.7277657530  | -8.9376886620  | H | 3.0237475769  | -6.6066512510  | -8.0259100466 |
| H | 0.8463828908  | -9.8056151992  | -6.5370943015  | H | 1.2747167317  | -10.5090036572 | -7.9777780339 |
| H | 7.9259385029  | -5.8327313535  | -5.9818325673  | H | 8.2985192035  | -6.7864926533  | -6.1613561964 |
| H | 6.3110993148  | -8.8991377993  | -3.4743476495  | H | 5.3135760051  | -8.2233590231  | -3.4580530081 |
| H | 5.8999284631  | -5.9382859304  | -7.3959313425  | H | 6.9228564033  | -7.5375932344  | -8.0742068004 |
| H | 4.2899544383  | -8.9962999548  | -4.8951683373  | H | 3.9367521558  | -8.9685050870  | -5.3661977179 |
| H | 8.6807789412  | -8.2499795899  | -3.2935780259  | H | 7.5395874506  | -7.5962808020  | -2.6407339960 |
| H | 9.3513901139  | -7.0035823436  | -4.3285150258  | H | 8.7821907656  | -7.0428455825  | -3.7473846340 |
| H | -1.2869195996 | -8.3201968223  | -9.9986627081  | H | -1.2431910736 | -7.0420704962  | -8.0976387406 |
| H | -2.0994968797 | -10.2330979193 | -8.7783474884  | H | -2.1491018761 | -9.2942670712  | -8.5907466913 |
| H | -1.0520288050 | -11.0612234283 | -7.6251198206  | H | -1.1264752617 | -10.7145303522 | -8.4786762114 |
| C | -2.3161763152 | -9.5613263718  | -6.7364147069  | C | -1.8651605762 | -10.0134701532 | -6.5821922285 |
| C | 8.3142404488  | -6.2463271068  | -2.6032280187  | C | 7.4104188126  | -5.5043723018  | -3.1290738290 |
| H | -2.7664225141 | -8.5970446733  | -6.9846226254  | H | -2.1276398140 | -9.0752741968  | -6.0844260935 |
| H | -1.7161931043 | -9.4310519797  | -5.8325139564  | H | -1.1015832862 | -10.5071682502 | -5.9740414361 |
| H | -3.1188785720 | -10.2677594549 | -6.5126753292  | H | -2.7539763710 | -10.6508553076 | -6.5940679134 |
| H | 8.1361021650  | -5.2448717942  | -3.0062319343  | H | 7.6085333596  | -4.8296497240  | -3.9670902454 |
| H | 9.2095379207  | -6.2054226420  | -1.9748466696  | H | 8.0223498972  | -5.1816265678  | -2.2816246376 |
| H | 7.4623538640  | -6.4992291631  | -1.9649920310  | H | 6.3584576679  | -5.3869915858  | -2.8528701259 |

• CI-S1/S0 optimized geometry for AZ1, AZ2 and AZ3 in trans and cis isomers

| AZ1-trans |               |                |                | AZ1-cis |              |               |               |
|-----------|---------------|----------------|----------------|---------|--------------|---------------|---------------|
| C         | -1.4882272078 | -7.4404176376  | -9.4437532190  | N       | 0.9481202912 | -0.4966659898 | -0.0904177278 |
| C         | -0.1653407561 | -7.8965753902  | -8.9040191083  | N       | 1.1668347245 | -0.3601946606 | 1.1258578701  |
| C         | 0.9964670135  | -7.1623140985  | -9.1255639798  | C       | 1.8905527641 | -0.0302612102 | -1.0105094190 |
| C         | -0.0435274842 | -9.0860168208  | -8.1882797585  | C       | 1.5792673095 | -0.2090812561 | -2.3564441671 |
| C         | 2.2283929206  | -7.5806303030  | -8.6636814759  | H       | 0.6326705351 | -0.6723611398 | -2.6068966578 |
| C         | 1.1728408299  | -9.5359172130  | -7.7191549688  | C       | 2.4722129173 | 0.1898413634  | -3.3335072642 |
| C         | 2.3354367384  | -8.7863072475  | -7.9480882611  | H       | 2.2248353263 | 0.0386758198  | -4.3784233732 |
| N         | 3.5276764809  | -9.2233615322  | -7.4900177494  | C       | 3.6835264264 | 0.7875222853  | -2.9958460838 |
| C         | 6.4813341208  | -6.4146684096  | -4.6530799091  | C       | 3.0989749292 | 0.5789989205  | -0.6559598507 |
| C         | 7.2012211361  | -6.9161441615  | -5.7341610723  | H       | 3.3252466686 | 0.7383487715  | 0.3907770578  |
| C         | 5.1344205761  | -6.7683825534  | -4.5306482819  | C       | 3.9759970756 | 0.9761016378  | -1.6415362917 |
| C         | 6.6020184065  | -7.7448594974  | -6.6640161677  | H       | 4.9121986069 | 1.4480350458  | -1.3617884322 |
| C         | 4.5209973834  | -7.5888536766  | -5.4523809947  | C       | 1.7233141603 | -1.0616979116 | 2.1358748586  |
| C         | 5.2548520231  | -8.0772794966  | -6.5382202846  | C       | 1.7249662140 | -0.5456470151 | 3.4387492943  |
| N         | 4.7235591001  | -8.8882462941  | -7.5440958844  | H       | 1.2722117529 | 0.4210317848  | 3.6201645995  |
| C         | 7.1306281266  | -5.5327306108  | -3.6304758308  | C       | 2.3002497064 | -1.2645997281 | 4.4669364781  |
| H         | -1.5747642669 | -6.3507670902  | -9.4231189437  | H       | 2.2944517584 | -0.8412822526 | 5.4662839737  |
| H         | -1.6272476061 | -7.7566021132  | -10.4843222739 | C       | 2.8823704177 | -2.5124631675 | 4.2598733488  |
| H         | 0.9392943232  | -6.2296091669  | -9.6786365248  | C       | 2.3094004187 | -2.3210036113 | 1.9098009278  |
| H         | -0.9293613660 | -9.6826915044  | -7.9946464499  | H       | 2.3094415628 | -2.7318530897 | 0.9077608148  |
| H         | 3.1195869679  | -6.9936907772  | -8.8479508495  | C       | 2.8682718266 | -3.0172496496 | 2.9613977747  |
| H         | 1.2488438678  | -10.4660917973 | -7.1701533566  | H       | 3.3109842702 | -3.9888473202 | 2.7635163146  |
| H         | 8.2473810724  | -6.6535914016  | -5.8461006191  | C       | 3.4864962233 | -3.2955359758 | 5.3872444605  |
| H         | 4.5617872829  | -6.3904773486  | -3.6900370603  | H       | 3.5726628442 | -2.6878053566 | 6.2904552806  |
| H         | 7.1516472008  | -8.1432385781  | -7.5081764357  | H       | 4.4866814817 | -3.6589214189 | 5.1326602016  |
| H         | 3.4807400288  | -7.8693643676  | -5.3453250437  | H       | 2.8798196500 | -4.1728424583 | 5.6378461560  |
| H         | 6.5319979012  | -4.6371638038  | -3.4424514166  | C       | 4.6516446641 | 1.2323031892  | -4.0496539007 |
| H         | 7.2379208937  | -6.0552238842  | -2.6741671161  | H       | 4.2994486884 | 0.9748031036  | -5.0498567157 |
| H         | -2.3183535654 | -7.8540205794  | -8.8661331752  | H       | 5.6317795462 | 0.7678329288  | -3.9057809837 |
| H         | 8.1247778575  | -5.2157626447  | -3.9501437891  | H       | 4.8009718395 | 2.3160223319  | -4.0143947208 |

| AZ2-trans |               |                |               | AZ2-cis |               |                |                |
|-----------|---------------|----------------|---------------|---------|---------------|----------------|----------------|
| C         | -0.2642340325 | -7.4591492383  | -8.5564957814 | C       | 0.4698233094  | -9.2665705884  | -9.0838607265  |
| C         | 0.9273843592  | -6.7468078920  | -8.5858386694 | C       | 1.6947785050  | -8.7239049860  | -9.4487787434  |
| C         | -0.3083918176 | -8.7742645735  | -8.0929835745 | C       | -0.1737397673 | -8.8278838687  | -7.9291122203  |
| C         | 2.1040967840  | -7.3263031053  | -8.1510113681 | C       | 2.3061496890  | -7.7546872324  | -8.6815022757  |
| C         | 0.8740391910  | -9.3540109118  | -7.6632756458 | C       | 0.4245449363  | -7.8482779860  | -7.1545832990  |
| C         | 2.0717346195  | -8.6385124753  | -7.6774397083 | C       | 1.6665340843  | -7.3056106787  | -7.5106852686  |
| N         | 3.1937358169  | -9.3238136698  | -7.1949447935 | N       | 2.2299743960  | -6.3608437970  | -6.7268286354  |
| C         | 6.6784061813  | -6.4772896673  | -4.6351639548 | C       | 6.7431362428  | -6.9704475020  | -4.7587521265  |
| C         | 7.1222149347  | -6.8547944006  | -5.8996042211 | C       | 6.6776243811  | -5.7399283013  | -5.4145036315  |
| C         | 5.4041663955  | -6.8925007231  | -4.2538887930 | C       | 5.6087168791  | -7.7820742083  | -4.7571191610  |
| C         | 6.3434779217  | -7.6099875546  | -6.7530538149 | C       | 5.5198102974  | -5.3316688282  | -6.0428297253  |
| C         | 4.5968526780  | -7.6401107823  | -5.0855336732 | C       | 4.4431769437  | -7.3897493877  | -5.3844421074  |
| C         | 5.0605548756  | -8.0139157186  | -6.3604817686 | C       | 4.3940281450  | -6.1580330586  | -6.0415840977  |
| N         | 4.2978667708  | -8.7558571683  | -7.1900811077 | N       | 3.2734743076  | -5.6809168606  | -6.7215331163  |
| C         | 7.5289665824  | -5.6521950281  | -3.7160663229 | C       | 7.9977028759  | -7.3926026473  | -4.0564542696  |
| H         | 0.9344328568  | -5.7294047801  | -8.9601080425 | H       | 2.1854027076  | -9.0667877790  | -10.3533952151 |
| C         | -1.6034594292 | -9.5305613833  | -8.0518324302 | C       | -1.4993769016 | -9.4007071295  | -7.5172597378  |
| H         | 3.0443828685  | -6.7912399064  | -8.1841483516 | H       | 3.2602369707  | -7.3283705641  | -8.9638502249  |
| H         | 0.9009671068  | -10.3750765838 | -7.3007952656 | H       | -0.0546174569 | -7.4872658343  | -6.2520286717  |
| H         | 8.1121883704  | -6.5533268495  | -6.2265574093 | H       | 7.5495660732  | -5.0947254394  | -5.4251271157  |
| H         | 5.0287356638  | -6.6241489995  | -3.2709254520 | H       | 5.6431870706  | -8.7397839957  | -4.2493577654  |
| H         | 6.7088309686  | -7.9011419838  | -7.7298750263 | H       | 5.4547920637  | -4.3780828353  | -6.5527707740  |
| H         | 3.6104633729  | -7.9543995271  | -4.7678962453 | H       | 3.5620063919  | -8.0182319639  | -5.3686372710  |
| H         | 7.1134677583  | -4.6481216344  | -3.5764213276 | H       | 8.1611074685  | -6.7950659903  | -3.1532050607  |
| H         | 7.6064351236  | -6.1083098593  | -2.7244101313 | H       | 7.9551370614  | -8.4412261145  | -3.7572638052  |
| H         | 8.5412857484  | -5.5378169988  | -4.1092905586 | H       | 8.8744266033  | -7.2563036020  | -4.6954484181  |
| H         | -1.1760016901 | -6.9878387154  | -8.9081962228 | H       | 0.0109066514  | -10.0319436852 | -9.6986099234  |
| H         | -2.1589495408 | -9.4171295218  | -8.9864593485 | H       | -1.8191051684 | -10.1939740390 | -8.1954006467  |
| H         | -2.2455258737 | -9.1637886307  | -7.2444549025 | H       | -2.2770198868 | -8.6308420030  | -7.5098127368  |
| H         | -1.4360245648 | -10.5960017172 | -7.8845260881 | H       | -1.4504481738 | -9.8209736936  | -6.5083439290  |

| AZ2-trans |               |                |               | AZ2-cis |               |                |               |
|-----------|---------------|----------------|---------------|---------|---------------|----------------|---------------|
| C         | -0.3208790831 | -7.4970843152  | -8.1344472063 | C       | -0.3086585509 | -7.4975246504  | -8.1144694650 |
| C         | 0.7624200653  | -6.6339577207  | -8.1927342914 | C       | 0.7802930979  | -6.6429455348  | -8.1783170452 |
| C         | -0.1146316835 | -8.8731433566  | -8.0315192169 | C       | -0.1121076398 | -8.8751210802  | -8.0065198465 |
| C         | 2.0591411675  | -7.1065784860  | -8.1444940918 | C       | 2.0740116832  | -7.1250656651  | -8.1327336398 |
| C         | 1.1789203705  | -9.3606271543  | -7.9924015723 | C       | 1.1776075289  | -9.3719871416  | -7.9696929296 |
| C         | 2.2796355800  | -8.4915060044  | -8.0427430491 | C       | 2.2847110666  | -8.5108529456  | -8.0286450646 |
| N         | 3.5313160510  | -8.9971145550  | -8.0036072112 | N       | 3.5337202283  | -9.0238478035  | -7.9959787657 |
| C         | 6.8658420415  | -7.4872887446  | -4.6474161100 | C       | 6.8964991116  | -7.4995127765  | -4.6762416605 |
| C         | 7.4111331611  | -7.4011861155  | -5.9273702975 | C       | 7.4255717498  | -7.4039170373  | -5.9621440606 |
| C         | 5.5598790142  | -7.9642624528  | -4.5130248070 | C       | 5.5989951621  | -7.9953832000  | -4.5273481242 |
| C         | 6.6798299238  | -7.7750206771  | -7.0374979286 | C       | 6.6867792385  | -7.7873695516  | -7.0643472560 |
| C         | 4.8142555178  | -8.3370901909  | -5.6115819218 | C       | 4.8450655870  | -8.3746613012  | -5.6177081805 |
| C         | 5.3707811558  | -8.2338489035  | -6.8902936887 | C       | 5.3853560594  | -8.2620552673  | -6.9025460343 |
| N         | 4.6959408725  | -8.5623287527  | -8.0661405139 | N       | 4.6995567001  | -8.5949085489  | -8.0710175306 |
| C         | 7.6487681563  | -7.0496900062  | -3.4421061153 | C       | 7.6853652157  | -7.0538142240  | -3.4776713489 |
| H         | 0.5952618463  | -5.5658837711  | -8.2828750817 | H       | 0.6203670277  | -5.5738900211  | -8.2701521803 |
| C         | -1.2837214410 | -9.8150592532  | -7.9255741926 | C       | -1.2900984922 | -9.8057514588  | -7.8979322033 |
| H         | 2.9065753284  | -6.4351150464  | -8.1965125957 | H       | 2.9262678190  | -6.4600591153  | -8.1882162953 |
| H         | 1.3661254842  | -10.4259574381 | -7.9252981207 | H       | 1.3566418992  | -10.4384607624 | -7.8994292230 |
| H         | 8.4278205163  | -7.0437551855  | -6.0513667990 | H       | 8.4350941135  | -7.0307944760  | -6.0977917747 |
| H         | 5.1264867400  | -8.0507825758  | -3.5219655787 | H       | 5.1796925321  | -8.0904749695  | -3.5310552975 |
| H         | 7.0942716553  | -7.7198568877  | -8.0367889745 | H       | 7.0884282864  | -7.7250169803  | -8.0684210775 |
| H         | 3.8082653981  | -8.7215374267  | -5.4997928920 | H       | 3.8453276873  | -8.7721291597  | -5.4962283627 |
| H         | 7.4005211247  | -7.6968883008  | -2.5950951186 | H       | 7.4847699214  | -7.7301684722  | -2.6406367199 |

|   |               |                |               |   |               |                |               |
|---|---------------|----------------|---------------|---|---------------|----------------|---------------|
| H | 8.7171309825  | -7.1845087607  | -3.6356298344 | H | 8.7541388496  | -7.1359784739  | -3.6960391335 |
| H | -1.3308583726 | -7.1053039498  | -8.1770353455 | H | -1.3155762790 | -7.0977152874  | -8.1563758970 |
| H | -2.1119518769 | -9.4315804336  | -8.5296653832 | H | -2.0819457218 | -9.4642189553  | -8.5723784963 |
| H | -1.0093577833 | -10.7842485653 | -8.3529641357 | H | -0.9979455218 | -10.8024003980 | -8.2416345236 |
| C | -1.7535691982 | -10.0088021478 | -6.4879443518 | C | -1.8396992660 | -9.8980769021  | -6.4786689016 |
| C | 7.3805972836  | -5.5960761293  | -3.0634202118 | C | 7.3609065020  | -5.6229983362  | -3.0587883003 |
| H | -2.0593247635 | -9.0569010712  | -6.0440629350 | H | -2.1673857978 | -8.9182407333  | -6.1192359100 |
| H | -0.9522351038 | -10.4201556130 | -5.8670977457 | H | -1.0751736647 | -10.2645677930 | -5.7873711688 |
| H | -2.6050416124 | -10.6941024092 | -6.4416850484 | H | -2.6950064580 | -10.5785185130 | -6.4319104185 |
| H | 7.6497086138  | -4.9209616750  | -3.8808499337 | H | 7.5861622800  | -4.9175762989  | -3.8637758388 |
| H | 7.9611995411  | -5.3105058822  | -2.1817781573 | H | 7.9438360285  | -5.3340997560  | -2.1798290677 |
| H | 6.3219533267  | -5.4374900419  | -2.8385895419 | H | 6.3006420163  | -5.5160964092  | -2.8121182574 |

• CI-S2/S1 optimized geometry for AZ1, AZ2 and AZ3 in trans and cis isomers

| AZ1-trans |               |               |                | AZ1-cis |              |               |               |
|-----------|---------------|---------------|----------------|---------|--------------|---------------|---------------|
| C         | -1.4589104623 | -8.4565145922 | -10.3807609523 | N       | 0.3259486892 | -0.1020576040 | -0.1151117171 |
| C         | -0.3269382469 | -8.2830412452 | -9.4191395631  | N       | 0.3277559586 | -0.1019105518 | 1.3532688066  |
| C         | 0.8605112329  | -7.6650647633 | -9.8172490565  | C       | 1.5147185453 | 0.0683349315  | -0.7408190387 |
| C         | -0.4339973339 | -8.7189174079 | -8.0907348913  | C       | 1.7983849879 | -0.7221759137 | -1.8779302151 |
| C         | 1.9059970222  | -7.4815989670 | -8.9436137290  | H       | 1.1034329151 | -1.5124359324 | -2.1342972198 |
| C         | 0.5944548612  | -8.5490802185 | -7.1995758613  | C       | 2.8988807221 | -0.4608286258 | -2.6651461782 |
| C         | 1.8014218654  | -7.9253630004 | -7.5982754666  | H       | 3.0776108742 | -1.0648781130 | -3.5483457263 |
| N         | 2.7769250020  | -7.7964913773 | -6.6837947208  | C       | 3.8030777529 | 0.5465796188  | -2.3328138072 |
| C         | 6.9862778065  | -6.7336459601 | -4.3932366135  | C       | 2.4201831016 | 1.1108901518  | -0.4265952512 |
| C         | 7.0889712068  | -6.2821998952 | -5.7178856070  | H       | 2.2146506908 | 1.7225559391  | 0.4430542514  |
| C         | 5.8008641183  | -7.3557011654 | -3.9986358729  | C       | 3.5375527577 | 1.3215613315  | -1.1913818974 |
| C         | 6.0578618203  | -6.4404494330 | -6.6068442134  | H       | 4.2305329112 | 2.1109184471  | -0.9174093572 |
| C         | 4.7504529317  | -7.5253930683 | -4.8704600139  | C       | 1.2797138062 | -0.8386015596 | 1.9737877184  |
| C         | 4.8517272400  | -7.0690597632 | -6.2113425882  | C       | 1.9263637282 | -0.2889766725 | 3.1043879825  |
| N         | 3.8789500884  | -7.2015165071 | -7.1282406777  | H       | 1.7182308814 | 0.7436060442  | 3.3569316510  |
| C         | 8.1084180703  | -6.5295481885 | -3.4263736068  | C       | 2.7571926632 | -1.0593318502 | 3.8891344728  |
| H         | -2.0065110028 | -7.5161253725 | -10.5164801405 | H       | 3.2199464664 | -0.6199756894 | 4.7664102126  |
| H         | -1.0983617236 | -8.7628401408 | -11.3665131771 | C       | 3.0379183054 | -2.3842103682 | 3.5603178520  |
| H         | 0.9600684807  | -7.3245454018 | -10.8429170440 | C       | 1.5456882069 | -2.1942434685 | 1.6621025536  |
| H         | -1.3491447257 | -9.2025950725 | -7.7662370126  | H       | 1.0565879840 | -2.6248499594 | 0.7973075152  |
| H         | 2.8291419786  | -7.0079927493 | -9.2445567742  | C       | 2.4144653969 | -2.9292648592 | 2.4248545317  |
| H         | 0.5159964900  | -8.8878319316 | -6.1739420354  | H       | 2.6206407545 | -3.9600497324 | 2.1548300772  |
| H         | 8.0057573867  | -5.8009744123 | -6.0417432711  | C       | 3.9913315903 | -3.2048530098 | 4.3688916858  |
| H         | 5.7077485892  | -7.7158351410 | -2.9792107217  | H       | 4.2305525081 | -2.7223690983 | 5.3180739029  |
| H         | 6.1354774641  | -6.0958576657 | -7.6305924378  | H       | 4.9317909382 | -3.3579065330 | 3.8271465995  |
| H         | 3.8305430884  | -8.0077839077 | -4.5736625977  | H       | 3.5806189835 | -4.1963660059 | 4.5808038708  |
| H         | 7.9808540466  | -5.5923336592 | -2.8706563532  | C       | 5.0383219229 | 0.7840314294  | -3.1419129733 |
| H         | 8.1543624266  | -7.3367677281 | -2.6914287558  | H       | 4.9714582463 | 0.3130312420  | -4.1242297625 |
| H         | -2.1741351484 | -9.2029355903 | -10.0295911864 | H       | 5.9199597050 | 0.3723613250  | -2.6367111444 |
| H         | 9.0722154266  | -6.4729956744 | -3.9373050584  | H       | 5.2220926061 | 1.8526190574  | -3.2844155675 |
| AZ2-trans |               |               |                | AZ1-cis |              |               |               |
| C         | -0.2644077479 | -8.3651615449 | -9.4528002604  | C       | 1.0499247521 | -9.0328563808 | -8.9443675727 |
| C         | 0.9025237044  | -7.7361509483 | -9.8599648529  | C       | 2.0346314488 | -8.1258925574 | -9.3385610863 |
| C         | -0.4197418853 | -8.8193321636 | -8.1323537190  | C       | 0.3479454509 | -8.8485953822 | -7.7509792359 |
| C         | 1.9433300519  | -7.5396110130 | -8.9771755102  | C       | 2.3239724835 | -7.0221488075 | -8.5741852354 |
| C         | 0.6137346098  | -8.6277249046 | -7.2474548420  | C       | 0.6721230144 | -7.7672764187 | -6.9553548183 |
| C         | 1.8166747747  | -7.9873450114 | -7.6368886109  | C       | 1.6493006502 | -6.8200023749 | -7.3477783877 |
| N         | 2.7731239076  | -7.8424320497 | -6.7038187318  | N       | 1.7669370527 | -5.7038212256 | -6.5957058941 |
| C         | 6.9211926059  | -6.7155442151 | -4.3476149450  | C       | 6.3288826556 | -7.2801469261 | -4.9721357332 |
| C         | 7.0448550668  | -6.2693500415 | -5.6752569582  | C       | 6.4750450314 | -6.3893536422 | -6.0361874168 |
| C         | 5.7376162750  | -7.3469249610 | -3.9705733695  | C       | 5.0337107501 | -7.4860066828 | -4.4526602221 |

|   |               |                |                |   |               |                |                |
|---|---------------|----------------|----------------|---|---------------|----------------|----------------|
| C | 6.0345621410  | -6.4459518625  | -6.5806723175  | C | 5.3883332096  | -5.7545881427  | -6.5918203369  |
| C | 4.7051740209  | -7.5368443602  | -4.8626111077  | C | 3.9498801942  | -6.8160114108  | -4.9440669114  |
| C | 4.8274489383  | -7.0878892128  | -6.2035049288  | C | 4.0877377703  | -5.9152729812  | -6.0384503707  |
| N | 3.8738202293  | -7.2317076236  | -7.1378411097  | N | 3.1146825631  | -5.0901805472  | -6.4554840163  |
| C | 8.0395599590  | -6.5101366664  | -3.3777298032  | C | 7.4970546239  | -8.0075892187  | -4.3909676137  |
| H | 0.9966128927  | -7.3953363793  | -10.8851556887 | H | 2.5716779705  | -8.2917220211  | -10.2660428155 |
| C | -1.6934332353 | -9.4929431201  | -7.7153445694  | C | -0.7252882367 | -9.8146725702  | -7.3428426429  |
| H | 2.8640271200  | -7.0535117609  | -9.2638730036  | H | 3.0753888385  | -6.3042652129  | -8.8764435357  |
| H | 0.5404718395  | -8.9615122366  | -6.2193226295  | H | 0.1565423326  | -7.5962883137  | -6.0173962521  |
| H | 7.9608275433  | -5.7759297955  | -5.9831019534  | H | 7.4625345105  | -6.2158811893  | -6.4502471894  |
| H | 5.6286037471  | -7.6966371548  | -2.9492874778  | H | 4.9021392317  | -8.1864817023  | -3.6341621020  |
| H | 6.1239592787  | -6.1044259089  | -7.6043213316  | H | 5.5033904001  | -5.0730006946  | -7.4253556713  |
| H | 3.7840329985  | -8.0248703565  | -4.5794893545  | H | 2.9600974933  | -6.9665472892  | -4.5323003149  |
| H | 8.2643306991  | -5.4449175584  | -3.2561588957  | H | 7.6387300847  | -7.7433267052  | -3.3371362699  |
| H | 7.7995422158  | -6.9192948437  | -2.3951934269  | H | 7.3450158615  | -9.0913094676  | -4.4275138740  |
| H | 8.9592327018  | -6.9893930589  | -3.7301372092  | H | 8.4208446791  | -7.7760893638  | -4.9234439194  |
| H | -1.0723269364 | -8.5102894895  | -10.1621918313 | H | 0.8308890991  | -9.8921469564  | -9.5687638098  |
| H | -2.5491350734 | -8.8204911630  | -7.8304569190  | H | -0.3981599838 | -10.8493448591 | -7.4765860005  |
| H | -1.6523306705 | -9.8095718653  | -6.6719233365  | H | -1.6263745325 | -9.6774081470  | -7.9493727093  |
| H | -1.8917817722 | -10.3765887300 | -8.3295413057  | H | -1.0056526996 | -9.6792574091  | -6.2967687461  |

#### AZ3-trans

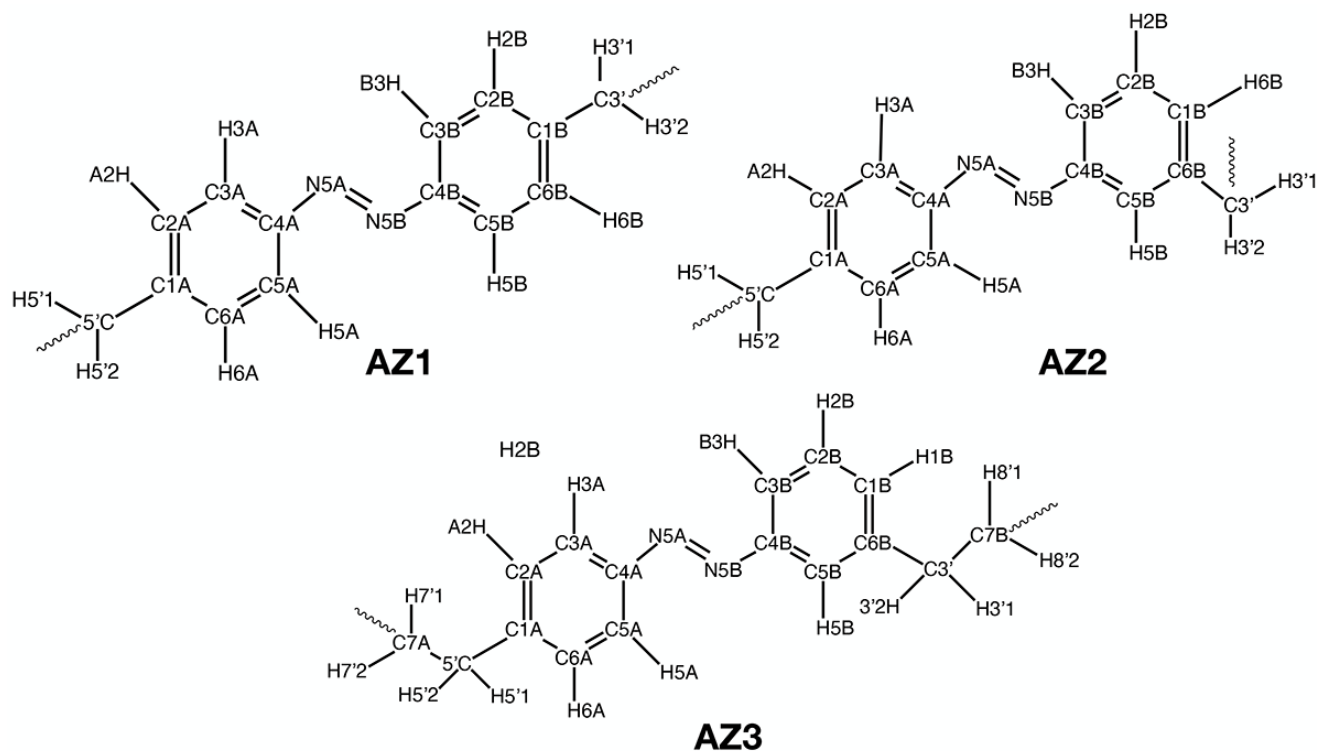
|   |               |                |                |
|---|---------------|----------------|----------------|
| C | -0.3935117088 | -8.3028157519  | -9.1778149475  |
| C | 0.6176707748  | -7.3919298700  | -9.4509938854  |
| C | -0.2855083843 | -9.2059191368  | -8.1084996909  |
| C | 1.7565245208  | -7.3506427036  | -8.6765746805  |
| C | 0.8485054564  | -9.1699172468  | -7.3314941123  |
| C | 1.8946093929  | -8.2492256878  | -7.5860085578  |
| N | 2.9626408895  | -8.2819784291  | -6.7709245722  |
| C | 7.2726783553  | -7.3852121287  | -4.6182795497  |
| C | 7.1477619748  | -6.5108836245  | -5.7110050499  |
| C | 6.2352112250  | -8.2832997082  | -4.3681305144  |
| C | 6.0369821830  | -6.5265952433  | -6.5111994325  |
| C | 5.1083841138  | -8.3210320570  | -5.1578126066  |
| C | 4.9760905560  | -7.4325084468  | -6.2582005547  |
| N | 3.9097588924  | -7.3950340365  | -7.0732675371  |
| C | 8.4749411180  | -7.3181474121  | -3.7259909960  |
| H | 0.5102277371  | -6.7077351244  | -10.2853823778 |
| C | -1.4053428825 | -10.1645290459 | -7.8095065211  |
| H | 2.5614837889  | -6.6554685122  | -8.8635325596  |
| H | 0.9786784633  | -9.8506675209  | -6.4983497857  |
| H | 7.9509891963  | -5.8125079919  | -5.9215954042  |
| H | 6.3216782496  | -8.9685405180  | -3.5310111140  |
| H | 5.9361013658  | -5.8571670827  | -7.3563068725  |
| H | 4.2991497391  | -9.0125032688  | -4.9739027945  |
| H | 8.6169226684  | -8.2842817679  | -3.2332438601  |
| H | 9.3680421141  | -7.1389017656  | -4.3337922410  |
| H | -1.2803248533 | -8.3243815007  | -9.8024700267  |
| H | -1.8334581999 | -10.5221217850 | -8.7517505411  |
| H | -1.0006966297 | -11.0426951400 | -7.2978914930  |
| C | -2.5058033686 | -9.5422797169  | -6.9570292514  |
| C | 8.3614109835  | -6.2217639975  | -2.6676815932  |
| H | -2.9406010708 | -8.6667939640  | -7.4487254131  |
| H | -2.1133216773 | -9.2153454352  | -5.9898309001  |
| H | -3.3104154838 | -10.2598657804 | -6.7726031915  |
| H | 8.2377923431  | -5.2387973731  | -3.1310880213  |
| H | 9.2587126440  | -6.1919151093  | -2.0430132036  |
| H | 7.4982455133  | -6.3927961163  | -2.0184661471  |

#### AZ1-cis

|   |               |                |               |
|---|---------------|----------------|---------------|
| C | 0.3648857792  | -7.2944674744  | -8.0566302867 |
| C | 1.5225258538  | -6.6921684188  | -8.5538975511 |
| C | 0.3546628335  | -8.6489524007  | -7.7242343410 |
| C | 2.6690654637  | -7.4222350447  | -8.7485430087 |
| C | 1.5223712811  | -9.3748658123  | -7.8740155822 |
| C | 2.6978201231  | -8.7928557856  | -8.4026277028 |
| N | 3.7260937703  | -9.6232116519  | -8.6945716469 |
| C | 6.4059799675  | -7.5527937710  | -4.8983220985 |
| C | 6.7501028106  | -6.9623513024  | -6.1167173617 |
| C | 5.5385491064  | -8.6628285664  | -4.9206329545 |
| C | 6.2315309998  | -7.4207045463  | -7.3043373700 |
| C | 5.0616621014  | -9.1757743163  | -6.0943030169 |
| C | 5.3938492263  | -8.5700696026  | -7.3387987006 |
| N | 5.1142071590  | -9.1156444425  | -8.5333896231 |
| C | 6.9034921097  | -7.0034622632  | -3.5962904662 |
| H | 1.5095926389  | -5.6370163787  | -8.8039741480 |
| C | -0.8828310503 | -9.2903154577  | -7.1566123594 |
| H | 3.5659634968  | -6.9719292360  | -9.1536397623 |
| H | 1.5518173474  | -10.4304875748 | -7.6284948423 |
| H | 7.4217977233  | -6.1103487621  | -6.1215506125 |
| H | 5.2576919340  | -9.1284428653  | -3.9812711767 |
| H | 6.4925631291  | -6.9566727406  | -8.2473468211 |
| H | 4.4098221467  | -10.0400903926 | -6.1086441240 |
| H | 7.1639246238  | -7.8341263970  | -2.9313479903 |
| H | 7.8238274835  | -6.4381934721  | -3.7683448251 |
| H | -0.5358481745 | -6.7033629069  | -7.9309050926 |
| H | -1.7657591949 | -8.8524540901  | -7.6326992353 |
| H | -0.8878723068 | -10.3539423220 | -7.4122980146 |
| C | -0.9909711850 | -9.1298596765  | -5.6441938952 |
| C | 5.8797330547  | -6.1079612122  | -2.9009704328 |
| H | -1.0131990110 | -8.0733053068  | -5.3609182217 |
| H | -0.1351227629 | -9.5882646126  | -5.1400368348 |
| H | -1.9018709106 | -9.6010200652  | -5.2638070262 |
| H | 5.6236315339  | -5.2470472065  | -3.5248920012 |
| H | 6.2736331501  | -5.7355421672  | -1.9512166596 |
| H | 4.9548877485  | -6.6534317578  | -2.6928942088 |

## 2 Azobenzene charges and GAFF parameters

The selected part of azobenzene derivatives for calculating the RESP charges and also QM/MM simulations are shown in Fig. S1.



**Fig. S1.** Atom labeling scheme of the azobenzene derivatives used in the force field and QM region of QM/MM simulations

**Table S1.** Atom names and RESP charges used for AZ1, AZ2 and AZ3 in MD simulations

| AZ1        |            |           | AZ2        |            |           | AZ3        |            |           |
|------------|------------|-----------|------------|------------|-----------|------------|------------|-----------|
| atom names | atom types | charge    | atom names | atom types | charge    | atom names | atom types | charge    |
| C5'        | c3         | 0.4030495 | C5'        | c3         | 0.4030495 | C5'        | c3         | -0.578415 |
| C1A        | ca         | -0.170015 | C1A        | ca         | -0.170015 | C1A        | ca         | -0.170015 |
| C2A        | ca         | -0.095668 | C2A        | ca         | -0.095668 | C2A        | ca         | -0.095668 |
| C6A        | ca         | -0.095668 | C6A        | ca         | -0.095668 | C6A        | ca         | -0.095668 |
| C3A        | ca         | -0.206585 | C3A        | ca         | -0.206585 | C3A        | ca         | -0.206585 |
| C5A        | ca         | -0.206585 | C5A        | ca         | -0.206585 | C5A        | ca         | -0.206585 |
| C4A        | ca         | 0.342622  | C4A        | ca         | 0.342622  | C4A        | ca         | 0.342622  |
| N5A        | ne         | -0.202255 | N5A        | ne         | -0.202255 | N5A        | ne         | -0.202255 |
| C1B        | ca         | -0.170015 | C1B        | ca         | -0.170015 | C1B        | ca         | -0.095668 |
| C2B        | ca         | -0.095668 | C2B        | ca         | -0.095668 | C2B        | ca         | -0.095668 |
| C6B        | ca         | -0.095668 | C6B        | ca         | -0.095668 | C6B        | ca         | -0.170015 |
| C3B        | ca         | -0.206585 | C3B        | ca         | -0.206585 | C3B        | ca         | -0.206585 |
| C5B        | ca         | -0.206585 | C5B        | ca         | -0.206585 | C5B        | ca         | -0.206585 |
| C4B        | ca         | 0.342622  | C4B        | ca         | 0.342622  | C4B        | ca         | 0.342622  |
| N5B        | nf         | -0.202255 | N5B        | nf         | -0.202255 | N5B        | nf         | -0.202255 |
| C3'        | c3         | 0.331041  | C3'        | c3         | 0.331041  | C3'        | c3         | -0.578415 |
| H5'1       | h1         | 0.038780  | H5'1       | h1         | 0.038780  | H5'1       | h1         | 0.015467  |
| H5'2       | h1         | 0.038780  | H5'2       | h1         | 0.038780  | H5'2       | h1         | 0.015467  |
| H2A        | ha         | 0.132519  | H2A        | ha         | 0.132519  | H2A        | ha         | 0.132519  |
| H6A        | ha         | 0.132519  | H6A        | ha         | 0.132519  | H6A        | ha         | 0.132519  |
| H3A        | ha         | 0.124774  | H3A        | ha         | 0.124774  | H3A        | ha         | 0.124774  |
| H5A        | ha         | 0.124774  | H5A        | ha         | 0.124774  | H5A        | ha         | 0.124774  |
| H2B        | ha         | 0.132519  | H2B        | ha         | 0.132519  | H2B        | ha         | 0.132519  |
| H6B        | ha         | 0.132519  | H6B        | ha         | 0.132519  | H6B        | ha         | 0.132519  |
| H3B        | ha         | 0.124774  | H3B        | ha         | 0.124774  | H3B        | ha         | 0.124774  |
| H5B        | ha         | 0.124774  | H5B        | ha         | 0.124774  | H5B        | ha         | 0.124774  |
| H3'1       | h1         | 0.038780  | H3'1       | h1         | 0.038780  | H3'1       | h1         | 0.015467  |
| H3'2       | h1         | 0.038780  | H3'2       | h1         | 0.038780  | H3'2       | h1         | 0.015467  |
|            |            |           |            |            |           | C7A        | c3         | 0.4030495 |
|            |            |           |            |            |           | H7'1       | h1         | 0.038780  |
|            |            |           |            |            |           | H7'2       | h1         | 0.038780  |
|            |            |           |            |            |           | C8B        | c3         | 0.4030495 |
|            |            |           |            |            |           | H8'1       | h1         | 0.038780  |
|            |            |           |            |            |           | H8'2       | h1         | 0.038780  |

**Table S2.** GAFF parameters for bonds of AZ1, AZ2 and AZ3. The force constants ( $K_b$ ) and equilibrium bonds ( $b_0$ ) are given in  $\text{kJ/mol.nm}^2$  and  $\text{nm}$ , respectively.

| AZ1        |            |            | AZ2        |            |            | AZ3        |            |            |
|------------|------------|------------|------------|------------|------------|------------|------------|------------|
| atom types | $b_0$      | $K_b$      | atom types | $b_0$      | $K_b$      | atom types | $b_0$      | $K_b$      |
| c3-ca      | 1.5156e-01 | 2.6861e+05 | c3-ca      | 1.5156e-01 | 2.6861e+05 | c3-ca      | 1.5156e-01 | 2.6861e+05 |
| c3-h1      | 1.0969e-01 | 2.7665e+05 | c3-h1      | 1.0969e-01 | 2.7665e+05 | c3-h1      | 1.0969e-01 | 2.7665e+05 |
| ca-ca      | 1.3984e-01 | 3.8585e+05 | ca-ca      | 1.3984e-01 | 3.8585e+05 | ca-ca      | 1.3984e-01 | 3.8585e+05 |
| ca-ha      | 1.0860e-01 | 2.8937e+05 | ca-ha      | 1.0860e-01 | 2.8937e+05 | ca-ha      | 1.0860e-01 | 2.8937e+05 |
| ne-nf      | 1.2632e-01 | 6.0450e+05 | ne-nf      | 1.2632e-01 | 6.0450e+05 | ne-nf      | 1.2632e-01 | 6.0450e+05 |
| ca-ne      | 1.4079e-01 | 3.2577e+05 | ca-ne      | 1.4079e-01 | 3.2577e+05 | ca-ne      | 1.4079e-01 | 3.2577e+05 |
| ca-nf      | 1.4079e-01 | 3.2577e+05 | ca-nf      | 1.4079e-01 | 3.2577e+05 | ca-nf      | 1.4079e-01 | 3.2577e+05 |
|            |            |            |            |            |            | c3-c3      | 1.5375e-01 | 2.5179e+05 |

**Table S3.** GAFF parameters for angles of AZ1, AZ2 and AZ3. The force constants ( $K_\theta$ ) and equilibrium angles ( $\theta_0$ ) are given in  $\text{kJ/mol.rad}^2$  and degree, respectively.

| AZ1        |            |            | AZ2        |            |            | AZ3        |            |            |
|------------|------------|------------|------------|------------|------------|------------|------------|------------|
| atom types | $\theta_0$ | $K_\theta$ | atom types | $\theta_0$ | $K_\theta$ | atom types | $\theta_0$ | $K_\theta$ |
| c3-ca-ca   | 1.2077e+02 | 5.3162e+02 | c3-ca-ca   | 1.2077e+02 | 5.3162e+02 | c3-c3-h1   | 1.0956e+02 | 3.8819e+02 |
| ca-c3-h1   | 1.0956e+02 | 3.9321e+02 | ca-c3-h1   | 1.0956e+02 | 3.9321e+02 | ca-c3-c3   | 1.1207e+02 | 5.2844e+02 |
| ca-ca-ca   | 1.2002e+02 | 5.5748e+02 | ca-ca-ca   | 1.2002e+02 | 5.5748e+02 | c3-ca-ca   | 1.2077e+02 | 5.3162e+02 |
| ca-ca-ha   | 1.1988e+02 | 4.0317e+02 | ca-ca-ha   | 1.1988e+02 | 4.0317e+02 | ca-c3-h1   | 1.0956e+02 | 3.9321e+02 |
| ca-ca-ne   | 1.2061e+02 | 5.6777e+02 | ca-ca-ne   | 1.2061e+02 | 5.6777e+02 | ca-ca-ca   | 1.2002e+02 | 5.5748e+02 |
| ca-ne-nf   | 1.1517e+02 | 5.8919e+02 | ca-ne-nf   | 1.1517e+02 | 5.8919e+02 | ca-ca-ha   | 1.1988e+02 | 4.0317e+02 |
| ca-ca-nf   | 1.2061e+02 | 5.6777e+02 | ca-ca-nf   | 1.2061e+02 | 5.6777e+02 | ca-ca-ne   | 1.2061e+02 | 5.6777e+02 |
| h1-c3-h1   | 1.0846e+02 | 3.2836e+02 | h1-c3-h1   | 1.0846e+02 | 3.2836e+02 | ca-ne-nf   | 1.1517e+02 | 5.8919e+02 |
| ne-nf-ca   | 1.1517e+02 | 5.8919e+02 | ne-nf-ca   | 1.1517e+02 | 5.8919e+02 | ca-ca-nf   | 1.2061e+02 | 5.6777e+02 |
|            |            |            |            |            |            | h1-c3-h1   | 1.0846e+02 | 3.2836e+02 |
|            |            |            |            |            |            | ne-nf-ca   | 1.1517e+02 | 5.8919e+02 |

**Table S4.** GAFF parameters for angles of AZ1, AZ2 and AZ3. The force constants ( $K_\phi$ ) and equilibrium angles ( $\phi_0$ ) are given in  $\text{kJ/mol}$  and degree, respectively.  $n$  is the multiplicity.

| AZ1         |          |          |     | AZ2         |          |          |     | AZ3         |          |          |     |
|-------------|----------|----------|-----|-------------|----------|----------|-----|-------------|----------|----------|-----|
| atom types  | $\phi_0$ | $K_\phi$ | $n$ | atom types  | $\phi_0$ | $K_\phi$ | $n$ | atom types  | $\phi_0$ | $K_\phi$ | $n$ |
| c3-ca-ca-ca | 180.00   | 15.16700 | 2   | c3-ca-ca-ca | 180.00   | 15.16700 | 2   | c3-ca-ca-ca | 180.00   | 15.16700 | 2   |
| c3-ca-ca-ca | 180.00   | 15.16700 | 2   | c3-ca-ca-ca | 180.00   | 15.16700 | 2   | c3-ca-ca-ha | 180.00   | 15.16700 | 2   |
| c3-ca-ca-ha | 180.00   | 15.16700 | 2   | c3-ca-ca-ha | 180.00   | 15.16700 | 2   | ca-ca-ca-ca | 180.00   | 15.16700 | 2   |
| ca-ca-ca-ca | 180.00   | 15.16700 | 2   | ca-ca-ca-ca | 180.00   | 15.16700 | 2   | ca-ca-ca-ha | 180.00   | 15.16700 | 2   |
| ca-ca-ca-ha | 180.00   | 15.16700 | 2   | ca-ca-ca-ha | 180.00   | 15.16700 | 2   | ca-ca-c3-h1 | 0.00     | 0.00000  | 0   |
| ca-ca-c3-h1 | 0.00     | 0.00000  | 0   | ca-ca-c3-h1 | 0.00     | 0.00000  | 0   | ca-ca-ca-ne | 180.00   | 15.16700 | 2   |
| ca-ca-ca-ne | 180.00   | 15.16700 | 2   | ca-ca-ca-ne | 180.00   | 15.16700 | 2   | ca-ca-ne-nf | 180.00   | 0.00000  | 3   |
| ca-ca-ne-nf | 180.00   | 0.00000  | 3   | ca-ca-ne-nf | 180.00   | 0.00000  | 3   | ca-ne-nf-ca | 180.00   | 86.80000 | 2   |
| ca-ne-nf-ca | 180.00   | 86.80000 | 2   | ca-ne-nf-ca | 180.00   | 86.80000 | 2   | ne-ca-ca-ha | 180.00   | 15.16700 | 2   |
| ne-ca-ca-ha | 180.00   | 15.16700 | 2   | ne-ca-ca-ha | 180.00   | 15.16700 | 2   | ne-nf-ca-ca | 180.00   | 0.00000  | 3   |
| ne-nf-ca-ca | 180.00   | 0.00000  | 3   | ne-nf-ca-ca | 180.00   | 0.00000  | 3   | nf-ca-ca-ha | 180.00   | 15.16700 | 2   |
| nf-ca-ca-ha | 180.00   | 15.16700 | 2   | nf-ca-ca-ha | 180.00   | 15.16700 | 2   | ha-ca-ca-ha | 180.00   | 15.16700 | 2   |
| ha-ca-ca-ha | 180.00   | 15.16700 | 2   | ha-ca-ca-ha | 180.00   | 15.16700 | 2   | ca-ca-ca-nf | 180.00   | 15.16700 | 2   |
| ca-ca-ca-nf | 180.00   | 15.16700 | 2   | ca-ca-ca-nf | 180.00   | 15.16700 | 2   | ca-c3-c3-h1 | 0.00     | 0.65084  | 3   |
|             |          |          |     |             |          |          |     | ca-ca-c3-c3 | 0.00     | 0.00000  | 0   |
|             |          |          |     |             |          |          |     | h1-c3-c3-h1 | 0.00     | 0.65084  | 3   |

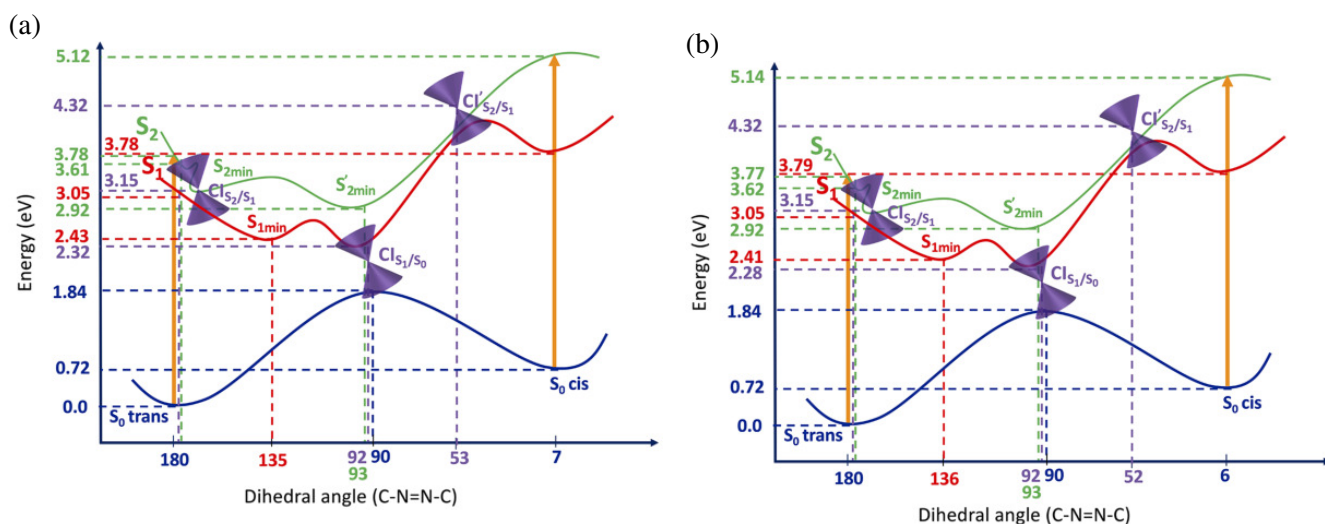
**Table S5.** Ion Lennard-Jones parameters and water models used in the MD simulations

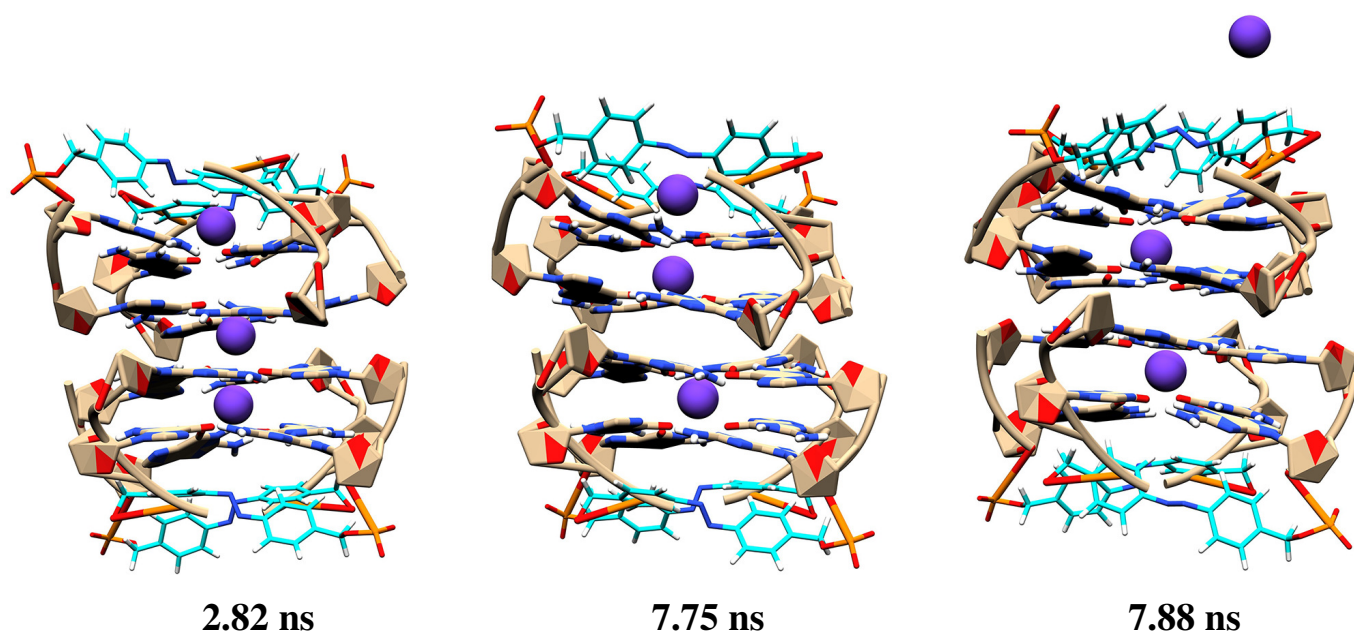
| simulation group     | ion parameters | ion type        | water model | $\sigma$ (nm)          | $\epsilon$ (kJ/mol)    |
|----------------------|----------------|-----------------|-------------|------------------------|------------------------|
| AZn-AAK <sup>+</sup> | AA             | K <sup>+</sup>  | TIP3P       | $4.736 \times 10^{-1}$ | $1.372 \times 10^{-3}$ |
| AZn-JCK <sup>+</sup> | JC             | K <sup>+</sup>  | SPC/E       | $2.838 \times 10^{-1}$ | $1.798 \times 10^{-0}$ |
| AZn-JCKCl            | JC             | K <sup>+</sup>  | SPC/E       | $2.838 \times 10^{-1}$ | $1.798 \times 10^{-0}$ |
|                      |                | Cl <sup>-</sup> |             | $4.830 \times 10^{-1}$ | $5.349 \times 10^{-2}$ |

Ion parameters are abbreviated as follows: AA: Amber-adapted Åqvist; JC: Joung and Cheatham. In AZn, n refers to the structure number of azobenzene derivatives AZ1, AZ2 and AZ3.

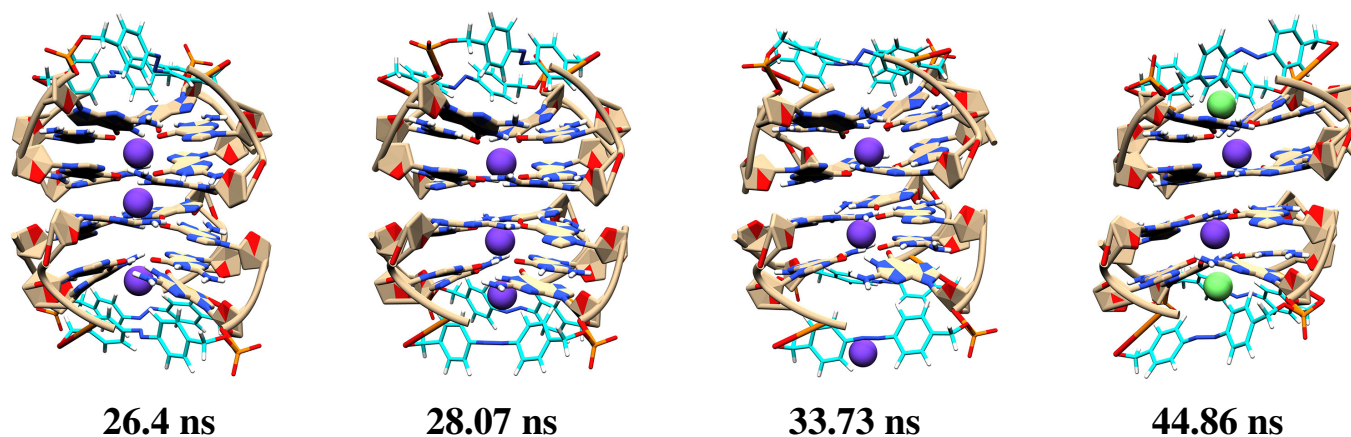
**Table S6.** Vertical excitation energies of S<sub>1</sub> and S<sub>2</sub> states and oscillator strengths (in parentheses) for AZ1 calculated at different levels of theory using the cc-pVDZ basis set. The energies are given in eV.

| method                 | trans          |                | cis            |                |
|------------------------|----------------|----------------|----------------|----------------|
|                        | S <sub>1</sub> | S <sub>2</sub> | S <sub>1</sub> | S <sub>2</sub> |
| TDDFT/BLYP             | 2.32 (0.001)   | 3.60 (0.964)   | 2.55 (0.070)   | 3.52 (0.007)   |
| TDDFT/B3LYP            | 2.68 (0.001)   | 3.90 (1.268)   | 2.76 (0.055)   | 4.19 (0.134)   |
| TDDFT/ $\omega$ B97X-D | 2.84 (0.001)   | 4.24 (1.238)   | 2.90 (0.037)   | 4.74 (0.223)   |
| TDDFT/CAM-B3LYP        | 2.87 (0.001)   | 4.23 (1.252)   | 2.88 (0.038)   | 4.74 (0.234)   |
| TDDFT/B5050LYP         | 3.05 (0.001)   | 4.27 (1.276)   | 3.01 (0.040)   | 4.87 (0.279)   |
| ADC(2)-s               | 2.97 (0.001)   | 4.25 (1.035)   | 3.03 (0.033)   | 4.72 (0.063)   |
| EOM-CCSD               | 3.07 (0.001)   | 4.59 (0.923)   | 3.12 (0.026)   | 4.83 (0.031)   |
| SF/ $\omega$ B97X-D    | 3.09           | 3.49           | 3.02           | 4.34           |
| SF/B5050LYP            | 3.07           | 3.73           | 3.05           | 4.4            |

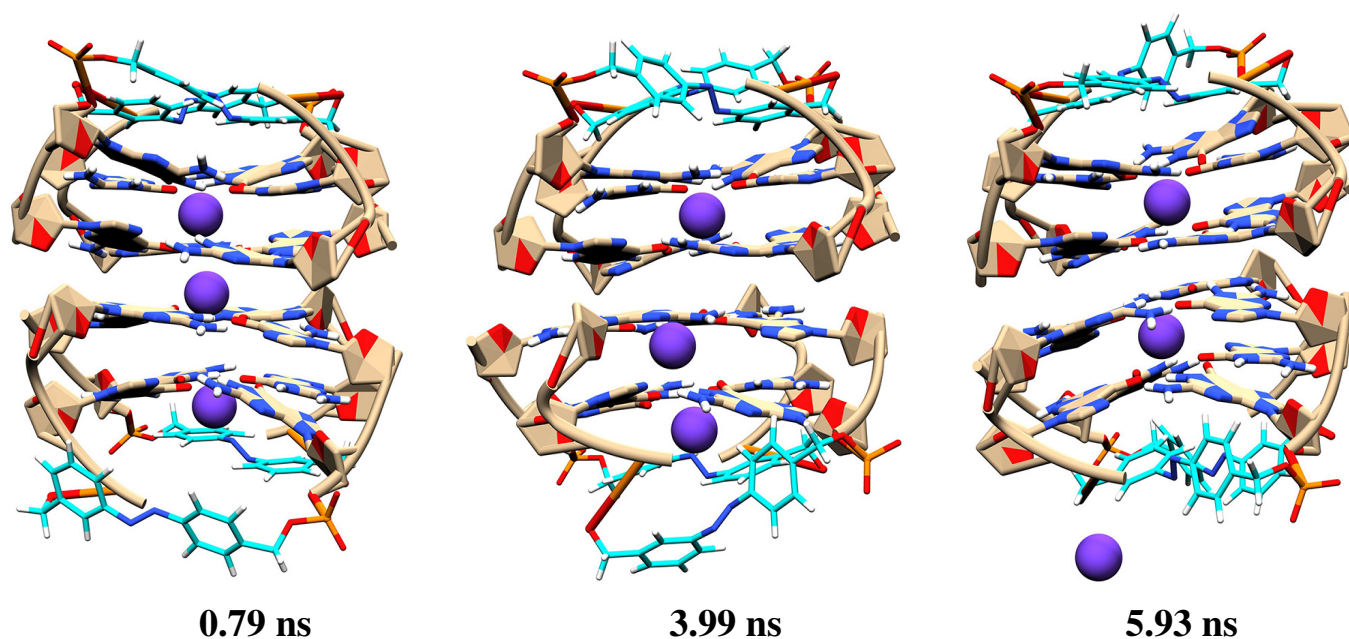
**Fig. S2.** Schematic representation of the PESs of the photoisomerization mechanism of (a) AZ2 and (b) AZ3 as function of CNNC dihedral angle. The ground state (S<sub>0</sub>), first (S<sub>1</sub>) and second (S<sub>2</sub>) excited states are shown in blue, red and green. The S<sub>0</sub> curve is a PES scan along dihedral angle obtained from SF-B5050LYP/ccpVDZ. The S<sub>1</sub> and S<sub>2</sub> curves are obtained through connection of the excited states optimized geometries and MECPs (shown in purple) calculated with SF-B5050LYP/cc-pVDZ.



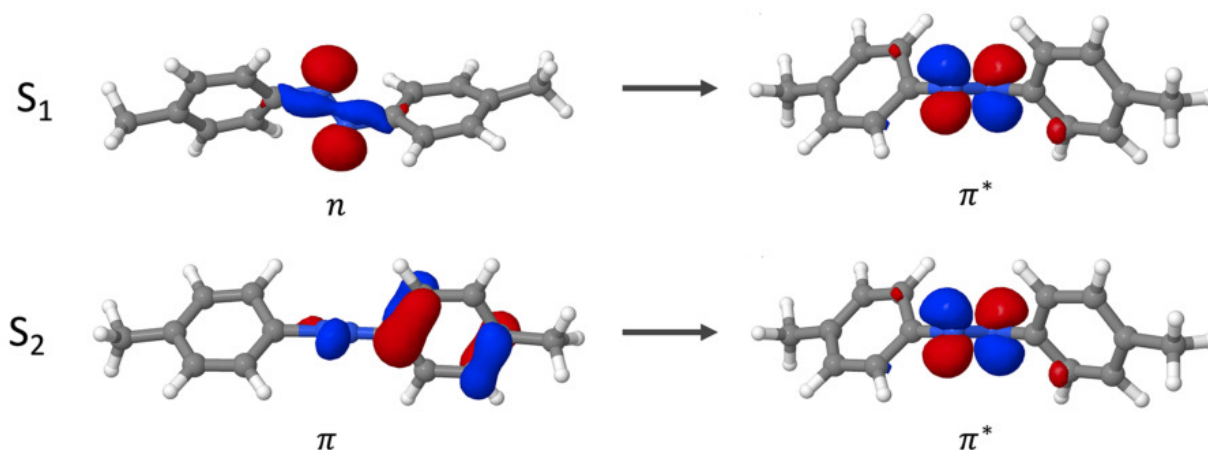
**Fig. S3.** Ion movement in AZ1-AAK<sup>+</sup> G-quadruplex. At 2.82 ns, the first/top K<sup>+</sup> moves up from the G-quadruplex channel and stays above the top G-quartet. At 7.75 ns simulation, the second/middle K<sup>+</sup> ion moves and occupies the empty coordination site of the first K<sup>+</sup> resulting to escape of K<sup>+</sup> through the top quartet at 7.88 ns simulation.



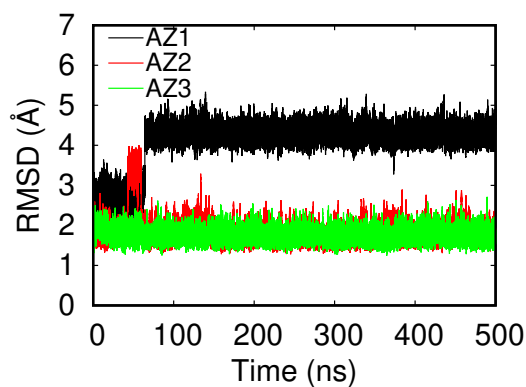
**Fig. S4.** Ion movement in AZ1-JCK<sup>+</sup> G-quadruplex. At 26.4 ns, third/bottom K<sup>+</sup> moves down from the G-quadruplex channel and stays close to the bottom G-quartet. At 28.07 ns simulation, the second/middle K<sup>+</sup> ion moves to the vacant position of third K<sup>+</sup>. After 5.66 ns, the third K<sup>+</sup> escapes from the G-quadruplex channel. Then, at 44.86 ns, two K<sup>+</sup> ions from the bulk water move to align near top and bottom G-quartets till the simulation end.



**Fig. S5.** Ion movement in AZ2-AAK<sup>+</sup> G-quadruplex. At 0.79 ns, third/bottom K<sup>+</sup> moves down from the G-quadruplex channel and stays close to the bottom G-quartet. At 3.99 ns simulation, the second/middle K<sup>+</sup> ion moves to the vacant position of third K<sup>+</sup> leading to escape of third K<sup>+</sup> from the structure at 5.93 ns simulation.



**Fig. S6.** Natural transition orbitals for the  $S_1$  and  $S_2$  transitions of one snapshot ( $\omega$ B97X-D/cc-pVDZ).



**Fig. S7.** RMSDs as a functional of simulation time for all atoms of the G-quadruplexes in JCKCl simulations.