Electronic Supplementary Information (ESI) For:

Ultrafast unidirectional chiral rotation in *Z*-*E* photoisomerization of two azoheteroarene photoswitches

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1. Detailed procedures of preparing excited state surface hopping molecular dynamics simulation for BMID and BHID

The ground-state geometry optimizations of the M-helical and P-helical Z-isomers of azoheteroarene BMID were first performed with the OM2/MRCI method. Then same number of samples pointed in the phase space (geometries and momenta) for the M-helical and P-helical Z-isomer of BMID were generated based on the Wigner distribution of the ground vibrational level of all normal modes near S_0 equilibrium geometry[S1]. This step gave the atomic initial coordinates and velocities. Next, the initial condition was prepared by vertically putting these geometries into the S_1 state, while whether a single geometry was chosen or not was relevant to its transition probability dependent on the oscillation strength and the S_0-S_1 energy gap. For more detailed discussions on the initial sampling, please refer to some previous works[S2-S4].

In our calculation, although the same number of samplings for the M-helical and P-helical Z-isomer of BMID were obtained using Wigner sampling method, less samplings were left as the initial conditions for the surface hopping dynamics, due to the filtering procedure basing on the S_0-S_1 transition probability. That's why different number of trajectories were employed in the surface hopping dynamics for the two BMID isomers.

Since either 764 or 694 trajectories are large enough to get the fully convergent results for all important quantities, such as the excited-state lifetime, the quantum yield of each channel, the chiral preference probability and etc, the difference of the trajectory numbers in two calculations should not affect our conclusions.

Because the same procedures were used for the initial sampling of the excited-state dynamics simulation of BHID, we do not need to discuss all details again.

2. Optimized geometries of azoheteroarene BMID

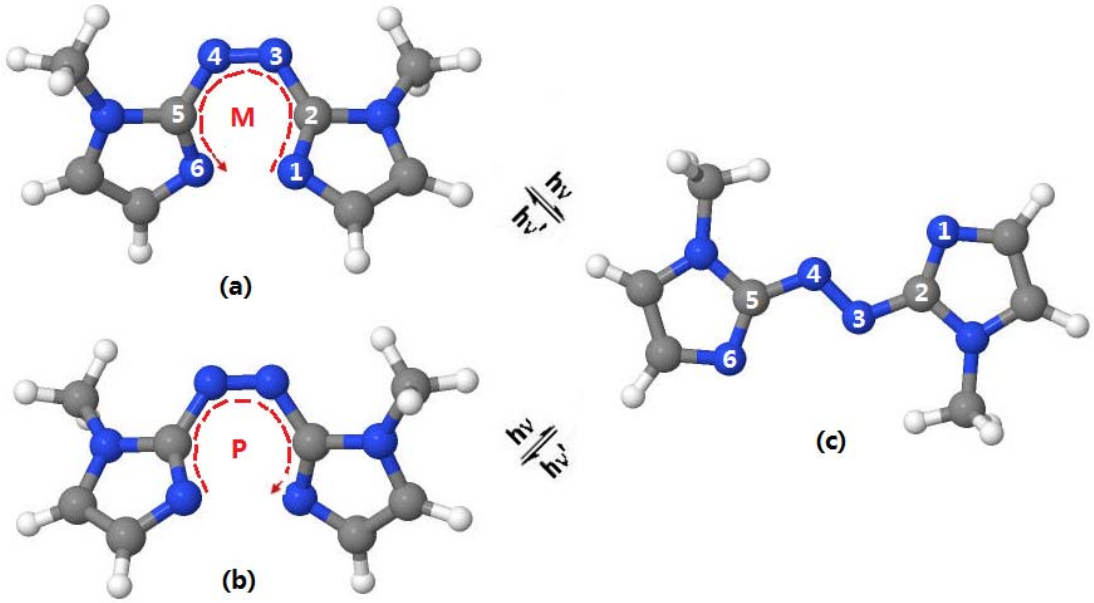

Fig. S1 Optimized geometries of (a) *Z*-isomer *M*-helical BMID; (b) *Z*-isomer *P*-helical BMID; and (c) *E*-isomer BMID calculated with OM2/MRCI method implemented in MNDO99 program[S5]. Atoms around central N=N are labelled.

Table S1. Optimized geometrical parameters of ground state azoheteroarene BMID, obtained from different methods. OM2/MRCI method is implemented in MNDO99 program[S5]; while B3LYP/6-311G(d,p) and CAM-B3LYP/6-311G(d,p) methods are implemented in Gaussian 03 program[S6]. The lengths are in angstroms; the dihedral angles and bond angles are in degrees.

(a) Z-isomer* azoheteroarene BMID *with M helicity

	OM2/MRCI	B3LYP/6-311G(d,p)	CAM-B3LYP/6-311G(d,p)	Reference[a]
N3N4	1.20	1.26	1.24	1.27
C2N3	1.42	1.39	1.40	1.39
N4C5	1.42	1.39	1.40	1.39
C2N3N4	123.1	124.5	122.6	125.8
N3N4C5	123.1	124.5	122.6	125.8
C2N3N4C5	-8.9	-17.3	-15.9	-16.2
N1C2N3N4	-39.8	-32.5	-40.1	-28.8
N3N4C5N6	-39.7	-32.5	-40.1	-28.8

***(b) E-isomer* azoheteroarene BMID**

	OM2/MRCI	B3LYP/6-311G(d,p)	CAM-B3LYP/6-311G(d,p)	Reference[a]
N3N4	1.22	1.26	1.25	1.27
C2N3	1.41	1.38	1.38	1.38
N4C5	1.41	1.38	1.38	1.38
C2N3N4	116.0	115.4	115.1	115.0
N3N4C5	116.0	115.4	115.1	115.0
C2N3N4C5	180.0	180.0	180.0	180.0
N1C2N3N4	0.0	0.0	0.0	0.0
N3N4C5N6	0.0	0.0	0.0	0.0

a) Calculated with B3LYP/6-31G(d,p) using a PCM continuum solvent model for water in Gaussian 09 by Weston et al.[S7].

3. Distribution of geometrical parameters and reaction pathways for the *Z*-*E* photoisomerization of azoheteroarene BMID

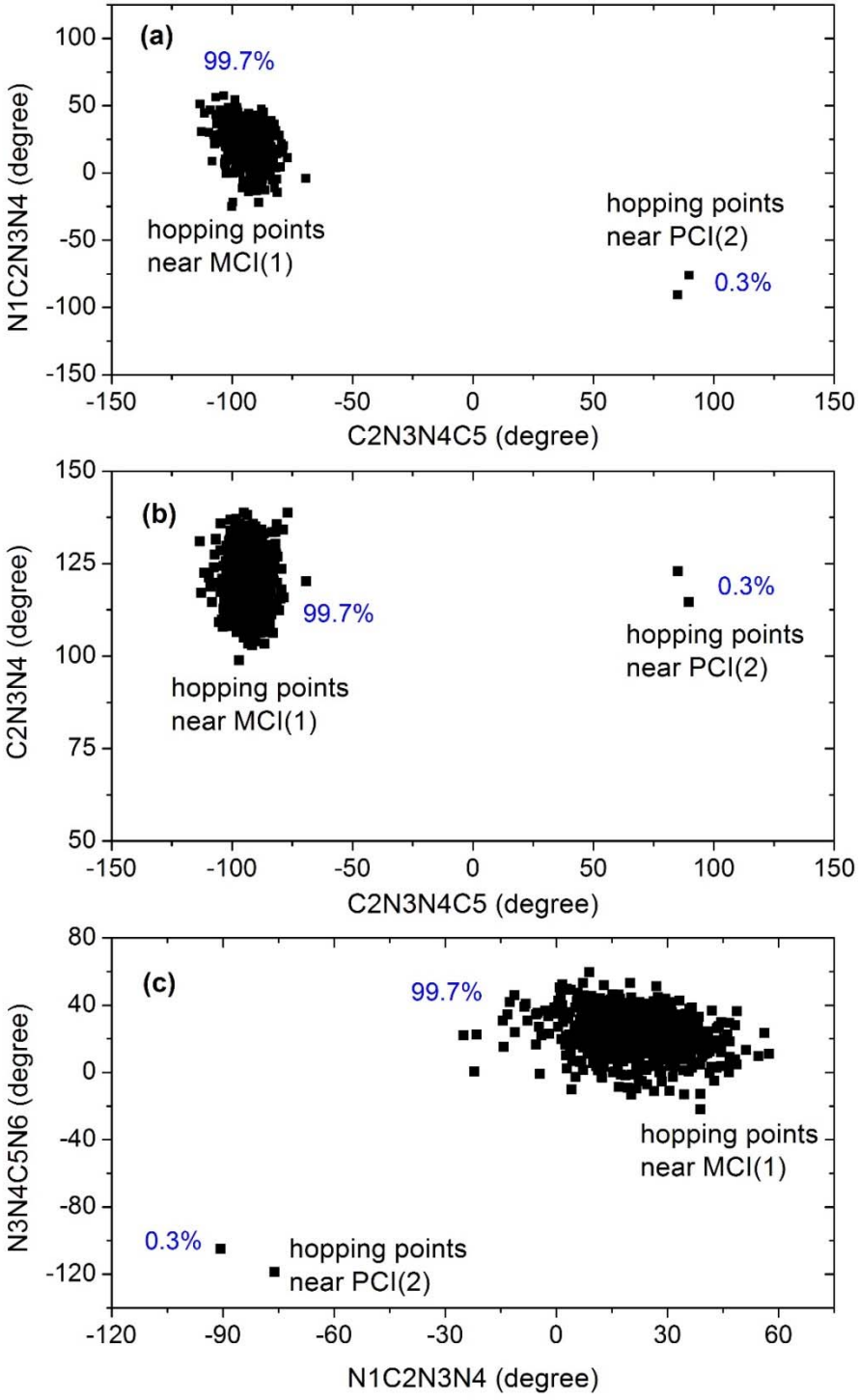

Fig. S2 Distributions of the (a) C2N3N4C5 and N1C2N3N4 dihedral angles; (b) C2N3N4C5 dihedral angle and C2N3N4 angle; (c) N1C2N3N4 and N3N4C5N6 dihedral angles at the hopping points of 764 trajectories starting from *M*-helical *Z*-isomer of azoheteroarene BMID.

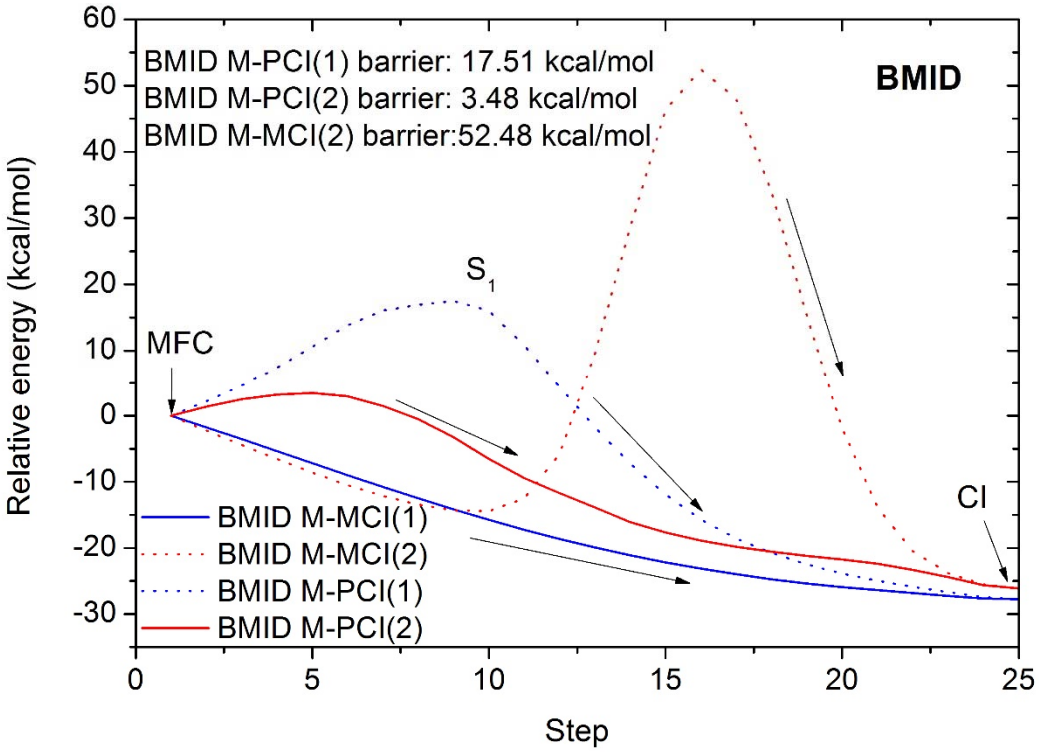

Fig. S3 OM2/MRCI energy profiles along four paths for azoheteroarene BMID, generated by linear interpolation between the Franck-Condon geometry of the M-helical Z-isomer (MFC) and four different S_1/S_0 conical intersections shown in Figure 3 in the main text of the article (MCI(1), PCI(1), MCI(2) and PCI(2)). Energies of BMID are relative to the S_1 excited-state energy of Franck-Condon geometry of its M-helical Z-isomer.

As can be seen in Fig. S3, there are very large barriers along the pathways connecting the Franck-Condon geometry of M-helical Z-isomer and PCI(1) and MCI(2). That's why we did not find reactions along these two pathways in all 764 trajectories.

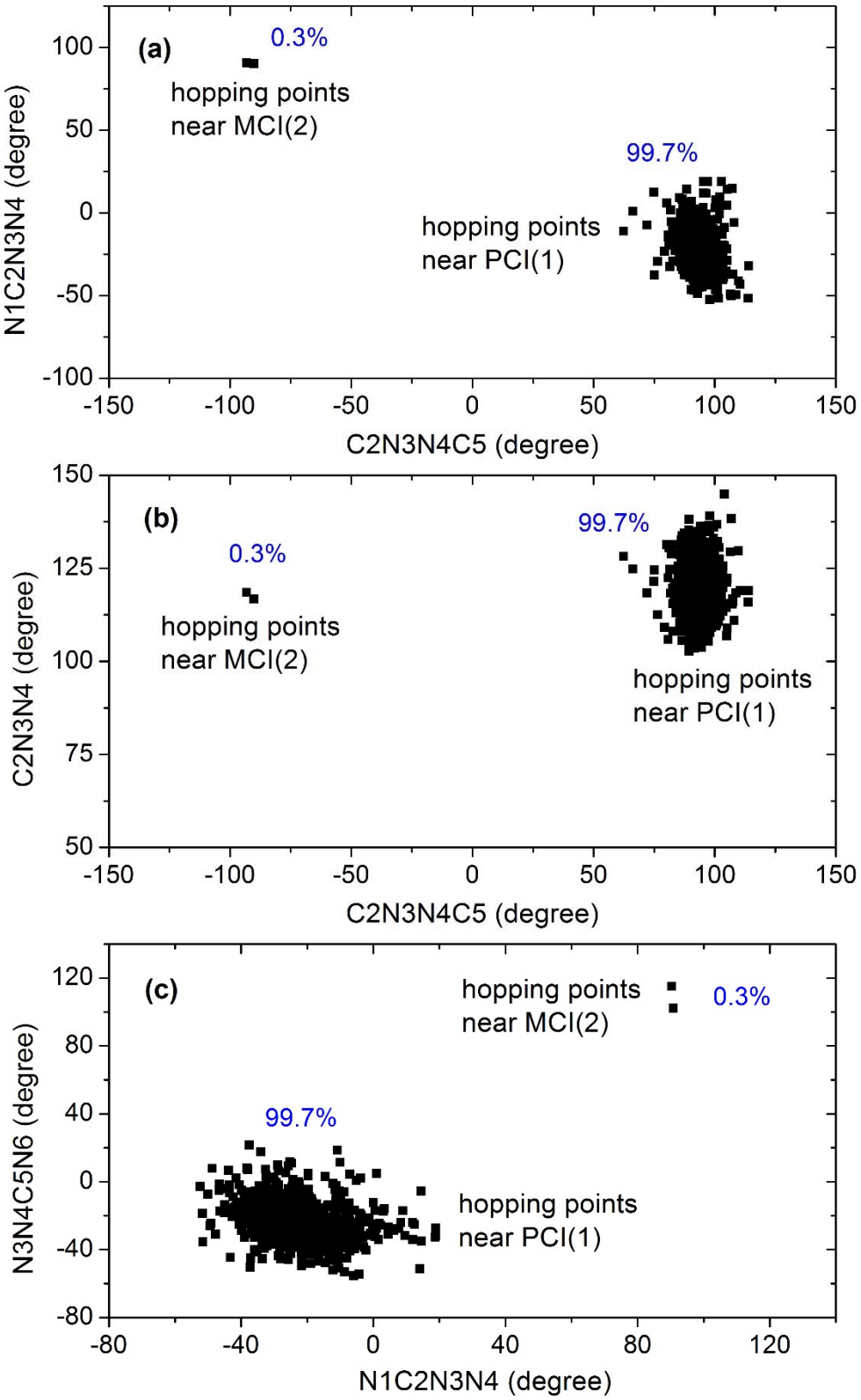

Fig. S4 Distributions of the (a) C2N3N4C5 and N1C2N3N4 dihedral angles; (b) C2N3N4C5 dihedral angle and C2N3N4 bond angle; (c) N1C2N3N4 and N3N4C5N6 dihedral angles at the hopping points of 694 trajectories starting from *P*-helical *Z*-isomer of azoheteroarene BMID.

4. Cartesian coordinates for several structures of azoheteroarene BMID optimized with the OM2/MRCI method

Unit of the Cartesian coordinate below is angstrom.

(1) Z-isomer M-helical azoheteroarene BMID at ground state

C	1.3608494666	-0.2576101052	-0.2204182680
N	1.0610530912	0.8278277525	-0.9603338064
C	2.1892132745	1.5745338008	-1.0077109797
C	3.2310976642	0.9391226343	-0.2901236684
N	2.7061205736	-0.2438823888	0.1758824753
C	3.3574834430	-1.2292123952	0.9955208980
H	4.2362706160	1.2874007007	-0.1137414616
N	0.5952977408	-1.4468374454	-0.0558852214
N	-0.5954066290	-1.4469066252	0.0557403998
C	-1.3609584537	-0.2577083737	0.2203609187
N	-2.7062443747	-0.2438792464	-0.1758393389
C	-3.2310428842	0.9392272807	0.2901297220
C	-2.1890598490	1.5745069463	1.0077270477
N	-1.0609996537	0.8276589437	0.9603045185
H	-2.2717812284	2.5184648830	1.5302023399
H	-4.2361341490	1.2876971618	0.1136592716
C	-3.3573422787	-1.2293869335	-0.9955024302
H	2.2720221754	2.5185542483	-1.5300704509
H	4.4020513505	-1.3792498787	0.6580608791
H	3.3670934606	-0.9009162174	2.0528030892
H	2.8204089122	-2.1911674375	0.9266815118
H	-4.4019459476	-1.3796007890	-0.6582705012
H	-3.3668012917	-0.9012130066	-2.0528276665
H	-2.8200738738	-2.1912242795	-0.9317569923

(2) Z-isomer P-helical azoheteroarene BMID at ground state

C	0.1255498377	0.0200647341	-0.3177081002
N	0.2019266958	0.4205375418	-1.6019724944
C	1.5206125388	0.5554118139	-1.8766136969
C	2.2961367341	0.2443210233	-0.7337938061
N	1.3992312875	-0.0589940920	0.2640974511
C	1.6920442760	-0.4782393235	1.6077535849
H	3.3696524712	0.2255101347	-0.6339256474
N	-1.0286138739	-0.0484028965	0.5133245489
N	-2.0954849515	-0.4190337221	0.1200905747
C	-2.2910795317	-1.0038298224	-1.1633280088
N	-3.5535733964	-0.9284780030	-1.7694369861
C	-3.4975540345	-1.7452484547	-2.8748786812
C	-2.2104304039	-2.3346160058	-2.8619266207

N	-1.4932889213	-1.8768836909	-1.8089557820
H	-1.8428815744	-3.0550362175	-3.5807986285
H	-4.2902742022	-1.8761970796	-3.5940418026
C	-4.6397275759	-0.0800349042	-1.3602894285
H	1.9132620388	0.8652528264	-2.8361668375
H	2.5316277234	0.1153015982	2.0204761769
H	1.9708858055	-1.5495743136	1.6216874930
H	0.8055727280	-0.3330733477	2.2492669921
H	-5.6075785505	-0.5999850258	-1.5030776244
H	-4.6429416913	0.8517742871	-1.9581253487
H	-4.5315605418	0.1823011852	-0.2987960306

(3) E-isomer azoheteroarene BMID at ground state

N	-1.1855277017	-1.5072958164	1.6934853498
C	-2.1582482665	-0.9384840512	0.9482359919
N	-3.3694561276	-0.8821791043	1.6566184064
C	-3.1208461669	-1.4409540354	2.8838745486
C	-1.7541470966	-1.8202538822	2.8774283492
N	-2.1320354006	-0.4214346948	-0.3669957242
N	-1.0633671516	-0.4899542273	-0.9458380933
C	-1.0371797439	0.0270479311	-2.2610868544
N	-2.0100278853	0.5952745373	-3.0065770214
C	-1.4413859212	0.9082965912	-4.1904898686
C	-0.0745074434	0.5296328533	-4.1966682514
N	0.1741727734	-0.0288487356	-2.9692908718
C	1.4209907163	-0.5686998687	-2.4848241879
C	-4.6160581970	-0.3415020514	1.1724803725
H	0.6483640318	0.6436990568	-4.9893095230
H	-1.2333149085	-2.2933877043	3.6996035958
H	-3.8436496160	-1.5548059522	3.6766091534
H	-1.9623198420	1.3810273332	-5.0128321342
H	1.7542016185	-1.4021752178	-3.1369310877
H	2.2010618817	0.2202389851	-2.4790662963
H	1.2898866523	-0.9486692102	-1.4582059497
H	-5.3968331314	-1.1298046958	1.1677091228
H	-4.9481940875	0.4926226054	1.8242641387
H	-4.4851557192	0.0377259766	0.1402781560

(4) Four different S_1/S_0 CIs for *Z*-*E* photoisomerization of azoheteroarene BMID, as shown in Figure 3.

MCI(1)

C	0.3126702909	0.2786540113	0.3187136227
N	0.4808896479	1.0218313033	1.4460104810
C	1.7568255525	1.4289348276	1.4402029095
C	2.4349718622	0.9444682226	0.2908958074
N	1.5121612770	0.2214181703	-0.4213189610

C	1.7211824512	-0.4937068468	-1.6500010048
H	3.4663354883	1.1012446592	0.0024783663
N	-0.8168824660	-0.3889447213	-0.1460248338
N	-1.8821179989	-0.2393932927	0.4629685976
C	-2.4138206225	-1.1048000774	1.3968853281
N	-3.7162684215	-0.9123285219	1.8961465308
C	-3.9420210159	-1.9546127782	2.7641327349
C	-2.7655178925	-2.7511770901	2.7468558677
N	-1.8484411742	-2.2348195852	1.9123067254
H	-2.6196915922	-3.6515899769	3.3304937855
H	-4.8474251826	-2.1088087549	3.3293339609
C	-4.6010675896	0.1758041796	1.5782303746
H	2.2080999961	2.0401523685	2.2101629082
H	2.0366244974	0.2027201065	-2.4543196041
H	2.5080481720	-1.2643907309	-1.5192986929
H	0.7881713814	-0.9894612388	-1.9558308900
H	-5.5167401665	-0.2054929649	1.0748284856
H	-4.8981465427	0.7130436441	2.5039082851
H	-4.0939742381	0.8868624545	0.9025442424

PCI(1)

C	0.3127074178	0.2792122525	-0.3194373535
N	0.4804356160	1.0218839239	-1.4471406262
C	1.7562999222	1.4292194249	-1.4419310747
C	2.4348974557	0.9454194990	-0.2926095280
N	1.5124417952	0.2225465880	0.4202441176
C	1.7219924811	-0.4919909974	1.6491780698
H	3.4663247131	1.1025169698	-0.0045959227
N	-0.8165808095	-0.3883594147	0.1459827707
N	-1.8820272275	-0.2393145320	-0.4627654363
C	-2.4138482407	-1.1052976608	-1.3960808842
N	-3.7164747037	-0.9133161872	-1.8950633029
C	-3.9422922118	-1.9560894199	-2.7624454706
C	-2.7656428185	-2.7524355226	-2.7450977793
N	-1.8484160588	-2.2354821459	-1.9110823853
H	-2.6198264133	-3.6531256079	-3.3283107672
H	-4.8478317078	-2.1107398061	-3.3273049587
C	-4.6013716493	0.1748293398	-1.5774628188
H	2.2072217594	2.0401506414	-2.2123246844
H	2.5087863846	-1.2627529286	1.5184979173
H	2.0378035373	0.2048156969	2.4530216549
H	0.7891086046	-0.9875831869	1.9556578385
H	-4.8987721083	0.7115601155	-2.5033325587
H	-5.5168546056	-0.2063683706	-1.0736411344
H	-4.0942241791	0.8863059560	-0.9022575368

MCI(2)

C	-0.5230534068	1.1465372666	2.7946338737

N	0.3469157172	1.1288321274	1.6491850267
C	1.6038952293	1.6941840223	1.5731035036
C	2.1131404203	1.3851357526	0.2917145559
N	1.2197651478	0.6429677482	-0.4160813819
C	0.1272345724	0.4923637397	0.4129851720
N	-1.0477821026	-0.1263118387	0.0152880625
N	-2.1256608492	0.0413336075	0.5970602102
C	-2.6558605036	-0.8818331747	1.4979722685
N	-2.0246995521	-1.8762653585	2.1601073002
C	-3.0053888487	-2.4732838091	2.8759646453
C	-4.2639507098	-1.8710271503	2.6430049485
N	-4.0316866251	-0.8433472929	1.7594232459
C	-4.9943439811	-0.0047213973	1.1042668744
H	2.0761555973	2.2526798028	2.3618313600
H	-2.8269249764	-3.3120369895	3.5379535961
H	-5.2229882385	-2.1481798536	3.0221928953
H	3.0653359391	1.7182505950	-0.1001055227
H	-0.0456086101	1.6963839306	3.6290238569
H	-1.4782640840	1.6501504493	2.5406485776
H	-0.7426249917	0.1150785656	3.1239721254
H	-5.7099394024	-0.6173464092	0.5262052058
H	-5.5597765922	0.5806085515	1.8475588082
H	-4.4855790886	0.6878787686	0.4180716434

PCI(2)

C	-0.5230506919	1.1465666479	-2.7946380481
N	0.3469250344	1.1288385985	-1.6491941108
C	1.6039052020	1.6941869457	-1.5731005124
C	2.1131433491	1.3851301148	-0.2917105766
N	1.2197514591	0.6429807962	0.4160855158
C	0.1272301926	0.4923763418	-0.4129939376
N	-1.0477925764	-0.1262906555	-0.0153044436
N	-2.1256683266	0.0413431301	-0.5970858404
C	-2.6558653261	-0.8818362995	-1.4979845479
N	-2.0246944907	-1.8762520208	-2.1601340933
C	-3.0053852738	-2.4732834570	-2.8759781040
C	-4.2639541099	-1.8710466168	-2.6430040377
N	-4.0316920425	-0.8433580382	-1.7594320510
C	-4.9943448344	-0.0047456766	-1.1042502672
H	2.0761743852	2.2526738307	-2.3618279658
H	-2.8269206998	-3.3120401744	-3.5379589824
H	-5.2229906156	-2.1482122408	-3.0221854329
H	3.0653423795	1.7182363034	0.1001118717
H	-1.4782429927	1.6502153680	-2.5406518437
H	-0.0455907008	1.6963830983	-3.6290418116
H	-0.7426760314	0.1151117755	-3.1239483084
H	-5.5597963877	0.5805949269	-1.8475194317
H	-5.7099187288	-0.6173893593	-0.5261846606
H	-4.4855758862	0.6878501605	-0.4180534011

5. Optimized geometries of azoheteroarene BHID

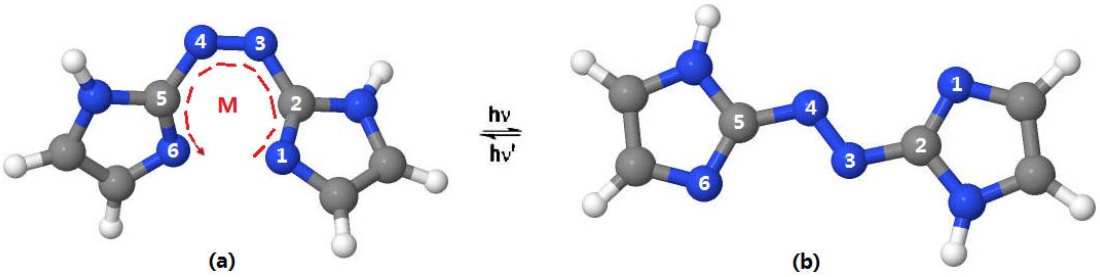

Fig. S5 Optimized geometries of (a) Z-isomer M-helical BHID and (b) E-isomer BHID calculated with OM2/MRCI method implemented in MNDO99 program[S5]. Atoms around central N=N bond are labelled.

Table S2. Optimized geometrical parameters of ground state azoheteroarene BHID, obtained from different methods. OM2/MRCI method is implemented in MNDO99 program[S5]; while B3LYP/6-311G(d,p) and CAM-B3LYP/6-311G(d,p) methods are implemented in Gaussian 03 program[S6]. The lengths are in angstroms; the dihedral angles and bond angles are in degrees.

(a) ***Z-isomer*** **azoheteroarene BHID** ***with M helicity***

	OM2/MRCI	B3LYP/6-311G(d,p)	CAM-B3LYP/6-311G(d,p)
N3N4	1.19	1.26	1.24
C2N3	1.42	1.39	1.40
N4C5	1.42	1.39	1.40
C2N3N4	123.2	125.3	123.4
N3N4C5	123.2	125.3	123.4
C2N3N4C5	-10.0	-15.1	-14.4
N1C2N3N4	-40.3	-28.7	-37.4
N3N4C5N6	-40.2	-28.7	-37.4

(b) ***E-isomer*** **azoheteroarene BHID**

	OM2/MRCI	B3LYP/6-311G(d,p)	CAM-B3LYP/6-311G(d,p)
N3N4	1.23	1.26	1.25
C2N3	1.41	1.38	1.39
N4C5	1.41	1.38	1.39
C2N3N4	115.8	115.1	114.9
N3N4C5	115.7	115.1	114.9
C2N3N4C5	180.0	180.0	180.0
N1C2N3N4	0.0	0.0	0.0
N3N4C5N6	0.0	0.0	0.0

6. Distribution of several geometrical parameters during the *Z*-*E* photoisomerization of azoheteroarene BHID

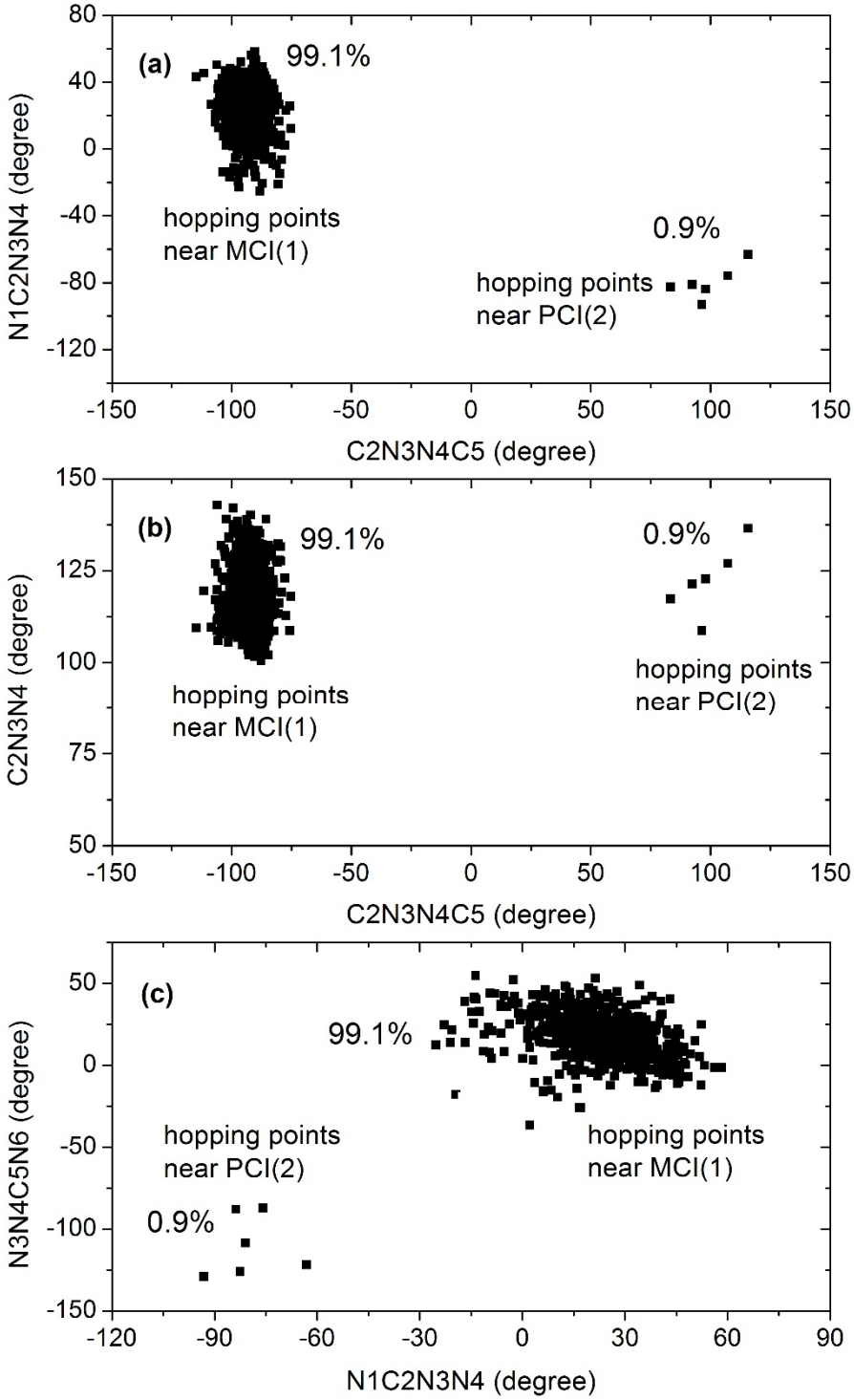

Fig. S6 Distributions of the (a) C2N3N4C5 and N1C2N3N4 dihedral angles; (b) C2N3N4C5 dihedral angle and C2N3N4 bond angle; (c) N1C2N3N4 and N3N4C5N6 dihedral angles at hopping points of 649 trajectories starting from *M*-helical *Z*-isomer of azoheteroarene BHID.

7. S_1/S_0 conical intersection related to the *Z*-*E* photoisomerization of azoheteroarene BHID

Basis on 649 geometries at hopping points as shown in Fig. 5(b) of the main text of the article, two optimized S_1/S_0 conical intersections are located, which are presented in following Fig. S7(a) and Fig. S7(c) respectively. The values of central dihedral angle C2N3N4C5 in Fig. S7(a) and Fig. S7(c) are -98.7° and 98.0° respectively. The enantiomers of them are also S_1/S_0 conical intersections, which are shown in Fig. S7(b) and Fig. S7(d) respectively. According to their helicities, the four conical intersections in Fig. S7 are named as MCI(1), PCI(1), MCI(2) and PCI(2), respectively. The Cartesian coordinates of them can be found in the ninth part of this electronic supplementary information.

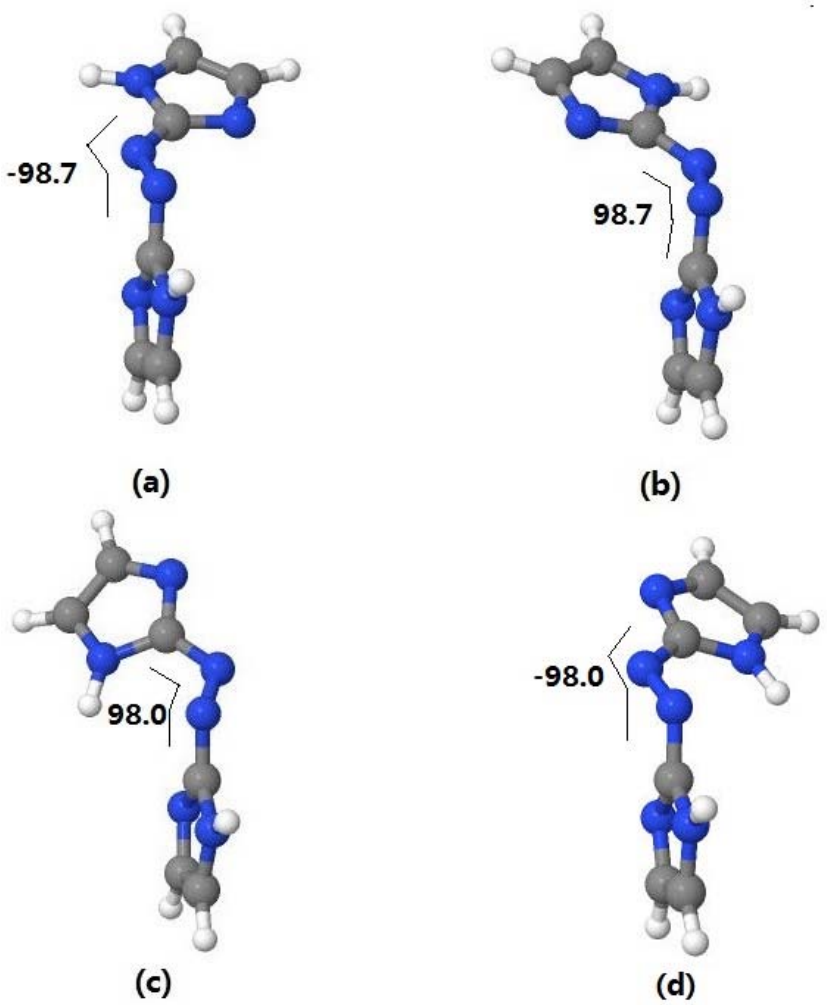

Fig. S7 Four different S_1/S_0 CIs for the Z-E photoisomerization of *M*-helical BHID. (a) MCI(1); (b) PCI(1), which is mirror invert of (a); (c) PCI(2), CI structure with P-helical, but not the mirror invert of (a); (d) MCI(2), which is mirror invert of (c).

8. Reaction pathways for the *Z*-*E* photoisomerization of azoheteroarene BHID

The energy profiles of BHID along different reaction paths connecting the initial M-helical Franck-Condon geometry and three relevant conical intersections generated by linear interpolation are presented in Fig. S8. For comparison, OM2/MRCI energy profiles for M-helical Z-isomer azobenzene connecting MFC and two S_1/S_0 conical intersections (MCI and PCI) are also presented. In Fig. S8, energies of BHID and azobenzene are relative to the energy of Franck-Condon geometry of their M-helical Z-isomer respectively. As we can see, the energy profile connecting MFC and MCI(1) is barrierless, and much steeper than that of azobenzene. But there is a barrier with a value of 3.97 kcal/mol along the energy profile connecting MFC and PCI(2), which is much larger than that along the reaction path of MFC-to-PCI for azobenzene. An even larger barrier with a value of 17.20 kcal/mol exists along the energy profile connecting MFC and PCI(1). We should emphasize that no trajectories decay around PCI(1) in our calculations. These two large barriers reduce the Z-E isomerization reactions through P-helical conical intersections, and also make the average lifetime of S_1 excited state for those trajectories through P-helical channels much longer than that through M-helical channels (ca. 115 fs vs 49 fs).

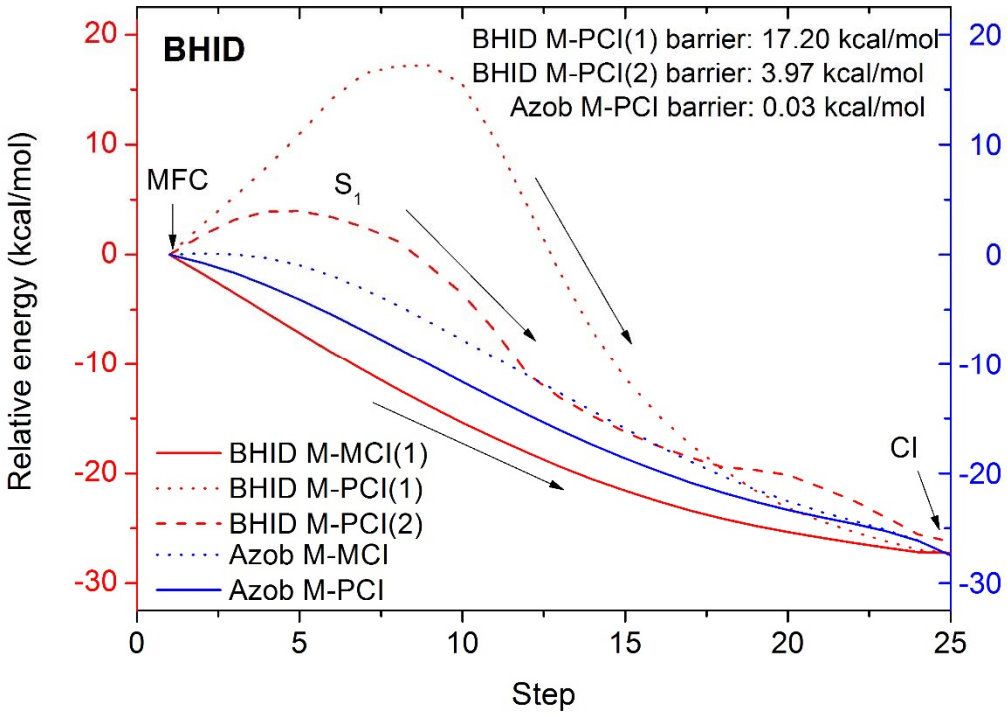

Fig. S8 OM2/MRCI energy profiles along three paths for azoheteroarene BHID (red lines, left), generated by linear interpolation between the Franck-Condon geometry of M-helical Z-isomer (MFC) and three different S_1/S_0 conical intersections (MCI(1), PCI(1) and PCI(2)). Energies of BHID are relative to the S_1 excited-state energy of Franck-Condon geometry of its M-helical Z-isomer. For comparison, OM2/MRCI relative energy profiles for M-helical Z-isomer azobenzene (Azob) connecting MFC and two S_1/S_0 conical intersections (MCI and PCI) are also presented, which were calculated with the OM2/MRCI method at the same active space as Weingart *et al.*[S3]. Energies of azobenzene are relative to the S_1 excited-state OM2/MRCI energy of Franck-Condon geometry of its M-helical Z-isomer.

9. Cartesian coordinates for several structures of azoheteroarene BHID optimized with the OM2/MRCI method

Unit of the Cartesian coordinate below is angstrom.

(1) *Z*-isomer M-helical azoheteroarene BHID at ground state

C	0.1327608634	0.0097678379	0.3430181943
N	0.2105783388	0.4368780684	1.6210887078
C	1.5371112439	0.5732051074	1.8785804305
C	2.3022516711	0.2521250021	0.7343313377
N	1.3924720527	-0.0698338646	-0.2405694294
H	3.3697261352	0.2586962588	0.6095334902
N	-1.0209008424	-0.0634658216	-0.4902373197
N	-2.0901451481	-0.4222198525	-0.0965259907
C	-2.2917106254	-1.0109732377	1.1853658174
N	-3.5475121973	-0.9267991819	1.7766668319
C	-3.5255902657	-1.7513591090	2.8727297628
C	-2.2478335207	-2.3554487898	2.8695431308
N	-1.5084596278	-1.9064058166	1.8227315840
H	-1.8960958878	-3.0842299047	3.5882032859
H	-4.3394890894	-1.8914513907	3.5605313985
H	1.9370274626	0.8953595806	2.8312143266
H	-4.3052894182	-0.3384876846	1.4661132206
H	1.5836505175	-0.3482258253	-1.1960034768

(2) *E*-isomer azoheteroarene BHID at ground state

N	-1.1744337253	-1.5052755964	1.7017227781
C	-2.1508737143	-0.9378505491	0.9510665103
N	-3.3510907914	-0.8861934378	1.6552403079
C	-3.1201611320	-1.4361314510	2.8796655803
C	-1.7522522859	-1.8155882429	2.8847990248
N	-2.1301052985	-0.4227994419	-0.3602861342
N	-1.0499817024	-0.4880747070	-0.9450541479
C	-1.0325840375	0.0279457700	-2.2563156063
N	-2.0127537387	0.5942509572	-3.0029746127
C	-1.4399448616	0.9066418082	-4.1877554052
C	-0.0712353688	0.5296901827	-4.1878049441
N	0.1652266020	-0.0207680595	-2.9646225172
H	0.6552494734	0.6434172355	-4.9785916932
H	-1.2372968412	-2.2860724977	3.7113440925
H	-3.8497675087	-1.5477590661	3.6678562059
H	-1.9586966570	1.3768154485	-5.0120730619
H	-4.2172941220	-0.5064686784	1.3001568156
H	1.0334561244	-0.3993344502	-2.6184563030

(3) Four different S_1/S_0 CIs for the *Z*-*E* photoisomerization of *M*-helical azoheteroarene BHID, as shown in Figure S7.

MCI(1)

C	0.4054184823	0.0228395754	0.4729545024
N	0.6051379553	0.8976086098	1.5035872938
C	1.9067235863	1.2197731726	1.4586193769
C	2.5578804486	0.5563064363	0.3807272270
N	1.5920344177	-0.1901116303	-0.2383503330
H	3.5929836014	0.6140779834	0.0831247546
N	-0.7706742956	-0.5744996413	0.0688783547
N	-1.8984951951	-0.3355735555	0.5122631755
C	-2.4286016406	-1.1937330098	1.4763628517
N	-3.7479520991	-1.0197596901	1.9127168498
C	-3.9742823084	-1.9642029472	2.8722678272
C	-2.7664762210	-2.7001625093	2.9833585044
N	-1.8412253068	-2.2264341250	2.1381561066
H	-2.6118154865	-3.5269079675	3.6592542276
H	-4.8994314782	-2.1092220196	3.4088756988
H	2.3947490196	1.8905838475	2.1545104331
H	-4.3876905480	-0.3154085420	1.5810147562
H	1.6951185287	-0.7956958840	-1.0379072262

PCI(1)

C	0.4054185223	0.0228395068	-0.4729544815
N	0.6051378751	0.8976086040	-1.5035872460
C	1.9067235020	1.2197732159	-1.4586194120
C	2.5578804820	0.5563064264	-0.3807273666
N	1.5920345255	-0.1901117187	0.2383502309
H	3.5929836609	0.6140779901	-0.0831249761
N	-0.7706742185	-0.5744997725	-0.0688782993
N	-1.8984951366	-0.3355736785	-0.5122630692
C	-2.4286015606	-1.1937330991	-1.4763627834
N	-3.7479519647	-1.0197596894	-1.9127169248
C	-3.9742821452	-1.9642029341	-2.8722679200
C	-2.7664760954	-2.7001625970	-2.9833584559
N	-1.8412252311	-2.2264342666	-2.1381559687
H	-2.6118153602	-3.5269080861	-3.6592541417
H	-4.8994312723	-2.1092219431	-3.4088758885
H	2.3947488503	1.8905839635	-2.1545104571
H	-4.3876903885	-0.3154084755	-1.5810149168
H	1.6951187239	-0.7956960132	1.0379070829

PCI(2)

C	0.3735500839	-0.2002608340	0.3257663466
N	0.8988515334	0.0017152947	1.5706022839
C	1.7548384860	1.0270535866	1.4469937787

C	1.7927980549	1.4946813469	0.1037898422
N	0.9128120263	0.7115161681	-0.5904336022
H	2.3818664279	2.2975749616	-0.3111587727
N	-0.5642873677	-1.1324833777	-0.0839532647
N	-0.8330936027	-2.1516602305	0.5819113171
C	-1.9332540338	-2.1753186803	1.4098520486
N	-2.6894608886	-1.0388879516	1.7723788793
C	-3.6478367476	-1.4638493640	2.6423254364
C	-3.4541176048	-2.8670551076	2.7774412109
N	-2.4322363844	-3.2859773856	2.0361462252
H	-4.0644891636	-3.5072453009	3.4006053539
H	-4.4060236953	-0.8500191442	3.1021618137
H	2.3354539150	1.4419486097	2.2614000118
H	-2.5220634763	-0.0911714158	1.4720452040
H	0.6937132197	0.7499142178	-1.5742393359

MCI(2)

C	0.3735500839	-0.2002608340	-0.3257663466
N	0.8988515334	0.0017152947	-1.5706022839
C	1.7548384860	1.0270535866	-1.4469937787
C	1.7927980549	1.4946813469	-0.1037898422
N	0.9128120263	0.7115161681	0.5904336022
H	2.3818664279	2.2975749616	0.3111587727
N	-0.5642873677	-1.1324833777	0.0839532647
N	-0.8330936027	-2.1516602305	-0.5819113171
C	-1.9332540338	-2.1753186803	-1.4098520486
N	-2.6894608886	-1.0388879516	-1.7723788793
C	-3.6478367476	-1.4638493640	-2.6423254364
C	-3.4541176048	-2.8670551076	-2.7774412109
N	-2.4322363844	-3.2859773856	-2.0361462252
H	-4.0644891636	-3.5072453009	-3.4006053539
H	-4.4060236953	-0.8500191442	-3.1021618137
H	2.3354539150	1.4419486097	-2.2614000118
H	-2.5220634763	-0.0911714158	-1.4720452040
H	0.6937132197	0.7499142178	1.5742393359

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