

Supplementary Information for

Theoretical Insights into the Structural and Fluorescence Properties of DNA Containing Fluorescent Nucleobases

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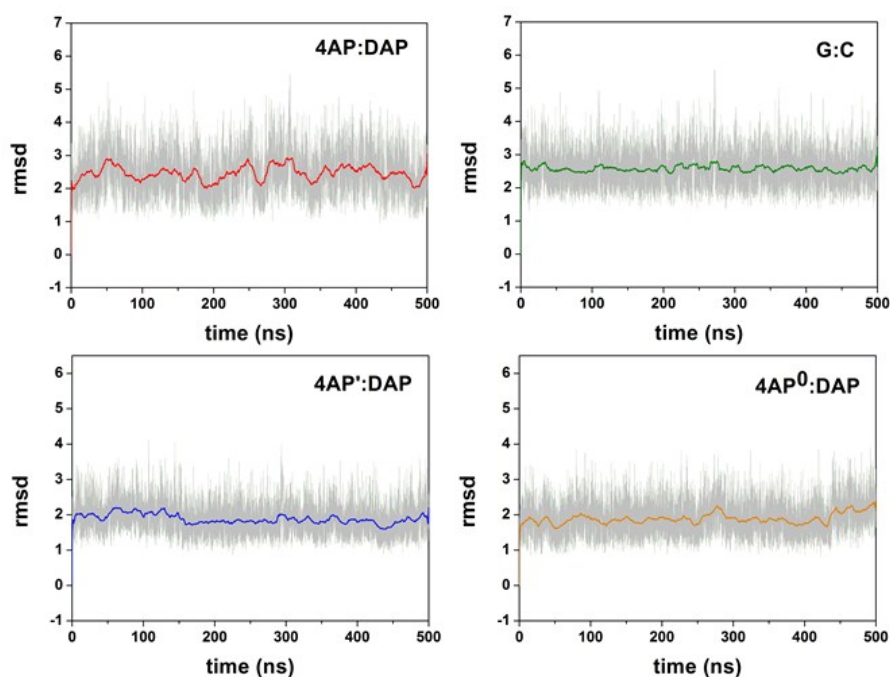


Fig. S1 RMSD values (Å) as a function of time for the oligonucleotides containing **4AP:DAP** (red), **G:C** (green) and **4AP':DAP** (blue) and **4AP⁰:DAP** (orange). The plots show the RMSD values of all atoms to the initial structure.

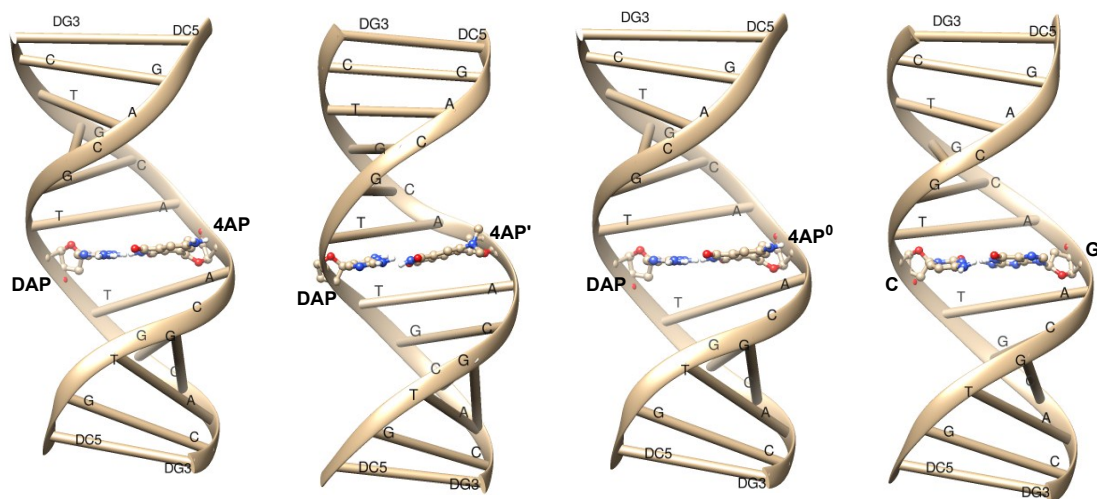


Fig. S2 Conformations of oligonucleotide containing **4AP/4AP'/4AP⁰:DAP** and **G:C** base pair from the cluster analysis of the production run.

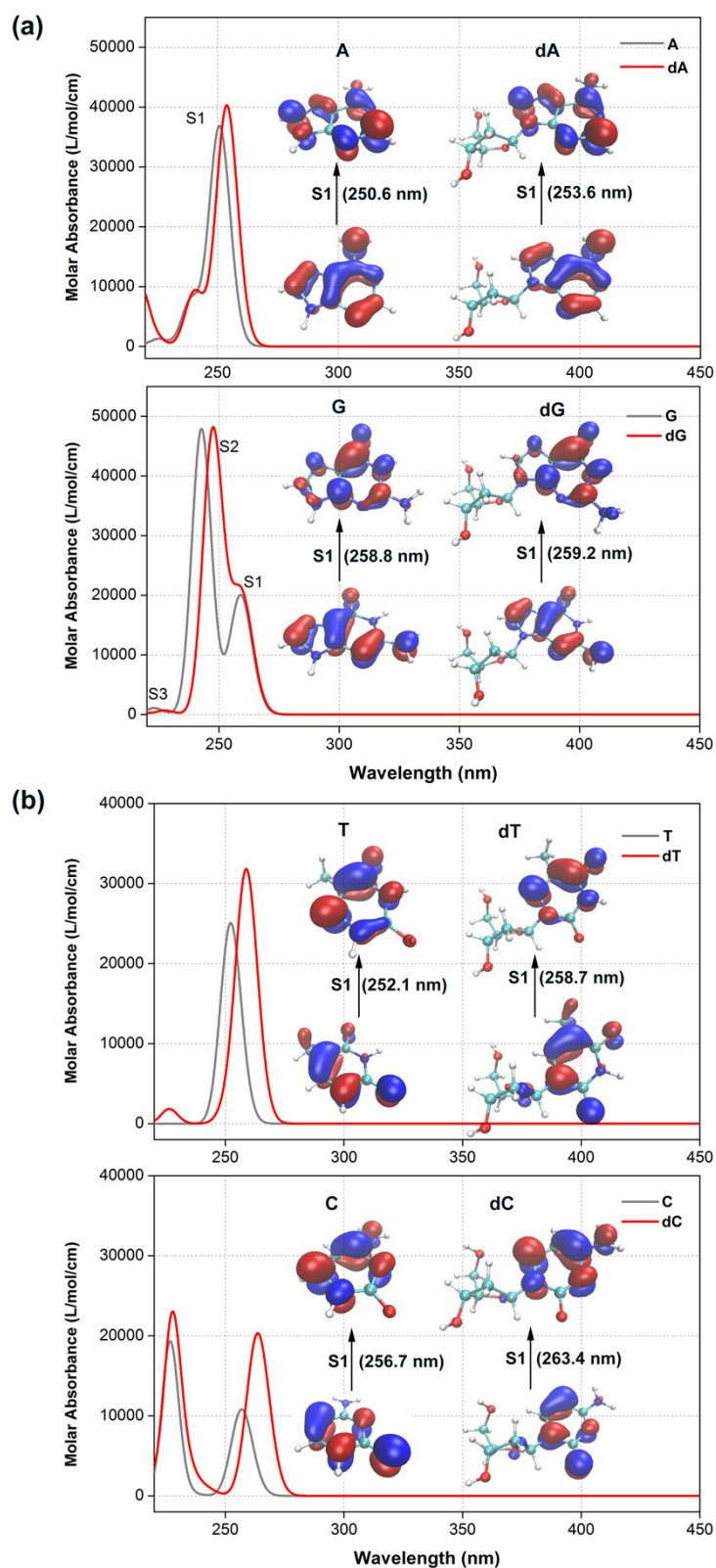


Fig. S3 The absorption spectrum of A/G/C/T and dA/dG/dC/dT in water determined at the TDB3LYP/6-311++G(d,p) level. The half-bandwidths were taken to be equal to 0.2 eV. Inserts: Natural transition orbitals (NTOs) involved in the first (S₁, ππ*) singlet transition.

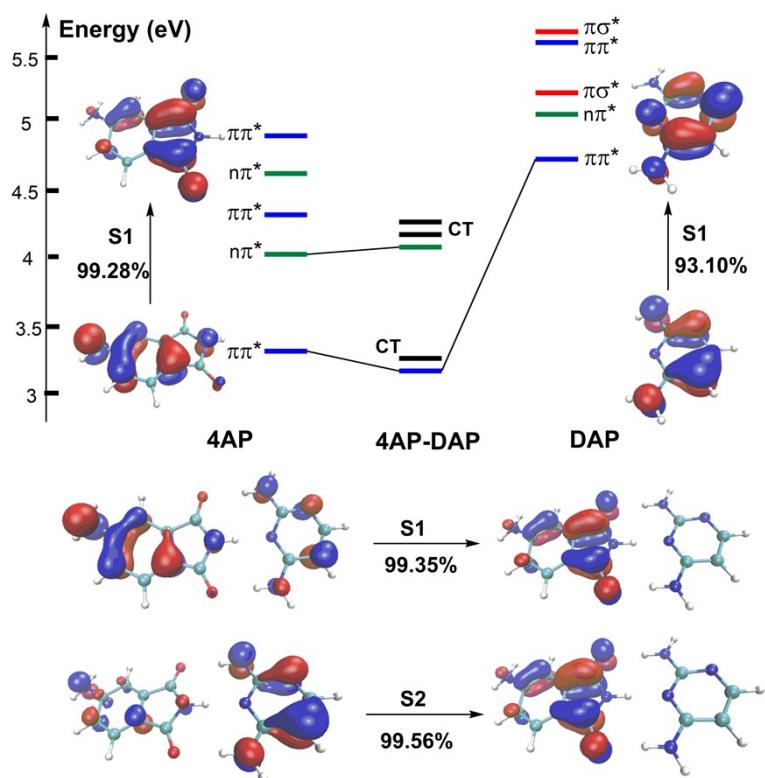


Fig. S4 Vertical transition energy diagrams for the **4AP:DAP** base pair and the isolated bases **4AP** and **DAP** calculated at the TD-B3LYP/6-311++G(d,p). The horizontal bars representing the excited electronic states are colored according to their character: blue for $\pi\pi^*$ states, green for $n\pi^*$ states, red for $\pi\sigma^*$ states. The black lines connect states of the same nature found in the isolated bases and in its base pairs. The inset plots show natural transition orbitals (NTO) for selected excited states of the bases and base pair.

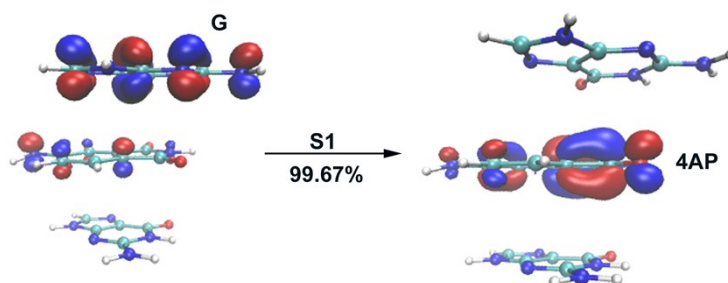


Fig. S5 Natural transition orbitals (NTOs) of the first transition for the stacking trimers **G_4AP_G**, calculated at the TD-B3LYP/6-311++G(d,p) level.

Table S1a: Vertical Transition Energies (E), Oscillator Strengths (f), and Assignments for **A** and **dA** in water, calculated at the TDB3LYP/6-311++G(d,p) level.

A				dA		
transitions	E/eV	f	assignment	E/eV	f	assignment
S ₁	4.9474	0.2726	$\pi\pi^*$	4.8887	0.2986	$\pi\pi^*$
S ₂	5.0968	0.0007	$n\pi^*$	5.0789	0.0009	$n\pi^*$
S ₃	5.1926	0.0567	$\pi\pi^*$	5.1611	0.0675	$\pi\pi^*$
S ₄	5.4942	0.0093	$\pi\sigma^*$	5.5193	0.0089	$\pi\sigma^*$
S ₅	5.6635	0.0019	$n\pi^*$	5.6484	0.0097	$n\pi^*$

Table S1b: Vertical Transition Energies (E), Oscillator Strengths (f), and Assignments for **G** and **dG** in water, calculated at the TDB3LYP/6-311++G(d,p) level.

G				dG		
transitions	E/eV	f	assignment	E/eV	f	assignment
S ₁	4.7913	0.1468	$\pi\pi^*$	4.7843	0.1486	$\pi\pi^*$
S ₂	5.1098	0.3367	$\pi\pi^*$	5.0143	0.3534	$\pi\pi^*$
S ₃	5.1652	0.0229	$\pi\sigma^*$	5.1454	0.0011	$\pi\sigma^*$
S ₄	5.4870	0.0003	$n\pi^*$	5.4528	0.0050	$n\pi^*$
S ₅	5.5642	0.0079	$\pi\sigma^*$	5.4965	0.0000	$\pi\sigma^*$

Table S1c: Vertical Transition Energies (E), Oscillator Strengths (f), and Assignments for **C** and **dC** in water, calculated at the TDB3LYP/6-311++G(d,p) level.

C				dC		
transitions	E/eV	f	assignment	E/eV	f	assignment
S ₁	4.8295	0.0803	$\pi\pi^*$	4.7058	0.1509	$\pi\pi^*$
S ₂	5.2629	0.0021	$n\pi^*$	5.1270	0.0064	$n\pi^*$
S ₃	5.4714	0.1430	$n\pi^*$	5.2833	0.0202	$n\pi^*$
S ₄	5.5135	0.0004	$n\pi^*$	5.4480	0.1668	$n\pi^*$
S ₅	5.7721	0.0043	$\pi\sigma^*$	5.6383	0.0125	$n\pi^*$

Table S1d: Vertical Transition Energies (E), Oscillator Strengths (f), and Assignments for **T** and **dT** in water, calculated at the TDB3LYP/6-311++G(d,p) level.

T				dT		
transitions	E/eV	f	assignment	E/eV	f	assignment
S ₁	4.9198	0.1861	$\pi\pi^*$	4.7919	0.2327	$\pi\pi^*$
S ₂	4.9702	0.0000	$n\pi^*$	4.9354	0.0142	$n\pi^*$
S ₃	5.8291	0.0003	$\pi\sigma^*$	5.4810	0.0137	$n\pi^*$
S ₄	6.0349	0.0001	$n\pi^*$	5.7888	0.0004	$\pi\sigma^*$
S ₅	6.0599	0.2421	$\pi\pi^*$	5.8948	0.0006	$n\pi^*$

Table S2: Emission wavelengths (λ , nm) and Oscillator strengths (f) for **A/G/C/T** and **dA/dG/dC/dT** in water, calculated at the TD-B3LYP/6-311++G(d,p) level.

Bases	E/eV	λ /nm	f	Bases	E/eV	λ /nm	f
A	4.1233	300.69	0.4770	dA	4.0169	308.66	0.4782
G	1.5759	786.73	0.0166	dG	1.9321	641.72	0.0394
C	3.6998	335.11	0.0605	dC	3.6812	336.81	0.0899
T	4.1935	295.66	0.3175	dT	3.5190	352.33	0.2753

Table S3: Absorption/Emission Energies (E), wavelengths (λ , nm), Oscillator Strengths (f) and Assignments of the **4AP:DAP** pair in water, calculated at the TD-B3LYP/6-311++G(d,p) level.

4AP:DAP pair				
transition	E/eV	λ /nm	f	assignment
Absorption				
S ₁	3.2330	383.49	0.0814	$\pi\pi^*$
S ₂	3.2612	380.18	0.0207	$\pi\pi^*(CT)$
S ₃	4.0666	304.89	0.0002	$n\pi^*$
S ₄	4.1423	299.31	0.0009	$n\pi^*(CT)$
S ₅	4.2351	292.76	0.0000	$n\pi^*(CT)$
Fluorescence				
S ₁ →S ₀	2.5699	482.44	0.1096	$\pi\pi^*$

Table S4: Vertical Transition Energies (E), Oscillator Strengths (f), and Assignments for **4AP:DAP** pair, **4AP** and **DAP** in water, calculated at the TD-CAM-B3LYP/6-311++G(d,p) level.

4AP:DAP pair			
transition	E/eV	f	assignment
S ₁	3.6587	0.1187	$\pi\pi^*$
S ₂	4.4634	0.0003	$n\pi^*$
S ₃	4.5013	0.0290	$\pi\pi^*$
S ₄	4.7695	0.0064	$n\pi^*$
S ₅	4.8726	0.1534	$\pi\pi^*$

4AP			
transitions	E/eV	f	assignment
S ₁	3.7218	0.1229	$\pi\pi^*$
S ₂	4.4118	0.0001	$n\pi^*$
S ₃	4.5257	0.0363	$\pi\pi^*$
S ₄	4.9831	0.0000	$n\pi^*$
S ₅	5.2703	0.6021	$\pi\pi^*$

DAP			
transitions	E/eV	f	assignment
S ₁	4.9584	0.1652	$\pi\pi^*$
S ₂	5.3820	0.0049	$n\pi^*$
S ₃	5.6365	0.0061	$\pi\sigma^*$
S ₄	5.8083	0.2138	$\pi\pi^*$
S ₅	6.0531	0.0032	$\pi\sigma^*$

Cartesian coordinates for absorption geometries involved in this study calculated at the TD-B3LYP/6-311++G(d,p) level.

4AP

O	-2.2073240	-0.2741690	0.6709740	O	-1.3027300	0.6702680	0.0578690
C	-0.0660300	0.5772980	-0.0028400	H	-1.3125700	1.5906740	0.6541450
C	-0.3890160	-0.7843950	-0.0020110	C	0.1147870	0.1489960	0.0254790
C	0.6215670	-1.7397910	-0.0004350	C	1.1411970	1.0321540	0.3660950
C	1.9424870	-1.3082520	-0.0010310	C	2.4640570	0.6262710	0.2640480
C	2.2733490	0.0676590	-0.0034030	C	2.7681880	-0.6676770	-0.1674260
C	1.2342810	1.0303340	-0.0044110	C	1.7879160	-1.5754470	-0.4933730
C	-1.3433300	1.3561000	0.0002260	C	0.4319750	-1.1772750	-0.3957620
C	-1.8575610	-0.9183870	0.0017280	N	-0.5561830	-2.0622730	-0.7475110
H	0.3930290	-2.7990040	0.0033560	H	-0.2934630	-3.0321080	-0.8425890
H	1.4633230	2.0898300	-0.0060410	H	-1.4680710	-1.8991960	-0.3407920
N	3.5848760	0.4676140	-0.0507230	H	2.0345180	-2.5806670	-0.8160390
H	3.8051830	1.4216780	0.1912150	C	4.2554750	-0.8183000	-0.1729980
H	4.3012570	-0.2026330	0.1837870	N	4.7442630	0.4102890	0.2600120
N	-2.3515490	0.3985140	0.0022020	C	3.7259730	1.3366140	0.5464190
H	-3.3372450	0.6230440	0.0043400	O	3.9175080	2.4707920	0.9409710
O	-1.5072190	2.5595010	0.0010560	H	5.7287420	0.6167910	0.3609730
O	-2.5550500	-1.9147250	0.0033510	O	4.9289520	-1.7808950	-0.4807980
H	2.7448310	-2.0374120	0.0007960	H	0.8965660	2.0341710	0.7011950

d4AP

O	-4.6123510	-1.5923670	1.7093020	C	-1.9606420	0.9499310	-1.3055550
C	-4.5200610	-0.9672730	0.4291370	H	-1.7017150	0.1636250	-2.0173860
H	-5.5001470	-0.5983910	0.1039480	H	-1.6619130	1.9115200	-1.7245850
H	-4.2042070	-1.7488310	-0.2655590	C	-3.4673720	0.9097690	-0.9836180
C	-3.5367080	0.1906040	0.3877030	H	-4.0186730	0.3580200	-1.7510340
H	-3.8166580	0.9424350	1.1382870	O	-4.0571700	2.2034230	-0.8134710
				H	-5.0034040	-0.9670570	2.3303970

H -4.1648200 2.6068100 -1.6823990

4AP'

C -0.7315460 0.5167200 -0.0000290

C -1.1688620 -0.8124460 0.0002680

C -0.2334680 -1.8422750 0.0006320

C 1.1174960 -1.5223460 0.0006000

C 1.5753200 -0.1716520 0.0001330

C 0.5982290 0.8682190 -0.0000720

C -1.9384640 1.4008860 -0.0004040

C -2.6397970 -0.8237450 0.0001250

H -0.5428040 -2.8810300 0.0010340

H 0.8828220 1.9105540 -0.0005110

N 2.9073820 0.1216890 -0.0002680

N -3.0229420 0.5317790 -0.0002200

H -3.9863530 0.8378250 -0.0005800

O -2.0012550 2.6146010 -0.0007870

O -3.4224640 -1.7562880 0.0002460

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C 3.3578600 1.5109510 0.0018280

H 4.4448230 1.5293180 0.0040810

H 3.0098910 2.0475930 -0.8869450

H 3.0063660 2.0458310 0.8902300

C 3.9017940 -0.9470670 -0.0019320

H 3.8138070 -1.5792150 0.8879100

H 3.8072140 -1.5819180 -0.8890720

H 4.8948660 -0.5047930 -0.0064310

d4AP'

O -4.6079190 1.2944050 -1.5799600

C -4.5710880 0.4696900 -0.4143720

H -5.5449050 -0.0193010 -0.3480020

H -4.4287280 1.0808150 0.4850610

C -3.4826880 -0.5849550 -0.4941330

H -3.6388590 -1.2138580 -1.3812400

O -2.2160210 0.0790960 -0.6045480

C -1.2343180 -0.8608200 -0.1638670

H -1.1511030 -1.6350370 -0.9389560

C 0.1688310 -0.2876600 -0.0116250

C 1.1691480 -1.2625730 -0.1357010

C 2.5067720 -0.9109690 -0.1262730

C 2.8678580 0.4310310 -0.0299440

C 1.9236710 1.4216460 0.1058600

C 0.5425720 1.0877200 0.1562140

N -0.3845560 2.1162700 0.3103960

C -1.3407010 2.0671100 1.4161340

H -2.2551580 2.5959190 1.1400860

H -1.5990750 1.0468080 1.6672110

H -0.9167490 2.5468330 2.3109300

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H 0.6448320 3.9325970 0.8073480

H 0.5803970 3.5218880 -0.9270500

H -0.8692280 4.0933890 -0.0952450

H 2.2386200 2.4503130 0.2076810

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N 4.7913870 -0.7980500 -0.2187780

C 3.7362640 -1.7234970 -0.2523400

O 3.8724280 -2.9264170 -0.3603660

H 5.7656170 -1.0621100 -0.2776870

O 5.0738840 1.4986990 -0.0385580

H 0.8839820 -2.2990290 -0.2803130
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H -1.6794540 -0.9485250 1.9818450
H -1.5082540 -2.5384200 1.2359760
C -3.3820800 -1.5210920 0.7333300
H -3.9721090 -1.1391890 1.5718800
O -3.8912200 -2.7991380 0.3381000
H -3.7375500 1.6998030 -1.6749420
H -4.0004350 -3.3426490 1.1266060

A

N -2.0759010 0.5800720 -0.0000030
C -2.2902110 -0.7768320 -0.0000290
N -1.1790430 -1.4752510 0.0000430
C -0.1767200 -0.5200070 -0.0000030
C 1.2312070 -0.6104440 -0.0000190
N 1.8855490 -1.7894720 -0.0000130
N 1.9448490 0.5326790 -0.0000110
C 1.2903360 1.7037740 0.0000030
N -0.0257450 1.9186930 0.0000120
C -0.7157550 0.7692690 0.0000130
H -3.2886500 -1.1871510 -0.0000420
H 2.8928730 -1.8035310 0.0000250
H 1.9190890 2.5891370 -0.0000030
H 1.3804090 -2.6601660 0.0000350
H -2.7848220 1.3000970 -0.0000050

dA

O 2.8430780 2.1575140 -0.2192190
C 3.5062220 1.4411030 0.8275580

H 3.2283240 1.8443580 1.8074060
H 4.5950400 1.5154060 0.7190420
C 3.1194830 -0.0287630 0.7771160
H 3.7107890 -0.5475680 1.5378990
O 1.7251690 -0.2065500 1.1149160
C 0.9899520 -0.7269360 0.0065870
H 0.6977160 -1.7577240 0.2142210
N -0.2600880 0.0106630 -0.1254420
C -0.4142750 1.3655840 -0.3472500
H 0.4483980 2.0039700 -0.4710280
N -1.6672840 1.7536630 -0.3576240
C -2.3882120 0.5946050 -0.1264480
C -3.7684840 0.3337850 -0.0139990
N -4.7082440 1.2932950 -0.1685880
H -5.6667830 1.0770450 0.0564990
H -4.4348250 2.2619560 -0.2114630
N -4.1630860 -0.9304230 0.2355680
C -3.2286590 -1.8839350 0.3624680
H -3.6049320 -2.8824000 0.5645420
N -1.9031350 -1.7625470 0.2740980
C -1.5335220 -0.4985770 0.0292920
C 3.3090250 -0.7136450 -0.5925810
H 4.0652360 -0.2062310 -1.1963600
C 1.9193480 -0.6294990 -1.2109180
H 1.7973450 0.3331660 -1.7060020
H 1.7407850 -1.4278800 -1.9305570
O 3.6386640 -2.1012680 -0.4491640
H 3.0908660 3.0862950 -0.1588630
H 4.5243380 -2.1728450 -0.0746250

G

N -1.7382870 -1.4985300 0.0006250
 C -2.7133150 -0.5241110 0.0007330
 N -2.2160860 0.6871440 0.0010120
 C -0.8441670 0.5014060 0.0007670
 C 0.2227980 1.4518440 0.0009370
 O 0.1787920 2.6803900 0.0004620
 N 1.4774720 0.7925330 0.0000220
 C 1.6780610 -0.5673850 -0.0006240
 N 2.9637760 -1.0041450 -0.0552310
 N 0.6897010 -1.4375640 0.0043460
 C -0.5299700 -0.8574930 0.0001210
 H -3.7624190 -0.7771200 0.0007310
 H 3.7160780 -0.3931090 0.2241780
 H 3.1053620 -1.9869810 0.1234580
 H 2.2799890 1.4106040 -0.0194850
 H -1.8858190 -2.4981480 0.0004000

dG

O 3.3701260 -1.9745460 0.1182170
 C 3.9066400 -1.1238910 -0.9005800
 H 3.6720880 -1.5175000 -1.8955100
 H 4.9965300 -1.0457530 -0.8069470
 C 3.3129050 0.2695300 -0.7766330
 H 3.8165210 0.9133990 -1.5026330
 O 1.9032940 0.2540080 -1.1033960
 C 1.1111760 0.6357910 0.0213410
 H 0.6915270 1.6293830 -0.1446260
 N -0.0325010 -0.2612550 0.1217280
 C -0.0038950 -1.6386040 0.2746940

H 0.9359580 -2.1656150 0.3465470

N -1.1971980 -2.1752000 0.2905180
 C -2.0654230 -1.1078940 0.1392180
 C -3.4917870 -1.0710850 0.0869950
 O -4.3042620 -1.9906010 0.1718020
 N -3.9509950 0.2586880 -0.0877150
 H -4.9588710 0.3577940 -0.1136150
 C -3.1621750 1.3786180 -0.1949850
 N -3.7956450 2.5762110 -0.3097660
 H -4.7472980 2.6119240 -0.6426690
 H -3.2127570 3.3600020 -0.5628350
 N -1.8471910 1.3350640 -0.1445690
 C -1.3587640 0.0877440 0.0252530
 C 3.4155920 0.9044000 0.6187310
 H 4.2342500 0.4748680 1.2009510
 C 2.0489670 0.6057970 1.2346860
 H 2.0605540 -0.3894410 1.6797880
 H 1.7589810 1.3298780 1.9968730
 O 3.6316240 2.3093050 0.4234020
 H 3.7476440 -2.8542590 0.0127730
 H 3.6839050 2.7330050 1.2880140

T

N -1.1145300 -1.2415790 -0.0000400
 C -1.6709170 0.0176820 0.0000120
 O -2.8761810 0.2239480 0.0001590
 N -0.7279530 1.0268750 -0.0000590
 C 0.6668070 0.8942930 -0.0003020
 O 1.3728330 1.8979040 0.0001790
 C 1.1561680 -0.4796510 -0.0000820

C 2.6374890 -0.7191170 0.0000410
C 0.2414720 -1.4762000 -0.0000580
H 2.8571020 -1.7876290 0.0001770
H 3.1071560 -0.2698770 0.8795200
H 3.1072590 -0.2700790 -0.8794850
H 0.5213260 -2.5217710 0.0000010
H -1.0923090 1.9723060 0.0000820
H -1.7624770 -2.0168820 0.0000230

dT

O -1.9123190 2.3561740 0.2551040
C -2.7654500 1.8331440 -0.7689380
H -2.4326080 2.1686500 -1.7570960
H -3.7995460 2.1662200 -0.6197620
C -2.7388850 0.3141050 -0.7309640
H -3.4697580 -0.0460180 -1.4617180
O -1.4387290 -0.1795870 -1.1294960
C -0.8483700 -0.9559900 -0.0881700
H -0.9030660 -2.0147610 -0.3332830
N 0.5855090 -0.6390420 -0.0260690
C 0.9851490 0.6765660 0.1249300
H 0.1672820 1.3836760 0.2009400
C 2.2771770 1.0741670 0.1578650
C 2.6884860 2.5084930 0.3244830
H 1.8136400 3.1548920 0.4066010
H 3.2999930 2.6397410 1.2217660
H 3.2889550 2.8460350 -0.5249660
C 3.3089770 0.0580110 0.0199710
O 4.5197880 0.2611680 0.0339860
N 2.8225710 -1.2423130 -0.1421530

H 3.5146480 -1.9752500 -0.2446040
C 1.5079520 -1.6645340 -0.1820090
O 1.2092940 -2.8410440 -0.3345010
C -3.0280550 -0.3157420 0.6507830
H -3.5798300 0.3702490 1.2975700
C -1.6352280 -0.6252010 1.1851970
H -1.2244800 0.2597140 1.6712200
H -1.6417620 -1.4526320 1.8941470
O -3.7332890 -1.5577520 0.5299470
H -4.6277310 -1.3789360 0.2173290
H -1.9307770 3.3181190 0.2101960

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O 2.2187720 -1.1809750 -0.0000240
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C -1.1391410 -0.2523390 0.0000260
N -2.3505570 -0.8429070 -0.0001360
C -1.0496930 1.1798640 -0.0000100
C 0.1990630 1.7078940 -0.0000150
H -3.2018610 -0.3059160 0.0005760
H -1.9279670 1.8083700 -0.0000420
H 0.3949490 2.7719230 -0.0000290
H -2.4119590 -1.8489920 0.0004510
H 2.2163000 1.2775940 -0.0000180

dC

O -2.0065910 2.4174480 0.3543250
C -2.8167890 1.7739440 -0.6370290

H	-2.5310640	2.2036120	-1.5995240	C	-2.2988900	0.9087830	-0.0087250
H	-3.8781470	1.9869640	-0.4732090	C	-3.4589920	1.6749410	-0.0057010
C	-2.6134230	0.2627030	-0.7074220	C	-4.6858800	1.0209540	0.0002110
H	-3.2959550	-0.1245260	-1.4722800	C	-4.7739340	-0.3909740	0.0044930
O	-1.2627460	-0.0309080	-1.1282690	C	-3.5838230	-1.1602590	0.0006740
C	-0.5860780	-0.8313620	-0.1565110	C	-0.9831900	-1.0245330	-0.0060300
H	-0.5206780	-1.8623270	-0.4967680	C	-0.8712000	1.2819960	-0.0103210
N	0.8011580	-0.3640650	-0.0479870	H	-3.4177500	2.7577790	-0.0059130
C	1.0471260	0.9618740	0.1591920	H	-3.6266120	-2.2433380	0.0033190
H	0.1734720	1.5970820	0.2439460	N	-5.9977000	-1.0108470	-0.0336320
C	2.3129530	1.4380390	0.2361790	H	-6.0500970	-1.9879060	0.2112380
H	2.5083540	2.4883180	0.3978000	H	-6.8161800	-0.4720230	0.2057250
C	3.3691500	0.4840220	0.0811290	N	-0.1579610	0.0825110	-0.0099380
N	4.6535000	0.8900590	0.1379410	H	0.8824020	0.0314550	-0.0077130
H	5.3937390	0.2156890	0.0229460	O	-0.6003310	-2.1837830	-0.0039660
H	4.8955520	1.8565250	0.2804670	O	-0.3443700	2.3857760	-0.0112340
N	3.1401620	-0.8095230	-0.1210270	H	-5.6026190	1.5998130	0.0025830
C	1.8699970	-1.2912640	-0.1867790	C	5.4065280	-0.2589660	0.0076830
O	1.6160090	-2.4877850	-0.3543090	H	6.4861270	-0.3816380	0.0101540
C	-2.8266490	-0.5095910	0.6139260	C	3.3536690	-1.2280440	-0.0024110
H	-3.4545470	0.0490360	1.3138130	N	2.5912790	-2.3507810	-0.0090110
C	-1.4073200	-0.7058580	1.1321800	H	1.5795690	-2.3146270	-0.0094820
H	-1.0919970	0.1712120	1.6994610	H	3.0522020	-3.2451010	-0.0114270
H	-1.3214010	-1.5865080	1.7682130	N	2.7043780	-0.0452350	0.0004890
O	-3.3895210	-1.8078880	0.3871960	C	3.4462850	1.0777760	0.0077860
H	-2.4974190	2.4722130	1.1808730	C	4.8586090	1.0057370	0.0118540
H	-4.2946610	-1.7045600	0.0710450	N	4.6884090	-1.3942220	0.0006030
				N	2.7921680	2.2616600	0.0118090
				H	3.3099970	3.1245410	0.0130580
4AP:DAP				H	1.7785070	2.3100160	0.0039370
C	-2.3816640	-0.4894500	-0.0051690				

H 5.4729500 1.8957300 0.0178200

A_4AP_A

N 4.2027390 1.6745450 0.1441550
C 4.7853280 1.0400990 1.2169980
H 5.2796540 1.6185230 1.9832240
N 4.6188690 -0.2468470 1.2218890
C 3.8759440 -0.4930350 0.0755310
C 3.3702650 -1.6747930 -0.4902210
N 3.5472120 -2.8882870 0.0514460
H 3.1599680 -3.7040660 -0.3999440
H 4.0675940 -2.9865880 0.9112530
N 2.6748410 -1.5642090 -1.6361800
C 2.5022810 -0.3552970 -2.1695540
H 1.9461210 -0.2433030 -3.0886110
N 2.9251630 0.8116030 -1.7343890
C 3.6191300 0.6728310 -0.5863520
N -4.3364530 1.3194360 -1.2393960
C -3.8065960 2.2824740 -0.4105330
H -3.8694280 3.3251200 -0.6864590
N -3.3162050 1.8147190 0.6951390
C -3.5287010 0.4468350 0.6045330
C -3.2300610 -0.6184710 1.4696490
N -2.6230520 -0.4608330 2.6539370
H -2.4336070 -1.2643290 3.2351280
H -2.3552370 0.4621660 2.9654600
N -3.5790160 -1.8556900 1.0708430
C -4.1820650 -2.0052600 -0.1071020
H -4.4710220 -2.9902040 -0.4445630
N -4.5101540 -1.0921840 -0.9943260

C -4.1494840 0.1369270 -0.5717070

C 0.3284050 0.1028170 0.5194070

C -0.3603590 0.0258920 -0.6956970

C -0.6088130 1.1804230 -1.4298890

C -0.1595490 2.3959130 -0.9273220

C 0.5367180 2.4777820 0.3028230

C 0.7836860 1.2936520 1.0391740

C 0.4486780 -1.2824330 1.0721260

C -0.6983330 -1.3857850 -0.9557610

H -1.1389730 1.1430830 -2.3746670

H 1.3150780 1.3316790 1.9840420

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H 1.6220050 3.7133160 1.5326570

H 0.9591980 4.4840640 0.1717660

N -0.1834890 -2.0996640 0.1407450

H -0.2654550 -3.1025370 0.2396930

O 0.9740060 -1.6545950 2.1020320

O -1.2894940 -1.8923370 -1.8899620

H -4.7642760 1.4532920 -2.1332910

H -0.3442880 3.2912210 -1.4833770

H 4.2047600 2.6538010 -0.0584610

G_4AP_G

N -4.4962570 1.3436470 -0.0895270

C -4.9874150 0.8007040 -1.2565540

H -5.5677280 1.4109890 -1.9331340

N -4.6831420 -0.4628360 -1.4265700

C -3.9372070 -0.7800410 -0.2923900

C -3.3307380 -2.0044550 0.0897240

O -3.3253970 -3.0788500 -0.5041520

N	-2.6687810	-1.8850210	1.3199460	C	0.7389340	-1.1931770	0.4521310
H	-2.2064900	-2.6986760	1.6738340	H	0.7590460	1.1440100	2.2238630
C	-2.6023580	-0.7341750	2.0809240	H	-1.4430400	1.6453490	-2.2422090
N	-1.9210000	-0.8271870	3.2251240	N	-1.4417190	3.8461290	-0.7285590
H	-1.4630260	-1.6479760	3.5942260	H	-2.0869310	3.8833150	-1.5029140
H	-1.8750990	0.0072190	3.7916110	H	-1.6112230	4.5290200	-0.0058180
N	-3.1718190	0.4137670	1.7211110	N	0.3866530	-1.8022690	-0.7657190
C	-3.8175430	0.3164390	0.5301170	H	0.6054060	-2.7632100	-0.9910070
N	4.0061930	1.6719390	1.5100620	O	-0.7048930	-1.2288380	-2.7310340
C	3.3932220	2.6792180	0.7973290	O	1.3371830	-1.7507070	1.3523760
H	3.2964280	3.6641950	1.2291320	H	4.3991970	1.7299640	2.4277660
N	2.9700590	2.3121750	-0.3889300	H	-0.2590460	3.2828840	1.5688800
C	3.3288780	0.9674310	-0.4666440	H	-4.6081740	2.2818930	0.2378390
C	3.1352140	0.0297730	-1.5142460				
O	2.6003770	0.1949700	-2.6068050	C_4AP_C			
N	3.6541070	-1.2285390	-1.1770240	N	3.7838310	1.6571120	-0.5350850
H	3.5672770	-1.9588510	-1.8549340	C	4.5808010	1.2161250	0.4746580
C	4.2771080	-1.5389000	0.0157190	H	5.0937230	1.9262420	1.1054660
N	4.7037250	-2.7978060	0.1440060	C	4.7460570	-0.1110460	0.7077620
H	4.6084680	-3.5436750	-0.5304450	H	5.3888930	-0.4459820	1.5213700
H	5.1525830	-3.0347950	1.0170680	C	4.0432920	-1.0128210	-0.1563730
N	4.4584770	-0.6584890	0.9982170	N	4.1582500	-2.3213220	0.0141660
C	3.9616250	0.5671400	0.6870920	H	3.6474850	-2.9235240	-0.6157610
C	-0.3890290	0.3517270	-0.8848990	H	4.7404290	-2.6894520	0.7530080
C	0.2336180	0.1889790	0.3578200	N	3.2609740	-0.5678230	-1.1472410
C	0.2845120	1.2499600	1.2554780	C	3.1098900	0.7640160	-1.3637810
C	-0.2918290	2.4593900	0.8864710	O	2.3961380	1.2130660	-2.2699250
C	-0.9210460	2.6285670	-0.3697430	N	-4.7984080	0.5888350	-0.9376520
C	-0.9663610	1.5395830	-1.2744350	C	-4.3410920	1.6738980	-0.2571870
C	-0.2931320	-0.9453020	-1.6241940	H	-4.5638060	2.6678810	-0.6153320

C	-3.6038140	1.5322050	0.8732760	T_4AP_T			
H	-3.2462150	2.4141800	1.4044600	N	3.7192150	1.5607420	-1.0397130
C	-3.3353610	0.1946510	1.3092290	C	4.5674250	1.4095580	0.0242680
N	-2.6228520	-0.0185260	2.4041170	H	5.0322150	2.2760530	0.4700760
H	-2.4560480	-0.9759700	2.6765190	C	4.7968610	0.2027690	0.5680910
H	-2.2648690	0.7607050	2.9383960	C	5.7237020	0.0261430	1.7348320
N	-3.7909980	-0.8675890	0.6314590	H	5.3604500	0.6110840	2.5794370
C	-4.5261500	-0.7037580	-0.4974630	H	5.7628110	-1.0270990	2.0129730
O	-4.9632500	-1.6602940	-1.1502510	H	6.7225300	0.3654860	1.4607340
C	0.4993190	-0.2575750	0.5723890	C	4.1519880	-0.9767280	0.0436410
C	-0.3863590	-0.4382020	-0.4960100	O	4.2994530	-2.1227470	0.4750150
C	-0.9115030	0.6654980	-1.1594360	N	3.3155140	-0.7331600	-1.0263860
C	-0.5370110	1.9346580	-0.7351190	H	2.8509050	-1.5153500	-1.4167920
C	0.3570800	2.1216730	0.3457290	C	3.0615340	0.4946900	-1.6058180
C	0.8850670	0.9888840	1.0123810	O	2.3037210	0.6108540	-2.5524490
C	0.8957400	-1.6083700	1.0785910	N	-4.8193470	0.1400530	-0.8588820
C	-0.5816010	-1.8849530	-0.7042980	C	-4.3872860	1.3843330	-0.4805600
H	-1.5962640	0.5475250	-1.9909170	H	-4.6982260	2.2547260	-1.0385790
H	1.5717110	1.1072970	1.8427380	C	-3.6227170	1.5556380	0.6099280
N	0.6748590	3.3854470	0.7749110	C	-3.1457350	2.9135380	1.0327190
H	1.4818370	3.5024400	1.3685490	H	-4.0043790	3.5554040	1.2305180
H	0.4868930	4.1636440	0.1613100	H	-2.5439840	2.8219550	1.9370870
N	0.2136820	-2.5122360	0.2715570	H	-2.5412900	3.3510500	0.2381160
H	0.2812750	-3.5157700	0.3733670	C	-3.2310580	0.4274680	1.4208220
O	1.6449810	-1.8956400	1.9902640	O	-2.5335720	0.4857950	2.4364690
O	-1.2644590	-2.4757780	-1.5190460	N	-3.7088540	-0.7852850	0.9685430
H	3.6799560	2.6403250	-0.6850960	H	-3.4651350	-1.5866120	1.4963470
H	-0.9344170	2.7914720	-1.2379500	C	-4.4955330	-0.9909730	-0.1485520
H	-5.3393490	0.7215630	-1.7681730	O	-4.8703550	-2.1052180	-0.4698440
				C	0.2177110	-0.4516850	0.3323640

C	-0.6604070	-0.6599890	-0.7372370	H	1.4531590	3.2844450	0.8342860
C	-1.0939150	0.4174220	-1.5022980	H	0.5286650	3.9087250	-0.4463840
C	-0.6367990	1.6887280	-1.1769020	N	-0.2234050	-2.6982500	0.2142600
C	0.2499550	1.9038490	-0.0952390	H	-0.2295320	-3.6917870	0.4009750
C	0.6841620	0.7976000	0.6755290	O	1.2190440	-2.0395640	1.9078460
C	0.5078250	-1.7790410	0.9584620	O	-1.6646190	-2.7106680	-1.6065200
C	-0.9551240	-2.1020030	-0.8284910	H	-5.3877230	0.0523960	-1.6769690
H	-1.7711860	0.2774580	-2.3364980	H	-0.9633010	2.5254510	-1.7584440
H	1.3633630	0.9377750	1.5086160	H	3.5735600	2.4753760	-1.4168460
N	0.6500450	3.1741780	0.2341560				

Cartesian coordinates for fluorescence geometries involved in this study calculated at the TD-B3LYP/6-311++G(d,p) level.

				H	-3.3129660	0.5582980	-0.0001680
				O	-1.5826240	2.5921980	0.0001030
4AP				O	-2.5077040	-1.9908550	-0.0001970
C	-0.0823590	0.6471220	0.0000160	H	2.7603060	-2.0247420	0.0005520
C	-0.3763020	-0.7684730	-0.0000740				
C	0.6334060	-1.7346640	0.0001010	d4AP			
C	1.9436200	-1.3137030	0.0002330	O	-4.7272240	-1.7979320	1.2161540
C	2.2539630	0.0996580	-0.0000480	C	-4.5478050	-0.9610330	0.0752340
C	1.2372230	1.0809440	-0.0000100	H	-5.5035430	-0.5373790	-0.2547660
C	-1.3293700	1.3677890	0.0000800	H	-4.1719400	-1.6090620	-0.7200260
C	-1.8393590	-0.9450740	-0.0000430	C	-3.5775710	0.1848740	0.3119600
H	0.3882040	-2.7894540	0.0001850	H	-3.9241580	0.8046330	1.1477860
H	1.4947170	2.1333450	0.0000640	O	-2.2717180	-0.3339220	0.6431260
N	3.5544390	0.4459750	-0.0001200	C	-1.3067660	0.6427670	0.2114060
H	3.8427180	1.4148830	-0.0011940	H	-1.3303060	1.4918150	0.9050720
H	4.2856080	-0.2521290	0.0002620	C	0.1001370	0.1091780	0.1846710
N	-2.3231380	0.3465200	0.0000500				

C 1.1359180 0.9976300 0.4324370
 C 2.4547220 0.5931210 0.2630980
 C 2.7957110 -0.7428550 -0.1642020
 C 1.7846890 -1.6652910 -0.3842510
 C 0.4413880 -1.2598470 -0.2021040
 N -0.5564490 -2.1445730 -0.3716210
 H -0.3616330 -3.0971200 -0.6478290
 H -1.5035380 -1.8789920 -0.1092070
 H 1.9979610 -2.6914220 -0.6596090
 C 4.2299320 -0.8420670 -0.2446250
 N 4.6902650 0.4512420 0.1384940
 C 3.7004590 1.3576130 0.4556460
 O 3.8572090 2.5366540 0.8104710
 H 5.6744260 0.6848700 0.1725270
 O 4.9837960 -1.7902010 -0.5576930
 H 0.9169780 2.0136660 0.7410260
 C -1.8628500 1.0965310 -1.1555540
 H -1.6043790 0.3636500 -1.9235650
 H -1.4862340 2.0724250 -1.4622680
 C -3.3840880 1.1119260 -0.9135430
 H -3.9220790 0.7370260 -1.7891290
 O -3.8901530 2.3996210 -0.5545990
 H -5.1879930 -1.2964990 1.8989310
 H -3.9287990 2.9466580 -1.3477790

4AP'

C -0.7469340 0.5810250 -0.0000640
 C -1.1603610 -0.7919920 0.0003140
 C -0.2334720 -1.8287880 0.0006840
 C 1.1144930 -1.5170470 0.0005030

C 1.5527370 -0.1484180 0.0000470
 C 0.6123810 0.9035480 -0.0001730
 C -1.9223270 1.4105450 -0.0004810
 C -2.6375610 -0.8398370 0.0001660
 H -0.5570380 -2.8626070 0.0011120
 H 0.9207970 1.9382640 -0.0007820
 N 2.9047280 0.1118870 0.0000000
 N -3.0085260 0.4860800 -0.0003440
 H -3.9746870 0.7852670 -0.0005840
 O -2.0646660 2.6542270 -0.0009660
 O -3.3933380 -1.8236110 0.0003850
 H 1.8397750 -2.3164870 0.0010460
 C 3.3815710 1.4884390 0.0021870
 H 4.4664830 1.4939310 0.0043720
 H 3.0216290 2.0178670 -0.8853280
 H 3.0179600 2.0163110 0.8890560
 C 3.9011400 -0.9602740 -0.0021480
 H 3.8011720 -1.5838070 0.8891360
 H 3.7937090 -1.5871200 -0.8900850
 H 4.8908140 -0.5155190 -0.0071070

d4AP'

O -4.6744680 1.1373240 -1.6039870
 C -4.4478410 0.5363550 -0.3285650
 H -5.4082150 0.1253080 -0.0117890
 H -4.1353900 1.2876690 0.4066600
 C -3.4276900 -0.5839610 -0.3786560
 H -3.6996810 -1.2908570 -1.1735760
 O -2.1304790 -0.0378230 -0.6720200
 C -1.1676050 -1.0158530 -0.2355190

H -1.1711740 -1.8473340 -0.9510900
C 0.2254460 -0.4431600 -0.1935830
C 1.3007600 -1.2935810 -0.4146290
C 2.6126530 -0.8365690 -0.2680620
C 2.8673040 0.5221260 0.1037310
C 1.8013380 1.4001070 0.3035790
C 0.5130920 0.9185200 0.1555850
N -0.5579270 1.8715040 0.3106240
C -1.0205510 2.2293040 1.6356030
H -2.0365010 2.6129480 1.5850560
H -0.9497650 1.3716830 2.2971980
H -0.3642740 3.0191260 2.0186290
C -0.8971850 2.7215030 -0.8131490
H -0.1041940 3.4696540 -0.9188970
H -0.9278560 2.1195990 -1.7174130
H -1.8439990 3.2237300 -0.6339380
H 1.9753130 2.4403560 0.5547770
C 4.2957880 0.7263970 0.1794660
N 4.8405980 -0.5249510 -0.1495990
C 3.8830190 -1.5109320 -0.4321090
O 4.1542110 -2.6864310 -0.7450490
H 5.8348450 -0.6999510 -0.1800940
O 4.9689260 1.7371720 0.4610800
H 1.1115520 -2.3252920 -0.6928110
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4AP:DAP

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C	3.2339300	0.3862480	-1.3653570	N	0.2137330	-2.6211160	-0.2238950
O	2.5356180	0.4502830	-2.3800930	H	0.2153940	-3.6206410	-0.3837600
N	3.7075800	-0.8296670	-0.9172290	O	-1.2717070	-2.0845960	-1.9837380
H	3.4602690	-1.6284690	-1.4471840	O	1.6816610	-2.5986050	1.6042370
C	4.4946300	-1.0417050	0.1984170	H	0.9981910	2.6249890	1.6001920