Supporting Information

Search a maximum of the D-π-A paradigm for second order nonlinear optical molecular materials

Cui-Cui Yang,[#ab] Xiao Su,[#b] Qi-Zheng Zheng,[b] Jiu Chen,[b] Wei Quan Tian,*[b] Wei-Qi Li,*[cde] Ling Yang*[f]

[a]College of Science, Chongqing University of Technology, Chongqing 400054, P. R. China

[b]Chongqing Key Laboratory of Theoretical and Computational Chemistry, College of Chemistry and Chemical Engineering, Chongqing University, Huxi Campus, Chongqing 401331, P. R. China

[c]School of Physics, Harbin Institute of Technology, Harbin 150001 P. R. China

[d]Technology Innovation Center of Materials and Devices at Extreme Environment, School of Materials Science and Engineering, Harbin Institute of Technology, Harbin 150001, China

[e]Collaborative Innovation Center of Extreme Optics, Shanxi University, Taiyuan 030006, P. R. China

[f]Wenzhou Institute, University of Chinese Academy of Sciences, 1 Jinlian Street, Wenzhou 325001, China

*Corresponding author: tianwq@cqu.edu.cn; tccliweiqi@hit.edu.cn; lyang@ucas.ac.cn

[#]C. C. Yang and X. Su contributed equally to this work.

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Fig. S1 Structure, frontier molecular orbitals and natural bond orbital (NBO) analysis of styrene.

Fig. S2 Structures of Da(Baz/Baz(r))Ac and D7Bb(n)A4 series of molecules predicted with B3LYP/6-31G(d,p).

Fig. S3 Evolution of the static first hyperpolarizability (<β_0>) with the numbers of excited states in D7BazA4.

Fig. S4 Evolution of the static first hyperpolarizability (<β_0>) [predicted with TD-CAM-B3LYP/6-31++G(d,p)-SOS] with the electron excitations and the transitional nature of the electron excitations with major contributions to the <β_0> of D7Bst(n=11)A4, D7(Betc/Betc')(n=11)A4 and D7Beae(n=11)A4, and the corresponding real space representation of electron (transparent cyan) and hole (transparent yellow) distributions of transition from ground state (S_0) to excited states (S_e) of these four molecules based on the electronic wavefunction predicted by using CAM-B3LYP/6–31++G(d,p) (plotted with isosurface value of 0.0005 a.u.). *f* is the oscillator strength (in a.u.). The red numbers are the distance ($D_{hole\text{-}ele}$, in Å) between the center of mass of hole (yellow sphere) and electron (cyan sphere).

Fig. S5 Hyperpolarizability density [$\rho_{xx}^{(2)}(\vec{r})$] (isovalue = 0.05 au) of (a) D7Bet(n=16)A4 and (b) D7Beta(n=11)A4. Blue and yellow colors indicate negative and positive spatial contributions,

respectively.

Fig. S6 Evolution of the static first hyperpolarizability (<β_0>) [predicted with TD-CAM-B3LYP/6-31++G(d,p)-SOS] with the electron excitations and the transitional nature of the electron excitations with major contributions to the <β_0> of D7Beta(r)(n=11)A4, D7Baet(n=11)A4 and D7Ba(r)et(n=11)A4, and the corresponding real space representation of electron (transparent cyan) and hole (transparent yellow) distributions of transition from ground state (S_0) to excited states (S_e) of these three molecules based on the electronic wavefunction predicted by using CAM-B3LYP/6–31++G(d,p) (plotted with isosurface value of 0.0005 a.u.). *f* is the oscillator strength (in a.u.). The red numbers are the distance ($D_{hole\text{-}ele}$, in Å) between the center of mass of hole (yellow sphere) and electron (cyan sphere).

Fig. S7 Evolution of the static first hyperpolarizability (<β_0>) with the electron excitation and the transition nature of the electron excitations with major contributions to the <β_0> of D7Baze(n=4)A4 and D7Bst(n=13)A4. *f* is the oscillator strength in a.u. unit.

Fig. S8 The static first hyperpolarizability per heavy atom (<β_0>/N), and the frequency-dependent first hyperpolarizability per heavy atom in the process of second harmonic generation (SHG) [$\beta(-2\omega; \omega, \omega)$] and electro-optical Pockels effect (EOPE) [$\beta(-\omega; \omega, 0)$] of D7Bet(n=16)A4 and D7Beta(n=11)A4 at 1064 nm predicted by using TD-CAM-B3LYP/6-31++G(d,p)-SOS, respectively.

Fig. S9 The contour plot of predicted two-dimensional second order nonlinear optical spectra (in 10^{-30} esu) of D7Bet(n=16) A4 and D7Beta(n=11)A4 in external fields up to 7.00 eV with a scanning step size of 0.05 eV.

Fig. S10 Two-dimensional second order NLO spectra of (a/b/c) D7Bet(n=16)A4 and (d/e) D7Beta(n=11)A4 with a step size of 0.005 eV. [(a) ω_1 scanned from 1.20 eV to 2.20 eV and ω_2 scanned from −0.50 eV to 0.50 eV; (b) ω_1 scanned from 1.90 eV to 2.90 eV and ω_2 scanned from −2.20 eV to −1.20 eV; (c) ω_1 scanned from 1.15 eV to 2.15 eV and ω_2 scanned from 0.30 eV to 1.30 eV; (d) ω_1 scanned from 1.15 eV to 2.15 eV and ω_2 scanned from 0.20 eV to 1.20 eV; (e) ω_1 scanned from 1.85 eV to 2.85 eV and ω_2 scanned from −2.15 eV to −1.15 eV].

Table S1 The electronic properties of styrene, different donors (D1 to D8) doped benzene, and different acceptors (A1 to A8) doped ethylene predicted with B3LYP/6-31G(d,p).

Table S2 The electronic properties [predicted with B3LYP/6-31G(d,p)] and static first hyperpolarizability per heavy atom (<β_0>/N, N is the numbers of heavy atoms) of D8(Baz/Baz(r))A4, D7(Baz/Baz(r))A4 and D7Bb(n)A4 predicted with using TD-CAM-B3LYP/6-31++G(d,p)-SOS.

Table S3 The electronic properties of DaAc, DaBaz(r)Ac and DaBazAc series of molecules predicted

with B3LYP/6-31G(d,p).

Table S4 The static first hyperpolarizability (<β_0>, in 10^{-30} esu), and the <β_0>/N (N is the numbers of heavy atoms) of DaAc, DaBaz(r)Ac and DaBazAc series of molecules predicted with using TD-CAM-B3LYP/6-31++G(d,p)-SOS and CAM-B3LYP/6-31++G(d,p)-CPKS (in brackets), respectively.

Table S5 The electronic properties [predicted with B3LYP/6-31G(d,p)] and static first hyperpolarizability (<β_0>) (×10^{-30} esu) [predicted with TD-CAM-B3LYP/6-31++G(d,p)-SOS] of D7Bb(n)A4 series of molecules.

Table S6 Major electronic excitations with transitional nature of D8(Baz/Baz(r))A4, D7(Baz/Baz(r))A4, Exp, BAY1 and D7Bb(n)A4 series of molecules. *f* is the oscillator strength in a.u. unit; E_t is the transition energy in eV (nm) unit; $<\beta_0>_{con}$ (contribution value to <β_0>) and $<\beta_0>_{total}$ are in 10^{-30} esu unit.

Table S7 Predicted major β_{ijk} [i, j, k∈(x, y, z)] (×10^{-30} esu) of D8(Baz/Baz(r))A4, D7(Baz/Baz(r))A4 and D7Bb(n)A4 series of molecules, and properties of the related states with important contributions to the β_{ijk} according to the SOS model. E_t is the transition energy in eV unit; m is the state number (m=0 is the ground state, m>0 is the mth excited state).

Table S8 Calculated electronic properties [predicted with B3LYP/6-31G(d,p)] and static first hyperpolarizability (<β_0>) (in 10^{-30} esu) and <β_0> per heavy atom (<β_0>/N) [predicted with TD-CAM-B3LYP/6-31++G(d,p)-SOS] for the experimentally and recently reported NLO molecules Exp and BAY1, respectively.

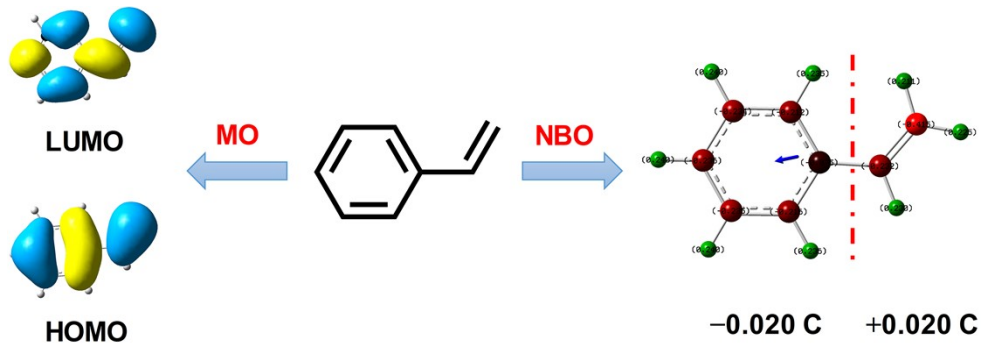


Fig. S1 Structure, frontier molecular orbitals and natural bond orbital (NBO) analysis of styrene.

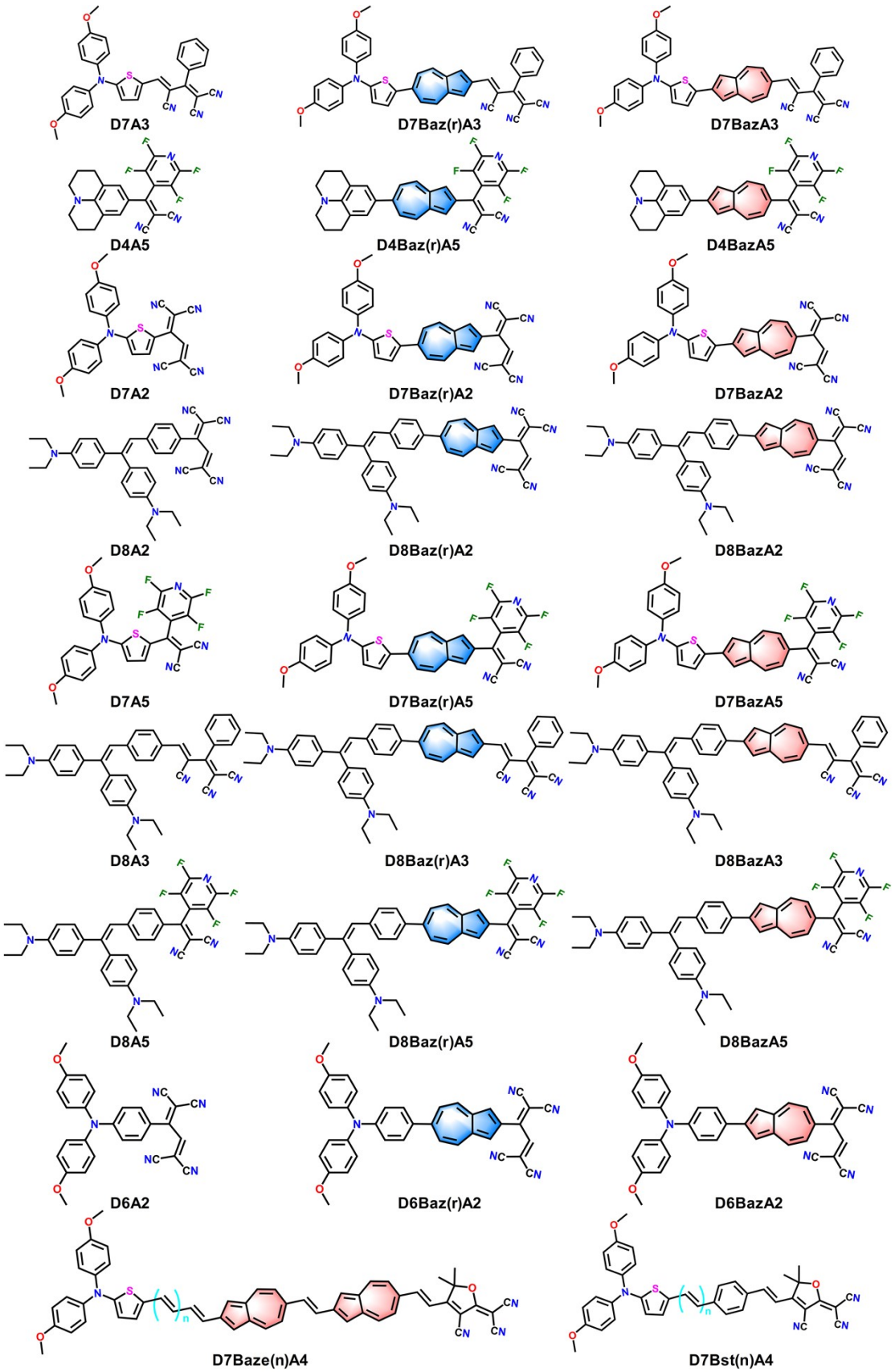


Fig. S2 Structures of Da(Baz/Baz(r))Ac and D7Bb(n)A4 series of molecules predicted with B3LYP/6-31G(d,p).

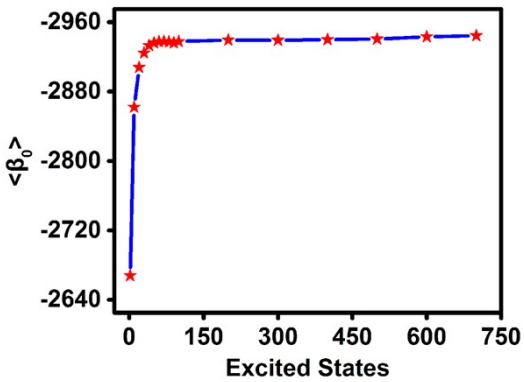
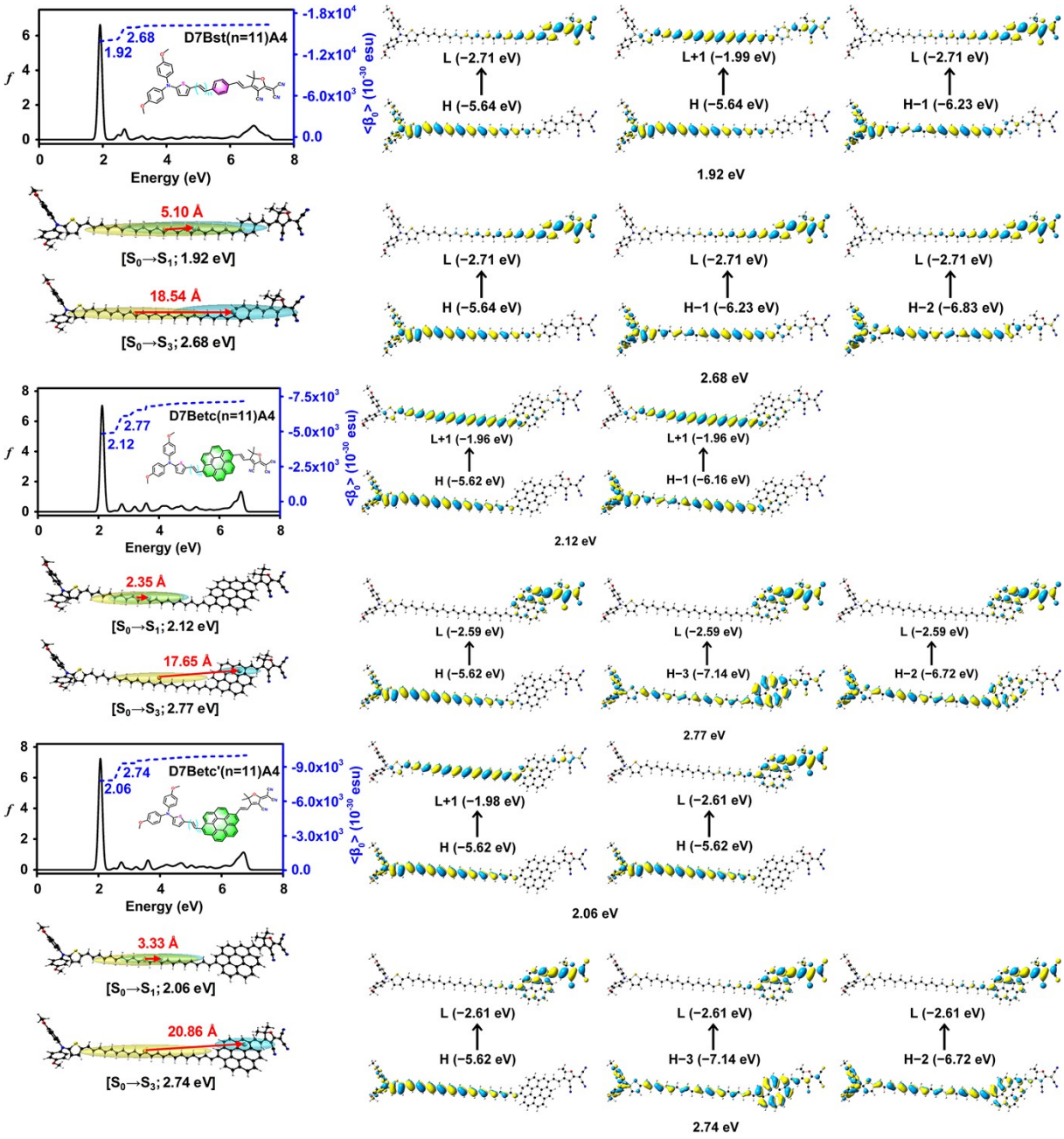


Fig. S3 Evolution of the static first hyperpolarizability (<β_0>) with the numbers of excited states in D7BazA4.



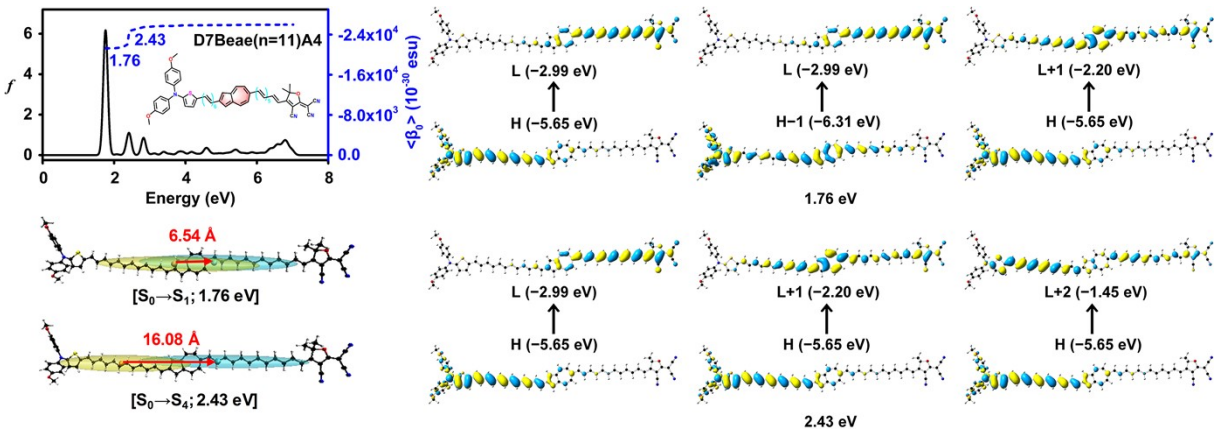
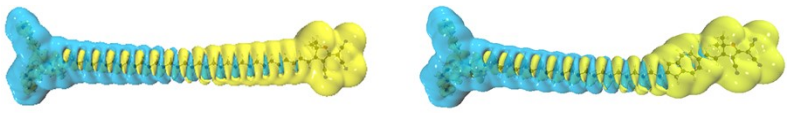


Fig. S4 Evolution of the static first hyperpolarizability (<β_0>) [predicted with TD-CAM-B3LYP/6-31++G(d,p)-SOS] with the electron excitations and the transitional nature of the electron excitations with major contributions to the <β_0> of D7Bst(n=11)A4, D7(Betc/Betc')(n=11)A4 and D7Beae(n=11)A4, and the corresponding real space representation of electron (transparent cyan) and hole (transparent yellow) distributions of transition from ground state (S_0) to excited states (S_e) of these four molecules based on the electronic wavefunction predicted by using CAM-B3LYP/6–31++G(d,p) (plotted with isosurface value of 0.0005 a.u.). *f* is the oscillator strength (in a.u.). The red numbers are the distance ($D_{hole\text{-}ele}$, in Å) between the center of mass of hole (yellow sphere) and electron (cyan sphere).



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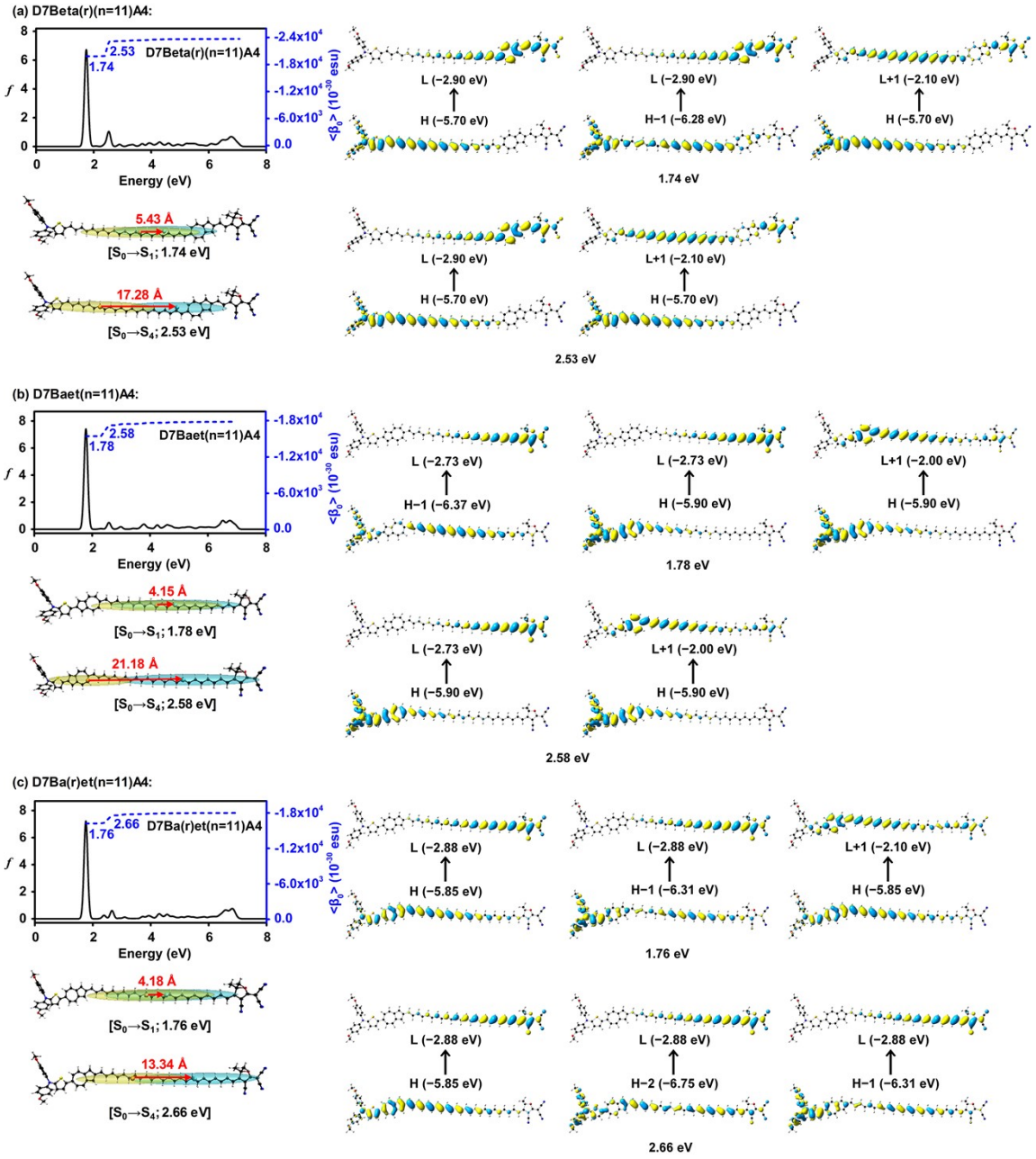

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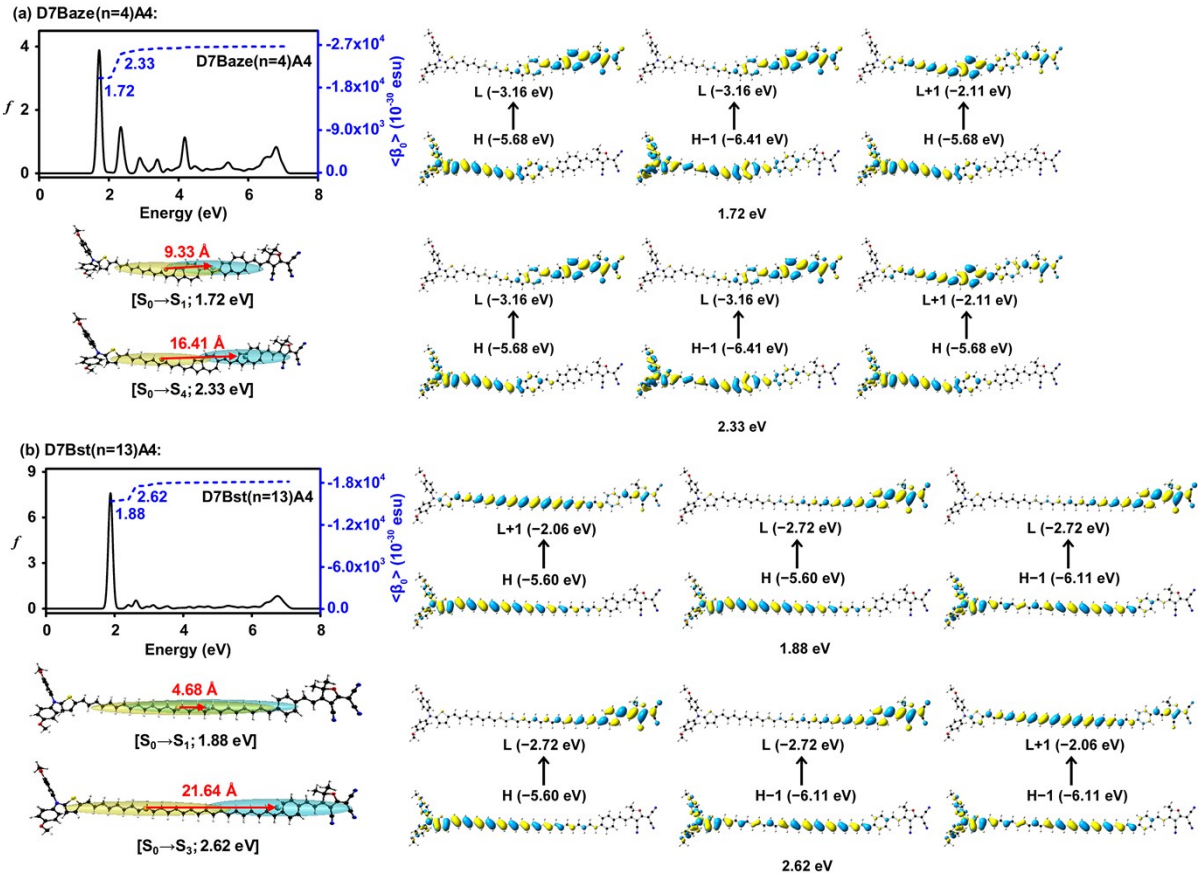

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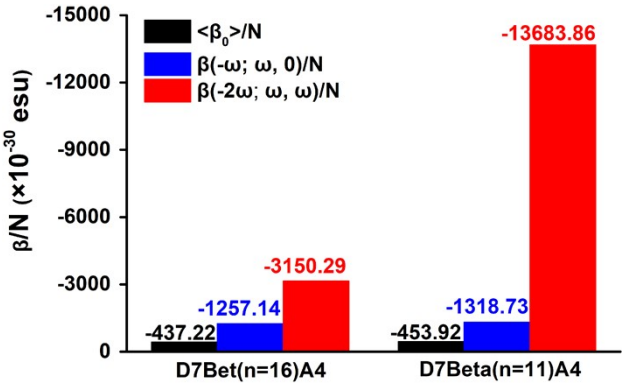

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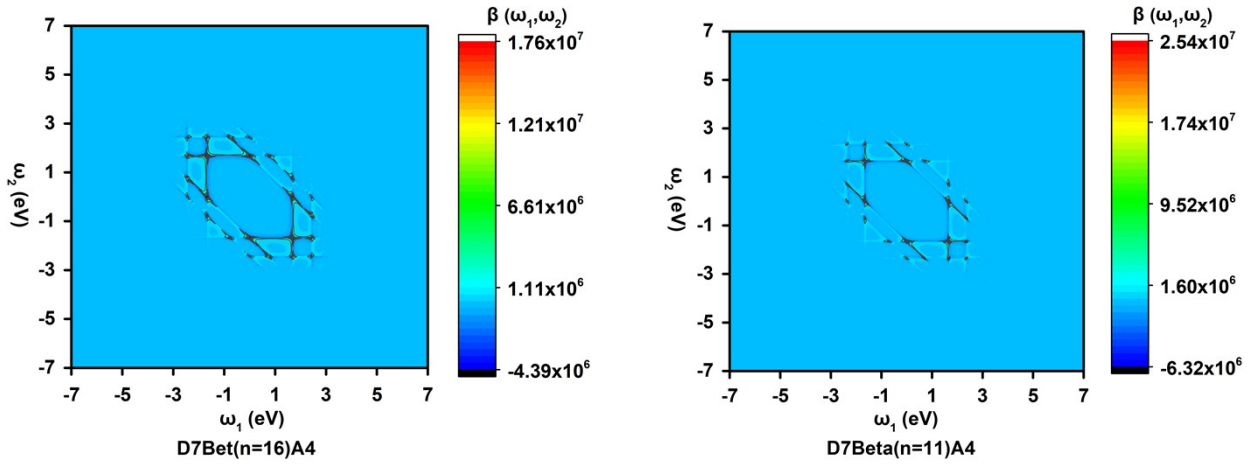

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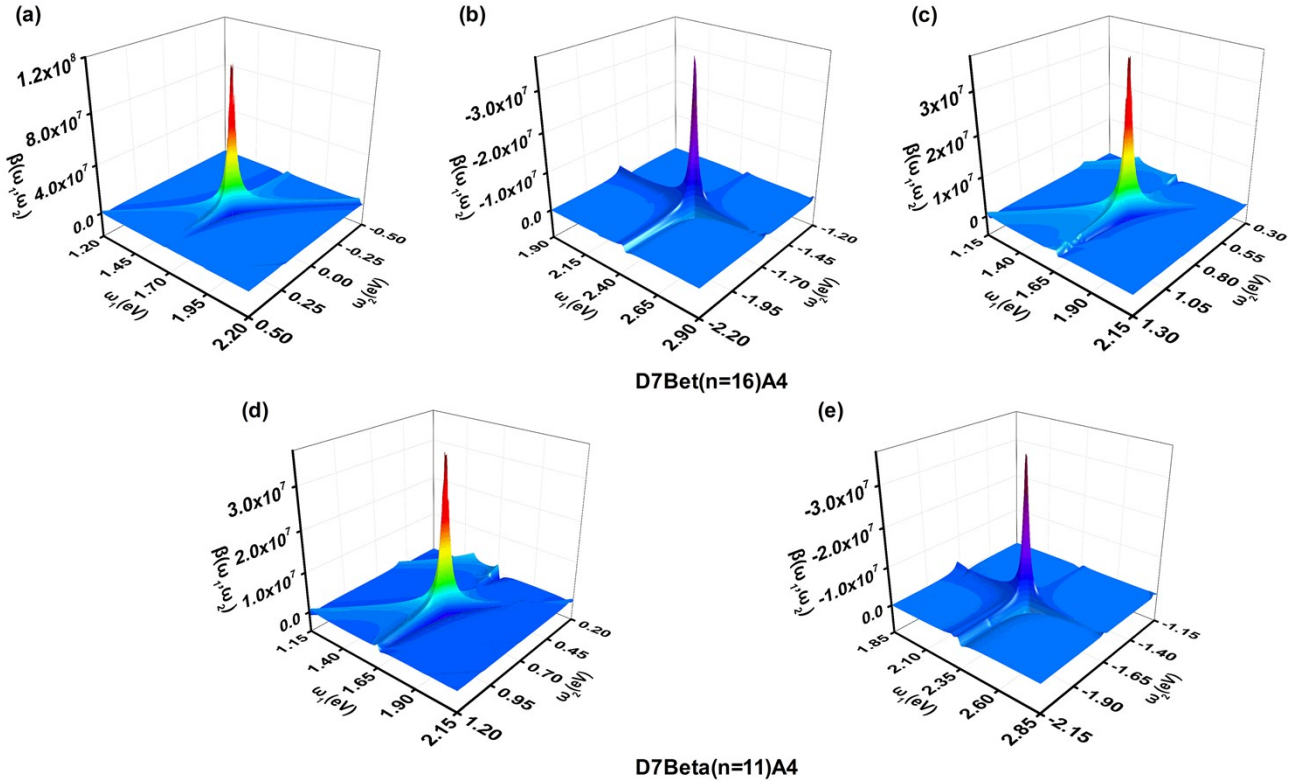

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Table S1 The electronic properties of styrene, different donors (D1 to D8) doped benzene, and different acceptors (A1 to A8) doped ethylene predicted with B3LYP/6-31G(d,p).

Compounds	BL (phenyl)	D_g (B3LYP)	NBO (phenyl)	NBO (donors)	Δq	E_{HOMO}	E_{LUMO}	E_{gap} (B3LYP)	IP (donor)
styrene (C_8H_8)	1.407	0.19	−0.020	0.020	0.040	−0.222	−0.031	5.19	10.38
D1 ($C_{18}H_{21}N_3$)	1.406	3.07	−0.010	0.009	0.019	−0.192	−0.039	4.17	7.02
D2 ($C_{16}H_{13}N$)	1.406	1.98	−0.002	0.002	0.004	−0.185	−0.056	3.52	6.92
D3 ($C_{14}H_{11}N$)	1.407	2.30	−0.020	0.020	0.040	−0.192	−0.014	4.85	7.43
D4 ($C_{18}H_{19}N$)	1.406	2.47	−0.026	0.024	0.050	−0.174	−0.010	4.47	6.59
D5 ($C_{24}H_{19}N$)	1.406	0.36	−0.006	0.011	0.017	−0.181	−0.028	4.16	6.42
D6 ($C_{26}H_{23}NO_2$)	1.406	2.60	−0.015	0.018	0.033	−0.169	−0.022	4.01	5.98
D7 ($C_{24}H_{21}NO_2S$)	1.408	2.69	−0.023	0.025	0.048	−0.168	−0.033	3.67	6.01
D8 ($C_{34}H_{38}N_2$)	1.406	3.71	−0.011	0.012	0.023	−0.168	−0.038	3.53	5.77
Compounds	**BL (ethenyl)**	**D_g (B3LYP)**	**NBO (acceptors)**	**NBO (ethenyl)**	**Δq**	**E_{HOMO}**	**E_{LUMO}**	**E_{gap} (B3LYP)**	**EA (acceptor)**
styrene (C_8H_8)	1.338	0.19	−0.020	0.020	0.040	−0.222	−0.031	5.19	−2.28
A1 ($C_{12}H_9NO_2$)	1.342	5.01	−0.107	0.059	0.166	−0.215	−0.114	2.73	1.31
A2 ($C_{10}H_4N_4$)	1.338	2.57	−0.128	0.127	0.255	−0.290	−0.165	3.40	2.87
A3 ($C_{15}H_9N_3$)	1.345	9.67	−0.100	0.100	0.200	−0.254	−0.123	3.58	1.64
A4 ($C_{14}H_{11}N_3O$)	1.344	12.29	−0.075	0.073	0.148	−0.242	−0.128	3.08	1.80
A5 ($C_{11}H_3F_4N_3$)	1.342	4.93	−0.618	0.135	0.753	−0.278	−0.129	4.08	1.89
A6 ($C_{14}H_7NO_5$)	1.338	3.23	−0.067	0.067	0.134	−0.256	−0.133	3.35	1.95
A7 ($C_{12}H_9N_3O_2$)	1.338	5.50	−0.057	0.058	0.115	−0.244	−0.102	3.87	1.02
A8 ($C_{11}H_6N_4O_2S$)	1.340	5.49	−0.080	0.082	0.162	−0.244	−0.128	3.17	1.77

BL is the bond length (in Å); D_g is the ground state dipole moment (in Debye); NBO is the charge of natural bond orbital analysis; Δq is the difference between positive and negative charge; E_{gap} is the energy gap between the highest occupied molecular orbital (E_{HOMO}) and the lowest unoccupied molecular orbital (E_{LUMO}) (in eV); EA is the electronic affinity. IP is the ionization potential.

Table S2 The electronic properties [predicted with B3LYP/6-31G(d,p)], static first hyperpolarizability per heavy atom (<β_0>/N, N is the numbers of heavy atoms) and β_{tot}/N of D8(Baz/Baz(r))A4, D7(Baz/Baz(r))A4 and D7Bb(n)A4 predicted with using TD-CAM-B3LYP/6-31++G(d,p)-SOS.

Compounds		ΔE_{OS-CS}	ΔE_{T-CS}	$<S^2>$	LVF	E_{gap}	D_g	<β_0>/N	β_{tot}/N
	D8A4	0.00	26.14	0.00	6.53	2.02	19.60	−28.27	29.93
D8(Baz/Baz(r))A4	D8Baz(r)A4	0.00	26.50	0.00	5.93	1.66	22.74	−41.41	43.46
	D8BazA4	0.00	21.67	0.00	5.77	1.45	21.08	−70.39	72.07
	D7A4	0.00	26.75	0.00	12.26	2.37	21.80	−12.09	12.48
D7(Baz/Baz(r))A4	D7Baz(r)A4	0.00	24.88	0.00	5.94	1.99	26.11	−27.74	29.20
	D7BazA4	0.00	20.17	0.00	4.56	1.68	23.61	−61.36	64.22
	D7Bet(n=16)A4	0.00	5.16	0.00	2.11	1.06	41.09	−437.22	440.28
	D7Beta(n=11)A4	0.00	7.54	0.00	2.42	1.01	35.66	−453.92	460.77
	D7Beta(r)(n=11)A4	0.00	8.69	0.00	1.98	1.14	39.27	−338.39	342.26
D7Bb(n)A4	D7Baet(n=11)A4	0.00	7.81	0.00	1.90	1.16	33.24	−254.71	258.43
	D7Ba(r)et(n=11)A4	0.00	8.10	0.00	2.04	1.28	37.26	−257.13	258.79
	D7Baze(n=4)A4	0.00	12.41	0.00	3.25	0.94	28.91	−381.34	397.10
	D7Bst(n=13)A4	0.00	7.66	0.00	2.04	1.13	32.46	−259.58	266.19

ΔE_{OS-CS} and ΔE_{T-CS} (in kcal/mol): the relative electronic energy differences between open-shell singlet (OS) or triplet (T) and closed-shell singlet (CS) (CS is taken as reference); $<S^2>$: the spin contamination of open-shell singlet obtained at UB3LYP/6-31G(d,p) level; LVF (in cm^{-1}): the lowest vibrational frequency; E_{gap} (in eV): the energy gap between the highest occupied molecular orbital and the lowest unoccupied molecular orbital; D_g (in Debye): the ground state dipole moment. <β_0>/N (in 10^{-30} esu): static first hyperpolarizability per heavy atom, N is the numbers of heavy atoms. β_{tot}/N is obtained through $[(\beta_{xxx}+\beta_{xyy}+\beta_{xzz})^2+(\beta_{yyy}+\beta_{yzz}+\beta_{yxx})^2+(\beta_{zzz}+\beta_{zxx}+\beta_{zyy})^2]^{1/2}$.

Table S3 The electronic properties of DaAc, DaBaz(r)Ac and DaBazAc series of molecules predicted with B3LYP/6-31G(d,p).

Compounds	D_g	E_{gap}	LVF	ΔE_{OS-CS}	ΔE_{T-CS}	$<S^2>$	Compounds	D_g	E_{gap}	LVF	ΔE_{OS-CS}	ΔE_{T-CS}	$<S^2>$
D7A3	17.31	2.61	8.92	0.00	30.91	0.00	D4A5	11.52	2.99	16.88	0.00	35.39	0.00
D7Baz(r)A3	21.12	2.08	7.56	0.00	27.15	0.00	D4Baz(r)A5	16.84	2.29	10.30	0.00	30.85	0.00
D7BazA3	18.90	1.79	6.72	0.00	21.76	0.00	D4BazA5	13.99	1.99	5.66	0.00	25.59	0.00
D7A2	13.30	2.07	11.58	0.00	22.15	0.00	D8A2	12.35	1.25	12.17	0.00	15.83	0.00
D7Baz(r)A2	18.80	1.70	7.66	0.00	24.28	0.00	D8Baz(r)A2	16.87	1.25	7.05	0.00	25.49	0.00
D7BazA2	15.09	1.16	8.46	0.00	18.75	0.00	D8BazA2	13.96	0.88	7.25	0.00	16.27	0.00
D7A5	13.83	2.78	9.34	0.00	31.95	0.00	D8A3	14.93	2.16	8.44	0.00	27.07	0.00
D7Baz(r)A5	19.61	2.13	6.62	0.00	28.11	0.00	D8Baz(r)A3	17.54	1.76	8.49	0.00	29.06	0.00
D7BazA5	15.41	1.82	6.94	0.00	23.05	0.00	D8BazA3	15.93	1.57	5.65	0.00	23.25	0.00
D8A5	13.45	2.19	6.87	0.00	27.87	0.00	D6A2	10.20	1.60	14.17	0.00	21.87	0.00
D8Baz(r)A5	17.86	1.74	5.21	0.00	30.49	0.00	D6Baz(r)A2	15.68	1.51	9.29	0.00	25.97	0.00
D8BazA5	14.28	1.59	7.26	0.00	24.68	0.00	D6BazA2	12.70	1.08	7.80	0.00	20.93	0.00

Table S4 The static first hyperpolarizability (<β_0>, in 10^{-30} esu), and the <β_0>/N (N is the numbers of heavy atoms) of DaAc, DaBaz(r)Ac and DaBazAc series of molecules predicted with using TD-CAM-B3LYP/6-31++G(d,p)-SOS and CAM-B3LYP/6-31++G(d,p)-CPKS (in brackets), respectively.

Compounds	<β_0>	<β_0>/N	Compounds	<β_0>	<β_0>/N	Compounds	<β_0>	<β_0>/N
D7A3	−253.62 (171.84)	−6.67 (4.52)	D8A4	−1300.31 (604.32)	−28.27 (13.14)	D4A5	−143.95 (58.69)	−4.96 (2.02)
D7Baz(r)A3	−1083.80 (692.89)	−22.58 (14.44)	D8Baz(r)A4	−2318.99 (826.45)	−41.41 (14.76)	D4Baz(r)A5	−787.49 (329.74)	−20.19 (8.45)
D7BazA3	−2001.68 (1139.16)	−41.70 (23.73)	D8BazA4	−3941.89 (1627.32)	−70.39 (29.06)	D4BazA5	−1161.22 (525.67)	−29.77 (13.48)
D7A2	−288.71 (126.63)	−8.49 (3.72)	D8A2	−1107.13 (458.99)	−26.36 (10.93)	D7A4	−459.49 (284.96)	−12.09 (7.50)
D7Baz(r)A2	−1567.34 (624.91)	−35.62 (14.20)	D8Baz(r)A2	−2534.99 (676.68)	−48.75 (13.01)	D7Baz(r)A4	−1331.47 (914.58)	−27.74 (19.05)
D7BazA2	−2444.51 (1072.44)	−55.56 (24.37)	D8BazA2	—	—	D7BazA4	−2945.31 (1567.86)	−61.36 (32.66)
D7A5	−180.01 (93.82)	−4.74 (2.47)	D8A3	−838.99 (433.95)	−18.24 (9.43)	D8A5	−755.85 (310.18)	−16.43 (6.74)
D7Baz(r)A5	−1005.58 (545.24)	−20.95 (11.36)	D8Baz(r)A3	−1844.29 (678.70)	−32.93 (12.12)	D8Baz(r)A5	−1957.93 (636.52)	−34.96 (11.37)
D7BazA5	−1717.46 (802.45)	−35.78 (16.72)	D8BazA3	−2716.70 (1220.38)	−48.51 (21.79)	D8BazA5	−2434.36 (866.06)	−43.47 (15.47)
D6A2	−505.12 (218.72)	−14.43 (6.25)	D6Baz(r)A2	−1578.57 (531.15)	−35.08 (11.80)	D6BazA2	−2090.11 (876.69)	−46.45 (19.48)

Table S5 The electronic properties [predicted with B3LYP/6-31G(d,p)] and static first hyperpolarizability (<β_0>) ($\times 10^{-30}$ esu) [predicted with TD-CAM-B3LYP/6-31++G(d,p)-SOS] of D7Bb(n)A4 series of molecules.

Compounds	ΔE_{OS-CS}	ΔE_{T-CS}	<S^2>	E_{gap}	D_g	<β_0>(<β_0>/N) (TDDFT/SOS)
D7Bet(n=1)A4 ($C_{32}H_{26}N_4O_3S$)	0.00	23.07	0.00	2.14 (4.06)	24.09	−1025.01 (−25.63)
D7Bet(n=2)A4 ($C_{34}H_{28}N_4O_3S$)	0.00	20.14	0.00	1.96 (3.82)	26.14	−1893.80 (−45.09)
D7Bet(n=3)A4 ($C_{36}H_{30}N_4O_3S$)	0.00	17.79	0.00	1.81 (3.62)	28.00	−3073.76 (−69.86)
D7Bet(n=4)A4 ($C_{38}H_{32}N_4O_3S$)	0.00	15.87	0.00	1.69 (3.46)	29.69	−4574.07 (−99.44)
D7Bet(n=5)A4 ($C_{40}H_{34}N_4O_3S$)	0.00	14.24	0.00	1.60 (3.33)	31.26	−6314.93 (−131.56)
D7Bet(n=6)A4 ($C_{42}H_{36}N_4O_3S$)	0.00	12.85	0.00	1.51 (3.22)	32.69	−8289.19 (−165.78)
D7Bet(n=7)A4 ($C_{44}H_{38}N_4O_3S$)	0.00	11.65	0.00	1.44 (3.13)	34.00	−10459.80 (−201.15)
D7Bet(n=8)A4 ($C_{46}H_{40}N_4O_3S$)	0.00	10.60	0.00	1.38 (3.05)	35.18	−12764.50 (−236.38)
D7Bet(n=9)A4 ($C_{48}H_{42}N_4O_3S$)	0.00	9.68	0.00	1.32 (2.99)	36.25	−15141.20 (−270.38)
D7Bet(n=10)A4 ($C_{50}H_{44}N_4O_3S$)	0.00	8.85	0.00	1.27 (2.93)	37.21	−17607.60 (−303.58)
D7Bet(n=11)A4 ($C_{52}H_{46}N_4O_3S$)	0.00	8.10	0.00	1.23 (2.88)	38.06	−20090.80 (−334.85)
D7Bet(n=12)A4 ($C_{54}H_{48}N_4O_3S$)	0.00	7.41	0.00	1.19 (2.83)	38.83	−22540.40 (−363.55)
D7Bet(n=13)A4 ($C_{56}H_{50}N_4O_3S$)	0.00	6.79	0.00	1.15 (2.79)	39.50	−24844.40 (−388.19)
D7Bet(n=14)A4 ($C_{58}H_{52}N_4O_3S$)	0.00	6.21	0.00	1.12 (2.76)	40.10	−26986.20 (−408.88)
D7Bet(n=15)A4 ($C_{60}H_{54}N_4O_3S$)	0.00	5.67	0.00	1.09 (2.73)	40.63	−28903.70 (−425.05)
D7Bet(n=16)A4 ($C_{62}H_{56}N_4O_3S$)	0.00	5.16	0.00	1.06 (2.70)	41.09	−30605.60 (−437.22)
D7Beta(n=1)A4 ($C_{42}H_{32}N_4O_3S$)	0.00	18.03	0.00	1.55 (3.24)	25.36	−3715.15 (−74.30)
D7Beta(n=2)A4 ($C_{44}H_{34}N_4O_3S$)	0.00	16.59	0.00	1.46 (3.11)	26.97	−6087.83 (−117.07)
D7Beta(n=3)A4 ($C_{46}H_{36}N_4O_3S$)	0.00	15.19	0.00	1.37 (3.00)	28.40	−8616.26 (−159.56)
D7Beta(n=4)A4 ($C_{48}H_{38}N_4O_3S$)	0.00	13.91	0.00	1.30 (2.91)	29.69	−11275.50 (−201.35)
D7Beta(n=5)A4 ($C_{50}H_{40}N_4O_3S$)	0.00	12.75	0.00	1.24 (2.83)	30.85	−14020.60 (−241.73)
D7Beta(n=6)A4 ($C_{52}H_{42}N_4O_3S$)	0.00	11.69	0.00	1.19 (2.77)	31.88	−16816.80 (−280.28)
D7Beta(n=7)A4 ($C_{54}H_{44}N_4O_3S$)	0.00	10.73	0.00	1.14 (2.72)	32.82	−19597.90 (−316.10)
D7Beta(n=8)A4 ($C_{56}H_{46}N_4O_3S$)	0.00	9.85	0.00	1.10 (2.67)	33.65	−22463.90 (−351.00)
D7Beta(n=9)A4 ($C_{58}H_{48}N_4O_3S$)	0.00	9.04	0.00	1.06 (2.63)	34.40	−25895.30 (−392.35)
D7Beta(n=10)A4 ($C_{60}H_{50}N_4O_3S$)	0.00	8.22	0.00	1.04 (2.61)	35.07	−29262.60 (−430.33)
D7Beta(n=11)A4 ($C_{62}H_{52}N_4O_3S$)	0.00	7.54	0.00	1.01 (2.58)	35.66	−31774.60 (−453.92)
D7Baze(n=4)A4 ($C_{62}H_{48}N_4O_3S$)	0.00	12.41	0.00	0.94 (2.52)	28.91	−26694.10 (−381.34)
D7Bst(n=13)A4 ($C_{62}H_{54}N_4O_3S$)	0.00	7.66	0.00	1.13 (2.74)	32.46	−18170.70 (−259.58)

Table S6 Major electronic excitations with transitional nature of D8(Baz/Baz(r))A4, D7(Baz/Baz(r))A4, Exp, BAY1 and D7Bb(n)A4 series of molecules. *f* is the oscillator strength in a.u. unit; E_t is the transition energy in eV (nm) unit; $<\beta_0>_{con}$ (contribution value to $<\beta_0>$) and $<\beta_0>_{total}$ are in 10^{-30} esu unit.

Compounds	*f*	E_t	Transition	Transition nature	$<\beta_0>_{con}$	$<\beta_0>_{total}$
D8A4 ($C_{40}H_{41}N_5O$)	1.50	2.45 (507.0)	$S_0 \rightarrow S_1$	H→L 83.36%	−1092.30	−1300.31
D8Baz(r)A4 ($C_{50}H_{47}N_5O$)	2.05	2.43 (509.4)	$S_0 \rightarrow S_2$	H→L 60.60% H−2→L 19.90%	−1921.68	−2318.99
D8BazA4 ($C_{50}H_{47}N_5O$)	1.86	2.11 (586.5)	$S_0 \rightarrow S_2$	H→L 72.91% H−2→L 16.11%	−3366.23	−3941.89
D7A4 ($C_{30}H_{24}N_4O_3S$)	1.64	2.53 (490.9)	$S_0 \rightarrow S_1$	H→L 94.16%	−477.22	−459.49
D7Baz(r)A4 ($C_{40}H_{30}N_4O_3S$)	2.21	2.25 (549.9)	$S_0 \rightarrow S_2$	H→L 80.90%	−1287.94	−1331.47
D7BazA4 ($C_{40}H_{30}N_4O_3S$)	1.88	2.01 (616.3)	$S_0 \rightarrow S_1$	H→L 82.82%	−2667.94	−2945.31
Exp ($C_{38}H_{30}N_4O_3S$)	1.97	2.24 (553.3)	$S_0 \rightarrow S_1$	H→L 74.51% H−1→L 18.48%	−1515.73	−1594.83
BAY1 ($C_{86}H_{89}F_3N_6O_3SSi_2$)	2.42	2.03 (611.7)	$S_0 \rightarrow S_1$	H→L 71.50% H−1→L 20.90%	−3756.03	−4114.91
	0.32	2.83 (438.3)	$S_0 \rightarrow S_2$	H−1→L 70.0% H→L 19.40%	−226.54	
D7Bet(n=16)A4 ($C_{62}H_{56}N_4O_3S$)	8.35	1.68 (738.8)	$S_0 \rightarrow S_1$	H→L 35.80% H−1→L 27.42% H→L+1 17.84%	−25772.40	−30605.60
	0.93	2.44 (508.5)	$S_0 \rightarrow S_3$	H→L 56.76% H→L+1 11.66%	−4001.80	
D7Beta(n=11)A4 ($C_{62}H_{52}N_4O_3S$)	5.73	1.66 (748.2)	$S_0 \rightarrow S_1$	H→L 46.43% H−1→L 23.90% H→L+1 14.56%	−25017.00	−31774.60
	1.16	2.35 (527.3)	$S_0 \rightarrow S_4$	H→L 49.20% H→L+1 16.97% H−1→L 12.42%	−5026.90	
D7Beta(r)(n=11)A4 ($C_{62}H_{52}N_4O_3S$)	6.72	1.74 (711.5)	$S_0 \rightarrow S_1$	H→L 44.40% H−1→L 22.40% H→L+1 16.70%	−19819.20	−23687.40
	1.03	2.53 (490.6)	$S_0 \rightarrow S_4$	H→L 48.30% H→L+1 18.80%	−3203.90	
D7Baet(n=11)A4 ($C_{62}H_{52}N_4O_3S$)	7.41	1.78 (695.3)	$S_0 \rightarrow S_1$	H−1→L 37.50% H→L 30.30% H→L+1 15.70%	−15427.20	−17830.00
	0.49	2.58 (480.8)	$S_0 \rightarrow S_4$	H→L 60.50% H→L+1 10.40%	−1770.70	
D7Ba(r)et(n=11)A4 ($C_{62}H_{52}N_4O_3S$)	7.22	1.76 (704.4)	$S_0 \rightarrow S_1$	H→L 54.90% H−1→L 15.70% H→L+1 14.80%	−16213.90	−17999.10
	0.60	2.66 (465.8)	$S_0 \rightarrow S_4$	H→L 34.00% H−2→L 21.10% H−1→L 16.90%	−1257.6	
D7Baze(n=4)A4 ($C_{62}H_{48}N_4O_3S$)	3.89	1.72 (720.1)	$S_0 \rightarrow S_1$	H→L 57.40% H−1→L 14.90% H→L+1 13.10%	−19997.90	−26694.10
	1.37	2.33 (531.2)	$S_0 \rightarrow S_4$	H→L 39.80% H−1→L 17.20%	−4999.90	

Compounds	f	E_t	Transition	Transition nature	$\langle\beta_0\rangle_{con}$	$\langle\beta_0\rangle_{total}$
				H→L+1 12.70% H−3→L 12.70%		
D7Bst(n=13)A4 ($C_{62}H_{54}N_4O_3S$)	7.60	1.88 (659.8)	S_0→S_1	H→L+1 33.10% H→L 29.70% H−1→L 16.10%	−15354.40	−18170.70
	0.54	2.62 (472.9)	S_0→S_3	H→L 55.70% H−1→L 13.00% H−1→L+1 10.10%	−1897.40	

Table S7 Predicted major β_{ijk} [i, j, k∈(x, y, z)] (×10^{-30} esu) of D8(Baz/Baz(r))A4, D7(Baz/Baz(r))A4 and D7Bb(n)A4 series of molecules, and properties of the related states with important contributions to the β_{ijk} according to the SOS model. E_t is the transition energy in eV unit; m is the state number (m=0 is the ground state, m>0 is the mth excited state).

Compounds (<β_0>)	β_{xxx}	State [S_m]	E_t	State dipole moment			Transition dipole moment		
				X	Y	Z	X	Y	Z
D8A4 (−1300.31)		S_0		17.87	−3.73	3.67			
	−1143.08	S_1 [S_0→S_1]	2.45	35.96	−0.73	3.70	12.72	0.74	0.63
D8Baz(r)A4 (−2318.99)		S_0		−20.85	−1.88	−7.10			
	2010.97	S_2 [S_0→S_2]	2.43	−43.95	−0.94	−6.38	14.86	0.22	1.13
D8BazA4 (−3941.89)		S_0		17.51	−4.68	4.10			
	−3544.62	S_2 [S_0→S_2]	2.11	46.75	−4.04	3.94	15.23	−0.39	0.54
D7A4 (−459.49)		S_0		20.82	4.53	2.81			
	−496.11	S_1 [S_0→S_1]	2.53	28.73	3.62	2.46	13.08	0.60	−0.15
D7Baz(r)A4 (−1331.47)		S_0		24.35	5.21	4.71			
	−1346.52	S_2 [S_0→S_2]	2.25	35.68	4.33	4.18	−16.07	−0.52	−0.12
D7BazA4 (−2945.31)		S_0		20.29	5.38	3.52			
	−2817.47	S_1 [S_0→S_1]	2.01	40.11	4.66	2.95	15.69	−0.05	−0.25
D7Bet(n=16)A4 (−30605.60)		S_0		31.49	2.46	3.48			
	−25991.70	S_1 [S_0→S_1]	1.68	55.42	1.42	3.22	36.18	1.22	0.51
	−3991.90	S_3 [S_0→S_3]	2.44	133.91	1.49	3.15	−9.96	−1.09	−0.36
D7Beta(n=11)A4 (−31774.60)		S_0		26.09	2.44	3.51			
	−25447.90	S_1 [S_0→S_1]	1.66	58.95	−0.35	2.70	−30.17	0.16	0.01
	−5058.90	S_4 [S_0→S_4]	2.35	118.73	0.00	2.61	11.37	0.93	0.28
D7Beta(r)(n=11)A4 (−23687.40)		S_0		31.63	2.64	4.44			
	−20082.30	S_1 [S_0→S_1]	1.74	57.38	1.66	4.10	−31.83	−0.73	−0.30
	−3206.40	S_4 [S_0→S_4]	2.53	114.34	1.65	3.88	10.29	1.16	0.37
D7Baet(n=11)A4 (−17830.00)		S_0		25.81	3.79	3.33			
	−15660.20	S_1 [S_0→S_1]	1.78	45.33	3.32	3.06	33.04	1.54	0.40
	−1777.10	S_4 [S_0→S_4]	2.58	127.39	3.48	2.88	−7.05	−0.70	−0.22
D7Ba(r)et(n=11)A4 (−17999.10)		S_0		−31.34	−3.75	2.74			
	16288.70	S_1 [S_0→S_1]	1.76	−51.44	−3.80	2.57	−32.78	−1.99	0.18
	1249.40	S_4 [S_0→S_4]	2.66	−95.20	−5.01	2.39	7.70	0.91	−0.17
D7Baze(n=4)A4 (−26694.10)		S_0		20.00	4.73	2.60			
	−20874.30	S_1 [S_0→S_1]	1.72	64.60	2.11	1.38	−24.37	0.23	0.31
	−5183.00	S_4 [S_0→S_4]	2.33	98.35	2.29	1.32	12.42	0.26	−0.11
D7Bst(n=13)A4 (−18170.70)		S_0		25.01	3.21	2.93			
	−15555.00	S_1 [S_0→S_1]	1.88	47.14	2.25	2.69	32.58	1.48	0.43
	−1912.80	S_3 [S_0→S_3]	2.62	128.66	1.58	2.36	7.37	0.39	0.24

(1) D8A4:

$$\beta_{XXX}\left[S_0 \rightarrow S_1\right]=6\times\frac{12.72\times(35.96-17.87)\times(-12.72)}{2.45^2}\times\frac{\left(10^{-18}\right)^3}{\left(1.602\times10^{-12}\right)^2}esu=-1140.01\times10^{-30}esu$$

(2) D8Baz(r)A4:

$$\beta_{XXX}\left[S_0 \rightarrow S_2\right]=6\times\frac{14.86\times\left[(-43.95)-(-20.85)\right]\times(-14.86)}{2.43^2}\times\frac{\left(10^{-18}\right)^3}{\left(1.602\times10^{-12}\right)^2}esu=2019.59\times10^{-30}esu$$

(3) D8BazA4:

$$\beta_{XXX}\left[S_0 \rightarrow S_2\right]=6\times\frac{15.23\times(46.75-17.51)\times(-15.23)}{2.11^2}\times\frac{\left(10^{-18}\right)^3}{\left(1.602\times10^{-12}\right)^2}esu=-3561.55\times10^{-30}esu$$

(4) D7A4:

$$\beta_{XXX}\left[S_0 \rightarrow S_1\right]=6\times\frac{13.08\times(28.73-20.82)\times(-13.08)}{2.53^2}\times\frac{\left(10^{-18}\right)^3}{\left(1.602\times10^{-12}\right)^2}esu=-494.28\times10^{-30}esu$$

(5) D7Baz(r)A4:

$$\beta_{XXX}\left[S_0 \rightarrow S_2\right]=6\times\frac{(-16.07)\times(35.68-24.35)\times16.07}{2.25^2}\times\frac{\left(10^{-18}\right)^3}{\left(1.602\times10^{-12}\right)^2}esu=-1351.21\times10^{-30}esu$$

(6) D7BazA4:

$$\beta_{XXX}\left[S_0 \rightarrow S_1\right]=6\times\frac{15.69\times(40.11-20.29)\times(-15.69)}{2.01^2}\times\frac{\left(10^{-18}\right)^3}{\left(1.602\times10^{-12}\right)^2}esu=-2823.47\times10^{-30}esu$$

(7) D7Bet(n=16)A4:

$$\beta_{XXX}\left[S_0 \rightarrow S_1\right]=6\times\frac{36.18\times(55.42-31.49)\times(-36.18)}{1.68^2}\times\frac{\left(10^{-18}\right)^3}{\left(1.602\times10^{-12}\right)^2}esu=-25947.02\times10^{-30}esu$$

$$\beta_{XXX}\left[S_0 \rightarrow S_3\right]=6\times\frac{(-9.96)\times(133.91-31.49)\times9.96}{2.44^2}\times\frac{\left(10^{-18}\right)^3}{\left(1.602\times10^{-12}\right)^2}esu=-3989.79\times10^{-30}esu$$

(8) D7Beta(n=11)A4:

$$\beta_{XXX}\left[S_0 \rightarrow S_1\right]=6\times\frac{(-30.17)\times(58.95-26.09)\times30.17}{1.66^2}\times\frac{\left(10^{-18}\right)^3}{\left(1.602\times10^{-12}\right)^2}esu=-25376.30\times10^{-30}esu$$

$$\beta_{XXX}\left[S_0 \rightarrow S_4\right]=6\times\frac{11.37\times(118.73-26.09)\times(-11.37)}{2.35^2}\times\frac{\left(10^{-18}\right)^3}{\left(1.602\times10^{-12}\right)^2}esu=-5070.02\times10^{-30}esu$$

(9) D7Beta(r)(n=11)A4:

$$\beta_{XXX}\left[S_0 \rightarrow S_1\right]=6\times\frac{(-31.83)\times(57.38-31.63)\times31.83}{1.74^2}\times\frac{\left(10^{-18}\right)^3}{\left(1.602\times10^{-12}\right)^2}esu=-20145.51\times10^{-30}esu$$

$$\beta_{XXX}\left[S_0 \rightarrow S_4\right]=6\times\frac{10.29\times\left(114.34-31.63\right)\times\left(-10.29\right)}{2.53^2}\times\frac{\left(10^{-18}\right)^3}{\left(1.602\times10^{-12}\right)^2}esu=-3198.70\times10^{-30}esu$$

(10) D7Baet(n=11)A4:

$$\beta_{XXX}\left[S_0 \rightarrow S_1\right]=6\times\frac{33.04\times\left(45.33-25.81\right)\times\left(-33.04\right)}{1.78^2}\times\frac{\left(10^{-18}\right)^3}{\left(1.602\times10^{-12}\right)^2}esu=-15723.39\times10^{-30}esu$$

$$\beta_{XXX}\left[S_0 \rightarrow S_4\right]=6\times\frac{\left(-7.05\right)\times\left(127.39-25.81\right)\times7.05}{2.58^2}\times\frac{\left(10^{-18}\right)^3}{\left(1.602\times10^{-12}\right)^2}esu=-1773.26\times10^{-30}esu$$

(11) D7Ba(r)et(n=11)A4:

$$\beta_{XXX}\left[S_0 \rightarrow S_1\right]=6\times\frac{\left(-32.78\right)\times\left[\left(-51.44\right)-\left(-31.34\right)\right]\times32.78}{1.76^2}\times\frac{\left(10^{-18}\right)^3}{\left(1.602\times10^{-12}\right)^2}esu=16301.02\times10^{-30}esu$$

$$\beta_{XXX}\left[S_0 \rightarrow S_4\right]=6\times\frac{7.70\times\left[\left(-95.20\right)-\left(-31.34\right)\right]\times\left(-7.70\right)}{2.66^2}\times\frac{\left(10^{-18}\right)^3}{\left(1.602\times10^{-12}\right)^2}esu=1251.05\times10^{-30}esu$$

(12) D7Baze(n=4)A4:

$$\beta_{XXX}\left[S_0 \rightarrow S_1\right]=6\times\frac{\left(-24.37\right)\times\left(64.60-20.00\right)\times24.37}{1.72^2}\times\frac{\left(10^{-18}\right)^3}{\left(1.602\times10^{-12}\right)^2}esu=-20932.22\times10^{-30}esu$$

$$\beta_{XXX}\left[S_0 \rightarrow S_4\right]=6\times\frac{12.42\times\left(98.35-20.00\right)\times\left(-12.42\right)}{2.33^2}\times\frac{\left(10^{-18}\right)^3}{\left(1.602\times10^{-12}\right)^2}esu=-5204.71\times10^{-30}esu$$

(13) D7Bst(n=13)A4:

$$\beta_{XXX}\left[S_0 \rightarrow S_1\right]=6\times\frac{32.58\times\left(47.14-25.01\right)\times\left(-32.58\right)}{1.88^2}\times\frac{\left(10^{-18}\right)^3}{\left(1.602\times10^{-12}\right)^2}esu=-15537.96\times10^{-30}esu$$

$$\beta_{XXX}\left[S_0 \rightarrow S_3\right]=6\times\frac{7.37\times\left(128.66-25.01\right)\times\left(-7.37\right)}{2.62^2}\times\frac{\left(10^{-18}\right)^3}{\left(1.602\times10^{-12}\right)^2}esu=-1917.47\times10^{-30}esu$$

Table S8 Calculated electronic properties [predicted with B3LYP/6-31G(d,p)] and static first hyperpolarizability (<β_0>) (in 10^{-30} esu) and <β_0> per heavy atom (<β_0>/N) [predicted with TD-CAM-B3LYP/6-31++G(d,p)-SOS] for the experimentally and recently reported NLO molecules Exp and BAY1, respectively.

Compounds	**E_{gap}**	**D_g**	**<β_0>/(<β_0>/N) (TDDFT/SOS)**
Exp ($C_{38}H_{30}N_4O_3S$)	1.85	21.93	−1594.83(−34.67)
BAY1 ($C_{86}H_{89}F_3N_6O_3SSi_2$)	1.56	29.05	−4114.91(−40.74)

E_{gap}: the energy gap between the highest occupied molecular orbital (E_{HOMO}) and the lowest unoccupied molecular orbital (E_{LUMO}) (in eV); D_g: the ground state dipole moment (in Debye).

Cartesian coordinates of all studied compounds optimized with B3LYP/6-31G(d,p)

	D7A3				D7Baz(r)A3		
N	2.705283	-0.092018	-0.061696	N	5.828741	-0.106065	-0.045063
C	3.772732	-1.023601	0.173725	C	6.921868	-0.995594	0.214076
C	3.724876	-1.910651	1.260395	C	6.831458	-1.9739	1.217675
C	4.889154	-1.029862	-0.663713	C	8.108001	-0.877617	-0.513489
C	4.769187	-2.794185	1.488472	C	7.901397	-2.8185	1.471824
H	2.865173	-1.904838	1.922265	H	5.91795	-2.068058	1.795152
C	5.950477	-1.905462	-0.431107	C	9.194783	-1.713449	-0.251075
H	4.933386	-0.34179	-1.501524	H	8.186713	-0.121488	-1.287586
C	5.89269	-2.798846	0.645968	C	9.094571	-2.69491	0.742052
H	4.745099	-3.485287	2.324071	H	7.843584	-3.57678	2.245369
H	6.80473	-1.886674	-1.096656	H	10.102194	-1.595272	-0.83062
C	3.031862	1.300176	-0.187145	C	6.092284	1.299377	-0.141535
C	2.663714	2.021446	-1.325009	C	5.700654	2.025975	-1.268539
C	3.754631	1.942823	0.829673	C	6.769263	1.959006	0.896383
C	2.986696	3.373896	-1.446753	C	5.955646	3.395374	-1.359862
H	2.120848	1.525731	-2.123088	H	5.190676	1.519537	-2.081519
C	4.092565	3.281527	0.708437	C	7.041731	3.31513	0.804805
H	4.049917	1.383646	1.71134	H	7.080002	1.398843	1.772127
C	3.706589	4.01096	-0.428328	C	6.632165	4.047185	-0.321535
H	2.685342	3.909689	-2.338365	H	5.636852	3.933311	-2.244254
H	4.648875	3.792207	1.486961	H	7.562111	3.837291	1.600465
C	1.410574	-0.533089	-0.151055	C	4.555188	-0.604659	-0.215132
C	0.97191	-1.841374	-0.376536	C	4.181795	-1.885861	-0.595947
S	0.055145	0.548839	0.090422	S	3.1417	0.374875	0.150862
C	-0.41894	-1.971325	-0.360636	C	2.787076	-2.071999	-0.60094
H	1.653522	-2.662108	-0.554604	H	4.897645	-2.648119	-0.87375
C	-1.109799	-0.777775	-0.132816	C	2.043226	-0.957536	-0.243212
H	-0.924098	-2.912302	-0.533253	H	2.331958	-3.001305	-0.921666
O	6.863893	-3.698075	0.96165	O	10.085898	-3.567466	1.076944
O	4.081636	5.318504	-0.444422	O	6.941276	5.373296	-0.307595
C	8.024899	-3.75384	0.143945	C	11.315732	-3.493322	0.370394
H	7.776845	-4.019668	-0.891099	H	11.178164	-3.685601	-0.701092
H	8.569413	-2.801368	0.151583	H	11.799112	-2.516981	0.501747
H	8.656346	-4.532272	0.573262	H	11.953258	-4.269417	0.7953
C	3.720274	6.112438	-1.566659	C	6.550399	6.169227	-1.417465
H	2.631291	6.168865	-1.686591	H	5.461104	6.171552	-1.548883
H	4.112058	7.110067	-1.366093	H	6.887362	7.181962	-1.193744
H	4.166203	5.728407	-2.492531	H	7.024567	5.827938	-2.346226
C	-2.48515	-0.45445	-0.09044	C	0.599241	-0.796845	-0.20878
C	-3.604251	-1.268229	-0.215333	C	0.077187	0.523712	-0.212018
H	-2.706971	0.599768	0.049932	C	-0.171576	-1.993467	-0.16923
C	-3.437375	-2.678174	-0.373918	C	-1.234155	0.970604	-0.186993
N	-3.238087	-3.824491	-0.438579	H	0.818712	1.315447	-0.265595
C	-4.948787	-0.701747	-0.14478	C	-1.542181	-2.174911	-0.155222
C	-6.042271	-1.278045	-0.769071	H	0.403974	-2.911194	-0.119009
C	-5.138014	0.546729	0.6444	C	-2.433617	0.245906	-0.161706
C	-4.684725	0.620066	1.973516	H	-1.351196	2.053606	-0.200955
C	-5.772541	1.665625	0.081086	C	-2.581431	-1.228313	-0.153017
C	-4.878335	1.777849	2.722986	H	-1.870638	-3.212922	-0.128354
H	-4.197541	-0.241362	2.418915	C	-3.721715	0.781268	-0.145547
C	-5.950782	2.82761	0.829348	C	-3.943987	-1.518664	-0.130441
H	-6.115902	1.625393	-0.947147	H	-3.970574	1.835933	-0.14797
C	-5.508938	2.88528	2.151831	C	-4.665162	-0.286397	-0.125601
H	-4.538754	1.814461	3.753626	H	-4.370566	-2.51051	-0.119705
H	-6.437248	3.686814	0.378135	C	-6.071683	-0.032149	-0.107043
H	-5.655042	3.789214	2.73555	C	-7.145877	-0.898565	-0.105584
C	-7.380818	-0.827718	-0.529729	H	-6.334538	1.022195	-0.111569
N	-8.486494	-0.503391	-0.359888	C	-6.939528	-2.314654	-0.070842
C	-5.948037	-2.332705	-1.731724	N	-6.745913	-3.45922	0.022285

N	-5.925621	-3.152032	-2.558898

C	-8.52124	-0.381825	-0.092123
C	-9.575486	-1.05702	-0.676609
C	-8.764831	0.916818	0.590352
C	-8.288933	1.127188	1.897132
C	-9.469274	1.949612	-0.050013
C	-8.531186	2.332334	2.55114
H	-7.744816	0.335153	2.401196
C	-9.69515	3.1601	0.602101
H	-9.826569	1.807084	-1.064184
C	-9.232017	3.352652	1.904363
H	-8.173233	2.47449	3.566247
H	-10.234032	3.951896	0.091167
H	-9.414993	4.294296	2.413278
C	-10.938078	-0.647731	-0.502555
N	-12.060664	-0.362822	-0.38231
C	-9.418301	-2.190845	-1.537061
N	-9.347726	-3.081024	-2.283918

D7BazA3

N	5.855371	-0.105893	-0.034121
C	6.947811	-0.980174	0.272717
C	6.854212	-1.90849	1.322604
C	8.136727	-0.897991	-0.455447
C	7.92324	-2.739575	1.621387
H	5.938486	-1.974436	1.900462
C	9.222727	-1.719491	-0.148465
H	8.218167	-0.181431	-1.266029
C	9.118927	-2.651713	0.890598
H	7.862559	-3.459221	2.430815
H	10.132164	-1.629264	-0.729918
C	6.118433	1.292667	-0.19746
C	5.717054	1.968048	-1.352712
C	6.80517	1.998719	0.803227
C	5.972799	3.331431	-1.508718
H	5.198937	1.426271	-2.137107
C	7.07839	3.348733	0.647233
H	7.122977	1.478931	1.701016
C	6.659653	4.028994	-0.507735
H	5.646051	3.82894	-2.413637
H	7.606402	3.905905	1.413608
C	4.582827	-0.614762	-0.189272
C	4.219204	-1.9168	-0.510094
S	3.161548	0.378062	0.111615
C	2.826266	-2.1104	-0.522396
H	4.943841	-2.688634	-0.733279
C	2.080037	-0.979344	-0.226882
H	2.365324	-3.059309	-0.771247
O	10.109327	-3.507163	1.27056
O	6.970928	5.35416	-0.557846
C	11.341225	-3.466271	0.565153
H	11.207049	-3.708116	-0.496734
H	11.824545	-2.48492	0.652228
H	11.977312	-4.221826	1.027649
C	6.57139	6.0976	-1.700325
H	5.480919	6.096545	-1.821738
H	6.912655	7.118979	-1.52815
H	7.035948	5.711273	-2.616257
C	-4.603031	-0.340305	-0.154105
C	-4.079818	-1.629507	-0.441502
C	-3.836342	0.830233	0.09758
C	-2.766881	-2.060318	-0.524236
H	-4.810645	-2.403674	-0.631783

D8A4

C	3.185093	-0.638472	0.149135
C	2.290108	-1.654423	0.359317
H	2.718535	-2.64005	0.528718
C	0.834303	-1.646386	0.382424
C	0.166637	-2.733904	0.992298
C	0.023559	-0.661612	-0.238581
C	-1.214512	-2.814631	1.018298
H	0.757646	-3.517562	1.458321
C	-1.354114	-0.747837	-0.22268
C	-2.019504	-1.821893	0.417369
H	-1.693142	-3.659135	1.508246
H	-1.928842	0.024133	-0.724191
C	2.810236	0.797086	0.184616
C	3.205277	1.689534	-0.825326
C	2.070093	1.336269	1.251096
C	2.849791	3.032985	-0.801473
C	1.716856	2.676573	1.29457
C	2.080519	3.571295	0.257609
H	3.206073	3.667523	-1.602785
H	1.13157	3.027604	2.13528
C	4.610492	-0.964084	-0.064579
C	5.640234	-0.105189	0.365911
C	5.015408	-2.153178	-0.699872
C	6.979716	-0.425086	0.207934
C	6.351772	-2.48064	-0.877953
H	4.2607	-2.81815	-1.109105
C	7.385317	-1.631816	-0.413234
H	7.721228	0.259639	0.600678
H	6.585343	-3.383784	-1.427338
N	8.733849	-1.942467	-0.552923
N	1.690769	4.90614	0.301185
C	9.149899	-3.230695	-1.108073
C	10.460642	-3.765244	-0.524949
H	9.231512	-3.176933	-2.207381
H	8.371408	-3.96071	-0.883406
H	10.674979	-4.745573	-0.962206
H	11.314756	-3.118235	-0.742587
H	10.385764	-3.883064	0.559983
C	9.72141	-0.857603	-0.589177
C	10.421357	-0.578917	0.746871
H	9.229507	0.053025	-0.947451
H	10.47155	-1.109566	-1.347977
H	11.122543	0.25599	0.638145

C	-2.464241	1.026392	0.154755
H	-4.423723	1.726287	0.283734
C	-1.567971	-1.350802	-0.348298
H	-2.643552	-3.115146	-0.76397
C	-1.425739	0.106544	-0.028674
H	-2.148103	2.044631	0.375267
C	-0.285963	-1.870626	-0.447919
C	-0.061952	0.373869	0.045813
H	-0.0465	-2.902463	-0.668934
C	0.658896	-0.825303	-0.209327
H	0.374839	1.341131	0.261025
C	-6.032833	-0.105332	-0.104041
C	-7.140016	-0.918055	-0.220505
H	-6.289848	0.938532	0.048176
C	-7.066979	-2.340988	-0.356242
N	-7.028735	-3.504663	-0.397522
C	-8.488561	-0.319255	-0.140555
C	-9.54513	-0.800005	-0.887288
C	-8.686599	0.825081	0.785427
C	-8.214551	0.749652	2.108968
C	-9.343723	1.993825	0.365145
C	-8.41743	1.806353	2.992206
H	-7.706124	-0.148307	2.444463
C	-9.529973	3.0554	1.248036
H	-9.694965	2.074897	-0.657717
C	-9.07336	2.962637	2.563528
H	-8.064099	1.726789	4.015672
H	-10.032351	3.954864	0.9062
H	-9.225545	3.788616	3.251764
C	-10.894689	-0.359753	-0.687831
N	-12.007447	-0.043051	-0.557747
C	-9.394277	-1.746024	-1.952218
N	-9.316206	-2.472138	-2.858595
H	9.700948	-0.318647	1.527263
H	10.982095	-1.45099	1.09255
C	1.978146	5.800124	-0.821257
C	0.940093	6.908198	-1.016488
H	1.988996	5.200548	-1.732552
H	2.981724	6.248747	-0.721121
H	1.205094	7.495947	-1.901066
H	-0.057006	6.486624	-1.172649
H	0.893469	7.598862	-0.17009
C	1.430957	5.536463	1.601189
C	-0.048096	5.604407	2.000615
H	1.848442	6.549597	1.57372
H	1.999011	5.00217	2.370434
H	-0.151096	6.070292	2.986949
H	-0.62745	6.192322	1.2846
H	-0.495382	4.607579	2.047145
H	0.494113	0.167408	-0.751371
H	1.764506	0.684993	2.064192
H	5.381778	0.823311	0.864341
H	3.804742	1.322217	-1.65318
C	-3.45558	-1.956002	0.473097
C	-4.381402	-1.095251	-0.046253
H	-3.804701	-2.845999	0.990659
H	-4.038482	-0.202389	-0.561757
C	-5.798048	-1.235809	0.012492
C	-6.698712	-0.334768	-0.526642
C	-6.598939	-2.359056	0.655815
C	-8.042408	-0.804892	-0.274612
O	-7.987478	-1.964662	0.401931
C	-6.317207	0.850879	-1.208477
N	-5.905461	1.796556	-1.748804
C	-6.412237	-3.719799	-0.025336
H	-6.567587	-3.632292	-1.103251
H	-5.408698	-4.113414	0.149147
H	-7.141349	-4.42773	0.376801
C	-9.272146	-0.274424	-0.602986
C	-9.41386	0.949646	-1.317319
N	-9.574518	1.94602	-1.898931
C	-10.461661	-0.963062	-0.220524
N	-11.436312	-1.520329	0.08904
C	-6.449064	-2.42821	2.180083
H	-5.446653	-2.756737	2.462512
H	-6.63161	-1.448084	2.627049
H	-7.177049	-3.137066	2.582639

D8Baz(r)A4

C	6.039441	-0.601207	0.026466
C	5.050257	-1.523008	0.217655
H	5.378273	-2.554247	0.332176
C	3.59717	-1.370816	0.288973
C	2.847498	-2.397492	0.902388
C	2.8685	-0.303955	-0.281081
C	1.463463	-2.346909	0.983341
H	3.372496	-3.252397	1.32044
C	1.483754	-0.264181	-0.219047
C	0.740901	-1.275443	0.424265
H	0.930447	-3.171012	1.447237
H	0.966272	0.58678	-0.650964
C	5.823753	0.868055	0.094981
C	6.312584	1.728061	-0.900732
C	5.154048	1.468256	1.174386
C	6.11482	3.103621	-0.850202

D8BazA4

C	6.088543	-0.585992	0.019773
C	5.113782	-1.533425	0.166123
H	5.461795	-2.558684	0.27548
C	3.658881	-1.4146	0.193161
C	2.912895	-2.471233	0.763039
C	2.924076	-0.352683	-0.382632
C	1.528669	-2.455431	0.794524
H	3.445565	-3.316247	1.191477
C	1.539879	-0.344165	-0.362691
C	0.7971	-1.387091	0.234364
H	1.002143	-3.292683	1.240766
H	1.018048	0.493567	-0.813569
C	5.837836	0.875037	0.119792
C	6.341898	1.77522	-0.832244
C	5.11904	1.428347	1.193122
C	6.115769	3.144595	-0.745763

C	4.951878	2.839715	1.240882	C	4.888934	2.7927	1.295664
C	5.413158	3.70548	0.219708	C	5.369228	3.699216	0.319394
H	6.542541	3.707686	-1.640063	H	6.556573	3.781353	-1.502078
H	4.410011	3.239339	2.089304	H	4.311102	3.155401	2.136833
C	7.423746	-1.070222	-0.215827	C	7.487572	-1.020395	-0.195064
C	8.541437	-0.359319	0.26009	C	8.578617	-0.291668	0.315313
C	7.693364	-2.254037	-0.92516	C	7.799899	-2.189771	-0.911659
C	9.83764	-0.817204	0.075631	C	9.888314	-0.718978	0.155554
C	8.986285	-2.716995	-1.131587	C	9.106734	-2.622568	-1.09239
H	6.868759	-2.804807	-1.367999	H	6.998189	-2.752495	-1.380631
C	10.106238	-2.019607	-0.621559	C	10.199273	-1.907363	-0.54829
H	10.651326	-0.245781	0.505397	H	10.679167	-0.135033	0.610406
H	9.117601	-3.605283	-1.736438	H	9.271147	-3.500507	-1.704131
N	11.414516	-2.471084	-0.787102	N	11.520367	-2.328426	-0.687891
N	5.173177	5.07785	0.28716	N	5.104496	5.0643	0.425294
C	11.67154	-3.760361	-1.427748	C	11.82192	-3.603412	-1.337845
C	12.9415	-4.459224	-0.935031	C	13.093547	-4.281044	-0.820315
H	11.712612	-3.656279	-2.52623	H	11.889817	-3.483517	-2.433356
H	10.830539	-4.418343	-1.203867	H	10.989862	-4.282196	-1.145043
H	13.029902	-5.4329	-1.427438	H	13.218279	-5.244652	-1.32453
H	13.850592	-3.896157	-1.163699	H	13.995186	-3.693633	-1.014863
H	12.901611	-4.624651	0.145575	H	13.027753	-4.46413	0.25618
C	12.510601	-1.495076	-0.800807	C	12.595	-1.329254	-0.660069
C	13.269906	-1.36352	0.525124	C	13.313992	-1.19626	0.688041
H	12.108975	-0.519637	-1.095677	H	12.180871	-0.359403	-0.956124
H	13.210567	-1.78146	-1.594626	H	13.323031	-1.592073	-1.436581
H	14.056145	-0.605405	0.436599	H	14.086834	-0.421711	0.62896
H	12.601709	-1.067427	1.338589	H	12.617603	-0.921902	1.485302
H	13.738809	-2.308541	0.810691	H	13.793753	-2.134625	0.97744
C	5.572909	5.949276	-0.817181	C	5.527275	5.98022	-0.633641
C	4.682387	7.182531	-0.990212	C	4.62428	7.206313	-0.792537
H	5.509247	5.370878	-1.740093	H	5.503323	5.434338	-1.578034
H	6.62504	6.267288	-0.711716	H	6.570294	6.309101	-0.481268
H	5.020197	7.750949	-1.862644	H	4.982588	7.811066	-1.631723
H	3.640656	6.891428	-1.154039	H	3.593187	6.906907	-1.002305
H	4.719478	7.856343	-0.129687	H	4.622031	7.848365	0.092719
C	5.01388	5.710252	1.602155	C	4.889978	5.647517	1.755238
C	3.560183	5.952664	2.026298	C	3.418724	5.852346	2.136638
H	5.552452	6.665133	1.586849	H	5.413227	6.610226	1.791981
H	5.521148	5.094973	2.353232	H	5.381038	5.013509	2.501481
H	3.528239	6.41053	3.021302	H	3.344869	6.27396	3.145319
H	3.048233	6.619775	1.328155	H	2.920055	6.535735	1.444696
H	2.9951	5.017166	2.064017	H	2.868464	4.907453	2.121885
H	3.397067	0.497624	-0.781548	H	3.451277	0.463873	-0.860056
H	4.778071	0.841895	1.977519	H	4.728454	0.769973	1.962874
H	8.38736	0.561428	0.813655	H	8.392013	0.618164	0.876723
H	6.865562	1.310384	-1.737014	H	6.929651	1.39463	-1.662486
C	-0.738927	-1.219401	0.499821	C	-5.936568	-1.27916	0.347278
C	-1.420568	-0.708185	-0.632528	C	-5.294864	-2.26271	1.140001
C	-2.77717	-0.527063	-0.857531	C	-3.945557	-2.538993	1.326355
C	-1.337164	-1.681247	1.693436	C	-5.29624	-0.321498	-0.480165
C	-3.871835	-0.807552	-0.026736	C	-2.827985	-1.912356	0.770754
C	-2.678141	-1.759656	2.054772	C	-3.947766	-0.097191	-0.707162
C	-3.821659	-1.391267	1.340159	C	-2.827972	-0.756219	-0.181599
H	-0.782	-0.442279	-1.468862	H	-5.9691	-2.907982	1.698946
H	-3.034584	-0.115275	-1.83251	H	-3.727585	-3.364715	2.001859
H	-0.640024	-1.99933	2.462235	H	-5.955903	0.342477	-1.028699
H	-2.865914	-2.156432	3.051829	H	-3.721457	0.714907	-1.396259
C	-5.214104	-0.594143	-0.338632	C	-1.493428	-2.244398	1.001207
H	-5.578519	-0.178401	-1.269162	H	-1.16193	-3.032063	1.664683
C	-6.007442	-1.013216	0.766906	C	-0.658445	-1.36755	0.260087
C	-7.437618	-0.976418	0.888851	C	-7.389687	-1.298923	0.426617

C	-8.304362	-0.515751	-0.061543	C	-8.279034	-0.440492	-0.152422
H	-7.831358	-1.354251	1.828748	H	-7.787839	-2.103781	1.037218
H	-7.89536	-0.141172	-0.996322	H	-7.914345	0.385588	-0.755718
C	-9.726239	-0.46776	0.03256	C	-9.701389	-0.502418	-0.044404
C	-10.561221	0.007664	-0.960972	C	-10.567306	0.393358	-0.641736
C	-10.598752	-0.909211	1.198685	C	-10.539933	-1.521294	0.714913
C	-11.932785	-0.098726	-0.512753	C	-11.927353	0.020634	-0.317147
O	-11.955826	-0.623551	0.723432	O	-11.912799	-1.075337	0.459231
C	-10.101927	0.51098	-2.207041	C	-10.145376	1.490158	-1.439372
N	-9.630889	0.904581	-3.196281	N	-9.702239	2.358339	-2.075959
C	-10.551518	-2.41728	1.470349	C	-10.443363	-2.943912	0.150945
H	-10.729755	-2.978609	0.550102	H	-10.623864	-2.941873	-0.926598
H	-9.581689	-2.714108	1.875315	H	-9.45762	-3.375919	0.336041
H	-11.327801	-2.677229	2.194442	H	-11.197165	-3.57337	0.630469
C	-13.120953	0.23573	-1.126406	C	-13.134681	0.586854	-0.664938
C	-13.178469	0.79707	-2.434312	C	-13.230342	1.748757	-1.483481
N	-13.270695	1.257599	-3.500164	N	-13.353064	2.696644	-2.149042
C	-14.353277	0.019459	-0.440492	C	-14.348332	0.001137	-0.195927
N	-15.362069	-0.15474	0.114596	N	-15.341724	-0.472916	0.184105
C	-10.406197	-0.06818	2.465973	C	-10.354073	-1.467287	2.235944
H	-9.425817	-0.247711	2.912404	H	-9.367279	-1.83333	2.52687
H	-10.492473	0.996405	2.235825	H	-10.465542	-0.44304	2.599405
H	-11.177091	-0.332036	3.19435	H	-11.113215	-2.092264	2.712875
C	-5.14381	-1.49701	1.783682	C	-1.497305	-0.463674	-0.456012
H	-5.45855	-1.884878	2.745173	H	-1.164717	0.314319	-1.130229

D4A5

C	4.63521	-2.181659	-0.394241	C	8.682532	-1.64799	-0.452364
C	5.421658	0.024167	0.429168	C	8.910997	0.439735	0.86243
C	3.637684	-2.779337	-1.381996	C	7.936798	-2.195613	-1.666193
C	3.01962	-0.345808	-0.034291	C	6.695134	-0.267449	0.031169
C	1.943949	-1.20294	-0.409731	C	5.86366	-1.216493	-0.624578
C	2.219182	-2.632248	-0.830424	C	6.469133	-2.428869	-1.304771
C	0.647898	-0.72174	-0.377764	C	4.488301	-1.031251	-0.633499
H	-0.147272	-1.391949	-0.689754	H	3.883833	-1.753096	-1.175671
C	0.330185	0.600144	0.007174	C	3.863084	0.071422	-0.022305
C	1.409784	1.421902	0.400449	C	4.706997	0.998163	0.617924
C	2.719196	0.979498	0.399909	C	6.085156	0.846439	0.67198
C	3.828868	1.894801	0.874703	C	6.930431	1.849899	1.431035
C	5.163785	1.514954	0.233298	C	8.370753	1.865904	0.916245
H	5.986536	2.086733	0.673639	H	9.009741	2.475805	1.56278
H	3.571605	2.934796	0.651118	H	6.481883	2.846382	1.356402
H	3.724946	-2.258033	-2.342098	H	8.014003	-1.474028	-2.487574
H	1.479788	-2.951844	-1.572157	H	5.887593	-2.683688	-2.197433
H	1.222265	2.429797	0.748959	H	4.270593	1.847365	1.13644
N	4.324122	-0.78331	-0.102732	N	8.075245	-0.407589	0.017961
H	3.921321	1.826386	1.96802	H	6.933856	1.595092	2.500595
H	5.143655	1.740136	-0.839094	H	8.40762	2.301315	-0.088962
H	6.336235	-0.277223	-0.092482	H	9.923286	0.430493	0.444023
H	5.576366	-0.195066	1.498692	H	8.98336	0.028026	1.884232
H	4.64845	-2.775607	0.534799	H	8.702889	-2.406318	0.349778
H	5.648677	-2.215817	-0.807581	H	9.724553	-1.430563	-0.710481
H	3.883251	-3.831684	-1.55534	H	8.409039	-3.125331	-1.999098
H	2.09814	-3.301348	0.033481	H	6.397637	-3.298062	-0.635233
C	-1.049603	1.053511	-0.009614	C	2.396464	0.246203	-0.052322
C	-1.483017	2.363281	-0.110834	C	1.606785	-0.928246	0.012007
C	-2.112068	0.005876	0.094249	C	1.905303	1.573796	-0.141324
C	-2.996821	-0.269194	-0.952218	C	0.227857	-1.085873	-0.000723
C	-2.261705	-0.760016	1.25454	H	2.167015	-1.850883	0.123278
C	-3.957037	-1.267082	-0.788856	C	0.603273	2.049137	-0.180123
C	-3.262478	-1.727494	1.309293	H	2.66999	2.339125	-0.225926
C	-2.871649	2.695544	-0.007842	C	-0.784485	-0.120704	-0.06897

D4Baz(r)A5

N	-3.99646	2.982816	0.082946
C	-0.627858	3.484248	-0.34881
N	0.030315	4.423719	-0.551031
F	-4.787578	-1.530201	-1.796934
F	-3.399261	-2.449361	2.422346
F	-1.460298	-0.565445	2.307786
F	-2.924351	0.405168	-2.103802
N	-4.083589	-1.975106	0.311997

D4BazA5

C	8.753436	-1.676519	-0.301731
C	8.988186	0.614864	0.612607
C	7.962849	-2.449191	-1.353773
C	6.755446	-0.258627	0.018075
C	5.916935	-1.31973	-0.425518
C	6.521287	-2.634133	-0.87802
C	4.541648	-1.148385	-0.428298
H	3.930294	-1.976759	-0.774093
C	3.918222	0.037423	0.007398
C	4.769706	1.067713	0.452524
C	6.150192	0.946434	0.473224
C	7.006561	2.085713	0.989489
C	8.424754	2.020319	0.420986
H	9.077813	2.747475	0.914115
H	6.536313	3.044369	0.745555
H	7.980545	-1.890436	-2.29663
H	5.905738	-3.072679	-1.670785
H	4.340117	2.006592	0.789228
N	8.135885	-0.383955	-0.02392
H	7.057558	2.039872	2.086895
H	8.414367	2.258566	-0.648845
H	9.983701	0.537647	0.162122
H	9.107256	0.401908	1.689322
H	8.838525	-2.278377	0.619936
H	9.773977	-1.48843	-0.652709
H	8.442465	-3.416428	-1.535124
H	6.507364	-3.353111	-0.046136
C	-2.765436	0.774638	-0.087438
C	-2.025365	1.814702	0.517213
C	-2.254533	-0.427653	-0.630878
C	-0.652826	1.945298	0.695987
H	-2.612219	2.624877	0.935172
C	-0.941439	-0.862041	-0.765516
H	-2.997583	-1.106506	-1.038577
C	0.382137	1.088145	0.312803
H	-0.338873	2.851666	1.210542
H	-0.121004	-2.115428	0.070316
C	-0.610835	1.347065	-0.154765
H	0.505552	3.130951	-0.259634
C	-2.158001	-0.368451	-0.062896
C	-1.882063	1.919507	-0.20993
H	-2.613914	-1.348045	-0.018788
C	-2.848889	0.874013	-0.153179
H	-2.079151	2.978726	-0.267153
C	-4.289502	0.979441	-0.178196
C	-5.031828	2.114243	-0.439829
C	-5.060235	-0.272321	0.104334
C	-5.766309	-0.947344	-0.893636
C	-5.099433	-0.828563	1.385188
C	-6.454266	-2.115547	-0.568873
C	-5.823646	-2.000192	1.595926
C	-6.462537	2.089952	-0.392946
N	-7.626153	2.088309	-0.352541
C	-4.474926	3.387018	-0.774722
N	-4.060597	4.439947	-1.049431
F	-7.1175	-2.75903	-1.529225
F	-5.855844	-2.524626	2.821826
F	-4.453793	-0.245881	2.401277
F	-5.783944	-0.484998	-2.147824
N	-6.478904	-2.626271	0.642733

D7A2

N	1.504616	-0.102559	0.188309
C	0.170243	-0.304865	0.397369
C	-0.447111	-1.450425	0.91095
S	-1.009952	0.916904	-0.0412
C	-1.836456	-1.352475	0.917246
H	0.105156	-2.311442	1.260565
C	-2.347357	-0.142608	0.43506
H	-2.47431	-2.137391	1.303861
C	-4.235179	1.535037	0.349091
C	-3.725003	0.231345	0.383086
C	-4.740866	-0.835464	0.38265
C	-4.720827	-1.992179	-0.332875
H	-5.638016	-0.650945	0.967351
C	-3.438931	2.712697	0.426785
N	-2.82455	3.701484	0.495794
C	-5.639046	1.760808	0.23444
N	-6.788969	1.936147	0.152534
C	-3.705301	-2.364703	-1.278802
N	-2.928084	-2.715041	-2.069596
C	-5.808533	-2.923228	-0.208789
N	-6.678387	-3.687385	-0.102092
C	2.032941	1.212465	-0.055769
C	2.764394	1.464778	-1.226008
C	1.841576	2.239982	0.870079
C	3.282496	2.727646	-1.465059
H	2.919835	0.666401	-1.943982
C	2.345536	3.517988	0.627165
H	1.290577	2.047335	1.784659
C	3.069949	3.768258	-0.545147
H	3.844842	2.941101	-2.367508
H	2.172344	4.299478	1.356113
C	2.407635	-1.219721	0.144413
C	3.570988	-1.201192	0.914959
C	2.153111	-2.315711	-0.694875
C	4.477093	-2.260709	0.860787
H	3.773621	-0.35097	1.557897

C	0.246666	-0.23826	-0.373504	C	3.043383	-3.377945	-0.742749
H	-0.819797	-1.829839	-1.249171	H	1.257515	-2.331193	-1.307319
C	1.743356	1.298137	0.512314	C	4.21363	-3.360124	0.033415
C	1.534819	-0.736757	-0.539503	H	5.372683	-2.220154	1.46842
H	2.163197	2.168409	0.998793	H	2.861146	-4.231025	-1.387216
C	2.473343	0.191903	-0.005896	O	3.607561	4.970199	-0.881152
H	1.770508	-1.678592	-1.01684	O	5.020967	-4.447585	-0.091781
C	-4.231771	0.934934	-0.155262	C	3.386498	6.076936	-0.01508
C	-4.873036	2.119566	-0.435054	H	3.875283	6.928721	-0.488776
C	-5.071603	-0.270913	0.100058	H	2.316815	6.289366	0.099345
C	-5.009229	-0.940451	1.327414	H	3.830996	5.90961	0.973851
C	-5.94087	-0.804492	-0.857194	C	6.22143	-4.490587	0.667992
C	-5.801712	-2.067844	1.530686	H	6.017431	-4.466638	1.745642
C	-6.680786	-1.944776	-0.545789	H	6.702261	-5.435759	0.414282
C	-6.300145	2.237017	-0.365286	H	6.892681	-3.662438	0.40883
N	-7.45622	2.353151	-0.300394				
C	-4.20279	3.31785	-0.846205				
N	-3.71907	4.315051	-1.201239				
F	-5.741321	-2.692248	2.706565				
F	-7.49613	-2.451666	-1.46894				
F	-6.054432	-0.245151	-2.065621				
F	-4.211765	-0.497147	2.304374				
N	-6.611515	-2.556192	0.616175				

	D7Baz(r)A2				**D7BazA2**		
N	-4.53579	-0.149517	-0.104876	N	-4.546389	-0.138621	-0.107848
C	-3.248787	-0.532904	-0.404527	C	-3.25699	-0.512981	-0.421202
C	-2.833768	-1.660897	-1.10226	C	-2.847041	-1.624599	-1.147899
S	-1.868078	0.380787	0.184713	S	-1.871812	0.386124	0.18605
C	-1.43531	-1.781901	-1.164474	C	-1.44829	-1.746657	-1.221
H	-3.525315	-2.356534	-1.558543	H	-3.544126	-2.311696	-1.608984
C	-0.726611	-0.763959	-0.540704	C	-0.743465	-0.743135	-0.572967
H	-0.951958	-2.582175	-1.711727	H	-0.953583	-2.544857	-1.762269
C	0.708241	-0.559285	-0.476567	C	5.883235	0.116067	-0.26439
C	1.180188	0.734545	-0.121649	C	5.42961	-1.044948	-0.93528
C	1.527142	-1.686031	-0.771731	C	5.097982	1.111589	0.353129
C	2.470792	1.215835	0.007657	C	4.136394	-1.484075	-1.175637
H	0.407787	1.477468	0.053796	H	6.210574	-1.675729	-1.351019
C	2.903998	-1.804361	-0.812848	C	3.715909	1.206785	0.47482
H	0.991332	-2.607831	-0.968761	H	5.653179	1.90853	0.837929
C	3.699524	0.565156	-0.183704	C	2.916048	-0.909868	-0.795166
H	2.546303	2.266152	0.285028	H	4.056198	-2.410146	-1.741935
C	3.901893	-0.84917	-0.55894	C	2.720572	0.355542	-0.013221
H	3.273419	-2.79759	-1.064418	H	3.357575	2.070498	1.031459
C	4.960777	1.14914	-0.047578	C	1.652868	-1.416559	-1.067283
C	5.277804	-1.06903	-0.606805	C	1.347671	0.526554	0.139105
H	5.145966	2.172961	0.242687	H	1.451337	-2.327908	-1.614788
C	5.942888	0.153469	-0.296991	C	0.671337	-0.547705	-0.5015
H	5.75466	-2.001106	-0.879262	H	0.876169	1.349759	0.661099
C	8.029427	1.507331	-0.624091	C	7.933162	1.506595	-0.645688
C	7.381495	0.319991	-0.300104	C	7.350532	0.312667	-0.241119
C	8.251681	-0.823583	0.000238	C	8.251946	-0.748473	0.18413
C	8.045759	-1.793196	0.932548	C	7.978931	-1.803283	1.007135
H	9.192098	-0.879195	-0.541474	H	9.283382	-0.672047	-0.148571
C	7.357913	2.697818	-1.035832	C	7.192925	2.588474	-1.215873
N	6.858709	3.692423	-1.379842	N	6.643848	3.493241	-1.701606
C	9.454314	1.610111	-0.571871	C	9.342443	1.732687	-0.544272
N	10.616781	1.682774	-0.537845	N	10.491444	1.907848	-0.468254
C	6.960896	-1.836617	1.873037	C	6.739424	-2.053349	1.684228
N	6.143874	-1.924205	2.695769	N	5.785857	-2.312846	2.297818
C	9.010839	-2.848627	1.076068	C	9.021348	-2.746661	1.29936
N	9.781771	-3.71211	1.186875	N	9.860683	-3.51766	1.531808

C	-4.852316	1.214991	0.201236	C	-4.869383	1.22231	0.19972
C	-5.53587	1.526965	1.386936	C	-5.57659	1.527816	1.373682
C	-4.507576	2.244482	-0.677724	C	-4.505991	2.258493	-0.664202
C	-5.859513	2.84169	1.683723	C	-5.90557	2.840715	1.672673
H	-5.811417	0.730679	2.070487	H	-5.866001	0.727512	2.046685
C	-4.814327	3.572503	-0.376924	C	-4.817852	3.584622	-0.360354
H	-3.993865	2.009413	-1.60419	H	-3.973463	2.029888	-1.581491
C	-5.496174	3.877626	0.807592	C	-5.523788	3.882373	0.811566
H	-6.385133	3.09686	2.597527	H	-6.44928	3.089791	2.577589
H	-4.53067	4.350344	-1.075177	H	-4.518632	4.366797	-1.047224
C	-5.590813	-1.120188	-0.090347	C	-5.592597	-1.117023	-0.08769
C	-6.785694	-0.864623	-0.766191	C	-6.798776	-0.867384	-0.746023
C	-5.453004	-2.321245	0.624105	C	-5.434999	-2.323785	0.613523
C	-7.835175	-1.784302	-0.735479	C	-7.839586	-1.796869	-0.709607
H	-6.900658	0.063385	-1.316439	H	-6.929145	0.063818	-1.287357
C	-6.485525	-3.246434	0.645005	C	-6.458716	-3.258488	0.639576
H	-4.532859	-2.523955	1.161811	H	-4.505562	-2.52314	1.136216
C	-7.687645	-2.986117	-0.032442	C	-7.672028	-3.003267	-0.019461
H	-8.751026	-1.556743	-1.267036	H	-8.764187	-1.573153	-1.227553
H	-6.391883	-4.176511	1.195276	H	-6.349078	-4.192728	1.179814
O	-5.853014	5.131881	1.196763	O	-5.887841	5.135047	1.20209
O	-8.639428	-3.955681	0.059871	O	-8.614129	-3.982896	0.07654
C	-5.509323	6.224107	0.354963	C	-5.525551	6.231466	0.374358
H	-5.878753	7.118074	0.858336	H	-5.904168	7.123183	0.875073
H	-4.423234	6.305905	0.223569	H	-4.43685	6.312717	0.265509
H	-5.986627	6.140396	-0.629395	H	-5.982266	6.154483	-0.620362
C	-9.881751	-3.746862	-0.596803	C	-9.86544	-3.779798	-0.563782
H	-9.7533	-3.64543	-1.681794	H	-9.750713	-3.667482	-1.649315
H	-10.483825	-4.631789	-0.387978	H	-10.457278	-4.671956	-0.356088
H	-10.398002	-2.859088	-0.210482	H	-10.385518	-2.900144	-0.164004

	D8A2				**D8Baz(r)A2**		
C	1.650005	-0.549187	0.004825	C	-4.379294	-0.606319	-0.070828
C	0.847957	-1.650626	0.162032	C	-3.374836	-1.522839	-0.203066
H	1.346731	-2.580417	0.426343	H	-3.688865	-2.557552	-0.324295
C	-0.598271	-1.770581	0.047798	C	-1.922395	-1.359666	-0.198759
C	-1.251187	-2.813837	0.744998	C	-1.133117	-2.393782	-0.747793
C	-1.401696	-0.941003	-0.770612	C	-1.232855	-0.274622	0.387237
C	-2.622477	-2.987815	0.681627	C	0.25265	-2.341778	-0.739782
H	-0.661236	-3.476209	1.371726	H	-1.629166	-3.247397	-1.201999
C	-2.7717	-1.105013	-0.829852	C	0.151972	-0.217383	0.386245
C	-3.421887	-2.121795	-0.092838	C	0.93589	-1.244861	-0.179803
H	-3.086231	-3.772678	1.26836	H	0.814164	-3.143222	-1.209595
H	-3.3535	-0.459831	-1.480756	H	0.641235	0.616903	0.879449
C	1.118374	0.83264	-0.042279	C	-4.169071	0.862893	-0.148816
C	1.578699	1.77494	-0.97823	C	-4.70953	1.734216	0.809793
C	0.134384	1.271508	0.862591	C	-3.453501	1.451493	-1.205146
C	1.060703	3.06258	-1.04273	C	-4.519659	3.110278	0.746601
C	-0.389187	2.552586	0.814444	C	-3.259379	2.823264	-1.284513
C	0.043039	3.492007	-0.155999	C	-3.775226	3.701256	-0.300381
H	1.478135	3.740128	-1.776295	H	-4.987053	3.723043	1.50674
H	-1.163531	2.809267	1.525138	H	-2.682386	3.214117	-2.113718
C	3.115101	-0.72944	-0.051467	C	-5.769915	-1.082368	0.109873
C	4.003261	0.229887	0.472901	C	-6.869422	-0.379248	-0.417689
C	3.698768	-1.877745	-0.61827	C	-6.0643	-2.266603	0.809162
C	5.3766	0.042405	0.463598	C	-8.169759	-0.844287	-0.290106
C	5.071977	-2.073225	-0.647144	C	-7.362108	-2.737127	0.957887
H	3.059992	-2.617061	-1.092085	H	-5.257436	-2.811294	1.29044
C	5.961321	-1.122652	-0.090424	C	-8.462298	-2.047002	0.397069
H	6.002071	0.797569	0.923486	H	-8.966913	-0.278708	-0.757022
H	5.450088	-2.95311	-1.151763	H	-7.515184	-3.624925	1.558227
N	7.341044	-1.300982	-0.080399	N	-9.773969	-2.504695	0.506092

N	-0.519782	4.76123	-0.211821
C	7.925903	-2.554402	-0.558188
C	9.240797	-2.930319	0.129545
H	8.076808	-2.528158	-1.651319
H	7.212049	-3.354265	-0.356071
H	9.581552	-3.897957	-0.252208
H	10.039208	-2.207426	-0.059268
H	9.104364	-3.018523	1.211279
C	8.215208	-0.121628	-0.070293
C	8.765816	0.260974	1.308969
H	7.666525	0.724406	-0.49766
H	9.049061	-0.313332	-0.755729
H	9.38825	1.159208	1.229596
H	7.958673	0.468118	2.017125
H	9.377727	-0.540147	1.73096
C	-0.132103	5.713258	-1.252502
C	-1.271624	6.623829	-1.719324
H	0.207593	5.147776	-2.120462
H	0.719754	6.330985	-0.920186
H	-0.908032	7.271449	-2.523606
H	-2.108303	6.034717	-2.105921
H	-1.647407	7.272973	-0.923845
C	-1.166264	5.318528	0.983037
C	-2.68618	5.124638	1.0447
H	-0.932236	6.388531	1.018993
H	-0.699092	4.881578	1.872152
H	-3.083226	5.567331	1.964789
H	-3.182552	5.602289	0.196071
H	-2.956561	4.065386	1.037152
H	-0.934059	-0.167838	-1.367226
H	-0.237489	0.589102	1.619419
H	3.602379	1.129944	0.927454
H	2.358428	1.490868	-1.678823
C	-4.875012	-2.279993	-0.175917
C	-5.489174	-3.522998	-0.299419
C	-4.771112	-4.745696	-0.471545
N	-4.234737	-5.76753	-0.629302
C	-6.912145	-3.662655	-0.28677
N	-8.072395	-3.76872	-0.285051
C	-5.758092	-1.119642	-0.163869
C	-5.5402	0.107789	0.393286
H	-6.738544	-1.254766	-0.612155
C	-4.400396	0.510516	1.16669
N	-3.53981	0.924015	1.831409
C	-6.555207	1.11709	0.2727
N	-7.367372	1.943496	0.170723

N	-3.545289	5.074442	-0.38051
C	-10.052133	-3.794859	1.136391
C	-11.296614	-4.499866	0.590506
H	-10.14048	-3.689854	2.231963
H	-9.199228	-4.44897	0.949194
H	-11.400593	-5.474303	1.07833
H	-12.217482	-3.941773	0.781088
H	-11.210474	-4.664444	-0.487523
C	-10.873632	-1.53313	0.472933
C	-11.577952	-1.405194	-0.883386
H	-10.487995	-0.555945	0.782942
H	-11.604733	-1.821191	1.237553
H	-12.368526	-0.648474	-0.828121
H	-10.877455	-1.108727	-1.66908
H	-12.033121	-2.351308	-1.186932
C	-4.004846	5.960209	0.688745
C	-3.137245	7.207052	0.879879
H	-3.976834	5.398843	1.623861
H	-5.054535	6.263457	0.529534
H	-3.522268	7.787101	1.724593
H	-2.10131	6.931474	1.098095
H	-3.141286	7.864345	0.005903
C	-3.333728	5.686135	-1.698068
C	-1.865206	5.941619	-2.058894
H	-3.885431	6.633138	-1.725182
H	-3.796854	5.050369	-2.460429
H	-1.792842	6.379659	-3.060657
H	-1.395443	6.630054	-1.351762
H	-1.286791	5.013534	-2.050936
H	-1.79286	0.51822	0.867191
H	-3.036253	0.815596	-1.979902
H	-6.696227	0.540696	-0.966829
H	-5.297264	1.325086	1.626338
C	2.415384	-1.176372	-0.177997
C	3.113594	-2.390802	0.028663
C	4.477425	-2.645118	0.070532
C	2.996649	0.097189	-0.383662
C	5.557088	-1.764933	-0.075788
C	4.331809	0.476506	-0.429825
C	5.487833	-0.300856	-0.296343
H	4.751489	-3.683751	0.249373
H	2.288602	0.900528	-0.559682
H	4.506586	1.537089	-0.605579
C	6.908612	-2.117339	-0.030902
H	7.288349	-3.114033	0.140357
C	7.681929	-0.938765	-0.194705
C	6.802739	0.167623	-0.353806
H	7.095363	1.193516	-0.533052
H	2.483658	-3.25559	0.210302
C	9.130341	-0.84084	-0.250646
C	9.949344	-1.83471	-0.769196
C	9.464722	-3.050563	-1.341217
N	9.124471	-4.055457	-1.82126
C	11.373031	-1.696726	-0.77277
N	12.531288	-1.572989	-0.782019
C	9.803234	0.380136	0.204032
C	9.456256	1.173316	1.254473
H	10.711847	0.66201	-0.321069
C	8.395867	0.917911	2.188957
N	7.59073	0.765572	3.01397
C	10.238965	2.344793	1.538362
N	10.86107	3.300998	1.763896

D8BazA2

C	4.399794	-0.61111	0.034455
C	3.399438	-1.525385	0.214156
H	3.718622	-2.539782	0.44504
C	1.94816	-1.378781	0.148606
C	1.148107	-2.355282	0.783705
C	1.271507	-0.366672	-0.570274
C	-0.235363	-2.304788	0.744712
H	1.636556	-3.163397	1.321898
C	-0.111373	-0.325221	-0.621038
C	-0.908678	-1.282853	0.043637
H	-0.806247	-3.080037	1.2452
H	-0.589203	0.474094	-1.178146
C	4.169995	0.856077	-0.024386
C	4.730141	1.650087	-1.037255
C	3.412875	1.521385	0.954967
C	4.520514	3.023648	-1.098233
C	3.200284	2.891692	0.911546
C	3.736608	3.689704	-0.127903
H	5.002559	3.577816	-1.893717
H	2.590882	3.342997	1.685088
C	5.800936	-1.081544	-0.045444
C	6.870176	-0.314922	0.455625
C	6.137179	-2.325074	-0.610832
C	8.178861	-0.773301	0.432797
C	7.444241	-2.791043	-0.654402
H	5.35766	-2.925866	-1.069865
C	8.512164	-2.035192	-0.115718
H	8.948585	-0.153682	0.876484
H	7.631919	-3.732448	-1.155266
N	9.830196	-2.486494	-0.116344
N	3.488921	5.061511	-0.171227
C	10.151454	-3.831378	-0.592514
C	11.358182	-4.466659	0.10321
H	10.312492	-3.836697	-1.684712
H	9.289202	-4.470311	-0.396815
H	11.498856	-5.483165	-0.277904
H	12.287663	-3.920088	-0.078686
H	11.199129	-4.525274	1.183887
C	10.922529	-1.506744	-0.111316
C	11.542528	-1.242233	1.266404
H	10.553686	-0.56765	-0.537716
H	11.699495	-1.861571	-0.798827
H	12.328143	-0.482409	1.187547
H	10.792565	-0.884282	1.977268
H	11.987139	-2.149181	1.683841
C	3.959758	5.856648	-1.30465
C	3.086581	7.075258	-1.61406
H	3.951053	5.216762	-2.188517
H	5.00464	6.181587	-1.155958
H	3.482006	7.585926	-2.49786
H	2.056633	6.773305	-1.825058
H	3.071414	7.802385	-0.797707
C	3.243434	5.781706	1.084345
C	1.76614	6.058273	1.389259
H	3.791621	6.730575	1.04396
H	3.691084	5.214942	1.90773
H	1.669646	6.575942	2.350169
H	1.30968	6.684868	0.618675
H	1.19083	5.129912	1.44396
H	1.843673	0.384738	-1.099941

D7A4

N	3.295508	-0.130059	-0.252199
C	3.827631	1.202395	-0.248902
C	3.531933	2.09363	-1.292616
C	4.671911	1.615792	0.78374
C	4.056464	3.377242	-1.285891
H	2.891834	1.772881	-2.107917
C	5.215879	2.900327	0.788926
H	4.909531	0.926417	1.587307
C	4.903911	3.791926	-0.245811
H	3.836672	4.076657	-2.085165
H	5.868373	3.194296	1.6017
C	4.20756	-1.232539	-0.141193
C	4.034502	-2.212367	0.838983
C	5.307036	-1.318196	-1.008745
C	4.930407	-3.276896	0.949079
H	3.192298	-2.148351	1.520123
C	6.210008	-2.36425	-0.894336
H	5.449684	-0.557542	-1.769177
C	6.027439	-3.356915	0.081978
H	4.769033	-4.023179	1.717271
H	7.063424	-2.442511	-1.559173
C	-0.577325	-0.199907	-0.163301
C	-0.10542	-1.441344	-0.581223
S	0.788338	0.884594	0.146185
C	1.288526	-1.534058	-0.67555
H	-0.767594	-2.259737	-0.840411
C	1.942603	-0.353982	-0.317824
H	1.81929	-2.418798	-1.000478
O	5.369571	5.06661	-0.338583
O	6.96374	-4.344158	0.103701
C	6.230902	5.549728	0.683731
H	5.736607	5.544355	1.663086
H	7.15599	4.962933	0.742527
H	6.473899	6.576722	0.409542
C	6.828426	-5.382822	1.064468
H	5.889353	-5.934334	0.932189
H	7.668297	-6.05756	0.896241
H	6.877314	-4.993639	2.089061
C	-1.906207	0.273871	0.003415
C	-3.047139	-0.478341	-0.141924
H	-2.002231	1.321654	0.274717
H	-2.946083	-1.529882	-0.398263
C	-4.382071	-0.028275	0.012616
C	-5.506882	-0.826714	-0.141048
C	-4.861479	1.37323	0.366902
C	-6.685133	-0.027846	0.091174
O	-6.319098	1.233685	0.381674
C	-8.028076	-0.345056	0.061339
C	-5.450621	-2.20486	-0.473461
N	-5.293157	-3.326018	-0.74723
C	-8.4994	-1.655004	-0.237877
N	-8.926368	-2.71209	-0.477679
C	-8.997113	0.664118	0.338489
N	-9.793137	1.483947	0.564326
C	-4.546171	2.423116	-0.704928
H	-5.067105	3.353332	-0.464116
H	-3.47414	2.626242	-0.756196
H	-4.880759	2.079274	-1.686494
C	-4.464412	1.823969	1.777621
H	-4.738515	1.064036	2.513199

H	2.977495	0.947003	1.766747	H	-3.38915	2.002564	1.848469
H	6.66464	0.652337	0.902606	H	-4.98917	2.751272	2.021139
H	5.348931	1.181298	-1.796926				
C	-7.61328	-1.013282	-0.143314				
C	-6.932948	-0.179113	-1.057538				
C	-5.567514	-0.020495	-1.267308				
C	-7.054414	-1.892172	0.806136				
C	-4.4944	-0.630399	-0.613655				
C	-5.717451	-2.157115	1.089725				
C	-4.566265	-1.64216	0.492521				
H	-5.295752	0.683629	-2.051691				
H	-7.767949	-2.423508	1.428357				
H	-5.546584	-2.872423	1.892038				
C	-3.14346	-0.412145	-0.868755				
H	-2.760657	0.253884	-1.630473				
C	-2.363523	-1.224385	0.000506				
C	-3.252473	-1.968071	0.822312				
H	-2.968543	-2.657944	1.60577				
H	-7.568326	0.412145	-1.711305				
C	-9.095615	-0.971007	-0.220578				
C	-9.843467	-2.126207	-0.385095				
C	-9.259529	-3.416487	-0.584091				
N	-8.840888	-4.487505	-0.765725				
C	-11.275056	-2.108336	-0.392105				
N	-12.439237	-2.087338	-0.4054				
C	-9.82428	0.286823	-0.156076				
C	-9.413728	1.47013	0.387568				
H	-10.83855	0.279853	-0.545321				
C	-8.178132	1.706891	1.076446				
N	-7.220875	1.979458	1.67845				
C	-10.297582	2.600855	0.340021				
N	-11.007404	3.521223	0.295878				

	D7Baz(r)A4				**D7BazA4**		
N	6.313214	-0.194298	-0.265429	N	-6.354265	0.17754	-0.263526
C	6.683238	1.18672	-0.357941	C	-6.718273	-1.207127	-0.293245
C	6.287675	1.965536	-1.457505	C	-6.321204	-2.031222	-1.358947
C	7.470618	1.768021	0.638839	C	-7.496826	-1.750154	0.731768
C	6.657281	3.299722	-1.540876	C	-6.681524	-3.370186	-1.382208
H	5.691624	1.518472	-2.246149	H	-5.730346	-1.614981	-2.1681
C	7.861048	3.104364	0.552659	C	-7.878035	-3.09188	0.7057
H	7.785123	1.169051	1.48715	H	-7.811028	-1.117406	1.555282
C	7.449379	3.880916	-0.538122	C	-7.465431	-3.912485	-0.351677
H	6.357429	3.911768	-2.384636	H	-6.380382	-4.016562	-2.19953
H	8.472367	3.52699	1.340581	H	-8.482503	-3.484008	1.514457
C	7.341911	-1.167088	-0.038295	C	-7.380028	1.155409	-0.053145
C	7.242026	-2.086538	1.00859	C	-7.242344	2.141939	0.926699
C	8.479847	-1.187896	-0.859267	C	-8.553916	1.116966	-0.821835
C	8.248653	-3.027356	1.231414	C	-8.24697	3.088276	1.133931
H	6.369278	-2.07202	1.6531	H	-6.341597	2.17544	1.530578
C	9.491625	-2.109176	-0.633432	C	-9.563386	2.044052	-0.609593
H	8.566001	-0.474323	-1.67206	H	-8.669274	0.352786	-1.583342
C	9.383417	-3.041327	0.410734	C	-9.417955	3.041552	0.367267
H	8.142023	-3.7283	2.050265	H	-8.110046	3.841655	1.900026
H	10.375738	-2.134991	-1.261344	H	-10.474567	2.023701	-1.197797
C	2.464716	-0.747625	-0.300255	C	-2.519187	0.755348	-0.379998
C	3.109263	-1.929507	-0.634645	C	-3.168196	1.902199	-0.813124
S	3.679316	0.512157	-0.007687	S	-3.71007	-0.482251	0.039851
C	4.512695	-1.855807	-0.679121	C	-4.570968	1.80992	-0.841255
H	2.578468	-2.851565	-0.837901	H	-2.629234	2.787332	-1.130773
C	4.998643	-0.593274	-0.366937	C	-5.042051	0.574737	-0.413434
H	5.156983	-2.689124	-0.92532	H	-5.228298	2.605634	-1.165911

O	7.765353	5.192591	-0.720389	O	-7.772364	-5.233738	-0.475088
O	10.426393	-3.907397	0.541466	O	-10.463134	3.906988	0.49053
C	8.564129	5.837343	0.261899	C	-8.561119	-5.840461	0.538576
H	8.070192	5.845756	1.241569	H	-8.063542	-5.799939	1.515644
H	9.547932	5.361232	0.358287	H	-9.5491	-5.369681	0.617721
H	8.693997	6.863463	-0.083621	H	-8.682833	-6.882423	0.240586
C	10.37668	-4.870876	1.584263	C	-10.374805	4.935614	1.466058
H	9.515981	-5.542352	1.473449	H	-9.526294	5.604016	1.272966
H	11.296804	-5.450276	1.501307	H	-11.303106	5.502761	1.389084
H	10.337428	-4.395116	2.572213	H	-10.285855	4.524806	2.47966
C	1.041971	-0.476675	-0.196059	C	4.088002	-0.324124	0.075236
C	0.160631	-1.457401	-0.73864	C	3.234839	-1.407803	0.401905
C	0.639452	0.729951	0.432297	C	3.6719	0.967347	-0.347342
C	-1.219176	-1.50682	-0.763217	C	1.849498	-1.504943	0.407187
H	0.645824	-2.294569	-1.227621	H	3.751159	-2.317734	0.700592
C	-0.626712	1.243218	0.670619	C	2.401814	1.479641	-0.535394
H	1.4472	1.35171	0.807725	H	4.469853	1.670776	-0.560384
C	-2.170223	-0.589397	-0.279137	C	0.890494	-0.539251	0.084712
H	-1.639925	-2.389265	-1.243485	H	1.45052	-2.472678	0.706672
C	-1.887434	0.705382	0.384116	C	1.148686	0.867212	-0.360341
H	-0.642749	2.209264	1.173842	H	2.362638	2.515064	-0.869775
C	-3.553534	-0.728535	-0.351302	C	-0.492425	-0.706761	0.11644
C	-3.122796	1.289061	0.681118	C	-0.087235	1.458726	-0.570831
H	-4.073852	-1.571743	-0.78725	H	-1.004687	-1.618174	0.398636
C	-4.156351	0.421718	0.239467	C	-1.114825	0.506034	-0.282723
H	-3.269417	2.24411	1.171697	H	-0.243696	2.478752	-0.896717
C	-5.551996	0.704334	0.392268	C	5.505182	-0.613285	0.199971
C	-6.579486	-0.112485	0.004525	C	6.563146	0.222338	-0.02794
H	-5.780924	1.656731	0.863596	H	5.723757	-1.628639	0.517188
H	-6.335006	-1.063414	-0.461842	H	6.381087	1.245221	-0.343599
C	-7.972082	0.14364	0.147794	C	7.94287	-0.108659	0.108484
C	-8.976313	-0.719014	-0.256213	C	8.9838	0.76971	-0.134442
C	-8.635956	1.372779	0.751968	C	8.550914	-1.438561	0.532461
C	-10.257665	-0.124109	0.049199	C	10.237535	0.091378	0.106148
O	-10.065465	1.074569	0.625387	O	9.991869	-1.173173	0.487917
C	-11.545597	-0.575545	-0.150562	C	11.542925	0.524388	0.007624
C	-8.738038	-1.977495	-0.868766	C	8.801764	2.114728	-0.551443
N	-8.442936	-2.989683	-1.362934	N	8.549731	3.199771	-0.890376
C	-11.83411	-1.833001	-0.753927	C	11.884586	1.8486	-0.39038
N	-12.115226	-2.852491	-1.242314	N	12.207617	2.920693	-0.711348
C	-12.64701	0.234422	0.256988	C	12.608075	-0.374531	0.312346
N	-13.550415	0.890868	0.587706	N	13.481551	-1.103872	0.560033
C	-8.397423	2.658591	-0.04793	C	8.299258	-2.578859	-0.461117
H	-9.039458	3.451712	0.343678	H	8.90813	-3.441934	-0.180355
H	-7.356678	2.981057	0.026669	H	7.248789	-2.877309	-0.46218
H	-8.637484	2.503308	-1.102439	H	8.573135	-2.272376	-1.473421
C	-8.36932	1.544556	2.251815	C	8.236435	-1.828221	1.981624
H	-8.58696	0.617562	2.787595	H	8.472648	-1.00457	2.659489
H	-7.328109	1.81629	2.437963	H	7.181548	-2.083661	2.102097
H	-9.013658	2.335247	2.644509	H	8.840717	-2.695009	2.260896

D7A5

C	4.337419	1.734729	-0.726061
C	3.645865	0.553752	-0.987727
C	3.480609	-0.380947	0.037402
C	4.03697	-0.057703	1.277151
C	4.707775	1.155411	1.425055
N	4.850707	2.025217	0.449171
F	3.143614	0.323905	-2.206105
F	4.488901	2.622574	-1.709453
F	5.227642	1.461615	2.613215
F	3.92692	-0.895244	2.312203

D7Baz(r)A5

C	7.64681	2.362686	-0.962327
C	7.076152	1.095014	-1.058004
C	6.995323	0.296231	0.084518
C	7.503171	0.83897	1.266215
C	8.049087	2.121415	1.246049
N	8.116228	2.861088	0.160666
F	6.615929	0.65165	-2.233051
F	7.721017	3.119588	-2.058351
F	8.523206	2.636635	2.380571
F	7.468411	0.141652	2.406428

C	2.75135	-1.670213	-0.190041
C	3.53697	-2.816912	-0.259484
C	3.006372	-4.128937	-0.420011
N	2.576063	-5.204173	-0.552695
C	4.959486	-2.737044	-0.171357
N	6.121495	-2.682283	-0.102898
C	1.333425	-1.601689	-0.306459
C	0.394667	-2.568554	-0.675574
S	0.502011	-0.064644	0.023775
C	-0.924582	-2.112934	-0.716968
H	0.668914	-3.581154	-0.937972
C	-1.054497	-0.766734	-0.365599
H	-1.767537	-2.726776	-1.003649
N	-2.207563	-0.035392	-0.263688
C	-3.478106	-0.694346	-0.144221
C	-3.690745	-1.670361	0.831497
C	-4.531897	-0.335818	-0.997893
C	-4.930312	-2.300964	0.949941
H	-2.883623	-1.944674	1.502825
C	-5.770356	-0.947025	-0.875361
H	-4.373418	0.426101	-1.753862
C	-5.979942	-1.93942	0.096014
H	-5.065764	-3.056327	1.71406
H	-6.59347	-0.680558	-1.529485
C	-2.176882	1.400598	-0.234477
C	-2.737403	2.089422	0.842542
C	-1.61442	2.124208	-1.297681
C	-2.73746	3.483991	0.873053
H	-3.180831	1.53161	1.660912
C	-1.597868	3.510351	-1.267266
H	-1.19245	1.594746	-2.14566
C	-2.160275	4.202578	-0.18244
H	-3.178657	3.99399	1.720422
H	-1.165673	4.083656	-2.080108
O	-7.227483	-2.481476	0.126455
O	-2.099825	5.558718	-0.255041
C	-7.501659	-3.495232	1.084494
H	-8.540768	-3.784567	0.924804
H	-6.856377	-4.370774	0.94106
H	-7.383622	-3.123663	2.109944
C	-2.643467	6.320627	0.815104
H	-2.133314	6.106261	1.762228
H	-2.483188	7.365819	0.549201
H	-3.718778	6.138437	0.9338

D7BazA5

C	6.387602	-1.071936	0.03971
C	7.270707	-2.134108	0.101298
C	6.88485	-3.509439	0.106043
N	6.608909	-4.640858	0.111016
C	8.683439	-1.91518	0.168276
N	9.835509	-1.75273	0.218798
C	-0.331677	-1.14802	-0.352553
C	0.329892	-2.407048	-0.444523
C	0.306839	0.109151	-0.177658
C	1.676561	-2.714352	-0.41558
H	-0.324653	-3.267585	-0.526281
C	1.650229	0.425604	-0.063311
H	-0.357843	0.967581	-0.149711
C	2.793988	-1.874013	-0.263179
H	1.911268	-3.773704	-0.508908
C	2.778355	-0.406426	-0.095977
H	1.864024	1.48652	0.059976
C	4.123184	-2.28945	-0.231738
C	4.106341	0.005542	0.021569
H	4.45304	-3.311523	-0.335169
C	4.951241	-1.139536	-0.056451
H	4.431043	1.026961	0.166013
C	-1.780219	-1.168794	-0.439187
C	-2.611554	-2.169774	-0.922882
S	-2.766418	0.215871	0.060039
C	-3.981737	-1.857125	-0.929681
H	-2.233886	-3.10291	-1.323
C	-4.249813	-0.588322	-0.431704
H	-4.754666	-2.519068	-1.297044
N	-5.476939	0.007152	-0.245795
C	-6.652276	-0.799993	-0.095082
C	-6.689544	-1.849766	0.825871
C	-7.794675	-0.52291	-0.86181
C	-7.839203	-2.626688	0.977043
H	-5.813375	-2.06581	1.428258
C	-8.945533	-1.280487	-0.705083
H	-7.774149	0.292391	-1.57731
C	-8.977606	-2.34267	0.212285
H	-7.837928	-3.434137	1.699093
H	-9.834506	-1.076063	-1.292033
C	-5.608141	1.43331	-0.183752
C	-6.26521	2.030711	0.894075
C	-5.105305	2.244351	-1.213807
C	-6.422112	3.415657	0.955982
H	-6.661479	1.407827	1.68927
C	-5.242205	3.622784	-1.150312
H	-4.608737	1.787086	-2.063279
C	-5.903594	4.221149	-0.065897
H	-6.93701	3.85088	1.803593
H	-4.857718	4.260665	-1.938804
O	-10.152342	-3.028301	0.282411
O	-5.991755	5.578833	-0.10495
C	-10.246611	-4.113323	1.194485
H	-11.255126	-4.512752	1.082417
H	-9.518424	-4.900506	0.962105
H	-10.101878	-3.78353	2.23093
C	-6.646417	6.24495	0.966005
H	-6.140781	6.064717	1.92284
H	-6.600074	7.308583	0.730113
H	-7.696732	5.9389	1.049886

D8A3

C	7.659539	2.115168	-1.430162	C	2.667586	-0.529075	0.1346
C	6.988815	0.907408	-1.251506	C	1.668596	-1.466378	0.166703
C	7.04027	0.272421	-0.005466	C	0.222751	-1.32166	0.077885
C	7.773673	0.920445	0.993927	C	-0.446898	-0.211175	-0.494655
C	8.398408	2.13287	0.703635	C	-0.583609	-2.400051	0.513598
N	8.341557	2.710897	-0.475966	C	-1.824237	-0.16226	-0.590862
F	6.316958	0.357913	-2.268224	H	0.133155	0.61511	-0.885029
F	7.611293	2.70693	-2.623482	C	-1.961382	-2.353177	0.424334
F	9.084122	2.747604	1.666005	C	-2.631151	-1.22868	-0.117591
F	7.865517	0.400125	2.221517	H	-2.281164	0.704032	-1.050515
C	6.328311	-1.018447	0.224544	H	-2.549157	-3.19588	0.779481
C	7.086318	-2.114392	0.573592	C	4.070292	-0.978735	0.001505
C	6.539576	-3.375656	0.977355	C	5.128599	-0.298443	0.630828
N	6.156159	-4.416162	1.331191	C	4.418374	-2.117534	-0.750223
C	8.51841	-2.061048	0.593695	C	6.443621	-0.735316	0.544573
N	9.682027	-2.03856	0.602771	C	5.726677	-2.564623	-0.84739
C	4.863532	-1.030427	0.05886	C	6.787748	-1.894075	-0.19074
C	4.184659	0.127181	0.506689	H	7.207914	-0.146554	1.035658
C	4.281598	-2.174497	-0.536966	H	5.924842	-3.453665	-1.43357
C	2.825519	0.413251	0.542898	C	2.428845	0.92631	0.284604
H	4.817644	0.90557	0.922058	C	3.022663	1.863486	-0.579289
C	2.949689	-2.467929	-0.791797	C	1.621519	1.43897	1.313573
H	4.980551	-2.928367	-0.880711	C	2.781144	3.224864	-0.461189
C	1.740939	-0.360403	0.117351	C	1.390779	2.799753	1.460141
H	2.565902	1.380882	0.968731	H	1.181935	0.752589	2.030825
C	1.798566	-1.719283	-0.514076	C	1.944155	3.74132	0.558432
H	2.773185	-3.422999	-1.283076	H	3.226981	3.891216	-1.189195
C	0.397613	-0.004639	0.18655	H	0.800155	3.127764	2.305867
C	0.489698	-2.093643	-0.788968	N	1.693888	5.105678	0.652294
H	0.017909	0.925242	0.591293	N	8.093487	-2.369243	-0.28168
C	-0.390051	-1.054071	-0.363708	C	0.74199	5.620852	1.637117
H	0.191833	-3.027934	-1.246397	C	-0.00666	6.876893	1.183807
C	-1.816127	-1.081223	-0.475867	H	1.241963	5.817351	2.601392
C	-2.621346	-2.049708	-1.055403	H	-0.004516	4.846659	1.818569
S	-2.816495	0.24744	0.123071	H	-0.723387	7.165577	1.959045
C	-3.995409	-1.749061	-1.057167	H	0.657288	7.730287	1.0205
H	-2.214973	-2.952044	-1.497696	H	-0.56109	6.688017	0.260257
C	-4.284226	-0.528624	-0.460082	C	2.671204	6.056899	0.111812
H	-4.758855	-2.387057	-1.482416	C	2.347303	6.58802	-1.290284
N	-5.525514	0.03461	-0.246605	H	3.658582	5.582339	0.109846
C	-6.686295	-0.801172	-0.163744	H	2.74623	6.897314	0.811796
C	-6.711477	-1.914421	0.680227	H	3.135989	7.270589	-1.626049
C	-7.827399	-0.493908	-0.921207	H	2.269399	5.774261	-2.016448
C	-7.84635	-2.722619	0.763444	H	1.399348	7.131556	-1.301534
H	-5.83643	-2.155811	1.274488	C	9.167003	-1.72905	0.478577
C	-8.964375	-1.282912	-0.830538	C	10.293542	-2.682008	0.886716
H	-7.816527	0.369728	-1.577823	H	8.733644	-1.326173	1.395091
C	-8.983211	-2.407801	0.008721	H	9.590666	-0.874904	-0.077735
H	-7.834767	-3.579369	1.426172	H	11.026976	-2.1347	1.487307
H	-9.851638	-1.054912	-1.411451	H	9.906034	-3.508466	1.489504
C	-5.6824	1.449836	-0.095733	H	10.824849	-3.101979	0.028255
C	-6.395686	1.965196	0.989296	C	8.491822	-3.146396	-1.461635
C	-5.146988	2.336945	-1.043842	C	8.492634	-4.666821	-1.261162
C	-6.577716	3.340539	1.137107	H	9.493914	-2.817253	-1.760395
H	-6.816232	1.285036	1.722582	H	7.83204	-2.882794	-2.295087
C	-5.308501	3.706028	-0.893425	H	8.780445	-5.169396	-2.191299
H	-4.605123	1.946061	-1.898591	H	9.19727	-4.96594	-0.481056
C	-6.027613	4.220631	0.196752	H	7.503308	-5.030756	-0.970048
H	-7.135939	3.709986	1.988694	H	-0.103318	-3.279308	0.933995
H	-4.898814	4.400796	-1.618667	H	3.644016	-2.653673	-1.290447
O	-10.144708	-3.120676	0.017618	H	3.66421	1.512782	-1.382241
O	-6.136832	5.577567	0.245222	H	4.91408	0.595171	1.20799

C	-10.223871	-4.268868	0.849662
H	-11.223123	-4.679513	0.700435
H	-9.47802	-5.023405	0.569465
H	-10.094074	-4.010982	1.908326
C	-6.850909	6.158231	1.327029
H	-6.385498	5.920974	2.291922
H	-6.814405	7.236284	1.166397
H	-7.898071	5.830649	1.342265

C	-4.069665	-1.285068	-0.156118
C	-5.027829	-0.381496	-0.56227
H	-4.47511	-2.230723	0.193697
C	-4.687932	0.940157	-0.994385
N	-4.410971	2.035517	-1.277609
C	-6.454329	-0.745023	-0.50244
C	-7.376679	-0.265235	-1.410987
C	-6.892647	-1.654603	0.588546
C	-7.673529	-2.790004	0.315627
C	-6.527759	-1.384538	1.920085
C	-8.082368	-3.630337	1.349153
H	-7.94716	-3.02024	-0.708362
C	-6.952777	-2.217513	2.951515
H	-5.925574	-0.509353	2.141182
C	-7.72863	-3.343862	2.668371
H	-8.678374	-4.508676	1.121935
H	-6.678878	-1.987	3.976503
H	-8.054436	-3.996358	3.472858
C	-7.021746	0.433295	-2.609918
N	-6.785633	0.958921	-3.621347
C	-8.78735	-0.463085	-1.250381
N	-9.941363	-0.587351	-1.15872
H	1.991051	-2.501067	0.263386

D8Baz(r)A3

C	5.61665	-0.599743	0.134202
C	4.593971	-1.498227	0.239621
C	3.144639	-1.305537	0.193708
C	2.497049	-0.21976	-0.435773
C	2.317332	-2.30912	0.741946
C	1.114106	-0.13327	-0.478709
H	3.088573	0.550369	-0.915141
C	0.933266	-2.226797	0.691924
C	0.291165	-1.129911	0.086191
H	0.658464	0.700172	-1.004443
H	0.340225	-3.004751	1.162643
C	7.005853	-1.09594	-0.004769
C	8.098524	-0.403403	0.545863
C	7.304401	-2.292278	-0.683677
C	9.400223	-0.879801	0.45353
C	8.597806	-2.782815	-0.780481
C	9.69414	-2.096612	-0.204389
H	10.192199	-0.277352	0.880151
H	8.755263	-3.717632	-1.304436
C	5.422926	0.872083	0.20916
C	5.990901	1.742032	-0.736898
C	4.692952	1.463157	1.252022
C	5.802113	3.116504	-0.675222
C	4.515776	2.838476	1.341054
H	4.271321	0.828733	2.025718
C	5.049807	3.712631	0.365383
H	6.227218	3.730721	-1.459717
H	3.985881	3.228339	2.200756
N	4.858008	5.093221	0.405056
N	10.985797	-2.613685	-0.296743
C	4.002837	5.687588	1.432013
C	3.305755	6.977369	0.991439
H	4.569625	5.874745	2.360958
H	3.223559	4.964555	1.67779
H	2.653796	7.327325	1.798075
H	4.009259	7.784435	0.769197
H	2.689588	6.803898	0.10446

D8BazA3

C	-5.641286	-0.603148	-0.109987
C	-4.61194	-1.500078	-0.169172
C	-3.165476	-1.303572	-0.122809
C	-2.520043	-0.180584	0.444001
C	-2.335369	-2.341144	-0.604238
C	-1.139256	-0.095999	0.49413
H	-3.114402	0.620643	0.865064
C	-0.953867	-2.254182	-0.557469
C	-0.311782	-1.123619	-0.010944
H	-0.68617	0.772319	0.961473
H	-0.359666	-3.065599	-0.965012
C	-7.027558	-1.103379	0.039802
C	-8.119092	-0.44914	-0.558292
C	-7.324253	-2.266272	0.775735
C	-9.417553	-0.932362	-0.457737
C	-8.614852	-2.762154	0.88297
C	-9.708854	-2.116395	0.258261
H	-10.210006	-0.360313	-0.923498
H	-8.771995	-3.670221	1.452402
C	-5.459545	0.865107	-0.247267
C	-6.047437	1.768678	0.654329
C	-4.724395	1.41897	-1.306992
C	-5.872733	3.141075	0.535566
C	-4.561587	2.791071	-1.453512
H	-4.287033	0.756829	-2.047996
C	-5.116082	3.700174	-0.522158
H	-6.311513	3.783673	1.289199
H	-4.026152	3.14966	-2.323388
N	-4.939587	5.079988	-0.61918
N	-10.997545	-2.639884	0.359789
C	-4.075914	5.639819	-1.65825
C	-3.396807	6.953204	-1.261588
H	-4.63178	5.783744	-2.601394
H	-3.287058	4.914717	-1.863836
H	-2.735951	7.275557	-2.072496
H	-4.110602	7.762182	-1.083144
H	-2.792441	6.822023	-0.359381

C	5.862253	5.970883	-0.207551	C	-5.963785	5.971089	-0.061465
C	5.500739	6.480138	-1.608325	C	-5.629123	6.550843	1.318434
H	6.8195	5.439583	-0.241752	H	-6.913896	5.428095	-0.014169
H	6.01951	6.825494	0.46103	H	-6.123975	6.790837	-0.771919
H	6.309077	7.105414	-2.003744	H	-6.451516	7.182573	1.672497
H	5.340455	5.651271	-2.303448	H	-5.467745	5.758147	2.054397
H	4.585792	7.077915	-1.590906	H	-4.722237	7.160068	1.285499
C	12.098822	-1.939482	0.370719	C	-12.101543	-2.017892	-0.37009
C	13.221409	-2.881018	0.81483	C	-13.213329	-2.993218	-0.765595
H	11.707841	-1.455236	1.266663	H	-11.69665	-1.595241	-1.290921
H	12.518515	-1.141627	-0.266735	H	-12.534643	-1.179321	0.203097
H	13.986388	-2.303463	1.343576	H	-13.970462	-2.458457	-1.347907
H	12.840982	-3.648268	1.49543	H	-12.817876	-3.805506	-1.382353
H	13.71362	-3.379449	-0.02477	H	-13.718902	-3.432606	0.098765
C	11.324612	-3.489803	-1.424311	C	-11.351633	-3.438175	1.539437
C	11.293634	-4.988754	-1.101793	C	-11.314272	-4.956028	1.32281
H	12.323751	-3.213819	-1.781285	H	-12.356294	-3.140473	1.862255
H	10.643382	-3.275012	-2.254662	H	-10.682386	-3.165484	2.362484
H	11.531075	-5.574035	-1.997233	H	-11.567736	-5.476796	2.253049
H	12.020253	-5.24332	-0.32604	H	-12.026549	-5.26688	0.554185
H	10.307304	-5.29742	-0.744249	H	-10.321416	-5.287992	1.00651
H	2.780739	-3.162797	1.22953	H	-2.798864	-3.226115	-1.032483
H	6.502416	-2.843896	-1.164935	H	-6.523159	-2.785534	1.293116
H	6.575157	1.329229	-1.554136	H	-6.63531	1.384593	1.482864
H	7.924359	0.534317	1.063737	H	-7.946102	0.462627	-1.12098
C	-1.186929	-1.02985	0.03423	C	6.402985	-0.631834	0.222023
C	-1.745254	0.261001	0.197254	C	5.857434	-1.917598	-0.039073
C	-3.071256	0.672303	0.192292	C	4.539565	-2.33661	-0.16249
C	-1.904087	-2.231021	-0.173846	C	5.666727	0.55247	0.473709
C	-4.243058	-0.078994	0.030944	C	3.358711	-1.598899	-0.042766
C	-3.2728	-2.453849	-0.264583	C	4.294332	0.758413	0.503132
C	-4.335202	-1.546987	-0.18247	C	3.243979	-0.140157	0.284406
H	-1.024418	1.050236	0.385286	H	6.594071	-2.704498	-0.182247
H	-3.228235	1.738527	0.349305	H	4.406379	-3.393779	-0.386791
H	-1.288506	-3.113473	-0.316426	H	6.251292	1.436316	0.690779
H	-3.562866	-3.489388	-0.438829	H	3.98761	1.77719	0.734213
C	-5.542887	0.428842	0.046533	C	2.06056	-2.083343	-0.183698
H	-5.80417	1.46755	0.18236	H	1.806648	-3.113327	-0.396486
C	-6.448187	-0.653865	-0.150496	C	1.139781	-1.024058	0.041837
C	-5.692525	-1.852761	-0.29074	C	1.885142	0.154305	0.3296
H	-6.109072	-2.839758	-0.452739	H	1.47309	1.135997	0.52159
C	-7.87963	-0.669095	-0.217359	C	7.857196	-0.622095	0.233045
C	-8.79575	0.354462	-0.117083	C	8.795557	0.381561	0.285342
H	-8.307909	-1.652515	-0.390758	H	8.295045	-1.615117	0.194104
C	-8.367907	1.695545	0.144875	C	8.466657	1.774464	0.241007
N	-8.001546	2.765737	0.421025	N	8.224296	2.908716	0.133907
C	-10.237776	0.079717	-0.227192	C	10.233525	0.03055	0.31463
C	-11.127483	0.997611	-0.748367	C	11.141373	0.764722	1.048196
C	-10.727932	-1.238519	0.253801	C	10.678808	-1.140197	-0.481968
C	-11.562273	-2.036044	-0.547069	C	11.516366	-2.121693	0.074829
C	-10.358438	-1.706835	1.527923	C	10.262887	-1.280349	-1.819176
C	-12.018922	-3.267817	-0.082916	C	11.932937	-3.209625	-0.689202
H	-11.839793	-1.696111	-1.538926	H	11.827308	-2.039685	1.110522
C	-10.830614	-2.930843	1.994096	C	10.695253	-2.360456	-2.583411
H	-9.71538	-1.098437	2.155431	H	9.616581	-0.528177	-2.259541
C	-11.659364	-3.715484	1.189019	C	11.529364	-3.328832	-2.019847
H	-12.655964	-3.876754	-0.716674	H	12.572839	-3.964204	-0.242746
H	-10.551885	-3.271827	2.986426	H	10.381714	-2.445752	-3.619259
H	-12.021624	-4.672852	1.551378	H	11.860901	-4.17428	-2.615071
C	-10.731839	2.195354	-1.426934	C	10.759876	1.768157	1.997101
N	-10.46783	3.154748	-2.030885	N	10.496178	2.554626	2.813476
C	-12.547378	0.808485	-0.689999	C	12.557381	0.560409	0.954217

N	-13.706797	0.707917	-0.65699	N	13.714302	0.441101	0.905742
H	4.884277	-2.538877	0.370092	H	-4.898694	-2.546239	-0.257301
		D8A5				**D8Baz(r)A5**	
C	2.30101	-0.409422	-0.013087	C	5.368105	-0.582769	0.150333
C	1.213782	-1.240935	-0.055406	C	4.314005	-1.449606	0.203811
C	-0.200767	-0.945978	-0.240027	C	2.876556	-1.210823	0.078651
C	-0.71162	0.227024	-0.845891	C	2.30163	-0.11893	-0.608198
C	-1.143773	-1.928027	0.14239	C	1.987204	-2.173841	0.60236
C	-2.067946	0.407311	-1.044354	C	0.927541	0.001602	-0.745649
H	-0.029066	1.001121	-1.171406	H	2.94361	0.635991	-1.044752
C	-2.503059	-1.739914	-0.029067	C	0.611234	-2.040012	0.487378
C	-3.008432	-0.569244	-0.639489	C	0.041263	-0.946703	-0.193515
H	-2.403392	1.329716	-1.500484	H	0.528953	0.86736	-1.265331
H	-3.186308	-2.521427	0.286056	H	-0.030494	-2.817666	0.88982
C	3.659335	-0.990816	-0.052132	C	6.746487	-1.120541	0.084806
C	4.739302	-0.391914	0.621988	C	7.829031	-0.460131	0.692268
C	3.942805	-2.179924	-0.751937	C	7.043644	-2.327034	-0.576942
C	6.009983	-0.950439	0.627255	C	9.118355	-0.976436	0.669848
C	5.205858	-2.749895	-0.755598	C	8.324769	-2.856487	-0.605478
C	6.286073	-2.160581	-0.052522	C	9.409248	-2.203052	0.028614
H	6.795425	-0.417869	1.147969	H	9.904927	-0.39796	1.137618
H	5.351808	-3.671455	-1.305368	H	8.481582	-3.796302	-1.120584
C	2.192111	1.062998	0.137061	C	5.213858	0.893989	0.215324
C	2.891477	1.946185	-0.703537	C	5.853512	1.746488	-0.700395
C	1.408395	1.639849	1.149279	C	4.44844	1.506307	1.219824
C	2.774932	3.323523	-0.577011	C	5.699413	3.125666	-0.648344
C	1.304717	3.015659	1.306576	C	4.30557	2.886034	1.300414
H	0.886406	0.991538	1.846553	H	3.970834	0.88469	1.971055
C	1.969284	3.907923	0.431139	C	4.912312	3.743799	0.353163
H	3.298076	3.951465	-1.287428	H	6.180041	3.727068	-1.410292
H	0.726652	3.389634	2.141732	H	3.743654	3.291223	2.132155
N	1.852419	5.290611	0.536545	N	4.757107	5.129157	0.382961
N	7.54277	-2.757648	-0.04831	N	10.687115	-2.759042	0.005513
C	0.947836	5.885536	1.520897	C	3.871633	5.749038	1.368565
C	0.339619	7.220356	1.082375	C	3.228689	7.054851	0.893998
H	1.453354	6.013411	2.493766	H	4.400879	5.925036	2.32147
H	0.122948	5.190351	1.681677	H	3.063647	5.047382	1.580802
H	-0.353025	7.569681	1.854636	H	2.553104	7.426084	1.671182
H	1.090798	8.002485	0.941846	H	3.962511	7.84165	0.698622
H	-0.218827	7.106892	0.148715	H	2.645616	6.89405	-0.017506
C	2.935116	6.143511	0.03254	C	5.813328	5.977733	-0.181425
C	2.696975	6.724946	-1.366457	C	5.534402	6.490405	-1.599594
H	3.86834	5.569977	0.042593	H	6.757146	5.421947	-0.166623
H	3.080837	6.961673	0.747429	H	5.959352	6.830682	0.491723
H	3.556354	7.330826	-1.674623	H	6.373676	7.099416	-1.953708
H	2.554738	5.934113	-2.108196	H	5.394363	5.663319	-2.301202
H	1.80776	7.359964	-1.387029	H	4.631069	7.105017	-1.629395
C	8.631861	-2.192149	0.748432	C	11.781046	-2.122045	0.738181
C	9.622071	-3.232947	1.278047	C	12.847972	-3.099605	1.23793
H	8.192066	-1.69379	1.613032	H	11.355318	-1.630123	1.613942
H	9.178058	-1.421113	0.178105	H	12.259689	-1.334499	0.130148
H	10.373237	-2.731251	1.896322	H	13.599282	-2.548525	1.812482
H	9.112247	-3.977533	1.896326	H	12.407014	-3.858394	1.890927
H	10.155359	-3.755613	0.479282	H	13.370862	-3.608412	0.423476
C	7.924254	-3.639332	-1.157835	C	11.061151	-3.644222	-1.103825
C	7.743539	-5.136567	-0.879423	C	10.962522	-5.142173	-0.790105
H	8.973265	-3.43752	-1.403288	H	12.087911	-3.400881	-1.400985
H	7.351713	-3.354387	-2.047005	H	10.436717	-3.405001	-1.971385
H	8.026913	-5.721661	-1.761355	H	11.2341	-5.732269	-1.672551
H	8.36368	-5.462734	-0.04064	H	11.632769	-5.422642	0.02643
H	6.704568	-5.372803	-0.633492	H	9.947201	-5.420027	-0.493775

H	-0.788325	-2.850909	0.592047
H	3.156009	-2.65889	-1.326776
H	3.518221	1.543189	-1.493676
H	4.577434	0.535343	1.161816
C	-4.447174	-0.413422	-0.823434
C	-5.067212	0.353999	-1.78837
C	-5.33656	-1.154229	0.122651
C	-6.17928	-2.188311	-0.295004
C	-5.353485	-0.848143	1.487011
C	-6.971305	-2.844296	0.646696
C	-6.192198	-1.56593	2.336719
C	-4.389022	1.02849	-2.852445
N	-3.889628	1.588171	-3.742975
C	-6.490621	0.514128	-1.808987
N	-7.644847	0.663921	-1.834134
H	1.420135	-2.303562	0.052989
F	-4.583222	0.130193	1.97506
F	-6.224733	-2.556788	-1.578844
F	-6.205659	-1.261497	3.634845
F	-7.762157	-3.836533	0.240597
N	-6.975402	-2.539534	1.925831

H	2.39513	-3.045364	1.107487
H	6.251664	-2.854916	-1.099614
H	6.466971	1.316535	-1.486852
H	7.65625	0.483666	1.199444
C	-1.426727	-0.806182	-0.336596
C	-1.903997	-0.283996	-1.563974
C	-3.200974	-0.032252	-1.987684
C	-2.219336	-1.207071	0.764673
C	-4.417107	-0.234974	-1.320795
C	-3.599146	-1.201181	0.926408
C	-4.601714	-0.783594	0.043579
H	-1.136274	-0.07558	-2.301969
H	-3.291315	0.369297	-2.995959
H	-1.661013	-1.54457	1.631916
H	-3.954195	-1.56244	1.89078
C	-5.682771	0.042934	-1.837892
H	-5.870561	0.461011	-2.814503
C	-6.655585	-0.301301	-0.855273
C	-5.97543	-0.802555	0.291341
H	-6.439023	-1.159709	1.20066
C	-8.09439	-0.191282	-0.937413
C	-8.837156	0.14388	-2.051804
C	-8.864553	-0.475884	0.314507
C	-9.613465	-1.64409	0.469722
C	-8.862661	0.415816	1.389379
C	-10.302237	-1.85675	1.662952
C	-9.592028	0.101543	2.534412
C	-8.287537	0.412113	-3.343536
N	-7.879611	0.639176	-4.41015
C	-10.263599	0.249693	-1.984695
N	-11.423213	0.345991	-1.945767
H	4.563934	-2.498016	0.354052
F	-8.172766	1.559883	1.32344
F	-9.67189	-2.551191	-0.510363
F	-9.585915	0.958606	3.556153
F	-11.007422	-2.978265	1.806871
N	-10.288542	-1.006372	2.666019

D8BazA5

C	5.393985	-0.614142	0.097686
C	4.323278	-1.462276	0.121682
C	2.890103	-1.194487	0.025894
C	2.323176	-0.046881	-0.573973
C	1.992229	-2.180895	0.491714
C	0.95089	0.109294	-0.669422
H	2.972305	0.716705	-0.98396
C	0.618979	-2.021554	0.400732
C	0.055375	-0.866041	-0.178146
H	0.559529	0.99392	-1.161264
H	-0.029299	-2.795896	0.797896
C	6.761413	-1.175222	0.001113
C	7.858219	-0.561764	0.631795
C	7.033631	-2.357811	-0.712616
C	9.137318	-1.101293	0.582974
C	8.304509	-2.909995	-0.767867
C	9.402427	-2.305006	-0.109935
H	9.936489	-0.55821	1.071347
H	8.442446	-3.830364	-1.322321
C	5.272012	0.861642	0.226384
C	5.916534	1.737054	-0.663862
C	4.537508	1.448284	1.268469
C	5.796034	3.116014	-0.551667

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N	-1.598594	-0.05416	-0.276995
C	-0.224263	-0.258001	-0.301044
C	0.633532	0.656257	-0.95769
C	0.362162	-1.376114	0.338115
C	2.002065	0.48289	-0.930484
H	0.209326	1.50055	-1.487062
C	1.731899	-1.553632	0.338035
H	-0.268235	-2.082726	0.863769
C	2.594985	-0.61974	-0.275035
H	2.629538	1.196503	-1.455171
H	2.147777	-2.398781	0.87493
C	-2.148129	1.264128	-0.383956
C	-1.672751	2.305228	0.419791
C	-3.198675	1.518961	-1.279609
C	-2.218405	3.586269	0.324601
H	-0.86403	2.120446	1.119976
C	-3.756793	2.785381	-1.366532
H	-3.575349	0.715278	-1.903739
C	-3.268857	3.832354	-0.56827
H	-1.826369	4.372398	0.958071
H	-4.568394	2.993967	-2.055327
C	-2.503032	-1.143846	-0.067492
C	-3.483438	-1.070911	0.92505

C	4.429416	2.826486	1.409375
H	4.056344	0.806692	2.000351
C	5.041195	3.708948	0.48874
H	6.277194	3.737946	-1.296744
H	3.89077	3.209147	2.266853
N	4.920573	5.095738	0.579111
N	10.669764	-2.884831	-0.158816
C	4.064259	5.694258	1.602484
C	3.44517	7.032553	1.190763
H	4.610775	5.819839	2.553719
H	3.243546	5.002756	1.798578
H	2.787892	7.386461	1.991426
H	4.194262	7.810204	1.017789
H	2.847679	6.92197	0.281166
C	5.992652	5.940907	0.040196
C	5.709105	6.530686	-1.346793
H	6.91954	5.357926	0.012122
H	6.174188	6.754794	0.752249
H	6.562817	7.128462	-1.685343
H	5.53087	5.743505	-2.084817
H	4.826579	7.175424	-1.332404
C	11.772683	-2.303945	0.60565
C	12.823402	-3.323014	1.054315
H	11.35328	-1.851408	1.505472
H	12.265093	-1.493318	0.040073
H	13.582057	-2.815045	1.658257
H	12.368924	-4.108285	1.66545
H	13.340097	-3.796424	0.214845
C	11.031183	-3.713422	-1.315035
C	10.916085	-5.225045	-1.082879
H	12.060062	-3.465764	-1.601901
H	10.407167	-3.421065	-2.166435
H	11.181601	-5.769137	-1.99624
H	11.582753	-5.557288	-0.282938
H	9.897514	-5.507474	-0.802336
H	2.39445	-3.083613	0.944079
H	6.230053	-2.847926	-1.254028
H	6.50622	1.326564	-1.4784
H	7.70499	0.362919	1.178882
C	-6.602199	-0.046158	-0.64263
C	-6.150426	-1.336827	-0.282668
C	-4.856014	-1.817858	-0.12033
C	-5.810953	1.09882	-0.87608
C	-3.636914	-1.147113	-0.243221
C	-4.427383	1.245637	-0.850468
C	-3.435491	0.29668	-0.596884
H	-6.929072	-2.079979	-0.138945
H	-4.781983	-2.871715	0.142805
H	-6.357354	2.013101	-1.078846
H	-4.066358	2.250809	-1.060565
C	-2.370368	-1.694091	-0.055702
H	-2.177166	-2.730211	0.188679
C	-1.387721	-0.689407	-0.275395
C	-2.060042	0.518614	-0.604007
H	-1.591948	1.47368	-0.801769
C	-8.068468	0.105582	-0.765566
C	-8.690618	0.834945	-1.750472
C	-8.919097	-0.57777	0.250121
C	-9.862558	-1.554789	-0.085205
C	-8.789033	-0.277609	1.611124
C	-10.604913	-2.161244	0.927808
C	-9.590594	-0.942394	2.536181
C	-2.438346	-2.289881	-0.877502
C	-4.388317	-2.115905	1.115807
H	-3.542924	-0.187626	1.552369
C	-3.323083	-3.33979	-0.682854
H	-1.688354	-2.351787	-1.659349
C	-4.308473	-3.261572	0.314247
H	-5.138357	-2.028882	1.892317
H	-3.280526	-4.229596	-1.30166
O	-3.880096	5.038086	-0.735807
C	-3.428707	6.136707	0.043959
H	-4.043837	6.987256	-0.251817
H	-3.560626	5.951289	1.11726
H	-2.374444	6.366521	-0.154657
O	-5.132018	-4.341113	0.416965
C	-6.142495	-4.327331	1.415377
H	-6.852073	-3.504629	1.261224
H	-6.669152	-5.277667	1.321901
H	-5.713844	-4.249446	2.422355
C	4.047069	-0.778449	-0.250617
C	4.674426	-2.002334	-0.464502
C	4.916619	0.368008	-0.008893
C	4.629298	1.504358	0.690965
H	5.933747	0.295876	-0.384101
C	3.973048	-3.185075	-0.850628
N	3.443727	-4.168465	-1.181659
C	6.089583	-2.154757	-0.331646
N	7.244793	-2.268191	-0.231352
C	3.412476	1.779501	1.401759
N	2.473314	2.071572	2.022932
C	5.630753	2.527372	0.806394
N	6.433634	3.364218	0.894986

C	-8.007347	1.419242	-2.867128
N	-7.513197	1.901371	-3.803865
C	-10.108703	1.047549	-1.749636
N	-11.255845	1.242154	-1.75655
H	4.556371	-2.520609	0.221805
F	-7.917738	0.648963	2.022537
F	-10.044383	-1.922916	-1.356906
F	-9.464824	-0.642555	3.82841
F	-11.491682	-3.098538	0.598787
N	-10.470809	-1.860796	2.200735

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N	-4.768809	-0.014563	-0.107871
C	-3.370951	-0.042354	-0.135724
C	-2.634684	0.915428	-0.866119
C	-2.647558	-1.032115	0.563889
C	-1.249931	0.883598	-0.883854
H	-3.160631	1.672079	-1.43627
C	-1.263375	-1.064281	0.519758
H	-3.181581	-1.764529	1.15764
C	-0.51686	-0.107894	-0.199103
H	-0.72498	1.613986	-1.491446
H	-0.746125	-1.81856	1.104186
C	-5.488061	1.203	-0.319216
C	-5.188933	2.352373	0.418257
C	-6.531399	1.25498	-1.258014
C	-5.896435	3.539421	0.218362
H	-4.392335	2.321895	1.154743
C	-7.252119	2.424393	-1.448768
H	-6.774773	0.367725	-1.833227
C	-6.93845	3.579587	-0.7158
H	-5.636971	4.412701	0.804508
H	-8.060067	2.472786	-2.171061
C	-5.52263	-1.204991	0.136965
C	-6.523229	-1.222391	1.111933
C	-5.294814	-2.367347	-0.619317
C	-7.289259	-2.36784	1.336216
H	-6.710317	-0.328501	1.697977
C	-6.038122	-3.51551	-0.389759
H	-4.529096	-2.363119	-1.3883
C	-7.04526	-3.525619	0.588027
H	-8.059692	-2.346695	2.09748
H	-5.869315	-4.417174	-0.968849
O	-7.701881	4.676914	-0.984369
C	-7.434873	5.873689	-0.26869
H	-8.151376	6.609612	-0.635508
H	-7.57638	5.739408	0.811249
H	-6.416482	6.237906	-0.454696
O	-7.724111	-4.699911	0.725858
C	-8.757225	-4.769528	1.697288
H	-9.557428	-4.048104	1.488777
H	-9.160681	-5.780891	1.635101
H	-8.372337	-4.596284	2.710242
C	0.960196	-0.144129	-0.23309
C	1.571535	-1.422627	-0.241748
C	2.912755	-1.776838	-0.263928
C	1.634992	1.100924	-0.253804
C	4.053993	-0.96479	-0.298267
C	2.993179	1.385139	-0.28751
C	4.09079	0.515941	-0.300145
H	0.88162	-2.259776	-0.268955
H	3.1102	-2.847714	-0.275965

D6BazA2

N	-4.788044	-0.020023	-0.123665
C	-3.389238	-0.061912	-0.145792
C	-2.642042	0.89468	-0.867749
C	-2.679158	-1.063337	0.552111
C	-1.259055	0.84922	-0.880719
H	-3.160177	1.663858	-1.428347
C	-1.295879	-1.099846	0.524347
H	-3.224909	-1.80152	1.127877
C	-0.53697	-0.146504	-0.187825
H	-0.723837	1.588442	-1.46753
H	-0.788423	-1.870266	1.095435
C	-5.491485	1.211806	-0.297006
C	-5.159485	2.341739	0.456744
C	-6.551436	1.299705	-1.214646
C	-5.850559	3.543726	0.293389
H	-4.349535	2.283986	1.176679
C	-7.255749	2.484443	-1.368697
H	-6.820155	0.428645	-1.80313
C	-6.909058	3.619653	-0.619697
H	-5.565058	4.400799	0.891286
H	-8.075798	2.560451	-2.074829
C	-5.554164	-1.207316	0.091857
C	-6.566209	-1.23426	1.055085
C	-5.325442	-2.358696	-0.681047
C	-7.342537	-2.377879	1.25112
H	-6.753443	-0.349516	1.654733
C	-6.079521	-3.505019	-0.479559
H	-4.550661	-2.347046	-1.440754
C	-7.097997	-3.5245	0.486205
H	-8.121131	-2.364139	2.004234
H	-5.910106	-4.397928	-1.071896
O	-7.658628	4.735007	-0.852238
C	-7.355279	5.913117	-0.120486
H	-8.06452	6.668991	-0.459946
H	-7.478649	5.761916	0.959484
H	-6.333821	6.261603	-0.319476
O	-7.786868	-4.696282	0.596348
C	-8.83176	-4.774111	1.554126
H	-9.624048	-4.043088	1.348589
H	-9.242175	-5.781151	1.470356
H	-8.457814	-4.620724	2.574417
C	6.17253	-0.319708	-0.254515
C	5.575255	0.855108	-0.763075
C	4.230579	1.178298	-0.901934
C	5.527861	-1.458838	0.269161
C	3.100005	0.437219	-0.548203
C	4.169285	-1.712082	0.43376
C	3.072113	-0.918727	0.093877
H	6.267065	1.609611	-1.127495
H	4.028866	2.148774	-1.351824

H	0.991021	1.972507	-0.197175	H	6.185658	-2.243486	0.629947
H	3.24479	2.444873	-0.283377	H	3.928541	-2.667178	0.896806
C	5.375924	-1.416164	-0.337623	C	1.775177	0.830336	-0.710067
H	5.682377	-2.452	-0.324242	H	1.462629	1.77833	-1.12736
C	6.233007	-0.284863	-0.336333	C	0.916685	-0.186118	-0.204543
C	5.435684	0.892806	-0.310404	C	1.73115	-1.244262	0.282884
H	5.801627	1.910447	-0.339692	H	1.380174	-2.174518	0.70935
C	7.683945	-0.282532	-0.399786	C	7.655011	-0.359055	-0.309503
C	8.428292	-1.244118	-1.06981	C	8.329924	-1.41096	-0.909213
C	8.44418	0.807491	0.221075	C	8.464178	0.719217	0.239218
C	8.160892	1.451727	1.386156	C	8.119972	1.620737	1.204978
H	9.365809	1.104456	-0.272031	H	9.484726	0.793949	-0.125752
C	7.856018	-2.325061	-1.807463	C	7.669129	-2.476114	-1.597714
N	7.442143	-3.221679	-2.424599	N	7.186744	-3.358166	-2.184817
C	9.858098	-1.207328	-1.071664	C	9.759055	-1.495663	-0.904283
N	11.022216	-1.164835	-1.077658	N	10.921998	-1.55546	-0.904768
C	7.092739	1.126336	2.28958	C	6.886664	1.654015	1.936716
N	6.285738	0.902131	3.096157	N	5.935399	1.734564	2.601268
C	9.024187	2.510994	1.831497	C	9.077081	2.615359	1.600964
N	9.712087	3.377502	2.189483	N	9.846586	3.42774	1.91836

D7Bet(n=16)A4

N	21.46375	0.16338	-0.172518	N	19.516784	0.443569	-0.058732
C	21.978729	1.494906	-0.242565	C	19.93607	1.791882	-0.281014
C	21.591248	2.36146	-1.278246	C	19.525059	2.490802	-1.428197
C	22.89004	1.950632	0.714161	C	20.775189	2.431699	0.635573
C	22.092351	3.653222	-1.339336	C	19.932459	3.799704	-1.638398
H	20.894692	2.01395	-2.033989	H	18.884335	1.999273	-2.152735
C	23.413852	3.242333	0.647097	C	21.205783	3.741481	0.419876
H	23.196536	1.287606	1.516455	H	21.099069	1.899332	1.523743
C	23.010664	4.105007	-0.379243	C	20.779911	4.436182	-0.718618
H	21.798153	4.330368	-2.13411	H	19.619447	4.348065	-2.520482
H	24.120044	3.564212	1.40286	H	21.857768	4.208286	1.148097
C	22.370533	-0.926716	0.012727	C	20.488103	-0.540604	0.305288
C	22.120842	-1.92076	0.963248	C	20.25732	-1.425523	1.362459
C	23.542614	-1.004496	-0.757166	C	21.704084	-0.621622	-0.393047
C	23.010333	-2.981881	1.140944	C	21.208856	-2.383806	1.715956
H	21.220347	-1.869759	1.566135	H	19.323653	-1.369712	1.912063
C	24.43983	-2.04613	-0.572329	C	22.661703	-1.55871	-0.034123
H	23.74625	-0.239174	-1.498644	H	21.893381	0.058935	-1.216391
C	24.180305	-3.04783	0.375031	C	22.421956	-2.452205	1.020607
H	22.786021	-3.736676	1.885039	H	20.997999	-3.055739	2.539136
H	25.347614	-2.113397	-1.162506	H	23.603699	-1.627714	-0.567798
C	17.576404	0.013135	-0.113233	C	15.652199	-0.003746	-0.102683
C	18.067796	-1.150858	-0.68182	C	16.251052	-1.17932	-0.527002
S	18.918921	1.063771	0.34875	S	16.89314	1.191782	0.284092
C	19.473902	-1.203261	-0.78478	C	17.659798	-1.131471	-0.580313
H	17.420758	-1.936589	-1.05521	H	15.679841	-2.049654	-0.829818
C	20.102872	-0.076726	-0.281681	C	18.182734	0.087804	-0.182978
H	20.021457	-2.029582	-1.220232	H	18.284632	-1.953826	-0.905326
O	23.449421	5.386976	-0.536389	O	21.131568	5.717901	-1.025755
O	25.12047	-4.03267	0.470604	O	23.424097	-3.340145	1.285545
C	24.37495	5.901244	0.408916	C	21.988152	6.412163	-0.131932
H	23.954427	5.912316	1.422533	H	21.534559	6.521194	0.861437
H	25.309952	5.326543	0.414711	H	22.958881	5.910368	-0.029758
H	24.585741	6.925006	0.09715	H	22.139621	7.400751	-0.567196
C	24.911279	-5.070125	1.415916	C	23.235498	-4.269371	2.341382
H	23.991079	-5.630355	1.206005	H	22.372223	-4.921661	2.157311
H	25.767376	-5.739608	1.322707	H	24.141882	-4.875281	2.374936
H	24.867856	-4.68139	2.441392	H	23.103485	-3.764629	3.307025
C	-23.182827	0.154947	0.04389	C	-17.604409	0.310271	0.161221
C	-24.445097	-0.344559	-0.179772	C	-16.508206	1.154598	0.483531

D7Beta(n=11)A4

H	-23.063004	1.164004	0.432096	C	-17.518941	-1.0245	-0.31072
H	-24.524267	-1.356606	-0.571794	C	-15.142276	0.929137	0.424505
C	-25.679614	0.315951	0.043113	H	-16.787832	2.146399	0.832475
C	-26.929187	-0.232679	-0.208183	C	-16.409089	-1.812422	-0.568649
C	-25.89764	1.719137	0.592597	H	-18.466646	-1.517554	-0.49977
C	-27.943688	0.730737	0.144581	C	-14.445143	-0.220492	0.026411
O	-27.356736	1.850227	0.603767	H	-14.51701	1.765844	0.732082
C	-29.321548	0.673784	0.083543	C	-15.044824	-1.512835	-0.438481
C	-27.127198	-1.537542	-0.729199	H	-16.625884	-2.817566	-0.926589
N	-27.186703	-2.618763	-1.157939	C	-13.064365	-0.374545	-0.006834
C	-30.022765	-0.471584	-0.389738	C	-13.985036	-2.365941	-0.720401
N	-30.636241	-1.38628	-0.769402	H	-12.348479	0.387002	0.27459
C	-30.092112	1.79689	0.506801	C	-12.755489	-1.690213	-0.464192
N	-30.72709	2.710682	0.851132	H	-14.072411	-3.383982	-1.080258
C	-25.378189	2.831392	-0.32565	C	-18.908421	0.919802	0.351577
H	-25.726465	3.798434	0.046088	C	-20.140314	0.381357	0.102437
H	-24.28642	2.840548	-0.35502	H	-18.870863	1.933706	0.738971
H	-25.751032	2.693338	-1.343299	H	-20.215997	-0.626765	-0.29409
C	-25.443341	1.886204	2.047088	C	-21.39601	1.022963	0.311016
H	-25.876735	1.103843	2.674587	C	-22.623503	0.445715	0.038974
H	-24.355478	1.831268	2.127611	C	-21.65429	2.419535	0.860034
H	-25.774445	2.858238	2.421534	C	-23.669784	1.384158	0.377795
C	-9.631958	-1.073287	-0.207741	O	-23.116876	2.514817	0.848041
C	-8.421114	-0.461896	0.003332	C	-25.042771	1.289559	0.293026
H	-9.63867	-2.106746	-0.553932	C	-22.782104	-0.863188	-0.487999
H	-8.419409	0.572612	0.348442	N	-22.808252	-1.944306	-0.91951
C	-7.158733	-1.080806	-0.196975	C	-25.703598	0.125845	-0.194581
C	-5.953547	-0.45893	0.013178	N	-26.283501	-0.805178	-0.586549
H	-7.156271	-2.115227	-0.540525	C	-25.851311	2.390411	0.70512
H	-5.960349	0.576288	0.356082	N	-26.516425	3.285745	1.040141
C	-4.685613	-1.06807	-0.18563	C	-21.149507	3.547056	-0.048256
C	-3.48551	-0.437068	0.023933	H	-21.531806	4.502702	0.319238
H	-4.675142	-2.102946	-0.527805	H	-20.058286	3.588112	-0.05872
H	-3.499916	0.598404	0.365842	H	-21.500654	3.400884	-1.072465
C	-2.212606	-1.037021	-0.174461	C	-21.228946	2.594658	2.322551
C	-1.01729	-0.39769	0.034882	H	-21.651112	1.799304	2.94131
H	-2.194797	-2.071912	-0.516406	H	-20.141713	2.570494	2.422201
H	-1.038857	0.63763	0.376899	H	-21.5937	3.556229	2.692457
C	0.260294	-0.988536	-0.164028	C	11.843933	-0.044424	-0.046042
C	1.450855	-0.341187	0.045505	C	10.746738	-0.835669	-0.254438
H	0.285206	-2.023036	-0.506808	H	11.681442	0.993042	0.2489
H	1.422155	0.693592	0.388671	H	10.899916	-1.873214	-0.551688
C	-10.887858	-0.443479	-0.004641	C	9.402623	-0.387398	-0.108779
C	-12.105225	-1.042376	-0.216919	C	8.290346	-1.158473	-0.319546
H	-10.876215	0.589778	0.344033	H	9.258223	0.650756	0.192954
H	-12.122851	-2.074259	-0.567168	H	8.425084	-2.196582	-0.623611
C	2.733086	-0.922533	-0.15473	C	6.955641	-0.688028	-0.167212
C	3.918659	-0.267047	0.055457	C	5.829238	-1.439128	-0.379418
H	2.765263	-1.95624	-0.499372	H	6.829901	0.35055	0.141217
H	3.882472	0.766798	0.400783	H	5.945544	-2.477519	-0.689941
C	-13.353303	-0.399933	-0.009463	C	4.503929	-0.946955	-0.220505
C	-14.578358	-0.983567	-0.223147	C	3.364107	-1.678187	-0.433631
H	-13.329679	0.631407	0.344295	H	4.39656	0.091813	0.094069
H	-14.609317	-2.013101	-0.579028	H	3.462257	-2.716629	-0.750105
C	-15.816764	-0.326071	-0.00946	C	2.04824	-1.164876	-0.268366
C	-17.050969	-0.890801	-0.224584	C	0.895728	-1.876548	-0.48204
H	-15.778389	0.70252	0.351036	H	1.95884	-0.126112	0.051718
H	-17.098496	-1.917003	-0.587758	H	0.976179	-2.914849	-0.803839
C	-18.277222	-0.215064	-0.002469	C	-0.410667	-1.342736	-0.310906
C	-19.52227	-0.756306	-0.218746	C	-1.575174	-2.03517	-0.524972
H	-18.220447	0.809756	0.366423	H	-0.4826	-0.304164	0.014107
H	-19.590567	-1.777922	-0.590764	H	-1.511971	-3.07313	-0.851589

C	5.205744	-0.838038	-0.146823	C	-2.872029	-1.481381	-0.348417
C	6.385825	-0.173899	0.064549	C	-4.04797	-2.154666	-0.562905
H	5.24572	-1.870529	-0.494346	H	-2.926875	-0.443232	-0.018801
H	6.34143	0.858588	0.41304	H	-4.001814	-3.192025	-0.894131
C	-20.733204	-0.058342	0.014212	C	-5.335094	-1.581113	-0.381094
C	-21.990723	-0.570725	-0.202503	C	-6.52211	-2.234864	-0.596157
H	-20.652945	0.961495	0.39291	H	-5.372898	-0.543709	-0.046805
H	-22.08576	-1.586143	-0.58454	H	-6.493226	-3.271245	-0.932191
C	7.678206	-0.733224	-0.140417	C	-7.799191	-1.641274	-0.408807
C	8.851996	-0.05955	0.07274	C	-8.997047	-2.274475	-0.62453
H	7.726863	-1.764037	-0.491841	H	-7.819452	-0.60508	-0.069337
H	8.798318	0.971108	0.425415	H	-8.986989	-3.309377	-0.966063
C	10.150353	-0.605424	-0.135497	C	-10.263737	-1.659609	-0.430402
C	11.316685	0.079012	0.080171	C	-11.465818	-2.278687	-0.650181
H	10.208918	-1.634033	-0.49188	H	-10.260034	-0.626525	-0.085105
H	11.252168	1.107339	0.437921	H	-11.451945	-3.310239	-0.999441
C	12.622046	-0.451177	-0.131512	C	13.197588	-0.470076	-0.186746
C	13.77906	0.246114	0.086804	C	14.268962	0.351532	0.021843
H	12.692099	-1.477061	-0.493628	H	13.364933	-1.506937	-0.474616
H	13.702386	1.271638	0.450294	H	14.061094	1.37934	0.317036
C	15.092735	-0.26571	-0.129325				
C	16.229337	0.457264	0.096791				
H	15.172116	-1.288883	-0.493822				
H	16.110832	1.471066	0.477517				

D7Beta(r)(n=11)A4

N	19.570516	0.3222	-0.127113	N	18.087418	-0.30562	-0.223193
C	20.023716	1.668559	-0.28722	C	18.533913	1.050417	-0.289083
C	19.617622	2.436553	-1.391129	C	18.145769	1.884691	-1.35068
C	20.893559	2.236393	0.647827	C	19.379574	1.563275	0.698525
C	20.06049	3.742285	-1.540963	C	18.581713	3.20013	-1.407455
H	18.952913	2.001483	-2.130068	H	17.499767	1.493932	-2.129786
C	21.35913	3.542687	0.492584	C	19.838358	2.879667	0.636685
H	21.214008	1.649988	1.502663	H	19.685701	0.925902	1.521498
C	20.938388	4.306593	-0.602768	C	19.434794	3.709176	-0.416437
H	19.751755	4.343724	-2.389313	H	18.285999	3.852476	-2.22216
H	22.034261	3.952732	1.233846	H	20.494362	3.245861	1.417127
C	20.52446	-0.706874	0.149233	C	19.042851	-1.343002	0.01379
C	20.307016	-1.637431	1.169329	C	18.810385	-2.331694	0.974187
C	21.710062	-0.786129	-0.599366	C	20.243972	-1.373391	-0.713289
C	21.241772	-2.639165	1.436609	C	19.745556	-3.342411	1.202877
H	19.39681	-1.583084	1.757183	H	17.887462	-2.31627	1.544217
C	22.651496	-1.767577	-0.326475	C	21.185741	-2.364385	-0.477841
H	21.888804	-0.069642	-1.394116	H	20.434246	-0.611634	-1.461985
C	22.424692	-2.706772	0.690859	C	20.943751	-3.361426	0.479003
H	21.042078	-3.3456	2.233287	H	19.533685	-4.09456	1.953242
H	23.570091	-1.83589	-0.899544	H	22.116133	-2.395271	-1.034923
C	15.695074	-0.01364	-0.110908	C	14.218291	-0.672679	-0.336989
C	16.251865	-1.190602	-0.585822	C	14.798563	-1.815719	-0.856242
S	16.977536	1.132904	0.290531	S	15.475757	0.462538	0.160465
C	17.659888	-1.181377	-0.664827	C	16.209739	-1.793613	-0.897207
H	15.650126	-2.033763	-0.905926	H	14.210516	-2.643648	-1.235353
C	18.225301	0.008823	-0.237059	C	16.748547	-0.623833	-0.391629
H	18.254199	-2.009875	-1.028922	H	16.820655	-2.598009	-1.286559
O	21.32284	5.591691	-0.849188	O	19.813968	5.010509	-0.571732
O	23.408132	-3.63558	0.871067	O	21.9286	-4.295037	0.626173
C	22.207191	6.216381	0.068869	C	20.67017	5.581669	0.405491
H	21.766666	6.286215	1.071558	H	20.206214	5.58146	1.400059
H	23.165076	5.684694	0.13412	H	21.632233	5.056068	0.458536
H	22.380741	7.221569	-0.317305	H	20.841705	6.611689	0.090196
C	23.23287	-4.60965	1.888201	C	21.736902	-5.326594	1.581581
H	22.342934	-5.226514	1.709143	H	20.8537	-5.935315	1.349038

D7Baet(n=11)A4

H	24.120435	-5.242796	1.854985	H	22.627901	-5.953775	1.530585
H	23.155679	-4.149047	2.881429	H	21.637061	-4.924384	2.597908
C	-12.790897	-1.290305	-0.237563	C	7.674365	0.784556	0.188732
C	-13.839917	-2.149073	-0.672603	C	8.59315	1.799348	0.549566
C	-12.963083	-0.002883	0.339758	C	8.015363	-0.515263	-0.270514
C	-15.211956	-1.972678	-0.671607	C	9.983491	1.807825	0.555797
H	-13.502933	-3.099231	-1.079772	H	8.134003	2.729278	0.877975
C	-14.118002	0.71286	0.600074	C	9.254366	-1.096192	-0.47765
H	-12.048881	0.502041	0.6334	H	7.175219	-1.163226	-0.499308
C	-15.976956	-0.880716	-0.229168	C	10.882672	0.799688	0.199184
H	-15.78798	-2.804048	-1.07562	H	10.4407	2.739153	0.887386
C	-15.46192	0.376477	0.369437	C	10.541769	-0.567446	-0.291229
H	-13.964067	1.689843	1.056879	H	9.230984	-2.122217	-0.843107
C	-17.367489	-0.785999	-0.26819	C	12.277299	0.883433	0.230209
C	-16.571148	1.168127	0.665766	C	11.743968	-1.224449	-0.529653
H	-18.03338	-1.549342	-0.649649	H	12.843219	1.754111	0.537998
C	-17.750563	0.471026	0.279558	C	12.823373	-0.34585	-0.215758
H	-16.543232	2.154412	1.113867	H	11.839157	-2.241202	-0.888706
C	-19.073366	0.995039	0.44041	C	-20.778032	-0.086991	0.000628
C	-20.231188	0.366513	0.067927	C	-22.004974	-0.674729	-0.197732
H	-19.128508	1.978439	0.900101	H	-20.722077	0.934776	0.369421
H	-20.159768	-0.614215	-0.39528	H	-22.020012	-1.696921	-0.5707
C	-21.556396	0.861871	0.220296	C	-23.279963	-0.096385	0.032287
C	-22.698416	0.188553	-0.178348	C	-24.490465	-0.735642	-0.189405
C	-21.992227	2.185149	0.833523	C	-23.587422	1.298526	0.559635
C	-23.854494	0.995401	0.13945	C	-25.565564	0.161373	0.161655
O	-23.452965	2.138739	0.720005	O	-25.051957	1.327537	0.591047
C	-25.202725	0.775983	-0.052658	C	-26.936225	0.005926	0.122851
C	-22.687515	-1.089571	-0.796351	C	-24.603899	-2.06099	-0.683753
N	-22.577461	-2.135735	-1.295594	N	-24.593634	-3.151593	-1.092047
C	-25.709824	-0.408512	-0.659448	C	-27.560594	-1.195544	-0.318152
N	-26.167667	-1.360502	-1.150376	N	-28.11208	-2.15903	-0.67113
C	-26.143671	1.762987	0.366465	C	-27.77872	1.079867	0.536878
N	-26.91702	2.56483	0.706218	N	-28.471935	1.953149	0.873721
C	-21.543149	3.414378	0.034971	C	-23.160295	2.42612	-0.387026
H	-22.036661	4.304026	0.434451	H	-23.570511	3.373432	-0.027956
H	-20.462127	3.553975	0.101282	H	-22.072379	2.511269	-0.433152
H	-21.814791	3.307361	-1.017889	H	-23.536832	2.242419	-1.39607
C	-21.685091	2.301	2.330914	C	-23.125121	1.524445	2.003519
H	-22.06016	1.426063	2.867117	H	-23.493089	0.725531	2.651628
H	-20.610204	2.380447	2.50649	H	-22.035068	1.547495	2.067702
H	-22.173334	3.192836	2.731903	H	-23.518292	2.477698	2.366023
C	11.889209	0.049202	0.016295	C	3.831186	0.908381	0.223269
C	10.767427	-0.706064	-0.196041	C	2.695483	0.190384	-0.031416
H	11.760453	1.081089	0.345446	H	3.726516	1.93212	0.583669
H	10.887844	-1.737875	-0.526413	H	2.795117	-0.83379	-0.391125
C	9.438308	-0.227918	-0.014734	C	1.374354	0.695908	0.144053
C	8.303985	-0.965786	-0.228117	C	0.230182	-0.013361	-0.104534
H	9.325243	0.804722	0.317679	H	1.27932	1.721338	0.502479
H	8.408962	-1.998258	-0.561637	H	0.320143	-1.039111	-0.462173
C	6.983316	-0.468809	-0.043567	C	-1.08441	0.503735	0.075172
C	5.837904	-1.190451	-0.257414	C	-2.23674	-0.196253	-0.166846
H	6.885493	0.564446	0.291641	H	-1.169162	1.530796	0.431598
H	5.928228	-2.223443	-0.593512	H	-2.157408	-1.223538	-0.52247
C	4.525208	-0.6757	-0.070194	C	-3.544762	0.333015	0.017621
C	3.36959	-1.381672	-0.284495	C	-4.705279	-0.357047	-0.217629
H	4.441757	0.358007	0.267419	H	-3.618655	1.361562	0.372236
H	3.445861	-2.414993	-0.622964	H	-4.637135	-1.385685	-0.571524
C	2.064652	-0.849909	-0.094827	C	-6.006442	0.184873	-0.027894
C	0.89942	-1.540452	-0.309735	C	-7.175297	-0.494526	-0.256451
H	1.995073	0.184032	0.245149	H	-6.068916	1.214665	0.325352
H	0.961955	-2.573859	-0.650639	H	-7.118946	-1.524228	-0.609164

C	-0.397772	-0.99207	-0.117654	C	-8.469136	0.060609	-0.060844
C	-1.572307	-1.666973	-0.333463	C	-9.646651	-0.607096	-0.282963
H	-0.453632	0.041818	0.224973	H	-8.519488	1.091301	0.291762
H	-1.523602	-2.700137	-0.677211	H	-9.602956	-1.637461	-0.635326
C	-2.861516	-1.101891	-0.138648	C	-10.93245	-0.037885	-0.080654
C	-4.045358	-1.760323	-0.355697	C	-12.119212	-0.692348	-0.296659
H	-2.903307	-0.068444	0.207293	H	-10.969609	0.993262	0.272328
H	-4.011167	-2.792782	-0.703107	H	-12.089541	-1.722854	-0.649792
C	-5.326025	-1.177833	-0.157299	C	-13.395867	-0.107662	-0.086448
C	-6.519498	-1.818043	-0.376062	C	-14.592846	-0.746551	-0.296584
H	-5.352702	-0.145384	0.193121	H	-13.418121	0.923371	0.268224
H	-6.501269	-2.849159	-0.728361	H	-14.579398	-1.776512	-0.651892
C	-7.790775	-1.216509	-0.172819	C	-15.858661	-0.144151	-0.076721
C	-8.994243	-1.836111	-0.392925	C	-17.067305	-0.764019	-0.280972
H	-7.800179	-0.185769	0.183551	H	-15.863294	0.886042	0.281239
H	-8.994436	-2.864998	-0.75185	H	-17.073529	-1.792501	-0.640094
C	-10.25562	-1.212234	-0.181047	C	-18.319802	-0.14057	-0.049027
C	-11.456112	-1.824826	-0.416576	C	-19.541884	-0.736715	-0.246909
H	-10.227275	-0.186306	0.18108	H	-18.302299	0.887888	0.314019
H	-11.413831	-2.842796	-0.800183	H	-19.57364	-1.762419	-0.611615
C	13.227456	-0.408707	-0.16246	C	5.159846	0.412256	0.051027
C	14.325538	0.375707	0.051984	C	6.272353	1.155017	0.316682
H	13.360121	-1.44002	-0.486037	H	5.250704	-0.609956	-0.310257
H	14.152312	1.39863	0.384186	H	6.099788	2.169179	0.67518

D7Ba(r)et(n=11)A4

N	18.017992	-0.445818	-0.206154
C	18.53445	0.887755	-0.177005
C	18.246319	1.789686	-1.214444
C	19.347104	1.308	0.879227
C	18.746939	3.082567	-1.181337
H	17.626934	1.468307	-2.045338
C	19.871063	2.601183	0.908894
H	19.576005	0.616612	1.683541
C	19.566474	3.499425	-0.121032
H	18.5291	3.787804	-1.976263
H	20.499725	2.896383	1.740046
C	18.909332	-1.545865	-0.004706
C	18.577821	-2.59363	0.859109
C	20.147126	-1.579566	-0.667348
C	19.451442	-3.664575	1.054809
H	17.626321	-2.576752	1.37992
C	21.02771	-2.631616	-0.462451
H	20.414759	-0.772549	-1.341103
C	20.686826	-3.687036	0.396681
H	19.163217	-4.461387	1.729769
H	21.98591	-2.66513	-0.97001
C	14.13731	-0.577119	-0.456022
C	14.671832	-1.701617	-1.057813
S	15.445022	0.427691	0.177965
C	16.083374	-1.762009	-1.058281
H	14.059742	-2.445442	-1.55398
C	16.671426	-0.676309	-0.437071
H	16.65771	-2.560556	-1.510402
O	20.013962	4.785804	-0.189903
O	21.618226	-4.676819	0.51987
C	20.842353	5.267201	0.857552
H	20.326377	5.241748	1.825757
H	21.775012	4.693617	0.932565
H	21.0774	6.301579	0.603649
C	21.327443	-5.769164	1.377991
H	20.432988	-6.31455	1.050651

D7Baze(n=4)A4

N	16.883764	0.412219	0.02738
C	17.27757	1.772894	-0.163798
C	16.905662	2.471149	-1.324659
C	18.053192	2.425903	0.798275
C	17.288498	3.792012	-1.504278
H	16.315161	1.96969	-2.084209
C	18.45921	3.748231	0.614396
H	18.346653	1.894115	1.697293
C	18.072076	4.441984	-0.538466
H	17.005387	4.33991	-2.396689
H	19.061787	4.225082	1.377845
C	17.862621	-0.548858	0.431673
C	17.606944	-1.443967	1.474381
C	19.110116	-0.596602	-0.211941
C	18.565021	-2.38041	1.866475
H	16.648427	-1.413952	1.981579
C	20.07357	-1.511771	0.18588
H	19.319108	0.0923	-1.023524
C	19.80909	-2.416023	1.225438
H	18.33428	-3.061341	2.676829
H	21.039785	-1.555262	-0.305508
C	13.040144	-0.141621	-0.208666
C	13.692219	-1.300093	-0.600235
S	14.226239	1.089569	0.234825
C	15.099759	-1.212651	-0.584055
H	13.161398	-2.185901	-0.930319
C	15.567924	0.021254	-0.163931
H	15.762757	-2.01723	-0.876142
O	18.404611	5.735147	-0.81737
O	20.819629	-3.280905	1.531107
C	19.197515	6.442681	0.123641
H	18.692576	6.530649	1.094053
H	20.174673	5.964861	0.269901
H	19.344571	7.438887	-0.295445
C	20.60677	-4.220316	2.573329
H	19.767995	-4.891438	2.348381

H	22.19145	-6.432738	1.324006	H	21.524819	-4.805101	2.643858
H	21.187957	-5.442986	2.416628	H	20.42076	-3.724229	3.534531
C	12.73616	-0.175592	-0.346782	C	-14.556226	0.579358	0.170942
C	11.774388	-1.217682	-0.438268	C	-13.574756	1.595439	0.310855
C	12.451498	1.196916	-0.157375	C	-14.308804	-0.791691	-0.086501
C	10.390831	-1.166506	-0.403743	C	-12.191044	1.535401	0.236352
H	12.187317	-2.217186	-0.5282	H	-13.973903	2.587799	0.508807
C	11.233765	1.853077	-0.020142	C	-13.109775	-1.465415	-0.263755
H	13.318407	1.851385	-0.135667	H	-15.187346	-1.424078	-0.157427
C	9.529475	-0.070562	-0.239064	C	-11.359626	0.433821	-0.001686
H	9.891928	-2.129835	-0.504902	H	-11.674317	2.482288	0.384675
C	9.930737	1.348089	-0.047927	C	-11.796159	-0.980112	-0.238215
H	11.306429	2.931366	0.117378	H	-13.201274	-2.533988	-0.451404
C	8.136819	-0.112661	-0.206643	C	-9.969601	0.44849	-0.061923
C	8.750487	2.085942	0.090787	C	-10.638375	-1.72767	-0.426952
H	7.539333	-1.009307	-0.313957	H	-9.353903	1.328925	0.068603
C	7.640846	1.208044	-0.005285	C	-9.504762	-0.87262	-0.32241
H	8.690761	3.157036	0.243995	H	-10.599941	-2.792644	-0.621541
C	-20.760532	-0.144301	0.037823	C	-15.927226	1.045172	0.314393
C	-21.973069	-0.777611	-0.104849	C	-17.079973	0.319924	0.218579
H	-20.729451	0.914572	0.2847	H	-16.014366	2.107672	0.52102
H	-21.961508	-1.838045	-0.348904	H	-17.030367	-0.744544	0.009237
C	-23.262608	-0.20311	0.030628	C	-18.407138	0.82447	0.367698
C	-24.456345	-0.894028	-0.118499	C	-19.549177	0.053891	0.26192
C	-23.607852	1.244199	0.352758	C	-18.838428	2.254434	0.662491
C	-25.555169	0.018376	0.088397	C	-20.706419	0.897246	0.470643
O	-25.073059	1.244296	0.358495	O	-20.300669	2.157014	0.699874
C	-26.921795	-0.171245	0.05151	C	-22.054418	0.610845	0.467139
C	-24.534251	-2.277229	-0.425452	C	-19.54082	-1.340334	-0.008708
N	-24.494779	-3.413442	-0.67799	N	-19.429934	-2.477304	-0.233105
C	-27.514491	-1.43575	-0.226719	C	-22.560182	-0.699767	0.231156
N	-28.040884	-2.450735	-0.449933	N	-23.014768	-1.755389	0.042729
C	-27.792525	0.930988	0.299155	C	-22.996722	1.655101	0.707044
N	-28.508796	1.827171	0.500456	N	-23.769711	2.50379	0.902416
C	-23.186117	2.234249	-0.738987	C	-18.5085	3.244699	-0.460684
H	-23.605647	3.218902	-0.517344	H	-19.001565	4.198255	-0.255792
H	-22.098666	2.320546	-0.792878	H	-17.432462	3.416306	-0.533026
H	-23.556175	1.907813	-1.713778	H	-18.864632	2.866492	-1.421818
C	-23.177657	1.68556	1.756437	C	-18.411075	2.7564	2.046776
H	-23.531042	0.974205	2.506648	H	-18.698621	2.040139	2.820068
H	-22.090344	1.756431	1.831678	H	-17.330358	2.905249	2.096863
H	-23.608459	2.666178	1.974074	H	-18.905103	3.709361	2.252172
C	3.828248	1.322122	0.088406	C	9.236367	-0.31608	-0.311929
C	2.707633	0.546048	-0.029239	C	8.182902	-1.160363	-0.536442
H	3.701533	2.388807	0.276628	H	9.020664	0.722261	-0.05706
H	2.829984	-0.520042	-0.220781	H	8.393271	-2.199157	-0.791546
C	1.376738	1.04213	0.081817	C	6.814669	-0.771777	-0.456984
C	0.246856	0.27849	-0.043685	C	5.752114	-1.607528	-0.675223
H	1.259759	2.108021	0.280498	H	6.608651	0.268273	-0.20127
H	0.358106	-0.78683	-0.245835	H	5.952613	-2.64804	-0.931152
C	-1.0772	0.78767	0.072462	C	4.388233	-1.207604	-0.586963
C	-2.216395	0.03761	-0.060273	C	3.317733	-2.035073	-0.798194
H	-1.182654	1.85272	0.281855	H	4.192247	-0.165988	-0.329964
H	-2.117182	-1.026769	-0.273154	H	3.507483	-3.077251	-1.055472
C	-3.533438	0.560677	0.061772	C	1.957319	-1.623488	-0.700243
C	-4.682038	-0.175047	-0.077315	C	0.887058	-2.449	-0.906054
H	-3.626605	1.624756	0.281674	H	1.77682	-0.580851	-0.441389
H	-4.59548	-1.238367	-0.300527	H	1.088555	-3.488045	-1.164357
C	-5.991755	0.362466	0.05094	C	-7.043456	-0.542496	-0.353243
C	-7.149792	-0.358474	-0.093423	C	-8.149233	-1.329702	-0.463687
H	-6.072108	1.425532	0.280578	H	-7.208671	0.510383	-0.134493
H	-7.076301	-1.420714	-0.326003	H	-8.039566	-2.391987	-0.666386

C	-8.451848	0.193908	0.040904	C	10.609854	-0.69256	-0.384168
C	-9.619329	-0.511986	-0.107416	C	11.642292	0.171169	-0.151084
H	-8.519024	1.256039	0.278953	H	10.826257	-1.729822	-0.635582
H	-9.559263	-1.573251	-0.347856	H	11.388288	1.197402	0.111737
C	-10.913317	0.055777	0.032484	C	-5.642416	-0.92004	-0.476855
C	-12.090346	-0.634755	-0.118227	C	-5.304975	-2.253112	-0.820592
H	-10.966896	1.117183	0.277144	C	-4.064708	-2.850073	-0.983669
H	-12.044278	-1.695277	-0.364574	C	-4.722066	0.131909	-0.23062
C	-13.375657	-0.050705	0.026541	C	-2.779524	-2.305087	-0.854508
C	-14.562607	-0.725154	-0.124716	C	-3.335149	0.14561	-0.240859
H	-13.41484	1.010312	0.275665	C	-2.432982	-0.893719	-0.504121
H	-14.531711	-1.78525	-0.374692	H	-6.145352	-2.918594	-0.989159
C	-15.838211	-0.123109	0.024203	H	-4.088848	-3.905045	-1.253565
C	-17.035903	-0.77991	-0.125404	H	-5.182755	1.087015	0.011746
H	-15.861377	0.937942	0.275403	H	-2.877572	1.106121	-0.007836
H	-17.022451	-1.839898	-0.376496	C	-1.575507	-2.980206	-1.031319
C	-18.300137	-0.156968	0.027137	H	-1.470995	-4.026278	-1.293611
C	-19.509812	-0.79334	-0.118252	C	-0.494541	-2.079104	-0.811002
H	-18.30391	0.904604	0.277909	C	-1.043477	-0.804174	-0.490271
H	-19.51852	-1.853441	-0.367709	H	-0.48213	0.094674	-0.26905
C	5.166236	0.837548	-0.018762				
C	6.270614	1.631711	0.090993				
H	5.293606	-0.228543	-0.200566				
H	6.11315	2.695787	0.26706				

D7Bst(n=13)A4

N	20.514973	0.234117	-0.165332	C	-10.56243	-1.453436	-0.280112
C	21.013291	1.571732	-0.231451	C	-9.364906	-0.820783	-0.077671
C	20.609301	2.438681	-1.260548	H	-10.553521	-2.49613	-0.597378
C	21.923474	2.034887	0.722932	H	-9.378884	0.222164	0.240864
C	21.093151	3.737211	-1.317577	C	-8.089266	-1.427155	-0.255836
H	19.913254	2.086087	-2.0144	C	-6.896443	-0.785108	-0.051763
C	22.430162	3.333614	0.659586	H	-8.07112	-2.468444	-0.577574
H	22.242695	1.372281	1.520582	H	-6.918902	0.256289	0.271258
C	22.010539	4.196191	-0.360127	C	-5.616408	-1.380142	-0.233756
H	20.785728	4.414387	-2.107323	C	-4.428025	-0.729968	-0.028175
H	23.135934	3.660767	1.413505	H	-5.59035	-2.419917	-0.560007
C	21.432689	-0.845645	0.024552	H	-4.457968	0.30981	0.299402
C	21.186046	-1.845389	0.969935	C	-3.143859	-1.314545	-0.214144
C	22.611739	-0.908871	-0.736099	C	-1.959862	-0.656842	-0.006931
C	22.085314	-2.897516	1.151711	H	-3.11055	-2.352666	-0.545103
H	20.280008	-1.806063	1.565332	H	-1.99692	0.381185	0.325443
C	23.518559	-1.941463	-0.546954	C	-0.671615	-1.231143	-0.19702
H	22.813048	-0.139428	-1.473941	C	0.507817	-0.566014	0.012116
C	23.262149	-2.948669	0.395317	H	-0.631183	-2.267415	-0.533038
H	21.862849	-3.656986	1.891602	H	0.463552	0.470066	0.349679
H	24.431659	-1.99732	-1.130104	C	-11.83329	-0.833955	-0.105514
C	16.629181	0.028607	-0.114447	C	-13.035753	-1.455054	-0.306053
C	17.137384	-1.118077	-0.7024	H	-11.836804	0.210513	0.208466
S	17.955808	1.089483	0.368213	H	-13.038946	-2.499062	-0.618734
C	18.544672	-1.148438	-0.804524	C	1.800294	-1.129657	-0.182259
H	16.501933	-1.905742	-1.09128	C	2.974758	-0.456814	0.029225
C	19.156957	-0.022545	-0.281421	H	1.848133	-2.163818	-0.523837
H	19.104489	-1.959167	-1.253669	H	2.92282	0.577042	0.372513
O	22.431923	5.484787	-0.512909	C	-14.301866	-0.818789	-0.134581
O	24.212053	-3.923954	0.495818	C	-15.500071	-1.43828	-0.334979
C	23.355312	6.005829	0.430564	H	-14.279887	0.225297	0.174753
H	22.939824	6.006037	1.446347	H	-15.479265	-2.483889	-0.639532
H	24.297711	5.443235	0.428794	C	4.271792	-1.008942	-0.169644
H	23.551439	7.033923	0.123425	C	5.44066	-0.32778	0.04472
C	24.005706	-4.966153	1.436362	H	4.327658	-2.040651	-0.517414
H	23.093042	-5.535196	1.217333	H	5.38027	0.703498	0.394392

H	24.869353	-5.626633	1.34846	C	6.742745	-0.86711	-0.158883
H	23.949742	-4.580933	2.462586	C	7.905158	-0.176759	0.058956
C	-20.795151	0.73181	0.188005	H	6.807536	-1.895952	-0.513577
C	-21.990124	0.096729	0.003995	H	7.835275	0.851506	0.415753
H	-20.800495	1.782143	0.467851	C	9.212953	-0.701622	-0.149678
H	-21.991258	-0.954489	-0.270987	C	10.367768	-0.00099	0.072302
C	-23.287796	0.673122	0.135301	H	9.2878	-1.727095	-0.512106
C	-24.471835	-0.01512	-0.053684	H	10.286996	1.023788	0.436864
C	-23.640205	2.110282	0.491194	C	11.682199	-0.509405	-0.141324
C	-25.580437	0.889451	0.158176	C	12.827668	0.203345	0.084734
O	-25.105711	2.107306	0.469365	H	11.768444	-1.531026	-0.511998
C	-26.943235	0.693493	0.090682	H	12.734999	1.224233	0.457412
C	-24.539392	-1.390542	-0.400465	C	14.149871	-0.286376	-0.134762
N	-24.489587	-2.518746	-0.683733	C	15.274998	0.450647	0.100386
C	-27.522168	-0.567173	-0.232617	H	14.244988	-1.304376	-0.509925
N	-28.03595	-1.579562	-0.492915	H	15.141562	1.458057	0.492892
C	-27.825486	1.784001	0.351756	C	-19.241248	-1.189761	-0.314104
N	-28.550153	2.670569	0.563892	C	-17.954059	-1.677084	-0.430325
C	-23.201184	3.131609	-0.56456	C	-16.819927	-0.862446	-0.190343
H	-23.629474	4.107688	-0.323093	C	-17.058636	0.483059	0.176837
H	-22.113436	3.22411	-0.594954	C	-18.346188	0.971465	0.292312
H	-23.551157	2.831675	-1.555151	C	-19.477192	0.155855	0.051925
C	-23.23851	2.51269	1.915119	H	-20.074743	-1.856191	-0.510153
H	-23.603695	1.779396	2.638064	H	-17.801088	-2.714556	-0.714286
H	-22.153341	2.58573	2.013849	H	-16.22405	1.148783	0.369667
H	-23.677745	3.485178	2.151099	H	-18.498441	2.010314	0.574598