Improper hydrogen bonded cyclohexane C-H_{ax}···Y_{ax} contacts: theoretical predictions and experimental evidence from ^{1}H NMR spectroscopy of suitable axial cyclohexane models

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Table S1. Geometrical parameters included by the C-H_{ax}···Y_{ax} contacts in the fully geometry optimized MP2/6-31G+** adamantane analogues **1-24** and second order perturbation analysis of the hyperconjugative interactions calculated at the same level of theory.

System	Hyperconjugative interaction (kcal mol^{-1})[1]	r(C-H$_{ax}$$\cdots$ O): r_1, r_2 Å	θ(C-H$_{ax}$$\cdots$O); θ_1, θ_2 deg	(ε_{σ^*}-ε_n) a.u.	$F_{n\sigma^*}$ a.u.
1	---	2.54, 2.54	89.0, 89.0	-	-
2	$E[\sigma(\text{C-H})_{\text{Me}} \rightarrow \sigma^*(\text{C4}'\text{-H}_{ax})] = 0.24$	2.25, 2.25	113.2, 113.2	1.40	0.016
	$E[\sigma(\text{C-H})_{\text{Me}} \rightarrow \sigma^*(\text{C9}'\text{-H}_{ax})] = 0.24$			1.40	0.016
3	$E[\sigma(\text{C4}'\text{-H}_{ax}) \rightarrow \sigma^*(\text{C2}'\text{-H})_{t\text{-Bu}}] = 0.10$	2.33, 2.12	125.7, 131.6	1.39	0.011
	$E[\sigma(\text{C4}'\text{-H}_{ax}) \rightarrow \sigma^*(\text{C2}'\text{-H})_{t\text{-Bu}}] = 0.34$			1.39	0.019
	$E[\sigma(\text{C9}'\text{-H}_{ax}) \rightarrow \sigma^*(\text{C2}'\text{-H})_{t\text{-Bu}}] = 0.58$			1.40	0.026
	$E[\sigma(\text{C2}'\text{-H})_{t\text{-Bu}} \rightarrow \sigma^*(\text{C4}'\text{-H}_{ax})] = 0.53$			1.42	0.025
	$E[\sigma(\text{C2}'\text{-H})_{t\text{-Bu}} \rightarrow \sigma^*(\text{C4}'\text{-H}_{ax})] = 0.20$			1.42	0.015
	$E[\sigma(\text{C2}'\text{-H})_{t\text{-Bu}} \rightarrow \sigma^*(\text{C9}'\text{-H}_{ax})] = 0.59$			1.41	0.026
4	$E[\pi(\text{C}\equiv\text{N}) \rightarrow \sigma^*(\text{C4}'\text{-H}_{ax})] = 0.18$	2.68, 2.68	96.1, 96.1	1.19	0.013
	$E[\pi(\text{C}\equiv\text{N}) \rightarrow \sigma^*(\text{C4}'\text{-H}_{ax})] = 0.27$			1.19	0.013
	$E[\pi(\text{C}\equiv\text{N}) \rightarrow \sigma^*(\text{C9}'\text{-H}_{ax})] = 0.18$				
5	$E[\pi(\text{C}\equiv\text{N}) \rightarrow \sigma^*(\text{C4}'\text{-H}_{ax})] = 0.11$	2.55, 2.55	96.9, 96.9	1.18	0.010
	$E[\pi(\text{C}\equiv\text{N}) \rightarrow \sigma^*(\text{C4}'\text{-H}_{ax})] = 0.27$			1.19	0.016
	$E[\pi(\text{C}\equiv\text{N}) \rightarrow \sigma^*(\text{C9}'\text{-H}_{ax})] = 0.11$			1.18	0.010
6	$E[n_a(\text{O}) \rightarrow \sigma^*(\text{C4}'\text{-H}_{ax})] = 0.32$	2.55, 2.63	96.4, 96.0	1.58	0.020
	$E[n_\beta(\text{O}) \rightarrow \sigma^*(\text{C9}'\text{-H}_{ax})] = 0.28$			1.22	0.017
	$\alpha = \text{sp}^{1.15}$, $\beta = \text{p}$				
7	$E[n_a(\text{O}) \rightarrow \sigma^*(\text{C4}'\text{-H}_{ax})] = 0.42$	2.53, 2.62	96.4, 96.4	1.52	0.023
	$E[n_\beta(\text{O}) \rightarrow \sigma^*(\text{C9}'\text{-H}_{ax})] = 0.22$			1.20	0.015
	$\alpha = \text{sp}^{1.44}$, $\beta = \text{p}$				
8	$E[n_a(\text{O}) \rightarrow \sigma^*(\text{C4}'\text{-H}_{ax})] = 0.50$	2.43, 2.51	97.1, 96.7	1.58	0.025
	$E[n_\beta(\text{O}) \rightarrow \sigma^*(\text{C9}'\text{-H}_{ax})] = 0.35$			1.22	0.019
	$\alpha = \text{sp}^{1.18}$, $\beta = \text{p}$				
9	$E[n_a(\text{O}) \rightarrow \sigma^*(\text{C4}'\text{-H}_{ax})] = 0.63$	2.31, 2.43	97.0, 96.2	1.57	0.028
	$E[n_\beta(\text{O}) \rightarrow \sigma^*(\text{C9}'\text{-H}_{ax})] = 0.33$			1.22	0.018
	$\alpha = \text{sp}^{1.22}$, $\beta = \text{p}$				
10	$E[n_a(\text{O}) \rightarrow \sigma^*(\text{C4}'\text{-H}_{ax})] = 0.33$	2.55, 2.60	96.1, 96.1	1.53	0.020
	$E[n_\beta(\text{O}) \rightarrow \sigma^*(\text{C9}'\text{-H}_{ax})] = 0.16$			1.21	0.013
	$\alpha = \text{sp}^{0.70}$, $\beta = \text{p}$				
11	$E[n_a(\text{N}) \rightarrow \sigma^*(\text{C4}'\text{-H}_{ax})] = 0.50$	2.62, 2.62	96.7, 96.7	1.22	0.022
	$E[n_\alpha(\text{N}) \rightarrow \sigma^*(\text{C9}'\text{-H}_{ax})] = 0.50$			1.22	0.022
	$\alpha = \text{sp}^{4.28}$				
12	$E[n_a(\text{N}) \rightarrow \sigma^*(\text{C4}'\text{-H}_{ax})] = 0.43$	2.62, 2.62	97.6, 97.6	1.17	0.020
	$E[n_\alpha(\text{N}) \rightarrow \sigma^*(\text{C9}'\text{-H}_{ax})] = 0.43$			1.17	0.020
	$\alpha = \text{sp}^{5.84}$				
13	$E[n_\alpha(\text{N}) \rightarrow \sigma^*(\text{C4}'\text{-H}_{ax})] = 0.31$, $\alpha = \text{p}$	2.70, 2.74	95.9, 93.7	1.09	0.017
14	$E[n_a(\text{F}) \rightarrow \sigma^*(\text{C4}'\text{-H}_{ax})] = 0.10$	2.57, 2.57	95.6, 95.6	1.34	0.011
	$E[n_a(\text{F}) \rightarrow \sigma^*(\text{C9}'\text{-H}_{ax})] = 0.10$			1.34	0.011
	$\alpha = \text{p}$				
15	$E[n_a(\text{Cl}) \rightarrow \sigma^*(\text{C4}'\text{-H}_{ax})] = 0.14$	2.84, 2.84	101.6, 101.6	1.87	0.014
	$E[n_a(\text{Cl}) \rightarrow \sigma^*(\text{C9}'\text{-H}_{ax})] = 0.14$			1.87	0.014
	$E[n_\beta(\text{Cl}) \rightarrow \sigma^*(\text{C4}'\text{-H}_{ax})] = 0.46$			1.17	0.021
	$E[n_\beta(\text{Cl}) \rightarrow \sigma^*(\text{C9}'\text{-H}_{ax})] = 0.46$			1.17	0.021
	$E[n_\gamma(\text{Cl}) \rightarrow \sigma^*(\text{C4}'\text{-H}_{ax})] = 0.20$			1.17	0.014
	$E[n_\gamma(\text{Cl}) \rightarrow \sigma^*(\text{C9}'\text{-H}_{ax})] = 0.20$			1.17	0.014
	$\alpha = \text{sp}^{0.22}$, $\beta = \gamma = \text{p}$				
16	$E[n_a(\text{S}) \rightarrow \sigma^*(\text{C4}'\text{-H}_{ax})] = 0.46$	2.83, 2.89	102.1, 102.3	1.52	0.024
	$E[n_a(\text{S}) \rightarrow \sigma^*(\text{C9}'\text{-H}_{ax})] = 0.17$			1.53	0.014
	$E[n_\beta(\text{S}) \rightarrow \sigma^*(\text{C4}'\text{-H}_{ax})] = 0.16$			1.09	0.012
	$E[n_\beta(\text{S}) \rightarrow \sigma^*(\text{C9}'\text{-H}_{ax})] = 0.95$			1.09	0.029
	$\alpha = \text{sp}^{0.51}$, $\beta = \text{p}$				
17	$E[n_a(\text{S}) \rightarrow \sigma^*(\text{C4}'\text{-H}_{ax})] = 0.50$	2.83, 2.89	102.2, 102.4	1.51	0.025
	$E[n_a(\text{S}) \rightarrow \sigma^*(\text{C9}'\text{-H}_{ax})] = 0.23$			1.51	0.017
	$E[n_\beta(\text{S}) \rightarrow \sigma^*(\text{C9}'\text{-H}_{ax})] = 0.98$			1.07	0.029
	$\alpha = \text{sp}^{0.51}$, $\beta = \text{p}$				
18	$E[n_a(\text{O}) \rightarrow \sigma^*(\text{C4}'\text{-H}_{ax})] = 1.22$	2.35, 2.35	118.8, 118.8	1.60	0.040
	$E[n_a(\text{O}) \rightarrow \sigma^*(\text{C9}'\text{-H}_{ax})] = 1.22$			1.60	0.039
	$E[n_\beta(\text{O}) \rightarrow \sigma^*(\text{C4}'\text{-H}_{ax})] = 0.51$			1.25	0.023
	$E[n_\beta(\text{O}) \rightarrow \sigma^*(\text{C9}'\text{-H}_{ax})] = 0.51$			1.25	0.023
	$\alpha = \text{sp}^{1.16}$, $\beta = \text{p}$				
19	$E[n_a(\text{O}) \rightarrow \sigma^*(\text{C4}'\text{-H}_{ax})] = 0.64$	2.38, 2.95	118.0, 112.9	1.70	0.030
	$E[n_\beta(\text{O}) \rightarrow \sigma^*(\text{C4}'\text{-H}_{ax})] = 0.95$			1.21	0.031
	$\alpha = \text{sp}^{0.75}$, $\beta = \text{p}$			1.27	0.010
	$E[\pi(\text{C=O}) \rightarrow \sigma^*(\text{C4}'\text{-H}_{ax})] = 0.11$			1.23	0.013
	$E[\pi(\text{C=O}) \rightarrow \sigma^*(\text{C9}'\text{-H}_{ax})] = 0.18$				

20	$E[n_a(O)\rightarrow\sigma^*(C4'\text{-}H_{ax})]=0.19$	2.58, 2.58	121.6, 121.6	1.68	0.016
	$E[n_a(O)\rightarrow\sigma^*(C9'\text{-}H_{ax})]=0.19$			1.68	0.016
	$E[n_\beta(O)\rightarrow\sigma^*(C4'\text{-}H_{ax})]=0.44$			1.18	0.021
	$E[n_\beta(O)\rightarrow\sigma^*(C9'\text{-}H_{ax})]=0.45$			1.18	0.021
	$\alpha = sp^{0.78}$, β = p			1.26	0.015
	$E[\pi(C{=}O\rightarrow\sigma^*(C4'\text{-}H_{ax})]=0.22$			1.26	0.015
	$E[\pi(C{=}O\rightarrow\sigma^*(C9'\text{-}H_{ax})]=0.21$				
21	$E[n_a(O)\rightarrow\sigma^*(C4'\text{-}H_{ax})]=0.82$	2.32, 2.46	120.2, 119.3	1.70	0.033
	$E[n_a(O)\rightarrow\sigma^*(C9'\text{-}H_{ax})]=0.27$			1.68	0.019
	$E[n_\beta(O)\rightarrow\sigma^*(C4'\text{-}H_{ax})]=1.20$			1.21	0.035
	$E[n_\beta(O)\rightarrow\sigma^*(C9'\text{-}H_{ax})]=0.20$			1.19	0.014
	$\alpha = sp^{0.74}$, β = p			1.25	0.026
	$E[\pi(C{=}O\rightarrow\sigma^*(C9'\text{-}H_{ax})]=0.65$				
22	$E[n_a(O)\rightarrow\sigma^*(C4'\text{-}H_{ax})]=0.53$	2.34, 3.17	117.1, 110.0	1.69	0.027
	$E[n_\beta(O)\rightarrow\sigma^*(C4'\text{-}H_{ax})]=0.50$			1.20	0.022
	$\alpha = sp^{0.77}$, β = p			1.27	0.023
	$E[\pi(C{=}O\rightarrow\sigma^*(C4'\text{-}H_{ax})]=0.54$				
23	$E[n_a(O)\rightarrow\sigma^*(C4'\text{-}H_{ax})]=0.89$	2.30, 2.44	120.6, 119.7	1.70	0.035
	$E[n_a(O)\rightarrow\sigma^*(C9'\text{-}H_{ax})]=0.29$			1.69	0.020
	$E[n_\beta(O)\rightarrow\sigma^*(C4'\text{-}H_{ax})]=1.24$			1.21	0.035
	$E[n_\beta(O)\rightarrow\sigma^*(C9'\text{-}H_{ax})]=0.19$			1.19	0.014
	$\alpha = sp^{0.74}$, β = p				
	$E[\pi(C{=}O\rightarrow\sigma^*(C9'\text{-}H_{ax})]=0.71$			1.25	0.027
24	$E[n_a(O)\rightarrow\sigma^*(C4'\text{-}H_{ax})]=0.84$	2.28, 2.98	118.9, 112.5	1.70	0.034
	$\alpha = sp^{0.75}$, β = p			1.28	0.018
	$E[\pi(C{=}O\rightarrow\sigma^*(C4'\text{-}H_{ax})] = 0.33$			1.24	0.012
	$E[\pi(C{=}O\rightarrow\sigma^*(C9'\text{-}H_{ax})] = 0.14$				

Table S2. Selected structural parameters[a,b] and hyperconjugative energies for the cyclohexane ring C-H_{ax}···O contacts included in the adamantane derivatives **1**-**24** calculated at the B3LYP/6-31G+** level.

System	C4-H_{ax}, C9-H_{ax} C4-H_{eq}, C9-H_{eq}	r(C4′H_{ax}···Y) r(C9′H_{ax}···Y) Å	θ(C4′H_{ax}···Y) θ(C9′H_{ax}···Y) deg	$\Delta r_{4'}$ $\Delta r_{9'}$[a] *m*Å	Δ% s-char.[b]	Hyperconjugative interaction (kcal mol^{-1})
1 adamantane (Y_1=**H**, A=H)[c]	1.0986, 1.0986 1.0986, 1.0986	2.56 2.56	88.9 88.9	0	0	---
2 (Y_1=C**H**$_3$, A=H)[c]	1.0972, 1.0972 1.0986,1.0986	2.86 2.86	95.8 95.8	-1.4 -1.4	0.31 0.31	$E[\sigma(\text{C-H})_{Me} \rightarrow \sigma^*(\text{C4′-H}_{ax})] = 0.21$ $E[\sigma(\text{C-H})_{Me} \rightarrow \sigma^*(\text{C9′-H}_{ax})] = 0.21$
3 (Y_1= C(C**H**$_3$)$_3$, A=H)[c]	1.0931, 1.0956 1.0990, 1.0990	2.64 2.94	120.2 117.1	-5.9 -3.4	0.97 0.61	$E[\sigma(\text{C4′-H}_{ax}) \rightarrow \sigma^*(\text{C2′-H})_{t\text{-Bu}}] = 0.20$ $E[\sigma(\text{C4′-H}_{ax}) \rightarrow \sigma^*(\text{C2′-H})_{t\text{-Bu}}] = 0.24$ $E[\sigma(\text{C9′-H}_{ax}) \rightarrow \sigma^*(\text{C2′-H})_{t\text{-Bu}}] = 0.56$ $E[\sigma(\text{C2′-H})_{t\text{-Bu}} \rightarrow \sigma^*(\text{C4′-H}_{ax})] = 0.60$ $E[\sigma(\text{C2′-H})_{t\text{-Bu}} \rightarrow \sigma^*(\text{C4′-H}_{ax})] = 0.11$ $E[\sigma(\text{C2′-H})_{t\text{-Bu}} \rightarrow \sigma^*(\text{C9′-H}_{ax})] = 0.63$
4 (Y_1= **C**N, A=H)[c]	1.0968, 1.0968 1.0976, 1.0976	2.74 2.74	95.9 95.9	-0.8 -0.8	0.37 0.37	$E[\pi(\text{C}\equiv\text{N}) \rightarrow \sigma^*(\text{C4′-H}_{ax})] = 0.11$ $E[\pi(\text{C}\equiv\text{N}) \rightarrow \sigma^*(\text{C9′-H}_{ax})] = 0.13$
5 (Y_1= **C**N, A=Me)[c]	1.0961, 1.0961 1.0977, 1.0977	2.60 2.60	96.9 96.9	-1.6 -1.6	0.60 0.60	$E[\pi(\text{C}\equiv\text{N}) \rightarrow \sigma^*(\text{C4′-H}_{ax})] = 0.21$ $E[\pi(\text{C}\equiv\text{N}) \rightarrow \sigma^*(\text{C9′-H}_{ax})] = 0.20$
6 (Y_1=**O**H, A=H)[c]	1.0954, 1.0959 1.0984, 1.0985	2.62 2.68	96.0 96.0	-3.0 -2.6	0.59 0.37	$E[n_\alpha(\text{O}) \rightarrow \sigma^*(\text{C4′-H}_{ax})] = 0.21$ $E[n_\beta(\text{O}) \rightarrow \sigma^*(\text{C9′-H}_{ax})] = 0.25$ $\alpha = sp^{1.1}$, β = p
7 (Y_1=**O**Me, A=H)[c]	1.0954, 1.0960 1.0985, 1.0985	2.60 2.68	96.1 95.9	-3.1 -2.5	0.65 0.46	$E[n_\alpha(\text{O}) \rightarrow \sigma^*(\text{C4′-H}_{ax})]=0.25$ $E[n_\beta(\text{O}) \rightarrow \sigma^*(\text{C9′-H}_{ax})]=0.18$ $\alpha = sp^{1.4}$, β = sp
8 (Y_1=**O**H, A=Me)[c]	1.0939, 1.0945 1.0984, 1.0984	2.55 2.49	97.0 97.1	-4.5 -3.9	0.94 0.70	$E[n_\alpha(\text{O}) \rightarrow \sigma^*(\text{C4′-H}_{ax})]=0.40$ $E[n_\beta(\text{O}) \rightarrow \sigma^*(\text{C9′-H}_{ax})]=0.37$ $\alpha = sp^{1.4}$, β = sp
9 (Y_1=**O**H, A= *t*-Bu)[c]	1.0919, 1.0935 1.0988, 1.0985	2.43 2.34	96.5 97.3	-6.9 -5.0	1.42 0.91	$E[n_\alpha(\text{O}) \rightarrow \sigma^*(\text{C4′-H}_{ax})]=0.54$ $E[n_\beta(\text{O}) \rightarrow \sigma^*(\text{C9′-H}_{ax})]=0.38$ $\alpha = sp^{1.1}$, β = p
10 (Y_1= **O**Ac, A=H)	1.0960, 1.0965 1.0981, 1.0981	2.63 2.68	95.8 95.6	-2.1 -1.6	0.41 0.29	$E[n_\alpha(\text{O}) \rightarrow \sigma^*(\text{C4′-H}_{ax})] = 0.21$ $E[n_\beta(\text{O}) \rightarrow \sigma^*(\text{C9′-H}_{ax})] = 0.11$ $\alpha = sp^{0.7}$, β = p
11 (Y_1= **N**H$_2$, A=H)[c]	1.0949, 1.0949 1.0987, 1.0987	2.67 2.67	96.7 96.7	-3.8 -3.8	0.71 0.71	$E[n_\alpha(\text{O}) \rightarrow \sigma^*(\text{C4′-H}_{ax})]=0.40$ $E[n_\alpha(\text{O}) \rightarrow \sigma^*(\text{C9′-H}_{ax})]=0.40$ $\alpha = sp^{4.3}$
12 (Y_1= **N**Me$_2$, A=H)[c]	1.0958, 1.0958 1.0987, 1.0987	2.71 2.71	97.2 97.2	-2.9 -2.9	0.64 0.64	$E[n_\alpha(\text{O}) \rightarrow \sigma^*(\text{C4′-H}_{ax})]=0.23$ $E[n_\alpha(\text{O}) \rightarrow \sigma^*(\text{C9′-H}_{ax})]=0.23$ $\alpha = sp^{6.2}$
13 (Y_1= **N**HAc, A=H)	1.0981, 1.0997 1.0979, 1.0980	2.77 2.79	95.3 93.8	-0.2 -1.7	-0.01 -0.30	$E[n_\alpha(\text{N}) \rightarrow \sigma^*(\text{C4′-H}_{ax})]=0.21$ α = p
14 (Y_1=**F**, A=H)	1.0957, 1.0957 1.0980, 1.0980	2.61 2.61	95.3 95.3	-2.3 -2.3	0.44 0.44	not located using a threshold of 0.1 kcal mol^{-1}
15 (Y_1=**Cl**, A=H)	1.0956, 1.0956 1.0978, 1.0978	2.88 2.88	102.2 102.2	-2.2 -2.2	0.55 0.55	$E[n_\alpha(\text{O}) \rightarrow \sigma^*(\text{C4′-H}_{ax})]=0.37$ $E[n_\alpha(\text{O}) \rightarrow \sigma^*(\text{C9′-H}_{ax})]=0.37$ $E[n_\beta(\text{O}) \rightarrow \sigma^*(\text{C4′-H}_{ax})]=0.15$ $E[n_\beta(\text{O}) \rightarrow \sigma^*(\text{C9′-H}_{ax})]=0.15$ $\alpha = \beta$ = p
16 (Y_1=**S**H, A=H)	1.0965, 1.0956 1.0981, 1.0982	2.86 2.89	103.3 103.4	-1.6 -2.6	0.47 0.60	$E[n_\alpha(\text{S}) \rightarrow \sigma^*(\text{C4′-H}_{ax})]=0.30$, $E[n_\alpha(\text{S}) \rightarrow \sigma^*(\text{C9′-H}_{ax})]=0.10$ $E[n_\beta(\text{S}) \rightarrow \sigma^*(\text{C4′-H}_{ax})]=0.11$ $E[n_\beta(\text{S}) \rightarrow \sigma^*(\text{C9′-H}_{ax})]=0.73$ $\alpha = sp^{0.45}$, β = p
17 (Y_1=**S**Me, A=H)	1.0942, 1.0943 1.0983, 1.0984	2.70 2.79	104.2 104.3	-4.1 -4.1	0.88 0.78	$E[n_\alpha(\text{S}) \rightarrow \sigma^*(\text{C4′-H}_{ax})]=0.59$ $E[n_\alpha(\text{S}) \rightarrow \sigma^*(\text{C9′-H}_{ax})]=0.10$ $E[n_\beta(\text{S}) \rightarrow \sigma^*(\text{C4′-H}_{ax})]=0.38$ $E[n_\beta(\text{S}) \rightarrow \sigma^*(\text{C9′-H}_{ax})]=1.00$ $\alpha = sp^{0.43}$, β = p
18 (Y_2=CMe$_2$**O**H, A=H)	1.0933, 1.0933 1.0993, 1.0993	2.41 2.41	118.9 118.9	-6.0 -6.0	1.39 1.38	$E[n_\alpha(\text{O}) \rightarrow \sigma^*(\text{C4′-H}_{ax})]=1.34$ $E[n_\alpha(\text{O}) \rightarrow \sigma^*(\text{C9′-H}_{ax})]=0.98$ $E[n_\beta(\text{O}) \rightarrow \sigma^*(\text{C4′-H}_{ax})]=0.66$ $E[n_\beta(\text{O}) \rightarrow \sigma^*(\text{C9′-H}_{ax})]=0.98$ $\alpha = sp^{1.2}$, β = p
19 (Y_2=C**O**Me, A=H)[c]	1.0924, 1.0963 1.0988, 1.0985	2.40 2.77	119.0 115.0	-6.4 -2.2	1.50 0.64	$E[n_\alpha(\text{O}) \rightarrow \sigma^*(\text{C4′-H}_{ax})] =0.49$ $E[n_\beta(\text{O}) \rightarrow \sigma^*(\text{C4′-H}_{ax})] =1.09$ $\alpha = sp^{0.7}$, β = p $E[\pi(\text{C=O} \rightarrow \sigma^*(\text{C4′-H}_{ax})]=0.19$
20 (Y_2,A =C**O**(CH$_2$)$_2$)	1.0952, 1.0963 1.0985, 1.0985	2.63 2.63	121.2 121.1	-3.3 -3.3	0.88 0.87	$E[n_\alpha(\text{O}) \rightarrow \sigma^*(\text{C4′-H}_{ax})]=0.10$ $E[n_\alpha(\text{O}) \rightarrow \sigma^*(\text{C9′-H}_{ax})]=0.11$ $E[n_\beta(\text{O}) \rightarrow \sigma^*(\text{C4′-H}_{ax})]=0.38$ $E[n_\beta(\text{O}) \rightarrow \sigma^*(\text{C9′-H}_{ax})]=0.39$ $\alpha = sp^{0.8}$, β = p $E[\pi(\text{C=O} \rightarrow \sigma^*(\text{C4′-H}_{ax})]=0.13$ $E[\pi(\text{C=O} \rightarrow \sigma^*(\text{C9′-H}_{ax})]=0.13$

21 (Y_2,A=C**O**$(CH_2)_3$)	1.0939, 1.0918	2.33	120.7	-7.0	1.59	$E[n_\alpha(O)\rightarrow\sigma^*(C4'\text{-}H_{ax})]$=0.20
	1.0985, 1.0988	2.46	119.2	-4.6	1.10	$E[n_\alpha(O)\rightarrow\sigma^*(C9'\text{-}H_{ax})]$=0.60
						$E[n_\beta(O)\rightarrow\sigma^*(C4'\text{-}H_{ax})]$=0.26
						$E[n_\beta(O)\rightarrow\sigma^*(C9'\text{-}H_{ax})]$=1.17
						$\alpha = sp^{0.8}$, β = p
						$E[\pi(C{=}O\rightarrow\sigma^*(C9'\text{-}H_{ax})]$=0.43
22 (Y_2,A=C**O**$(CH_2)_4$)	1.0920, 1.0983	2.35	117.6	-6.5	1.46	$E[n_\alpha(O)\rightarrow\sigma^*(C4'\text{-}H_{ax})]$=0.42
	1.0985, 1.0983	3.17	109.9	0.0	0.18	$E[n_\beta(O)\rightarrow\sigma^*(C4'\text{-}H_{ax})]$=0.58
						$\alpha = sp^{0.8}$, β = p
						$E[\pi(C{=}O\rightarrow\sigma^*(C9'\text{-}H_{ax})]$=0.37
23 (Y_2,A=C**O**$CH_2C_6H_4$)	1.0919, 1.0928	2.32	120.7	-6.8	1.62	$E[n_\alpha(O)\rightarrow\sigma^*(C4'\text{-}H_{ax})]$=0.37
	1.0987, 1.0985	2.38	120.2	-5.7	1.36	$E[n_\alpha(O)\rightarrow\sigma^*(C9'\text{-}H_{ax})]$=0.47
						$E[n_\beta(O)\rightarrow\sigma^*(C4'\text{-}H_{ax})]$=0.59
						$E[n_\beta(O)\rightarrow\sigma^*(C9'\text{-}H_{ax})]$=0.98
						$\alpha = sp^{0.7}$, β = p
						$E[\pi(C{=}O\rightarrow\sigma^*(C4'\text{-}H_{ax})]$=0.21
						$E[\pi(C{=}O\rightarrow\sigma^*(C9'\text{-}H_{ax})]$=0.45
24 (Y_2,A=C**O**$(CH_2)_2C_6H_4$)	1.0905, 1.0971	2.27	119.3	-8.3	1.81	$E[n_\alpha(O)\rightarrow\sigma^*(C4'\text{-}H_{ax})]$=0.75
	1.0988, 1.0983	2.96	112.2	-1.2	0.41	$E[n_\beta(O)\rightarrow\sigma^*(C9'\text{-}H_{ax})]$=1.06
						$\alpha = sp^{0.8}$, β = p
						$E[\pi(C{=}O\rightarrow\sigma^*(C4'\text{-}H_{ax})]$ = 0.12
						$E[\pi(C{=}O\rightarrow\sigma^*(C9'\text{-}H_{ax})]$ = 0.19

[a] $\Delta r_{4'} = r(C_{4'}\text{-}H_{ax}) - r(C_{4'}\text{-}H_{eq})]$, Δ% s-char.=(% s-char. $C_{4'}\text{-}H_{ax}$ – % s-char $C_{4'}\text{-}H_{eq})]$

Table S3. Geometrical parameters included by the C-H_{ax}···Y_{ax} contacts in the fully geometry optimized B3LYP/6-31G+** adamantane analogues **1-24** and second order perturbation analysis of the hyperconjugative interactions calculated at the same level of theory.

System	Hyperconjugative interaction (kcal mol^{-1})[1]	r(C-H_{ax}··· O): r_1, r_2 Å	θ(C-H_{ax}···O); θ_1, θ_2 deg	(ε_{σ^*}-ε_n) a.u.	$F_{n\sigma^*}$ a.u.
1	---	2.56, 2.56	95.8, 95.8	0.95	0.013
				0.95	0.013
2	$E[\sigma(C\text{-}H)_{Me} \rightarrow \sigma^*(C4'\text{-}H_{ax})] = 0.21$	2.86, 2.86	95.8, 95.8	0.95	0.013
	$E[\sigma(C\text{-}H)_{Me} \rightarrow \sigma^*(C9'\text{-}H_{ax})] = 0.21$			0.95	0.013
3	$E[\sigma(C4'\text{-}H_{ax}) \rightarrow \sigma^*(C2'\text{-}H)_{t\text{-}Bu}] = 0.20$	2.64, 2.94	120.2, 117.1	0.95	0.012
	$E[\sigma(C4'\text{-}H_{ax}) \rightarrow \sigma^*(C2'\text{-}H)_{t\text{-}Bu}] = 0.24$			0.94	0.013
	$E[\sigma(C9'\text{-}H_{ax}) \rightarrow \sigma^*(C2'\text{-}H)_{t\text{-}Bu}] = 0.56$			0.96	0.021
	$E[\sigma(C2'\text{-}H)_{t\text{-}Bu} \rightarrow \sigma^*(C4'\text{-}H_{ax})] = 0.60$			0.97	0.022
	$E[\sigma(C2'\text{-}H)_{t\text{-}Bu} \rightarrow \sigma^*(C4'\text{-}H_{ax})] = 0.11$			0.96	0.009
	$E[\sigma(C2'\text{-}H)_{t\text{-}Bu} \rightarrow \sigma^*(C9'\text{-}H_{ax})] = 0.63$			0.96	0.022
6	$E[\pi(C\equiv N) \rightarrow \sigma^*(C4'\text{-}H_{ax})] = 0.11$	2.74, 2.74	95.9, 95.9	0.79	0.008
	$E[\pi(C\equiv N) \rightarrow \sigma^*(C9'\text{-}H_{ax})] = 0.13$			0.79	0.009
5	$E[\pi(C\equiv N) \rightarrow \sigma^*(C4'\text{-}H_{ax})] = 0.21$	2.60, 2.60	96.9, 96.9	0.80	0.011
	$E[\pi(C\equiv N) \rightarrow \sigma^*(C9'\text{-}H_{ax})] = 0.20$			0.80	0.011
7	$E[n_a(O) \rightarrow \sigma^*(C4'\text{-}H_{ax})] = 0.21$, $\alpha = sp^{1.1}$	2.62, 2.68	96.0, 96.0	1.07	0.013
	$E[n_\beta(O) \rightarrow \sigma^*(C9'\text{-}H_{ax})] = 0.25$, $\beta = p$			0.76	0.012
7	$E[n_a(O) \rightarrow \sigma^*(C4'\text{-}H_{ax})] = 0.25$, $\alpha = sp^{1.36}$	2.60, 2.68	96.1, 95.9	1.02	0.014
	$E[n_\beta(O) \rightarrow \sigma^*(C9'\text{-}H_{ax})] = 0.18$, $\beta = p$			0.75	0.010
8	$E[n_a(O) \rightarrow \sigma^*(C4'\text{-}H_{ax})] = 0.40$, $\alpha = sp^{1.1}$	2.55, 2.49	97.0, 97.1	1.07	0.019
	$E[n_\beta(O) \rightarrow \sigma^*(C9'\text{-}H_{ax})] = 0.37$, $\beta = p$			0.76	0.015
9	$E[n_a(O) \rightarrow \sigma^*(C4'\text{-}H_{ax})] = 0.54$, $\alpha = sp^{1.12}$	2.60, 2.68	96.1, 95.9	1.07	0.022
	$E[n_\beta(O) \rightarrow \sigma^*(C9'\text{-}H_{ax})] = 0.38$, $\beta = p$			0.76	0.015
10	$E[n_a(O) \rightarrow \sigma^*(C4'\text{-}H_{ax})] = 0.21$, $\alpha = sp^{0.69}$	2.63, 2.68	95.8, 95.6	1.02	0.013
	$E[n_\beta(O) \rightarrow \sigma^*(C9'\text{-}H_{ax})] = 0.11$, $\beta = p$			0.78	0.009
11	$E[n_a(O) \rightarrow \sigma^*(C4'\text{-}H_{ax})] = 0.40$	2.67, 2.67	96.7, 96.7	0.78	0.016
	$E[n_\alpha(O) \rightarrow \sigma^*(C9'\text{-}H_{ax})] = 0.40$, $\alpha = sp^{4.3}$			0.78	0.016
12	$E[n_a(O) \rightarrow \sigma^*(C4'\text{-}H_{ax})] = 0.23$	2.71, 2.71	97.2, 97.2	0.74	0.012
	$E[n_\alpha(O) \rightarrow \sigma^*(C9'\text{-}H_{ax})] = 0.23$, $\alpha = sp^{6.18}$			0.74	0.012
13	$E[n_\alpha(N) \rightarrow \sigma^*(C4'\text{-}H_{ax})] = 0.21$, $\alpha = p$	2.77, 2.79	95.3, 93.8	0.70	0.012
14	not located using a threshold of 0.1 kcal mol^{-1}	2.61, 2.61	102.2, 102.2	---	---
15	$E[n_a(Cl) \rightarrow \sigma^*(C4'\text{-}H_{ax})] = 0.37$, $\alpha = p$	2.88, 2.88	95.3, 95.3	0.76	0.015
	$E[n_a(Cl) \rightarrow \sigma^*(C9'\text{-}H_{ax})] = 0.37$			0.76	0.015
	$E[n_\beta(Cl) \rightarrow \sigma^*(C4'\text{-}H_{ax})] = 0.15$, $\beta = p$			0.76	0.010
	$E[n_\beta(Cl) \rightarrow \sigma^*(C9'\text{-}H_{ax})] = 0.15$			0.76	0.010
16	$E[n_a(S) \rightarrow \sigma^*(C4'\text{-}H_{ax})] = 0.30$, $\alpha = sp^{0.45}$	2.86, 2.89	103.3, 103.4	1.09	0.016
	$E[n_a(S) \rightarrow \sigma^*(C9'\text{-}H_{ax})] = 0.10$			1.09	0.010
	$E[n_a(S) \rightarrow \sigma^*(C4'\text{-}H_{ax})] = 0.11$, $\beta = p$			0.70	0.008
	$E[n_\beta(S) \rightarrow \sigma^*(C9'\text{-}H_{ax})] = 0.73$			0.71	0.020
17	$E[n_a(S) \rightarrow \sigma^*(C4'\text{-}H_{ax})] = 0.59$, $\alpha = sp^{0.43}$	2.70, 2.79	104.2, 104.3	1.08	0.023
	$E[n_a(S) \rightarrow \sigma^*(C9'\text{-}H_{ax})] = 0.10$			1.08	0.009
	$E[n_\beta(S) \rightarrow \sigma^*(C4'\text{-}H_{ax})] = 0.38$, $\beta = p$			0.69	0.015
	$E[n_\beta(S) \rightarrow \sigma^*(C9'\text{-}H_{ax})] = 1.00$			0.69	0.024
18	$E[n_a(O) \rightarrow \sigma^*(C4'\text{-}H_{ax})] = 1.34$	2.41, 2.41	118.9, 118.9	1.08	0.034
	$E[n_a(O) \rightarrow \sigma^*(C9'\text{-}H_{ax})] = 0.98$, $\alpha = sp^{1.2}$			1.08	0.029
	$E[n_\beta(O) \rightarrow \sigma^*(C4'\text{-}H_{ax})] = 0.66$			0.80	0.021
	$E[n_\beta(O) \rightarrow \sigma^*(C9'\text{-}H_{ax})] = 0.98$, $\beta = p$			0.80	0.019
19	$E[n_a(O) \rightarrow \sigma^*(C4'\text{-}H_{ax})] = 0.49$, $\alpha = sp^{0.74}$	2.40, 2.77	119.0, 115.0	1.18	0.021
	$E[n_\beta(O) \rightarrow \sigma^*(C4'\text{-}H_{ax})] = 1.09$, $\beta = p$			0.75	0.026
	$E[\pi(C{=}O \rightarrow \sigma^*(C4'\text{-}H_{ax})] = 0.19$			0.84	0.011
20	$E[n_a(O) \rightarrow \sigma^*(C4'\text{-}H_{ax})] = 0.10$	2.63, 2.63	121.2, 121.2	1.16	0.010
	$E[n_a(O) \rightarrow \sigma^*(C9'\text{-}H_{ax})] = 0.11$, $\alpha = sp^{0.8}$			1.16	0.010
	$E[n_\beta(O) \rightarrow \sigma^*(C4'\text{-}H_{ax})] = 0.38$			0.74	0.016
	$E[n_\beta(O) \rightarrow \sigma^*(C9'\text{-}H_{ax})] = 0.39$, $\beta = p$			0.74	0.016
	$E[\pi(C{=}O \rightarrow \sigma^*(C4'\text{-}H_{ax})] = 0.13$			0.86	0.009
	$E[\pi(C{=}O \rightarrow \sigma^*(C4'\text{-}H_{ax})] = 0.13$			0.86	0.009
21	$E[n_a(O) \rightarrow \sigma^*(C4'\text{-}H_{ax})] = 0.20$	2.33, 2.46	120.7, 119.2	1.16	0.014
	$E[n_a(O) \rightarrow \sigma^*(C9'\text{-}H_{ax})] = 0.60$, $\alpha = sp^{0.8}$			1.18	0.024
	$E[n_\beta(O) \rightarrow \sigma^*(C4'\text{-}H_{ax})] = 0.26$			0.74	0.013
	$E[n_\beta(O) \rightarrow \sigma^*(C9'\text{-}H_{ax})] = 1.17$, $\beta = p$			0.76	0.027
	$E[\pi(C{=}O \rightarrow \sigma^*(C9'\text{-}H_{ax})] = 0.43$			0.86	0.017
22	$E[n_a(O) \rightarrow \sigma^*(C4'\text{-}H_{ax})] = 0.42$, $\alpha = sp^{0.8}$	2.35, 3.17	117.6, 108.9	1.17	0.020
	$E[n_\beta(O) \rightarrow \sigma^*(C4'\text{-}H_{ax})] = 0.58$, $\beta = p$			0.75	0.019
	$E[\pi(C{=}O \rightarrow \sigma^*(C9'\text{-}H_{ax})] = 0.37$			0.87	0.016

23	$E[n_a(O) \rightarrow \sigma^*(C4'\text{-}H_{ax})] = 0.37$	2.32, 2.38	120.7, 120.2	1.17	0.019
	$E[n_a(O) \rightarrow \sigma^*(C9'\text{-}H_{ax})] = 0.47$, $\alpha = sp^{0.7}$			0.75	0.017
	$E[n_\beta(O) \rightarrow \sigma^*(C4'\text{-}H_{ax})] = 0.59$			1.18	0.024
	$E[n_\beta(O) \rightarrow \sigma^*(C9'\text{-}H_{ax})] = 0.98$, $\beta = p$			0.75	0.025
	$E[\pi(C{=}O \rightarrow \sigma^*(C4'\text{-}H_{ax})] = 0.21$			0.86	0.012
	$E[\pi(C{=}O \rightarrow \sigma^*(C9'\text{-}H_{ax})] = 0.45$			0.86	0.018
24	$E[n_a(O) \rightarrow \sigma^*(C4'\text{-}H_{ax})] = 0.75$, $\alpha = sp^{0.8}$	2.27, 2.96	119.2, 112.2	1.18	0.027
	$E[n_\beta(O) \rightarrow \sigma^*(C9'\text{-}H_{ax})] = 1.06$, $\beta = p$			0.76	0.026
	$E[\pi(C{=}O \rightarrow \sigma^*(C4'\text{-}H_{ax})] = 0.12$			0.84	0.009
	$E[\pi(C{=}O \rightarrow \sigma^*(C9'\text{-}H_{ax})] = 0.19$			0.88	0.012

Cartesian coordinates of the optimized compounds 1-24 at the MP2/6-31+G** level

Compound 1 ($E_{el,MP2}$ = -389.47593989 a.u.)

#

Ad

0 1

C	-0.82588400	-1.52293500	0.36830600
C	-0.64022100	-0.93507900	-1.03700900
H	-1.09664900	-1.60171800	-1.77635900
C	-0.18678900	-0.59014300	1.40584700
H	-0.32003700	-1.01082100	2.40816500
C	1.31101800	-0.44354700	1.10532100
H	1.80371700	-1.41983800	1.17111800
H	1.78089500	0.20708900	1.85103700
C	0.85826400	-0.78798100	-1.33400600
H	1.00256600	-0.38504500	-2.34248000
H	1.34411700	-1.76947200	-1.30497000
C	1.49973000	0.14597000	-0.29893200
H	2.56890700	0.25001500	-0.51207200
C	0.82583100	1.52297300	-0.36830700
H	1.28832200	2.20338000	0.35513800
H	0.96962300	1.96082400	-1.36220000
C	-1.31101300	0.44353900	-1.10534100
H	-2.38506900	0.34759800	-0.91191000
H	-1.19944900	0.86506900	-2.11036000
C	-0.85824500	0.78799900	1.33402600
H	-1.92543800	0.69721000	1.56440200
H	-0.42111400	1.45723400	2.08318900
C	-0.67269000	1.37922000	-0.06990900
H	-1.15222300	2.36256200	-0.11975900
H	-1.89261900	-1.64859600	0.58406200
H	-0.36556300	-2.51558300	0.42301400

Compound 2 ($E_{el,MP2}$ = -428.66138864 a.u.)

#

2-MeAd

0 1

C	-1.35595100	-0.66171800	0.00026000
C	-0.52595200	-0.31522300	1.25034100
H	-1.11844100	-0.53996300	2.14535200
C	-0.52595700	-0.31618300	-1.25009400
H	-1.11845900	-0.54160800	-2.14492300
C	-0.13399900	1.16885900	-1.25331400
H	-1.02133900	1.80748200	-1.29132300
H	0.45173500	1.38916200	-2.15273800

C	-0.13398700	1.16981900	1.25242300
H	0.45175600	1.39080800	2.15167300
H	-1.02132400	1.80847500	1.28995400
C	0.69406800	1.48582800	-0.00057000
H	0.96883200	2.54610600	-0.00097900
C	1.96509200	0.62653800	-0.00024600
H	2.57301100	0.85627600	-0.88231300
H	2.57301500	0.85695500	0.88164200
C	0.75097500	-1.16754800	1.25387200
H	0.48980900	-2.23123100	1.27995800
H	1.34081700	-0.95667800	2.15294800
C	0.75096800	-1.16850600	-1.25298300
H	0.48981000	-2.23221000	-1.27825200
H	1.34081200	-0.95832100	-2.15221900
C	1.58043300	-0.85879400	0.00032600
H	2.48711800	-1.47324400	0.00055500
C	-2.74368900	-0.02401900	0.00000900
H	-3.30507300	-0.33571700	-0.88342700
H	-3.30511500	-0.33509400	0.88363800
H	-2.70330000	1.06480300	-0.00037100
H	-1.50567800	-1.75031600	0.00067900

Compound 3 ($E_{el,MP2}$ = -546.20949397 a.u.)

#

2-t-Bu-Ad

0 1

C	-0.63136300	-0.02705300	-0.54205300
C	0.24133000	1.23250000	-0.33479300
H	-0.33539000	2.12949300	-0.57198000
C	0.21696100	-1.25439400	-0.13315500
H	-0.38636400	-2.16562700	-0.20561600
C	1.39696500	-1.35749800	-1.11598700
H	1.02350500	-1.47800100	-2.13870300
H	2.00038900	-2.24253900	-0.88392000
C	1.42134700	1.14584000	-1.31890400
H	2.04260900	2.04497700	-1.23425000
H	1.04441300	1.10881500	-2.34687800
C	2.26703700	-0.09625300	-1.01462100
H	3.09308000	-0.16363600	-1.73094000
C	2.82657400	0.02680200	0.40820400
H	3.45367400	-0.84002000	0.64422900
H	3.46052300	0.91716200	0.48492300
C	0.80200600	1.34471100	1.08972500
H	-0.00294600	1.44001000	1.82354300
H	1.40825100	2.25491800	1.16696900
C	0.80008200	-1.14299800	1.28719500
H	0.01763900	-1.12681600	2.04491600
H	1.41250900	-2.03084800	1.48409600
C	1.66476400	0.11619600	1.40523100
H	2.06019200	0.19538500	2.42366300
C	-2.11036000	0.00132500	-0.04326000

C	-2.72647100	1.37775200	-0.31906000
H	-3.80615800	1.33884400	-0.15556500
H	-2.31868400	2.14451200	0.34180400
H	-2.55449700	1.68746100	-1.35306200
C	-2.89556500	-1.03163200	-0.86711100
H	-3.93765600	-1.06538300	-0.54034000
H	-2.88226400	-0.77238800	-1.92836100
H	-2.47987400	-2.03461300	-0.75609200
C	-2.32991900	-0.33286300	1.43707200
H	-2.04036300	-1.35920700	1.66519900
H	-1.78795600	0.33867200	2.10223300
H	-3.39421300	-0.23558700	1.66714100
H	-0.75075900	-0.10019100	-1.63391400

Compound 4 ($E_{el,MP2}$ = -481.48836332 a.u.)

#

2-CN-Ad

0 1

C	-1.06945700	-0.84227000	0.00164300
C	-0.29107700	-0.40885800	-1.26177700
H	-0.85685300	-0.71260200	-2.14796500
C	-0.29188400	-0.40248700	1.26336300
H	-0.85823700	-0.70176100	2.15070200
C	1.07476200	-1.09962200	1.25380900
H	0.94381600	-2.18707300	1.27866900
H	1.63002000	-0.82102400	2.15532800
C	1.07557300	-1.10591400	-1.24786800
H	1.63140800	-0.83184000	-2.15041800
H	0.94465400	-2.19347700	-1.26735100
C	1.85940200	-0.68649200	0.00217600
H	2.83624300	-1.18074500	0.00373600
C	2.05130100	0.83627400	-0.00159700
H	2.62558700	1.14249200	0.87931700
H	2.62614600	1.13805100	-0.88367800
C	-0.10015300	1.11298100	-1.25614300
H	-1.06983400	1.61931300	-1.28496100
H	0.44567100	1.41113300	-2.15726500
C	-0.10093600	1.11930100	1.25018700
H	-1.07062700	1.62577800	1.27586900
H	0.44433900	1.42196900	2.15013500
C	0.68264100	1.53020000	-0.00377600
H	0.82094000	2.61599500	-0.00647100
C	-2.42924200	-0.29396000	-0.00004300
N	-3.52762500	0.14764000	0.00002200
H	-1.16547000	-1.93461900	0.00436100

Compound 5 ($E_{el,MP2}$ = -520.67487284 a.u.)

#

2-Me-2-CN-Ad

0 1

C	-1.09152400	0.46417200	-0.00000400
C	-0.21843600	0.19567800	1.25663700
H	-0.82834200	0.38659500	2.14697000
C	-0.21833300	0.19586300	-1.25661900
H	-0.82817400	0.38691200	-2.14697000
C	1.00800000	1.12119100	-1.25304900
H	0.71318600	2.17241400	-1.30643200
H	1.60090300	0.91734600	-2.15094500
C	1.00789700	1.12100400	1.25329800
H	1.60072300	0.91703100	2.15121700
H	0.71307800	2.17222100	1.30680900
C	1.85387700	0.85949700	0.00014000
H	2.72274000	1.52582700	0.00022500
C	2.32375000	-0.60070000	0.00004900
H	2.94386300	-0.79412000	-0.88187400
H	2.94379900	-0.79424200	0.88199000
C	0.26083100	-1.26347800	1.25472400
H	-0.59176400	-1.94723100	1.29513600
H	0.86117300	-1.44485800	2.15250400
C	0.26093100	-1.26329100	-1.25488300
H	-0.59166300	-1.94703500	-1.29546800
H	0.86134600	-1.44453900	-2.15264200
C	1.10350100	-1.52996500	-0.00006500
H	1.43430300	-2.57349300	-0.00012500
C	-2.22542900	-0.47452200	-0.00012500
N	-3.16179300	-1.19997200	-0.00025100
C	-1.70379200	1.87463300	0.00007600
H	-2.32697800	2.01110600	-0.88516000
H	-2.32706800	2.01096800	0.88527000
H	-0.93621800	2.64440900	0.00018000

Compound 6 ($E_{el,MP2}$ = -464.51934851 a.u.)

#

2AdOH

0 1

C	-1.33667700	-0.61936800	0.32782800
C	-0.52586900	0.26062100	1.27645400
H	-1.12252800	0.43244100	2.17762800
C	-0.54261400	-0.86398400	-0.96014100
H	-1.14292500	-1.48778600	-1.63509000
C	-0.21666500	0.47373900	-1.63618600
H	-1.13865800	0.99353700	-1.90791900
H	0.34327100	0.28946400	-2.55960400
C	-0.19996400	1.59763700	0.59810700

H	0.37503500	2.22426200	1.28861900
H	-1.12350500	2.12987100	0.35990100
C	0.61188700	1.33990800	-0.67834000
H	0.84831100	2.29385000	-1.16118600
C	1.91303500	0.60865200	-0.32265900
H	2.50551400	0.43433600	-1.22768400
H	2.51978200	1.22737500	0.34755600
C	0.77604000	-0.47144500	1.63141400
H	0.55438900	-1.41927600	2.13434900
H	1.35870000	0.13593000	2.33173600
C	0.75789000	-1.59743600	-0.60126900
H	0.53262700	-2.56212600	-0.13292400
H	1.32714300	-1.80685800	-1.51293400
C	1.58659300	-0.72918900	0.35450300
H	2.51555600	-1.25036100	0.60857800
O	-2.58000000	0.05724400	0.07923400
H	-3.11361700	-0.50474400	-0.50026200
H	-1.54104200	-1.58267900	0.81710000

Compound 7 ($E_{el,MP2}$ = -503.68771001 a.u.)

#

2AdOMe

0 1

C	-1.03451500	0.03736500	-0.64174900
C	-0.01176600	-1.07229300	-0.88224400
H	-0.48038100	-1.83451200	-1.51247100
C	-0.42062600	1.12351900	0.25234200
H	-1.15033400	1.92249200	0.41839400
C	-0.00339300	0.50651400	1.59281700
H	-0.87735600	0.09344100	2.10399400
H	0.42091200	1.28363100	2.23833100
C	0.40926900	-1.68604300	0.45961300
H	1.13606500	-2.48633400	0.28117700
H	-0.45755000	-2.13039700	0.95391400
C	1.03195700	-0.59943700	1.34607900
H	1.33490000	-1.03614500	2.30354800
C	2.25936200	-0.00513300	0.64222400
H	2.71980900	0.76286500	1.27371300
H	3.01150900	-0.78501200	0.47997200
C	1.21529100	-0.47869300	-1.58747700
H	0.92925600	-0.05419200	-2.55632600
H	1.94301200	-1.27265300	-1.78583200
C	0.80667200	1.71049500	-0.46040800
H	0.50958100	2.16300900	-1.41333900
H	1.23958000	2.50783100	0.15314600
C	1.84177900	0.60587000	-0.70223100
H	2.71905400	1.02856000	-1.20328500
O	-2.18597800	-0.58193100	-0.05802900
H	-1.33169000	0.48287600	-1.60609700
C	-3.31421300	0.28124900	0.01776700
H	-4.16168600	-0.34380500	0.28922300

H	-3.18764600	1.05820800	0.77637800
H	-3.50811700	0.75511200	-0.95061000

Compound 8 ($E_{el,MP2}$ = -503.70889767 a.u.)

#

2-Me-2AdOH

0 1

C	-1.30476100	-0.03372500	-0.00752300
C	-0.40362900	-0.00369200	-1.25078400
H	-1.05041000	-0.02125300	-2.13504900
C	-0.40877300	-0.00492700	1.24634700
H	-1.05649800	-0.01915900	2.13363800
C	0.51068000	-1.23519200	1.25352800
H	-0.08189000	-2.15156600	1.28092800
H	1.13345000	-1.21517100	2.15494500
C	0.51555400	-1.23459200	-1.25212600
H	1.14378700	-1.21214000	-2.14963500
H	-0.08019100	-2.14812500	-1.28744600
C	1.39893300	-1.21712700	0.00253700
H	2.04799800	-2.09917900	0.00437800
C	2.25801300	0.05345000	0.00648800
H	2.90555900	0.06786900	0.89025000
H	2.90955100	0.06990700	-0.87415700
C	0.46441800	1.26449400	-1.24996200
H	-0.15100400	2.16703300	-1.30142800
H	1.09463400	1.26358700	-2.14574000
C	0.45949800	1.26390300	1.25744200
H	-0.15678900	2.16588800	1.30649200
H	1.08526000	1.26168100	2.15653100
C	1.34679900	1.28741800	0.00545200
H	1.95751000	2.19657900	0.00759900
C	-2.35050000	1.07707300	-0.01115600
H	-2.97425000	0.97626800	-0.90034500
H	-2.98736300	0.98688500	0.87368900
H	-1.91531800	2.07391300	-0.00199900
O	-2.01009800	-1.29482800	-0.08134800
H	-2.66065100	-1.30688200	0.63667300

Compound 9 ($E_{el,MP2}$ = -621.24982365 a.u.)

#

2-tBu-2AdOH

0 1

C	0.58951400	-0.45753400	0.00091600
C	-0.29276400	-0.18049500	1.24184500
H	0.29434400	-0.37136700	2.14241100
C	-0.27993900	-0.14911800	-1.24766400
H	0.32335600	-0.29067600	-2.15389800
C	-1.47854500	-1.11955600	-1.27721700

H	-1.14557100	-2.15661000	-1.33912400
H	-2.07462700	-0.91283200	-2.17347200
C	-1.49363000	-1.14622400	1.23432900
H	-2.10187300	-0.94930700	2.12492200
H	-1.15025800	-2.17848600	1.28933800
C	-2.34083000	-0.91849000	-0.02237400
H	-3.17355300	-1.62995500	-0.03813400
C	-2.88595100	0.51377500	0.00421900
H	-3.51436400	0.69997800	-0.87389200
H	-3.51256300	0.65970500	0.89101300
C	-0.84419800	1.25273900	1.26200200
H	-0.04591100	1.99441200	1.32703900
H	-1.45428300	1.37646600	2.16396900
C	-0.86457700	1.27770200	-1.24120800
H	-0.09586100	2.04206500	-1.31468800
H	-1.49782500	1.38764100	-2.12914700
C	-1.70976000	1.49640400	0.01803100
H	-2.08680400	2.52485200	0.02906600
C	2.03424900	0.18505600	0.00971200
O	0.80458800	-1.89176000	0.08334200
H	1.21151700	-2.17961600	-0.74610400
C	2.64805000	0.04556400	1.40885300
H	3.71472300	0.27853600	1.36110100
H	2.19315700	0.73814300	2.11945500
H	2.53679200	-0.97171900	1.78544300
C	2.94112500	-0.58390200	-0.97209300
H	3.88358000	-0.04446800	-1.08316100
H	3.18427100	-1.58240300	-0.60858700
H	2.49771300	-0.66044500	-1.96847200
C	2.14042300	1.66027700	-0.40765100
H	1.91674300	1.79941600	-1.46580700
H	1.50752900	2.32440300	0.17562500
H	3.17405700	1.97916600	-0.25183600

Compound 10 ($E_{el,MP2}$ = -616.76443100 a.u.)

#

2-ADOAc

0 1

C	-2.81136200	0.18548900	0.05782000
O	-2.91926500	1.40119400	-0.02761700
C	-3.92907200	-0.80382400	-0.13232900
H	-4.87762200	-0.27553400	-0.13744000
H	-3.91079800	-1.55140000	0.65790400
H	-3.79299500	-1.31678800	-1.08434400
O	-1.64430300	-0.45919100	0.32479700
C	0.95793900	-1.67286300	0.58067600
C	1.59091800	-1.28604200	-0.76264300
C	0.55915800	-0.52193800	-1.60332300
C	0.52910700	-0.40412900	1.32968700
C	-0.47110200	0.38798100	0.49426200
C	0.13122700	0.75154600	-0.86265900

C	2.81371400	-0.39260500	-0.51528700
C	2.38586300	0.87750100	0.23226600
C	1.35641900	1.64306700	-0.60862700
C	1.75296400	0.49127800	1.57560000
H	1.67866100	-2.22753400	1.19119300
H	0.09552500	-2.32506200	0.41972800
H	1.89988200	-2.19118600	-1.29566400
H	-0.31029300	-1.15623400	-1.79875600
H	0.98854700	-0.24995100	-2.57359400
H	0.05760500	-0.66819900	2.28170900
H	-0.61379200	1.30176000	-1.44386500
H	3.28106500	-0.12440700	-1.46905600
H	3.56220500	-0.93685100	0.07095600
H	3.25976900	1.51295900	0.40909900
H	1.79575700	1.94073600	-1.56634500
H	1.05270800	2.56104200	-0.09386100
H	2.47848300	-0.04552200	2.19555900
H	1.45964300	1.39118200	2.12714800
H	-0.79044800	1.29219700	1.01952700

Compound 11 ($E_{el,MP2}$ = -444.68169268 a.u.)

#

2AdNH2

0 1

C	-1.30525100	0.75876100	0.00000000
C	-0.56206800	0.26696200	1.25042600
H	-1.08754200	0.63465900	2.14114600
C	-0.56206800	0.26696200	-1.25042600
H	-1.08754200	0.63465900	-2.14114600
C	0.88327800	0.78247000	-1.25088400
H	0.89384000	1.87421000	-1.26778900
H	1.39513500	0.42863400	-2.15292100
C	0.88327800	0.78247000	1.25088400
H	1.39513500	0.42863400	2.15292100
H	0.89384000	1.87421000	1.26778900
C	1.60818900	0.26827700	0.00000000
H	2.64056700	0.63384300	0.00000000
C	1.60763800	-1.26603500	0.00000000
H	2.13804300	-1.64202800	-0.88196800
H	2.13804300	-1.64202800	0.88196800
C	-0.56206800	-1.26780500	1.25176900
H	-1.58987300	-1.64675000	1.27420900
H	-0.06160600	-1.63762900	2.15303600
C	-0.56206800	-1.26780500	-1.25176900
H	-1.58987300	-1.64675000	-1.27420900
H	-0.06160600	-1.63762900	-2.15303600
C	0.16208400	-1.78123400	0.00000000
H	0.16101000	-2.87650200	0.00000000
N	-1.37678900	2.22415000	0.00000000
H	-1.88963600	2.54820600	-0.81603200
H	-1.88963600	2.54820600	0.81603200

H	-2.30645400	0.29686600	0.00000000

Compound 12 ($E_{el,MP2}$ = -523.03066905 a.u.)

#

2-AdNMe2

0 1

C	-0.29407700	-0.02972000	1.24739200
H	-0.52366300	0.53881300	2.15147600
C	-0.29407700	-0.02972000	-1.24739200
H	-0.52366300	0.53881300	-2.15147600
C	1.18075300	-0.45277500	-1.25242200
H	1.82596600	0.42929300	-1.27220300
H	1.38938500	-1.04187700	-2.15292500
C	1.18075300	-0.45277500	1.25242200
H	1.38938500	-1.04187700	2.15292500
H	1.82596600	0.42929300	1.27220300
C	1.47376900	-1.29027500	0.00000000
H	2.52657500	-1.59217100	0.00000000
C	0.58225000	-2.53982700	0.00000000
H	0.79719400	-3.15345200	-0.88199200
H	0.79719400	-3.15345200	0.88199200
C	-1.18903200	-1.27669000	1.23999500
H	-2.24438900	-0.98210000	1.25318100
H	-1.00463900	-1.85754800	2.15037800
C	-1.18903200	-1.27669000	-1.23999500
H	-2.24438900	-0.98210000	-1.25318100
H	-1.00463900	-1.85754800	-2.15037800
C	-0.89472400	-2.12356700	0.00000000
H	-1.53007600	-3.01568400	0.00000000
N	0.21677200	2.06493900	0.00000000
C	-0.04561100	2.87331600	1.18865100
H	0.47742300	3.82358800	1.08784100
H	-1.12074100	3.08132600	1.32670400
H	0.33061000	2.38304900	2.08331800
C	-0.04561100	2.87331600	-1.18865100
H	-1.12074100	3.08132600	-1.32670400
H	0.47742300	3.82358800	-1.08784100
H	0.33061000	2.38304900	-2.08331800
C	-0.58305900	0.82808300	0.00000000
H	-1.66200700	1.09504300	0.00000000

Compound 13 ($E_{el,MP2}$ = -594.87851782 a.u.)

#

2-AdNHCOMe

0 1

C	1.04634800	-1.70303700	0.48788400
C	1.67609000	-1.22363100	-0.82693200
C	0.63078700	-0.44305500	-1.63555700

C	0.55764200	-0.49212300	1.29804000
C	-0.46789400	0.31896000	0.49608100
C	0.15835100	0.77487900	-0.83307100
C	2.86848900	-0.30991600	-0.51383300
C	2.39242800	0.90185900	0.29820500
C	1.35301100	1.68357300	-0.51526000
C	1.75508400	0.41839400	1.60774700
N	-1.69001600	-0.44696200	0.29559300
H	1.78138900	-2.26023800	1.07860600
H	0.22977300	-2.40364000	0.27709700
H	2.01889400	-2.08891100	-1.40389800
H	-0.21957000	-1.08810000	-1.88053300
H	1.06271000	-0.11205100	-2.58603800
H	0.09316200	-0.82429100	2.23334800
H	-0.59778100	1.33143800	-1.39359700
H	3.33632900	0.02494900	-1.44586400
H	3.62748400	-0.86452500	0.04894400
H	3.24531300	1.54960100	0.52602100
H	1.80033800	2.04777800	-1.44619700
H	1.01411200	2.56168200	0.04493600
H	2.49065700	-0.13277500	2.20350200
H	1.42757800	1.27393500	2.20765200
C	-2.88747700	0.16660100	0.06011400
O	-2.99757100	1.39925300	0.00054100
C	-4.07349600	-0.75180400	-0.14413100
H	-1.65856900	-1.45401700	0.33156100
H	-4.38238200	-0.69529500	-1.18733100
H	-4.89688200	-0.39299900	0.46971700
H	-3.85918900	-1.78982500	0.10766000
H	-0.75887100	1.20779100	1.06522400

Compound 14 ($E_{el,MP2}$ = -488.50351541 a.u.)

#

2AdF

0 1

C	-1.31974700	-0.71868600	0.00000500
C	-0.54054100	-0.34859100	1.25393300
H	-1.14203800	-0.60997600	2.12984400
C	-0.54053800	-0.34860700	-1.25392700
H	-1.14203600	-0.61000200	-2.12983400
C	-0.23200400	1.15429200	-1.25004100
H	-1.16221100	1.72741600	-1.26899500
H	0.32969600	1.41106400	-2.15436200
C	-0.23200700	1.15430800	1.25002900
H	0.32968900	1.41109300	2.15434800
H	-1.16221500	1.72743200	1.26897100
C	0.58505800	1.50695500	-0.00000700
H	0.80884100	2.57859700	-0.00001100
C	1.89514600	0.70809400	-0.00000500
H	2.49189600	0.96608000	-0.88163700
H	2.49190900	0.96609500	0.88161100

C	0.77059000	-1.15088000	1.24996500
H	0.55986900	-2.22587500	1.26873100
H	1.34106300	-0.91945700	2.15497600
C	0.77059300	-1.15089500	-1.24995000
H	0.55987400	-2.22589000	-1.26870900
H	1.34106500	-0.91947800	-2.15496300
C	1.58630800	-0.79517400	0.00000600
H	2.52164200	-1.36420300	0.00001400
F	-2.56027200	-0.02180300	-0.00000400
H	-1.58173200	-1.78156800	0.00000800

Compound 15 ($E_{el,MP2}$ = -848.50782788 a.u.)

#

2AdCl

0 1

C	-1.02959400	-0.73341500	0.00000400
C	-0.24811500	-0.34267100	1.25488700
H	-0.83956400	-0.59862300	2.13888700
C	-0.24811500	-0.34268700	-1.25488300
H	-0.83956500	-0.59864900	-2.13888000
C	0.07692400	1.15600000	-1.25115800
H	-0.84294100	1.74535100	-1.27932300
H	0.64667800	1.40132000	-2.15354500
C	0.07692400	1.15601500	1.25114400
H	0.64667700	1.40134700	2.15352700
H	-0.84294200	1.74536600	1.27930100
C	0.89443900	1.50315700	-0.00000900
H	1.12424600	2.57353000	-0.00001600
C	2.19999800	0.69727200	-0.00000300
H	2.79828100	0.95138600	-0.88169700
H	2.79827900	0.95139600	0.88168900
C	1.06075200	-1.14984700	1.25051100
H	0.84295000	-2.22315500	1.27482200
H	1.63304300	-0.91605000	2.15414200
C	1.06075200	-1.14986100	-1.25049700
H	0.84295100	-2.22317000	-1.27479600
H	1.63304300	-0.91607500	-2.15413200
C	1.87843800	-0.80299900	0.00000500
H	2.80856200	-1.38053400	0.00000800
H	-1.21069700	-1.81067800	0.00001100
Cl	-2.67843700	-0.00285600	0.00000000

Compound 16 ($E_{el,MP2}$ = -787.11384357 a.u.)

#

2-AdSH

0 1

C	1.06313700	-0.26075400	-1.68031300
C	1.88414900	0.50794500	-0.63767200

C	-0.24037600	-0.76726200	-1.04478600
C	-1.03965100	0.45238100	-0.56074100
C	-0.23590800	1.19356600	0.51840700
C	1.06543500	1.69918100	-0.12406800
C	2.21899800	-0.42505400	0.53347500
C	0.92014400	-0.93188100	1.17352500
C	0.10336300	0.26075100	1.68732600
C	0.09794800	-1.69796000	0.12841700
S	-2.70610400	-0.08171800	-0.01212200
H	1.63919700	-1.11149900	-2.05980500
H	0.83720200	0.38479700	-2.53591500
H	2.80960000	0.87118600	-1.09656700
H	-0.82693600	-1.30759000	-1.79487300
H	-0.81861400	2.04722500	0.88257000
H	0.83756500	2.38359600	-0.94880800
H	1.64446000	2.26399200	0.61435400
H	2.81989000	0.10878100	1.27778000
H	2.81860800	-1.27041000	0.17854800
H	1.15880200	-1.59805300	2.00902600
H	0.67971000	0.81523000	2.43573100
H	-0.81130300	-0.08836400	2.17243600
H	0.67013100	-2.55368900	-0.24593100
H	-0.81267100	-2.09677500	0.58437800
H	-1.19293100	1.12144500	-1.41335200
H	-3.17847500	1.15214000	0.17296200

Compound 17 ($E_{el,MP2}$ = -826.29646132 a.u.)

#

2-AdSMe

0 1

C	1.40317800	-0.13579300	-1.68068800
C	2.06534500	0.77635900	-0.64101500
C	0.22065400	-0.87914300	-1.04190000
C	-0.79911400	0.16183400	-0.55356900
C	-0.14472600	1.04944100	0.51792600
C	1.03547200	1.79106600	-0.12920900
C	2.57182600	-0.07415600	0.53146400
C	1.39384800	-0.81778500	1.17459000
C	0.36632700	0.19929400	1.68745200
C	0.73072100	-1.72741800	0.13162300
S	-2.33199400	-0.67016200	-0.01071200
C	-3.43631200	0.76230200	0.01332300
H	2.12970800	-0.86233800	-2.06068400
H	1.05698600	0.45395500	-2.53654100
H	2.90520600	1.30752100	-1.10115900
H	-0.25602400	-1.52158900	-1.78902100
H	-0.87083900	1.78231200	0.88501800
H	0.67951300	2.41609800	-0.95596400
H	1.49781900	2.45913000	0.60562600
H	3.06138400	0.56540100	1.27411100
H	3.32060900	-0.79100400	0.17689700

H	1.75628100	-1.42494600	2.01066200
H	0.82768000	0.85302500	2.43580700
H	-0.46694800	-0.31590100	2.17210900
H	1.45408200	-2.46107100	-0.24079500
H	-0.08967300	-2.28919800	0.58796200
H	-4.43967100	0.39143200	0.21647300
H	-3.16756900	1.47207000	0.79357800
H	-3.44276000	1.26421500	-0.95422000
H	-1.08719200	0.78746500	-1.40845100

Compound 18 ($E_{el,MP2}$ = -582.07303388 a.u.)

#

2-CMe2OH-Ad

0 1

C	-0.62981300	0.00020200	-0.59660000
C	0.22211400	-1.24915800	-0.27807900
H	-0.35878700	-2.15631700	-0.46480300
C	0.22212500	1.24934900	-0.27723900
H	-0.35877300	2.15663600	-0.46333800
C	0.72400300	1.25072600	1.17523400
H	-0.11578000	1.28267900	1.86975100
H	1.33130800	2.14899100	1.33931400
C	0.72398200	-1.25151900	1.17439500
H	1.33126000	-2.14990900	1.33789100
H	-0.11581200	-1.28389000	1.86887800
C	1.57507500	-0.00048800	1.42772900
H	1.92524800	-0.00084100	2.46561200
C	2.78111100	-0.00017600	0.47930900
H	3.40445500	0.88205300	0.66340000
H	3.40444400	-0.88253800	0.66280100
C	1.43761700	-1.25040100	-1.22041000
H	1.10423200	-1.28181600	-2.26410200
H	2.03783500	-2.15035300	-1.04495800
C	1.43762700	1.25121700	-1.21956900
H	1.10424400	1.28333900	-2.26323900
H	2.03785600	2.15104300	-1.04351000
C	2.28938900	0.00032100	-0.97412000
H	3.14792600	0.00054600	-1.65466600
C	-2.07667000	0.00004300	-0.05299700
C	-2.83166200	-1.24628200	-0.51840900
H	-3.87792300	-1.18042800	-0.20942400
H	-2.80836400	-1.33575400	-1.60631300
H	-2.40590800	-2.14585300	-0.07881500
C	-2.83172000	1.24654500	-0.51787500
H	-2.80842900	1.33649200	-1.60574300
H	-3.87796400	1.18054400	-0.20888300
H	-2.40598300	2.14592600	-0.07788300
H	-0.78025200	0.00056600	-1.68713100
O	-2.02871200	-0.00026300	1.39320800
H	-2.94421700	-0.00128400	1.71128500

Compound 19 ($E_{el,MP2}$ = -541.69965615 a.u.)

#

2-Ad-COMe

0 1

C	-0.29722800	0.02936600	-1.69601700
C	-1.25451100	-0.99029300	-1.06440500
C	0.12663800	1.06412100	-0.64488200
C	0.85364600	0.36485000	0.53120500
C	-0.07625900	-0.70291100	1.13156400
C	-0.53245800	-1.71968900	0.07378200
C	-2.48732600	-0.26765100	-0.50630100
C	-2.04991000	0.74422800	0.56116400
C	-1.31306300	0.01453400	1.69413500
C	-1.11428500	1.77318800	-0.08506000
C	2.22672900	-0.13907100	0.12611800
O	2.48763800	-1.33470500	-0.02513100
H	-0.78896600	0.54340100	-2.52925400
H	0.57860700	-0.48477500	-2.10540700
H	-1.56645100	-1.71427100	-1.82429800
H	0.78888700	1.80570900	-1.10353800
H	0.45311400	-1.22535000	1.93499900
H	0.32277200	-2.27701400	-0.30788500
H	-1.21407300	-2.43731500	0.54430500
H	-3.17983500	-0.99653600	-0.07179100
H	-3.02246100	0.24841300	-1.31126800
H	-2.92925300	1.25566500	0.96674200
H	-1.98167300	-0.71573400	2.16257600
H	-1.01810000	0.72796300	2.47209100
H	-1.63659400	2.29524200	-0.89438600
H	-0.81253000	2.52941600	0.64802200
H	1.03982300	1.13522300	1.29493700
C	3.30692200	0.91051100	-0.03831100
H	3.66619800	1.19236200	0.95428500
H	4.13550300	0.49586700	-0.60744200
H	2.93055100	1.81227300	-0.51958800

Compound 20 ($E_{el,MP2}$ = -579.67316488 a.u.)

#

adamantane-spirocyclobutanone

0 1

C	0.68845800	1.24256400	-1.25268100
C	1.56500500	1.38753100	-0.00191000
C	0.02332000	-0.14080900	-1.25476300
C	-0.85277400	-0.29922500	0.00115900
C	0.02457200	-0.13808300	1.25572900
C	0.68979100	1.24524100	1.25008600
C	2.64287300	0.29577900	-0.00126700
C	1.97756400	-1.08685300	0.00053300

C	1.10170000	-1.23179100	1.25187000
C	1.10057600	-1.23439000	-1.24969500
C	-1.79945700	-1.54215600	0.00243200
C	-2.11610500	0.57225200	0.00004000
C	-3.05632000	-0.63063100	-0.00233200
O	-2.30699200	1.77928600	0.00126100
H	1.30117000	1.35037800	-2.15481200
H	-0.07209300	2.02725300	-1.27341200
H	2.04002200	2.37403300	-0.00323500
H	-0.61032200	-0.24783500	-2.14463800
H	-0.60820300	-0.24315200	2.14643600
H	-0.07072300	2.02996700	1.27002000
H	1.30350400	1.35486000	2.15132200
H	3.28468200	0.40232200	0.88025100
H	3.28384600	0.40040100	-0.88362400
H	2.74681200	-1.86636700	0.00098600
H	1.71600900	-1.14089500	2.15458300
H	0.64029900	-2.22474700	1.27564000
H	1.71403700	-1.14516400	-2.15315200
H	0.63933900	-2.22745900	-1.27110800
H	-1.70541100	-2.16720900	0.89127500
H	-1.70186900	-2.17264200	-0.88215900
H	-3.68666800	-0.68781700	-0.89153000
H	-3.69371500	-0.68678700	0.88186800

Compound 21 ($E_{el,MP2}$ = -618.88369499 a.u.)

#

adamantane-spirocyclopentanone

0 1

C	0.84776500	1.00980500	-1.42674900
C	1.88428200	1.24411900	-0.31932600
C	0.05726900	-0.27802000	-1.14253600
C	-0.69805800	-0.16132800	0.21819300
C	0.35095600	0.12092500	1.31525900
C	1.16599700	1.39107900	1.02710100
C	2.84866400	0.05387200	-0.25131800
C	2.05610400	-1.22513700	0.04612000
C	1.32061300	-1.07143200	1.38668800
C	1.04587900	-1.45378600	-1.08624000
C	-1.55874000	-1.40758400	0.51906900
C	-1.78254200	0.91628700	0.08043700
C	-3.14122700	0.26337500	-0.15481200
C	-2.84226600	-1.22673600	-0.30200000
O	-1.62307400	2.13333400	0.15099600
H	1.35210600	0.90589600	-2.39412600
H	0.17842600	1.86984300	-1.49888500
H	2.44417400	2.15974300	-0.53681100
H	-0.66610000	-0.44593800	-1.95004000
H	-0.17258500	0.22962500	2.27349800
H	0.52039200	2.26841900	1.02093900
H	1.90412800	1.52215300	1.82689000

H	3.59702600	0.22341800	0.53056100
H	3.38708900	-0.05407800	-1.19955000
H	2.74018400	-2.07882800	0.10134000
H	2.04875500	-0.89294600	2.18580300
H	0.79173600	-1.99443900	1.64224400
H	1.57488400	-1.51493000	-2.04405500
H	0.52787200	-2.40712800	-0.95624200
H	-1.80466200	-1.40675300	1.58832000
H	-1.05978800	-2.35103900	0.30714500
H	-3.64364900	0.73173300	-1.00200900
H	-3.74950600	0.46222900	0.73331500
H	-3.65390000	-1.86305400	0.05228100
H	-2.66016800	-1.48323700	-1.34790000

Compound 22 ($E_{el,MP2}$ = -658.07162734 a.u.)

#

adamantane-spirocyclohexanone

0 1

C	1.48021600	1.53367200	-0.70234300
C	2.09373800	1.13198600	0.64330600
C	0.66849100	0.35866300	-1.27549100
C	-0.46581800	-0.05164900	-0.30889200
C	0.18923600	-0.46111900	1.03736900
C	0.97108000	0.73199100	1.60951600
C	3.04213600	-0.05544700	0.43673200
C	2.26080100	-1.23482200	-0.15613100
C	1.15477900	-1.63712200	0.82675700
C	1.63606800	-0.81674500	-1.49501800
C	-1.34146000	-1.18810900	-0.90720500
C	-1.47338100	1.08364700	-0.11430000
C	-2.61685300	0.80149400	0.83746600
C	-3.42916200	-0.37294400	0.26436500
O	-1.46391000	2.11069800	-0.79872500
H	2.27753400	1.79033100	-1.40918000
H	0.85070400	2.41641300	-0.59185500
H	2.64897100	1.97836300	1.06142800
H	0.21989600	0.66047800	-2.22784700
H	-0.57778600	-0.76321100	1.75515800
H	0.30264800	1.58443600	1.77941900
H	1.39201100	0.45701900	2.58342300
H	3.49635000	-0.34996400	1.38956900
H	3.85666400	0.23264100	-0.23658100
H	2.93650000	-2.08225300	-0.31420900
H	0.62220600	-2.52347100	0.46985700
H	1.59849300	-1.90717400	1.79191900
H	2.42510500	-0.49900700	-2.18562500
H	1.13704400	-1.66788400	-1.96586400
H	-1.71235600	-0.84109300	-1.88032900
H	-0.73287000	-2.07014300	-1.10661200
H	-3.22157500	1.70513500	0.91773100
H	-4.23389500	-0.64278300	0.95229800

H	-3.90051800	-0.04466800	-0.66757800
C	-2.52905900	-1.57354900	-0.02214300
H	-2.24164100	0.54194100	1.83040500
H	-2.17069600	-2.00190000	0.91864000
H	-3.10638900	-2.35846400	-0.51829900

Compound 23 ($E_{el,MP2}$ = -770.87515389 a.u.)

#

spirobenzenecyclopentanone

0 1

O	0.50187500	2.29490700	-0.44134300
C	0.77670100	1.09966000	-0.30824100
C	-0.20292600	-0.09000200	-0.30454000
C	-0.83156200	-0.18607700	1.12074400
C	-1.69965400	1.05244300	1.39875500
C	-2.83818900	1.13455200	0.37067800
C	-2.25091100	1.24292000	-1.04184500
C	-3.70756500	-0.12552500	0.45515300
C	2.11341100	-0.82526300	-0.22773300
C	4.47377200	-0.87351200	0.23055000
C	4.48866900	0.52730900	0.35540900
C	3.31578000	1.26608900	0.18928500
C	2.13975500	0.56471500	-0.09149000
H	-1.68531500	2.16712000	-1.15159200
H	-4.15962600	-0.21145300	1.44959300
H	-4.52595500	-0.06369000	-0.27054200
H	-3.44941000	2.01866400	0.58027200
H	-2.11563500	0.97084300	2.40930100
H	-1.10091700	1.96517100	1.36637800
H	-0.02203700	-0.25156000	1.85946200
H	3.30095500	2.34601100	0.28052500
H	5.41975900	1.03160300	0.58442000
H	5.39488000	-1.42856800	0.36486300
C	3.29015500	-1.56004400	-0.06663900
H	3.29414100	-2.64005400	-0.16800800
C	-2.22190200	-1.24474100	-1.23161600
H	-1.63249700	-2.13921600	-1.45825500
H	-3.01708700	-1.19067200	-1.98344900
C	-2.84053200	-1.35766200	0.17039800
H	-3.45498400	-2.26282700	0.22543100
C	-1.72746500	-1.43178100	1.22249200
H	-1.15209900	-2.35358900	1.10628100
H	-2.16732500	-1.46511100	2.22562500
C	-1.35714300	0.02470000	-1.32254100
H	-0.92555500	0.10802200	-2.32808600
H	-3.06385100	1.25683100	-1.77725900
C	0.73018400	-1.29703600	-0.59642900
H	0.69161400	-1.54053500	-1.66474100
H	0.45247400	-2.20071100	-0.05381300

Compound 24 ($E_{el,MP2}$ = -810.06288135 a.u.)

#

spirobenzenecyclohexanone

0 1

C	-2.83076500	0.84955200	-1.07932100
C	-3.08680800	1.07414300	0.41847100
C	-1.78047400	1.47991700	1.11335600
C	-1.76253800	-0.24288100	-1.26925100
C	-0.43983600	0.18306800	-0.59166700
C	-0.72517600	0.38050800	0.92227200
C	-3.60161300	-0.22478100	1.05110800
C	-2.56302100	-1.33462900	0.84915700
C	-1.24651000	-0.93295100	1.52547100
C	-2.31845800	-1.53915500	-0.64998700
C	0.66880600	-0.84550700	-0.77826100
C	0.16531200	1.45169000	-1.24407300
C	2.00467600	-0.45606200	-0.23367900
O	0.53095400	-1.91763600	-1.37738700
H	-2.54582500	1.78788400	-1.56197400
H	-3.75675600	0.52185500	-1.56460600
H	-3.83096600	1.86750000	0.54760200
H	-1.95948900	1.62057400	2.18556900
H	-1.42108000	2.43892000	0.72697700
H	-1.57225300	-0.40290500	-2.33699700
H	0.19729400	0.66129900	1.43993100
H	-4.55208700	-0.51567500	0.59082800
H	-3.79085900	-0.07022300	2.11942800
H	-2.93011000	-2.26732300	1.29057300
H	-0.50219100	-1.72879700	1.40818800
H	-1.40141800	-0.79735400	2.60201400
H	-1.63487900	-2.36954400	-0.81908700
H	-3.26406400	-1.78579700	-1.14653300
H	0.46444100	1.19443300	-2.26782000
H	-0.58227000	2.24021400	-1.33010000
C	1.37260700	1.98513400	-0.47369600
C	2.35776700	0.90129900	-0.11081600
H	1.03240000	2.48083800	0.44219200
H	1.87748300	2.75393300	-1.06620800
C	2.91813600	-1.46683900	0.10727800
C	4.18098000	-1.13285800	0.59239300
C	4.54292800	0.21531000	0.71812600
C	3.63846800	1.21861200	0.36287700
H	2.61890900	-2.50071200	-0.01779900
H	4.88200000	-1.91189500	0.86653600
H	5.52745100	0.48168100	1.08405200
H	3.92974600	2.26075700	0.44777400

Cartesian coordinates of the optimized compounds 1-24 at the B3LYP/6-31+G** level

Compound 1 ($E_{el,B3LYP}$ = -390.75426694 a.u.)

#

Ad

0 1

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.54396725
H	1.03436755	0.00000000	1.91250271
C	-1.45349760	-0.00238611	-0.52153267
H	-1.45054009	-0.00373694	-1.61957017
C	-2.18256263	-1.26215672	-0.00372859
H	-1.68452968	-2.16687375	-0.37864696
H	-3.21316831	-1.28462248	-0.38356183
C	-0.73308138	-1.25957003	2.05679598
H	-0.72407496	-1.27978172	3.15514257
H	-0.21080494	-2.16425305	1.71648470
C	-2.18839546	-1.26310047	1.54034988
H	-2.70713549	-2.15904967	1.90628960
C	-2.91489631	0.00079198	2.05012615
H	-3.95774382	0.00137787	1.70428254
H	-2.94345457	0.00232100	3.14841273
C	-0.73176816	1.26103398	2.05435871
H	-0.20843626	2.16450597	1.71232442
H	-0.72242698	1.28335150	3.15269022
C	-2.18209623	1.25887488	-0.00654895
H	-1.68394917	2.16196389	-0.38509779
H	-3.21256847	1.27963946	-0.38679034
C	-2.18710030	1.26312692	1.53758898
H	-2.70541594	2.16037956	1.90118171
H	0.53494973	0.88290834	-0.37719822
H	0.53726725	-0.88193446	-0.37662535

Compound 2 ($E_{el,B3LYP}$ = -430.06962513 a.u.)

#

2-MeAd

0 1

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.55227104
H	1.03822074	0.00000000	1.91242816
C	-1.47310614	-0.02940405	-0.48783042
H	-1.48827903	-0.05023732	-1.58640343
C	-2.21221763	-1.27058583	0.06205950
H	-1.74965615	-2.19527543	-0.30500248
H	-3.24770530	-1.27307560	-0.30479557
C	-0.73762435	-1.24129178	2.10381545
H	-0.71478027	-1.22345161	3.20198713

H	-0.23147821	-2.16496137	1.79654103
C	-2.19949758	-1.24326110	1.60620116
H	-2.71945310	-2.12917487	1.99437514
C	-2.91139442	0.03342875	2.10212282
H	-3.95857389	0.03441045	1.76986307
H	-2.92430766	0.05469097	3.20048129
C	-0.71895910	1.27161104	2.05518517
H	-0.19299500	2.16767616	1.69826136
H	-0.69693175	1.30586841	3.15307607
C	-2.19394656	1.24210223	0.01207874
H	-1.70140481	2.13755032	-0.39113379
H	-3.22950211	1.25621894	-0.35461581
C	-2.18011758	1.27905016	1.55594615
H	-2.68496504	2.18854235	1.90760520
C	0.87548445	-1.09992570	-0.61786380
H	0.87513765	-1.02533838	-1.71194406
H	1.91408829	-1.00432594	-0.27938828
H	0.53775147	-2.10804065	-0.35847929
H	0.42936404	0.96026011	-0.32388709

Compound 3 ($E_{el,B3LYP}$ = -548.00757978 a.u.)

#

2-t-Bu-Ad

0 1

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.55985231
H	1.02860537	0.00000000	1.93464005
C	-1.48906866	0.07059574	-0.45953160
H	-1.54195505	0.13531914	-1.55292468
C	-2.18745553	-1.23419708	-0.00245171
H	-1.69225814	-2.10494678	-0.45259000
H	-3.22902776	-1.24258610	-0.35199662
C	-0.68834142	-1.30592127	2.02797591
H	-0.66118014	-1.36856887	3.12461992
H	-0.13970549	-2.17698742	1.64524658
C	-2.15187122	-1.33782547	1.53867910
H	-2.62780443	-2.27526162	1.85565435
C	-2.90757770	-0.13830202	2.14792828
H	-3.95862187	-0.15042750	1.82857668
H	-2.90459942	-0.20811884	3.24431411
C	-0.76666903	1.19521940	2.16953940
H	-0.29539959	2.14652761	1.89901037
H	-0.72528610	1.12836805	3.26567907
C	-2.26370394	1.26109379	0.15761371
H	-1.85292607	2.22008009	-0.16881806
H	-3.30309771	1.22999105	-0.19809630
C	-2.23498846	1.17462391	1.69647588
H	-2.77320354	2.03088567	2.12404686
C	1.04101726	0.91171707	-0.75907190
C	2.42691833	0.77952070	-0.08814152
H	3.19595539	1.24523011	-0.71542921

H	2.46120270	1.27212929	0.88893038
H	2.70593256	-0.27173120	0.05345137
C	1.17611129	0.37497805	-2.20503836
H	1.91214540	0.96309219	-2.76530687
H	1.51017542	-0.66929170	-2.21125457
H	0.23008838	0.42786832	-2.75347722
C	0.69437781	2.41306806	-0.85351760
H	-0.21750695	2.58544662	-1.43249637
H	0.57064196	2.87904725	0.12797819
H	1.50674844	2.94357185	-1.36511620
H	0.34151246	-1.01030788	-0.27332062

Compound 4 ($E_{el,B3LYP}$ = -482.99773978 a.u.)

#

2-CN-Ad

0 1

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.55965043
H	1.03665266	0.00000000	1.91600440
C	-1.47186900	0.02775435	-0.51520615
H	-1.46546082	0.04723987	-1.61120350
C	-2.17896456	-1.24957931	-0.01380629
H	-1.67774417	-2.14242280	-0.41162573
H	-3.20856314	-1.26751662	-0.39363182
C	-0.72311381	-1.27698680	2.03860951
H	-0.70535826	-1.31449074	3.13539525
H	-0.19325640	-2.17046496	1.68138403
C	-2.17981447	-1.27866399	1.52914288
H	-2.68821033	-2.18655291	1.87768315
C	-2.91402921	-0.03108958	2.06661110
H	-3.95795699	-0.03364727	1.72550162
H	-2.93737037	-0.05286259	3.16439757
C	-0.74049567	1.24689970	2.08627878
H	-0.22442182	2.15976758	1.76478343
H	-0.72323171	1.24157261	3.18374294
C	-2.19793071	1.27437327	0.03177751
H	-1.71249849	2.18780397	-0.33292087
H	-3.22798812	1.28870240	-0.34709898
C	-2.19763603	1.24603685	1.57554282
H	-2.71875520	2.13284198	1.95714785
C	0.79427105	1.10689437	-0.54900257
N	1.42413056	1.98103565	-0.98556178
H	0.47875142	-0.92422859	-0.35196551

Compound 5 ($E_{el,B3LYP}$ = -522.31078015 a.u.)

#

2-Me-2AdCN

0 1

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.57045646
H	1.04065546	0.00000000	1.91785874
C	-1.49845721	0.00000000	-0.46991191
H	-1.51853406	0.00000000	-1.56683725
C	-2.22030826	-1.25550671	0.06730940
H	-1.77232086	-2.17341435	-0.32980522
H	-3.25831098	-1.24021301	-0.28935050
C	-0.72868514	-1.25539874	2.09866934
H	-0.69913825	-1.23973964	3.19583302
H	-0.21569116	-2.17342954	1.79048103
C	-2.19379601	-1.26219160	1.61118285
H	-2.70046440	-2.16172529	1.98327622
C	-2.91224262	-0.00242628	2.13871818
H	-3.96143677	-0.00278285	1.81423678
H	-2.91678565	-0.00276711	3.23693379
C	-0.72918407	1.25585560	2.09885550
H	-0.21488807	2.16576377	1.76871253
H	-0.69729951	1.25318274	3.19605425
C	-2.22089433	1.25584002	0.06769728
H	-1.75193771	2.16572074	-0.32424832
H	-3.25826027	1.25318248	-0.29109532
C	-2.19461447	1.25738596	1.61173145
H	-2.70097914	2.15691088	1.98360182
C	0.66549821	1.22551183	-0.48876095
N	1.21460048	2.16758651	-0.89210635
C	0.81103549	-1.17796140	-0.59571522
H	0.80078226	-1.13366500	-1.68910359
H	1.85279335	-1.13011125	-0.26406257
H	0.40263241	-2.14244417	-0.29183489

Compound 6 ($E_{el,B3LYP}$ = -465.97581558 a.u.)

#

2-AdOH

0 1

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.53861968
H	1.04046388	0.00000000	1.88564382
C	-1.45509490	-0.03889077	-0.51710311
H	-1.44518066	-0.06003093	-1.61713887
C	-2.17932153	-1.29029635	0.02289585
H	-1.67206503	-2.19639598	-0.32725063
H	-3.20613224	-1.31990831	-0.36617842
C	-0.73205043	-1.25011292	2.07341549

H	-0.71264056	-1.24383558	3.17161281
H	-0.21189413	-2.15584533	1.74329754
C	-2.18950342	-1.25546047	1.56569247
H	-2.70964513	-2.14282596	1.94941593
C	-2.91399846	0.01873932	2.04923934
H	-3.95631947	0.01522946	1.70174922
H	-2.94386179	0.04193093	3.14717749
C	-0.72702091	1.27365947	2.02566465
H	-0.20484977	2.17092249	1.66618962
H	-0.70858474	1.31307921	3.12260313
C	-2.17548984	1.23857481	-0.02942255
H	-1.66692974	2.13142174	-0.41883434
H	-3.20134665	1.26233727	-0.42003989
C	-2.18411649	1.26993279	1.51441224
H	-2.69916371	2.17548274	1.86056253
O	0.77756167	-1.12071521	-0.44511311
H	0.86005280	-1.07813575	-1.40664909
H	0.47742823	0.92932399	-0.35153902

Compound 7 ($E_{el,B3LYP}$ = -506.27907094 a.u.)

#

2AdOMe

0 1

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.54030905
H	1.04175329	0.00000000	1.88359366
C	-1.45900989	-0.02447390	-0.51514335
H	-1.46285240	-0.03036301	-1.61258642
C	-2.18291789	-1.27868776	0.01836155
H	-1.68264561	-2.18367182	-0.34493968
H	-3.21260954	-1.29996367	-0.36375808
C	-0.72919474	-1.25358272	2.06995676
H	-0.71009894	-1.25109141	3.16831156
H	-0.20649119	-2.15675360	1.73699228
C	-2.18681881	-1.25793844	1.56238112
H	-2.70583770	-2.14846970	1.94029634
C	-2.91081726	0.01273793	2.05787747
H	-3.95460787	0.01102423	1.71478201
H	-2.93630680	0.02748224	3.15618804
C	-0.72561625	1.26919958	2.03799412
H	-0.20381568	2.16996100	1.68659438
H	-0.70538829	1.29729030	3.13538433
C	-2.17726554	1.24799682	-0.01276586
H	-1.67647531	2.14594054	-0.40056968
H	-3.20561820	1.26749826	-0.39753579
C	-2.18320937	1.26865399	1.53051826
H	-2.69784874	2.17145558	1.88471575
O	0.77200499	-1.12239802	-0.43642114
H	0.49408572	0.91945905	-0.36141836
C	1.17554740	-1.07737858	-1.79275951
H	1.84384611	-1.92707296	-1.95280866

H	0.32783004	-1.16219927	-2.48743030
H	1.72129914	-0.14734022	-2.01663913

Compound 8 ($E_{el,B3LYP}$ = -505.29280806 a.u.)

#

2-Me-2AdOH

0 1

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.55072064
H	1.04318875	0.00000000	1.89190066
C	-1.48026979	0.00547417	-0.48077786
H	-1.49015659	0.01385608	-1.58135997
C	-2.20176866	-1.25979568	0.03732283
H	-1.71444969	-2.15918718	-0.35194266
H	-3.23757591	-1.26256491	-0.32819640
C	-0.71950781	-1.26535971	2.07252546
H	-0.69184906	-1.26911422	3.17059566
H	-0.19672540	-2.16243802	1.72823886
C	-2.18306099	-1.27251306	1.58102226
H	-2.68806442	-2.17669833	1.94536573
C	-2.91159737	-0.02081676	2.11315538
H	-3.96023319	-0.02397241	1.78483944
H	-2.92109867	-0.02688269	3.21180801
C	-0.73652326	1.24786917	2.09016196
H	-0.23056495	2.17134782	1.78414340
H	-0.71156360	1.22980542	3.18766247
C	-2.22122276	1.25376195	0.05395548
H	-1.77192421	2.17688340	-0.33105362
H	-3.25841244	1.23898104	-0.30647039
C	-2.20000389	1.24813303	1.59789623
H	-2.71485696	2.14148900	1.97508631
C	0.82394227	1.15158505	-0.59428411
H	1.86057853	1.07628934	-0.25044088
H	0.82302025	1.09105432	-1.69076721
H	0.44429828	2.13936383	-0.32519371
O	0.64430521	-1.23408932	-0.38956543
H	0.74305440	-1.23682170	-1.35143153

Compound 9 ($E_{el,B3LYP}$ = -623.22202346 a.u.)

#

2-tBu-2AdOH

0 1

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.56361675
H	1.03418777	0.00000000	1.91972417
C	-1.50507993	0.03724669	-0.43789855
H	-1.56507077	0.08496384	-1.53422733
C	-2.20665582	-1.25635694	0.05350612

H	-1.73726629	-2.14500536	-0.37750297
H	-3.25087391	-1.24313479	-0.28737116
C	-0.69150982	-1.29150745	2.07159908
H	-0.65882294	-1.29648717	3.16988404
H	-0.15003087	-2.17337292	1.72339344
C	-2.15871221	-1.32917178	1.59621185
H	-2.63189425	-2.26136745	1.93176303
C	-2.90868459	-0.12081636	2.19132004
H	-3.96314186	-0.13402056	1.88295436
H	-2.89363290	-0.16957963	3.28869377
C	-0.76242547	1.20336647	2.16364443
H	-0.29360803	2.15536108	1.89735698
H	-0.71224602	1.13451251	3.25869070
C	-2.28853067	1.23152165	0.16683029
H	-1.91510486	2.19209302	-0.18875296
H	-3.33187827	1.16333524	-0.17049257
C	-2.23650034	1.17899295	1.70660321
H	-2.76472181	2.04812567	2.12032406
C	0.97222267	1.05463763	-0.71742928
O	0.55143991	-1.30077328	-0.32699027
H	0.45199349	-1.45193353	-1.27506689
C	2.34904387	1.04326284	-0.01515125
H	3.08016613	1.58620922	-0.62517518
H	2.31367682	1.53547471	0.96238797
H	2.71329045	0.02165074	0.12390939
C	1.19876565	0.62620228	-2.19316628
H	1.75306117	1.41061139	-2.71931521
H	1.79474109	-0.28784509	-2.27668491
H	0.25616007	0.48594150	-2.73544367
C	0.48847187	2.52279871	-0.78436016
H	-0.37679949	2.64358685	-1.44250388
H	0.24203128	2.94592002	0.19065559
H	1.29587712	3.13447820	-1.20393762

Compound 10 ($E_{el,B3LYP}$ = -618.64859028 a.u.)

#

AD2OAc

0 1

C	-2.85925300	0.18474900	0.03440700
O	-2.98974100	1.39130700	-0.03056200
C	-3.98489600	-0.81406800	-0.09313400
H	-4.92293900	-0.28399900	-0.25682900
H	-4.05231300	-1.42071600	0.81517400
H	-3.79034600	-1.49510300	-0.92729300
O	-1.67736100	-0.44003200	0.23958100
C	0.97517300	-1.66356400	0.63567500
C	1.67302200	-1.31216600	-0.69577500
C	0.66199500	-0.59299000	-1.61483700
C	0.48701400	-0.37001200	1.32357300
C	-0.49105600	0.39089300	0.41498100
C	0.17335100	0.70559700	-0.93806000

C	2.87532700	-0.38322400	-0.42111700
C	2.38794600	0.91241700	0.26311800
C	1.38046200	1.63121600	-0.66000900
C	1.69264500	0.55838500	1.59542800
H	1.67023900	-2.19104200	1.30237700
H	0.12903000	-2.33637400	0.45491100
H	2.02136300	-2.23269000	-1.18168700
H	-0.18742800	-1.25227900	-1.82958500
H	1.12993900	-0.34828800	-2.57760000
H	-0.02051900	-0.61142300	2.26581900
H	-0.55128500	1.22245500	-1.57728800
H	3.38722300	-0.14132000	-1.36242000
H	3.60788300	-0.89406600	0.21857900
H	3.24277200	1.57242800	0.45887900
H	1.86050100	1.90174600	-1.60930300
H	1.04064600	2.56720600	-0.19724300
H	2.39708100	0.05593300	2.27080700
H	1.36100800	1.47372000	2.10387600
H	-0.81642300	1.32021300	0.89117400

Compound 11 ($E_{el,B3LYP}$ = -446.10748703 a.u.)

#

2AdNH2

0 1

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.54758049
H	1.04049919	0.00000000	1.90445151
C	-1.46489999	-0.02978607	-0.49818288
H	-1.46746543	-0.05099489	-1.59797336
C	-2.19873911	-1.27435602	0.04719688
H	-1.70798701	-2.18585720	-0.30947999
H	-3.23086909	-1.28498778	-0.32930329
C	-0.73552620	-1.24460426	2.09060420
H	-0.71153730	-1.23376177	3.18899606
H	-0.22722678	-2.15574864	1.75843253
C	-2.19596721	-1.24151875	1.59053211
H	-2.71883021	-2.12585346	1.97781192
C	-2.90758197	0.03702954	2.08147918
H	-3.95351364	0.04070960	1.74481868
H	-2.92594830	0.06160326	3.17983509
C	-0.71365709	1.27717925	2.04105546
H	-0.18649917	2.17128331	1.68085839
H	-0.69247056	1.31400013	3.13829836
C	-2.17954675	1.24737306	-0.00609000
H	-1.68107044	2.14089392	-0.40634154
H	-3.21185009	1.26277314	-0.38006766
C	-2.17356113	1.28252074	1.53773818
H	-2.67925114	2.19256345	1.88659509
N	0.75036671	-1.15274257	-0.52052771
H	0.76608637	-1.14027212	-1.53786030
H	1.71824051	-1.12091180	-0.20815720

H	0.44471099	0.95599849	-0.33236129

Compound 12 ($E_{el,B3LYP}$ = -524.71987569 a.u.)

#

2-AdNMe2

0 1

C	0.00000000	0.00000000	0.00000000
H	0.00000000	0.00000000	1.09465954
C	1.39612617	0.00000000	-2.08302901
H	2.40864757	0.00000000	-2.49905775
C	0.61542700	-1.22396896	-2.60905846
H	1.11151222	-2.15014270	-2.29764824
H	0.60566516	-1.20848075	-3.70760029
C	-0.78326579	-1.22396896	-0.52220003
H	-1.80308820	-1.20848075	-0.11372517
H	-0.30668362	-2.15014270	-0.18169114
C	-0.82859617	-1.18849811	-2.06474026
H	-1.38351113	-2.05981431	-2.43666561
C	-1.52587501	0.10725927	-2.53208336
H	-1.57760334	0.13230800	-3.62927323
H	-2.56039638	0.13230800	-2.16293984
C	-0.69523695	1.29506805	-0.47232598
H	-0.15965984	2.17436823	-0.08920785
H	-1.71001680	1.33399061	-0.05401524
C	0.69501437	1.29506805	-2.54658967
H	1.25293285	2.17436823	-2.19680500
H	0.69626680	1.33399061	-3.64420548
C	-0.74866361	1.33568591	-2.01116639
H	-1.24448263	2.25727952	-2.34348337
N	2.22512234	-1.18740650	-0.01802065
C	2.26189133	-1.23970445	1.44276885
H	2.88834238	-2.08007134	1.75539195
H	2.67787689	-0.31710691	1.89597078
H	1.26639986	-1.40447718	1.85925080
C	3.59027518	-1.23970445	-0.53918820
H	4.16756756	-0.31710691	-0.32665705
H	4.11752517	-2.08007134	-0.07855649
H	3.59716666	-1.40447718	-1.61826789
C	1.46174189	-0.02874940	-0.52966759
H	1.96346594	0.90528848	-0.19339283

Compound 13 ($E_{el,B3LYP}$ = -598.78321912 a.u.)

#

2-AdNHCOMe

0 1

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.54399694
C	1.45937640	0.00000000	2.04909583

C	0.73479428	1.25624005	-0.52285456
C	2.19343498	1.29559873	-0.01033679
C	2.19057444	1.26025276	1.54035933
C	-0.72294423	1.26402418	2.05624615
C	0.00368944	2.52472290	1.53965194
C	1.46022225	2.52117913	2.05106487
C	0.00583952	2.51592337	-0.00410033
N	2.99904569	0.22962852	-0.60711061
H	-1.02924526	-0.00606948	-0.38228120
H	0.46643185	-0.92278243	-0.37459080
H	-0.51856811	-0.89543697	1.91042644
H	1.97883923	-0.90663279	1.71147451
H	1.47874541	-0.02020489	3.14666153
H	0.74206177	1.25939884	-1.62074321
H	3.22950887	1.26378632	1.88812340
H	-0.74332403	1.26490278	3.15433216
H	-1.76797246	1.26437927	1.71735516
H	-0.51283985	3.42352215	1.90013918
H	1.47560276	2.54017845	3.14876823
H	1.98528080	3.42301880	1.71001006
H	-1.02411411	2.52883246	-0.38457616
H	0.49941868	3.41854389	-0.38743115
C	4.33889941	0.36034429	-0.84056574
O	4.96783732	1.37437189	-0.54216326
C	5.01692655	-0.82723475	-1.50680494
H	2.54806145	-0.63130231	-0.87772673
H	5.84594586	-1.15803515	-0.87515283
H	5.44180931	-0.49738941	-2.45931338
H	4.34746606	-1.67317757	-1.68994138
H	2.66422950	2.23124734	-0.32971547

Compound 14 ($E_{el,B3LYP}$ = -489.99955581 a.u.)

#

2AdF

0 1

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.53214328
H	1.03840094	0.00000000	1.88561539
C	-1.43170135	-0.03172722	-0.54505646
H	-1.39229295	-0.05393856	-1.64104577
C	-2.17089804	-1.27783375	-0.01120968
H	-1.67359833	-2.18819240	-0.36403519
H	-3.19423747	-1.29336938	-0.40883138
C	-0.74403800	-1.24628692	2.05896931
H	-0.73673580	-1.23870360	3.15691417
H	-0.22438479	-2.15626623	1.73892658
C	-2.19535115	-1.24455735	1.53217033
H	-2.72394296	-2.12913304	1.90991778
C	-2.91676315	0.03428640	2.01038438
H	-3.95648308	0.03635824	1.65596042
H	-2.95372822	0.05869210	3.10796001

C	-0.72505078	1.28111669	2.00703686
H	-0.19343006	2.17537950	1.65382815
H	-0.71658408	1.32047235	3.10384617
C	-2.15180774	1.24941369	-0.06296523
H	-1.64481993	2.14287637	-0.45252922
H	-3.17406284	1.26631065	-0.46207345
C	-2.17642138	1.28202347	1.48040581
H	-2.68956594	2.19082747	1.82005369
F	0.71185767	-1.13433621	-0.47328534
H	0.54666643	0.86783721	-0.38992760

Compound 15 ($E_{el,B3LYP}$ = -850.35301371 a.u.)

#

2AdCl

0 1

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.53818132
H	1.03464872	0.00000000	1.89937869
C	-1.44000458	-0.05622861	-0.53775174
H	-1.41540961	-0.09564419	-1.63264908
C	-2.19140357	-1.28148706	0.02395133
H	-1.71202745	-2.20639116	-0.31535669
H	-3.21653007	-1.28787593	-0.36882510
C	-0.75826160	-1.22550453	2.09002026
H	-0.74979216	-1.19152576	3.18727540
H	-0.24909361	-2.14925696	1.79367967
C	-2.21044617	-1.22020012	1.56634823
H	-2.74512927	-2.09357038	1.96090969
C	-2.91996301	0.07274227	2.02341643
H	-3.96014850	0.07816879	1.67063562
H	-2.95471123	0.11740373	3.12034850
C	-0.71676081	1.29633090	1.99235272
H	-0.17578076	2.17911984	1.62566919
H	-0.70572901	1.35013405	3.08868404
C	-2.14932528	1.24042168	-0.07293550
H	-1.63870395	2.12201684	-0.48341066
H	-3.17317694	1.25387851	-0.46854909
C	-2.16848681	1.30268182	1.46891702
H	-2.67135281	2.22287469	1.79284793
H	0.50759102	0.89172996	-0.37626568
Cl	1.02497764	-1.37747425	-0.67372452

Compound 16 ($E_{el,B3LYP}$ = -788.94029963 a.u.)

#

2-AdSH

0 1

C	1.06571600	-0.19625800	-1.70121100
C	1.89767600	0.53939500	-0.62928300

C	-0.24201300	-0.73574400	-1.07534700
C	-1.04663600	0.47275900	-0.53979500
C	-0.23465200	1.17873800	0.57142900
C	1.07154900	1.71409700	-0.06379200
C	2.24364000	-0.44131600	0.51195200
C	0.94229100	-0.98007700	1.14342300
C	0.11663800	0.19611400	1.70794600
C	0.11169600	-1.71317500	0.06793800
S	-2.74413400	-0.08334600	-0.01325000
H	1.64225100	-1.03214500	-2.11906900
H	0.83569100	0.48090400	-2.53466100
H	2.82117900	0.92421400	-1.08106600
H	-0.83039700	-1.25216600	-1.84334700
H	-0.81737400	2.01831300	0.97193900
H	0.83769900	2.43202300	-0.86186300
H	1.65154500	2.25776000	0.69369000
H	2.85084500	0.06592900	1.27404400
H	2.84796100	-1.27216000	0.12302400
H	1.18727900	-1.67802800	1.95433800
H	0.68976100	0.72405000	2.48175400
H	-0.79873200	-0.17610600	2.18101300
H	0.68343300	-2.55660300	-0.34145900
H	-0.79774400	-2.13337900	0.51370400
H	-1.21185300	1.17281900	-1.36613800
H	-3.24083600	1.15091700	0.20653600

Compound 17 ($E_{el,B3LYP}$ = -828.25627408 a.u.)

#

2-AdSMe

0 1

C	1.57531600	1.20192900	-1.04155300
C	2.21911400	0.81702600	0.30828600
C	0.33106700	0.31666100	-1.30722400
C	-0.72459100	0.53483500	-0.17646900
C	-0.05760900	0.10888100	1.16787300
C	1.18718300	0.99404400	1.44230400
C	2.66686200	-0.65841600	0.25609800
C	1.43980900	-1.55419800	-0.01230000
C	0.40831900	-1.36448000	1.12057800
C	0.80251800	-1.15696000	-1.36108100
S	-2.19958100	-0.55195600	-0.62632900
C	-3.34958700	-0.32402100	0.77437200
H	2.29617200	1.04795100	-1.85536400
H	1.31819400	2.26665900	-1.05587600
H	3.08719200	1.46195600	0.49799300
H	-0.11836800	0.59751500	-2.26867700
H	-0.77553300	0.24399600	1.98719100
H	0.91111700	2.04841000	1.55182500
H	1.63071600	0.69051100	2.39992300
H	3.14308100	-0.94165400	1.20471700
H	3.41742900	-0.79707800	-0.53397400

H	1.75087100	-2.60623300	-0.05095500
H	0.86036600	-1.62927600	2.08600100
H	-0.44573900	-2.03125600	0.96750400
H	1.53928800	-1.26422500	-2.16852900
H	-0.02981000	-1.82622100	-1.59887700
H	-4.21479000	-0.95172200	0.54645000
H	-2.91612900	-0.66523400	1.71809600
H	-3.68976400	0.70967000	0.87310900
H	-1.08180134	1.54324608	-0.15627340

Compound 18 ($E_{el,B3LYP}$ = -583.91989814 a.u.)

#

2-CMe2OH-Ad

0 1

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.57826659
H	1.03508769	0.00000000	1.94230267
C	-1.51985807	-0.01997037	-0.41013306
H	-1.59916957	-0.03424047	-1.50365146
C	-2.28852822	-1.23097536	0.18024590
H	-1.88534983	-2.17748044	-0.18149843
H	-3.33482099	-1.16773647	-0.15027766
C	-0.76003226	-1.20612424	2.18821290
H	-0.71777697	-1.12461580	3.28420948
H	-0.29731501	-2.15028991	1.90837771
C	-2.23183759	-1.19207081	1.72420156
H	-2.74901055	-2.07154579	2.13020501
C	-2.91681591	0.09276532	2.22984504
H	-3.97198099	0.10853467	1.92302237
H	-2.89966576	0.12469818	3.32792779
C	-0.70350938	1.27306215	2.12332230
H	-0.17630253	2.18845351	1.83696193
H	-0.67687150	1.24162986	3.22130702
C	-2.24203801	1.25299609	0.10934153
H	-1.83384930	2.16635446	-0.33463374
H	-3.29415684	1.20937282	-0.20470223
C	-2.17487050	1.31372504	1.65137601
H	-2.64836284	2.24065122	2.00238822
C	0.86765963	-1.19137502	-0.66842736
C	2.34880947	-1.13007264	-0.21329869
H	2.90559537	-1.93240609	-0.70976076
H	2.84150587	-0.18964967	-0.46647969
H	2.44337627	-1.27801493	0.86864825
C	0.84806743	-1.07429796	-2.21400903
H	1.26325209	-0.13069906	-2.57685958
H	1.45188438	-1.88273535	-2.64081233
H	-0.16793395	-1.16973041	-2.61275004
H	0.43641180	0.91217611	-0.34982779
O	0.37810713	-2.49168120	-0.33013431
H	0.92065541	-3.15923442	-0.75629634

Compound 19 ($E_{el,B3LYP}$ = -543.40090345 a.u.)

#

2-Ad-COMe

0 1

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.54394522
C	1.45163313	0.00000000	-0.52647608
C	2.22033431	-1.26810817	-0.02702930
C	2.16283153	-1.30227574	1.52375825
C	0.70941514	-1.27339643	2.04816982
C	0.74575836	1.24734313	2.06319737
C	2.20192938	1.22884812	1.54980254
C	2.90760163	-0.05266912	2.04805531
C	2.19258320	1.24610257	0.00652931
C	1.74196301	-2.53084104	-0.73925464
O	0.86474317	-3.25916960	-0.30133579
H	-0.51903690	0.89066333	-0.37936689
H	-0.54704216	-0.87304124	-0.37469222
H	-1.03565822	0.01173858	1.90710839
H	1.44811748	0.02074307	-1.62433421
H	2.66306334	-2.21089316	1.88197163
H	0.17327239	-2.16666635	1.71966767
H	0.72668478	-1.28138459	3.14676024
H	0.73303080	1.26292445	3.16129186
H	0.24045019	2.16220505	1.72414299
H	2.73861373	2.11109147	1.92239554
H	2.92419948	-0.06782943	3.14586685
H	3.95423670	-0.06249866	1.71324929
H	1.69304139	2.15451771	-0.35615234
H	3.21986023	1.26942280	-0.38150051
H	3.27083573	-1.13505469	-0.32563049
C	2.42496951	-2.85079866	-2.05991983
H	3.46725600	-3.13720440	-1.87082639
H	1.90979902	-3.67431940	-2.55705648
H	2.45138730	-1.97363430	-2.71655908

Compound 20 ($E_{el,B3LYP}$ = -581.48214208 a.u.)

#

adamantane-spirocyclobutanone

0 1

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.54306034
C	1.45362845	0.00000000	-0.52166029
C	2.19858774	-1.27042858	-0.02249124
C	2.18143433	-1.27170462	1.53235338
C	0.72473301	-1.26628110	2.04535251
C	0.73282839	1.25599942	2.06100640
C	2.18761426	1.25492657	1.54484664

C	2.91187180	-0.01162657	2.04763570
C	2.18681119	1.25517308	0.00164314
C	3.59786502	-1.54026164	-0.68582166
C	1.72168991	-2.58851018	-0.67031691
C	3.07731648	-2.86227418	-1.32346194
O	0.67213925	-3.19149538	-0.66972304
H	-0.52003634	0.89042829	-0.37868957
H	-0.53791334	-0.87658830	-0.37636800
H	-1.03482683	-0.00211218	1.90840783
H	1.45165331	0.00659394	-1.62045234
H	2.69775733	-2.17077895	1.89629571
H	0.19824278	-2.16279559	1.70116701
H	0.72805744	-1.29017807	3.14359010
H	0.72372276	1.27346121	3.15933276
H	0.21447740	2.16329005	1.72211283
H	2.71240571	2.14679034	1.91106421
H	2.93109234	-0.02660343	3.14559663
H	3.95735794	-0.00743875	1.71289816
H	1.68267558	2.15439391	-0.37698967
H	3.21670721	1.28669913	-0.37705090
H	4.41163757	-1.68103920	0.03048956
H	3.90113498	-0.78285376	-1.41346333
H	3.03752062	-2.88901154	-2.41791536
H	3.55120189	-3.78715351	-0.97689222

Compound 21 ($E_{el,B3LYP}$ = -620.81983853 a.u.)

#

adamantane-spirocyclopentanone

0 1

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.54391490
C	1.45296491	0.00000000	-0.53165698
C	2.22374501	-1.28672646	-0.04454223
C	2.17644776	-1.28257809	1.51508624
C	0.72673431	-1.26235153	2.05146040
C	0.73035912	1.25431637	2.06587654
C	2.18254276	1.25034589	1.54488308
C	2.90599781	-0.02211275	2.03993527
C	2.16089582	1.26871466	0.00212328
C	3.67282848	-1.36035752	-0.60716483
C	1.58799983	-2.54470086	-0.69061891
C	2.47766429	-3.06530398	-1.82126919
C	3.55766495	-1.99469847	-2.00678182
O	0.53925463	-3.07499689	-0.37183529
H	-0.51218262	0.89599853	-0.37614741
H	-0.55139574	-0.86813561	-0.37263776
H	-1.03613350	-0.00329819	1.90608675
H	1.43982384	0.02647552	-1.62956235
H	2.68999335	-2.18172793	1.88239369
H	0.19063621	-2.16044396	1.73829635
H	0.75692614	-1.25897577	3.14984619

H	0.72163679	1.26724092	3.16431045
H	0.21439711	2.16476064	1.73079668
H	2.71188542	2.13910077	1.91286337
H	2.91177801	-0.04265329	3.13783701
H	3.95556675	-0.01250782	1.72185456
H	1.61376503	2.15250878	-0.35260829
H	3.17805020	1.35838333	-0.39494874
H	4.26734287	-2.01905828	0.04197862
H	4.18635095	-0.39822286	-0.63179981
H	1.87604604	-3.29477919	-2.70577101
H	2.91009862	-4.01498168	-1.47616848
H	4.51069309	-2.39889401	-2.36079902
H	3.23214109	-1.24617095	-2.73874614

Compound 22 ($E_{el,B3LYP}$ = -660.13746102 a.u.)

#

adamantane-spirocyclohexanone

0 1

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.54168845
C	1.45584710	0.00000000	-0.52876232
C	2.23246422	-1.26136512	-0.03670781
C	2.21777047	-1.22343680	1.53152807
C	0.75818419	-1.24647894	2.04473322
C	0.70208686	1.27352464	2.05639474
C	2.15146223	1.30702809	1.52801020
C	2.90097695	0.06346554	2.04856145
C	2.13840056	1.29155493	-0.01669533
C	3.68816083	-1.30164018	-0.62031086
C	1.61216966	-2.56687985	-0.58221424
C	2.30343617	-3.86253593	-0.17733793
C	3.76136298	-3.84297519	-0.69162110
O	0.70515763	-2.58060630	-1.40000856
H	-0.51201151	0.89776771	-0.37225528
H	-0.54634318	-0.86249643	-0.38724372
H	-1.03346363	-0.02830057	1.91071564
H	1.43891737	-0.00497671	-1.62493535
H	2.75201665	-2.08947583	1.93624814
H	0.24416751	-2.15812966	1.71161747
H	0.76164932	-1.27061002	3.14278265
H	0.70150106	1.29326677	3.15502880
H	0.15590181	2.16480376	1.71956877
H	2.65515874	2.21532596	1.88372702
H	3.95623338	0.09707205	1.75304486
H	2.88946906	0.05345609	3.14691114
H	1.57960476	2.15913174	-0.39181788
H	3.15725495	1.39240442	-0.40747965
H	3.60792366	-1.23566476	-1.71498680
H	4.24568984	-0.41702114	-0.30475127
H	1.73930488	-4.69545892	-0.60484980
H	4.29308175	-4.73537254	-0.34156986

H	3.74540240	-3.89354822	-1.78849529
C	4.48429791	-2.56392347	-0.25100355
H	2.30204683	-3.96927109	0.91428357
H	4.66193835	-2.59239364	0.83182239
H	5.47420001	-2.51454120	-0.72097419

Compound 23 ($E_{el,B3LYP}$ = -773.26109588 a.u.)

#

cycl-spiro-benzene-cyclopentanone

0 1

O	-0.54734800	1.93027200	-0.02315000
C	-0.04119800	0.81688700	-0.01423900
C	-0.80698400	-0.53097600	-0.00760300
C	-1.68534100	-0.65327100	1.26918100
C	-2.90933200	0.27462100	1.27802200
C	-3.76887500	0.07944000	0.01957400
C	-2.93482300	0.26598900	-1.25718500
C	1.63066100	-0.84549500	-0.00422800
C	4.00004200	-0.43019200	0.00968600
C	3.77161000	0.95740700	0.00725700
C	2.46952800	1.45222700	-0.00073300
C	1.41218400	0.53512500	-0.00607800
H	-2.60785500	1.30877400	-1.32883200
H	-4.61199500	0.78076300	0.02566200
H	-3.50305900	0.07366500	2.17867300
H	-2.57978200	1.31755900	1.33543600
H	-1.06632700	-0.48110000	2.15961800
H	2.26248100	2.51829100	-0.00269100
H	4.61597400	1.64035700	0.01178500
H	5.02130500	-0.80129800	0.01606800
C	2.93801900	-1.33906000	0.00390900
H	3.13201600	-2.40862700	0.00553800
C	-1.70913900	-0.65992600	-1.26616700
H	-1.10726100	-0.49054800	-2.16881400
H	-3.54617000	0.05738400	-2.14420200
C	0.32411000	-1.60657900	-0.01460300
H	0.25674400	-2.24991200	-0.90106400
H	0.25142900	-2.27045300	0.85599000
H	-4.20217200	-0.93264100	0.02761800
H	-2.05105800	-1.70456700	-1.31253800
H	-2.02824600	-1.69699500	1.32619600

Compound 24 ($E_{el,B3LYP}$ = -812.57522736 a.u.)

#

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0 1

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.54577184

C	1.45419777	0.00000000	2.06287141
C	0.76192672	-1.24037891	-0.53128445
C	2.24593930	-1.21313361	-0.04056058
C	2.20657702	-1.24165995	1.52981200
C	-0.71367920	-1.26674411	2.06090889
C	0.01638575	-2.51521472	1.52523181
C	1.47683348	-2.51190893	2.02343838
C	0.00975754	-2.49318643	-0.01626204
C	3.07055845	-2.39875921	-0.57904144
C	3.01464165	0.02647969	-0.58928526
C	4.54854810	-2.36021626	-0.32365993
O	2.58970896	-3.32715464	-1.21650907
H	0.42479010	0.93576851	-0.38119622
H	-1.03327648	-0.03745653	-0.36933061
H	-0.51965705	0.89478085	1.91288469
H	1.45939796	-0.02613722	3.16093447
H	1.96541542	0.92619203	1.77387032
H	0.75490492	-1.24166082	-1.62858604
H	3.22768328	-1.24638711	1.92672493
H	-1.76041146	-1.27158259	1.72864051
H	-0.72571465	-1.27120367	3.15969811
H	-0.48958443	-3.42179467	1.88180257
H	1.99447554	-3.41556010	1.67836761
H	1.50240347	-2.53465203	3.12124046
H	0.46074341	-3.40108705	-0.41818882
H	-1.02565312	-2.45425128	-0.38191198
H	3.05685865	-0.05848955	-1.68420101
H	2.46875703	0.94765071	-0.37854284
C	4.44065240	0.15443941	-0.03389763
C	5.21252213	-1.14620268	-0.06684044
H	4.40538652	0.52065470	1.00168734
H	4.98795448	0.91881419	-0.59897916
C	5.27216458	-3.56424967	-0.37568437
C	6.64427748	-3.57369484	-0.14937940
C	7.30923792	-2.36821632	0.11081422
C	6.59878520	-1.16873148	0.14325179
H	4.73258014	-4.48018204	-0.59429178
H	7.19676673	-4.50814924	-0.17872664
H	8.38249340	-2.36472453	0.27980267
H	7.12455282	-0.23468264	0.32753133

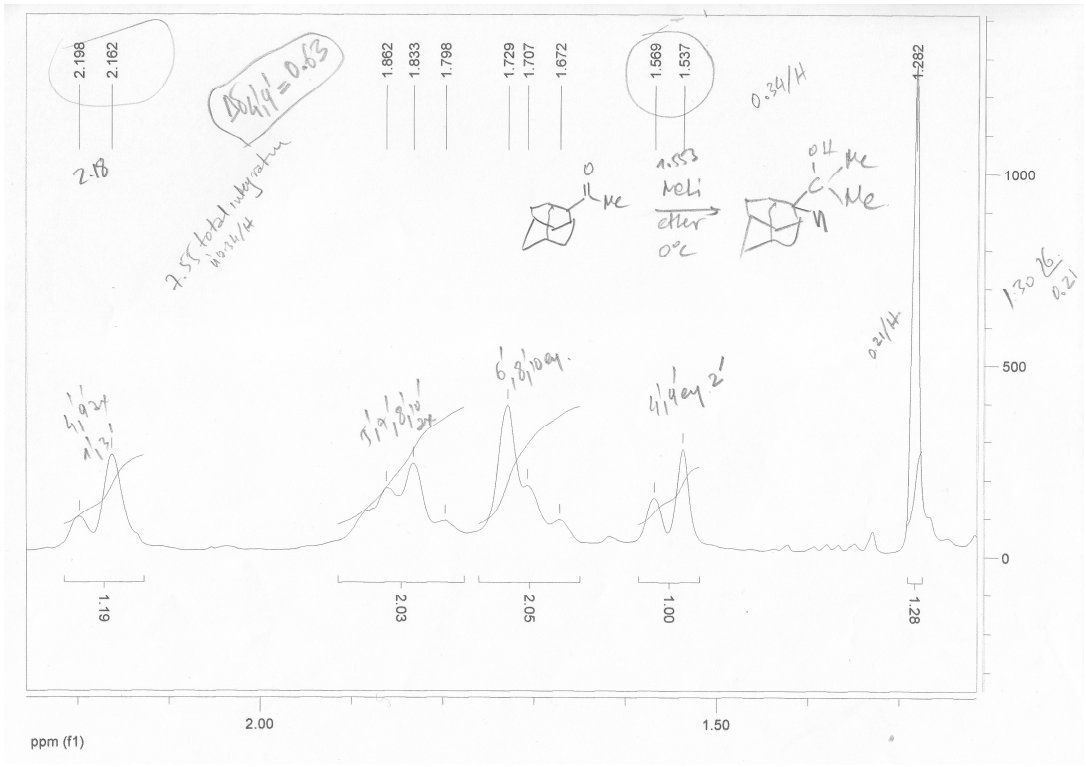
Synthesis of compound 18

2-(2-Adamantyl-2-propanol, 18. To a stirred solution of sodium ethoxide (220 mg, 9.60 mmol) in absolute ethanol (5 mL) and anhydrous THF (11 mL), a solution of 2-adamantanone (960 mg, 6.40 mmol) and toluenesulfonylmethyl isocyanide (TOSMIC) (1.49 g, 7.68 mmol) in anhydrous THF (25 mL) at room temperature. The mixture was stirred at room temperature for 2 h, then solvent was evaporated in vacuo and water (15 mL) was added. The mixture was extracted with ether and the organic solution was dried (Na_2SO_4). Solvent was removed to afford quantitatively 2-cyanoadamantane (ethanol – water).

To a stirred solution of 2-cyanoadamantane (350 mg, 2.17 mmol) in anhydrous ether was added during a 2 min period, under an argon atmosphere, a solution of MeLi 1.6 M in ether (4.1 mL, 6.56 mmol) at 0 ºC. The yellow complex formed was stirred for 90 min at ambient temperature and hydrolyzed with water (8 mL) at 0 ºC. The residue was treated with a mixture of acetone (5 mL) and HCl 6N (5 mL) and the mixture was refluxed for 2 h. Acetone was removed in vacuo and the resulting mixture was extracted with ether. The organic solution was washed with water and brine, was dried (Na_2SO_4) and evaporated in vacuo to afford 2-acetyladamantane **19** (302 mg, 78 %).

To a stirred solution of 2-acetyladamantane **19** (590 mg, 3.31 mmol) in anhydrous ether (40 mL) was added dropwise, under an argon atmosphere, a solution of MeLi 5 % in ether (4.4 mL, 10.0 mmol) at 0 ºC. The mixture was stirred overnight at ambient temperature, then a saturated solution of NH_4Cl (50 mL) was added at 0 ºC. The organic phase was separated, washed with water, brine and dried over Na_2SO_4. After solvent evaporation the liquid alcohol **18** (502 mg, 78 %) was obtained; MS (ESI) m/z consistent to $C_{13}H_{22}O$.

Compound 18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1.672
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1.282
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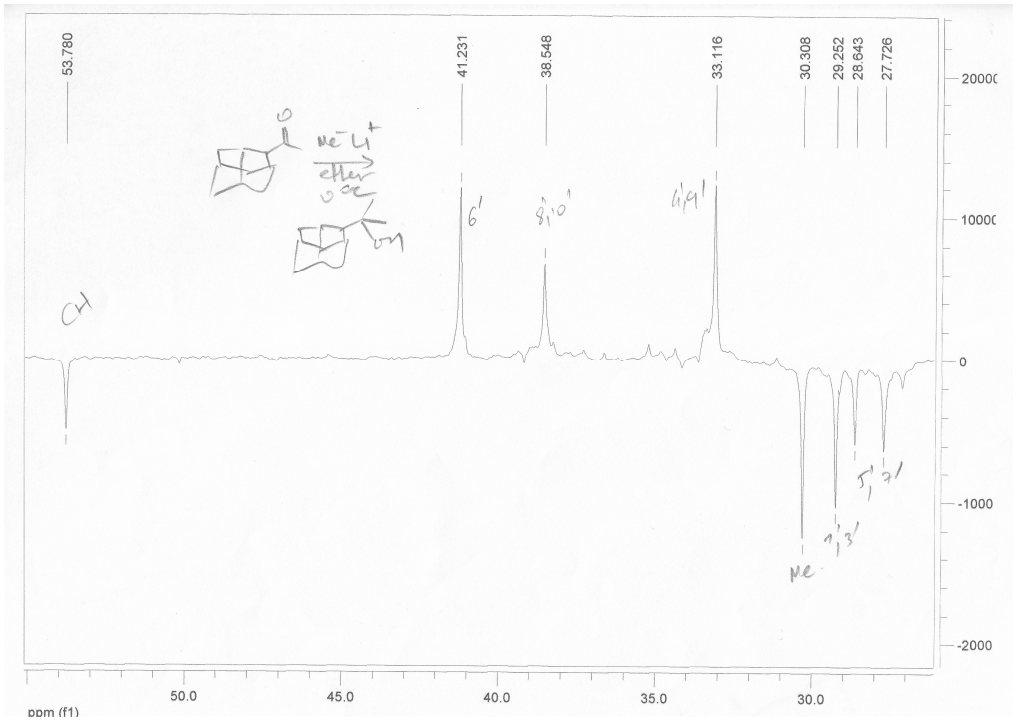
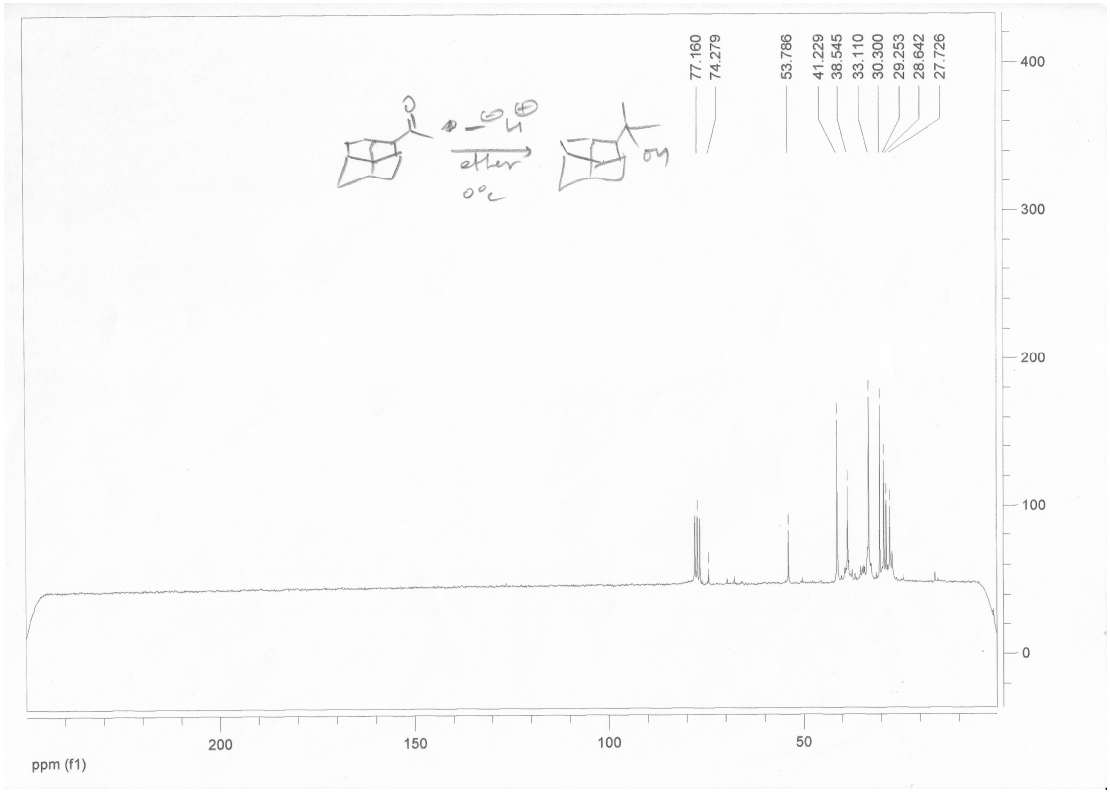
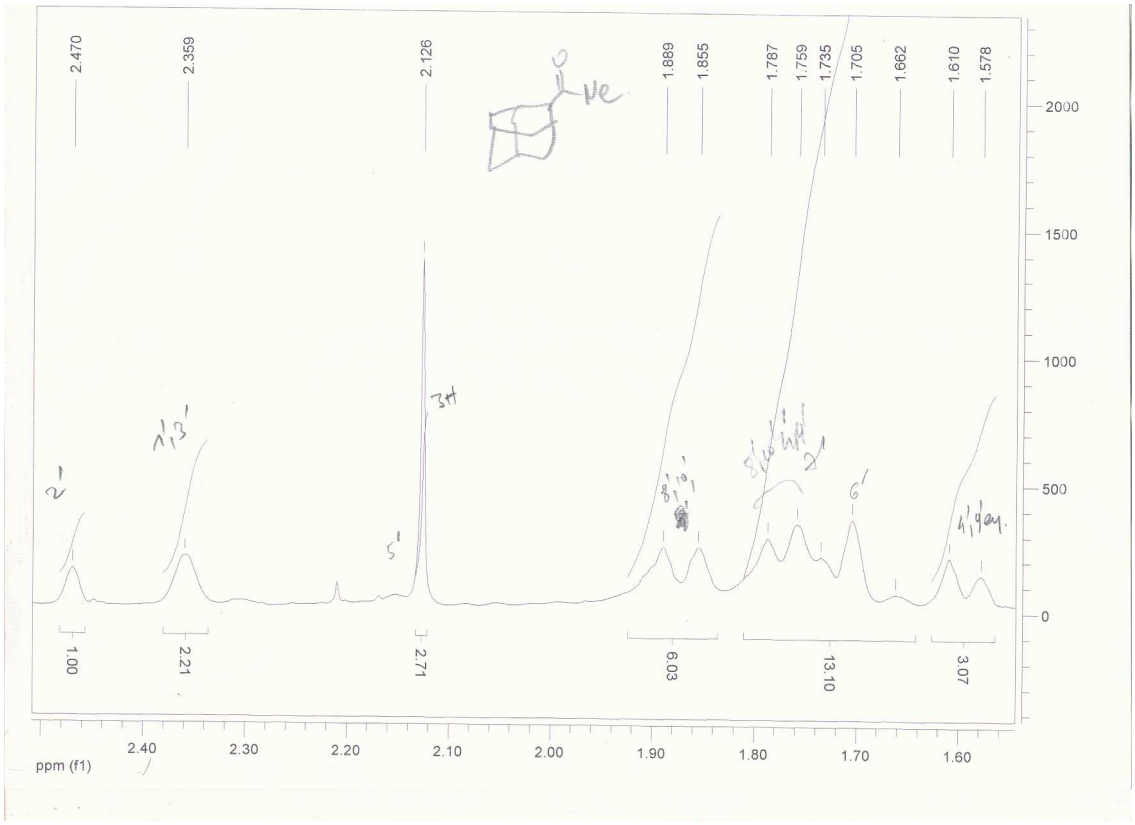
2.05
1.00
1.28
2.00
1.50
ppm (f1)


53.780
41.231
38.548
33.116
30.308
29.252
28.643
27.726
50.0
45.0
40.0
35.0
30.0
ppm (f1)


77.160
74.279
53.786
41.229
38.545
33.110
30.300
29.253
28.642
27.726
400
300
200
100
0
200
150
100
50
ppm (f1)

Compound 19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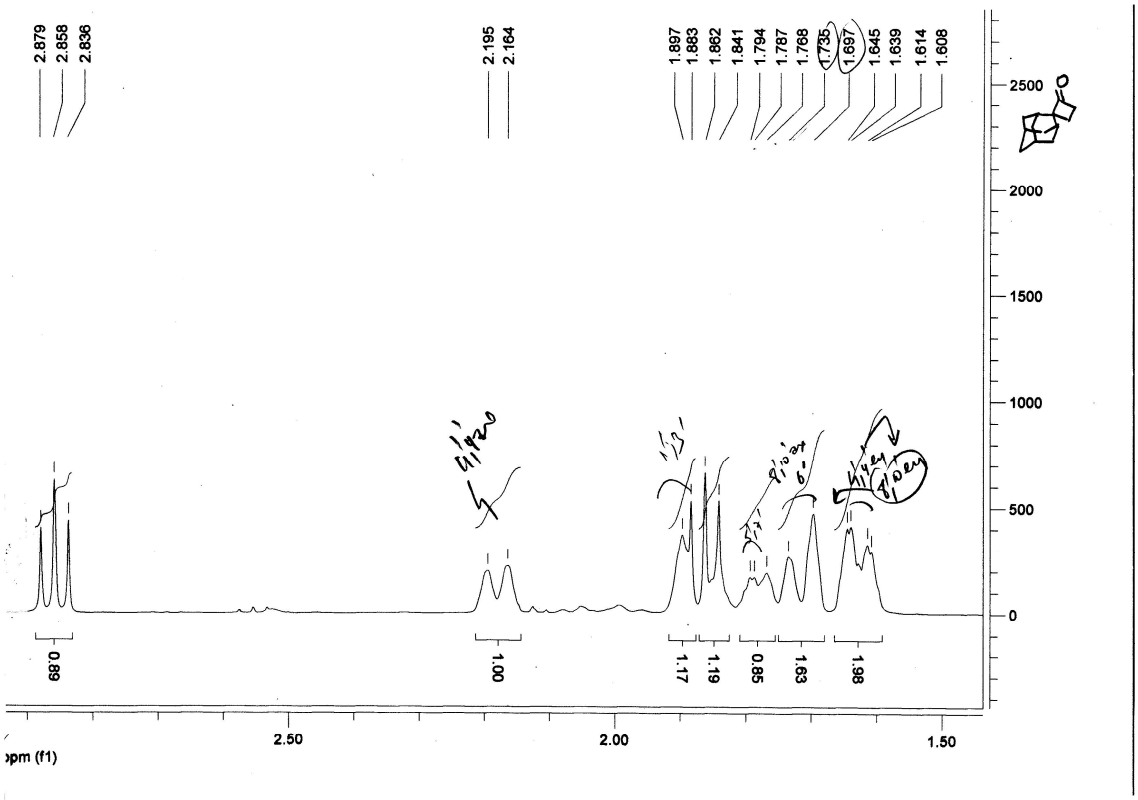
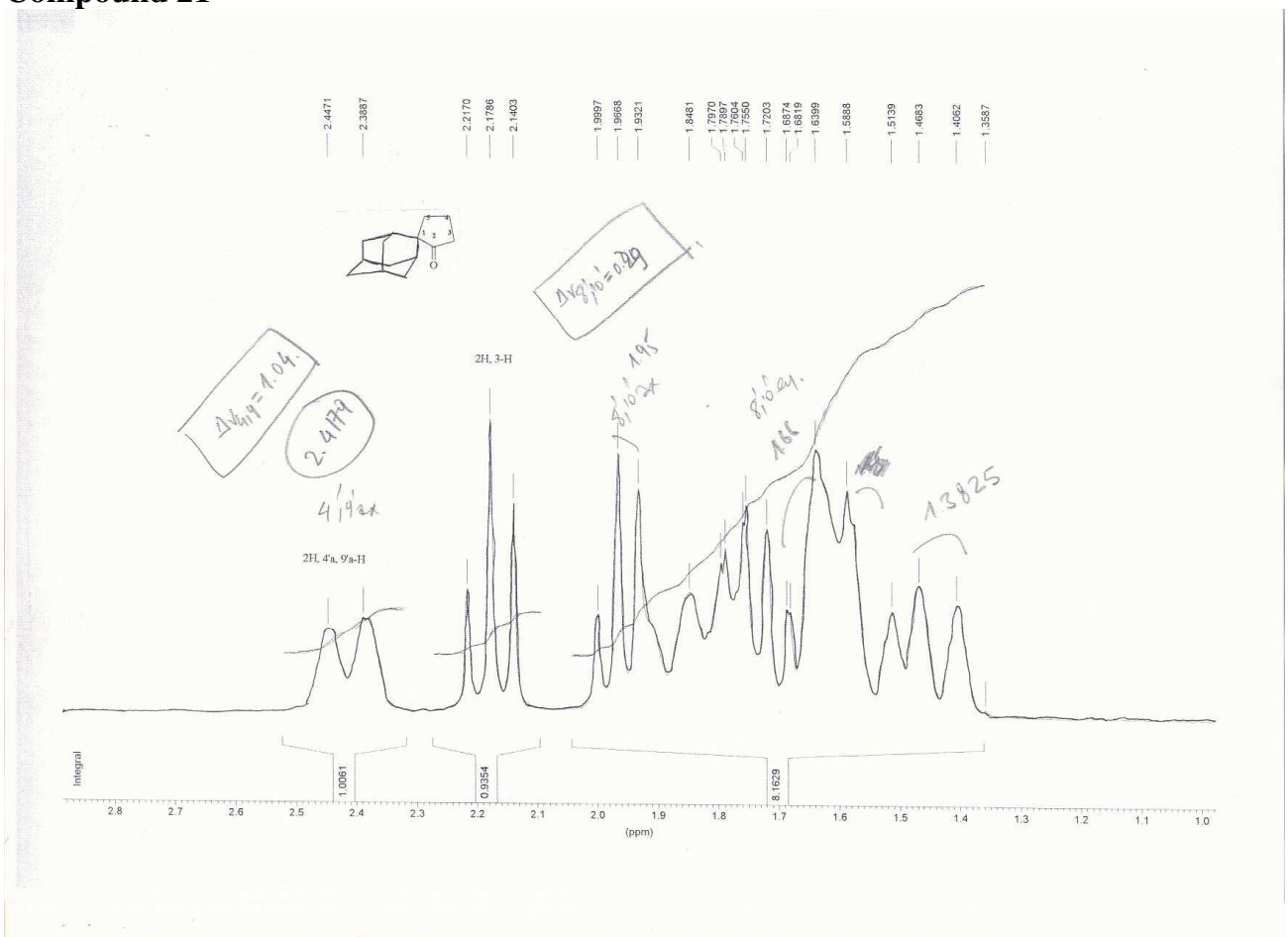
2.359
2.126
1.889
1.855
1.787
1.759
1.735
1.705
1.662
1.610
1.578
2000
1500
1000
500
0
1.00
2.21
2.71
6.03
13.10
3.07
2.40
2.30
2.20
2.10
2.00
1.90
1.80
1.70
1.60
ppm (f1)

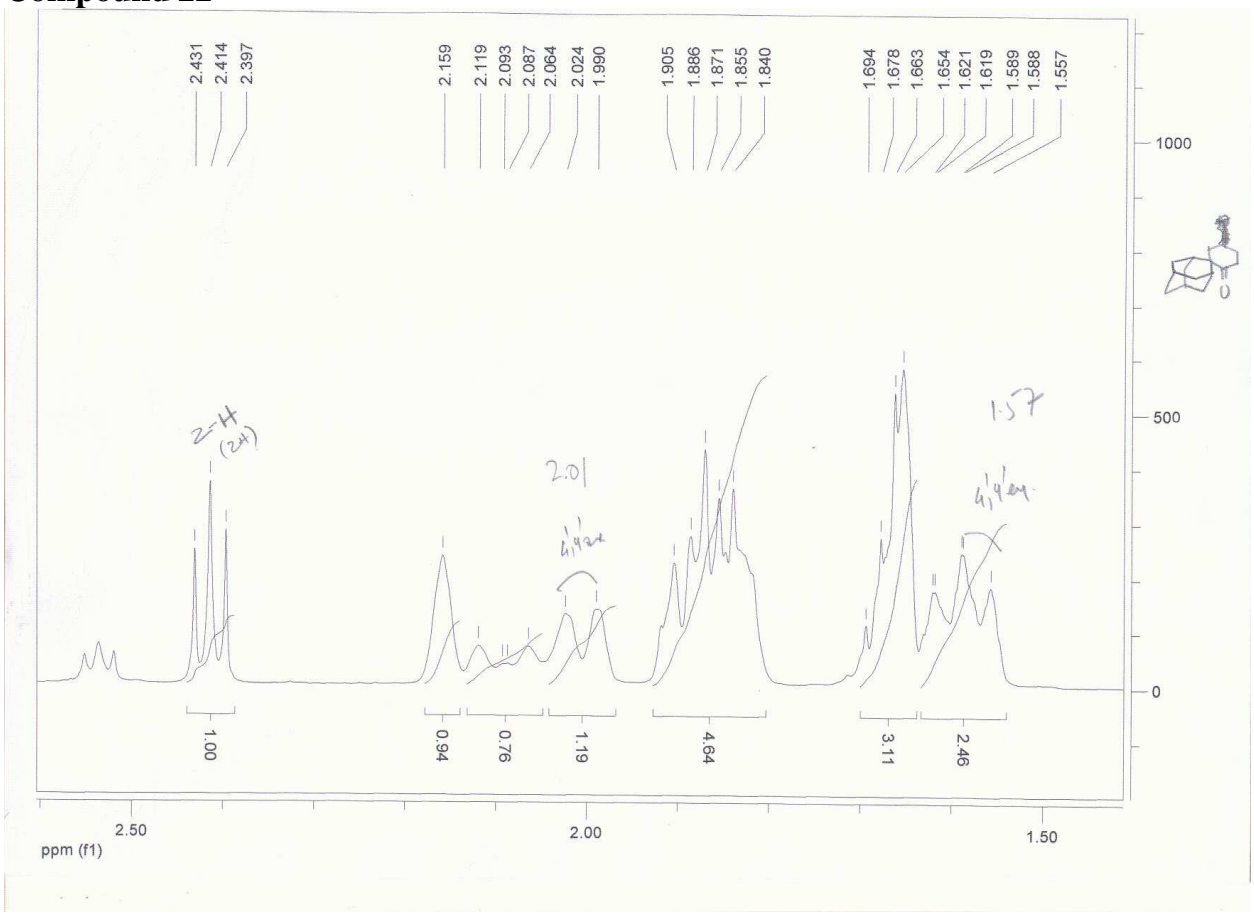
Compound 20



Compound 21



Compound 22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2.064
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1.990
1.905
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1.855
1.840
1.694
1.678
1.663
1.654
1.621
1.619
1.589
1.588
1.557
1000
500
0
1.00
0.94
0.76
1.19
4.64
3.11
2.46
2.50
2.00
1.50
ppm (f1)