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# Substituted adenine quartets: interplay between substituent effect, hydrogen bonding and aromaticity

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## Electronic Supplementary Information

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**Table S1.** Hydrogen bonds engaged in stabilizing freely optimized structures with total ($E_{tot}$) and relative ($\Delta E_{rel}$) energy values. $\Delta E_{rel,X}$ is calculated for each substituent X separately, $\Delta E_{rel,A4}$ – calculated by reference to $A_4$-N3 tetramers.

| | | X | DH…A | DH /Å | DA /Å | DHA /° | AH /Å | $E_{tot}$ / kcal/mol | $\Delta E_{rel,X}$ / kcal/mol | $\Delta E_{rel,A4}$ / kcal/mol |
|---|---|---|---|---|---|---|---|---|---|---|
| $A_4$-N1 | C8 | $NO_2$ | N10H···N1 | 1.035 | 2.930 | 160.85 | 1.933 | -10525.41 | 10.04 | 4.61 |
| | | Cl | | 1.033 | 2.942 | 160.02 | 1.950 | -9043.68 | 15.00 | 2.60 |
| | | F | | 1.032 | 2.940 | 160.11 | 1.948 | -9222.11 | 32.71 | 2.02 |
| | | H | | 1.033 | 2.937 | 160.21 | 1.944 | -9205.35 | 2.69 | 2.69 |
| | | Me | | 1.033 | 2.940 | 160.12 | 1.948 | -10686.01 | 1.81 | 1.81 |
| | | $NH_2$ | | 1.032 | 2.940 | 159.95 | 1.949 | -10282.16 | 21.64 | -0.15 |
| | N9 | $NO_2$ | | 1.033 | 2.935 | 159.88 | 1.944 | -10434.73 | 100.72 | 16.08 |
| | | Cl | | 1.032 | 2.944 | 159.67 | 1.954 | -8930.14 | 128.54 | 7.13 |
| | | F | | 1.034 | 2.928 | 160.44 | 1.934 | -9007.05 | 247.77 | 6.82 |
| | | H | | 1.033 | 2.937 | 160.21 | 1.944 | -9205.35 | 2.69 | 2.69 |
| | | Me | | 1.033 | 2.939 | 159.79 | 1.948 | -10655.25 | 32.57 | 3.66 |
| | | $NH_2$ | | 1.033 | 2.932 | 160.17 | 1.939 | -10171.84 | 131.96 | 2.11 |
| $A_4$-N3 | C8 | $NO_2$ | N10H···N3 | 1.030 | 3.039 | 171.15 | 2.017 | -10530.02 | 5.43 | **0.00** |
| | | Cl | | 1.028 | 3.064 | 172.02 | 2.042 | -9046.28 | 12.40 | **0.00** |
| | | F | | 1.028 | 3.061 | 171.89 | 2.040 | -9224.13 | 30.69 | **0.00** |
| | | H | | 1.029 | 3.055 | 171.80 | 2.034 | -9208.04 | **0.00** | **0.00** |
| | | Me | | 1.029 | 3.060 | 172.16 | 2.037 | -10687.82 | **0.00** | **0.00** |
| | | $NH_2$ | | 1.028 | 3.064 | 172.19 | 2.042 | -10282.01 | 21.79 | **0.00** |
| | N9 | $NO_2$ | | 1.031 | 3.024 | 167.61 | 2.009 | -10450.81 | 84.64 | **0.00** |
| | | Cl | | 1.030 | 3.048 | 170.49 | 2.028 | -8937.27 | 121.41 | **0.00** |
| | | F | | 1.030 | 3.037 | 170.21 | 2.017 | -9013.87 | 240.95 | **0.00** |
| | | H | | 1.029 | 3.055 | 171.80 | 2.034 | -9208.04 | **0.00** | **0.00** |
| | | Me | | 1.030 | 3.046 | 171.34 | 2.025 | -10658.91 | 28.91 | **0.00** |
| | | $NH_2$ | | 1.030 | 3.039 | 171.29 | 2.018 | -10173.95 | 129.85 | **0.00** |
| $A_4$-N7 | C2 | $NO_2$ | N10H···N7 | 1.038 | 3.028 | 170.85 | 1.839 | -10535.45 | **0.00** | -5.43 |
| | | Cl | | 1.036 | 3.109 | 179.05 | 1.874 | -9058.68 | **0.00** | -12.40 |
| | | F | | 1.036 | 3.103 | 179.50 | 1.868 | -9254.82 | **0.00** | -30.69 |
| | | H | | 1.033 | 2.932 | 178.89 | 1.899 | -9207.62 | 0.42 | 0.42 |
| | | Me | | 1.033 | 3.122 | 178.84 | 1.897 | -10683.34 | 4.48 | 4.48 |
| | | $NH_2$ | | 1.033 | 3.123 | 178.86 | 1.901 | -10303.80 | **0.00** | -21.79 |
| | N9 | $NO_2$ | | 1.031 | 3.075 | 179.60 | 1.909 | -10434.04 | 101.41 | 16.77 |
| | | Cl | | 1.032 | 3.108 | 177.85 | 1.902 | -8930.84 | 127.84 | 6.43 |
| | | F | | 1.032 | 3.105 | 179.52 | 1.898 | -9006.72 | 248.10 | 7.15 |
| | | H | | 1.033 | 2.932 | 178.89 | 1.899 | -9207.62 | 0.42 | 0.42 |
| | | Me | | 1.034 | 3.120 | 178.93 | 1.889 | -10658.73 | 29.09 | 0.18 |
| | | $NH_2$ | | 1.034 | 3.108 | 177.20 | 1.891 | -10173.58 | 130.22 | 0.37 |

**Table S2.** Interaction energy and cSAR values of analyzed systems. All energy values are given in kcal/mol.

| | | X | $E_{int}$ | $E_{prep}$ | $E_{HB}$ | cSAR(X) | cSAR($NH_2$) |
|---|---|---|---|---|---|---|---|
| $A_4$-N1 | C8 | $NO_2$ | -34.55 | 4.58 | -29.97 | -0.031 | 0.237 |
| | | Cl | -34.54 | 4.34 | -30.20 | 0.094 | 0.215 |
| | | F | -34.17 | 3.98 | -30.19 | 0.135 | 0.211 |
| | | H | -34.04 | 4.53 | -29.51 | 0.138 | 0.216 |
| | | Me | -34.33 | 4.68 | -29.65 | 0.172 | 0.208 |
| | | $NH_2$ | -34.16 | 4.12 | -30.04 | 0.245 | 0.200 |
| | N9 | $NO_2$ | -32.82 | 4.61 | -28.21 | -0.028 | 0.226 |
| | | Cl | -33.97 | 4.71 | -29.26 | 0.030 | 0.220 |
| | | F | -34.23 | 4.50 | -29.73 | 0.039 | 0.224 |
| | | H | -34.04 | 4.53 | -29.51 | 0.100 | 0.216 |
| | | Me | -33.73 | 4.80 | -28.93 | 0.126 | 0.210 |
| | | $NH_2$ | -34.06 | 4.66 | -29.40 | 0.115 | 0.216 |
| $A_4$-N3 | C8 | $NO_2$ | -36.28 | 1.70 | -34.58 | -0.040 | 0.287 |
| | | Cl | -34.37 | 1.57 | -32.8 | 0.089 | 0.248 |
| | | F | -33.77 | 1.56 | -32.21 | 0.130 | 0.244 |
| | | H | -33.84 | 1.64 | -32.20 | 0.130 | 0.241 |
| | | Me | -33.10 | 1.64 | -31.46 | 0.163 | 0.231 |
| | | $NH_2$ | -31.77 | 1.88 | -29.89 | 0.230 | 0.218 |
| | N9 | $NO_2$ | -46.86 | 2.57 | -44.29 | -0.048 | 0.273 |
| | | Cl | -38.19 | 1.80 | -36.39 | 0.021 | 0.260 |
| | | F | -38.41 | 1.86 | -36.55 | 0.028 | 0.267 |
| | | H | -33.84 | 1.64 | -32.2 | 0.095 | 0.241 |
| | | Me | -34.27 | 1.68 | -32.59 | 0.123 | 0.236 |
| | | $NH_2$ | -33.26 | 1.75 | -31.51 | 0.114 | 0.232 |
| $A_4$-N7 | C2 | $NO_2$ | -45.97 | 6.88 | -39.09 | -0.020 | 0.222 |
| | | Cl | -37.37 | 2.65 | -34.72 | 0.069 | 0.228 |
| | | F | -36.56 | 2.54 | -34.02 | 0.119 | 0.229 |
| | | H | -34.21 | 2.43 | -31.78 | 0.148 | 0.216 |
| | | Me | -34.14 | 2.40 | -31.74 | 0.163 | 0.213 |
| | | $NH_2$ | -32.77 | 2.57 | -30.20 | 0.255 | 0.217 |
| | N9 | $NO_2$ | -29.44 | 1.92 | -27.52 | -0.015 | 0.229 |
| | | Cl | -32.24 | 2.28 | -29.96 | 0.042 | 0.222 |
| | | F | -31.48 | 2.08 | -29.40 | 0.048 | 0.227 |
| | | H | -34.21 | 2.43 | -31.78 | 0.110 | 0.216 |
| | | Me | -35.01 | 2.60 | -32.41 | 0.138 | 0.211 |
| | | $NH_2$ | -33.82 | 2.68 | -31.14 | 0.124 | 0.216 |

**Table S3.** HOMA aromaticity index observed in the molecules of substituted adenine.

| X | $A_4$-N1 | | $A_4$-N3 | | $A_4$-N7 | | monomer | | |
|---|---|---|---|---|---|---|---|---|---|
| | C8-X | N9-X | C8 | N9 | C2 | N9 | C2 | C8 | N9 |
| | 5 ring | 5 ring | 5 ring | 5 ring | 5 ring | 5 ring | 5 ring | 5 ring | 5 ring |
| $NO_2$ | 0.831 | 0.691 | 0.833 | 0.666 | 0.841 | 0.708 | 0.827 | 0.833 | 0.684 |
| Cl | 0.790 | 0.779 | 0.788 | 0.778 | 0.831 | 0.794 | 0.818 | 0.793 | 0.781 |
| F | 0.762 | 0.822 | 0.758 | 0.826 | 0.830 | 0.837 | 0.814 | 0.764 | 0.825 |
| H | 0.809 | 0.809 | 0.808 | 0.808 | 0.824 | 0.824 | 0.814 | 0.814 | 0.814 |
| Me | 0.798 | 0.810 | 0.796 | 0.811 | 0.824 | 0.827 | 0.812 | 0.803 | 0.815 |
| $NH_2$ | 0.778 | 0.800 | 0.773 | 0.801 | 0.812 | 0.813 | 0.797 | 0.781 | 0.802 |
| *range* | *0.069* | *0.131* | *0.075* | *0.160* | *0.029* | *0.129* | *0.030* | *0.069* | *0.141* |
| *average* | *0.795* | *0.785* | *0.793* | *0.782* | *0.827* | *0.801* | *0.814* | *0.798* | *0.787* |
| *SD* | *0.022* | *0.044* | *0.024* | *0.054* | *0.009* | *0.043* | *0.009* | *0.022* | *0.048* |

| X | $A_4$-N1 | | $A_4$-N3 | | $A_4$-N7 | | monomer | | |
|---|---|---|---|---|---|---|---|---|---|
| | C8-X | N9-X | C8 | N9 | C2 | N9 | C2 | C8 | N9 |
| | 6 ring | 6 ring | 6 ring | 6 ring | 6 ring | 6 ring | 6 ring | 6 ring | 6 ring |
| $NO_2$ | 0.904 | 0.939 | 0.889 | 0.919 | 0.944 | 0.942 | 0.938 | 0.907 | 0.947 |
| Cl | 0.936 | 0.933 | 0.931 | 0.923 | 0.944 | 0.937 | 0.949 | 0.947 | 0.942 |
| F | 0.942 | 0.926 | 0.938 | 0.917 | 0.941 | 0.932 | 0.945 | 0.953 | 0.935 |
| H | 0.931 | 0.931 | 0.927 | 0.927 | 0.936 | 0.936 | 0.944 | 0.944 | 0.944 |
| Me | 0.936 | 0.930 | 0.933 | 0.927 | 0.936 | 0.936 | 0.942 | 0.949 | 0.942 |
| $NH_2$ | 0.945 | 0.934 | 0.942 | 0.931 | 0.928 | 0.938 | 0.937 | 0.957 | 0.947 |
| *range* | *0.041* | *0.013* | *0.053* | *0.014* | *0.016* | *0.010* | *0.012* | *0.050* | *0.012* |
| *average* | *0.932* | *0.932* | *0.927* | *0.924* | *0.938* | *0.937* | *0.943* | *0.943* | *0.943* |
| *SD* | *0.013* | *0.004* | *0.018* | *0.005* | *0.006* | *0.003* | *0.004* | *0.017* | *0.004* |

**Table S4.** cSAR values of X-substituted monomer and $A_4$-N1, $A_4$-N3, $A_4$-N7 systems. Given **Δ** values corresponds to the difference between maxima and minima in given data set.

| | **Monomer** | | **$A_4$-N1** | **$A_4$-N3** | **$A_4$-N7** | **Δ** |
|---|---|---|---|---|---|---|
| **X** | C2-X | C8-X | C8-X | C8-X | C2-X | |
| $NO_2$ | -0.020 | -0.045 | -0.031 | -0.040 | -0.020 | 0.025 |
| Cl | 0.075 | 0.094 | 0.094 | 0.089 | 0.069 | 0.025 |
| F | 0.124 | 0.135 | 0.135 | 0.130 | 0.119 | 0.016 |
| H | 0.151 | 0.140 | 0.138 | 0.130 | 0.148 | 0.021 |
| Me | 0.171 | 0.173 | 0.172 | 0.163 | 0.163 | 0.010 |
| $NH_2$ | 0.268 | 0.247 | 0.245 | 0.230 | 0.255 | 0.038 |
| **Δ** | 0.288 | 0.292 | 0.276 | 0.270 | 0.275 | |

| | **Monomer** | **$A_4$-N1** | **$A_4$-N3** | **$A_4$-N7** | **Δ** |
|---|---|---|---|---|---|
| **X** | N9-X | | | | |
| $NO_2$ | -0.038 | -0.028 | -0.048 | -0.015 | 0.033 |
| Cl | 0.029 | 0.030 | 0.021 | 0.042 | 0.021 |
| F | 0.036 | 0.039 | 0.028 | 0.048 | 0.020 |
| H | 0.101 | 0.100 | 0.095 | 0.110 | 0.015 |
| Me | 0.129 | 0.126 | 0.123 | 0.138 | 0.015 |
| $NH_2$ | 0.117 | 0.115 | 0.114 | 0.124 | 0.010 |
| **Δ** | 0.167 | 0.154 | 0.171 | 0.153 | |

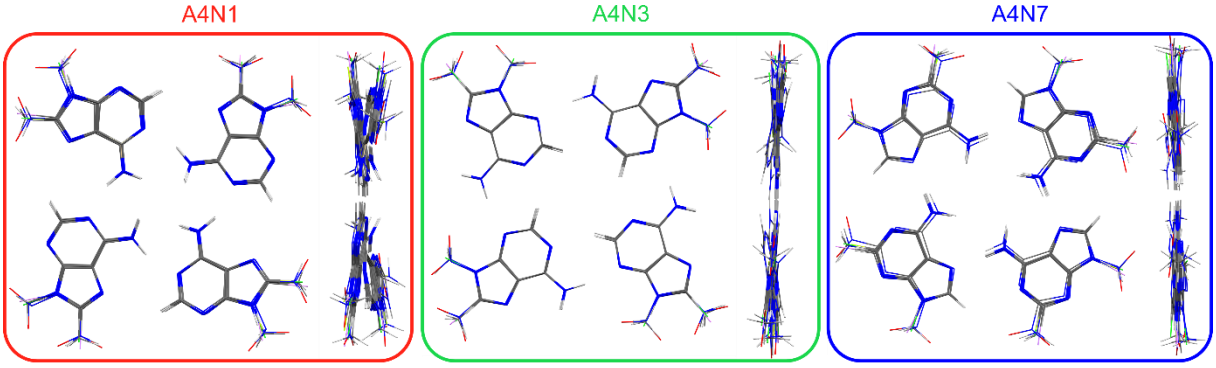



**Figure S1.** Superposition of optimized structures of the substituted adenine tetramer depending on its type.

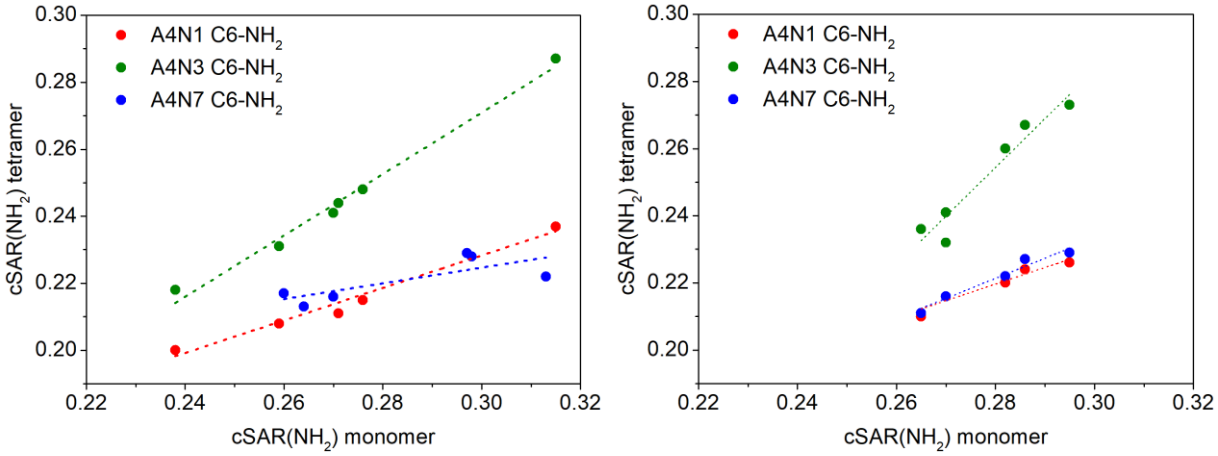



**Figure S2**. Comparison of cSAR($NH_2$) values calculated for tetramers and monomers substituted at positions C-X (a) and N-X (b).

**Table S5.** Slope values, *a*, and determination coefficients, $R^2$, of $cSAR_{tetramer}(NH_2)$ and $cSAR_{monomer}(NH_2)$ correlations.

| Substitution position | C2/C8 | | N9 | |
|---|---|---|---|---|
| Quartet type | *a* | $R^2$ | *a* | $R^2$ |
| $A_4$-N1 | 0.485 | 0.969 | 0.492 | 0.932 |
| $A_4$-N3 | 0.916 | 0.988 | 1.449 | 0.929 |
| $A_4$-N7 | 0.234 | 0.596 | 0.598 | 0.964 |

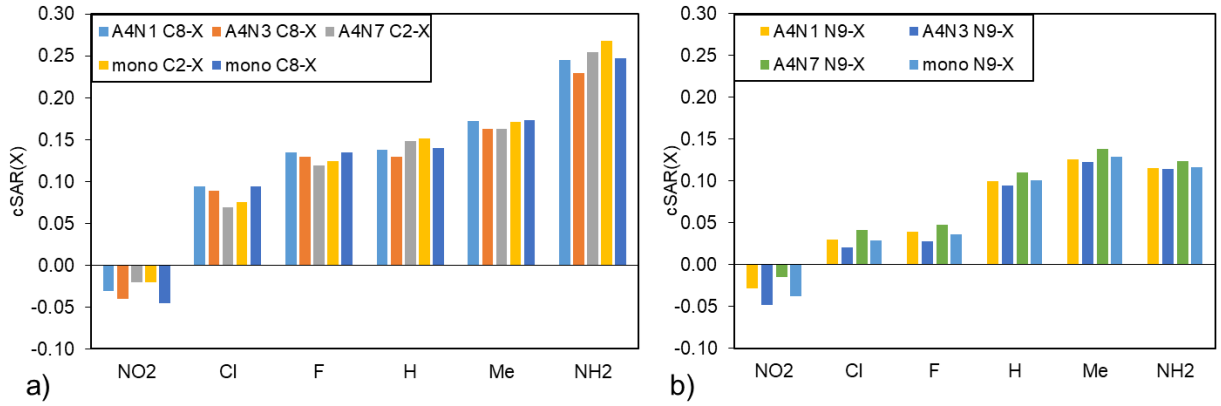



**Figure S3.** Changes in cSAR(X) values depending on the substitution position and type of adenine tetramer.

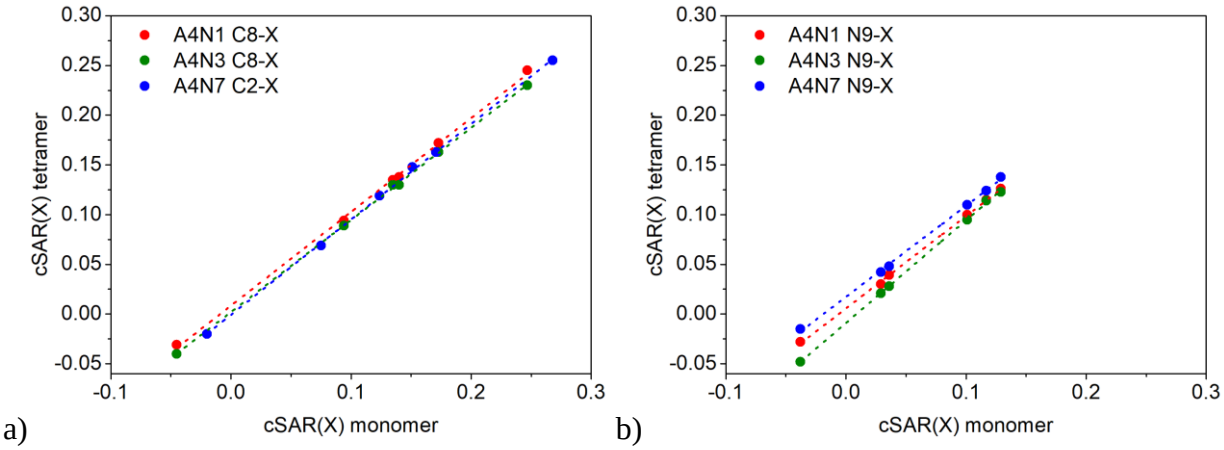
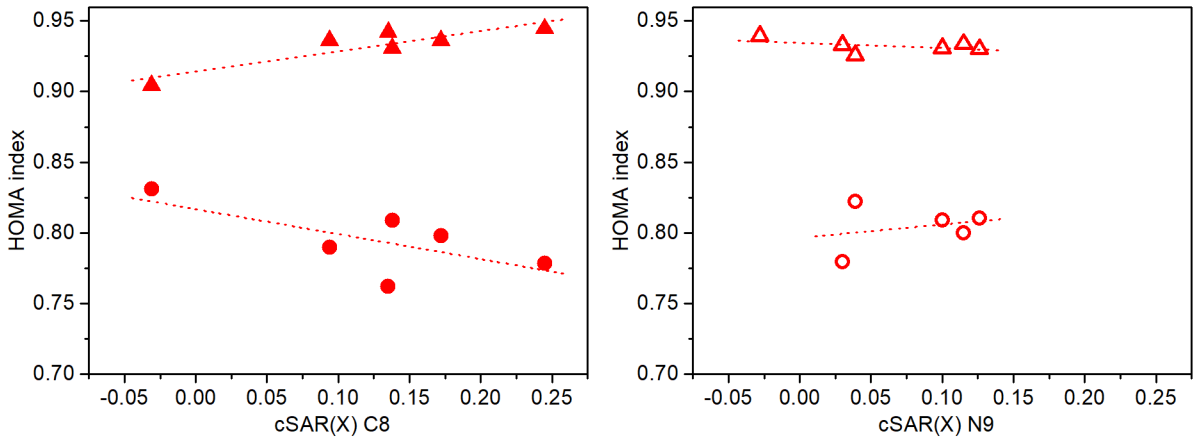



**Figure S4**. Comparison of cSAR(X) values calculated for tetramers and monomers substituted at C2/C8 (a) and N9 (b) positions.

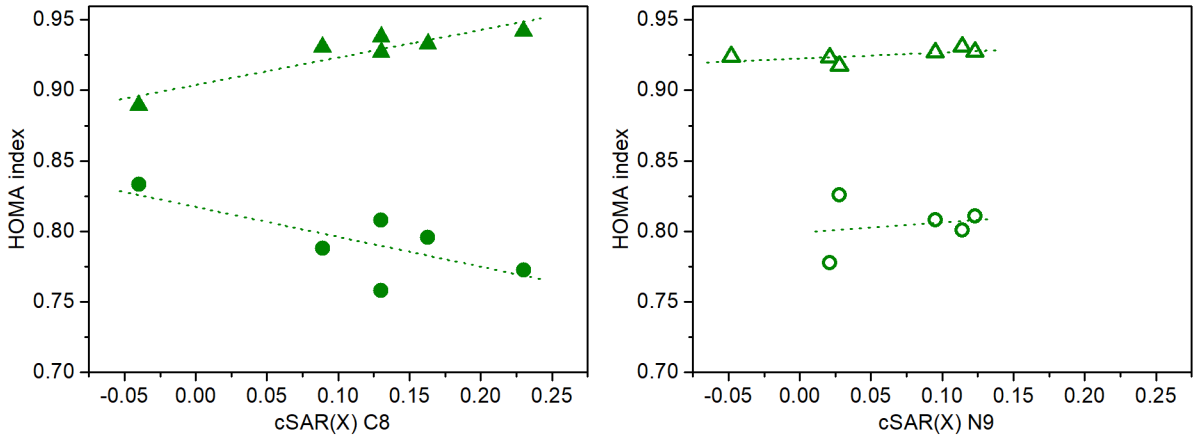
**Table S6.** Slope values, *a*, and determination coefficients, $R^2$, of $cSAR_{tetramer}(X)$ vs $cSAR_{monomer}(X)$ correlations.

| | C2/C8 | | N9 | |
|---|---|---|---|---|
| | $cSAR_{tetramer}(X)$ *vs* $cSAR_{monomer}(X)$ | | | |
| | *a* | $R^2$ | *A* | $R^2$ |
| $A_4$-N1 | 0.943 | 0.999 | 0.930 | 0.999 |
| $A_4$-N3 | 0.926 | 1.000 | 1.033 | 1.000 |
| $A_4$-N7 | 0.960 | 0.999 | 0.917 | 0.999 |

a) $A_4N1$ substituted derivatives




b) $A_4N3$ substituted derivatives




c) $A_4N7$ substituted derivatives

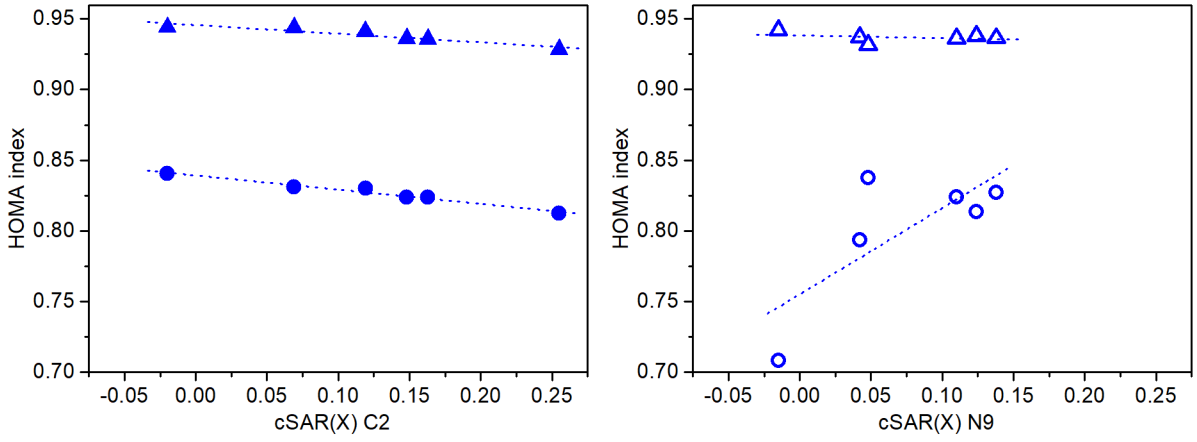
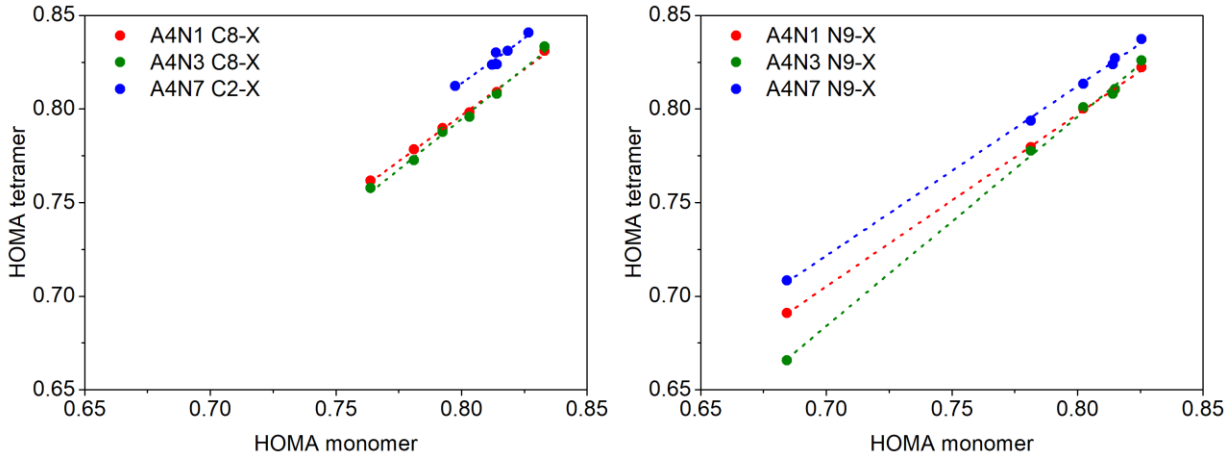



**Figure S5.** Comparison of HOMA indices for both 5- and 6-membered rings (denoted by circles and triangles, respectively) calculated for tetramers substituted at the C2/C8 and N9 positions.

**Table S7.** Slope values, *a*, and determination coefficients, $R^2$, of $HOMA_{tetramer}(X)$ and cSAR(X) correlations for 5- and 6-membered rings.

| Substitution position | C2/C8 | | N9 | |
|---|---|---|---|---|
| Quartet type | *a* | $R^2$ | *a* | $R^2$ |
| | 5-membered rings | | | |
| $A_4$-N1 | -0.177 | 0.453 | 0.618 | 0.587 |
| $A_4$-N3 | -0.212 | 0.516 | 0.678 | 0.588 |
| $A_4$-N7 | -0.101 | 0.971 | 0.609 | 0.573 |
| | 6-membered rings | | | |
| $A_4$-N1 | 0.142 | 0.804 | -0.035 | 0.220 |
| $A_4$-N3 | 0.195 | 0.853 | 0.043 | 0.382 |
| $A_4$-N7 | -0.061 | 0.874 | -0.019 | 0.117 |

(a) For five-membered rings




(b) For six-membered rings

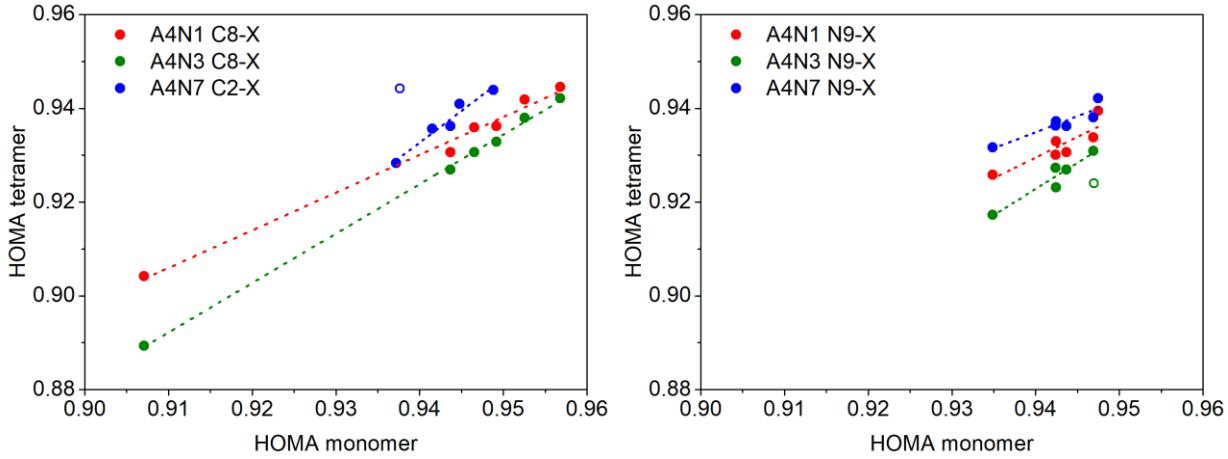



**Figure S6**. Comparison of HOMA values for five- and six-membered rings calculated for substituted monomers and tetramers.

**Table S8.** Slope values, *a*, and determination coefficients, $R^2$, of $HOMA_{tetramer}(X)$ and $HOMA_{monomer}(X)$ correlations for 5- and 6-membered rings.

| Substitution position | C2/C8 | | N9 | |
|---|---|---|---|---|
| Quartet type | *a* | $R^2$ | *a* | $R^2$ |
| | 5-membered rings | | | |
| $A_4$-N1 | 0.981 | 0.997 | 0.921 | 0.999 |
| $A_4$-N3 | 1.081 | 0.993 | 1.119 | 0.998 |
| $A_4$-N7 | 0.960 | 0.939 | 0.906 | 0.999 |
| | 6-membered rings | | | |
| $A_4$-N1 | 0.805 | 0.989 | 0.879 | 0.771 |
| $A_4$-N3 | 1.056 | 0.999 | 1.115 | 0.914 |
| $A_4$-N7 | 1.353 | 0.950 | 0.683 | 0.847 |

Cartesian coordinates of equilibrium geometries of C8-$NO_2$ and N9-$NO_2$ substituted derivatives of the $A_4N1$ tetramer

| | C8-$NO_2$ | | | | N9-$NO_2$ | | |
|---|---|---|---|---|---|---|---|
| N | -3.635420 | -0.530605 | -0.006233 | N | -3.648254 | -0.530091 | -0.071077 |
| C | -4.962249 | -0.557903 | 0.257157 | C | -4.977806 | -0.534344 | 0.138687 |
| N | -5.730011 | -1.626533 | 0.524056 | N | -5.773258 | -1.589663 | 0.388399 |
| C | -5.019508 | -2.762324 | 0.515117 | C | -5.079992 | -2.731352 | 0.422517 |
| C | -3.631362 | -2.890810 | 0.261110 | C | -3.696038 | -2.886039 | 0.230084 |
| C | -2.930845 | -1.689348 | -0.026578 | C | -2.964712 | -1.705553 | -0.043709 |
| N | -5.454484 | -4.056275 | 0.718891 | N | -5.520588 | -4.056204 | 0.624164 |
| C | -4.338510 | -4.857366 | 0.573890 | C | -4.396228 | -4.895082 | 0.537112 |
| N | -3.229383 | -4.208366 | 0.298868 | N | -3.299434 | -4.223300 | 0.303322 |
| H | -5.454256 | 0.413926 | 0.246774 | H | -5.456546 | 0.443155 | 0.102364 |
| N | -1.613000 | -1.664396 | -0.317042 | H | -4.496219 | -5.964862 | 0.657476 |
| H | -1.016185 | -2.507351 | -0.257681 | N | -1.632777 | -1.694597 | -0.273941 |
| H | -1.233797 | -0.819941 | -0.726861 | H | -1.043568 | -2.539025 | -0.195621 |
| H | -6.394215 | -4.383130 | 0.922762 | H | -1.236520 | -0.863975 | -0.695379 |
| N | -0.530456 | 3.634841 | 0.010795 | N | -0.530179 | 3.648349 | 0.071874 |
| C | -0.556475 | 4.961044 | -0.255638 | C | -0.534249 | 4.977759 | -0.138646 |
| N | -1.624306 | 5.728930 | -0.525243 | N | -1.589415 | 5.773125 | -0.389112 |
| C | -2.760670 | 5.019338 | -0.515769 | C | -2.731149 | 5.079926 | -0.423255 |
| C | -2.890430 | 3.631912 | -0.258736 | C | -2.886020 | 3.696109 | -0.230089 |
| C | -1.689749 | 2.931205 | 0.031686 | C | -1.705684 | 2.964870 | 0.044581 |
| N | -4.054125 | 5.454818 | -0.721692 | N | -4.055898 | 5.520494 | -0.625635 |
| C | -4.856219 | 4.339839 | -0.574621 | C | -4.894904 | 4.396263 | -0.538193 |
| N | -4.208282 | 3.230891 | -0.296639 | N | -4.223291 | 3.299570 | -0.303584 |
| H | 0.415752 | 5.452281 | -0.245518 | H | 0.443276 | 5.456442 | -0.102312 |
| N | -1.666043 | 1.614042 | 0.325379 | H | -5.964635 | 4.496266 | -0.658960 |
| H | -0.822422 | 1.235179 | 0.737160 | N | -1.694910 | 1.633094 | 0.275780 |
| H | -2.509095 | 1.017504 | 0.265602 | H | -0.864374 | 1.237036 | 0.697592 |
| H | -4.380101 | 6.394284 | -0.928118 | H | -2.539251 | 1.043798 | 0.197247 |
| N | 3.635589 | 0.530755 | -0.007453 | N | 3.648241 | 0.530099 | -0.070742 |
| C | 4.962467 | 0.558459 | 0.255245 | C | 4.977781 | 0.534343 | 0.139073 |
| N | 5.730154 | 1.627397 | 0.520961 | N | 5.773219 | 1.589654 | 0.388793 |
| C | 5.019505 | 2.763094 | 0.511621 | C | 5.079953 | 2.731343 | 0.422897 |
| C | 3.631274 | 2.891176 | 0.258159 | C | 3.696011 | 2.886041 | 0.230412 |
| C | 2.930870 | 1.689405 | -0.028431 | C | 2.964695 | 1.705560 | -0.043439 |
| N | 5.454348 | 4.057277 | 0.714443 | N | 5.520539 | 4.056188 | 0.624571 |
| C | 4.338200 | 4.858090 | 0.569321 | C | 4.396193 | 4.895077 | 0.537497 |
| N | 3.229106 | 4.208691 | 0.295180 | N | 3.299409 | 4.223304 | 0.303643 |
| H | 5.454614 | -0.413301 | 0.245354 | H | 5.456522 | -0.443156 | 0.102778 |
| N | 1.613032 | 1.664191 | -0.318631 | H | 4.496184 | 5.964856 | 0.657890 |
| H | 1.016149 | 2.507043 | -0.259227 | N | 1.632766 | 1.694598 | -0.273803 |
| H | 1.233601 | 0.819242 | -0.727097 | H | 1.043551 | 2.539030 | -0.195564 |
| H | 6.394070 | 4.384425 | 0.917884 | H | 1.236595 | 0.863993 | -0.695328 |
| N | 0.530776 | -3.634984 | 0.012025 | N | 0.530153 | -3.648291 | 0.072108 |
| C | 0.556564 | -4.961268 | -0.254190 | C | 0.534257 | -4.977734 | -0.138447 |
| N | 1.624192 | -5.729332 | -0.524006 | N | 1.589456 | -5.773135 | -0.388855 |
| C | 2.760614 | -5.019828 | -0.515090 | C | 2.731191 | -5.079938 | -0.422828 |
| C | 2.890618 | -3.632337 | -0.258408 | C | 2.886033 | -3.696098 | -0.229653 |
| C | 1.690139 | -2.931436 | 0.032265 | C | 1.705661 | -2.964823 | 0.044847 |
| N | 4.053927 | -5.455495 | -0.721391 | N | 4.055959 | -5.520522 | -0.624974 |
| C | 4.856202 | -4.340562 | -0.575071 | C | 4.894954 | -4.396283 | -0.537532 |
| N | 4.208495 | -3.231457 | -0.296871 | N | 4.223312 | -3.299566 | -0.303008 |
| H | -0.415689 | -5.452440 | -0.243668 | H | -0.443271 | -5.456418 | -0.102200 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| N | 1.666643 | -1.614198 | 0.325562 | H | 5.964703 | -4.496299 | -0.658197 |
| H | 0.823150 | -1.235107 | 0.737355 | N | 1.694847 | -1.633010 | 0.275855 |
| H | 2.509656 | -1.017651 | 0.265211 | H | 0.864335 | -1.236915 | 0.697666 |
| H | 4.379713 | -6.395055 | -0.927604 | H | 2.539233 | -1.043767 | 0.197416 |
| N | -4.454652 | -6.303738 | 0.718643 | N | -6.891377 | -4.541066 | 0.868247 |
| O | -5.601886 | -6.729557 | 0.984342 | O | -6.984530 | -5.761619 | 0.974582 |
| O | -3.435990 | -6.988380 | 0.570549 | O | -7.756540 | -3.686836 | 0.934587 |
| N | -6.302405 | 4.456801 | -0.720684 | N | -4.540553 | 6.891157 | -0.870786 |
| O | -6.726929 | 5.603467 | -0.991269 | O | -5.761057 | 6.984348 | -0.977643 |
| O | -6.988104 | 3.439341 | -0.568906 | O | -3.686220 | 7.756194 | -0.937349 |
| N | 4.454102 | 6.304570 | 0.713096 | N | 6.891328 | 4.541033 | 0.868627 |
| O | 5.601394 | 6.730822 | 0.978422 | O | 6.984496 | 5.761580 | 0.974926 |
| O | 3.435181 | 6.988883 | 0.564639 | O | 7.756472 | 3.686789 | 0.934961 |
| N | 6.302325 | -4.457763 | -0.721929 | N | 4.540645 | -6.891211 | -0.869840 |
| O | 6.726629 | -5.604602 | -0.991973 | O | 3.686317 | -7.756250 | -0.936459 |
| O | 6.988205 | -3.440322 | -0.571264 | O | 5.761163 | -6.984415 | -0.976414 |

Cartesian coordinates of equilibrium geometries of C8-Cl and N9-Cl substituted derivatives of the $A_4N1$ tetramer

| | C8-Cl | | | | N9-Cl | | |
|---|---|---|---|---|---|---|---|
| N | -3.648263 | -0.584644 | -0.028330 | N | -3.645809 | -0.585960 | -0.116480 |
| C | -4.977293 | -0.599049 | 0.198737 | C | -4.984195 | -0.598053 | 0.054686 |
| N | -5.756161 | -1.660967 | 0.464962 | N | -5.776709 | -1.658819 | 0.274837 |
| C | -5.043417 | -2.796659 | 0.493841 | C | -5.071004 | -2.795243 | 0.324536 |
| C | -3.659273 | -2.938300 | 0.282205 | C | -3.679902 | -2.945289 | 0.177903 |
| C | -2.946691 | -1.749906 | -0.005270 | C | -2.953089 | -1.754591 | -0.072472 |
| N | -5.498065 | -4.090265 | 0.710572 | N | -5.519655 | -4.099825 | 0.505986 |
| C | -4.384305 | -4.911008 | 0.612745 | C | -4.410914 | -4.944540 | 0.460401 |
| N | -3.269379 | -4.276046 | 0.359032 | N | -3.293497 | -4.280758 | 0.262870 |
| H | -5.463618 | 0.374778 | 0.160159 | H | -5.464759 | 0.378241 | 0.009314 |
| N | -1.616281 | -1.718180 | -0.252009 | H | -4.522206 | -6.014969 | 0.577976 |
| H | -1.013510 | -2.554189 | -0.188702 | N | -1.614337 | -1.729459 | -0.267460 |
| H | -1.238494 | -0.880966 | -0.677497 | H | -1.014339 | -2.563918 | -0.172330 |
| H | -6.453645 | -4.377116 | 0.889954 | H | -1.216995 | -0.892774 | -0.674850 |
| N | -0.584722 | 3.648554 | 0.034162 | N | -0.585911 | 3.646144 | 0.117485 |
| C | -0.598575 | 4.977085 | -0.195573 | C | -0.598105 | 4.984513 | -0.053408 |
| N | -1.660042 | 5.755610 | -0.464724 | N | -1.658918 | 5.776891 | -0.273777 |
| C | -2.795866 | 5.043077 | -0.493688 | C | -2.795260 | 5.071062 | -0.324052 |
| C | -2.938001 | 3.659368 | -0.279612 | C | -2.945187 | 3.679942 | -0.177374 |
| C | -1.750089 | 2.947155 | 0.010984 | C | -1.754462 | 2.953300 | 0.073313 |
| N | -4.089176 | 5.497601 | -0.712675 | N | -4.099836 | 5.519574 | -0.506461 |
| C | -4.910267 | 4.384237 | -0.613360 | C | -4.944454 | 4.410745 | -0.461133 |
| N | -4.275785 | 3.269682 | -0.357220 | N | -4.280594 | 3.293407 | -0.262836 |
| H | 0.375331 | 5.463261 | -0.156739 | H | 0.378138 | 5.465166 | -0.007579 |
| N | -1.718905 | 1.617245 | 0.260755 | H | -6.014869 | 4.521927 | -0.579506 |
| H | -0.882463 | 1.240317 | 0.688687 | N | -1.729105 | 1.614574 | 0.268319 |
| H | -2.554716 | 1.014265 | 0.196585 | H | -0.891914 | 1.217447 | 0.675758 |
| H | -4.375683 | 6.452947 | -0.893957 | H | -2.563599 | 1.014420 | 0.174232 |
| N | 3.648333 | 0.584635 | -0.030498 | N | 3.646177 | 0.586107 | -0.119756 |
| C | 4.977392 | 0.598968 | 0.196109 | C | 4.984513 | 0.598121 | 0.051558 |
| N | 5.756234 | 1.660742 | 0.462555 | N | 5.776751 | 1.658634 | 0.273489 |
| C | 5.043405 | 2.796351 | 0.492400 | C | 5.070805 | 2.794819 | 0.325401 |
| C | 3.659223 | 2.938063 | 0.281510 | C | 3.679741 | 2.944939 | 0.178898 |
| C | 2.946667 | 1.749823 | -0.006570 | C | 2.953258 | 1.754541 | -0.073966 |
| N | 5.497995 | 4.089844 | 0.709485 | N | 5.519112 | 4.099119 | 0.509584 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | 4.384183 | 4.910575 | 0.612744 | C | 4.410256 | 4.943726 | 0.465529 |
| N | 3.269247 | 4.275730 | 0.359315 | N | 3.293060 | 4.280163 | 0.266730 |
| H | 5.463788 | -0.374790 | 0.156815 | H | 5.465263 | -0.377997 | 0.004638 |
| N | 1.616203 | 1.718193 | -0.253207 | H | 4.521272 | 6.013901 | 0.585349 |
| H | 1.013448 | 2.554137 | -0.189030 | N | 1.614560 | 1.729330 | -0.269501 |
| H | 1.238520 | 0.881442 | -0.679311 | H | 1.014425 | 2.563799 | -0.174077 |
| H | 6.453573 | 4.376635 | 0.888403 | H | 1.217900 | 0.893610 | -0.678961 |
| N | 0.585119 | -3.648388 | 0.032315 | N | 0.586268 | -3.646056 | 0.119676 |
| C | 0.598592 | -4.976807 | -0.198182 | C | 0.598232 | -4.984346 | -0.051834 |
| N | 1.659656 | -5.755250 | -0.468951 | N | 1.658724 | -5.776580 | -0.274047 |
| C | 2.795484 | -5.042770 | -0.498836 | C | 2.794982 | -5.070713 | -0.325972 |
| C | 2.937990 | -3.659182 | -0.284346 | C | 2.945127 | -3.679686 | -0.179264 |
| C | 1.750483 | -2.947051 | 0.008072 | C | 1.754734 | -2.953174 | 0.073786 |
| N | 4.088483 | -5.497218 | -0.719294 | N | 4.099311 | -5.519054 | -0.510379 |
| C | 4.909794 | -4.383982 | -0.620770 | C | 4.943971 | -4.410249 | -0.466056 |
| N | 4.275698 | -3.269526 | -0.363427 | N | 4.280397 | -3.293065 | -0.267043 |
| H | -0.375292 | -5.462940 | -0.158524 | H | -0.377921 | -5.465062 | -0.004889 |
| N | 1.719670 | -1.617201 | 0.258475 | H | 6.014188 | -4.521301 | -0.585853 |
| H | 0.884063 | -1.240675 | 0.688247 | N | 1.729684 | -1.614474 | 0.269387 |
| H | 2.555582 | -1.014467 | 0.194037 | H | 0.894136 | -1.217564 | 0.678946 |
| H | 4.374701 | -6.452454 | -0.900923 | H | 2.564061 | -1.014466 | 0.173146 |
| Cl | -4.547908 | -6.624144 | 0.815277 | Cl | -7.162491 | -4.584595 | 0.720944 |
| Cl | -6.623203 | 4.547842 | -0.817220 | Cl | -4.584702 | 7.162366 | -0.722142 |
| Cl | 4.547730 | 6.623607 | 0.816064 | Cl | 7.161763 | 4.583739 | 0.725895 |
| Cl | 6.622501 | -4.547633 | -0.826759 | Cl | 4.583931 | -7.161687 | -0.727112 |

Cartesian coordinates of equilibrium geometries of C8-F and N9-F substituted derivatives of the $A_4N1$ tetramer

| | C8-F | | | | N9-F | | |
|---|---|---|---|---|---|---|---|
| N | -3.650180 | -0.585492 | -0.023712 | N | -3.637809 | -0.560003 | -0.026500 |
| C | -4.976010 | -0.596408 | 0.213198 | C | -4.963120 | -0.569520 | 0.228999 |
| N | -5.747942 | -1.653438 | 0.521200 | N | -5.742431 | -1.624834 | 0.511586 |
| C | -5.029592 | -2.781762 | 0.583571 | C | -5.029260 | -2.759028 | 0.525055 |
| C | -3.647169 | -2.926014 | 0.365662 | C | -3.648693 | -2.917816 | 0.285274 |
| C | -2.942972 | -1.747303 | 0.032852 | C | -2.941460 | -1.726821 | -0.016971 |
| N | -5.478830 | -4.073851 | 0.854831 | N | -5.429301 | -4.063070 | 0.744251 |
| C | -4.357852 | -4.872672 | 0.776066 | C | -4.352815 | -4.921921 | 0.636926 |
| N | -3.248231 | -4.264748 | 0.491249 | N | -3.252594 | -4.251016 | 0.355009 |
| H | -5.467730 | 0.372963 | 0.145860 | H | -5.444740 | 0.406911 | 0.201397 |
| N | -1.612829 | -1.716188 | -0.221127 | H | -4.463149 | -5.989637 | 0.773309 |
| H | -1.012160 | -2.553378 | -0.156558 | N | -1.618379 | -1.703761 | -0.291654 |
| H | -1.243557 | -0.894068 | -0.682370 | H | -1.015265 | -2.540166 | -0.220549 |
| H | -6.428988 | -4.365556 | 1.053915 | H | -1.239710 | -0.864707 | -0.713234 |
| N | -0.585894 | 3.651350 | 0.030937 | N | -0.562285 | 3.638909 | 0.026038 |
| C | -0.597260 | 4.976986 | -0.206931 | C | -0.574283 | 4.965983 | -0.221488 |
| N | -1.654395 | 5.748206 | -0.516028 | N | -1.631271 | 5.746071 | -0.496349 |
| C | -2.782340 | 5.029290 | -0.578633 | C | -2.764547 | 5.031539 | -0.510549 |
| C | -2.926133 | 3.646968 | -0.359822 | C | -2.920948 | 3.649202 | -0.278799 |
| C | -1.747340 | 2.943560 | -0.025727 | C | -1.728288 | 2.941159 | 0.015630 |
| N | -4.074420 | 5.477742 | -0.851086 | N | -4.069835 | 5.431595 | -0.722287 |
| C | -4.872802 | 4.356473 | -0.772190 | C | -4.926838 | 4.353224 | -0.618582 |
| N | -4.264590 | 3.247326 | -0.485892 | N | -4.253843 | 3.251792 | -0.346515 |
| H | 0.371812 | 5.469248 | -0.139383 | H | 0.401452 | 5.448965 | -0.193388 |
| N | -1.715849 | 1.613638 | 0.229592 | H | -5.995023 | 4.463103 | -0.750089 |
| H | -0.893746 | 1.245161 | 0.691396 | N | -1.703464 | 1.616213 | 0.282565 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | -2.552614 | 1.012391 | 0.164137 | H | -0.863390 | 1.236461 | 0.699695 |
| H | -4.366396 | 6.427605 | -1.050984 | H | -2.540318 | 1.013823 | 0.212634 |
| N | 3.651116 | 0.586017 | -0.029123 | N | 3.636618 | 0.560203 | -0.037094 |
| C | 4.977143 | 0.596598 | 0.206874 | C | 4.963785 | 0.567629 | 0.208730 |
| N | 5.749097 | 1.652937 | 0.516854 | N | 5.746525 | 1.621504 | 0.487060 |
| C | 5.030521 | 2.780915 | 0.582499 | C | 5.034951 | 2.756638 | 0.507113 |
| C | 3.647909 | 2.925465 | 0.365768 | C | 3.652844 | 2.917435 | 0.277589 |
| C | 2.943678 | 1.747490 | 0.030595 | C | 2.941894 | 1.727944 | -0.021227 |
| N | 5.479639 | 4.072305 | 0.856937 | N | 5.438095 | 4.059757 | 0.725585 |
| C | 4.358416 | 4.871091 | 0.781179 | C | 4.361662 | 4.919963 | 0.627507 |
| N | 3.248728 | 4.263727 | 0.494954 | N | 3.258728 | 4.250868 | 0.352508 |
| H | 5.469062 | -0.372457 | 0.136797 | H | 5.443793 | -0.409457 | 0.176517 |
| N | 1.613227 | 1.716737 | -0.222585 | H | 4.474194 | 5.987229 | 0.764706 |
| H | 1.012768 | 2.553958 | -0.156514 | N | 1.616762 | 1.706920 | -0.286382 |
| H | 1.244240 | 0.895829 | -0.686161 | H | 1.015401 | 2.544275 | -0.213190 |
| H | 6.429820 | 4.363631 | 1.056311 | H | 1.234602 | 0.869006 | -0.706341 |
| N | 0.586276 | -3.650830 | 0.026931 | N | 0.559266 | -3.636815 | 0.020020 |
| C | 0.596649 | -4.976346 | -0.212082 | C | 0.570135 | -4.963874 | -0.225532 |
| N | 1.652717 | -5.747578 | -0.525398 | N | 1.626535 | -5.744660 | -0.499280 |
| C | 2.780555 | -5.028792 | -0.590955 | C | 2.760387 | -5.030980 | -0.515076 |
| C | 2.925227 | -3.646576 | -0.371592 | C | 2.917812 | -3.648655 | -0.285351 |
| C | 1.747614 | -2.943196 | -0.033201 | C | 1.725798 | -2.939956 | 0.008953 |
| N | 4.071649 | -5.477251 | -0.867828 | N | 4.065282 | -5.431917 | -0.727364 |
| C | 4.870421 | -4.356108 | -0.790664 | C | 4.923207 | -4.354165 | -0.625711 |
| N | 4.263311 | -3.247052 | -0.501841 | N | 4.250977 | -3.252267 | -0.354294 |
| H | -0.372327 | -5.468434 | -0.141771 | H | -0.406082 | -5.445867 | -0.196926 |
| N | 1.717035 | -1.613260 | 0.222484 | H | 5.991314 | -4.464903 | -0.757972 |
| H | 0.897267 | -1.245296 | 0.688989 | N | 1.701756 | -1.615160 | 0.275088 |
| H | 2.554198 | -1.012710 | 0.156395 | H | 0.861467 | -1.234506 | 0.692289 |
| H | 4.362821 | -6.427027 | -1.069425 | H | 2.538370 | -1.012592 | 0.203358 |
| F | -4.489531 | -6.188100 | 0.990982 | F | -6.732721 | -4.463672 | 1.033188 |
| F | -6.188140 | 4.487410 | -0.988402 | F | -4.473061 | 6.736463 | -1.001546 |
| F | 4.489938 | 6.185928 | 1.000060 | F | 6.743897 | 4.458160 | 1.006888 |
| F | 6.184967 | -4.487050 | -1.011090 | F | 4.467413 | -6.737200 | -1.005231 |

Cartesian coordinates of equilibrium geometries of C8-H and N9-H substituted derivatives of the $A_4N1$ tetramer

C8-H / N9-H

| | | | |
|---|---|---|---|
| N | -3.639812 | -0.589874 | -0.054963 |
| C | -4.970931 | -0.602642 | 0.165863 |
| N | -5.753605 | -1.661755 | 0.425273 |
| C | -5.042533 | -2.802412 | 0.455918 |
| C | -3.656905 | -2.946799 | 0.251483 |
| C | -2.941979 | -1.756547 | -0.029985 |
| N | -5.499071 | -4.091715 | 0.668243 |
| C | -4.394581 | -4.928699 | 0.581263 |
| N | -3.273669 | -4.282532 | 0.331237 |
| H | -5.452303 | 0.373861 | 0.128217 |
| H | -4.485339 | -6.000837 | 0.709546 |
| N | -1.611224 | -1.727027 | -0.271989 |
| H | -1.004210 | -2.558453 | -0.188432 |
| H | -1.225954 | -0.883187 | -0.676968 |
| N | -0.590567 | 3.641156 | 0.063624 |
| C | -0.601809 | 4.971309 | -0.162640 |
| N | -1.659585 | 5.753470 | -0.428715 |

| | | | |
|---|---|---|---|
| C | -2.800531 | 5.042893 | -0.460657 |
| C | -2.946384 | 3.658162 | -0.251481 |
| C | -1.757574 | 2.943837 | 0.037516 |
| N | -4.088715 | 5.499131 | -0.679469 |
| C | -4.926633 | 4.395409 | -0.591337 |
| N | -4.281991 | 3.275308 | -0.335104 |
| H | 0.374904 | 5.452176 | -0.123797 |
| H | -5.998201 | 4.486126 | -0.723820 |
| N | -1.729516 | 1.614302 | 0.286106 |
| H | -0.886593 | 1.230146 | 0.693416 |
| H | -2.560162 | 1.006627 | 0.200304 |
| N | 3.639435 | 0.590376 | -0.062659 |
| C | 4.969987 | 0.601704 | 0.162297 |
| N | 5.752309 | 1.659330 | 0.428329 |
| C | 5.041568 | 2.800135 | 0.461575 |
| C | 3.656553 | 2.945937 | 0.253549 |
| C | 2.941894 | 1.757180 | -0.034992 |
| N | 5.497889 | 4.088191 | 0.681120 |
| C | 4.393898 | 4.925988 | 0.594449 |
| N | 3.273567 | 4.281423 | 0.338280 |
| H | 5.451017 | -0.374851 | 0.122443 |
| H | 4.484650 | 5.997470 | 0.727714 |
| N | 1.611767 | 1.729070 | -0.281171 |
| H | 1.004348 | 2.559815 | -0.193980 |
| H | 1.227104 | 0.886273 | -0.688333 |
| N | 0.591319 | -3.640672 | 0.064046 |
| C | 0.602645 | -4.970821 | -0.162553 |
| N | 1.660292 | -5.752692 | -0.430299 |
| C | 2.801012 | -5.041820 | -0.463604 |
| C | 2.946702 | -3.657017 | -0.254350 |
| C | 1.758079 | -2.943013 | 0.036314 |
| N | 4.089114 | -5.497795 | -0.684123 |
| C | 4.926839 | -4.393867 | -0.596544 |
| N | 4.282153 | -3.273865 | -0.339242 |
| H | -0.373884 | -5.451961 | -0.122620 |
| H | 5.998330 | -4.484359 | -0.730181 |
| N | 1.730088 | -1.613463 | 0.284813 |
| H | 0.887751 | -1.229240 | 0.693991 |
| H | 2.560130 | -1.005410 | 0.196135 |
| H | -6.461128 | -4.356163 | 0.846456 |
| H | -4.351945 | 6.460588 | -0.862106 |
| H | 6.459502 | 4.351396 | 0.863560 |
| H | 4.352487 | -6.459302 | -0.866967 |

Cartesian coordinates of equilibrium geometries of C8-Me and N9-Me substituted derivatives of the $A_4N1$ tetramer

| | C8-Me | | | | N9-Me | | |
|---|---|---|---|---|---|---|---|
| N | -3.644380 | -0.571956 | -0.037863 | N | -3.638436 | -0.603671 | -0.129354 |
| C | -4.973557 | -0.583921 | 0.185620 | C | -4.978134 | -0.617973 | 0.032393 |
| N | -5.760929 | -1.646917 | 0.420562 | N | -5.770884 | -1.679897 | 0.246496 |
| C | -5.055213 | -2.790679 | 0.420106 | C | -5.059793 | -2.821257 | 0.303314 |
| C | -3.671559 | -2.935742 | 0.210175 | C | -3.665068 | -2.962123 | 0.167090 |
| C | -2.952302 | -1.743840 | -0.042480 | C | -2.940962 | -1.770284 | -0.079889 |
| N | -5.515977 | -4.083958 | 0.596433 | N | -5.539876 | -4.108201 | 0.481397 |
| C | -4.417707 | -4.936722 | 0.483389 | C | -4.426967 | -4.938956 | 0.443483 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| N | -3.297276 | -4.276122 | 0.251330 | N | -3.289035 | -4.297106 | 0.256738 |
| H | -5.450738 | 0.395330 | 0.173115 | H | -5.457104 | 0.359277 | -0.017114 |
| N | -1.620722 | -1.713296 | -0.286959 | H | -4.529481 | -6.012116 | 0.559066 |
| H | -1.017372 | -2.548611 | -0.220781 | N | -1.600798 | -1.736449 | -0.268474 |
| H | -1.234687 | -0.864129 | -0.679391 | H | -0.995572 | -2.567084 | -0.168306 |
| H | -6.480371 | -4.346471 | 0.763981 | H | -1.205502 | -0.895690 | -0.669603 |
| N | -0.571907 | 3.644205 | 0.038059 | N | -0.603675 | 3.638509 | 0.130865 |
| C | -0.583679 | 4.973383 | -0.185417 | C | -0.617880 | 4.978135 | -0.031884 |
| N | -1.646584 | 5.760911 | -0.420116 | N | -1.679735 | 5.770833 | -0.247172 |
| C | -2.790458 | 5.055375 | -0.419568 | C | -2.821111 | 5.059765 | -0.303790 |
| C | -2.935721 | 3.671740 | -0.209735 | C | -2.962058 | 3.665105 | -0.166679 |
| C | -1.743895 | 2.952309 | 0.042758 | C | -1.770310 | 2.941080 | 0.081212 |
| N | -4.083689 | 5.516353 | -0.595686 | N | -4.107976 | 5.539820 | -0.482376 |
| C | -4.936628 | 4.418235 | -0.482628 | C | -4.938789 | 4.426962 | -0.444175 |
| N | -4.276175 | 3.297689 | -0.250782 | N | -4.297037 | 3.289091 | -0.256570 |
| H | 0.395644 | 5.450416 | -0.173120 | H | 0.359398 | 5.457067 | 0.017780 |
| N | -1.713451 | 1.620741 | 0.287110 | H | -6.011919 | 4.529473 | -0.560166 |
| H | -0.864326 | 1.234502 | 0.679490 | N | -1.736501 | 1.601030 | 0.270381 |
| H | -2.548783 | 1.017358 | 0.220873 | H | -0.895875 | 1.205721 | 0.671938 |
| H | -4.346067 | 6.480787 | -0.763136 | H | -2.567027 | 0.995576 | 0.169845 |
| N | 3.644037 | 0.571797 | -0.037772 | N | 3.638209 | 0.603700 | -0.129452 |
| C | 4.973258 | 0.583622 | 0.185516 | C | 4.977938 | 0.617997 | 0.032514 |
| N | 5.760834 | 1.646567 | 0.420007 | N | 5.770757 | 1.679920 | 0.246915 |
| C | 5.055290 | 2.790437 | 0.419296 | C | 5.059704 | 2.821297 | 0.303480 |
| C | 3.671616 | 2.935647 | 0.209514 | C | 3.664969 | 2.962174 | 0.167056 |
| C | 2.952133 | 1.743785 | -0.042646 | C | 2.940790 | 1.770340 | -0.080005 |
| N | 5.516284 | 4.083699 | 0.595203 | N | 5.539816 | 4.108229 | 0.481282 |
| C | 4.418114 | 4.936590 | 0.482013 | C | 4.426907 | 4.938985 | 0.443412 |
| N | 3.297534 | 4.276093 | 0.250276 | N | 3.288949 | 4.297160 | 0.256708 |
| H | 5.450294 | -0.395702 | 0.173236 | H | 5.456880 | -0.359274 | -0.017102 |
| N | 1.620520 | 1.713391 | -0.286928 | H | 4.529440 | 6.012144 | 0.558928 |
| H | 1.017325 | 2.548761 | -0.220908 | N | 1.600597 | 1.736563 | -0.268687 |
| H | 1.234328 | 0.864102 | -0.678925 | H | 0.995507 | 2.567249 | -0.168784 |
| H | 6.480748 | 4.346123 | 0.762617 | H | 1.205406 | 0.895705 | -0.669795 |
| N | 0.571796 | -3.644216 | 0.038110 | N | 0.603801 | -3.638412 | 0.130781 |
| C | 0.583571 | -4.973342 | -0.185539 | C | 0.617962 | -4.978054 | -0.031954 |
| N | 1.646462 | -5.760791 | -0.420438 | N | 1.679768 | -5.770820 | -0.247115 |
| C | 2.790322 | -5.055227 | -0.419922 | C | 2.821165 | -5.059801 | -0.303697 |
| C | 2.935568 | -3.671633 | -0.209816 | C | 2.962164 | -3.665142 | -0.166585 |
| C | 1.743764 | -2.952284 | 0.042921 | C | 1.770466 | -2.941035 | 0.081315 |
| N | 4.083546 | -5.516125 | -0.596393 | N | 4.108011 | -5.539903 | -0.482191 |
| C | 4.936459 | -4.417992 | -0.483170 | C | 4.938846 | -4.427063 | -0.444038 |
| N | 4.275996 | -3.297521 | -0.250882 | N | 4.297146 | -3.289161 | -0.256456 |
| H | -0.395740 | -5.450398 | -0.173217 | H | -0.359322 | -5.456962 | 0.017650 |
| N | 1.713381 | -1.620756 | 0.287689 | H | 6.011965 | -4.529603 | -0.560022 |
| H | 0.864236 | -1.234735 | 0.680187 | N | 1.736837 | -1.600960 | 0.270791 |
| H | 2.548708 | -1.017451 | 0.221523 | H | 0.896178 | -1.205897 | 0.672444 |
| H | 4.345940 | -6.480521 | -0.764142 | H | 2.567446 | -0.995803 | 0.170577 |
| C | -4.549363 | -6.421900 | 0.607376 | C | -6.943848 | -4.483553 | 0.641927 |
| H | -4.977411 | -6.705798 | 1.577989 | H | -7.362737 | -4.005944 | 1.533574 |
| H | -5.199872 | -6.829895 | -0.178268 | H | -7.520475 | -4.160886 | -0.231240 |
| H | -3.559823 | -6.875535 | 0.512707 | H | -7.010863 | -5.569764 | 0.743234 |
| C | -6.421806 | 4.550197 | -0.606314 | C | -4.483213 | 6.943736 | -0.643525 |
| H | -6.829599 | 5.200146 | 0.179901 | H | -4.160746 | 7.520676 | 0.229487 |
| H | -6.705777 | 4.979066 | -1.576538 | H | -4.005365 | 7.362279 | -1.535187 |
| H | -6.875587 | 3.560662 | -0.512349 | H | -5.569379 | 7.010733 | -0.745125 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | 4.550036 | 6.421786 | 0.605469 | C | 6.943787 | 4.483578 | 0.641531 |
| H | 4.978946 | 6.705917 | 1.575647 | H | 7.362848 | 4.006101 | 1.533129 |
| H | 5.199934 | 6.829471 | -0.180855 | H | 7.520271 | 4.160821 | -0.231657 |
| H | 3.560461 | 6.875511 | 0.511487 | H | 7.010761 | 5.569776 | 0.742678 |
| C | 6.421629 | -4.549839 | -0.607176 | C | 4.483227 | -6.943821 | -0.643266 |
| H | 6.829596 | -5.200244 | 0.178620 | H | 4.160767 | -7.520707 | 0.229773 |
| H | 6.705468 | -4.978129 | -1.577731 | H | 4.005383 | -7.362421 | -1.534891 |
| H | 6.875355 | -3.560307 | -0.512712 | H | 5.569388 | -7.010814 | -0.744859 |

Cartesian coordinates of equilibrium geometries of C8-$NH_2$ and N9-$NH_2$ substituted derivatives of the $A_4$N1 tetramer

| | C8-$NH_2$ | | | | N9-$NH_2$ | | |
|---|---|---|---|---|---|---|---|
| N | -3.637548 | -0.549606 | -0.087614 | N | -3.636071 | -0.659311 | -0.032192 |
| C | -4.924688 | -0.509278 | 0.300703 | C | -4.962142 | -0.688000 | 0.210492 |
| N | -5.683690 | -1.531547 | 0.738387 | N | -5.723745 | -1.759054 | 0.492025 |
| C | -4.993985 | -2.680804 | 0.756244 | C | -4.989381 | -2.883069 | 0.521791 |
| C | -3.652402 | -2.877484 | 0.384880 | C | -3.606808 | -3.013453 | 0.300422 |
| C | -2.961423 | -1.731737 | -0.066038 | C | -2.917630 | -1.814967 | -0.007329 |
| N | -5.445930 | -3.944547 | 1.127282 | N | -5.427894 | -4.181013 | 0.752206 |
| C | -4.374020 | -4.815922 | 0.950384 | C | -4.313314 | -5.004304 | 0.658290 |
| N | -3.281482 | -4.216889 | 0.518386 | N | -3.204615 | -4.344077 | 0.388099 |
| H | -5.390383 | 0.474108 | 0.255051 | H | -5.458665 | 0.280815 | 0.172478 |
| N | -1.664306 | -1.745985 | -0.466988 | H | -4.408929 | -6.073972 | 0.799469 |
| H | -1.073411 | -2.590222 | -0.418256 | N | -1.592549 | -1.763405 | -0.275343 |
| H | -1.329716 | -0.953284 | -1.000507 | H | -0.968238 | -2.581569 | -0.188813 |
| H | -6.406013 | -4.184068 | 1.344479 | H | -1.229597 | -0.918130 | -0.696986 |
| N | -0.555458 | 3.667823 | -0.221977 | N | -0.645953 | 3.614789 | 0.055018 |
| C | -0.600329 | 5.002065 | -0.384995 | C | -0.685095 | 4.949039 | -0.135447 |
| N | -1.689096 | 5.775372 | -0.554942 | N | -1.765297 | 5.715396 | -0.362914 |
| C | -2.812710 | 5.044797 | -0.555734 | C | -2.886773 | 4.977376 | -0.395357 |
| C | -2.925323 | 3.652617 | -0.401926 | C | -3.006834 | 3.586913 | -0.224966 |
| C | -1.713874 | 2.950192 | -0.216179 | C | -1.798781 | 2.892492 | 0.028505 |
| N | -4.125280 | 5.493532 | -0.678599 | N | -4.191141 | 5.419452 | -0.575145 |
| C | -4.938659 | 4.366818 | -0.594502 | C | -5.008772 | 4.299707 | -0.502846 |
| N | -4.262102 | 3.248554 | -0.417496 | N | -4.337992 | 3.183524 | -0.294214 |
| H | 0.366134 | 5.504104 | -0.375281 | H | 0.282400 | 5.448358 | -0.099342 |
| N | -1.648247 | 1.605961 | -0.042701 | H | -6.082167 | 4.396240 | -0.612291 |
| H | -0.785190 | 1.225641 | 0.325624 | N | -1.735584 | 1.557225 | 0.241221 |
| H | -2.490165 | 1.008525 | -0.033526 | H | -0.886743 | 1.189048 | 0.651759 |
| H | -4.405008 | 6.442911 | -0.894858 | H | -2.563247 | 0.941119 | 0.182535 |
| N | 3.637519 | 0.549903 | -0.088604 | N | 3.635179 | 0.656568 | -0.012882 |
| C | 4.924940 | 0.509389 | 0.298980 | C | 4.958375 | 0.687353 | 0.244425 |
| N | 5.684381 | 1.531538 | 0.736232 | N | 5.717760 | 1.761055 | 0.521295 |
| C | 4.994825 | 2.680870 | 0.754585 | C | 4.984479 | 2.886231 | 0.527672 |
| C | 3.652989 | 2.877739 | 0.384123 | C | 3.605110 | 3.015452 | 0.286451 |
| C | 2.961548 | 1.732107 | -0.066425 | C | 2.917623 | 1.813338 | -0.012015 |
| N | 5.447191 | 3.944541 | 1.125369 | N | 5.423299 | 4.187209 | 0.740234 |
| C | 4.375267 | 4.816062 | 0.949185 | C | 4.312000 | 5.011210 | 0.616681 |
| N | 3.282348 | 4.217191 | 0.518004 | N | 3.204641 | 4.348230 | 0.346775 |
| H | 5.390507 | -0.474034 | 0.253043 | H | 5.454696 | -0.282068 | 0.223199 |
| N | 1.664098 | 1.746476 | -0.466347 | H | 4.408084 | 6.083099 | 0.739209 |
| H | 1.073513 | 2.590919 | -0.417725 | N | 1.596436 | 1.759670 | -0.297230 |
| H | 1.329266 | 0.954074 | -1.000186 | H | 0.968047 | 2.574934 | -0.214550 |
| H | 6.407503 | 4.183972 | 1.341738 | H | 1.235481 | 0.903899 | -0.698706 |
| N | 0.554865 | -3.667300 | -0.221840 | N | 0.649669 | -3.619408 | 0.077371 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | 0.599372 | -5.001647 | -0.384112 | C | 0.690100 | -4.953639 | -0.113406 |
| N | 1.687951 | -5.775322 | -0.553665 | N | 1.770167 | -5.718147 | -0.348102 |
| C | 2.811738 | -5.045020 | -0.554922 | C | 2.890251 | -4.978412 | -0.385908 |
| C | 2.924709 | -3.652766 | -0.401966 | C | 3.009379 | -3.588276 | -0.212442 |
| C | 1.713444 | -2.949941 | -0.216539 | C | 1.801303 | -2.895321 | 0.045074 |
| N | 4.124188 | -5.494166 | -0.677461 | N | 4.194349 | -5.418519 | -0.573083 |
| C | 4.937862 | -4.367619 | -0.594024 | C | 5.010926 | -4.297925 | -0.500403 |
| N | 4.261597 | -3.249066 | -0.417818 | N | 4.339836 | -3.183039 | -0.286647 |
| H | -0.367230 | -5.503405 | -0.374047 | H | -0.276033 | -5.454990 | -0.071025 |
| N | 1.648056 | -1.605555 | -0.043909 | H | 6.083924 | -4.392901 | -0.614507 |
| H | 0.785316 | -1.225054 | 0.324994 | N | 1.736454 | -1.559222 | 0.254611 |
| H | 2.490151 | -1.008372 | -0.034563 | H | 0.889691 | -1.193790 | 0.672616 |
| H | 4.403671 | -6.443770 | -0.893005 | H | 2.564700 | -0.943881 | 0.198998 |
| N | -4.516540 | -6.181356 | 1.148951 | N | -6.742760 | -4.628777 | 1.020704 |
| H | -3.624386 | -6.666999 | 1.103741 | H | -7.079851 | -4.132710 | 1.850239 |
| H | -5.064689 | -6.457165 | 1.959180 | H | -7.336016 | -4.336956 | 0.239309 |
| N | -6.313414 | 4.457739 | -0.757808 | N | -4.648367 | 6.746689 | -0.762189 |
| H | -6.778956 | 3.577067 | -0.554114 | H | -4.290830 | 7.304971 | 0.017877 |
| H | -6.762772 | 5.244960 | -0.297877 | H | -4.202859 | 7.111722 | -1.608905 |
| N | 4.518079 | 6.181467 | 1.147694 | N | 6.736207 | 4.636718 | 1.015777 |
| H | 3.625971 | 6.667179 | 1.103230 | H | 7.035924 | 4.213563 | 1.898827 |
| H | 5.066800 | 6.457158 | 1.957587 | H | 7.349570 | 4.264701 | 0.285809 |
| N | 6.312592 | -4.459018 | -0.757128 | N | 4.651903 | -6.744489 | -0.767218 |
| H | 6.778358 | -3.578339 | -0.553941 | H | 4.281983 | -7.311246 | 0.000917 |
| H | 6.761676 | -5.246083 | -0.296674 | H | 4.220727 | -7.100064 | -1.624745 |

Cartesian coordinates of equilibrium geometries of C8-$NO_2$ and N9-$NO_2$ substituted derivatives of the $A_4$N3 tetramer

| | C8-$NO_2$ | | | | N9-$NO_2$ | | |
|---|---|---|---|---|---|---|---|
| N | 0.762105 | -2.997601 | -0.002039 | N | 0.799313 | -2.963521 | 0.010903 |
| C | -0.578206 | -2.999225 | -0.059629 | C | -0.534085 | -2.924275 | -0.040614 |
| N | -1.419908 | -4.059815 | -0.036391 | N | -1.403494 | -3.965737 | -0.037838 |
| C | -0.752158 | -5.219820 | 0.061837 | C | -0.762712 | -5.136236 | 0.028657 |
| C | 0.654024 | -5.368452 | 0.135661 | C | 0.624975 | -5.332023 | 0.091592 |
| C | 1.430617 | -4.173428 | 0.096003 | C | 1.437816 | -4.164939 | 0.077500 |
| N | -1.241600 | -6.507720 | 0.119584 | N | -1.276103 | -6.451618 | 0.059465 |
| C | -0.134223 | -7.330055 | 0.224998 | C | -0.176217 | -7.333685 | 0.139607 |
| N | 1.015280 | -6.693851 | 0.238115 | N | 0.957875 | -6.688678 | 0.158914 |
| N | 2.773196 | -4.171586 | 0.153559 | N | 2.780201 | -4.184198 | 0.127636 |
| H | -1.065189 | -2.026954 | -0.123311 | H | -1.005436 | -1.944114 | -0.083269 |
| H | 3.263227 | -5.053825 | 0.235659 | H | -0.329387 | -8.403161 | 0.177467 |
| H | 3.302994 | -3.288643 | 0.115847 | H | 3.269847 | -5.068731 | 0.176567 |
| H | -2.204019 | -6.829164 | 0.094854 | H | 3.315670 | -3.303319 | 0.102994 |
| N | -2.996881 | -0.760308 | -0.014188 | N | -2.964151 | -0.799955 | -0.003116 |
| C | -2.998740 | 0.580316 | 0.037428 | C | -2.923994 | 0.533403 | 0.051222 |
| N | -4.059900 | 1.421416 | 0.020093 | N | -3.964902 | 1.403414 | 0.045906 |
| C | -5.220345 | 0.752481 | -0.064311 | C | -5.135402 | 0.763214 | -0.025804 |
| C | -5.368833 | -0.654287 | -0.127679 | C | -5.332002 | -0.624311 | -0.091174 |
| C | -4.173205 | -1.430091 | -0.096832 | C | -4.165303 | -1.437767 | -0.076350 |
| N | -6.509017 | 1.240749 | -0.114816 | N | -6.450348 | 1.277435 | -0.062302 |
| C | -7.331591 | 0.132135 | -0.204808 | C | -7.332793 | 0.178390 | -0.145793 |
| N | -6.694834 | -1.017016 | -0.213638 | N | -6.688477 | -0.956146 | -0.163219 |
| N | -4.171222 | -2.772999 | -0.149312 | N | -4.184074 | -2.779847 | -0.135836 |
| H | -2.026336 | 1.068241 | 0.091559 | H | -1.943722 | 1.004204 | 0.097293 |
| H | -5.054737 | -3.261589 | -0.218608 | H | -8.402035 | 0.332395 | -0.187213 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | -3.287399 | -3.301608 | -0.118932 | H | -5.069048 | -3.267438 | -0.191756 |
| H | -6.830792 | 2.203143 | -0.094996 | H | -3.302823 | -3.314325 | -0.106735 |
| N | -0.759776 | 2.997737 | 0.003785 | N | -0.801308 | 2.964202 | 0.002640 |
| C | 0.580961 | 2.999483 | -0.044991 | C | 0.531823 | 2.923806 | -0.054912 |
| N | 1.422140 | 4.060497 | -0.024282 | N | 1.402080 | 3.964435 | -0.049171 |
| C | 0.753202 | 5.220823 | 0.061781 | C | 0.762773 | 5.134960 | 0.027703 |
| C | -0.653653 | 5.369347 | 0.123871 | C | -0.624380 | 5.331798 | 0.097495 |
| C | -1.429593 | 4.173903 | 0.087656 | C | -1.438315 | 4.165455 | 0.080041 |
| N | 1.241447 | 6.509371 | 0.114912 | N | 1.277713 | 6.449473 | 0.066958 |
| C | 0.132712 | 7.331824 | 0.205678 | C | 0.179380 | 7.332019 | 0.157047 |
| N | -1.016528 | 6.695149 | 0.213498 | N | -0.955389 | 6.688050 | 0.175580 |
| N | -2.772600 | 4.172406 | 0.136196 | N | -2.780392 | 4.184957 | 0.139416 |
| H | 1.068843 | 2.027051 | -0.099322 | H | 1.001996 | 1.943430 | -0.104446 |
| H | -3.262605 | 5.055664 | 0.201473 | H | 0.333926 | 8.400993 | 0.201928 |
| H | -3.302018 | 3.289220 | 0.098833 | H | -3.268322 | 5.069596 | 0.194413 |
| H | 2.203901 | 6.831136 | 0.096307 | H | -3.315573 | 3.304169 | 0.110295 |
| N | 2.998411 | 0.761256 | 0.009838 | N | 2.962692 | 0.799851 | -0.010968 |
| C | 2.999771 | -0.579197 | 0.064333 | C | 2.923196 | -0.533440 | 0.044959 |
| N | 4.060160 | -1.421043 | 0.038777 | N | 3.964572 | -1.402950 | 0.043495 |
| C | 5.220249 | -0.753228 | -0.059034 | C | 5.135042 | -0.762374 | -0.026927 |
| C | 5.369129 | 0.653158 | -0.129460 | C | 5.331056 | 0.625163 | -0.092985 |
| C | 4.174284 | 1.429862 | -0.087364 | C | 4.163979 | 1.438083 | -0.080767 |
| N | 6.508043 | -1.242721 | -0.119529 | N | 6.450285 | -1.275980 | -0.060856 |
| C | 7.330578 | -0.135184 | -0.221938 | C | 7.332365 | -0.176406 | -0.144076 |
| N | 6.694585 | 1.014456 | -0.231199 | N | 6.687527 | 0.957776 | -0.163494 |
| N | 4.172626 | 2.772612 | -0.141834 | N | 4.182829 | 2.780209 | -0.137051 |
| H | 2.027394 | -1.066136 | 0.126753 | H | 1.943073 | -1.004633 | 0.090026 |
| H | 5.055067 | 3.261640 | -0.224256 | H | 8.401742 | -0.329876 | -0.184184 |
| H | 3.289809 | 3.302394 | -0.103494 | H | 5.067248 | 3.269211 | -0.189890 |
| H | 6.829268 | -2.205281 | -0.098355 | H | 3.301509 | 3.314909 | -0.114036 |
| N | -0.313748 | -8.772510 | 0.311842 | N | -2.665018 | -6.870839 | 0.013885 |
| O | -1.503346 | -9.169775 | 0.271397 | O | -2.843737 | -8.086337 | 0.071053 |
| O | 0.690182 | -9.484238 | 0.416541 | O | -3.498596 | -5.977319 | -0.076619 |
| N | -8.775026 | 0.310163 | -0.281266 | N | -6.868902 | 2.666577 | -0.020123 |
| O | -9.172553 | 1.499879 | -0.253283 | O | -5.975133 | 3.499837 | 0.071509 |
| O | -9.487292 | -0.695415 | -0.365394 | O | -8.084245 | 2.845712 | -0.081468 |
| N | 0.310522 | 8.775079 | 0.283860 | N | 2.666898 | 6.867612 | 0.019941 |
| O | 1.500329 | 9.172635 | 0.255462 | O | 3.499227 | 5.973743 | -0.077366 |
| O | -0.695260 | 9.487189 | 0.369966 | O | 2.846992 | 8.082611 | 0.083466 |
| N | 8.773027 | -0.314698 | -0.309565 | N | 6.869406 | -2.664895 | -0.016419 |
| O | 9.170058 | -1.504488 | -0.274638 | O | 5.975878 | -3.498527 | 0.074912 |
| O | 9.484994 | 0.689537 | -0.409269 | O | 8.084911 | -2.843489 | -0.075710 |

Cartesian coordinates of equilibrium geometries of C8-Cl and N9-Cl substituted derivatives of the $A_4N3$ tetramer

| | | C8-Cl | | | | N9-Cl | |
|---|---|---|---|---|---|---|---|
| N | 0.735872 | -3.022739 | 0.001552 | N | 0.750554 | -3.000770 | 0.025582 |
| C | -0.604686 | -3.017709 | -0.040982 | C | -0.588385 | -2.985604 | -0.048320 |
| N | -1.444221 | -4.079073 | 0.003686 | N | -1.432707 | -4.042876 | -0.080110 |
| C | -0.770387 | -5.236444 | 0.107485 | C | -0.765852 | -5.203982 | -0.023888 |
| C | 0.624595 | -5.389078 | 0.163935 | C | 0.625017 | -5.375259 | 0.060474 |
| C | 1.399902 | -4.202396 | 0.103089 | C | 1.407151 | -4.187659 | 0.080557 |
| N | -1.268537 | -6.530947 | 0.190454 | N | -1.253768 | -6.507534 | -0.031862 |
| C | -0.162179 | -7.363293 | 0.292361 | C | -0.163517 | -7.376446 | 0.045644 |
| N | 0.982729 | -6.733328 | 0.280105 | N | 0.974878 | -6.723459 | 0.102667 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| N | 2.749272 | -4.200213 | 0.145023 | N | 2.753414 | -4.193842 | 0.151967 |
| H | -1.089943 | -2.044803 | -0.109207 | H | -1.070373 | -2.009577 | -0.083291 |
| H | 3.236857 | -5.082346 | 0.228342 | H | -0.305554 | -8.449429 | 0.055169 |
| H | 3.279620 | -3.320679 | 0.093590 | H | 3.238433 | -5.081158 | 0.183702 |
| H | -2.240746 | -6.815872 | 0.184804 | H | 3.288405 | -3.314415 | 0.138125 |
| N | -3.023003 | -0.736871 | 0.004938 | N | -3.000781 | -0.749170 | -0.054412 |
| C | -3.017885 | 0.603669 | 0.049103 | C | -2.985938 | 0.589890 | 0.016383 |
| N | -4.079026 | 1.443303 | 0.002171 | N | -4.043512 | 1.433266 | 0.062817 |
| C | -5.236132 | 0.769550 | -0.105967 | C | -5.204584 | 0.764995 | 0.026242 |
| C | -5.388805 | -0.625426 | -0.164601 | C | -5.375677 | -0.626169 | -0.053033 |
| C | -4.202350 | -1.400849 | -0.101105 | C | -4.187680 | -1.407147 | -0.089621 |
| N | -6.530364 | 1.267822 | -0.191901 | N | -6.508427 | 1.251526 | 0.055516 |
| C | -7.362618 | 0.161568 | -0.297819 | C | -7.377189 | 0.160349 | -0.005700 |
| N | -6.732826 | -0.983411 | -0.285144 | N | -6.724038 | -0.977522 | -0.072013 |
| N | -4.199937 | -2.750172 | -0.145201 | N | -4.193537 | -2.753604 | -0.158298 |
| H | -2.045089 | 1.088727 | 0.121155 | H | -2.010056 | 1.072941 | 0.036162 |
| H | -5.081617 | -3.237535 | -0.229103 | H | -8.450292 | 0.301147 | 0.002854 |
| H | -3.320384 | -3.280377 | -0.090793 | H | -5.080231 | -3.239748 | -0.173201 |
| H | -6.815202 | 2.240068 | -0.185645 | H | -3.313518 | -3.287921 | -0.148095 |
| N | -0.734625 | 3.022148 | 0.009933 | N | -0.750604 | 3.001021 | 0.018315 |
| C | 0.606141 | 3.017981 | -0.026371 | C | 0.588401 | 2.985947 | -0.052749 |
| N | 1.444568 | 4.080436 | 0.013239 | N | 1.432953 | 4.043131 | -0.080998 |
| C | 0.769187 | 5.237984 | 0.105126 | C | 0.766202 | 5.204210 | -0.024574 |
| C | -0.626261 | 5.389787 | 0.153621 | C | -0.624770 | 5.375374 | 0.057239 |
| C | -1.400278 | 4.202084 | 0.098135 | C | -1.407093 | 4.187867 | 0.074218 |
| N | 1.265581 | 6.533633 | 0.180480 | N | 1.254324 | 6.507661 | -0.029855 |
| C | 0.157895 | 7.365681 | 0.270801 | C | 0.163994 | 7.376516 | 0.046691 |
| N | -0.986319 | 6.734537 | 0.257595 | N | -0.974509 | 6.723524 | 0.100749 |
| N | -2.749827 | 4.199375 | 0.131260 | N | -2.753357 | 4.194113 | 0.143619 |
| H | 1.092494 | 2.044993 | -0.085831 | H | 1.070260 | 2.009970 | -0.087726 |
| H | -3.237903 | 5.081563 | 0.208447 | H | 0.306170 | 8.449421 | 0.057887 |
| H | -3.279400 | 3.318847 | 0.087959 | H | -3.238048 | 5.081164 | 0.177987 |
| H | 2.237505 | 6.819578 | 0.177394 | H | -3.288452 | 3.314711 | 0.130142 |
| N | 3.024148 | 0.735724 | 0.010038 | N | 3.000558 | 0.749679 | -0.049984 |
| C | 3.019251 | -0.604879 | 0.051882 | C | 2.985436 | -0.589335 | 0.023553 |
| N | 4.080424 | -1.444418 | 0.003567 | N | 4.042949 | -1.432930 | 0.067082 |
| C | 5.237491 | -0.770519 | -0.103449 | C | 5.204108 | -0.765098 | 0.024151 |
| C | 5.389954 | 0.624506 | -0.160268 | C | 5.375463 | 0.625891 | -0.058519 |
| C | 4.203466 | 1.399811 | -0.095374 | C | 4.187540 | 1.407221 | -0.091486 |
| N | 6.531811 | -1.268639 | -0.189286 | N | 6.507947 | -1.252058 | 0.047943 |
| C | 7.363907 | -0.162163 | -0.293428 | C | 7.376896 | -0.161336 | -0.019435 |
| N | 6.734000 | 0.982749 | -0.279855 | N | 6.723825 | 0.976700 | -0.084463 |
| N | 4.201142 | 2.749275 | -0.136996 | N | 4.193563 | 2.753583 | -0.163226 |
| H | 2.046486 | -1.090028 | 0.122572 | H | 2.009430 | -1.072067 | 0.048042 |
| H | 5.082707 | 3.236817 | -0.222991 | H | 8.450014 | -0.302514 | -0.015937 |
| H | 3.321840 | 3.279568 | -0.082209 | H | 5.080653 | 3.239094 | -0.183643 |
| H | 6.816849 | -2.240830 | -0.183460 | H | 3.313686 | 3.288034 | -0.150667 |
| Cl | -0.375914 | -9.078668 | 0.425418 | Cl | -2.917291 | -6.962519 | -0.142977 |
| Cl | -9.077717 | 0.375499 | -0.435187 | Cl | -6.963283 | 2.914761 | 0.170198 |
| Cl | 0.369353 | 9.082260 | 0.392924 | Cl | 2.918087 | 6.962663 | -0.137239 |
| Cl | 9.079134 | -0.375840 | -0.430009 | Cl | 6.962710 | -2.915222 | 0.163645 |

Cartesian coordinates of equilibrium geometries of C8-F and N9-F substituted derivatives of the $A_4N3$ tetramer

| | C8-F | | | | N9-F | | |
|---|---|---|---|---|---|---|---|
| N | 0.739801 | -3.017661 | 0.023226 | N | 0.763584 | -2.996309 | 0.002570 |
| C | -0.599853 | -3.009637 | -0.011493 | C | -0.576530 | -2.980047 | -0.046231 |
| N | -1.438694 | -4.073142 | 0.012762 | N | -1.427185 | -4.031583 | -0.004670 |
| C | -0.763794 | -5.230032 | 0.083287 | C | -0.756809 | -5.188193 | 0.103031 |
| C | 0.630717 | -5.385752 | 0.126962 | C | 0.637590 | -5.365836 | 0.168493 |
| C | 1.404671 | -4.200468 | 0.091961 | C | 1.420346 | -4.179643 | 0.108859 |
| N | -1.265313 | -6.531714 | 0.131811 | N | -1.213697 | -6.488558 | 0.184631 |
| C | -0.154187 | -7.347460 | 0.200078 | C | -0.152927 | -7.368799 | 0.294530 |
| N | 0.990664 | -6.740493 | 0.200299 | N | 0.988374 | -6.708910 | 0.285133 |
| N | 2.755279 | -4.197381 | 0.126455 | N | 2.766255 | -4.184003 | 0.156925 |
| H | -1.086299 | -2.036316 | -0.058725 | H | -1.056271 | -2.005053 | -0.118455 |
| H | 3.243339 | -5.081472 | 0.177200 | H | -0.305901 | -8.436860 | 0.372263 |
| H | 3.283023 | -3.316058 | 0.083706 | H | 3.252828 | -5.067478 | 0.234328 |
| H | -2.235529 | -6.823303 | 0.124568 | H | 3.298104 | -3.304058 | 0.098595 |
| N | -3.018162 | -0.740259 | -0.010856 | N | -2.995109 | -0.763189 | -0.014299 |
| C | -3.009933 | 0.599373 | 0.027992 | C | -2.978835 | 0.576973 | 0.032262 |
| N | -4.073045 | 1.438532 | -0.000786 | N | -4.030759 | 1.427394 | -0.004255 |
| C | -5.229751 | 0.764198 | -0.081001 | C | -5.187875 | 0.756605 | -0.104501 |
| C | -5.385599 | -0.630141 | -0.129743 | C | -5.365617 | -0.637943 | -0.166291 |
| C | -4.200751 | -1.404525 | -0.089080 | C | -4.178959 | -1.420351 | -0.112148 |
| N | -6.530926 | 1.266236 | -0.138032 | N | -6.488813 | 1.213007 | -0.179818 |
| C | -7.346494 | 0.155551 | -0.215711 | C | -7.369472 | 0.151816 | -0.282164 |
| N | -6.739839 | -0.989519 | -0.214703 | N | -6.709311 | -0.989301 | -0.274711 |
| N | -4.198055 | -2.755075 | -0.127867 | N | -4.183277 | -2.766273 | -0.157549 |
| H | -2.036636 | 1.085462 | 0.082124 | H | -2.003654 | 1.057069 | 0.098500 |
| H | -5.081245 | -3.243130 | -0.183723 | H | -8.438022 | 0.304374 | -0.353700 |
| H | -3.316966 | -3.282884 | -0.080948 | H | -5.067368 | -3.252562 | -0.230954 |
| H | -6.822278 | 2.236540 | -0.130273 | H | -3.302787 | -3.297696 | -0.105067 |
| N | -0.740405 | 3.018024 | 0.016186 | N | -0.764132 | 2.995690 | 0.005576 |
| C | 0.599085 | 3.009878 | -0.024271 | C | 0.576001 | 2.979297 | -0.042590 |
| N | 1.438278 | 4.073071 | 0.002353 | N | 1.426641 | 4.030867 | -0.001592 |
| C | 0.764156 | 5.229836 | 0.082086 | C | 0.756146 | 5.187576 | 0.105860 |
| C | -0.630052 | 5.385626 | 0.132595 | C | -0.638321 | 5.365271 | 0.171047 |
| C | -1.404473 | 4.200715 | 0.094059 | C | -1.421040 | 4.179089 | 0.110799 |
| N | 1.266289 | 6.531057 | 0.136166 | N | 1.212833 | 6.488023 | 0.186444 |
| C | 0.155710 | 7.346659 | 0.214466 | C | 0.151888 | 7.368409 | 0.296126 |
| N | -0.989343 | 6.739991 | 0.216514 | N | -0.989348 | 6.708495 | 0.287637 |
| N | -2.754949 | 4.198048 | 0.133955 | N | -2.766928 | 4.183642 | 0.156679 |
| H | 1.085012 | 2.036614 | -0.078114 | H | 1.055776 | 2.004272 | -0.114333 |
| H | -3.243627 | 5.081290 | 0.190112 | H | 0.304730 | 8.436574 | 0.373018 |
| H | -3.282981 | 3.317014 | 0.088943 | H | -3.253758 | 5.067018 | 0.233184 |
| H | 2.236566 | 6.822442 | 0.126356 | H | -3.299151 | 3.303866 | 0.097834 |
| N | 3.017216 | 0.740152 | -0.023805 | N | 2.995683 | 0.763263 | -0.016892 |
| C | 3.009062 | -0.599374 | 0.013173 | C | 2.979473 | -0.576971 | 0.029743 |
| N | 4.072416 | -1.438452 | -0.011124 | N | 4.031597 | -1.427219 | -0.005630 |
| C | 5.229369 | -0.764052 | -0.084091 | C | 5.188629 | -0.756202 | -0.105289 |
| C | 5.385218 | 0.630266 | -0.130128 | C | 5.366259 | 0.638387 | -0.167969 |
| C | 4.200153 | 1.404549 | -0.094923 | C | 4.179588 | 1.420718 | -0.113762 |
| N | 6.530830 | -1.265998 | -0.133375 | N | 6.489790 | -1.212319 | -0.178563 |
| C | 7.346685 | -0.155227 | -0.204520 | C | 7.370383 | -0.151019 | -0.281023 |
| N | 6.739958 | 0.989725 | -0.206000 | N | 6.709981 | 0.989975 | -0.275223 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| N | 4.197476 | 2.755104 | -0.130804 | N | 4.184269 | 2.766782 | -0.156623 |
| H | 2.035717 | -1.085516 | 0.062578 | H | 2.004216 | -1.057257 | 0.095370 |
| H | 5.081242 | 3.243122 | -0.183505 | H | 8.439041 | -0.303405 | -0.351519 |
| H | 3.316293 | 3.283178 | -0.089199 | H | 5.067597 | 3.253943 | -0.232891 |
| H | 6.822199 | -2.236258 | -0.125286 | H | 3.303664 | 3.298376 | -0.103272 |
| F | -0.334902 | -8.674415 | 0.260215 | F | -2.560773 | -6.862075 | 0.168551 |
| F | -8.672847 | 0.336831 | -0.285824 | F | -6.862439 | 2.560066 | -0.165257 |
| F | 0.337078 | 8.673092 | 0.281927 | F | 2.559943 | 6.861481 | 0.170409 |
| F | 8.673424 | -0.336463 | -0.266202 | F | 6.863856 | -2.559209 | -0.161154 |

Cartesian coordinates of equilibrium geometries of C8-H / N9-H substituted derivatives of the $A_4N3$ tetramer

C8-H / N9-H

| | | | |
|---|---|---|---|
| N | 0.736640 | -3.015814 | 0.007581 |
| C | -0.605347 | -3.011075 | -0.027876 |
| N | -1.443541 | -4.071621 | 0.011378 |
| C | -0.769091 | -5.232895 | 0.100710 |
| C | 0.626882 | -5.386283 | 0.148535 |
| C | 1.399524 | -4.196133 | 0.094868 |
| N | -1.265048 | -6.524378 | 0.171611 |
| C | -0.167218 | -7.372604 | 0.258535 |
| N | 0.981700 | -6.728928 | 0.246885 |
| N | 2.749669 | -4.194339 | 0.129786 |
| H | -1.090573 | -2.037506 | -0.086329 |
| H | -0.286596 | -8.447247 | 0.327640 |
| H | 3.234053 | -5.079048 | 0.202607 |
| H | 3.280720 | -3.314275 | 0.082310 |
| N | -3.016778 | -0.737370 | 0.006564 |
| C | -3.012008 | 0.604562 | 0.044687 |
| N | -4.071994 | 1.443060 | -0.002410 |
| C | -5.232580 | 0.768955 | -0.103467 |
| C | -5.385806 | -0.626900 | -0.155171 |
| C | -4.196417 | -1.399912 | -0.092440 |
| N | -6.523309 | 1.265306 | -0.185121 |
| C | -7.371055 | 0.167706 | -0.280847 |
| N | -6.727776 | -0.981344 | -0.265766 |
| N | -4.194611 | -2.750067 | -0.129595 |
| H | -2.038794 | 1.089435 | 0.112293 |
| H | -8.445018 | 0.287424 | -0.358721 |
| H | -5.078529 | -3.233660 | -0.213214 |
| H | -3.314778 | -3.281229 | -0.079444 |
| N | -0.736728 | 3.016131 | 0.010790 |
| C | 0.605261 | 3.011474 | -0.026603 |
| N | 1.443385 | 4.072138 | 0.011726 |
| C | 0.768900 | 5.233386 | 0.102074 |
| C | -0.627031 | 5.386661 | 0.152017 |
| C | -1.399641 | 4.196442 | 0.099159 |
| N | 1.264762 | 6.524978 | 0.172278 |
| C | 0.166990 | 7.373172 | 0.260550 |
| N | -0.981848 | 6.729326 | 0.250676 |
| N | -2.749781 | 4.194499 | 0.135871 |
| H | 1.090505 | 2.037889 | -0.086310 |
| H | 0.286346 | 8.447865 | 0.329259 |
| H | -3.234262 | 5.078788 | 0.209967 |
| H | -3.280793 | 3.314494 | 0.087313 |

| | | | |
|---|---|---|---|
| N | 3.016311 | 0.736870 | 0.001849 |
| C | 3.011319 | -0.605137 | 0.038303 |
| N | 4.071439 | -1.443575 | -0.005104 |
| C | 5.232492 | -0.769383 | -0.100513 |
| C | 5.386105 | 0.626547 | -0.149725 |
| C | 4.196389 | 1.399479 | -0.091032 |
| N | 6.523496 | -1.265647 | -0.177696 |
| C | 7.371734 | -0.167980 | -0.268906 |
| N | 6.728484 | 0.981133 | -0.254912 |
| N | 4.194959 | 2.749614 | -0.126594 |
| H | 2.037898 | -1.090078 | 0.101601 |
| H | 8.445996 | -0.287607 | -0.343129 |
| H | 5.079852 | 3.233289 | -0.199854 |
| H | 3.315321 | 3.281052 | -0.076882 |
| H | -2.243081 | -6.788354 | 0.165498 |
| H | -6.787082 | 2.243397 | -0.180026 |
| H | 2.242740 | 6.789070 | 0.164662 |
| H | 6.787239 | -2.243751 | -0.171897 |

Cartesian coordinates of equilibrium geometries of C8-Me and N9-Me substituted derivatives of the $A_4N3$ tetramer

| | C8-Me | | | | N9-Me | | |
|---|---|---|---|---|---|---|---|
| N | 0.732237 | -3.021613 | -0.022270 | N | 0.755783 | -3.006819 | -0.000775 |
| C | -0.608990 | -3.015581 | -0.058305 | C | -0.585663 | -2.998129 | -0.052526 |
| N | -1.446970 | -4.078168 | -0.032672 | N | -1.425401 | -4.057645 | -0.028369 |
| C | -0.772202 | -5.239504 | 0.039093 | C | -0.752688 | -5.220685 | 0.062833 |
| C | 0.622727 | -5.393774 | 0.083772 | C | 0.642646 | -5.377828 | 0.127562 |
| C | 1.394265 | -4.204591 | 0.049791 | C | 1.416487 | -4.188486 | 0.089599 |
| N | -1.266826 | -6.532808 | 0.092292 | N | -1.268580 | -6.505177 | 0.118594 |
| C | -0.171509 | -7.395189 | 0.167683 | C | -0.171191 | -7.354237 | 0.213815 |
| N | 0.974719 | -6.739358 | 0.163192 | N | 0.986601 | -6.721846 | 0.221067 |
| N | 2.745880 | -4.201695 | 0.090177 | N | 2.767106 | -4.183831 | 0.143522 |
| H | -1.094788 | -2.041599 | -0.104275 | H | -1.069028 | -2.023903 | -0.110610 |
| H | 3.230215 | -5.086401 | 0.157632 | H | -0.301935 | -8.428930 | 0.274131 |
| H | 3.276076 | -3.320683 | 0.067603 | H | 3.252496 | -5.068013 | 0.214872 |
| H | -2.245674 | -6.793505 | 0.082782 | H | 3.294000 | -3.300243 | 0.102420 |
| N | -3.019974 | -0.732317 | 0.012827 | N | -3.005350 | -0.754919 | 0.001755 |
| C | -3.013800 | 0.608991 | 0.045653 | C | -2.996188 | 0.586772 | 0.047389 |
| N | -4.076403 | 1.446968 | 0.021265 | N | -4.055776 | 1.426463 | 0.023419 |
| C | -5.238042 | 0.772086 | -0.045303 | C | -5.219304 | 0.753463 | -0.060267 |
| C | -5.392599 | -0.623036 | -0.086061 | C | -5.377050 | -0.642276 | -0.116422 |
| C | -4.203272 | -1.394489 | -0.053852 | C | -4.187579 | -1.416006 | -0.079737 |
| N | -6.531366 | 1.266731 | -0.095106 | N | -6.503725 | 1.269312 | -0.115802 |
| C | -7.394209 | 0.171299 | -0.164960 | C | -7.353447 | 0.171564 | -0.201830 |
| N | -6.738568 | -0.975020 | -0.160448 | N | -6.721427 | -0.986453 | -0.204900 |
| N | -4.200223 | -2.746157 | -0.090572 | N | -4.183767 | -2.766918 | -0.125748 |
| H | -2.039671 | 1.094824 | 0.088222 | H | -2.021728 | 1.070396 | 0.100724 |
| H | -5.085469 | -3.230737 | -0.154806 | H | -8.428246 | 0.302280 | -0.259778 |
| H | -3.319148 | -3.276376 | -0.069291 | H | -5.068643 | -3.252045 | -0.190362 |
| H | -6.791848 | 2.245660 | -0.086598 | H | -3.300051 | -3.294135 | -0.093743 |
| N | -0.732565 | 3.021460 | -0.020126 | N | -0.755398 | 3.006740 | -0.005826 |
| C | 0.608616 | 3.015658 | -0.057328 | C | 0.586124 | 2.997855 | -0.054508 |
| N | 1.446431 | 4.078345 | -0.031358 | N | 1.425970 | 4.057277 | -0.028449 |
| C | 0.771539 | 5.239528 | 0.041603 | C | 0.753191 | 5.220472 | 0.061465 |
| C | -0.623384 | 5.393567 | 0.087250 | C | -0.642364 | 5.377880 | 0.122029 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | -1.394776 | 4.204283 | 0.053458 | C | -1.416234 | 4.188647 | 0.082364 |
| N | 1.266011 | 6.532892 | 0.094553 | N | 1.269235 | 6.504699 | 0.120126 |
| C | 0.170607 | 7.395125 | 0.169892 | C | 0.171693 | 7.354021 | 0.212825 |
| N | -0.975490 | 6.739116 | 0.166587 | N | -0.986262 | 6.721973 | 0.216166 |
| N | -2.746309 | 4.200816 | 0.096340 | N | -2.767023 | 4.184216 | 0.131734 |
| H | 1.094432 | 2.041721 | -0.104560 | H | 1.069508 | 2.023585 | -0.111837 |
| H | -3.231065 | 5.085320 | 0.165050 | H | 0.302585 | 8.428603 | 0.274448 |
| H | -3.275810 | 3.319385 | 0.069100 | H | -3.251776 | 5.068736 | 0.205306 |
| H | 2.244787 | 6.793748 | 0.084602 | H | -3.293518 | 3.300176 | 0.097104 |
| N | 3.020398 | 0.731513 | 0.013899 | N | 3.005232 | 0.755981 | -0.000473 |
| C | 3.014749 | -0.609715 | 0.050451 | C | 2.996024 | -0.585539 | 0.048500 |
| N | 4.077713 | -1.447301 | 0.028384 | N | 4.055311 | -1.425594 | 0.023217 |
| C | 5.239031 | -0.772095 | -0.040555 | C | 5.218663 | -0.753038 | -0.066661 |
| C | 5.392959 | 0.622884 | -0.085196 | C | 5.376355 | 0.642397 | -0.128426 |
| C | 4.203412 | 1.393996 | -0.054675 | C | 4.187324 | 1.416568 | -0.088549 |
| N | 6.532664 | -1.266236 | -0.090324 | N | 6.502945 | -1.269243 | -0.123425 |
| C | 7.394833 | -0.170589 | -0.163757 | C | 7.352526 | -0.171921 | -0.216323 |
| N | 6.738629 | 0.975405 | -0.161438 | N | 6.720622 | 0.986094 | -0.221712 |
| N | 4.200092 | 2.745636 | -0.095416 | N | 4.183511 | 2.767381 | -0.136596 |
| H | 2.040785 | -1.095836 | 0.093785 | H | 2.021658 | -1.068780 | 0.105664 |
| H | 5.085534 | 3.229447 | -0.160683 | H | 8.427197 | -0.302974 | -0.276500 |
| H | 3.318881 | 3.275471 | -0.074549 | H | 5.067324 | 3.252380 | -0.213723 |
| H | 6.793693 | -2.245009 | -0.079967 | H | 3.299804 | 3.294518 | -0.100844 |
| C | -0.334431 | -8.880640 | 0.246125 | C | -2.685368 | -6.858440 | 0.084460 |
| H | -0.897642 | -9.174080 | 1.142510 | H | -3.204749 | -6.428771 | 0.948137 |
| H | -0.870598 | -9.271363 | -0.629403 | H | -3.146304 | -6.474132 | -0.831953 |
| H | 0.654535 | -9.343841 | 0.286975 | H | -2.782040 | -7.947012 | 0.108591 |
| C | -8.879845 | 0.334534 | -0.238355 | C | -6.856147 | 2.686573 | -0.090600 |
| H | -9.266793 | 0.875286 | 0.636057 | H | -6.484282 | 3.150801 | 0.829390 |
| H | -9.176453 | 0.893516 | -1.136402 | H | -6.413833 | 3.202134 | -0.950171 |
| H | -9.343801 | -0.654409 | -0.272493 | H | -7.944181 | 2.784126 | -0.130546 |
| C | 0.333477 | 8.880688 | 0.246090 | C | 2.686452 | 6.857183 | 0.094391 |
| H | 0.897030 | 9.175666 | 1.141728 | H | 3.201797 | 6.419372 | 0.956437 |
| H | 0.869280 | 9.269933 | -0.630329 | H | 3.150967 | 6.480597 | -0.823495 |
| H | -0.655516 | 9.343820 | 0.286498 | H | 2.783851 | 7.945441 | 0.128608 |
| C | 8.880569 | -0.332924 | -0.238221 | C | 6.855348 | -2.686373 | -0.093948 |
| H | 9.269617 | -0.865678 | 0.640133 | H | 6.477024 | -3.148851 | 0.824241 |
| H | 9.176358 | -0.899162 | -1.131881 | H | 6.419231 | -3.203676 | -0.955650 |
| H | 9.343244 | 0.656158 | -0.281517 | H | 7.943653 | -2.783808 | -0.125821 |

Cartesian coordinates of equilibrium geometries of C8-$NH_2$ and N9-$NH_2$ substituted derivatives of the $A_4$N3 tetramer

| | C8-$NH_2$ | | | | N9-$NH_2$ | | |
|---|---|---|---|---|---|---|---|
| N | 0.713832 | -3.025822 | 0.124576 | N | 0.781520 | -2.992879 | -0.423647 |
| C | -0.625599 | -3.015279 | 0.090101 | C | -0.560517 | -2.987877 | -0.419921 |
| N | -1.461049 | -4.080932 | 0.022071 | N | -1.394812 | -4.041796 | -0.258847 |
| C | -0.784341 | -5.239080 | -0.002709 | C | -0.711661 | -5.187804 | -0.095307 |
| C | 0.608360 | -5.398061 | 0.032150 | C | 0.682528 | -5.344126 | -0.076640 |
| C | 1.376509 | -4.211565 | 0.094531 | C | 1.449191 | -4.162125 | -0.247408 |
| N | -1.286967 | -6.537786 | -0.079437 | N | -1.209473 | -6.471261 | 0.092330 |
| C | -0.185198 | -7.389531 | -0.078094 | C | -0.111177 | -7.315905 | 0.211029 |
| N | 0.965440 | -6.749434 | -0.025216 | N | 1.037775 | -6.677120 | 0.117547 |
| N | 2.730938 | -4.209896 | 0.126162 | N | 2.800710 | -4.155773 | -0.246256 |
| H | -1.114002 | -2.042077 | 0.118197 | H | -1.050856 | -2.024779 | -0.555508 |
| H | 3.217582 | -5.095396 | 0.099190 | H | -0.250876 | -8.379172 | 0.363267 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | 3.260220 | -3.328662 | 0.134098 | H | 3.285215 | -5.028915 | -0.086740 |
| H | -2.262315 | -6.800546 | -0.006126 | H | 3.323890 | -3.270859 | -0.296830 |
| N | -3.025267 | -0.723413 | 0.103739 | N | -3.031021 | -0.772975 | -0.466190 |
| C | -3.007654 | 0.615526 | 0.148773 | C | -3.036565 | 0.567949 | -0.514891 |
| N | -4.067503 | 1.459197 | 0.098135 | N | -4.084941 | 1.401927 | -0.320944 |
| C | -5.226812 | 0.792106 | -0.004028 | C | -5.212675 | 0.719338 | -0.058289 |
| C | -5.392797 | -0.599073 | -0.059250 | C | -5.355373 | -0.673818 | 0.027944 |
| C | -4.211855 | -1.376439 | -0.002500 | C | -4.180999 | -1.439656 | -0.188447 |
| N | -6.519578 | 1.306794 | -0.092615 | N | -6.485584 | 1.216611 | 0.193871 |
| C | -7.375738 | 0.212889 | -0.191038 | C | -7.310596 | 0.118958 | 0.414296 |
| N | -6.742938 | -0.943025 | -0.185332 | N | -6.669622 | -1.028934 | 0.325829 |
| N | -4.215741 | -2.730497 | -0.053724 | N | -4.162316 | -2.790590 | -0.135409 |
| H | -2.033167 | 1.096049 | 0.225121 | H | -2.084368 | 1.057057 | -0.715823 |
| H | -5.101476 | -3.209832 | -0.130807 | H | -8.362546 | 0.258200 | 0.631899 |
| H | -3.338703 | -3.265355 | -0.023010 | H | -5.006925 | -3.270429 | 0.145406 |
| H | -6.779402 | 2.279288 | 0.019317 | H | -3.271621 | -3.303204 | -0.199066 |
| N | -0.712792 | 3.026204 | 0.124109 | N | -0.783207 | 2.998178 | -0.466459 |
| C | 0.626837 | 3.016325 | 0.095469 | C | 0.558781 | 2.991970 | -0.470568 |
| N | 1.462081 | 4.082208 | 0.027569 | N | 1.394790 | 4.040751 | -0.287247 |
| C | 0.784921 | 5.240028 | -0.002902 | C | 0.713759 | 5.182591 | -0.090367 |
| C | -0.607992 | 5.398305 | 0.025927 | C | -0.680011 | 5.339513 | -0.059663 |
| C | -1.375903 | 4.211585 | 0.087749 | C | -1.448768 | 4.162970 | -0.255475 |
| N | 1.287105 | 6.538842 | -0.080724 | N | 1.214105 | 6.460006 | 0.129238 |
| C | 0.184818 | 7.389929 | -0.086092 | C | 0.117129 | 7.301972 | 0.277661 |
| N | -0.965621 | 6.749283 | -0.036557 | N | -1.032936 | 6.667251 | 0.172764 |
| N | -2.730461 | 4.209697 | 0.113060 | N | -2.800456 | 4.157672 | -0.245293 |
| H | 1.115574 | 2.043401 | 0.128478 | H | 1.047678 | 2.031809 | -0.629701 |
| H | -3.217340 | 5.095151 | 0.076959 | H | 0.258687 | 8.360444 | 0.458838 |
| H | -3.259788 | 3.328455 | 0.120319 | H | -3.282080 | 5.023738 | -0.043927 |
| H | 2.261897 | 6.802501 | -0.002633 | H | -3.323943 | 3.272888 | -0.298265 |
| N | 3.026353 | 0.723514 | 0.119755 | N | 3.028697 | 0.774694 | -0.482278 |
| C | 3.008886 | -0.615427 | 0.166235 | C | 3.034954 | -0.566467 | -0.522219 |
| N | 4.068314 | -1.459256 | 0.110393 | N | 4.083782 | -1.398995 | -0.324590 |
| C | 5.227122 | -0.792449 | 0.000992 | C | 5.211220 | -0.714237 | -0.066198 |
| C | 5.392879 | 0.598638 | -0.056508 | C | 5.353247 | 0.679469 | 0.011622 |
| C | 4.212386 | 1.376220 | 0.006077 | C | 4.178680 | 1.443598 | -0.209697 |
| N | 6.519191 | -1.307390 | -0.095055 | N | 6.482807 | -1.209517 | 0.196061 |
| C | 7.374878 | -0.213616 | -0.200045 | C | 7.306151 | -0.110242 | 0.415261 |
| N | 6.742239 | 0.942340 | -0.191595 | N | 6.665846 | 1.036981 | 0.313709 |
| N | 4.216484 | 2.730241 | -0.046421 | N | 4.159418 | 2.794566 | -0.163567 |
| H | 2.034688 | -1.095750 | 0.247455 | H | 2.082487 | -1.057201 | -0.716566 |
| H | 5.102097 | 3.209392 | -0.129351 | H | 8.356477 | -0.247895 | 0.641754 |
| H | 3.339851 | 3.265576 | -0.013919 | H | 5.006663 | 3.277384 | 0.104724 |
| H | 6.779699 | -2.279693 | 0.017224 | H | 3.268563 | 3.307029 | -0.227233 |
| N | -0.345634 | -8.770839 | -0.060074 | N | -2.558989 | -6.889890 | 0.150529 |
| H | -1.049590 | -9.136227 | -0.696802 | H | -3.008251 | -6.402440 | 0.929861 |
| H | 0.544427 | -9.250731 | -0.167612 | H | -3.021496 | -6.583435 | -0.709250 |
| N | -8.755609 | 0.381653 | -0.214991 | N | -6.912044 | 2.564579 | 0.224020 |
| H | -9.093331 | 1.130413 | -0.815172 | H | -6.369306 | 3.053010 | 0.941079 |
| H | -9.236491 | -0.495636 | -0.398124 | H | -6.678541 | 2.988652 | -0.677432 |
| N | 0.344430 | 8.771487 | -0.070264 | N | 2.564233 | 6.874414 | 0.197726 |
| H | 1.048027 | 9.135923 | -0.707794 | H | 3.014673 | 6.361408 | 0.960226 |
| H | -0.546043 | 9.249914 | -0.180362 | H | 3.024176 | 6.597084 | -0.672983 |
| N | 8.754520 | -0.382644 | -0.233116 | N | 6.908357 | -2.557403 | 0.242269 |
| H | 9.088139 | -1.131583 | -0.834948 | H | 6.332327 | -3.046061 | 0.932851 |
| H | 9.233973 | 0.493867 | -0.420221 | H | 6.716037 | -2.980884 | -0.669705 |

Cartesian coordinates of equilibrium geometries of C2-$NO_2$ and N9-$NO_2$ substituted derivatives of the $A_4N7$ tetramer

| | C2-$NO_2$ | | | | N9-$NO_2$ | | |
|---|---|---|---|---|---|---|---|
| N | -2.882640 | -4.070288 | 0.112133 | N | -3.068526 | -4.272155 | -0.041273 |
| C | -2.941541 | -5.388763 | 0.234678 | C | -3.117654 | -5.616488 | -0.043280 |
| N | -1.987965 | -6.313372 | 0.262797 | N | -2.099527 | -6.502509 | -0.010282 |
| C | -0.779413 | -5.734954 | 0.160238 | C | -0.917402 | -5.885231 | 0.025904 |
| C | -0.532251 | -4.357882 | 0.035753 | C | -0.702488 | -4.500784 | 0.033213 |
| C | -1.658911 | -3.500939 | -0.006785 | C | -1.851892 | -3.672570 | 0.000013 |
| N | 0.480399 | -6.316385 | 0.166491 | N | 0.396124 | -6.411100 | 0.069403 |
| C | 1.406070 | -5.293324 | 0.060873 | C | 1.290475 | -5.336719 | 0.097697 |
| N | 0.825715 | -4.106441 | -0.016880 | N | 0.657454 | -4.188920 | 0.075236 |
| N | -1.573983 | -2.160288 | -0.146981 | N | -1.770637 | -2.324778 | 0.008828 |
| H | 2.479965 | -5.453698 | 0.045689 | H | -4.115923 | -6.051269 | -0.075084 |
| H | -0.705109 | -1.761276 | -0.475273 | H | 2.363162 | -5.475276 | 0.128921 |
| H | -2.461917 | -1.623706 | -0.173139 | H | -0.856762 | -1.897639 | 0.054932 |
| H | 0.677690 | -7.308568 | 0.243331 | H | -2.617938 | -1.737320 | -0.018678 |
| N | -4.069601 | 2.882747 | -0.108369 | N | -4.269261 | 3.068450 | 0.047739 |
| C | -5.387709 | 2.942153 | -0.234254 | C | -5.613508 | 3.119722 | 0.044813 |
| N | -6.312608 | 1.988953 | -0.264933 | N | -6.500908 | 2.102995 | 0.007368 |
| C | -5.734892 | 0.780157 | -0.161235 | C | -5.885315 | 0.919983 | -0.027796 |
| C | -4.358258 | 0.532423 | -0.033226 | C | -4.501164 | 0.702842 | -0.030523 |
| C | -3.500980 | 1.658763 | 0.011861 | C | -3.671370 | 1.851003 | 0.007257 |
| N | -6.316771 | -0.479431 | -0.169790 | N | -6.413184 | -0.392578 | -0.075341 |
| C | -5.294333 | -1.405535 | -0.061938 | C | -5.340118 | -1.288676 | -0.099235 |
| N | -4.107454 | -0.825677 | 0.019281 | N | -4.191380 | -0.657575 | -0.073196 |
| N | -2.160841 | 1.573475 | 0.155746 | N | -2.323612 | 1.767940 | 0.004498 |
| H | -5.455179 | -2.479369 | -0.047812 | H | -6.046811 | 4.118648 | 0.076166 |
| H | -1.762233 | 0.703953 | 0.482735 | H | -5.480474 | -2.361055 | -0.131018 |
| H | -1.623625 | 2.461028 | 0.180669 | H | -1.897131 | 0.853915 | -0.045368 |
| H | -7.308830 | -0.676290 | -0.249381 | H | -1.735072 | 2.614982 | 0.030079 |
| N | 2.882582 | 4.070264 | 0.109697 | N | 3.068087 | 4.268739 | -0.052181 |
| C | 2.941529 | 5.388695 | 0.232607 | C | 3.118498 | 5.613055 | -0.052276 |
| N | 1.987943 | 6.313257 | 0.261952 | N | 2.101464 | 6.500017 | -0.012387 |
| C | 0.779309 | 5.734802 | 0.160488 | C | 0.918942 | 5.883824 | 0.029230 |
| C | 0.532088 | 4.357761 | 0.035879 | C | 0.702748 | 4.499607 | 0.035463 |
| C | 1.658752 | 3.500887 | -0.008201 | C | 1.851121 | 3.670275 | -0.005292 |
| N | -0.480528 | 6.316163 | 0.168234 | N | -0.393852 | 6.410902 | 0.080291 |
| C | -1.406263 | 5.293088 | 0.063272 | C | -1.289090 | 5.337270 | 0.110540 |
| N | -0.825922 | 4.106256 | -0.015358 | N | -0.657276 | 4.188899 | 0.083090 |
| N | 1.573835 | 2.160366 | -0.149094 | N | 1.768542 | 2.322541 | 0.000440 |
| H | -2.480180 | 5.453419 | 0.049114 | H | 4.116977 | 6.046914 | -0.088712 |
| H | 0.704345 | 1.761120 | -0.475457 | H | -2.361482 | 5.476894 | 0.146578 |
| H | 2.461653 | 1.623622 | -0.175192 | H | 0.854619 | 1.896510 | 0.056718 |
| H | -0.677785 | 7.308323 | 0.245476 | H | 2.614903 | 1.734327 | -0.028815 |
| N | 4.069890 | -2.882717 | -0.110295 | N | 4.268873 | -3.067405 | 0.043529 |
| C | 5.388126 | -2.942008 | -0.235057 | C | 5.613160 | -3.118274 | 0.042965 |
| N | 6.312924 | -1.988693 | -0.265361 | N | 6.500388 | -2.101387 | 0.005798 |
| C | 5.734977 | -0.779935 | -0.162484 | C | 5.884552 | -0.918581 | -0.032125 |
| C | 4.358212 | -0.532347 | -0.035553 | C | 4.500373 | -0.701914 | -0.037540 |
| C | 3.501038 | -1.658775 | 0.009078 | C | 3.670746 | -1.850149 | 0.000751 |
| N | 6.316694 | 0.479729 | -0.170809 | N | 6.412035 | 0.394127 | -0.080474 |
| C | 5.294064 | 1.405727 | -0.063885 | C | 5.338702 | 1.289798 | -0.107758 |
| N | 4.107200 | 0.825725 | 0.016556 | N | 4.190191 | 0.658268 | -0.082678 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| N | 2.160721 | -1.573539 | 0.151646 | N | 2.323012 | -1.767192 | -0.003286 |
| H | 5.454755 | 2.479586 | -0.049804 | H | 6.046686 | -4.117028 | 0.076303 |
| H | 1.762043 | -0.704193 | 0.479022 | H | 5.478529 | 2.362204 | -0.140986 |
| H | 1.623703 | -2.461203 | 0.177429 | H | 1.896691 | -0.853234 | -0.055640 |
| H | 7.308779 | 0.676710 | -0.249667 | H | 1.734973 | -2.614136 | 0.022406 |
| N | -4.384873 | -5.936439 | 0.350813 | N | 0.818810 | -7.828320 | 0.082593 |
| O | -4.517008 | -7.148960 | 0.527328 | O | -0.078075 | -8.647655 | 0.019355 |
| O | -5.308662 | -5.113330 | 0.255693 | O | 2.032764 | -7.992630 | 0.155864 |
| N | -5.934524 | 4.385752 | -0.351818 | N | -7.831094 | -0.813111 | -0.087362 |
| O | -7.146921 | 4.518469 | -0.528524 | O | -8.648960 | 0.085079 | -0.024366 |
| O | -5.110880 | 5.309160 | -0.257591 | O | -7.997415 | -2.026906 | -0.159984 |
| N | 4.384961 | 5.936405 | 0.347542 | N | -0.815161 | 7.828450 | 0.096081 |
| O | 4.517276 | 7.149135 | 0.522557 | O | 0.082381 | 8.647015 | 0.032103 |
| O | 5.308654 | 5.113103 | 0.253035 | O | -2.028822 | 7.993862 | 0.172174 |
| N | 5.935242 | -4.385581 | -0.351356 | N | 7.829741 | 0.815184 | -0.090968 |
| O | 7.148022 | -4.518264 | -0.525634 | O | 8.647896 | -0.082643 | -0.026354 |
| O | 5.111436 | -5.309008 | -0.258547 | O | 7.995665 | 2.028963 | -0.164083 |

Cartesian coordinates of equilibrium geometries of C2-Cl and N9-Cl substituted derivatives of the $A_4N7$ tetramer

| | C2-Cl | | | | N9-Cl | | |
|---|---|---|---|---|---|---|---|
| N | -3.016211 | -4.262713 | -0.213764 | N | -3.041396 | -4.286097 | -0.191212 |
| C | -3.040985 | -5.598041 | -0.251981 | C | -3.078520 | -5.630134 | -0.297912 |
| N | -2.044970 | -6.482725 | -0.186497 | N | -2.054160 | -6.504557 | -0.311429 |
| C | -0.860270 | -5.855976 | -0.073505 | C | -0.878480 | -5.876807 | -0.208931 |
| C | -0.654410 | -4.471218 | -0.024698 | C | -0.672399 | -4.495495 | -0.095125 |
| C | -1.809660 | -3.652036 | -0.093139 | C | -1.833424 | -3.679593 | -0.081477 |
| N | 0.409578 | -6.405688 | 0.015533 | N | 0.416262 | -6.401952 | -0.193761 |
| C | 1.304727 | -5.353350 | 0.108144 | C | 1.311126 | -5.346056 | -0.080645 |
| N | 0.699543 | -4.179471 | 0.086589 | N | 0.682808 | -4.188803 | -0.020133 |
| N | -1.750948 | -2.305165 | -0.048012 | N | -1.763518 | -2.334077 | 0.029633 |
| H | 2.377107 | -5.491283 | 0.183776 | H | -4.073381 | -6.066566 | -0.380868 |
| H | -0.856787 | -1.876221 | 0.145288 | H | 2.384049 | -5.489452 | -0.050813 |
| H | -2.612411 | -1.730493 | -0.065843 | H | -0.865191 | -1.915561 | 0.226205 |
| H | 0.629841 | -7.395355 | 0.009641 | H | -2.617353 | -1.754806 | 0.046238 |
| N | -4.264338 | 3.015289 | 0.198164 | N | -4.283354 | 3.041609 | 0.188651 |
| C | -5.599483 | 3.037191 | 0.245745 | C | -5.626606 | 3.078809 | 0.304493 |
| N | -6.482443 | 2.039657 | 0.180212 | N | -6.501272 | 2.054693 | 0.320147 |
| C | -5.854038 | 0.856865 | 0.056239 | C | -5.874589 | 0.879183 | 0.210046 |
| C | -4.469171 | 0.654217 | -0.003273 | C | -4.494087 | 0.672990 | 0.086862 |
| C | -3.652037 | 1.810839 | 0.065497 | C | -3.678004 | 1.833873 | 0.070680 |
| N | -6.401737 | -0.413672 | -0.035970 | N | -6.400249 | -0.415324 | 0.195223 |
| C | -5.348237 | -1.306185 | -0.138688 | C | -5.345373 | -1.310262 | 0.073644 |
| N | -4.175526 | -0.698522 | -0.121999 | N | -4.188317 | -0.682161 | 0.007160 |
| N | -2.305239 | 1.755471 | 0.009874 | N | -2.333393 | 1.764301 | -0.050757 |
| H | -5.484327 | -2.378643 | -0.216567 | H | -6.062067 | 4.073500 | 0.394094 |
| H | -1.876213 | 0.865507 | -0.201445 | H | -5.489293 | -2.383097 | 0.043109 |
| H | -1.732799 | 2.618104 | 0.034553 | H | -1.916126 | 0.866939 | -0.253924 |
| H | -7.390871 | -0.636070 | -0.024758 | H | -1.754257 | 2.618347 | -0.063288 |
| N | 3.015365 | 4.259621 | -0.188982 | N | 3.041195 | 4.283471 | -0.184091 |
| C | 3.040863 | 5.594701 | -0.236340 | C | 3.079400 | 5.626905 | -0.297934 |
| N | 2.045439 | 6.480282 | -0.174740 | N | 2.055772 | 6.502119 | -0.315389 |
| C | 0.860543 | 5.854922 | -0.056591 | C | 0.879606 | 5.875828 | -0.209802 |
| C | 0.653925 | 4.470564 | 0.000811 | C | 0.672394 | 4.495214 | -0.089352 |
| C | 1.808762 | 3.650408 | -0.061919 | C | 1.832788 | 3.678526 | -0.070745 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| N | -0.408905 | 6.405905 | 0.029691 | N | -0.414707 | 6.402049 | -0.197982 |
| C | -1.304684 | 5.354619 | 0.127776 | C | -1.310466 | 5.347356 | -0.080607 |
| N | -0.700181 | 4.180311 | 0.113132 | N | -0.683094 | 4.189901 | -0.013979 |
| N | 1.749738 | 2.303775 | -0.005114 | N | 1.761991 | 2.333752 | 0.048485 |
| H | -2.377049 | 5.493655 | 0.201258 | H | 4.074583 | 6.062042 | -0.383885 |
| H | 0.857637 | 1.876927 | 0.202781 | H | -2.383297 | 5.491749 | -0.052737 |
| H | 2.611330 | 1.729211 | -0.023254 | H | 0.863839 | 1.917029 | 0.249430 |
| H | -0.628592 | 7.395649 | 0.018007 | H | 2.615670 | 1.754248 | 0.064352 |
| N | 4.263759 | -3.015743 | 0.205288 | N | 4.283744 | -3.041538 | 0.185607 |
| C | 5.598706 | -3.037933 | 0.258570 | C | 5.627111 | -3.078777 | 0.300326 |
| N | 6.481982 | -2.040004 | 0.203523 | N | 6.501477 | -2.054472 | 0.319944 |
| C | 5.854112 | -0.856358 | 0.085193 | C | 5.874316 | -0.878660 | 0.215573 |
| C | 4.469573 | -0.653242 | 0.022232 | C | 4.493652 | -0.672408 | 0.094398 |
| C | 3.652100 | -1.810311 | 0.078912 | C | 3.677926 | -1.833475 | 0.073415 |
| N | 6.402158 | 0.414798 | 0.003444 | N | 6.399476 | 0.416099 | 0.205956 |
| C | 5.349057 | 1.308028 | -0.097440 | C | 5.344199 | 1.311171 | 0.088939 |
| N | 4.176277 | 0.700324 | -0.088415 | N | 4.187303 | 0.682922 | 0.020675 |
| N | 2.305647 | -1.754091 | 0.017326 | N | 2.333383 | -1.763660 | -0.047643 |
| H | 5.485396 | 2.380958 | -0.169028 | H | 6.062981 | -4.073712 | 0.385141 |
| H | 1.877719 | -0.861086 | -0.184025 | H | 5.487719 | 2.384157 | 0.062469 |
| H | 1.732035 | -2.616138 | 0.031312 | H | 1.915519 | -0.864727 | -0.242742 |
| H | 7.391259 | 0.637069 | 0.019016 | H | 1.753851 | -2.617345 | -0.062373 |
| Cl | -4.665444 | -6.302292 | -0.409510 | Cl | 0.836254 | -8.070185 | -0.318894 |
| Cl | -6.306122 | 4.659294 | 0.416423 | Cl | -8.067953 | -0.835025 | 0.328504 |
| Cl | 4.665351 | 6.296941 | -0.400746 | Cl | -0.833283 | 8.070160 | -0.330113 |
| Cl | 6.304562 | -4.661074 | 0.422294 | Cl | 8.067213 | 0.835840 | 0.339146 |

Cartesian coordinates of equilibrium geometries of C2-F and N9-F substituted derivatives of the $A_4N7$ tetramer

| | | C2-F | | | | N9-F | |
|---|---|---|---|---|---|---|---|
| N | -3.031888 | -4.260080 | -0.068338 | N | -3.052185 | -4.293960 | -0.061429 |
| C | -3.046596 | -5.590828 | -0.043781 | C | -3.092615 | -5.642605 | -0.053767 |
| N | -2.063643 | -6.479536 | 0.036587 | N | -2.073827 | -6.520399 | 0.012596 |
| C | -0.873953 | -5.851746 | 0.096648 | C | -0.898614 | -5.883642 | 0.070107 |
| C | -0.666855 | -4.466465 | 0.082202 | C | -0.683300 | -4.495748 | 0.068869 |
| C | -1.822241 | -3.647625 | -0.001982 | C | -1.844558 | -3.681639 | 0.004282 |
| N | 0.395161 | -6.399291 | 0.182899 | B | 0.396639 | -6.373199 | 0.141887 |
| C | 1.294457 | -5.345342 | 0.212467 | C | 1.306170 | -5.341506 | 0.175320 |
| N | 0.690218 | -4.173344 | 0.154126 | N | 0.670923 | -4.182171 | 0.132939 |
| N | -1.759730 | -2.301401 | -0.021777 | N | -1.772108 | -2.333409 | 0.002480 |
| H | 2.367761 | -5.483487 | 0.270249 | H | -4.088340 | -6.081425 | -0.107232 |
| H | -0.851991 | -1.867344 | 0.063340 | H | 2.377174 | -5.492168 | 0.222921 |
| H | -2.617273 | -1.721255 | -0.071496 | H | -0.863938 | -1.902539 | 0.098499 |
| H | 0.613747 | -7.388778 | 0.212216 | H | -2.622027 | -1.749550 | -0.041445 |
| N | -4.262566 | 3.032086 | 0.063181 | N | -4.294787 | 3.052567 | 0.060142 |
| C | -5.593391 | 3.045288 | 0.041975 | C | -5.643488 | 3.092026 | 0.054127 |
| N | -6.481304 | 2.061116 | -0.034252 | N | -6.520747 | 2.072555 | -0.011427 |
| C | -5.852375 | 0.871941 | -0.093754 | C | -5.883229 | 0.897754 | -0.070090 |
| C | -4.466811 | 0.666411 | -0.082868 | C | -4.495189 | 0.683452 | -0.070713 |
| C | -3.649004 | 1.822907 | -0.002777 | C | -3.681773 | 1.845256 | -0.006821 |
| N | -6.398745 | -0.398059 | -0.175940 | N | -6.371922 | -0.397991 | -0.141824 |
| C | -5.343881 | -1.296251 | -0.206754 | C | -5.339509 | -1.306682 | -0.176417 |
| N | -4.172395 | -0.690533 | -0.153358 | N | -4.180545 | -0.670530 | -0.135156 |
| N | -2.302687 | 1.761770 | 0.012915 | N | -2.333547 | 1.773323 | -0.007246 |
| H | -5.480809 | -2.369884 | -0.262083 | H | -6.082938 | 4.087501 | 0.108273 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | -1.867813 | 0.854164 | -0.070146 | H | -5.489258 | -2.377837 | -0.224174 |
| H | -1.722575 | 2.619182 | 0.062476 | H | -1.902428 | 0.865190 | -0.103905 |
| H | -7.388061 | -0.617863 | -0.202116 | H | -1.749205 | 2.622314 | 0.036685 |
| N | 3.032333 | 4.262422 | -0.063592 | N | 3.052371 | 4.294902 | -0.059064 |
| C | 3.046130 | 5.593219 | -0.041328 | C | 3.091910 | 5.643600 | -0.052990 |
| N | 2.062352 | 6.481467 | 0.034698 | N | 2.072387 | 6.520897 | 0.011560 |
| C | 0.872875 | 5.853011 | 0.092206 | C | 0.897448 | 5.883475 | 0.068993 |
| C | 0.666628 | 4.467549 | 0.079523 | C | 0.683067 | 4.495433 | 0.069578 |
| C | 1.822877 | 3.649312 | 0.000340 | C | 1.844945 | 3.681934 | 0.007205 |
| N | -0.396807 | 6.399905 | 0.173553 | N | -0.398373 | 6.372283 | 0.138970 |
| C | -1.295586 | 5.345480 | 0.202613 | C | -1.307248 | 5.339993 | 0.172566 |
| N | -0.690514 | 4.173769 | 0.148779 | N | -0.671085 | 4.181006 | 0.132453 |
| N | 1.761287 | 2.303014 | -0.016477 | N | 1.773015 | 2.333691 | 0.008939 |
| H | -2.369131 | 5.483028 | 0.257036 | H | 4.087485 | 6.082997 | -0.106006 |
| H | 0.853536 | 1.868457 | 0.064935 | H | -2.378501 | 5.489837 | 0.218829 |
| H | 2.619395 | 1.723304 | -0.065434 | H | 0.864886 | 1.902472 | 0.106107 |
| H | -0.616009 | 7.389289 | 0.200593 | H | 2.621350 | 1.748519 | -0.034667 |
| N | 4.262060 | -3.032977 | 0.067540 | N | 4.295806 | -3.052476 | 0.059673 |
| C | 5.592834 | -3.046840 | 0.043552 | C | 5.644495 | -3.091796 | 0.053175 |
| N | 6.481019 | -2.063184 | -0.035098 | N | 6.521565 | -2.072090 | -0.011159 |
| C | 5.852539 | -0.873775 | -0.093706 | C | 5.883881 | -0.897279 | -0.067840 |
| C | 4.467102 | -0.667487 | -0.079749 | C | 4.495796 | -0.683104 | -0.068017 |
| C | 3.648927 | -1.823604 | 0.002349 | C | 3.682577 | -1.845177 | -0.005937 |
| N | 6.399401 | 0.395800 | -0.177586 | N | 6.372460 | 0.398628 | -0.137255 |
| C | 5.344971 | 1.294550 | -0.206587 | C | 5.340032 | 1.307344 | -0.170134 |
| N | 4.173269 | 0.689573 | -0.150365 | N | 4.181130 | 0.671030 | -0.130197 |
| N | 2.302626 | -1.761981 | 0.021109 | N | 2.334308 | -1.773633 | -0.007304 |
| H | 5.482533 | 2.368018 | -0.262639 | H | 6.084091 | -4.087304 | 0.105613 |
| H | 1.868039 | -0.854308 | -0.062002 | H | 5.489731 | 2.378620 | -0.215801 |
| H | 1.723433 | -2.619144 | 0.071406 | H | 1.902736 | -0.865635 | -0.103663 |
| H | 7.388777 | 0.614957 | -0.205995 | H | 1.749212 | -2.622763 | 0.036053 |
| F | -4.293056 | -6.129693 | -0.113067 | F | 0.744366 | -7.719414 | 0.166620 |
| F | -6.133448 | 4.291351 | 0.110140 | F | -7.717937 | -0.746829 | -0.165415 |
| F | 4.292414 | 6.132815 | -0.108038 | F | -0.747164 | 7.718305 | 0.161787 |
| F | 6.132439 | -4.293051 | 0.111430 | F | 7.718433 | 0.747599 | -0.160152 |

Cartesian coordinates of equilibrium geometries of C2-H / N9-H substituted derivatives of the $A_4N7$ tetramer

C2-H / N9-H

| | | | |
|---|---|---|---|
| N | -3.055222 | -4.331704 | -0.054295 |
| C | -3.077421 | -5.680540 | -0.037879 |
| N | -2.046794 | -6.544174 | 0.027301 |
| C | -0.871341 | -5.896006 | 0.076876 |
| C | -0.685539 | -4.506732 | 0.067874 |
| C | -1.853122 | -3.703843 | 0.001665 |
| N | 0.412514 | -6.422090 | 0.145532 |
| C | 1.290986 | -5.354193 | 0.171074 |
| N | 0.668023 | -4.190352 | 0.126495 |
| N | -1.796914 | -2.354129 | -0.010741 |
| H | -4.068782 | -6.131237 | -0.082814 |
| H | 2.367498 | -5.471244 | 0.217717 |
| H | -0.890410 | -1.915867 | 0.069859 |
| H | -2.648942 | -1.770743 | -0.047899 |
| N | -4.329216 | 3.054890 | 0.055997 |
| C | -5.677995 | 3.079275 | 0.036890 |

| | | | |
|---|---|---|---|
| N | -6.543088 | 2.050102 | -0.029825 |
| C | -5.896719 | 0.873583 | -0.077070 |
| C | -4.507777 | 0.685450 | -0.064430 |
| C | -3.703136 | 1.851816 | 0.002115 |
| N | -6.424781 | -0.409294 | -0.145958 |
| C | -5.358310 | -1.289610 | -0.168458 |
| N | -4.193567 | -0.668680 | -0.121610 |
| N | -2.353483 | 1.793700 | 0.016924 |
| H | -6.127175 | 4.071341 | 0.080721 |
| H | -5.477248 | -2.365911 | -0.214455 |
| H | -1.916519 | 0.886657 | -0.064039 |
| H | -1.769794 | 2.645639 | 0.052994 |
| N | 3.056059 | 4.331517 | -0.058644 |
| C | 3.079037 | 5.680312 | -0.040456 |
| N | 2.048848 | 6.544445 | 0.026245 |
| C | 0.872992 | 5.896865 | 0.074997 |
| C | 0.686338 | 4.507702 | 0.063768 |
| C | 1.853585 | 3.704262 | -0.003337 |
| N | -0.410604 | 6.423660 | 0.144665 |
| C | -1.289757 | 5.356271 | 0.168442 |
| N | -0.667530 | 4.192066 | 0.121963 |
| N | 1.796792 | 2.354589 | -0.016712 |
| H | 4.070685 | 6.130495 | -0.085122 |
| H | -2.366237 | 5.474002 | 0.215331 |
| H | 0.890096 | 1.916628 | 0.062778 |
| H | 2.649170 | 1.770827 | -0.053761 |
| N | 4.327441 | -3.054986 | 0.062845 |
| C | 5.676156 | -3.080075 | 0.040066 |
| N | 6.541496 | -2.051559 | -0.032020 |
| C | 5.895557 | -0.874894 | -0.080906 |
| C | 4.506749 | -0.686056 | -0.064722 |
| C | 3.701776 | -1.851822 | 0.007654 |
| N | 6.424007 | 0.407419 | -0.155413 |
| C | 5.357900 | 1.288189 | -0.178103 |
| N | 4.193038 | 0.667981 | -0.125678 |
| N | 2.352168 | -1.793126 | 0.027172 |
| H | 6.124972 | -4.072208 | 0.085663 |
| H | 5.477283 | 2.364256 | -0.228073 |
| H | 1.915323 | -0.886259 | -0.055449 |
| H | 1.769158 | -2.645782 | 0.063707 |
| H | 0.647594 | -7.407802 | 0.166450 |
| H | -7.410826 | -0.642628 | -0.169025 |
| H | -0.645086 | 7.409493 | 0.167197 |
| H | 7.410095 | 0.640113 | -0.182083 |

Cartesian coordinates of equilibrium geometries of C2-Me and N9-Me substituted derivatives of the $A_4N7$ tetramer

| C2-Me | | | | N9-Me | | | |
|---|---|---|---|---|---|---|---|
| N | -3.046491 | -4.333552 | 0.001361 | N | -3.041476 | -4.326437 | -0.126051 |
| C | -3.090428 | -5.688314 | 0.030697 | C | -3.060363 | -5.675069 | -0.157773 |
| N | -2.042411 | -6.540536 | 0.059975 | N | -2.027930 | -6.538395 | -0.118198 |
| C | -0.866212 | -5.893614 | 0.058741 | C | -0.852997 | -5.888851 | -0.041802 |
| C | -0.675559 | -4.507331 | 0.031550 | C | -0.671466 | -4.499596 | -0.003105 |
| C | -1.846583 | -3.707622 | 0.000105 | C | -1.840303 | -3.697704 | -0.045134 |
| N | 0.417687 | -6.424252 | 0.088083 | N | 0.427504 | -6.428467 | 0.009808 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | 1.301232 | -5.358914 | 0.078914 | C | 1.298464 | -5.355830 | 0.076548 |
| N | 0.679935 | -4.194118 | 0.045013 | N | 0.679435 | -4.186362 | 0.069720 |
| N | -1.790826 | -2.357512 | -0.031258 | N | -1.787483 | -2.347981 | -0.011242 |
| H | 2.378285 | -5.478848 | 0.096656 | H | -4.050858 | -6.125728 | -0.222025 |
| H | -0.880567 | -1.920283 | -0.045012 | H | 2.375025 | -5.477263 | 0.122576 |
| H | -2.644268 | -1.775071 | -0.044525 | H | -0.884161 | -1.912917 | 0.112103 |
| H | 0.649344 | -7.410566 | 0.109989 | H | -2.642216 | -1.766341 | -0.027608 |
| N | -4.334091 | 3.045785 | -0.004351 | N | -4.326038 | 3.041071 | 0.123907 |
| C | -5.688898 | 3.089295 | -0.032018 | C | -5.674665 | 3.059748 | 0.156605 |
| N | -6.540779 | 2.040924 | -0.058187 | N | -6.537889 | 2.027180 | 0.117257 |
| C | -5.893383 | 0.864976 | -0.056357 | C | -5.888238 | 0.852318 | 0.039641 |
| C | -4.506922 | 0.674782 | -0.031888 | C | -4.498968 | 0.671036 | -0.000613 |
| C | -3.707528 | 1.846199 | -0.002525 | C | -3.697196 | 1.839954 | 0.041793 |
| N | -6.423634 | -0.419156 | -0.082181 | N | -6.427658 | -0.428313 | -0.012104 |
| C | -5.357983 | -1.302357 | -0.072688 | C | -5.354919 | -1.299063 | -0.080386 |
| N | -4.193334 | -0.680654 | -0.044846 | N | -4.185595 | -0.679770 | -0.074384 |
| N | -2.357167 | 1.791423 | 0.027085 | N | -2.347422 | 1.787216 | 0.007518 |
| H | -5.477536 | -2.379475 | -0.086566 | H | -6.125418 | 4.050220 | 0.221511 |
| H | -1.919733 | 0.881245 | 0.043473 | H | -5.476087 | -2.375656 | -0.126955 |
| H | -1.775163 | 2.644732 | 0.040113 | H | -1.912305 | 0.884132 | -0.118413 |
| H | -7.409938 | -0.651194 | -0.101217 | H | -1.765558 | 2.641253 | 0.023797 |
| N | 3.046693 | 4.333484 | 0.000246 | N | 3.041562 | 4.328409 | -0.117079 |
| C | 3.090912 | 5.688250 | 0.030329 | C | 3.059361 | 5.677017 | -0.150987 |
| N | 2.043051 | 6.540641 | 0.060438 | N | 2.026134 | 6.539572 | -0.114768 |
| C | 0.866737 | 5.893922 | 0.059146 | C | 0.851552 | 5.889234 | -0.039237 |
| C | 0.675791 | 4.507674 | 0.031047 | C | 0.671155 | 4.499899 | 0.001802 |
| C | 1.846673 | 3.707741 | -0.000770 | C | 1.840726 | 3.698861 | -0.037123 |
| N | -0.417060 | 6.424819 | 0.089296 | N | -0.429576 | 6.427837 | 0.008770 |
| C | -1.300824 | 5.359663 | 0.079203 | C | -1.299733 | 5.354571 | 0.075853 |
| N | -0.679794 | 4.194720 | 0.044149 | N | -0.679630 | 4.185658 | 0.072390 |
| N | 1.790677 | 2.357619 | -0.031675 | N | 1.788791 | 2.349128 | -0.001269 |
| H | -2.377850 | 5.479845 | 0.097049 | H | 4.049627 | 6.128385 | -0.214107 |
| H | 0.880350 | 1.920603 | -0.045576 | H | -2.376524 | 5.475069 | 0.119752 |
| H | 2.643608 | 1.774653 | -0.045547 | H | 0.885574 | 1.913554 | 0.121416 |
| H | -0.648520 | 7.411176 | 0.112148 | H | 2.643347 | 1.767638 | -0.017667 |
| N | 4.333299 | -3.045801 | -0.002800 | N | 4.328237 | -3.042072 | 0.118534 |
| C | 5.688076 | -3.089692 | -0.031283 | C | 5.676854 | -3.060265 | 0.151510 |
| N | 6.540242 | -2.041596 | -0.059181 | N | 6.539647 | -2.027233 | 0.115411 |
| C | 5.893221 | -0.865451 | -0.058012 | C | 5.889520 | -0.852420 | 0.041433 |
| C | 4.506860 | -0.674843 | -0.032236 | C | 4.500182 | -0.671563 | 0.001574 |
| C | 3.707188 | -1.845972 | -0.001410 | C | 3.698909 | -1.841010 | 0.039721 |
| N | 6.423851 | 0.418498 | -0.086171 | N | 6.428466 | 0.428576 | -0.005730 |
| C | 5.358467 | 1.301999 | -0.077336 | C | 5.355386 | 1.299114 | -0.070913 |
| N | 4.193650 | 0.680663 | -0.045773 | N | 4.186259 | 0.679411 | -0.067314 |
| N | 2.356974 | -1.790472 | 0.029434 | N | 2.349172 | -1.788808 | 0.004095 |
| H | 5.478294 | 2.379076 | -0.093825 | H | 6.128018 | -4.050705 | 0.213613 |
| H | 1.919769 | -0.880218 | 0.044643 | H | 5.476230 | 2.375906 | -0.113690 |
| H | 1.775222 | -2.644066 | 0.042760 | H | 1.913674 | -0.885346 | -0.117358 |
| H | 7.410199 | 0.650228 | -0.106817 | H | 1.767301 | -2.643032 | 0.020269 |
| C | -4.472680 | -6.302594 | 0.025991 | C | 0.753722 | -7.854771 | 0.010156 |
| H | -5.055538 | -5.929116 | 0.877112 | H | 0.397004 | -8.325032 | 0.932724 |
| H | -5.009817 | -6.014284 | -0.886631 | H | 0.270357 | -8.343090 | -0.841441 |
| H | -4.407443 | -7.391948 | 0.078536 | H | 1.837463 | -7.971010 | -0.065649 |
| C | -6.303660 | 4.471364 | -0.028872 | C | -7.853871 | -0.754937 | -0.011250 |
| H | -6.014918 | 5.009895 | 0.882781 | H | -8.341482 | -0.272501 | 0.841259 |
| H | -5.931014 | 5.053182 | -0.881056 | H | -8.325199 | -0.397585 | -0.932981 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | -7.393031 | 4.405679 | -0.080481 | H | -7.969653 | -1.838733 | 0.063748 |
| C | 4.473242 | 6.302382 | 0.025634 | C | -0.757402 | 7.853796 | 0.005195 |
| H | 5.056594 | 5.927933 | 0.875986 | H | -0.404018 | 8.326475 | 0.927760 |
| H | 5.009798 | 6.015031 | -0.887623 | H | -0.272149 | 8.340874 | -0.846014 |
| H | 4.408187 | 7.391677 | 0.079364 | H | -1.840997 | 7.968559 | -0.074073 |
| C | 6.302454 | -4.471907 | -0.027175 | C | 7.854543 | 0.755910 | -0.003112 |
| H | 6.013229 | -5.009976 | 0.884608 | H | 8.342233 | 0.269687 | 0.847202 |
| H | 5.929923 | -5.053948 | -0.879266 | H | 8.326249 | 0.403191 | -0.926440 |
| H | 7.391869 | -4.406525 | -0.078522 | H | 7.969759 | 1.839398 | 0.077027 |

Cartesian coordinates of equilibrium geometries of C2-$NH_2$ and N9-$NH_2$ substituted derivatives of the $A_4$N7 tetramer

| | C2-$NH_2$ | | | | N9-$NH_2$ | | |
|---|---|---|---|---|---|---|---|
| N | -3.071790 | -4.332025 | 0.021371 | N | -2.989439 | -4.321744 | -0.290951 |
| C | -3.102319 | -5.688209 | 0.082708 | C | -3.015410 | -5.662563 | -0.157248 |
| N | -2.058948 | -6.551183 | 0.125502 | N | -1.983134 | -6.517576 | -0.011182 |
| C | -0.887935 | -5.901111 | 0.092127 | C | -0.812301 | -5.862361 | -0.018153 |
| C | -0.698575 | -4.514580 | 0.028569 | C | -0.619055 | -4.482981 | -0.156372 |
| C | -1.871116 | -3.714317 | -0.007927 | C | -1.786914 | -3.689596 | -0.291914 |
| N | 0.395929 | -6.429121 | 0.117591 | N | 0.473729 | -6.386458 | 0.112413 |
| C | 1.281433 | -5.360671 | 0.069263 | C | 1.355987 | -5.323195 | 0.047665 |
| N | 0.657729 | -4.200100 | 0.016323 | N | 0.735735 | -4.167108 | -0.114534 |
| N | -1.809081 | -2.365642 | -0.069801 | N | -1.736424 | -2.345060 | -0.431471 |
| H | 2.357921 | -5.480805 | 0.077563 | H | -4.007026 | -6.114651 | -0.165506 |
| H | -0.895120 | -1.936551 | -0.096289 | H | 2.428077 | -5.456040 | 0.126956 |
| H | -2.655769 | -1.775823 | -0.115878 | H | -0.842362 | -1.893608 | -0.295700 |
| H | 0.628421 | -7.414329 | 0.156405 | H | -2.600256 | -1.776782 | -0.412941 |
| N | -4.322272 | 3.057898 | 0.135173 | N | -4.312189 | 2.950842 | 0.251981 |
| C | -5.679524 | 3.086638 | 0.156716 | C | -5.624853 | 2.933267 | 0.554110 |
| N | -6.543042 | 2.046058 | 0.078785 | N | -6.471065 | 1.883877 | 0.587108 |
| C | -5.892498 | 0.880855 | -0.037828 | C | -5.835836 | 0.745063 | 0.273419 |
| C | -4.504527 | 0.694183 | -0.074756 | C | -4.484498 | 0.598152 | -0.060294 |
| C | -3.703728 | 1.863459 | 0.016646 | C | -3.701589 | 1.780662 | -0.070758 |
| N | -6.421077 | -0.399275 | -0.138800 | N | -6.353611 | -0.548799 | 0.221470 |
| C | -5.351575 | -1.280303 | -0.227149 | C | -5.312159 | -1.391861 | -0.122457 |
| N | -4.190138 | -0.657115 | -0.191041 | N | -4.177009 | -0.738313 | -0.299885 |
| N | -2.353258 | 1.804686 | -0.003344 | N | -2.387375 | 1.776722 | -0.384088 |
| H | -5.471793 | -2.354024 | -0.305625 | H | -6.060680 | 3.900516 | 0.803821 |
| H | -1.924177 | 0.901329 | -0.145863 | H | -5.441710 | -2.463536 | -0.212831 |
| H | -1.765953 | 2.654747 | 0.010490 | H | -1.973306 | 0.910855 | -0.698856 |
| H | -7.406963 | -0.631972 | -0.147483 | H | -1.815676 | 2.636428 | -0.326753 |
| N | 3.070527 | 4.334261 | 0.040455 | N | 2.979654 | 4.327292 | -0.149054 |
| C | 3.099998 | 5.690637 | 0.098523 | C | 3.004729 | 5.666434 | 0.001080 |
| N | 2.055946 | 6.552875 | 0.139456 | N | 1.970401 | 6.521999 | 0.128751 |
| C | 0.885437 | 5.901817 | 0.107227 | C | 0.798977 | 5.869931 | 0.078323 |
| C | 0.697152 | 4.514945 | 0.046659 | C | 0.606571 | 4.493035 | -0.086805 |
| C | 1.870441 | 3.715469 | 0.012759 | C | 1.776362 | 3.698142 | -0.193444 |
| N | -0.398774 | 6.429043 | 0.129734 | N | -0.488734 | 6.395719 | 0.175988 |
| C | -1.283612 | 5.359950 | 0.082878 | C | -1.371757 | 5.336565 | 0.066724 |
| N | -0.659040 | 4.199695 | 0.033965 | N | -0.749860 | 4.181128 | -0.092531 |
| N | 1.809856 | 2.366517 | -0.045127 | N | 1.728084 | 2.354950 | -0.346613 |
| H | -2.360167 | 5.479615 | 0.088608 | H | 3.997059 | 6.116226 | 0.026739 |
| H | 0.896484 | 1.935822 | -0.064302 | H | -2.445338 | 5.471893 | 0.115896 |
| H | 2.657095 | 1.777250 | -0.090524 | H | 0.830668 | 1.903519 | -0.234406 |
| H | -0.631860 | 7.414232 | 0.165484 | H | 2.591827 | 1.787414 | -0.302533 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| N | 4.323858 | -3.060041 | 0.125769 | N | 4.331638 | -2.964695 | 0.164070 |
| C | 5.681008 | -3.088626 | 0.154029 | C | 5.656729 | -2.960119 | 0.406291 |
| N | 6.544560 | -2.047136 | 0.089651 | N | 6.502715 | -1.911510 | 0.461053 |
| C | 5.894280 | -0.881152 | -0.019827 | C | 5.853071 | -0.758462 | 0.240763 |
| C | 4.506465 | -0.694462 | -0.061718 | C | 4.487597 | -0.596691 | -0.020488 |
| C | 3.705624 | -1.864809 | 0.014777 | C | 3.706594 | -1.779737 | -0.064150 |
| N | 6.422959 | 0.399771 | -0.107415 | N | 6.366281 | 0.538017 | 0.244696 |
| C | 5.353743 | 1.281384 | -0.193493 | C | 5.310190 | 1.396361 | -0.001588 |
| N | 4.192287 | 0.657692 | -0.168322 | N | 4.169130 | 0.749716 | -0.170629 |
| N | 2.355343 | -1.806301 | -0.013067 | N | 2.380896 | -1.760381 | -0.320483 |
| H | 5.474387 | 2.355674 | -0.262835 | H | 6.103796 | -3.938528 | 0.581394 |
| H | 1.926381 | -0.900976 | -0.142663 | H | 5.434612 | 2.471912 | -0.037422 |
| H | 1.767518 | -2.655842 | -0.002647 | H | 1.946863 | -0.869931 | -0.520360 |
| H | 7.408844 | 0.632615 | -0.109424 | H | 1.806739 | -2.619480 | -0.282979 |
| N | -4.361302 | -6.257633 | 0.065385 | N | 0.853049 | -7.738317 | 0.290162 |
| H | -4.419988 | -7.224897 | 0.356833 | H | 0.377133 | -8.084391 | 1.128147 |
| H | -5.132139 | -5.651861 | 0.314284 | H | 0.479656 | -8.271344 | -0.500400 |
| N | -6.248202 | 4.344570 | 0.232805 | N | -7.680789 | -0.970940 | 0.474335 |
| H | -7.223522 | 4.377712 | 0.502913 | H | -7.915411 | -0.694638 | 1.431925 |
| H | -5.650770 | 5.086101 | 0.576075 | H | -8.296867 | -0.437167 | -0.144758 |
| N | 4.358606 | 6.260921 | 0.079280 | N | -0.869069 | 7.745919 | 0.368351 |
| H | 4.417377 | 7.228598 | 0.370757 | H | -0.465912 | 8.055861 | 1.257442 |
| H | 5.130398 | 5.655779 | 0.327024 | H | -0.416326 | 8.300277 | -0.363731 |
| N | 6.249365 | -4.346888 | 0.222726 | N | 7.703866 | 0.945908 | 0.469168 |
| H | 7.223176 | -4.382969 | 0.497236 | H | 8.020697 | 0.485650 | 1.327223 |
| H | 5.650002 | -5.092052 | 0.553858 | H | 8.274830 | 0.568313 | -0.291958 |

Cartesian coordinates of equilibrium geometries substituted C2- $NO_2$, C8- $NO_2$ and N9- $NO_2$ derivatives of adenine 9H

| | | C2-$NO_2$ | | | | C8-$NO_2$ | |
|---|---|---|---|---|---|---|---|
| N | -2.978850 | -4.278003 | -0.303890 | N | -3.638244 | -0.662093 | -0.229155 |
| C | -3.012150 | -5.582720 | -0.053149 | C | -4.981924 | -0.677291 | -0.113788 |
| N | -2.046080 | -6.459376 | 0.190784 | N | -5.807003 | -1.733964 | 0.015828 |
| C | -0.852392 | -5.840674 | 0.180708 | C | -5.125999 | -2.885688 | 0.019032 |
| C | -0.619902 | -4.475890 | -0.071809 | C | -3.722264 | -3.035261 | -0.096424 |
| C | -1.764340 | -3.681463 | -0.334055 | C | -2.971190 | -1.834834 | -0.222135 |
| N | 0.401176 | -6.374950 | 0.404416 | N | -5.602626 | -4.176056 | 0.135427 |
| C | 1.307614 | -5.330845 | 0.278402 | C | -4.492121 | -4.995930 | 0.085137 |
| N | 0.733604 | -4.178405 | -0.006591 | N | -3.348922 | -4.360996 | -0.052636 |
| N | -1.690338 | -2.360480 | -0.615791 | H | -5.461550 | 0.300477 | -0.127092 |
| H | 2.371805 | -5.486757 | 0.407353 | N | -1.622542 | -1.832485 | -0.324692 |
| H | -0.795463 | -1.890224 | -0.613272 | H | -1.108143 | -2.703172 | -0.354090 |
| H | -2.542021 | -1.831794 | -0.753080 | H | -1.136466 | -0.951431 | -0.432484 |
| H | 0.603677 | -7.345430 | 0.616842 | H | -6.562304 | -4.490754 | 0.238429 |
| N | -4.413269 | -6.174489 | -0.035170 | N | -4.654563 | -6.439930 | 0.186394 |
| O | -4.611993 | -7.155501 | -0.761734 | O | -5.835767 | -6.842335 | 0.312078 |
| O | -5.236894 | -5.627373 | 0.707382 | O | -3.642645 | -7.148466 | 0.143675 |
| | | N9-$NO_2$ | | | | | |
| N | -3.591864 | -0.639604 | -0.269938 | | | | |
| C | -4.933295 | -0.615886 | -0.191457 | | | | |
| N | -5.789117 | -1.651291 | -0.062028 | | | | |
| C | -5.140021 | -2.815370 | -0.011988 | | | | |
| C | -3.750718 | -3.004836 | -0.078250 | | | | |

| | | | |
|---|---|---|---|
| C | -2.963867 | -1.836913 | -0.214336 |
| N | -5.631487 | -4.134115 | 0.118932 |
| C | -4.524000 | -5.000539 | 0.122334 |
| N | -3.394701 | -4.352999 | 0.005653 |
| H | -5.391469 | 0.370989 | -0.239747 |
| H | -4.661403 | -6.068927 | 0.213298 |
| N | -1.611248 | -1.876037 | -0.288439 |
| H | -1.122103 | -2.760680 | -0.269504 |
| H | -1.097393 | -1.012268 | -0.405730 |
| N | -7.023315 | -4.584044 | 0.225862 |
| O | -7.157209 | -5.800789 | 0.349525 |
| O | -7.874011 | -3.712431 | 0.179318 |

Cartesian coordinates of equilibrium geometries substituted C2-Cl, C8-Cl and N9-Cl derivatives of adenine 9H

| | | C2-Cl | | | | C8-Cl | |
|---|---|---|---|---|---|---|---|
| N | -2.982693 | -4.254082 | -0.228673 | N | -3.639915 | -0.660538 | -0.212706 |
| C | -3.023574 | -5.588934 | -0.179258 | C | -4.983229 | -0.667517 | -0.110784 |
| N | -2.031168 | -6.471324 | -0.060169 | N | -5.809212 | -1.723182 | 0.020379 |
| C | -0.843697 | -5.845578 | 0.013071 | C | -5.125628 | -2.874909 | 0.043205 |
| C | -0.620751 | -4.458967 | -0.024000 | C | -3.732107 | -3.030138 | -0.052152 |
| C | -1.775147 | -3.650121 | -0.150687 | C | -2.979185 | -1.840429 | -0.184581 |
| N | 0.416821 | -6.399609 | 0.137062 | N | -5.613431 | -4.170388 | 0.163420 |
| C | 1.317488 | -5.341128 | 0.168391 | C | -4.504930 | -5.002754 | 0.135319 |
| N | 0.734036 | -4.163359 | 0.073932 | N | -3.364127 | -4.374818 | 0.007821 |
| N | -1.717278 | -2.296571 | -0.193474 | H | -5.460626 | 0.311293 | -0.138893 |
| H | 2.383777 | -5.508405 | 0.260405 | N | -1.623556 | -1.838875 | -0.273908 |
| H | -0.822958 | -1.826024 | -0.164499 | H | -1.114087 | -2.710817 | -0.316253 |
| H | -2.569767 | -1.765932 | -0.317156 | H | -1.141752 | -0.961872 | -0.422754 |
| H | 0.626419 | -7.389709 | 0.195762 | H | -6.583173 | -4.449768 | 0.258633 |
| Cl | -4.649220 | -6.289333 | -0.293363 | Cl | -4.704862 | -6.719284 | 0.266758 |

| | | N9-Cl | |
|---|---|---|---|
| N | -3.631700 | -0.662832 | -0.307890 |
| C | -4.975645 | -0.658028 | -0.203392 |
| N | -5.805889 | -1.701711 | -0.021796 |
| C | -5.129913 | -2.852518 | 0.053493 |
| C | -3.738129 | -3.025140 | -0.033713 |
| C | -2.980329 | -1.843670 | -0.224496 |
| N | -5.604521 | -4.149990 | 0.230501 |
| C | -4.507001 | -5.009805 | 0.241447 |
| N | -3.372661 | -4.363580 | 0.084191 |
| H | -5.448702 | 0.320426 | -0.277159 |
| H | -4.638253 | -6.076922 | 0.366450 |
| N | -1.625653 | -1.858682 | -0.316847 |
| H | -1.124399 | -2.736987 | -0.313332 |
| H | -1.134797 | -0.994063 | -0.503158 |
| Cl | -7.258538 | -4.609199 | 0.409204 |

Cartesian coordinates of equilibrium geometries substituted C2-F, C8-F and N9-F derivatives of adenine 9H

| | | C2-F | | | | C8-F | |
|---|---|---|---|---|---|---|---|
| N | -2.985738 | -4.256464 | -0.240968 | N | -3.642757 | -0.669902 | -0.301539 |
| C | -3.011337 | -5.586743 | -0.191960 | C | -4.983548 | -0.670780 | -0.185020 |
| N | -2.031519 | -6.473836 | -0.071644 | N | -5.806979 | -1.721261 | 0.002865 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | -0.842903 | -5.847194 | 0.007849 | C | -5.122537 | -2.868143 | 0.068705 |
| C | -0.623717 | -4.459718 | -0.025840 | C | -3.730408 | -3.028486 | -0.033032 |
| C | -1.779373 | -3.651372 | -0.155955 | C | -2.980807 | -1.848078 | -0.225489 |
| N | 0.416325 | -6.398365 | 0.139429 | N | -5.612088 | -4.162737 | 0.247417 |
| C | 1.316302 | -5.337030 | 0.178701 | C | -4.499433 | -4.976561 | 0.239966 |
| N | 0.730944 | -4.161777 | 0.082018 | N | -3.360339 | -4.376807 | 0.078971 |
| N | -1.723281 | -2.297999 | -0.193368 | H | -5.462825 | 0.304953 | -0.252886 |
| H | 2.382133 | -5.503446 | 0.278015 | N | -1.624201 | -1.846978 | -0.322226 |
| H | -0.829130 | -1.827476 | -0.162818 | H | -1.115657 | -2.719783 | -0.352433 |
| H | -2.574359 | -1.768387 | -0.323819 | H | -1.150562 | -0.979571 | -0.537705 |
| H | 0.626804 | -7.387948 | 0.199340 | H | -6.578598 | -4.445468 | 0.361650 |
| F | -4.255434 | -6.122053 | -0.281637 | F | -4.667213 | -6.296539 | 0.394257 |

N9-F

| | | | |
|---|---|---|---|
| N | -3.626711 | -0.652616 | -0.212447 |
| C | -4.971635 | -0.648150 | -0.113202 |
| N | -5.809209 | -1.693218 | 0.016671 |
| C | -5.131832 | -2.846820 | 0.039669 |
| C | -3.737559 | -3.025928 | -0.051957 |
| C | -2.977635 | -1.836863 | -0.182889 |
| N | -5.574935 | -4.150980 | 0.157419 |
| C | -4.507567 | -5.026889 | 0.132497 |
| N | -3.371509 | -4.367863 | 0.006691 |
| H | -5.440288 | 0.334683 | -0.142464 |
| H | -4.650053 | -6.096757 | 0.209438 |
| N | -1.623995 | -1.852714 | -0.273339 |
| H | -1.123638 | -2.731282 | -0.283627 |
| H | -1.126249 | -0.980178 | -0.393714 |
| F | -6.907895 | -4.538767 | 0.274759 |

Cartesian coordinates of equilibrium geometries substituted C2-H / C8-H / N9-H derivatives of adenine 9H

C2-H / C8-H / N9-H

| | | | |
|---|---|---|---|
| N | -3.634160 | -0.656588 | -0.193865 |
| C | -4.979778 | -0.662677 | -0.101923 |
| N | -5.807593 | -1.715775 | 0.017707 |
| C | -5.126372 | -2.872367 | 0.039636 |
| C | -3.731862 | -3.029213 | -0.045946 |
| C | -2.978063 | -1.837521 | -0.165020 |
| N | -5.614481 | -4.163923 | 0.147690 |
| C | -4.515988 | -5.012037 | 0.123071 |
| N | -3.369796 | -4.371588 | 0.007447 |
| H | -5.454780 | 0.317409 | -0.129367 |
| H | -4.629204 | -6.087167 | 0.193006 |
| N | -1.620387 | -1.840907 | -0.235793 |
| H | -1.121422 | -2.717388 | -0.303310 |
| H | -1.136060 | -0.967993 | -0.401667 |
| H | -6.590718 | -4.422600 | 0.231836 |

Cartesian coordinates of equilibrium geometries substituted C2-Me, C8-Me and N9-Me derivatives of adenine 9H

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| | | C2-Me | | | | C8-Me | |
| N | -2.978969 | -4.265416 | -0.176116 | N | -3.630197 | -0.657202 | -0.264202 |
| C | -3.059990 | -5.617088 | -0.092603 | C | -4.974141 | -0.662384 | -0.161619 |
| N | -2.031892 | -6.482829 | 0.033041 | N | -5.800124 | -1.716521 | -0.024440 |
| C | -0.844877 | -5.857926 | 0.069586 | C | -5.118086 | -2.871457 | 0.002997 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | -0.616364 | -4.474725 | -0.005862 | C | -3.724908 | -3.028456 | -0.091577 |
| C | -1.772507 | -3.667926 | -0.129754 | C | -2.974196 | -1.839218 | -0.227579 |
| N | 0.419339 | -6.412430 | 0.186231 | N | -5.603473 | -4.162921 | 0.126063 |
| C | 1.323533 | -5.357665 | 0.174910 | C | -4.507517 | -5.023918 | 0.101660 |
| N | 0.742586 | -4.180740 | 0.061167 | N | -3.364981 | -4.371579 | -0.028861 |
| N | -1.705657 | -2.308914 | -0.185513 | H | -5.450798 | 0.316730 | -0.195734 |
| H | 2.390874 | -5.525856 | 0.253050 | N | -1.613610 | -1.838907 | -0.301948 |
| H | -0.805477 | -1.855373 | -0.265620 | H | -1.118795 | -2.714706 | -0.401737 |
| H | -2.549574 | -1.790160 | -0.391389 | H | -1.140227 | -0.970136 | -0.512052 |
| H | 0.626546 | -7.401005 | 0.265690 | H | -6.579560 | -4.418607 | 0.220428 |
| C | -4.454084 | -6.199657 | -0.135977 | C | -4.662692 | -6.507713 | 0.214019 |
| H | -5.013072 | -5.897566 | 0.759432 | H | -5.153831 | -6.785880 | 1.155849 |
| H | -5.001793 | -5.812075 | -1.002573 | H | -5.267798 | -6.908126 | -0.610227 |
| H | -4.411831 | -7.290534 | -0.180355 | H | -3.674524 | -6.972521 | 0.182464 |

N9-Me

| | | | |
|---|---|---|---|
| N | -3.626489 | -0.665754 | -0.275160 |
| C | -4.974571 | -0.676151 | -0.235032 |
| N | -5.801746 | -1.730623 | -0.118255 |
| C | -5.115767 | -2.883592 | -0.038531 |
| C | -3.717163 | -3.034388 | -0.063443 |
| C | -2.966300 | -1.841785 | -0.186474 |
| N | -5.617290 | -4.169818 | 0.083875 |
| C | -4.510686 | -5.007679 | 0.128008 |
| N | -3.356708 | -4.371755 | 0.041093 |
| H | -5.451952 | 0.300633 | -0.308043 |
| H | -4.628711 | -6.081238 | 0.222067 |
| N | -1.605783 | -1.835118 | -0.198927 |
| H | -1.099659 | -2.709236 | -0.242164 |
| H | -1.124412 | -0.965376 | -0.385825 |
| C | -7.030555 | -4.532050 | 0.173684 |
| H | -7.475174 | -4.100090 | 1.076286 |
| H | -7.569914 | -4.150148 | -0.698703 |
| H | -7.116644 | -5.621028 | 0.209047 |

Cartesian coordinates of equilibrium geometries substituted C2-$NH_2$, C8-$NH_2$ and N9-$NH_2$ derivatives of adenine 9H

| | | C2-$NH_2$ | | | | C8-$NH_2$ | |
|---|---|---|---|---|---|---|---|
| N | -2.985327 | -4.244441 | -0.121774 | N | -3.628862 | -0.669289 | -0.273969 |
| C | -3.058527 | -5.598244 | -0.021824 | C | -4.972567 | -0.663341 | -0.217595 |
| N | -2.038442 | -6.478702 | 0.103858 | N | -5.805565 | -1.714433 | -0.068472 |
| C | -0.851829 | -5.857080 | 0.108032 | C | -5.129904 | -2.865272 | 0.017972 |
| C | -0.620075 | -4.474370 | 0.009643 | C | -3.735688 | -3.032159 | -0.027100 |
| C | -1.773692 | -3.662696 | -0.104413 | C | -2.979218 | -1.852196 | -0.173566 |
| N | 0.412050 | -6.413115 | 0.206679 | N | -5.633367 | -4.155001 | 0.172501 |
| C | 1.323541 | -5.358888 | 0.160764 | C | -4.534296 | -5.008672 | 0.199494 |
| N | 0.742005 | -4.184073 | 0.043650 | N | -3.380508 | -4.376716 | 0.095831 |
| N | -1.692751 | -2.303240 | -0.173981 | H | -5.446059 | 0.313777 | -0.304009 |
| H | 2.391331 | -5.531743 | 0.218597 | N | -1.610099 | -1.853622 | -0.181904 |
| H | -0.786311 | -1.872127 | -0.298525 | H | -1.128841 | -2.734166 | -0.312718 |
| H | -2.527067 | -1.779592 | -0.406218 | H | -1.146348 | -1.003983 | -0.480115 |
| H | 0.618706 | -7.401499 | 0.290213 | H | -6.612551 | -4.412823 | 0.134695 |
| N | -4.327379 | -6.131495 | -0.092455 | N | -4.692779 | -6.384309 | 0.259802 |
| H | -4.439645 | -7.091431 | 0.206892 | H | -3.808325 | -6.865143 | 0.402004 |
| H | -5.100731 | -5.495972 | 0.051017 | H | -5.420904 | -6.721390 | 0.883461 |

N9-$NH_2$

| | | | |
|---|---|---|---|
| N | -2.908042 | -4.251952 | 0.426168 |
| C | -2.885502 | -5.570280 | 0.704248 |
| N | -1.856412 | -6.432286 | 0.592853 |
| C | -0.755298 | -5.813027 | 0.142061 |
| C | -0.618901 | -4.456802 | -0.192953 |
| C | -1.779003 | -3.663426 | -0.030639 |
| N | 0.501529 | -6.357435 | -0.098843 |
| C | 1.306640 | -5.321857 | -0.554924 |
| N | 0.673422 | -4.167067 | -0.623934 |
| N | -1.801906 | -2.337577 | -0.329376 |
| H | -3.824182 | -5.989884 | 1.064376 |
| H | 2.343440 | -5.505257 | -0.810767 |
| H | -0.949318 | -1.865544 | -0.595478 |
| H | -2.634088 | -1.801443 | -0.122152 |
| N | 0.927152 | -7.696269 | 0.068121 |
| H | 0.763652 | -7.956283 | 1.045011 |
| H | 0.318951 | -8.289400 | -0.503616 |