Electronic Supplementary Material (ESI) for Analyst.

Supporting Information for

Isomer Differentiation through Supramolecular Self-assembly in Microdroplets of Milliseconds Life-time

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1 Chemicals and Reagents

Thymine, uracil, 6-methyluracil, imidazole, pyrazole, 1,2,3-triazole, 1,2,4-triazole, N,N,N',N'-tetramethyl-1,2-ethylenediamine, 1,3-propanediamine and 1,2-propanediamine were purchased from Sigma Aldrich (Saint Louis, USA), which were of analytical grade or higher. HPLC grade Methanol was purchased from Fisher Scientific (Shanghai, China). Water was obtained from Wahaha Company (Hangzhou, China). All reagents were used as received. Analyte solutions were prepared in MeOH/water (1:1 v/v), and were freshly prepared and analyzed.

Dual pipettes were fabricated from quartz theta capillaries (1.2 mm outer diameter, 0.90 mm inner diameter) using a laser-based P-2000 pipette puller (Sutter Instrument Co.) Microscopic image of the tip end was shown in Fig S1. Each dual pipette was used for only one time to avoid cross contamination.

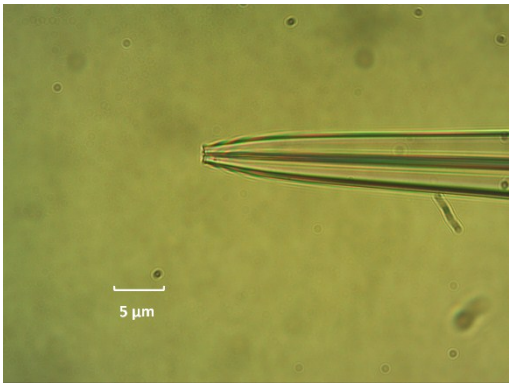

Fig S1 The theta capillary tip used in the experiment.

2 Mass Spectrometry

MS experiment was done using a Thermo Finnigan LCQ Advantage MAX ion trap mass spectrometer (San Jose, CA, USA). MS instrument parameters could greatly influence the clusters formation. Experiments have shown when the voltage of the tube lens offset varied from -100 V to 0V, and the inlet capillary temperature was set below 150 °C, the clusters were hardly affected. Typically, the voltage of tube lens offset was set at -80V, and the inlet temperature was 100 °C. A platinum electrode was inserted into either of the two barrels, and in both ways identical mass spectra could be obtained. High voltage of 1.5 kV was applied to induce nanospray. Note that higher voltage may cause the breakdown of the tip end. All mass spectra were acquired in positive mode with 3 microscans and were recorded by the instrument software (Xcalibur version 1.4 SR1).

3 Theoretical Calculations

Due to the complexity of the self-assemblies, followed by pioneering works by Schalley et al. [1], molecular dynamics was used in our calculations. Augmented MM2 force field implemented in the hyperchem program package was applied. The structures were established according to our previous publications[2-5]. 5 or 6 uracil molecules (or analogs) were assemble in cycles via double complementary hydrogen bonding under the supramolecular inducement of the central cation. The positive charge centers were always put in the center of the host cycles. Each established model was optimized carefully and should be converged down to 0.1 kJ/mol. Gibbs free energy was calculated at 300 K and no solvent conditions applied.

4 Additional Results and Discussions

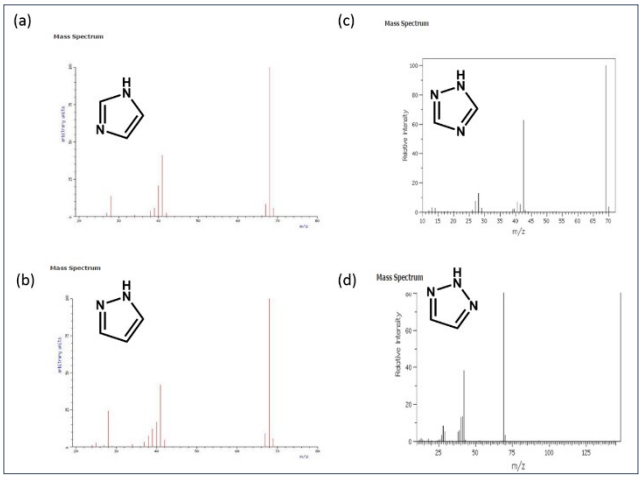

Fig S2 EI-MS spectra of (a) imidazole, (b) pyrazole, (c) 1,2,4-triazole, (d) 1,2,3-triaozle.

Discussions:

The mass spectra in Fig S2a and 2b were obtained from Wiley Subscription Services, Inc. (USA) through the SciFinder search engine. Note that the EI-MS spectra of imidazole and pyrazole are very similar. It is very hard to differentiate them. The mass spectra in Fig S2c and 2d were obtained from the National Institute of Advanced Industrial Science and Technology (Japan) through the Scifinder search engine. Note that the EI-MS spectra of 1,2,4-triazole and 1,2,3-triazole are also very similar. It is very hard to differentiate them, too. However, by supramolecular recognition by uracil as discussed in the main text, these two groups of isomers can be much easier to clearly differentiate.

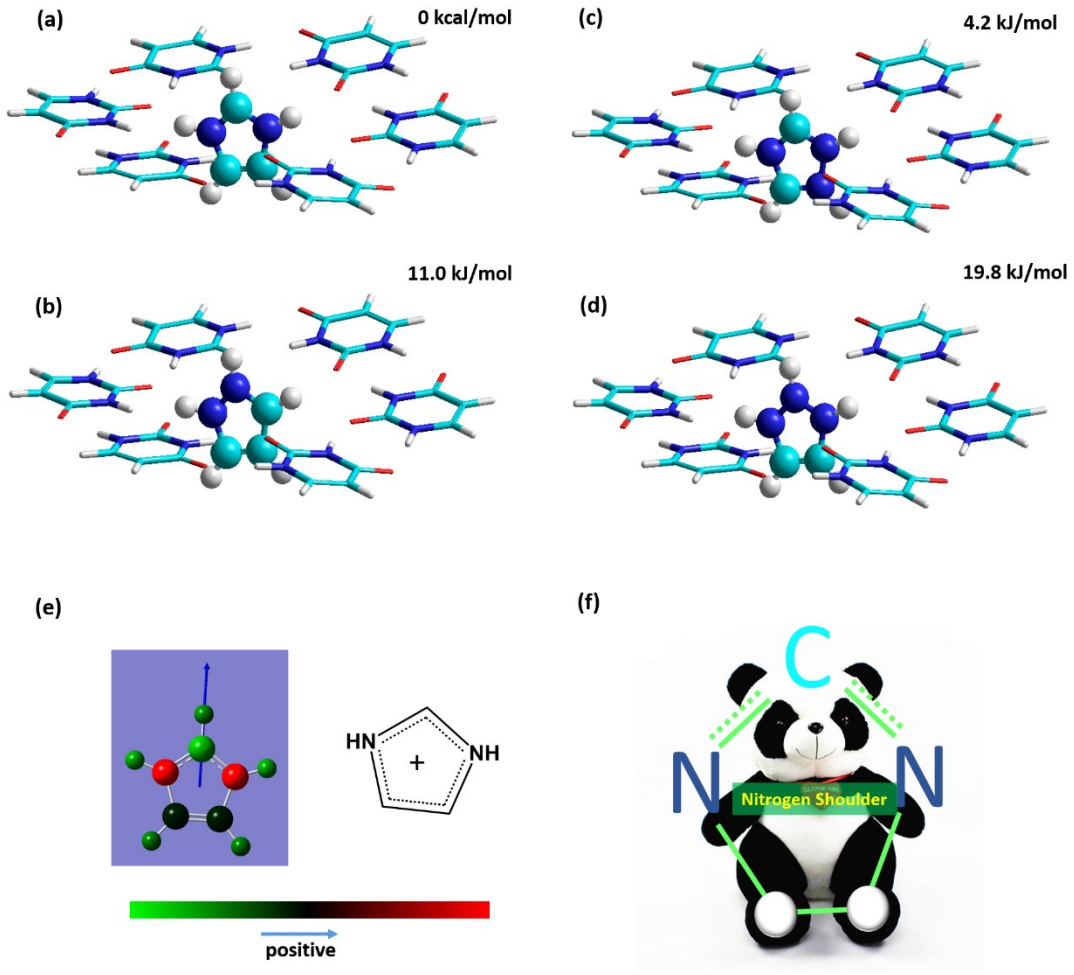

Fig S3 Theoretically optimized structures of (a) imidazole, (b) pyrazole, (c) 1,2,4-triazole, and (d) 1,2,3-triazole self-assemblies with uracil. (e) Calculated charge distribution of imidazole. The arrow shows the dipole moment. (f) Schematic illustration of the "nitrogen shoulder" model (see discussions below).

Discussions:

From the calculations shown in Fig S3, the 6-mer corresponding to imidazole is the most stable one, and followed by 1,2,4-triazole. In the optimized structure, the nitrogen atoms in the "nitrogen shoulder" are in the plane formed by the uracil molecules. The partial positive charges on the nitrogen shoulder, as shown in Fig S3e, would stabilize the whole self-assembly by charge-dipole interactions. If the heterocycle in the center do not have nitrogen shoulder, the relative Gibbs free energy of the self-assembly become higher, and such cluster can barely be seen in mass spectra.

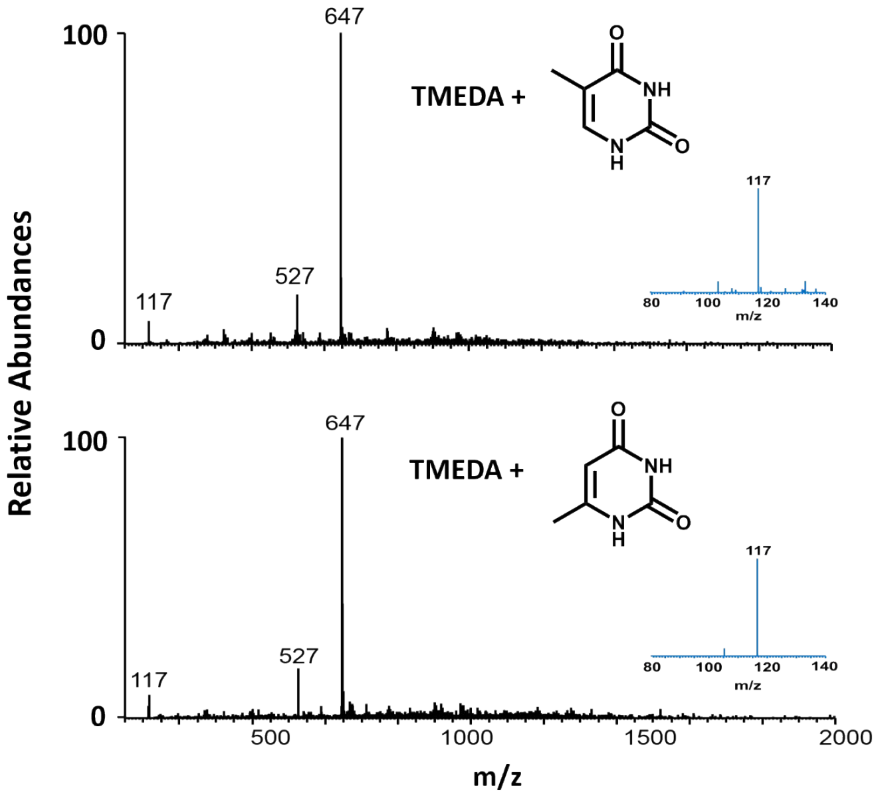

Fig S4 Single-barrel nano-ESI analyses of mixed solution of (a) TMEDA and thymine, (b) TMEDA and 6MU. Insets show the mass spectra at lower mass range. Ions: $[TMEDA+H]^+$ (m/z 117), $[T_4/6MU_4 + Na\ ]^+$ (m/z 527), $[T_5/6MU_5 + NH_4]^+$ (m/z 647).

5 Coordinates of Calculated Models

Di-protonated 1,3-propanediamine

C	−2.48815171	−0.45023696	0.00000000
H	−2.13149729	−1.45904696	0.00000000
H	−3.55815171	−0.45022378	0.00000000
C	−1.97480949	0.27571931	1.25740497
H	−0.90481130	0.27401225	1.25838332
H	−2.32986605	1.28509233	1.25642758
C	−2.49044893	−0.44861033	2.51480806
H	−2.13570049	−1.45809184	2.51559626
H	−3.56044671	−0.44657699	2.51401810
N	−2.00001782	0.24404871	3.71505835
H	−2.77759780	0.56016406	4.25860270
H	−1.44613870	−0.38528866	4.26017521
N	−1.99814323	0.24272130	−1.20025020
H	−1.44213590	−0.38566243	−1.74429959
H	−2.77591701	0.55651288	−1.74486272
H	−1.44269034	1.02846737	3.44289395
H	−1.44303768	1.02871363	−0.92808502

Di-protonated 1,2-propanediamine

C	−2.48815171	−0.45023696	0.00000000
H	−2.13149743	−1.45904701	−0.00000031
H	−3.55815171	−0.45022382	−0.00000002
C	−1.97480949	0.27571931	1.25740497
H	−0.90481130	0.27401225	1.25838332
C	−2.49044893	−0.44861033	2.51480806
H	−2.13570049	−1.45809184	2.51559626
H	−3.56044671	−0.44657699	2.51401810
N	−2.00001782	0.24404871	3.71505835
H	−2.77759780	0.56016406	4.25860270
H	−1.44613870	−0.38528866	4.26017521
H	−1.44269034	1.02846737	3.44289395
H	−2.13147883	0.05416177	−0.87365118
N	−2.46259747	1.66242803	1.25606220
H	−1.69918465	2.28415086	1.08095769
H	−3.15277898	1.77231221	0.54081752
H	−2.86765735	1.87416029	2.14549795

6-mer induced by 1,3-propanediamine

O	6.75920000	-8.55110000	0.40510000
O	6.06090000	-4.50970000	2.31610000
N	6.25370000	-6.80580000	-0.89390000
C	5.95250000	-5.53190000	-1.08400000
C	5.87870000	-4.65000000	-0.02960000
C	5.55650000	-3.18900000	-0.21840000
H	6.61390000	-6.99570000	2.27910000
H	6.30610000	-7.40070000	-1.68960000
H	5.76940000	-5.19100000	-2.06250000
H	5.42670000	-2.95240000	-1.27470000
H	6.37340000	-2.58810000	0.18310000
H	4.63710000	-2.95060000	0.31720000
O	7.38040000	-12.08770000	-1.54310000
O	6.06390000	-8.51980000	-3.99870000
C	6.42450000	-9.69360000	-3.94350000
N	6.75570000	-10.29220000	-2.70650000
C	7.08780000	-11.57000000	-2.65600000
N	7.11730000	-12.31980000	-3.74670000
C	6.83620000	-11.85270000	-4.95210000
C	6.47950000	-10.53680000	-5.14370000
C	6.15100000	-9.97600000	-6.50490000
H	6.73010000	-9.75180000	-1.87290000
H	7.36090000	-13.28130000	-3.65770000
H	6.88410000	-12.50440000	-5.77710000
H	6.20370000	-10.75110000	-7.26960000
H	5.14240000	-9.56160000	-6.48690000
H	6.86090000	-9.18450000	-6.74840000
O	7.16990000	-15.83380000	0.56300000
O	8.11030000	-15.76880000	-3.86010000
C	7.79360000	-16.39430000	-2.85050000
O	6.62760000	-15.62310000	9.00240000
C	6.64030000	-14.39680000	8.91350000
N	6.59180000	-13.76160000	7.65290000
C	6.62030000	-12.44340000	7.57390000
N	6.70080000	-11.68730000	8.65740000
C	6.74640000	-12.18370000	9.88270000
C	6.71470000	-13.54160000	10.10410000
C	6.75190000	-14.13490000	11.48950000
H	6.53380000	-14.30740000	6.82480000
H	6.72370000	-10.69870000	8.55020000
H	6.80370000	-11.52270000	10.69970000
H	6.77900000	-13.35110000	12.24690000
H	5.86190000	-14.74690000	11.64200000
H	7.64010000	-14.75940000	11.58910000
C	6.14040000	-5.20370000	1.30440000
N	6.43970000	-6.58190000	1.39360000
C	6.48780000	-7.32320000	0.30180000
N	7.62260000	-15.73570000	-1.61240000
C	7.31860000	-16.43790000	-0.53430000
N	7.16010000	-17.74930000	-0.57840000
C	7.26750000	-18.45010000	-1.69760000
C	7.58030000	-17.84710000	-2.89370000
C	7.67700000	-18.61680000	-4.18920000
H	7.73220000	-14.74720000	-1.55150000
H	6.93710000	-18.23940000	0.26200000
H	7.10710000	-19.48660000	-1.66590000
H	7.63860000	-19.69220000	-4.00700000
H	8.61820000	-18.37260000	-4.68310000
H	6.84470000	-18.33290000	-4.83500000
O	6.42780000	-15.45720000	4.62510000
O	6.87390000	-19.46020000	2.57680000
C	6.72550000	-18.81140000	3.61030000
N	6.60930000	-17.40510000	3.56700000
C	6.52250000	-16.71340000	4.68850000
N	6.53870000	-17.30770000	5.87120000
C	6.64510000	-18.61820000	6.01970000
C	6.73940000	-19.45440000	4.93010000
C	6.85830000	-20.95180000	5.06360000
H	6.59560000	-16.93530000	2.69130000
H	6.46950000	-16.74550000	6.68930000
H	6.65890000	-19.02150000	6.99180000
H	6.81570000	-21.25290000	6.11060000
H	6.03960000	-21.42850000	4.52250000
H	7.80760000	-21.27690000	4.63650000
O	6.56560000	-11.89490000	6.43940000
O	6.73540000	-8.54780000	4.32290000
O	6.77460000	-8.13940000	8.82920000
C	6.70970000	-7.61740000	7.71830000
N	6.77120000	-8.40210000	6.54460000
C	6.68090000	-7.82850000	5.35820000
N	6.52910000	-6.51900000	5.23510000
C	6.44190000	-5.70010000	6.26960000
C	6.52500000	-6.17000000	7.56040000
C	6.43750000	-5.25780000	8.75720000
H	6.88330000	-9.38690000	6.61160000
H	6.47470000	-6.12650000	4.32330000
H	6.30720000	-4.67090000	6.09660000
H	6.34470000	-4.21680000	8.44690000
H	7.33980000	-5.37070000	9.35920000

H	5.56790000	-5.53140000	9.35560000
O	11.98350000	-12.19500000	-1.14090000
O	13.04870000	-8.97680000	-4.13520000
C	12.97010000	-10.17050000	-3.84880000
N	12.42060000	-10.57760000	-2.61130000
C	12.45560000	-11.85030000	-2.26000000
N	12.98790000	-12.77130000	-3.04830000
C	13.52420000	-12.49330000	-4.22510000
C	13.55650000	-11.20450000	-4.70900000
C	14.19970000	-10.85150000	-6.02880000
H	12.02010000	-9.90190000	-2.00130000
H	12.99790000	-13.71830000	-2.73710000
H	13.94130000	-13.27350000	-4.79240000
H	14.44930000	-11.74790000	-6.59600000
H	13.51470000	-10.24090000	-6.61710000
H	15.11200000	-10.28430000	-5.84380000
O	12.90840000	-8.72970000	0.23680000
O	13.12530000	-4.60450000	2.09170000
C	13.18070000	-5.32620000	1.09710000
N	12.99160000	-6.72210000	1.20570000
C	13.04450000	-7.48080000	0.12540000
N	13.25580000	-6.96580000	-1.07500000
C	13.46800000	-5.67610000	-1.27990000
C	13.45920000	-4.77730000	-0.23680000
C	15.27670000	-14.85600000	5.84260000
N	14.25960000	-14.03900000	5.29750000
C	14.02240000	-12.84610000	5.81360000
N	14.71090000	-12.39040000	6.84870000
C	15.67960000	-13.07820000	7.43050000
C	16.03340000	-14.33220000	6.98570000
C	17.16530000	-15.12050000	7.60000000
H	13.73050000	-14.36020000	4.51900000
H	14.49910000	-11.48160000	7.19930000
H	16.19370000	-12.64820000	8.24050000
H	17.56430000	-14.61450000	8.47900000
H	16.80590000	-16.10760000	7.89140000
H	17.96250000	-15.23390000	6.86490000
O	12.97490000	-14.36110000	1.94270000
O	13.75140000	-16.31930000	-2.06180000
C	13.95110000	-16.27420000	-0.84810000
N	13.27320000	-15.33040000	-0.04240000
C	13.56640000	-15.22800000	1.24180000
N	14.47580000	-16.00550000	1.80940000
C	15.16130000	-16.92100000	1.14460000
C	14.95920000	-17.12390000	-0.20200000
C	13.73360000	-3.30690000	-0.43020000
H	12.82440000	-7.13090000	2.09640000
H	13.27200000	-7.57820000	-1.86040000
H	13.65450000	-5.33950000	-2.25930000
H	13.82520000	-3.06400000	-1.48840000
H	12.91480000	-2.72930000	-0.00160000
H	14.66220000	-3.04450000	0.07770000
O	12.15880000	-8.14740000	4.39320000
O	14.57860000	-8.94300000	8.13720000
C	14.18110000	-8.15650000	7.27760000
N	13.27970000	-8.58180000	6.27430000
C	12.96790000	-7.76640000	5.28250000
N	13.47930000	-6.54820000	5.19840000
C	14.30000000	-6.04530000	6.10600000
C	14.69910000	-6.78540000	7.19570000
C	15.65910000	-6.24870000	8.23140000
H	12.88680000	-9.49550000	6.31420000
H	13.23350000	-5.98100000	4.41670000
H	14.65170000	-5.06210000	5.98380000
H	15.85900000	-5.18920000	8.07100000
H	15.23630000	-6.38070000	9.22780000
H	16.59810000	-6.79870000	8.16850000
O	13.12770000	-12.11700000	5.30400000
O	15.57730000	-15.92240000	5.30820000
C	15.74700000	-18.14240000	-0.98940000
H	12.58060000	-14.74070000	-0.44490000
H	14.65960000	-15.89310000	2.78200000
H	15.87510000	-17.49790000	1.65900000
H	16.31260000	-18.79640000	-0.32600000
H	15.06210000	-18.74850000	-1.58260000
H	16.43870000	-17.62700000	-1.65610000
C	9.33850000	-10.97480000	2.47880000
C	10.63030000	-11.80700000	2.64390000
H	10.66030000	-12.58450000	1.87660000
H	10.65020000	-12.26300000	3.63910000
N	11.81140000	-10.93300000	2.50210000
H	12.65450000	-11.50330000	2.46370000
H	11.74680000	-10.38180000	1.64950000
H	11.87410000	-10.31670000	3.30890000
H	7.22390000	-11.07440000	2.93760000
H	8.23300000	-12.13970000	3.92950000
C	8.07810000	-11.75820000	2.91760000
N	7.76140000	-12.88890000	2.01960000
H	6.93150000	-13.36860000	2.36690000
H	7.57590000	-12.55100000	1.07590000

H	8.53430000	-13.55350000	1.99350000

6-mer induced by 1,2-propanediamine

O	5.88940000	-8.84130000	0.26270000
O	5.29800000	-4.98080000	2.64930000
C	5.32100000	-5.53020000	1.55300000
N	5.57170000	-6.92610000	1.43190000
C	5.61950000	-7.57160000	0.27140000
N	5.39350000	-6.88790000	-0.85530000
C	5.14280000	-5.56220000	-0.86640000
C	5.10020000	-4.81440000	0.31320000
C	4.83870000	-3.33580000	0.35290000
H	5.71250000	-7.40290000	2.29030000
H	5.40470000	-7.35810000	-1.75030000
H	4.96650000	-5.03130000	-1.79100000
H	4.69370000	-2.95310000	-0.67100000
H	5.70520000	-2.83110000	0.82190000
H	3.92950000	-3.14810000	0.95550000
O	6.50670000	-12.29780000	-1.04610000
O	5.41100000	-8.42670000	-3.24230000
C	5.66030000	-9.62590000	-3.30990000
N	5.95230000	-10.38710000	-2.14250000
C	6.23790000	-11.68530000	-2.15910000
N	6.24680000	-12.32610000	-3.33270000
C	5.97790000	-11.71340000	-4.50410000
C	5.67610000	-10.35040000	-4.56420000
C	5.37820000	-9.61930000	-5.84170000
H	5.92940000	-9.87820000	-1.29190000
H	6.46160000	-13.31300000	-3.37310000
H	5.98690000	-12.25650000	-5.43840000
H	5.43270000	-10.31640000	-6.69430000
H	4.36220000	-9.18480000	-5.77760000
H	6.12060000	-8.80870000	-5.97260000
O	6.32830000	-15.25190000	1.36330000
O	6.82130000	-15.09870000	-3.19170000
C	6.68960000	-15.78250000	-2.18220000
N	6.57070000	-15.18530000	-0.89420000
C	6.42620000	-15.87960000	0.23050000
N	6.38490000	-17.21480000	0.16040000
C	6.48310000	-17.89170000	-1.00250000
C	6.64010000	-17.22940000	-2.22280000
C	6.74840000	-17.93480000	-3.54380000
H	6.60370000	-14.19250000	-0.88520000
H	6.27550000	-17.76640000	1.00070000
H	6.44370000	-18.97130000	-1.03140000
H	6.69260000	-19.02570000	-3.39210000
H	7.71560000	-17.67110000	-4.01270000
H	5.91740000	-17.60430000	-4.19610000
O	5.83600000	-14.70240000	5.03520000
O	6.12510000	-18.59290000	2.63680000
C	6.02630000	-18.05380000	3.73440000
N	5.97410000	-16.63630000	3.85900000
C	5.87930000	-15.99990000	5.02210000
N	5.82680000	-16.71980000	6.14800000
C	5.86930000	-18.06830000	6.15560000
C	5.95960000	-18.80470000	4.97130000
C	6.00570000	-20.30530000	4.92750000
H	6.01200000	-16.13700000	3.00200000
H	5.75060000	-16.25990000	7.04610000
H	5.83520000	-18.62740000	7.08000000
H	5.94390000	-20.71250000	5.95050000
H	5.15210000	-20.67300000	4.32630000
H	6.95540000	-20.62150000	4.45520000
O	5.82550000	-11.19650000	6.36020000
O	5.79970000	-15.21140000	8.56580000
C	5.82800000	-13.98680000	8.63700000
N	5.81580000	-13.17870000	7.46460000
C	5.83990000	-11.84960000	7.48190000
N	5.87130000	-11.22150000	8.66180000
C	5.89350000	-11.87980000	9.83890000
C	5.87370000	-13.27570000	9.89850000
C	5.90210000	-14.05300000	11.18340000
H	5.78650000	-13.67990000	6.60890000
H	5.87950000	-10.21140000	8.70280000
H	5.92800000	-11.34860000	10.77950000
H	5.93560000	-13.35960000	12.04030000
H	4.99160000	-14.67930000	11.24410000
H	6.79930000	-14.70130000	11.19100000
O	5.79460000	-8.28280000	3.95220000
O	5.83120000	-8.38840000	8.53280000
C	5.77160000	-7.71490000	7.50970000

N	5.80000000	-8.32140000	6.22130000
C	5.74060000	-7.64110000	5.08080000
N	5.62500000	-6.31010000	5.13210000
C	5.59150000	-5.62410000	6.29350000
C	5.66990000	-6.27030000	7.52970000
C	5.64890000	-5.55050000	8.84800000
H	5.86850000	-9.31150000	6.22560000
H	5.55850000	-5.76910000	4.28090000
H	5.50290000	-4.54720000	6.30740000
H	5.56830000	-4.46360000	8.68030000
H	6.58460000	-5.77640000	9.39480000
H	4.78080000	-5.90430000	9.43650000
O	12.51050000	-12.53260000	-0.67050000
O	13.28660000	-9.01610000	-3.45030000
C	13.24880000	-10.23960000	-3.32760000
N	12.83850000	-10.82630000	-2.10130000
C	12.84870000	-12.12950000	-1.85220000
N	13.21060000	-12.96660000	-2.83060000
C	13.58730000	-12.53160000	-4.05260000
C	13.61440000	-11.17000000	-4.37690000
C	14.03250000	-10.64460000	-5.72020000
H	12.52500000	-10.18400000	-1.41530000
H	13.20630000	-13.97280000	-2.67310000
H	13.88520000	-13.22310000	-4.82850000
H	14.27290000	-11.48440000	-6.39340000
H	13.20290000	-10.04890000	-6.14670000
H	14.92370000	-10.00080000	-5.59170000
O	12.71870000	-9.15480000	0.13450000
O	13.28420000	-5.17050000	2.27430000
C	13.22970000	-5.76290000	1.19690000
N	12.95420000	-7.15540000	1.15620000
C	12.93600000	-7.88570000	0.04650000
N	13.14550000	-7.27220000	-1.12400000
C	13.38470000	-5.94750000	-1.21810000
C	13.43570000	-5.12350000	-0.08730000
C	13.70520000	-3.64770000	-0.14600000
H	12.76520000	-7.57170000	2.02990000
H	13.12570000	-7.80670000	-1.98680000
H	13.54760000	-5.47170000	-2.17500000
H	13.83580000	-3.33140000	-1.19450000
H	12.84960000	-3.10860000	0.30370000
H	14.62540000	-3.42820000	0.42860000
O	12.63320000	-8.46370000	3.58030000
O	14.60070000	-9.31120000	7.59110000
C	14.28260000	-8.45760000	6.76370000

N	13.54350000	-8.82100000	5.60700000
C	13.24670000	-7.99280000	4.61350000
N	13.59580000	-6.70650000	4.72840000
C	14.26050000	-6.22930000	5.80270000
C	14.62730000	-7.05410000	6.87270000
C	15.37710000	-6.56520000	8.07850000
H	13.24250000	-9.76370000	5.58350000
H	13.35890000	-6.04480000	3.99420000
H	14.53720000	-5.18680000	5.87470000
H	15.55260000	-5.47950000	7.99640000
H	14.77900000	-6.78010000	8.98460000
H	16.34570000	-7.09750000	8.13840000
O	13.23030000	-11.52710000	5.01250000
O	15.39200000	-15.54020000	4.84280000
C	15.20520000	-14.49410000	5.46070000
N	14.28580000	-13.52320000	4.97790000
C	14.06470000	-12.34800000	5.55690000
N	14.71820000	-12.06160000	6.68900000
C	15.60390000	-12.90940000	7.25340000
C	15.88830000	-14.16010000	6.69390000
C	16.86870000	-15.13110000	7.28610000
H	13.79500000	-13.78050000	4.15660000
H	14.55390000	-11.17760000	7.16140000
H	16.12950000	-12.65110000	8.16200000
H	17.29040000	-14.71750000	8.21750000
H	16.34560000	-16.08220000	7.50230000
H	17.68020000	-15.31170000	6.55540000
O	13.32560000	-13.93920000	2.35650000
O	13.83940000	-15.66590000	-1.82730000
C	14.08310000	-15.79130000	-0.62620000
N	13.54490000	-14.86990000	0.31080000
C	13.81360000	-14.87420000	1.61170000
N	14.58600000	-15.85240000	2.09740000
C	15.13480000	-16.80310000	1.31260000
C	14.91760000	-16.83800000	-0.07010000
C	15.52780000	-17.86540000	-0.97930000
H	12.92590000	-14.19880000	-0.06900000
H	14.77590000	-15.90120000	3.09300000
H	15.76800000	-17.57580000	1.72540000
H	16.12640000	-18.58010000	-0.38990000
H	14.71790000	-18.40260000	-1.50860000
H	16.17570000	-17.35240000	-1.71570000
C	9.14600000	-11.22380000	2.55960000
C	10.55140000	-11.81390000	2.74320000
C	9.00100000	-9.74830000	2.19890000

H	10.62910000	-12.65560000	2.01930000
H	10.57210000	-12.08840000	3.81630000
H	7.92770000	-9.49910000	2.11150000
H	9.50500000	-9.55350000	1.23170000
H	9.46310000	-9.12470000	2.98850000
N	11.77350000	-10.94700000	2.55610000
N	7.92480000	-12.08860000	2.74340000
H	12.54500000	-11.49610000	2.18960000
H	11.58560000	-10.19400000	1.91660000
H	12.06260000	-10.55420000	3.44240000
H	8.04730000	-12.98430000	2.28480000
H	7.10730000	-11.63960000	2.34620000
H	7.74760000	-12.25700000	3.72670000

16-mer induced by 1,3-propanediamine

O	1.43310000	-3.47120000	-0.70850000
O	-1.40790000	-6.32600000	1.45570000
C	-0.37570000	-6.17890000	0.80950000
N	0.02890000	-4.89450000	0.34940000
C	1.14000000	-4.68460000	-0.34650000
N	1.92470000	-5.71790000	-0.65350000
C	1.64110000	-6.97800000	-0.26870000
C	0.49460000	-7.28460000	0.47680000
H	-0.58630000	-4.13940000	0.58880000
H	2.78210000	-5.54650000	-1.18890000
H	2.31880000	-7.75740000	-0.54440000
C	0.12970000	-8.66210000	0.93510000
H	0.03950000	-8.68490000	2.02240000
H	-0.84040000	-8.95080000	0.52760000
H	0.87400000	-9.39180000	0.62660000
O	3.46580000	-0.72020000	-2.20680000
O	4.33320000	-5.20440000	-2.09670000
C	4.70680000	-4.08190000	-2.41810000
N	3.90400000	-2.93590000	-2.15950000
C	4.27040000	-1.70240000	-2.47940000
N	5.44770000	-1.50210000	-3.06790000
C	6.28920000	-2.51240000	-3.36340000
C	5.97590000	-3.84630000	-3.06840000
H	3.03900000	-3.10810000	-1.68260000
H	5.72630000	-0.54280000	-3.28450000
H	7.21930000	-2.27980000	-3.83290000
C	6.86740000	-5.00920000	-3.37320000
H	7.11240000	-5.54750000	-2.45620000
H	6.35620000	-5.71400000	-4.03090000
H	7.78940000	-4.68660000	-3.85020000
O	2.51430000	2.79850000	-1.29070000
O	6.15690000	1.18410000	-3.53520000
C	5.56960000	2.15270000	-3.06970000
N	4.32620000	2.00630000	-2.39320000
C	3.65050000	3.02550000	-1.88010000
N	4.15100000	4.25460000	-1.98400000
C	5.31940000	4.51390000	-2.60400000
C	6.09210000	3.49570000	-3.17890000
H	3.98100000	1.06980000	-2.32790000
H	3.61760000	5.02960000	-1.58680000
H	5.65670000	5.52550000	-2.65560000
C	7.39480000	3.71970000	-3.88110000
H	8.19180000	3.16400000	-3.38470000
H	7.33770000	3.35190000	-4.90680000
H	7.65880000	4.77390000	-3.89940000
O	-0.72320000	3.53770000	0.47670000
O	2.60580000	6.36290000	-0.87060000
C	1.51430000	6.22340000	-0.32950000
N	0.92160000	4.93980000	-0.19000000
C	-0.25450000	4.74330000	0.39240000
N	-0.92540000	5.78720000	0.87770000
C	-0.46290000	7.04890000	0.79490000
C	0.76860000	7.34320000	0.19400000
H	1.45490000	4.17780000	-0.56280000
H	-1.82590000	5.61890000	1.33520000
H	-1.05730000	7.83830000	1.20000000
C	1.34170000	8.71720000	0.06900000
H	2.30670000	8.76620000	0.57460000
H	1.51590000	8.95520000	-0.98110000
H	0.67970000	9.46410000	0.49630000
O	-3.12460000	0.75440000	1.49530000
O	-3.41840000	5.25380000	2.21240000
C	-3.91430000	4.14180000	2.36540000
N	-3.29170000	2.98250000	1.82800000
C	-3.77300000	1.75660000	1.98850000
N	-4.90910000	1.58320000	2.65820000
C	-5.58800000	2.60810000	3.20810000
C	-5.14280000	3.93310000	3.09660000
H	-2.42900000	3.14450000	1.34140000
H	-5.23770000	0.62710000	2.80210000
H	-6.48630000	2.39790000	3.74320000
C	-5.84650000	5.11190000	3.69060000

H	-5.18950000	5.62480000	4.39460000
H	-6.10270000	5.83050000	2.91050000
H	-6.75350000	4.81310000	4.20970000
O	-1.80180000	-2.71940000	1.04000000
O	-5.57880000	-1.13900000	3.07280000
C	-4.88930000	-2.11030000	2.78120000
N	-3.68480000	-1.95420000	2.04060000
C	-2.88600000	-2.96340000	1.71240000
N	-3.21520000	-4.19900000	2.08890000
C	-4.33740000	-4.46920000	2.78550000
C	-5.23550000	-3.46160000	3.16580000
H	-3.46810000	-1.01410000	1.78460000
H	-2.58220000	-4.96820000	1.85050000
H	-4.53690000	-5.48460000	3.05300000
C	-6.49680000	-3.70630000	3.93540000
H	-6.48430000	-3.14290000	4.86970000
H	-7.35990000	-3.35940000	3.36470000
H	-6.62550000	-4.76220000	4.16120000
C	0.09200000	0.42000000	1.17800000
C	-0.00850000	-0.18100000	-0.24190000
C	-1.21930000	0.47820000	-0.94140000
H	-0.83800000	0.25390000	1.72140000
H	0.26000000	1.49730000	1.12010000
H	-0.15480000	-1.25840000	-0.18170000
H	0.90560000	0.02030000	-0.80080000
H	-2.11420000	0.35730000	-0.33540000
H	-1.04510000	1.54780000	-1.07170000
H	-1.73380000	-1.08440000	-2.26950000
H	-2.33060000	0.40320000	-2.66600000
H	-0.74270000	0.04200000	-2.93890000
N	-1.51500000	-0.08610000	-2.28650000
H	1.20350000	0.40730000	2.88920000
H	1.00410000	-1.13920000	2.30800000
H	2.11470000	-0.09920000	1.58830000
N	1.18080000	-0.15720000	2.02540000
O	0.62480000	0.22950000	-4.22410000
O	1.36130000	-3.97410000	-5.79860000
C	1.66600000	-2.78330000	-5.84880000
N	1.05580000	-1.85350000	-4.96650000
C	1.26710000	-0.54370000	-5.01950000
N	2.12840000	-0.05770000	-5.91220000
C	2.80070000	-0.84790000	-6.76600000
C	2.63020000	-2.24160000	-6.78330000
C	3.35130000	-3.15950000	-7.71960000
H	0.36130000	-2.22790000	-4.35300000
H	2.23000000	0.96010000	-5.99430000
H	3.47570000	-0.39050000	-7.45390000
H	4.03950000	-2.61110000	-8.35960000
H	3.91170000	-3.90620000	-7.15480000
H	2.63710000	-3.69700000	-8.34540000
O	-1.17790000	-2.81250000	-3.52950000
O	-4.98100000	-5.30910000	-3.53700000
C	-3.80600000	-5.22170000	-3.88820000
N	-3.03610000	-4.08480000	-3.52390000
C	-1.77870000	-3.89260000	-3.90010000
N	-1.18100000	-4.81620000	-4.65280000
C	-1.80120000	-5.94660000	-5.03830000
C	-3.12930000	-6.22860000	-4.67890000
C	-3.85800000	-7.47400000	-5.07830000
H	-3.51530000	-3.38150000	-3.00540000
H	-0.23030000	-4.63640000	-4.99180000
H	-1.26020000	-6.64300000	-5.63920000
H	-3.22200000	-8.13730000	-5.66110000
H	-4.20360000	-8.00600000	-4.19040000
H	-4.74140000	-7.22300000	-5.66730000
O	-4.39580000	-2.01110000	-2.31680000
O	-8.12440000	0.55690000	-1.90540000
C	-7.66270000	-0.56960000	-2.07520000
N	-6.25670000	-0.77730000	-2.07430000
C	-5.68670000	-1.94800000	-2.31740000
N	-6.45520000	-3.00820000	-2.56160000
C	-7.79960000	-2.94160000	-2.54800000
C	-8.48270000	-1.74220000	-2.29260000
C	-9.97440000	-1.61880000	-2.26480000
H	-5.69080000	0.03750000	-1.95840000
H	-6.00890000	-3.89480000	-2.81700000
H	-8.35520000	-3.83100000	-2.74470000
H	-10.45460000	-2.57870000	-2.44270000
H	-10.30060000	-1.23470000	-1.29680000
H	-10.30990000	-0.90900000	-3.02270000
O	-4.64130000	1.53260000	-2.13900000
O	-4.02610000	5.50740000	-4.25770000
C	-4.82140000	4.74820000	-3.70850000
N	-4.36760000	3.53120000	-3.13320000
C	-5.16760000	2.62670000	-2.58800000
N	-6.47680000	2.86950000	-2.53070000
C	-7.01920000	4.00510000	-3.00920000
C	-6.24200000	5.01010000	-3.60680000
C	-6.80230000	6.28770000	-4.15030000
H	-3.39770000	3.33440000	-3.24240000

H	-7.10350000	2.13490000	-2.18340000
H	-8.07620000	4.13320000	-2.93360000
H	-7.87780000	6.34620000	-3.99600000
H	-6.32900000	7.14220000	-3.66340000
H	-6.59290000	6.36820000	-5.21800000
O	-1.75080000	2.76370000	-3.69110000
O	1.98550000	2.82770000	-6.26470000
C	0.98570000	3.44120000	-5.89550000
N	0.10340000	2.85640000	-4.94990000
C	-1.02440000	3.41470000	-4.53980000
N	-1.36810000	4.60960000	-5.01600000
C	-0.59120000	5.28230000	-5.88680000
C	0.62110000	4.76090000	-6.36760000
C	1.51630000	5.47920000	-7.32930000
H	0.35760000	1.95520000	-4.61900000
H	-2.26710000	5.01640000	-4.73380000
H	-0.91850000	6.24180000	-6.22000000
H	1.11930000	6.45990000	-7.58260000
H	2.51000000	5.60260000	-6.89540000
H	1.63410000	4.89830000	-8.24520000
O	-1.06750000	0.16190000	4.31400000
O	-1.70190000	-4.03980000	5.92190000
C	-2.02580000	-2.85490000	5.98370000
N	-1.45360000	-1.90850000	5.08990000
C	-1.69120000	-0.60690000	5.14340000

N	-2.54700000	-0.13600000	6.04780000
C	-3.18250000	-0.94100000	6.91950000
C	-2.97770000	-2.32990000	6.94090000
C	-3.65600000	-3.25750000	7.90090000
H	-0.76490000	-2.25740000	4.45650000
H	-2.67860000	0.87820000	6.12350000
H	-3.85610000	-0.49910000	7.61890000
H	-4.35350000	-2.72230000	8.54200000
H	-4.20000000	-4.03040000	7.35590000
H	-2.91820000	-3.76270000	8.52650000
O	0.74900000	-2.74930000	3.50470000
O	4.67740000	-5.04710000	3.59510000
C	3.49930000	-5.00460000	3.94340000
N	2.67550000	-3.91870000	3.54190000
C	1.40820000	-3.77890000	3.91170000
N	0.85920000	-4.70370000	4.70130000
C	1.53430000	-5.78710000	5.12350000
C	2.87320000	-6.01680000	4.76840000
C	3.66150000	-7.21090000	5.20880000
H	3.12430000	-3.20600000	3.00860000
H	-0.09960000	-4.56570000	5.03950000
H	1.02780000	-6.48630000	5.75130000
H	3.05760000	-7.88320000	5.81470000
H	4.03250000	-7.75580000	4.33920000
H	4.53140000	-6.89790000	5.78810000
O	3.96000000	-1.80240000	2.31100000
O	7.61380000	0.86130000	1.82720000
C	7.18910000	-0.27600000	2.02340000
N	5.78970000	-0.52530000	2.02330000
C	5.24850000	-1.70230000	2.30360000
N	6.04700000	-2.73280000	2.57590000
C	7.38920000	-2.62970000	2.55800000
C	8.04170000	-1.41980000	2.27160000
C	9.53050000	-1.26020000	2.23950000
H	5.20640000	0.26890000	1.87450000
H	5.62640000	-3.62410000	2.85160000
H	7.96760000	-3.49910000	2.77660000
H	10.03490000	-2.20350000	2.43920000
H	9.84710000	-0.89130000	1.26250000
H	9.84970000	-0.52500000	2.97990000
O	4.13330000	1.70130000	1.95300000
O	3.29470000	5.62770000	4.09370000
C	4.12940000	4.90900000	3.55090000
N	3.74430000	3.66700000	2.97620000
C	4.59550000	2.81570000	2.42340000
N	5.89050000	3.12620000	2.38170000
C	6.36930000	4.28710000	2.86820000
C	5.53410000	5.24850000	3.45860000
C	6.02010000	6.55490000	4.00640000
H	2.78950000	3.40620000	3.09890000
H	6.55750000	2.42500000	2.04270000
H	7.41860000	4.47160000	2.80330000
H	7.09180000	6.67230000	3.85910000
H	5.50470000	7.38290000	3.51630000
H	5.80020000	6.62430000	5.07290000
O	1.18300000	2.74270000	3.65390000
O	-2.52990000	2.75160000	6.27260000
C	-1.55780000	3.38570000	5.86890000
N	-0.66360000	2.79930000	4.93350000
C	0.43320000	3.39090000	4.48490000
N	0.72710000	4.61920000	4.90830000
C	-0.06190000	5.28930000	5.76900000

C	-1.24150000	4.73470000	6.29040000
C	-2.14620000	5.44860000	7.24660000
H	-0.87880000	1.87260000	4.64780000
H	1.60290000	5.05540000	4.60240000
H	0.23110000	6.27240000	6.06300000
H	-1.78030000	6.44980000	7.46530000
H	-3.15060000	5.52480000	6.82720000
H	-2.22800000	4.89050000	8.18060000

16-mer induced by 1,2-propanediamine

O	1.43560000	-3.47360000	-0.70730000
O	-1.40790000	-6.32600000	1.45570000
C	-0.37570000	-6.17890000	0.80950000
N	0.02890000	-4.89450000	0.34940000
C	1.14000000	-4.68490000	-0.34640000
N	1.92470000	-5.71790000	-0.65350000
C	1.64110000	-6.97800000	-0.26880000
C	0.49460000	-7.28460000	0.47680000
H	-0.58620000	-4.13990000	0.58890000
H	2.78200000	-5.54650000	-1.18890000
H	2.31880000	-7.75740000	-0.54440000
C	0.12970000	-8.66210000	0.93510000
H	0.03950000	-8.68490000	2.02240000
H	-0.84040000	-8.95080000	0.52760000
H	0.87400000	-9.39180000	0.62660000
O	3.46570000	-0.72020000	-2.20680000
O	4.33320000	-5.20440000	-2.09670000
C	4.70680000	-4.08190000	-2.41810000
N	3.90390000	-2.93580000	-2.15950000
C	4.27040000	-1.70250000	-2.47940000
N	5.44770000	-1.50210000	-3.06790000
C	6.28920000	-2.51230000	-3.36340000
C	5.97590000	-3.84630000	-3.06830000
H	3.03900000	-3.10810000	-1.68260000
H	5.72630000	-0.54290000	-3.28450000
H	7.21930000	-2.27990000	-3.83290000
C	6.86740000	-5.00920000	-3.37320000
H	7.11240000	-5.54750000	-2.45620000
H	6.35620000	-5.71400000	-4.03090000
H	7.78940000	-4.68660000	-3.85020000
O	2.51430000	2.79850000	-1.29070000
O	6.15690000	1.18410000	-3.53520000
C	5.56960000	2.15270000	-3.06970000
N	4.32620000	2.00630000	-2.39310000
C	3.65060000	3.02550000	-1.88010000
N	4.15100000	4.25450000	-1.98400000
C	5.31930000	4.51390000	-2.60390000
C	6.09210000	3.49570000	-3.17890000
H	3.98100000	1.06990000	-2.32790000
H	3.61760000	5.02960000	-1.58680000
H	5.65670000	5.52550000	-2.65560000
C	7.39480000	3.71970000	-3.88110000
H	8.19180000	3.16400000	-3.38470000
H	7.33770000	3.35190000	-4.90680000
H	7.65880000	4.77390000	-3.89940000
O	-0.72380000	3.54030000	0.47710000
O	2.60570000	6.36300000	-0.87060000
C	1.51430000	6.22340000	-0.32950000
N	0.92160000	4.93980000	-0.19000000
C	-0.25440000	4.74350000	0.39240000
N	-0.92540000	5.78720000	0.87760000
C	-0.46300000	7.04880000	0.79490000
C	0.76860000	7.34320000	0.19390000
H	1.45480000	4.17790000	-0.56280000
H	-1.82580000	5.61890000	1.33520000
H	-1.05730000	7.83830000	1.20000000
C	1.34170000	8.71720000	0.06900000
H	2.30670000	8.76620000	0.57460000
H	1.51590000	8.95520000	-0.98110000
H	0.67970000	9.46410000	0.49630000
O	-3.12720000	0.75480000	1.49460000
O	-3.41840000	5.25380000	2.21250000
C	-3.91430000	4.14180000	2.36540000
N	-3.29170000	2.98250000	1.82800000
C	-3.77300000	1.75670000	1.98850000
N	-4.90910000	1.58320000	2.65820000
C	-5.58800000	2.60800000	3.20810000
C	-5.14280000	3.93310000	3.09660000
H	-2.42910000	3.14460000	1.34140000
H	-5.23770000	0.62710000	2.80210000
H	-6.48630000	2.39790000	3.74320000
C	-5.84650000	5.11190000	3.69060000
H	-5.18950000	5.62480000	4.39460000
H	-6.10270000	5.83050000	2.91050000
H	-6.75350000	4.81310000	4.20970000
O	-1.80910000	-2.72500000	1.04780000
O	-5.57880000	-1.13900000	3.07280000
C	-4.88930000	-2.11030000	2.78120000
N	-3.68470000	-1.95420000	2.04050000

C	-2.88620000	-2.96350000	1.71250000
N	-3.21510000	-4.19900000	2.08880000
C	-4.33730000	-4.46920000	2.78550000
C	-5.23550000	-3.46160000	3.16580000
H	-3.46820000	-1.01410000	1.78460000
H	-2.58220000	-4.96820000	1.85050000
H	-4.53690000	-5.48460000	3.05300000
C	-6.49680000	-3.70630000	3.93540000
H	-6.48430000	-3.14290000	4.86970000
H	-7.35990000	-3.35940000	3.36470000
H	-6.62550000	-4.76220000	4.16120000
C	-0.36390000	0.47860000	0.33950000
C	-0.46510000	-0.12390000	-1.07980000
C	-1.66740000	0.53610000	-1.76590000
H	-1.29050000	0.30990000	0.88120000
H	-0.19600000	1.55100000	0.28050000
C	1.26690000	-0.54370000	-5.01930000
N	2.12840000	-0.05780000	-5.91220000
C	2.80070000	-0.84790000	-6.76590000
C	2.63020000	-2.24160000	-6.78330000
C	3.35130000	-3.15950000	-7.71960000
H	0.36130000	-2.22780000	-4.35300000
H	2.23010000	0.96010000	-5.99430000
H	3.47570000	-0.39050000	-7.45390000
H	4.03950000	-2.61110000	-8.35960000
H	3.91170000	-3.90620000	-7.15480000
H	2.63710000	-3.69700000	-8.34540000
O	-1.17890000	-2.81120000	-3.53020000
O	-4.98100000	-5.30910000	-3.53700000
C	-3.80590000	-5.22170000	-3.88820000
N	-3.03600000	-4.08470000	-3.52380000
C	-1.77870000	-3.89270000	-3.90020000
N	-1.18100000	-4.81620000	-4.65270000
C	-1.80110000	-5.94660000	-5.03830000
C	-3.12930000	-6.22860000	-4.67890000
C	-3.85800000	-7.47400000	-5.07830000
H	-3.51520000	-3.38150000	-3.00540000
H	-0.23030000	-4.63640000	-4.99180000
H	-1.26020000	-6.64300000	-5.63920000
H	-3.22200000	-8.13730000	-5.66110000
H	-4.20360000	-8.00600000	-4.19040000
H	-4.74140000	-7.22300000	-5.66730000
O	-4.39570000	-2.01100000	-2.31680000
O	-8.12440000	0.55680000	-1.90540000
C	-7.66270000	-0.56960000	-2.07520000
H	0.44930000	0.07790000	-1.63930000
H	-2.54790000	0.40410000	-1.15740000
H	-1.47870000	1.58680000	-1.89150000
H	0.74670000	0.46460000	2.05060000
H	0.54780000	-1.08590000	1.47320000
H	1.65870000	-0.04260000	0.74960000
N	0.72480000	-0.10000000	1.18740000
H	-1.82880000	0.08210000	-2.72740000
N	-0.66030000	-1.57050000	-1.00210000
H	-1.56130000	-1.81790000	-1.37750000
H	0.05660000	-2.03830000	-1.53010000
H	-0.60650000	-1.86790000	-0.04810000
O	0.61810000	0.22850000	-4.21840000
O	1.36130000	-3.97410000	-5.79860000
C	1.66600000	-2.78330000	-5.84880000
N	1.05580000	-1.85340000	-4.96650000
N	-6.25670000	-0.77730000	-2.07430000
C	-5.68680000	-1.94800000	-2.31740000
N	-6.45520000	-3.00820000	-2.56160000
C	-7.79950000	-2.94160000	-2.54800000
C	-8.48270000	-1.74220000	-2.29260000
C	-9.97440000	-1.61880000	-2.26480000
H	-5.69080000	0.03750000	-1.95840000
H	-6.00900000	-3.89480000	-2.81700000
H	-8.35520000	-3.83100000	-2.74470000
H	-10.45460000	-2.57870000	-2.44270000
H	-10.30060000	-1.23470000	-1.29680000
H	-10.30990000	-0.90900000	-3.02270000
O	-4.64160000	1.53270000	-2.13930000
O	-4.02610000	5.50740000	-4.25770000
C	-4.82140000	4.74820000	-3.70850000
N	-4.36760000	3.53110000	-3.13320000
C	-5.16760000	2.62670000	-2.58800000
N	-6.47670000	2.86950000	-2.53070000
C	-7.01920000	4.00510000	-3.00920000
C	-6.24190000	5.01010000	-3.60680000
C	-6.80230000	6.28770000	-4.15030000
H	-3.39770000	3.33440000	-3.24240000
H	-7.10350000	2.13490000	-2.18340000
H	-8.07610000	4.13320000	-2.93360000
H	-7.87780000	6.34620000	-3.99600000
H	-6.32900000	7.14220000	-3.66340000
H	-6.59290000	6.36820000	-5.21800000
O	-1.75120000	2.76530000	-3.69360000
O	1.98550000	2.82770000	-6.26470000

C	0.98570000	3.44130000	-5.89550000
N	0.10330000	2.85630000	-4.94990000
C	-1.02440000	3.41480000	-4.54000000
N	-1.36810000	4.60960000	-5.01600000
C	-0.59130000	5.28230000	-5.88680000
C	0.62110000	4.76080000	-6.36760000
C	1.51630000	5.47920000	-7.32930000
H	0.35760000	1.95520000	-4.61890000
H	-2.26710000	5.01640000	-4.73380000
H	-0.91850000	6.24180000	-6.22000000
H	1.11930000	6.45990000	-7.58260000
H	2.51000000	5.60260000	-6.89540000
H	1.63410000	4.89830000	-8.24520000
O	-1.06710000	0.16190000	4.31330000
O	-1.70190000	-4.03980000	5.92190000
C	-2.02580000	-2.85490000	5.98370000
N	-1.45360000	-1.90850000	5.08980000
N	0.85920000	-4.70370000	4.70130000
C	1.53420000	-5.78710000	5.12350000
C	2.87330000	-6.01680000	4.76840000
C	3.66150000	-7.21090000	5.20890000
H	3.12430000	-3.20600000	3.00860000
H	-0.09950000	-4.56570000	5.03950000
H	1.02780000	-6.48630000	5.75130000
H	3.05760000	-7.88320000	5.81470000
H	4.03250000	-7.75580000	4.33920000
H	4.53140000	-6.89790000	5.78810000
O	3.95960000	-1.80200000	2.31080000
O	7.61380000	0.86130000	1.82720000
C	7.18910000	-0.27610000	2.02340000
N	5.78960000	-0.52530000	2.02330000
C	5.24860000	-1.70220000	2.30360000
N	6.04710000	-2.73280000	2.57590000
C	7.38910000	-2.62980000	2.55800000
C	8.04170000	-1.41980000	2.27160000
C	9.53050000	-1.26020000	2.23950000
H	5.20640000	0.26890000	1.87450000
H	5.62640000	-3.62410000	2.85160000
H	7.96760000	-3.49900000	2.77660000
H	10.03490000	-2.20360000	2.43920000
H	9.84710000	-0.89130000	1.26250000
H	9.84970000	-0.52500000	2.97990000
O	4.13310000	1.70110000	1.95290000
O	3.29470000	5.62770000	4.09370000
C	4.12940000	4.90900000	3.55090000
C	-1.69120000	-0.60700000	5.14350000
N	-2.54700000	-0.13610000	6.04780000
C	-3.18250000	-0.94090000	6.91950000
C	-2.97770000	-2.32990000	6.94090000
C	-3.65600000	-3.25750000	7.90090000
H	-0.76500000	-2.25740000	4.45650000
H	-2.67860000	0.87820000	6.12350000
H	-3.85610000	-0.49920000	7.61890000
H	-4.35350000	-2.72230000	8.54200000
H	-4.20000000	-4.03040000	7.35590000
H	-2.91820000	-3.76270000	8.52650000
O	0.74970000	-2.74510000	3.50170000
O	4.67740000	-5.04720000	3.59510000
C	3.49930000	-5.00460000	3.94340000
N	2.67540000	-3.91870000	3.54190000
C	1.40820000	-3.77880000	3.91160000
N	3.74430000	3.66700000	2.97620000
C	4.59550000	2.81580000	2.42340000
N	5.89050000	3.12620000	2.38170000
C	6.36930000	4.28710000	2.86820000
C	5.53400000	5.24850000	3.45860000
C	6.02010000	6.55490000	4.00640000
H	2.78960000	3.40620000	3.09890000
H	6.55750000	2.42500000	2.04270000
H	7.41860000	4.47160000	2.80330000
H	7.09180000	6.67230000	3.85910000
H	5.50470000	7.38290000	3.51630000
H	5.80020000	6.62430000	5.07290000
O	1.18300000	2.74190000	3.65360000
O	-2.52990000	2.75170000	6.27260000
C	-1.55780000	3.38570000	5.86890000
N	-0.66360000	2.79930000	4.93350000
C	0.43310000	3.39090000	4.48500000
N	0.72710000	4.61920000	4.90840000
C	-0.06190000	5.28930000	5.76900000
C	-1.24150000	4.73470000	6.29040000
C	-2.14620000	5.44860000	7.24660000
H	-0.87880000	1.87260000	4.64780000
H	1.60290000	5.05540000	4.60240000
H	0.23110000	6.27240000	6.06300000
H	-1.78030000	6.44980000	7.46530000
H	-3.15060000	5.52480000	6.82720000
H	-2.22800000	4.89050000	8.18060000

6-mer induced by imidazole

O	0.54770000	-4.00270000	-1.12800000
O	-3.76030000	-5.35670000	-1.71430000
C	-2.53740000	-5.57320000	-1.55650000
N	-1.59120000	-4.55840000	-1.43560000
C	-0.33730000	-4.86510000	-1.23640000
N	0.06110000	-6.10250000	-1.14980000
C	-0.74440000	-7.11850000	-1.27710000
C	-2.10580000	-6.89280000	-1.49040000
H	-1.84610000	-3.62880000	-1.49720000
H	1.00190000	-6.25480000	-0.98310000
H	-0.35930000	-8.07870000	-1.21140000
H	-2.77570000	-7.67440000	-1.58830000
O	3.72040000	-2.15740000	-1.21770000
O	2.85190000	-6.55980000	-0.77130000
C	3.66050000	-5.61030000	-0.85940000
N	3.28640000	-4.27610000	-1.00400000
C	4.17200000	-3.32340000	-1.08350000
N	5.44950000	-3.63270000	-1.02220000
C	5.90550000	-4.85860000	-0.88690000
C	5.00920000	-5.92540000	-0.79780000
H	2.36370000	-4.01090000	-1.04830000
H	6.10320000	-2.92230000	-1.07700000
H	6.93100000	-5.04310000	-0.84720000
H	5.31770000	-6.91170000	-0.69120000
O	4.01040000	1.45580000	-1.39290000
O	7.37070000	-1.53850000	-1.36480000
C	6.96280000	-0.35730000	-1.41850000
N	5.61450000	-0.00060000	-1.40390000
C	5.25030000	1.25220000	-1.43210000
N	6.16860000	2.19560000	-1.49140000
C	7.46140000	1.95720000	-1.54110000
C	7.92380000	0.64040000	-1.50310000
H	4.91330000	-0.66750000	-1.35950000
H	5.88950000	3.12390000	-1.49960000
H	8.14600000	2.74230000	-1.60130000
H	8.93460000	0.40020000	-1.52980000
O	1.04930000	3.49350000	-1.29740000
O	5.31470000	4.94680000	-1.38200000
C	4.08400000	5.17310000	-1.37100000
N	3.11800000	4.16880000	-1.35300000
C	1.84620000	4.45950000	-1.33100000
N	1.46170000	5.71620000	-1.32970000
C	2.29350000	6.73220000	-1.35940000
C	3.67000000	6.49850000	-1.38140000
H	3.36350000	3.23410000	-1.35260000
H	0.51350000	5.91100000	-1.30220000
H	1.93160000	7.70970000	-1.36240000
H	4.36520000	7.26920000	-1.40190000
O	-2.21900000	1.80950000	-1.85060000
O	-1.36430000	6.18750000	-1.19680000
C	-2.16110000	5.25600000	-1.44460000
N	-1.77790000	3.91740000	-1.52290000
C	-2.65660000	2.98280000	-1.76460000
N	-3.92320000	3.30460000	-1.91940000
C	-4.37970000	4.53540000	-1.86220000
C	-3.49700000	5.58960000	-1.61850000
H	-0.85610000	3.64820000	-1.39610000
H	-4.56690000	2.60190000	-2.08890000
H	-5.39480000	4.73150000	-1.99580000
H	-3.80950000	6.57900000	-1.56020000
O	-2.49550000	-1.87520000	-1.65830000
O	-5.75110000	1.14440000	-2.31340000
C	-5.36830000	-0.03850000	-2.18760000
N	-4.04320000	-0.40310000	-1.96210000
C	-3.71620000	-1.65920000	-1.83410000
N	-4.63670000	-2.59820000	-1.90150000
C	-5.90920000	-2.34770000	-2.11380000
C	-6.33720000	-1.02830000	-2.27570000
H	-3.33270000	0.25420000	-1.89710000
H	-4.37560000	-3.52740000	-1.79360000
H	-6.60150000	-3.12490000	-2.16410000
H	-7.33060000	-0.77870000	-2.44950000
H	0.46340000	1.44110000	-1.99200000
H	-0.08530000	-2.33420000	-1.04950000
C	-0.17850000	-0.72720000	0.23230000
H	-0.42720000	-1.18210000	1.14370000
C	0.35210000	-0.60430000	-1.95290000
N	0.06180000	-1.40450000	-0.96060000
H	0.55520000	-0.88560000	-2.89720000
H	-0.11600000	1.38450000	0.54400000
N	0.31160000	0.59220000	-1.46580000
C	-0.02140000	0.56060000	-0.07190000

6-mer induced by pyrazole

O	0.54770000	-4.00270000	-1.12800000
O	-3.76030000	-5.35670000	-1.71430000
C	-2.53740000	-5.57320000	-1.55650000

N	-1.59120000	-4.55840000	-1.43560000
C	-0.33730000	-4.86510000	-1.23640000
N	0.06110000	-6.10250000	-1.14980000
C	-0.74440000	-7.11850000	-1.27710000
C	-2.10580000	-6.89280000	-1.49040000
H	-1.84610000	-3.62880000	-1.49720000
H	1.00190000	-6.25480000	-0.98310000
H	-0.35930000	-8.07870000	-1.21140000
H	-2.77570000	-7.67440000	-1.58830000
O	3.72040000	-2.15740000	-1.21770000
O	2.85190000	-6.55980000	-0.77130000
C	3.66050000	-5.61030000	-0.85940000
N	3.28640000	-4.27610000	-1.00400000
C	4.17200000	-3.32340000	-1.08350000
N	5.44950000	-3.63270000	-1.02220000
C	5.90550000	-4.85860000	-0.88690000
C	5.00920000	-5.92540000	-0.79780000
O	5.31470000	4.94680000	-1.38200000
C	4.08400000	5.17310000	-1.37100000
N	3.11800000	4.16880000	-1.35300000
C	1.84620000	4.45950000	-1.33100000
N	1.46170000	5.71620000	-1.32970000
C	2.29350000	6.73220000	-1.35940000
C	3.67000000	6.49850000	-1.38140000
H	3.36350000	3.23410000	-1.35260000
H	0.51350000	5.91100000	-1.30220000
H	1.93160000	7.70970000	-1.36240000
H	4.36520000	7.26920000	-1.40190000
O	-2.21900000	1.80950000	-1.85060000
O	-1.36430000	6.18750000	-1.19680000
C	-2.16110000	5.25600000	-1.44460000
N	-1.77790000	3.91740000	-1.52290000
C	-2.65660000	2.98280000	-1.76460000
N	-3.92320000	3.30460000	-1.91940000
C	-4.37970000	4.53540000	-1.86220000
C	-3.49700000	5.58960000	-1.61850000
H	-0.85610000	3.64820000	-1.39610000
H	-4.56690000	2.60190000	-2.08890000
H	-5.39480000	4.73150000	-1.99580000
H	-3.80950000	6.57900000	-1.56020000
O	-2.49550000	-1.87520000	-1.65830000
O	-5.75110000	1.14440000	-2.31340000
C	-5.36830000	-0.03850000	-2.18760000
N	-4.04320000	-0.40310000	-1.96210000
C	-3.71620000	-1.65920000	-1.83410000
H	2.36370000	-4.01090000	-1.04830000
H	6.10320000	-2.92230000	-1.07700000
H	6.93100000	-5.04310000	-0.84720000
H	5.31770000	-6.91170000	-0.69120000
O	4.01040000	1.45580000	-1.39290000
O	7.37070000	-1.53850000	-1.36480000
C	6.96280000	-0.35730000	-1.41850000
N	5.61450000	-0.00060000	-1.40390000
C	5.25030000	1.25220000	-1.43210000
N	6.16860000	2.19560000	-1.49140000
C	7.46140000	1.95720000	-1.54110000
C	7.92380000	0.64040000	-1.50310000
H	4.91330000	-0.66750000	-1.35950000
H	5.88950000	3.12390000	-1.49960000
H	8.14600000	2.74230000	-1.60130000
H	8.93460000	0.40020000	-1.52980000
O	1.04930000	3.49350000	-1.29740000
N	-4.63670000	-2.59820000	-1.90150000
C	-5.90920000	-2.34770000	-2.11380000
C	-6.33720000	-1.02830000	-2.27570000
H	-3.33270000	0.25420000	-1.89710000
H	-4.37560000	-3.52740000	-1.79360000
H	-6.60150000	-3.12490000	-2.16410000
H	-7.33060000	-0.77870000	-2.44950000
H	0.46340000	1.44110000	-1.99200000
H	-0.08530000	-2.33420000	-1.04950000
C	-0.17850000	-0.72720000	0.23230000
H	-0.42720000	-1.18210000	1.14370000
N	0.06180000	-1.40450000	-0.96060000
H	-0.11600000	1.38450000	0.54400000
C	-0.02140000	0.56060000	-0.07190000
C	0.31160000	0.59220000	-1.46580000
N	0.35210000	-0.60430000	-1.95290000
H	1.26448158	-0.81474147	-2.30400432

6-mer induced by 1,2,4-triazole

O	0.54770000	-4.00270000	-1.12800000
O	-3.76030000	-5.35670000	-1.71430000
C	-2.53740000	-5.57320000	-1.55650000
N	-1.59120000	-4.55840000	-1.43560000
C	-0.33730000	-4.86510000	-1.23640000
N	0.06110000	-6.10250000	-1.14980000
C	-0.74440000	-7.11850000	-1.27710000
C	-2.10580000	-6.89280000	-1.49040000

H	-1.84610000	-3.62880000	-1.49720000
H	1.00190000	-6.25480000	-0.98310000
H	-0.35930000	-8.07870000	-1.21140000
H	-2.77570000	-7.67440000	-1.58830000
O	3.72040000	-2.15740000	-1.21770000
O	2.85190000	-6.55980000	-0.77130000
C	3.66050000	-5.61030000	-0.85940000
N	3.28640000	-4.27610000	-1.00400000
C	4.17200000	-3.32340000	-1.08350000
N	5.44950000	-3.63270000	-1.02220000
C	5.90550000	-4.85860000	-0.88690000
C	5.00920000	-5.92540000	-0.79780000
H	2.36370000	-4.01090000	-1.04830000
H	6.10320000	-2.92230000	-1.07700000
H	6.93100000	-5.04310000	-0.84720000
H	5.31770000	-6.91170000	-0.69120000
O	4.01040000	1.45580000	-1.39290000
O	7.37070000	-1.53850000	-1.36480000
C	6.96280000	-0.35730000	-1.41850000
N	5.61450000	-0.00060000	-1.40390000
C	5.25030000	1.25220000	-1.43210000
N	6.16860000	2.19560000	-1.49140000
C	7.46140000	1.95720000	-1.54110000
C	7.92380000	0.64040000	-1.50310000
H	4.91330000	-0.66750000	-1.35950000
H	5.88950000	3.12390000	-1.49960000
H	8.14600000	2.74230000	-1.60130000
H	8.93460000	0.40020000	-1.52980000
O	1.04930000	3.49350000	-1.29740000
O	5.31470000	4.94680000	-1.38200000
C	4.08400000	5.17310000	-1.37100000
N	3.11800000	4.16880000	-1.35300000
C	1.84620000	4.45950000	-1.33100000
N	1.46170000	5.71620000	-1.32970000
C	2.29350000	6.73220000	-1.35940000
C	3.67000000	6.49850000	-1.38140000
H	3.36350000	3.23410000	-1.35260000
H	0.51350000	5.91100000	-1.30220000
H	1.93160000	7.70970000	-1.36240000
H	4.36520000	7.26920000	-1.40190000
O	-2.21900000	1.80950000	-1.85060000
O	-1.36430000	6.18750000	-1.19680000
C	-2.16110000	5.25600000	-1.44460000
N	-1.77790000	3.91740000	-1.52290000
C	-2.65660000	2.98280000	-1.76460000
N	-3.92320000	3.30460000	-1.91940000
C	-4.37970000	4.53540000	-1.86220000
C	-3.49700000	5.58960000	-1.61850000
H	-0.85610000	3.64820000	-1.39610000
H	-4.56690000	2.60190000	-2.08890000
H	-5.39480000	4.73150000	-1.99580000
H	-3.80950000	6.57900000	-1.56020000
O	-2.49550000	-1.87520000	-1.65830000
O	-5.75110000	1.14440000	-2.31340000
C	-5.36830000	-0.03850000	-2.18760000
N	-4.04320000	-0.40310000	-1.96210000
C	-3.71620000	-1.65920000	-1.83410000
N	-4.63670000	-2.59820000	-1.90150000
C	-5.90920000	-2.34770000	-2.11380000
C	-6.33720000	-1.02830000	-2.27570000
H	-3.33270000	0.25420000	-1.89710000
H	-4.37560000	-3.52740000	-1.79360000
H	-6.60150000	-3.12490000	-2.16410000
H	-7.33060000	-0.77870000	-2.44950000
H	0.46340000	1.44110000	-1.99200000
H	-0.08530000	-2.33420000	-1.04950000
C	-0.17850000	-0.72720000	0.23230000
H	-0.42720000	-1.18210000	1.14370000
N	0.06180000	-1.40450000	-0.96060000
H	-0.11600000	1.38450000	0.54400000
C	0.31160000	0.59220000	-1.46580000
N	0.35210000	-0.60430000	-1.95290000
N	-0.02140000	0.56060000	-0.07190000
H	0.56231982	-0.86454188	-2.89528092

6-mer induced by 1,2,3-triazole

O	0.54770000	-4.00270000	-1.12800000
O	-3.76030000	-5.35670000	-1.71430000
C	-2.53740000	-5.57320000	-1.55650000
N	-1.59120000	-4.55840000	-1.43560000
C	-0.33730000	-4.86510000	-1.23640000
N	0.06110000	-6.10250000	-1.14980000
C	-0.74440000	-7.11850000	-1.27710000
C	-2.10580000	-6.89280000	-1.49040000
H	-1.84610000	-3.62880000	-1.49720000
H	1.00190000	-6.25480000	-0.98310000
H	-0.35930000	-8.07870000	-1.21140000
H	-2.77570000	-7.67440000	-1.58830000
O	3.72040000	-2.15740000	-1.21770000

O	2.85190000	-6.55980000	-0.77130000
C	3.66050000	-5.61030000	-0.85940000
N	3.28640000	-4.27610000	-1.00400000
C	4.17200000	-3.32340000	-1.08350000
N	5.44950000	-3.63270000	-1.02220000
C	5.90550000	-4.85860000	-0.88690000
C	5.00920000	-5.92540000	-0.79780000
H	2.36370000	-4.01090000	-1.04830000
H	6.10320000	-2.92230000	-1.07700000
H	6.93100000	-5.04310000	-0.84720000
H	5.31770000	-6.91170000	-0.69120000
O	4.01040000	1.45580000	-1.39290000
O	7.37070000	-1.53850000	-1.36480000
C	6.96280000	-0.35730000	-1.41850000
N	5.61450000	-0.00060000	-1.40390000
C	5.25030000	1.25220000	-1.43210000
N	6.16860000	2.19560000	-1.49140000
C	7.46140000	1.95720000	-1.54110000
C	7.92380000	0.64040000	-1.50310000
H	4.91330000	-0.66750000	-1.35950000
H	5.88950000	3.12390000	-1.49960000
H	8.14600000	2.74230000	-1.60130000
H	8.93460000	0.40020000	-1.52980000
O	1.04930000	3.49350000	-1.29740000
O	5.31470000	4.94680000	-1.38200000
C	4.08400000	5.17310000	-1.37100000
N	3.11800000	4.16880000	-1.35300000
C	1.84620000	4.45950000	-1.33100000
N	1.46170000	5.71620000	-1.32970000
C	2.29350000	6.73220000	-1.35940000
C	3.67000000	6.49850000	-1.38140000
H	3.36350000	3.23410000	-1.35260000
H	0.51350000	5.91100000	-1.30220000
H	1.93160000	7.70970000	-1.36240000
H	4.36520000	7.26920000	-1.40190000
O	-2.21900000	1.80950000	-1.85060000
O	-1.36430000	6.18750000	-1.19680000
C	-2.16110000	5.25600000	-1.44460000
N	-1.77790000	3.91740000	-1.52290000
C	-2.65660000	2.98280000	-1.76460000
N	-3.92320000	3.30460000	-1.91940000
C	-4.37970000	4.53540000	-1.86220000
C	-3.49700000	5.58960000	-1.61850000
H	-0.85610000	3.64820000	-1.39610000
H	-4.56690000	2.60190000	-2.08890000
H	-5.39480000	4.73150000	-1.99580000
H	-3.80950000	6.57900000	-1.56020000
O	-2.49550000	-1.87520000	-1.65830000
O	-5.75110000	1.14440000	-2.31340000
C	-5.36830000	-0.03850000	-2.18760000
N	-4.04320000	-0.40310000	-1.96210000
C	-3.71620000	-1.65920000	-1.83410000
N	-4.63670000	-2.59820000	-1.90150000
C	-5.90920000	-2.34770000	-2.11380000
C	-6.33720000	-1.02830000	-2.27570000
H	-3.33270000	0.25420000	-1.89710000
H	-4.37560000	-3.52740000	-1.79360000
H	-6.60150000	-3.12490000	-2.16410000
H	-7.33060000	-0.77870000	-2.44950000
H	0.46340000	1.44110000	-1.99200000
H	-0.08530000	-2.33420000	-1.04950000
C	-0.17850000	-0.72720000	0.23230000
H	-0.42720000	-1.18210000	1.14370000
N	0.06180000	-1.40450000	-0.96060000
H	-0.11600000	1.38450000	0.54400000
N	0.35210000	-0.60430000	-1.95290000
N	0.31160000	0.59220000	-1.46580000
C	-0.02140000	0.56060000	-0.07190000
H	0.56231982	-0.86454188	-2.89528092

References

1 C. A. Schalley, T. Muller, P. Linnartz, M. Witt, M. Schafer, A. Lutzen, *Chem Eur J* **2002**, *8*, 3538-3551.

2 B. Qiu, J. Liu, Z. Qin, G. B. Wang, H. Luo, *Chem Commun* **2009**, 2863-2865.

3 Z. Qin, J. Liu, B. Qiu, H. Luo, *J Mass Spectrom* **2012**, *47*, 552-554.
4 B. Qiu, Z. Qin, J. Liu, H. Luo, *J Mass Spectrom* **2011**, *46*, 587-594.
5 Z. Qin, B. Qiu, J. M. Sun, W. B. Zhao, H. Luo, *J Mass Spectrom* **2014**, *49*, 266-273.