

Supporting Information for

**Exploring the influence of steric hindrance and
electronic nature of the substituents in the
supramolecular arrangements of
5-(substituted phenyl)-2-formylpyrroles**

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Table S1 Details of data collection and structure refinement for compounds **1-4**.

	1	2	3	4
Formula	C ₁₁ H ₉ NO	C ₁₃ H ₁₃ NO	C ₁₃ H ₇ F ₆ NO	C ₂₀ H ₂₇ NO
<i>M</i>	171.19	199.24	307.20	297.42
λ (Å)	0.71073	0.71073	0.71073	0.71073
<i>T</i> (K)	150(2)	150(2)	150(2)	150(2)
Crystal system	Monoclinic	Monoclinic	Monoclinic	Triclinic
Space group	<i>P</i> 2 ₁ / <i>c</i>	<i>P</i> 2 ₁ / <i>n</i>	<i>P</i> 2 ₁ / <i>c</i>	<i>P</i> -1
<i>a</i> (Å)	11.328(5)	8.0139(18)	13.086(2)	8.6799(13)
<i>b</i> (Å)	5.042(2)	13.509(2)	4.7468(7)	9.8371(13)
<i>c</i> (Å)	15.578(7)	10.342(2)	19.887(3)	12.608(2)
α (°)	90	90	90	72.477(7)
β (°)	109.947(11)	102.552(9)	105.901(9)°	70.308(5)
γ (°)	90	90	90	65.232(4)
<i>V</i> (Å ³)	836.2(6)	1092.9(4)	1188.1(3)	904.1(2)
<i>Z</i>	4	4	4	2
ρ_{calc} (g.cm ⁻³)	1.360	1.211	1.717	1.093
μ (mm ⁻¹)	0.088	0.077	0.173	0.066
Crystal size	0.35×0.25×0.20	0.20×0.12×0.08	0.60×0.18×0.08	0.16×0.16×0.12
Crystal colour	Colourless	Colourless	Colourless	Colourless
Crystal description	Prism	Prism	Needle	Prism
θ_{max} (°)	32.434	26.389	25.788	25.741
Total data	12299	7793	10048	7972
Unique data	2994	2202	2257	3402
<i>R</i> _{int}	0.0358	0.1412	0.0806	0.0432
<i>R</i> [<i>I</i> >2σ(<i>I</i>)]	0.0443	0.1218	0.0446	0.0498
<i>R</i> _w	0.1191	0.2843	0.0863	0.1036
Goodness of fit	1.065	0.897	0.948	0.942
ρ_{min}	-0.336	-0.349	-0.280	-0.199
ρ_{max}	0.457	0.437	0.225	0.194

Table S2 Details of data collection and structure refinement for compounds 5-7.

	5	6	7
Formula	C ₁₃ H ₁₃ NO	C ₁₂ H ₁₁ NO ₂	C ₁₁ H ₈ FNO
<i>M</i>	199.24	201.22	189.18
λ (Å)	0.71073	0.71073	0.71073
<i>T</i> (K)	150(2)	150(2)	150(2)
Crystal system	Monoclinic	Orthorhombic	Orthorhombic
Space group	<i>P</i> 2 ₁ / <i>c</i>	<i>P</i> 2 ₁ 2 ₁ 2 ₁	<i>P</i> 2 ₁ 2 ₁ 2 ₁
<i>a</i> (Å)	7.9115(7)	5.5376(3)	5.5758(89)
<i>b</i> (Å)	23.9817(18)	6.4429(3)	6.3791(6)
<i>c</i> (Å)	11.4591(10)	27.5008(14)	24.0493(3)
α (°)	90	90	90
β (°)	96.844(3)	90	90
γ (°)	90	90	90
<i>V</i> (Å ³)	2158.7(3)	981.18(9)	871.20(19)
<i>Z</i>	8	4	4
ρ_{calc} (g.cm ⁻³)	1.226	1.362	1.442
μ (mm ⁻¹)	0.078	0.094	0.108
Crystal size	0.22×0.12×0.10	0.24×0.20×0.12	0.24×0.10×0.06
Crystal colour	Orange	Colourless	Yellow
Crystal description	Prism	Prism	Prism
θ_{max} (°)	25.755	25.684	25.581
Total data	10811	4846	2893
Unique data	4112	1804	1574
<i>R</i> _{int}	0.0709	0.0409	0.0430
<i>R</i> [<i>I</i> > 2 σ (<i>I</i>)]	0.0521	0.0426	0.0500
<i>R</i> _w	0.0941	0.0818	0.0785
Goodness of fit	0.913	1.011	0.948
ρ_{min}	-0.211	-0.226	-0.198
ρ_{max}	0.203	0.169	0.215

Table S3 Selected bond lengths (Å) and angles (°) for compounds **1-7**.

	1	2	3	4	5		6	7
					A	B		
<i>Lengths (Å)</i>								
N1-C2	1.3731(13)	1.386(5)	1.363(3)	1.381(2)	1.378(3)	1.379(3)	1.386(4)	1.383(5)
C2-C3	1.3828(14)	1.354(6)	1.383(3)	1.373(2)	1.378(3)	1.377(3)	1.380(4)	1.376(5)
C3-C4	1.3945(15)	1.402(6)	1.380(3)	1.393(2)	1.400(3)	1.389(3)	1.392(4)	1.401(6)
C4-C5	1.3911(14)	1.391(6)	1.386(3)	1.376(2)	1.386(3)	1.377(3)	1.394(4)	1.399(5)
C5-N1	1.3571(13)	1.349(5)	1.356(3)	1.349(2)	1.365(3)	1.362(3)	1.359(4)	1.354(5)
C5-C7	1.4609(14)	1.467(5)	1.459(3)	1.491(2)	1.481(3)	1.479(3)	1.467(4)	1.471(5)
C2-C6	1.4259(15)	1.415(6)	1.429(3)	1.416(3)	1.428(3)	1.423(3)	1.422(4)	1.427(5)
C6-O1	1.2182(13)	1.219(6)	1.220(3)	1.223(2)	1.232(3)	1.236(3)	1.233(3)	1.223(5)
<i>Angles (°)</i>								
C5-N1-C2	109.67(8)	109.7(3)	109.8(2)	109.75(15)	109.56(18)	108.99(19)	109.5(3)	109.7(3)
N1-C2-C3	107.71(9)	107.3(3)	107.5(2)	106.89(15)	107.4(2)	107.52(19)	107.4(3)	107.6(4)
C2-C3-C4	107.33(9)	108.5(4)	107.5(2)	107.88(16)	107.90(19)	107.7(2)	107.7(3)	107.7(4)
C3-C4-C5	107.81(9)	106.9(4)	108.0(2)	107.72(16)	107.5(2)	108.0(2)	108.0(3)	107.4(4)
C4-C5-N1	107.47(8)	107.6(3)	107.2(2)	107.75(15)	107.6(2)	107.86(19)	107.4(2)	107.6(3)
C7-C5-C4	128.70(9)	128.9(4)	128.7(2)	129.72(15)	131.3(2)	129.6(2)	129.6(3)	128.9(3)
C7-C5-N1	123.81(8)	123.5(4)	124.0(2)	122.51(15)	121.07(18)	122.5(2)	123.0(3)	123.5(4)
N1-C2-C6	124.00(9)	124.2(4)	123.7(2)	123.96(16)	125.1(2)	123.6(2)	123.1(3)	122.8(3)
C3-C2-C6	128.27(9)	128.5(4)	128.8(2)	129.14(16)	127.5(2)	128.9(2)	129.4(3)	129.5(4)
C2-C6-O1	125.84(10)	125.8(4)	125.2(2)	126.54(17)	125.9(2)	125.2(2)	124.6(3)	125.4(4)

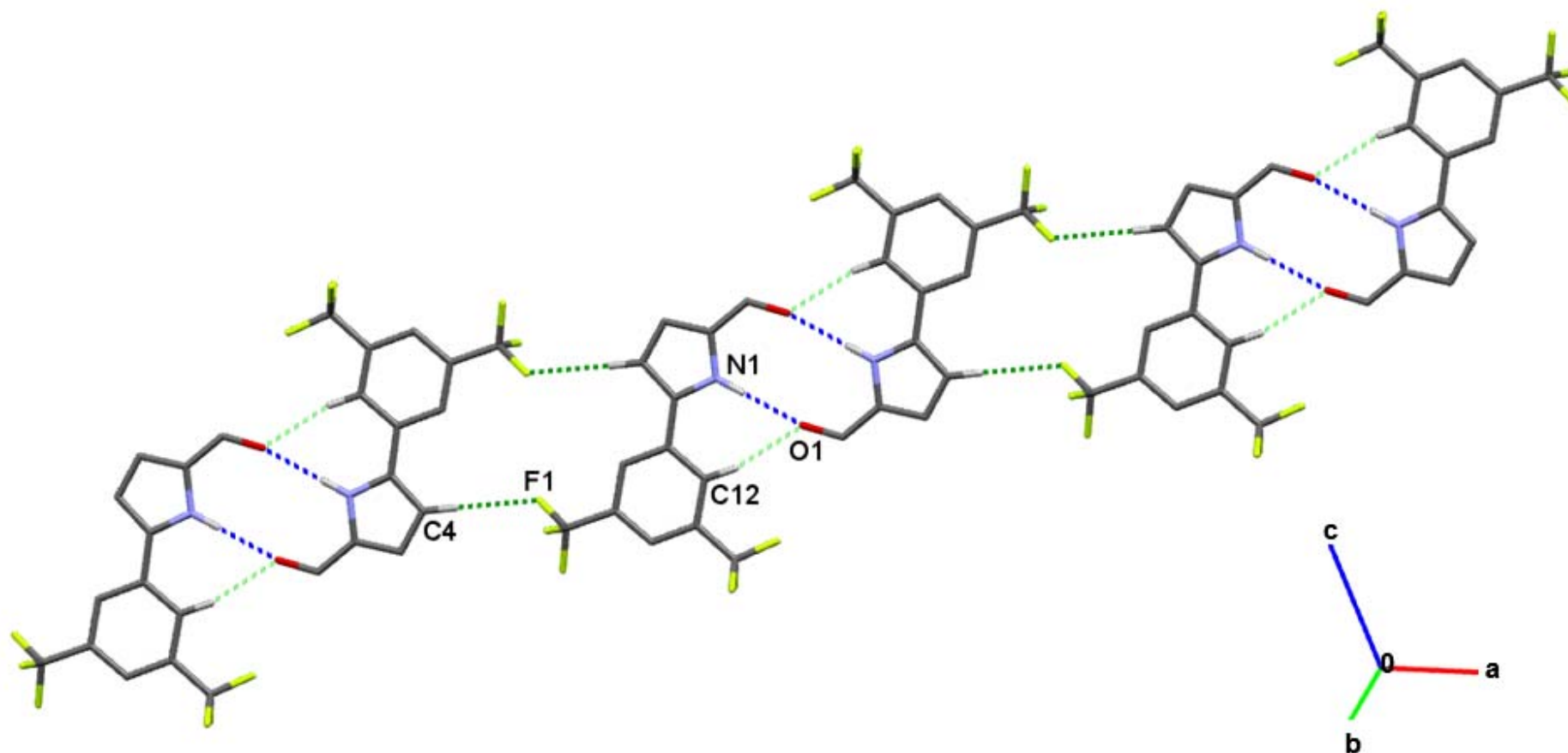


Figure S1 Consecutive $R^2_2(10)$ and $R^2_2(16)$ chain synthons along the a direction of the crystalline structure of **3**. Donor and acceptor atoms are identified. Blue dashed lines represent the $N_1-H_1 \cdots O_1$ hydrogen-bonds, light-green and green dashed lines representing the $C_{12}-H_{12} \cdots O_1$ and $C_4-H_4 \cdots F_1$, respectively.

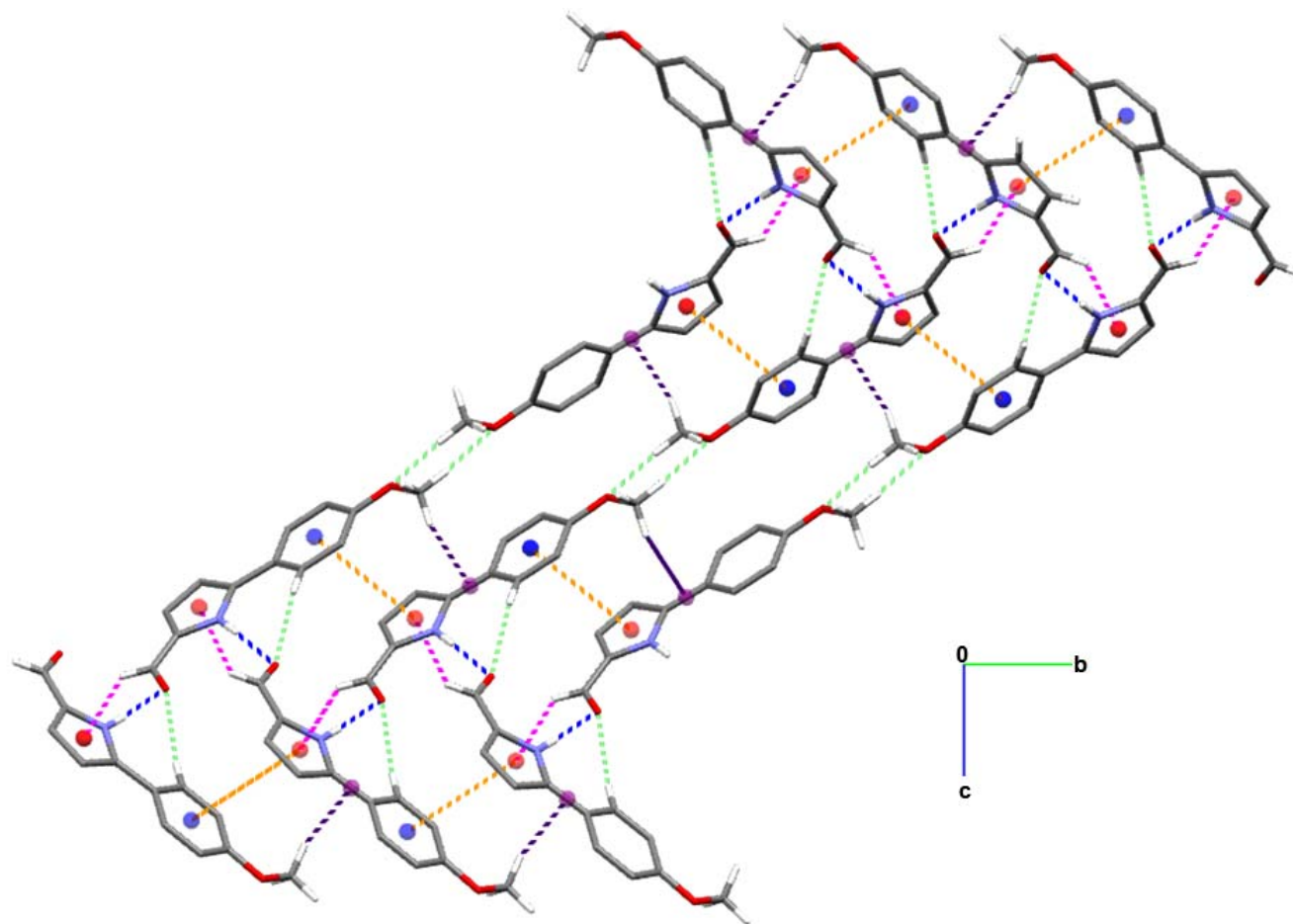


Figure S2 View along plane 011 of compound **6**, showing the 2D grid with intercalated zigzag and linear chains. All interactions are represented: N₁-H₁⋯O₁ (blue), both the C₁₂-H₁₂⋯O₁ and the C₁₃-H_{13B}⋯O₂ (light-green), the C₆-H₆⋯C_g(Pyr) (pink), the C₁₃-H_{13C}⋯π C_g(C5-C7) (purple) and the π⋯π interaction between the centroids of the pyrrole and aryl ring (orange dashed lines).

Atomic Coordinates for all the optimised molecules (M06-2X/6-31G)

Monomer 1

O	2.233564	3.398545	1.226398
N	0.663591	1.136086	0.629053
H	1.309566	1.394730	-0.102218
C	0.533510	1.866092	1.794281
C	-0.483880	1.281316	2.541785
H	-0.821206	1.613399	3.510976
C	-0.972396	0.182887	1.802694
H	-1.743414	-0.507129	2.104525
C	-0.243061	0.109690	0.612252
C	1.370761	3.012435	2.034323
H	1.207953	3.542066	2.982336
C	-0.339289	-0.844932	-0.492922
C	-1.552508	-1.503283	-0.743931
H	-2.417683	-1.273617	-0.131782
C	-1.656005	-2.422462	-1.784229
H	-2.600251	-2.921795	-1.967776
C	-0.552735	-2.691709	-2.596900
H	-0.635369	-3.404459	-3.408909
C	0.657373	-2.039272	-2.357007
H	1.520517	-2.249939	-2.977768
C	0.766289	-1.126450	-1.310154
H	1.722673	-0.654196	-1.109028

Monomer 2

O	3.573069	3.273913	0.035573
N	1.479377	1.450732	0.516872
H	2.056274	1.214217	-0.276829
C	1.674151	2.598478	1.260563
C	0.669082	2.647434	2.221753
H	0.549724	3.418323	2.966811
C	-0.142512	1.507307	2.042353
H	-0.994656	1.220733	2.636729
C	0.379476	0.773870	0.972734
C	2.765383	3.486412	0.957297
H	2.853701	4.379986	1.589544
C	-0.075542	-0.487122	0.385168
C	-1.422280	-0.857495	0.488735
H	-2.123133	-0.190219	0.980483
C	-1.881202	-2.056813	-0.059728
C	-0.972034	-2.881278	-0.730919
H	-1.322719	-3.812018	-1.170126
C	0.378725	-2.535712	-0.849400
C	0.816921	-1.337169	-0.283092
H	1.871202	-1.081044	-0.339925
C	-3.328623	-2.462679	0.072183
H	-3.704976	-2.891776	-0.860527
H	-3.957042	-1.607206	0.330860
H	-3.453114	-3.217520	0.856147
C	1.340396	-3.454625	-1.562328
H	1.448833	-4.402585	-1.025448
H	2.331145	-3.002613	-1.648259
H	0.986376	-3.687532	-2.571222

Monomer 4

O	1.624935	-4.086428	2.983923
N	1.303129	-1.947489	1.169624
C	2.513086	-2.573315	1.406581
C	3.465617	-1.949418	0.608986
H	4.512003	-2.208498	0.562982
C	2.806893	-0.928738	-0.116924
H	3.242316	-0.255802	-0.837818
C	1.461191	-0.945242	0.249819
C	2.603754	-3.659897	2.346785
H	3.599198	-4.104380	2.479123
C	0.321940	-0.110916	-0.197946
C	-0.510652	-0.564618	-1.239033

C	-1.587991	0.235396	-1.636420
H	-2.243273	-0.107421	-2.432358
C	-1.848536	1.467056	-1.036321
C	-1.006056	1.899597	-0.006047
H	-1.200897	2.856650	0.468935
C	0.072482	1.129180	0.430759
C	-0.286157	-1.917254	-1.901276
H	0.713719	-2.267182	-1.619971
C	0.988082	1.642717	1.534042
H	1.486517	0.776562	1.985250
C	-0.334131	-1.833230	-3.434503
H	-1.336123	-1.570111	-3.788929
H	-0.073080	-2.802496	-3.870445
H	0.368106	-1.083914	-3.810223
C	-1.310603	-2.942708	-1.383226
H	-1.240779	-3.056978	-0.297066
H	-1.142155	-3.921637	-1.842670
H	-2.329240	-2.619523	-1.624908
C	2.077923	2.550931	0.935557
H	2.669725	2.012790	0.189961
H	2.752244	2.911212	1.719076
H	1.619137	3.418328	0.447915
C	0.232416	2.378962	2.649749
H	-0.159978	3.339680	2.300633
H	0.910378	2.586687	3.482911
H	-0.604859	1.783154	3.024241
C	-3.023851	2.318005	-1.485645
H	-3.518599	1.784111	-2.307741
C	-2.557758	3.682681	-2.019129
H	-2.081964	4.266311	-1.223519
H	-3.409391	4.258373	-2.395182
H	-1.833709	3.561603	-2.829576
H	0.444895	-2.209708	1.632490
C	-4.047642	2.498705	-0.352577
H	-4.911335	3.072439	-0.703263
H	-3.600313	3.041046	0.487541
H	-4.398916	1.531630	0.017634

Monomer 5

C	-2.798897	2.618643	0.328080
C	-2.769145	1.408626	1.016204
H	-3.657941	3.273773	0.418851
C	-1.723106	2.987737	-0.476155
H	-3.601790	1.122829	1.650444
C	-1.669853	0.550879	0.908521
H	-1.746275	3.928307	-1.016242
C	-0.606545	2.156805	-0.605979
C	-1.648480	-0.748874	1.679160
C	-0.586411	0.930675	0.089489
C	0.544616	2.576132	-1.489004
C	0.584534	0.038110	-0.035253
C	1.908308	0.213087	0.369746
N	0.497387	-1.201525	-0.611286
H	2.292006	1.088217	0.868850
C	2.625034	-0.955788	0.024328
C	1.729779	-1.826017	-0.588535
H	3.671372	-1.152196	0.199078
C	1.895282	-3.141026	-1.151245
H	-0.323688	-1.618126	-1.025648
O	0.962937	-3.774822	-1.675388
H	2.905862	-3.567710	-1.096224
H	-1.902085	-1.605310	1.044586
H	-0.658477	-0.942243	2.102245
H	-2.374183	-0.720396	2.495034
H	0.871487	1.757045	-2.135681
H	0.254656	3.420459	-2.118530
H	1.413619	2.881710	-0.897447

Dimer 1

O	-0.509640	1.362274	1.033324
N	-2.023403	-1.039310	0.320868
H	-1.259296	-0.895017	-0.346065
C	-2.293426	-0.175677	1.368305
C	-3.407524	-0.674796	2.053533
H	-3.865585	-0.218815	2.917595
C	-3.802419	-1.852385	1.407978
H	-4.641668	-2.477583	1.663743
C	-2.925484	-2.062291	0.328244
C	-1.526870	0.985432	1.659196
H	-1.883318	1.578895	2.511593
C	-2.931960	-3.150362	-0.653008
C	-3.643826	-4.327253	-0.372125
H	-4.152994	-4.431278	0.579414
C	-3.682727	-5.369218	-1.293564
H	-4.235130	-6.272267	-1.060877
C	-3.005395	-5.254906	-2.509224
H	-3.034412	-6.066492	-3.227064
C	-2.289237	-4.091132	-2.792298
H	-1.760997	-3.995779	-3.734129
C	-2.250566	-3.042230	-1.875282
H	-1.691105	-2.142526	-2.108896
N	1.794360	1.323729	-0.567759
C	2.892044	2.107848	-0.365135
C	3.051718	3.002902	0.783978
C	3.775261	1.893209	-1.438878
C	3.182326	0.959399	-2.296896
C	1.955408	3.389045	1.570978
C	4.326525	3.495291	1.104818
C	2.138338	4.250920	2.650762
C	4.502272	4.359655	2.181182
C	3.407541	4.741748	2.959310
C	1.945905	0.607650	-1.742303
H	4.722891	2.386112	-1.579032
H	3.586008	0.572215	-3.219762
H	0.962699	3.016667	1.341272
H	5.184425	3.186136	0.518336
H	1.283597	4.542697	3.250343
H	5.493304	4.729758	2.417305
H	3.543846	5.414373	3.798258
C	0.990907	-0.323273	-2.235035
H	0.963879	1.258663	0.028408
O	-0.083017	-0.634538	-1.670521
H	1.248745	-0.792491	-3.193895

Dimer 2

O	0.165064	1.482221	0.801077
N	-2.068841	-0.399169	0.976006
H	-1.375755	-0.735473	0.301530
C	-1.927251	0.778924	1.688924
C	-3.058456	0.921162	2.501517
H	-3.240430	1.738657	3.182068
C	-3.883532	-0.184928	2.267215
H	-4.824572	-0.399830	2.745414
C	-3.249073	-0.996823	1.309286
C	-0.816975	1.656549	1.558677
H	-0.858197	2.557366	2.185789
C	-3.710449	-2.263566	0.735458
C	-5.054681	-2.637195	0.875967
H	-5.747749	-1.975220	1.385097
C	-5.526590	-3.837820	0.344455
C	-4.633174	-4.665158	-0.345472
H	-4.994365	-5.597472	-0.773091
C	-3.289007	-4.313442	-0.501881
C	-2.834715	-3.110343	0.043603
H	-1.793574	-2.832341	-0.083370
C	-6.970636	-4.243896	0.511731
H	-7.373935	-4.658270	-0.416621
H	-7.590134	-3.391192	0.799946

H	-7.075915	-5.010292	1.287296
C	-2.336298	-5.225501	-1.235932
H	-2.051243	-6.080755	-0.613543
H	-1.422132	-4.693075	-1.510224
H	-2.790052	-5.620023	-2.149722
N	2.068771	0.399140	-0.975769
C	3.248425	0.997349	-1.310074
C	3.710139	2.263735	-0.735746
C	3.881892	0.186415	-2.269457
C	3.056796	-0.919704	-2.503592
C	2.834630	3.110375	-0.043463
C	5.054454	2.637109	-0.876187
C	3.289241	4.313106	0.502593
C	5.526674	3.837351	-0.344113
C	4.633481	4.664555	0.346292
C	1.926582	-0.778429	-1.689438
H	4.822232	0.402042	-2.748709
H	3.238079	-1.736586	-3.185061
H	1.793433	2.832510	0.083398
H	5.747306	1.975160	-1.385652
C	2.336723	5.225073	1.237001
C	6.970811	4.243176	-0.511203
H	4.994925	5.596562	0.774367
C	0.816798	-1.656576	-1.558505
H	1.376635	0.734811	-0.300007
O	-0.164425	-1.483247	-0.799623
H	0.857674	-2.556930	-2.186302
H	2.791300	5.620825	2.149840
H	1.423320	4.692170	1.512918
H	2.050190	6.079503	0.614151
H	7.076157	5.010526	-1.285811
H	7.589971	3.390641	-0.800633
H	7.374454	4.656245	0.417585

Dimer 4

O	0.671530	-2.637362	-0.941145
N	0.581456	0.074341	-1.874855
C	1.739843	-0.662784	-1.687617
C	2.821712	0.207030	-1.856199
H	3.862002	-0.063210	-1.757389
C	2.297254	1.480376	-2.143411
H	2.845536	2.388778	-2.333478
C	0.899707	1.369183	-2.154646
C	1.716559	-2.022873	-1.263886
H	2.683943	-2.536408	-1.210423
C	-0.144523	2.376719	-2.455991
C	-0.732123	2.403467	-3.734593
C	-1.725093	3.353694	-3.999922
H	-2.184231	3.380829	-4.984737
C	-2.145982	4.266550	-3.035112
C	-1.547935	4.222032	-1.770761
H	-1.868905	4.925377	-1.008272
C	-0.551645	3.295204	-1.462164
C	-0.322310	1.432450	-4.833145
H	0.470501	0.785751	-4.441819
C	0.022166	3.230084	-0.052888
H	1.022652	2.787129	-0.119869
C	0.250726	2.178584	-6.049373
H	-0.503949	2.832849	-6.498815
H	0.574958	1.464371	-6.812868
H	1.108382	2.794818	-5.763519
C	-1.503066	0.533585	-5.238496
H	-1.912449	0.016352	-4.366380
H	-1.178066	-0.208064	-5.975518
H	-2.303321	1.129464	-5.692113
C	0.166123	4.606862	0.610655
H	0.695448	5.310276	-0.038724
H	0.725957	4.509405	1.546322
H	-0.809997	5.037202	0.858690
C	-0.842716	2.301483	0.820048
H	-1.881290	2.652448	0.835114

H	-0.470788	2.281359	1.850925
H	-0.834928	1.276197	0.435120
C	-3.234121	5.280206	-3.344303
H	-3.528885	5.132755	-4.391712
C	-2.721967	6.721740	-3.192708
H	-2.436163	6.922735	-2.154508
H	-3.501916	7.437495	-3.471719
H	-1.846707	6.896362	-3.824509
H	-0.377563	-0.294966	-1.897649
C	-4.474845	5.049825	-2.465460
H	-5.269761	5.754691	-2.729413
H	-4.229595	5.197715	-1.408019
H	-4.856761	4.032236	-2.586052
C	-2.508604	-0.734588	0.325578
H	-2.376405	-0.951032	3.625265
C	-1.108670	-4.494292	1.851528
C	1.157706	-0.041882	2.970097
H	1.180071	-5.447984	2.893229
H	2.582713	-4.777787	5.972463
H	3.947594	-5.847720	5.585482
H	2.364619	-6.120821	4.839234
H	2.825718	0.028147	1.570368
H	1.899085	1.541620	1.662195
H	1.236364	0.145638	0.789843
H	1.471493	0.161207	5.124626
H	2.941979	0.391995	4.159645
H	1.711327	1.655083	4.194933
H	-0.177833	-4.770798	-0.097055
H	-1.518391	-5.895430	0.240982
H	0.055923	-6.137330	1.012338
C	1.167268	-4.361384	2.920768
H	-2.626479	-5.886124	2.553234
H	-2.123314	-4.697508	3.774249
H	-3.888353	0.136593	-1.078303
O	-2.164455	-0.430080	-1.994293
H	4.171732	-3.687155	4.380642
C	3.065031	-5.348041	5.173785
C	-1.133578	-1.550377	1.905769
H	0.120286	0.312233	2.971805
C	1.817842	0.448429	1.667376
C	1.861992	0.570875	4.188581
H	-1.862059	-3.795543	1.472550
C	-0.657828	-5.376905	0.675889
C	0.037579	-2.277619	2.449474
H	-0.689774	-1.799621	-0.143713
H	-4.032680	0.045382	1.717733
C	-2.895853	-0.318945	-0.981041
C	3.459292	-4.432563	4.003047
H	3.066302	-1.744829	3.904638
C	-2.235205	-0.977687	2.556867
H	-1.063920	-6.060338	3.370855
N	-1.312332	-1.391213	0.564916
C	-3.097486	-0.471842	1.566449
C	0.054866	-3.686953	2.411487
C	1.126938	-1.564362	2.991560
C	2.219614	-2.281428	3.487424
C	2.257777	-3.677039	3.461128
C	-1.771637	-5.333945	2.956542
C	4.155972	-5.238436	2.894168
H	5.045567	-5.742430	3.285183
H	4.457679	-4.589100	2.067534
H	3.481568	-6.003010	2.493749

Dimer 5

O	-0.141643	1.128044	1.398991
N	-1.770697	-1.131399	0.570598
H	-1.094892	-0.918589	-0.171241
C	-1.879672	-0.448932	1.769109
C	-2.923467	-1.035305	2.494887
H	-3.252054	-0.728334	3.475932
C	-3.441959	-2.079210	1.712755

H	-4.245198	-2.751069	1.968361
C	-2.705970	-2.119517	0.517577
C	-1.052236	0.655217	2.117679
H	-1.252855	1.110745	3.095948
C	-2.824695	-3.039336	-0.632519
C	-4.020195	-3.074256	-1.378727
C	-5.182996	-2.168735	-1.046326
C	-4.118189	-3.960141	-2.455880
H	-5.033287	-3.982666	-3.038419
C	-3.058597	-4.800621	-2.787561
H	-3.149069	-5.483885	-3.624596
C	-1.883112	-4.762772	-2.042055
H	-1.057902	-5.420637	-2.293705
C	-1.746620	-3.887010	-0.961130
C	-0.465377	-3.872345	-0.162959
N	1.711045	1.232605	-0.652020
C	2.715281	2.145286	-0.540730
C	2.830054	3.059683	0.613938
C	3.514169	2.047521	-1.691386
C	2.961190	1.048083	-2.507398
C	1.797682	3.984470	0.873543
C	3.976933	3.013976	1.432650
C	1.930873	4.856258	1.958278
C	4.072505	3.897918	2.511351
C	3.057649	4.814725	2.774973
C	1.834840	0.544544	-1.845646
H	4.379841	2.655572	-1.898455
H	3.320593	0.716994	-3.469660
C	0.567372	4.054559	0.001851
C	5.087491	2.022756	1.174603
H	1.141825	5.574211	2.155922
H	4.950131	3.860097	3.148240
H	3.145987	5.496096	3.613776
C	0.944679	-0.491190	-2.245747
H	0.977328	1.075385	0.047256
O	-0.030766	-0.901831	-1.575410
H	1.155498	-0.950656	-3.220104
H	-5.890244	-2.137462	-1.878432
H	-4.849023	-1.148804	-0.836903
H	-5.725132	-2.516874	-0.160750
H	0.121697	-4.770578	-0.369022
H	-0.664934	-3.829126	0.912052
H	0.142979	-3.000249	-0.423071
H	0.056847	5.010699	0.140258
H	-0.133429	3.253409	0.258641
H	0.820426	3.947923	-1.057235
H	5.753988	1.964878	2.038302
H	5.689885	2.308255	0.305959
H	4.691722	1.023020	0.974559

Tetramer 1

O	-2.812139	-0.580487	-0.145225
N	-2.011238	-2.773622	-1.820642
H	-1.154355	-2.282662	-1.546050
C	-3.249930	-2.640492	-1.223569
C	-4.063287	-3.670920	-1.699645
H	-5.100471	-3.819139	-1.441742
C	-3.293939	-4.434960	-2.598518
H	-3.617661	-5.285407	-3.176777
C	-2.019622	-3.856846	-2.653315
C	-3.575329	-1.541587	-0.365528
H	-4.573155	-1.570941	0.092341
C	-0.844713	-4.227749	-3.446079
C	-0.521134	-5.576745	-3.649320
C	0.604783	-5.926457	-4.393664
H	0.850169	-6.972118	-4.539425
C	1.419316	-4.933257	-4.941545
H	2.296738	-5.205866	-5.516434
C	1.097446	-3.587198	-4.751202
H	1.721861	-2.812722	-5.181074
C	-0.030625	-3.234400	-4.013241

H	-1.142846	-6.343853	-3.200082
H	-0.284407	-2.189534	-3.870007
O	0.642945	-2.314454	-1.099242
N	2.814743	-2.489548	0.834969
H	2.330272	-1.599159	0.999930
C	2.583883	-3.357172	-0.215587
C	3.577491	-4.340004	-0.182471
H	3.655047	-5.169555	-0.868287
C	4.421262	-4.050126	0.903763
H	5.273810	-4.617231	1.241122
C	3.921839	-2.896763	1.522508
C	1.498112	-3.226141	-1.134080
H	1.444771	-4.001943	-1.911946
C	4.415098	-2.180457	2.704370
C	5.787792	-1.939436	2.858132
C	6.259191	-1.222500	3.957187
H	7.321513	-2.033865	4.061843
C	5.364409	-0.736983	4.913341
H	5.729129	-0.170619	5.762620
C	3.996893	-0.986756	4.775083
H	3.298588	-0.613519	5.515090
C	3.524650	-1.711664	3.682790
H	6.475058	-2.294684	2.097714
H	2.463002	-1.902704	3.570705
N	-2.335794	-2.069939	-1.034080
C	-2.989825	2.385272	-2.189683
C	-3.589523	1.384038	-3.074854
C	-2.935168	3.778566	-2.349472
C	-2.225212	4.301906	-1.257773
C	-3.051982	0.092502	-3.178250
C	-4.707201	1.720164	-3.853955
C	-3.632807	-0.849454	-4.025665
C	-5.275899	0.782977	-4.712952
C	-4.743822	-0.505539	-4.798208
C	-1.858365	3.225586	-0.444096
H	-3.335575	4.323852	-3.188665
H	-1.982618	5.336622	-1.070790
H	-2.178944	-0.171855	-2.590862
H	-5.138655	2.711333	-3.764306
H	-3.216575	-1.850768	-4.081652
H	-6.141256	1.053735	-5.307087
H	-5.191824	-1.236911	-5.460928
C	-1.103826	3.228163	0.765202
H	-2.286524	1.141938	-0.607185
O	-0.804267	2.199080	1.412584
H	-0.777350	4.215913	1.122401
N	1.495591	2.609202	2.952489
C	1.544823	3.755978	3.692347
C	0.356655	4.559885	3.988252
C	2.878113	3.964803	4.075691
C	3.640744	2.912565	3.541428
C	-0.921484	3.979443	4.025947
C	0.486674	5.933337	4.246388
C	-2.041823	4.761529	4.300877
C	-0.633934	6.708542	4.534017
C	-1.902896	6.126310	4.558683
C	2.765636	2.078167	2.840759
H	3.229513	4.771933	4.697806
H	4.701147	2.747047	3.655305
H	-1.037368	2.918298	3.835720
H	1.468258	6.392423	4.198889
H	-3.022815	4.301025	4.323182
H	-0.518469	7.768631	4.728781
H	-2.775301	6.730844	4.778192
C	3.046403	0.866887	2.137043
H	0.665117	2.250251	2.462178
O	2.174888	0.144762	1.606524
H	4.106381	0.577124	2.102567

Tetramer 2

O	-2.407743	-0.513491	-0.963353
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N	-1.847747	-2.917004	-2.474061
H	-0.980513	-2.620447	-2.008919
C	-3.103073	-2.397114	-2.223672
C	-4.030981	-3.158397	-2.937689
H	-5.093504	-2.971665	-2.970677
C	-3.316004	-4.155900	-3.624749
H	-3.715085	-4.898051	-4.297307
C	-1.958517	-3.985266	-3.319596
C	-3.320477	-1.211526	-1.453470
H	-4.372672	-0.910741	-1.343926
C	-0.796124	-4.745405	-3.784903
C	-0.923953	-6.107519	-4.094302
C	0.173120	-6.848383	-4.534649
C	0.026552	-8.306481	-4.894867
C	1.417066	-6.212066	-4.642994
H	2.281122	-6.786665	-4.966617
C	1.571209	-4.856121	-4.341918
C	2.921503	-4.187039	-4.422409
C	0.450892	-4.125536	-3.931474
H	-1.885690	-6.594451	-3.964554
H	0.555176	-3.067857	-3.708575
O	0.639186	-2.634933	-1.177459
N	2.646972	-2.391371	0.888544
H	2.183564	-1.483057	0.767334
C	2.445730	-3.499311	0.086872
C	3.379279	-4.471215	0.461064
H	3.461335	-5.456875	0.029021
C	4.152998	-3.931493	1.501905
H	4.943754	-4.418085	2.049663
C	3.674166	-2.637740	1.753664
C	1.429832	-3.567363	-0.912086
H	1.371200	-4.513657	-1.469316
C	4.116720	-1.660303	2.753319
C	5.479681	-1.511563	3.034249
C	5.918850	-0.559750	3.960486
C	7.387724	-0.416654	4.276900
C	4.971023	0.252915	4.590251
H	5.305275	1.013713	5.291559
C	3.600104	0.115670	4.335385
C	2.601338	1.016814	5.017347
C	3.183898	-0.856055	3.424112
H	6.202908	-2.123371	2.503020
H	2.125824	-0.973269	3.211055
N	-2.919483	2.282128	-0.890311
C	-3.896836	2.585176	-1.795196
C	-4.306971	1.669843	-2.865789
C	-4.374785	3.870656	-1.505235
C	-3.654032	4.347345	-0.398282
C	-3.361809	0.902143	-3.557108
C	-5.664930	1.548100	-3.192711
C	-3.760097	-0.008422	-4.541497
C	-6.084140	0.658824	-4.184216
C	-5.121930	-0.120640	-4.838692
C	-2.752400	3.346503	-0.022887
H	-5.130083	4.393066	-2.069707
H	-3.749252	5.311138	0.078016
H	-2.309345	0.993404	-3.304388
H	-6.397949	2.131085	-2.643034
C	-2.737637	-0.857505	-5.254883
C	-7.544225	0.537777	-4.546341
H	-5.441449	-0.835481	-5.592914
C	-1.791246	3.370299	1.031301
H	-2.482744	1.359454	-0.786896
O	-1.000827	2.437893	1.297165
H	-1.772469	4.291972	1.631663
N	1.614250	2.845604	2.277098
C	1.799109	3.991447	2.997414
C	0.688659	4.742517	3.586906
C	3.178088	4.239552	3.066641
C	3.828019	3.209090	2.363738
C	-0.501592	4.098342	3.943499

C	0.814754	6.122319	3.810794	N	2.884867	-2.307255	0.647689
C	-1.569338	4.817858	4.492917	H	2.645755	-1.323215	0.492261
C	-0.228335	6.854655	4.375567	C	2.339540	-3.398604	-0.000596
C	-1.418609	6.190264	4.703798	C	2.888123	-4.549892	0.572052
C	2.839845	2.351045	1.875784	H	2.656341	-5.561419	0.272595
H	3.639835	5.056603	3.597193	C	3.769805	-4.133820	1.587991
H	4.890937	3.069917	2.238779	H	4.374699	-4.754767	2.229116
H	-0.605374	3.029594	3.779902	C	3.743534	-2.734513	1.617578
H	1.728654	6.629139	3.516385	C	1.348066	-3.316138	-1.025139
C	-2.854674	4.108340	4.842717	H	1.049008	-4.278845	-1.459875
C	-0.085141	8.334363	4.635203	C	4.523352	-1.790623	2.453099
H	-2.242225	6.756236	5.131364	C	5.761393	-1.326057	1.957520
C	2.986086	1.119301	1.164515	C	6.513147	-0.425568	2.721528
H	0.705069	2.477315	1.973937	H	7.460059	-0.068500	2.330545
O	2.035002	0.370940	0.855714	C	6.058622	0.038151	3.957596
H	4.020617	0.833887	0.925167	C	6.876331	0.989362	4.816094
H	0.909092	-8.878830	-4.596377	C	4.824995	-0.426324	4.421521
H	-0.096559	-8.431537	-5.976383	H	4.450279	-0.058154	5.373970
H	-0.846632	-8.748350	-4.408533	C	4.043695	-1.337599	3.702100
H	2.845518	-3.197914	-4.882329	C	6.237093	-1.705963	0.561237
H	3.626279	-4.783588	-5.006620	H	5.706433	-2.615285	0.258681
H	3.348853	-4.048773	-3.421692	C	5.858224	-0.586160	-0.427076
H	7.635519	0.613439	4.546525	C	7.742003	-2.002633	0.495229
H	8.006882	-0.704645	3.423311	C	2.739162	-1.797143	4.348249
H	7.669801	-1.055546	5.121078	C	2.911409	-3.183778	4.996257
H	1.587901	0.823936	4.656644	H	2.553694	-1.079785	5.159080
H	2.832361	2.069527	4.817726	C	1.490940	-1.774204	3.448032
H	2.612018	0.871215	6.102677	N	-2.872104	2.586103	-0.823642
H	-3.209658	-1.718371	-5.734852	C	-3.750464	3.018123	-1.774968
H	-1.988196	-1.239016	-4.553287	C	-4.320381	2.091789	-2.780037
H	-2.213895	-0.281005	-6.025460	C	-3.956111	4.389816	-1.579893
H	-7.804460	-0.493552	-4.800143	C	-3.173815	4.780706	-0.475357
H	-7.784940	1.160845	-5.414749	C	-3.480916	1.540932	-3.780467
H	-8.184909	0.858175	-3.720918	C	-5.675252	1.718035	-2.709921
H	-3.597802	4.806344	5.235026	C	-4.023150	0.625956	-4.680513
H	-2.684575	3.334635	5.597962	C	-6.180298	0.800931	-3.646339
H	-3.282904	3.615022	3.963383	C	-5.369807	0.240089	-4.630577
H	-0.991681	8.875822	4.350289	C	-2.498665	3.644028	-0.020153
H	0.752614	8.755186	4.073974	H	-4.595907	5.012527	-2.185007
H	0.093853	8.529571	5.698139	H	-3.077001	5.770759	-0.054846
Tetramer 4				C	-2.020864	1.958662	-3.898345
O	-2.440676	-0.138170	-1.298225	C	-6.611099	2.259494	-1.637172
N	-1.725848	-2.594389	-2.614905	H	-3.382904	0.173829	-5.432617
H	-0.891082	-2.231888	-2.138695	H	-7.225539	0.515793	-3.583650
C	-2.993498	-2.048024	-2.579231	C	-5.886421	-0.749010	-5.663806
C	-3.830417	-2.867971	-3.339318	C	-1.515754	3.541100	1.011805
H	-4.883235	-2.695251	-3.507586	H	-2.552436	1.613547	-0.744839
C	-3.043051	-3.926102	-3.836618	O	-0.845963	2.509880	1.247423
H	-3.360821	-4.740197	-4.468301	H	-1.352464	4.451345	1.600961
C	-1.738806	-3.732741	-3.367734	H	-1.663233	2.232544	-2.902072
C	-3.296359	-0.835595	-1.886724	C	-1.917951	3.207202	-4.795347
H	-4.349416	-0.523502	-1.914126	C	-1.100420	0.841195	-4.406570
C	-0.503143	-4.520141	-3.566649	C	-7.303309	1.129058	-0.858049
C	-0.345625	-5.773527	-2.932313	C	-7.650302	3.210009	-2.255806
C	0.862047	-6.460758	-3.084697	H	-6.012905	2.835066	-0.924040
H	0.983746	-7.425465	-2.598631	N	1.609803	2.677219	2.621222
C	1.924325	-5.927334	-3.820777	C	1.505312	3.689734	3.532152
C	3.248514	-6.663598	-3.919831	C	0.219235	4.387980	3.756106
C	1.743672	-4.691231	-4.443049	C	2.759696	3.865809	4.127872
H	2.560365	-4.272620	-5.025218	C	3.638929	2.935647	3.540808
C	0.543510	-3.980176	-4.342987	C	-0.840851	3.703719	4.387293
C	-1.436655	-6.379740	-2.059322	C	0.040760	5.711586	3.293326
C	-0.914865	-6.729383	-0.655285	C	-2.081486	4.338783	4.500020
C	-2.050452	-7.616981	-2.736068	C	-1.212352	6.314198	3.447609
H	-2.229182	-5.634103	-1.940823	C	-2.288151	5.637306	4.029715
C	0.397417	-2.668979	-5.105881	C	2.907852	2.203288	2.602391
C	0.485634	-2.918845	-6.622050	H	2.982582	4.584205	4.900580
C	1.438777	-1.629406	-4.661824	H	4.684604	2.783884	3.764763
H	-0.596079	-2.256825	-4.898692	C	-0.669678	2.304850	4.966979
O	0.817222	-2.255209	-1.423888	C	1.154389	6.428426	2.538156
				H	-2.904577	3.804496	4.968015

H	-1.368684	7.327224	3.091022	H	2.444353	-8.689116	-3.956104
C	-3.655592	6.289997	4.128862	H	4.892784	-7.261883	-2.618459
C	3.364221	1.144499	1.758908	H	3.291760	-7.405079	-1.873209
H	0.830662	2.367567	2.030610	H	4.031825	-5.805951	-2.069401
O	2.631138	0.474963	0.996669	C	-7.187769	-1.447905	-5.255650
H	4.439420	0.930940	1.820321	H	-5.109059	-1.518233	-5.781200
C	-0.943243	2.309757	6.481321	C	-6.066766	-0.045906	-7.022929
H	0.371705	1.998516	4.821023	H	-0.878308	3.541959	-4.868360
C	-1.565653	1.280265	4.251727	H	-2.518727	4.027625	-4.390395
H	2.107922	6.132831	2.988338	H	-2.280648	2.978595	-5.803873
C	1.057983	7.957476	2.605197	H	-0.058433	1.165223	-4.327813
C	1.169828	5.960699	1.068618	H	-1.291908	0.597997	-5.458358
H	-3.575089	7.287757	3.677161	H	-1.216233	-0.069299	-3.808457
C	-4.093170	6.463487	5.592275	H	-7.902774	1.546230	-0.042761
C	-4.704821	5.489960	3.338100	H	-6.568338	0.441936	-0.427798
H	-0.760038	1.315539	6.901013	H	-7.974000	0.551550	-1.502873
H	-1.984905	2.575896	6.690616	H	-8.310694	3.614772	-1.482337
H	-0.298732	3.028897	6.995328	H	-8.267786	2.679183	-2.989105
H	-1.417910	0.284799	4.683062	H	-7.161807	4.044691	-2.767486
H	-1.340567	1.239383	3.183050	H	-7.433627	-2.233167	-5.976316
H	-2.623629	1.542978	4.367670	H	-8.024544	-0.740962	-5.240270
H	1.962331	8.403021	2.180567	H	-7.110827	-1.902828	-4.262625
H	0.950788	8.308837	3.635791	H	-6.389722	-0.759538	-7.787723
H	0.207159	8.330186	2.024713	H	-5.134350	0.420086	-7.353695
H	1.990170	6.437377	0.522580	H	-6.826621	0.738513	-6.938000
H	0.227364	6.233399	0.577635	Tetramer 5			
H	1.292637	4.875419	0.996198	O	-2.454735	-0.288976	-1.169305
H	-5.061692	6.970698	5.646593	N	-1.647659	-2.730918	-2.501012
H	-3.360808	7.048754	6.155200	H	-0.824179	-2.365580	-2.011446
H	-4.194924	5.487909	6.079851	C	-2.933581	-2.233026	-2.437157
H	-5.666331	6.013160	3.334888	C	-3.753164	-3.076595	-3.191425
H	-4.857996	4.504922	3.792218	H	-4.812003	-2.935319	-3.346634
H	-4.386848	5.333289	2.302623	C	-2.937794	-4.098913	-3.711554
C	7.771962	0.188196	5.779951	H	-3.237625	-4.912339	-4.352449
H	6.165264	1.569175	5.421725	C	-1.631313	-3.861273	-3.265756
C	7.720509	1.975693	3.998644	C	-3.281242	-1.033946	-1.742013
H	6.143091	-0.858500	-1.448375	H	-4.348892	-0.774691	-1.753526
H	6.380351	0.340995	-0.160952	C	-0.381718	-4.606006	-3.521699
H	4.781200	-0.389354	-0.407454	C	-0.257430	-5.940887	-3.082171
H	8.001922	-2.383873	-0.497028	C	0.949116	-6.616067	-3.299126
H	8.032605	-2.749455	1.239796	H	1.050077	-7.639358	-2.952659
H	8.338335	-1.099877	0.664445	C	2.012884	-5.988419	-3.944858
H	2.005874	-3.458101	5.547476	H	2.942757	-6.522264	-4.105727
H	3.757920	-3.193290	5.689419	C	1.877829	-4.673780	-4.386054
H	3.083156	-3.941649	4.225993	H	2.701556	-4.183029	-4.893681
H	0.596174	-1.803264	4.078761	C	0.688227	-3.966411	-4.183796
H	1.454430	-2.643378	2.785677	C	-1.387712	-6.638288	-2.362593
H	1.446622	-0.871153	2.831493	H	-1.811456	-6.004501	-1.578443
H	8.346748	0.860149	6.425344	H	-1.035218	-7.566968	-1.907875
H	8.474964	-0.428632	5.209409	H	-2.205151	-6.888079	-3.046203
H	7.173852	-0.475285	6.410947	C	0.580007	-2.535604	-4.651099
H	8.171889	2.721936	4.659106	H	0.756662	-1.845747	-3.818569
H	7.118106	2.496619	3.247318	H	-0.413563	-2.320357	-5.054270
H	8.535845	1.460103	3.480241	H	1.322868	-2.329738	-5.425427
H	3.909019	-6.062913	-4.558663	O	0.886941	-2.473389	-1.315925
C	3.082097	-8.045676	-4.571850	N	3.001341	-2.432091	0.683202
C	3.909385	-6.788079	-2.536337	H	2.607420	-1.485751	0.639766
H	-1.736104	-7.086601	-0.026167	C	2.637124	-3.512801	-0.096006
H	-0.467628	-5.855590	-0.170480	C	3.450809	-4.590103	0.265109
H	-0.158595	-7.520834	-0.696951	H	3.399124	-5.578026	-0.166824
H	-2.851102	-8.035301	-2.117833	C	4.316299	-4.141553	1.279784
H	-1.290911	-8.393182	-2.882741	H	5.066492	-4.713031	1.802228
H	-2.465406	-7.361773	-3.715789	C	4.012682	-2.796421	1.523852
H	0.322946	-1.983398	-7.167243	C	1.581002	-3.482194	-1.056923
H	-0.265336	-3.645691	-6.945575	H	1.391924	-4.430701	-1.576823
H	1.473539	-3.303591	-6.897698	C	4.579891	-1.856300	2.512935
H	1.307170	-0.702246	-5.229322	C	5.916910	-1.427806	2.389537
H	2.456246	-1.993335	-4.845648	C	6.421077	-0.508059	3.317129
H	1.340488	-1.407442	-3.595733	H	7.447270	-0.168975	3.220587
H	4.053438	-8.538660	-4.679371	C	5.619978	-0.026431	4.350618
H	2.623335	-7.960793	-5.560830				

H	6.020680	0.688240	5.061176
C	4.302460	-0.463837	4.471280
H	3.674948	-0.085296	5.271271
C	3.765327	-1.381876	3.562537
C	6.795625	-1.928579	1.268082
H	6.280050	-1.875177	0.304922
H	7.712137	-1.337333	1.205696
H	7.079531	-2.974912	1.419685
C	2.326229	-1.814745	3.692280
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H	2.206898	-2.878191	3.466863
H	1.960140	-1.629188	4.704726
N	-3.001758	2.433077	-0.682969
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C	-4.580188	1.857266	-2.512764
C	-4.316775	4.142503	-1.279510
C	-3.451313	4.591055	-0.264807
C	-3.765461	1.382841	-3.562235
C	-5.917197	1.428700	-2.389514
C	-4.302421	0.464739	-4.471016
C	-6.421194	0.508897	-3.317146
C	-5.619933	0.027273	-4.350512
C	-2.637551	3.513788	0.096241
H	-5.066976	4.713971	-1.801953
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C	-2.326358	1.815757	-3.691751
C	-6.796081	1.929458	-1.268185
H	-3.674783	0.086202	-5.270910
H	-7.447381	0.169760	-3.220726
H	-6.020503	-0.687446	-5.061098
C	-1.581358	3.483186	1.057077
H	-2.607780	1.486756	-0.639595
O	-0.887250	2.474383	1.315975
H	-1.392229	4.431690	1.576963
H	-1.960075	1.630146	-4.704116
H	-1.691129	1.258072	-2.993315
H	-2.207116	2.879224	-3.466383
H	-7.712600	1.338208	-1.205942
H	-7.079965	2.975792	-1.419817
H	-6.280650	1.876047	-0.304947
N	1.647214	2.731795	2.501340
C	1.630731	3.862011	3.266284
C	0.381052	4.606576	3.522292
C	2.937167	4.099684	3.712195
C	3.752647	3.077518	3.191938
C	-0.688896	3.966716	4.184126
C	0.256671	5.941544	3.083053
C	-1.878593	4.673914	4.386423
C	-0.949971	6.616546	3.300033
C	-2.013741	5.988640	3.945511
C	2.933172	2.233994	2.437502
H	3.236898	4.913019	4.353252
H	4.811486	2.936298	3.347195
C	-0.580581	2.535800	4.651077
C	1.386951	6.639232	2.363752
H	-2.702324	4.182960	4.893849
H	-1.051006	7.639903	2.953782
H	-2.943689	6.522349	4.106401
C	3.280959	1.035029	1.742219
H	0.823792	2.366508	2.011639
O	2.454541	0.290066	1.169375
H	4.348621	0.775821	1.753803
H	-1.323528	2.329652	5.425248
H	0.412958	2.320561	5.054331
H	-0.757039	1.846137	3.818343
H	2.204275	6.888987	3.047512
H	1.034394	7.567961	1.909182
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