

## Supplementary Information

### High chemical recyclability of vinyl lactone acrylic bioplastics

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#### Materials and Methods

The synthesis of air and moisture sensitive materials were carried out in flame-dried Schlenk glassware on a dual-manifold Schlenk line or in an inert gas (Ar or N<sub>2</sub>) glovebox. Organic solvents were dried with CaH<sub>2</sub> or sodium/potassium alloy (for hexanes) between 24 and 48 h before being distilled and stored under nitrogen atmosphere. NMR solvents (CDCl<sub>3</sub>, dimethyl sulfoxide-*d*<sub>6</sub>, and benzene-*d*<sub>6</sub>) were used as received. NMR spectra were recorded on a Varian Inova 400 MHz spectrometer. Chemical shifts for <sup>1</sup>H and <sup>13</sup>C NMR spectra were referenced to internal <sup>13</sup>C solvent resonances.

Triethyl aluminum, methyl trimethylsilyl dimethylketene acetal (<sup>m</sup>eSKA), *n*-butyllithium, Mmethyl  $\alpha$ -bromophenylacetate (MBPA), N,N,N',N'',N''-pentamethyldiethylenetriamine (PMEDTA), and galvinoxyl were purchased from Sigma-Aldrich Chemical Co. Copper(II) bromide and zinc(II) chloride were purchased from Alfa-Aesar. Iron(III) chloride was purchased from Spectrum Chemical Mfg. Corp. Polyethylene (*M*<sub>w</sub> = 35 kDa), poly(methyl methacrylate) (*M*<sub>w</sub> = 15 kDa), poly(ethylene terephthalate) (granular), isotactic polypropylene (*M*<sub>w</sub> = 12 kDa), and Merrifield peptide resin (PS) were purchased from Sigma-Aldrich Chemical Co. The above commercial reagents were used as received.  $\alpha$ -Methylene- $\gamma$ -butyrolactone (MBL) and  $\gamma$ -methyl- $\alpha$ -methylene- $\gamma$ -butyrolactone ( $\gamma$ MMBL) were purchased from TCI America, dried over CaH<sub>2</sub> overnight, vacuum distilled, and stored over activated Davison 4 Å molecular sieves in a brown bottle inside a freezer of the glovebox for further use.

Tris(pentafluorophenyl)borane, B(C<sub>6</sub>F<sub>5</sub>)<sub>3</sub>, was obtained as a research gift from Boulder Scientific Co. and was further purified by sublimation (twice). Tris(pentafluorophenyl)alane, Al(C<sub>6</sub>F<sub>5</sub>)<sub>3</sub> (unsolvated form) was prepared by the ligand exchange reaction between B(C<sub>6</sub>F<sub>5</sub>)<sub>3</sub> and either AlMe<sub>3</sub> or AlEt<sub>3</sub> in dry hexanes, following literature procedures.<sup>1,2</sup> *As the unsolvated alane is thermal and shock sensitive, extreme caution should be exercised while handling this material!*

### Polymer Samples Prepared by Group Transfer Polymerization (GTP)<sup>3,4</sup>

All GTP reactions were carried out in an inert gas (Ar or N<sub>2</sub>) glovebox at room temperature in 500 mL oven-dried glass reactors. In a typical polymerization, monomer was premixed with Al(C<sub>6</sub>F<sub>5</sub>)<sub>3</sub> (2 equiv. relative to initiator) in CH<sub>2</sub>Cl<sub>2</sub>. <sup>m</sup>eSKA was dissolved in CH<sub>2</sub>Cl<sub>2</sub> before being added to the vigorously stirring monomer solution to start the polymerization (1.0 M). Polymerizations were quenched with 100 mL of 5% HCl in methanol. The polymers were precipitated into 500 mL of methanol and collected by filtration before being washed with excess methanol to remove catalyst residue and unreacted monomer. The polymers were then dried overnight in a vacuum oven at 50 °C to consistent weights before NMR and GPC analyses were performed. Polymer characterization data are summarized in Table S1.

### Polymer Samples Prepared by Atom Transfer Radical Polymerization (ATRP)<sup>5</sup>

All ATRP reactions were performed in septum sealed, argon filled, oven-dried, 20 mL scintillation vials at 45 °C in a silicon oil bath. In a typical polymerization, the vial was brought into an inert gas (Ar or N<sub>2</sub>) filled glovebox, and a magnetic stir bar was wrapped with around 2 cm of concentrated HCl washed copper wire before being loaded into the vial. Then monomer, MBPA (1 equiv.), and copper(II) bromide (0.05 equiv.) were loaded into the vial before it was covered with a rubber septum and sealed with electrical tape. The vial was removed from the glovebox and a solution of PMEDTA (0.36 equiv.) in isopropanol (equal volume solvent to monomer) was added to the vial before it was heated to 45 °C and polymerization was left to proceed. Polymerizations were quenched by dissolving any solid that had precipitated in CHCl<sub>3</sub> and passed the resulting solution through a column of neutral alumina. The quenched solution was concentrated and then precipitated into methanol before polymers were collected by filtration and washed with excess methanol to remove impurities. The polymers were then dried overnight in a vacuum oven at 50 °C to consistent weights before NMR and GPC analyses were performed. Polymer characterization data are summarized in Table S1.

**Table S1 Summary of polymerization method and data**

Entry	Polymer	Method	[monomer]:[initiator]: [catalyst]	M <sub>n</sub> (kDa)	Đ
1	PMMA	GTP	500:1:1	44.8	1.18
2	PMBL	GTP	200:1:1	11.7	1.40
3	PyMMBL	GTP	800:1:1	120	3.43
4	PyMMBL	ATRP	50:1:0.05	9.73	1.10

### **Polymer and Pyrolysis Residue Characterization**

Polymer number-average molecular weights ( $M_n$ ), weight-average molecular weights ( $M_w$ ), and dispersities ( $D = M_w/M_n$ ) were obtained from gel permeation chromatography (GPC) analyses carried out at 40 °C with a flow rate of 1.0 mL/min, with DMF as the eluent, on a Waters University 1500 GPC equipped with four PL gel 5  $\mu$ m mixed-C columns (Polymer Laboratories). Chromatograms were processed with Waters Empower software (version 2002). Chromatogram files were processed with Origin for presentation. Ten molecular weight PMMA standards were acquired from Polymer Laboratories. To obtain a calibration curve, three different molecular weight sample sets were dissolved in DMF to known concentration.

### **Matrix-assisted Laser Desorption/Ionization Time of Flight Mass Spectrometry (MALDI-TOF MS)**

MALDI-TOF MS was performed on a Ultraflex MALDI-TOF mass spectrometer (Bruker Daltonics) operated in positive ion reflector mode using a Nd:TAG laser at 355 nm and 25 kV accelerating voltage. Samples were prepared on a 96-well plate by first depositing a layer of NaI solution (1%), followed by 0.5  $\mu$ L of a solution of polymer or pyrolysis sample and dithranol matrix in  $\text{CHCl}_3$  on top of the NaI crystals. Calibrants were prepared by depositing a layer of NaI solution (1%) on the plate before 0.5  $\mu$ L of a solution of peptide calibration mixture and  $\alpha$ -cyano-4-hydroxycinnamic acid (HCCA) matrix was deposited on top of the NaI crystals. Obtained spectra were processed using mMass processing software.

### **Typical Procedure for Acrylic Plastic Chemical Recycling**

Depolymerization experiments were performed in 25 to 50 mL oven-dried round-bottom flasks fixed with Teflon-coated magnetic stir bars. Additives (if used) were loaded into the flask inside an inert gas (Ar or  $\text{N}_2$ ) filled glovebox before the vessel was sealed, brought outside the glovebox, loaded with polymer sample, and fixed with a microdistillation apparatus (short path, no Vigreux) with a collection flask and thermometer. The reaction flask was wrapped in aluminum foil before the reaction apparatus was slowly evacuated to between 50 and 100 mTorr. The collection flask was submerged in dry ice while a heating mantle (100 mL, 115 V, Glas-Col, hemispheric) in circuit with a thermocouple was heated to a predetermined temperature and held there. The reaction flask was introduced to the heating mantle before being wrapped in glass wool. After the reaction was complete, the residues in the condenser and reaction flask were isolated and analyzed with NMR and GPC (Figure S2 to S3). The distillate in the collection flask was weighed and analyzed by NMR spectroscopy.

### Radical Trapping of Depolymerization Residues with galvinoxyl for MALDI-TOF Analysis

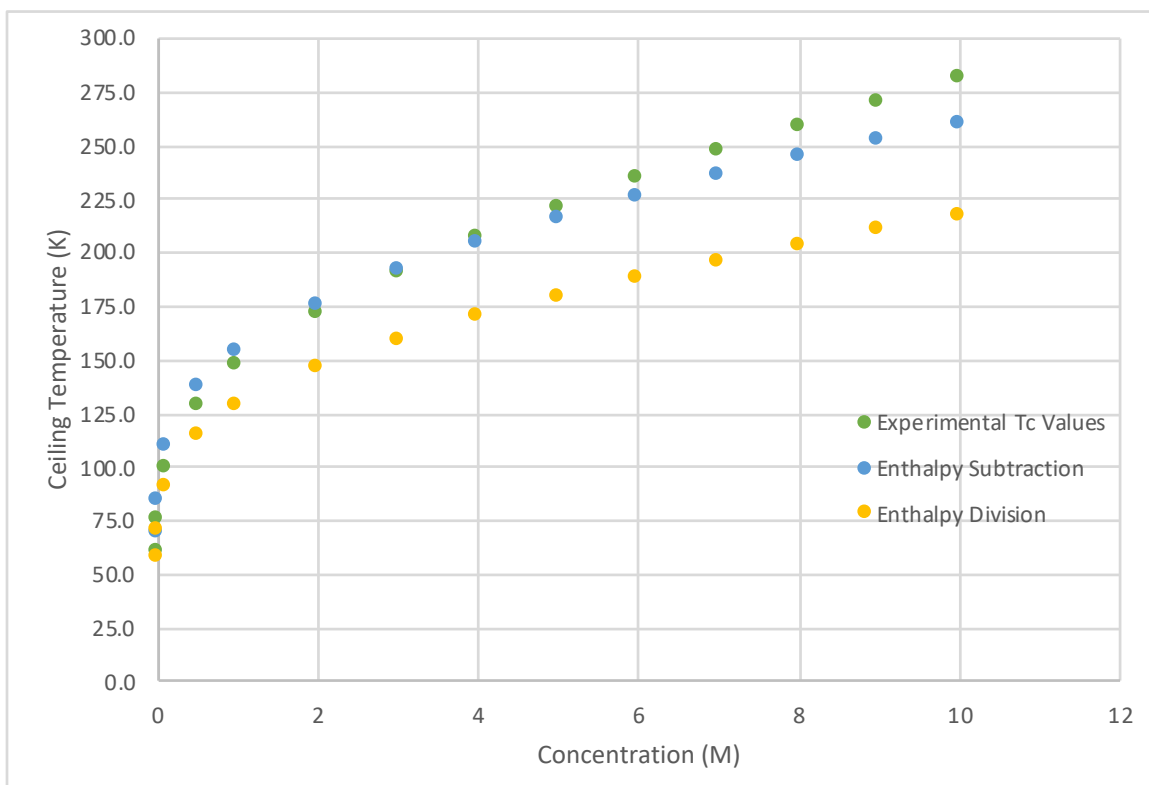
A typical procedure for chemical recycling of acrylic polymers was followed (500 mg polymer). Upon depolymerization for 30 min, the vacuum was released and galvinoxyl (50 mg for all experiments) was added to the reaction flask and heat was removed. The apparatus was allowed to cool to room temperature before the reaction flask was extracted with chloroform and the solution was analyzed via MALDI-TOF MS.

### Thermal Analysis

Thermal gravimetric analysis (TGA) was performed on a Q50 TGA Analyzer (TA Instruments) to obtain decomposition temperatures ( $T_d$ , defined by the temperature of 5 % weight loss) and maximum rate decomposition temperatures ( $T_{max}$ ) of the polymers. Between 5 and 10 mg of polymer sample was heated from 30 °C to 700 °C at 10 °C/min while the mass of the sample was continuously measured. Values of  $T_{max}$  were obtained from derivative (wt %/°C) vs. temperature (°C) plots by selecting the peak values, while  $T_d$  values were obtained from wt % vs. temperature (°C) plots by selecting the point of the weight percent versus temperature (°C) plots indicating 95 weight percent of sample remaining (Figures S2-S4). Differential scanning calorimetry (DSC) was performed on an Auto Q20 (TA Instruments) to obtain the glass transition temperature ( $T_g$ ) and melting temperature ( $T_m$ ). Between 3 and 10 mg of polymer sample was weighed into an aluminum pan and sealed with an aluminum lid. Samples were then heated at 10-20 °C/min from room temperature to 250 °C and cooled to -40 °C to remove thermal history before being reheated to 250 °C. During this time, the thermal response was measured relative to a reference pan.

### Computational Details

All the density functional theory (DFT) calculations were performed using ORCA 4.2.<sup>6</sup> Geometry optimizations were performed using the BP86 functional with the def2-SVPD basis set.<sup>7-9</sup> The dispersion correction scheme of D3BJ was employed. Geometry minima were confirmed with frequency calculations and all energies are BP86/SVPD electronic energies calculated at 298 K using the BP86/SVPD method. All structures modeled a charge of zero and were capped with a proton for simplicity of calculation. Computational details are summarized in Table S2.



**Figure S1** Test of fitting the DFT calculated  $T_c$  values as a function of monomer concentration [M] for the ring-opening polymerization of MBL against the full set of experimental data at various [M] concentrations. The best fitting correction made to the computed  $T_c$  values was found with  $\Delta H_p$  correction by subtraction and  $\Delta S_p$  correction by division.

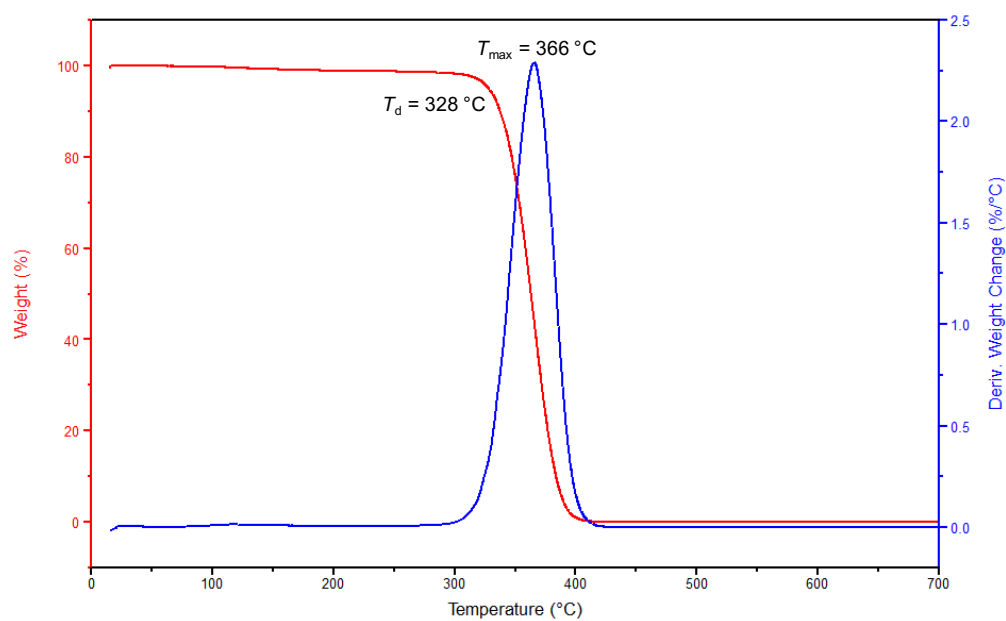


Figure S2 TGA thermograph for PMMA used in this study.

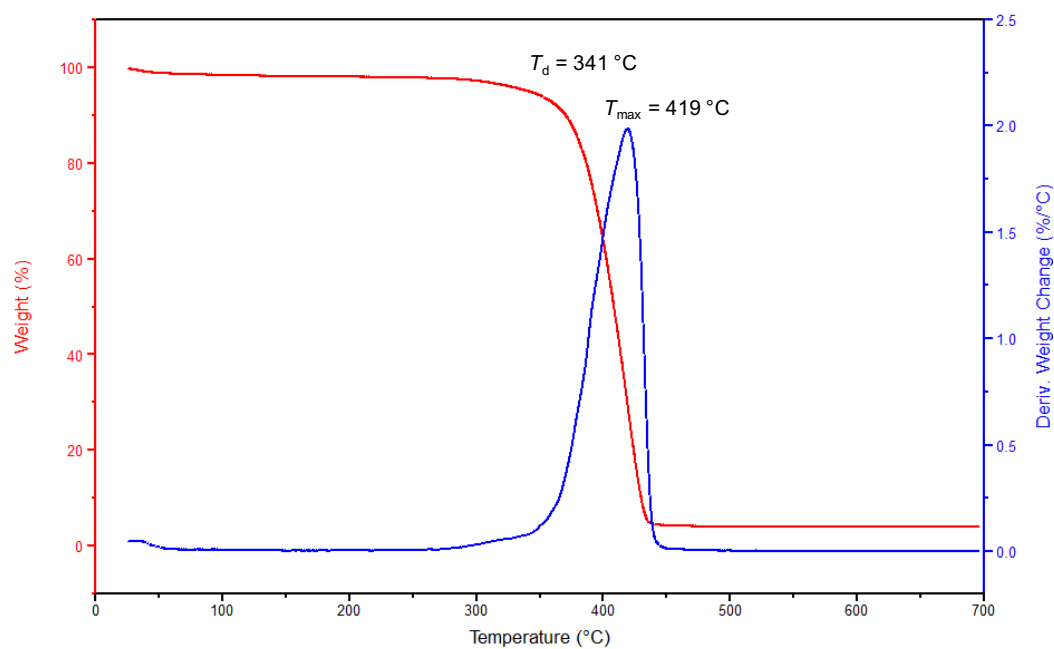


Figure S3 TGA Thermograph for PMBL used in this study.

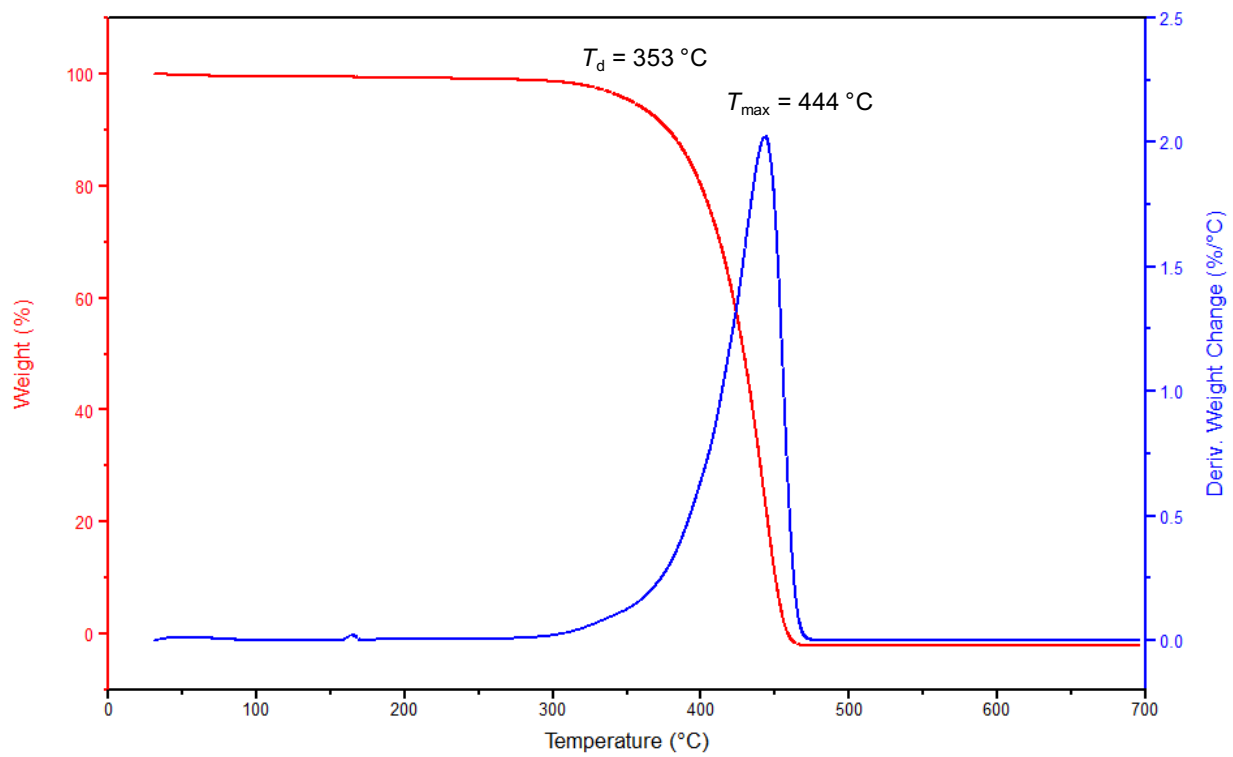
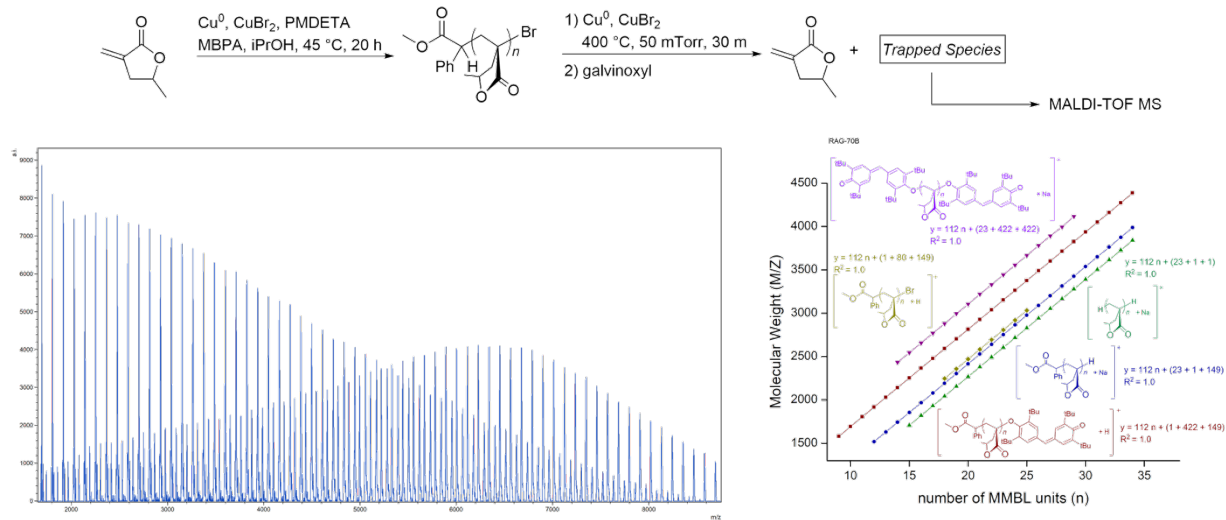


Figure S4 TGA Thermograph for PyMMBL.



**Figure S5** MALDI-TOF MS spectrum and chain-end analysis of polymer residues from catalyzed depolymerization of P $\gamma$ MMBL synthesized by ATRP.



**Table S2. Cartesian coordinates of species reported in the manuscript and in reference to Table 2**

<b>MBL</b>				H	-1.72506	0.56387	-2.40040
C	-0.35134	-0.03306	0.21783	H	-1.22051	-1.07216	-1.89151
C	-0.43551	-0.51821	1.46941	H	0.00558	0.13861	-2.39917
C	-0.07211	1.36916	-0.26205	H	-2.08670	0.48157	1.41646
C	-0.54506	-0.91325	-0.98155	H	-2.98979	0.80003	-0.09618
C	-0.11859	1.23679	-1.80601	H	-2.44480	-0.85405	0.27317
O	-0.40402	-0.14792	-2.11290				
O	-0.78659	-2.10026	-1.02623				
H	-0.29566	0.11840	2.35388	<b>PMBL Dimer</b>			
H	-0.65105	-1.58577	1.61955	C	0.03786	-1.46603	1.22764
H	0.91482	1.73012	0.08690	C	-1.02959	-2.13599	2.12439
H	-0.83096	2.08491	0.10900	C	1.34141	-1.84404	1.98787
H	0.84385	1.49078	-2.28843	C	-0.26469	-3.30676	2.75625
H	-0.91679	1.84890	-2.26592	O	1.10674	-2.85405	2.86364
				O	2.43116	-1.32514	1.86584
				C	0.00008	0.07758	1.18797
<b>PMBL Monomer</b>				C	0.06339	-2.15162	-0.16669
C	0.46550	-1.68414	0.30963	C	-1.10015	2.25638	1.00247
C	-0.43700	-2.46265	1.28230	O	-1.95139	2.74493	1.72496
C	1.87513	-2.15888	0.70120	O	0.02938	2.91622	0.64140
C	0.40276	-3.71138	1.59356	C	0.18249	4.23976	1.18746
O	1.78488	-3.30305	1.44639	C	-1.13081	0.83254	0.41601
O	2.93694	-1.65005	0.42190	C	1.36140	-1.97047	-0.97345
C	0.38654	-0.15470	0.31404	C	-0.86262	0.93422	-1.10388
C	-0.59440	1.99864	-0.41412	C	-2.53140	0.25171	0.66494
O	-0.47813	2.69481	-1.40727	C	2.18269	-3.26461	-1.01453
O	-0.51613	2.49613	0.84765	C	1.25933	-1.60507	-2.46242
C	-0.26372	3.90995	0.94623	O	2.87899	-3.32458	-2.19029
C	-0.84041	0.48019	-0.40269	C	2.58054	-2.16500	-3.00966
C	-0.94746	-0.00141	-1.85794	O	2.22562	-4.14490	-0.18432
C	-2.16540	0.21206	0.34884	H	-1.91937	-2.47647	1.56707
H	0.31672	-2.06208	-0.72575	H	-1.36743	-1.43427	2.90874
H	-1.42274	-2.72700	0.86268	H	-0.60586	-3.57081	3.77145
H	-0.60413	-1.86445	2.19874	H	-0.27155	-4.21573	2.12355
H	0.27832	-4.09698	2.62020	H	0.97539	0.43470	0.80954
H	0.20931	-4.53416	0.87539	H	-0.03202	0.40718	2.24623
H	1.31120	0.21707	-0.17036	H	-0.09664	-3.23609	-0.01873
H	0.41676	0.20258	1.36134	H	-0.80357	-1.78646	-0.74417
H	-0.22277	4.13191	2.02474	H	1.14031	4.61606	0.79399
H	0.69521	4.16323	0.45789	H	-0.65481	4.88654	0.86759
H	-1.07567	4.48064	0.45927	H	0.20191	4.19857	2.29204

H	2.01812	-1.23321	-0.46254	H	-2.41262	-1.40300	3.39192
H	-1.54696	1.67080	-1.56496	H	-0.94866	-2.27325	2.82539
H	-1.03945	-0.03184	-1.60512	H	0.16688	1.58548	-0.27762
H	0.17203	1.25844	-1.30736	H	-1.22640	1.91998	0.73461
H	-2.76556	0.19742	1.74157	H	1.58091	-0.33785	0.77475
H	-3.29990	0.88926	0.19356	H	0.73342	-1.73517	1.41791
H	-2.61398	-0.75900	0.22860	H	-0.23935	5.37086	-1.87525
H	1.15888	-0.52192	-2.64485	H	-1.97809	5.20875	-2.37694
H	0.39485	-2.11907	-2.92751	H	-1.55885	5.29539	-0.62899
H	3.41290	-1.44044	-2.89983	H	-1.80717	1.19876	-3.41015
H	2.53417	-2.50577	-4.05829	H	-0.96173	-0.17902	-2.68702
				H	-0.16015	1.41395	-2.73312
				H	-3.65726	0.79825	-0.19079
				H	-3.75130	0.75443	-1.96037
				H	-2.94650	-0.58088	-1.10460
				H	1.63642	-3.78403	-0.13201
				H	2.80024	-2.47032	0.18656
				H	2.04577	-3.60614	-2.59646
				H	3.68846	-3.27954	-1.93906
				H	0.14329	-4.40327	-1.62602
				H	-0.69086	-3.49340	0.99711
				H	-0.52481	-5.17857	0.46249
				H	-2.89164	-5.31079	0.70425
				H	-3.08425	-3.52925	0.65838
				H	-1.16434	-1.65130	-1.20729
				H	-0.17729	-2.19685	-2.54914
<b>PMBL Trimer</b>							
C	-0.55573	-0.07840	0.90755				
C	-1.80724	-0.88565	1.32172				
C	-0.13661	0.48658	2.30556				
C	-1.51195	-1.31941	2.75981				
O	-0.68783	-0.26851	3.30707				
O	0.59450	1.41981	2.53727				
C	-0.81409	1.18078	0.02008				
C	0.69518	-0.97903	0.60807				
C	-2.11118	2.76973	-1.29067				
O	-3.20825	3.25627	-1.07179				
O	-1.02196	3.51382	-1.59477				
C	-1.21995	4.93885	-1.61918				
C	-1.76857	1.26380	-1.23495				
C	0.95740	-1.73130	-0.71929				
C	-1.12333	0.90474	-2.59148				
C	-3.10309	0.51175	-1.10041				
C	1.74583	-0.82699	-1.70207				
C	2.03108	-2.83132	-0.52315				
O	2.59806	-1.59913	-2.44677				
C	2.63539	-2.95008	-1.92529				
O	1.71552	0.37548	-1.81716				
C	-0.66051	-3.77258	-1.20517				
C	-1.01227	-4.21555	0.22818				
C	-1.92061	-4.10363	-2.01775				
C	-2.54765	-4.38681	0.20757				
O	-2.93778	-4.46887	-1.18085				
O	-2.05352	-4.04879	-3.21859				
C	-0.30265	-2.29140	-1.45484				
H	-2.03815	-1.73434	0.66339				
H	-2.68566	-0.22063	1.32234				
				<b>PMBL Tetramer</b>			
				C	0.95925	1.29544	-1.12331
				C	-0.08015	1.72992	-2.18913
				C	1.77181	2.58514	-0.94891
				C	0.68228	2.79330	-2.98612
				O	1.60358	3.39494	-2.03669
				O	2.45785	2.92424	-0.00723
				C	1.80251	0.13959	-1.75760
				C	0.30467	0.76694	0.17147
				C	3.55353	-1.59619	-1.83018
				O	4.41863	-1.87295	-2.64068
				O	2.72423	-2.54380	-1.29908
				C	2.94822	-3.88921	-1.75508
				C	3.24697	-0.19561	-1.26889
				C	-0.22798	1.72185	1.25883
				C	4.26644	0.79191	-1.86419

C	3.41349	-0.26053	0.26711	H	-3.87970	2.20231	3.08031
C	0.91864	2.10651	2.23111	H	-5.36142	1.24097	2.75278
C	-0.76560	3.10291	0.82536	H	-0.66129	0.36373	2.92381
O	0.79654	3.40221	2.61512	H	-1.68308	1.78148	2.85585
C	-0.33956	4.03095	1.97727	H	0.06113	-1.19007	1.90921
O	1.74858	1.35522	2.69480	H	0.57417	-2.73243	0.12642
C	-2.39580	0.11090	1.66801	H	-0.93108	-3.66942	0.41073
C	-3.48731	0.04404	2.76428	H	0.59595	-5.00581	1.78024
C	-3.13725	0.89352	0.56530	H	1.59792	-3.56357	2.18452
C	-4.28502	1.33089	2.52982	H	-1.80463	-1.17929	0.02909
O	-4.16230	1.60804	1.10545	H	-2.82973	-1.96559	1.22272
O	-2.88602	0.92883	-0.62293				
C	-1.23135	0.99654	2.22098				
C	-0.73371	-1.94239	1.73043	<b>MMA</b>			
C	-0.12830	-3.08576	0.90226	C	-0.57253	0.65236	0.73023
C	-0.97178	-2.59350	3.09275	C	0.74786	0.15852	0.21076
C	0.56824	-3.92177	1.98369	C	-0.53225	1.43039	1.83409
O	-0.21839	-3.72905	3.19069	C	-1.86447	0.27236	0.03666
O	-1.69436	-2.21446	3.99057	O	0.60252	-0.61581	-0.90100
C	-1.96994	-1.27641	1.11784	O	1.83984	0.40184	0.70218
H	-0.98529	2.14541	-1.71692	C	1.82411	-1.13397	-1.45369
H	-0.40820	0.88196	-2.81567	H	-1.45282	1.83182	2.28059
H	1.28058	2.36507	-3.81415	H	0.42954	1.67439	2.30450
H	0.04975	3.60337	-3.38671	H	-1.68087	-0.30730	-0.88099
H	1.87904	0.32179	-2.84703	H	-2.50245	-0.33821	0.70611
H	1.16631	-0.75834	-1.64552	H	-2.44167	1.17703	-0.23550
H	-0.52320	0.14229	-0.18741	H	1.52697	-1.72345	-2.33602
H	1.01819	0.10368	0.68363	H	2.49722	-0.30557	-1.74350
H	2.20417	-4.51116	-1.23124	H	2.34269	-1.76930	-0.71132
H	2.81066	-3.95535	-2.84999				
H	3.97441	-4.21449	-1.50413	<b>PMMA Dimer</b>			
H	5.29626	0.46576	-1.63692	C	-5.03952	-1.77722	0.10990
H	4.12903	1.79780	-1.43594	C	-4.83940	-2.88640	1.15276
H	4.17383	0.84876	-2.96379	O	-3.92409	-3.80479	0.73820
H	3.20948	0.71946	0.72784	O	-5.42952	-2.98032	2.21439
H	2.75012	-1.01383	0.72525	C	-3.69558	-4.90288	1.63937
H	4.45487	-0.53962	0.51225	C	-5.86921	-0.64818	0.74194
H	-1.85674	3.12132	0.66798	C	-3.66773	-1.27954	-0.41477
H	-0.29700	3.44550	-0.10929	C	-2.66687	-0.77969	0.64381
H	-0.01766	5.03033	1.63905	C	-3.05088	0.54250	1.29328
H	-1.13032	4.15213	2.74436	C	-1.25809	-0.63926	0.02904
H	-4.12993	-0.84066	2.60361	O	-3.39711	1.47649	0.36767
H	-3.06724	-0.03864	3.78015	O	-3.01268	0.77592	2.48946
				C	-3.76425	2.76459	0.89229

C	-5.81484	-2.39568	-1.07879	H	-5.99265	9.93518	2.01922
H	-2.94071	-5.53958	1.14966	H	-4.82499	10.27895	0.66817
H	-3.32280	-4.53089	2.61122	H	-7.33231	6.85821	-3.63544
H	-4.63263	-5.46447	1.80882	H	-7.35163	8.63987	-3.48029
H	-5.97636	0.18396	0.02233	H	-5.80069	7.78831	-3.58173
H	-6.87563	-1.01062	1.01305	H	-6.91921	5.49075	-1.14308
H	-5.40743	-0.26612	1.66828	H	-5.92908	6.43983	-0.03690
H	-3.84958	-0.47253	-1.15057	H	-3.61222	3.94818	-1.47852
H	-3.18541	-2.10858	-0.96517	H	-4.24629	4.66925	0.03129
H	-2.61142	-1.50086	1.48207	H	-5.32568	3.71264	-1.01978
H	-0.53171	-0.25422	0.76833	H	-6.84883	4.73749	-5.26948
H	-0.90504	-1.62652	-0.32165	H	-5.94976	3.23865	-4.85093
H	-1.27689	0.04915	-0.83703	H	-7.68600	3.41703	-4.34508
H	-4.65358	2.67081	1.54348	H	-8.37233	7.38508	-0.06628
H	-2.93334	3.19411	1.48147	H	-8.84036	8.49426	-1.39200
H	-3.98813	3.39233	0.01488	H	-8.84011	6.72444	-1.66626
H	-6.80652	-2.76251	-0.75557	H	-3.09507	6.41459	-2.78174
H	-5.97166	-1.62589	-1.85879	H	-4.09318	7.71947	-2.16269
H	-5.25526	-3.23763	-1.52464	H	-2.02640	7.67751	-1.05036

**PMMA Trimer**

C	-6.84160	7.58871	-1.64300
C	-6.18219	8.84133	-1.04694
O	-6.39399	8.92891	0.29321
O	-5.56448	9.69012	-1.66866
C	-5.88362	10.10976	0.93651
C	-6.82214	7.72038	-3.17401
C	-6.15587	6.28924	-1.10634
C	-4.88317	5.72184	-1.79560
C	-5.21009	5.21484	-3.21702
C	-4.49023	4.43445	-1.01828
O	-6.37451	4.51076	-3.23906
O	-4.50874	5.34017	-4.20523
C	-6.73127	3.94183	-4.51005
C	-8.31212	7.55124	-1.15606
C	-3.69822	6.71945	-1.91081
C	-1.82843	5.68516	-0.46658
C	-2.73403	6.88922	-0.71150
C	-3.36378	7.37329	0.59628
O	-1.27102	5.23954	-1.62307
O	-1.58024	5.18932	0.62017
C	-0.37771	4.12096	-1.49549
H	-6.47237	10.99164	0.62334

H	-2.58593	7.56673	1.35499
H	-4.05912	6.63096	1.02606
H	-3.91524	8.30945	0.41424
H	-0.08129	3.85650	-2.52269
H	0.50537	4.39952	-0.89127
H	-0.89013	3.27271	-1.00432

**PMMA Tetramer**

C	-3.13212	-4.92667	4.97094
C	-1.98984	-3.92037	4.77868
O	-2.17459	-2.79807	5.52976
O	-1.00043	-4.08842	4.08822
C	-1.14838	-1.79912	5.40986
C	-2.95595	-5.51359	6.39641
C	-4.52040	-4.23144	4.94117
C	-5.05257	-3.68444	3.59232
C	-5.47811	-4.82742	2.65023
C	-4.01954	-2.82888	2.83576
O	-6.17121	-5.79409	3.30318
O	-5.29110	-4.85118	1.44540
C	-6.68723	-6.85397	2.48029
C	-2.98774	-6.05024	3.93378
C	-6.39916	-2.91202	3.81900
C	-6.63445	-2.55631	6.28970

C	-6.52130	-1.84002	4.93978	H	-9.11468	-2.24321	8.94557
C	-5.37378	-0.81212	4.91640	H	-8.69567	-0.48746	9.16644
O	-5.86440	-1.98246	7.24828	H	-10.39322	-0.99181	8.76711
O	-7.34599	-3.52794	6.48767				
C	-5.86883	-2.57956	8.55532	<b>PMMA Pentamer</b>			
C	-7.83810	-1.01925	4.70251	C	14.48110	-23.61024	-8.13672
C	-9.62588	-1.88576	6.37301	C	13.00694	-23.74223	-7.72804
C	-9.24022	-1.63347	4.91781	O	12.81788	-24.69313	-6.77189
C	-9.62376	-2.84287	4.05177	O	12.09511	-23.10759	-8.22766
O	-8.96796	-1.05365	7.23018	C	11.46899	-24.94350	-6.33937
O	-10.47747	-2.67183	6.74305	C	14.49902	-23.68863	-9.68018
C	-9.32004	-1.20864	8.61495	C	15.15612	-22.30220	-7.59488
H	-0.17088	-2.20921	5.72090	C	14.67151	-20.84500	-7.88089
H	-1.07138	-1.45345	4.36222	C	14.40630	-20.65185	-9.39196
H	-1.45513	-0.97288	6.07107	C	15.88724	-19.91872	-7.56846
H	-3.07644	-4.73121	7.16737	O	15.53068	-20.89242	-10.12720
H	-3.72340	-6.29037	6.56935	O	13.36245	-20.29849	-9.90515
H	-1.95904	-5.97726	6.51558	C	15.37620	-20.75316	-11.54713
H	-4.46209	-3.39725	5.65938	C	15.32795	-24.76947	-7.56909
H	-5.26176	-4.94142	5.34679	C	13.37402	-20.35952	-7.16827
H	-3.61658	-2.02624	3.46868	C	11.90815	-19.54941	-5.36838
H	-3.17748	-3.44429	2.47586	C	13.14014	-20.44820	-5.62670
H	-4.47965	-2.37446	1.94191	C	12.75718	-21.87943	-5.19199
H	-7.22908	-7.52598	3.16533	O	11.43146	-19.70772	-4.09744
H	-7.36766	-6.44754	1.70967	O	11.37271	-18.80847	-6.16749
H	-5.85879	-7.38770	1.97936	C	10.31678	-18.86717	-3.75615
H	-3.78746	-6.79709	4.08069	C	14.38432	-19.92574	-4.84924
H	-3.04310	-5.67117	2.89930	C	13.60602	-18.23113	-3.16823
H	-2.01020	-6.55088	4.04233	C	14.38298	-19.53844	-3.34472
H	-6.65560	-2.42085	2.86051	C	13.89406	-20.64968	-2.39832
H	-7.17915	-3.66089	4.01543	O	13.25004	-18.02400	-1.87037
H	-4.40541	-1.25696	5.19335	O	13.37594	-17.42375	-4.04932
H	-5.57250	0.00892	5.62622	C	12.63474	-16.75104	-1.60167
H	-5.28806	-0.37601	3.90444	C	15.88958	-19.22706	-3.03470
H	-6.43405	-3.52692	8.54117	C	16.25395	-18.72260	-1.63075
H	-4.81626	-2.75439	8.83797	C	15.99596	-17.23232	-1.46048
H	-6.33109	-1.86820	9.26262	C	17.74995	-18.97738	-1.33536
H	-7.77652	-0.11157	5.32873	O	15.82093	-16.91779	-0.14899
H	-7.78801	-0.67108	3.65203	O	16.01131	-16.39720	-2.34798
H	-9.92700	-0.80315	4.63290	C	15.72330	-15.51326	0.14772
H	-9.16780	-3.76937	4.44035	H	11.32190	-26.03730	-6.35273
H	-9.29875	-2.69186	3.00647	H	11.35497	-24.56577	-5.30743
H	-10.71734	-2.98693	4.06326	H	10.75142	-24.44036	-7.01038

H	14.19774	-24.70060	-10.00771	C	0.22083	-0.98259	-0.24846
H	13.79198	-22.97313	-10.13081	C	0.41955	0.41625	0.27831
H	15.51511	-23.48590	-10.05999	C	1.23754	0.34642	1.52463
H	16.19431	-22.36383	-7.97386	O	1.61516	1.24444	2.24844
H	15.24620	-22.40218	-6.49654	C	-0.01950	1.59515	-0.21163
H	16.26755	-20.08157	-6.54763	C	-0.84075	1.78502	-1.44535
H	16.71063	-20.12311	-8.27135	H	1.82361	-2.41703	0.32629
H	15.60308	-18.85490	-7.66858	H	0.32488	-2.57578	1.30388
H	14.61209	-21.45924	-11.92347	H	-0.85150	-1.25655	-0.29862
H	15.06318	-19.72466	-11.80231	H	0.63416	-1.10209	-1.26937
H	16.36313	-20.98136	-11.98127	H	0.26248	2.49294	0.36384
H	16.36426	-24.68644	-7.94551	H	-1.07453	0.83251	-1.95449
H	15.35878	-24.74907	-6.46499	H	-1.79642	2.29601	-1.20404
H	14.92530	-25.74898	-7.88006	H	-0.31596	2.44642	-2.16629
H	13.26419	-19.29578	-7.43982				
H	12.52107	-20.85723	-7.65571				
H	13.59931	-22.57354	-5.34690	O	-0.44051	-2.44276	3.13052
H	11.89732	-22.23404	-5.78324	C	-1.24434	-3.04244	2.09000
H	12.47964	-21.91973	-4.13047	C	-1.46159	-1.94269	1.04019
H	10.54031	-17.81753	-4.01852	C	-0.30980	-0.92957	1.27382
H	9.41381	-19.18967	-4.30571	C	0.13062	-1.26986	2.71642
H	10.17100	-18.98970	-2.67037	O	0.88128	-0.65240	3.43883
H	15.16447	-20.70278	-4.96187	C	0.89186	-1.17265	0.32513
H	14.74520	-19.03148	-5.38171	C	1.49064	-2.58222	0.36380
H	14.13204	-20.41881	-1.34671	C	-0.88177	0.51851	1.17212
H	14.39328	-21.60246	-2.65694	C	0.02419	1.74970	0.89155
H	12.80536	-20.78875	-2.46845	C	0.64090	1.70069	-0.51384
H	12.54891	-16.68890	-0.50501	C	1.13481	1.97165	1.92818
H	11.63626	-16.70234	-2.07080	C	-0.90917	2.99314	0.89364
H	13.25971	-15.93584	-2.00714	O	1.78655	1.99881	-0.80048
H	16.43390	-20.17645	-3.20522	O	-0.27603	1.33820	-1.45618
H	16.26738	-18.49911	-3.77835	C	0.20554	1.31448	-2.81042
H	15.65942	-19.24228	-0.85667	H	-2.17873	-3.39720	2.55971
H	18.38623	-18.49271	-2.09957	H	-0.69300	-3.91678	1.69501
H	17.95650	-20.06341	-1.35193	H	-1.46972	-2.33992	0.00872
H	18.03545	-18.58615	-0.34281	H	-2.43546	-1.44751	1.21177
H	14.86777	-15.06013	-0.38524	H	1.68493	-0.44509	0.57362
H	16.64791	-14.99014	-0.16011	H	0.55342	-0.94224	-0.70329
H	15.58227	-15.44751	1.23861	H	2.37461	-2.63767	-0.29698
				H	0.77457	-3.35009	0.01547
				H	1.82351	-2.85737	1.38269
<b>EBL</b>				H	-1.64097	0.50031	0.36870
O	1.54013	-0.97186	1.77725	H	-1.43305	0.73001	2.10953
C	0.98352	-1.85803	0.77967				

H	1.67228	2.91093	1.70936	H	-0.68435	1.92144	1.40309
H	1.86978	1.15231	1.94547	H	3.02620	2.45502	0.73236
H	0.69513	2.03442	2.93859	H	2.55605	0.83332	1.32914
H	-0.34174	3.90651	0.63647	H	1.88563	2.29098	2.09372
H	-1.74024	2.88017	0.17431	H	1.80296	0.22548	-1.18840
H	-1.33398	3.12979	1.90599	H	0.75136	1.40792	-2.02256
H	-0.64617	0.98359	-3.42631	H	2.41740	1.85035	-1.56515
H	0.54410	2.32060	-3.11867	H	-1.58195	4.65454	-2.10837
H	1.05445	0.61161	-2.90593	H	-1.14429	5.26600	-0.45404
<b>PEBL Dimer</b>				H	0.06691	5.34188	-1.77978
O	-1.05176	-0.68820	3.64630	H	-2.23721	-3.38731	-1.06757
C	-2.19842	-1.08958	2.87223	H	-2.12848	-3.04392	0.67973
C	-2.05823	-0.35038	1.54202	H	-1.84100	-0.44723	-1.07623
C	-0.51935	-0.18628	1.35223	H	-0.21391	-0.35883	-1.76116
C	-0.08084	-0.13718	2.84732	C	-1.57083	-1.59916	-2.88053
O	0.94464	0.28198	3.33116	H	-0.23675	-4.57874	0.95479
C	0.09718	-1.53369	0.80269	H	-1.11097	-5.41319	-0.37706
C	1.63314	-1.59755	0.87058	H	-1.84100	-0.76352	-3.55162
C	-0.29555	1.20133	0.65444	H	-0.80638	-2.20526	-3.39960
C	1.03720	1.83880	0.12214	H	-2.47812	-2.21937	-2.75569
C	0.64566	3.31480	-0.13392	<b>PEBL Trimer</b>			
C	2.19239	1.85139	1.13203	O	-0.10212	-2.77450	3.06992
C	1.52103	1.28952	-1.24113	C	-1.12203	-1.77019	2.85307
O	1.14535	4.28975	0.39654	C	-0.54251	-0.84557	1.78107
O	-0.35243	3.41871	-1.05621	C	0.31696	-1.80231	0.91561
C	-0.77538	4.75863	-1.36454	C	0.79006	-2.77888	2.03066
C	-0.52390	-2.10450	-0.55496	O	1.77966	-3.47466	2.04784
C	0.58492	-2.90959	-1.27588	C	-0.57946	-2.68518	-0.06823
C	-1.53403	-3.23351	-0.23015	C	0.04608	-4.07506	-0.31229
C	-1.04596	-1.04630	-1.55060	C	1.55112	-1.19003	0.22579
O	0.48297	-4.23764	-0.96689	C	2.33105	-0.05892	0.94067
C	-0.63376	-4.46586	-0.07407	C	1.48584	1.21877	0.93371
O	1.43980	-2.48706	-2.02150	C	2.83933	-0.44041	2.34208
H	-3.10287	-0.81467	3.44230	C	3.55292	0.27422	0.03974
H	-2.17608	-2.19336	2.76119	O	0.74057	1.55984	0.02527
H	-2.55966	-0.87831	0.71661	O	1.68846	1.99405	2.02758
H	-2.52351	0.64970	1.62277	C	0.97181	3.24159	2.04749
H	-0.22903	-2.27501	1.56027	C	-1.07855	-2.08602	-1.46888
H	1.97414	-2.64483	0.78622	C	0.01244	-2.40194	-2.52820
H	1.99251	-1.21346	1.83814	C	-2.27825	-2.95726	-1.95490
H	2.12596	-1.03624	0.06428	C	-1.46013	-0.56540	-1.34332
H	-1.01223	1.25467	-0.18102	O	-0.47294	-3.21507	-3.50119

C	-1.88108	-3.49914	-3.33532	H	-0.55090	-0.81022	-4.10139
O	1.17765	-2.06084	-2.54093	H	0.29014	0.96008	-5.55764
C	-1.56434	0.38460	-2.60079	H	-1.46407	1.18228	-5.35806
C	-2.77196	-0.44190	-0.53019	H	-0.31216	2.24350	-4.48562
C	-1.59951	1.85733	-2.10033				
C	-2.78230	2.50399	-2.84046				
O	-3.56541	1.42301	-3.40663	<b>PEBL Tetramer</b>			
C	-2.90893	0.23427	-3.33308	O	1.54506	-0.17999	5.46692
C	-0.45615	0.19862	-3.66615	C	1.50163	1.07385	4.74715
O	-3.37329	-0.77301	-3.83159	C	1.62255	0.68060	3.27454
C	-0.49601	1.20594	-4.82149	C	0.90005	-0.68912	3.20898
H	-1.30615	-1.27210	3.82055	C	1.28590	-1.22568	4.62083
H	-2.05434	-2.27808	2.53450	O	1.34865	-2.37366	4.99503
H	0.10569	-0.10556	2.27944	C	-0.69094	-0.55316	3.25160
H	-1.31471	-0.28936	1.24013	C	-1.35409	-1.82744	3.81672
H	-1.52118	-2.85963	0.48721	C	1.36028	-1.68660	2.13226
H	0.06153	-4.67994	0.60819	C	2.86841	-1.84423	1.74937
H	-0.52834	-4.64736	-1.06116	C	2.87622	-3.10520	0.86162
H	1.08471	-3.99406	-0.67490	C	3.42502	-0.68339	0.88437
H	1.27656	-0.82223	-0.76996	C	3.78438	-2.10828	2.95239
H	2.26357	-2.01397	0.04397	O	3.40000	-4.17088	1.13162
H	2.02334	-0.59116	3.07066	O	2.19151	-2.88835	-0.29114
H	3.49965	0.34469	2.74835	C	2.04651	-4.02094	-1.16284
H	3.40768	-1.38427	2.27919	C	-1.54297	-0.07061	1.96911
H	4.22019	-0.60573	-0.00670	C	-1.89869	-1.32790	1.13242
H	3.22990	0.52139	-0.98720	C	-2.94014	0.37318	2.51264
H	4.12979	1.12396	0.44945	C	-0.83059	1.09010	1.16993
H	1.23848	3.85386	1.16715	O	-3.22163	-1.59818	1.18741
H	1.27262	3.74436	2.98006	C	-3.95459	-0.66565	2.00855
H	-0.11862	3.05702	2.03726	O	-1.14891	-2.06564	0.52200
H	-2.47607	-3.78217	-1.24936	C	-1.26767	1.49402	-0.32139
H	-3.20435	-2.37234	-2.04253	C	-0.86296	2.34933	2.07024
H	-0.64101	-0.09801	-0.77156	C	-0.50539	2.77895	-0.74220
H	-2.00432	-4.59239	-3.43470	C	-1.50354	3.93179	-0.53219
H	-2.42519	-2.98681	-4.14724	O	-2.80434	3.32303	-0.31421
H	-2.86615	-1.22453	0.24038	C	-2.72557	1.96539	-0.27601
H	-3.66256	-0.53635	-1.17594	C	-1.07441	0.33788	-1.35194
H	-2.84891	0.53366	-0.01979	O	-3.72340	1.27705	-0.18547
H	-0.64763	2.37288	-2.30476	C	0.37114	-0.17721	-1.31284
H	-1.74111	1.90809	-1.01028	C	-1.50057	0.54049	-2.86646
H	-3.45646	3.08079	-2.18262	C	-0.32719	1.01234	-3.75553
H	-2.46466	3.15266	-3.67808	C	-1.81184	-0.87072	-3.44243
H	0.52241	0.24016	-3.15562	C	-1.06501	-0.94020	-4.78398
				O	-0.09942	0.13892	-4.77142



O	0.32561	2.03389	-3.65579	C	-3.08112	1.66633	-4.59353
H	2.33671	1.69597	5.11231	H	-3.89251	2.41017	-4.68597
H	0.54858	1.58606	4.99058	H	-2.24130	2.01422	-5.22452
H	1.24597	1.45515	2.59789	H	-3.46246	0.71881	-5.01733
H	2.68752	0.53571	3.04165				
H	-0.88136	0.24772	3.99136				
H	-2.44948	-1.71609	3.87332	<b>MMBL</b>			
H	-1.00483	-2.05190	4.83499	C	1.08890	-0.44020	0.68930
H	-1.13663	-2.71150	3.19298	C	1.44510	-0.86370	1.90860
H	1.01057	-2.67775	2.47821	H	1.47580	-0.15570	2.75080
H	0.79817	-1.50213	1.20816	H	1.71600	-1.90890	2.11890
H	3.69132	0.19390	1.49742	C	0.69720	0.95790	0.31210
H	4.35081	-1.00310	0.37061	C	1.00490	-1.20700	-0.42420
H	2.70500	-0.36660	0.11305	C	0.47420	0.82830	-1.20140
H	3.43490	-2.96840	3.54513	O	0.63090	-0.52450	-1.54220
H	4.81261	-2.32302	2.61107	O	1.23770	-2.39870	-0.45220
H	3.83010	-1.22696	3.61740	C	-0.89950	1.32130	-1.64930
H	1.46599	-3.65860	-2.02630	H	1.50750	1.68110	0.55940
H	1.50431	-4.83315	-0.64541	H	-0.23370	1.24320	0.85310
H	3.03707	-4.39293	-1.48267	H	1.26240	1.40080	-1.75040
H	-3.22305	1.36962	2.14951	H	-1.02470	1.20900	-2.75080
H	-2.94138	0.42652	3.61436	H	-1.03480	2.39870	-1.40020
H	0.21956	0.77973	1.04348	H	-1.71600	0.74760	-1.15430
H	-4.42171	-1.25039	2.82276				
H	-4.73894	-0.21842	1.37699	<b>PMMBL Monomer</b>			
H	-0.75030	2.08970	3.13371	C	0.36860	0.11140	-1.24630
H	-1.81745	2.89547	1.98507	C	-0.09000	-0.51160	0.08340
H	-0.05407	3.05647	1.82461	C	0.25550	0.22260	1.40180
H	0.42498	2.92711	-0.16971	C	-0.11050	-0.75890	2.53060
H	-0.21130	2.71263	-1.80184	O	0.98710	-1.40200	3.01850
H	-1.28279	4.56358	0.34700	C	0.77270	-2.37130	4.01670
H	-1.59851	4.58538	-1.41771	O	-1.24320	-0.94910	2.91550
H	-1.74498	-0.46836	-1.01886	C	1.74230	0.62830	1.45240
H	0.56698	-0.73798	-0.39357	C	-0.60300	1.48630	1.61910
H	1.09548	0.65039	-1.41409	C	-0.30270	1.42950	-1.63240
H	0.57216	-0.88675	-2.13437	C	0.05480	-0.76410	-2.45200
C	-2.67522	1.51697	-3.12246	C	-0.27190	1.38020	-3.15470
H	-2.89760	-1.02812	-3.56524	O	-0.28290	0.02850	-3.50300
H	-1.44801	-1.65611	-2.75779	O	0.10540	-1.97380	-2.48610
H	-0.50232	-1.87895	-4.92924	C	-1.44060	2.11020	-3.80850
H	-1.72416	-0.78262	-5.65776	H	1.47900	0.22680	-1.26390
H	-3.54278	1.17073	-2.53489	H	0.38500	-1.52150	0.14490
H	-2.39932	2.51632	-2.74095	H	-1.19000	-0.69060	0.03350
				H	1.76090	-2.80240	4.29280

H	0.32350	-1.89940	4.91920	H	-2.17860	-0.86240	-1.29610
H	0.12350	-3.18640	3.62550	H	-2.33430	-0.57000	3.07700
H	2.01760	1.03860	2.45060	H	-3.67280	-1.31010	2.13790
H	1.97220	1.42580	0.71110	H	-2.09490	-2.14990	2.26440
H	2.41770	-0.22820	1.22870	H	0.20020	1.56980	-1.94380
H	-1.68650	1.29430	1.45020	H	-1.38110	1.39990	-1.14400
H	-0.48480	1.87380	2.65690	H	-0.65540	2.85560	0.71540
H	-0.30780	2.31740	0.94450	H	0.46440	4.84610	-0.27660
H	0.22370	2.32690	-1.23750	H	-0.79070	4.22560	-1.41020
H	-1.35840	1.43410	-1.27430	H	0.95360	3.90090	-1.72660
H	0.69050	1.81180	-3.52630	H	0.29450	-2.73840	-0.20270
H	-1.37420	2.05360	-4.91920	H	-0.02420	-0.98300	-1.86730
H	-1.44410	3.18640	-3.52040	H	1.63790	-0.41110	-1.72730
H	-2.41770	1.67000	-3.50490	H	1.62000	-4.12780	-1.54190
				H	1.47200	-2.78950	-2.73970
				H	3.60010	-1.81690	-2.03180
				H	5.28680	-3.64840	-1.81650
				H	4.07420	-4.07890	-3.07700
				H	3.99590	-4.84610	-1.44850
				H	-5.28680	1.92490	-1.12650
				H	-5.19540	2.22590	0.65560
				H	-3.94460	2.95000	-0.47750
<b>PMMBL Dimer</b>				<b>PMMBL Trimer</b>			
C	0.31630	0.30790	-0.16470	C	1.43910	0.32210	1.30650
C	-0.55980	-0.15090	1.02800	C	-0.03430	0.59050	1.72950
C	-2.08330	-0.42500	0.87470	C	-0.82260	-0.18340	2.82400
C	-2.88160	0.88790	0.85380	C	-2.01750	0.73460	3.17090
O	-3.80830	0.90860	-0.14480	O	-3.10420	0.46490	2.39290
O	-2.70780	1.79480	1.63700	O	-1.97830	1.61770	3.99920
C	-2.40850	-1.34160	-0.32040	C	-1.36120	-1.55860	2.37300
C	-2.57060	-1.14880	2.15520	C	-0.03230	-0.39530	4.12880
C	-0.29420	1.48420	-0.94720	C	1.85600	1.34800	0.23580
C	1.55320	1.04540	0.37190	C	2.38880	0.79750	2.42230
C	0.07620	2.70040	-0.11160	C	2.25380	2.58750	1.02410
O	1.30280	2.37870	0.46460	O	2.71610	2.10510	2.24510
O	2.61270	0.53400	0.65620	O	2.81210	0.11960	3.33310
C	0.18370	3.98550	-0.92620	C	3.33010	3.42330	0.33710
C	1.19240	-2.20860	-0.59700	C	1.51320	-1.81120	-0.43810
C	0.78960	-0.81280	-1.12380	C	1.81290	-1.13350	0.93320
C	1.82800	-3.04520	-1.71730	C	2.68860	-1.72840	-1.42630
C	2.27890	-2.30090	0.46540	C	1.56540	-3.32020	-0.12830
C	3.31140	-2.76240	-1.51030	C	3.60390	-2.88120	-1.04200
O	3.47110	-2.55410	-0.13850				
O	2.11340	-2.20000	1.66160				
C	4.21390	-3.89590	-1.98700				
C	-4.59390	2.07020	-0.26790				
H	-0.10310	-1.07890	1.43170				
H	-0.43190	0.58240	1.85840				
H	-3.48360	-1.63000	-0.34430				
H	-1.84080	-2.29510	-0.26460				

O	2.77550	-3.83820	-0.46140	H	-3.49180	0.26880	-3.77650
O	0.66160	-3.95660	0.36950	H	-0.56900	-1.28370	-0.25390
C	4.36310	-3.47900	-2.22290	H	-0.28820	-2.45690	-1.51760
C	-4.23670	1.28350	2.56260				
C	0.03540	-0.45470	-2.17850				
C	-1.22640	0.41030	-2.08230	<b>PMMBL Tetramer</b>			
C	-0.09810	-0.98870	-3.60030	C	0.88170	-2.69290	1.83310
C	-1.40040	0.87850	-3.52060	C	-0.25400	-1.70690	2.21770
O	-0.88770	-0.14610	-4.31840	C	-1.56290	-2.09500	2.95150
O	0.42050	-1.99070	-4.04050	C	-2.39640	-0.79290	2.95650
C	-2.85030	1.17210	-3.89080	O	-3.12760	-0.66610	1.81220
C	0.13350	-1.52370	-1.07580	O	-2.36880	0.03240	3.84270
H	-0.05620	1.65920	2.05150	C	-2.36000	-3.21630	2.25860
H	-0.66510	0.57570	0.81350	C	-1.32880	-2.48200	4.42760
H	-2.03540	-1.99410	3.14550	C	2.25320	-2.00050	1.93690
H	-0.55510	-2.30490	2.22230	C	1.08820	-3.73590	2.93510
H	-1.93970	-1.50920	1.42500	C	2.58060	-2.09230	3.42150
H	0.45540	0.54070	4.48150	O	1.99000	-3.28060	3.84500
H	-0.69680	-0.75200	4.94880	O	0.54310	-4.81590	3.00380
H	0.74820	-1.17720	4.00830	C	4.07840	-2.10560	3.71220
H	2.74880	0.98160	-0.31700	C	0.94100	-2.77030	-0.92200
H	1.06070	1.58460	-0.50110	C	0.63940	-3.40990	0.47530
H	1.36590	3.23570	1.22290	C	2.35590	-3.13250	-1.39870
H	3.59250	4.31570	0.95040	C	0.07760	-3.60420	-1.88180
H	2.97500	3.78300	-0.65580	C	2.18490	-4.44250	-2.15620
H	4.26400	2.83810	0.17620	O	0.84380	-4.51930	-2.52860
H	2.91740	-1.22590	1.06690	O	-1.12400	-3.49670	-2.01170
H	1.40360	-1.76360	1.75210	C	3.08300	-4.55610	-3.38500
H	2.33180	-1.91010	-2.46250	C	-3.80830	0.55010	1.61610
H	3.21970	-0.75420	-1.43260	C	0.96590	-0.33950	-2.22250
H	4.33770	-2.55170	-0.26600	C	2.33210	0.32810	-1.98620
H	5.01980	-4.31570	-1.89110	C	1.22070	-1.09300	-3.52760
H	5.00750	-2.71000	-2.70730	C	3.09450	0.20510	-3.29860
H	3.66830	-3.88140	-2.99510	O	2.41290	-0.73480	-4.06700
H	-5.01980	0.93500	1.85270	O	0.46770	-1.89100	-4.03790
H	-4.62670	1.18820	3.60080	C	3.21960	1.50760	-4.08560
H	-3.98360	2.34100	2.32450	C	0.56630	-1.27080	-1.03910
H	0.93860	0.19650	-2.19000	C	-0.43150	1.95740	-1.74790
H	-1.13830	1.25700	-1.36660	C	-0.16630	0.67480	-2.56980
H	-2.09640	-0.22010	-1.78240	C	0.26040	3.20700	-2.30530
H	-0.77690	1.78920	-3.70020	C	-0.10770	2.01000	-0.26840
H	-2.92970	1.51230	-4.94880	C	0.47450	4.07220	-1.07180
H	-3.26810	1.97460	-3.24080	O	0.44790	3.21360	0.02760
				O	-0.31640	1.14060	0.54480

C	1.78470	4.85350	-1.09960				
H	0.18740	-0.86490	2.80040				
H	-0.58780	-1.24650	1.26690	<b>Methyl 2-ethacrylate</b>			
H	-3.36010	-3.34420	2.73210	O	-0.53119	1.81396	0.64941
H	-1.84830	-4.19880	2.33800	C	-0.91330	1.06369	-0.24055
H	-2.52210	-3.01850	1.17550	O	-2.17801	1.06881	-0.72080
H	-0.64090	-1.77410	4.94280	C	-3.08461	2.02467	-0.13408
H	-2.28800	-2.50010	4.99380	H	-3.18747	1.84193	0.95088
H	-0.89700	-3.49740	4.54220	H	-4.04910	1.88008	-0.64507
H	3.01850	-2.58430	1.38020	H	-2.71503	3.05338	-0.29862
H	2.28260	-0.95290	1.56740	C	-0.06527	0.04239	-0.93964
H	2.10790	-1.25390	3.98840	C	0.81632	-0.65315	-0.19046
H	4.27010	-2.18050	4.80720	H	0.91130	-0.48138	0.88964
H	4.55870	-1.17030	3.34380	H	1.45511	-1.42107	-0.64900
H	4.58440	-2.96770	3.22120	C	-0.27297	-0.17199	-2.42190
H	1.19890	-4.37560	0.49880	C	-0.32615	1.12809	-3.23572
H	-0.43020	-3.71670	0.49530	H	-1.20509	-0.75183	-2.59600
H	2.76280	-2.36740	-2.08750	H	0.56566	-0.80429	-2.77118
H	3.10600	-3.22590	-0.58720	H	-1.23321	1.71933	-3.01555
H	2.39030	-5.30420	-1.47380	H	-0.34328	0.89017	-4.31678
H	2.93310	-5.53330	-3.89870	H	0.56892	1.75194	-3.04059
H	4.15680	-4.48200	-3.09800				
H	2.86880	-3.75100	-4.12410	<b>PMEA Monomer</b>			
H	-4.30680	0.50620	0.62200	C	-4.26880	-0.41947	-0.42191
H	-4.58440	0.68660	2.40210	C	-2.97756	0.21529	0.14726
H	-3.08580	1.39690	1.61390	C	-5.44441	0.48250	-0.01186
H	2.26120	1.36910	-1.61290	O	-5.35033	1.55069	0.58117
H	2.90470	-0.21910	-1.20100	O	-6.63138	-0.02855	-0.40124
H	4.12530	-0.18600	-3.11120	C	-7.80555	0.75066	-0.08454
H	3.84880	1.36310	-4.99380	H	-7.89197	0.88110	1.00929
H	3.69540	2.30530	-3.47080	H	-8.65791	0.17272	-0.47468
H	2.22800	1.87380	-4.43230	H	-7.74878	1.74031	-0.57277
H	-0.53900	-1.21710	-0.91220	C	-4.50760	-1.84308	0.12977
H	1.00380	-0.78200	-0.14490	H	-4.49660	-1.85200	1.23529
H	-1.53290	2.16600	-1.77510	H	-3.72175	-2.52801	-0.23718
H	-1.12070	0.09590	-2.61590	H	-5.47852	-2.23812	-0.21393
H	-0.02400	1.02230	-3.62170	C	-4.22677	-0.45527	-1.96877
H	-0.33240	3.71940	-3.09670	H	-4.09342	0.56021	-2.38696
H	1.24570	2.94970	-2.74620	H	-5.15706	-0.88578	-2.37867
H	-0.38150	4.78260	-0.95850	H	-3.38267	-1.08260	-2.30992
H	1.89650	5.47650	-0.18260	C	-1.67657	-0.57632	-0.08628
H	1.82080	5.53330	-1.98140	C	-1.52299	-1.71102	0.91289
H	2.66420	4.17180	-1.15450	O	-1.19835	-2.87766	0.31370
				O	-1.63347	-1.59596	2.12808

C	-0.99728	-4.01220	1.18691	C	-0.40341	0.82360	1.08311
H	-0.16621	-3.81165	1.88680	C	0.95165	0.46986	1.70778
H	-0.75307	-4.85620	0.52365	H	-1.09306	1.09676	1.90382
H	-1.92074	-4.21816	1.75780	H	-0.30603	1.72741	0.44869
H	-3.09767	0.38009	1.23454	H	0.91250	-0.49349	2.25074
H	-2.85486	1.21700	-0.30551	H	1.22995	1.24584	2.44469
C	-0.44751	0.35995	0.04497	H	1.77041	0.41889	0.96961
H	-1.65995	-1.02056	-1.09962	C	-0.49149	-0.46375	-1.16234
C	0.90055	-0.34115	-0.13982	C	0.97239	-0.98505	-1.20242
H	-0.48984	0.85709	1.03526	H	-0.54168	0.50972	-1.68669
H	-0.56692	1.15718	-0.71469	H	-1.11899	-1.14848	-1.74928
H	1.08208	-1.09399	0.65206	C	1.91503	0.03589	-1.87929
H	1.72977	0.38945	-0.09843	C	3.38829	-0.37615	-1.88223
H	0.94963	-0.85982	-1.11710	H	1.79477	0.99493	-1.33510

**PMEA Dimer**

C	-3.65808	-0.38263	-0.83461
C	-2.59373	0.30787	0.07609
C	-4.98827	0.27205	-0.42108
O	-5.15212	1.47690	-0.31357
O	-5.98681	-0.62281	-0.22148
C	-7.26394	-0.05708	0.13021
H	-7.18908	0.49501	1.08486
H	-7.95193	-0.91240	0.22661
H	-7.60696	0.63730	-0.65851
C	-3.69058	-1.91023	-0.66427
H	-3.86224	-2.19851	0.38761
H	-2.73380	-2.34988	-0.99480
H	-4.49342	-2.35684	-1.27495
C	-3.50904	-0.01887	-2.33713
H	-3.38316	1.07082	-2.46558
H	-4.41096	-0.32979	-2.89789
H	-2.64665	-0.53260	-2.79343
C	-1.14402	-0.25385	0.21987
C	-1.21247	-1.53362	1.06320
O	-0.65506	-2.59969	0.44322
O	-1.69759	-1.59575	2.18117
C	-0.65300	-3.84069	1.16983
H	-0.19395	-3.70017	2.16449
H	-0.05795	-4.53602	0.55749
H	-1.68904	-4.20438	1.29995
H	-3.00055	0.33011	1.10455
H	-2.51607	1.36446	-0.23974

H	1.55749	0.22156	-2.91208
H	3.75480	-0.54357	-0.85075
H	4.01671	0.40724	-2.34534
H	3.54969	-1.31650	-2.44264
C	1.09099	-2.33794	-1.88248
H	1.34305	-1.17704	-0.18388
O	1.72073	-3.29375	-1.46006
O	0.44029	-2.36115	-3.07963
C	0.52846	-3.59481	-3.81213
H	1.58348	-3.83819	-4.03483
H	-0.03964	-3.43346	-4.74256
H	0.08902	-4.42299	-3.22588

**PMEA Trimer**

C	-0.86460	0.33510	-0.62281
C	-1.46189	1.74925	-0.41835
O	-2.67455	1.86851	-0.99596
C	-3.33411	3.14577	-0.85585
H	-2.72207	3.94199	-1.31637
H	-3.49683	3.37420	0.21287
H	-4.29553	3.04086	-1.38224
O	-0.93429	2.66980	0.19371
C	-0.82702	0.06431	-2.14411
H	-1.83429	0.17582	-2.57890
H	-0.49229	-0.96471	-2.35193
H	-0.13929	0.75885	-2.65873
C	-1.83822	-0.65448	0.06340
H	-2.86814	-0.48954	-0.29561
H	-1.82666	-0.53420	1.16227

H	-1.57565	-1.69821	-0.17807	H	7.21938	2.05314	0.31119
C	0.54535	0.39915	0.02622	H	5.66099	2.60207	-0.34191
C	1.57098	-0.79838	0.07983	H	8.00364	1.44488	-2.02236
H	0.40464	0.70696	1.07875	H	7.48071	3.15088	-1.96201
H	1.07445	1.23512	-0.46481	H	6.40877	1.91002	-2.68375
C	1.08042	-1.84253	1.11811	C	6.91356	-0.59316	-0.64066
C	1.83550	-3.16740	1.29666	H	5.08030	0.33028	-1.07763
H	0.02055	-2.06730	0.93334	O	7.85577	-0.69302	0.31864
H	1.06249	-1.30465	2.08608	C	8.88211	-1.68578	0.11036
H	2.10350	-3.64185	0.33988	H	9.52788	-1.63574	1.00080
H	1.19989	-3.87798	1.85563	H	9.45803	-1.45456	-0.80349
H	2.76511	-3.05352	1.87737	H	8.42176	-2.68567	0.01804
C	1.83165	-1.23315	-1.39017	O	6.94271	-1.25555	-1.67243
O	2.40359	-0.46809	-2.15669				
O	1.47403	-2.43101	-1.92548				
C	0.40335	-3.30975	-1.53688	<b>PM Eaton Tetramer</b>			
H	-0.31433	-3.33809	-2.37590	O	1.52396	1.99692	0.04194
H	-0.11299	-2.97940	-0.62758	C	1.74091	1.47624	-1.19391
H	0.82358	-4.31710	-1.38275	C	1.43653	3.43105	0.10953
C	2.87774	-0.05478	0.56331	H	2.37460	3.89105	-0.25261
C	4.10569	-0.70436	1.27202	H	1.26838	3.67033	1.17191
H	2.53601	0.71421	1.28078	H	0.59778	3.79480	-0.51200
H	3.23291	0.50062	-0.31837	O	1.84487	2.17127	-2.19023
C	3.81774	-0.80936	2.80381	C	1.85793	-0.06185	-1.15274
C	4.85728	-1.46521	3.71690	C	1.82744	-0.55911	-2.61108
H	2.84506	-1.30641	2.95592	H	0.95926	-0.12646	-3.13840
H	3.66248	0.23819	3.13124	H	1.72609	-1.65547	-2.64524
H	4.92020	-2.55381	3.55094	H	2.73408	-0.25597	-3.16246
H	4.57252	-1.29290	4.77212	C	0.63983	-0.62943	-0.39040
H	5.87002	-1.04644	3.57145	H	-0.29402	-0.29856	-0.88241
C	4.60985	-2.01293	0.66638	H	0.61307	-0.28344	0.65629
O	4.09843	-2.23754	-0.55740	H	0.65873	-1.73284	-0.40969
C	4.55000	-3.41883	-1.24901	C	3.24261	-0.29680	-0.45981
H	3.98773	-3.43466	-2.19407	C	3.76869	-1.71961	-0.00232
H	4.32737	-4.31721	-0.64634	C	3.07026	-2.06392	1.34065
H	5.63450	-3.34757	-1.43643	C	3.17860	-3.48311	1.89963
O	5.44743	-2.75101	1.17178	H	2.00031	-1.83428	1.23012
C	5.27878	0.31946	1.10231	H	3.46735	-1.34579	2.08166
C	5.87025	0.46484	-0.31443	H	2.76424	-4.22526	1.19644
H	6.09051	0.06842	1.80562	H	2.59843	-3.54307	2.83891
H	4.87600	1.30155	1.41671	H	4.20879	-3.77549	2.15096
C	6.48337	1.87638	-0.49866	C	3.40281	-2.70922	-1.10105
C	7.12964	2.10651	-1.86637	O	2.42888	-3.44663	-1.09988
				O	4.26223	-2.64854	-2.15542

C	3.96277	-3.52523	-3.25251	H	10.39632	-1.65002	4.31826
H	3.95626	-4.57693	-2.91127	H	11.07486	-0.67156	3.00046
H	4.76092	-3.35956	-3.99341	C	9.67967	-3.01295	0.44096
H	2.97454	-3.28409	-3.68461	O	9.70467	-3.00931	-0.91480
H	3.26817	0.31195	0.46306	O	10.04533	-3.97253	1.10284
H	3.99753	0.13387	-1.14517	C	9.98838	-0.51211	0.41722
C	5.30865	-1.45510	0.10824	C	11.51365	-0.73867	0.27988
C	6.43890	-2.36973	0.71994	H	9.81660	0.34866	1.09200
H	5.37844	-0.51387	0.67913	H	9.59231	-0.21058	-0.56779
H	5.65028	-1.22987	-0.91671	C	12.28362	0.57726	0.55201
C	6.63966	-3.69375	-0.06109	C	13.80340	0.45156	0.43017
C	5.56461	-4.78384	-0.03671	H	12.01286	0.90402	1.57623
H	7.59343	-4.15131	0.24726	H	11.90150	1.35739	-0.13645
H	6.79410	-3.38878	-1.11387	H	14.19100	-0.34535	1.09374
H	5.33621	-5.14999	0.97645	H	14.30007	1.39997	0.70659
H	5.91296	-5.64870	-0.63124	H	14.11216	0.19945	-0.60228
H	4.60759	-4.46067	-0.46608	C	11.92530	-1.29018	-1.07755
C	6.21635	-2.42801	2.25436	H	11.86555	-1.49765	1.00017
O	5.79217	-1.44440	2.83724	O	12.66037	-2.24855	-1.25517
O	6.44754	-3.52781	3.02811	O	11.43375	-0.54026	-2.09724
C	7.28394	-4.66873	2.76591	C	11.79189	-0.97339	-3.41945
H	7.50461	-5.08763	3.76166	H	11.30264	-0.26723	-4.10923
H	8.23444	-4.39696	2.27859	H	11.43150	-2.00347	-3.59585
H	6.75331	-5.43127	2.17111	H	12.88933	-0.95314	-3.54952
C	7.69310	-1.43967	0.45632	C	10.19554	-4.21386	-1.53393
C	9.13773	-1.69528	0.98971	H	9.63441	-5.08887	-1.15975
H	7.42343	-0.43386	0.82672	H	11.27061	-4.33386	-1.31507
H	7.76958	-1.36143	-0.64330	H	10.03174	-4.07935	-2.61437
C	9.16555	-1.67304	2.53655				
C	10.53403	-1.60957	3.22230				
H	8.63986	-2.55851	2.92075				
H	8.55732	-0.80346	2.85186				
H	11.17177	-2.46410	2.93435				

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