Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Toward High-level Theoretical Studies of Large Biodiesel Molecules: An ONIOM [QCISD(T)/CBS:DFT] Study of Hydrogen Abstraction Reactions of $C_nH_{2n+1}COOC_mH_{2m+1}$ + H

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Method	MF		MA		MB							
	α		α		α		α'		β'		γ'	
	EB	HR	EB	HR	EB	HR	EB	HR	EB	HR	EB	HR
[QCISD(T)/CBS]$_1$	11.02	-4.83	10.60	-5.27								
[QCISD(T)/CBS]$_2$	10.94	-4.93	10.52	-5.37	10.37	-5.52	7.10	-10.19	8.29	-6.00	10.20	-3.49
ONIOM			10.54	-5.29	10.40	-5.45	7.14	-10.16	8.26	-6.05	10.22	-3.55
Experiment[1]	12.90				10.32	-5.54	6.97	-10.38	8.10	-6.16	10.09	-3.63
QCISD(T)/6-311++G(2d,2p)[2]	11.60	-4.20			10.32	-5.10	7.30	-9.83	8.24	-5.70	10.15	-3.38
MRSDCI+DS/CBS[a,3]	12.10	-3.30										
MRACPF/CBS[b,3]	12.00	-3.50										
CCSD(T)/CBS[4]			10.53	-4.96								
CCSD(T)/CBS[a,5]					10.32	-5.54	6.97	-10.38	8.10	-6.16	10.09	-3.63
CCSD(T)/CBS[b,5]					10.32	-5.10	7.30	-9.83	8.24	-5.70	10.15	-3.38

Table S1: Comparison of Energy Barriers for Hydrogen Abstraction Reactions of MF+H, MA+H and MB+H. (Unit : kcal/mol)

[2] QCISD(T)/6-311++G(2d,2p)//MP2/6-311++G(2d,dp),
[a,3] MRSDCI+DS/CBS//B3LYP/cc-pVTZ,

[b,3] MRACPF/CBS//B3LYP/cc-pVTZ,

[4] CCSD(T)/CBS//MP2/aug-cc-pVTZ,

[a,5] CCSD(T)/CBS//B3LYP/6-311++G(d,p),

[b,5] CCSD(T)/CBS//MP2/cc-pVTZ.

MF: $HCOOCH_3 + H \rightarrow HCOOC\cdot H_2 + H_2$

MA: $CH_3COOCH_3 + H \rightarrow CH3COOC\cdot H_2 + H_2$

MB: α $CH_3CH_2CH_2COOCH_3 + H \rightarrow CH_3CH_2CH_2COOC\cdot H_2 + H_2$

α' $CH_3CH_2CH_2COOCH_3 + H \rightarrow CH_3CH_2C\cdot HCOOCH_3 + H_2$

β' $CH_3CH_2CH_2COOCH_3 + H \rightarrow CH_3C\cdot HCH_2COOCH_3 + H_2$

γ' $CH_3CH_2CH_2COOCH_3 + H \rightarrow C\cdot H_2CH_2CH_2COOCH_3 + H_2$

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2. D. A. Good and J. S. Francisco, *The Journal of Physical Chemistry A*, 2002, **106**, 1733-1738.
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Reactions		1	2	3	4	5
$H+CH_3(CH_2)_{14}COOCH_3$ $\rightarrow H_2+CH_3(CH_2)_{11}CH(CH_2)_2COOCH_3$ (ONIOM)	$CH_3(CH_2)_{14}COOCH_3$	**929**	**114**	**455**	**232**	**57**
	$CH_3(CH_2)_{11}CH(CH_2)_2COOCH_3$	**1803**	**202**	**701**	**440**	**97**
	TS	**3085**	**264**	**935**	**441**	**109**
$H+CH_3(CH_2)_8COOCH_3$ $\rightarrow H_2+CH_3(CH_2)_5CH(CH)_2COOCH_3$ (ONIOM)	$CH_3(CH_2)_8COOCH_3$	**1335**	**93**	**455**	**87**	**51**
	$CH_3(CH_2)_5CH(CH)_2COOCH_3$	**2558**	**180**	**753**	**151**	**86**
	TS	**5757**	**236**	**1090**	**166**	**103**
$H + CH_3(CH_2)_4COOCH_3$ $\rightarrow H_2+CH_3CH_2CH(CH_2)_2COOCH_3$	ONIOM					
	$CH_3(CH_2)_4COOCH_3$	**890**	**105**	**462**	**71**	**34**
	$CH_3CH_2CH(CH_2)_2COOCH_3$	**2466**	**226**	**940**	**110**	**52**
	TS	**7254**	**304**	**1388**	**151**	**66**
	Full QCISD(T)/CBS					
	$CH_3(CH_2)_4COOCH_3$	**21241**	**692**	**1211**	**116**	**9**
	$CH_3CH_2CH(CH_2)_2COOCH_3$	**25144**	**1646**	**2183**	**208**	**20**
	TS	**38223**	**2089**	**3291**	**250**	**25**

Table S2: Comparison of computation times with the ONIOM and QCISD(T)/CBS methods. (Unit : minutes)

2× 6 core CPU Intel(R) Xeon(R) CPU E5-2620 0 @ 2.00GHz

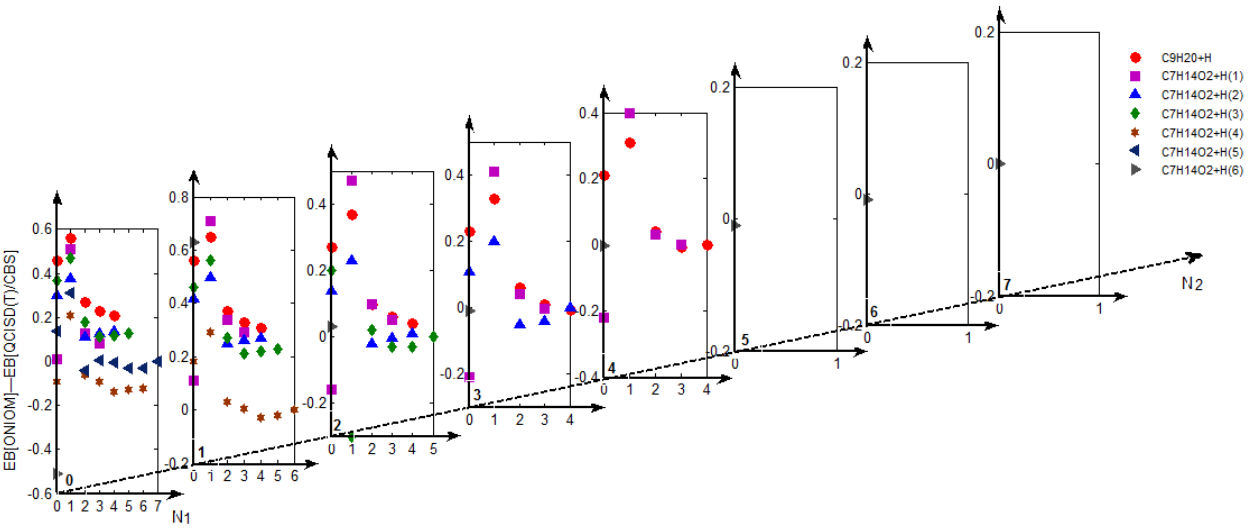
1: QCISD(T)/CC-PVTZ

2: QCISD(T)/CC-PVDZ

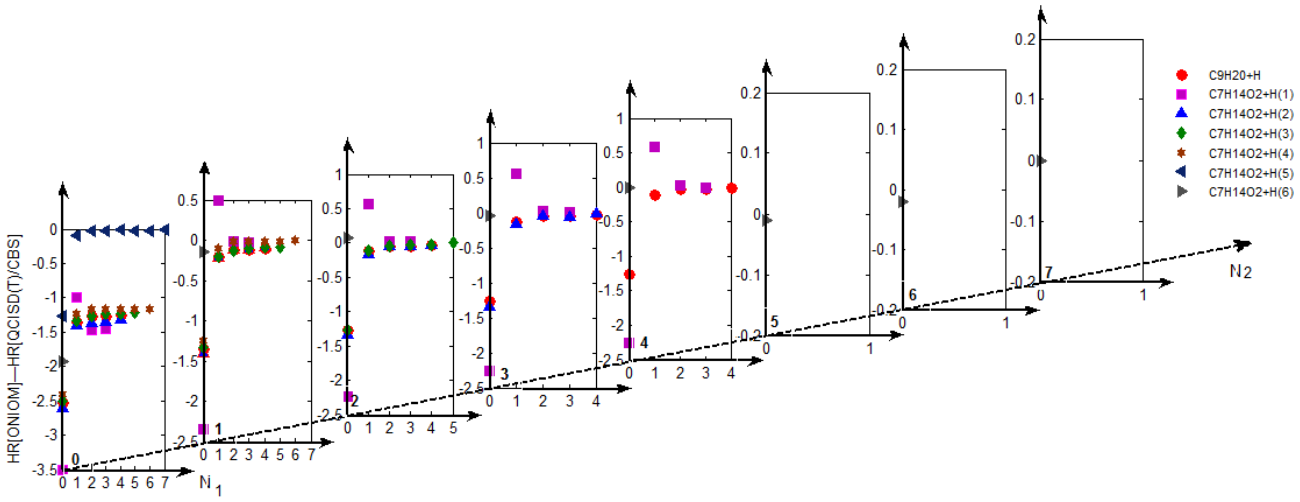
3: MP2/CC-PVQZ

4: MP2/CC-PVTZ

5: MP2/CC-PVDZ



(a)



(b)

Figure S1 (a) Variation of the difference of the calculated energy barriers, EB[ONIOM/CAP(N_1, N_2)] - EB[QCISD(T)/CBS], with N_1 and N_2, (b) Variation of the difference of the calculated heat of reaction, HR[ONIOM/CAP(N_1, N_2)] - HR[QCISD(T)/CBS] with N_1 and N_2, for the five reactions including C_9H_{20} + H → $C_4H_9C{\cdot}HC_4H_9$ + H_2, $C_7H_{14}O_2$ + H → $C_4H_9C{\cdot}HCOOCH_3$ + H_2 (1), $C_3H_7C{\cdot}HCH_2COOCH_3$ + H_2 (2), $C_2H_5C{\cdot}H(CH_2)_2COOCH3$ + H_2 (3), $CH_3C{\cdot}H(CH_2)_3COOCH_3$ + H_2 (4), $C{\cdot}H_2(CH_2)_4COOCH_3$ + H_2 (5), and $CH_3(CH_2)_4COOC{\cdot}H_2$ + H_2 (6). Each two-dimensional plane represents a constant N_2 plane (N_2=0-7 from left to right).

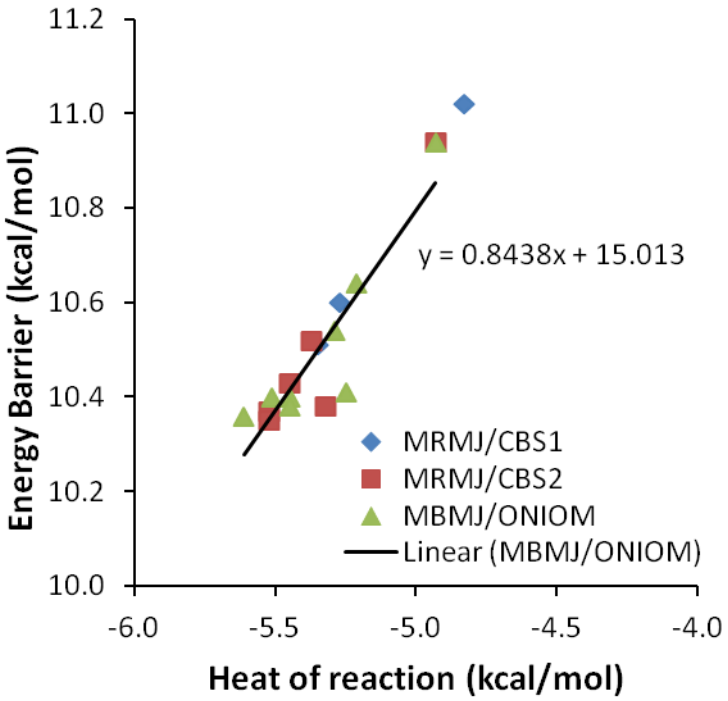


Figure S2. Evans-Polanyi Plot for the reactions $C_nH_{2n+1}COOCH_3 + H \rightarrow C_nH_{2n+1}COOC{\cdot}H_2 + H_2$.

The optimized geometries at B3LYP/6-311++G(d,p) level.

$HCOOCH_3$(n=0,m=1)

$H + HCOOCH_3 \rightarrow H_2 + HCOOCH_2$ (TS2-1)

$HCOOCH_3$

C	-0.9459	-3.8721	-0.7334
O	-0.3140	-4.9791	-0.3217
O	-1.9305	-3.8381	-1.4212
C	-0.8832	-6.2335	-0.7544
H	-1.9039	-6.3333	-0.3833
H	-0.8878	-6.2909	-1.8434
H	-0.2426	-7.0029	-0.3308
H	-0.4193	-2.9913	-0.3409

$HCOOCH_2$

C	-0.6673	-3.8097	-0.9831
O	-0.0301	-4.9391	-0.5615
O	-1.5892	-3.7814	-1.7465
C	-0.4540	-6.1486	-1.0292
H	-1.2796	-6.1835	-1.7211
H	0.1030	-6.9858	-0.6459
H	-0.1924	-2.9459	-0.5059

TS1-1

C	-0.7162	-3.8233	-0.9187
O	-0.0844	-4.9423	-0.4905
O	-1.6737	-3.7953	-1.6377
C	-0.6071	-6.1790	-0.8976
H	-1.6071	-6.4954	-0.0798
H	-1.0642	-6.1605	-1.8840
H	0.1405	-6.9476	-0.7295
H	-2.3154	-6.6954	0.5286
H	-0.1998	-2.9494	-0.5035

$HCOOCHCH_3$(n=0,m=2)

$H + HCOOCH_2CH_3 \rightarrow H_2 + HCOOCHCH_3$ (TS3-1)

$H + HCOOCH_2CH_3 \rightarrow H_2 + HCOOCH_2CH_2$ (TS3-2)

$HCOOCH_2CH_3$

C	-0.9272	-3.8912	-0.7215
O	-0.2940	-4.9952	-0.3068
O	-1.9101	-3.8568	-1.4128
C	-0.8527	-6.2677	-0.7365
H	-1.8843	-6.3277	-0.3828
H	-0.8702	-6.2848	-1.8284
C	0.0146	-7.3668	-0.1606
H	0.0252	-7.3268	0.9308
H	-0.3784	-8.3406	-0.4646
H	1.0425	-7.2845	-0.5204
H	-0.4047	-3.0075	-0.3283

$HCOOCHCH_3$

C	-0.9881	-3.8545	-0.4127
O	-0.3110	-4.9806	-0.0657
O	-2.0662	-3.8241	-0.9367
C	-0.8650	-6.2105	-0.3405
H	-1.8821	-6.2113	-0.7032
C	-0.1327	-7.3699	0.2111
H	-0.1786	-7.4055	1.3105
H	-0.5624	-8.2980	-0.1702
H	0.9278	-7.3407	-0.0625
H	-0.3828	-2.9849	-0.1330

TS3-1

C	-0.9758	-3.8707	-0.4153
O	-0.2715	-4.9907	-0.1390
O	-2.0517	-3.8298	-0.9422
C	-0.8269	-6.2359	-0.5242
H	-1.9150	-6.2233	-0.4726
H	-0.5909	-6.3645	-1.7906
C	-0.1299	-7.3635	0.1808
H	-0.3030	-7.3159	1.2609
H	-0.5122	-8.3191	-0.1858
H	0.9475	-7.3298	0.0041
H	-0.3574	-6.4632	-2.7473
H	-0.4024	-3.0013	-0.0696

$HCOOCH_2CH_2$

C	-1.1827	-3.9258	-0.6169
O	-0.5885	-5.0433	-0.1774
O	-2.1423	-3.8728	-1.3384
C	-1.1729	-6.3011	-0.6169
H	-2.2433	-6.2791	-0.3651
H	-1.1097	-6.3609	-1.7079
C	-0.4566	-7.4089	0.0474
H	-0.0429	-7.2747	1.0378
H	-0.4626	-8.3950	-0.3971
H	-0.6507	-3.0540	-0.2116

TS3-2

C	-1.1940	-3.9206	-0.6198
O	-0.5777	-5.0268	-0.1792
O	-2.1512	-3.8889	-1.3450
C	-1.1247	-6.2927	-0.6305
H	-2.1742	-6.3466	-0.3183
H	-1.1075	-6.3171	-1.7232
C	-0.3076	-7.3905	-0.0271
H	-0.1216	-7.3037	1.0414
H	-0.6110	-8.3896	-0.3344
H	0.9565	-7.2965	-0.5684
H	1.7792	-7.2295	-0.9610
H	-0.6826	-3.0391	-0.2098

CH_3COOCH_3(n=1,m=1)

$H + CH_3COOCH_3 \rightarrow H_2 + CH_2COOCH_3$ (TS3-3)

$H + CH_3COOCH_3 \rightarrow H_2 + CH_3COOCH_2$ (TS3-4)

CH_3COOCH_3

C	-0.1581	-2.6600	-0.1438
H	-0.1596	-2.6889	0.9484
H	0.8843	-2.6707	-0.4697
C	-0.8828	-3.8633	-0.6892
O	-0.2801	-5.0095	-0.2985
O	-1.8707	-3.8380	-1.3812
C	-0.8877	-6.2315	-0.7573
H	-1.9112	-6.3110	-0.3881
H	-0.8972	-6.2675	-1.8475
H	-0.2717	-7.0317	-0.3529
H	-0.6484	-1.7529	-0.4908

CH_2COOCH_3

C	0.1322	-2.6578	-0.4998
H	1.1613	-2.7382	-0.1784
C	-0.6395	-3.8348	-0.8292
O	0.0853	-4.9751	-0.6796
O	-1.8004	-3.8255	-1.1978
C	-0.6048	-6.1975	-0.9849
H	-0.9316	-6.2030	-2.0263
H	0.1170	-6.9914	-0.8061
H	-0.3477	-1.6934	-0.5831
H	-1.4760	-6.3172	-0.3386

TS3-3

C	0.0953	-2.6529	-0.3002
H	-0.1093	-2.5843	0.9806
H	1.1770	-2.7355	-0.3598
C	-0.6625	-3.8398	-0.7653
O	0.0584	-4.9749	-0.6120
O	-1.7934	-3.8194	-1.1949
C	-0.6032	-6.1958	-0.9906
H	-0.8685	-6.1733	-2.0485
H	0.1150	-6.9882	-0.7923
H	-0.3144	-1.7151	-0.6622
H	-1.5079	-6.3389	-0.3979
H	-0.2336	-2.4922	1.9406

CH_3COOCH_2

C	0.0482	-2.6219	-0.2751
H	-0.0149	-2.7155	0.8116
H	1.1077	-2.5863	-0.5398
C	-0.6075	-3.8025	-0.9327
O	0.0039	-4.9714	-0.5363
O	-1.5325	-3.7811	-1.6993
C	-0.4583	-6.1542	-1.0332
H	-1.2863	-6.1449	-1.7230
H	0.0733	-7.0184	-0.6738
H	-0.4462	-1.7084	-0.5984

TS3-4

C	0.0599	-2.6238	-0.2916
H	0.0020	-2.6575	0.7990
H	1.1173	-2.6447	-0.5642
C	-0.6489	-3.8147	-0.8747
O	-0.0477	-4.9762	-0.4690
O	-1.6073	-3.7926	-1.6003
C	-0.6132	-6.1817	-0.8995
H	-1.6100	-6.4921	-0.0815
H	-1.0821	-6.1237	-1.8790
H	0.1113	-6.9788	-0.7622
H	-2.3193	-6.6929	0.5335
H	-0.4040	-1.7110	-0.6586

$CH_3COOCH_2CH_3$(n=1,m=2)

$H + CH_3COOCH_2CH_3 \rightarrow H_2 + CH_2COOCH_2CH_3$ (TS4-1)

$H + CH_3COOCH_2CH_3 \rightarrow H_2 + CH_3COOCHCH_3$ (TS4-2)

$H + CH_3COOCH_2CH_3 \rightarrow H_2 + CH_3COOCH_2CH_2$ (TS4-3)

$CH_3COOCH_2CH_3$

C	-0.1691	-2.6519	-0.1480
H	-0.1631	-2.6747	0.9444
H	0.8717	-2.6452	-0.4799
C	-0.8744	-3.8720	-0.6837
O	-0.2568	-5.0048	-0.2805
O	-1.8606	-3.8638	-1.3794
C	-0.8389	-6.2549	-0.7263
H	-1.8722	-6.3036	-0.3746
H	-0.8593	-6.2605	-1.8186
H	-0.6774	-1.7556	-0.4974
C	0.0059	-7.3809	-0.1673
H	0.0190	-7.3575	0.9249
H	-0.4069	-8.3426	-0.4843
H	1.0356	-7.3154	-0.5263

$CH_2COOCH_2CH_3$

C	0.1210	-2.6443	-0.4921
H	1.1451	-2.7152	-0.1527
C	-0.6367	-3.8293	-0.8287
O	0.0925	-4.9628	-0.6612
O	-1.7918	-3.8258	-1.2172
C	-0.5770	-6.2065	-0.9723
H	-0.9079	-6.1750	-2.0135
H	-0.3643	-1.6838	-0.5889
H	-1.4677	-6.2911	-0.3446
C	0.4052	-7.3323	-0.7215
H	-0.0685	-8.2910	-0.9490
H	1.2899	-7.2284	-1.3538
H	0.7259	-7.3475	0.3226

TS4-1

C	0.0877	-2.6400	-0.3009
H	-0.1200	-2.5674	0.9793
H	1.1703	-2.7140	-0.3580
C	-0.6605	-3.8355	-0.7625
O	0.0686	-4.9632	-0.6059
O	-1.7920	-3.8209	-1.1923
C	-0.5772	-6.2061	-0.9794
H	-0.8636	-6.1468	-2.0319
H	-0.3287	-1.7068	-0.6674
H	-1.4913	-6.3137	-0.3908
H	-0.2465	-2.4720	1.9387
C	0.4052	-7.3294	-0.7186
H	-0.0497	-8.2854	-0.9907
H	1.3136	-7.2013	-1.3113
H	0.6832	-7.3701	0.3368

$CH_3COOCHCH_3$

C	-0.1230	-2.6376	0.0425
H	0.1710	-2.6972	1.0925
H	0.7930	-2.6075	-0.5534
C	-0.9402	-3.8395	-0.3430
O	-0.2715	-4.9951	-0.0266
O	-2.0250	-3.8308	-0.8635
C	-0.8392	-6.2071	-0.3495
H	-1.8605	-6.1797	-0.7001
C	-0.1421	-7.3917	0.1975
H	-0.2227	-7.4538	1.2942
H	-0.5741	-8.3038	-0.2190
H	0.9267	-7.3743	-0.0427
H	-0.7038	-1.7348	-0.1341

TS4-2

C	-0.1263	-2.6510	0.0582
H	0.1588	-2.7506	1.1075
H	0.7942	-2.5819	-0.5267
C	-0.9166	-3.8526	-0.3844
O	-0.2268	-5.0026	-0.1242
O	-2.0049	-3.8378	-0.8974
C	-0.8110	-6.2269	-0.5181
H	-1.8985	-6.1904	-0.4640
H	-0.5832	-6.3560	-1.7823
C	-0.1401	-7.3786	0.1755
H	-0.3097	-7.3367	1.2565
H	-0.5458	-8.3216	-0.1987
H	0.9376	-7.3698	-0.0030
H	-0.3517	-6.4599	-2.7448
H	-0.7221	-1.7524	-0.0864

$CH_3COOCH_2CH_2$

C	-0.4452	-2.6914	-0.0260
H	-0.4075	-2.7404	1.0642
H	0.5852	-2.6700	-0.3889
C	-1.1540	-3.9021	-0.5769
O	-0.5691	-5.0427	-0.1455
O	-2.1125	-3.8834	-1.3099
C	-1.1560	-6.2826	-0.6116
H	-2.2300	-6.2619	-0.3744
H	-1.0834	-6.3272	-1.7036
C	-0.4556	-7.4092	0.0397
H	-0.0035	-7.2823	1.0142
H	-0.5134	-8.3985	-0.3943
H	-0.9665	-1.7907	-0.3432

TS4-3

C	-0.4529	-2.6799	-0.0306
H	-0.4050	-2.7301	1.0592
H	0.5740	-2.6432	-0.4022
C	-1.1481	-3.8997	-0.5776
O	-0.5452	-5.0334	-0.1498
O	-2.1111	-3.8959	-1.3044
C	-1.1095	-6.2781	-0.6221
H	-2.1613	-6.3246	-0.3158
H	-1.0908	-6.2888	-1.7154
C	-0.3129	-7.4001	-0.0344
H	-0.1260	-7.3329	1.0355
H	-0.6326	-8.3894	-0.3568
H	0.9535	-7.3197	-0.5714
H	1.7792	-7.2614	-0.9606
H	-0.9900	-1.7864	-0.3417

$CH_3CH_2COOCH_3$(n=2,m=1)

$H + CH_3CH_2COOCH_3 \rightarrow H_2 + CH_3CHCOOCH_3$ (TS4-4)

$H + CH_3CH_2COOCH_3 \rightarrow H_2 + CH_2CH_2COOCH_3$ (TS4-5)

$H + CH_3CH_2COOCH_3 \rightarrow H_2 + CH_3CH_2COOCH_2$ (TS4-6)

$CH_3CH_2COOCH_3$

C	-0.7618	-1.3332	-0.5645
H	-1.7974	-1.2537	-0.2282
H	-0.7614	-1.2279	-1.6511
C	-0.1443	-2.6626	-0.1389
H	-0.1250	-2.7634	0.9514
H	0.9008	-2.7384	-0.4571
C	-0.8747	-3.8678	-0.6917
O	-0.2821	-5.0158	-0.2908
O	-1.8543	-3.8410	-1.3958
C	-0.8888	-6.2363	-0.7535
H	-1.9179	-6.3102	-0.3989
H	-0.8829	-6.2768	-1.8437
H	-0.2824	-7.0379	-0.3376
H	-0.1970	-0.5008	-0.1382

$CH_3CHCOOCH_3$

C	-0.7563	-1.3265	-0.5888
H	-1.8350	-1.3980	-0.7286
H	-0.3317	-0.7186	-1.3984
C	-0.1333	-2.6701	-0.5533
H	0.9376	-2.7785	-0.4266
C	-0.9199	-3.8786	-0.6836
O	-0.1406	-4.9940	-0.6219
O	-2.1295	-3.9228	-0.8311
C	-0.8336	-6.2453	-0.7418
H	-1.5614	-6.3604	0.0636
H	-1.3531	-6.3069	-1.6998
H	-0.0647	-7.0121	-0.6741
H	-0.5545	-0.7761	0.3397

TS4-4

C	-0.7583	-1.3359	-0.5584
H	-1.8175	-1.2823	-0.3034
H	-0.6717	-1.1925	-1.6401
C	-0.1682	-2.6675	-0.1483
H	-0.2100	-2.7226	1.0959
H	0.9009	-2.7749	-0.3323
C	-0.9290	-3.8789	-0.5843
O	-0.1735	-4.9950	-0.4750
O	-2.0798	-3.8862	-0.9556
C	-0.8257	-6.2337	-0.8109
H	-1.6878	-6.3986	-0.1631
H	-1.1563	-6.2210	-1.8504
H	-0.0765	-7.0070	-0.6564
H	-0.2259	-2.6853	2.1418
H	-0.2325	-0.5144	-0.0666

$CH_2CH_2COOCH_3$

C	-0.6559	-1.3386	-0.7670
H	-1.4486	-1.3266	-1.5015
C	-0.1514	-2.6255	-0.2247
H	0.9309	-2.7426	-0.3846
C	-0.8306	-3.8497	-0.8086
O	-0.3086	-4.9778	-0.2797
O	-1.7141	-3.8473	-1.6287
C	-0.8705	-6.2168	-0.7517
H	-1.9366	-6.2629	-0.5255
H	-0.7282	-6.3141	-1.8288
H	-0.3323	-6.9996	-0.2218
H	-0.2304	-0.4057	-0.4219
H	-0.2628	-2.6815	0.8690

TS4-5

C	-0.8584	-1.3435	-0.5905
H	-2.0012	-1.3133	0.1589
H	-1.2493	-1.2811	-1.6029
C	-0.1487	-2.6272	-0.2481
H	0.8763	-2.6190	-0.6471
C	-0.8194	-3.8591	-0.8241
O	-0.3670	-4.9783	-0.2203
O	-1.6280	-3.8650	-1.7188
C	-0.8974	-6.2228	-0.7155
H	-1.9809	-6.2498	-0.5937
H	-0.6518	-6.3487	-1.7709
H	-0.4245	-6.9978	-0.1166
H	-0.3525	-0.4388	-0.2593
H	-0.0373	-2.7579	0.8321
H	-2.7475	-1.3218	0.7002

$CH_3CH_2COOCH_2$

C	-0.5061	-1.2864	-0.7345
H	-1.5673	-1.2262	-0.4859
H	-0.4125	-1.1455	-1.8130
C	0.0873	-2.6238	-0.2996
H	0.0146	-2.7599	0.7850
H	1.1568	-2.6815	-0.5290
C	-0.5813	-3.8096	-0.9501
O	0.0108	-4.9800	-0.5288
O	-1.4984	-3.7894	-1.7264
C	-0.4626	-6.1650	-1.0097
H	-1.2829	-6.1568	-1.7086
H	0.0567	-7.0299	-0.6342
H	0.0114	-0.4647	-0.2345

TS4-6

C	-0.4928	-1.2905	-0.7540
H	-1.5460	-1.1986	-0.4826
H	-0.4223	-1.1857	-1.8384
C	0.0813	-2.6265	-0.2900
H	0.0320	-2.7262	0.7997
H	1.1428	-2.7181	-0.5429
C	-0.6317	-3.8195	-0.8807
O	-0.0440	-4.9830	-0.4597
O	-1.5789	-3.7966	-1.6210
C	-0.6108	-6.1872	-0.8909
H	-1.6221	-6.4861	-0.0877
H	-1.0636	-6.1331	-1.8783
H	0.1059	-6.9885	-0.7373
H	-2.3436	-6.6794	0.5170
H	0.0546	-0.4653	-0.2931

$CH_3CH_2COOCH_2CH3$(n=2,m=2)

$H + CH_3CH_2COOCH_2CH_3 \rightarrow H_2 + CH_3CHCOOCH_2CH_3$ (TS5-1)

$H + CH_3CH_2COOCH_2CH_3 \rightarrow H_2 + CH_2CH_2COOCH_2CH_3$ (TS5-2)

$H + CH_3CH_2COOCH_2CH_3 \rightarrow H_2 + CH_3CH_2COOCHCH_3$ (TS5-3)

$H + CH_3CH_2COOCH_2CH_3 \rightarrow H_2 + CH_3CH_2COOCH_2CH_2$ (TS5-4)

$CH_3CH_2COOCH_2CH_3$

C	-0.7823	-1.3375	-0.5693
H	-1.8198	-1.2665	-0.2375
H	-0.7790	-1.2376	-1.6564
C	-0.1537	-2.6589	-0.1349
H	-0.1363	-2.7524	0.9562
H	0.8928	-2.7270	-0.4500
C	-0.8733	-3.8747	-0.6809
O	-0.2626	-5.0138	-0.2859
O	-1.8608	-3.8568	-1.3753
C	-0.8539	-6.2577	-0.7370
H	-1.8853	-6.3037	-0.3797
H	-0.8796	-6.2563	-1.8292
C	-0.0113	-7.3914	-0.1894
H	0.0078	-7.3739	0.9026
H	-0.4304	-8.3492	-0.5098
H	1.0164	-7.3279	-0.5540
H	-0.2272	-0.4973	-0.1454

$CH_3CHCOOCH_2CH_3$

C	0.0066	-0.0017	0.0077
H	-0.3486	-0.5822	0.8694
H	1.0753	0.1804	0.1211
C	-0.7401	1.2718	-0.1172
H	-1.8172	1.2699	-0.2385
C	-0.0697	2.5555	-0.0833
O	-0.9491	3.5851	-0.2188
O	1.1321	2.7187	0.0490
C	-0.3843	4.9148	-0.2000
H	0.1401	5.0607	0.7480
H	0.3547	4.9943	-1.0014
C	-1.5215	5.9004	-0.3769
H	-2.2508	5.8068	0.4309
H	-1.1290	6.9208	-0.3684
H	-2.0356	5.7388	-1.3271
H	-0.1542	-0.6385	-0.8722

TS5-1

C	0.0055	0.0069	-0.0130
H	-0.0346	-0.0562	1.0791
H	1.0570	0.0320	-0.3023
C	-0.7210	1.2407	-0.5024
H	-1.7890	1.2637	-0.2850
H	-0.7241	1.1971	-1.7475
C	-0.0642	2.5495	-0.1935
O	-0.9269	3.5773	-0.3481
O	1.0957	2.6886	0.1210
C	-0.3923	4.9082	-0.1365
H	0.0057	4.9658	0.8792
H	0.4381	5.0637	-0.8293
C	-1.5175	5.8961	-0.3647
H	-2.3395	5.7227	0.3335
H	-1.1486	6.9142	-0.2137
H	-1.9061	5.8197	-1.3826
H	-0.7383	1.0757	-2.7876
H	-0.4536	-0.8970	-0.4196

$CH_2CH_2COOCH_2CH_3$

C	-0.9359	-1.3528	-0.3514
H	-1.9114	-1.3473	-0.8167
C	-0.2274	-2.6340	-0.1042
H	0.0108	-2.7722	0.9613
H	0.7553	-2.6610	-0.5988
C	-0.9951	-3.8621	-0.5589
O	-0.2933	-4.9837	-0.2930
O	-2.0799	-3.8616	-1.0859
C	-0.9079	-6.2403	-0.6760
H	-1.8707	-6.3258	-0.1671
H	-1.0992	-6.2208	-1.7513
C	0.0430	-7.3532	-0.2868
H	0.2267	-7.3539	0.7900
H	-0.3899	-8.3188	-0.5614
H	1.0010	-7.2487	-0.8010
H	-0.4735	-0.4177	-0.0647

TS5-2

C	-0.8184	-1.3532	-0.6272
H	-1.9030	-1.2990	-0.6763
H	-0.4712	-1.3097	-1.9482
C	-0.2590	-2.6373	-0.0730
H	-0.3104	-2.6366	1.0257
H	0.8011	-2.7592	-0.3130
C	-1.0116	-3.8719	-0.5332
O	-0.2863	-4.9866	-0.3112
O	-2.1205	-3.8774	-1.0089
C	-0.9112	-6.2484	-0.6617
H	-1.8387	-6.3466	-0.0929
H	-1.1707	-6.2242	-1.7224
C	0.0744	-7.3527	-0.3406
H	0.3259	-7.3579	0.7224
H	-0.3645	-8.3214	-0.5939
H	0.9965	-7.2339	-0.9139
H	-0.3507	-0.4478	-0.2456
H	-0.1941	-1.3086	-2.8279

$CH_3CH_2COOCHCH_3$

C	-0.8466	-1.3132	-0.1659
H	-1.7698	-1.2586	0.4143
H	-1.1122	-1.1921	-1.2176
C	-0.1241	-2.6369	0.0710
H	0.1597	-2.7572	1.1217
H	0.8149	-2.6833	-0.4919
C	-0.9448	-3.8416	-0.3249
O	-0.2703	-4.9979	-0.0226
O	-2.0331	-3.8331	-0.8382
C	-0.8346	-6.2093	-0.3537
H	-1.8592	-6.1830	-0.6951
C	-0.1331	-7.3953	0.1849
H	-0.2138	-7.4659	1.2812
H	-0.5612	-8.3061	-0.2384
H	0.9356	-7.3717	-0.0547
H	-0.2073	-0.4771	0.1266

TS5-3

C	-0.8545	-1.3265	-0.1424
H	-1.7871	-1.3042	0.4245
H	-1.1052	-1.1730	-1.1934
C	-0.1168	-2.6473	0.0607
H	0.1545	-2.7995	1.1106
H	0.8298	-2.6645	-0.4903
C	-0.9142	-3.8517	-0.3844
O	-0.2244	-5.0025	-0.1261
O	-2.0044	-3.8375	-0.8938
C	-0.8103	-6.2265	-0.5171
H	-1.8976	-6.1906	-0.4570
H	-0.5900	-6.3563	-1.7819
C	-0.1359	-7.3784	0.1729
H	-0.2997	-7.3365	1.2547
H	-0.5435	-8.3214	-0.1992
H	0.9409	-7.3695	-0.0112
H	-0.3645	-6.4615	-2.7468
H	-0.2316	-0.4924	0.1885

$CH_3CH_2COOCH_2CH_2$

C	-1.0627	-1.3658	-0.4784
H	-2.1073	-1.2868	-0.1716
H	-1.0330	-1.2752	-1.5659
C	-0.4507	-2.6862	-0.0180
H	-0.4610	-2.7722	1.0738
H	0.6029	-2.7613	-0.3066
C	-1.1604	-3.9027	-0.5741
O	-0.5706	-5.0416	-0.1442
O	-2.1221	-3.8883	-1.3033
C	-1.1579	-6.2835	-0.6028
H	-2.2286	-6.2691	-0.3502
H	-1.1013	-6.3273	-1.6958
C	-0.4427	-7.4073	0.0372
H	0.0310	-7.2764	1.0008
H	-0.5075	-8.3979	-0.3928
H	-0.5134	-0.5250	-0.0483

TS5-4

C	-1.0759	-1.3621	-0.4778
H	-2.1188	-1.2949	-0.1624
H	-1.0558	-1.2698	-1.5653
C	-0.4458	-2.6762	-0.0242
H	-0.4462	-2.7640	1.0674
H	0.6063	-2.7394	-0.3212
C	-1.1457	-3.8993	-0.5769
O	-0.5430	-5.0334	-0.1491
O	-2.1105	-3.8965	-1.3017
C	-1.1109	-6.2783	-0.6149
H	-2.1593	-6.3267	-0.2970
H	-1.1044	-6.2897	-1.7083
C	-0.3068	-7.3995	-0.0359
H	-0.1066	-7.3311	1.0315
H	-0.6298	-8.3895	-0.3532
H	0.9528	-7.3189	-0.5884
H	1.7736	-7.2604	-0.9881
H	-0.5324	-0.5160	-0.0510

$CH_3CH_2CH_2COOCH_3$(n=3,m=1)

H + $CH_3CH_2CH_2COOCH_3 \rightarrow H_2 + CH_3CH_2CHCOOCH_3$ (TS5-5)

H + $CH_3CH_2CH_2COOCH_3 \rightarrow H_2 + CH_3CHCH_2COOCH_3$ (TS5-6)

H + $CH_3CH_2CH_2COOCH_3 \rightarrow H_2 + CH_2CH_2CH_2COOCH_3$ (TS5-7)

H + $CH_3CH_2CH_2COOCH_3 \rightarrow H_2 + CH_3CH_2CH_2COOCH_2$ (TS5-8)

$CH_3CH_2CH_2COOCH_3$

C	3.2470	-0.3001	-0.0018
H	3.3579	-0.9302	0.8865
H	4.0785	0.4092	-0.0099
H	3.3538	-0.9453	-0.8797
C	1.9017	0.4304	-0.0050
H	1.8330	1.0939	0.8618
H	1.8286	1.0779	-0.8836
C	0.7164	-0.5354	0.0065
H	0.7496	-1.1898	0.8852
H	0.7465	-1.2080	-0.8583
C	-0.6305	0.1544	0.0028
O	-1.6357	-0.7513	-0.0010
O	-0.8171	1.3467	0.0035
C	-2.9710	-0.2138	-0.0039
H	-3.1400	0.3955	0.8852
H	-3.1350	0.3979	-0.8923
H	-3.6319	-1.0778	-0.0069

$CH_3CH_2CHCOOCH_3$

C	3.0661	-0.2721	0.4977
H	2.7636	-0.1911	1.5446
H	3.9901	0.2965	0.3667
H	3.2852	-1.3232	0.2897
C	1.9664	0.2689	-0.4376
H	1.7679	1.3226	-0.2306
H	2.3357	0.2129	-1.4731
C	0.6962	-0.4942	-0.3455
H	0.6956	-1.5710	-0.4780
C	-0.5737	0.1503	-0.0842
O	-1.5976	-0.7483	-0.0597
O	-0.7382	1.3453	0.0954
C	-2.9004	-0.2011	0.1921
H	-2.9296	0.2908	1.1662
H	-3.1686	0.5240	-0.5786
H	-3.5818	-1.0492	0.1722

TS5-5

C	3.2273	-0.2596	-0.0934
H	3.3646	-0.7242	0.8873
H	4.0528	0.4392	-0.2490
H	3.3109	-1.0465	-0.8492
C	1.8799	0.4614	-0.1829
H	1.8220	1.2655	0.5554
H	1.7850	0.9494	-1.1613
C	0.6970	-0.4691	0.0038
H	0.8056	-0.9767	1.1415
H	0.7074	-1.3556	-0.6320
C	-0.6492	0.1797	0.0324
O	-1.6331	-0.7262	-0.1710
O	-0.8569	1.3526	0.2417
C	-2.9791	-0.2198	-0.1051
H	-3.1779	0.2085	0.8784
H	-3.1365	0.5451	-0.8668
H	-3.6213	-1.0788	-0.2860
H	0.9525	-1.3938	2.0870

$CH_3CHCH_2COOCH_3$

C	3.2988	-0.2019	-0.0455
H	3.5674	-0.6437	0.9282
H	4.0429	0.5651	-0.2687
H	3.4141	-1.0088	-0.7825
C	1.9181	0.3548	-0.0432
H	1.7468	1.4231	-0.0262
C	0.7427	-0.5492	0.0827
H	0.7625	-1.1123	1.0322
H	0.7437	-1.3336	-0.6881
C	-0.5968	0.1587	0.0271
O	-1.6065	-0.7389	-0.0158
O	-0.7713	1.3517	0.0314
C	-2.9380	-0.1922	-0.0470
H	-3.1280	0.4024	0.8477
H	-3.0723	0.4356	-0.9289
H	-3.6036	-1.0518	-0.0838

TS5-6

C	3.2219	-0.2870	-0.0902
H	3.3276	-1.1916	0.5165
H	4.0141	0.4076	0.1993
H	3.3971	-0.5701	-1.1360
C	1.8566	0.3397	0.0782
H	1.7756	0.6719	1.3489
H	1.7439	1.3119	-0.4012
C	0.6764	-0.5735	-0.1689
H	0.6612	-1.4140	0.5311
H	0.7511	-1.0241	-1.1702
C	-0.6622	0.1356	-0.1193
O	-1.6648	-0.7420	0.0977
O	-0.8367	1.3185	-0.2787
C	-2.9953	-0.1900	0.1159
H	-3.0870	0.5547	0.9075
H	-3.2284	0.2751	-0.8429
H	-3.6562	-1.0332	0.3039
H	1.7283	0.8513	2.2960

$CH_2CH_2CH_2COOCH_3$

C	3.2792	-0.3118	0.0016
H	4.1851	0.1965	0.3078
H	3.3805	-1.2888	-0.4572
C	1.9684	0.3934	0.0341
H	1.9040	1.0373	0.9185
H	1.8846	1.0884	-0.8170
C	0.7722	-0.5619	0.0027
H	0.7868	-1.2390	0.8626
H	0.8128	-1.2077	-0.8818
C	-0.5645	0.1466	-0.0116
O	-1.5803	-0.7447	0.0280
O	-0.7336	1.3408	-0.0545
C	-2.9095	-0.1913	0.0140
H	-3.0628	0.4553	0.8792
H	-3.0738	0.3856	-0.8972
H	-3.5802	-1.0468	0.0517

TS5-7

C	3.1756	-0.1531	-0.1735
H	3.3304	-1.0193	0.8725
H	4.0353	0.5020	-0.0401
H	3.2875	-0.8139	-1.0339
C	1.8267	0.5040	-0.0112
H	1.7719	1.0171	0.9538
H	1.7072	1.2920	-0.7660
C	0.6669	-0.4859	-0.1331
H	0.7371	-1.2705	0.6271
H	0.6948	-1.0069	-1.0969
C	-0.6930	0.1655	-0.0057
O	-1.6768	-0.7582	-0.0745
O	-0.9012	1.3460	0.1353
C	-3.0233	-0.2586	0.0295
H	-3.1707	0.2446	0.9861
H	-3.2343	0.4419	-0.7797
H	-3.6640	-1.1344	-0.0452
H	3.4112	-1.5862	1.6008

$CH_3CH_2CH_2COOCH_2$

C	-3.1829	-0.3258	0.0009
H	-3.2808	-0.9693	-0.8810
H	-4.0245	0.3713	-0.0058
H	-3.2835	-0.9599	0.8857
C	-1.8493	0.4257	-0.0029
H	-1.7872	1.0769	-0.8795
H	-1.7898	1.0865	0.8668
C	-0.6502	-0.5232	0.0039
H	-0.6713	-1.1932	-0.8637
H	-0.6731	-1.1823	0.8798
C	0.6807	0.1861	0.0014
O	1.7087	-0.7317	-0.0008
O	0.8718	1.3727	0.0014
C	2.9944	-0.2771	-0.0024
H	3.1745	0.7854	0.0018
H	3.7357	-1.0576	-0.0039

TS5-8

C	3.3053	-0.3123	0.0816
H	3.3757	-0.9143	0.9930
H	4.1427	0.3900	0.0836
H	3.4397	-0.9855	-0.7711
C	1.9684	0.4293	0.0036
H	1.8721	1.1193	0.8467
H	1.9356	1.0494	-0.8970
C	0.7755	-0.5272	-0.0009
H	0.7705	-1.1566	0.8968
H	0.8289	-1.2252	-0.8442
C	-0.5609	0.1716	-0.0678
O	-1.5774	-0.7464	-0.1112
O	-0.7526	1.3586	-0.0868
C	-2.8885	-0.2593	-0.1384
H	-2.9951	0.6930	-0.6528
H	-3.5528	-1.0546	-0.4635
H	-3.2649	0.0017	1.1053
H	-3.5116	0.1724	2.0185

$CH_3CH_2CH_2COOCH_2CH_3$(n=3,m=2)

$H + CH_3CH_2CH_2COOCH_2CH_3 \rightarrow H_2 + CH_3CH_2CHCOOCH_2CH_3$ (TS6-1)

$H + CH_3CH_2CH_2COOCH_2CH_3 \rightarrow H_2 + CH_3CHCH_2COOCH_2CH_3$ (TS6-2)

$H + CH_3CH_2CH_2COOCH_2CH_3 \rightarrow H_2 + CH_2CH_2CH_2COOCH_2CH_3$ (TS6-3)

$H + CH_3CH_2CH_2COOCH_2CH_3 \rightarrow H_2 + CH_3CH_2CH_2COOCHCH_3$ (TS6-4)

$H + CH_3CH_2CH_2COOCH_2CH_3 \rightarrow H_2 + CH_3CH_2CH_2COOCH_2CH_2$ (TS6-5)

$CH_3CH_2CH_2COOCH_2CH_3$

C	-0.0379	-0.1213	0.0032
H	-0.0414	-0.1339	1.0978
H	1.0068	-0.1045	-0.3236
C	-0.7845	-1.3279	-0.5719
H	-1.8325	-1.3042	-0.2597
H	-0.7970	-1.2749	-1.6645
C	-0.1615	-2.6554	-0.1399
H	-0.1439	-2.7447	0.9526
H	0.8866	-2.7208	-0.4535
C	-0.8793	-3.8725	-0.6841
O	-0.2657	-5.0101	-0.2884
O	-1.8677	-3.8586	-1.3775
C	-0.8551	-6.2557	-0.7374
H	-1.8861	-6.3033	-0.3791
H	-0.8819	-6.2558	-1.8295
C	-0.0099	-7.3872	-0.1891
H	0.0103	-7.3681	0.9029
H	-0.4274	-8.3461	-0.5078
H	1.0174	-7.3222	-0.5548
H	-0.4999	0.8158	-0.3181

$CH_3CH_2CHCOOCH_2CH_3$

C	-0.2031	-0.2751	-0.0287
H	0.1927	-0.2368	0.9902
H	0.6204	-0.5279	-0.7010
C	-1.3476	-1.2997	-0.1481
H	-2.1730	-0.9737	0.5042
H	-1.7453	-1.3213	-1.1651
C	-0.9459	-2.6732	0.2478
H	-0.4484	-2.8435	1.1968
C	-1.2077	-3.8259	-0.5895
O	-0.7690	-4.9774	-0.0106
O	-1.7520	-3.7959	-1.6810
C	-0.9820	-6.1923	-0.7628
H	-2.0533	-6.3088	-0.9464
H	-0.4896	-6.0961	-1.7339
C	-0.4172	-7.3407	0.0486
H	-0.9182	-7.4207	1.0160
H	-0.5624	-8.2800	-0.4918
H	0.6528	-7.2076	0.2236
H	-0.5582	0.7250	-0.2892

TS6-1

C	-0.3576	-0.1330	0.1880
H	-0.1948	-0.2192	1.2668
H	0.6221	-0.0440	-0.2903
C	-1.1354	-1.3330	-0.3585
H	-2.1260	-1.3778	0.1118
H	-1.3215	-1.2173	-1.4295
C	-0.4310	-2.6542	-0.1176
H	-0.1241	-2.8271	0.9150
H	0.6738	-2.5903	-0.6996
C	-1.0776	-3.8630	-0.7157
O	-0.6105	-4.9977	-0.1495
O	-1.8897	-3.8471	-1.6126
C	-1.1176	-6.2451	-0.6865
H	-2.2046	-6.2545	-0.5782
H	-0.8888	-6.2830	-1.7541
C	-0.4593	-7.3748	0.0782
H	-0.6945	-7.3165	1.1434
H	-0.8209	-8.3345	-0.3007
H	0.6263	-7.3471	-0.0384
H	-0.9016	0.7973	0.0077
H	1.5956	-2.4809	-1.1775

$CH_3CHCH_2COOCH_2CH_3$

C	0.0342	-0.0609	-0.1782
H	-0.0964	-0.0005	0.9124
H	1.1178	0.0310	-0.3549
C	-0.5158	-1.3275	-0.7345
H	-1.2217	-1.3202	-1.5543
C	-0.0505	-2.6420	-0.2155
H	-0.1993	-2.7287	0.8720
H	1.0377	-2.7690	-0.3422
C	-0.7154	-3.8410	-0.8652
O	-0.2811	-4.9878	-0.2996
O	-1.5180	-3.8046	-1.7649
C	-0.8275	-6.2211	-0.8311
H	-1.9144	-6.1951	-0.7250
H	-0.5977	-6.2729	-1.8978
C	-0.2076	-7.3675	-0.0588
H	-0.4431	-7.2961	1.0054
H	-0.5988	-8.3171	-0.4337
H	0.8787	-7.3754	-0.1729
H	-0.4442	0.8155	-0.6193

TS6-2

C	-0.0531	-0.0860	-0.0697
H	0.1656	-0.1543	1.0005
H	0.8967	0.0975	-0.5882
C	-0.7158	-1.3433	-0.5843
H	-1.8516	-1.4378	0.0724
H	-1.0717	-1.2772	-1.6123
C	0.0123	-2.6387	-0.3009
H	0.1189	-2.8160	0.7731
H	1.0378	-2.5879	-0.6976
C	-0.6332	-3.8510	-0.9442
O	-0.2858	-4.9832	-0.2994
O	-1.3418	-3.8279	-1.9210
C	-0.7991	-6.2251	-0.8466
H	-1.8894	-6.1680	-0.8731
H	-0.4446	-6.3246	-1.8752
C	-0.3084	-7.3529	0.0375
H	-0.6687	-7.2330	1.0616
H	-0.6779	-8.3076	-0.3464
H	0.7831	-7.3906	0.0568
H	-2.6504	-1.5065	0.6109
H	-0.6882	0.7888	-0.2287

$CH_2CH_2CH_2COOCH_2CH_3$

C	-0.0304	-0.1223	-0.4428
H	1.0502	-0.1478	-0.3574
C	-0.7964	-1.3196	-0.8860
H	-1.8042	-1.3076	-0.4560
H	-0.9624	-1.2892	-1.9749
C	-0.1020	-2.6393	-0.5378
H	0.0301	-2.7423	0.5437
H	0.9080	-2.6698	-0.9628
C	-0.8426	-3.8603	-1.0407
O	-0.2475	-4.9941	-0.6114
O	-1.8296	-3.8494	-1.7363
C	-0.8487	-6.2438	-1.0348
H	-1.8871	-6.2633	-0.6961
H	-0.8536	-6.2760	-2.1268
C	-0.0332	-7.3711	-0.4358
H	-0.0356	-7.3199	0.6553
H	-0.4597	-8.3324	-0.7349
H	1.0023	-7.3331	-0.7814
H	-0.5207	0.8374	-0.3363

TS6-3

C	-0.0342	-0.1210	-0.3346
H	-0.0771	-0.1678	1.0303
H	1.0392	-0.1107	-0.5272
C	-0.7895	-1.3234	-0.8458
H	-1.8171	-1.3099	-0.4701
H	-0.8794	-1.2646	-1.9382
C	-0.1219	-2.6470	-0.4686
H	-0.0412	-2.7519	0.6181
H	0.9065	-2.6890	-0.8454
C	-0.8530	-3.8613	-1.0013
O	-0.2533	-5.0001	-0.5942
O	-1.8380	-3.8398	-1.6994
C	-0.8506	-6.2445	-1.0388
H	-1.8861	-6.2768	-0.6926
H	-0.8636	-6.2542	-2.1311
C	-0.0242	-7.3789	-0.4690
H	-0.0178	-7.3494	0.6229
H	-0.4480	-8.3364	-0.7838
H	1.0082	-7.3284	-0.8222
H	-0.4993	0.8438	-0.5319
H	-0.1367	-0.2194	1.9539

$CH_3CH_2CH_2COOCHCH_3$

C	-0.0047	-0.1053	0.2731
H	0.2704	-0.1504	1.3317
H	0.9219	-0.0611	-0.3080
C	-0.8623	-1.3064	-0.1341
H	-1.7971	-1.3088	0.4342
H	-1.1508	-1.2228	-1.1856
C	-0.1384	-2.6355	0.0836
H	0.1492	-2.7639	1.1331
H	0.8013	-2.6666	-0.4813
C	-0.9510	-3.8404	-0.3261
O	-0.2772	-4.9963	-0.0184
O	-2.0324	-3.8346	-0.8541
C	-0.8328	-6.2079	-0.3627
H	-1.8524	-6.1835	-0.7187
C	-0.1354	-7.3941	0.1809
H	-0.2322	-7.4700	1.2755
H	-0.5541	-8.3044	-0.2528
H	0.9367	-7.3660	-0.0426
H	-0.5419	0.8325	0.1107

TS6-4

C	-0.0173	-0.1181	0.3054
H	0.2561	-0.1880	1.3630
H	0.9099	-0.0485	-0.2722
C	-0.8607	-1.3173	-0.1354
H	-1.7973	-1.3442	0.4293
H	-1.1466	-1.2097	-1.1854
C	-0.1228	-2.6434	0.0506
H	0.1622	-2.7967	1.0976
H	0.8189	-2.6515	-0.5109
C	-0.9187	-3.8489	-0.3922
O	-0.2288	-4.9989	-0.1275
O	-2.0068	-3.8385	-0.9062
C	-0.8110	-6.2242	-0.5194
H	-1.8987	-6.1894	-0.4664
H	-0.5824	-6.3568	-1.7820
C	-0.1400	-7.3740	0.1777
H	-0.3111	-7.3298	1.2583
H	-0.5441	-8.3182	-0.1950
H	0.9380	-7.3643	0.0008
H	-0.5644	0.8178	0.1664
H	-0.3501	-6.4642	-2.7456

$CH_3CH_2CH_2COOCH_2CH_2$

C	-0.3345	-0.1461	0.0960
H	-0.3879	-0.1407	1.1894
H	0.7240	-0.1428	-0.1831
C	-1.0646	-1.3559	-0.4931
H	-2.1250	-1.3201	-0.2278
H	-1.0281	-1.3199	-1.5858
C	-0.4710	-2.6808	-0.0137
H	-0.5024	-2.7533	1.0798
H	0.5891	-2.7591	-0.2798
C	-1.1742	-3.9005	-0.5693
O	-0.5762	-5.0363	-0.1414
O	-2.1385	-3.8931	-1.2953
C	-1.1599	-6.2815	-0.5959
H	-2.2282	-6.2746	-0.3327
H	-1.1140	-6.3237	-1.6895
C	-0.4310	-7.4012	0.0356
H	0.0541	-7.2675	0.9931
H	-0.4960	-8.3925	-0.3930
H	-0.7735	0.7891	-0.2610

TS6-5

C	-0.3455	-0.1382	0.0945
H	-0.3894	-0.1354	1.1884
H	0.7104	-0.1248	-0.1939
C	-1.0698	-1.3534	-0.4908
H	-2.1282	-1.3274	-0.2165
H	-1.0428	-1.3150	-1.5836
C	-0.4603	-2.6737	-0.0190
H	-0.4818	-2.7488	1.0745
H	0.5983	-2.7421	-0.2940
C	-1.1564	-3.8983	-0.5718
O	-0.5478	-5.0307	-0.1465
O	-2.1237	-3.9000	-1.2932
C	-1.1145	-6.2774	-0.6089
H	-2.1598	-6.3309	-0.2816
H	-1.1180	-6.2874	-1.7023
C	-0.3003	-7.3959	-0.0387
H	-0.0898	-7.3277	1.0267
H	-0.6223	-8.3869	-0.3539
H	0.9533	-7.3095	-0.6034
H	-0.7961	0.7936	-0.2567
H	1.7698	-7.2471	-1.0114

$CH_3CH_2CH_2CH_2COOCH_3$(n=4,m=1)

$H + CH_3CH_2CH_2CH_2COOCH_3 \rightarrow H_2 + CH_3CH_2CH_2CHCOOCH_3$ (TS6-6)

$H + CH_3CH_2CH_2CH_2COOCH_3 \rightarrow H_2 + CH_3CH_2CHCH_2COOCH_3$ (TS6-7)

$H + CH_3CH_2CH_2CH_2COOCH_3 \rightarrow H_2 + CH_3CHCH_2CH_2COOCH_3$ (TS6-8)

$H + CH_3CH_2CH_2CH_2COOCH_3 \rightarrow H_2 + CH_2CH_2CH_2CH_2COOCH_3$ (TS6-9)

$H + CH_3CH_2CH_2CH_2COOCH_3 \rightarrow H_2 + CH_3CH_2CH_2CH_2COOCH_2$ (TS6-10)

$CH_3CH_2CH_2CH_2COOCH_3$

C	-0.0204	-0.1234	-0.0024
H	-0.0187	-0.1845	1.0930
H	1.0316	-0.1678	-0.3103
C	-0.7703	-1.3298	-0.5778
H	-1.8208	-1.2944	-0.2717
H	-0.7757	-1.2752	-1.6714
C	-0.1617	-2.6622	-0.1416
H	-0.1529	-2.7529	0.9508
H	0.8878	-2.7376	-0.4476
C	-0.8854	-3.8724	-0.6906
O	-0.2784	-5.0156	-0.2955
O	-1.8714	-3.8559	-1.3861
C	-0.8789	-6.2413	-0.7523
H	-1.9028	-6.3257	-0.3852
H	-0.8862	-6.2806	-1.8426
H	-0.2597	-7.0375	-0.3449
C	-0.6214	1.2164	-0.4364
H	-0.6062	1.3221	-1.5255
H	-1.6624	1.3068	-0.1109
H	-0.0664	2.0579	-0.0128

$CH_3CH_2CH_2CHCOOCH_3$

C	-4.0610	-2.3434	-0.0382
H	-4.7483	-1.9180	0.7001
H	-3.9045	-1.5708	-0.7994
C	-2.7141	-2.6586	0.6564
H	-2.8644	-3.4088	1.4366
H	-2.0404	-3.0965	-0.0951
C	-2.0667	-1.4605	1.2450
H	-1.7627	-0.6350	0.6104
C	-1.8406	-1.3287	2.6690
O	-1.2352	-0.1468	2.9750
O	-2.1426	-2.1547	3.5140
C	-0.9688	0.0737	4.3680
H	-1.8970	0.0714	4.9424
H	-0.3080	-0.7014	4.7607
H	-0.4886	1.0485	4.4225
C	-4.6891	-3.5830	-0.6795
H	-5.6409	-3.3380	-1.1583
H	-4.0319	-4.0106	-1.4431
H	-4.8817	-4.3596	0.0666

TS6-6

C	-4.1215	-2.3646	-0.2394
H	-5.0459	-1.8759	0.0897
H	-3.6726	-1.6980	-0.9857
C	-3.1713	-2.5048	0.9554
H	-3.6061	-3.1619	1.7145
H	-2.2456	-2.9989	0.6302
C	-2.8098	-1.1778	1.5928
H	-3.8754	-0.6564	1.9872
H	-2.4408	-0.4215	0.8986
C	-1.9746	-1.2506	2.8303
O	-1.3960	-0.0578	3.1003
O	-1.8455	-2.2270	3.5322
C	-0.6127	0.0036	4.3065
H	-1.2333	-0.2170	5.1762
H	0.2102	-0.7113	4.2638
H	-0.2336	1.0220	4.3547
H	-4.7926	-0.2489	2.2751
C	-4.4571	-3.7088	-0.8911
H	-5.1373	-3.5802	-1.7370
H	-3.5554	-4.2056	-1.2618
H	-4.9376	-4.3848	-0.1774

$CH_3CH_2CHCH_2COOCH_3$

C	-4.2445	-2.1814	-0.3414
H	-5.1532	-1.6325	-0.0492
H	-3.8541	-1.6223	-1.2104
C	-3.2526	-2.1425	0.7711
H	-2.6964	-3.0304	1.0474
C	-2.8984	-0.8553	1.4285
H	-3.7841	-0.3401	1.8282
H	-2.4754	-0.1327	0.7094
C	-1.8914	-0.9880	2.5542
O	-1.7291	0.1952	3.1875
O	-1.2945	-1.9899	2.8602
C	-0.7784	0.2083	4.2686
H	-1.0778	-0.4931	5.0485
H	0.2149	-0.0613	3.9070
H	-0.7843	1.2279	4.6478
C	-4.6199	-3.5992	-0.7854
H	-5.3393	-3.5790	-1.6081
H	-3.7374	-4.1486	-1.1254
H	-5.0660	-4.1624	0.0389

TS6-7

C	-4.2524	-2.1989	-0.2980
H	-5.1328	-1.5873	-0.0648
H	-3.7439	-1.6849	-1.1275
C	-3.3239	-2.2264	0.8979
H	-4.0311	-2.7552	1.8782
H	-2.5039	-2.9407	0.8132
C	-2.8768	-0.8808	1.4242
H	-3.7214	-0.2818	1.7767
H	-2.4141	-0.2936	0.6166
C	-1.8431	-0.9736	2.5287
O	-1.8098	0.1645	3.2544
O	-1.1162	-1.9141	2.7339
C	-0.8279	0.2143	4.3073
H	-1.0033	-0.5848	5.0286
H	0.1775	0.1123	3.8965
H	-0.9540	1.1881	4.7752
H	-4.5926	-3.0710	2.5954
C	-4.6944	-3.5913	-0.7579
H	-5.3518	-3.5279	-1.6288
H	-3.8326	-4.2065	-1.0332
H	-5.2372	-4.1140	0.0344

$CH_3CHCH_2CH_2COOCH_3$

C	-3.9613	-2.4837	-0.2673
H	-3.8884	-1.5961	-0.8891
C	-3.1272	-2.5661	0.9678
H	-3.6553	-3.1360	1.7429
H	-2.2108	-3.1495	0.7770
C	-2.7316	-1.1952	1.5199
H	-3.6189	-0.6005	1.7616
H	-2.1836	-0.6139	0.7701
C	-1.8717	-1.2679	2.7620
O	-1.5577	-0.0278	3.2014
O	-1.5007	-2.2766	3.3112
C	-0.7407	0.0366	4.3848
H	-1.2456	-0.4432	5.2245
H	0.2176	-0.4564	4.2151
H	-0.5962	1.0969	4.5805
C	-4.6407	-3.6914	-0.8156
H	-5.1627	-4.2519	-0.0304
H	-5.3671	-3.4344	-1.5905
H	-3.9237	-4.3971	-1.2683

TS6-8

C	-4.1014	-2.4083	-0.2303
H	-5.1747	-1.7540	0.1567
H	-3.7023	-1.7273	-0.9874
C	-3.2250	-2.5162	1.0003
H	-3.7520	-3.0711	1.7836
H	-2.3366	-3.1169	0.7643
C	-2.7844	-1.1562	1.5427
H	-3.6484	-0.5413	1.8146
H	-2.2446	-0.5837	0.7798
C	-1.8863	-1.2571	2.7563
O	-1.5638	-0.0288	3.2188
O	-1.4927	-2.2795	3.2628
C	-0.7056	0.0077	4.3743
H	-1.1768	-0.5015	5.2161
H	0.2499	-0.4714	4.1558
H	-0.5628	1.0629	4.5964
H	-5.9801	-1.3117	0.4669
C	-4.6125	-3.7089	-0.8091
H	-5.1299	-4.3046	-0.0511
H	-5.3064	-3.5348	-1.6354
H	-3.7845	-4.3169	-1.1947

$CH_2CH_2CH_2CH_2COOCH_3$

C	-4.0828	-2.3735	-0.2749
H	-3.5605	-1.7562	-1.0286
C	-3.1793	-2.5121	0.9588
H	-3.6932	-3.0986	1.7259
H	-2.2814	-3.0792	0.6956
C	-2.7713	-1.1584	1.5385
H	-3.6468	-0.5743	1.8421
H	-2.2589	-0.5468	0.7863
C	-1.8496	-1.2651	2.7341
O	-1.6023	-0.0441	3.2612
O	-1.3777	-2.2834	3.1772
C	-0.7215	-0.0134	4.3996
H	-1.1358	-0.6023	5.2191
H	0.2595	-0.4105	4.1347
H	-0.6468	1.0347	4.6808
C	-4.4759	-3.6769	-0.8788
H	-5.3239	-3.7461	-1.5492
H	-3.8529	-4.5557	-0.7578
H	-4.9825	-1.7970	-0.0187

TS6-9

C	-4.1083	-2.3951	-0.2391
H	-3.5623	-1.8527	-1.0262
C	-3.2139	-2.5221	1.0000
H	-3.7460	-3.0711	1.7829
H	-2.3300	-3.1204	0.7595
C	-2.7722	-1.1635	1.5431
H	-3.6309	-0.5530	1.8407
H	-2.2532	-0.5829	0.7706
C	-1.8359	-1.2624	2.7283
O	-1.6155	-0.0433	3.2707
O	-1.3302	-2.2740	3.1489
C	-0.7177	-0.0047	4.3956
H	-1.1006	-0.6199	5.2109
H	0.2706	-0.3667	4.1084
H	-0.6706	1.0404	4.6937
C	-4.5655	-3.7250	-0.7882
H	-5.3916	-4.2799	0.1481
H	-5.2246	-3.6793	-1.6544
H	-3.7934	-4.4877	-0.8917
H	-4.9836	-1.7752	-0.0075
H	-5.9643	-4.6187	0.7916

$CH_3CH_2CH_2CH_2COOCH_2$

C	-4.4393	-2.5071	-0.1156
H	-5.0587	-1.6020	-0.1358
H	-3.7324	-2.4102	-0.9488
C	-3.6643	-2.5637	1.2053
H	-4.3641	-2.6567	2.0421
H	-3.0430	-3.4648	1.2324
C	-2.7811	-1.3347	1.4202
H	-3.3753	-0.4134	1.4108
H	-2.0563	-1.2203	0.6057
C	-2.0096	-1.3652	2.7157
O	-1.2379	-0.2292	2.8359
O	-2.0286	-2.2264	3.5535
C	-0.4656	-0.0756	3.9490
H	-0.4780	-0.8428	4.7058
H	0.1054	0.8368	3.9647
C	-5.3252	-3.7357	-0.3403
H	-6.0655	-3.8408	0.4588
H	-5.8662	-3.6682	-1.2880
H	-4.7299	-4.6537	-0.3615

TS6-10

C	-4.4292	-2.5120	-0.1188
H	-5.0625	-1.6172	-0.1573
H	-3.7066	-2.4082	-0.9377
C	-3.6817	-2.5481	1.2186
H	-4.3972	-2.6451	2.0414
H	-3.0485	-3.4402	1.2650
C	-2.8209	-1.3050	1.4426
H	-3.4283	-0.3928	1.4092
H	-2.0762	-1.1867	0.6475
C	-2.0876	-1.3051	2.7621
O	-1.2843	-0.1990	2.8606
O	-2.1643	-2.1347	3.6292
C	-0.5635	-0.0263	4.0470
H	-0.2659	-0.9581	4.5223
H	0.2287	0.6966	3.8756
H	-1.3553	0.5524	4.9384
H	-1.9508	0.9809	5.5596
C	-5.2902	-3.7560	-0.3547
H	-6.0450	-3.8690	0.4296
H	-5.8126	-3.7024	-1.3137
H	-4.6799	-4.6644	-0.3586

$CH_3CH_2CH_2CH_2COOCH_2CH_3$(n=4,m=2)

$H + CH_3CH_2CH_2CH_2COOCH_2CH_3 \rightarrow H_2 + CH_3CH_2CH_2CHCOOCH_2CH_3$ (TS7-1)

$H + CH_3CH_2CH_2CH_2COOCH_2CH_3 \rightarrow H_2 + CH_3CH_2CHCH_2COOCH_2CH_3$ (TS7-2)

$H + CH_3CH_2CH_2CH_2COOCH_2CH_3 \rightarrow H_2 + CH_3CHCH_2CH_2COOCH_2CH_3$ (TS7-3)

$H + CH_3CH_2CH_2CH_2COOCH_2CH_3 \rightarrow H_2 + CH_2CH_2CH_2CH_2COOCH_2CH_3$ (TS7-4)

$H + CH_3CH_2CH_2CH_2COOCH_2CH_3 \rightarrow H_2 + CH_3CH_2CH_2CH_2COOCHCH_3$ (TS7-5)

$H + CH_3CH_2CH_2CH_2COOCH_2CH_3 \rightarrow H_2 + CH_3CH_2CH_2CH_2COOCH_2CH_2$ (TS7-6)

$CH_3CH_2CH_2CH_2COOCH_2CH_3$

C	-0.0284	-0.1128	0.0005
H	-0.0489	-0.1631	1.0962
H	1.0296	-0.1612	-0.2855
C	-0.7680	-1.3242	-0.5779
H	-1.8241	-1.2858	-0.2923
H	-0.7527	-1.2791	-1.6719
C	-0.1686	-2.6530	-0.1188
H	-0.1782	-2.7315	0.9747
H	0.8855	-2.7337	-0.4066
C	-0.8885	-3.8684	-0.6640
O	-0.2666	-5.0068	-0.2829
O	-1.8855	-3.8536	-1.3448
C	-0.8603	-6.2514	-0.7290
H	-1.8831	-6.3063	-0.3488
H	-0.9109	-6.2431	-1.8202
C	-0.6189	1.2233	-0.4588
H	-0.5812	1.3183	-1.5484
H	-1.6663	1.3176	-0.1557
H	-0.0720	2.0686	-0.0322
C	0.0013	-7.3834	-0.2081
H	0.0461	-7.3723	0.8832
H	-0.4196	-8.3417	-0.5245
H	1.0198	-7.3116	-0.5964

$CH_3CH_2CH_2CHCOOCH_2CH_3$

C	-0.1465	-0.2970	-0.2325
H	-0.5639	-0.6866	0.7016
H	0.9413	-0.2761	-0.1025
C	-0.5062	-1.2672	-1.3834
H	-1.5911	-1.3141	-1.5051
H	-0.0887	-0.8566	-2.3149
C	0.0239	-2.6379	-1.1790
H	1.0934	-2.8074	-1.1149
C	-0.8469	-3.7861	-1.0307
O	-0.1389	-4.9350	-0.8511
O	-2.0664	-3.7547	-1.0595
C	-0.9129	-6.1445	-0.6932
H	-1.5736	-6.0295	0.1700
H	-1.5437	-6.2763	-1.5761
C	-0.6665	1.1206	-0.4825
H	-0.2401	1.5442	-1.3972
H	-1.7553	1.1289	-0.5885
H	-0.4073	1.7862	0.3452
C	0.0595	-7.2928	-0.5139
H	0.6823	-7.1442	0.3712
H	-0.4935	-8.2280	-0.3913
H	0.7129	-7.3922	-1.3836

TS7-1

C	-0.0149	-0.1105	-0.2575
H	-0.1308	-0.1312	0.8323
H	1.0612	-0.1950	-0.4521
C	-0.7391	-1.3170	-0.8658
H	-1.8151	-1.2507	-0.6789
H	-0.6262	-1.2982	-1.9583
C	-0.2251	-2.6469	-0.3516
H	-0.4008	-2.6557	0.8861
H	0.8560	-2.7770	-0.4186
C	-0.9607	-3.8625	-0.8191
O	-0.2330	-4.9825	-0.6125
O	-2.0749	-3.8655	-1.2905
C	-0.8646	-6.2386	-0.9654
H	-1.7959	-6.3303	-0.4016
H	-1.1193	-6.2143	-2.0275
C	-0.5289	1.2252	-0.8013
H	-0.3947	1.2897	-1.8856
H	-1.5954	1.3526	-0.5922
H	0.0015	2.0680	-0.3502
C	0.1111	-7.3503	-0.6391
H	0.3573	-7.3562	0.4251
H	-0.3337	-8.3160	-0.8938
H	1.0371	-7.2390	-1.2078
H	-0.5420	-2.6063	1.9194

$CH_3CH_2CHCH_2COOCH_2CH_3$

C	-0.0032	-0.0542	-0.0864
H	0.0328	-0.1147	1.0124
H	1.0533	0.0551	-0.3899
C	-0.5605	-1.3203	-0.6428
H	-1.2713	-1.2986	-1.4603
C	-0.0430	-2.6407	-0.1923
H	-0.1199	-2.7609	0.8985
H	1.0371	-2.7461	-0.3933
C	-0.7249	-3.8319	-0.8387
O	-0.2822	-4.9851	-0.2928
O	-1.5431	-3.7854	-1.7238
C	-0.8365	-6.2123	-0.8303
H	-1.9212	-6.1898	-0.7030
H	-0.6273	-6.2493	-1.9019
C	-0.7768	1.1999	-0.5078
H	-0.7868	1.3056	-1.5964
H	-1.8150	1.1520	-0.1682
H	-0.3259	2.1028	-0.0880
C	-0.1999	-7.3677	-0.0856
H	-0.4149	-7.3111	0.9838
H	-0.5967	-8.3130	-0.4656
H	0.8840	-7.3720	-0.2207

TS7-2

C	-0.0454	-0.0761	-0.0757
H	0.1309	-0.1609	1.0038
H	0.9516	0.0039	-0.5347
C	-0.7124	-1.3379	-0.5812
H	-1.8446	-1.4293	0.0887
H	-1.0738	-1.2737	-1.6084
C	0.0115	-2.6349	-0.2953
H	0.1142	-2.8136	0.7788
H	1.0382	-2.5879	-0.6889
C	-0.6358	-3.8457	-0.9399
O	-0.2851	-4.9795	-0.2993
O	-1.3480	-3.8211	-1.9140
C	-0.7996	-6.2202	-0.8479
H	-1.8901	-6.1639	-0.8700
H	-0.4491	-6.3166	-1.8782
C	-0.8447	1.1962	-0.3727
H	-0.9993	1.3214	-1.4485
H	-1.8283	1.1635	0.1035
H	-0.3235	2.0835	-0.0045
C	-0.3046	-7.3501	0.0310
H	-0.6610	-7.2333	1.0569
H	-0.6748	-8.3040	-0.3541
H	0.7870	-7.3869	0.0460
H	-2.6273	-1.5140	0.6466

$CH_3CHCH_2CH_2COOCH_2CH_3$

C	-0.0145	-0.1232	-0.2281
H	1.0502	-0.2121	-0.0318
C	-0.7622	-1.3286	-0.6923
H	-1.7989	-1.2904	-0.3345
H	-0.8529	-1.3282	-1.7915
C	-0.1169	-2.6446	-0.2538
H	-0.0488	-2.7027	0.8376
H	0.9146	-2.7150	-0.6167
C	-0.8573	-3.8729	-0.7379
O	-0.2502	-5.0005	-0.3069
O	-1.8560	-3.8743	-1.4167
C	-0.8582	-6.2562	-0.7002
H	-1.8875	-6.2751	-0.3346
H	-0.8914	-6.3013	-1.7912
C	-0.6159	1.2370	-0.3229
H	-0.6758	1.5894	-1.3666
H	-1.6435	1.2509	0.0607
H	-0.0360	1.9792	0.2312
C	-0.0241	-7.3745	-0.1097
H	0.0027	-7.3101	0.9804
H	-0.4557	-8.3403	-0.3858
H	1.0017	-7.3381	-0.4834

TS7-3

C	-0.0268	-0.1177	-0.0522
H	-0.0789	-0.2058	1.2588
H	1.0524	-0.1702	-0.2227
C	-0.7749	-1.3281	-0.5710
H	-1.8130	-1.3004	-0.2237
H	-0.8324	-1.2793	-1.6666
C	-0.1303	-2.6517	-0.1583
H	-0.0791	-2.7412	0.9318
H	0.9068	-2.7112	-0.5070
C	-0.8613	-3.8672	-0.6881
O	-0.2560	-5.0049	-0.2853
O	-1.8514	-3.8487	-1.3792
C	-0.8557	-6.2505	-0.7226
H	-1.8865	-6.2860	-0.3628
H	-0.8832	-6.2598	-1.8146
C	-0.6169	1.2342	-0.3868
H	-0.5866	1.4164	-1.4684
H	-1.6632	1.2996	-0.0736
H	-0.0662	2.0434	0.0994
C	-0.0188	-7.3831	-0.1644
H	0.0026	-7.3538	0.9272
H	-0.4446	-8.3415	-0.4737
H	1.0084	-7.3300	-0.5319
H	-0.1644	-0.2588	2.2237

$CH_2CH_2CH_2CH_2COOCH_2CH_3$

C	0.0026	-0.1012	-0.0685
H	-0.0121	-0.1468	1.0294
H	1.0728	-0.1707	-0.3364
C	-0.7313	-1.3163	-0.6535
H	-1.7877	-1.2778	-0.3724
H	-0.7076	-1.2684	-1.7464
C	-0.1274	-2.6411	-0.1903
H	-0.1561	-2.7308	0.9013
H	0.9332	-2.7067	-0.4603
C	-0.8173	-3.8584	-0.7696
O	-0.2750	-4.9959	-0.2813
O	-1.7267	-3.8436	-1.5634
C	-0.8377	-6.2421	-0.7625
H	-1.9041	-6.2578	-0.5263
H	-0.7370	-6.2736	-1.8499
C	-0.5450	1.2065	-0.5248
H	-1.0770	1.2886	-1.4657
H	-0.3218	2.1206	0.0117
C	-0.0889	-7.3738	-0.0891
H	-0.1980	-7.3249	0.9967
H	-0.4871	-8.3330	-0.4309
H	0.9756	-7.3387	-0.3314

TS7-4

C	-0.0430	-0.1026	-0.0502
H	-0.0074	-0.1639	1.0448
H	1.0068	-0.1266	-0.3814
C	-0.7796	-1.3216	-0.6188
H	-1.8256	-1.3025	-0.2981
H	-0.7983	-1.2656	-1.7114
C	-0.1396	-2.6413	-0.1901
H	-0.1402	-2.7492	0.8999
H	0.9153	-2.6809	-0.4872
C	-0.8163	-3.8623	-0.7776
O	-0.2786	-4.9968	-0.2783
O	-1.7105	-3.8513	-1.5886
C	-0.8245	-6.2460	-0.7717
H	-1.8954	-6.2674	-0.5571
H	-0.7016	-6.2759	-1.8569
C	-0.6553	1.2147	-0.4608
H	-0.9030	1.3149	-1.5178
H	-1.8854	1.2842	0.1287
H	-0.1758	2.1066	-0.0592
C	-0.0833	-7.3739	-0.0838
H	-0.2145	-7.3263	0.9995
H	-0.4693	-8.3350	-0.4342
H	0.9857	-7.3329	-0.3046
H	-2.7042	1.3114	0.5609

$CH_3CH_2CH_2CH_2COOCHCH_3$

C	-0.0794	-0.1015	0.0450
H	-0.2514	-0.1634	1.1267
H	1.0078	-0.1516	-0.0930
C	-0.7357	-1.3030	-0.6438
H	-1.8211	-1.2612	-0.5083
H	-0.5663	-1.2486	-1.7243
C	-0.2122	-2.6391	-0.1173
H	-0.3796	-2.7295	0.9627
H	0.8726	-2.7201	-0.2506
C	-0.8480	-3.8399	-0.7759
O	-0.2963	-4.9982	-0.2867
O	-1.7161	-3.8304	-1.6091
C	-0.7740	-6.2093	-0.7340
H	-1.4538	-6.1761	-1.5728
C	-0.5974	1.2416	-0.4769
H	-0.4085	1.3479	-1.5496
H	-1.6764	1.3364	-0.3209
H	-0.1129	2.0800	0.0308
C	0.0038	-7.3896	-0.2970
H	0.1454	-7.3964	0.7894
H	-0.5167	-8.3059	-0.5823
H	1.0072	-7.4194	-0.7505

TS7-5

C	-0.0691	-0.1104	0.0365
H	-0.2309	-0.1566	1.1205
H	1.0159	-0.1767	-0.1118
C	-0.7484	-1.3115	-0.6305
H	-1.8319	-1.2526	-0.4854
H	-0.5884	-1.2738	-1.7130
C	-0.2392	-2.6475	-0.0900
H	-0.3974	-2.7225	0.9920
H	0.8430	-2.7470	-0.2327
C	-0.8964	-3.8503	-0.7257
O	-0.3786	-5.0049	-0.2084
O	-1.7523	-3.8354	-1.5716
C	-0.9095	-6.2302	-0.6672
H	-2.0215	-6.4111	-0.0388
H	-1.2208	-6.1703	-1.7096
C	-0.5747	1.2329	-0.4970
H	-0.3950	1.3238	-1.5727
H	-1.6508	1.3436	-0.3317
H	-0.0745	2.0709	-0.0042
C	-0.0001	-7.3692	-0.3015
H	0.1896	-7.3895	0.7742
H	-0.4612	-8.3168	-0.5902
H	0.9615	-7.2835	-0.8182
H	-2.8503	-6.5564	0.4956

$CH_3CH_2CH_2CH_2COOCH_2CH_2$

C	-0.0261	-0.1163	-0.0181
H	0.0086	-0.1877	1.0761
H	1.0172	-0.1387	-0.3567
C	-0.7708	-1.3307	-0.5837
H	-1.8128	-1.3160	-0.2480
H	-0.8077	-1.2669	-1.6760
C	-0.1277	-2.6560	-0.1761
H	-0.0875	-2.7574	0.9144
H	0.9142	-2.7098	-0.5117
C	-0.8438	-3.8737	-0.7196
O	-0.2278	-5.0106	-0.3203
O	-1.8307	-3.8649	-1.4146
C	-0.8135	-6.2541	-0.7762
H	-1.8365	-6.3333	-0.3927
H	-0.8982	-6.2106	-1.8724
C	-0.6633	1.2164	-0.4212
H	-0.6814	1.3327	-1.5093
H	-1.6959	1.2846	-0.0651
H	-0.1116	2.0638	-0.0054
C	0.0399	-7.3716	-0.3212
H	-0.3665	-8.3734	-0.2794
H	1.0989	-7.2208	-0.1605

TS7-6

C	-0.0345	-0.1099	-0.0131
H	-0.0338	-0.1624	1.0827
H	1.0185	-0.1445	-0.3190
C	-0.7696	-1.3293	-0.5801
H	-1.8206	-1.3043	-0.2748
H	-0.7749	-1.2825	-1.6741
C	-0.1454	-2.6512	-0.1339
H	-0.1355	-2.7334	0.9593
H	0.9046	-2.7178	-0.4397
C	-0.8578	-3.8734	-0.6707
O	-0.2227	-5.0067	-0.2884
O	-1.8578	-3.8736	-1.3462
C	-0.8138	-6.2520	-0.7232
H	-1.8386	-6.3145	-0.3466
H	-0.8713	-6.2502	-1.8182
C	-0.6503	1.2194	-0.4586
H	-0.6345	1.3167	-1.5486
H	-1.6927	1.3002	-0.1354
H	-0.1058	2.0706	-0.0409
C	0.0401	-7.3720	-0.2179
H	-0.0530	-7.3628	1.1567
H	-0.3357	-8.3639	-0.4628
H	1.1092	-7.2603	-0.3876
H	-0.1510	-7.3532	2.0662

$CH_3CH_2CH_2CH_2CH_2COOCH_3$(n=5,m=1)

$H + CH_3CH_2CH_2CH_2CH_2COOCH_3 \rightarrow H_2 + CH_3CH_2CH_2CH_2CHCOOCH_3$ (TS7-7)

$H + CH_3CH_2CH_2CH_2CH_2COOCH_3 \rightarrow H_2 + CH_3CH_2CH_2CHCH_2COOCH_3$ (TS7-8)

$H + CH_3CH_2CH_2CH_2CH_2COOCH_3 \rightarrow H_2 + CH_3CH_2CHCH_2CH_2COOCH_3$ (TS7-9)

$H + CH_3CH_2CH_2CH_2CH_2COOCH_3 \rightarrow H_2 + CH_3CHCH_2CH_2CH_2COOCH_3$ (TS7-10)

$H + CH_3CH_2CH_2CH_2CH_2COOCH_3 \rightarrow H_2 + CH_2CH_2CH_2CH_2CH_2COOCH_3$ (TS7-11)

$H + CH_3CH_2CH_2CH_2CH_2COOCH_3 \rightarrow H_2 + CH_3CH_2CH_2CH_2CH_2COOCH_2$ (TS7-12)

$CH_3CH_2CH_2CH_2CH_2COOCH_3$

C	-0.0290	-0.1187	-0.0080
H	-0.0279	-0.1770	1.0886
H	1.0247	-0.1599	-0.3143
C	-0.7763	-1.3266	-0.5830
H	-1.8269	-1.2942	-0.2773
H	-0.7812	-1.2740	-1.6766
C	-0.1646	-2.6572	-0.1451
H	-0.1546	-2.7462	0.9474
H	0.8847	-2.7312	-0.4520
C	-0.8867	-3.8695	-0.6915
O	-0.2771	-5.0111	-0.2954
O	-1.8737	-3.8559	-1.3857
C	-0.8761	-6.2385	-0.7496
H	-1.8991	-6.3245	-0.3802
H	-0.8856	-6.2791	-1.8398
H	-0.2546	-7.0330	-0.3425
C	-0.6251	1.2261	-0.4389
H	-0.6255	1.2853	-1.5340
H	-1.6772	1.2681	-0.1326
C	0.1234	2.4312	0.1376
H	0.1112	2.4184	1.2321
H	1.1708	2.4362	-0.1805
H	-0.3262	3.3734	-0.1877

$CH_3CH_2CH_2CH_2CHCOOCH_3$

C	-3.8410	-2.4085	-0.2197
H	-4.5762	-1.9293	0.4363
H	-3.5892	-1.6739	-0.9942
C	-2.5743	-2.7420	0.6050
H	-2.8226	-3.4563	1.3935
H	-1.8506	-3.2280	-0.0655
C	-1.9439	-1.5428	1.2099
H	-1.5362	-0.7606	0.5787
C	-1.8783	-1.3483	2.6431
O	-1.2656	-0.1741	2.9641
O	-2.3090	-2.1202	3.4835
C	-1.1542	0.1066	4.3672
H	-2.1419	0.1586	4.8290
H	-0.5694	-0.6665	4.8691
H	-0.6508	1.0690	4.4332
C	-4.4644	-3.6479	-0.8710
H	-3.7228	-4.1249	-1.5231
H	-4.7032	-4.3814	-0.0920
C	-5.7265	-3.3289	-1.6773
H	-5.5127	-2.6253	-2.4880
H	-6.1501	-4.2320	-2.1251
H	-6.4974	-2.8796	-1.0437

TS7-7

C	-4.1214	-2.3534	-0.2379
H	-5.0467	-1.8635	0.0902
H	-3.6722	-1.6872	-0.9858
C	-3.1718	-2.4970	0.9565
H	-3.6067	-3.1550	1.7146
H	-2.2459	-2.9904	0.6311
C	-2.8092	-1.1718	1.5974
H	-3.8739	-0.6510	1.9946
H	-2.4402	-0.4136	0.9053
C	-1.9728	-1.2497	2.8339
O	-1.3913	-0.0589	3.1067
O	-1.8448	-2.2283	3.5328
C	-0.6059	-0.0031	4.3119
H	-1.2257	-0.2253	5.1819
H	0.2152	-0.7197	4.2655
H	-0.2245	1.0143	4.3628
H	-4.7903	-0.2432	2.2849
C	-4.4651	-3.6938	-0.8972
H	-3.5392	-4.1831	-1.2228
H	-4.9126	-4.3584	-0.1486
C	-5.4152	-3.5531	-2.0897
H	-4.9802	-2.9210	-2.8701
H	-5.6396	-4.5250	-2.5371
H	-6.3645	-3.0994	-1.7882

$CH_3CH_2CH_2CHCH_2COOCH_3$

C	-4.2348	-2.1487	-0.3538
H	-5.1438	-1.5907	-0.0759
H	-3.8257	-1.5928	-1.2174
C	-3.2597	-2.1248	0.7735
H	-2.7260	-3.0222	1.0627
C	-2.8952	-0.8433	1.4363
H	-3.7774	-0.3205	1.8346
H	-2.4629	-0.1223	0.7214
C	-1.8954	-0.9896	2.5666
O	-1.7082	0.1950	3.1908
O	-1.3233	-2.0024	2.8841
C	-0.7627	0.1948	4.2765
H	-1.0833	-0.4916	5.0615
H	0.2253	-0.1028	3.9226
H	-0.7451	1.2177	4.6460
C	-4.6247	-3.5599	-0.8134
H	-3.7165	-4.1049	-1.0952
H	-5.0573	-4.1034	0.0339
C	-5.6097	-3.5614	-1.9848
H	-5.8654	-4.5803	-2.2880
H	-6.5413	-3.0508	-1.7208
H	-5.1892	-3.0512	-2.8574

TS7-8

C	-4.2556	-2.1884	-0.2925
H	-5.1391	-1.5793	-0.0601
H	-3.7469	-1.6702	-1.1207
C	-3.3295	-2.2211	0.9046
H	-4.0378	-2.7497	1.8837
H	-2.5104	-2.9363	0.8198
C	-2.8800	-0.8775	1.4343
H	-3.7231	-0.2789	1.7915
H	-2.4197	-0.2876	0.6273
C	-1.8429	-0.9743	2.5352
O	-1.8014	0.1643	3.2596
O	-1.1196	-1.9181	2.7387
C	-0.8150	0.2106	4.3084
H	-0.9911	-0.5867	5.0314
H	0.1882	0.1033	3.8935
H	-0.9344	1.1856	4.7756
H	-4.5999	-3.0657	2.6002
C	-4.7001	-3.5769	-0.7686
H	-3.8120	-4.1771	-0.9982
H	-5.2126	-4.0905	0.0523
C	-5.6162	-3.5250	-1.9941
H	-5.9149	-4.5282	-2.3091
H	-6.5285	-2.9585	-1.7830
H	-5.1177	-3.0453	-2.8423

$CH_3CH_2CHCH_2CH_2COOCH_3$

C	-3.9270	-2.5126	-0.2892
H	-3.8411	-1.6324	-0.9223
C	-3.1103	-2.5841	0.9582
H	-3.6501	-3.1431	1.7328
H	-2.1929	-3.1718	0.7865
C	-2.7180	-1.2081	1.5003
H	-3.6071	-0.6059	1.7158
H	-2.1513	-0.6391	0.7554
C	-1.8874	-1.2695	2.7629
O	-1.5516	-0.0264	3.1771
O	-1.5558	-2.2721	3.3472
C	-0.7638	0.0491	4.3794
H	-1.3046	-0.3902	5.2190
H	0.1832	-0.4768	4.2498
H	-0.5924	1.1100	4.5481
C	-4.5974	-3.7238	-0.8470
H	-5.0745	-4.2861	-0.0323
H	-3.8378	-4.4148	-1.2554
C	-5.6272	-3.4182	-1.9411
H	-5.1634	-2.8908	-2.7802
H	-6.0742	-4.3363	-2.3314
H	-6.4333	-2.7876	-1.5559

TS7-9

C	-4.1244	-2.3942	-0.2147
H	-5.1925	-1.7373	0.1941
H	-3.7314	-1.7136	-0.9768
C	-3.2346	-2.5084	1.0057
H	-3.7519	-3.0679	1.7921
H	-2.3472	-3.1052	0.7574
C	-2.7911	-1.1503	1.5510
H	-3.6527	-0.5401	1.8398
H	-2.2644	-0.5712	0.7838
C	-1.8734	-1.2564	2.7494
O	-1.5655	-0.0307	3.2289
O	-1.4536	-2.2801	3.2315
C	-0.6886	0.0007	4.3705
H	-1.1349	-0.5348	5.2095
H	0.2726	-0.4540	4.1265
H	-0.5637	1.0541	4.6113
H	-5.9844	-1.3010	0.5422
C	-4.6552	-3.6897	-0.7938
H	-5.1985	-4.2374	-0.0144
H	-3.8019	-4.3285	-1.0660
C	-5.5558	-3.4939	-2.0169
H	-5.0195	-2.9867	-2.8248
H	-5.9094	-4.4531	-2.4037
H	-6.4327	-2.8895	-1.7685

$CH_3CH_2CHCH_2CH_2COOCH_3$

C	-4.0542	-2.3480	-0.3059
H	-3.5228	-1.7294	-1.0538
C	-3.1653	-2.4982	0.9356
H	-3.6907	-3.0860	1.6941
H	-2.2672	-3.0683	0.6801
C	-2.7562	-1.1503	1.5282
H	-3.6318	-0.5621	1.8234
H	-2.2303	-0.5381	0.7859
C	-1.8506	-1.2682	2.7347
O	-1.6095	-0.0519	3.2763
O	-1.3847	-2.2905	3.1754
C	-0.7438	-0.0322	4.4262
H	-1.1686	-0.6289	5.2347
H	0.2407	-0.4268	4.1705
H	-0.6727	1.0132	4.7184
C	-4.4603	-3.6461	-0.9203
H	-3.8428	-4.5207	-0.7394
H	-4.9531	-1.7649	-0.0535
C	-5.5108	-3.7065	-1.9755
H	-5.8182	-4.7333	-2.1876
H	-6.4040	-3.1363	-1.6895
H	-5.1647	-3.2706	-2.9282

TS7-10

C	-4.1208	-2.3939	-0.2332
H	-3.5781	-1.8573	-1.0273
C	-3.2194	-2.5226	0.9997
H	-3.7456	-3.0742	1.7849
H	-2.3346	-3.1169	0.7538
C	-2.7784	-1.1638	1.5438
H	-3.6356	-0.5590	1.8557
H	-2.2724	-0.5780	0.7662
C	-1.8219	-1.2627	2.7128
O	-1.6447	-0.0543	3.2939
O	-1.2662	-2.2650	3.0904
C	-0.7281	-0.0148	4.4035
H	-1.0684	-0.6737	5.2035
H	0.2693	-0.3229	4.0866
H	-0.7207	1.0206	4.7372
C	-4.5963	-3.7234	-0.7827
H	-5.3467	-4.2429	0.1637
H	-3.7990	-4.4679	-0.8538
H	-4.9930	-1.7698	0.0026
H	-5.9424	-4.5880	0.8452
C	-5.4810	-3.6737	-2.0088
H	-5.8502	-4.6667	-2.2778
H	-6.3463	-3.0231	-1.8485
H	-4.9304	-3.2806	-2.8729

$CH_2CH_2CH_2CH_2CH_2COOCH_3$

C	-4.0768	-2.4081	-0.2611
H	-3.5364	-1.8578	-1.0419
C	-3.1953	-2.5305	0.9856
H	-3.7288	-3.0830	1.7658
H	-2.3043	-3.1234	0.7554
C	-2.7672	-1.1702	1.5357
H	-3.6371	-0.5569	1.7960
H	-2.2196	-0.5933	0.7818
C	-1.8888	-1.2619	2.7647
O	-1.5510	-0.0290	3.2075
O	-1.5213	-2.2790	3.3002
C	-0.7105	0.0155	4.3753
H	-1.2038	-0.4675	5.2201
H	0.2391	-0.4856	4.1820
H	-0.5511	1.0722	4.5783
C	-4.5167	-3.7682	-0.8247
H	-3.6121	-4.3705	-1.0250
H	-4.9683	-1.8132	-0.0287
C	-5.3424	-3.6718	-2.0603
H	-5.9883	-4.4861	-2.3656
H	-5.2159	-2.8435	-2.7485
H	-5.0614	-4.3299	-0.0545

TS7-11

C	-4.1100	-2.3866	-0.2442
H	-3.5734	-1.8385	-1.0293
C	-3.2169	-2.5165	0.9936
H	-3.7473	-3.0661	1.7779
H	-2.3321	-3.1152	0.7548
C	-2.7740	-1.1601	1.5417
H	-3.6362	-0.5422	1.8158
H	-2.2332	-0.5846	0.7815
C	-1.8767	-1.2613	2.7562
O	-1.5548	-0.0322	3.2204
O	-1.4821	-2.2828	3.2635
C	-0.6954	0.0030	4.3748
H	-1.1646	-0.5086	5.2164
H	0.2604	-0.4745	4.1543
H	-0.5535	1.0579	4.5990
C	-4.5654	-3.7412	-0.8016
H	-3.6786	-4.3453	-1.0465
H	-4.9939	-1.7846	-0.0010
C	-5.4382	-3.6305	-2.0282
H	-5.8170	-4.5701	-2.4291
H	-6.5969	-3.0179	-1.6398
H	-5.0785	-2.9606	-2.8099
H	-5.0965	-4.3011	-0.0221
H	-7.3779	-2.6183	-1.3430

$CH_3CH_2CH_2CH_2CH_2COOCH_2$

C	-4.3676	-2.5839	-0.1677
H	-4.8251	-1.5892	-0.2507
H	-3.6568	-2.6612	-1.0010
C	-3.6109	-2.6900	1.1607
H	-4.3138	-2.6112	1.9962
H	-3.1509	-3.6796	1.2479
C	-2.5312	-1.6182	1.3081
H	-2.9604	-0.6114	1.2442
H	-1.8021	-1.6749	0.4914
C	-1.7685	-1.7070	2.6064
O	-0.8122	-0.7159	2.6650
O	-1.9296	-2.5040	3.4914
C	-0.0191	-0.6345	3.7713
H	-0.1445	-1.3576	4.5606
H	0.7121	0.1544	3.7299
C	-5.4540	-3.6523	-0.3330
H	-6.1658	-3.5735	0.4974
H	-4.9977	-4.6458	-0.2482
C	-6.2067	-3.5475	-1.6625
H	-6.9759	-4.3200	-1.7474
H	-6.7002	-2.5756	-1.7627
H	-5.5268	-3.6617	-2.5127

TS7-12

C	-4.4235	-2.5037	-0.1201
H	-5.0578	-1.6082	-0.1579
H	-3.7017	-2.3987	-0.9409
C	-3.6766	-2.5437	1.2172
H	-4.3916	-2.6420	2.0401
H	-3.0430	-3.4355	1.2621
C	-2.8155	-1.3013	1.4447
H	-3.4223	-0.3887	1.4110
H	-2.0687	-1.1822	0.6518
C	-2.0862	-1.3036	2.7664
O	-1.2786	-0.2008	2.8670
O	-2.1692	-2.1323	3.6338
C	-0.5614	-0.0304	4.0559
H	-0.2694	-0.9632	4.5328
H	0.2344	0.6892	3.8870
H	-1.3541	0.5520	4.9441
H	-1.9501	0.9831	5.5632
C	-5.2893	-3.7441	-0.3680
H	-6.0088	-3.8504	0.4527
H	-4.6554	-4.6383	-0.3331
C	-6.0387	-3.7007	-1.7026
H	-6.6458	-4.5982	-1.8481
H	-6.7076	-2.8359	-1.7530
H	-5.3435	-3.6301	-2.5450

C_9H_{22}

H+CH3(CH2)7CH3→H_2+$CH_3(CH_2)_3CH(CH_2)_3CH_3$ (TS9-1)

$CH_3(CH_2)_7CH_3$

C	-0.0355	-0.0737	-0.0131
H	-0.0338	-0.1416	1.0827
H	1.0174	-0.1233	-0.3207
C	-0.7891	-1.2757	-0.5932
H	-1.8415	-1.2256	-0.2848
H	-0.7907	-1.2069	-1.6889
C	-0.2049	-2.6296	-0.1740
H	-0.2018	-2.6986	0.9218
H	0.8474	-2.6810	-0.4834
C	-0.6186	1.2808	-0.4321
H	-0.6202	1.3494	-1.5269
H	-1.6701	1.3312	-0.1239
C	0.1412	2.4754	0.1521
H	0.1312	2.4535	1.2465
H	1.1882	2.4729	-0.1677
H	-0.2999	3.4248	-0.1645
C	-0.9602	-3.8315	-0.7528
H	-2.0122	-3.7807	-0.4425
H	-0.9640	-3.7625	-1.8486
C	-0.3757	-5.1853	-0.3346
H	-0.3695	-5.2545	0.7613
H	0.6758	-5.2382	-0.6470
C	-1.1324	-6.3878	-0.9100
H	-2.1824	-6.3365	-0.5964
H	-1.1395	-6.3192	-2.0049
C	-0.5402	-7.7356	-0.4880
H	-0.5497	-7.8483	0.6010
H	-1.1037	-8.5713	-0.9129
H	0.4986	-7.8328	-0.8203

$CH_3(CH_2)_3CH(CH_2)_3CH_3$

C	-0.0172	-0.1166	-0.0643
H	0.0128	-0.3176	1.0135
H	1.0255	-0.1293	-0.4067
C	-0.7889	-1.2444	-0.7636
H	-1.8382	-1.2329	-0.4327
H	-0.8362	-1.0204	-1.8460
C	-0.2135	-2.6052	-0.5515
C	-0.6120	1.2748	-0.3060
H	-0.6435	1.4719	-1.3847
H	-1.6545	1.2854	0.0350
C	0.1642	2.3940	0.3942
H	0.1848	2.2428	1.4781
H	1.2016	2.4329	0.0470
H	-0.2859	3.3724	0.2042
C	-0.9614	-3.8408	-0.9282
H	-2.0068	-3.7537	-0.5963
H	-1.0248	-3.9210	-2.0298
C	-0.3543	-5.1389	-0.3779
H	-0.3118	-5.0789	0.7165
H	0.6853	-5.2221	-0.7197
C	-1.1242	-6.3983	-0.7891
H	-2.1637	-6.3125	-0.4494
H	-1.1665	-6.4546	-1.8838
C	-0.5127	-7.6886	-0.2356
H	-0.4875	-7.6766	0.8587
H	-1.0856	-8.5674	-0.5446
H	0.5152	-7.8219	-0.5875
H	0.8473	-2.6898	-0.3269

TS9-1

C	-0.0248	-0.0856	-0.0056
H	-0.0069	-0.1728	1.0876
H	1.0208	-0.1485	-0.3341
C	-0.8090	-1.2651	-0.5929
H	-1.8574	-1.2070	-0.2724
H	-0.8284	-1.1754	-1.6903
C	-0.2474	-2.6234	-0.2256
H	-0.3615	-2.6994	1.0855
C	-0.5951	1.2824	-0.3958
H	-0.6160	1.3671	-1.4893
H	-1.6394	1.3448	-0.0664
C	0.1950	2.4555	0.1914
H	0.2055	2.4170	1.2852
H	1.2353	2.4419	-0.1491
H	-0.2377	3.4158	-0.1027
C	-0.9798	-3.8391	-0.7554
H	-2.0284	-3.7997	-0.4327
H	-1.0052	-3.7858	-1.8550
C	-0.3601	-5.1756	-0.3301
H	-0.3291	-5.2263	0.7650
H	0.6840	-5.2126	-0.6672
C	-1.1098	-6.3971	-0.8731
H	-2.1528	-6.3584	-0.5357
H	-1.1428	-6.3440	-1.9683
C	-0.4853	-7.7283	-0.4455
H	-0.4687	-7.8251	0.6447
H	-1.0444	-8.5787	-0.8456
H	0.5468	-7.8135	-0.7999
H	-0.5144	-2.7503	2.0398
H	0.8380	-2.6872	-0.3513

$CH_3(CH_2)_8COOCH_3$(n=9,m=1)

$H + CH_3(CH_2)_8COOCH_3 \rightarrow H_2 + CH_3(CH_2)_7CHCOOCH_3$ (TS11-1)

$H + CH_3(CH_2)_8COOCH_3 \rightarrow H_2 + CH_3(CH_2)_6CHCH_2COOCH_3$ (TS11-2)

$H + CH_3(CH_2)_8COOCH_3 \rightarrow H_2 + CH_3(CH_2)_5CH(CH_2)_2COOCH_3$ (TS11-3)

$H + CH_3(CH_2)_8COOCH_3 \rightarrow H_2 + CH_3(CH_2)_4CH(CH_2)_3COOCH_3$ (TS11-4)

$H + CH_3(CH_2)_8COOCH_3 \rightarrow H_2 + CH_3(CH_2)_3CH(CH_2)_4COOCH_3$ (TS11-5)

$H + CH_3(CH_2)_8COOCH_3 \rightarrow H_2 + CH_3(CH_2)_2CH(CH_2)_5COOCH_3$ (TS11-6)

$H + CH_3(CH_2)_8COOCH_3 \rightarrow H_2 + CH_3CH_2CH(CH_2)_6COOCH_3$ (TS11-7)

$H + CH_3(CH_2)_8COOCH_3 \rightarrow H_2 + CH_3CH(CH_2)_7COOCH_3$ (TS11-8)

$H + CH_3(CH_2)_8COOCH_3 \rightarrow H_2 + CH_2(CH_2)_8COOCH_3$ (TS11-9)

$H + CH_3(CH_2)_8COOCH_3 \rightarrow H_2 + CH_3(CH_2)_8COOCH_2$ (TS11-10)

$CH_3(CH_2)_8COOCH_3$

C	0.0533	-0.1229	-0.1994
H	0.1304	-0.2285	0.8908
H	1.0839	-0.1291	-0.5780
C	-0.7089	-1.3215	-0.7748
H	-1.7389	-1.3195	-0.4035
H	-0.7831	-1.2284	-1.8629
C	-0.0506	-2.6562	-0.4259
H	0.0276	-2.7879	0.6590
H	0.9796	-2.6970	-0.7985
C	-0.7799	-3.8600	-0.9815
O	-0.1781	-5.0082	-0.5929
O	-1.7638	-3.8352	-1.6798
C	-0.7785	-6.2283	-1.0648
H	-1.8066	-6.3110	-0.7094
H	-0.7740	-6.2601	-2.1553
H	-0.1669	-7.0299	-0.6563
C	-0.5971	1.2253	-0.5296
H	-0.6720	1.3334	-1.6192
H	-1.6280	1.2299	-0.1532
C	0.1578	2.4276	0.0482
H	0.2356	2.3158	1.1375
H	1.1880	2.4249	-0.3311
C	-0.4954	3.7763	-0.2748
H	-0.5707	3.8903	-1.3640
H	-1.5265	3.7774	0.1019

C	0.2560	4.9783	0.3081
H	0.3329	4.8636	1.3974
H	1.2869	4.9795	-0.0697
C	-0.3980	6.3277	-0.0106
H	-0.4726	6.4439	-1.0988
H	-1.4283	6.3264	0.3656
C	0.3582	7.5219	0.5788
H	-0.1333	8.4675	0.3335
H	0.4187	7.4525	1.6696
H	1.3821	7.5707	0.1945

$CH_3(CH_2)_7CHCOOCH_3$

C	0.0641	-0.0722	-0.6020
H	-0.0676	-0.2409	0.4725
H	1.1454	-0.0310	-0.7800
C	-0.5380	-1.2697	-1.3754
H	-1.6120	-1.3354	-1.1857
H	-0.4055	-1.0799	-2.4509
C	0.1007	-2.5639	-1.0317
H	1.1578	-2.7195	-1.2184
C	-0.6371	-3.6477	-0.4181
O	0.1562	-4.7328	-0.1929
O	-1.8215	-3.6237	-0.1273
C	-0.4910	-5.8622	0.4118
H	-0.8927	-5.5969	1.3915
H	-1.3060	-6.2219	-0.2190
H	0.2808	-6.6231	0.5091
C	-0.5735	1.2645	-0.9956
H	-0.4458	1.4231	-2.0743
H	-1.6553	1.2133	-0.8209
C	0.0072	2.4618	-0.2347
H	-0.1165	2.2993	0.8437
H	1.0893	2.5137	-0.4119
C	-0.6331	3.8003	-0.6205
H	-0.5107	3.9625	-1.6993
H	-1.7149	3.7476	-0.4425
C	-0.0544	4.9994	0.1390
H	-0.1757	4.8375	1.2181
H	1.0276	5.0538	-0.0393
C	-0.6956	6.3381	-0.2443
H	-0.5743	6.5002	-1.3223
H	-1.7764	6.2841	-0.0656
C	-0.1119	7.5304	0.5193
H	-0.5904	8.4680	0.2232
H	-0.2494	7.4143	1.5991
H	0.9619	7.6325	0.3329

TS11-1

C	-0.0552	-0.1224	-0.3148
H	-0.0919	-0.1762	0.7803
H	1.0067	-0.1742	-0.5875
C	-0.7941	-1.3281	-0.9066
H	-1.8521	-1.3032	-0.6295
H	-0.7728	-1.2682	-2.0033
C	-0.2005	-2.6587	-0.4883
H	-0.2650	-2.7166	0.7587
H	0.8733	-2.7537	-0.6554
C	-0.9411	-3.8780	-0.9343
O	-0.1600	-4.9801	-0.8539
O	-2.0961	-3.9058	-1.2916
C	-0.7904	-6.2261	-1.2034
H	-1.6341	-6.4258	-0.5412
H	-1.1441	-6.1989	-2.2350
H	-0.0204	-6.9847	-1.0821
C	-0.6306	1.2208	-0.7771
H	-0.5910	1.2730	-1.8728
H	-1.6937	1.2699	-0.5093
C	0.0972	2.4334	-0.1864
H	0.0508	2.3849	0.9092
H	1.1621	2.3787	-0.4475
C	-0.4692	3.7777	-0.6574
H	-0.4226	3.8252	-1.7532
H	-1.5341	3.8328	-0.3967
C	0.2584	4.9911	-0.0683
H	0.2097	4.9464	1.0276
H	1.3242	4.9350	-0.3264
C	-0.3037	6.3362	-0.5425
H	-0.2552	6.3812	-1.6374
H	-1.3680	6.3933	-0.2836
C	0.4306	7.5424	0.0502
H	0.0064	8.4847	-0.3076
H	0.3694	7.5447	1.1432
H	1.4913	7.5318	-0.2203
H	-0.3128	-2.7091	1.8020

$CH_3(CH_2)_6CHCH_2COOCH_3$

C	-4.2294	-2.1083	-0.3428
H	-5.1211	-1.5135	-0.0877
H	-3.7818	-1.5767	-1.2027
C	-3.2752	-2.1096	0.8027
C	-2.9020	-0.8389	1.4816
H	-3.7809	-0.3126	1.8823
H	-2.4604	-0.1141	0.7763
C	-1.9073	-1.0065	2.6134
O	-1.7187	0.1674	3.2570
O	-1.3393	-2.0259	2.9168
C	-0.7755	0.1475	4.3446
H	-1.0990	-0.5510	5.1175
H	0.2127	-0.1462	3.9878
H	-0.7566	1.1642	4.7308
C	-4.6620	-3.5088	-0.7969
H	-3.7681	-4.0950	-1.0430
H	-5.1438	-4.0240	0.0427
C	-5.6089	-3.4947	-2.0012
H	-6.4993	-2.9009	-1.7566
H	-5.1212	-2.9790	-2.8387
C	-6.0442	-4.8928	-2.4546
H	-5.1535	-5.4892	-2.6913
H	-6.5393	-5.4060	-1.6200
C	-6.9809	-4.8810	-3.6677
H	-6.4856	-4.3678	-4.5025
H	-7.8724	-4.2850	-3.4322
C	-7.4160	-6.2784	-4.1238
H	-7.9144	-6.7903	-3.2916
H	-6.5253	-6.8747	-4.3567
C	-8.3471	-6.2561	-5.3396
H	-7.8637	-5.7810	-6.1992
H	-8.6382	-7.2667	-5.6395
H	-9.2633	-5.6965	-5.1259
H	-2.7520	-3.0152	1.0850

TS11-2

C	-4.2553	-2.1752	-0.2645
H	-5.1370	-1.5657	-0.0270
H	-3.7498	-1.6561	-1.0940
C	-3.3230	-2.2085	0.9279
H	-4.0253	-2.7384	1.9108
H	-2.5039	-2.9231	0.8380
C	-2.8713	-0.8651	1.4562
H	-3.7119	-0.2690	1.8230
H	-2.4202	-0.2727	0.6459
C	-1.8228	-0.9619	2.5462
O	-1.7793	0.1737	3.2755
O	-1.0928	-1.9030	2.7381
C	-0.7820	0.2199	4.3140
H	-0.9467	-0.5815	5.0353
H	0.2172	0.1192	3.8881
H	-0.9011	1.1922	4.7869
H	-4.5827	-3.0553	2.6305
C	-4.7014	-3.5636	-0.7385
H	-3.8138	-4.1660	-0.9687
H	-5.2144	-4.0771	0.0833
C	-5.6189	-3.5210	-1.9652
H	-6.5061	-2.9174	-1.7338
H	-5.1043	-3.0025	-2.7848
C	-6.0629	-4.9074	-2.4454
H	-5.1754	-5.5123	-2.6718
H	-6.5814	-5.4242	-1.6276
C	-6.9746	-4.8677	-3.6768
H	-6.4570	-4.3488	-4.4943
H	-7.8639	-4.2649	-3.4507
C	-7.4161	-6.2536	-4.1609
H	-7.9355	-6.7717	-3.3455
H	-6.5276	-6.8563	-4.3857
C	-8.3240	-6.2039	-5.3933
H	-7.8196	-5.7224	-6.2371
H	-8.6203	-7.2070	-5.7127
H	-9.2380	-5.6373	-5.1887

$CH_3(CH_2)_5CH(CH_2)_2COOCH_3$

C	-0.4445	-0.1084	-0.0996
C	-1.0061	-1.3527	-0.7032
H	-2.0579	-1.4892	-0.4008
H	-1.0475	-1.2581	-1.7956
C	-0.2211	-2.6113	-0.3281
H	-0.1844	-2.7415	0.7590
H	0.8228	-2.5316	-0.6496
C	-0.7914	-3.8798	-0.9230
O	-0.0623	-4.9559	-0.5487
O	-1.7608	-3.9558	-1.6380
C	-0.5071	-6.2283	-1.0543
H	-1.5225	-6.4398	-0.7160
H	-0.4851	-6.2354	-2.1450
H	0.1903	-6.9601	-0.6527
C	-0.9069	1.2419	-0.5353
H	-0.9574	1.2769	-1.6335
H	-1.9489	1.4060	-0.2032
C	-0.0399	2.4002	-0.0220
H	0.0007	2.3590	1.0738
H	0.9898	2.2583	-0.3718
C	-0.5423	3.7801	-0.4595
H	-0.5880	3.8174	-1.5557
H	-1.5730	3.9186	-0.1081
C	0.3242	4.9377	0.0486
H	0.3696	4.9025	1.1451
H	1.3554	4.7994	-0.3017
C	-0.1750	6.3191	-0.3901
H	-0.2206	6.3544	-1.4854
H	-1.2049	6.4585	-0.0392
C	0.6975	7.4693	0.1211
H	0.3149	8.4391	-0.2093
H	0.7339	7.4821	1.2151
H	1.7261	7.3771	-0.2419
H	0.1332	-0.1861	0.8186

TS11-3

C	-0.0790	-0.1230	-0.2885
H	-0.1717	-0.1986	1.0247
H	1.0056	-0.1665	-0.4302
C	-0.8013	-1.3487	-0.8087
H	-1.8485	-1.3283	-0.4896
H	-0.8291	-1.3182	-1.9059
C	-0.1533	-2.6580	-0.3573
H	-0.1319	-2.7300	0.7352
H	0.8938	-2.7108	-0.6756
C	-0.8548	-3.8896	-0.8870
O	-0.2420	-5.0144	-0.4550
O	-1.8288	-3.8989	-1.5997
C	-0.8199	-6.2584	-0.8925
H	-1.8496	-6.3450	-0.5427
H	-0.8052	-6.3248	-1.9813
H	-0.1999	-7.0367	-0.4530
C	-0.6712	1.2226	-0.6535
H	-0.7138	1.3034	-1.7506
H	-1.7137	1.2647	-0.3129
C	0.1058	2.4185	-0.0898
H	0.1461	2.3394	1.0032
H	1.1452	2.3687	-0.4387
C	-0.4949	3.7734	-0.4802
H	-0.5411	3.8477	-1.5745
H	-1.5335	3.8234	-0.1285
C	0.2843	4.9708	0.0747
H	0.3306	4.8973	1.1690
H	1.3235	4.9210	-0.2764
C	-0.3133	6.3278	-0.3141
H	-0.3610	6.4010	-1.4075
H	-1.3506	6.3793	0.0389
C	0.4738	7.5178	0.2425
H	0.0213	8.4692	-0.0509
H	0.5105	7.4911	1.3362
H	1.5060	7.5148	-0.1222
H	-0.3051	-0.2588	1.9819

$CH_3(CH_2)_4CH(CH_2)_3COOCH_3$

C	-0.0484	-0.1822	0.2701
H	-0.0749	-0.3764	1.3590
H	1.0214	-0.1978	0.0123
C	-0.7736	-1.3247	-0.4537
H	-1.8356	-1.3126	-0.1903
H	-0.7287	-1.1623	-1.5345
C	-0.1844	-2.6941	-0.1184
H	-0.2198	-2.8849	0.9607
H	0.8760	-2.7476	-0.3885
C	-0.8909	-3.8442	-0.8024
O	-0.2837	-5.0193	-0.5163
O	-1.8659	-3.7604	-1.5083
C	-0.8720	-6.1946	-1.1031
H	-1.9013	-6.3177	-0.7628
H	-0.8618	-6.1247	-2.1918
H	-0.2562	-7.0261	-0.7674
C	-0.6111	1.1701	-0.0170
C	0.1040	2.4159	0.3876
H	0.1106	2.5044	1.4901
H	1.1662	2.3372	0.1106
C	-0.4870	3.7030	-0.2044
H	-0.4750	3.6316	-1.2987
H	-1.5426	3.7784	0.0856
C	0.2517	4.9720	0.2324
H	0.2412	5.0396	1.3283
H	1.3083	4.8939	-0.0560
C	-0.3357	6.2595	-0.3568
H	-0.3278	6.1910	-1.4514
H	-1.3900	6.3411	-0.0656
C	0.4130	7.5220	0.0803
H	-0.0292	8.4211	-0.3578
H	0.3916	7.6381	1.1686
H	1.4631	7.4851	-0.2266
H	-1.6482	1.2435	-0.3346

TS11-4

C	0.0016	-0.1599	0.0277
H	-0.0079	-0.2348	1.1231
H	1.0621	-0.2126	-0.2647
C	-0.7524	-1.3464	-0.5838
H	-1.8100	-1.2936	-0.3084
H	-0.7212	-1.2824	-1.6756
C	-0.1788	-2.6918	-0.1403
H	-0.2357	-2.8110	0.9469
H	0.8873	-2.7646	-0.3869
C	-0.8656	-3.8819	-0.7746
O	-0.4009	-5.0399	-0.2521
O	-1.7089	-3.8378	-1.6365
C	-0.9673	-6.2491	-0.7902
H	-2.0448	-6.2744	-0.6214
H	-0.7717	-6.3194	-1.8612
H	-0.4774	-7.0613	-0.2576
C	-0.5519	1.1886	-0.3857
H	-0.7647	1.2549	-1.4570
H	-1.7654	1.2297	0.1259
C	0.1485	2.4161	0.1599
H	0.1645	2.3685	1.2566
H	1.2035	2.3904	-0.1543
C	-0.4780	3.7418	-0.2894
H	-0.4863	3.7819	-1.3861
H	-1.5281	3.7685	0.0251
C	0.2481	4.9758	0.2567
H	0.2564	4.9359	1.3538
H	1.3003	4.9466	-0.0558
C	-0.3742	6.3025	-0.1935
H	-0.3838	6.3425	-1.2896
H	-1.4246	6.3321	0.1203
C	0.3569	7.5312	0.3552
H	-0.1120	8.4594	0.0169
H	0.3534	7.5375	1.4498
H	1.4016	7.5489	0.0287
H	-2.6247	1.2521	0.5707

$CH_3(CH_2)_3CH(CH_2)_4COOCH_3$

C	-0.0260	-0.0919	-0.2922
H	-0.0379	-0.0568	0.8040
H	1.0298	-0.1577	-0.5847
C	-0.7715	-1.3394	-0.7766
H	-1.8259	-1.2784	-0.4889
H	-0.7617	-1.3775	-1.8708
C	-0.1727	-2.6318	-0.2222
H	-0.1780	-2.6301	0.8740
H	0.8799	-2.7362	-0.5076
C	-0.8967	-3.8808	-0.6758
O	-0.2872	-4.9906	-0.1983
O	-1.8856	-3.9173	-1.3665
C	-0.8890	-6.2474	-0.5589
H	-1.9119	-6.3035	-0.1834
H	-0.8994	-6.3691	-1.6430
H	-0.2686	-7.0105	-0.0941
C	-0.6164	1.2149	-0.8401
H	-0.6269	1.1606	-1.9447
C	0.1047	2.4447	-0.3979
C	-0.4711	3.8065	-0.6021
H	-0.4687	4.0578	-1.6794
H	-1.5348	3.8020	-0.3213
C	0.2575	4.9210	0.1617
H	0.2383	4.6922	1.2342
H	1.3152	4.9249	-0.1312
C	-0.3373	6.3137	-0.0723
H	-0.3199	6.5383	-1.1458
H	-1.3948	6.3078	0.2192
C	0.3954	7.4201	0.6920
H	-0.0535	8.3997	0.5057
H	0.3660	7.2413	1.7715
H	1.4477	7.4754	0.3955
H	-1.6765	1.2869	-0.5562
H	1.1555	2.3613	-0.1300

TS11-5

C	-0.0534	-0.1280	-0.1292
H	-0.0541	-0.1734	0.9666
H	1.0002	-0.1590	-0.4358
C	-0.7875	-1.3483	-0.6946
H	-1.8392	-1.3226	-0.3925
H	-0.7892	-1.3087	-1.7888
C	-0.1646	-2.6674	-0.2385
H	-0.1603	-2.7446	0.8547
H	0.8872	-2.7340	-0.5388
C	-0.8715	-3.8919	-0.7778
O	-0.2624	-5.0237	-0.3554
O	-1.8470	-3.8934	-1.4883
C	-0.8472	-6.2613	-0.8008
H	-1.8758	-6.3471	-0.4474
H	-0.8379	-6.3186	-1.8902
H	-0.2285	-7.0460	-0.3710
C	-0.6674	1.2040	-0.5765
H	-0.6649	1.2520	-1.6763
C	0.0484	2.4232	-0.0323
H	-0.0932	2.3478	1.2767
H	1.1366	2.3639	-0.1346
C	-0.5109	3.7784	-0.4139
H	-0.5067	3.8660	-1.5116
H	-1.5663	3.8326	-0.1166
C	0.2558	4.9619	0.1883
H	0.2486	4.8776	1.2818
H	1.3088	4.9017	-0.1159
C	-0.3099	6.3269	-0.2188
H	-0.3052	6.4087	-1.3127
H	-1.3619	6.3865	0.0857
C	0.4624	7.5040	0.3839
H	0.0342	8.4620	0.0764
H	0.4464	7.4688	1.4778
H	1.5106	7.4924	0.0688
H	-1.7237	1.2403	-0.2806
H	-0.2645	2.2944	2.2274

$CH_3(CH_2)_2CH(CH_2)_5COOCH_3$

C	0.0591	-0.1556	-0.0262
H	0.0241	-0.1993	1.0704
H	1.1179	-0.2532	-0.2999
C	-0.7289	-1.3336	-0.6092
H	-1.7861	-1.2434	-0.3401
H	-0.6945	-1.2987	-1.7028
C	-0.2004	-2.6858	-0.1312
H	-0.2407	-2.7629	0.9613
H	0.8566	-2.8117	-0.3924
C	-0.9523	-3.8696	-0.6998
O	-0.4423	-5.0327	-0.2324
O	-1.8821	-3.8187	-1.4673
C	-1.0742	-6.2361	-0.7060
H	-2.1280	-6.2515	-0.4242
H	-0.9938	-6.3084	-1.7916
H	-0.5383	-7.0531	-0.2276
C	-0.4599	1.2081	-0.4934
H	-0.4266	1.2527	-1.5891
C	0.3289	2.3930	0.0807
H	1.3958	2.2695	-0.1838
C	-0.1556	3.7289	-0.3761
C	0.3460	4.9957	0.2328
H	0.3762	4.8932	1.3280
H	1.3998	5.1626	-0.0601
C	-0.4675	6.2425	-0.1431
H	-0.4922	6.3356	-1.2353
H	-1.5062	6.0997	0.1752
C	0.0871	7.5317	0.4680
H	-0.5137	8.3993	0.1816
H	0.0950	7.4805	1.5614
H	1.1148	7.7162	0.1388
H	-1.5154	1.3118	-0.2152
H	0.3101	2.3504	1.1803
H	-0.7170	3.7875	-1.3056

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C	-0.0271	-0.1493	0.0072
H	-0.0654	-0.2128	1.1026
H	1.0361	-0.1995	-0.2628
C	-0.7645	-1.3478	-0.5998
H	-1.8259	-1.3034	-0.3358
H	-0.7255	-1.2938	-1.6924
C	-0.1856	-2.6856	-0.1401
H	-0.2277	-2.7813	0.9508
H	0.8766	-2.7663	-0.3982
C	-0.8887	-3.8884	-0.7308
O	-0.3388	-5.0381	-0.2759
O	-1.8144	-3.8610	-1.5044
C	-0.9232	-6.2575	-0.7695
H	-1.9763	-6.3171	-0.4909
H	-0.8376	-6.3104	-1.8558
H	-0.3577	-7.0606	-0.3017
C	-0.5995	1.2002	-0.4394
H	-0.5689	1.2621	-1.5345
C	0.1437	2.4031	0.1539
H	1.2044	2.3526	-0.1373
C	-0.4166	3.7441	-0.2745
H	-0.6195	3.8014	-1.3485
H	-1.6356	3.7796	0.2237
C	0.2674	4.9821	0.2680
H	0.2761	4.9419	1.3652
H	1.3251	4.9655	-0.0382
C	-0.3676	6.3000	-0.1925
H	-0.3667	6.3350	-1.2885
H	-1.4197	6.3170	0.1130
C	0.3470	7.5365	0.3594
H	-0.1284	8.4583	0.0137
H	0.3324	7.5463	1.4538
H	1.3946	7.5640	0.0428
H	-1.6581	1.2562	-0.1597
H	0.1337	2.3395	1.2499
H	-2.5020	3.7994	0.6562

$CH_3CH_2CH(CH_2)_6COOCH_3$

C	-0.0187	-0.1221	-0.0656
H	-0.0093	-0.1474	1.0319
H	1.0322	-0.1757	-0.3790
C	-0.7730	-1.3455	-0.5975
H	-1.8208	-1.3021	-0.2837
H	-0.7876	-1.3261	-1.6920
C	-0.1595	-2.6635	-0.1252
H	-0.1396	-2.7195	0.9694
H	0.8867	-2.7491	-0.4394
C	-0.8896	-3.8899	-0.6277
O	-0.2720	-5.0207	-0.2137
O	-1.8887	-3.8946	-1.3046
C	-0.8778	-6.2596	-0.6259
H	-1.8947	-6.3359	-0.2380
H	-0.9048	-6.3285	-1.7144
H	-0.2494	-7.0433	-0.2084
C	-0.6168	1.2091	-0.5339
H	-0.6234	1.2361	-1.6311
C	0.1302	2.4358	-0.0004
H	1.1806	2.3871	-0.3144
C	-0.4704	3.7696	-0.4671
H	-0.5016	3.7741	-1.5728
C	0.2594	4.9747	0.0256
C	-0.3270	6.3437	-0.0745
H	-0.3811	6.6514	-1.1348
H	-1.3740	6.3195	0.2601
C	0.4439	7.4112	0.7111
H	-0.0114	8.3979	0.5920
H	0.4626	7.1749	1.7788
H	1.4804	7.4788	0.3670
H	-1.6682	1.2612	-0.2232
H	0.1375	2.4117	1.0959
H	-1.5250	3.8265	-0.1595
H	1.3187	4.8809	0.2541

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C	-0.0163	-0.1393	-0.0290
H	0.0137	-0.1960	1.0669
H	1.0288	-0.1786	-0.3632
C	-0.7749	-1.3504	-0.5824
H	-1.8178	-1.3191	-0.2511
H	-0.8067	-1.3017	-1.6756
C	-0.1500	-2.6782	-0.1549
H	-0.1162	-2.7659	0.9370
H	0.8928	-2.7491	-0.4843
C	-0.8784	-3.8934	-0.6865
O	-0.2746	-5.0331	-0.2771
O	-1.8645	-3.8828	-1.3822
C	-0.8776	-6.2629	-0.7197
H	-1.9027	-6.3396	-0.3541
H	-0.8823	-6.3162	-1.8094
H	-0.2618	-7.0556	-0.3006
C	-0.6292	1.2019	-0.4470
H	-0.6591	1.2600	-1.5426
C	0.1248	2.4160	0.1060
H	1.1690	2.3794	-0.2305
C	-0.4909	3.7573	-0.3107
H	-0.5177	3.8173	-1.4099
C	0.2469	4.9666	0.2257
H	0.1400	4.8811	1.5375
H	1.3317	4.9025	0.0937
C	-0.3135	6.3296	-0.1262
H	-0.3369	6.4285	-1.2217
H	-1.3596	6.3856	0.1990
C	0.4798	7.4951	0.4728
H	0.0457	8.4569	0.1873
H	0.4907	7.4438	1.5651
H	1.5186	7.4830	0.1286
H	-1.6737	1.2411	-0.1124
H	0.1543	2.3589	1.2006
H	-1.5388	3.7985	0.0139
H	-0.0070	4.8221	2.4922

$CH_3CH(CH_2)_7COOCH_3$

C	-0.0097	-0.1506	-0.0219
H	0.0307	-0.2124	1.0736
H	1.0315	-0.1995	-0.3667
C	-0.7859	-1.3521	-0.5722
H	-1.8246	-1.3129	-0.2291
H	-0.8296	-1.2975	-1.6647
C	-0.1681	-2.6875	-0.1585
H	-0.1223	-2.7805	0.9327
H	0.8701	-2.7663	-0.5003
C	-0.9137	-3.8941	-0.6859
O	-0.3073	-5.0406	-0.2992
O	-1.9142	-3.8726	-1.3603
C	-0.9261	-6.2632	-0.7398
H	-1.9434	-6.3382	-0.3529
H	-0.9545	-6.3066	-1.8295
H	-0.3055	-7.0628	-0.3412
C	-0.6124	1.1987	-0.4288
H	-0.6531	1.2605	-1.5238
C	0.1605	2.4043	0.1177
H	1.2017	2.3530	-0.2268
C	-0.4411	3.7531	-0.2901
H	-0.4770	3.8188	-1.3849
C	0.3323	4.9602	0.2583
H	1.3873	4.8810	-0.0655
C	-0.2246	6.2831	-0.1507
C	0.2315	7.5485	0.4913
H	-0.3972	8.3981	0.2139
H	0.2318	7.4687	1.5859
H	1.2657	7.8070	0.2058
H	-1.6529	1.2485	-0.0836
H	0.2001	2.3419	1.2131
H	-1.4810	3.8089	0.0536
H	0.3751	4.9033	1.3564
H	-0.8088	6.3387	-1.0647

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C	-0.0318	-0.1468	-0.0033
H	-0.0318	-0.2094	1.0928
H	1.0218	-0.1887	-0.3093
C	-0.7797	-1.3524	-0.5829
H	-1.8305	-1.3202	-0.2778
H	-0.7839	-1.2966	-1.6762
C	-0.1690	-2.6845	-0.1484
H	-0.1602	-2.7771	0.9438
H	0.8806	-2.7580	-0.4545
C	-0.8909	-3.8948	-0.6998
O	-0.2862	-5.0380	-0.3012
O	-1.8736	-3.8783	-1.3999
C	-0.8854	-6.2638	-0.7599
H	-1.9107	-6.3478	-0.3963
H	-0.8889	-6.3035	-1.8501
H	-0.2680	-7.0601	-0.3499
C	-0.6279	1.1989	-0.4313
H	-0.6282	1.2616	-1.5270
C	0.1160	2.4088	0.1448
H	1.1693	2.3660	-0.1622
C	-0.4816	3.7540	-0.2821
H	-0.4843	3.8185	-1.3777
C	0.2675	4.9628	0.2910
H	1.3213	4.9196	-0.0267
C	-0.3098	6.3009	-0.1226
H	-0.5331	6.3595	-1.1916
H	-1.5189	6.3342	0.3903
C	0.3815	7.5364	0.4107
H	-0.1572	8.4477	0.1382
H	0.4642	7.5058	1.5015
H	1.3985	7.6206	0.0070
H	-1.6808	1.2416	-0.1249
H	0.1164	2.3451	1.2407
H	-1.5319	3.8008	0.0292
H	0.2864	4.9008	1.3870
H	-2.3887	6.3715	0.8189

$CH_2(CH_2)_8COOCH_3$

C	0.0092	-0.0004	0.0032
H	0.0143	-0.0041	1.1011
H	1.0631	0.0008	-0.3047
C	-0.6706	-1.2753	-0.5079
H	-1.7212	-1.2854	-0.2009
H	-0.6792	-1.2783	-1.6027
C	0.0131	-2.5469	-0.0060
H	0.0295	-2.5798	1.0896
H	1.0643	-2.5799	-0.3133
C	-0.6446	-3.8221	-0.4870
O	0.0289	-4.9084	-0.0423
O	-1.6353	-3.8957	-1.1721
C	-0.5059	-6.1869	-0.4311
H	-1.5206	-6.3090	-0.0494
H	-0.5195	-6.2813	-1.5179
H	0.1598	-6.9263	0.0089
C	-0.6624	1.2848	-0.4937
H	-0.6668	1.2886	-1.5911
H	-1.7160	1.2833	-0.1866
C	0.0111	2.5646	0.0143
H	0.0146	2.5607	1.1120
H	1.0651	2.5652	-0.2923
C	-0.6600	3.8496	-0.4837
H	-0.6641	3.8537	-1.5814
H	-1.7140	3.8489	-0.1767
C	0.0136	5.1285	0.0244
H	0.0191	5.1297	1.1209
H	1.0659	5.1346	-0.2870
C	-0.6615	6.4158	-0.4741
H	-0.6908	6.3883	-1.5787
H	-1.7156	6.4250	-0.1669
C	0.0079	7.6664	-0.0204
H	1.0752	7.6857	0.1705
H	-0.5250	8.6093	0.0036

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C	0.0211	0.0016	-0.0097
H	0.0467	0.0012	1.0879
H	1.0691	-0.0009	-0.3372
C	-0.6713	-1.2729	-0.5046
H	-1.7167	-1.2781	-0.1800
H	-0.6982	-1.2802	-1.5990
C	0.0165	-2.5448	-0.0091
H	0.0473	-2.5765	1.0861
H	1.0636	-2.5797	-0.3303
C	-0.6480	-3.8196	-0.4817
O	0.0155	-4.9066	-0.0239
O	-1.6351	-3.8923	-1.1722
C	-0.5242	-6.1847	-0.4070
H	-1.5431	-6.2972	-0.0333
H	-0.5288	-6.2879	-1.4930
H	0.1328	-6.9247	0.0449
C	-0.6564	1.2870	-0.4977
H	-0.6831	1.2868	-1.5949
H	-1.7035	1.2901	-0.1693
C	0.0312	2.5666	-0.0083
H	0.0582	2.5662	1.0890
H	1.0784	2.5634	-0.3375
C	-0.6475	3.8517	-0.4956
H	-0.6754	3.8523	-1.5931
H	-1.6943	3.8548	-0.1656
C	0.0399	5.1306	-0.0058
H	0.0673	5.1335	1.0905
H	1.0861	5.1316	-0.3376
C	-0.6417	6.4153	-0.4938
H	-0.6714	6.4110	-1.5943
H	-1.6903	6.4225	-0.1716
C	0.0380	7.6803	-0.0285
H	-0.4405	8.6142	-0.3218
H	-0.0923	7.7286	1.3309
H	1.1210	7.7118	-0.1528
H	-0.2131	7.7453	2.2491

$CH_3(CH_2)_8COOCH_2$

C	-4.2299	-2.6052	-0.1926
H	-4.7446	-1.6467	-0.3395
H	-3.4725	-2.6676	-0.9849
C	-3.5395	-2.6085	1.1757
H	-4.2898	-2.5461	1.9704
H	-3.0195	-3.5596	1.3280
C	-2.5436	-1.4593	1.3324
H	-3.0335	-0.4880	1.1979
H	-1.7663	-1.5016	0.5604
C	-1.8525	-1.4402	2.6729
O	-0.9959	-0.3630	2.7515
O	-1.9910	-2.2236	3.5737
C	-0.2753	-0.1806	3.8946
C	-5.2355	-3.7491	-0.3643
H	-5.9903	-3.6877	0.4300
H	-4.7205	-4.7074	-0.2196
C	-5.9353	-3.7514	-1.7281
H	-6.4484	-2.7918	-1.8728
H	-5.1805	-3.8147	-2.5227
C	-6.9436	-4.8936	-1.8971
H	-6.4302	-5.8532	-1.7540
H	-7.6966	-4.8310	-1.1009
C	-7.6478	-4.8963	-3.2586
H	-8.1604	-3.9361	-3.4032
H	-6.8959	-4.9613	-4.0560
C	-8.6587	-6.0365	-3.4260
H	-8.1469	-6.9959	-3.2823
H	-9.4101	-5.9712	-2.6297
C	-9.3578	-6.0312	-4.7886
H	-10.0700	-6.8565	-4.8763
H	-9.9091	-5.0989	-4.9469
H	-8.6346	-6.1290	-5.6046
H	0.3617	0.6870	3.8782
H	-0.3989	-0.8760	4.7086

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C	-4.2408	-2.5874	-0.2010
H	-4.7904	-1.6427	-0.3039
H	-3.5014	-2.5987	-1.0123
C	-3.5181	-2.6119	1.1503
H	-4.2509	-2.6049	1.9634
H	-2.9606	-3.5479	1.2571
C	-2.5619	-1.4322	1.3260
H	-3.0902	-0.4761	1.2364
H	-1.7998	-1.4176	0.5382
C	-1.8445	-1.4286	2.6542
O	-1.0094	-0.3455	2.7430
O	-1.9540	-2.2406	3.5345
C	-0.2914	-0.1791	3.9320
H	-0.0178	-1.1134	4.4170
H	0.5181	0.5239	3.7589
H	-1.0746	0.4243	4.8147
H	-1.6635	0.8703	5.4298
C	-5.2122	-3.7586	-0.3862
H	-5.9486	-3.7474	0.4273
H	-4.6627	-4.7032	-0.2847
C	-5.9453	-3.7417	-1.7323
H	-6.4912	-2.7948	-1.8348
H	-5.2093	-3.7575	-2.5465
C	-6.9222	-4.9094	-1.9114
H	-6.3762	-5.8564	-1.8110
H	-7.6556	-4.8945	-1.0949
C	-7.6616	-4.8932	-3.2539
H	-8.2066	-3.9456	-3.3560
H	-6.9295	-4.9112	-4.0720
C	-8.6417	-6.0587	-3.4302
H	-8.0973	-7.0057	-3.3306
H	-9.3723	-6.0414	-2.6123
C	-9.3786	-6.0333	-4.7726
H	-10.0672	-6.8776	-4.8672
H	-9.9624	-5.1143	-4.8860
H	-8.6759	-6.0828	-5.6105

$CH_3(CH_2)_{14}COOCH_3$(n=15,m=1)

$H + CH_3(CH_2)_{14}COOCH_3 \rightarrow H_2 + CH_3(CH_2)_{13}CHCOOCH_3$ (TS17-1)

$H + CH_3(CH_2)_{14}COOCH_3 \rightarrow H_2 + CH_3(CH_2)_{12}CHCH_2COOCH_3$ (TS17-2)

$H + CH_3(CH_2)_{14}COOCH_3 \rightarrow H_2 + CH_3(CH_2)_{11}CH(CH_2)_2COOCH_3$ (TS17-3)

$H + CH_3(CH_2)_{14}COOCH_3 \rightarrow H_2 + CH_3(CH_2)_{10}CH(CH_2)_3COOCH_3$ (TS17-4)

$H + CH_3(CH_2)_{14}COOCH_3 \rightarrow H_2 + CH_3(CH_2)_9CH(CH_2)_4COOCH_3$ (TS17-5)

$H + CH_3(CH_2)_{14}COOCH_3 \rightarrow H_2 + CH_3(CH_2)_8CH(CH_2)_5COOCH_3$ (TS17-6)

$H + CH_3(CH_2)_{14}COOCH_3 \rightarrow H_2 + CH_3(CH_2)_7CH(CH_2)_6COOCH_3$ (TS17-7)

$H + CH_3(CH_2)_{14}COOCH_3 \rightarrow H_2 + CH_3(CH_2)_6CH(CH_2)_7COOCH_3$ (TS17-8)

$H + CH_3(CH_2)_{14}COOCH_3 \rightarrow H_2 + CH_3(CH_2)_5CH(CH_2)_8COOCH_3$ (TS17-9)

$H + CH_3(CH_2)_{14}COOCH_3 \rightarrow H_2 + CH_3(CH_2)_4CH(CH_2)_9COOCH_3$ (TS17-10)

$H + CH_3(CH_2)_{14}COOCH_3 \rightarrow H_2 + CH_3(CH_2)_3CH(CH_2)_{10}COOCH_3$ (TS17-11)

$H + CH_3(CH_2)_{14}COOCH_3 \rightarrow H_2 + CH_3(CH_2)_2CH(CH_2)_{11}COOCH_3$ (TS17-12)

$H + CH_3(CH_2)_{14}COOCH_3 \rightarrow H_2 + CH_3CH_2\ CH(CH_2)_{12}COOCH_3$ (TS17-13)

$H + CH_3(CH_2)_{14}COOCH_3 \rightarrow H_2 + CH_3CH(CH_2)_{13}COOCH_3$ (TS17-14)

$H + CH_3(CH_2)_{14}COOCH_3 \rightarrow H_2 + CH_2\ (CH_2)_{14}COOCH_3$ (TS17-15)

$H + CH_3(CH_2)_{14}COOCH_3 \rightarrow H_2 + CH_3(CH_2)_{14}COOCH_2$ (TS17-16)

$CH_3(CH_2)_{14}COOCH_3$

C	-0.5093	-0.0822	0.1951
H	-0.5593	-0.1116	1.2915
H	0.5527	-0.1882	-0.0627
C	-1.2954	-1.2642	-0.3824
H	-2.3545	-1.1693	-0.1228
H	-1.2521	-1.2405	-1.4762
C	-0.7737	-2.6125	0.1139
H	-0.8103	-2.6703	1.2080
H	0.2809	-2.7511	-0.1489
C	-1.5402	-3.8000	-0.4266
O	-0.9988	-4.9609	0.0102
O	-2.5068	-3.7537	-1.1476
C	-1.6469	-6.1674	-0.4327
H	-2.6824	-6.1933	-0.0903

H	-1.6292	-6.2336	-1.5215
H	-1.0775	-6.9821	0.0094
C	-1.0131	1.2798	-0.2958
H	-0.9570	1.3121	-1.3914
H	-2.0762	1.3836	-0.0437
C	-0.2368	2.4661	0.2867
H	-0.2966	2.4340	1.3824
H	0.8272	2.3598	0.0381
C	-0.7361	3.8292	-0.2059
H	-0.6695	3.8645	-1.3011
H	-1.8018	3.9327	0.0362
C	0.0335	5.0153	0.3861
H	-0.0363	4.9805	1.4811
H	1.0999	4.9103	0.1471
C	-0.4622	6.3792	-0.1078
H	-0.3857	6.4173	-1.2022
H	-1.5301	6.4815	0.1249
C	0.3011	7.5646	0.4939
H	0.2221	7.5268	1.5882
H	1.3696	7.4612	0.2638
C	-0.1917	8.9294	-0.0005
H	-1.2614	9.0305	0.2244
H	-0.1070	8.9700	-1.0943
C	0.5664	10.1139	0.6092
H	0.4801	10.0734	1.7029
H	1.6365	10.0121	0.3861
C	0.0757	11.4795	0.1148
H	-0.9952	11.5799	0.3348
H	0.1656	11.5220	-0.9785
C	0.8302	12.6633	0.7297
H	0.7399	12.6218	1.8232
H	1.9015	12.5638	0.5107
C	0.3412	14.0299	0.2364
H	-0.7291	14.1299	0.4547
H	0.4331	14.0728	-0.8558
C	1.1003	15.2057	0.8583
H	0.9986	15.2097	1.9483
H	2.1690	15.1531	0.6273
H	0.7276	16.1645	0.4869

$CH_3(CH_2)_{13}CHCOOCH_3$

C	-3.4529	-2.5815	-0.3434
H	-4.3473	-2.1044	0.0718
H	-3.0435	-1.8851	-1.0849
C	-2.4218	-2.7859	0.7945
H	-2.8360	-3.4600	1.5481
H	-1.5330	-3.2697	0.3659
C	-2.0189	-1.5131	1.4419
C	-2.4064	-1.1858	2.7978
O	-1.9386	0.0378	3.1743
O	-3.0689	-1.8956	3.5361
C	-2.2740	0.4492	4.5077
H	-3.3570	0.5067	4.6320
H	-1.8707	-0.2527	5.2399
H	-1.8229	1.4316	4.6320
C	-3.8418	-3.8953	-1.0302
H	-2.9413	-4.3728	-1.4375
H	-4.2430	-4.5887	-0.2807
C	-4.8699	-3.7093	-2.1518
H	-4.4644	-3.0216	-2.9051
H	-5.7638	-3.2204	-1.7440
C	-5.2792	-5.0209	-2.8323
H	-5.6862	-5.7067	-2.0782
H	-4.3863	-5.5128	-3.2396
C	-6.3086	-4.8329	-3.9524
H	-5.8968	-4.1567	-4.7129
H	-7.1948	-4.3281	-3.5462
C	-6.7382	-6.1439	-4.6208
H	-7.1512	-6.8184	-3.8595
H	-5.8536	-6.6511	-5.0274
C	-7.7697	-5.9523	-5.7385
H	-7.3520	-5.2884	-6.5065
H	-8.6473	-5.4319	-5.3334
C	-8.2196	-7.2631	-6.3937
H	-8.6381	-7.9256	-5.6249
H	-7.3436	-7.7855	-6.7997
C	-9.2533	-7.0678	-7.5087
H	-8.8312	-6.4142	-8.2831
H	-10.1235	-6.5347	-7.1040
C	-9.7202	-8.3781	-8.1531
H	-10.1425	-9.0309	-7.3781
H	-8.8514	-8.9124	-8.5590
C	-10.7561	-8.1800	-9.2653
H	-10.3322	-7.5330	-10.0446

H	-11.6219	-7.6392	-8.8610
C	-11.2344	-9.4891	-9.9036
H	-11.6581	-10.1355	-9.1252
H	-10.3705	-10.0297	-10.3094
C	-12.2703	-9.2792	-11.0119
H	-11.8632	-8.6667	-11.8227
H	-12.5921	-10.2306	-11.4448
H	-13.1608	-8.7701	-10.6296
H	-1.4491	-0.7731	0.8905

TS17-1

C	-4.0627	-2.3098	-0.1867
H	-4.9704	-1.7655	0.1020
H	-3.5614	-1.6892	-0.9405
C	-3.1518	-2.4622	1.0366
H	-3.6334	-3.0821	1.7986
H	-2.2392	-3.0016	0.7490
C	-2.7510	-1.1369	1.6543
H	-3.8021	-0.5691	2.0213
H	-2.3427	-0.4086	0.9522
C	-1.9384	-1.2172	2.9064
O	-1.3183	-0.0423	3.1631
O	-1.8572	-2.1839	3.6285
C	-0.5496	0.0116	4.3790
H	-1.1893	-0.1716	5.2435
H	0.2473	-0.7331	4.3596
H	-0.1345	1.0164	4.4155
H	-4.7086	-0.1231	2.2869
C	-4.4543	-3.6521	-0.8143
H	-3.5448	-4.2032	-1.0862
H	-4.9672	-4.2655	-0.0627
C	-5.3490	-3.5119	-2.0510
H	-4.8294	-2.9085	-2.8067
H	-6.2526	-2.9495	-1.7828
C	-5.7554	-4.8549	-2.6683
H	-6.2878	-5.4513	-1.9161
H	-4.8519	-5.4243	-2.9221
C	-6.6328	-4.7170	-3.9178
H	-6.0941	-4.1325	-4.6749
H	-7.5299	-4.1357	-3.6682
C	-7.0551	-6.0607	-4.5228
H	-7.6038	-6.6394	-3.7684
H	-6.1585	-6.6476	-4.7611
C	-7.9189	-5.9248	-5.7819
H	-7.3651	-5.3568	-6.5407
H	-8.8097	-5.3279	-5.5472
C	-8.3550	-7.2692	-6.3755
H	-8.9155	-7.8329	-5.6184
H	-7.4647	-7.8700	-6.6023
C	-9.2099	-7.1358	-7.6409
H	-8.6462	-6.5799	-8.4013
H	-10.0963	-6.5282	-7.4166
C	-9.6556	-8.4810	-8.2256
H	-10.2225	-9.0346	-7.4658

H	-8.7695	-9.0905	-8.4458
C	-10.5063	-8.3504	-9.4939
H	-9.9386	-7.8010	-10.2564
H	-11.3911	-7.7380	-9.2759
C	-10.9569	-9.6958	-10.0745
H	-11.5254	-10.2441	-9.3134
H	-10.0733	-10.3080	-10.2924
C	-11.8055	-9.5559	-11.3417
H	-11.2513	-9.0435	-12.1345
H	-12.1113	-10.5320	-11.7287
H	-12.7138	-8.9765	-11.1475

$CH_3(CH_2)_{12}CHCH_2COOCH_3$

C	-4.2100	-2.0730	-0.2919
H	-5.1013	-1.4852	-0.0198
H	-3.7722	-1.5271	-1.1478
C	-3.2450	-2.0874	0.8445
C	-2.8733	-0.8258	1.5409
H	-3.7509	-0.3156	1.9649
H	-2.4500	-0.0839	0.8423
C	-1.8597	-1.0041	2.6541
O	-1.6686	0.1611	3.3127
O	-1.2805	-2.0243	2.9329
C	-0.7084	0.1308	4.3850
H	-1.0144	-0.5826	5.1515
H	0.2763	-0.1493	4.0082
H	-0.6911	1.1413	4.7875
C	-4.6419	-3.4682	-0.7627
H	-3.7481	-4.0486	-1.0224
H	-5.1173	-3.9962	0.0726
C	-5.5960	-3.4396	-1.9610
H	-6.4847	-2.8485	-1.7041
H	-5.1130	-2.9137	-2.7951
C	-6.0346	-4.8318	-2.4291
H	-5.1455	-5.4273	-2.6735
H	-6.5296	-5.3530	-1.5995
C	-6.9726	-4.8041	-3.6412
H	-6.4744	-4.2857	-4.4708
H	-7.8600	-4.2048	-3.3991
C	-7.4154	-6.1951	-4.1091
H	-7.9232	-6.7100	-3.2832
H	-6.5276	-6.7976	-4.3412
C	-8.3396	-6.1662	-5.3317
H	-7.8297	-5.6525	-6.1571
H	-9.2266	-5.5620	-5.1010
C	-8.7840	-7.5563	-5.8009
H	-9.3003	-8.0680	-4.9782
H	-7.8967	-8.1626	-6.0251
C	-9.6987	-7.5262	-7.0306
H	-9.1817	-7.0140	-7.8525
H	-10.5862	-6.9201	-6.8069
C	-10.1423	-8.9158	-7.5023
H	-10.6632	-9.4270	-6.6821
H	-9.2546	-9.5230	-7.7223
C	-11.0513	-8.8850	-8.7360
H	-10.5312	-8.3729	-9.5562

H	-11.9403	-8.2793	-8.5167
C	-11.4936	-10.2739	-9.2110
H	-12.0156	-10.7853	-8.3930
H	-10.6056	-10.8795	-9.4294
C	-12.3988	-10.2322	-10.4457
H	-11.8918	-9.7574	-11.2919
H	-12.6961	-11.2371	-10.7585
H	-13.3123	-9.6625	-10.2474
H	-2.7135	-2.9943	1.1067

TS17-2

C	-4.2332	-2.1467	-0.2159
H	-5.1134	-1.5405	0.0350
H	-3.7405	-1.6241	-1.0509
C	-3.2845	-2.1796	0.9635
H	-3.9704	-2.7158	1.9546
H	-2.4634	-2.8900	0.8599
C	-2.8316	-0.8357	1.4894
H	-3.6694	-0.2452	1.8714
H	-2.3963	-0.2382	0.6741
C	-1.7653	-0.9305	2.5623
O	-1.7175	0.2021	3.2959
O	-1.0264	-1.8677	2.7382
C	-0.7040	0.2503	4.3185
H	-0.8517	-0.5554	5.0386
H	0.2889	0.1582	3.8760
H	-0.8218	1.2196	4.7977
H	-4.5157	-3.0375	2.6813
C	-4.6817	-3.5353	-0.6875
H	-3.7955	-4.1357	-0.9279
H	-5.1854	-4.0510	0.1386
C	-5.6116	-3.4915	-1.9048
H	-6.4955	-2.8866	-1.6645
H	-5.1045	-2.9737	-2.7294
C	-6.0627	-4.8770	-2.3809
H	-5.1785	-5.4850	-2.6120
H	-6.5780	-5.3915	-1.5596
C	-6.9812	-4.8349	-3.6074
H	-6.4643	-4.3200	-4.4278
H	-7.8653	-4.2263	-3.3772
C	-7.4322	-6.2196	-4.0860
H	-7.9549	-6.7325	-3.2682
H	-6.5478	-6.8300	-4.3101
C	-8.3419	-6.1769	-5.3191
H	-7.8187	-5.6628	-6.1359
H	-9.2269	-5.5672	-5.0954
C	-8.7913	-7.5612	-5.8007
H	-9.3182	-8.0743	-4.9857
H	-7.9060	-8.1719	-6.0206
C	-9.6950	-7.5179	-7.0382
H	-9.1682	-7.0028	-7.8520
H	-10.5813	-6.9088	-6.8180
C	-10.1414	-8.9020	-7.5230
H	-10.6703	-9.4167	-6.7102

H	-9.2549	-9.5116	-7.7410
C	-11.0416	-8.8586	-8.7628
H	-10.5139	-8.3423	-9.5755
H	-11.9299	-8.2512	-8.5451
C	-11.4856	-10.2422	-9.2512
H	-12.0144	-10.7582	-8.4404
H	-10.5983	-10.8491	-9.4687
C	-12.3830	-10.1880	-10.4911
H	-11.8692	-9.7086	-11.3305
H	-12.6816	-11.1895	-10.8134
H	-13.2958	-9.6168	-10.2941

$CH_3(CH_2)_{11}CH(CH_2)_2COOCH_3$

C	-3.5666	-2.6390	-0.3885
C	-2.9468	-2.6008	0.9690
H	-3.5923	-3.1119	1.6943
H	-2.0076	-3.1792	0.9843
C	-2.6559	-1.1796	1.4550
H	-3.5732	-0.5811	1.4778
H	-1.9822	-0.6582	0.7667
C	-2.0397	-1.1250	2.8352
O	-1.7582	0.1510	3.1852
O	-1.8205	-2.0699	3.5536
C	-1.1759	0.3360	4.4886
H	-1.8544	-0.0215	5.2645
H	-0.2302	-0.2024	4.5648
H	-1.0153	1.4076	4.5853
C	-4.1320	-3.8974	-0.9574
H	-4.6163	-4.4775	-0.1596
H	-3.3143	-4.5461	-1.3228
C	-5.1252	-3.6713	-2.1077
H	-4.6365	-3.0800	-2.8924
H	-5.9602	-3.0619	-1.7418
C	-5.6674	-4.9696	-2.7147
H	-4.8308	-5.5698	-3.0955
H	-6.1368	-5.5702	-1.9248
C	-6.6801	-4.7386	-3.8420
H	-7.5161	-4.1401	-3.4576
H	-6.2127	-4.1344	-4.6305
C	-7.2267	-6.0327	-4.4555
H	-7.6864	-6.6409	-3.6658
H	-6.3925	-6.6277	-4.8495
C	-8.2506	-5.7961	-5.5716
H	-9.0841	-5.2014	-5.1757
H	-7.7917	-5.1862	-6.3605
C	-8.8006	-7.0873	-6.1880
H	-9.2553	-7.6996	-5.3984
H	-7.9685	-7.6801	-6.5896
C	-9.8312	-6.8469	-7.2971
H	-10.6621	-6.2528	-6.8948
H	-9.3766	-6.2351	-8.0872
C	-10.3852	-8.1364	-7.9135
H	-9.5553	-8.7293	-8.3195
H	-10.8371	-8.7495	-7.1229
C	-11.4201	-7.8942	-9.0180
H	-10.9687	-7.2825	-9.8102

H	-12.2496	-7.3000	-8.6127
C	-11.9781	-9.1824	-9.6338
H	-11.1501	-9.7756	-10.0410
H	-12.4285	-9.7940	-8.8425
C	-13.0128	-8.9291	-10.7341
H	-12.5818	-8.3495	-11.5566
H	-13.3910	-9.8665	-11.1517
H	-13.8700	-8.3676	-10.3491
H	-3.4043	-1.7996	-1.0612

TS17-3

C	-3.9676	-2.3803	-0.2316
H	-5.0308	-1.6971	0.1439
H	-3.5444	-1.7184	-0.9938
C	-3.1092	-2.4915	1.0117
H	-3.6573	-3.0243	1.7956
H	-2.2300	-3.1125	0.7956
C	-2.6486	-1.1333	1.5425
H	-3.5037	-0.4964	1.7903
H	-2.0835	-0.5836	0.7812
C	-1.7742	-1.2353	2.7731
O	-1.4363	-0.0071	3.2256
O	-1.4095	-2.2580	3.3003
C	-0.5992	0.0282	4.3964
H	-1.0962	-0.4599	5.2359
H	0.3504	-0.4725	4.2026
H	-0.4396	1.0834	4.6071
H	-5.8209	-1.2395	0.4682
C	-4.5070	-3.6755	-0.8027
H	-5.0722	-4.2059	-0.0256
H	-3.6587	-4.3313	-1.0525
C	-5.3867	-3.4914	-2.0449
H	-4.8140	-2.9633	-2.8180
H	-6.2324	-2.8404	-1.7928
C	-5.9145	-4.8111	-2.6183
H	-5.0670	-5.4557	-2.8858
H	-6.4688	-5.3476	-1.8375
C	-6.8191	-4.6283	-3.8420
H	-7.6704	-3.9918	-3.5676
H	-6.2710	-4.0820	-4.6205
C	-7.3422	-5.9468	-4.4233
H	-7.8615	-6.5078	-3.6354
H	-6.4923	-6.5706	-4.7294
C	-8.2891	-5.7591	-5.6140
H	-9.1434	-5.1456	-5.2996
H	-7.7776	-5.1863	-6.3984
C	-8.8052	-7.0759	-6.2054
H	-9.2871	-7.6633	-5.4130
H	-7.9539	-7.6760	-6.5522
C	-9.7939	-6.8831	-7.3609
H	-10.6477	-6.2904	-7.0075
H	-9.3180	-6.2870	-8.1504
C	-10.3064	-8.1976	-7.9603
H	-9.4554	-8.7813	-8.3349

H	-10.7630	-8.8029	-7.1663
C	-11.3221	-8.0014	-9.0913
H	-10.8692	-7.3924	-9.8848
H	-12.1745	-7.4213	-8.7141
C	-11.8348	-9.3137	-9.6954
H	-10.9848	-9.8896	-10.0817
H	-12.2800	-9.9261	-8.9016
C	-12.8597	-9.1055	-10.8141
H	-12.4332	-8.5250	-11.6384
H	-13.2045	-10.0591	-11.2240
H	-13.7382	-8.5638	-10.4495

$CH_3(CH_2)_{10}CH(CH_2)_3COOCH_3$

C	-4.3510	-2.1991	-0.0273
H	-3.8472	-1.7555	-0.8996
C	-3.3298	-2.4519	1.0899
H	-3.8349	-2.8798	1.9610
H	-2.6049	-3.2025	0.7618
C	-2.5938	-1.1790	1.5062
H	-3.2993	-0.4076	1.8370
H	-2.0543	-0.7367	0.6616
C	-1.6006	-1.3901	2.6279
O	-0.9182	-0.2504	2.8862
O	-1.4209	-2.4180	3.2338
C	0.0507	-0.3198	3.9483
H	-0.4327	-0.5817	4.8906
H	0.8154	-1.0638	3.7204
H	0.4894	0.6740	4.0066
C	-5.0974	-3.4202	-0.4514
H	-5.0619	-1.4207	0.3085
C	-5.9643	-3.4268	-1.6659
H	-6.8774	-2.8305	-1.4805
H	-5.4526	-2.9029	-2.4869
C	-6.3824	-4.8287	-2.1329
H	-5.4822	-5.4182	-2.3438
H	-6.8977	-5.3410	-1.3106
C	-7.2863	-4.8164	-3.3701
H	-8.1879	-4.2282	-3.1553
H	-6.7720	-4.2951	-4.1881
C	-7.6959	-6.2156	-3.8438
H	-6.7935	-6.8043	-4.0533
H	-8.2147	-6.7362	-3.0284
C	-8.5918	-6.2052	-5.0878
H	-9.4961	-5.6194	-4.8778
H	-8.0735	-5.6811	-5.9013
C	-8.9959	-7.6043	-5.5664
H	-9.5158	-8.1285	-4.7539
H	-8.0912	-8.1902	-5.7745
C	-9.8883	-7.5934	-6.8128
H	-10.7944	-7.0101	-6.6039
H	-9.3692	-7.0664	-7.6239
C	-10.2885	-8.9923	-7.2956
H	-10.8082	-9.5197	-6.4851
H	-9.3821	-9.5756	-7.5041
C	-11.1793	-8.9807	-8.5428
H	-12.0873	-8.3998	-8.3344

H	-10.6609	-8.4514	-9.3532
C	-11.5771	-10.3788	-9.0297
H	-12.0959	-10.9081	-8.2210
H	-10.6700	-10.9592	-9.2387
C	-12.4665	-10.3561	-10.2763
H	-12.7313	-11.3674	-10.5978
H	-13.3981	-9.8132	-10.0876
H	-11.9616	-9.8633	-11.1134
H	-5.1770	-4.2484	0.2485

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C	-4.1613	-2.3479	-0.1079
H	-3.6680	-1.8183	-0.9378
C	-3.1809	-2.4763	1.0634
H	-3.6552	-3.0248	1.8832
H	-2.3155	-3.0730	0.7605
C	-2.7013	-1.1173	1.5734
H	-3.5316	-0.5145	1.9539
H	-2.2602	-0.5301	0.7581
C	-1.6512	-1.2149	2.6592
O	-1.4577	-0.0146	3.2520
O	-1.0401	-2.2091	2.9664
C	-0.4513	0.0274	4.2807
H	-0.7023	-0.6610	5.0888
H	0.5241	-0.2413	3.8723
H	-0.4460	1.0542	4.6399
C	-4.6788	-3.6779	-0.6171
H	-5.3907	-4.1691	0.3776
H	-3.8945	-4.4343	-0.7172
H	-5.0116	-1.7167	0.1824
H	-5.9551	-4.4678	1.1041
C	-5.6233	-3.6377	-1.8007
H	-6.4779	-2.9910	-1.5626
H	-5.1092	-3.1519	-2.6447
C	-6.1284	-5.0156	-2.2459
H	-5.2680	-5.6579	-2.4730
H	-6.6545	-5.4936	-1.4110
C	-7.0539	-4.9586	-3.4661
H	-7.9104	-4.3099	-3.2411
H	-6.5233	-4.4816	-4.3005
C	-7.5657	-6.3327	-3.9128
H	-6.7094	-6.9849	-4.1282
H	-8.1050	-6.8052	-3.0818
C	-8.4795	-6.2767	-5.1423
H	-9.3343	-5.6219	-4.9284
H	-7.9380	-5.8060	-5.9732
C	-8.9950	-7.6494	-5.5893
H	-9.5419	-8.1178	-4.7608
H	-8.1403	-8.3061	-5.7976
C	-9.9008	-7.5927	-6.8247
H	-10.7549	-6.9350	-6.6171
H	-9.3528	-7.1248	-7.6529
C	-10.4176	-8.9645	-7.2730
H	-10.9689	-9.4312	-6.4463

H	-9.5636	-9.6232	-7.4775
C	-11.3186	-8.9071	-8.5116
H	-12.1732	-8.2485	-8.3081
H	-10.7676	-8.4408	-9.3389
C	-11.8365	-10.2779	-8.9619
H	-12.3889	-10.7435	-8.1365
H	-10.9833	-10.9365	-9.1651
C	-12.7342	-10.2093	-10.2009
H	-13.0876	-11.2016	-10.4948
H	-13.6141	-9.5844	-10.0175
H	-12.1984	-9.7815	-11.0542

$CH_3(CH_2)_9CH(CH_2)_4COOCH_3$

C	-0.0427	-0.1144	-0.2008
H	-0.0037	-0.0350	0.8926
H	0.9989	-0.1810	-0.5400
C	-0.7940	-1.3888	-0.5985
H	-1.8321	-1.3320	-0.2562
H	-0.8425	-1.4664	-1.6897
C	-0.1450	-2.6514	-0.0322
H	-0.0898	-2.6084	1.0619
H	0.8916	-2.7522	-0.3718
C	-0.8744	-3.9263	-0.3963
O	-0.2043	-5.0107	0.0579
O	-1.9145	-4.0007	-1.0039
C	-0.8061	-6.2883	-0.2202
H	-1.7917	-6.3558	0.2429
H	-0.9061	-6.4374	-1.2962
H	-0.1312	-7.0265	0.2076
C	-0.6732	1.1623	-0.7730
H	-0.7310	1.0658	-1.8730
H	-1.7221	1.2324	-0.4474
C	0.0493	2.4171	-0.4102
C	-0.5086	3.7630	-0.7337
H	-0.4613	3.9352	-1.8254
H	-1.5825	3.7849	-0.4961
C	0.1995	4.9262	-0.0244
H	0.1137	4.7895	1.0603
H	1.2719	4.8846	-0.2537
C	-0.3471	6.3040	-0.4124
H	-0.2538	6.4368	-1.4982
H	-1.4222	6.3432	-0.1936
C	0.3558	7.4648	0.3004
H	0.2483	7.3412	1.3858
H	1.4331	7.4150	0.0952
C	-0.1710	8.8458	-0.1061
H	-1.2489	8.8964	0.0955
H	-0.0596	8.9691	-1.1912
C	0.5317	10.0059	0.6081
H	0.4107	9.8895	1.6930
H	1.6110	9.9475	0.4159
C	0.0193	11.3882	0.1880
H	-1.0601	11.4480	0.3795
H	0.1413	11.5039	-0.8969
C	0.7236	12.5478	0.9011
H	0.5971	12.4368	1.9861

H	1.8038	12.4851	0.7145
C	0.2195	13.9313	0.4750
H	-0.8594	13.9955	0.6624
H	0.3460	14.0427	-0.6089
C	0.9308	15.0827	1.1918
H	0.7912	15.0206	2.2758
H	2.0078	15.0645	0.9968
H	0.5507	16.0544	0.8638
H	1.0908	2.3479	-0.1050

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C	-0.0662	-0.1626	-0.0258
H	-0.1048	-0.1938	1.0698
H	0.9976	-0.1910	-0.2952
C	-0.7736	-1.3945	-0.5997
H	-1.8344	-1.3733	-0.3311
H	-0.7412	-1.3672	-1.6939
C	-0.1563	-2.7040	-0.1094
H	-0.1802	-2.7648	0.9848
H	0.9030	-2.7705	-0.3812
C	-0.8464	-3.9394	-0.6457
O	-0.2200	-5.0617	-0.2233
O	-1.8245	-3.9559	-1.3524
C	-0.7918	-6.3082	-0.6606
H	-1.8158	-6.4073	-0.2973
H	-0.7919	-6.3678	-1.7499
H	-0.1585	-7.0834	-0.2348
C	-0.6717	1.1598	-0.5118
H	-0.6274	1.1951	-1.6112
H	-1.7387	1.1918	-0.2570
C	0.0145	2.3904	0.0450
H	-0.1836	2.3329	1.3476
H	1.1063	2.3351	-0.0089
C	-0.5334	3.7369	-0.3812
H	-0.4714	3.8117	-1.4781
H	-1.6033	3.7866	-0.1409
C	0.1922	4.9331	0.2467
H	0.1196	4.8652	1.3388
H	1.2616	4.8717	0.0071
C	-0.3526	6.2886	-0.2165
H	-0.2746	6.3563	-1.3095
H	-1.4240	6.3466	0.0154
C	0.3664	7.4851	0.4166
H	0.2803	7.4213	1.5091
H	1.4393	7.4218	0.1931
C	-0.1672	8.8429	-0.0539
H	-1.2410	8.9057	0.1658
H	-0.0771	8.9079	-1.1461
C	0.5496	10.0383	0.5839
H	0.4550	9.9757	1.6759
H	1.6241	9.9722	0.3689
C	0.0230	11.3972	0.1087
H	-1.0517	11.4637	0.3228
H	0.1188	11.4602	-0.9832

C	0.7399	12.5916	0.7477
H	0.6428	12.5307	1.8397
H	1.8152	12.5247	0.5355
C	0.2172	13.9517	0.2715
H	-0.8566	14.0198	0.4847
H	0.3142	14.0131	-0.8194
C	0.9411	15.1380	0.9151
H	0.8325	15.1239	2.0043
H	2.0123	15.1166	0.6905
H	0.5456	16.0918	0.5547
H	-0.3949	2.2907	2.2908

$CH_3(CH_2)_8CH(CH_2)_5COOCH_3$

C	-0.1723	-0.1645	0.4287
H	-0.1018	-0.1724	1.5244
H	0.8449	-0.3470	0.0579
C	-1.0937	-1.2989	-0.0325
H	-2.1102	-1.1252	0.3346
H	-1.1658	-1.2978	-1.1247
C	-0.6149	-2.6721	0.4386
H	-0.5567	-2.7182	1.5319
H	0.4016	-2.8782	0.0844
C	-1.4952	-3.8140	-0.0208
O	-1.0306	-4.9970	0.4439
O	-2.4817	-3.7179	-0.7093
C	-1.7841	-6.1641	0.0671
H	-2.8086	-6.0935	0.4353
H	-1.8016	-6.2739	-1.0183
H	-1.2688	-7.0040	0.5281
C	-0.6381	1.2187	-0.0374
H	-0.7155	1.2245	-1.1317
H	-1.6489	1.4105	0.3417
C	0.2895	2.3583	0.4048
H	0.3777	2.3572	1.5024
H	1.3130	2.1431	0.0453
C	-0.1363	3.7107	-0.0618
C	0.5670	4.9493	0.3839
H	0.7471	4.9025	1.4685
H	1.5777	4.9874	-0.0642
C	-0.1702	6.2514	0.0406
H	-0.3589	6.2802	-1.0401
H	-1.1551	6.2429	0.5226
C	0.5921	7.5146	0.4545
H	0.7898	7.4820	1.5339
H	1.5753	7.5197	-0.0338
C	-0.1465	8.8144	0.1157
H	-1.1245	8.8150	0.6141
H	-0.3555	8.8405	-0.9617
C	0.6230	10.0802	0.5104
H	0.8354	10.0539	1.5872
H	1.5994	10.0803	0.0088
C	-0.1174	11.3796	0.1735
H	-1.0906	11.3831	0.6812
H	-0.3367	11.4017	-0.9020
C	0.6566	12.6460	0.5562
H	0.8775	12.6251	1.6315

H	1.6294	12.6436	0.0473
C	-0.0834	13.9459	0.2200
H	-1.0538	13.9508	0.7312
H	-0.3062	13.9661	-0.8538
C	0.7003	15.2053	0.6013
H	0.9068	15.2326	1.6759
H	1.6619	15.2454	0.0798
H	0.1469	16.1137	0.3468
H	-0.8306	3.7791	-0.8959

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C	-0.2244	-0.1571	0.4115
H	-0.0960	-0.1877	1.5015
H	0.7812	-0.2647	-0.0157
C	-1.0965	-1.3364	-0.0326
H	-2.1010	-1.2361	0.3905
H	-1.2260	-1.3139	-1.1193
C	-0.5095	-2.6868	0.3774
H	-0.3753	-2.7454	1.4638
H	0.4905	-2.8302	-0.0470
C	-1.3569	-3.8699	-0.0378
O	-0.7640	-5.0337	0.3160
O	-2.4206	-3.8175	-0.6053
C	-1.4792	-6.2363	-0.0224
H	-2.4537	-6.2525	0.4677
H	-1.6211	-6.3058	-1.1018
H	-0.8575	-7.0542	0.3352
C	-0.8009	1.2044	0.0087
H	-0.9256	1.2390	-1.0799
H	-1.8062	1.3120	0.4351
C	0.0645	2.3889	0.4554
H	0.1932	2.3510	1.5484
H	1.0735	2.2887	0.0345
C	-0.5039	3.7420	0.0796
H	-0.5145	3.7567	-1.2376
H	-1.5707	3.8364	0.3056
C	0.2987	4.9631	0.4802
H	0.4415	4.9504	1.5719
H	1.3058	4.8932	0.0488
C	-0.3470	6.2930	0.0726
H	-0.4982	6.3017	-1.0135
H	-1.3467	6.3584	0.5207
C	0.4721	7.5219	0.4822
H	0.6388	7.5019	1.5671
H	1.4665	7.4643	0.0211
C	-0.1880	8.8510	0.0979
H	-1.1802	8.9085	0.5639
H	-0.3610	8.8685	-0.9859
C	0.6297	10.0840	0.4988
H	0.8131	10.0604	1.5810
H	1.6175	10.0338	0.0228
C	-0.0425	11.4116	0.1304
H	-1.0284	11.4621	0.6106
H	-0.2310	11.4335	-0.9509

C	0.7745	12.6468	0.5251
H	0.9689	12.6230	1.6055
H	1.7582	12.6014	0.0396
C	0.0966	13.9740	0.1656
H	-0.8847	14.0207	0.6533
H	-0.0995	13.9978	-0.9133
C	0.9212	15.2026	0.5608
H	1.1035	15.2263	1.6400
H	1.8956	15.2019	0.0620
H	0.4109	16.1313	0.2903
H	-0.4505	3.7611	-2.2040

$CH_3(CH_2)_7CH(CH_2)_6COOCH_3$

C	-0.0411	-0.1023	-0.1577
H	-0.0282	-0.1960	0.9361
H	1.0093	-0.0266	-0.4678
C	-0.6647	-1.3613	-0.7700
H	-1.7130	-1.4424	-0.4651
H	-0.6763	-1.2779	-1.8614
C	0.0762	-2.6368	-0.3694
H	0.0964	-2.7574	0.7196
H	1.1276	-2.5961	-0.6766
C	-0.5201	-3.8975	-0.9567
O	0.1626	-4.9906	-0.5434
O	-1.4726	-3.9558	-1.6953
C	-0.3124	-6.2565	-1.0368
H	-1.3433	-6.4266	-0.7229
H	-0.2615	-6.2863	-2.1262
H	0.3480	-7.0040	-0.6025
C	-0.7750	1.1867	-0.5438
H	-0.7856	1.2824	-1.6371
H	-1.8257	1.1098	-0.2360
C	-0.1581	2.4477	0.0699
H	-0.1509	2.3530	1.1632
H	0.8918	2.5285	-0.2367
C	-0.8922	3.7398	-0.3149
C	-0.3214	4.9740	0.3008
C	-0.7321	6.3369	-0.1482
H	-0.7117	6.3852	-1.2475
H	-1.7907	6.5164	0.1175
C	0.1195	7.4744	0.4324
H	0.0874	7.4210	1.5279
H	1.1673	7.3172	0.1492
C	-0.3283	8.8682	-0.0199
H	-1.3797	9.0187	0.2578
H	-0.2936	8.9220	-1.1159
C	0.5164	10.0040	0.5684
H	0.4807	9.9500	1.6643
H	1.5679	9.8535	0.2918
C	0.0706	11.3997	0.1176
H	-0.9827	11.5478	0.3891
H	0.1119	11.4563	-0.9780
C	0.9093	12.5356	0.7140
H	0.8677	12.4796	1.8097
H	1.9632	12.3888	0.4433
C	0.4646	13.9321	0.2647

H	-0.5888	14.0785	0.5331
H	0.5094	13.9900	-0.8297
C	1.3058	15.0599	0.8696
H	1.2526	15.0502	1.9630
H	2.3596	14.9610	0.5902
H	0.9635	16.0414	0.5297
H	-0.9040	3.8450	-1.4100
H	-1.9572	3.6377	-0.0338
H	0.2362	4.8795	1.2297

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C	0.0298	-0.1466	-0.1999
H	0.1330	-0.2185	0.8908
H	1.0514	-0.1442	-0.6014
C	-0.7218	-1.3755	-0.7229
H	-1.7389	-1.3898	-0.3184
H	-0.8329	-1.3089	-1.8098
C	-0.0196	-2.6860	-0.3676
H	0.0999	-2.7896	0.7169
H	0.9971	-2.7127	-0.7758
C	-0.7421	-3.9187	-0.8658
O	-0.0757	-5.0422	-0.5125
O	-1.7723	-3.9333	-1.4942
C	-0.6657	-6.2863	-0.9320
H	-1.6627	-6.4002	-0.5041
H	-0.7371	-6.3282	-2.0199
H	0.0003	-7.0629	-0.5623
C	-0.6528	1.1789	-0.5558
H	-0.7459	1.2549	-1.6467
H	-1.6777	1.1752	-0.1631
C	0.0912	2.4084	-0.0238
H	0.1692	2.3404	1.0688
H	1.1196	2.4047	-0.4041
C	-0.5770	3.7370	-0.3990
C	0.1378	4.9585	0.1419
H	0.3895	4.8727	1.2036
H	1.3329	4.9296	-0.4110
C	-0.4317	6.3132	-0.2270
H	-0.4659	6.4065	-1.3203
H	-1.4794	6.3615	0.1083
C	0.3430	7.4956	0.3675
H	0.3471	7.4085	1.4616
H	1.3915	7.4332	0.0523
C	-0.2253	8.8620	-0.0306
H	-1.2789	8.9206	0.2728
H	-0.2192	8.9506	-1.1247
C	0.5419	10.0423	0.5760
H	0.5235	9.9610	1.6706
H	1.5981	9.9738	0.2849
C	-0.0072	11.4122	0.1618
H	-1.0651	11.4802	0.4474
H	0.0172	11.4952	-0.9326
C	0.7579	12.5906	0.7745
H	0.7278	12.5121	1.8692

H	1.8173	12.5190	0.4951
C	0.2187	13.9623	0.3534
H	-0.8399	14.0347	0.6316
H	0.2508	14.0419	-0.7402
C	0.9894	15.1321	0.9722
H	0.9459	15.1003	2.0656
H	2.0451	15.1068	0.6837
H	0.5810	16.0947	0.6519
H	-0.6544	3.8149	-1.4911
H	-1.6130	3.7393	-0.0261
H	2.1809	4.9162	-0.8800

$CH_3(CH_2)_6CH(CH_2)_7COOCH_3$

C	0.5462	-0.0752	-1.0574
H	0.6194	-0.2082	0.0300
H	1.5743	-0.1302	-1.4391
C	-0.2816	-1.2175	-1.6564
H	-1.3081	-1.1705	-1.2787
H	-0.3561	-1.0938	-2.7414
C	0.3075	-2.5929	-1.3445
H	0.3819	-2.7558	-0.2634
H	1.3330	-2.6783	-1.7220
C	-0.4860	-3.7431	-1.9252
O	0.0741	-4.9294	-1.5925
O	-1.4840	-3.6507	-2.5973
C	-0.5907	-6.1049	-2.0906
H	-1.6122	-6.1565	-1.7112
H	-0.6149	-6.0977	-3.1813
H	-0.0046	-6.9461	-1.7267
C	-0.0287	1.3136	-1.3576
H	-0.1017	1.4471	-2.4445
H	-1.0560	1.3695	-0.9757
C	0.7963	2.4595	-0.7613
H	0.8672	2.3259	0.3261
H	1.8246	2.4010	-1.1416
C	0.2245	3.8484	-1.0638
H	0.1577	3.9846	-2.1505
H	-0.8024	3.9123	-0.6842
C	1.0518	4.9952	-0.4661
H	1.1243	4.8679	0.6245
H	2.0937	4.9034	-0.8265
C	0.5268	6.3573	-0.7772
C	1.0466	7.5735	-0.0855
H	1.0912	7.3905	0.9988
H	2.0980	7.7516	-0.3797
C	0.2387	8.8497	-0.3586
H	-0.7992	8.6913	-0.0416
H	0.2044	9.0261	-1.4411
C	0.8028	10.0916	0.3395
H	0.8360	9.9146	1.4225
H	1.8439	10.2416	0.0250
C	0.0029	11.3693	0.0614
H	-1.0379	11.2207	0.3771
H	-0.0312	11.5454	-1.0217
C	0.5691	12.6122	0.7570
H	0.6005	12.4385	1.8406

H	1.6111	12.7593	0.4437
C	-0.2259	13.8923	0.4756
H	-1.2666	13.7471	0.7903
H	-0.2581	14.0657	-0.6071
C	0.3496	15.1286	1.1727
H	0.3613	15.0002	2.2598
H	1.3788	15.3197	0.8524
H	-0.2384	16.0236	0.9508
H	-0.0825	6.4871	-1.6686

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C	0.5318	-0.0757	-1.0888
H	0.6705	-0.2251	-0.0099
H	1.5396	-0.0550	-1.5240
C	-0.2508	-1.2579	-1.6707
H	-1.2582	-1.2827	-1.2425
H	-0.3868	-1.1213	-2.7480
C	0.4383	-2.5983	-1.4148
H	0.5763	-2.7757	-0.3426
H	1.4471	-2.6098	-1.8438
C	-0.3064	-3.7857	-1.9852
O	0.3064	-4.9444	-1.6482
O	-1.3089	-3.7409	-2.6554
C	-0.3047	-6.1503	-2.1421
H	-1.3239	-6.2448	-1.7646
H	-0.3267	-6.1494	-3.2329
H	0.3168	-6.9632	-1.7728
C	-0.1480	1.2775	-1.3259
H	-0.2831	1.4303	-2.4042
H	-1.1566	1.2553	-0.8940
C	0.6269	2.4625	-0.7387
H	0.7627	2.3065	0.3393
H	1.6355	2.4865	-1.1716
C	-0.0559	3.8151	-0.9699
H	-0.1860	3.9766	-2.0476
H	-1.0644	3.7913	-0.5404
C	0.7171	4.9973	-0.3727
H	0.8594	4.8377	0.7040
H	1.7292	5.0239	-0.8056
C	0.0574	6.3430	-0.5955
H	-0.2697	6.4959	-1.6287
H	-1.0976	6.2664	0.0345
C	0.7493	7.5542	-0.0041
H	0.8677	7.4109	1.0779
H	1.7714	7.6114	-0.4096
C	0.0266	8.8800	-0.2718
H	-0.9968	8.8169	0.1170
H	-0.0664	9.0267	-1.3555
C	0.7308	10.0928	0.3462
H	0.8183	9.9451	1.4304
H	1.7584	10.1501	-0.0361
C	0.0160	11.4214	0.0745
H	-1.0142	11.3601	0.4483
H	-0.0634	11.5743	-1.0097

C	0.7108	12.6329	0.7059
H	0.7880	12.4810	1.7905
H	1.7422	12.6941	0.3346
C	-0.0015	13.9628	0.4338
H	-1.0326	13.9012	0.8026
H	-0.0756	14.1169	-0.6497
C	0.6972	15.1664	1.0730
H	0.7534	15.0593	2.1610
H	1.7205	15.2744	0.6993
H	0.1659	16.0979	0.8587
H	-1.9099	6.2025	0.5573

$CH_3(CH_2)_5CH(CH_2)_8COOCH_3$

C	0.0354	-0.1110	-0.1875
H	0.0683	-0.1015	0.9099
H	1.0792	-0.1785	-0.5213
C	-0.7337	-1.3480	-0.6640
H	-1.7748	-1.2899	-0.3308
H	-0.7705	-1.3638	-1.7581
C	-0.1159	-2.6530	-0.1623
H	-0.0756	-2.6750	0.9329
H	0.9238	-2.7527	-0.4932
C	-0.8597	-3.8914	-0.6127
O	-0.2382	-5.0116	-0.1760
O	-1.8715	-3.9129	-1.2702
C	-0.8556	-6.2599	-0.5395
H	-1.8659	-6.3201	-0.1322
H	-0.9016	-6.3619	-1.6247
H	-0.2230	-7.0331	-0.1090
C	-0.5691	1.2065	-0.6853
H	-0.5994	1.1978	-1.7823
H	-1.6134	1.2722	-0.3541
C	0.1909	2.4497	-0.2094
H	0.2201	2.4577	0.8879
H	1.2357	2.3843	-0.5400
C	-0.4155	3.7663	-0.7074
H	-0.4378	3.7621	-1.8049
H	-1.4627	3.8262	-0.3834
C	0.3345	5.0106	-0.2206
H	0.3579	5.0176	0.8758
H	1.3805	4.9571	-0.5484
C	-0.2794	6.3280	-0.7156
H	-0.3205	6.3041	-1.8208
H	-1.3319	6.3846	-0.4005
C	0.4437	7.5517	-0.2600
C	-0.1545	8.9124	-0.3957
H	-1.2081	8.8839	-0.0806
H	-0.1907	9.2029	-1.4626
C	0.5852	10.0086	0.3844
H	0.6050	9.7395	1.4474
H	1.6321	10.0375	0.0567
C	-0.0369	11.3995	0.2209
H	-1.0849	11.3670	0.5461
H	-0.0582	11.6636	-0.8445
C	0.6979	12.4970	0.9983
H	0.7221	12.2326	2.0636

H	1.7454	12.5337	0.6716
C	0.0722	13.8876	0.8394
H	-0.9740	13.8512	1.1672
H	0.0475	14.1521	-0.2248
C	0.8128	14.9782	1.6187
H	0.8226	14.7605	2.6915
H	1.8537	15.0616	1.2899
H	0.3429	15.9564	1.4832
H	1.5044	7.4722	-0.0328

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C	0.0157	-0.1538	-0.1711
H	0.0184	-0.2206	0.9248
H	1.0695	-0.1780	-0.4786
C	-0.7143	-1.3689	-0.7536
H	-1.7644	-1.3553	-0.4450
H	-0.7230	-1.3086	-1.8467
C	-0.0807	-2.6928	-0.3265
H	-0.0618	-2.7867	0.7655
H	0.9673	-2.7507	-0.6410
C	-0.7901	-3.9126	-0.8730
O	-0.1608	-5.0473	-0.4884
O	-1.7836	-3.9096	-1.5582
C	-0.7475	-6.2809	-0.9420
H	-1.7651	-6.3829	-0.5621
H	-0.7681	-6.3168	-2.0322
H	-0.1106	-7.0686	-0.5452
C	-0.6014	1.1844	-0.5928
H	-0.5987	1.2541	-1.6882
H	-1.6561	1.2070	-0.2903
C	0.1199	2.4026	-0.0055
H	0.1129	2.3337	1.0900
H	1.1760	2.3767	-0.3041
C	-0.4916	3.7425	-0.4301
H	-0.4797	3.8150	-1.5254
H	-1.5488	3.7669	-0.1358
C	0.2267	4.9577	0.1666
H	0.2090	4.8894	1.2610
H	1.2848	4.9325	-0.1240
C	-0.3803	6.2987	-0.2634
H	-0.3570	6.3706	-1.3620
H	-1.4423	6.3288	0.0129
C	0.3234	7.5073	0.3191
H	0.1474	7.4111	1.6221
H	1.4137	7.4465	0.2444
C	-0.2217	8.8705	-0.0547
H	-1.2856	8.9221	0.2111
H	-0.1836	8.9778	-1.1500
C	0.5287	10.0411	0.5921
H	0.4827	9.9390	1.6830
H	1.5912	9.9793	0.3240
C	-0.0163	11.4147	0.1860
H	-1.0798	11.4752	0.4511
H	0.0302	11.5147	-0.9064

C	0.7323	12.5855	0.8324
H	0.6815	12.4888	1.9248
H	1.7972	12.5225	0.5723
C	0.1954	13.9616	0.4232
H	-0.8682	14.0257	0.6837
H	0.2466	14.0587	-0.6683
C	0.9506	15.1242	1.0739
H	0.8876	15.0751	2.1657
H	2.0113	15.1072	0.8039
H	0.5442	16.0902	0.7615
H	-0.0492	7.3442	2.5673

$CH_3(CH_2)_4CH(CH_2)_9COOCH_3$

C	0.0027	-0.1609	-0.1363
H	-0.0275	-0.2206	0.9596
H	1.0605	-0.2535	-0.4156
C	-0.7865	-1.3316	-0.7325
H	-1.8421	-1.2488	-0.4547
H	-0.7599	-1.2792	-1.8258
C	-0.2510	-2.6896	-0.2794
H	-0.2756	-2.7790	0.8127
H	0.8019	-2.8129	-0.5570
C	-1.0133	-3.8669	-0.8475
O	-0.4733	-5.0356	-0.4302
O	-1.9750	-3.8074	-1.5741
C	-1.1156	-6.2339	-0.9028
H	-2.1546	-6.2673	-0.5715
H	-1.0867	-6.2792	-1.9924
H	-0.5498	-7.0564	-0.4706
C	-0.5177	1.2106	-0.5807
H	-0.4887	1.2700	-1.6763
H	-1.5746	1.3041	-0.3002
C	0.2691	2.3855	0.0108
H	0.2417	2.3244	1.1066
H	1.3258	2.2919	-0.2717
C	-0.2518	3.7578	-0.4310
H	-0.2281	3.8179	-1.5268
H	-1.3074	3.8528	-0.1452
C	0.5380	4.9329	0.1562
H	0.5191	4.8693	1.2521
H	1.5927	4.8408	-0.1346
C	0.0107	6.3040	-0.2791
H	0.0273	6.3687	-1.3744
H	-1.0408	6.4017	0.0168
C	0.8057	7.4808	0.3033
H	0.8058	7.4176	1.4021
H	1.8683	7.3650	0.0188
C	0.3107	8.8239	-0.1200
C	0.8197	10.0803	0.5046
H	0.8694	9.9559	1.5966
H	1.8678	10.2548	0.1965
C	-0.0038	11.3311	0.1663
H	-1.0369	11.1808	0.5022
H	-0.0503	11.4440	-0.9243
C	0.5531	12.6172	0.7851
H	0.6045	12.5028	1.8760

H	1.5874	12.7643	0.4471
C	-0.2685	13.8669	0.4491
H	-1.3007	13.7225	0.7907
H	-0.3227	13.9800	-0.6406
C	0.2984	15.1486	1.0667
H	0.3319	15.0803	2.1588
H	1.3182	15.3384	0.7169
H	-0.3089	16.0204	0.8077
H	-0.2655	8.8988	-1.0393

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C	0.0181	-0.1700	-0.1476
H	-0.0212	-0.2425	0.9473
H	1.0810	-0.2272	-0.4171
C	-0.7295	-1.3573	-0.7641
H	-1.7903	-1.3072	-0.4985
H	-0.6914	-1.2940	-1.8564
C	-0.1610	-2.7037	-0.3165
H	-0.1938	-2.8026	0.7747
H	0.8975	-2.7960	-0.5847
C	-0.8857	-3.8966	-0.9011
O	-0.3192	-5.0536	-0.4865
O	-1.8412	-3.8571	-1.6371
C	-0.9253	-6.2649	-0.9735
H	-1.9651	-6.3294	-0.6494
H	-0.8881	-6.3003	-2.0632
H	-0.3402	-7.0754	-0.5442
C	-0.5404	1.1895	-0.5825
H	-0.5019	1.2626	-1.6769
H	-1.6026	1.2460	-0.3124
C	0.2015	2.3823	0.0309
H	0.1711	2.3031	1.1255
H	1.2622	2.3312	-0.2474
C	-0.3682	3.7410	-0.3920
H	-0.3437	3.8190	-1.4867
H	-1.4273	3.7921	-0.1084
C	0.3746	4.9360	0.2162
H	0.3638	4.8495	1.3104
H	1.4306	4.8957	-0.0813
C	-0.2161	6.2912	-0.1878
H	-0.2148	6.3767	-1.2820
H	-1.2675	6.3348	0.1206
C	0.5330	7.4883	0.4102
H	0.5603	7.3976	1.5039
H	1.5839	7.4579	0.0831
C	-0.0574	8.8321	0.0344
H	-1.2583	8.8390	0.5746
H	-0.2992	8.9126	-1.0301
C	0.6288	10.0667	0.5823
H	0.6890	9.9936	1.6760
H	1.6710	10.0794	0.2271
C	-0.0532	11.3836	0.1911
H	-1.0903	11.3697	0.5468
H	-0.1064	11.4503	-0.9031

C	0.6558	12.6262	0.7401
H	0.7176	12.5548	1.8339
H	1.6924	12.6437	0.3783
C	-0.0328	13.9421	0.3604
H	-1.0671	13.9246	0.7246
H	-0.0971	14.0134	-0.7323
C	0.6807	15.1803	0.9110
H	0.7316	15.1541	2.0041
H	1.7066	15.2464	0.5347
H	0.1631	16.1002	0.6252
H	-2.1108	8.8362	1.0360

$CH_3(CH_2)_3CH(CH_2)_{10}COOCH_3$

C	0.0127	-0.1477	-0.1307
H	-0.0209	-0.2083	0.9651
H	1.0762	-0.1679	-0.4026
C	-0.6912	-1.3700	-0.7301
H	-1.7508	-1.3612	-0.4557
H	-0.6650	-1.3147	-1.8233
C	-0.0642	-2.6883	-0.2769
H	-0.0780	-2.7756	0.8159
H	0.9930	-2.7430	-0.5591
C	-0.7524	-3.9146	-0.8355
O	-0.1156	-5.0433	-0.4453
O	-1.7373	-3.9212	-1.5328
C	-0.6845	-6.2822	-0.9068
H	-1.7048	-6.3956	-0.5373
H	-0.6938	-6.3165	-1.9971
H	-0.0434	-7.0638	-0.5049
C	-0.5970	1.1846	-0.5809
H	-0.5594	1.2469	-1.6760
H	-1.6611	1.2039	-0.3128
C	0.0990	2.4109	0.0201
H	0.0583	2.3493	1.1155
H	1.1640	2.3887	-0.2452
C	-0.5059	3.7445	-0.4331
H	-0.4651	3.8062	-1.5283
H	-1.5708	3.7674	-0.1678
C	0.1913	4.9701	0.1682
H	0.1505	4.9082	1.2635
H	1.2563	4.9462	-0.0969
C	-0.4112	6.3050	-0.2844
H	-0.3741	6.3654	-1.3799
H	-1.4752	6.3311	-0.0153
C	0.2924	7.5276	0.3135
H	0.2580	7.4686	1.4083
H	1.3546	7.5052	0.0393
C	-0.3109	8.8651	-0.1346
H	-1.3801	8.8911	0.1345
H	-0.3061	8.9107	-1.2381
C	0.3778	10.0663	0.4223
C	-0.1392	11.4455	0.1809
H	-1.1567	11.5404	0.5986
H	-0.2731	11.6089	-0.9021
C	0.7451	12.5604	0.7537
H	0.8673	12.4020	1.8326

H	1.7488	12.4811	0.3175
C	0.1958	13.9693	0.5079
H	-0.8059	14.0483	0.9480
H	0.0663	14.1234	-0.5704
C	1.0905	15.0747	1.0762
H	1.2132	14.9671	2.1586
H	2.0882	15.0460	0.6268
H	0.6701	16.0664	0.8870
H	1.2902	9.9353	0.9970

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C	0.0355	-0.1566	-0.1707
H	0.0615	-0.2170	0.9252
H	1.0821	-0.1914	-0.5008
C	-0.7166	-1.3691	-0.7301
H	-1.7609	-1.3424	-0.4027
H	-0.7447	-1.3175	-1.8233
C	-0.0886	-2.6958	-0.3037
H	-0.0543	-2.7835	0.7883
H	0.9543	-2.7645	-0.6333
C	-0.8151	-3.9127	-0.8338
O	-0.2013	-5.0509	-0.4344
O	-1.8079	-3.9051	-1.5198
C	-0.8028	-6.2821	-0.8749
H	-1.8235	-6.3653	-0.4986
H	-0.8189	-6.3317	-1.9646
H	-0.1786	-7.0732	-0.4651
C	-0.5800	1.1841	-0.5867
H	-0.6027	1.2471	-1.6822
H	-1.6271	1.2173	-0.2596
C	0.1644	2.4003	-0.0243
H	0.1891	2.3338	1.0712
H	1.2112	2.3682	-0.3535
C	-0.4530	3.7423	-0.4336
H	-0.4740	3.8123	-1.5290
H	-1.5008	3.7721	-0.1079
C	0.2874	4.9571	0.1372
H	0.3120	4.8832	1.2321
H	1.3344	4.9303	-0.1918
C	-0.3337	6.3002	-0.2627
H	-0.3544	6.3786	-1.3575
H	-1.3817	6.3244	0.0630
C	0.4032	7.5114	0.3193
H	0.4257	7.4319	1.4128
H	1.4500	7.4923	-0.0100
C	-0.2232	8.8549	-0.0739
H	-1.2744	8.8780	0.2416
H	-0.2405	8.9389	-1.1717
C	0.4970	10.0599	0.4958
H	0.3772	9.9437	1.8033
H	1.5835	10.0080	0.3739
C	-0.0735	11.4243	0.1673
H	-1.1236	11.4645	0.4848
H	-0.0889	11.5476	-0.9268

C	0.6991	12.5911	0.7944
H	0.7169	12.4673	1.8840
H	1.7455	12.5491	0.4651
C	0.1161	13.9659	0.4499
H	-0.9289	14.0071	0.7805
H	0.0949	14.0873	-0.6401
C	0.8947	15.1260	1.0769
H	0.9058	15.0504	2.1688
H	1.9351	15.1342	0.7363
H	0.4527	16.0914	0.8155
H	0.2203	9.8632	2.7551

$CH_3(CH_2)_2CH(CH_2)_{11}COOCH_3$

C	0.0074	-0.1623	-0.1542
H	0.0266	-0.2314	0.9414
H	1.0544	-0.2211	-0.4797
C	-0.7720	-1.3513	-0.7263
H	-1.8165	-1.3023	-0.4023
H	-0.7946	-1.2899	-1.8191
C	-0.1773	-2.6962	-0.3090
H	-0.1506	-2.7941	0.7824
H	0.8654	-2.7863	-0.6339
C	-0.9292	-3.8914	-0.8527
O	-0.3371	-5.0465	-0.4695
O	-1.9236	-3.8555	-1.5354
C	-0.9642	-6.2600	-0.9233
H	-1.9853	-6.3276	-0.5449
H	-0.9845	-6.2957	-2.0135
H	-0.3546	-7.0683	-0.5253
C	-0.5717	1.1967	-0.5633
H	-0.5900	1.2665	-1.6585
H	-1.6184	1.2557	-0.2385
C	0.2035	2.3895	0.0072
H	0.2221	2.3183	1.1026
H	1.2503	2.3295	-0.3181
C	-0.3744	3.7496	-0.4001
H	-0.3938	3.8209	-1.4954
H	-1.4208	3.8101	-0.0741
C	0.4019	4.9422	0.1699
H	0.4229	4.8697	1.2651
H	1.4480	4.8824	-0.1577
C	-0.1769	6.3028	-0.2346
H	-0.1998	6.3751	-1.3298
H	-1.2223	6.3633	0.0948
C	0.6011	7.4950	0.3338
H	0.6273	7.4201	1.4287
H	1.6457	7.4368	0.0010
C	0.0177	8.8543	-0.0656
H	-1.0246	8.9174	0.2694
H	-0.0077	8.9316	-1.1600
C	0.7985	10.0479	0.5019
H	0.8367	9.9754	1.5992
H	1.8539	9.9639	0.1810
C	0.2530	11.3803	0.1079
C	0.7279	12.6432	0.7457
H	0.7941	12.5052	1.8353

H	1.7661	12.8578	0.4291
C	-0.1391	13.8721	0.4364
H	-1.1628	13.6812	0.7775
H	-0.1981	14.0019	-0.6508
C	0.3870	15.1587	1.0777
H	0.4265	15.0704	2.1682
H	1.3984	15.3907	0.7287
H	-0.2510	16.0138	0.8379
H	-0.3356	11.4506	-0.8040

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C	0.0291	-0.1662	-0.1682
H	0.0366	-0.2372	0.9275
H	1.0803	-0.2131	-0.4819
C	-0.7314	-1.3623	-0.7509
H	-1.7803	-1.3234	-0.4400
H	-0.7410	-1.3002	-1.8439
C	-0.1297	-2.7019	-0.3269
H	-0.1136	-2.7994	0.7648
H	0.9170	-2.7834	-0.6409
C	-0.8660	-3.9034	-0.8781
O	-0.2717	-5.0538	-0.4840
O	-1.8510	-3.8756	-1.5747
C	-0.8849	-6.2723	-0.9434
H	-1.9101	-6.3461	-0.5775
H	-0.8913	-6.3101	-2.0336
H	-0.2749	-7.0758	-0.5362
C	-0.5606	1.1869	-0.5812
H	-0.5655	1.2600	-1.6762
H	-1.6121	1.2322	-0.2700
C	0.1917	2.3877	0.0033
H	0.2002	2.3107	1.0984
H	1.2426	2.3450	-0.3116
C	-0.4031	3.7410	-0.4022
H	-0.4107	3.8197	-1.4971
H	-1.4543	3.7817	-0.0885
C	0.3453	4.9426	0.1857
H	0.3594	4.8591	1.2803
H	1.3949	4.9075	-0.1344
C	-0.2593	6.2949	-0.2088
H	-0.2742	6.3794	-1.3032
H	-1.3085	6.3284	0.1119
C	0.4862	7.4976	0.3806
H	0.5088	7.4078	1.4744
H	1.5335	7.4712	0.0522
C	-0.1319	8.8469	-0.0017
H	-1.1763	8.8751	0.3311
H	-0.1569	8.9382	-1.0952
C	0.6155	10.0501	0.5859
H	0.6595	9.9590	1.6790
H	1.6619	10.0285	0.2435
C	0.0102	11.3898	0.2192
H	-1.1875	11.3856	0.7673
H	-0.2391	11.4720	-0.8434

C	0.6900	12.6278	0.7672
H	0.7489	12.5563	1.8612
H	1.7329	12.6455	0.4141
C	0.0049	13.9427	0.3748
H	-1.0331	13.9240	0.7251
H	-0.0423	14.0102	-0.7187
C	0.7130	15.1798	0.9336
H	0.7460	15.1563	2.0274
H	1.7447	15.2437	0.5733
H	0.2008	16.0993	0.6375
H	-2.0371	11.3763	1.2335

CH_3CH_2 $CH(CH_2)_{12}COOCH_3$

C	0.0219	-0.1520	-0.1413
H	0.0303	-0.2121	0.9550
H	1.0736	-0.1866	-0.4546
C	-0.7210	-1.3648	-0.7123
H	-1.7694	-1.3407	-0.3985
H	-0.7349	-1.3110	-1.8057
C	-0.0960	-2.6912	-0.2806
H	-0.0737	-2.7797	0.8118
H	0.9505	-2.7585	-0.5986
C	-0.8160	-3.9085	-0.8186
O	-0.1947	-5.0459	-0.4288
O	-1.8105	-3.9019	-1.5021
C	-0.7909	-6.2774	-0.8755
H	-1.8092	-6.3695	-0.4949
H	-0.8121	-6.3190	-1.9655
H	-0.1600	-7.0678	-0.4746
C	-0.5868	1.1885	-0.5681
H	-0.5918	1.2502	-1.6639
H	-1.6391	1.2223	-0.2581
C	0.1488	2.4052	0.0043
H	0.1512	2.3437	1.1004
H	1.2020	2.3690	-0.3034
C	-0.4560	3.7469	-0.4245
H	-0.4566	3.8094	-1.5204
H	-1.5097	3.7829	-0.1186
C	0.2787	4.9632	0.1506
H	0.2780	4.9009	1.2466
H	1.3327	4.9260	-0.1541
C	-0.3235	6.3058	-0.2789
H	-0.3228	6.3684	-1.3749
H	-1.3775	6.3435	0.0259
C	0.4123	7.5210	0.2969
H	0.4122	7.4577	1.3928
H	1.4662	7.4834	-0.0084
C	-0.1893	8.8644	-0.1308
H	-1.2428	8.9022	0.1757
H	-0.1902	8.9281	-1.2268
C	0.5487	10.0770	0.4459
H	0.5530	10.0160	1.5408
H	1.6003	10.0441	0.1340
C	-0.0569	11.4230	0.0224
H	-1.1112	11.4670	0.3331
H	-0.0898	11.4620	-1.0828

C	0.6701	12.6146	0.5507
C	0.0773	13.9835	0.4998
H	-0.9642	13.9455	0.8502
H	0.0049	14.3214	-0.5503
C	0.8567	15.0309	1.3036
H	0.8948	14.7629	2.3633
H	1.8869	15.1137	0.9441
H	0.3952	16.0186	1.2219
H	1.7309	12.5177	0.7710

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C	0.0314	-0.1600	-0.1658
H	0.0411	-0.2239	0.9303
H	1.0826	-0.1991	-0.4806
C	-0.7186	-1.3669	-0.7398
H	-1.7673	-1.3361	-0.4273
H	-0.7306	-1.3116	-1.8331
C	-0.1033	-2.6979	-0.3086
H	-0.0839	-2.7882	0.7836
H	0.9435	-2.7716	-0.6244
C	-0.8297	-3.9099	-0.8502
O	-0.2206	-5.0519	-0.4546
O	-1.8193	-3.8958	-1.5408
C	-0.8236	-6.2790	-0.9044
H	-1.8456	-6.3620	-0.5318
H	-0.8364	-6.3220	-1.9944
H	-0.2025	-7.0740	-0.4974
C	-0.5712	1.1852	-0.5864
H	-0.5780	1.2514	-1.6819
H	-1.6227	1.2229	-0.2742
C	0.1714	2.3959	-0.0101
H	0.1813	2.3257	1.0855
H	1.2223	2.3599	-0.3254
C	-0.4342	3.7422	-0.4232
H	-0.4424	3.8147	-1.5185
H	-1.4856	3.7766	-0.1095
C	0.3057	4.9521	0.1583
H	0.3197	4.8746	1.2533
H	1.3557	4.9219	-0.1608
C	-0.3061	6.2990	-0.2434
H	-0.3194	6.3788	-1.3383
H	-1.3562	6.3279	0.0753
C	0.4324	7.5076	0.3429
H	0.4525	7.4226	1.4371
H	1.4807	7.4838	0.0178
C	-0.1870	8.8548	-0.0459
H	-1.2351	8.8774	0.2795
H	-0.2071	8.9424	-1.1401
C	0.5509	10.0607	0.5458
H	0.5747	9.9720	1.6385
H	1.5973	10.0443	0.2150
C	-0.0759	11.4073	0.1642
H	-1.1256	11.4293	0.4849
H	-0.0985	11.4980	-0.9330

C	0.6476	12.6086	0.7371
H	0.5351	12.4876	2.0453
H	1.7336	12.5581	0.6088
C	0.0760	13.9753	0.4191
H	-0.9716	14.0132	0.7423
H	0.0549	14.1027	-0.6735
C	0.8567	15.1318	1.0511
H	0.8664	15.0507	2.1416
H	1.8961	15.1393	0.7087
H	0.4137	16.0968	0.7912
H	0.3835	12.4032	2.9975

$CH_3CH(CH_2)_{13}COOCH_3$

C	0.0303	-0.1671	-0.1779
H	0.1079	-0.2520	0.9140
H	1.0603	-0.1909	-0.5575
C	-0.7440	-1.3692	-0.7292
H	-1.7717	-1.3544	-0.3522
H	-0.8239	-1.2927	-1.8182
C	-0.0925	-2.7028	-0.3638
H	-0.0104	-2.8189	0.7228
H	0.9356	-2.7562	-0.7399
C	-0.8330	-3.9101	-0.8967
O	-0.2187	-5.0557	-0.5198
O	-1.8351	-3.8899	-1.5688
C	-0.8294	-6.2787	-0.9702
H	-1.8469	-6.3624	-0.5857
H	-0.8557	-6.3145	-2.0603
H	-0.2048	-7.0775	-0.5762
C	-0.6067	1.1807	-0.5347
H	-0.6829	1.2664	-1.6262
H	-1.6366	1.2050	-0.1562
C	0.1634	2.3866	0.0151
H	0.2354	2.3024	1.1074
H	1.1949	2.3584	-0.3596
C	-0.4673	3.7361	-0.3470
H	-0.5367	3.8210	-1.4392
H	-1.4996	3.7646	0.0252
C	0.3024	4.9412	0.2053
H	0.3650	4.8602	1.2983
H	1.3369	4.9076	-0.1606
C	-0.3198	6.2920	-0.1665
H	-0.3789	6.3739	-1.2596
H	-1.3554	6.3258	0.1962
C	0.4494	7.4961	0.3889
H	0.5008	7.4189	1.4827
H	1.4874	7.4568	0.0334
C	-0.1636	8.8480	0.0059
H	-1.2026	8.8872	0.3580
H	-0.2113	8.9261	-1.0880
C	0.6046	10.0510	0.5647
H	0.6460	9.9762	1.6593
H	1.6456	10.0078	0.2186
C	-0.0024	11.4022	0.1728
H	-1.0430	11.4495	0.5157
H	-0.0371	11.4810	-0.9212

C	0.7651	12.6062	0.7364
H	0.8035	12.5385	1.8341
H	1.8217	12.5330	0.4163
C	0.2064	13.9315	0.3379
C	0.6541	15.1916	0.9963
H	0.6453	15.1010	2.0900
H	1.6900	15.4553	0.7222
H	0.0257	16.0425	0.7220
H	-0.3711	13.9950	-0.5798

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C	0.0319	-0.1649	-0.1757
H	0.0822	-0.2448	0.9181
H	1.0711	-0.1912	-0.5294
C	-0.7297	-1.3692	-0.7401
H	-1.7657	-1.3529	-0.3867
H	-0.7847	-1.2966	-1.8310
C	-0.0868	-2.7013	-0.3548
H	-0.0249	-2.8100	0.7341
H	0.9478	-2.7592	-0.7115
C	-0.8210	-3.9109	-0.8910
O	-0.2013	-5.0544	-0.5166
O	-1.8237	-3.8941	-1.5624
C	-0.8082	-6.2794	-0.9666
H	-1.8237	-6.3685	-0.5778
H	-0.8390	-6.3136	-2.0566
H	-0.1783	-7.0760	-0.5765
C	-0.5949	1.1816	-0.5546
H	-0.6396	1.2643	-1.6480
H	-1.6354	1.2064	-0.2061
C	0.1583	2.3893	0.0144
H	0.1970	2.3083	1.1086
H	1.2008	2.3600	-0.3286
C	-0.4613	3.7375	-0.3706
H	-0.4932	3.8214	-1.4646
H	-1.5058	3.7650	-0.0341
C	0.2872	4.9440	0.2072
H	0.3115	4.8636	1.3018
H	1.3340	4.9117	-0.1220
C	-0.3236	6.2937	-0.1866
H	-0.3412	6.3768	-1.2811
H	-1.3723	6.3246	0.1363
C	0.4207	7.4988	0.3995
H	0.4308	7.4195	1.4944
H	1.4716	7.4632	0.0836
C	-0.1816	8.8495	-0.0035
H	-1.2336	8.8845	0.3079
H	-0.1869	8.9308	-1.0983
C	0.5600	10.0532	0.5887
H	0.5598	9.9746	1.6836
H	1.6136	10.0156	0.2821
C	-0.0382	11.4036	0.1794
H	-1.0901	11.4442	0.4866
H	-0.0361	11.4845	-0.9151

C	0.7063	12.6051	0.7736
H	0.7160	12.5295	1.8689
H	1.7627	12.5653	0.4644
C	0.1336	13.9487	0.3717
H	-1.0810	13.9764	0.8724
H	-0.0789	14.0213	-0.6987
C	0.8197	15.1770	0.9280
H	0.8907	15.1325	2.0191
H	1.8410	15.2655	0.5363
H	0.2845	16.0921	0.6613
H	-1.9555	14.0096	1.2914

$CH_2\ (CH_2)_{14}COOCH_3$

C	0.0405	-0.1613	-0.1788
H	0.0621	-0.2225	0.9172
H	1.0876	-0.2102	-0.5056
C	-0.7263	-1.3633	-0.7410
H	-1.7714	-1.3218	-0.4177
H	-0.7492	-1.3116	-1.8343
C	-0.1188	-2.6985	-0.3116
H	-0.0900	-2.7861	0.7806
H	0.9242	-2.7822	-0.6371
C	-0.8604	-3.9055	-0.8438
O	-0.2634	-5.0519	-0.4424
O	-1.8510	-3.8845	-1.5326
C	-0.8803	-6.2748	-0.8846
H	-1.9033	-6.3439	-0.5119
H	-0.8933	-6.3245	-1.9744
H	-0.2684	-7.0743	-0.4726
C	-0.5559	1.1877	-0.5959
H	-0.5739	1.2518	-1.6914
H	-1.6037	1.2341	-0.2725
C	0.2016	2.3940	-0.0298
H	0.2246	2.3244	1.0656
H	1.2483	2.3513	-0.3582
C	-0.4012	3.7436	-0.4361
H	-0.4207	3.8168	-1.5312
H	-1.4492	3.7827	-0.1114
C	0.3497	4.9500	0.1386
H	0.3774	4.8696	1.2332
H	1.3954	4.9180	-0.1940
C	-0.2644	6.2993	-0.2516
H	-0.2891	6.3835	-1.3459
H	-1.3113	6.3275	0.0778
C	0.4799	7.5056	0.3320
H	0.5142	7.4137	1.4254
H	1.5240	7.4856	-0.0065
C	-0.1472	8.8538	-0.0406
H	-1.1921	8.8706	0.2957
H	-0.1794	8.9490	-1.1338
C	0.5916	10.0599	0.5504
H	0.6319	9.9588	1.6427
H	1.6341	10.0504	0.2065
C	-0.0466	11.4068	0.1922
H	-1.0895	11.4139	0.5351
H	-0.0859	11.5105	-0.9001

C	0.6889	12.6115	0.7882
H	0.7337	12.5108	1.8791
H	1.7289	12.6141	0.4381
C	0.0403	13.9595	0.4360
H	-1.0010	13.9723	0.7840
H	-0.0298	14.0346	-0.6646
C	0.7674	15.1422	0.9751
H	1.8418	15.1136	1.1190
H	0.2663	16.0929	1.1116

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C	0.0363	-0.1596	-0.1744
H	0.0431	-0.2140	0.9222
H	1.0876	-0.2127	-0.4868
C	-0.7256	-1.3634	-0.7393
H	-1.7749	-1.3175	-0.4307
H	-0.7333	-1.3187	-1.8331
C	-0.1271	-2.6971	-0.2929
H	-0.1130	-2.7770	0.8002
H	0.9199	-2.7858	-0.6039
C	-0.8653	-3.9059	-0.8255
O	-0.2697	-5.0509	-0.4182
O	-1.8529	-3.8872	-1.5188
C	-0.8847	-6.2753	-0.8588
H	-1.9089	-6.3437	-0.4891
H	-0.8942	-6.3282	-1.9484
H	-0.2739	-7.0734	-0.4423
C	-0.5513	1.1882	-0.6077
H	-0.5553	1.2455	-1.7037
H	-1.6030	1.2392	-0.2979
C	0.2020	2.3960	-0.0394
H	0.2131	2.3317	1.0565
H	1.2522	2.3499	-0.3562
C	-0.3941	3.7448	-0.4581
H	-0.4030	3.8128	-1.5537
H	-1.4449	3.7877	-0.1435
C	0.3542	4.9522	0.1181
H	0.3755	4.8742	1.2130
H	1.4018	4.9186	-0.2083
C	-0.2568	6.3011	-0.2781
H	-0.2767	6.3832	-1.3726
H	-1.3050	6.3311	0.0470
C	0.4865	7.5075	0.3067
H	0.5214	7.4142	1.3999
H	1.5305	7.4890	-0.0323
C	-0.1421	8.8559	-0.0630
H	-1.1863	8.8713	0.2754
H	-0.1764	8.9529	-1.1560
C	0.5973	10.0610	0.5292
H	0.6445	9.9546	1.6207
H	1.6376	10.0558	0.1789
C	-0.0467	11.4082	0.1825
H	-1.0870	11.4111	0.5328
H	-0.0937	11.5179	-0.9089

C	0.6901	12.6109	0.7813
H	0.7435	12.5000	1.8710
H	1.7278	12.6178	0.4237
C	0.0354	13.9570	0.4458
H	-1.0041	13.9595	0.7964
H	-0.0219	14.0666	-0.6482
C	0.7641	15.1486	1.0183
H	0.6703	15.0601	2.3786
H	1.8440	15.1633	0.8671
H	0.3064	16.1205	0.8359
H	0.5738	14.9856	3.2969

$CH_3(CH_2)_{14}COOCH_2$

C	-4.3660	-2.4879	-0.0501
H	-4.9467	-1.5608	-0.1428
H	-3.6194	-2.4600	-0.8546
C	-3.6536	-2.5097	1.3066
H	-4.3922	-2.5258	2.1144
H	-3.0767	-3.4344	1.4089
C	-2.7232	-1.3120	1.4984
H	-3.2713	-0.3664	1.4133
H	-1.9582	-1.2751	0.7140
C	-2.0124	-1.3078	2.8286
O	-1.1940	-0.2028	2.9271
O	-2.1092	-2.1216	3.7076
C	-0.4667	-0.0250	4.0667
C	-5.2934	-3.6890	-0.2661
H	-6.0362	-3.7222	0.5412
H	-4.7104	-4.6148	-0.1797
C	-6.0150	-3.6698	-1.6183
H	-6.6126	-2.7522	-1.6964
H	-5.2714	-3.6167	-2.4242
C	-6.9203	-4.8851	-1.8490
H	-6.3190	-5.8009	-1.7811
H	-7.6583	-4.9465	-1.0387
C	-7.6501	-4.8591	-3.1968
H	-8.2704	-3.9552	-3.2546
H	-6.9125	-4.7723	-4.0053
C	-8.5266	-6.0917	-3.4464
H	-7.9021	-6.9934	-3.4011
H	-9.2571	-6.1883	-2.6326
C	-9.2667	-6.0572	-4.7884
H	-9.9092	-5.1678	-4.8238
H	-8.5374	-5.9361	-5.6001
C	-10.1149	-7.3055	-5.0564
H	-9.4686	-8.1926	-5.0328
H	-10.8371	-7.4354	-4.2398
C	-10.8655	-7.2633	-6.3923
H	-11.5250	-6.3858	-6.4086
H	-10.1448	-7.1153	-7.2072
C	-11.6925	-8.5228	-6.6740
H	-11.0305	-9.3985	-6.6661
H	-12.4080	-8.6768	-5.8557
C	-12.4509	-8.4759	-8.0051
H	-13.1206	-7.6059	-8.0101
H	-11.7372	-8.3128	-8.8234

C	-13.2670	-9.7408	-8.2948
H	-12.5974	-10.6096	-8.2938
H	-13.9788	-9.9060	-7.4767
C	-14.0240	-9.6827	-9.6248
H	-14.5946	-10.5989	-9.8010
H	-14.7280	-8.8446	-9.6429
H	-13.3359	-9.5532	-10.4663
H	0.1500	0.8573	4.0607
H	-0.5438	-0.7539	4.8568

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C	-4.3753	-2.4758	-0.0533
H	-4.9820	-1.5632	-0.1210
H	-3.6382	-2.4108	-0.8644
C	-3.6500	-2.5044	1.2964
H	-4.3795	-2.5460	2.1109
H	-3.0551	-3.4201	1.3787
C	-2.7400	-1.2924	1.4970
H	-3.3066	-0.3572	1.4115
H	-1.9694	-1.2369	0.7205
C	-2.0489	-1.2689	2.8388
O	-1.1470	-0.2381	2.8927
O	-2.2318	-2.0235	3.7571
C	-0.4552	-0.0458	4.0932
H	-0.2675	-0.9634	4.6461
H	0.4097	0.5834	3.9046
H	-1.2175	0.6709	4.9065
H	-1.7898	1.1995	5.4700
C	-5.2716	-3.6974	-0.2852
H	-5.9983	-3.7736	0.5336
H	-4.6607	-4.6077	-0.2340
C	-6.0183	-3.6632	-1.6234
H	-6.6474	-2.7644	-1.6633
H	-5.2922	-3.5613	-2.4406
C	-6.8871	-4.9009	-1.8741
H	-6.2535	-5.7970	-1.8509
H	-7.6026	-5.0146	-1.0494
C	-7.6504	-4.8562	-3.2026
H	-8.3015	-3.9724	-3.2154
H	-6.9367	-4.7183	-4.0254
C	-8.4921	-6.1088	-3.4714
H	-7.8374	-6.9900	-3.4716
H	-9.1975	-6.2560	-2.6432
C	-9.2681	-6.0561	-4.7923
H	-9.9357	-5.1847	-4.7846
H	-8.5643	-5.8909	-5.6186
C	-10.0888	-7.3196	-5.0748
H	-9.4188	-8.1890	-5.0910
H	-10.7869	-7.4909	-4.2451
C	-10.8729	-7.2621	-6.3907
H	-11.5512	-6.3993	-6.3699
H	-10.1761	-7.0795	-7.2191
C	-11.6802	-8.5324	-6.6819
H	-11.0005	-9.3941	-6.7075

H	-12.3739	-8.7185	-5.8516
C	-12.4690	-8.4730	-7.9948
H	-13.1535	-7.6150	-7.9678
H	-11.7768	-8.2817	-8.8253
C	-13.2696	-9.7462	-8.2910
H	-12.5857	-10.6032	-8.3206
H	-13.9608	-9.9386	-7.4613
C	-14.0560	-9.6765	-9.6034
H	-14.6151	-10.5989	-9.7845
H	-14.7740	-8.8503	-9.5909
H	-13.3884	-9.5202	-10.4568