Supporting Information

TITLE: 6-Endo Or Not 6-Endo: That is the Question

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Contents:

(1) Cartesion coordinates from 6-31G* optimization,
Hartree-Fock 6-31G* energy in a.u. (Hartrees),
and MP2/6-31G* energy in a.u. (Hartrees), for:

each conformation of compound 6,

beginning with conformation C, (minima)
followed by the seven intermediate conformations for the first ring inversion,
followed by conformation A. (minima)
followed by the seven intermediate conformations for the second ring inversion,
followed by conformation B. (minima)
finally the data for conformation D. (minima)

(barriers to conformation D were not determined due to its high relative energy)

(2) 1H and 13C NMR, and HRMS specta of synthesized compounds.

C-A-B_PROF.1 (6-C)

		Cartesian Coordinates (Angstroms)		
Atom	Label	X	Y	Z
O	O2	-2.1086202	-1.5417334	-2.0895777
C	C1	-1.4539528	-0.9895998	-1.2863928
C	C6	-0.0791656	-1.4982815	-0.8067395
C	C2	0.8988588	-0.3301696	-0.6423896
H	H1	1.8146171	-0.6983178	-0.2005730
C	C4	0.3305260	0.8546231	0.1761810
Cl	Cl1	0.6244717	2.3764760	-0.7787648
C	C5	1.0212659	1.0225921	1.5267698
H	H6	2.0765027	1.2206394	1.3905707
H	H7	0.9112319	0.1167282	2.1123545
H	H8	0.5900696	1.8490602	2.0792189
C	C3	-1.1774960	0.7091258	0.3767554
H	H3	-1.3727552	0.0856232	1.2371253
H	H4	-1.6372802	1.6687320	0.5376344
O	O1	-1.8310157	0.1636699	-0.7518651
H	H5	1.1347182	0.0014803	-1.6422464
Cl	Cl2	0.5907822	-2.6378612	-1.9817151
Cl	Cl3	-0.3327585	-2.3727867	0.7436544

E(HF) = -1759.4457851 a.u.
E(MP2) = -1760.9715055 a.u.

C-A-B_PROF.2

Atom	Label	Cartesian Coordinates (Angstroms) X	Y	Z
O	O2	-2.1198870	-1.6755632	-1.9640275
C	C1	-1.4466433	-1.0543751	-1.2296722
C	C6	-0.0417379	-1.4894922	-0.7770052
C	C2	0.8831527	-0.2710152	-0.7017315
H	H1	1.8603440	-0.5807843	-0.3576317
C	C4	0.3344715	0.8794127	0.1732615
Cl	Cl1	0.7338058	2.4373823	-0.6735422
C	C5	0.9962849	0.9205135	1.5496641
H	H6	2.0611513	1.0868124	1.4503425
H	H7	0.8372341	-0.0150713	2.0693576
H	H8	0.5846733	1.7251322	2.1486222
C	C3	-1.1899034	0.7702520	0.3186880
H	H3	-1.4359146	0.2756016	1.2483547
H	H4	-1.6329207	1.7508091	0.3524354
O	O1	-1.8298423	0.1259369	-0.7631041
H	H5	0.9930126	0.0712609	-1.7210111
Cl	Cl2	0.6382123	-2.6445893	-1.9313201
Cl	Cl3	-0.2254933	-2.3122230	0.8083200

E(HF) = -1759.4447073 a.u.
E(MP2) = -1760.9704675 a.u.

C-A-B_PROF.3

Atom	Label	Cartesian Coordinates (Angstroms) X	Y	Z
O	O2	-2.1286909	-1.7792391	-1.8492831
C	C1	-1.4419368	-1.1103572	-1.1710834
C	C6	-0.0074959	-1.4849125	-0.7698592
C	C2	0.8715675	-0.2308915	-0.7360481
H	H1	1.8798060	-0.5006807	-0.4540761
C	C4	0.3357905	0.8929606	0.1769827
Cl	Cl1	0.8161137	2.4681376	-0.5898363
C	C5	0.9731554	0.8481726	1.5662721
H	H6	2.0468565	0.9620961	1.4901000
H	H7	0.7553642	-0.0901269	2.0544691
H	H8	0.5942989	1.6550543	2.1837521
C	C3	-1.2006439	0.8222452	0.2789414
H	H3	-1.4917160	0.4753992	1.2617342
H	H4	-1.6183016	1.8088915	0.1730222
O	O1	-1.8448837	0.0712846	-0.7289419
H	H5	0.9047720	0.1217391	-1.7578110
Cl	Cl2	0.6762130	-2.6167473	-1.9460630
Cl	Cl3	-0.1202688	-2.3130256	0.8177284

E(HF) = -1759.4419032 a.u.
E(MP2) = -1760.9675999 a.u.

C-A-B_PROF.4

Atom	Label	Cartesian Coordinates (Angstroms) X	Y	Z
O	O2	-2.1617909	-1.9519914	-1.5682424
C	C1	-1.4383050	-1.1924869	-1.0394305
C	C6	0.0482359	-1.4821928	-0.7809800
C	C2	0.8645523	-0.1873845	-0.7734008
H	H1	1.9013675	-0.4102681	-0.5637915
C	C4	0.3431365	0.8960635	0.1873473
Cl	Cl1	0.9483646	2.4816198	-0.4696323
C	C5	0.9088931	0.7675883	1.6029084
H	H6	1.9910863	0.7587464	1.5791688
H	H7	0.5625789	-0.1378573	2.0766821
H	H8	0.5933842	1.6111030	2.2060296
C	C3	-1.2026553	0.9145338	0.2042693
H	H3	-1.5648480	0.7708282	1.2134557
H	H4	-1.5628735	1.8756858	-0.1183364
O	O1	-1.8551733	0.0048395	-0.6623957
H	H5	0.8121791	0.1902289	-1.7858399
Cl	Cl2	0.6814092	-2.5221982	-2.0705542
Cl	Cl3	0.1304586	-2.3868578	0.7627428

E(HF) = -1759.4381871 a.u.
E(MP2) = -1760.9635797 a.u.

C-A-B_PROF.5

Atom	Label	Cartesian Coordinates (Angstroms) X	Y	Z
O	O2	-2.1645712	-1.8897275	-1.5859943
C	C1	-1.4370532	-1.2192265	-0.9524113
C	C6	0.0680062	-1.4930971	-0.8210699
C	C2	0.8628776	-0.1892571	-0.7889988
H	H1	1.9069253	-0.4012688	-0.6050103
C	C4	0.3456252	0.8572497	0.2068644
Cl	Cl1	0.9982435	2.4575989	-0.4031050
C	C5	0.8733229	0.7429617	1.6371791
H	H6	1.9530236	0.6660139	1.6429332
H	H7	0.4618277	-0.1272476	2.1306185
H	H8	0.5897277	1.6222696	2.2005651
C	C3	-1.1920686	0.9746648	0.1761036
H	H3	-1.5664266	1.1374993	1.1737220
H	H4	-1.5173970	1.7595976	-0.4849508
O	O1	-1.8830131	-0.2095830	-0.2232349
H	H5	0.7878885	0.2235946	-1.7866384
Cl	Cl2	0.6378366	-2.4575244	-2.1932063
Cl	Cl3	0.2752251	-2.4545179	0.6766343

E(HF) = -1759.4377441 a.u.
E(MP2) = -1760.9625838 a.u.

C-A-B_PROF.6

Atom	Label	Cartesian Coordinates (Angstroms) X	Y	Z
O	O2	-2.1983263	-1.8908812	-1.4405751
C	C1	-1.4320591	-1.2322920	-0.8432557
C	C6	0.0852676	-1.4819215	-0.8384077
C	C2	0.8711301	-0.1695119	-0.8005932
H	H1	1.9192974	-0.3773788	-0.6363239
C	C4	0.3546285	0.8590321	0.2138129
Cl	Cl1	1.0354649	2.4660237	-0.3414324
C	C5	0.8249712	0.7074637	1.6587980
H	H6	1.9001852	0.5906470	1.7042121
H	H7	0.3644475	-0.1550841	2.1227924
H	H8	0.5501704	1.5883145	2.2234234
C	C3	-1.1698046	0.9993111	0.1202541
H	H3	-1.5744180	1.3466923	1.0561816
H	H4	-1.4707437	1.6321149	-0.6995592
O	O1	-1.8216326	-0.2643995	-0.0208750
H	H5	0.7775717	0.2615312	-1.7889553
Cl	Cl2	0.5658780	-2.3802866	-2.2881166
Cl	Cl3	0.4179719	-2.4993748	0.5986197

E(HF) = -1759.4414988 a.u.
E(MP2) = -1760.9663351 a.u.

C-A-B_PROF.7

Atom	Label	Cartesian Coordinates (Angstroms) X	Y	Z
O	O2	-2.2116665	-1.9609326	-1.2237806
C	C1	-1.4232397	-1.2486328	-0.7262984
C	C6	0.0998797	-1.4559155	-0.8445988
C	C2	0.8814890	-0.1369574	-0.8135114
H	H1	1.9323923	-0.3437459	-0.6666797
C	C4	0.3662917	0.8782350	0.2147280
Cl	Cl1	1.0753783	2.4853743	-0.2731472
C	C5	0.7727442	0.6559147	1.6688157
H	H6	1.8411417	0.5022638	1.7523064
H	H7	0.2665442	-0.2073851	2.0794466
H	H8	0.5029265	1.5229983	2.2572736
C	C3	-1.1457684	1.0213604	0.0612185
H	H3	-1.5766853	1.5237765	0.9112793
H	H4	-1.4092011	1.5308100	-0.8545632
O	O1	-1.7795116	-0.2548949	0.0846167
H	H5	0.7717574	0.3049471	-1.7953242
Cl	Cl2	0.4816111	-2.2985114	-2.3575520
Cl	Cl3	0.5539166	-2.5187044	0.5257709

E(HF) = -1759.4450123 a.u.
E(MP2) = -1760.9702929 a.u.

C-A-B_PROF.8 (6-A)

Atom	Label	Cartesian Coordinates (Angstroms) X	Y	Z
O	O2	-2.2013718	-2.0414329	-0.9889147
C	C1	-1.4124895	-1.2598165	-0.6109570
C	C6	0.1079245	-1.4252410	-0.8454642
C	C2	0.8944570	-0.1043203	-0.8194286
H	H1	1.9448842	-0.3164654	-0.6777746
C	C4	0.3758261	0.9019373	0.2164011
Cl	Cl1	1.1080955	2.5062956	-0.2064058
C	C5	0.7250711	0.6037469	1.6713268
H	H6	1.7879937	0.4328693	1.7849741
H	H7	0.1945911	-0.2703433	2.0212975
H	H8	0.4444934	1.4441982	2.2934065
C	C3	-1.1256833	1.0390857	0.0051196
H	H3	-1.5779987	1.6757736	0.7477710
H	H4	-1.3428307	1.4373753	-0.9777096
O	O1	-1.7584734	-0.2229375	0.1506743
H	H5	0.7822009	0.3451227	-1.7970380
Cl	Cl2	0.3814847	-2.2115505	-2.4136459
Cl	Cl3	0.6718253	-2.5342968	0.4463678

E(HF) = -1759.4463559 a.u.
E(MP2) = -1760.9723128 a.u.

C-A-B_PROF.9

Atom	Label	Cartesian Coordinates (Angstroms) X	Y	Z
O	O2	-2.1393268	-2.1740156	-0.6258256
C	C1	-1.3933820	-1.2806604	-0.4726292
C	C6	0.1059097	-1.4027969	-0.8549849
C	C2	0.9248516	-0.0957058	-0.8123800
H	H1	1.9551355	-0.3296314	-0.5876390
C	C4	0.3791037	0.9127548	0.2048898
Cl	Cl1	1.1554328	2.5078140	-0.1590583
C	C5	0.6626190	0.5744914	1.6652283
H	H6	1.7241394	0.4344909	1.8250878
H	H7	0.1493282	-0.3318548	1.9576154
H	H8	0.3221654	1.3791021	2.3048745
C	C3	-1.1068942	1.0798444	-0.0687865
H	H3	-1.5686969	1.7625815	0.6256407
H	H4	-1.2756504	1.4365850	-1.0767439
O	O1	-1.7792531	-0.1544337	0.1134570
H	H5	0.8814476	0.3574957	-1.7915411
Cl	Cl2	0.1905457	-2.0655027	-2.5085986
Cl	Cl3	0.8125248	-2.6105583	0.2613939

E(HF) = -1759.4454179 a.u.
E(MP2) = -1760.9717095 a.u.

C-A-B_PROF.10

Atom	Label	Cartesian Coordinates (Angstroms) X	Y	Z
O	O2	-2.0052168	-2.2540713	-0.1868741
C	C1	-1.3383605	-1.2948333	-0.3095535
C	C6	0.1093871	-1.3882455	-0.8662771
C	C2	0.9630754	-0.0972010	-0.7903419
H	H1	1.9739730	-0.3510626	-0.5096897
C	C4	0.3812184	0.9163705	0.1967397
Cl	Cl1	1.1983230	2.5011049	-0.1058230
C	C5	0.5863154	0.5482651	1.6633904
H	H6	1.6416801	0.4464061	1.8816321
H	H7	0.0994235	-0.3891629	1.9031865
H	H8	0.1745161	1.3164281	2.3058247
C	C3	-1.0844993	1.1077653	-0.1595097
H	H3	-1.5634714	1.8275427	0.4842317
H	H4	-1.1901870	1.4291440	-1.1875355
O	O1	-1.7962469	-0.1010126	0.0332067
H	H5	0.9873423	0.3568791	-1.7685444
Cl	Cl2	-0.0671637	-1.8628624	-2.5850785
Cl	Cl3	0.9298913	-2.7114543	0.0010159

E(HF) = -1759.4439532 a.u.
E(MP2) = -1760.9704582 a.u.

C-A-B_PROF.11

Atom	Label	Cartesian Coordinates (Angstroms) X	Y	Z
O	O2	-1.8588614	-2.2799324	0.1330380
C	C1	-1.2761184	-1.3124547	-0.1898866
C	C6	0.0992825	-1.3786657	-0.9054277
C	C2	1.0071649	-0.1273479	-0.7372740
H	H1	1.9788649	-0.4297250	-0.3779505
C	C4	0.3816308	0.9131075	0.1931026
Cl	Cl1	1.2049195	2.4939710	-0.1072314
C	C5	0.5316757	0.5726743	1.6738453
H	H6	1.5798379	0.5240133	1.9397469
H	H7	0.0812709	-0.3857002	1.9056473
H	H8	0.0549498	1.3259504	2.2884335
C	C3	-1.0708549	1.0888549	-0.2263700
H	H3	-1.5682232	1.8443974	0.3597303
H	H4	-1.1389345	1.3515608	-1.2738911
O	O1	-1.7875213	-0.1083144	0.0140307
H	H5	1.1485025	0.3200505	-1.7082714
Cl	Cl2	-0.3182121	-1.5830264	-2.6412235
Cl	Cl3	0.9506266	-2.8294134	-0.3400484

E(HF) = -1759.4435542 a.u.
E(MP2) = -1760.9700600 a.u.

C-A-B_PROF.12

Atom	Label	Cartesian Coordinates (Angstroms) X	Y	Z
O	O2	-1.7594601	-2.3189409	0.2548275
C	C1	-1.2366785	-1.3457677	-0.1443727
C	C6	0.0808933	-1.3692889	-0.9568452
C	C2	1.0382348	-0.1772839	-0.6732564
H	H1	1.9381652	-0.5437034	-0.2029791
C	C4	0.3794026	0.9090489	0.1860058
Cl	Cl1	1.1845759	2.4873177	-0.1725605
C	C5	0.5133950	0.6386757	1.6833668
H	H6	1.5580360	0.6287046	1.9670842
H	H7	0.0826573	-0.3204965	1.9477263
H	H8	0.0080084	1.4050231	2.2575807
C	C3	-1.0739622	1.0480306	-0.2475063
H	H3	-1.5804255	1.8214528	0.3062923
H	H4	-1.1460759	1.2635237	-1.3046432
O	O1	-1.7698460	-0.1489338	0.0527127
H	H5	1.3296419	0.2431680	-1.6226369
Cl	Cl2	-0.4608156	-1.3180529	-2.6719734
Cl	Cl3	0.9142534	-2.9024773	-0.6588222

E(HF) = -1759.4443639 a.u.
E(MP2) = -1760.9709573 a.u.

C-A-B_PROF.13

Atom	Label	Cartesian Coordinates (Angstroms) X	Y	Z
O	O2	-1.7164921	-2.3814173	0.2359568
C	C1	-1.2215094	-1.3909725	-0.1561028
C	C6	0.0644566	-1.3611837	-1.0104831
C	C2	1.0524769	-0.2377991	-0.6056906
H	H1	1.8404821	-0.6708638	-0.0074309
C	C4	0.3743628	0.9050529	0.1749032
Cl	Cl1	1.1467825	2.4743357	-0.2842740
C	C5	0.5257318	0.7281315	1.6849552
H	H6	1.5729332	0.7343169	1.9597392
H	H7	0.0951069	-0.2141638	2.0052844
H	H8	0.0259017	1.5277464	2.2170705
C	C3	-1.0910897	1.0050078	-0.2311635
H	H3	-1.5987416	1.7724364	0.3297767
H	H4	-1.1967108	1.2103412	-1.2857063
O	O1	-1.7526241	-0.2040988	0.1018708
H	H5	1.5097439	0.1362477	-1.5078516
Cl	Cl2	-0.5068006	-1.1027954	-2.6979099
Cl	Cl3	0.8759901	-2.9303221	-0.9229440

E(HF) = -1759.4452271 a.u.
E(MP2) = -1760.9717444 a.u.

C-A-B_PROF.14

Atom	Label	Cartesian Coordinates (Angstroms) X	Y	Z
O	O2	-1.7574838	-2.4830057	0.0126471
C	C1	-1.2380713	-1.4631402	-0.2511612
C	C6	0.0530959	-1.3506844	-1.0873249
C	C2	1.0422216	-0.3257681	-0.4986139
H	H1	1.6396129	-0.8453859	0.2375203
C	C4	0.3629754	0.8945949	0.1698515
Cl	Cl1	1.0650498	2.4288905	-0.4873187
C	C5	0.5872706	0.8831301	1.6809423
H	H6	1.6459567	0.8826802	1.9086081
H	H7	0.1406779	-0.0059216	2.1137681
H	H8	0.1372664	1.7530462	2.1427719
C	C3	-1.1272868	0.9332823	-0.1588183
H	H3	-1.6330565	1.6676788	0.4464557
H	H4	-1.3013342	1.1581212	-1.1981355
O	O1	-1.7247339	-0.3071334	0.1802213
H	H5	1.7124407	-0.0203546	-1.2866450
Cl	Cl2	-0.4519076	-0.8706314	-2.7436002
Cl	Cl3	0.8473065	-2.9293991	-1.1811686

E(HF) = -1759.4457210 a.u.
E(MP2) = -1760.9718143 a.u.

C-A-B_PROF.15 (6B)

Atom	Label	Cartesian Coordinates (Angstroms) X	Y	Z
O	O2	-2.2282889	-2.2247642	-0.1655259
C	C1	-1.4613394	-1.3506078	-0.3264654
C	C6	-0.0231930	-1.5507035	-0.8464950
C	C2	0.9487057	-0.6448719	-0.0816511
C	C4	0.4801755	0.8225514	0.0619807
Cl	Cl1	1.5096384	1.9205192	-0.9474046
C	C5	0.6018258	1.2739332	1.5158391
H	H6	1.6101460	1.1250898	1.8830637
H	H7	-0.0810358	0.6960323	2.1304578
H	H8	0.3529449	2.3227234	1.6142860
C	C3	-0.9556121	0.9876502	-0.4445025
H	H3	-1.4112310	1.8685148	-0.0222912
H	H4	-0.9926379	1.0598005	-1.5183734
O	O1	-1.7599146	-0.0954852	-0.0078712
H	H2	1.9246925	-0.7049903	-0.5379785
H	H9	1.0310879	-1.0726911	0.9099561
Cl	Cl2	-0.0178595	-1.1979575	-2.6032580
Cl	Cl3	0.4718957	-3.2347430	-0.6137663

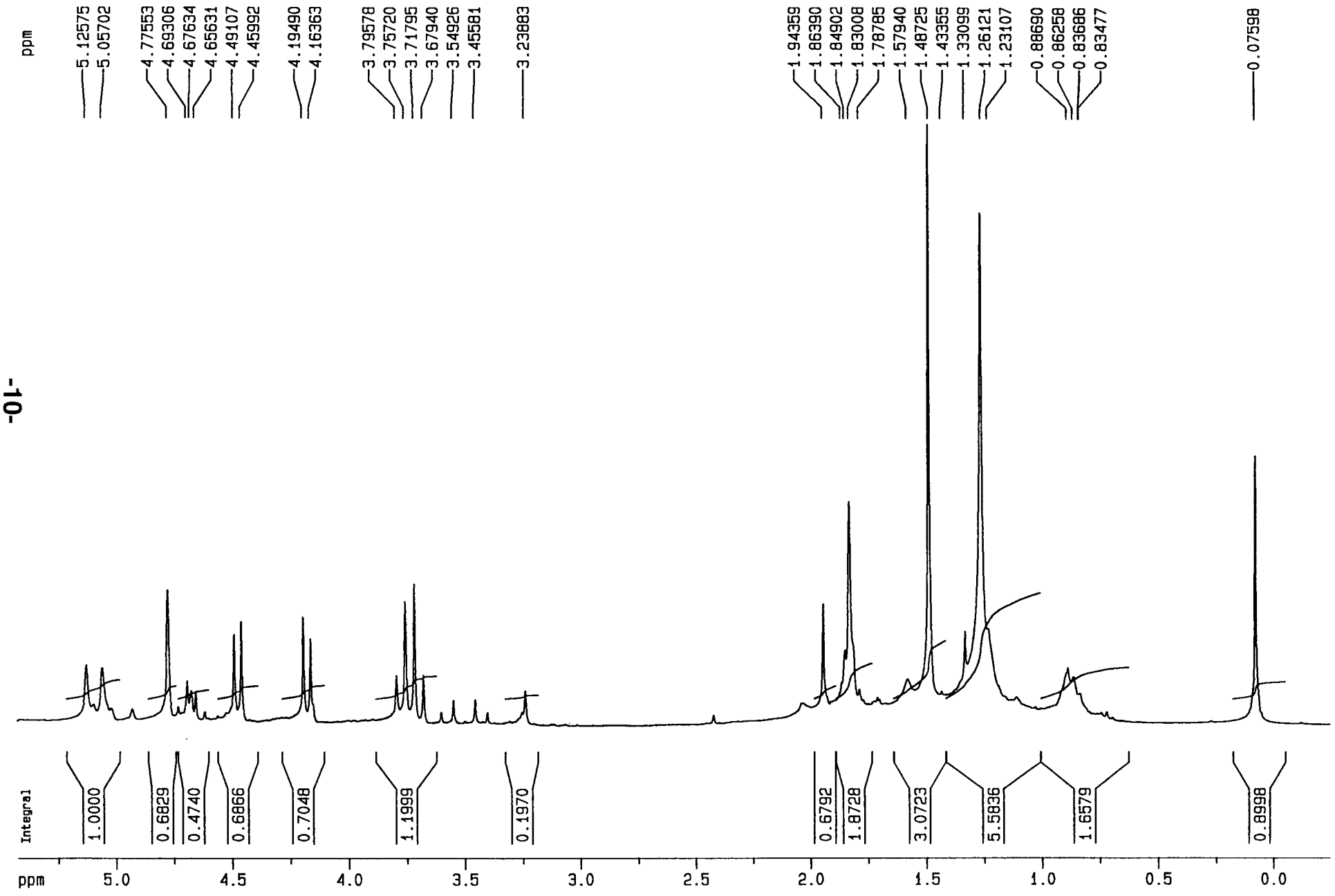
E(HF) = -1759.4461836 a.u.
E(MP2) = -1760.9721983 a.u.

6D

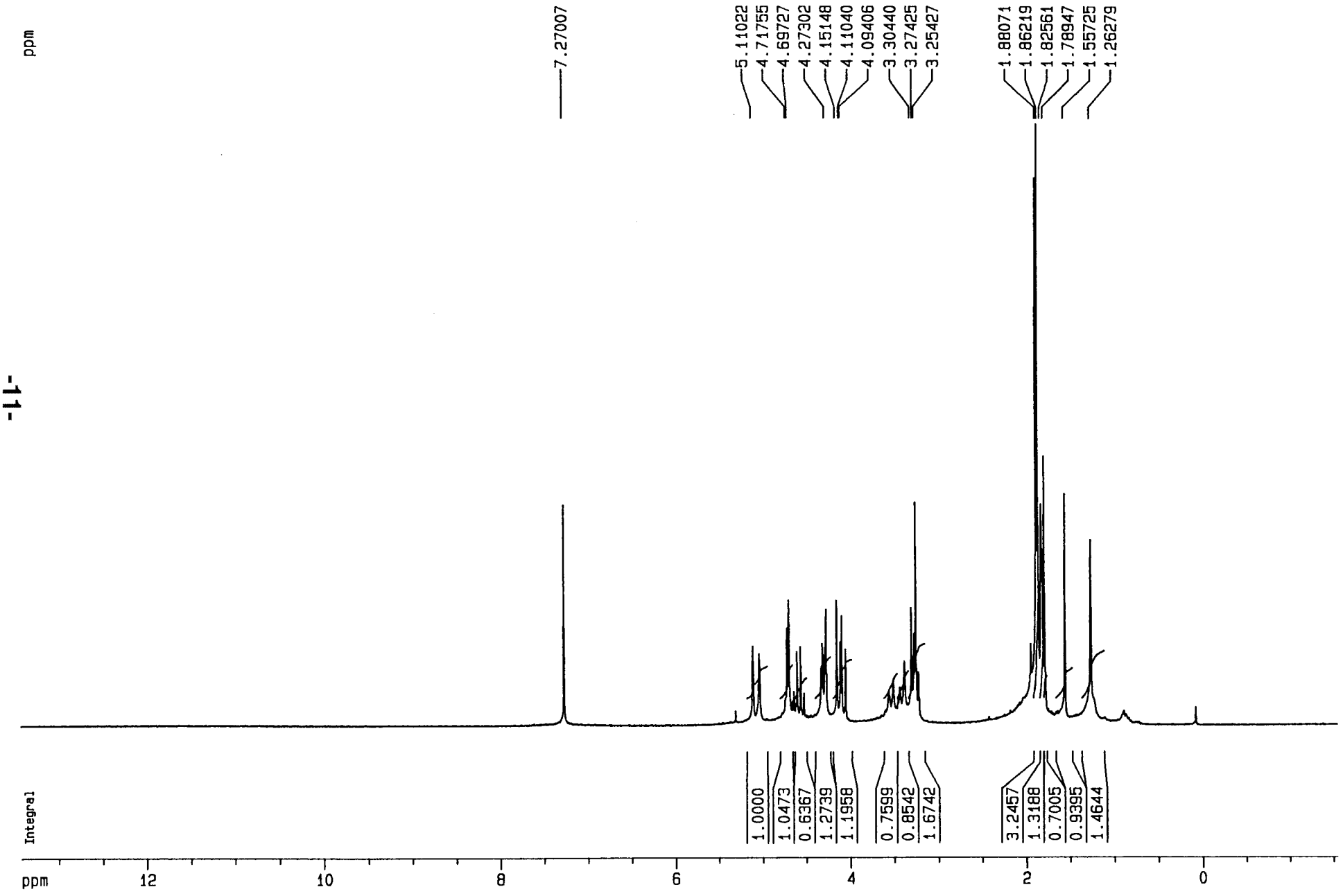
Atom	Label	Cartesian Coordinates (Angstroms) X	Y	Z
O	O2	-2.0128113	-2.6749503	0.0132847
C	C1	-1.3467625	-1.7198489	-0.1335853
C	C6	0.1915696	-1.7968213	-0.2776293
C	C5	0.9284333	-0.4908276	0.0632851
H	H5	1.0576560	-0.4798881	1.1394904
H	H6	1.9138673	-0.5108340	-0.3800448
C	C4	0.1804831	0.7980241	-0.2846212
C	C3	-1.2556280	0.6554530	0.1891579
H	H3	-1.2680041	0.6402137	1.2743172
H	H4	-1.8686937	1.4729567	-0.1520418
O	O1	-1.8842362	-0.5137513	-0.2906890
Cl	Cl1	0.1806519	1.1165314	-2.0641874
C	C2	0.8457838	1.9952831	0.3921278
H	H1	1.8701844	2.0976957	0.0574824
H	H2	0.8466964	1.8678049	1.4699611
H	H10	0.3188580	2.9104900	0.1520549
Cl	Cl2	0.4927042	-2.2927883	-1.9668380
Cl	Cl3	0.8092481	-3.0747426	0.7984750

E(HF) = -1759.4433497 a.u.
E(MP2) = -1760.9689031 a.u.

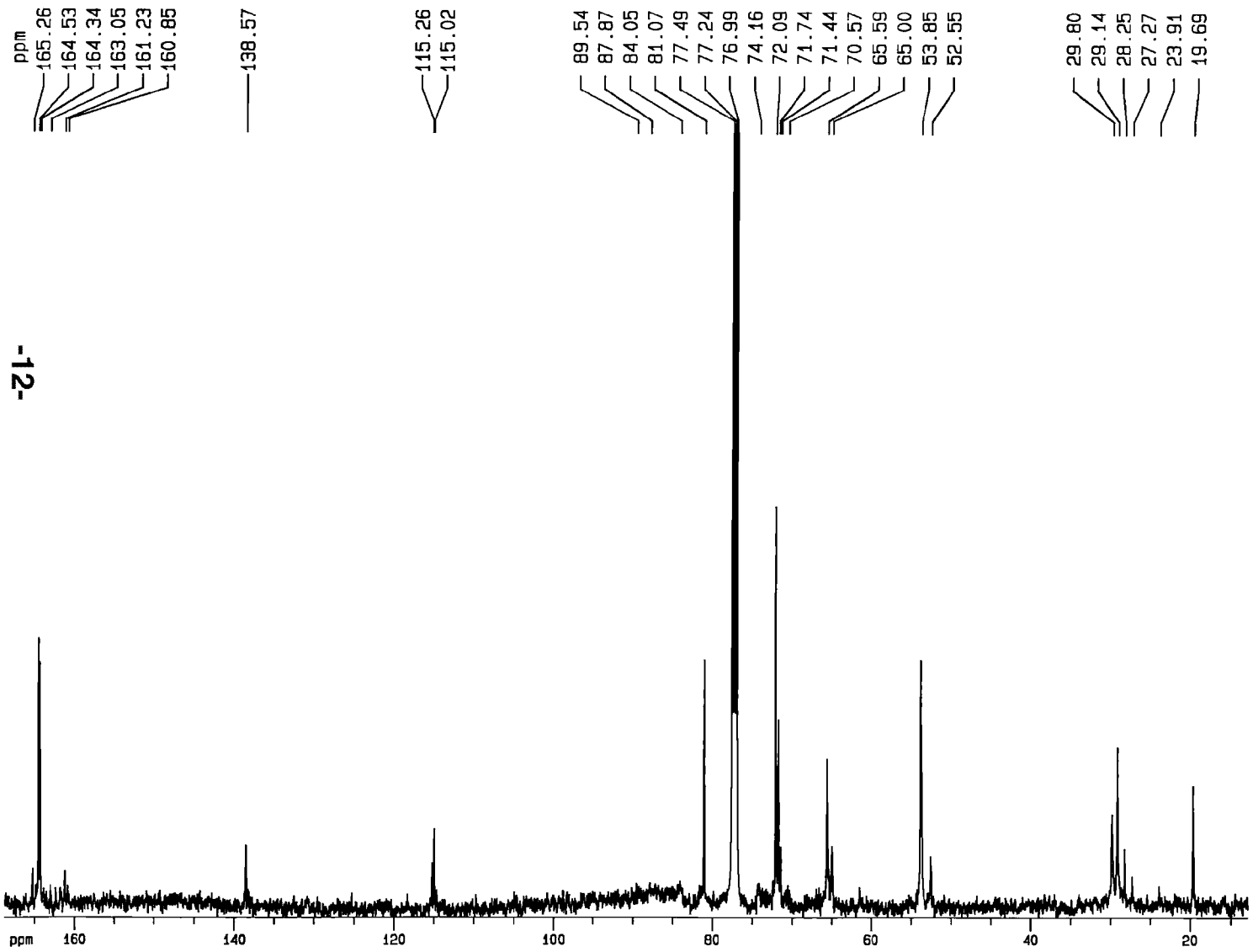
Chenbo 06-02-04 Cyclization of Allyl trichloroacetate 2nd pot
five-memberd ring CDCl3



Chenbo 06-02-04 Cyclization of Allyl trichloroacetate 2nd pot
six-memberd ring mixture CDCl3 7a + 7b



Chenbo 090904, 125 MHz, C13, cdcl3, rt



Current Data Parameters

NAME	Chenbo090904
EXPNO	2
PROCNO	1

F2 - Acquisition Parameters

Date_	500000
Time	15.17
INSTRUM	spect
PROBHD	5 mm TXI 13C
PULPROG	c13wonoe
TD	32768
SOLVENT	CDCl3
NS	6282
DS	2
SWH	32679.738 Hz
FIDRES	0.997306 Hz
AQ	0.5014004 sec
RG	32768
DW	15.300 usec
DE	6.00 usec
TE	290.0 K
D3	0.00100000 sec
PL12	6.00 dB
D1	10.00000000 sec
CPDPRG2	waltz16
PCPD2	100.00 usec
SFO2	500.1330008 MHz
NUC2	1H
PL2	120.00 dB
P1	17.00 usec
DE	6.00 usec
SFO1	125.7715724 MHz
NUC1	13C
PL1	0.00 dB

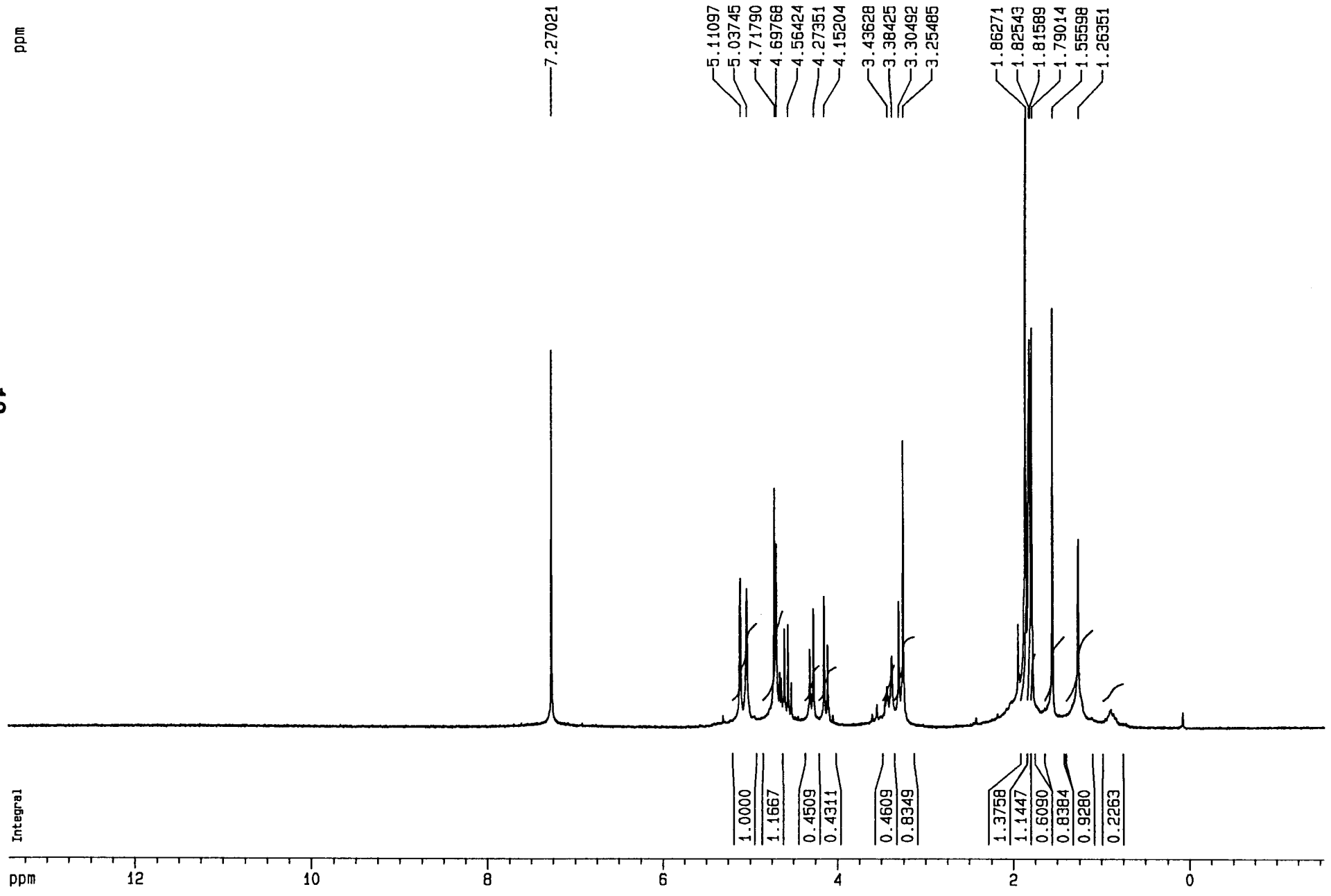
F2 - Processing parameters

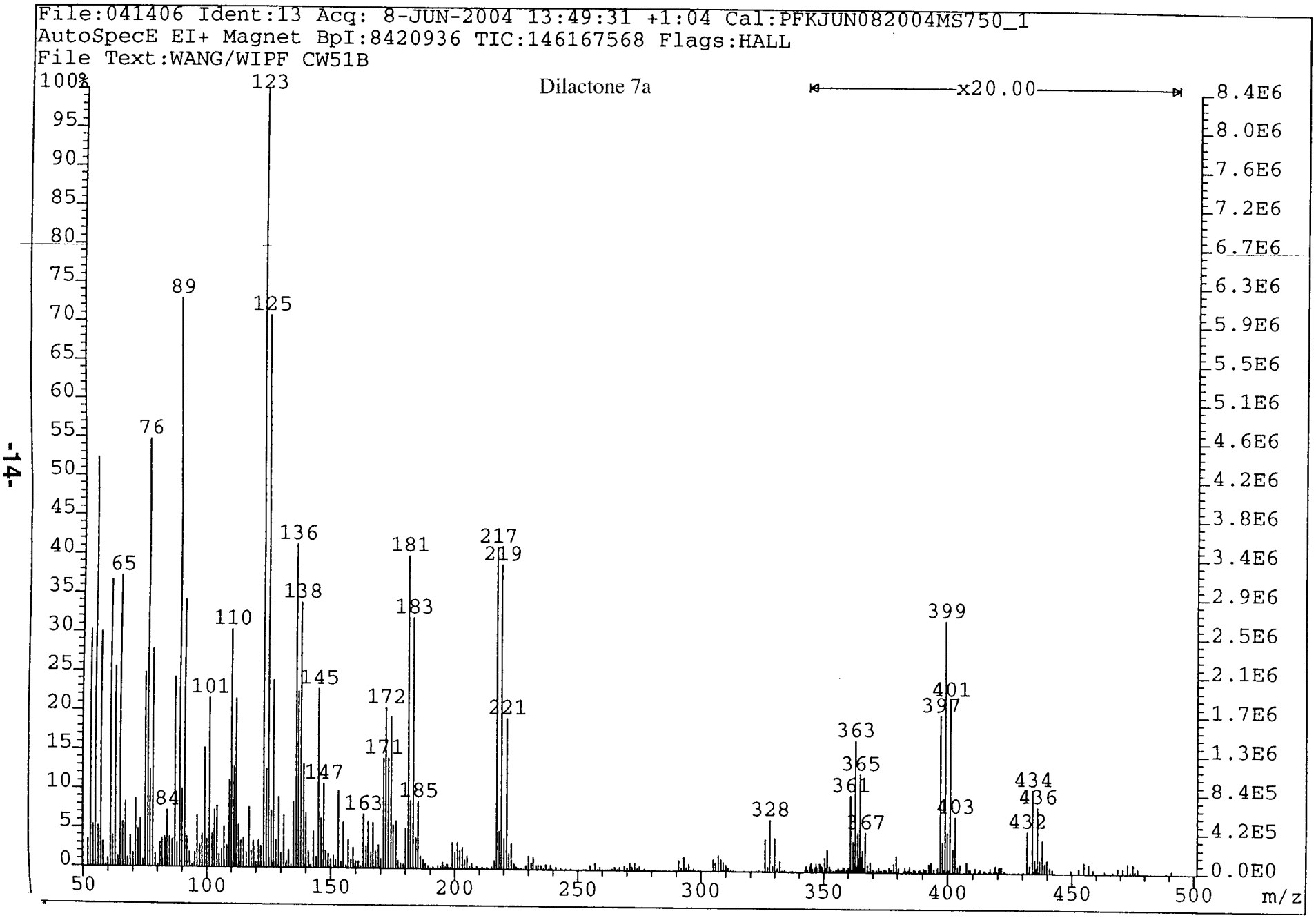
SI	8192
SF	125.7577671 MHz
WDW	EM
SSB	0
LB	4.00 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	20.00 cm
F1P	168.836 ppm
F1	21232.43 Hz
F2P	12.861 ppm
F2	1617.43 Hz
PPMCM	7.79872 ppm/cm
HZCM	980.75006 Hz/cm

Chenbo 06-02-04 Cyclization of Allyl trichloroacetate 2nd pot
six-memberd ring high Rf CDCl3 7a

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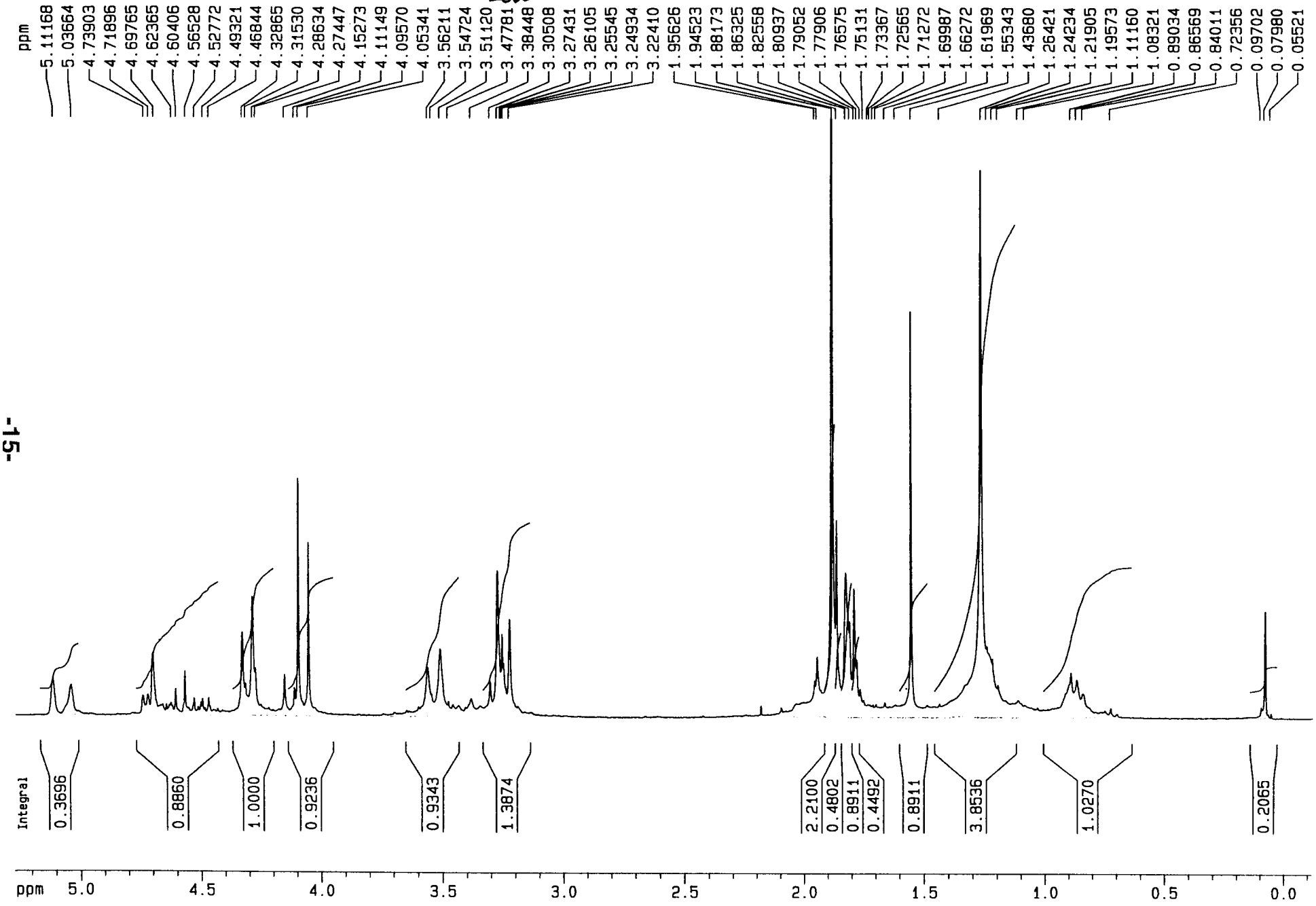
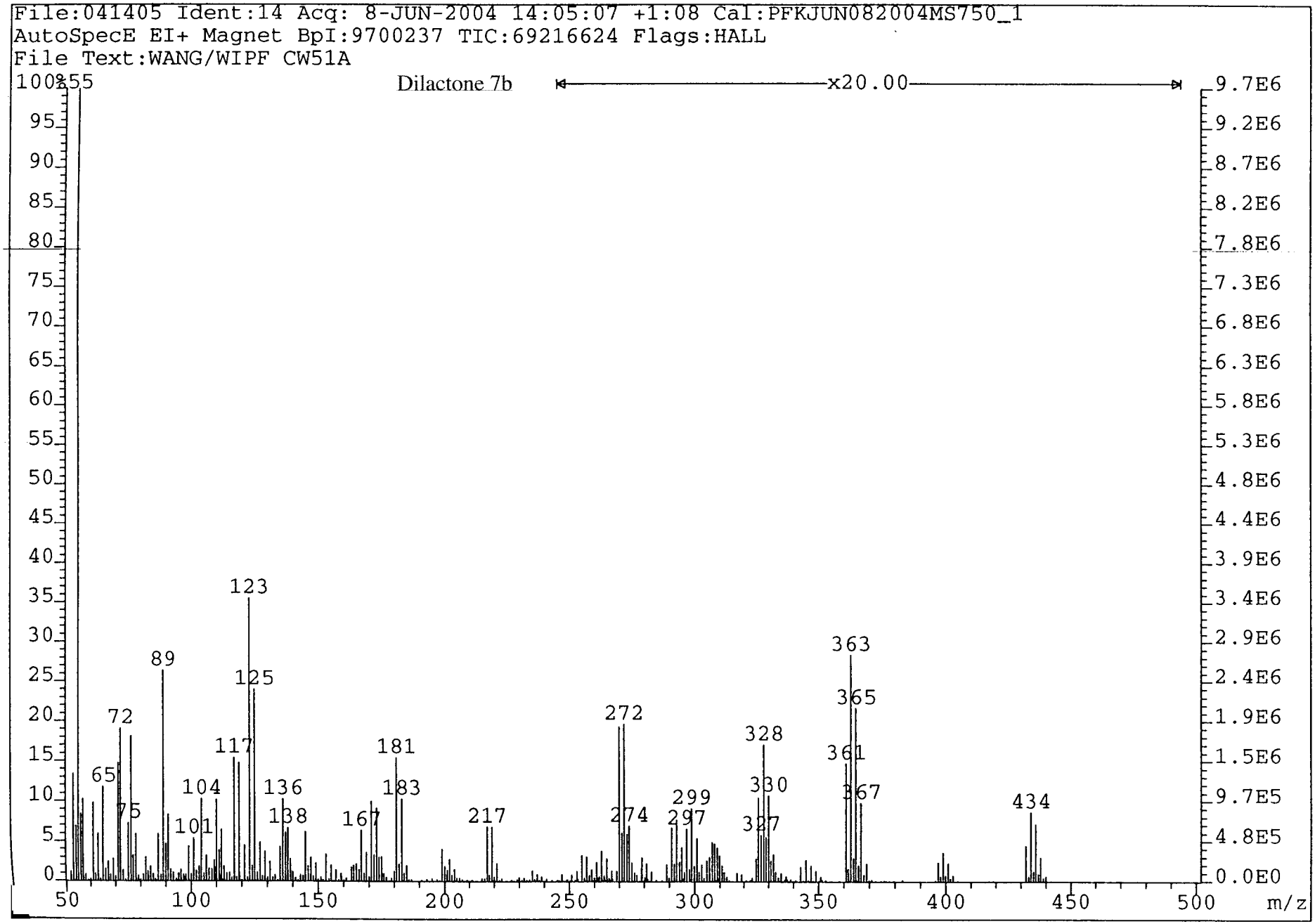
File Text:WANG/WIPF CW51B
Dilactone 7a
x20.00
100%
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
5
0
8.4E6
8.0E6
7.6E6
7.2E6
6.7E6
6.3E6
5.9E6
5.5E6
5.1E6
4.6E6
4.2E6
3.8E6
3.4E6
2.9E6
2.5E6
2.1E6
1.7E6
1.3E6
8.4E5
4.2E5
0.0E0
50
100
150
200
250
300
350
400
450
500
m/z
123
89
125
76
65
136
138
110
181
183
217
219
399
101
145
172
221
401
397
363
171
365
361
147
185
84
163
328
434
436
403
432
367

Chenbo 06-03-04 Cyclization of Allyl trichloroacetate 2nd pot 7b

12-memberd ring ~~high~~ low Rf in CDCl3

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x20.00
100%
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89
125
72
117
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2.4E6
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9.7E5
4.8E5
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m/z