

Stereocontrol of Intramolecular Diels–Alder Reactions by an Allylic Diphenylcyclopropyl Group

Regis Tripoli,^a Tory N. Cayzer,^a Anthony C. Willis,^{a,‡} Michael S. Sherburn,^{*,a,b}
and Michael N. Paddon-Row^{**c}

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^a Research School of Chemistry, Australian National University, Canberra, ACT 0200, Australia

^b ARC Centre of Excellence for Free Radical Chemistry and Biotechnology. E-mail: sherburn@rsc.anu.edu.au (synthetic)

^c School of Chemistry, The University of New South Wales, Sydney, NSW 2052, Australia. E-mail: m.paddonrow@unsw.edu.au (computational)

‡ Author to whom correspondence should be addressed regarding X-ray crystal structures. E-mail: willis@rsc.anu.edu.au

1. Coordinates, scf energies, scf energies + zpe, and thermally corrected enthalpies and Gibbs free energies (298.15 K) for B3LYP/6-31G(d) optimized TSs for the IMDA reactions of 5a, 5b, 5c, 5d, 6a, 6b, 6c, and 6d.¹

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TS-cis-5a-in B3LYP/6-31G(d)

SCF Energy (no zpe) = -577.9131811 au; Energy+zpe (0K) = -577.6870811 au

Enthalpy (298K) = -577.6742851 au; Gibbs free energy (298K) = -577.7251981 au

C;1.159553;-1.283007;-0.547157

C;0.570112;-1.539455;0.687202

C;-0.739388;-1.139207;0.983018

C;-1.545055;-0.437179;0.092216

C;-0.133974;1.392191;-0.312379

C;1.079962;0.867582;-0.728668

C;2.304123;0.941045;0.134964

O;2.549088;1.821077;0.925454

O;3.189128;-0.089873;-0.028025

C;2.658346;-1.254044;-0.706470

C;-2.882924;0.068846;0.477953

C;-4.127587;-0.459480;-0.230085

C;-3.683329;0.956604;-0.452527

H;0.562805;-1.377686;-1.449434

H;1.217986;-1.801397;1.523420

H;-1.064558;-1.200750;2.020825

H;-1.396486;-0.584349;-0.974624

H;-0.850452;1.755667;-1.039643

H;-0.225779;1.792791;0.690869

H;1.282530;0.799478;-1.796969

H;2.950884;-1.220760;-1.762707

H;3.158491;-2.108110;-0.238028

H;-3.002223;0.265831;1.541623

H;-5.009967;-0.643882;0.376460

H;-3.981263;-1.176657;-1.033293

H;-3.242669;1.205073;-1.415097

H;-4.264069;1.761732;-0.011229

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TS-trans-5a-in B3LYP/6-31G(d)

SCF Energy (no zpe) = -577.9127655 au; Energy+zpe (0K) = -577.6865535 au

Enthalpy (298K) = -577.6737795 au; Gibbs free energy (298K) = -577.7247485 au

C;0.060563;-1.082717;0.923196

C;1.572827;0.494283;-0.072786

C;1.025471;1.683728;0.398854

C;-0.322998;2.037200;0.237651

C;-1.196003;1.166172;-0.404086

C;-1.201629;-0.509295;0.843492

C;-2.695939;1.225738;-0.412996

C;-2.309977;-1.077027;0.002118

O;-3.183355;-0.134562;-0.476441

C;2.961943;0.089845;0.243608

O;-2.479835;-2.242626;-0.259232

C;3.967735;-0.120734;-0.885265

C;3.467082;-1.297123;-0.100526
H;0.325814;-1.888383;0.246089
H;0.640212;-1.011223;1.834371
H;1.152617;0.035280;-0.963778
H;1.622659;2.275568;1.091890
H;-0.722040;2.842384;0.853274
H;-0.800607;0.600072;-1.245829
H;-1.561281;0.051371;1.704800
H;-3.110766;1.722287;-1.297327
H;-3.092517;1.722999;0.481736
H;3.367832;0.531455;1.152010
H;4.985234;0.223981;-0.722394
H;3.611304;0.008074;-1.903689
H;2.772025;-1.976537;-0.587225
H;4.140582;-1.780249;0.601884

#####

TS-cis-5a-ou B3LYP/6-31G(d)

SCF Energy (no zpe) = -577.9114151 au; Energy+zpe (0K) = -577.6851181 au

Enthalpy (298K) = -577.6723261 au; Gibbs free energy (298K) = -577.7235751 au

C;-1.204790;-1.356480;0.429385
C;-0.362006;-1.429996;-0.674065
C;0.960454;-0.963861;-0.640744
C;1.519637;-0.365126;0.482397
C;-0.011994;1.363532;0.823010
C;-1.261299;0.769963;0.901234
C;-2.277234;0.928741;-0.189623
O;-2.387950;1.897333;-0.903327
O;-3.131562;-0.128862;-0.346141
C;-2.703421;-1.366917;0.272122
C;2.875692;0.244292;0.524832
C;3.569358;0.782425;-0.708032
C;4.081915;-0.476470;-0.070577
H;-0.803564;-1.552020;1.419112
H;-0.810960;-1.592489;-1.653869
H;1.481050;-0.883590;-1.593446
H;1.139817;-0.665734;1.454122
H;0.519621;1.632922;1.729318
H;0.270051;1.900139;-0.075724
H;-1.677514;0.546219;1.882584
H;-3.208755;-1.481474;1.238381
H;-3.060802;-2.155790;-0.398030
H;3.079206;0.787351;1.445104
H;4.151145;1.693448;-0.598177
H;3.050043;0.704440;-1.659332
H;3.890343;-1.420299;-0.573521
H;5.018548;-0.441511;0.479592

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TS-trans-ou B3LYP/6-31G(d)

SCF Energy (no zpe) = -577.9107791 au; Energy+zpe (0K) = -577.6844921 au

Enthalpy (298K) = -577.6717311 au; Gibbs free energy (298K) = -577.7227471 au

C;-0.088244;-1.382558;0.544561
C;1.497853;0.066738;-0.483197
C;1.240918;1.256818;0.188771

C;-0.039263;1.830140;0.271128
C;-1.125805;1.203326;-0.323242
C;-1.238719;-0.629823;0.729543
C;-2.581078;1.475816;-0.079206
C;-2.525829;-0.897516;0.004708
O;-3.288288;0.221339;-0.215840
C;2.803235;-0.646158;-0.461242
O;-2.919857;-1.975337;-0.368597
C;3.772865;-0.537398;0.697213
C;4.120084;0.108879;-0.612822
H;-0.054467;-2.120639;-0.251347
H;0.614285;-1.519115;1.356793
H;0.875253;-0.182316;-1.336514
H;2.006293;1.660414;0.850016
H;-0.209726;2.597047;1.025815
H;-0.952146;0.694845;-1.270030
H;-1.376685;-0.132972;1.688156
H;-3.034080;2.142509;-0.821718
H;-2.758246;1.897922;0.918589
H;2.775190;-1.616062;-0.952231
H;4.309496;-1.435508;0.990873
H;3.497755;0.103906;1.530741
H;4.060112;1.191436;-0.683002
H;4.896018;-0.339072;-1.227936

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TS-cis-5a-an B3LYP/6-31G(d)

SCF Energy (no zpe) = -577.9088832 au; Energy+zpe (0K) = -577.6824572 au

Enthalpy (298K) = -577.6697402 au; Gibbs free energy (298K) = -577.7206442 au

C;1.326253;-1.311506;-0.478379
C;0.542095;-1.560211;0.644515
C;-0.834764;-1.297601;0.660851
C;-1.520455;-0.734715;-0.409675
C;-0.223268;1.212486;-0.719167
C;1.088481;0.784560;-0.856865
C;2.114568;1.056917;0.203801
O;2.121546;2.014196;0.940229
O;3.104108;0.117318;0.299389
C;2.820327;-1.137939;-0.363644
C;-2.984716;-0.432771;-0.349914
C;-3.570560;0.967864;-0.336188
C;-3.661273;0.096755;0.890869
H;0.922612;-1.534496;-1.461616
H;1.041344;-1.703906;1.602571
H;-1.352372;-1.362654;1.615942
H;-1.142150;-0.910631;-1.413004
H;-0.819714;1.439181;-1.594930
H;-0.528310;1.681175;0.209638
H;1.494607;0.664551;-1.860624
H;3.304669;-1.144403;-1.347237
H;3.294883;-1.903295;0.258967
H;-3.577547;-1.143461;-0.929089
H;-4.471467;1.142283;-0.918182
H;-2.892244;1.813626;-0.302394
H;-3.033816;0.365297;1.736517
H;-4.625853;-0.318413;1.169276

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TS-trans-5a-an B3LYP/6-31G(d)

SCF Energy (no zpe) = -577.9081482 au; Energy+zpe (0K) = -577.6818082 au

Enthalpy (298K) = -577.6690622 au; Gibbs free energy (298K) = -577.7203652 au

C;0.153310;-1.196305;0.531679
C;1.521943;0.449871;-0.599714
C;1.115866;1.598949;0.069086
C;-0.226486;1.989759;0.202161
C;-1.231667;1.197024;-0.338756
C;-1.078365;-0.585676;0.729168
C;-2.705844;1.289139;-0.068485
C;-2.340405;-1.048507;0.055125
O;-3.248676;-0.046720;-0.169046
C;2.962501;0.050177;-0.665364
O;-2.597944;-2.180458;-0.272180
C;3.492702;-1.283128;-0.182284
C;3.840198;-0.015655;0.560654
H;0.268334;-1.937498;-0.252564
H;0.874855;-1.228443;1.337823
H;0.912849;0.076888;-1.418629
H;1.858641;2.119845;0.671325
H;-0.476089;2.742176;0.949239
H;-1.015549;0.705785;-1.285903
H;-1.257251;-0.106024;1.690215
H;-3.249911;1.880198;-0.813510
H;-2.916620;1.704308;0.925580
H;3.456413;0.415616;-1.568487
H;4.266935;-1.761613;-0.775760
H;2.804849;-1.977316;0.288464
H;3.367577;0.143748;1.526552
H;4.855416;0.365876;0.495843

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TS-trans-5b-in B3LYP/6-31G(d)

SCF Energy (no zpe) = -805.8000102 au; Energy+zpe (0K) = -805.5306852 au

Enthalpy (298K) = -805.5132232 au; Gibbs free energy (298K) = -805.5755512 au

C;0.233418;0.880210;-0.481432
C;-1.048485;-1.504697;0.091526
C;-0.417677;-1.639898;1.314137
C;0.970866;-1.551216;1.500079
C;1.829250;-1.243600;0.435220
C;1.518092;0.607807;0.006605
C;3.322558;-1.081868;0.561378
C;2.739938;0.666688;-0.887944
O;3.737549;-0.169848;-0.476944
C;-0.714885;1.542652;0.403975
C;-2.507612;-1.474983;-0.061230
O;2.881943;1.371546;-1.853418
O;-0.542789;1.755461;1.596738
O;-1.841527;1.934044;-0.258004
C;-2.798830;2.633930;0.543397
C;-3.166146;-2.355477;-1.131851
C;-3.143339;-0.872672;-1.303968
H;0.002182;0.805571;-1.537662

H;-0.480213;-1.611100;-0.827528
H;-1.042059;-1.683098;2.204509
H;1.345547;-1.481075;2.519676
H;1.550294;-1.652142;-0.536235
H;1.706035;1.029639;0.995771
H;3.874797;-2.010021;0.384539
H;3.610010;-0.680910;1.541719
H;-3.066375;-1.361772;0.864944
H;-2.363586;3.546443;0.961099
H;-3.152004;2.007495;1.368016
H;-3.622497;2.879685;-0.128886
H;-4.099073;-2.841929;-0.860995
H;-2.509484;-2.961543;-1.750022
H;-2.473699;-0.441506;-2.041782
H;-4.064165;-0.314611;-1.163483

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TS-cis-5b-in B3LYP/6-31G(d)
SCF Energy (no zpe) = -805.7985669 au; Energy+zpe (0K) = -805.5288939 au
Enthalpy (298K) = -805.5115419 au; Gibbs free energy (298K) = -805.5732799 au
C;-1.868529;-1.097721;0.861694
C;-1.557154;-1.972803;-0.189585
C;-0.250006;-2.169181;-0.650834
C;0.859641;-1.548217;-0.102820
C;-0.160754;0.877546;-0.421165
C;-1.386456;0.736316;0.236388
C;-2.686137;0.881493;-0.516886
O;-2.855796;1.540460;-1.512030
O;-3.719528;0.188367;0.043383
C;-3.310776;-0.708167;1.101772
C;2.215341;-1.721176;-0.645974
C;0.961200;1.472990;0.300195
O;1.088069;1.508744;1.517776
O;1.871979;2.013434;-0.552023
C;2.949031;2.726954;0.066640
C;3.281489;-2.395226;0.230451
C;3.385178;-0.937665;-0.084157
H;-1.201367;-1.065266;1.719387
H;-2.372456;-2.326660;-0.819961
H;-0.115017;-2.740316;-1.568231
H;0.798657;-1.113733;0.890845
H;-0.110981;0.843478;-1.502531
H;-1.412442;1.155815;1.243659
H;-3.437263;-0.207166;2.068473
H;-4.002420;-1.554260;1.054253
H;2.262646;-1.977299;-1.702113
H;2.565995;3.494964;0.743965
H;3.596615;2.050921;0.633128
H;3.506608;3.182465;-0.752916
H;3.947668;-3.094687;-0.266670
H;2.993136;-2.687361;1.236193
H;3.165856;-0.237264;0.715869
H;4.144561;-0.602536;-0.784501

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TS-trans-5b-ou B3LYP/6-31G(d)

SCF Energy (no zpe) = -805.7974006 au; Energy+zpe (0K) = -805.5278676 au

Enthalpy (298K) = -805.5104356 au; Gibbs free energy (298K) = -805.5729096 au

C;0.390347;0.979783;-0.461980
C;-0.993167;-1.343447;-0.613372
C;-0.574394;-1.817890;0.615508
C;0.773064;-1.874884;1.010305
C;1.794601;-1.400051;0.182932
C;1.576109;0.555493;0.143088
C;3.249431;-1.329529;0.563647
C;2.922178;0.726791;-0.526937
O;3.829209;-0.227693;-0.166063
C;-0.677506;1.508723;0.381045
C;-2.401023;-1.137016;-1.009359
O;3.226287;1.608590;-1.288573
O;-0.711277;1.460973;1.602438
O;-1.651905;2.104100;-0.362503
C;-2.692321;2.733253;0.392981
C;-3.496818;-0.862873;0.004245
C;-3.459651;-2.194338;-0.675593
H;0.332577;1.142455;-1.532271
H;-0.280296;-1.295334;-1.428438
H;-1.320211;-2.016404;1.382446
H;0.987264;-2.060551;2.061480
H;1.659145;-1.548464;-0.887848
H;1.611886;0.725153;1.220206
H;3.818292;-2.215897;0.265145
H;3.383879;-1.171379;1.641308
H;-2.522242;-0.649693;-1.972320
H;-2.280634;3.498069;1.057802
H;-3.237023;2.001784;0.996789
H;-3.356550;3.188183;-0.343690
H;-4.268548;-0.155489;-0.285489
H;-3.205726;-0.800100;1.049050
H;-3.124706;-3.057408;-0.107107
H;-4.200724;-2.416776;-1.438508

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TS-cis-5b-ou B3LYP/6-31G(d)

SCF Energy (no zpe) = -805.7977005 au; Energy+zpe (0K) = -805.5278425 au

Enthalpy (298K) = -805.5104795 au; Gibbs free energy (298K) = -805.5728495 au

C;1.833732;-0.866039;-1.103298
C;1.319813;-1.941187;-0.366481
C;-0.042148;-2.095159;-0.076977
C;-1.014848;-1.205302;-0.500867
C;0.133655;0.912043;0.470234
C;1.429484;0.805144;-0.036060
C;2.611656;0.568508;0.865333
O;2.694543;0.894155;2.023508
O;3.649893;-0.065393;0.244903
C;3.319421;-0.585499;-1.064770
C;-2.438216;-1.258528;-0.108041
C;-0.828945;1.736553;-0.258831
O;-0.701782;2.113921;-1.416028
O;-1.919643;2.035258;0.496069
C;-2.887273;2.880374;-0.140604

C;-2.900795;-1.888424;1.192131
C;-3.194818;-2.590681;-0.095613
H;1.282848;-0.518291;-1.973397
H;2.022067;-2.543108;0.209835
H;-0.310736;-2.865264;0.643843
H;-0.797524;-0.562137;-1.346542
H;-0.095034;0.623403;1.488353
H;1.639286;1.450449;-0.890107
H;3.612224;0.144083;-1.828453
H;3.934255;-1.482181;-1.185825
H;-3.019123;-0.405044;-0.443640
H;-2.440492;3.839261;-0.417658
H;-3.286582;2.407654;-1.042847
H;-3.677967;3.027409;0.596329
H;-3.715131;-1.395140;1.715079
H;-2.141651;-2.304754;1.848718
H;-2.622308;-3.480526;-0.341834
H;-4.212528;-2.590149;-0.476411

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TS-trans-5b-an B3LYP/6-31G(d)

SCF Energy (no zpe) = -805.7936722 au; Energy+zpe (0K) = -805.5242932 au

Enthalpy (298K) = -805.5068682 au; Gibbs free energy (298K) = -805.5691452 au

C;0.270654;0.898553;-0.466367
C;-0.915357;-1.691126;-0.500064
C;-0.421792;-1.968048;0.758730
C;0.923829;-1.815468;1.132200
C;1.865385;-1.276993;0.237273
C;1.513896;0.555230;0.096375
C;3.331683;-1.105623;0.556084
C;2.815166;0.835478;-0.636721
O;3.810388;-0.021259;-0.265224
C;-0.752221;1.400506;0.439850
C;-2.345265;-1.876867;-0.867080
O;3.011792;1.711430;-1.437156
O;-0.714030;1.319401;1.661009
O;-1.770725;2.021591;-0.223361
C;-2.784903;2.593046;0.612431
C;-3.251240;-0.747884;-1.313959
C;-3.481201;-1.426663;0.016312
H;0.143555;1.024317;-1.534951
H;-0.231324;-1.581851;-1.336845
H;-1.137082;-2.225149;1.536817
H;1.179670;-1.900515;2.186618
H;1.720584;-1.545623;-0.809487
H;1.584278;0.821804;1.153478
H;3.933553;-1.979374;0.289561
H;3.498513;-0.868351;1.614517
H;-2.508467;-2.812336;-1.408346
H;-2.343611;3.274146;1.344673
H;-3.337969;1.812818;1.144420
H;-3.450647;3.133186;-0.062147
H;-3.943281;-0.958654;-2.124760
H;-2.851619;0.259911;-1.305576
H;-3.226098;-0.867104;0.912586
H;-4.341259;-2.081384;0.126916

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TS-trans-5c-in B3LYP/6-31G(d)

SCF Energy (no zpe) = -805.7998301 au; Energy+zpe (0K) = -805.5303661 au

Enthalpy (298K) = -805.5129191 au; Gibbs free energy (298K) = -805.5750601 au

C;-0.260220;0.551874;-1.036969

C;1.547328;-1.473375;0.113508

C;0.714458;-2.523222;-0.205256

C;-0.675664;-2.546091;0.018906

C;-1.394009;-1.442743;0.501167

C;-1.462239;-0.164043;-0.908017

C;-2.879300;-1.533338;0.751516

C;-2.732045;0.517325;-0.376907

O;-3.473991;-0.259975;0.450331

C;0.107458;1.514975;-0.019592

C;2.963208;-1.439495;-0.266153

O;-0.395345;1.577975;1.099114

O;-3.111387;1.605270;-0.718412

O;1.119255;2.343039;-0.410156

C;1.490031;3.341695;0.550249

C;3.992286;-0.843300;0.696383

C;3.658890;-0.112009;-0.561597

H;0.362811;0.449826;-1.915769

H;1.201111;-0.692189;0.782976

H;1.142726;-3.358137;-0.758863

H;-1.235048;-3.386731;-0.390846

H;-0.894071;-0.776799;1.204428

H;-1.714266;-0.774684;-1.777691

H;-3.114165;-1.739050;1.800412

H;-3.352485;-2.303677;0.128437

H;3.300668;-2.288216;-0.857145

H;2.281707;3.923733;0.076486

H;1.853507;2.881717;1.473950

H;0.635802;3.980702;0.789552

H;4.947632;-1.355166;0.771320

H;3.619968;-0.450622;1.638696

H;3.052502;0.786395;-0.504086

H;4.382236;-0.117101;-1.372296

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TS-trans-5c-ou B3LYP/6-31G(d)

SCF Energy (no zpe) = -805.7962720 au; Energy+zpe (0K) = -805.5267560 au

Enthalpy (298K) = -805.5092530 au; Gibbs free energy (298K) = -805.5722310 au

C;0.322069;0.584089;0.975965

C;-1.674188;-0.763992;-0.398564

C;-1.249141;-2.029122;-0.056769

C;0.085113;-2.465840;-0.194456

C;1.115250;-1.609690;-0.584952

C;1.358289;-0.351642;0.927017

C;2.553726;-2.042620;-0.656089

C;2.776644;0.009922;0.486292

O;3.387431;-0.931377;-0.279585

C;0.251736;1.651120;-0.010756

C;-3.002003;-0.187082;-0.106471

O;0.865414;1.664050;-1.071906

O;3.370515;0.989718;0.850930
 O;-0.627597;2.627374;0.341498
 C;-0.727966;3.717047;-0.585645
 C;-3.897617;-0.710276;1.000388
 C;-4.282230;-0.967029;-0.422941
 H;-0.389756;0.586496;1.790943
 H;-1.064876;-0.181409;-1.079789
 H;-1.931018;-2.691232;0.475053
 H;0.346805;-3.431415;0.237443
 H;0.884638;-0.804704;-1.281709
 H;1.391428;-1.042708;1.771051
 H;2.861395;-2.315622;-1.670769
 H;2.760846;-2.889524;0.011288
 H;-3.058015;0.882792;-0.286909
 H;-1.454511;4.405206;-0.151350
 H;-1.068546;3.367341;-1.564710
 H;0.240352;4.210045;-0.707432
 H;-4.462850;0.024448;1.567004
 H;-3.531576;-1.542396;1.595754
 H;-4.155889;-1.970963;-0.818376
 H;-5.112614;-0.413777;-0.853110

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TS-cis-5c-in B3LYP/6-31G(d)
 SCF Energy (no zpe) = -805.7944067 au; Energy+zpe (0K) = -805.5251947 au
 Enthalpy (298K) = -805.5077427 au; Gibbs free energy (298K) = -805.5701447 au
 C;1.373077;-1.781433;0.179498
 C;0.666578;-1.438831;1.341949
 C;-0.719973;-1.216946;1.354527
 C;-1.513600;-1.256780;0.228199
 C;0.127827;0.488834;-1.050769
 C;1.314522;-0.254072;-1.083522
 C;2.645766;0.336128;-0.624589
 O;3.037061;1.438880;-0.903345
 O;3.443360;-0.538603;0.042115
 C;2.884846;-1.853526;0.222779
 C;-2.931366;-0.873654;0.224096
 C;-0.078925;1.464544;0.004890
 O;0.613463;1.549347;1.011193
 O;-1.157572;2.263914;-0.223503
 C;-1.401653;3.248758;0.786563
 C;-3.955720;-1.762975;-0.486227
 C;-3.608059;-0.428213;-1.062514
 H;0.883759;-2.469294;-0.506711
 H;1.231360;-1.135243;2.220479
 H;-1.157984;-0.831164;2.273043
 H;-1.149247;-1.742023;-0.672732
 H;-0.591504;0.432900;-1.857683
 H;1.458765;-0.824915;-2.004394
 H;3.278434;-2.509931;-0.562635
 H;3.260260;-2.205918;1.187506
 H;-3.278891;-0.390027;1.134082
 H;-1.629848;2.775958;1.747008
 H;-0.530444;3.897110;0.915622
 H;-2.258336;3.825886;0.434829
 H;-4.918072;-1.892266;0.001018

H;-3.583582;-2.655083;-0.982696
H;-2.997566;-0.396891;-1.960661
H;-4.327541;0.381603;-0.987046

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TS-cis-5c-ou B3LYP/6-31G(d)

SCF Energy (no zpe) = -805.7916979 au; Energy+zpe (0K) = -805.5222959 au

Enthalpy (298K) = -805.5049109 au; Gibbs free energy (298K) = -805.5670449 au

C;-1.471511;-1.783710;0.014880
C;-0.539774;-1.631335;-1.019616
C;0.836151;-1.463843;-0.790597
C;1.383633;-1.369788;0.471377
C;-0.309972;0.592480;1.167457
C;-1.532710;-0.080449;1.075507
C;-2.715185;0.492049;0.300487
O;-3.073120;1.639665;0.353354
O;-3.439333;-0.430265;-0.384928
C;-2.950432;-1.782854;-0.302524
C;2.793932;-1.056038;0.777300
C;0.139261;1.424833;0.061952
O;-0.340150;1.398780;-1.063439
O;1.183892;2.227326;0.405632
C;1.644514;3.096276;-0.635011
C;3.656349;-0.218299;-0.149683
C;3.931883;-1.683124;-0.035215
H;-1.166967;-2.382227;0.870371
H;-0.909436;-1.429930;-2.022750
H;1.455558;-1.229219;-1.653763
H;0.799947;-1.713367;1.317941
H;0.248340;0.616036;2.094983
H;-1.875932;-0.520983;2.014626
H;-3.526471;-2.313724;0.464749
H;-3.169832;-2.235786;-1.273542
H;3.000014;-0.937844;1.837660
H;2.041836;2.521945;-1.477823
H;0.831551;3.731144;-0.998215
H;2.432052;3.703010;-0.185382
H;4.344484;0.481470;0.315642
H;3.193196;0.151925;-1.059723
H;3.643300;-2.330305;-0.858752
H;4.811218;-2.013373;0.511150

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TS-cis-5c-an B3LYP/6-31G(d)

SCF Energy (no zpe) = -805.7908449 au; Energy+zpe (0K) = -805.5214309 au

Enthalpy (298K) = -805.5040709 au; Gibbs free energy (298K) = -805.5661389 au

C;1.492657;-1.699043;0.046574
C;0.586717;-1.552399;1.114139
C;-0.809285;-1.540420;0.931364
C;-1.415602;-1.601274;-0.300965
C;0.238750;0.540376;-1.152332
C;1.469703;-0.136192;-1.084187
C;2.684513;0.533262;-0.434131
O;3.009202;1.677662;-0.611035
O;3.462890;-0.313421;0.284237

C;2.981239;-1.667679;0.340281
C;-2.875072;-1.539147;-0.551334
C;-0.150969;1.352432;-0.022215
O;0.405477;1.304746;1.070990
O;-1.222031;2.160899;-0.267275
C;-1.614263;2.994220;0.830903
C;-3.598255;-0.230343;-0.860723
C;-3.865301;-0.957546;0.428320
H;1.189930;-2.391329;-0.736695
H;0.973523;-1.289120;2.095183
H;-1.429556;-1.362810;1.806407
H;-0.822591;-1.885683;-1.165533
H;-0.372388;0.527614;-2.045545
H;1.770030;-0.599919;-2.027732
H;3.546297;-2.265771;-0.384460
H;3.214810;-2.029914;1.345034
H;-3.235249;-2.382221;-1.142436
H;-1.959393;2.391042;1.676379
H;-0.777407;3.615176;1.161602
H;-2.426767;3.615966;0.452281
H;-4.354735;-0.256235;-1.640346
H;-3.013869;0.682595;-0.817858
H;-3.482657;-0.512173;1.342324
H;-4.813277;-1.473799;0.551886

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TS-trans-5d-in B3LYP/6-31G(d)

SCF Energy (no zpe) = -1033.6806887 au; Energy+zpe (0K) = -1033.3680917 au

Enthalpy (298K) = -1033.3460007 au; Gibbs free energy (298K) = -1033.4187527 au

C;-0.406040;-0.677001;0.531770
C;1.155076;1.814868;-0.621531
C;0.382158;2.632454;0.161108
C;-1.029409;2.552222;0.267683
C;-1.811976;1.597705;-0.377180
C;-1.655925;-0.050985;0.675327
C;-3.317637;1.634872;-0.332804
C;-2.932392;-0.640081;0.086293
O;-3.813380;0.285267;-0.368081
C;-0.135954;-1.354607;-0.744796
C;2.615588;1.854760;-0.643954
O;-0.724825;-1.059016;-1.781557
O;-3.204791;-1.811172;0.098821
O;0.799549;-2.325713;-0.704841
C;1.009596;-3.019429;-1.944433
C;0.497064;-0.546330;1.688293
O;0.201527;0.073686;2.702066
O;1.696594;-1.157912;1.543723
C;2.565932;-1.052756;2.677910
C;3.354420;1.545155;-1.949571
C;3.406037;0.557361;-0.835364
H;0.681354;1.125176;-1.315709
H;0.885996;3.348237;0.808207
H;-1.504771;3.192192;1.010408
H;-1.423632;1.142411;-1.286788
H;-1.818367;0.330338;1.684007
H;-3.746221;2.133389;-1.207897

H;-3.688727;2.133482;0.572145
H;3.074193;2.598503;0.003510
H;1.770569;-3.770067;-1.728286
H;1.356902;-2.333153;-2.722056
H;0.084076;-3.493990;-2.280291
H;2.095276;-1.477934;3.568489
H;2.818895;-0.007862;2.879862
H;3.459664;-1.618915;2.411508
H;4.234784;2.144651;-2.163250
H;2.745712;1.316603;-2.820075
H;2.834281;-0.361946;-0.906967
H;4.323395;0.468524;-0.260374

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TS-trans-5d-ou B3LYP/6-31G(d)
SCF Energy (no zpe) = -1033.6761311 au; Energy+zpe (0K) = -1033.3635741 au
Enthalpy (298K) = -1033.3413981 au; Gibbs free energy (298K) = -1033.4150671 au
C;0.532813;0.652715;0.472385
C;-1.383755;-1.253574;-0.966834
C;-1.004388;-2.284733;-0.145456
C;0.341753;-2.619089;0.142245
C;1.438613;-1.905767;-0.334295
C;1.543961;-0.275542;0.767052
C;2.857248;-2.332447;-0.064013
C;3.001125;-0.034251;0.393969
O;3.678074;-1.155101;0.039438
C;0.656017;1.416460;-0.782424
C;-2.765478;-0.800958;-1.192868
O;1.238916;0.969643;-1.766435
O;3.556492;1.028881;0.482712
O;0.100884;2.641020;-0.767357
C;0.251471;3.395083;-1.979355
C;-0.544687;0.760773;1.471527
O;-0.580116;0.093971;2.497805
O;-1.512409;1.653212;1.156198
C;-2.534018;1.811728;2.147167
C;-3.848425;-0.954076;-0.131727
C;-3.905598;-1.816037;-1.347207
H;-0.629817;-0.754132;-1.566562
H;-1.767599;-2.831704;0.405024
H;0.510774;-3.376057;0.907476
H;1.329010;-1.352159;-1.265280
H;1.446600;-0.699586;1.766991
H;3.279950;-2.918868;-0.885946
H;2.941281;-2.915212;0.862523
H;-2.846512;0.082714;-1.818485
H;-0.249020;4.345540;-1.791382
H;-0.214372;2.875054;-2.821306
H;1.309334;3.554146;-2.203917
H;-2.102701;2.117703;3.104269
H;-3.085844;0.878752;2.293911
H;-3.194623;2.589430;1.760859
H;-4.558872;-0.137730;-0.037552
H;-3.552113;-1.401908;0.812700
H;-3.638046;-2.864864;-1.255116
H;-4.652071;-1.605838;-2.108085

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TS-cis-5d-in B3LYP/6-31G(d)

SCF Energy (no zpe) = -1033.6751125 au; Energy+zpe (0K) = -1033.3627375 au

Enthalpy (298K) = -1033.3405465 au; Gibbs free energy (298K) = -1033.4140825 au

C;-1.613682;1.821147;-0.543950

C;-1.177340;2.046560;0.763415

C;0.182881;2.083522;1.163137

C;1.238161;1.815086;0.335479

C;-0.365166;-0.794464;-0.373560

C;-1.457227;-0.125601;-0.951165

C;-2.889581;-0.452918;-0.550774

O;-3.305719;-1.569931;-0.387657

O;-3.719794;0.617870;-0.515369

C;-3.096658;1.871347;-0.851197

C;2.635528;1.805008;0.765040

C;-0.466420;-1.083410;1.057482

O;-1.350289;-0.580822;1.748223

O;0.487139;-1.884452;1.576068

C;0.369784;-2.130544;2.982894

C;0.769160;-1.079998;-1.270782

O;0.963403;-0.480498;-2.324046

O;1.563623;-2.091000;-0.861423

C;2.606992;-2.463804;-1.770411

C;3.693576;2.473612;-0.124078

C;3.661802;0.987521;-0.013339

H;-0.948238;2.124510;-1.348189

H;-1.924411;2.099475;1.551445

H;0.384036;2.255533;2.218881

H;1.066049;1.638438;-0.724094

H;-1.358014;-0.006233;-2.031227

H;-3.271439;2.074888;-1.914192

H;-3.621854;2.629076;-0.263745

H;2.799695;1.894399;1.836307

H;0.471750;-1.201321;3.551668

H;-0.597724;-2.581964;3.218580

H;1.182477;-2.816697;3.225187

H;3.343558;-1.661735;-1.877771

H;2.197232;-2.697929;-2.756377

H;3.072669;-3.345128;-1.327688

H;4.474181;3.026624;0.390485

H;3.352510;2.931247;-1.048249

H;3.290705;0.424926;-0.864019

H;4.429056;0.484152;0.567490

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TS-trans-5d-an B3LYP/6-31G(d)

SCF Energy (no zpe) = -1033.6742829 au; Energy+zpe (0K) = -1033.3617379 au

Enthalpy (298K) = -1033.3396169 au; Gibbs free energy (298K) = -1033.4129009 au

C;0.429356;0.670598;0.489475

C;-1.152893;-1.653632;-1.122344

C;-0.608051;-2.500668;-0.196811

C;0.772337;-2.554148;0.133554

C;1.721842;-1.654061;-0.353627

C;1.597893;-0.084155;0.723356

C;3.201638;-1.857806;-0.137413
 C;2.982802;0.422110;0.324737
 O;3.827130;-0.566181;-0.065871
 C;0.346655;1.413161;-0.775417
 C;-2.592261;-1.571588;-1.455450
 O;1.054397;1.137842;-1.741482
 O;3.351810;1.559807;0.435231
 O;-0.559136;2.409365;-0.807062
 C;-0.623695;3.133752;-2.043962
 C;-0.581141;0.571559;1.554231
 O;-0.474484;-0.198599;2.502203
 O;-1.647115;1.397985;1.422283
 C;-2.593129;1.338836;2.499072
 C;-3.466560;-0.449029;-0.909019
 C;-3.686664;-1.872823;-0.464360
 H;-0.498035;-1.048616;-1.745817
 H;-1.274987;-3.157623;0.356808
 H;1.071347;-3.251021;0.915447
 H;1.502778;-1.143910;-1.290810
 H;1.616188;-0.507785;1.728515
 H;3.673152;-2.378108;-0.976527
 H;3.409951;-2.414729;0.785512
 H;-2.799612;-1.818126;-2.498234
 H;-1.389034;3.895684;-1.891839
 H;-0.900064;2.470943;-2.868989
 H;0.340522;3.596111;-2.270676
 H;-2.106268;1.556912;3.453124
 H;-3.057245;0.349990;2.558381
 H;-3.341198;2.098033;2.267303
 H;-4.181718;-0.003249;-1.594716
 H;-3.008947;0.248044;-0.215025
 H;-3.398622;-2.129088;0.551471
 H;-4.567793;-2.397855;-0.822468

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TS-cis-5d-an B3LYP/6-31G(d)
 SCF Energy (no zpe) = -1033.6725286 au; Energy+zpe (0K) = -1033.3599266 au
 Enthalpy (298K) = -1033.3378926 au; Gibbs free energy (298K) = -1033.4104756 au
 C;-1.854809;1.424289;-0.994621
 C;-1.191832;2.131933;0.011074
 C;0.213941;2.325911;0.072084
 C;1.106703;1.773371;-0.802295
 C;-0.361058;-0.901307;-0.180150
 C;-1.613333;-0.519676;-0.691341
 C;-2.895379;-0.689389;0.110121
 O;-3.163581;-1.664684;0.761381
 O;-3.796391;0.308385;-0.066940
 C;-3.368786;1.345374;-0.969447
 C;2.577361;1.871495;-0.724423
 C;-0.152976;-0.657316;1.248057
 O;-0.916814;0.060395;1.889101
 O;0.929843;-1.237287;1.812893
 C;1.070370;-1.007194;3.222555
 C;0.599175;-1.430095;-1.166211
 O;0.412583;-1.375470;-2.376880
 O;1.708383;-1.987162;-0.634715

C;2.632540;-2.527087;-1.589250
C;3.374685;0.934890;0.191666
C;3.319901;2.406660;0.477609
H;-1.389939;1.408364;-1.977477
H;-1.773488;2.478883;0.861583
H;0.591400;2.890686;0.920817
H;0.735535;1.240943;-1.675042
H;-1.745045;-0.814912;-1.733603
H;-3.768116;1.128304;-1.967007
H;-3.831676;2.265746;-0.604058
H;3.048602;2.038084;-1.692219
H;1.215665;0.056464;3.432722
H;0.183990;-1.354500;3.759730
H;1.949804;-1.578949;3.521338
H;3.002746;-1.745120;-2.258236
H;2.157187;-3.307451;-2.189509
H;3.448344;-2.943584;-0.997069
H;4.290207;0.514156;-0.214750
H;2.803785;0.257049;0.817159
H;2.745072;2.734179;1.338825
H;4.204726;3.007088;0.285516

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TS-cis-6a-ul-in B3LYP/6-31G(d)
SCF Energy (no zpe) = -808.9654861 au; Energy+zpe (0K) = -808.6581171 au
Enthalpy (298K) = -808.6408031 au; Gibbs free energy (298K) = -808.7041891 au

C;1.973386;-1.411897;0.182833
C;1.749680;-0.826126;1.425300
C;0.806945;0.194174;1.604490
C;0.044698;0.722551;0.566769
C;1.781773;1.369539;-0.869925
C;2.558764;0.240275;-1.077655
C;3.942830;0.124077;-0.510964
O;4.699472;1.046646;-0.321577
O;4.337967;-1.150432;-0.208041
C;3.267112;-2.121854;-0.124841
C;-0.856648;1.877133;0.783177
C;-2.377488;1.750804;0.557205
C;-1.539044;2.578595;-0.372340
H;1.127730;-1.607520;-0.469423
H;2.500506;-0.962022;2.203452
H;0.819640;0.733046;2.551321
H;-0.205548;0.084741;-0.275048
H;1.038777;1.662328;-1.602393
H;2.145368;2.154529;-0.216508
H;2.382395;-0.359529;-1.969846
H;3.208003;-2.675867;-1.069149
H;3.575066;-2.817129;0.663068
H;-0.579153;2.508751;1.624955
H;-2.962219;2.311774;1.285932
H;-1.349201;2.182957;-1.367020
H;-1.629008;3.660785;-0.338089
C;-3.015128;0.460510;0.138006
C;-3.215573;-0.556153;1.085331
C;-3.455268;0.243539;-1.173916
C;-3.834216;-1.753639;0.730608

H;-2.875922;-0.403833;2.106909
C;-4.073517;-0.956392;-1.533615
H;-3.324036;1.025215;-1.917357
C;-4.264549;-1.958961;-0.582931
H;-3.978108;-2.529038;1.478609
H;-4.410169;-1.103354;-2.556684
H;-4.746164;-2.892618;-0.860991

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TS-trans-6a-ul-in B3LYP/6-31G(d)

SCF Energy (no zpe) = -808.9649778 au; Energy+zpe (0K) = -808.6575148 au
Enthalpy (298K) = -808.6402168 au; Gibbs free energy (298K) = -808.7039088 au

C;1.863576;1.388958;-0.943948
C;-0.006116;1.143229;0.544762
C;0.655842;1.161076;1.769300
C;1.727289;0.312257;2.085261
C;2.194344;-0.594830;1.140584
C;2.892027;0.633799;-0.395810
C;3.483982;-1.362055;1.180574
C;3.456269;-0.590315;-1.061237
O;3.931697;-1.530575;-0.184314
C;-1.029899;2.156678;0.206569
O;3.525241;-0.786100;-2.249814
C;-2.472130;1.739946;-0.158108
C;-1.558283;2.304397;-1.205153
H;1.329008;1.013542;-1.810699
H;1.815080;2.456910;-0.775125
H;-0.073206;0.210859;-0.006005
H;0.463145;1.999768;2.437929
H;2.349314;0.563851;2.943394
H;1.452189;-1.065253;0.497818
H;3.610191;1.142265;0.245581
H;3.377894;-2.378018;1.577046
H;4.254166;-0.840683;1.763802
H;-0.961250;3.075077;0.786964
H;-3.220580;2.430198;0.230061
H;-1.154250;1.624218;-1.950181
H;-1.750857;3.305451;-1.581214
C;-2.912941;0.307925;-0.143554
C;-3.292689;-0.283903;1.071972
C;-2.987829;-0.463788;-1.309972
C;-3.728871;-1.606400;1.120102
H;-3.238582;0.301791;1.986701
C;-3.420880;-1.791290;-1.264917
H;-2.717508;-0.020376;-2.264273
C;-3.792250;-2.367255;-0.050391
H;-4.016659;-2.045603;2.071841
H;-3.472048;-2.371738;-2.182436
H;-4.130207;-3.399429;-0.014380

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TS-cis-6a-lk-in B3LYP/6-31G(d)

SCF Energy (no zpe) = -808.9654048 au; Energy+zpe (0K) = -808.6578298 au
Enthalpy (298K) = -808.6405788 au; Gibbs free energy (298K) = -808.7030288 au
C;2.368317;0.156827;1.339995

C;2.446602;1.454749;0.846391
 C;1.343804;2.095125;0.264478
 C;0.101157;1.488802;0.111423
 C;0.764098;-0.396992;-1.115646
 C;1.755961;-1.019188;-0.374437
 C;3.187206;-1.022008;-0.820804
 O;3.560959;-1.007795;-1.969739
 O;4.109747;-1.051993;0.190364
 C;3.600386;-0.697011;1.498508
 C;-0.994622;2.160665;-0.629034
 C;-2.177607;2.766728;0.107273
 C;-2.403818;1.559507;-0.760487
 H;1.470444;-0.159256;1.862012
 H;3.433337;1.875473;0.653756
 H;1.526047;3.026575;-0.270368
 H;-0.204471;0.727402;0.822271
 H;-0.257937;-0.753289;-1.068690
 H;1.480018;-1.846758;0.277933
 H;3.386041;-1.612096;2.063243
 H;4.426245;-0.173967;1.992082
 H;-0.661222;2.720770;-1.501007
 H;-2.558096;3.724880;-0.236447
 H;-2.207924;2.645237;1.186115
 H;-2.861378;1.768080;-1.725577
 C;-2.777221;0.211384;-0.231156
 C;-3.103686;-0.802933;-1.147742
 C;-2.827121;-0.099743;1.136149
 C;-3.454892;-2.081579;-0.717721
 H;-3.082010;-0.581077;-2.212458
 C;-3.174483;-1.380844;1.569885
 H;-2.611432;0.665343;1.876160
 C;-3.488437;-2.378107;0.646523
 H;-3.704843;-2.845616;-1.449099
 H;-3.208943;-1.594193;2.635187
 H;-3.763404;-3.373127;0.985310
 H;1.040015;0.171639;-1.997010

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TS-trans-6a-lk-in B3LYP/6-31G(d)

SCF Energy (no zpe) = -808.9642030 au; Energy+zpe (0K) = -808.6566760 au

Enthalpy (298K) = -808.6394120 au; Gibbs free energy (298K) = -808.7021000 au

C;0.798161;-0.034358;-1.414805
 C;0.086124;1.758920;0.031651
 C;1.260979;2.502578;0.081018
 C;2.506562;1.965849;0.442976
 C;2.617390;0.613883;0.745141
 C;2.108287;-0.321144;-1.055862
 C;3.881748;-0.186169;0.862215
 C;2.529942;-1.630542;-0.449058
 O;3.592322;-1.529253;0.413008
 C;-1.164987;2.337099;-0.515485
 O;2.036870;-2.709253;-0.668659
 C;-2.309353;2.734589;0.403935
 C;-2.498380;1.571596;-0.529357
 H;-0.005668;-0.696927;-1.112211
 H;0.594863;0.617503;-2.255140

H;-0.036883;0.910905;0.697583
 H;1.252337;3.496733;-0.365292
 H;3.402707;2.539647;0.209874
 H;1.783847;0.152162;1.271448
 H;2.907244;0.166593;-1.612562
 H;4.236610;-0.296728;1.893161
 H;4.694330;0.241403;0.260373
 H;-1.014815;2.996210;-1.369208
 H;-2.840720;3.657968;0.189051
 H;-2.186106;2.536738;1.464593
 H;-3.096909;1.785748;-1.412784
 C;-2.633582;0.152388;-0.076315
 C;-2.922674;-0.833389;-1.034909
 C;-2.489220;-0.252440;1.258920
 C;-3.047876;-2.174744;-0.677706
 H;-3.047622;-0.540130;-2.075024
 C;-2.609717;-1.596218;1.619279
 H;-2.295145;0.484326;2.032997
 C;-2.886958;-2.563620;0.653824
 H;-3.268979;-2.916905;-1.440075
 H;-2.491987;-1.884030;2.660736
 H;-2.979306;-3.608837;0.934905

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TS-cis-6a-lk-ou B3LYP/6-31G(d)
 SCF Energy (no zpe) = -808.9622481 au; Energy+zpe (0K) = -808.6547581 au
 Enthalpy (298K) = -808.6374601 au; Gibbs free energy (298K) = -808.7007631 au
 C;2.125966;-1.327479;-0.703042
 C;1.184529;-1.217885;0.315147
 C;0.208575;-0.211482;0.330563
 C;0.124295;0.765601;-0.654940
 C;2.282735;1.651945;-0.529823
 C;3.153450;0.584137;-0.680692
 C;3.974450;0.072111;0.464412
 O;4.388015;0.741701;1.381175
 O;4.259903;-1.265581;0.419553
 C;3.434931;-2.041771;-0.483149
 C;-0.799203;1.929860;-0.637345
 C;-1.422651;2.486364;0.621769
 C;-2.318747;1.818271;-0.382677
 H;1.823138;-1.143101;-1.729259
 H;1.376822;-1.742263;1.250985
 H;-0.359482;-0.085691;1.248587
 H;0.471977;0.502474;-1.649598
 H;2.054811;2.290775;-1.376258
 H;3.570366;0.381217;-1.666309
 H;3.974634;-2.193123;-1.425507
 H;3.317862;-3.014533;0.005842
 H;-0.550951;2.673296;-1.392169
 H;-1.473654;3.566029;0.733775
 H;-1.220008;1.959655;1.550383
 H;-2.899161;2.494566;-1.010511
 C;-3.010535;0.516759;-0.115517
 C;-3.280234;-0.361033;-1.176839
 C;-3.449330;0.163855;1.166792
 C;-3.962500;-1.557086;-0.962126

H;-2.946825;-0.100416;-2.178705
C;-4.131192;-1.035169;1.386883
H;-3.265594;0.839208;1.998196
C;-4.389392;-1.899821;0.323432
H;-4.159196;-2.224282;-1.797413
H;-4.463907;-1.289443;2.389956
H;-4.920057;-2.832909;0.492821
H;2.135002;2.086525;0.452281

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TS-trans-6a-lk-ou B3LYP/6-31G(d)

SCF Energy (no zpe) = -808.9617695 au; Energy+zpe (0K) = -808.6542115 au
Enthalpy (298K) = -808.6369415 au; Gibbs free energy (298K) = -808.7000635 au

C;-2.293278;1.621932;-0.246493
C;-0.137247;0.735951;0.270745
C;-0.025730;-0.263359;-0.690005
C;-0.994577;-1.265799;-0.862278
C;-2.135939;-1.280274;-0.070863
C;-3.086764;0.531360;-0.574210
C;-3.398722;-2.055612;-0.309030
C;-4.255929;0.084725;0.255220
O;-4.497470;-1.264258;0.199675
C;0.762005;1.912035;0.401440
O;-4.965793;0.794933;0.924596
C;1.590138;2.466853;-0.735455
C;2.303041;1.822688;0.420624
H;-2.418815;2.104141;0.718399
H;-1.828169;2.215037;-1.023499
H;-0.674532;0.501201;1.184255
H;0.730289;-0.166448;-1.465283
H;-0.975759;-1.842193;-1.786430
H;-2.023687;-0.982097;0.970072
H;-3.173648;0.261008;-1.625122
H;-3.445006;-3.000632;0.243869
H;-3.554257;-2.269763;-1.374427
H;0.373262;2.658946;1.090282
H;1.645958;3.546008;-0.851311
H;1.564488;1.925326;-1.677549
H;2.754999;2.514321;1.131902
C;3.050871;0.531085;0.291017
C;3.103549;-0.360103;1.373703
C;3.753415;0.202796;-0.875426
C;3.832701;-1.545068;1.291384
H;2.562777;-0.119411;2.285891
C;4.483561;-0.984725;-0.962921
H;3.737238;0.889108;-1.718100
C;4.524996;-1.862790;0.120075
H;3.858515;-2.223300;2.140393
H;5.023266;-1.219683;-1.876784
H;5.092650;-2.787138;0.054096

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TS-cis-6a-ul-ou B3LYP/6-31G(d)

SCF Energy (no zpe) = -808.9611117 au; Energy+zpe (0K) = -808.6533747 au
Enthalpy (298K) = -808.6361617 au; Gibbs free energy (298K) = -808.6983767 au

C;2.695804;-0.892718;1.005388
C;1.478478;-0.504167;1.556336
C;0.246952;-0.955094;1.059292
C;0.155032;-1.796451;-0.044946
C;1.337717;-0.529611;-1.624512
C;2.576150;-0.264452;-1.061145
C;2.957056;1.116960;-0.617866
O;2.573417;2.143744;-1.126126
O;3.819710;1.166597;0.442727
C;3.939963;-0.063780;1.197355
C;-1.099297;-2.265814;-0.693080
C;-2.423423;-1.495085;-0.795993
C;-2.322489;-2.685489;0.112546
H;2.826086;-1.920119;0.678615
H;1.464507;0.372549;2.203767
H;-0.648884;-0.463679;1.426975
H;0.994271;-2.458950;-0.233088
H;1.224400;-1.340612;-2.335835
H;0.593487;0.256668;-1.664970
H;3.418665;-0.904782;-1.320212
H;4.837393;-0.601401;0.868922
H;4.089800;0.253696;2.234577
H;-0.903910;-2.887436;-1.564535
H;-2.929376;-1.688863;-1.742107
H;-2.269728;-2.504636;1.182647
H;-2.834030;-3.605059;-0.159818
C;-2.641257;-0.095180;-0.304744
C;-2.216931;0.990228;-1.086825
C;-3.314948;0.173565;0.894126
C;-2.437116;2.303161;-0.673176
H;-1.709594;0.800660;-2.029645
C;-3.537177;1.487536;1.312450
H;-3.674681;-0.652608;1.501548
C;-3.095683;2.556583;0.532355
H;-2.090013;3.127844;-1.289644
H;-4.061028;1.673635;2.246547
H;-3.265373;3.579208;0.858092

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TS-trans-6a-ul-ou B3LYP/6-31G(d)

SCF Energy (no zpe) = -808.9607477 au; Energy+zpe (0K) = -808.6529737 au

Enthalpy (298K) = -808.6357687 au; Gibbs free energy (298K) = -808.6981827 au

C;-1.287061;0.145692;-1.376697
C;-0.173111;1.535013;0.233427
C;-0.064258;0.659954;1.309745
C;-1.167725;-0.027415;1.842195
C;-2.432816;0.136898;1.290810
C;-2.210911;-0.599973;-0.656996
C;-3.642553;-0.720195;1.526438
C;-3.696396;-0.459774;-0.830787
O;-4.417474;-0.724341;0.305180
C;0.951355;2.217522;-0.461587
O;-4.268646;-0.156159;-1.848942
C;2.346427;1.631689;-0.743419
C;2.183754;2.720962;0.275907
H;-1.626529;0.976268;-1.988349

H;-0.320389;-0.274155;-1.619541
H;-1.118038;2.051247;0.100304
H;0.922178;0.336862;1.630138
H;-0.973333;-0.880632;2.491018
H;-2.694731;1.132260;0.935571
H;-1.908064;-1.588026;-0.314460
H;-4.317643;-0.326030;2.294375
H;-3.370164;-1.748138;1.798935
H;0.604625;2.874177;-1.256358
H;2.735605;1.964984;-1.705443
H;2.251188;2.452758;1.326636
H;2.555788;3.716360;0.047559
C;2.770948;0.233431;-0.410962
C;2.498733;-0.803430;-1.317743
C;3.490856;-0.076629;0.750517
C;2.910961;-2.110419;-1.061914
H;1.965288;-0.577192;-2.238283
C;3.903180;-1.385188;1.012400
H;3.741555;0.714838;1.451494
C;3.611813;-2.407739;0.109302
H;2.687315;-2.896620;-1.778317
H;4.460907;-1.601748;1.919917
H;3.934217;-3.425620;0.311094

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TS-cis-6a-lk-an B3LYP/6-31G(d)

SCF Energy (no zpe) = -808.9583346 au; Energy+zpe (0K) = -808.6505256 au

Enthalpy (298K) = -808.6333626 au; Gibbs free energy (298K) = -808.6956186 au

C;-2.753395;0.704199;1.075360
C;-1.571433;0.281398;1.676664
C;-0.328027;0.840852;1.349997
C;-0.170937;1.819386;0.374945
C;-1.196667;0.727648;-1.452052
C;-2.461591;0.359942;-1.018427
C;-2.828549;-1.079423;-0.801737
O;-2.379005;-2.016283;-1.417169
O;-3.761753;-1.292233;0.175429
C;-3.980861;-0.172413;1.065750
C;1.151416;2.436914;0.039391
C;1.805666;2.378858;-1.323627
C;2.479993;1.702135;-0.155669
H;-2.895474;1.763428;0.882118
H;-1.572728;-0.671225;2.206079
H;0.563061;0.354803;1.736818
H;-1.008924;2.483720;0.179695
H;-1.064614;1.628999;-2.039242
H;-3.303822;1.006662;-1.262833
H;-4.869388;0.380277;0.738159
H;-4.194428;-0.620902;2.041420
H;1.270755;3.402876;0.535692
H;2.254916;3.283131;-1.725506
H;1.341872;1.749318;-2.075119
H;3.320553;2.254109;0.262881
C;2.669217;0.219379;-0.042687
C;3.229489;-0.297865;1.137821
C;2.349799;-0.680686;-1.067356

C;3.437397;-1.666503;1.299171
H;3.502886;0.386574;1.938433
C;2.551117;-2.053600;-0.907698
H;1.953514;-0.311852;-2.008420
C;3.092084;-2.553178;0.276449
H;3.871026;-2.040775;2.223040
H;2.287453;-2.730815;-1.715523
H;3.249600;-3.621106;0.399639
H;-0.428502;-0.031358;-1.541178

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TS-trans-6a-lk-an B3LYP/6-31G(d)

SCF Energy (no zpe) = -808.9582665 au; Energy+zpe (0K) = -808.6505055 au

Enthalpy (298K) = -808.6333525 au; Gibbs free energy (298K) = -808.6954455 au

C;1.047485;0.340920;1.180643
C;0.170188;1.473566;-0.776476
C;0.183324;0.430655;-1.695363
C;1.319150;-0.352175;-1.959560
C;2.505707;-0.103862;-1.279075
C;2.037496;-0.508610;0.703563
C;3.719326;-0.987127;-1.224309
C;3.492941;-0.343590;1.043301
O;4.343109;-0.788757;0.064336
C;-1.050458;2.300191;-0.514252
O;3.938588;0.117605;2.064993
C;-1.598079;2.583225;0.864890
C;-2.430451;1.781494;-0.106527
H;1.327045;1.259692;1.686715
H;0.055431;-0.044490;1.372049
H;1.096815;2.008409;-0.586044
H;-0.769401;0.086665;-2.089799
H;1.183779;-1.300546;-2.477973
H;2.743479;0.937245;-1.066602
H;1.759174;-1.541247;0.498994
H;4.485209;-0.721765;-1.961514
H;3.462745;-2.046285;-1.355765
H;-1.102367;3.158090;-1.189172
H;-1.914230;3.594855;1.104510
H;-1.141702;2.058009;1.697296
H;-3.239851;2.338827;-0.577266
C;-2.780342;0.337377;0.095010
C;-3.311972;-0.392698;-0.981481
C;-2.660111;-0.309526;1.331709
C;-3.683826;-1.727670;-0.835037
H;-3.437010;0.098906;-1.944174
C;-3.027511;-1.649469;1.482396
H;-2.295851;0.242284;2.193420
C;-3.536906;-2.365205;0.399679
H;-4.091833;-2.270371;-1.683949
H;-2.924479;-2.128073;2.452848
H;-3.826289;-3.405965;0.517133

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TS-trans-6b-ul-in B3LYP/6-31G(d)

SCF Energy (no zpe) = -1036.8525927 au; Energy+zpe (0K) = -1036.5019827 au

Enthalpy (298K) = -1036.4799817 au; Gibbs free energy (298K) = -1036.5550627 au
 C;1.837004;0.311989;-0.734175
 C;-0.345828;0.526218;0.983654
 C;0.399802;0.181327;2.095693
 C;1.226720;-0.950413;2.169582
 C;1.403447;-1.797457;1.065588
 C;2.463802;-0.823729;-0.203665
 C;2.299055;-3.010162;1.059986
 C;2.709367;-2.061809;-1.043351
 O;2.736245;-3.206702;-0.300932
 C;2.269050;1.620314;-0.264644
 C;-1.107819;1.774824;0.899039
 O;2.892760;-2.090334;-2.232771
 O;3.039788;1.822842;0.664267
 O;1.727848;2.632009;-1.004517
 C;2.147681;3.946642;-0.625285
 C;-2.562675;1.771569;0.340301
 C;-1.455361;2.395286;-0.442565
 H;1.201264;0.249462;-1.609641
 H;-0.549926;-0.212227;0.216658
 H;0.452370;0.895933;2.915055
 H;1.912434;-1.027697;3.011486
 H;0.528694;-1.940700;0.431320
 H;3.310110;-0.587692;0.444429
 H;1.780737;-3.930772;1.345335
 H;3.171724;-2.878734;1.712413
 H;-0.938131;2.470221;1.718080
 H;3.233878;4.046914;-0.706105
 H;1.852915;4.169673;0.404599
 H;1.651020;4.626567;-1.319512
 H;-3.203765;2.466512;0.880637
 H;-1.073655;1.886340;-1.321439
 H;-1.417418;3.478259;-0.515361
 C;-3.258260;0.506926;-0.054965
 C;-3.154617;-0.046554;-1.337997
 C;-4.062225;-0.151568;0.889968
 C;-3.822210;-1.229637;-1.664134
 H;-2.561658;0.456345;-2.096395
 C;-4.733261;-1.328698;0.566295
 H;-4.156818;0.266835;1.889570
 C;-4.612554;-1.875589;-0.714025
 H;-3.728650;-1.639844;-2.666216
 H;-5.350514;-1.820788;1.313434
 H;-5.134452;-2.794017;-0.968513

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TS-trans-6b-lk-in B3LYP/6-31G(d)
 SCF Energy (no zpe) = -1036.8524428 au; Energy+zpe (0K) = -1036.5015638 au
 Enthalpy (298K) = -1036.4797048 au; Gibbs free energy (298K) = -1036.5528178 au
 C;1.031519;0.253821;-0.906871
 C;-0.160125;0.811461;1.509804
 C;1.018730;1.299814;2.041968
 C;2.232961;0.593210;2.049433
 C;2.348363;-0.648976;1.414917
 C;2.260185;-0.271914;-0.492660
 C;3.619726;-1.448689;1.304875

C;2.694953;-1.678899;-0.841945
 O;3.529623;-2.224881;0.091425
 C;0.966368;1.680171;-1.198066
 C;-1.371773;1.637500;1.384792
 O;2.394739;-2.290869;-1.834333
 O;1.857152;2.490598;-0.982043
 O;-0.220618;2.038291;-1.774434
 C;-0.320046;3.419229;-2.140766
 C;-2.585876;1.345127;2.270688
 C;-2.680807;1.094119;0.797948
 H;0.205733;-0.385481;-1.192977
 H;-0.289528;-0.255168;1.354812
 H;1.046162;2.344266;2.347143
 H;3.136387;1.132428;2.328600
 H;1.468382;-1.290561;1.447894
 H;3.082865;0.443631;-0.537622
 H;3.745384;-2.174039;2.114933
 H;4.507761;-0.804952;1.266904
 H;-1.184103;2.693679;1.203653
 H;0.461653;3.688691;-2.856709
 H;-0.225444;4.065729;-1.263206
 H;-1.305976;3.533892;-2.594071
 H;-3.110303;2.196496;2.695740
 H;-2.507340;0.493760;2.940019
 H;-3.224853;1.848854;0.232332
 C;-2.802530;-0.282044;0.214195
 C;-2.542278;-0.471141;-1.153928
 C;-3.205554;-1.388476;0.973069
 C;-2.670477;-1.729920;-1.738885
 H;-2.218328;0.375697;-1.752520
 C;-3.331382;-2.651655;0.388932
 H;-3.442138;-1.263520;2.025814
 C;-3.063167;-2.827414;-0.967826
 H;-2.458958;-1.855667;-2.797390
 H;-3.646827;-3.495671;0.996883
 H;-3.160435;-3.809118;-1.423191

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TS-cis-6b-ul-in B3LYP/6-31G(d)

SCF Energy (no zpe) = -1036.8516512 au; Energy+zpe (0K) = -1036.5006242 au

Enthalpy (298K) = -1036.4787712 au; Gibbs free energy (298K) = -1036.5521832 au

C;1.751871;-1.907467;-0.250008
 C;1.499881;-2.039464;1.126823
 C;0.575707;-1.242071;1.809726
 C;-0.192459;-0.262469;1.202182
 C;1.972368;0.955848;0.128332
 C;2.555965;-0.134894;-0.529350
 C;3.933570;-0.617113;-0.138416
 O;4.802028;0.049878;0.365010
 O;4.141358;-1.934814;-0.424645
 C;2.943591;-2.624167;-0.849512
 C;-1.122393;0.574822;1.963377
 C;1.122023;1.860000;-0.634281
 O;0.537972;1.583456;-1.677204
 O;1.050718;3.091326;-0.059284
 C;0.346278;4.085247;-0.812646

C;-2.633659;0.657602;1.553375
 C;-1.731826;1.838635;1.397282
 H;0.902335;-1.736494;-0.906809
 H;2.202289;-2.621422;1.722824
 H;0.541047;-1.320162;2.895396
 H;-0.297492;-0.256656;0.123894
 H;2.359714;1.296500;1.080578
 H;2.382143;-0.150425;-1.607267
 H;2.900429;-2.631781;-1.944792
 H;3.053318;-3.653632;-0.497107
 H;-0.967315;0.560809;3.040087
 H;0.755725;4.167276;-1.823030
 H;-0.719593;3.847019;-0.886196
 H;0.484628;5.018939;-0.265857
 H;-3.279361;0.674635;2.428833
 H;-1.436506;2.119344;0.393244
 H;-1.856552;2.680078;2.073124
 C;-3.218493;-0.111561;0.415062
 C;-4.213954;-1.061393;0.695185
 C;-2.830309;0.065869;-0.922988
 C;-4.801481;-1.813679;-0.320579
 H;-4.531252;-1.209141;1.725240
 C;-3.414141;-0.691612;-1.939630
 H;-2.069305;0.794095;-1.188217
 C;-4.401439;-1.633068;-1.645675
 H;-5.572749;-2.539488;-0.076080
 H;-3.097144;-0.536192;-2.967522
 H;-4.857564;-2.216448;-2.440906

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TS-trans-6b-lk-ou B3LYP/6-31G(d)
 SCF Energy (no zpe) = -1036.8486738 au; Energy+zpe (0K) = -1036.4979278 au
 Enthalpy (298K) = -1036.4759708 au; Gibbs free energy (298K) = -1036.5509628 au
 C;2.382610;0.619013;-0.450862
 C;-0.270256;0.129805;-0.567635
 C;-0.346473;-0.470147;0.674934
 C;0.499987;-1.515241;1.082389
 C;1.525550;-1.987272;0.257098
 C;2.850505;-0.541265;0.172056
 C;2.539553;-3.027560;0.652739
 C;3.859675;-1.454649;-0.489136
 O;3.742557;-2.757352;-0.097482
 C;2.081395;1.783946;0.374985
 C;-1.019131;1.323493;-1.007125
 O;4.715160;-1.119910;-1.267794
 O;2.059095;1.803581;1.597151
 O;1.842043;2.889951;-0.385924
 C;1.602428;4.091685;0.354103
 C;-1.739498;2.261862;-0.066786
 C;-2.571091;1.400305;-0.969006
 H;2.450462;0.748470;-1.525028
 H;0.225641;-0.400818;-1.372729
 H;-0.980914;-0.025626;1.436100
 H;0.509054;-1.777969;2.138853
 H;1.314522;-2.011505;-0.811537
 H;3.015196;-0.432183;1.245144

H;2.242411;-4.045819;0.382329
H;2.759357;-2.998286;1.727517
H;-0.590824;1.791254;-1.889358
H;2.455517;4.329228;0.996154
H;0.710488;3.994200;0.979887
H;1.460285;4.874239;-0.393090
H;-1.677668;3.326468;-0.274633
H;-1.714985;2.020801;0.992164
H;-2.978789;1.898658;-1.848128
C;-3.427877;0.279849;-0.467111
C;-3.701001;-0.814195;-1.303109
C;-4.011351;0.305993;0.805707
C;-4.526527;-1.852848;-0.877420
H;-3.257139;-0.847858;-2.295477
C;-4.837633;-0.734497;1.237106
H;-3.829346;1.154201;1.460133
C;-5.097100;-1.817494;0.397755
H;-4.724064;-2.691780;-1.539680
H;-5.282082;-0.693439;2.228170
H;-5.740555;-2.627093;0.731490

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TS-cis-6b-lk-ou B3LYP/6-31G(d)

SCF Energy (no zpe) = -1036.8487766 au; Energy+zpe (0K) = -1036.4979316 au

Enthalpy (298K) = -1036.4759746 au; Gibbs free energy (298K) = -1036.5507436 au

C;1.415763;-1.909460;-0.939946
C;0.358951;-1.980833;-0.021338
C;-0.420930;-0.876993;0.346527
C;-0.233256;0.390467;-0.178100
C;2.313252;0.526609;0.384539
C;2.791734;-0.672207;-0.147584
C;3.338602;-1.763834;0.733726
O;3.845098;-1.613014;1.817624
O;3.227842;-3.008770;0.183834
C;2.409870;-3.047889;-1.009547
C;-0.920310;1.619832;0.263687
C;2.409196;1.733067;-0.434078
O;2.605563;1.754199;-1.642021
O;2.236579;2.864800;0.301405
C;2.371088;4.091123;-0.429206
C;-1.579368;1.772884;1.617481
C;-2.462257;1.729576;0.407887
H;1.288828;-1.304568;-1.834199
H;0.297230;-2.865185;0.612421
H;-1.098823;-1.007410;1.185716
H;0.290007;0.484988;-1.123572
H;2.117216;0.630963;1.444166
H;3.311121;-0.568727;-1.101371
H;3.054284;-2.967722;-1.892541
H;1.939670;-4.035537;-1.009406
H;-0.466035;2.524070;-0.130223
H;3.369382;4.171916;-0.868335
H;1.630598;4.152241;-1.232172
H;2.211016;4.885984;0.300543
H;-1.443660;2.717135;2.137383
H;-1.570343;0.905865;2.272363

H;-2.836796;2.694429;0.066257
C;-3.393388;0.592603;0.119790
C;-3.686311;0.247490;-1.208587
C;-4.030571;-0.113934;1.147704
C;-4.585252;-0.776672;-1.500378
H;-3.199421;0.787367;-2.017356
C;-4.930486;-1.142573;0.859189
H;-3.830000;0.151852;2.182256
C;-5.209991;-1.477620;-0.465522
H;-4.797045;-1.030457;-2.535797
H;-5.415713;-1.677508;1.671465
H;-5.910200;-2.277238;-0.691770

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TS-cis-6b-ul-ou B3LYP/6-31G(d)
SCF Energy (no zpe) = -1036.8493855 au; Energy+zpe (0K) = -1036.4981855 au
Enthalpy (298K) = -1036.4763615 au; Gibbs free energy (298K) = -1036.5492755 au
C;-2.473985;-0.844993;1.466431
C;-1.234259;-1.462105;1.697864
C;-0.024245;-0.758883;1.760631
C;0.050472;0.615727;1.603863
C;-1.238599;0.627413;-0.703213
C;-2.410566;-0.053927;-0.364269
C;-2.754313;-1.370838;-1.015377
O;-2.422476;-1.721344;-2.120186
O;-3.524139;-2.178998;-0.230536
C;-3.675201;-1.699998;1.125567
C;1.274198;1.439596;1.585313
C;-1.219052;2.083529;-0.639593
O;-2.040155;2.784609;-0.063108
O;-0.144668;2.605678;-1.298953
C;-0.072174;4.036850;-1.305564
C;2.601052;1.073192;0.882280
C;2.525384;1.059542;2.373992
H;-2.672315;0.105757;1.955299
H;-1.177780;-2.545588;1.595987
H;0.891841;-1.341864;1.793966
H;-0.858764;1.193725;1.723281
H;-0.434874;0.118395;-1.218534
H;-3.274593;0.589094;-0.187003
H;-4.609395;-1.132137;1.204902
H;-3.758541;-2.596809;1.746252
H;1.061326;2.504503;1.558096
H;-0.960121;4.467616;-1.776417
H;0.007697;4.429386;-0.287312
H;0.821353;4.283351;-1.880793
H;3.074851;1.955855;0.454020
H;2.497485;0.098188;2.879273
H;3.023284;1.843679;2.938125
C;2.792310;-0.154003;0.046089
C;2.361555;-0.148854;-1.290284
C;3.442773;-1.294091;0.534771
C;2.558567;-1.261123;-2.107360
H;1.863058;0.734258;-1.682078
C;3.640338;-2.410068;-0.282144
H;3.810102;-1.305179;1.557684

C;3.195988;-2.398307;-1.604179
H;2.210563;-1.242163;-3.136585
H;4.147827;-3.285285;0.115312
H;3.347056;-3.266289;-2.240109

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TS-trans-6b-ul-ou B3LYP/6-31G(d)

SCF Energy (no zpe) = -1036.8473559 au; Energy+zpe (0K) = -1036.4962799 au
Enthalpy (298K) = -1036.4744409 au; Gibbs free energy (298K) = -1036.5470849 au

C;-2.017071;1.041986;0.149673
C;-0.037084;-0.346531;1.473931
C;0.087358;-1.375400;0.561599
C;-1.012322;-2.072608;0.029236
C;-2.334389;-1.753372;0.356846
C;-2.706615;-0.014013;-0.453442
C;-3.529487;-2.433484;-0.258111
C;-4.201355;-0.184377;-0.245658
O;-4.613064;-1.482993;-0.270168
C;-0.964110;1.741799;-0.572405
C;1.025080;0.563367;1.952941
O;-4.992767;0.710563;-0.096472
O;-0.494737;1.423913;-1.657307
O;-0.565927;2.858551;0.105629
C;0.385368;3.686056;-0.573208
C;2.460349;0.694414;1.443760
C;2.208694;0.047062;2.775817
H;-2.396076;1.502531;1.055648
H;-0.959700;-0.261075;2.038453
H;1.054050;-1.560728;0.107866
H;-0.829184;-2.709775;-0.834918
H;-2.519468;-1.440551;1.384246
H;-2.396591;-0.224602;-1.478667
H;-3.887077;-3.287019;0.326571
H;-3.324303;-2.769876;-1.282312
H;0.615996;1.502438;2.317583
H;0.037496;3.932462;-1.579921
H;1.357096;3.188608;-0.648188
H;0.473278;4.589586;0.032381
H;2.806186;1.727150;1.507893
H;2.314542;-1.033184;2.829062
H;2.466153;0.572159;3.691865
C;3.085691;-0.046655;0.294977
C;4.144480;-0.936622;0.523511
C;2.686727;0.195426;-1.029464
C;4.789179;-1.573348;-0.538614
H;4.469934;-1.125076;1.543358
C;3.330409;-0.441739;-2.091069
H;1.847475;0.854693;-1.233453
C;4.384068;-1.326679;-1.850884
H;5.608440;-2.259403;-0.339172
H;3.000668;-0.248686;-3.108534
H;4.883227;-1.821618;-2.679831

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TS-cis-6b-lk-an B3LYP/6-31G(d)

SCF Energy (no zpe) = -1036.8444102 au; Energy+zpe (0K) = -1036.4933702 au
 Enthalpy (298K) = -1036.4715402 au; Gibbs free energy (298K) = -1036.5453872 au
 C;2.078537;-1.462215;-1.441708
 C;0.710224;-1.773626;-1.537772
 C;-0.299487;-0.804427;-1.586621
 C;-0.063498;0.557960;-1.547944
 C;1.512217;0.446640;0.635706
 C;2.384407;-0.587244;0.268344
 C;2.413955;-1.891636;1.027851
 O;2.088417;-2.057777;2.175967
 O;2.882158;-2.927584;0.272084
 C;3.050867;-2.581057;-1.121918
 C;-1.142075;1.582868;-1.617915
 C;1.953287;1.819739;0.412621
 O;2.835782;2.158005;-0.365618
 O;1.268754;2.711767;1.178550
 C;1.662043;4.081690;1.017238
 C;-1.526752;2.506112;-0.481437
 C;-2.528046;1.491077;-0.971974
 H;2.455173;-0.636837;-2.042032
 H;0.406720;-2.801861;-1.342993
 H;-1.328091;-1.147669;-1.531740
 H;0.928998;0.935458;-1.777005
 H;0.679026;0.258172;1.300524
 H;3.377867;-0.236812;-0.019298
 H;4.089614;-2.277587;-1.296368
 H;2.854481;-3.498920;-1.682660
 H;-1.148551;2.072896;-2.594674
 H;2.715956;4.212944;1.277005
 H;1.509887;4.410240;-0.014683
 H;1.027651;4.650595;1.698126
 H;-1.703863;3.553647;-0.710831
 H;-1.046163;2.340955;0.475389
 H;-3.309366;1.895626;-1.613469
 C;-3.016996;0.341021;-0.145628
 C;-4.021407;-0.485653;-0.676307
 C;-2.538010;0.051827;1.139784
 C;-4.515658;-1.574107;0.041437
 H;-4.417545;-0.269624;-1.666450
 C;-3.027771;-1.039159;1.859622
 H;-1.782405;0.685578;1.593315
 C;-4.016250;-1.858876;1.313883
 H;-5.293467;-2.197269;-0.392479
 H;-2.636231;-1.244075;2.852401
 H;-4.398096;-2.706343;1.876481

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TS-trans-6c-ul-in B3LYP/6-31G(d)
 SCF Energy (no zpe) = -1036.8515898 au; Energy+zpe (0K) = -1036.5008928 au
 Enthalpy (298K) = -1036.4789638 au; Gibbs free energy (298K) = -1036.5527618 au
 C;-1.806406;0.575806;-1.189686
 C;0.336339;-1.421476;-0.976508
 C;-0.543707;-2.480527;-0.923004
 C;-1.696003;-2.537127;-0.115841
 C;-2.154275;-1.452465;0.644834
 C;-2.835789;-0.171338;-0.594401

C;-3.390369;-1.574133;1.501475
 C;-3.792153;0.470397;0.421426
 O;-4.092880;-0.320449;1.480854
 C;-1.085553;1.545536;-0.389177
 C;1.420885;-1.361968;-1.961626
 O;-1.122142;1.602518;0.836234
 O;-4.321326;1.538830;0.270228
 O;-0.317343;2.390437;-1.135484
 C;0.372417;3.398894;-0.382875
 C;2.828059;-0.847490;-1.582906
 C;1.950329;-0.024067;-2.468662
 H;-1.589448;0.495132;-2.246584
 H;0.332535;-0.670225;-0.194253
 H;-0.397784;-3.293622;-1.633764
 H;-2.365906;-3.384515;-0.259820
 H;-1.414031;-0.777898;1.074280
 H;-3.406268;-0.786486;-1.293297
 H;-3.151950;-1.772884;2.550933
 H;-4.062269;-2.363146;1.138800
 H;1.414409;-2.171616;-2.688420
 H;0.909518;3.997400;-1.120460
 H;1.069334;2.945586;0.327484
 H;-0.338789;4.020567;0.167753
 H;3.616254;-1.402587;-2.091883
 H;1.479340;0.863675;-2.056862
 H;2.188318;0.043704;-3.526701
 C;3.184495;-0.436227;-0.185992
 C;3.322089;-1.403831;0.820806
 C;3.439229;0.903098;0.135369
 C;3.696872;-1.041263;2.113740
 H;3.126251;-2.447249;0.585689
 C;3.815327;1.269593;1.429662
 H;3.351529;1.661365;-0.638017
 C;3.943438;0.298601;2.423025
 H;3.793514;-1.804200;2.881784
 H;4.010917;2.313752;1.659557
 H;4.232719;0.582488;3.431177

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TS-trans-6c-lk-ou B3LYP/6-31G(d)
 SCF Energy (no zpe) = -1036.8476709 au; Energy+zpe (0K) = -1036.4969189 au
 Enthalpy (298K) = -1036.4749159 au; Gibbs free energy (298K) = -1036.5498749 au
 C;-2.226255;0.573825;-0.936285
 C;0.436095;0.370490;-0.146601
 C;0.646087;-0.879051;-0.686748
 C;-0.217126;-1.972692;-0.466509
 C;-1.423829;-1.848889;0.223939
 C;-2.599583;-0.772877;-0.944977
 C;-2.383712;-2.994023;0.396436
 C;-3.866955;-1.280589;-0.256635
 O;-3.726385;-2.476048;0.372916
 C;-2.486152;1.398047;0.233173
 C;1.164824;1.610604;-0.475724
 O;-2.771257;0.966844;1.344835
 O;-4.940232;-0.743684;-0.330632
 O;-2.320380;2.725496;-0.018912

C;-2.584805;3.591320;1.093363
 C;2.008026;1.787700;-1.720079
 C;2.709609;1.736219;-0.396823
 H;-1.816064;1.045011;-1.819759
 H;-0.218181;0.453414;0.713753
 H;1.436374;-1.014215;-1.421313
 H;-0.041768;-2.877332;-1.048035
 H;-1.484006;-1.126189;1.036835
 H;-2.465042;-1.278075;-1.903034
 H;-2.273243;-3.493020;1.364687
 H;-2.274271;-3.744380;-0.397596
 H;0.643429;2.502700;-0.138386
 H;-2.419305;4.603812;0.722431
 H;-1.911345;3.373608;1.927572
 H;-3.616277;3.473872;1.436649
 H;1.941259;2.738182;-2.242458
 H;2.103828;0.929119;-2.379352
 H;3.025568;2.698815;0.004920
 C;3.595283;0.597845;0.006513
 C;3.685375;0.224712;1.356313
 C;4.385281;-0.084276;-0.927480
 C;4.536764;-0.802241;1.759585
 H;3.076897;0.744145;2.092786
 C;5.238378;-1.115522;-0.527392
 H;4.341812;0.203212;-1.974726
 C;5.316268;-1.478067;0.817124
 H;4.590249;-1.078134;2.809498
 H;5.845033;-1.630843;-1.267599
 H;5.979646;-2.279781;1.130305

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TS-cis-6c-ul-in B3LYP/6-31G(d)
 SCF Energy (no zpe) = -1036.8469377 au; Energy+zpe (0K) = -1036.4965687 au
 Enthalpy (298K) = -1036.4745507 au; Gibbs free energy (298K) = -1036.5498247 au
 C;1.179425;-1.960979;0.647744
 C;1.202886;-1.065379;1.728055
 C;0.378046;0.068834;1.795800
 C;-0.486356;0.448798;0.791241
 C;1.518584;0.316708;-1.053598
 C;1.847262;-1.042554;-0.970465
 C;3.289682;-1.511543;-0.794413
 O;4.233208;-1.062804;-1.390463
 O;3.428066;-2.589956;0.020274
 C;2.199377;-3.078775;0.590326
 C;-1.227173;1.715069;0.816522
 C;2.278227;1.288922;-0.289353
 O;3.069792;1.002611;0.600062
 O;1.990181;2.573483;-0.641483
 C;2.718457;3.572878;0.079587
 C;-2.719148;1.770244;0.400860
 C;-1.673244;2.386216;-0.471667
 H;0.204705;-2.184359;0.219442
 H;2.019507;-1.136403;2.443037
 H;0.552665;0.767832;2.611695
 H;-0.774930;-0.263906;0.026583
 H;0.775522;0.670020;-1.756981

H;1.340757;-1.668600;-1.709546
 H;1.841966;-3.917757;-0.018759
 H;2.461749;-3.458641;1.581597
 H;-0.955166;2.384441;1.629551
 H;2.476859;3.539756;1.146664
 H;3.796244;3.429275;-0.038118
 H;2.411848;4.528401;-0.349120
 H;-3.291673;2.467553;1.011618
 H;-1.408930;1.881540;-1.396317
 H;-1.600854;3.468496;-0.524215
 C;-3.481689;0.538035;0.019283
 C;-4.015905;-0.283948;1.024785
 C;-3.709456;0.187299;-1.317486
 C;-4.750065;-1.423774;0.703356
 H;-3.847473;-0.024709;2.067448
 C;-4.442614;-0.956566;-1.643208
 H;-3.323304;0.821174;-2.110905
 C;-4.964358;-1.766141;-0.634655
 H;-5.154263;-2.047022;1.496794
 H;-4.610455;-1.208869;-2.687039
 H;-5.536380;-2.654967;-0.886838

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TS-cis-6c-lk-in B3LYP/6-31G(d)
 SCF Energy (no zpe) = -1036.8470960 au; Energy+zpe (0K) = -1036.4965080 au
 Enthalpy (298K) = -1036.4745760 au; Gibbs free energy (298K) = -1036.5486720 au
 C;2.019264;-1.175392;1.524430
 C;2.059664;0.143762;2.000214
 C;0.926469;0.970714;2.048999
 C;-0.327054;0.597868;1.610527
 C;0.727598;-0.132149;-0.805429
 C;1.609486;-1.145444;-0.408335
 C;3.071308;-1.165142;-0.846112
 O;3.458743;-0.925670;-1.959402
 O;3.931105;-1.605296;0.110913
 C;3.313397;-1.945771;1.366082
 C;-1.447263;1.549347;1.557564
 C;1.218910;1.221741;-0.984479
 O;2.319207;1.616761;-0.621602
 O;0.299514;2.039158;-1.578123
 C;0.742300;3.383610;-1.793341
 C;-2.718395;1.279104;2.363061
 C;-2.787260;1.238014;0.868822
 H;1.142533;-1.764846;1.783834
 H;3.030264;0.613275;2.143793
 H;1.084769;2.017216;2.303139
 H;-0.568250;-0.450051;1.462347
 H;-0.293349;-0.360380;-1.078771
 H;1.186659;-2.151008;-0.478383
 H;3.141668;-3.028725;1.388896
 H;4.047824;-1.695996;2.136842
 H;-1.145342;2.593264;1.510099
 H;0.956115;3.882995;-0.843089
 H;1.647634;3.401284;-2.406636
 H;-0.077613;3.885863;-2.309534
 H;-3.170182;2.117223;2.886419

H;-2.755477;0.343657;2.913434
H;-3.217906;2.123003;0.403394
C;-3.040544;-0.011371;0.082935
C;-2.866341;0.020361;-1.311358
C;-3.479166;-1.205537;0.669453
C;-3.113945;-1.108101;-2.090985
H;-2.512768;0.935710;-1.779642
C;-3.723185;-2.339730;-0.109540
H;-3.653421;-1.249851;1.740617
C;-3.541793;-2.295937;-1.491325
H;-2.970432;-1.061068;-3.167186
H;-4.065885;-3.254610;0.366969
H;-3.736084;-3.176246;-2.097926

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TS-trans-6c-ul-ou B3LYP/6-31G(d)

SCF Energy (no zpe) = -1036.8474014 au; Energy+zpe (0K) = -1036.4964914 au

Enthalpy (298K) = -1036.4745354 au; Gibbs free energy (298K) = -1036.5486564 au

C;1.040897;0.299915;0.794414
C;-0.375184;0.397080;-1.693467
C;-0.470371;-0.972907;-1.812657
C;0.623659;-1.845622;-1.642931
C;1.886919;-1.405020;-1.232416
C;1.724276;-0.911597;0.630457
C;3.046556;-2.349824;-1.053336
C;3.227796;-1.039375;0.889364
O;3.872001;-1.858177;0.017216
C;1.667463;1.557399;0.432553
C;-1.478269;1.373736;-1.735948
O;2.669107;1.670348;-0.267186
O;3.803936;-0.553857;1.825818
O;0.984132;2.633086;0.914778
C;1.554197;3.907427;0.592425
C;-2.779689;1.292881;-0.887256
C;-2.830964;1.075197;-2.364007
H;0.059075;0.319303;1.246440
H;0.610710;0.845513;-1.724199
H;-1.448833;-1.428969;-1.939553
H;0.417693;-2.915460;-1.630647
H;2.207682;-0.411399;-1.544985
H;1.203525;-1.777974;1.043433
H;3.692219;-2.394253;-1.936159
H;2.712851;-3.367680;-0.811823
H;-1.130671;2.395695;-1.859703
H;0.906487;4.647454;1.065005
H;1.582929;4.061097;-0.490783
H;2.572604;3.986335;0.982711
H;-3.093078;2.281418;-0.554674
H;-2.981273;0.065270;-2.734437
H;-3.274230;1.843151;-2.992230
C;-3.038463;0.229718;0.131033
C;-2.631503;0.448325;1.457735
C;-3.717712;-0.957882;-0.167701
C;-2.880996;-0.498201;2.449917
H;-2.112605;1.371359;1.706902
C;-3.967512;-1.909848;0.823910

H;-4.074423;-1.134057;-1.178841
C;-3.548211;-1.685155;2.134779
H;-2.556676;-0.308710;3.469723
H;-4.499548;-2.823177;0.570435
H;-3.745184;-2.423603;2.907172

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TS-trans-6c-lk-an B3LYP/6-31G(d)

SCF Energy (no zpe) = -1036.8449425 au; Energy+zpe (0K) = -1036.4940925 au
Enthalpy (298K) = -1036.4722145 au; Gibbs free energy (298K) = -1036.5457275 au

C;0.990542;0.279799;0.748917
C;-0.369093;0.290438;-1.778015
C;-0.446503;-1.081304;-1.848969
C;0.641770;-1.948905;-1.623886
C;1.888368;-1.487353;-1.182683
C;1.658343;-0.949096;0.638808
C;3.043048;-2.427978;-0.945178
C;3.149172;-1.082270;0.973508
O;3.826983;-1.918912;0.146923
C;1.672390;1.512237;0.394512
C;-1.540815;1.188263;-1.984254
O;2.685903;1.579453;-0.292449
O;3.681528;-0.582089;1.927593
O;1.037563;2.616527;0.876347
C;1.664102;3.866553;0.555483
C;-1.876546;2.314436;-1.037923
C;-2.837797;1.157072;-1.171940
H;0.003767;0.330858;1.187796
H;0.602655;0.773760;-1.814230
H;-1.427433;-1.532669;-1.979178
H;0.437839;-3.018314;-1.582078
H;2.216286;-0.504876;-1.521882
H;1.109733;-1.793422;1.061193
H;3.718319;-2.484266;-1.804560
H;2.701661;-3.442108;-0.699543
H;-1.692272;1.423431;-3.040891
H;1.048189;4.632786;1.028099
H;1.699678;4.017458;-0.527332
H;2.683459;3.897535;0.949205
H;-2.169618;3.273999;-1.455507
H;-1.277086;2.388634;-0.136172
H;-3.717530;1.364740;-1.780184
C;-3.120212;0.180439;-0.071057
C;-3.825059;-0.997486;-0.369330
C;-2.754442;0.409885;1.261670
C;-4.132631;-1.925542;0.624047
H;-4.137947;-1.182723;-1.395068
C;-3.057696;-0.519573;2.260177
H;-2.244560;1.330944;1.528354
C;-3.744180;-1.692164;1.945627
H;-4.679294;-2.829473;0.367604
H;-2.764693;-0.317883;3.287254
H;-3.983530;-2.412951;2.722750

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TS-cis-6c-lk-ou B3LYP/6-31G(d)

SCF Energy (no zpe) = -1036.8428024 au; Energy+zpe (0K) = -1036.4922494 au

Enthalpy (298K) = -1036.4702944 au; Gibbs free energy (298K) = -1036.5447844 au

C;1.489287;-2.061333;-0.390411
C;0.609995;-1.502253;0.546079
C;-0.308801;-0.488327;0.227210
C;-0.384427;0.086188;-1.023843
C;2.238893;0.644061;-1.048438
C;2.777115;-0.645788;-0.990043
C;3.849423;-1.030349;0.024338
O;4.809795;-0.355856;0.290209
O;3.713817;-2.279545;0.540200
C;2.566962;-3.016140;0.074009
C;-1.200104;1.253329;-1.410424
C;2.111164;1.428113;0.169981
O;2.214948;0.972260;1.300565
O;1.828997;2.736799;-0.079818
C;1.720417;3.562271;1.084856
C;-1.714620;2.278529;-0.423227
C;-2.714624;1.384420;-1.088879
H;1.103738;-2.228799;-1.393395
H;0.780677;-1.707820;1.600673
H;-0.854362;-0.038917;1.051629
H;0.060965;-0.441006;-1.860435
H;2.033772;1.122581;-1.997935
H;3.008728;-1.080787;-1.965256
H;2.888433;-3.683708;-0.734397
H;2.245580;-3.629384;0.920594
H;-0.940269;1.647829;-2.389563
H;0.881570;3.245401;1.712554
H;2.637175;3.517074;1.679350
H;1.554794;4.575106;0.714164
H;-1.666132;3.324092;-0.713951
H;-1.492431;2.102209;0.625596
H;-3.269464;1.833790;-1.912366
C;-3.485570;0.332286;-0.353660
C;-3.885963;-0.835426;-1.021187
C;-3.868818;0.499799;0.983011
C;-4.642269;-1.808516;-0.370728
H;-3.596275;-0.979246;-2.059535
C;-4.624685;-0.474393;1.639253
H;-3.583312;1.405776;1.510944
C;-5.013131;-1.631740;0.964842
H;-4.940812;-2.706968;-0.904653
H;-4.912734;-0.324479;2.676496
H;-5.601557;-2.390394;1.473803

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TS-trans-6d-ul-in B3LYP/6-31G(d)

SCF Energy (no zpe) = -1264.7323010 au; Energy+zpe (0K) = -1264.3385680 au

Enthalpy (298K) = -1264.3119540 au; Gibbs free energy (298K) = -1264.3965850 au

C;-1.840157;0.433382;0.430066
C;0.578554;0.321935;-1.613938
C;-0.318177;-0.027190;-2.590020
C;-1.306205;-1.037131;-2.470720
C;-1.554701;-1.762439;-1.308839

C;-2.619042;-0.580780;-0.152341
 C;-2.538065;-2.903318;-1.278367
 C;-3.181729;-1.743768;0.657819
 O;-3.179660;-2.933117;0.007812
 C;-0.911847;0.026324;1.494593
 C;1.497485;1.449934;-1.749873
 O;-0.552698;-1.139253;1.634887
 O;-3.687424;-1.623650;1.742051
 O;-0.478925;1.011222;2.310326
 C;0.373420;0.574660;3.380831
 C;-2.050146;1.782123;-0.124465
 O;-2.823896;2.015228;-1.044538
 O;-1.315708;2.758282;0.460281
 C;-1.552968;4.075986;-0.050017
 C;2.917659;1.408446;-1.138404
 C;1.876689;2.280993;-0.522828
 H;0.671977;-0.282989;-0.716375
 H;-0.331586;0.564206;-3.504075
 H;-2.006025;-1.139495;-3.299689
 H;-0.751447;-1.869829;-0.581854
 H;-3.354858;-0.192260;-0.857091
 H;-2.046486;-3.874914;-1.389934
 H;-3.302601;-2.805225;-2.060141
 H;1.415387;1.997586;-2.686003
 H;0.630242;1.480850;3.931086
 H;1.271682;0.089800;2.989241
 H;-0.154851;-0.130586;4.027882
 H;-2.605416;4.351245;0.059846
 H;-1.282852;4.139911;-1.108126
 H;-0.922006;4.736115;0.547099
 H;3.643540;1.921304;-1.769540
 H;1.421903;1.980520;0.415856
 H;1.940713;3.356410;-0.662355
 C;3.462844;0.189878;-0.455780
 C;3.676163;0.166206;0.928263
 C;3.820513;-0.939055;-1.208358
 C;4.225531;-0.958542;1.548031
 H;3.419641;1.039745;1.521553
 C;4.368487;-2.063195;-0.592561
 H;3.660521;-0.933920;-2.283966
 C;4.571249;-2.077019;0.789713
 H;4.385185;-0.958254;2.623068
 H;4.635113;-2.930514;-1.190824
 H;4.995374;-2.953983;1.270972

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TS-trans-6d-lk-ou B3LYP/6-31G(d)
 SCF Energy (no zpe) = -1264.7275100 au; Energy+zpe (0K) = -1264.3337920 au
 Enthalpy (298K) = -1264.3070740 au; Gibbs free energy (298K) = -1264.3930070 au
 C;2.200804;-0.268635;-0.333454
 C;-0.765197;-0.193396;0.377384
 C;-1.019482;0.658703;-0.666783
 C;-0.265803;1.828930;-0.932093
 C;0.854203;2.216579;-0.200789
 C;2.324471;1.049484;-0.800390
 C;1.592316;3.499932;-0.475857

C;3.389478;2.002356;-0.273283
 O;2.988490;3.295820;-0.192692
 C;2.498092;-0.517425;1.088302
 C;-1.418627;-1.484276;0.638769
 O;2.353094;0.345392;1.949659
 O;4.523018;1.683659;-0.027845
 O;2.955244;-1.750257;1.372467
 C;3.279119;-1.978502;2.751878
 C;1.781387;-1.263642;-1.335826
 O;1.567371;-0.987953;-2.509159
 O;1.629660;-2.518491;-0.849576
 C;1.260149;-3.501245;-1.823391
 C;-2.174942;-2.274215;-0.412019
 C;-2.966181;-1.655077;0.694403
 H;-0.064077;0.117568;1.145177
 H;-1.777412;0.393268;-1.398419
 H;-0.483702;2.356351;-1.860241
 H;0.930738;1.894293;0.836217
 H;2.214369;1.123768;-1.882743
 H;1.271235;4.314436;0.181147
 H;1.477845;3.824036;-1.518425
 H;-0.898216;-2.082335;1.381412
 H;3.629147;-3.010267;2.798861
 H;2.398557;-1.841934;3.386177
 H;4.061911;-1.290546;3.081761
 H;1.999803;-3.549773;-2.627275
 H;0.283445;-3.271424;-2.259290
 H;1.223953;-4.447584;-1.281450
 H;-2.036024;-3.351791;-0.419258
 H;-2.244637;-1.830771;-1.401486
 H;-3.268547;-2.332863;1.492314
 C;-3.916870;-0.518723;0.479635
 C;-4.124860;0.422457;1.499535
 C;-4.653126;-0.392606;-0.705202
 C;-5.039038;1.461700;1.337692
 H;-3.559262;0.337878;2.424420
 C;-5.568928;0.648974;-0.871580
 H;-4.518360;-1.123045;-1.498567
 C;-5.764033;1.579467;0.148868
 H;-5.184505;2.182188;2.138277
 H;-6.132379;0.728131;-1.797619
 H;-6.476478;2.390009;0.021376

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TS-cis-6d-ul-in B3LYP/6-31G(d)

SCF Energy (no zpe) = -1264.7286949 au; Energy+zpe (0K) = -1264.3348749 au

Enthalpy (298K) = -1264.3082789 au; Gibbs free energy (298K) = -1264.3925269 au

C;0.970443;2.286381;-0.378574
 C;1.022792;1.733771;-1.658929
 C;0.187942;0.684365;-2.122402
 C;-0.704187;0.007154;-1.337626
 C;1.745838;-0.325855;0.652776
 C;1.901575;1.047741;0.897483
 C;3.253720;1.733597;0.765202
 O;4.288562;1.264675;1.161523
 O;3.196459;2.996027;0.275667

C;1.868797;3.457480;-0.037478
 C;-1.522013;-1.101897;-1.815815
 C;2.518390;-0.877634;-0.462812
 O;3.088711;-0.145087;-1.267629
 O;2.529216;-2.221624;-0.576818
 C;3.280506;-2.727329;-1.687614
 C;0.786573;-1.030601;1.520102
 O;-0.064168;-0.453781;2.193322
 O;0.935152;-2.372044;1.551735
 C;0.100767;-3.064647;2.489165
 C;-3.002957;-1.268061;-1.340736
 C;-1.950104;-2.215071;-0.871261
 H;0.018405;2.243553;0.144226
 H;1.817529;2.060637;-2.325091
 H;0.335230;0.351737;-3.148265
 H;-0.863146;0.323387;-0.311301
 H;1.360628;1.385174;1.782872
 H;1.479008;4.013555;0.823183
 H;1.988352;4.153124;-0.872220
 H;-1.349625;-1.390616;-2.850196
 H;2.852768;-2.386714;-2.635368
 H;4.321721;-2.398205;-1.633766
 H;3.216807;-3.813492;-1.609120
 H;-0.954398;-2.998484;2.206098
 H;0.220445;-2.651193;3.493826
 H;0.433352;-4.102837;2.457433
 H;-3.630352;-1.641005;-2.147729
 H;-1.604690;-2.140592;0.154068
 H;-1.948471;-3.226881;-1.266787
 C;-3.705361;-0.274126;-0.474199
 C;-4.805843;0.413072;-1.011397
 C;-3.327534;0.007700;0.848144
 C;-5.505711;1.354882;-0.259288
 H;-5.115955;0.203262;-2.032866
 C;-4.024372;0.956089;1.599113
 H;-2.487008;-0.502265;1.309095
 C;-5.115165;1.632734;1.051967
 H;-6.356596;1.869922;-0.697584
 H;-3.711561;1.158420;2.619967
 H;-5.658455;2.365707;1.642207

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TS-trans-6d-lk-in B3LYP/6-31G(d)

SCF Energy (no zpe) = -1264.7252964 au; Energy+zpe (0K) = -1264.3317194 au

Enthalpy (298K) = -1264.3050084 au; Gibbs free energy (298K) = -1264.3901634 au

C;-1.501801;-0.012868;0.869839
 C;0.268128;1.533936;-1.206972
 C;-0.888800;2.145247;-1.618364
 C;-2.086485;1.482081;-1.973840
 C;-2.300322;0.114062;-1.790310
 C;-2.664592;-0.100919;0.079405
 C;-3.559907;-0.558045;-2.278280
 C;-3.403565;-1.424514;-0.108373
 O;-3.912381;-1.599957;-1.353347
 C;-0.600906;-1.179825;0.861178
 C;1.415632;2.324566;-0.722148

O;-0.530844;-1.940003;-0.099620
 O;-3.611115;-2.217096;0.771157
 O;0.089854;-1.375072;1.996161
 C;0.887708;-2.569476;2.025877
 C;-1.346011;1.229442;1.640302
 O;-2.164695;2.141048;1.621172
 O;-0.203445;1.301767;2.364674
 C;-0.068461;2.483773;3.160951
 C;2.611352;2.619529;-1.625657
 C;2.802789;1.746508;-0.417404
 H;0.387895;0.457920;-1.301978
 H;-0.921370;3.233572;-1.599934
 H;-2.941535;2.106497;-2.230325
 H;-1.436027;-0.548667;-1.789182
 H;-3.360365;0.716723;0.271838
 H;-3.419502;-1.046668;-3.247352
 H;-4.395512;0.149347;-2.358561
 H;1.129761;3.164454;-0.091260
 H;1.376072;-2.563133;3.001230
 H;1.628356;-2.561136;1.223941
 H;0.251506;-3.452761;1.921585
 H;-0.895191;2.571429;3.871524
 H;-0.052018;3.380782;2.534443
 H;0.878326;2.370267;3.691207
 H;3.010376;3.630105;-1.612070
 H;2.631087;2.147062;-2.603148
 H;3.277761;2.234350;0.430805
 C;3.172761;0.301622;-0.522071
 C;3.820424;-0.302644;0.566783
 C;2.952811;-0.475106;-1.670603
 C;4.243432;-1.630120;0.509919
 H;4.004163;0.281676;1.465256
 C;3.360489;-1.808149;-1.724441
 H;2.471274;-0.040796;-2.542129
 C;4.012935;-2.391327;-0.637579
 H;4.755286;-2.068276;1.362852
 H;3.174370;-2.388787;-2.623768
 H;4.340620;-3.426073;-0.685812

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TS-trans-ul-ou B3LYP/6-31G(d)
 SCF Energy (no zpe) = -1264.7259888 au; Energy+zpe (0K) = -1264.3318978 au
 Enthalpy (298K) = -1264.3053018 au; Gibbs free energy (298K) = -1264.3893478 au
 C;1.776721;0.310369;0.570683
 C;-0.497216;-0.004696;-1.481132
 C;-0.847700;-1.263385;-1.065320
 C;0.093901;-2.278345;-0.759759
 C;1.476596;-2.135680;-0.844690
 C;2.043707;-1.061577;0.715830
 C;2.398743;-3.293369;-0.563643
 C;3.472462;-1.594497;0.650330
 O;3.604652;-2.796514;0.042594
 C;2.610907;1.056738;-0.391289
 C;-1.375715;1.164503;-1.651202
 O;3.098920;0.522365;-1.383459
 O;4.412995;-1.047697;1.164503

O;2.816258;2.352408;-0.099119
C;3.660003;3.060188;-1.020241
C;0.721432;0.876700;1.425696
O;0.095612;0.230521;2.257568
O;0.489652;2.194444;1.209550
C;-0.428915;2.819268;2.114296
C;-2.812283;1.338749;-1.141831
C;-2.575731;1.143540;-2.607463
H;0.533220;0.174511;-1.772451
H;-1.885267;-1.478292;-0.835769
H;-0.298143;-3.174975;-0.279357
H;1.883054;-1.420801;-1.557987
H;1.472364;-1.523668;1.521550
H;2.714350;-3.804033;-1.479010
H;1.937552;-4.029839;0.107035
H;-0.814790;2.095265;-1.675010
H;3.717216;4.078322;-0.633885
H;3.229187;3.053585;-2.025426
H;4.653379;2.605714;-1.057877
H;-0.160429;2.602798;3.151387
H;-1.452675;2.477966;1.935510
H;-0.350334;3.888850;1.913327
H;-2.998897;2.373018;-0.849455
H;-2.826983;0.173516;-3.027876
H;-2.689748;1.978457;-3.293606
C;-3.592898;0.354173;-0.317983
C;-4.787914;-0.181829;-0.819279
C;-3.198133;0.010788;0.984592
C;-5.571960;-1.037068;-0.043281
H;-5.108093;0.081371;-1.824256
C;-3.980933;-0.845750;1.760098
H;-2.259866;0.380586;1.387578
C;-5.170596;-1.370868;1.251067
H;-6.495778;-1.440074;-0.450281
H;-3.652706;-1.106580;2.762689
H;-5.778204;-2.037638;1.857202

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TS-cis-6d-lk-ou B3LYP/6-31G(d)

SCF Energy (no zpe) = -1264.7232856 au; Energy+zpe (0K) = -1264.3296806 au

Enthalpy (298K) = -1264.3029666 au; Gibbs free energy (298K) = -1264.3891296 au

C;-0.843747;2.160023;-0.932701
C;0.043762;1.883984;0.108455
C;0.826023;0.707551;0.216833
C;0.733012;-0.347580;-0.650718
C;-2.256530;-0.269839;-0.205018
C;-2.484067;1.026165;-0.692234
C;-3.242350;2.074473;0.104323
O;-4.248101;1.856796;0.728129
O;-2.767874;3.337139;-0.042671
C;-1.628903;3.454953;-0.916941
C;1.418719;-1.643939;-0.544159
C;-2.017719;-0.391654;1.238277
O;-1.760438;0.589855;1.928697
O;-2.079655;-1.638091;1.749374
C;-1.853932;-1.722766;3.162031

C;-2.229759;-1.337256;-1.222711
 O;-2.213151;-1.110708;-2.428338
 O;-2.220713;-2.594584;-0.730666
 C;-2.235668;-3.632937;-1.718579
 C;1.960404;-2.199317;0.760292
 C;2.947157;-1.783929;-0.281354
 H;-0.614303;1.746551;-1.911567
 H;0.047159;2.553448;0.965597
 H;1.442306;0.615628;1.106281
 H;0.137701;-0.232039;-1.551260
 H;-2.761995;1.035212;-1.747147
 H;-1.983768;3.713172;-1.921547
 H;-1.046537;4.295182;-0.529495
 H;1.037912;-2.386348;-1.239915
 H;-0.844567;-1.385738;3.417139
 H;-2.576416;-1.109941;3.707768
 H;-1.978161;-2.777285;3.412057
 H;-1.353186;-3.574710;-2.362741
 H;-3.129359;-3.560634;-2.344365
 H;-2.237785;-4.567048;-1.155363
 H;1.807354;-3.257769;0.951185
 H;1.849224;-1.570400;1.639300
 H;3.383010;-2.594578;-0.864899
 C;3.855391;-0.604417;-0.122292
 C;4.255133;0.128526;-1.250181
 C;4.366559;-0.236043;1.128642
 C;5.136515;1.201282;-1.130169
 H;3.865730;-0.145810;-2.227758
 C;5.248455;0.840012;1.252932
 H;4.082037;-0.803782;2.010594
 C;5.635395;1.562217;0.124228
 H;5.432863;1.758194;-2.015192
 H;5.635435;1.109056;2.232253
 H;6.321698;2.399325;0.219128

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TS-cis-6d-ul-ou B3LYP/6-31G(d)

SCF Energy (no zpe) = -1264.7212463 au; Energy+zpe (0K) = -1264.3272373 au

Enthalpy (298K) = -1264.3006473 au; Gibbs free energy (298K) = -1264.3850953 au

C;1.934937;-1.274473;-1.844504
 C;0.656910;-1.690343;-1.456622
 C;-0.492947;-0.859281;-1.445839
 C;-0.432872;0.488738;-1.682519
 C;1.866649;0.585911;0.377630
 C;2.753968;-0.178348;-0.400610
 C;3.544277;-1.326675;0.211160
 O;4.095302;-1.268486;1.279885
 O;3.696814;-2.400509;-0.598372
 C;3.065354;-2.284171;-1.886338
 C;-1.526236;1.472251;-1.711070
 C;1.119813;-0.156901;1.396885
 O;1.043958;-1.381954;1.357792
 O;0.535087;0.570295;2.372618
 C;-0.061422;-0.208407;3.419807
 C;1.775883;2.016854;0.046686
 O;2.296444;2.511361;-0.948615

O;1.062130;2.756556;0.924236
 C;1.005290;4.158121;0.632083
 C;-2.940815;1.325283;-1.128841
 C;-2.754097;1.260219;-2.608952
 H;1.985125;-0.481483;-2.586239
 H;0.545902;-2.690823;-1.045345
 H;-1.432706;-1.314710;-1.150138
 H;0.524914;0.918890;-1.958416
 H;3.371754;0.436913;-1.056345
 H;3.826888;-1.991166;-2.618259
 H;2.715078;-3.289245;-2.136254
 H;-1.160664;2.495891;-1.702628
 H;-0.827681;-0.877072;3.020850
 H;0.698166;-0.808079;3.929674
 H;-0.497940;0.517890;4.107110
 H;0.527178;4.339019;-0.335395
 H;2.008810;4.591778;0.611130
 H;0.415708;4.597576;1.437785
 H;-3.308191;2.283326;-0.760226
 H;-2.820414;0.286544;-3.086314
 H;-3.075206;2.091731;-3.230291
 C;-3.426549;0.168926;-0.308710
 C;-3.038775;0.052040;1.034829
 C;-4.334320;-0.762891;-0.829140
 C;-3.548925;-0.970293;1.834162
 H;-2.324309;0.761351;1.445276
 C;-4.838245;-1.792816;-0.031927
 H;-4.657939;-0.673812;-1.862714
 C;-4.448493;-1.898144;1.303184
 H;-3.244434;-1.044588;2.874523
 H;-5.541611;-2.506093;-0.453492
 H;-4.842613;-2.695535;1.927226

#####

TS-cis-6d-lk-in B3LYP/6-31G(d)
 SCF Energy (no zpe) = -1264.7188902 au; Energy+zpe (0K) = -1264.3253582 au
 Enthalpy (298K) = -1264.2987752 au; Gibbs free energy (298K) = -1264.3835342 au
 C;-2.132285;1.549411;-1.221243
 C;-1.863298;2.231680;-0.028265
 C;-0.593882;2.609139;0.497703
 C;0.638226;2.344983;-0.022310
 C;-1.495153;-1.017930;-0.073750
 C;-2.438610;-0.346162;-0.873103
 C;-3.885890;-0.161530;-0.440103
 O;-4.530873;-0.950330;0.195792
 O;-4.451959;0.960862;-0.965425
 C;-3.537189;1.696563;-1.793238
 C;1.855381;2.911601;0.560953
 C;-1.474879;-0.661763;1.334490
 O;-2.175197;0.252473;1.775699
 O;-0.604399;-1.338778;2.119906
 C;-0.624520;-0.963576;3.502641
 C;-0.600407;-1.934301;-0.805462
 O;-0.490558;-1.931643;-2.025195
 O;0.030965;-2.844627;-0.030270
 C;0.745639;-3.852058;-0.759943

C;3.006446;3.353189;-0.349035
C;3.222281;2.205059;0.580144
H;-1.327901;1.462874;-1.948619
H;-2.722760;2.531760;0.565043
H;-0.629992;3.191437;1.417238
H;0.743185;1.739359;-0.920904
H;-2.383283;-0.669583;-1.915666
H;-3.580241;1.311277;-2.819546
H;-3.894852;2.728749;-1.794675
H;1.674414;3.547698;1.424635
H;-0.316841;0.078764;3.630890
H;-1.625819;-1.087235;3.924337
H;0.082931;-1.632760;3.994614
H;1.533934;-3.406591;-1.370981
H;0.065016;-4.409347;-1.409936
H;1.170519;-4.511566;-0.001451
H;3.471198;4.312052;-0.137159
H;2.894219;3.131755;-1.407217
H;3.780263;2.447051;1.485276
C;3.447471;0.803023;0.103314
C;2.858288;-0.277643;0.773878
C;4.325509;0.541539;-0.956793
C;3.155532;-1.588863;0.405954
H;2.158432;-0.093097;1.584319
C;4.620676;-0.770370;-1.330603
H;4.790447;1.372398;-1.481434
C;4.041550;-1.838962;-0.644864
H;2.684414;-2.409295;0.937491
H;5.306393;-0.956452;-2.153018
H;4.277199;-2.861074;-0.929494

#####

2. Anisotropic Displacement Ellipsoid Plots for 17a, 17c, and 18b

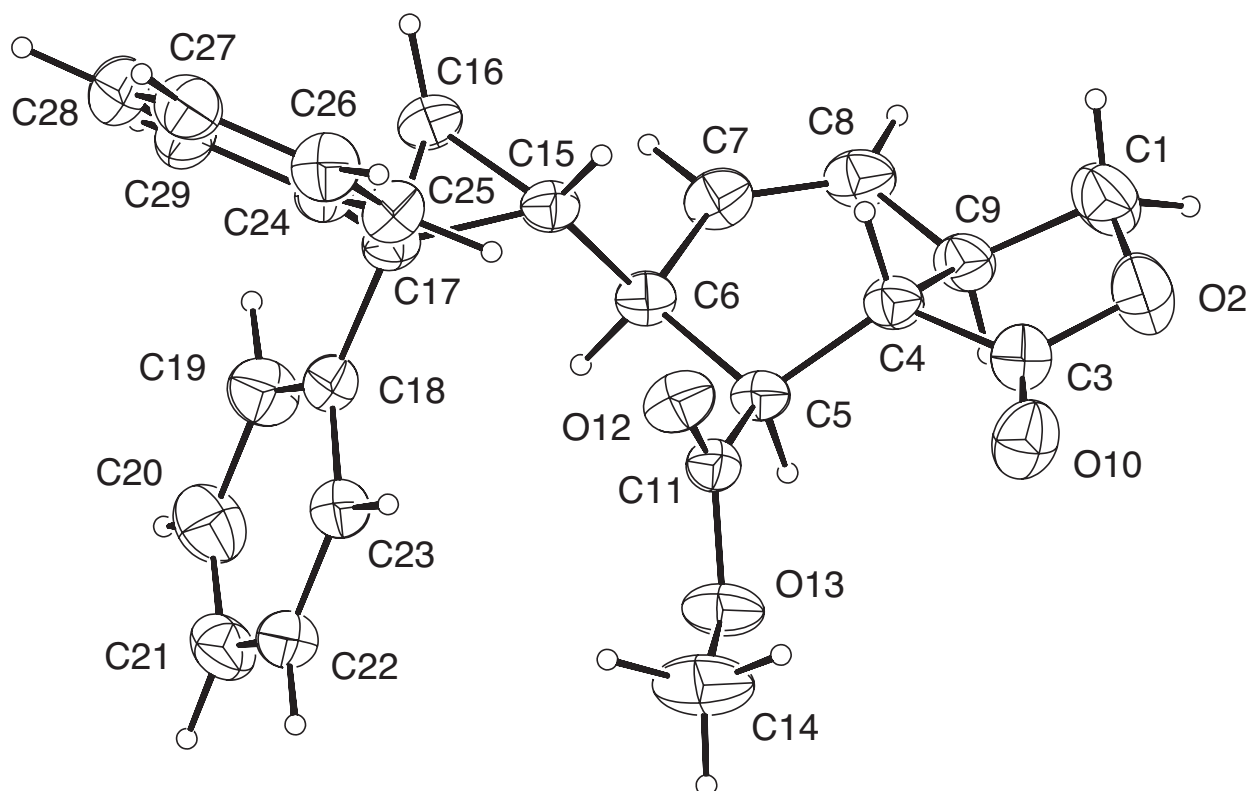


FIGURE S1. Anisotropic displacement ellipsoid plot of compound **17a** (CCDC 644828) with labeling of selected atoms. Ellipsoids show 50% probability levels. Hydrogen atoms are drawn as circles with small radii.

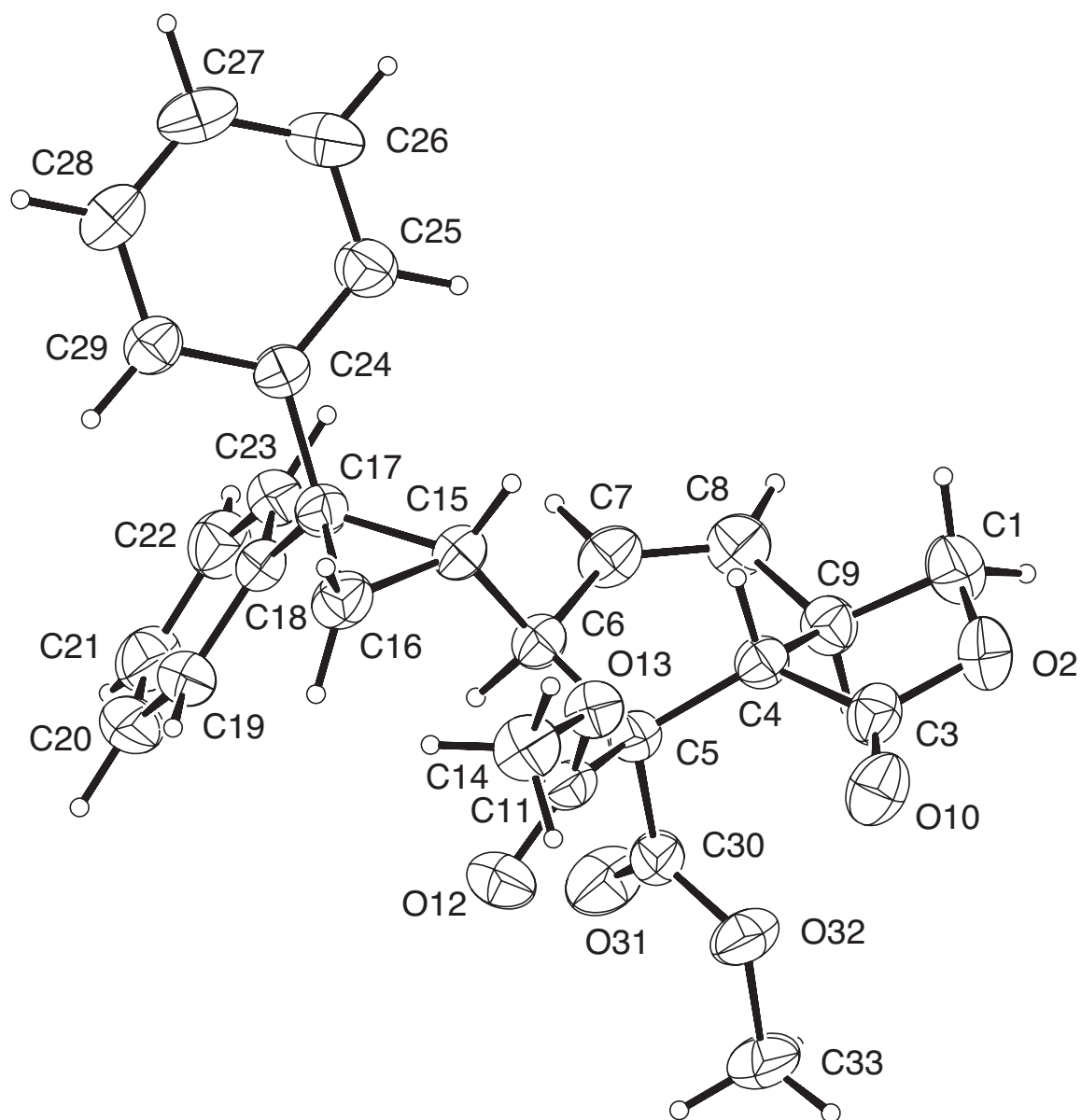


FIGURE S2. Anisotropic displacement ellipsoid plot of compound **17c** (CCDC 644829) with labeling of selected atoms. Ellipsoids show 50% probability levels. Hydrogen atoms are drawn as circles with small radii.

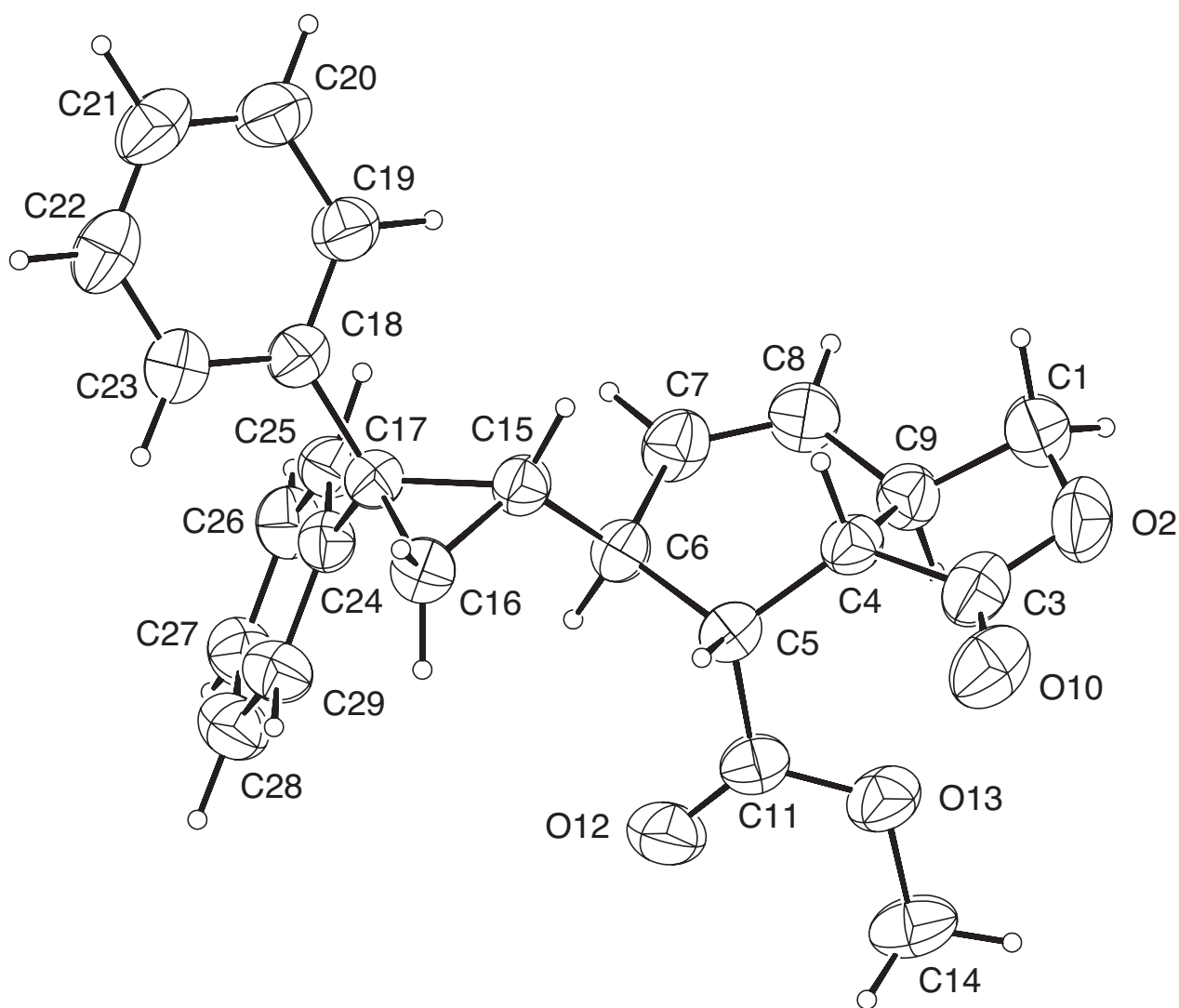
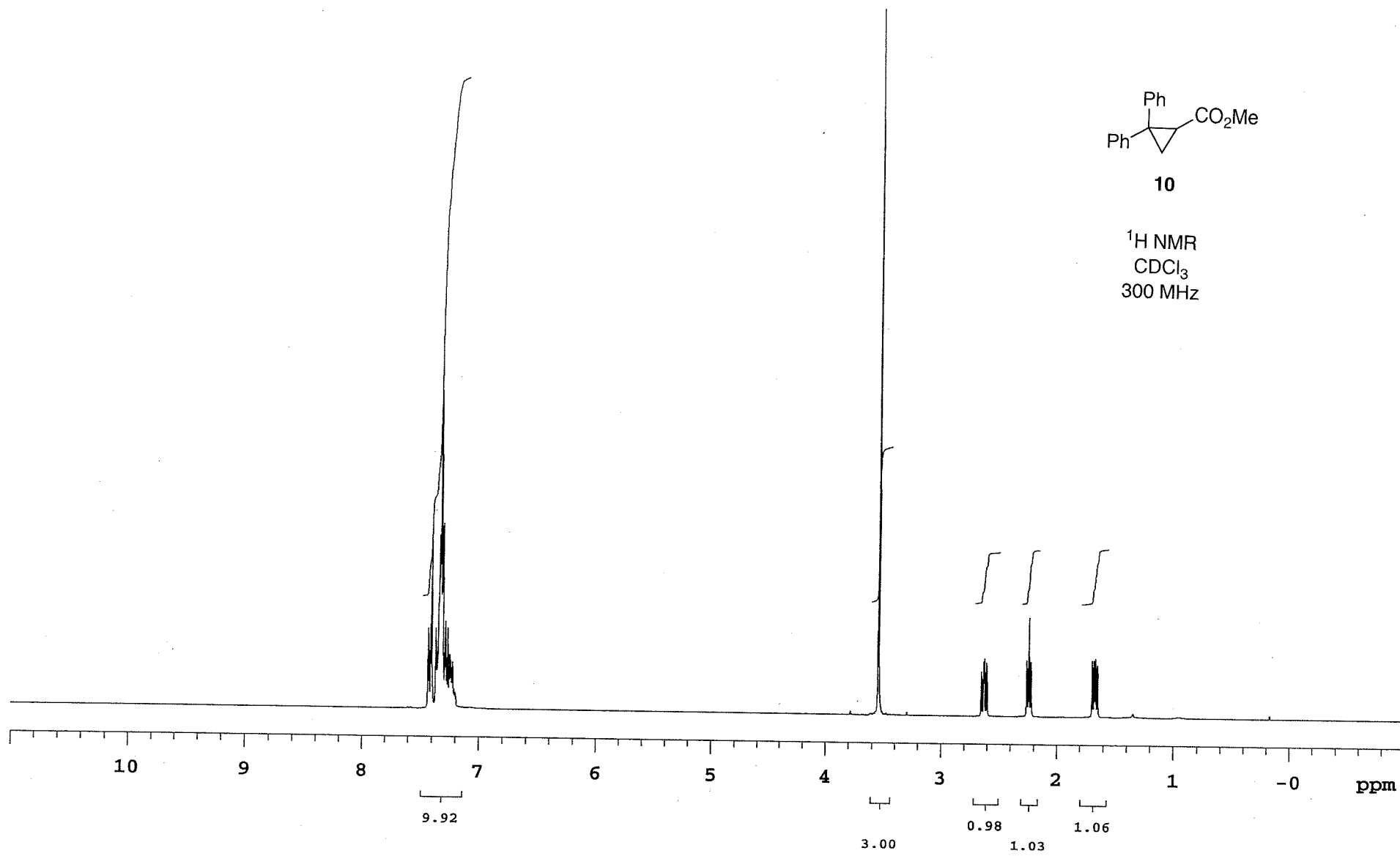
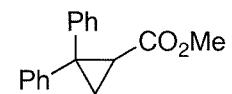


FIGURE S3. Anisotropic displacement ellipsoid plot of compound **18b** (CCDC 644830) with labeling of selected atoms. Ellipsoids show 50% probability levels. Hydrogen atoms are drawn as circles with small radii.

3. References

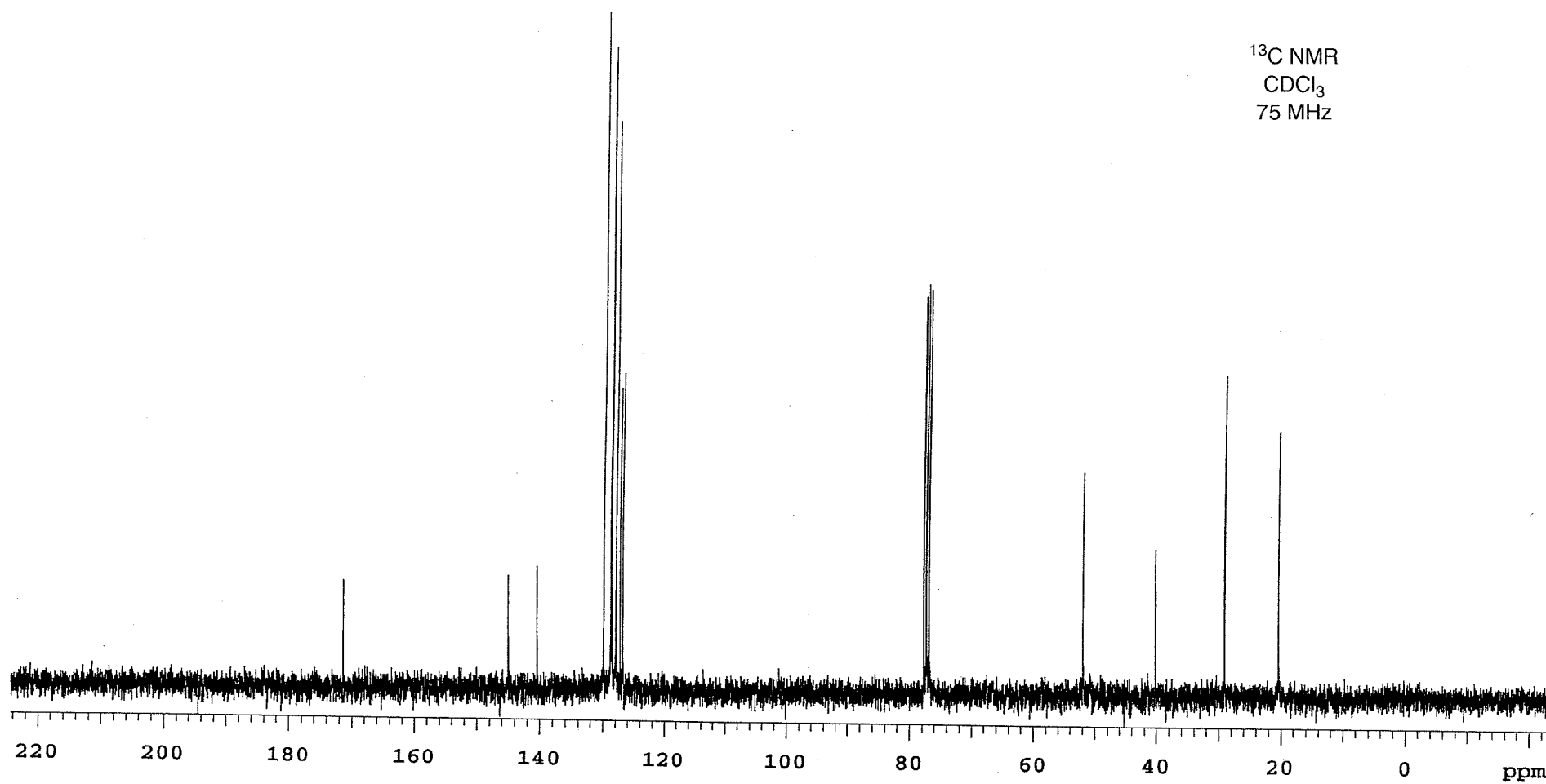
- 1 M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez and J. A. Pople, *Gaussian 2003*, Revision D.01, Gaussian, Inc., Pittsburgh, PA, 2003.

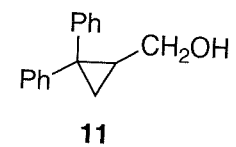




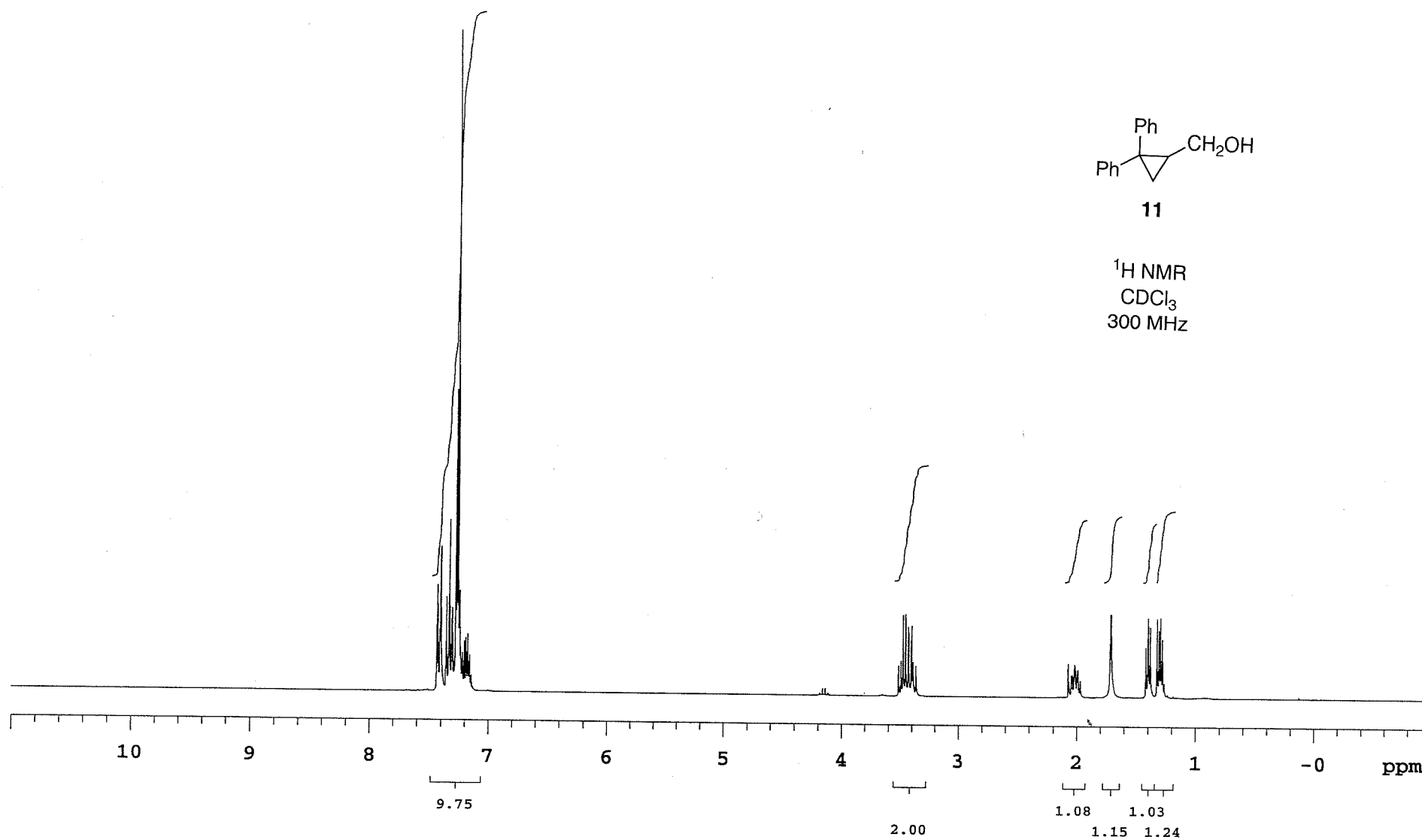
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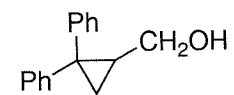
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 CDCl_3
75 MHz





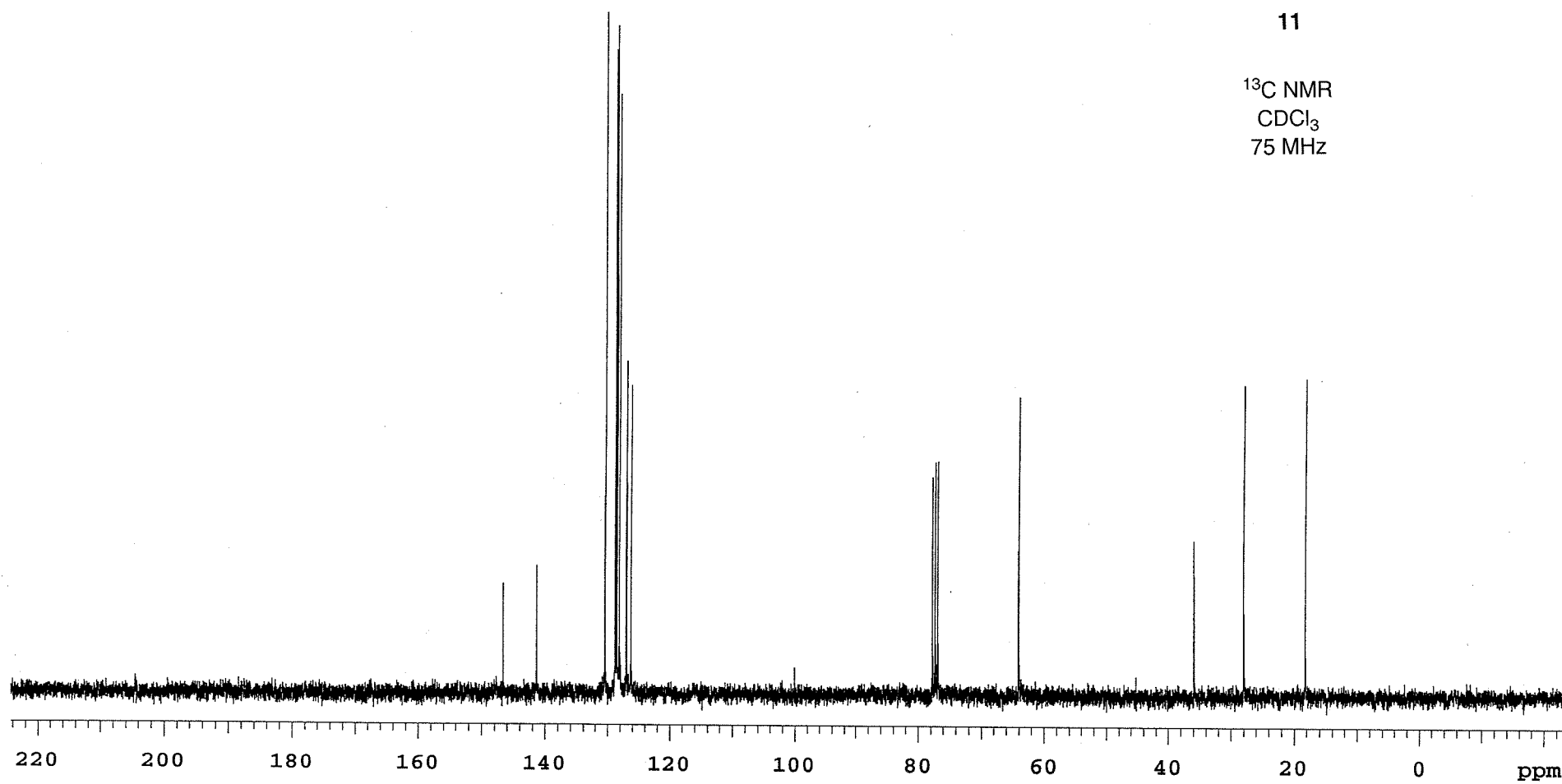
^1H NMR
 CDCl_3
300 MHz

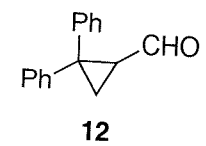




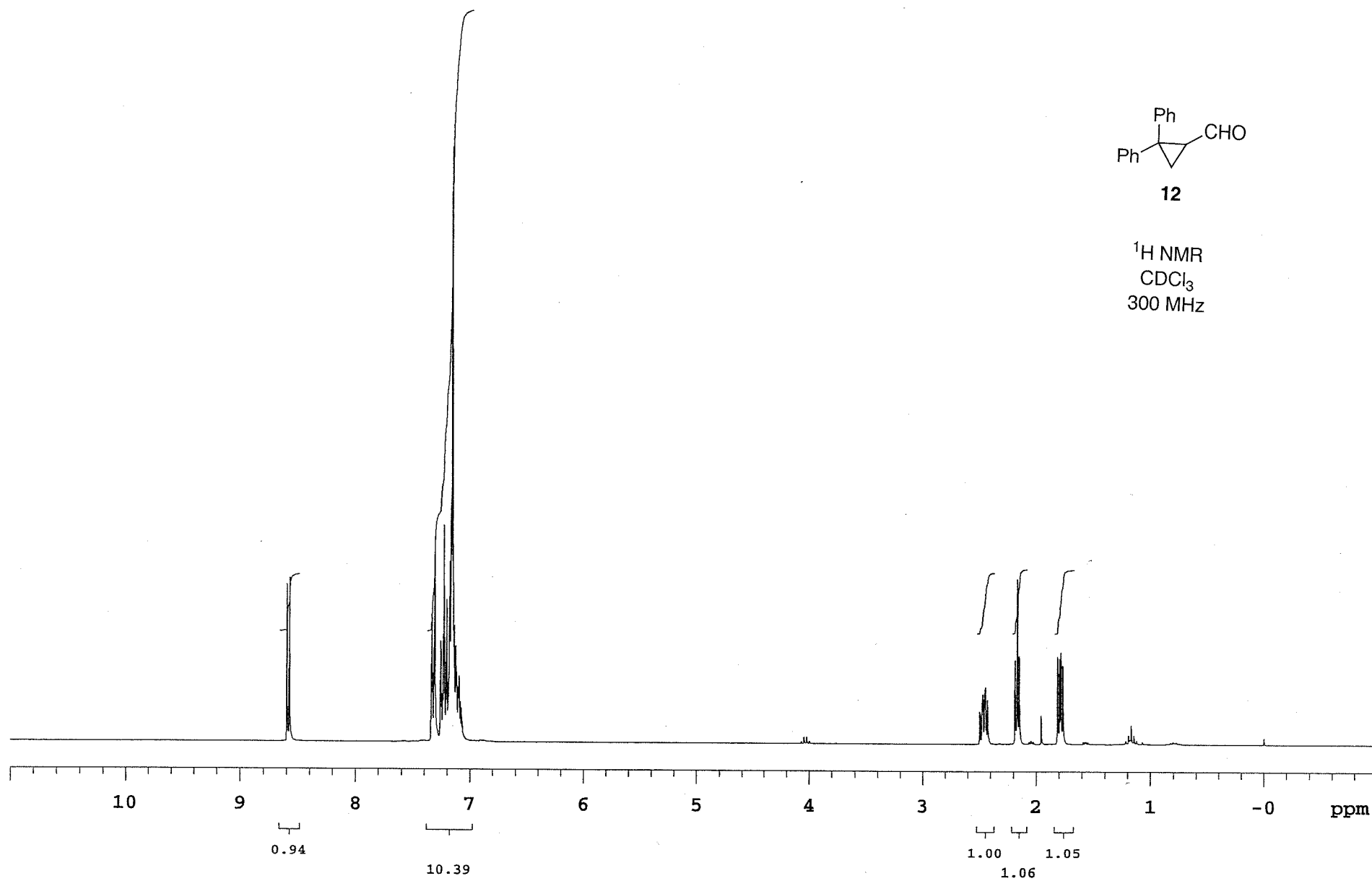
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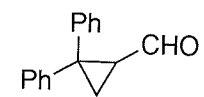
^{13}C NMR
 CDCl_3
75 MHz





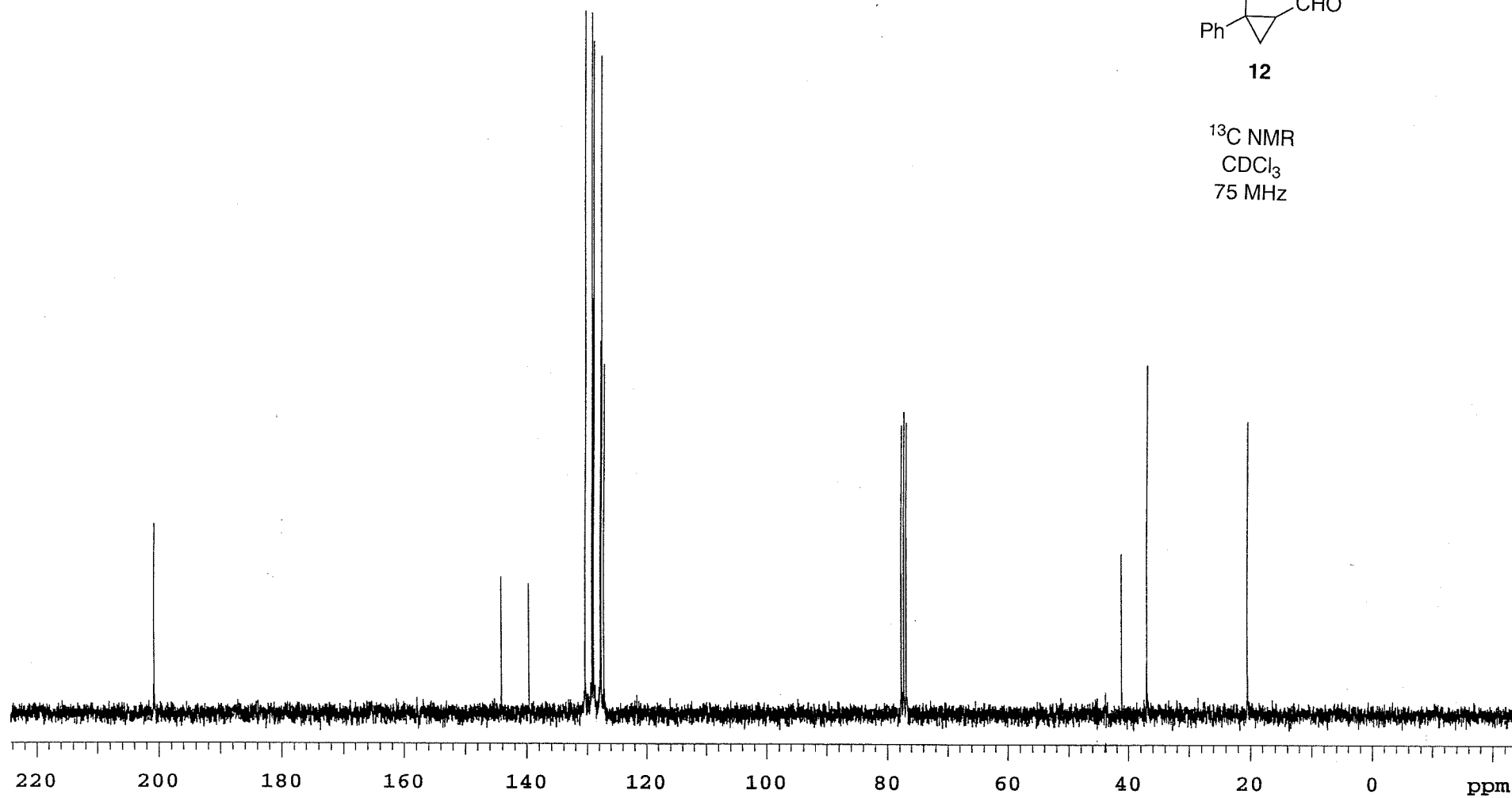
^1H NMR
 CDCl_3
300 MHz

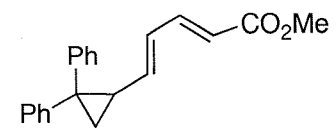




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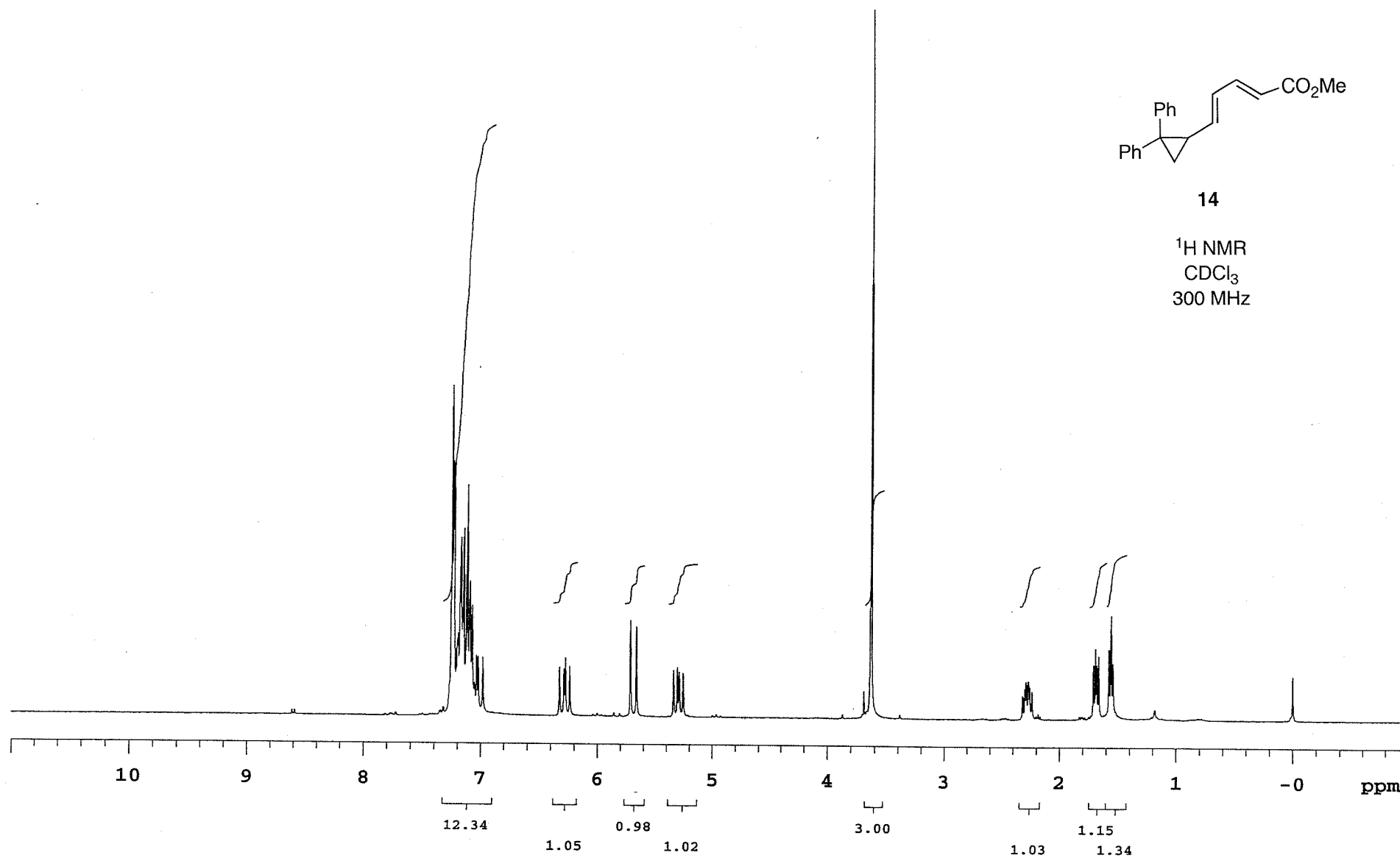
^{13}C NMR
 CDCl_3
75 MHz

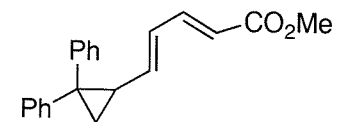




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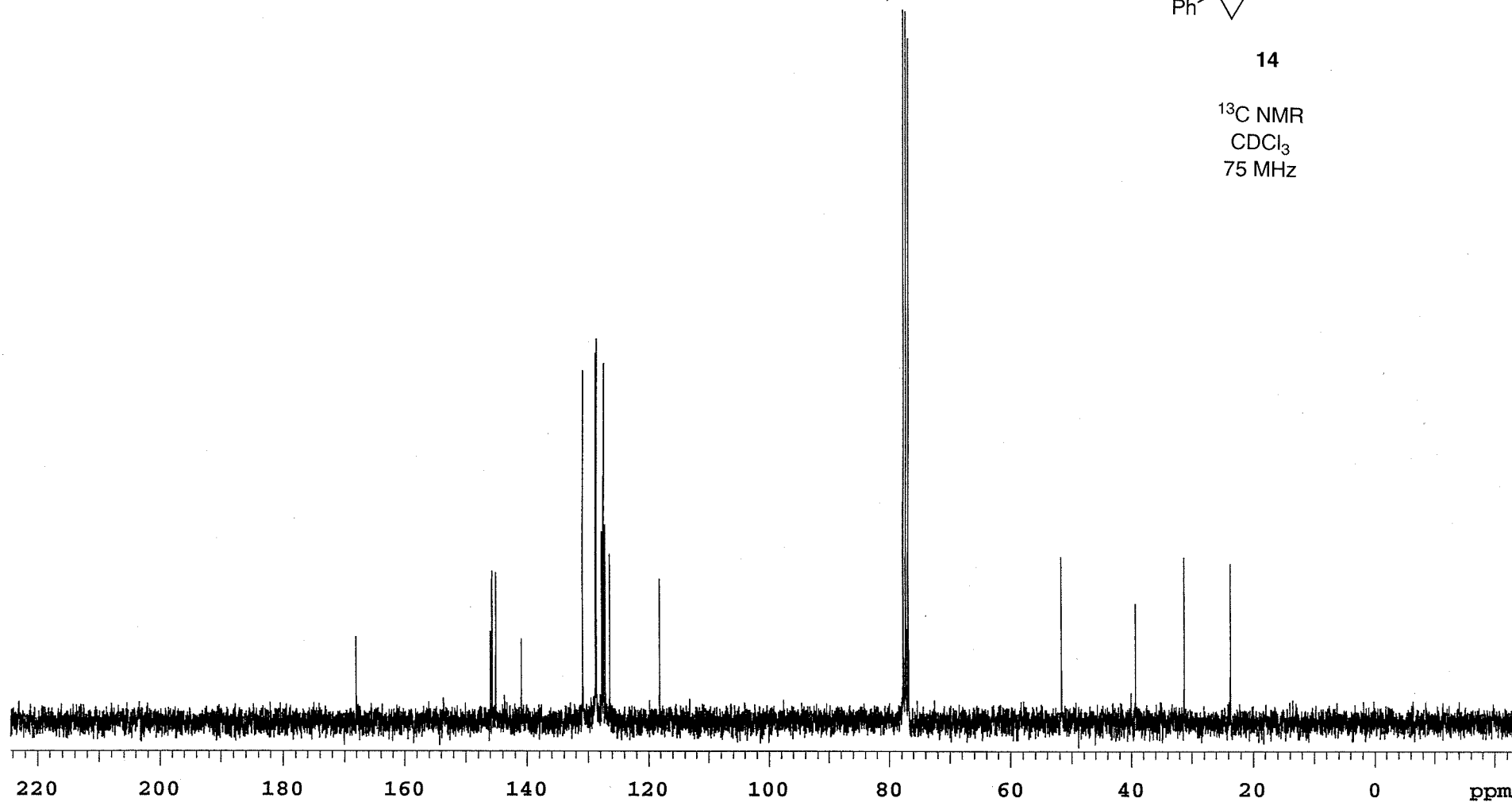
¹H NMR
CDCl₃
300 MHz

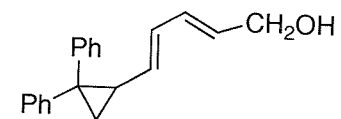




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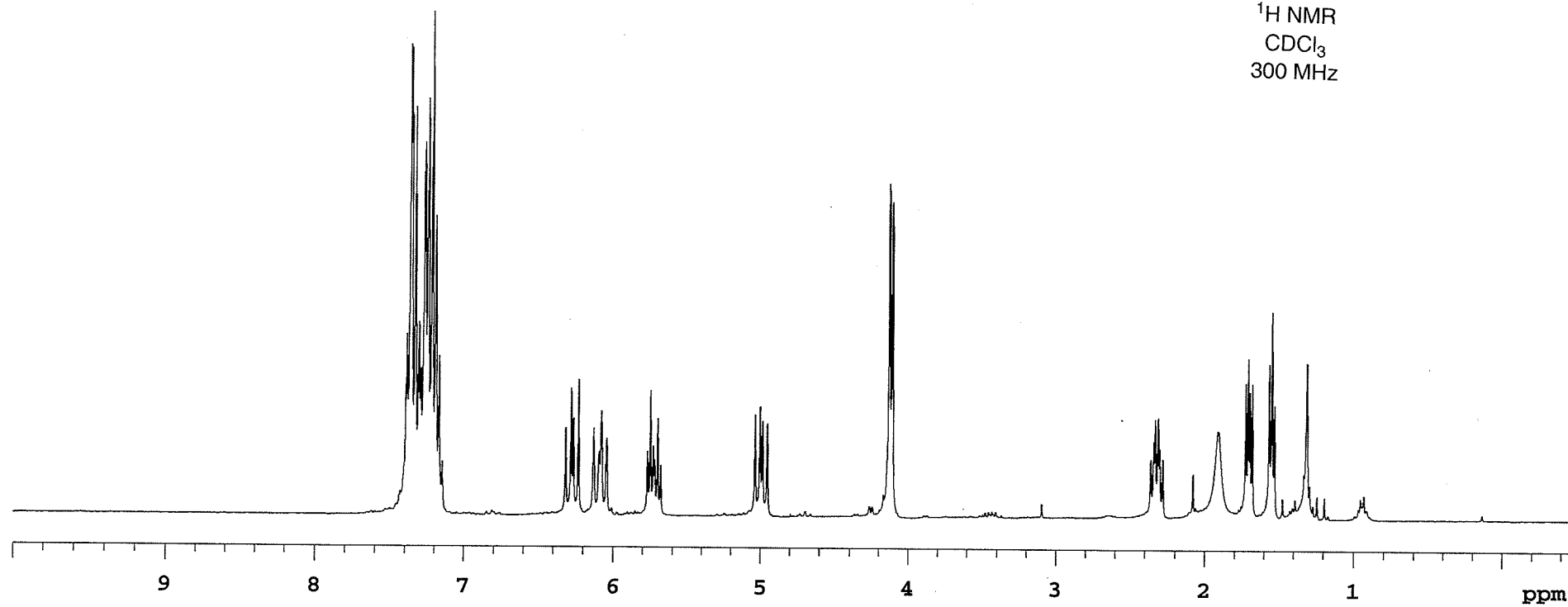
^{13}C NMR
 CDCl_3
75 MHz

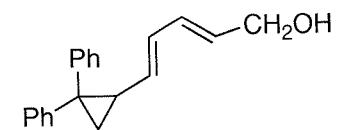




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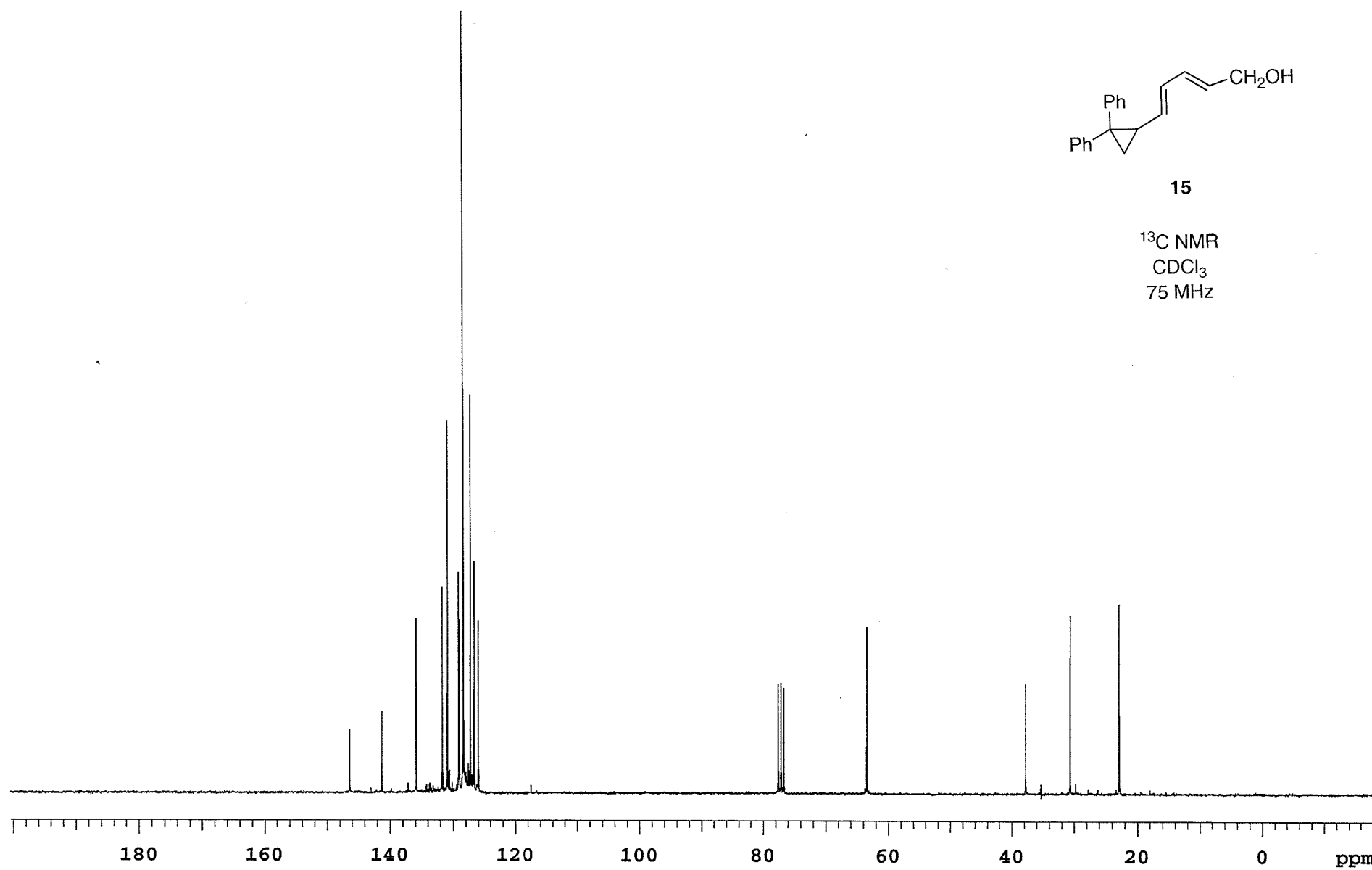
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 CDCl_3
300 MHz

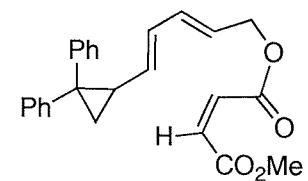




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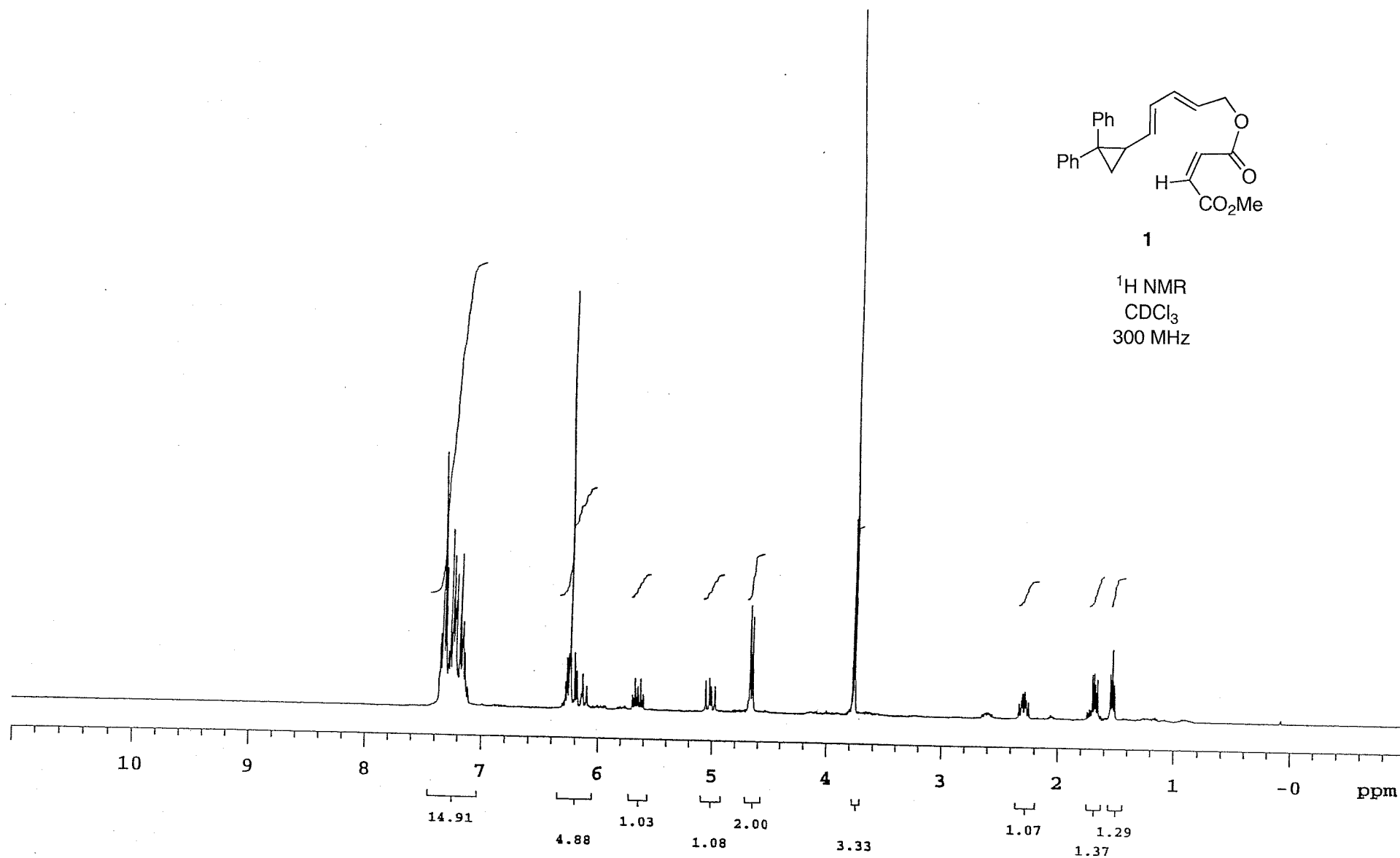
^{13}C NMR
 CDCl_3
75 MHz

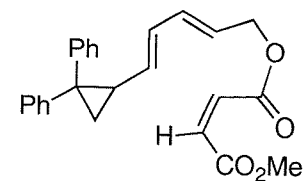




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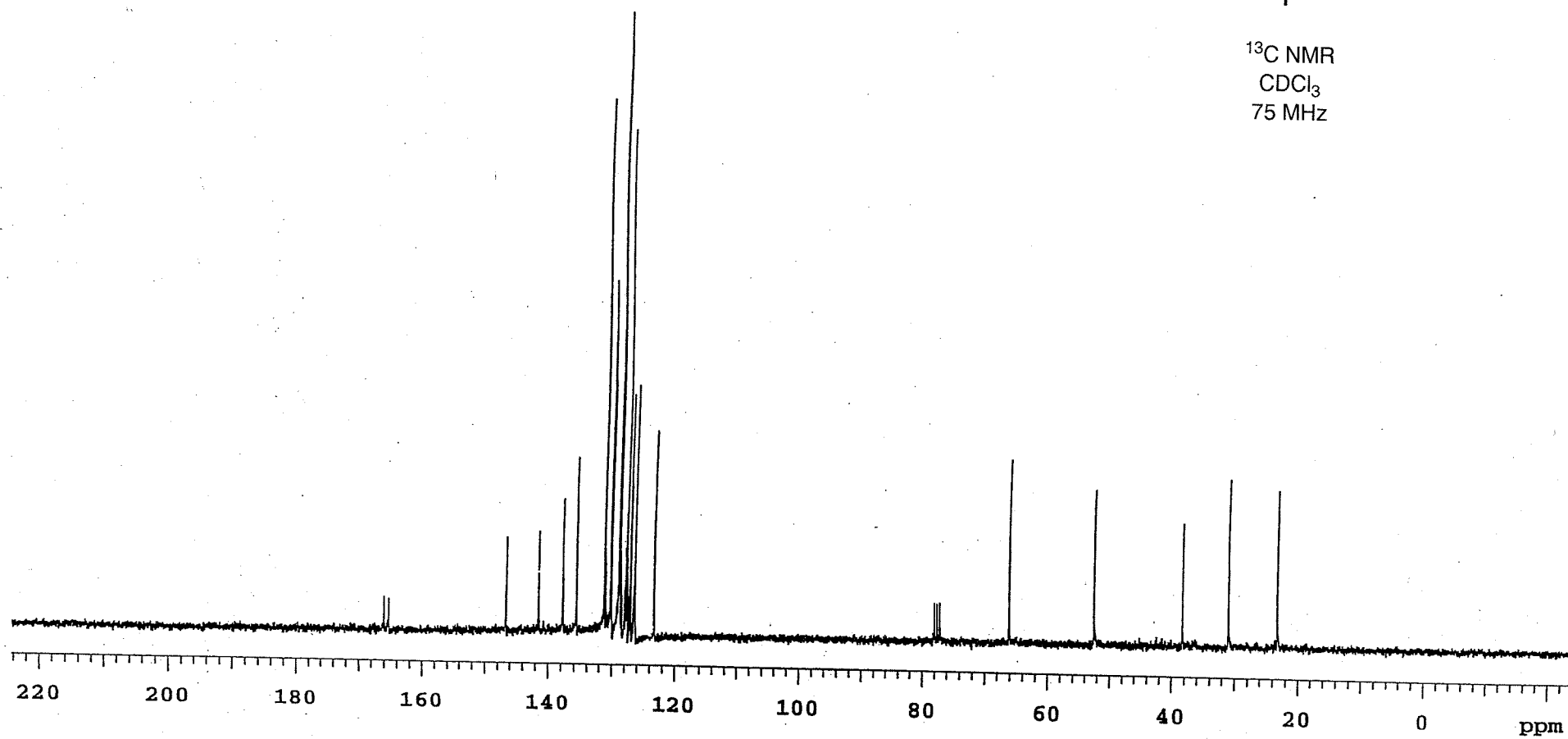
^1H NMR
 CDCl_3
 300 MHz

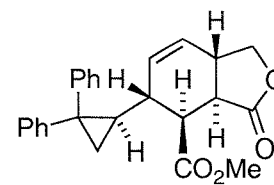




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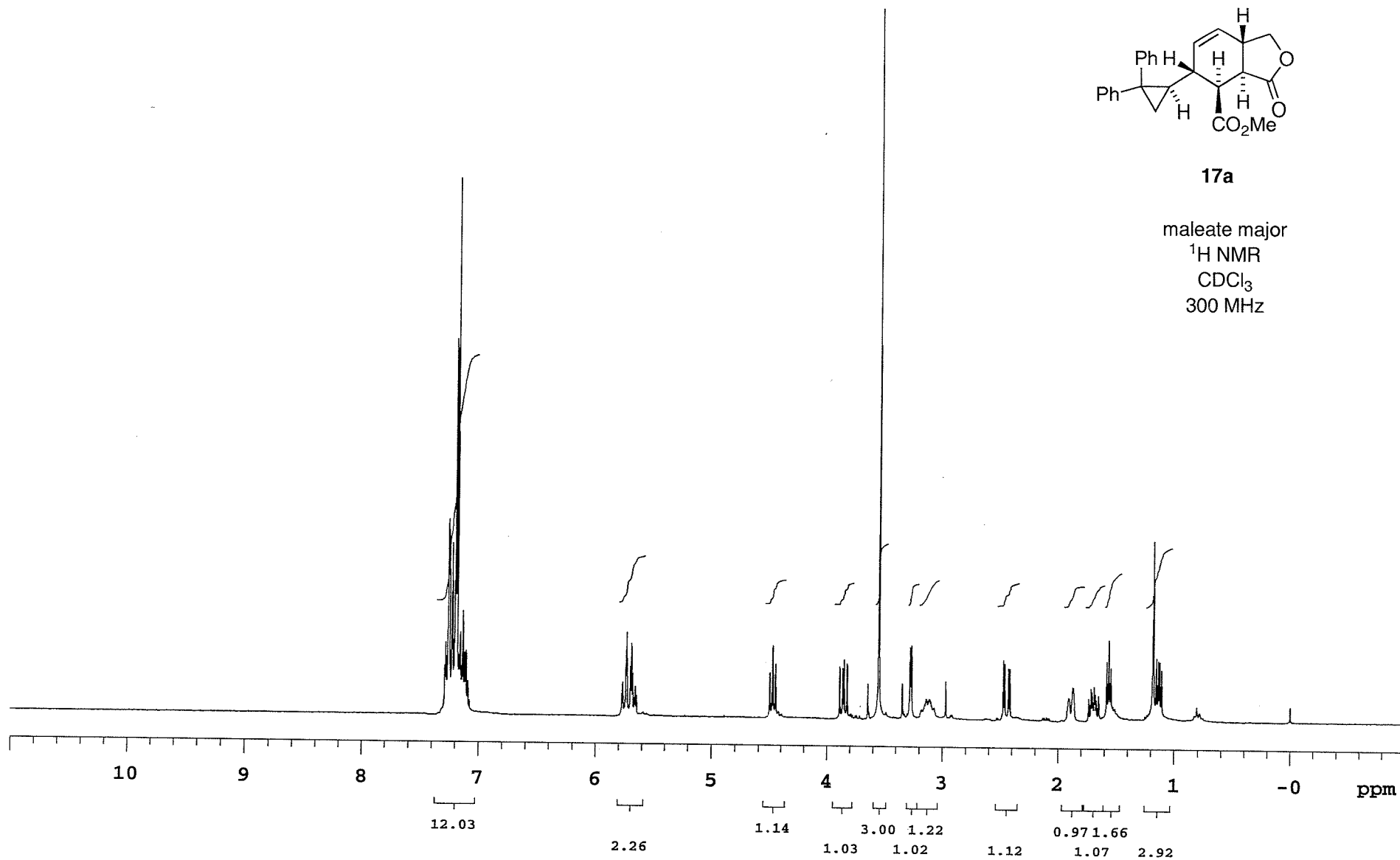
^{13}C NMR
 CDCl_3
 75 MHz





17a

maleate major
 ^1H NMR
 CDCl_3
 300 MHz

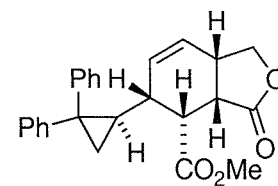




17a

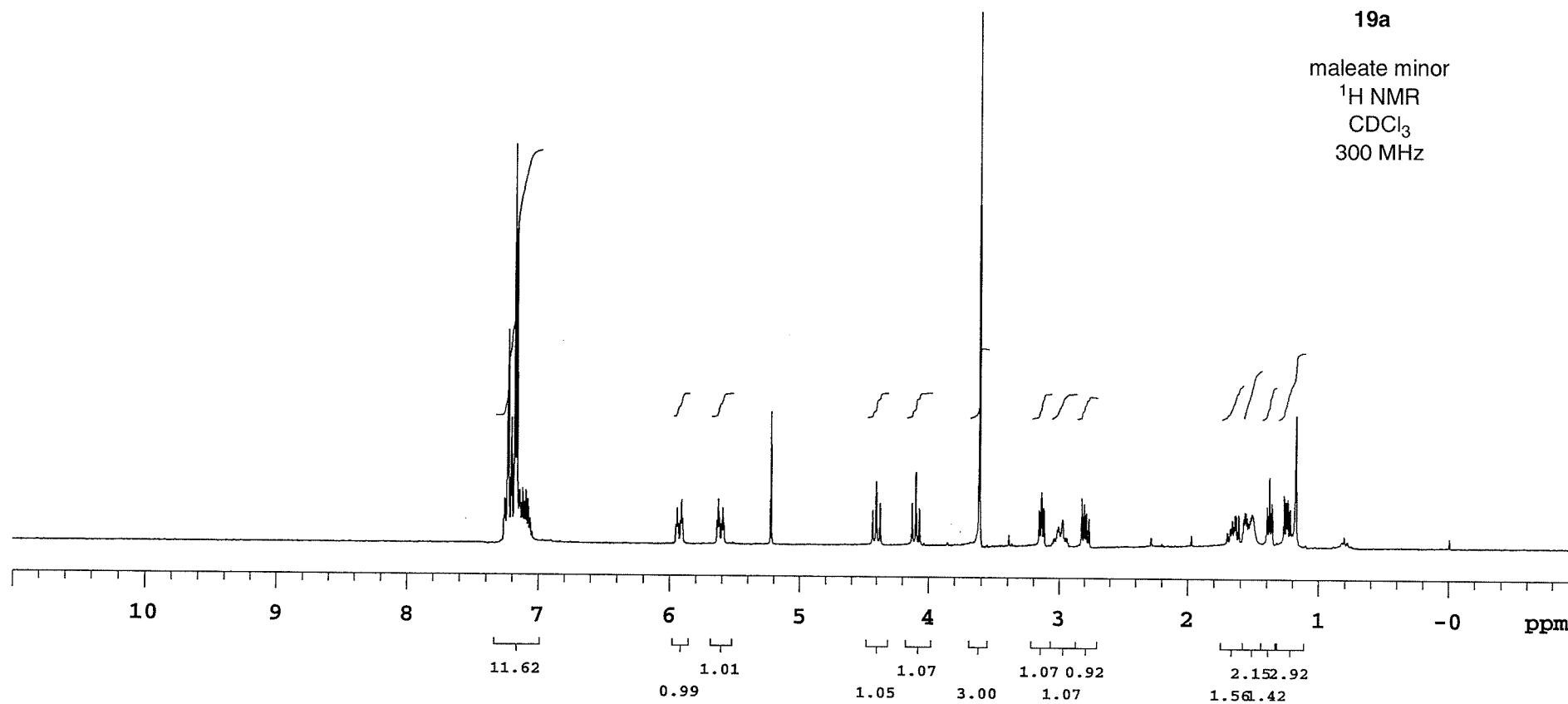
maleate major
¹³C NMR
CDCl₃
75 MHz

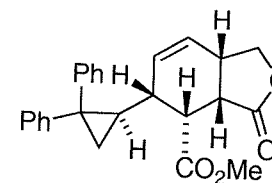
Chemical structure of **17a** is shown in the top right corner. It is a complex polycyclic molecule featuring a cyclopropane ring, a cyclohexene ring, and a five-membered lactone ring, with various substituents including phenyl groups and a methyl ester group.



19a

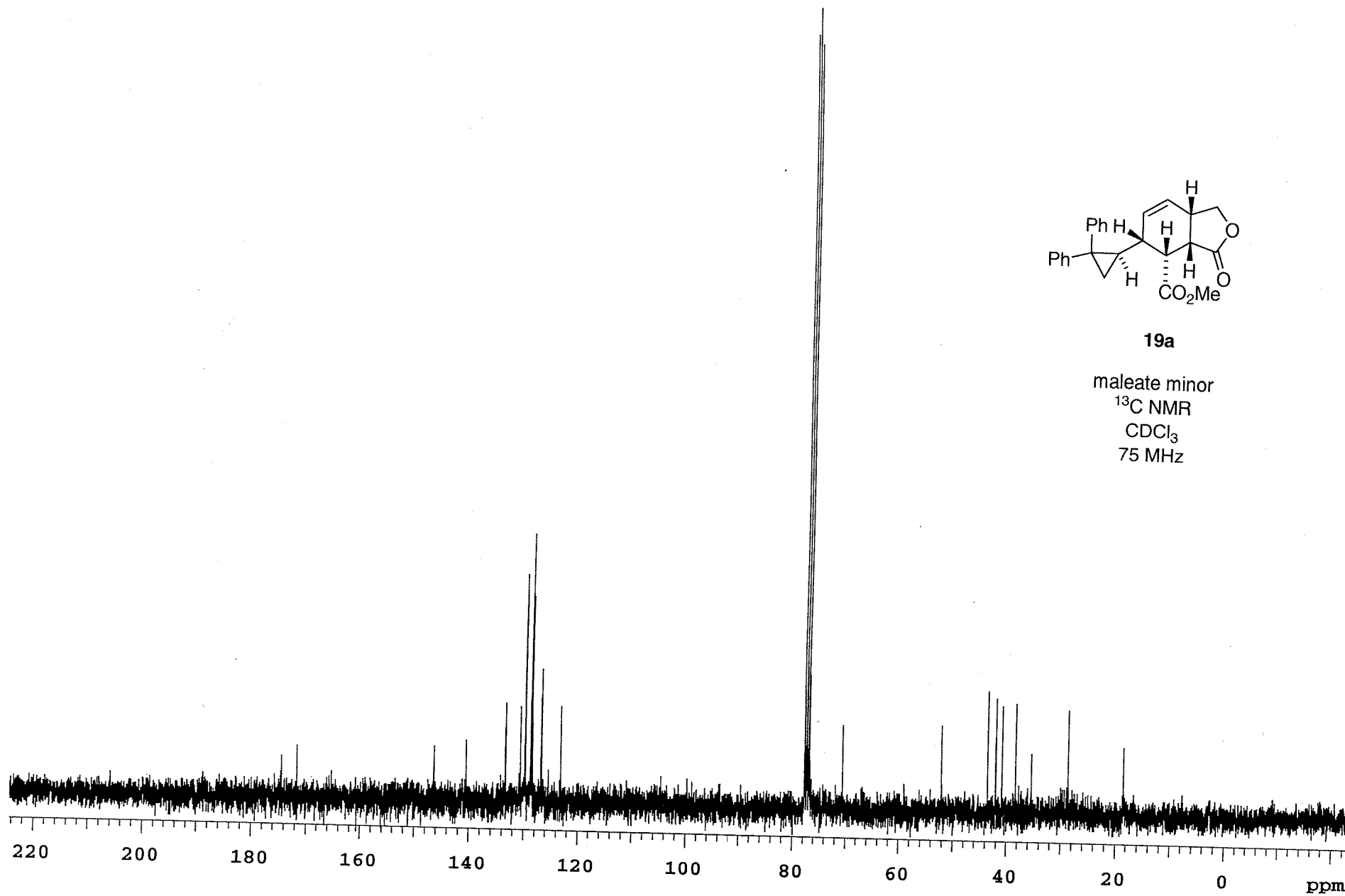
maleate minor
¹H NMR
 CDCl₃
 300 MHz





19a

maleate minor
¹³C NMR
 CDCl₃
 75 MHz

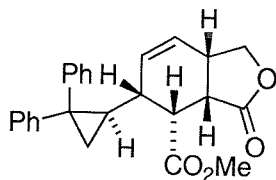


TCH126G
Inova 600
26 June 2006

Pulse Sequence: gDQCOSY

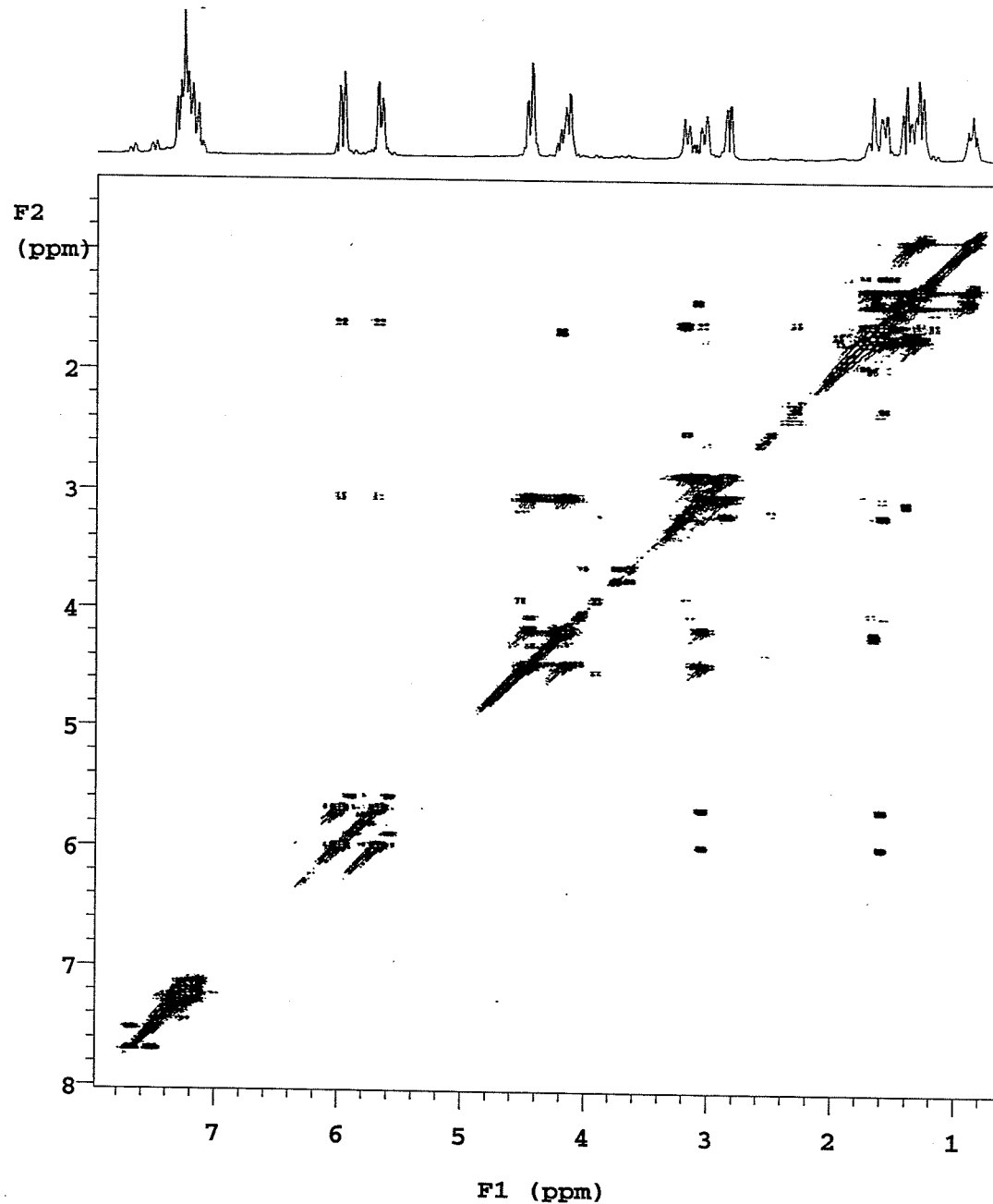
Solvent: CDCl₃
Ambient temperature
Operator: easton
File: TCH126G_600cosy
INOVA-500 "bloch"

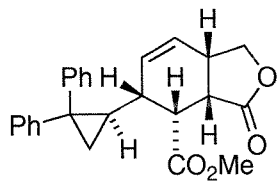
Relax. delay 2.000 sec
Acq. time 0.178 sec
Width 5760.4 Hz
2D Width 5760.4 Hz
16 repetitions
2 x 144 increments
OBSERVE H1, 599.9849024 MHz
DATA PROCESSING
Sq. sine bell 0.133 sec
Shifted by -0.089 sec
F1 DATA PROCESSING
Sq. sine bell 0.037 sec
Shifted by -0.025 sec
FT size 2048 x 2048
Total time 2 hr, 51 min, 12 sec



19a

maleate minor
¹H-¹H COSY
CDCl₃
600 MHz





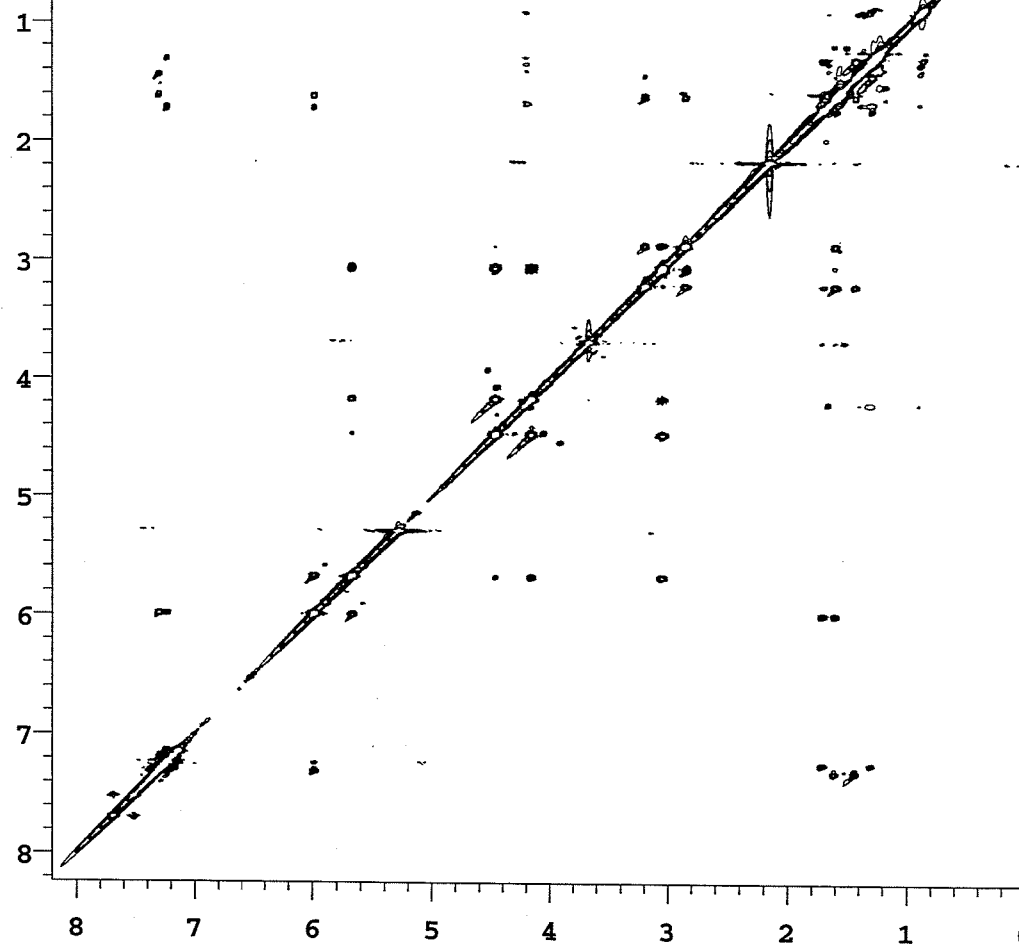
19a

maleate minor
NOESY
CDCl₃
600 MHz

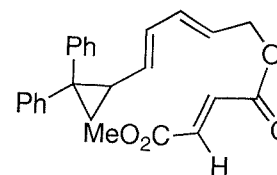
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Mixing 1.000 sec
Acq. time 0.178 sec
Width 5760.4 Hz
2D Width 5760.4 Hz
32 repetitions
2 x 200 increments
OBSERVE H1, 599.9849024 MHz
DATA PROCESSING
Gauss apodization 0.082 sec
F1 DATA PROCESSING
Gauss apodization 0.032 sec
FT size 2048 x 2048
Total time 13 hr, 13 min, 59 sec

F2

(ppm)

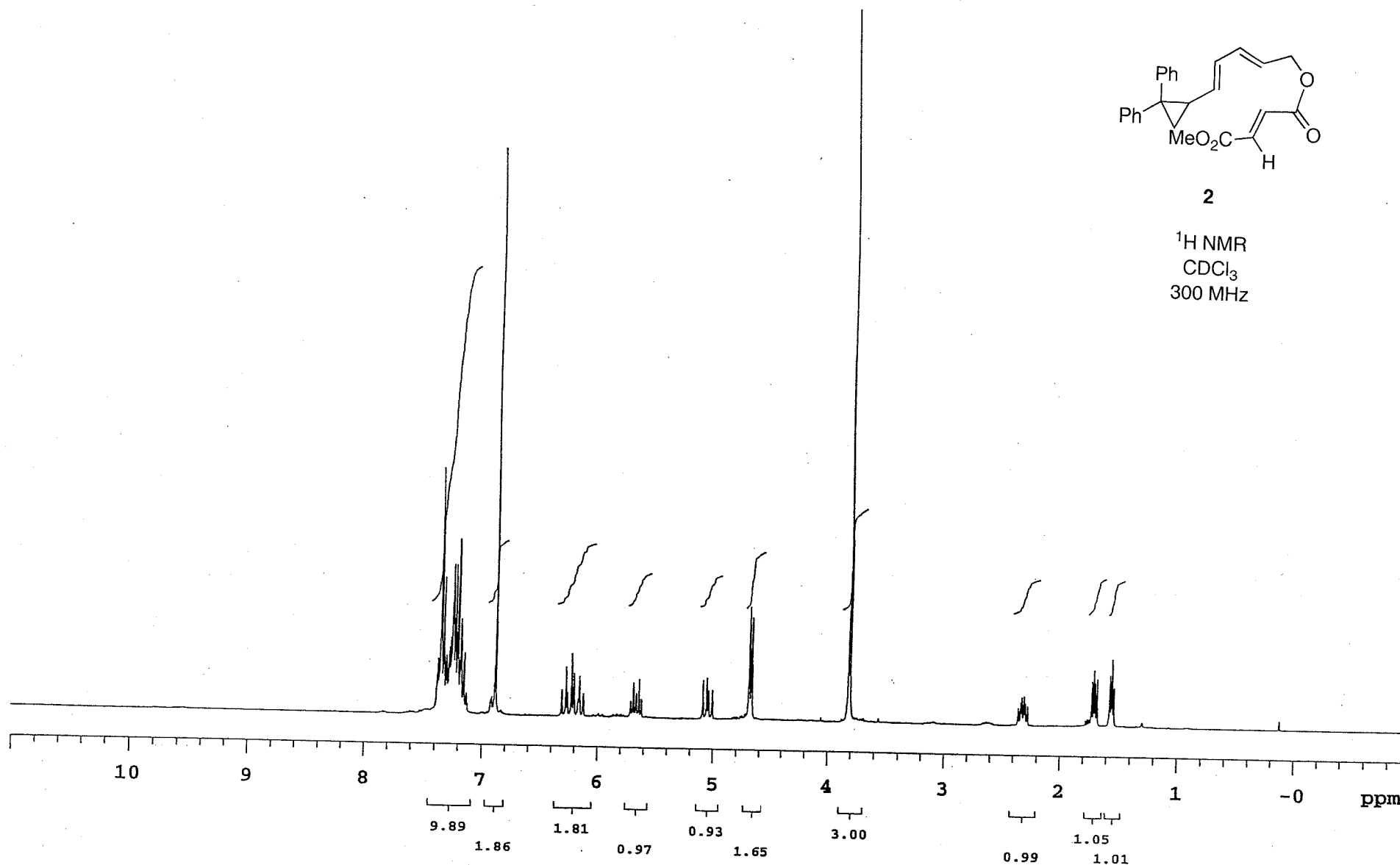


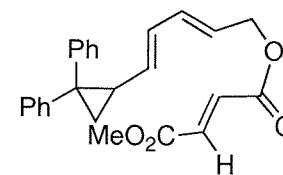
F1 (ppm)



2

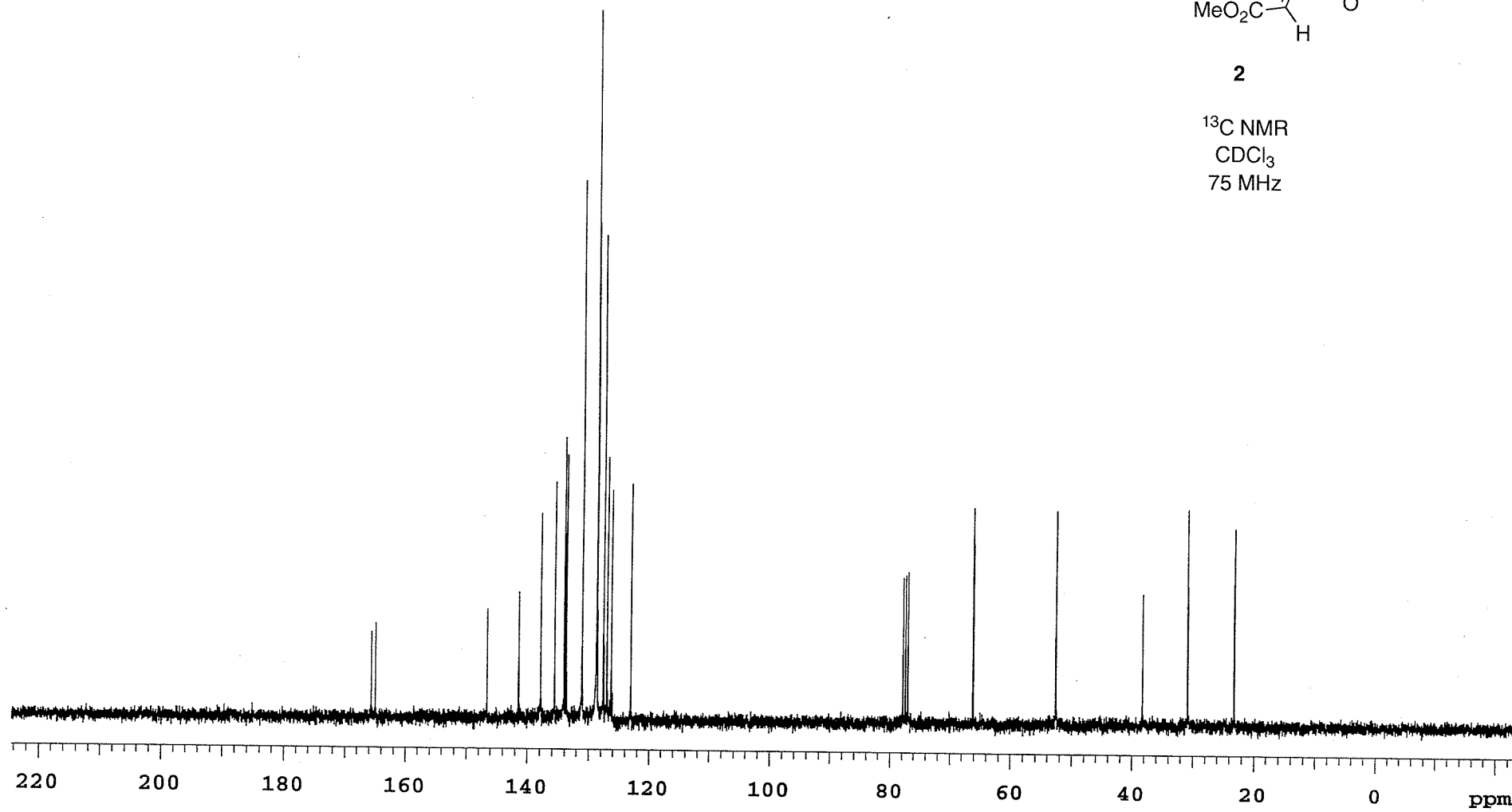
^1H NMR
 CDCl_3
 300 MHz



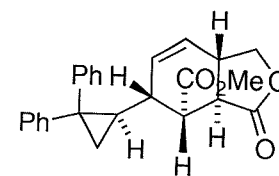


2

^{13}C NMR
 CDCl_3
 75 MHz

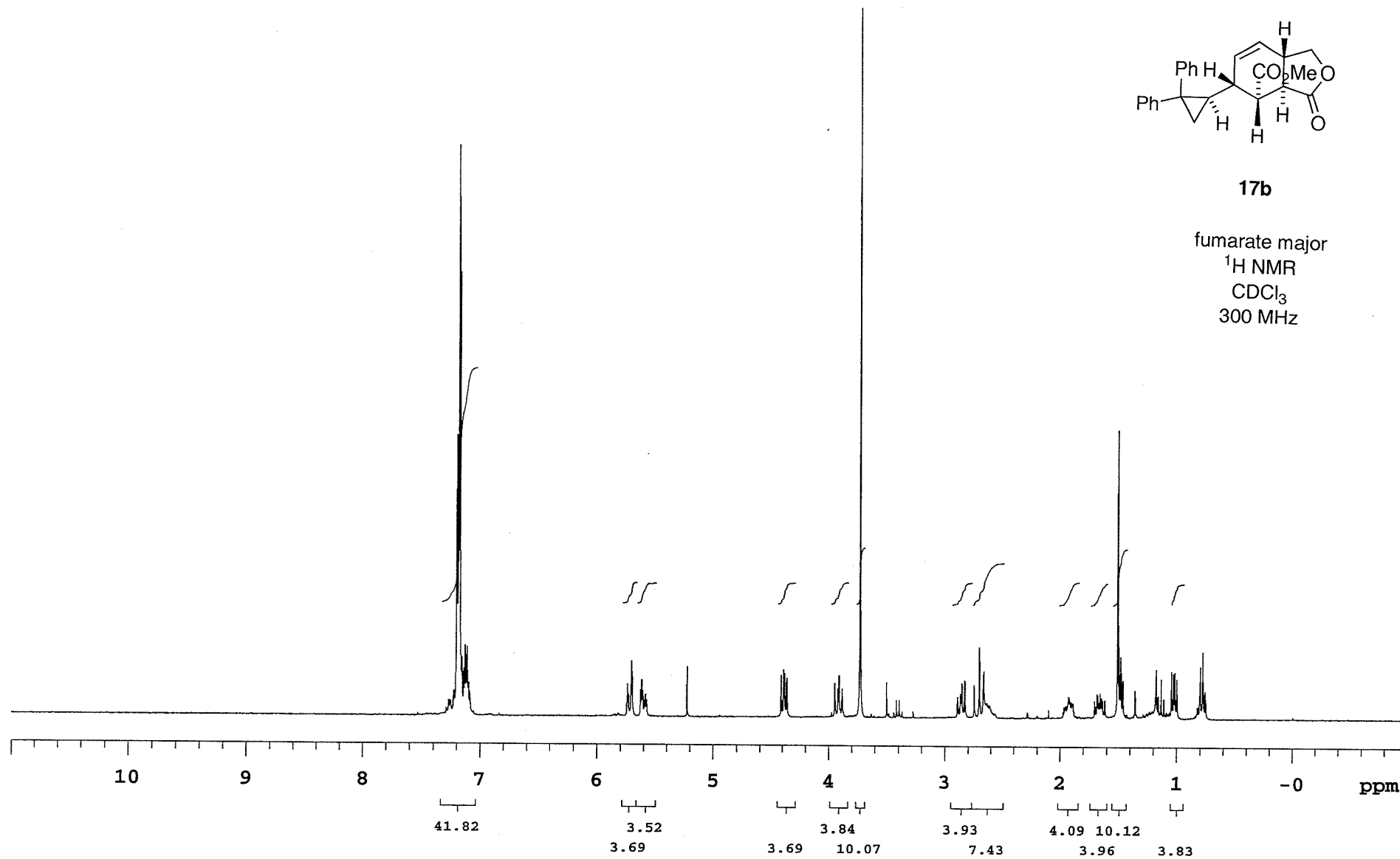


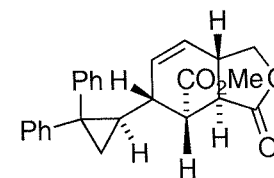
6001204002



17b

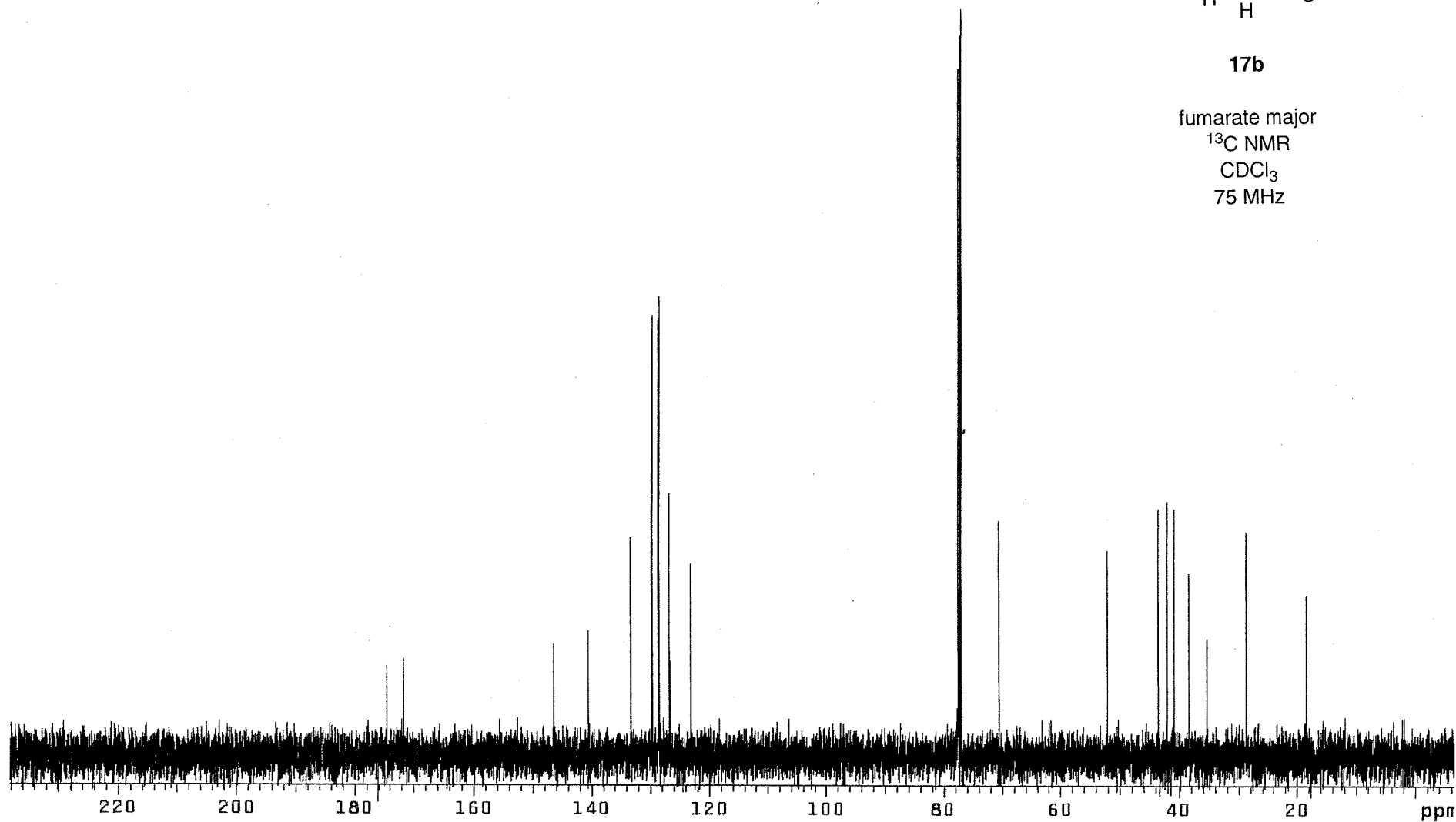
fumarate major
¹H NMR
 CDCl₃
 300 MHz

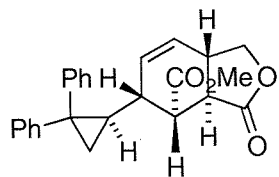




17b

fumarate major
 ^{13}C NMR
 CDCl_3
 75 MHz





17b

fumarate major

^1H - ^1H COSY

CDCl_3

600 MHz

Relax. delay 1.500 sec

Acq. time 0.184 sec

Width 5562.5 Hz

2D Width 5562.5 Hz

16 repetitions

2 x 139 increments

OBSERVE H1, 599.9849026 MHz

DATA PROCESSING

Sq. sine bell 0.138 sec

Shifted by -0.092 sec

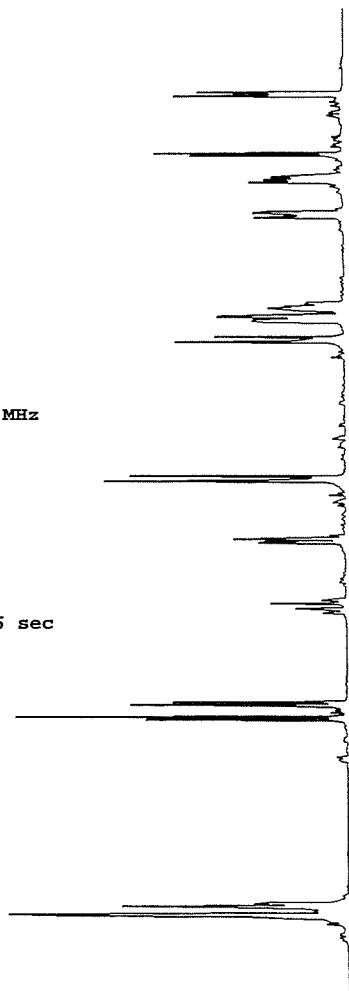
F1 DATA PROCESSING

Sq. sine bell 0.037 sec

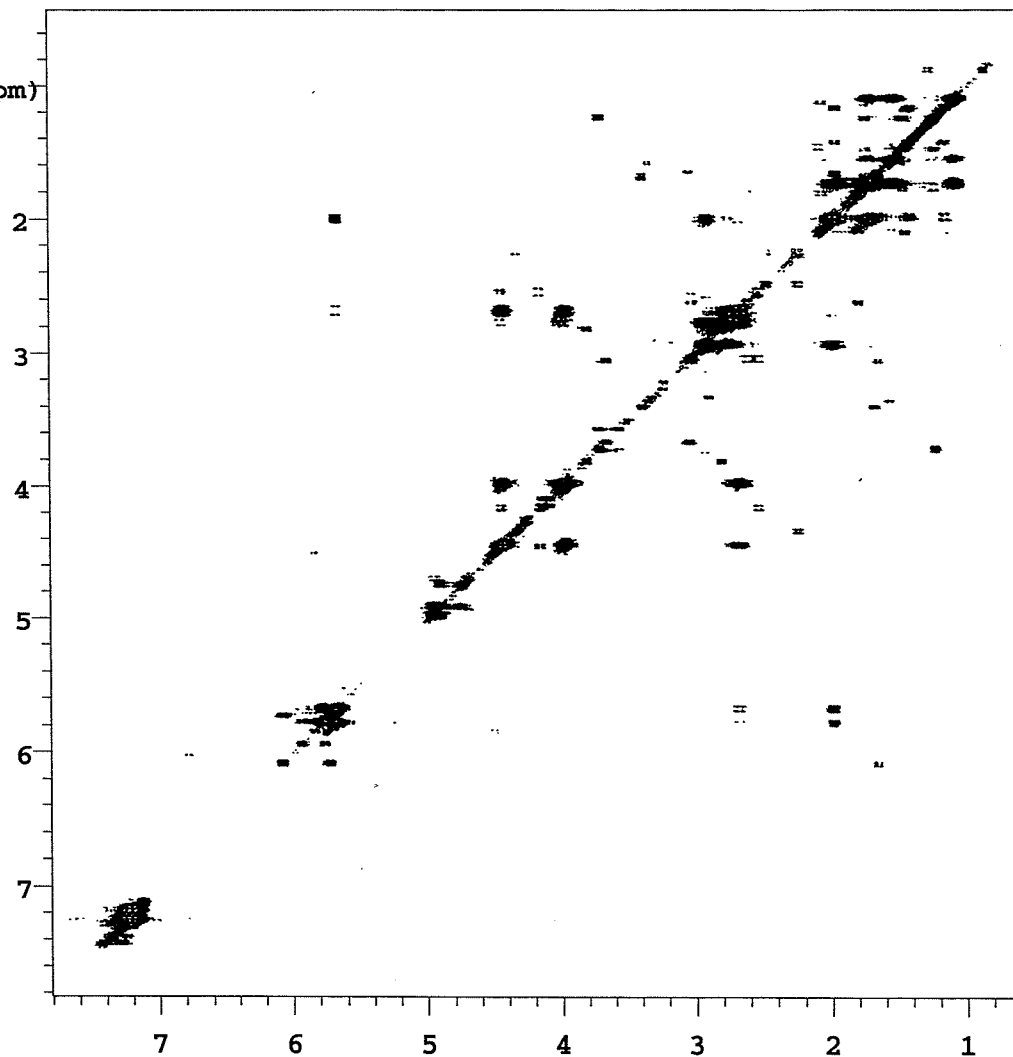
Shifted by -0.025 sec

FT size 2048 x 2048

Total time 2 hr, 8 min, 26 sec

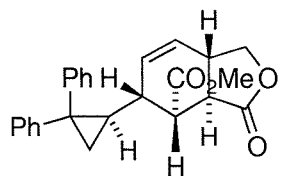


F2
(ppm)



F1 (ppm)

[12]



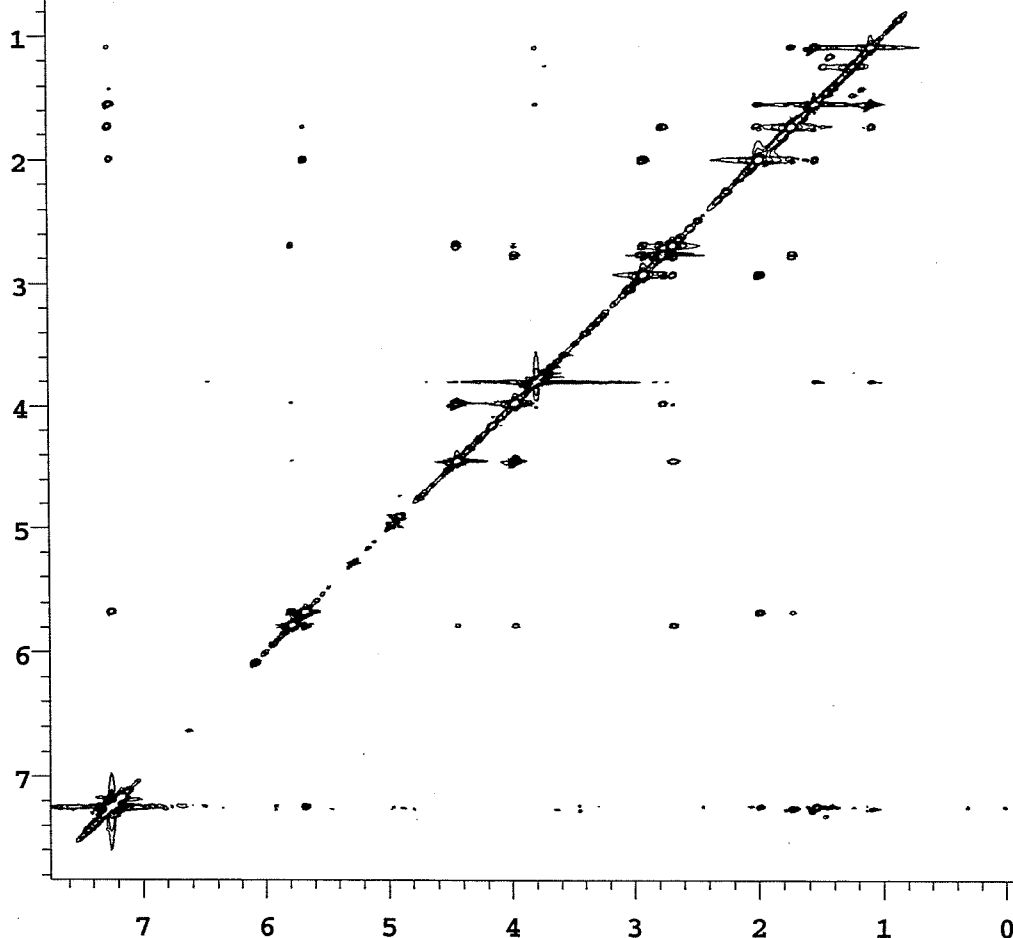
17b

fumarate major
NOESY
CDCl₃
600 MHz

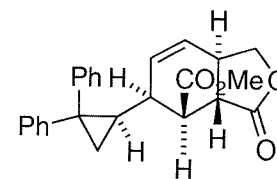
Relax. delay 1.000 sec
Mixing 1.000 sec
Acq. time 0.184 sec
Width 5562.5 Hz
2D Width 5562.5 Hz
64 repetitions
2 x 200 increments
OBSERVE H1, 599.9849026 MHz
DATA PROCESSING
~~Gauss apodization 0.085 sec~~
F1 DATA PROCESSING
Gauss apodization 0.033 sec
FT size 2048 x 2048
Total time 15 hr, 48 min, 9 sec

F2

(ppm)

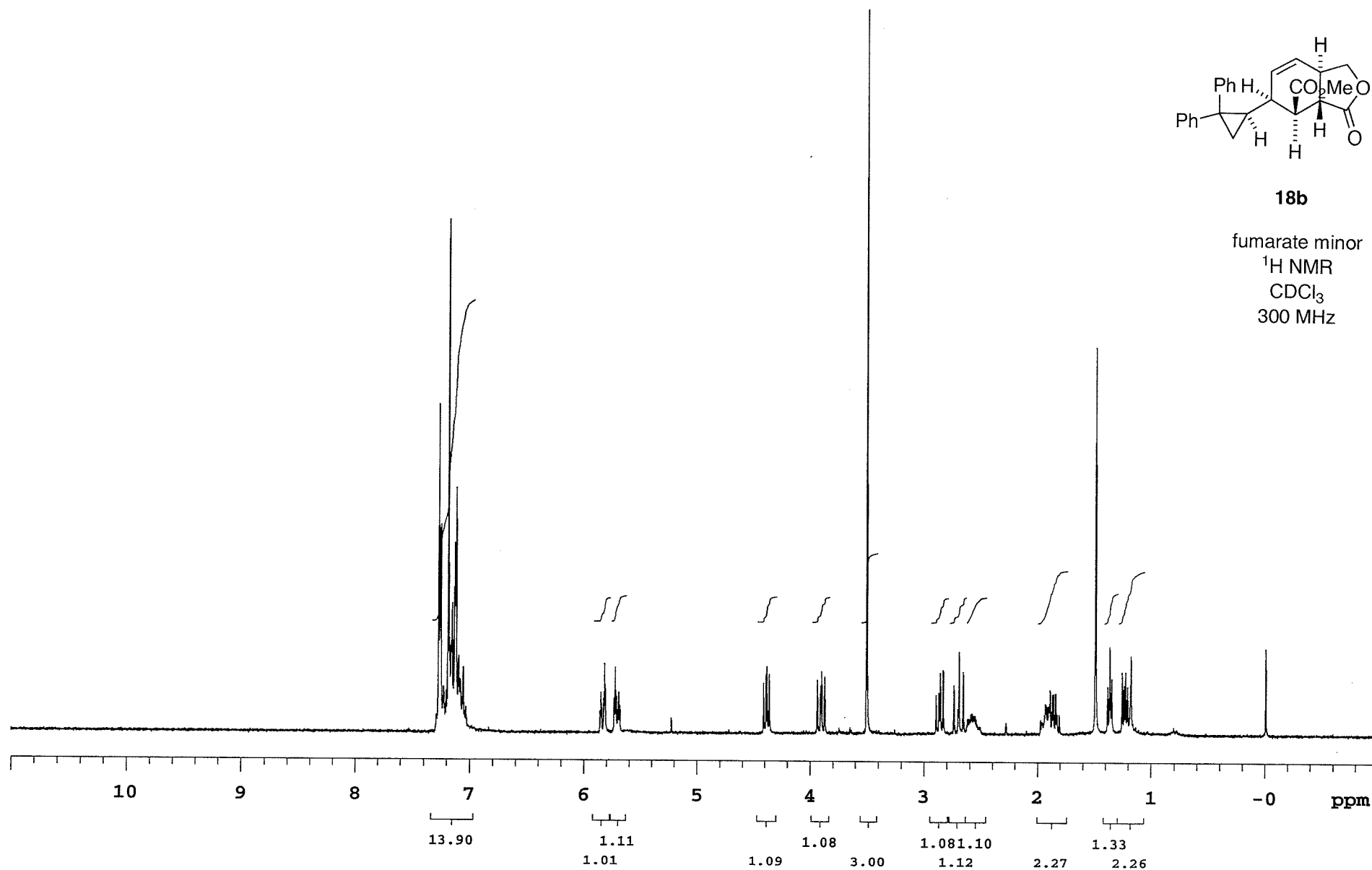


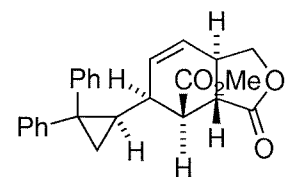
F1 (ppm)



18b

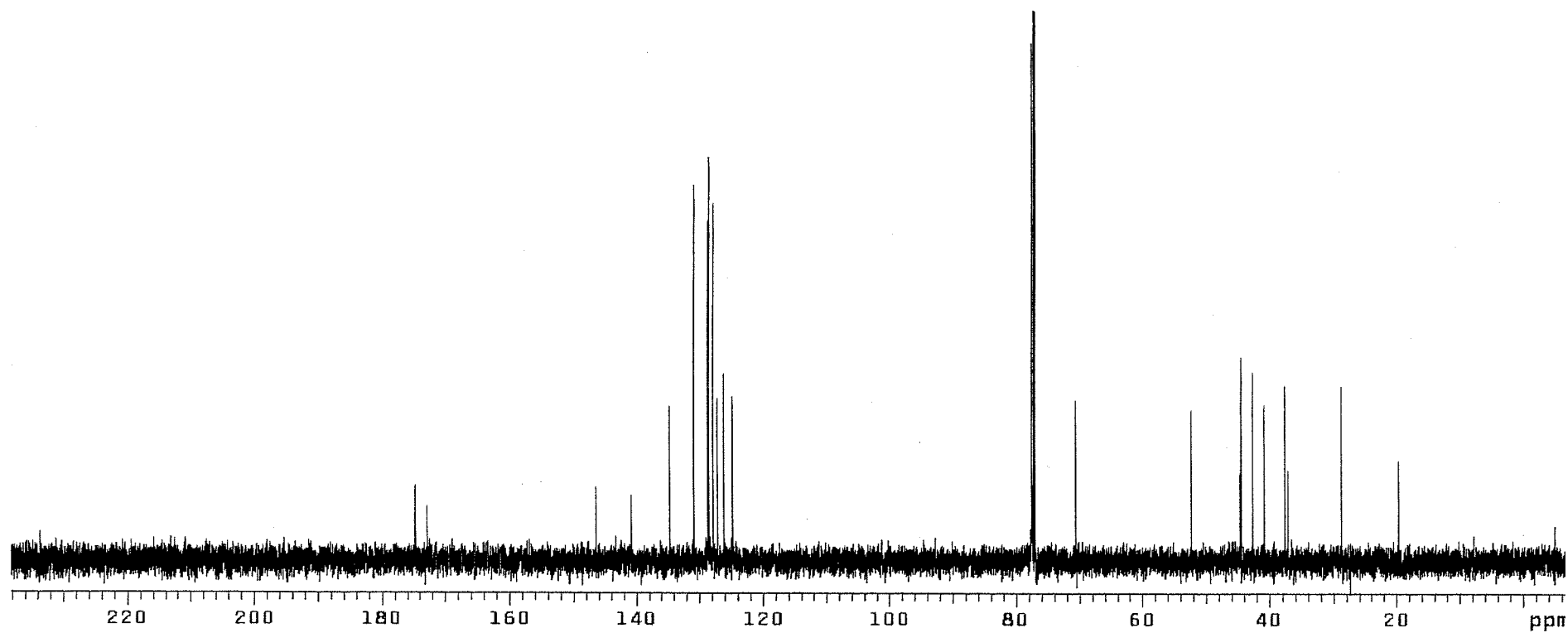
fumarate minor
 ^1H NMR
 CDCl_3
 300 MHz





18b

fumarate minor
 ^{13}C NMR
 CDCl_3
 75 MHz



TCH158CR
CDC13 06-11-06

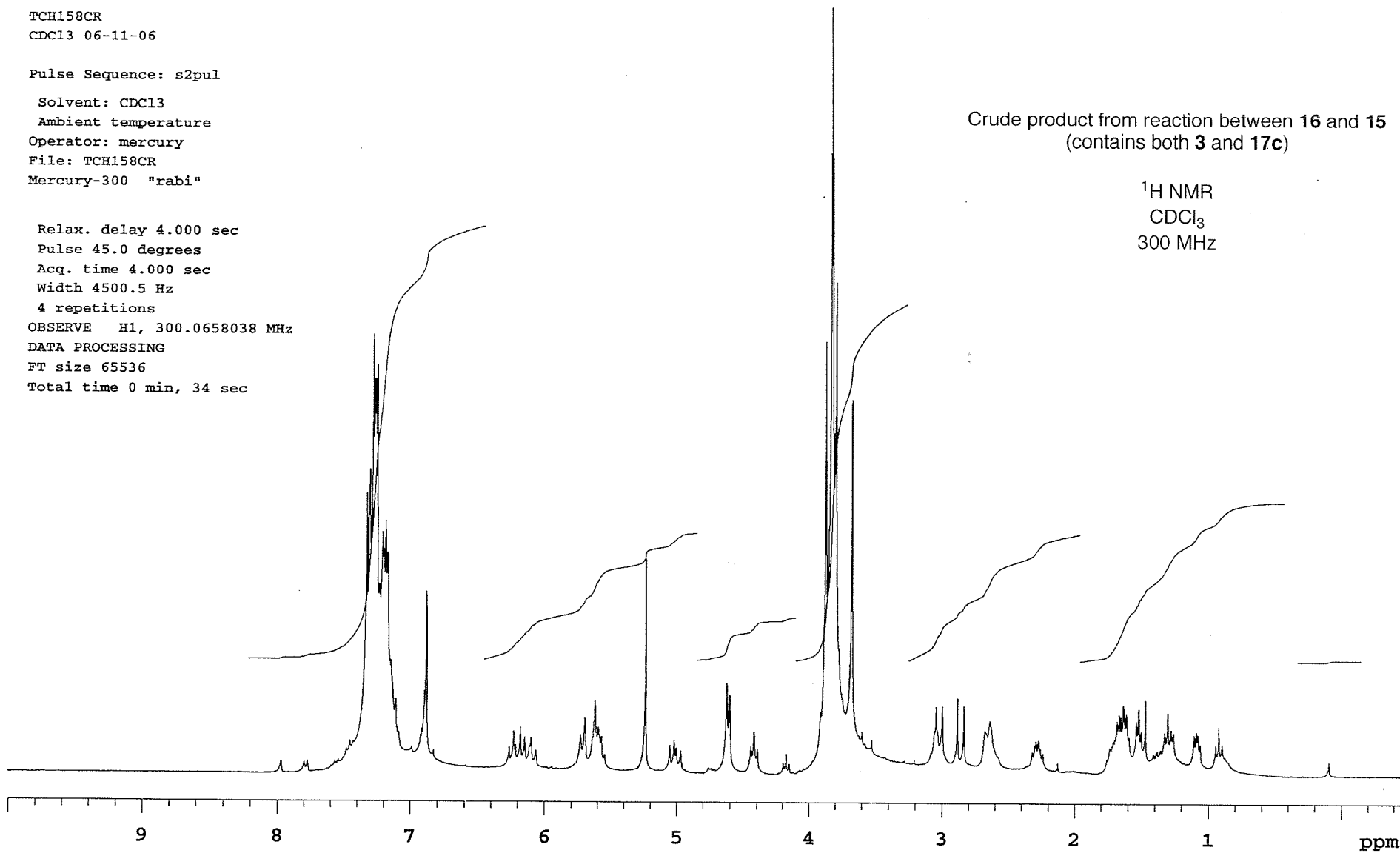
Pulse Sequence: s2pul

Solvent: CDC13
Ambient temperature
Operator: mercury
File: TCH158CR
Mercury-300 "rabi"

Relax. delay 4.000 sec
Pulse 45.0 degrees
Acq. time 4.000 sec
Width 4500.5 Hz
4 repetitions
OBSERVE H1, 300.0658038 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 34 sec

Crude product from reaction between **16** and **15**
(contains both **3** and **17c**)

^1H NMR
 CDCl_3
300 MHz



TCH160CR
CDC13 13-11-06

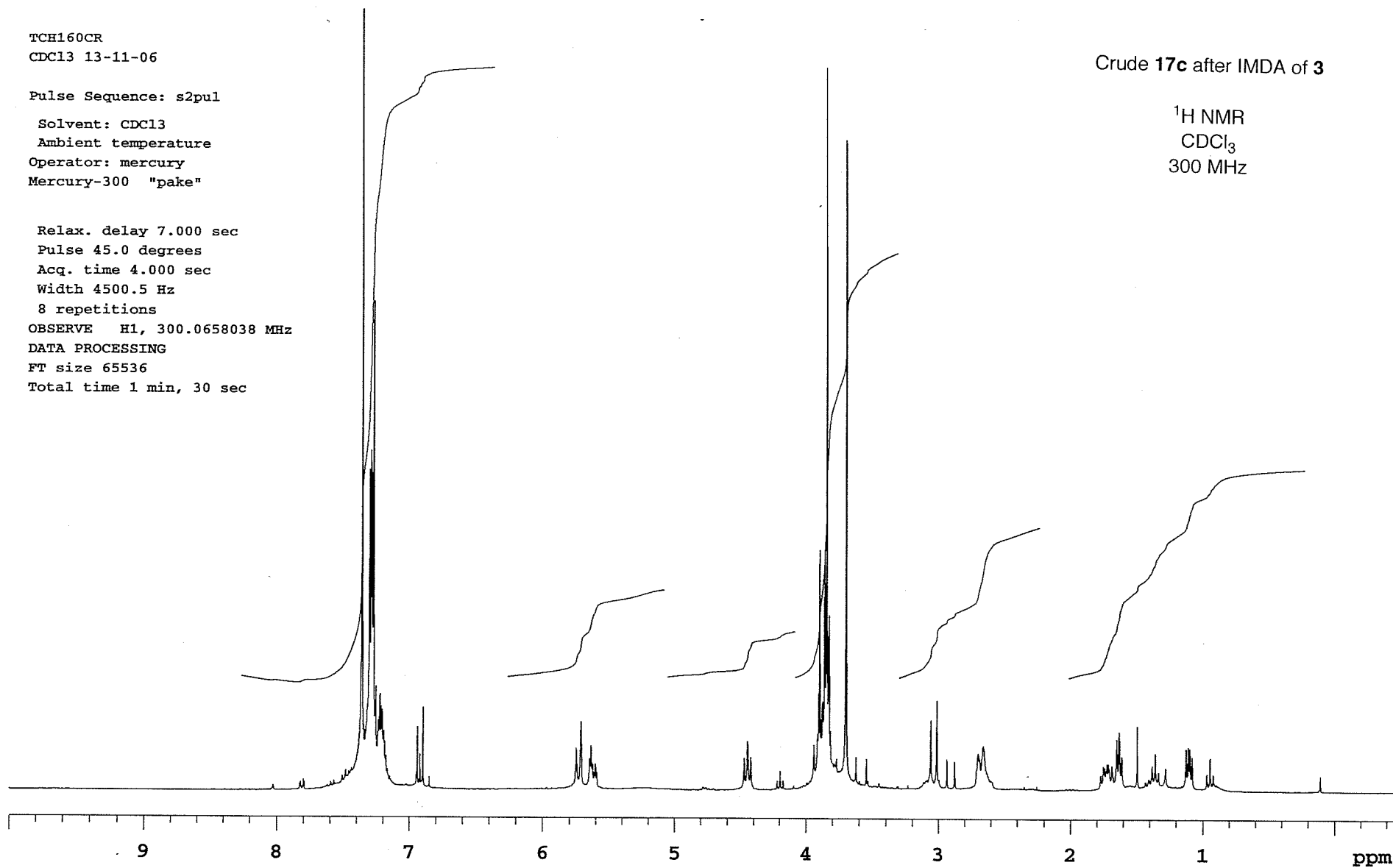
Pulse Sequence: s2pul

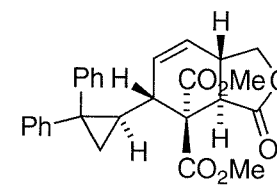
Solvent: CDC13
Ambient temperature
Operator: mercury
Mercury-300 "pake"

Relax. delay 7.000 sec
Pulse 45.0 degrees
Acq. time 4.000 sec
Width 4500.5 Hz
8 repetitions
OBSERVE H1, 300.0658038 MHz
DATA PROCESSING
FT size 65536
Total time 1 min, 30 sec

Crude **17c** after IMDA of **3**

^1H NMR
 CDCl_3
300 MHz

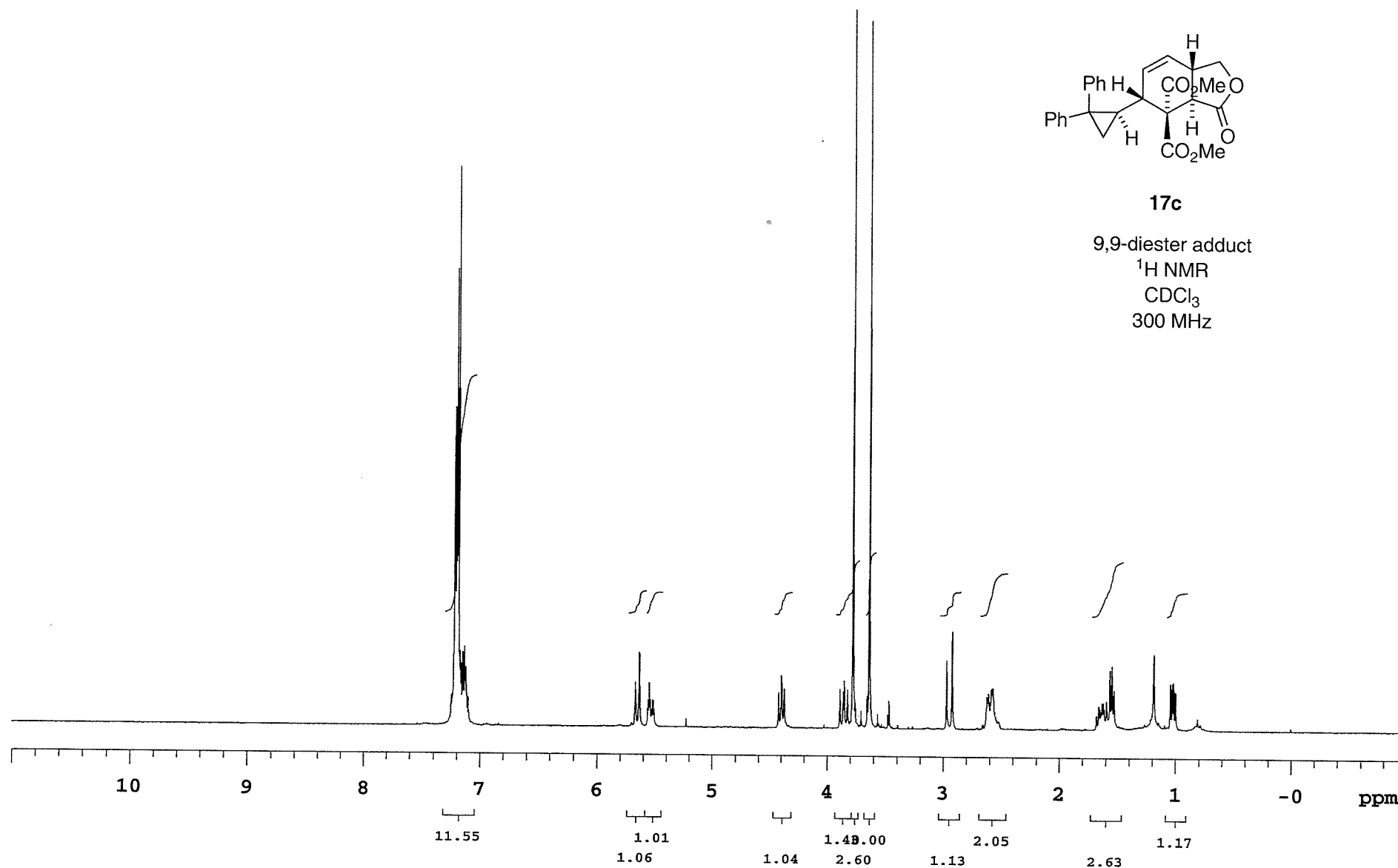


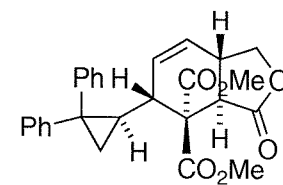
**17c**

9,9-diester adduct

¹H NMRCDCl₃

300 MHz





17c

9,9-diester adduct

^{13}C NMR

CDCl_3

75 MHz

