Evidence for Nonstatistical Dynamics in the Wolff Rearrangement of a Carbene

*Aviva E. Litovitz, Ivan Keresztes, Barry K. Carpenter**[‡]

Department of Chemistry and Chemical Biology,

Baker Laboratory, Cornell University, Ithaca, New York 14853-1301

Supporting Information

Table of contents:

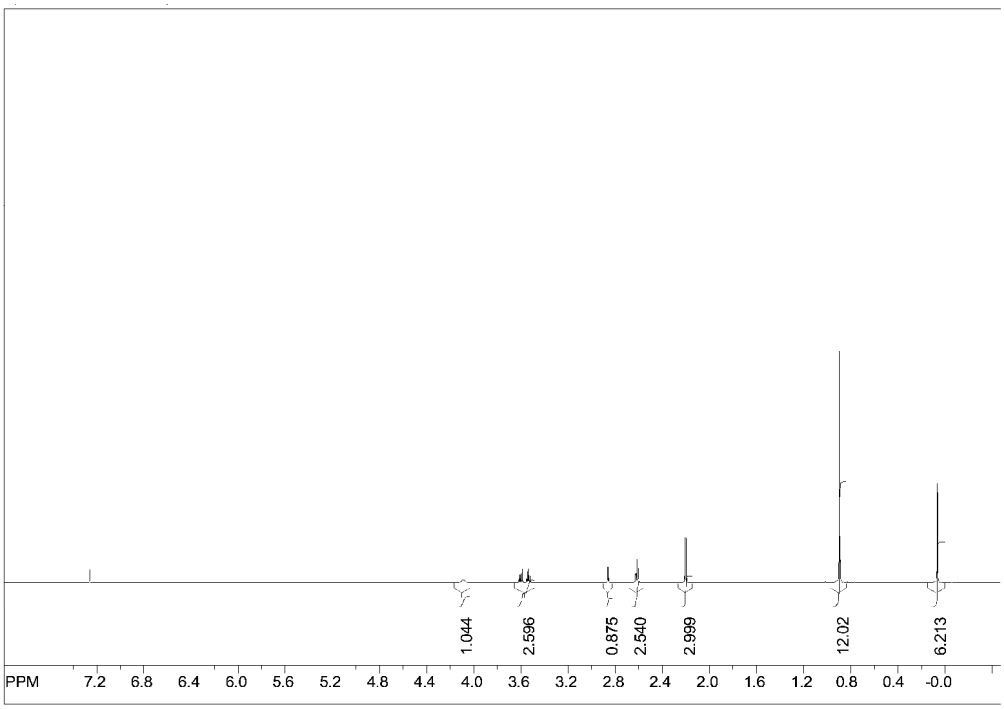

Figure S1: ^{1}H NMR spectrum of 5-(*tert*-butyldimethylsilyloxy)-4-hydroxypentan-2-one-2-^{13}C (**14**)

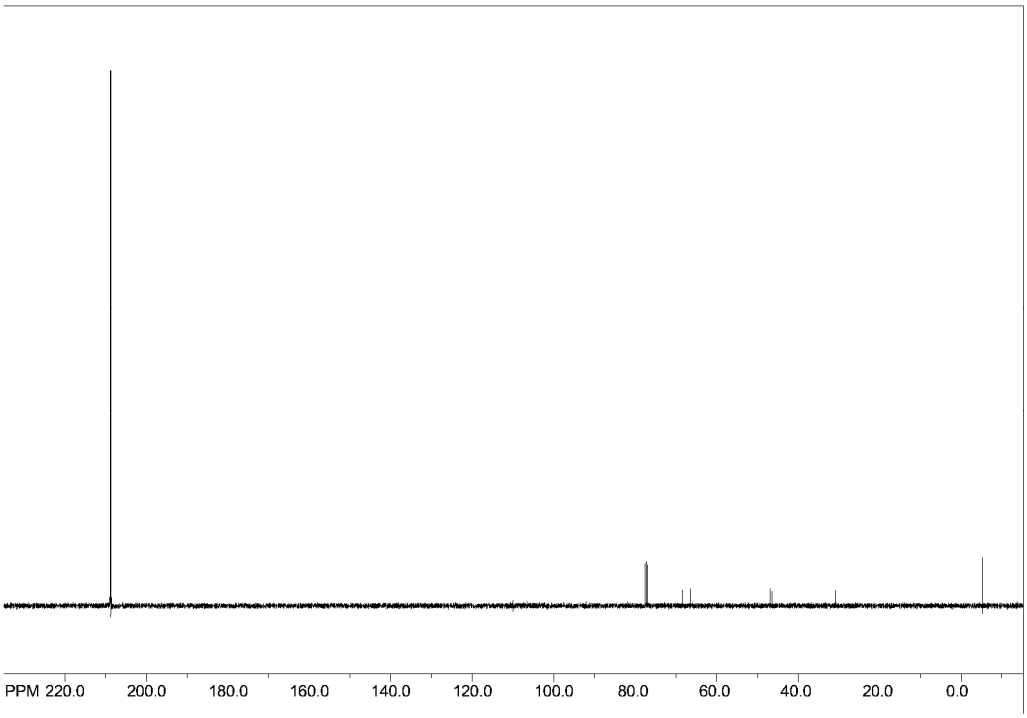

Figure S2: ^{13}C NMR spectrum of 5-(*tert*-butyldimethylsilyloxy)-4-hydroxypentan-2-one-2-^{13}C (**14**)

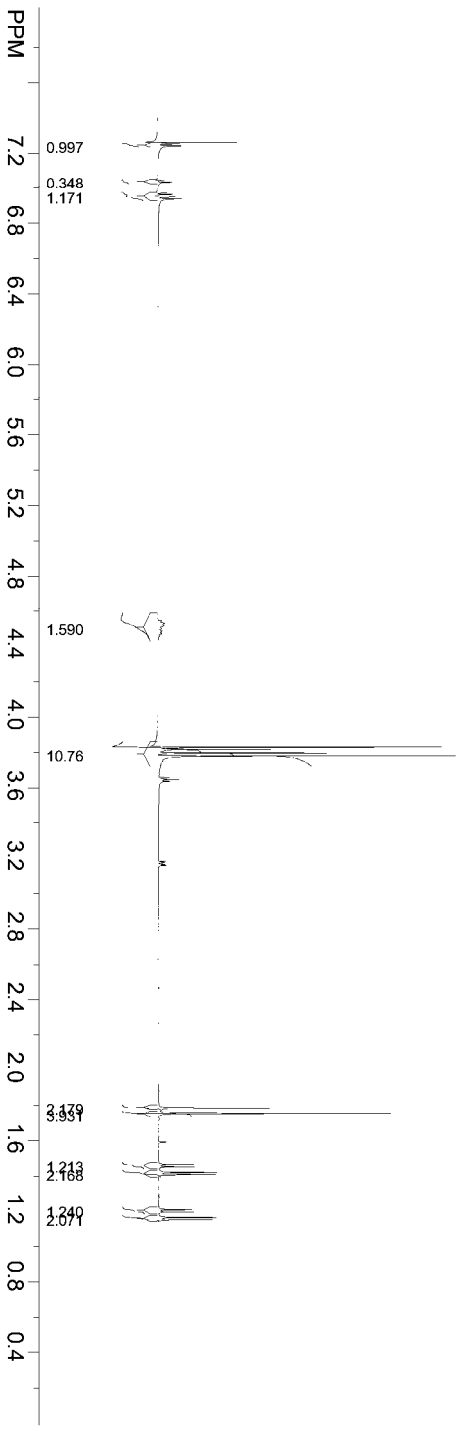

Figure S3: ^{1}H NMR spectrum of dimethyl 1-(1-hydroxyethyl-2-^{13}C)-4-methyl-7-oxabicyclo-[2.2.1]hepta-2,5-diene-2,3-dicarboxylate (**7a**)

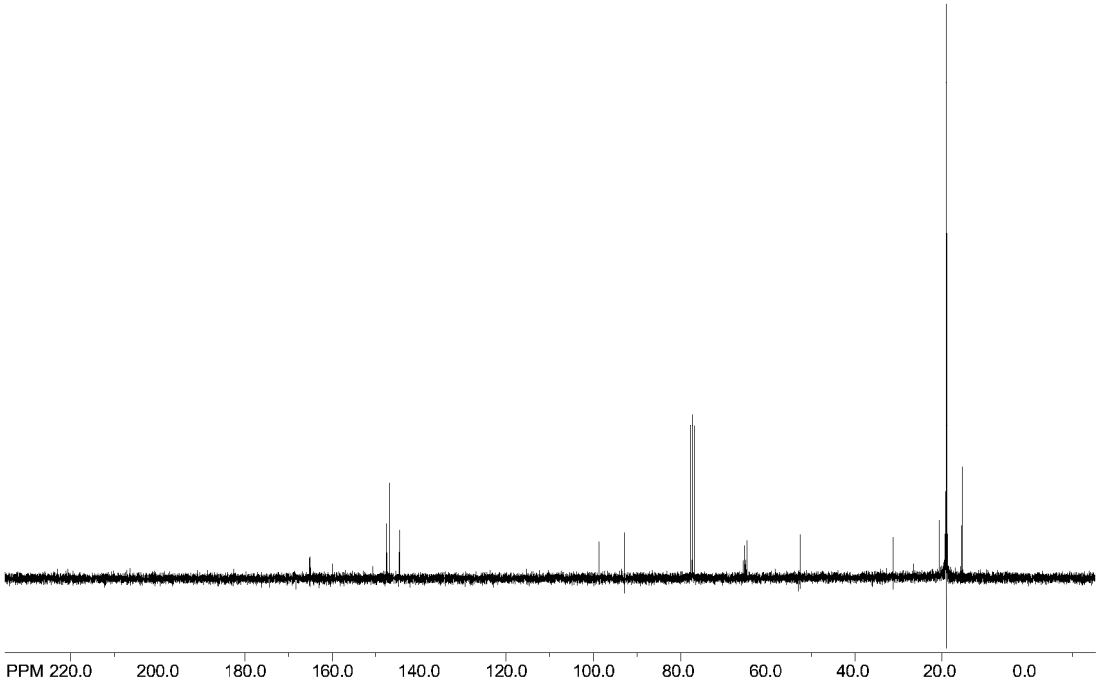

Figure S4: ^{13}C NMR spectrum of dimethyl 1-(1-hydroxyethyl-2-^{13}*C*)-4-methyl-7-oxabicyclo-[2.2.1]hepta-2,5-diene-2,3-dicarboxylate (**7a**)

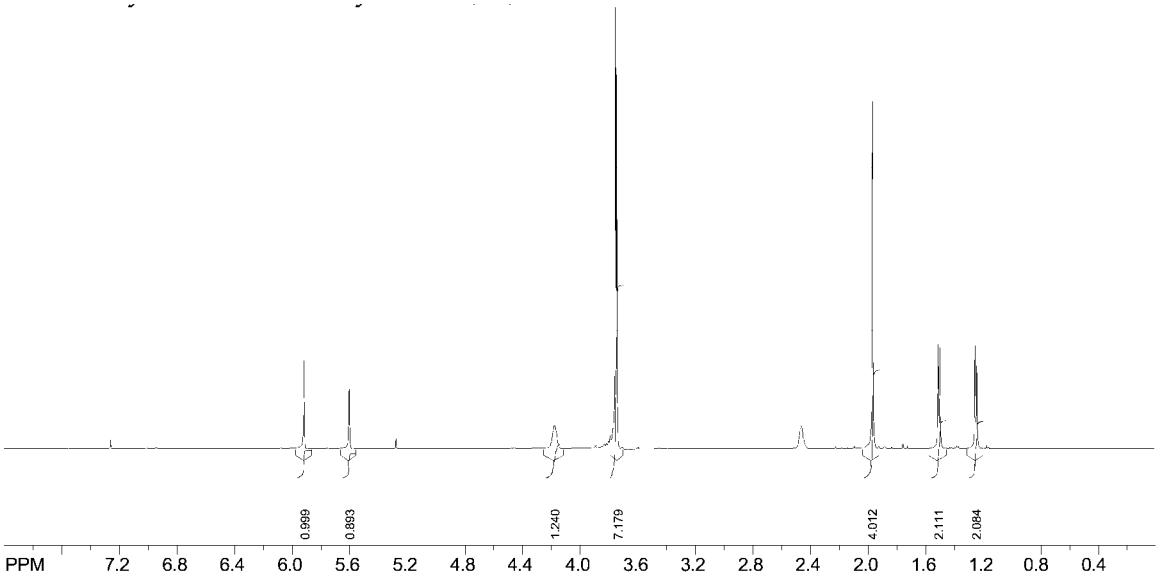

Figure S5: ^{1}H NMR spectrum of dimethyl 1-(1-hydroxyethyl-2-^{13}*C*)-7-methyloxepin-4,5-dicarboxylate (**9a**)

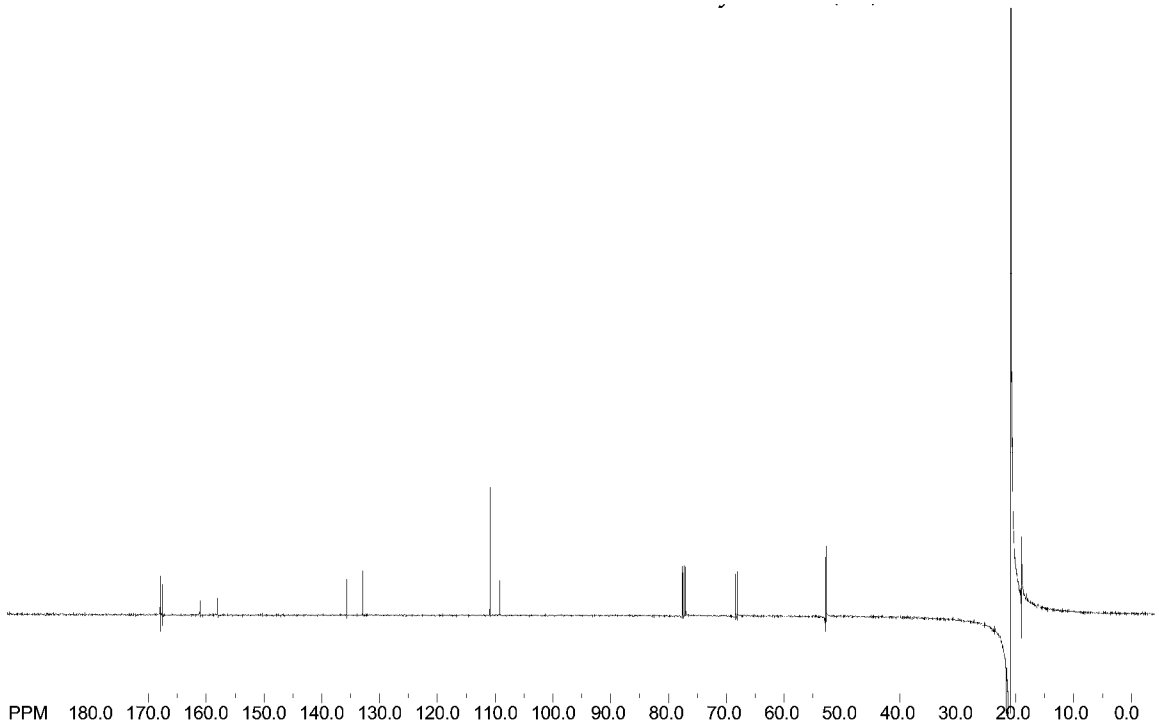

Figure S6: ^{13}C NMR spectrum of dimethyl 1-(1-hydroxyethyl-2-*^{13}C*)-7-methyloxepin-4,5-dicarboxylate (**9a**)

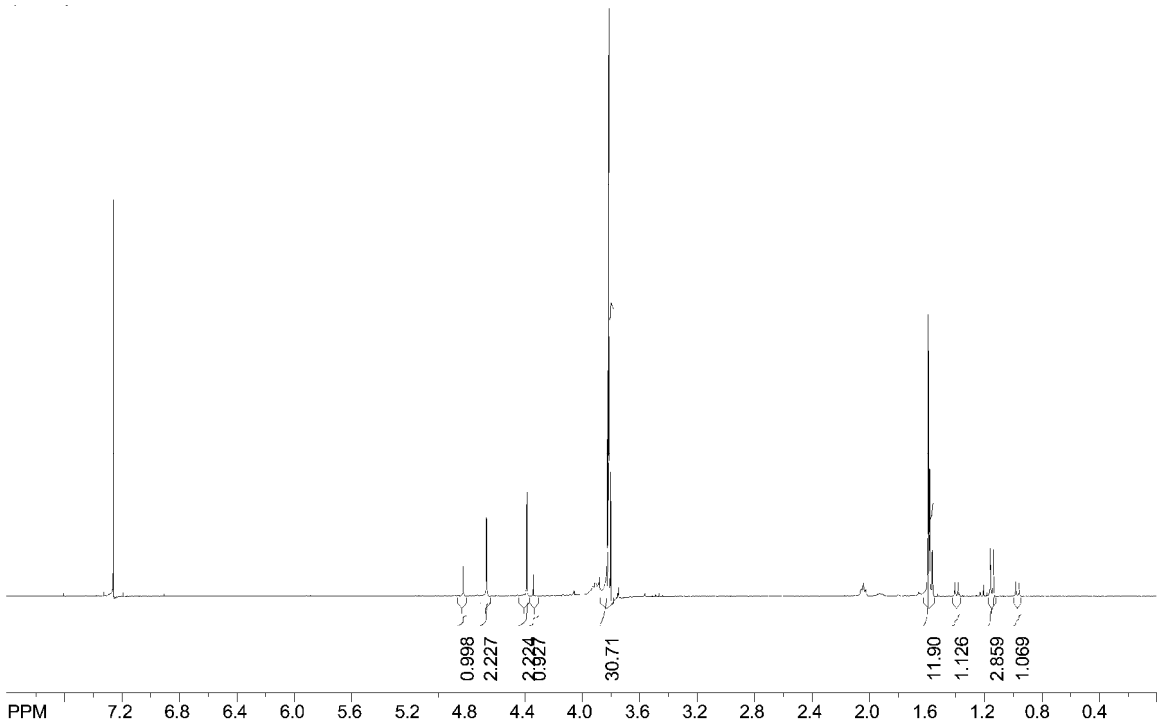

Figure S7: ^{1}H NMR spectrum of tetramethyl 2-(1-hydroxyethyl-2-*^{13}C*)-4-methyl-3-oxatricyclo-[3.2.2.0^{2,4}]nona-6,8-diene-6,7,8,9-tetracarboxylate (**10a**)

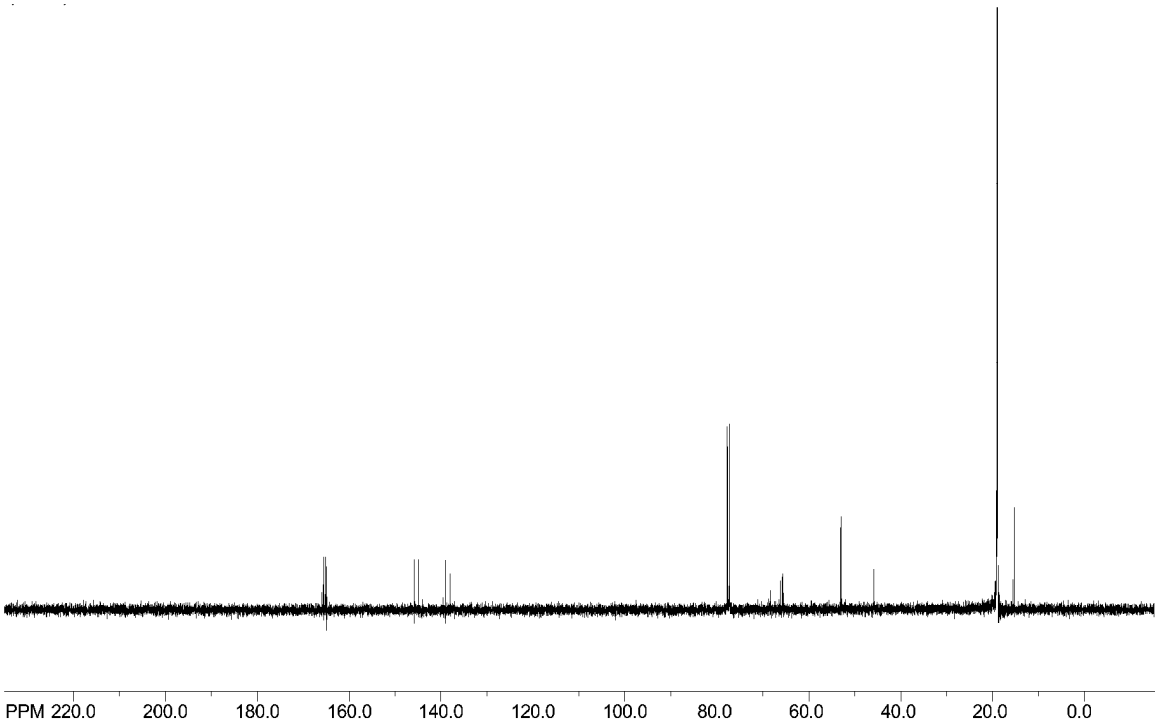

Figure S8: ^{13}C NMR spectrum of tetramethyl 2-(1-hydroxyethyl-2-*^{13}C*)-4-methyl-3-oxatricyclo-[3.2.2.0^{2,4}]nona-6,8-diene-6,7,8,9-tetracarboxylate (**10a**)

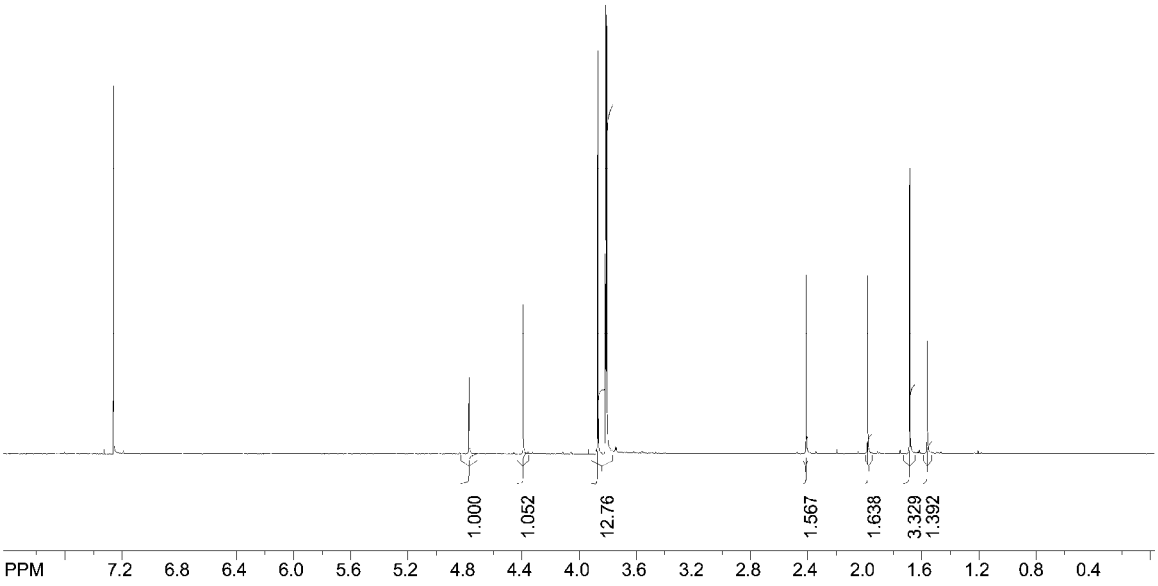

Figure S9: ^{1}H NMR spectrum of tetramethyl 2-(acetyl-2-*^{13}C*)-4-methyl-3-oxatricyclo[3.2.2.0^{2,4}]nona-6,8-diene-6,7,8,9-tetracarbox-ylate (**1a**)

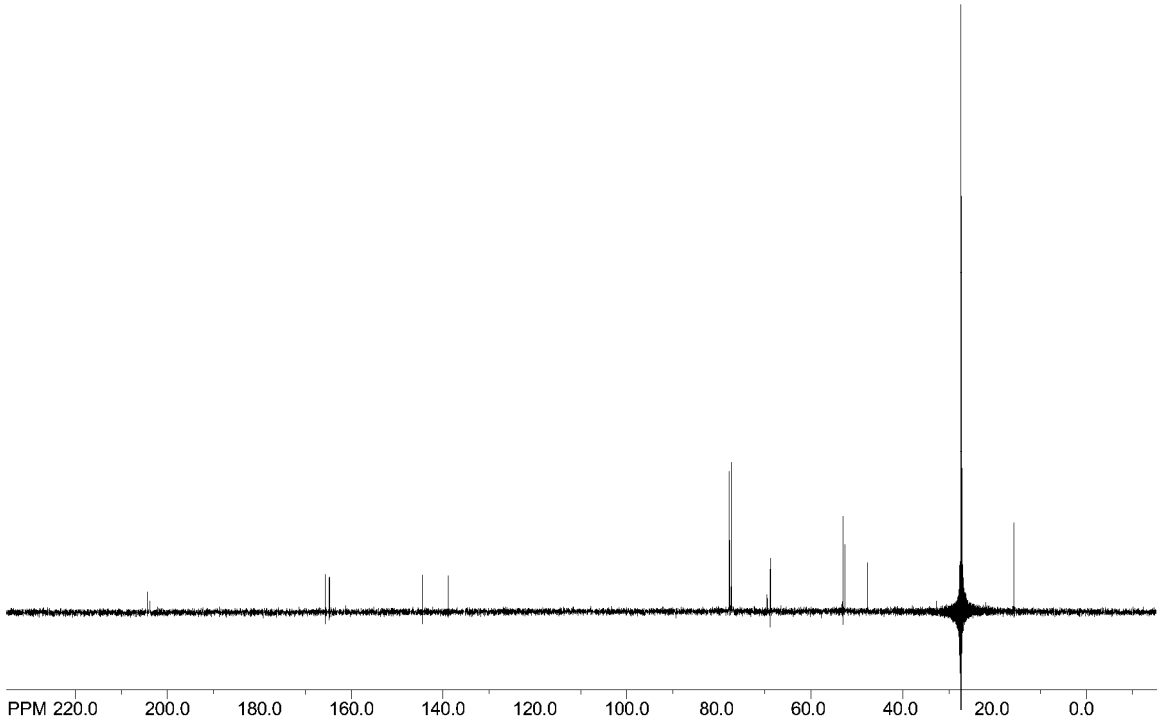

Figure S10: ^{13}C NMR spectrum of tetramethyl 2-(acetyl-2-^{13}C)-4-methyl-3-oxatricyclo[3.2.2.0^{2,4}]nona-6,8-diene-6,7,8,9-tetracarbox-ylate (**1a**)

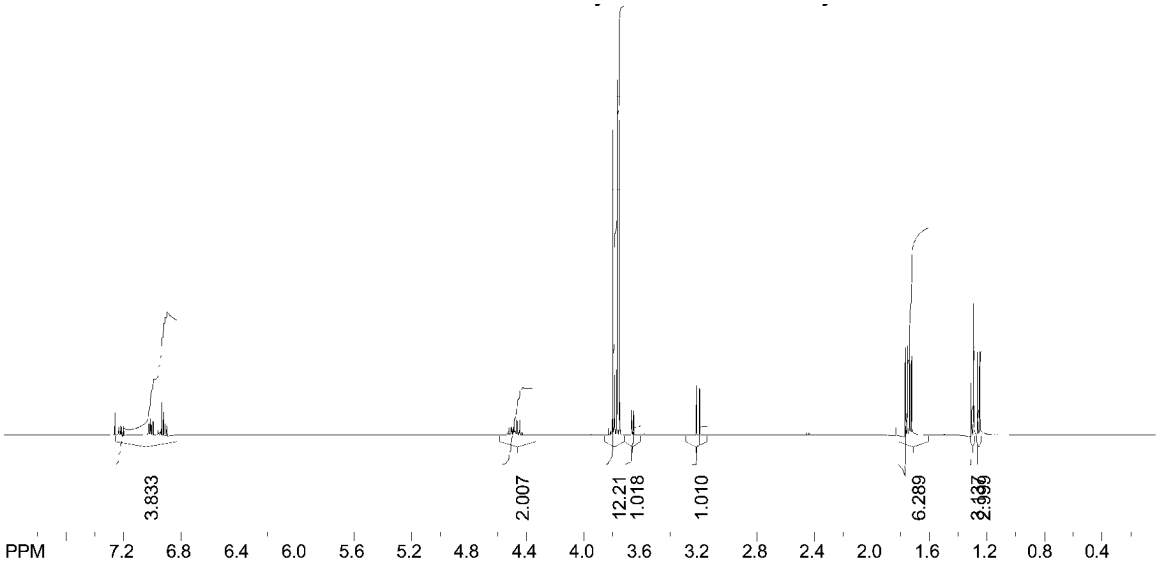

Figure S11: ^{1}H NMR spectrum of dimethyl 1-(1-hydroxyethyl)-4-methyl-7-oxabicyclo[2.2.1]hepta-2,5-diene-2,3-dicarboxylate-4-^{13}C (**7b**)

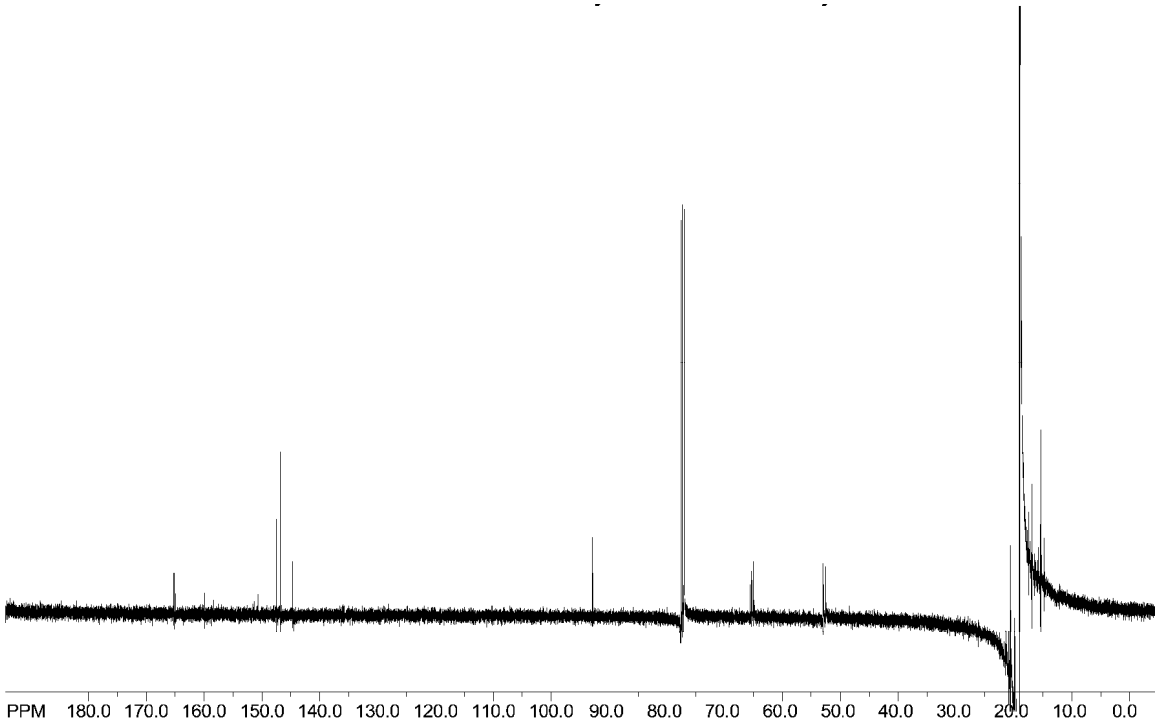

Figure S12: ^{13}C NMR spectrum of dimethyl 1-(1-hydroxyethyl)-4-methyl-7-oxabicyclo[2.2.1]hepta-2,5-diene-2,3-dicarboxylate-4-^{13}C (**7b**)

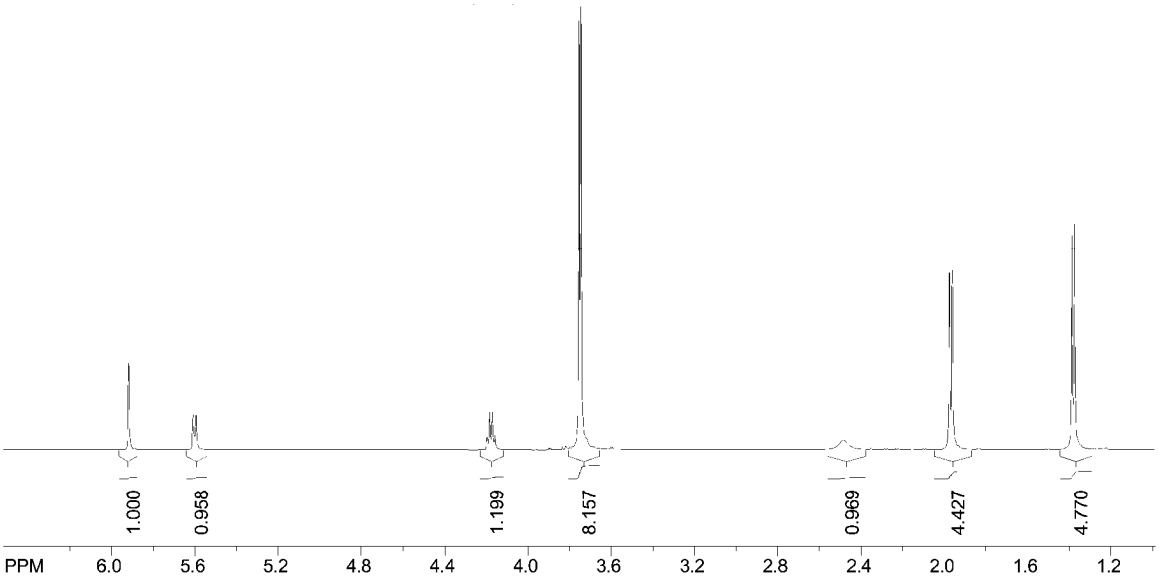

Figure S13: ^{1}H NMR spectrum of dimethyl 2-acetyl-7-methyl-7-oxepin-4,5-dicarboxylate-^{13}C (**9b**)

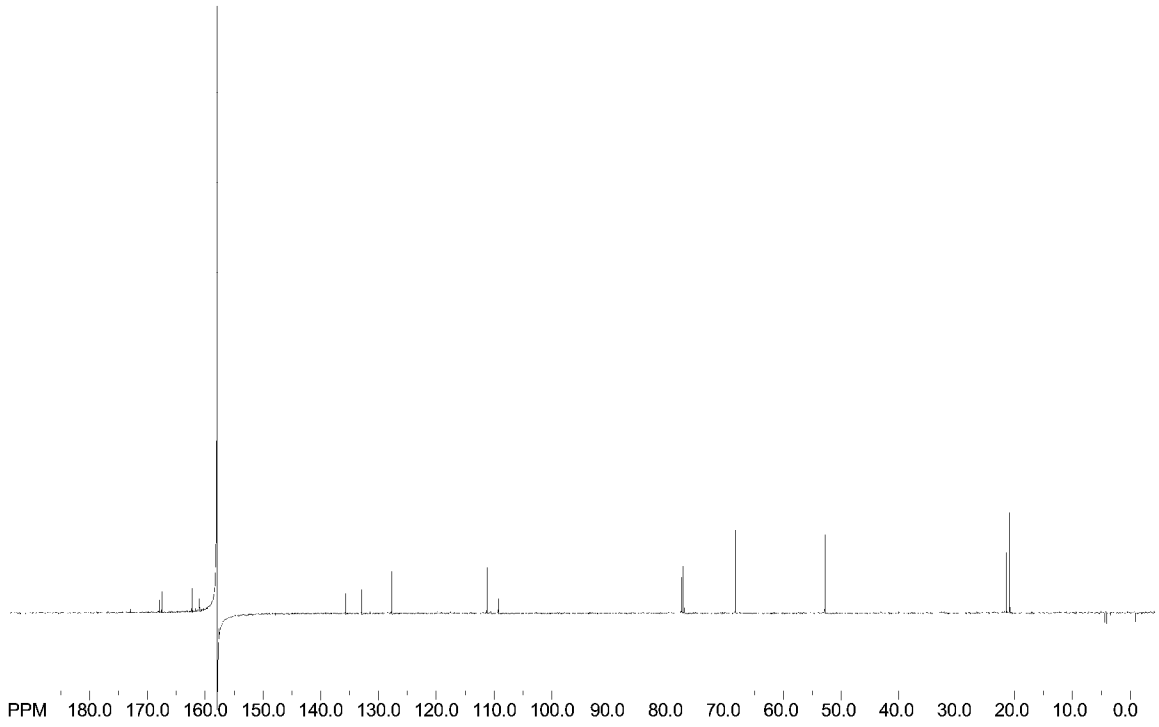

Figure S14: ^{13}C NMR spectrum of dimethyl 2-acetyl-7-methyl-7-oxepin-4,5-dicarboxylate-^{13}C (**9b**)

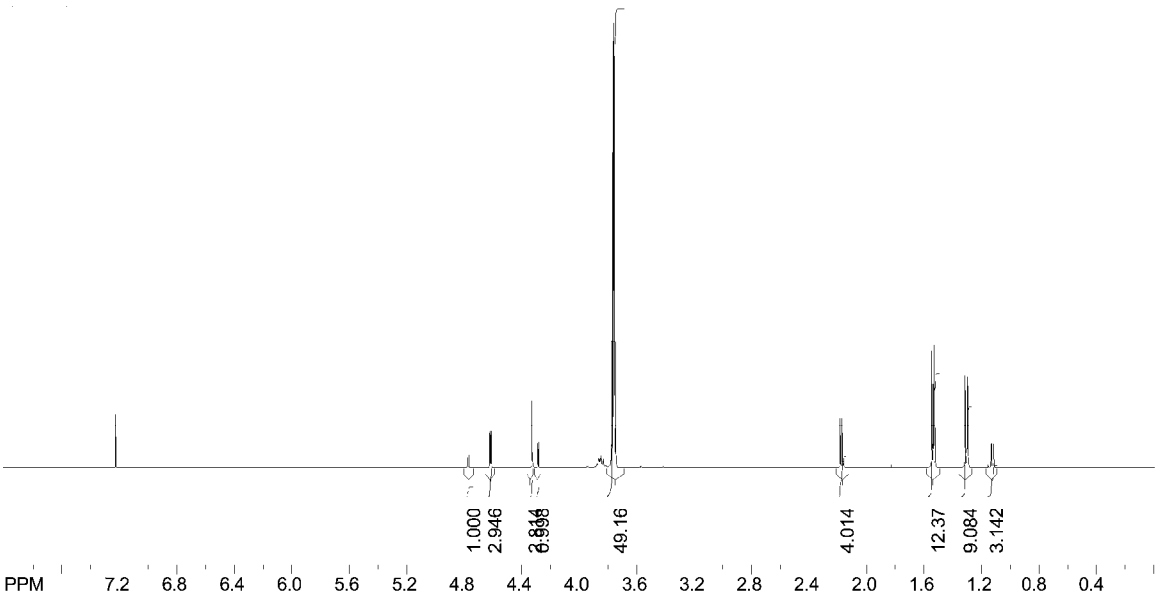

Figure S15: ^{1}H NMR spectrum of tetramethyl 2-(1-hydroxyethyl)-4-methyl-3-oxatricyclo-[3.2.2.0^{2,4}]nona-6,8-diene-6,7,8,9-tetra-carboxylate-4-^{13}C (**10b**)

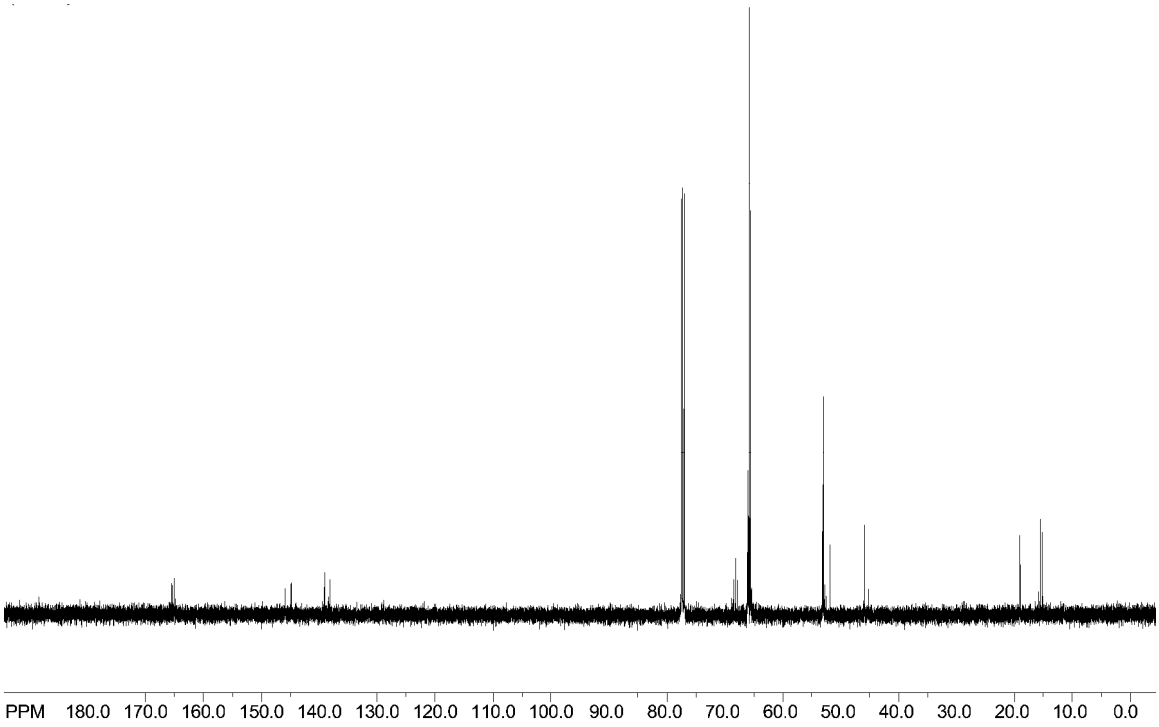

Figure S16: ^{13}C NMR spectrum of tetramethyl 2-(1-hydroxyethyl)-4-methyl-3-oxatricyclo-[3.2.2.0^{2,4}]nona-6,8-diene-6,7,8,9-tetra-carboxylate-4-*^{13}C* (**10b**)

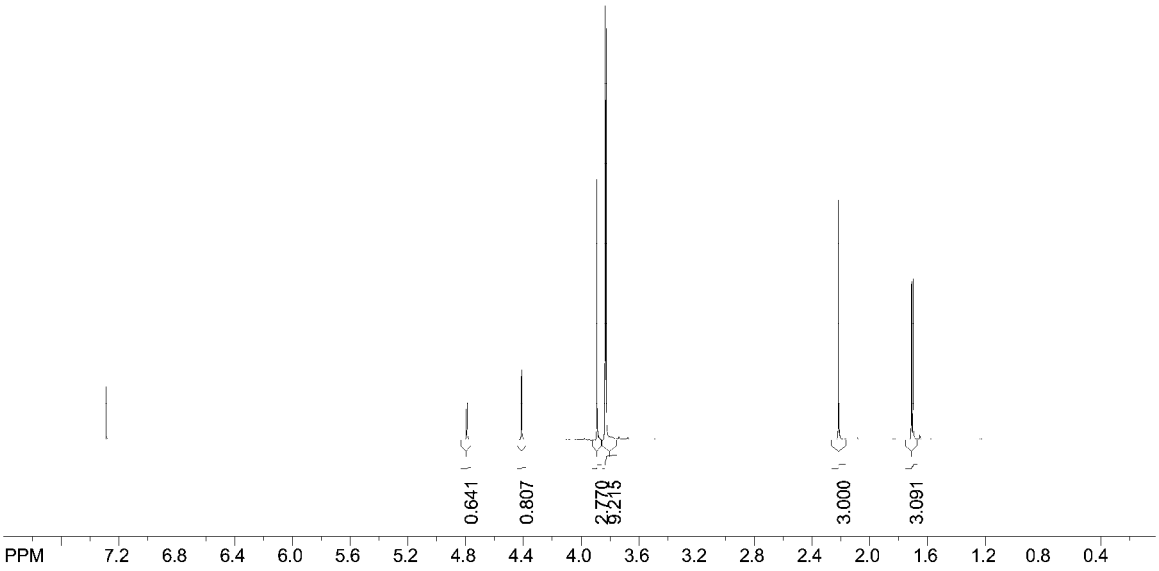

Figure S17: ^{1}H NMR spectrum of tetramethyl 2-acetyl-4-methyl-3-oxatricyclo[3.2.2.0^{2,4}]nona-6,8-diene-6,7,8,9-tetracarboxylate-4-*^{13}C* (**1b**)

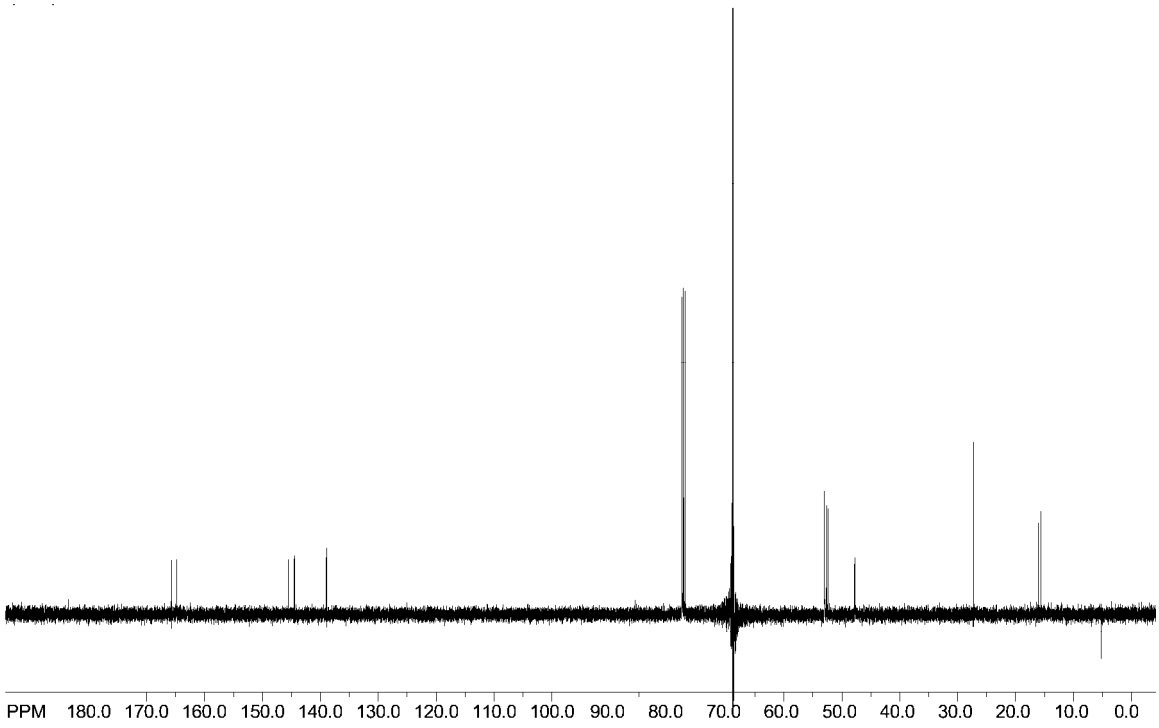

Figure S18: ^{13}C NMR spectrum of tetramethyl 2-acetyl-4-methyl-3-oxatricyclo[3.2.2.0^{2,4}]nona-6,8-diene-6,7,8,9-tetracarboxylate-4-*^{13}C* (**1b**)

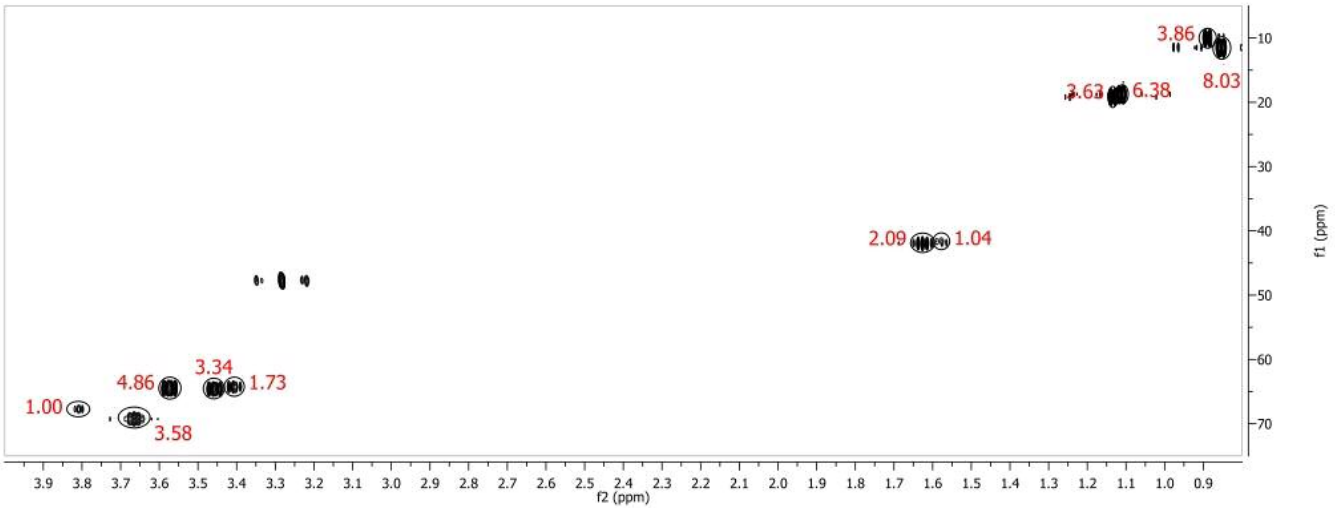

***Figure S19*:** HSQC-AD spectrum of 2-methylbutane-1,3-diol (**16**)

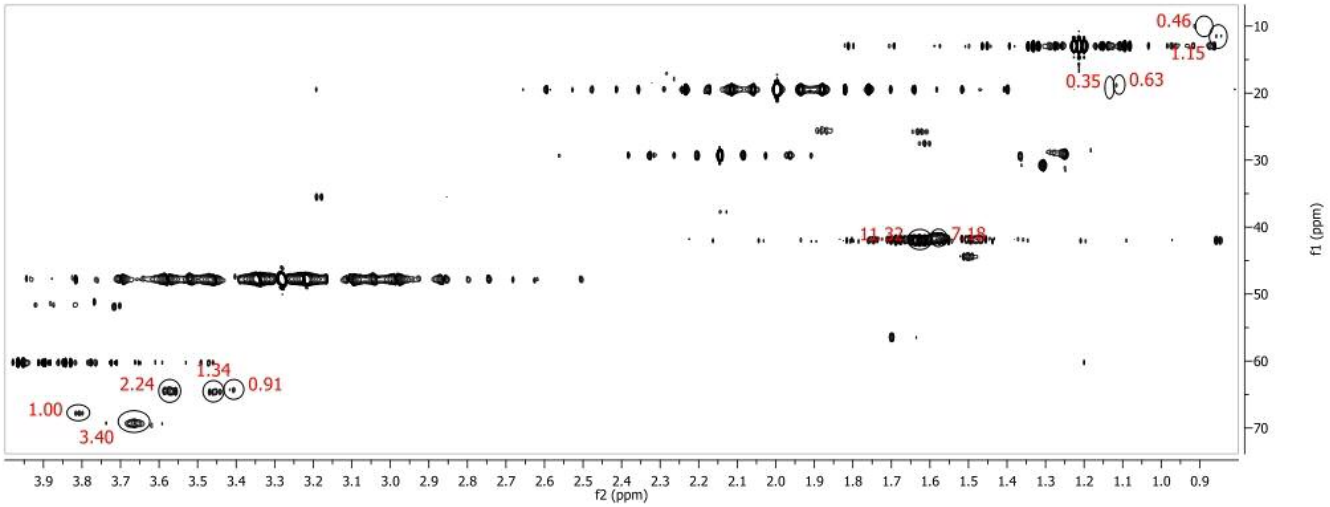

Figure S20: HSQC-AD spectrum of ^{13}C-labeled 2-methylbutane-1,3-diols derived from thermolysis of compound **1b**, followed by methanol trapping and DIBAL reduction

COMPUTATIONAL WORK

Coupled cluster calculations were carried out with MOLPRO.[1] All DFT calculations were carried out with Gaussian 03.[2b]

Acetylmethyloxirene/benzene adduct; MPWB1K/6-31+G(d,p):

O	-0.321607	0.872813	-1.252778
C	-0.472587	-0.171941	-0.307572
C	0.180980	1.078603	0.048907
C	0.536498	-1.343065	-0.309083
C	1.695565	0.824003	0.265620
C	1.102864	-1.317961	1.095623
C	1.718275	-0.184193	1.396482
C	1.625384	-0.972694	-1.273192
C	2.231146	0.164636	-0.974098
H	0.040977	-2.278514	-0.540753
H	2.207228	1.749463	0.511932
H	0.984379	-2.159409	1.757218
H	2.190726	0.031882	2.340808
H	1.828232	-1.567277	-2.148763
H	2.999611	0.629231	-1.569959
C	-1.866562	-0.529635	0.083213
O	-2.046013	-1.447599	0.845931
C	-2.990108	0.212493	-0.565478
H	-3.911772	0.016107	-0.030838
H	-2.793292	1.275308	-0.647289
H	-3.082524	-0.154713	-1.587672
C	-0.408279	2.182000	0.863436
H	-0.135753	2.050989	1.907706
H	-0.016300	3.139427	0.526381
H	-1.489614	2.212315	0.792858

Energy: -576.510967

Enthalpy: -576.288998

Retro-Diels-Alder transition state for acetylmethyloxirene/benzene adduct; MPWB1K/6-31+G(d,p):

O	0.453338	1.111069	1.221689
C	0.706869	0.148586	0.120332
C	-0.020714	1.241469	-0.075289
C	-0.578552	-1.643550	0.321929
C	-2.224912	0.414583	-0.189511
C	-1.081085	-1.510506	-0.997777
C	-1.905448	-0.460764	-1.252428
C	-1.282488	-1.078848	1.401567
C	-2.104596	-0.021968	1.138188
H	0.140406	-2.425711	0.516854
H	-2.825025	1.288828	-0.397738
H	-0.714669	-2.154538	-1.779971
H	-2.246164	-0.242222	-2.252784
H	-1.066977	-1.384098	2.412530
H	-2.565040	0.537810	1.936681
C	2.010520	-0.350329	-0.265315
O	2.167232	-0.987602	-1.284533
C	3.111674	-0.053685	0.705121
H	4.066549	-0.234736	0.225938
H	3.040392	0.967874	1.070477
H	3.013929	-0.704586	1.572433
C	-0.168646	2.478052	-0.851011
H	-0.387222	2.244391	-1.887409
H	-0.960905	3.101849	-0.448944
H	0.764438	3.039169	-0.800164

Energy: -576.419828
Enthalpy: -576.201861

TS for Singelton rearrangement of acetylmethyloxirene/benzene adduct to 7-methyl-7-pyruvoylnorcaradiene; MPWB1K/6-31+G(d,p):

O	-0.490511	0.273025	-1.730923
C	-0.428703	-0.142086	-0.495134
C	0.297959	1.013295	0.068681
C	0.545010	-1.397542	-0.063676
C	1.764108	0.875374	0.118615
C	0.832855	-0.992457	1.322300
C	1.384485	0.239077	1.445111
C	1.748767	-1.254716	-0.925841
C	2.363575	-0.087917	-0.840875
H	0.038930	-2.350564	-0.147123
H	2.284300	1.818583	0.225638
H	0.521618	-1.581504	2.167941
H	1.555655	0.745649	2.379833
H	2.030769	-2.038105	-1.609325
H	3.217580	0.204100	-1.428551
C	-1.778546	-0.434434	0.181083
O	-1.846183	-0.954723	1.268981
C	-2.976294	-0.041869	-0.612563
H	-3.881624	-0.306185	-0.079656
H	-2.942430	1.024935	-0.824508
H	-2.926662	-0.523133	-1.586355
C	-0.358724	2.310638	0.360671
H	0.314572	2.978294	0.889757

H	-0.619435	2.775545	-0.586825
H	-1.266673	2.181794	0.944480

Energy: -576.450983
Enthalpy: -576.232147

TS for Singelton rearrangement of acetylmethyloxirene/benzene adduct to 7,7-diacetylnorcaradiene; MPWB1K/6-31+G(d,p):

O	0.050846	1.361441	-1.311695
C	-0.223559	1.089740	-0.080631
C	0.423500	-0.240175	-0.056583
C	-1.842592	0.604026	0.340662
C	-0.402819	-1.424575	-0.389256
C	-1.487357	-0.278999	1.434608
C	-0.632315	-1.284509	1.099075
C	-2.325730	-0.123634	-0.851319
C	-1.598391	-1.165943	-1.218771
H	-2.431546	1.468748	0.618968
H	0.197712	-2.285513	-0.647909
H	-1.744036	-0.063241	2.460227
H	-0.139321	-1.946946	1.789389
H	-3.186551	0.232554	-1.392719
H	-1.798222	-1.786568	-2.075739
C	0.157860	2.119950	0.966676
C	1.888284	-0.465324	0.030268
H	0.004422	1.759693	1.980899
H	-0.446071	3.009994	0.812298
H	1.198330	2.408934	0.850009
O	2.272401	-1.451205	0.619105
C	2.817600	0.475493	-0.656973
H	2.508903	1.508543	-0.551100
H	3.822580	0.309935	-0.285775
H	2.780931	0.265688	-1.724350

Energy: -576.446398
Enthalpy: -576.227499

Endo-7-methyl-7-pyruvoylnorcaradiene; MPWB1K/6-31+G(d,p):

O	-0.625319	-0.087932	-1.882714
C	-0.689473	0.241645	-0.728623
C	0.281698	1.162913	-0.066475
C	1.103029	-1.772354	0.769120
C	1.741192	0.854957	-0.151530
C	0.733255	-0.744402	1.550148
C	0.954401	0.649397	1.161004
C	1.902574	-1.572918	-0.416072
C	2.260353	-0.343324	-0.805380
H	0.892434	-2.782806	1.086283
H	2.366916	1.733997	-0.215265
H	0.268387	-0.927294	2.507424
H	1.083832	1.363469	1.961717
H	2.280592	-2.438566	-0.937164
H	2.970273	-0.208291	-1.607100
C	-1.887646	-0.215253	0.110420
O	-2.207165	0.428149	1.076674
C	-2.620189	-1.411465	-0.387579
H	-2.892574	-1.270079	-1.430043

H	-1.956388	-2.273757	-0.354707
H	-3.496297	-1.587639	0.224332
C	-0.137289	2.608519	-0.108856
H	0.607622	3.223353	0.391275
H	-0.228044	2.955897	-1.135651
H	-1.088316	2.743695	0.400150

Energy: -576.526850
Enthalpy: -576.305217

TS for methylpyruvoylcarbene extrusion from *endo*-7-methyl-7-pyruvoylnorcaradiene; MPWB1K/6-31+G(d,p):

O	0.406838	-1.213264	-0.535580
C	1.010250	-0.227037	-0.153259
C	0.794067	0.946906	0.483519
C	-2.838477	-0.960273	-0.770259
C	-1.664384	0.904110	0.913854
C	-2.489856	0.284248	-1.259355
C	-1.912089	1.220877	-0.418066
C	-2.585830	-1.284571	0.554274
C	-1.995001	-0.360988	1.392767
H	-3.291615	-1.688651	-1.424694
H	-1.307544	1.657768	1.599064
H	-2.675931	0.531305	-2.293019
H	-1.677328	2.206273	-0.791334
H	-2.843171	-2.263404	0.927850
H	-1.798375	-0.609509	2.424133
C	2.607896	-0.370602	-0.118469
O	3.365427	0.478367	-0.489333
C	3.012065	-1.748839	0.284770
H	2.608817	-1.971907	1.269418
H	2.574191	-2.463957	-0.404513
H	4.093344	-1.816134	0.284690
C	1.113415	2.318998	0.158859
H	0.897209	3.022674	0.956893
H	2.205337	2.265531	0.034155
H	0.724604	2.672207	-0.795148

Energy: -576.439078
Enthalpy: -576.221828

Benzene; MPWB1K/6-31+G(d,p):

C	0.000000	1.385234	0.000000
C	1.199648	0.692617	0.000000
C	1.199648	-0.692617	0.000000
C	0.000000	-1.385234	0.000000
C	-1.199648	-0.692617	0.000000
C	-1.199648	0.692617	0.000000
H	0.000000	2.464214	0.000000
H	2.134072	1.232107	0.000000
H	2.134072	-1.232107	0.000000
H	0.000000	-2.464214	0.000000
H	-2.134072	-1.232107	0.000000
H	-2.134072	1.232107	0.000000

Energy: -232.137687

Enthalpy: -232.029118

Acetylmethyloxirene (**2**); MPWB1K/6-31+G(d,p):

C	-0.093931	0.050009	-0.000465
C	-1.375514	-0.025136	-0.000102
C	1.303967	0.334246	-0.000063
O	-0.938227	-1.303077	-0.000168
O	1.693365	1.484327	-0.000042
C	-2.725161	0.515630	0.000268
C	2.208308	-0.855667	0.000283
H	-3.252640	0.150030	-0.877876
H	-3.252124	0.150073	0.878742
H	-2.708799	1.598514	0.000238
H	3.237287	-0.516684	0.000867
H	2.014104	-1.473338	0.874420
H	2.015049	-1.473082	-0.874244

Energy: -344.308035
Enthalpy: -344.199534

Diacetylcarbene C_2 (**3**); MPWB1K/6-31+G(d,p):

C	.000000	.000000	.820634
C	.725280	.993739	.120581
C	-.725280	-.993739	.120581
C	-2.130500	-.877262	-.330209
C	2.130500	.877262	-.330209
H	-2.786928	-.942907	.534624
H	2.786928	.942907	.534624
H	-2.299405	.088689	-.800033
H	2.299405	-.088689	-.800033
H	2.353236	1.687333	-1.016007
H	-2.353236	-1.687333	-1.016007
O	.000000	1.973775	.009660
O	.000000	-1.973775	.009660

Energy: -344.308822
Enthalpy: -344.201722

Diacetylcarbene C_1 (**3**); MPWB1K/6-31+G(d,p):

C	2.005103	0.889789	0.337215
C	-0.033409	-0.104585	-0.785952
C	1.216902	-0.292872	-0.105542
C	-1.222140	0.149825	-0.125662
O	-1.128880	1.384724	-0.091456
C	-2.334928	-0.690249	0.345137
O	1.560414	-1.453502	0.013481
H	2.433233	1.380751	-0.533695
H	2.799891	0.554112	0.993990
H	1.362219	1.612511	0.833716
H	-2.991907	-0.101482	0.975594
H	-1.955113	-1.555708	0.881021
H	-2.889762	-1.051405	-0.518005

Energy: -344.308969
Enthalpy: -344.200815

Diacetylcarbene C_2 (**3**); B3LYP/6-31+G(d,p):

C	0.000000	0.000000	0.732237
C	0.741187	1.027471	0.104874
C	-0.741187	-1.027471	0.104874
C	-2.179872	-0.959970	-0.301010
C	2.179872	0.959970	-0.301010
H	-2.810413	-1.024347	0.592933
H	2.810413	1.024347	0.592933
H	-2.399133	-0.007403	-0.793929
H	2.399133	0.007403	-0.793929
H	2.406007	1.799993	-0.962034
H	-2.406007	-1.799993	-0.962034
O	0.000000	2.024166	0.017892
O	0.000000	-2.024166	0.017892

Energy: -344.498305
Enthalpy: -344.392847

Diacetylcarbene C_2 (**3**); O3LYP/6-31+G(d,p):

C	.000000	.000000	.669397
C	.754803	1.036518	.092799
C	-.754803	-1.036518	.092799
C	-2.198821	-1.001944	-.293456
C	2.198821	1.001944	-.293456
H	-2.815027	-1.071800	.609624
H	2.815027	1.071800	.609624
H	-2.447879	-.061181	-.792750
H	2.447879	.061181	-.792750
H	2.419861	1.853271	-.940975
H	-2.419861	-1.853271	-.940975
O	.000000	2.029497	.039982
O	.000000	-2.029497	.039982

Energy: -344.384449
Enthalpy: -344.279016

Diacetylcarbene C_2 (**3**); CCSD(T)/cc-pVTZ//CCSD/cc-pVDZ:

C	0.000000	0.000000	0.929478
C	0.712105	0.992870	0.130345
C	-0.712105	-0.992870	0.130345
C	-2.133702	-0.805783	-0.326046
C	2.133702	0.805783	-0.326046
H	-2.390152	-1.581599	-1.065002
H	2.390152	1.581599	-1.065002
H	-2.804146	-0.887240	0.547791
H	2.804146	0.887240	0.547791
H	2.256424	-0.204958	-0.753570
H	-2.256424	0.204958	-0.753570
O	0.000000	1.980535	-0.042931
O	0.000000	-1.980535	-0.042931

CCSD(T) Energy: -343.906259
CCSD Energy: -343.527674
CCSD Enthalpy: -343.424154

TS between diacetylcarbene (**3**) and acetylmethylketene (**4**) MPWB1K/6-31+G(d,p):

C	-1.884555	1.038712	-0.102063
C	-0.006472	-0.107353	0.748501
C	-1.241636	-0.315839	0.093570
C	1.210801	0.223316	0.095211
O	1.448608	1.383754	-0.181569
C	2.140771	-0.927027	-0.132169
O	-1.736082	-1.376307	-0.216894
H	-2.682744	1.149027	0.626073
H	-2.298267	1.048782	-1.106521
H	-1.179809	1.861079	0.011543
H	2.611923	-0.789268	-1.100609
H	1.629127	-1.886552	-0.100663
H	2.906105	-0.913488	0.639582

Energy: -344.30474
Enthalpy: -344.198210

Acetylmethylketene (**4**) MPWB1K/6-31+G(d,p):

C	0.298994	1.989959	0.025548
C	0.280253	0.490095	0.001370
C	1.395526	-0.212991	-0.007204
C	-1.010643	-0.203491	-0.016025
O	-2.029023	0.449316	-0.035879
C	-1.037859	-1.703534	0.027318
O	2.371801	-0.828179	-0.018794
H	-0.278104	2.368710	-0.813066
H	1.307662	2.385249	-0.033182
H	-0.167525	2.351855	0.937617
H	-0.929690	-2.033766	1.058951
H	-0.236737	-2.152653	-0.554777
H	-1.995456	-2.048718	-0.344203

Energy: -344.413428
Enthalpy: -344.302663

TS between acetylmethyloxirene (**2**) and methylpyruvoylcarbene (**13**) MPWB1K/6-31+G(d,p):

C	-2.311126	-0.573906	0.148662
C	-1.180456	0.378797	-0.008275
O	-1.280781	1.576854	-0.062454
C	0.171050	-0.248092	-0.088826
O	0.473397	-1.498975	-0.093172
C	1.398045	0.165462	-0.279701
C	2.744016	0.360933	0.185289
H	-2.154134	-1.189421	1.032408
H	-2.330638	-1.256525	-0.698885
H	-3.244902	-0.030812	0.222690
H	3.494590	0.085258	-0.550172
H	2.922996	-0.163778	1.124064
H	2.841989	1.433079	0.372012

Energy: -344.289704
Enthalpy: -344.182902

Methylpyruvoylcarbene (**13**) MPWB1K/6-31+G(d,p):

O	-0.205586	1.813770	-0.232936
C	0.163116	0.690500	0.069102
C	1.399760	0.296277	0.589998
C	-0.841624	-0.487713	0.011013
O	-0.441087	-1.614376	-0.130066
C	-2.271515	-0.088850	0.069636
H	-2.490559	0.294680	1.064908
H	-2.454068	0.727708	-0.622582
H	-2.898496	-0.945091	-0.146856
C	2.423362	-0.361821	-0.147369
H	3.373002	-0.488958	0.358911
H	1.882813	-1.339668	-0.095682
H	2.522105	-0.134185	-1.208964

Energy: -344.297414
Enthalpy: -344.190692

Methylpyruvoylcarbene (**13**) CCSD(T)/cc-pVTZ//CCSD/cc-pVDZ:

O	-0.040745	1.786888	0.078237
C	-0.197460	0.593737	-0.159360
C	-1.461888	0.075639	-0.678427
C	0.938201	-0.440990	-0.037593
O	0.641349	-1.623198	-0.058053
C	2.335469	0.104281	0.139609
H	2.633050	0.644903	-0.777017
H	2.348640	0.837989	0.963150
H	3.035025	-0.722145	0.336163
C	-2.435940	-0.381345	0.331702
H	-3.470648	-0.459970	-0.037114
H	-2.040756	-1.423756	0.452788
H	-2.380436	0.105532	1.324976

CCSD(T) Energy: -343.892344

TS for acetyl migration in methylpyruvoylcarbene; CCSD(T)/cc-pVTZ//CCSD/cc-pVDZ:

O	-0.341458	1.829568	-0.439652
C	0.176548	0.814402	-0.002251
C	1.311918	0.380165	0.716215
C	-0.750980	-0.524299	-0.031488
O	-0.359680	-1.595999	-0.433886
C	-2.186149	-0.210832	0.344056
H	-2.217365	0.131864	1.393965
H	-2.556631	0.611937	-0.288500
H	-2.798312	-1.116772	0.213410
C	2.359574	-0.388981	0.010623
H	3.225169	-0.633814	0.646676
H	1.820316	-1.335636	-0.242094
H	2.670466	0.051135	-0.958080

CCSD(T) Energy: -343.893324

TS connecting methylpyruvoylcarbene and diacetylcarbene; CCSD(T)/cc-pVTZ//CCSD/cc-pVDZ:

C	-2.331999	-0.653862	0.140962
C	-1.230736	0.372879	-0.003999

O	-1.395658	1.576037	-0.062271
C	0.157318	-0.196298	-0.072061
O	0.575825	-1.458154	-0.106914
C	1.405411	0.186641	-0.235852
C	2.806636	0.373909	0.169288
H	-2.152325	-1.265356	1.043569
H	-2.306457	-1.342458	-0.722705
H	-3.307816	-0.149979	0.204356
H	3.508693	0.047711	-0.616358
H	3.011148	-0.185140	1.101036
H	2.965646	1.452546	0.353555

CCSD(T) Energy: -343.891645

TS connecting methylpyruvoylcarbene and dimethylcyclopropenone epoxide; CCSD(T)/cc-pVTZ//CCSD/cc-pVDZ:

O	-0.251701	2.066174	0.000000
C	0.000000	0.860185	0.000000
C	1.080369	-0.029910	0.000000
C	-0.912489	-0.386351	0.000000
O	-0.045972	-1.304523	0.000000
C	-2.377051	-0.610475	0.000000
H	-2.798054	-0.102476	0.886210
H	-2.798054	-0.102476	-0.886210
H	-2.630281	-1.681442	0.000000
C	2.522330	-0.341586	0.000000
H	2.845518	-0.897611	0.900594
H	2.845518	-0.897611	-0.900594
H	3.037778	0.637241	0.000000

CCSD(T) Energy: -343.889812

Dimethylcyclopropenone epoxide (**17**): CCSD(T)/cc-pVTZ//CCSD/cc-pVDZ:

C	-0.279140	0.969121	1.806719
C	-0.279140	0.969121	-1.806719
C	-0.279140	-0.123389	0.787444
C	-0.279140	-0.123389	-0.787444
C	0.750976	-0.825088	0.000000
O	-1.428088	-0.436805	0.000000
O	1.913941	-1.143980	0.000000
H	-0.859770	1.833529	1.438904
H	-0.859770	1.833529	-1.438904
H	-0.744228	0.613548	2.742949
H	-0.744228	0.613548	-2.742949
H	0.757334	1.276934	2.026361
H	0.757334	1.276934	-2.026361

CCSD(T) Energy: -343.915479
CCSD Energy: -343.531417
CCSD Enthalpy: -343.424715

1. MOLPRO, version 2006.1, Werner, H.-J.; Knowles, P. J.; Lindh, R.; Manby, F. R.; Schütz, M.; Celani, P.; Korona, T.; Rauhut, G.; Amos, R. D.; Bernhardsson, A.; Berning, A.; Cooper, D. L.; Deegan, M. J. O.; Dobbyn, A. J.; Eckert, F.; Hampel, C.; Hetzer, G.; Lloyd, A. W.; McNicholas, S. J.; Meyer, W.; Mura, M. E.; Nicklass, A.; Palmieri, P.; Pitzer, R.; Schumann, U.; Stoll, H.; Stone, A. J.; Tarroni, R.; Thorsteinsson T., see http://www.molpro.net.

11b. *Gaussian 03* (Revision B.04); Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, J. A.; Vreven, Jr., T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai,

H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A. Gaussian, Inc., Pittsburgh PA, 2003.