Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Effect of Conformational Rigidity on the Stereoselectivity of Nucleophilic Additions to Five-membered Ring Bicyclic Oxocarbenium Ion Intermediates.

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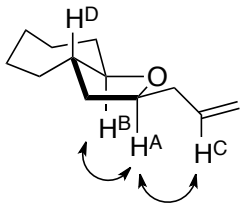
Table of Contents

Stereochemical Proof of Allyl Products

The stereochemistry of **20** was determined by analysis of nOe data: Relevant DPFGSE-nOe data (mixing time 0.5 s): (the peaks in the ^{1}H NMR spectra were assigned using ^{1}H NMR chemical shifts, ^{13}C NMR chemical shifts, COSY, and HSQC)



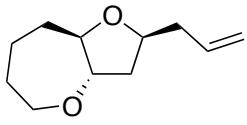
20

H^{A} irradiated: H^{B} (0.4%) H^{C} (0.2%)

H^{B} irradiated: H^{A} (0.8%)

Note: There was no nOe observed between H^{A} and H^{D}

Stereochemical Proof of Allyl Product 21 by ^{13}C NMR Prediction



21

Stereochemistry of **21** was assigned by ^{13}C NMR prediction. Gas phase low energy conformers of **21**-*cis* and **21**-*trans* diastereomers were located using conformational search option in Spartan'10[1] software package at PM3 level of theory. Conformers were further optimized using B3LYP/6-31G** method[2] in Gaussian09.[3] Polarizable Continuum Model[4] (PCM) was used to introduce benzene as an implicit solvent with the use of *SCRF=(Solvent=Benzene)* keywords. NMR shielding tensor calculations were done at the same level of theory employing *giao* command. Shielding constants were first Boltzmann averaged and the averages were used to calculate the chemical shifts according to the procedure described by Smith et al.[5] Cartesian

coordinates for the optimized geometries of the lowest energy conformations and diagnostic chemical shifts, both experimental and theoretical, are reported below.

References:

1. *Spartan'10*, Wavefunction, Inc. Irvine, CA.
2. Gaussian 09, Revision B.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2009.
3. (a) Becke, A. D. *J. Chem. Phys.* **1993**, *98,* 1372–1377. (b) Becke, A. D. *J. Chem. Phys.* **1993**, *98,* 5648–5652. (c) Lee, C.; Yang, W.; Parr, R. G. *Phys. Rev. B* **1988**, *37,* 785–789. (d) Stephens, P. J.; Devlin, F. J.; Chabalowski, C. F.; Frisch, M. J. *J. Phys. Chem.* **1994**, *98,* 11623–11627.
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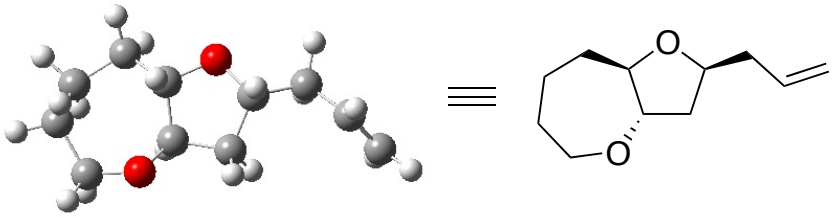

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Sum of electronic and thermal Enthalpies= -580.153010
Sum of electronic and thermal Free Energies= -580.205944

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C	3.13039700	0.93349100	0.59930100
H	3.06108800	0.59765800	1.64208100
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H	4.57854600	-0.50858200	-0.08471900
C	2.74989300	-1.57762400	0.06620500
H	2.82711900	-1.77240200	1.14991400
H	3.21351300	-2.42114200	-0.45489000
O	1.38342000	-1.61260300	-0.33081000
C	0.56603900	-0.62465000	0.28170300
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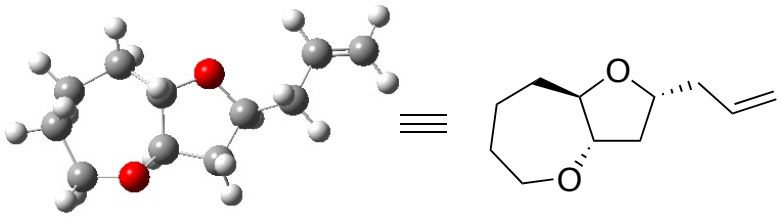
C	0.74301400	0.76284500	-0.37375300
H	0.94968900	0.56395400	-1.43962200
C	-0.92515800	-0.93532400	0.04497100
H	-1.01930800	-1.76629000	-0.65840300
H	-1.42887900	-1.22372200	0.97157200
C	-1.51102100	0.37988100	-0.52483200
H	-1.62061500	0.29001600	-1.61850800
O	-0.53056000	1.39006300	-0.24321400
C	-2.84419500	0.82581900	0.07918600

H	-3.04468500	1.84283500	-0.28496700
H	-2.73834300	0.88693700	1.16858300
C	-3.98558000	-0.08125300	-0.28866600
H	-4.18519300	-0.18665900	-1.35611200
C	-4.74743900	-0.74836100	0.57889900
H	-4.58851900	-0.67408100	1.65223200
H	-5.56231400	-1.38656700	0.25006400

	Calculated chemical shift, ppm	Observed chemical shift, ppm
C-4	83.13	83.75
C-3	78.93	80.60



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Zero-point correction= 0.276558 (Hartree/Particle)
Thermal correction to Energy= 0.289191
Thermal correction to Enthalpy= 0.290136
Thermal correction to Gibbs Free Energy= 0.236391
Sum of electronic and zero-point Energies= -580.166504
Sum of electronic and thermal Energies= -580.153871
Sum of electronic and thermal Enthalpies= -580.152927
Sum of electronic and thermal Free Energies= -580.206672

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C	2.83475000	1.46919400	0.38402600
H	2.95941400	1.20294800	1.44196700
H	3.39653200	2.39987700	0.24733700
C	3.49262700	0.35729300	-0.45670500
H	3.24384500	0.46135000	-1.52020400

H	4.58247000	0.46676400	-0.38316400
C	3.17005000	-1.07056400	0.00711100
H	3.38741200	-1.15486700	1.08574700
H	3.81480400	-1.78315200	-0.51661400
O	1.84502800	-1.52331900	-0.25296400
C	0.82219800	-0.78277800	0.39067000
H	1.08386900	-0.60708400	1.44711900
C	0.51048100	0.54752700	-0.32057400
H	0.65522400	0.35675800	-1.39564400
C	-0.51367800	-1.51674500	0.27996100
H	-0.56442600	-1.98615200	-0.70960900
H	-0.64611300	-2.29514700	1.03538000
C	-1.54321100	-0.38679100	0.39995900
O	-0.87721800	0.80847600	-0.06692200
H	-1.81239300	-0.22749500	1.45487100
C	-2.82928600	-0.60909800	-0.40633200
H	-3.29517100	-1.54700800	-0.07877400
H	-2.53908400	-0.73789300	-1.45881800
C	-3.80756700	0.52617300	-0.28144600
H	-3.42323800	1.50518000	-0.56358700
C	-5.06437800	0.40946600	0.14811100
H	-5.72591100	1.26802400	0.21931700
H	-5.48143000	-0.55175500	0.44107700

	Calculated chemical shift, ppm	Observed chemical shift, ppm
C-4	82.36	81.73
C-3	80.33	81.10

Computational details

1. Conformational Analysis of Oxocarbenium Ions

To locate low energy conformations of oxocarbenium ion intermediates, initial guess structures were generated using semi-empirical PM3 method in Spartan'10.[1] The conformational search was performed several times until an adequate sampling of conformational space was achieved. Conformers within 10 kcal/mol of each other were carried forward for optimization at the higher level of theory. Usually, the number of unique conformations found in the searches would not exceed three structures. The final structures were subjected to optimization using B3LYP[2] hybrid functional in Gaussian G09-B01[3] software package using Pople's[4] 6-31+G** basis set. B3LYP methods have been shown to reproduce successfully experimental geometries in a range of molecules.[5] To better simulate experimental conditions carried out in this work, we used Polarizable Continuum Model (PCM)[6] for introducing dichloromethane as an implicit solvent with the use of *SCRF=(Solvent=Dichloromethane)* keywords. Obtained structures were characterized as local minima by harmonic frequency analysis. All local minima had zero negative frequencies.

2. Transition States Structures for Nucleophilic Additions of Allyltrimethylsilane to Oxocarbenium Ions 26 and 29

Transition states were modeled using geometries of the lowest energy conformations found in the previous search and the optimized structure of allyltrimethylsilane. Both synclinal (60°) and antiperiplanar (180°) torsional angles between the approaching nucleophile and the oxocarbenium ion were considered.[7,8] The nucleophile was oriented such as to minimize the possible steric interactions, and the electrophilic attack was modeled to be anti to the silyl group, in accordance with the previous studies.[9] Several geometries for synclinal and antiperiplanar transition states were considered, but the synclinal transition states where the silyl group is gauche to the oxygen atom were the lowest energy (by up to 1.5 kcal/mol). Starting geometries containing single imaginary

frequency were generated by constraining the distance between the two reactive carbons that form the new bond to 1.8 Å, and allowing for optimization with constrain (using *AddRedundant* option in Gaussian). The resulting structures were next subjected to the transition state search with no constrains imposed. For both optimizations with constrain and the transition state searches, the B3LYP computational method was replaced with M06-2X method for several reasons. Previous computational studies on the addition of allylic silanes to oxocarbenium ions reported failure of B3LYP method to locate transition states.[7] M06-2X has shown accuracy comparable to CCSD methods, but at a lower computational cost,[10] and was recently used to simulate transition states of allyltrimethylsilane additions to propargylic cations.[11] Both optimizations with constrain and transition state search calculations were performed in solvent using *SCRF=(Solvent=Dichloromethane)* keywords. Because energies calculated in solvent medium are temperature dependent, relative energies were computed both at T=273 K, and T=195 K. Due to pseudorotation, seven-membered rings exhibit low frequency modes. To achieve satisfactory convergence and reliable imaginary frequencies, the integration grid was set equal to "*UltraFine*" using a "*Tight"* optimization criteria.[12] Harmonic frequency analysis verified that transition state structures were optimized to the first-order saddle points. Gibbs free energies were calculated as the sums of electronic and thermal free energies, including zero-point correction. Structures reported in the manuscript were visualized using GaussView5[13] software.

References:

1. *Spartan'10*, Wavefunction, Inc. Irvine, CA.

2. (a) Becke, A. D. *J. Chem. Phys.* **1993**, *98,* 1372–1377. (b) Becke, A. D. *J. Chem. Phys.* **1993**, *98,* 5648–5652. (c) Lee, C.; Yang, W.; Parr, R. G. *Phys. Rev. B* **1988**, *37,* 785–789. (d) Stephens, P. J.; Devlin, F. J.; Chabalowski, C. F.; Frisch, M. J. *J. Phys. Chem.* **1994**, *98,* 11623–11627.

3. Gaussian 09, Revision B.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov,

A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2009.

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11. Nitsch, D.; Huber, S. M.; Pothig, A.; Narayanan, A.; Olah, G. A.; Prakash, G. K.; Bach, T. *J. Am. Chem. Soc.* **2014**, *136*, 2851–2857.
12. Æ. Fisher, G. W. Frisch, G. W. Trucks, Gaussian 03 User's Reference, Gaussian, Inc., Pittsburgh, PA, 2003.
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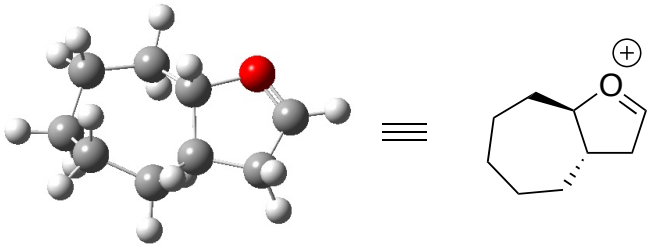
1. Low Energy Conformers of Oxocarbenium Ions using PCM(CH_2Cl_2)-M062X/631+G method**



26

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Number of imaginary frequencies = 0

Zero-point correction= 0.233740 (Hartree/Particle)
Thermal correction to Energy= 0.242379
Thermal correction to Enthalpy= 0.243323
Thermal correction to Gibbs Free Energy= 0.200551
Sum of electronic and zero-point Energies= -425.463922
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C	-2.36805600	0.07818400	0.44058200
H	-3.45953100	0.09367800	0.41741300
H	-2.08425800	0.25368800	1.48300700
C	-1.85477000	1.20930800	-0.46441900
H	-2.55344400	2.04726500	-0.43296300
H	-1.86628200	0.84988100	-1.49781400
C	-0.45724100	1.75717400	-0.13237100
H	-0.04183100	2.23926400	-1.02103100
H	-0.53201200	2.52529600	0.63990500
C	0.52518900	0.69752800	0.36991400
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C	0.44954700	-0.61527200	-0.39851100
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C	2.00720900	1.09373500	0.27750600
H	2.22704100	1.72204500	-0.59703000
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O	1.89628500	-1.13884300	-0.30715800
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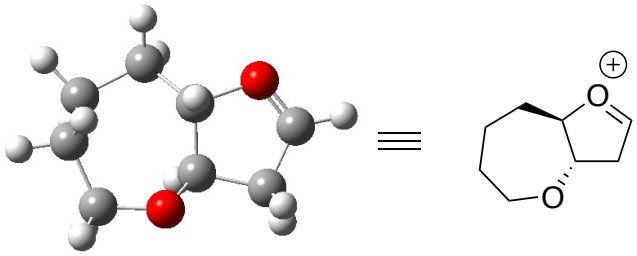

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H	-0.03009200	2.19238800	1.01060200
C	1.82430500	1.19991600	0.47475200
H	1.83411600	0.88492600	1.52083400
H	2.53037900	2.02697700	0.39985000
C	2.32600600	0.02927400	-0.38716800
H	2.12719300	0.19685400	-1.44915000
H	3.41284400	-0.02155700	-0.28382300
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H	1.97488700	-1.49809400	1.10175400
H	2.33787600	-2.12775900	-0.51792900
O	0.41910900	-1.60132000	-0.26635100
C	-0.44551600	-0.68027000	0.36183600
H	-0.16465300	-0.52918500	1.41034400
C	-0.45450200	0.64955800	-0.39874900

H	-0.32507800	0.46054100	-1.46468300
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H	-2.03121500	-1.79238300	-0.62307500
H	-2.28039600	-1.70360400	1.12356300
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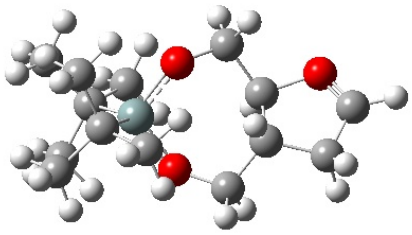

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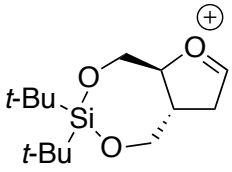

S1

(oxocarbenium ion intermediate resulting from acetate 6)

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Zero-point correction= 0.395897 (Hartree/Particle)
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Thermal correction to Enthalpy= 0.418209
Thermal correction to Gibbs Free Energy= 0.347380
Sum of electronic and zero-point Energies= -1064.455314
Sum of electronic and thermal Energies= -1064.433945
Sum of electronic and thermal Enthalpies= -1064.433001
Sum of electronic and thermal Free Energies= -1064.503830

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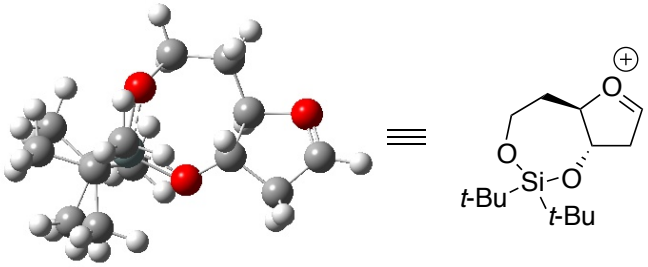
C	2.29224000	0.64230700	0.43794300
C	2.25778100	-0.68192700	-0.33834300
O	3.69873900	-0.87705100	-0.77990000
C	4.45777200	-0.07112000	-0.17893400
H	4.07821600	0.51982200	1.77469600
H	1.96756500	1.44678200	-0.22760000
H	2.07899700	-1.54928800	0.30044200
H	5.52222900	-0.14093500	-0.39865400
C	1.37558700	0.59237500	1.67010300
H	1.26773900	1.59886400	2.08925100

H	1.83003600	-0.04569500	2.43739900
C	1.38220000	-0.69204800	-1.59779000
H	1.25534400	-1.71780300	-1.95880000
H	1.88457600	-0.11147000	-2.37989800
O	0.10290200	0.04019400	1.37518100
Si	-0.87348000	0.00305900	0.00763200
O	0.13422700	-0.08338100	-1.34440100
C	-1.80991000	1.65481800	-0.25338100
C	-0.80591200	2.82200600	-0.09529100
H	-0.37806300	2.86555300	0.91195200
H	-1.32186500	3.77593100	-0.26863400
H	0.01282500	2.75971900	-0.82035100
C	-2.41915700	1.73118200	-1.67347900
H	-3.16638800	0.95195100	-1.85128200
H	-1.65046400	1.64571800	-2.44782000
H	-2.92017800	2.70014700	-1.80436900
C	-2.93440300	1.83311100	0.79241300
H	-3.72837600	1.08894000	0.67629100
H	-3.39660800	2.82200500	0.66995600
H	-2.55955300	1.77201800	1.82048400
C	-1.87877600	-1.61189000	0.23246300
C	-0.90754600	-2.81239900	0.12537300
H	-1.45994700	-3.74736400	0.28958300
H	-0.11489300	-2.76702100	0.88026000
H	-0.44505600	-2.88315900	-0.86487100
C	-2.55022200	-1.65848600	1.62540200
H	-3.08318800	-2.61204800	1.74241900
H	-3.28232400	-0.85738900	1.76343000
H	-1.81372400	-1.58656100	2.43175900
C	-2.96306000	-1.76201800	-0.85940400
H	-3.46166100	-2.73477300	-0.75136100
H	-2.54296700	-1.71985900	-1.87078100
H	-3.73732700	-0.99224300	-0.78182200



S2

(oxocarbenium ion intermediate resulting from acetate 7)

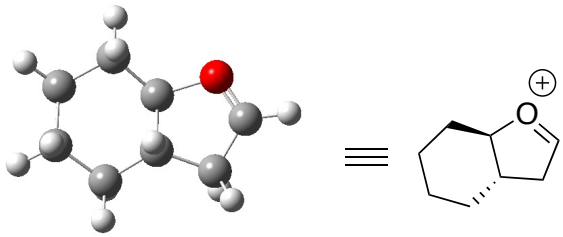
#p b3lyp/6-31+g(d,p) opt freq scrf=(solvent=dichloromethane)
Number of imaginary frequencies = 0

Zero-point correction= 0.395921 (Hartree/Particle)
Thermal correction to Energy= 0.417022
Thermal correction to Enthalpy= 0.417966
Thermal correction to Gibbs Free Energy= 0.347911
Sum of electronic and zero-point Energies= -1064.460753
Sum of electronic and thermal Energies= -1064.439652
Sum of electronic and thermal Enthalpies= -1064.438708
Sum of electronic and thermal Free Energies= -1064.508763

1 1

H	-2.80743600	1.99547800	-1.92423600
C	-2.78888000	0.95485800	-1.58969000
C	-1.78313600	0.60929300	-0.47003200
C	-2.49638400	-0.53731400	0.28171900
O	-3.96553500	-0.22454000	0.00775600
C	-4.06466200	0.53388300	-0.99612100
H	-2.61899600	0.33114400	-2.48467000
H	-1.69836500	1.47316400	0.20005800
H	-5.07240200	0.78849700	-1.32217000
H	-2.34850900	-1.48883900	-0.23807200
C	-2.26698000	-0.65601600	1.77152300
H	-2.96911000	-1.38316100	2.19370800
H	-2.43774500	0.30982600	2.25848400
O	-0.53277800	0.21166600	-0.95993400
Si	0.81025700	0.00433700	0.08170500
O	0.16228100	-0.24169200	1.60895900
C	-0.83966600	-1.14799500	2.06880300
H	-0.72522100	-1.23104600	3.15267200
H	-0.69008800	-2.14730600	1.64419900
C	1.72897700	-1.54188500	-0.58912000
C	2.61402800	-1.19336400	-1.80924500
H	3.41926200	-0.49735700	-1.55617200
H	2.03375400	-0.75933000	-2.63116300
H	3.08515500	-2.10964900	-2.18944700
C	0.70854500	-2.61760600	-1.03716500
H	0.04499500	-2.25115000	-1.82584500
H	0.08817800	-2.97950500	-0.21052900
H	1.25073800	-3.48779600	-1.43088600
C	2.61884100	-2.14677600	0.52468900
H	3.39700200	-1.45550100	0.86234500
H	3.12277500	-3.04458800	0.14252700
H	2.03438700	-2.44510800	1.40143400

C	1.76292800	1.66098000	0.22099700
C	2.01114000	2.26512100	-1.18183700
H	2.50929700	3.23826300	-1.07710000
H	1.07392800	2.42996700	-1.72405300
H	2.65382900	1.63646300	-1.80414200
C	3.11611200	1.46529800	0.94380200
H	3.61372000	2.43750200	1.06042100
H	3.79872700	0.81843200	0.38376100
H	2.98870500	1.03975200	1.94530500
C	0.92040500	2.67212000	1.03724000
H	1.47776000	3.61383800	1.13166800
H	0.70174500	2.30699700	2.04451100
H	-0.02904000	2.91322500	0.54590900



S3

(oxocarbenium ion intermediate leading to allylated product 3)

#p mp2/6-31+g(d,p) opt freq scrf=(solvent=dichloromethane)
Number of imaginary frequencies = 0

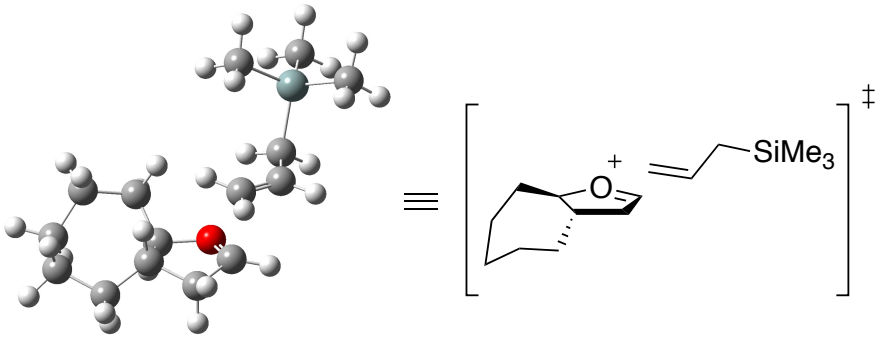
Zero-point correction= 0.204087 (Hartree/Particle)
Thermal correction to Energy= 0.211473
Thermal correction to Enthalpy= 0.212418
Thermal correction to Gibbs Free Energy= 0.172572
Sum of electronic and zero-point Energies= -386.310722
Sum of electronic and thermal Energies= -386.303335
Sum of electronic and thermal Enthalpies= -386.302391
Sum of electronic and thermal Free Energies= -386.342237

1 1

H	-0.83568600	-2.50777700	0.20943900
C	-0.84708300	-1.50484400	-0.21610600
C	-2.14907900	0.72031100	-0.24436600
C	0.31097400	0.73005900	-0.27583500
C	-0.90678300	1.50406100	0.21150900
C	0.26341900	-0.65665600	0.31830500
C	-2.13110000	-0.74887300	0.20302100

H	-2.20858200	0.76499400	-1.33593100
H	0.23485200	0.62664400	-1.36440400
H	-0.88444700	1.59562900	1.30121800
H	0.27485400	-0.64283000	1.41151300
H	-2.22626400	-0.79935800	1.29164500
H	-0.77748300	-1.57725200	-1.30287800
H	-3.04981800	1.20030400	0.14164900
H	-0.91237400	2.51150100	-0.20629900
H	-2.99311200	-1.27193200	-0.21240900
C	1.74559000	1.15782800	0.04387600
H	2.18751500	1.91340500	-0.60340800
H	1.86707300	1.49136300	1.08462300
O	1.68636000	-1.16279300	0.00584900
C	2.43707200	-0.14632800	-0.07942200
H	3.49452800	-0.33569600	-0.22744300

2. Transition States for Nucleophilic Additions of Allyltrimethylsilane to Oxocarbenium Ions 26 and 29 Calculated with PCM(CH_2Cl_2)-M062X/631+G method at 195 K**



S4

(synclinal transition state for the inside attack of the allyltrimethylsilane to oxocarbenium ion 26)

#p M062x/6-31+G opt=(readfc,ts,noeigen) Temperature=195 freq guess=(mix,always) SCRF=(Solvent=Dichloromethane) scf=novaracc SCF=Tight int=grid=ultrafine iop(1/8=5)*

Number of imaginary frequencies = 1

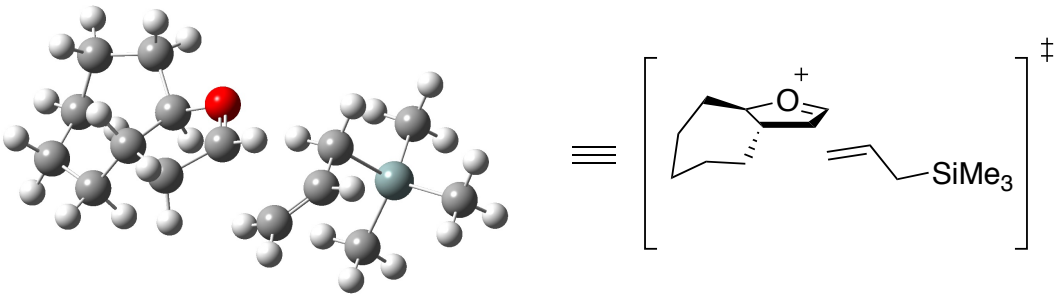
Zero-point correction= 0.415944 (Hartree/Particle)
Thermal correction to Energy= 0.425782
Thermal correction to Enthalpy= 0.426399

Thermal correction to Gibbs Free Energy= 0.388304
Sum of electronic and zero-point Energies= -952.827213
Sum of electronic and thermal Energies= -952.817376
Sum of electronic and thermal Enthalpies= -952.816758
Sum of electronic and thermal Free Energies= -952.854854

1 1

H	-1.47314500	1.90276100	-1.62744900
C	-1.61551500	1.41694500	-0.65699900
H	-0.64661400	1.43088800	-0.14261700
C	-2.65229400	2.18480600	0.18615800
H	-2.42215800	2.05387300	1.25089100
H	-2.51675200	3.25012800	-0.02233600
C	-4.12752500	1.80044900	-0.03715600
H	-4.32524700	1.61363200	-1.10226700
H	-4.74398000	2.66422500	0.23294800
C	-4.60366900	0.61400600	0.81761000
H	-4.33868400	0.81984700	1.86359800
H	-5.69756000	0.56494200	0.78117800
C	-2.53424500	-0.81309000	0.31882100
H	-2.08768000	-0.40933700	1.23696200
C	-2.03167100	-0.02107500	-0.89276500
H	-2.74647700	-0.09616400	-1.71842400
C	-1.96032500	-2.21268600	0.05788500
H	-2.62971400	-2.79712900	-0.59589900
H	-1.75181900	-2.81489700	0.94119100
O	-0.86115000	-0.79429000	-1.39219700
C	-0.76752200	-1.91760600	-0.78559600
H	-0.08707200	-2.64437100	-1.21409000
C	0.67980400	-1.37452500	1.04889500
H	0.43233000	-2.15663200	1.75958500
H	0.20281400	-0.40542700	1.18345900
C	1.70193600	-1.52273900	0.17152300
C	-4.05893200	-0.76457700	0.42936100
H	-4.48763800	-1.07984600	-0.53202500
H	-4.38388700	-1.49929000	1.17465300
H	2.20433700	-2.49046100	0.13447900
C	2.20671300	-0.47754500	-0.73297600
H	2.57230700	-0.90051800	-1.67556400
H	1.44195900	0.27944800	-0.94929100
Si	3.67117100	0.46790200	0.08886300
C	4.36742200	1.62955100	-1.21146200
H	5.18851100	2.22377800	-0.79538000
H	4.75625300	1.07054000	-2.06941300
H	3.59981800	2.32167200	-1.57433700
C	4.96139600	-0.77580100	0.65120900

H	4.56424800	-1.43741900	1.42922000
H	5.30285800	-1.39720300	-0.18413600
H	5.83500300	-0.26026700	1.06527400
C	2.97353700	1.42170300	1.54910900
H	3.75637600	2.02602600	2.02088200
H	2.17180100	2.09829500	1.23069700
H	2.56795800	0.74569900	2.31000800



S5

(synclinal transition state for the outside attack of the allyltrimethylsilane to oxocarbenium ion 26)

#p M062x/6-31+G opt=(readfc,ts,noeigen) Temperature=195 freq guess=(mix,always) SCRF=(Solvent=Dichloromethane) scf=novaracc SCF=Tight int=grid=ultrafine iop(1/8=5)*

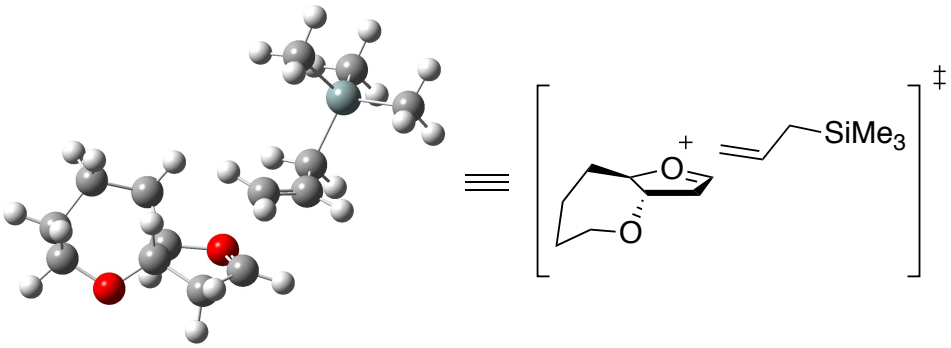
Number of imaginary frequencies = 1

Zero-point correction= 0.416028 (Hartree/Particle)
Thermal correction to Energy= 0.425942
Thermal correction to Enthalpy= 0.426559
Thermal correction to Gibbs Free Energy= 0.388159
Sum of electronic and zero-point Energies= -952.824548
Sum of electronic and thermal Energies= -952.814634
Sum of electronic and thermal Enthalpies= -952.814016
Sum of electronic and thermal Free Energies= -952.852416

1 1

H	1.63208500	1.91395000	-1.66599500
C	2.39897500	1.15341500	-1.48630900
H	2.65262900	0.70912700	-2.45535500
C	3.65455600	1.79172000	-0.86258500
H	4.53930400	1.21306800	-1.15543800
H	3.77761900	2.77989300	-1.31558200
C	3.65484300	1.92531600	0.67191200

H	2.66006600	2.21598100	1.03884100
H	4.32309000	2.75097300	0.93828000
C	4.15881000	0.67359800	1.40913700
H	5.12697600	0.38991100	0.97467900
H	4.35518300	0.93102300	2.45588900
C	2.76573300	-0.95662900	-0.00480000
H	3.62905600	-1.06762000	-0.67284300
C	1.80806800	0.07647000	-0.60149600
H	1.18240800	0.51341000	0.18646400
C	1.94278400	-2.26412600	-0.03274400
H	1.61217800	-2.58816100	0.95645000
H	2.48503400	-3.10588200	-0.47804100
O	0.86074800	-0.73155800	-1.40497000
C	0.80244000	-1.92390800	-0.94475100
H	0.21648000	-2.63284900	-1.51850300
C	-0.85862100	-1.80454300	0.77484300
H	-0.78386900	-2.82878700	1.12782700
H	-0.32283800	-1.04131900	1.33956200
C	3.23291100	-0.54690500	1.39306900
H	2.34384800	-0.35187500	2.01058600
H	3.75400800	-1.39294100	1.85478100
C	-2.02356900	-0.09415700	-0.64714000
H	-1.22587500	0.60518600	-0.36692600
H	-2.17103000	-0.05848700	-1.73326000
C	-1.75131500	-1.46191200	-0.18479200
H	-2.32100700	-2.26225000	-0.65969100
Si	-3.64220000	0.57798300	0.15996000
C	-3.95666300	2.26845400	-0.59361500
H	-4.10344100	2.19647000	-1.67668200
H	-4.85579000	2.72009800	-0.15994600
H	-3.11576800	2.94519100	-0.40697100
C	-5.04680700	-0.60957500	-0.22019400
H	-5.15772200	-0.76171700	-1.29958000
H	-4.88240800	-1.58643900	0.24793300
H	-5.99392700	-0.21233200	0.16144300
C	-3.34654000	0.70207400	2.01004900
H	-2.49106200	1.35099700	2.22961400
H	-4.22523600	1.12287300	2.51137600
H	-3.14881700	-0.28254000	2.44790600



S6

(synclinal transition state for the outside attack of the allyltrimethylsilane to oxocarbenium ion 27)

#p M062x/6-31+G opt=(readfc,ts,noeigen) Temperature=195 freq guess=(mix,always) SCRF=(Solvent=Dichloromethane) scf=novaracc SCF=Tight int=grid=ultrafine iop(1/8=5)*

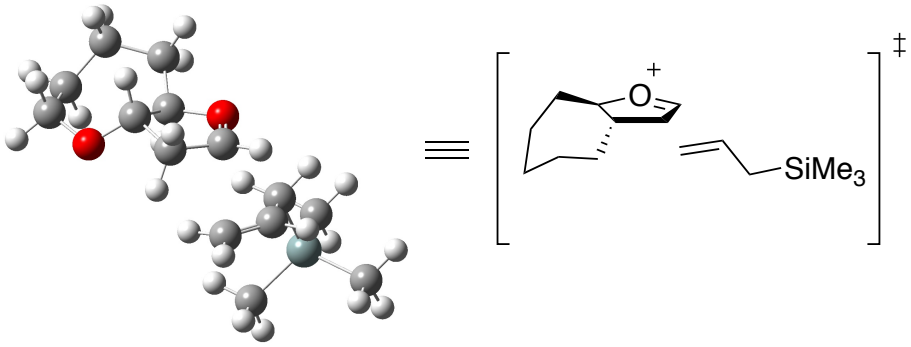
Number of imaginary frequencies = 1

Zero-point correction= 0.392001 (Hartree/Particle)
Thermal correction to Energy= 0.412474
Thermal correction to Enthalpy= 0.413418
Thermal correction to Gibbs Free Energy= 0.341819
Sum of electronic and zero-point Energies= -988.737221
Sum of electronic and thermal Energies= -988.716748
Sum of electronic and thermal Enthalpies= -988.715804
Sum of electronic and thermal Free Energies= -988.787404

1 1

H	-1.64552500	2.01885600	-1.60899700
C	-1.74165500	1.49799400	-0.65197500
H	-0.76872300	1.55521900	-0.15061400
C	-2.81746600	2.16542400	0.23149000
H	-2.54229400	2.05329400	1.28758800
H	-2.79670800	3.23919900	0.02682700
C	-4.25573800	1.64470100	0.05010100
H	-4.50611600	1.51742600	-1.01079800
H	-4.94202000	2.40730500	0.43537400
C	-4.58553700	0.36409100	0.82205500
H	-4.29944600	0.48629500	1.87732700
H	-5.65768900	0.16495800	0.77689700
C	-2.58232400	-0.77450600	0.28938400
H	-2.19487400	-0.36562600	1.23407400
C	-2.08662100	0.04757500	-0.91443800
H	-2.81289000	-0.05837600	-1.72553400
C	-1.98491700	-2.15565300	0.01919700

H	-2.66225900	-2.72043200	-0.64262900
H	-1.77190200	-2.76893400	0.89283300
O	-0.89650300	-0.68939500	-1.39722400
C	-0.79731500	-1.82239000	-0.81180900
H	-0.08343300	-2.52473700	-1.22553800
C	0.63435400	-1.26241700	1.11319800
H	0.37935600	-2.06339600	1.80008200
H	0.16826100	-0.29180800	1.28035100
C	1.63656000	-1.40069000	0.21382000
H	2.12085700	-2.37572000	0.13661700
C	2.15114000	-0.33545500	-0.66413200
H	2.40835300	-0.72349200	-1.65741900
H	1.43291000	0.48684900	-0.77422600
Si	3.75664600	0.42736000	0.07777400
C	4.40035400	1.66905200	-1.17485900
H	5.30994000	2.15351000	-0.80295200
H	4.64254400	1.17973300	-2.12443900
H	3.65847700	2.45020000	-1.37291400
C	5.00075100	-0.94995400	0.36895400
H	4.64350200	-1.65826900	1.12479600
H	5.19964600	-1.50630100	-0.55380700
H	5.95155600	-0.53626700	0.72283700
C	3.29300000	1.26499800	1.69328000
H	4.16690100	1.75404100	2.13778400
H	2.52406000	2.02962200	1.53448400
H	2.90805300	0.54032200	2.41924100
O	-3.97988400	-0.82849500	0.31826300



S7

(synclinal transition state for the outside attack of the allyltrimethylsilane to oxocarbenium ion 27)

#p M062x/6-31+G opt=(readfc,ts,noeigen) Temperature=195 freq guess=(mix,always) SCRF=(Solvent=Dichloromethane) scf=novaracc SCF=Tight int=grid=ultrafine iop(1/8=5)*

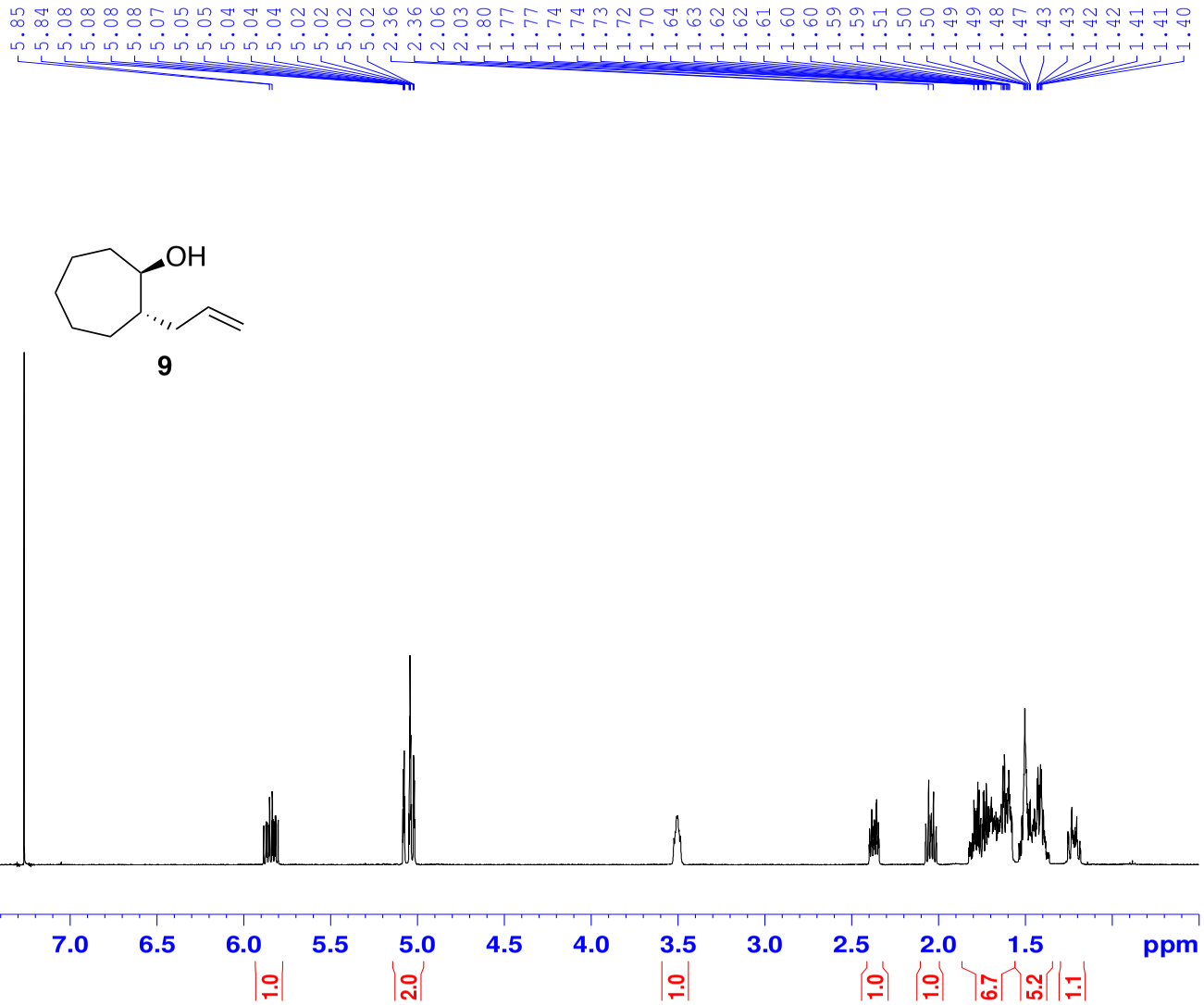
Number of imaginary frequencies = 1

Zero-point correction= 0.392021 (Hartree/Particle)
Thermal correction to Energy= 0.412558
Thermal correction to Enthalpy= 0.413503
Thermal correction to Gibbs Free Energy= 0.341579
Sum of electronic and zero-point Energies= -988.735062
Sum of electronic and thermal Energies= -988.714524
Sum of electronic and thermal Enthalpies= -988.713580
Sum of electronic and thermal Free Energies= -988.785503

1 1

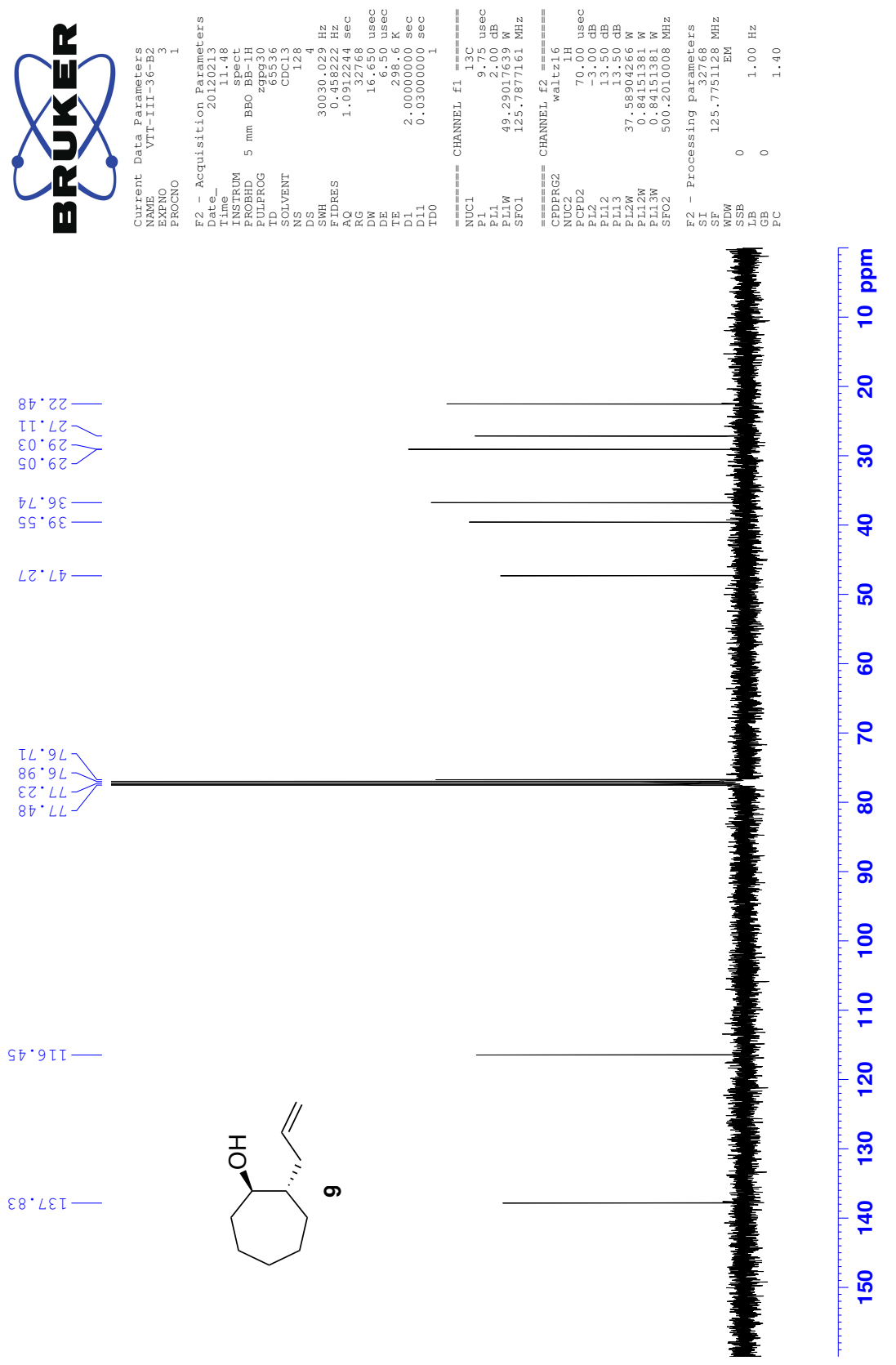
H	1.65357800	2.04792400	-1.55382800
C	2.40999200	1.26886800	-1.42081800
H	2.66441300	0.88288800	-2.41378400
C	3.67310100	1.84239300	-0.74343300
H	4.55756800	1.30763900	-1.11032100
H	3.78777100	2.87787900	-1.07499400
C	3.69090800	1.80098800	0.79586700
H	2.73049100	2.12313100	1.21841600
H	4.43496400	2.52618700	1.14446400
C	4.10648800	0.45825000	1.40394900
H	5.04936100	0.12404500	0.94591200
H	4.26522400	0.56647700	2.47840100
C	2.79644300	-0.89455400	-0.03166500
H	3.69350000	-0.96041500	-0.66414800
C	1.81859900	0.14996800	-0.59310600
H	1.20959100	0.53205100	0.23404100
C	1.99823100	-2.20684100	-0.09605600
H	1.67783600	-2.52533800	0.89824200
H	2.54991800	-3.03900900	-0.54597200
O	0.88199800	-0.64917700	-1.40954300
C	0.86011600	-1.85652400	-0.99822200
H	0.25082700	-2.55212400	-1.56374300
C	-0.84754300	-1.81031600	0.82004200
H	-0.75639500	-2.84631200	1.13406600
H	-0.31601200	-1.06175300	1.40774200
C	-1.99736200	-0.06652200	-0.57744100
H	-1.22622300	0.63493000	-0.23430600
H	-2.08214000	0.00319500	-1.66919000
C	-1.71629200	-1.44914600	-0.15005000
H	-2.26854900	-2.23948300	-0.66128500

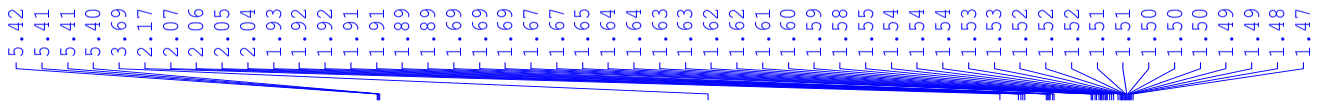
Si	-3.66924600	0.54925800	0.15226200
C	-3.96845400	2.26697000	-0.54605900
H	-4.04208500	2.24145400	-1.63873300
H	-4.90323800	2.68343000	-0.15455600
H	-3.15586800	2.94970100	-0.27469800
C	-5.03099600	-0.63648100	-0.36790500
H	-5.07154200	-0.74058000	-1.45789600
H	-4.88345200	-1.63195500	0.06533800
H	-6.00558600	-0.26718300	-0.02960700
C	-3.50120600	0.59675800	2.02204000
H	-2.68044800	1.25517700	2.32817800
H	-4.42251800	0.97192900	2.48132000
H	-3.30535900	-0.40203600	2.42743700
O	3.14446000	-0.59261300	1.29066400

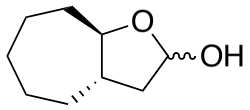


BRUKER

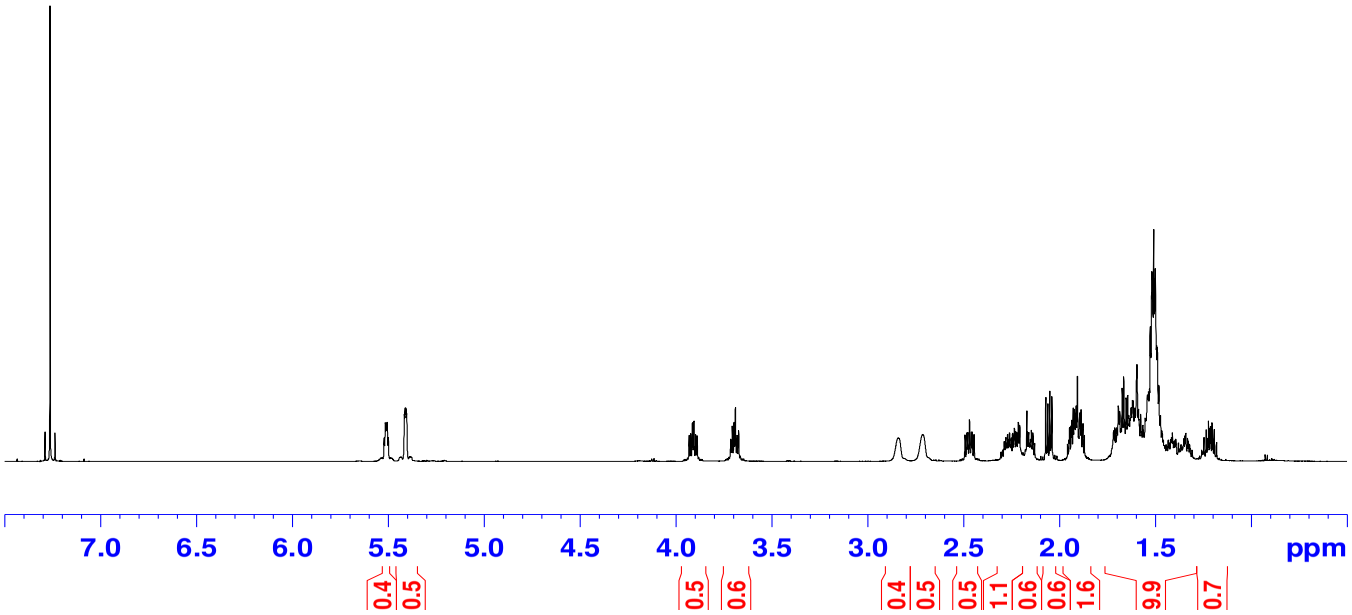
```
Current Data Parameters
NAME       VTT-III-36-B2
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20120213
Time               11.46
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH            10330.578 Hz
FIDRES          0.157632 Hz
AQ             3.1719923 sec
RG                 228.1
DW                48.400 usec
DE                 6.50 usec
TE                298.2 K
D1            2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 9.20 usec
PL1               -3.00 dB
PL1W        37.58904266 W
SFO1        500.2020889 MHz

F2 - Processing parameters
SI                 32768
SF          500.1990130 MHz
WDW                   no
SSB        0
LB         0 Hz
GB         0
PC                 1.00
```


Current Data Parameters
NAME VTT-III-36-B2
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120213
Time_ 11.48
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912244 sec
RG 32768
DW 16.650 usec
DE 6.50 usec
TE 298.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.75 usec
PL1 2.00 dB
PL1W 49.29017639 W
SFO1 125.7877161 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL2 -3.00 dB
PL12 13.50 dB
PL13 13.50 dB
PL2W 37.58904266 W
PL12W 0.84151381 W
PL13W 0.84151381 W
SFO2 500.2010008 MHz
F2 - Processing parameters
SI 32768
SF 125.7751128 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
22.48
27.11
29.03
29.05
36.74
39.55
47.27
76.71
76.98
77.23
77.48
116.45
137.83
OH
9
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10 ppm

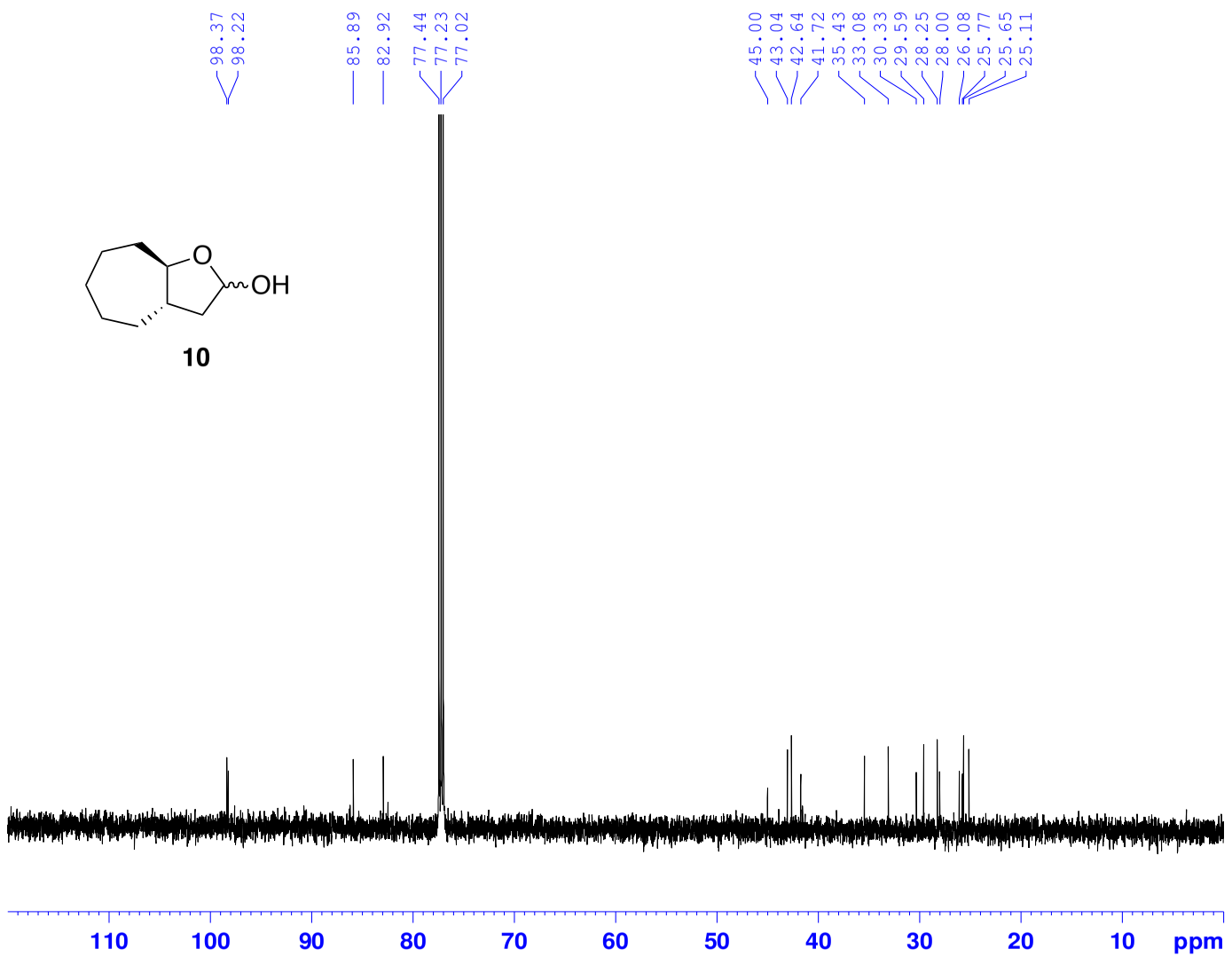




10




```
Current Data Parameters
NAME         VTT-III-39-A
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20120208
Time               13.03
INSTRUM            spect
PROBHD   5 mm PAQXI 1H/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH            12335.526 Hz
FIDRES          0.188225 Hz
AQ             2.6564426 sec
RG                113.19
DW                40.533 usec
DE                 6.50 usec
TE                298.1 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                  9.79 usec
PLW1          9.30000019 W
SFO1        600.1937064 MHz

F2 - Processing parameters
SI                 65536
SF           600.1900131 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```



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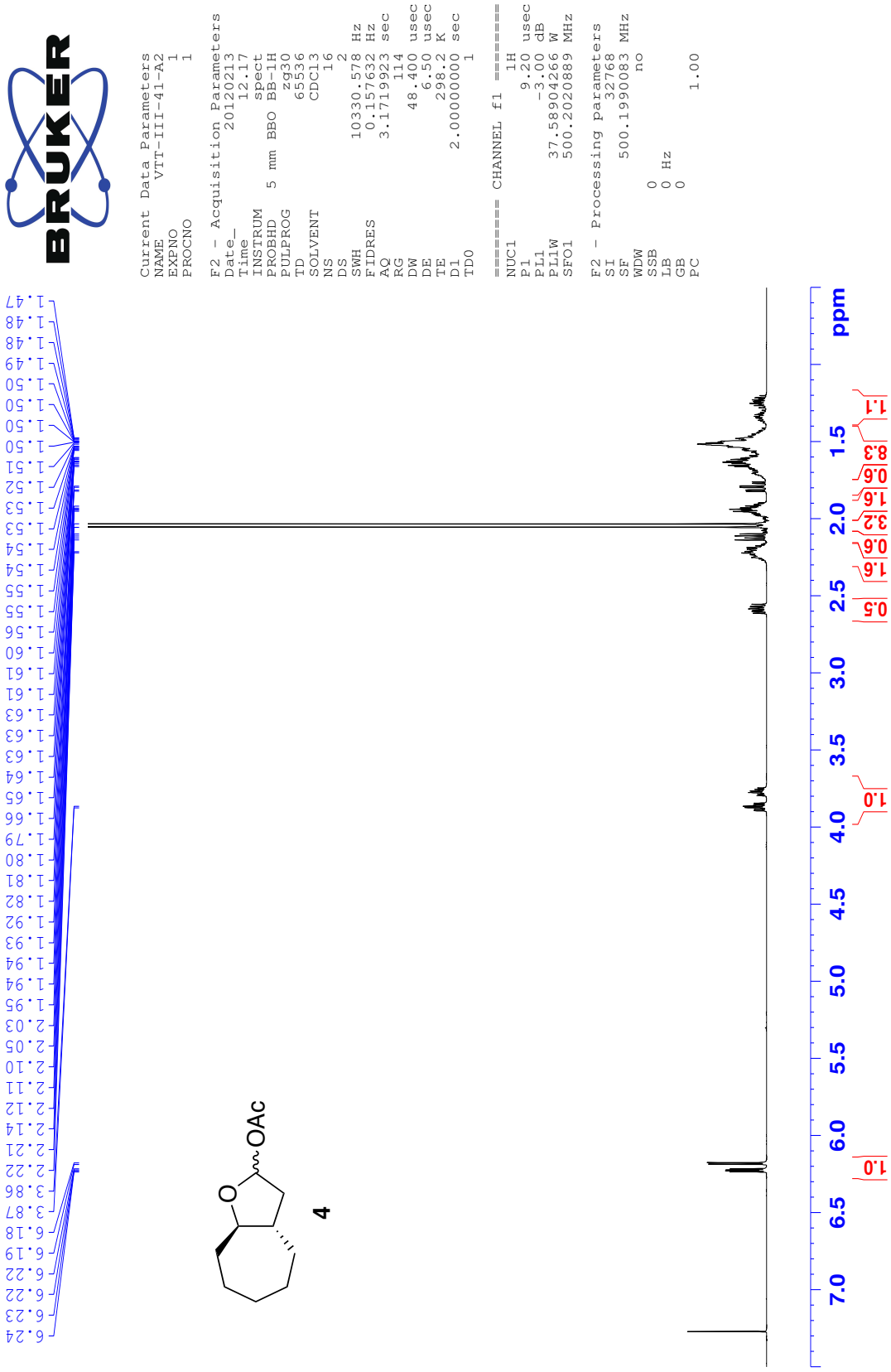
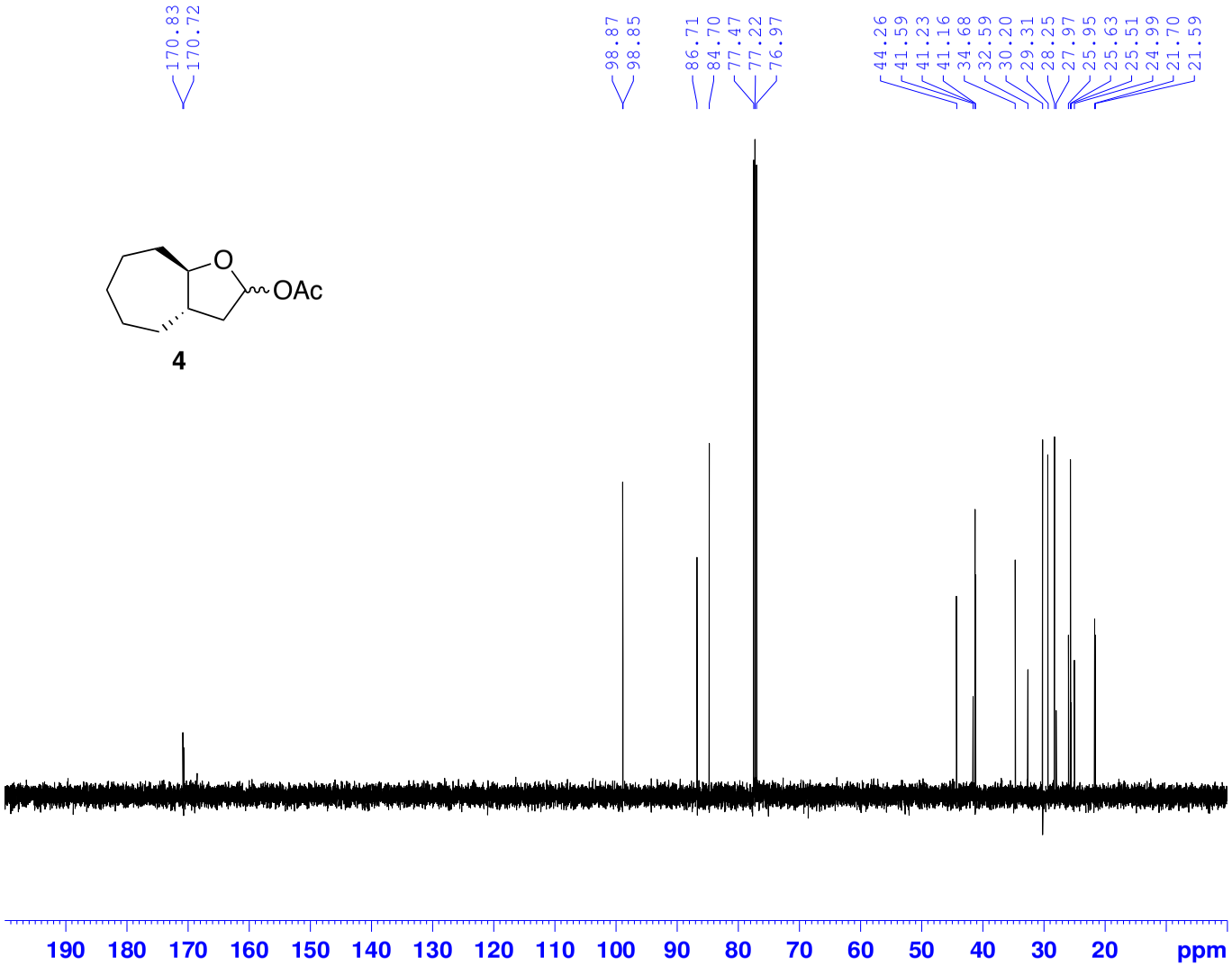
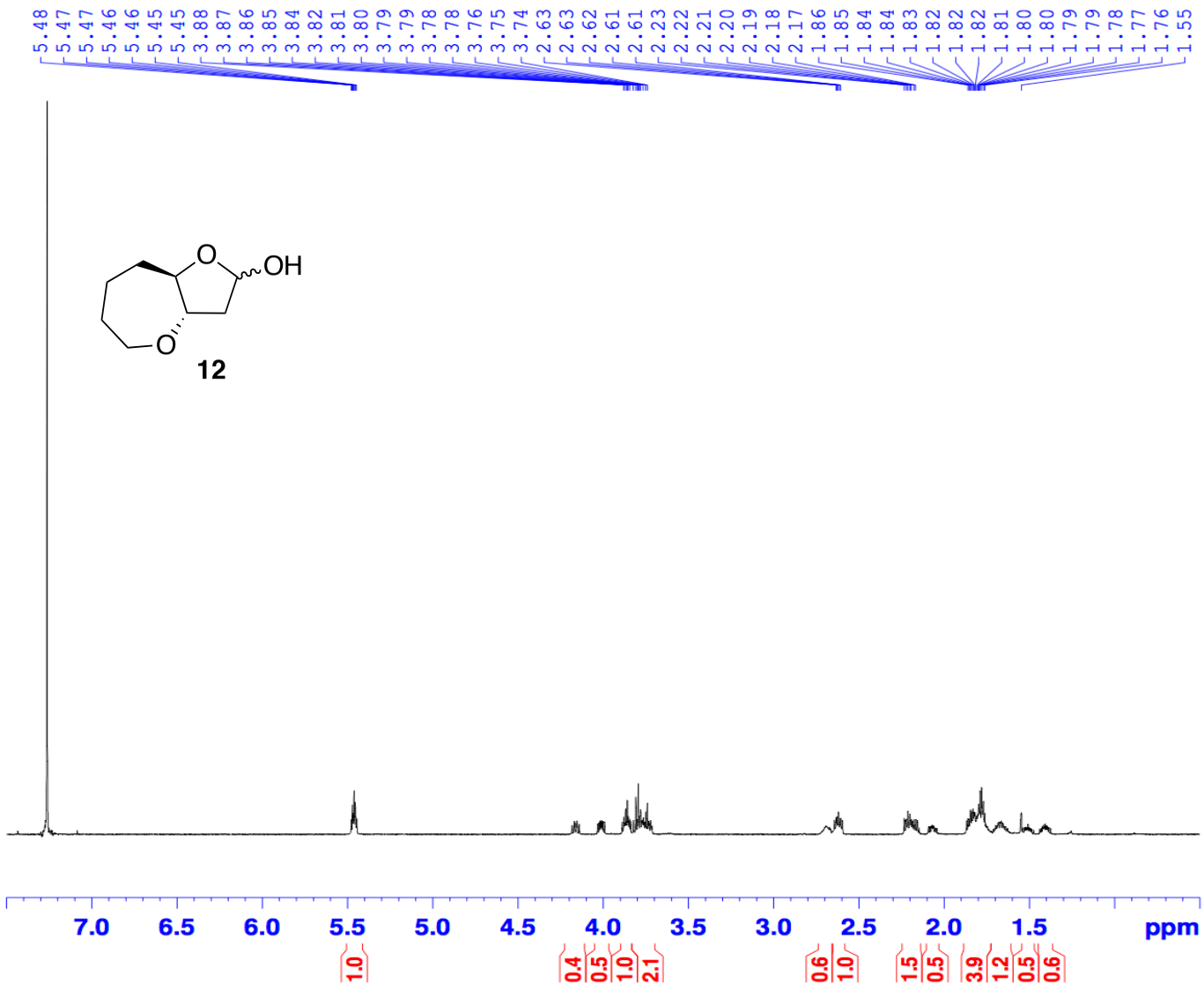
```
Current Data Parameters
NAME        VTT-III-39-A
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20120208
Time               13.05
INSTRUM            spect
PROBHD   5 mm PAQXI 1H/
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  111
DS                    4
SWH           36057.691 Hz
FIDRES         0.550197 Hz
AQ            0.9088159 sec
RG                184.65
DW               13.867 usec
DE                6.50 usec
TE               298.1 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                15.00 usec
PLW1       106.00000000 W
SFO1        150.9329866 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             70.00 usec
PLW2          9.30000019 W
PLW12         0.18190999 W
PLW13         0.08913500 W
SFO2        600.1924008 MHz

F2 - Processing parameters
SI                32768
SF          150.9178639 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

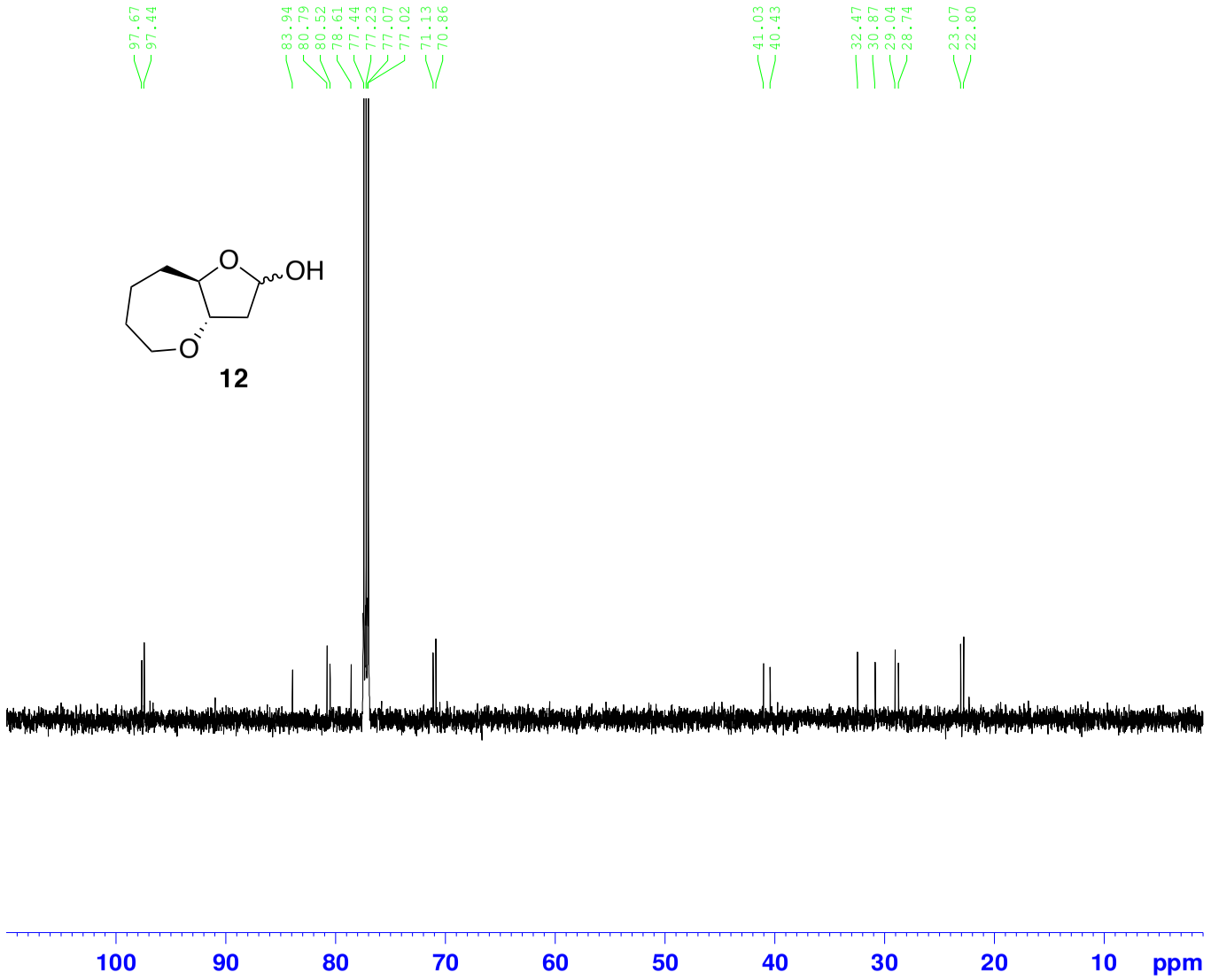

Current Data Parameters
NAME VTT-III-41-A2
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120213
Time 12.17
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 114
DW 48.400 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
TDO 1
======== CHANNEL f1 ========
NUC1 1H
P1 9.20 usec
PL1 -3.00 dB
PL1W 37.58904266 W
SFO1 500.2020889 MHz
F2 - Processing parameters
SI 32768
SF 500.1990083 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
OAc
4
ppm




```
Current Data Parameters
NAME      VTT-III-41-A2
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20120213
Time              12.19
INSTRUM           spect
PROBHD   5 mm BBO BB-1H
PULPROG         zgpg30
TD                65536
SOLVENT           CDCl3
NS                  128
DS                    4
SWH           30030.029 Hz
FIDRES         0.458222 Hz
AQ             1.0912244 sec
RG                32768
DW               16.650 usec
DE                6.50 usec
TE                298.5 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                 9.75 usec
PL1                2.00 dB
PL1W        49.29017639 W
SFO1       125.7877161 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             70.00 usec
PL2               -3.00 dB
PL12              13.50 dB
PL13              13.50 dB
PL2W        37.58904266 W
PL12W        0.84151381 W
PL13W        0.84151381 W
SFO2       500.2010008 MHz

F2 - Processing parameters
SI                32768
SF         125.7751165 MHz
WDW                  no
SSB       0
LB        0 Hz
GB        0
PC                1.40
```




```
Current Data Parameters
NAME        VTT-IV-73-A2
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20130228
Time               14.16
INSTRUM            spect
PROBHD   5 mm PAQXI 1H/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     8
DS                     0
SWH            12335.526 Hz
FIDRES          0.188225 Hz
AQ             2.6564426 sec
RG                184.65
DW                40.533 usec
DE                 6.50 usec
TE                298.2 K
D1            2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                  9.79 usec
PLW1          9.30000019 W
SFO1        600.1937064 MHz

F2 - Processing parameters
SI                 65536
SF          600.1900139 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```



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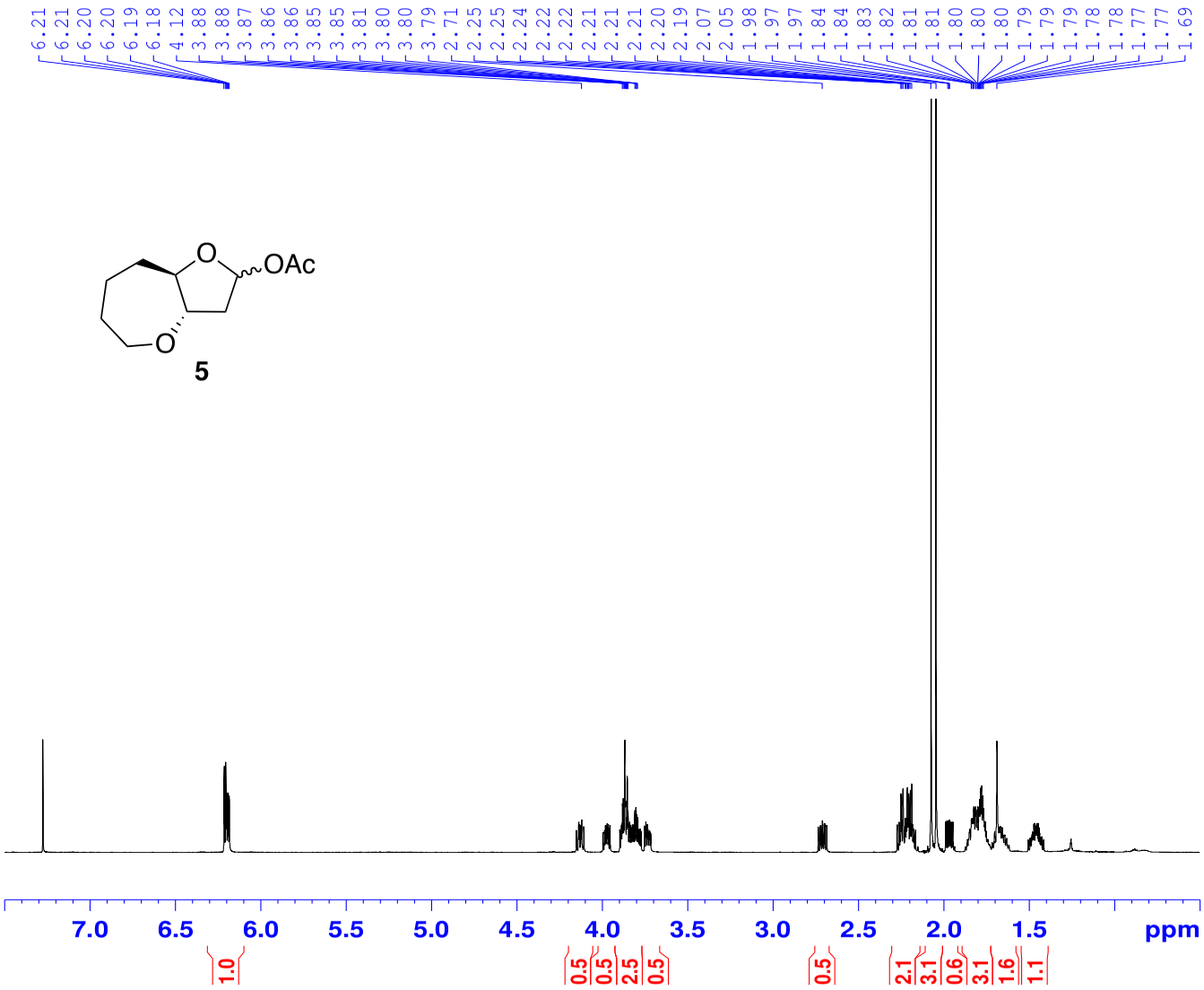
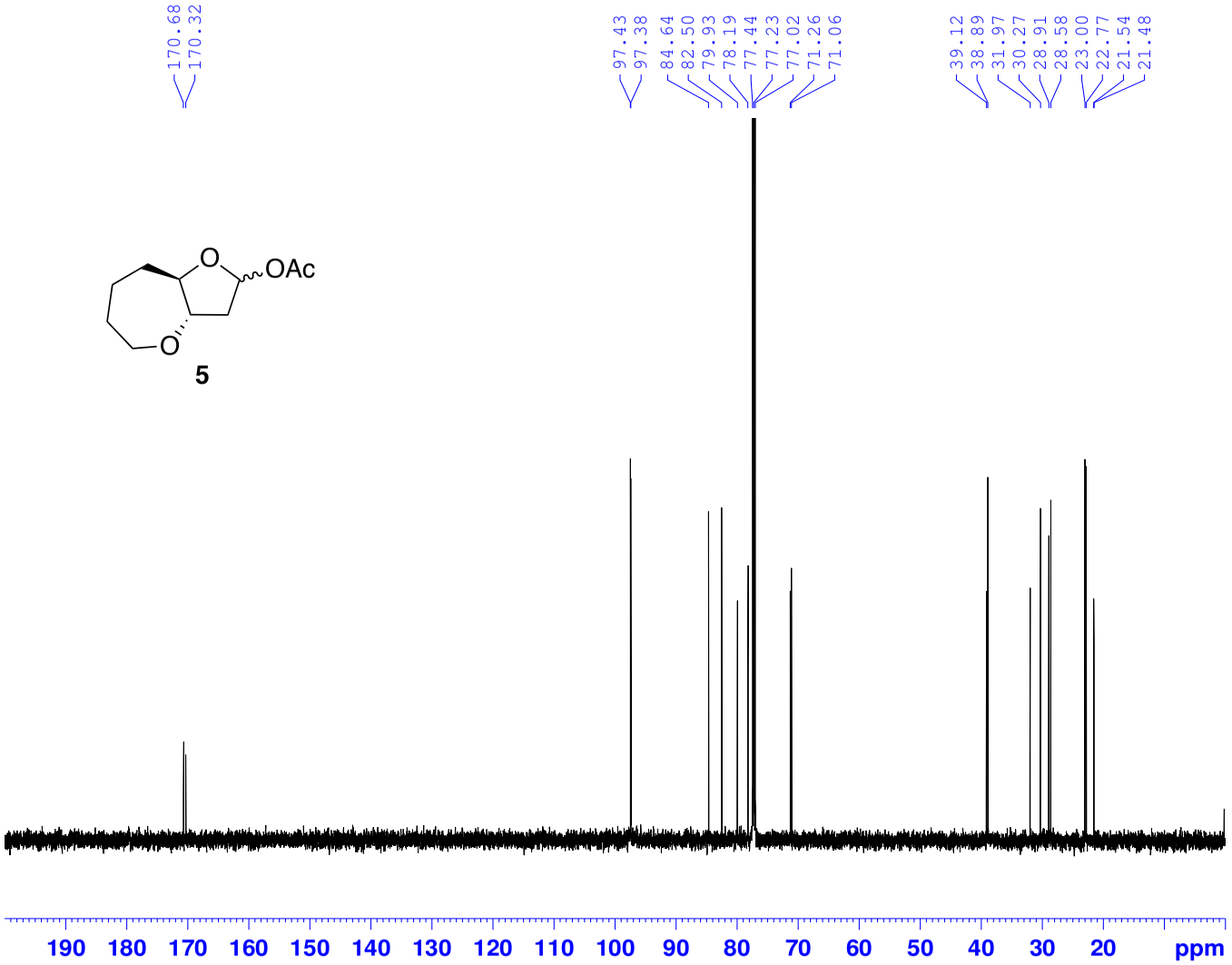
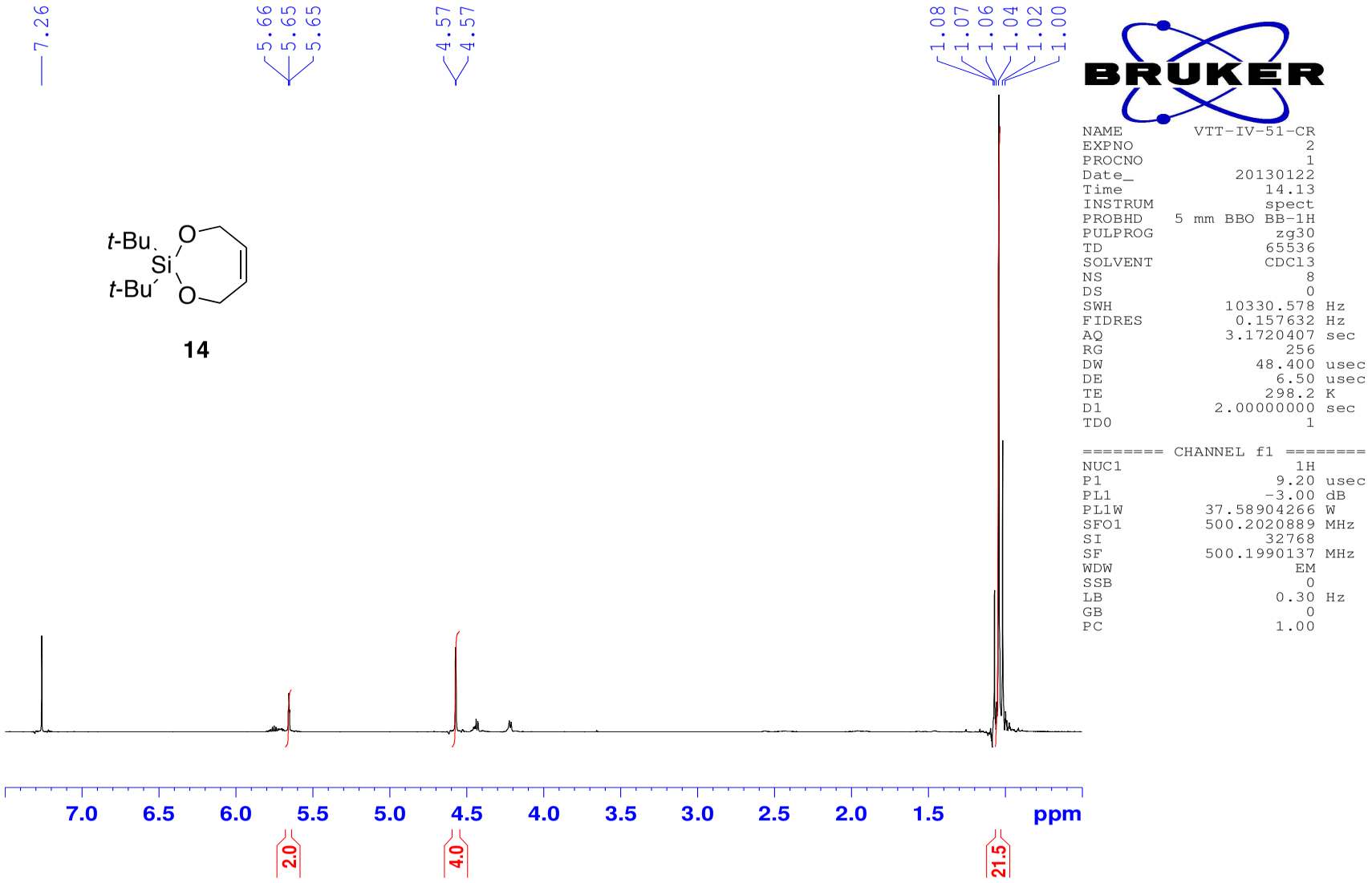
```
Current Data Parameters
NAME         VTT-IV-73-A
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20130213
Time               17.20
INSTRUM            spect
PROBHD   5 mm PAQXI 1H/
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  128
DS                    0
SWH           36057.691 Hz
FIDRES         0.550197 Hz
AQ            0.9088159 sec
RG               184.65
DW               13.867 usec
DE                 6.50 usec
TE                298.1 K
D1           2.50000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                15.00 usec
PLW1       106.00000000 W
SFO1        150.9329866 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             70.00 usec
PLW2          9.30000019 W
PLW12         0.18190999 W
PLW13         0.08913500 W
SFO2        600.1924008 MHz

F2 - Processing parameters
SI                32768
SF          150.9178634 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

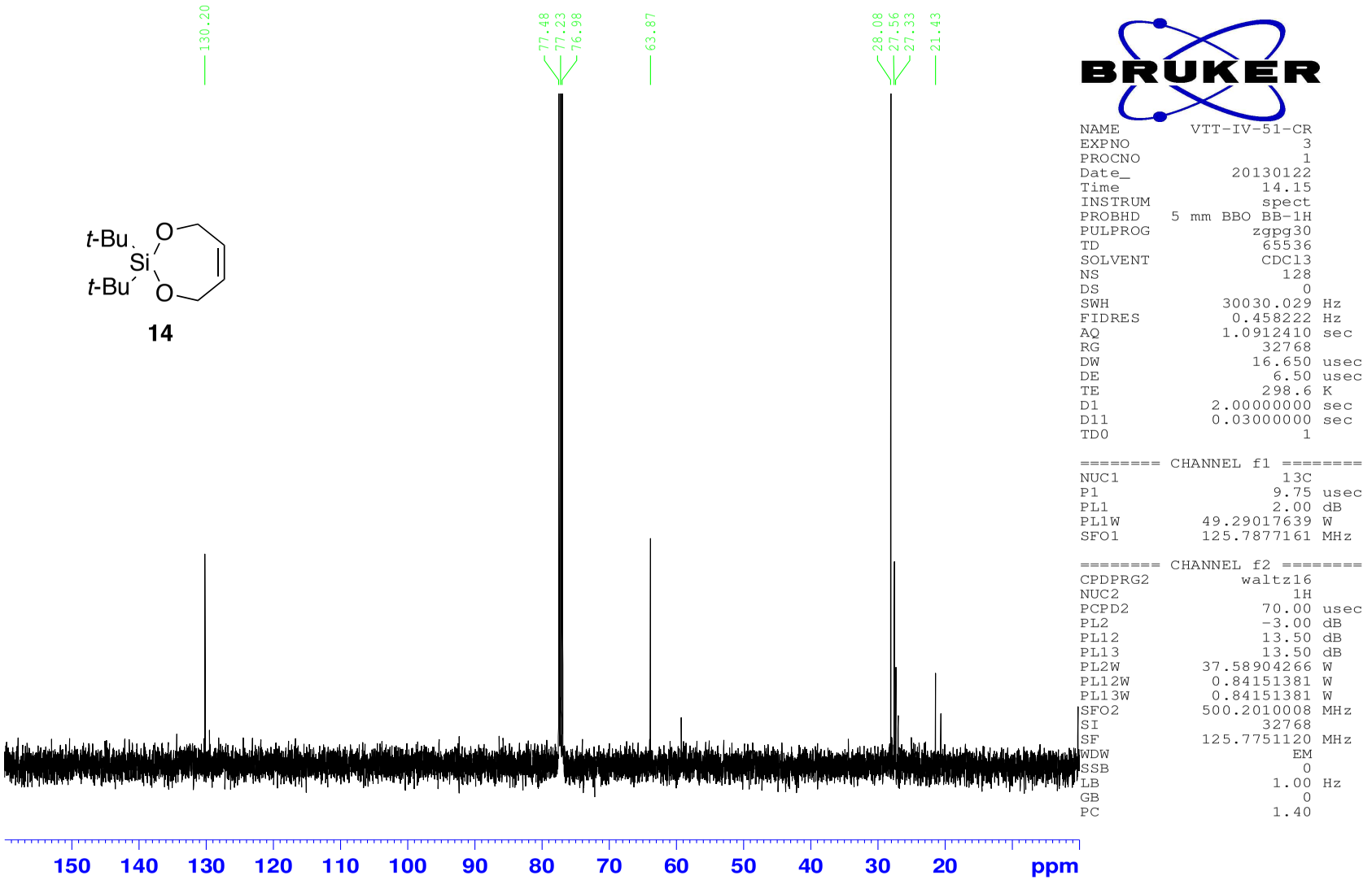



```
Current Data Parameters
NAME       VTT-III-186-A
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20120730
Time               21.54
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     8
DS                     0
SWH           12335.526 Hz
FIDRES         0.188225 Hz
AQ            2.6564426 sec
RG                 56.41
DW                40.533 usec
DE                 6.50 usec
TE                298.1 K
D1           2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                11.00 usec
PLW1         26.50000000 W
SFO1         600.1937064 MHz

F2 - Processing parameters
SI                 65536
SF           600.1900066 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```




```
Current Data Parameters
NAME       VTT-III-186-A
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20120730
Time               21.59
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  128
DS                    0
SWH           36057.691 Hz
FIDRES         0.550197 Hz
AQ             0.9088159 sec
RG                184.65
DW                13.867 usec
DE                 6.50 usec
TE                298.1 K
D1           2.50000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                 10.65 usec
PLW1       104.00000000 W
SFO1        150.9329866 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2              70.00 usec
PLW2        26.50000000 W
PLW12        0.65438998 W
PLW13        0.32065001 W
SFO2        600.1924008 MHz

F2 - Processing parameters
SI                 32768
SF          150.9178676 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```


7.26
5.66
5.65
5.65
4.57
4.57
1.08
1.07
1.06
1.04
1.02
1.00
t-Bu
Si
t-Bu
O
O
14
BRUKER
NAME VTT-IV-51-CR
EXPNO 2
PROCNO 1
Date_ 20130122
Time 14.13
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 256
DW 48.400 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 9.20 usec
PL1 -3.00 dB
PL1W 37.58904266 W
SFO1 500.2020889 MHz
SI 32768
SF 500.1990137 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
ppm
2.0
4.0
21.5



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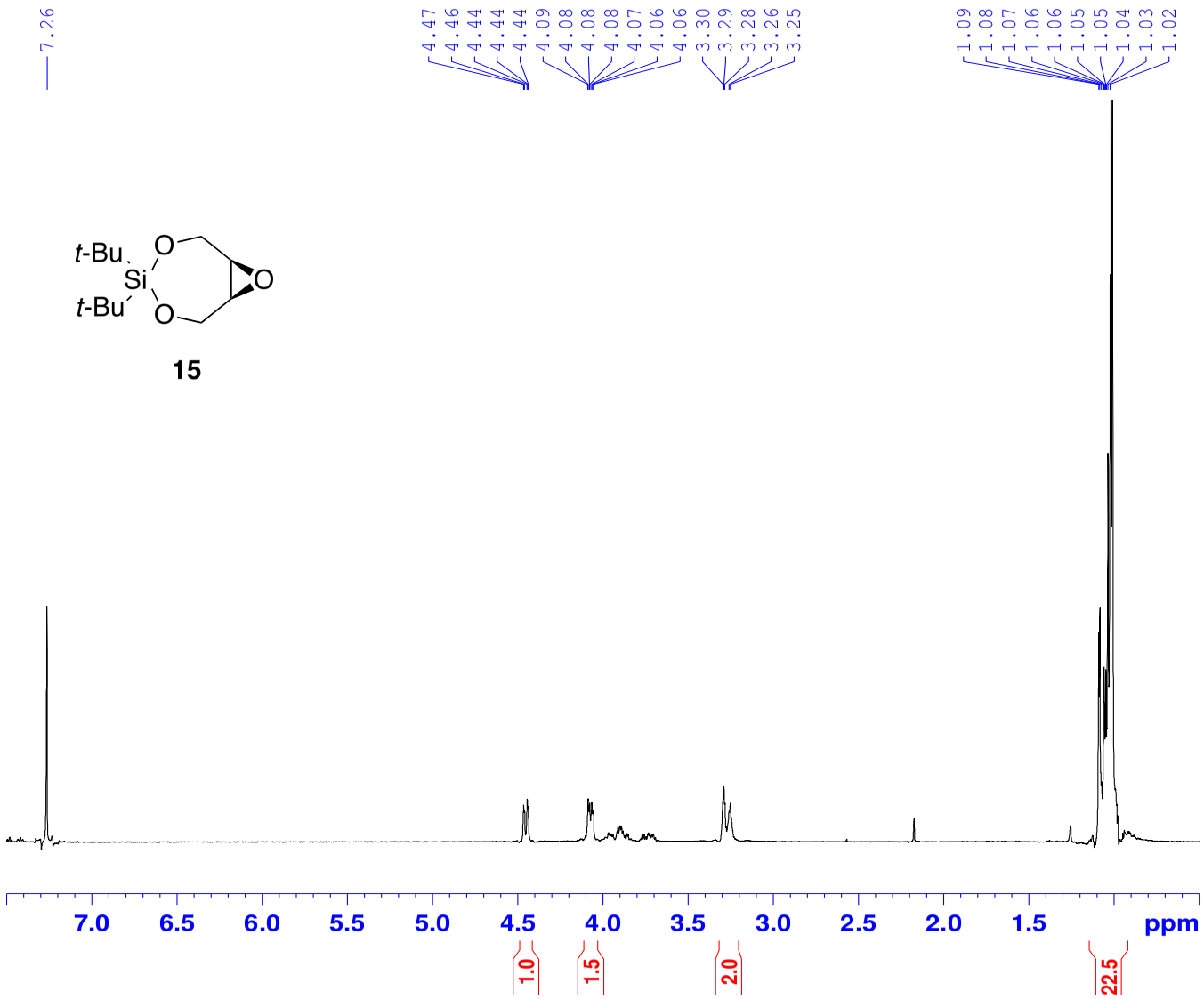
NAME	VTT-IV-51-CR
EXPNO	3
PROCNO	1
Date_	20130122
Time	14.15
INSTRUM	spect
PROBHD	5 mm BBO BB-1H
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	128
DS	0
SWH	30030.029 Hz
FIDRES	0.458222 Hz
AQ	1.0912410 sec
RG	32768
DW	16.650 usec
DE	6.50 usec
TE	298.6 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.75 usec
PL1	2.00 dB
PL1W	49.29017639 W
SFO1	125.7877161 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	70.00 usec
PL2	-3.00 dB
PL12	13.50 dB
PL13	13.50 dB
PL2W	37.58904266 W
PL12W	0.84151381 W
PL13W	0.84151381 W
SFO2	500.2010008 MHz
SI	32768
SF	125.7751120 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



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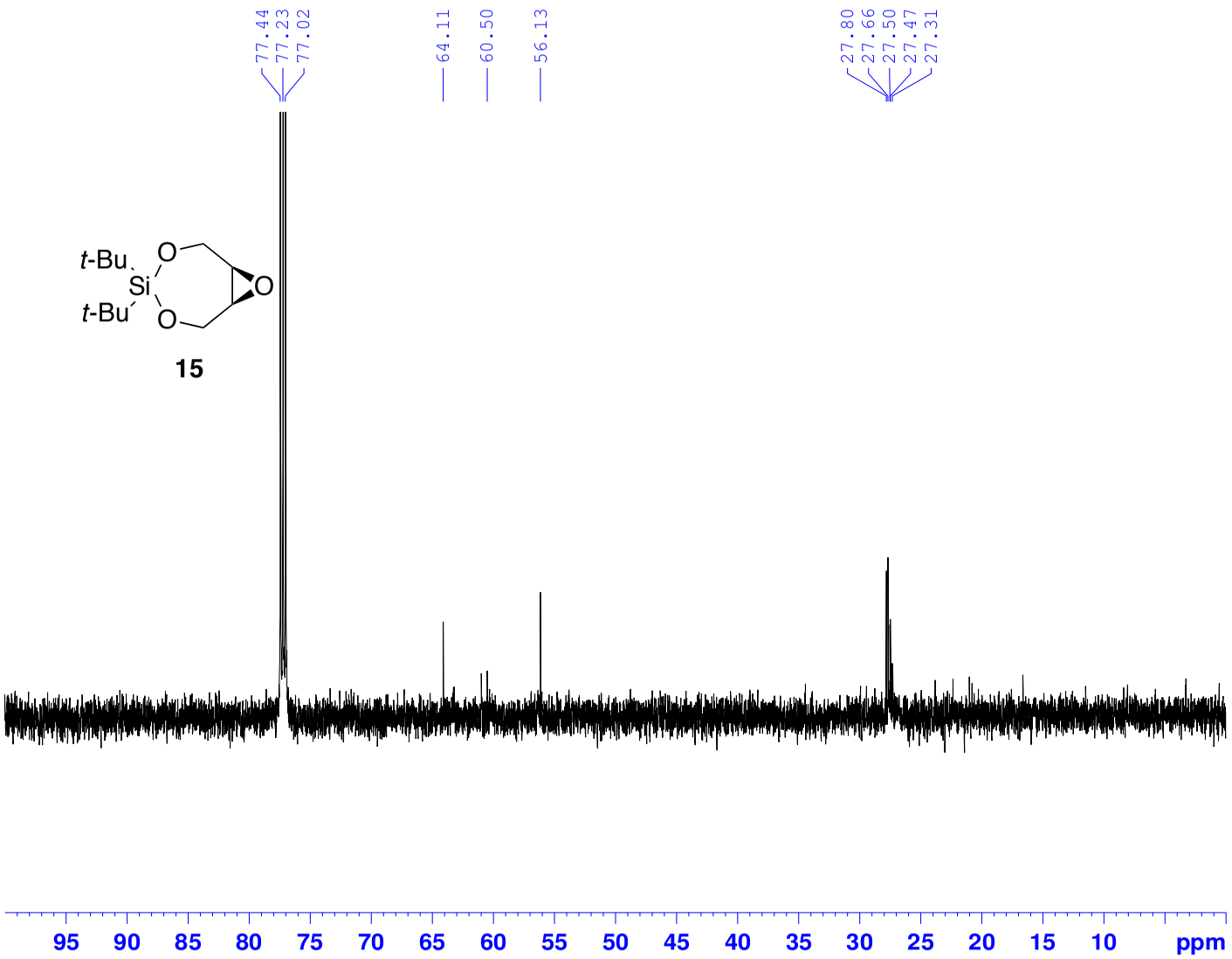
```
Current Data Parameters
NAME       VTT-IV-53-CR2
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20130124
Time               15.10
INSTRUM            spect
PROBHD   5 mm PAQXI 1H/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     8
DS                     0
SWH            12335.526 Hz
FIDRES          0.188225 Hz
AQ             2.6564426 sec
RG                126.35
DW                40.533 usec
DE                 6.50 usec
TE                298.2 K
D1            2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 9.79 usec
PLW1          9.30000019 W
SFO1         600.1937064 MHz

F2 - Processing parameters
SI                 65536
SF           600.1900130 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```



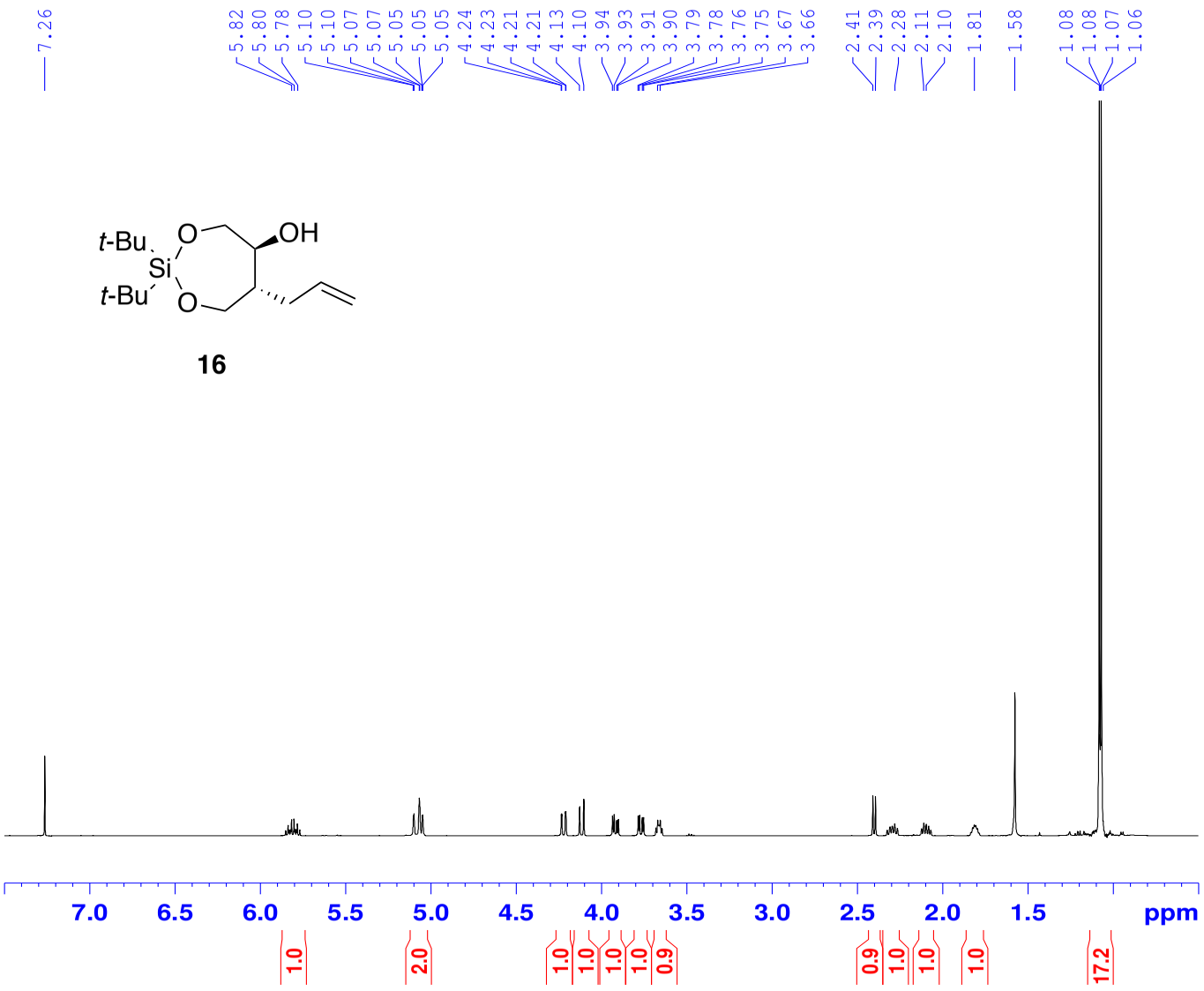

```
Current Data Parameters
NAME       VTT-IV-53-CR2
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20130124
Time               15.12
INSTRUM            spect
PROBHD   5 mm PAQXI 1H/
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  128
DS                    0
SWH           36057.691 Hz
FIDRES         0.550197 Hz
AQ            0.9088159 sec
RG               184.65
DW               13.867 usec
DE                6.50 usec
TE                298.2 K
D1           2.50000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                15.00 usec
PLW1       106.00000000 W
SFO1        150.9329866 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             70.00 usec
PLW2          9.30000019 W
PLW12         0.18190999 W
PLW13         0.08913500 W
SFO2         600.1924008 MHz

F2 - Processing parameters
SI                32768
SF          150.9178633 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```



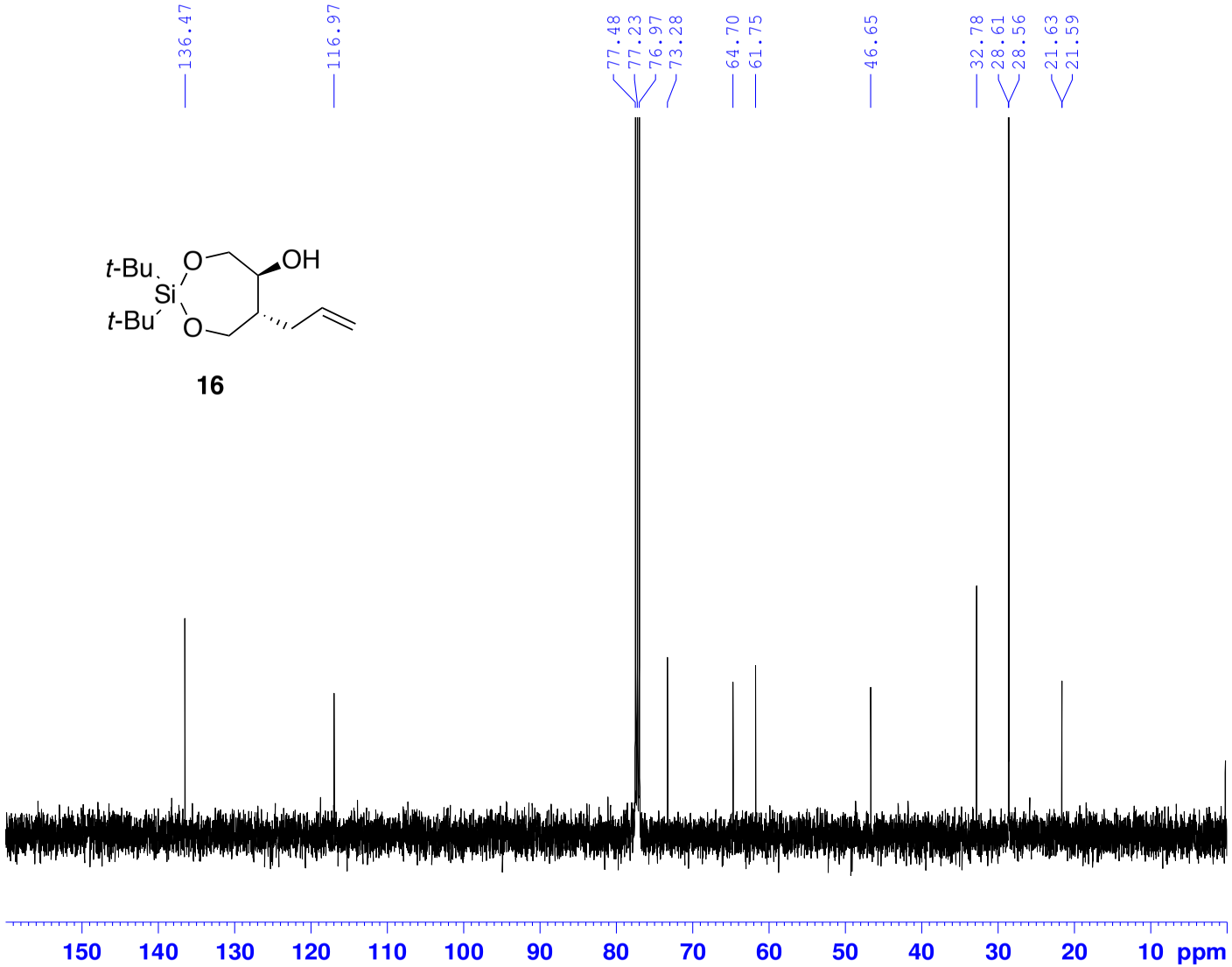
BRUKER

```
Current Data Parameters
NAME        VTT-II-135-C
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20110822
Time               14.15
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH           10330.578 Hz
FIDRES         0.157632 Hz
AQ             3.1719923 sec
RG                   256
DW                48.400 usec
DE                 6.50 usec
TE                298.2 K
D1            2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 9.20 usec
PL1               -3.00 dB
PL1W        37.58904266 W
SFO1        500.2020889 MHz

F2 - Processing parameters
SI                 32768
SF          500.1990134 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```



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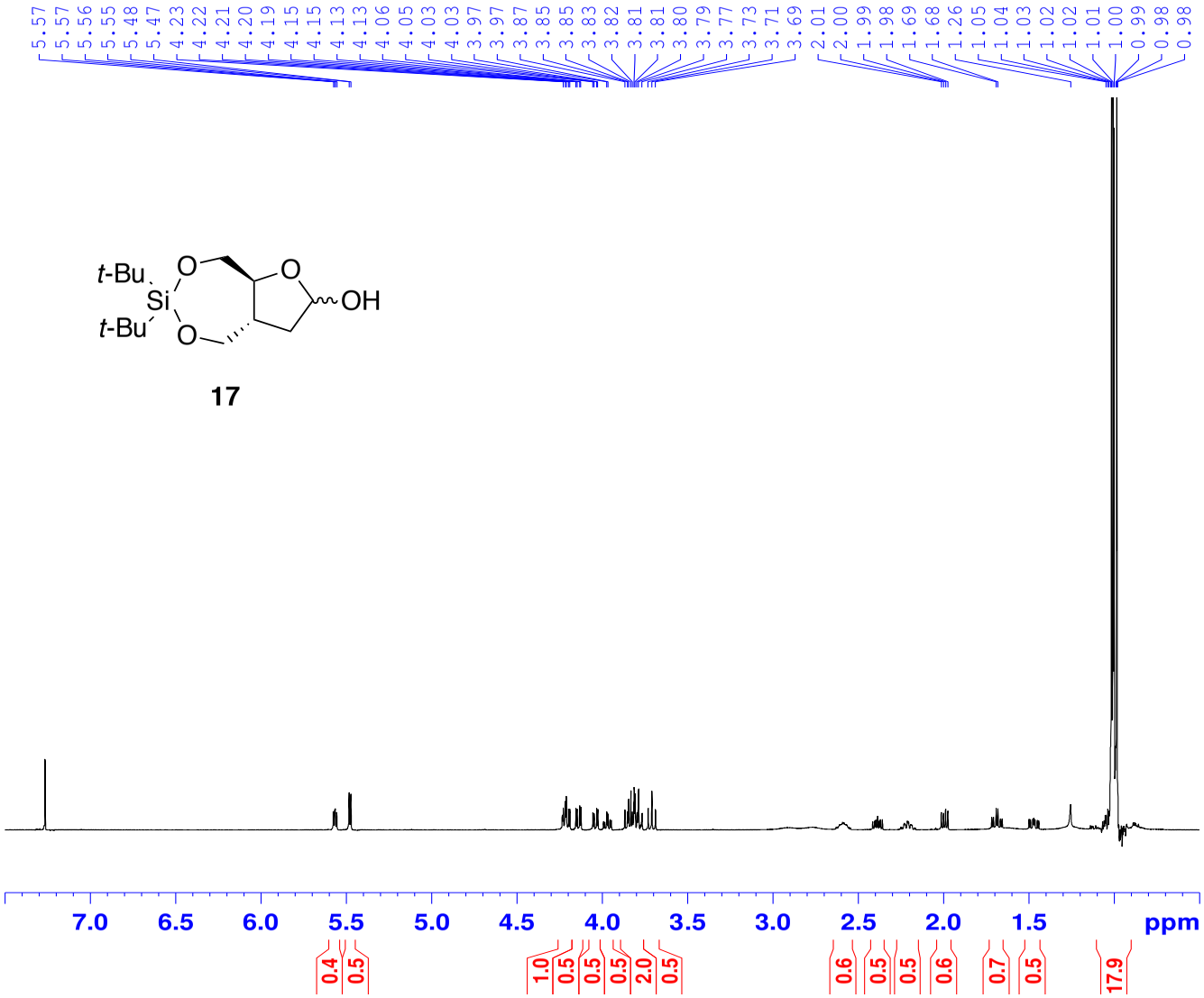
```
Current Data Parameters
NAME        VTT-II-135-C
EXPNO                  3
PROCNO                 1

F2 - Acquisition Parameters
Date_           20110822
Time               14.24
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  177
DS                    4
SWH           30030.029 Hz
FIDRES         0.458222 Hz
AQ             1.0912244 sec
RG                16384
DW               16.650 usec
DE                6.50 usec
TE                298.7 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                 10.25 usec
PL1                 2.00 dB
PL1W        49.29017639 W
SFO1       125.7877161 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2              70.00 usec
PL2                -3.00 dB
PL12               14.63 dB
PL13               14.91 dB
PL2W        37.58904266 W
PL12W        0.64872593 W
PL13W        0.60822082 W
SFO2       500.2010008 MHz

F2 - Processing parameters
SI                 32768
SF         125.7751116 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```



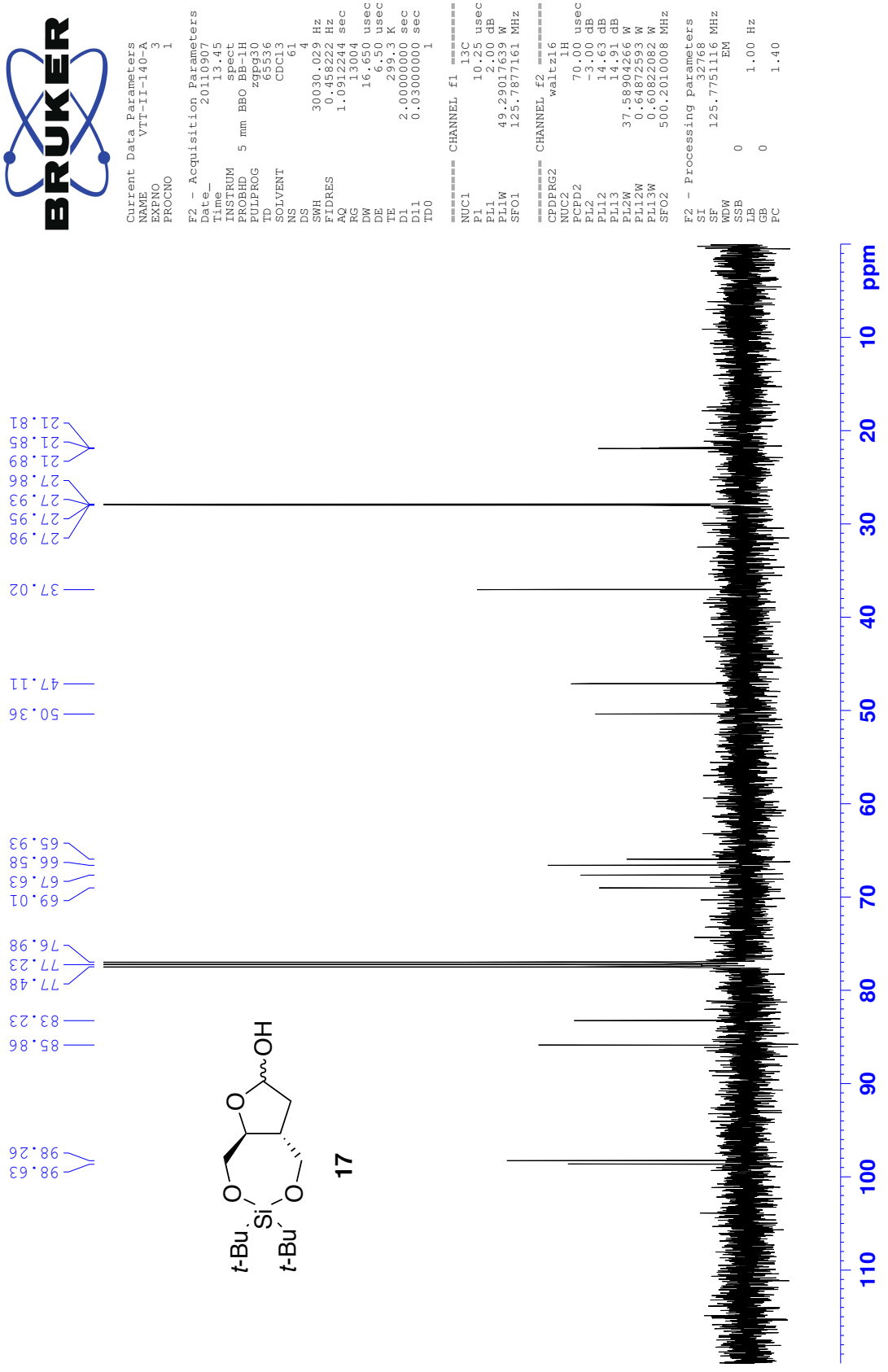
17

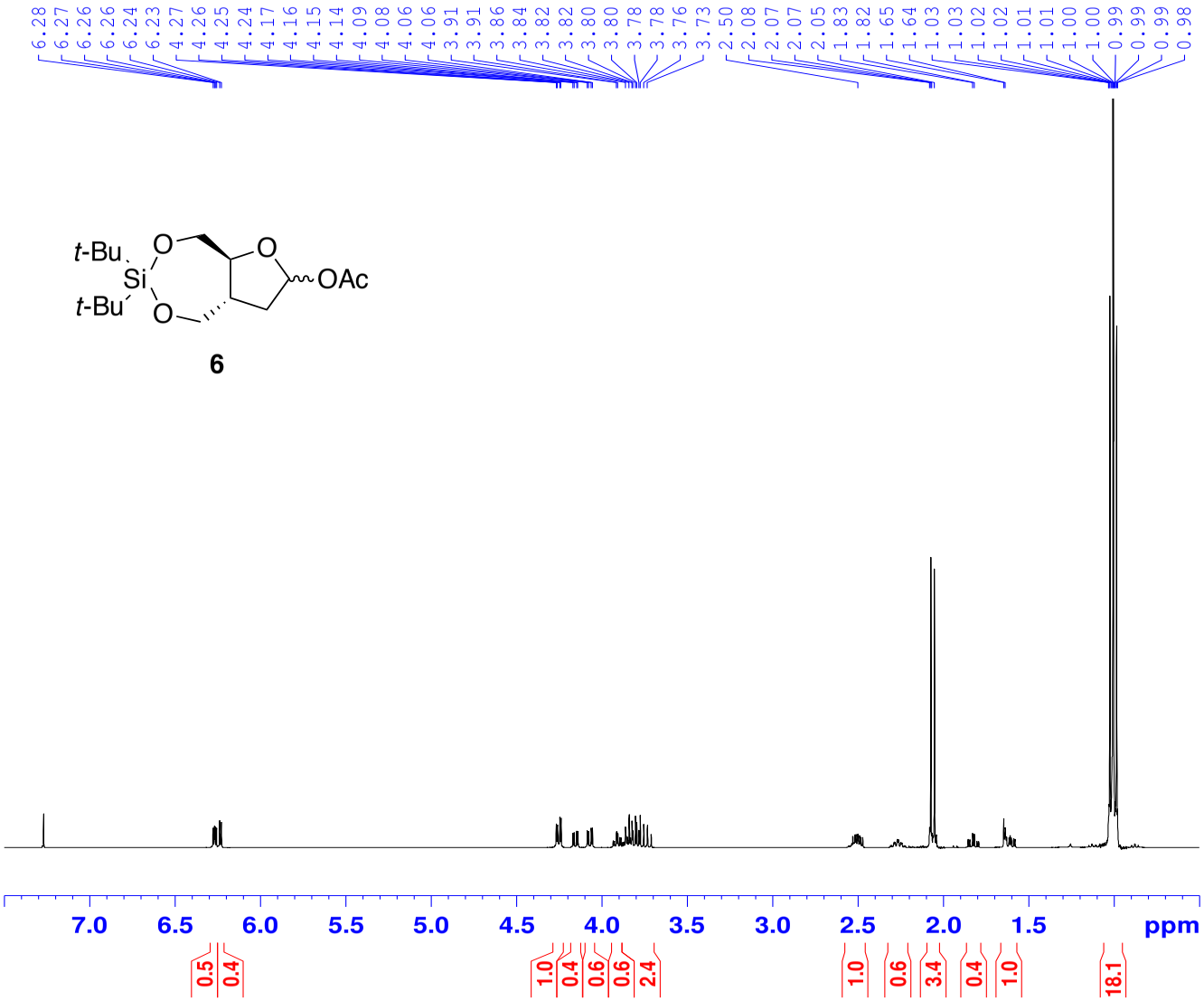
```
Current Data Parameters
NAME        VTT-II-140-A
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20110907
Time               13.38
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH           10330.578 Hz
FIDRES         0.157632 Hz
AQ            3.1719923 sec
RG                  90.5
DW                48.400 usec
DE                 6.50 usec
TE                298.2 K
D1           2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 9.20 usec
PL1               -3.00 dB
PL1W        37.58904266 W
SFO1       500.2020889 MHz

F2 - Processing parameters
SI                 32768
SF         500.1990127 MHz
WDW                   no
SSB       0
LB        0 Hz
GB        0
PC                 1.00
```


Current Data Parameters
NAME VTT-II-140-A
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110907
Time 13.45
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 61
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912244 sec
RG 13004
DW 16.650 usec
DE 6.50 usec
TE 299.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 10.25 usec
PL1 2.00 dB
PL1W 49.29017639 W
SFO1 125.7877161 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL2 -3.00 dB
PL12 14.63 dB
PL13 14.91 dB
PL2W 37.58904266 W
PL12W 0.64872593 W
PL13W 0.60822082 W
SFO2 500.2010008 MHz
F2 - Processing parameters
SI 32768
SF 125.7751116 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
21.81
21.85
21.89
27.86
27.93
27.95
27.98
37.02
47.11
50.36
65.93
66.58
67.63
69.01
76.98
77.23
77.48
83.23
85.86
98.26
98.63
OH
O
O
O
Si
t-Bu
t-Bu
17
ppm
10
20
30
40
50
60
70
80
90
100
110



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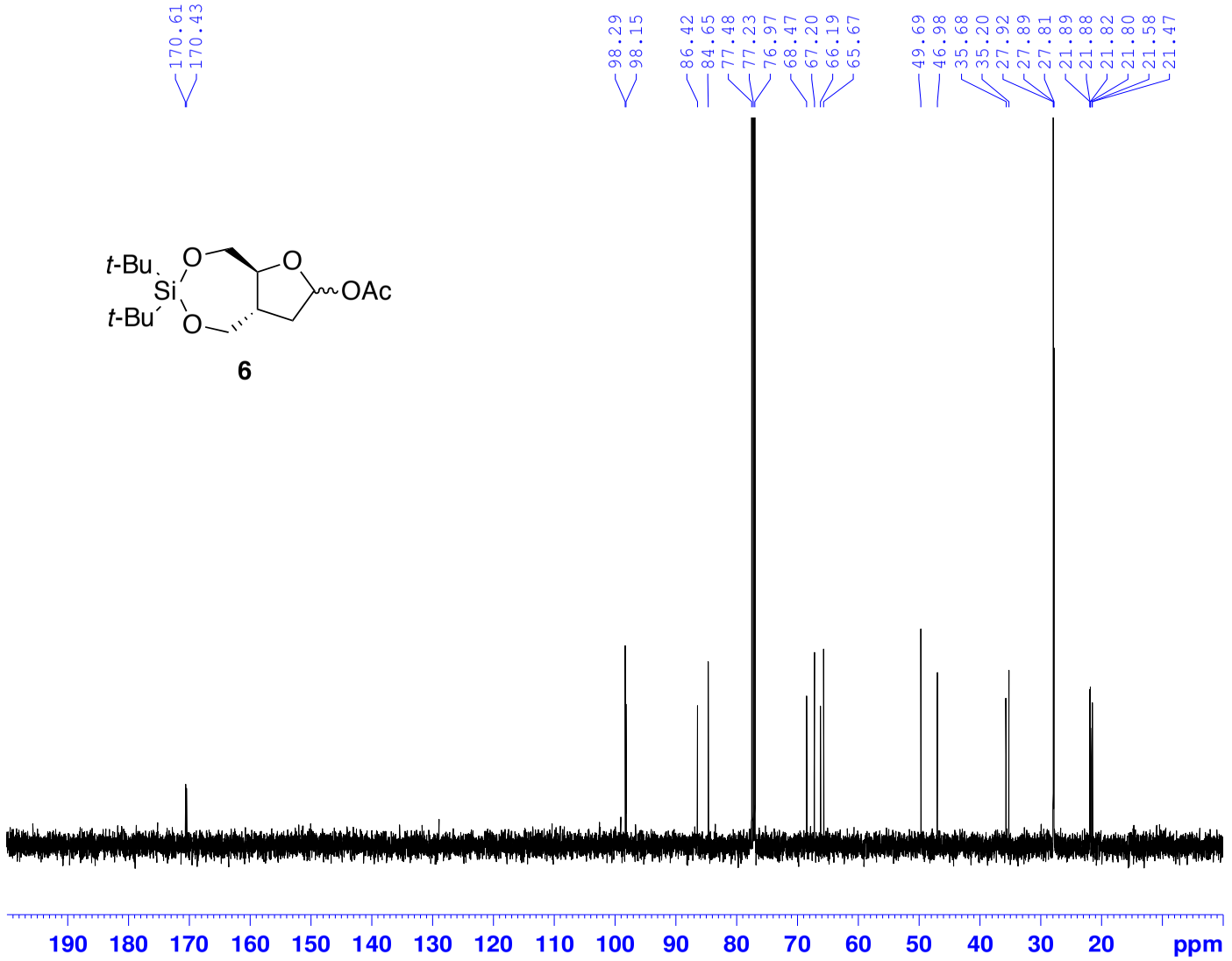
```
Current Data Parameters
NAME        VTT-II-145-A
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20110912
Time               12.53
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH            10330.578 Hz
FIDRES          0.157632 Hz
AQ             3.1719923 sec
RG                    64
DW                48.400 usec
DE                 6.50 usec
TE                298.1 K
D1             2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 9.20 usec
PL1               -3.00 dB
PL1W        37.58904266 W
SFO1        500.2020889 MHz

F2 - Processing parameters
SI                 32768
SF          500.1990100 MHz
WDW                   no
SSB       0
LB        0 Hz
GB        0
PC                 1.00
```



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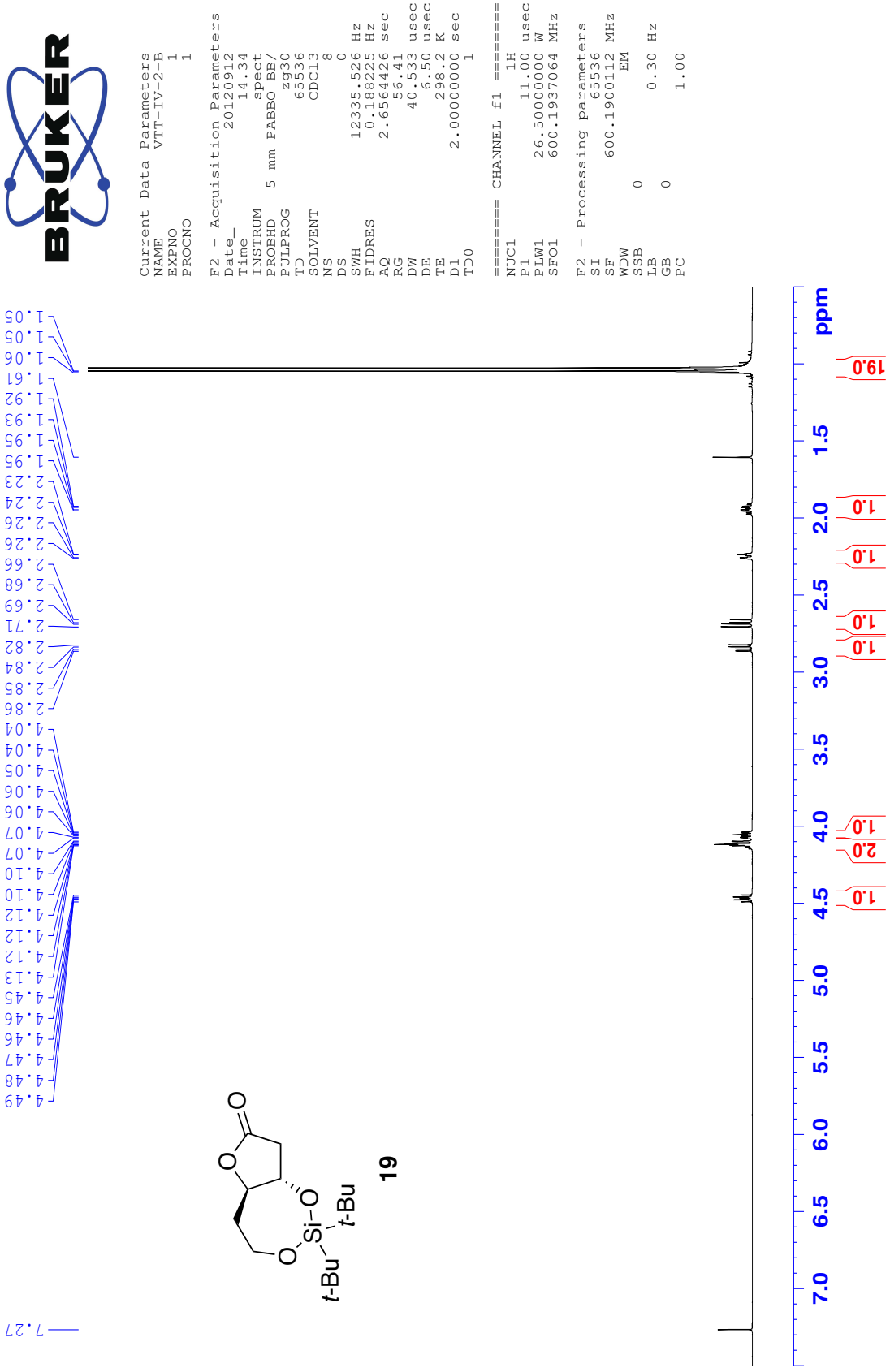
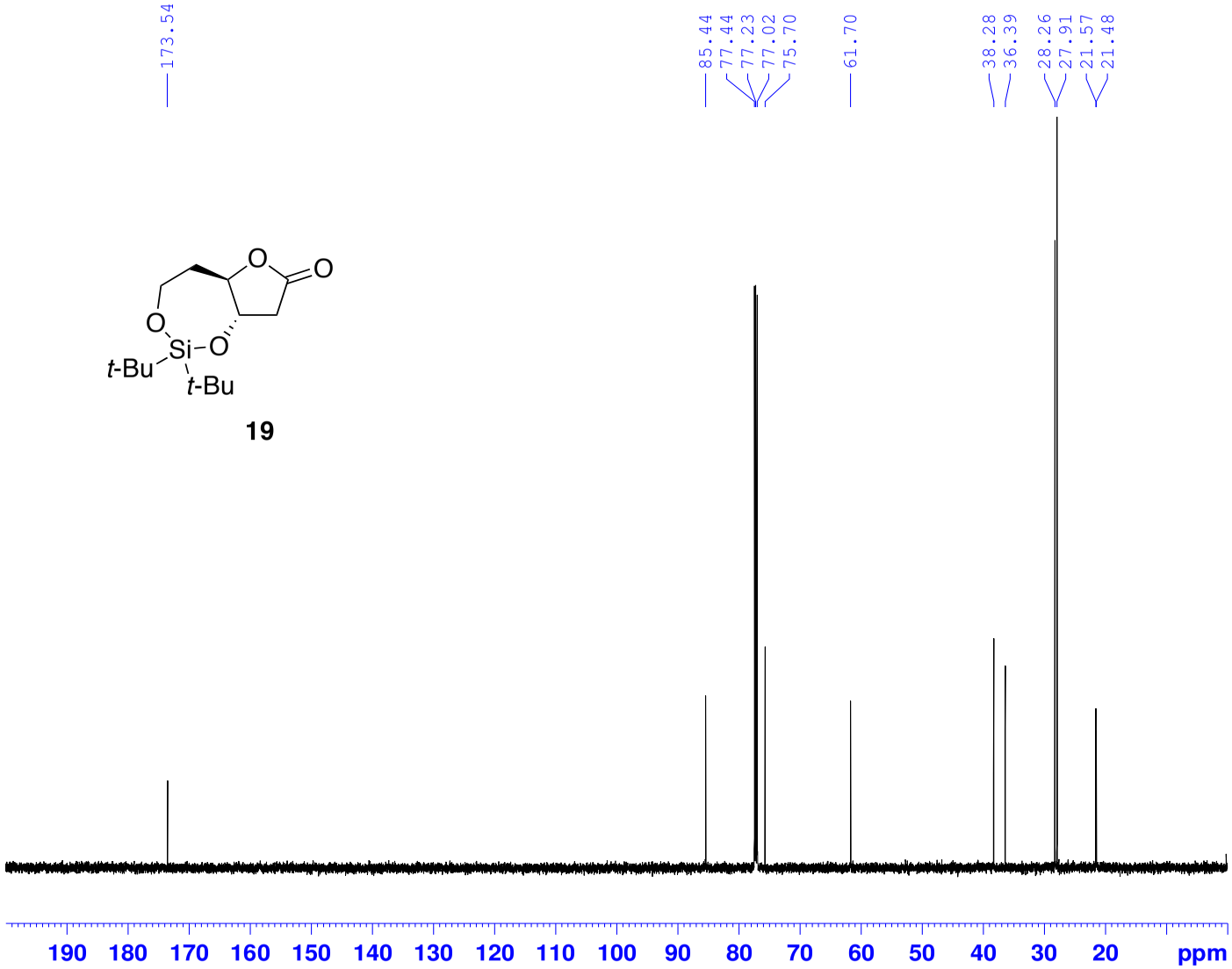
```
Current Data Parameters
NAME        VTT-II-145-A
EXPNO                  3
PROCNO                 1

F2 - Acquisition Parameters
Date_           20110912
Time               12.56
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                   51
DS                    4
SWH           30030.029 Hz
FIDRES            0.458222 Hz
AQ             1.0912244 sec
RG                5160.6
DW                16.650 usec
DE                 6.50 usec
TE                298.4 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                 10.25 usec
PL1                 2.00 dB
PL1W         49.29017639 W
SFO1        125.7877161 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2              70.00 usec
PL2                -3.00 dB
PL12               14.63 dB
PL13               14.91 dB
PL2W         37.58904266 W
PL12W         0.64872593 W
PL13W         0.60822082 W
SFO2        500.2010008 MHz

F2 - Processing parameters
SI                 32768
SF          125.7751143 MHz
WDW                EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```


Current Data Parameters
NAME VTT-IV-2-B
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120912
Time 14.34
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 12335.526 Hz
FIDRES 0.188225 Hz
AQ 2.6564426 sec
RG 56.41
DW 40.533 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 11.00 usec
PLW1 26.50000000 W
SFO1 600.1937064 MHz
F2 - Processing parameters
SI 65536
SF 600.1900112 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1.05
1.05
1.06
1.61
1.92
1.93
1.95
1.95
2.23
2.24
2.26
2.26
2.66
2.68
2.69
2.71
2.82
2.84
2.85
2.86
4.04
4.04
4.05
4.06
4.06
4.07
4.07
4.10
4.10
4.12
4.12
4.12
4.13
4.45
4.46
4.46
4.47
4.48
4.49
7.27
19.0
1.0
1.0
1.0
1.0
2.0
1.0
ppm
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
O
O
O
Si
O
t-Bu
t-Bu
19



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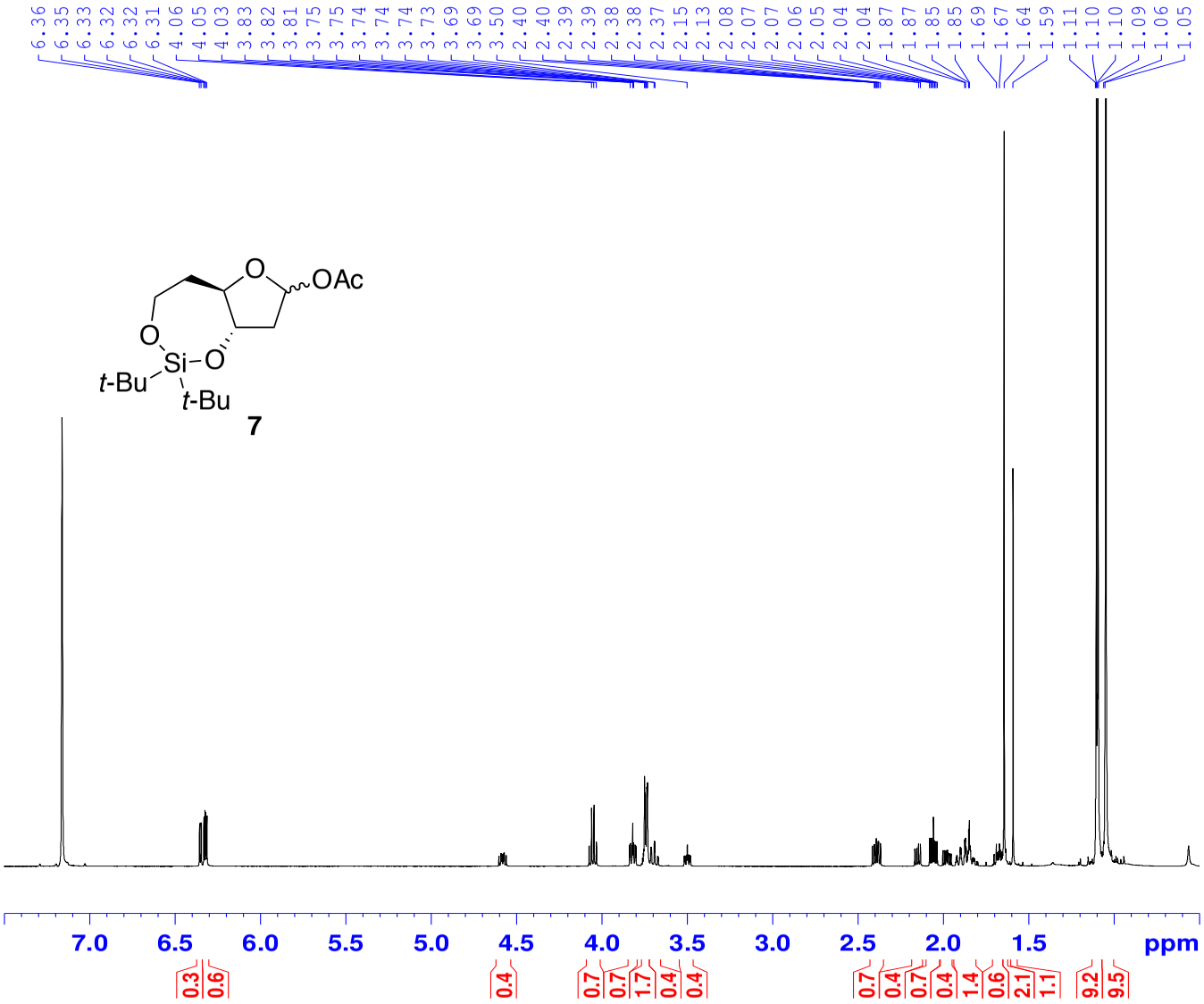
```
Current Data Parameters
NAME          VTT-IV-2-B
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20120912
Time               15.12
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD                65536
SOLVENT           CDCl3
NS                  128
DS                    0
SWH           36057.691 Hz
FIDRES         0.550197 Hz
AQ             0.9088159 sec
RG               184.65
DW              13.867 usec
DE                6.50 usec
TE               298.3 K
D1           2.50000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                10.65 usec
PLW1       104.00000000 W
SFO1        150.9329866 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             70.00 usec
PLW2        26.50000000 W
PLW12        0.65438998 W
PLW13        0.32065001 W
SFO2        600.1924008 MHz

F2 - Processing parameters
SI                32768
SF          150.9178655 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```



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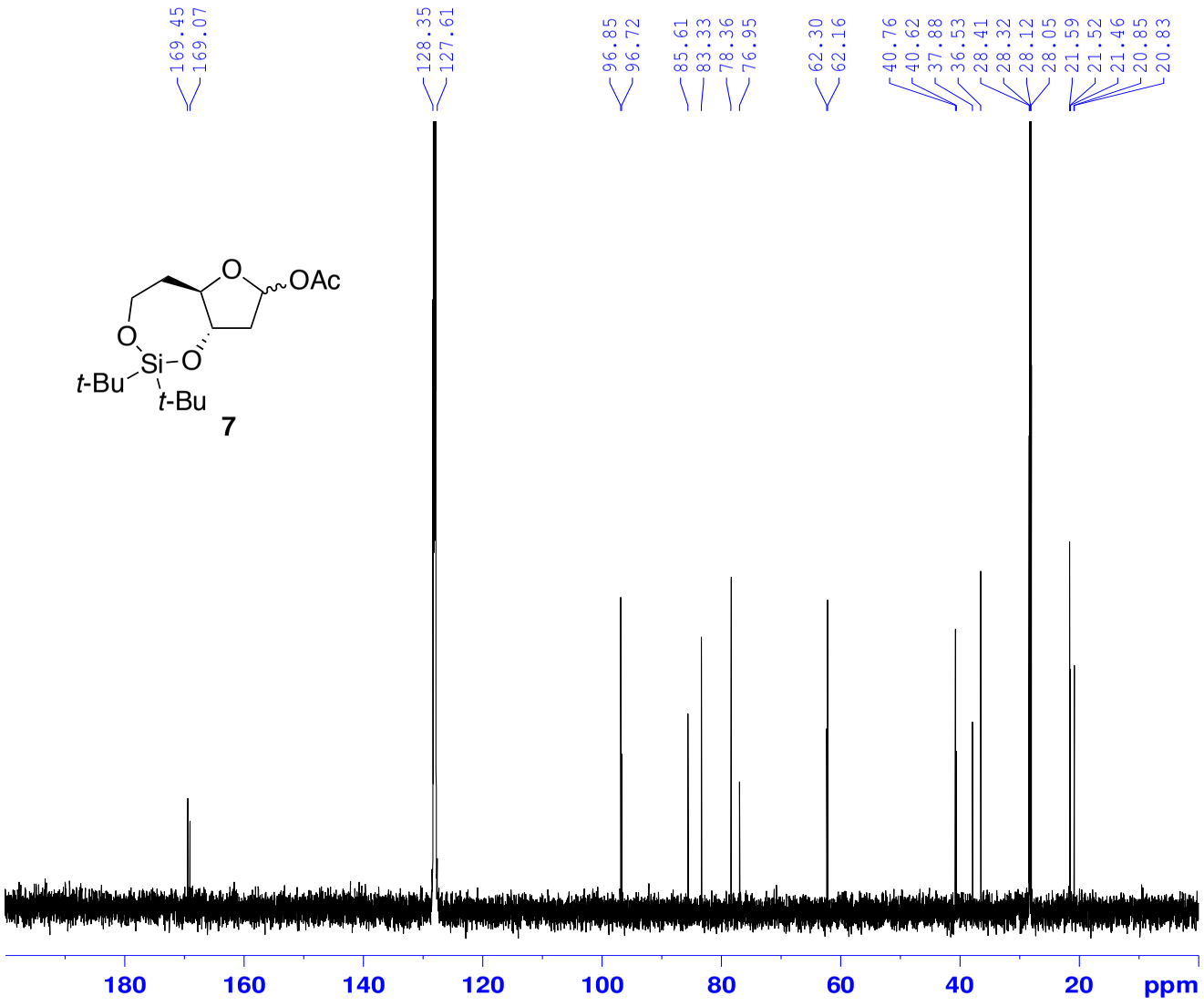
```
Current Data Parameters
NAME         VTT-IV-16-A
EXPNO                  5
PROCNO                 1

F2 - Acquisition Parameters
Date_           20120917
Time               16.41
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT             C6D6
NS                     8
DS                     0
SWH            12335.526 Hz
FIDRES          0.188225 Hz
AQ             2.6564426 sec
RG                 56.41
DW                40.533 usec
DE                 6.50 usec
TE                298.2 K
D1            2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 11.00 usec
PLW1         26.50000000 W
SFO1         600.1937064 MHz

F2 - Processing parameters
SI                 65536
SF           600.1899953 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```



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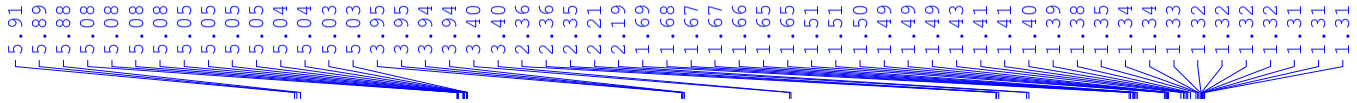
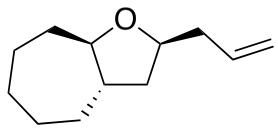
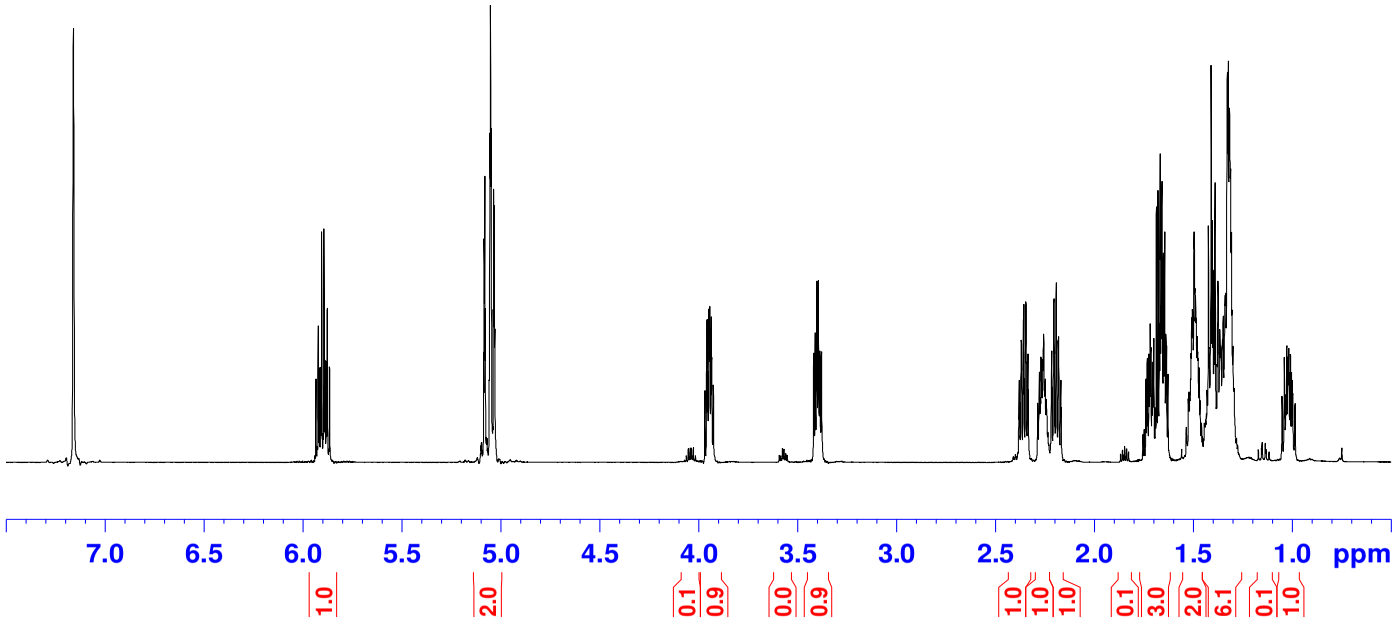
```
Current Data Parameters
NAME         VTT-IV-16-A
EXPNO                  6
PROCNO                 1

F2 - Acquisition Parameters
Date_           20120917
Time               16.41
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT             C6D6
NS                   128
DS                     0
SWH            36057.691 Hz
FIDRES          0.550197 Hz
AQ             0.9088159 sec
RG                184.65
DW                13.867 usec
DE                 6.50 usec
TE                298.5 K
D1            2.50000000 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                10.65 usec
PLW1        104.00000000 W
SFO1         150.9329866 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             70.00 usec
PLW2         26.50000000 W
PLW12         0.65438998 W
PLW13         0.32065001 W
SFO2         600.1924008 MHz

F2 - Processing parameters
SI                 32768
SF           150.9178394 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

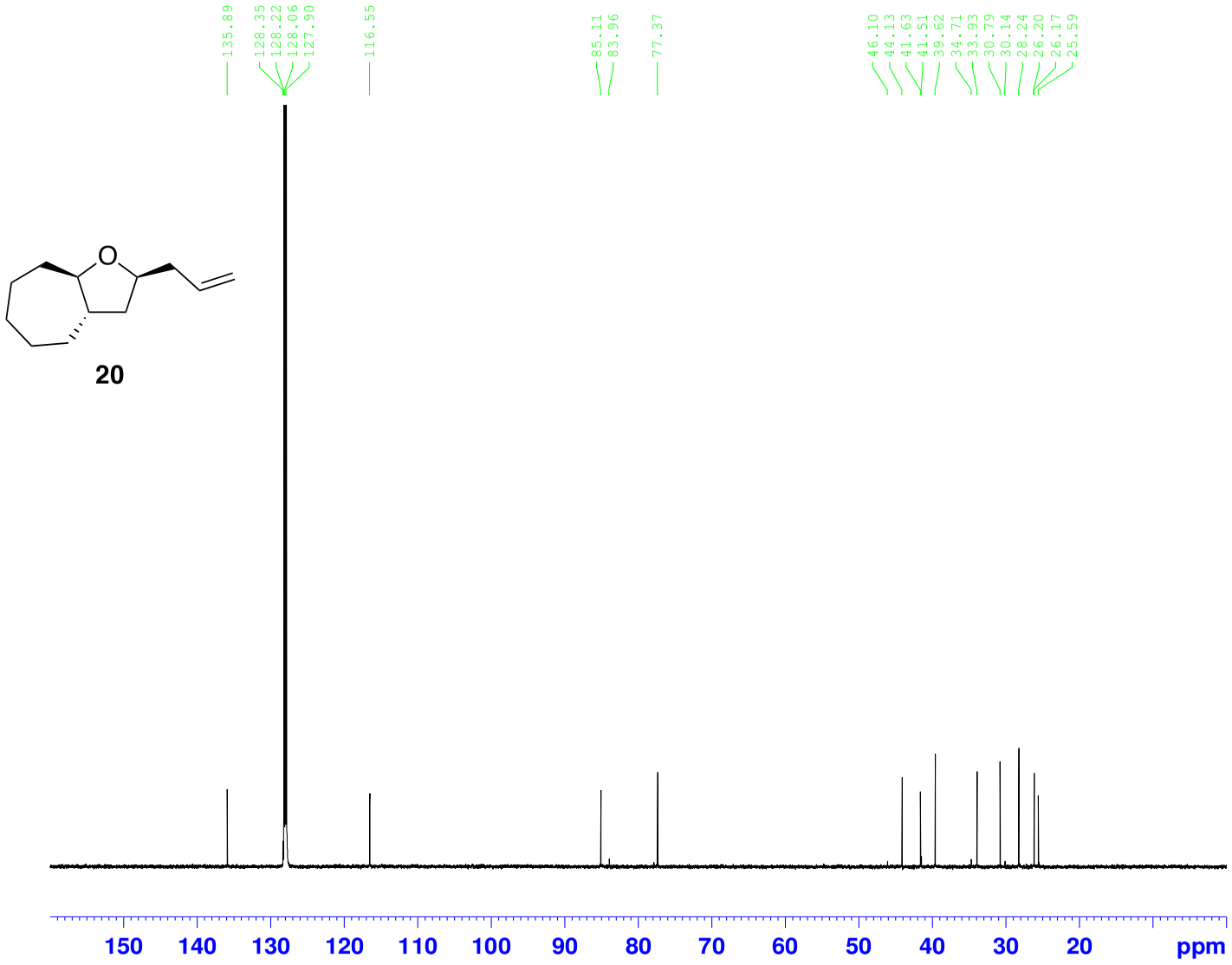




20




```
Current Data Parameters
NAME         VTT-IV-85-A
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20130307
Time               18.42
INSTRUM            spect
PROBHD   5 mm PAQXI 1H/
PULPROG             zg30
TD                 65536
SOLVENT             C6D6
NS                     8
DS                     0
SWH            12335.526 Hz
FIDRES          0.188225 Hz
AQ             2.6564426 sec
RG                 33.59
DW                40.533 usec
DE                 6.50 usec
TE                298.2 K
D1            2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 9.79 usec
PLW1          9.30000019 W
SFO1        600.1937064 MHz

F2 - Processing parameters
SI                 65536
SF          600.1899947 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```



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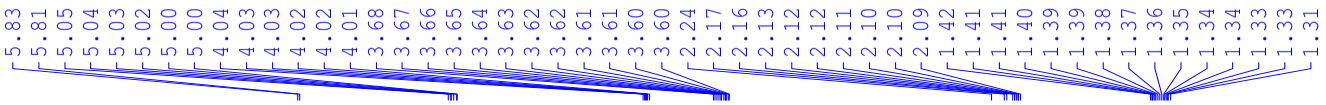
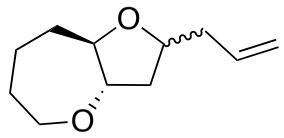
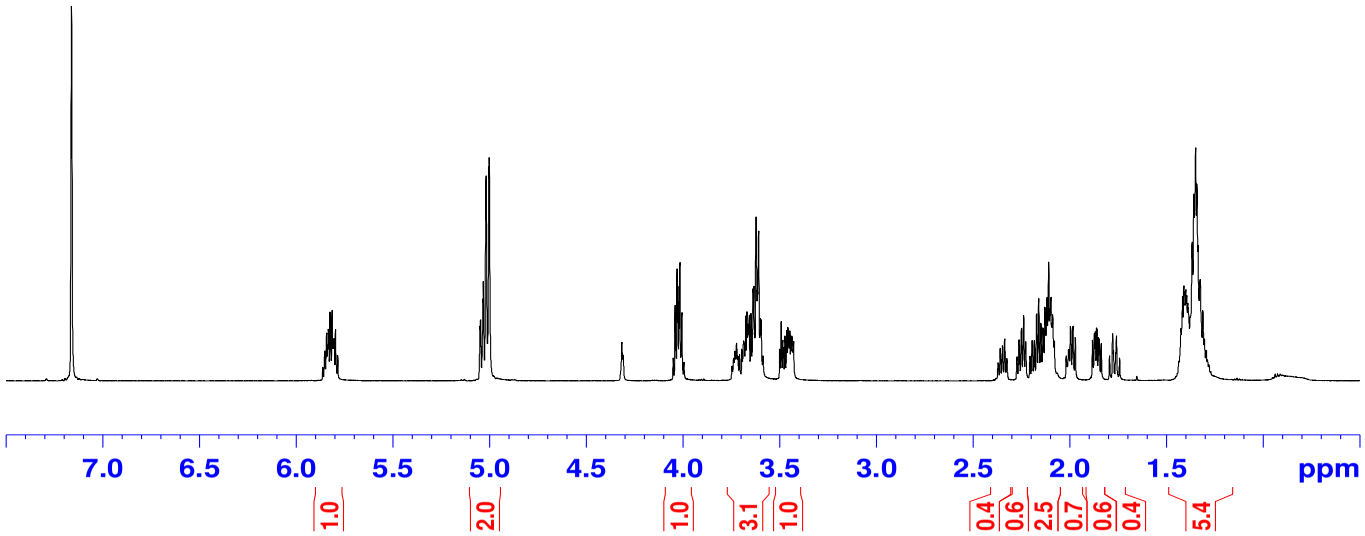
```
Current Data Parameters
NAME         VTT-IV-85-A
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20130307
Time               18.44
INSTRUM            spect
PROBHD   5 mm PAQXI 1H/
PULPROG          zgpg30
TD                65536
SOLVENT             C6D6
NS                   128
DS                     0
SWH            36057.691 Hz
FIDRES          0.550197 Hz
AQ              0.9088159 sec
RG                184.65
DW                13.867 usec
DE                 6.50 usec
TE                298.2 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                 15.00 usec
PLW1        106.00000000 W
SFO1         150.9329866 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                  1H
PCPD2              70.00 usec
PLW2           9.30000019 W
PLW12          0.18190999 W
PLW13          0.08913500 W
SFO2          600.1924008 MHz

F2 - Processing parameters
SI                 32768
SF           150.9178381 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

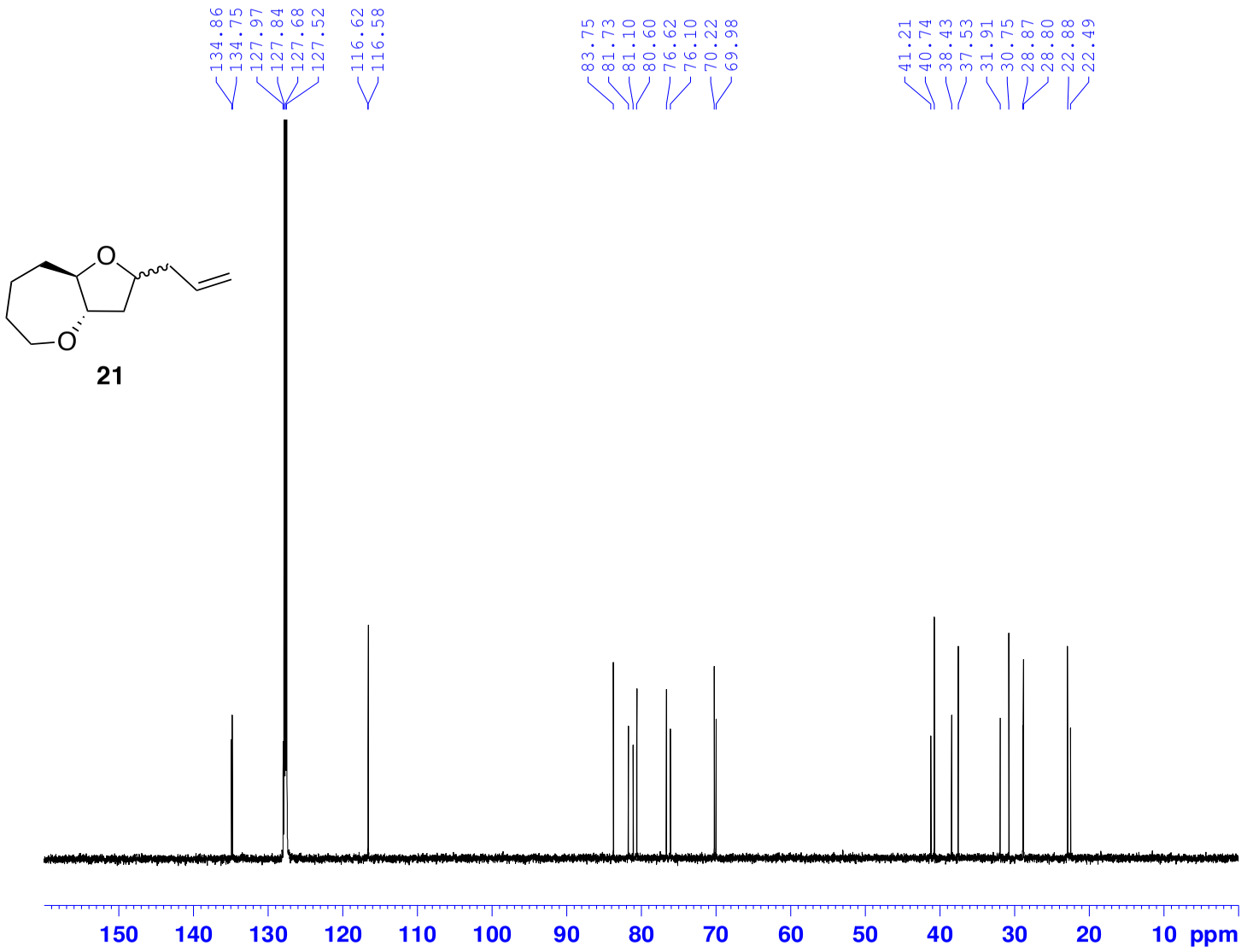




21

```
Current Data Parameters
NAME       VTT-III-200-A
EXPNO                  5
PROCNO                 1

F2 - Acquisition Parameters
Date_           20120813
Time               15.58
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT             C6D6
NS                     8
DS                     0
SWH            12335.526 Hz
FIDRES          0.188225 Hz
AQ             2.6564426 sec
RG                 76.07
DW                40.533 usec
DE                 6.50 usec
TE                298.1 K
D1            2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                11.00 usec
PLW1         26.50000000 W
SFO1         600.1937064 MHz

F2 - Processing parameters
SI                 65536
SF           600.1899954 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```





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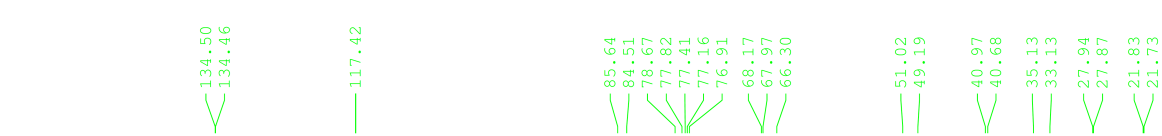
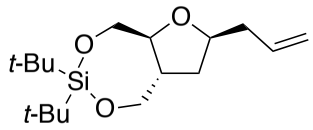
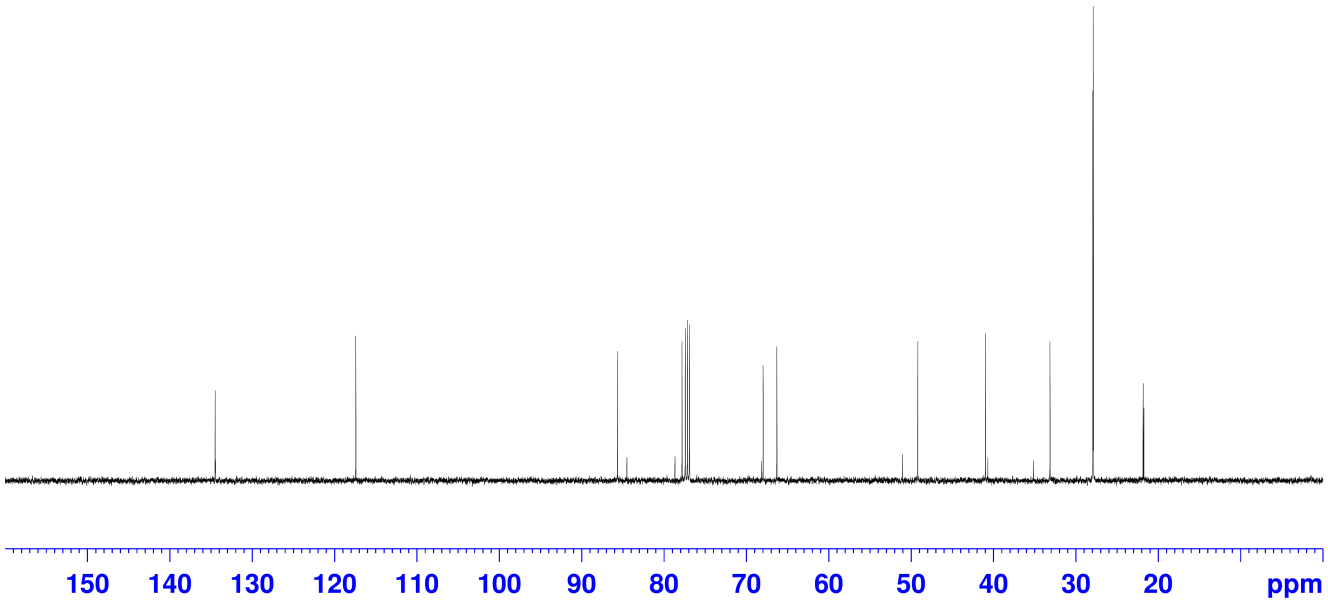
```
Current Data Parameters
NAME      VTT-III-200-A
EXPNO                 6
PROCNO                1

F2 - Acquisition Parameters
Date_          20120813
Time              16.00
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD               65536
SOLVENT           C6D6
NS                 128
DS                   0
SWH          36057.691 Hz
FIDRES        0.550197 Hz
AQ           0.9088159 sec
RG              184.65
DW              13.867 usec
DE                6.50 usec
TE              298.2 K
D1          2.00000000 sec
D11         0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                13C
P1                10.65 usec
PLW1       104.00000000 W
SFO1        150.9329866 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2            70.00 usec
PLW2        26.50000000 W
PLW12        0.65438998 W
PLW13        0.32065001 W
SFO2        600.1924008 MHz

F2 - Processing parameters
SI                32768
SF          150.9178960 MHz
WDW                EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

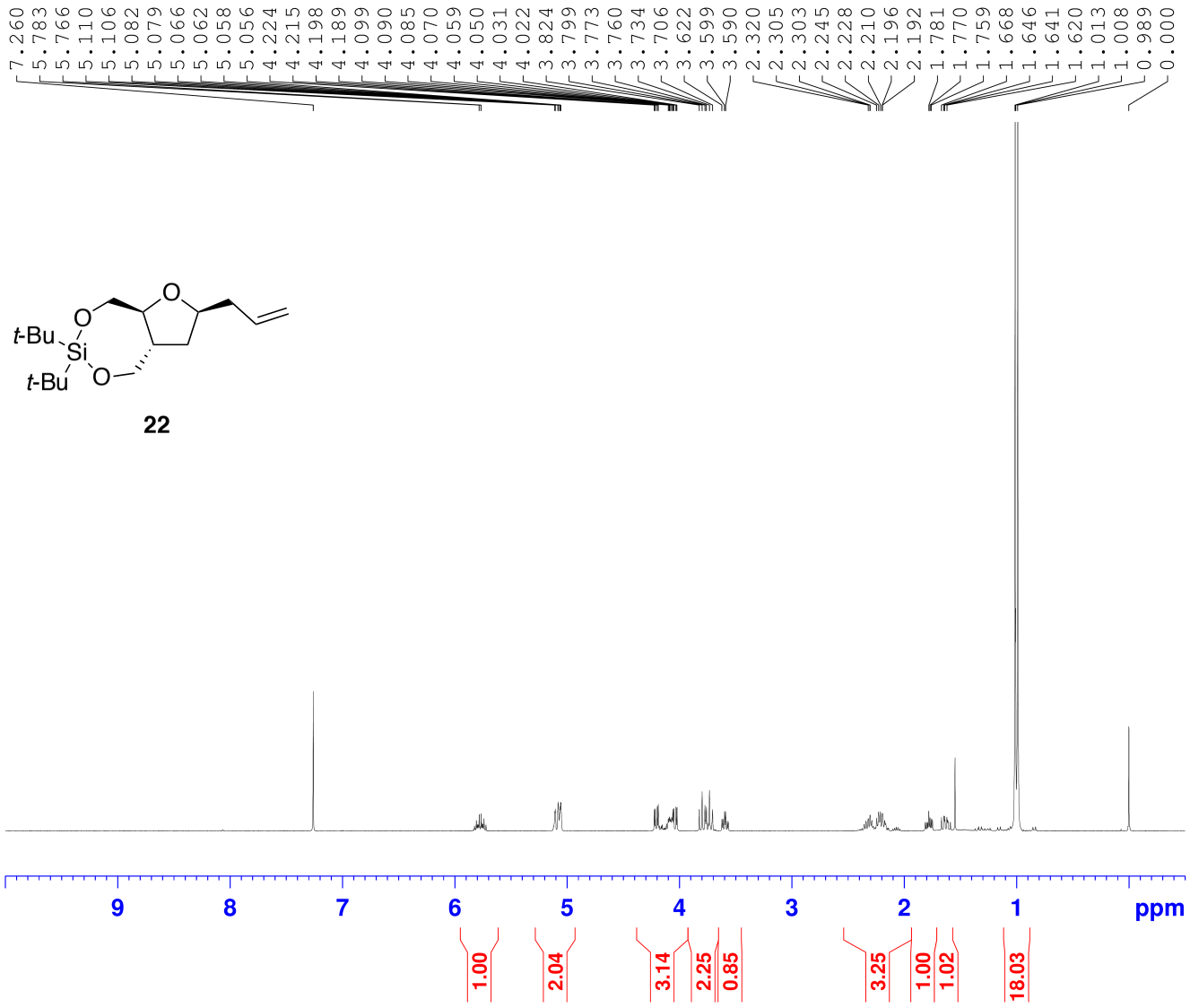




22

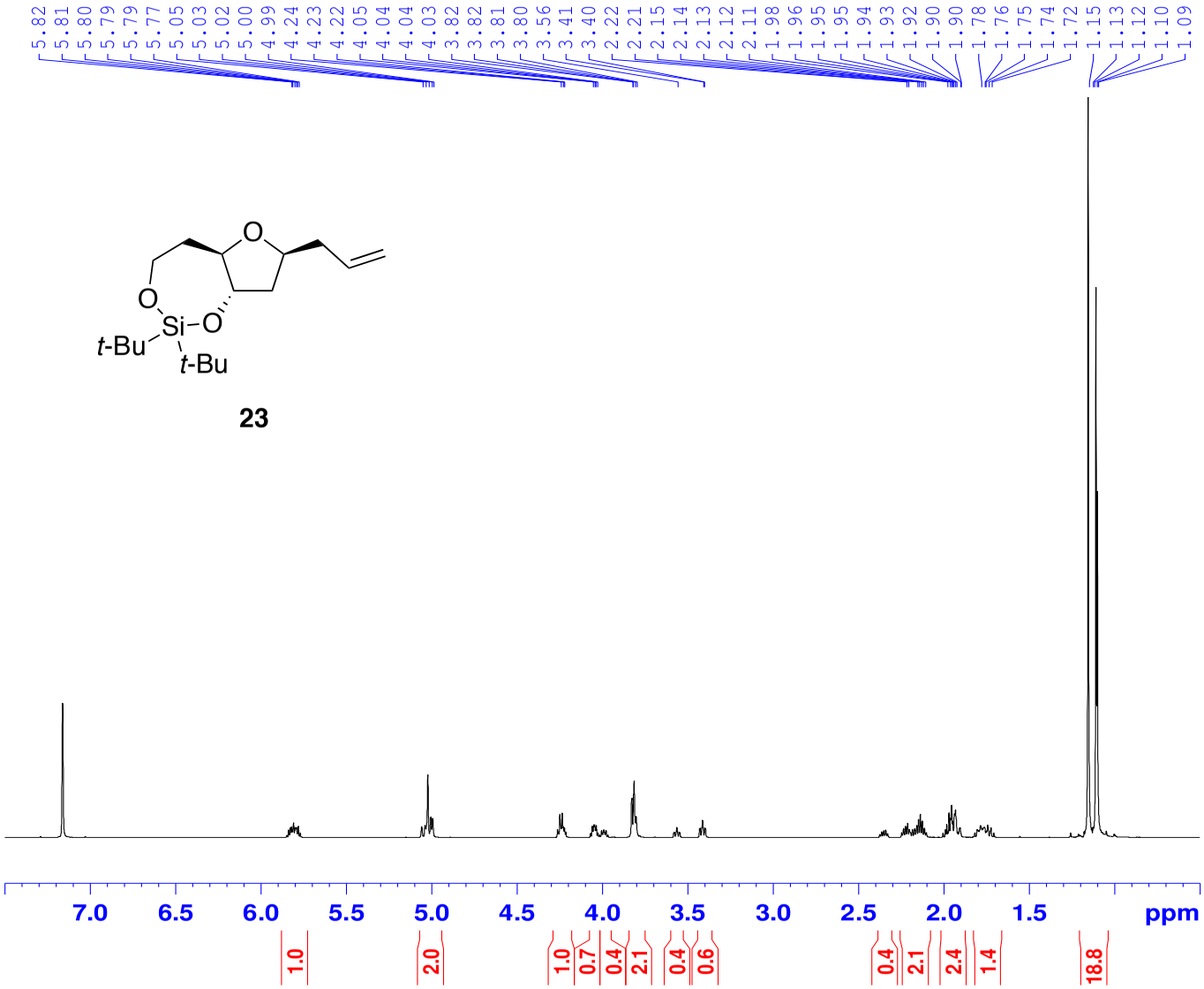



```
Current Data Parameters
NAME       VTT-II-153-A2
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20110921
Time               15.43
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                   35
DS                    4
SWH           30030.029 Hz
FIDRES         0.458222 Hz
AQ             1.0912244 sec
RG                32768
DW               16.650 usec
DE                6.50 usec
TE                298.5 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                10.25 usec
PL1                2.00 dB
PL1W        49.29017639 W
SFO1       125.7877161 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             70.00 usec
PL2               -3.00 dB
PL12              14.63 dB
PL13              14.91 dB
PL2W        37.58904266 W
PL12W        0.64872593 W
PL13W        0.60822082 W
SFO2       500.2010008 MHz

F2 - Processing parameters
SI                32768
SF         125.7751222 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```



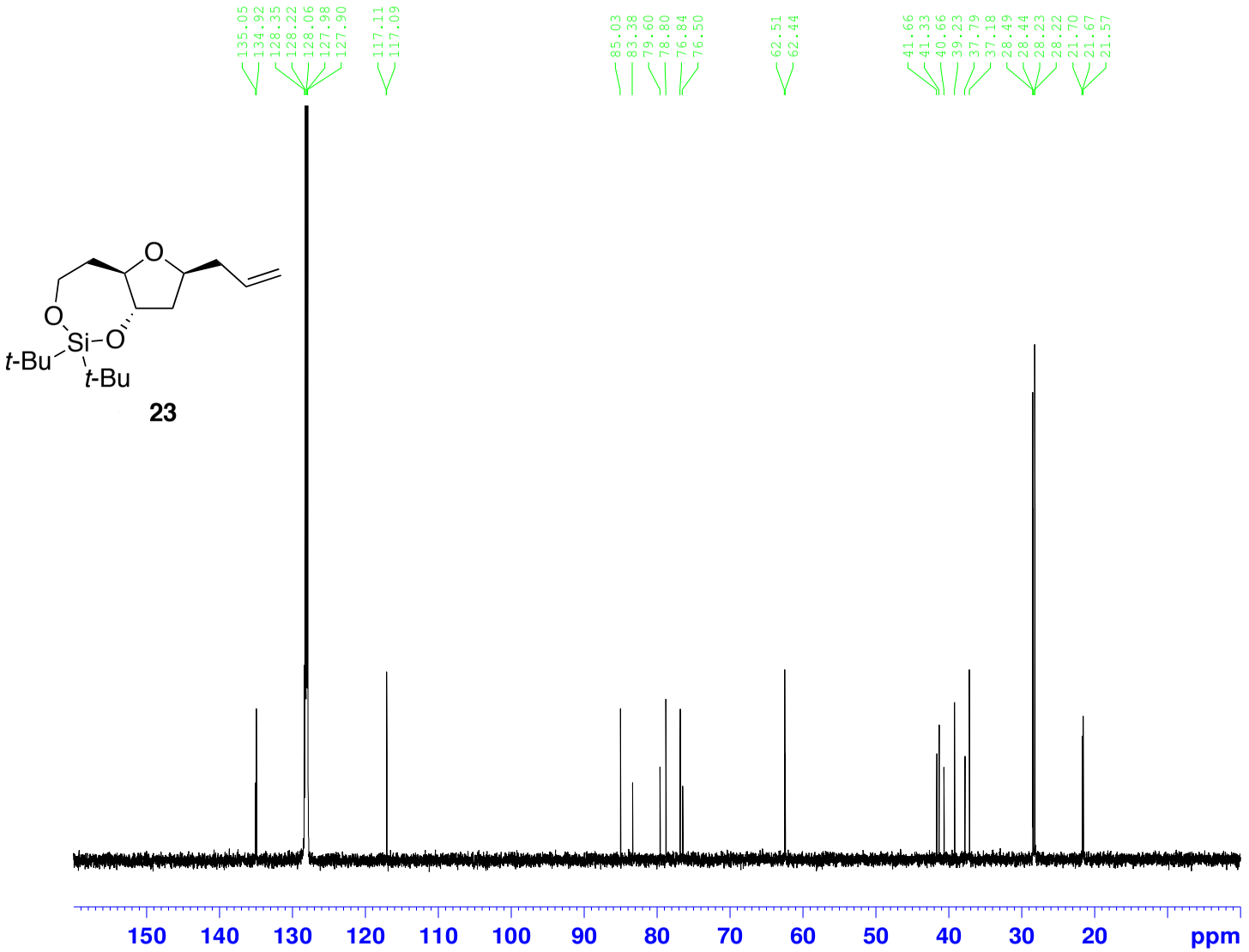
BRUKER

```
Current Data Parameters
NAME        VTT-II-186-A
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameter
Date_           20111103
Time               18.21
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8278.146 Hz
FIDRES          0.126314 Hz
AQ              3.9584243 se
RG                   256
DW                60.400 us
DE                 6.50 us
TE                298.2 K
D1           2.00000000 se
TD0                    1

======== CHANNEL f1 ======
NUC1                  1H
P1                 8.10 us
PL1               -5.00 dE
PL1W        31.77312851 W
SFO1       400.1324710 MH

F2 - Processing parameters
SI                 32768
SF          400.1300091 MH
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```



23

```
Current Data Parameters
NAME         VTT-IV-95-A
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20130321
Time               19.50
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT             C6D6
NS                     8
DS                     0
SWH            12335.526 Hz
FIDRES          0.188225 Hz
AQ             2.6564426 sec
RG                 33.59
DW                40.533 usec
DE                 6.50 usec
TE                298.1 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 11.00 usec
PLW1         26.50000000 W
SFO1        600.1937064 MHz

F2 - Processing parameters
SI                 65536
SF          600.1899953 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```



23

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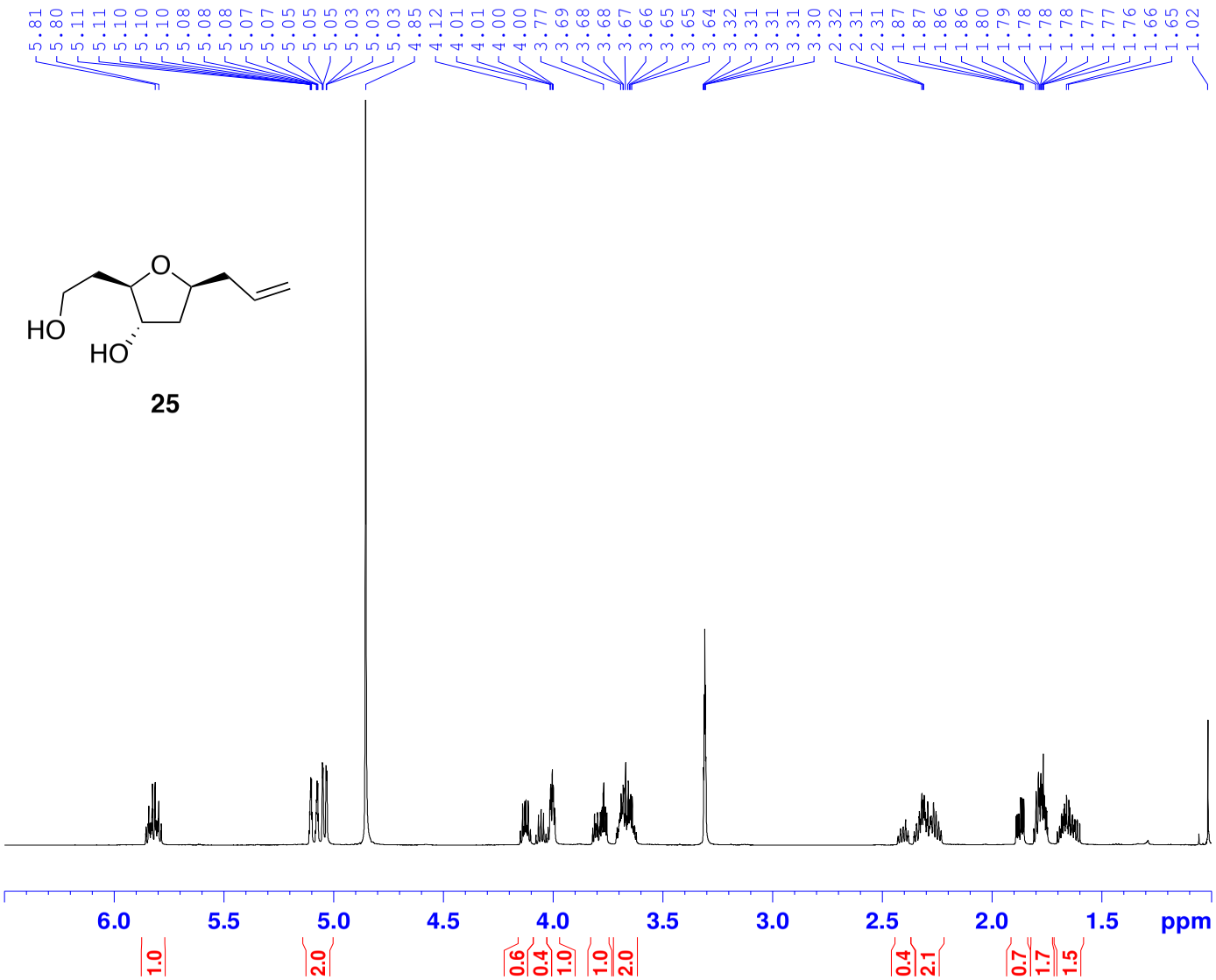
```
Current Data Parameters
NAME          VTT-IV-95-A
EXPNO                   6
PROCNO                  1

F2 - Acquisition Parameters
Date_            20130321
Time                21.39
INSTRUM             spect
PROBHD    5 mm PABBO BB/
PULPROG           zgpg30
TD                 65536
SOLVENT              C6D6
NS                    128
DS                      0
SWH             36057.691 Hz
FIDRES          0.550197 Hz
AQ              0.9088159 sec
RG                 184.65
DW                 13.867 usec
DE                   6.50 usec
TE                  298.1 K
D1             2.50000000 sec
D11            0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   13C
P1                   10.65 usec
PLW1         104.00000000 W
SFO1          150.9329866 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                   1H
PCPD2                70.00 usec
PLW2          26.50000000 W
PLW12          0.65438998 W
PLW13          0.32065001 W
SFO2          600.1924008 MHz

F2 - Processing parameters
SI                    32768
SF            150.9178388 MHz
WDW                     EM
SSB       0
LB                   1.00 Hz
GB        0
PC                   1.40
```



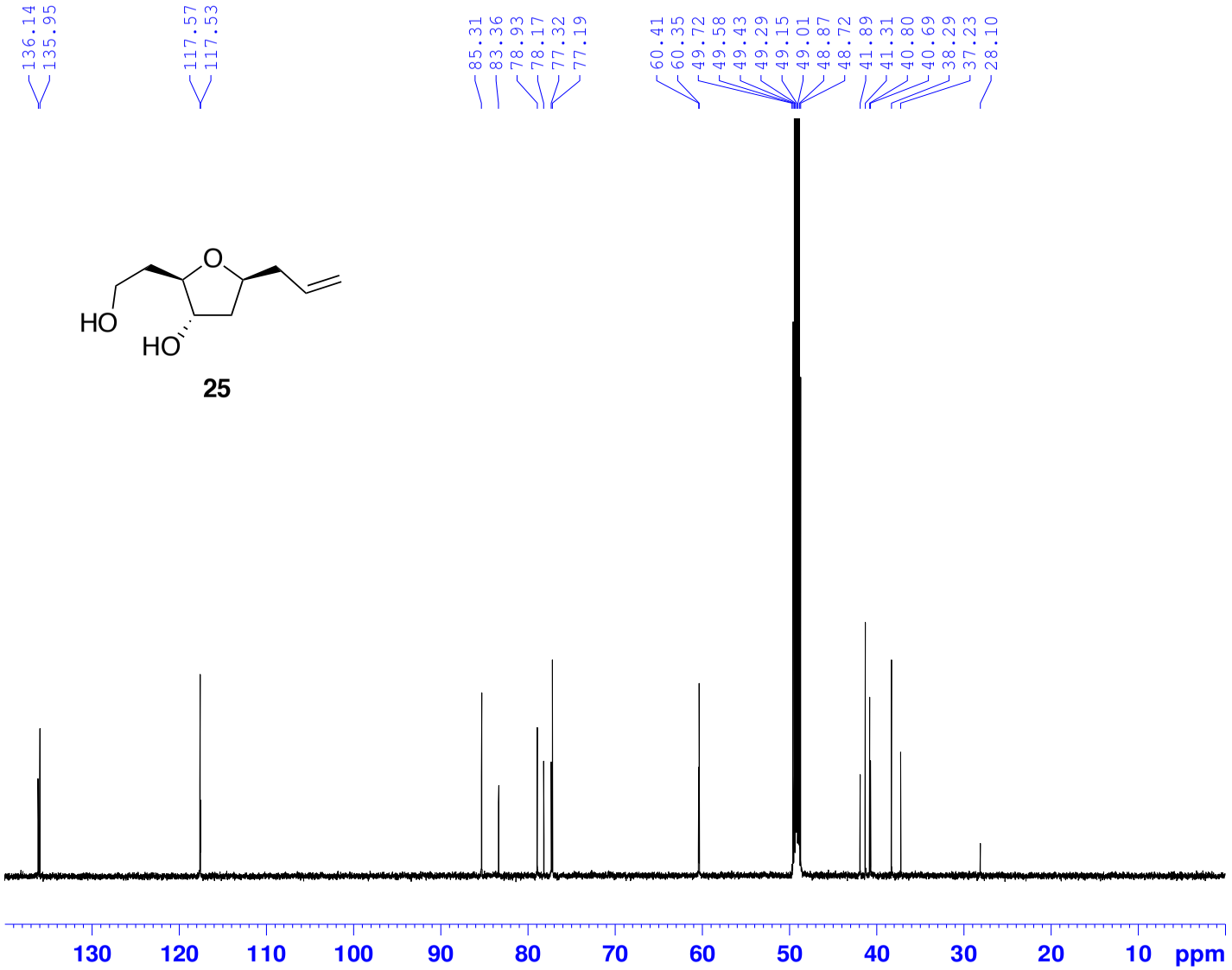
BRUKER

```
Current Data Parameters
NAME         VTT-IV-97-A
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20130328
Time               21.04
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT             MeOD
NS                    16
DS                     0
SWH            12335.526 Hz
FIDRES          0.188225 Hz
AQ             2.6564426 sec
RG                 33.59
DW                40.533 usec
DE                 6.50 usec
TE                298.1 K
D1             2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 11.00 usec
PLW1         26.50000000 W
SFO1         600.1937064 MHz

F2 - Processing parameters
SI                 65536
SF           600.1900117 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```



BRUKER

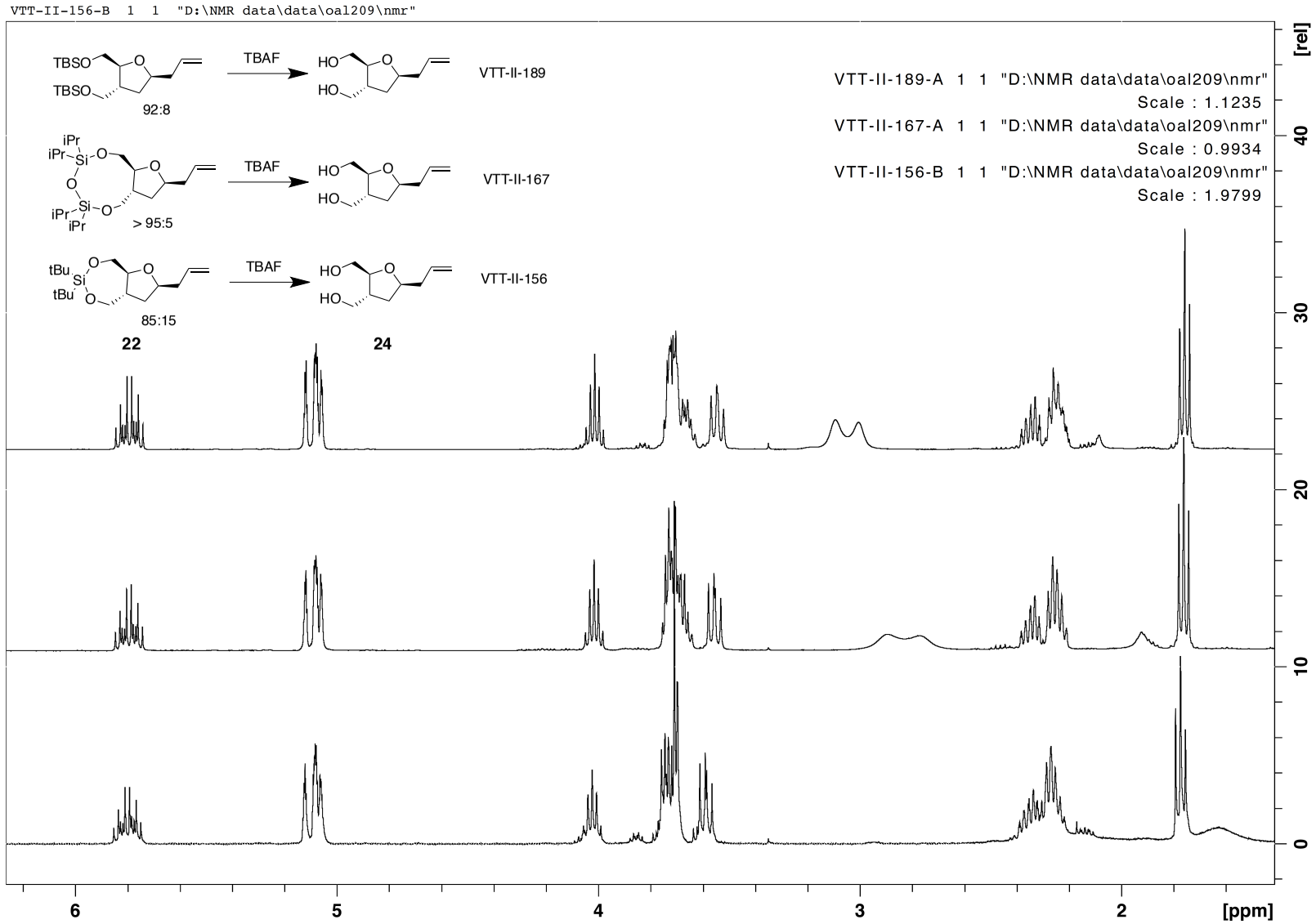
```
Current Data Parameters
NAME         VTT-IV-97-A
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20130328
Time               21.07
INSTRUM            spect
PROBHD    5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT             MeOD
NS                   955
DS                     0
SWH            36057.691 Hz
FIDRES         0.550197 Hz
AQ             0.9088159 sec
RG                184.65
DW                13.867 usec
DE                 6.50 usec
TE                298.1 K
D1            2.50000000 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                10.65 usec
PLW1        104.00000000 W
SFO1         150.9329866 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2             70.00 usec
PLW2         26.50000000 W
PLW12         0.65438998 W
PLW13         0.32065001 W
SFO2         600.1924008 MHz

F2 - Processing parameters
SI                 32768
SF           150.9176618 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```


VTT-II-156-B 1 1 "D:\NMR data\data\oal209\nmr"
TBSO
TBSO
92:8
TBAF
HO
HO
VTT-II-189
iPr
iPr
Si
O
O
Si
iPr
iPr
> 95:5
TBAF
VTT-II-167
tBu
Si
tBu
85:15
TBAF
VTT-II-156
22
24
VTT-II-189-A 1 1 "D:\NMR data\data\oal209\nmr"
Scale : 1.1235
VTT-II-167-A 1 1 "D:\NMR data\data\oal209\nmr"
Scale : 0.9934
VTT-II-156-B 1 1 "D:\NMR data\data\oal209\nmr"
Scale : 1.9799
[rel]
40
30
20
10
0
6
5
4
3
2
[ppm]