Electronic Supplementary Information

Triphenylphosphine-mediated Reaction of Dialkyl Azodicarboxylate with Activated Alkenes Leading to Pyrazolines

Shoko Yamazaki,*[a] Yuta Maenaka,[a] Ken Fujinami,[a] and Yuji Mikata[b]

[a]*Department of Chemistry, Nara University of Education, Takabatake-cho, Nara 630-8528, Japan,* [b]*KYOUSEI Science Center, Nara Women's University, Nara 630-8506, Japan*

yamazaks@nara-edu.ac.jp

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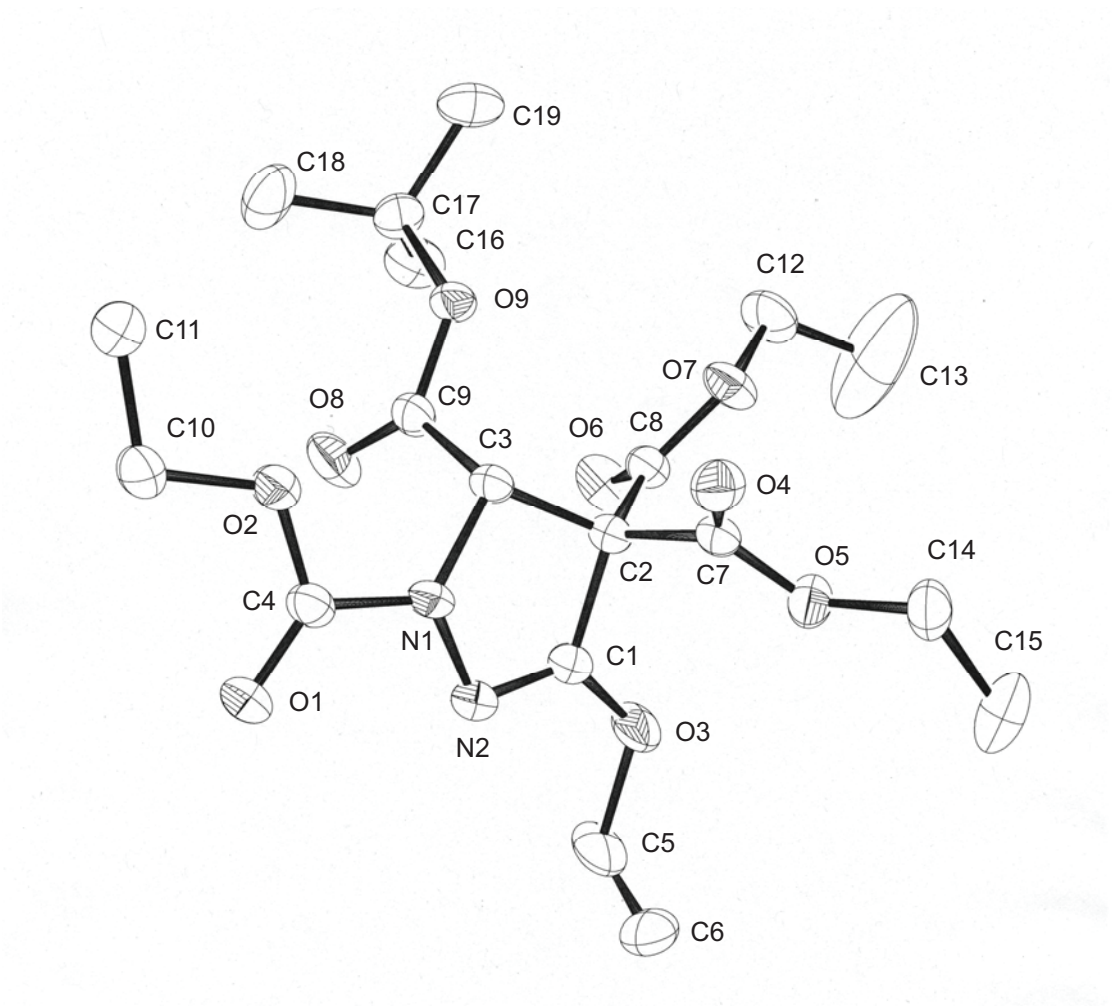


Figure S1. ORTEP drawing of the pyrazoline derivative **3a** (thermal ellipsoids are drawn at 50% probability). Hydrogen and disordered carbon (C20) atoms were omitted for clarity.

X-ray Structure Report

for

Compound **3a**

(CCDC 877668)

Experimental

Data Collection

A colorless unknown crystal of $C_{19}H_{30}N_2O_9$ having approximate dimensions of 0.600 x 0.300 x 0.300 mm was mounted on a glass fiber. All measurements were made on a Rigaku Mercury70 diffractometer using graphite monochromated Mo-Kα radiation.

The crystal-to-detector distance was 45.01 mm.

Cell constants and an orientation matrix for data collection corresponded to a primitive triclinic cell with dimensions:

a	=	9.214(2) Å	α	=	99.651(2)^o
b	=	9.256(2) Å	β	=	96.668(2)^o
c	=	14.723(3) Å	γ	=	112.748(2)^o
V	=	1118.7(4) Å^3			

For Z = 2 and F.W. = 430.45, the calculated density is 1.278 g/cm^3. Based on a statistical analysis of intensity distribution, and the successful solution and refinement of the structure, the space group was determined to be:

P-1 (#2)

The data were collected at a temperature of -149 $\pm$ 1^{o}C to a maximum 2θ value of 54.9^o. A total of 720 oscillation images were collected. A sweep of data was done using ω oscillations from -70.0 to 110.0^o in 0.5^o steps. The exposure rate was 60.0 [sec./^{o}]. The detector swing angle was 20.10^o. A second sweep was performed using ω oscillations from -70.0 to 110.0^o in 0.5^o steps. The exposure rate was 60.0 [sec./^{o}]. The detector swing angle was 20.10^o. The crystal-to-detector distance was 45.01 mm. Readout was performed in the 0.137 mm pixel mode.

Data Reduction

Of the 8677 reflections that were collected, 4855 were unique (R_{int} = 0.0122); equivalent reflections were merged. Data were collected and processed using CrystalClear (Rigaku).

The linear absorption coefficient, μ, for Mo-Kα radiation is 1.015 cm^{-1}. An empirical absorption correction was applied which resulted in transmission factors ranging from 0.836 to 0.970. The data were corrected for Lorentz and polarization effects.

Structure Solution and Refinement

The structure was solved by direct methods[2] and expanded using Fourier techniques. The non-hydrogen atoms were refined anisotropically. Hydrogen atoms were refined using the riding model. The final cycle of full-matrix least-squares refinement[3] on F^2 was based on 4855 observed reflections and 280 variable parameters and converged (largest parameter shift was 0.00 times its esd) with unweighted and weighted agreement factors of:

$$R1 = \Sigma \, ||Fo| - |Fc|| \, / \, \Sigma \, |Fo| = 0.0600$$

$$wR2 = [\Sigma \, (w \, (Fo^2 - Fc^2)^2 \,) / \, \Sigma \, w(Fo^2)^2]^{1/2} = 0.1697$$

The standard deviation of an observation of unit weight[4] was 1.06. Unit weights were used. The maximum and minimum peaks on the final difference Fourier map corresponded to 0.71 and -0.58 $e^-/Å^3$, respectively.

Neutral atom scattering factors were taken from Cromer and Waber[5]. Anomalous dispersion effects were included in Fcalc[6]; the values for Δf' and Δf'' were those of Creagh and McAuley[7]. The values for the mass attenuation coefficients are those of Creagh and Hubbell[8]. All calculations were performed using the CrystalStructure[9] crystallographic software package except for refinement, which was performed using SHELXL-97[10].

References

(1) CrystalClear: Rigaku Corporation, 1999. CrystalClear Software User's Guide, Molecular Structure Corporation, (c) 2000.J.W.Pflugrath (1999) Acta Cryst. D55, 1718-1725.

(2) SHELX97: Sheldrick, G.M. (2008). Acta Cryst. A64, 112-122.

(3) Least Squares function minimized: (SHELXL97)

$\Sigma w(F_o^2-F_c^2)^2$ where w = Least Squares weights.

(4) Standard deviation of an observation of unit weight:

$[\Sigma w(F_o^2-F_c^2)^2/(N_o-N_v)]^{1/2}$

where: N_o = number of observations
N_v = number of variables

(5) Cromer, D. T. & Waber, J. T.; "International Tables for X-ray Crystallography", Vol. IV, The Kynoch Press, Birmingham, England, Table 2.2 A (1974).

(6) Ibers, J. A. & Hamilton, W. C.; Acta Crystallogr., 17, 781 (1964).

(7) Creagh, D. C. & McAuley, W.J .; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.6.8, pages 219-222 (1992).

(8) Creagh, D. C. & Hubbell, J.H..; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.4.3, pages 200-206 (1992).

(9) CrystalStructure 4.0: Crystal Structure Analysis Package, Rigaku Corporation (2000-2010). Tokyo 196-8666, Japan.

(10) SHELX97: Sheldrick, G.M. (2008). Acta Cryst. A64, 112-122.

EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	$C_{19}H_{30}N_2O_9$
Formula Weight	430.45
Crystal Color, Habit	colorless, unknown
Crystal Dimensions	0.600 X 0.300 X 0.300 mm
Crystal System	triclinic
Lattice Type	Primitive
Lattice Parameters	a = 9.214(2) Å b = 9.256(2) Å c = 14.723(3) Å α = 99.651(2) ^{o} β = 96.668(2) ^{o} γ = 112.748(2) ^{o} V = 1118.7(4) Å^3
Space Group	P-1 (#2)
Z value	2
D_{calc}	1.278 g/cm^3
F_{000}	460.00
μ(MoKα)	1.015 cm^{-1}

B. Intensity Measurements

Diffractometer	Mercury70
Radiation	MoKα (λ = 0.71070 Å) graphite monochromated
Voltage, Current	50kV, 40mA
Temperature	-149.8°C
Detector Aperture	70 x 70 mm
Data Images	720 exposures
ω oscillation Range	-70.0 - 110.0°
Exposure Rate	60.0 sec./°
Detector Swing Angle	20.10°
ω oscillation Range	-70.0 - 110.0°
Exposure Rate	60.0 sec./°
Detector Swing Angle	20.10°
Detector Position	45.01 mm
Pixel Size	0.137 mm
$2\theta_{max}$	54.9°
No. of Reflections Measured	Total: 8677 Unique: 4855 (R_{int} = 0.0122)
Corrections	Lorentz-polarization Absorption (trans. factors: 0.836 - 0.970)

C. Structure Solution and Refinement

Structure Solution	Direct Methods (SHELX97)
Refinement	Full-matrix least-squares on F^2
Function Minimized	Σ w $(Fo^2 - Fc^2)^2$
Least Squares Weights	$w = 1/ [\sigma^2(Fo^2) + (0.0885 \cdot P)^2 + 0.6683 \cdot P]$ where $P = (Max(Fo^2,0) + 2Fc^2)/3$
$2\theta_{max}$ cutoff	54.9^o
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (All reflections)	4855
No. Variables	280
Reflection/Parameter Ratio	17.34
Residuals: R1 (I>2.00σ(I))	0.0600
Residuals: R (All reflections)	0.0657
Residuals: wR2 (All reflections)	0.1697
Goodness of Fit Indicator	1.060
Max Shift/Error in Final Cycle	0.000
Maximum peak in Final Diff. Map	0.71 $e^-/Å^3$
Minimum peak in Final Diff. Map	-0.58 $e^-/Å^3$

Table 1. Atomic coordinates and B_{iso}/B_{eq} and occupancy

atom	x	y	z	B_{eq}	occ
O1	1.3811(2)	0.8598(2)	0.32493(10)	2.83(3)	1
O2	1.2688(2)	0.7015(2)	0.42230(9)	2.38(3)	1
O3	0.8735(2)	0.5759(3)	0.07240(10)	3.70(4)	1
O4	0.7458(2)	0.6433(2)	0.33988(10)	2.61(3)	1
O5	0.6415(2)	0.5850(2)	0.18534(10)	2.55(3)	1
O6	0.7917(2)	0.2529(2)	0.12336(11)	3.25(3)	1
O7	0.6198(2)	0.2735(2)	0.21596(10)	2.72(3)	1
O8	1.1548(2)	0.4003(2)	0.26677(12)	3.27(3)	1
O9	0.9488(2)	0.2928(2)	0.34072(9)	2.07(3)	1
N1	1.1144(2)	0.6860(2)	0.29192(11)	2.08(3)	1
N2	1.0897(2)	0.7010(2)	0.19835(11)	2.38(3)	1
C1	0.9462(3)	0.6010(3)	0.16077(13)	2.32(3)	1
C2	0.8504(2)	0.5086(2)	0.22580(12)	1.92(3)	1
C3	0.9892(2)	0.5407(2)	0.30700(12)	1.86(3)	1
C4	1.2676(2)	0.7581(2)	0.34412(13)	2.09(3)	1
C5	0.9669(3)	0.6752(5)	0.0147(3)	6.45(10)	1
C6	0.9506(5)	0.8118(5)	0.0162(3)	3.33(7)	0.600
C7	0.7399(2)	0.5874(2)	0.25912(13)	2.04(3)	1
C8	0.7508(2)	0.3297(2)	0.18031(12)	2.12(3)	1
C9	1.0444(2)	0.4032(2)	0.30159(13)	2.05(3)	1
C10	1.4246(3)	0.7558(3)	0.4832(2)	2.85(4)	1
C11	1.4003(3)	0.6573(3)	0.5549(2)	3.35(4)	1
C12	0.5134(3)	0.1025(3)	0.1815(2)	3.37(4)	1
C13	0.3815(6)	0.0802(6)	0.1161(6)	15.3(4)	1
C14	0.5222(3)	0.6481(3)	0.2041(2)	2.90(4)	1
C15	0.4575(4)	0.6734(4)	0.1124(2)	4.33(6)	1
C16	0.9441(3)	0.0430(3)	0.2488(2)	3.23(4)	1
C17	0.9696(3)	0.1425(2)	0.3468(2)	2.46(4)	1
C18	1.1336(3)	0.1867(3)	0.4052(2)	4.34(6)	1
C19	0.8372(3)	0.0600(3)	0.3968(2)	3.20(4)	1
C20	0.8666(8)	0.7038(9)	-0.0553(5)	3.82(11)	0.400

$B_{eq} = 8/3\ \pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos\gamma + 2U_{13}(aa^*cc^*)\cos\beta + 2U_{23}(bb^*cc^*)\cos\alpha)$

Table 2. Atomic coordinates and B_{iso} involving hydrogen atoms

atom	x	y	z	B_{iso}	occ
H3	0.9588	0.5645	0.3690	2.23	1
H10A	1.4654	0.8716	0.5139	3.41	1
H10B	1.5030	0.7400	0.4466	3.41	1
H11A	1.3043	0.6520	0.5792	4.02	1
H11B	1.4941	0.7067	0.6066	4.02	1
H11C	1.3866	0.5482	0.5260	4.02	1
H12A	0.5734	0.0449	0.1524	4.04	1
H12B	0.4767	0.0563	0.2350	4.04	1
H13A	0.3314	-0.0318	0.0798	18.35	1
H13B	0.4159	0.1523	0.0736	18.35	1
H13C	0.3037	0.1044	0.1486	18.35	1
H14A	0.5725	0.7511	0.2521	3.49	1
H14B	0.4348	0.5704	0.2272	3.49	1
H15A	0.4228	0.5746	0.0633	5.19	1
H15B	0.5416	0.7618	0.0951	5.19	1
H15C	0.3658	0.7004	0.1191	5.19	1
H16A	1.0269	0.1027	0.2165	3.88	1
H16B	0.8378	0.0206	0.2135	3.88	1
H16C	0.9509	-0.0588	0.2530	3.88	1
H18A	1.2167	0.2373	0.3705	5.21	1
H18B	1.1411	0.0892	0.4184	5.21	1
H18C	1.1492	0.2622	0.4646	5.21	1
H19A	0.7331	0.0395	0.3594	3.84	1
H19B	0.8538	0.1295	0.4586	3.84	1
H19C	0.8390	-0.0423	0.4048	3.84	1

Table 3. Anisotropic displacement parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
O1	0.0252(7)	0.0319(7)	0.0459(9)	0.0031(6)	0.0078(6)	0.0181(7)
O2	0.0247(7)	0.0307(7)	0.0302(7)	0.0053(6)	0.0042(6)	0.0110(6)
O3	0.0264(8)	0.0773(12)	0.0344(8)	0.0104(8)	0.0094(6)	0.0316(8)
O4	0.0367(8)	0.0338(7)	0.0343(8)	0.0189(6)	0.0109(6)	0.0095(6)
O5	0.0274(7)	0.0350(7)	0.0371(8)	0.0156(6)	0.0044(6)	0.0095(6)
O6	0.0377(8)	0.0344(8)	0.0411(9)	0.0072(7)	0.0143(7)	-0.0028(7)
O7	0.0294(7)	0.0251(7)	0.0446(8)	0.0039(6)	0.0155(6)	0.0097(6)
O8	0.0312(8)	0.0308(7)	0.0692(11)	0.0139(6)	0.0258(8)	0.0161(7)
O9	0.0274(7)	0.0207(6)	0.0334(7)	0.0100(5)	0.0091(6)	0.0113(5)
N1	0.0236(8)	0.0226(7)	0.0306(8)	0.0042(6)	0.0064(6)	0.0127(6)
N2	0.0258(8)	0.0335(8)	0.0331(9)	0.0097(7)	0.0087(7)	0.0176(7)
C1	0.0249(9)	0.0356(10)	0.0300(9)	0.0109(8)	0.0088(8)	0.0159(8)
C2	0.0232(9)	0.0246(8)	0.0265(9)	0.0086(7)	0.0085(7)	0.0103(7)
C3	0.0224(8)	0.0196(8)	0.0283(9)	0.0064(7)	0.0071(7)	0.0092(7)
C4	0.0254(9)	0.0216(8)	0.0323(9)	0.0080(7)	0.0084(8)	0.0085(7)
C5	0.0341(13)	0.153(4)	0.067(2)	0.022(2)	0.0200(13)	0.085(3)
C6	0.049(3)	0.052(2)	0.038(2)	0.026(2)	0.016(2)	0.026(2)
C7	0.0222(9)	0.0216(8)	0.0338(10)	0.0065(7)	0.0079(7)	0.0116(7)
C8	0.0239(9)	0.0268(9)	0.0280(9)	0.0077(7)	0.0062(7)	0.0085(7)
C9	0.0225(9)	0.0219(8)	0.0323(9)	0.0070(7)	0.0062(7)	0.0081(7)
C10	0.0245(9)	0.0380(11)	0.0366(11)	0.0036(8)	0.0013(8)	0.0113(9)
C11	0.0331(11)	0.0534(13)	0.0408(12)	0.0147(10)	0.0055(9)	0.0202(10)
C12	0.0333(11)	0.0258(10)	0.058(2)	-0.0001(9)	0.0100(10)	0.0109(10)
C13	0.088(3)	0.063(3)	0.342(10)	-0.017(3)	-0.127(5)	0.055(4)
C14	0.0257(10)	0.0345(10)	0.0519(12)	0.0151(8)	0.0060(9)	0.0092(9)
C15	0.052(2)	0.058(2)	0.057(2)	0.0354(13)	-0.0116(12)	0.0006(12)
C16	0.0507(13)	0.0277(10)	0.0484(13)	0.0180(10)	0.0187(11)	0.0090(9)
C17	0.0354(10)	0.0201(8)	0.0412(11)	0.0132(8)	0.0070(9)	0.0112(8)
C18	0.047(2)	0.0375(12)	0.080(2)	0.0193(11)	-0.0088(13)	0.0206(12)
C19	0.057(2)	0.0258(9)	0.0433(12)	0.0164(10)	0.0184(10)	0.0162(9)
C20	0.046(4)	0.063(4)	0.041(3)	0.021(3)	0.012(3)	0.029(3)

The general temperature factor expression: $\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$

Table 4. Bond lengths (Å)

atom	atom	distance	atom	atom	distance
O1	C4	1.206(3)	O2	C4	1.343(3)
O2	C10	1.452(3)	O3	C1	1.331(3)
O3	C5	1.458(4)	O4	C7	1.201(3)
O5	C7	1.323(3)	O5	C14	1.462(4)
O6	C8	1.196(3)	O7	C8	1.325(3)
O7	C12	1.463(3)	O8	C9	1.198(3)
O9	C9	1.331(3)	O9	C17	1.491(3)
N1	N2	1.409(3)	N1	C3	1.466(2)
N1	C4	1.370(3)	N2	C1	1.274(2)
C1	C2	1.521(3)	C2	C3	1.544(3)
C2	C7	1.543(3)	C2	C8	1.531(3)
C3	C9	1.537(3)	C5	C6	1.327(7)
C5	C20	1.430(9)	C6	C20	1.251(7)
C10	C11	1.488(4)	C12	C13	1.384(7)
C14	C15	1.503(4)	C16	C17	1.514(3)
C17	C18	1.514(4)	C17	C19	1.513(4)

Table 5. Bond lengths involving hydrogens (Å)

atom	atom	distance	atom	atom	distance
C3	H3	1.000	C10	H10A	0.990
C10	H10B	0.990	C11	H11A	0.980
C11	H11B	0.980	C11	H11C	0.980
C12	H12A	0.990	C12	H12B	0.990
C13	H13A	0.980	C13	H13B	0.980
C13	H13C	0.980	C14	H14A	0.990
C14	H14B	0.990	C15	H15A	0.980
C15	H15B	0.980	C15	H15C	0.980
C16	H16A	0.980	C16	H16B	0.980
C16	H16C	0.980	C18	H18A	0.980
C18	H18B	0.980	C18	H18C	0.980
C19	H19A	0.980	C19	H19B	0.980
C19	H19C	0.980			

Table 6. Bond angles (°)

atom	atom	atom	angle	atom	atom	atom	angle
C4	O2	C10	116.23(15)	C1	O3	C5	116.40(16)
C7	O5	C14	116.96(17)	C8	O7	C12	117.22(17)
C9	O9	C17	122.05(17)	N2	N1	C3	112.21(12)
N2	N1	C4	118.55(15)	C3	N1	C4	123.53(17)
N1	N2	C1	106.10(16)	O3	C1	N2	125.95(19)
O3	C1	C2	118.48(14)	N2	C1	C2	115.52(17)
C1	C2	C3	99.56(14)	C1	C2	C7	109.22(18)
C1	C2	C8	113.26(15)	C3	C2	C7	110.75(15)
C3	C2	C8	113.71(17)	C7	C2	C8	109.93(14)
N1	C3	C2	100.88(15)	N1	C3	C9	111.04(16)
C2	C3	C9	113.54(13)	O1	C4	O2	125.68(16)
O1	C4	N1	125.80(19)	O2	C4	N1	108.46(15)
O3	C5	C6	114.6(4)	O3	C5	C20	111.8(4)
C6	C5	C20	53.8(4)	C5	C6	C20	67.3(5)
O4	C7	O5	126.3(2)	O4	C7	C2	124.30(19)
O5	C7	C2	109.43(16)	O6	C8	O7	126.04(16)
O6	C8	C2	123.47(17)	O7	C8	C2	110.43(16)
O8	C9	O9	127.8(2)	O8	C9	C3	123.95(18)
O9	C9	C3	108.28(17)	O2	C10	C11	106.44(16)
O7	C12	C13	111.1(3)	O5	C14	C15	106.5(2)
O9	C17	C16	109.69(18)	O9	C17	C18	109.11(15)
O9	C17	C19	102.14(19)	C16	C17	C18	112.8(3)
C16	C17	C19	111.25(15)	C18	C17	C19	111.3(2)
C5	C20	C6	58.9(4)				

Table 7. Bond angles involving hydrogens (°)

atom	atom	atom	angle	atom	atom	atom	angle
N1	C3	H3	110.4	C2	C3	H3	110.4
C9	C3	H3	110.3	O2	C10	H10A	110.4
O2	C10	H10B	110.4	C11	C10	H10A	110.4
C11	C10	H10B	110.4	H10A	C10	H10B	108.6
C10	C11	H11A	109.5	C10	C11	H11B	109.5
C10	C11	H11C	109.5	H11A	C11	H11B	109.5
H11A	C11	H11C	109.5	H11B	C11	H11C	109.5
O7	C12	H12A	109.4	O7	C12	H12B	109.4
C13	C12	H12A	109.4	C13	C12	H12B	109.4
H12A	C12	H12B	108.0	C12	C13	H13A	109.5
C12	C13	H13B	109.5	C12	C13	H13C	109.5
H13A	C13	H13B	109.5	H13A	C13	H13C	109.5
H13B	C13	H13C	109.5	O5	C14	H14A	110.4
O5	C14	H14B	110.4	C15	C14	H14A	110.4
C15	C14	H14B	110.4	H14A	C14	H14B	108.6
C14	C15	H15A	109.5	C14	C15	H15B	109.5
C14	C15	H15C	109.5	H15A	C15	H15B	109.5
H15A	C15	H15C	109.5	H15B	C15	H15C	109.5
C17	C16	H16A	109.5	C17	C16	H16B	109.5
C17	C16	H16C	109.5	H16A	C16	H16B	109.5
H16A	C16	H16C	109.5	H16B	C16	H16C	109.5
C17	C18	H18A	109.5	C17	C18	H18B	109.5
C17	C18	H18C	109.5	H18A	C18	H18B	109.5
H18A	C18	H18C	109.5	H18B	C18	H18C	109.5
C17	C19	H19A	109.5	C17	C19	H19B	109.5
C17	C19	H19C	109.5	H19A	C19	H19B	109.5
H19A	C19	H19C	109.5	H19B	C19	H19C	109.5

Table 8. Torsion Angles(°)
(Those having bond angles > 160 or < 20 degrees are excluded.)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
C4	O2	C10	C11	-170.47(15)	C10	O2	C4	O1	-7.0(3)
C10	O2	C4	N1	175.54(16)	C1	O3	C5	C6	-90.8(3)
C1	O3	C5	C20	-149.7(3)	C5	O3	C1	N2	-1.4(4)
C5	O3	C1	C2	176.0(3)	C7	O5	C14	C15	165.22(13)
C14	O5	C7	O4	-3.8(3)	C14	O5	C7	C2	177.08(12)
C8	O7	C12	C13	-101.4(3)	C12	O7	C8	O6	-1.1(3)
C12	O7	C8	C2	-178.40(16)	C9	O9	C17	C16	-62.64(18)
C9	O9	C17	C18	61.4(2)	C9	O9	C17	C19	179.28(12)
C17	O9	C9	O8	0.4(3)	C17	O9	C9	C3	179.85(12)
N2	N1	C3	C2	-23.2(2)	N2	N1	C3	C9	97.41(18)
C3	N1	N2	C1	13.9(3)	N2	N1	C4	O1	15.4(3)
N2	N1	C4	O2	-167.17(15)	C4	N1	N2	C1	168.28(16)
C3	N1	C4	O1	166.66(18)	C3	N1	C4	O2	-15.9(3)
C4	N1	C3	C2	-176.08(17)	C4	N1	C3	C9	-55.4(3)
N1	N2	C1	O3	-179.9(2)	N1	N2	C1	C2	2.6(3)
O3	C1	C2	C3	166.00(19)	O3	C1	C2	C7	-77.9(3)
O3	C1	C2	C8	44.9(3)	N2	C1	C2	C3	-16.3(3)
N2	C1	C2	C7	99.7(2)	N2	C1	C2	C8	-137.38(19)
C1	C2	C3	N1	21.49(17)	C1	C2	C3	C9	-97.36(16)
C1	C2	C7	O4	-119.73(17)	C1	C2	C7	O5	59.43(15)
C1	C2	C8	O6	32.6(3)	C1	C2	C8	O7	-150.07(17)
C3	C2	C7	O4	-11.1(3)	C3	C2	C7	O5	168.10(12)
C7	C2	C3	N1	-93.39(15)	C7	C2	C3	C9	147.76(13)
C3	C2	C8	O6	-80.1(3)	C3	C2	C8	O7	97.22(19)
C8	C2	C3	N1	142.24(15)	C8	C2	C3	C9	23.4(2)
C7	C2	C8	O6	155.06(18)	C7	C2	C8	O7	-27.6(2)
C8	C2	C7	O4	115.43(17)	C8	C2	C7	O5	-65.41(18)
N1	C3	C9	O8	-17.6(3)	N1	C3	C9	O9	162.92(12)
C2	C3	C9	O8	95.28(18)	C2	C3	C9	O9	-84.24(17)
O3	C5	C6	C20	-99.8(3)	O3	C5	C20	C6	105.3(4)
C6	C5	C20	C6	0.0(3)	C20	C5	C6	C20	0.0(4)
C5	C6	C20	C5	-0.00(15)					

Table 9. Intramolecular contacts less than 3.60 Å

atom	atom	distance	atom	atom	distance
O1	N2	2.7769(19)	O1	C10	2.711(3)
O2	O8	3.026(2)	O2	N2	3.510(3)
O2	C3	2.6281(19)	O2	C9	2.8535(18)
O3	O5	2.874(3)	O3	O6	3.035(3)
O3	N1	3.448(2)	O3	C7	3.142(3)
O3	C8	2.939(3)	O4	O7	3.2762(19)
O4	N1	3.436(3)	O4	C1	3.444(3)
O4	C3	2.813(3)	O4	C8	3.434(3)
O4	C14	2.718(3)	O5	O7	2.927(3)
O5	C1	2.822(3)	O5	C8	2.899(3)
O6	O8	3.373(2)	O6	O9	3.254(3)
O6	C1	2.896(3)	O6	C3	3.227(2)
O6	C9	3.016(3)	O6	C12	2.719(3)
O6	C13	3.468(6)	O6	C16	3.445(4)
O7	O9	3.283(2)	O7	C3	3.2890(19)
O7	C7	2.608(3)	O8	N1	2.781(3)
O8	N2	3.348(3)	O8	C1	3.552(3)
O8	C2	3.350(3)	O8	C4	3.024(3)
O8	C8	3.556(3)	O8	C16	3.066(3)
O8	C17	2.873(3)	O8	C18	3.041(4)
O9	N1	3.595(2)	O9	C2	3.139(3)
O9	C8	2.962(3)	N1	C7	3.163(3)
N1	C10	3.551(3)	N2	C5	2.741(4)
N2	C6	3.321(5)	N2	C7	3.265(3)
N2	C8	3.582(3)	N2	C9	3.277(3)
C1	C4	3.416(3)	C1	C6	3.113(5)
C1	C9	3.254(4)	C1	C20	3.546(8)
C4	C9	3.033(3)	C7	C15	3.598(4)
C8	C9	2.831(3)	C8	C13	3.201(5)
C9	C16	3.026(3)	C9	C18	3.004(4)

Table 10. Intramolecular contacts less than 3.60 Å involving hydrogens

atom	atom	distance	atom	atom	distance
O1	H10A	2.772	O1	H10B	2.619
O2	H3	2.593	O2	H11A	2.440
O2	H11B	3.200	O2	H11C	2.656
O4	H3	2.364	O4	H14A	2.529
O4	H14B	2.906	O5	H15A	2.500
O5	H15B	2.627	O5	H15C	3.228
O6	H12A	2.326	O6	H12B	3.530
O6	H13B	3.175	O6	H16A	3.285
O6	H16B	2.845	O7	H3	3.452
O7	H13A	3.181	O7	H13B	2.419
O7	H13C	2.683	O8	H3	3.134
O8	H16A	2.476	O8	H16B	3.479
O8	H18A	2.483	O8	H18C	3.369
O9	H3	2.442	O9	H16A	2.676
O9	H16B	2.623	O9	H16C	3.302
O9	H18A	2.711	O9	H18B	3.291
O9	H18C	2.570	O9	H19A	2.503
O9	H19B	2.505	O9	H19C	3.211
N2	H3	3.155	C1	H3	3.134
C4	H3	2.821	C4	H10A	2.693
C4	H10B	2.571	C7	H3	2.534
C7	H14A	2.551	C7	H14B	2.734
C8	H3	3.104	C8	H12A	2.436
C8	H12B	3.105	C8	H13B	2.963
C8	H16B	3.349	C9	H16A	2.788
C9	H16B	3.243	C9	H18A	2.818
C9	H18C	3.143	C11	H18C	3.407
C12	H16B	3.357	C12	H19A	3.390
C16	H12A	3.551	C16	H18A	2.671
C16	H18B	2.775	C16	H18C	3.355
C16	H19A	2.671	C16	H19B	3.340
C16	H19C	2.714	C18	H11C	3.286
C18	H16A	2.709	C18	H16B	3.358
C18	H16C	2.734	C18	H19A	3.340
C18	H19B	2.665	C18	H19C	2.721
C19	H16A	3.339	C19	H16B	2.663
C19	H16C	2.723	C19	H18A	3.340

Table 10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C19	H18B	2.682	C19	H18C	2.703
H10A	H11A	2.432	H10A	H11B	2.277
H10A	H11C	2.836	H10B	H11A	2.836
H10B	H11B	2.433	H10B	H11C	2.277
H11A	H18C	3.364	H11C	H18A	3.073
H11C	H18C	2.621	H12A	H13A	2.141
H12A	H13B	2.356	H12A	H13C	2.742
H12A	H16B	2.603	H12A	H19A	3.245
H12B	H13A	2.345	H12B	H13B	2.745
H12B	H13C	2.150	H12B	H16B	3.512
H12B	H19A	2.887	H14A	H15A	2.854
H14A	H15B	2.320	H14A	H15C	2.412
H14B	H15A	2.411	H14B	H15B	2.854
H14B	H15C	2.321	H16A	H18A	2.490
H16A	H18B	3.075	H16A	H18C	3.569
H16A	H19A	3.551	H16B	H18A	3.565
H16B	H19A	2.462	H16B	H19B	3.550
H16B	H19C	2.969	H16C	H18A	2.956
H16C	H18B	2.629	H16C	H19A	2.996
H16C	H19C	2.573	H18A	H19B	3.567
H18A	H19C	3.598	H18B	H19A	3.587
H18B	H19B	2.925	H18B	H19C	2.537
H18C	H19A	3.575	H18C	H19B	2.500
H18C	H19C	3.040			

Table 11. Intermolecular contacts less than 3.60 Å

atom	atom	distance	atom	atom	distance
O1	C12[1]	3.326(3)	O1	C14[2]	3.168(3)
O1	C15[2]	3.592(4)	O3	C5[3]	3.360(5)
O3	C15[4]	3.543(3)	O4	C11[5]	3.315(3)
O4	C19[6]	3.539(3)	O6	C5[3]	3.143(4)
O6	C6[3]	3.470(5)	O6	C20[3]	3.312(8)
O7	C11[5]	3.368(3)	O8	C20[3]	3.060(7)
C5	O3[3]	3.360(5)	C5	O6[3]	3.143(4)
C5	C5[3]	3.493(7)	C6	O6[3]	3.470(5)
C6	C6[7]	3.376(7)	C11	O4[5]	3.315(3)
C11	O7[5]	3.368(3)	C12	O1[8]	3.326(3)
C14	O1[9]	3.168(3)	C15	O1[9]	3.592(4)
C15	O3[4]	3.543(3)	C15	C20[4]	3.491(7)
C19	O4[10]	3.539(3)	C20	O6[3]	3.312(8)
C20	O8[3]	3.060(7)	C20	C15[4]	3.491(7)

Symmetry Operators:

(1)	X+1,Y+1,Z	(2)	X+1,Y,Z
(3)	-X+2,-Y+1,-Z	(4)	-X+1,-Y+1,-Z
(5)	-X+2,-Y+1,-Z+1	(6)	X,Y+1,Z
(7)	-X+2,-Y+2,-Z	(8)	X-1,Y-1,Z
(9)	X-1,Y,Z	(10)	X,Y-1,Z

Table 12. Intermolecular contacts less than 3.60 Å involving hydrogens

atom	atom	distance	atom	atom	distance
O1	H10A[1]	2.887	O1	H12A[2]	3.562
O1	H12B[2]	2.383	O1	H14A[3]	2.592
O1	H14B[3]	3.064	O1	H15C[3]	3.102
O1	H19A[2]	2.951	O2	H19B[4]	2.775
O3	H15A[5]	2.871	O3	H15C[5]	3.336
O4	H10B[6]	3.188	O4	H11A[4]	3.057
O4	H11B[4]	3.425	O4	H11C[4]	2.931
O4	H16C[7]	3.243	O4	H18C[4]	2.801
O4	H19C[7]	2.657	O5	H15A[5]	3.597
O5	H16C[7]	3.310	O6	H13A[8]	3.128
O7	H11A[4]	2.915	O7	H11B[4]	2.930
O8	H14B[3]	2.643	O9	H11A[4]	2.907
N1	H16C[7]	3.344	N2	H13A[2]	3.495
N2	H15C[3]	2.921	N2	H16C[7]	3.010
C1	H16C[7]	3.195	C3	H11A[4]	3.409
C4	H10A[1]	3.472	C4	H12B[2]	3.465
C4	H14A[3]	3.275	C4	H14B[3]	3.168
C4	H15C[3]	3.543	C4	H19B[4]	3.378
C5	H13A[2]	3.300	C5	H15A[5]	3.360
C6	H13A[2]	3.185	C6	H13C[2]	3.416
C6	H13C[5]	3.563	C6	H16A[7]	3.440
C6	H16C[7]	3.491	C7	H11A[4]	3.469
C7	H16C[7]	3.118	C7	H19C[7]	3.441
C10	H10A[1]	3.188	C10	H19A[4]	3.537
C10	H19B[4]	3.279	C11	H3[4]	3.578
C11	H11C[9]	3.400	C11	H12B[4]	3.464
C11	H18A[9]	3.269	C11	H19A[4]	3.581
C12	H11B[4]	3.340	C12	H15B[10]	3.316
C12	H15C[10]	3.345	C13	H15C[10]	3.470
C14	H10B[6]	3.570	C14	H16B[7]	3.515
C14	H19A[7]	3.589	C15	H12A[7]	3.105
C15	H13A[7]	3.433	C15	H13B[5]	3.496
C16	H14A[10]	3.457	C18	H10B[9]	3.533
C18	H11B[9]	3.217	C18	H19C[11]	3.321
C19	H10A[4]	3.442	C19	H11A[4]	3.377
C19	H14A[10]	3.166	C19	H18B[11]	3.271
C20	H13B[5]	3.356	C20	H13C[5]	3.158

Table 12. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C20	H14B^{5}	3.365	C20	H15A^{5}	2.877
C20	H15C^{5}	3.409	C20	H16A^{12}	3.227
H3	C11^{4}	3.578	H3	H11A^{4}	2.767
H3	H11C^{4}	3.567	H3	H18C^{4}	3.170
H3	H19B^{4}	3.199	H10A	O1^{1}	2.887
H10A	C4^{1}	3.472	H10A	C10^{1}	3.188
H10A	C19^{4}	3.442	H10A	H10A^{1}	2.332
H10A	H10B^{1}	3.435	H10A	H12B^{4}	3.583
H10A	H18B^{9}	3.506	H10A	H19A^{4}	2.991
H10A	H19B^{4}	3.011	H10B	O4^{3}	3.188
H10B	C14^{3}	3.570	H10B	C18^{9}	3.533
H10B	H10A^{1}	3.435	H10B	H11C^{9}	3.268
H10B	H14A^{3}	3.015	H10B	H14B^{3}	3.218
H10B	H18A^{9}	3.427	H10B	H18B^{9}	3.260
H10B	H18C^{9}	3.327	H10B	H19A^{2}	3.333
H10B	H19C^{2}	3.171	H11A	O4^{4}	3.057
H11A	O7^{4}	2.915	H11A	O9^{4}	2.907
H11A	C3^{4}	3.409	H11A	C7^{4}	3.469
H11A	C19^{4}	3.377	H11A	H3^{4}	2.767
H11A	H12B^{4}	3.297	H11A	H19A^{4}	3.009
H11A	H19B^{4}	2.998	H11B	O4^{4}	3.425
H11B	O7^{4}	2.930	H11B	C12^{4}	3.340
H11B	C18^{9}	3.217	H11B	H11C^{9}	3.398
H11B	H12B^{4}	2.830	H11B	H18A^{9}	2.479
H11B	H18B^{9}	3.257	H11B	H18C^{9}	3.486
H11C	O4^{4}	2.931	H11C	C11^{9}	3.400
H11C	H3^{4}	3.567	H11C	H10B^{9}	3.268
H11C	H11B^{9}	3.398	H11C	H11C^{9}	2.708
H11C	H18A^{9}	3.421	H12A	O1^{13}	3.562
H12A	C15^{10}	3.105	H12A	H13B^{8}	3.547
H12A	H14A^{10}	3.298	H12A	H15B^{10}	2.504
H12A	H15C^{10}	2.934	H12B	O1^{13}	2.383
H12B	C4^{13}	3.465	H12B	C11^{4}	3.464
H12B	H10A^{4}	3.583	H12B	H11A^{4}	3.297
H12B	H11B^{4}	2.830	H12B	H14A^{10}	3.307
H12B	H15B^{10}	3.420	H12B	H15C^{10}	3.149
H13A	O6^{8}	3.128	H13A	N2^{13}	3.495

Table 12. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

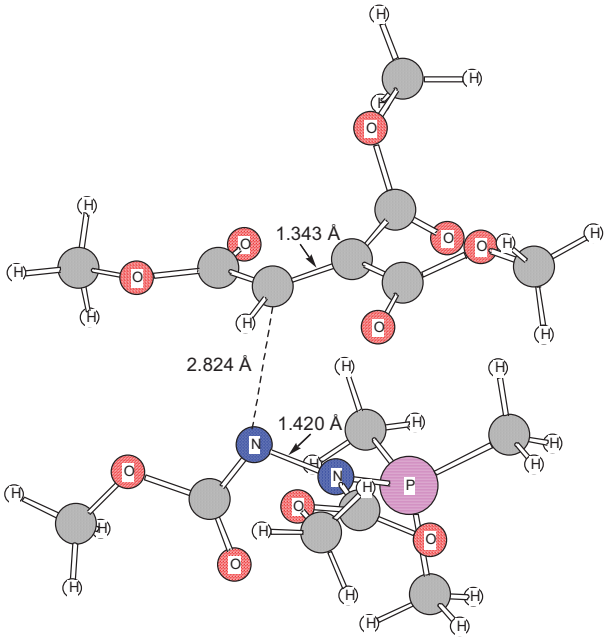
atom	atom	distance	atom	atom	distance
H13A	C5[13]	3.300	H13A	C6[13]	3.185
H13A	C15[10]	3.433	H13A	H15B[10]	3.218
H13A	H15C[10]	2.761	H13B	C15[5]	3.496
H13B	C20[5]	3.356	H13B	H12A[8]	3.547
H13B	H15A[5]	3.486	H13B	H15B[5]	2.756
H13C	C6[13]	3.416	H13C	C6[5]	3.563
H13C	C20[5]	3.158	H13C	H16A[6]	2.841
H13C	H18A[6]	3.585	H14A	O1[6]	2.592
H14A	C4[6]	3.275	H14A	C16[7]	3.457
H14A	C19[7]	3.166	H14A	H10B[6]	3.015
H14A	H12A[7]	3.298	H14A	H12B[7]	3.307
H14A	H16B[7]	2.934	H14A	H16C[7]	3.239
H14A	H19A[7]	2.608	H14A	H19C[7]	2.896
H14B	O1[6]	3.064	H14B	O8[6]	2.643
H14B	C4[6]	3.168	H14B	C20[5]	3.365
H14B	H10B[6]	3.218	H15A	O3[5]	2.871
H15A	O5[5]	3.597	H15A	C5[5]	3.360
H15A	C20[5]	2.877	H15A	H13B[5]	3.486
H15A	H15A[5]	2.945	H15B	C12[7]	3.316
H15B	H12A[7]	2.504	H15B	H12B[7]	3.420
H15B	H13A[7]	3.218	H15B	H13B[5]	2.756
H15B	H16B[7]	2.944	H15C	O1[6]	3.102
H15C	O3[5]	3.336	H15C	N2[6]	2.921
H15C	C4[6]	3.543	H15C	C12[7]	3.345
H15C	C13[7]	3.470	H15C	C20[5]	3.409
H15C	H12A[7]	2.934	H15C	H12B[7]	3.149
H15C	H13A[7]	2.761	H16A	C6[10]	3.440
H16A	C20[12]	3.227	H16A	H13C[3]	2.841
H16B	C14[10]	3.515	H16B	H14A[10]	2.934
H16B	H15B[10]	2.944	H16C	O4[10]	3.243
H16C	O5[10]	3.310	H16C	N1[10]	3.344
H16C	N2[10]	3.010	H16C	C1[10]	3.195
H16C	C6[10]	3.491	H16C	C7[10]	3.118
H16C	H14A[10]	3.239	H18A	C11[9]	3.269
H18A	H10B[9]	3.427	H18A	H11B[9]	2.479
H18A	H11C[9]	3.421	H18A	H13C[3]	3.585
H18B	C19[11]	3.271	H18B	H10A[9]	3.506

Table 12. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H18B	H10B[9]	3.260	H18B	H11B[9]	3.257
H18B	H19B[11]	2.943	H18B	H19C[11]	2.707
H18C	O4[4]	2.801	H18C	H3[4]	3.170
H18C	H10B[9]	3.327	H18C	H11B[9]	3.486
H18C	H19C[11]	3.048	H19A	O1[13]	2.951
H19A	C10[4]	3.537	H19A	C11[4]	3.581
H19A	C14[10]	3.589	H19A	H10A[4]	2.991
H19A	H10B[13]	3.333	H19A	H11A[4]	3.009
H19A	H14A[10]	2.608	H19B	O2[4]	2.775
H19B	C4[4]	3.378	H19B	C10[4]	3.279
H19B	H3[4]	3.199	H19B	H10A[4]	3.011
H19B	H11A[4]	2.998	H19B	H18B[11]	2.943
H19C	O4[10]	2.657	H19C	C7[10]	3.441
H19C	C18[11]	3.321	H19C	H10B[13]	3.171
H19C	H14A[10]	2.896	H19C	H18B[11]	2.707
H19C	H18C[11]	3.048	H19C	H19C[11]	3.579

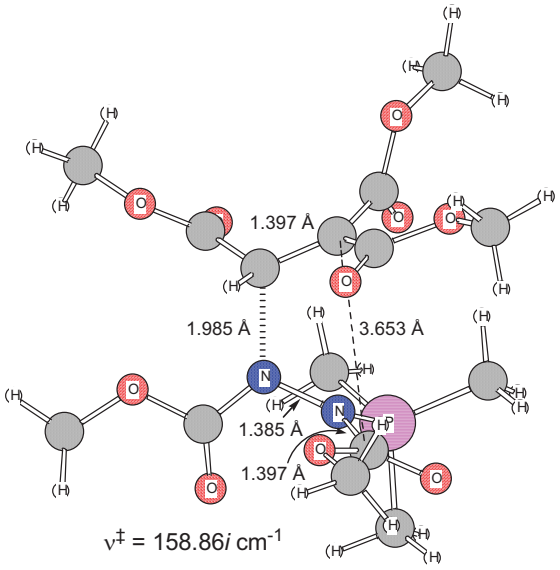
Symmetry Operators:

(1) -X+3,-Y+2,-Z+1
(2) X+1,Y+1,Z
(3) X+1,Y,Z
(4) -X+2,-Y+1,-Z+1
(5) -X+1,-Y+1,-Z
(6) X-1,Y,Z
(7) X,Y+1,Z
(8) -X+1,-Y,-Z
(9) -X+3,-Y+1,-Z+1
(10) X,Y-1,Z
(11) -X+2,-Y,-Z+1
(12) -X+2,-Y+1,-Z
(13) X-1,Y-1,Z



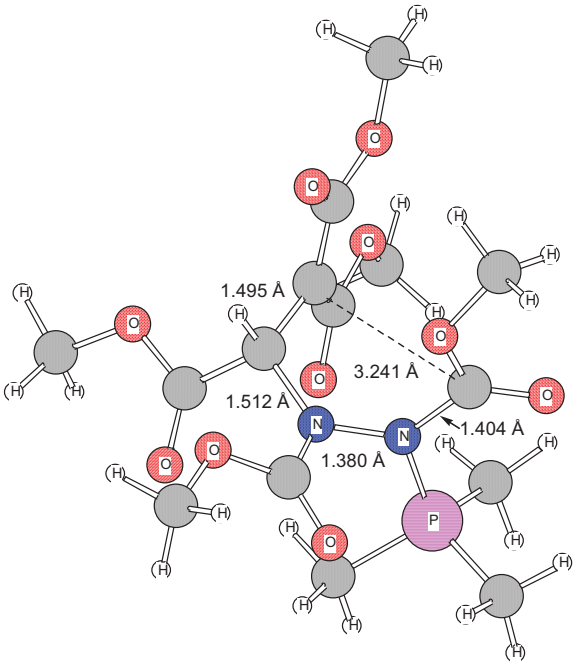
1m + A

[ΔG° = 0 kcal/mol]



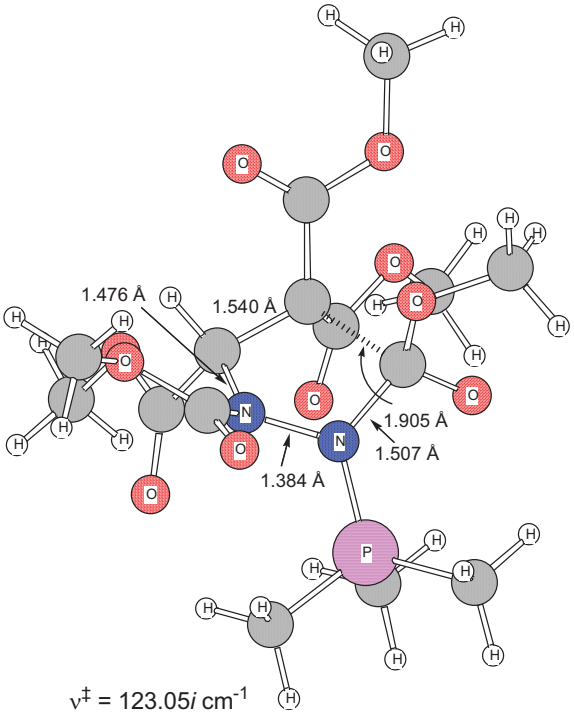
TS1

[ΔG‡ = +10.10 kcal/mol]



Int1

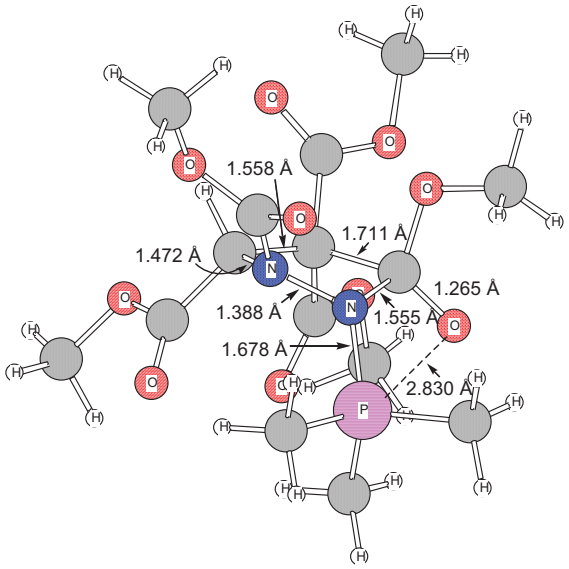
[ΔG° = -1.57 kcal/mol]



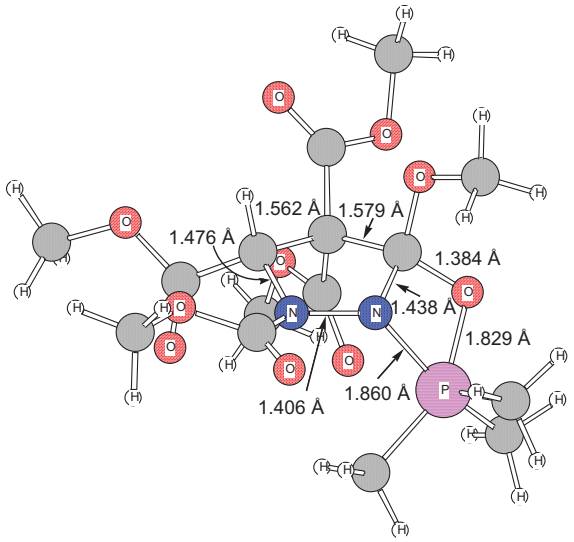
TS2

[[ΔG‡ = +14.55 kcal/mol]

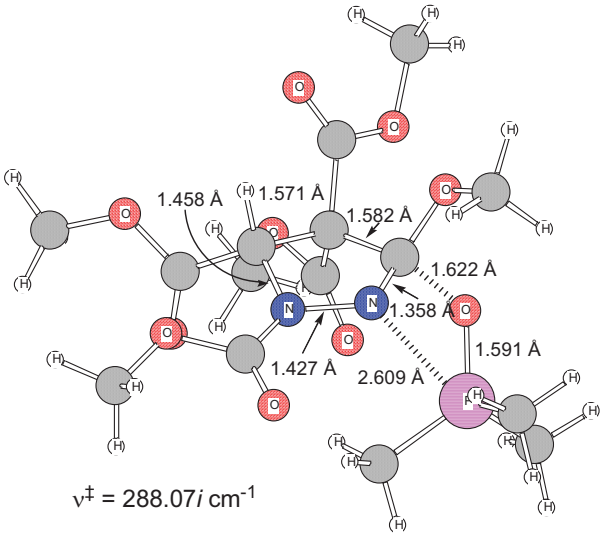
Figure S2. continued.



Int2
[ΔG° = +13.28 kcal/mol]

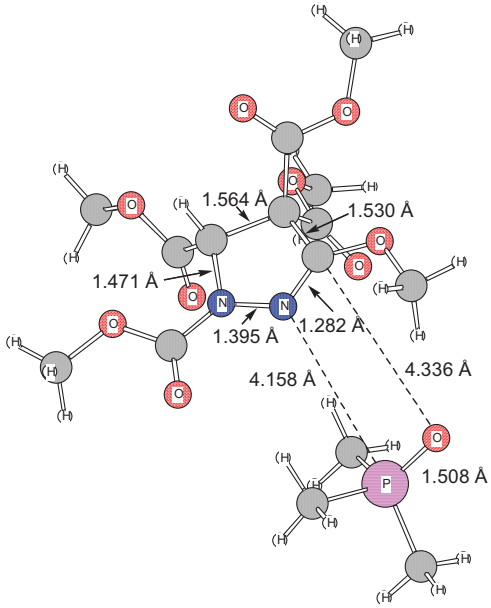


Int3
[ΔG° = +18.82 kcal/mol]



$\nu^{\ddagger}$ = 288.07*i* cm^{-1}

TS3
[$\Delta G^{\ddagger}$ = +28.26 kcal/mol]



3m + Me_3PO
[ΔG° = -20.71 kcal/mol]

Figure S2. continued.

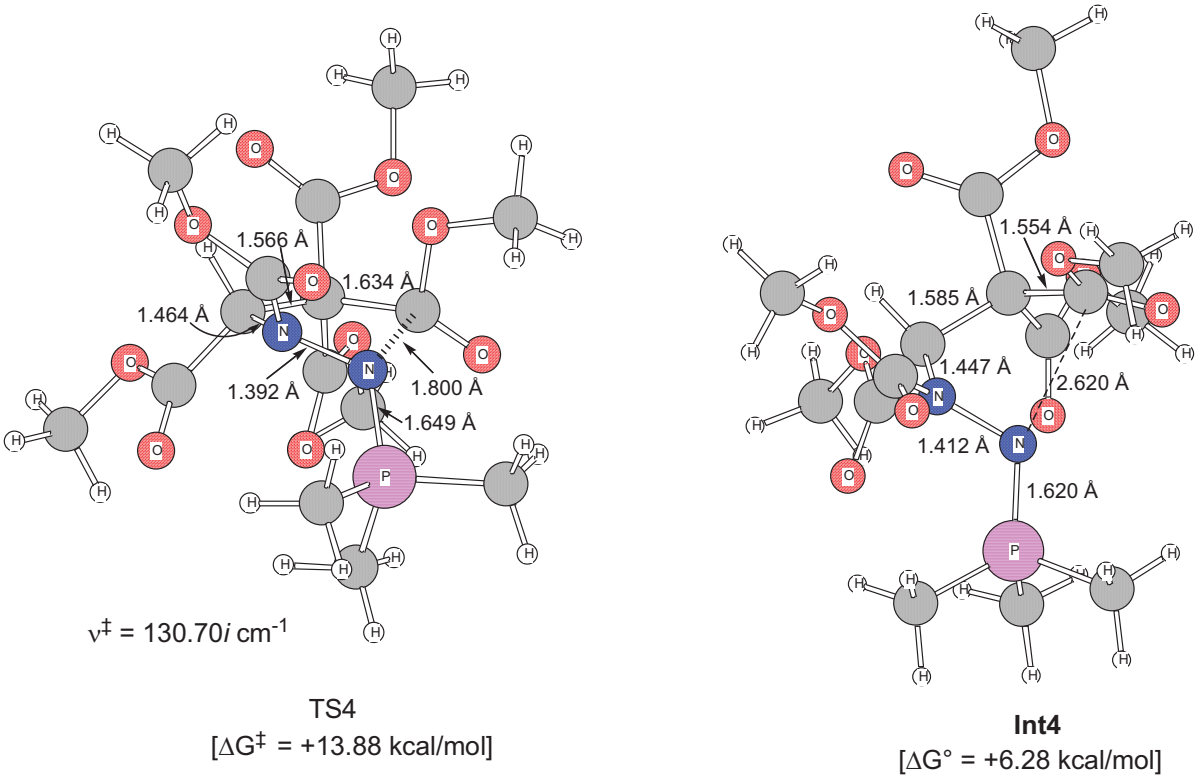
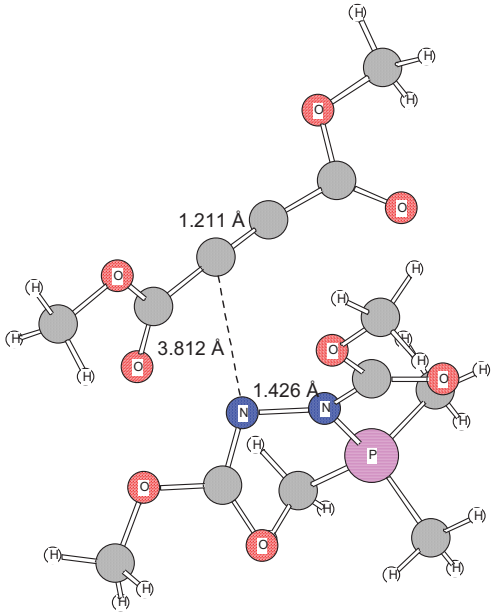
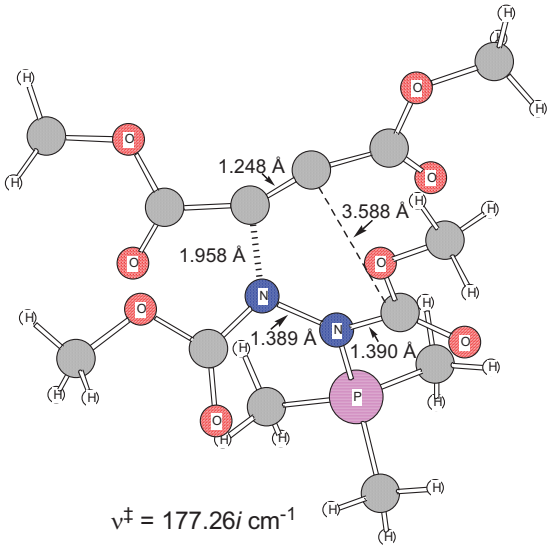


Figure S2. B3LYP/6-31G*-optimized structures in Scheme 2.[S1,S2]



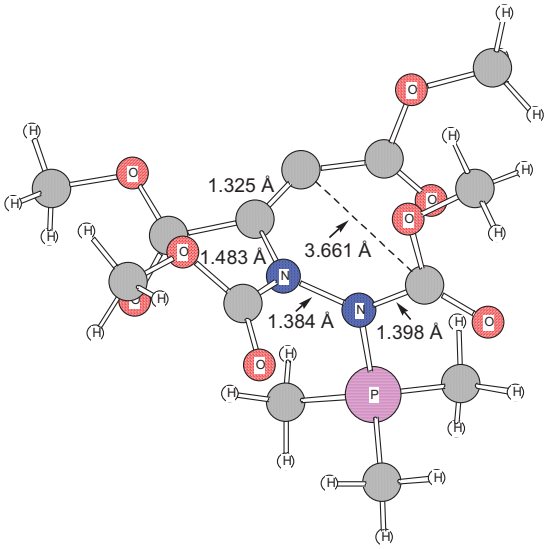
9 + A

[ΔG° = 0 kcal/mol]



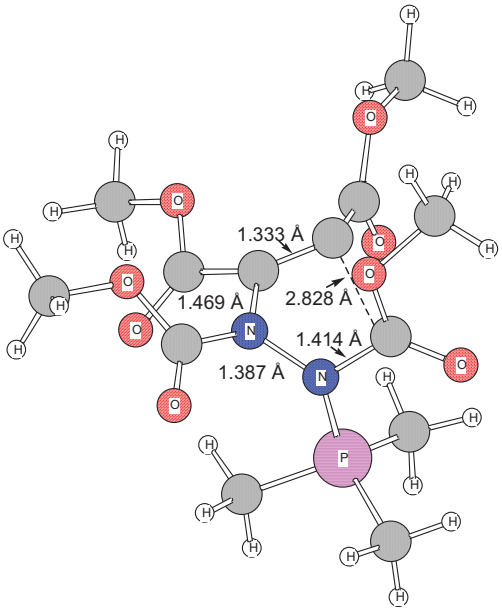
TS1a

[ΔG‡ = +12.07 kcal/mol]



Int1a

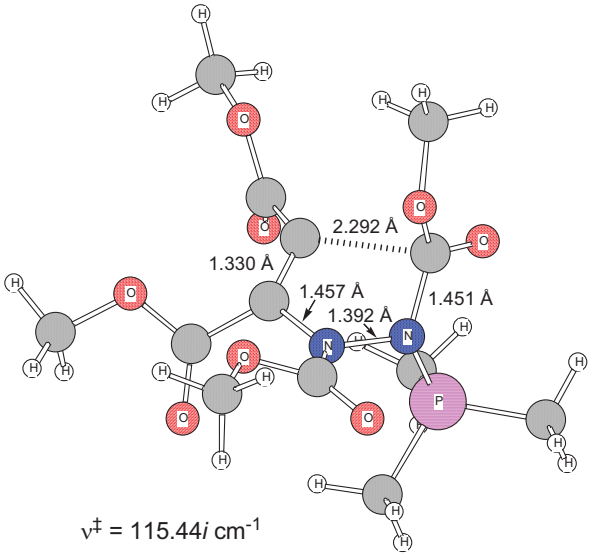
[ΔG° = +4.19 kcal/mol]



Int1a*i*

[ΔG° = +1.63 kcal/mol]

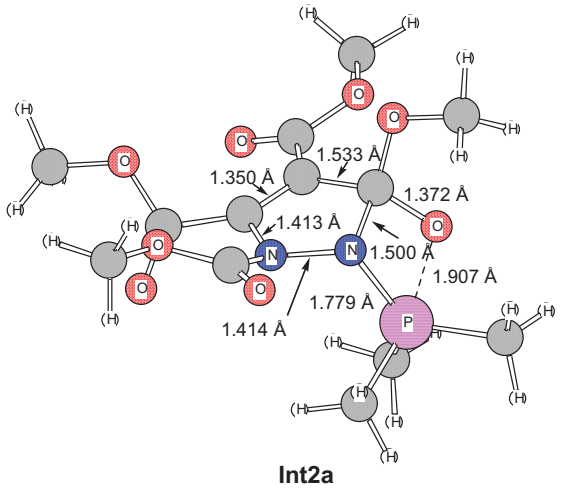
Figure S3. continued.



$\nu^{\ddagger}$ = 115.44*i* cm^{-1}

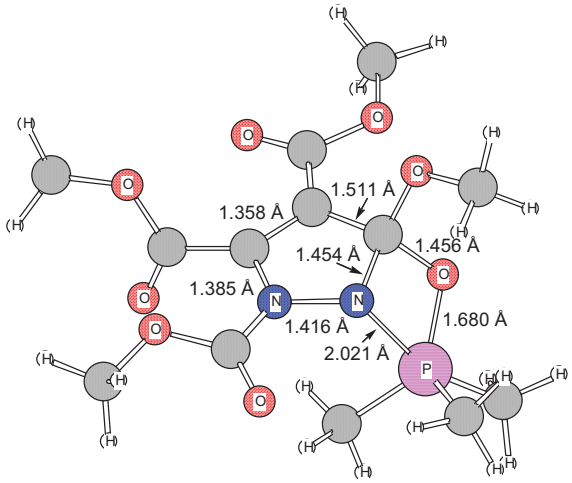
TS2a

[ΔG° = +3.82 kcal/mol]



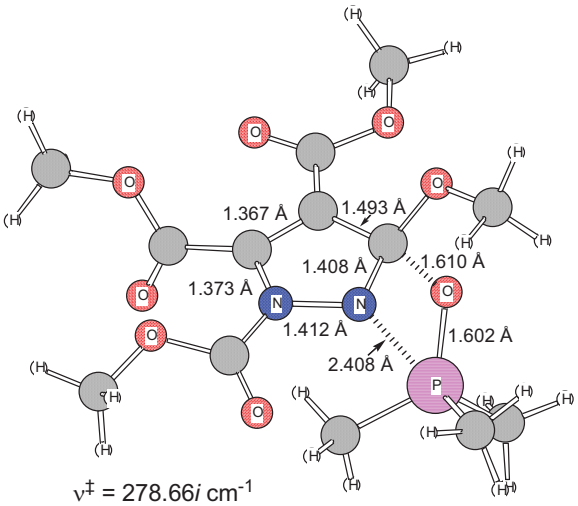
Int2a

[ΔG° = -13.80 kcal/mol]



Int3a

[ΔG° = -15.24 kcal/mol]

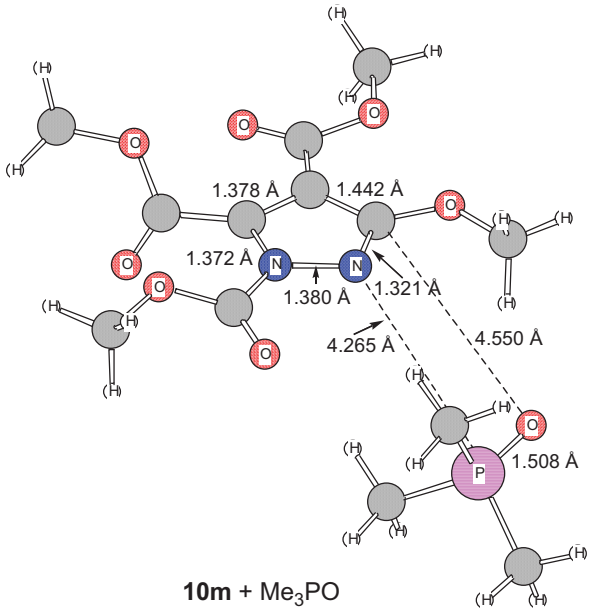


$\nu^{\ddagger}$ = 278.66*i* cm^{-1}

TS3a

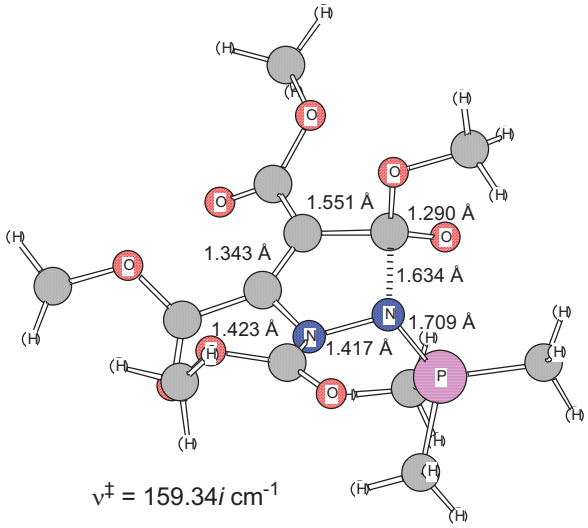
[ΔG‡ = -13.37 kcal/mol]

Figure S3. continued.



10m + Me_3PO

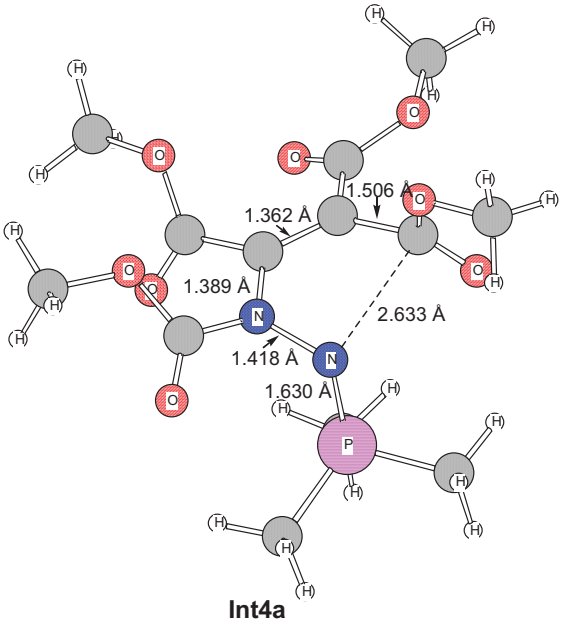
[$\Delta G°$ = -67.14 kcal/mol]



$\nu^{\ddagger}$ = 159.34*i* cm^{-1}

TS4a

[$\Delta G^{\ddagger}$ = -11.58 kcal/mol]



Int4a

[$\Delta G°$ = -28.48 kcal/mol]

Figure S3. B3LYP/6-31G*-optimized structures in Scheme 4.[S1,S2]

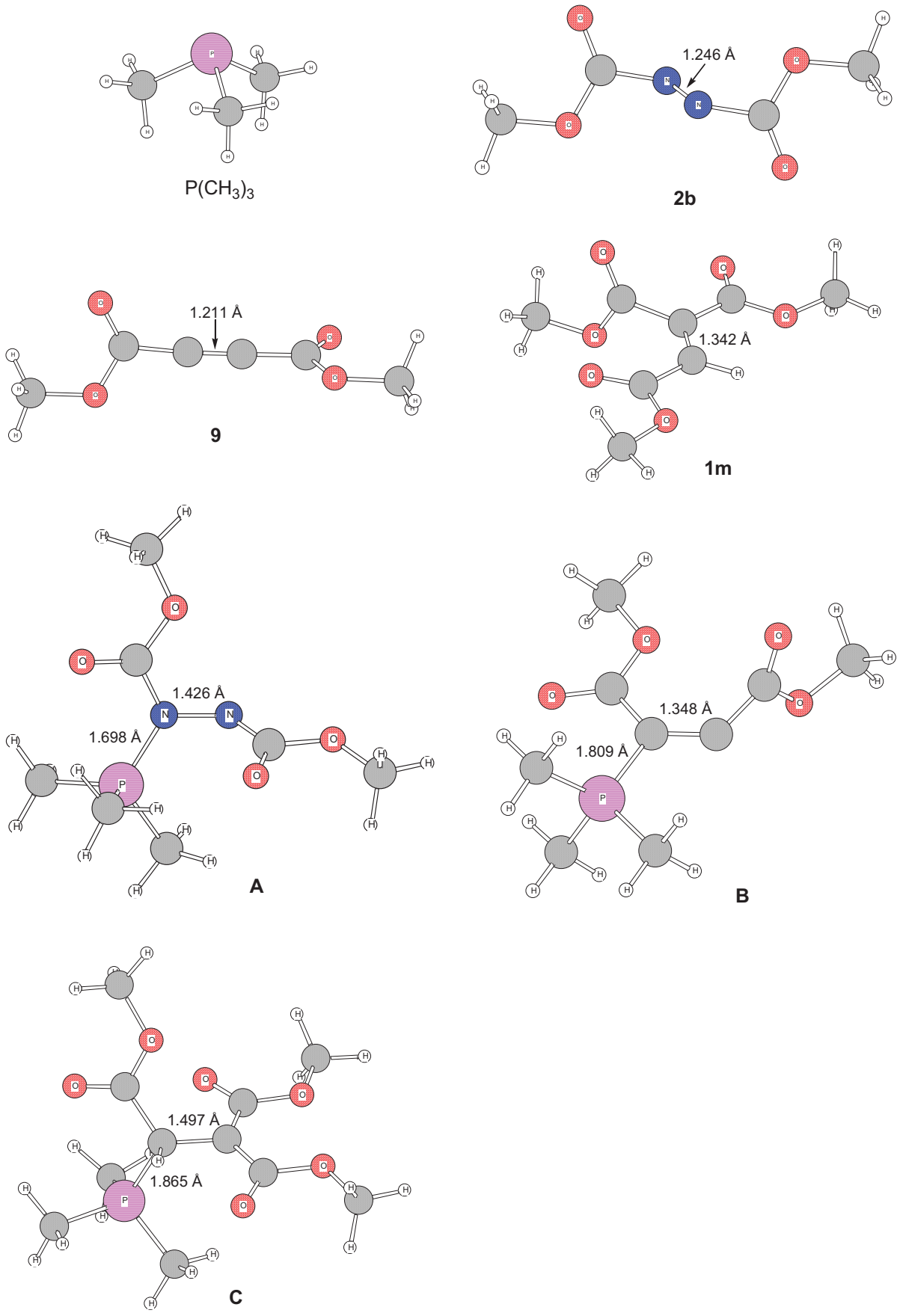
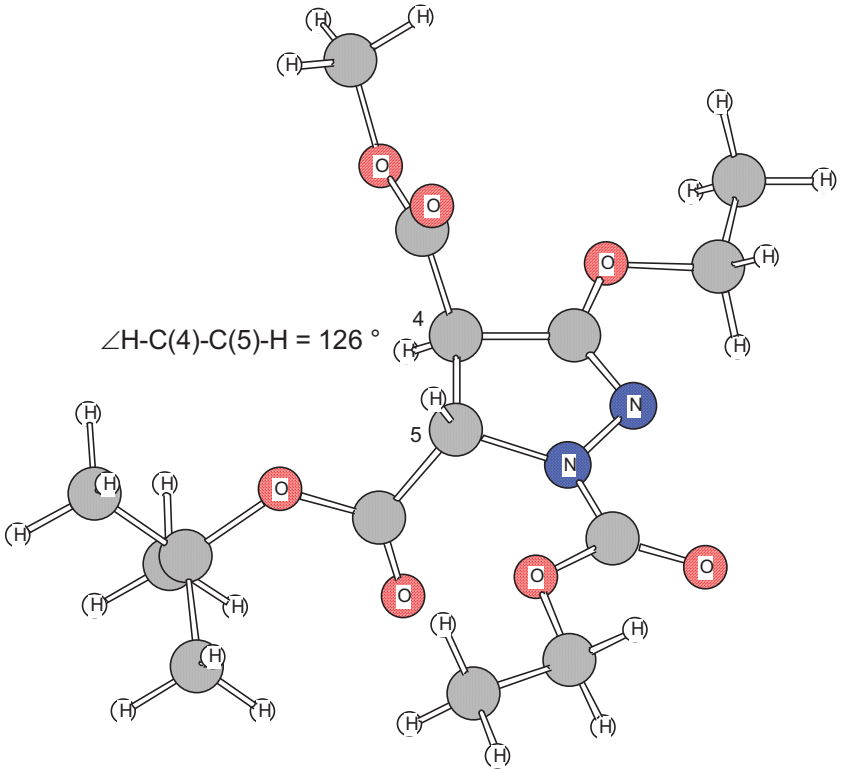
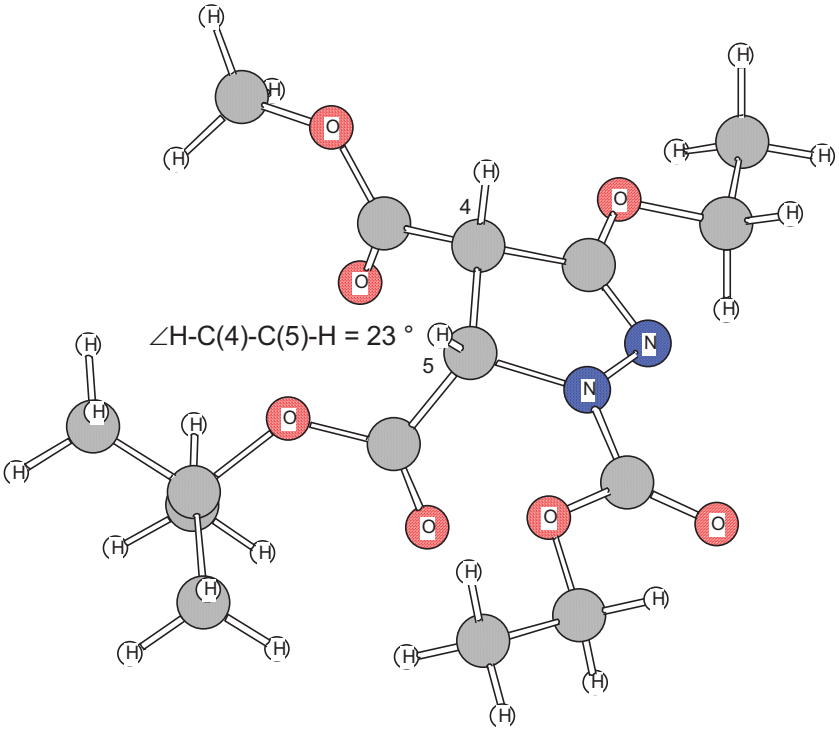


Figure S4. B3LYP/6-31G*-optimized structures in Scheme 5.[S1,S2]



trans-**12**



cis-**12**

Figure S5. B3LYP/6-31G*-optimized structures of *trans*-**12** and *cis*-**12**. The atom-numbering is different from that of Cartesian coordinates of the optimized geometries**.**

References

[S1] (a) A. D. Becke, *J. Chem. Phys*., 1993, **98**, 5648. (b) C. Lee, W. Yang and R. G. Parr, *Phys. Rev. B*, 1998, **37**, 785.

[S1] Gaussian 03, Revision C.02, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, Gaussian, Inc., Wallingford CT, 2004.

Cartesian coordinates of the optimized geometries of Figures S2-5

1m + A (DEADTS1nnRRR.rev.log)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	1.180134	-1.392135	1.756199
2	8	0	0.685780	-3.226730	-0.320059
3	8	0	1.077764	-1.792639	-2.042641
4	8	0	3.683334	-0.199658	0.477209
5	8	0	3.238663	1.662647	-0.754133
6	7	0	1.200989	-1.040854	0.090674
7	7	0	1.555788	0.243885	-0.398261
8	6	0	0.716834	-2.839710	-2.960636
9	6	0	0.970593	-2.112819	-0.754885
10	6	0	4.607152	2.010949	-0.561940
11	6	0	2.865601	0.470126	-0.179042
12	1	0	1.286651	-3.748369	-2.752945
13	1	0	0.963152	-2.446499	-3.947102
14	1	0	-0.353737	-3.041557	-2.888558
15	6	0	2.522975	-2.516882	2.248841
16	1	0	4.848696	2.126000	0.500216
17	1	0	5.274470	1.254008	-0.985739
18	1	0	4.744094	2.962191	-1.082020
19	6	0	1.362557	0.201254	2.595417
20	6	0	-0.402924	-2.109986	2.295796
21	1	0	3.455868	-2.070703	1.898069
22	1	0	2.362670	-3.483878	1.766752
23	1	0	2.529873	-2.639831	3.337123
24	1	0	-0.580544	-3.037773	1.751638
25	1	0	-1.203170	-1.387538	2.104619
26	1	0	-0.347433	-2.312025	3.371523
27	1	0	0.643714	0.912199	2.178839
28	1	0	2.379303	0.566580	2.444792
29	1	0	1.165921	0.054996	3.662338
30	6	0	-1.011883	1.116869	-1.184973
31	6	0	-2.027621	0.509752	-0.549334
32	6	0	-2.576239	1.001138	0.763361
33	6	0	-2.592916	-0.741431	-1.128797
34	6	0	-0.363380	2.348048	-0.661112
35	8	0	-2.354398	0.473925	1.836372
36	8	0	-2.184628	-1.297164	-2.129522
37	8	0	-3.368795	2.067519	0.600871
38	8	0	-3.640999	-1.188222	-0.403293
39	6	0	-4.253820	-2.395324	-0.883909
40	6	0	-3.849237	2.669791	1.815694
41	8	0	-0.462836	2.757035	0.483248
42	8	0	0.302067	2.980400	-1.635998
43	6	0	1.047366	4.137736	-1.227230
44	1	0	-0.627118	0.702703	-2.108539
45	1	0	-3.527693	-3.212361	-0.897373
46	1	0	-4.645615	-2.249395	-1.893998
47	1	0	-5.062108	-2.609496	-0.184477
48	1	0	-3.005328	3.053881	2.394264
49	1	0	-4.403017	1.942031	2.413857
50	1	0	-4.500046	3.484394	1.497554
51	1	0	1.461274	4.554496	-2.145823
52	1	0	1.848020	3.830675	-0.552011
53	1	0	0.394693	4.862108	-0.732826

TS1 (DEADTS1nn.log)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	1.176564	-1.543736	1.768464
2	8	0	0.549956	-3.320458	-0.363719
3	8	0	0.891584	-1.804840	-2.033277

4	8	0	3.498433	-0.168404	-0.010871
5	8	0	2.667757	1.688169	-1.036215
6	7	0	0.986424	-1.131902	0.120021
7	7	0	1.218615	0.159914	-0.322605
8	6	0	0.483645	-2.758113	-3.033877
9	6	0	0.784096	-2.189128	-0.770601
10	6	0	4.008731	2.176092	-1.123913
11	6	0	2.534455	0.478871	-0.427359
12	1	0	0.782667	-3.767543	-2.746675
13	1	0	0.985703	-2.446408	-3.949800
14	1	0	-0.598507	-2.685407	-3.155960
15	6	0	2.597383	-2.663363	1.965657
16	1	0	4.441138	2.321085	-0.129018
17	1	0	4.641228	1.482712	-1.684913
18	1	0	3.936653	3.130897	-1.647492
19	6	0	1.513397	0.003896	2.634352
20	6	0	-0.304133	-2.327832	2.467711
21	1	0	3.454479	-2.183696	1.485798
22	1	0	2.378557	-3.613751	1.474794
23	1	0	2.796810	-2.829615	3.029453
24	1	0	-0.552276	-3.211392	1.878112
25	1	0	-1.115080	-1.595660	2.437402
26	1	0	-0.096569	-2.613788	3.504859
27	1	0	0.752354	0.742493	2.365292
28	1	0	2.506133	0.359095	2.350822
29	1	0	1.479299	-0.195677	3.710489
30	6	0	-0.410839	1.188046	-0.799539
31	6	0	-1.590515	0.560432	-0.391587
32	6	0	-2.168928	0.748448	0.959881
33	6	0	-2.241527	-0.331868	-1.342606
34	6	0	-0.013901	2.493987	-0.171552
35	8	0	-1.619391	0.494277	2.026040
36	8	0	-1.871049	-0.562798	-2.488356
37	8	0	-3.418917	1.260087	0.921743
38	8	0	-3.335297	-0.956941	-0.807093
39	6	0	-4.033656	-1.830973	-1.694607
40	6	0	-4.077827	1.386932	2.187591
41	8	0	0.191551	2.709375	1.005776
42	8	0	0.035987	3.454985	-1.118621
43	6	0	0.367848	4.765632	-0.641228
44	1	0	-0.219521	1.130209	-1.863742
45	1	0	-3.414383	-2.691601	-1.968911
46	1	0	-4.330035	-1.309008	-2.608847
47	1	0	-4.915557	-2.165390	-1.144803
48	1	0	-3.521581	2.056897	2.849003
49	1	0	-4.176190	0.411481	2.673758
50	1	0	-5.062579	1.799920	1.964158
51	1	0	0.358388	5.408898	-1.521859
52	1	0	1.357817	4.763002	-0.176622
53	1	0	-0.366968	5.108224	0.092620

Int1 (DEADTS10b.for.log)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	1.846969	-1.269102	1.485456
2	8	0	0.674944	-3.156908	-0.311337
3	8	0	0.295712	-1.656521	-1.987979
4	8	0	3.227774	0.191406	-1.091297
5	8	0	1.919351	1.869719	-1.887919
6	7	0	1.062663	-0.929815	0.001425
7	7	0	1.006460	0.350701	-0.509088
8	6	0	-0.338409	-2.639152	-2.831101
9	6	0	0.653447	-2.027063	-0.773521
10	6	0	3.077897	2.444883	-2.509804
11	6	0	2.146847	0.760643	-1.170059
12	1	0	0.420400	-3.113439	-3.459224
13	1	0	-1.050428	-2.070596	-3.427696
14	1	0	-0.841740	-3.391301	-2.221918
15	6	0	3.311943	-2.291826	1.144167
16	1	0	3.808399	2.743008	-1.753259
17	1	0	3.538192	1.732704	-3.198722
18	1	0	2.709079	3.317581	-3.048829

19	6	0	2.373812	0.306478	2.183473
20	6	0	0.772874	-2.126703	2.666776
21	1	0	3.913109	-1.772015	0.393845
22	1	0	2.996532	-3.263694	0.760243
23	1	0	3.887979	-2.426026	2.065587
24	1	0	0.369929	-3.026581	2.199342
25	1	0	-0.029224	-1.429369	2.927558
26	1	0	1.363365	-2.393372	3.550284
27	1	0	1.505540	0.963321	2.267099
28	1	0	3.123378	0.766041	1.537235
29	1	0	2.801766	0.103227	3.171073
30	6	0	-0.302034	1.108707	-0.512682
31	6	0	-1.504946	0.304748	-0.135977
32	6	0	-1.711299	0.106055	1.254166
33	6	0	-2.360700	-0.055123	-1.239519
34	6	0	-0.089867	2.380766	0.322111
35	8	0	-0.863793	0.410361	2.129424
36	8	0	-2.110841	0.176884	-2.428256
37	8	0	-2.898576	-0.448840	1.636363
38	8	0	-3.507378	-0.720616	-0.897085
39	6	0	-4.365074	-1.041228	-1.988038
40	6	0	-3.106552	-0.573984	3.038524
41	8	0	0.952724	2.738533	0.834641
42	8	0	-1.211084	3.120002	0.341158
43	6	0	-1.125334	4.346589	1.078516
44	1	0	-0.454855	1.422377	-1.549063
45	1	0	-3.891198	-1.744886	-2.682013
46	1	0	-4.648353	-0.146536	-2.551075
47	1	0	-5.248497	-1.501337	-1.539156
48	1	0	-2.929435	0.372233	3.558158
49	1	0	-2.456596	-1.339076	3.481337
50	1	0	-4.149388	-0.879155	3.151078
51	1	0	-2.104447	4.816297	0.978025
52	1	0	-0.344319	4.993071	0.668251
53	1	0	-0.903891	4.142957	2.129763

TS2 (DEADTS10b.log)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	1.916523	-1.254829	-1.470477
2	8	0	-0.672267	-0.611026	-2.261131
3	8	0	-0.484390	1.631518	-1.733669
4	8	0	2.929335	2.010648	-0.286224
5	8	0	1.950084	2.185404	1.759463
6	7	0	1.072809	0.095398	-0.920764
7	7	0	1.255555	0.564884	0.368370
8	6	0	-1.189869	1.894765	-2.943611
9	6	0	-0.334944	0.267301	-1.430188
10	6	0	2.819486	3.290104	2.045041
11	6	0	2.102899	1.648485	0.529584
12	1	0	-0.645837	1.517615	-3.816973
13	1	0	-1.265656	2.983608	-3.001759
14	1	0	-2.188359	1.449409	-2.930612
15	6	0	2.222668	-0.989627	-3.240949
16	1	0	3.866768	2.984704	1.973297
17	1	0	2.636613	4.112160	1.348662
18	1	0	2.575578	3.591417	3.064121
19	6	0	3.501427	-1.212560	-0.588629
20	6	0	1.217660	-2.919668	-1.241917
21	1	0	2.745506	-0.038010	-3.367651
22	1	0	1.255983	-0.947921	-3.746310
23	1	0	2.830203	-1.806030	-3.644585
24	1	0	0.255121	-2.967889	-1.750269
25	1	0	1.065459	-3.094035	-0.175433
26	1	0	1.918932	-3.654225	-1.654887
27	1	0	3.304073	-1.408876	0.468666
28	1	0	3.953341	-0.224309	-0.701897
29	1	0	4.162424	-1.984755	-0.994640
30	6	0	0.090727	0.261577	1.222439
31	6	0	-1.135120	0.168771	0.295774
32	6	0	-1.774023	-1.174147	0.229839
33	6	0	-1.995146	1.395138	0.468486

34	6	0	0.407707	-0.960287	2.085405
35	8	0	-1.176680	-2.213769	0.480874
36	8	0	-1.748036	2.296664	1.251518
37	8	0	-3.041871	-1.173800	-0.208496
38	8	0	-3.051950	1.445117	-0.365436
39	6	0	-3.853520	2.627890	-0.253805
40	6	0	-3.611958	-2.467427	-0.441333
41	8	0	1.403000	-1.652962	1.995136
42	8	0	-0.522024	-1.103516	3.042362
43	6	0	-0.391290	-2.275001	3.862029
44	1	0	-0.064451	1.105952	1.894833
45	1	0	-3.262610	3.518370	-0.485735
46	1	0	-4.259582	2.728066	0.756590
47	1	0	-4.658945	2.501550	-0.978725
48	1	0	-3.614161	-3.064800	0.474672
49	1	0	-3.048938	-2.997331	-1.213985
50	1	0	-4.632167	-2.276645	-0.776750
51	1	0	-1.198022	-2.212059	4.592957
52	1	0	0.580742	-2.291012	4.361373
53	1	0	-0.500236	-3.170603	3.244784

Int2 (DEADTS10b.rev.log)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	1.939571	-1.481625	-1.196570
2	8	0	-0.490187	-0.550082	-2.308681
3	8	0	-0.169030	1.671254	-1.668523
4	8	0	3.074388	1.757842	0.044959
5	8	0	1.847919	2.086940	1.932378
6	7	0	1.186769	-0.043328	-0.771140
7	7	0	1.255847	0.426977	0.533297
8	6	0	0.406438	1.997231	-2.924008
9	6	0	-0.205228	0.270758	-1.388774
10	6	0	2.734593	3.158539	2.283525
11	6	0	2.130327	1.479563	0.759461
12	1	0	1.490904	1.815894	-2.921331
13	1	0	0.228689	3.065402	-3.074646
14	1	0	-0.061260	1.422180	-3.729276
15	6	0	2.476639	-1.299072	-2.921238
16	1	0	3.762698	2.796104	2.365780
17	1	0	2.692775	3.952401	1.533662
18	1	0	2.377028	3.523851	3.246615
19	6	0	3.398697	-1.597918	-0.122437
20	6	0	1.040811	-3.058996	-1.054337
21	1	0	3.137547	-0.431882	-2.998582
22	1	0	1.580361	-1.133977	-3.523001
23	1	0	3.002397	-2.200009	-3.253548
24	1	0	0.149751	-3.004100	-1.679618
25	1	0	0.738101	-3.202691	-0.016004
26	1	0	1.699201	-3.872996	-1.379176
27	1	0	3.049680	-1.749178	0.902853
28	1	0	3.966721	-0.666299	-0.182090
29	1	0	4.020207	-2.443274	-0.433920
30	6	0	-0.051538	0.281615	1.192934
31	6	0	-1.118932	0.263862	0.057536
32	6	0	-1.897152	-1.036316	-0.023707
33	6	0	-1.953873	1.547376	0.147768
34	6	0	-0.008807	-0.926026	2.130985
35	8	0	-1.443784	-2.107254	0.345059
36	8	0	-1.795462	2.395180	1.006527
37	8	0	-3.100677	-0.924103	-0.588649
38	8	0	-2.861581	1.663282	-0.828652
39	6	0	-3.583668	2.900618	-0.843754
40	6	0	-3.786431	-2.160824	-0.831737
41	8	0	0.906822	-1.718731	2.223908
42	8	0	-1.092039	-0.929745	2.925084
43	6	0	-1.218232	-2.066301	3.793940
44	1	0	-0.239944	1.163209	1.806084
45	1	0	-2.897767	3.739159	-0.993233
46	1	0	-4.125968	3.047089	0.094440
47	1	0	-4.278114	2.819975	-1.680883
48	1	0	-3.941564	-2.709083	0.101324

49	1	0	-3.209892	-2.779812	-1.523571
50	1	0	-4.740760	-1.877659	-1.276368
51	1	0	-2.117612	-1.885573	4.383348
52	1	0	-0.343359	-2.154862	4.442713
53	1	0	-1.324514	-2.976367	3.197653

Int3 (DEADTS6nn.rev.log)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	2.580737	-0.453190	0.814410
2	8	0	1.715658	-1.772280	-0.111493
3	8	0	0.706872	-1.225405	-2.154113
4	8	0	1.929993	3.026634	-0.775875
5	8	0	-0.330828	3.326684	-0.808995
6	7	0	1.468846	0.318863	-0.460778
7	7	0	0.479150	1.303141	-0.287988
8	6	0	1.916712	-1.257424	-2.907408
9	6	0	0.848160	-0.935270	-0.790931
10	6	0	-0.109813	4.721691	-1.059534
11	6	0	0.801340	2.589017	-0.659945
12	1	0	2.463817	-0.313455	-2.806985
13	1	0	1.614967	-1.399463	-3.947363
14	1	0	2.554451	-2.090056	-2.591781
15	6	0	4.178725	-0.215770	-0.056692
16	1	0	0.441235	5.178012	-0.232931
17	1	0	0.453532	4.861944	-1.985427
18	1	0	-1.104158	5.161093	-1.146253
19	6	0	2.499818	1.014079	1.960088
20	6	0	3.024901	-1.749377	2.079782
21	1	0	4.140152	0.712772	-0.630204
22	1	0	4.362515	-1.055139	-0.732852
23	1	0	4.993695	-0.165883	0.672329
24	1	0	3.313200	-2.673708	1.572689
25	1	0	2.162551	-1.952952	2.716130
26	1	0	3.854466	-1.393345	2.699740
27	1	0	1.511826	1.061738	2.425187
28	1	0	2.662140	1.931597	1.387487
29	1	0	3.258396	0.924323	2.743620
30	6	0	-0.873162	0.743169	-0.477794
31	6	0	-0.658302	-0.791497	-0.281387
32	6	0	-0.802708	-1.141720	1.201155
33	6	0	-1.623031	-1.607666	-1.144526
34	6	0	-1.880500	1.372373	0.491219
35	8	0	0.066932	-1.027077	2.036111
36	8	0	-2.448115	-1.149308	-1.900630
37	8	0	-2.061098	-1.510351	1.490797
38	8	0	-1.412118	-2.920547	-0.951254
39	6	0	-2.215009	-3.796112	-1.757875
40	6	0	-2.343102	-1.697686	2.891229
41	8	0	-1.673419	1.591454	1.664926
42	8	0	-3.040274	1.619402	-0.134103
43	6	0	-4.082077	2.165548	0.690651
44	1	0	-1.231117	0.899992	-1.497619
45	1	0	-2.019387	-3.618425	-2.818504
46	1	0	-3.277555	-3.635871	-1.556558
47	1	0	-1.917109	-4.806245	-1.476149
48	1	0	-2.179807	-0.759860	3.427116
49	1	0	-1.700883	-2.476939	3.307888
50	1	0	-3.390356	-1.996519	2.936467
51	1	0	-4.937323	2.298928	0.028292
52	1	0	-3.769079	3.121976	1.117497
53	1	0	-4.327731	1.475535	1.502241

TS3 (DEADTS6nn.log)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	2.900903	0.601143	0.851139

2	8	0	2.288923	-0.743978	0.261563
3	8	0	1.475920	-1.297323	-1.842675
4	8	0	0.352457	3.571138	-0.791161
5	8	0	-1.833700	2.896702	-0.822417
6	7	0	1.086903	0.892961	-1.001806
7	7	0	-0.216579	1.352596	-0.647652
8	6	0	2.387257	-0.763292	-2.795577
9	6	0	1.097334	-0.450043	-0.799220
10	6	0	-2.213435	4.272830	-0.736711
11	6	0	-0.481654	2.675049	-0.764381
12	1	0	2.078706	0.241796	-3.098438
13	1	0	2.366267	-1.447639	-3.646609
14	1	0	3.406460	-0.727801	-2.389175
15	6	0	4.005420	1.501877	-0.287009
16	1	0	-1.923599	4.699114	0.228763
17	1	0	-1.746125	4.854004	-1.535497
18	1	0	-3.299678	4.282797	-0.842531
19	6	0	1.873024	1.839086	1.704868
20	6	0	3.992168	-0.097017	2.141084
21	1	0	3.394520	2.043060	-1.010711
22	1	0	4.661140	0.795545	-0.804736
23	1	0	4.621046	2.202386	0.288617
24	1	0	4.674397	-0.828031	1.699100
25	1	0	3.370366	-0.604668	2.883827
26	1	0	4.572327	0.691621	2.630997
27	1	0	0.986539	1.354341	2.115799
28	1	0	1.572304	2.614879	0.997611
29	1	0	2.464422	2.267984	2.522632
30	6	0	-1.190725	0.268087	-0.659260
31	6	0	-0.299755	-0.962607	-0.260964
32	6	0	-0.396496	-1.249658	1.251548
33	6	0	-0.731532	-2.220375	-1.037716
34	6	0	-2.359824	0.535535	0.292555
35	8	0	0.335235	-0.871288	2.135658
36	8	0	-1.539173	-2.243118	-1.937165
37	8	0	-1.511822	-1.974221	1.484228
38	8	0	-0.074220	-3.298300	-0.579710
39	6	0	-0.330290	-4.519917	-1.288015
40	6	0	-1.830629	-2.186255	2.869922
41	8	0	-2.251002	0.901495	1.443208
42	8	0	-3.528396	0.273778	-0.311443
43	6	0	-4.696733	0.470994	0.498831
44	1	0	-1.583240	0.076638	-1.662762
45	1	0	-0.036009	-4.417642	-2.335765
46	1	0	-1.390980	-4.779664	-1.235737
47	1	0	0.276826	-5.277275	-0.791422
48	1	0	-2.019226	-1.225686	3.355267
49	1	0	-1.010570	-2.700344	3.376771
50	1	0	-2.729201	-2.803938	2.868779
51	1	0	-5.542171	0.223614	-0.143325
52	1	0	-4.756381	1.509623	0.834480
53	1	0	-4.672503	-0.185611	1.372780

3m + Me3PO (DEADTS6nn.for.log)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	4.342029	-0.575420	0.546849
2	8	0	4.057915	-1.894767	-0.126974
3	8	0	0.142954	-2.366262	-1.246185
4	8	0	1.604205	2.490074	-1.693819
5	8	0	-0.452955	3.242857	-1.056230
6	7	0	0.643481	-0.096938	-1.292569
7	7	0	-0.028434	1.062105	-0.903504
8	6	0	1.426247	-2.666761	-1.852124
9	6	0	-0.111642	-1.091846	-1.004007
10	6	0	-0.002266	4.581068	-1.307063
11	6	0	0.486644	2.279349	-1.268892
12	1	0	1.516742	-2.127697	-2.800119
13	1	0	1.405954	-3.743317	-2.022632
14	1	0	2.245220	-2.389448	-1.181246
15	6	0	4.445240	0.852428	-0.590311
16	1	0	0.822708	4.841755	-0.638607

17	1	0	0.329245	4.687263	-2.342830
18	1	0	-0.866414	5.217791	-1.113972
19	6	0	3.109854	-0.100926	1.815054
20	6	0	5.944566	-0.569979	1.444528
21	1	0	3.475731	1.032726	-1.065488
22	1	0	5.183821	0.632599	-1.368187
23	1	0	4.749760	1.761734	-0.059929
24	1	0	6.755417	-0.770639	0.737187
25	1	0	5.939935	-1.366487	2.195233
26	1	0	6.132981	0.388255	1.940776
27	1	0	3.093261	-0.859957	2.603454
28	1	0	2.114439	-0.061664	1.364222
29	1	0	3.342084	0.873322	2.258774
30	6	0	-1.426450	0.814405	-0.518308
31	6	0	-1.431145	-0.736364	-0.316772
32	6	0	-1.362775	-1.167794	1.163315
33	6	0	-2.625755	-1.387569	-1.037975
34	6	0	-1.816668	1.615401	0.726510
35	8	0	-0.376244	-1.584587	1.716566
36	8	0	-3.298961	-0.839678	-1.880806
37	8	0	-2.556190	-0.977373	1.756371
38	8	0	-2.781258	-2.655754	-0.641623
39	6	0	-3.823320	-3.394310	-1.307059
40	6	0	-2.585292	-1.250699	3.170981
41	8	0	-1.124948	1.742113	1.711199
42	8	0	-3.046289	2.131534	0.581141
43	6	0	-3.539001	2.875156	1.708262
44	1	0	-2.113512	1.055660	-1.333888
45	1	0	-3.627694	-3.438865	-2.381030
46	1	0	-4.792675	-2.920193	-1.134657
47	1	0	-3.795433	-4.391035	-0.867823
48	1	0	-1.909386	-0.569636	3.693560
49	1	0	-2.285568	-2.283263	3.363385
50	1	0	-3.618270	-1.084445	3.477064
51	1	0	-4.527859	3.227518	1.415080
52	1	0	-2.876927	3.716499	1.927694
53	1	0	-3.604573	2.232060	2.589798

TS4 (DEADTS7n.log)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	2.168437	-1.352160	-1.149375
2	8	0	-0.559311	-0.180095	-2.450775
3	8	0	-0.092576	1.857277	-1.456226
4	8	0	3.053802	1.815249	0.308519
5	8	0	1.667648	2.022406	2.099444
6	7	0	1.302897	-0.008294	-0.744392
7	7	0	1.248136	0.405716	0.583561
8	6	0	0.520481	2.344610	-2.643133
9	6	0	-0.291822	0.468266	-1.429496
10	6	0	2.495310	3.095484	2.565570
11	6	0	2.064014	1.469808	0.927094
12	1	0	1.582903	2.070435	-2.664010
13	1	0	0.430388	3.432975	-2.608379
14	1	0	0.016951	1.949603	-3.530150
15	6	0	2.463105	-1.148138	-2.928917
16	1	0	3.521148	2.751516	2.723021
17	1	0	2.501435	3.918577	1.846381
18	1	0	2.049086	3.415455	3.507873
19	6	0	3.735760	-1.354607	-0.222819
20	6	0	1.467155	-3.027266	-0.934394
21	1	0	3.123265	-0.293059	-3.094664
22	1	0	1.487743	-0.941928	-3.382394
23	1	0	2.903283	-2.051548	-3.361142
24	1	0	0.535209	-3.106411	-1.496127
25	1	0	1.246411	-3.190323	0.122315
26	1	0	2.191979	-3.769193	-1.289624
27	1	0	3.504571	-1.560894	0.826659
28	1	0	4.195959	-0.366969	-0.297954
29	1	0	4.406857	-2.129308	-0.607310
30	6	0	-0.090272	0.210096	1.142393
31	6	0	-1.117487	0.233379	-0.039106

32	6	0	-1.815020	-1.112185	-0.238024
33	6	0	-2.093626	1.407497	0.173636
34	6	0	-0.091989	-1.047379	2.015985
35	8	0	-1.253791	-2.179724	-0.079535
36	8	0	-2.154482	2.065046	1.193324
37	8	0	-3.089157	-1.010589	-0.624936
38	8	0	-2.862555	1.638971	-0.896821
39	6	0	-3.755963	2.753935	-0.779594
40	6	0	-3.739276	-2.251053	-0.943381
41	8	0	0.853933	-1.786192	2.191208
42	8	0	-1.272588	-1.170415	2.649039
43	6	0	-1.418299	-2.343973	3.464400
44	1	0	-0.336280	1.044369	1.800224
45	1	0	-3.194017	3.677799	-0.617289
46	1	0	-4.450039	2.608033	0.052711
47	1	0	-4.294625	2.793789	-1.726845
48	1	0	-3.745783	-2.916955	-0.076452
49	1	0	-3.224950	-2.741958	-1.773073
50	1	0	-4.755508	-1.978851	-1.228895
51	1	0	-2.404544	-2.261523	3.921996
52	1	0	-0.639648	-2.378805	4.230295
53	1	0	-1.355376	-3.240700	2.842048

Int4 (DEADTS7n.rev.log)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	2.752967	-1.089821	-0.812934
2	8	0	-1.009063	0.204217	-2.604605
3	8	0	-0.426608	2.007348	-1.358107
4	8	0	2.810132	2.211965	0.257351
5	8	0	1.164913	2.368454	1.818358
6	7	0	1.566827	0.014206	-0.820432
7	7	0	1.188636	0.582284	0.415981
8	6	0	0.120639	2.640581	-2.527062
9	6	0	-0.845071	0.744897	-1.536369
10	6	0	1.782123	3.579543	2.262536
11	6	0	1.797662	1.762645	0.768417
12	1	0	1.030058	2.111908	-2.821462
13	1	0	0.353242	3.661417	-2.223432
14	1	0	-0.605220	2.631133	-3.343721
15	6	0	3.467618	-0.976033	-2.486954
16	1	0	2.809925	3.396620	2.588390
17	1	0	1.793852	4.327099	1.464409
18	1	0	1.172716	3.925787	3.098994
19	6	0	4.092372	-0.810280	0.403429
20	6	0	2.324082	-2.869996	-0.622976
21	1	0	3.934794	0.004368	-2.609757
22	1	0	2.656181	-1.068496	-3.214974
23	1	0	4.204467	-1.765608	-2.663415
24	1	0	1.511495	-3.115372	-1.311004
25	1	0	1.970138	-3.042214	0.395511
26	1	0	3.194212	-3.504470	-0.827801
27	1	0	3.666437	-0.937886	1.402984
28	1	0	4.457235	0.214234	0.301862
29	1	0	4.908114	-1.527398	0.264311
30	6	0	-0.112100	0.207238	0.926979
31	6	0	-1.251257	0.122530	-0.172179
32	6	0	-1.629867	-1.336972	-0.510941
33	6	0	-2.484687	0.902338	0.353900
34	6	0	0.011597	-1.058199	1.790822
35	8	0	-0.842227	-2.255352	-0.525015
36	8	0	-2.709411	1.123569	1.522255
37	8	0	-2.929488	-1.463458	-0.808948
38	8	0	-3.271294	1.320015	-0.649789
39	6	0	-4.456720	2.027922	-0.252222
40	6	0	-3.336858	-2.770698	-1.247619
41	8	0	1.055824	-1.589671	2.102693
42	8	0	-1.189234	-1.441427	2.260057
43	6	0	-1.187257	-2.610891	3.094157
44	1	0	-0.431086	0.979190	1.627686
45	1	0	-4.194954	2.919350	0.323508
46	1	0	-5.097655	1.383680	0.355298

47	1	0	-4.955987	2.300913	-1.181921
48	1	0	-3.128203	-3.516251	-0.476149
49	1	0	-2.806427	-3.039179	-2.164279
50	1	0	-4.408506	-2.693609	-1.431364
51	1	0	-2.217323	-2.730429	3.430776
52	1	0	-0.516410	-2.473059	3.945398
53	1	0	-0.865854	-3.482859	2.517808

9 + A (ADEADTS1c.rev.log)
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.769426	-1.603186	-1.272103
2	8	0	-0.818408	-2.945662	1.187600
3	8	0	-1.519973	-1.185537	2.443664
4	8	0	-3.427686	-0.229322	-0.766143
5	8	0	-3.216843	1.863213	0.104938
6	7	0	-1.079079	-0.883351	0.239356
7	7	0	-1.488906	0.478172	0.352258
8	6	0	-1.560866	-2.065113	3.577485
9	6	0	-1.127500	-1.761382	1.305737
10	6	0	-4.489620	2.145463	-0.468692
11	6	0	-2.738756	0.594917	-0.135486
12	1	0	-2.254873	-2.891125	3.401207
13	1	0	-1.905177	-1.445168	4.405517
14	1	0	-0.567731	-2.470559	3.788724
15	6	0	-1.999790	-2.859206	-1.744770
16	1	0	-4.462278	2.075311	-1.561705
17	1	0	-5.254847	1.456824	-0.097954
18	1	0	-4.727705	3.168688	-0.168305
19	6	0	-0.794164	-0.263528	-2.488855
20	6	0	0.874408	-2.386678	-1.316264
21	1	0	-2.978629	-2.378168	-1.691061
22	1	0	-1.946846	-3.688167	-1.036441
23	1	0	-1.794807	-3.219001	-2.758819
24	1	0	0.889183	-3.211242	-0.602323
25	1	0	1.657919	-1.671907	-1.049526
26	1	0	1.063298	-2.766336	-2.326521
27	1	0	-0.201698	0.586056	-2.139094
28	1	0	-1.829229	0.055049	-2.623790
29	1	0	-0.389555	-0.644201	-3.432261
30	6	0	2.109913	1.673296	-0.036617
31	6	0	3.073302	0.939086	-0.035168
32	6	0	4.146146	-0.028075	-0.067594
33	6	0	0.958875	2.555608	-0.177729
34	8	0	3.992010	-1.188412	-0.399848
35	8	0	5.315643	0.512974	0.306388
36	6	0	6.440455	-0.387813	0.293381
37	8	0	0.456298	2.781057	-1.260859
38	8	0	0.600996	3.073006	0.991895
39	6	0	-0.612483	3.862705	0.979333
40	1	0	6.603913	-0.778421	-0.714156
41	1	0	6.268405	-1.220906	0.979299
42	1	0	7.290265	0.211743	0.618224
43	1	0	-0.704858	4.245853	1.995454
44	1	0	-1.456392	3.220601	0.720637
45	1	0	-0.516914	4.682921	0.263495

TS1a (ADEADTS1c.log)
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.700710	-1.849289	-1.288715
2	8	0	2.576362	-1.715984	0.796727
3	8	0	1.291215	-0.550841	2.268688
4	8	0	-1.781489	-2.454621	0.575713
5	8	0	-2.791707	-0.540037	1.278826
6	7	0	0.476189	-1.053314	0.212376
7	7	0	-0.700059	-0.390930	0.539392

8	6	0	2.385634	-0.565854	3.201755
9	6	0	1.539931	-1.138425	1.103295
10	6	0	-4.012697	-1.276214	1.388354
11	6	0	-1.742177	-1.237695	0.779326
12	1	0	2.684188	-1.592352	3.428253
13	1	0	2.003666	-0.068370	4.092730
14	1	0	3.239430	-0.019328	2.793872
15	6	0	0.865367	-3.642962	-1.038066
16	1	0	-4.375932	-1.577392	0.400734
17	1	0	-3.877910	-2.167253	2.006718
18	1	0	-4.723329	-0.592651	1.856062
19	6	0	-0.790593	-1.539620	-2.264609
20	6	0	2.140239	-1.217756	-2.195659
21	1	0	-0.012295	-3.973213	-0.476657
22	1	0	1.774150	-3.842549	-0.467266
23	1	0	0.913268	-4.151064	-2.006990
24	1	0	3.052574	-1.544985	-1.695281
25	1	0	2.119020	-0.119351	-2.207035
26	1	0	2.109773	-1.609434	-3.218475
27	1	0	-1.076239	-0.485364	-2.224226
28	1	0	-1.609008	-2.132288	-1.852153
29	1	0	-0.588409	-1.837355	-3.298442
30	6	0	-0.663598	1.429147	-0.182554
31	6	0	0.455807	1.947808	-0.370429
32	6	0	1.827883	2.199020	-0.563265
33	6	0	-2.075498	1.667905	-0.519963
34	8	0	2.481379	1.868551	-1.555975
35	8	0	2.383351	2.901375	0.466444
36	6	0	3.765490	3.230944	0.292801
37	8	0	-2.725325	0.986932	-1.293222
38	8	0	-2.552182	2.773250	0.078955
39	6	0	-3.905030	3.114237	-0.260257
40	1	0	3.912053	3.854902	-0.593873
41	1	0	4.377334	2.329442	0.189192
42	1	0	4.047689	3.780215	1.192747
43	1	0	-4.127365	4.017568	0.308535
44	1	0	-4.584855	2.304975	0.019635
45	1	0	-3.998745	3.302656	-1.333346

Int1a (ADEADTS1cR.for.log)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.917921	-1.567075	-1.526496
2	8	0	2.864480	-1.255772	0.493811
3	8	0	1.566424	-0.084821	1.951217
4	8	0	-0.915132	-2.421847	1.271618
5	8	0	-2.177830	-0.636346	1.893586
6	7	0	0.708542	-0.751658	-0.035280
7	7	0	-0.539969	-0.326917	0.386294
8	6	0	2.685718	0.040272	2.849362
9	6	0	1.816196	-0.721755	0.817748
10	6	0	-3.082101	-1.522300	2.568872
11	6	0	-1.206291	-1.237415	1.195636
12	1	0	3.058683	-0.947253	3.130720
13	1	0	2.292679	0.570288	3.715704
14	1	0	3.483354	0.616268	2.375581
15	6	0	1.062883	-3.356393	-1.243036
16	1	0	-3.645602	-2.111296	1.840101
17	1	0	-2.538276	-2.190614	3.240233
18	1	0	-3.753432	-0.872962	3.131202
19	6	0	-0.571124	-1.211946	-2.485804
20	6	0	2.339388	-0.914974	-2.437226
21	1	0	0.211174	-3.675321	-0.636502
22	1	0	1.986836	-3.547575	-0.692373
23	1	0	1.082511	-3.888949	-2.199485
24	1	0	3.269000	-1.291863	-2.011131
25	1	0	2.296031	0.179670	-2.332250
26	1	0	2.246614	-1.211481	-3.487724
27	1	0	-0.532949	-0.166020	-2.802478
28	1	0	-1.478772	-1.355392	-1.891190
29	1	0	-0.579827	-1.865775	-3.363779
30	6	0	-1.041129	0.980133	-0.101854

31	6	0	-0.280288	2.027569	-0.386036
32	6	0	1.106948	2.247754	-0.424900
33	6	0	-2.472011	0.878456	-0.493111
34	8	0	1.867186	1.942729	-1.365716
35	8	0	1.579471	2.993732	0.634709
36	6	0	2.917064	3.465449	0.489021
37	8	0	-3.050758	-0.167250	-0.777721
38	8	0	-3.085798	2.073761	-0.549349
39	6	0	-4.438468	2.044688	-1.015234
40	1	0	3.018477	4.117899	-0.384762
41	1	0	3.630707	2.640690	0.381373
42	1	0	3.130511	4.029458	1.400400
43	1	0	-4.776369	3.081531	-0.989116
44	1	0	-5.061829	1.421895	-0.366773
45	1	0	-4.493395	1.652222	-2.035274

Int1a*i* (ADEADTS2.for.log)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-1.822012	-0.877684	-1.480817
2	8	0	-1.786050	-2.630631	0.715083
3	8	0	-1.277790	-1.078312	2.307375
4	8	0	-2.613546	2.018012	0.626048
5	8	0	-0.555886	2.704171	1.315025
6	7	0	-1.556167	-0.427424	0.150549
7	7	0	-0.751945	0.679391	0.379605
8	6	0	-0.867484	-2.100700	3.234050
9	6	0	-1.498835	-1.498984	1.070589
10	6	0	-1.101674	4.003536	1.580073
11	6	0	-1.418638	1.828170	0.771151
12	1	0	-1.576883	-2.930792	3.231621
13	1	0	-0.841999	-1.612965	4.208104
14	1	0	0.130151	-2.444775	2.947895
15	6	0	-3.501225	-1.560224	-1.615792
16	1	0	-1.427803	4.478015	0.650489
17	1	0	-1.948221	3.933052	2.267306
18	1	0	-0.286776	4.570869	2.030518
19	6	0	-1.777863	0.681877	-2.393207
20	6	0	-0.618808	-2.057472	-2.158677
21	1	0	-4.208665	-0.835905	-1.202499
22	1	0	-3.561642	-2.494251	-1.055631
23	1	0	-3.735284	-1.739672	-2.670307
24	1	0	-0.755434	-3.016877	-1.655793
25	1	0	0.410472	-1.718170	-1.977750
26	1	0	-0.803802	-2.165612	-3.233607
27	1	0	-0.806675	1.176018	-2.274898
28	1	0	-2.547064	1.343183	-1.984196
29	1	0	-1.976966	0.477101	-3.449888
30	6	0	0.692520	0.460986	0.226234
31	6	0	1.165333	-0.760209	0.475151
32	6	0	2.406592	-1.276842	-0.005892
33	6	0	1.349005	1.560454	-0.527119
34	8	0	2.571184	-1.678079	-1.164355
35	8	0	3.363406	-1.443070	0.953473
36	6	0	4.556319	-2.092363	0.510558
37	8	0	0.785036	2.320560	-1.306700
38	8	0	2.676271	1.605764	-0.307234
39	6	0	3.404198	2.533119	-1.121437
40	1	0	5.051354	-1.518663	-0.279450
41	1	0	4.343273	-3.095475	0.127365
42	1	0	5.201374	-2.153646	1.389741
43	1	0	4.443580	2.445544	-0.803122
44	1	0	3.039334	3.552477	-0.968194
45	1	0	3.306990	2.276635	-2.180333

TS2a (ADEADTS2.log)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	15	0	-1.875246	-1.201841	-1.285057
2	8	0	-0.750539	-2.795629	0.638194
3	8	0	-0.619116	-1.237869	2.323503
4	8	0	-2.890198	1.584061	0.989816
5	8	0	-0.904734	2.652620	1.299121
6	7	0	-1.444795	-0.636714	0.270947
7	7	0	-0.899390	0.643382	0.306154
8	6	0	0.265060	-2.042537	3.111546
9	6	0	-0.713001	-1.630118	1.035393
10	6	0	-1.623770	3.803627	1.764083
11	6	0	-1.677995	1.626706	0.897214
12	1	0	-0.040020	-3.092056	3.084692
13	1	0	0.198034	-1.648878	4.126533
14	1	0	1.285991	-1.937416	2.727788
15	6	0	-3.293835	-2.317343	-1.089884
16	1	0	-2.257786	4.207122	0.969932
17	1	0	-2.244703	3.546237	2.625601
18	1	0	-0.857779	4.526911	2.044982
19	6	0	-2.415022	0.296117	-2.151540
20	6	0	-0.578388	-2.021872	-2.268981
21	1	0	-4.097476	-1.782340	-0.576903
22	1	0	-2.978011	-3.171883	-0.488606
23	1	0	-3.640160	-2.655587	-2.071858
24	1	0	-0.464828	-3.047759	-1.917334
25	1	0	0.384226	-1.514109	-2.137758
26	1	0	-0.872958	-2.004199	-3.324287
27	1	0	-1.566136	0.976963	-2.274396
28	1	0	-3.175459	0.798681	-1.547350
29	1	0	-2.825567	0.022378	-3.128365
30	6	0	0.540046	0.650927	0.081603
31	6	0	1.152380	-0.504145	0.325169
32	6	0	2.442191	-0.929716	-0.145161
33	6	0	1.007918	1.808294	-0.722637
34	8	0	2.665917	-1.281601	-1.302389
35	8	0	3.372517	-1.046879	0.843240
36	6	0	4.631793	-1.587281	0.429544
37	8	0	0.304043	2.448688	-1.488918
38	8	0	2.324623	2.037975	-0.562498
39	6	0	2.881892	3.042069	-1.421578
40	1	0	5.105352	-0.948860	-0.322357
41	1	0	4.508967	-2.589941	0.009146
42	1	0	5.244804	-1.625878	1.331865
43	1	0	3.936403	3.103669	-1.150882
44	1	0	2.386489	4.003639	-1.262293
45	1	0	2.772878	2.754949	-2.471191

Int2a (ADEADTS2.rev.log)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	2.245528	-0.800082	-0.929152
2	8	0	2.309998	0.877583	-0.024557
3	8	0	1.264487	0.957447	2.066625
4	8	0	-0.119574	-3.277020	1.059708
5	8	0	-2.132696	-2.275306	0.714315
6	7	0	1.091322	-0.846789	0.423962
7	7	0	-0.262009	-1.156489	0.156429
8	6	0	2.485486	0.616353	2.717879
9	6	0	1.186626	0.621193	0.719657
10	6	0	-2.786223	-3.481759	1.142829
11	6	0	-0.785586	-2.333284	0.702337
12	1	0	2.661796	-0.466768	2.687729
13	1	0	2.362905	0.930059	3.756974
14	1	0	3.335093	1.138933	2.268586
15	6	0	4.020008	-1.070599	-0.549531
16	1	0	-2.525495	-4.312704	0.482604
17	1	0	-2.496139	-3.728329	2.166871
18	1	0	-3.852968	-3.265478	1.086097
19	6	0	1.828928	-2.524837	-1.536578
20	6	0	1.971285	0.090958	-2.516685
21	1	0	4.082114	-1.520311	0.446805
22	1	0	4.545442	-0.114823	-0.532159

23	1	0	4.476333	-1.754695	-1.270290
24	1	0	2.518098	1.034517	-2.516343
25	1	0	0.901735	0.310165	-2.606546
26	1	0	2.263609	-0.535490	-3.364652
27	1	0	0.812766	-2.553337	-1.944053
28	1	0	1.881916	-3.249073	-0.719086
29	1	0	2.521318	-2.822321	-2.331866
30	6	0	-0.957600	0.056022	-0.046841
31	6	0	-0.168065	1.121480	0.205622
32	6	0	-0.549948	2.516348	-0.066232
33	6	0	-2.315479	0.049679	-0.691257
34	8	0	-1.527035	2.852911	-0.713868
35	8	0	0.324850	3.387516	0.471760
36	6	0	0.035952	4.771641	0.231867
37	8	0	-2.491294	-0.380159	-1.809334
38	8	0	-3.247484	0.585425	0.098801
39	6	0	-4.533499	0.777165	-0.516421
40	1	0	-0.930352	5.044169	0.665303
41	1	0	0.014176	4.980750	-0.841305
42	1	0	0.842317	5.323937	0.714979
43	1	0	-5.173024	1.178678	0.269486
44	1	0	-4.926299	-0.171485	-0.890809
45	1	0	-4.444780	1.488438	-1.341250

Int3a (ADEADTS4.rev.log)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	2.320870	-0.909456	-0.793147
2	8	0	2.277448	0.650234	-0.169342
3	8	0	1.468224	1.148642	1.965251
4	8	0	-0.331957	-3.321896	0.642610
5	8	0	-2.333177	-2.239023	0.529321
6	7	0	0.944035	-0.864903	0.685709
7	7	0	-0.432757	-1.042229	0.405078
8	6	0	2.557912	0.561761	2.670364
9	6	0	1.145513	0.573995	0.743670
10	6	0	-2.998084	-3.512608	0.520598
11	6	0	-0.985377	-2.301622	0.545511
12	1	0	2.402917	-0.514914	2.805320
13	1	0	2.580855	1.053089	3.645409
14	1	0	3.509373	0.739284	2.154540
15	6	0	3.725660	-0.405692	-1.921315
16	1	0	-2.706070	-4.092442	-0.358797
17	1	0	-2.752362	-4.076282	1.423598
18	1	0	-4.062451	-3.279895	0.489481
19	6	0	3.133945	-2.326270	0.052327
20	6	0	1.130901	-1.516435	-2.059567
21	1	0	4.581491	-0.056921	-1.334596
22	1	0	3.413518	0.412347	-2.578096
23	1	0	4.046002	-1.251758	-2.539202
24	1	0	0.371447	-0.757203	-2.270396
25	1	0	0.629280	-2.410463	-1.682288
26	1	0	1.659943	-1.752466	-2.986267
27	1	0	2.366959	-3.021779	0.398171
28	1	0	3.671916	-1.946713	0.927032
29	1	0	3.850384	-2.818173	-0.612502
30	6	0	-1.034750	0.165302	0.093809
31	6	0	-0.140631	1.178430	0.229864
32	6	0	-0.423341	2.572758	-0.114133
33	6	0	-2.408964	0.253014	-0.511830
34	8	0	-1.481164	2.968214	-0.578894
35	8	0	0.631818	3.379744	0.124512
36	6	0	0.428409	4.761156	-0.199325
37	8	0	-2.622831	-0.073716	-1.657875
38	8	0	-3.303061	0.745525	0.345075
39	6	0	-4.600850	1.016294	-0.214384
40	1	0	-0.392764	5.178892	0.389870
41	1	0	0.196629	4.879596	-1.261622
42	1	0	1.367349	5.258175	0.046476
43	1	0	-5.204311	1.378375	0.617746
44	1	0	-5.032553	0.107539	-0.641199
45	1	0	-4.513998	1.781182	-0.989796

TS3a (ADEADTS4.log)
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	2.435966	-0.934527	-0.869408
2	8	0	2.275085	0.535773	-0.252817
3	8	0	1.620520	1.156546	1.915479
4	8	0	-0.489752	-3.301378	0.653105
5	8	0	-2.465957	-2.180084	0.491574
6	7	0	0.813060	-0.882355	0.909083
7	7	0	-0.545873	-1.006321	0.547375
8	6	0	2.576571	0.439942	2.686710
9	6	0	1.082161	0.497623	0.827816
10	6	0	-3.143479	-3.439427	0.365314
11	6	0	-1.120525	-2.264633	0.573919
12	1	0	2.206699	-0.561094	2.932698
13	1	0	2.721940	1.021413	3.599795
14	1	0	3.535702	0.362739	2.157459
15	6	0	3.772674	-0.526143	-2.068103
16	1	0	-2.817355	-3.963522	-0.537079
17	1	0	-2.947234	-4.066858	1.237934
18	1	0	-4.202677	-3.190321	0.300124
19	6	0	3.186415	-2.278081	0.120082
20	6	0	1.111071	-1.612941	-1.931958
21	1	0	4.648998	-0.144950	-1.536089
22	1	0	3.426114	0.250672	-2.755609
23	1	0	4.062518	-1.411077	-2.644562
24	1	0	0.327233	-0.865628	-2.085734
25	1	0	0.671520	-2.487637	-1.448709
26	1	0	1.527258	-1.892188	-2.905061
27	1	0	2.398047	-2.866202	0.589324
28	1	0	3.811299	-1.834361	0.900696
29	1	0	3.818135	-2.899895	-0.524328
30	6	0	-1.090585	0.195916	0.167789
31	6	0	-0.140465	1.169981	0.297675
32	6	0	-0.347931	2.563564	-0.087002
33	6	0	-2.430505	0.329006	-0.497330
34	8	0	-1.384169	2.997229	-0.569400
35	8	0	0.742095	3.330910	0.133793
36	6	0	0.599089	4.708416	-0.230950
37	8	0	-2.607955	0.010124	-1.652727
38	8	0	-3.347261	0.852380	0.318010
39	6	0	-4.607755	1.163257	-0.300976
40	1	0	-0.211620	5.177026	0.334274
41	1	0	0.385638	4.807831	-1.299276
42	1	0	1.554407	5.174387	0.013651
43	1	0	-5.234825	1.554400	0.500127
44	1	0	-5.052651	0.266272	-0.739345
45	1	0	-4.460212	1.916760	-1.078444

10m + Me3PO (ADEADTS4.for.log)
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-4.501145	0.334609	0.395831
2	8	0	-4.058779	1.773965	0.322815
3	8	0	-0.007049	2.618743	-0.757036
4	8	0	-1.285277	-2.288421	-0.632366
5	8	0	0.876289	-2.959096	-0.455805
6	7	0	-0.382148	0.314411	-0.709329
7	7	0	0.429486	-0.755194	-0.390889
8	6	0	-1.364275	2.799469	-1.219483
9	6	0	0.390180	1.372670	-0.541029
10	6	0	0.443908	-4.332272	-0.450159
11	6	0	-0.108628	-2.053125	-0.505143
12	1	0	-1.504297	2.278798	-2.172427
13	1	0	-1.468560	3.875893	-1.359593
14	1	0	-2.091888	2.432330	-0.490458

15	6	0	-6.270964	0.153705	0.851527
16	1	0	-0.204649	-4.521325	0.408266
17	1	0	-0.093549	-4.561582	-1.373092
18	1	0	1.359166	-4.918659	-0.377657
19	6	0	-4.312862	-0.590041	-1.171231
20	6	0	-3.593253	-0.666113	1.630895
21	1	0	-6.888384	0.673599	0.112285
22	1	0	-6.441140	0.619884	1.827152
23	1	0	-6.577720	-0.896844	0.898682
24	1	0	-3.663753	-0.185662	2.611730
25	1	0	-2.542983	-0.716774	1.331823
26	1	0	-3.989525	-1.684988	1.696979
27	1	0	-3.248344	-0.654022	-1.413930
28	1	0	-4.835897	-0.057655	-1.971752
29	1	0	-4.714333	-1.606298	-1.091956
30	6	0	1.692989	-0.361004	-0.029066
31	6	0	1.717358	1.014786	-0.105808
32	6	0	2.884771	1.833248	0.257889
33	6	0	2.765003	-1.273265	0.497993
34	8	0	3.910722	1.374830	0.728960
35	8	0	2.691060	3.141979	0.014615
36	6	0	3.788469	3.998872	0.367079
37	8	0	2.734612	-1.763279	1.602174
38	8	0	3.739404	-1.430299	-0.403330
39	6	0	4.897398	-2.143852	0.067910
40	1	0	4.683082	3.731984	-0.201939
41	1	0	4.009512	3.919950	1.434752
42	1	0	3.459403	5.007126	0.115750
43	1	0	5.570861	-2.198213	-0.787148
44	1	0	4.620300	-3.144730	0.408441
45	1	0	5.360092	-1.592315	0.889702

TS4a (ADEADTS3.log)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-2.389765	-0.014605	-1.038646
2	8	0	-1.515051	-2.091867	-0.009251
3	8	0	-0.685512	-1.411750	2.053858
4	8	0	-1.450693	2.880990	1.171354
5	8	0	0.819182	2.824004	1.036507
6	7	0	-1.429630	0.204529	0.358096
7	7	0	-0.356790	1.110700	0.168167
8	6	0	-1.830375	-1.980767	2.675817
9	6	0	-0.784514	-1.265947	0.660758
10	6	0	0.865823	4.139999	1.611100
11	6	0	-0.421388	2.328691	0.849523
12	1	0	-2.684316	-1.288362	2.649611
13	1	0	-1.549728	-2.158842	3.717046
14	1	0	-2.115777	-2.919633	2.193465
15	6	0	-3.987071	-0.780400	-0.626629
16	1	0	0.358755	4.859316	0.962781
17	1	0	0.390622	4.142299	2.594750
18	1	0	1.925948	4.379225	1.695016
19	6	0	-2.808923	1.699172	-1.533980
20	6	0	-1.643166	-0.726854	-2.548348
21	1	0	-4.329685	-0.349862	0.318881
22	1	0	-3.848460	-1.853078	-0.504847
23	1	0	-4.718783	-0.555108	-1.410017
24	1	0	-1.500301	-1.796418	-2.406041
25	1	0	-0.672871	-0.245794	-2.711702
26	1	0	-2.287853	-0.515502	-3.408806
27	1	0	-1.915522	2.202656	-1.913647
28	1	0	-3.175280	2.257368	-0.669820
29	1	0	-3.567377	1.683280	-2.323561
30	6	0	0.834060	0.361741	-0.045428
31	6	0	0.655687	-0.950677	0.177711
32	6	0	1.652659	-1.987102	-0.157074
33	6	0	1.985404	1.043301	-0.718315
34	8	0	2.522805	-1.864850	-1.002459
35	8	0	1.475148	-3.102553	0.573757
36	6	0	2.376843	-4.177373	0.278730
37	8	0	1.849314	1.661765	-1.753414

38	8	0	3.137253	0.862546	-0.067615
39	6	0	4.310509	1.324306	-0.758129
40	1	0	3.410573	-3.879143	0.475332
41	1	0	2.288335	-4.478025	-0.768984
42	1	0	2.081015	-4.993501	0.938417
43	1	0	5.139215	1.144870	-0.073201
44	1	0	4.225133	2.387902	-0.994396
45	1	0	4.444918	0.754027	-1.680741

Int4a (ADEADTS3.for.log)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-2.334531	-1.177394	-0.888398
2	8	0	0.610049	-2.867617	0.066363
3	8	0	0.654323	-1.811633	2.069532
4	8	0	-2.901682	1.701464	0.839513
5	8	0	-0.874391	2.646915	1.233994
6	7	0	-1.610395	-0.731311	0.502331
7	7	0	-0.956086	0.525142	0.436678
8	6	0	0.170531	-3.008650	2.694688
9	6	0	0.757129	-1.859186	0.732390
10	6	0	-1.534591	3.892635	1.502951
11	6	0	-1.689862	1.644752	0.837634
12	1	0	-0.872596	-3.175129	2.411842
13	1	0	0.247408	-2.830014	3.767771
14	1	0	0.773874	-3.871248	2.400919
15	6	0	-2.735865	-2.930322	-0.624733
16	1	0	-2.036060	4.263367	0.604770
17	1	0	-2.269355	3.768104	2.301672
18	1	0	-0.743421	4.576939	1.810575
19	6	0	-3.909969	-0.341273	-1.327648
20	6	0	-1.303706	-1.062509	-2.401596
21	1	0	-3.371188	-3.022123	0.260664
22	1	0	-1.801097	-3.470965	-0.454695
23	1	0	-3.259115	-3.345046	-1.491374
24	1	0	-0.441690	-1.724758	-2.283307
25	1	0	-0.944053	-0.034278	-2.517700
26	1	0	-1.872752	-1.345543	-3.293273
27	1	0	-3.721832	0.717476	-1.520589
28	1	0	-4.593050	-0.406414	-0.476978
29	1	0	-4.365547	-0.803224	-2.210884
30	6	0	0.398795	0.563293	0.131205
31	6	0	1.203584	-0.534500	0.172039
32	6	0	2.551729	-0.505167	-0.433997
33	6	0	0.873248	1.853287	-0.516008
34	8	0	2.948566	0.285943	-1.272279
35	8	0	3.324167	-1.502791	0.056653
36	6	0	4.639454	-1.595275	-0.505729
37	8	0	0.362237	2.276637	-1.531619
38	8	0	1.872124	2.432223	0.152075
39	6	0	2.487629	3.544210	-0.518634
40	1	0	5.214034	-0.689515	-0.292577
41	1	0	4.586437	-1.734953	-1.588840
42	1	0	5.099518	-2.461518	-0.029233
43	1	0	3.238434	3.922697	0.175207
44	1	0	1.747474	4.315151	-0.747057
45	1	0	2.956118	3.198184	-1.443245

P(CH3)3 (PMe.log)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.000480	-0.000397	-0.605678
2	6	0	-1.574478	-0.475113	0.281019
3	6	0	1.199518	-1.124826	0.280574
4	6	0	0.375637	1.600431	0.280396
5	1	0	-1.871110	-1.487270	-0.014768

6	1	0	-2.380866	0.205360	-0.013252
7	1	0	-1.470797	-0.444990	1.373085
8	1	0	-0.356901	2.361487	-0.009547
9	1	0	1.365234	1.962192	-0.019102
10	1	0	0.356875	1.493305	1.372310
11	1	0	2.223932	-0.874793	-0.016161
12	1	0	1.014480	-2.164077	-0.011814
13	1	0	1.122285	-1.048210	1.372480

2b (DEAD2.log)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.157073	1.576093	0.073248
2	8	0	-2.392909	-0.679306	-0.134343
3	8	0	2.157088	-1.576091	-0.073246
4	8	0	2.392903	0.679309	0.134341
5	7	0	-0.330835	0.253401	-0.462981
6	7	0	0.330831	-0.253409	0.462954
7	6	0	-3.814628	-0.559217	0.087392
8	6	0	-1.719005	0.469118	-0.109659
9	6	0	3.814624	0.559224	-0.087366
10	6	0	1.719002	-0.469125	0.109650
11	1	0	-4.006937	-0.184119	1.095259
12	1	0	-4.208985	-1.567689	-0.031472
13	1	0	-4.254923	0.121324	-0.645135
14	1	0	4.254914	-0.121316	0.645166
15	1	0	4.006956	0.184129	-1.095229
16	1	0	4.208979	1.567696	0.031506

9 (AM.log)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.602331	0.192487	0.060967
2	6	0	0.602340	0.192534	-0.060923
3	6	0	2.035030	0.249064	-0.278917
4	6	0	-2.035021	0.248904	0.279039
5	8	0	2.562516	0.977301	-1.091259
6	8	0	2.679136	-0.606623	0.533369
7	6	0	4.113091	-0.619669	0.389136
8	8	0	-2.562493	0.976750	1.091735
9	8	0	-2.679151	-0.606386	-0.533639
10	6	0	-4.113109	-0.619437	-0.389427
11	1	0	4.526721	0.367054	0.611813
12	1	0	4.390737	-0.904888	-0.628608
13	1	0	4.466107	-1.358323	1.108203
14	1	0	-4.466211	-1.357168	-1.109398
15	1	0	-4.526641	0.367602	-0.610861
16	1	0	-4.390778	-0.905904	0.627961

1m (MeEster.log)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.444426	-1.021849	-0.030744
2	6	0	0.525801	-0.102555	0.086213
3	6	0	0.270522	1.363590	0.352894
4	6	0	1.977847	-0.453258	0.016832
5	6	0	-1.886024	-0.670959	0.014478
6	8	0	0.269413	1.836347	1.464284
7	8	0	2.861928	0.377304	0.044882
8	8	0	0.108548	2.043965	-0.788388
9	8	0	2.191125	-1.779360	-0.091576
10	6	0	3.572668	-2.171315	-0.176040

11	1	0	4.114390	-1.850693	0.717308
12	1	0	4.041983	-1.727005	-1.057530
13	1	0	3.561335	-3.258625	-0.251492
14	6	0	-0.156047	3.449878	-0.625203
15	1	0	0.656839	3.929324	-0.074509
16	1	0	-1.095909	3.590997	-0.085829
17	1	0	-0.227526	3.850355	-1.636454
18	8	0	-2.341205	0.448276	0.139708
19	8	0	-2.641535	-1.783611	-0.104757
20	6	0	-4.062073	-1.566209	-0.068443
21	1	0	-4.511094	-2.554553	-0.166797
22	1	0	-4.370106	-0.917843	-0.893037
23	1	0	-4.352672	-1.101266	0.877238
24	1	0	-0.193054	-2.067990	-0.162045

A (3dMeR.log)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.838768	-1.417299	-0.041872
2	8	0	-2.378169	0.851665	0.462747
3	8	0	-0.862672	2.381300	-0.269765
4	8	0	1.694088	-0.289839	1.018330
5	8	0	3.024512	0.686681	-0.551736
6	7	0	-0.411557	0.168667	-0.473767
7	7	0	0.862495	0.475933	-1.036555
8	6	0	-1.768295	3.418243	0.138017
9	6	0	-1.296081	1.140991	-0.048774
10	6	0	4.115322	0.433083	0.326103
11	6	0	1.805049	0.262392	-0.097621
12	1	0	-2.713615	3.342049	-0.405880
13	1	0	-1.259880	4.350849	-0.106881
14	1	0	-1.966068	3.358450	1.211470
15	6	0	-2.393940	-1.911707	-0.863316
16	1	0	3.973848	0.923127	1.294870
17	1	0	4.252147	-0.640114	0.502090
18	1	0	4.996030	0.841909	-0.174975
19	6	0	0.459169	-2.490406	-0.708380
20	6	0	-1.019116	-1.704515	1.746024
21	1	0	-2.269990	-1.817123	-1.946142
22	1	0	-3.199309	-1.255438	-0.531792
23	1	0	-2.631264	-2.952251	-0.617281
24	1	0	-1.853309	-1.107027	2.118480
25	1	0	-0.084125	-1.381375	2.208796
26	1	0	-1.202318	-2.767348	1.937669
27	1	0	1.341085	-2.402214	-0.072331
28	1	0	0.710942	-2.150595	-1.715781
29	1	0	0.096054	-3.522532	-0.730898

B (AMPMe.log)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	2.054493	-0.567247	0.046766
2	8	0	1.089313	2.148199	0.096193
3	8	0	-1.135171	1.777000	-0.050968
4	8	0	-2.532463	-0.945491	-1.467301
5	8	0	-2.678030	-1.072374	0.804726
6	6	0	0.310163	-0.098983	-0.051076
7	6	0	-0.563418	-1.118291	-0.178275
8	6	0	-1.342296	3.196452	-0.022156
9	6	0	0.139960	1.370910	0.004951
10	6	0	-4.098974	-1.114985	0.653569
11	6	0	-1.982179	-0.986715	-0.374606
12	1	0	-0.961069	3.622909	0.909902
13	1	0	-2.421458	3.332641	-0.093641
14	1	0	-0.838155	3.676141	-0.865459
15	6	0	2.158351	-2.381893	-0.017316
16	1	0	-4.475201	-0.202749	0.179725

17	1	0	-4.406717	-1.972091	0.046330
18	1	0	-4.500096	-1.205944	1.665318
19	6	0	3.069324	0.073747	-1.335438
20	6	0	2.883261	-0.038833	1.591395
21	1	0	1.688901	-2.734774	-0.937575
22	1	0	1.594376	-2.804697	0.816500
23	1	0	3.205870	-2.697757	0.028191
24	1	0	2.356250	-0.472881	2.446343
25	1	0	2.832984	1.050079	1.655411
26	1	0	3.927652	-0.366344	1.607189
27	1	0	3.020593	1.164549	-1.322537
28	1	0	2.654905	-0.291915	-2.279632
29	1	0	4.109422	-0.255584	-1.245055

C (MeEsterPMe.log)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.644307	-0.245423	-0.621708
2	6	0	-0.768955	-0.002804	-0.190426
3	6	0	-0.947587	1.040811	0.767688
4	6	0	-1.723880	-0.874290	-0.812288
5	6	0	1.530858	0.963630	-0.890579
6	8	0	0.004704	1.652865	1.289062
7	8	0	-1.409111	-1.823904	-1.551245
8	8	0	-2.231238	1.346563	1.105320
9	8	0	-3.033509	-0.619564	-0.534663
10	6	0	-3.964423	-1.508697	-1.149859
11	1	0	-3.793548	-2.544381	-0.838026
12	1	0	-3.896935	-1.462967	-2.241299
13	1	0	-4.949329	-1.172670	-0.818577
14	6	0	-2.370746	2.393316	2.064649
15	1	0	-1.928825	3.326778	1.702636
16	1	0	-1.892076	2.132194	3.014490
17	1	0	-3.446608	2.515065	2.206966
18	8	0	2.709278	1.016364	-0.572142
19	8	0	0.907483	1.905379	-1.595943
20	6	0	1.670029	3.097948	-1.846348
21	1	0	1.014466	3.741889	-2.432545
22	1	0	2.581845	2.864783	-2.402448
23	1	0	1.932880	3.575256	-0.899181
24	1	0	0.590470	-0.846063	-1.542281
25	15	0	1.566798	-1.351928	0.562135
26	6	0	0.415353	-2.686252	1.027174
27	6	0	3.019296	-2.154984	-0.209809
28	6	0	2.102918	-0.509219	2.084077
29	1	0	-0.097031	-3.039792	0.127685
30	1	0	-0.338225	-2.289048	1.710949
31	1	0	0.960399	-3.501938	1.511802
32	1	0	3.714913	-1.377676	-0.532438
33	1	0	2.695001	-2.737011	-1.078084
34	1	0	3.512916	-2.823545	0.502987
35	1	0	1.284353	0.131513	2.422506
36	1	0	2.956136	0.129460	1.849497
37	1	0	2.373356	-1.248764	2.844788

trans-12 (transpyr.log)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-3.389537	0.201532	-0.719560
2	8	0	0.154174	3.800904	-0.048836
3	8	0	1.694642	2.270989	0.667388
4	7	0	-1.607049	1.664464	-0.424908
5	7	0	-0.277374	1.534289	-0.044818
6	6	0	-4.222175	1.323487	-1.101876
7	6	0	-2.124536	0.494525	-0.408015
8	6	0	2.631617	3.346898	0.878110

9	6	0	0.485689	2.655750	0.167269
10	1	0	-4.233211	2.044947	-0.277732
11	6	0	-5.603096	0.779970	-1.410955
12	1	0	-3.765060	1.815568	-1.967189
13	1	0	2.795694	3.865411	-0.071788
14	1	0	2.194738	4.066437	1.577835
15	6	0	3.910280	2.734296	1.418516
16	6	0	0.114938	0.155005	0.265119
17	6	0	-1.191606	-0.638272	-0.007920
18	6	0	-1.703799	-1.387767	1.219784
19	1	0	-1.101079	-1.349689	-0.834907
20	6	0	1.255765	-0.342156	-0.631539
21	8	0	-1.488184	-1.065565	2.366381
22	8	0	-2.445919	-2.445572	0.851802
23	6	0	-3.039752	-3.188580	1.932769
24	8	0	1.558896	0.147183	-1.694697
25	8	0	1.800178	-1.429733	-0.059093
26	6	0	2.895232	-2.186936	-0.706323
27	1	0	0.404426	0.053935	1.313671
28	1	0	-3.718534	-2.550566	2.504254
29	1	0	-2.265148	-3.575639	2.599412
30	1	0	-3.585633	-4.004298	1.458966
31	6	0	3.168772	-3.302834	0.303874
32	6	0	4.120041	-1.282013	-0.869764
33	6	0	2.410660	-2.761383	-2.040914
34	1	0	2.275061	-3.917159	0.453774
35	1	0	3.465670	-2.884642	1.270873
36	1	0	3.975920	-3.948346	-0.058090
37	1	0	4.400145	-0.843752	0.094328
38	1	0	3.925544	-0.477547	-1.580902
39	1	0	4.966836	-1.875263	-1.232792
40	1	0	2.196608	-1.968729	-2.759779
41	1	0	1.506473	-3.362449	-1.892710
42	1	0	3.184473	-3.414181	-2.460025
43	1	0	-6.035830	0.288543	-0.533684
44	1	0	-5.563798	0.055025	-2.230201
45	1	0	-6.264300	1.601110	-1.707756
46	1	0	4.332719	2.019512	0.704645
47	1	0	3.725371	2.212251	2.363144
48	1	0	4.651700	3.520417	1.598830

cis-12 (cispyr.log)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-3.367490	-0.782718	0.017523
2	8	0	0.724509	-3.786888	0.425174
3	8	0	2.078608	-2.239950	-0.572270
4	7	0	-1.390985	-2.005465	0.072822
5	7	0	-0.095050	-1.792002	-0.401387
6	6	0	-4.027355	-1.841968	0.752975
7	6	0	-2.070567	-0.965561	-0.233510
8	6	0	3.208681	-3.098210	-0.315108
9	6	0	0.887266	-2.711978	-0.106550
10	1	0	-3.955499	-2.766505	0.169671
11	6	0	-5.463654	-1.412610	0.977565
12	1	0	-3.487311	-1.998036	1.692737
13	1	0	3.300277	-3.248309	0.765214
14	1	0	3.023906	-4.075670	-0.771850
15	6	0	4.434506	-2.421084	-0.899249
16	6	0	0.142573	-0.395769	-0.783602
17	6	0	-1.319098	0.102081	-1.009754
18	6	0	-1.639116	1.514767	-0.542645
19	1	0	-1.578343	0.021891	-2.070877
20	6	0	0.930541	0.361630	0.311132
21	8	0	-1.583003	1.891691	0.606156
22	8	0	-2.019926	2.286013	-1.577632
23	6	0	-2.376735	3.638409	-1.239749
24	8	0	1.135707	-0.067414	1.420752
25	8	0	1.372542	1.518684	-0.206293
26	6	0	2.195550	2.462862	0.587527
27	1	0	0.722936	-0.338066	-1.704971

28	1	0	-1.510837	4.170585	-0.836998
29	1	0	-3.179086	3.646785	-0.498116
30	1	0	-2.706736	4.094262	-2.173177
31	6	0	2.405900	3.619721	-0.391353
32	6	0	3.527528	1.793270	0.939133
33	6	0	1.428754	2.925047	1.829834
34	1	0	1.447743	4.070099	-0.671008
35	1	0	2.902806	3.271977	-1.302899
36	1	0	3.029024	4.393026	0.069777
37	1	0	4.028621	1.436583	0.032363
38	1	0	3.375971	0.950734	1.616204
39	1	0	4.185118	2.520905	1.427866
40	1	0	1.297664	2.108562	2.541220
41	1	0	0.440164	3.301699	1.552696
42	1	0	1.987673	3.731977	2.317743
43	1	0	-5.978987	-1.253133	0.024875
44	1	0	-5.507080	-0.484322	1.555882
45	1	0	-5.998021	-2.191025	1.532656
46	1	0	4.602639	-1.445671	-0.430918
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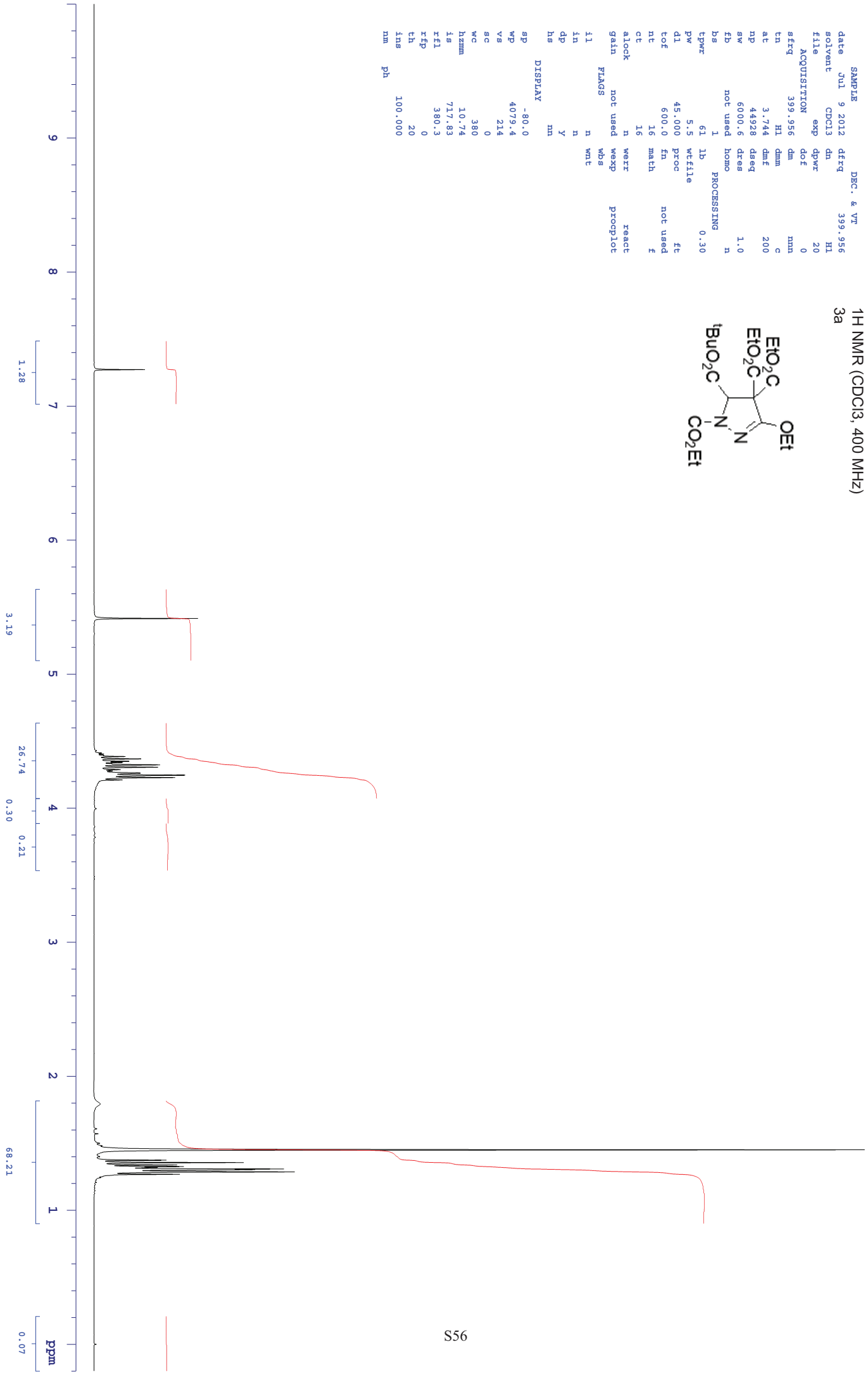
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maenaka/tBuDEADr

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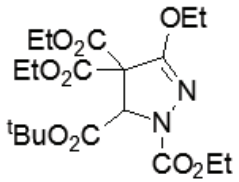

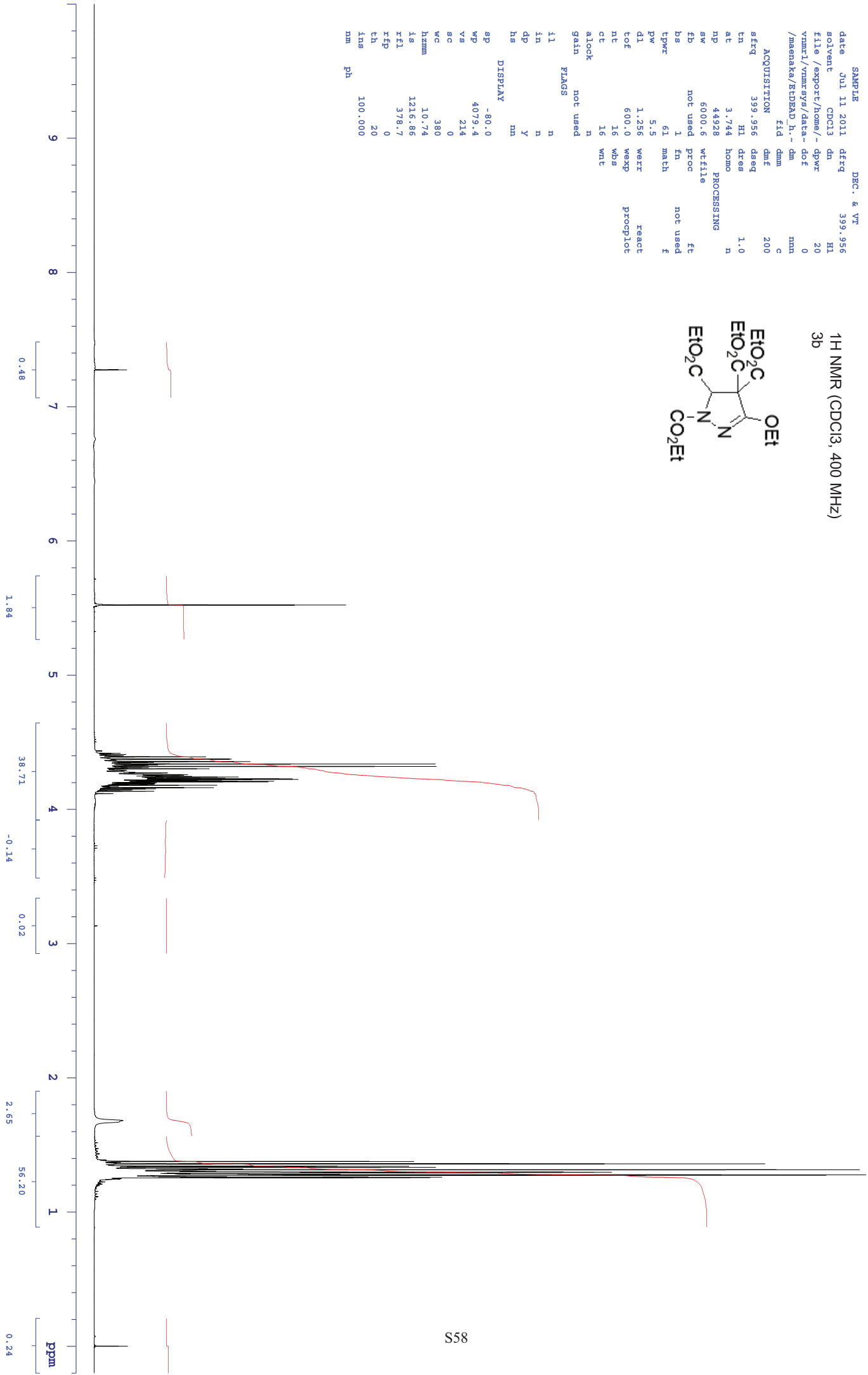

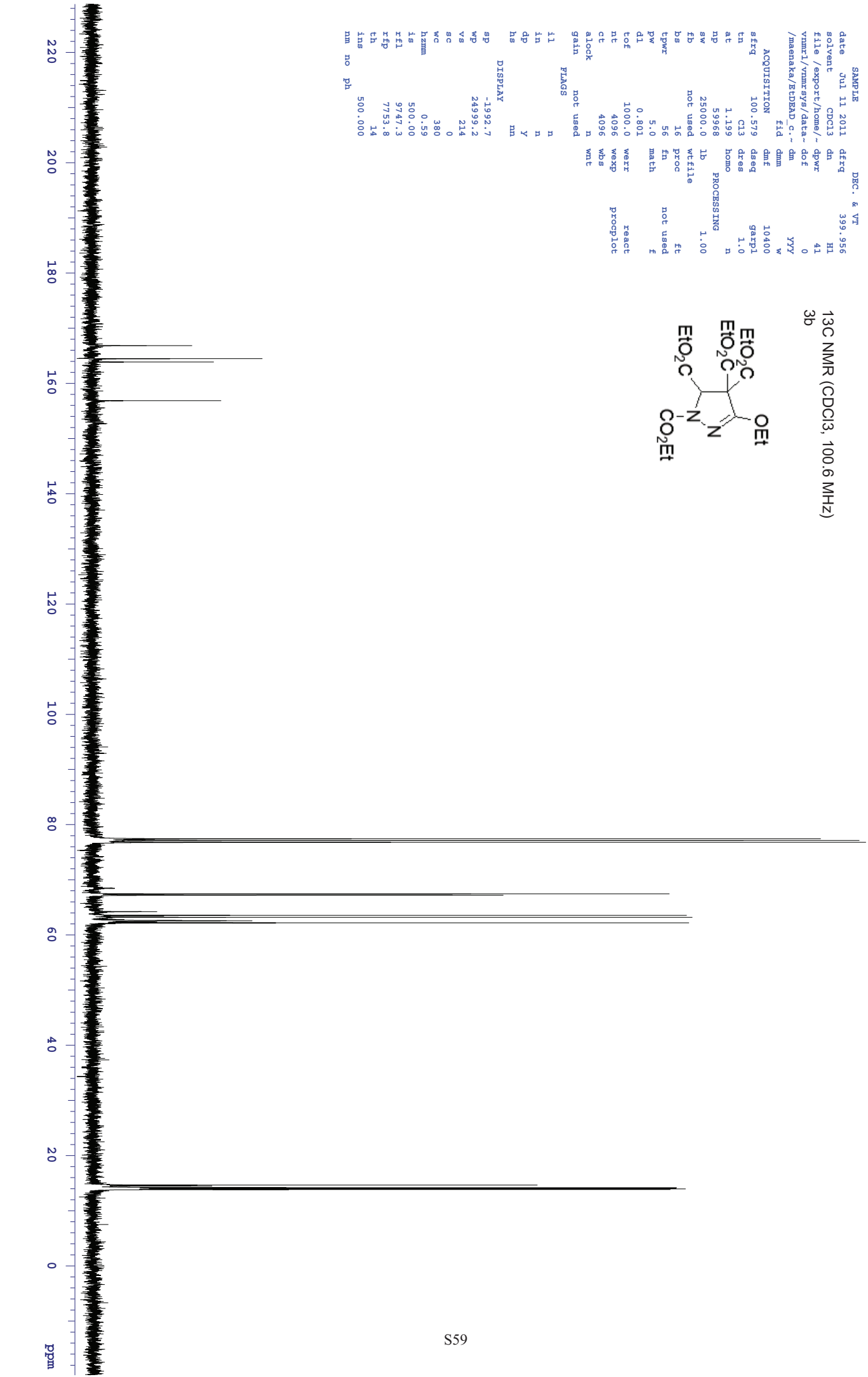
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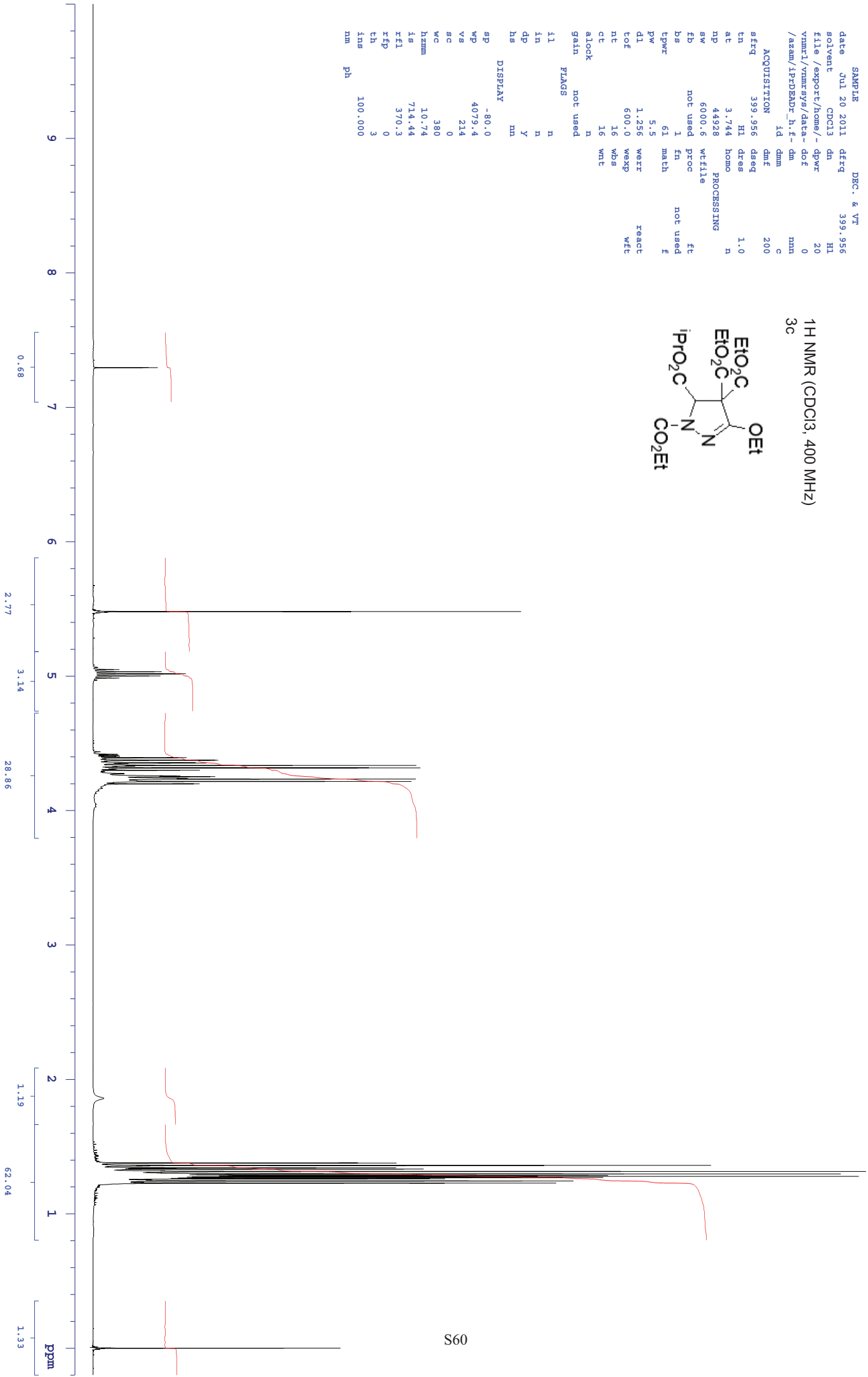
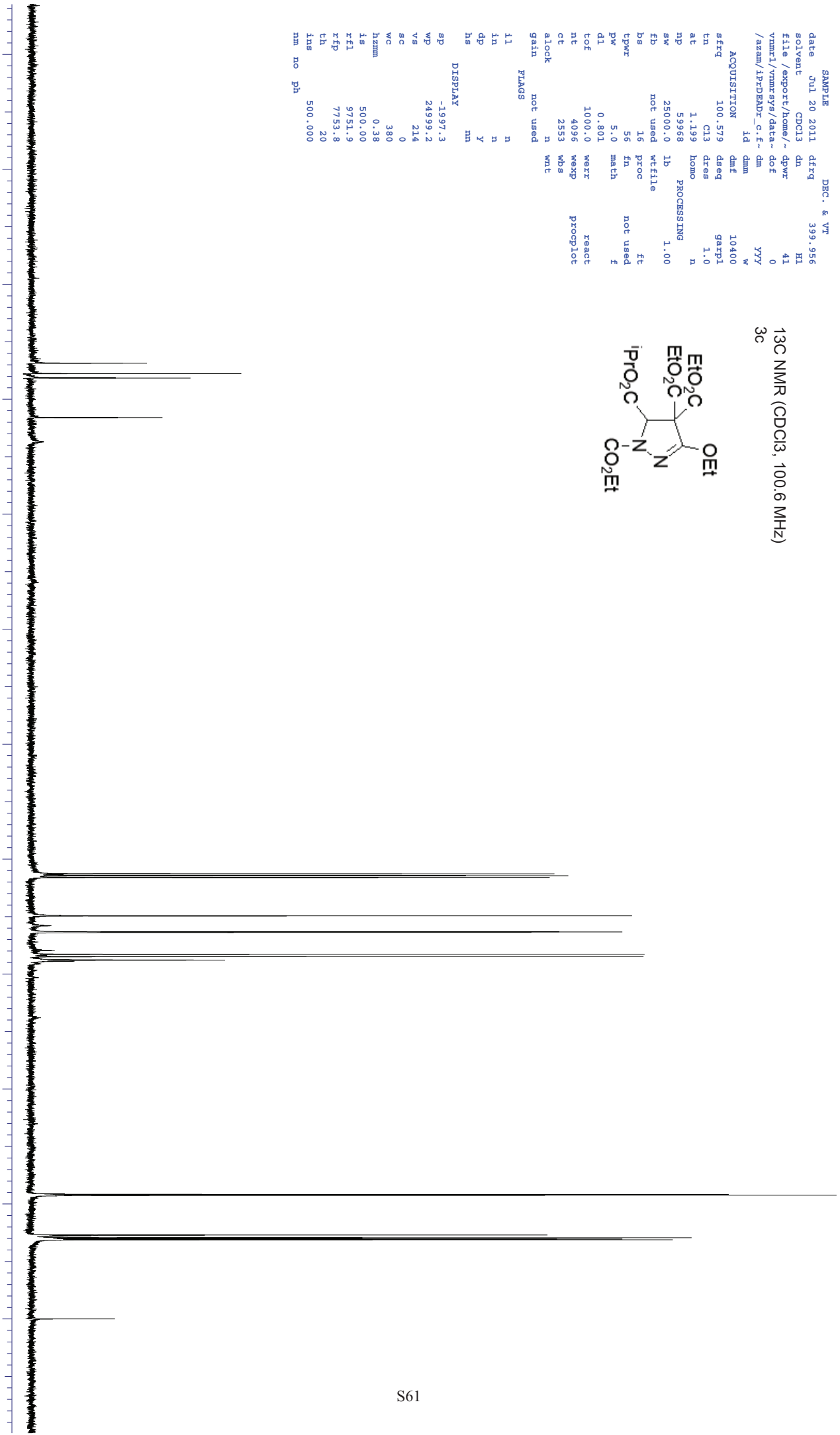
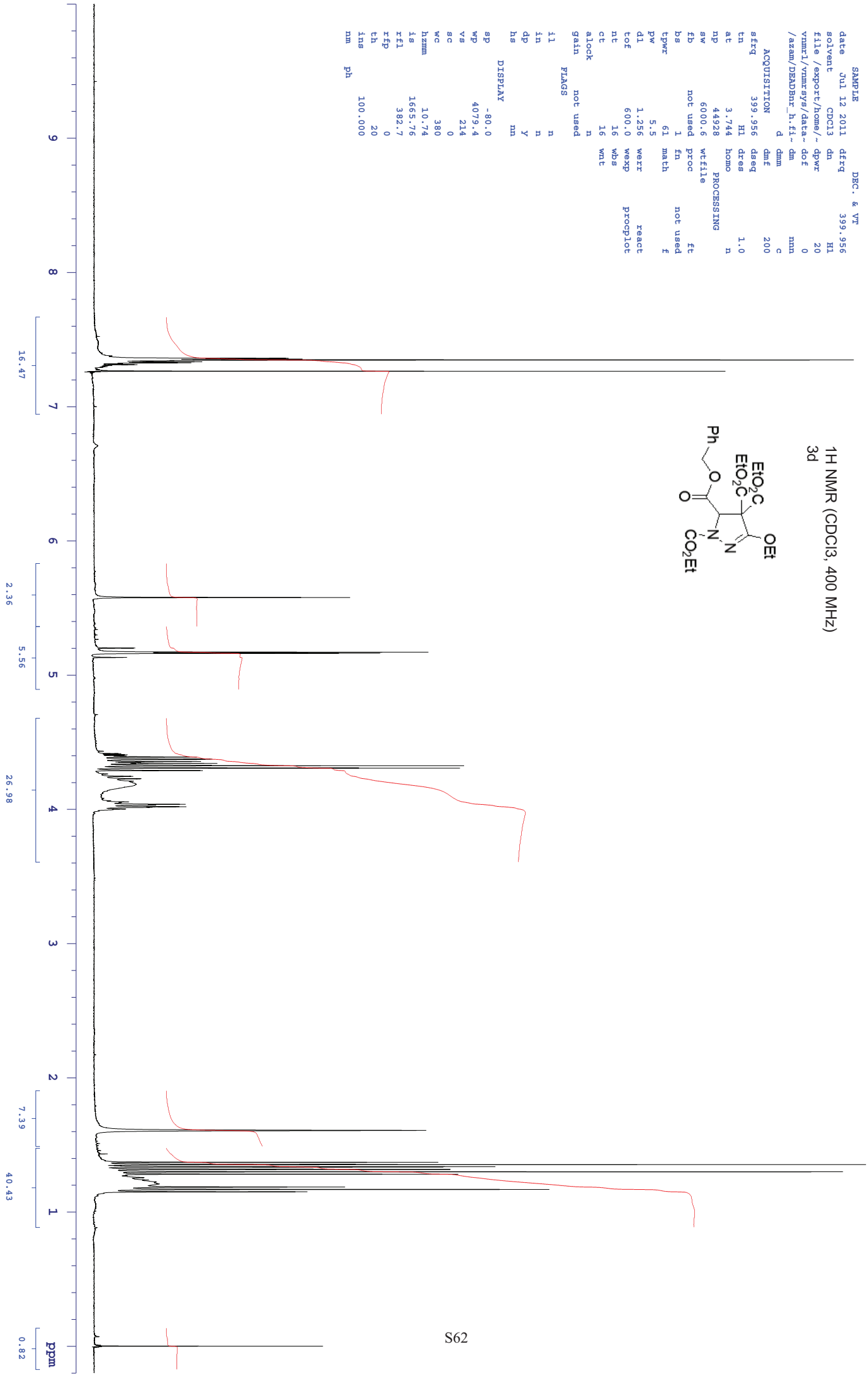
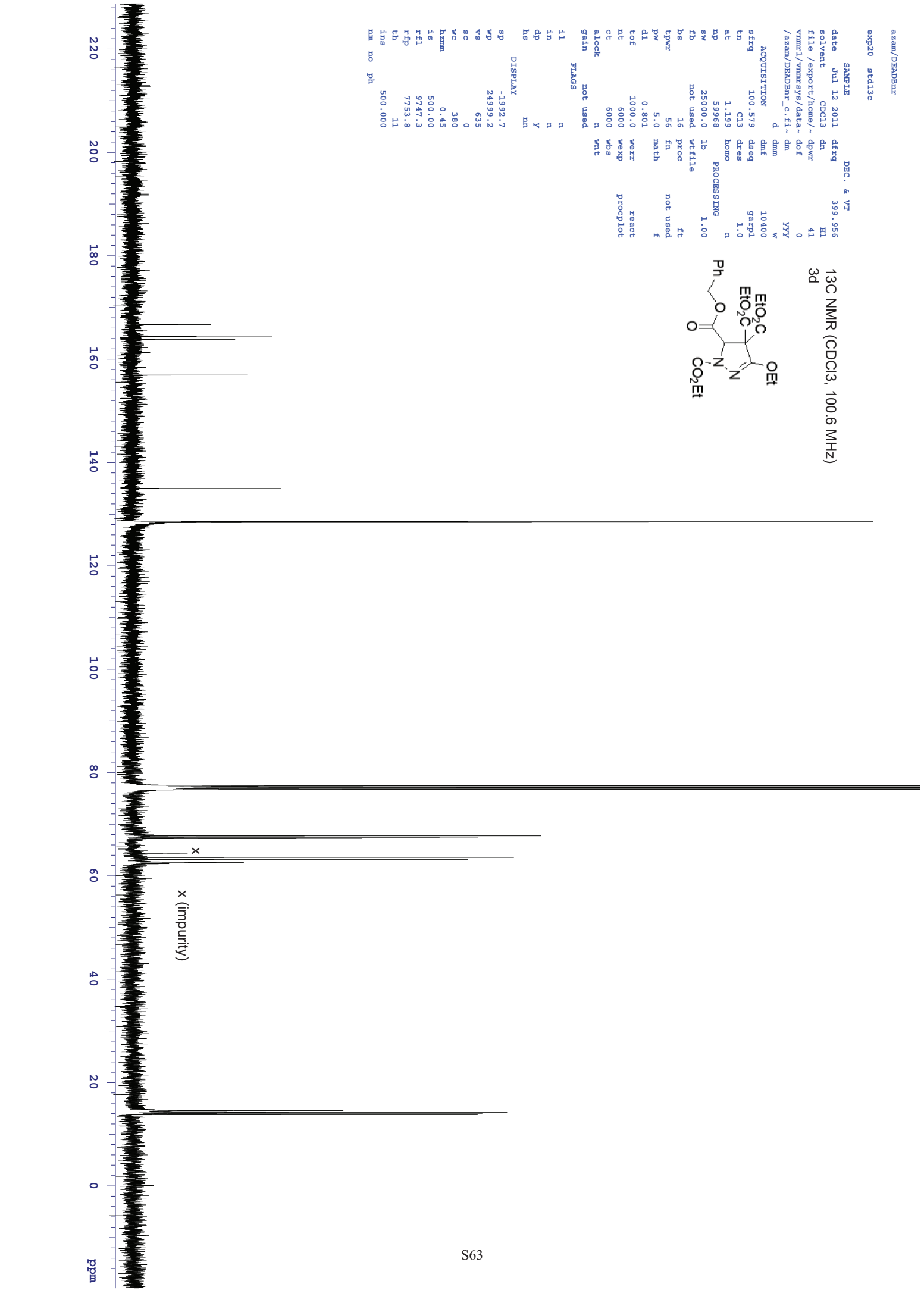
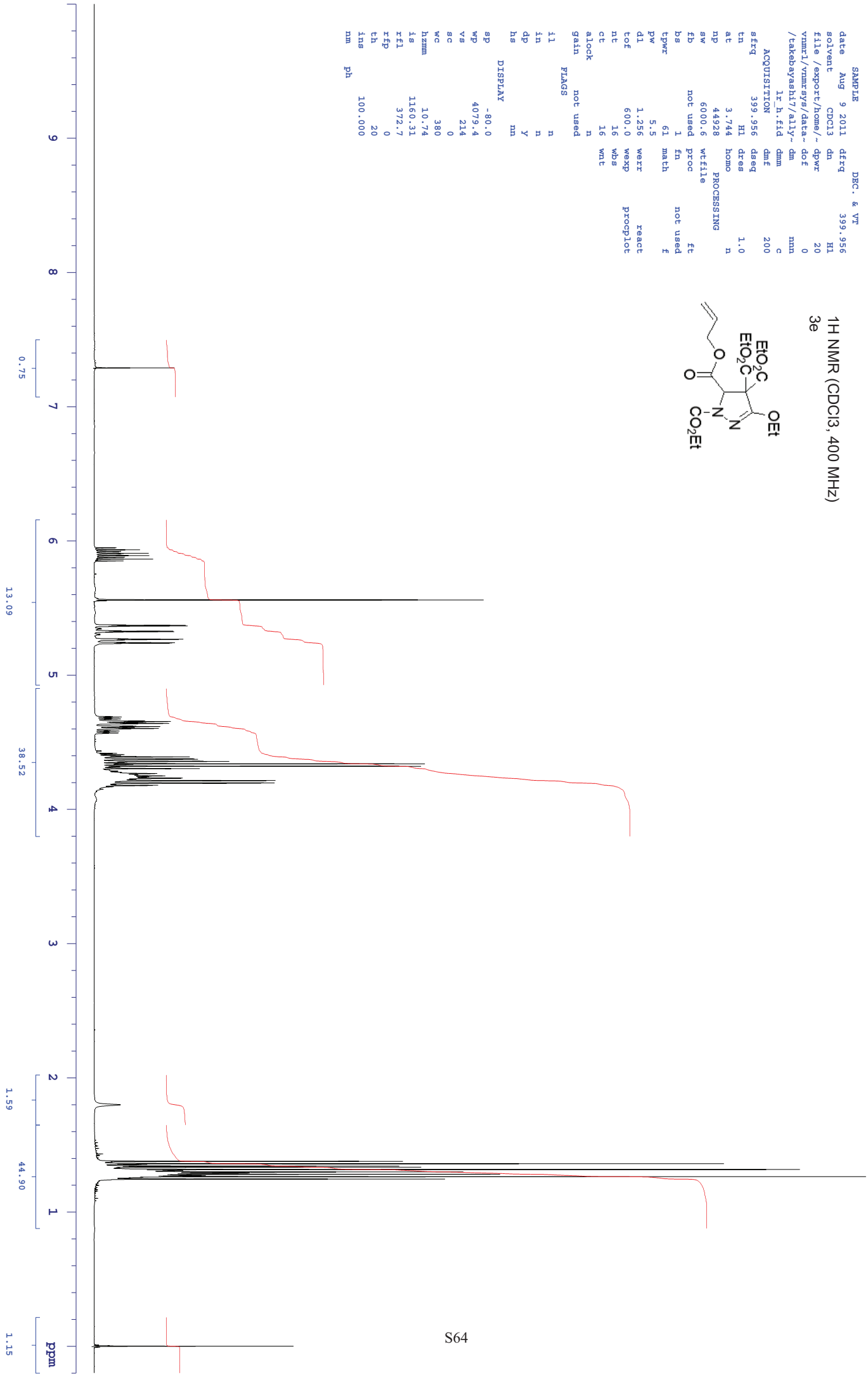
dp y
hs nn
DISPLAY
sp -1992.7
wp 24999.2
vs 214
sc 0
wc 380
hzmm 0.59
is 500.00
rfl 9747.3
rfp 7753.8
th 14
ins 500.000
nm no ph
13C NMR (CDCl3, 100.6 MHz)
3b
EtO2C
EtO2C
OEt
N
N
EtO2C
CO2Et
220
200
180
160
140
120
100
80
60
40
20
0
ppm

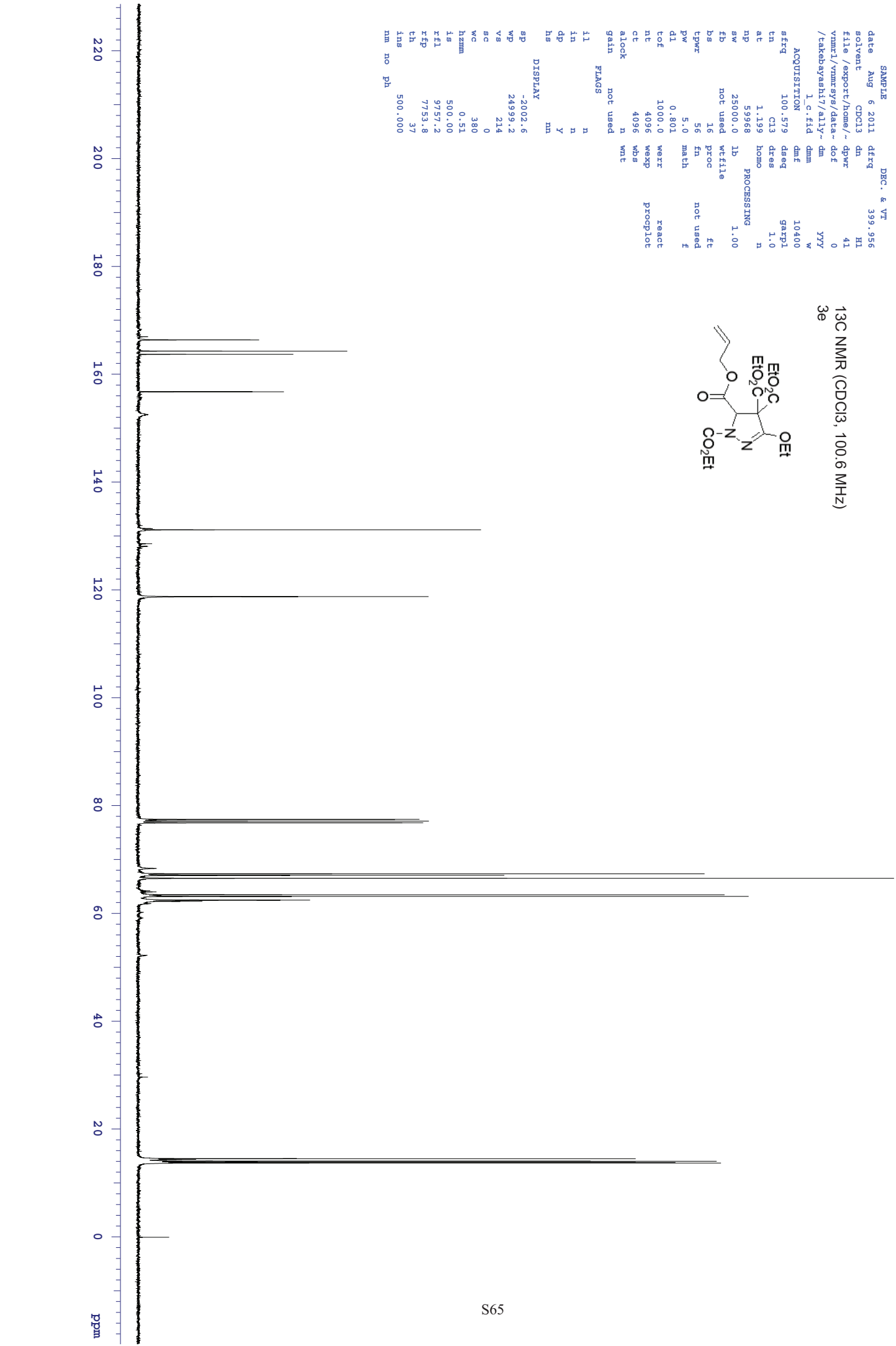

azam/iPrDEADr
exp20 std1h
SAMPLE DEC. & VT
date Jul 20 2011 dfrq 399.956
solvent CDCl3 dn H1
file /export/home/~ dpwr 20
vnmr1/vnmrsys/data~ dof 0
/azam/iPrDEADr_h.f~ dm nnn
id dmm c
ACQUISITION dmf 200
sfrq 399.956 dseq 1.0
tn H1 dres n
at 3.744 homo
np 44928 PROCESSING
sw 6000.6 wtfile
fb not used proc ft
bs not used fn not used
tpwr 61 math f
pw 5.5
d1 1.256 werr react
tof 600.0 wexp wft
nt 16 wbs
ct 16 wnt
alock n
gain not used
FLAGS
il n
in n
dp y
hs nn
DISPLAY
sp -80.0
wp 4079.4
vs 214
sc 0
wc 380
hzmm 10.74
is 714.44
rfl 370.3
rfp 0
th 3
ins 100.000
nm ph
1H NMR (CDCl3, 400 MHz)
3c
EtO2C
EtO2C
OEt
iPrO2C
N
N
CO2Et
9
8
7
6
5
4
3
2
1
ppm
0.68
2.77
3.14
28.86
1.19
62.04
1.33

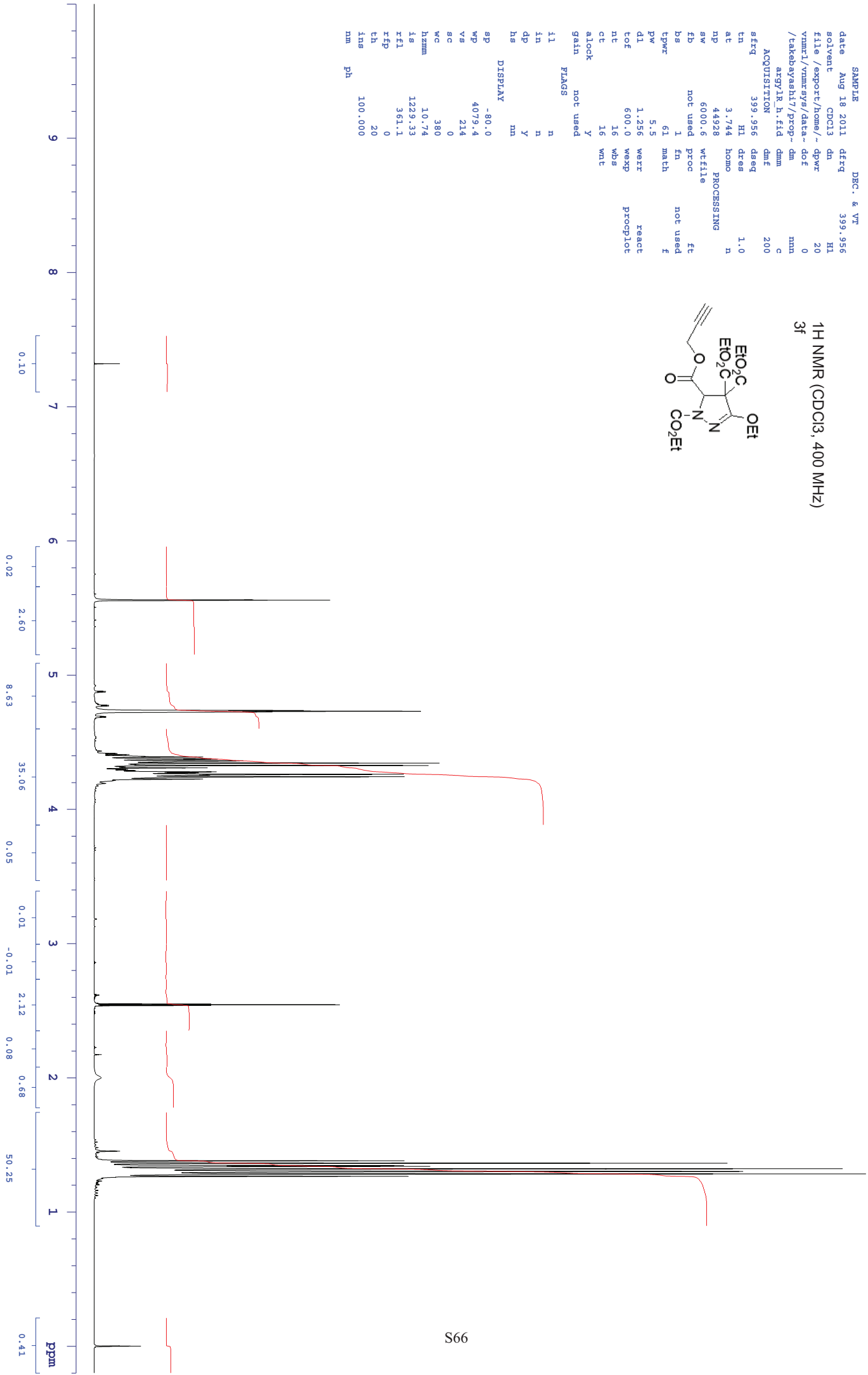

azam/iPrDEADr
exp20 std13c
SAMPLE DEC. & VT
date Jul 20 2011 dfrq 399.956
solvent CDCl3 dn H1
file /export/home/~ dpwr 41
vnmr1/vnmrsys/data~ dof 0
/azam/iPrDEADr_c.f~ dm yyy
id dmm w
ACQUISITION dmf 10400
sfrq 100.579 dseq garp1
tn C13 dres 1.0
at 1.199 homo n
np 59968 PROCESSING
sw 25000.0 lb 1.00
fb not used wtfile
bs ft
tpwr 16 proc
pw 56 fn not used
d1 5.0 math f
tof 0.801
nt 1000.0 werr
ct 4096 wexp react
alock 2553 wbs procplot
gain n wnt
not used
FLAGS
il n
in n
dp y
hs nn
DISPLAY
sp -1997.3
wp 24999.2
vs 214
sc 0
wc 380
hzmm 0.38
is 500.00
rfl 9751.9
rfp 7753.8
th 20
ins 500.000
nm no ph
13C NMR (CDCl3, 100.6 MHz)
3c
EtO2C
EtO2C
OEt
iPrO2C
N
N
CO2Et
220
200
180
160
140
120
100
80
60
40
20
0
ppm

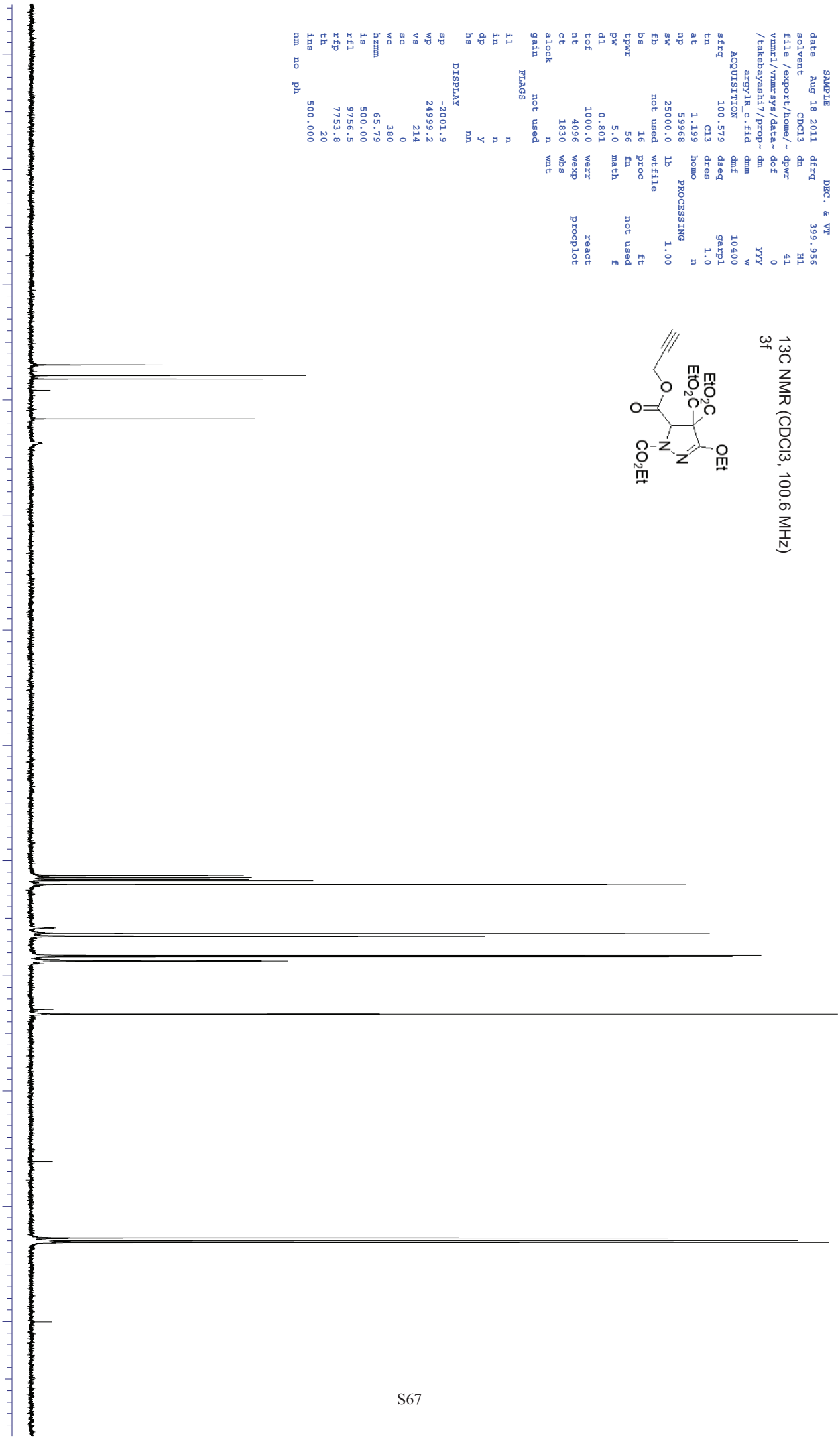


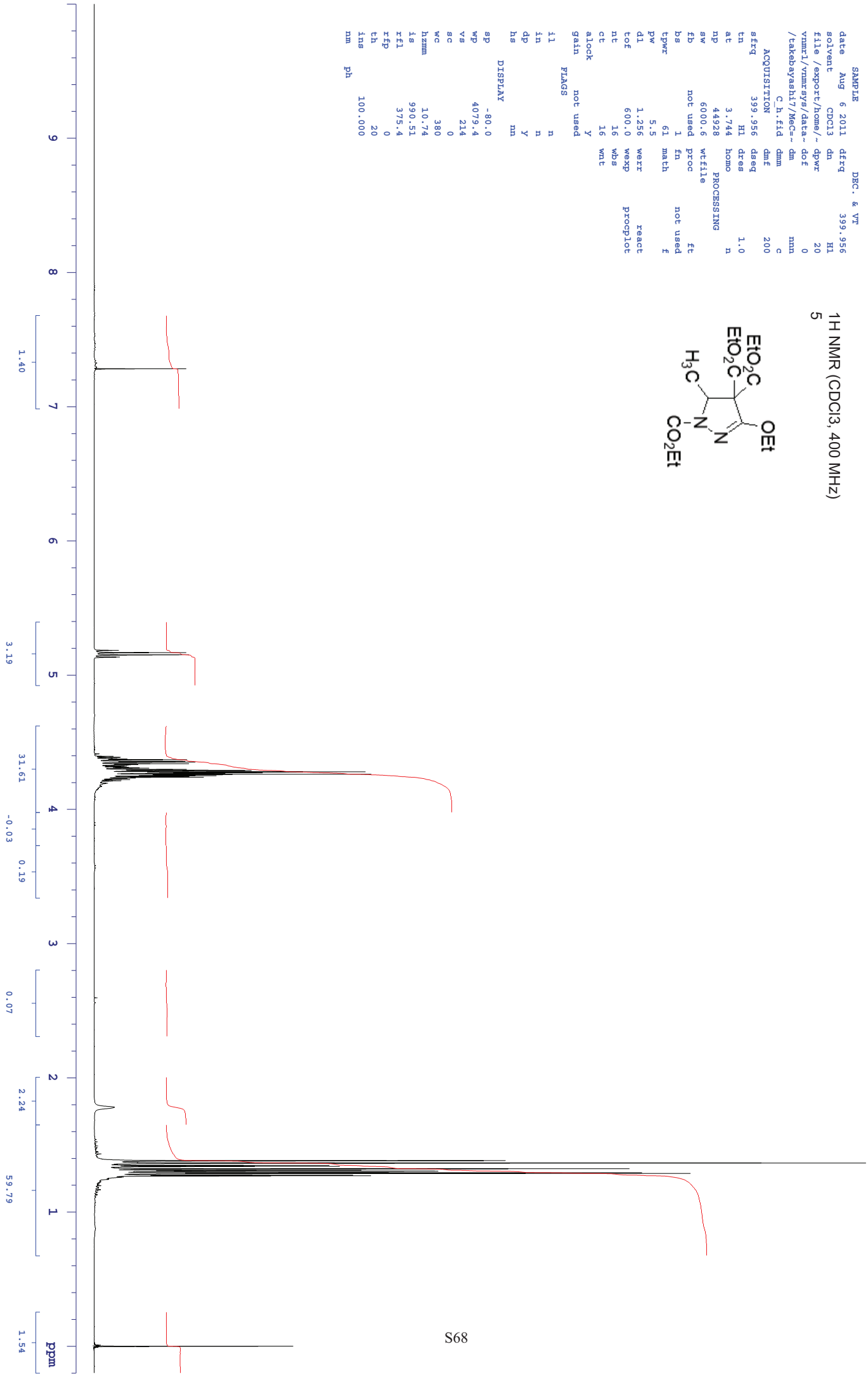









takebayashi7/propargylR
exp20 std13c
SAMPLE DEC. & VT
date Aug 18 2011 dfrq 399.956
solvent CDCl3 dn H1
file /export/home/~ dpwr 41
vnmr1/vnmrsys/data~ dof 0
/takebayashi7/prop~ dm yyy
argylR_c.fid dmm w
ACQUISITION dmf 10400
sfrq 100.579 dseq garp1
tn C13 dres 1.0
at 1.199 homo n
np 59968 PROCESSING
sw 25000.0 lb 1.00
fb not used wtfile
bs ft
tpwr 56 fn not used
pw 5.0 math f
d1 0.801
tof 1000.0 werr react
nt 4096 wexp procplot
ct 1830 wbs
alock n wnt
gain not used
FLAGS
il n
in n
dp y
hs nn
DISPLAY
sp -2001.9
wp 24999.2
vs 214
sc 0
wc 380
hzmm 65.79
is 500.00
rfl 9756.5
rfp 7753.8
th 20
ins 500.000
nm no ph
13C NMR (CDCl3, 100.6 MHz)
3f
EtO2C
EtO2C
OEt
O
O
N
N
CO2Et
220
200
180
160
140
120
100
80
60
40
20
0
ppm

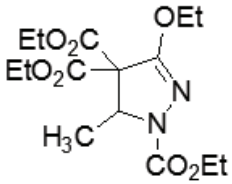


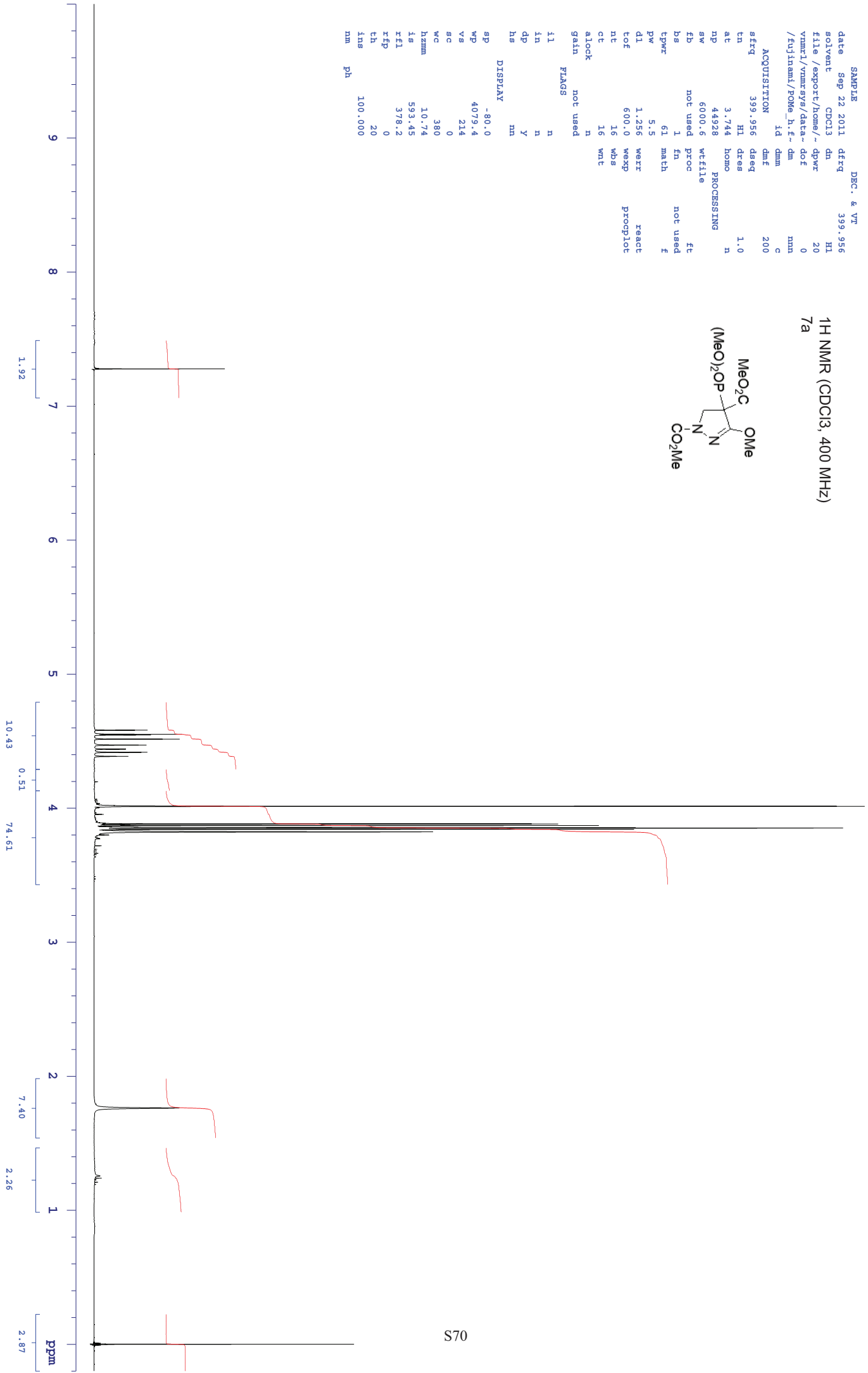
takebayashi7/MeC=C

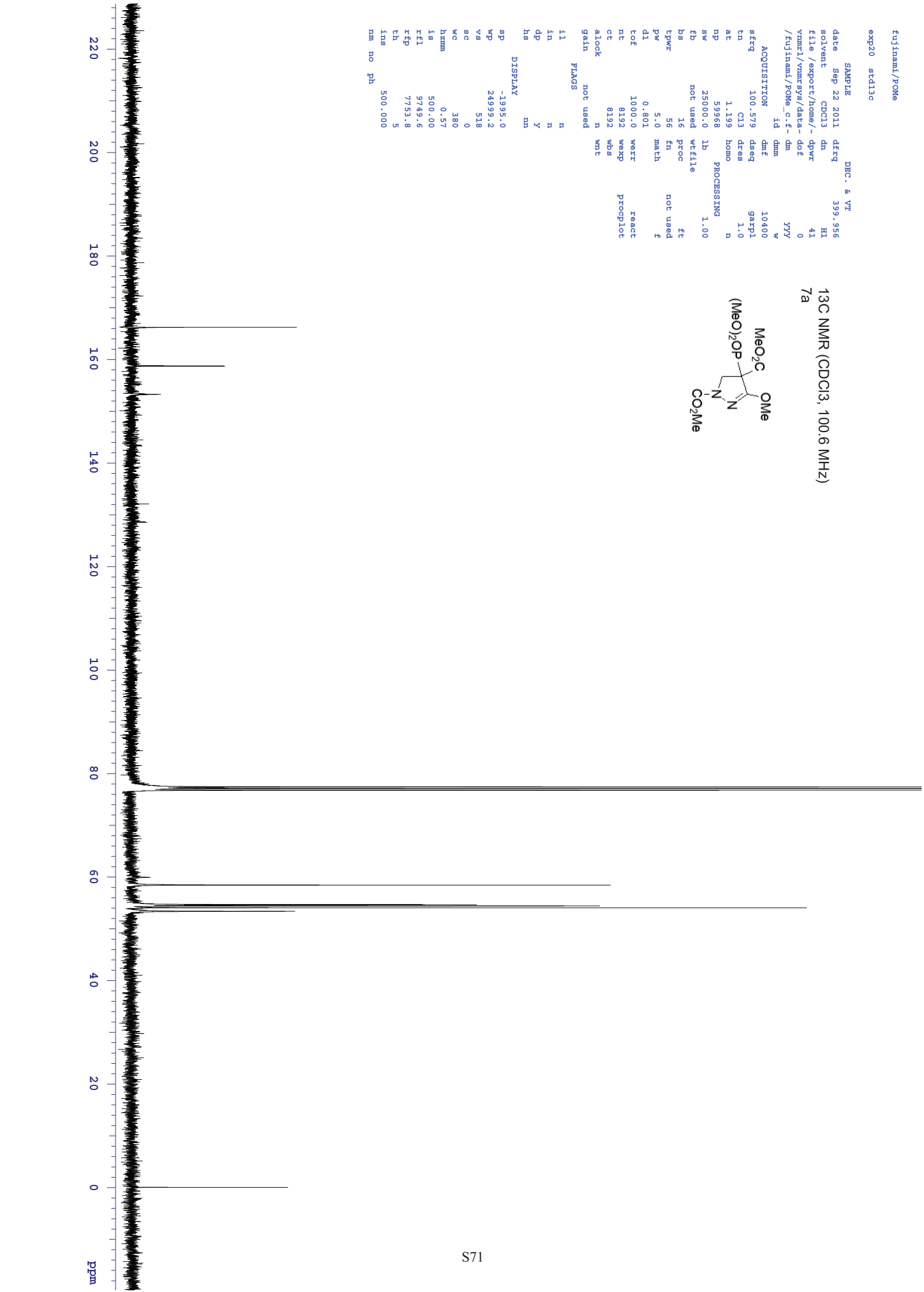
exp20 std13c

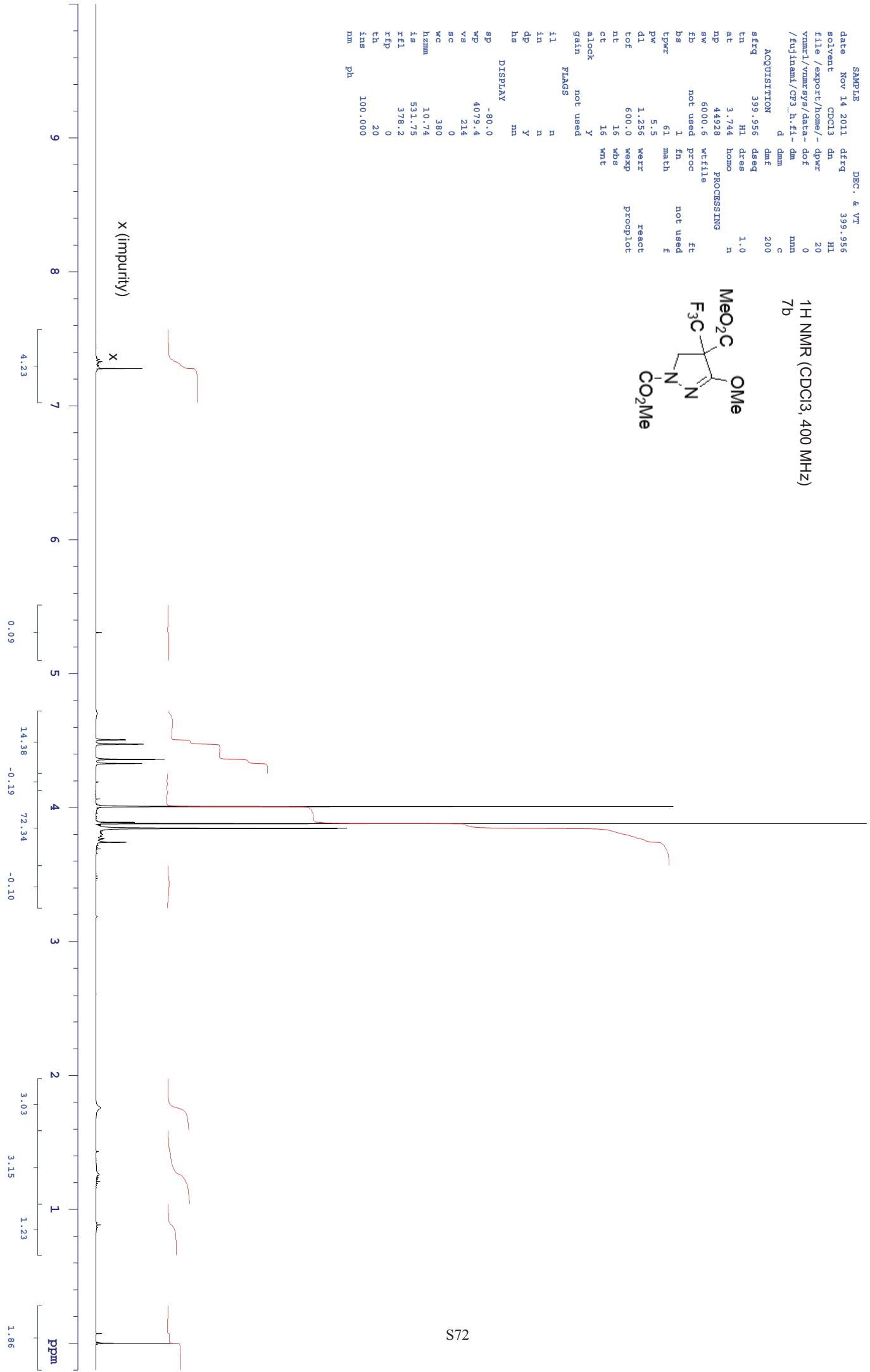
SAMPLE		DEC. & VT	
date	Aug 6 2011	dfrq	399.956
solvent	CDCl3	dn	H1
file	/export/home/~	dpwr	41
vnmrl/vnmrsys/data~		dof	0
/takebayashi7/MeC=~		dm	yyy
	C_c.fid	dmm	w
ACQUISITION		dmf	10400
sfrq	100.579	dseq	garp1
tn	C13	dres	1.0
at	1.199	homo	n
np	59968	PROCESSING	
sw	25000.0	lb	1.00
fb	not used	wtfile	
bs	16	proc	ft
tpwr	56	fn	not used
pw	5.0	math	f
d1	0.801		
tof	1000.0	werr	react
nt	2048	wexp	procplot
ct	2048	wbs	
alock	n	wnt	
gain	not used		
FLAGS			
il	n		
in	n		
dp	y		
hs	nn		
DISPLAY			
sp	-1995.0		
wp	24999.2		
vs	214		
sc	0		
wc	380		
hzmm	1.51		
is	500.00		
rfl	9749.6		
rfp	7753.8		
th	20		
ins	500.000		
nm no ph			

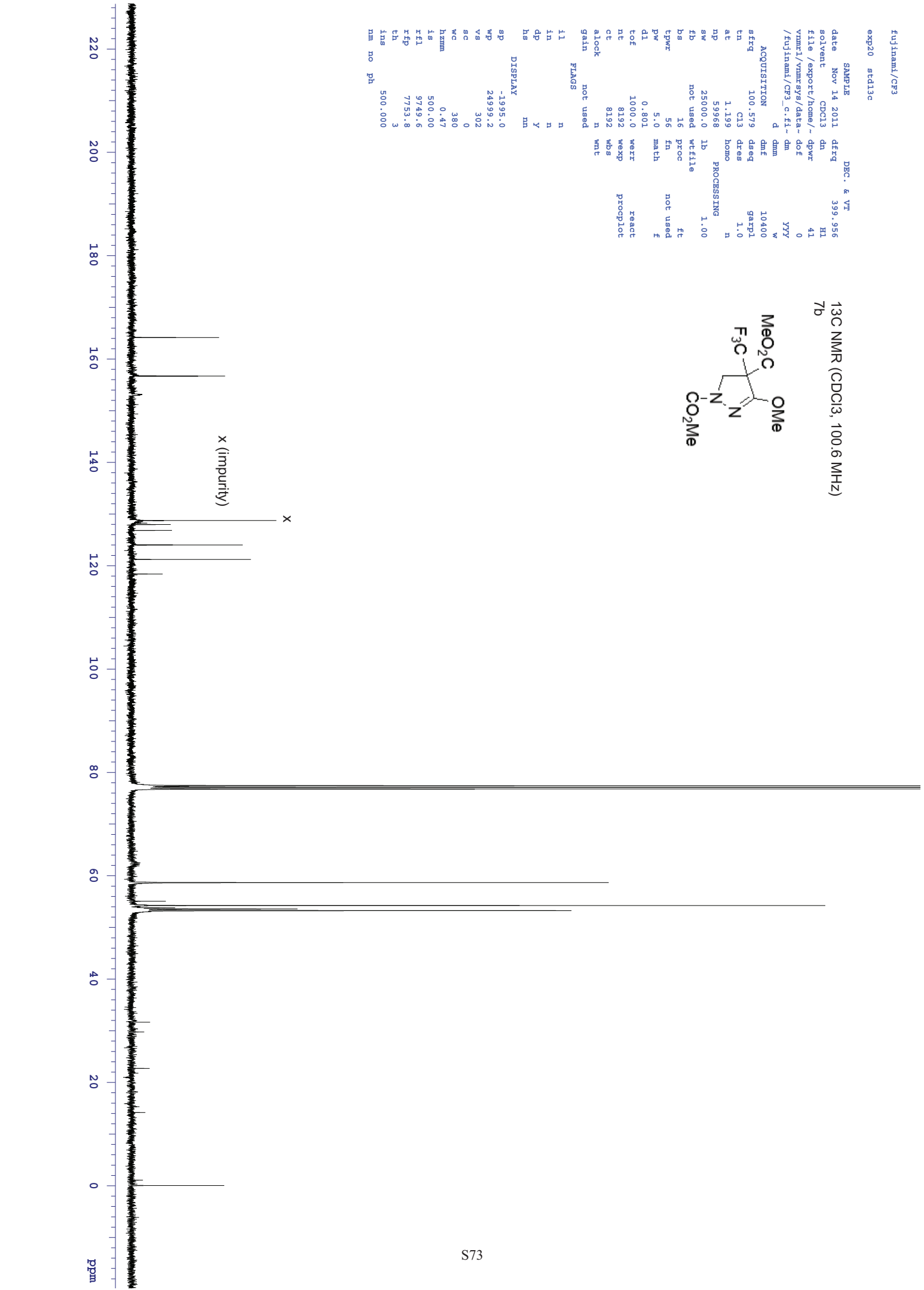
13C NMR (CDCl3, 100.6 MHz)
5

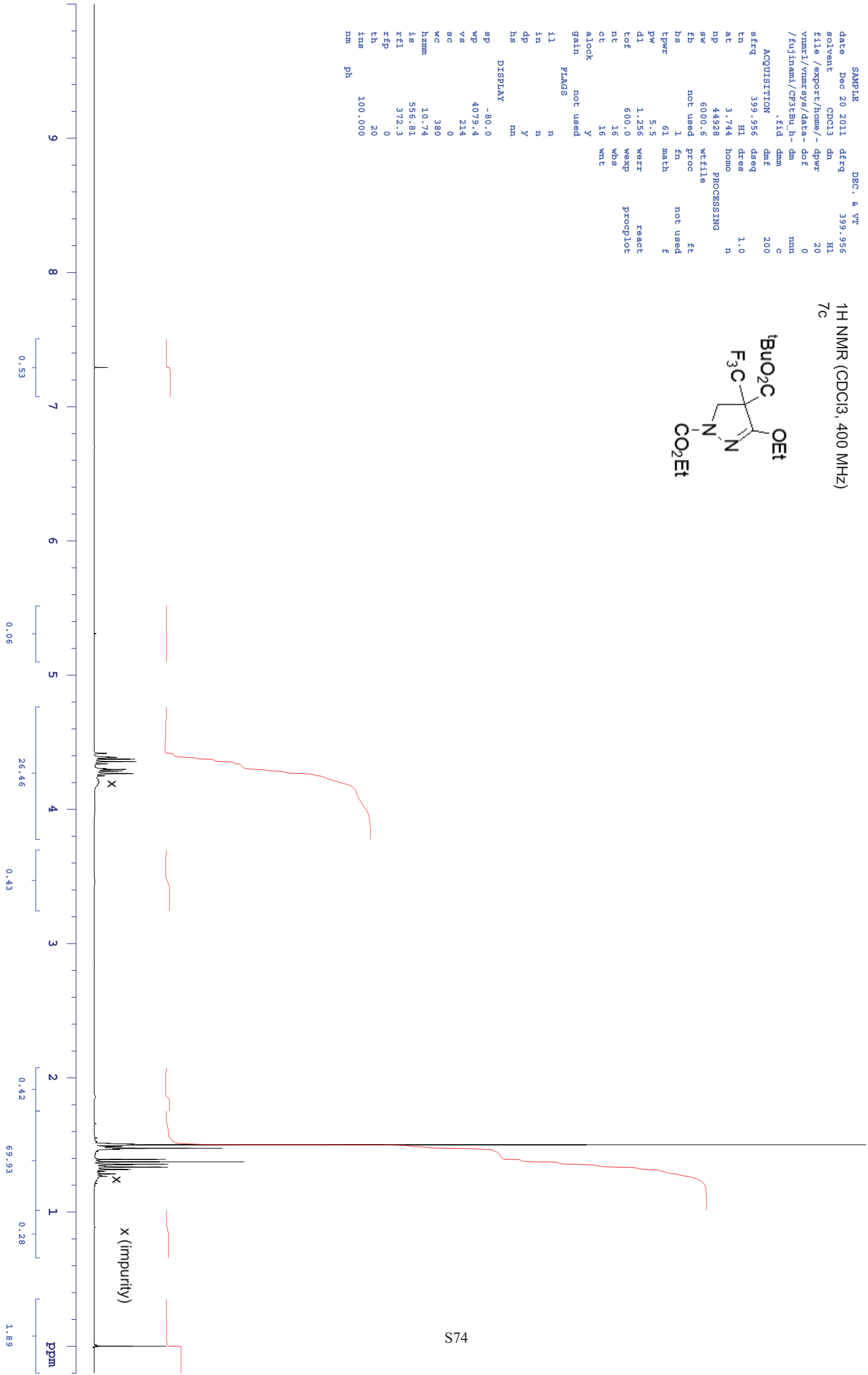




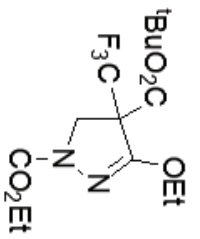








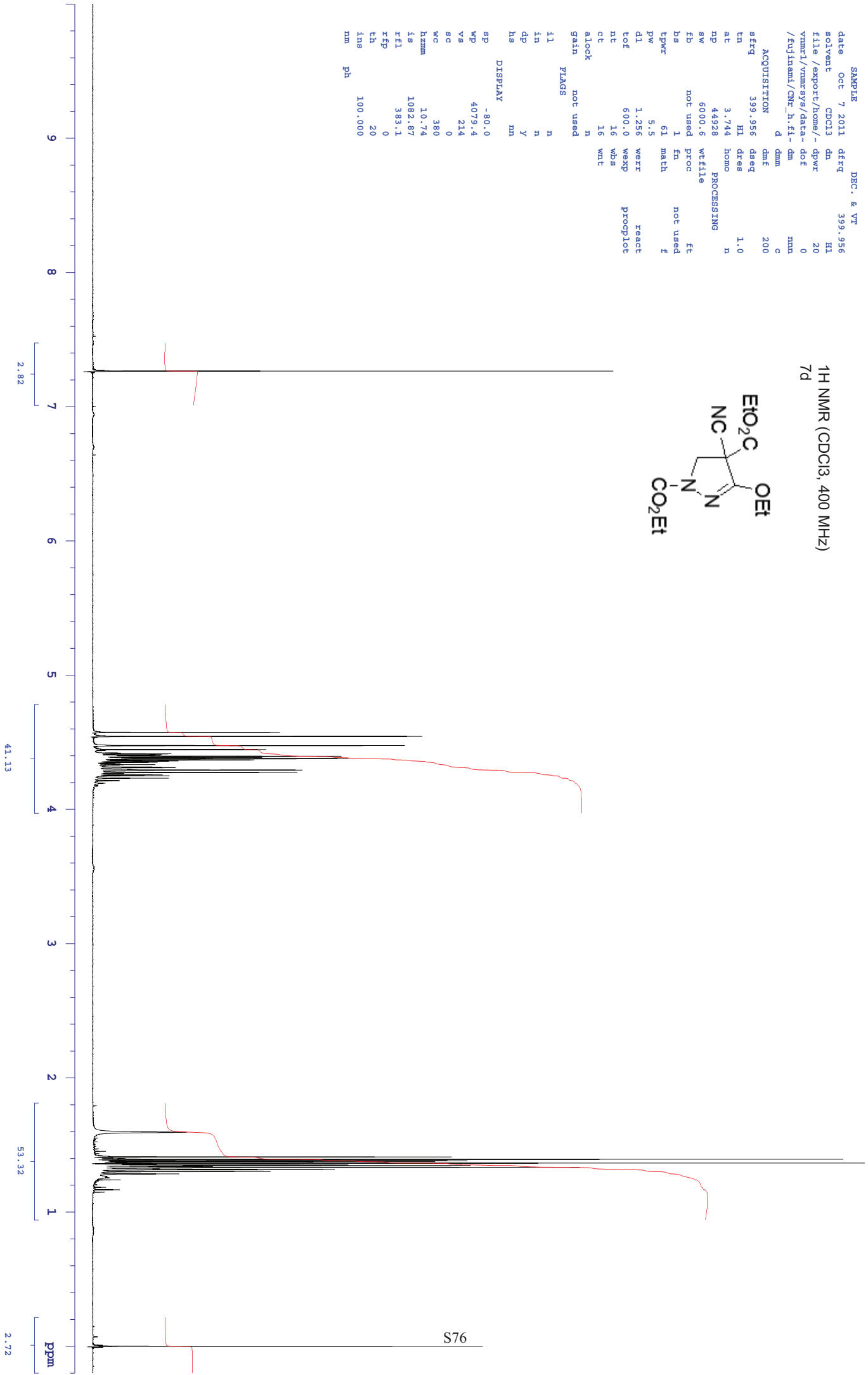
13C NMR (CDCl3, 100.6 MHz)
7c

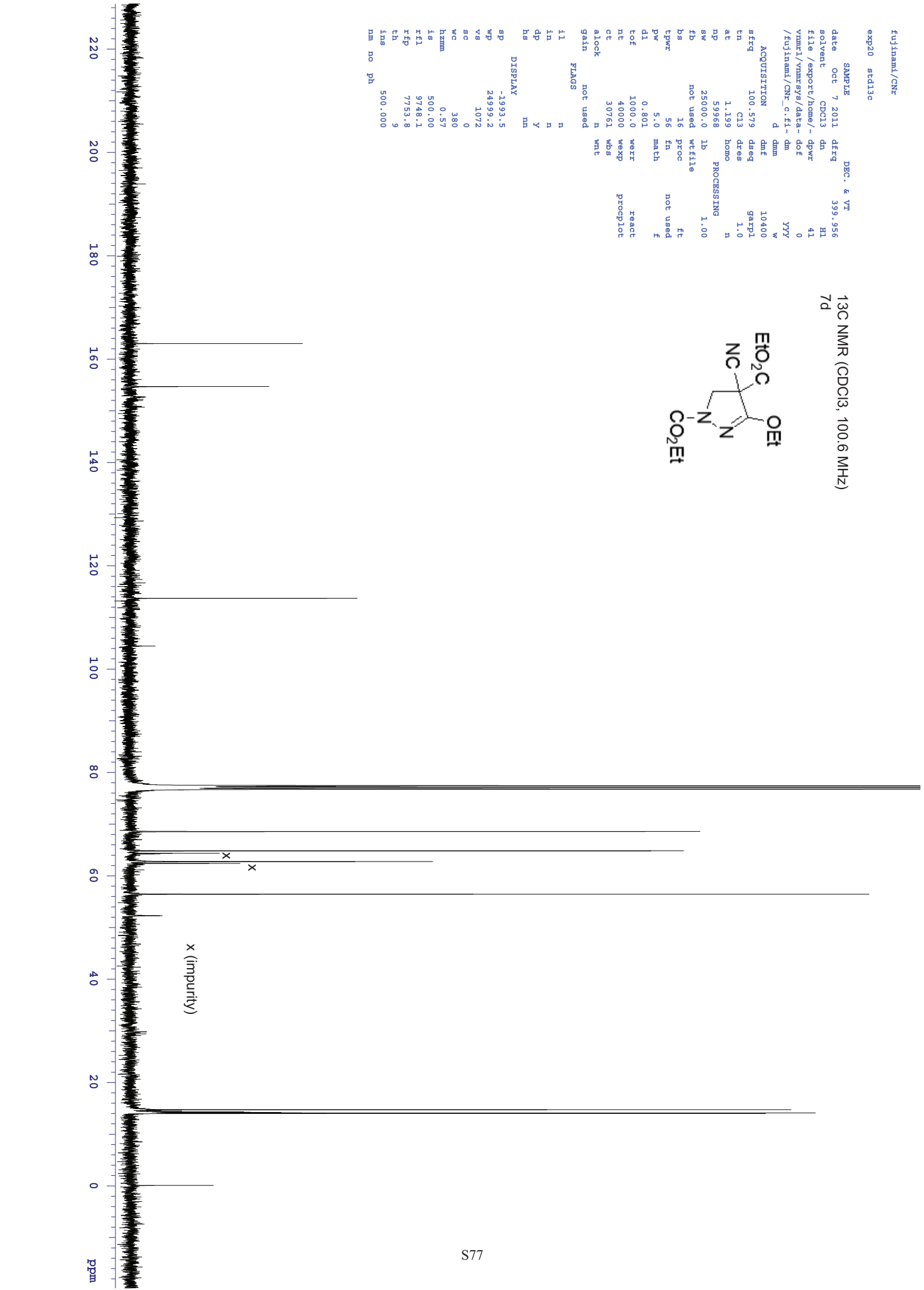


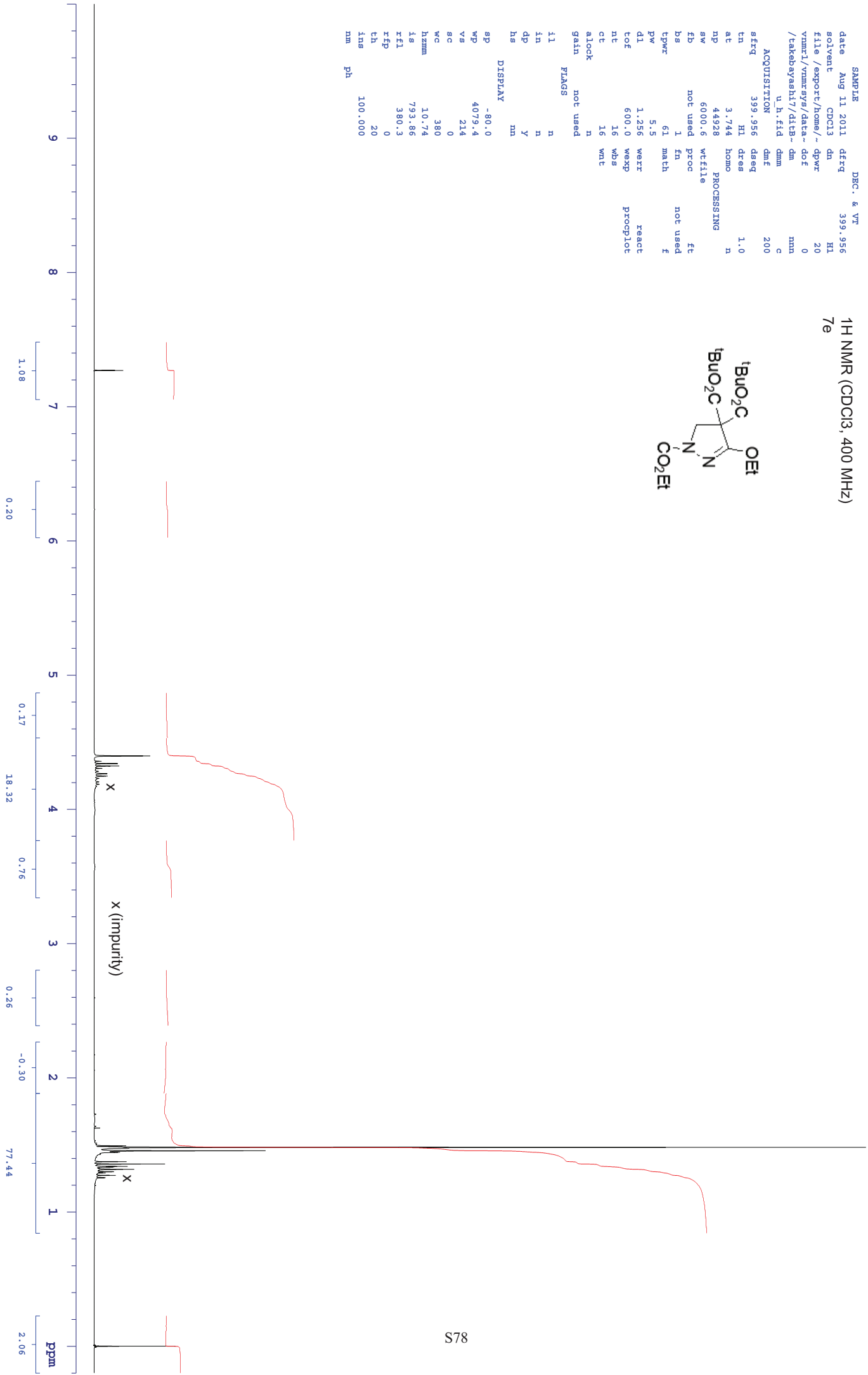

```
fujinami/CF3tBu

exp20  std13c

                SAMPLE                          DEC. & VT
date    Dec 20 2011   dfrq      399.956
solvent       CDCl3   dn             H1
file /export/home/~ dpwr             41
vnmrj/vnmrsys/data~ dof               0
/fujinami/CF3tBu_c~ dm              yyy
                .fid  dmm               w
    ACQUISITION       dmf         11088
sfrq      100.579     dseq        garp1
tn            C13     dres          1.0
at          1.199     homo             n
np          59968          PROCESSING
sw       25000.0     lb            1.00
fb     not used     wtfile
bs                  16   proc          ft
tpwr                56   fn      not used
pw                 5.0   math           f
d1               0.801
tof             1000.0   werr       react
nt                4096   wexp     procplot
ct                4096   wbs
alock                n   wnt
gain        not used
              FLAGS
il                   n
in                   n
dp                   y
hs                  nn
            DISPLAY
sp              -1995.8
wp              24999.2
vs                  214
sc                    0
wc                  380
hzmm                2.40
is                500.00
rfl               9750.4
rfp               7753.8
th                    20
ins              500.000
nm  no  ph
```





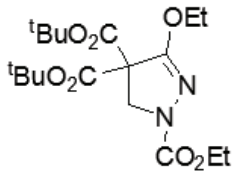


takebayashi7/ditBu

exp20 std13c

SAMPLE		DEC. & VT	
date	Aug 11 2011	dfrq	399.956
solvent	CDCl3	dn	H1
file	/export/home/~	dpwr	41
vnmrl/vnmrsys/data~		dof	0
/takebayashi7/ditB~		dm	yyy
	u_c.fid	dmm	w
ACQUISITION		dmf	10400
sfrq	100.579	dseq	garp1
tn	C13	dres	1.0
at	1.199	homo	n
np	59968	PROCESSING	
sw	25000.0	lb	1.00
fb	not used	wtfile	
bs	16	proc	ft
tpwr	56	fn	not used
pw	5.0	math	f
d1	0.801		
tof	1000.0	werr	react
nt	4096	wexp	procplot
ct	4096	wbs	
alock	n	wnt	
gain	not used		
FLAGS			
il	n		
in	n		
dp	y		
hs	nn		
DISPLAY			
sp	-1992.7		
wp	24999.2		
vs	214		
sc	0		
wc	380		
hzmm	0.69		
is	500.00		
rfl	9747.3		
rfp	7753.8		
th	48		
ins	500.000		
nm no ph			

13C NMR (CDCl3, 100.6 MHz)
7e



takebayashi7/ditBuMeR

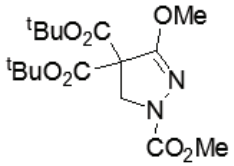
exp10 std1h

SAMPLE		DEC. & VT	
date	Aug 23 2011	dfrq	399.956
solvent	CDCl3	dn	H1
file	/export/home/~	dpwr	20
vnmrl/vnmrsys/data~		dof	0
/takebayashi7/ditB~		dm	nnn
	uMeR_h.fid	dmm	c
ACQUISITION		dmf	200
sfrq	399.956	dseq	
tn	H1	dres	1.0
at	3.744	homo	n
np	44928	PROCESSING	
sw	6000.6	wtfile	
fb	not used	proc	ft
bs	16	fn	not used
tpwr	61	math	f
pw	5.5		
d1	1.256	werr	react
tof	600.0	wexp	wft
nt	16	wbs	
ct	16	wnt	
alock	n		
gain	not used		

FLAGS	
il	n
in	n
dp	y
hs	nn

DISPLAY	
sp	-80.0
wp	4079.4
vs	214
sc	0
wc	380
hzmm	10.74
is	671.74
rfl	370.3
rfp	0
th	5
ins	100.000
nm	ph

1H NMR (CDCl3, 400 MHz)
7f

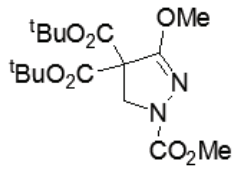


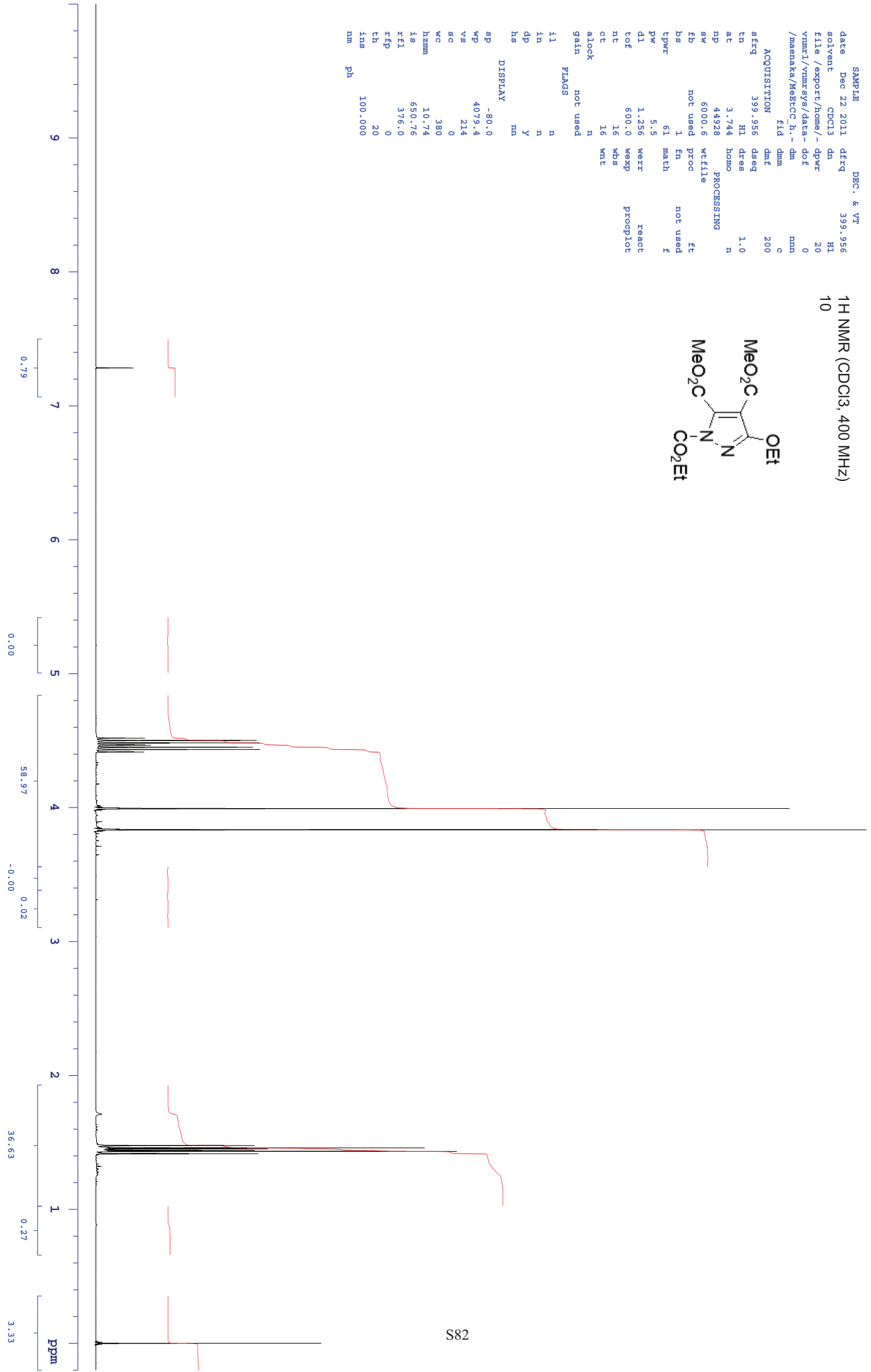
takebayashi7/ditBuMeR

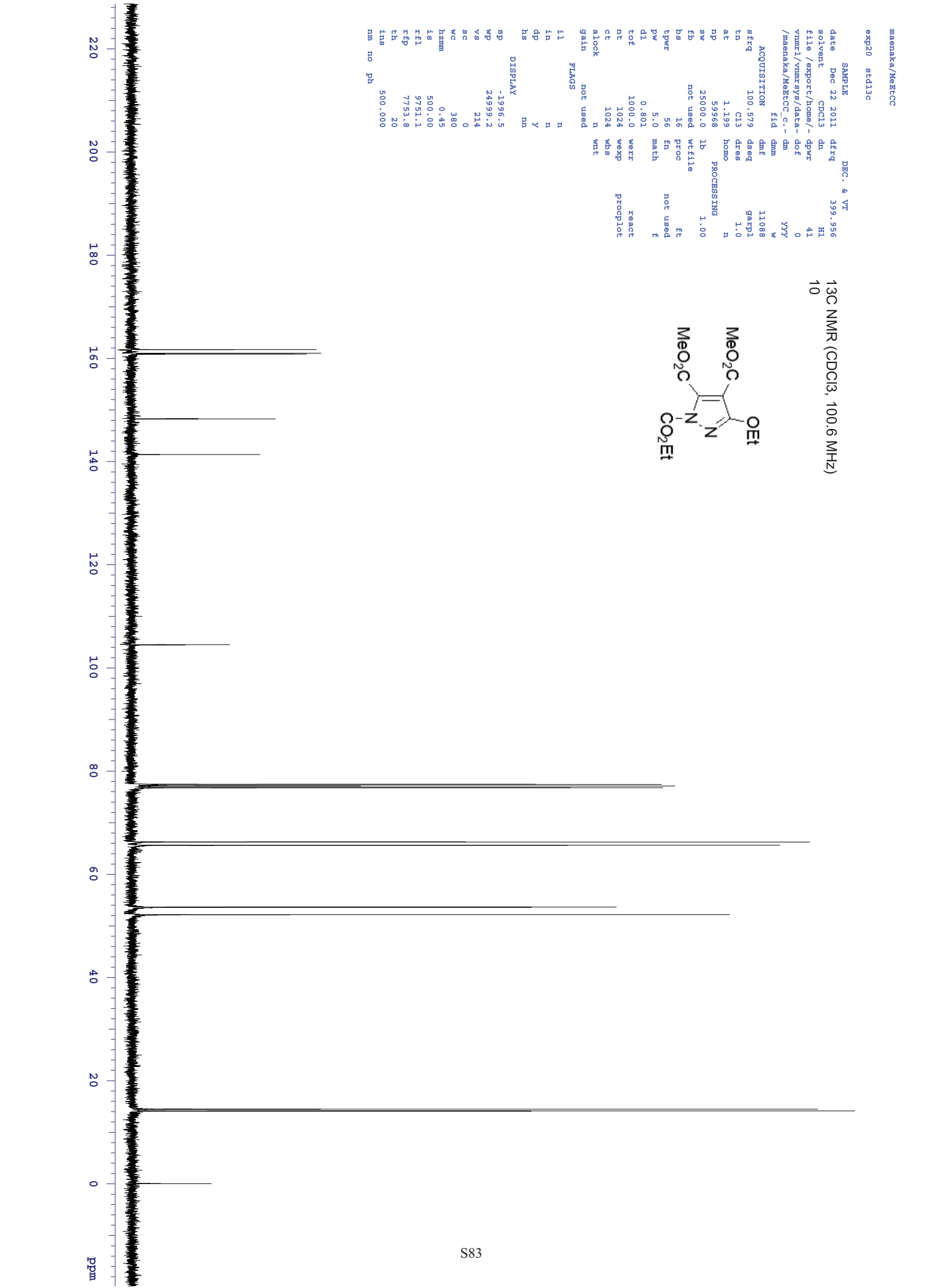
exp10 std13c

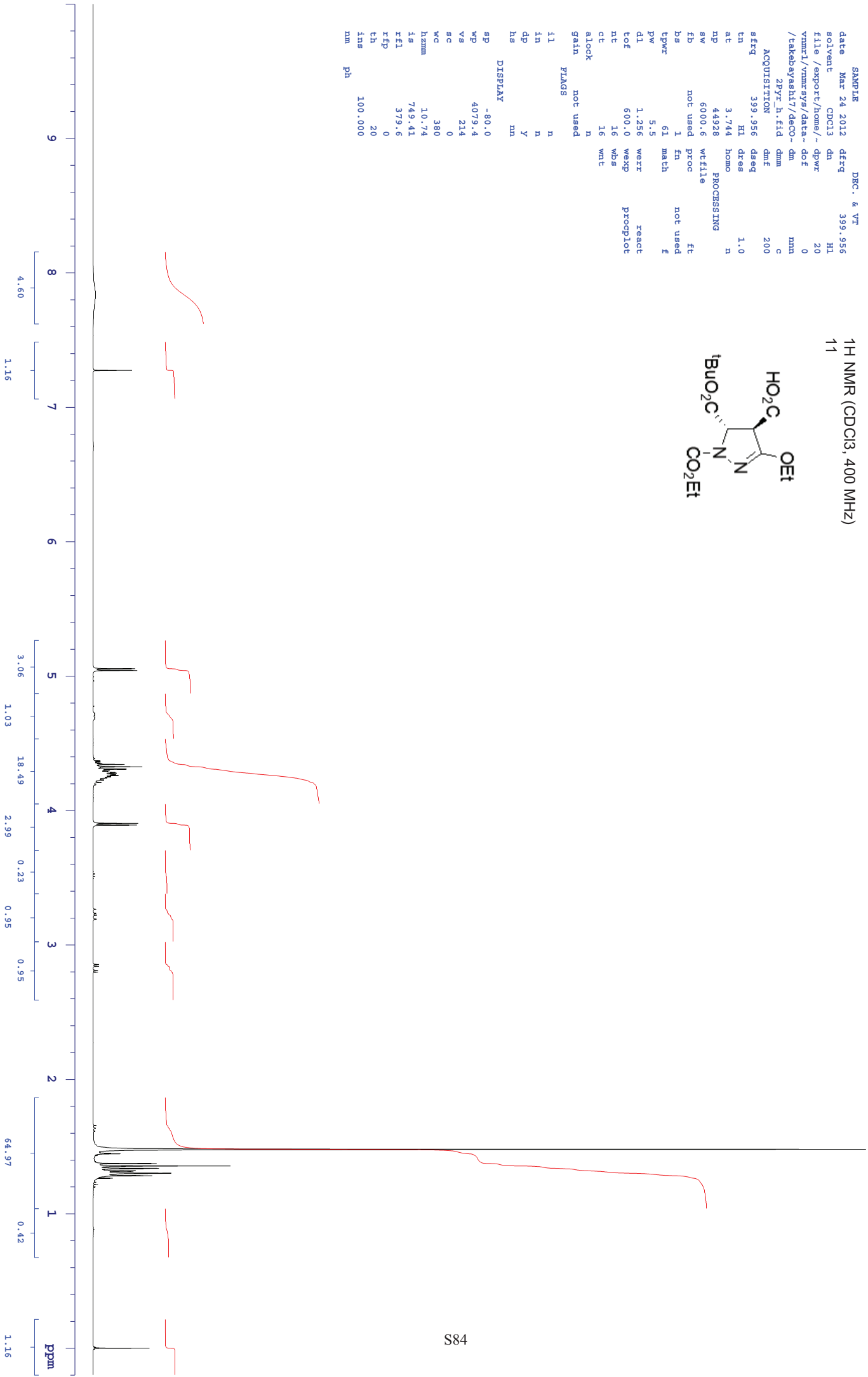
SAMPLE		DEC. & VT	
date	Aug 23 2011	dfrq	399.956
solvent	CDCl3	dn	H1
file	/export/home/~	dpwr	41
vnmrl/vnmrsys/data~		dof	0
/takebayashi7/ditB~		dm	yyy
	uMeR_c.fid	dmm	w
ACQUISITION		dmf	10400
sfrq	100.579	dseq	garp1
tn	C13	dres	1.0
at	1.199	homo	n
np	59968	PROCESSING	
sw	25000.0	lb	1.00
fb	not used	wtfile	
bs	16	proc	ft
tpwr	56	fn	not used
pw	5.0	math	f
d1	0.801		
tof	1000.0	werr	react
nt	8192	wexp	procplot
ct	8192	wbs	
alock	n	wnt	
gain	not used		
FLAGS			
il	n		
in	n		
dp	y		
hs	nn		
DISPLAY			
sp	-1998.1		
wp	24999.2		
vs	214		
sc	0		
wc	380		
hzmm	0.41		
is	500.00		
rfl	9752.7		
rfp	7753.8		
th	2		
ins	500.000		
nm no ph			

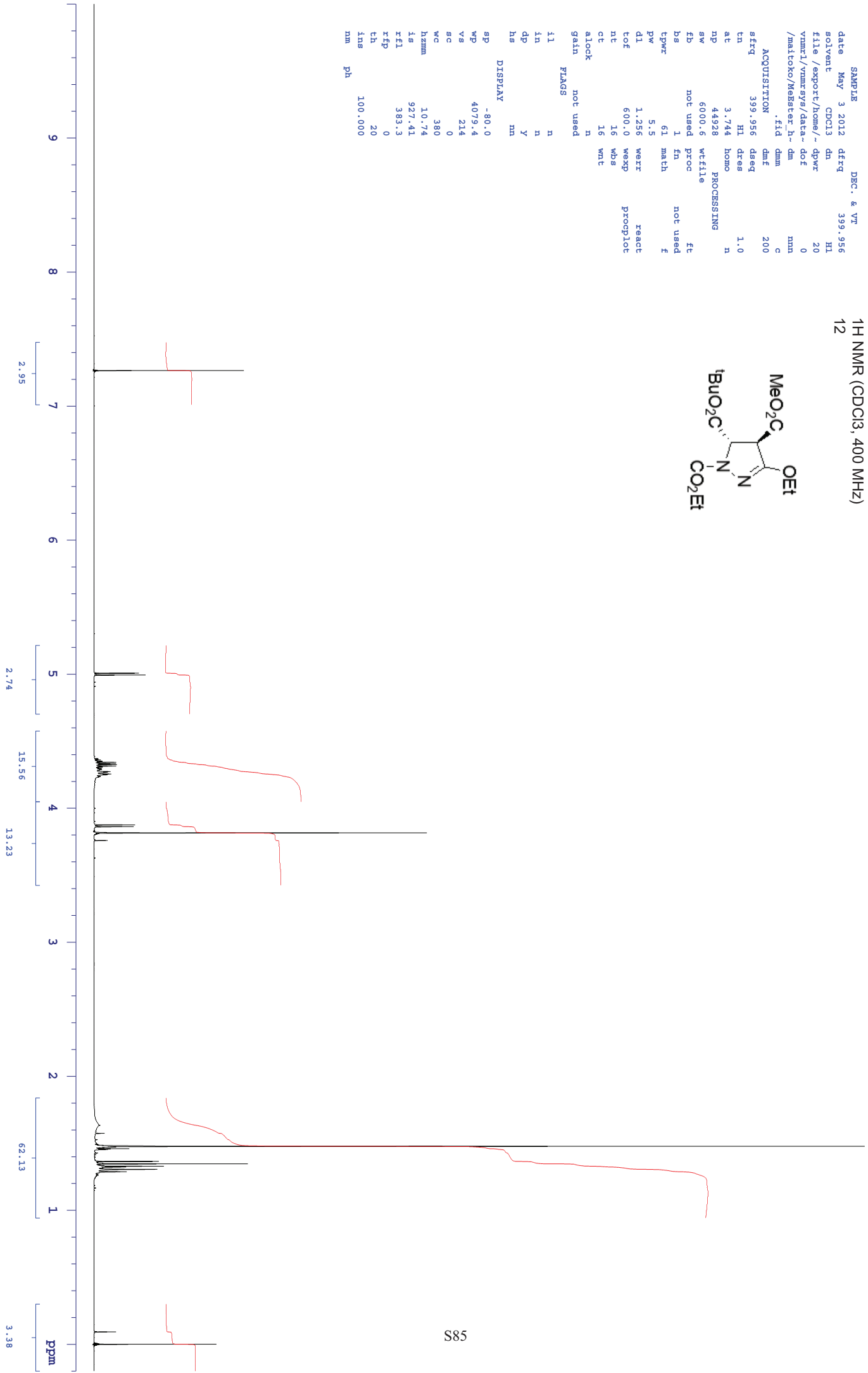
13C NMR (CDCl3, 100.6 MHz)
7f

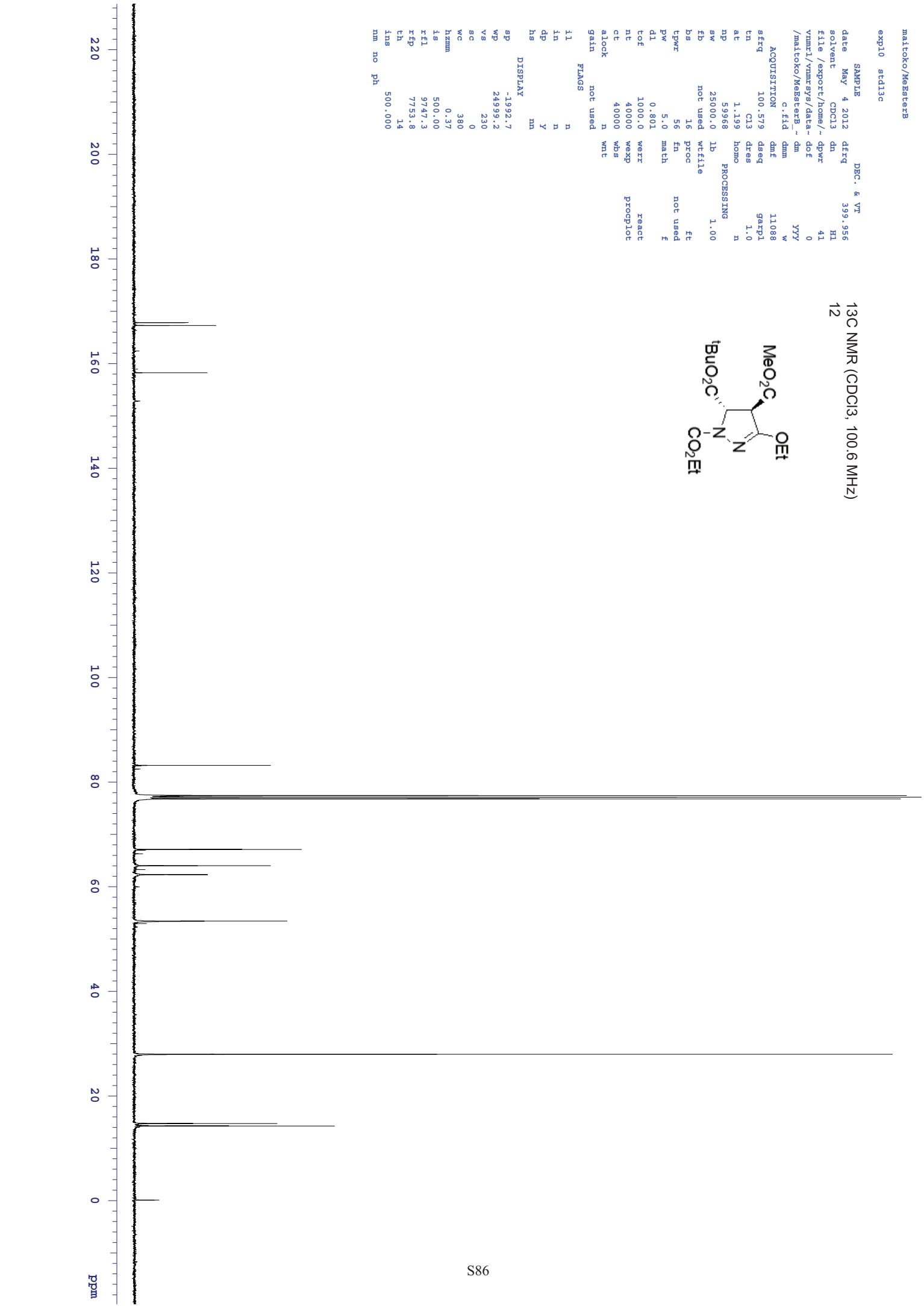


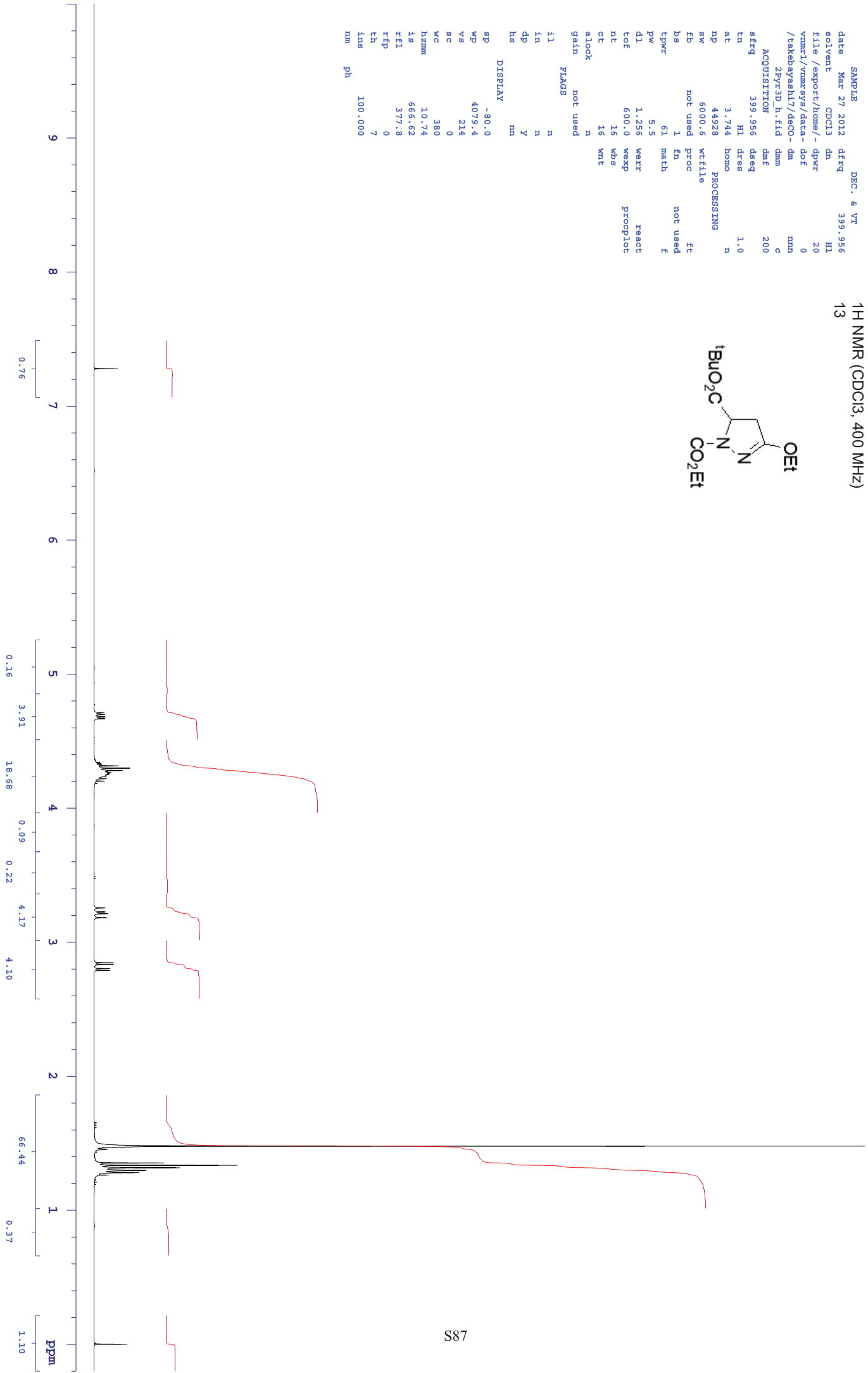

maenaka/MeEtCC
exp20 std1h
SAMPLE DEC. & VT
date Dec 22 2011 dfrq 399.956
solvent CDCl3 dn H1
file /export/home/~ dpwr 20
vnmr1/vnmrsys/data~ dof 0
/maenaka/MeEtCC_h.~ dm nnn
fid dmm c
ACQUISITION dmf 200
sfrq 399.956 dseq 1.0
tn H1 dres n
at 3.744 homo
np 44928 PROCESSING
sw 6000.6 wtfile
fb not used proc ft
bs not used fn not used
tpwr 61 math f
pw 5.5 react
d1 1.256 werr
tof 600.0 wexp procplot
nt 16 wbs
ct 16 wnt
alock n
gain not used
FLAGS
il n
in n
dp y
hs nn
DISPLAY
sp -80.0
wp 4079.4
vs 214
sc 0
wc 380
hzmm 10.74
is 650.76
rfl 376.0
rfp 0
th 20
ins 100.000
nm ph
1H NMR (CDCl3, 400 MHz)
10
MeO2C
MeO2C
OEt
CO2Et
N
N
0.79
0.00
58.97
-0.00
0.02
36.63
0.27
3.33
9
8
7
6
5
4
3
2
1
ppm




takebayashi7/deCO2Pyr
exp1D stdih
SAMPLE DEC. & VT
date Mar 24 2012 dfrq 399.956
solvent CDCl3 dn H1
file /export/home/~ dpwr 20
vnmr1/vnmrsys/data~ dof 0
/takebayashi7/deCO~ dm nnn
2Pyr_h.fid dmm c
ACQUISITION dmf 200
sfrq 399.956 dseq
tn H1 dres 1.0
at 3.744 homo n
np 44928 PROCESSING
sw 6000.6 wtfile
fb not used proc ft
bs not used fn not used
tpwr 61 math f
pw 5.5
d1 1.256 werr react
tof 600.0 wexp procplot
nt 16 wbs
ct 16 wnt
alock n
gain not used
FLAGS
il n
in n
dp y
hs nn
DISPLAY
sp -80.0
wp 4079.4
vs 214
sc 0
wc 380
hzmm 10.74
is 749.41
rfl 379.6
rfp 0
th 20
ins 100.000
nm ph
HO2C
OEt
tBuO2C
N
N
CO2Et
1H NMR (CDCl3, 400 MHz)
11
4.60
1.16
3.06
1.03
18.49
2.99
0.23
0.95
0.95
64.97
0.42
1.16
9
8
7
6
5
4
3
2
1
ppm


maitoko/MeEster
exp10 std1h
SAMPLE DEC. & VT
date May 3 2012 dfrq 399.956
solvent CDCl3 dn H1
file /export/home/~ dpwr 20
vnmr1/vnmrsys/data~ dof 0
/maitoko/MeEster_h~ dm nnn
.fid dmm c
ACQUISITION dmf 200
sfrq 399.956 dseq
tn H1 dres 1.0
at 3.744 homo n
np 44928 PROCESSING
sw 6000.6 wtfile
fb not used proc ft
bs not used fn not used
tpwr 61 math f
pw 5.5
d1 1.256 werr react
tof 600.0 wexp procplot
nt 16 wbs
ct 16 wnt
alock n
gain not used
FLAGS
il n
in n
dp y
hs nn
DISPLAY
sp -80.0
wp 4079.4
vs 214
sc 0
wc 380
hzmm 10.74
is 927.41
rfl 383.3
rfp 0
th 20
ins 100.000
nm ph
1H NMR (CDCl3, 400 MHz)
12
MeO2C
OEt
tBuO2C
N
N
CO2Et
9
8
7
6
5
4
3
2
1
ppm
2.95
2.74
15.56
13.23
62.13
3.38


maitoko/MeEsterB
exp10 std13c
SAMPLE DEC. & VT
date May 4 2012 dfrq 399.956
solvent CDCl3 dn H1
file /export/home/~ dpwr 41
vnmr1/vnmrsys/data~ dof 0
/maitoko/MeEsterB_~ dm yyy
c.fid dmm w
ACQUISITION dmf 11088
sfrq 100.579 dseq garp1
tn C13 dres 1.0
at 1.199 homo n
np 59968 PROCESSING
sw 25000.0 lb 1.00
fb not used wtfile
bs 16 proc ft
tpwr 56 fn not used
pw 5.0 math f
d1 0.801
tof 1000.0 werr react
nt 40000 wexp procplot
ct 40000 wbs
alock n wnt
gain not used
FLAGS
il n
in n
dp y
hs nn
DISPLAY
sp -1992.7
wp 24999.2
vs 230
sc 0
wc 380
hzmm 0.37
is 500.00
rfl 9747.3
rfp 7753.8
th 14
ins 500.000
nm no ph
13C NMR (CDCl3, 100.6 MHz)
12
MeO2C
OEt
tBuO2C
N
N
CO2Et
220
200
180
160
140
120
100
80
60
40
20
0
ppm


takebayashi7/deCO2Pyr3D
exp1 std1h
SAMPLE DEC. & VT
date Mar 27 2012 dfrq 399.956
solvent CDCl3 dn H1
file /export/home/~ dpwr 20
vnmr1/vnmrsys/data~ dof 0
/takebayashi7/deCO~ dm nnn
2Pyr3D_h.fid dmm c
ACQUISITION dmf 200
sfrq 399.956 dseq 1.0
tn H1 dres n
at 3.744 homo
np 44928 PROCESSING
sw 6000.6 wtfile
fb not used proc ft
bs not used fn not used
tpwr 61 math f
pw 5.5
d1 1.256 werr react
tof 600.0 wexp procplot
nt 16 wbs
ct 16 wnt
alock n
gain not used
FLAGS
il n
in n
dp y
hs nn
DISPLAY
sp -80.0
wp 4079.4
vs 214
sc 0
wc 380
hzmm 10.74
is 666.62
rfl 377.8
rfp 0
th 7
ins 100.000
nm ph
1H NMR (CDCl3, 400 MHz)
13
OEt
N
N
CO2Et
tBuO2C
0.76
0.16
3.91
18.68
0.09
0.22
4.17
4.10
66.44
0.37
1.10
ppm

takebayashi7/deCO2Pyr3D

exp10 std13c

SAMPLE		DEC. & VT	
date	Mar 27 2012	dfrq	399.956
solvent	CDCl3	dn	H1
file	/export/home/~	dpwr	41
vnmrl/vnmrsys/data~		dof	0
/takebayashi7/deCO~		dm	yyy
2Pyr3Dr_c.fid		dmm	w
ACQUISITION		dmf	11088
sfrq	100.579	dseq	garp1
tn	C13	dres	1.0
at	1.199	homo	n
np	59968	**PROCESSING**	
sw	25000.0	lb	1.00
fb	not used	wtfile	
bs	16	proc	ft
tpwr	56	fn	not used
pw	5.0	math	f
d1	0.801		
tof	1000.0	werr	react
nt	8192	wexp	procplot
ct	8192	wbs	
alock	n	wnt	
gain	not used		
FLAGS			
il	n		
in	n		
dp	y		
hs	nn		
DISPLAY			
sp	-1995.8		
wp	24999.2		
vs	214		
sc	0		
wc	380		
hzmm	1.55		
is	500.00		
rfl	9750.4		
rfp	7753.8		
th	2		
ins	500.000		
nm no ph			

13C NMR (CDCl3, 100.6 MHz)
13