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Fragmentation of chloroperoxides: Hypochlorite-mediated dehydration of hydroperoxyacetals to esters

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Abstract

Hypochlorites efficiently dehydrate hydroperoxyacetals to furnish the corresponding esters. The reaction, which can be accomplished with stoichiometric $\text{Ca}(\text{OCl})_2$ or with catalytic amounts of *t*-BuOCl, appears to involve formation and heterolytic fragmentation of secondary chloroperoxides, species not previously described in solution chemistry.

Keywords: hypochlorite, hydroperoxyacetal, chloroperoxide, fragmentation, ester

1. Introduction

Hydroperoxyacetals, readily available intermediates,¹ are substrates for a number of useful fragmentations, including Fe(II)-mediated cleavage to alkoxy radicals,^{1(c), 2} heterolytic C–O bond migrations of tertiary peresters, or persulfonates (Criegee rearrangement),³ and the base-promoted dehydration of hydroperoxyacetals, or derived peresters, or persulfonates.^{1(c), 4, 5} In the course of investigations into the addition of oxygen nucleophiles to ozonolysis-derived carbonyl oxides,⁶ we observed the rapid dehydration of secondary hydroperoxyacetals in the presence of commercial bleach.⁷ We now report that $\text{Ca}(\text{OCl})_2$, *t*-BuOCl, and trichloroisocyanuric acid mediate the rapid heterolytic dehydration of hydroperoxyacetals through the apparent intermediacy of secondary chloroperoxides, species whose solution chemistry has not been previously described.

2. Results and discussion

Most of the substrates employed in this study were prepared via ozonolysis of alkenes in the presence of an alcohol.^{1a} Addition of $\text{Ca}(\text{OCl})_2$ (1.3 equiv) to CH_3CN solutions of hydroperoxyacetals **1a–h** furnished esters **2a–h** (Table 1) after evaporation of solvent and filtration through a short silica column.^{7, 8} The reaction could also be conducted in $\text{CH}_3\text{OH}/\text{CH}_2\text{Cl}_2$; however the reaction in CH_2Cl_2 , THF,

or toluene was limited by the solubility of $\text{Ca}(\text{OCl})_2$. The dehydration proved compatible with a free primary alcohol (entry 4) or a chloroethyl acetal (entry 8). Little reaction was observed with aq NaOCl.

Comparable yields were available with *t*-BuOCl (Table 2).⁹ Reactions, although conducted for the same duration as for $\text{Ca}(\text{OCl})_2$, were now complete within 1 min (TLC).¹⁰ The rate and yield were not affected by protection from laboratory light (entry 2), use of CH_2Cl_2 as solvent (entry 3), or the presence of acid (entry 4). However, the presence of methanol slowed reactions considerably (not shown). Dehydration could be conducted with catalytic (0.25 equiv) quantities of *t*-BuOCl (entries 5 and 8), although the reactions now required 15 min for completion.

Table 1. Fragmentation of hydroperoxyacetals with $\text{Ca}(\text{OCl})_2$

Entry	Substrate	R ¹	R ²	Product	Yield ^a
1	1a	Octyl	Me	2a	75% (91)
2	1b	Octyl	Et	2b	86% (90)
3	1c	Octyl	<i>i</i> -Pr	2c	83% (93)
4	1d	Octyl	(CH ₂) ₂ OH	2d	83% (86)
5	1e	AcO(CH ₂) ₈	Me	2e	85% (93)
6	1f	BnO(CH ₂) ₃	Me	2f	81% (94)
7	1g	Ph(CH ₂) ₂	Me	2g	80% (93)
8	1h	Octyl	(CH ₂) ₂ Cl	2h	82% (92)

a. Isolated yields on 0.5 mmol or (5 mmol) scale.

Table 2. Fragmentation of hydroperoxyacetals with *t*-BuOCl

$\begin{array}{c} \text{H} \\ \diagup \\ \text{C} \text{---} \text{OOH} \\ \diagdown \\ \text{O} \end{array} \xrightarrow[\text{CH}_3\text{CN, rt}]{t\text{-BuOCl (0.25 - 1.2 eq)}} \begin{array}{c} \text{O} \\ \parallel \\ \text{C} \text{---} \text{O} \end{array}$					
Entry	Substrate	<i>t</i> -BuOCl (equiv)	<i>t</i> (min)	Product	Yield ^a (%)
1	1a	1.2	10	2a	77
2 ^b	1a	1.2	10	2a	77
3 ^c	1a	1.2	10	2a	79
4 ^d	1a	1.2	10	2a	84
5	1a	0.25	15	2a	78
6	1b	1.2	10	2b	85
7	1d	1.2	10	2d	84
8	1e	0.25	15	2e	85
9	1h	1.2	10	2h	84

a. Isolated yields on 0.5 mmol scale.

b. Protected from light (Al foil over flask).

c. CH₂Cl₂ as solvent.

d. Added HOAc (≥ 2 equiv).

No reaction was observed between *t*-BuOCl and a silylated hydroperoxyacetal (**1i**, Scheme 1). However, a secondary hydroperoxide (**1j**)¹¹ underwent rapid dehydration; the low yield likely reflects product volatility. Dehydration of secondary allylic hydroperoxides (not shown) required excess *t*-BuOCl and furnished the expected α,β -unsaturated ketones as mixtures with significant amounts of byproducts lacking unsaturation.

The fragmentation can be combined with alkene ozonolysis to afford a convenient one-pot synthesis of esters (Scheme 2).

The fragmentation is likely to involve the initial formation of chloroperoxides, species previously prepared only in tertiary systems.¹² The intermediacy of ROOCl is consistent with the lack of reaction of silylated hydroperoxyacetal **1i**. In an effort to access chloroperoxides with reagents other than hypochlorites, we discovered that commercially available trichloroisocyanuric acid promotes the dehydrative fragmentation as or more efficiently than *t*-BuOCl (Scheme 3).

Scheme 1. Substrates other than hydroperoxyacetals. **Scheme 2.** Application in tandem with ozonolysis. **Scheme 3.** Dehydration with trichloroisocyanuric acid.

The conversion of the chloroperoxides to esters could in principle proceed through either homolytic or heterolytic pathways (Scheme 4), and several additional experiments were conducted to discriminate between these possibilities (Scheme 5).

Chloroperoxides are reported to undergo homolytic scission to generate ROO[•] and Cl[•].^{12, 13} For this reason, we initially hypothesized the dehydrations involved a radical chain initiated by abstraction of the acetal C-H; the resulting carbon radical would be expected to fragment to the product ester and a propagating radical ([•]OCl). However, the dehydrations were insensitive to the presence or the absence of visible light and did not occur in the presence of PhI(OTFA)₂, a reagent known to promote peroxy radical formation.¹⁴ Perhaps most convincingly, dehydration of **1k**, a hydroperoxyacetal substrate incorporating a fast radical clock (Scheme 5), proceeded with no detectable formation of ring-opened products.¹⁵

The potential role of alkoxy radicals was probed with hydroperoxyacetals **1l** and **1m**¹⁶ (Scheme 5); the α -oxygenated alkoxy radicals derived from either substrate would be expected to readily undergo β -scission.¹⁷ However, both **1l** and **1m** undergo dehydration with no signs of radical cleavage. In contrast, a hydroperoxyketal unable to dehydrate (**1n**) undergoes a much slower (30 min) reaction to furnish chloroalkanoate **3**, the product of alkoxy radical cleavage.

The results support fragmentation through the heterolytic pathway illustrated in Scheme 4, presumably through a mechanism analogous to Criegee or Hock fragmentation (activation of hydroperoxides by protonation or Lewis acid

Scheme 4. Mechanistic possibilities. **Scheme 5.** Additional substrates.

complexation).^{3, 18} The specificity for migration of hydrogen relative to Ph or Bn (**1j**, **1l**) under nonbasic conditions is interesting. However, as has recently been demonstrated for Baeyer-Villiger rearrangements of alkoxybromanes derived from hemiacetals,¹⁹ the nature of the activating reagents can have a strong influence on rearrangements to electron-deficient oxygen. The proposed mechanism predicts the regeneration of HOCl,²⁰ and is consistent with the high conversion obtained in the presence of substoichiometric *t*-BuOCl or trichloroisocyanuric acid. The results may be of relevance to atmospheric decomposition of primary chloroperoxides.²¹

3. Conclusions

We have developed a new fragmentation of hydroperoxyacetals to esters based upon heterolytic fragmentation of intermediate chloroperoxides.

⚠ **CAUTION:** While we experienced no hazards in the course of this work, any preparative work with peroxides should be conducted with an awareness of the potential for spontaneous and exothermic decomposition reactions.²²

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8. Typical procedure for reactions with $\text{Ca}(\text{OCl})_2$: To a flame-dried 8 mL vial equipped with stirbar and screw-top septa cap containing technical grade $\text{Ca}(\text{OCl})_2$ (1.3 equiv, 1.0 mmol, 143 mg of 65% reagent) is added CH_3CN (2 mL). A solution of the hydroperoxy acetal (1.0 equiv, 0.50 mmol) in CH_3CN (1 mL) is added as a single portion via syringe. The reaction is stirred vigorously for 10 min at which time the partially heterogeneous solution is filtered through a short plug of silica. The reaction vial is rinsed with a small amount of CH_2Cl_2 and this solution is also filtered through the silica plug. The silica plug is rinsed with another small portion of CH_2Cl_2 and the filtrate is concentrated.
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Supplementary data — ^1H and ^{13}C NMR spectra for **1a-i**, **1k-n**, **2a-I**, **2k-m**, & **3** are presented in the following pages.

Supporting Information
 “Fragmentation of chloroperoxides: hypochlorite-mediated dehydration of
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P1 9.50 usec
PL1 0.00 dB
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL2 -4.00 dB
PL12 12.90 dB
PL13 13.82 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Current Data Parameters
NAME TFish0444_product_062409
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20090624
Time_ 14.03
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 128
DW 60.400 usec
DE 6.50 usec
TE 295.9 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 12.50 usec
PL1 -2.50 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Current Data Parameters
NAME TFish0444_product_062409
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20090626
Time_ 15.25
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 187
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 5792.6
DW 20.850 usec
DE 6.50 usec
TE 296.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 10.00 usec
PL1 0.00 dB
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.50 dB
PL12 13.62 dB
PL13 13.62 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Current Data Parameters
 NAME TFish0425_product_060609
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20090606
 Time_ 16.45
 INSTRUM spect
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 6172.839 Hz
 FIDRES 0.094190 Hz
 AQ 5.3084660 sec
 RG 228.1
 DW 81.000 usec
 DE 6.50 usec
 TE 298.0 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 8.14 usec
 PL1 0.60 dB
 SFO1 300.1318534 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Current Data Parameters
 NAME TFish0425_product_060609
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20090606
 Time_ 16.51
 INSTRUM spect
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 32768
 SOLVENT CDC13
 NS 113
 DS 4
 SWH 17985.611 Hz
 FIDRES 0.548877 Hz
 AQ 0.9110004 sec
 RG 13004
 DW 27.800 usec
 DE 6.50 usec
 TE 298.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 6.25 usec
 PL1 0.00 dB
 SFO1 75.4752953 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 0.60 dB
 PL12 20.45 dB
 PL13 20.55 dB
 SFO2 300.1312005 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4677490 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Current Data Parameters
 NAME TFish0452_product_dry_062909
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20090629
 Time_ 12.48
 INSTRUM spect
 PROBHD 5 mm Multinucl
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8278.146 Hz
 FIDRES 0.126314 Hz
 AQ 3.9584243 sec
 RG 90.5
 DW 60.400 usec
 DE 6.50 usec
 TE 294.8 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 12.50 usec
 PL1 -2.50 dB
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Current Data Parameters
NAME TFish0452_product_dry_062909
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20090629
Time_ 12.15
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 170
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 5160.6
DW 20.850 usec
DE 6.50 usec
TE 295.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 10.00 usec
PL1 0.00 dB
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.50 dB
PL12 13.62 dB
PL13 13.62 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Current Data Parameters
 NAME TFish0640_product_061010
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20090611
 Time_ 12.56
 INSTRUM spect
 PROBHD 5 mm Multinucl
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 16
 DS 2
 SWH 8278.146 Hz
 FIDRES 0.126314 Hz
 AQ 3.9584243 sec
 RG 90.5
 DW 60.400 usec
 DE 6.50 usec
 TE 294.6 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 12.50 usec
 PL1 -2.50 dB
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Current Data Parameters
 NAME TFish0640_product_061010
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20090611
 Time_ 12.41
 INSTRUM spect
 PROBHD 5 mm Multinucl
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 158
 DS 4
 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 5792.6
 DW 20.850 usec
 DE 6.50 usec
 TE 295.3 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 10.00 usec
 PL1 0.00 dB
 SFO1 100.6228298 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -2.50 dB
 PL12 13.62 dB
 PL13 13.62 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127690 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

4.774
4.760
4.746

3.575

1.635
1.614
1.600
1.286
0.970
0.915
0.898
0.880
0.203
0.192

Current Data Parameters
NAME TFish0459_Product_063009
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20090630
Time_ 19.58
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 71.8
DW 60.400 usec
DE 6.50 usec
TE 295.5 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 12.50 usec
PL1 -2.50 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0PC

1i

Current Data Parameters
 NAME TFish0459_Product_063009
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20090630
 Time_ 20.02
 INSTRUM spect
 PROBHD 5 mm Multinucl
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 165
 DS 4
 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 4597.6
 DW 20.850 usec
 DE 6.50 usec
 TE 295.8 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 10.00 usec
 PL1 0.00 dB
 SFO1 100.6228298 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -2.50 dB
 PL12 13.62 dB
 PL13 13.62 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127690 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

8.416
8.379
7.292
7.196
7.127
4.667
4.654
4.644
3.580
3.552
2.043
2.033
2.021
1.544
1.536
1.533
1.522
1.519
1.510
1.508
1.505
1.497
1.494
1.483
1.471
1.232
1.218
1.209
1.205
1.196
1.183
1.121
1.107
1.098
1.084
1.070
1.056
1.048
1.043
1.041
1.034
1.027
1.021
1.019

Current Data Parameters
NAME TFish0529_product_111409
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20091114
Time_ 17.54
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 90.5
DW 60.400 usec
DE 6.50 usec
TE 293.9 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 12.00 usec
PL1 -3.35 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Current Data Parameters
 NAME TFish0529_product_111409
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20091114
 Time 18.03
 INSTRUM spect
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 232
 DS 4
 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 1024
 DW 20.850 usec
 DE 6.50 usec
 TE 295.1 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 10.00 usec
 PL1 0.50 dB
 SFO1 100.6228298 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 70.00 usec
 PL2 -3.35 dB
 PL12 11.97 dB
 PL13 11.97 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127690 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

141.50
141.48
128.40
126.14
125.97
125.95
109.24
109.15
56.15
55.93
22.85
22.81
19.75
19.68
12.12
11.85

Current Data Parameters
 NAME TFish0514_product_091109
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20090911
 Time_ 20.50
 INSTRUM spect
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8278.146 Hz
 FIDRES 0.126314 Hz
 AQ 3.9584243 sec
 RG 128
 DW 60.400 usec
 DE 6.50 usec
 TE 293.9 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 12.00 usec
 PL1 -3.35 dB
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

11

136.13
129.52
128.47
126.70

109.11

77.36
77.04
76.73

56.40

38.22

Current Data Parameters
NAME TFish0514_product_091109
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20090911
Time_ 20.57
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 94
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 1024
DW 20.850 usec
DE 6.50 usec
TE 294.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 10.00 usec
PL1 0.00 dB
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL2 -3.35 dB
PL12 11.97 dB
PL13 11.97 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

200 180 160 140 120 100 80 60 40 20 0 ppm

Current Data Parameters
 NAME TFish0587_product_031010
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20100310
 Time_ 12.19
 INSTRUM spect
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 16
 DS 2
 SWH 8278.146 Hz
 FIDRES 0.126314 Hz
 AQ 3.9584243 sec
 RG 90.5
 DW 60.400 usec
 DE 6.50 usec
 TE 298.0 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.25 usec
 PL1 -3.35 dB
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 131072
 SF 400.1300000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1m

102.58

62.88

27.35
25.01
19.58

Current Data Parameters
NAME TFish0587_product_031010
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20100310
Time_ 12.25
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 82
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 812.7
DW 20.850 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 10.00 usec
PL1 0.50 dB
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL2 -3.35 dB
PL12 13.34 dB
PL13 13.34 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

200 180 160 140 120 100 80 60 40 20 0 ppm

7.503
7.478
3.344
3.308
2.259
2.251
2.224
2.216
2.162
2.154
2.127
2.124
2.119
2.111
1.740
1.734
1.720
1.708
1.622
1.423
1.413
1.406
1.389
1.379
1.356
1.346
1.276
1.241
1.235
1.210
1.203
1.178
1.170
1.145
1.137
1.091
1.084
1.076
1.061
1.054
1.047
1.041
1.024
0.887

Current Data Parameters
NAME TFish0580_product_030310
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20100303
Time_ 19.46
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 90.5
DW 60.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 12.00 usec
PL1 -3.35 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Current Data Parameters
 NAME TFish0580_product_030310
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20100303
 Time_ 19.56
 INSTRUM spect
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 379
 DS 4
 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 1149.4
 DW 20.850 usec
 DE 6.50 usec
 TE 298.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 10.00 usec
 PL1 0.50 dB
 SFO1 100.6228298 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 70.00 usec
 PL2 -3.35 dB
 PL12 11.97 dB
 PL13 11.97 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 65536
 SF 100.6127690 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Current Data Parameters
NAME TFish0448_crude_062609
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20090626
Time_ 13.07
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 71.8
DW 60.400 usec
DE 6.50 usec
TE 295.4 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 12.50 usec
PL1 -2.50 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

3.00
2.00
2.16
10.64
3.05

Current Data Parameters
NAME TFish0448_crude_062609
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20090626
Time_ 13.11
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 117
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 4597.6
DW 20.850 usec
DE 6.50 usec
TE 295.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 10.00 usec
PL1 0.00 dB
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.50 dB
PL12 13.62 dB
PL13 13.62 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

2a

4.165
4.147
4.129
4.111
2.318
2.300
2.281
1.649
1.631
1.612
1.310
1.300
1.286
1.269
1.251
0.909
0.892
0.875

Current Data Parameters
NAME TFish0454_crude_063009
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20090630
Time_ 10.23
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 64
DW 60.400 usec
DE 6.50 usec
TE 295.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 12.50 usec
PL1 -2.50 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1.98
2.00
2.14
13.37
3.06

Current Data Parameters
NAME TFish0454_crude_063009
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20090630
Time_ 10.27
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 194
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 5792.6
DW 20.850 usec
DE 6.50 usec
TE 295.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 10.00 usec
PL1 0.00 dB
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.50 dB
PL12 13.62 dB
PL13 13.62 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Current Data Parameters
NAME TFish0455_crude_063009
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20090630
Time_ 18.57
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 57
DW 60.400 usec
DE 6.50 usec
TE 295.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 12.50 usec
PL1 -2.50 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Current Data Parameters
NAME TFish0455_crude_063009
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20090630
Time_ 19.02
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 222
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 5160.6
DW 20.850 usec
DE 6.50 usec
TE 296.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 10.00 usec
PL1 0.00 dB
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.50 dB
PL12 13.62 dB
PL13 13.62 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Current Data Parameters
NAME TFish0456_crude_063009
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20090630
Time_ 19.15
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 71.8
DW 60.400 usec
DE 6.50 usec
TE 295.4 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 12.50 usec
PL1 -2.50 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.130000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Current Data Parameters
NAME TFish0456_crude_063009
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20090630
Time_ 19.24
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 132
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 5160.6
DW 20.850 usec
DE 6.50 usec
TE 296.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 10.00 usec
PL1 0.00 dB
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.50 dB
PL12 13.62 dB
PL13 13.62 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Current Data Parameters
NAME TFish0445_crude_062409
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20090624
Time_ 17.19
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 90.5
DW 60.400 usec
DE 6.50 usec
TE 296.1 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 12.50 usec
PL1 -2.50 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

4.077
4.061
4.044
3.681
2.336
2.318
2.299
2.060
1.659
1.644
1.627
1.613
1.326

Current Data Parameters
NAME TFish0445_crude_062409
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20090626
Time_ 15.44
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 205
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 5160.6
DW 20.850 usec
DE 6.50 usec
TE 296.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 10.00 usec
PL1 0.00 dB
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.50 dB
PL12 13.62 dB
PL13 13.62 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Current Data Parameters
 NAME TFish0457_crude_063009
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20090630
 Time_ 19.31
 INSTRUM spect
 PROBHD 5 mm Multinucl
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8278.146 Hz
 FIDRES 0.126314 Hz
 AQ 3.9584243 sec
 RG 71.8
 DW 60.400 usec
 DE 6.50 usec
 TE 295.4 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 12.50 usec
 PL1 -2.50 dB
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

4.520
 3.678
 3.550
 3.534
 3.519
 2.485
 2.466
 2.448
 2.003
 1.988
 1.985
 1.976
 1.970
 1.954
 1.951
 1.936

Current Data Parameters
NAME TFish0457_crude_063009
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20090630
Time_ 19.35
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 157
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 4597.6
DW 20.850 usec
DE 6.50 usec
TE 296.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 10.00 usec
PL1 0.00 dB
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.50 dB
PL12 13.62 dB
PL13 13.62 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Current Data Parameters
NAME TFish0458_crude_063009
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20090630
Time_ 19.46
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 71.8
DW 60.400 usec
DE 6.50 usec
TE 295.4 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 12.50 usec
PL1 -2.50 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Current Data Parameters
NAME TFish0458_crude_063009
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20090630
Time_ 19.49
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 123
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 4597.6
DW 20.850 usec
DE 6.50 usec
TE 295.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 10.00 usec
PL1 0.00 dB
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.50 dB
PL12 13.62 dB
PL13 13.62 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

2h

4.361
4.347
4.333
3.716
3.703
3.701
3.687
2.389
2.370
2.351
1.692
1.673
1.655
1.637
1.618
1.315
1.304
1.298
1.288
0.913
0.897
0.879

Current Data Parameters
NAME TFish0641_crude_061010
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20100603
Time_ 11.23
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 71.8
DW 60.400 usec
DE 6.50 usec
TE 294.1 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.25 usec
PL1 -3.35 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Current Data Parameters
 NAME TFish0641_crude_061010
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20100603
 Time_ 11.29
 INSTRUM spect
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 153
 DS 4
 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 32768
 DW 20.850 usec
 DE 6.50 usec
 TE 294.8 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 10.00 usec
 PL1 0.50 dB
 SFO1 100.6228298 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 70.00 usec
 PL2 -3.35 dB
 PL12 13.34 dB
 PL13 13.34 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127690 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Current Data Parameters
 NAME TFish0530_crude_111409
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20091114
 Time_ 19.41
 INSTRUM spect
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 16
 DS 2
 SWH 8278.146 Hz
 FIDRES 0.126314 Hz
 AQ 3.9584243 sec
 RG 90.5
 DW 60.400 usec
 DE 6.50 usec
 TE 293.9 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 12.00 usec
 PL1 -3.35 dB
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

173.88

140.00

128.49

126.53

126.21

51.92

26.29

23.96

17.04

Current Data Parameters
NAME TFish0530_crude_111409
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20091114
Time_ 19.46
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 112
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 1024
DW 20.850 usec
DE 6.50 usec
TE 295.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 10.00 usec
PL1 0.50 dB
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL2 -3.35 dB
PL12 11.97 dB
PL13 11.97 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

2l

7.325

3.724
3.666

Current Data Parameters
NAME TFish0515_crude_091409
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20090914
Time_ 14.20
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 71.8
DW 60.400 usec
DE 6.50 usec
TE 293.9 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 12.00 usec
PL1 -3.35 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

6.64

3.00
1.98

Current Data Parameters
NAME TFish0515_crude_091409
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20090914
Time 14.23
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 54
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 812.7
DW 20.850 usec
DE 6.50 usec
TE 294.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 10.00 usec
PL1 0.00 dB
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL2 -3.35 dB
PL12 11.97 dB
PL13 11.97 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

2l

172.08

134.00
129.70
129.53
129.48
129.28
128.61
128.49
128.40
127.14
126.79

52.08

41.22

2m

4.321
4.301
4.282
2.533
2.510
2.487
1.916
1.898
1.892
1.873
1.853
1.843
1.836
1.818
1.802
1.798
1.790

Current Data Parameters
NAME TFish0593_crude_031810
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20100318
Time_ 18.45
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 114
DW 81.000 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 9.00 usec
PL1 0.60 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 65536
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

2m

171.39

69.43

29.80

22.27

19.05

Current Data Parameters
NAME TFish0593_crude_031810
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20100318
Time_ 18.48
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 32768
SOLVENT CDC13
NS 46
DS 4
SWH 17985.611 Hz
FIDRES 0.548877 Hz
AQ 0.9110004 sec
RG 13004
DW 27.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 6.25 usec
PL1 0.00 dB
SFO1 75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL2 0.60 dB
PL12 18.42 dB
PL13 18.42 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

200 180 160 140 120 100 80 60 40 20 0 ppm

3.692
3.595
3.580
3.574
3.568
3.559
3.549
3.530
3.522
2.436
2.422
2.412
2.397
2.372
2.356
2.348
2.332
2.000
1.998
1.992
1.982
1.980
1.974
1.964
1.903
1.893
1.884
1.877
1.868
1.565
1.546
1.529
1.510
1.386
1.383
1.378
1.366
1.363
1.129
1.120
1.112
1.102
1.093
0.910

Current Data Parameters
NAME TFish0589_10-17_031510
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20100315
Time_ 20.08
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 64
DW 60.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.25 usec
PL1 -3.35 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

10 9 8 7 6 5 4 3 2 1 0 ppm

3.00 2.01 2.11 2.12 1.03 1.13 1.04 8.99

Current Data Parameters
 NAME TFish0589_10-17_031510
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20100315
 Time_ 20.13
 INSTRUM spect
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 58
 DS 4
 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 812.7
 DW 20.850 usec
 DE 6.50 usec
 TE 298.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 10.00 usec
 PL1 0.50 dB
 SFO1 100.6228298 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 70.00 usec
 PL2 -3.35 dB
 PL12 13.34 dB
 PL13 13.34 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127690 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40