Supplementary

Information

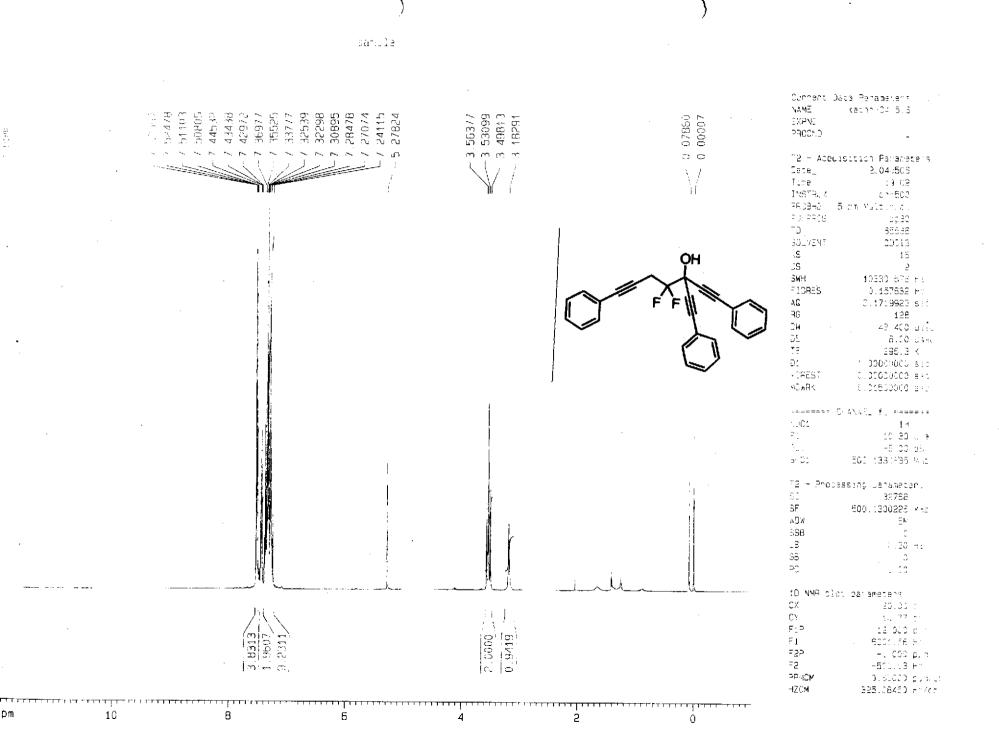
Easy Accesses to Various CF₂-containing Molecules Based on the Reaction of 2,2,3,3-Tetrafluorooxetane with Various Nucleophiles

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E-mail: ishihara@kit.ac.jp



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Current Data Parameters NAME

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OH FF

EXPNO 2 PROCNO 1 F2 - Acquisition Parameters Date_ 20040608 15.46 Time INSTRUM drx500 PROBHD 5 mm Multinucl PULPROG zgpg30 TD 65536 SOLVENT CDC13 256 NS 2 DS S₩H 30030.029 Hz FIDRES 0.458222 Hz AQ 1.0912244 sec RG 3649.1 DW DE 16.650 usec 6.00 usec ΤE 298.2 К D1 0.50000000 sec d11 0.03000000 sec MCREST 0.00000000 sec MCWRK 0.01500000 sec ====== CHANNEL f1 ======= NUC1 1 3C P1 5.70 usec PL1 -2.00 dB SF01 125.7703643 MHz ====== CHANNEL f2 ======== CPDPRG2 waltz16 NUC2 1H 100.00 usec PCPD2 PL2 -6.00 dB PL12 13.74 dB PL13 13.74 dB SF02 500.1320005 MHz F2 - Processing parameters SI 32768 SF 125.7578097 MHz WDW ЕΜ SSB 0 LB 1.00 Hz GB 0

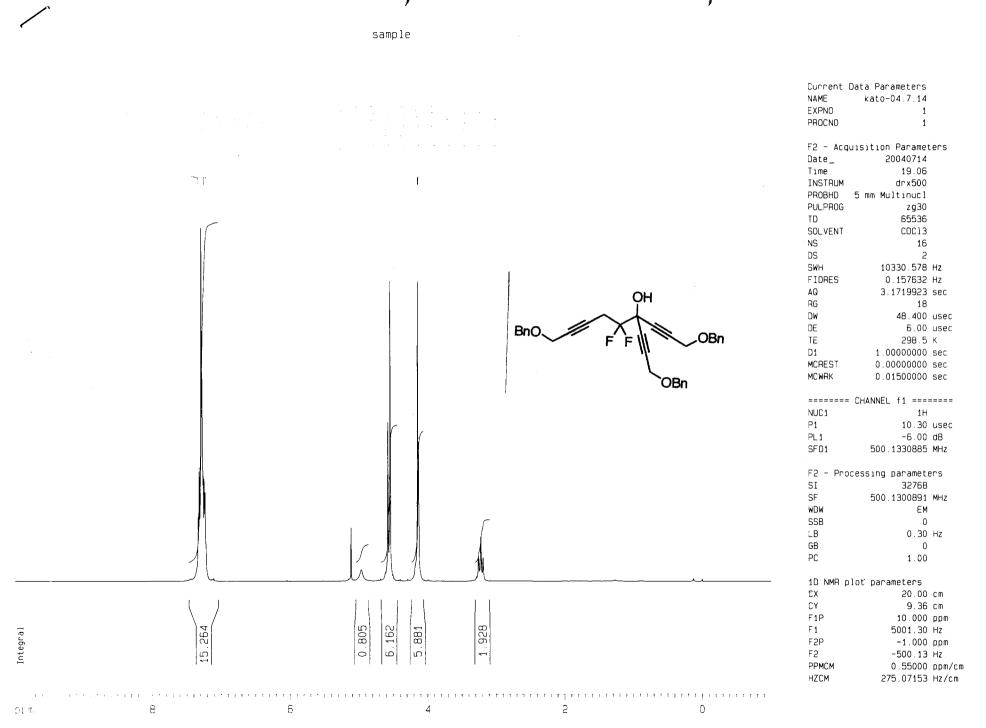
kato-04.6.8

1D NMR plot parameters СХ 20.00 cm CY 10.**4**1 cm F1P 200.000 ppm F 1 25151.56 Hz F2P -10.000 ppm F2 -1257.58 Hz PPMCM 10.50000 ppm/cm HZCM 1320.45703 Hz/cm

1.40

РС

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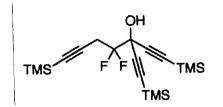
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		F2 - Acquisition Parameters
		Date_ 20040714 Time 19.14
		INSTRUM drx500
		PROBHD 5 mm Multinucl
		PULPROG zgpg30
		TD 65536
		SOLVENT CDC13
		NS 256
		DS 2
	ÓН	SWH 30030.029 Hz FIDRES 0.458222 Hz
		FIDRES 0.458222 Hz AQ 1.0912244 sec
	BnO, X	96 3649 1
		N DW 16.650 used
	BnO F F OB	DE 6.00 used
		ТЕ 299.5 К
		Di 0.5000000 sec
	OBn	d11 0.03000000 sec
		MCREST 0.0000000 sec
		MCWRK 0.01500000 sec
		====== CHANNEL f1 =======
		NUC1 13C
		P1 5.70 used
		PL1 -2.00 dB
		SF01 125.7703643 MHz
		====== CHANNEL f2 =======
		•CPDPRG2 waltz16
		NUC2 1H PCPD2 100.00 used
		PCPD2 100.00 used PL2 -6.00 dB
		PL12 13.74 dB
		PL13 13.74 dB
		SF02 500.1320005 MHz
		F2 - Processing parameters SI 32768
		SF 125.7578482 MHz
		WDW EM
		SSB 0
		LB 1.00 Hz
		GB 0
		PC 1.40
		1D NMR plot parameters
		CX 20.00 cm
		F1P 200.000 ppm
		F1 25151.57 Hz
e a a production	, i a a constant o constant i de accaracter constant e constant e constant e constant e constant e constant e c	F2P -10.000 ppm F2 -1257.58 Hz
	150 125 100 75 50 25 0	FZ -1207.08 HZ
m 175	150 125 100 75 50 25 0	PPMCM 10.50000 ppm

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Current Data NAME k EXPNO PROCNO	a Parameters kato-04.7.16 1 1	
Date_ Time INSTRUM	ition Paramet 20040716 15.45 drx500 mm Multinucl zg30 65536 CDC13 16 2 10330.578 0.157632 3.1719923 16 48.400 6.00 299.3 1.0000000 0.0000000 0.01500000	Hz Hz sec usec k sec sec sec
===== CH/ NUC1	ANNEL f1 ==== 1H	
P1 PL1 SF01	10.30 -6.00 500.1330885	dB
F2 - Process SI	sing paramete 32768	ers
SF WDW SSB LB GB PC	500.1300137 EM 0.30 0.30 0 1.00	-
1D NMR plot CX CY F1P F1 F2P F2 PPMCM HZCM	parameters 20.00 9.97 10.000 5001.30 -1.000 -500.13 0.55000 275.07150	cm ppm Hz ppm Hz ppm/cm

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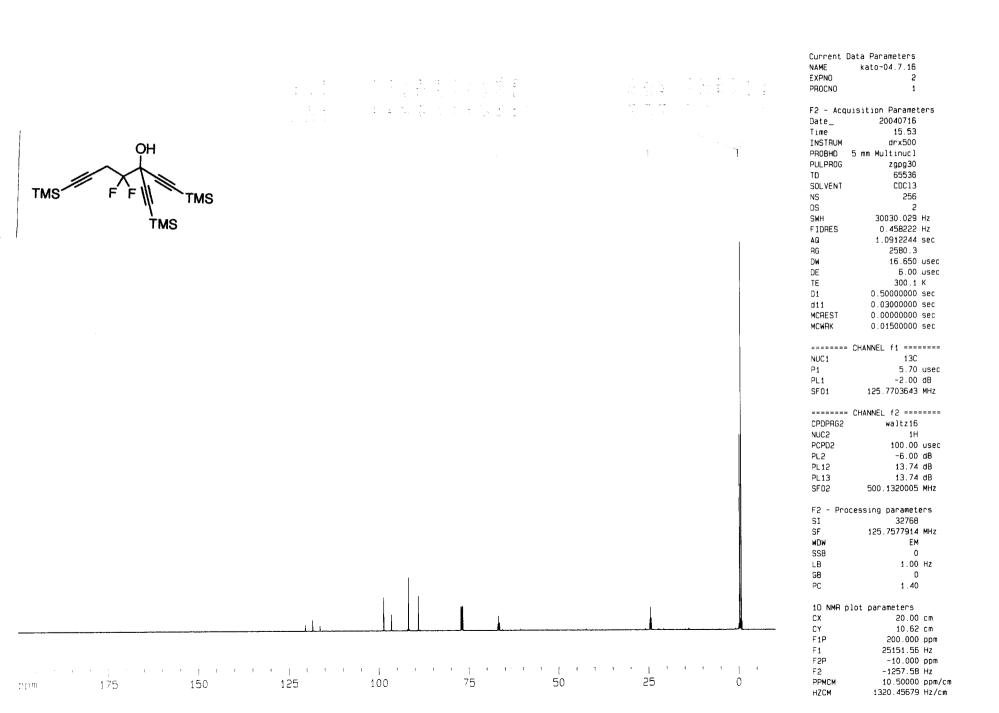
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<u>1.051</u> 2.259

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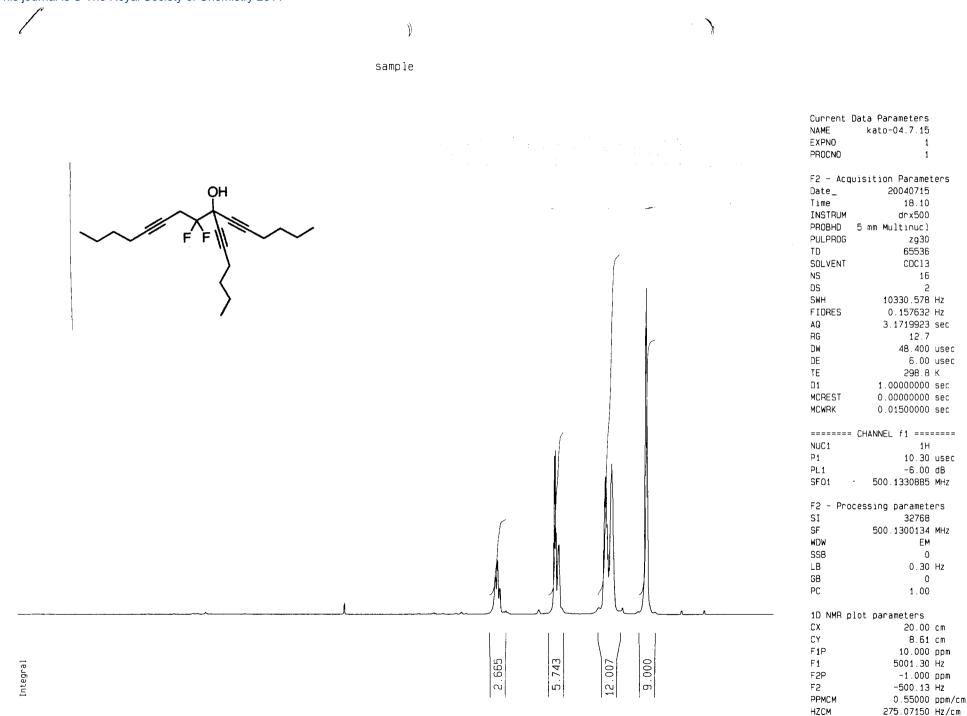
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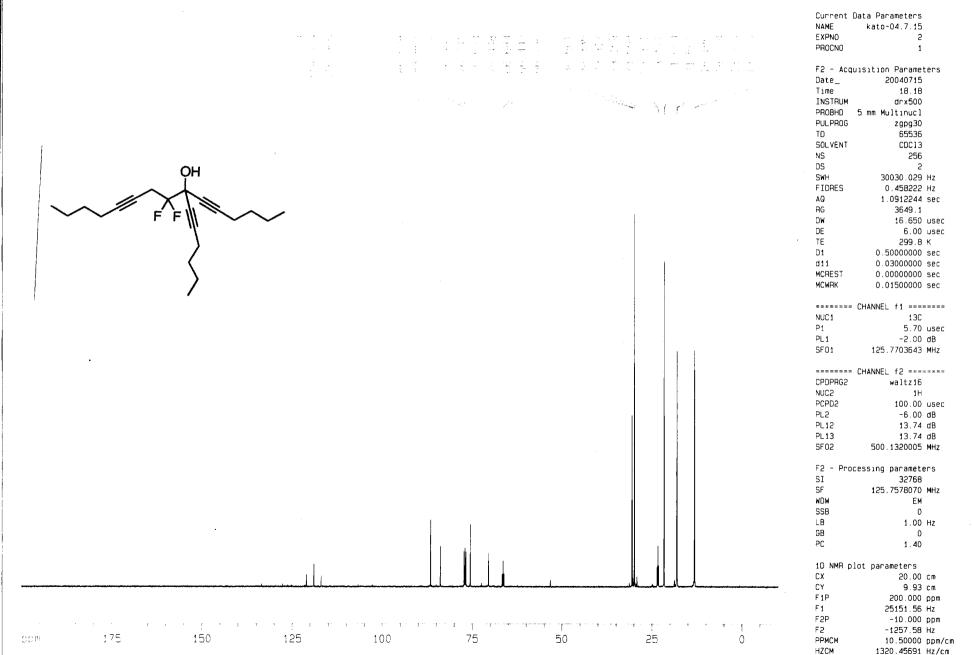
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HZCM

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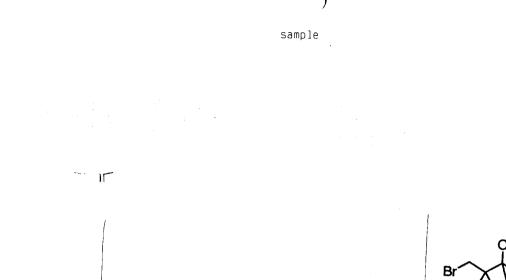
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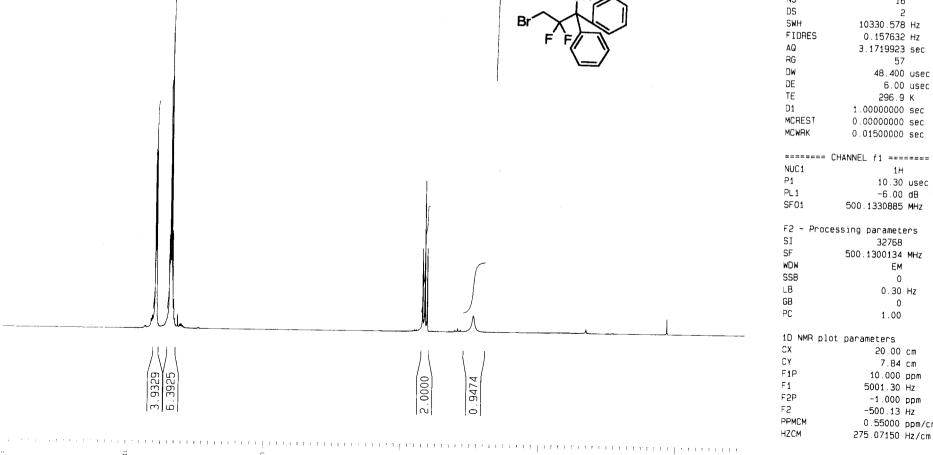
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NAME kato-04.10.22 EXPNO 1 PROCNO 1 F2 - Acquisition Parameters Date_ 20041022 Time 15.45 INSTRUM drx500 PROBHD 5 mm Multinucl PULPROG 2q30 TD 65536 SOLVENT CDC13 NS 16 DS 2 SWH 10330.578 Hz FIDRES 0.157632 Hz AQ 3.1719923 sec RG 57 DW 48.400 usec DE 6.00 usec ΤE 296.9 К D1 1.00000000 sec MCREST 0.00000000 sec MCWRK 0.01500000 sec ======= CHANNEL f1 ======== NUC1 1H Ρ1 10.30 usec PL1 -6.00 dB SF01 500.1330885 MHz F2 - Processing parameters SI 32768 SF 500.1300134 MHz WDW EM SSB 0 LВ 0.30 Hz GB 0 PC 1.00 1D NMR plot parameters СХ 20.00 cm CY 7.84 cm F1P 10.000 ppm F1 5001.30 Hz F2P -1.000 ppm F2 -500.13 Hz PPMCM 0.55000 ppm/cm

Current Data Parameters



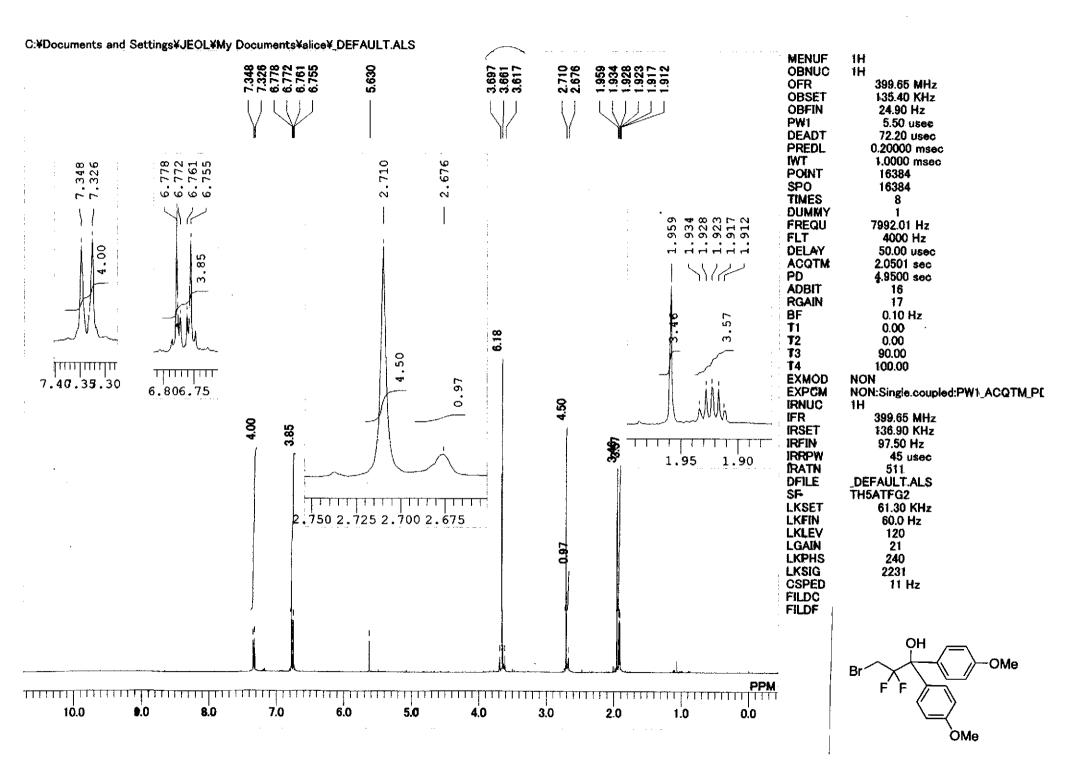
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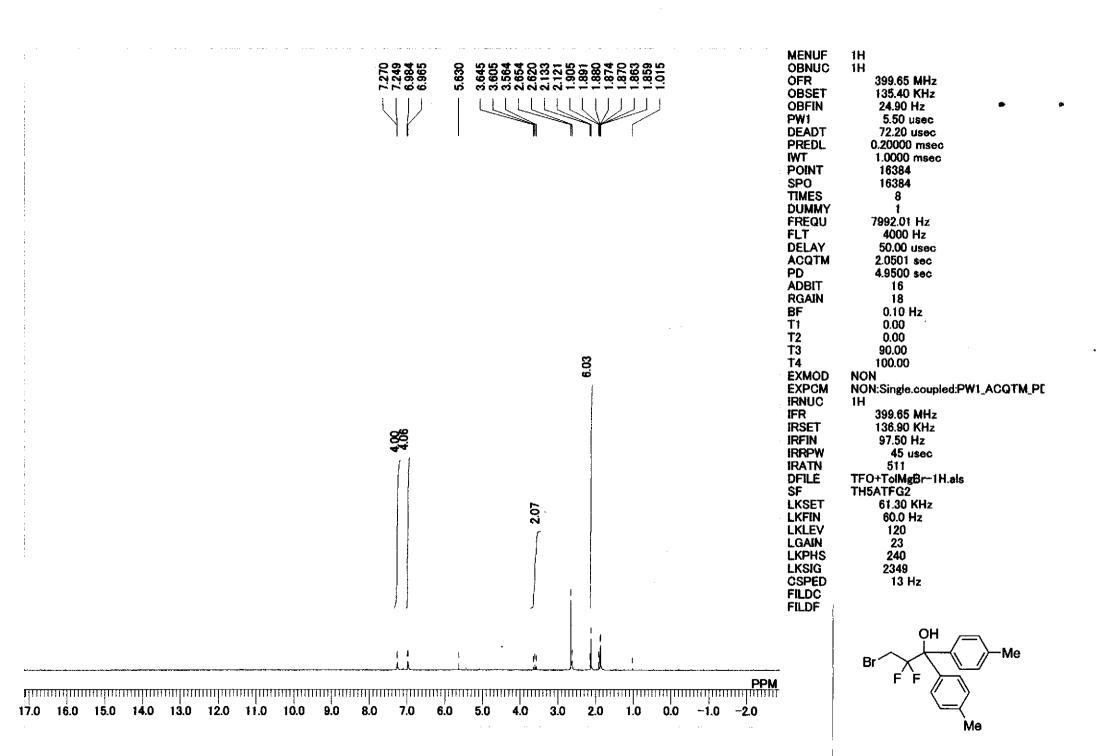
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	Current Data Parameters NAME kato-04.10.22 EXPNO 2 PROCNO 1 F2 - Acquisition Parameters Date_ 20041022 Time 15.53
Br F F	INSTRUM drx500 PROBHD 5 mm Multinuc1 PULPROG 2gpg30 TD 65536 SOLVENT CDC13 NS 2256 DS 2 SWH 30030.029 Hz FIDRES 0.458222 Hz AQ 1.0912244 sec AQ 1.0912244 sec AQ 3649.1 DW 16.650 usec DE 6.00 usec TE 297.9 K D1 0.5000000 sec d11 0.0300000 sec
	MCWRK 0.01500000 sec CHANNEL f1 = NUC1 13C P1 5.70 usec PL1 -2.00 dB SF01 125.7703643 MHz
	F2 - Processing parameters SI 32768 SF 125.7578015 MHz WDW EM SSB 0 LB 1.00 Hz GB 0 PC 1.40 1D NMR plot parameters CX 20.00 cm CY 10.11 cm
1 ' ' ' 1 ' ' ' ' ' ' 150 100 50	F1P 200.000 ppm F1 25151.56 Hz F2P -10.000 ppm F2 -1257.58 Hz PPMCM 10.50000 ppm/cm HZCM 1320.45691 Hz/cm

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				PW1 DEADT PREDL IWT POINT SPO TIMES DUMMY FREQU FLT DELAY ACQTM PD ADBIT RGAIN BF T1 T2 T3 T4 EXMOD EXPCM IRNUC IFR IRSET IRFIN IRRPW IRATN DFILE SF LKSET LKSET LKFIN LKLEV LGAIN LKPHS LKSIG CSPED FILDC	6.20 usec 19.00 usec 0.20000 msec 32768 32768 32768 20000 1 27118.64 Hz 13550 Hz 14.80 usec 1.2083 sec 1.7920 sec 16 23 0.10 Hz 0.00 0.00 90.00 100.00 BCM Bilevel.complete.decoupling:Set_IRRF 1H 399.65 MHz 124.00 KHz 10500.00 Hz 45 usec 511 TFO-AnisMgBr=13C(20100302).als TH5ATFG2 61.30 KHz 60.0 Hz 120 23 240 627 14 Hz
1	. .			FILDF	Br OH OMe



- 208.390	139.944 138.273 129.472 128.303	23.25 23.25 23.119 23.136 23.749 23.749 23.749 23.749 23.749 23.749 23.749 23.749 23.749 23.749 21.064 21.064	MENUF OBNUC OFR OBSET OBFIN PW1	13C 13C 100.40 MHz 125.00 KHz 10500.00 Hz 6.20 usec
	Y Y		DEADT PREDL IWT POINT SPO TIMES	19.00 usec 0.20000 msec 1.0000 msec 32768 32768 20000
		· · · · · · · · · · · · · · · · · · ·	DUMMY FREQU FLT DELAY ACQTM PD ADBIT	1 27118.64 Hz 13550 Hz 14.80 usec 1.2083 sec 1.7920 sec
			ADBIT RGAIN BF T1 T2 T3 T3 T4	16 24 0.10 Hz 0.00 0.00 90.00 \$00.00
			EXMOD EXPCM IRNUC IFR IRSET IRFIN	BCM Bilevel.complete.decoupling:Set_IRRF TH 399.65 MHz 124.00 KHz 10500.00 Hz
			IRFIN IRRPW IRATN DFILE SF LKSET LKSET	45 usec 511 TFO+ToIMgBr~13C.als TH5ATFG2 61.30 KHz 60.0 Hz
			LKLEV LGAIN LKPHS LKSIG CSPED	60.0 Hz 120 23 240 1132 13 Hz
			FILDC FILDF	OHMe
220.0 210.0 200.0 190.0 180.0 1		РРМ 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0.0		

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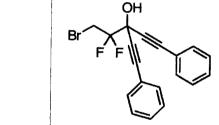
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Current Data Parameters NAME kato-05.2.17 EXPNO 1 PROCNO 1 F2 - Acquisition Parameters Date_ 20050217 Time 17.31 INSTRUM drx500 PROBHD 5 mm Multinucl PULPROG zg30 TD 65536 SOLVENT CDC13 NS 16 DS 2 SWH 10330.578 Hz FIDRES 0.157632 Hz AQ 3.1719923 sec RG 128 D₩ 48.400 usec DE 6.00 usec ΤE 295.7 K D1 1.00000000 sec d11 0.03000000 sec MCREST 0.00000000 sec MCWRK 0.01500000 sec ======= CHANNEL f1 ======= NUC1 1H P1 10.30 usec PL1 -6.00 dB SF01 500.1330885 MHz ====== CHANNEL f2 ======== CPDPRG2 NUC2 off PCPD2 100.00 usec PL2 120.00 dB PL12 120.00 dB PL13 120.00 dB SF02 500.1330885 MHz F2 - Processing parameters SΙ 32768 SF 500.1300129 MHz WDW ЕM SSB 0 ∟В 1.00 Hz GB 0 PC 1.00 1D NMR plot parameters СХ 20.00 cm ĊΥ 7.63 cm F1P 10.000 ppm 5001.30 Hz E1 F2P -1.000 ppm

F2

PPMCM

HZCM

0

-500.13 Hz

275.07150 Hz/cm

0.55000 ppm/cm

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			Current Data Parameters NAME kato-05.2.17 EXPNO 2 PROCNO 1
		Br + F + F + F + F + F + F + F + F + F +	F2 - Acquisition Parameters Date_ 20050217 Time 17.41 INSTRUM drx500 PROBHD 5 mm Multinucl PULPROG zgpg30 TD 65536 SOLVENT CDC13 NS 256 DS 2 SWH 30030.029 Hz FIDRES 0.458222 Hz AQ 1.0912244 sec RG 3649.1 DW 16.650 usec DE 6.00 usec TE 296.8 K D1 0.5000000 sec d11 0.3000000 sec MCREST 0.01500000 sec MCREST 0.01500000 sec P1 5.70 usec PL1 -2.00 dB SF01 125.7703643 MHz ETE 29DPR62 Waltz16 NUC2 NUC2 1H PCPD2 100.00 usec PL2 -6.00 dB PL12 13.74 dB
			PL13 13.74 dB SF02 500.1320005 MHz F2 - Processing parameters SI 32768 SF 125.7577987 MHz WDW EM SSB 0 LB 1.00 Hz GB 0 PC 1.40
r 1 - 1 - 1 - 1 - 1 - 1 r 175 - 150		25 0	1D NMR plot parameters CX 20.00 cm CY 10.21 cm F1P 200.000 ppm F1 25151.56 Hz F2P -10.000 ppm F2 -1257.58 Hz PPMCM 10.50000 ppm/cm HZCM 1320.45679 Hz/cm

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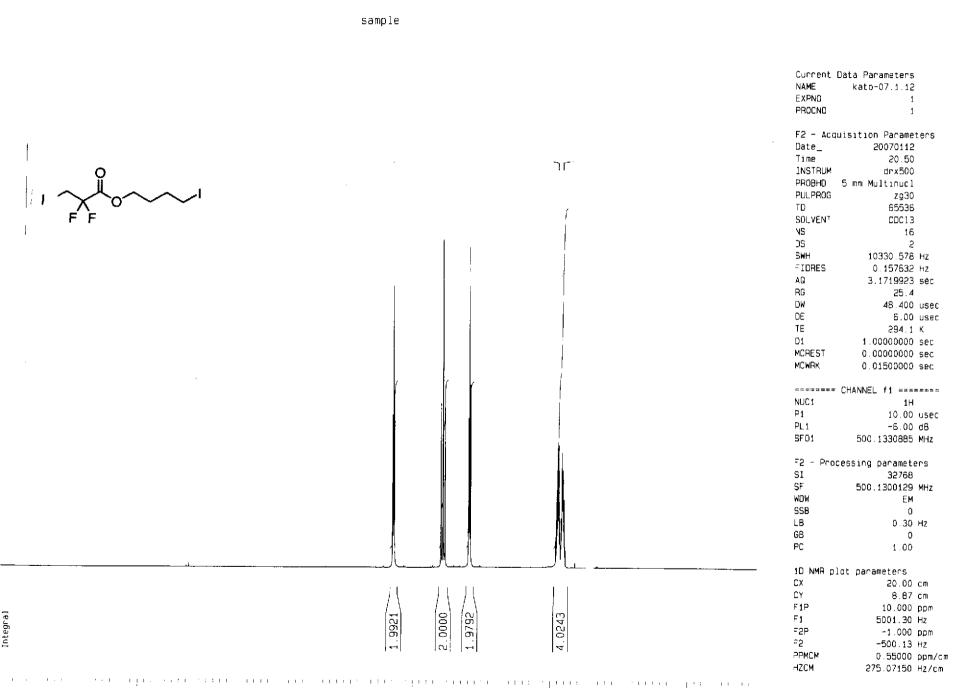
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			Current Data Paramet NAME kato-06.1 EXPNO PROCNO	
Br Br			F2 - Acquisition Par Date_ 20060 Time 16 INSTRUM dry PROBHD 5 mm Multin PULPROG 2 TD 65 SOLVENT CC NS DS SWH 10330 FIDRES 0.157 AQ 3.1719 RG DW 48 DE 6 TE 22 D1 1.00000 MCREST 0.00000	rameters 0111 5.36 x500
				1H 0.30 usec 5.00 dB
			SF 500.1300 WDW SSB LB 00 GB PC 1	2768 D131 MHz EM 0.30 Hz 0 1.00
	2.0000 1.9865	4.0760	CY 9 F1P 10 F1 5001 F2P -1 F2 -500 PPMCM 0.55	ers 0.00 cm 0.78 cm 0.000 ppm 1.30 Hz 0.000 ppm 0.13 Hz 5000 ppm/cm 7150 Hz/cm

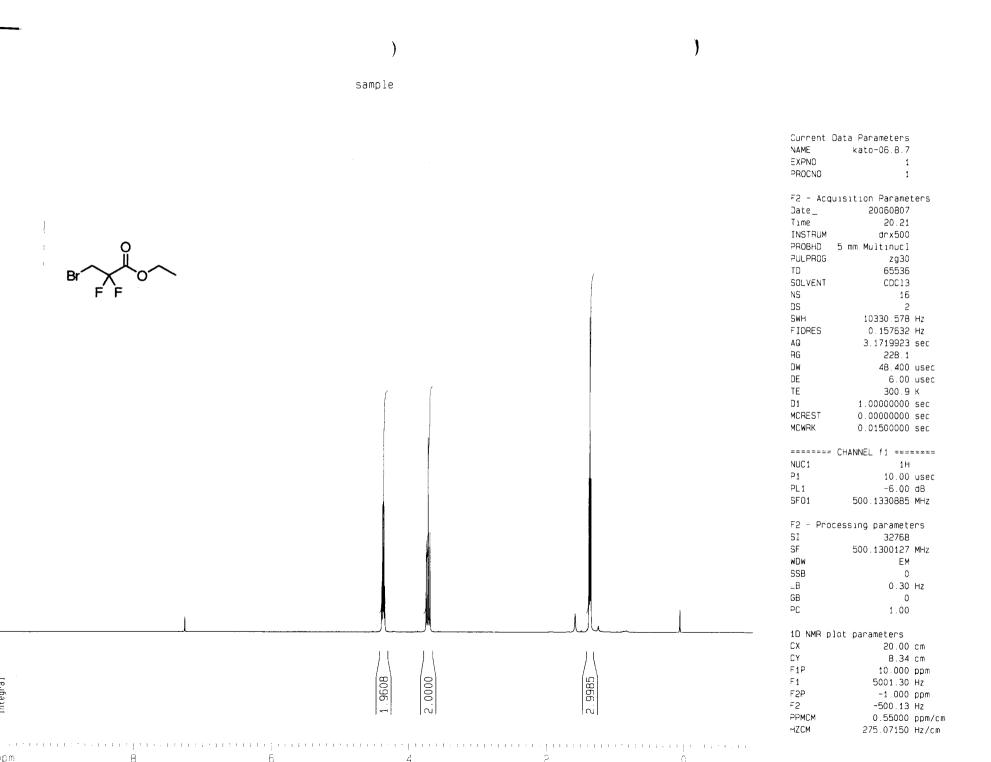
Current Data Parameters NAME kato-06.1.11 EXPNO 2 PROCNO 1 F2 - Acquisition Parameters Date_ 20060111 16.44 drx500 Time INSTRUM Ηz Ηz sec usec Jsec sec

	PROBHD 5 mm Multinu	
	PUL PROG zgpg	
	TD 655	536
	- SOLVENT CDC	213
0		256
0	DS	2
	SWH 30030.0	
F F l	40 1.09122	
	RG 3649	
		550 usec
	DE 6.	.00 usec
		4.2 K
	D1 0.500000	
	d11 0.030000	
	MCWRK 0.015000	DOO sec
	######## CHANNEL f1 =	******
	NUC1 1	13C
	P1 5.	.70 usec
		.00 dB
	SF01 125.77036	
	5.01 125.77050	
	SERVICE F2 =	
	CPDPRG2 waltz	
	NUC2	1H
	PCPD2 100.	.00 usec
		.00 dB
		.74 dB
		.74 dB .74 dB
	SF02 500.13200	DOS MHZ
	F2 - Processing param	neters
	, SI 327	
	SF 125.7579	
		EM
	SSB	0
		.00 Hz
	GB	0
	PC 1.	. 40
	1D NMR plot parameter	~ S
A REAL AND A		.00 cm
ne ne servente en		.92 cm
we have been been and the method of the method of the second state of the method of the second state of the se		
		000 ppm
	F1 25151.	
	F2P -10.0	000 ppm
алар алар такаралар (такаралар) 179 — 189 — 125 — 100 — 75	F2 -1257.	
17: 18) 125 100 75		000 ppm/cm
	HZCM 1320.456	579 Hz/cm



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Current Data Parameters NAME kato-07.1.12 EXPNO 2 PROCNO 1 F2 - Acquisition Parameters Date_ 20070112 20.5B Time INSTRUM dr x500 PROBHD 5 mm Multinucl PULPROG zgpg30 TD 65536 SOLVENT CDC13 256 NS DS 2 S₩H 30030.029 Hz FIDRES 0.458222 Hz AQ 1.0912244 sec RG 1448.2 D₩ 16.650 Lsec ΩE 6.00 usec. TE 294.5 K 01 0.50000000 sec di1 0.03000000 sec MCREST 0.00000000 sec MCWRK 0.01500000 sec HERE CHANNEL f1 HERE VUCi 13C 21 11.00 usec PL1 -3.00 dB 125.7703643 MHz SF01 ---- CHANNEL f2 -----CPDPRG2 waltz16 NUC2 1H PCP02 100.00 usec PL2 -6.00 dB PL12 17.00 dB PL13 19.00 dB SF02 500.1320005 MHz F2 - Processing parameters 51 32768 SF 125.7578271 MHz WDW ЕМ ۵ SSØ LB 1.00 Hz 68 Q PC 1.40 10 NMR plot parameters СX 20.00 cm CΥ 9.44 cm ° 1P 219.089 ppm F1 27552.18 Hz F2P -19.703 ppm . . **. .** 2 I i F2 -2477.85 Hz 75 200 175 150 125 100 50 2ä ppm 0 PPMCM 11.93963 ppm/cm HZCM 1501.50159 Hz/cm

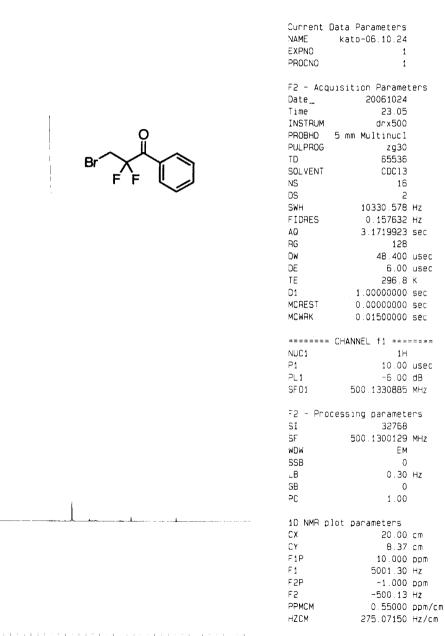


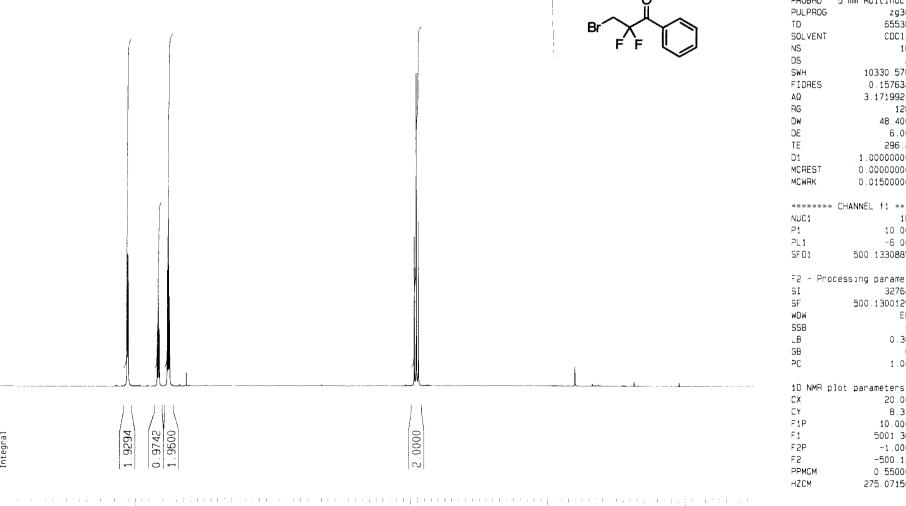
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					PROCNO	1
					F2 - Acq	uisition Parameter
					Date_	20060807
					Time	20.3B
					INSTRUM	drx500
					PROBHD	5 mm Multinucl
					PULPROG	zgpg30
					TD SOLVENT	65536
	-				NS	CDC13
	0				DS	512
					SWH	2
Br	$\sim \sim \sim \sim$				FIDRES	30030.029 H
DI					AQ	0.458222 H.
					AG	1.0912244 si
					DW	2048
					DE	16.650 u: 6.00 u:
					TE	301.2 K
					D1	0.50000000 s
					d11	0.03000000 s
					MCREST	0.00000000 s
					MCWRK	0.01500000 s
					=========	CHANNEL f1 =====
					NUC1	130
					P1	11.00 us
			I		PL1	-3.00 dE
					SF01	125.7703643 MH
					3====22	CHANNEL f2 =====
					CPDPRG2	waltz16
					NUC2	1H
					PCPD2	100.00 us
					PL2	-6.00 df
					PL12	17.00 di
					PL13	19.00 df
					SF02	500.1320005 M
					F2 - Proc	essing parameters
				1	SI	32768
					SF	125.7577905 M∤
				l í	WDW	EM
					SSB	0
					LB	1.00 Hz
					GB - PC	0
		I				1.40
	L		l Í		10 NMA pl	ot parameters
	an a		the second se		CX	20.00 cm
			and the second		CY	9.89 cr
					F1P	219.381 pp
					F1	27588.83 Hz
	175 150	125 100	75 50		F2P F2	-19.412 pp
200			75 50	25 0		-2441.20 Hz

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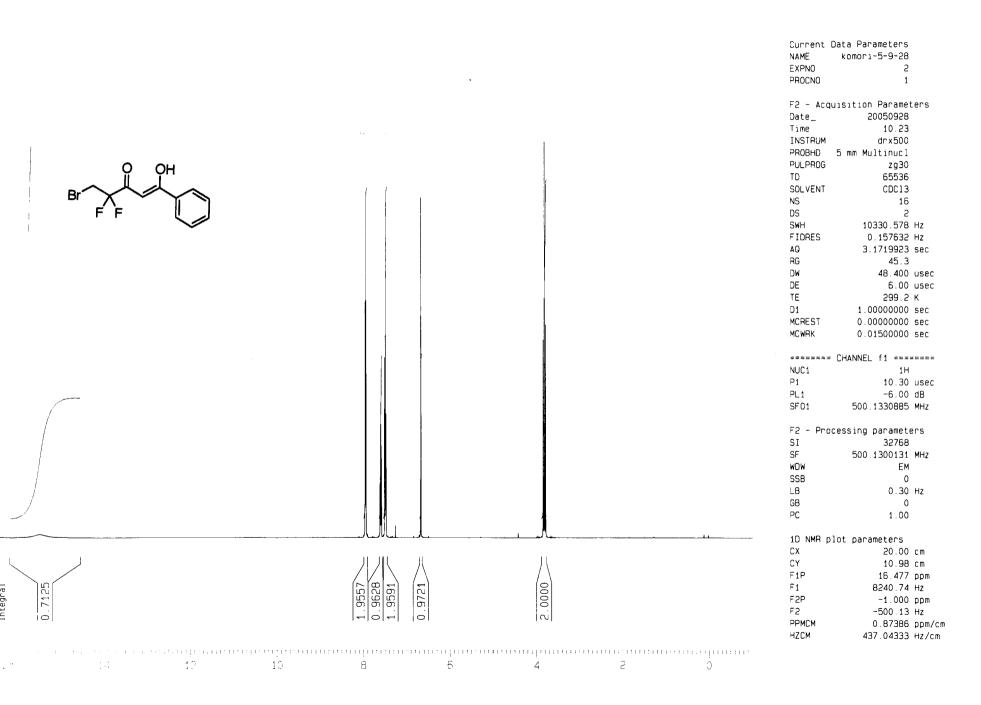
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		Br	NAME EXPNO PROCNO F2 - Acqu Date Time INSTRUM PROBHD PULPROG TD SOLVENT NS DS SWH FIDRES	ata Parameters kato-06.10.24 2 1 1sition Parameters 20061024 23.13 drx500 5 mm Multinucl 2gpg30 65536 CDC13 256 2 30030.029 Hz 0.458222 Hz
		F F	A0 RG DW DE TE D1 d11 MCREST MCWRK	1.0912244 sec 1625.5 16.650 usec 297.1 K 0.5000000 sec 0.0300000 sec 0.01500000 sec CHANNEL f1 ====== 13C 11.00 usec -3.00 dB 125.7703643 MHz
				CHANNEL f2 ======= walt216 1H 100.00 usec ~6.00 dB 17.00 dB 19.00 dB 500.1320005 MHz
	1		SI SF WDW SSB LB GB PC	essing parameters 32768 125.7577332 MHz EM 0 1.00 Hz 0 1.40 pt parameters
рот 200 175 150	, , , , , , , , , , , , , , , , , , ,		CX CY F1P F1 F2P	ot parameters 20.00 cm 8.95 cm 219.359 ppm 27586.10 Hz -19.434 ppm -2443.93 Hz 11.93963 ppm/cm 1501.50146 Hz/cm

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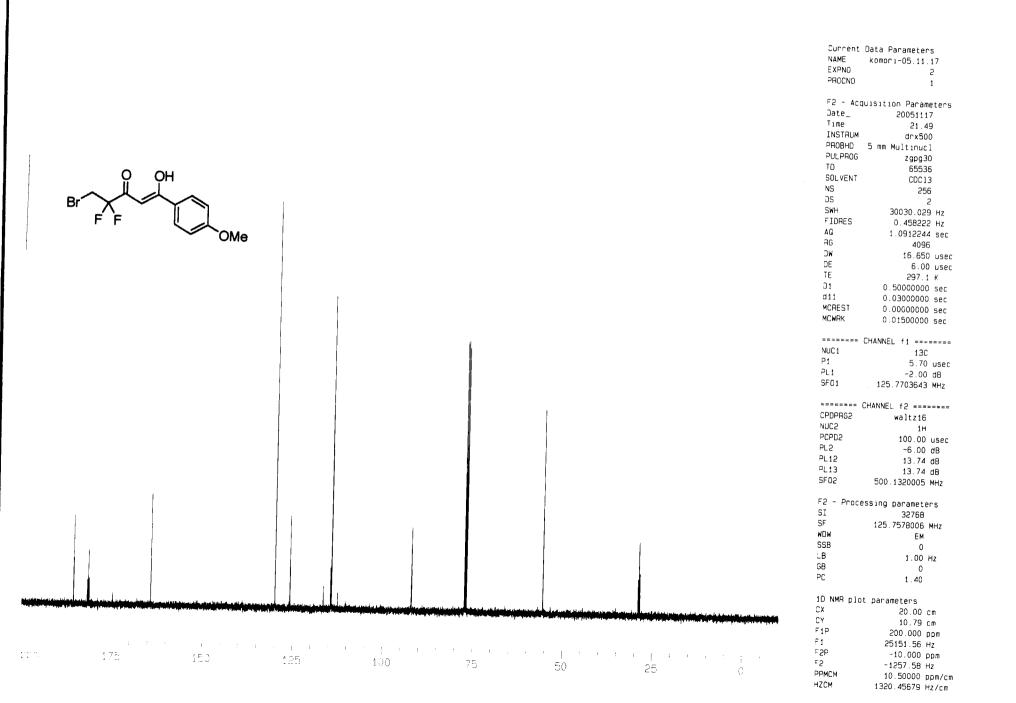


			NAME K EXPNO PROCNO F2 - Acquis Date_ Time INSTRUM PROBHD 5 PULPROG TD SOLVENT NS SWH FIDRES A0 A6 DW DE TE D1 d11 MCREST MCWRK	<pre>ca Parameters comori-5-9-28 3 1 sition Parameters 20050928 10.35 drx500 mm Multinucl zgpg30 65536 CDC13 256 2 30030.029 Hz 0.458222 Hz 1.0912244 sec 3649.1 16.650 usec 6.00 usec 299.9 K 0.5000000 sec 0.03000000 sec 0.0000000 sec 0.01500000 sec 34NNEL f1 ======</pre>
			NUC1 P1	13C 5.70 usec
			PL1 SF01	~2.00 dB 125.7703643 MHz
			CPDPAG2 NUC2 PCPD2 PL2 PL12 PL13 SF02	HANNEL f2 ======= waltz16 1H 100.00 usec -6.00 dB 13.74 dB 13.74 dB 500.1320005 MHz
			F2 - Proces SI	sing parameters 32768
			SF WDW	125.7578024 MHz EM
			SSB LB	0 1.00 Hz
			GB PC	0
	11			parameters
www.			CX	20.00 cm 10.41 cm
			F1P F1	219.286 ppm 27576.91 Hz
			F2P F2	-19.507 ppm
:::	176 15 0	125 100 75 50 25 0	F2 PPMCM HZCM	-2453.12 Hz 11.93963 ppm/cm 1501.50159 Hz/cm

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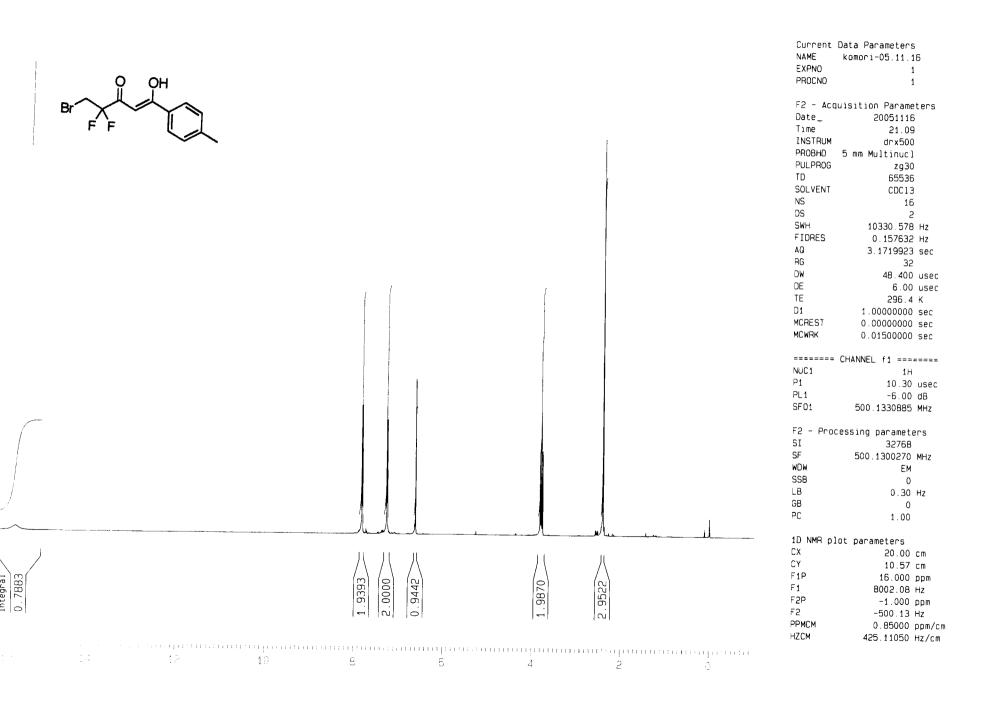
		Current Data Parameters NAME komori-05.11.17 EXPNO 1 PROCNO 1
$ \begin{array}{c} & & \\ & \\ & \\ & \\ & \\ & \\ & \\ & \\ & \\ $		F2 - Acquisition Parameters Date_ 20051117 Time 21.41 INSTRUM drx500 PROBHD 5 mm Multinucl PULPROG zg30 TD 65536 SOLVENT CDC13 NS 16 DS 2 SWH 10330.578 FIDRES 0.157632 AQ 3.1719923 AQ 3.1719923 DW 48 AQ 3.1719923 DW 48 DE 6.00 DE 6.00 DE 6.00 DE 6.00 DE 296.3 MCREST 0.0000000 MCREST 0.001500000 MCWRK 0.01500000 MCWRK 0.01500000 SF01 500.1330885 SF01 500.1330885 SI 32768
		SF 500.1300131 MHz WDW EM SSB 0 LB 0.30 Hz GB 0 PC 1.00 1.00 1.00 1.00
Integral 0.7864	<u> 1.9886</u> <u> 2.0000</u> <u> 0.9932</u> <u> 2.0713</u>	1D NMR plot parameters CX 20.00 cm CY 11.02 cm F1P 16.000 ppm F1 8002.08 Hz F2P -1.000 ppm F2 -500.13 Hz PPMCM 0.85000 ppm/cm HZCM 425.11047 Hz/cm
14 12 10 10 10 10 10 10 10 10 10 10 10 10 10	' ! ' ' I ' ' I ' ' I ' ' I ' ' I ' ' I ' ' I ' ' I ' ' I ' ' I ' ' I ' ' I ' ' I ' ' I ' ' I ' ' I ' ' I ' ' I 8 6 4 2 0	120H 423.1104/ HZ/CM

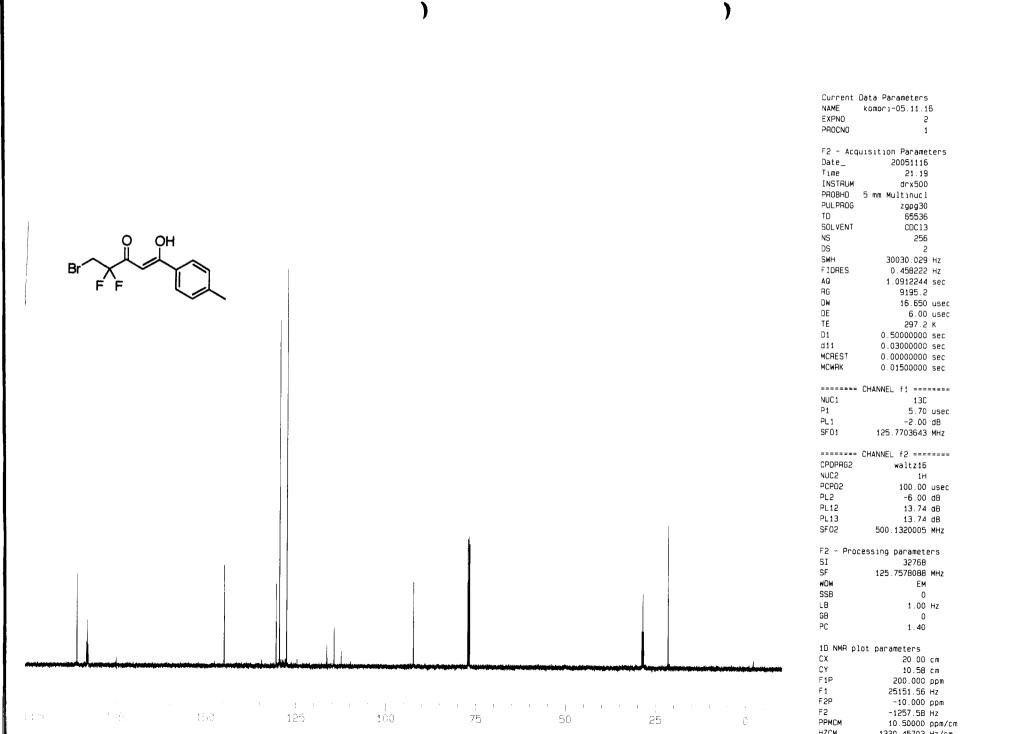
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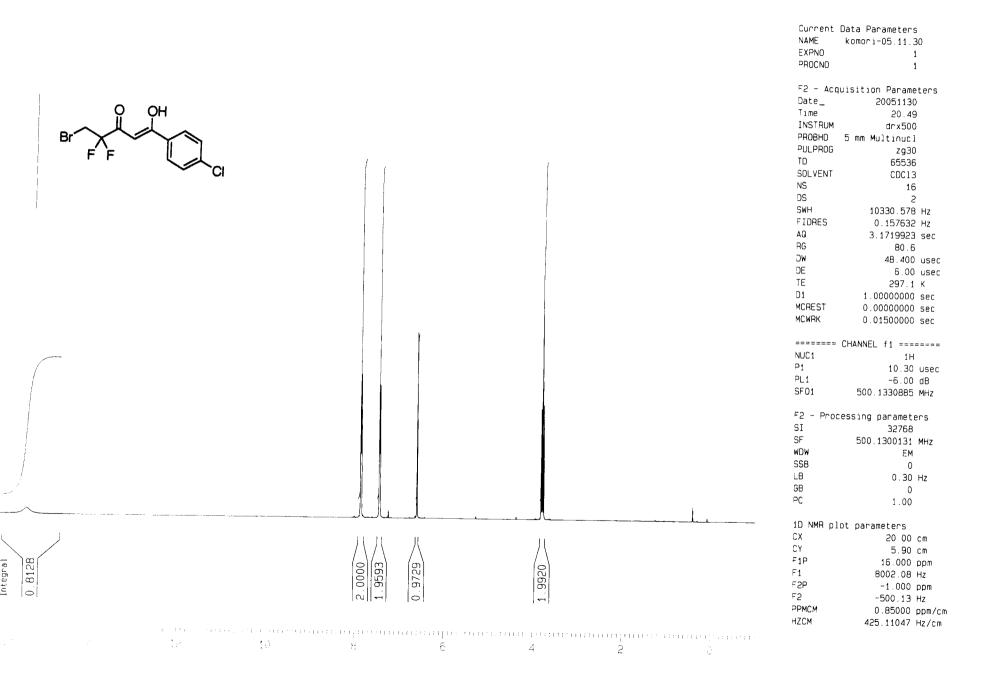


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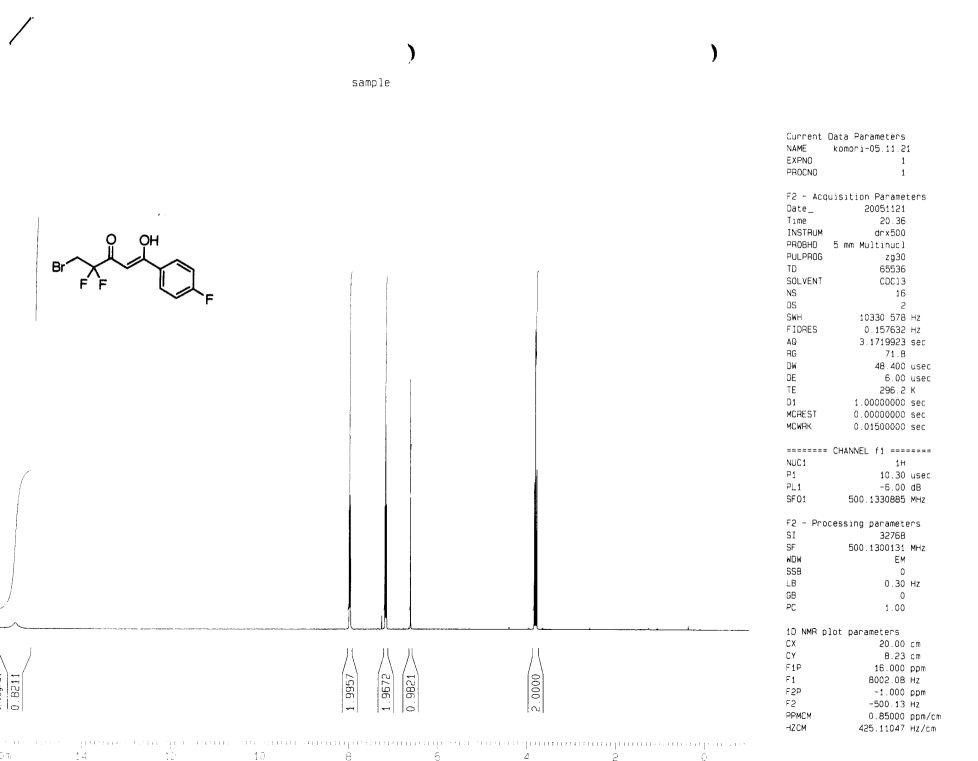
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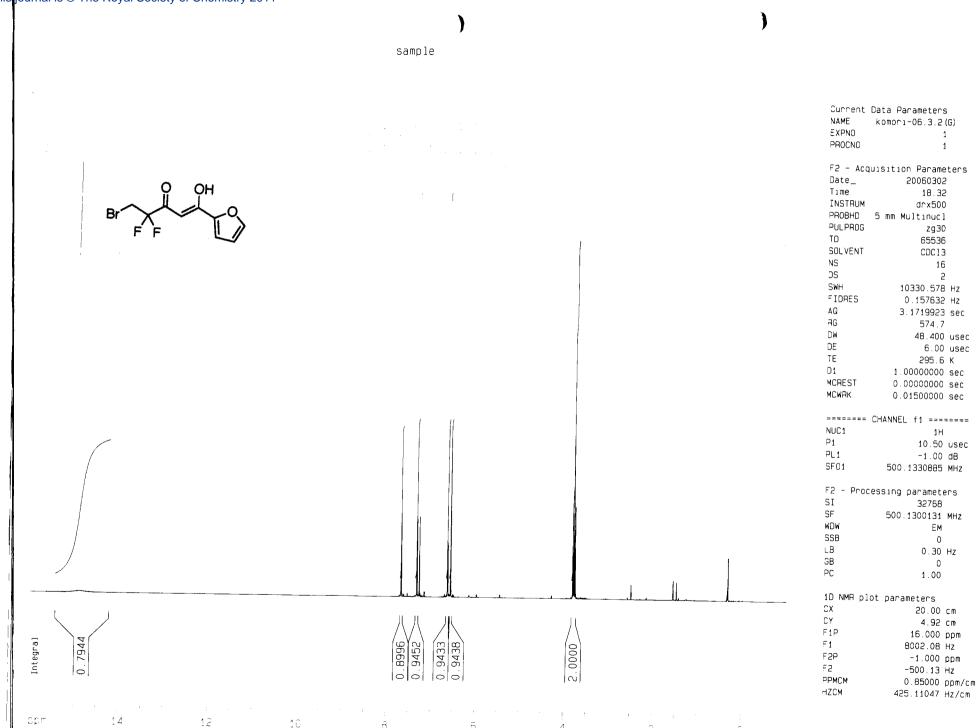
$Br \xrightarrow{O}_{F} \xrightarrow{O}_{F} \xrightarrow{O}_{F} \xrightarrow{O}_{C}$		Current Data Parameters NAME komori-05.11.30 EXPNO 2 PROCNO 1 F2 - Acquisition Parameters Date 20.58 INSTRUM drx500 PROBHD 5 mm Multinuc1 PULPROG 2gpg30 TD 65536 SOLVENT CDC13 NS 256 DS 2 SWH 30030.029 Hz FIDRES 0.458222 Hz AQ 1.0912244 sec RG 4597.6 DW 16.650 usec DE 6.00 usec TE 297.8 K D1 0.5000000 sec MCHEST 0.000000 sec MCMEST 0.000000 sec MCWRK 0.01500000 sec NUC1 13C P1 5.70 usec PL1 -2.00 dB
		SF01 125.7703643 MHz CPDPR62 waltz16 NUC2 1H PCPD2 100.00 usec PL2 -6.00 dB PL13 13.74 dB SF02 500.1320005 MHz F2 - Processing parameters SI 32768 SF 125.7577987 MHz WDW EM SSB 0 LB 1.00 Hz GB 0 PC 1.40
nakon a porten andre andre andre andre porten andre andre andre andre and andre and and and and and and and and 1986 - 1980 - 1980 - 1980 - 1980 - 1980 - 1980 - 1980 - 1980 - 1980 - 1980 - 1980 - 1980 - 1980 - 1980 - 1980 - 1	анна и и и и и и и и и и и и и и и и и и	CX 20.00 cm CY 10.55 cm F1P 200.000 ppm F1 25151.56 Hz F2P ~10.000 ppm F2 ~1257.58 Hz PPMCM 10.50000 ppm/cm HZCM 1320.45679 Hz/cm

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Current Data Parameters



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$Br \underbrace{F}_{F} \underbrace{F}_{F} \underbrace{O}_{F} \underbrace{O}_{F} \underbrace{O}_{F}$			Current Data Parameters NAME komori-05.11.21 EXPNO 2 PROCNO 1 F2 - Acquisition Parameters Date_ 20051121 Time 20.44 INSTRUM drx500 PROBHD 5 mm Multinucl PULPROG zgpg30 TD 65536 SOLVENT CDC13 NS 256 DS 2 SWH 30030.029 Hz FIDRES 0.458222 Hz AQ 1.0912244 sec RG 3649.1 DW 16.650 usec DE 6.00 usec TE 296.9 K D1 0.5000000 sec d11 0.0300000 sec MCREST 0.000000 sec MCWRK 0.01500000 sec
			P1 5.70 usec PL1 -2.00 dB SF01 125.7703643 MHz CHANNEL f2 ======= CPDPR62 waltz16 NUC2 1H PCPD2 100.00 usec PL2 -6.00 dB PL12 13.74 dB PL13 13.74 dB SF02 500.1320005 MHz F2 - Processing parameters SI 32768 SF 125.7577978 MHz WDW EM SSB 0 LB 1.00 Hz GB 0 PC 1.40
			CX 20.00 cm CY 10.19 cm F1P 200.000 ppm F1 25151.56 Hz F2P -10.000 ppm F2 -1257.58 Hz PPMCM 10.50000 ppm/cm HZCM 1320.45679 Hz/cm



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Current Data Parameters NAME komor:-06.3.11-G EXPNO 5 PROCNO 1 F2 - Acquisition Parameters Date_ 20060311 Time 13.10 INSTRUM drx500 PROBHD 5 mm Multinucl PULPROG zgpg30 TD 65536 SOLVENT CDC13 NS 256 DS 2 SWH 30030.029 Hz FIDRES 0.458222 Hz AQ 1.0912244 sec RG 2580.3 ЭW 16.650 usec DE 6.00 usec ΤE 298.0 К **D1** 0.50000000 sec d11 0.03000000 sec MCREST 0.00000000 sec MCWRK 0.01500000 sec ----- CHANNEL f1 +-+--** NUC1 1 3C 21 9.00 usec PL1 -1.00 dB SF01 125.7703643 MHz ====== CHANNEL f2 ======= CPDPRG2 waltz16 NUC2 1H PCPD2 100.00 usec PL2 -6.00 dB PL12 18.58 dB PL13 19.00 dB SF02 500.1320005 MHz F2 ~ Processing parameters SI 32768 SF 125.7577923 MHz WDW EM SSB 0 LB 1.00 Hz GB 0 PC 1.40 1D NMR plot parameters СХ 20.00 cm CY 10.17 cm F1P 200.000 ppm F1 25151.56 Hz F2P -10.000 ppm T. F2 -1257.58 Hz

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PPMCM

нгсм

10.50000 ppm/cm

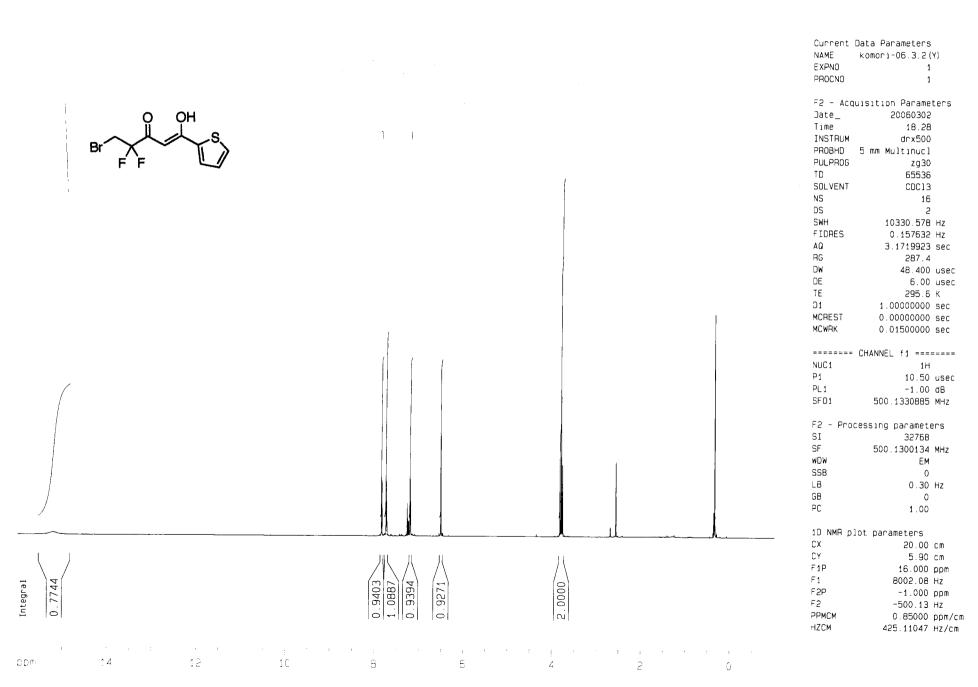
1320.45679 Hz/cm

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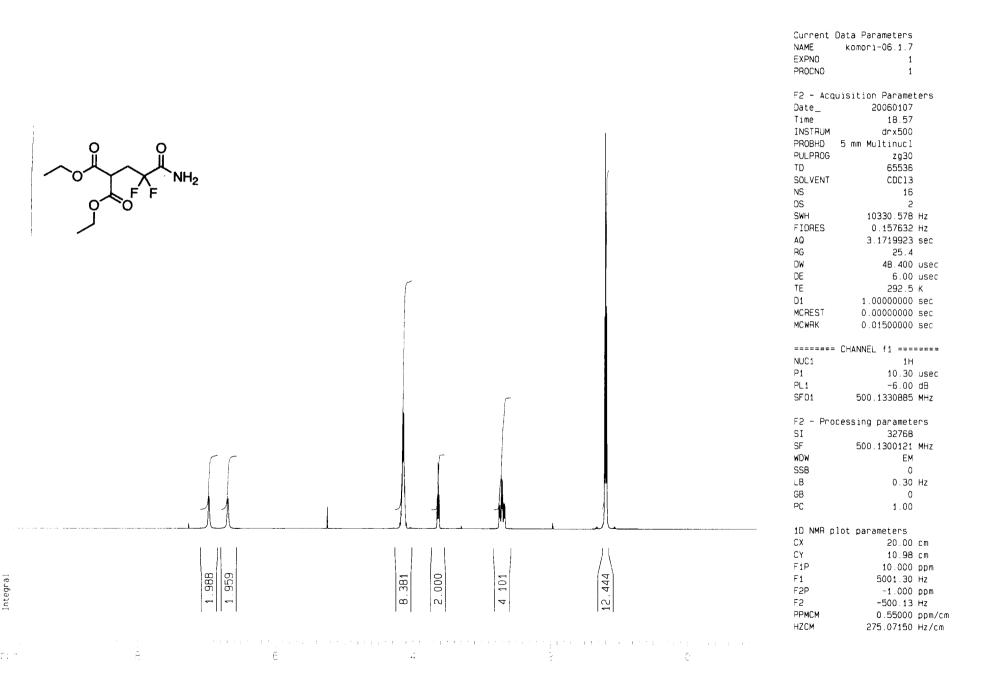
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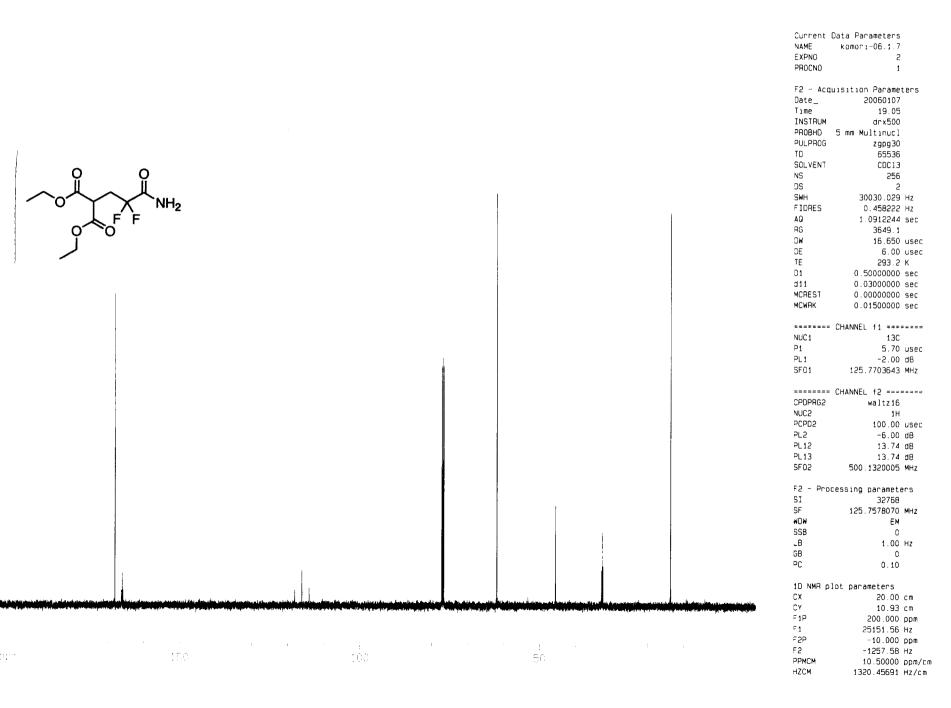
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		EXPN0 1 PROCN0 1
		F2 - Acquisition Parameters
		Date_ 20060311
		Time 13.20
		INSTRUM drx500
		PROBHD 5 mm Multinucl
		PULPROG zgpg30
		TD 65536
		SOLVENT CDC13
		NS 256
ООН		DS 2
		SWH 30030.029 Hz
		FIDRES 0.458222 Hz
	\	AG 1.0912244 sec RG 3649.1
FF		
		DW 16.650 usec DE 6.00 usec
		TE 298.1 K
		D1 0.5000000 sec
		d11 0.03000000 sec
		MCREST 0.0000000 sec
		MCWRK 0.01500000 sec
		======= CHANNEL f1 =======
		NUC1 13C
		P1 9.00 usec
		PL1 -1.00 dB
		SF01 125.7703643 MHz
		======= CHANNEL f2 ========
		CPDPRG2 waltz16
		NUC2 1H
		PCPD2 100.00 usec
		PL2 -6.00 dB
		PL12 18.58 dB
		PL13 19.00 dB
		SF02 500.1320005 MHz
		F2 - Processing parameters
		SI 32768
		SF 125.7577951 MHz
		WDW EM
1		SSB 0
1		LB 1.00 Hz
		GB 0
		PC 1.40
		1D NMR plot parameters
		1D NMR plot parameters CX 20.00 cm
, u, a.,		СХ 20.00 cm СУ 11.10 cm
nan anna an a' suara khara na Dinan can an bhara an an an		СХ 20.00 cm СУ 11.10 cm рак и мар и и и и и и и и и и и и и и и и и и и
y na na dana sa ang sa ang Ta ang sa gang sa gang sa gang sa gang sa ang sa		СХ 20.00 cm СУ 11.10 cm F1P 200.000 ppm F1 25151.56 Hz
y any starting site in the second starting of the second starting		CX 20.00 cm CY 11.10 cm CY 11.10 cm F1P 200.00 pm F1 25151.56 Hz F2P -10.000 pm
		CX 20.00 cm CY 11.10 cm CY 11.10 cm F1P 200.000 pm F1 25151.56 Hz F2P -10.000 pm

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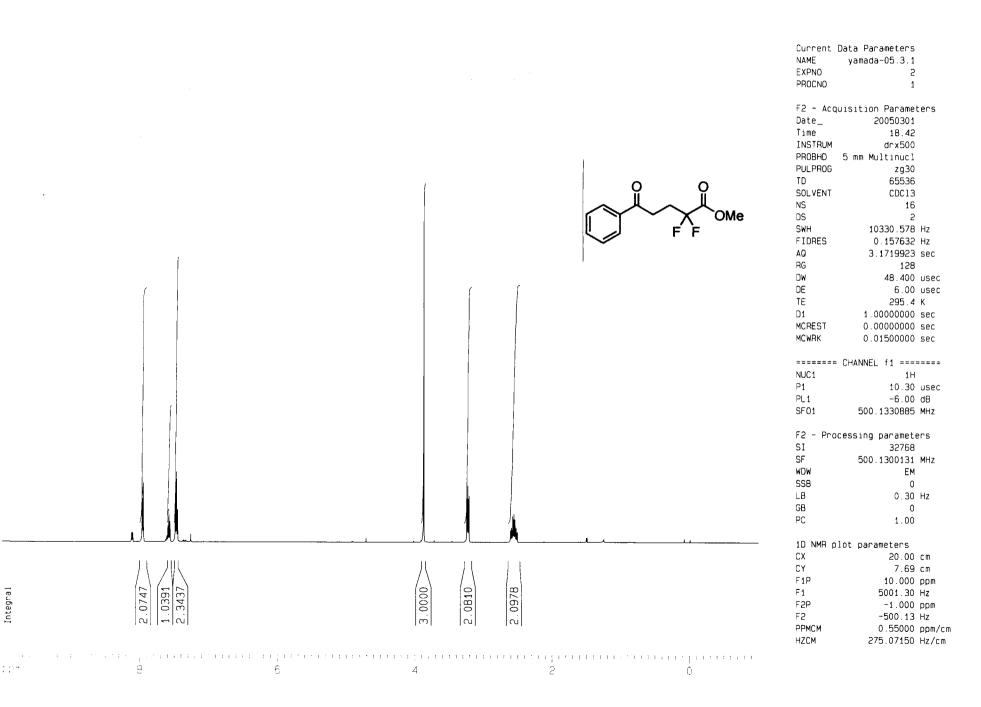




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Current Data Parameters NAME yamada-05.3.1 EXPN0 3 PROCNO 1 F2 - Acquisition Parameters Date_ 20050301 18.51 Time INSTRUM drx500 PROBHD 5 mm Multinucl PULPROG zgpg30 TD 65536 SOLVENT CDC13 256 NS DS 2 SWH 30030.029 Hz FIDRES 0.458222 Hz AQ 1.0912244 sec **`OMe** RG 3649.1 FF D₩ DE 16.650 usec 6.00 usec ΤE 296.4 K D1 0.50000000 sec 0.03000000 sec d11 MCREST 0.00000000 sec MCWRK 0.01500000 sec ======= CHANNEL f1 ======= NUC1 13C P1 5.70 usec PL1 -2.00 dB SF01 125.7703643 MHz ======= CHANNEL f2 ======== CPDPRG2 waltz16 NUC2 1H PCPD2 100.00 usec PL2 -6.00 dB PL12 13.74 dB PL13 13.74 dB SF02 500.1320005 MHz F2 - Processing parameters SI 32768 SF 125.7577987 MHz WDW ЕM SSB 0 LB 1.00 Hz GB 0 PC 1.40 1D NMA plot parameters СХ 20.00 cm CY 6.51 cm F1P 210.000 ppm F1 26409.14 Hz F2P -10.000 ppm E i E F2 -1257.58 Hz C PPMCM 11.00000 ppm/cm HZCM 1383.33569 Hz/cm

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		Current Data Parameters
		NAME yamada-05.3.2
		EXPNO 2
		PROCNO 1
		F2 - Acquisition Parameters
		Date20050302
		Time 15.15
		INSTRUM drx500 PROBHD 5 mm Multinucl
		PULPROG Zg30
		TD 65536
-		SOLVENT CDC13
o o		NS 16
		DS 2
OMe		SWH 10330.578 Hz
F F		FIDRES 0.157632 Hz
eO		AQ 3.1719923 sec
eO		RG 228.1
		DW 48.400 usec
		DE 6.00 usec
		ТЕ 295.5 К
		D1 1.00000000 sec
		MCREST 0.00000000 sec
		MCWRK 0.01500000 sec
		====== CHANNEL f1 =======
		NUC1 1H
		NUC1 1H P1 10.30 usec
		NUC1 1H P1 10.30 usec PL1 -6.00 dB
		NUC1 1H P1 10.30 usec
		NUC1 1H P1 10.30 usec PL1 -6.00 dB SF01 500.1330885 MHz F2 - Processing parameters
		NUC1 1H P1 10.30 usec PL1 -6.00 dB SFD1 500.1330885 MHz F2 - Processing parameters SI 32768
		NUC1 1H P1 10.30 usec PL1 -6.00 dB SFD1 500.1330885 MHz F2 - Processing parameters SI 32768 SF 500.1300106 MHz
		NUC1 1H P1 10.30 usec PL1 -6.00 dB SFD1 500.1330885 MHz F2 - Processing parameters SI 32768 SF 500.1300106 MHz WDW EM
		NUC1 1H P1 10.30 usec PL1 -6.00 dB SF01 500.1330885 MHz F2 Processing parameters SI 32768 SF 500.1300106 MHz WDW EM SSB 0
		NUC1 1H P1 10.30 usec PL1 -6.00 dB SF01 500.1330885 MHz F2 Processing parameters SI 32768 SF 500.1300106 MHz WDW EM SSB 0 LB 0.30 Hz
		NUC1 1H P1 10.30 usec PL1 -6.00 dB SF01 500.1330885 MHz F2 Processing parameters SI 32768 SF 500.1300106 MHz WDW EM SSB 0 LB 0.30 Hz GB 0
		NUC1 1H P1 10.30 usec PL1 -6.00 dB SFD1 500.1330885 MHz F2 Processing parameters SI 32768 SF 500.1300106 MHz WDW EM SSB 0 LB 0.30 Hz GB 0 PC 1.00
		NUC1 1H P1 10.30 usec PL1 -6.00 dB SFD1 500.1330885 MHz F2 - Processing parameters SI SF 500.1300106 MHz WDW EM SSB 0 LB 0.30 Hz GB 0 PC 1.00
		NUC1 1H P1 10.30 usec PL1 -6.00 dB SFD1 500.1330885 MHz F2 - Processing parameters SI 32768 SF 500.1300106 MHz WDW EM SSB 0 LB 0.30 Hz GB 0 PC 1.00 LL 1D NMR plot parameters CX 20.00 cm
		NUC1 1H P1 10.30 usec PL1 -6.00 dB SFD1 500.1330885 MHz F2 Processing parameters SI 32768 SF 500.1300106 MHz WDW EM SSB 0 LB 0.30 Hz GB 0 PC 1.00 L 10 NMR plot parameters CX 20.00 cm CY 7.17 cm
		NUC1 1H P1 10.30 usec PL1 -6.00 dB SFD1 500.1330885 MHz F2 Processing parameters SI 32768 SF 500.1300106 MHz WDW EM SSB 0 LB 0.30 Hz G8 0 PC 1.00 L 10 NMR plot parameters CX 20.00 cm CY 7.17 cm F1P 10.000 ppm
		NUC1 1H P1 10.30 usec PL1 -6.00 dB SFD1 500.1330885 MHz F2 Processing parameters SI 32768 SF 500.1300106 MHz WDW EM SSB 0 LB 0.30 Hz GB 0 PC 1.00 L 10 NMR plot parameters CX 20.00 cm CY 7.17 cm F1P 10.000 ppm F1 5001.30 Hz
		NUC1 1H P1 10.30 usec PL1 -6.00 dB SFD1 500.1330885 MHz F2 Processing parameters SI 32768 SF 500.1300106 MHz WDW EM SSB 0 LB 0.30 Hz GB 0 PC 1.00 1D NMR plot parameters CX CY 7.17 cm F1P 10.000 ppm F1 5001.30 Hz F2P -1.000 ppm
<u>2.0000</u> <u>1.983</u>	5.9022	NUC1 1H P1 10.30 usec PL1 -6.00 dB SF01 500.1330885 MHz F2 Processing parameters SI 32768 SF 500.1300106 MHz WDW EM SSB 0 LB 0.30 Hz GB 0 PC 1.00 1D NMR plot parameters CX 20.00 cm CY 7.17 cm F1P 10.000 ppm F1 5001.30 Hz F2P -1.000 ppm F2 -500.13 Hz
<u> </u>	5.9022	NUC1 1H P1 10.30 usec PL1 -6.00 dB SF01 500.1330885 MHz F2 Processing parameters SI 32768 SF 500.1300106 MHz WDW EM SSB 0 LB 0.30 Hz GB 0 PC 1.00 1D NMR plot parameters CX 20.00 cm CY 7.17 cm F1P 10.000 ppm F1 5001.30 Hz F2P -1.000 ppm F2 -500.13 Hz PPMCM 0.55000 ppm/cm
		NUC1 1H P1 10.30 usec PL1 -6.00 dB SFD1 500.1330885 MHz F2 Processing parameters SI 32768 SF 500.1300106 MHz WDW EM WDW EM SSB 0 LB 0.30 Hz GB 0 PC 1.00 L 1D NMR plot parameters CX 20.00 cm CY 7.17 cm F1P 10.000 ppm F1 5001.30 Hz F2P -1.000 ppm F1 5001.30 Hz F2P -500.13 Hz PPMCM 0.55000 ppm/cm HZCM 275.07150 Hz/cm
		NUC1 1H P1 10.30 usec PL1 -6.00 dB SFD1 500.1330885 MHz F2 Processing parameters SI 32768 SF 500.1300106 MHz WDW EM WDW EM SSB 0 LB 0.30 Hz GB 0 PC 1.00 L 1D NMR plot parameters CX 20.00 cm CY 7.17 cm F1P 10.000 ppm F1 5001.30 Hz F2P -1.000 ppm F1 5001.30 Hz F2P -500.13 Hz PPMCM 0.55000 ppm/cm HZCM 275.07150 Hz/cm

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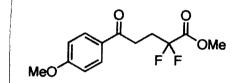
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Current Data Parameters NAME yamada-05.3.2 EXPNO 3 PROCNO 1 F2 ~ Acquisition Parameters Date_ 20050302 Time 15.23 INSTRUM drx500 PROBHD 5 mm Multinucl PULPROG zgpg30 TD 65536 SOLVENT CDC13 NS 256 DS 2 SWH 30030.029 Hz FIDRES 0.458222 Hz AQ 1.0912244 sec RG 3649.1 DW 16.650 usec DE 6.00 usec ΤE 296.5 K D1 0.50000000 sec d11 0.03000000 sec MCREST 0.00000000 sec MCWRK 0.01500000 sec ======= CHANNEL f1 ******* NUC1 13C P1 5.70 usec PL1 -2.00 dB SF01 125.7703643 MHz ======= CHANNEL f2 ======= CPDPRG2 waltz16 NUC2 1H PCPD2 100.00 usec PL2 -6.00 dB PL12 13.74 dB PL13 13.74 dB SF02 500.1320005 MHz F2 - Processing parameters SI 32768 SF 125.7577942 MHz WDW ЕΜ SSB 0 LB 1.00 Hz GB 0 PC 1.40 1D NMR plot parameters СХ 20.00 cm CY 10.44 cm F1P 210.000 ppm F1 26409.14 Hz F2P -10.000 ppm a to detail produce para a para an and a second second F2 -1257.58 Hz 75 50 25 0 PPMCM 11.00000 ppm/cm

HZCM

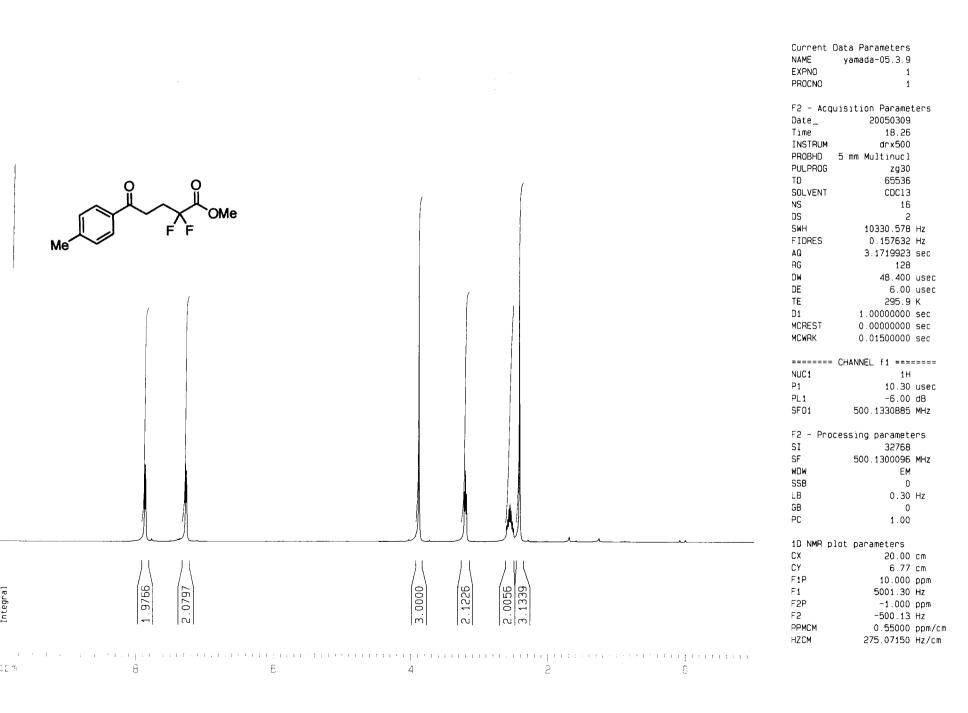
1383.33569 Hz/cm



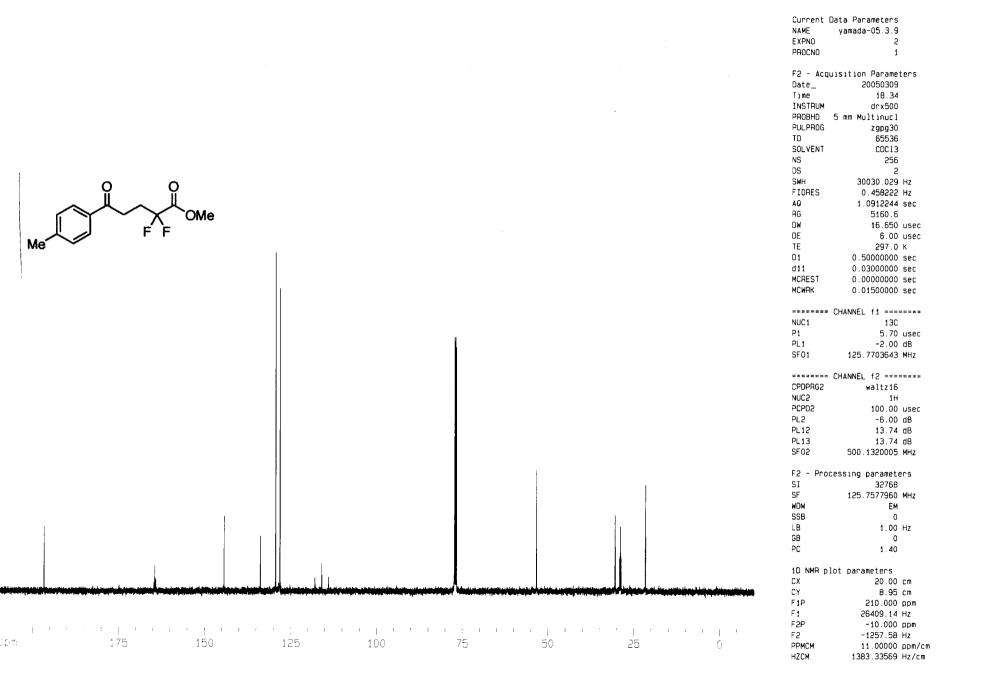
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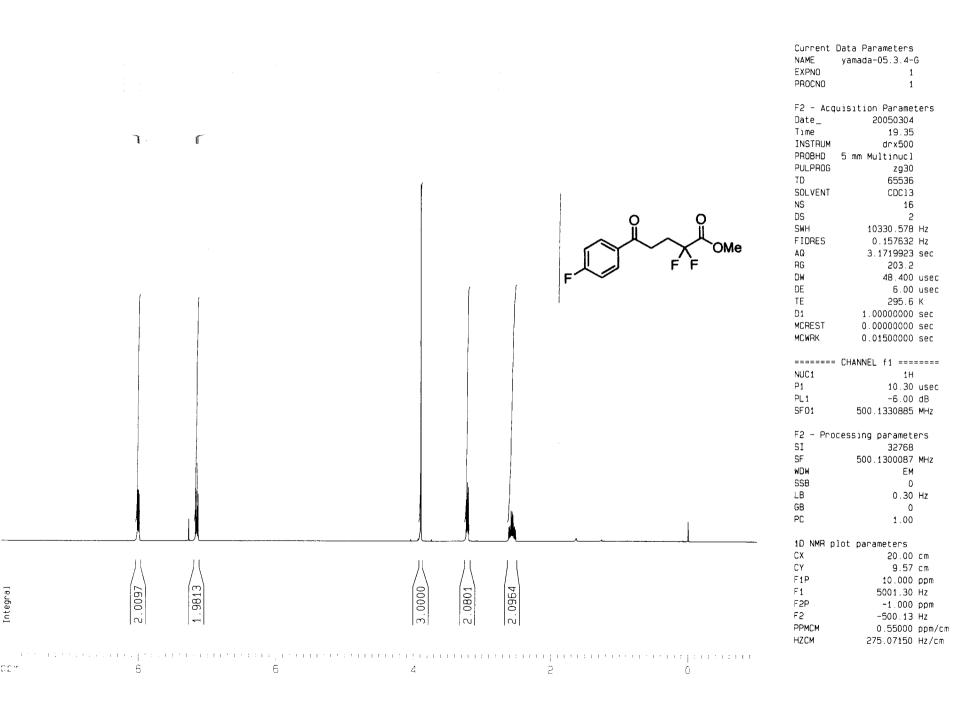
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Current Data Parameters yamada-05.3.7 NAME EXPNO 3 PROCNO 1 F2 - Acquisition Parameters Date_ 20050307 Time 19.13 INSTRUM drx500 ſ 1 PROBHD 5 mm Multinucl PULPROG zgpg30 TD 65536 SOLVENT CDC13 . NS 256 DS 2 SWH 30030.029 Hz FIDRES 0.458222 Hz AQ 1.0912244 sec RG DW DE TE 6502 16.650 usec 6.00 usec 296.8 К D1 0.50000000 sec d11 0.03000000 sec MCREST 0.00000000 sec MCWRK 0.01500000 sec ======= CHANNEL f1 ======= NUC1 130 Ρ1 5.70 usec PL1 -2.00 dB SF01 125.7703643 MHz ======= CHANNEL f2 ======== waltz16 CPDPRG2 NUC2 1H PCPD2 100.00 usec PL2 ~6.00 dB PL12 13.74 dB PL13 13.74 dB SF02 500.1320005 MHz F2 - Processing parameters SI 32768 SF 125.7577951 MHz WDW ЕM SSB 0 LB 1.00 Hz GB 0 PC 1.40 1D NMR plot parameters СХ 20.00 cm СΥ 9.99 cm F1P 210.000 ppm F 1 26409.14 Hz F2P -10.000 ppm , reacher and the construction of the second s F2 -1257.58 Hz 125 100 75 50 175 150 ppm. 25 0 PPMCM 11.00000 ppm/cm HZCM 1383.33569 Hz/cm

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Current Data Parameters NAME yamada-05.3.3-G EXPNO 1 PROCNO 1 F2 - Acquisition Parameters Date_ 20050303 Time 21.37 INSTRUM drx500 PROBHD 5 mm Multinucl PULPROG zg30 TD 65536 SOLVENT CDC13 NS 16 ОМе DS 2 SWH 10330.578 Hz FIDRES 0.157632 Hz AQ 3.1719923 sec RG 287.4 DW 48.400 usec DE 6.00 usec ΤE 295.6 К D1 1.00000000 sec MCREST 0.00000000 sec MCWRK 0.01500000 sec ======= CHANNEL f1 ======== NUC1 1H P1 10.30 usec PL1 -6.00 dB SF01 500.1330885 MHz F2 - Processing parameters SI 32768 SF 500.1300153 MHz WDW ЕM SSB 0 LВ 0.30 Hz GB 0 PC 1.00 1D NMR plot parameters СХ 20.00 cm CY 7.95 cm F1P 10.000 ppm 0.8970 0254 8449 0730 3.0000 0589 F1

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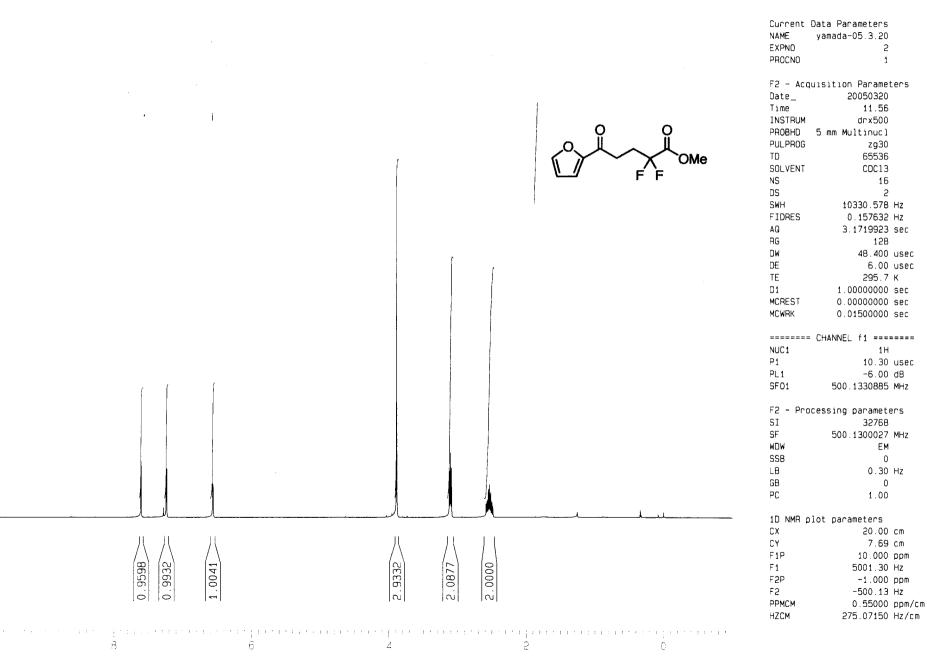
5001.30 Hz F2P -1.000 ppm F2 -500.13 Hz PPMCM 0.55000 ppm/cm HZCM 275.07150 Hz/cm

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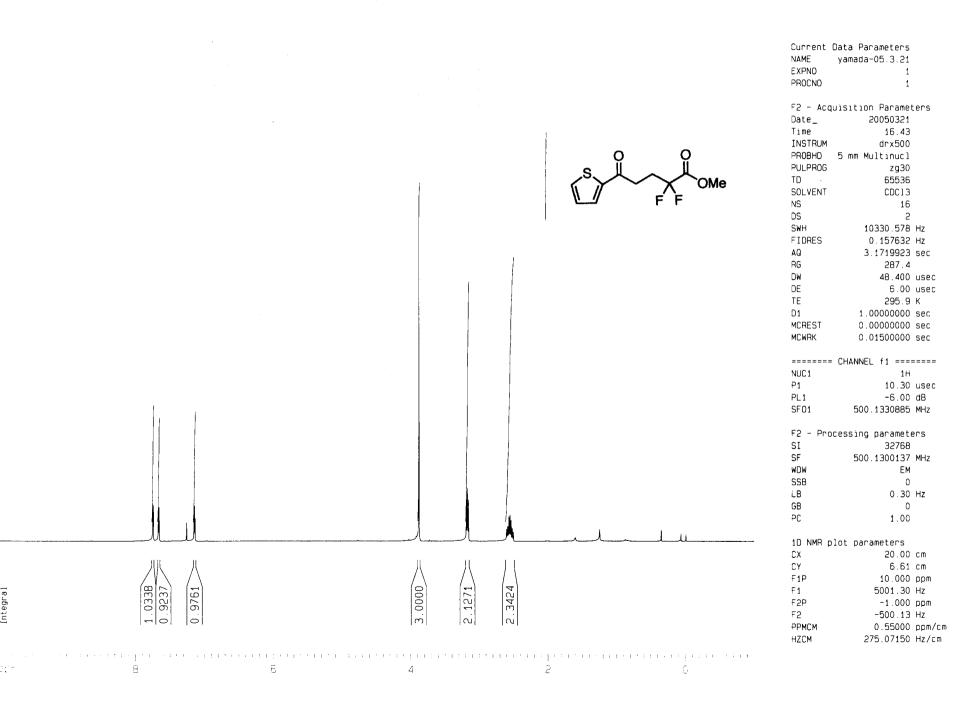
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	PROCNO 1
	F2 - Acquisition Parameters
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	Time 18.45
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	PULPROG zgpg30
	TD 65536
	SOLVENT CDC13
	NS 256 DS 2
	SWH 30030.029 Hz
	FIDRES 0.458222 Hz
	AQ 1.0912244 sec
	RG 3649.1 DW 16.650 usec
F F	DW 16.650 usec DE 6.00 usec
\sim	TE 297.1 K
	D1 0.5000000 sec
	d11 0.03000000 sec MCREST 0.00000000 sec
	MCREST 0.00000000 sec MCWRK 0.01500000 sec
	====== CHANNEL f1 ======
	NUC1 13C P1 5.70 usec
	PL1 -2.00 dB
	SF01 125.7703643 MHz
	======= CHANNEL f2 =======
	CPDPRG2 waltz16
	NUC2 1H
	PCPD2 100.00 usec
	PL2 -6.00 dB PL12 13.74 dB
	PL13 13.74 dB
	SF02 500.1320005 MHz
	F2 - Processing parameters SI 32768
	SF 125.7577969 MHz
	WDW EM
	SSB 0
	LB 1.00 Hz GB 0
	PC 1.40
	1D NMR plot parameters CX 20.00 cm
	CX 20.00 cm
	F1P 210.000 ppm
	F1 26409.14 Hz
en en en la companya de la companya	F2P -10.000 ppm F2 -1257.58 Hz
r 176 150 125 100 75 50 25 0	PPMCM 11.00000 ppm/cm
	HZCM 1383.33569 Hz/cm

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			f = f = F	Current Data Parameters NAME yamada-05.3.20 EXPNO 3 PROCNO 1 F2 - Acquisition Parameters Date_ 20050320 Time 12.04 INSTRUM drx500 PROBHD 5 mm Multinuc1 PULPROG zgpg30 TD 65536 SOLVENT CDC13 NS 256 DS 2 SWH 30030.029 Hz FIDRES 0.458222 Hz AQ 1.0912244 sec RG 9195.2 DW 16.650 usec DE 6.00 usec TE 296.8 K D1 0.5000000 sec d11 0.0300000 sec MCREST 0.001500000 sec MCREST 0.001500000 sec
				NUC1 13C P1 5.70 usec PL1 -2.00 dB SF01 125.7703643 MHz
таради и и и порта и страната с 1 - 1 - 1 - 1 - 1 - 1 - 1 - 1 150	· : · · · · · · · · · · · · · · · · · ·	аласконоронция инстриронорона I I I I I I I I I I I I I 75	serve de la construction	F1P 200.000 ppm F1 25151.56 Hz F2P -10.000 ppm F2 -1257.58 Hz PPMCM 10.50000 ppm/cm HZCM 1320.45679 Hz/cm



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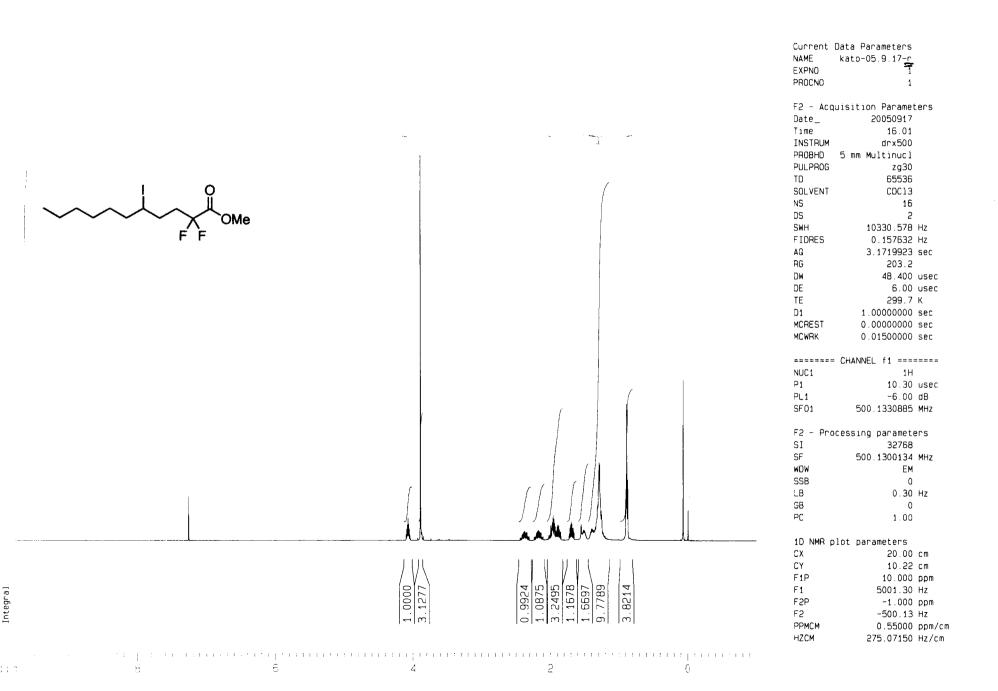
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	Current Data Parameters
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	PROCNO 1
	F2 - Acquisition Parameters
	Date20050321
	Time 16.51
	INSTRUM drx500
	PROBHD 5 mm Multinucl
	PULPROG zgpg30
`	TD 65536
	SOLVENT CDC13
i i i i i i i i i i i i i i i i i i i	NS 256
0 0	DS 2
	SWH 30030.029 Hz
	FIDRES 0.458222 Hz
	AQ 1.0912244 sec
	RG 5160.6
	DW 16.650 usec
	DE 6.00 usec
	ТЕ 297.0 K
	D1 0.5000000 sec
	d11 0.03000000 sec
	MCREST 0.0000000 sec
	MCWRK 0.01500000 sec
	====== CHANNEL f1 =======
	NUC1 13C
	P1 5.70 usec
	PL1 -2.00 dB
	SF01 125.7703643 MHz
	======= CHANNEL f2 ========
	CPDPRG2 waltz16
	NUC2 1H
	PCPD2 100.00 usec
	PL2 -6.00 dB
	PL12 13.74 dB
	PL13 13.74 dB
	SF02 500.1320005 MHz
	3F02 300.1320003 MHZ
	F2 - Processing parameters
	SI 3276B
	SF 125.7577942 MHz
	WDW EM
	SSB 0
	LB 1.00 Hz
	GB 0
	PC 1.40
	1D NMR plot parameters
	CX 20.00 cm
المارية المرابعة المرابع	CY 10.83 cm
	F1P 200.000 ppm
	F1 25151.56 Hz
	F2P -10.000 ppm
	F2 -1257.58 Hz
100 75 50 25 0	PPMCM 10.50000 ppm/cm
	HZCM 1320.45679 Hz/cm
	1204 IS20.43075 (1270)

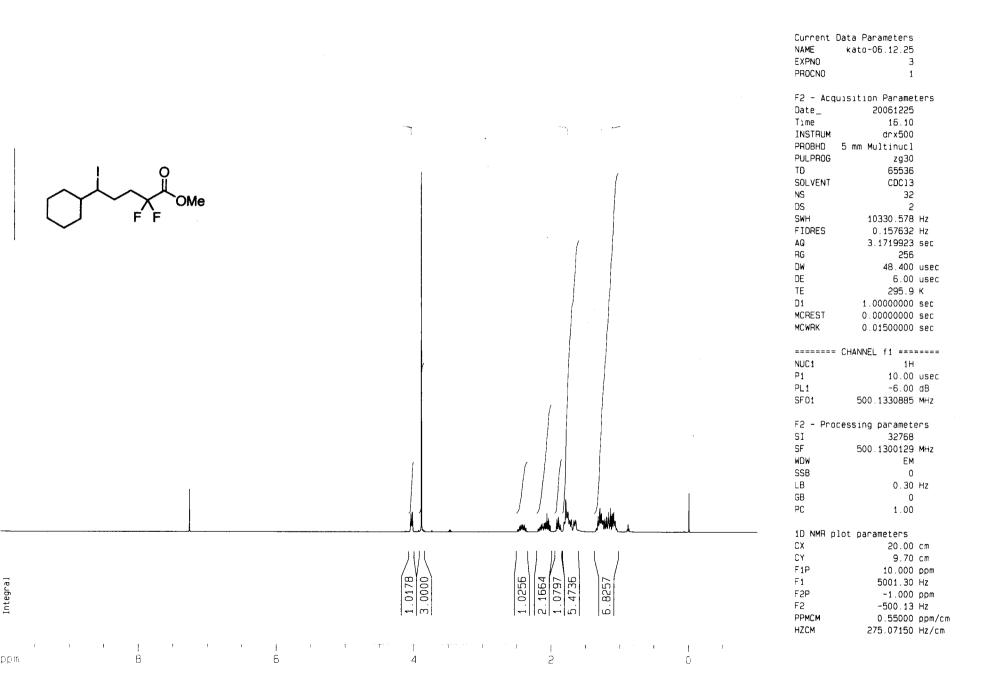
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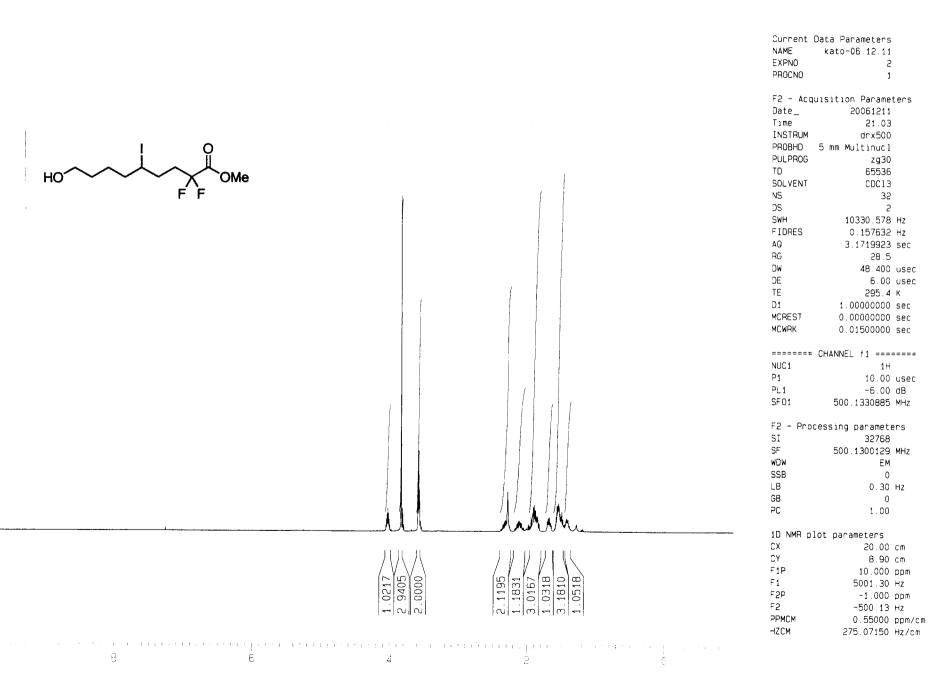
Current Data Parameters kato-06.12.25 NAME EXPNO 2 PROCNO 1 F2 - Acquisition Parameters Date_ 20061225 Time 16.04 INSTRUM drx500 PROBHD 5 mm Multinucl PULPROG zgpg30 ΤD 65536 SOLVENT CDC13 NS 256 DS 2 `OMe SWH 30030.029 Hz FIDRES 0.458222 Hz AQ 1.0912244 sec RG 5160.6 DW 16.650 usec DE 6.00 usec ΤE 296.2 к D1 0.50000000 sec d11 0.03000000 sec MCREST 0.00000000 sec MCWRK 0.01500000 sec ====== CHANNEL f1 ======= NUC1 130 P1 11.00 usec PL1 -3.00 dB SF01 125.7703643 MHz ********* CHANNEL f2 ******* waltz16 CPDPRG2 NUC2 1H PCPD2 100.00 usec PL2 -6.00 dB PL12 17.00 dB PL13 19.00 dB SF02 500.1320005 MHz F2 - Processing parameters SI 32768 SF 125.7577932 MHz WDW ЕМ SSB 0 LB 1.00 Hz GB 0 PC 1.40 1D NMR plot parameters 20.00 cm СХ CY 10.38 cm F1P 219.359 ppm F1 27586.10 Hz F2P -19.434 ppm F2 -2443.93 Hz 200 175 150 125 100 75 50 25 ppm. 0 PPMCM 11.93963 ppm/cm HZCM 1501.50134 Hz/cm

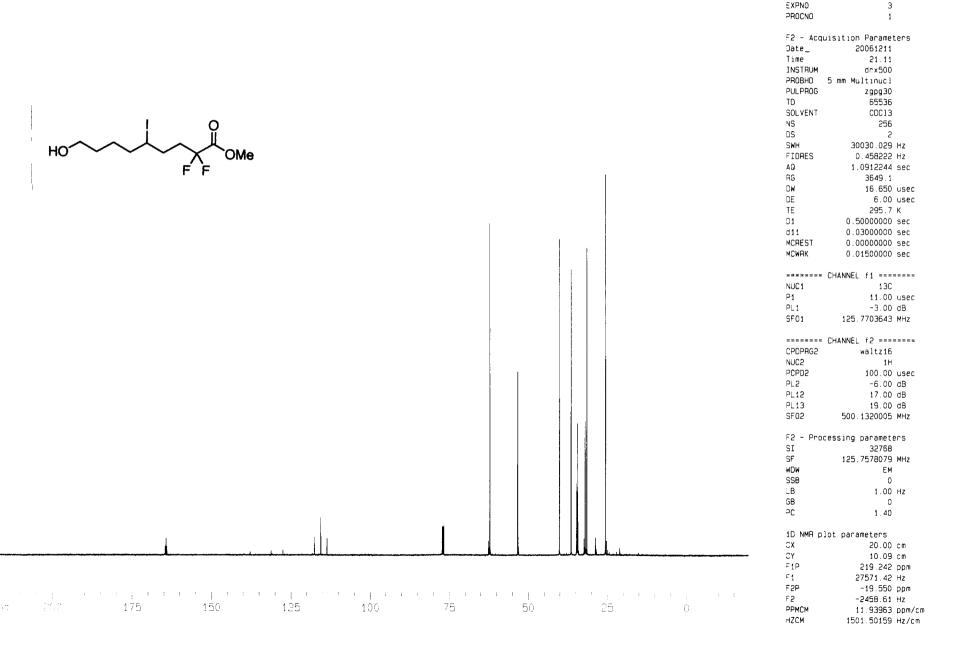
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sample



Current Data Parameters NAME kato-06.12.25 EXPNO 4 PROCNO 1 F2 - Acquisition Parameters 20061225 Date_ Time 16.23 INSTRUM drx500 PROBHD 5 mm Multinucl PULPROG zgpg30 TD 65536 SOLVENT CDC13 NS 300 DS 2 OMe SWH 30030.029 Hz FIDRES 0.458222 Hz AQ 1.0912244 sec ЯG 2896.3 DW 16.650 usec DE 6.00 usec ΤE 296.3 К D1 0.50000000 sec d11 0.03000000 sec MCREST 0.00000000 sec MCWRK 0.01500000 sec ====== CHANNEL f1 ======= NUC1 130 P1 11.00 usec PL1 -3.00 dB SF01 125.7703643 MHz ====== CHANNEL f2 ======= CPDPRG2 waltzi6 NUC2 1H PCPD2 100.00 usec PL2 -6.00 dB PL12 17.00 dB PL13 19.00 dB SF02 500.1320005 MHz F2 - Processing parameters SI 32768 SF 125.7577932 MHz WDW ЕМ SSB 0 СΒ 1.00 Hz GB 0 РС 1.40 1D NMR plot parameters СХ 20.00 cm CY 10.06 cm F1P 219.359 ppm F 1 27586.10 Hz F2P -19.434 ppm 150 mqc 200 175 F2 100 125 -2443.93 Hz 75 50 25 0 PPMCM 11.93963 ppm/cm HZCM 1501.50134 Hz/cm





Current Data Parameters

kato-06.12.11

NAME