Desymmetrization of *meso*-1,2-Diols by a Chiral *N*,*N*-4-Dimethylaminopyridine Derivative Containing a 1,1′-Binaphthyl Unit: Importance of Two Hydroxy Groups

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SUPPORTING INFORMATION

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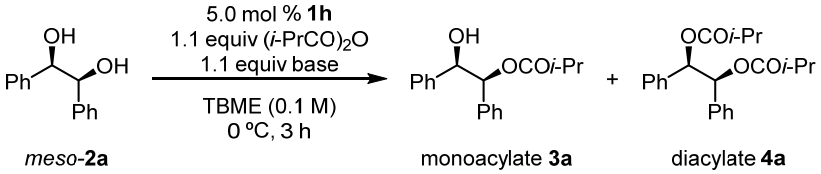
The details of optimization of reaction conditions

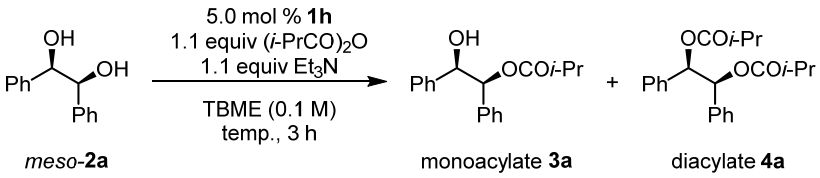
Table S1. Base screening for the desymmetrization of *meso*-**2a**[a)]



Entry	Base	**3a** [%][b)]	**4a** [%][b)]	**2a** [%][b)]	**3a**/**4a**	Er of **3a**[c)]
1	Et_3N	86	10	8	8.6	94:6
2	*i*-Pr_2EtN	84	5	13	16.8	94:6
3	pyridine	85	15	2	5.7	95:5
4	DBU	45	17	35	2.6	50:50
5	NMI	68	16	13	4.3	86:14
6	TMEDA	83	9	7	9.2	89:11
7	proton-sponge	85	8	7	10.6	94.5:5.5
8	Cs_2CO_3	34	3	43	11.3	50:50
9	K_2CO_3	74	8	19	9.3	50:50
10	K_3PO_4	86	9	7	9.6	55:45
11	KO*t*-Bu	55	13	27	4.2	69:31
12	KOAc	84	8	8	11	92:8
13	none	84	6	12	14	95:5

[a)] Reactions were performed on a 0.1 mmol scale in solvent (0.1 M) under an argon atmosphere. [b)] NMR yield were determined by ^1H NMR analysis using 2-methoxynaphthalene as an internal standard. [c)] Enantiomer ratio was determined by HPLC analysis using CHIRALCEL OJ-H.

Table S2. The effects of reaction temperature screening of the desymmetrization of *meso*-**2a**[a)]

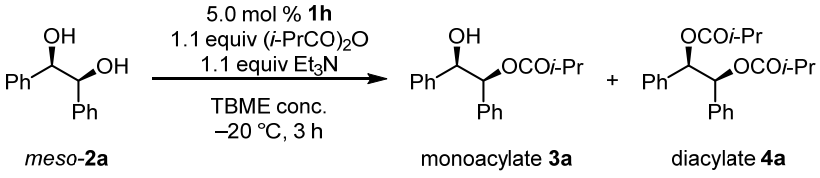


meso-**2a** monoacylate **3a** diacylate **4a**

Entry	temp. [°C]	**3a** [%][b)]	**4a** [%][b)]	**2a** [%][b)]	**3a**/**4a**	Er of **3a**[c)]
1	0	86	10	8	8.6	94:6
2	–20	85	6	9	14.2	98:2
3	–40	85	5	7	17	98:2
4	–60	78	4	21	19.5	98:2

[a)] Reactions were performed on a 0.1 mmol scale in solvent (0.1 M) under an argon atmosphere. [b)] NMR yield were determined by ^{1}H NMR analysis using 2-methoxynaphthalene as an internal standard. [c)] Enantiomer ratio was determined by HPLC analysis using CHIRALCEL OJ-H.

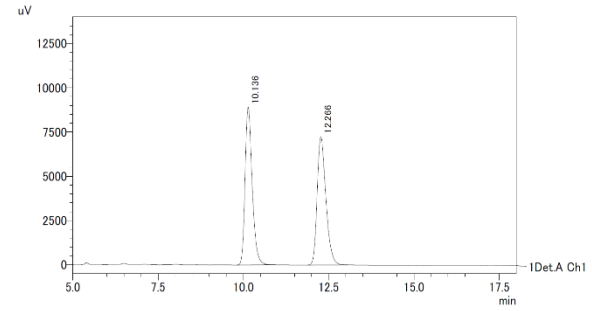
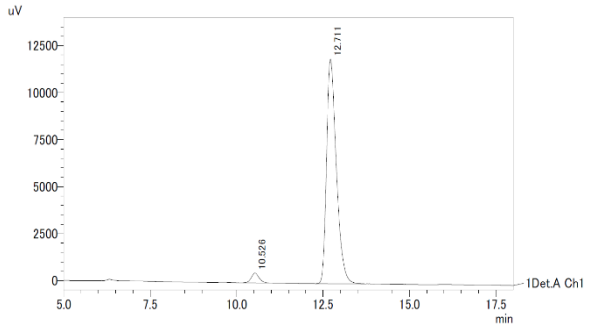
Table S3. The effects of substrate concentration screening of the desymmetrization of *meso*-**2a**[a)]



meso-**2a** monoacylate **3a** diacylate **4a**

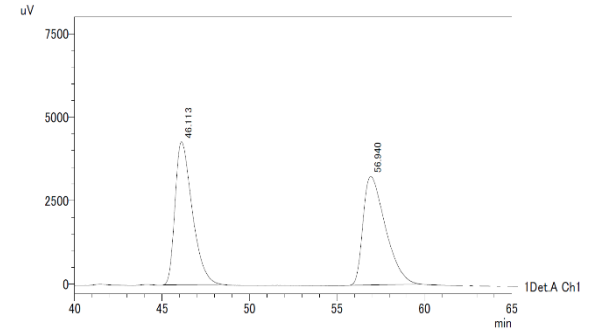
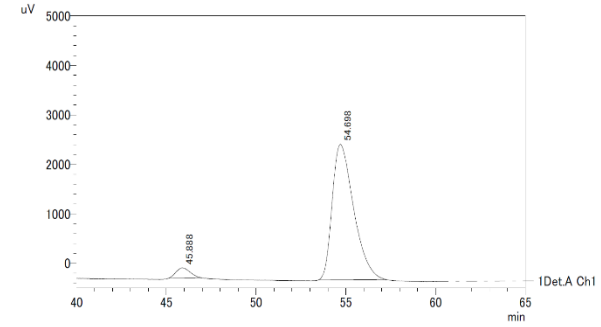
Entry	conc. [M]	**3a** [%][b)]	**4a** [%][b)]	**2a** [%][b)]	**3a**/**4a**	Er of **3a**[c)]
1	0.05	81	13	7	6.2	97:3
2	0.1	84	6	12	14	97:3
3	0.2	89	10	2	8.9	96:4

[a)] Reactions were performed on a 0.1 mmol scale in solvent (0.1 M) under an argon atmosphere. [b)] NMR yield were determined by ^{1}H NMR analysis using 2-methoxynaphthalene as an internal standard. [c)] Enantiomer ratio was determined by HPLC analysis using CHIRALCEL OJ-H.

Racemic sample of **3b**	Figure 2, **3b**
	

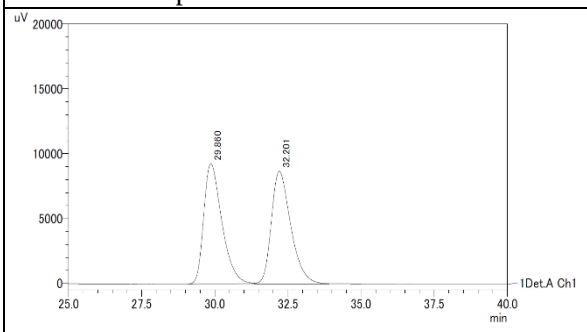
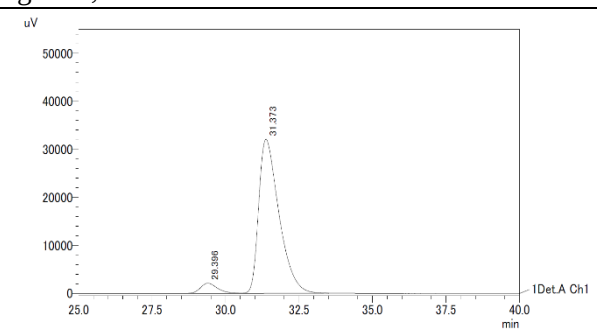
Peak	**Ret. Time**	**Area**	**Area %**
1	10.136	129328	50.129
2	12.266	128660	49.871

Peak #	**Ret. Time**	**Area**	**Area %**
1	10.526	8126	3.344
2	12.711	234887	96.656

Racemic sample of **3c**	Figure 2, **3c**
	

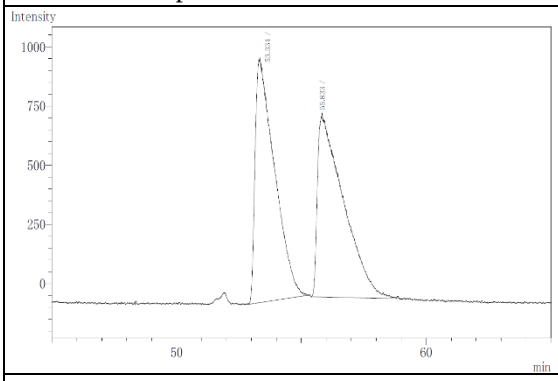
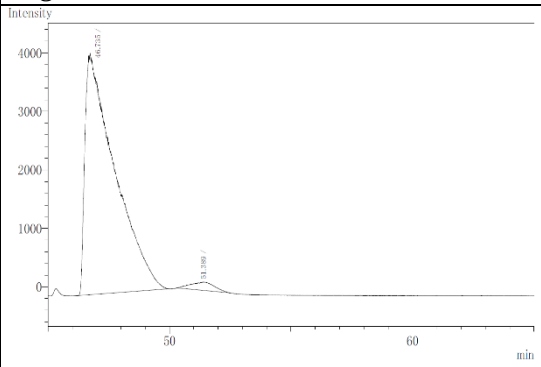
Peak	**Ret. Time**	**Area**	**Area %**
1	46.113	293838	50.293
2	56.940	290418	49.707

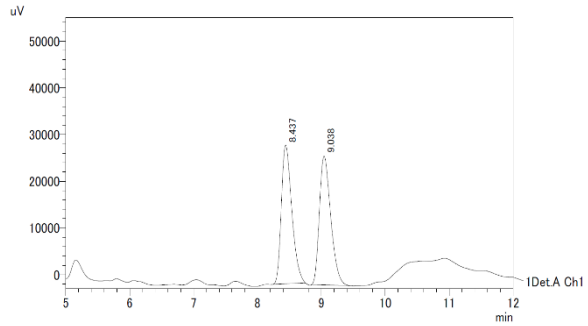
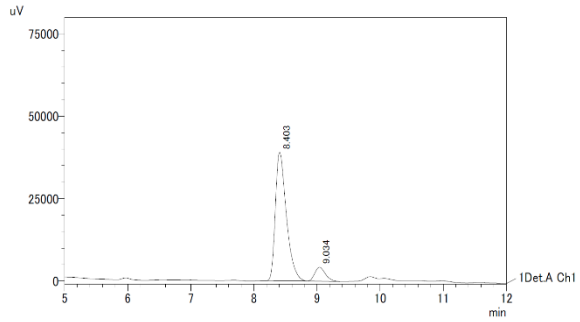
Peak	**Ret. Time**	**Area**	**Area %**
1	45.888	10866	4.555
2	54.698	227671	95.445

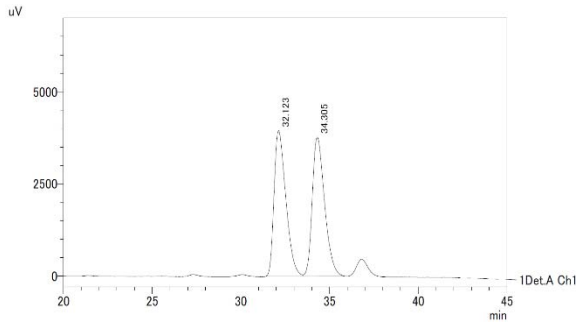
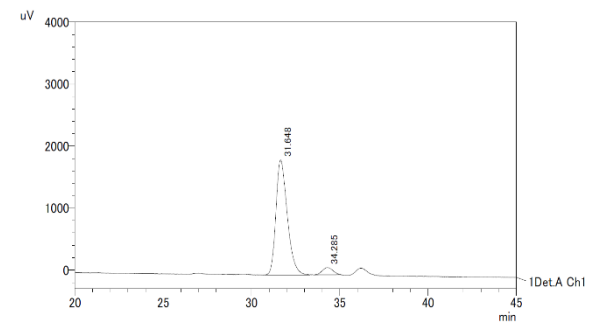
Racemic sample of **3d**	Figure 2, **3d**
	

Peak	**Ret. Time**	**Area**	**Area %**
1	29.860	400005	50.044
2	32.201	399309	49.956

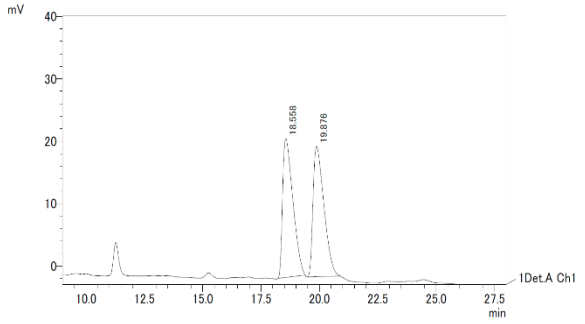
Peak	**Ret. Time**	**Area**	**Area %**
1	29.396	83925	5.171
2	31.373	1539164	94.829

Racemic sample of **3e**				Figure 2, **3e**			
							
Peak	**Ret. Time**	**Area**	**Conc. %**	**Peak**	**Ret. Time**	**Area**	**Conc. %**
1	53.334	55657	49.905	1	46.735	350018	97.348
2	55.833	55868	50.095	2	51.389	9537	2.652

Racemic sample of **3f**				Figure 2, **3f**			
							
Peak	**Ret. Time**	**Area**	**Area %**	**Peak**	**Ret. Time**	**Area**	**Area %**
1	8.437	337935	49.837	1	8.403	473272	90.562
2	9.0385	340139	50.163	2	9.034	49324	9.438

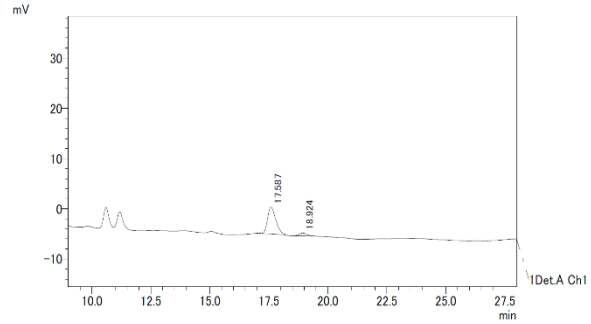
Racemic sample of **3g**				Figure 2, **3g**			
							
Peak	**Ret. Time**	**Area**	**Area %**	**Peak**	**Ret. Time**	**Area**	**Area %**
1	32.123	182395	50.009	1	31.648	82460	94.452
2	34.305	182326	49.991	2	34.285	4843	5.548

Racemic sample of **3h**



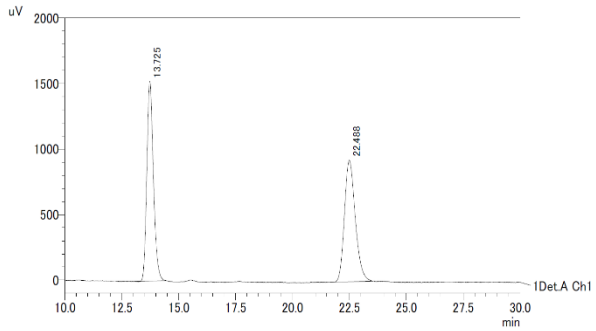
Peak	Ret. Time	Area	Area %
1	18.558	680693	50.111
2	19.876	677688	49.889

Figure 2, **3h**



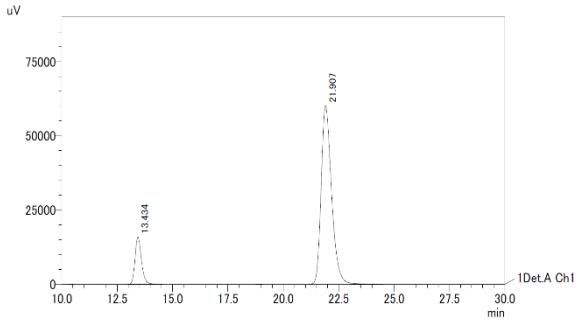
Peak	Ret. Time	Area	Area %
1	17.587	128958	90.866
2	18.924	12963	9.134

Racemic sample of **3i** (benzoate derivative)



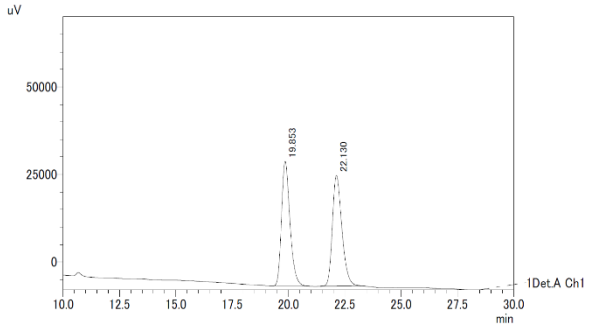
Peak	Ret. Time	Area	Area %
1	13.725	30561	49.884
2	22.488	30702	50.116

Figure 2, **3i** (benzoate derivative)



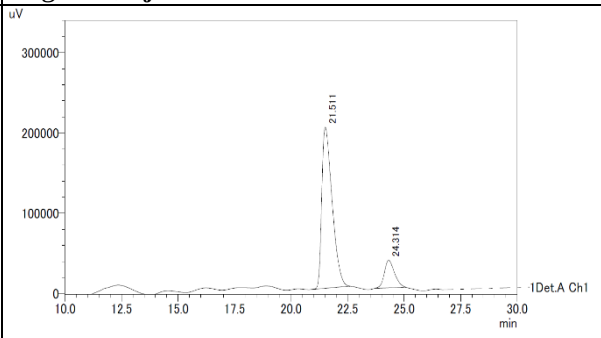
Peak	Ret. Time	Area	Area %
1	13.434	318497	13.995
2	21.907	1957297	86.005

Racemic sample of **3j**

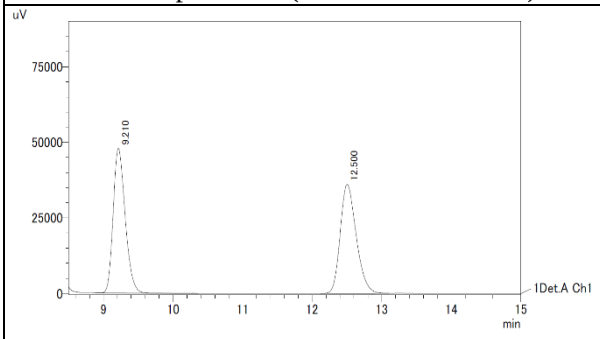
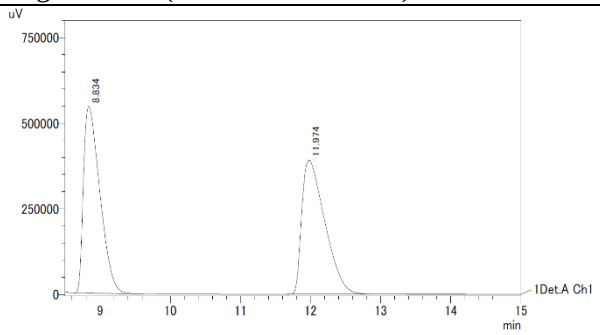


Peak	Ret. Time	Area	Area %
1	19.853	929324	49.923
2	22.130	932206	50.077

Figure 2, **3j**

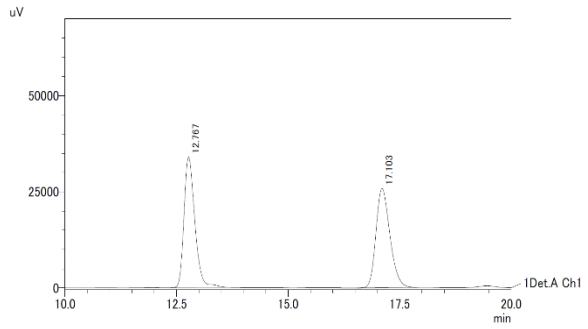
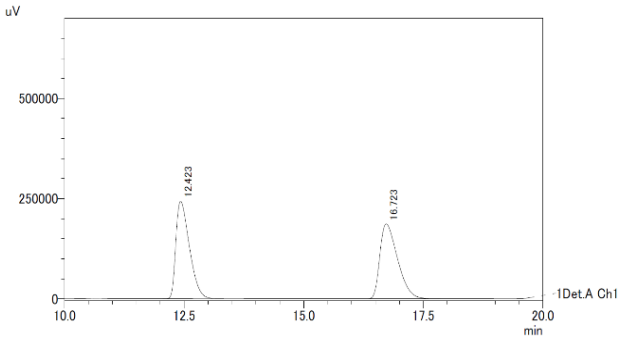


Peak	Ret. Time	Area	Area %
1	21.511	6407334	85.652
2	24.314	1073333	14.587

Racemic sample of **3k** (benzoate derivative)	Figure 2, **3k** (benzoate derivative)
	

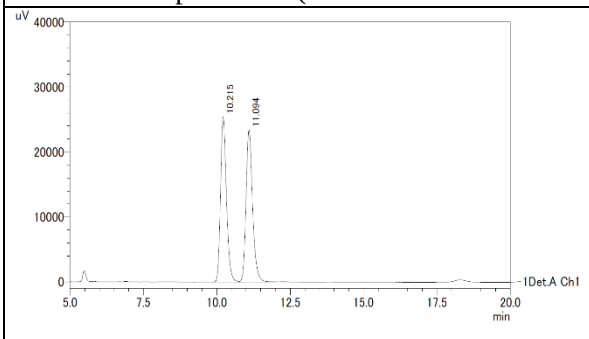
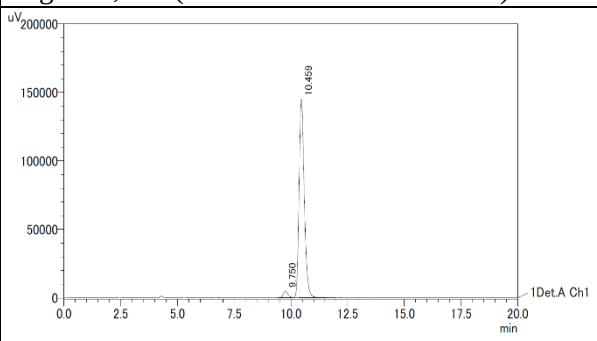
Peak	**Ret. Time**	**Area**	**Area %**
1	9.210	575853	49.974
2	12.500	576454	50.026

Peak	**Ret. Time**	**Area**	**Area %**
1	8.834	8869599	49.802
2	11.974	8940265	50.198

Racemic sample of **3l** (benzoate derivative)	Figure 2, **3l** (benzoate derivative)
	

Peak	**Ret. Time**	**Area**	**Area %**
1	12.767	570268	50.413
2	17.103	560919	49.587

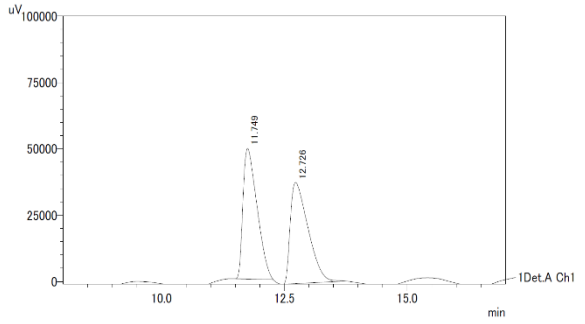
Peak	**Ret. Time**	**Area**	**Area %**
1	12.423	4776406	49.871
2	16.723	4801202	50.129

Racemic sample of **3m** (4-nitro benzoate derivative)	Figure 2, **3m** (4-nitro benzoate derivative)
	

Peak	**Ret. Time**	**Area**	**Area %**
1	10.215	356784	49.607
2	11.094	362439	50.393

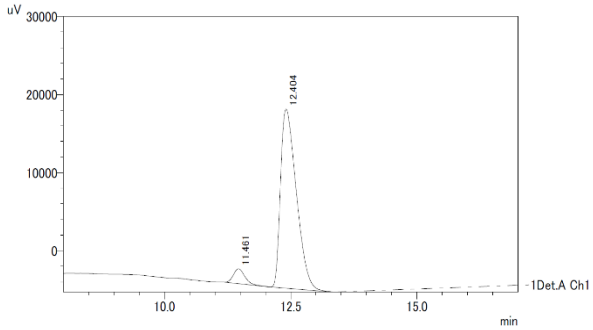
Peak	**Ret. Time**	**Area**	**Area %**
1	9.750	72220	3.034
2	10.459	2308280	96.966

Racemic sample of **3n**



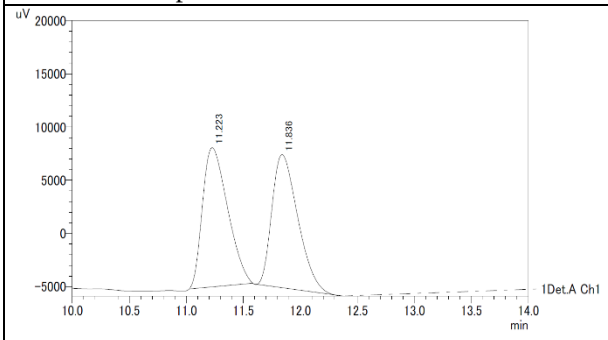
Peak	Ret. Time	Area	Area %
1	11.749	976812	50.372
2	12.726	962371	49.628

Figure 2, **3n**



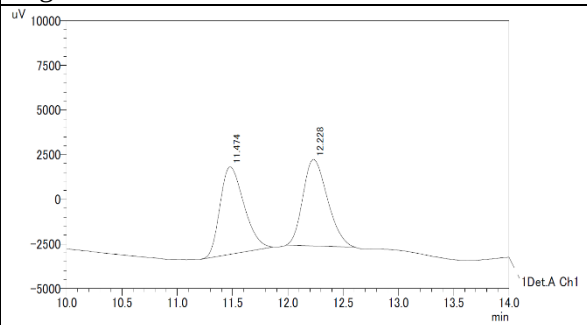
Peak	Ret. Time	Area	Area %
1	11.461	29917	5.652
2	12.404	499413	94.348

Racemic sample of **3o**



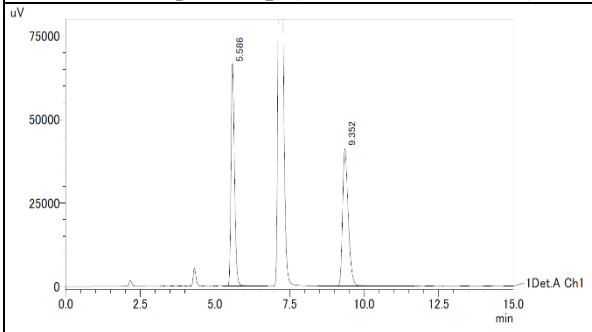
Peak	Ret. Time	Area	Area %
1	11.223	200455	50.354
2	11.836	197634	49.646

Figure 2, **3o**



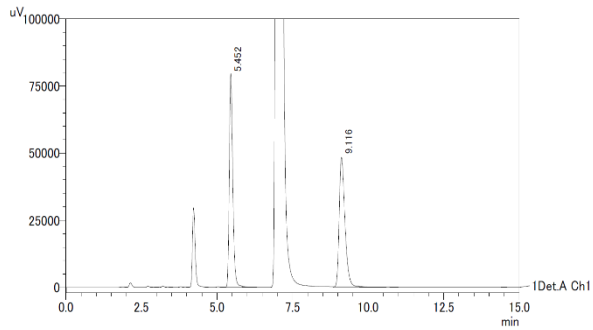
Peak	Ret. Time	Area	Area %
1	11.474	73987	49.611
2	12.228	75147	50.389

Racemic sample of **3p** (benzoate derivative)



Peak	Ret. Time	Area	Area %
1	5.586	539216	49.912
2	9.352	541114	50.088

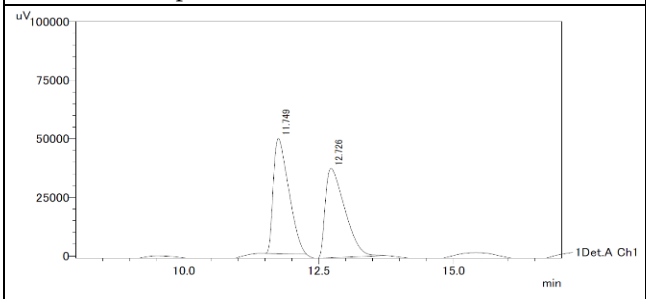
Figure 2, **3p** (benzoate derivative)



Peak	Ret. Time	Area	Area %
1	5.452	636151	49.914
2	9.116	638344	50.086

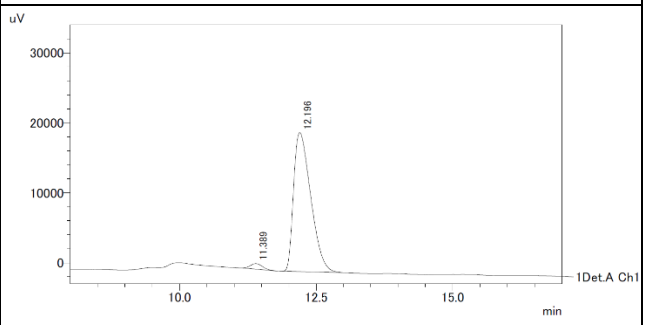
Investigation of intramolecular acyl migration (Scheme 2)

Racemic sample of **3n**



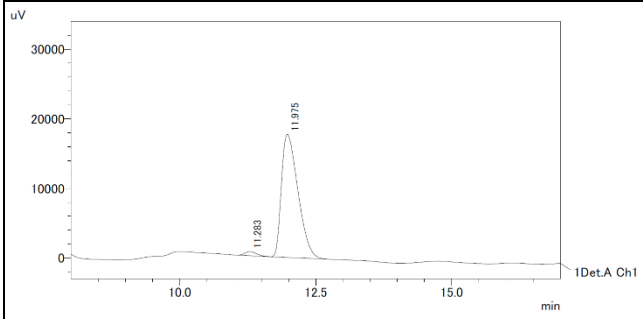
Peak	Ret. Time	Area	Area %
1	11.749	976812	50.372
2	12.726	962371	49.628

Scheme 2, **3n**



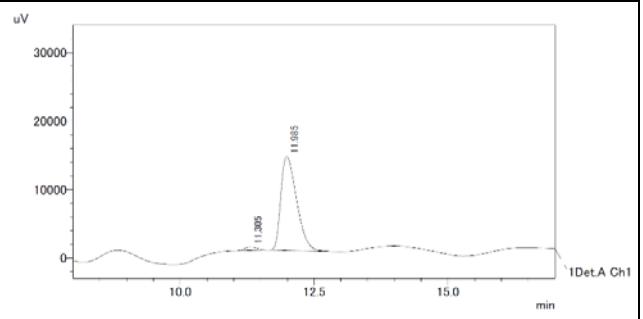
Peak	Ret. Time	Area	Area %
1	11.389	11986	2.689
2	12.196	433756	97.311

Scheme 2, **3n**, step a



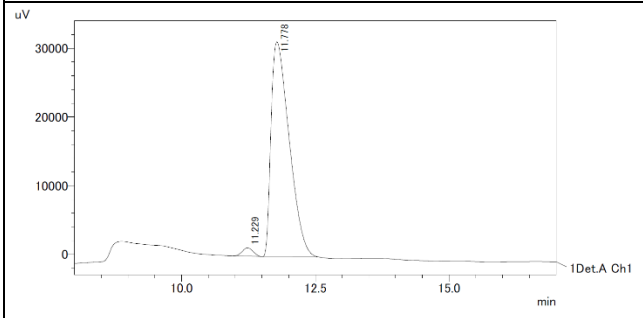
Peak	Ret. Time	Area	Area %
1	11.283	8846	2.317
2	11.975	373017	97.683

Scheme 2, **3n**, step b



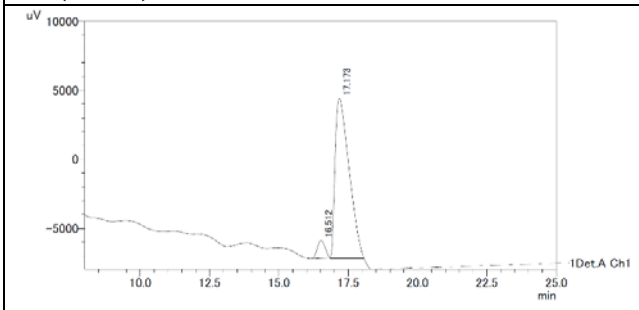
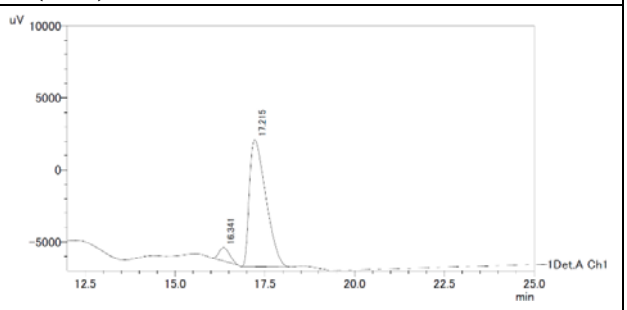
Peak	Ret. Time	Area	Area %
1	11.305	7272	2.528
2	11.985	280391	97.472

Scheme 2, **3n**, step c

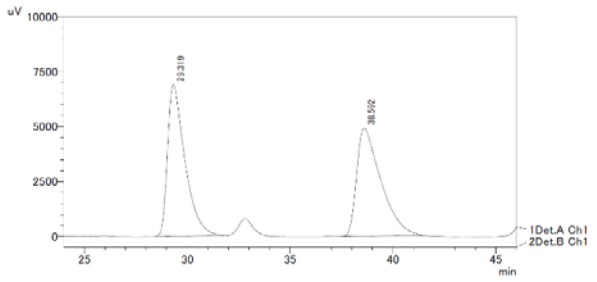
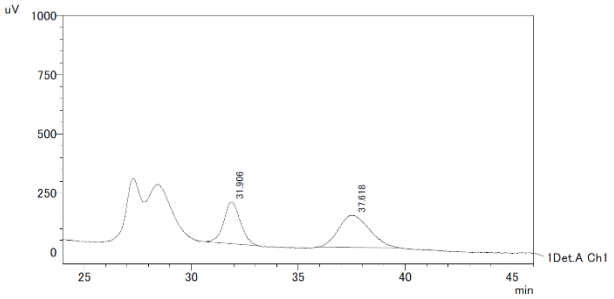


Peak	Ret. Time	Area	Area %
1	11.229	16625	2.198
2	11.778	739830	97.802

Investigation of intramolecular acyl migration with *ent*-1h (eq.1)

3n (before)				**3n** (after)			
							
Peak	**Ret. Time**	**Area**	**Area %**	**Peak**	**Ret. Time**	**Area**	**Area %**
1	16.512	24122	5.664	1	16.341	18852	6.260
2	17.173	401784	94.336	2	17.215	282302	93.740

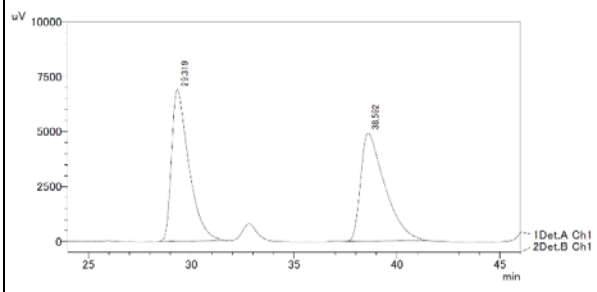
Investigation of second acylation step (eq.2)

Racemic sample of **3a** (before)				Recovered **3a** (after)			
							
Peak	**Ret. Time**	**Area**	**Area %**	**Peak**	**Ret. Time**	**Area**	**Area %**
1	29.319	405052	50.262	1	31.906	9497	40.971
2	38.592	400827	49.738	2	37.618	13683	59.029

Effects of the *tert*-alcohol unit(s) of the catalyst in the desymmetrization of *meso*-2a (Table 4)

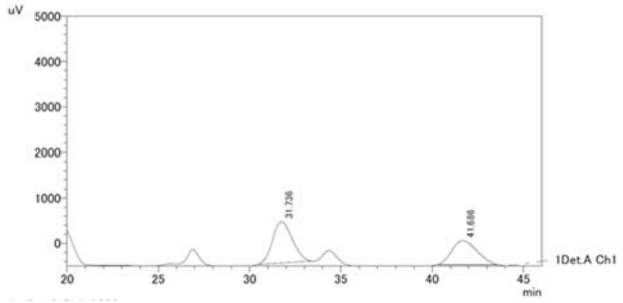
The crude product of **3a** was subjected to HPLC with DAICEL CHIRALPAK® OJ-H (For entries 2 and 3, hexane/i-PrOH = 98/2, v/v, flow rate = 1.0 mL/min, 30 °C, UV = 254 nm; For entries 4 and 5, hexane/i-PrOH = 98.5/1.5, v/v, flow rate = 1.0 mL/min, 30 °C, UV = 254 nm).

Racemic sample of **3a** for entries 2 and 3



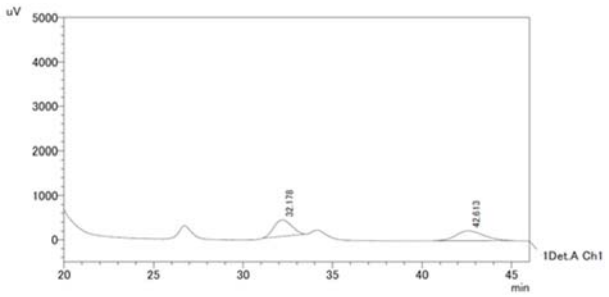
Peak	Ret. Time	Area	Area %
1	29.319	405052	50.262
2	38.592	400827	49.738

3a from **1h′** (entry 2)



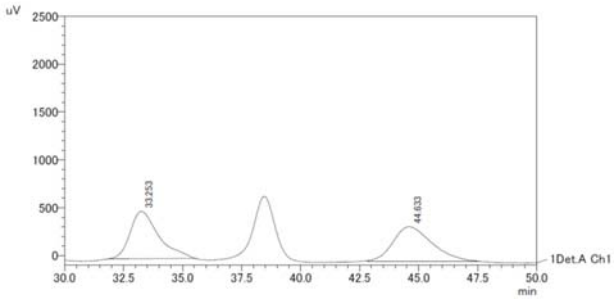
Peak	Ret. Time	Area	Area %
1	31.736	68598	57.685
2	41.686	50319	42.315

3a from **1h″** (entry 3)



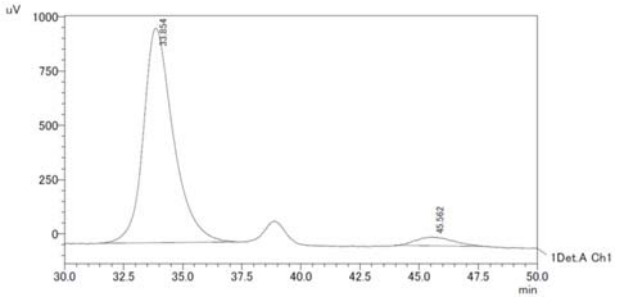
Peak	Ret. Time	Area	Area %
1	32.178	25864	52.400
2	42.613	23495	47.600

Racemic sample of **3a** for entries 4 and 5



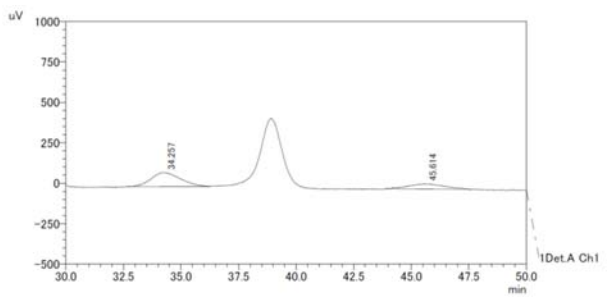
Peak	Ret. Time	Area	Area %
1	33.253	41715	49.937
2	44.633	41820	50.063

3a from **1h‴** (entry 4)

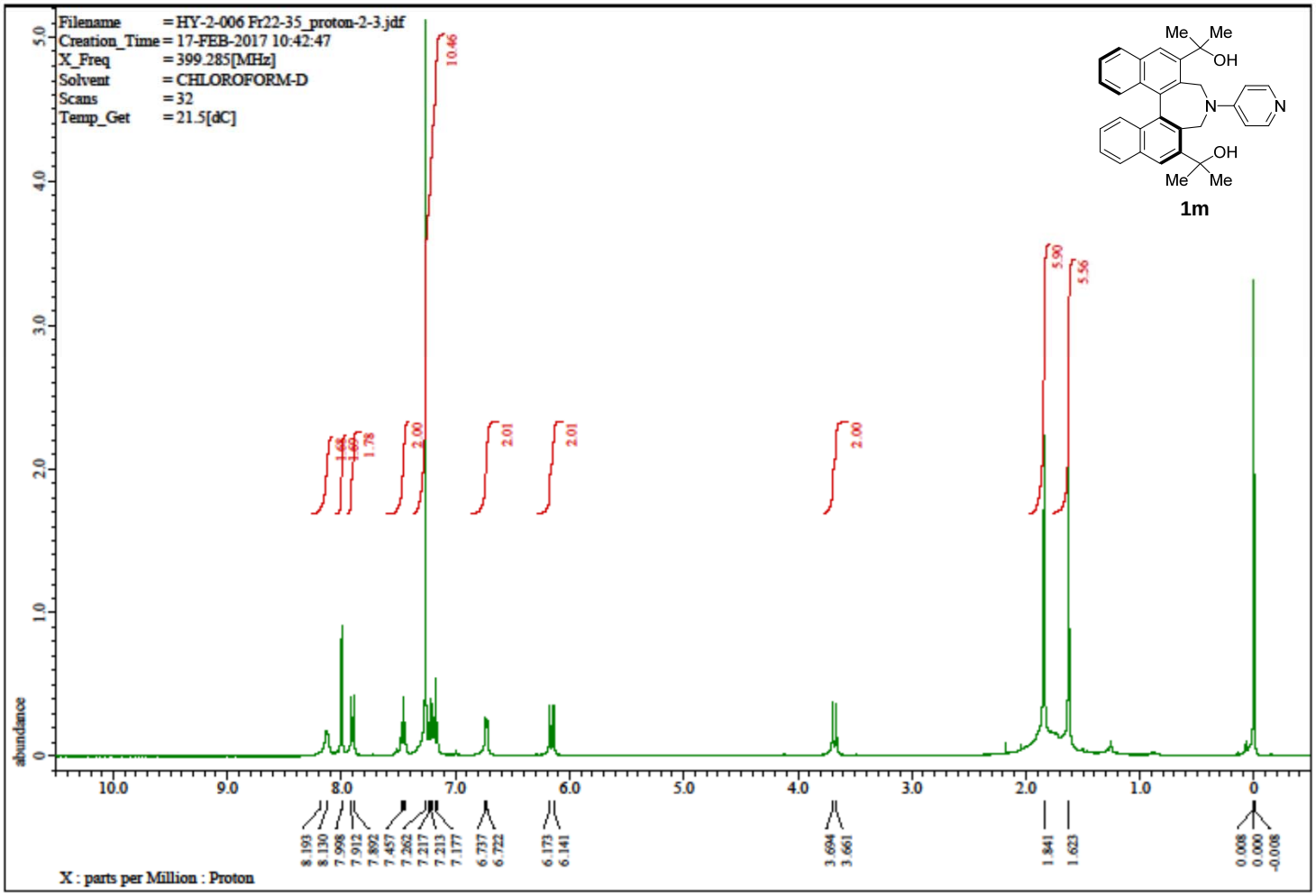


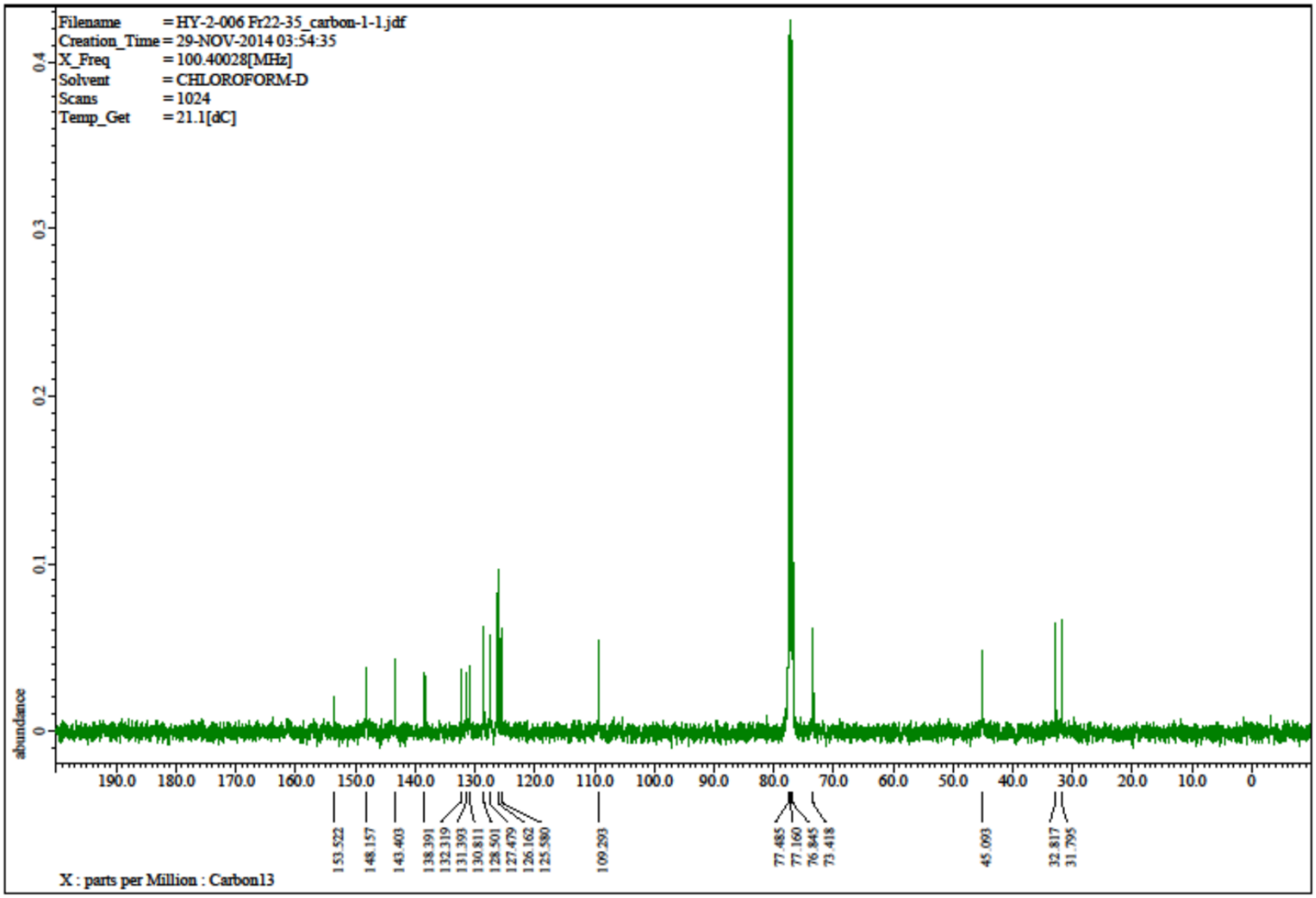
Peak	Ret. Time	Area	Area %
1	33.854	87208	95.235
2	45.562	4364	4.765

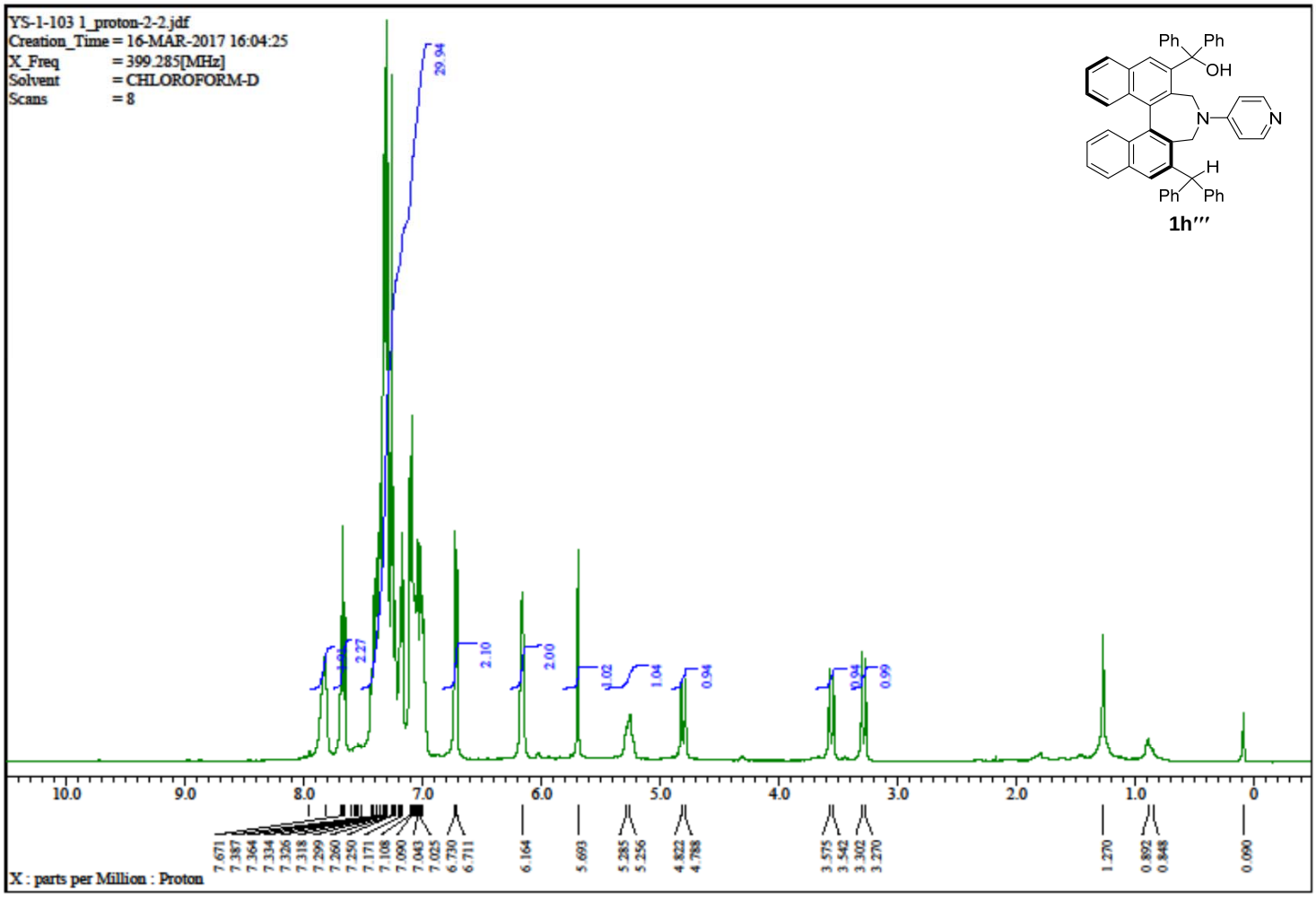
3a from **1h⁗** (entry 5)

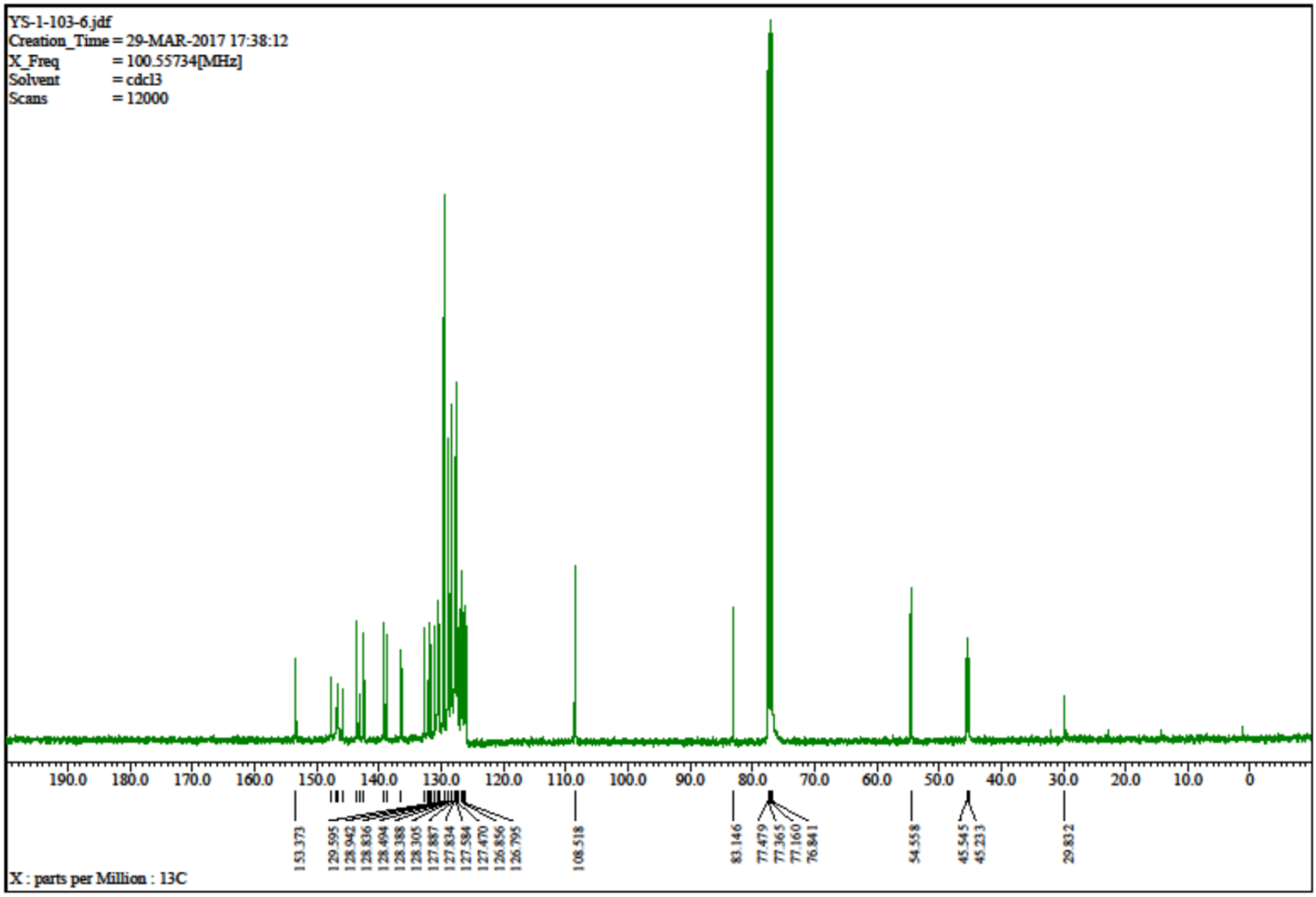


Peak	Ret. Time	Area	Area %
1	34.257	7647	69.394
2	45.614	3373	30.606


Filename = HY-2-006 Fr22-35_proton-2-3.jdf
Creation_Time = 17-FEB-2017 10:42:47
X_Freq = 399.285[MHz]
Solvent = CHLOROFORM-D
Scans = 32
Temp_Get = 21.5[dC]
Me Me
OH
N
N
OH
Me Me
1m
X : parts per Million : Proton
abundance


Filename = HY-2-006 Fr22-35_carbon-1-1.jdf
Creation_Time = 29-NOV-2014 03:54:35
X_Freq = 100.40028[MHz]
Solvent = CHLOROFORM-D
Scans = 1024
Temp_Get = 21.1[dC]
X : parts per Million : Carbon13
abundance


YS-1-103 1_proton-2-2.jdf
Creation_Time = 16-MAR-2017 16:04:25
X_Freq = 399.285[MHz]
Solvent = CHLOROFORM-D
Scans = 8
Ph
Ph
OH
N
N
H
Ph
Ph
1h'''
X : parts per Million : Proton


YS-1-103-6.jdf
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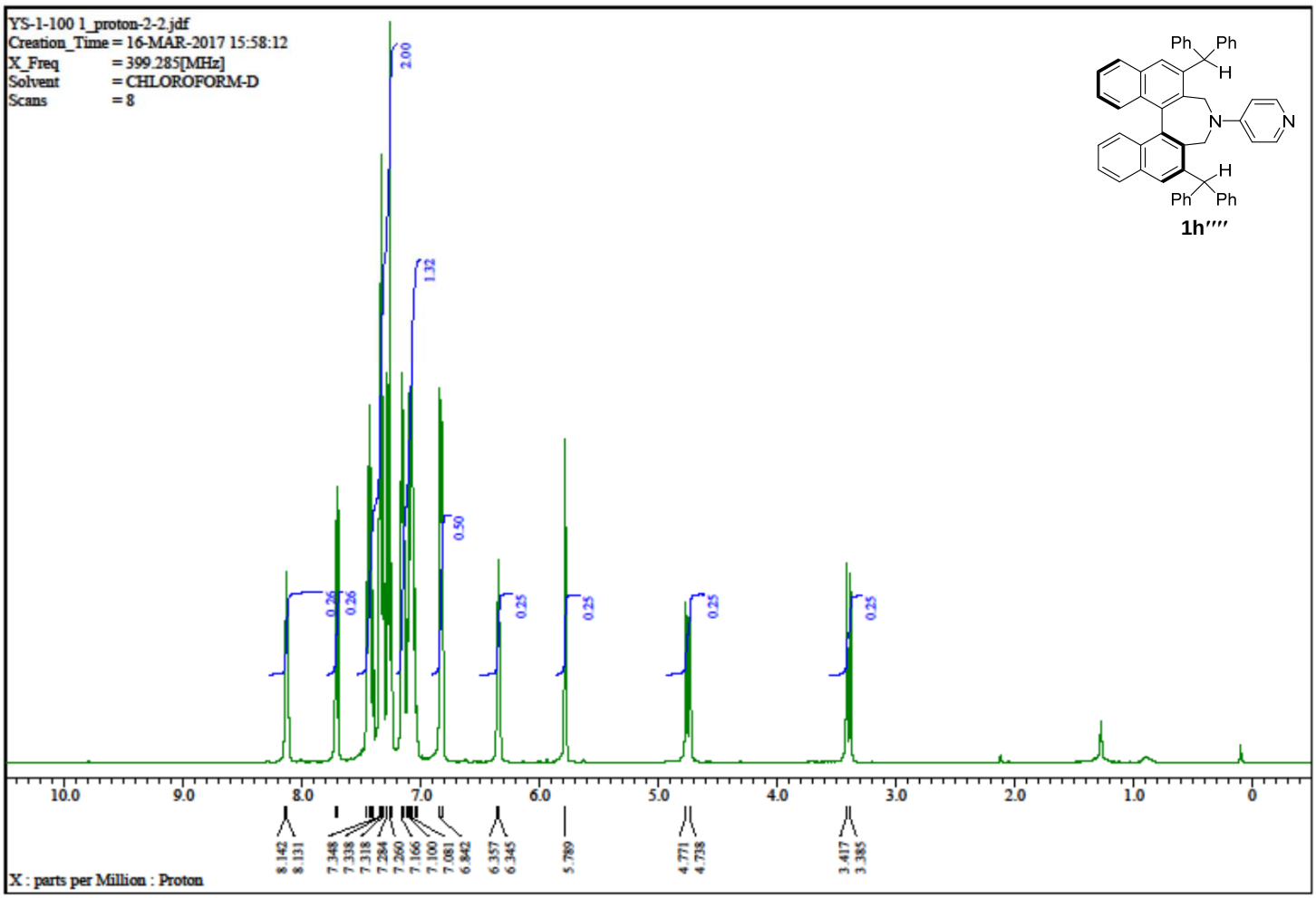
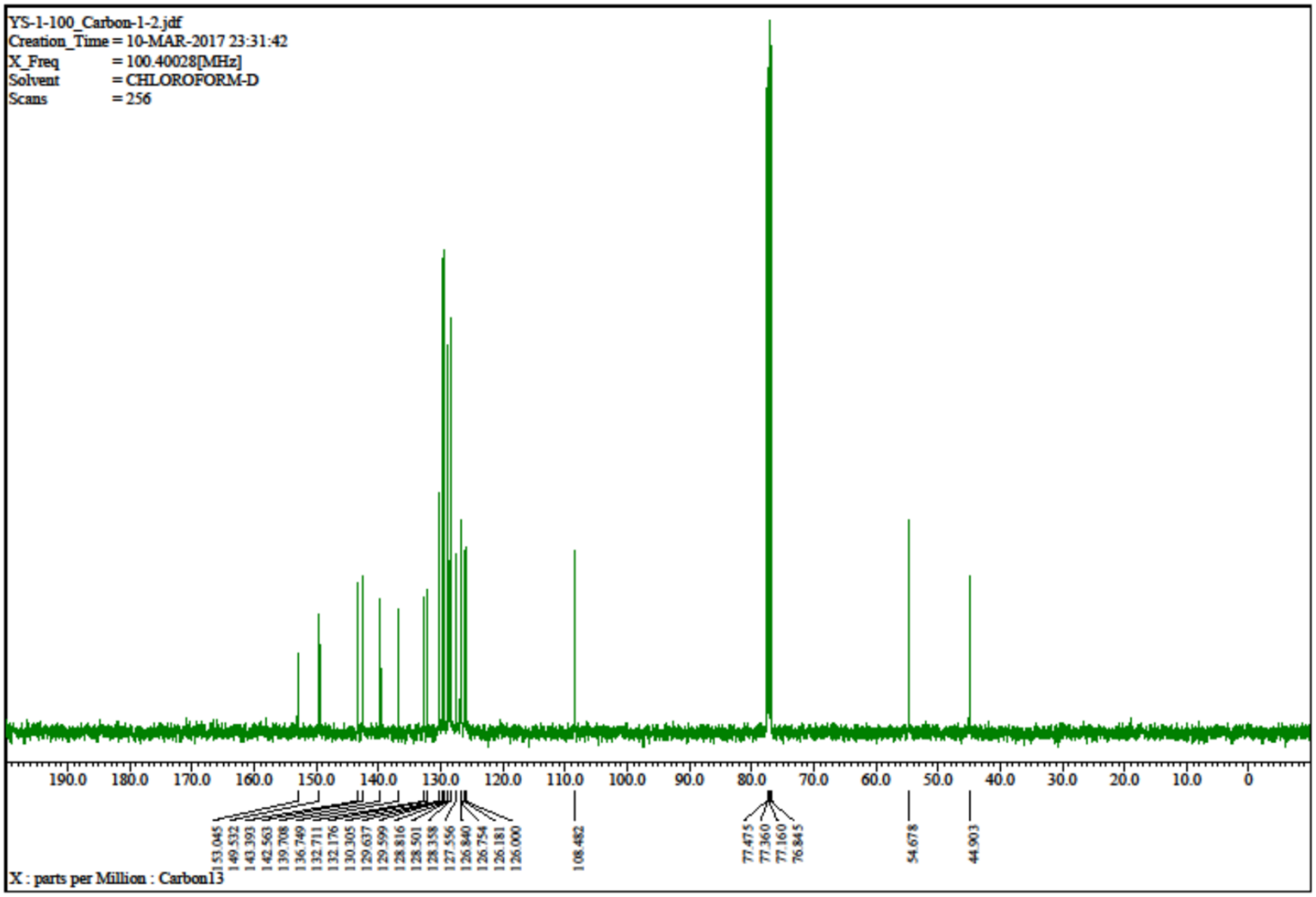
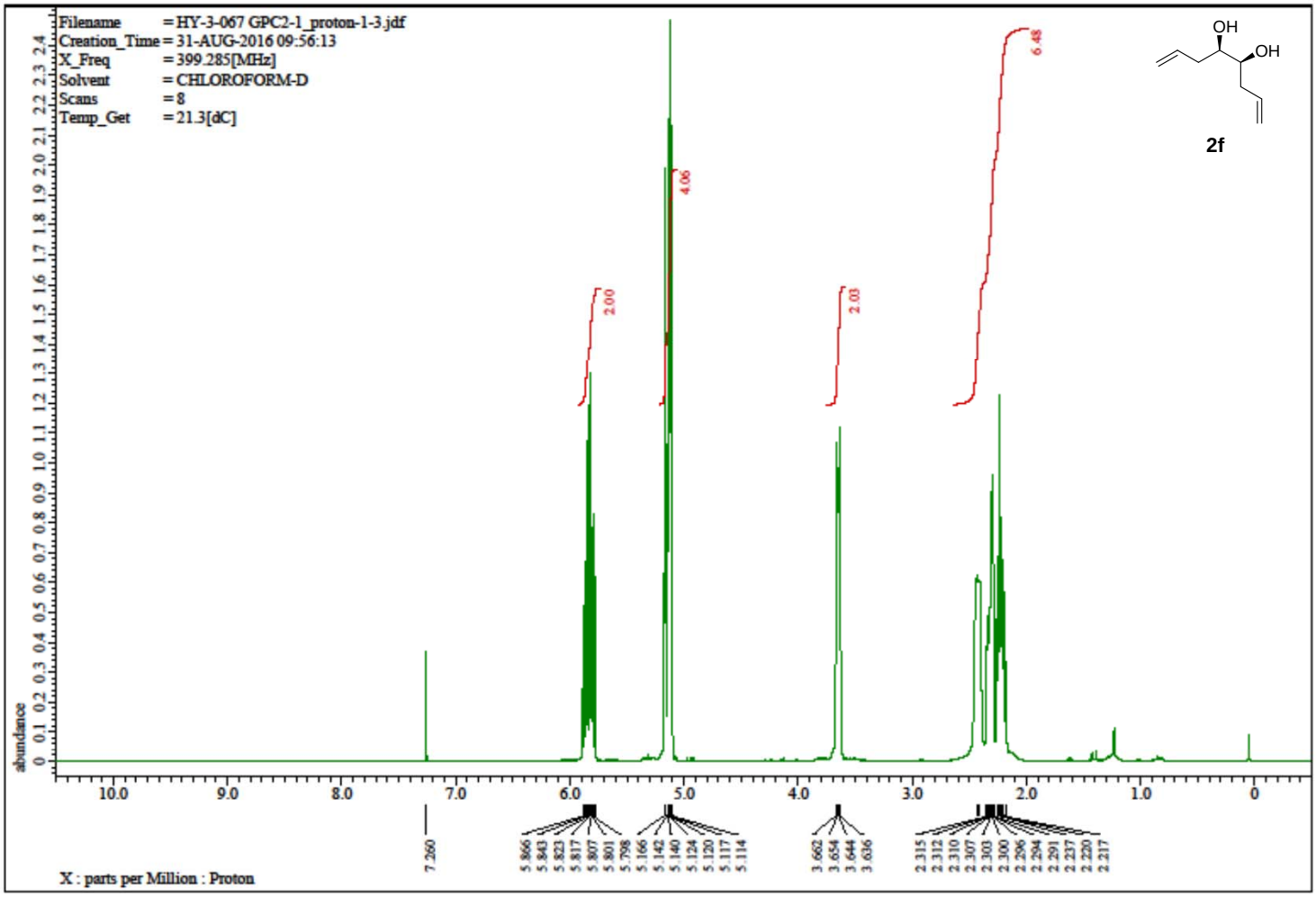
X_Freq = 100.55734[MHz]
Solvent = cdcl3
Scans = 12000
X : parts per Million : 13C


YS-1-100 1_proton-2-2.jdf
Creation_Time = 16-MAR-2017 15:58:12
X_Freq = 399.285[MHz]
Solvent = CHLOROFORM-D
Scans = 8
Ph
Ph
H
N
N
H
Ph
Ph
1h''''
2.00
1.32
0.50
0.26
0.26
0.25
0.25
0.25
0.25
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
8.142
8.131
7.348
7.338
7.318
7.284
7.260
7.166
7.100
7.081
6.842
6.357
6.345
5.789
4.771
4.738
3.417
3.385
X : parts per Million : Proton


YS-1-100_Carbon-1-2.jdf
Creation_Time = 10-MAR-2017 23:31:42
X_Freq = 100.40028[MHz]
Solvent = CHLOROFORM-D
Scans = 256
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
153.045
149.532
143.393
142.563
139.708
136.749
132.711
132.176
130.305
129.637
129.599
128.816
128.501
128.358
127.556
126.840
126.754
126.181
126.000
108.482
77.475
77.360
77.160
76.845
54.678
44.903
X : parts per Million : Carbon13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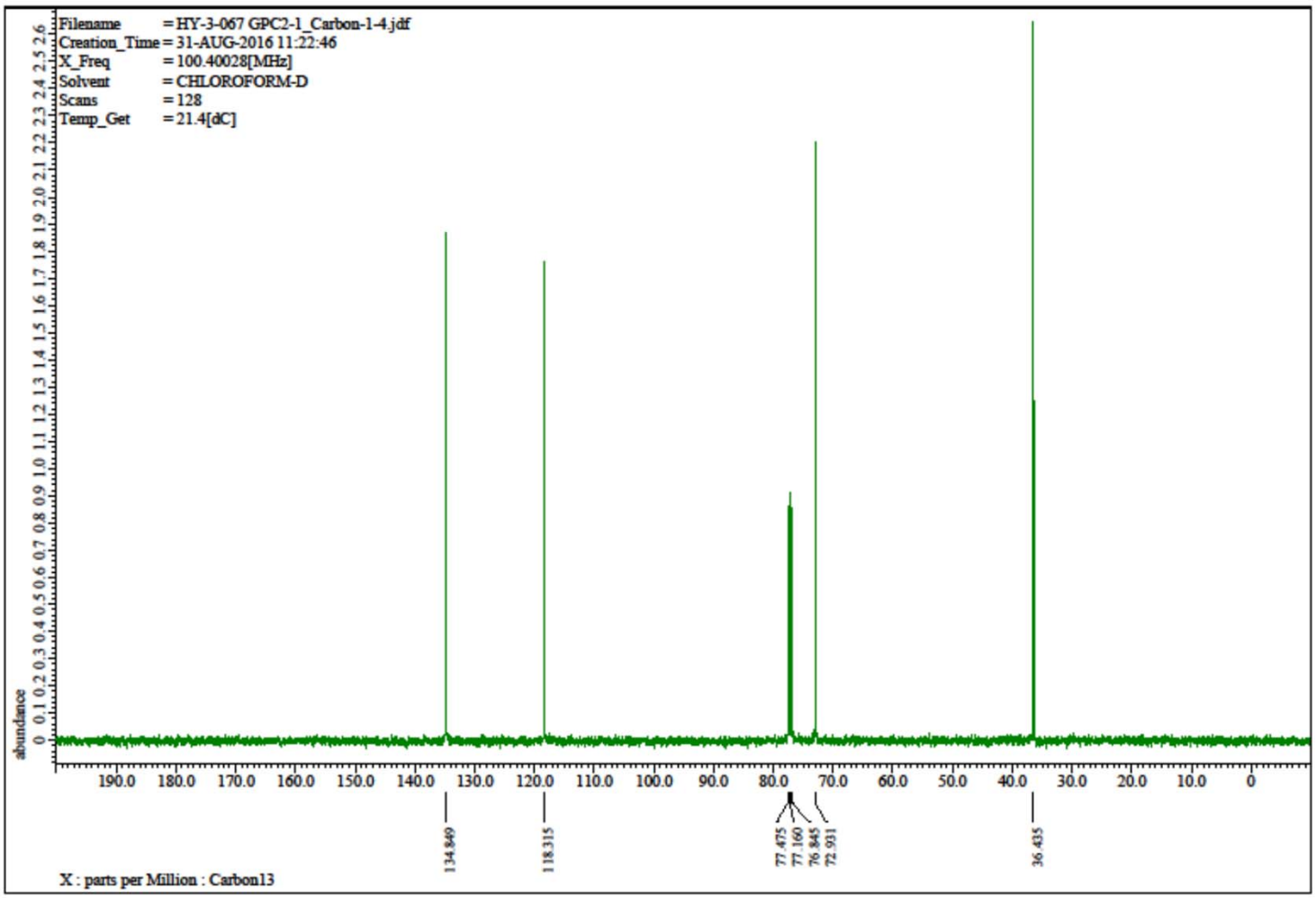
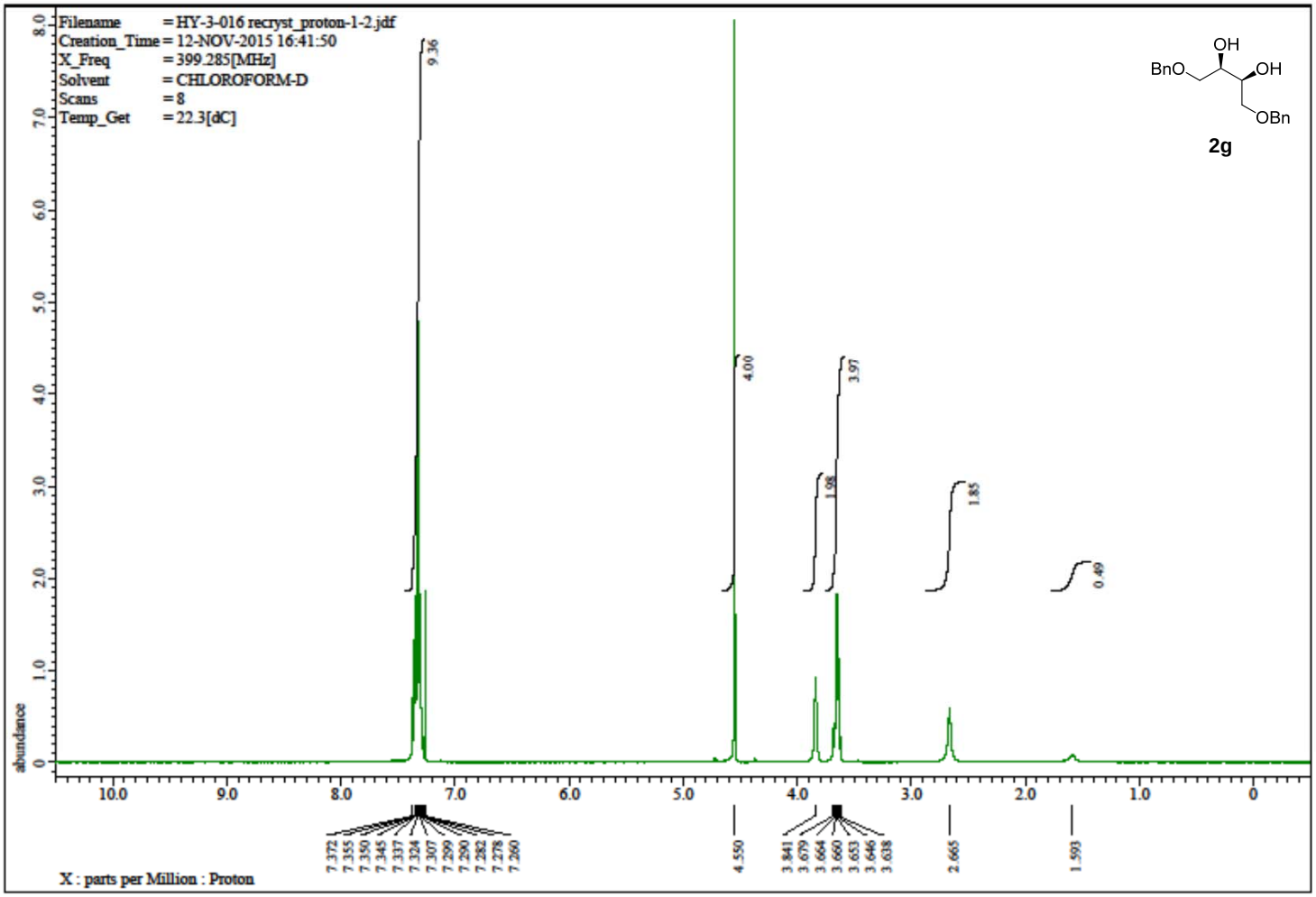
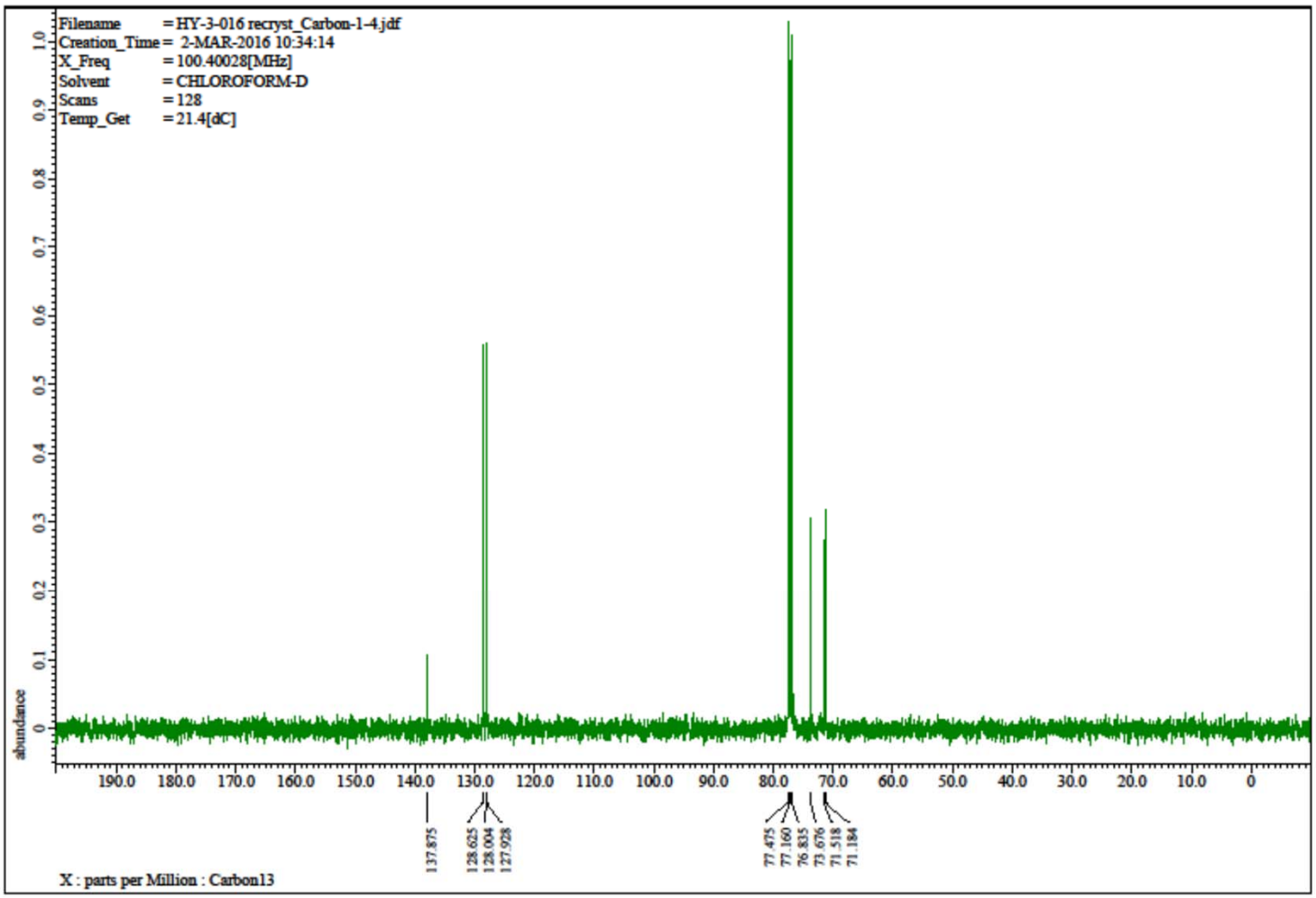
Creation_Time = 31-AUG-2016 09:56:13
X_Freq = 399.285[MHz]
Solvent = CHLOROFORM-D
Scans = 8
Temp_Get = 21.3[dC]
OH
OH
2f
2.00
4.06
2.03
6.48
abundance
X : parts per Million : Proton


Filename = HY-3-067 GPC2-1_Carbon-1-4.jdf
Creation_Time = 31-AUG-2016 11:22:46
X_Freq = 100.40028[MHz]
Solvent = CHLOROFORM-D
Scans = 128
Temp_Get = 21.4[dC]
abundance
X : parts per Million : Carbon13


Filename = HY-3-016 recryst_proton-1-2.jdf
Creation_Time = 12-NOV-2015 16:41:50
X_Freq = 399.285[MHz]
Solvent = CHLOROFORM-D
Scans = 8
Temp_Get = 22.3[dC]
9.36
4.00
3.97
1.98
1.85
0.49
OH
BnO
OH
OBn
2g
abundance
X : parts per Million : Proton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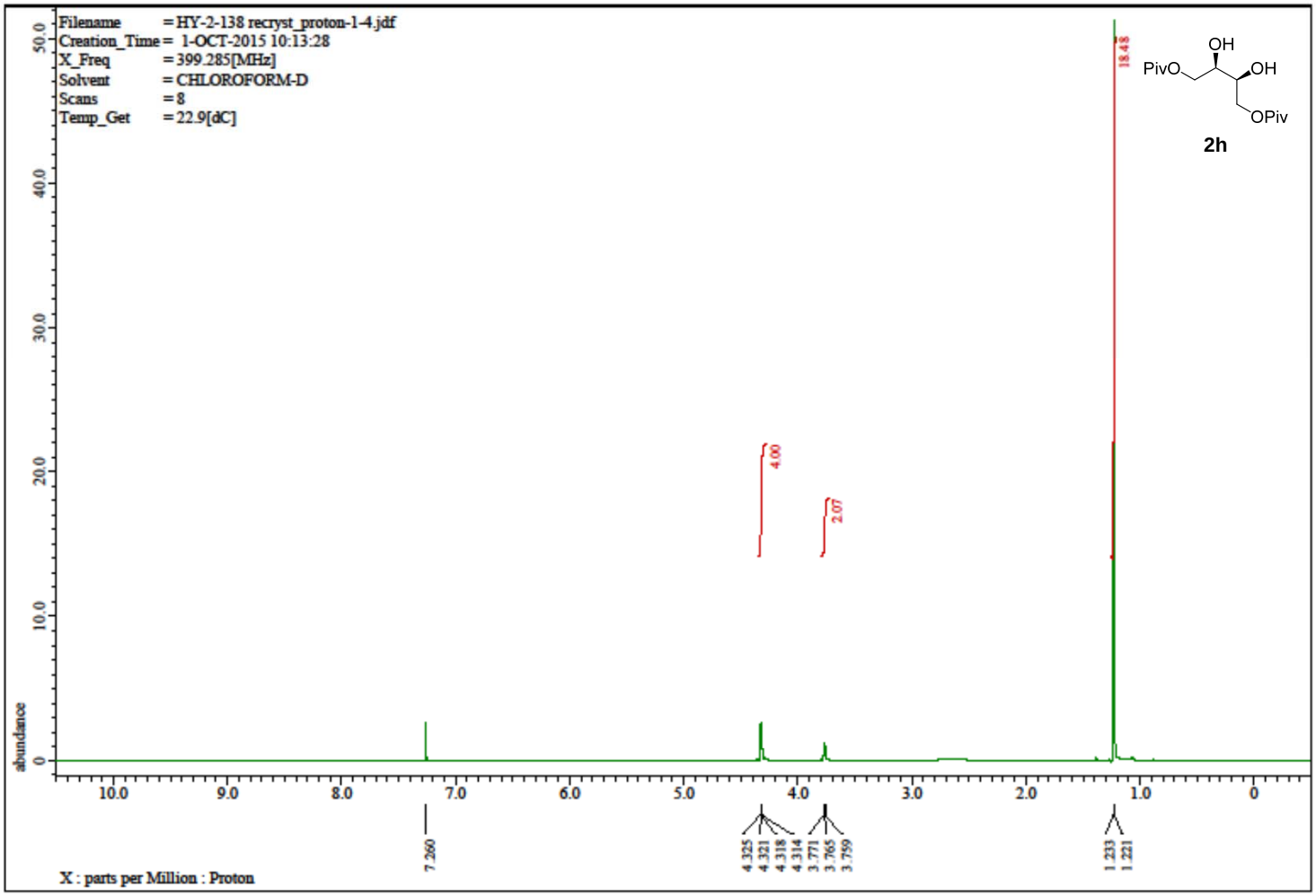
Creation_Time = 2-MAR-2016 10:34:14
X_Freq = 100.40028[MHz]
Solvent = CHLOROFORM-D
Scans = 128
Temp_Get = 21.4[dC]
abundance
X : parts per Million : Carbon13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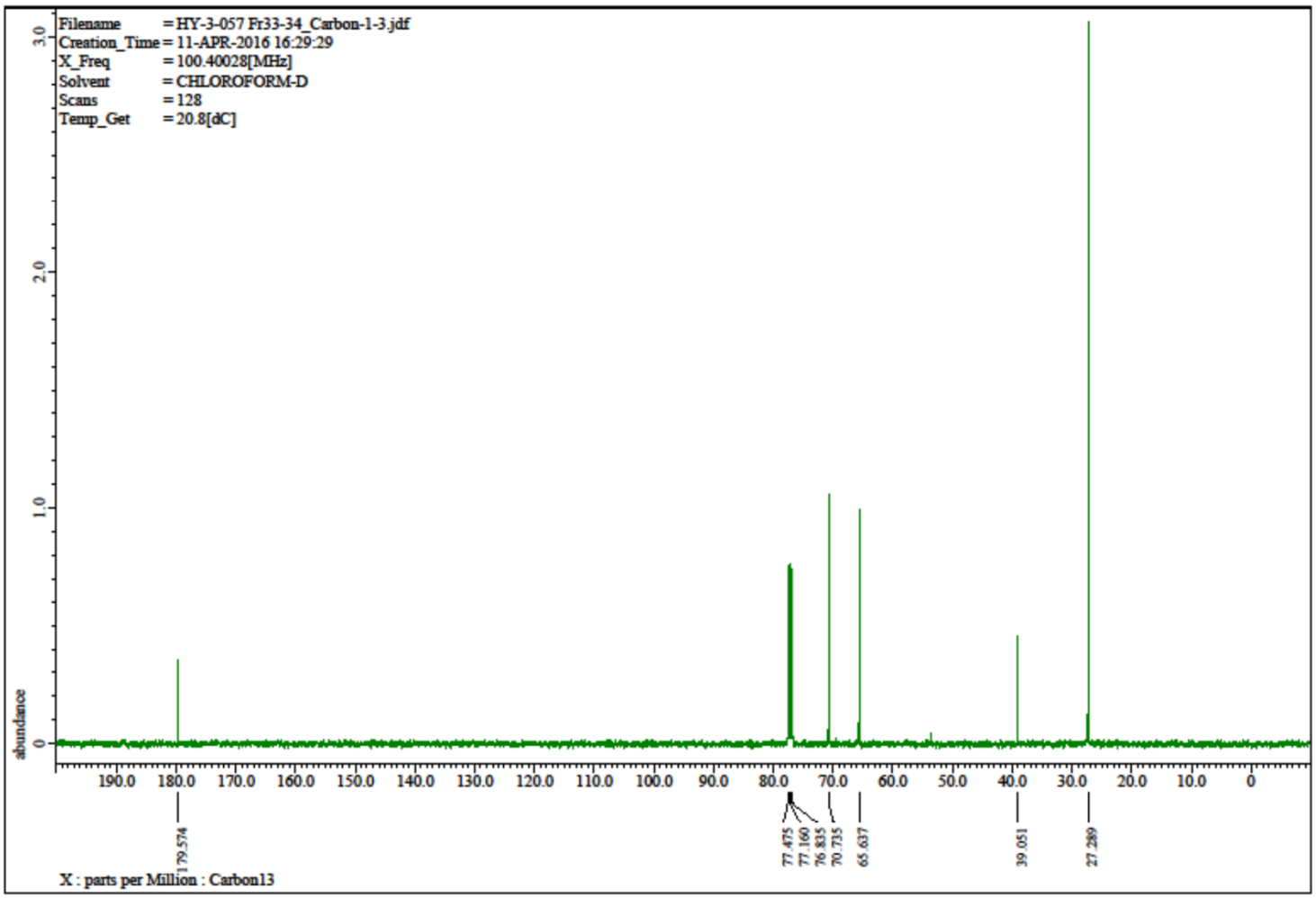
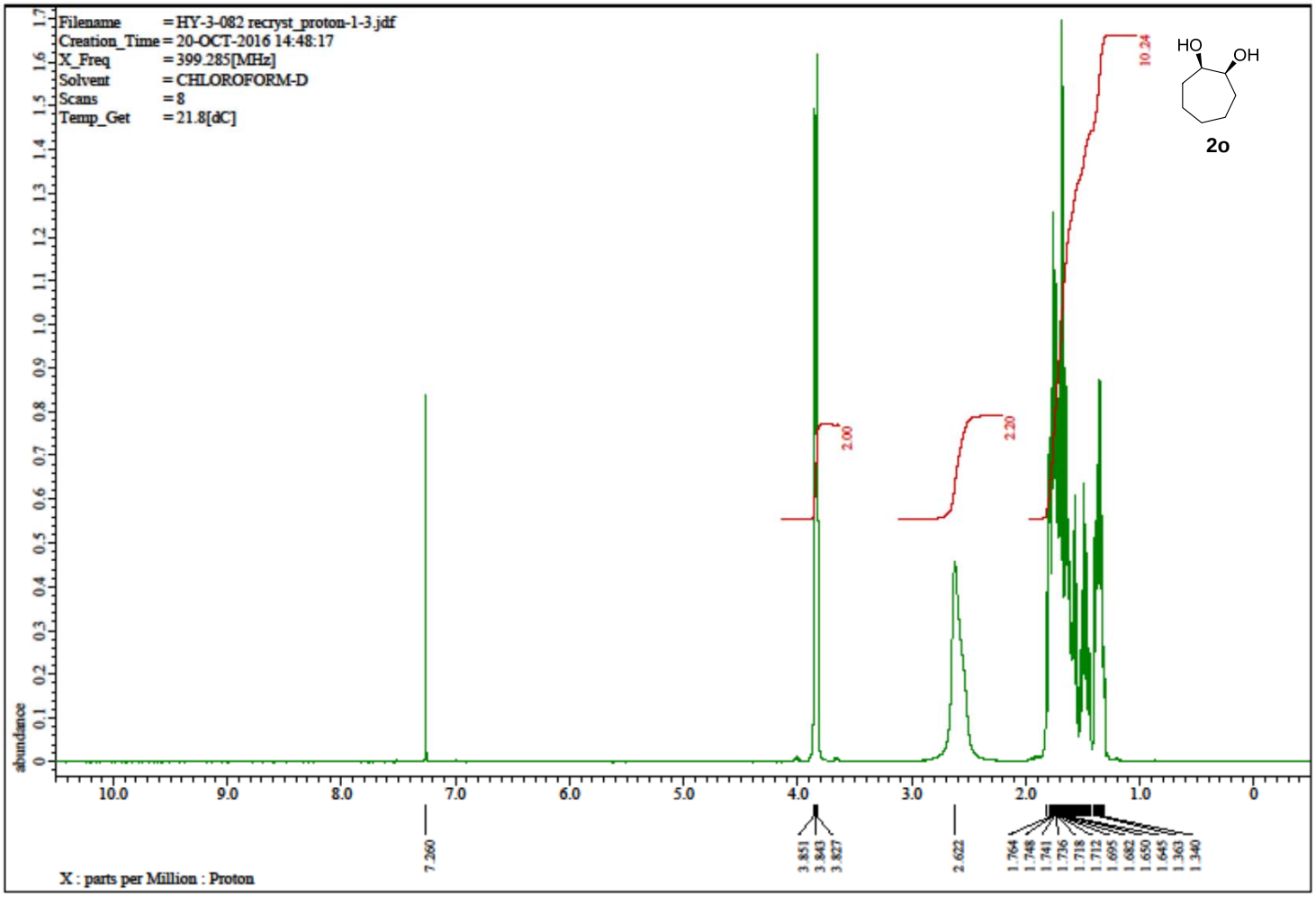
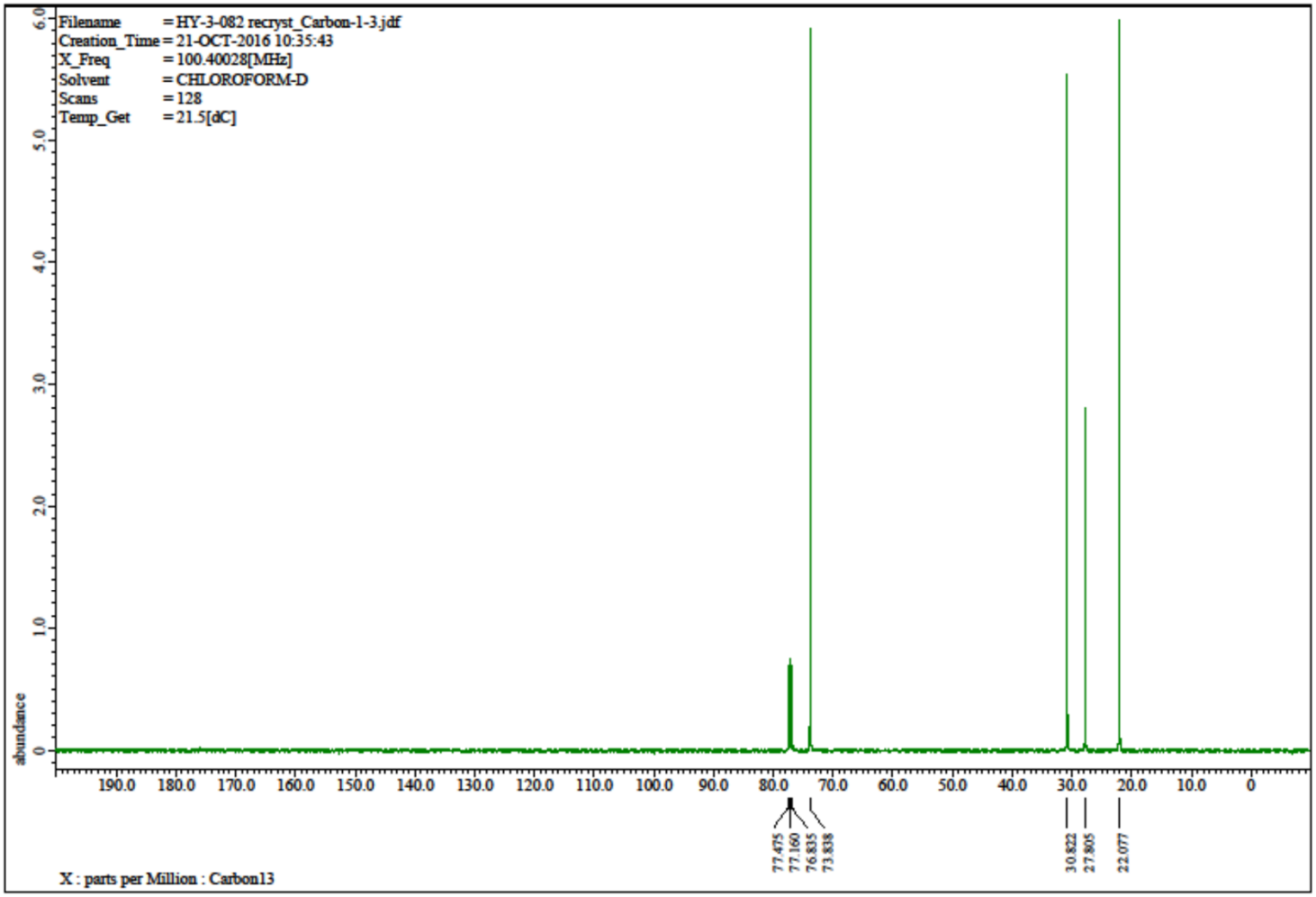
Creation_Time = 1-OCT-2015 10:13:28
X_Freq = 399.285[MHz]
Solvent = CHLOROFORM-D
Scans = 8
Temp_Get = 22.9[dC]
OH
PivO
OH
OPiv
2h
18.48
4.00
2.07
abundance
7.260
4.325
4.321
4.318
4.314
3.771
3.765
3.759
1.233
1.221
X : parts per Million : Proton


Filename = HY-3-057 Fr33-34_Carbon-1-3.jdf
Creation_Time = 11-APR-2016 16:29:29
X_Freq = 100.40028[MHz]
Solvent = CHLOROFORM-D
Scans = 128
Temp_Get = 20.8[dC]
abundance
179.574
77.475
77.160
76.835
70.735
65.637
39.051
27.289
X : parts per Million : Carbon13


Filename = HY-3-082 recryst_proton-1-3.jdf
Creation_Time = 20-OCT-2016 14:48:17
X_Freq = 399.285[MHz]
Solvent = CHLOROFORM-D
Scans = 8
Temp_Get = 21.8[dC]
HO
OH
2o
10.24
2.00
2.20
abundance
7.260
3.851
3.843
3.827
2.622
1.764
1.748
1.741
1.736
1.718
1.712
1.695
1.682
1.650
1.645
1.363
1.340
X : parts per Million : Proton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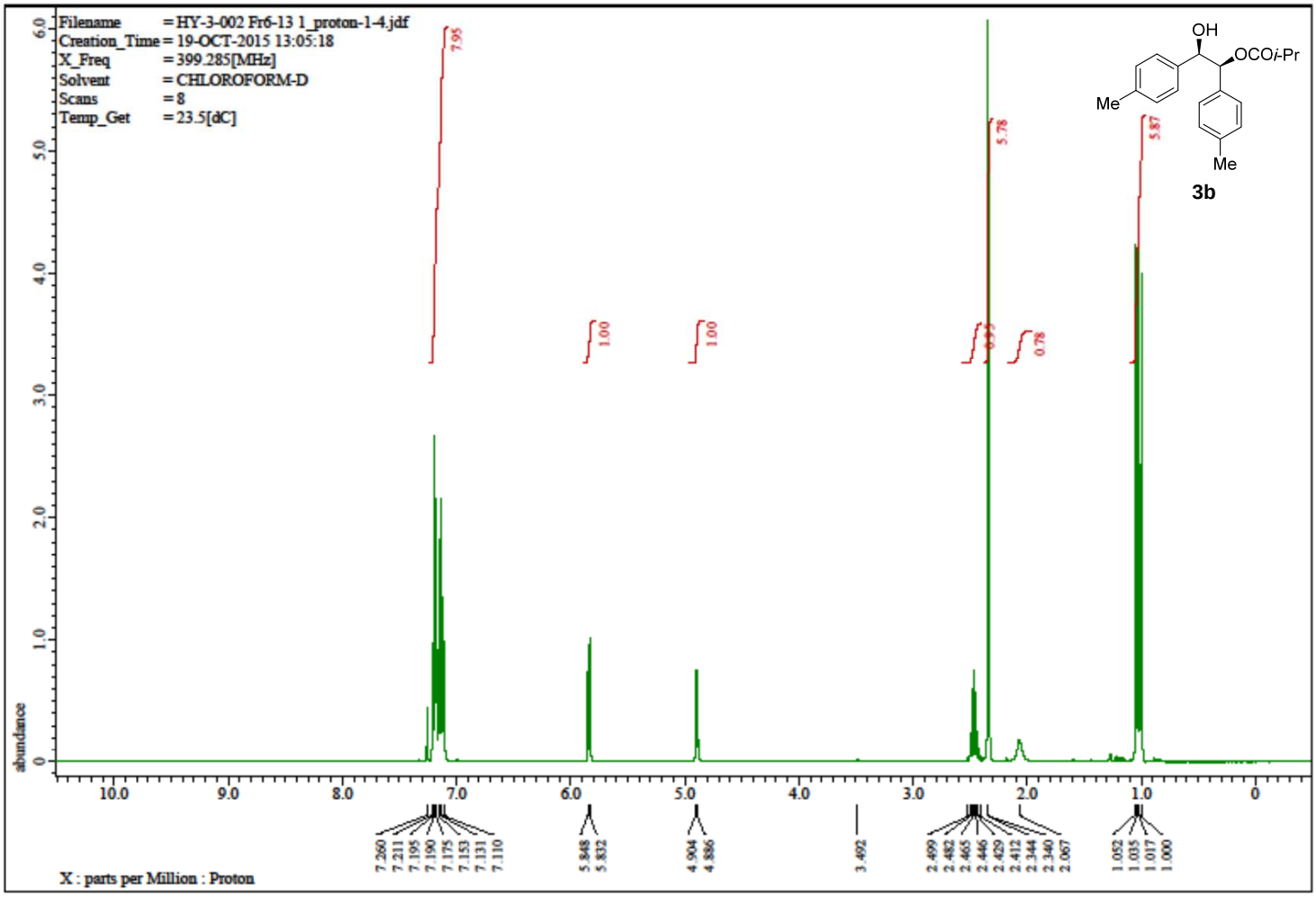
Creation_Time = 21-OCT-2016 10:35:43
X_Freq = 100.40028[MHz]
Solvent = CHLOROFORM-D
Scans = 128
Temp_Get = 21.5[dC]
abundance
77.475
77.160
76.835
73.838
30.822
27.805
22.077
X : parts per Million : Carbon13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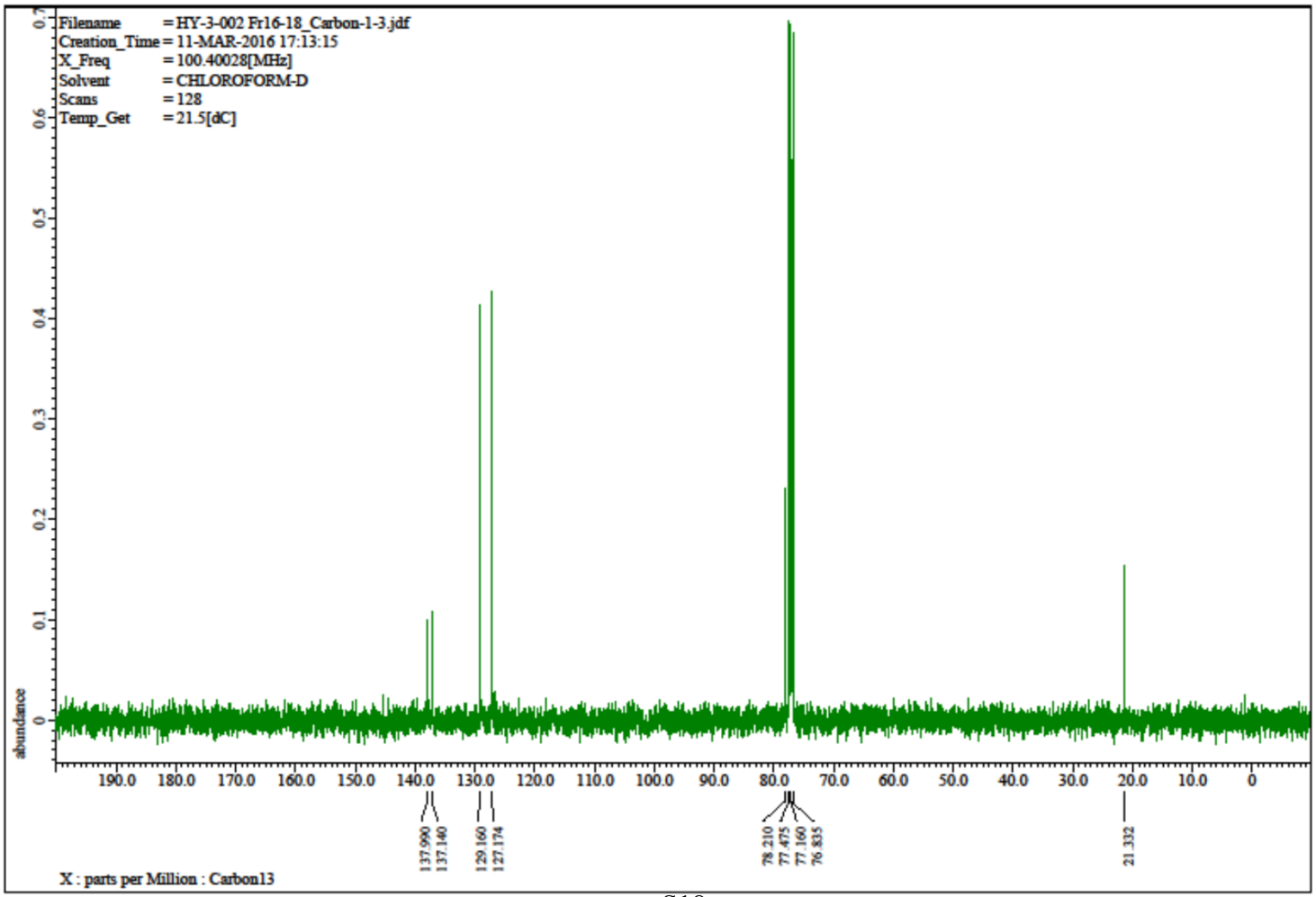
Creation_Time = 19-OCT-2015 13:05:18
X_Freq = 399.285[MHz]
Solvent = CHLOROFORM-D
Scans = 8
Temp_Get = 23.5[dC]
OH
OCOi-Pr
Me
Me
3b
X : parts per Million : Proton


Filename = HY-3-002 Fr16-18_Carbon-1-3.jdf
Creation_Time = 11-MAR-2016 17:13:15
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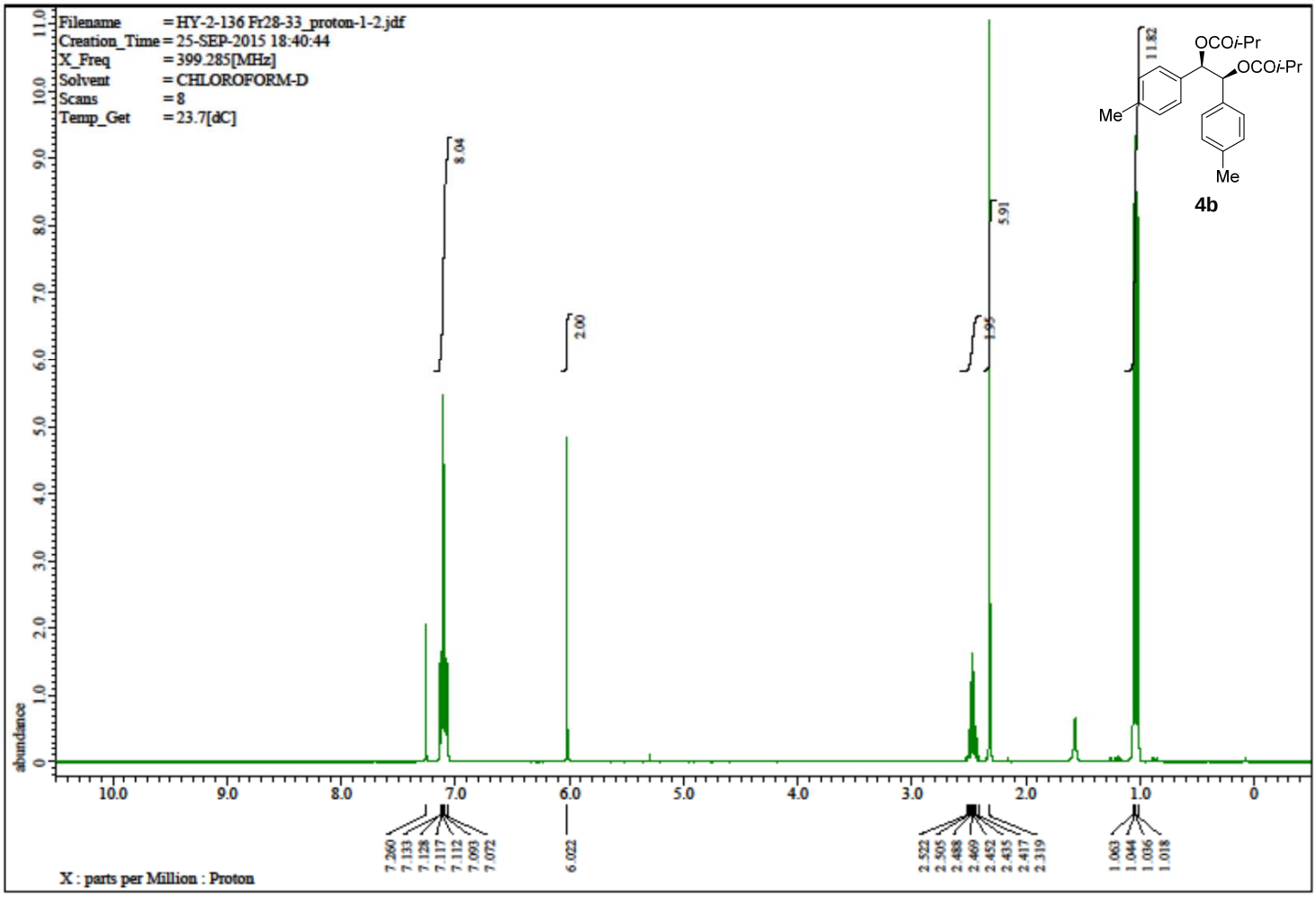
Scans = 128
Temp_Get = 21.5[dC]
X : parts per Million : Carbon13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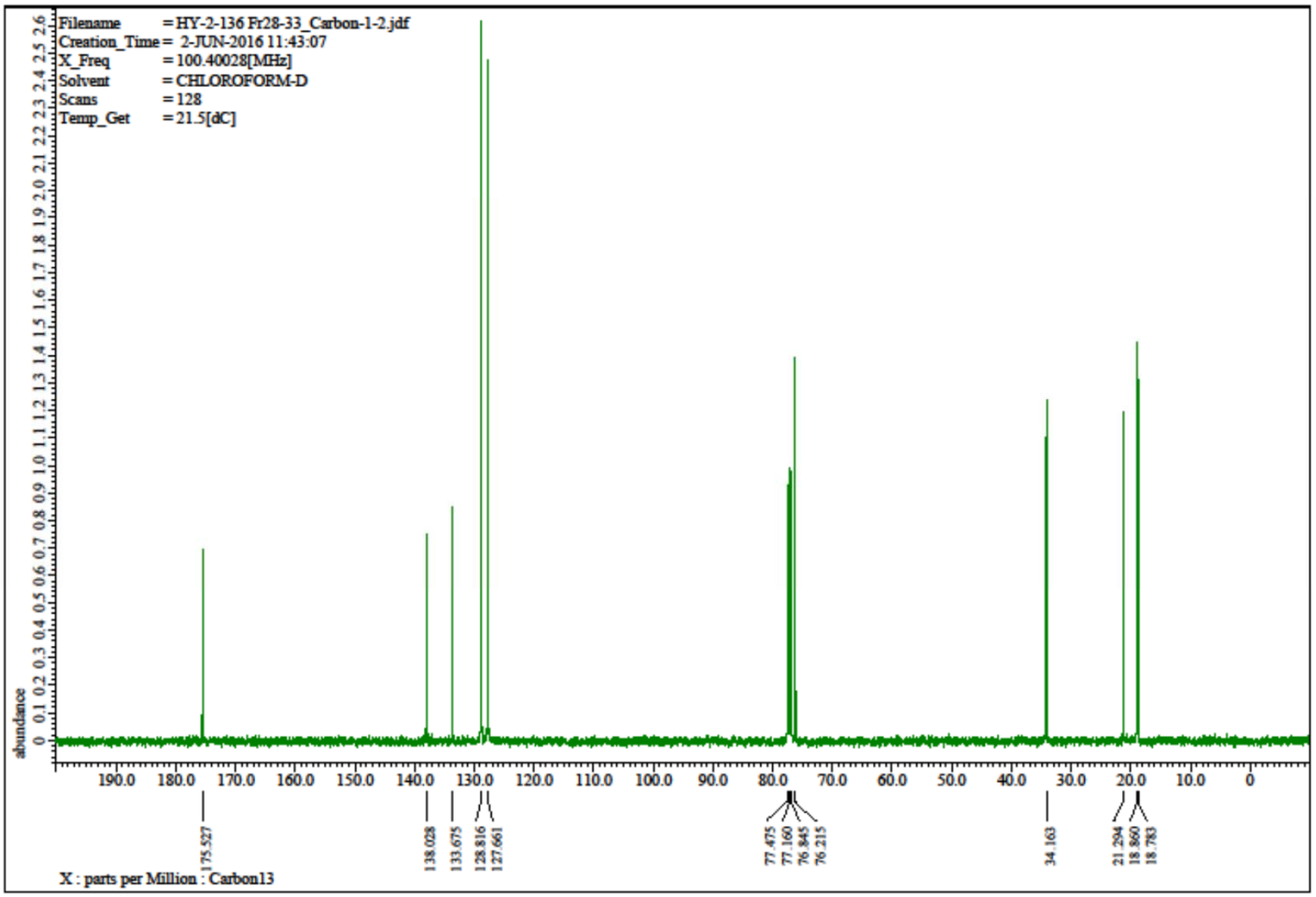
Creation_Time = 25-SEP-2015 18:40:44
X_Freq = 399.285[MHz]
Solvent = CHLOROFORM-D
Scans = 8
Temp_Get = 23.7[dC]
OCOi-Pr
OCOi-Pr
Me
Me
4b
X : parts per Million : Proton
abundance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Creation_Time = 2-JUN-2016 11:43:07
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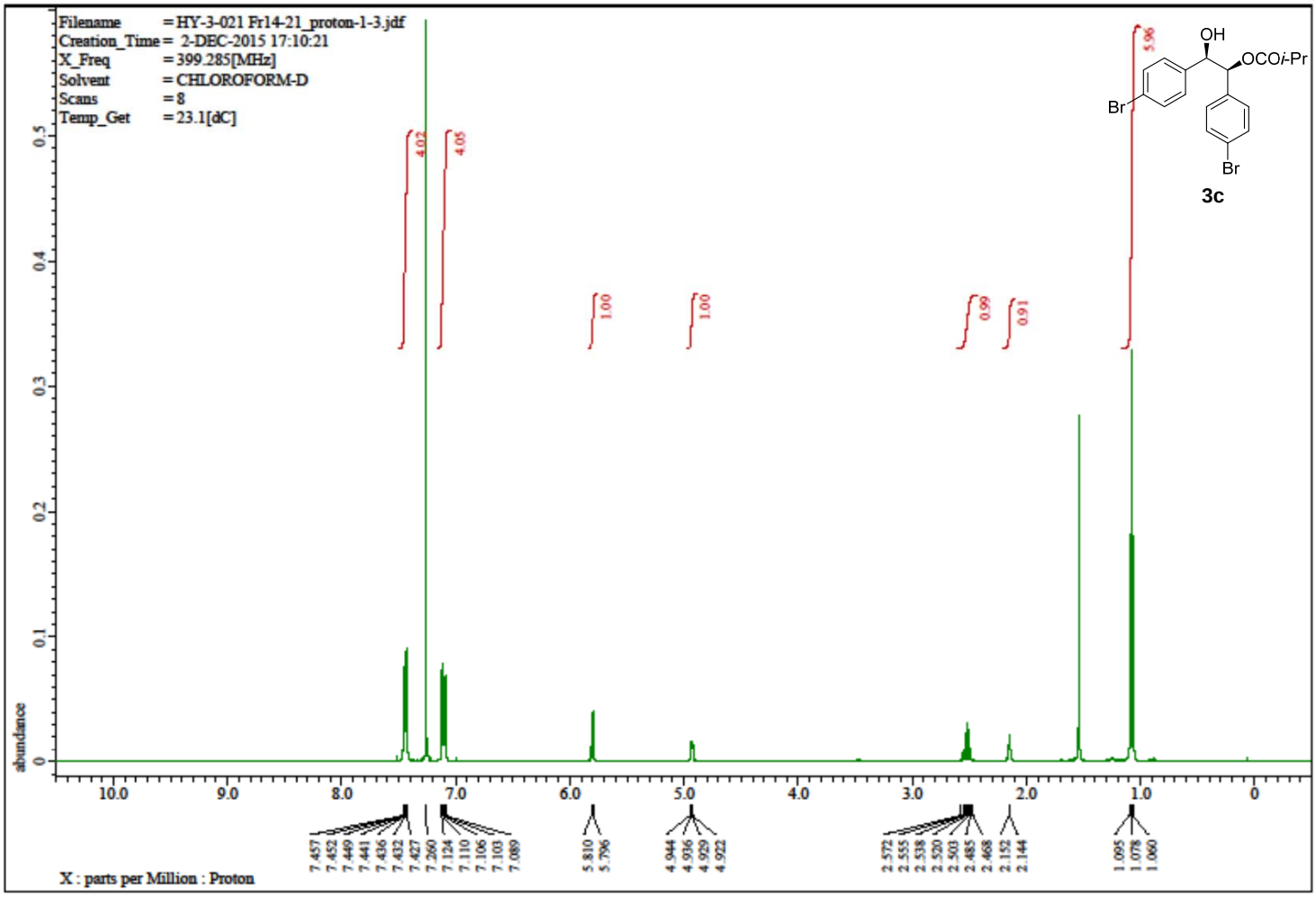
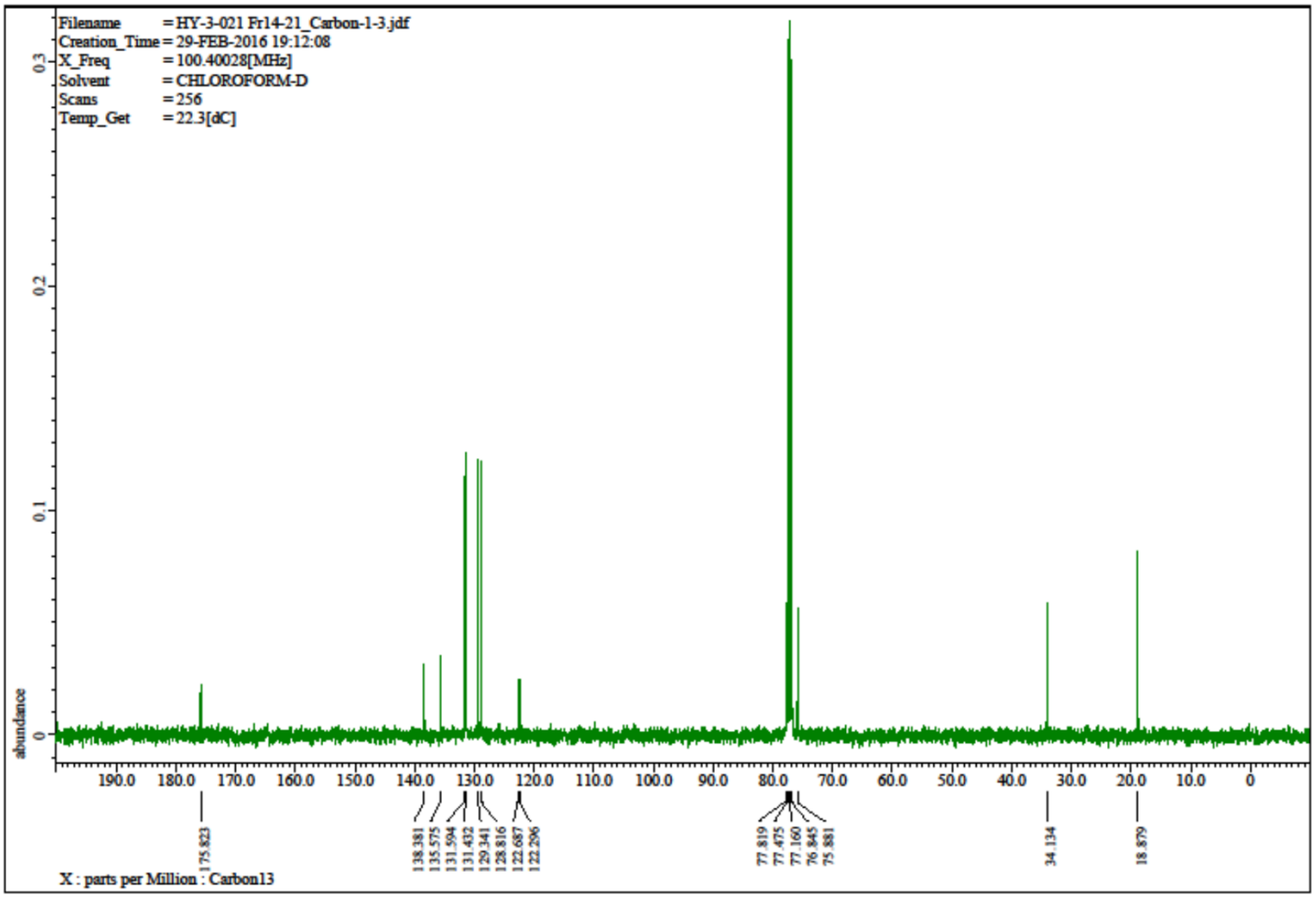
Solvent = CHLOROFORM-D
Scans = 128
Temp_Get = 21.5[dC]
X : parts per Million : Carbon13
abundance


Filename = HY-3-021 Fr14-21_proton-1-3.jdf
Creation_Time = 2-DEC-2015 17:10:21
X_Freq = 399.285[MHz]
Solvent = CHLOROFORM-D
Scans = 8
Temp_Get = 23.1[dC]
OH
OCOi-Pr
Br
Br
3c
X : parts per Million : Proton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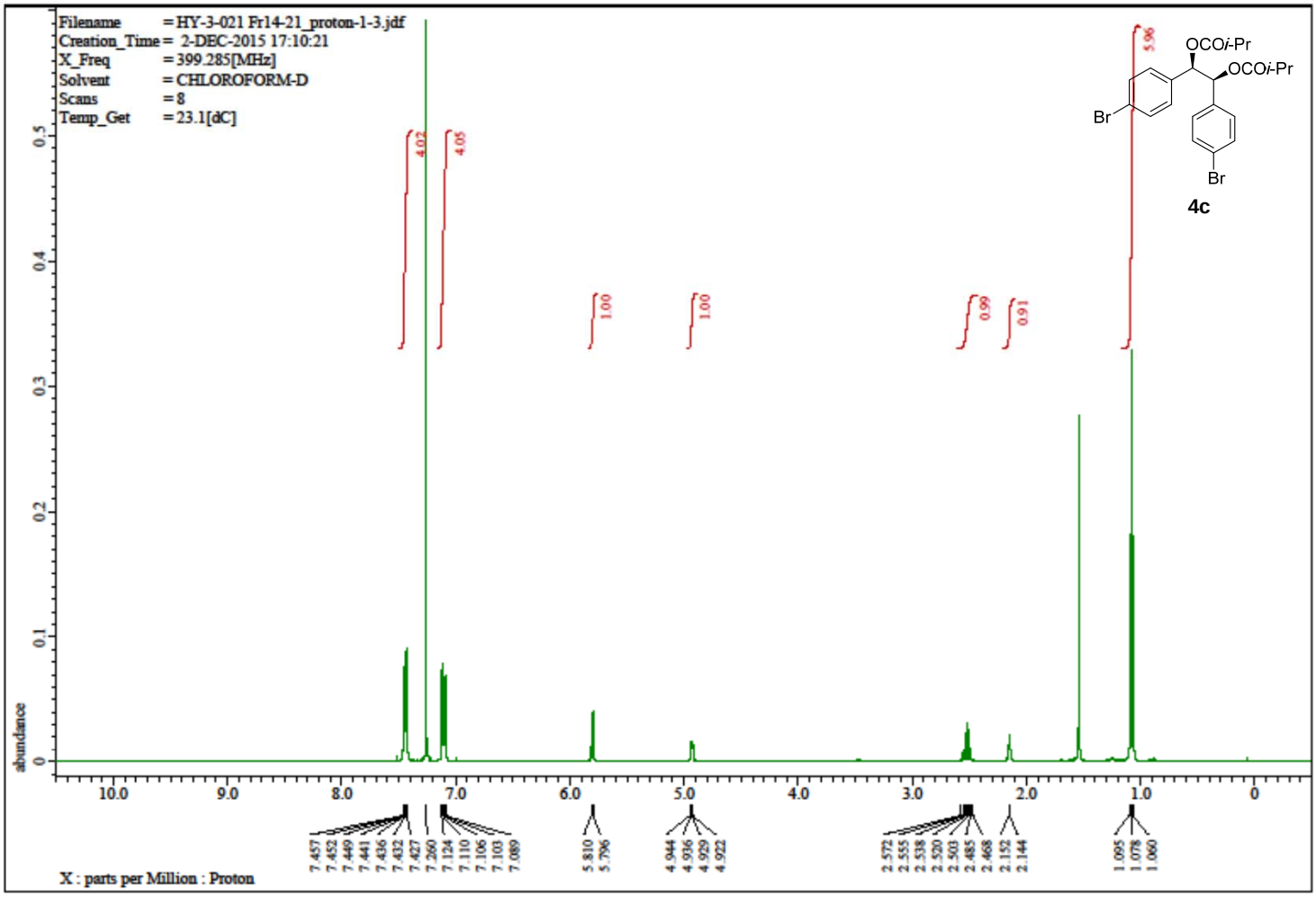
Creation_Time = 29-FEB-2016 19:12:08
X_Freq = 100.40028[MHz]
Solvent = CHLOROFORM-D
Scans = 256
Temp_Get = 22.3[dC]
X : parts per Million : Carbon13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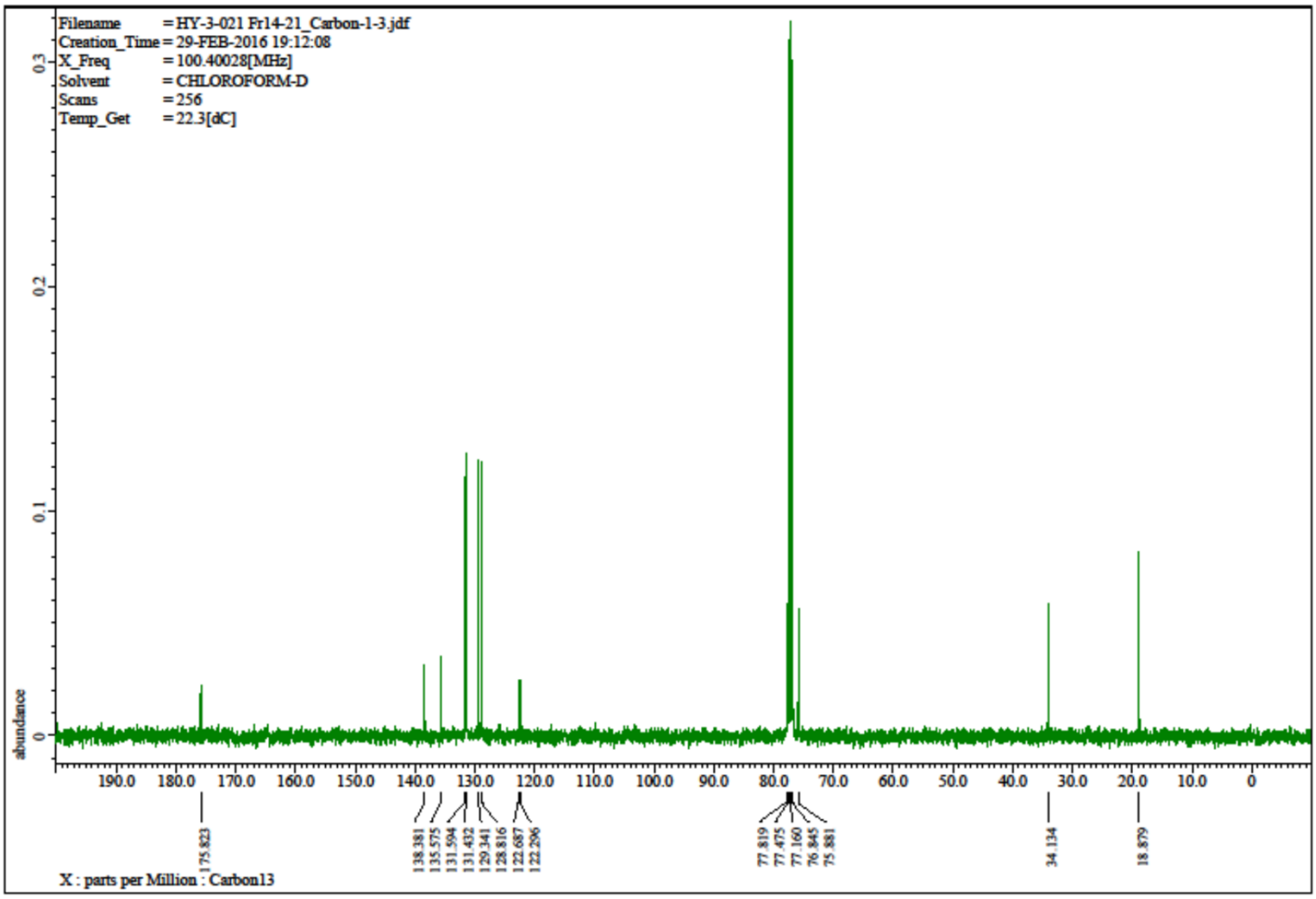
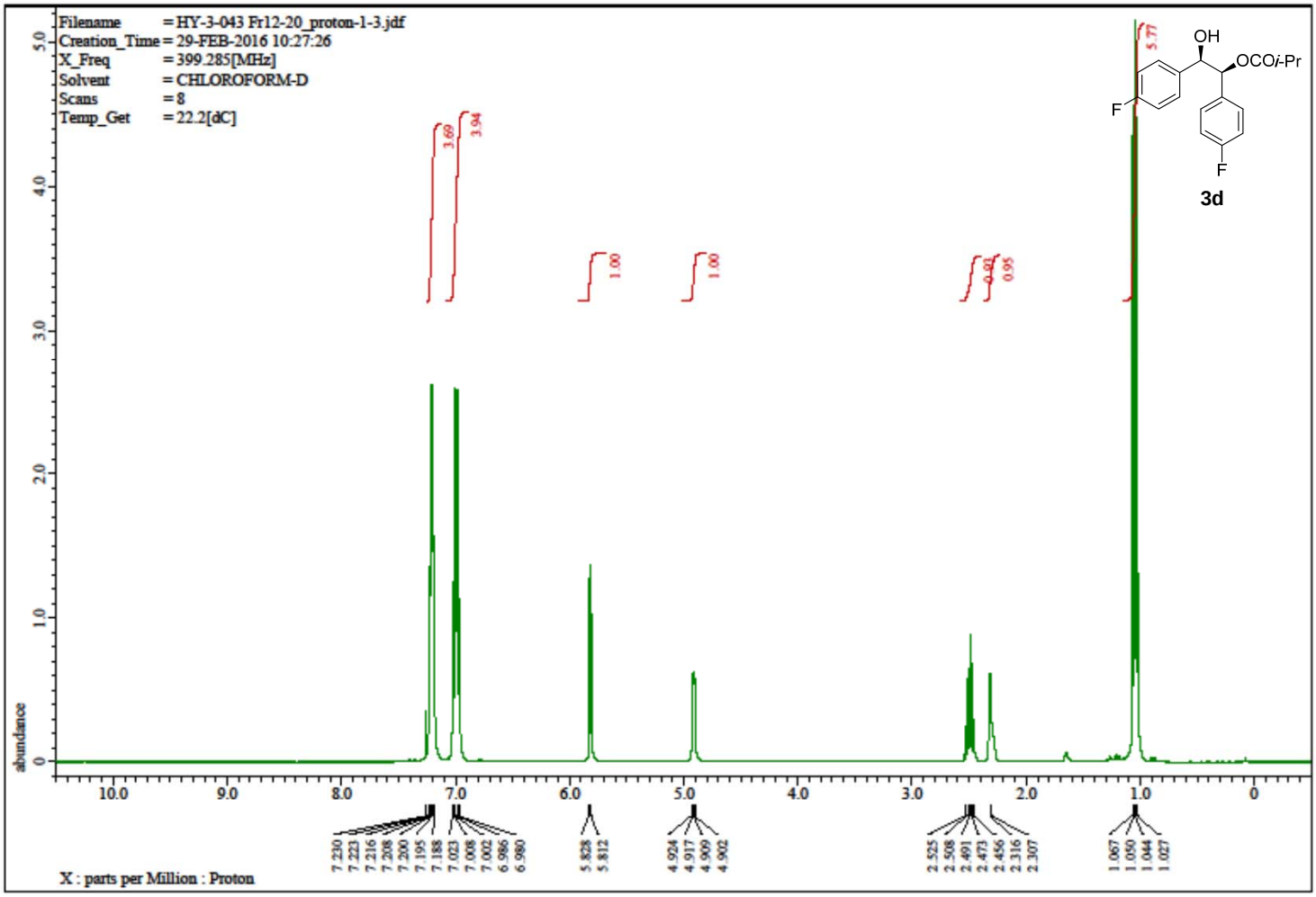
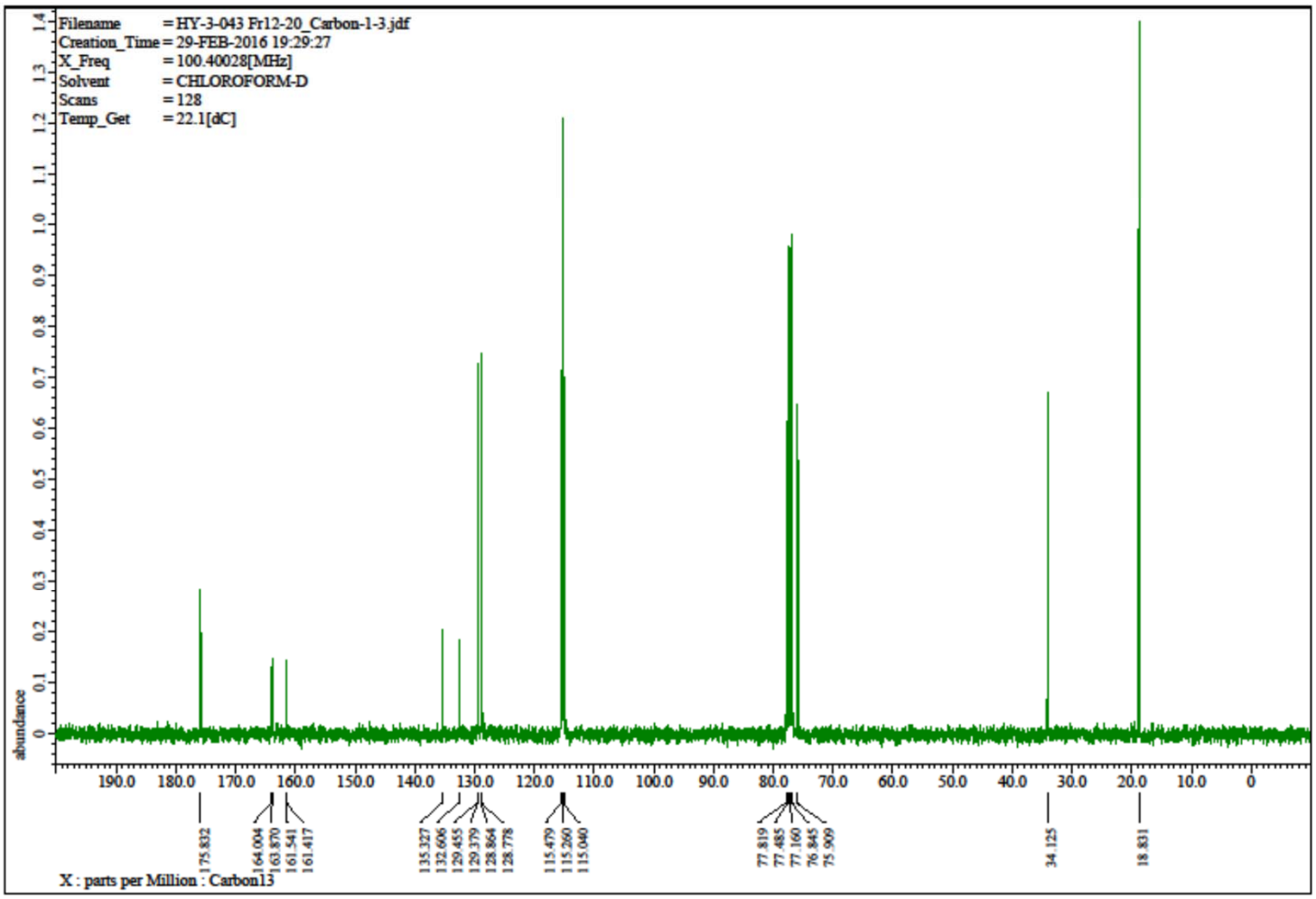
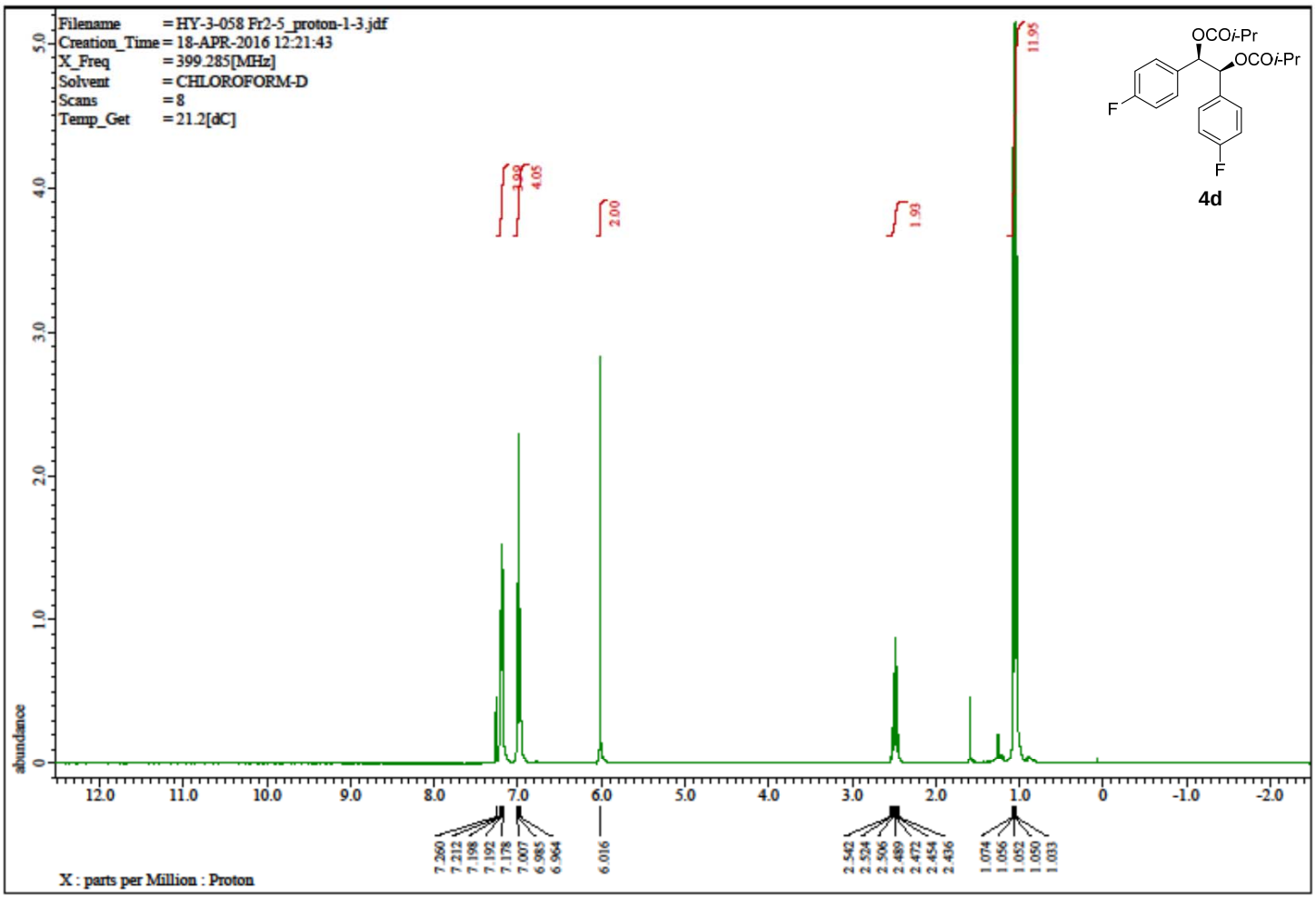
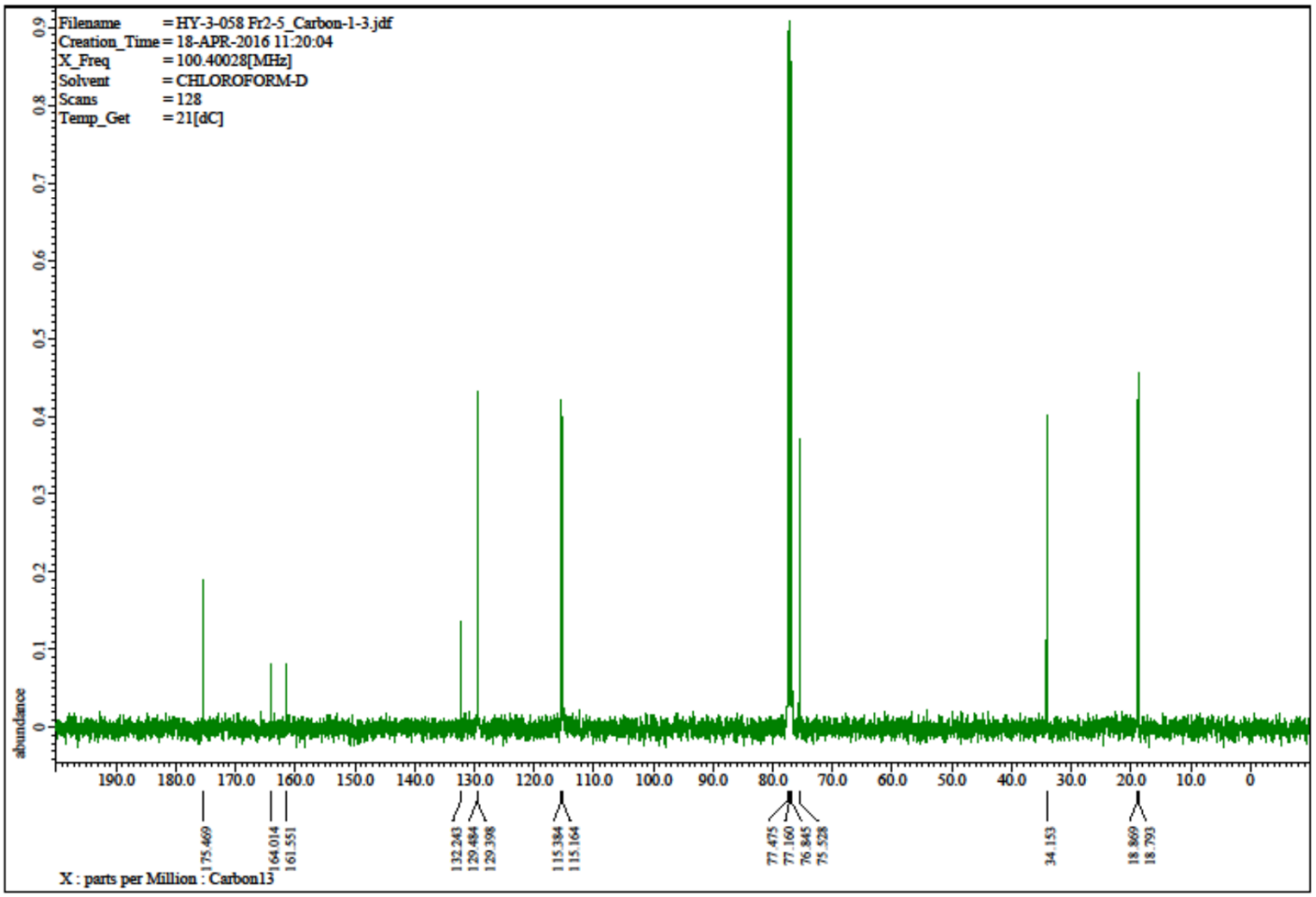
Creation_Time = 2-DEC-2015 17:10:21
X_Freq = 399.285[MHz]
Solvent = CHLOROFORM-D
Scans = 8
Temp_Get = 23.1[dC]
OCOi-Pr
OCOi-Pr
Br
Br
4c
abundance
X : parts per Million : Proton

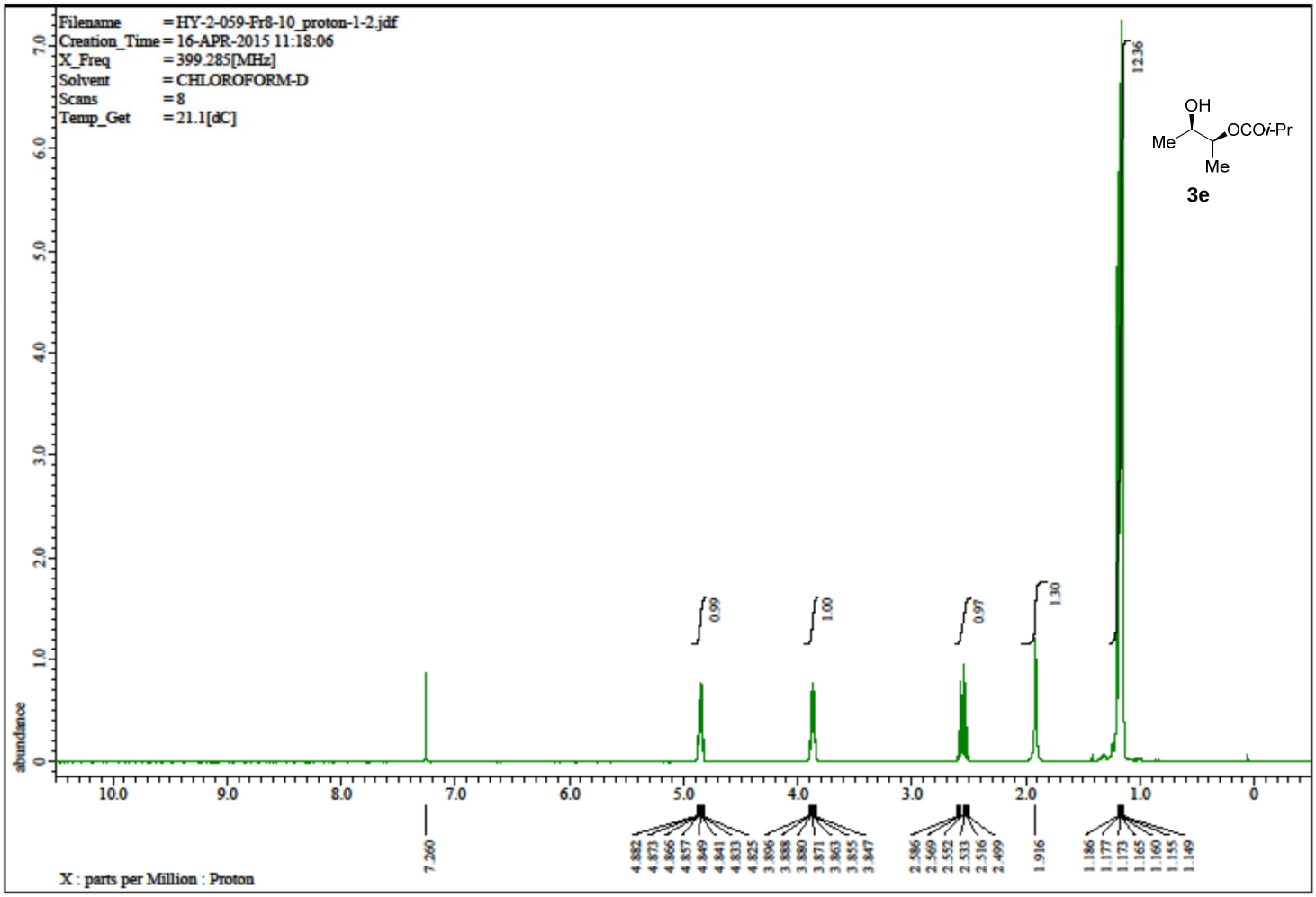

Filename = HY-3-021 Fr14-21_Carbon-1-3.jdf
Creation_Time = 29-FEB-2016 19:12:08
X_Freq = 100.40028[MHz]
Solvent = CHLOROFORM-D
Scans = 256
Temp_Get = 22.3[dC]
abundance
X : parts per Million : Carbon13

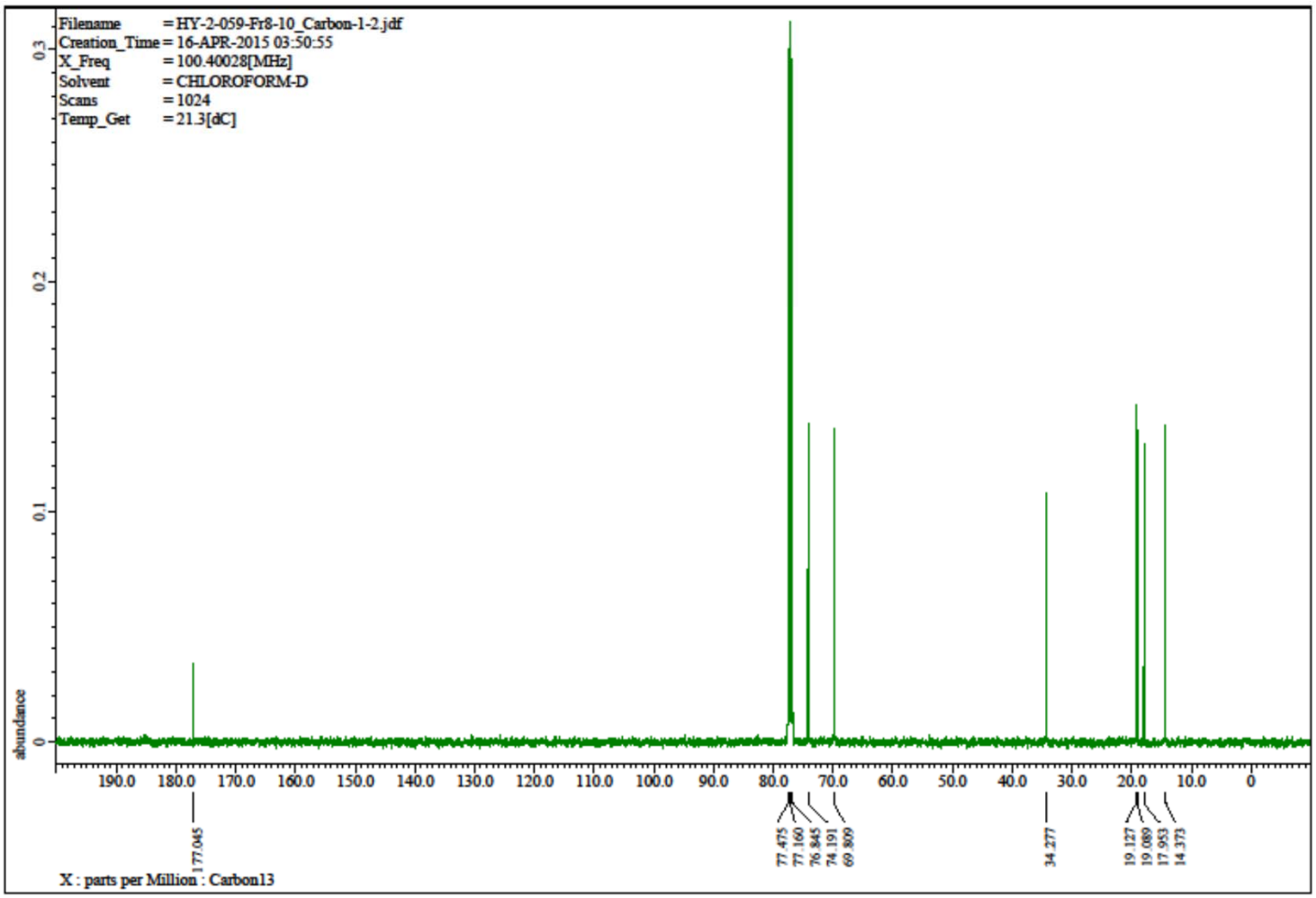

Filename = HY-3-043 Fr12-20_proton-1-3.jdf
Creation_Time = 29-FEB-2016 10:27:26
X_Freq = 399.285[MHz]
Solvent = CHLOROFORM-D
Scans = 8
Temp_Get = 22.2[dC]
OH
OCOi-Pr
F
F
3d
X : parts per Million : Proton
abundance

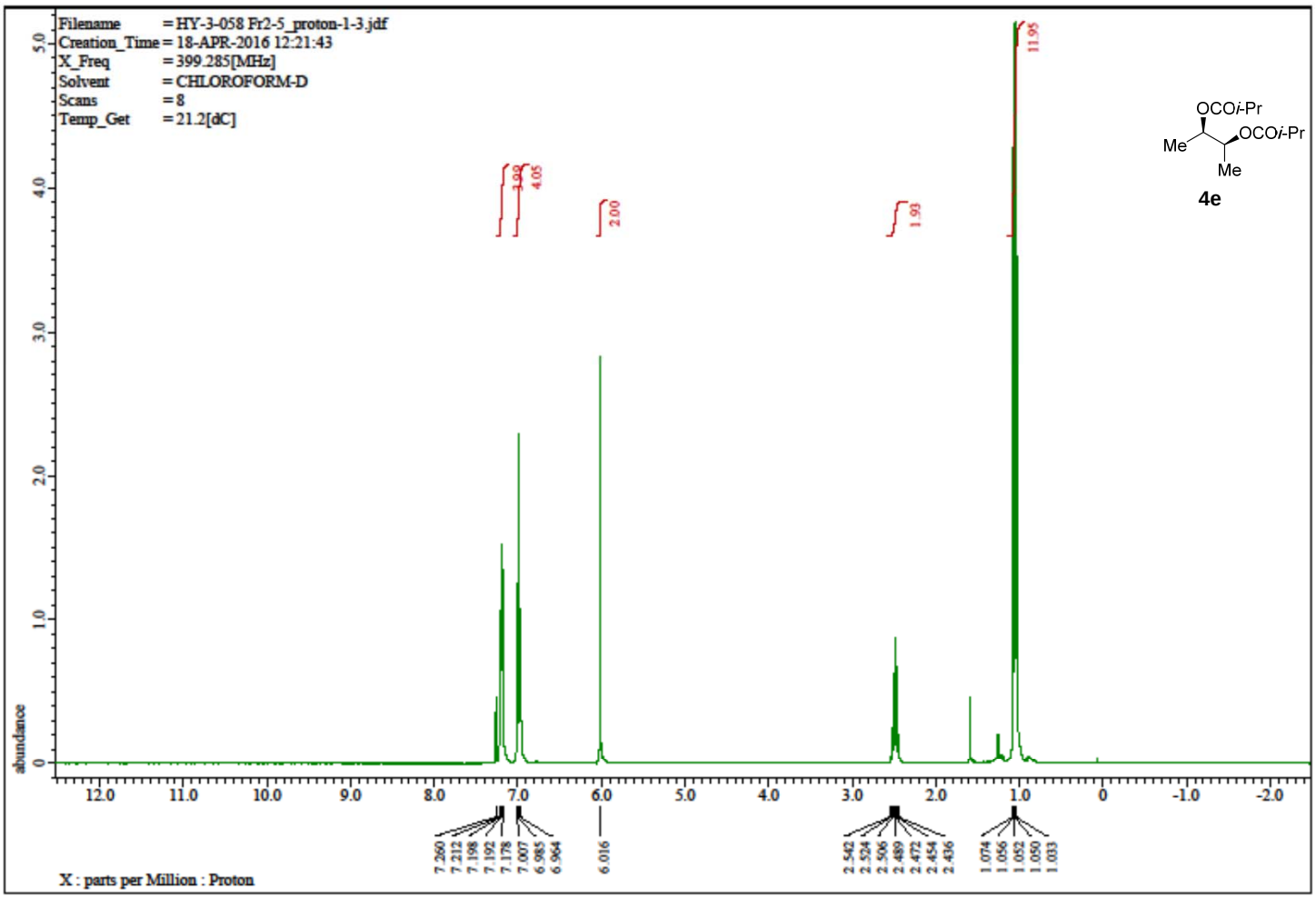

Filename = HY-3-043 Fr12-20_Carbon-1-3.jdf
Creation_Time = 29-FEB-2016 19:29:27
X_Freq = 100.40028[MHz]
Solvent = CHLOROFORM-D
Scans = 128
Temp_Get = 22.1[dC]
X : parts per Million : Carbon13
abundance

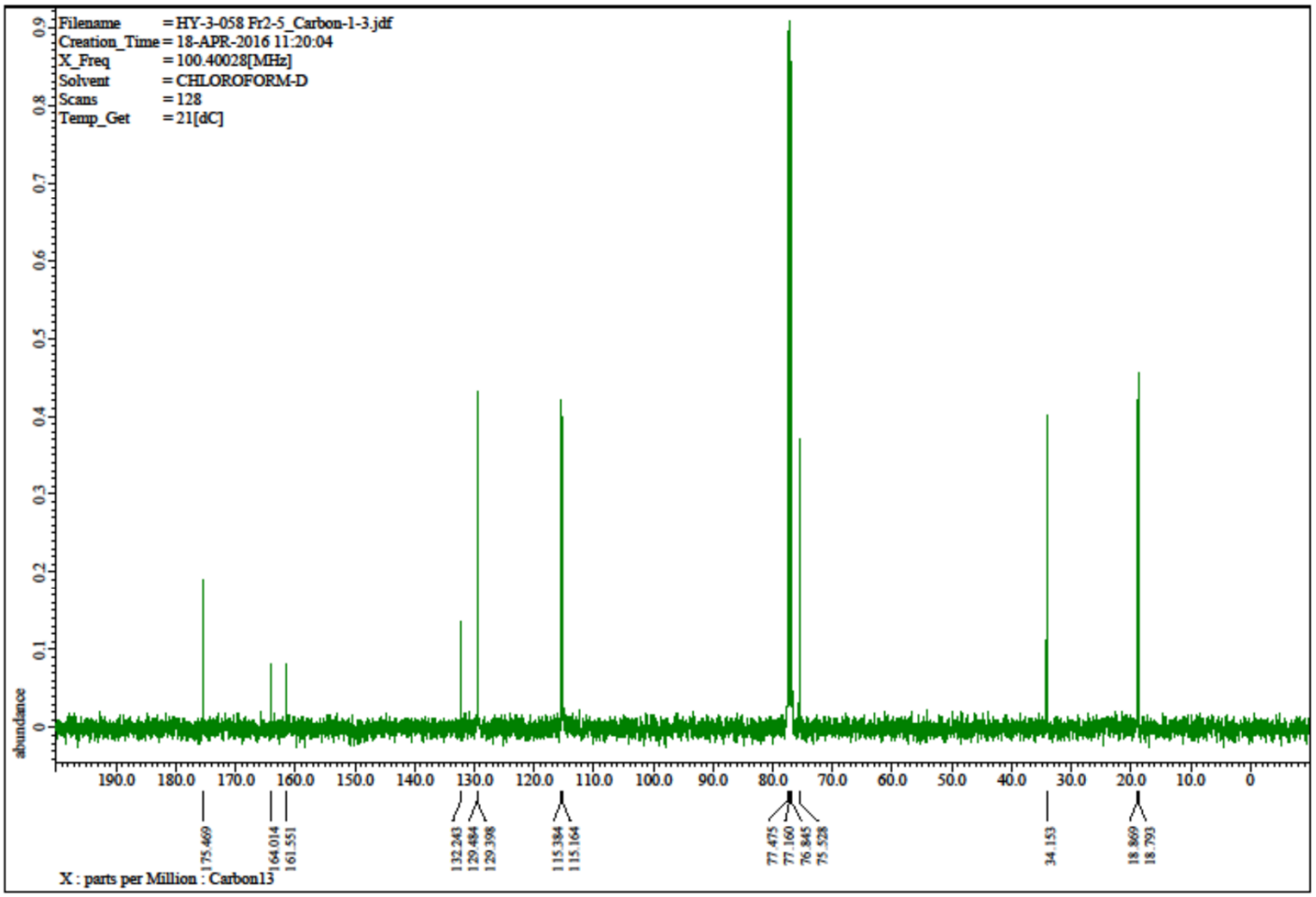

Filename = HY-3-058 Fr2-5_proton-1-3.jdf
Creation_Time = 18-APR-2016 12:21:43
X_Freq = 399.285[MHz]
Solvent = CHLOROFORM-D
Scans = 8
Temp_Get = 21.2[dC]
OCOi-Pr
OCOi-Pr
F
F
4d
X : parts per Million : Proton
abundance

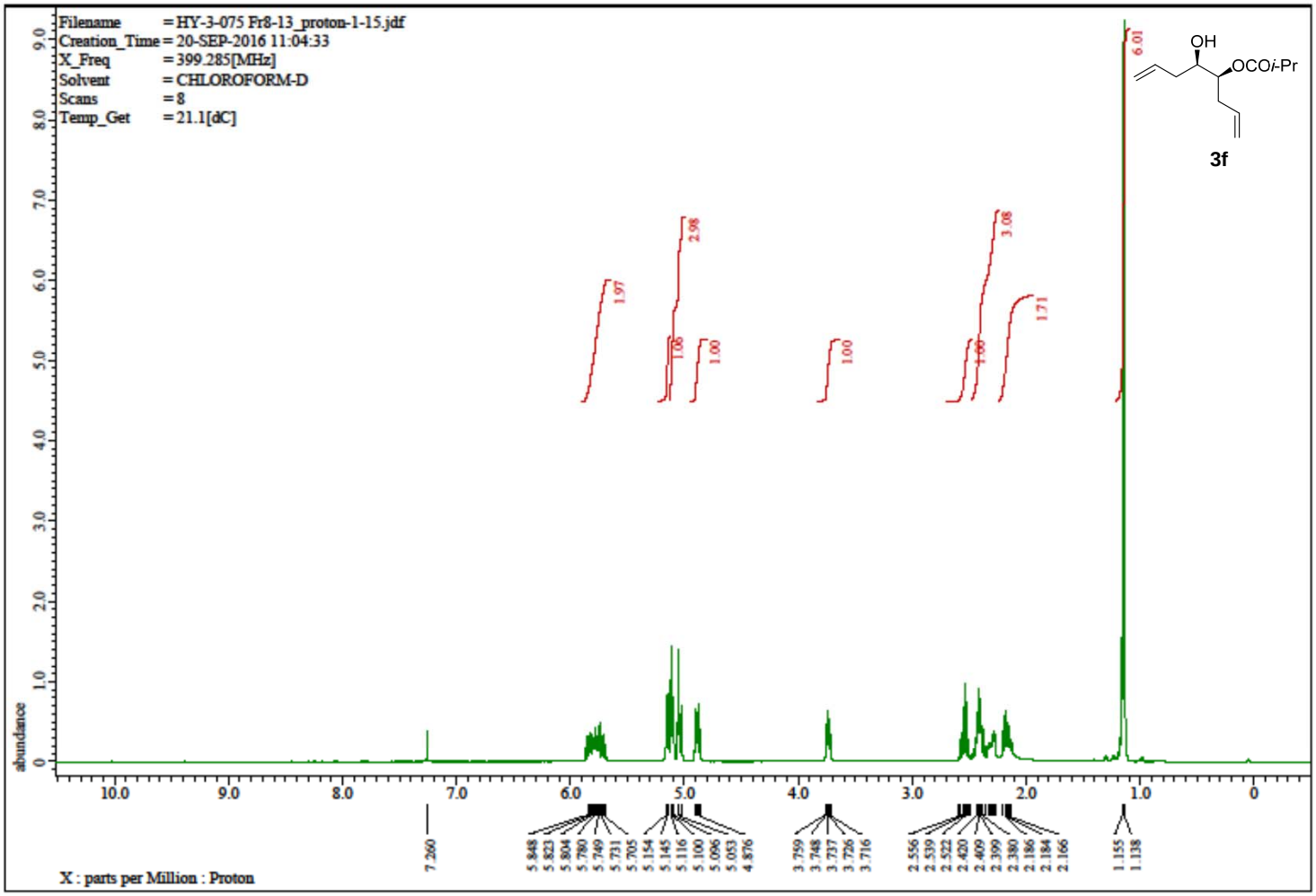

Filename = HY-3-058 Fr2-5_Carbon-1-3.jdf
Creation_Time = 18-APR-2016 11:20:04
X_Freq = 100.40028[MHz]
Solvent = CHLOROFORM-D
Scans = 128
Temp_Get = 21[dC]
X : parts per Million : Carbon13
abundance

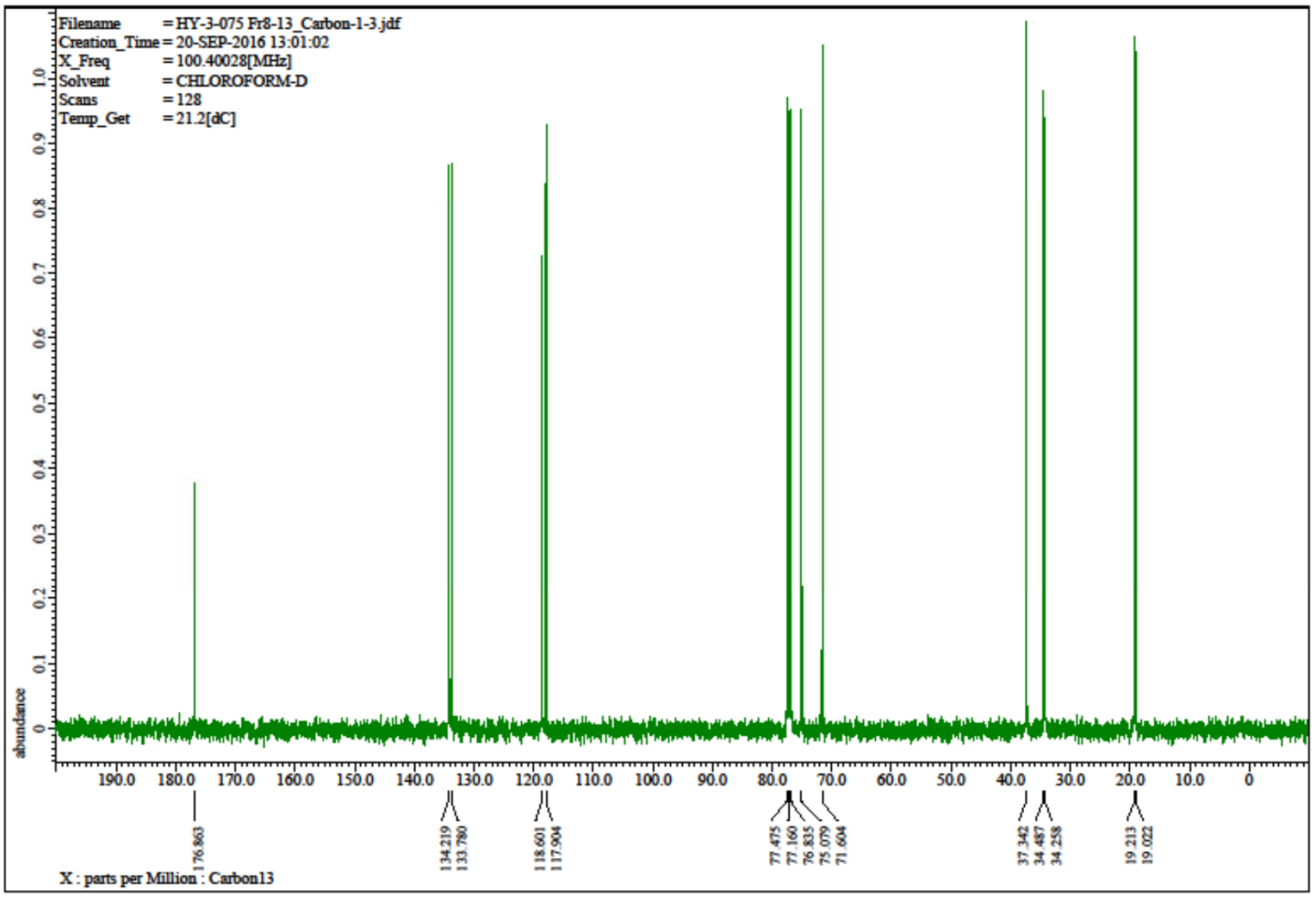

Filename = HY-2-059-Fr8-10_proton-1-2.jdf
Creation_Time = 16-APR-2015 11:18:06
X_Freq = 399.285[MHz]
Solvent = CHLOROFORM-D
Scans = 8
Temp_Get = 21.1[dC]
OH
Me
OCO*i*-Pr
Me
3e
12.36
0.99
1.00
0.97
1.30
7.260
4.882
4.873
4.866
4.857
4.849
4.841
4.833
4.825
3.896
3.888
3.880
3.871
3.863
3.855
3.847
2.586
2.569
2.552
2.533
2.516
2.499
1.916
1.186
1.177
1.173
1.165
1.160
1.155
1.149
abundance
X : parts per Million : Proton

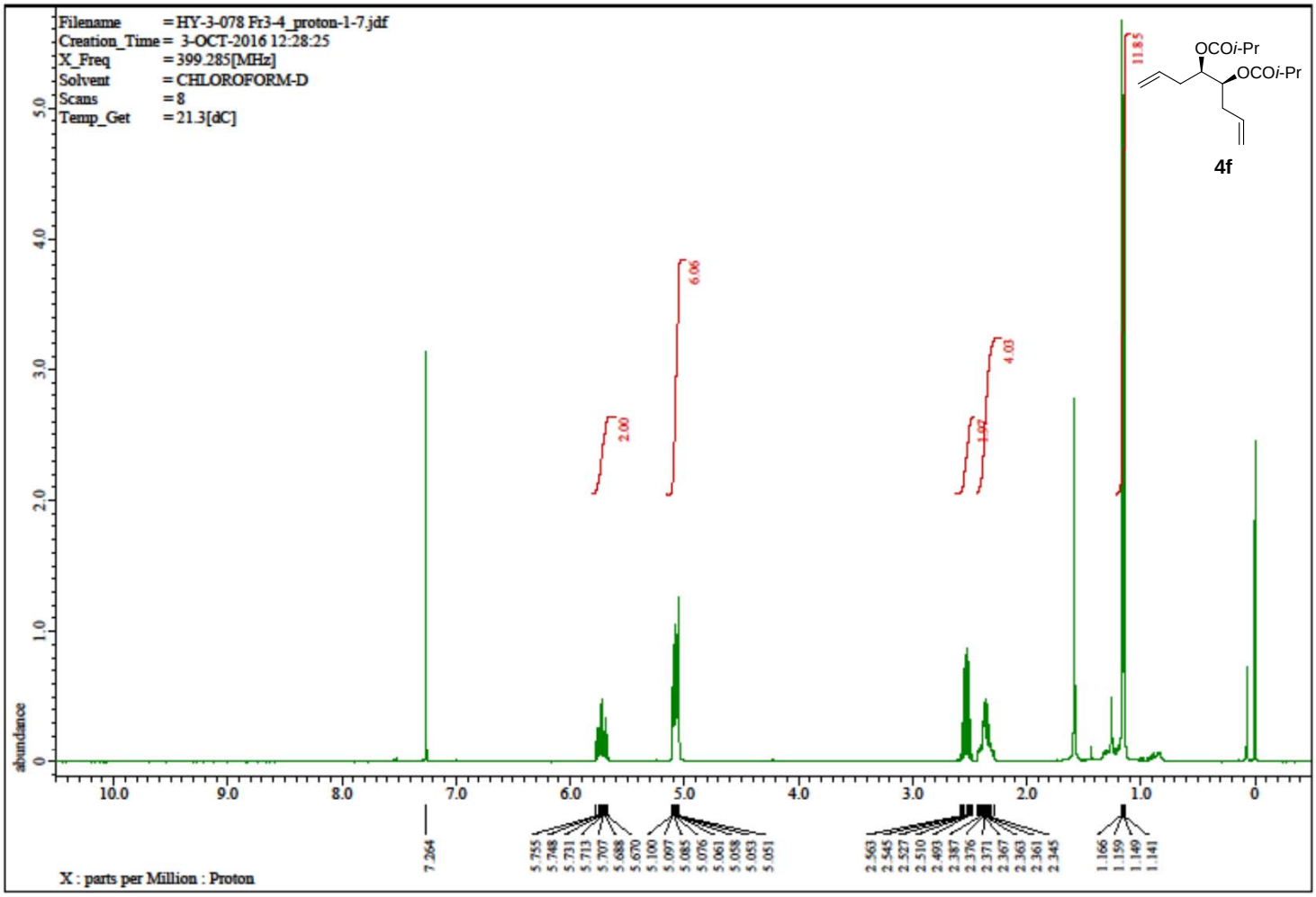

Filename = HY-2-059-Fr8-10_Carbon-1-2.jdf
Creation_Time = 16-APR-2015 03:50:55
X_Freq = 100.40028[MHz]
Solvent = CHLOROFORM-D
Scans = 1024
Temp_Get = 21.3[dC]
177.045
77.475
77.160
76.845
74.191
69.809
34.277
19.127
19.089
17.953
14.373
abundance
X : parts per Million : Carbon13

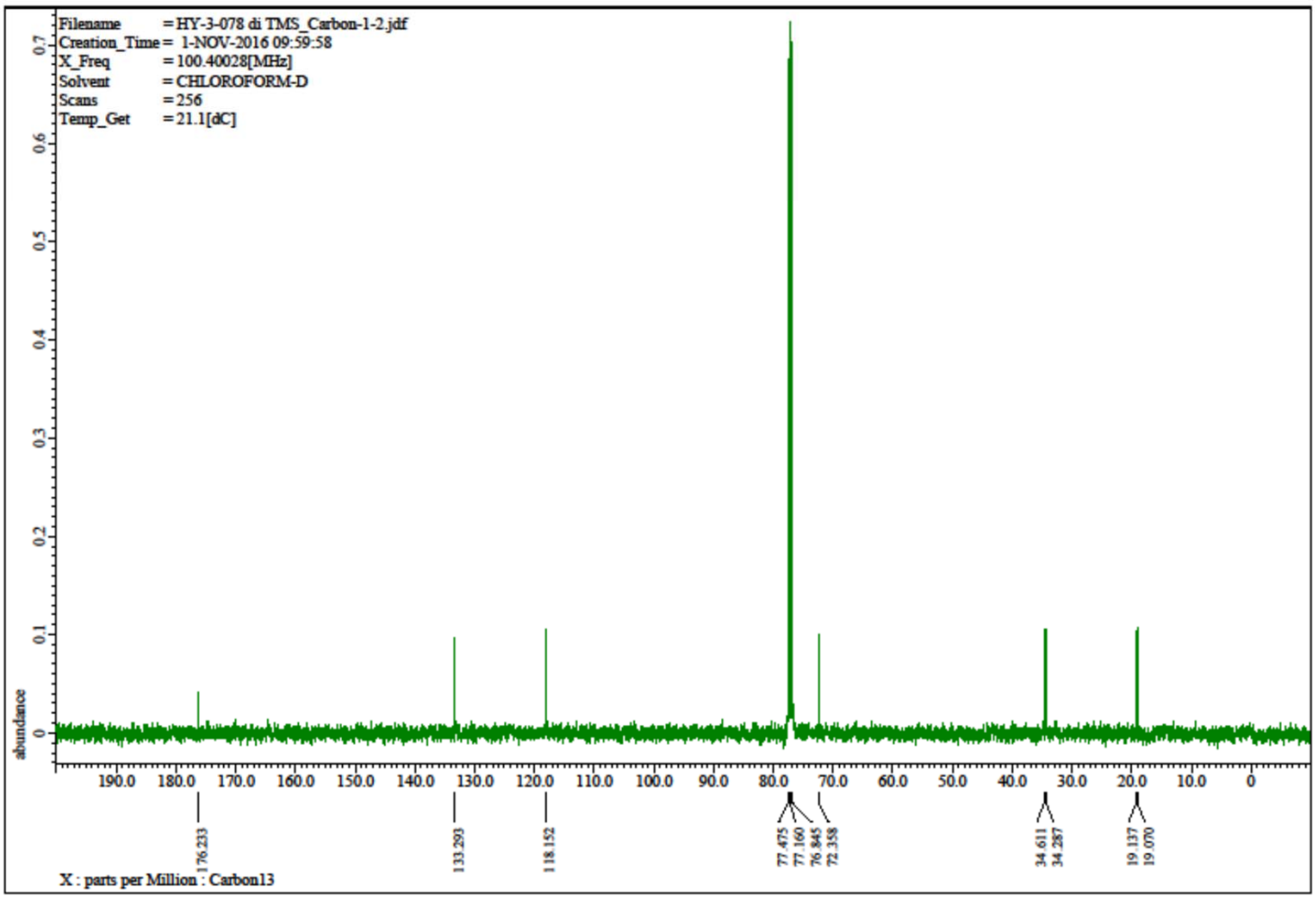

Filename = HY-3-058 Fr2-5_proton-1-3.jdf
Creation_Time = 18-APR-2016 12:21:43
X_Freq = 399.285[MHz]
Solvent = CHLOROFORM-D
Scans = 8
Temp_Get = 21.2[dC]
OCOi-Pr
OCOi-Pr
Me
Me
4e
X : parts per Million : Proton
abundance

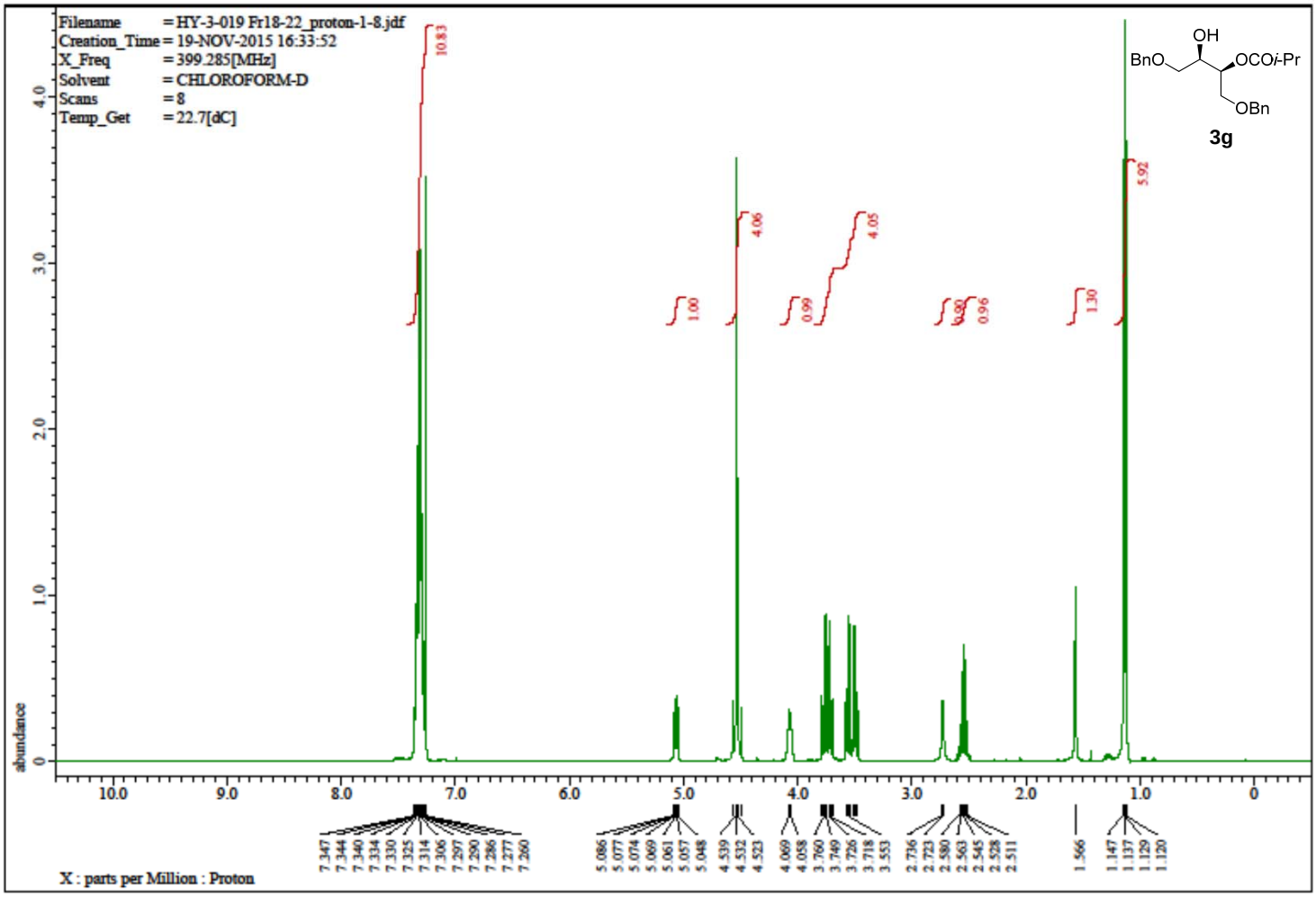

Filename = HY-3-058 Fr2-5_Carbon-1-3.jdf
Creation_Time = 18-APR-2016 11:20:04
X_Freq = 100.40028[MHz]
Solvent = CHLOROFORM-D
Scans = 128
Temp_Get = 21[dC]
X : parts per Million : Carbon13
abundance

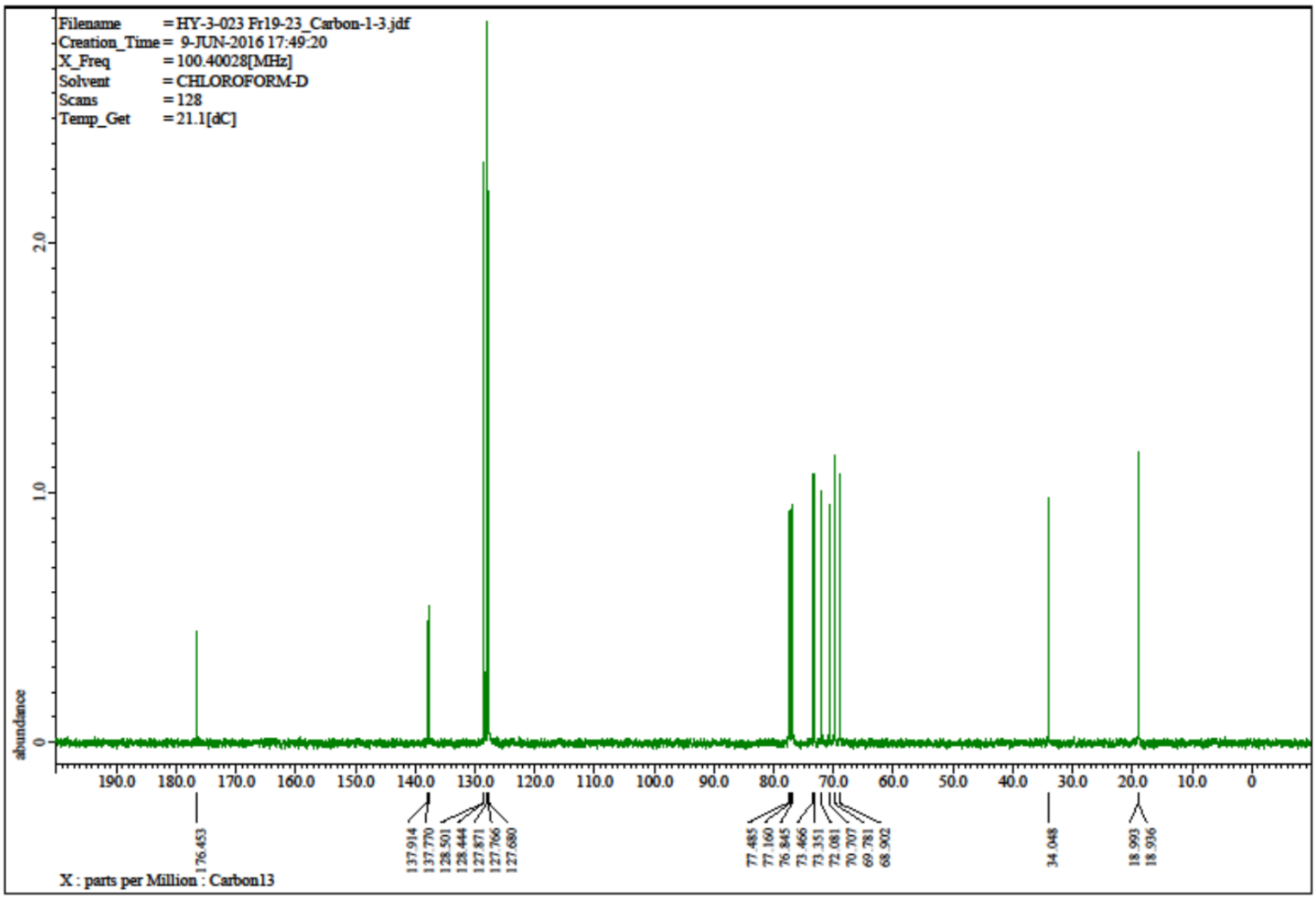

Filename = HY-3-075 Fr8-13_proton-1-15.jdf
Creation_Time = 20-SEP-2016 11:04:33
X_Freq = 399.285[MHz]
Solvent = CHLOROFORM-D
Scans = 8
Temp_Get = 21.1[dC]
OH
OCOi-Pr
3f
6.01
2.98
3.08
1.97
1.71
1.06
1.00
1.00
1.00
1.00
abundance
X : parts per Million : Proton
7.260
5.848 5.823 5.804 5.780 5.749 5.731 5.705
5.154 5.145 5.116 5.100 5.096 5.053 4.876
3.759 3.748 3.737 3.726 3.716
2.556 2.539 2.522 2.420 2.409 2.399 2.380 2.186 2.184 2.166
1.155 1.138

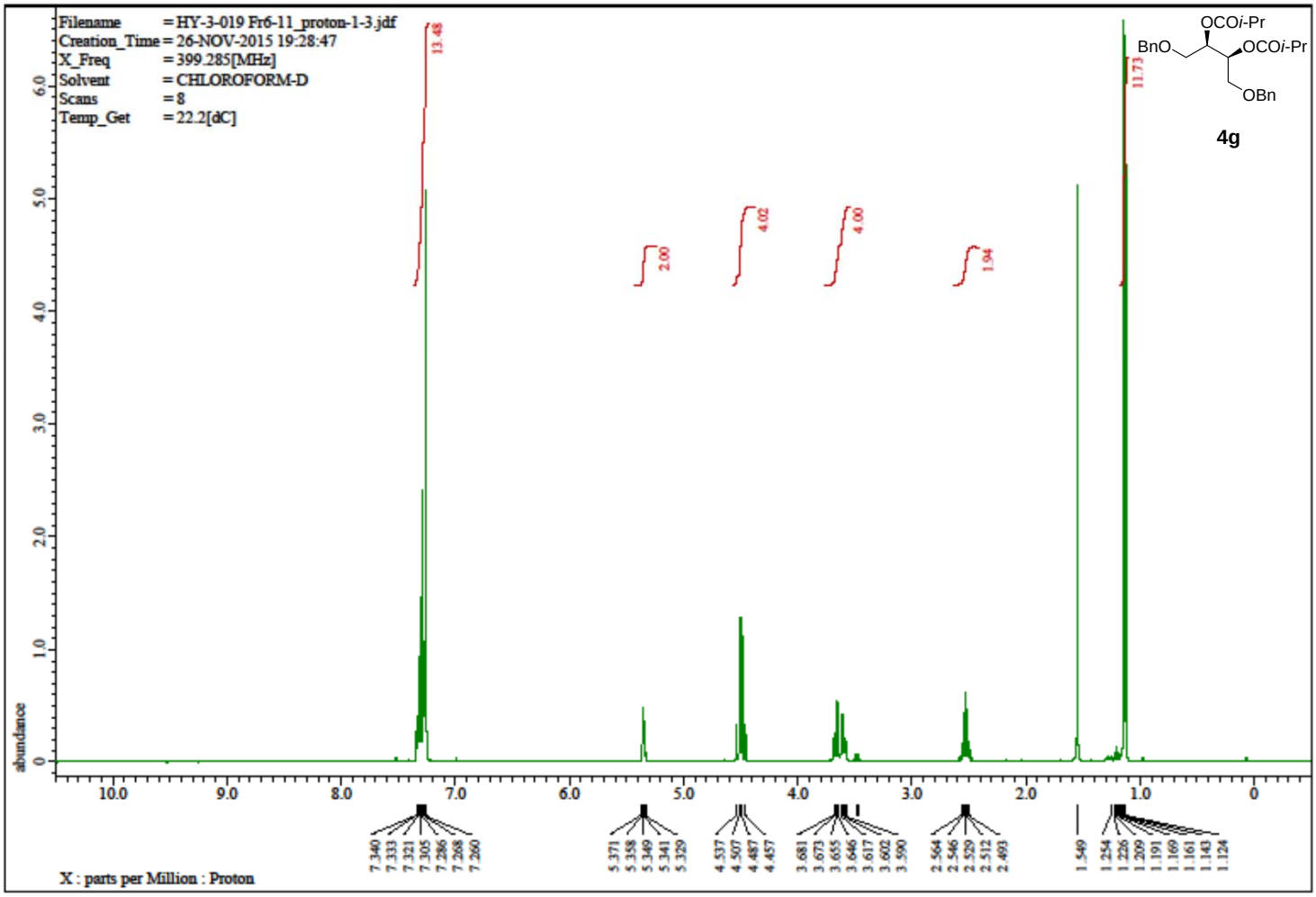

Filename = HY-3-075 Fr8-13_Carbon-1-3.jdf
Creation_Time = 20-SEP-2016 13:01:02
X_Freq = 100.40028[MHz]
Solvent = CHLOROFORM-D
Scans = 128
Temp_Get = 21.2[dC]
abundance
X : parts per Million : Carbon13
176.863
134.219 133.780
118.601 117.904
77.475 77.160 76.835 75.079 71.604
37.342 34.487 34.258
19.213 19.022

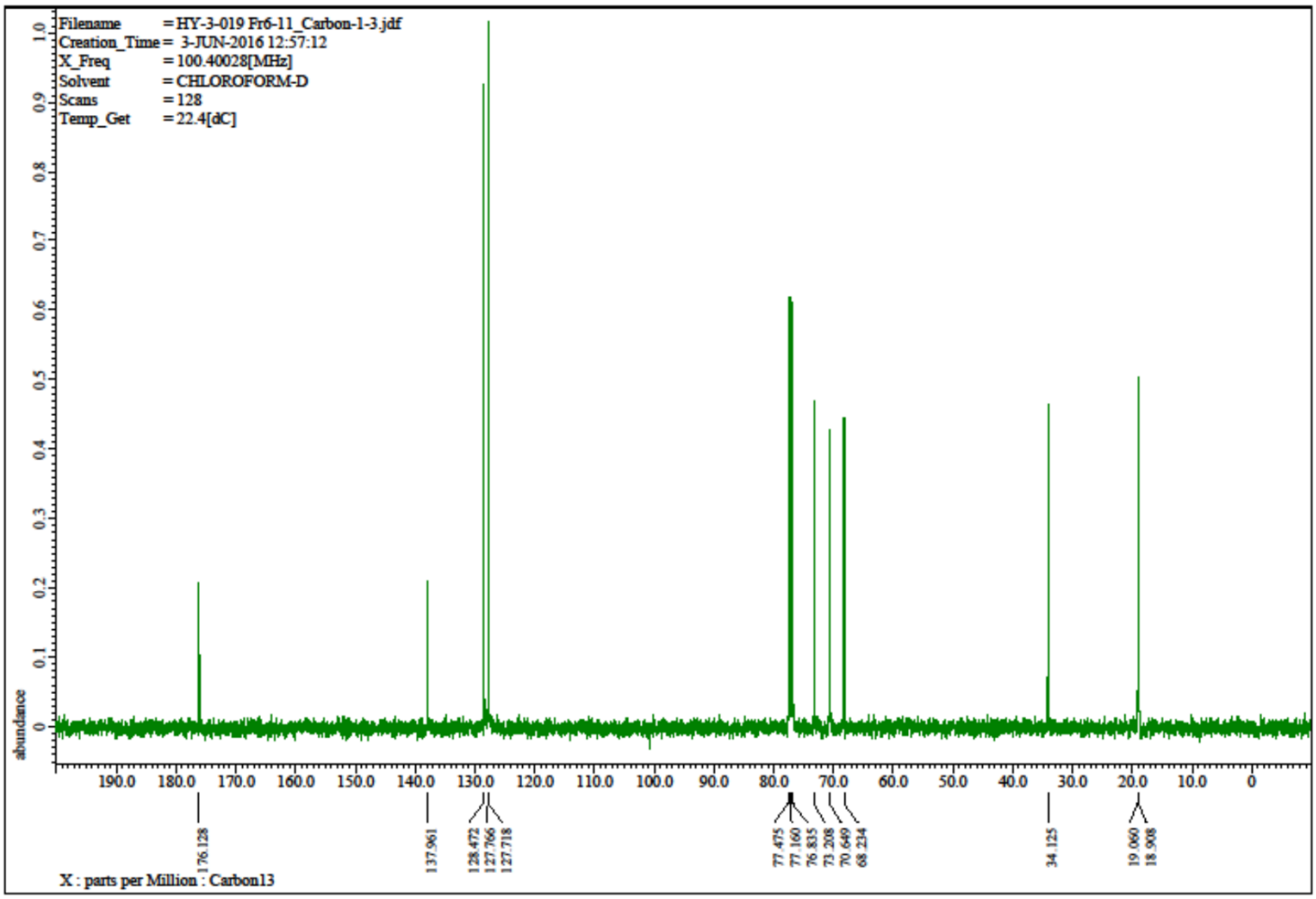

Filename = HY-3-078 Fr3-4_proton-1-7.jdf
Creation_Time = 3-OCT-2016 12:28:25
X_Freq = 399.285[MHz]
Solvent = CHLOROFORM-D
Scans = 8
Temp_Get = 21.3[dC]
OCOi-Pr
OCOi-Pr
4f
11.85
6.06
4.03
2.00
1.07
abundance
7.264
5.755
5.748
5.731
5.713
5.707
5.688
5.670
5.100
5.097
5.085
5.076
5.061
5.058
5.053
5.051
2.563
2.545
2.527
2.510
2.491
2.387
2.376
2.371
2.367
2.363
2.361
2.345
1.166
1.159
1.149
1.141
X : parts per Million : Proton

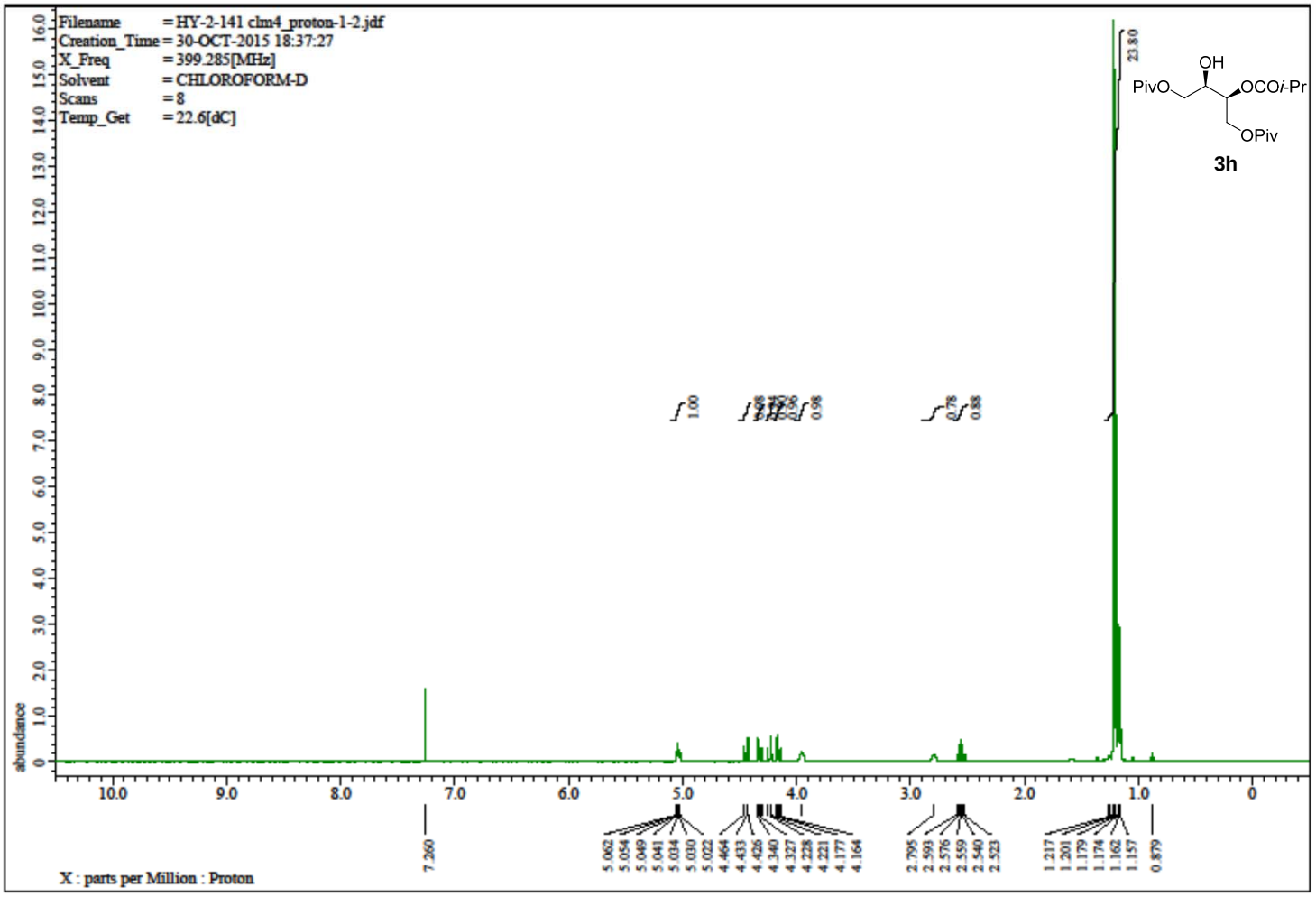

Filename = HY-3-078 di TMS_Carbon-1-2.jdf
Creation_Time = 1-NOV-2016 09:59:58
X_Freq = 100.40028[MHz]
Solvent = CHLOROFORM-D
Scans = 256
Temp_Get = 21.1[dC]
abundance
176.233
133.293
118.152
77.475
77.160
76.845
72.358
34.611
34.287
19.137
19.070
X : parts per Million : Carbon13

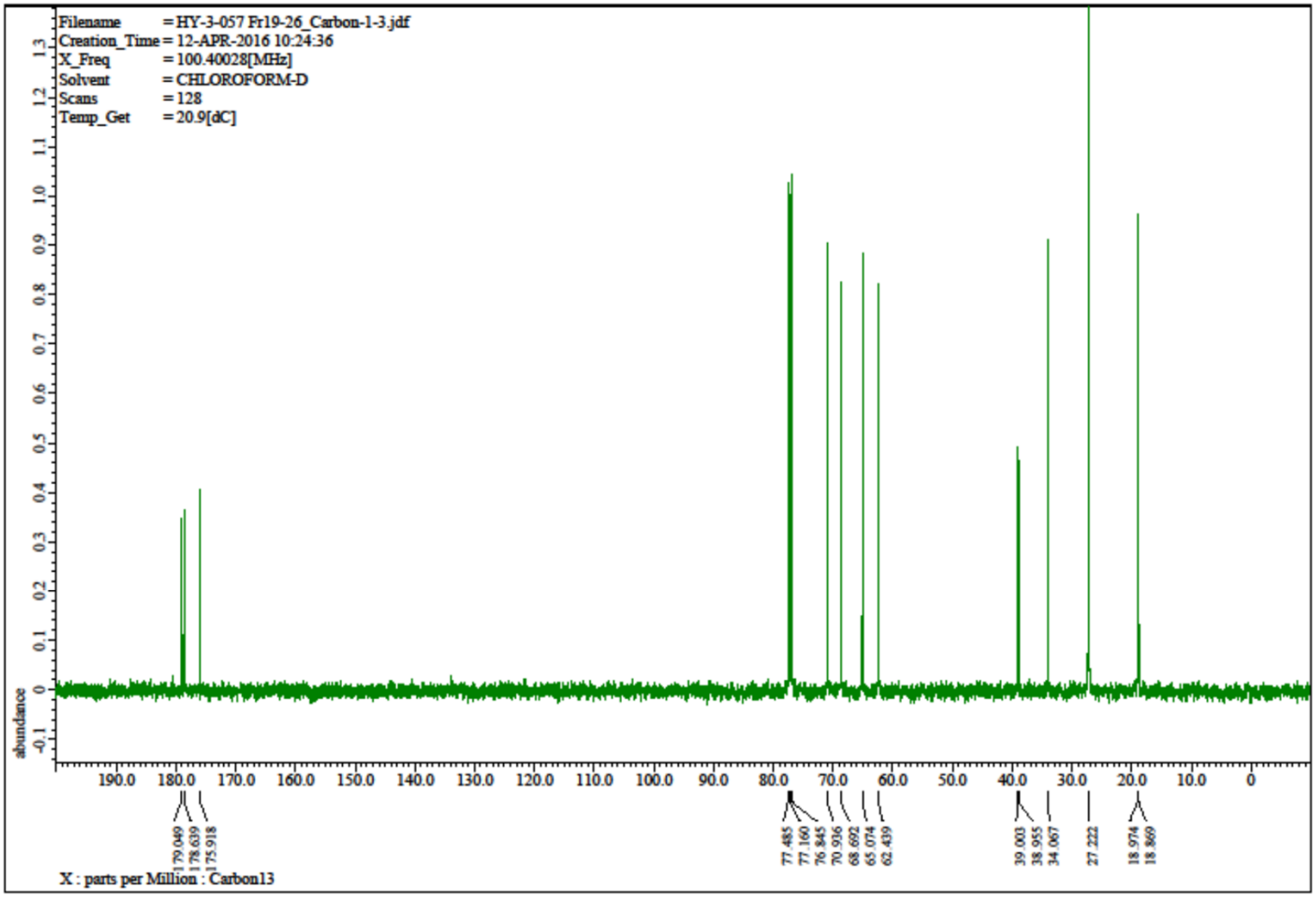

Filename = HY-3-019 Fr18-22_proton-1-8.jdf
Creation_Time = 19-NOV-2015 16:33:52
X_Freq = 399.285[MHz]
Solvent = CHLOROFORM-D
Scans = 8
Temp_Get = 22.7[dC]
OH
BnO
OCOi-Pr
OBn
3g
X : parts per Million : Proton
abundance

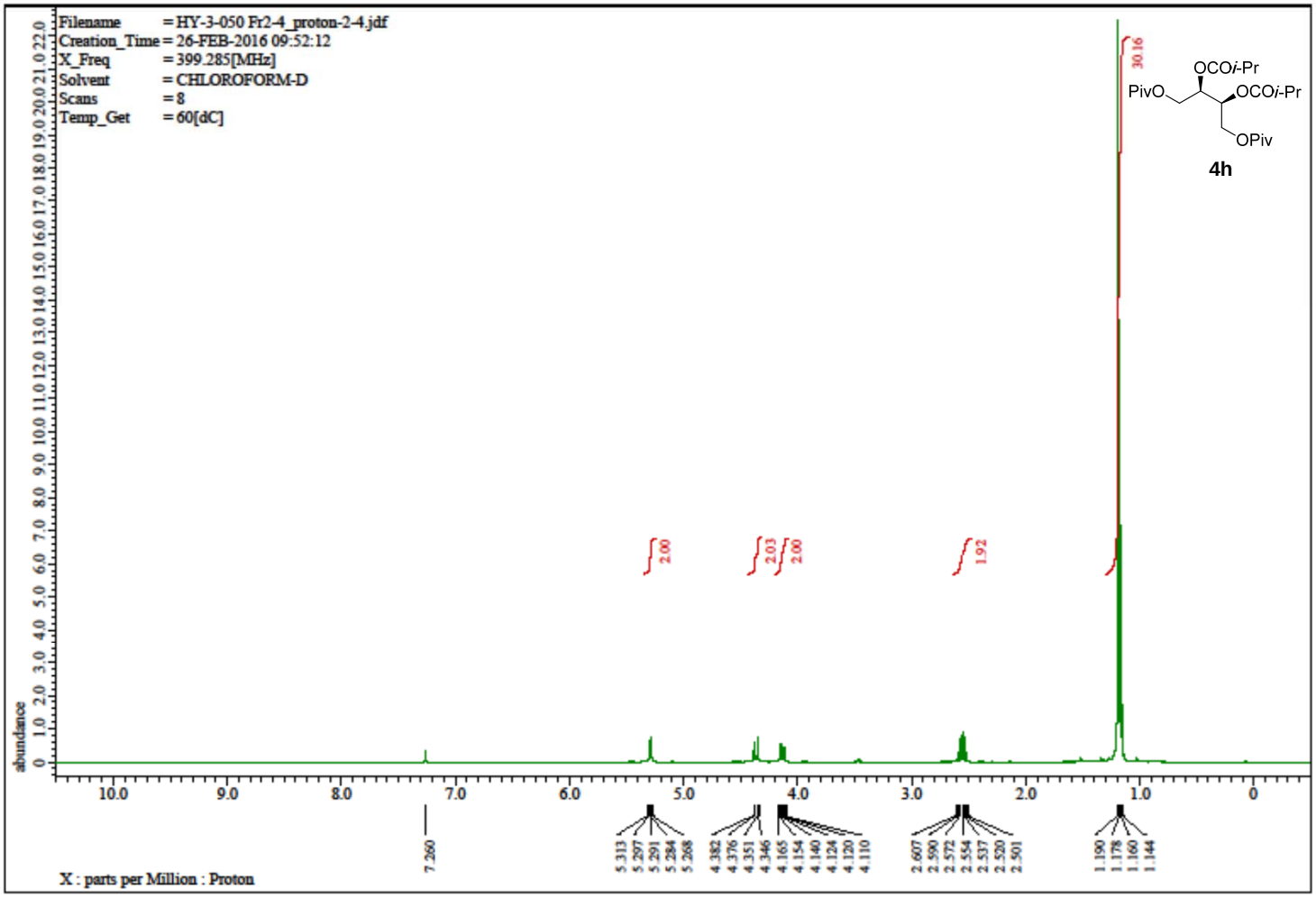

Filename = HY-3-023 Fr19-23_Carbon-1-3.jdf
Creation_Time = 9-JUN-2016 17:49:20
X_Freq = 100.40028[MHz]
Solvent = CHLOROFORM-D
Scans = 128
Temp_Get = 21.1[dC]
X : parts per Million : Carbon13
abundance

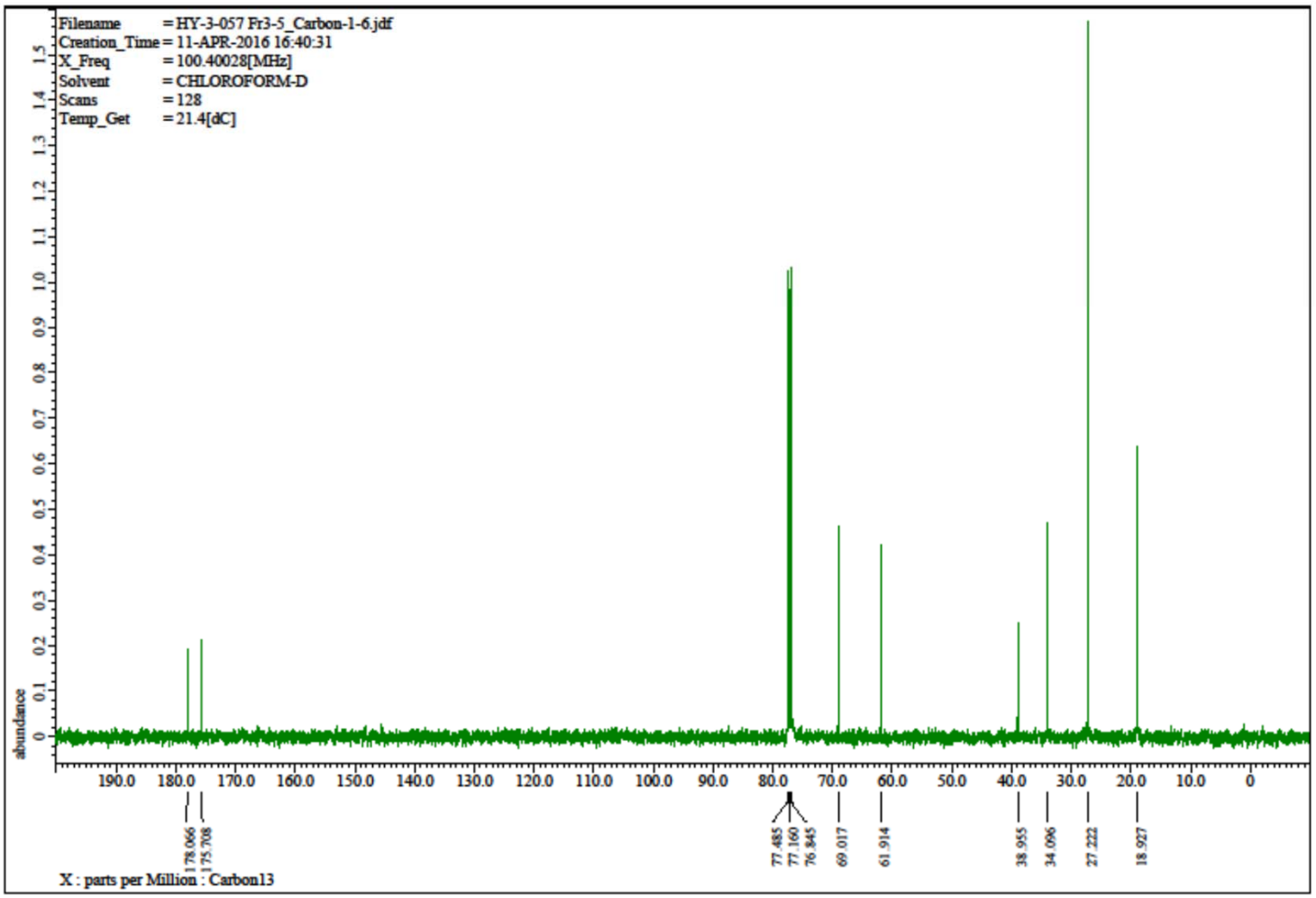

Filename = HY-3-019 Fr6-11_proton-1-3.jdf
Creation_Time = 26-NOV-2015 19:28:47
X_Freq = 399.285[MHz]
Solvent = CHLOROFORM-D
Scans = 8
Temp_Get = 22.2[dC]
OCOi-Pr
BnO
OCOi-Pr
OBn
4g
13.48
11.73
2.00
4.02
4.00
1.94
abundance
X : parts per Million : Proton

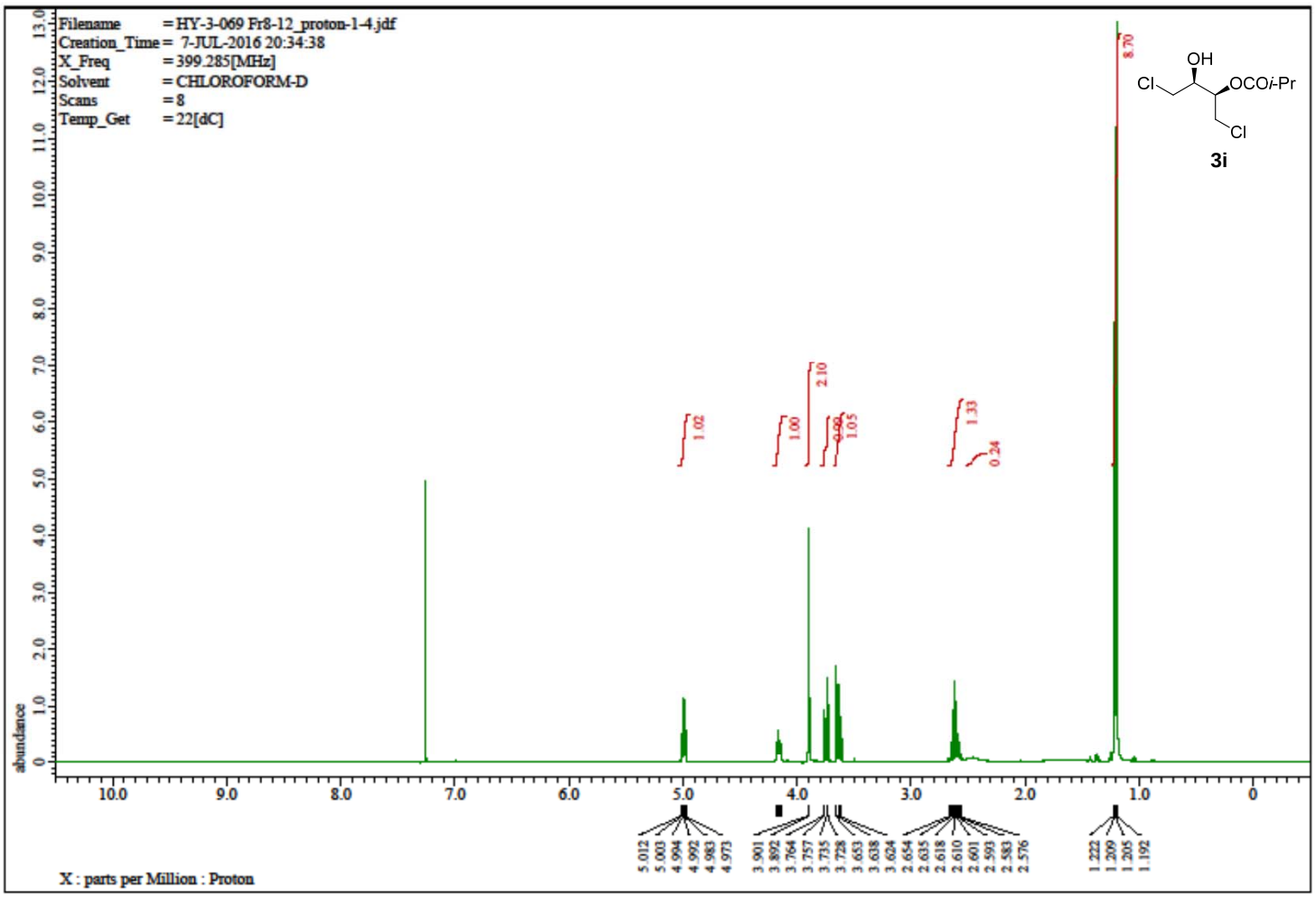

Filename = HY-3-019 Fr6-11_Carbon-1-3.jdf
Creation_Time = 3-JUN-2016 12:57:12
X_Freq = 100.40028[MHz]
Solvent = CHLOROFORM-D
Scans = 128
Temp_Get = 22.4[dC]
abundance
X : parts per Million : Carbon13

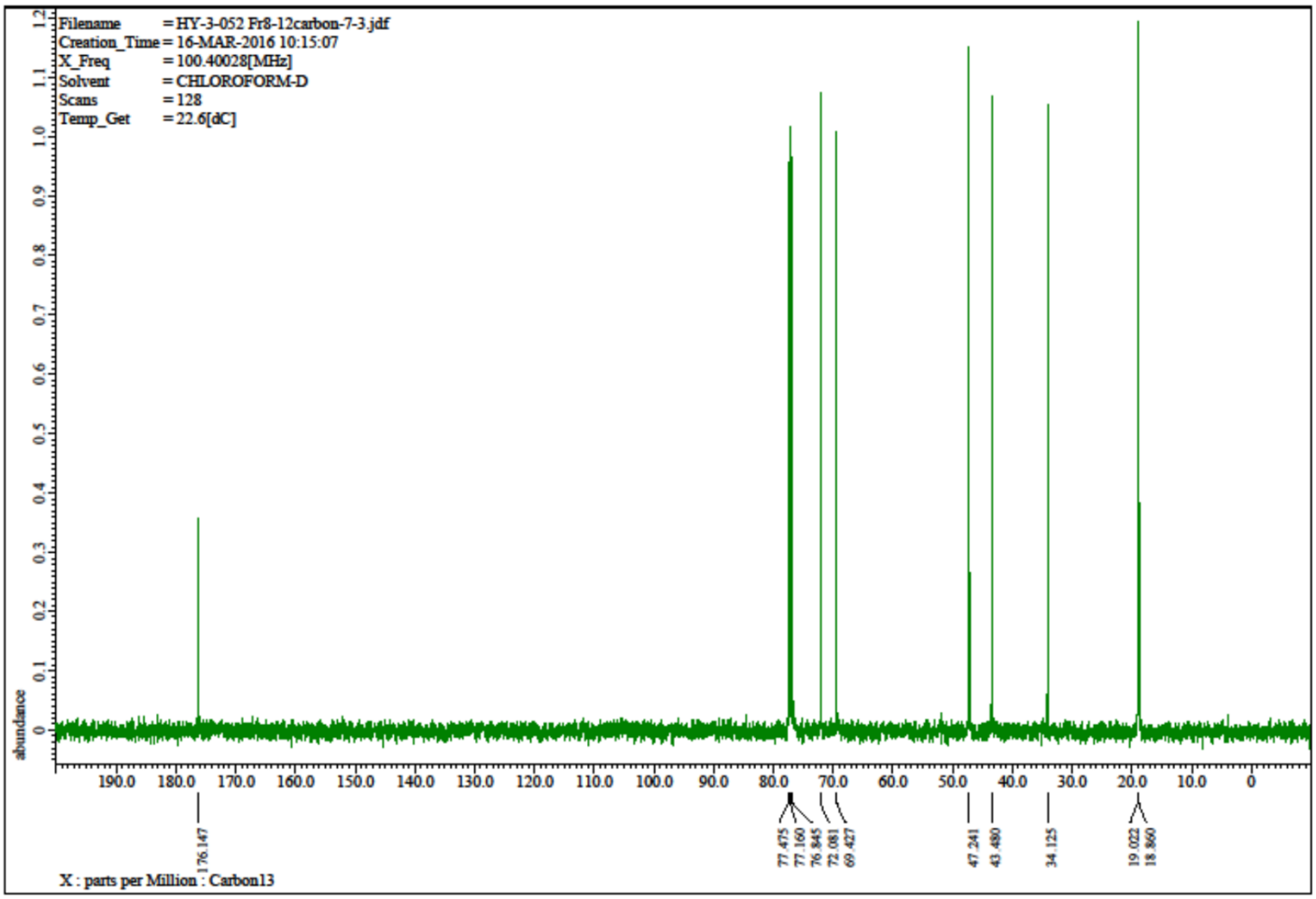

Filename = HY-2-141 clm4_proton-1-2.jdf
Creation_Time = 30-OCT-2015 18:37:27
X_Freq = 399.285[MHz]
Solvent = CHLOROFORM-D
Scans = 8
Temp_Get = 22.6[dC]
PivO
OH
OCO-i-Pr
OPiv
3h
X : parts per Million : Proton
abundance

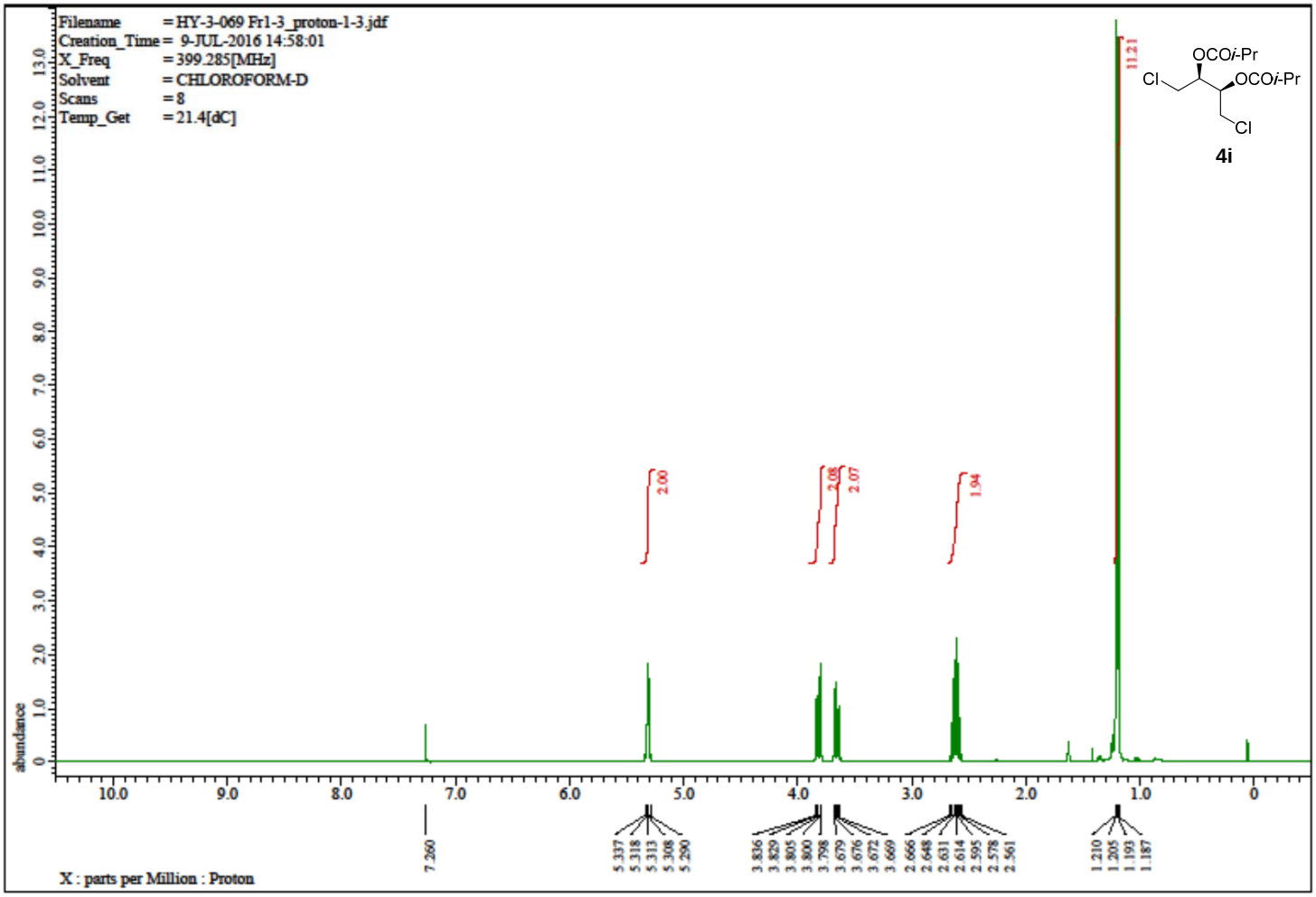

Filename = HY-3-057 Fr19-26_Carbon-1-3.jdf
Creation_Time = 12-APR-2016 10:24:36
X_Freq = 100.40028[MHz]
Solvent = CHLOROFORM-D
Scans = 128
Temp_Get = 20.9[dC]
X : parts per Million : Carbon13
abundance

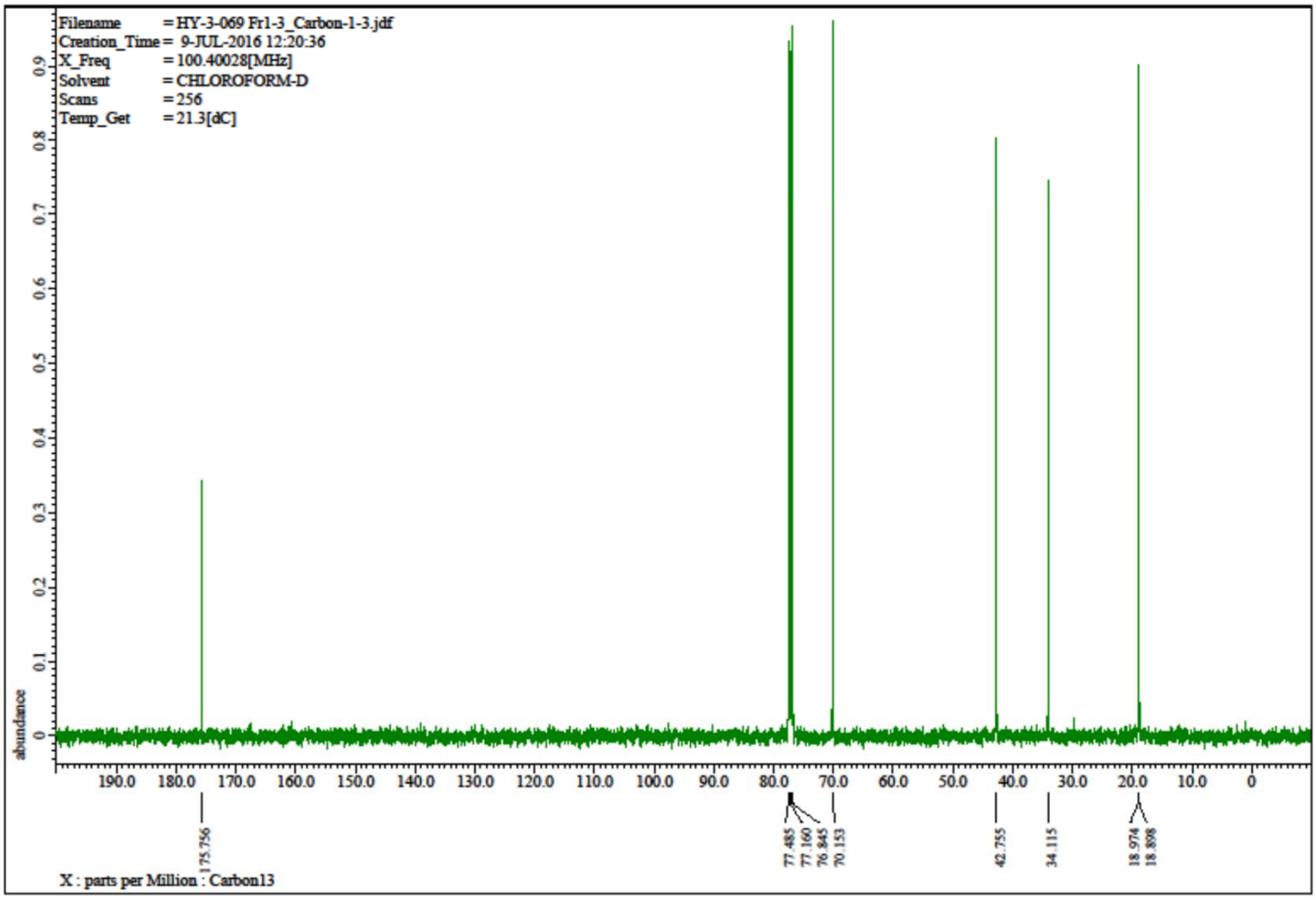

Filename = HY-3-050 Fr2-4_proton-2-4.jdf
Creation_Time = 26-FEB-2016 09:52:12
X_Freq = 399.285[MHz]
Solvent = CHLOROFORM-D
Scans = 8
Temp_Get = 60[dC]
OCOi-Pr
PivO
OCOi-Pr
OPiv
4h
30.16
2.00
2.03
2.00
1.92
7.260
5.313
5.297
5.291
5.284
5.268
4.382
4.376
4.351
4.346
4.165
4.154
4.140
4.124
4.120
4.110
2.607
2.590
2.572
2.554
2.537
2.520
2.501
1.190
1.178
1.160
1.144
abundance
X : parts per Million : Proton

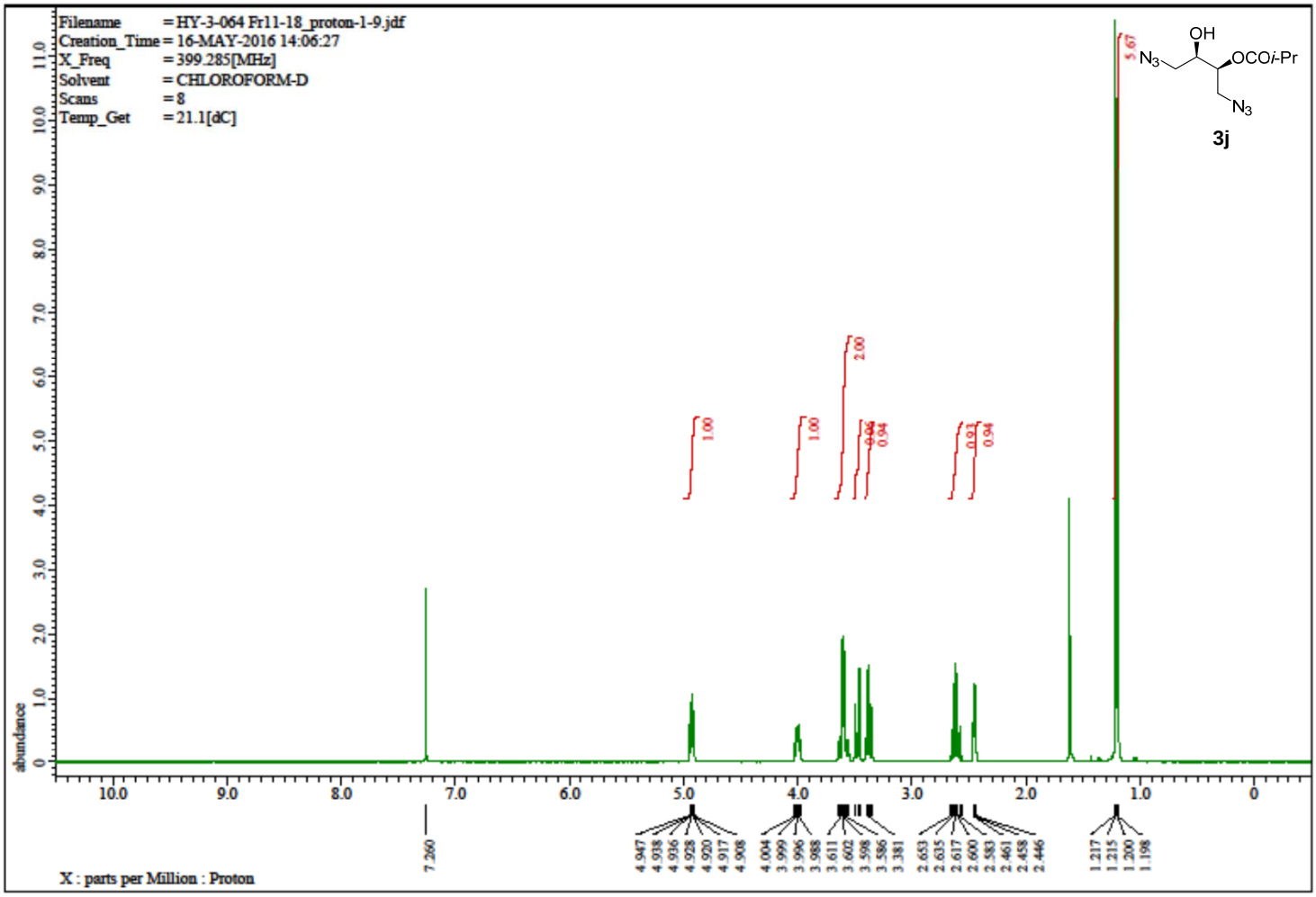

Filename = HY-3-057 Fr3-5_Carbon-1-6.jdf
Creation_Time = 11-APR-2016 16:40:31
X_Freq = 100.40028[MHz]
Solvent = CHLOROFORM-D
Scans = 128
Temp_Get = 21.4[dC]
178.066
175.708
77.485
77.160
76.845
69.017
61.914
38.955
34.096
27.222
18.927
abundance
X : parts per Million : Carbon13

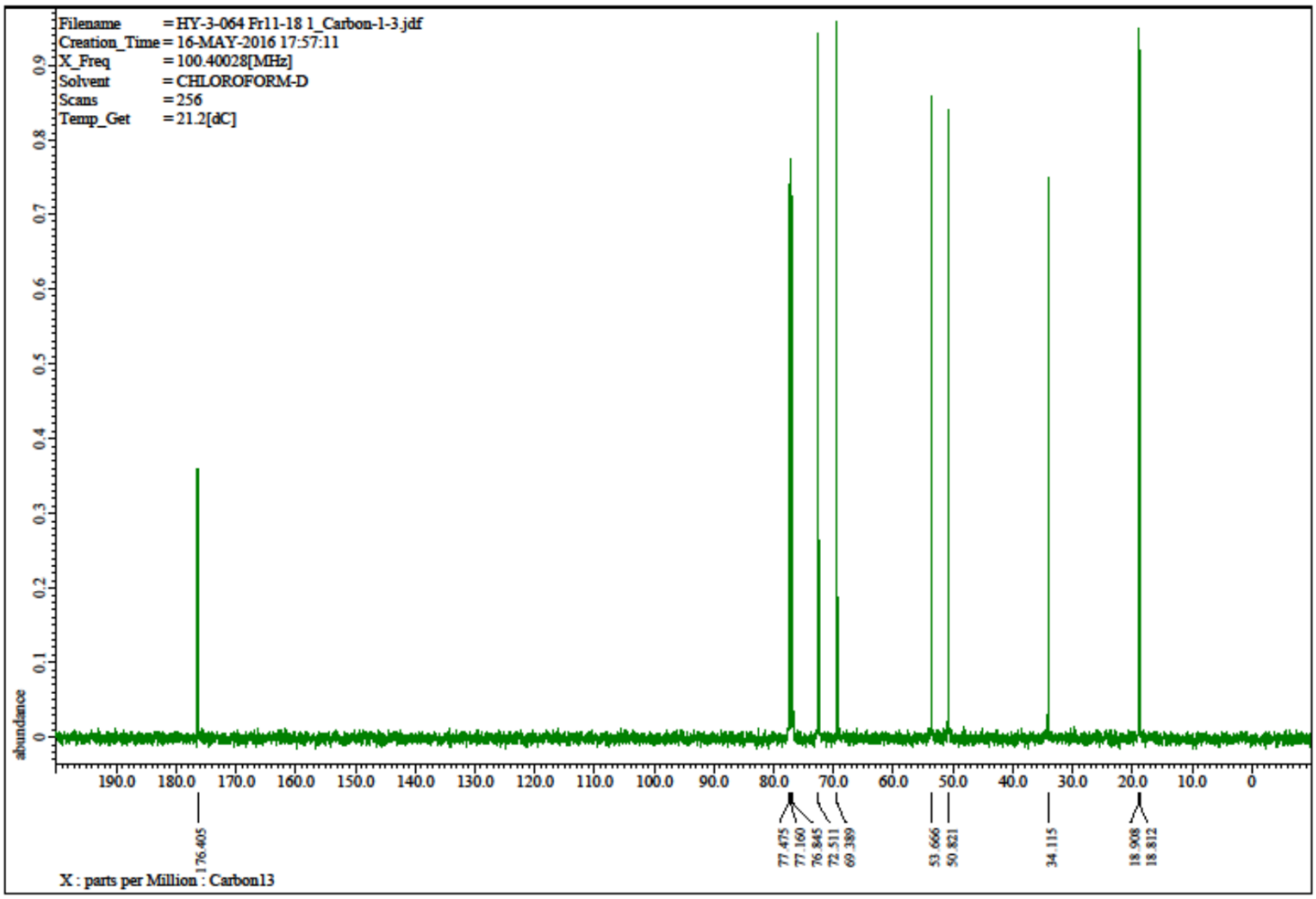

Filename = HY-3-069 Fr8-12_proton-1-4.jdf
Creation_Time = 7-JUL-2016 20:34:38
X_Freq = 399.285[MHz]
Solvent = CHLOROFORM-D
Scans = 8
Temp_Get = 22[dC]
OH
Cl
OCOi-Pr
Cl
3i
X : parts per Million : Proton

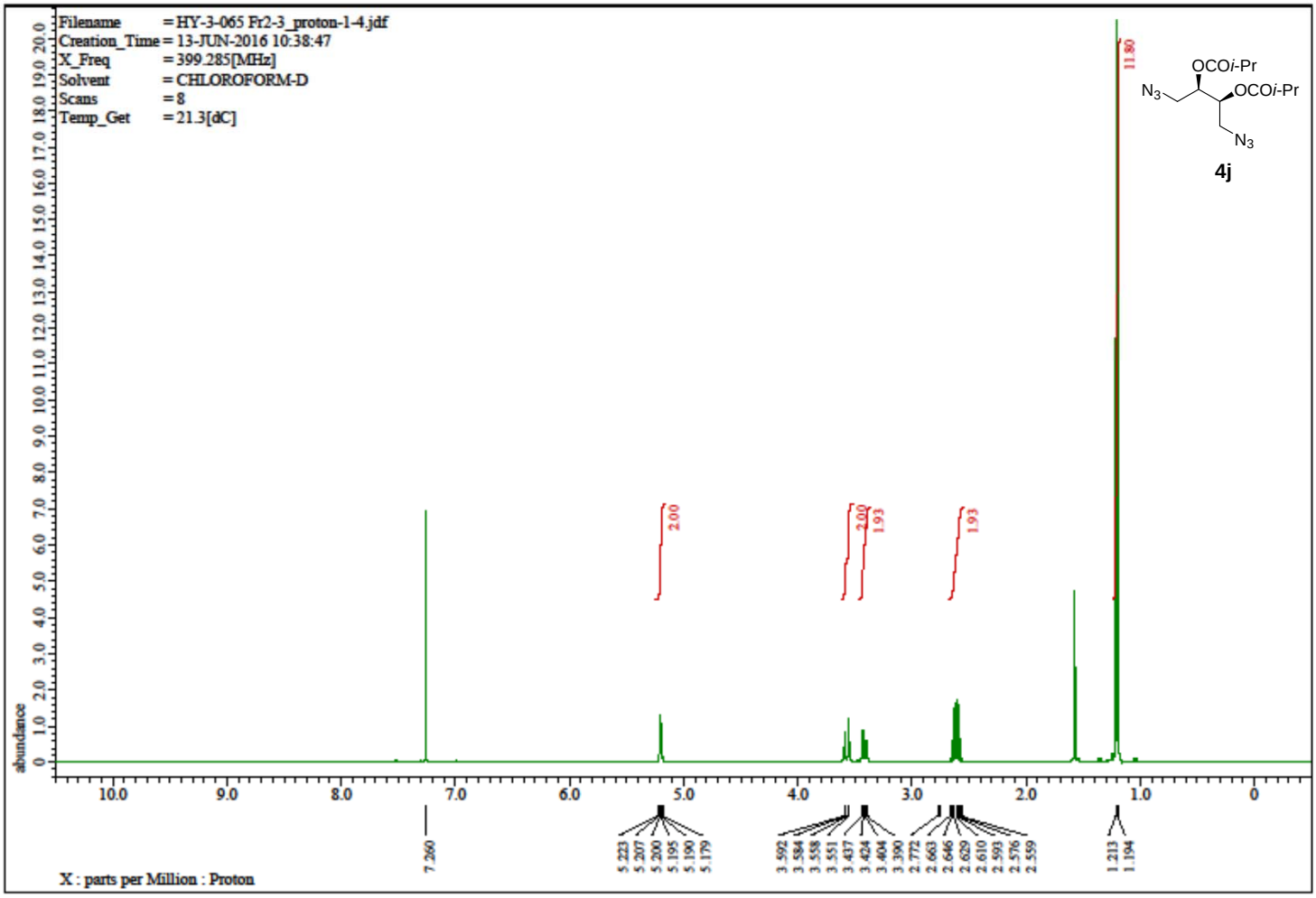

Filename = HY-3-052 Fr8-12carbon-7-3.jdf
Creation_Time = 16-MAR-2016 10:15:07
X_Freq = 100.40028[MHz]
Solvent = CHLOROFORM-D
Scans = 128
Temp_Get = 22.6[dC]
X : parts per Million : Carbon13

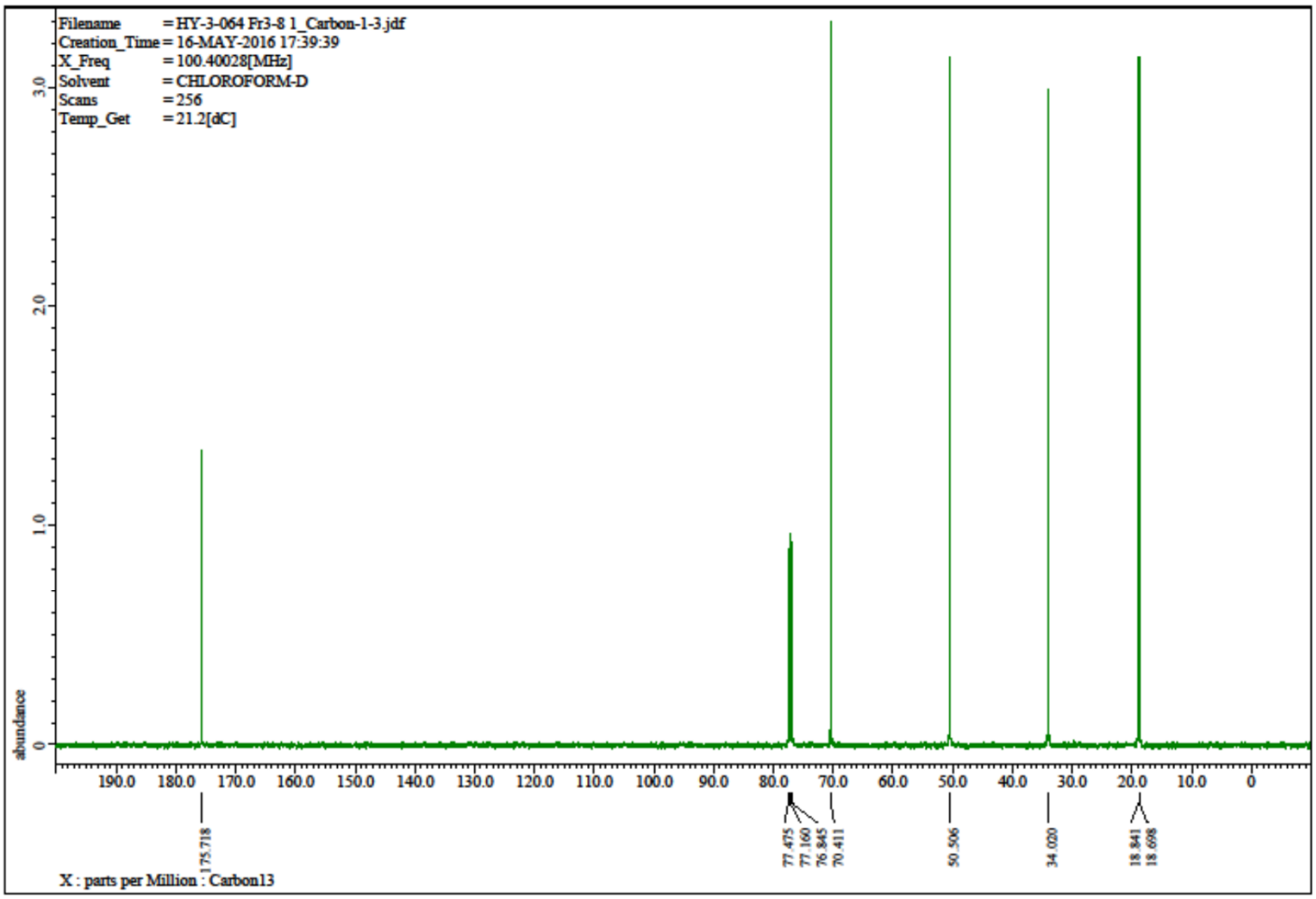

Filename = HY-3-069 Fr1-3_proton-1-3.jdf
Creation_Time = 9-JUL-2016 14:58:01
X_Freq = 399.285[MHz]
Solvent = CHLOROFORM-D
Scans = 8
Temp_Get = 21.4[dC]
OCOi-Pr
Cl
OCOi-Pr
Cl
4i
11.21
2.00
2.08
2.07
1.94
abundance
X : parts per Million : Proton

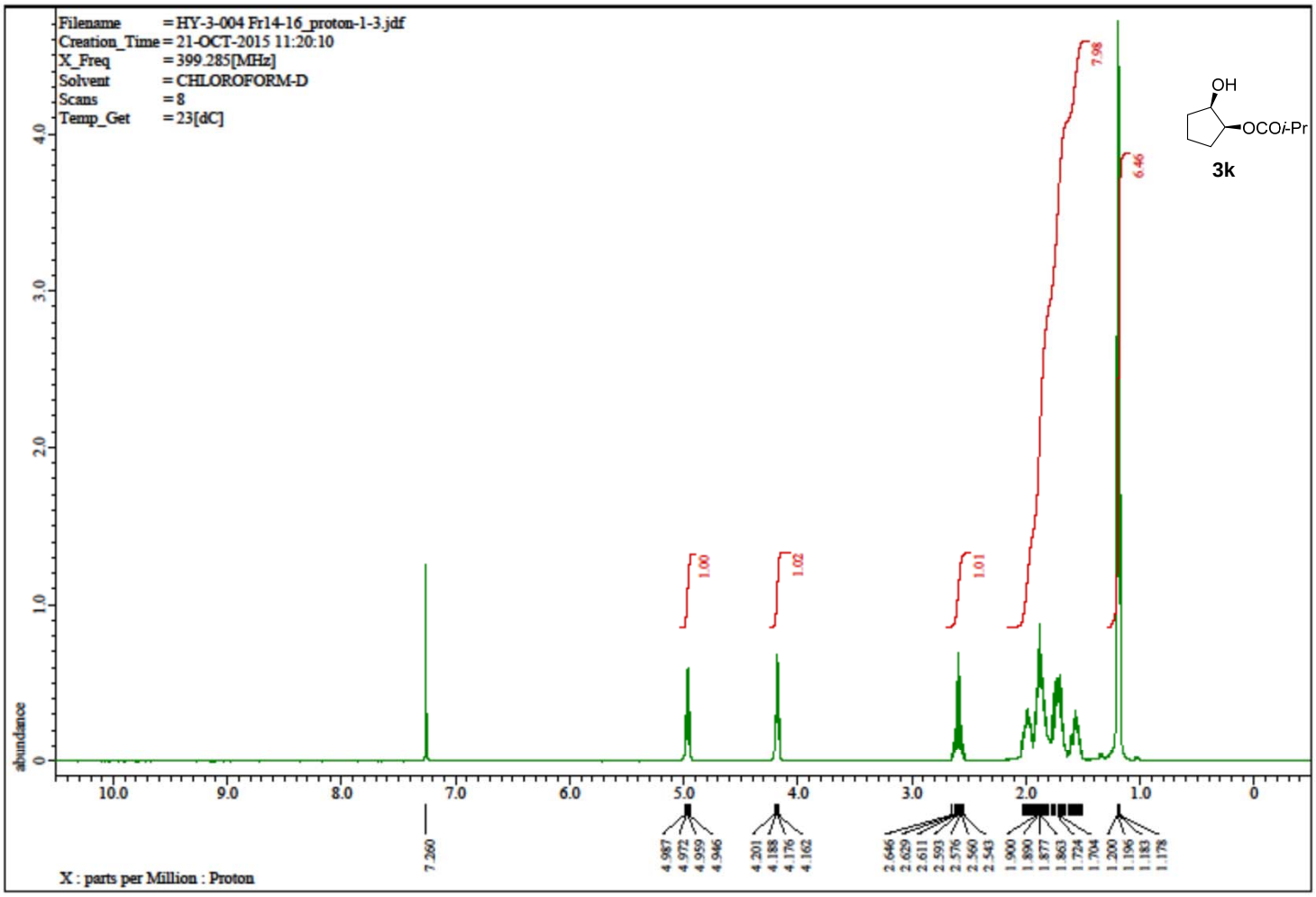

Filename = HY-3-069 Fr1-3_Carbon-1-3.jdf
Creation_Time = 9-JUL-2016 12:20:36
X_Freq = 100.40028[MHz]
Solvent = CHLOROFORM-D
Scans = 256
Temp_Get = 21.3[dC]
abundance
X : parts per Million : Carbon13

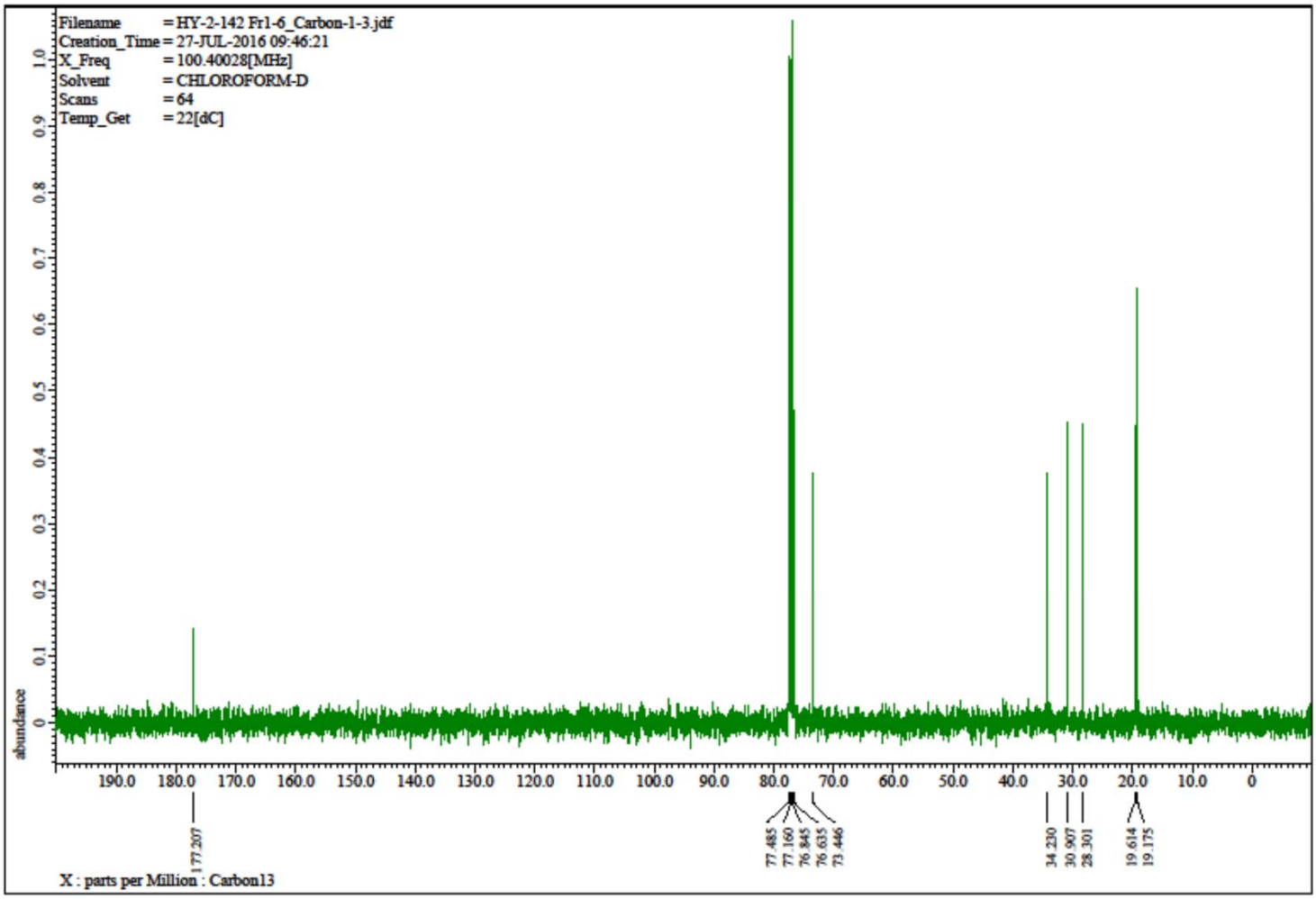

Filename = HY-3-064 Fr11-18_proton-1-9.jdf
Creation_Time = 16-MAY-2016 14:06:27
X_Freq = 399.285[MHz]
Solvent = CHLOROFORM-D
Scans = 8
Temp_Get = 21.1[dC]
OH
N3
OCOi-Pr
N3
3j
X : parts per Million : Proton

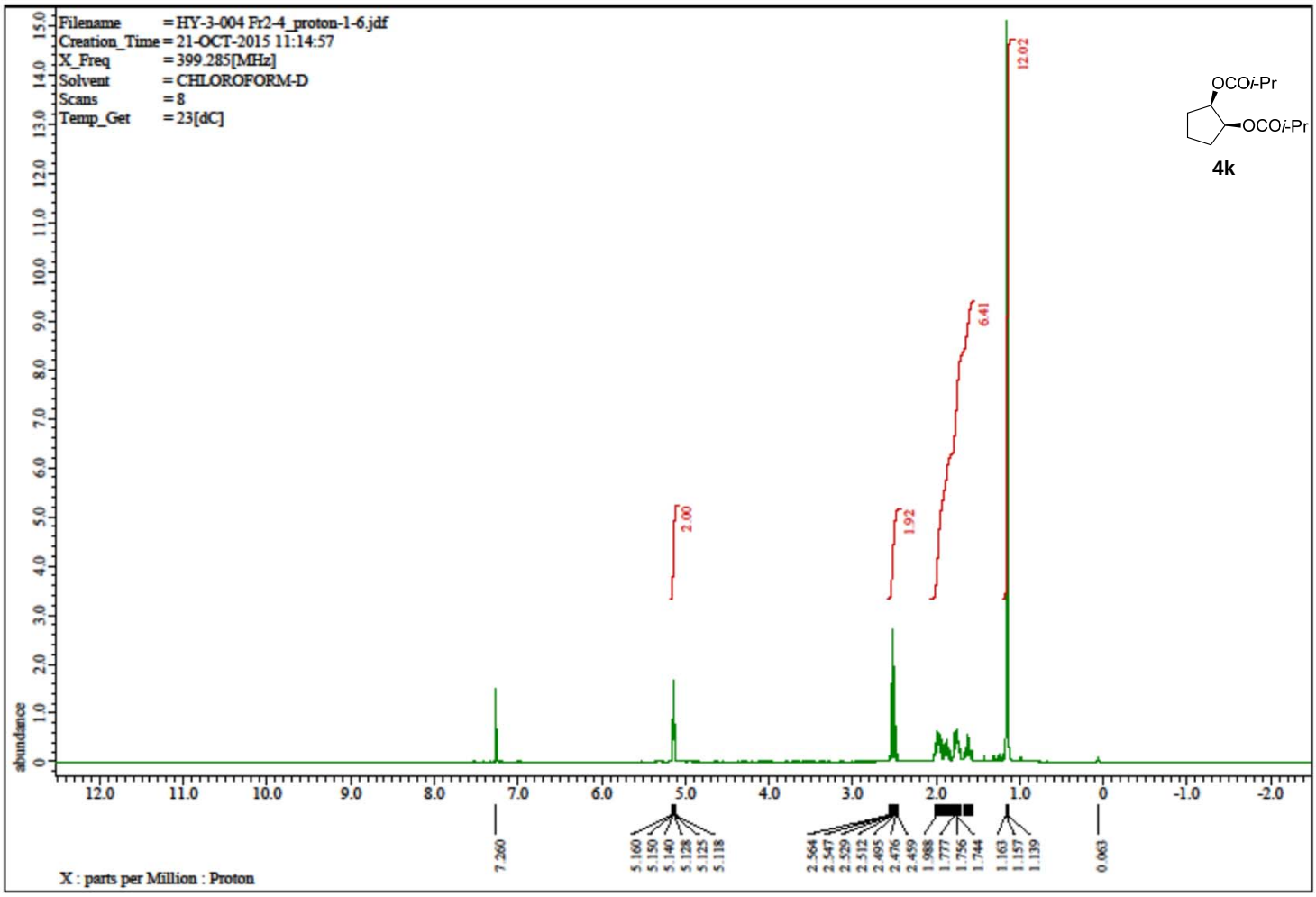

Filename = HY-3-064 Fr11-18 1_Carbon-1-3.jdf
Creation_Time = 16-MAY-2016 17:57:11
X_Freq = 100.40028[MHz]
Solvent = CHLOROFORM-D
Scans = 256
Temp_Get = 21.2[dC]
X : parts per Million : Carbon13

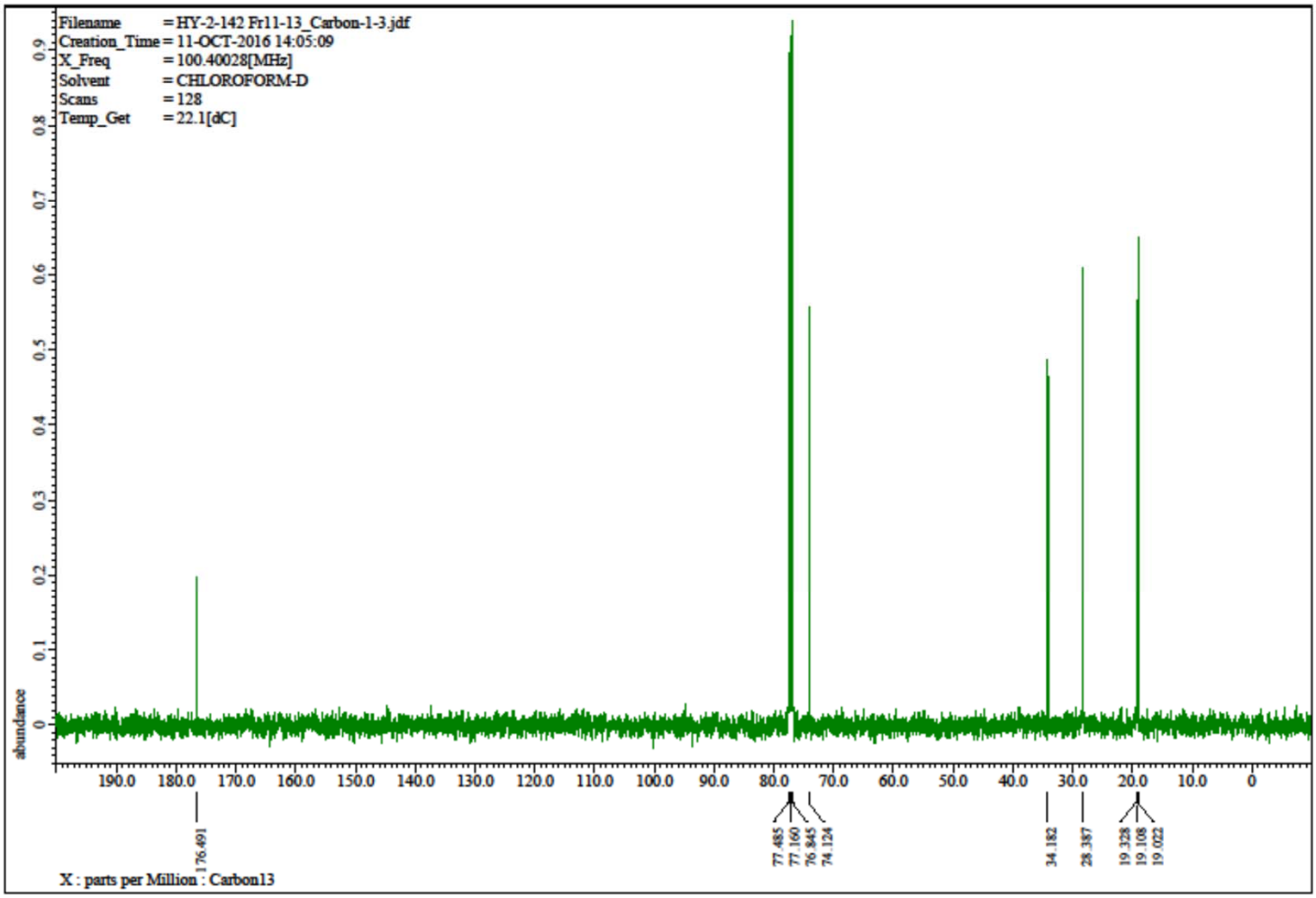

Filename = HY-3-065 Fr2-3_proton-1-4.jdf
Creation_Time = 13-JUN-2016 10:38:47
X_Freq = 399.285[MHz]
Solvent = CHLOROFORM-D
Scans = 8
Temp_Get = 21.3[dC]
OCO*i*-Pr
N3
OCO*i*-Pr
N3
4j
11.80
2.00
2.00
1.93
1.93
abundance
X : parts per Million : Proton

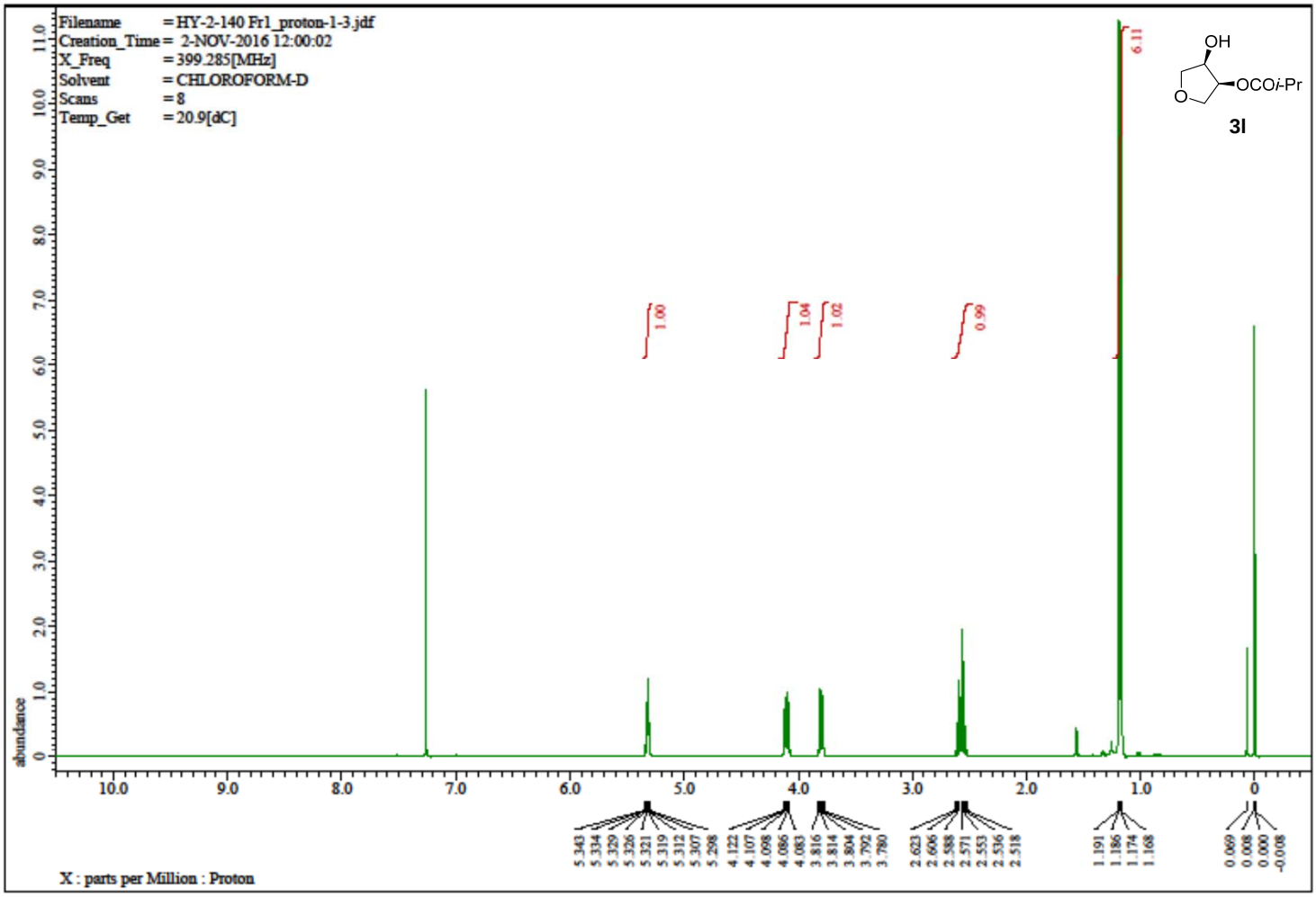

Filename = HY-3-064 Fr3-8 1_Carbon-1-3.jdf
Creation_Time = 16-MAY-2016 17:39:39
X_Freq = 100.40028[MHz]
Solvent = CHLOROFORM-D
Scans = 256
Temp_Get = 21.2[dC]
abundance
X : parts per Million : Carbon13

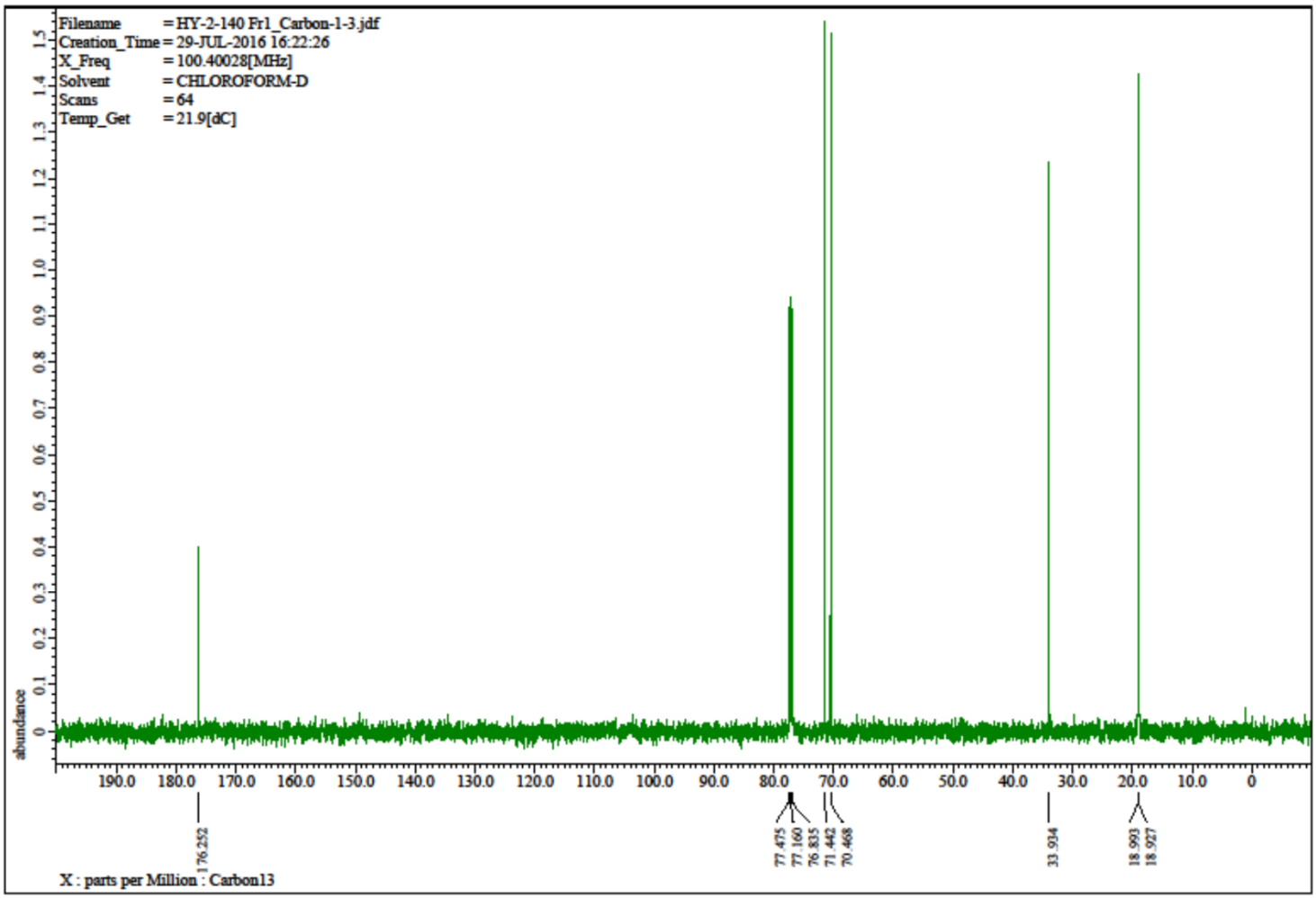

Filename = HY-3-004 Fr14-16_proton-1-3.jdf
Creation_Time = 21-OCT-2015 11:20:10
X_Freq = 399.285[MHz]
Solvent = CHLOROFORM-D
Scans = 8
Temp_Get = 23[dC]
OH
OCOi-Pr
3k
7.98
6.46
1.00
1.02
1.01
abundance
7.260
4.987
4.972
4.959
4.946
4.201
4.188
4.176
4.162
2.646
2.629
2.611
2.591
2.576
2.560
2.543
1.900
1.890
1.877
1.863
1.724
1.704
1.200
1.196
1.183
1.178
X : parts per Million : Proton

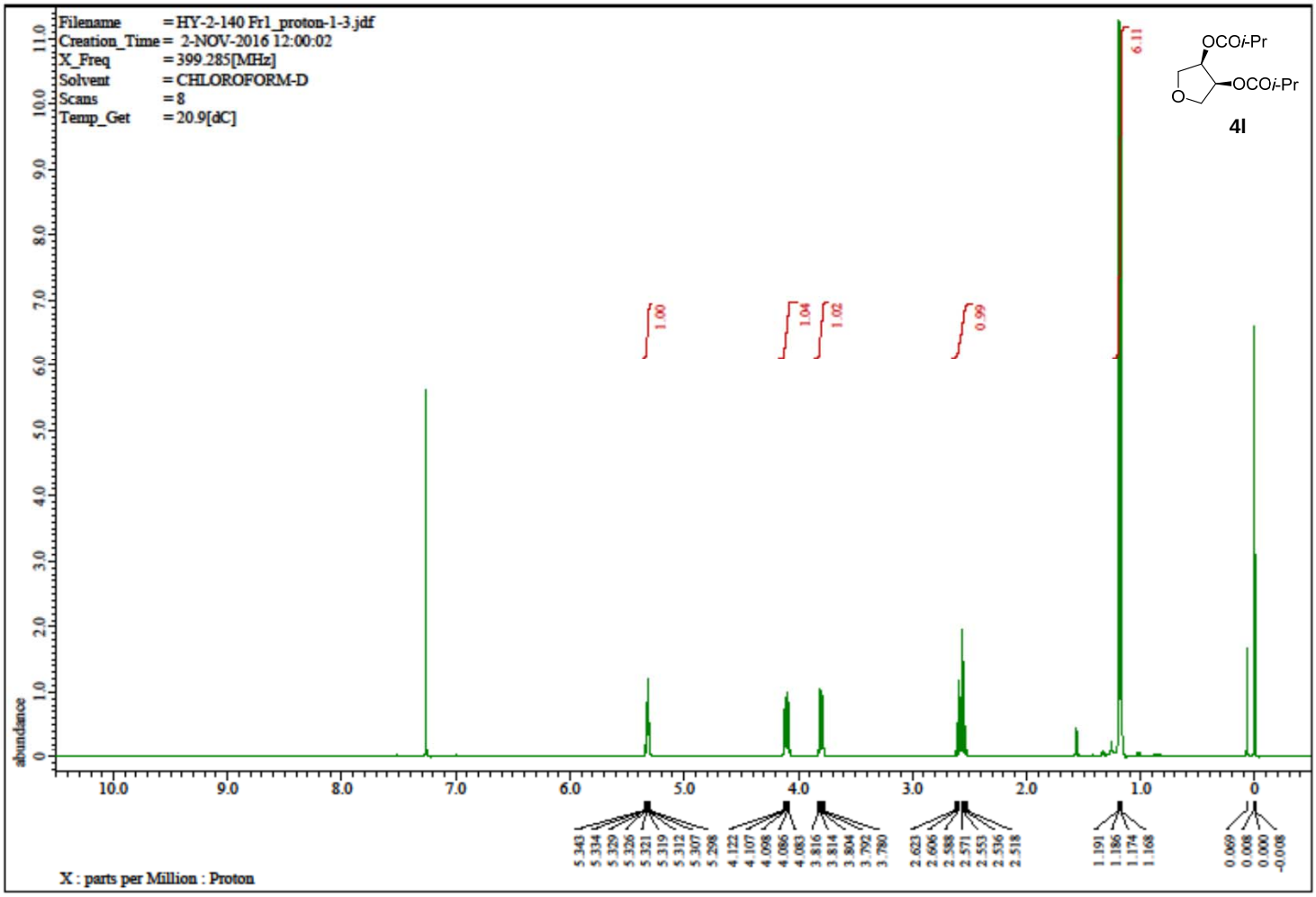

Filename = HY-2-142 Fr1-6_Carbon-1-3.jdf
Creation_Time = 27-JUL-2016 09:46:21
X_Freq = 100.40028[MHz]
Solvent = CHLOROFORM-D
Scans = 64
Temp_Get = 22[dC]
abundance
177.207
77.485
77.160
76.845
76.635
73.446
34.230
30.907
28.301
19.614
19.175
X : parts per Million : Carbon13

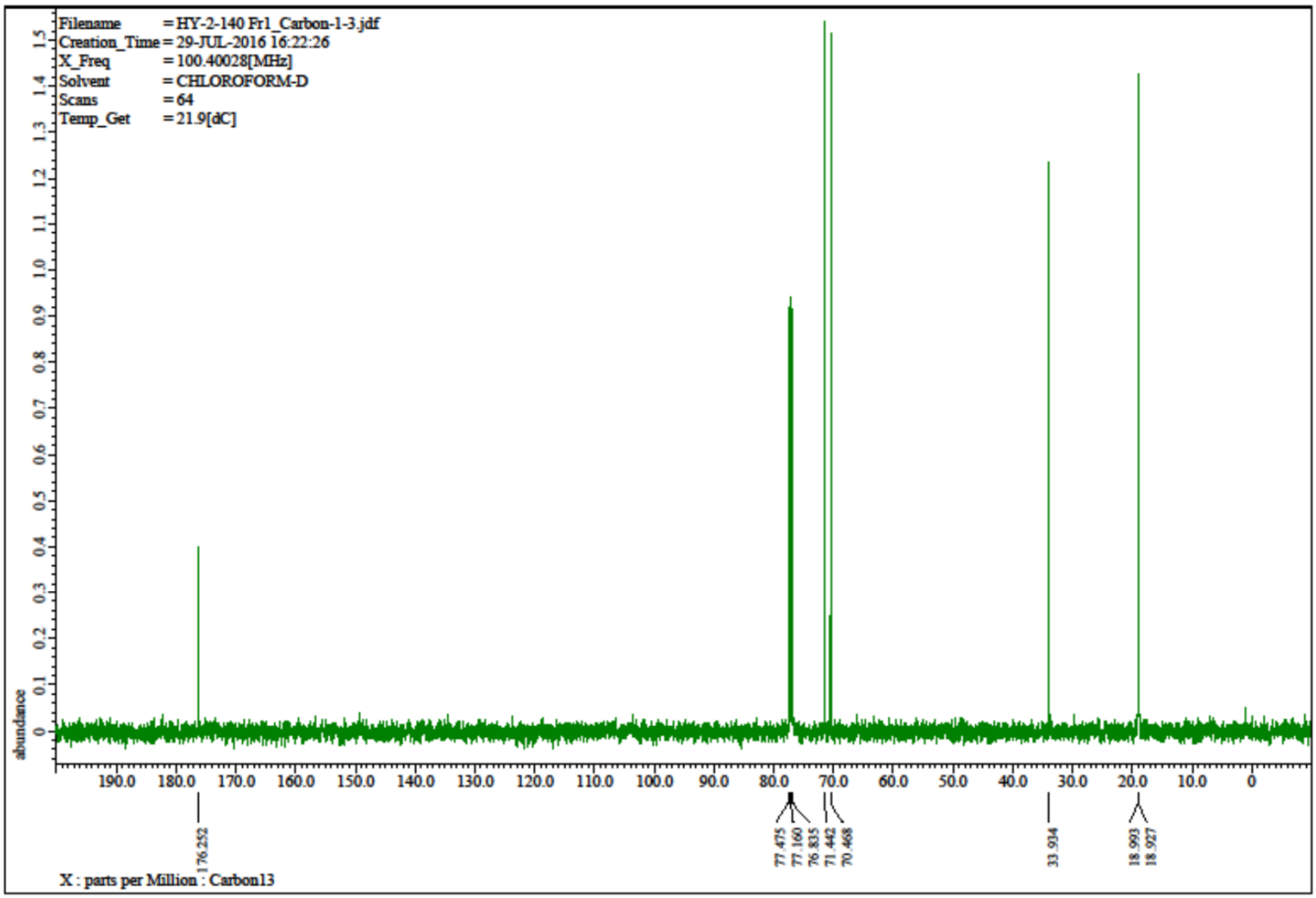

Filename = HY-3-004 Fr2-4_proton-1-6.jdf
Creation_Time = 21-OCT-2015 11:14:57
X_Freq = 399.285[MHz]
Solvent = CHLOROFORM-D
Scans = 8
Temp_Get = 23[dC]
OCOi-Pr
OCOi-Pr
4k
12.02
6.41
2.00
1.92
7.260
5.160
5.150
5.140
5.128
5.125
5.118
2.564
2.547
2.529
2.512
2.495
2.476
2.459
1.988
1.777
1.756
1.744
1.163
1.157
1.139
0.063
abundance
X : parts per Million : Proton

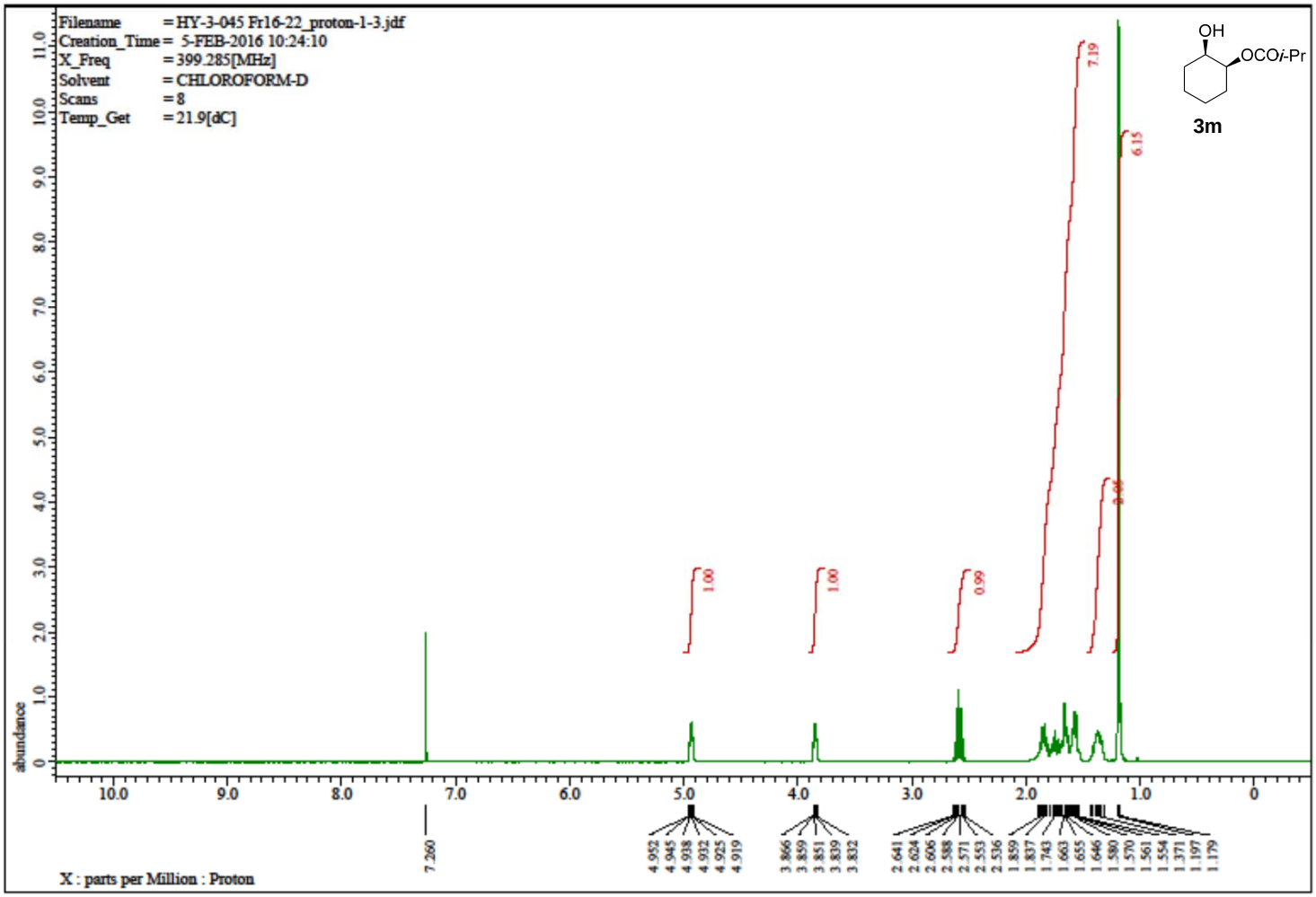

Filename = HY-2-142 Fr11-13_Carbon-1-3.jdf
Creation_Time = 11-OCT-2016 14:05:09
X_Freq = 100.40028[MHz]
Solvent = CHLOROFORM-D
Scans = 128
Temp_Get = 22.1[dC]
176.491
77.485
77.160
76.845
74.124
34.182
28.387
19.328
19.108
19.022
abundance
X : parts per Million : Carbon13

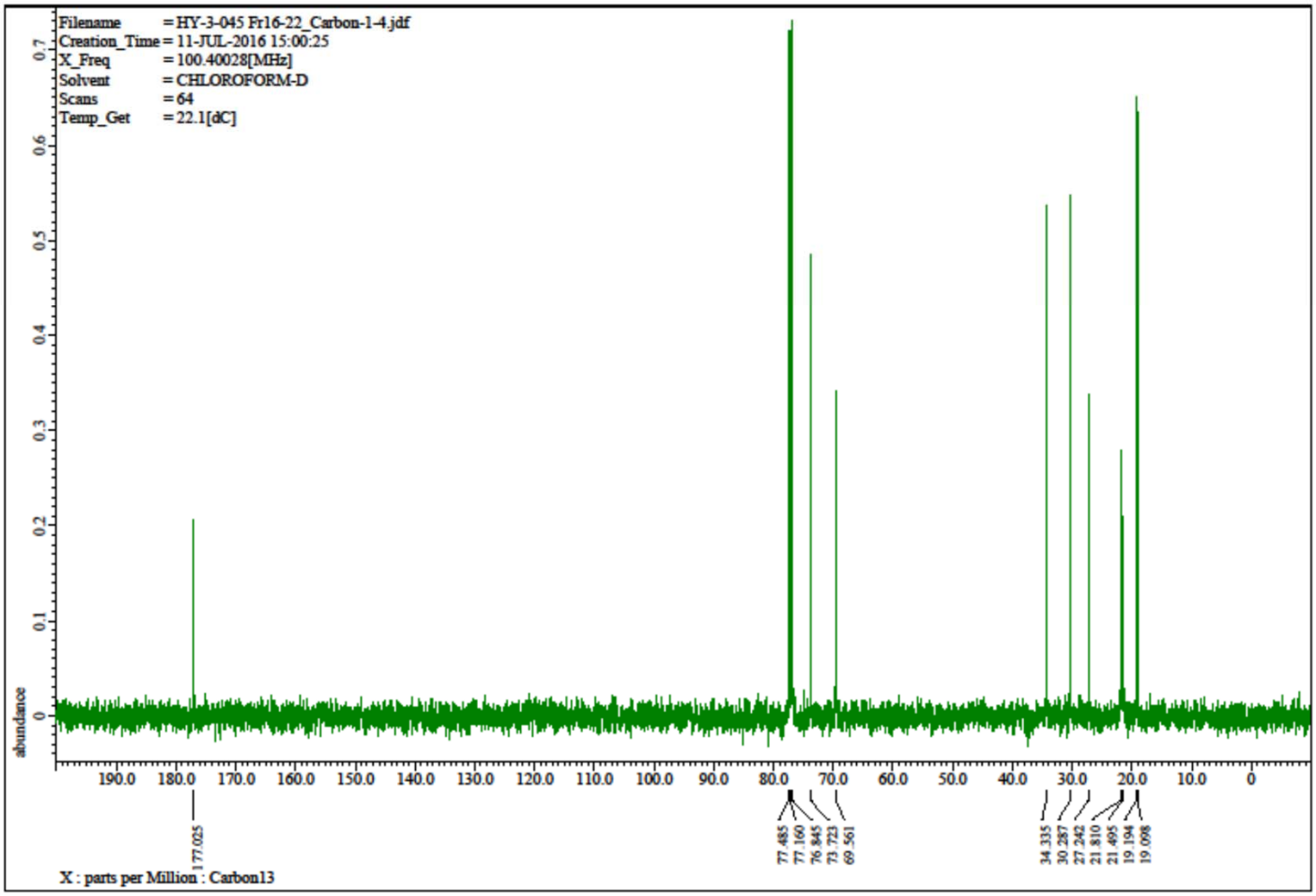

Filename = HY-2-140 Fr1_proton-1-3.jdf
Creation_Time = 2-NOV-2016 12:00:02
X_Freq = 399.285[MHz]
Solvent = CHLOROFORM-D
Scans = 8
Temp_Get = 20.9[dC]
OH
OCOi-Pr
3l
6.11
1.00
1.04
1.02
0.99
abundance
X : parts per Million : Proton

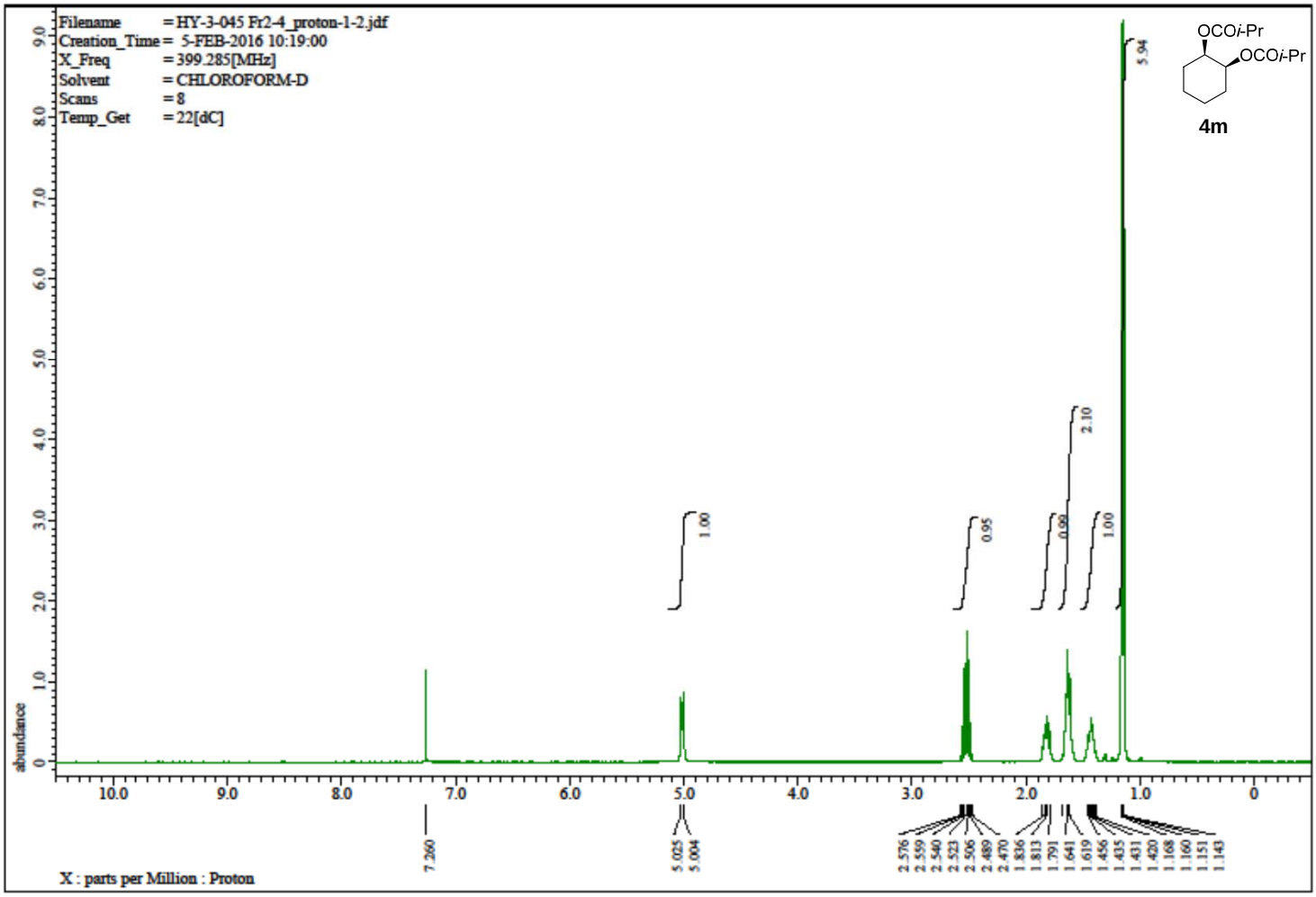

Filename = HY-2-140 Fr1_Carbon-1-3.jdf
Creation_Time = 29-JUL-2016 16:22:26
X_Freq = 100.40028[MHz]
Solvent = CHLOROFORM-D
Scans = 64
Temp_Get = 21.9[dC]
abundance
X : parts per Million : Carbon13

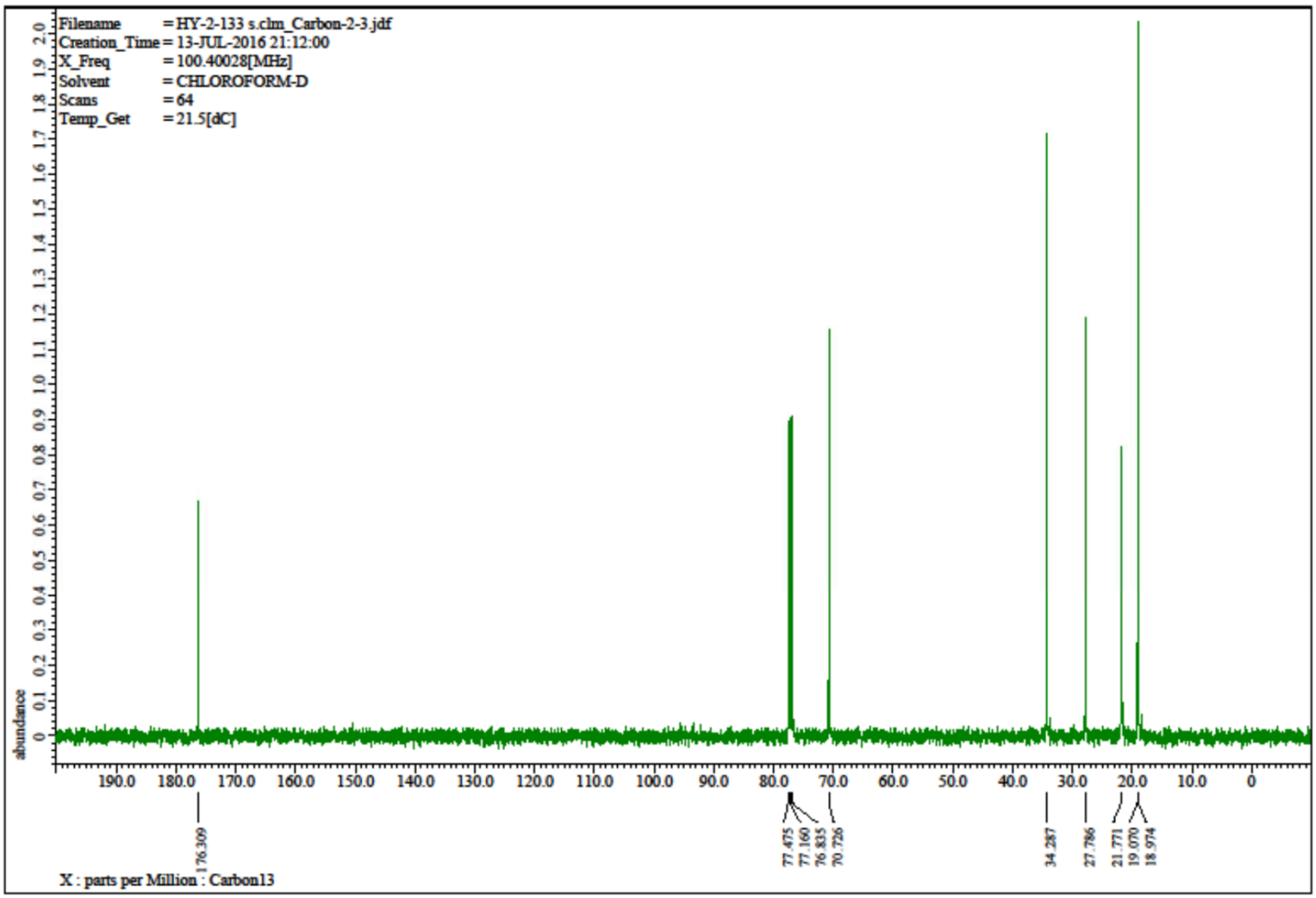

Filename = HY-2-140 Fr1_proton-1-3.jdf
Creation_Time = 2-NOV-2016 12:00:02
X_Freq = 399.285[MHz]
Solvent = CHLOROFORM-D
Scans = 8
Temp_Get = 20.9[dC]
OCOi-Pr
OCOi-Pr
4l
1.00
1.04
1.02
0.99
6.11
abundance
X : parts per Million : Proton

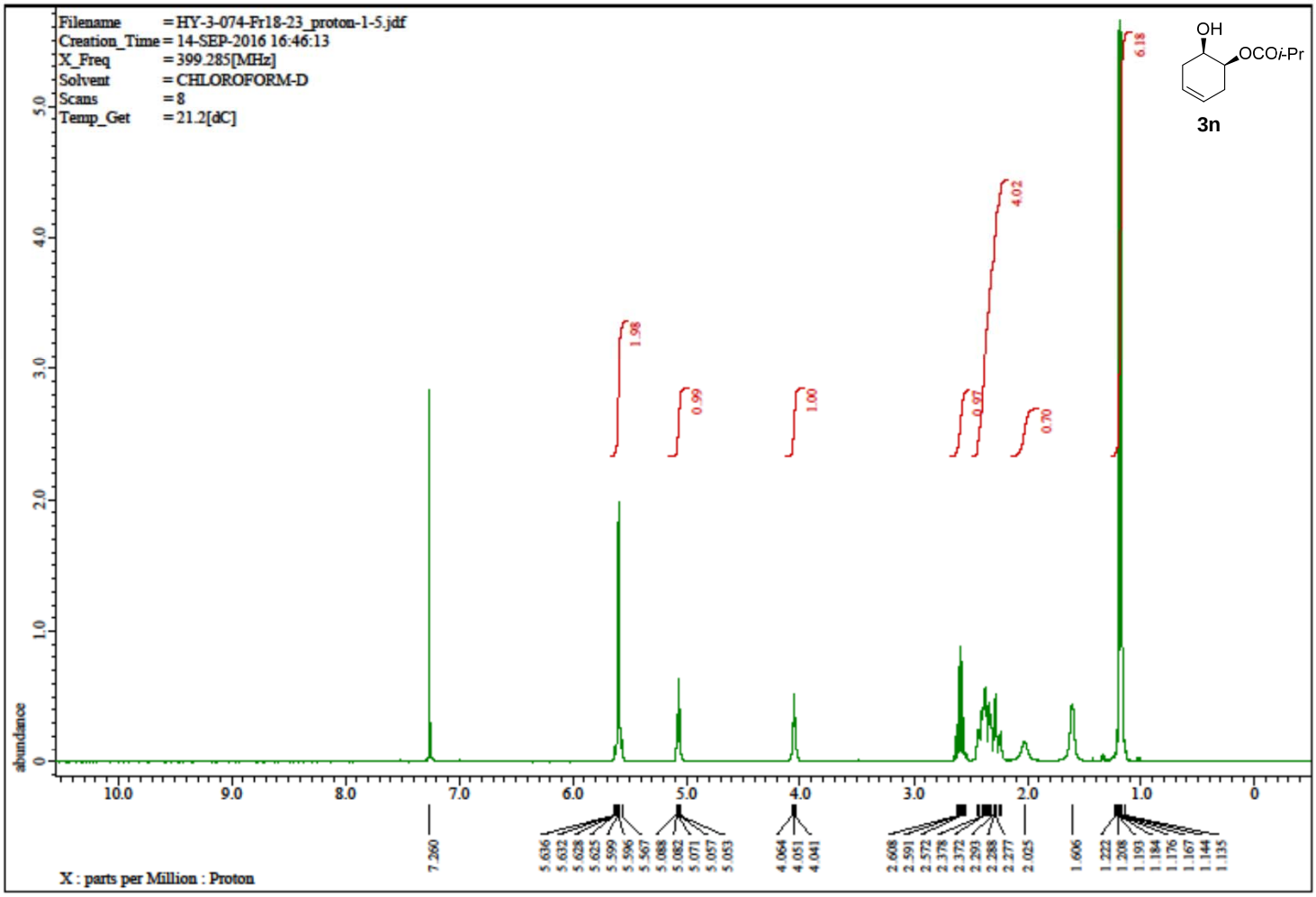

Filename = HY-2-140 Fr1_Carbon-1-3.jdf
Creation_Time = 29-JUL-2016 16:22:26
X_Freq = 100.40028[MHz]
Solvent = CHLOROFORM-D
Scans = 64
Temp_Get = 21.9[dC]
abundance
X : parts per Million : Carbon13

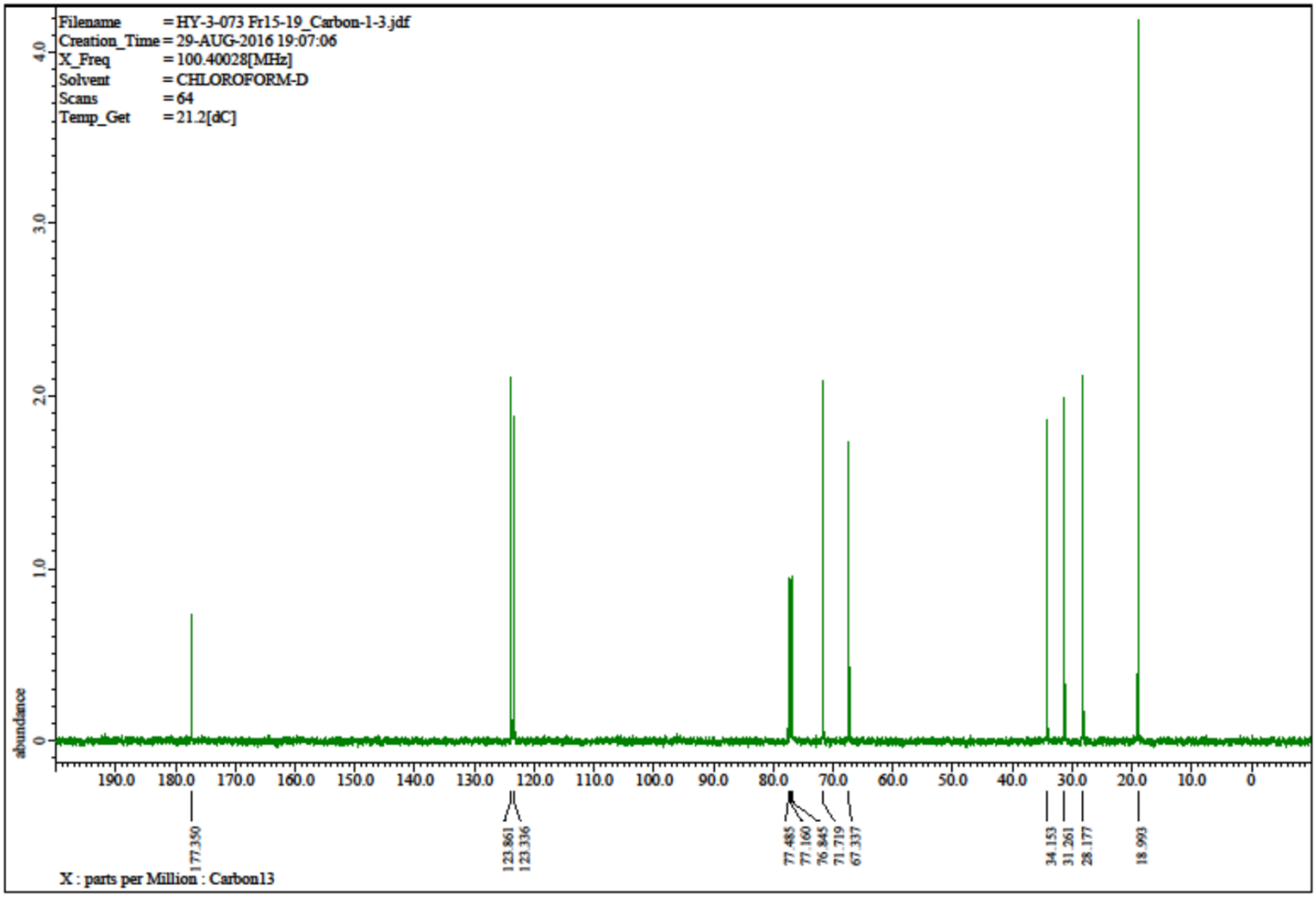

Filename = HY-3-045 Fr16-22_proton-1-3.jdf
Creation_Time = 5-FEB-2016 10:24:10
X_Freq = 399.285[MHz]
Solvent = CHLOROFORM-D
Scans = 8
Temp_Get = 21.9[dC]
OH
OCOi-Pr
3m
7.19
6.15
8.48
1.00
1.00
0.99
abundance
7.260
4.952
4.945
4.938
4.932
4.925
4.919
3.866
3.859
3.851
3.839
3.832
2.641
2.624
2.606
2.588
2.571
2.553
2.536
1.859
1.837
1.743
1.663
1.655
1.646
1.580
1.570
1.561
1.554
1.371
1.197
1.179
X : parts per Million : Proton

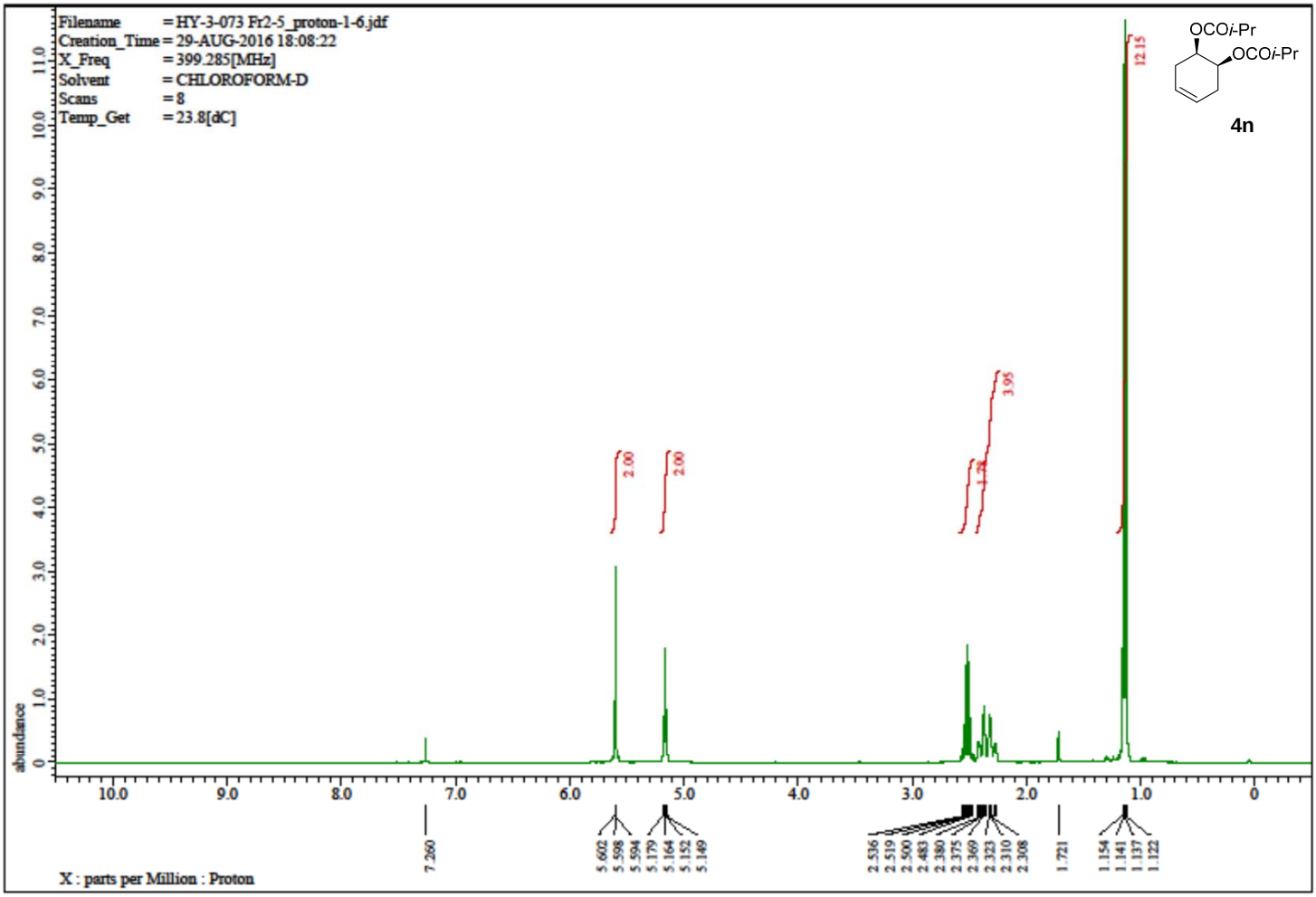

Filename = HY-3-045 Fr16-22_Carbon-1-4.jdf
Creation_Time = 11-JUL-2016 15:00:25
X_Freq = 100.40028[MHz]
Solvent = CHLOROFORM-D
Scans = 64
Temp_Get = 22.1[dC]
abundance
177.025
77.485
77.160
76.845
73.723
69.561
34.335
30.287
27.242
21.810
21.495
19.194
19.098
X : parts per Million : Carbon13

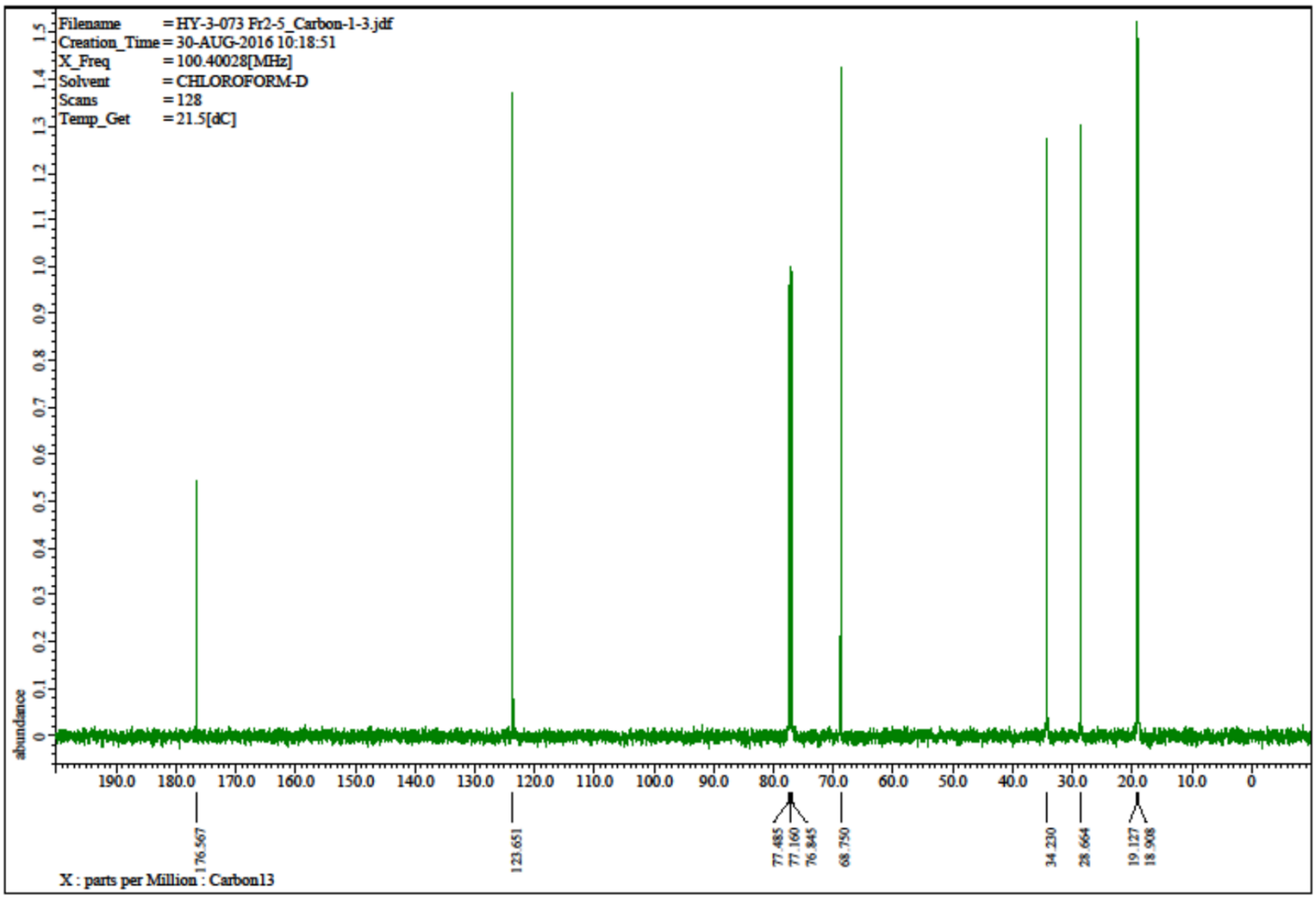

Filename = HY-3-045 Fr2-4_proton-1-2.jdf
Creation_Time = 5-FEB-2016 10:19:00
X_Freq = 399.285[MHz]
Solvent = CHLOROFORM-D
Scans = 8
Temp_Get = 22[dC]
OCOi-Pr
OCOi-Pr
4m
5.94
2.10
1.00
0.95
0.99
1.00
abundance
7.260
5.025
5.004
2.576
2.559
2.540
2.523
2.506
2.489
2.470
1.836
1.813
1.791
1.641
1.619
1.456
1.435
1.431
1.420
1.168
1.160
1.151
1.143
X : parts per Million : Proton

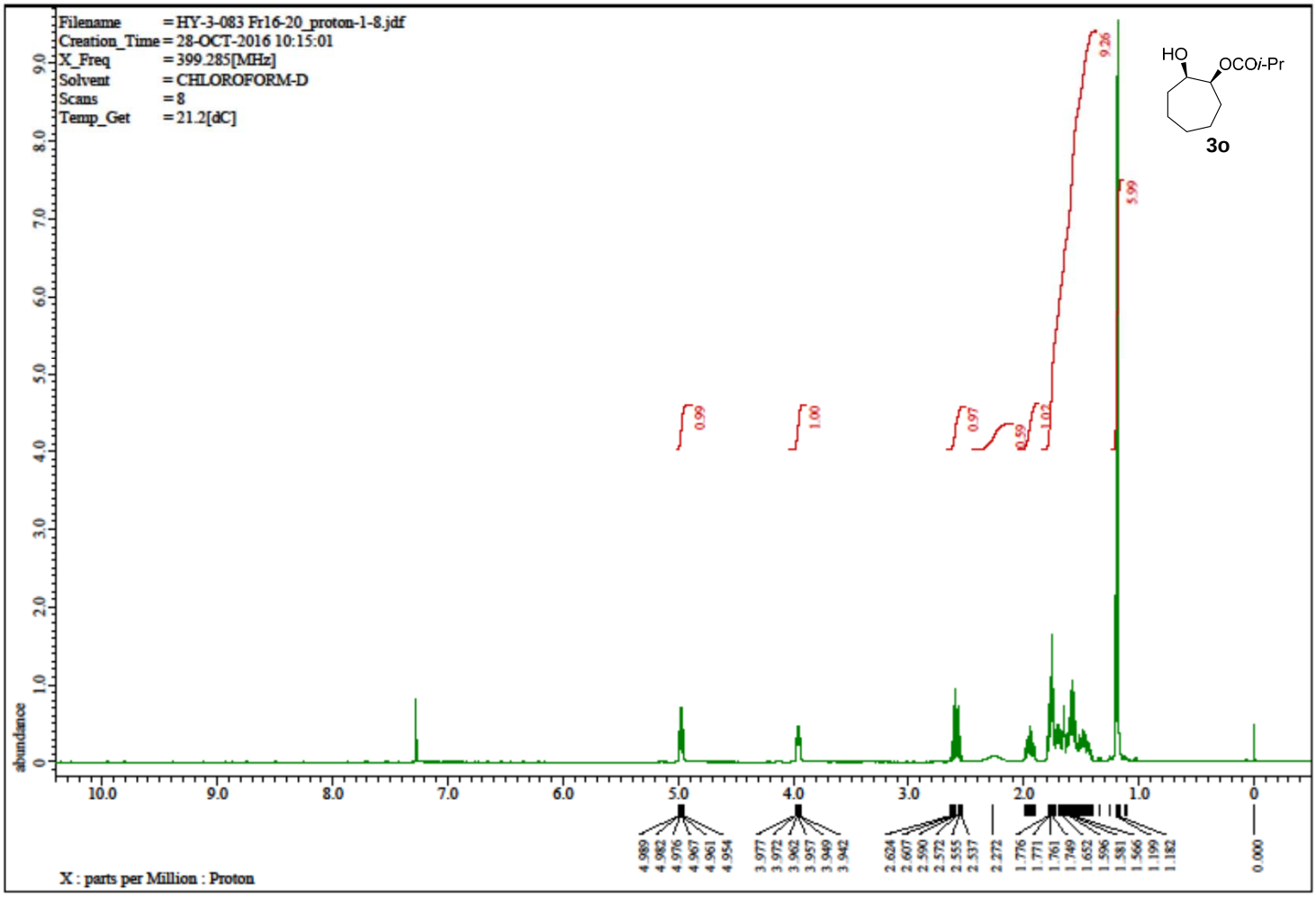

Filename = HY-2-133 s.clm_Carbon-2-3.jdf
Creation_Time = 13-JUL-2016 21:12:00
X_Freq = 100.40028[MHz]
Solvent = CHLOROFORM-D
Scans = 64
Temp_Get = 21.5[dC]
abundance
176.309
77.475
77.160
76.835
70.726
34.287
27.786
21.771
19.070
18.974
X : parts per Million : Carbon13

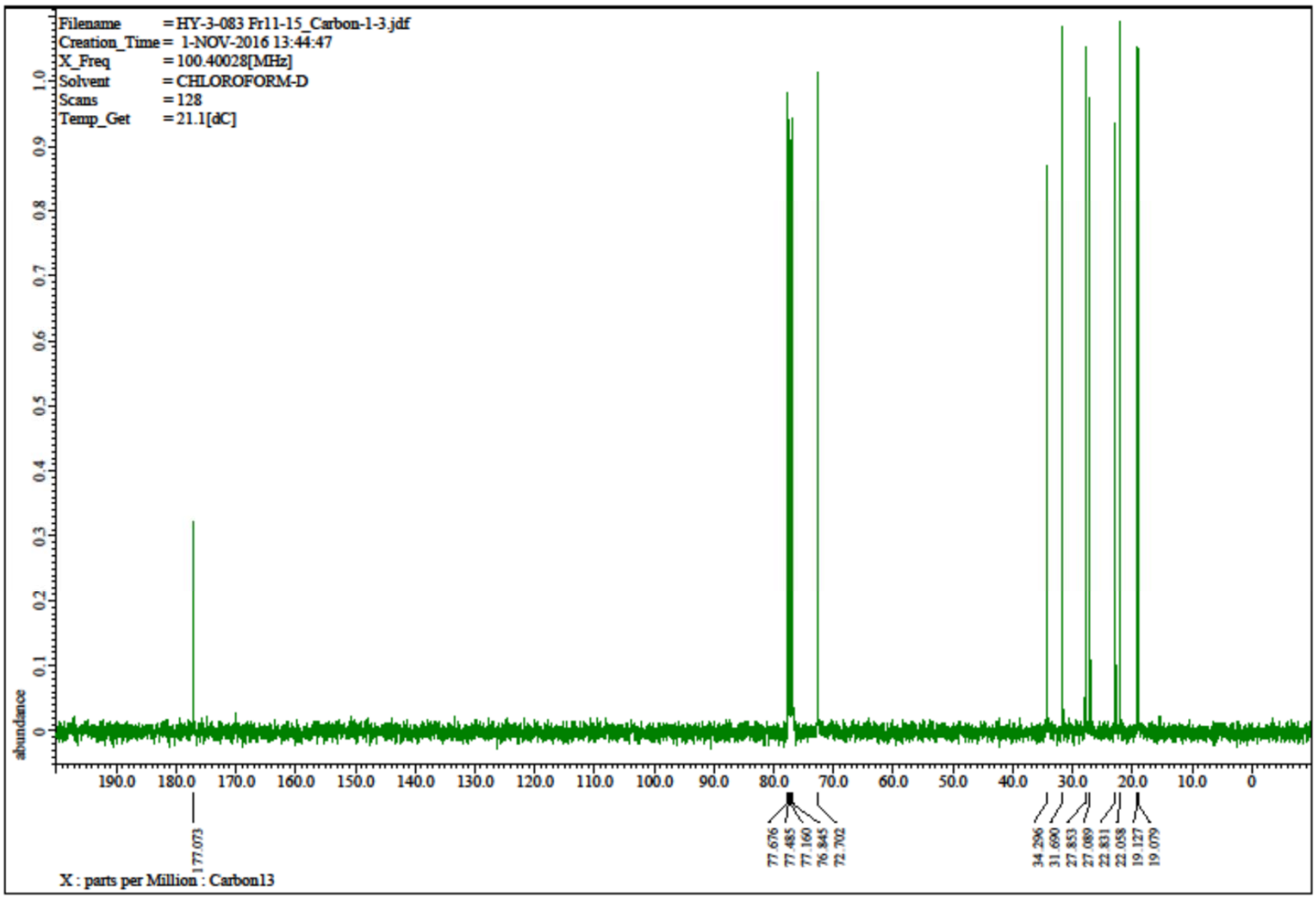

Filename = HY-3-074-Fr18-23_proton-1-5.jdf
Creation_Time = 14-SEP-2016 16:46:13
X_Freq = 399.285[MHz]
Solvent = CHLOROFORM-D
Scans = 8
Temp_Get = 21.2[dC]
OH
OCOi-Pr
3n
X : parts per Million : Proton

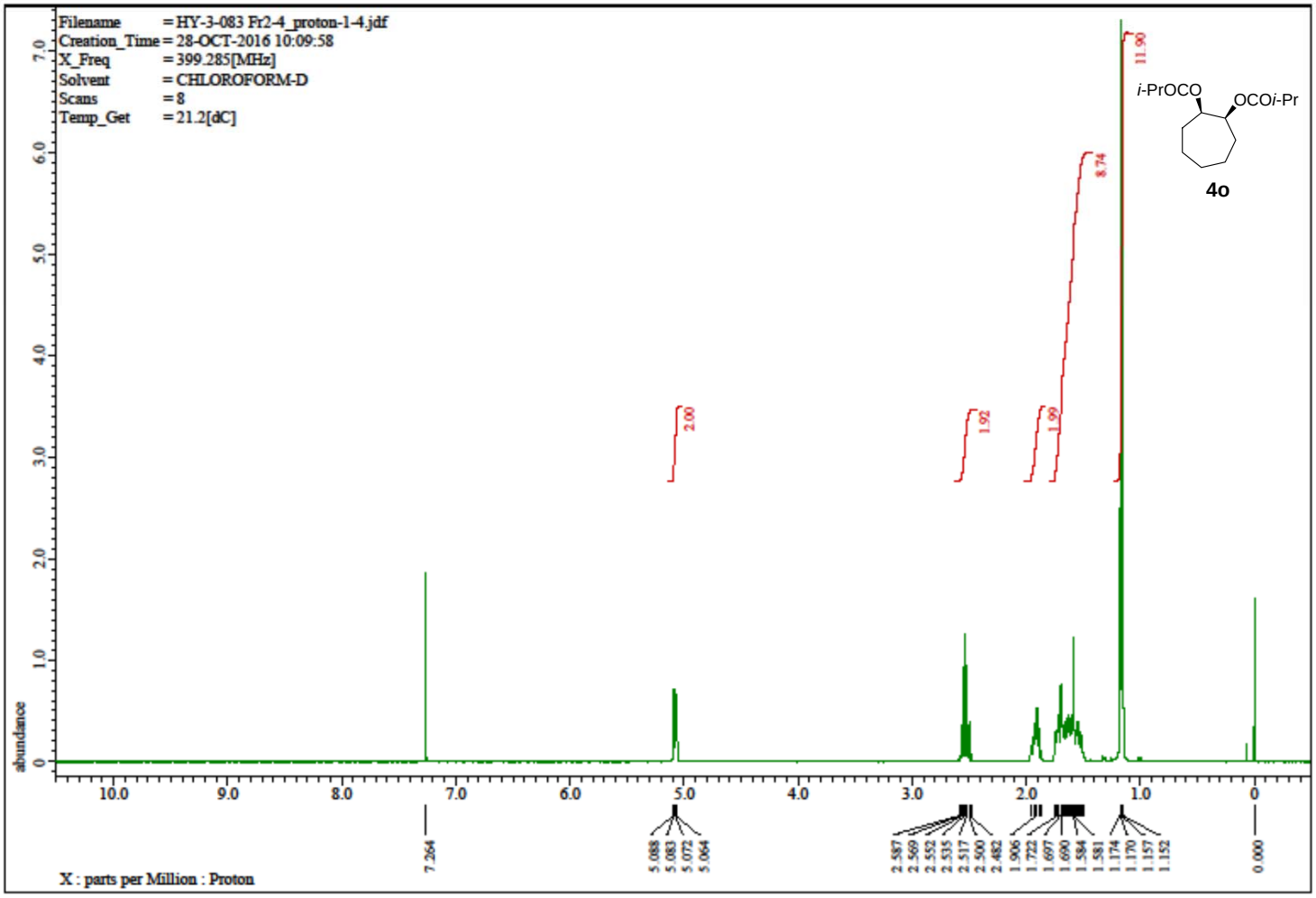

Filename = HY-3-073 Fr15-19_Carbon-1-3.jdf
Creation_Time = 29-AUG-2016 19:07:06
X_Freq = 100.40028[MHz]
Solvent = CHLOROFORM-D
Scans = 64
Temp_Get = 21.2[dC]
X : parts per Million : Carbon13

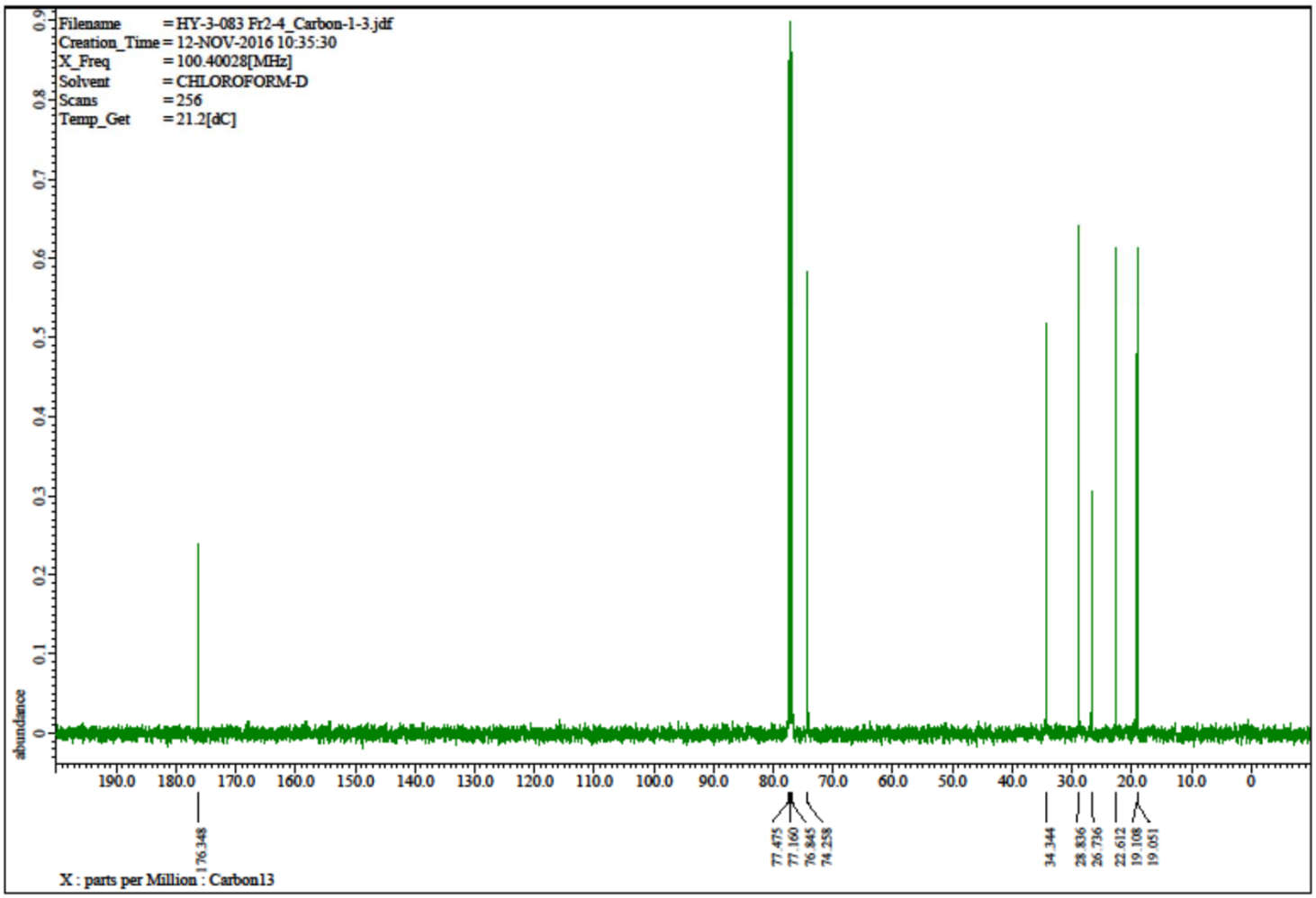

Filename = HY-3-073 Fr2-5_proton-1-6.jdf
Creation_Time = 29-AUG-2016 18:08:22
X_Freq = 399.285[MHz]
Solvent = CHLOROFORM-D
Scans = 8
Temp_Get = 23.8[dC]
OCOi-Pr
OCOi-Pr
4n
X : parts per Million : Proton

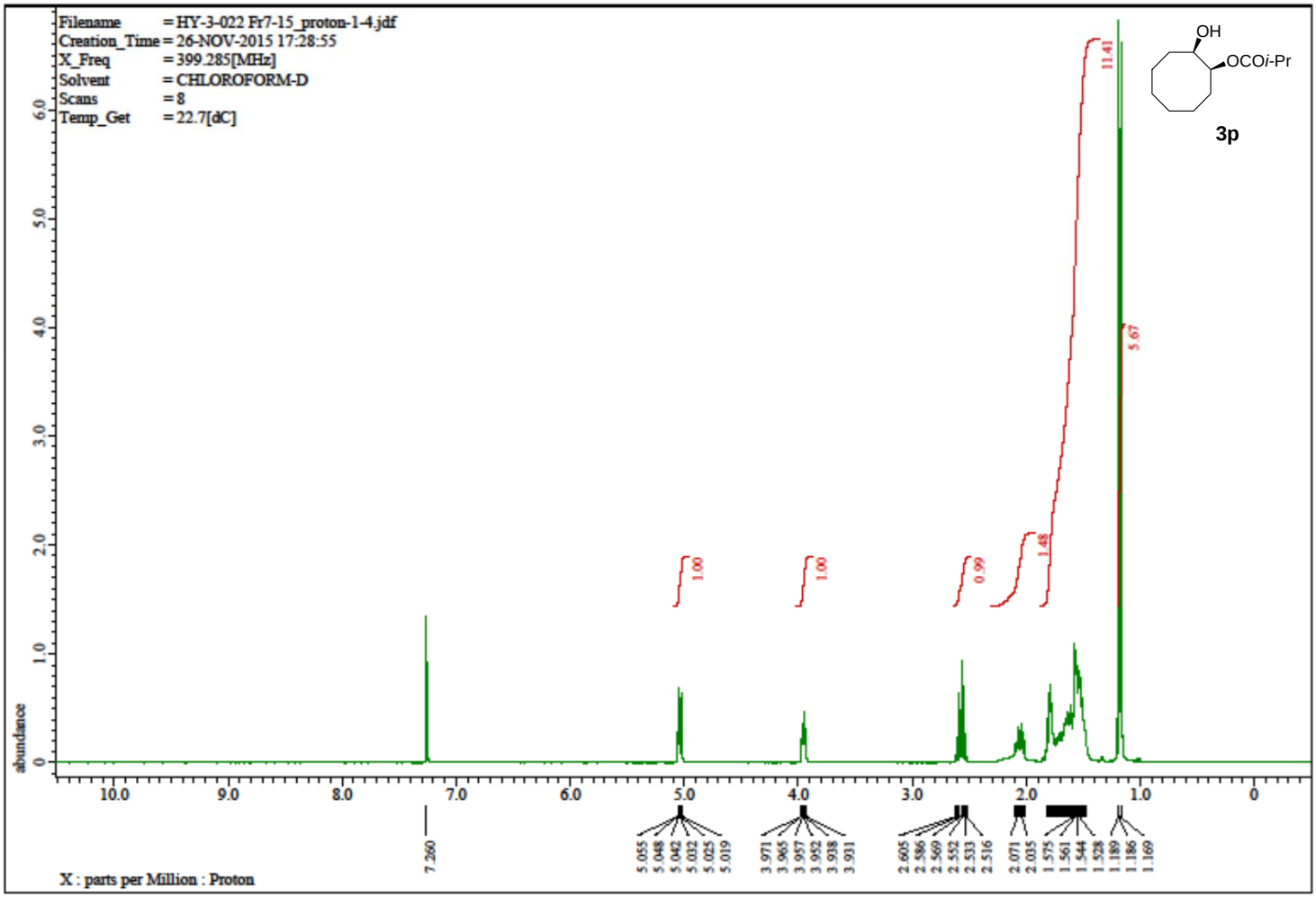

Filename = HY-3-073 Fr2-5_Carbon-1-3.jdf
Creation_Time = 30-AUG-2016 10:18:51
X_Freq = 100.40028[MHz]
Solvent = CHLOROFORM-D
Scans = 128
Temp_Get = 21.5[dC]
X : parts per Million : Carbon13

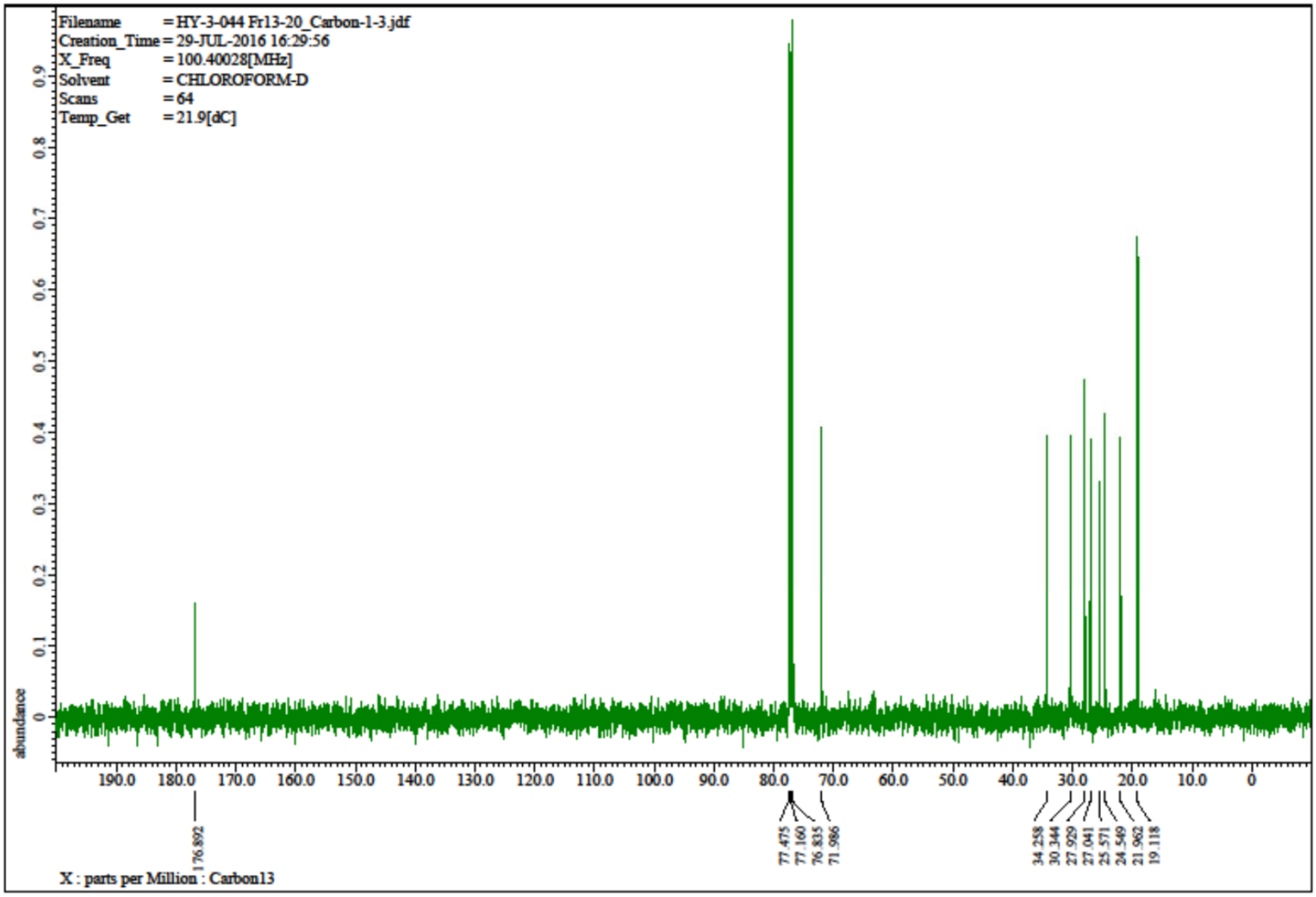

Filename = HY-3-083 Fr16-20_proton-1-8.jdf
Creation_Time = 28-OCT-2016 10:15:01
X_Freq = 399.285[MHz]
Solvent = CHLOROFORM-D
Scans = 8
Temp_Get = 21.2[dC]
HO
OCOi-Pr
3o
9.26
5.99
0.99
1.00
0.97
0.59
1.02
abundance
X : parts per Million : Proton

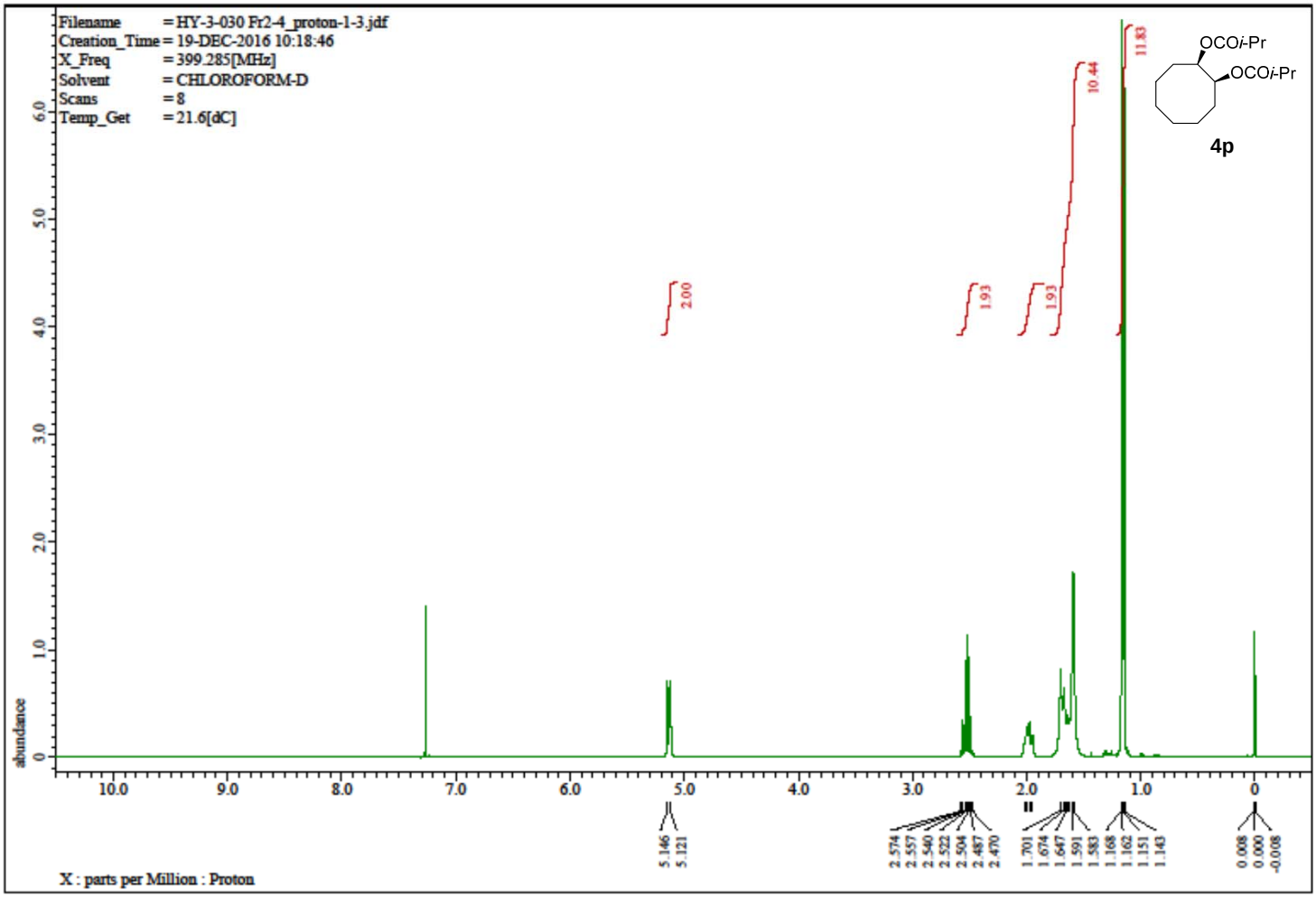

Filename = HY-3-083 Fr11-15_Carbon-1-3.jdf
Creation_Time = 1-NOV-2016 13:44:47
X_Freq = 100.40028[MHz]
Solvent = CHLOROFORM-D
Scans = 128
Temp_Get = 21.1[dC]
abundance
X : parts per Million : Carbon13

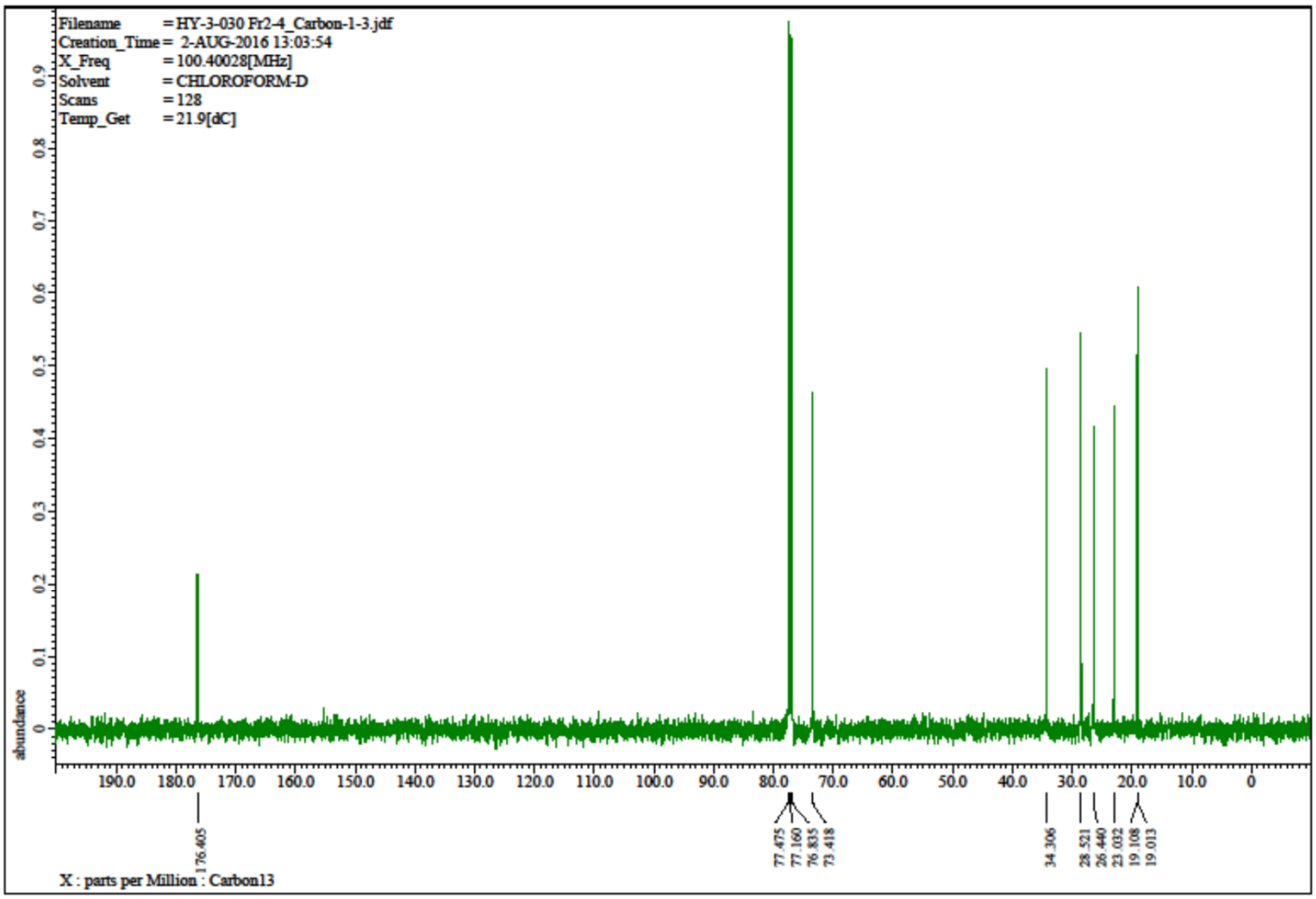

Filename = HY-3-083 Fr2-4_proton-1-4.jdf
Creation_Time = 28-OCT-2016 10:09:58
X_Freq = 399.285[MHz]
Solvent = CHLOROFORM-D
Scans = 8
Temp_Get = 21.2[dC]
i-PrOCO
OCOi-Pr
4o
11.90
8.74
2.00
1.92
1.99
abundance
X : parts per Million : Proton


Filename = HY-3-083 Fr2-4_Carbon-1-3.jdf
Creation_Time = 12-NOV-2016 10:35:30
X_Freq = 100.40028[MHz]
Solvent = CHLOROFORM-D
Scans = 256
Temp_Get = 21.2[dC]
abundance
X : parts per Million : Carbon13


Filename = HY-3-022 Fr7-15_proton-1-4.jdf
Creation_Time = 26-NOV-2015 17:28:55
X_Freq = 399.285[MHz]
Solvent = CHLOROFORM-D
Scans = 8
Temp_Get = 22.7[dC]
OH
OCOi-Pr
3p
11.41
5.67
1.00
1.00
0.99
1.48
abundance
7.260
5.055
5.048
5.042
5.032
5.025
5.019
3.971
3.965
3.957
3.952
3.938
3.931
2.605
2.586
2.569
2.552
2.533
2.516
2.071
2.035
1.575
1.561
1.544
1.528
1.189
1.186
1.169
X : parts per Million : Proton


Filename = HY-3-044 Fr13-20_Carbon-1-3.jdf
Creation_Time = 29-JUL-2016 16:29:56
X_Freq = 100.40028[MHz]
Solvent = CHLOROFORM-D
Scans = 64
Temp_Get = 21.9[dC]
abundance
176.892
77.475
77.160
76.835
71.986
34.258
30.344
27.929
27.041
25.571
24.569
21.962
19.118
X : parts per Million : Carbon13


Filename = HY-3-030 Fr2-4_proton-1-3.jdf
Creation_Time = 19-DEC-2016 10:18:46
X_Freq = 399.285[MHz]
Solvent = CHLOROFORM-D
Scans = 8
Temp_Get = 21.6[dC]
OCOi-Pr
OCOi-Pr
4p
2.00
1.93
1.93
10.44
11.83
abundance
X : parts per Million : Proton


Filename = HY-3-030 Fr2-4_Carbon-1-3.jdf
Creation_Time = 2-AUG-2016 13:03:54
X_Freq = 100.40028[MHz]
Solvent = CHLOROFORM-D
Scans = 128
Temp_Get = 21.9[dC]
abundance
X : parts per Million : Carbon13