Supporting information for

Oxidative Rearrangement of Malondialdehyde: Substrate Scope and Mechanistic Insights

Xin Yu,[a] Zheng Liu,[b] Zilei Xia,[c] Zhigao Shen,[c] Xixian Pan,[a] Hui Zhang*[a] and Weiqing Xie*[b]

[a] Department of Chemistry, School of Science & Instrumental Analysis and Research Center, Shanghai University, Shanghai 200444, China. E-mail: yehao7171@163.com.
[b] State Key Laboratory of Bioorganic & Natural Products Chemistry, Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences, Shanghai 200032, China. E-mail: xiewq@sioc.ac.cn.
[c] State Key Laboratory of Natural Medicines, Center of Drug Discovery, China Pharmaceutical University, Nanjing 210009, China.

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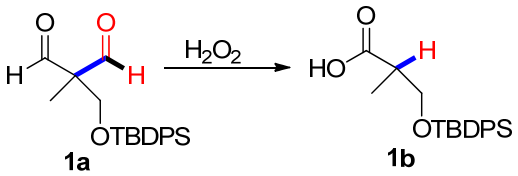
1. Reaction Condition Optimization.

Table S1. Catalyst and Solvent Evaluation.



Entry	Catalyst (equiv)	solvent	Time (h)	Yield[b] (%)
1	--	$CHCl_3$	5	82(80)
2	PhCOOH (0.1)	$CHCl_3$	12	62
3	$[(C_6H_5)O]_2PO_2H$ (0.1)	$CHCl_3$	2	86
4	8H-R-TRIP (0.1)	$CHCl_3$	2	65[c]
5	CF_3COOH (0.1)	$CHCl_3$	5	72
6	$4\text{-}CH_3(C_6H_4)SO_3H$ (0.1)	$CHCl_3$	2	79
7	HCl (0.1)	$CHCl_3$	2	60
8	HBF_4 (0.1)	$CHCl_3$	2	82
9	TfOH (0.1)	$CHCl_3$	2	55
10	*dl*-CSA (0.1)	$CHCl_3$	1	91
11	Ag(OTf)	$CHCl_3$	12	56
12	$Zn(OTf)_2$	$CHCl_3$	12	54
13	$FeCl_3$	$CHCl_3$	12	NR
14	$Cu(OTf)_2$	$CHCl_3$	6	72
15	*dl*-CSA (0.1)	EA	1	97
16	*dl*-CSA (0.1)	MeOH	1	75
17	*dl*-CSA (0.1)	Acetone	2	86
18	*dl*-CSA (0.05)	EA	1	97(93)
19	cis-Hexahydro-phthalic acid (0.1)	$CHCl_3$	6	82
20	*L*-Malic acid	$CHCl_3$	6	70
21	$(Tf)_2NH$	$CHCl_3$	2	complex
22	H_2SO_4	$CHCl_3$	2	67
23	$HClO_4$	$CHCl_3$	2	72
24	*dl*-CSA	DCM	2	85
25	*dl*-CSA	Et_2O	2	88
26	*dl*-CSA	Toluene	overnight	80
27	*dl*-CSA	EtOH	2	83
28	*dl*-CSA	Hexane	overnight	90
29	*dl*-CSA	THF	2	83
30	*dl*-CSA	Acetone	2	86
31	*dl*-CSA	CH_3CN	1	89
32	NO	EA	5.5	82(80)

Reaction conditions: Malondialdehyde (0.2mmol), catalyst (0.02mmol), H_2O_2 (0.24mmol), solvent (2ml). *dl*-CSA = *dl*-10-camphorsulfonic acid. [a]NMR yields, isolated yields are shown in parentheses.

Table S2. Optimization of Reaction Condition by Screening of Oxidant1

Entry	Oxidant	Temp. (°C)	t (h)	Yield[a] (%)
1	TBHP	19	2	NR
2	MCPBA	19	40min	Complex
3	NO	19	2h	NR

Reaction conditions: Malondialdehyde (0.2mmol), CSA (0.02mmol), H_2O_2 (0.24mmol), EA (2ml). [a]NMR yields.

Table S3. Optimization of Reaction Condition by Screening of Concentration and Catalyst's Amount.

Entry	Catalyst (eq.)	Den. (M)	Solvent	Time (h)	Temp. (°C)	Yield [a] (%)
1	0.1	0.2	EA	1	18	94
2	0.1	0.1	EA	1	18	97
3	0.1	0.05	EA	1	18	97
4	0.1	0.025	EA	1	18	96
5	0.02	0.05	EA	1	18	94
6	0.05	0.05	EA	1	18	97
7	0.08	0.05	EA	1	18	96

Reaction conditions: Malondialdehyde (0.2mmol), CSA (indicated in Table S3), H_2O_2 (0.24mmol), EA (indicated in Table S3). [a]NMR yields.

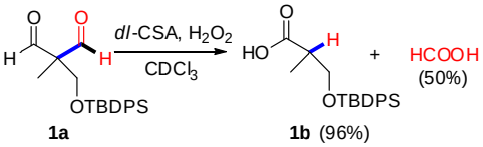
Table S4. Effect of Temperature and Oxidant's Amount.

Entry	H_2O_2(30%) (eq.)	Temp. (°C)	Time (h)	Yield[a] (%)
1	1.2	16	1	97
2	1.2	0	2	90
3	2.0	17	1	86
4	3.0	17	1	90

Reaction conditions: Malondialdehyde (0.2mmol), CSA (0.02mmol), H_2O_2 (indicated in Table S4), EA (2ml). [a]NMR yields.

2. Mechanistic studies.

2.1 NMR Studies of Crude Reaction Mixture.



1a **1b** (96%)

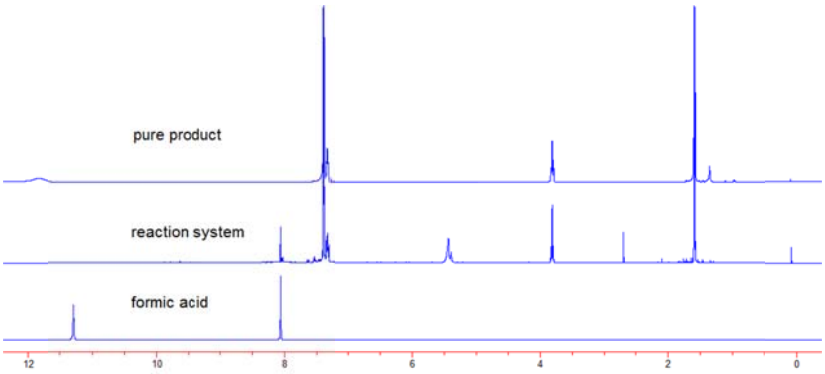


Figure S1. ^{1}HNMR Spectra of Product 2a, Reaction Mixture and Formic Acid.

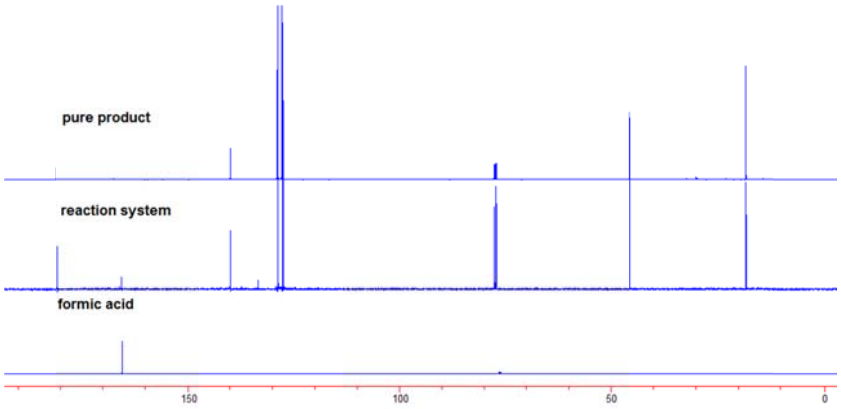
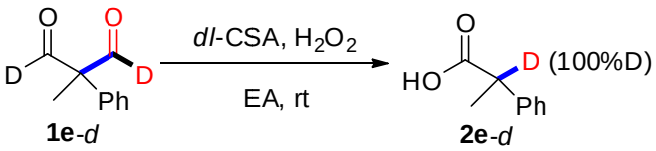


Figure S2. ^{13}CNMR Spectra of Product 2a, Reaction Mixture and Formic acid.



1e-*d* **2e-*d***

Scheme S1. Deuterated Experiment.

To determine the fate of both aldehydes, oxidative decarbonylation of **1a** was performed in NMR tube by using $CDCl_3$ as solvent. After completion of reaction, NMR spectra were collected. Besides the desired product **2a**, formic acid was also found by comparing with the standard spectra, which indicating that the other aldehyde was converted to formic acid (Figure S1 and S2). Subjection of deuterated malondialdehyde **1e-*d*** to the standard reaction condition led to carboxylic acid **2e-*d*** with complete deuterium on α-position as judged by ^{1}H NMR (Scheme S1). This reaction implied that one of aldehyde proton shifted to α-position of resulting carboxylic acid during the course of oxidative decarbonylation reaction.

2. 2 Monitoring the Reaction by ^{1}HNMR Spectra

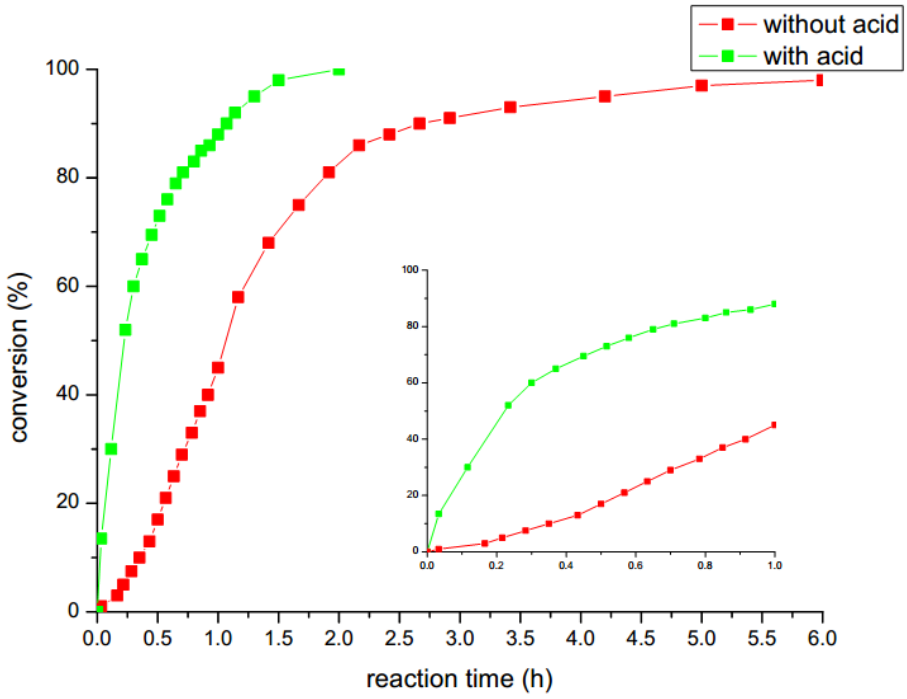


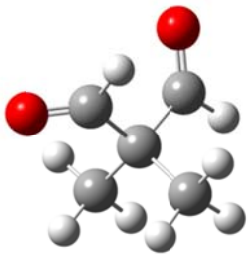
Figure S3. Reaction Progress of Oxidative Decarbonylation of 1a Monitored by ^{1}H NMR.

To further gain insight into the reaction mechanism, reaction progress was monitored by ^{1}H NMR spectroscopy using $CDCl_3$ as solvent (Figure S3). The diagram showed that an accelerating effect was obviously observed (Figure S3, green line) when catalytic CSA was added to the reaction mixture. In the absence of catalyst, the reaction was very slow at the beginning and acceleration could be observed once carboxylic acid produced, which was ascribed the self-catalytic effect of products (Figure S3, read line).

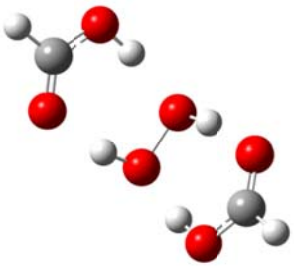
2.3. Computational Details.[1]

Geometry optimizations were carried out by the density functional theory (DFT) method with the B3LYP functional and the 6-31g(d) basis set. Frequency calculations were carried out for each stationary structure at the same level to make sure that it is an equilibrium structure or a transition state. For simplification, 2,2-dimethyl-malondialdehyde and formic acid as catalyst were used for calculation. All the calculations were carried out by the *Gaussian 09* program. Cartesian coordinates and Gibbs energy are provided.

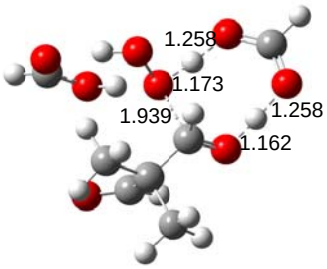
Figures of the Optimized Geomtries



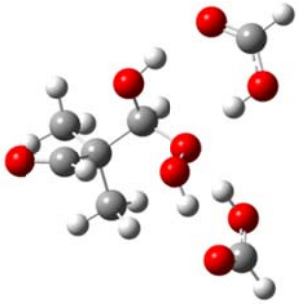
Dial



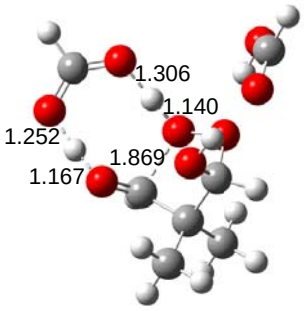
HOOH·2HCOOH



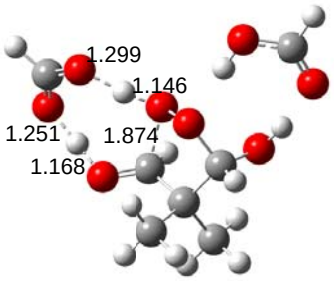
T1



I1



T2-cis



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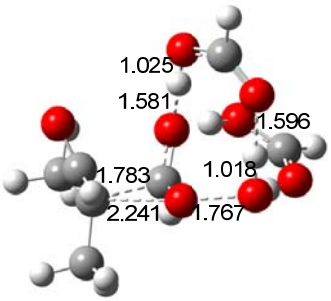
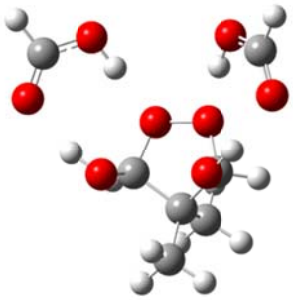


T-BV



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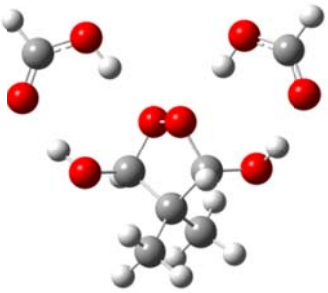

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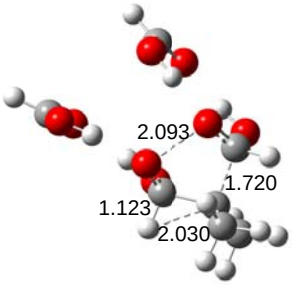

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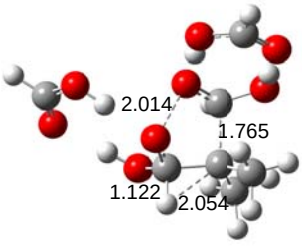
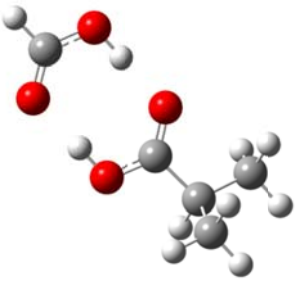


T3-trans



Product

Cartesian Coordinate

Dial

C	0.00458900	0.37634600	-0.00318100

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C	-0.54421500	0.90944000	1.33127800
C	1.44153800	-0.09463600	0.20785600
C	-0.83059500	-0.79194100	-0.52500200
O	-1.86376600	-1.16754000	-0.02095000
O	1.82903000	-1.23315700	0.07357400
H	0.34000700	1.09947700	-2.05753300
H	0.71141000	2.28953400	-0.79644100
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H	0.07724400	1.72998300	1.70720200
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H	-0.43291300	-1.27146500	-1.44388600

HOOH·2HCOOH

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O	2.06727300	-1.16037600	-0.44558600
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T1

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O	2.44137500	-2.13150700	0.85985600
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I1

C	-1.85500800	-0.31474100	0.40179200
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O	-3.60052200	-0.94292000	-1.15729700
O	-0.28825000	-1.97630900	-0.24185300
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T2-cis

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O	0.45248500	0.41783400	1.22633500
C	1.84186600	-0.34252100	0.23450700
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O	0.12511100	2.63600100	0.27915300
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C	-3.84934600	0.25016000	-0.21592000
O	-3.37586500	-0.47814700	-1.07074900
H	-2.29565500	0.39098800	0.88249000
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T2-trans

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C	-1.00868600	1.06581900	0.26100000
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O	-1.66369200	1.12855500	-0.94264800
O	-2.79952000	-2.11864100	0.43029600

C	-3.87786900	-1.50962500	-0.03134000
O	-3.95504200	-0.35491800	-0.41550600
O	0.31641200	-0.68954600	-0.33926400
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H	3.64967700	-3.21823800	-0.03481100

T-BV

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C	-0.37659500	-0.76100300	0.16367500
O	-0.41367900	-0.05381300	1.32062200
C	-2.58223100	0.72607700	0.16931100
O	-2.78120300	1.42341500	-0.79968100
O	0.23068400	-0.24632700	-0.86632800
H	-2.65224800	-1.06429800	2.18682900
H	-2.22875500	-2.53565800	1.29494700
H	-3.79689900	-1.77097600	1.02414300
H	-1.93783100	-0.70251400	-2.07256000
H	-3.47930600	-1.34984700	-1.47565600
H	-2.00905500	-2.34117200	-1.37042500
H	-0.20491500	-1.84124600	0.31772100
H	-2.70158500	1.12088300	1.19956000
O	1.22583300	0.16992300	1.94082700
H	1.37948500	1.06726500	1.48496600
H	1.77660400	-0.49963400	1.42126200
O	2.82378300	-1.52264200	0.65649100
C	3.03071900	-1.85980900	-0.50713200

O	2.29267100	-1.60952100	-1.55392000
H	3.91978100	-2.45030500	-0.76794300
H	1.45309100	-1.05840300	-1.30863800
O	1.64029300	2.48047200	0.79179000
C	1.22748500	2.93110100	-0.27511000
O	0.56028600	2.31009700	-1.20680300
H	1.41115900	3.98042700	-0.54218100
H	0.38934000	1.32152600	-0.99817200

I2-cis

C	0.00703800	2.10284300	0.15530400
C	0.00776200	2.87493800	1.48802100
C	0.01157400	3.05896600	-1.03998100
C	-1.18215700	1.12010900	0.13351600
O	-0.74488800	0.02694500	0.99173600
O	0.74414300	0.02160900	0.99252800
C	1.19033000	1.11287100	0.13640400
O	1.49778200	0.69738400	-1.13490100
O	-1.48840300	0.70576200	-1.13841300
H	0.00438900	2.19909000	2.34857000
H	-0.87408100	3.52149600	1.55485200
H	0.89359200	3.51577000	1.55726000
H	0.01068300	2.51019600	-1.98084500
H	0.89948900	3.70010500	-1.00598500
H	-0.87194100	3.70625900	-1.00781900
H	-2.05829400	1.50038100	0.67821800
H	2.06716700	1.48775100	0.68367300
H	2.28520400	0.11168000	-1.08175100
H	-2.27891200	0.12406300	-1.08707000
O	-1.97723500	-2.43614800	0.53675300
C	-3.08541100	-2.25768800	-0.16369400
O	-3.45735100	-1.22181400	-0.68694600
H	-1.47830900	-1.58013300	0.61413000
H	-3.66186900	-3.19115000	-0.21946700
O	1.95593300	-2.44971500	0.53125300
C	3.06824200	-2.27867900	-0.16444300
O	3.45227200	-1.24388400	-0.68108600
H	1.46493200	-1.58927500	0.61105300
H	3.63565300	-3.21750700	-0.22297700

I2-trans

C	0.00977900	1.97265200	0.04832500
C	0.31223900	2.69810900	1.37050100
C	-0.22073100	2.98616600	-1.08202000

C	-1.20414700	1.02631500	0.24686800
O	-0.58752000	-0.24939700	0.57754500
O	0.50654900	-0.33136500	-0.40269500
C	1.15218200	0.97617400	-0.32917400
O	2.17863100	1.00380100	0.58375000
O	-1.99609800	0.95764200	-0.87207600
H	0.42304500	1.99316400	2.19887100
H	-0.50431500	3.39124300	1.60270300
H	1.24022400	3.26979600	1.29647100
H	-0.43138800	2.48727000	-2.03098000
H	0.66739100	3.61716700	-1.20094500
H	-1.07065400	3.63597000	-0.85187200
H	-1.76987200	1.24204800	1.16415000
H	1.50160500	1.10562100	-1.36224000
H	2.89351600	0.41253100	0.25708300
H	-2.76769900	0.38402400	-0.66408500
O	2.19572300	-2.52817900	-0.02148000
C	3.45548200	-2.16062500	-0.18771800
O	3.87248500	-1.02154300	-0.30745300
H	1.59961400	-1.73337800	-0.04129500
H	4.11491200	-3.03885100	-0.21032600
O	-2.27259500	-2.46791500	0.34550400
C	-3.51527700	-2.08074900	0.11088500
O	-3.89356900	-0.94467700	-0.11716100
H	-1.66061000	-1.68448400	0.33869600
H	-4.20179900	-2.93730700	0.15029300

T3-cis

C	-2.24659000	-0.45498000	0.05183100
C	-0.83051000	-1.12118600	0.30738600
C	-1.62599100	1.04000500	-0.53095800
H	-1.22584100	-2.16009700	0.46493800
O	-0.72936300	0.76189300	-1.42849000
O	-0.10928600	-1.13202700	-0.78786000
C	-2.99008100	-1.14157900	-1.09002800
C	-3.08469200	-0.25352800	1.29777200
O	-0.26678100	-0.64618400	1.47563800
O	-1.36320100	1.87301800	0.51740200
H	-2.58752700	1.34558700	-0.99353200
H	-2.36706600	-1.20325700	-1.98385400
H	-3.91051100	-0.59681200	-1.32426900
H	-3.28911000	-2.15383700	-0.79604900
H	-2.50809600	0.23296200	2.08331000
H	-3.45412800	-1.22004500	1.66134800

H	-3.96356200	0.35840200	1.06681300
H	0.71570000	-0.70926700	1.39922700
H	-0.38540400	1.97821300	0.64322800
O	1.93387700	1.35221800	-1.19225700
C	2.16620200	1.99960100	-0.06417800
O	1.33800400	2.33864800	0.76368300
H	0.95816000	1.15371700	-1.27900400
H	3.23650900	2.21636700	0.05244100
O	2.49877300	-1.87555400	-0.85609000
C	3.05273500	-1.56636400	0.29904500
O	2.50740500	-1.02528600	1.24825800
H	1.54895700	-1.56206500	-0.86398900
H	4.11006900	-1.86550200	0.32189900

T3-trans

C	-0.51943300	1.80870100	0.29261300
C	0.84215200	1.19940800	0.72937900
C	-0.78805600	0.71432900	-1.06569000
O	-0.18745800	-0.41700900	-0.79015700
O	0.71584000	-0.09513800	0.98067500
C	-1.62851000	1.57169800	1.30869300
C	-0.47722500	3.23704200	-0.20870100
O	1.85381300	1.62598500	-0.10461700
O	-2.15117000	0.72698800	-1.27520900
H	0.93173800	1.67862000	1.74015700
H	-0.28681000	1.28318100	-1.86628100
H	-1.66376400	0.53034300	1.63475800
H	-2.59290900	1.84450000	0.87731300
H	-1.46560400	2.20734100	2.18733300
H	0.36365600	3.40184900	-0.88507500
H	-0.39783600	3.93971100	0.62952300
H	-1.41492800	3.46050000	-0.72974000
H	2.53554200	0.91436300	-0.19817900
H	-2.56254800	-0.06904800	-0.85440800
O	2.49971300	-2.04221100	0.31099200
C	3.58154600	-1.51040500	-0.22210700
O	3.78460800	-0.32385000	-0.42504500
H	1.84549500	-1.31994000	0.53281100
H	4.32057900	-2.28359300	-0.47318300
O	-1.38733300	-2.68036800	0.15416700
C	-2.68867400	-2.49571800	0.24862100
O	-3.30333100	-1.48131600	-0.04301900
H	-0.95222100	-1.84980600	-0.19257900
H	-3.18863600	-3.39299900	0.63840900

Product

C	2.12870900	-0.14977600	-0.30638500
C	0.61420000	-0.08004800	-0.21413200
O	0.00729800	0.93728300	0.12139200
C	2.75298400	1.24614800	-0.37817800
C	2.67018600	-0.96912600	0.88519700
O	0.02385500	-1.23026300	-0.50444800
H	2.37728700	1.80942700	-1.23819600
H	3.84150200	1.16583300	-0.46908100
H	2.52183200	1.82313400	0.52242000
H	2.23243700	-1.97117600	0.90985700
H	2.44649400	-0.46844400	1.83440700
H	3.75777100	-1.06864900	0.80461200
H	-0.96774700	-1.14778000	-0.39781200
O	-2.64629600	1.17383200	0.38218500
C	-3.22330400	0.02616200	0.10736500
O	-2.66718900	-1.01278500	-0.22374100
H	-1.64646500	1.09005600	0.28330900
H	-4.31512700	0.09025300	0.20873500
H	2.35401500	-0.70734600	-1.22455300

3. Experimental part

3.1 General considerations

Unless otherwise specified, all reactions were carried out in open flask. Ethyl acetate and hydrogen peroxide (30%) were used directly as received form the regent company. Anhydrous solvents were treated as followed: dimethylformamide was distilled over calcium hydride under reduced pressure, tetrahydrofuran was distilled from benzophenone ketyl under nitrogen atmosphere. Column chromatography was carried out by normal silica gel (40-60 μm, 230-400 mesh, Silicycle P60). ^{1}H and ^{19}F NMR spectra were recorded on Angilent instrument (500 MHz and 400 MHz, respectively). ^{13}C NMR spectra were recorded on Angilent instrument (125 MHz). Chemical shifts (δ) are reported in ppm relative to TMS (δ 0.00) for the ^{1}H NMR and to chloroform (δ 77.0) for the ^{13}C NMR measurements. Low resolution mass spectra were obtained on Agilent Technologies 5973N spectrometer in EI mode. High resolution mass spectra were obtained on Waters Micromass GCT premier spectrometer.

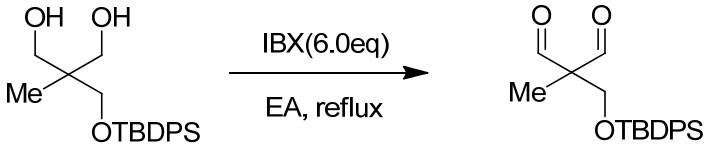
3.2 General Procedure for the synthesis of 1,3-diol

S1a [2], **S1b** [3], **S1c** [2] and S**1d** [2] are known compounds and they are synthesized according to related literature. The rest of 1,3-diols are synthesized by the method as followed:

Under nitrogen atmosphere, diethyl ester (or dimethyl ester, 10 mmol) dissolved in THF (20 ml) was added to a suspension of $LiAlH_4$ (1.14 g, 30 mmol) in THF (40ml) slowly at 0 ^{o}C. The reaction mixture was stirred for addition 30 min, then removed the ice-bath and warmed to room temperature. H_2O (1.2 ml) was added dropwise to quenched the reaction until the TLC showed the starting material was completely consumed, 20% aqueous KOH (1.2 ml) and H_2O (3 ml) was added successively. The precipitated white solid was filtered and washed with EtOAc, the filtrate was concentrated in vacuo and purified by column chromatography (EtOAc : PE = 1:3) to afford the corresponding 1,3-diol .

All of the diethyl esters (or dimethyl esters) are synthesized according to the related literatures[4].

3.3 General Procedure for the synthesis of Malondialdehydes

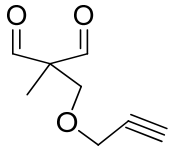


S1a **1a**

To a mixture of IBX (6 mmol, 1.68 g) and **S1a** (1 mmol) in a round bottom flask was added EtOAc (15 ml) via cannula. The reaction suspension was heated to reflux overnight. Then the reaction mixture was cooled in an ice bath for a while and then filtered. The filter cake was washed with EtOAc and the combined filtrates concentrated to give the **1a** as colorless oil (99%), which was used without further purification.

2-(((tert-butyldiphenylsilyl)oxy)methyl)-2-methylmalonaldehyde (1a).[2]

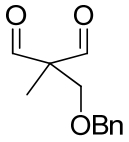
^{1}H NMR (500 MHz, $CDCl_3$): δ9.82 (s, 2H), 7.63-7.64 (m, 4H), 7.41-7.47 (m, 6H), 4.03 (s, 2H), 1.25 (s, 3H), 1.05 (s, 9H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 200.5, 135.6, 132.3, 130.1, 127.9, 65.3, 64.1, 26.7, 12.8; IR(film): 3071, 2931, 2857, 1732, 1471, 1427 cm^{-1}; HRMS(EI): calcd for $C_{17}H_{17}O_3Si[M-C_4H_9]^+$: 297.0947, found: 297.0950.



2-methyl-2-((prop-2-yn-1-yloxy)methyl)malonaldehyde (1b).

Following the general procedure, the title product was synthesized from **S1b**, as yellow oil (99%).

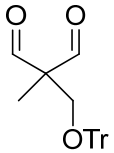
^{1}H NMR (500 MHz, $CDCl_3$): δ 9.72 (s, 2H), 4.16 (d, *J* = 2.5 Hz, 2H), 3.91 (s, 2H), 2.48 (t, *J* = 2.5 Hz, 1H), 1.29 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 199.8, 78.6, 75.5, 70.2, 62.6, 58.8, 13.4; IR(film): 3438, 3289,2859, 1728, 1454, 1359 cm^{-1}; HRMS(EI): calcd for $C_8H_{11}O_3[M]^+$: 155.0708, found: 155.0706.



2-((benzyloxy)methyl)-2-methylmalonaldehyde (1c).[2]

Following the general procedure, the title product was synthesized from **S1c**, as colorless oil (99%).

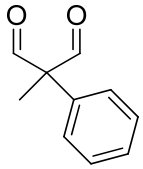
^{1}H NMR (500 MHz, $CDCl_3$): δ 9.75 (s, 2H), 7.38-7.28 (m, 5H), 4.54 (s, 2H), 3.83 (s, 2H), 1.28 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 200.1, 137.2, 128.5, 128.0, 127.7, 73.7, 70.8, 62.9, 13.4; IR(film): 3031, 2859, 2725, 1734, 1712, 1454 cm^{-1}; HRMS(EI): calcd for $C_{12}H_{13}O_3[M-H]^+$: 205.0870, found: 205.0869.



2-methyl-2-((trityloxy)methyl)malonaldehyde (1d).[2]

Following the general procedure, the title product was synthesized from **S1d**, as colorless oil (99%).

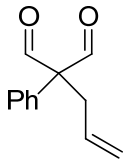
^{1}H NMR (500 MHz, $CDCl_3$): δ 9.76 (s, 2H), 7.44-7.27 (m, 15H), 3.6 (s, 2H), 1.25 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 200.3, 143.0, 128.7, 128.6, 128.0, 127.4, 87.3, 64.6, 62.8, 13.4; IR(film): 3059, 2931, 2871, 2722, 1733, 1712, 1569, 1491, 1449 cm^{-1}; HRMS(EI): calcd for $C_{24}H_{22}O_3[M]^+$: 358.1569, found: 358.1571.



2-methyl-2-phenylmalonaldehyde (1e).[5]

Following the general procedure, the title product was synthesized from **S1e**, as colorless oil (99%).

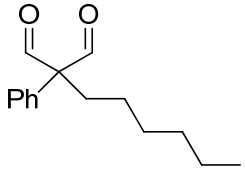
^{1}H NMR (500 MHz, $CDCl_3$): δ 9.76 (s, 2H), 7.49 (t, J = 7.5 Hz, 2H), 7.42 (t, J = 7.5 Hz, 1H), 7.32 (d, J = 7.5 Hz, 2H), 1.70 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 198.1, 133.0, 129.6, 128.7, 127.4, 66.1, 14.0; IR(film): 3061, 2833, 2722, 1735, 1711, 1598, 1494, 1446 cm^{-1}; HRMS(EI): calcd for $C_{10}H_{10}O_2[M]^+$: 162.0681, found: 162.0678.



2-allyl-2-phenylmalonaldehyde (1f).

Following the general procedure, the title product was synthesized from **S1f**, as pale yellow oil (99%).

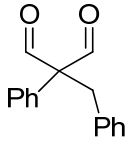
^{1}H NMR (500 MHz, $CDCl_3$): δ 9.84 (s, 2H), 7.48 (t, *J* = 7.5 Hz, 2H), 7.41 (t, *J* = 7.5 Hz, 1H), 7.28-7.26 (m, 2H), 5.80-5.74 (m, 1H), 5.23-5.15 (m, 2H), 3.08 (d, *J* = 7.5 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 198.3, 132.3, 131.6, 129.7, 128.7, 127.7, 120.1, 68.5, 34.3; IR(film): 3080, 2837, 2728, 1730, 1712, 1597, 1494, 1448 cm^{-1}; HRMS(EI): calcd for $C_{12}H_{12}O_2[M]^+$: 188.0837, found: 188.0835.



2-hexyl-2-phenylmalonaldehyde (1g).

Following the general procedure, the title product was synthesized from **S1g**, as colorless oil (99%).

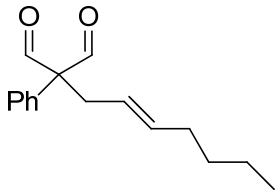
^{1}H NMR (500 MHz, $CDCl_3$): δ 9.85 (s, 2H), 7.46 (t, *J* = 7.5 Hz, 2H), 7.40-7.38 (m, 1H), 7.27-7.24 (m, 2H), 2.29-2.25 (m, 2H), 1.40-1.28 (m, 8H), 0.89 (t, *J* = 6.5 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 198.7, 133.0, 129.5, 128.5, 127.8, 69.3, 31.4, 29.9, 24.4, 22.5, 14.0; IR(film): 2929, 2857, 2726, 1731, 1713, 1598, 1495, 1448 cm^{-1}; HRMS(EI): calcd for $C_{15}H_{20}O_2[M]^+$: 232.1463, found: 232.1468.



2-benzyl-2-phenylmalonaldehyde (1h).

Following the general procedure, the title product was synthesized from **S1h**, as colorless oil (99%).

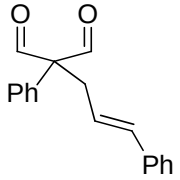
^{1}H NMR (500 MHz, $CDCl_3$): δ 9.93 (s, 2H), 7.48-7.40 (m, 3H), 7.25-7.21 (m, 5H), 7.08-7.06 (m, 2H), 3.67 (s, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 198.3, 134.9, 133.1, 130.4, 129.6, 129.0, 128.8, 128.5, 127.9, 127.2, 69.9, 36.8; IR(film): 3061, 2842, 2725, 1728, 1682, 1582, 1496, 1453 cm^{-1}; HRMS(EI): calcd for $C_{16}H_{14}O_2[M]^+$: 238.0994, found: 238.0997.



(E)-2-(hept-2-en-1-yl)-2-phenylmalonaldehyde (1i).

Following the general procedure, the title product was synthesized from **S1i**, as pale yellow oil (99%).

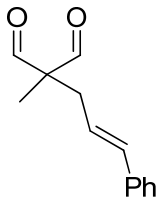
^{1}H NMR (500 MHz, $CDCl_3$): δ 9.82 (s, 2H), 7.45 (t, *J* = 7.5 Hz, 2H), 7.38 (t, *J* = 7.5 Hz, 1H), 7.26 (d, *J* = 7.5 Hz, 2H), 3.02 (d, *J* = 7.0 Hz, 2H), 1.98-1.94 (m. 2 H), 1.31-1.22 (m, 4H), 0.86 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 198.7, 136.6, 132.6, 129.5, 128.6, 127.8, 122.6, 68.6, 33.3, 32.2, 31.3, 22.1, 13.8; IR(film): 2926, 2854, 2728, 1731, 1714, 1495, 1447 cm^{-1}; HRMS(EI): calcd for $C_{16}H_{20}O_2[M]^+$: 244.1463, found: 244.1461.



2-cinnamyl-2-phenylmalonaldehyde (1j).

Following the general procedure, the title product was synthesized from **S1j**, as pale yellow oil (98%).

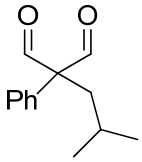
^{1}H NMR (500 MHz, $CDCl_3$): δ 9.90 (s, 2H), 7.50 (t, *J* = 7.5 Hz, 2H), 7.43 (t, *J* = 7.5 Hz, 1H), 7.32-7.23 (m, 7H), 6.56 (d, *J* = 16.0 Hz, 1H), 6.14 (dt, *J* = 16.0 Hz, 7.5 Hz, 1H), 3.24 (d, *J* = 6.5 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 198.4, 136.6, 135.0, 132.5, 129.8, 128.8, 128.6, 127.8, 126.4, 122.9, 69.1, 33.7; IR(film): 3027, 2829, 2725, 1731, 1712, 1494, 1447 cm^{-1} ; HRMS(EI): calcd for $C_{18}H_{16}O_2[M]^+$: 264.1150, found: 264.1152.



2-cinnamyl-2-methylmalonaldehyde (1k).

Following the general procedure, the title product was synthesized from **S1k**, as pale yellow oil (99%).

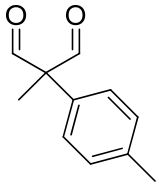
^{1}H NMR (500 MHz, $CDCl_3$): δ 9.70 (s, 2H), 7.35-7.23 (m, 5H), 6.51 (d, *J* = 15.5 Hz, 1H), 6.06 (dt, *J* = 15.5 Hz, 7.5 Hz, 1H), 2.75 (d, *J* = 7.5 Hz, 2H), 1.37 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 200.4, 136.5, 135.0, 128.6, 127.8, 126.3, 122.1, 62.5, 35.9, 14.9; IR(film): 3027, 2969, 2828, 1732, 1708, 1598, 1495, 1450 cm^{-1}; HRMS(EI): calcd for $C_{13}H_{14}O_2[M]^+$: 202.0994, found: 202.0091.



2-isobutyl-2-phenylmalonaldehyde (1l).

Following the general procedure, the title product was synthesized from **S1l**, as colorless oil (98%).

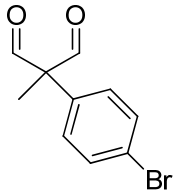
^{1}H NMR (500 MHz, $CDCl_3$): δ 9.91 (s, 2H), 7.43 (t, *J* = 7.5 Hz, 2H), 7.36 (t, *J* = 7.5 Hz, 1H), 7.25 (d, *J* = 7.5 Hz, 2H), 2.28 (d, *J* = 6.5 Hz, 2H), 1.75-1.70 (m, 1H), 0.92 (d, *J* = 6.5 Hz, 6H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 198.7, 133.4, 129.5, 128.5, 127.8, 68.9, 39.4, 24.9, 24.0; IR(film): 3060, 2960, 2723, 1728, 1597, 1495, 1468 cm^{-1}; HRMS(EI): calcd for $C_{13}H_{16}O_2[M]^+$: 204.1150, found: 204.1152.



2-methyl-2-(p-tolyl)malonaldehyde (1m).

Following the general procedure, the title product was synthesized from **S1m**, as colorless oil (99%).

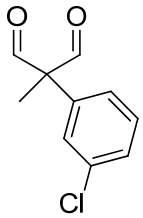
^{1}H NMR (500 MHz, $CDCl_3$): δ 9.74 (s, 2H), 7.29 (d, *J* = 8.0 Hz, 2H), 7.21-7.19 (m, 2H), 2.39 (s, 3H), 1.68 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 198.2, 138.7, 130.3, 129.9, 127.3, 65.7, 21.0, 13.9; IR(film): 2983, 2834, 2721, 1735, 1711, 1513, 1452 cm^{-1}; HRMS(EI): calcd for $C_{11}H_{12}O_2[M]^+$: 176.0837, found: 176.0842.



2-(4-bromophenyl)-2-methylmalonaldehyde (1n).

Following the general procedure, the title product was synthesized from **S1n**, as colorless oil (99%).

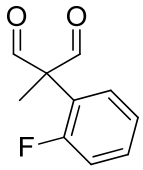
^{1}H NMR (500 MHz, $CDCl_3$): δ 9.72 (s, 2H), 7.62-7.60 (m, 2H), 7.19-7.18 (m, 2H), 1.70 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 197.5, 132.7, 132.0, 129.1, 123.2, 65.7, 14.2; IR(film): 2833, 2725, 1736, 1711, 1592, 1490, 1456 cm^{-1}; HRMS(EI): calcd for $C_{10}H_9BrO_2[M]^+$: 239.9786, found: 239.9790.



2-(3-chlorophenyl)-2-methylmalonaldehyde (1o).

Following the general procedure, the title product was synthesized from **S1o**, as colorless oil (99%).

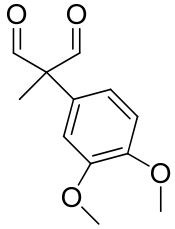
^{1}H NMR (500 MHz, $CDCl_3$): δ 9.73 (s, 2H), 7.43-7.19 (m, 4H), 1.70 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 197.4, 135.6, 135.0, 130.7, 129.0, 127.6, 125.8, 65.8, 14.2; IR(film): 2833, 2721, 1730, 1713, 1593, 1480, 1416 cm^{-1}; HRMS(EI): calcd for $C_{10}H_9ClO_2[M]^+$: 196.0291, found: 196.0287.



2-(2-fluorophenyl)-2-methylmalonaldehyde (1p).

Following the general procedure, the title product was synthesized from **S1p**, as colorless oil (99%).

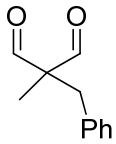
^{1}H NMR (500 MHz, $CDCl_3$): δ 9.38 (d, J = 3.5 Hz, 2H), 7.44-7.40 (m, 1H), 7.28-7.26 (m, 2H), 7.20-7.16 (m, 1H), 1.66 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 197.38 and 197.36, 161.8, 159.8, 130.90 and 130.83, 128.73 and 128.69, 125.27 and 125.25, 116.33 and 116.16, 64.10 and 64.08, 15.3; ^{19}F NMR (400 MHz, $CDCl_3$) δ -113.5 (s, 1F); IR(film): 2987, 2834, 2722, 1738, 1716, 1581, 1489, 1454 cm^{-1}; HRMS(EI): calcd for $C_{10}H_9FO_2[M]^+$: 180.0587, found: 180.0587.



2-(3,4-dimethoxyphenyl)-2-methylmalonaldehyde (1q).

Following the general procedure, the title product was synthesized from **S1q**, as colorless oil (99%).

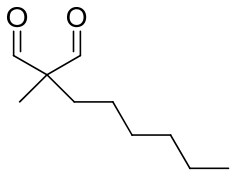
^{1}H NMR (500 MHz, $CDCl_3$): δ 9.72 (s, 2H), 6.95 (d, *J* = 8.0 Hz, 1H), 6.84 (dd, *J* = 8.5 Hz, 2.0 Hz, 1H), 6.75 (d, *J* = 2.5 Hz, 1H), 3.89 (s, 6H), 1.66 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 198.1, 149.9, 149.5, 124.9, 120.1, 111.9, 110.2, 65.4, 56.0, 55.9, 14.0; IR(film): 2938, 2838, 2720, 1735, 1708, 1589, 1518, 1465, 1413 cm^{-1}; HRMS(EI): calcd for $C_{12}H_{14}O_4[M]^+$: 222.0892, found: 222.0890.



2-benzyl-2-methylmalonaldehyde (1r).

Following the general procedure, the title product was synthesized from **S1r**, as yellow oil (99%).

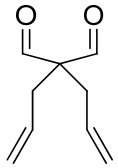
^{1}H NMR (500 MHz, $CDCl_3$): δ 9.71 (s, 2H), 7.31-7.25 (m, 3H), 7.10 (d, *J* = 7.0Hz, 2H), 3.17 (s, 2H), 1.30 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 200.7, 134.5, 130.1, 128.7, 127.3, 63.0, 38.5, 14.9; IR(film): 3063, 2932, 2830, 2727, 1753, 1709, 1603, 1496, 1453 cm^{-1}; HRMS(EI): calcd for $C_{11}H_{12}O_2[M]^+$: 176.0837, found: 176.0840.



2-hexyl-2-methylmalonaldehyde (1s).

Following the general procedure, the title product was synthesized from **S1s**, as colorless oil (99%).

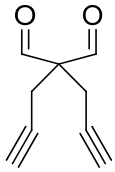
^{1}H NMR (500 MHz, $CDCl_3$): δ 9.65 (s, 2H), 1.82-1.79 (m, 2H), 1.29-1.21 (m, 11H), 0.86 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 201.0, 62.4, 32.5, 31.4, 29.6, 23.7, 22.4, 14.4, 14.0, 13.9; IR(film): 2958, 2931, 2859, 1711, 1467, 1260 cm^{-1}; HRMS(EI): calcd for $C_{10}H_{18}O_2[M]^+$: 170.1307, found: 170.1310.



2,2-diallylmalonaldehyde (1t).

Following the general procedure, the title product was synthesized from **S1t**, as pale yellow oil (99%).

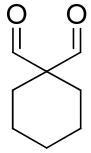
^{1}H NMR (500 MHz, $CDCl_3$): δ 9.71 (s, 2H), 5.74-5.65 (m, 2H), 5.20-5.16 (m, 4H), 2.62 (d, *J* = 8.0 Hz, 4H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 200.5, 130.8, 120.2, 64.4, 34.7; IR(film): 3488, 3076, 2924, 2096, 1724, 1639, 1442 cm^{-1}; HRMS(EI): calcd for $C_9H_{12}O_2[M]^+$: 152.0837, found: 152.0840.



2,2-di(prop-2-yn-1-yl)malonaldehyde (1u).

Following the general procedure, the title product was synthesized from **S1u**, as colorless oil (99%).

^{1}H NMR (500 MHz, $CDCl_3$): δ 9.68 (s, 2H), 2.93 (d, *J* = 3.0 Hz, 4H), 2.13 (t, *J* = 3.0 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 197.0, 77.2, 73.1, 64.0, 19.3; IR(film): 3289, 1713, 1683, 1651, 1429, 1260 cm^{-1}; HRMS(EI): calcd for $C_9H_7O_2[M-H]^+$: 147.0446, found: 147.0048.

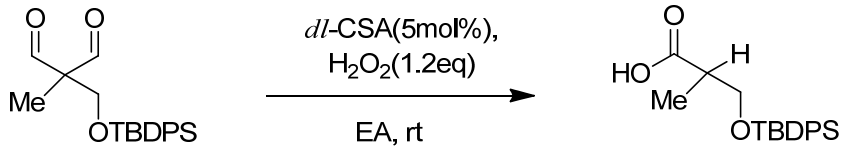


cyclohexane-1,1-dicarbaldehyde (1v).

Following the general procedure, the title product was synthesized from **S1v**, as colorless oil (99%).

^{1}H NMR (500 MHz, $CDCl_3$): δ 9.52 (s, 2H), 1.93 (t, *J* = 6.0 Hz, 4H), 1.54-1.50 (m, 4H), 1.46-1.43 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 200.6, 63.7, 26.6, 24.9, 21.8; IR(film): 2936, 2858, 1726, 1692, 1582, 1450 cm^{-1}; HRMS(EI): calcd for $C_8H_{12}O_2[M]^+$: 140.0837, found: 140.0832.

2.4 General Procedure for the synthesis of carboxylic acids



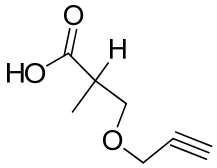
1a **2a**

H_2O_2 (0.24mmol) was added to the solution of **1a** (0.2mmol) and *dl*-CSA (0.01mmol) in EtOAc (2ml). The reaction mixture was stirred at room temperature until the TLC showed the starting material was completely consumed. Remove the solvent under reduced pressure, the resulting residue was purified by column chromatography (EtOAc : PE = 1 : 2) to afford the **2a** (66 mg, 93%) as a white solid.

3-((tert-butyldiphenylsilyl)oxy)-2-methylpropanoic acid (2a).

^{1}H NMR (500 MHz, $CDCl_3$): δ 7.72 (d, *J* = 6.5 Hz, 4H), 7.48-7.41 (m, 6H), 3.80 (dd, *J* = 9.5 Hz, 7.0 Hz, 1H), 3.81 (dd, *J* = 9.5 Hz, 6.0 Hz, 1H), 2.82-2.75 (m, 1H), 1.24 (d, *J* = 7.0 Hz, 3H), 1.09 (s, 9H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 181.2, 135.6, 133.3,

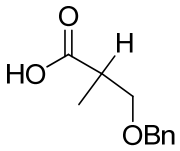
129.8, 127.8, 65.7, 42.3, 26.8, 19.3, 13.3; IR(film): 3072, 2958, 2858, 1711, 1472, 1423 cm^{-1}; HRMS(EI): calcd for $C_{16}H_{17}O_3Si[M-C_4H_9]^+$: 285.0947, found: 285.0952.



2-methyl-3-(prop-2-yn-1-yloxy)propanoic acid (2b).

Following the general procedure, the title product was synthesized from **1b** (reaction time 1h). Chromatographic purification (EtOAc : PE = 1 : 2) gave 22.5 mg (79%) as pale yellow oil.

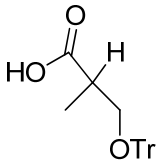
^1H NMR (500 MHz, $CDCl_3$): δ 11.16 (brs, 1H), 4.17 (s, 2H), 3.72 (t, *J* = 7.5 Hz, 1H), 3.64-3.61 (m, 1H), 2.81-2.78 (m, 1H), 2.44 (s, 2H), 1.23 (d, *J* = 7.5 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 180.9, 79.3, 74.7, 71.2, 58.4, 39.9, 13.7; IR(film): 3296, 2976, 2879, 2636, 1712, 1651, 1471 cm^{-1}; HRMS(EI): calcd for $C_7H_9O_3[M-H]^+$: 141.0552, found: 141.0549.



3-(benzyloxy)-2-methylpropanoic acid (2c).

Following the general procedure, the title product was synthesized from **1c** (reaction time 1.5h). Chromatographic purification (EtOAc : PE = 1 : 2) gave 32.6 mg (84%) as white solid.

^1H NMR (500 MHz, $CDCl_3$): δ 11.66 (brs, 1H), 7.40-7.32 (m, 5H), 4.59 (s, 2H), 3.74-3.71 (m, 1H), 3.60-3.57 (m, 1H), 2.88-2.84 (m, 1H), 1.27 (d, *J* = 6.0 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 181.1, 138.0, 128.4, 127.7, 73.2, 71.6, 40.2, 13.8; IR(film): 3064, 2979, 2867, 1709, 1497, 1459, 1453 cm^{-1}; HRMS(EI): calcd for $C_{11}H_{14}O_3[M]^+$: 194.0943, found: 194.0944.

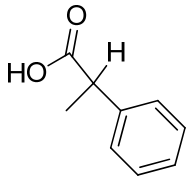


2-methyl-3-(trityloxy)propanoic acid (2d).

Following the general procedure, the title product was synthesized from **1d** (reaction time 1h). Chromatographic purification (EtOAc : PE = 1 : 2) gave 59.5 mg (86%) as colorless oil.

^1H NMR (500 MHz, Acetone-d_6): δ 7.49-7.47 (m, 6H), 7.36-7.33 (m, 6H), 7.29-7.25 (m, 3H), 3.33 (dd, *J* = 8.5 Hz, 7.5 Hz, 1H), 3.21 (dd, *J* = 8.5 Hz, 6.0 Hz, 1H), 2.77-2.73 (m, 1H), 1.15 (d, *J* = 7.0 Hz, 3H); ^{13}C NMR (125 MHz, Acetone-d6): δ 205.3, 144.2, 128.6, 127.7, 127.0, 86.3, 65.4, 39.9, 13.6; IR(film): 3058, 2933, 2878,

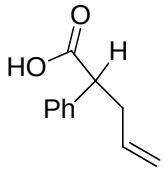
1708, 1597, 1491, 1449 cm^{-1}; HRMS(EI): calcd for $C_{23}H_{22}O_3[M]^+$: 346.1569, found: 346.1570.



2-phenylpropanoic acid (2e).[6a]

Following the general procedure, the title product was synthesized from **1e** (reaction time 1h). Chromatographic purification (EtOAc : PE = 1 : 2) gave 26.6 mg (89%) as colorless oil.

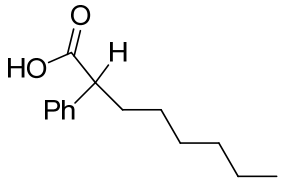
^1H NMR (500 MHz, $CDCl_3$): δ 11.84 (brs, 1H), 7.40-7.32 (m, 5H), 3.80 (q, *J* = 7.5 Hz, 1H), 1.58 (d, *J* = 7.0 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 181.3, 139.8, 128.8, 127.7, 127.5, 45.5, 18.1; IR(film): 3030, 2979, 2935, 1705, 1601, 1496, 1454, 1413 cm^{-1}; HRMS(EI): calcd for $C_9H_{10}O_2[M]^+$: 150.0681, found: 150.0678.



2-phenylpent-4-enoic acid (2f).[6b]

Following the general procedure, the title product was synthesized from **1f** (reaction time 1h). Chromatographic purification (EtOAc : PE = 1 : 2) gave 30.6 mg (87%) as white solid.

^1H NMR (500 MHz, $CDCl_3$): δ 7.36-7.27 (m, 5H), 5.76-5.70 (m, 1H), 5.10 (d, *J* = 17.0 Hz, 1H), 5.02 (d, *J* = 10.0 Hz, 1H), 3.66 (t, *J* = 7.5 Hz, 1H), 2.86-2.80 (m, 1H), 2.57-2.51 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 180.1, 137.9, 134.9, 128.8, 128.1, 127.7, 117.4, 51.5, 37.1; IR(film): 3077, 2973, 2921, 1708, 1634, 1497, 1455 cm^{-1}; HRMS(EI): calcd for $C_{11}H_{12}O_2[M]^+$: 176.0837, found: 176.0836.

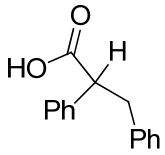


2-phenyloctanoic acid (2g).[6c]

Following the general procedure, the title product was synthesized from **1g** (reaction time 1h). Chromatographic purification (EtOAc : PE = 1 : 2) gave 37.9 mg (86%) as white solid.

^1H NMR (500 MHz, $CDCl_3$): δ 11.71 (brs, 1H), 7.36-7.26 (m, 5H), 3.55 (t, *J* = 7.5 Hz, 1H), 2.12-2.05 (m, 1H), 1.83-1.76 (m, 1H), 1.34-1.26 (m, 8H), 0.88 (t, *J* = 7.5 Hz 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 180.8, 138.6, 128.6, 128.1, 127.4, 51.7, 33.1, 31.6,

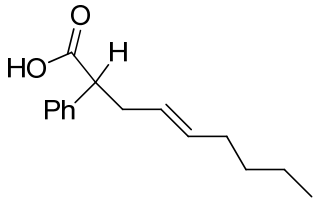
29.0, 27.5, 22.6, 14.1; IR(film): 3030, 2927, 2857, 1707, 1496, 1455 cm^{-1}; HRMS(EI): calcd for $C_{14}H_{20}O_2[M]^+$: 220.1463, found: 220.1460.



2,3-diphenylpropanoic acid (2h).[6d]

Following the general procedure, the title product was synthesized from **1h** (reaction time 4h). Chromatographic purification (EtOAc : PE = 1 : 2) gave 37.5 mg (83%) as white solid.

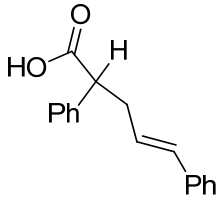
^1H NMR (500 MHz, $CDCl_3$): δ 7.33-7.11 (m, 10H), 3.88 (t, *J* = 7.5 Hz, 1H), 3.42 (dd, *J* = 13.5 Hz, 9.0 Hz, 1H), 3.05 (dd, *J* = 13.5 Hz, 7.0 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 179.8, 138.7, 138.0, 129.0, 128.8, 128.5, 128.2, 127.7, 126.5, 53.6, 39.3; IR(film): 3036, 3029, 1706, 1601, 1496, 1454, 1414 cm^{-1}; HRMS(EI): calcd for $C_{15}H_{14}O_2[M]^+$: 226.0994, found: 226.0992.



(E)-2-phenylnon-4-enoic acid (2i).

Following the general procedure, the title product was synthesized from **1i** (reaction time 1h). Chromatographic purification (EtOAc : PE = 1 : 2) gave 40.4 mg (87%) as white solid.

^1H NMR (500 MHz, $CDCl_3$): δ 7.35-7.27 (m, 5H), 5.51-5.45 (m, 1H), 5.35-5.29 (m, 1H), 3.60 (t, *J* = 7.5 Hz, 1H), 2.79-2.73 (m, 1H), 2.49-2.44 (m, 1H), 1.96-1.92 (m, 2H), 1.28-1.20 (,m, 4H), 0.85 (t, *J* = 7.5 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 180.0, 138.1, 133.7, 128.6, 128.1, 127.5, 126.1, 52.1, 36.2, 32.1, 31.4, 22.0, 13.9; IR(film): 3083, 2957, 2857, 1708, 1601, 1496, 1455 cm^{-1}; HRMS(EI): calcd for $C_{15}H_{20}O_2[M]^+$: 232.1463, found: 236.1461.

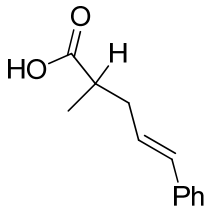


(E)-2,5-diphenylpent-4-enoic acid (2j).[6e]

Following the general procedure, the title product was synthesized from **1j** (reaction time 5h). Chromatographic purification (EtOAc : PE = 1 : 2) gave 40.9 mg (81%) as white solid.

^1H NMR (500 MHz, $CDCl_3$): δ 7.36-7.19 (m, 10H), 6.45 (d, *J* = 10.5 Hz, 1H), 6.14-6.08 (m, 1H), 3.74 (t, *J* = 7.5 Hz, 1H), 3.00 (dt, *J* = 14.5 Hz, 7.5 Hz, 1H), 2.73-2.67 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 179.7, 137.9, 137.3, 132.5, 128.8,

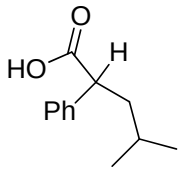
128.5, 128.1, 127.7, 127.3, 126.5, 126.2, 51.8, 36.5; IR(film): 3027, 2919, 1738, 1705, 1599, 1459, 1453 cm^{-1}; HRMS(EI): calcd for $C_{17}H_{16}O_2[M]^+$: 252.1150, found: 252.1146.



(E)-2-methyl-5-phenylpent-4-enoic acid (2k).[6e]

Following the general procedure, the title product was synthesized from **1k** (reaction time 1h). Chromatographic purification (EtOAc : PE = 1 : 2) gave 36.5 mg (96%) as pale yellow oil.

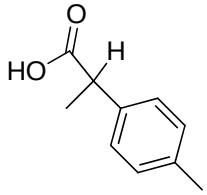
^{1}H NMR (500 MHz, $CDCl_3$): δ 11.47 (brs, 1H), 7.41 (d, *J* = 7,5 Hz, 2H), 7.35 (t, *J* = 7.5 Hz, 2H), 7.27 (t, *J* = 7.0 Hz, 1H), 6.51 (d, *J* = 16.0 Hz, 1H), 6.26-6.20 (m, 1H), 2.71-2.64 (m, 2H), 2.46-2.40 (m, 1H), 1.30 (d, *J* = 6.0Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 182.8, 137.4, 132.5, 128.6, 127.3, 126.9, 126.2, 39.6, 36.7, 16.5; IR(film): 3026, 2976, 2936, 1705, 1597, 1495, 1462 cm^{-1}; HRMS(EI): calcd for $C_{12}H_{14}O_2[M]^+$: 190.0994, found: 190.0992.



4-methyl-2-phenylpentanoic acid (2l).

Following the general procedure, the title product was synthesized from **1l** (reaction time 3h). Chromatographic purification (EtOAc : PE = 1 : 2) gave 21.5 mg (56%) as white solid.

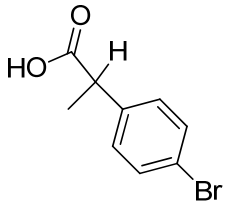
^{1}H NMR (500 MHz, $CDCl_3$): δ 7.35-7.27 (m, 5H), 3.67 (t, *J* = 8.0 Hz, 1H), 2.00-1.94 (m, 1H), 1.73-1.68 (m, 1H), 1.53-1.47 (m, 1H), 0.92 (d, *J* = 6.0 Hz, 6H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 180.5, 138.6, 128.6, 128.1, 127.4, 49.5, 42.0, 25.8, 22.6, 22.2; IR(film): 3029, 2957, 2871, 1693, 1453, 1410 cm^{-1}; HRMS(EI): calcd for $C_{12}H_{16}O_2[M]^+$: 192.1150, found: 192.1152.



2-(p-tolyl)propanoic acid (2m).[6f]

Following the general procedure, the title product was synthesized from **1m** (reaction time 1h). Chromatographic purification (EtOAc : PE = 1 : 2) gave 27.6 mg (84%) as white solid.

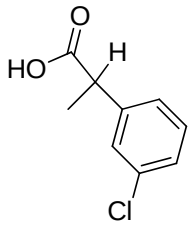
^{1}H NMR (500 MHz, $CDCl_3$): δ 7.24 (d, *J* = 8.5 Hz, 2H), 7.17 (d, J = 8.0 Hz, 2H), 3.73 (q, *J* = 7.0 Hz, 1H), 2.36 (s, 3H), 1.53 (d, *J* = 7.0 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 181.1, 137.1, 136.8, 129.4, 127.5, 45.0, 21.1, 18.1; IR(film): 2982, 2937, 1706, 1514, 1458, 1412 cm^{-1}; HRMS(EI): calcd for $C_{10}H_{12}O_2[M]^+$: 164.0837, found: 164.0842.



2-(4-bromophenyl)propanoic acid (2n).[6g]

Following the general procedure, the title product was synthesized from **1n** (reaction time 1h). Chromatographic purification (EtOAc : PE = 1 : 2) gave 42.9 mg (94%) as white solid.

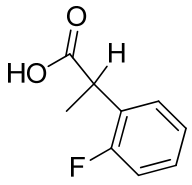
^{1}H NMR (500 MHz, $CDCl_3$): δ 7.47 (d, *J*= 8.5 Hz, 2H), 7.20 (d, *J* = 8.5 Hz, 2H), 3.71 (q, *J* = 7.5 Hz, 1H), 1.51 (d, *J* = 7.0 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 180.4, 138.6, 131.8, 129.4, 121.4, 44.8, 18.0; IR(film): 2981, 2937, 1707, 1489, 1459, 1404 cm^{-1}; HRMS(EI): calcd for $C_9H_9BrO_2[M]^+$: 227.9786, found: 227.9787.



2-(3-chlorophenyl)propanoic acid (2o).[6h]

Following the general procedure, the title product was synthesized from **1o** (reaction time 1h). Chromatographic purification (EtOAc : PE = 1 : 2) gave 32.8 mg (89%) as white solid.

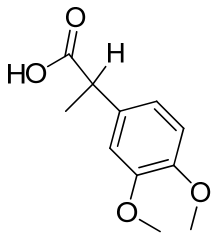
^{1}H NMR (500 MHz, $CDCl_3$): δ 7.34-7.21 (m, 4H), 3.73 (q, *J* = 7.0 Hz, 1H), 1.53 (d, *J* = 7.5 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 180.3, 141.5, 134.5, 129.9, 127.9, 127.7, 125.9, 45.1, 18.0; IR(film): 2983, 2937, 1709, 1596, 1478, 1412 cm^{-1}; HRMS(EI): calcd for $C_9H_9ClO_2[M]^+$: 184.0291, found: 184.0290.



2-(2-fluorophenyl)propanoic acid (2p).

Following the general procedure, the title product was synthesized from **1p** (reaction time 1h). Chromatographic purification (EtOAc : PE = 1 : 2) gave 31.9 mg (95%) as white solid.

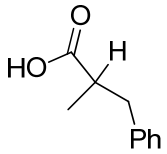
^{1}H NMR (500 MHz, $CDCl_3$): δ 7.35-7.32 (m, 1H), 7.28-7.25 (m, 1H), 7.14 (t, *J* = 7.5 Hz, 1H), 7.07 (t, *J* = 9.0 Hz, 1H), 4.08 (q, *J* = 7.5 Hz, 1H), 1.55 (d, *J* = 7.0 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 180.1, 161.4, 159.4, 128.97 and 128.90, 128.78 and 128.75, 127.13 and 127.01, 124.34 and 124.31, 115.61 and 115.43, 38.41 and 38.38, 17.1; ^{19}F NMR (400 MHz, $CDCl_3$) δ -117.8 (s, 1F); IR(film): 2986, 2935, 1711, 1587, 1493, 1456, 1415 cm^{-1}; HRMS(EI): calcd for $C_9H_9FO_2[M]^+$: 168.0587, found: 168.0590.



2-(3,4-dimethoxyphenyl)propanoic acid (2q).[6f]

Following the general procedure, the title product was synthesized from **1q** (reaction time 1h). Chromatographic purification (EtOAc : PE = 1 : 2) gave 38.7 mg (92%) as white solid.

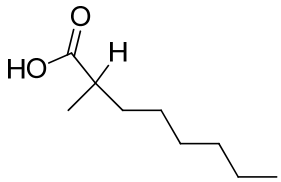
^{1}H NMR (500 MHz, $CDCl_3$): δ 6.88-6.82 (m, 3H), 3.87 (d, *J* = 9.0 Hz, 6H), 3.68 (q, *J* = 7.0 Hz, 1H), 1.51 (d, *J* = 7.5 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 180.8, 149.0, 148.4, 132.3, 119.7, 111.2, 110.8, 55.9, 44.9, 18.1; IR(film): 3529, 2937, 2837, 1707, 1592, 1517, 1464, 1420 cm^{-1}; HRMS(EI): calcd for $C_{11}H_{14}O_4[M]^+$: 210.0892, found: 210.0888.



2-methyl-3-phenylpropanoic acid (2r).

Following the general procedure, the title product was synthesized from **1r** (reaction time 1h). Chromatographic purification (EtOAc : PE = 1 : 2) gave 28.6 mg (87%) as yellow oil.

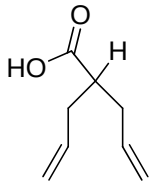
^{1}H NMR (500 MHz, $CDCl_3$): δ 7.33-7.20 (m, 5H), 3.10 (dd, *J* = 13.5 Hz, 6.5 Hz, 1H), 2.83-2.76 (m, 1H), 2.69 (dd, *J* = 13.5 Hz, 8.0 Hz, 1H), 1.20 (d, *J* = 6.5 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 182.7, 139.0, 129.0, 128.4, 126.5, 41.3, 39.3, 16.5; IR(film): 3029, 2977, 2937, 1707, 1496, 1454, 1416 cm^{-1}; HRMS(EI): calcd for $C_{10}H_{12}O_2[M]^+$: 164.0837, found: 164.0835.



2-methyloctanoic acid (2s).[6i]

Following the general procedure, the title product was synthesized from **1s** (reaction time 1h). Chromatographic purification (EtOAc : PE = 1 : 5) gave 28.5 mg (94%) as colorless oil.

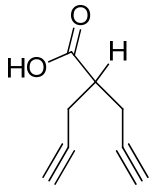
^{1}H NMR (500 MHz, $CDCl_3$): δ 2.48-2.44 (m, 1H), 1.71-1.66 (m, 1H), 1.46-1.40 (m, 1H), 1.34-1.28 (m, 8H), 1.18 (d, J = 7.0 Hz, 3H), 0.89 (t, J = 7.0 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 183.7, 39.4, 33.3, 31.7, 29.1, 27.1, 22.6, 16.8, 14.0; IR(film): 2930, 2859, 1708, 1467, 1417 cm^{-1}; HRMS(EI): calcd for $C_9H_{18}O_2[M]^+$: 158.1307, found: 158.1310.



2-allylpent-4-enoic acid (2t).[6j]

Following the general procedure, the title product was synthesized from **1t** (reaction time 1h). Chromatographic purification (EtOAc : PE = 1 : 2) gave 25.8 mg (92%) as pale yellow oil.

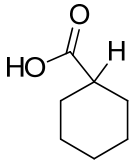
^{1}H NMR (500 MHz, $CDCl_3$): δ 11.69 (brs, 1H), 5.82-5.74 (m, 2H), 5.12-5.06 (m, 4H), 2.57-2.53 (m, 1H), 2.43-2.38 (m, 2H), 2.32-2.27 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 181.6, 134.8, 117.3, 44.8, 35.4; IR(film): 3080, 2982, 2917, 1709, 1643, 1444 cm^{-1}; HRMS(EI): calcd for $C_8H_{12}O_2[M]^+$: 140.0837, found: 140.0835.



2-(prop-2-yn-1-yl)pent-4-ynoic acid (2u).

Following the general procedure, the title product was synthesized from **1u** (reaction time 1h). Chromatographic purification (EtOAc : PE = 1 : 2) gave 22.3 mg (82%) as white solid.

^{1}H NMR (500 MHz, $CDCl_3$): δ 2.86-2.81 (m, 1H), 2.74-2.64 (m, 4H), 2.06 (t, J = 2.5 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 178.2, 80.1, 70.8, 42.8, 19.6; IR(film): 3297, 2928, 2852, 1713, 1434, 1281 cm^{-1}; HRMS(EI): calcd for $C_8H_7O_2[M\text{-}H]^+$: 135.0446, found: 135.0445.

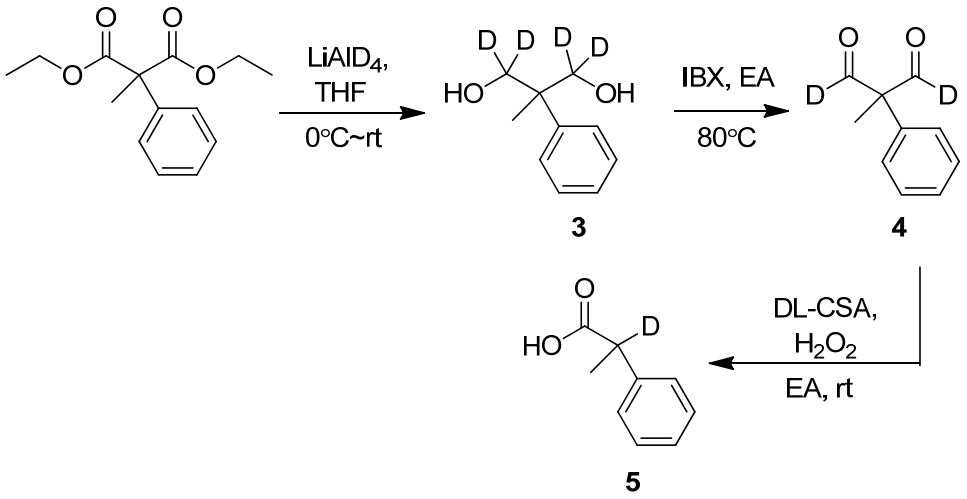


cyclohexanecarboxylic acid (2v).[6k]

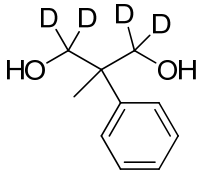
Following the general procedure, the title product was synthesized from **1v** (reaction time 1h). Chromatographic purification (EtOAc : PE = 1 : 5) gave 20.5 mg (80%) as colorless oil.

^{1}H NMR (500 MHz, $CDCl_3$): δ 2.37- 2.31 (m, 1H), 1.96-1.93 (m, 2H), 1.79-1.76 (m, 2H), 1.67-1.64 (m, 1H), 1.50-1.43 (m, 2H), 1.34-1.22 (m, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 182.8, 42.9, 28.7, 25.7, 25.3; IR(film): 2934, 2857, 1704, 1452, 1418 cm^{-1}; HRMS(EI): calcd for $C_7H_{12}O_2[M]^+$: 128.0837, found: 128.0836.

3.5 Date for deuterated compounds



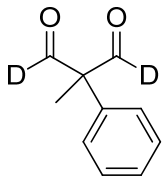
Following the general procedures, deuterated compound **5** is synthesized from diethyl 2-methyl-2-phenylmalonate (use the $LiAlD_4$ instead of $LiAlH_4$ in the first step).



1,1,3,3-4-deuterio-2-methyl-2-phenylpropane-1,3-diol. (3)

Synthesis from diethyl 2-methyl-2-phenylmalonate, 76% yield as white solid. Chromatographic purification (EtOAc : PE = 1 : 3).

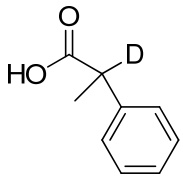
^{1}H NMR (500 MHz, $CDCl_3$): δ 7.41-7.35 (m, 4H), 7.25 (t, *J* = 7.0 Hz, 1H), 2.86 (brs, 2H), 1.28 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 143.2, 128.6, 126.7, 126.6, 69.03 and 68.87 and 68.69, 44.1, 20.6; IR(film): 3328, 2974, 2206, 2091, 1498, 1444, 1370 cm^{-1}; HRMS(EI): calcd for $C_{10}H_{10}D_4O_2[M]^+$: 170.1245, found: 170.1248.



2-methyl-2-phenyl-deuteratedmalonaldehyde (4).

Synthesis from deuterated compound **3**, 92% yield as colorless oil.

^{1}H NMR (500 MHz, $CDCl_3$): δ 7.49 (t, *J* = 7.5 Hz, 2H), 7.42 (t, *J* = 7.5 Hz, 1H), 7.32 (d, *J* = 7.0 Hz, 2H), 1.70 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 198.05 and 197.83 and 197.61, 133.0, 129.6, 128.7, 127.4, 13.9; IR(film): 2116, 2067, 1720, 1697, 1597, 1493, 1446 cm^{-1}; HRMS(EI): calcd for $C_{10}H_8D_2O_2[M]^+$: 164.0806, found: 164.0809.



2-deuterio-2-phenylpropanoic acid (5).

Synthesis from deuterated compound **4**, 80% as white solid.

^{1}H NMR (500 MHz, $CDCl_3$): δ 7.37-7.27 (m, 5H), 1.53 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 180.8, 139.7, 128.7, 127.6, 45.16 and 45.01 and 44.85, 18.0; IR(film): 3027, 2980, 1705, 1601, 1497, 1448 cm^{-1}; HRMS(EI): calcd for $C_9H_9DO_2[M]^+$: 151.0744, found: 151.0748.

3. Reference:

[1] Gaussian 09, Revision A.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

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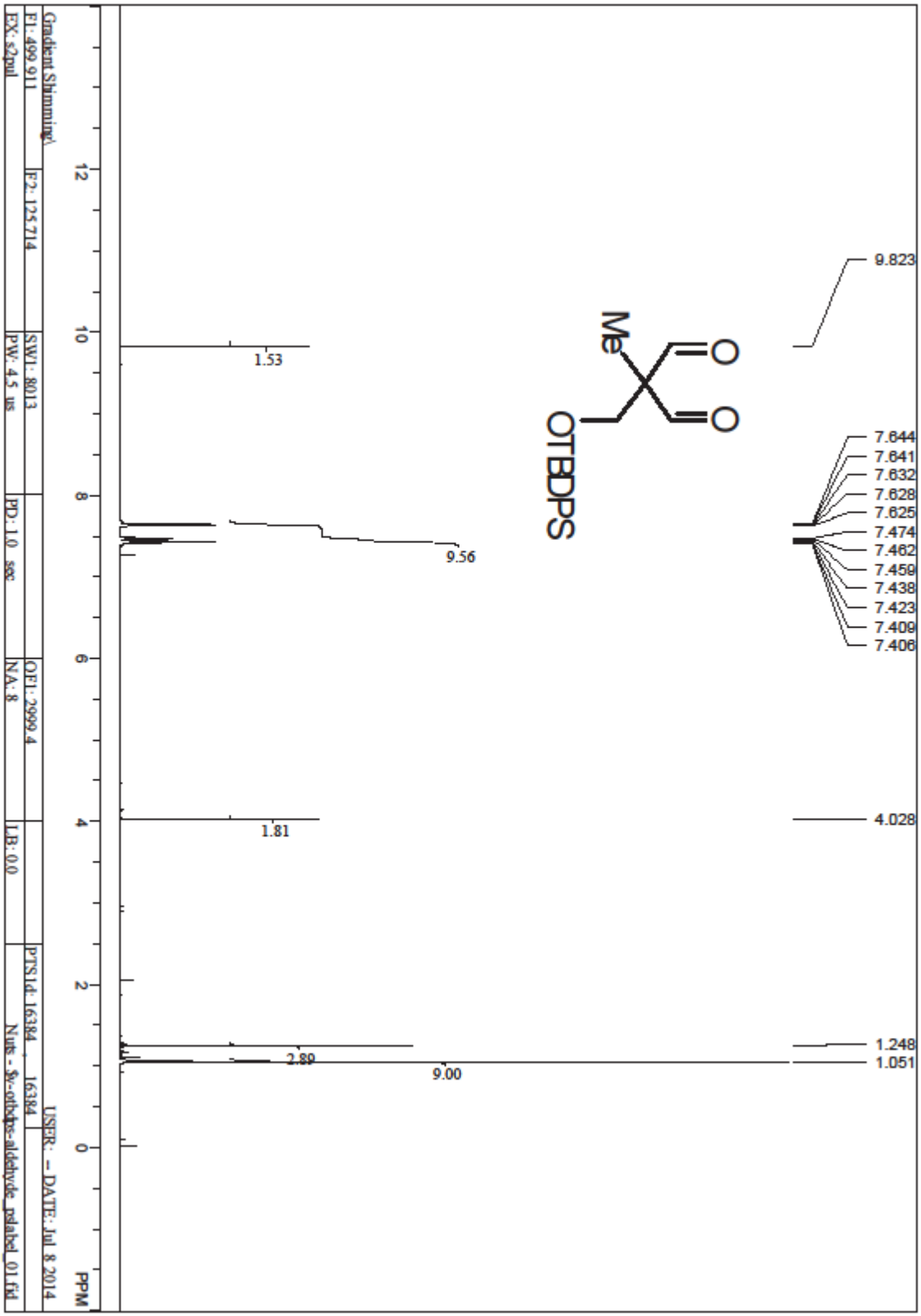
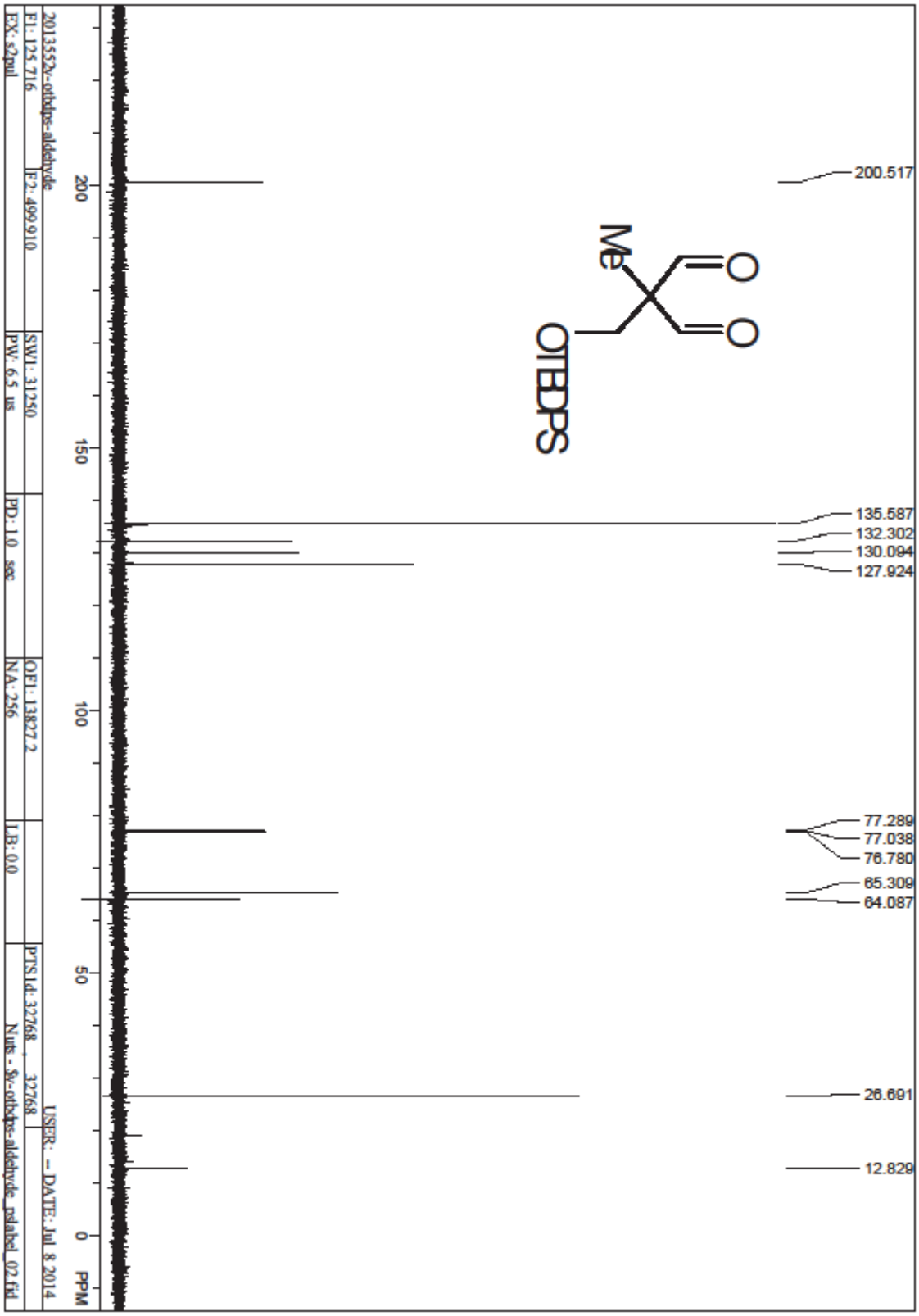
4. Copies of NMR for all compounds.

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Me
OTBDPS
O
O
200
150
100
50
0
PPM
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DATE: Jul 8 2014
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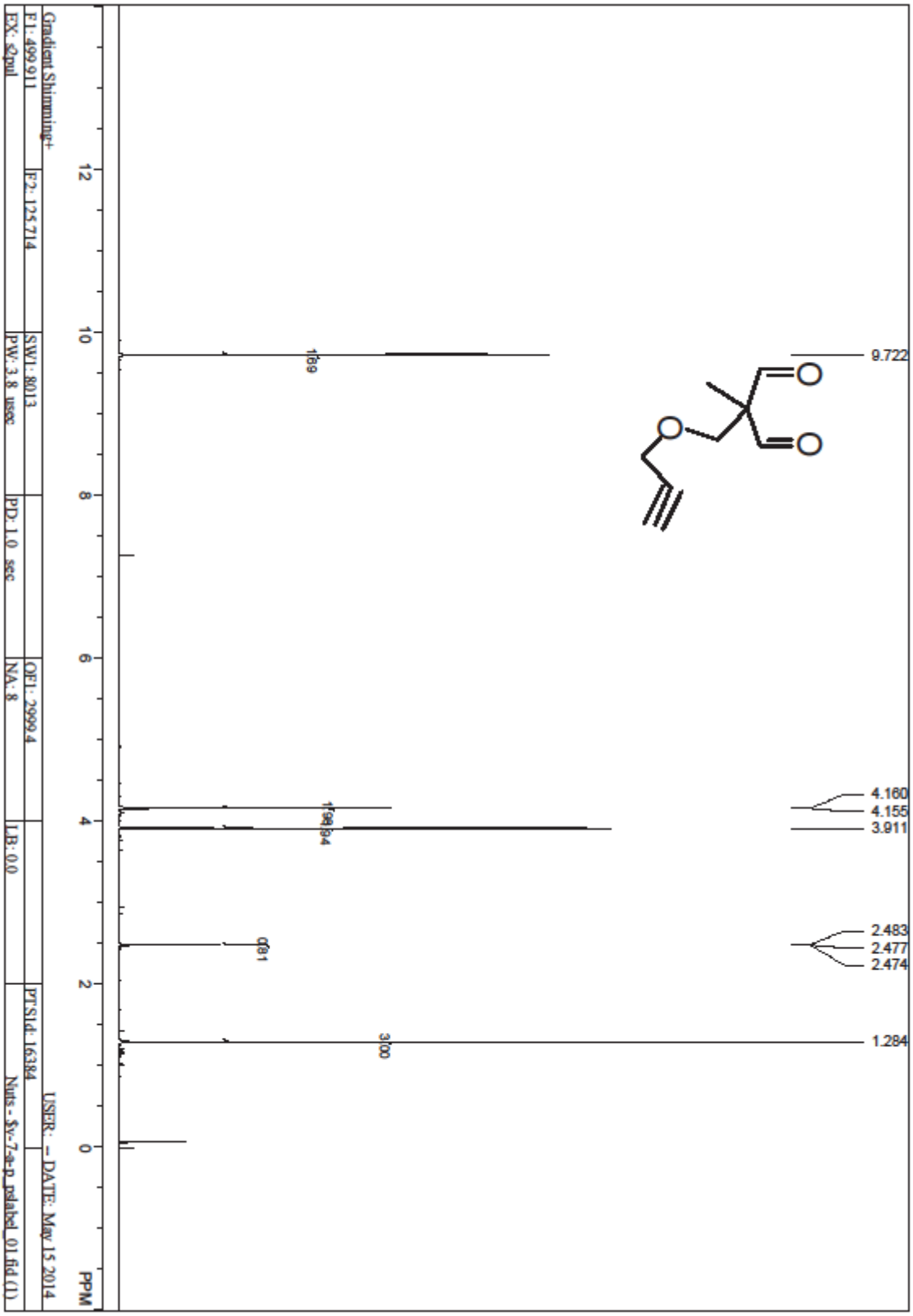
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1.84
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12
10
8
6
4
2
0
PPM
Gradient Shimming+
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F2: 125.714
SW1: 8013
PW: 3.8 usec
PD: 1.0 sec
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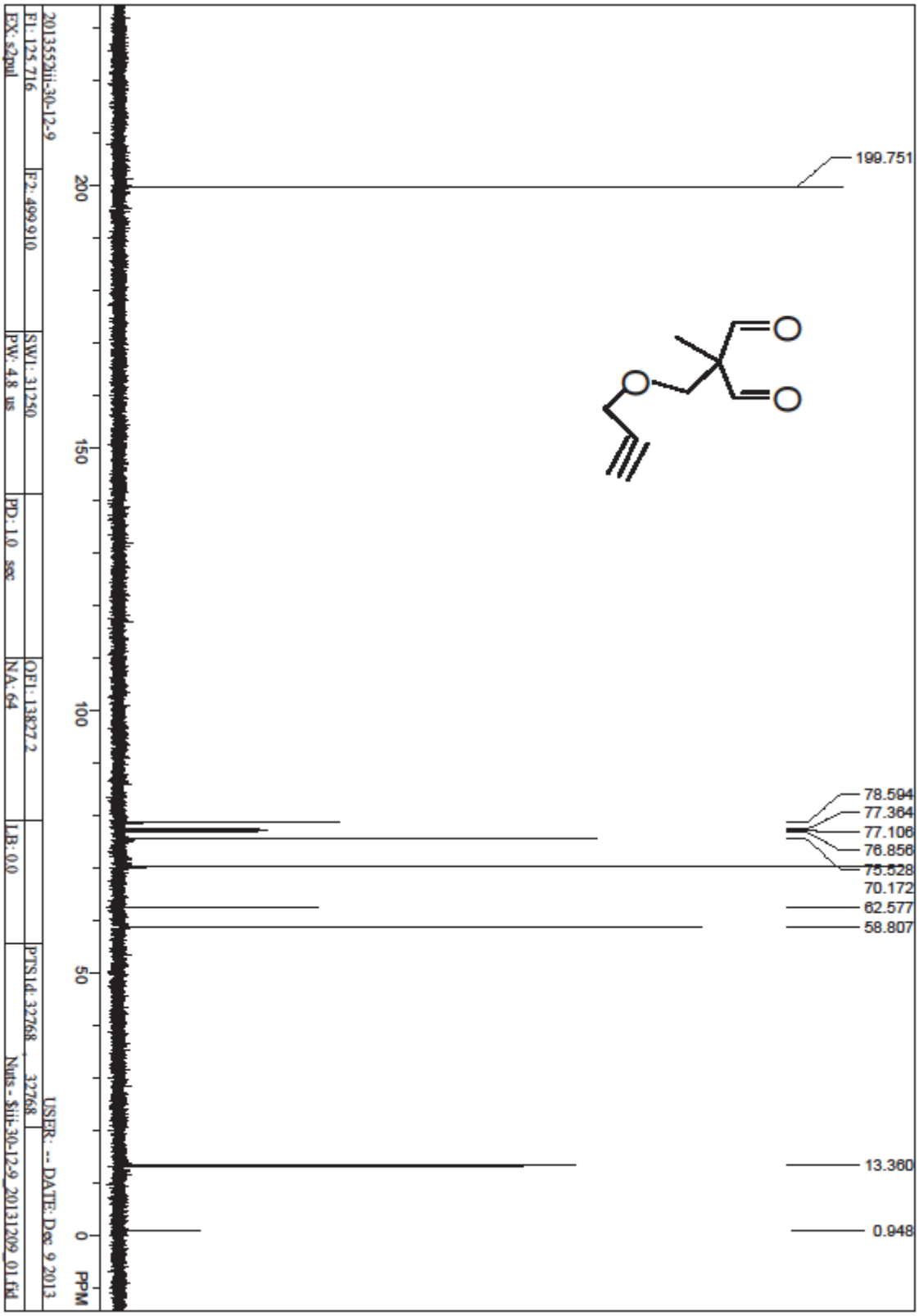
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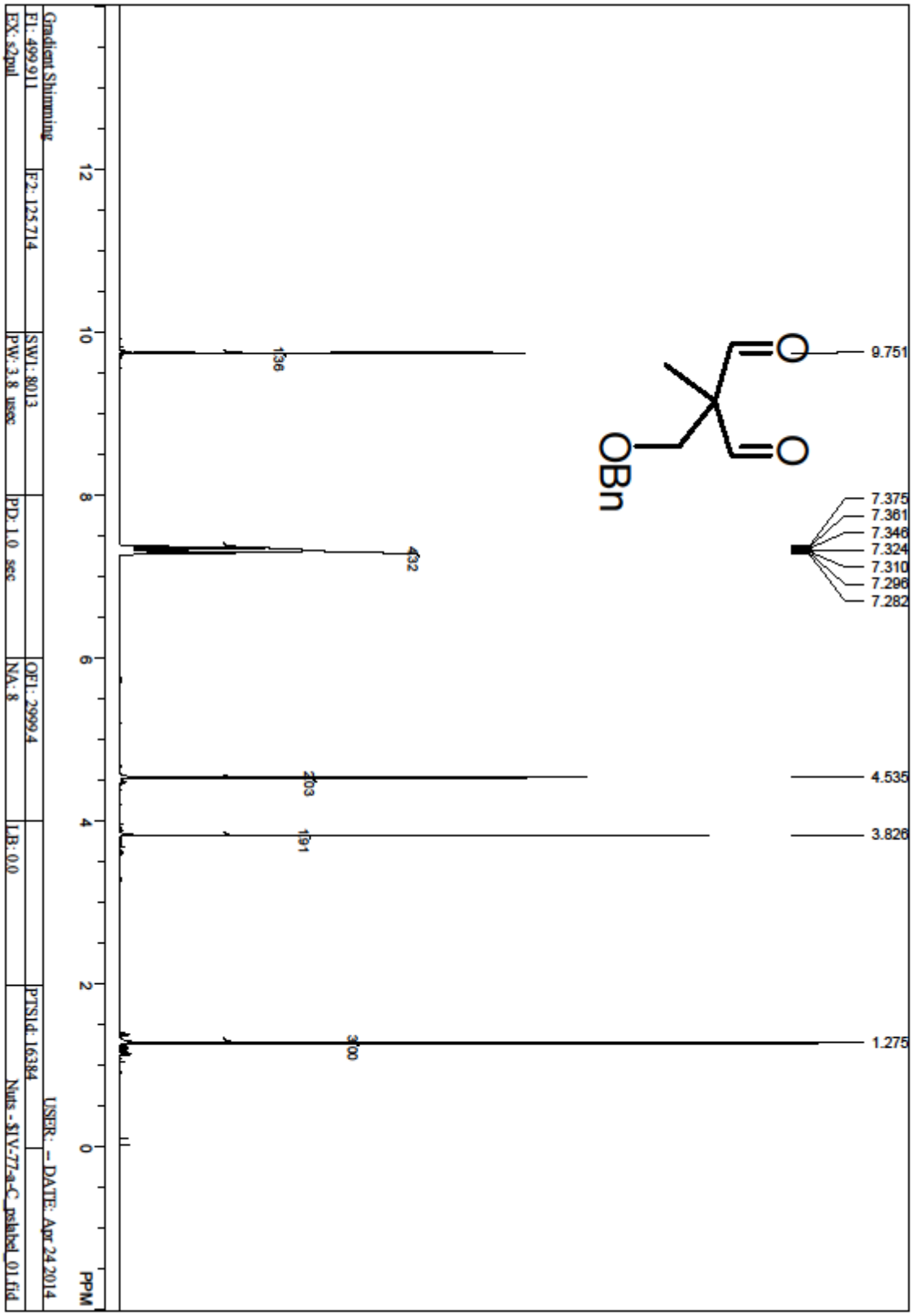
50
0
PPM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PTS1d: 16384
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8
6
4
2
0
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7.310
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7.282
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3.826
1.275
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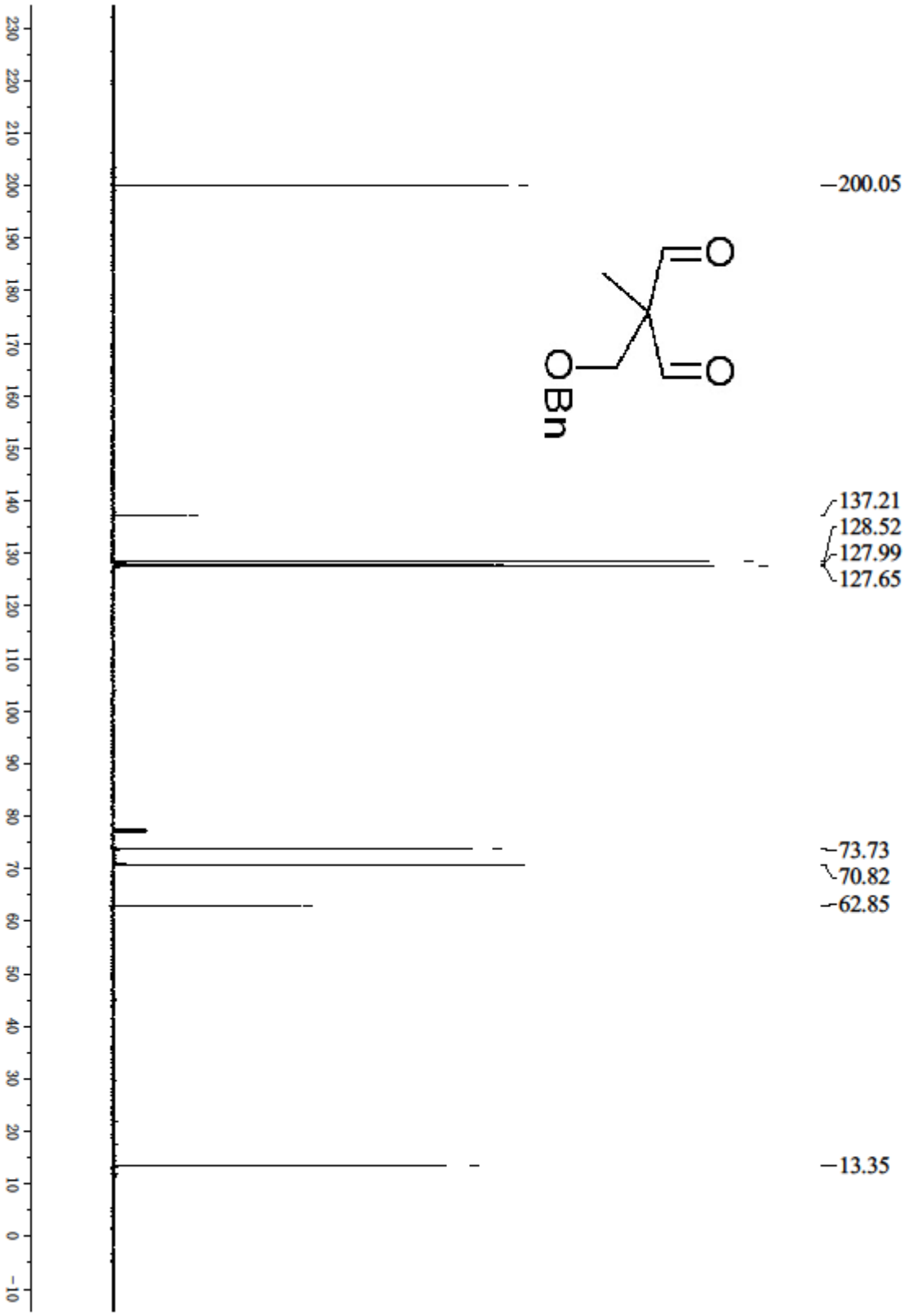
432
203
191
300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62.85
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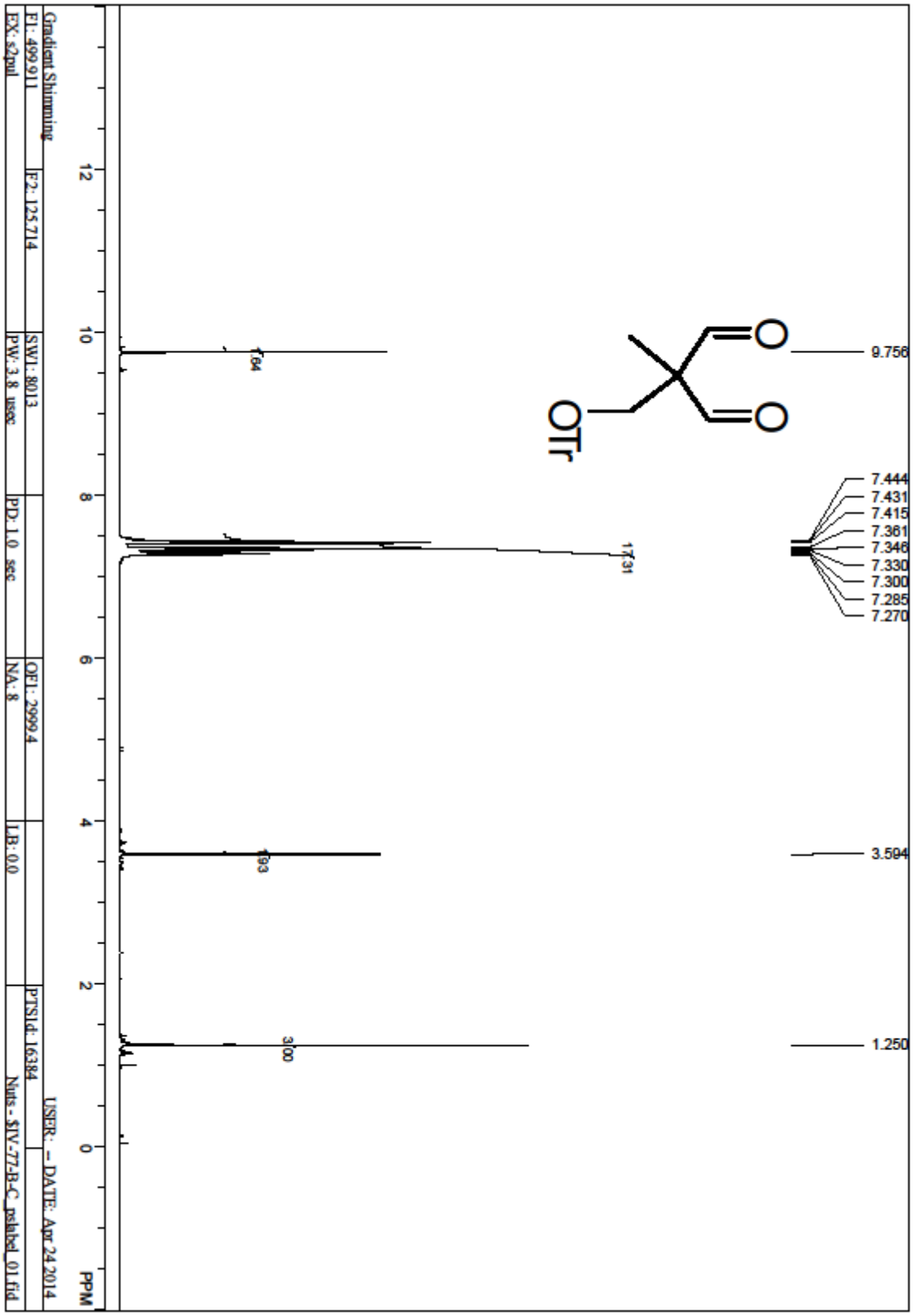
O
O
Bn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8
6
4
2
0
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7.444
7.431
7.415
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7.330
7.300
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3.594
1.250
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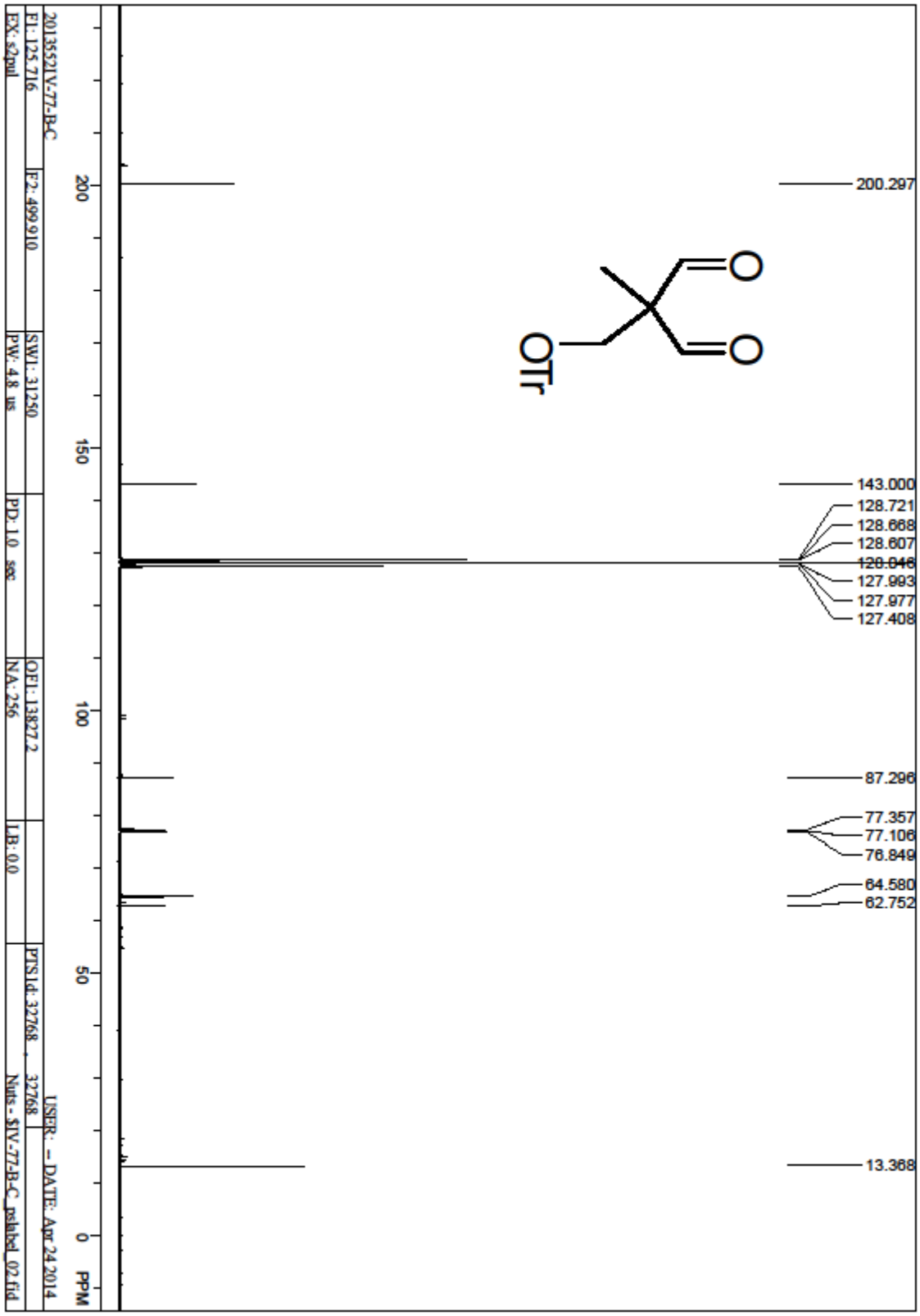
17.31
1.93
3.00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76.849
64.580
62.752
13.368
OTr
O
O
200
150
100
50
0
PPM
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PW: 4.8 us
PD: 1.0 sec
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LB: 0.0
PTS1d: 32768 * 32768
USER: -- DATE: Apr 24 2014
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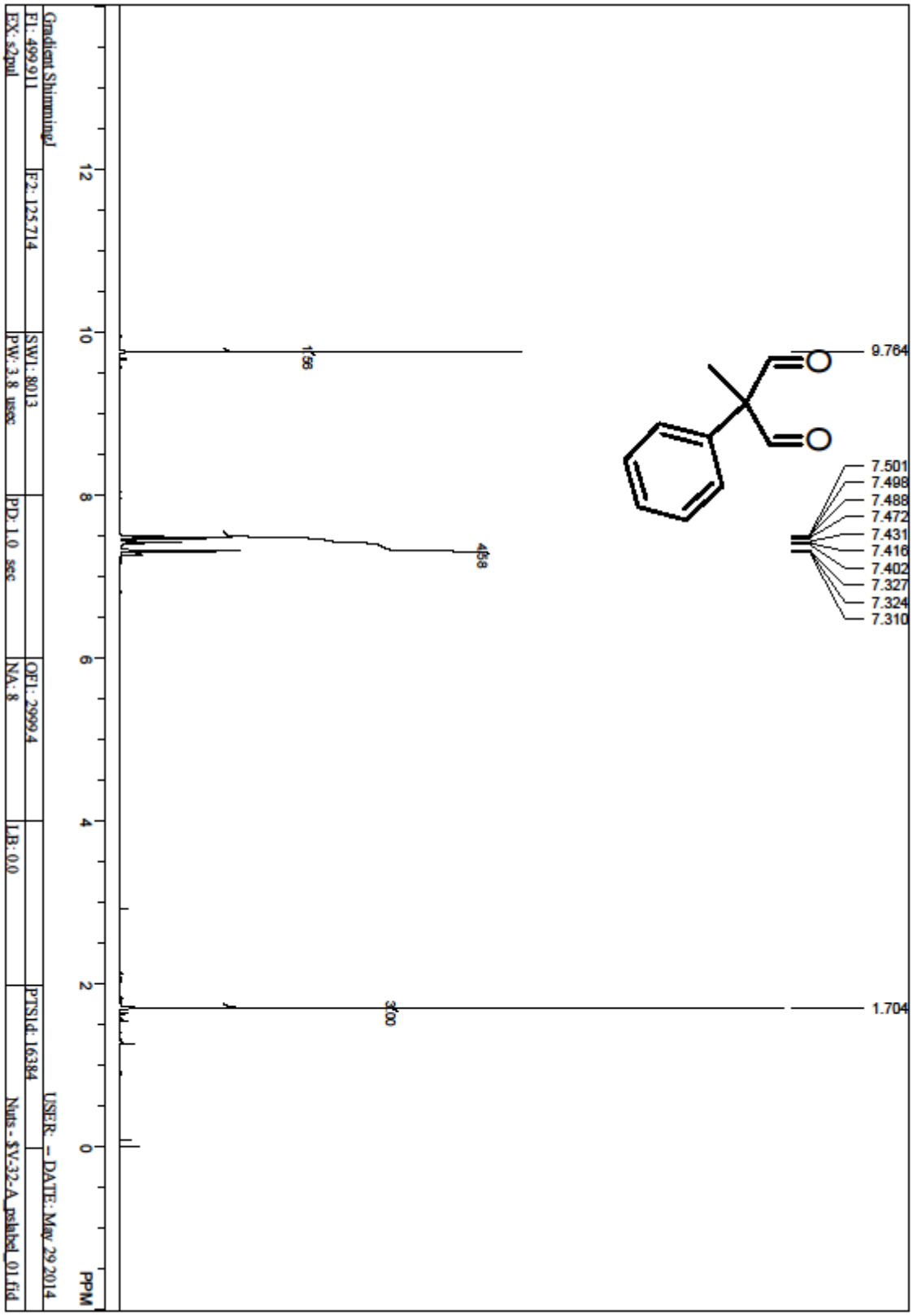
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7.402
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7.324
7.310
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1.56
4.58
3.00
PPM
Gradient Shimming]
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F2: 125.714
SW1: 8013
PW: 3.8 usec
PD: 1.0 sec
OF1: 2999.4
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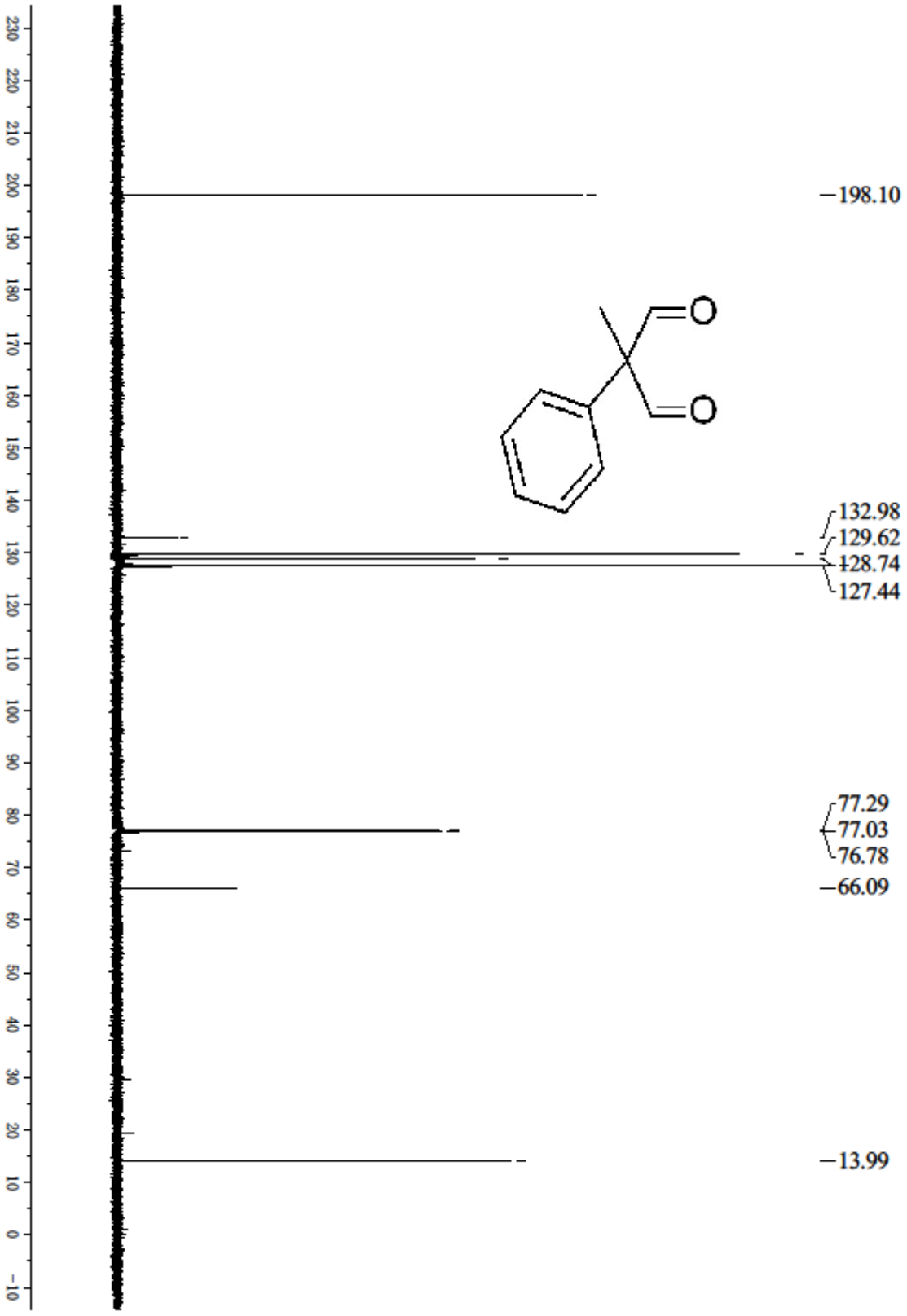
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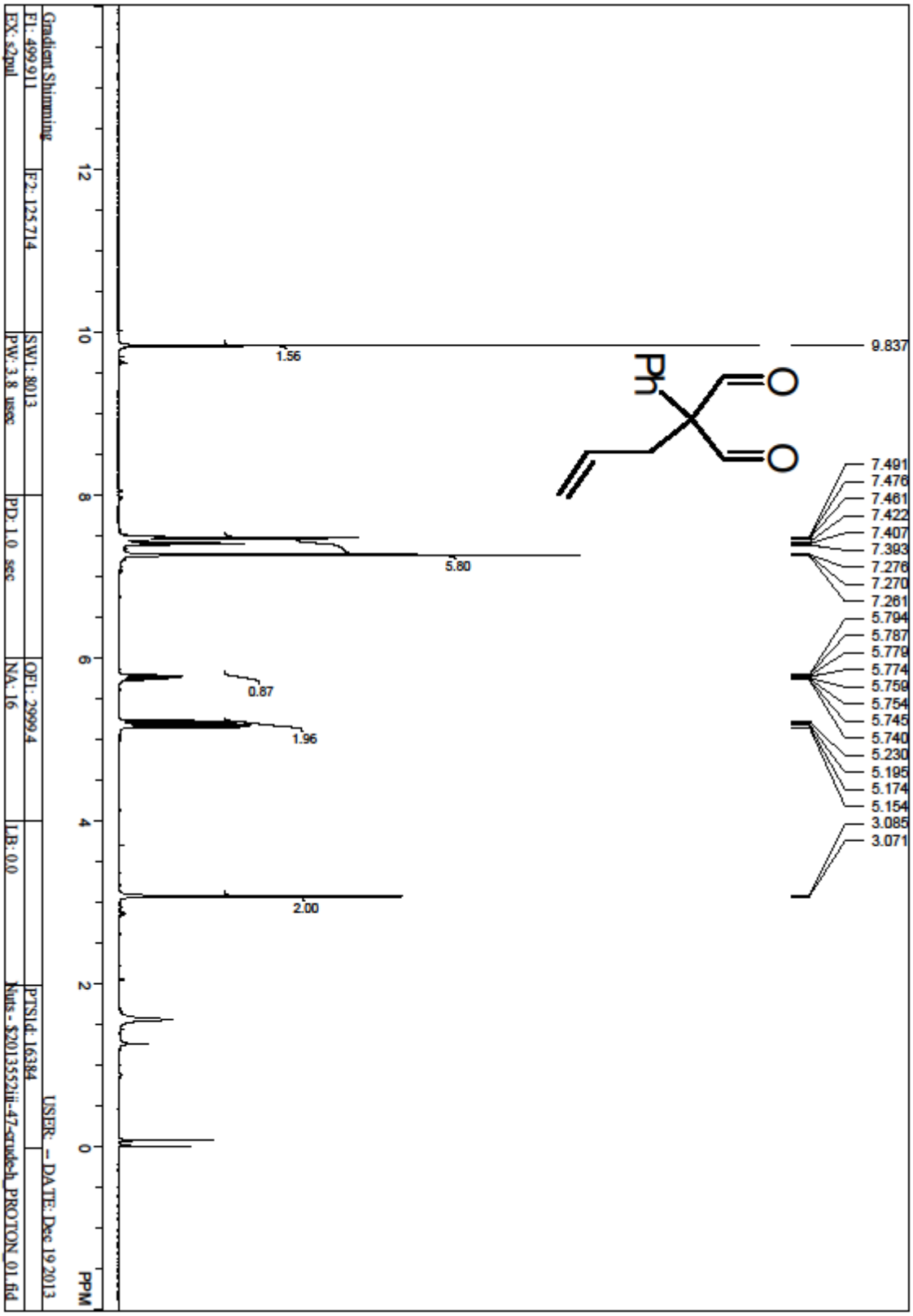
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2
4
6
8
10
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2.00
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7.491
7.476
7.461
7.422
7.407
7.393
7.276
7.270
7.261
5.794
5.787
5.779
5.774
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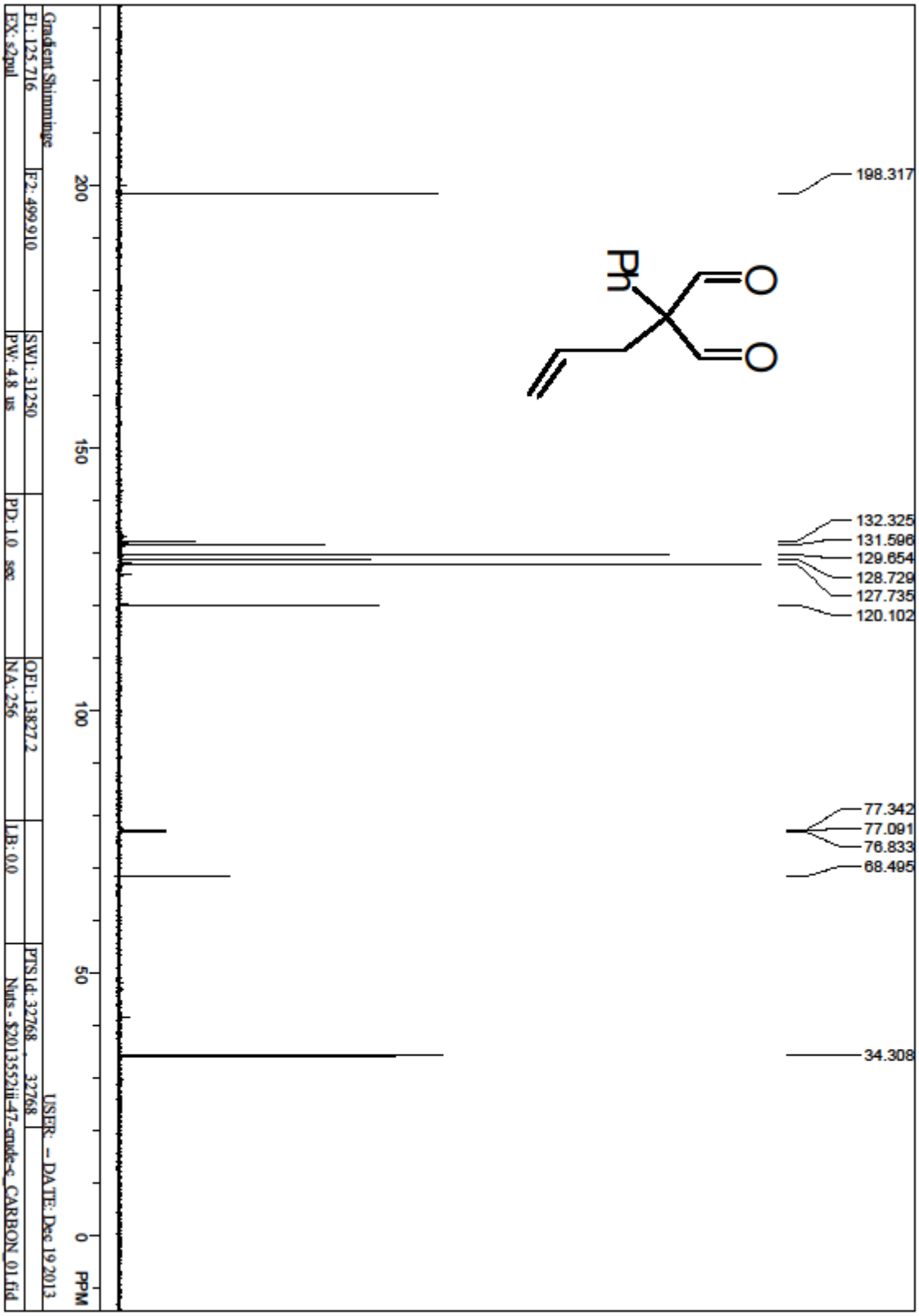
Ph
O
O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USER: -- DATE: Dec 19 2013
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O
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129.654
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68.495
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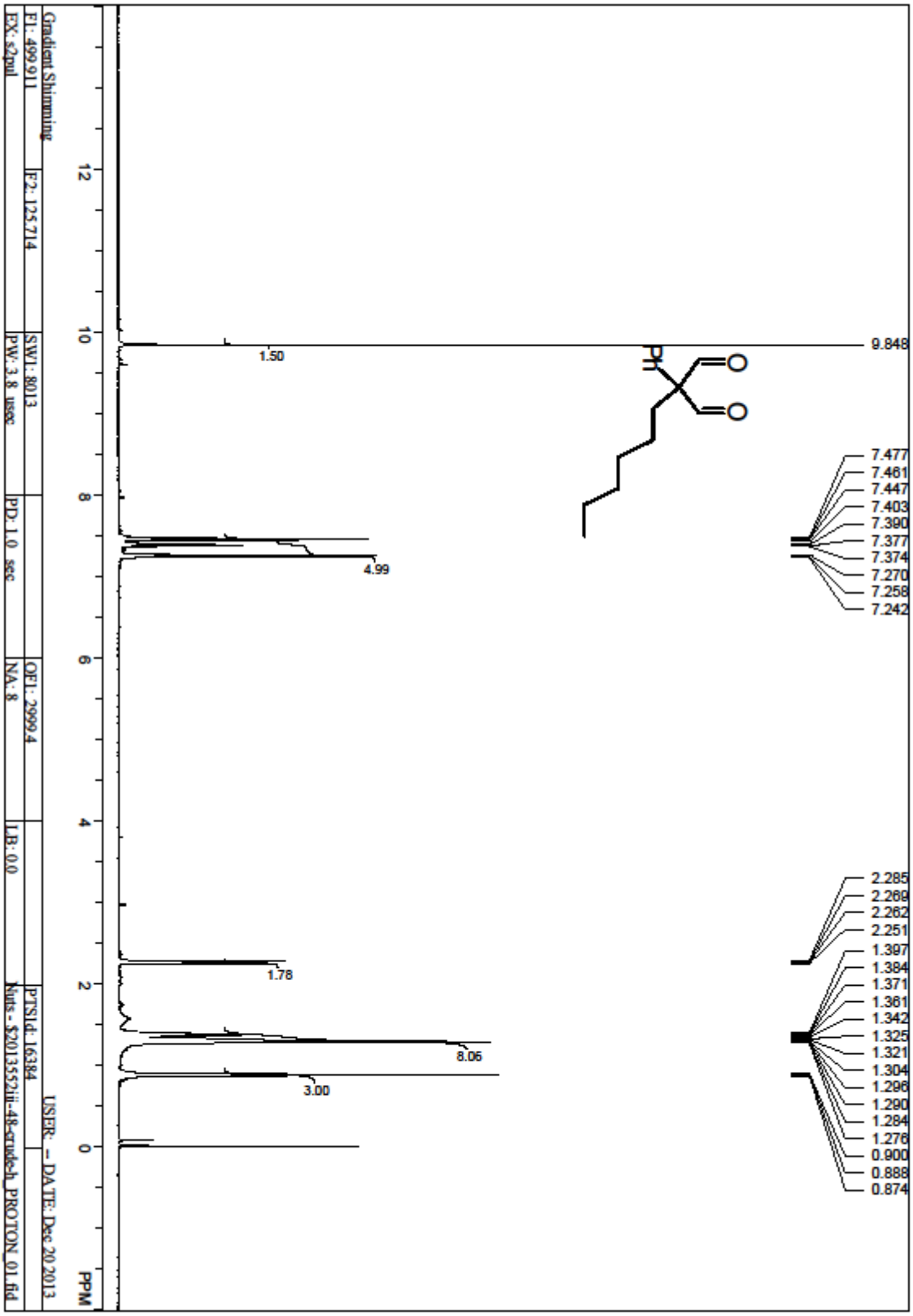
100
50
0
PPM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4
6
8
10
12
1.50
4.99
1.78
8.06
3.00
9.848
7.477
7.461
7.447
7.403
7.390
7.377
7.374
7.270
7.258
7.242
2.285
2.269
2.262
2.251
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1.384
1.371
1.361
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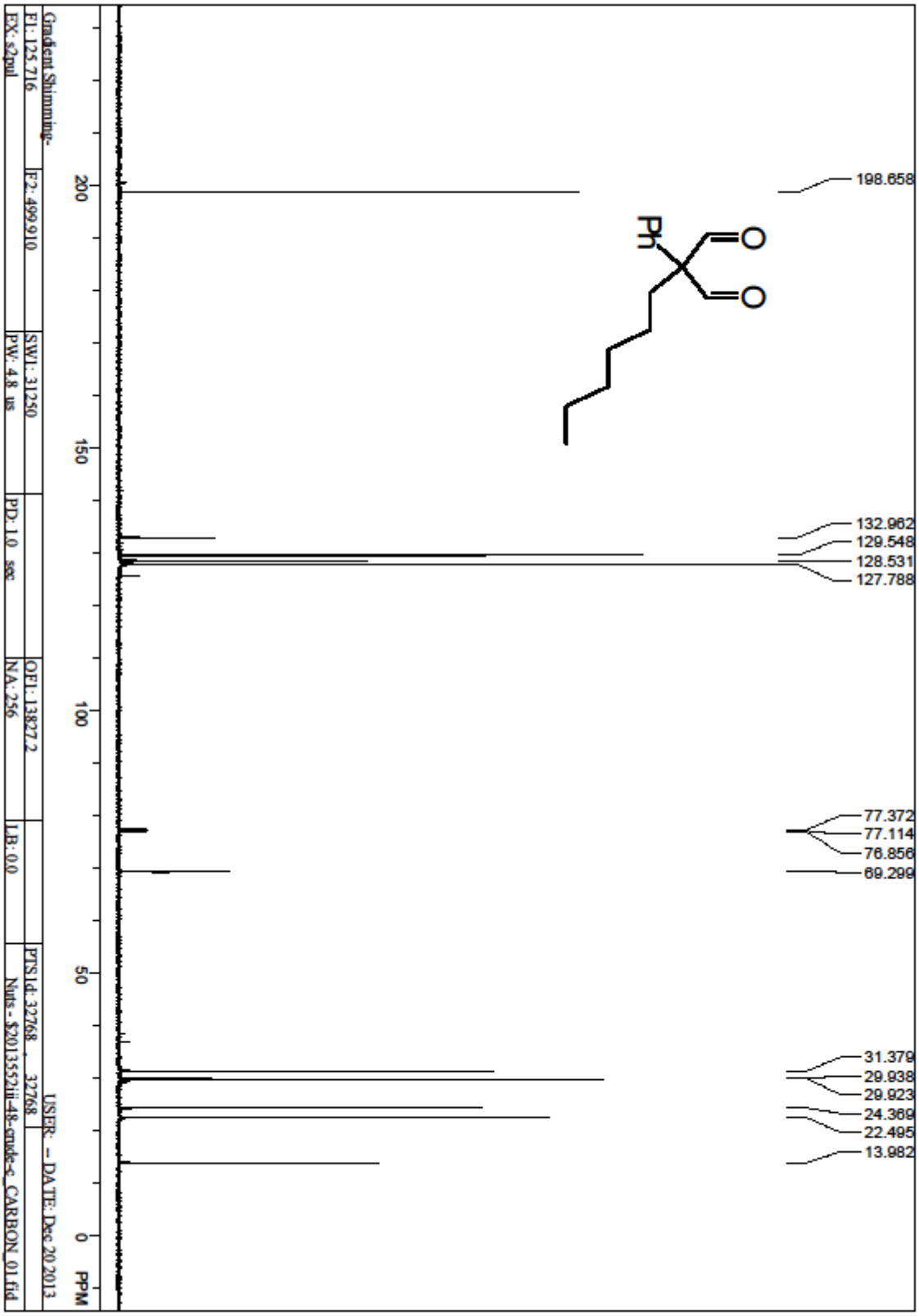
O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O
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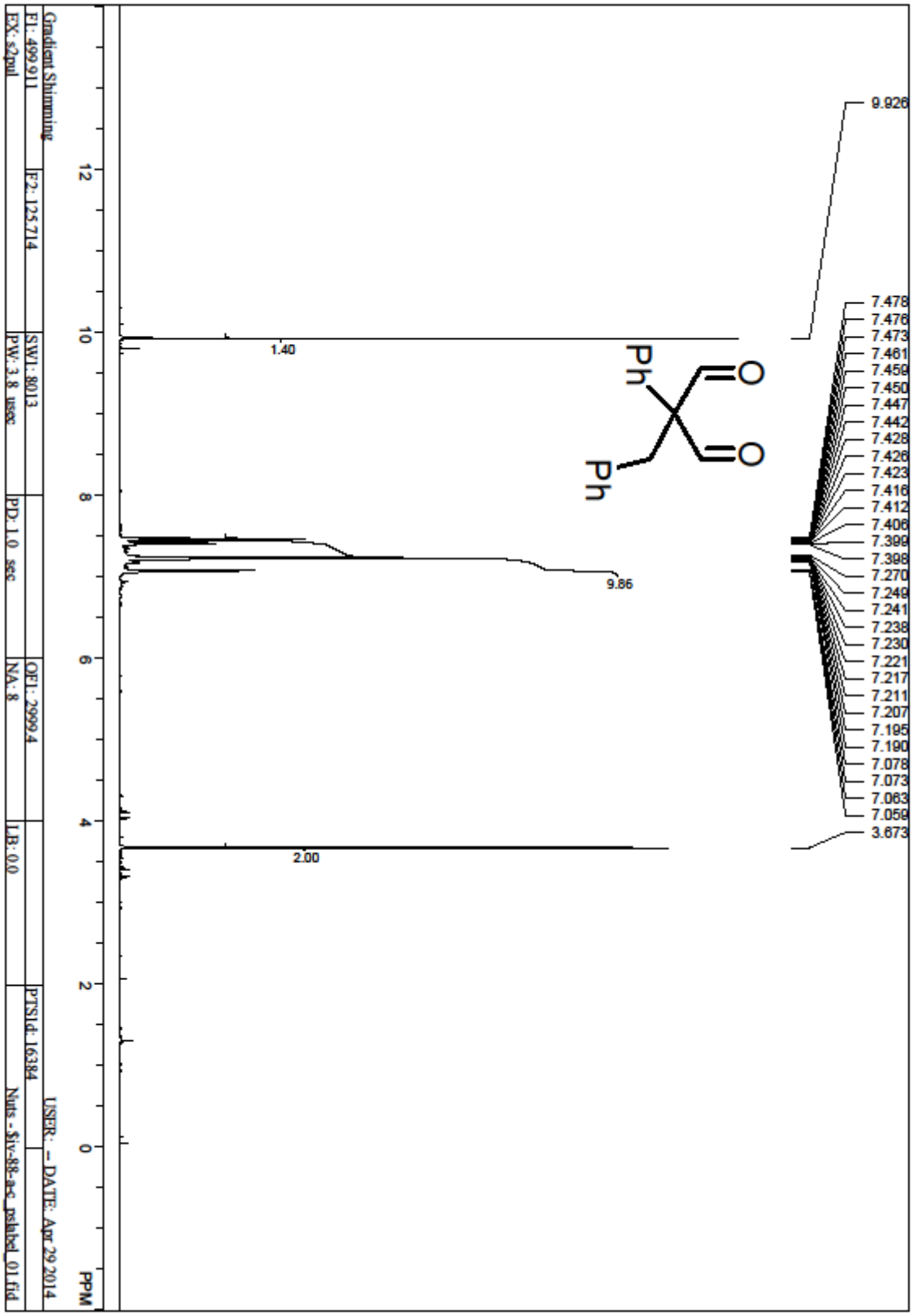
150
100
50
0
PPM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7.412
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7.238
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7.217
7.211
7.207
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7.190
7.078
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7.063
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2.00
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Ph
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10
8
6
4
2
0
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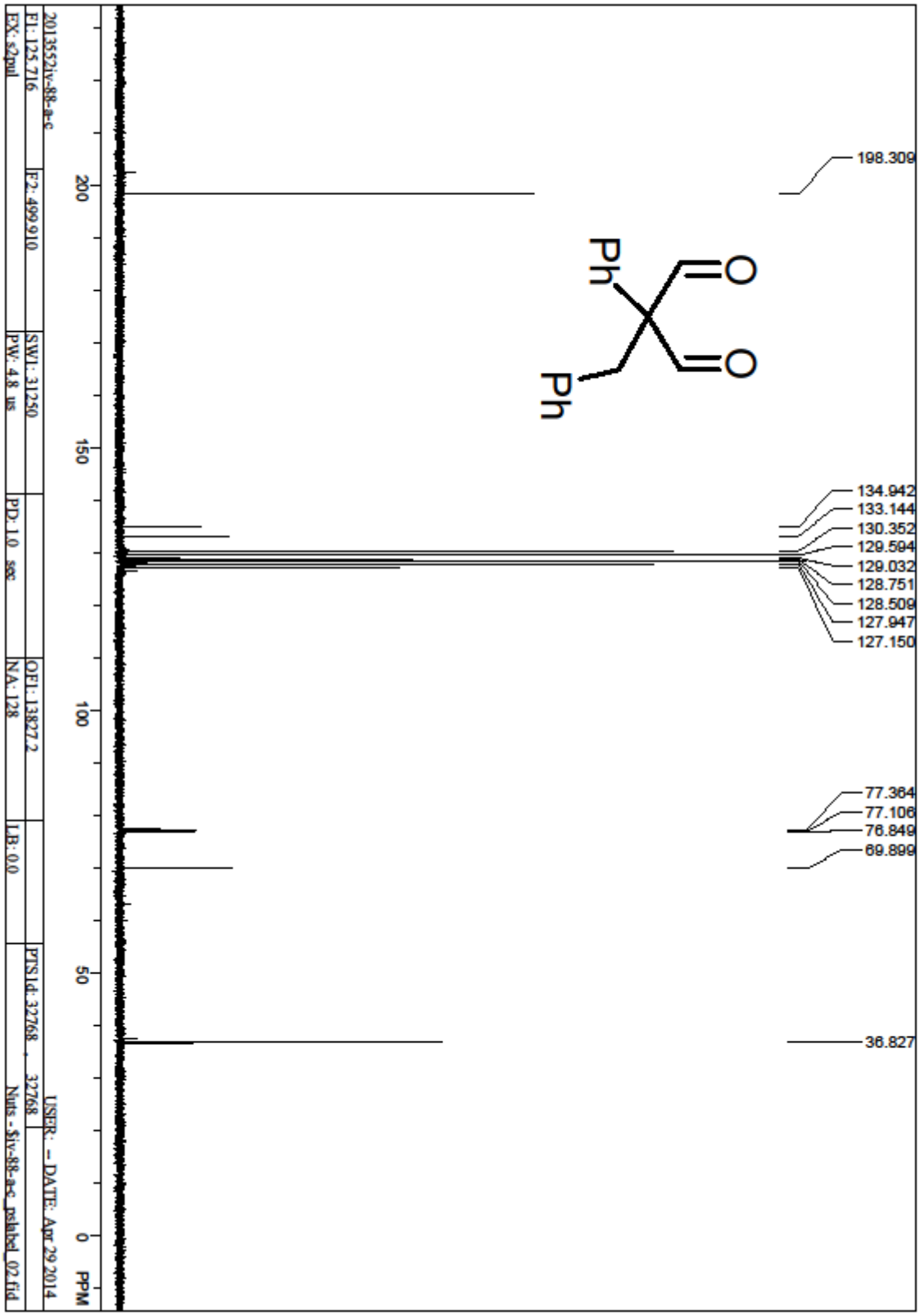
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77.106
76.849
69.899
36.827
Ph
Ph
O
O
200
150
100
50
0
PPM
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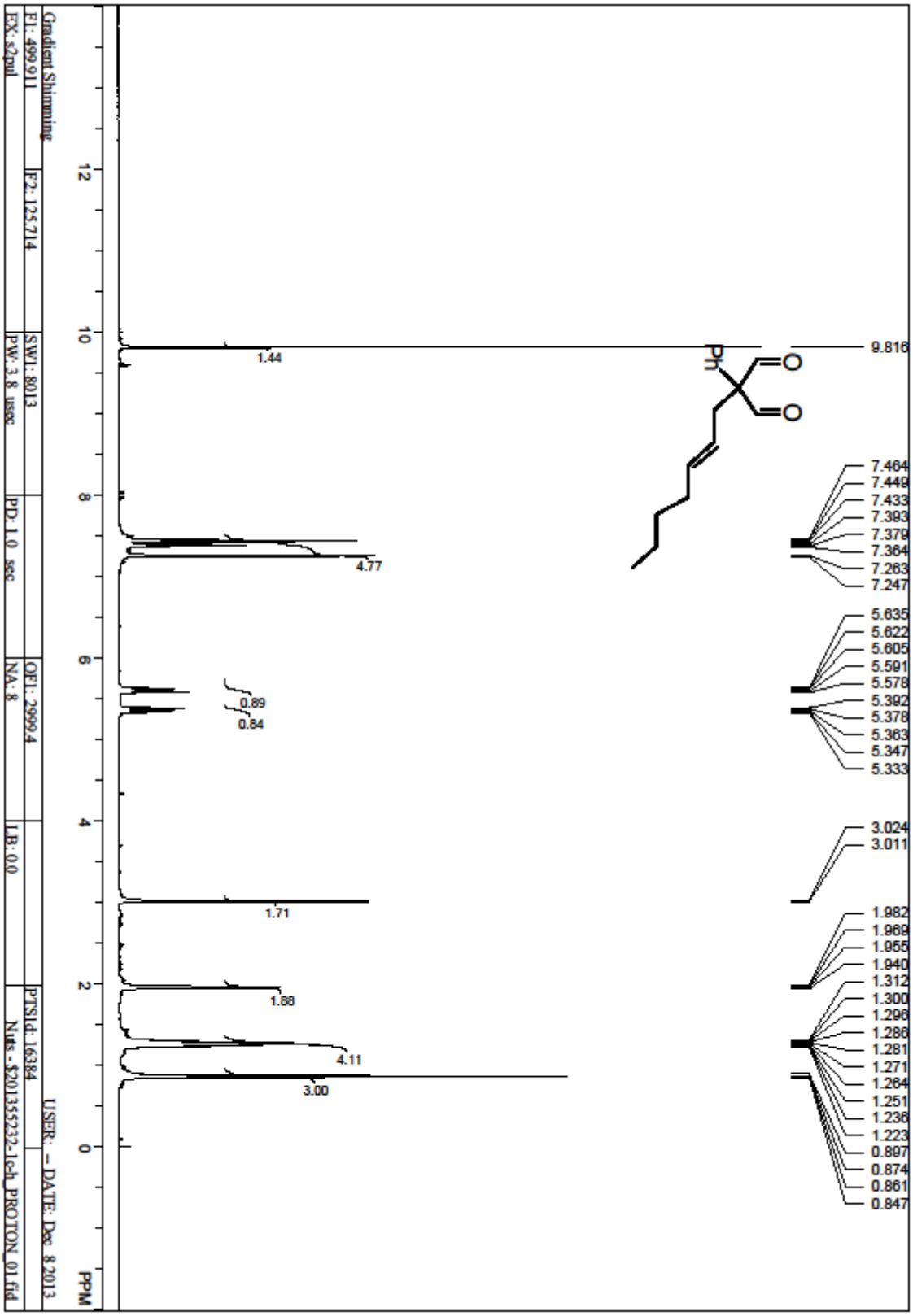
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8
6
4
2
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4.77
0.89
0.84
1.71
1.88
4.11
3.00
Ph
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O
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7.464
7.449
7.433
7.393
7.379
7.364
7.263
7.247
5.635
5.622
5.605
5.591
5.578
5.392
5.378
5.363
5.347
5.333
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3.011
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1.969
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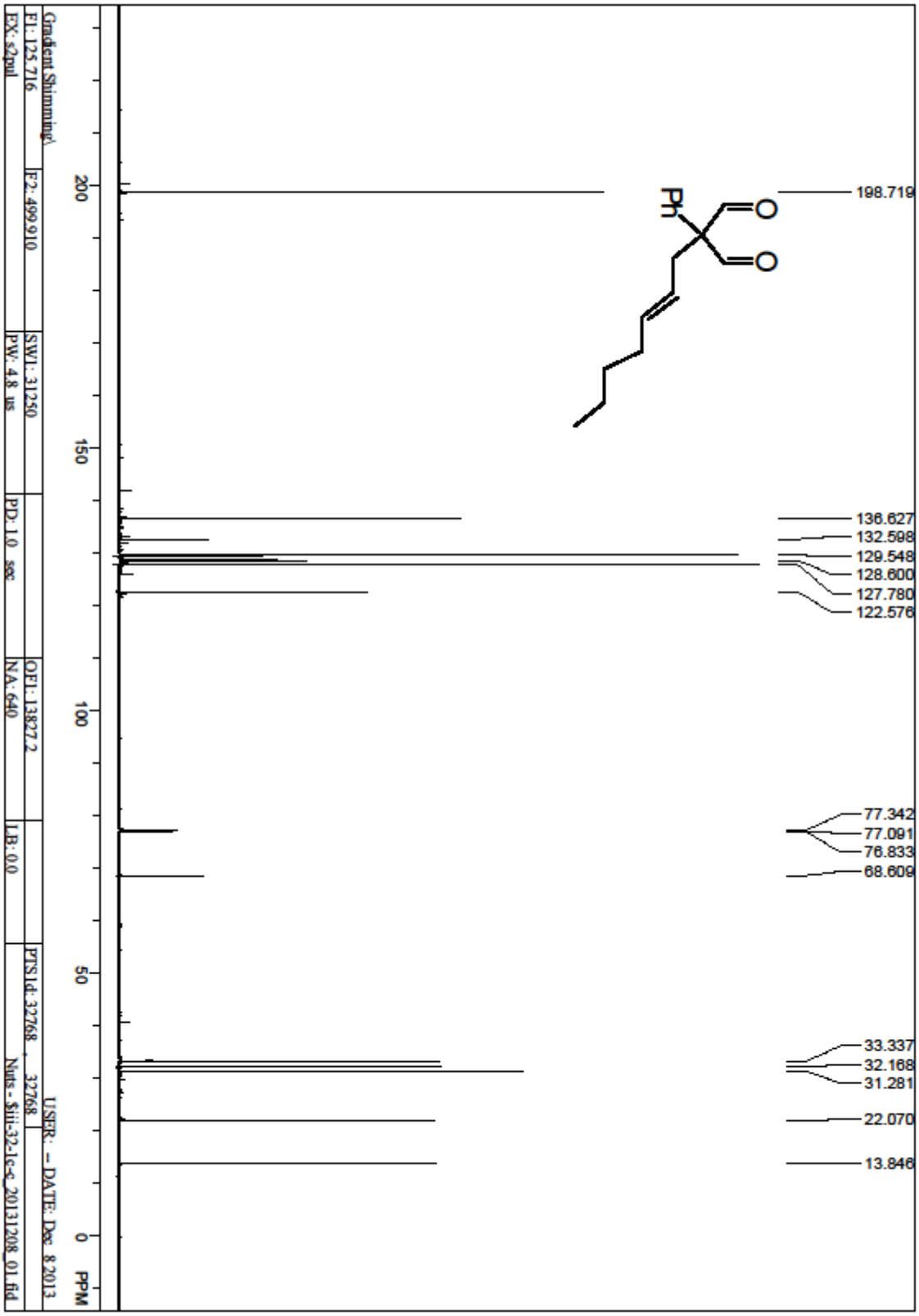
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77.091
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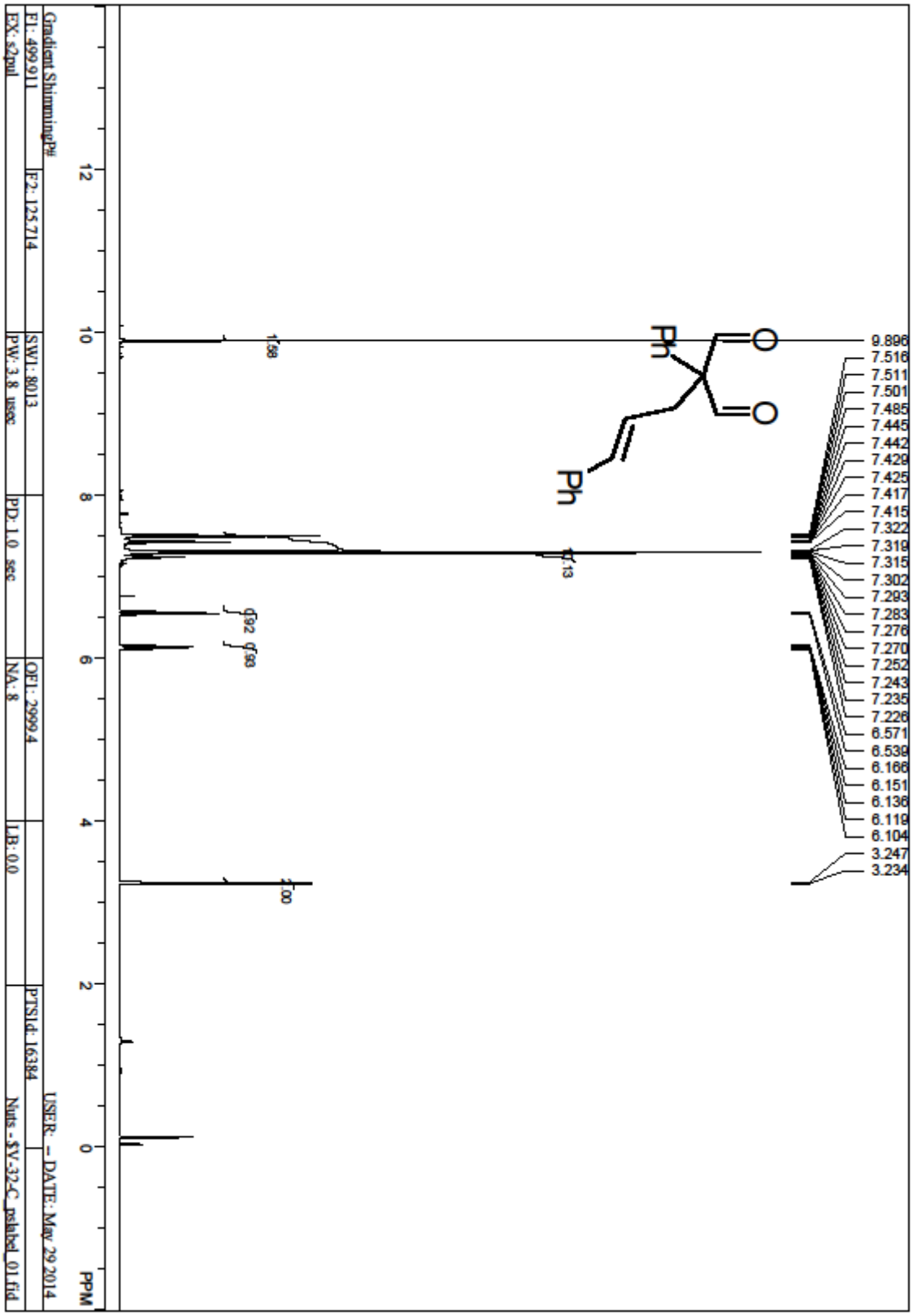
0
PPM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6
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0.93
1.00
Ph
Ph
O
O
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7.511
7.501
7.485
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7.442
7.429
7.425
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3.247
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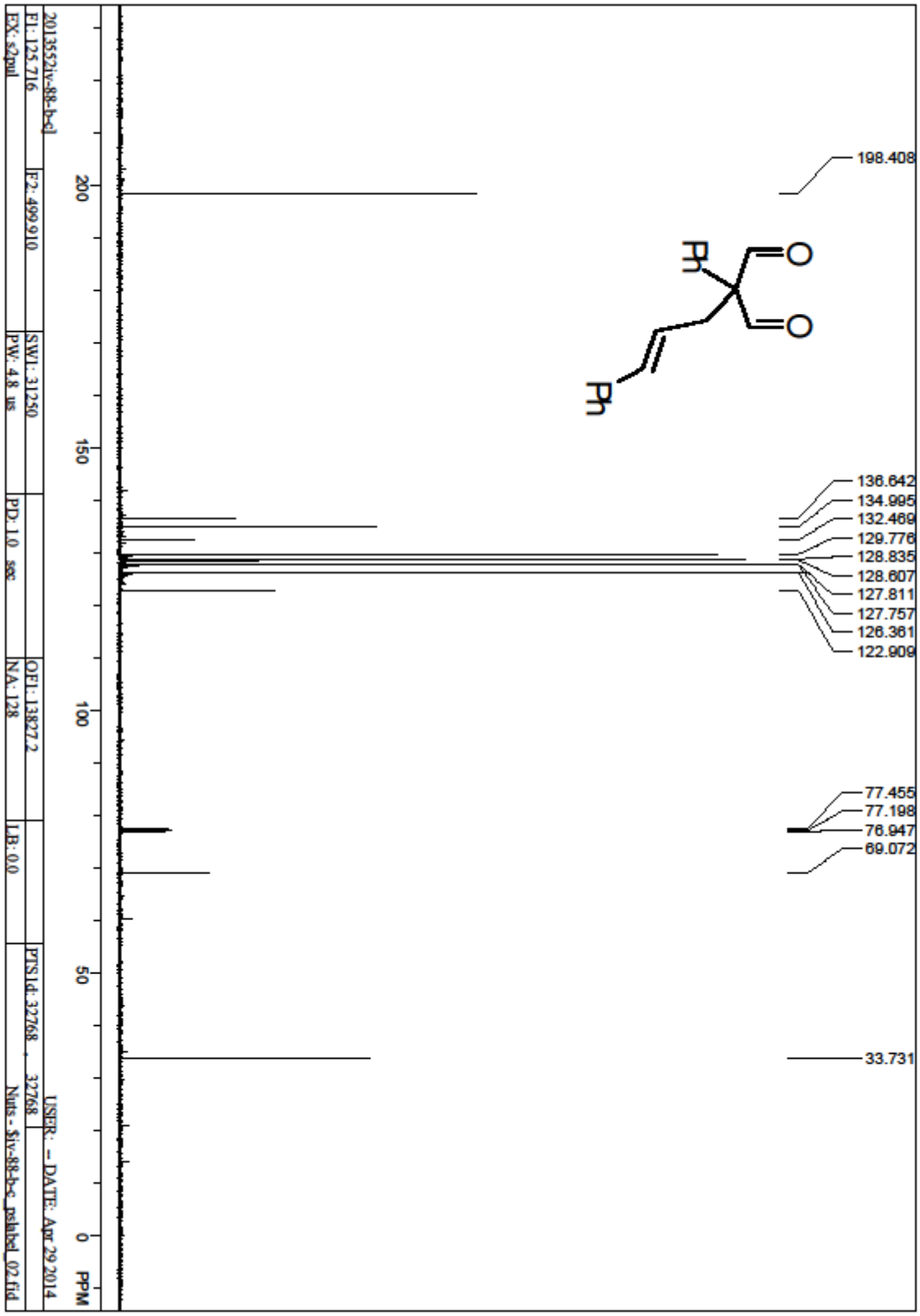
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76.947
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Ph
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O
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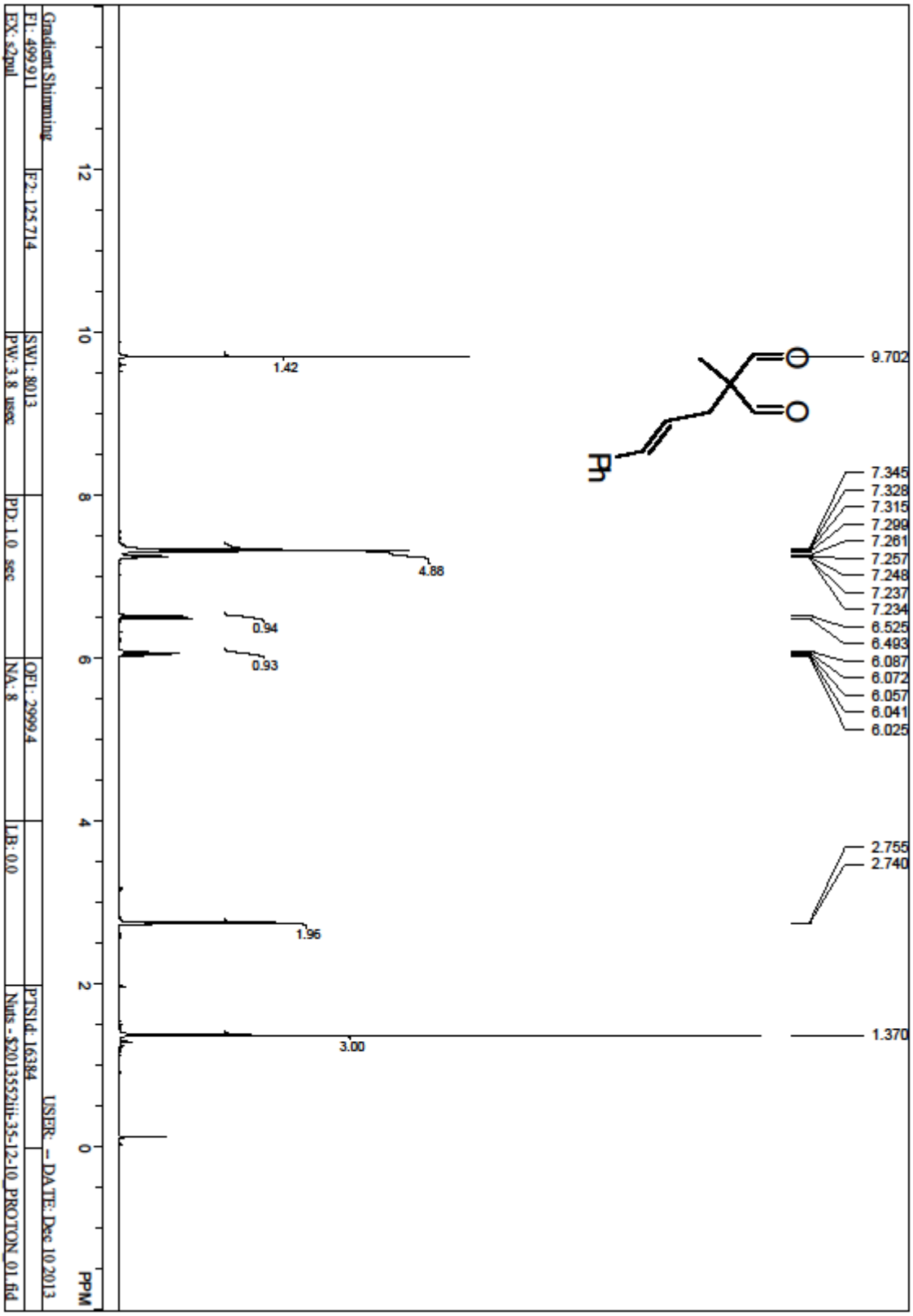
150
100
50
0
PPM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NA: 8
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4
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0.94
0.93
1.96
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Ph
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O
9.702
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7.328
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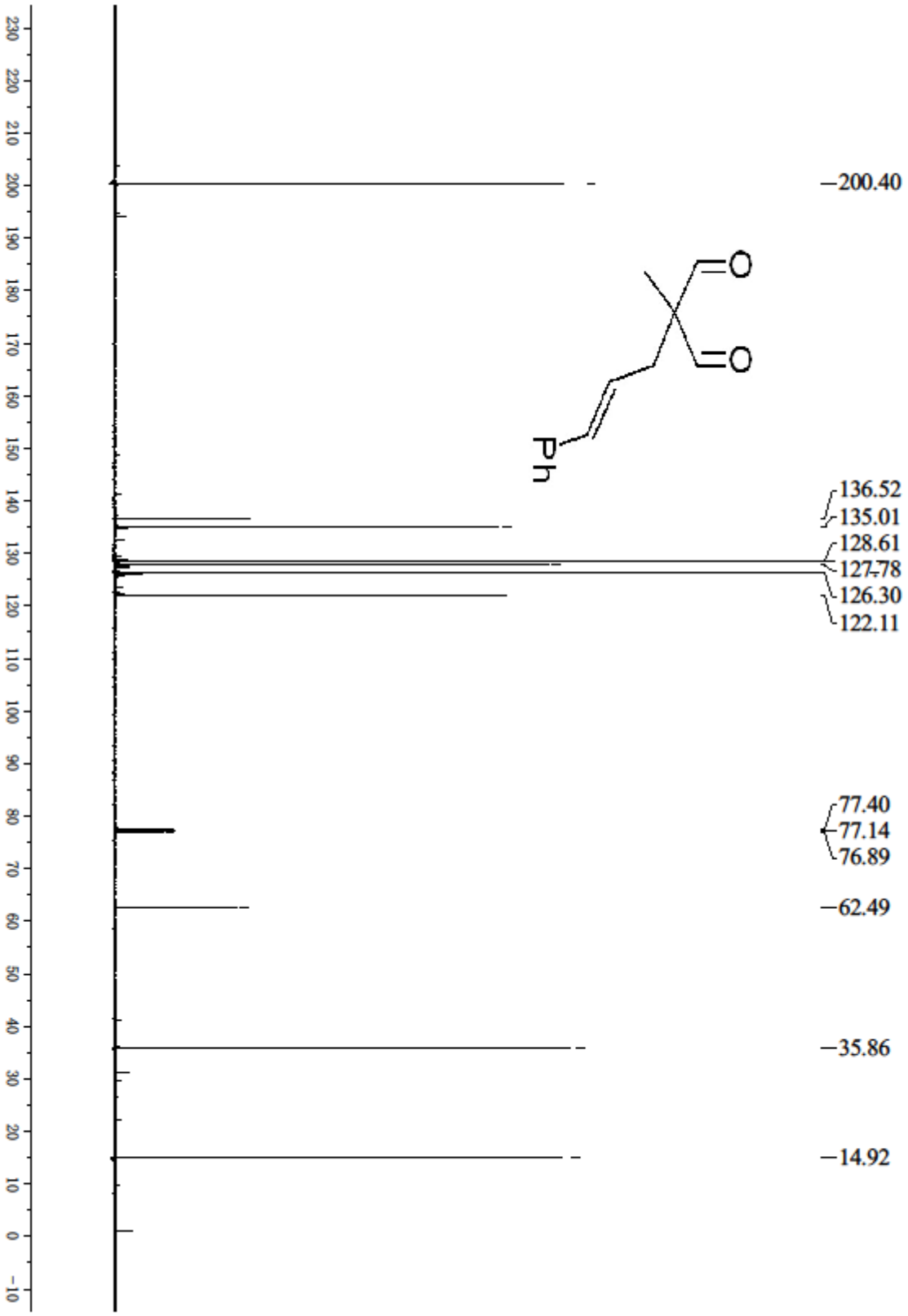
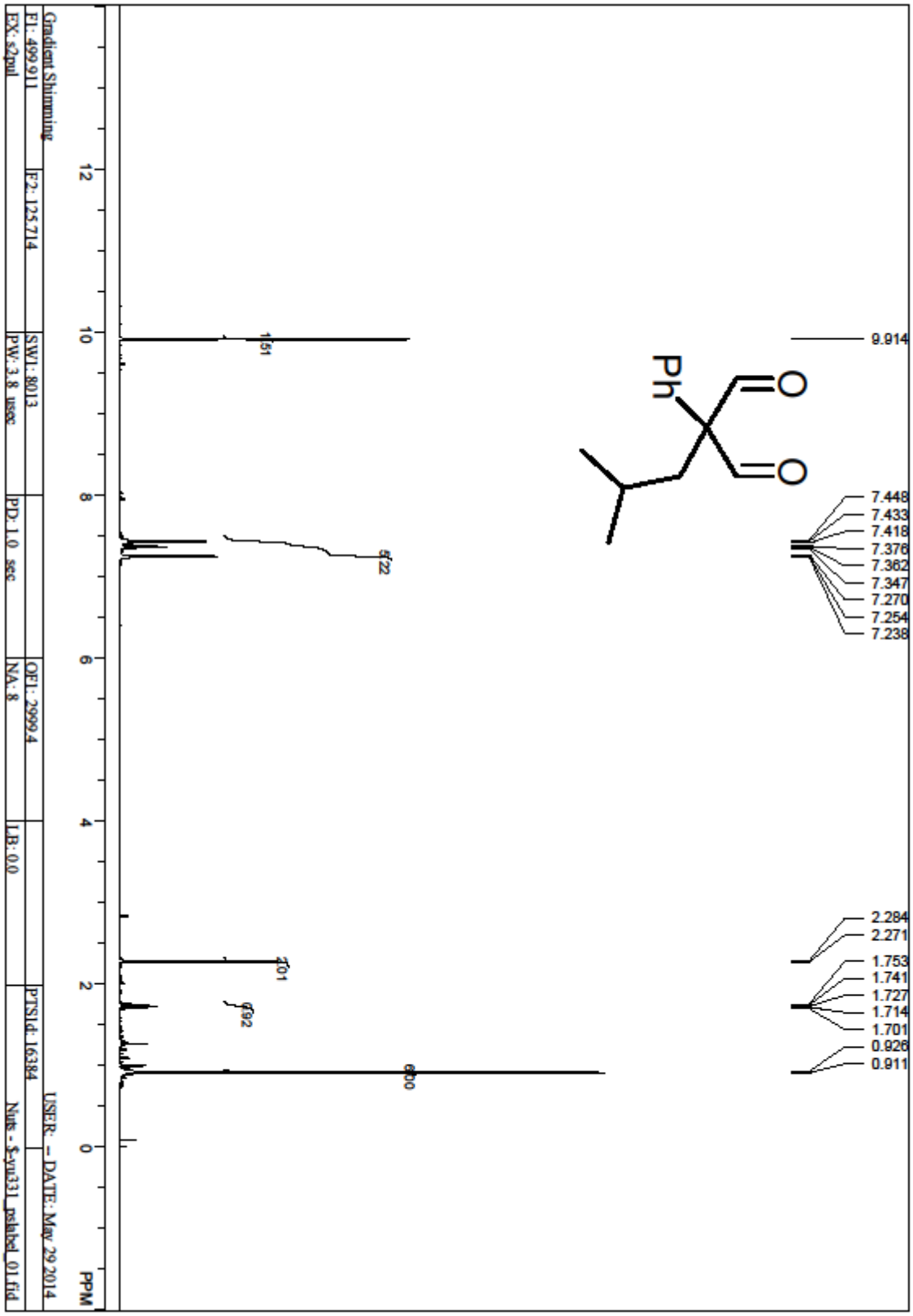
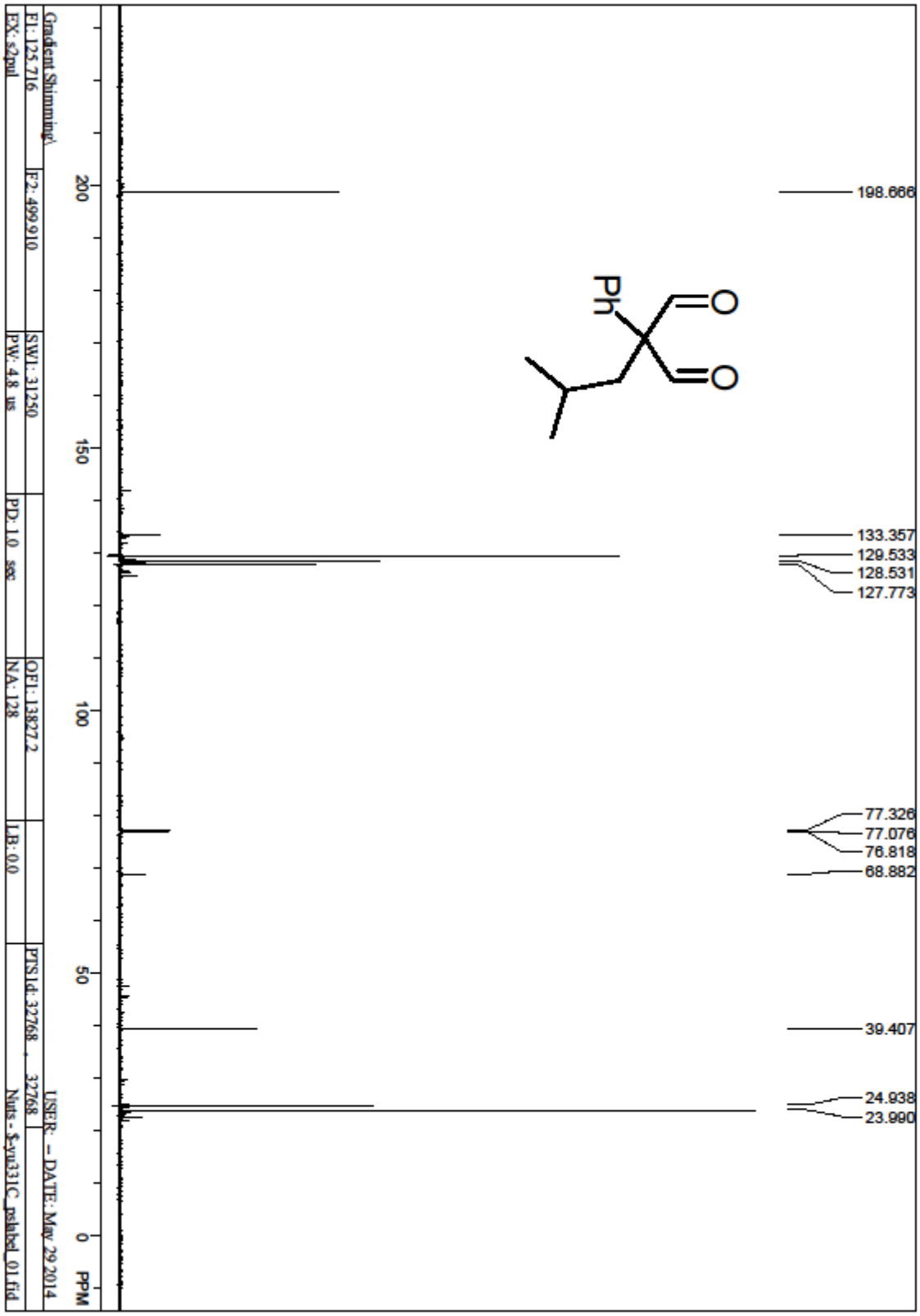
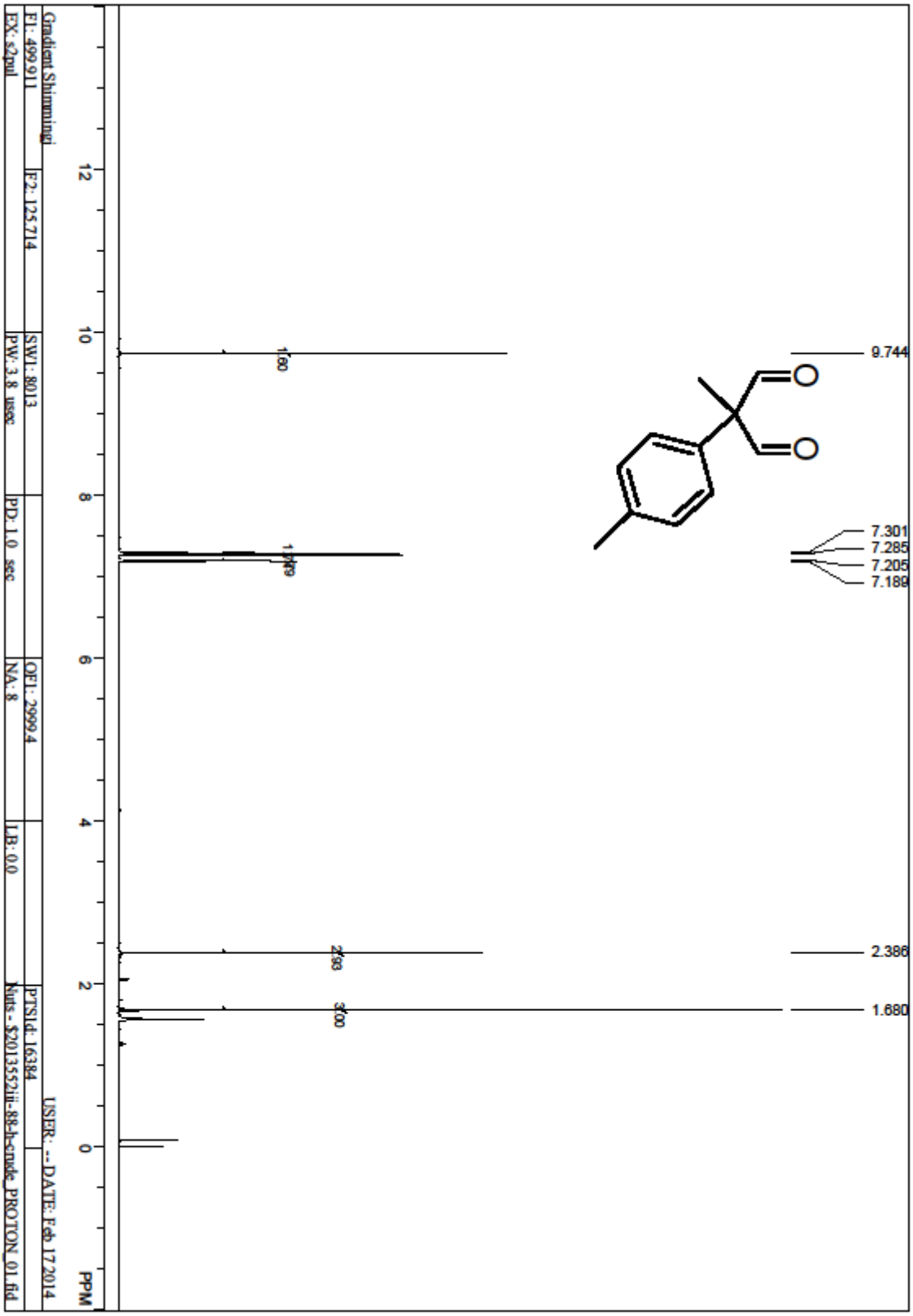
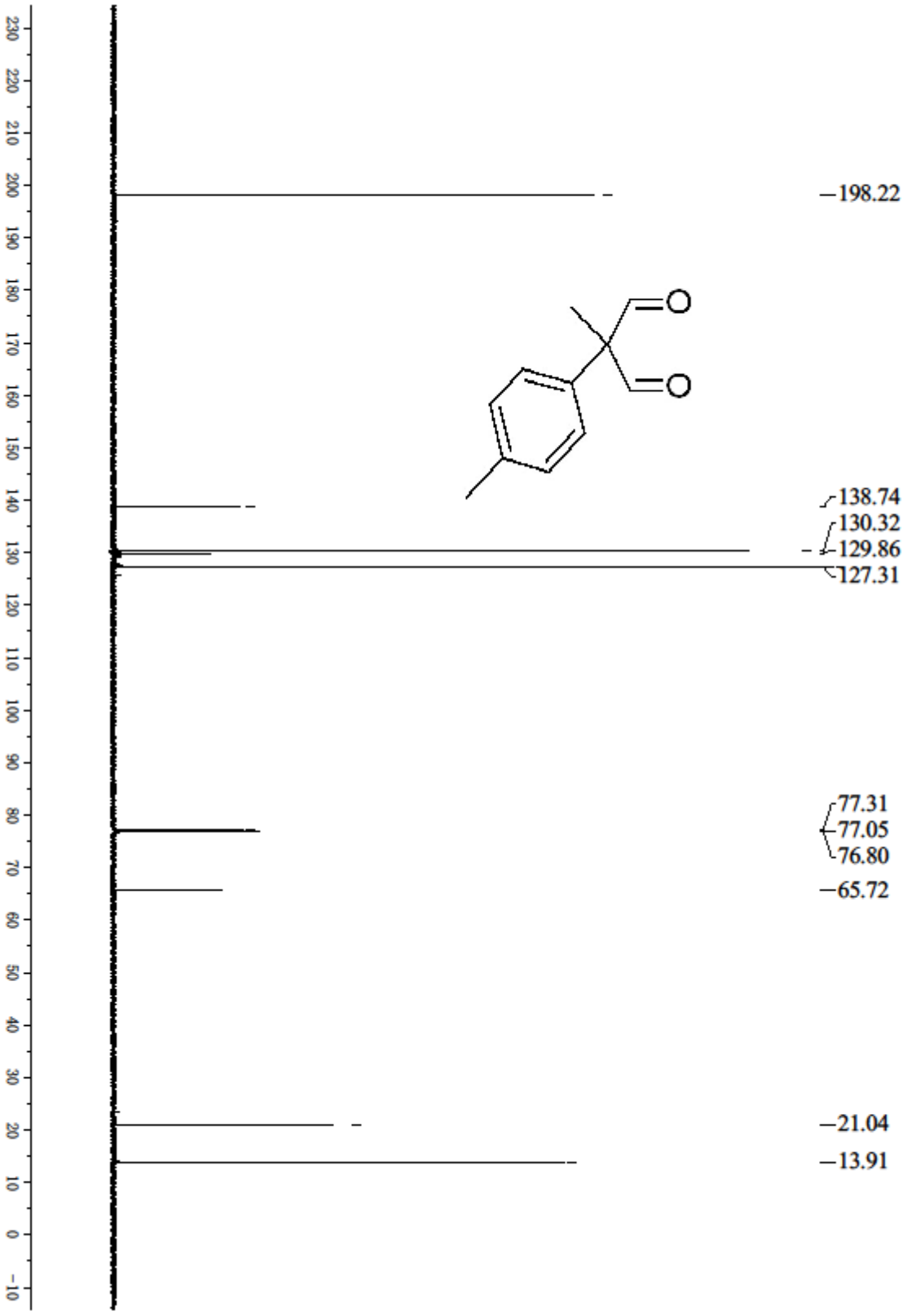
7.299
7.261
7.257
7.248
7.237
7.234
6.525
6.493
6.087
6.072
6.057
6.041
6.025
2.755
2.740
1.370

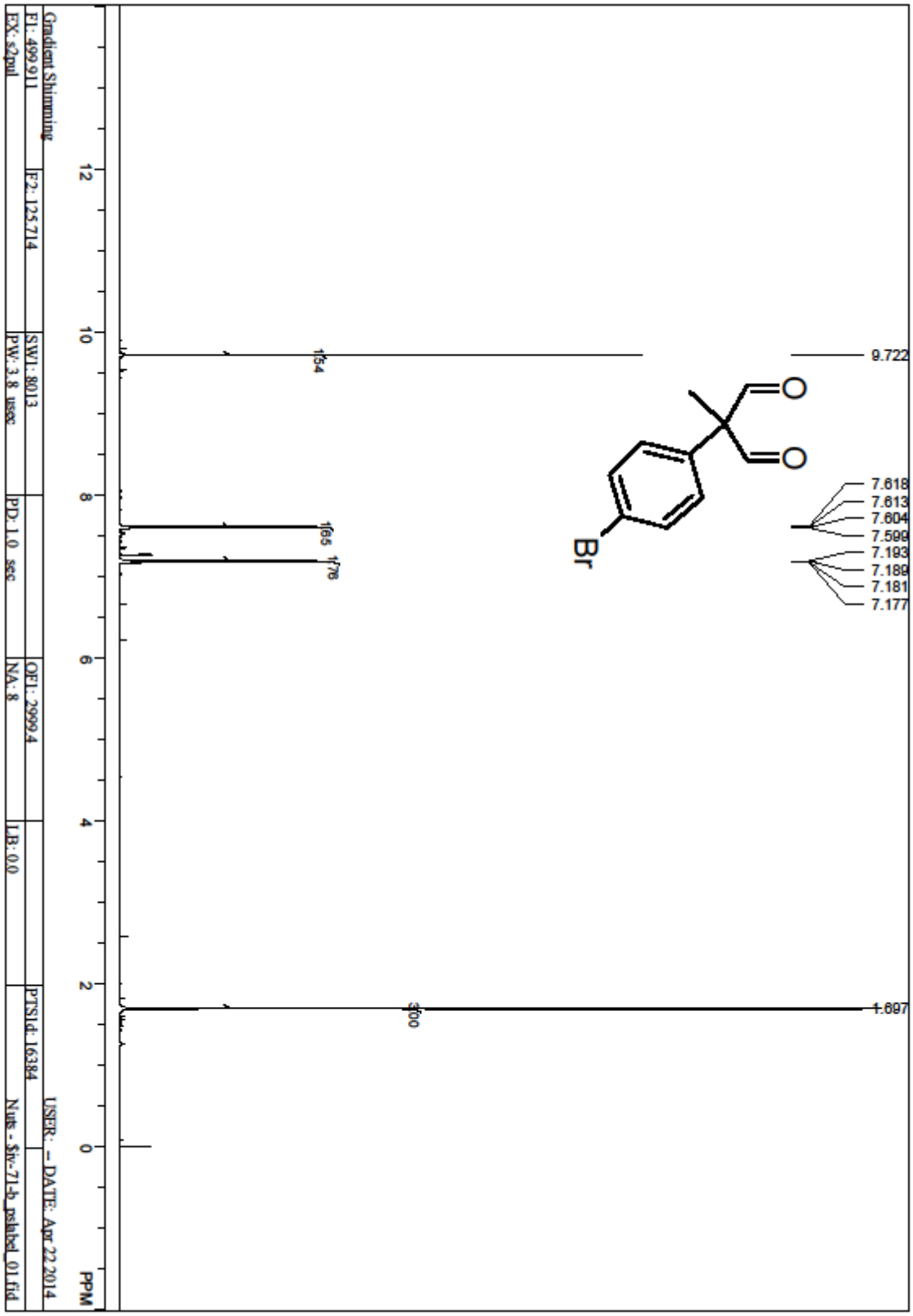

200.40
O
O
Ph
136.52
135.01
128.61
127.78
126.30
122.11
77.40
77.14
76.89
62.49
35.86
14.92

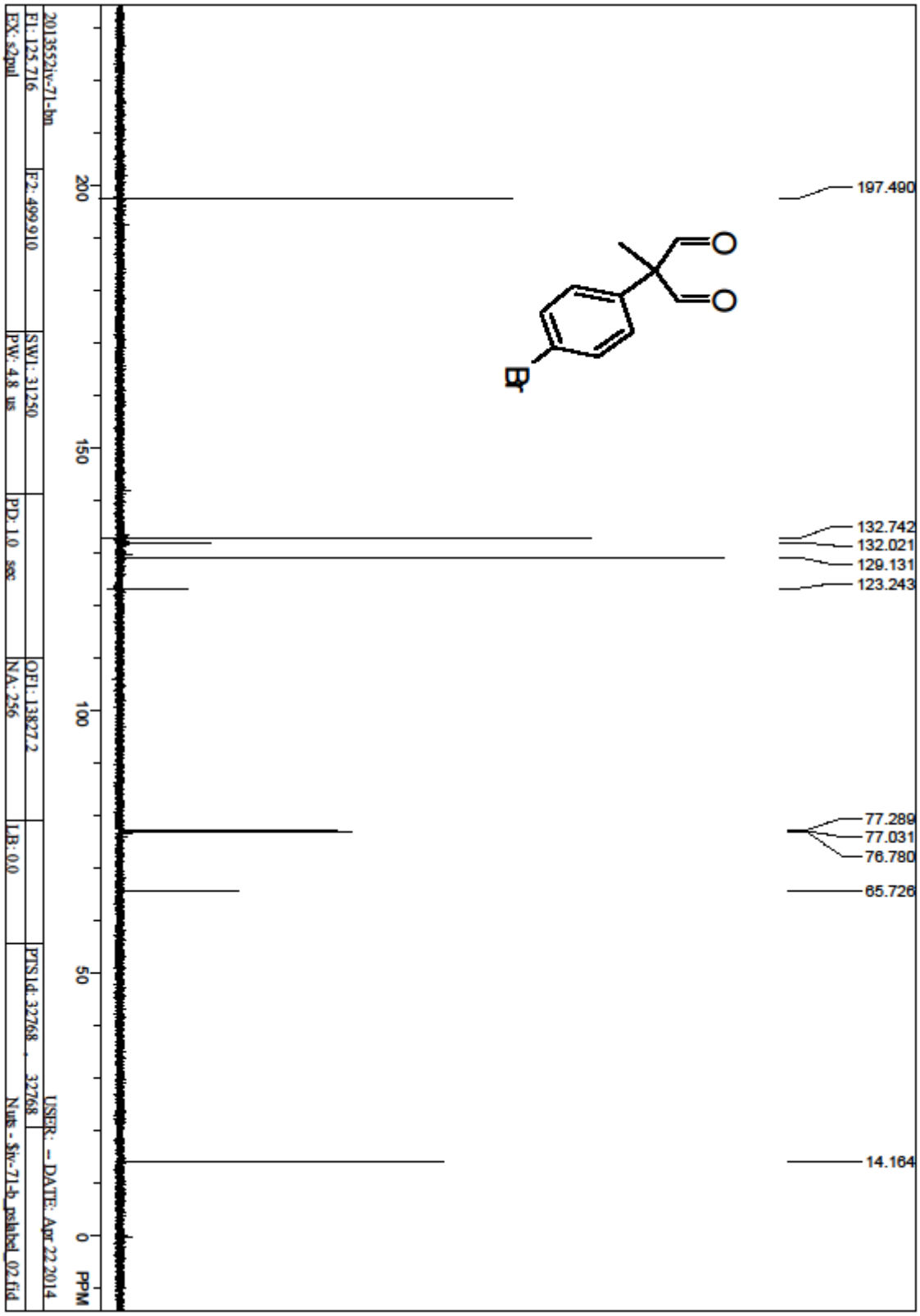

9.914
7.448
7.433
7.418
7.376
7.362
7.347
7.270
7.254
7.238
2.284
2.271
1.753
1.741
1.727
1.714
1.701
0.926
0.911
Ph
O
O
1.51
6.22
2.01
0.92
6.00
12
10
8
6
4
2
0
PPM
Gradient Shimming
F1: 499.911
F2: 125.714
SW1: 8013
PW: 3.8 usec
PD: 1.0 sec
OF1: 2999.4
NA: 8
LB: 0.0
PTS1d: 16384
USER: -- DATE: May 29 2014
EX: s2pul
Nuts - $cyu331_pslabel_01.fid

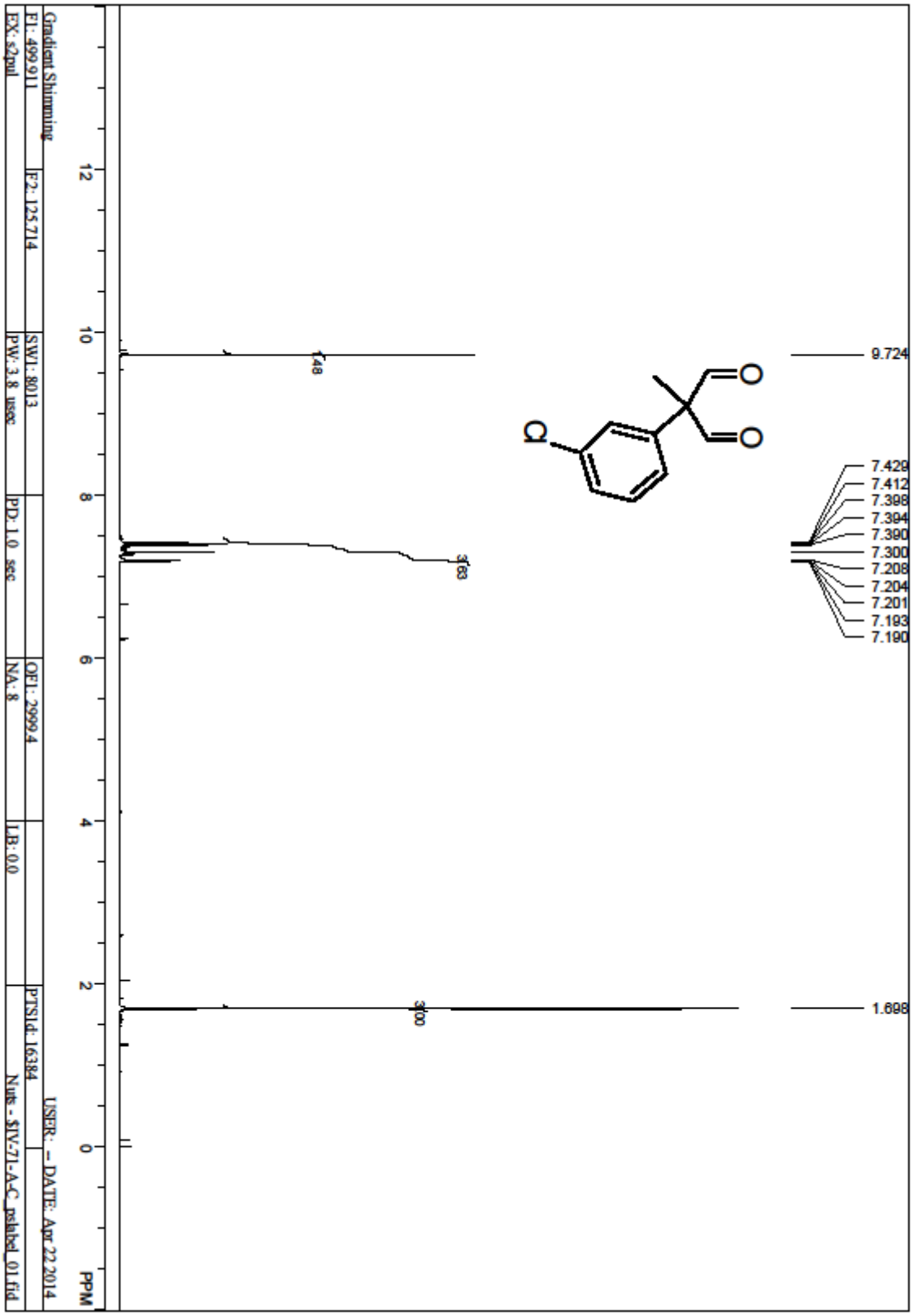

Gradient Shimming\
F1: 125.716
F2: 499.910
EX: s2pul
SW1: 31250
PW: 4.8 us
PD: 1.0 sec
QF1: 13827.2
NA: 128
LB: 0.0
PTS1d: 32768 , 32768
USER: -- DATE: May 29 2014
Nuts - $cyu331C_pslabel_01.fid
Ph
O
O
198.666
133.357
129.533
128.531
127.773
77.326
77.076
76.818
68.882
39.407
24.938
23.990
200
150
100
50
0
PPM

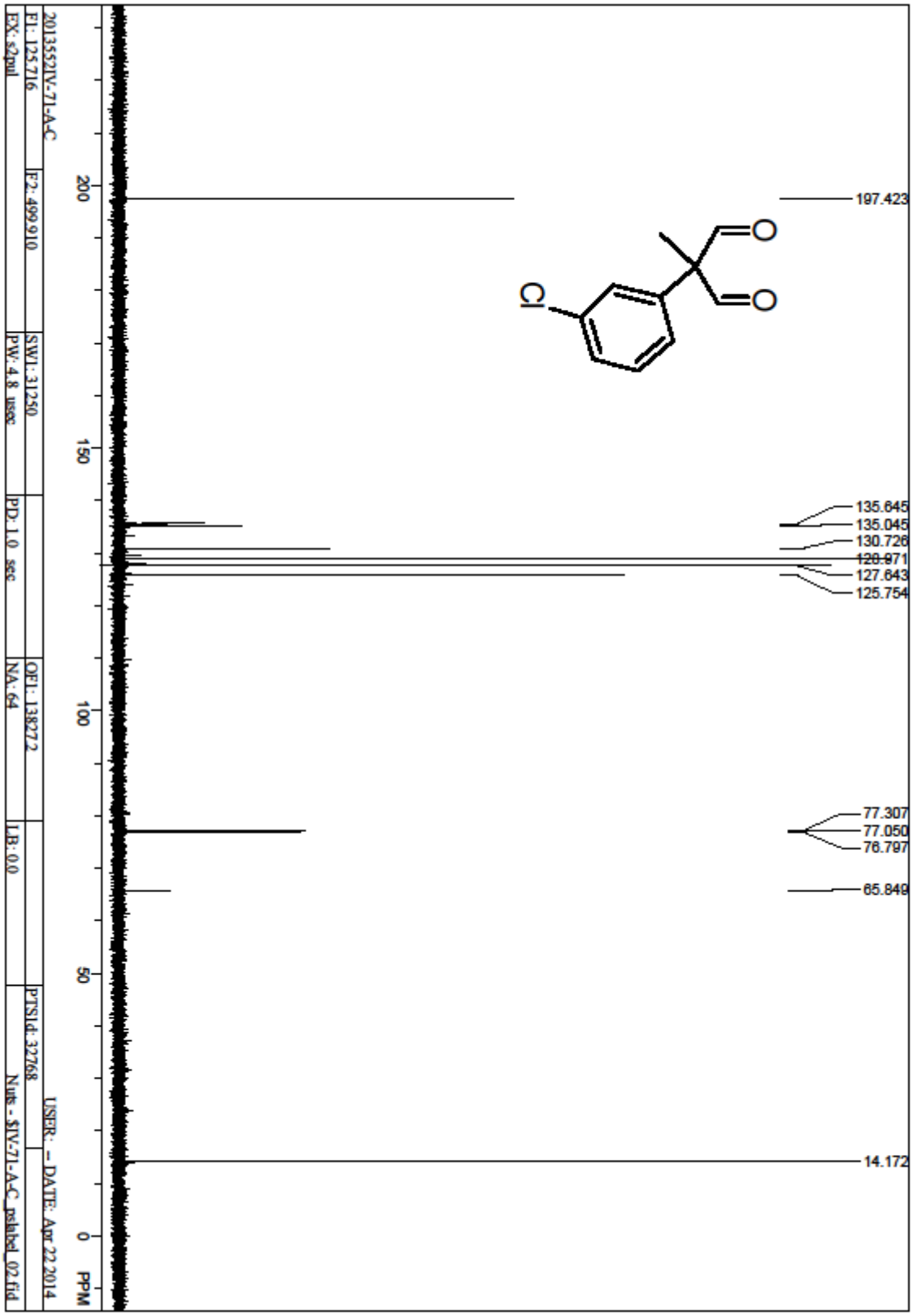

Gradient Shimming
FI: 499.911
F2: 125.714
EX: s2pul
SW1: 8013
PW: 3.8 usec
PD: 1.0 sec
OF1: 2999.4
NA: 8
PTS1d: 16384
LB: 0.0
USER: --DATE: Feb 17 2014
Nuts - $20135521ii-88-hcmde_PROTON_01.fid
PPM
12
10
8
6
4
2
0
9.744
7.301
7.285
7.205
7.189
2.386
1.680
1.00
2.93
3.00

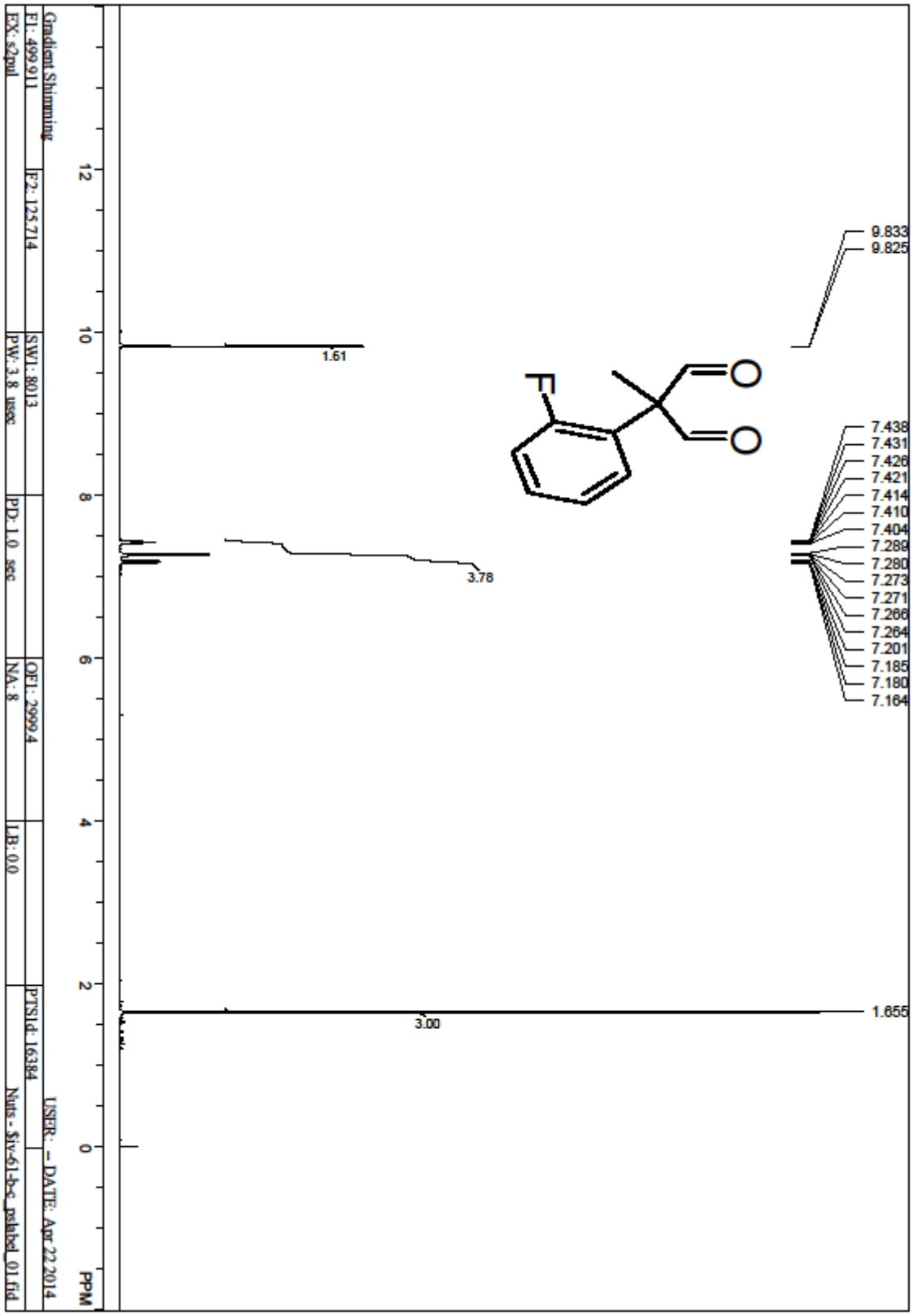

198.22
138.74
130.32
129.86
127.31
77.31
77.05
76.80
65.72
21.04
13.91

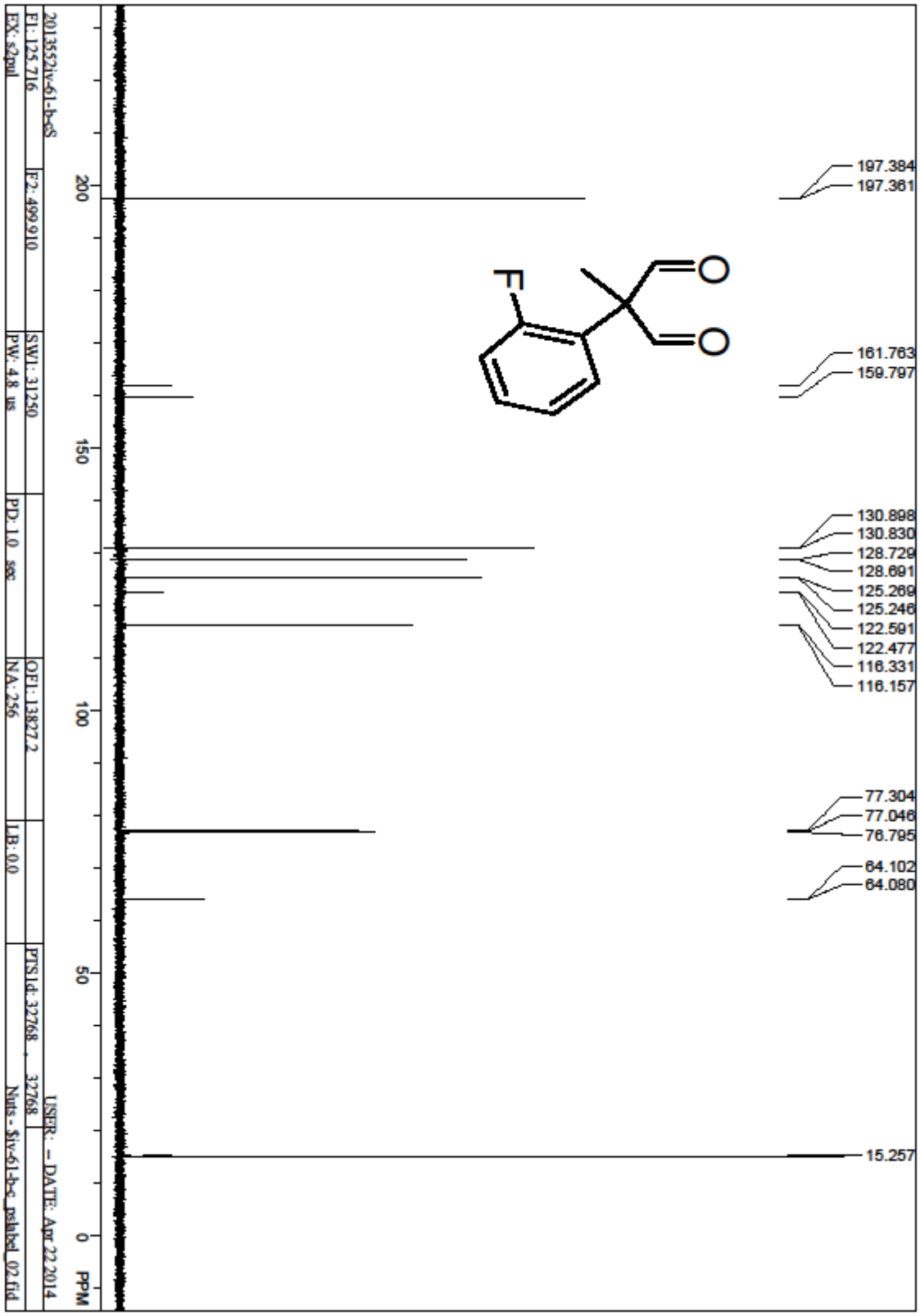

9.722
7.618
7.613
7.604
7.599
7.193
7.189
7.181
7.177
1.697
1.54
1.65
1.78
3.00
O
O
Br
12
10
8
6
4
2
0
PPM
Gradient Shimming
F1: 499.911
F2: 125.714
SW1: 8013
PW: 3.8 usec
PD: 1.0 sec
OF1: 2999.4
NA: 8
LB: 0.0
PTS1d: 16384
USER: -- DATE: Apr 22 2014
EX: s2pul
Nuts - Shv-71-b_pslabel_01.fid

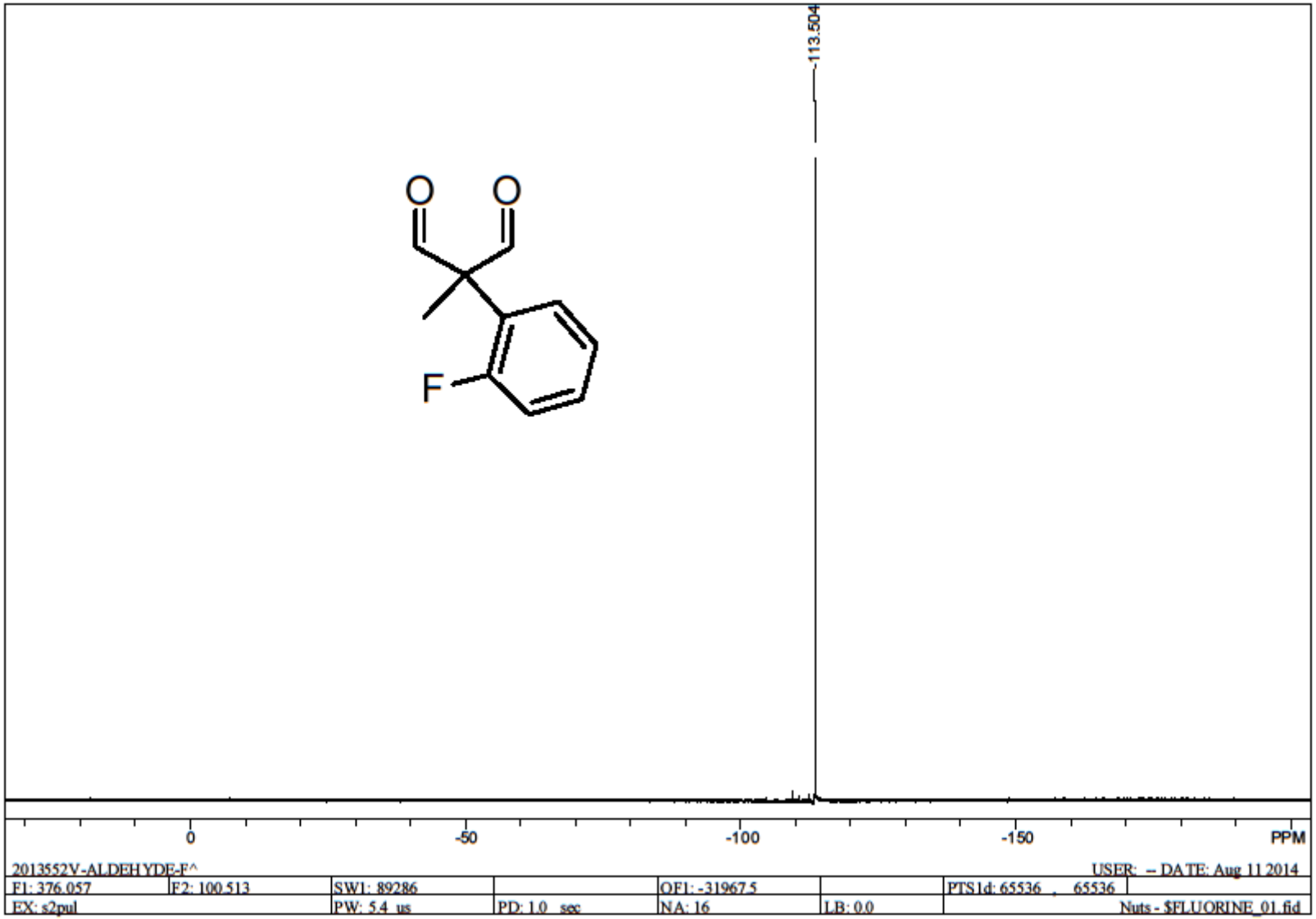

197.490
132.742
132.021
129.131
123.243
77.289
77.031
76.780
65.726
14.164
Br
O
O
200
150
100
50
0
PPM
20130521v-71-bm
F1: 125.716
F2: 499.910
SW1: 31250
PW: 4.8 us
PD: 1.0 sec
QF1: 13827.2
NA: 256
LB: 0.0
PTS1d: 32768 , 32768
USER: -- DATE: Apr 22 2014
EX: s2pul
Nuts - $tv-71-b_pslabel_02.fid

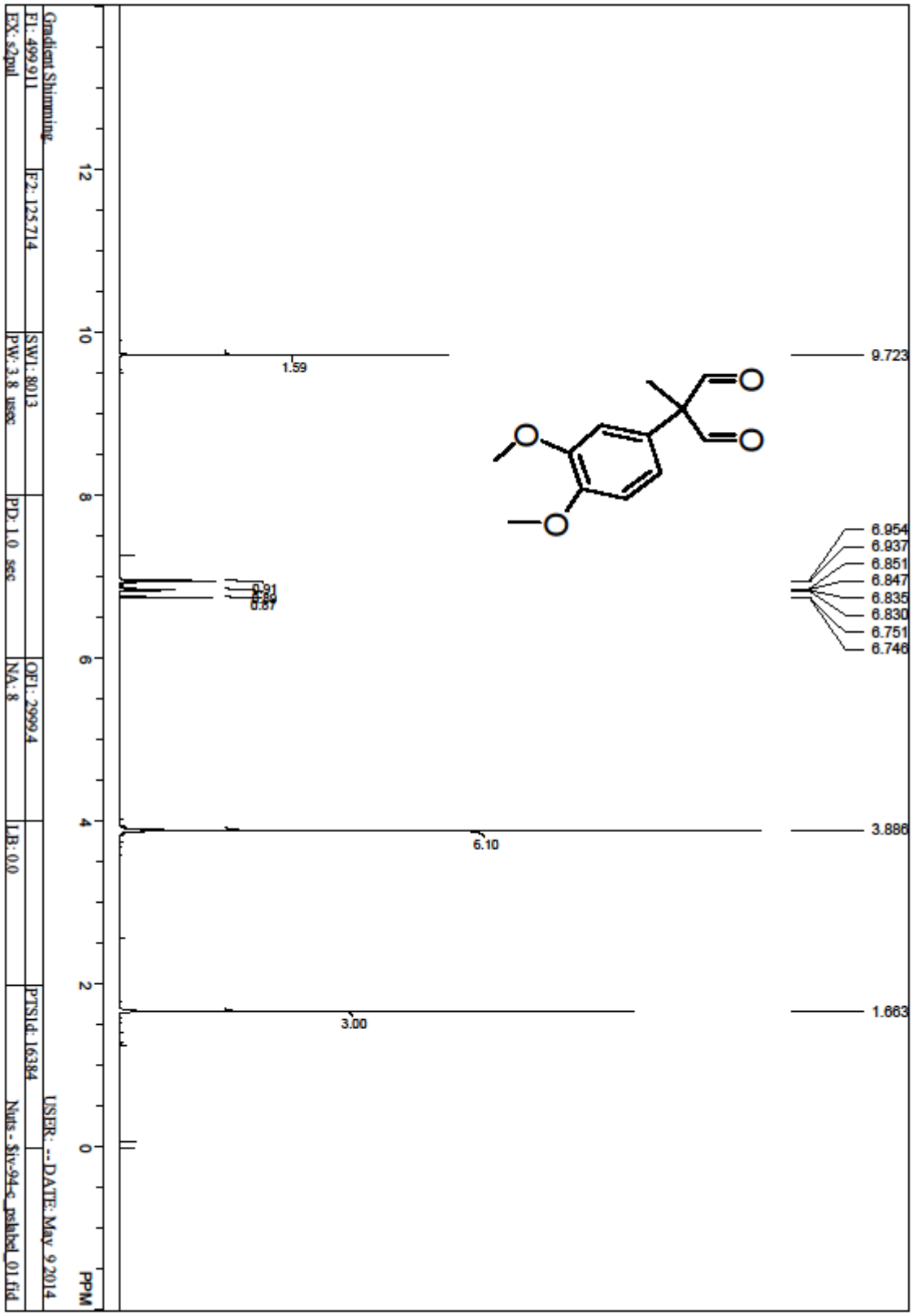

9.724
7.429
7.412
7.398
7.394
7.390
7.300
7.208
7.204
7.201
7.193
7.190
1.698
1.48
3.63
3.00
O
O
Cl
12
10
8
6
4
2
0
PPM
Gradient Shimming
F1: 499.911
F2: 125.714
SW1: 8013
PW: 3.8 usec
PD: 1.0 sec
OF1: 2999.4
NA: 8
LB: 0.0
PTS1d: 16384
USER: -- DATE: Apr 22 2014
EX: s2pul
Nuts - SIV-71-A-C_pslabel_01.fid

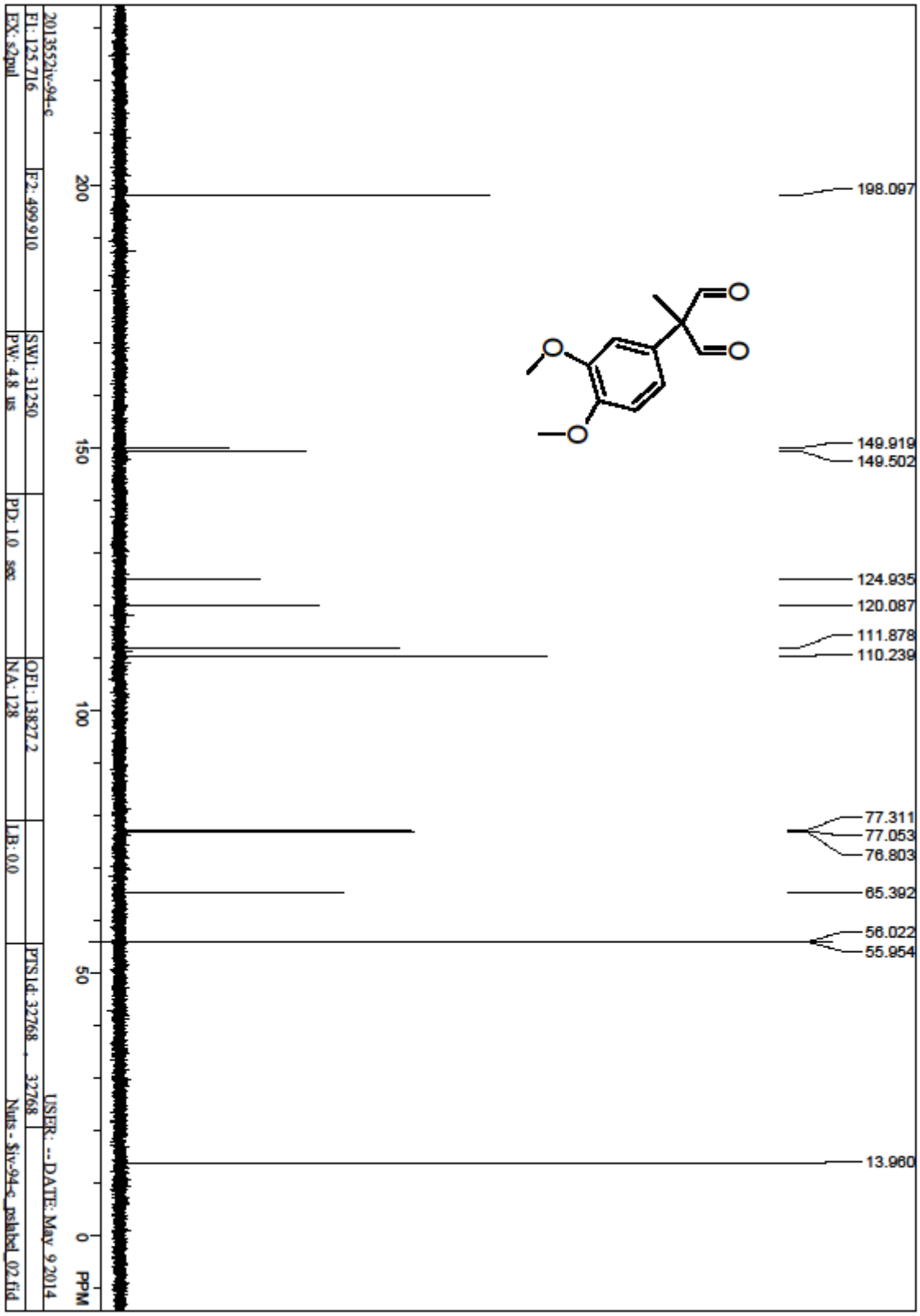

197.423
135.645
135.045
130.726
128.971
127.643
125.754
77.307
77.050
76.797
65.849
14.172
Cl
O
O
200
150
100
50
0
PPM
2013552IV-71-A-C
EL: 125.716
F2: 499.910
SW1: 31250
PW: 4.8 usec
PD: 1.0 sec
OF1: 138272
NA: 64
LB: 0.0
PTS1d: 32768
USER: --
DATE: Apr 22 2014
EX: s2pul
Nuts - SIV-71-A-C_pslabel_02.fid

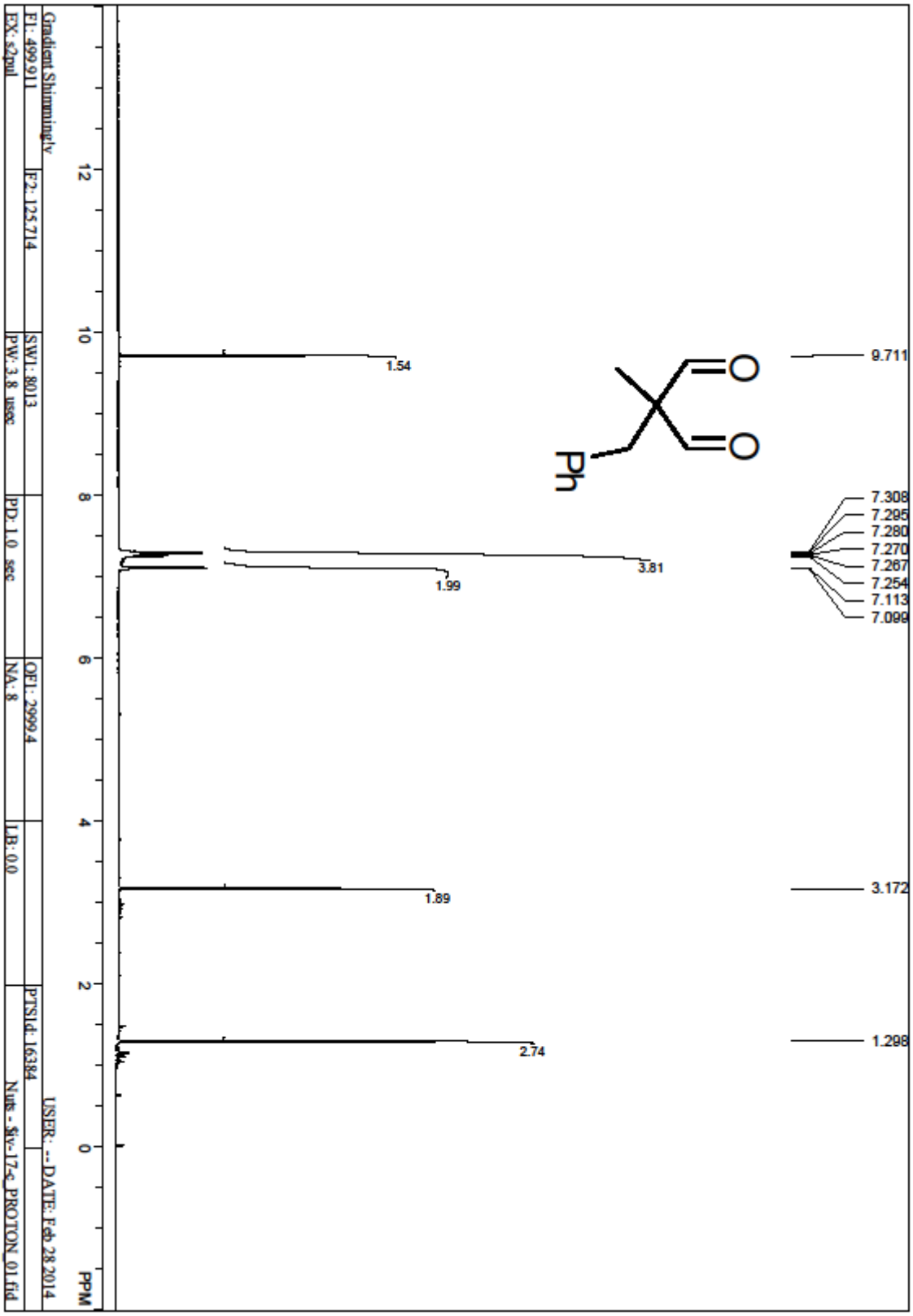

Gradient Shimming
F1: 499.911
F2: 125.714
SW1: 8013
PW: 3.8 usec
PD: 1.0 sec
OF1: 2999.4
NA: 8
LB: 0.0
PTS1d: 16384
USER: -- DATE: Apr 22 2014
EX: s2pul
Nuts - $hv-61-bcs_pslabel_01.fid
PPM
12
10
8
6
4
2
0
9.833
9.825
7.438
7.431
7.426
7.421
7.414
7.410
7.404
7.289
7.280
7.273
7.271
7.266
7.264
7.201
7.185
7.180
7.164
1.655
1.61
3.78
3.00
F
O
O

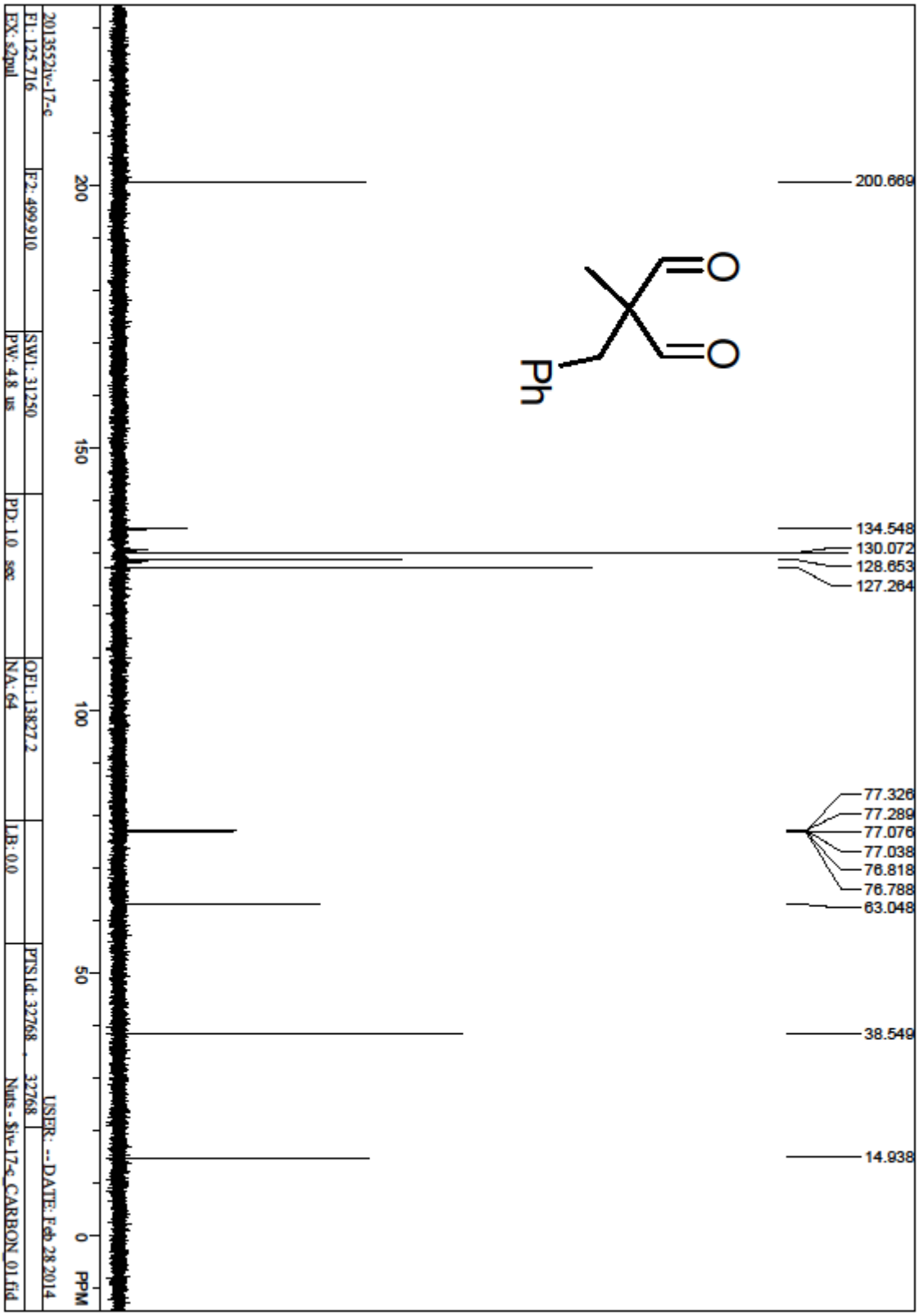

197.384
197.361
161.763
159.797
130.898
130.830
128.729
128.691
125.269
125.246
122.591
122.477
116.331
116.157
77.304
77.046
76.795
64.102
64.080
15.257
F
O
O
200
150
100
50
0
PPM
2013552iv-61-bc-S
EX: s2pul
F1: 125.716
F2: 499.910
PW: 4.8 us
SW1: 31250
PD: 1.0 sec
NA: 256
OF1: 13827.2
LB: 0.0
PTS1d: 32768 , 32768
USER: -- DATE: Apr 22 2014
Nuts - $iv-61-bc-s_pslabel_02.fid

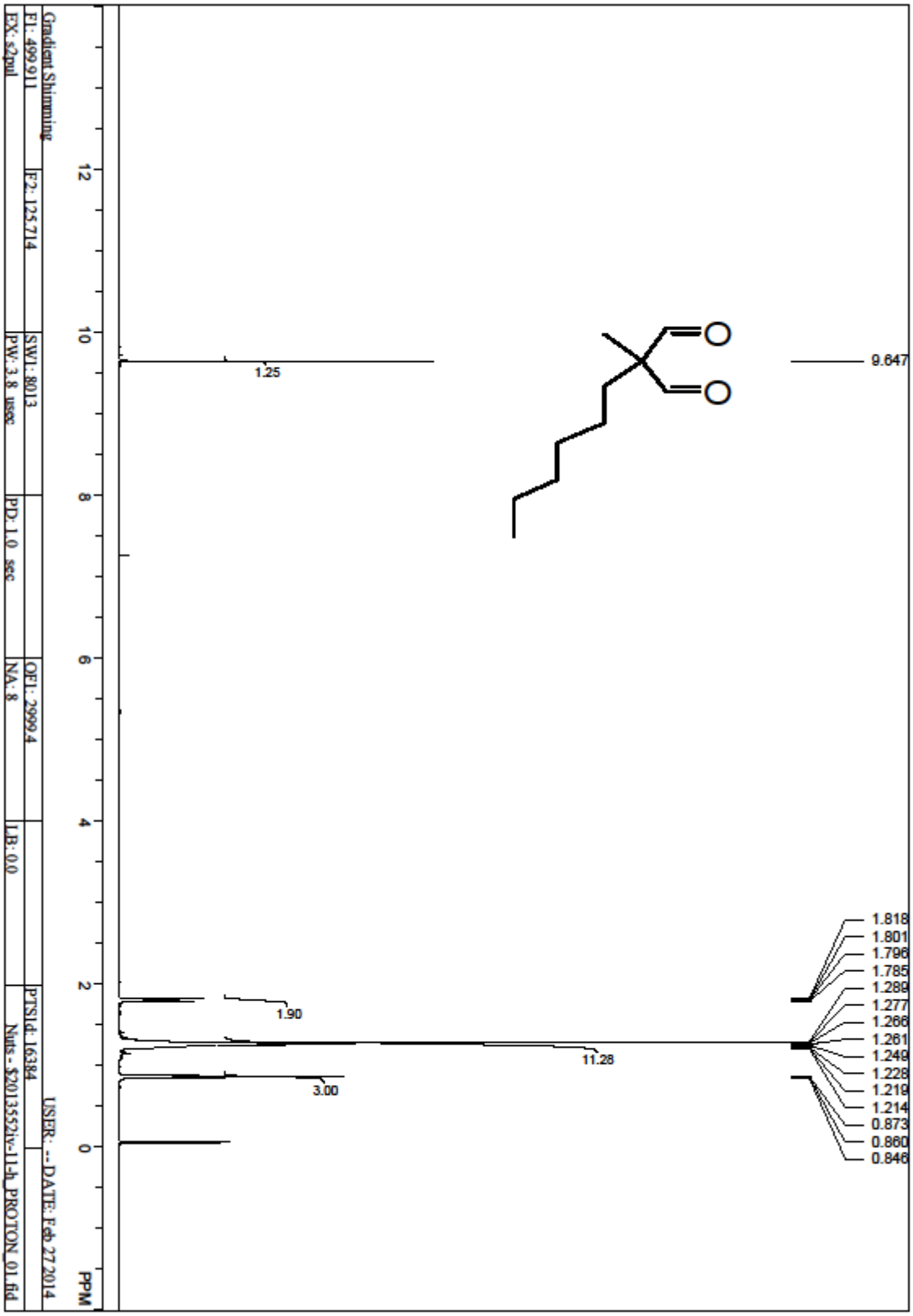

-113.504
O
O
F
0
-50
-100
-150
PPM
2013552V-ALDEHYDE-F^
USER: -- DATE: Aug 11 2014
F1: 376.057
F2: 100.513
SW1: 89286
OF1: -31967.5
PTS1d: 65536 , 65536
EX: s2pul
PW: 5.4 us
PD: 1.0 sec
NA: 16
LB: 0.0
Nuts - $FLUORINE_01.fid

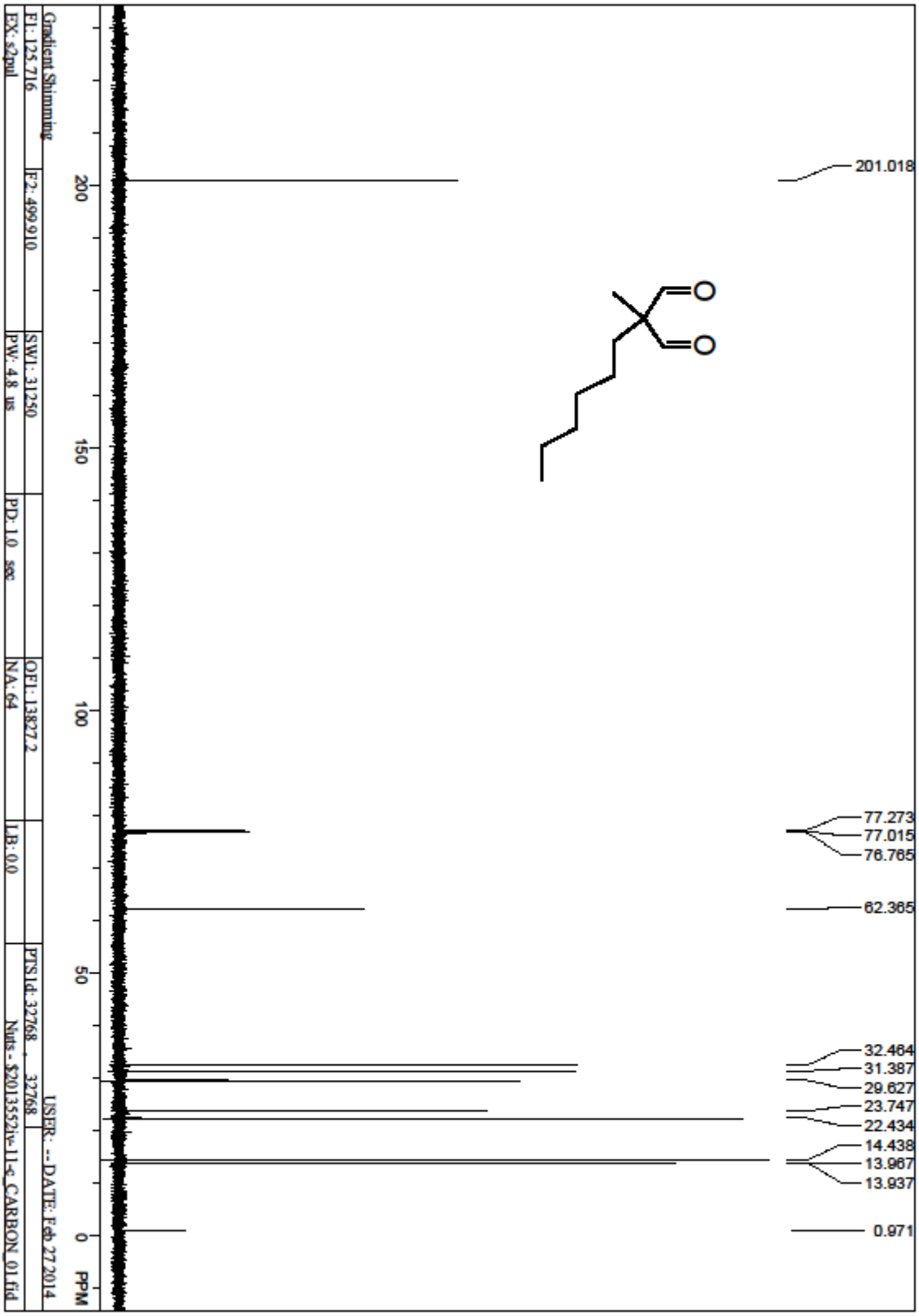

Gradient Shimming
F1: 499.911
F2: 125.714
SW1: 8013
PW: 3.8 usec
PD: 1.0 sec
OF1: 2999.4
NA: 8
LB: 0.0
PTS1d: 16384
USER: -- DATE: May 9 2014
EX: s2pul
Nuts - $iv-94-c_pslabel_01.fid
PPM
12
10
8
6
4
2
0
9.723
6.954
6.937
6.851
6.847
6.835
6.830
6.751
6.746
3.886
1.663
1.59
6.10
3.00
0.91
0.87

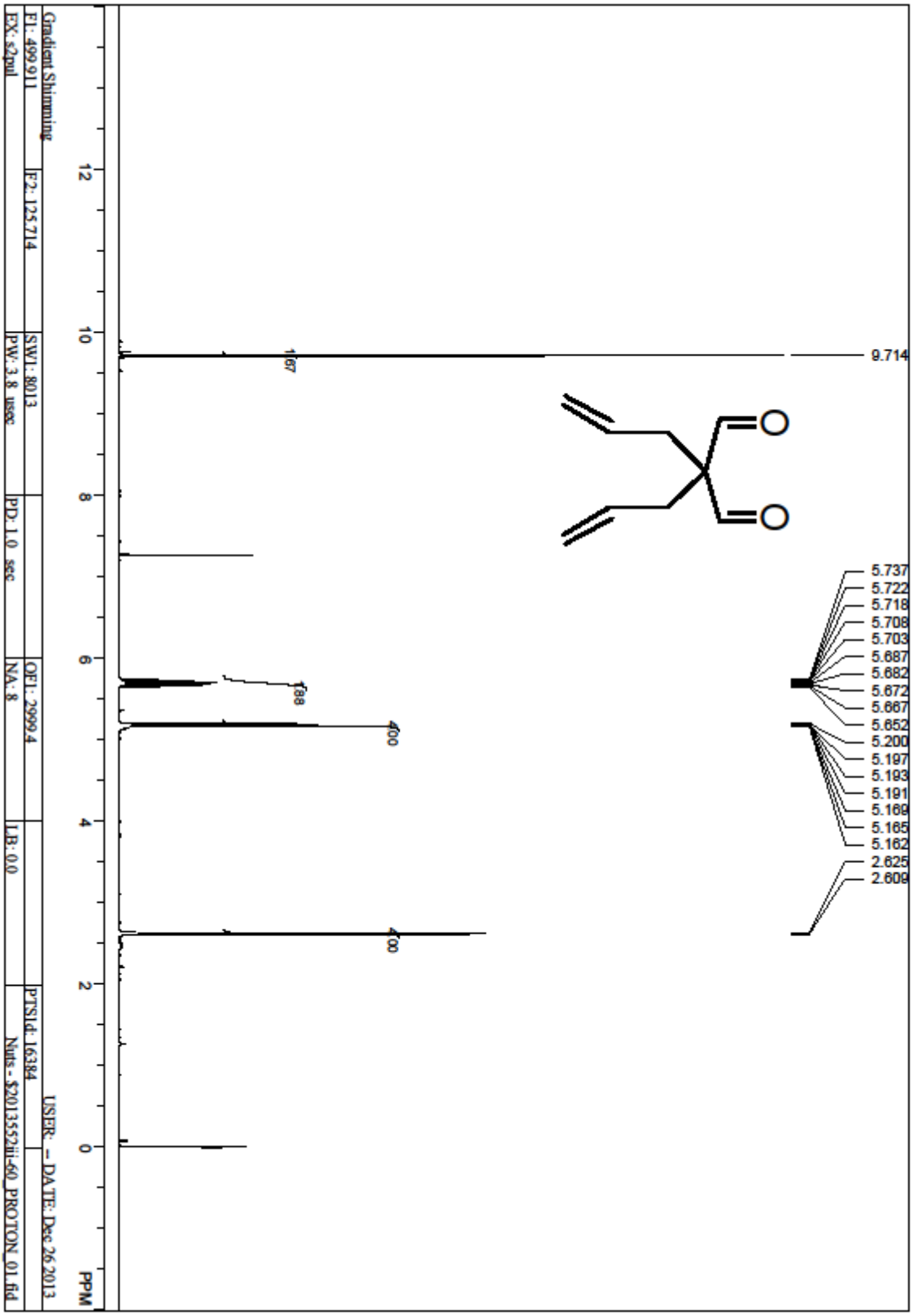

198.097
149.919
149.502
124.935
120.087
111.878
110.239
77.311
77.053
76.803
65.392
56.022
55.954
13.960
200
150
100
50
0
PPM

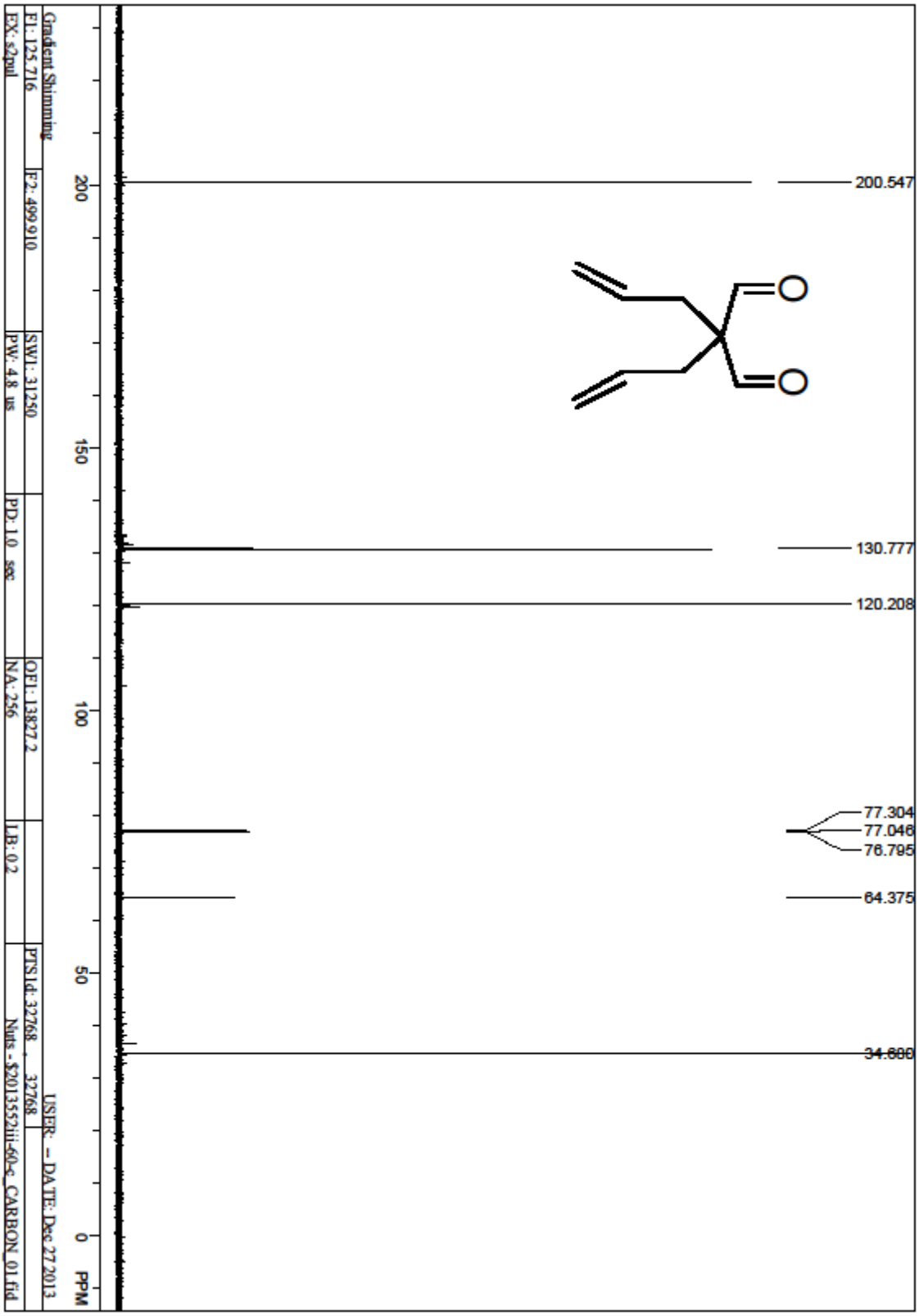

Gradient Shimming!y
FI: 499911
F2: 125.714
EX: s2pul
SW1: 8013
PW: 3.8 usec
PD: 1.0 sec
OF1: 2999.4
NA: 8
LB: 0.0
PTS1d: 16384
USER: --DATE: Feb 28 2014
Nuts - $ky-17-c_PROTON_01.fid
PPM
12
10
8
6
4
2
0
1.54
3.81
1.99
1.89
2.74
Ph
O
O
9.711
7.308
7.295
7.280
7.270
7.267
7.254
7.113
7.099
3.172
1.298

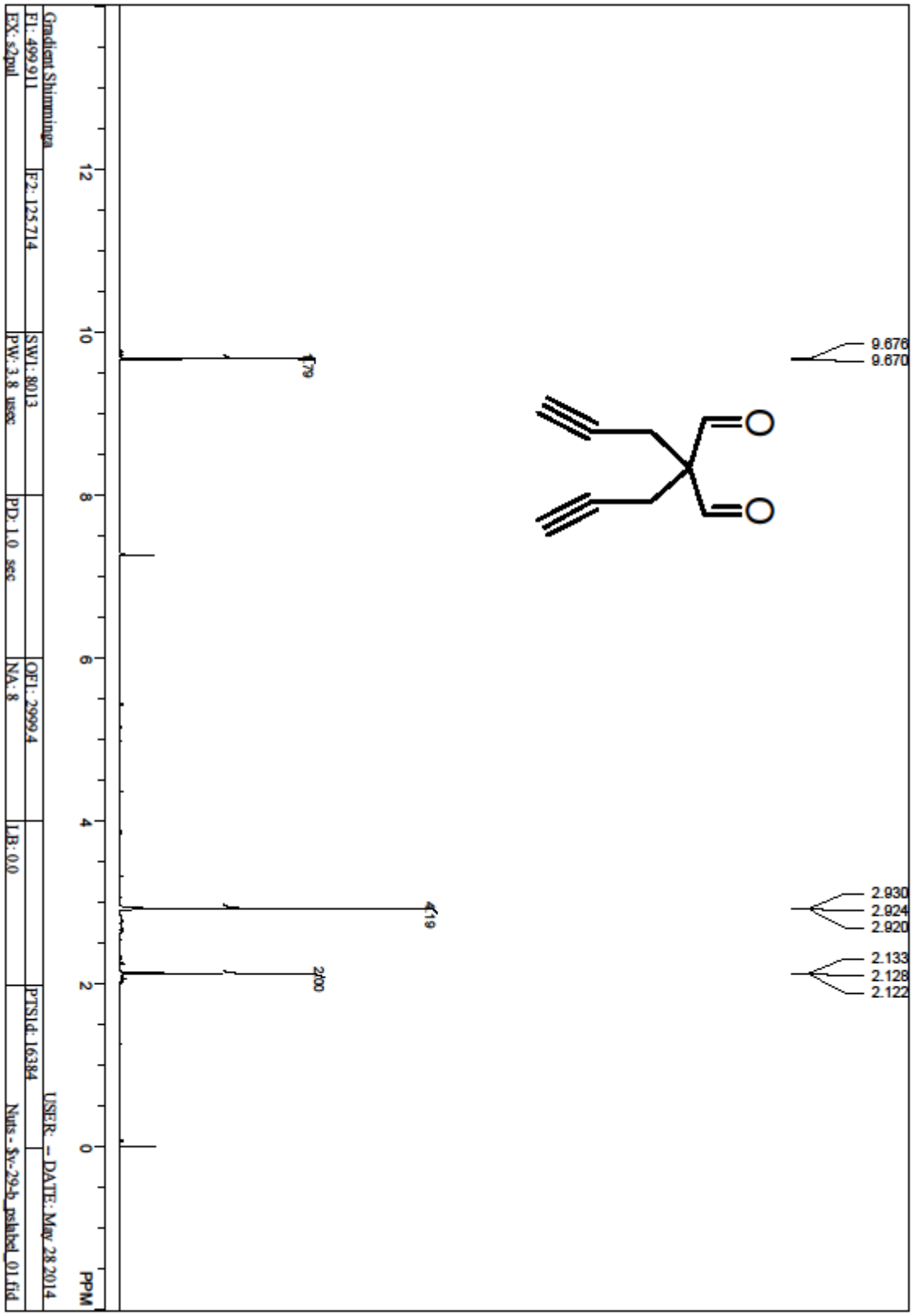

200.669
134.548
130.072
128.653
127.264
77.326
77.289
77.076
77.038
76.818
76.788
63.048
38.549
14.938
Ph
O
O
200
150
100
50
0
PPM
2013552iv-17-c
EL: 125.716
F2: 499.910
SW1: 31250
PW: 4.8 us
PD: 1.0 sec
NA: 64
QF1: 13827.2
LB: 0.0
PTS1d: 32768
32768
USER: --DATE: Feb 28 2014
EX: s2pul
Nuts - $iv-17-c_CARBON_01.fid

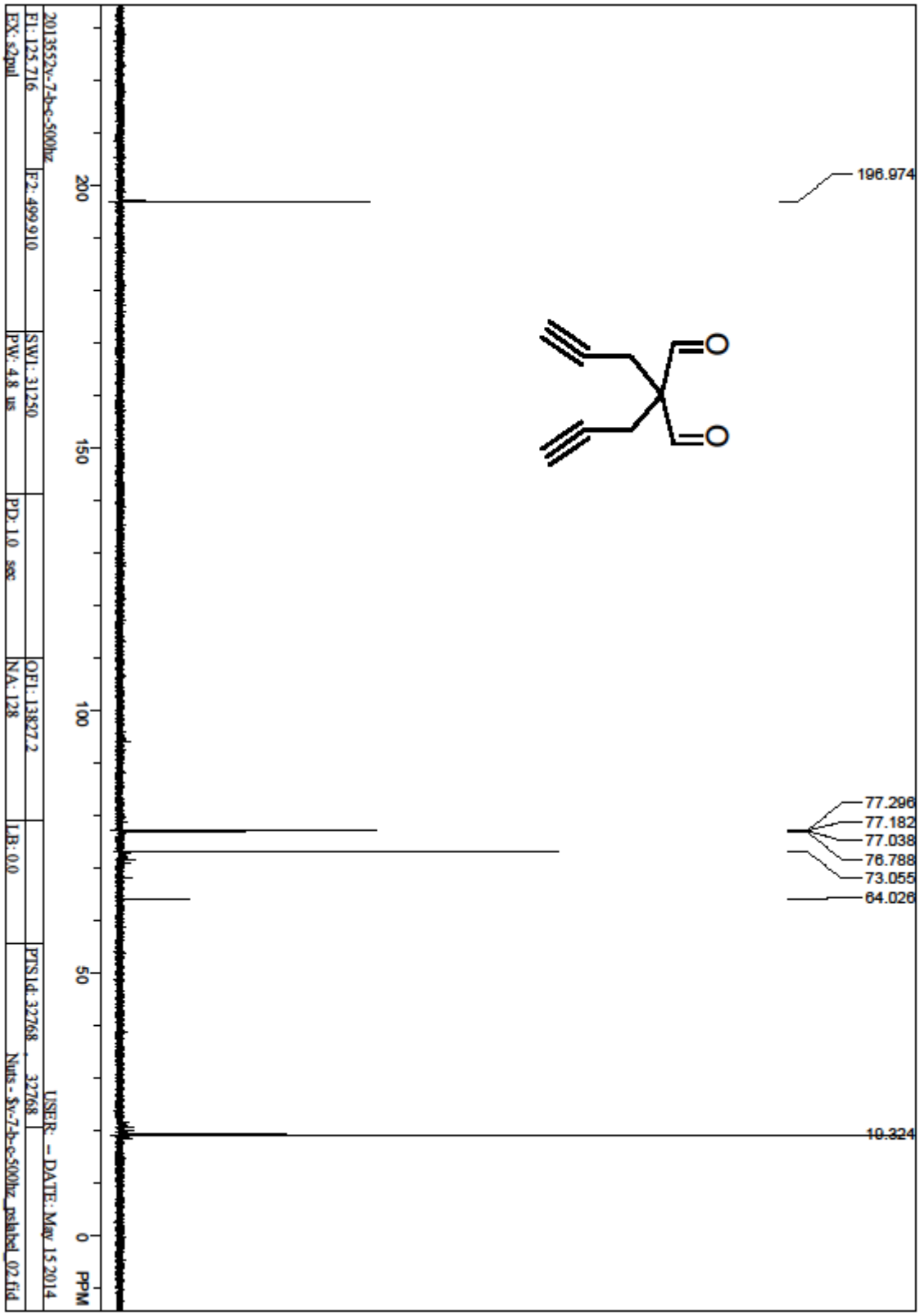

Gradient Shimming
EL: 499911
F2: 125.714
SW1: 8013
PW: 3.8 usec
PD: 1.0 sec
OF1: 2999.4
NA: 8
LB: 0.0
PTS1d: 16384
USER: --DATE: Feb 27 2014
EX: s2pul
Nuts - $20135521v-11-h_PROTON_01.fid
PPM
12
10
8
6
4
2
0
1.25
9.647
1.90
11.28
3.00
1.818
1.801
1.796
1.785
1.289
1.277
1.266
1.261
1.249
1.228
1.219
1.214
0.873
0.860
0.846

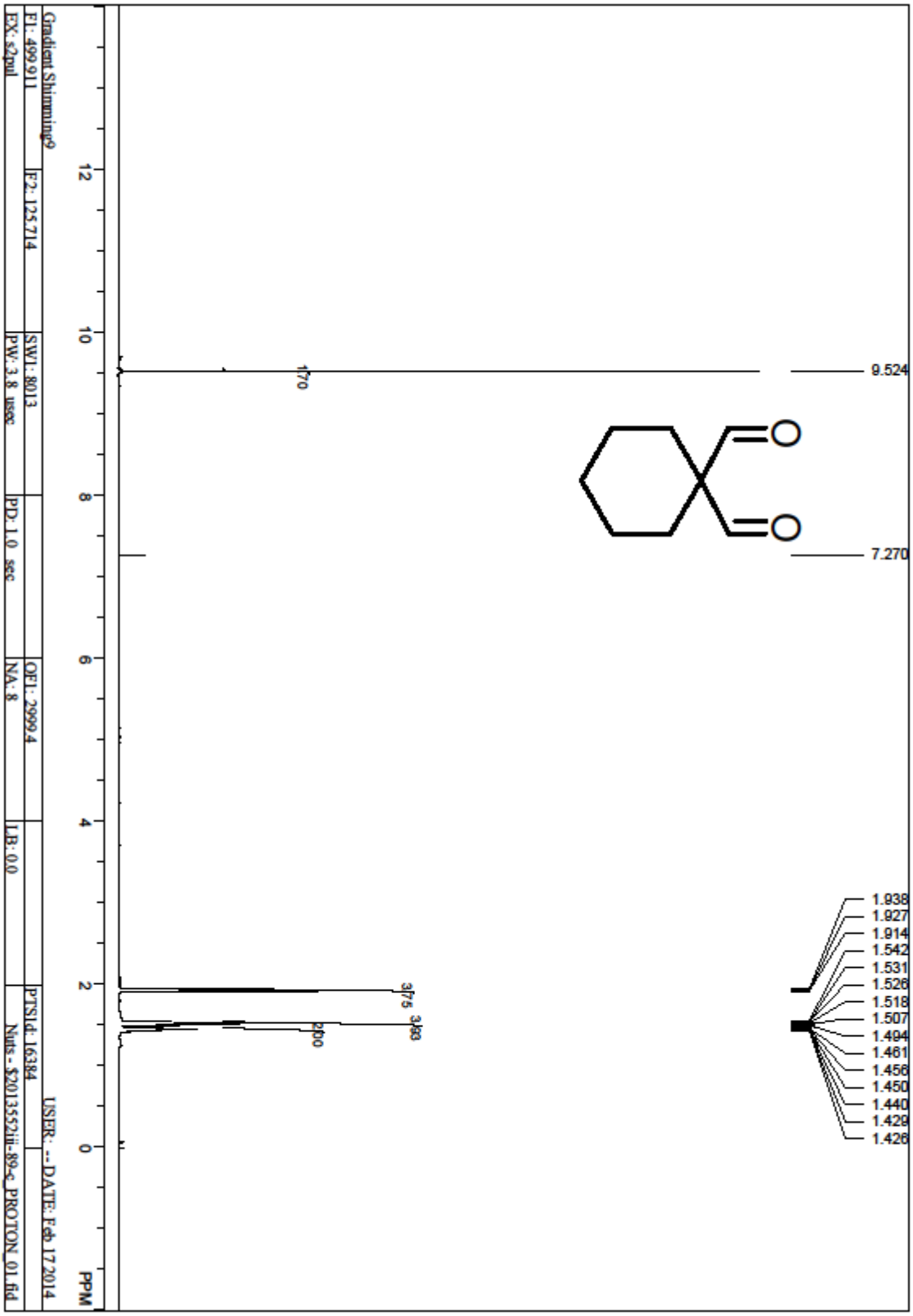

Gradient Shimming
F1: 125.716
F2: 499.910
SW1: 31250
PW: 4.8 us
PD: 1.0 sec
NA: 64
OF1: 13827.2
LB: 0.0
PTS1d: 32768
32768
USER: --DATE: Feb 27 2014
EX: s2pul
Nuts - $20135521ve-11-c_CARBON_01.fid
201.018
77.273
77.015
76.765
62.365
32.464
31.387
29.627
23.747
22.434
14.438
13.967
13.937
0.971
200
150
100
50
0
PPM

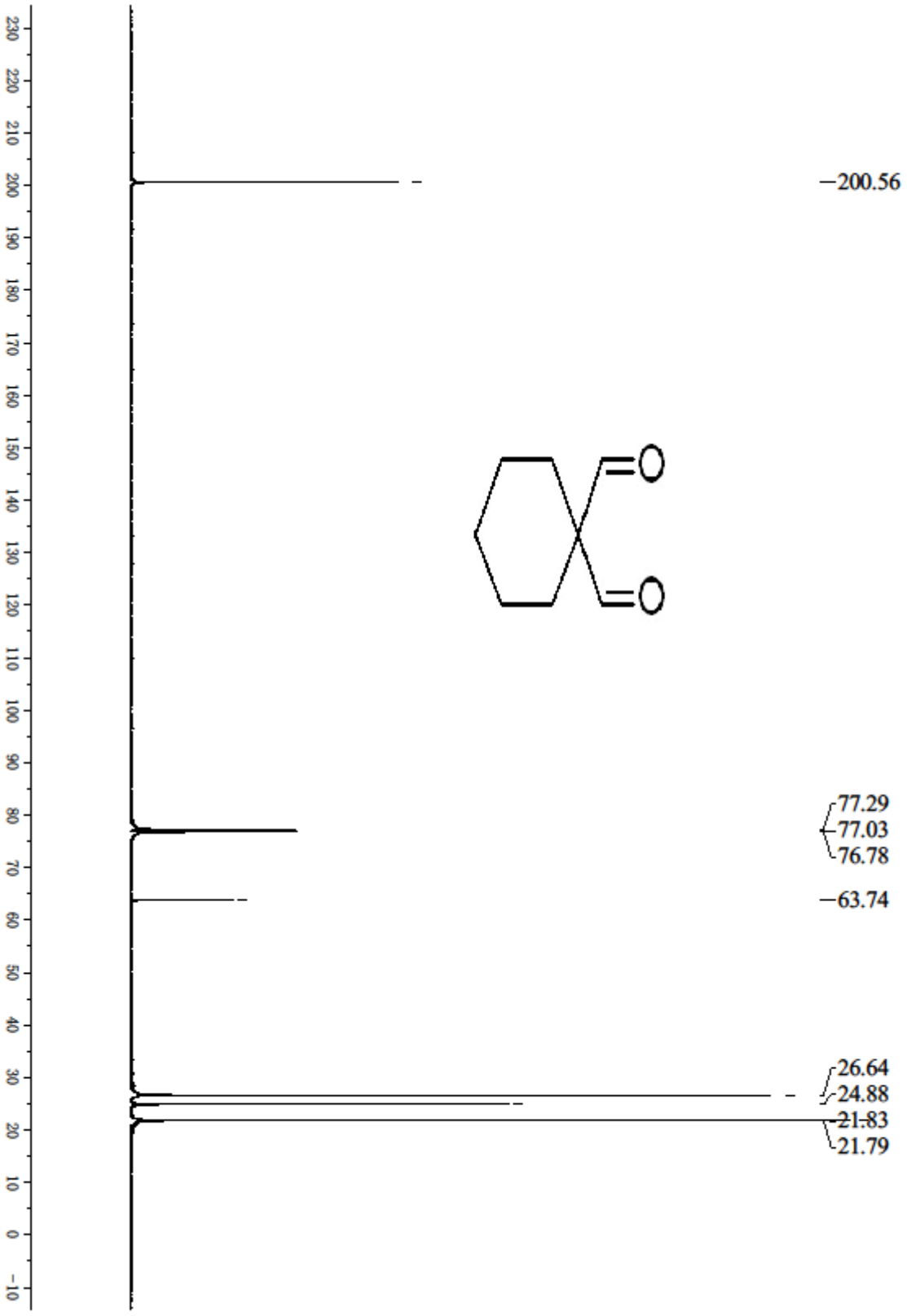

9.714
5.737
5.722
5.718
5.708
5.703
5.687
5.682
5.672
5.667
5.652
5.200
5.197
5.193
5.191
5.169
5.165
5.162
2.625
2.609
1.67
1.88
4.00
4.00
12
10
8
6
4
2
0
PPM
Gradient Shimming
F1: 499.911
F2: 125.714
SW1: 8013
PW: 3.8 usec
PD: 1.0 sec
OF1: 29994
NA: 8
LB: 0.0
PTS1d: 16384
USER: -- DATE: Dec 26 2013
EX: s2pul
Nuts - $20135528ii-60_PROTON_01.fid

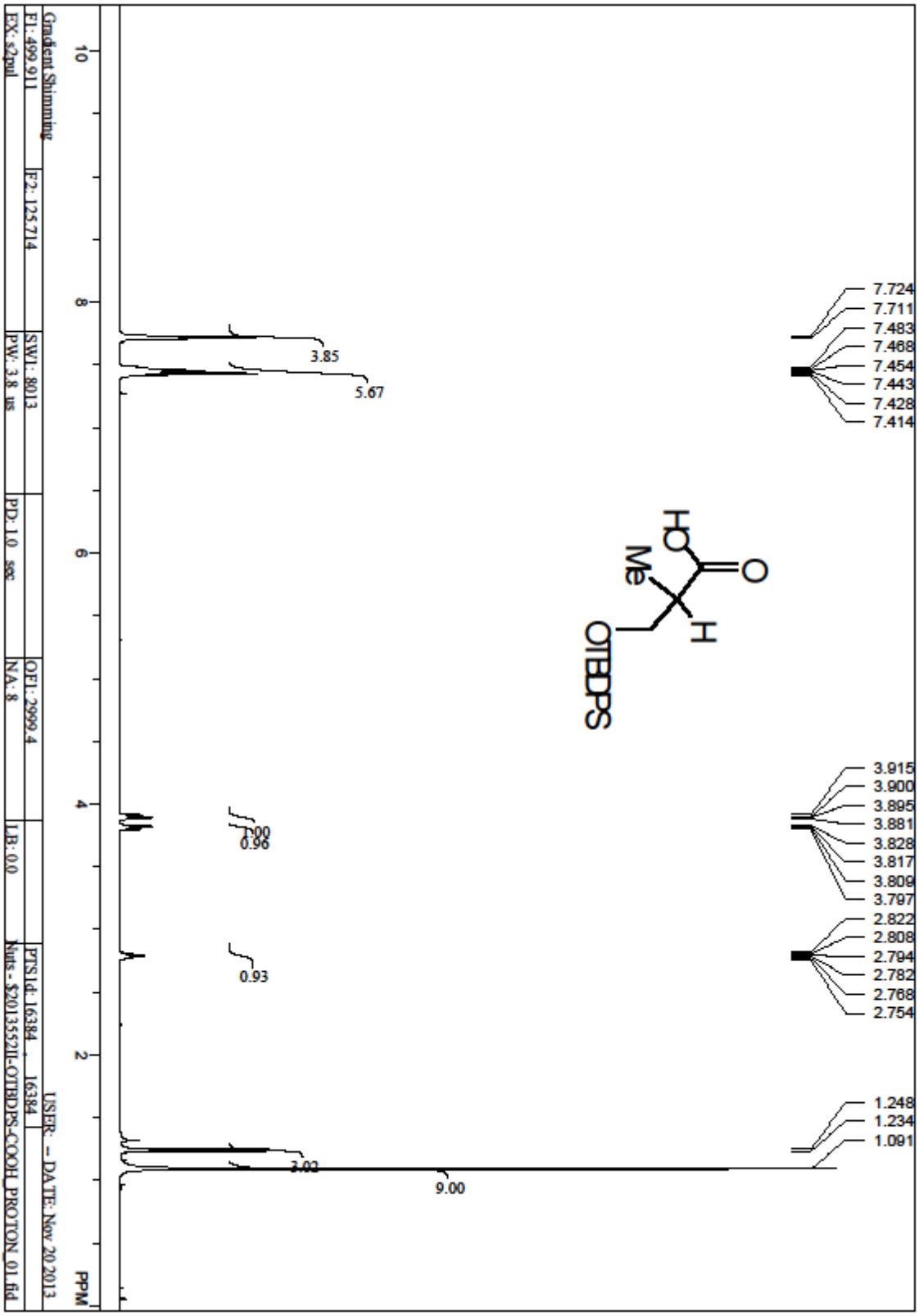

Gradient Shimming
F1: 125.716
F2: 499.910
SW1: 31250
PW: 4.8 us
PD: 1.0 sec
OF1: 13827.2
NA: 256
LB: 0.2
PTS1d: 32768
Nuts - $20135521iii-60-c_CARBON_01.fid
USER: -- DATE: Dec 27 2013
EX: s2pul
200.547
130.777
120.208
77.304
77.046
76.795
64.375
34.680
200
150
100
50
0
PPM

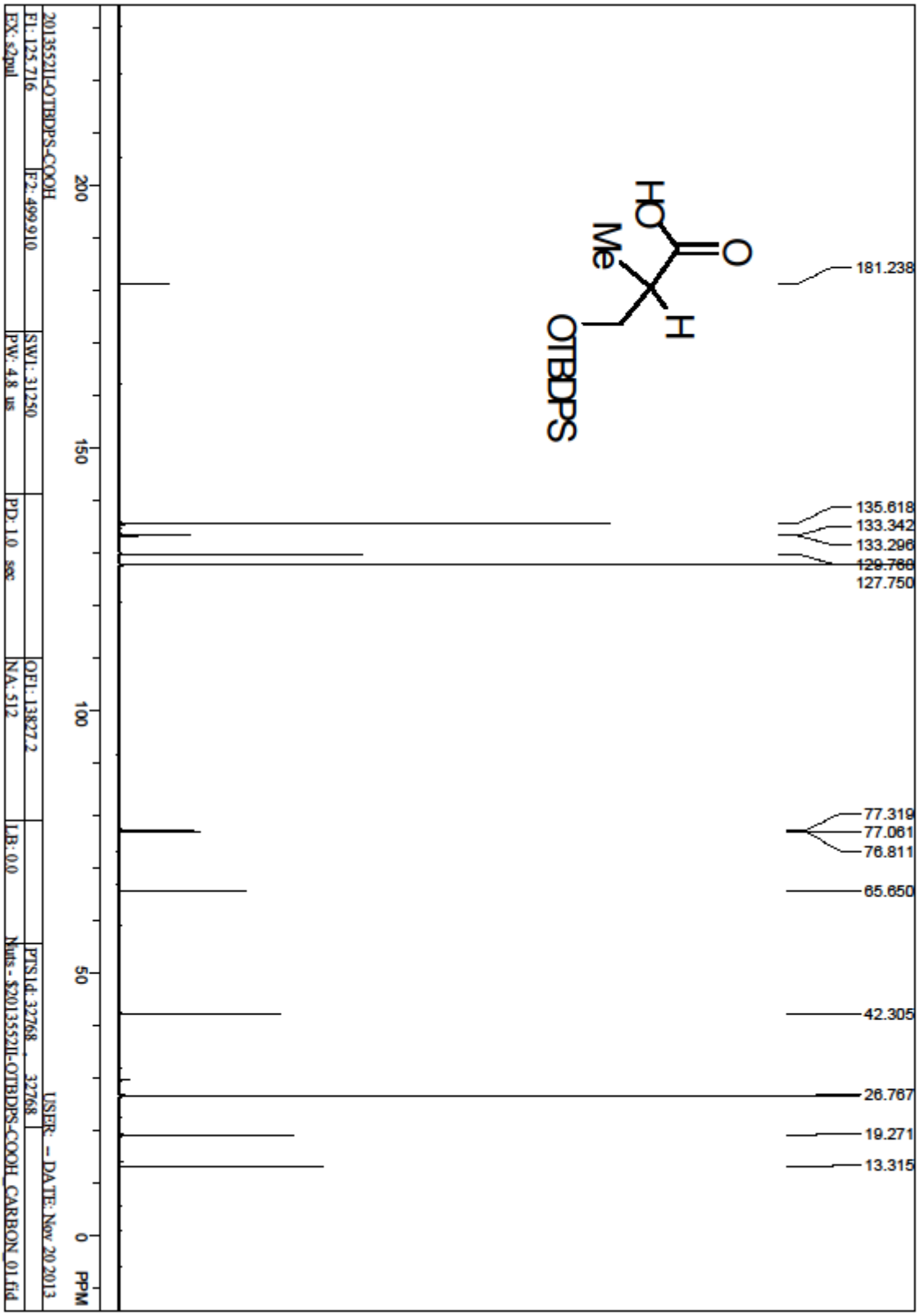

9.676
9.670
2.930
2.924
2.920
2.133
2.128
2.122
1.79
4.19
2.00
12
10
8
6
4
2
0
PPM
Gradient Shimming
F1: 499.911
F2: 125.714
SW1: 8013
PW: 3.8 usec
PD: 1.0 sec
OF1: 2999.4
NA: 8
LB: 0.0
PTS1d: 16384
USER: -- DATE: May 28 2014
EX: s2pul
Nuts--$v-29-b_pslabel_01.fid

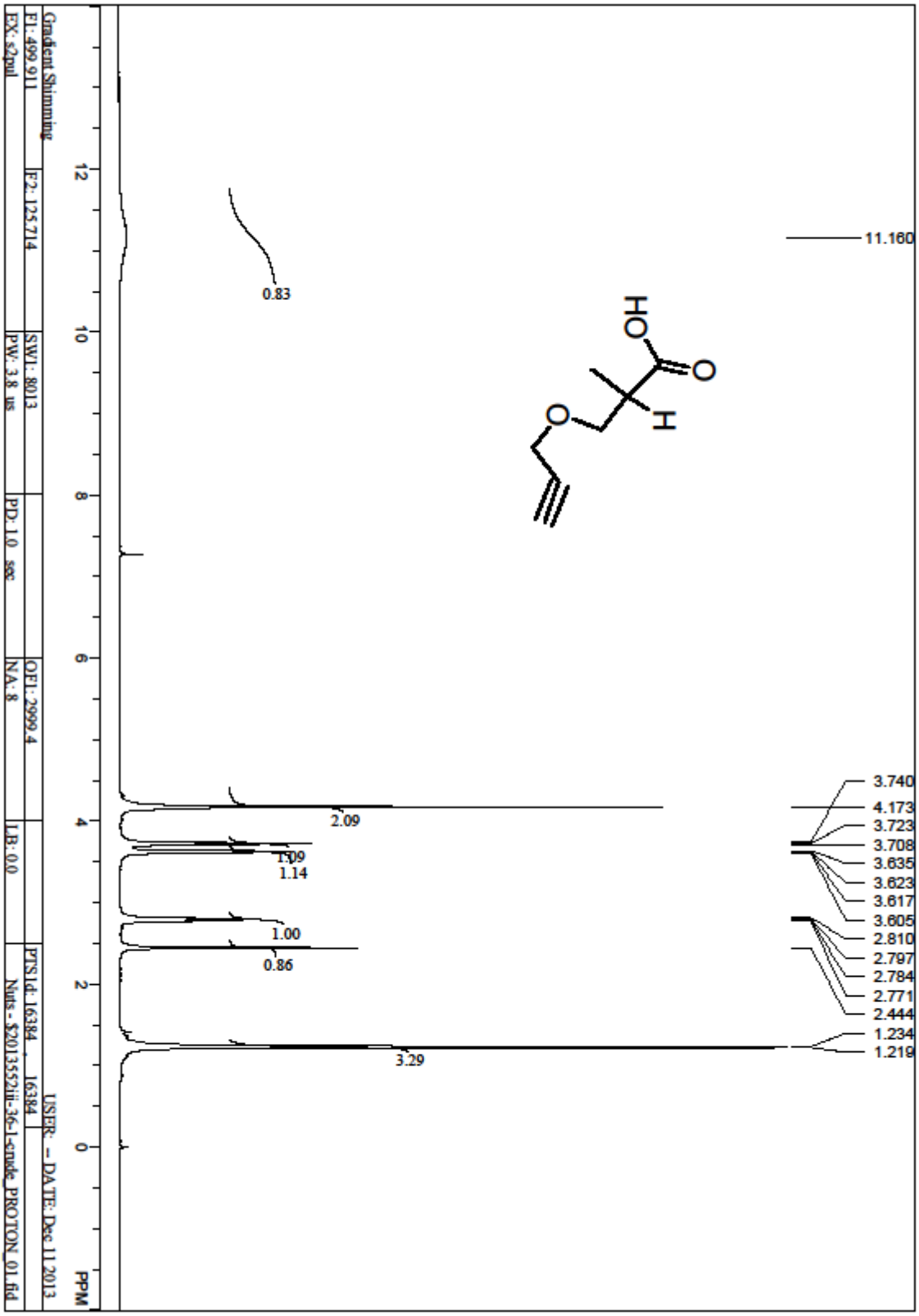

196.974
77.296
77.182
77.038
76.788
73.055
64.026
10.324
200
150
100
50
0
PPM
2013552v-7-bc-500hz
F1: 125.716
F2: 499.910
SW1: 31250
PW: 4.8 us
PD: 1.0 sec
QF1: 13827.2
NA: 128
LB: 0.0
PTS1d: 32768 _ 32768
EX: s2pul
USER: – DATE: May 15 2014
Nitts - $v-7-bc-500hz_pslabel_02.fid

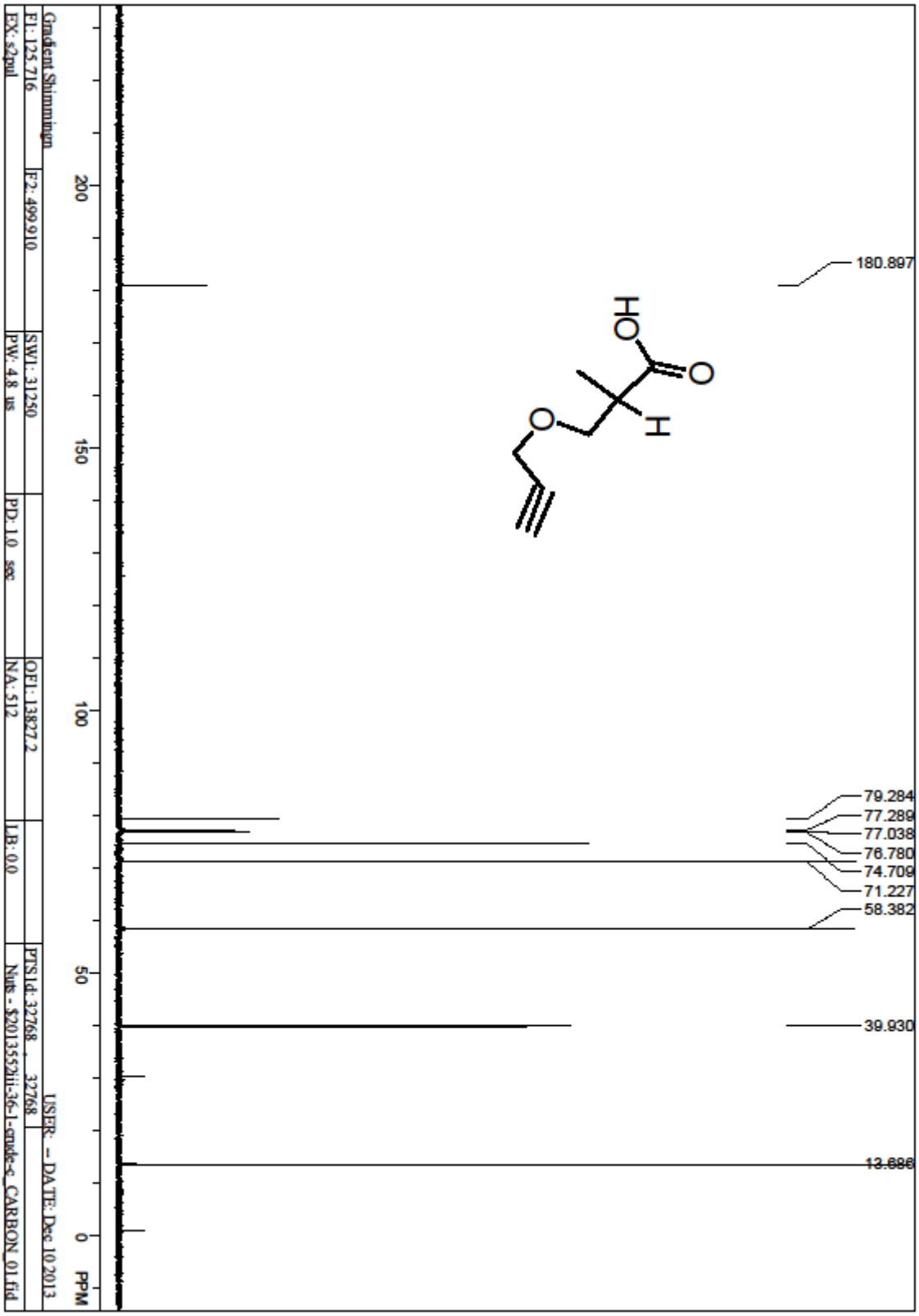

Gradient Shimming9
F1: 499.911
F2: 125.714
SW1: 8013
PW: 3.8 usec
PD: 1.0 sec
OF1: 2999.4
NA: 8
PTS1d: 16384
LB: 0.0
USER: --DATE: Feb 17 2014
Nuts--$20135521ii-89-c_PROTON_01.fid
EX: s2pul
PPM
12
10
8
6
4
2
0
9.524
7.270
1.938
1.927
1.914
1.542
1.531
1.526
1.518
1.507
1.494
1.461
1.456
1.450
1.440
1.429
1.426
1.70
3.75
3.69
2.00

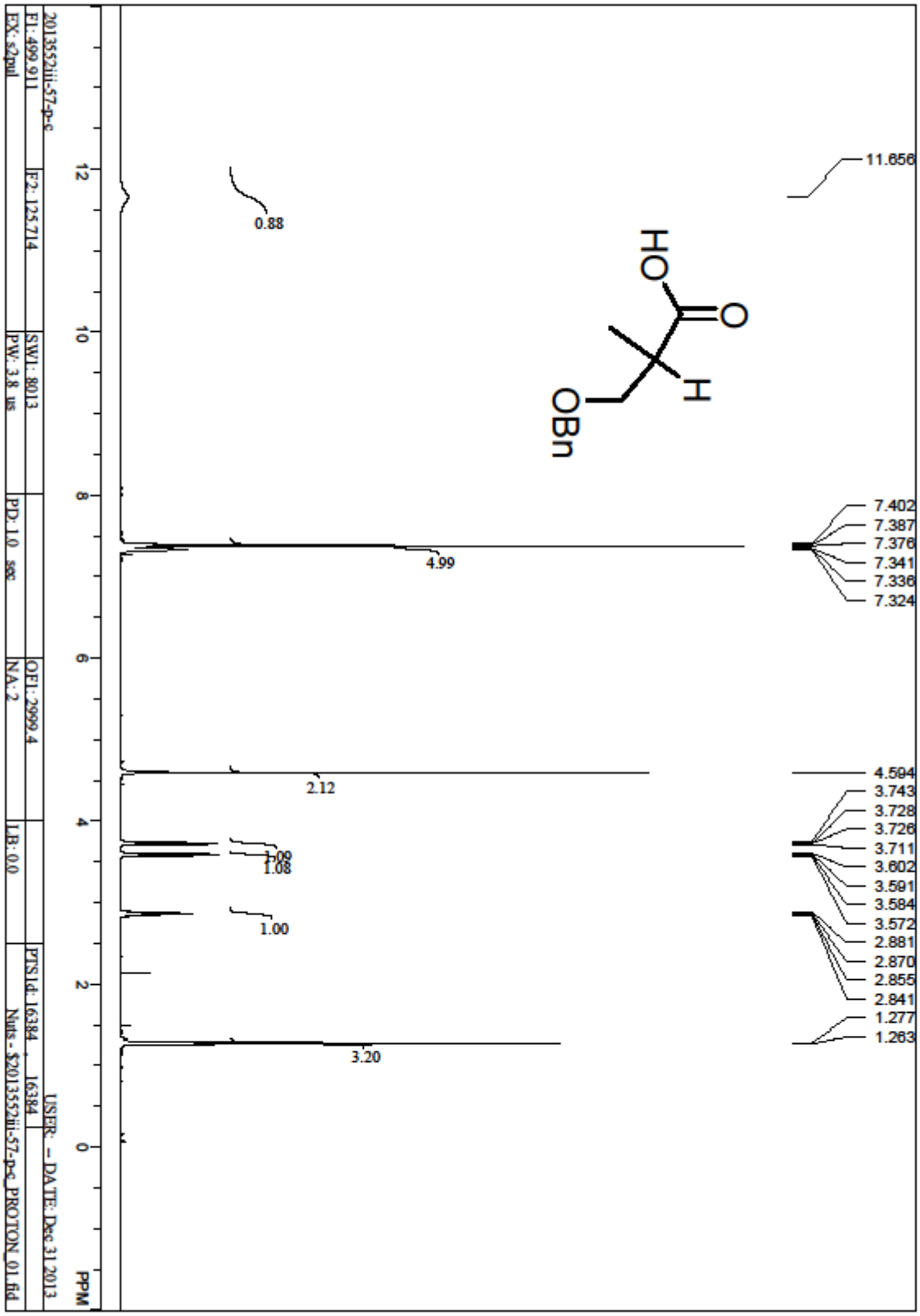

200.56
77.29
77.03
76.78
63.74
26.64
24.88
21.83
21.79

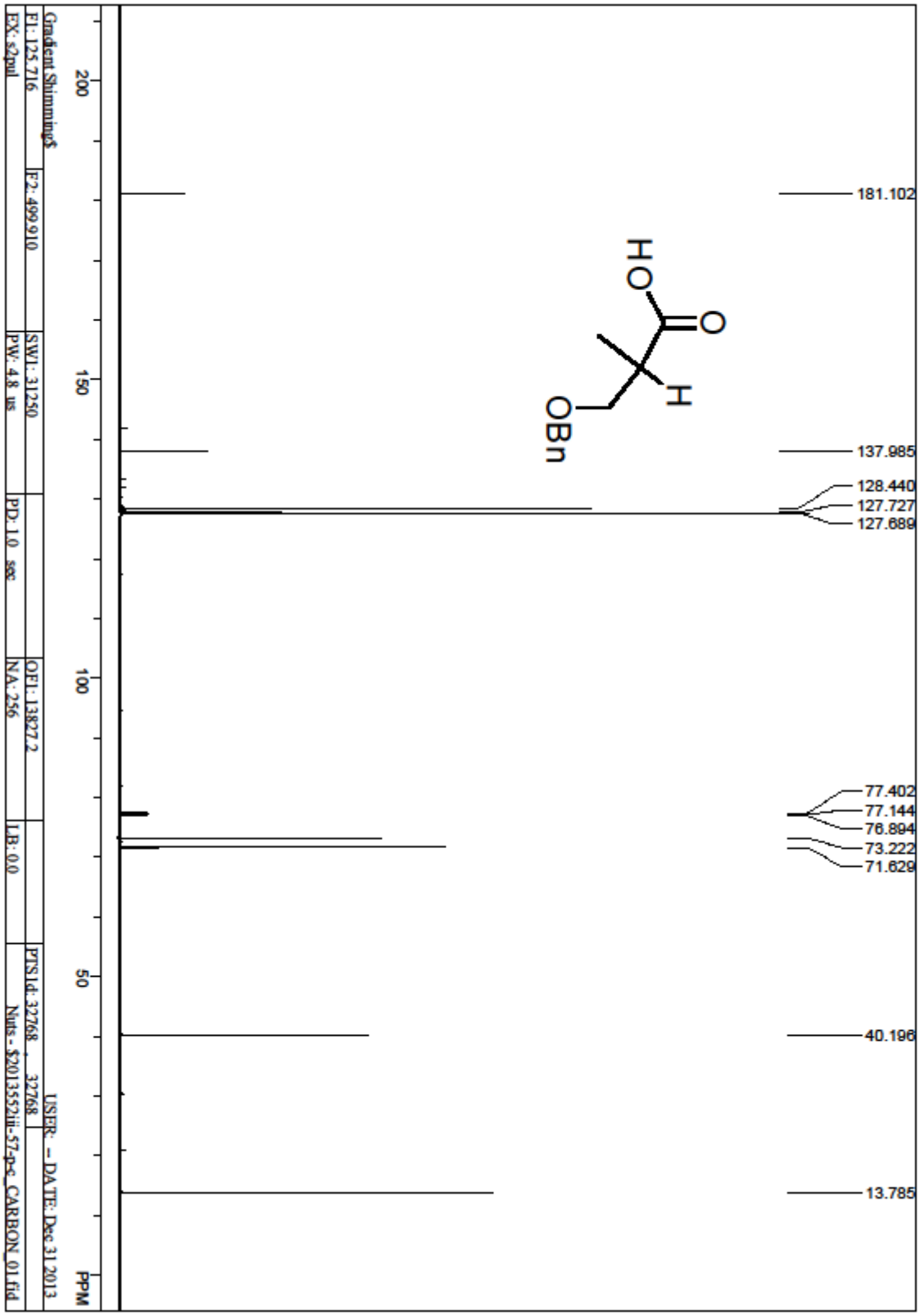

Gradient Shimming
F1: 499.911
F2: 125.714
SW1: 8013
PW: 3.8 us
PD: 1.0 sec
OF1: 2999.4
NA: 8
LB: 0.0
PTS1d: 16384
16384
EX: s2pul
USER: -- DATE: Nov 20 2013
Nuts - $20135521L-OTBDPS-COOH_PROTON_01.fid
PPM
10
8
6
4
2
3.85
5.67
1.00
0.96
0.93
3.02
9.00
7.724
7.711
7.483
7.468
7.454
7.443
7.428
7.414
3.915
3.900
3.895
3.881
3.828
3.817
3.809
3.797
2.822
2.808
2.794
2.782
2.768
2.754
1.248
1.234
1.091
HO
O
Me
H
OTBDPS

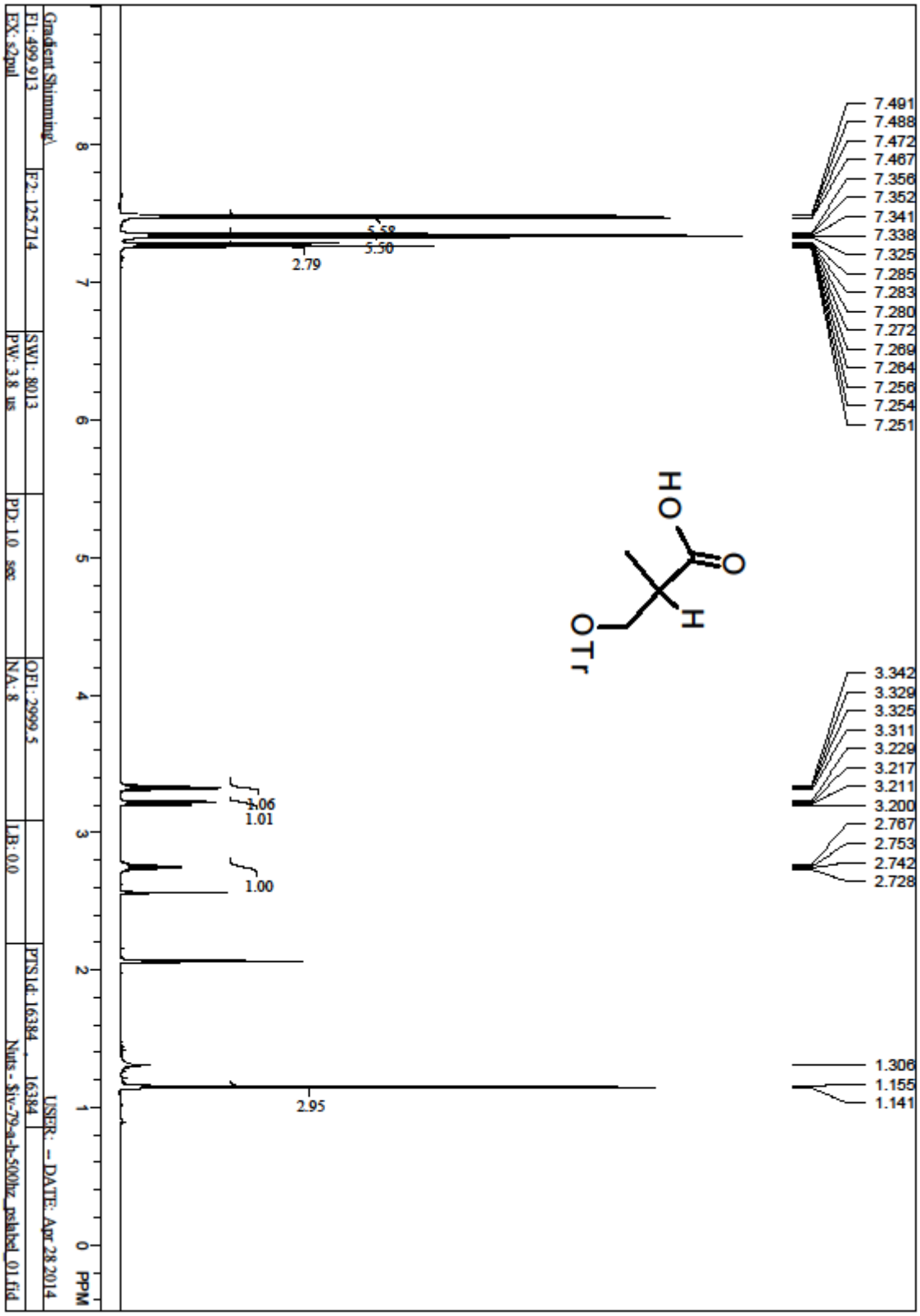

20135521I-OTBDPS-COOH
F1: 125.716
F2: 499.910
SW1: 31250
PW: 4.8 us
PD: 1.0 sec
OF1: 13827.2
NA: 512
LB: 0.0
PTS1d: 32768 → 32768
USER: -- DATE: Nov 20 2013
EX: s2pul
Nuts - $20135521I-OTBDPS-COOH_CARBON_01.fid
HO
O
Me
H
OTBDPS
181.238
135.618
133.342
133.296
129.766
127.750
77.319
77.061
76.811
65.650
42.305
26.767
19.271
13.315
200
150
100
50
0
PPM

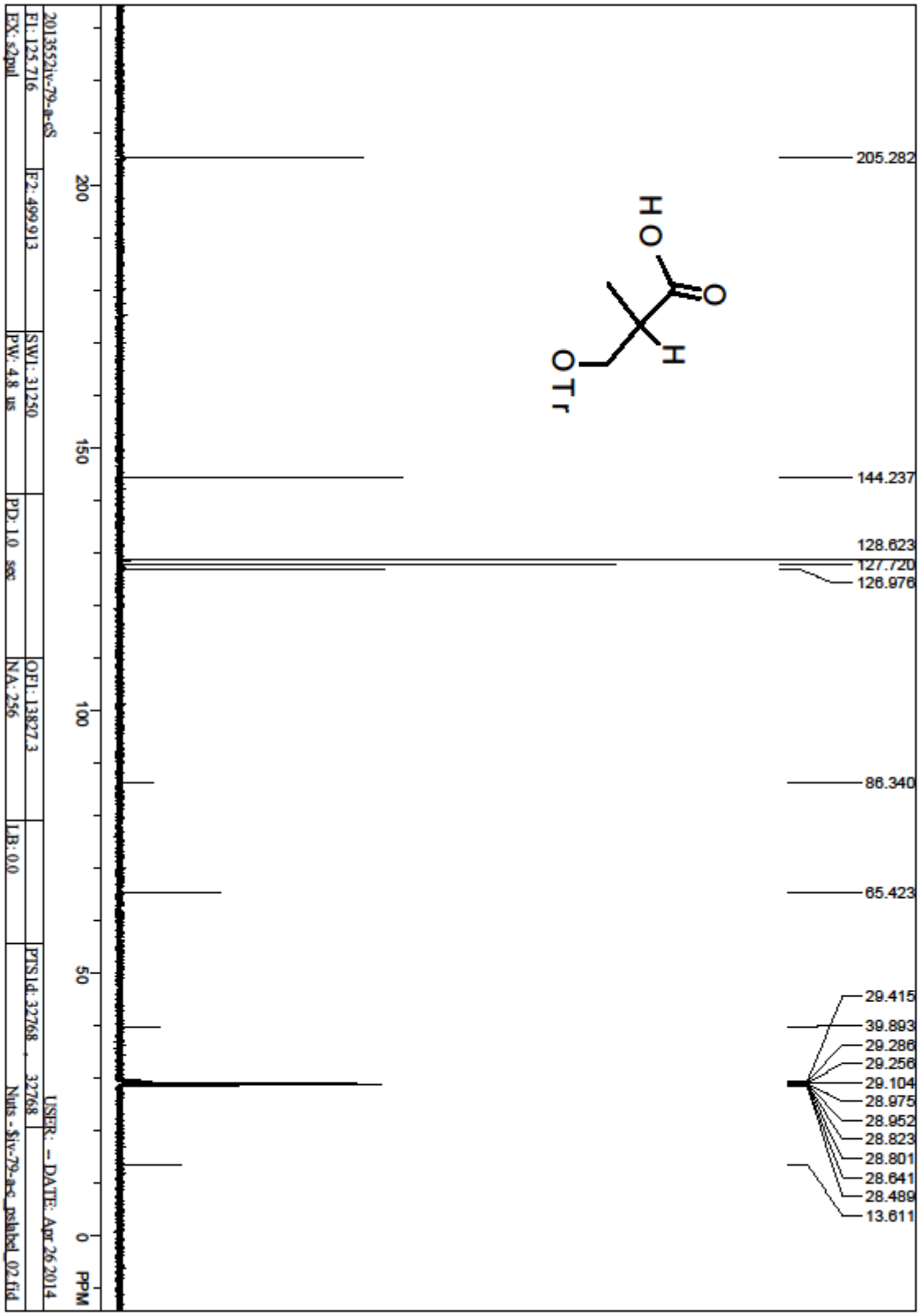

Gradient Shimming
EX: s2pul
F1: 499.911
F2: 125.714
PW: 3.8 us
SW1: 8013
PD: 1.0 sec
NA: 8
OF1: 2999.4
LB: 0.0
PTS1d: 16384
16384
Nuts - $20135521iii-36-1-cmde_PROTON_01.fid
USER: -- DATE: Dec 11 2013
PPM
0.83
11.160
2.09
1.09
1.14
1.00
0.86
3.29
3.740
4.173
3.723
3.708
3.635
3.623
3.617
3.605
2.810
2.797
2.784
2.771
2.444
1.234
1.219
HO
O
O
H

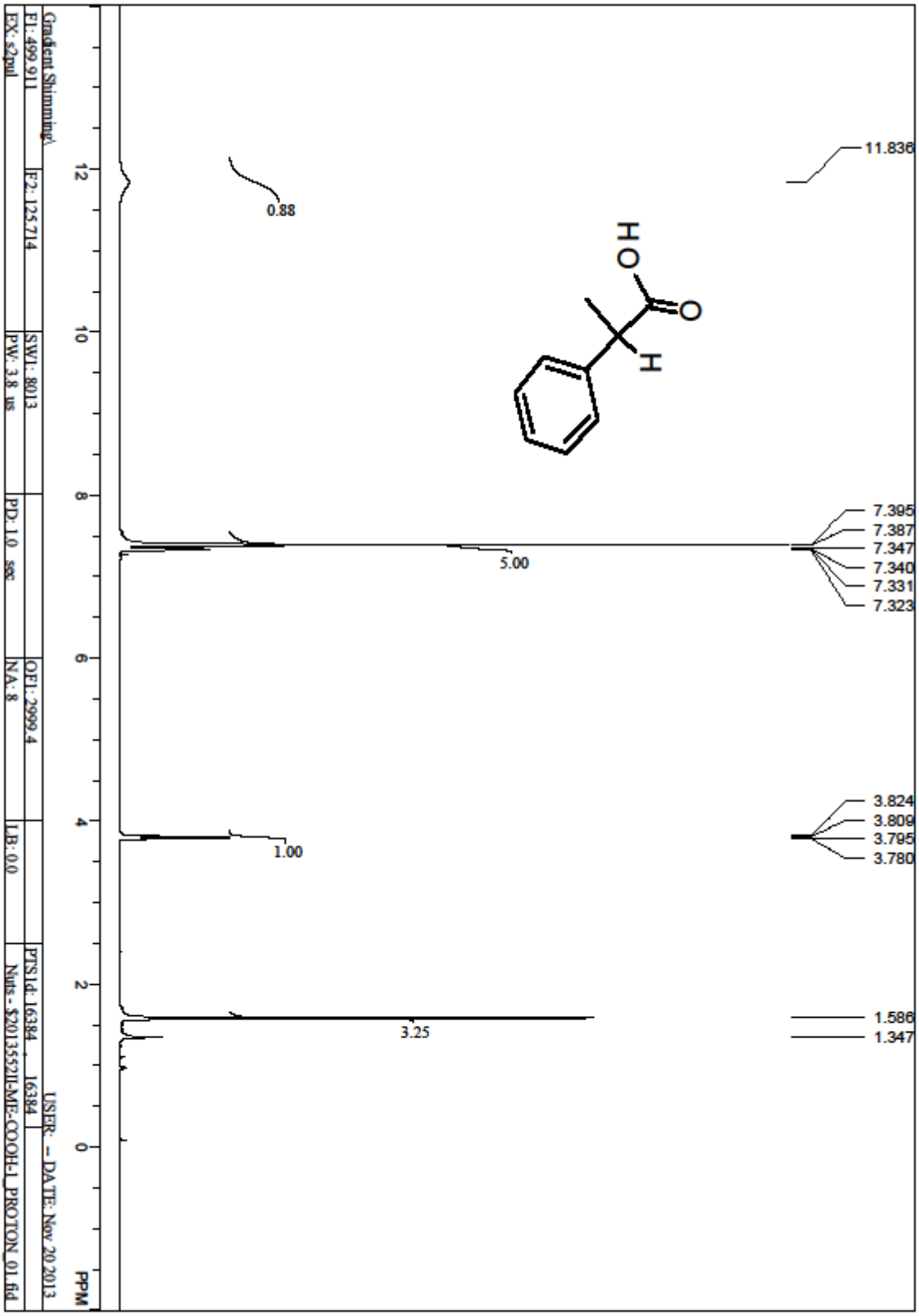

180.897
79.284
77.289
77.038
76.780
74.709
71.227
58.382
39.930
13.686
200
150
100
50
0
PPM
Gradient Shimming
F1: 125.716
F2: 499.910
SW1: 31250
PW: 4.8 us
PD: 1.0 sec
QF1: 13827.2
NA: 512
LB: 0.0
PTS1d: 32768 → 32768
EX: s2pul
Nuts - $20135520iii-36-1-crude-c_CARBON_01.fid
USER: -- DATE: Dec 10 2013

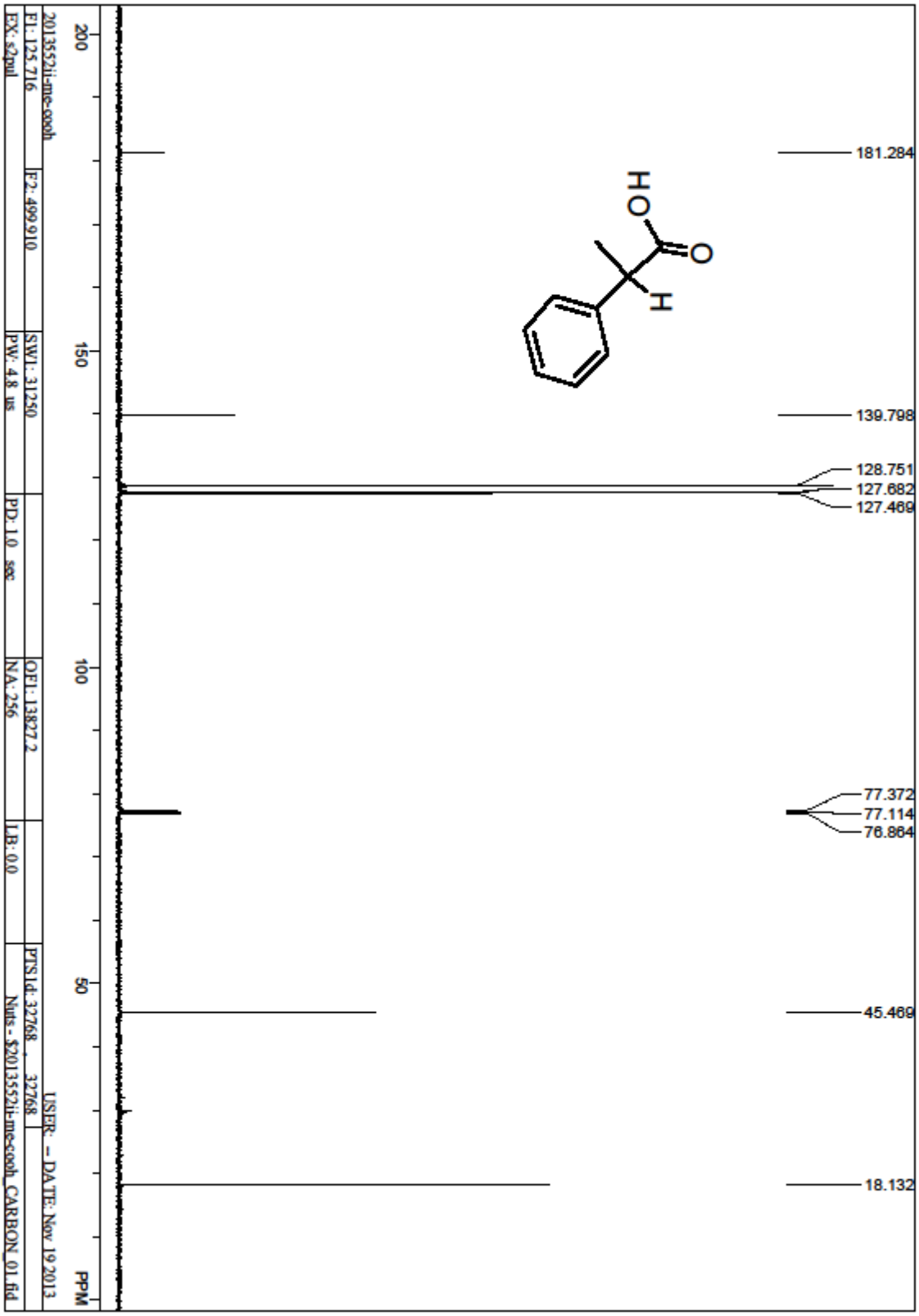

11.656
0.88
HO
O
H
OBn
7.402
7.387
7.376
7.341
7.336
7.324
4.99
4.594
3.743
3.728
3.726
3.711
3.602
3.591
3.584
3.572
2.881
2.870
2.855
2.841
1.277
1.263
2.12
1.09
1.08
1.00
3.20
PPM
20135521ii-57-pc-c
F1: 499.911
F2: 125.714
SW1: 8013
PW: 3.8 us
PD: 1.0 sec
OF1: 2999.4
NA: 2
LB: 0.0
PTS1d: 16384
16384
EX: s2pul
USER: -- DATE: Dec 31 2013
Nuts - $20135521ii-57-pc_PROTON_01.fid

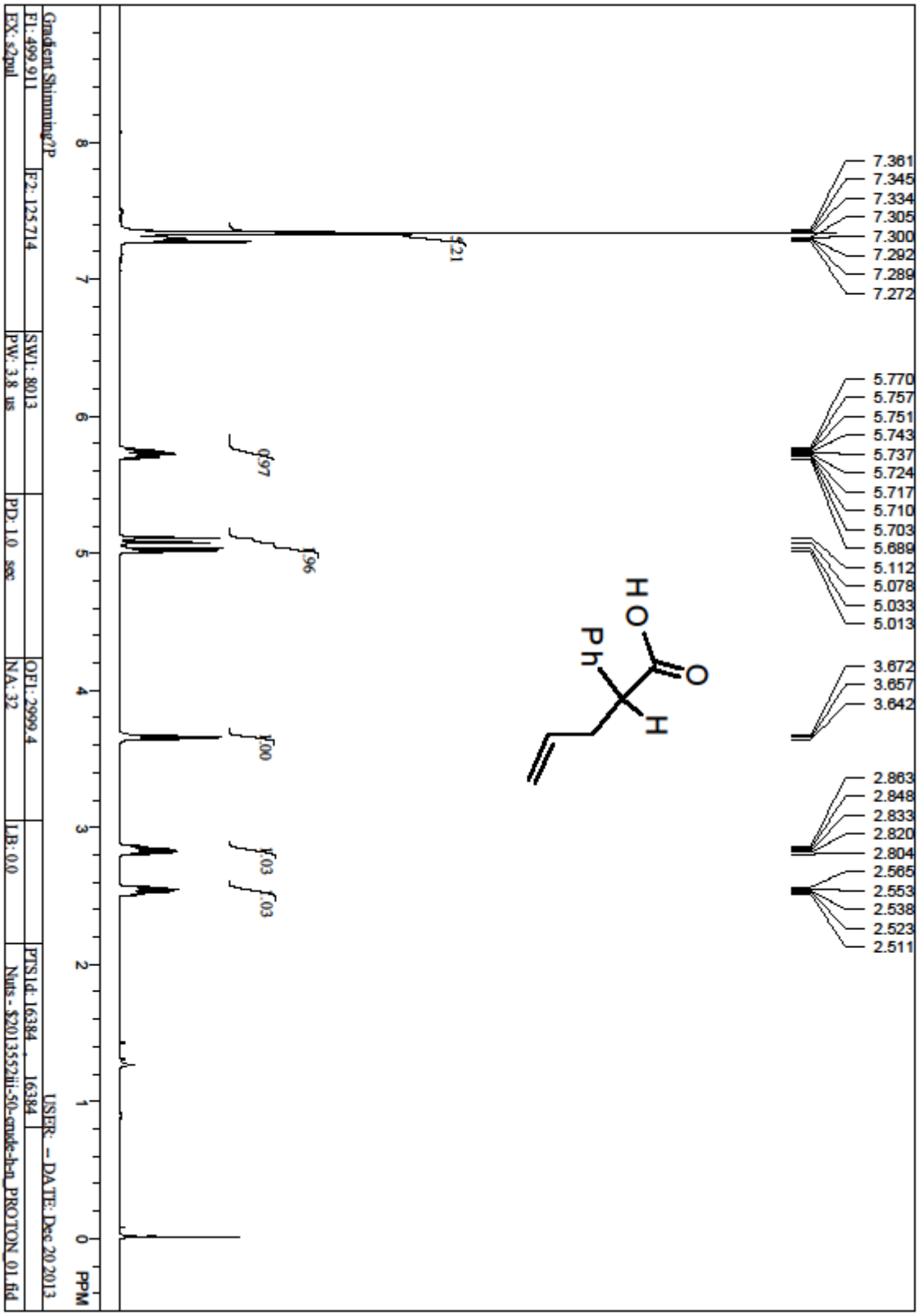

181.102
137.985
128.440
127.727
127.689
77.402
77.144
76.894
73.222
71.629
40.196
13.785
HO
O
H
OBn
200
150
100
50
PPM
Gradient Shimming$
F1: 125.716
F2: 499.910
EX: s2pul
SW1: 31250
PW: 4.8 us
PD: 1.0 sec
OF1: 13827.2
NA: 256
LB: 0.0
PTS1d: 32768
32768
USER: -- DATE: Dec 31 2013
Nuts - $20135521ii-57-pc_CARBON_01.fid

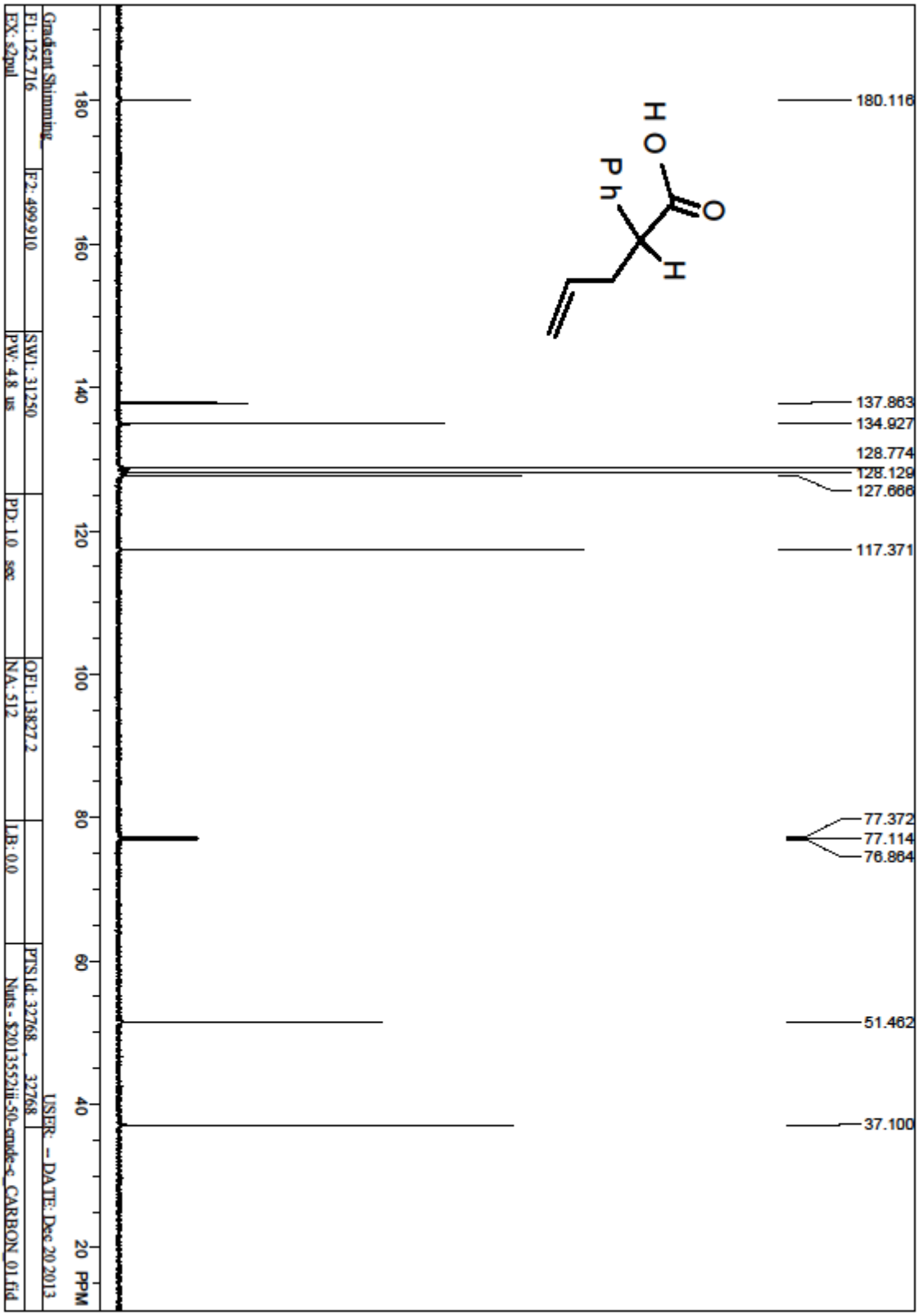

Gradient Shimming\
F1: 499.913
F2: 125.714
EX: s2pul
SW1: 8013
PW: 3.8 us
PD: 1.0 sec
OF1: 2999.5
NA: 8
LB: 0.0
PTS1d: 16384
16384
USER: -- DATE: Apr 28 2014
Nuts - Siv-79-a-hr-500hz_pslabel_01.fid
PPM
7.491
7.488
7.472
7.467
7.356
7.352
7.341
7.338
7.325
7.285
7.283
7.280
7.272
7.269
7.264
7.256
7.254
7.251
5.58
5.50
2.79
3.342
3.329
3.325
3.311
3.229
3.217
3.211
3.200
2.767
2.753
2.742
2.728
1.06
1.01
1.00
1.306
1.155
1.141
2.95
HO
O
H
OTr

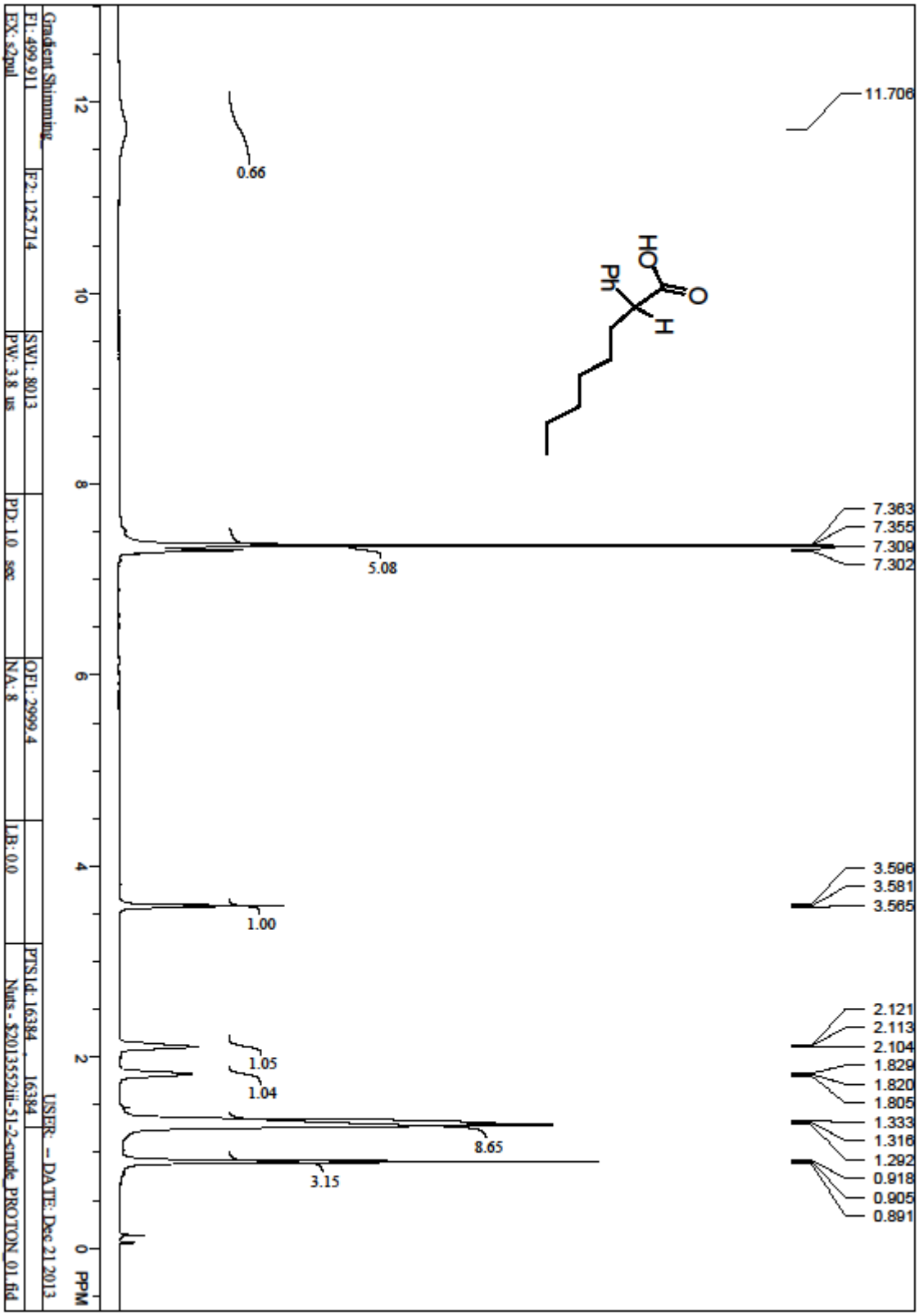

205.282
144.237
128.623
127.720
126.976
86.340
65.423
29.415
39.893
29.286
29.256
29.104
28.975
28.952
28.823
28.801
28.641
28.489
13.611
HO
O
H
OTr
200
150
100
50
0
PPM

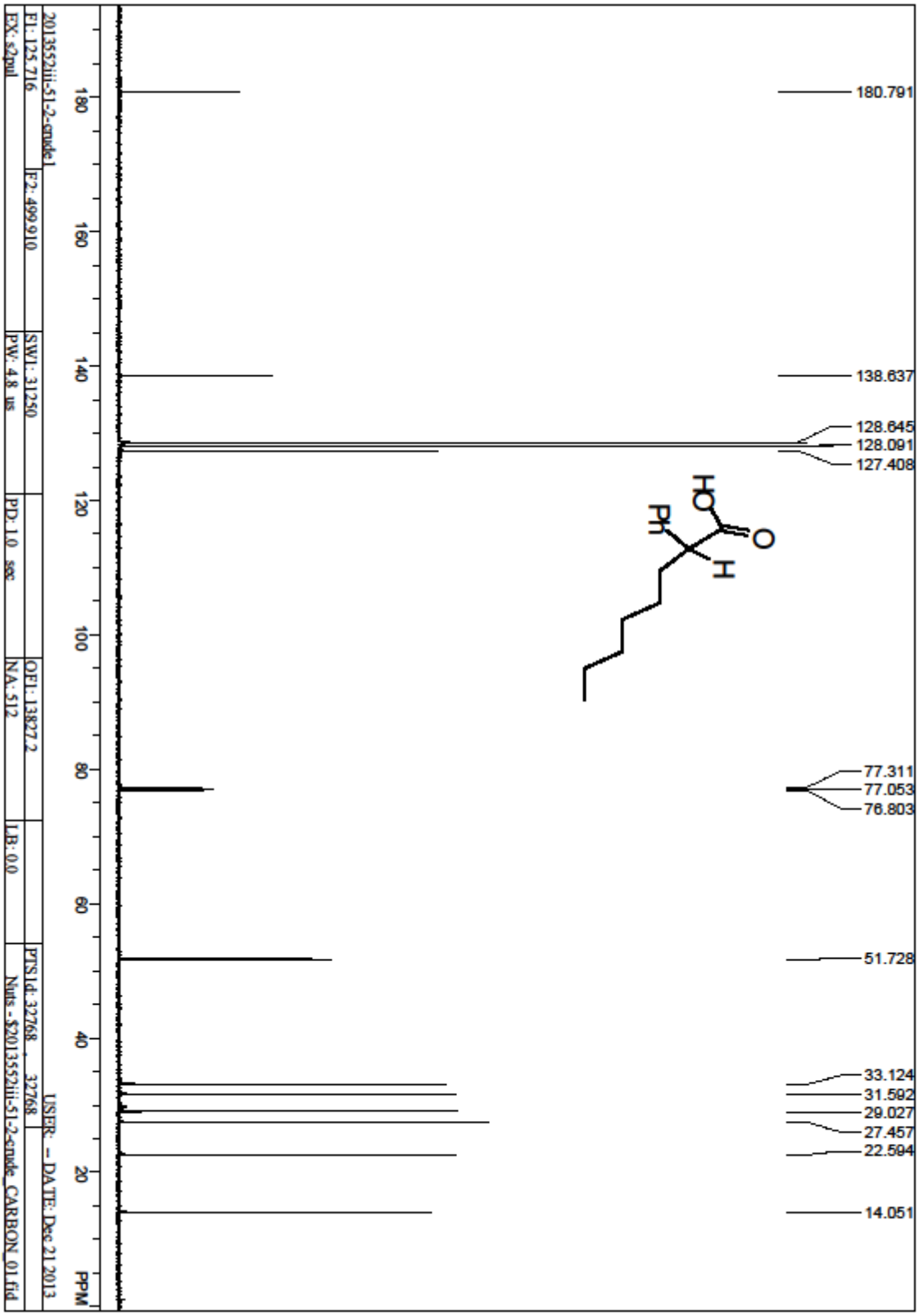

Gradient Shimming\
F1: 499.911
F2: 125.714
SW1: 8013
PW: 3.8 us
PD: 1.0 sec
NA: 8
OF1: 2999.4
LB: 0.0
PTS1d: 16384
16384
EX: s2pul
Nuts - $20135521IL-ME-COOH-L_PROTON_01.fid
USER: -- DATE: Nov 20 2013
PPM
0.88
5.00
1.00
3.25
11.836
7.395
7.387
7.347
7.340
7.331
7.323
3.824
3.809
3.795
3.780
1.586
1.347
HO
O
H

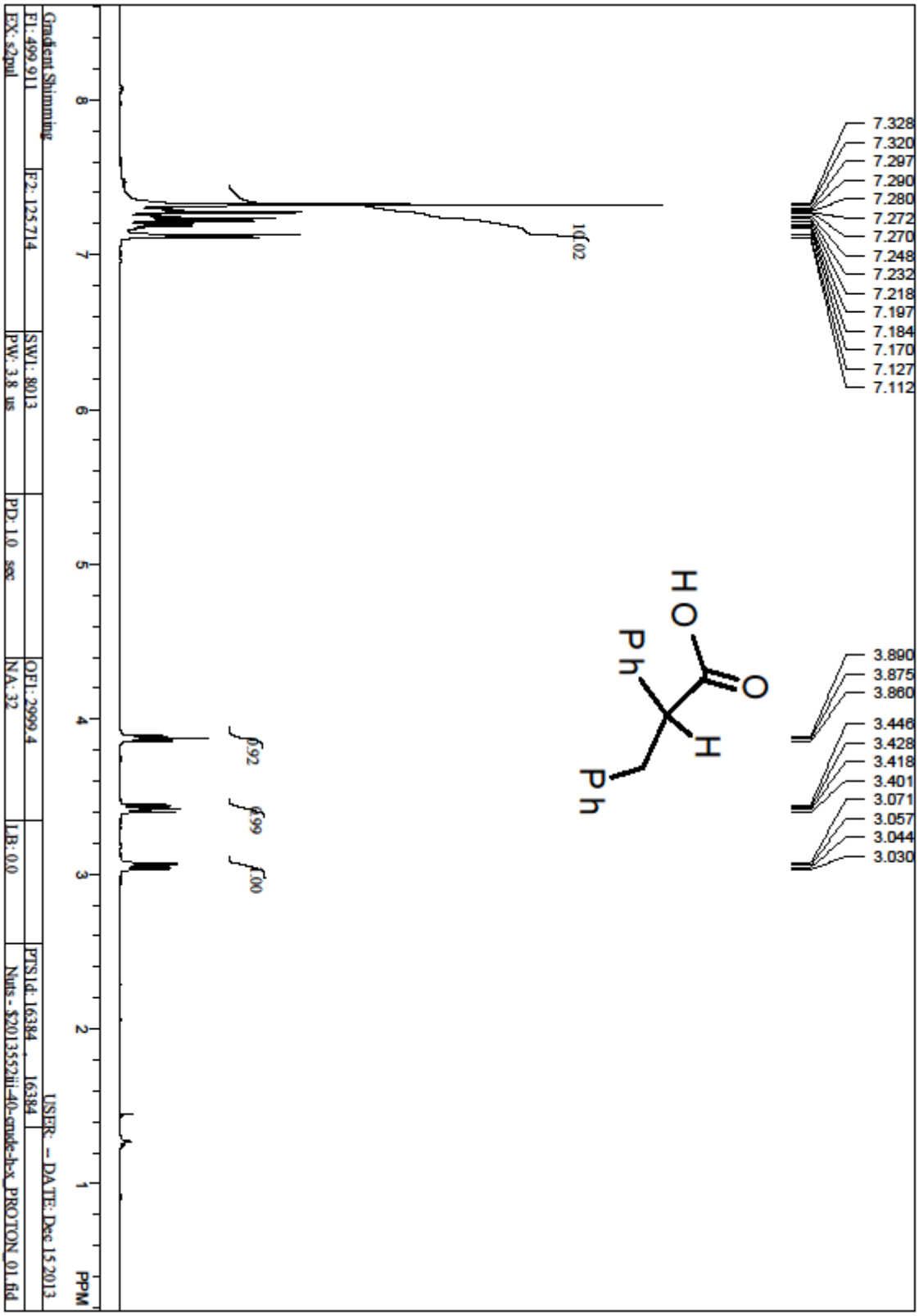

181.284
139.798
128.751
127.682
127.469
77.372
77.114
76.864
45.469
18.132
200
150
100
50
PPM
20133521i-me-cooh
F1: 125.716
F2: 499.910
SW1: 31250
PW: 4.8 us
PD: 1.0 sec
OF1: 13827.2
NA: 256
LB: 0.0
PTS1d: 32768 _ 32768
USER: -- DATE: Nov 19 2013
EX: s2pul
Nitts - $20133521i-me-cooh_CARBON_01.fid

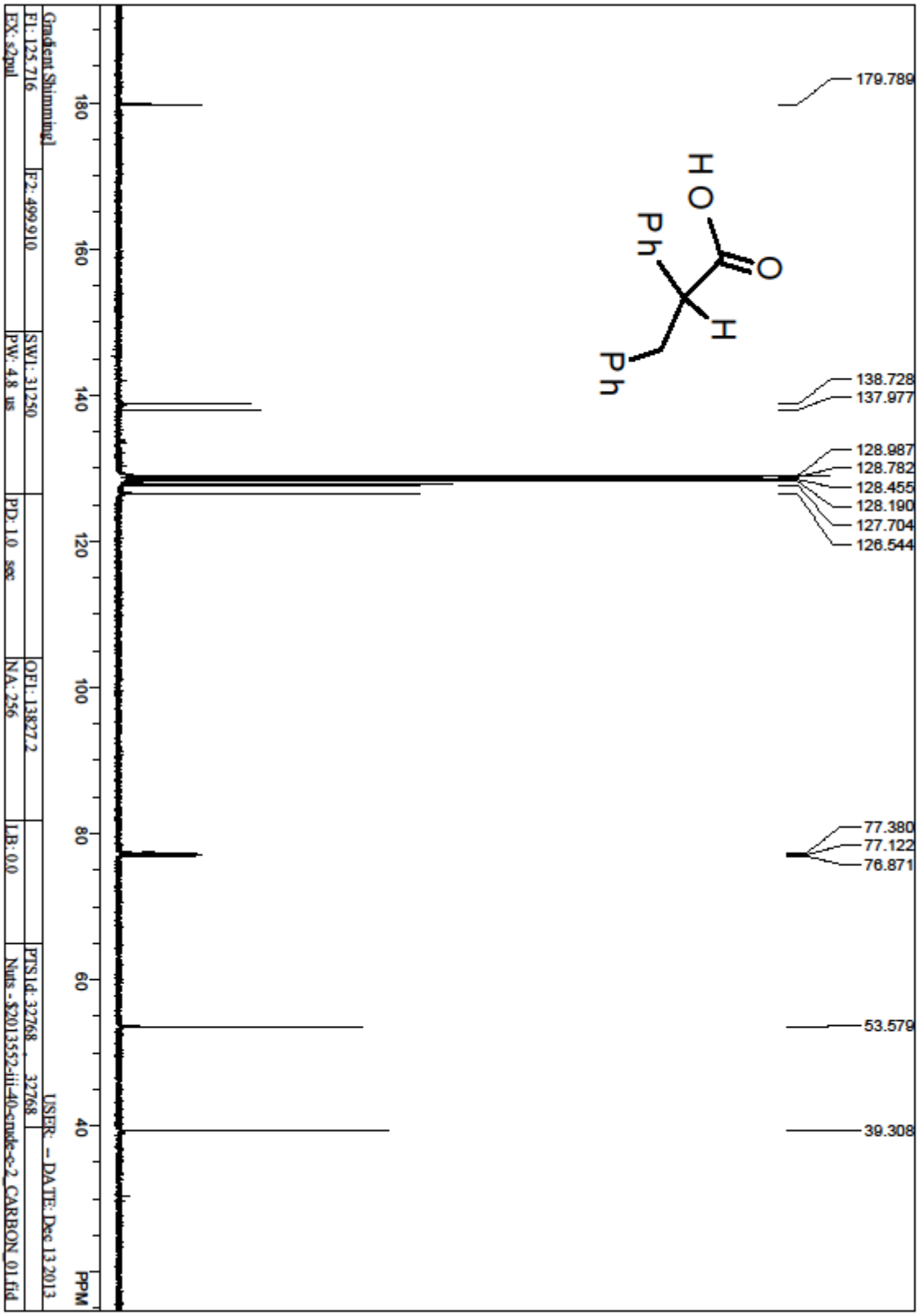

7.361
7.345
7.334
7.305
7.300
7.292
7.289
7.272
5.770
5.757
5.751
5.743
5.737
5.724
5.717
5.710
5.703
5.689
5.112
5.078
5.033
5.013
3.672
3.657
3.642
2.863
2.848
2.833
2.820
2.804
2.565
2.553
2.538
2.523
2.511
HO
O
Ph
H
21.00
1.97
0.96
1.00
1.03
1.03
8
7
6
5
4
3
2
1
0
PPM
Gradient Shimming?P
F1: 499.911
F2: 125.714
SW1: 8013
PW: 3.8 us
PD: 1.0 sec
OF1: 2999.4
NA: 32
LB: 0.0
PTS1d: 16384
16384
USER: -- DATE: Dec 20 2013
EX: s2pul
Nuts - $20135521iii-50-cmake-hen_PROTON_01.fid

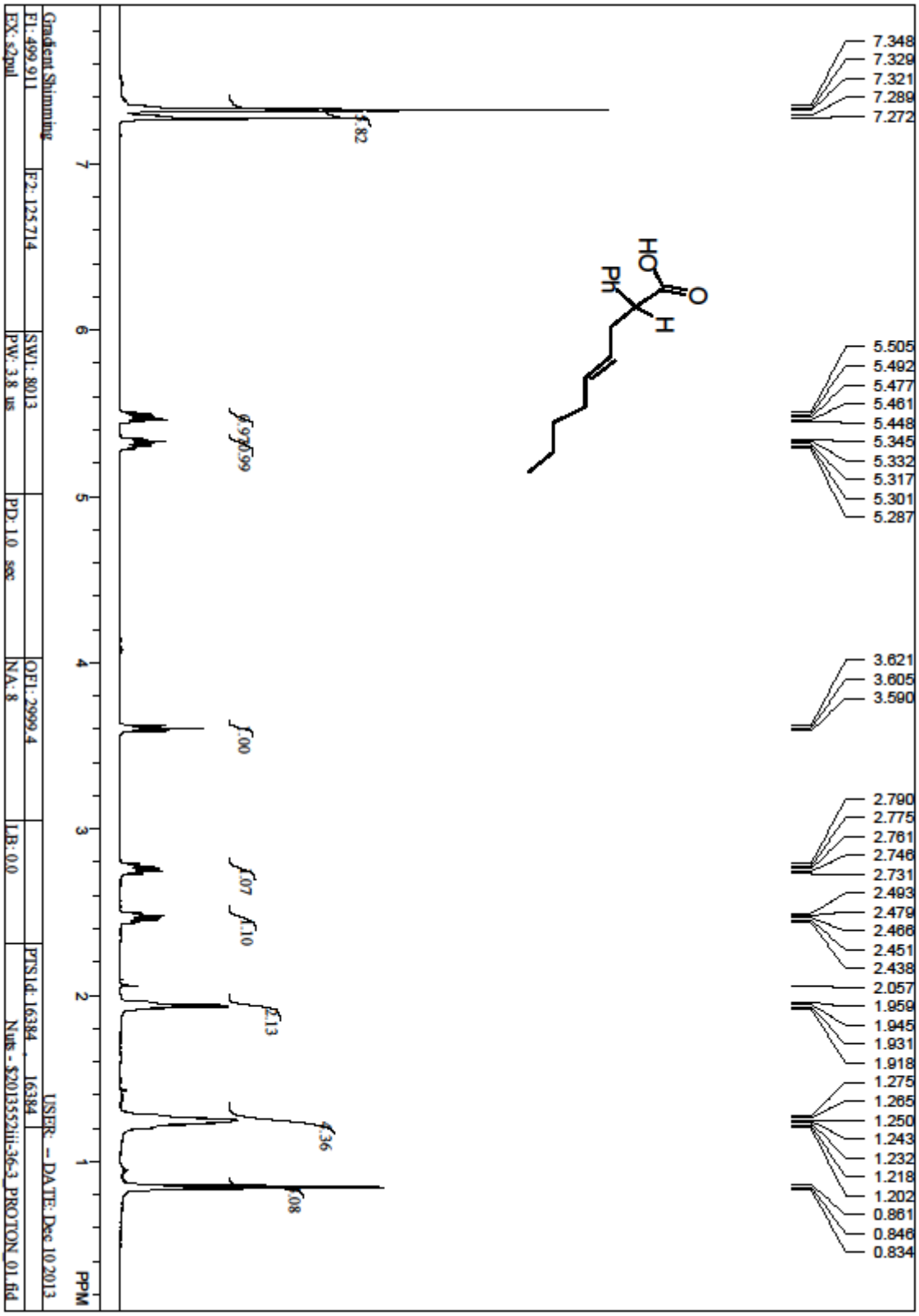

180.116
137.863
134.927
128.774
128.129
127.666
117.371
77.372
77.114
76.864
51.462
37.100
O
H
O
Ph
H
180
160
140
120
100
80
60
40
20
PPM
Gradient Shimming
F1: 125.716
F2: 499.910
SW1: 31250
PW: 4.8 us
PD: 1.0 sec
OF1: 13827.2
NA: 512
LB: 0.0
PTS1d: 32768 -- 32768
EX: s2pul
Nuts - $20135521iii-50-cmdte-c_CARBON_01.fid
USER: -- DATE: Dec 20 2013

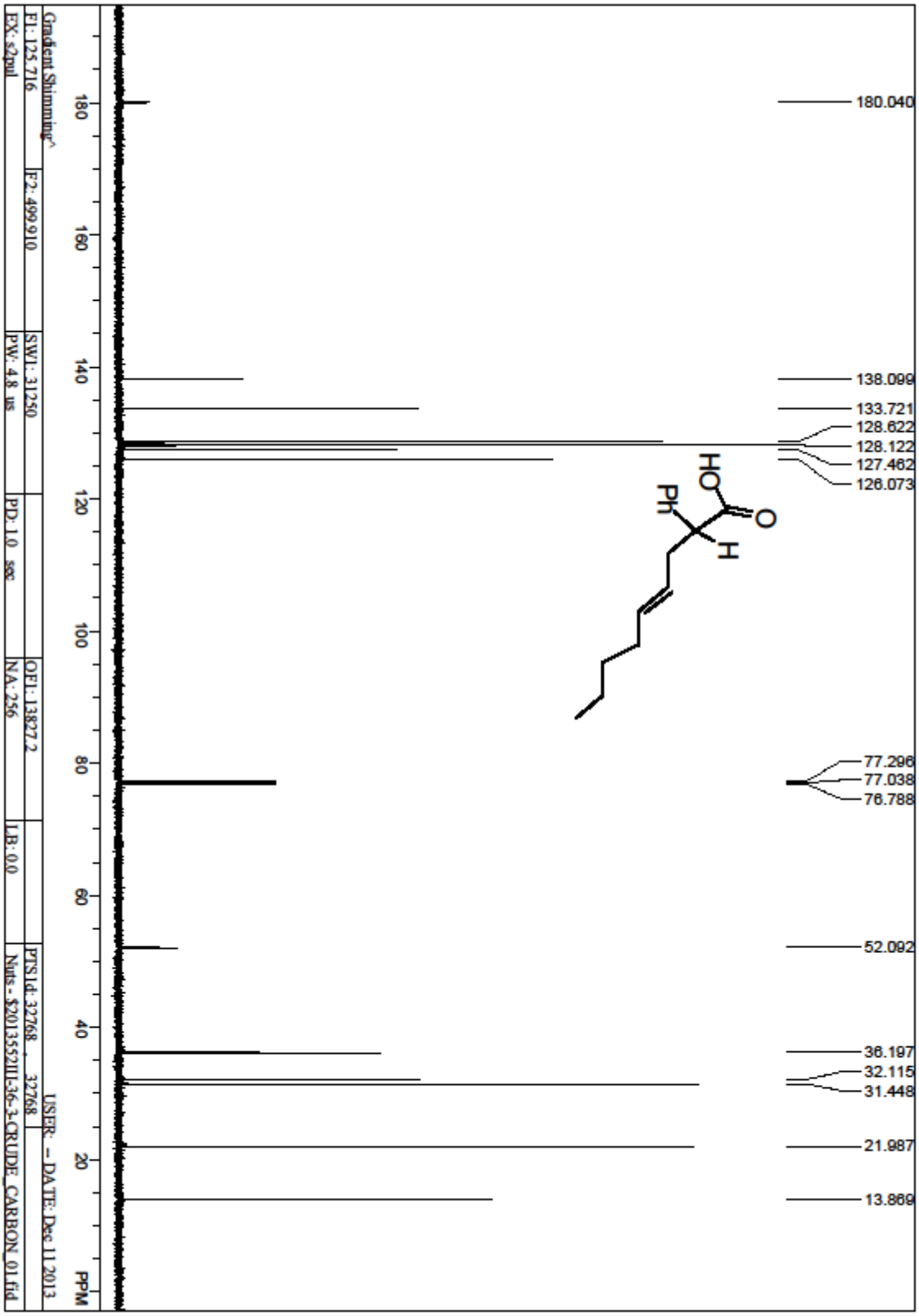

Gradient Shimming
F1: 499.911
F2: 125.714
SW1: 8013
PW: 3.8 us
PD: 1.0 sec
OF1: 2999.4
NA: 8
LB: 0.0
PTS1d: 16384
16384
USER: -- DATE: Dec 21 2013
EX: s2pul
Nuts - $20135521ii-51-2-crude_PROTON_01.fid
PPM
0.66
11.706
HO
O
Ph
H
7.363
7.355
7.309
7.302
5.08
3.596
3.581
3.565
1.00
2.121
2.113
2.104
1.829
1.820
1.805
1.05
1.04
1.333
1.316
1.292
0.918
0.905
0.891
8.65
3.15

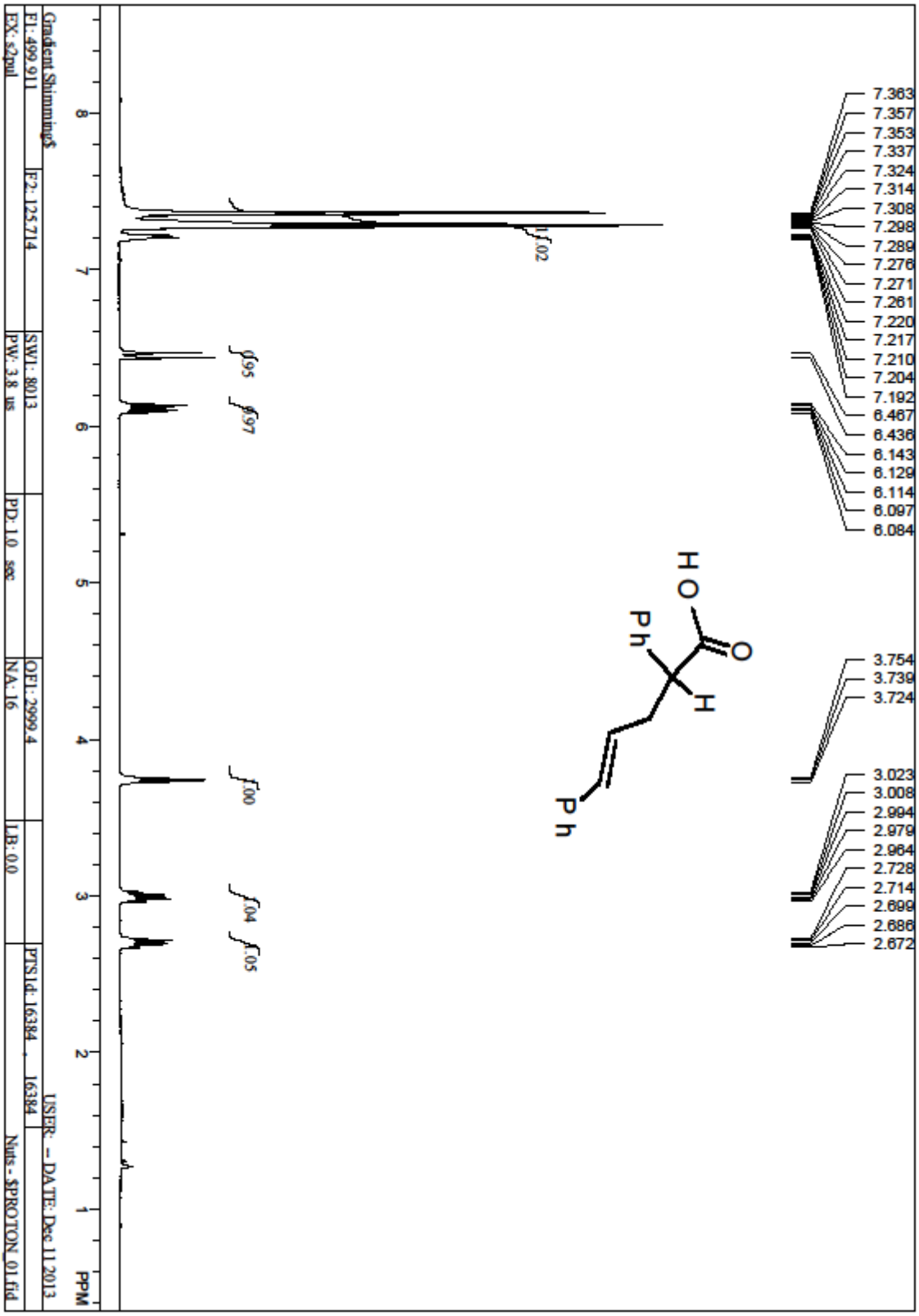

180.791
138.637
128.645
128.091
127.408
77.311
77.053
76.803
51.728
33.124
31.592
29.027
27.457
22.594
14.051
OH
O
PH
H
180
160
140
120
100
80
60
40
20
PPM
20135521ii-51-2-crude1
F1: 125.716
F2: 499.910
EX: s2pul
SW1: 31250
PW: 4.8 us
PD: 1.0 sec
OF1: 13827.2
NA: 512
LB: 0.0
PTS1d: 32768 ... 32768
USER: -- DATE: Dec 21 2013
Nuts - $20135521ii-51-2-crude_CARBON_01.fid

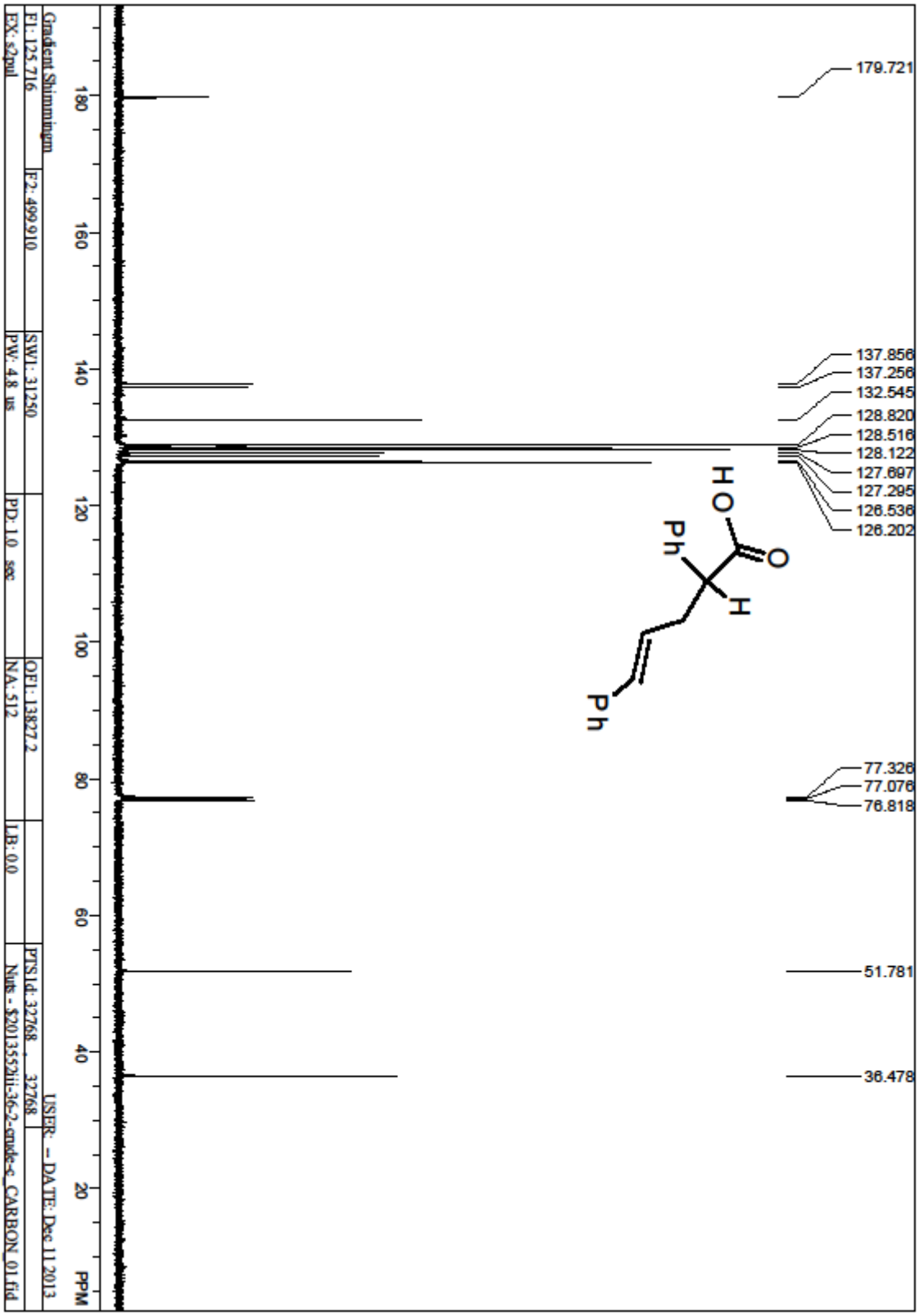

7.328
7.320
7.297
7.290
7.280
7.272
7.270
7.248
7.232
7.218
7.197
7.184
7.170
7.127
7.112
3.890
3.875
3.860
3.446
3.428
3.418
3.401
3.071
3.057
3.044
3.030
10.02
0.92
0.99
1.00
O
H
O
Ph
Ph
PPM
Gradient Shimming
F1: 499.911
F2: 125.714
SW1: 8013
PW: 3.8 us
PD: 1.0 sec
OF1: 2999.4
NA: 32
LB: 0.0
PTS1d: 16384
16384
USER: -- DATE: Dec 15 2013
EX: s2pul
Nuts - $20135521iii-40-cmde-hex_PROTON_01.fid

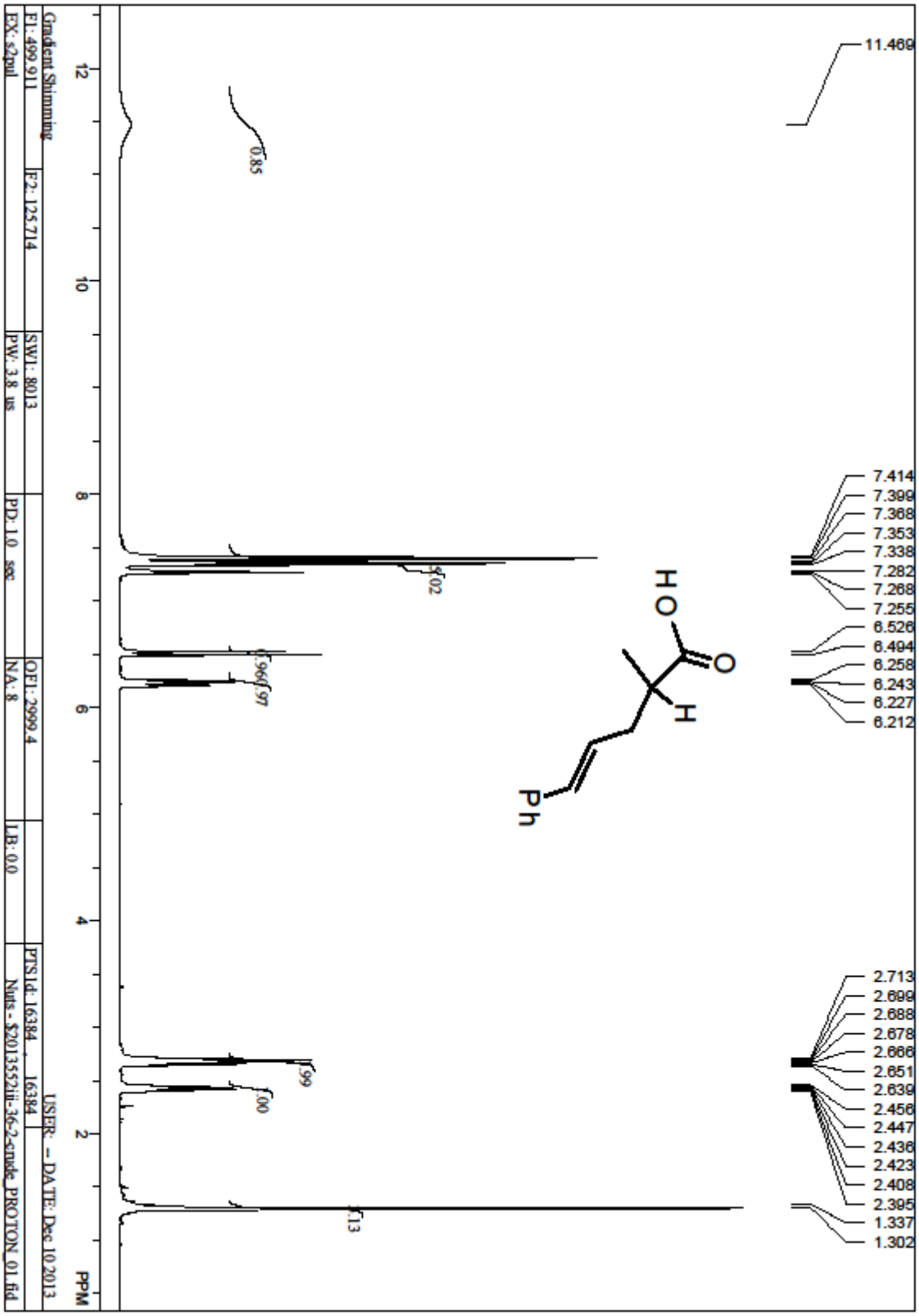

179.789
138.728
137.977
128.987
128.782
128.455
128.190
127.704
126.544
77.380
77.122
76.871
53.579
39.308
HO
O
H
Ph
Ph
180
160
140
120
100
80
60
40
PPM
Gradient Shimming]
F1: 125.716
F2: 499.910
EX: s2pul
SW1: 31250
PW: 4.8 us
PD: 1.0 sec
OF1: 13827.2
NA: 256
LB: 0.0
PTS1d: 32768 -- 32768
Nuts - $20133552-iii-40-nmfe-c-2_CARBON_01.fid
USER: -- DATE: Dec 13 2013

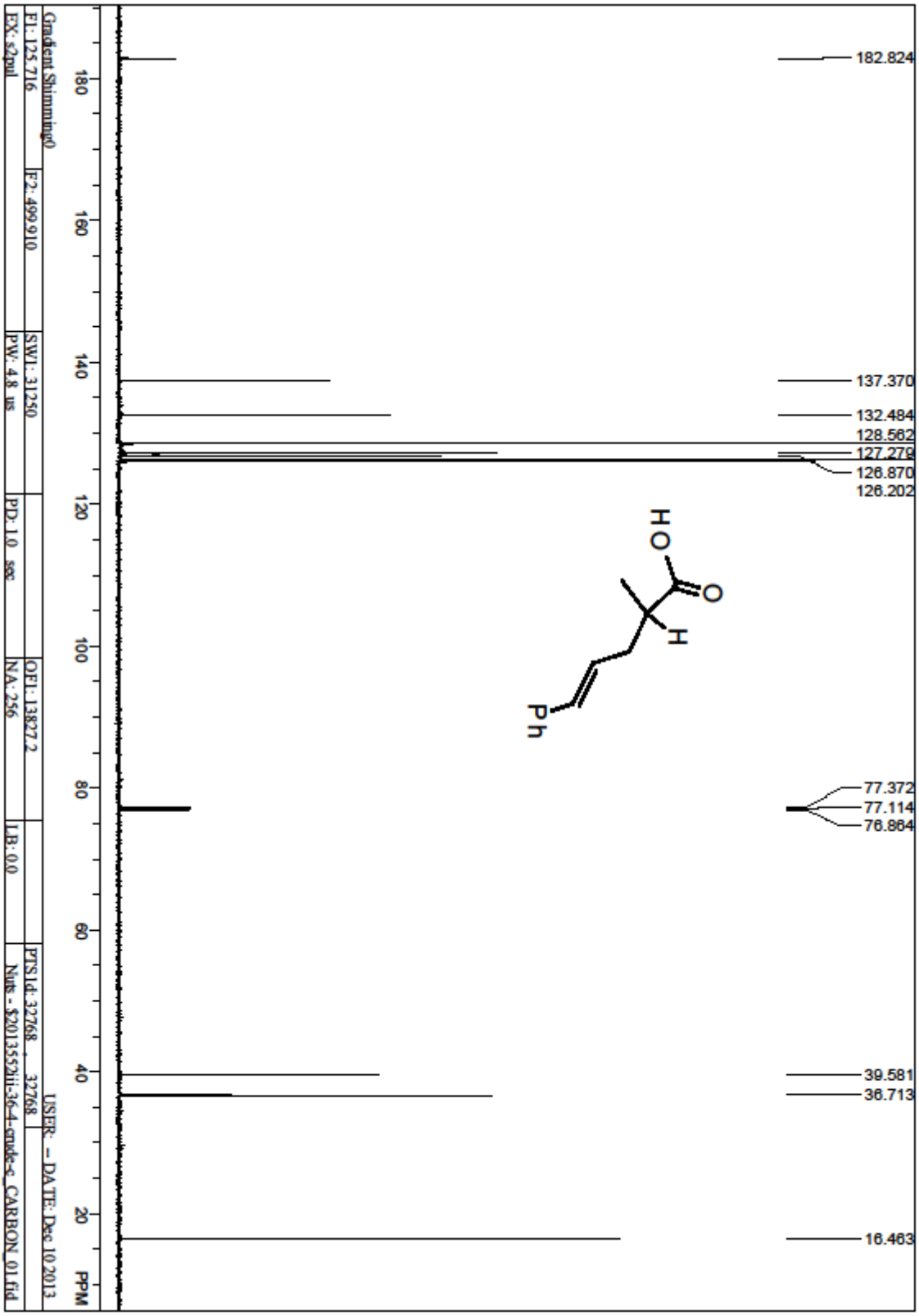

Gradient Shimming
F1: 499.911
F2: 125.714
SW1: 8013
PW: 3.8 us
PD: 1.0 sec
OF1: 2999.4
NA: 8
LB: 0.0
PTS1d: 16384
16384
USER: -- DATE: Dec 10 2013
EX: s2pul
Nuts - $20135521iii-36-3_PROTON_01.fid
PPM
7.348
7.329
7.321
7.289
7.272
5.505
5.492
5.477
5.461
5.448
5.345
5.332
5.317
5.301
5.287
3.621
3.605
3.590
2.790
2.775
2.761
2.746
2.731
2.493
2.479
2.466
2.451
2.438
2.057
1.959
1.945
1.931
1.918
1.275
1.265
1.250
1.243
1.232
1.218
1.202
0.861
0.846
0.834
1.82
9.97
9.99
1.00
1.07
1.10
1.13
4.36
3.08

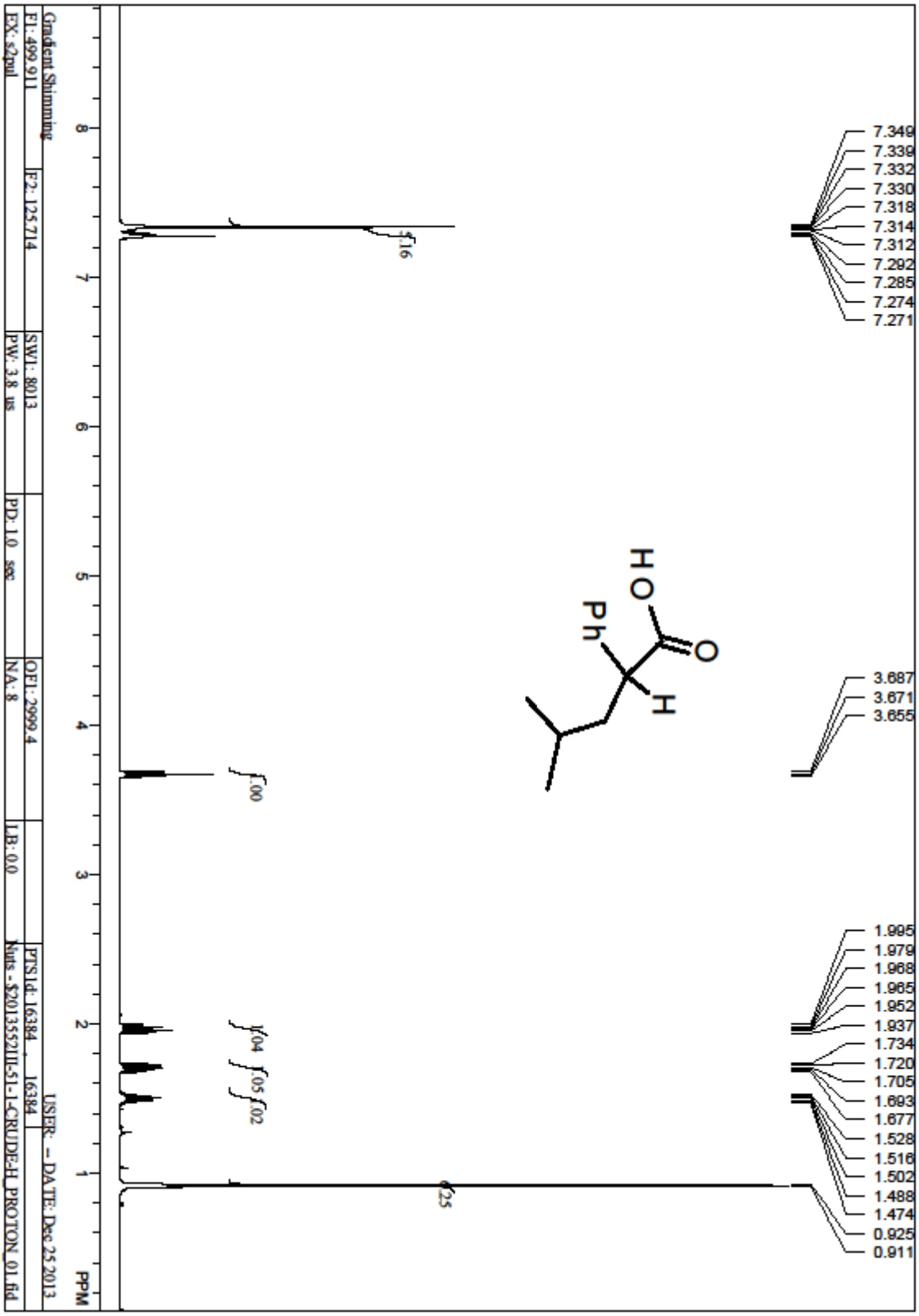

Gradient Shimming^
F1: 125.716
F2: 499.910
EX: s2pul
SW1: 31250
PW: 4.8 us
PD: 1.0 sec
OF1: 13827.2
NA: 256
LB: 0.0
PTS1d: 32768
32768
Nuts - $20135520IIU36-3-CRUDE_CARBON_01.fid
USER: -- DATE: Dec 11 2013
180.040
138.099
133.721
128.622
128.122
127.462
126.073
77.296
77.038
76.788
52.092
36.197
32.115
31.448
21.987
13.869
HO
O
H
Ph
180
160
140
120
100
80
60
40
20
PPM

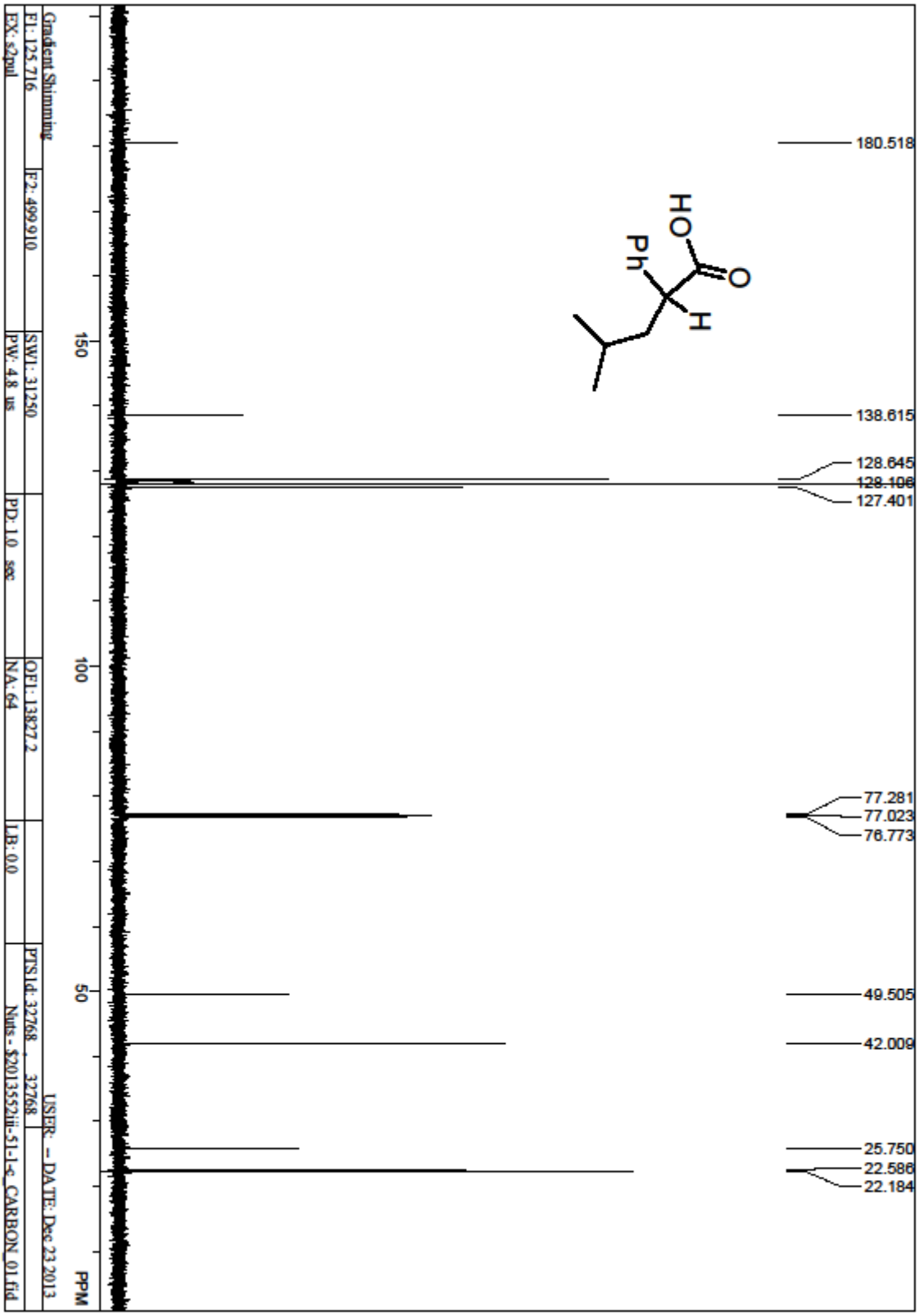

7.363
7.357
7.353
7.337
7.324
7.314
7.308
7.298
7.289
7.276
7.271
7.261
7.220
7.217
7.210
7.204
7.192
6.467
6.436
6.143
6.129
6.114
6.097
6.084
3.754
3.739
3.724
3.023
3.008
2.994
2.979
2.964
2.728
2.714
2.699
2.686
2.672
1.02
.95
.97
1.00
1.04
1.05
O
H
Ph
Ph
PPM
Gradient Shimming$
F1: 499.911
F2: 125.714
SW1: 8013
PW: 3.8 us
PD: 1.0 sec
OF1: 2999.4
NA: 16
LB: 0.0
PTS1d: 16384
16384
USER: -- DATE: Dec 11 2013
EX: s2pul
Nuts - $PROTON_01.fid

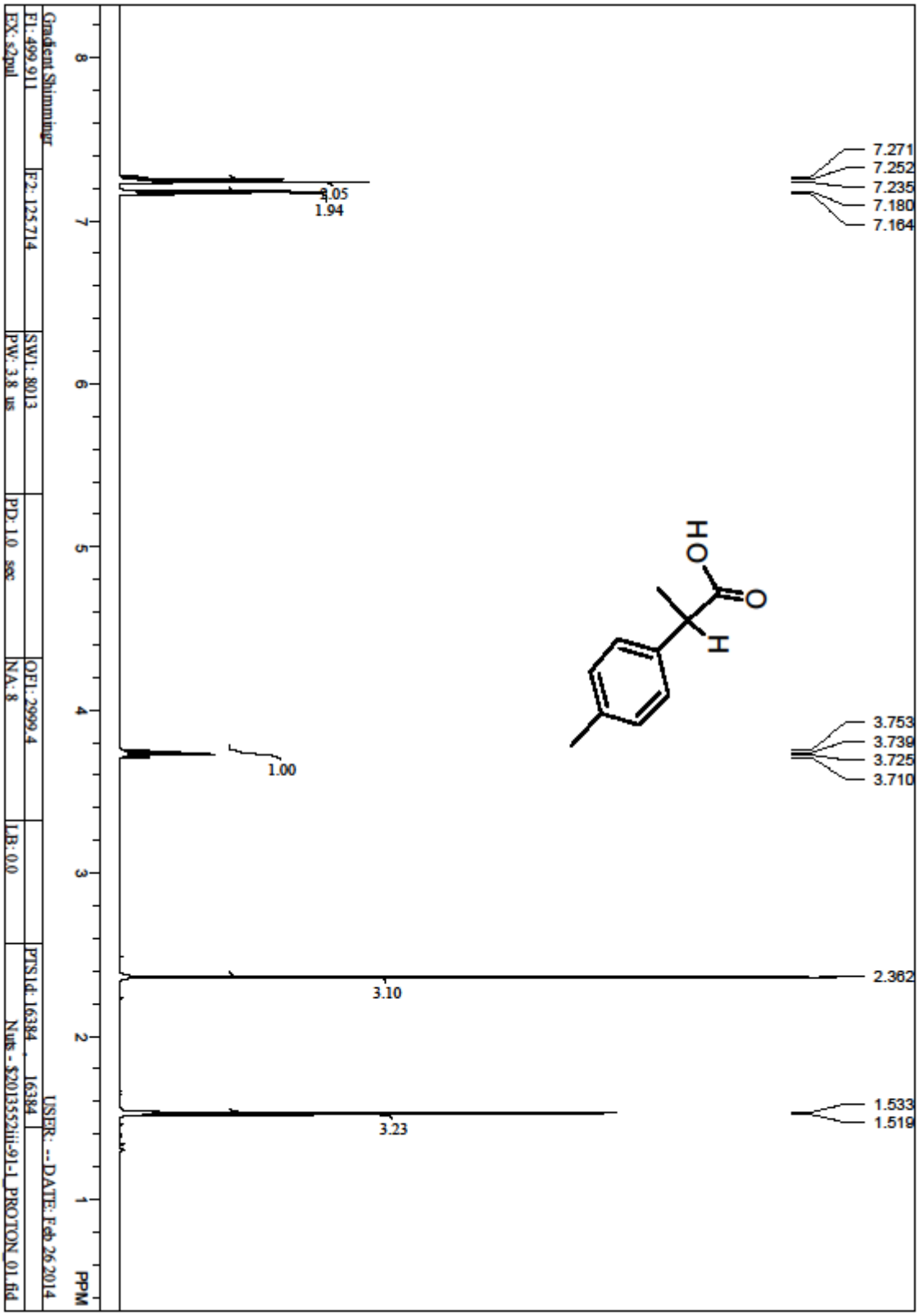

179.721
137.856
137.256
132.545
128.820
128.516
128.122
127.697
127.295
126.536
126.202
77.326
77.076
76.818
51.781
36.478
HO
O
Ph
H
Ph
180
160
140
120
100
80
60
40
20
PPM
Gradient Shimming
F1: 125.716
F2: 499.910
EX: s2pul
SW1: 31250
PW: 4.8 us
PD: 1.0 sec
OF1: 13827.2
NA: 512
LB: 0.0
PTS1d: 32768 → 32768
Nuts - $20135520iii-36-2-cmdcs_CARBON_01.fid
USER: -- DATE: Dec 11 2013

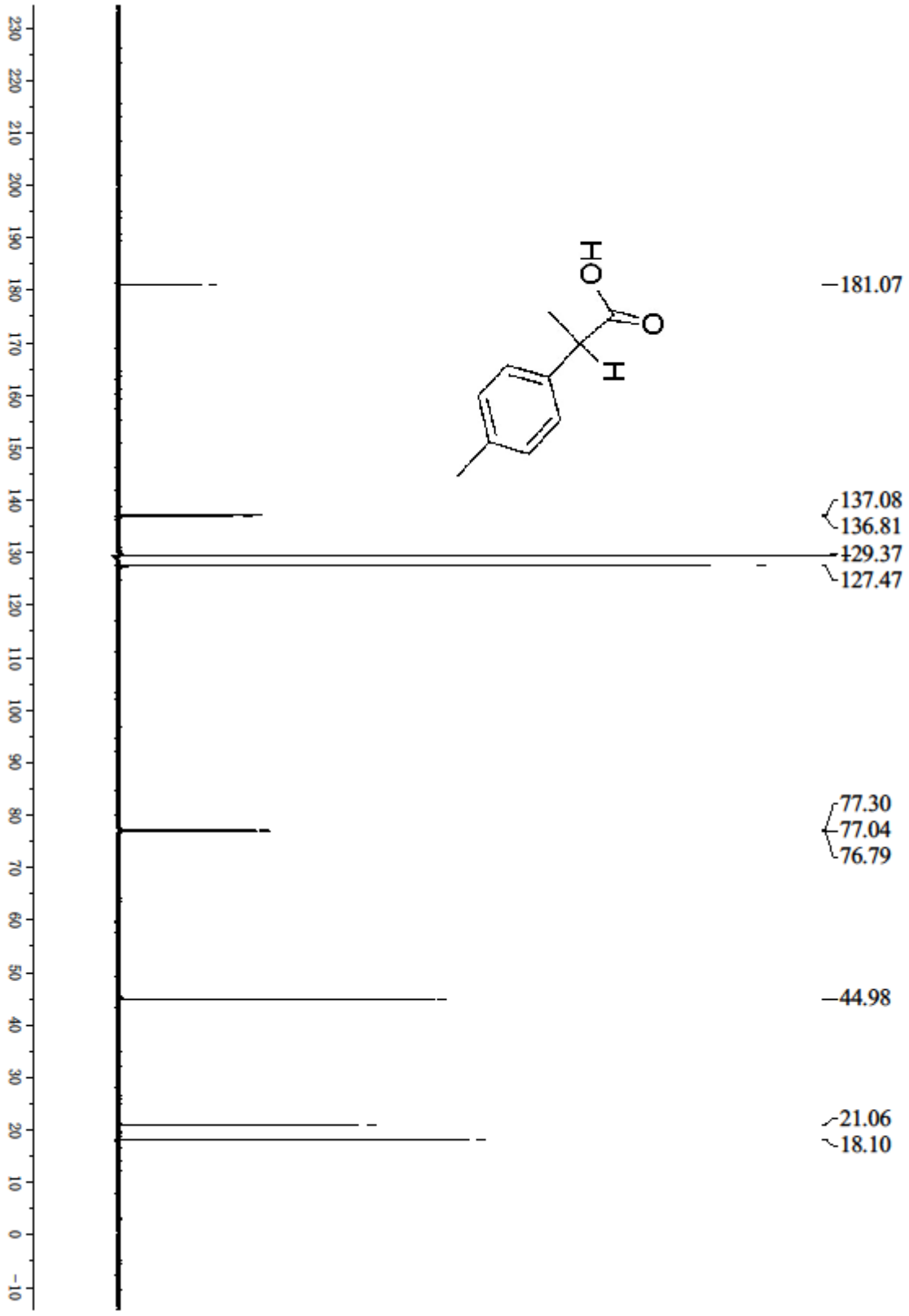

11.469
7.414
7.399
7.368
7.353
7.338
7.282
7.268
7.255
6.526
6.494
6.258
6.243
6.227
6.212
2.713
2.699
2.688
2.678
2.666
2.651
2.639
2.456
2.447
2.436
2.423
2.408
2.395
1.337
1.302
0.85
5.02
1.96
1.97
1.99
1.00
4.13
HO
O
H
Ph
12
10
8
6
4
2
PPM
Gradient Shimming
F1: 499.911
F2: 125.714
SW1: 8013
PW: 3.8 us
PD: 1.0 sec
QE1: 2999.4
NA: 8
LB: 0.0
PTS1d: 16384
16384
USER: -- DATE: Dec 10 2013
EX: s2pul
Nuts - $20135521ii-36-2-crude_PROTON_01.fid

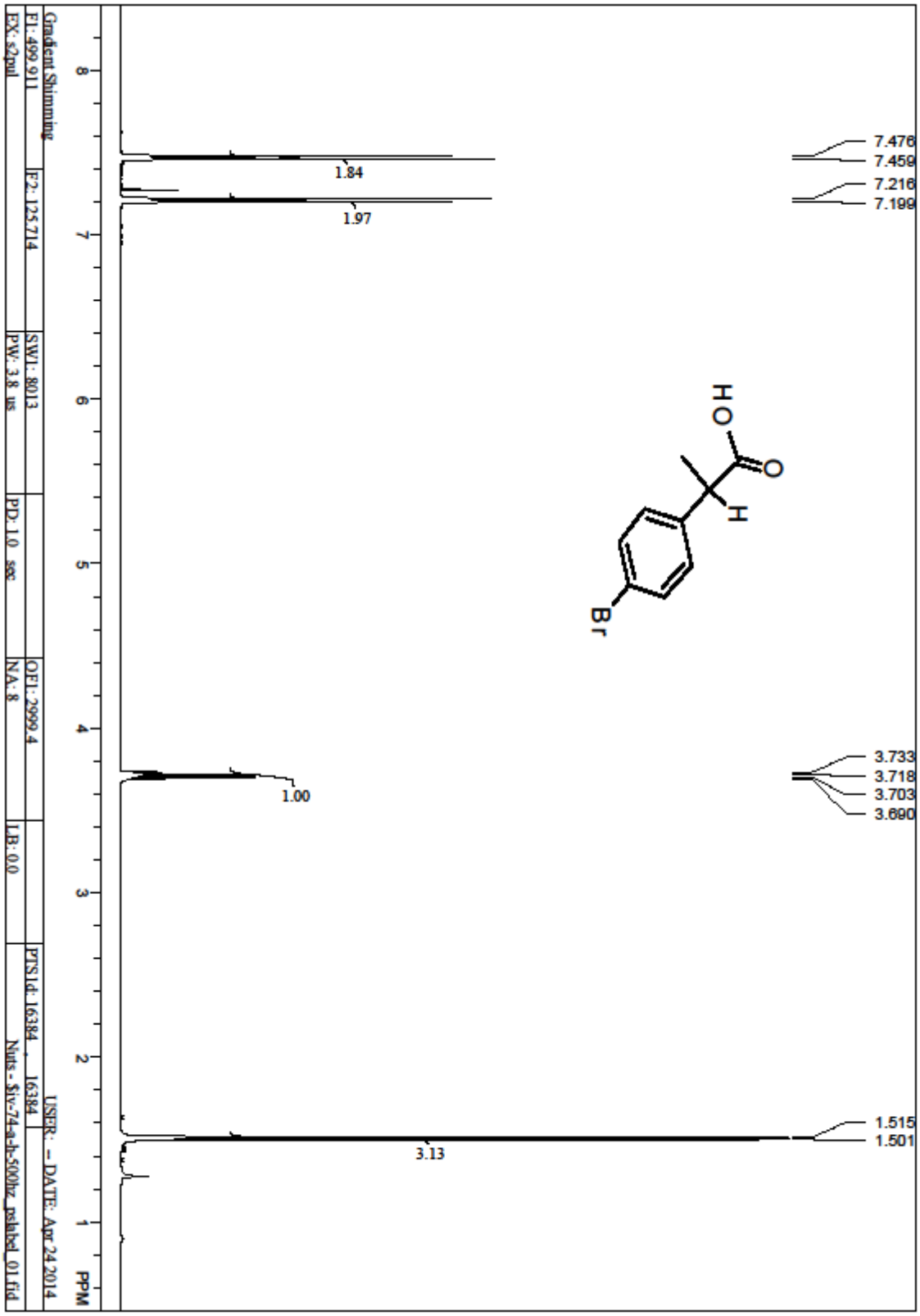

182.824
137.370
132.484
128.562
127.279
126.870
126.202
77.372
77.114
76.864
39.581
36.713
16.463
HO
O
H
Ph
180
160
140
120
100
80
60
40
20
PPM
Gradient Shimming0
F1: 125.716
F2: 499.910
SW1: 31250
PW: 4.8 us
PD: 1.0 sec
QF1: 13827.2
NA: 256
LB: 0.0
PTS1d: 32768 → 32768
Nuts - $20135230ii-36-4-cmdcs_CARBON_01.fid
EX: s2pul
USER: -- DATE: Dec 10 2013

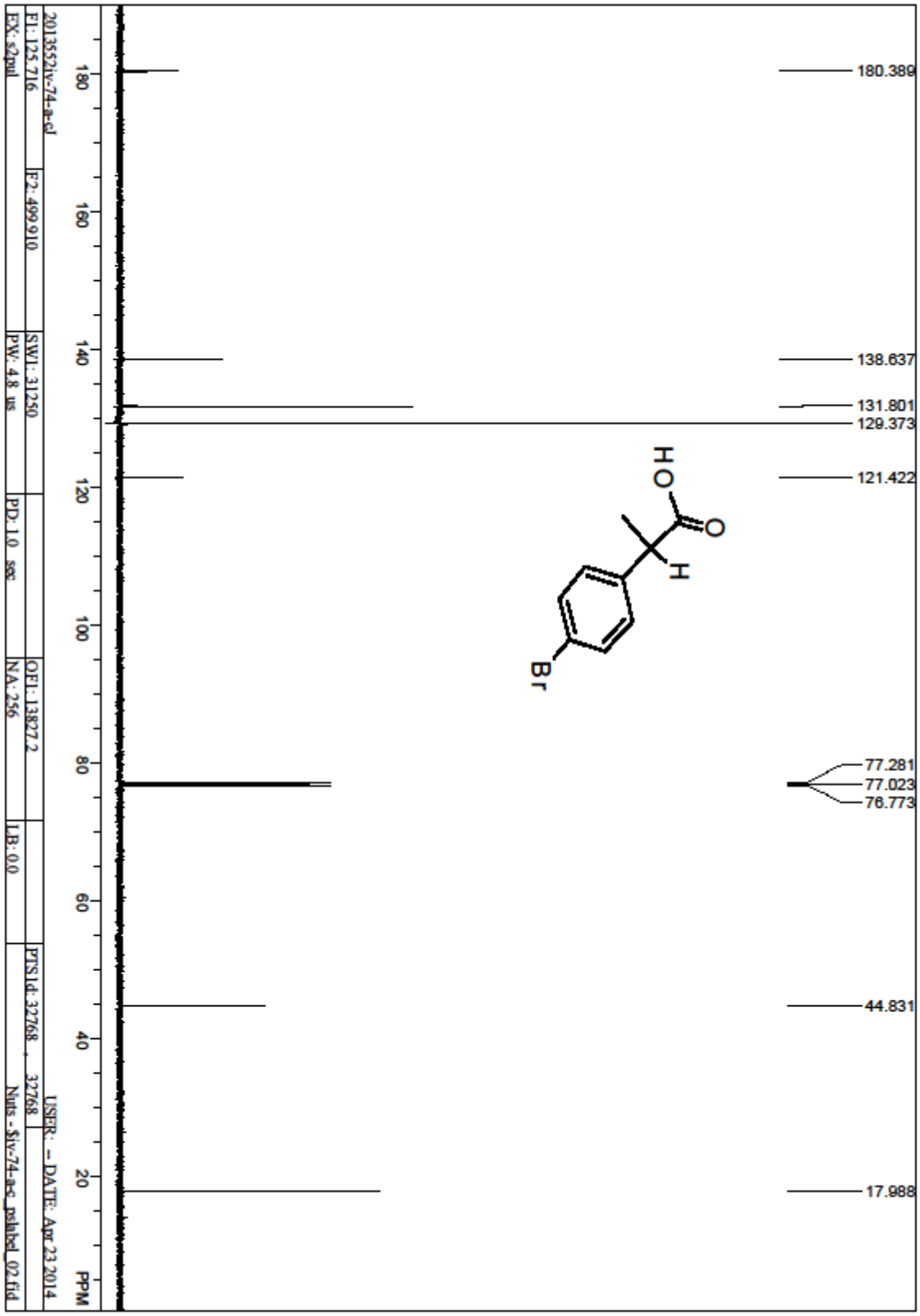

7.349
7.339
7.332
7.330
7.318
7.314
7.312
7.292
7.285
7.274
7.271
3.687
3.671
3.655
1.995
1.979
1.968
1.965
1.952
1.937
1.734
1.720
1.705
1.693
1.677
1.528
1.516
1.502
1.488
1.474
0.925
0.911
HO
O
Ph
H
1.16
1.00
2.04
2.05
2.02
6.25
PPM
Gradient Shimming
F1: 499.911
F2: 125.714
SW1: 8013
PW: 3.8 us
PD: 1.0 sec
OF1: 2999.4
NA: 8
LB: 0.0
PTS1d: 16384
16384
USER: -- DATE: Dec 25 2013
EX: s2pul
Nuts - $20135520III-51-1-CRUDE-H_PROTON_01.fid

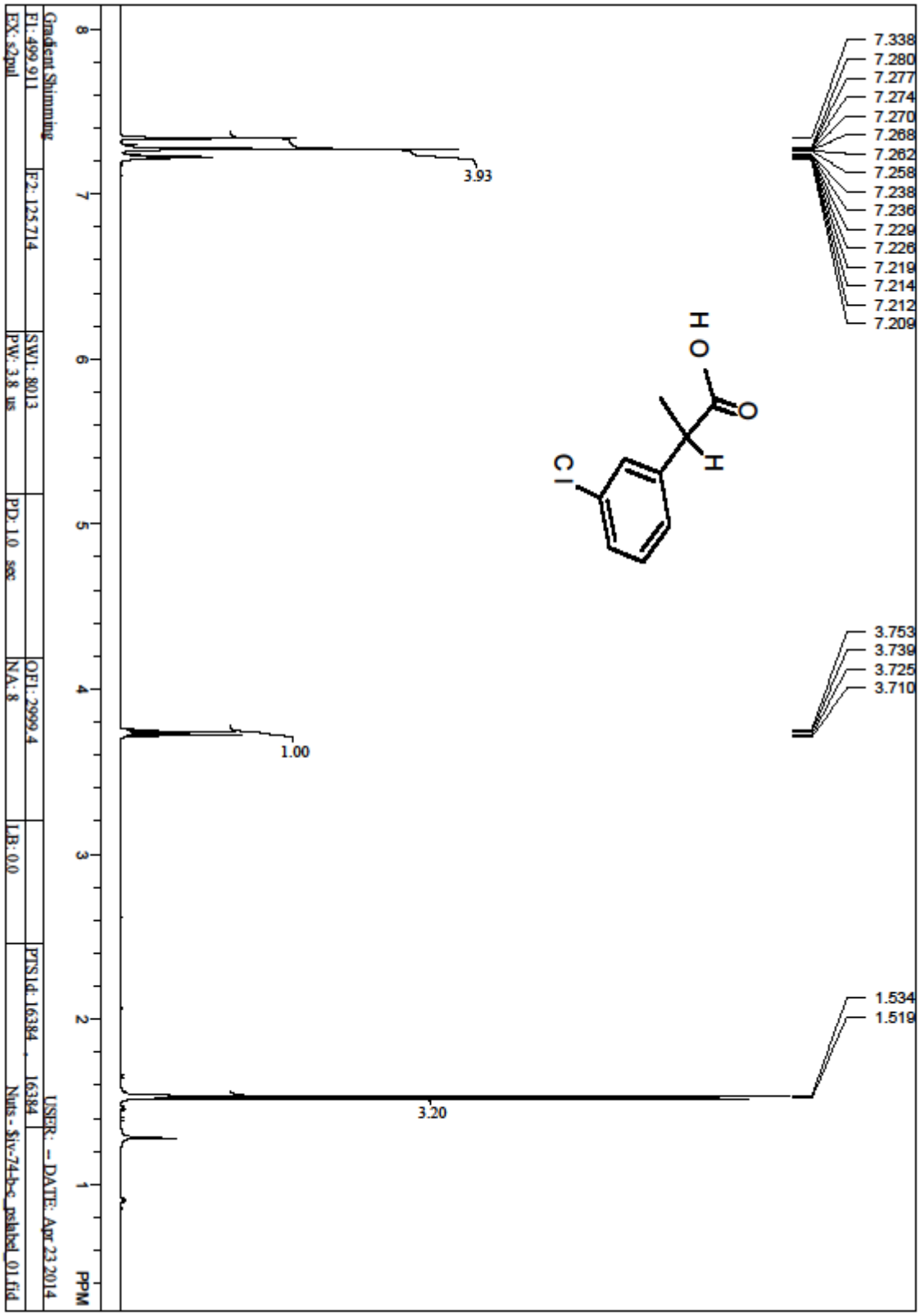

Gradient Shimming
F1: 125.716
F2: 499.910
SW1: 31250
PW: 4.8 us
PD: 1.0 sec
OF1: 13827.2
NA: 64
LB: 0.0
PTS1d: 32768 → 32768
EX: s2pul
Nuts - $20133552iii-51-1-c_CARBON_01.fid
USER: -- DATE: Dec 23 2013
PPM
150
100
50
180.518
138.615
128.645
128.106
127.401
77.281
77.023
76.773
49.505
42.009
25.750
22.586
22.184
HO
O
Ph
H

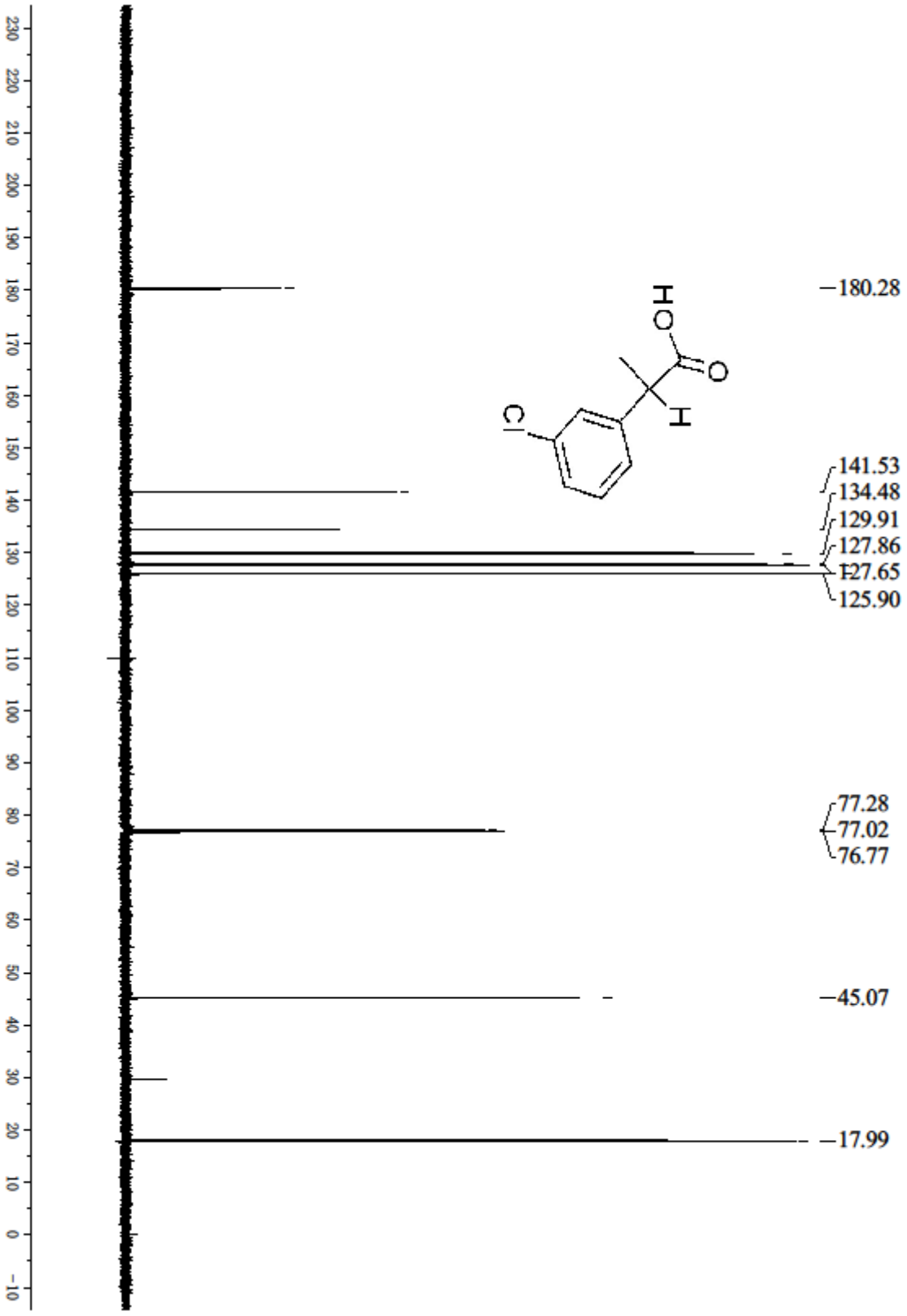

Gradient Shimming
F1: 499.911
F2: 125.714
SW1: 8013
PW: 3.8 us
PD: 1.0 sec
OF1: 2999.4
NA: 8
LB: 0.0
PTS1d: 16384
16384
USER: -- DATE: Feb 26 2014
EX: s2pul
Nuts -$20135521iii-91-1_PROTON_01.fid
PPM
8
7
6
5
4
3
2
1
7.271
7.252
7.235
7.180
7.164
3.753
3.739
3.725
3.710
2.362
1.533
1.519
2.05
1.94
1.00
3.10
3.23
HO
O
H

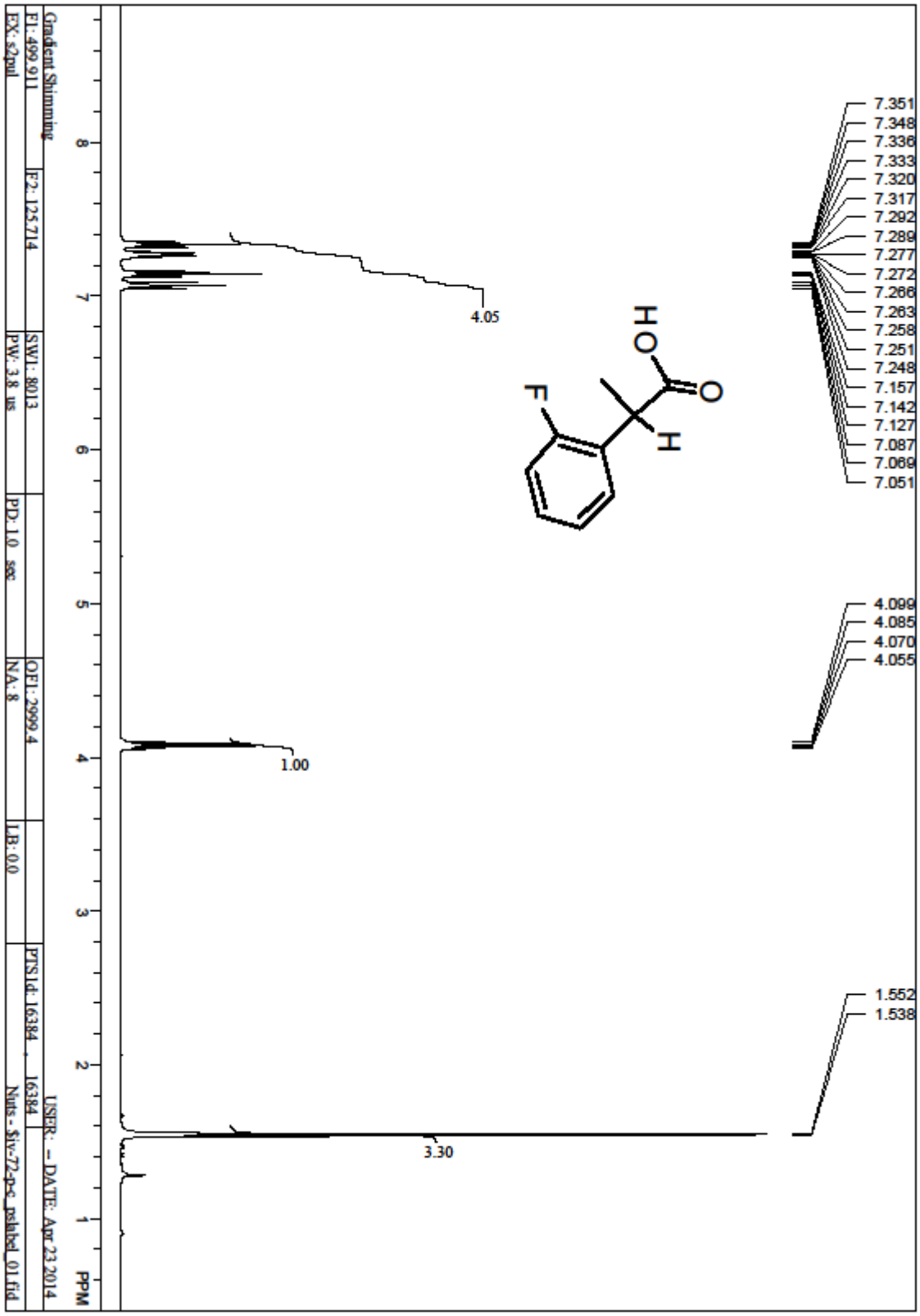

181.07
137.08
136.81
129.37
127.47
77.30
77.04
76.79
44.98
21.06
18.10

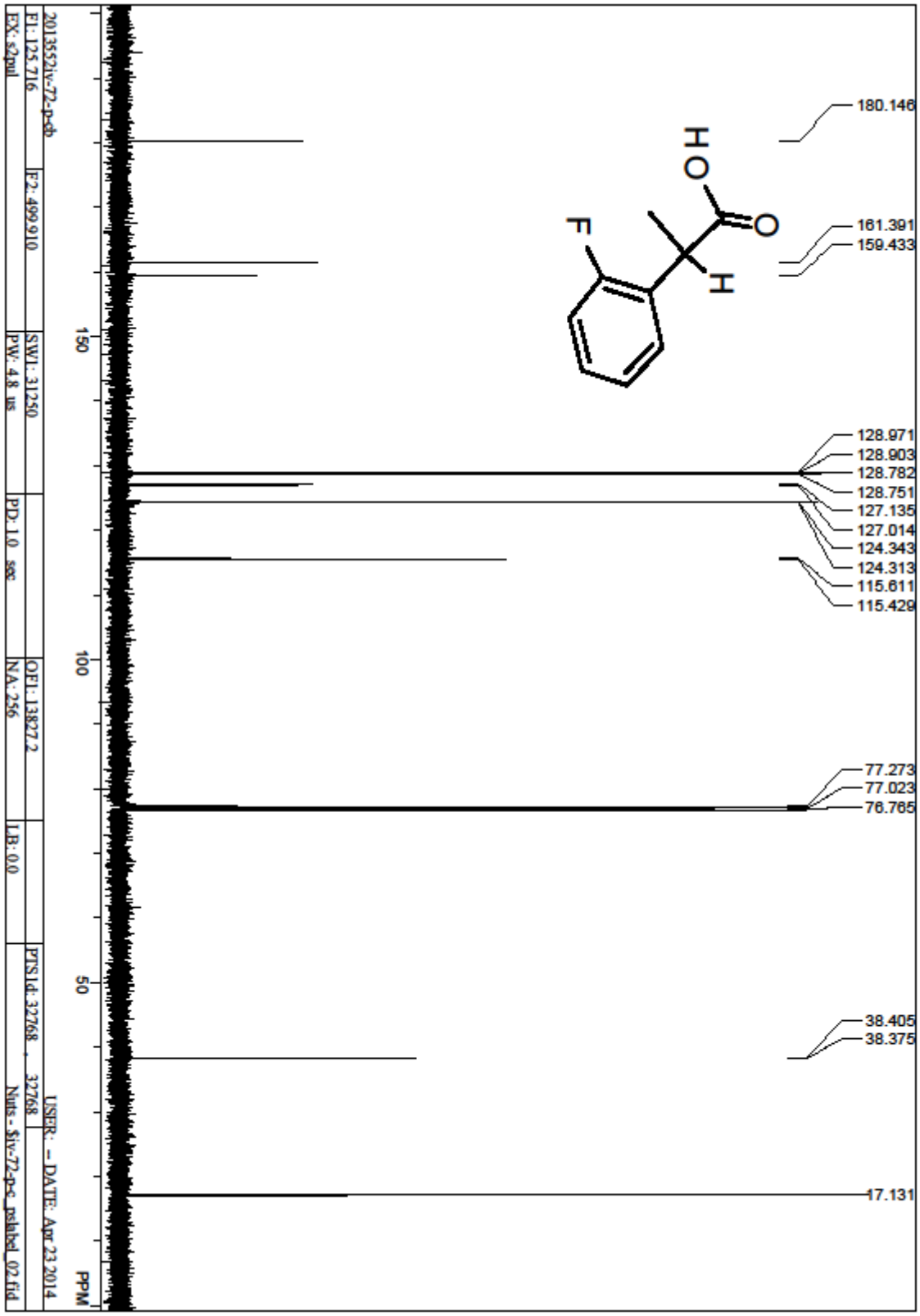

Gradient Shimming
F1: 499.911
F2: 125.714
SW1: 8013
PW: 3.8 us
PD: 1.0 sec
OF1: 2999.4
NA: 8
LB: 0.0
PTS1d: 16384 _ 16384
EX: s2pul
USER: -- DATE: Apr 24 2014
Nuts - $tv-74-a-hr-500hz_pslabel_01.fid
PPM
1.84
1.97
1.00
3.13
7.476
7.459
7.216
7.199
3.733
3.718
3.703
3.690
1.515
1.501
HO
O
H
Br

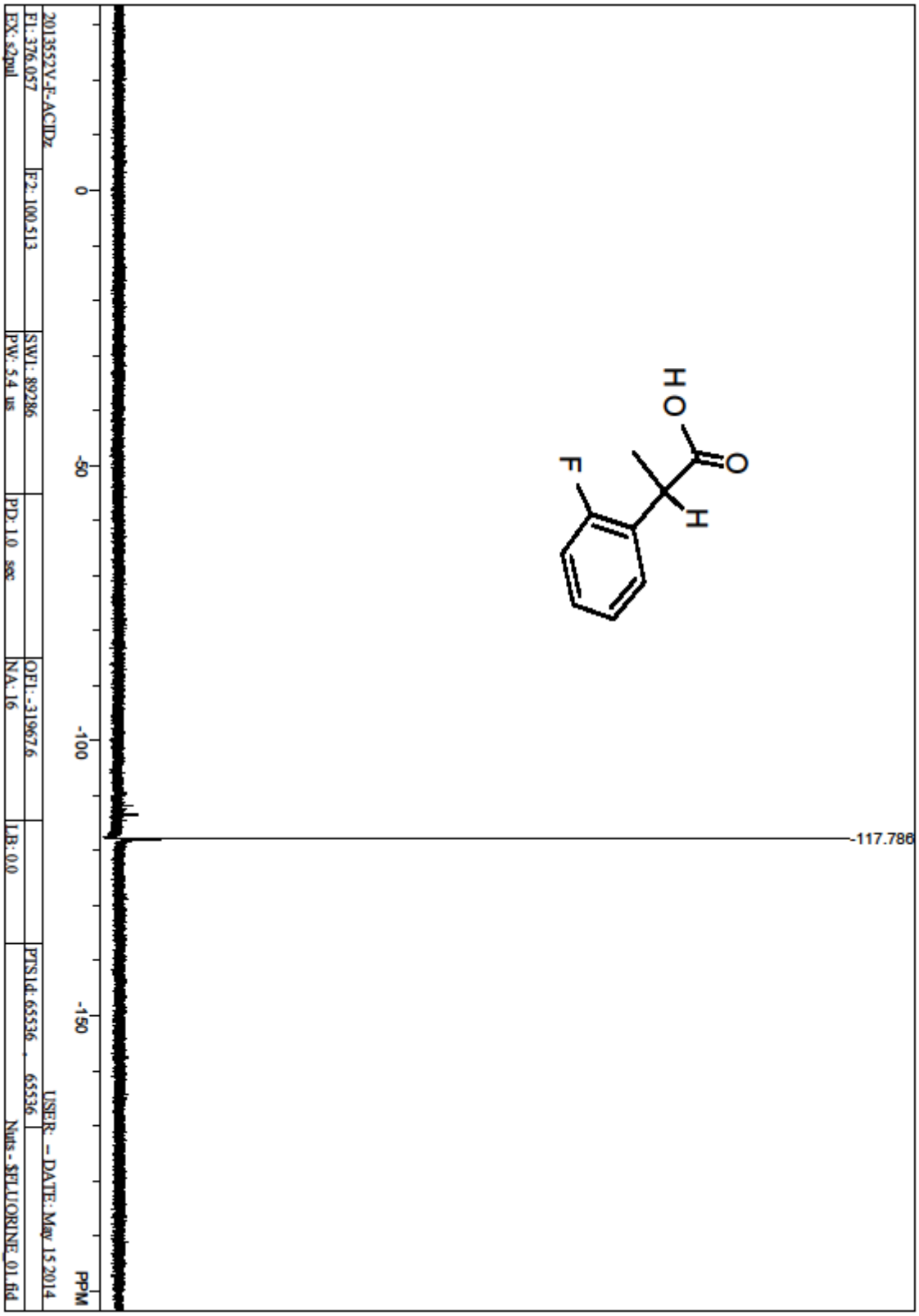

180.389
138.637
131.801
129.373
121.422
77.281
77.023
76.773
44.831
17.988
HO
O
H
Br
PPM
USER: -- DATE: Apr 23 2014
Nuts - $iv-74-ac_pslabel_02.fid
2013552iv-74-ac-cl
EX: s2pul
F1: 125.716
F2: 499.910
PW: 4.8 us
SW1: 31250
PD: 1.0 sec
NA: 256
OF1: 13827.2
LB: 0.0
PTS1d: 32768 , 32768

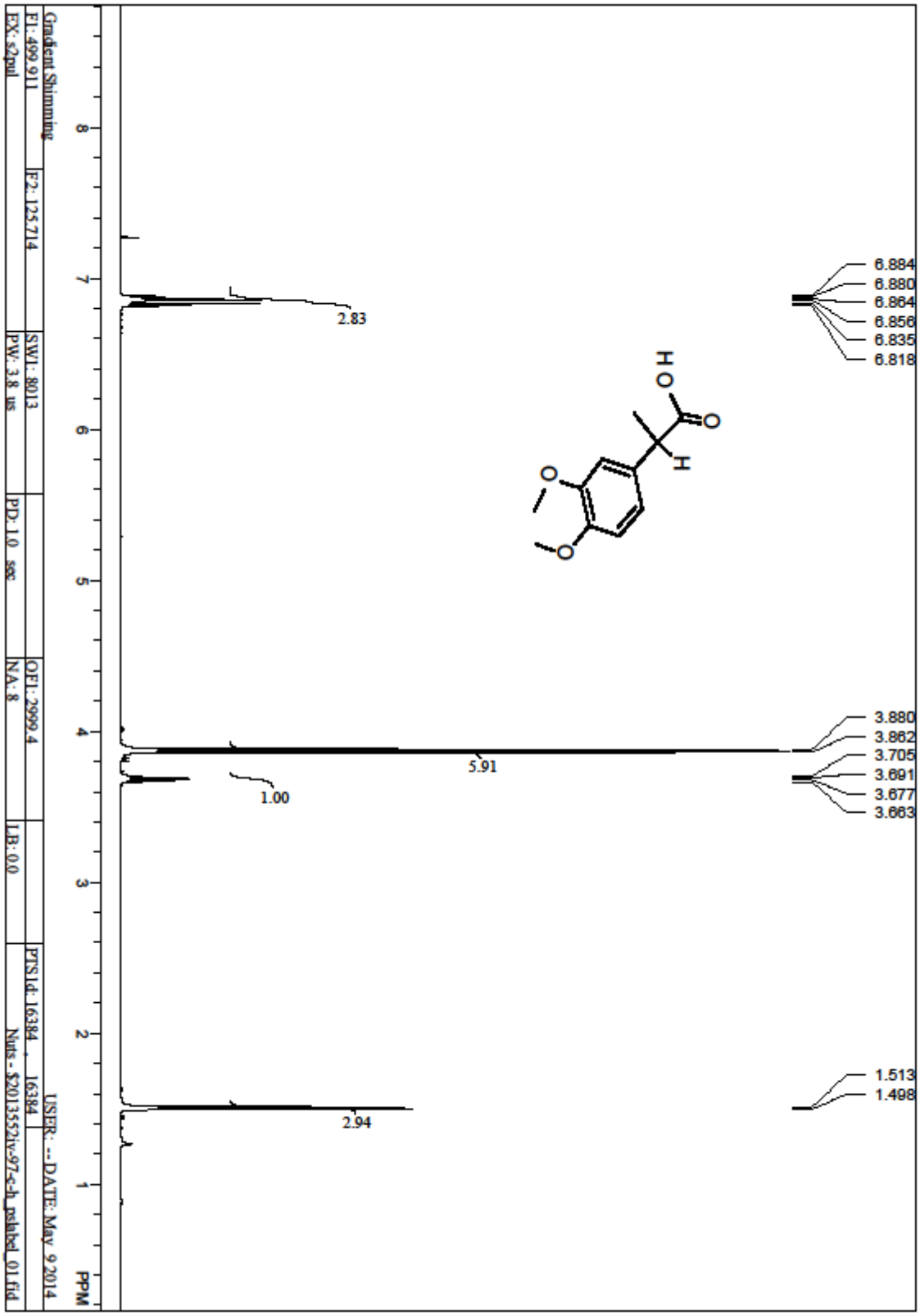

Gradient Shimming
F1: 499.911
F2: 125.714
SW1: 8013
PW: 3.8 us
PD: 1.0 sec
OF1: 2999.4
NA: 8
LB: 0.0
PTS1d: 16384
16384
EX: s2pul
USER: -- DATE: Apr 23 2014
Nuts - Siv-74-bcs_pslabel_01.fid
PPM
8
7
6
5
4
3
2
1
3.93
1.00
3.20
7.338
7.280
7.277
7.274
7.270
7.268
7.262
7.258
7.238
7.236
7.229
7.226
7.219
7.214
7.212
7.209
3.753
3.739
3.725
3.710
1.534
1.519
O
H
O
Cl

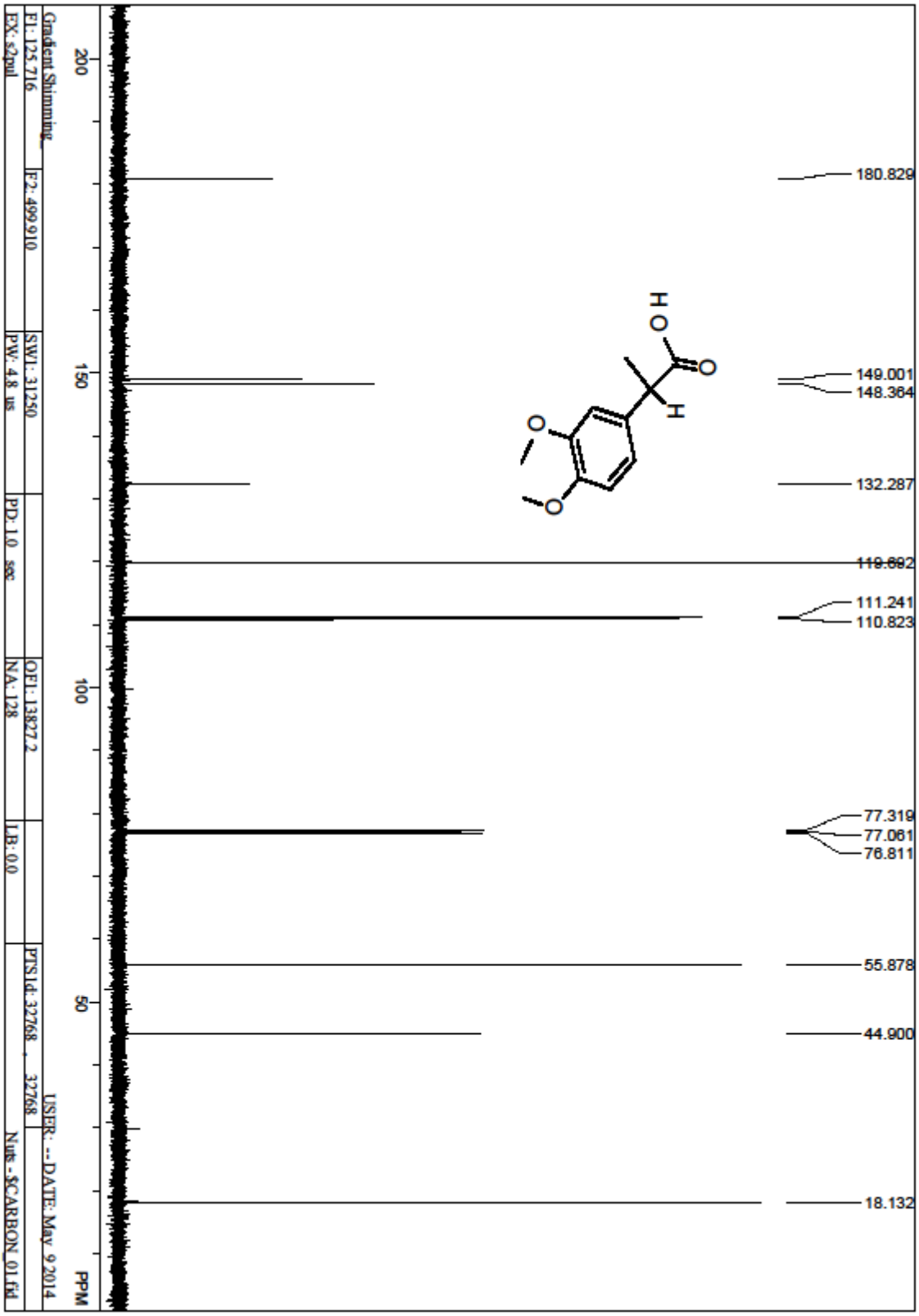

180.28
141.53
134.48
129.91
127.86
127.65
125.90
77.28
77.02
76.77
45.07
17.99
O
H
O
H
Cl

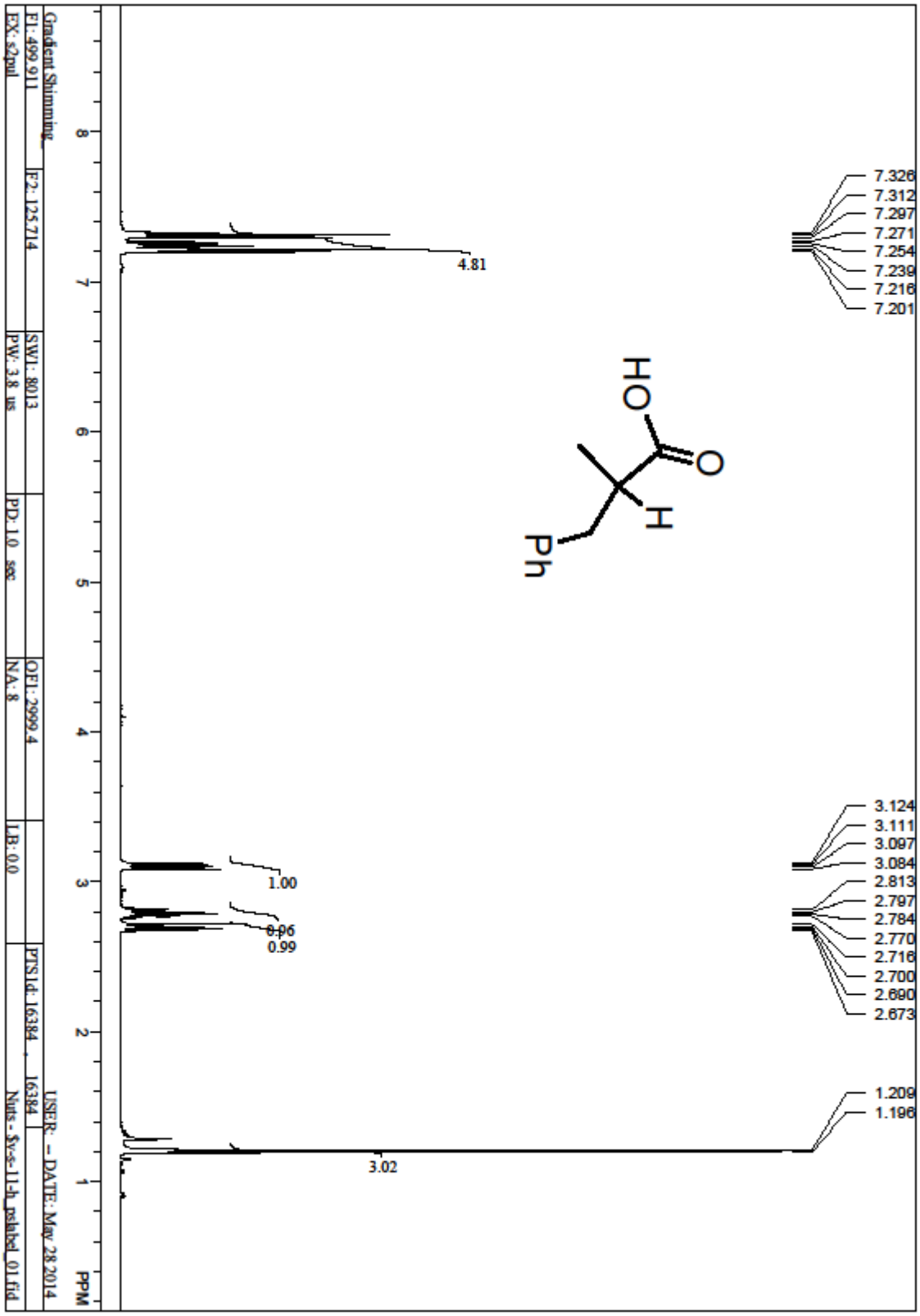

Gradient Shimming
F1: 499.911
F2: 125.714
EX: s2pul
SW1: 8013
PW: 3.8 us
PD: 1.0 sec
OF1: 2999.4
NA: 8
LB: 0.0
PTS1d: 16384
16384
USER: -- DATE: Apr 23 2014
Nuts - Siv-72-pc_pslabel_01.fid
PPM
7.351
7.348
7.336
7.333
7.320
7.317
7.292
7.289
7.277
7.272
7.266
7.263
7.258
7.251
7.248
7.157
7.142
7.127
7.087
7.069
7.051
4.099
4.085
4.070
4.055
1.552
1.538
4.05
1.00
3.30
F
HO
O
H

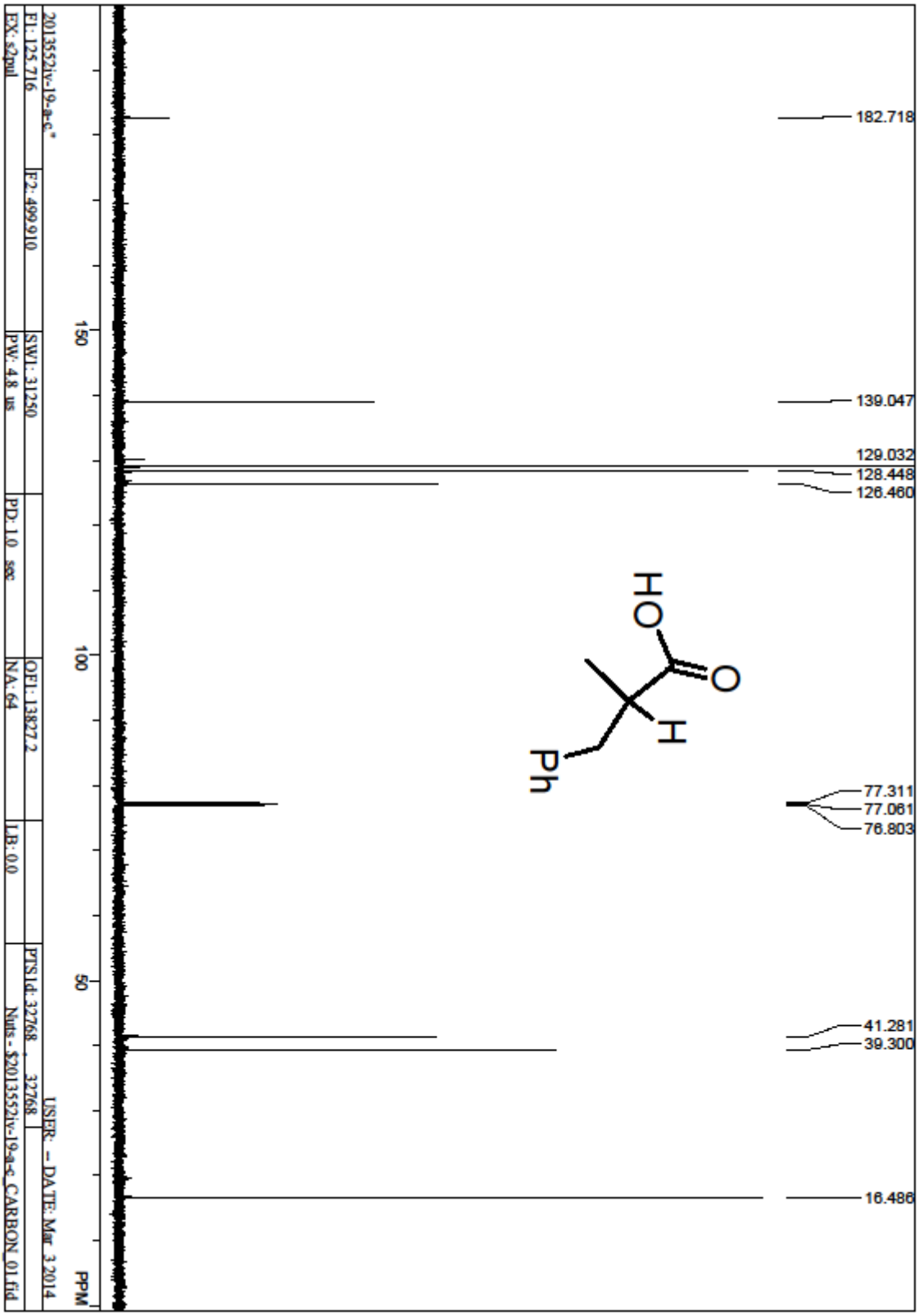

180.146
161.391
159.433
128.971
128.903
128.782
128.751
127.135
127.014
124.343
124.313
115.611
115.429
77.273
77.023
76.765
38.405
38.375
17.131
150
100
50
PPM
F
O
H
O
H
2013552iv-72-pc4h
F1: 125.716
F2: 499.910
SW1: 31250
PW: 4.8 us
PD: 1.0 sec
OF1: 13827.2
NA: 256
LB: 0.0
PTS1d: 32768 , 32768
USER: -- DATE: Apr 23 2014
EX: s2pul
Nuts - $iv-72-pc_pslabel_02.fid

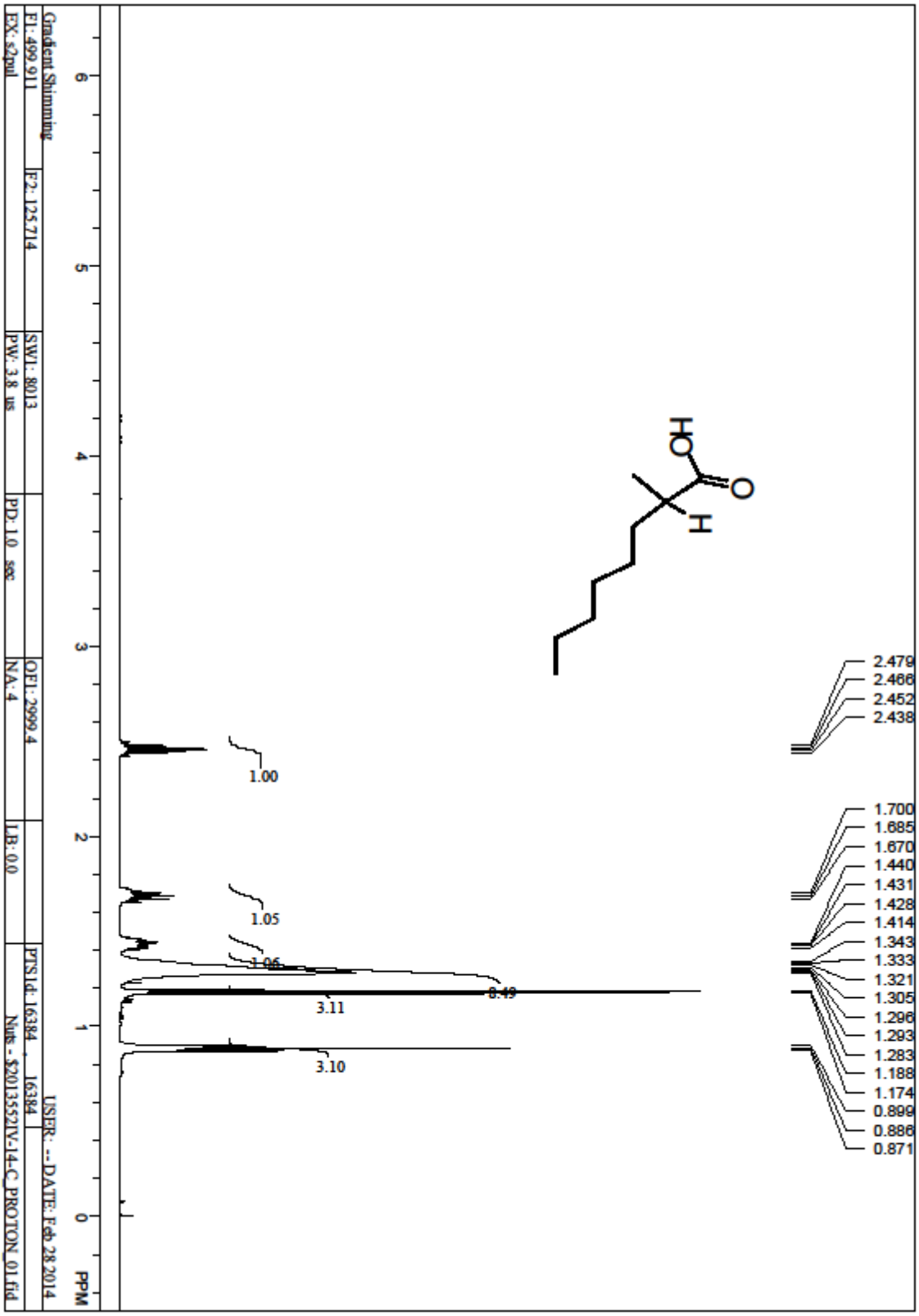

20133521V-F-ACIDz
F1: 376.057
F2: 100.513
SW1: 89286
PW: 5.4 us
PD: 1.0 sec
OF1: -319676
NA: 16
LB: 0.0
PTS1d: 65536
65536
USER: -- DATE: May 15 2014
EX: s2pul
Nuts - $FLUORINE_01.fid
-117.786
0
-50
-100
-150
PPM
H
O
O
H
F

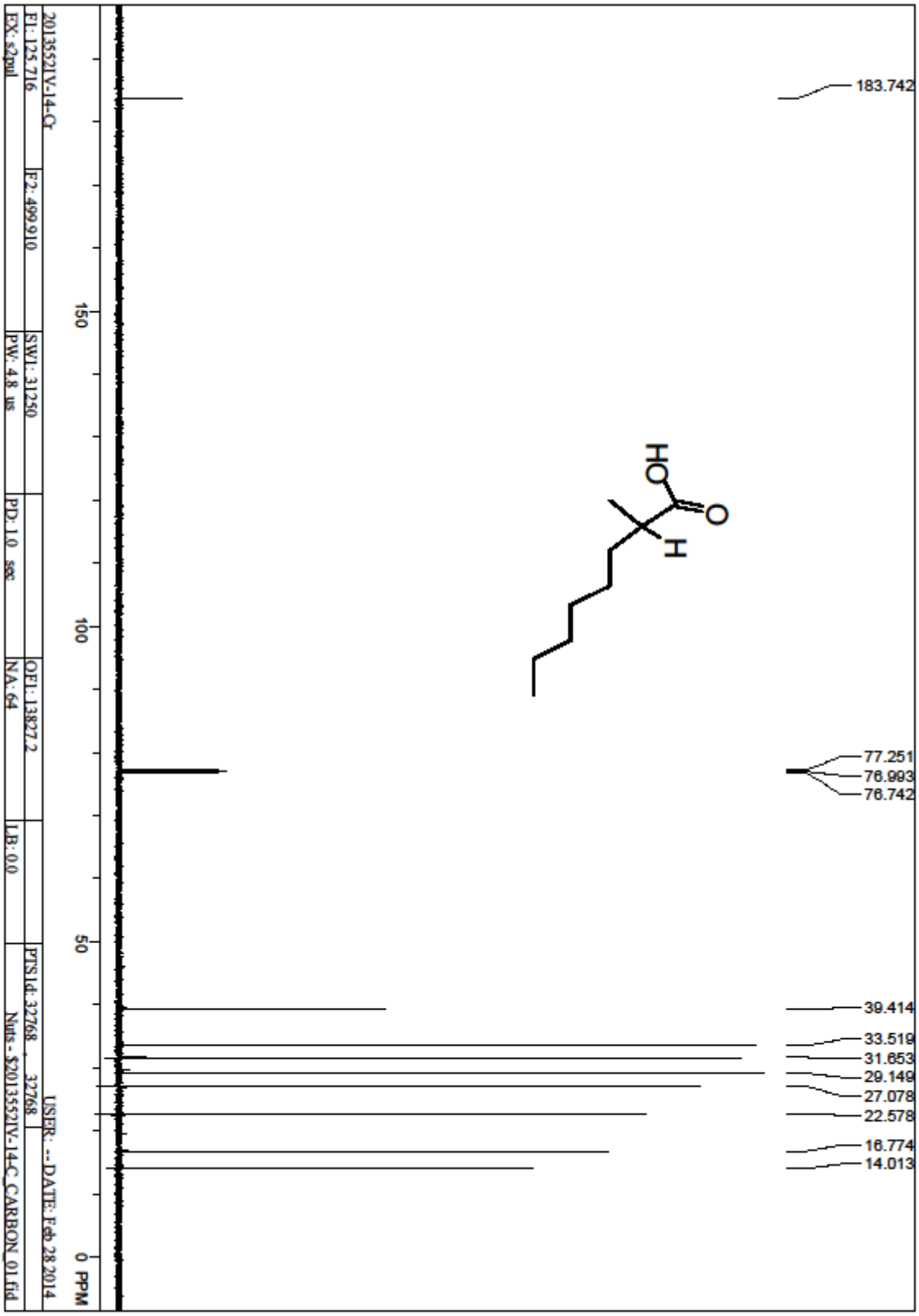

Gradient Shimming
F1: 499.911
F2: 125.714
SW1: 8013
PW: 3.8 us
PD: 1.0 sec
NA: 8
OF1: 2999.4
LB: 0.0
PTS1d: 16384
16384
EX: s2pul
Nuts - $20135521v-97-c-h_pslabel_01.fid
USER: --DATE: May 9 2014
PPM
8
7
6
5
4
3
2
1
2.83
5.91
1.00
2.94
6.884
6.880
6.864
6.856
6.835
6.818
3.880
3.862
3.705
3.691
3.677
3.663
1.513
1.498
H
O
O
H
O
O

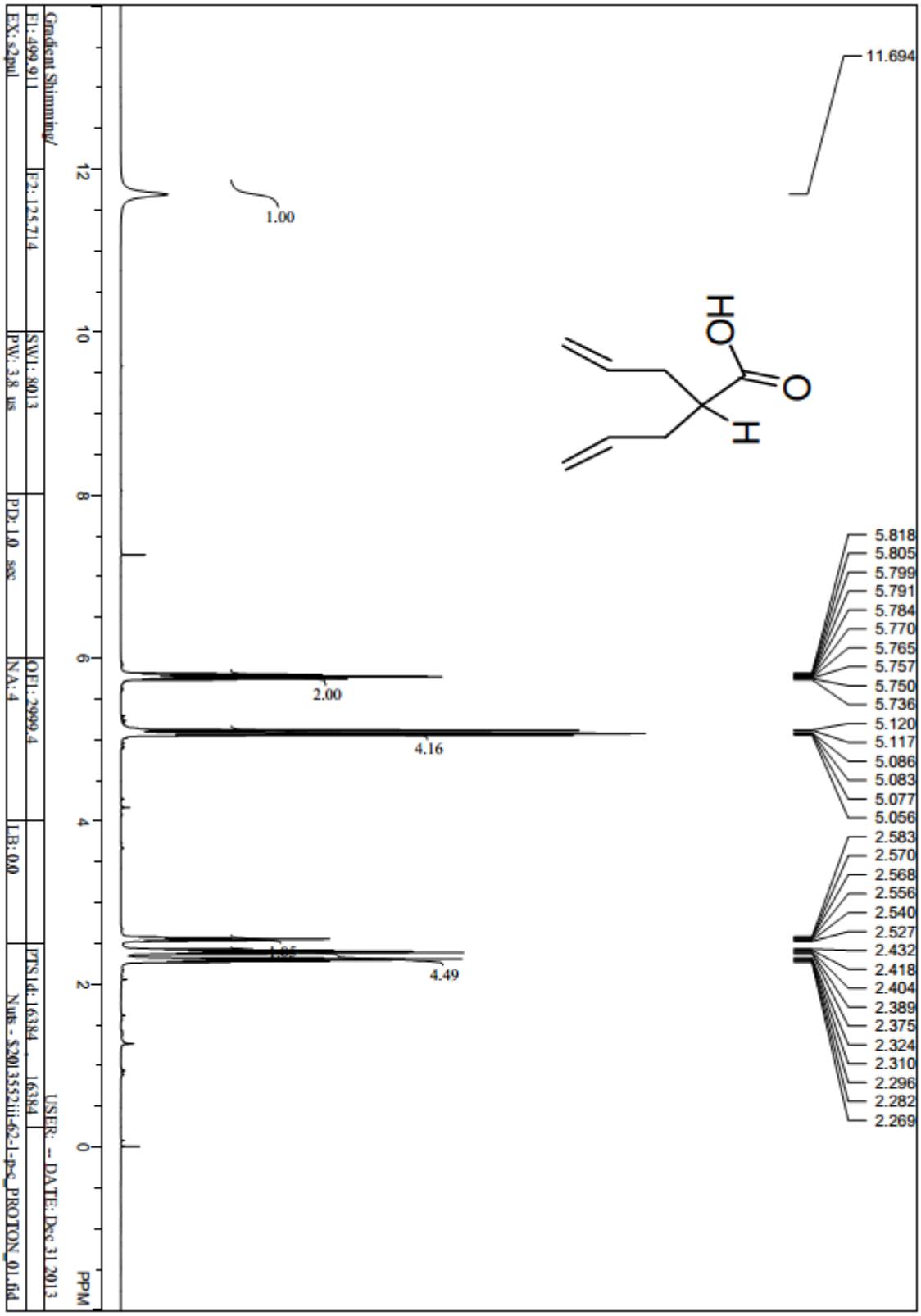

Gradient Shimming
EX: s2pul
F1: 125.716
F2: 499.910
PW: 4.8 us
SW1: 31250
PD: 1.0 sec
NA: 128
QF1: 13827.2
LB: 0.0
PTS1d: 32768
32768
USER: -- DATE: May 9 2014
Nuts -$CARBON_01.fid
200
150
100
50
PPM
180.829
149.001
148.364
132.287
119.682
111.241
110.823
77.319
77.061
76.811
55.878
44.900
18.132
H
O
O
O
O
H

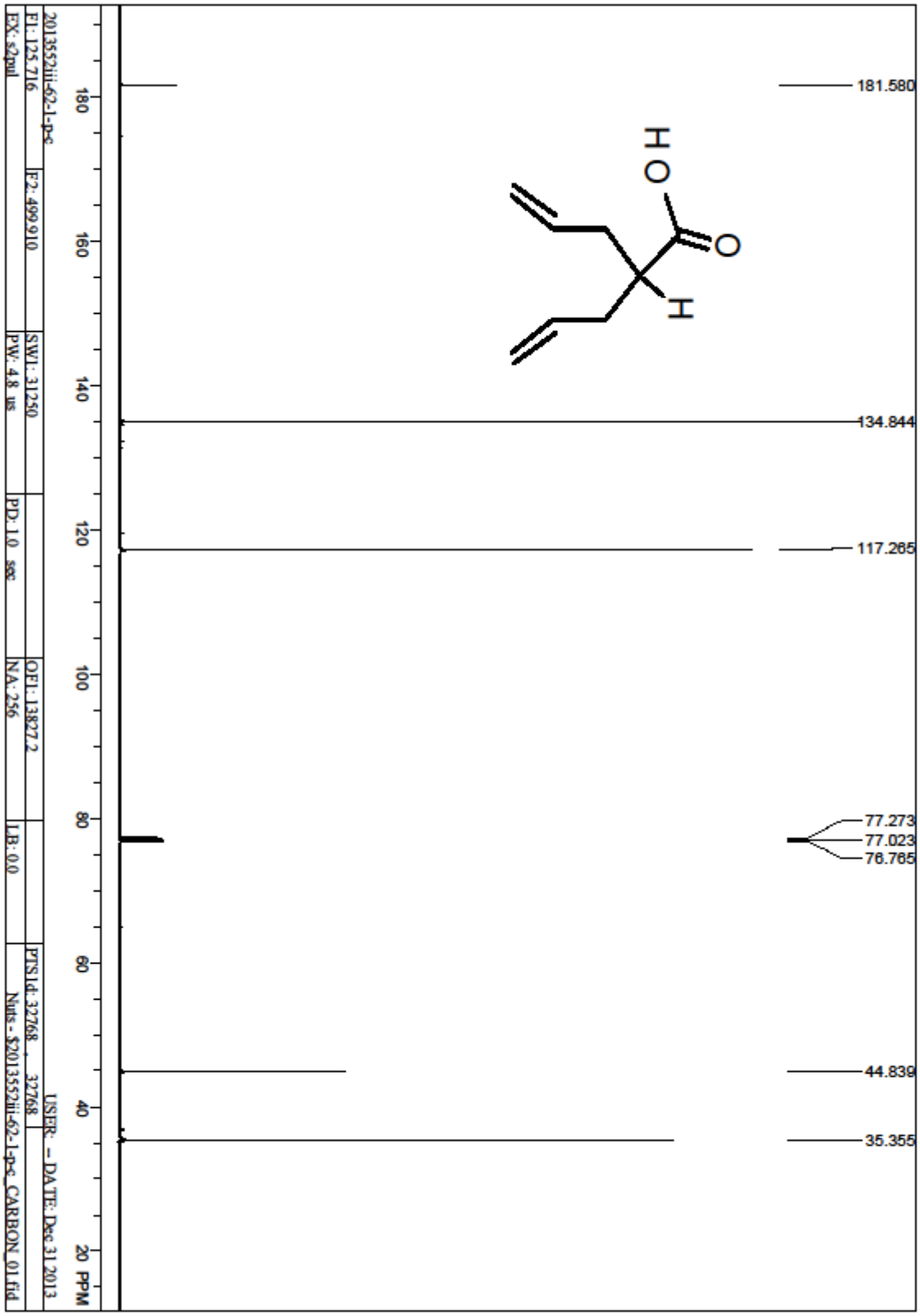

Gradient Shimming
F1: 499.911
F2: 125.714
SW1: 8013
PW: 3.8 us
PD: 1.0 sec
NA: 8
QF1: 2999.4
LB: 0.0
PTS1d: 16384
16384
USER: -- DATE: May 28 2014
EX: s2pul
Nuts-$ycs-11h_pslabel_01.fid
PPM
4.81
1.00
0.96
0.99
3.02
7.326
7.312
7.297
7.271
7.254
7.239
7.216
7.201
3.124
3.111
3.097
3.084
2.813
2.797
2.784
2.770
2.716
2.700
2.690
2.673
1.209
1.196
HO
O
H
Ph

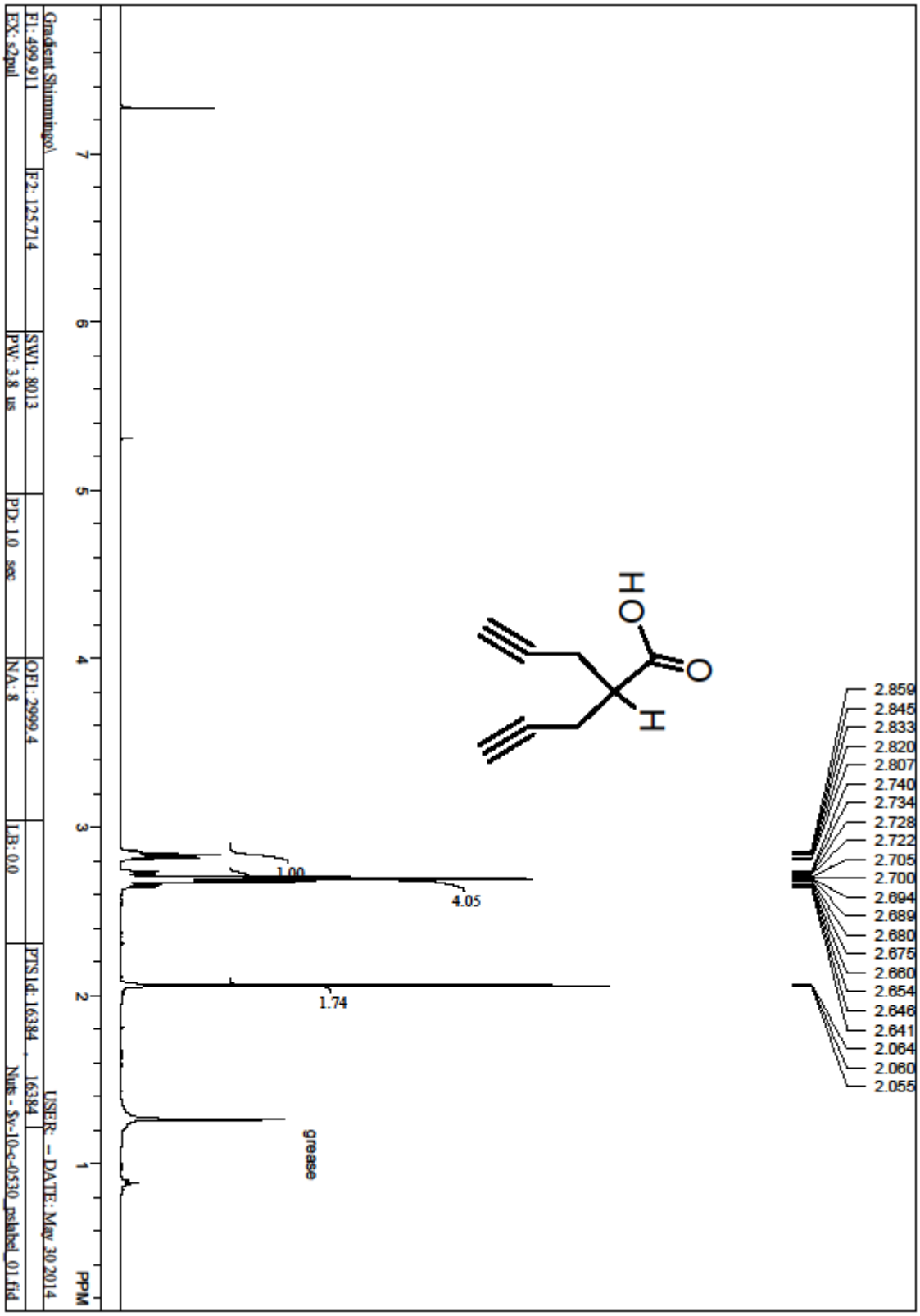

182.718
139.047
129.032
128.448
126.460
77.311
77.061
76.803
41.281
39.300
16.486
HO
O
H
Ph
150
100
50
PPM
2013552iv-19-a-c.*
EX: s2pul
F1: 125.716
F2: 499.910
PW: 4.8 us
SW1: 31250
PD: 1.0 sec
NA: 64
OF1: 13827.2
LB: 0.0
PTS1d: 32768
32768
USER: – DATE: Mar 3 2014
Nuts - $2013552iv-19-a-c_CARBON_01.fid

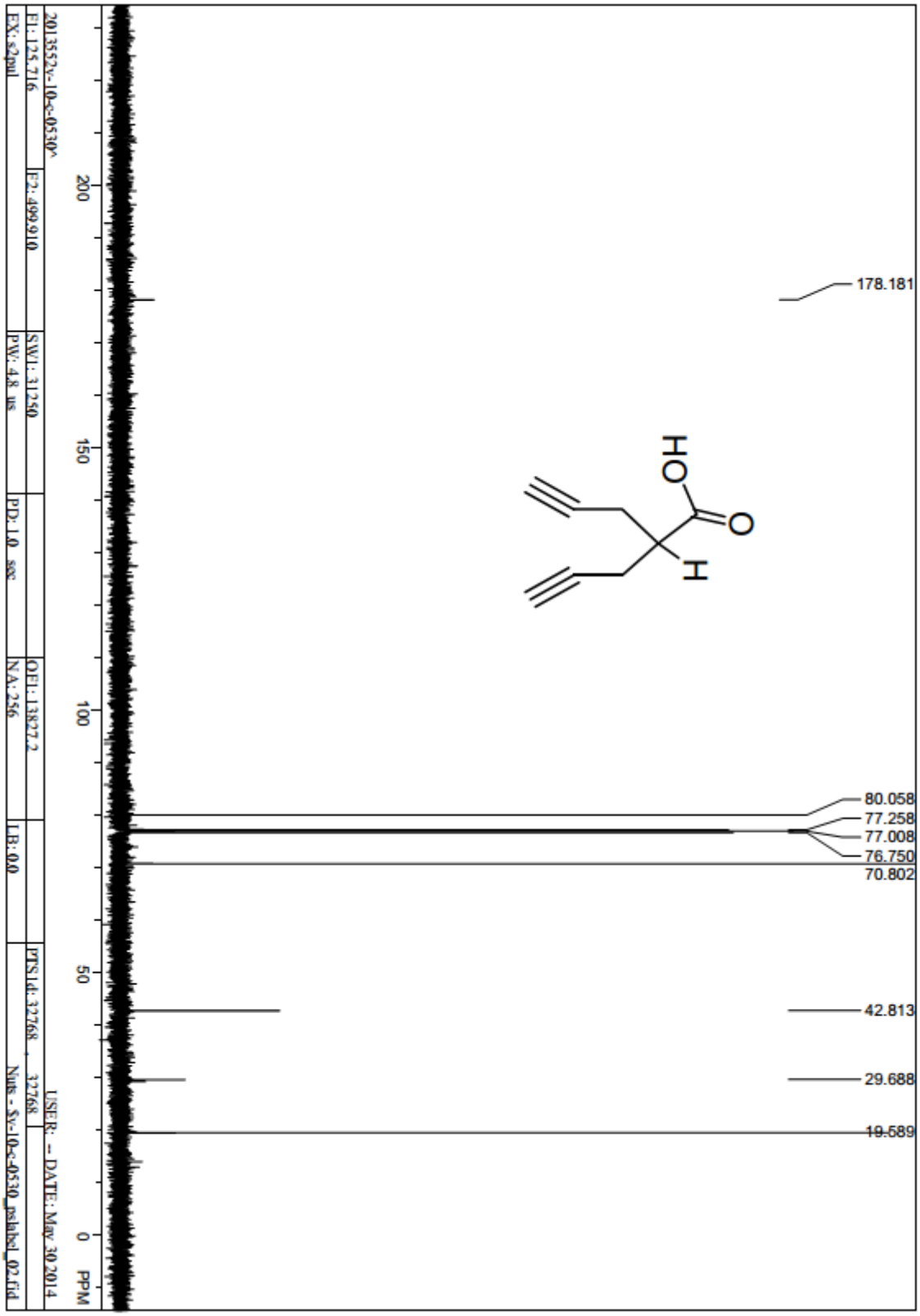

Gradient Shimming
F1: 499.911
F2: 125.714
EX: s2pul
SW1: 8013
PW: 3.8 us
PD: 1.0 sec
OF1: 2999.4
NA: 4
LB: 0.0
PTS1d: 16384
16384
Nuts - $20135521V-14-C_PROTON_01.fid
USER: --DATE: Feb 28 2014
PPM
0
1
2
3
4
5
6
1.00
1.05
1.06
8.49
3.11
3.10
2.479
2.466
2.452
2.438
1.700
1.685
1.670
1.440
1.431
1.428
1.414
1.343
1.333
1.321
1.305
1.296
1.293
1.283
1.188
1.174
0.899
0.886
0.871
HO
O
H

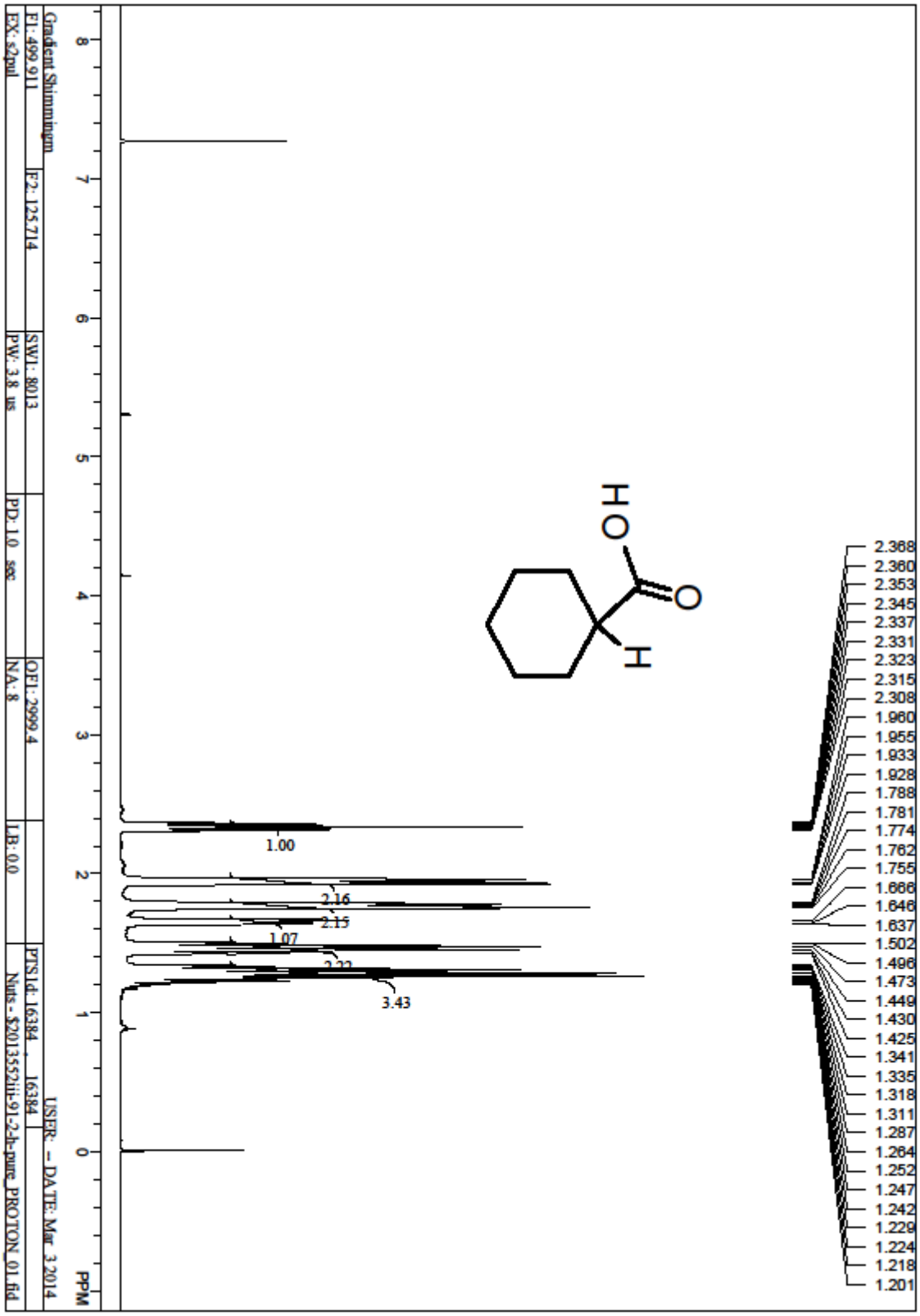

183.742
77.251
76.993
76.742
39.414
33.519
31.653
29.149
27.078
22.578
16.774
14.013
HO
O
H
150
100
50
0 PPM
2013552IV-14-Cr
F1: 125.716
F2: 499.910
SW1: 31250
PW: 4.8 us
PD: 1.0 sec
QE1: 13827.2
NA: 64
LB: 0.0
PTS1d: 32768
32768
USER: --DATE: Feb 28 2014
EX: s2pul
Nuts - $2013552IV-14-C_CARBON_01.fid

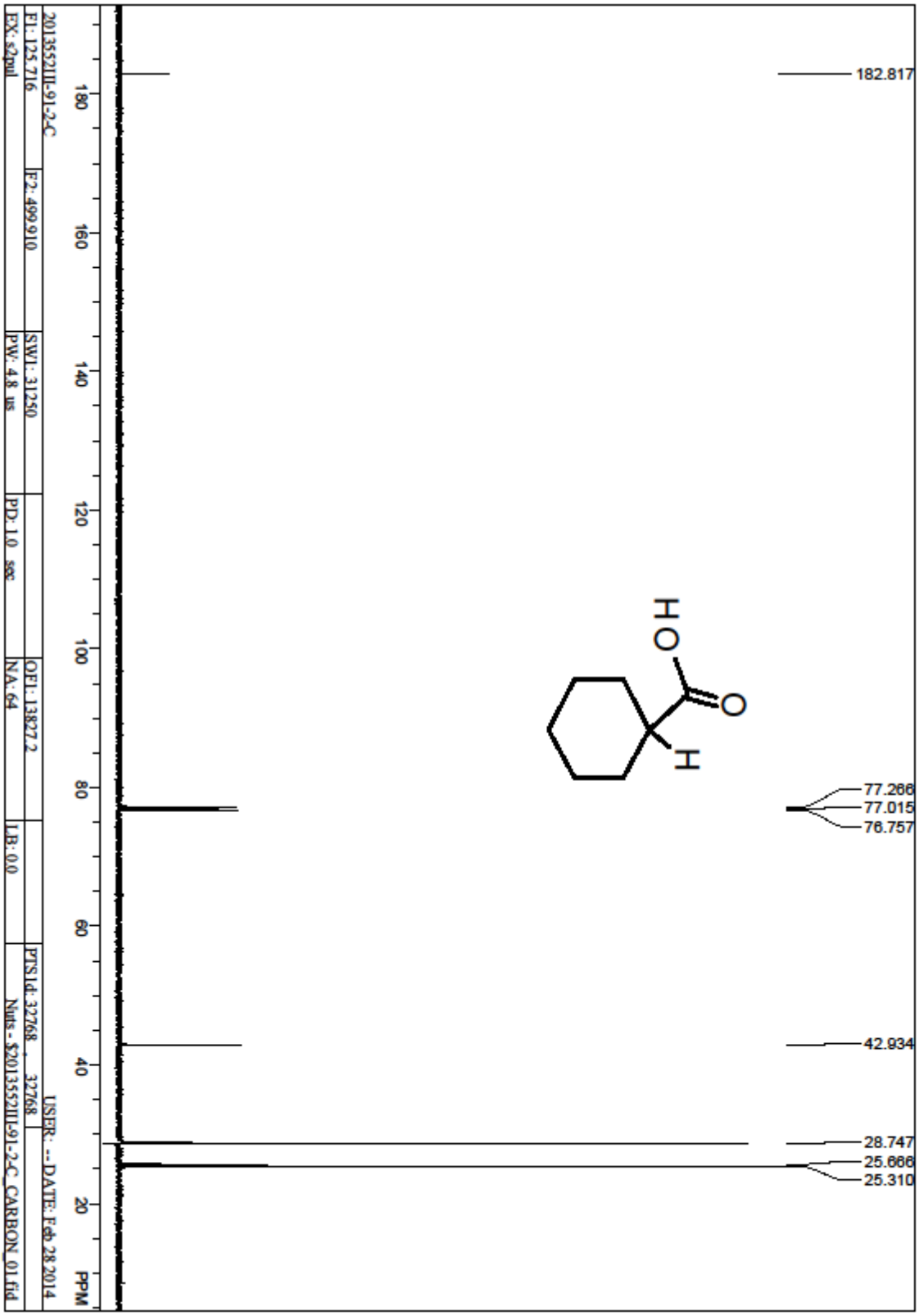

Gradient Shimming/
F1: 499.911
F2: 125.714
SW1: 8013
PW: 3.8 us
PD: 1.0 sec
NA: 4
OE1: 2999.4
LB: 0.0
PTS1d: 16384
16384
Nuts - S20135521ii-62-1-pcs_PROTON_01.fid
USER: -- DATE: Dec 31 2013
EX: s2pul
PPM
0
2
4
6
8
10
12
11.694
1.00
2.00
4.16
1.85
4.49
5.818
5.805
5.799
5.791
5.784
5.770
5.765
5.757
5.750
5.736
5.120
5.117
5.086
5.083
5.077
5.056
2.583
2.570
2.568
2.556
2.540
2.527
2.432
2.418
2.404
2.389
2.375
2.324
2.310
2.296
2.282
2.269
OH
O
H

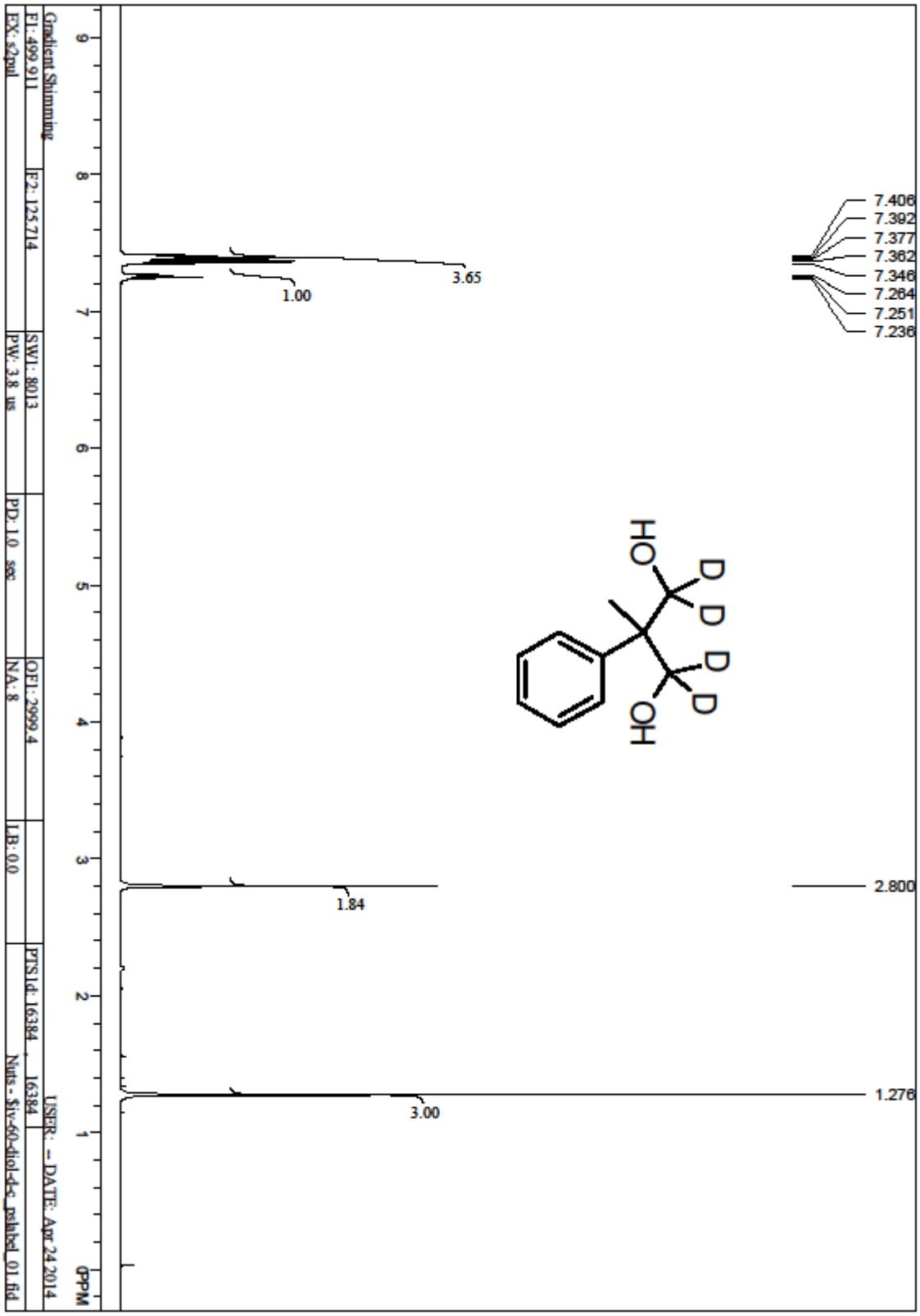

181.580
134.844
117.265
77.273
77.023
76.765
44.839
35.355
180
160
140
120
100
80
60
40
20 PPM
O
H
O
H
20135521ii-62-1-pc
F1: 125.716
F2: 499.910
SW1: 31250
PW: 4.8 us
PD: 1.0 sec
QF1: 13827.2
NA: 256
LB: 0.0
PTS1d: 32768 x 32768
USER: -- DATE: Dec 31 2013
EX: s2pul
Nuts - $20135521ii-62-1-pc_CARBON_01.fid

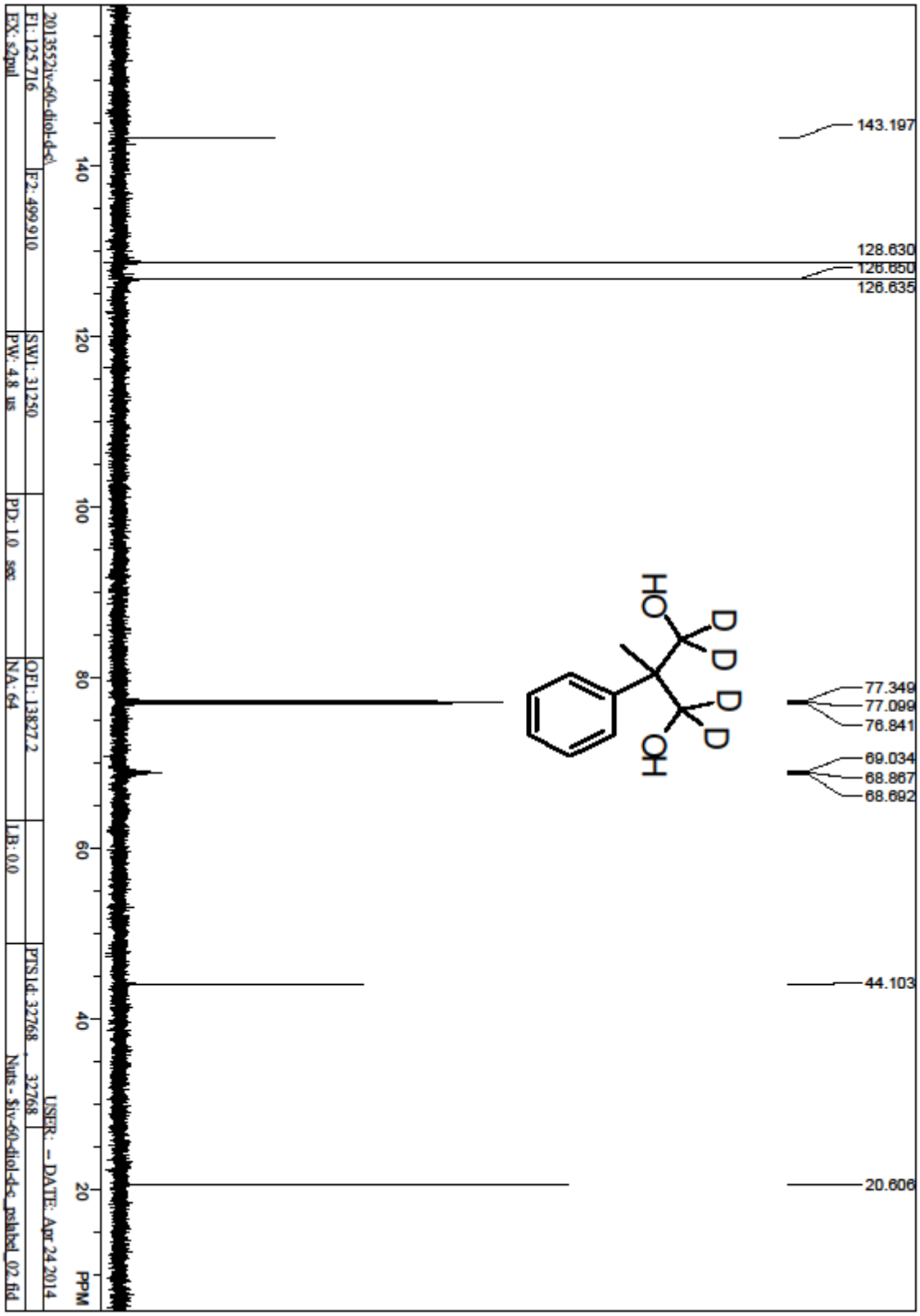

Gradient Shimming\
F1: 499.911
F2: 125.714
SW1: 8013
PW: 3.8 us
PD: 1.0 sec
OF1: 2999.4
NA: 8
LB: 0.0
PTS1d: 16384
16384
USER: -- DATE: May 30 2014
EX: s2pul
Nuts - $y-10-c-0530_pslabel_01.fid
PPM
1.00
4.05
1.74
grease
2.859
2.845
2.833
2.820
2.807
2.740
2.734
2.728
2.722
2.705
2.700
2.694
2.689
2.680
2.675
2.660
2.654
2.646
2.641
2.064
2.060
2.055

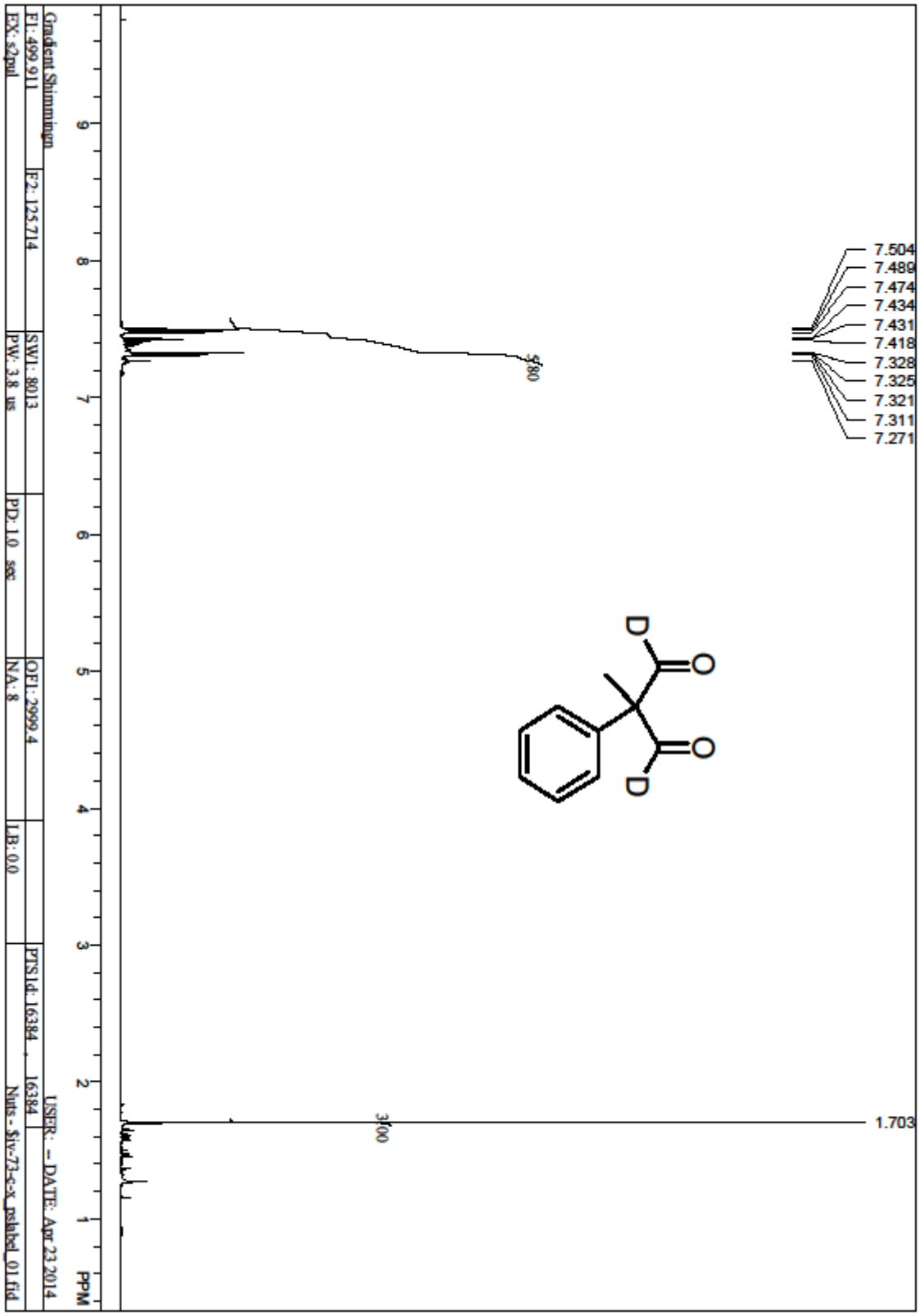

178.181
80.058
77.258
77.008
76.750
70.802
42.813
29.688
19.589
200
150
100
50
0
PPM
HO
O
H
USER: -- DATE: May 30 2014
20133527c-10-c-0530^
EX: s2pul
F1: 125.716
F2: 499.910
SW1: 31250
PW: 4.8 us
PD: 1.0 sec
OF1: 13827.2
NA: 256
LB: 0.0
PTS1d: 32768
32768
Nuts - $c-10-c-0530_pslabel_02.fid

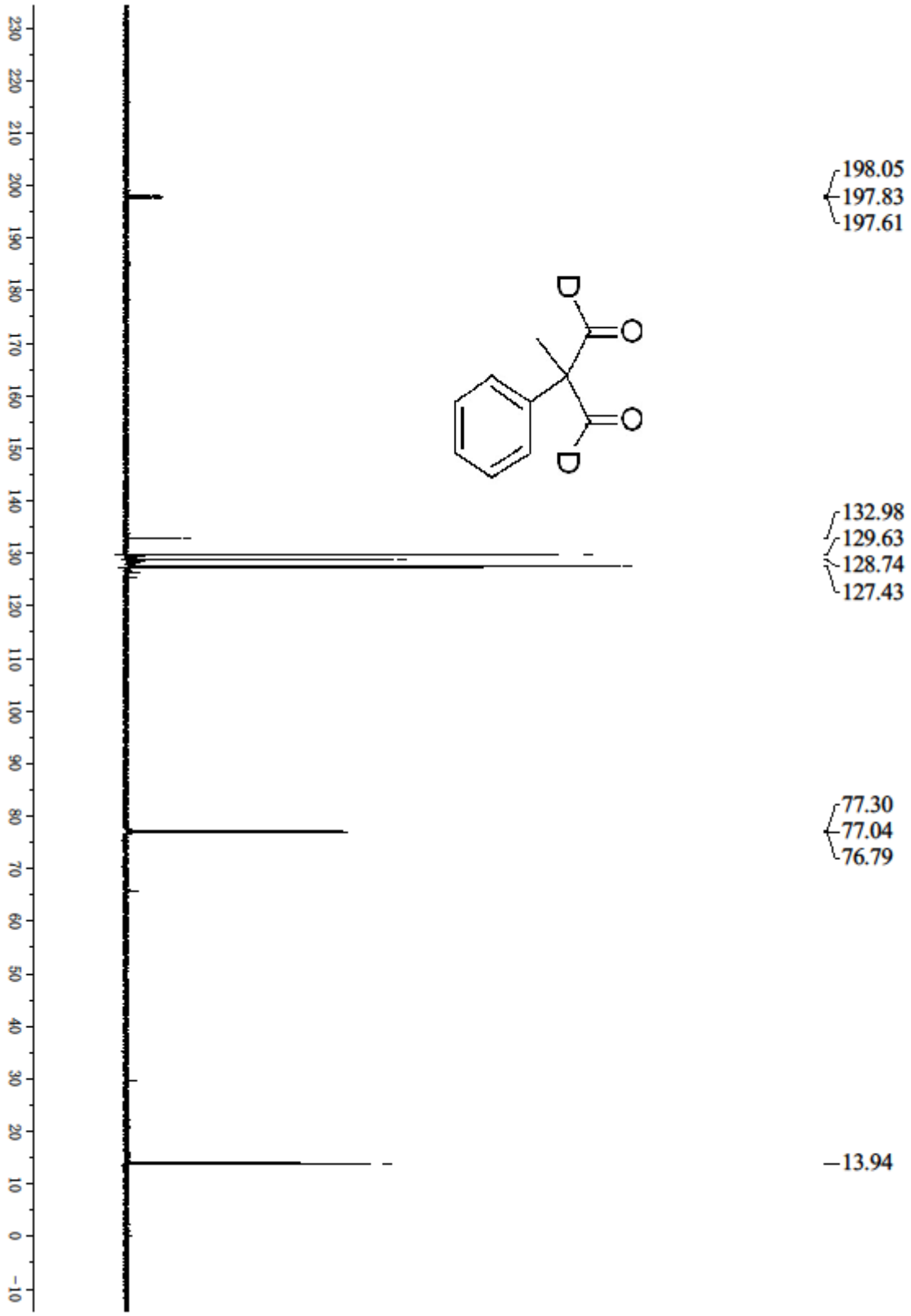

Gradient Shimmingpm
F1: 499.911
F2: 125.714
SW1: 8013
PW: 3.8 us
PD: 1.0 sec
OF1: 2999.4
NA: 8
LB: 0.0
PTS1d: 16384
16384
USER: – DATE: Mar 3 2014
EX: s2pul
Nmts - $20133552iit-91-2-h-pure_PROTON_01.fid
PPM
1.00
2.16
2.15
1.07
3.43
2.368
2.360
2.353
2.345
2.337
2.331
2.323
2.315
2.308
1.960
1.955
1.933
1.928
1.788
1.781
1.774
1.762
1.755
1.666
1.646
1.637
1.502
1.496
1.473
1.449
1.430
1.425
1.341
1.335
1.318
1.311
1.287
1.264
1.252
1.247
1.242
1.229
1.224
1.218
1.201

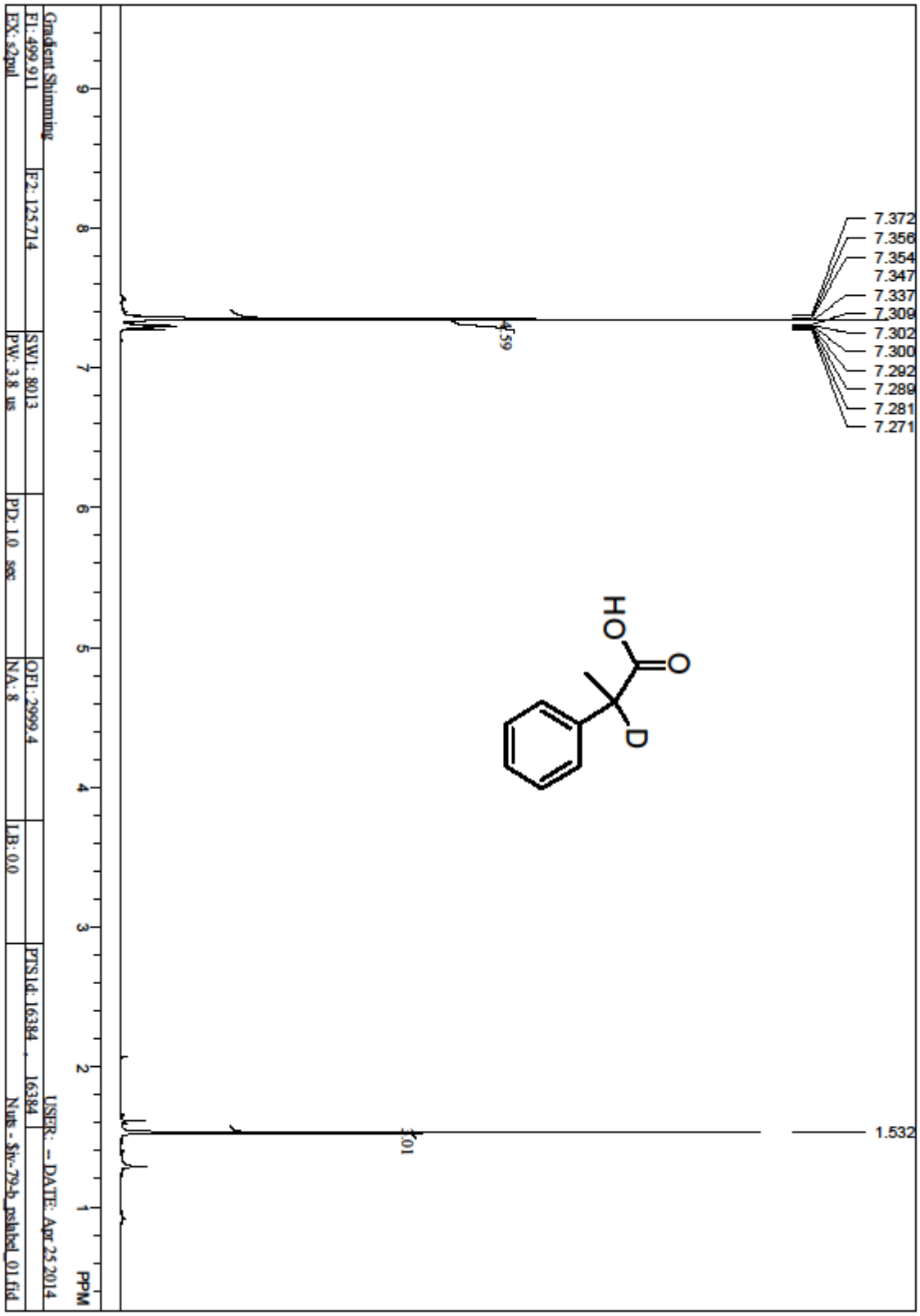

182.817
77.266
77.015
76.757
42.934
28.747
25.666
25.310
O
H
O
H
180
160
140
120
100
80
60
40
20
PPM
20135521II-91-2-C
EX: s2pul
F1: 125.716
F2: 499.910
SW1: 31250
PW: 4.8 us
PD: 1.0 sec
OF1: 13827.2
NA: 64
LB: 0.0
PTS1d: 32768 → 32768
USER: --DATE: Feb 28 2014
Nuts-$20135521II-91-2-C_CARBON_01.fid

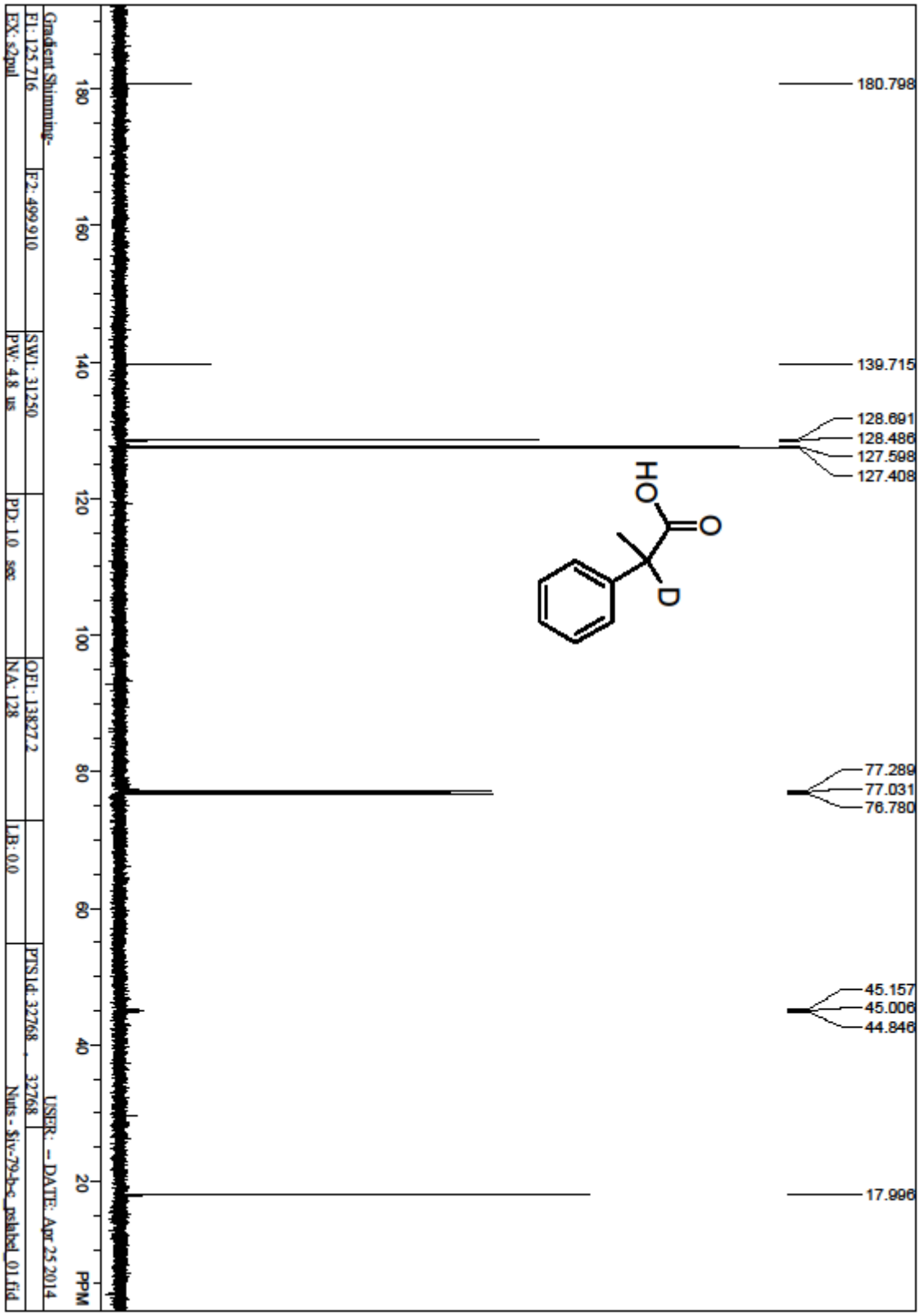

Gradient Shimming
F1: 499.911
F2: 125.714
EX: s2pul
SW1: 8013
PW: 3.8 us
PD: 1.0 sec
OF1: 2999.4
NA: 8
LB: 0.0
PTS1d: 16384
16384
USER: -- DATE: Apr 24 2014
Nuts - $iv-60-diol-dc_pslabel_01.fid
PPM
1.00
3.65
1.84
3.00
7.406
7.392
7.377
7.362
7.346
7.264
7.251
7.236
2.800
1.276
HO
D
D
D
D
OH


143.197
128.630
126.650
126.635
77.349
77.099
76.841
69.034
68.867
68.692
44.103
20.606
HO
D D D D
OH
140
120
100
80
60
40
20
PPM
2013552iv-60-diol-dc\
F1: 125.716
F2: 499.910
SW1: 31250
PW: 4.8 us
PD: 1.0 sec
OF1: 13827.2
NA: 64
LB: 0.0
PTS1d: 32768 _ 32768
EX: s2pul
USER: -- DATE: Apr 24 2014
Nuts - $iv-60-diol-dc_pslabel_02.fid


Gradient Shimming
F1: 499.911
F2: 125.714
SW1: 8013
PW: 3.8 us
PD: 1.0 sec
OF1: 2999.4
NA: 8
LB: 0.0
PTS1d: 16384
16384
USER: -- DATE: Apr 23 2014
EX: s2pul
Nuts - Siv-73-c-x_pslabel_01.fid
7.504
7.489
7.474
7.434
7.431
7.418
7.328
7.325
7.321
7.311
7.271
1.703
3.00
9.80
PPM
D
O
O
D


198.05
197.83
197.61
132.98
129.63
128.74
127.43
77.30
77.04
76.79
13.94


Gradient Shimming
F1: 499.911
F2: 125.714
SW1: 8013
PW: 3.8 us
PD: 1.0 sec
QF1: 2999.4
NA: 8
LB: 0.0
PTS1d: 16384
16384
USER: -- DATE: Apr 25 2014
EX: s2pul
Nuts - $hc-79-b_pslabel_01.fid
PPM
7.372
7.356
7.354
7.347
7.337
7.309
7.302
7.300
7.292
7.289
7.281
7.271
4.59
1.01
1.532
HO
O
D


Gradient Shimming-
EX: s2pul
F1: 125.716
F2: 499.910
PW: 4.8 us
SW1: 31250
PD: 1.0 sec
OF1: 13827.2
NA: 128
LB: 0.0
PTS1d: 32768 , 32768
USER: -- DATE: Apr 25 2014
Nuts - Siv-79-bc_pslabel_01.fid
PPM
180.798
139.715
128.691
128.486
127.598
127.408
77.289
77.031
76.780
45.157
45.006
44.846
17.996
HO
O
D