Electronic Supporting Information for "Characterization of Phosphonic Acid Binding to Zinc Oxide"

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Instrumentation Details

XPS Peak Fitting

Peak fitting was accomplished using eXPFit, a set of macros designed for use with Microsoft Excel. Parameters for peak fitting of the O(1s) peak of the various ZnO substrates are listed in the table below.

Sample	Solvent Cleaned ZnO		Oxygen plasma etched ZnO			ODPA modified ZnO		
Binding Energy (eV)	529.98	531.66	529.96	531.65	532.40	529.80	531.00	531.50
Height (a.u.)	9530	4080	10820	3400	1400	3420	1700	2.1
LFWHM (eV)	1.276	1.792	1.150	1.900	1.900	1.400	2.300	2.100
RFWHM (eV)	1.276	1.792	1.150	1.900	1.900	1.400	2.300	2.100
LGaussian	0.912	0.863	0.900	1.000	1.600	0.900	0.950	0.800
RGaussian	0.912	0.863	0.900	1.000	1.600	0.900	0.950	0.800
Area (a.u.)	13412	8217	13787	6876	2136	5305	4247	2273

AFM

All AFM images were acquired under atmospheric conditions using a commercial MultiMode AFM (Veeco, CA) Dimension 3100 equipped with a NanoScope III controller. The microscope was housed within an acoustic isolation hood and stabilized on a floating nitrogen table (Micro-g, Technical Manufacturing Corporation, MA). The AFM piezo scanner was calibrated using a 3D reference silicon grating (Veeco, part number 498-000-026) with a 10 μm lateral pitch and a step height of 200 nm. Cantilevers (NSC35/NoAl, Mikromasch, CA) were made from n-type silicon (phosphorus doped), utilizing cantilevers 110 and 130 ± 5 μm in length, which have a typical probe radius of 10 nm and typical spring constants of 7.5 and 4.5 N/m, respectively. Image processing was performed using NanoScope III version 5.30r1 from Digital Instruments.

Lateral force microscopy images (LFM) were obtained in contact mode with a deflection set point of 0.5 V for each sample using the same tip (NSC35/NoAl, 130 ± 5 μm cantilever length) for measurements on all four sample types. These 10 μm images were collected at a speed of 20 μm/s with a 90° scan angle. The LFM retrace was subtracted from the LFM trace and the resulting image flattened using a first order polynomial background. Each sample was examined in three areas to ensure data consistency across the entire surface.

Additional Experimental Data

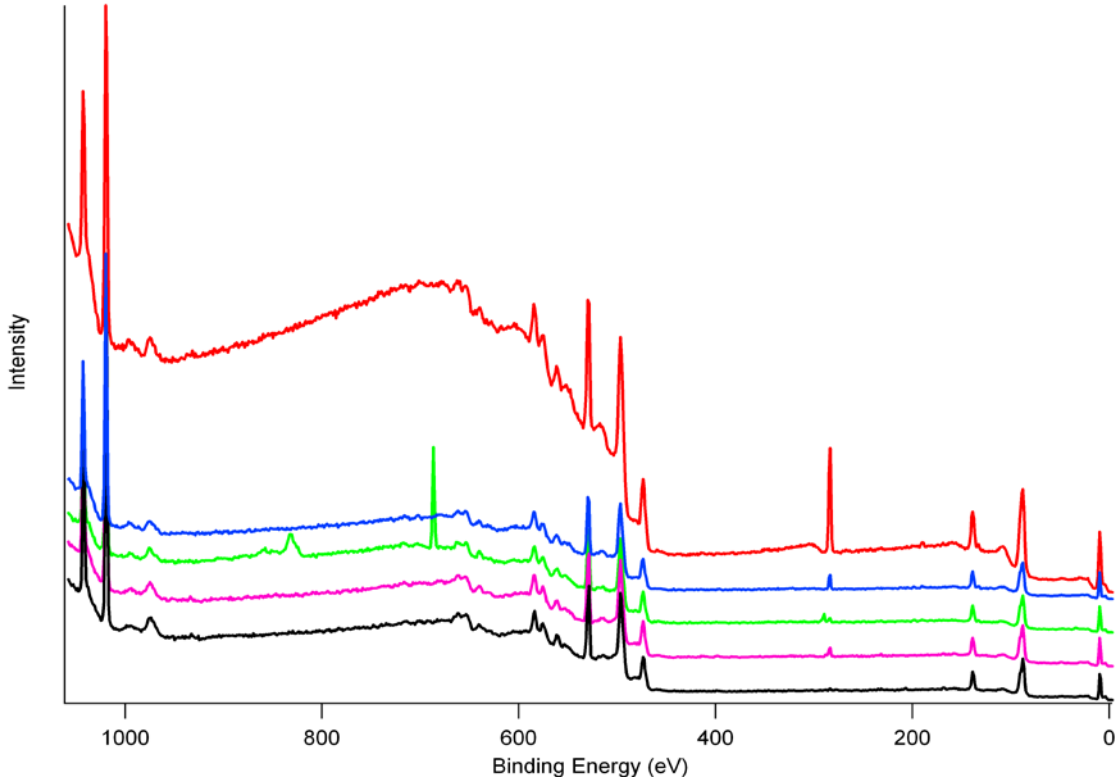


Figure SI-1. XPS spectra of ZnO (pink), oxygen plasma etched ZnO (black), OPA–modified ZnO (blue), ODPA–modified ZnO (red), and FHOPA–modified ZnO (green). The spectra have been offset for clarity.

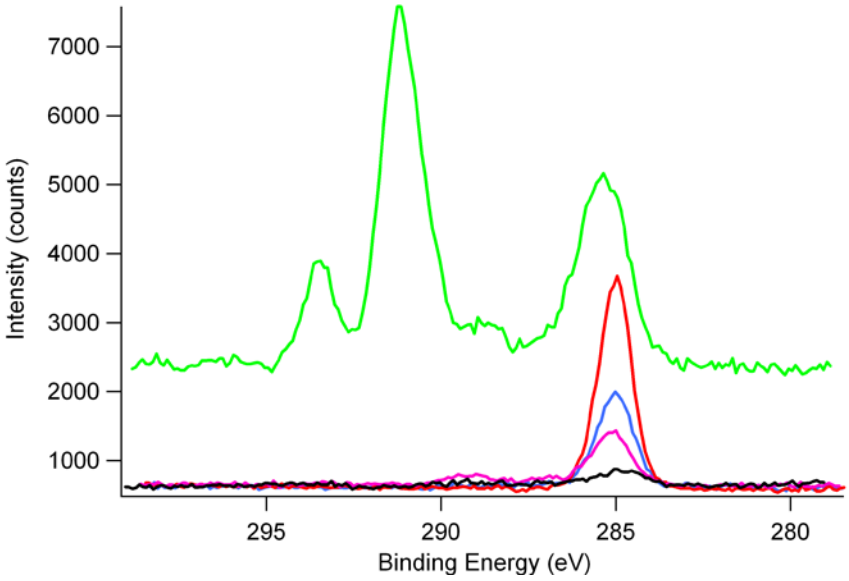


Figure SI-2. XPS C(1s) peaks of ZnO (pink), oxygen plasma etched ZnO (black), OPA–modified ZnO (blue), ODPA–modified ZnO (red), and FHOPA–modified ZnO (green).

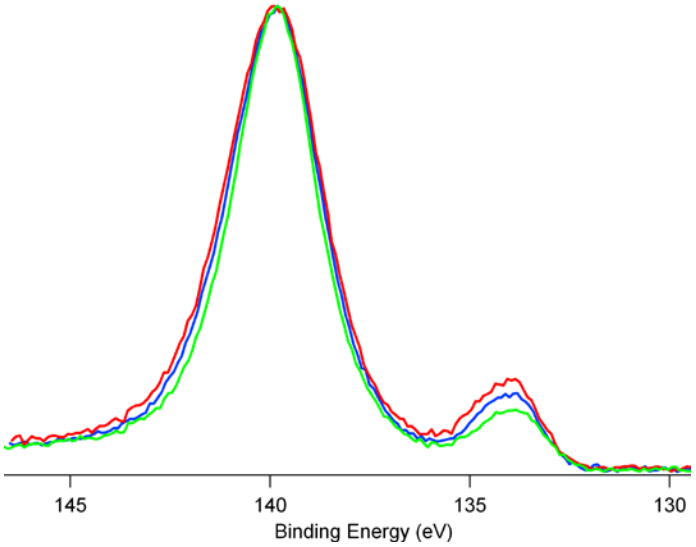


Figure SI-3. XPS P(2p) peaks (~ 134 eV) of OPA–modified ZnO (blue), ODPA–modified ZnO (red), and FHOPA–modified ZnO (green). The Zn(3s) peaks (~140 eV) were normalized.

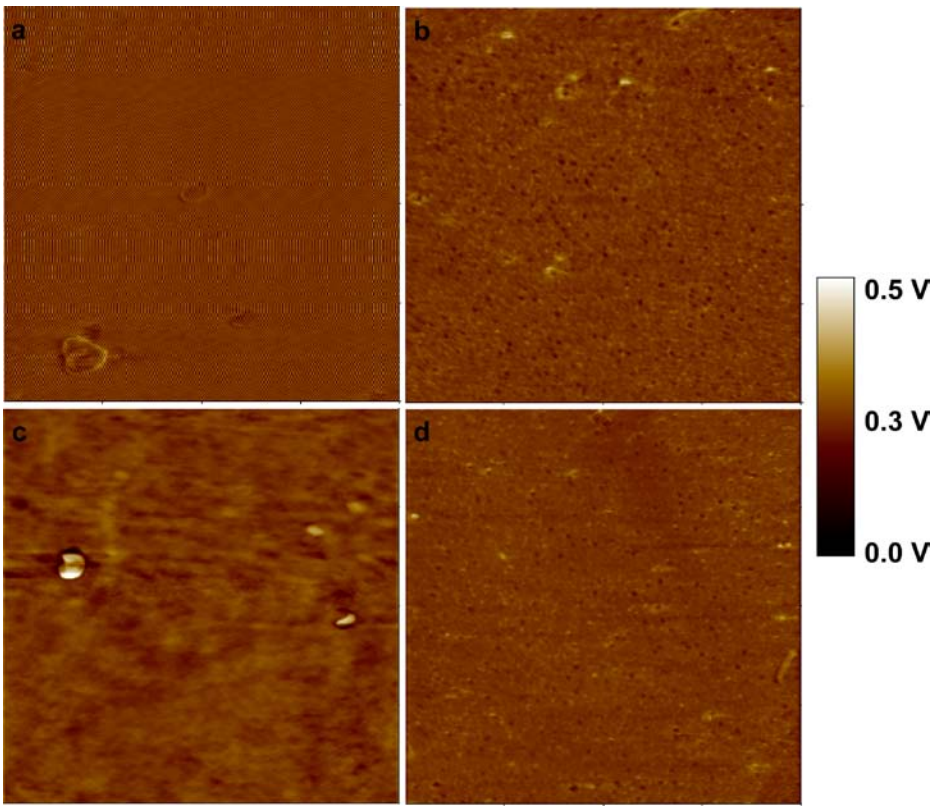
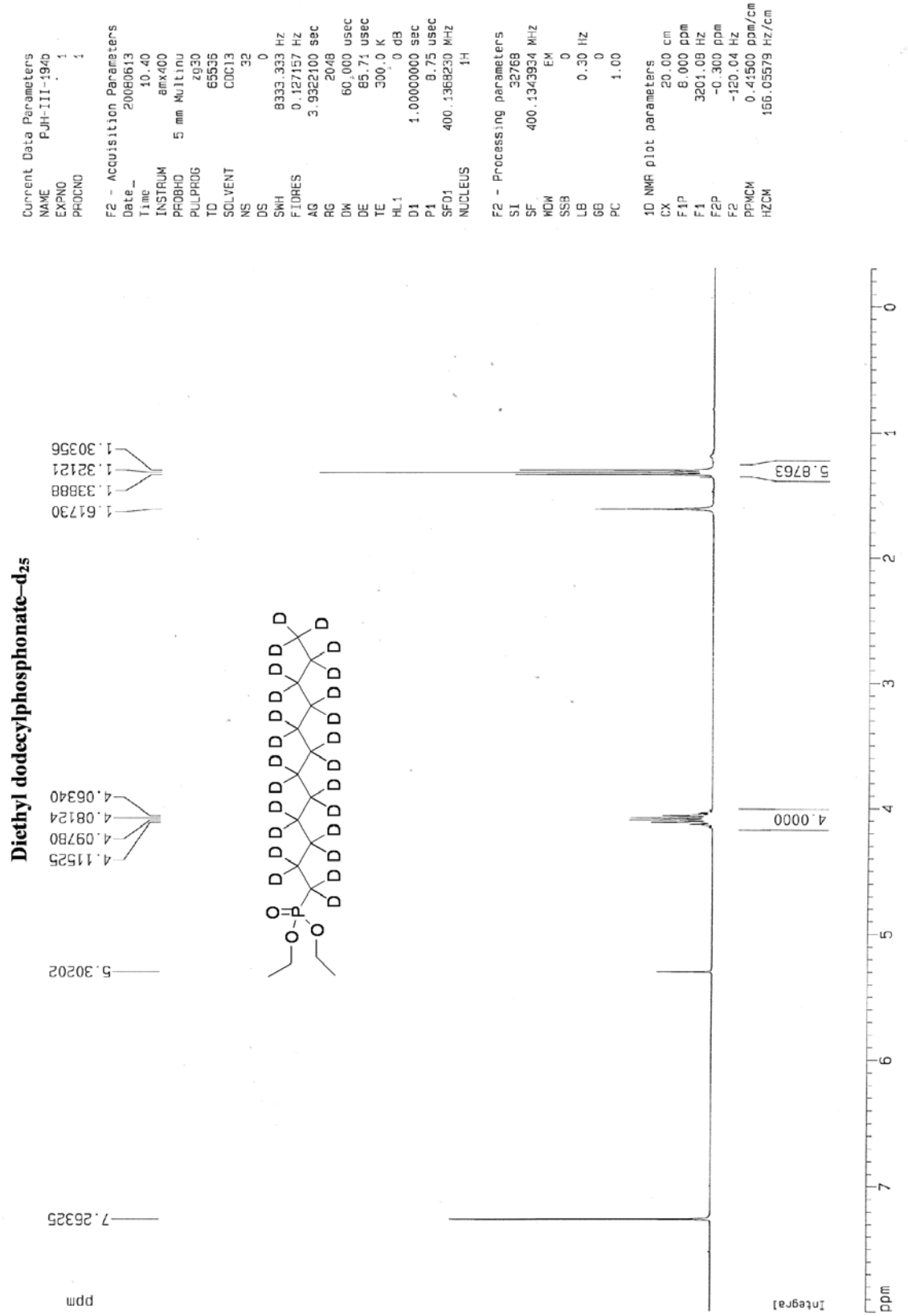


Figure SI-4. Lateral Force Microscopy images of unmodified ZnO (a), and ZnO modified with OPA (b), ODPA (c), and FHOPA (d). Images are 10 μm × 10 μm.

Characterization data for diethyl dodecylphosphonate-d_{25} is presented below.


Diethyl dodecylphosphonate–d25
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PROCNO 1
F2 - Acquisition Parameters
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Time 10.40
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PROBHD 5 mm Multinu
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 0
SWH 8333.333 Hz
FIDRES 0.127157 Hz
AG 3.9322100 sec
RG 2048
DW 60.000 usec
DE 85.71 usec
TE 300.0 K
HL1 0 dB
D1 1.00000000 sec
P1 8.75 usec
SFO1 400.1368230 MHz
NUCLEUS 1H
F2 - Processing parameters
SI 32768
SF 400.1343934 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
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F1P 8.000 ppm
F1 3201.08 Hz
F2P -0.300 ppm
F2 -120.04 Hz
PPMCM 0.41500 ppm/cm
HZCM 166.05579 Hz/cm
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1.32121
1.33888
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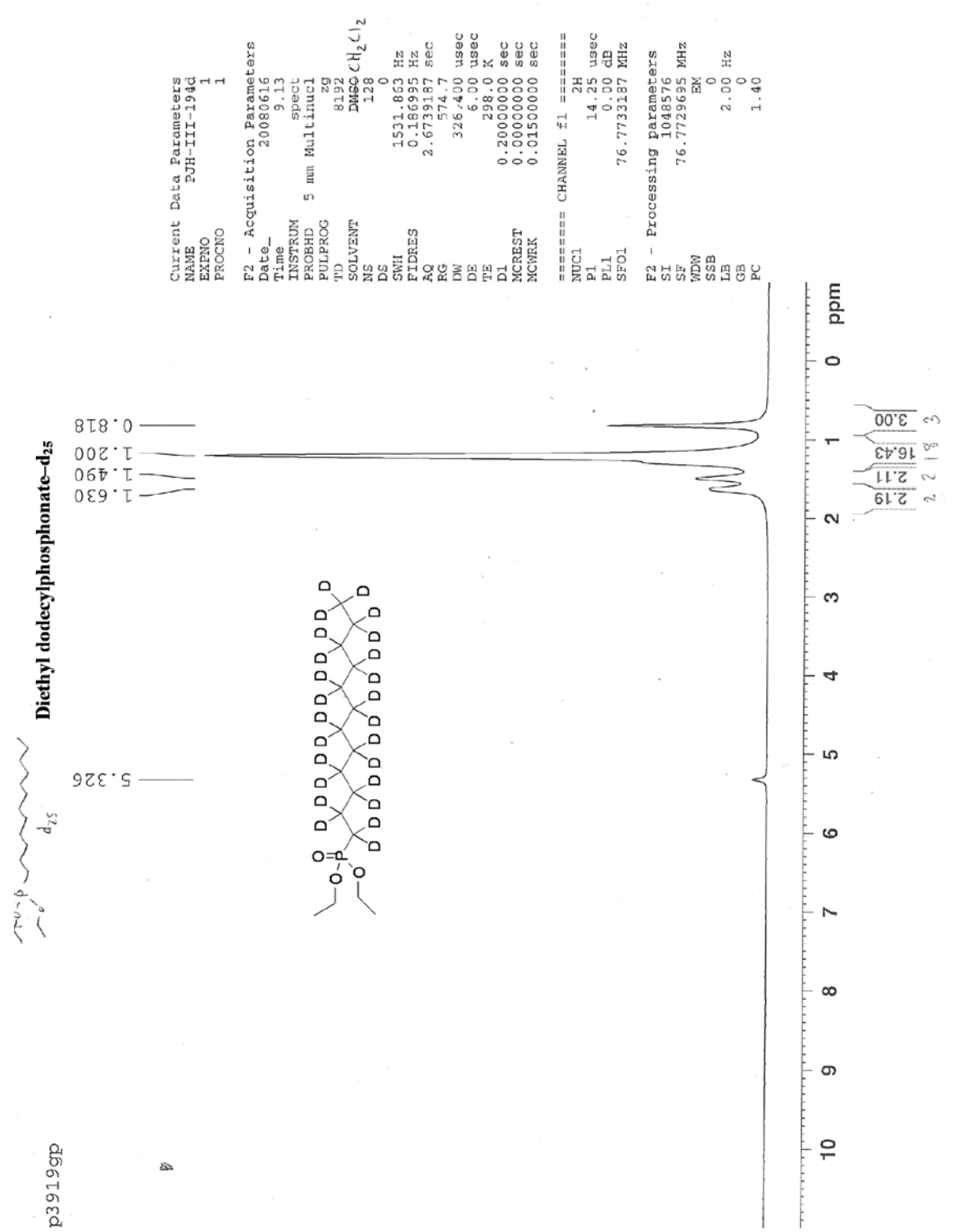
5.30202
7.26325
5.8763
4.0000
ppm
Integral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p3919gp
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PROCNO 1
F2 - Acquisition Parameters
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INSTRUM spect
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PULPROG zg
TD 8192
SOLVENT DMSO CH2Cl2
NS 128
DS 0
SWH 1531.863 Hz
FIDRES 0.186995 Hz
AQ 2.67391187 sec
RG 574.7
DW 326.400 usec
DE 6.00 usec
TE 298.0 K
D1 0.20000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 2H
P1 14.25 usec
PL1 0.00 dB
SFO1 76.7733187 MHz
F2 - Processing parameters
SI 1048576
SF 76.7729695 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40
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1.200
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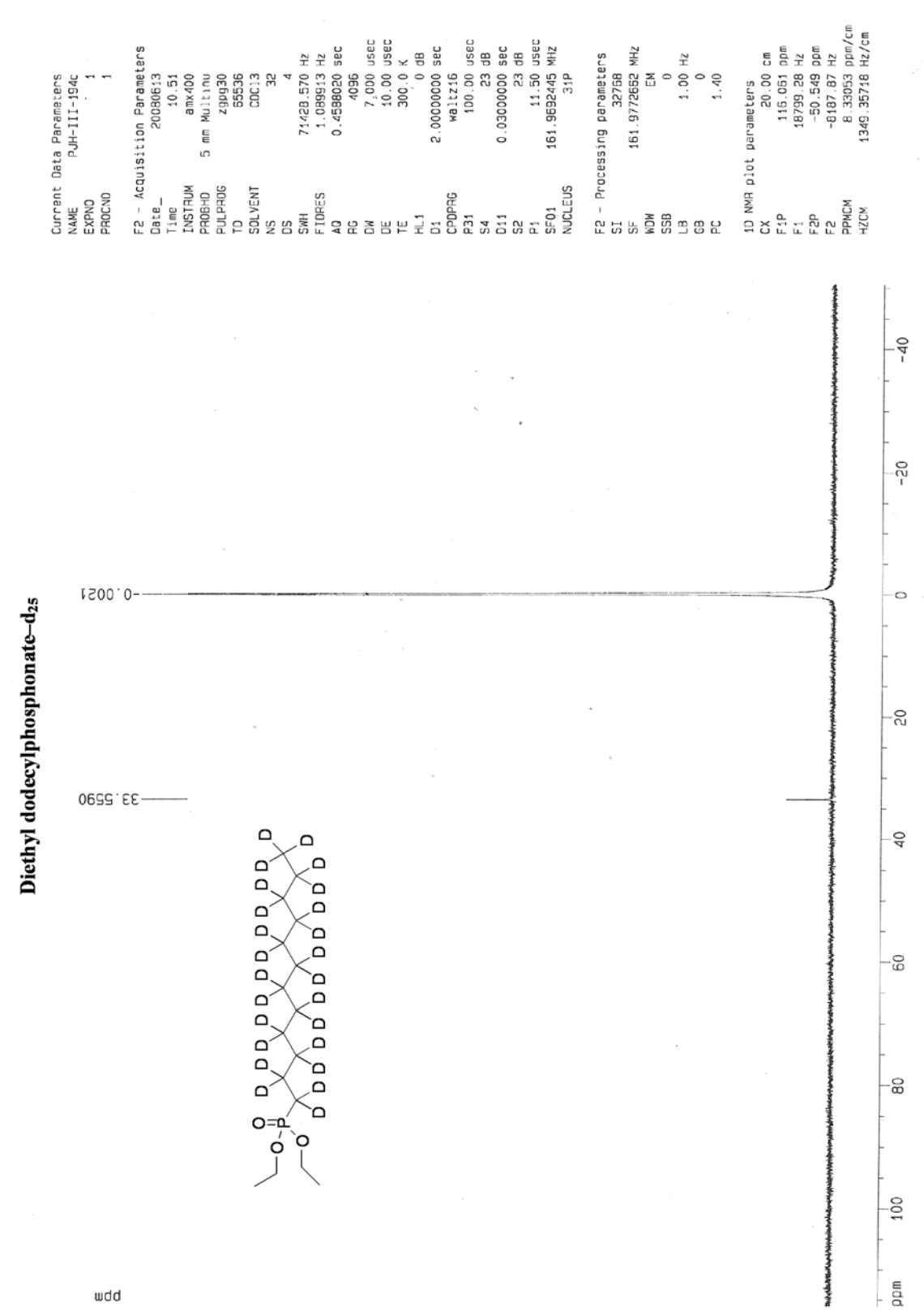
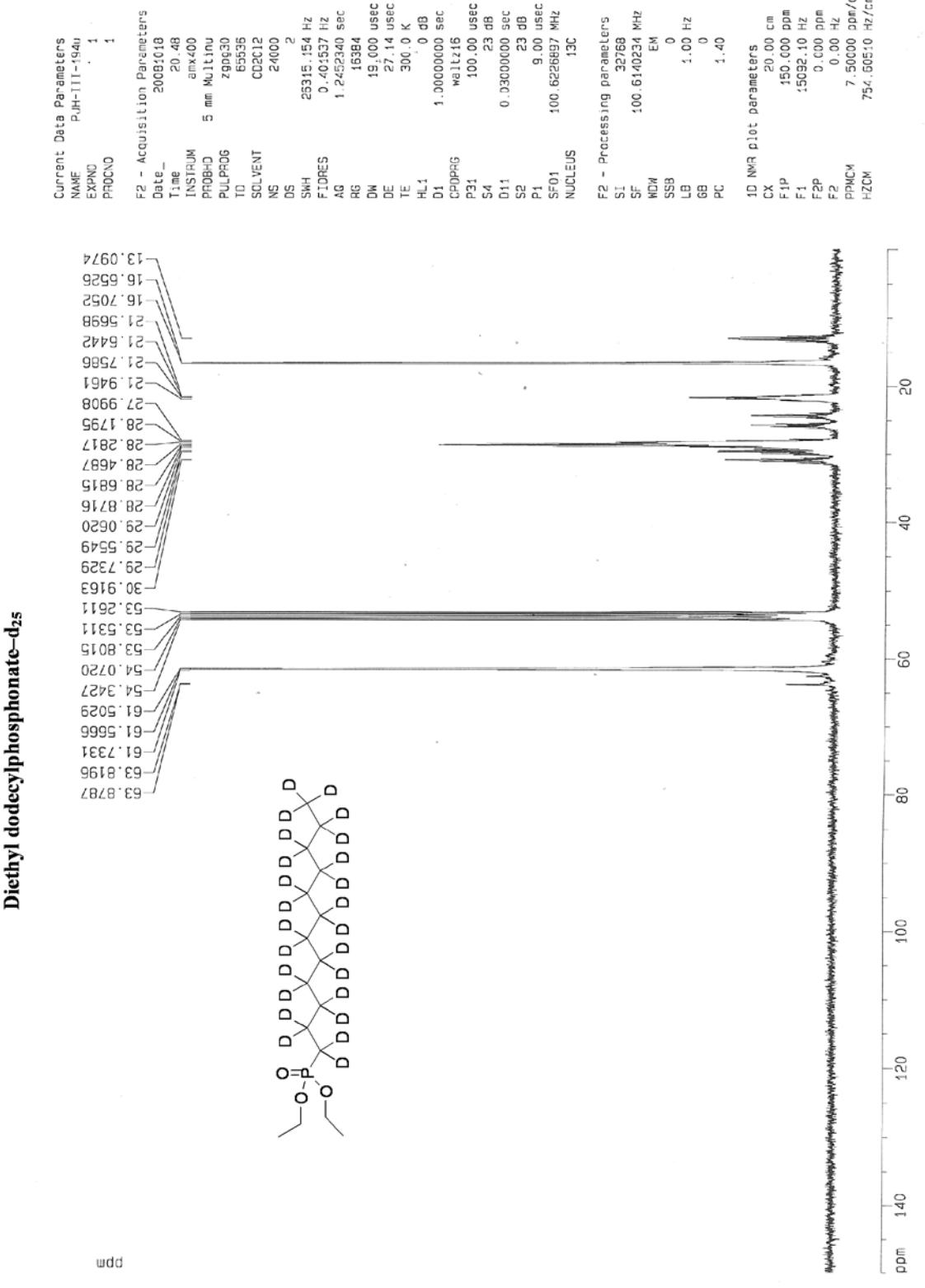
2.19
2.11
16.43
3.00
ppm

Diethyl dodecylphosphonate–d_{25}



Diethyl dodecylphosphonate–d_{25}



Diethyl dodecylphosphonate–d_{25}