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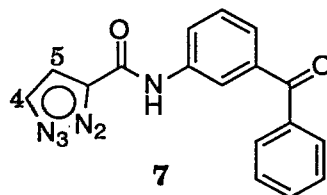
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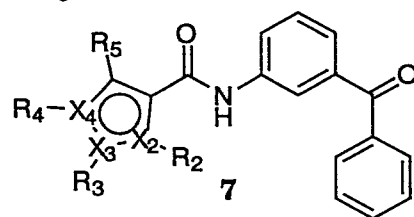
Supplemental Material

Table 1. Carboxamides 32a-r containing a pyrazole heterocycle prepared by the synthesis in Scheme 3.



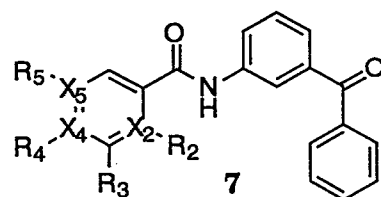
cpd	N ₂	N ₃	R ₄	R ₅	MS base peak	MS other peak	MS parent ion	% yld ^b
7a	Me	-	neopent	H	123	360 (-Me)	375	86
7b	Me	-	Me	H	123	-	319	93
7c^a	Me	-	Me	Br	201	318 (-Br)	397	93
7d^a	Me	-	H	H	109	-	305	77
7e	Me	-	CF ₃	H	177	-	373	99
7f^a	Me	-	CF ₃	Cl	211	-	407	88
7g^a	Me	-	4-Cl-2-F-benzene	Cl	-	-	-	67
7h^a	Et	-	H	H	-	-	-	63
7i	PhCH ₂	-	<i>t</i> -Bu	H	212	422 (-Me)	437	91
7j	<i>t</i> -Bu	-	Me	H	109	346 (-Me)	361	69
7k	-	Me	<i>t</i> -Bu	H	165	-	361	48
7l	-	Me	<i>neo</i> -pent	H	179	360 (-Me)	375	100
7m	-	Me	Me	H	123	-	319	93
7n^a	-	Me	Cl	Cl	177	-	373	82
7o^a	-	Me	CO ₂ Me	H	167	332 (-OMe)	363	82
7p^a	-	Me	CF ₃	H	177	-	373	81
7q^a	-	Me	CF ₃	Br	257	-	451	66
7r^a	-	Ph	Me	H	185	-	381	77

^a Addition of 11 was required for removal of aniline.^b Yields were based on mass recovery.

Table 2. Carboxamides 7A-Z containing a 5-membered heterocyclic ring prepared by the synthesis in Scheme 3.

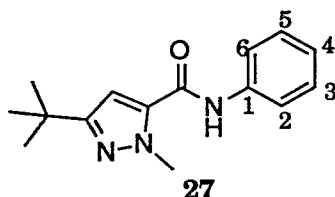
cpd	X ₂	X ₃	X ₄	R ₂	R ₃	R ₄	R ₅	MS base peak	MS other peak	MS parent ion	% yld ^b
7A^a	S	C	C	-	H	H	H	111	-	307	100
7B	S	C	C	-	<i>t</i> -Bu	H	H	167	-	363	66
7C^a	S	C	C	-	Cl	H	H	145	-	341	87
7D^a	S	C	C	-	H	3-thiophene	H	193	-	389	60
7E^a	O	C	C	-	H	H	H	95	-	291	100
7F^a	O	C	C	-	H	<i>t</i> -Bu	H	151	332 (-Me)	347	75
7G^a	O	C	C	-	<i>t</i> -Bu	H	H	151	332 (-Me)	347	83
7H^a	O	C	C	-	SiMe ₃	H	H	167	348 (-Me)	363	80
7I^a	O	C	C	-	Cl	Cl	H	105	-	359	84
7J	O	C	C	-	Me	Me	H	123	-	319	93
7K^a	C	O	C	Me	-	Me	H	123	-	319	53
7L^a	C	O	C	Me	-	Ph	H	105	-	381	78
7M	S	C	N	-	Me	-	Me	140	-	336	100
7N^a	S	C	N	-	<i>i</i> -Pr	-	Me	168	-	364	83
7O^a	S	C	N	-	OMe	-	CF ₃	210	-	406	75
7P^a	S	C	N	-	Cl	-	<i>i</i> -Pr	188	349 (-Cl)	384	79
7Q^a	S	C	N	-	H	-	Me	126	-	322	94
7R^a	S	C	N	-	H	-	Br	192	-	388	36
7S	S	C	N	-	4-Cl-Ph	-	Me	-	-	-	70
7T	S	C	N	-	Ph	-	Me	202	-	398	77
7U	S	C	N	-	4-CF ₃ -Ph	-	Me	202	-	466	65
7V	S	C	N	-	3-CF ₃ -Ph	-	Me	202	-	466	64
7W^a	S	C	N	-	Cl	-	Ph	222	-	418	72
7X^a	O	C	N	-	NH <i>t</i> -Bu	-	CF ₃	255	-	431	70
7Y^a	S	N	C	-	-	Cl	Cl	105	-	376	35
7Z^a	N	N	N	-	-	3-CF ₃ -Ph	Me	145	-	450	67

^a Addition of 11 was required for removal of aniline. ^b Yields were based on mass recovery.

Table 3. Carboxamides 7aa-ll containing a 6-membered ring prepared by the synthesis in Scheme 3.

cpd	X ₂	X ₄	X ₅	R ₂	R ₃	R ₄	R ₅	MS base peak	MS other peak	MS parent ion	% yld ^b
7aa	C	C	C	CF ₃	H	H	H	292	-	369	49
7ab	C	C	C	H	CF ₃	H	H	173	-	369	81
7cc	C	C	C	H	H	CF ₃	H	292	-	369	100
7dd	C	C	C	Cl	H	Cl	H	105	-	370	93
7ee	C	C	C	F	H	F	H	141	-	337	96
7ff	C	C	C	NO ₂	H	CF ₃	H	165	-	414	97
7gg^a	C	C	C	<i>t</i> -Bu	H	<i>t</i> -Bu	H	217	-	414	73
7hh	C	C	C	H	CHMe(CN)	H	H	158	-	354	86
7ii	N	C	N	-	H	H	-	79	-	303	100
7jj	N	C	N	-	H	Me	-	93	-	317	95
7kk^a	N	C	C	-	Cl	H	CF ₃	105	-	404	71
7ll	C	N	C	H	Cl	-	Cl	105	-	371	83

^a Addition of 11 was required for removal of aniline. ^b Yields were based on mass recovery.

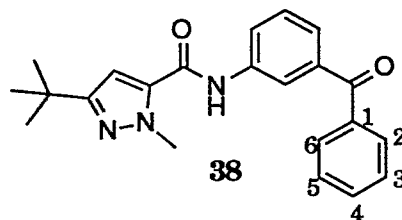
Table 4. Pyrazolecarboxamides 27 prepared by the synthesis in Scheme 6.

cpd	R ₂	R ₃	R ₄	R ₅	R ₆	MS base peak	MS other peak	MS parent ion	% yld ^b
27a	H	H	H	H	H	165	242 (-Me)	257	100
27b	H	COMe	H	H	H	165	284 (-Me)	299	100
27c	H	COMe	NO ₂	H	H	165	329 (-Me)	344	62
27d	H	COMe	Me	H	Me	165	312 (-Me)	327	100
27e	H	COMe	H	H	Cl	-	-	-	88
27f	H	COPr	H	H	H	-	-	-	92
27g	H	COCH ₂ CH ₂ -		H	H	165	296 (-Me)	311	82
27h	H	COCH ₂ CH ₂ CH ₂ CH ₂ -		H	H	165	324 (-Me)	339	88
27i	H	COOCH ₂ -		H	H	-	-	-	96
27j	H	CONMeCO-		H	H	165	325 (-Me)	340	75
27k	H	COCONH-		H	H		delete		79
27l	H	CO ₂ Me	H	H	H	165	300 (-Me)	315	43
27m	H	CO ₂ Et	H	H	H	165	314 (-Me)	329	100
27n	H	CONH ₂	H	H	H	165	285 (-Me)	300	100
27o	H	CONEt ₂	H	H	H	165	-	356	98
27p	H	COCH ₂ CONH-2- isothiazole	H	H	H	165	298 (-amide)	-	70
27q	H	COCH ₂ CO ₂ Et	H	H	H	165	298 (-CO ₂ Et)	300	93
27r	H	NHCO ₂ - <i>t</i> -Bu	H	H	H	165	272 (-CO ₂ - <i>t</i> -Bu)	372	81
27s	H	OMe	OMe	H	H	165	312 (-Me)	317	94
27t	H	OMe	H	H	H	165	272 (-Me)	287	82
27u	H	OCH(Me) ₂	H	H	H	165	404 (-Me)	419	100
27v	H	CF ₃	H	H	H	165	310 (-Me)	325	100
27w	H	NO ₂	H	H	H	165	287 (-Me)	302	99
27x	SiMe ₃	H	H	H	H	258	314 (-Me)	329	96
27y ^a	CF ₃	H	NO ₂	H	H	165	355 (-Me)	370	68
27z	Cl	H	Cl	H	H	-	-	-	96
27aa ^a	Cl	H	SO ₂ Me	H	H	165	354 (-Me)	369	86
27bb	Cl	H	F	OMe	H	165	324 (-Me)	339	100
27cc	F	H	F	H	H	165	278 (-Me)	293	80
27dd	H	Ph	H	H	H	165	318 (-Me)	333	87
27ee	H	SO ₂ Ph	H	H	H	165	383 (-Me)	398	75

27ff	H	OPh	H	H	H	165	334 (-Me)	349	100
27gg	H	NHCOPh	H	H	H	105	-	376	81
27hh	H	CONHPh	H	H	H	284	-	376	69
27ii	COPh	H	H	H	H	165	346 (-Me)	361	82
27jj	H	H	COPh	H	H	165	346 (-Me)	361	84

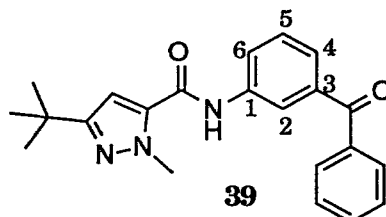
^a Prepared by reacting **25** with the aniline **26** in pyridine at 80°C.

^b Yields were based on mass recovery.

Table 5. Pyrazolecarboxamides 38 prepared by the synthesis in Scheme 8.

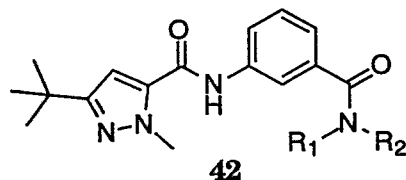
cpd	R ₂	R ₃	R ₄	R ₅	R ₆	MS base peak	MS other peak	MS parent ion	% yld ^c
38a	H	H	Me	H	H	165	360 (-Me)	375	80
38b	H	H	F	H	H	165	364 (-Me)	379	79
38c	H	H	OMe	H	H	165	376 (-Me)	391	76
38d	OMe	H	OMe	H	H	165	-	421	72
38e	Cl	H	F	Me	H	165	412 (-Me)	427	69
38f	H	Cl	Cl	H	H	165	414 (-Me)	429	70
38g	F	H	Cl	Me	H	165	412 (-Me)	427	65
38h	F	H	H	OH	H	165	380 (-Me)	395	67
38i	F	H	OH	H	H	165	380 (-Me)	395	69
38j^a	F	H	OMe	H	H	165	394 (-Me)	409	60
38k^b	F	H	H	Me	H	165	378 (-Me)	393	61
38l	H	H	cyclohexyl	H	H	165	428 (-Me)	443	93
38m	Me	Me	Me	H	H	165	388 (-Me)	403	87
38n	H	H	pentyl	H	H	165	416 (-Me)	431	84
38o	CH(Me) ₂	H	CH(Me) ₂	H	H	280	-	445	94
38p	cyclohexyl	H	cyclohexyl	H	H	-	-	-	86
38q	H	H	CH ₂ (cyclohexyl)	H	H	165	442 (-Me)	457	92
38r	H	H	OBu	H	H	165	-	433	88
38s	H	OMe	OMe	H	H	165	406 (-Me)	421	62

^a A 61:39 mixture of regioisomers determined by ¹H NMR.^b A 70:30 mixture of regioisomers determined by ¹H NMR.^c Yields were based on mass recovery.

Table 6. Pyrazolecarboxamides 39 prepared by the synthesis in Scheme 8.

cpd	R ₂	R ₄	R ₅	R ₆	MS base peak	MS other peak	MS parent ion	% yld ^a
39a	H	Cl	H	H	165	380 (-Me)	395	75
39b	H	H	H	Cl	165	380 (-Me)	395	91
39c	H	H	H	CF ₃	149	414 (-Me)	429	35
39d	Me	H	H	H	165	360 (-Me)	375	88
39e	H	H	CF ₃	H	165	414 (-Me)	429	100
39f	H	H	H	Me	165	360 (-Me)	375	80
39g	CO ₂ Me	H	H	H	165	404 (-Me)	419	95
39h	H	H	CO ₂ Me	H	165	404 (-Me)	419	81
39i	H	H	H	OMe	165	376 (-Me)	391	79
39j	H	H	H	CO ₂ Me	149	404 (-Me)	419	95
39k	OMe	OMe	H	H	165	406 (-Me)	421	100
39l	H	H	H	N(CH ₂) ₅	-	-	-	86
39m	H	H	H	SO ₂ Me	149	424 (-Me)	439	84

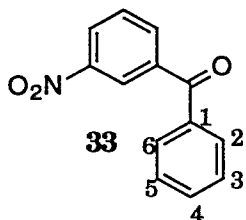
^a Yields were based on mass recovery.

Table 7. 3-[[[3-(1,1-Dimethylethyl)-1-methyl-1H-pyrazol-5-yl]carbonyl]amino]-benzamides 42a-l prepared by the synthesis in Scheme 9.

cpd	R ₁	R ₂	MS base peak	MS other peak	MS parent ion	% yld ^a
42a	Pr	H	165	-	342	78
42b	Ph	H	284	-	376	69
42c	Me	H	165	-	314	82
42d	Me	Me	-	-	-	99
42e	Me	Ph	-	-	-	63
42f	Me	CH ₂ CHCH ₂	284	-	354	58
42g	Me	CH ₂ CCH	165	-	352	77
42h	Et	Et	165	-	356	98
42i	CH ₂ CHCH ₂	CH ₂ CHCH ₂	284	-	380	65
42j	-(CH ₂) ₂ NMe(CH ₂) ₂ -		284	-	383	72
42k	-(CH ₂) ₂ O(CH ₂) ₂ -		165	355 (-Me)	-	71
42l	-(CH ₂) ₅ -		257	-	368	68

^a Yields were based on mass recovery.

Friedel-Crafts Acylation with 3-Nitrobenzoyl Chloride (31) to Afford the Substituted 3-Nitrobenzophenone 33 (Scheme 7).

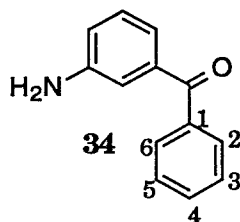


cpd	R ₂	R ₃	R ₄	R ₅	R ₆	MS base peak	MS other peak	MS parent ion	regio- isomer ratio
33a	H	H	Me	H	H	119	-	241	88:12
33b	H	H	F	H	H	-	-	-	65:35
33d	OMe	H	OMe	H	H	165	-	287	-
33e	Cl	H	F	Me	H	-	-	-	-
33f	H	Cl	Cl	H	H	173	-	295	-
33g	F	H	Cl	Me	H	-	-	-	-
33h	F	H	H	OH	H	-	-	-	-
33i	F	H	OH	H	H	-	-	-	-
33j	F	H	OMe	H	H	153	-	275	50:50
33k	F	H	H	Me	H	-	-	-	70:30
33l	H	H	cyclohexyl	H	H	-	-	-	-
33m	Me	Me	Me	H	H	-	-	-	80:20
33n	H	H	pentyl	H	H	-	-	-	-
33o	CH(Me) ₂	H	CH(Me) ₂	H	H	294	-	311	-
33p	cyclohexyl	H	cyclohexyl	H	H	-	-	-	-
33q	H	H	CH ₂ (cyclohexyl)	H	H	-	-	-	-
33r	H	H	OBu	H	H	-	-	-	-
33s	H	OMe	OMe	H	H	-	-	-	81:19

2,4-Diisopropyl-3'-nitrobenzophenone (33o). General procedure C yielded a clear oil. ¹H NMR (CDCl₃) ppm: 1.27 (d, 6H), 1.36 (d, 6H), 3.04 (sept, 1H), 3.19 (sept, 1H), 7.19 (m, 2H), 7.39 (s, 1H), 7.72 (t, 1H), 8.23 (m, 1H), 8.48 (m, 1H), 8.69 (m, 1H).

Reduction of the 3-Nitrobenzophenone **33** with Iron to Afford the 3-Aminobenzophenone **34**

(Scheme 7).



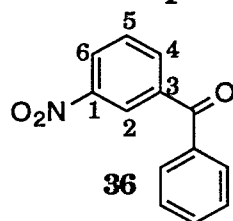
cpd	R ₂	R ₃	R ₄	R ₅	R ₆	MS base peak	MS other peak	MS parent ion	regio- isomers
34a	H	H	Me	H	H	-	-	-	
34b	H	H	F	H	H	-	-	215	
34c	H	H	OMe	H	H	-	-	-	
34d	OMe	H	OMe	H	H	-	-	-	
34e	Cl	H	F	Me	H	228	-	263	
34f	H	Cl	Cl	H	H	-	-	265	
34g	F	H	Cl	Me	H	-	-	263	
34h	F	H	H	OH	H	-	-	231	
34i	F	H	OH	H	H	-	-	231	
34j	F	H	OMe	H	H	153	-	245	61:39
34k	F	H	H	Me	H	-	-	229	70:30
34l	H	H	cyclohexyl	H	H	-	-	279	
34m	Me	Me	Me	H	H	-	-	239	
34n	H	H	pentyl	H	H	175	-	267	
34o	CH(Me) ₂	H	CH(Me) ₂	H	H	-	-	281	
34p	cyclohexyl	H	cyclohexyl	H	H	-	-	361	
34q	H	H	CH ₂ (cyclohexyl)	H	H	-	-	293	
34r	H	H	OBu	H	H	121	-	269	
34s	H	OMe	OMe	H	H	151	-	257	

3-Amino-4'-methoxybenzophenone (34c). General procedure D yielded a yellow solid. ¹H NMR (CDCl₃) ppm: 3.85 (bs, 2H), 3.94 (s, 3H), 6.91 (m, 1H), 7.01 (d, 2H), 7.13 (m, 2H), 7.27 (t, 1H), 7.90 (d, 2H).

3-Amino-2'-fluoro-4'-hydroxybenzophenone (34i). General procedure D yielded a white solid. ¹H NMR (CDCl₃) ppm: 3.91 (bs, 2H), 6.64 (m, 1H), 6.81 (dd, 1H), 6.93 (m, 1H), 6.99 (m, 1H), 7.05 (m, 1H), 7.32 (m, 1H), 7.73 (dd, 1H).

3-Amino-2'-fluoro-4'-methoxybenzophenone (34j). General procedure D yielded a yellow solid. ¹H NMR (CDCl₃) ppm: 3.86 (bs, 2H), 3.92 (s, 3H), 6.79 (m, 2H), 6.92 (m, 2H), 7.19 (m, 2H), 7.58 (t, 1H).

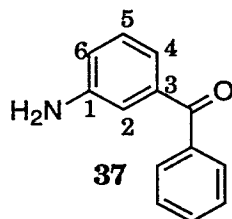
Friedel-Crafts Acylation with Substituted 3-Nitrobenzoyl Chlorides 35b and Benzene to Afford the Substituted 3-Nitrobenzophenone 36 (Scheme 7).



cpd	R ₂	R ₄	R ₅	R ₆	MS base peak	MS other peak	MS parent ion
36a	H	Cl	H	H	105	-	231
36b	H	H	H	Cl	-	-	231
36c	H	H	H	CF ₃	105	-	295
36d	Me	H	H	H	-	-	-
36e	H	H	CF ₃	H	105	-	295
36f	H	H	H	Me	-	-	-
36g	CO ₂ Me	H	H	H	-	-	-
36h	H	H	CO ₂ Me	H	-	-	-
36i	H	H	H	OMe	-	-	-
36j	H	H	H	CO ₂ Me	-	-	-
36k	OMe	OMe	H	H	-	-	-
36l	H	H	H	N(CH ₂) ₅	-	-	-
36m	H	H	H	SO ₂ Me	-	-	-

Reduction of the 3-Nitrobenzophenone **36** with Iron to Afford the 3-Aminobenzophenone **37**

(Scheme 7).



cpd	R ₂	R ₄	R ₅	R ₆	MS base peak	MS other peak	MS parent ion
37a	H	Cl	H	H	105	-	231
37b	H	H	H	Cl	-	-	231
37c	H	H	H	CF ₃	-	-	265
37d	Me	H	H	H	-	-	211
37e	H	H	CF ₃	H	105	-	265
37f	H	H	H	Me	134	-	211
37g	CO ₂ Me	H	H	H	222	-	255
37h	H	H	CO ₂ Me	H	-	-	255
37i	H	H	H	OMe	-	-	227
37j	H	H	H	CO ₂ Me	-	-	255
37k	OMe	OMe	H	H	227	-	257
37l	H	H	H	N(CH ₂) ₅	-	-	280
37m	H	H	H	SO ₂ Me	105	-	275

3-Amino-4'-chlorobenzophenone (37a). General procedure D yielded a white solid. ¹H NMR (CDCl₃) ppm: 3.84 (bs, 2H), 6.71 (d, 1H), 6.79 (dd, 1H), 7.25 (d, 1H), 7.54 (m, 2H), 7.64 (m, 1H), 7.91 (m, 2H).

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dof

dm

dmm

dmf

dpwr

dpwrf

temp

PROCESSING

lb

wtfile

proc

fn

math

werr

msm_acq

rrr

msm_std

q_completed

s_proton_data

save_data

msm_test

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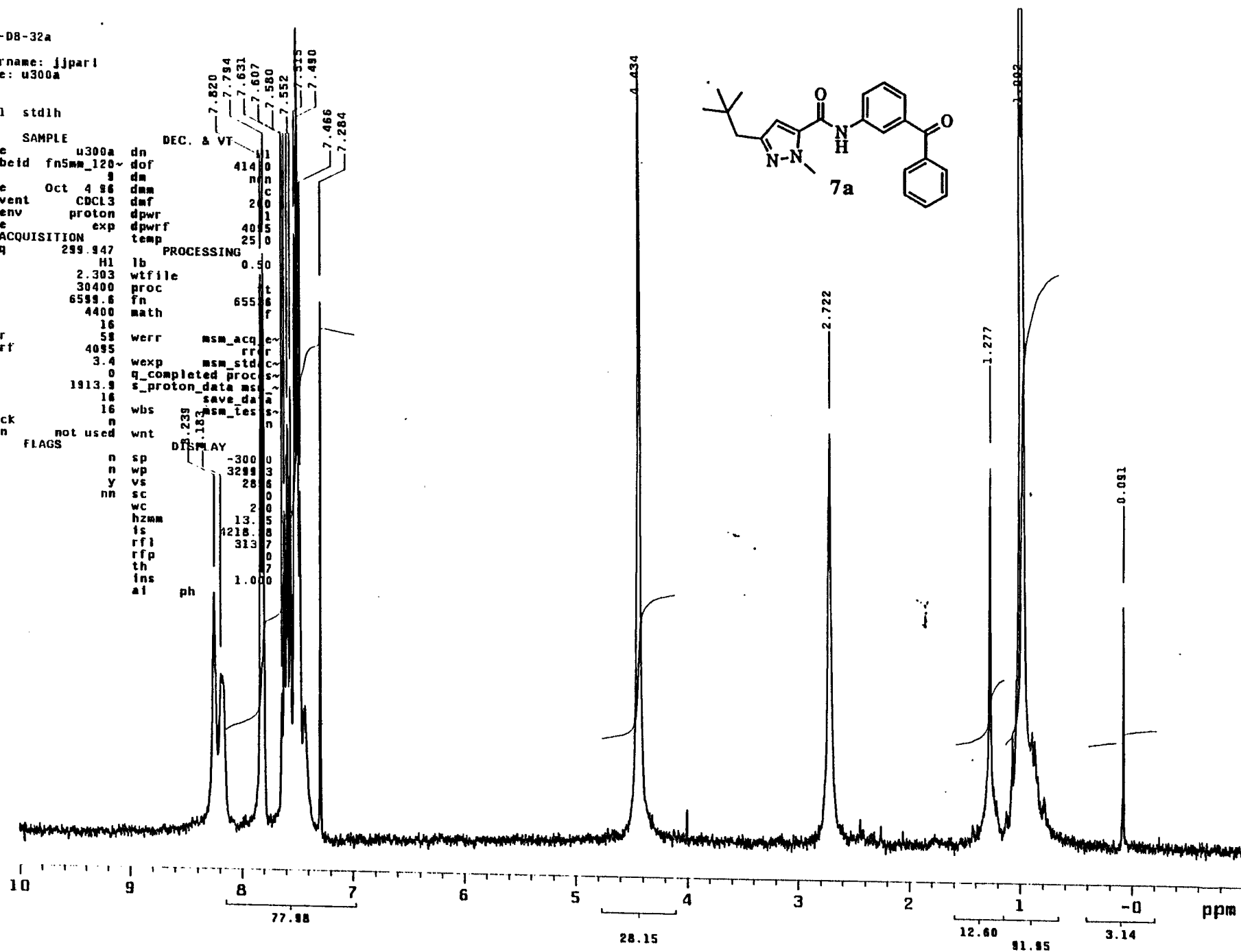
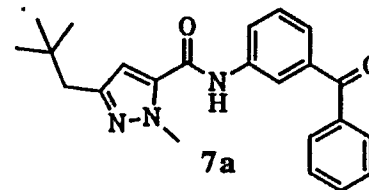
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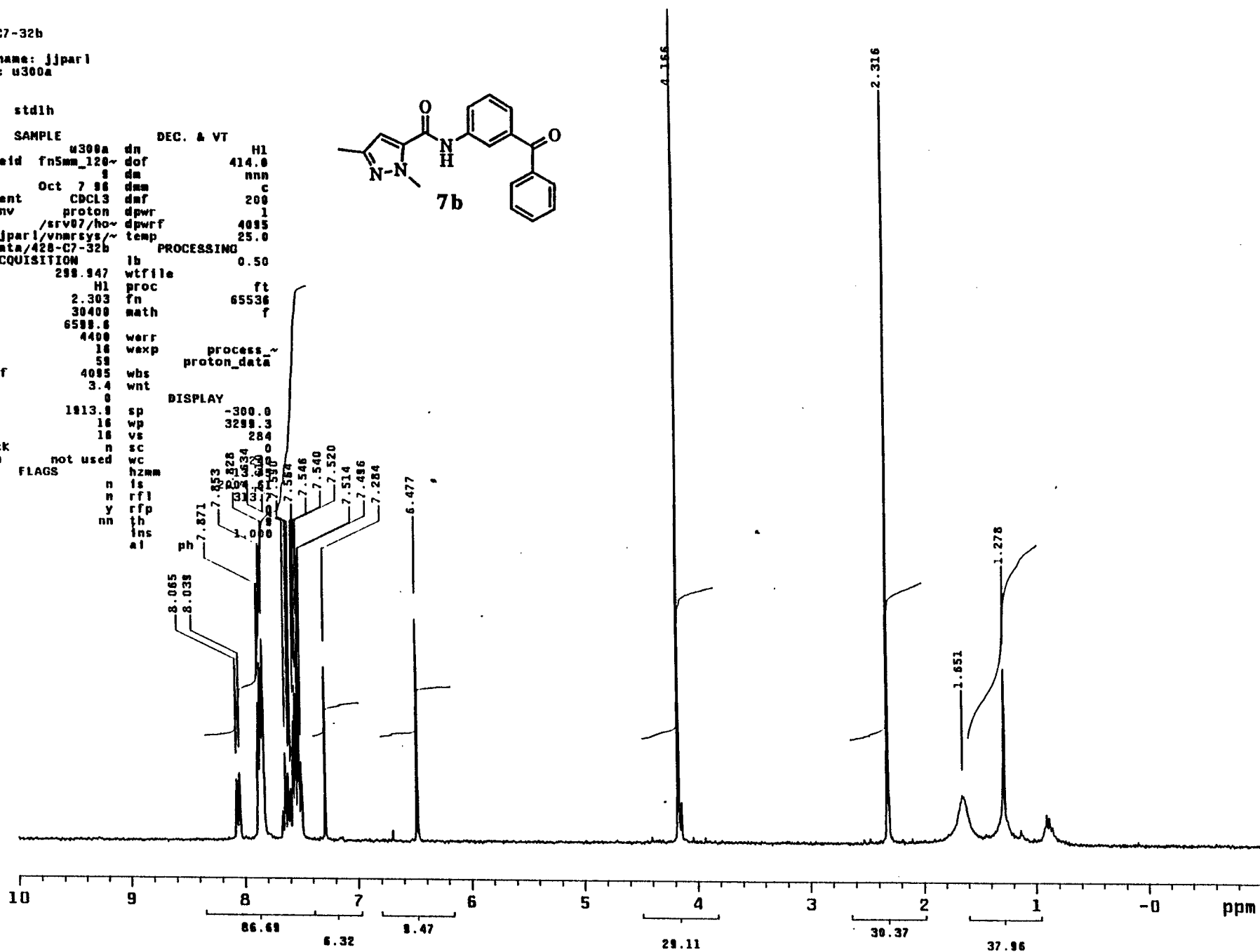
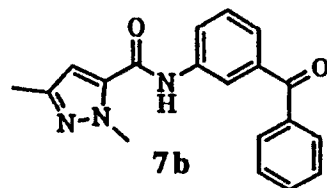


428-C7-32b

Username: jiparl
Node: u300a

exp3 std1h

SAMPLE DEC. & VT
node u300a dn H1
probeid fn5mm_120~ dof 414.0
date Oct 7 98 dm nnn
solvent CDCl3 dmf 200
acqenv proton dpwr 1
file /srv07/hv~ dpwrf 4095
me/jiparl/vnmrsys/~ temp 25.0
data/428-C7-32b PROCESSING
ACQUISITION lb 0.50
sfrq 299.947 wtfile
tn H1 proc ft
at 2.303 fn 65536
np 30400 math f
sw 6598.6
fb 4400 werr
bs 16 wexp
tpwr 59 process_~
tpwrf 4095 wbs proton_data
pw 3.4 wnt
dl 0
tof 1913.0 sp
nt 16 wp -300.0
ct 18 vs 3299.3
a-lock n sc 284
gain not used n wc
ll n hzmm
in n is
dp y rfi
hs nn rfp
th
ins
ai



517-A3-32d-32d

Username: jjparl
Mode: u300a

exp5 std1h

SAMPLE DEC. & VT

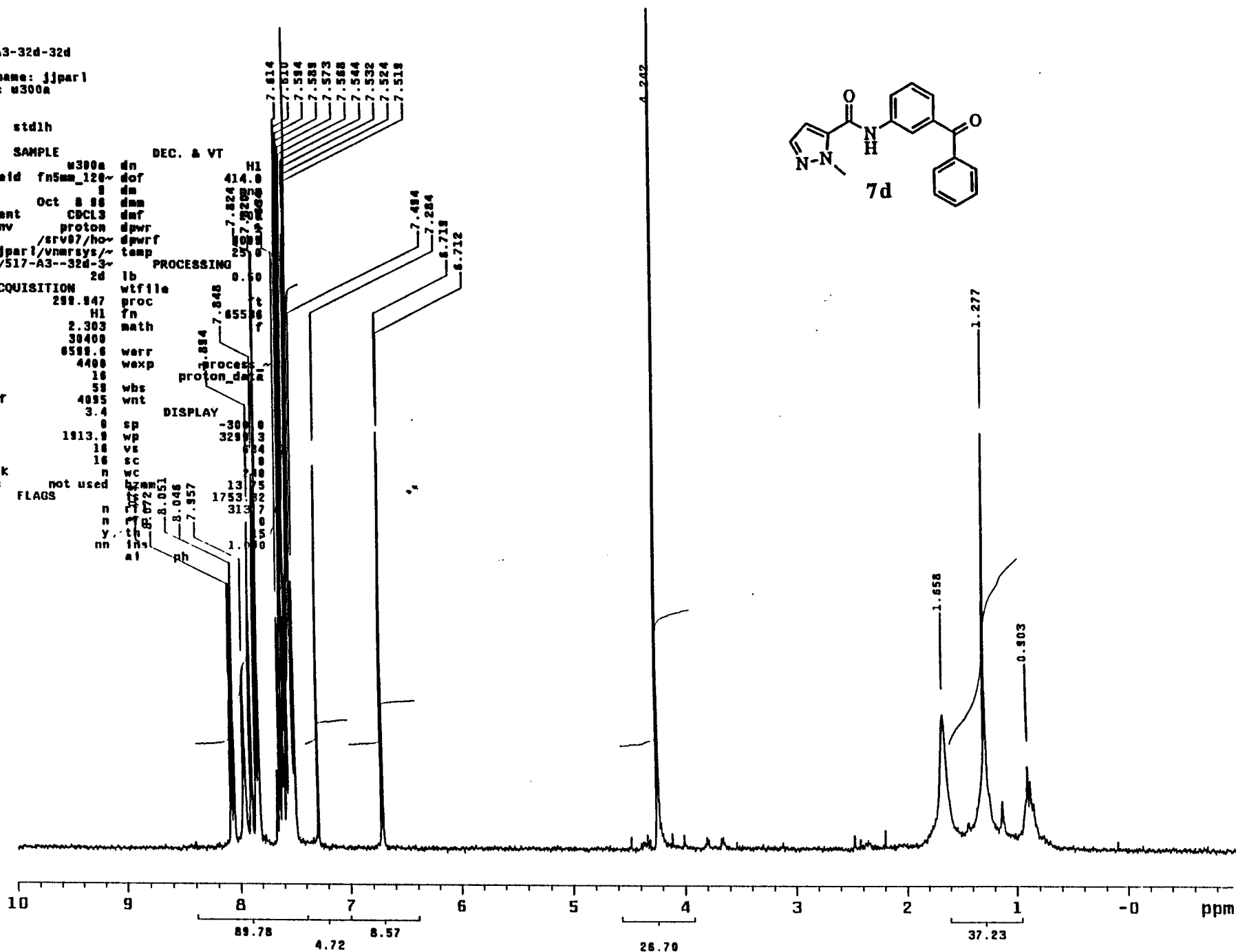
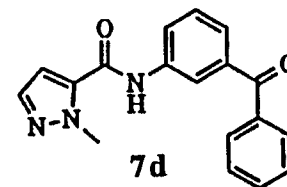
node u300a dn H1
probelid fn5mm_120~ dof 414.0
date Oct 8 86 dm 7.8244
solvent CDCl3 dnf 7.8244
acqenv proton dpwr 7.8244
file /srv07/hw dpwr 7.8244
me/jjparl/vnmrSYS~ temp 25.0
data/517-A3--32d-3~

PROCESSING

2d lb
ACQUISITION 258.947 wtfile
sfrq 258.947 proc
tn H1 fn
at 2.303 math
np 30400
sw 6588.6 warr
fb 4400 wexp
bs 16
tpwr 58 wbs
tpwrf 4095 wnt
pw 3.4
d1 0 sp
tof 1813.8 wp
nt 18 vs
ct 18 sc
clock 18 wc
gain not used
FLAGS
il n
in n
dp y
hs nn
at

DISPLAY
-304.0
328.0
13.75
1753.32
313.7
1.000

ph



485-B10-321

Username: jjparl
Node: u300a

expl stdlh

SAMPLE

node u300a dn
probeid fn5mm_120~ dof 414.0
date Oct 4 98 dm
solvent CDCL3 dmf 200
acqenv proton dpwr 1
file exp dpwrf 4095
temp 25.0

ACQUISITION
sfrq 299.947
tn H1
at 2.303
np 30400
sw 6599.00
fb 4400
bs 16
tpwr 59
tpwrf 4095
pw 3.4
d1 0
tof 1913.9
nt 16
ct 16
alock n
gain not used

PROCESSING

HL
lb
wv file
t
f
math
f
wv
msm_acq_e~
rror
wexp
msm_stdac~
q_completed proces~
s_proton_data ms~
save_data
msm tes~
n

DISPLAY

sp
wp
vs
sc
wc
hzmm
ls
rfl
rfp
th
ins
ai

ph

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2.0
13.5
2987.9
313.7
0
3
1.0 0

not used

wnt

wbs

s_proton_data

save_data

msm tes

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sc

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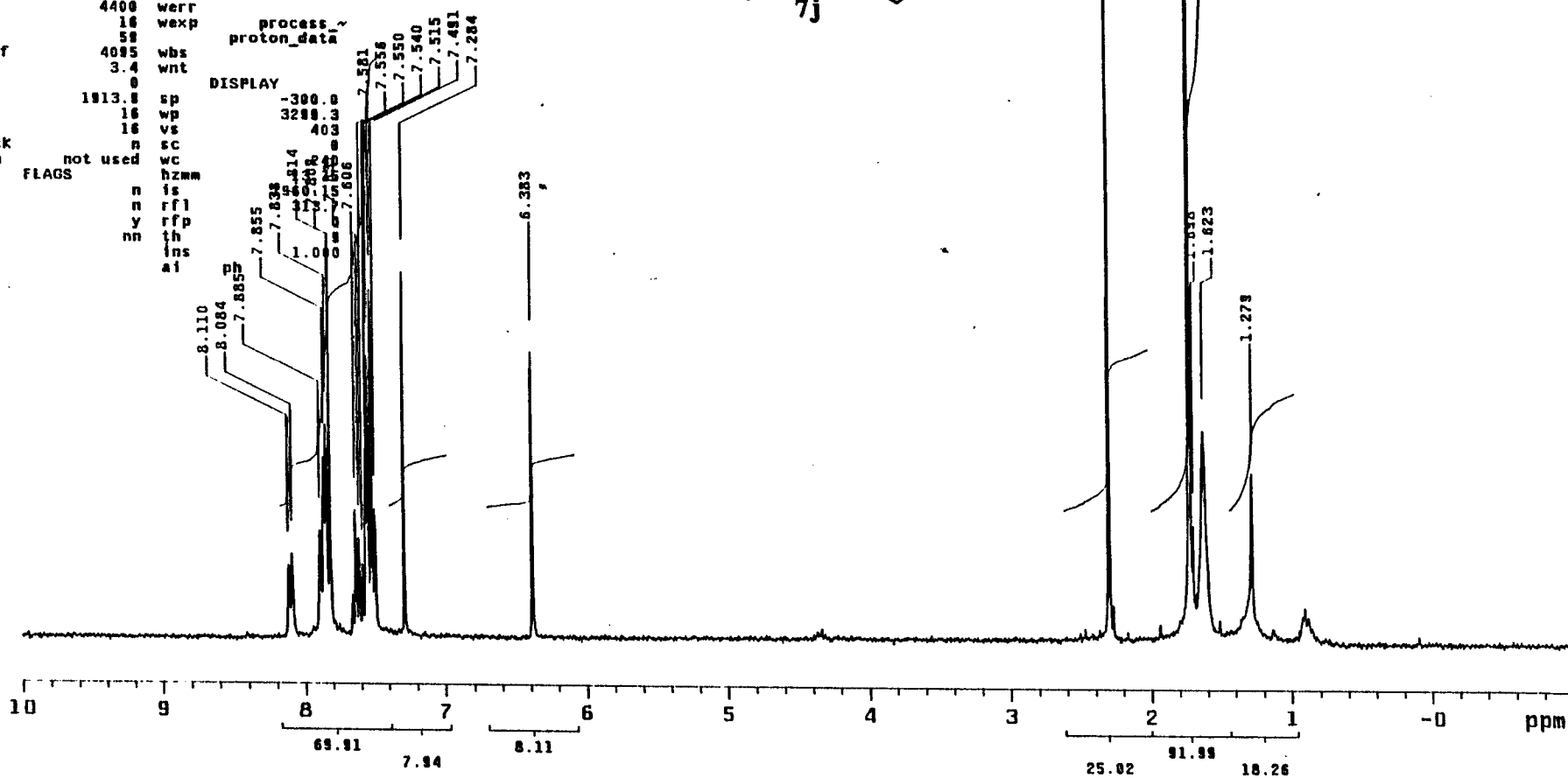
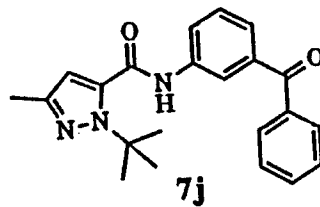
rfp

485-C2-32j

Username: jjparl
Node: u300a

exp3 std1h

SAMPLE		DEC. & VT	
node	u300a	dn	H1
probeid	fn5mm_120~	dof	414.0
		dm	nnn
date	Oct 7 96	dum	c
solvent	CDCl3	daf	200
acqenv	proton	dpwr	1
file	/srv07/ho~	dpwrf	4095
me/jjparl/vmarsys/~	data/485-C2-32j	temp	25.0
ACQUISITION		PROCESSING	
sfrq	299.947	lb	0.50
tn	H1	wtfile	
at	2.303	fn	ft
np	30400	math	65536
sw	6599.6		f
fb	4400	werr	
bs	16	wexp	
tpwr	58	process ~	
tpwrf	4095	proton_data	
pw	3.4	wnt	
dl	0	DISPLAY	
tof	1913.8	sp	-300.0
nt	16	wp	3298.3
ct	16	vs	403
clock	n	sc	
gain	not used	wc	
FLAGS		hzmm	
il	n	is	
in	n	rfl	
dp	y	rff	
hs	nn	th	
		ins	
		ai	



428-B9-32k

Username: jjparl
Node: u300a

exp3 std1h

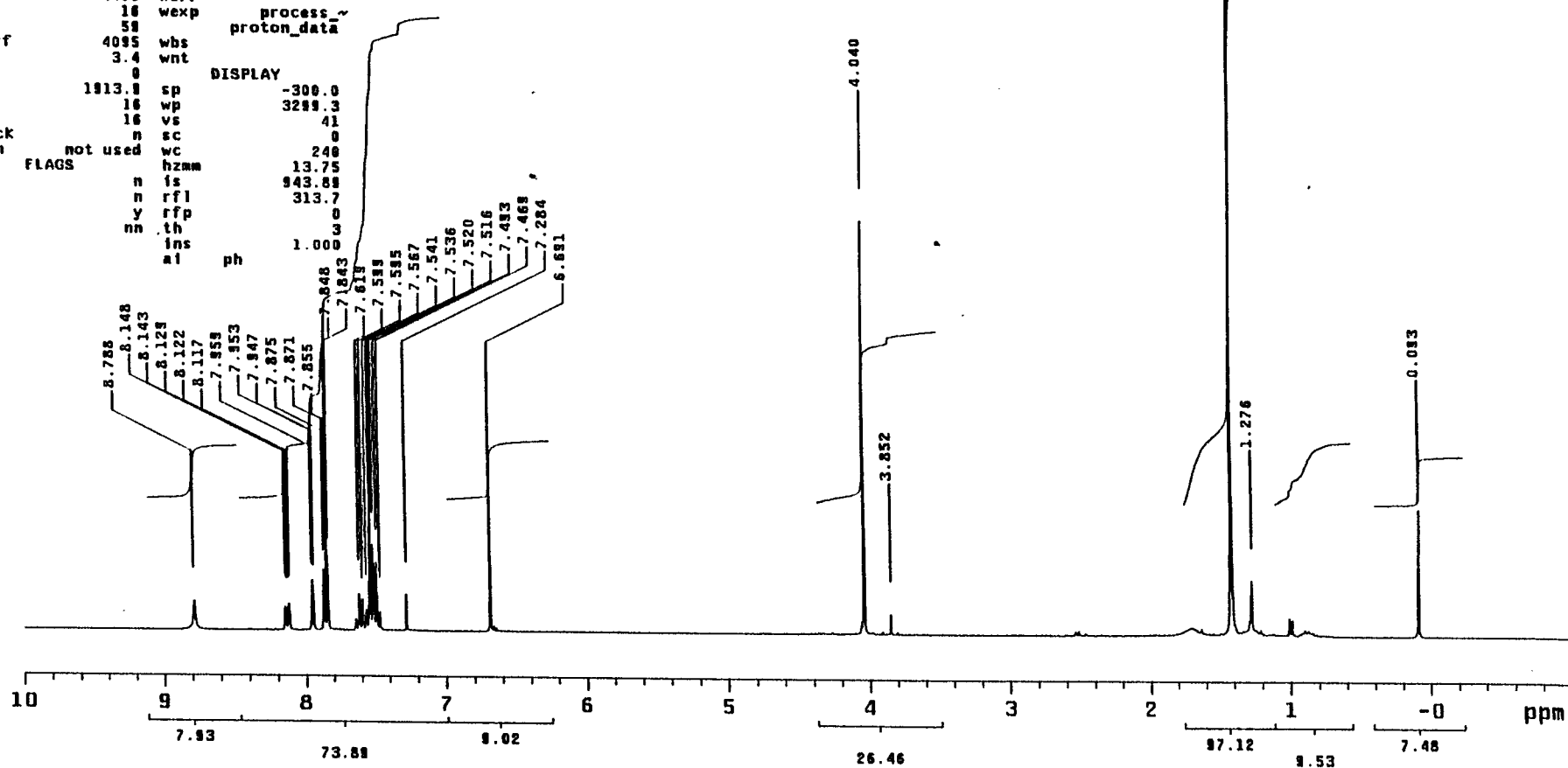
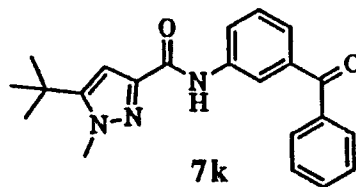
SAMPLE DEC. & VT

node	u300a	dn	H1
probeid	fn5mm_120	dof	414.0
		dm	nnn
date	Oct 7 96	dmm	c
solvent	CDCl3	dmf	200
acqenv	proton	dpwr	1
file	/srv07/hov	dpwrf	4095
me/jjparl/vnmrsvs/~		temp	25.0
data/428-B9-32k		PROCESSING	
ACQUISITION	lb		0.50
sfrq	299.947	wtfile	
tn	H1	proc	ft
at	2.303	fn	65536
np	38400	math	f
sw	6588.6		
fb	4400	werr	
bs	16	wexp	
tpwr	58		
tpwrf	4095	wbs	
pw	3.4	wnt	
d1	0		
tof	1913.0	sp	-300.0
nt	16	wp	3289.3
ct	16	vs	41
alock	n	sc	0
gain	not used	wc	240
FLAGS		hzmm	13.75
il	n	is	943.88
in	n	rfl	313.7
dp	y	rfp	
hs	nn	th	3
		ins	1.000
		al	

process_~
proton_data

DISPLAY

ph



485-G2-32o
 Username: jiparl
 Mode: u300a

exp5 std1h

SAMPLE DEC. & VT
 node u300a dn H1
 probeid fn5mm_120~ dof 414.0
 date Oct 4 86 dm nnn
 solvent CDCl3 dmf 200
 acqenv proton dpwr 1
 file /srv07/hov dpwrf 4095
 me/jiparl/vnmrsvs/~ temp 25.0
 data/485-G2-32o PROCESSING
 ACQUISITION lb 0.50
 sfrq 299.947 wfile
 tn H1 proc ft
 at 2.303 fn 65536
 np 30400 math f
 sw 6598.6
 fb 4400 werr
 bs 16 wexp
 tpwr 59
 tpwrf 4095 wbs
 pw 3.4 wnt
 dl 0
 tof 1913.9 sp
 nt 16 wp
 ct 16 vs
 alock n sc
 gain not used wc
 FLAGS hzm
 il n
 in is
 hs 13.75
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485-G11-32p

Username: jjparl
Node: u300a

exp3 stdlh

SAMPLE DEC. & VT

node u300a dn H1
 probeid fn5mm_120~ dof 414.0
 date Oct 7 96 dm nnn
 solvent CDCL3 dmf 200
 acqenv proton dpwr 1
 file /srv07/ho~ dpwrf 4095
 me/jjparl/vnmrsys/~ temp 25.0

data/485-G11-32p PROCESSING
 ACQUISITION lb 0.50

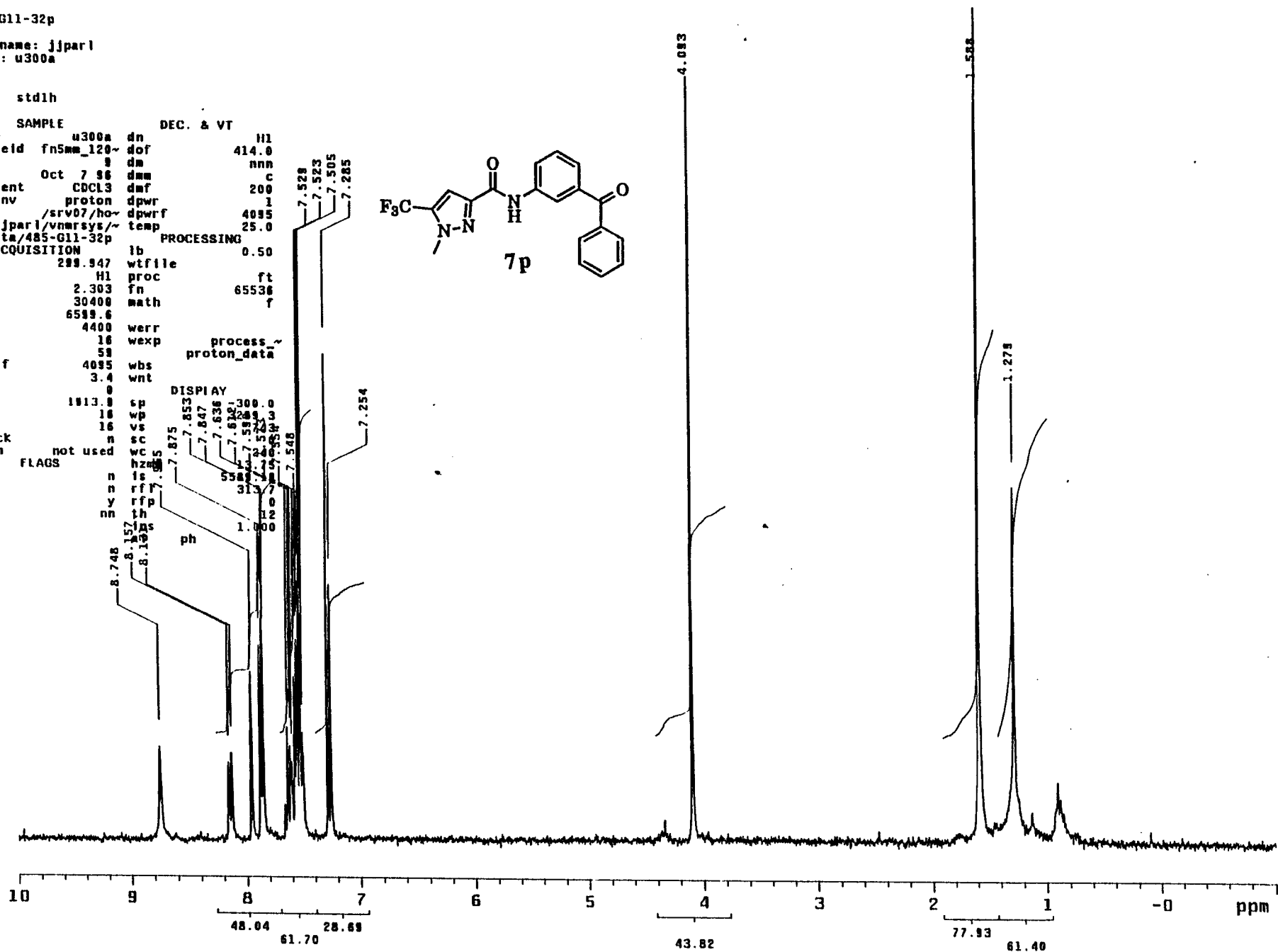
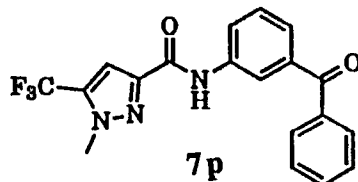
sfrq 299.947 wtfile
 tn H1 proc ft
 at 2.303 fn 65536
 np 30400 math f

sw 6599.6
 fb 4400 werr
 bs 16 wexp
 tpwr 59
 tpwrf 4095 wbs
 pw 3.4 wnt
 dl 0

process
 proton_data
 DISPLAY

sp 300.0
 vs 300.0
 sc 300.0
 wc 300.0
 hzm 300.0
 is 300.0
 rf 300.0
 rf 300.0
 th 300.0
 ms 300.0

not used
 FLAGS
 ll
 in
 dp
 hs




```
Username: jjparl
Node: u300a
```

expl stdlh

```

      SAMPLE
node      u300a
probeid   fn5mm_120
          8
date      Oct  7 16
solvent    CDCl3
acqenv     proton
file       exp

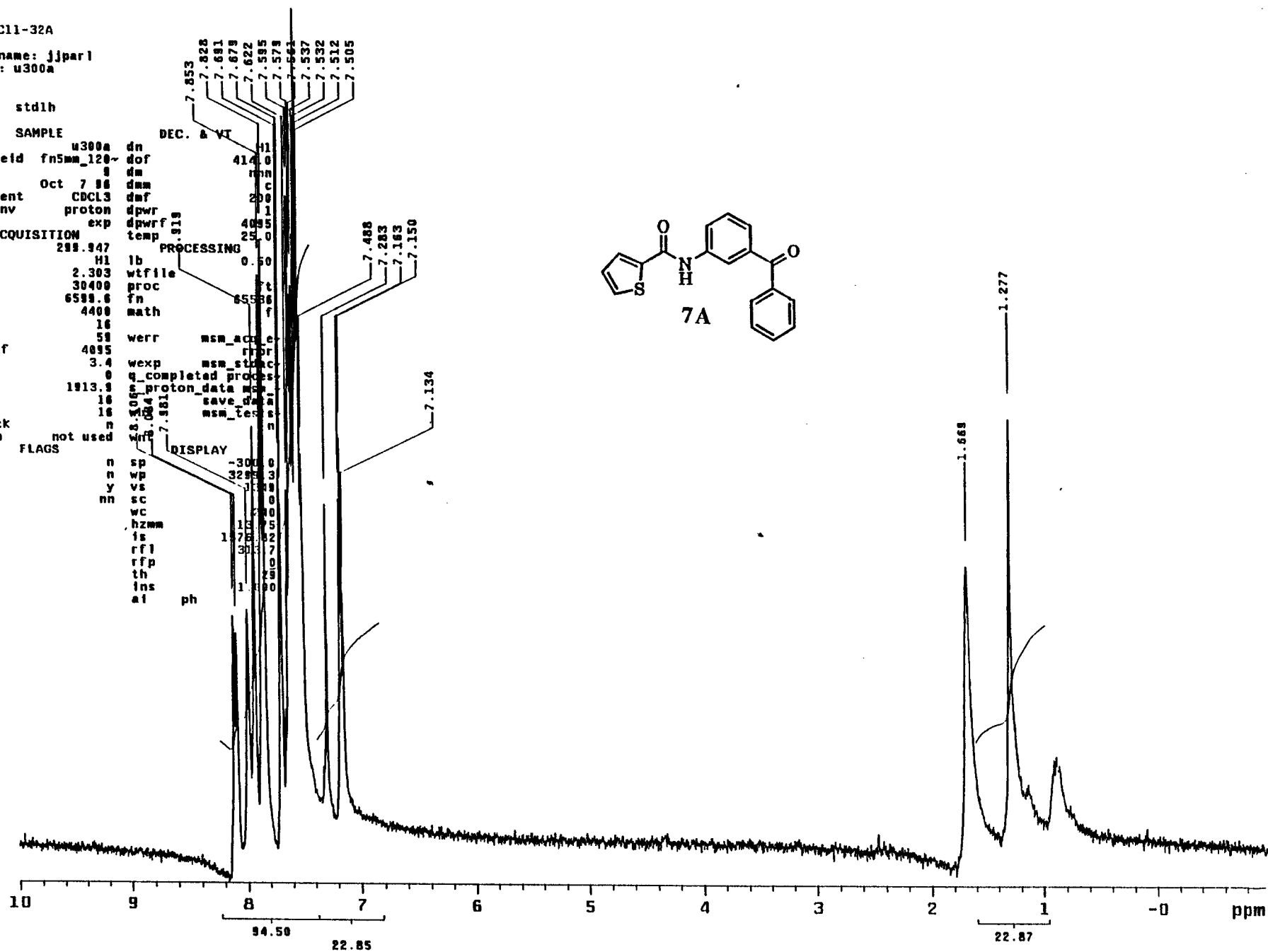
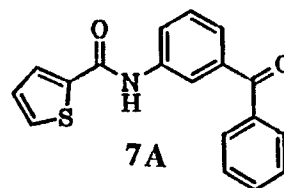
```

~~DEC. 6 VI~~

PROCESSING

DISPLAY

ph



485-C8-32c

Username: jjparl
Node: u300a

expl stdlh

SAMPLE

node	u300a	dn	41
probeid	fn5mm_120~	dof	414
		dm	0
date	Oct 7 86	dmm	0
solvent	CDCL3	dmf	2
acqenv	proton	dpwr	1
file	exp	dpwrf	40
		temp	25

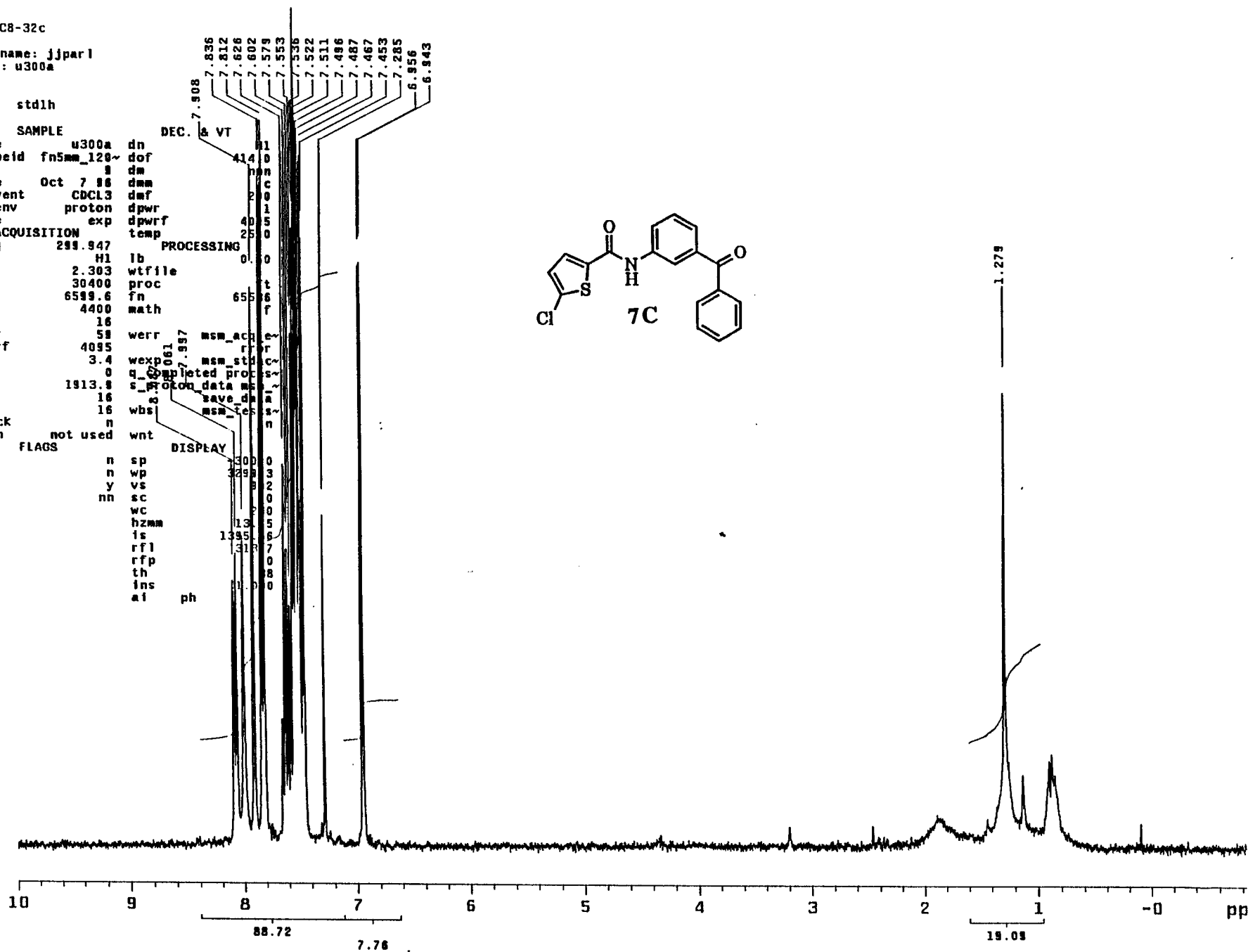
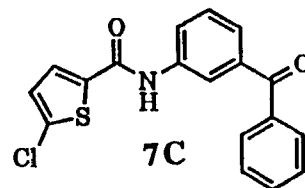
ACQUISITION

sfrq	299.947	PROCESSING	0
tn	H1	lb	0
at	2.303	wtfile	
np	30400	proc	t
sw	6599.6	fn	655
fb	4400	math	f
bs	16		
tpwr	58	werr	
tpwrf	4095	wexp	0.061
pw	3.4	msm_std	c
d1	0	q_completed	proce
tof	1913.8	s_proton_data	ms
nt	16	save_da	a
ct	16	msm_ses	s
alock	n	wbs	n
gain	not used	wnt	

DISPLAY

ll	n	sp	0
ln	n	wp	3
dp	y	vs	8
hs	nn	sc	0
		wc	0
		hzmm	13
		is	1395
		rfl	318
		rfp	7
		th	0
		ins	0
		ai	0

ph



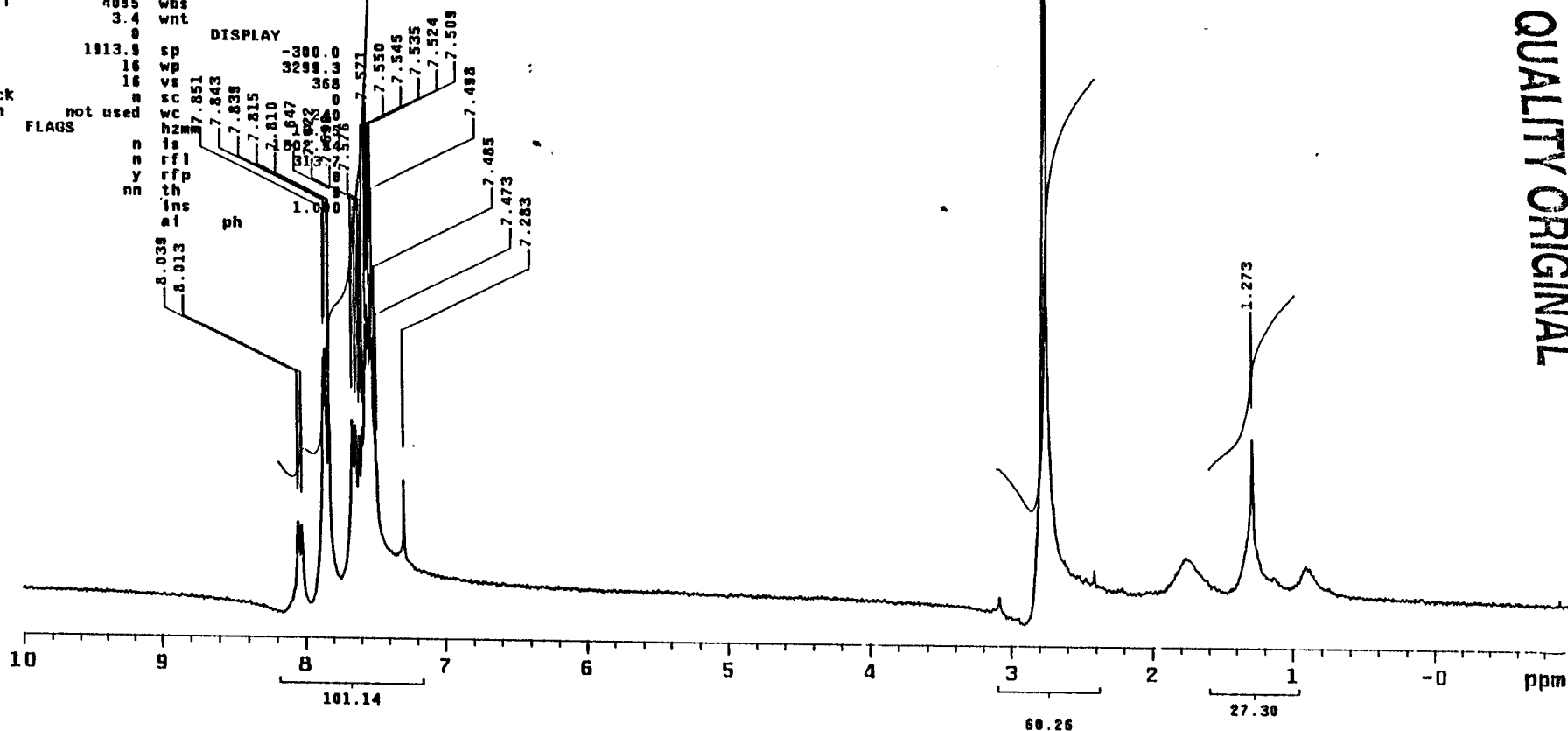
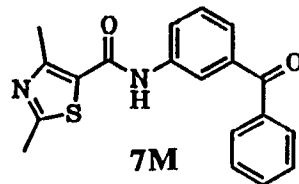
POOR QUALITY ORIGINAL

485-D7-32M

Username: jjparl
Node: u300a

exp3 std1h

SAMPLE		DEC. & VT	
node	u300a	dn	H1
probeid	fn5mm_120~	dof	414.0
		dm	nmr
date	Oct 7 96	dsm	c
solvent	CDCL3	daf	200
acqenv	proton	dpwr	1
file	/srv07/ho~	dpwrf	4095
me/jjparl/vnmrsvs/~		temp	25.0
data/485-D7-32M			
ACQUISITION		lb	0.50
sfrq	299.947	wtfile	
tn	H1	proc	ft
at	2.303	fn	65538
np	30400	math	f
sw	6599.6		
fb	4400	werr	
bs	16	wexp	
tpwr	59	process ~	
tpwrf	4095	proton_data	
pw	3.4	wbs	
dl	0	wnt	
tof	1913.9	DISPLAY	
nt	16	sp	-300.0
ct	16	wp	3299.3
alock	16	vs	368
gain	not used	sc	0
		wc	0
hzm	7.851	hzm	7.851
ts	7.838	ts	7.838
rfl	7.815	rfl	7.815
rff	7.810	rff	7.810
th	7.807	th	7.807
ins	7.804	ins	7.804
al	7.801	al	7.801
ph	1.000	ph	1.000

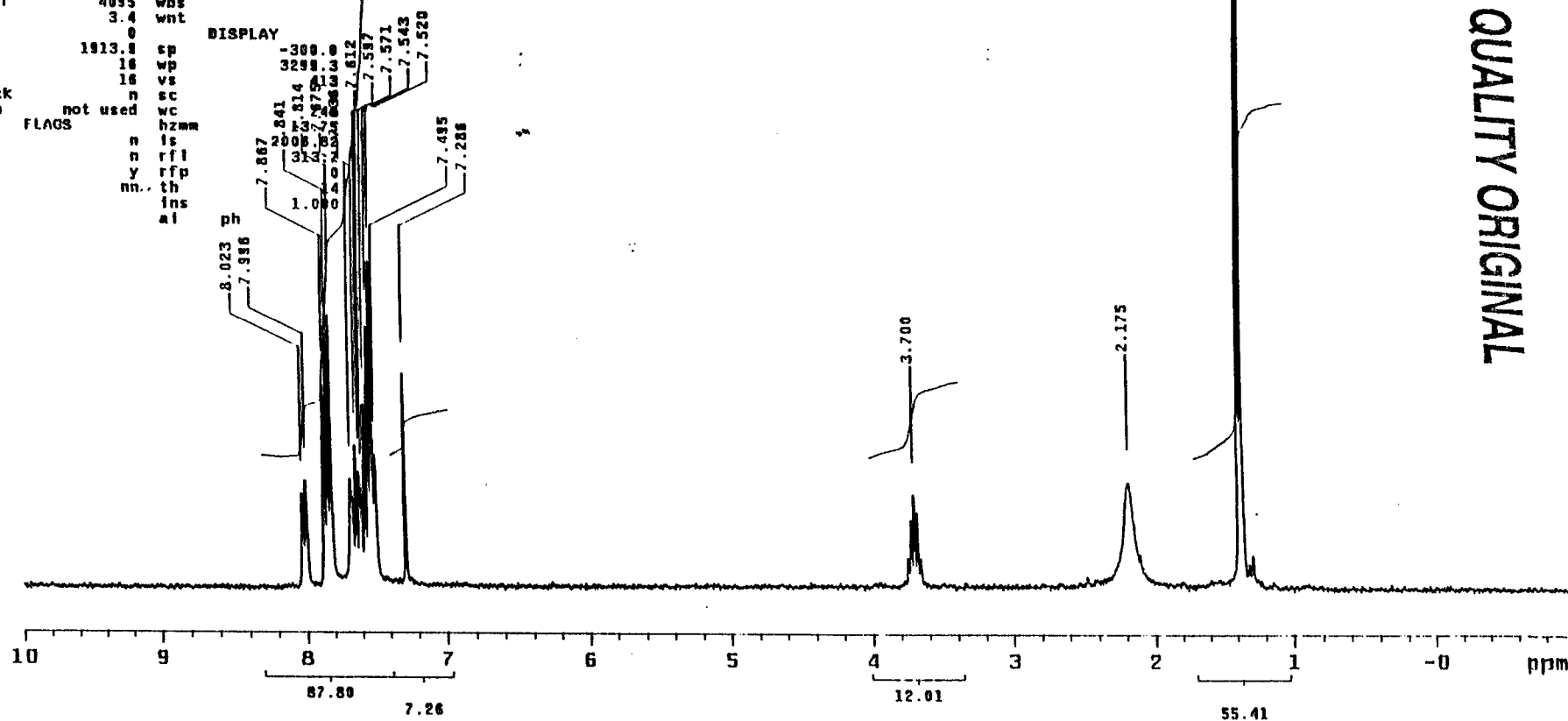
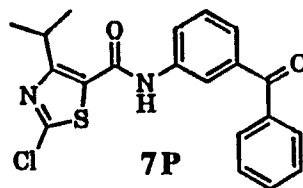


485-B6-32P

Username: jiparl
Node: u300a

exp3 stdlh

SAMPLE		DEC. & VT	
mode	u300a	dn	H1
probeid	fn5mm_120~	dof	414.0
		dm	nmn
date	Oct 7 98	dmm	c
solvent	CDCl3	dmf	200
acqenv	proton	dpwr	1
file	/srv07/hw~	dpwrf	4095
me/jiparl/vnarsys/~		temp	25.0
data/485-B6-32P		PROCESSING	
ACQUISITION	lb	0.50	
sfrq	299.947	wtfile	
tn	H1	proc	ft
at	2.303	fn	65536
np	30400	math	f
sw	6588.6		
fb	4400	werr	
bs	16	wexp	
tpwr	58	process ~	
tpwrf	4095	proton_data	
pw	3.4	wbs	
dl	0	wnt	
tor	1913.8	DISPLAY	
nt	16	ep	-300.0
ct	16	wp	3298.3
clock	n	vs	3298.3
gain	not used	sc	3298.3
	FLAGS	wc	3298.3
il	n	hzmm	3298.3
in	n	ls	3298.3
dp	y	rfl	3298.3
hs	nn	rff	3298.3
		th	3298.3
		ins	3298.3
		al	3298.3



POOR QUALITY ORIGINAL

POOR QUALITY ORIGINAL

485-05-32W

Username: jiparl
Node: u300a

expl stdlh

SAMPLE

node u300a
probeid fn5mm_120-
date Oct 7 86
solvent CDCL3
acqenv proton
file exp

ACQUISITION

sfrq 289.947
tn H1
at 2.303
np 30400
sw 6598.6
fb 4400
bs 16
tpwr 59
tpwrf 4095
pw 3.4
dl 0
tof 1913.8
nt 16
ct 16
alock n
gain not used

PROCESSING

lb
wtfile
proc
fn
math

werr msm_acq
wexp msm_std
q_completed process
s_proton_data msm
save data
msm_test

DISPLAY
-300.0
3298.6
825
240
13.26
1175.0
313.7
25
1.000
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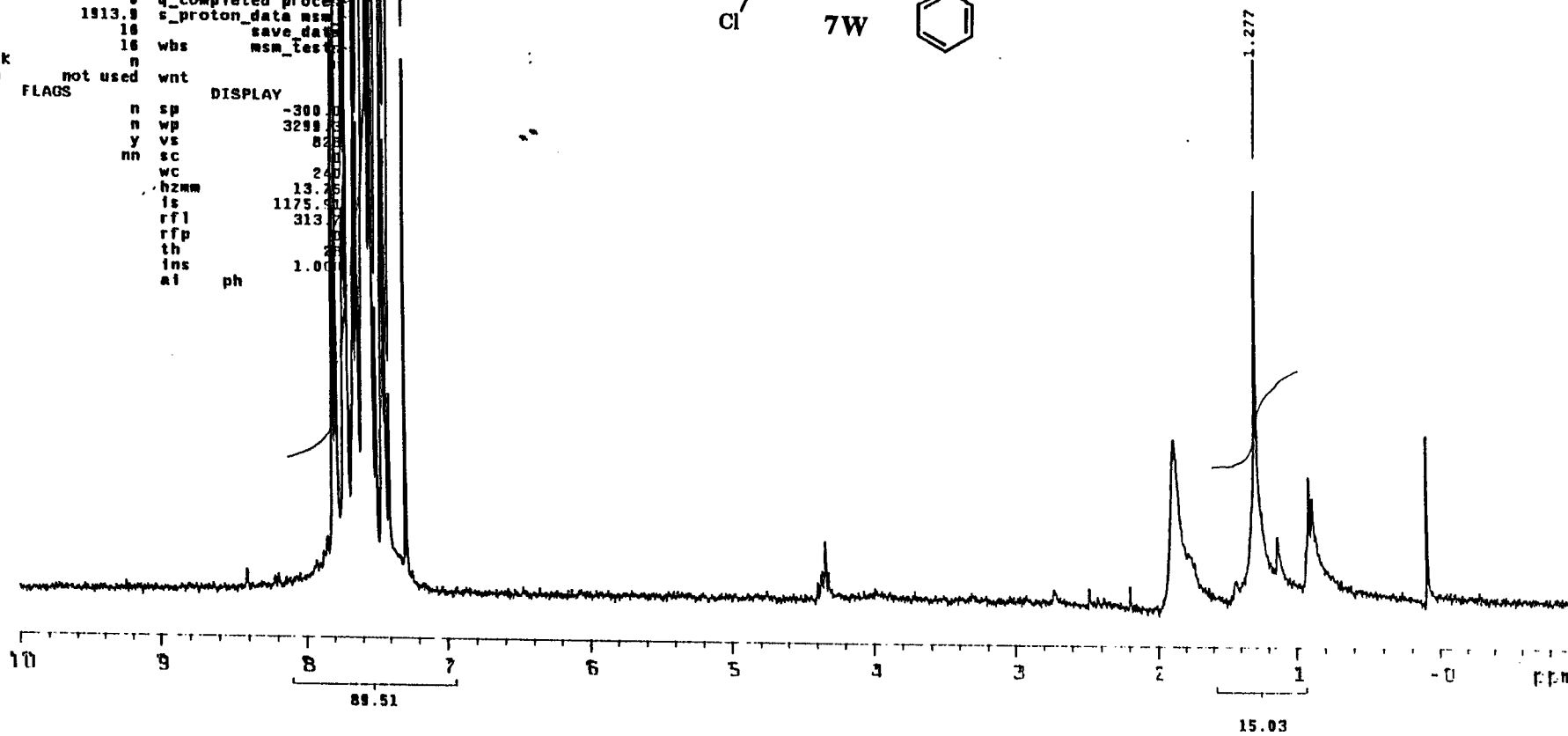
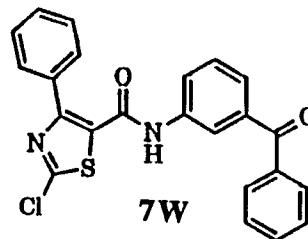
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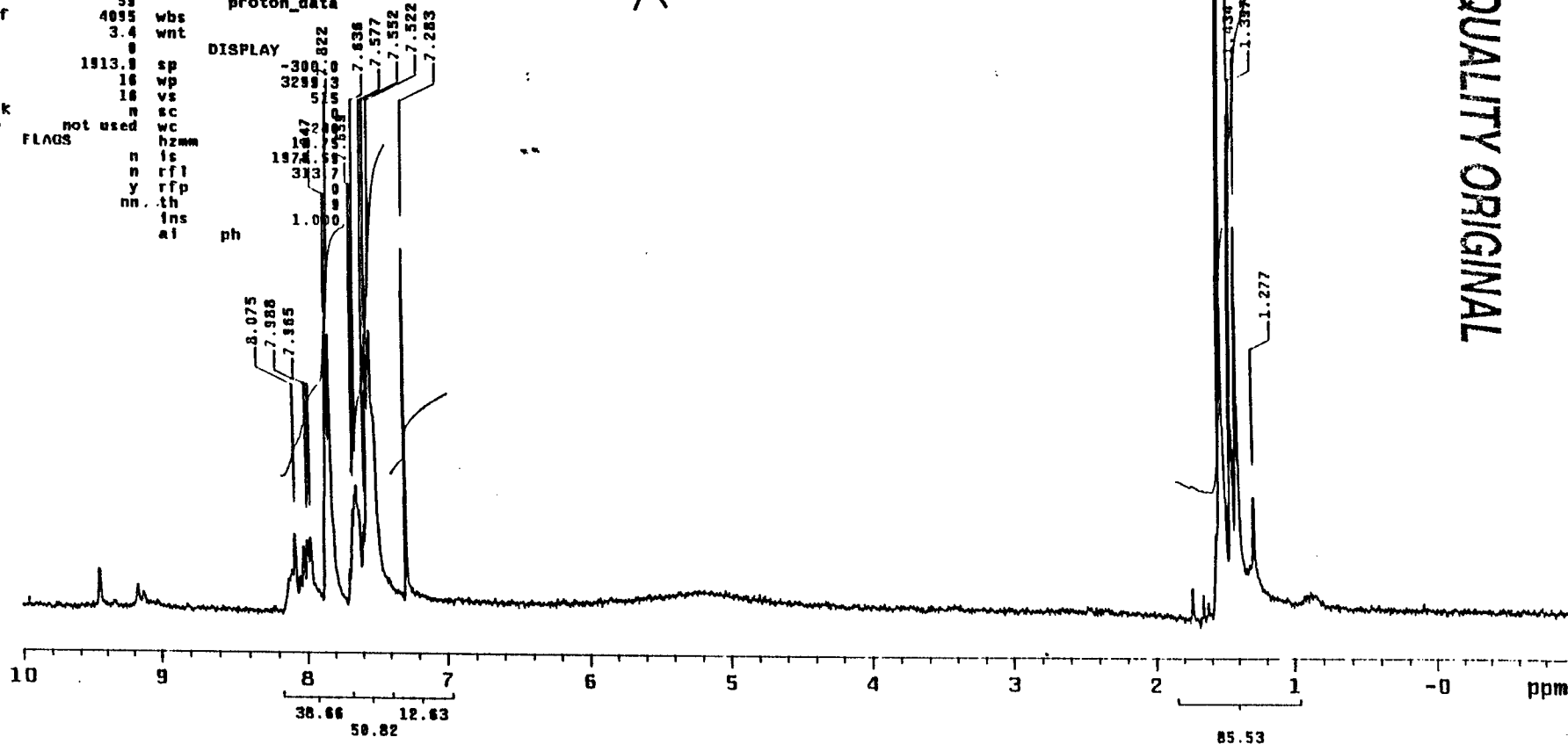
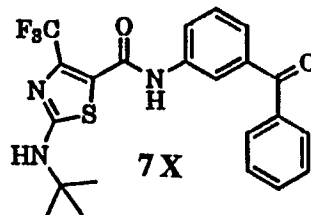


485-B4-32X

Username: jjparl
Node: u300a

exp3 std1h

SAMPLE		DEC. & VT	
node	u300a	dn	H1
probed	fn5mm_120~	dof	414.0
		da	nmr
date	Oct 7 98	dms	c
solvent	CDCL3	dmf	200
acqenv	proton	dpwr	1
file	/srv07/hw~	dpwrf	4095
me/jjparl/vnmr/sys~		temp	25.0
data/485-B4-32X			
ACQUISITION		PROCESSING	
sfrq	299.947	lb	0.50
tn	H1	wtfile	
at	2.303	proc	ft
np	30400	fn	65538
sw	6599.6	math	f
fb	4400	werr	
bs	16	wexp	
tpwr	59		
tpwrf	4095	wbs	
pw	3.4	wnt	
di	0		
tof	1913.8	sp	-300.0
nt	16	wp	3299.3
ct	16	vs	515
clock	n	sc	147
gain	not used	wc	1974.5
		hzmm	313.7
ll	n	ls	0.0
in	n	rfl	0.0
dp	y	rfp	0.0
hs	nn	th	0.0
		ins	1.000
		ai	



POOR QUALITY ORIGINAL

POOR QUALITY ORIGINAL

485-G12-322

Username: jiparl
Node: u300a

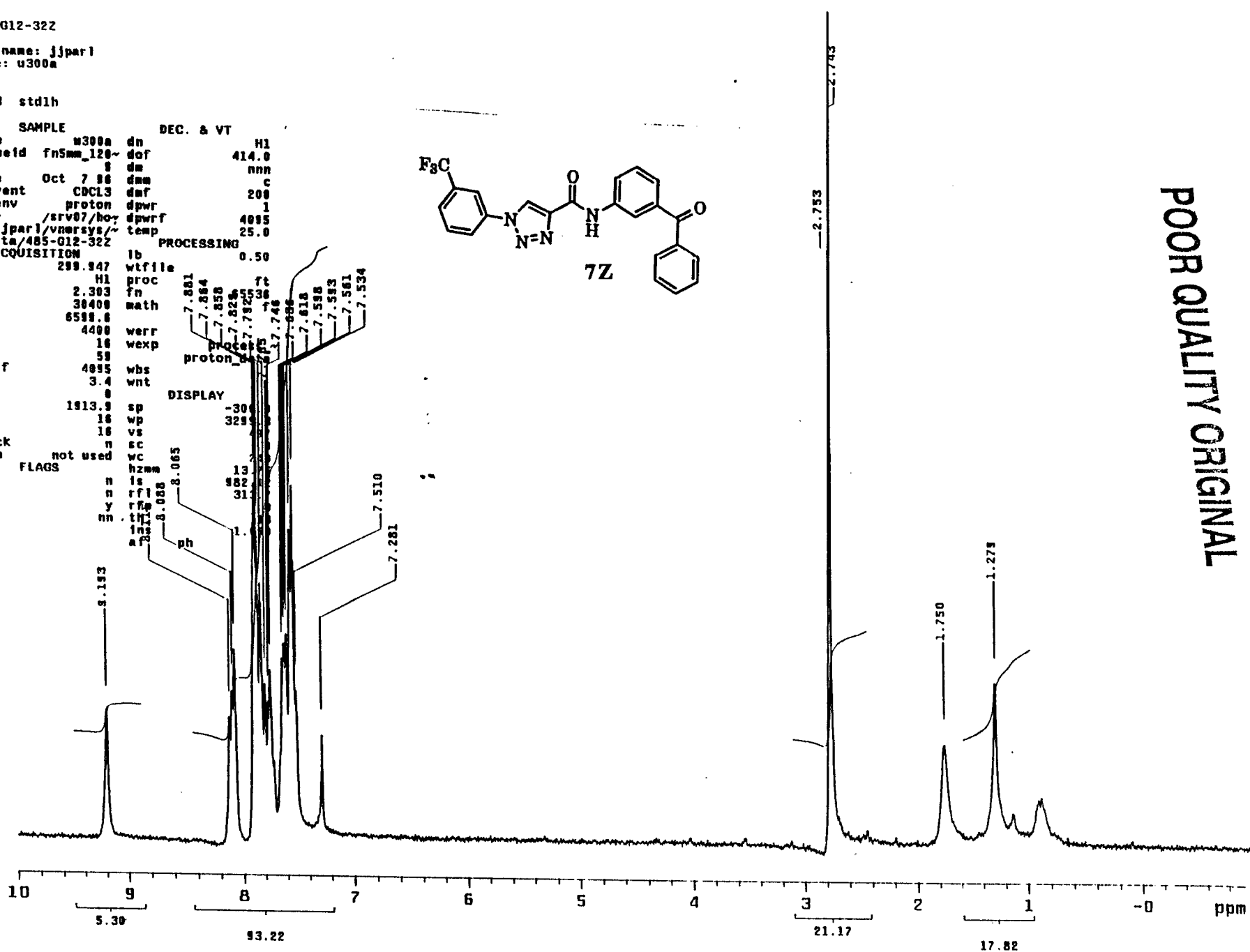
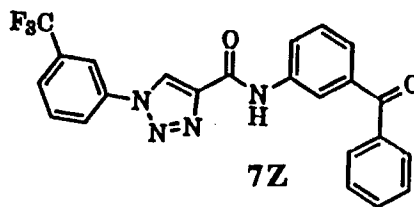
exp3 std1h

SAMPLE DEC. & VT

node u300a dn H1
probeid fn5mm_120~ dof 414.0
date Oct 7 96 dm nnn
solvent CDCl3 dmf c
acqenv proton dpwr 1
file /srv07/box dpwr 4095
me/jiparl/vnrsys/~ temp 25.0
data/485-G12-322

ACQUISITION lb 0.50
sfrq 299.947 wf file
tn H1 proc
at 2.303 fn
np 30400 math
sw 6589.6
fb 4400 werr
bs 16 wexp
tpwr 59
tpwrf 4095 wbs
pw 3.4 wnt
dl 0
tof 1913.9 sp
nt 16 wp
ct 16 vs
alock n sc
gain not used vc
FLAGS n hzmm
ii n is
in n rf
dp y r
hs nn t
a 3.216
ph 8.088
8.065

PROCESSING
DISPLAY
-30
329
13
982
31
7.881
7.864
7.858
7.826
7.792
7.748
7.686
7.618
7.598
7.583
7.561
7.534
7.510
7.281



542-C5-32aa

Username: jjparl
Node: u300a

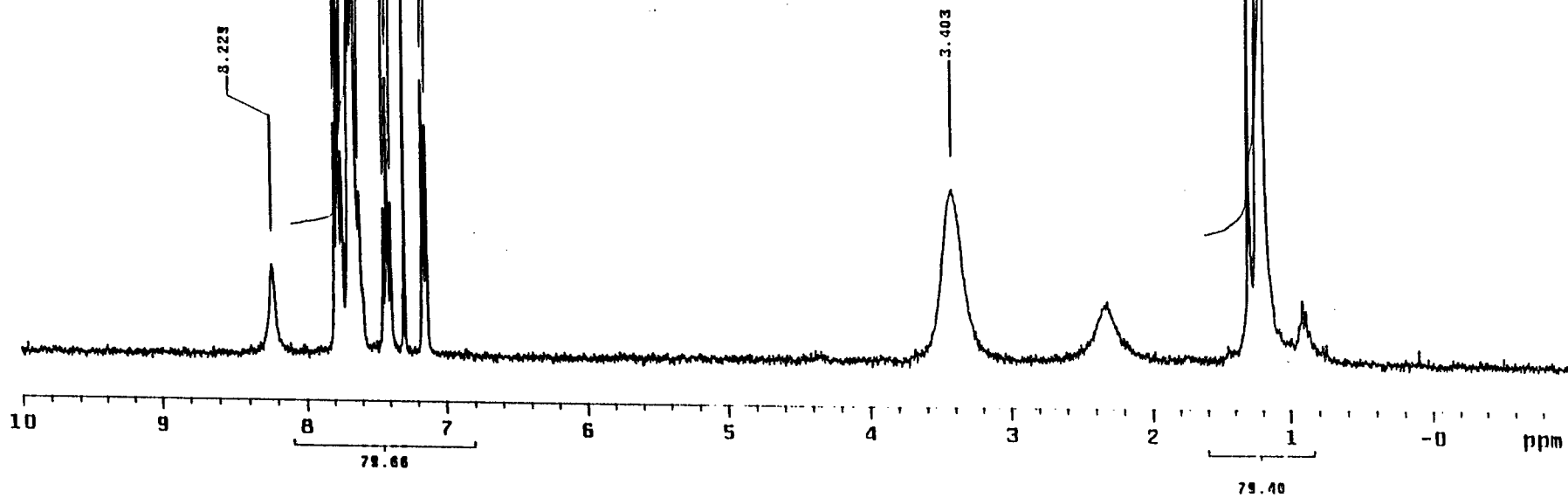
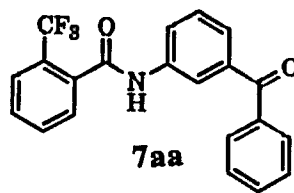
exp3 std1h

SAMPLE DEC. & VT
node u300a dn H1
probeid fn5mm_120~ dof 414.0
date Oct 7 98 dm nnn
solvent CDCl3 dmf 200
acqenv proton dpwr 1
file /srv07/hc~ dpwrf 4095
me/jjparl/vnmrsys~ temp 25.0
data/542-C5-32aa
ACQUISITION lb PROCESSING 0.50
sfrq 299.847 wtfile
tn H1 proc
at 2.303 fn
np 30400 math
sw 6588.6
fb 4400 werr
bs 16 wexp
tpwr 50
tpwrf 4095 wbs
pw 3.4 wnt
d1 0
tof 1913.8 sp
nt 16 wp
ct 16 vs
alock n sc
gain not used wc
FLAGS n hzwm
n ls
n rfl
y rfp
nn. th
al ins
ph al

PROCESSING

DISPLAY

ph



428-D2-32bb

Username: jjparl
Node: u300a

expl std1h

SAMPLE DEC. & VT

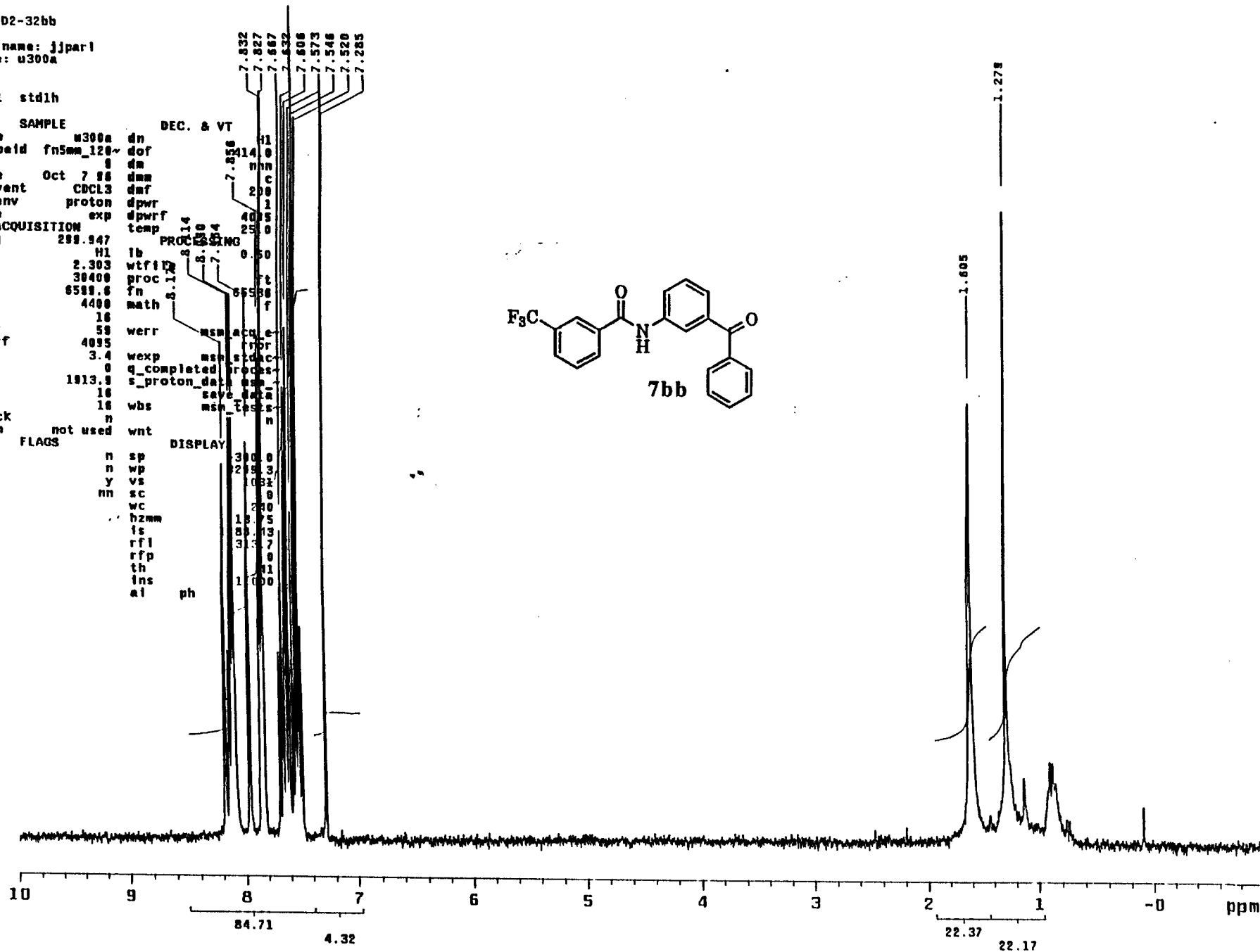
node u300a dn 41
 probeld fn5mm_120~ dor 0.14
 date Oct 7 86 dm 230
 solvent CDCL3 dmf 1
 acqenv proton dpwr 40.5
 file exp dpwrf 25.0
 ACQUISITION temp 25.0

sfreq 289.947
 tn H1
 at 2.303
 np 30400
 sw 6589.6
 fb 4400
 bs 16
 tpwr 59
 tpwrf 4095
 pw 3.4
 di 0
 tof 1913.9
 nt 16
 ct 16
 alock n
 gain not used
 wnt n

PROCESSING
 lb 0.50
 wtfile
 proc
 fn 65556
 math f
 werr
 msh
 wexp
 q_completed
 s_proton_data
 save_data
 wbs
 msh
 test
 n

DISPLAY
 sp 300.0
 wp 229.3
 vs 1031
 sc 0
 wc 240
 hzmm 15.5
 is 89.13
 rfl 313.7
 rfp 0
 th 1
 ins 1000
 al

ph



428-B10-32jj

Username: jip
Node: u300a

expl stdlh

SAMPLE

```

node u300a dn H1
probed fn5m 120~ dof 414.0
date Oct 7 86 dm mn
solvent CDCl3 dmf c
acqenv proton dpwr 1
file exp dpwr 4095
ACQUISITION temp 25.0
sfrq 295.947 PROCESSING 0.50
tn H1 lb wtfile
at 2.303 wfile
np 30400 proc ft
sw 8598.6 fn 5536
fb 4400 math f
bs 16
tpwr 58 werr mma acc e
tpwr 4095 rwr
pw 3.4 wexp mma stac
dl 0 q_completed probes
tof 1513.8 s_proton_data mma
nt 16 save_data mma
ct 16 mma tests
alock n
gain not used wnt n

```

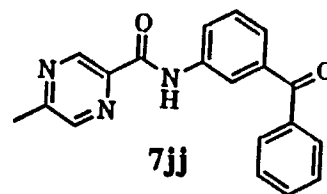
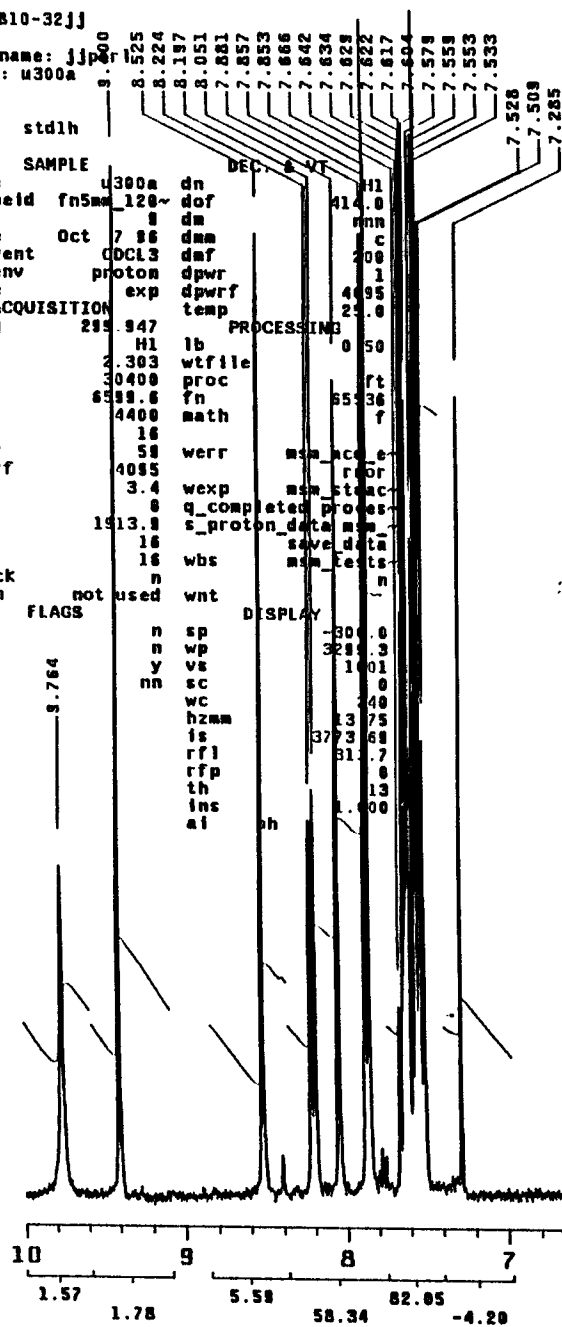
FLAGS

DISPLAY

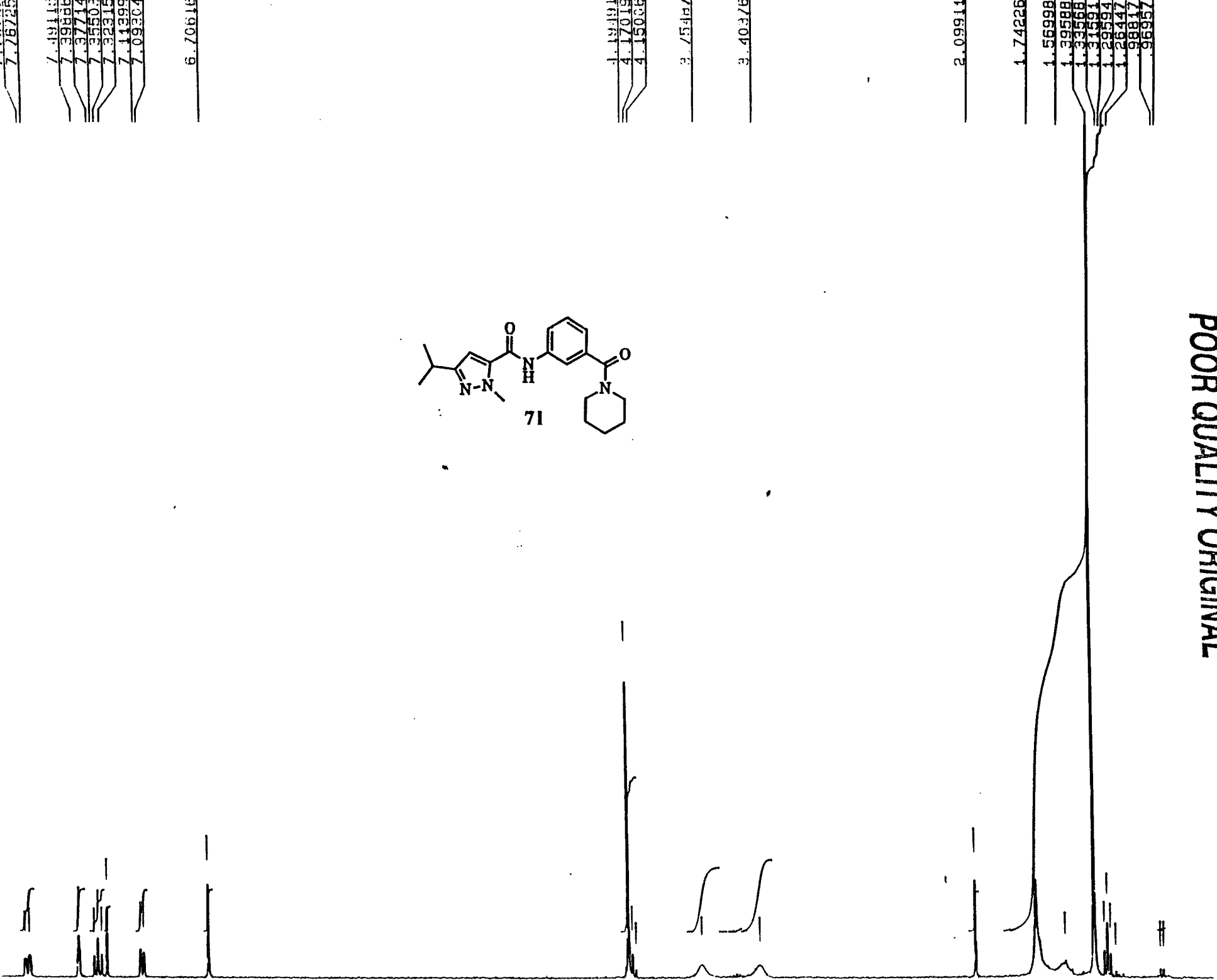
```

il n
in n
dp y
hs nn

```



POOR QUALITY ORIGINAL

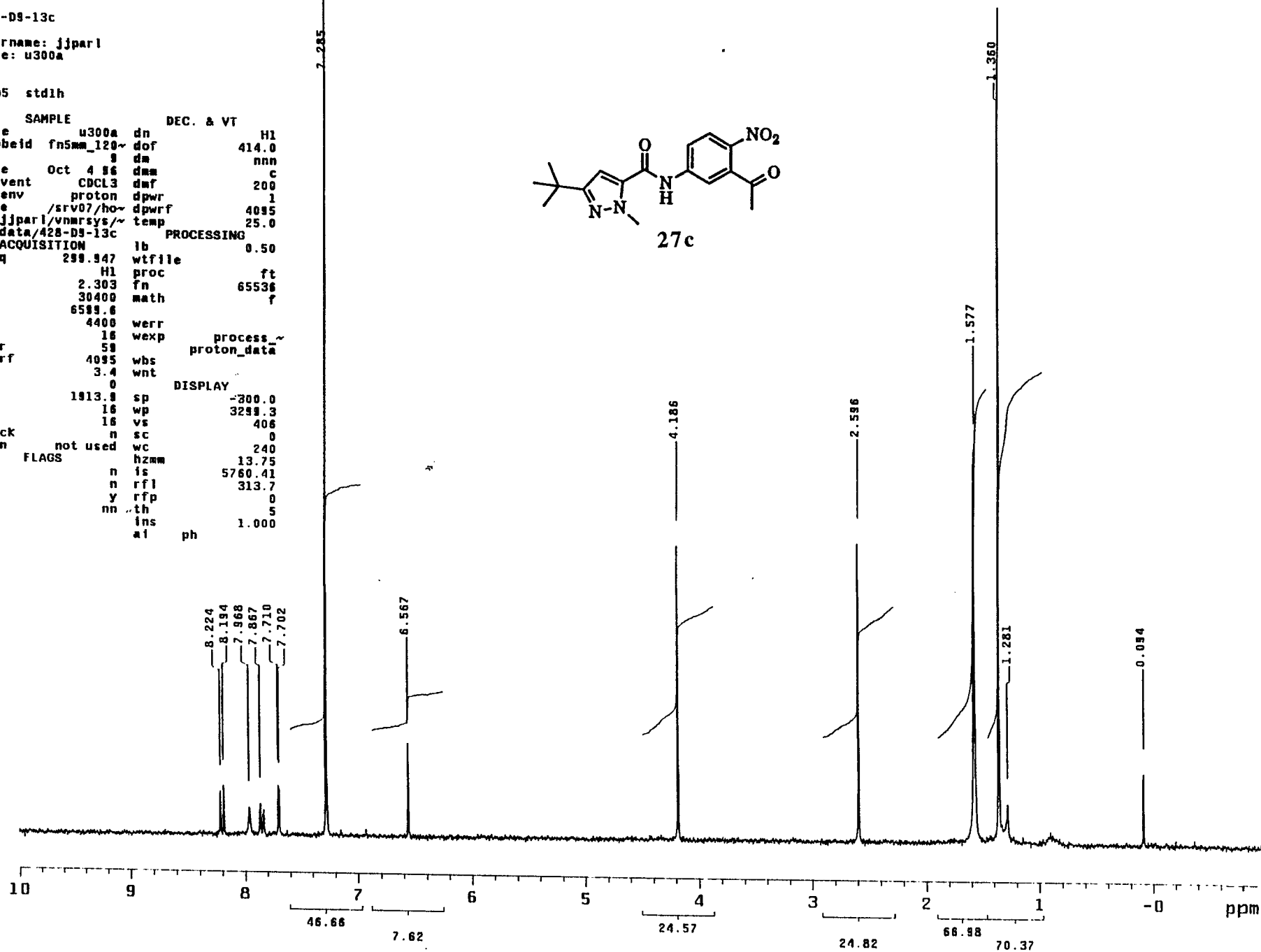
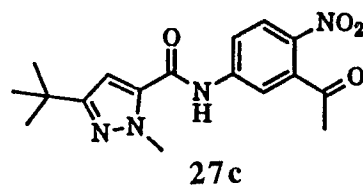


428-D9-13c

Username: jiparl
Node: u300a

exp5 std1h

SAMPLE		DEC. & VT	
node	u300a	dn	H1
probeid	fn5mm_120~	dof	414.0
		dm	nnn
date	Oct 4 86	dmm	c
solvent	CDCL3	dmf	200
acqenv	proton	dpwr	1
file	/srv07/ho~	dpwrf	4095
me/jiparl/vnmrsvs/~		temp	25.0
data/428-D9-13c		PROCESSING	
ACQUISITION	lb		0.50
sfrq	299.947	wtfile	
tn	H1	proc	ft
at	2.303	fn	65536
np	30400	math	f
sw	6599.6		
fb	4400	werr	
bs	18	wexp	process_~
tpwr	59		proton_data
tpwrf	4095	wbs	
pw	3.4	wnt	
d1	0	DISPLAY	
tof	1913.9	sp	-300.0
nt	16	wp	3299.3
ct	16	vs	406
alock	n	sc	0
gain	not used	wc	240
il	FLAGS	hzmm	13.75
in	n	is	5760.41
dp	y	rfl	313.7
hs	nn	rpf	0
		th	5
		ins	1.000
		ai	
		ph	



485-B1-13e

Username: jjparl
Node: u300a

exp5 std1h

SAMPLE DEC. & VT

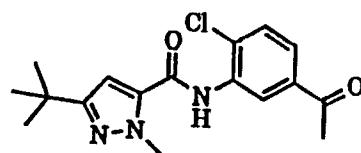
node u300a dn H1
probeid fn5mm_128~ dof 414.0
date Oct 4 96 dnm nnn
solvent CDCL3 dmf c
acqenv proton dmf 200
file /srv07/hov dpwrf 1
me/jjparl/vnmrsvs/~ temp 4095
data/485-B1-13e temp 25.0

PROCESSING

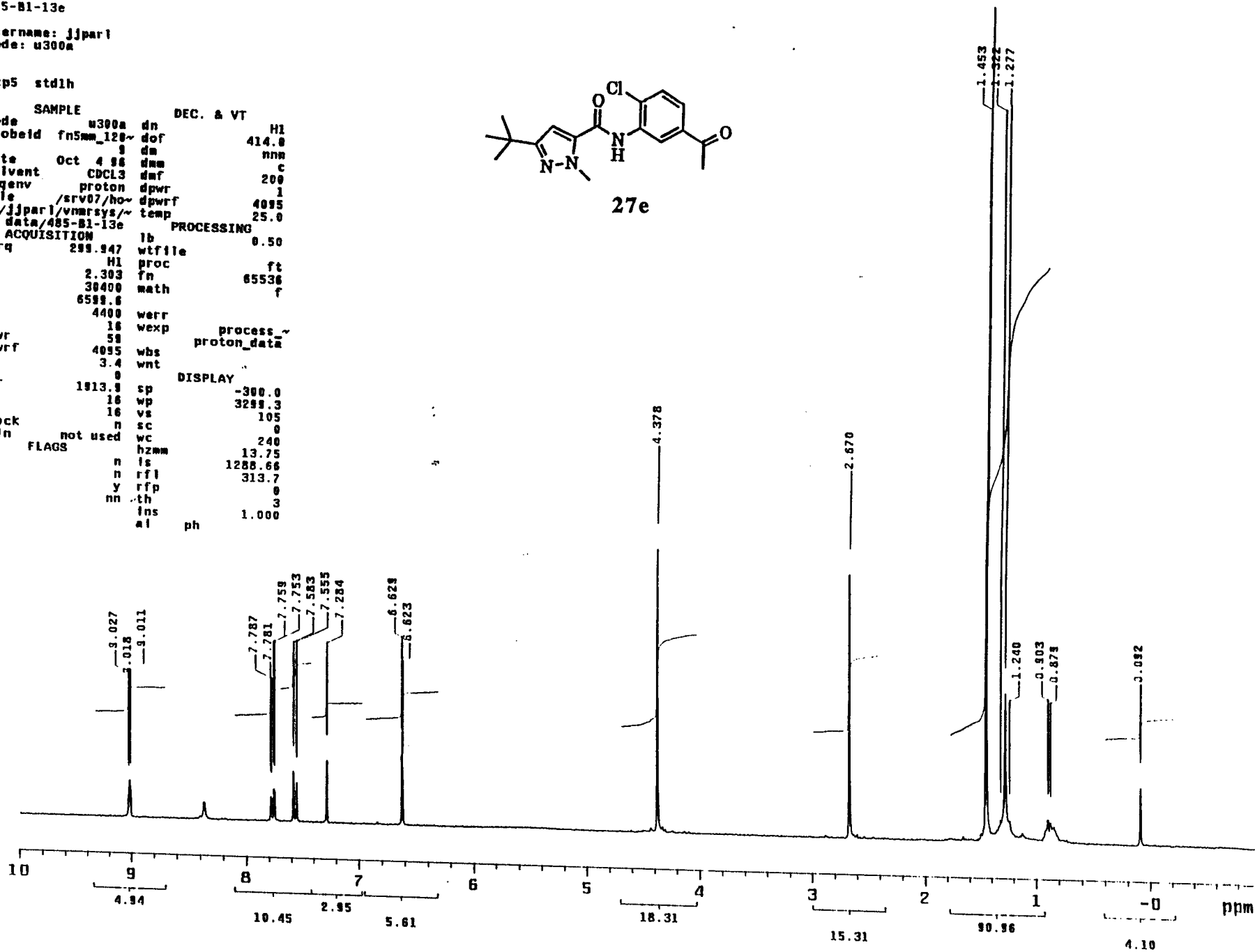
ACQUISITION lb 0.50
sfrq 299.947 wtfile
tn H1 proc
at 2.303 fn ft
np 30400 fn 65536
sw 6599.6 math f
fb 4400 werr
bs 16 wexp
tpwr 50 process ~
tpwrf 4095 wbs proton_data
pw 3.4 wnt
dl 0
tof 1913.9
nt 16 sp
ct 16 wp
a lock 16 vs
gain not used wc
il n hzmm
in n ls
dp y rfi
hs nn rfp
th 0
ins 3
al 1.000
ph

DISPLAY

sp -300.0
wp 3299.3
vs 105
sc 0
wc 240
hzmm 13.75
ls 1288.66
rfi 313.7
rfp 0
th 3
ins 1.000
al



27e



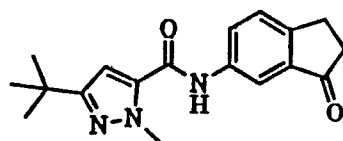
428-A8-13g

Username: jjparl

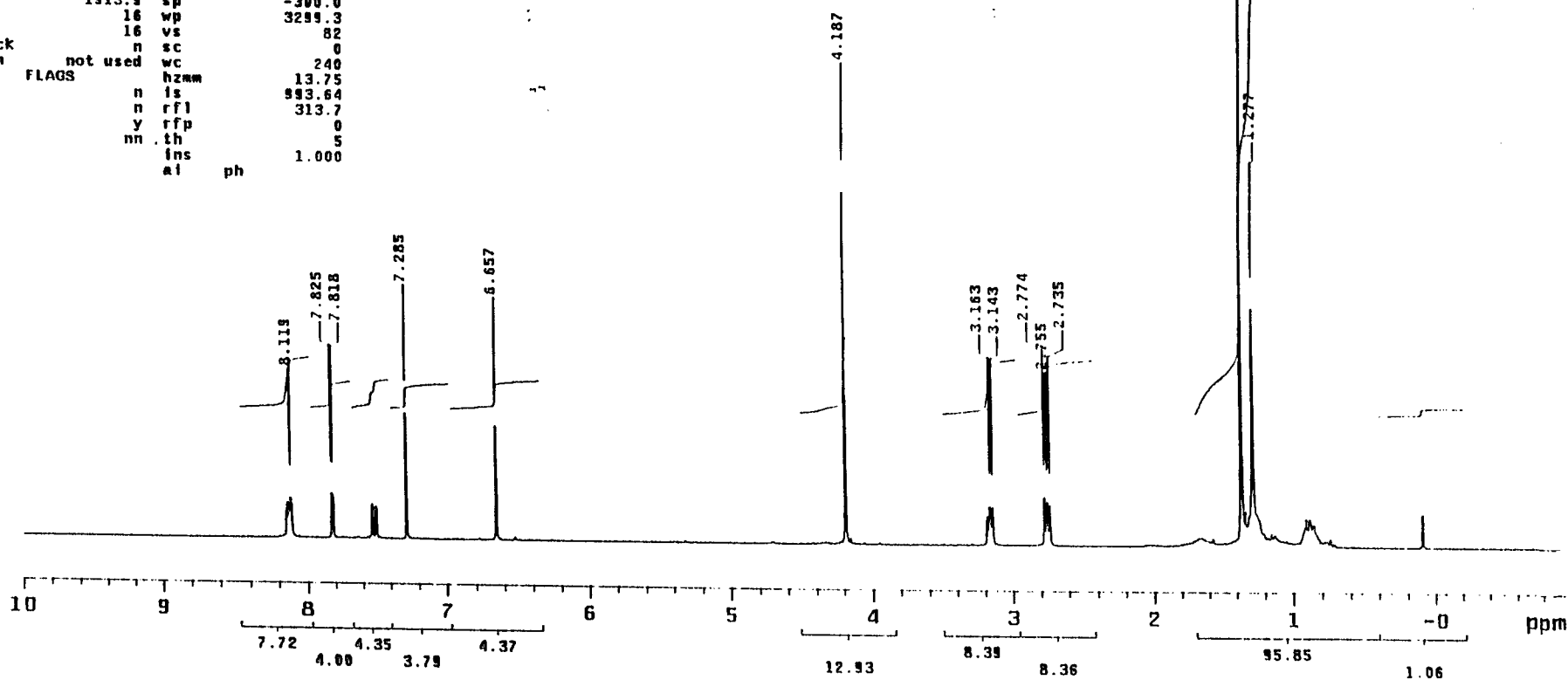
Node: u300a

exp5 std1h

SAMPLE		DEC. & VT	
node	u300a	dn	H1
probeid	fn5mm_120~	dof	414.0
		dm	nnn
date	Oct 4 98	dmm	C
solvent	CDCl3	dmf	200
acqenv	proton	dpwr	1
file	/srv07/hom	dpwrf	4095
me/jjparl/vnmrsvs/~		temp	25.0
data/428-A8-13g		PROCESSING	
ACQUISITION	lb		0.50
sfrq	299.947	wtfile	
tn	H1	proc	ft
at	2.303	fn	65536
np	30400	math	f
sw	6599.6		
fb	4400	werr	
bs	16	wexp	
tpwr	59	process_~	
tpwrf	4095	proton_data	
pw	3.4		
d1	0		
tof	1913.9	sp	-300.0
nt	16	wp	3299.3
ct	16	vs	82
alock	n	sc	0
gain	not used	wc	240
FLAGS		hzmm	13.75
il	n	ls	993.64
in	n	rfl	313.7
dp	y	rfp	0
hs	nn	th	5
		ins	1.000
		ai	ph



27g

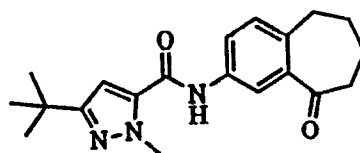


428-C2-13h

Username: jjparl
Node: u300a

exp5 std1h

SAMPLE		DEC. & VT	
node	u300a	dn	H1
probeid	fn5mm_120	dof	414.0
		dm	nnn
date	Oct 4 96	dmm	c
solvent	CDCl3	dmf	200
acqenv	proton	dpwr	1
file	/srv07/ho~	dpwrf	4095
me/jjparl/vnmrsvs/~		temp	25.0
data/428-C2-13h			
ACQUISITION		PROCESSING	
sfrq	299.947	lb	0.50
tn	H1	wtfile	
at	2.303	proc	ft
np	30400	fn	65536
sw	6599.6	math	f
fb	4400		
bs	16	werr	
tpwr	59	wexp	
tpwrf	4095	process	~
pw	3.4	proton_data	
d1	0	wbs	
tof	1913.9	wnt	
nt	16	DISPLAY	
ct	16	sp	-300.0
alock	n	wp	3299.3
gain	not used	vs	82
	FLAGS	sc	0
		wc	0
		hzmm	0
il	n	ls	0
in	n	rfl	0
dp	y	rfp	0
hs	nn	th	0
		ins	0
		ai	0



27h

