Supporting Information

General: Caffeic acide phenethyl ester (CAPE), dihydrocaffeic acid phenethyl ester (DHC), SB 203580 and BIRB-796 were obtained from commercial suppliers and used without further purification. All solvents were distilled prior to use. Nuclear magnetic resonance (NMR) spectroscopy was performed on either Varian Unity+ 300 (300 MHz) or Varian DirectDrive 400 (400 MHz) instruments. Melting points were obtained using a Buchi B-540 apparatus and are uncorrected. Mass spectrometry services were provided by the Mass Spectrometry Facility at the University of Texas at Austin. HPLC was performed on a Varian Prostar 320 system.

4-(4-fluorophenyl)-5-(4-pyridyl)-1-ethynyl-1H-imidazole (2): To a solution of 5 mg (0.01 mmol) of 4-(4-fluorophenyl)-5-(4-pyridyl)-2-(2-triisolpropylsilanyl)-1H-imidazole[S1] in 2 mL THF at -78 °C was added a solution of 1.0 M tetrabutylammonium fluoride in THF (0.012 mL, 0.012 mmol). The reaction mixture was stirred at -78 °C until completion (*ca*. 30 min). Water (2 mL) was added to the reaction mixture, which was allowed to warm to room temperature and extracted 3 x CH_2Cl_2. The organic layers were combined, dried over Na_2SO_4, and the solvent was evaporated under reduced pressure. The residue was purified by flash chromatography (0-50% EtOAc/hexane) to afford 4-(4-fluorophenyl)-5-(4-pyridyl)-1-ethynyl-1H-imidazole (3 mg, 96 % yield) as a light yellow solid: mp = 123-124 °C; ^{1}H NMR (300 MHz, $CDCl_3$) d: 8.69 (br s, 2H, pyridine 2-,6-**H**), 7.94 (s, 1H, imidazole 2-**H**), 7.48-7.39 (m, 2H, pyridine 3-,5-**H**), 7.40-7.39 (m, 2H, Ar 2-,6-**H**), 7.02-6.98 (m, 2H, Ar 3-,5-**H**); MS m/z: 264 (M^+, 100); HRMS (CI) calcd for $C_{16}H_{11}N_3F$ (M^+) 264.0937, found 264.0932.

***N*-(4-hydroxy-3-methoxyphenethyl)-2-(4-hydroxyphenyl)acetamide (Mis-042):** A mixture of 32 mg (0.19 mmol) of 2(4-hydroxy-3-methoxyphenyl)ethylamine and 29 mg (0.19 mmol) of 4-hydroxyphenylacetic acid was heated under Ar at 190 °C for 2 h. After cooling to room temperature, the reaction mixture was dissolved in EtOAc and washed with 1 N HCl, $NaHCO_3$ (sat), and brine. The organic layer was dried over Na_2SO_4 and evaporated. The residue was recrystallized from EtOAc to afford 18 mg (32 % yield) of MIS-042 as tan crystals: mp = 131.9-133.5 °C (lit.[S2] 132-134 °C); ^{1}H NMR (300 MHz, CD_3CN) d 7.01 (d, 2H, J = 8.2 Hz, phenol 3,-5-**H**), 6.74-6.68 (m, 3H, phenol 2-,6-H, catechol 4-**H**), 6.56 (d, 1H, J = 8.0 Hz, catechol 3-**H**), 6.39 (br s, 1H, catechol 6-**H**), 3.78 (s, 3H, catechol O**Me**), 3.33-3.28 (m, 4H, NHC**H**$_2$, C**H**$_2$CO), 2.62 (t, 2H, J = 7.0 Hz, NCH$_2$C**H**$_2$); ^{13}C NMR (75 MHz, CD_3CN) d 172.2, 156.6, 147.9, 145.3, 131.9, 131.1, 127.8, 122.0, 116.0, 115.3, 113.0, 56.3, 42.8, 41.4, 35.5; MS (ESI) *m/z* 302 ($MH,^+$ 21), 324 ([M+Na],$^+$ 100); HRMS (ESI) calcd for $C_{17}H_{20}NO_4$ $(MH)^+$ 302.13868, found 302.13858.

General Procedure for Synthesis of MIS-103, 108, 109, 112, and 113: (*E*)-Phenethyl 3-(4-fluoro-3-methoxyphenyl)acrylate (Mis-108): 4-Fluoro-3-methoxybenzaldehyde (100 mg, 0.648 mmol), (carboxymethyl)triphenylphosphonium chloride β-phenylethyl ester,[S3] (0.973 mg, 0.648 mmol) and

$KHCO_3$ (211.7 mg, 2.11 mmol) were dissolved in 2 mL of dioxane and 2 mL of $CHCl_3$. The resulting mixture was refluxed at 80 °C for 18 hours. The reaction mixture was allowed to cool to room temperature, poured into water, and extracted with $CHCl_3$. The combined extracts were washed with brine, dried over anhydrous Na_2SO_4, filtered and evaporated. The residue was subjected to flash chromatography (4.5:0.5 hexane/EtOAc) to afford a mixture of *E*/*Z* isomers (1:0.14). Recrystallization from EtOAc/hexane afforded pure *E*- isomer as a white crystalline solid (122 mg, 63% yield): mp 70.0-71.1 °C; IR: 2962, 1705, 1474, 1216, 780 cm^{-1}. ^1H NMR (300 MHz, d_6-acetone): δ 3.01 (t, J = 6.8 Hz, 2 H), 3.96 (s, 3 H), 4.38 (t, J = 6.8 Hz, 2 H), 6.52 (d, J = 16 Hz, 1 H), 7.16-7.31 (m, 2 H), 7.31 (d, J = 4.5 Hz, 4 H), 7.51 (dd, J_1 = 8.2 Hz, J_2 = 6.4 Hz, 1 H), 7.62 (d, J = 16 Hz, 1 H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 166.7, 153.7 (J_{C-F} = 250 Hz), 147.9 (J_{C-F} = 11 Hz), 143.9, 137.8, 131.0 (J_{C-F} = 4 Hz), 128.9, 128.5, 126.6, 121.6 (J_{C-F} = 7 Hz), 117.8, 116.4 (J_{C-F} = 18 Hz), 112.2, 65.0, 56.2, 35.2; CI-MS *m/z* 301(MH^+, 65), HRMS (CI) calcd for $C_{18}H_{17}FO_3$ $(MH)^+$ 301.1240, found 301.1239.

(*E*)-3-(3-fluoro-4-methoxyphenyl)-*N*-phenethylacrylamide (Mis-103). Following the general procedure above, but substituting (2-oxo-2-(phenethylamino)ethyl)triphenylphosphonium chloride[S4] for (carboxymethyl)triphenylphosphonium chloride β-phenylethyl ester, afforded after flash chromatography (4.5:0.5 hexane/EtOAc) and recrystallization from CH_2Cl_2/hexane **Mis-103** as a white crystalline solid (89 mg, 80 % yield): mp 152-152.4 °C; ^1H NMR (300 MHz, $CDCl_3$): δ 7.51 (d, 1H, J = 15.6 Hz, ArC**H**=CH), 7.34-7.16 (m, 7H, ArH), 6.51 (t, 1H, J = 8.4 Hz, Ar**H**), 6.16 (d, 1H, J = 15.6 Hz, CH=C**H**CO), 5.58 (brs, 1H, N**H**), 3.89 (s, 3H, O**Me**), 3.64 (dt, 2H, J = 6.9, 6.3 Hz, NHC$\mathbf{H_2}$), 2.87 (t, 2H, J = 6.9 Hz, $CH_2C\mathbf{H_2}$Ph); ^{13}C NMR (75 MHz, $CDCl_3$): δ 165.9, 152.5 (J_{C-F} = 247 Hz), 149.2 (J_{C-F} = 9.0 Hz), 140.0, 139.1, 129.0, 128.9, 128.3 (J_{C-F} = 7 Hz), 126.8, 125.3 (J_{C-F} = 3 Hz), 119.8, 114.4 (J_{C-F} = 19 Hz), 113.4 (J_{C-F} = 2 Hz), 56.5, 41.0, 35.9; MS (CI) m/z 300 (MH^+, 100); HRMS (CI) calcd for $C_{18}H_{19}FNO_2$ $(MH)^+$ 300.1400, found 301.1399.

(*E*)-Phenethyl 3-(3-fluoro-4-methoxyphenyl)acrylate (Mis-109). Following the general procedure above, flash chromatography (4:1 hexane/EtOAc) and recrystallization from EtOAc/hexane afforded **Mis-109** as a white crystalline solid (202 mg, 52% yield): mp 76.3-77.6 °C; IR 2935, 1705, 1516, 1458, 1278, 1167, 1127, 1020 cm^{-1}. ^1H NMR (300 MHz, d_6-acetone): δ 3.00 (t, J = 7.0 Hz, 2 H), 3.94 (s, 3 H), 4.37 (t, J = 7.0 Hz, 2 H), 6.44 (d, J = 16 Hz, 1 H), 7.17 (d, J = 8.6 Hz, 1H), 7.22 (dd, J_1 = 10.1 Hz, J_2 = 6.1 Hz, 1 H), 7.31 (d, J = 4.5 Hz, 4 H), 7.44 (dd, J_1 = 8.41 Hz, J_2 = 1.37 Hz, 1 H), 7.54 (dd, J = 12.7 Hz, J_2 =10.3 Hz, 1 H), 7.58 (d, J = 16.8 Hz, 1 H). ^{13}C NMR (75 MHz, d_6-acetone): δ 166.4, 152.4 (d, J_{C-F} = 245 Hz), 149.8 (J_{C-F} = 10 Hz), 143.4 (J_{C-F} = 2 Hz), 138.5, 129.2, 128.6, 127.9 (J_{C-F} = 6 Hz), 126.6, 126.0 (J_{C-F} = 3 Hz), 117.2, 114.8 (J_{C-F} = 18 Hz), 113.8, 64.9, 55.9, 35.1; MS (CI) *m/z* 301 (MH^+, 65); HRMS (CI) calcd for $C_{18}H_{17}FO_3$ 301.1240, found: 301.1239.

(*E*)-3-(3,4-difluorophenyl)-*N*-phenethylacrylamide (Mis-112A). Following the general procedure above, but substituting (2-oxo-2-(phenethylamino)ethyl)triphenylphosphonium chloride[S4] for (carboxymethyl)triphenylphosphonium chloride β-phenylethyl ester, afforded after flash chromatography (4.5:0.5 hexane/EtOAc) and recrystallization from CH_2Cl_2/hexane **Mis-112A** as a white crystalline solid (399 mg, 79 % yield): mp 143.5-145.0 °C; IR 3303, 1656, 1622, 1550, 1518, 1297, 1275, 1197, 966 cm^{-1}; ^1H NMR (300 MHz, d_6-acetone): δ 2.85 (t, J = 7.4 Hz, 2 H), 3.86 (dt, 2 H), 6.65 (d, J = 15.6 Hz, 1 H), 7.17-7.43 (m, 7 H), 7.47 (d, J = 15.6 Hz, 1 H), 7.52-7.57 (td, 1H). ^{13}C NMR (75MHz, d_6-acetone, missing two $\mathbf{C}_{ipso}$-F due to coupling): δ 164.8, 139.8, 137.2, 133.6 (m), 128.9, 128.6, 126.4, 124.9 (m), 123.7, 117.9 (J_{C-F} = 18 Hz), 116.11 (J_{C-F} = 17 Hz), 41.0, 35.8; MS (CI) *m/z* 288 (MH^+, 15), HRMS (CI) calcd for $C_{19}H_{19}FO_4$; $(MH)^+$ 288.1200, found 288.1200.

(*E*)-Phenethyl 3-(3,4-difluorophenyl)acrylate (Mis-113A).[S5] Following the general procedure above, flash chromatography (4.5:0.5 hexane/EtOAc) and recrystallization from EtOAc/hexane afforded **Mis-113A** as a colorless crystalline solid (300 mg, 75% yield): mp 57.8-59.2 °C (lit.[S5] 53-57 °C); IR 3086, 2947, 1711, 1642, 1518, 1274, 1213, 1184, 1113, 983, 701 cm^{-1}; ^1H NMR (400 MHz, d_6-acetone): δ 2.99 (t, J = 7.0 Hz, 2 H), 4.40 (t, J = 7.0 Hz, 2 H), 6.31 (d, J = 15.8 Hz, 1 H), 7.12-7.24 (m, 7 H), 7.28-7.34 (m, 3 H), 7.54 (d, J = 15.8 Hz, 1 H); ^{13}C NMR (75 MHz, d_6-acetone, missing two $\mathbf{C}_{ipso}$-F due to coupling): δ 166.0, 142.4, 138.4, 132.5 (m), 129.2, 128.6, 126.6, 125.9 (m), 119.8, 118.0 (d, J_{C-F} = 18 Hz), 116.7 (d, J_{C-F} = 18 Hz), 65.1, 35.1; MS (CI) *m/z* 289 (MH^+, 20), HRMS (CI) calcd for $C_{17}H_{14}F_2O_2$ $(MH)^+$ 289.0995, found 289.1040.

African Potato Extract (APE): Following the procedure of Drewes and co-workers[S6] dried, ground *H. hemerocallidea* corms (20 g) were extracted with 50 mL of EtOH at room temperature for 48 h. Filtration and evaporation of the solvent afforded 338 mg of APE as a brown solid.

Rooperol: Following the procedure of Drewes and co-workers,[S6] APE (300 mg) was dissolved in 190 mL of 10 mM sodium acetate buffer, pH 4.5, and treated with 1 g of cellulase at 37 °C overnight. The resulting mixture was carefully extracted with EtOAc (5 x 50 mL) and the combined extracts were dried over Na_2SO_4 and filtered. The residue upon evaporation of the solvent was subjected to repeated flash chromatography (5-50% EtOAc/Hexance) to afford 14 mg of rooperol as a pale yellow solid: mp = 148 °C (lit.[S6] 148 °C); ^1H NMR ($CDCl_3$): d 6.84 (d, 1H, J = 1.6 Hz, catechol 3-**H**), 6.81 (d, 1H, J = 1.9 Hz, catechol' 3**H**), 6.75 (dd, 1H, J = 8.1, 1.9 Hz, catechol'-5**H**), 6.70-6.60 (m, 3H, catechol 5-,6-**H**, catechol' 6-**H**), 6.50 (dt, 1H, J = 15.4, 1.5 Hz, CH=C**H**-Ar), 6.00 (dt, 1H, J = 15.6, 5.6 Hz, C**H**=CHAr), 3.23 (dd, 2H, J = 5.7, 1.8 Hz, C**H$_2$**CH=); ^{13}C NMR (75 MHz, CD_3OD): d 145.4, 144.9, 144.6 (2X), 130.7, 129.5,

123.3, 121.2, 118.1, 117.9, 114.9, 114.8, 114.7, 112.4, 83.6, 82.4, 21.9; MS *m/z*: 283 (MH^+, 100); HRMS (CI) calcd for $C_{17}H_{15}O_4$ (MH^+) 283.0970, found 283.0961.

Nyasol:[S7] Also isolated from the flash chromatographic purification of rooperol as a yellow oil (2 mg): ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.17 (d, 2H, J = 8.4 Hz, Ar**H**), 7.11 (d, 2H, J = 8.7 Hz, Ar**H**), 6.80-8.76 (m, 4H, Ar**H**), 6.50 (d, 1H, J = 11.5 Hz, ArC**H**=CH), 6.01 (ddd, 1H, J = 16.7, 10.6, 6.0 Hz, C**H**=CH_2), 5.67 (dd, 1H, J = 11.5, 10.0, C**H**=CHAr), 5.17-5.14 (m, 2H, CH=C**H$_2$**), 4.80 (brs, 1H, ArO**H**), 4.69 (brs, 1H, ArO**H**), 4.49 (1H, dd, J = 10.0, 6.0 Hz, ArC**H**CH=CH_2) (matches lit.[S8]); MS (CI) m/z 252 (M^+, 100); HRMS (CI) calcd for $C_{17}H_{16}O_2$ $[M^+]_+$: 253.1150, Found: 253.1151.

MALDI-MS on p38α•2 adduct

In order to identify the site of adduction, the sample of unactivated p38α treated with compound **2** was digested with chymotrypsin and further analyzed by MALDI-MS/MS. The MASCOT generated chymotrypsin digest coverage based on MS values showed 88 % coverage of the protein in the untreated sample (p38α alone), with peptides 36-59, 130-132, 208-216, 271-274 unobserved. For the treated digest (modified p38α by compound **2**), the coverage was 83 %, with peptides 36-59, 105-132, 208-216 unobserved. The major difference in coverage was the absence of peptide 105-129 in the treated sample. Comparative MALDI analysis and de novo sequencing identified the modification site. In the untreated sample, the peptide 104-129 is seen at 2952.476, with sequence confirmed by MS/MS. This peptide is absent from the treated sample. However, a new peptide is observed at 3215.553 (Figure S13). De novo sequencing identified the peptide as residues 104-129 with modification of Cys119 by a mass addition of 263 Da (Figure S2). The modification at Cys119 was observed in five additional peptide sequences for peptides only in the treated sample. They were observed with same modification of 263 Da, and at lower signal intensity with modification of 261 Da: residues 115-119 at 965.435/967.450, 110-119 at 1435.6/1437.660, 115-129 at 2048.960/2050.976, 111-129 at 2464.155, and 110-129 at 2519.171/2521.178. However, none of these peptides were observed in the untreated sample. The MS of the treated protein chymotrypsin digest does not contain peptide 104-129 in an unlabeled form, only the labeled peptide, implying that this site is modified stoichiometrically. Thus, it is unlikely that any other site on the protein is modified.

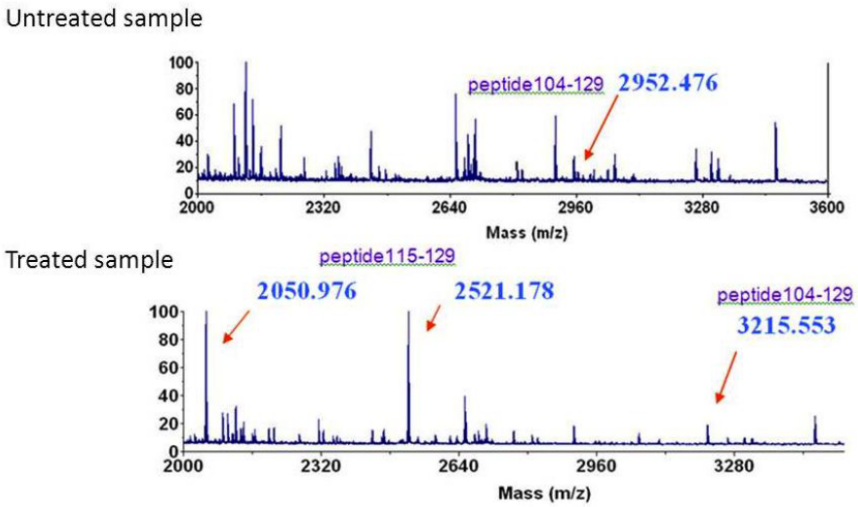
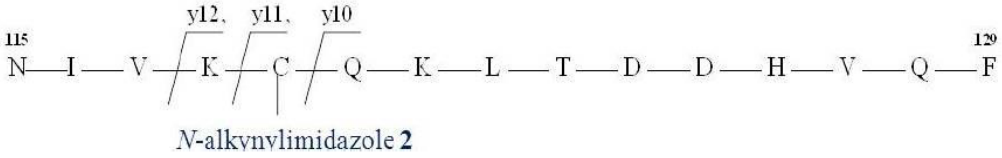


Figure S1. MALDI-MS spectra of p38α treated with *N*-alkynylimidazole **2** and untreated p38α after digestion with chymotrypsin.



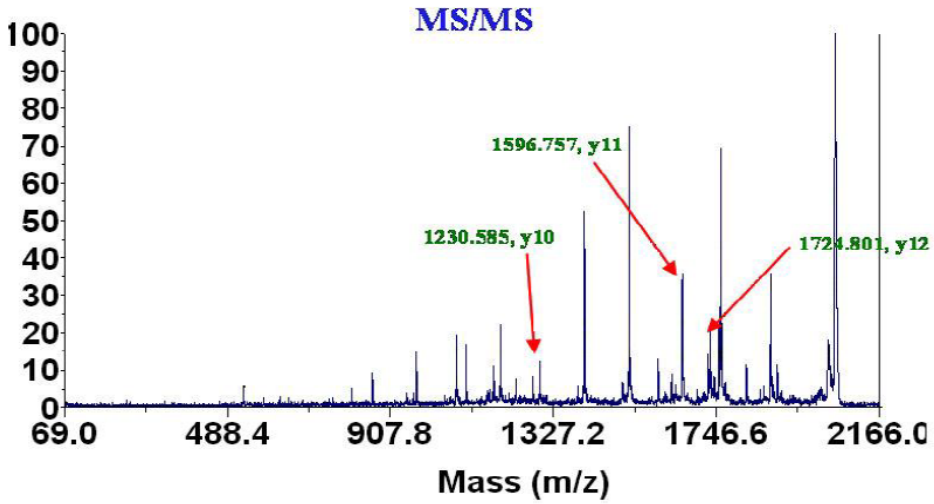


Figure S2. MALDI-MS/MS spectrum of *N*-alkynylimidazole **2** adducted p38α after digestion with chymotrypsin.

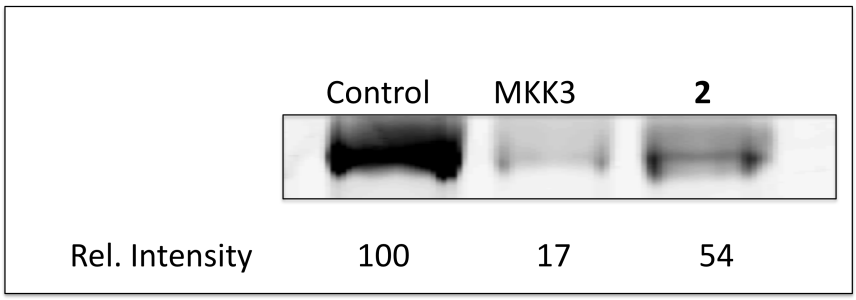


Figure S3. Competition between Compounds **3** and **2** for adduction of p38α. p38α (5 μM) was incubated in the presence of **3** (100 μM) alone (**Control**) or in the presence of an equimolar concentration of MKK3 peptide or compound **2** for 16 h followed by click reaction and in-gel fluorescence SDS-PAGE analysis.

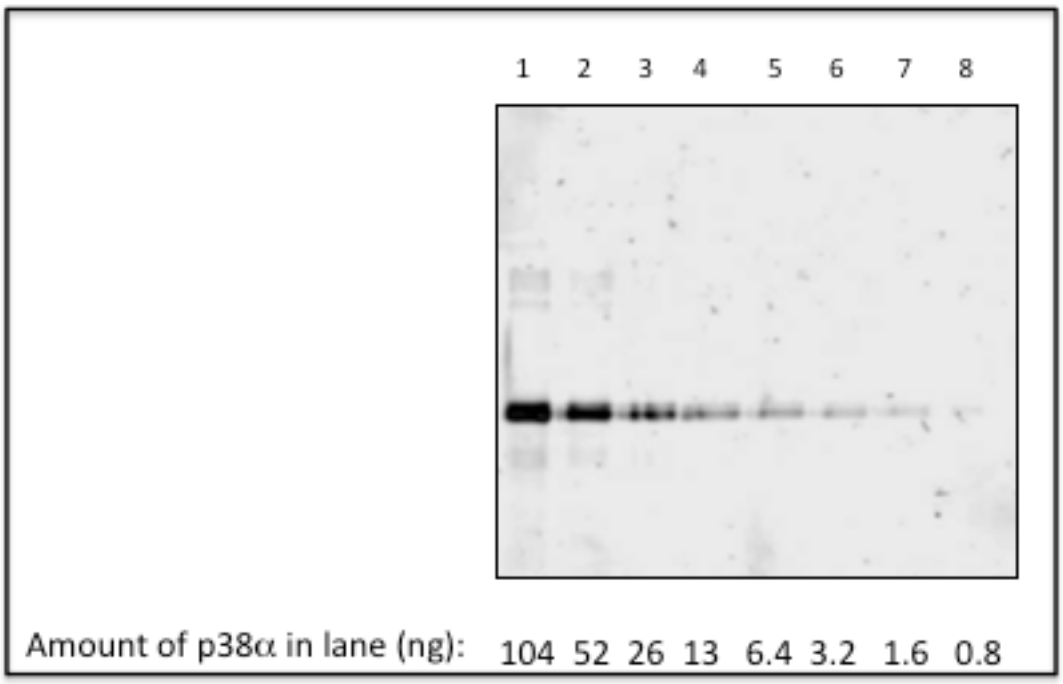


Figure S4. Limit of detection of p38α after incubation with **3** and click reaction with Alexa594-azide.

One issue that arose when studying the kinetics of the adduction of p38α by **3** was the possibility of adduction of p38α by **3** during the click reaction. In order to address this, we have carried out parallel experiments in which samples from adduction reactions were either directly treated under click reaction conditions, or first subjected to spin-column purification to remove unadducts **3** and then treated under click reaction conditions. As shown in **Figure S5** (below), there was no significant difference in the adducts formed under the two different conditions. Presumably, the click reaction of unadducted **3** is fast relative to adduct formation, and once unadducted **3** undergoes click reaction, it is no longer able to form adducts with p38α.

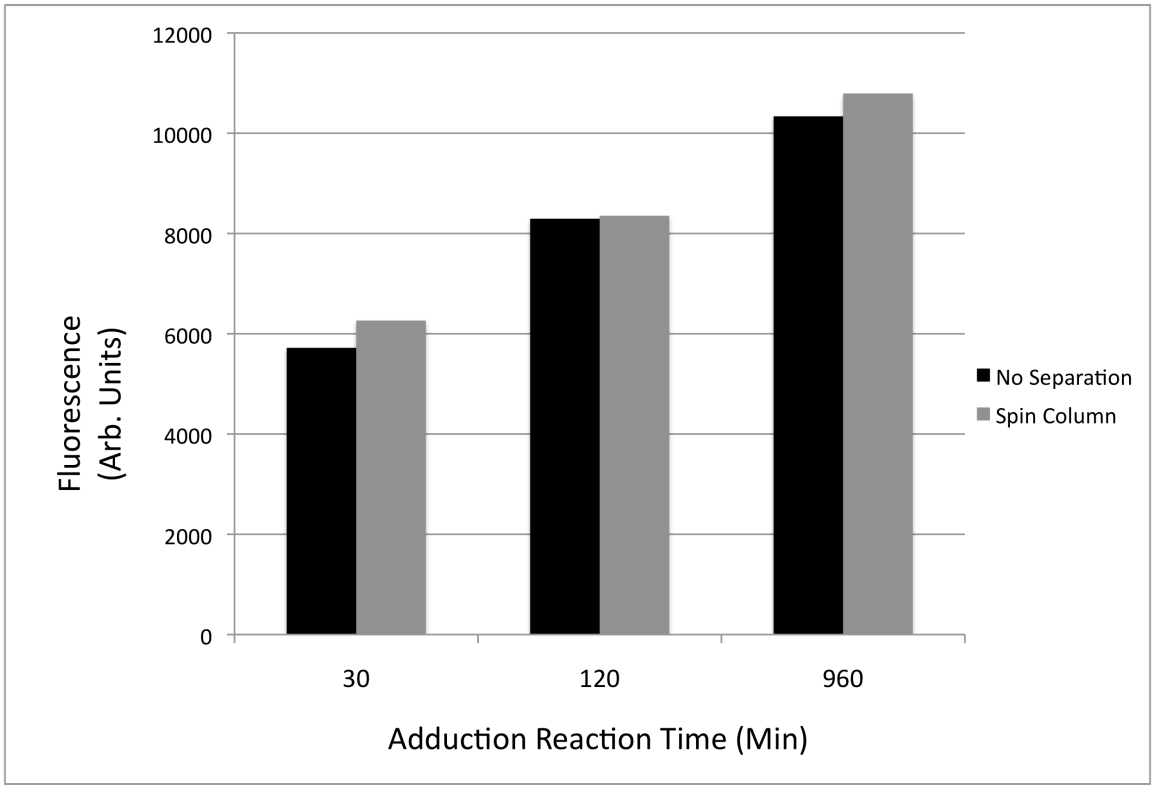


Figure S5. Comparison of p38α adduction by compound **3** with and without removal of non-adducted **3** prior to click chemistry. Black bars: Fluorescence intensity of bands from in-gel fluorescence SDS-PAGE analysis of click reactions run directly on adduction incubations containing 5 μM p38α and 100 μM **3** at 30, 120, and 960 min. Gray bars: Adduction reactions containing 5 μM p38α and 100 μM **3** at 30, 120, and 960 min were first subjected to spin column removal of unadducted **3** and then subjected to click reaction.

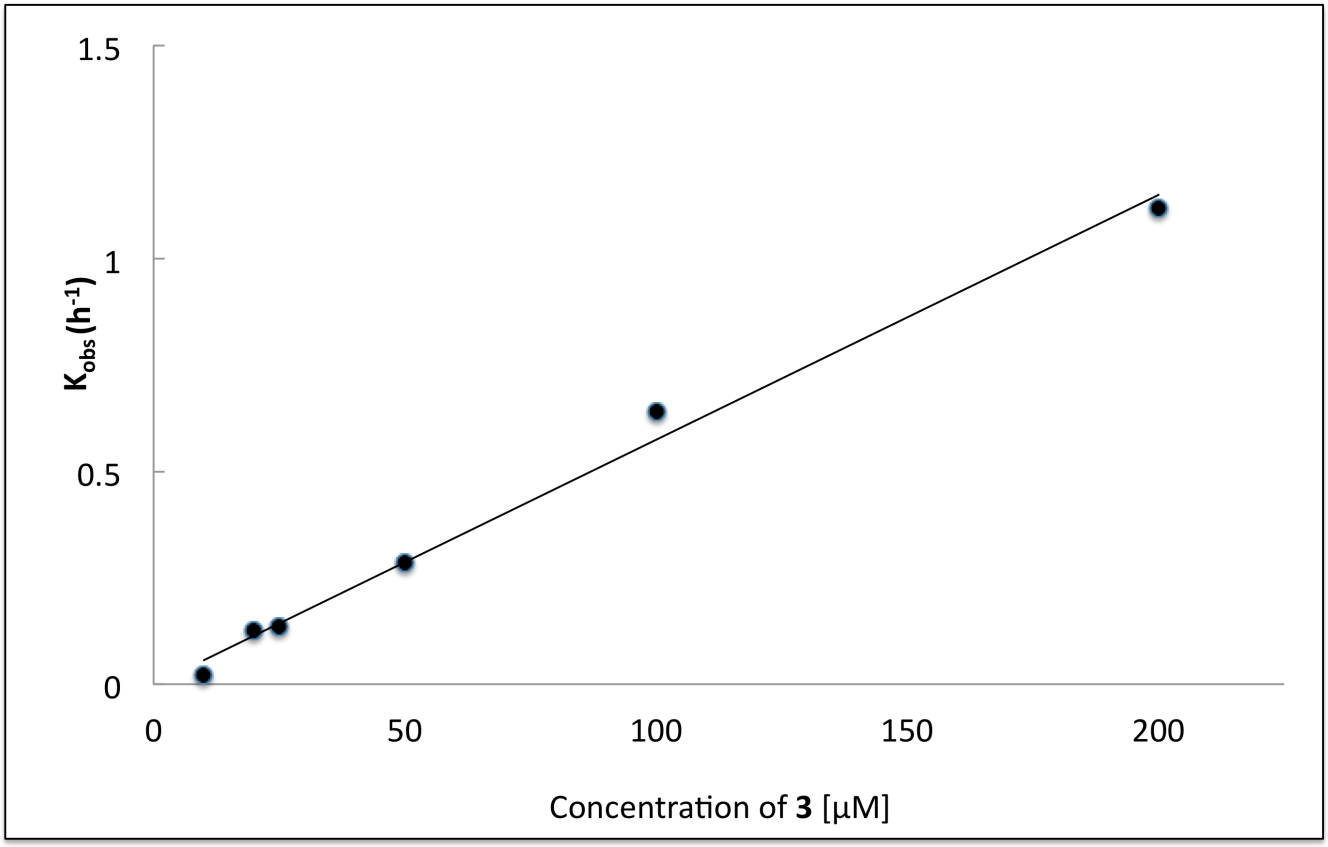


Figure S6. Concentration dependence of the observed pseudo-first order rate of p38α adduct formation by **3**.

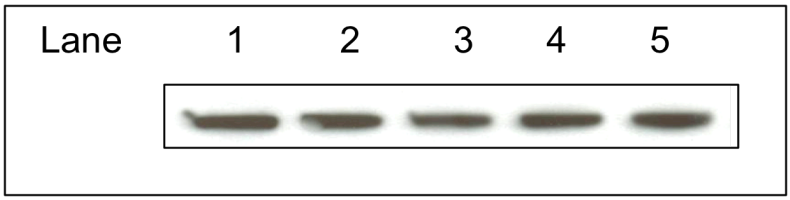


Figure S7. Anti-FLAG Western blot of samples from Figure 6 in the paper. HEK 293T cells over-expressing Flag-tagged p38α were treated with **3** and then subjected to lysis, immunoprecipitation, and click reaction with Alexa594-azide. Lane 1. Cells treated with vehicle (0.05 % DMSO); 2. Cells treated with 1 μM 3. Lane 3. Cells treated with 5 μM **3**. Lane 4. Cells treated with 50 μM 3. Lane 5. Isolated flag-tagged p38α (~0.6 μg) treated with 50 μM 3 *in vitro*.

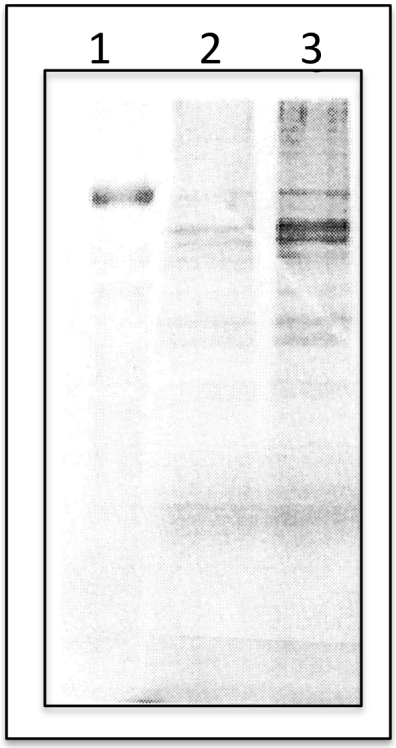
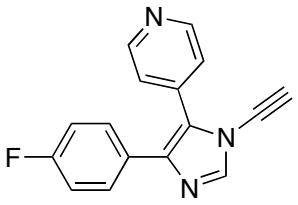


Figure S8. Selectivity of adduction by compound **3**. Cell lysate from transfected HEK293 cells (200 μg protein) was incubated with 100 μM **3** for 1-3 hours and then subjected to click reaction with Alexa594-azide. Lane 1: Protien marker of authentic p38α•3 adduct after click reaction. Lane 2: cell lysate after 1 hour incubation with 100 μM compound **3**. Lane 3: cell lysate after 3 hour incubation with 100 μM compound **3**.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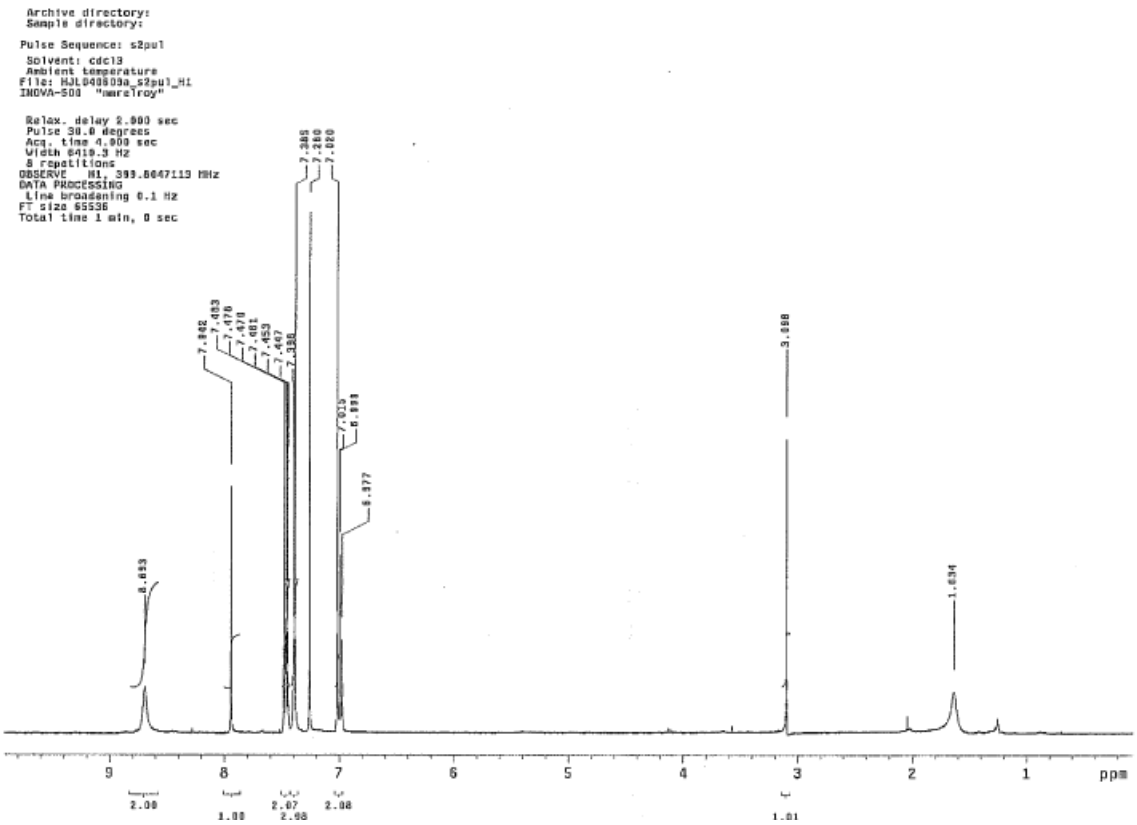
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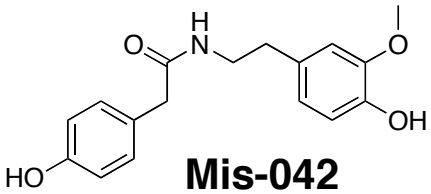
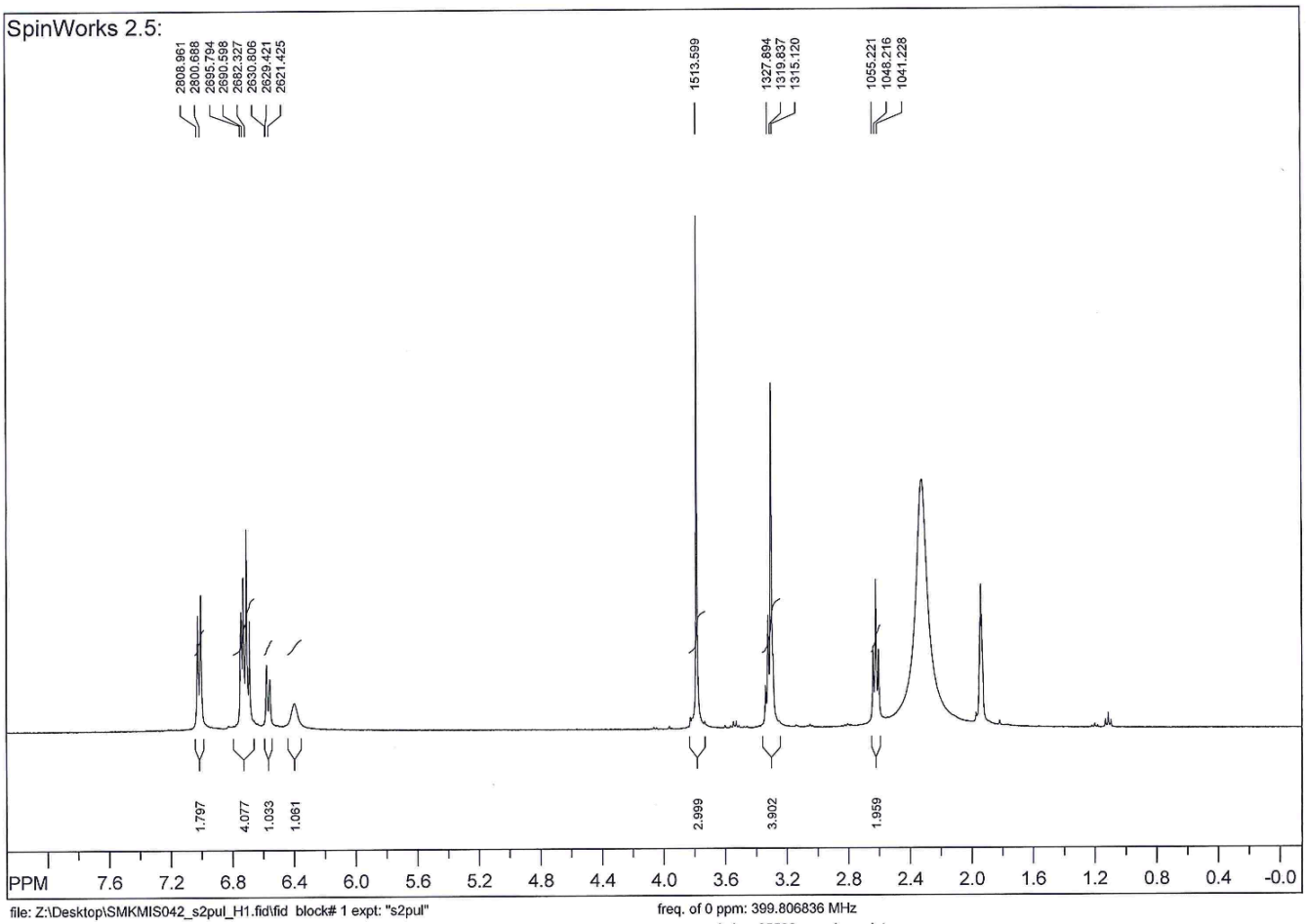


Mis-042



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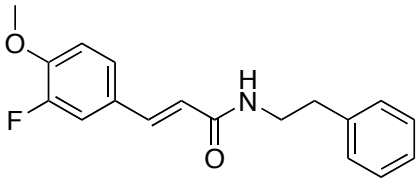
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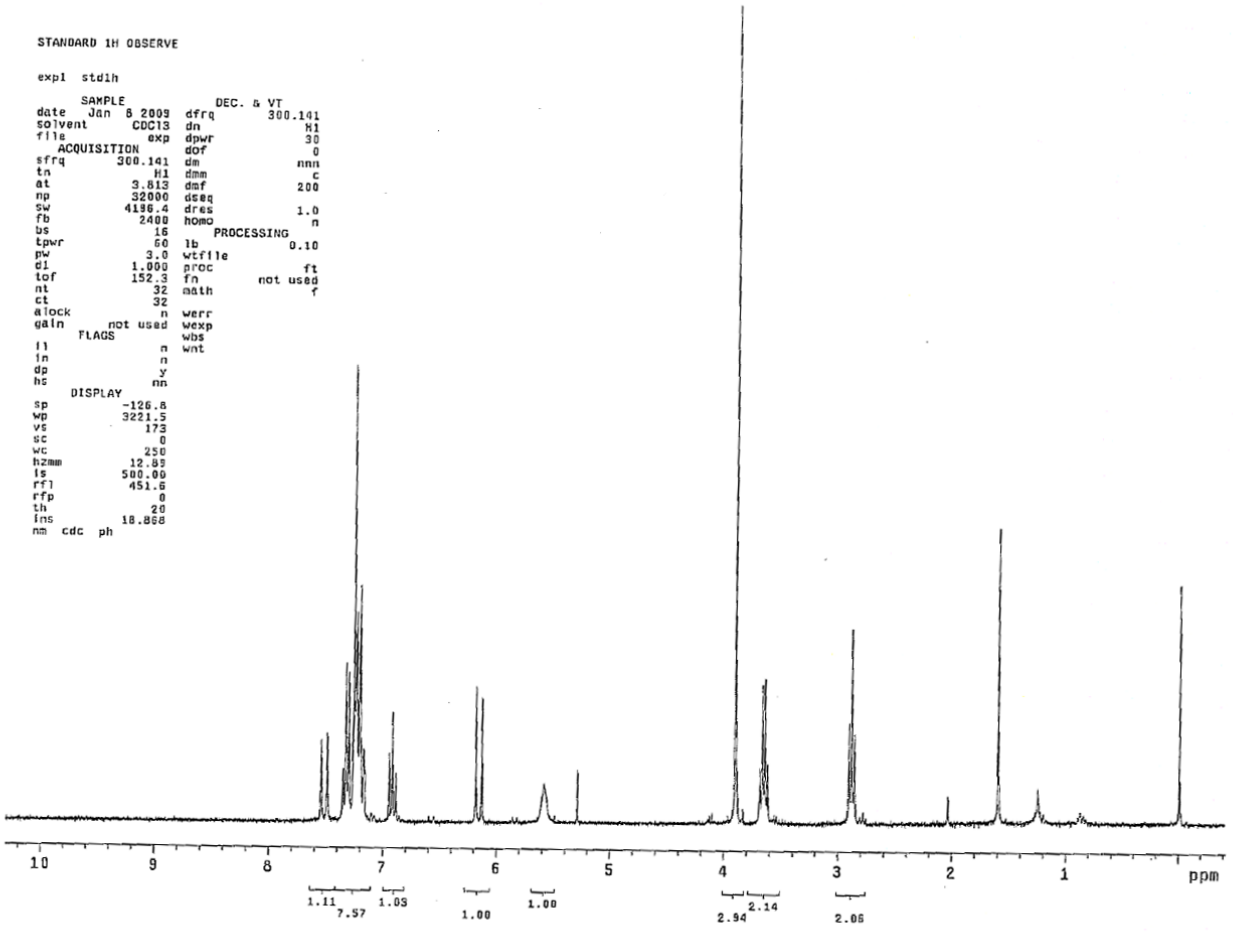
Mis-103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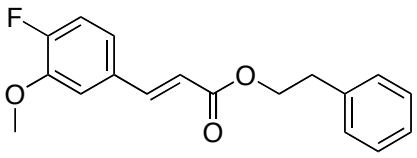
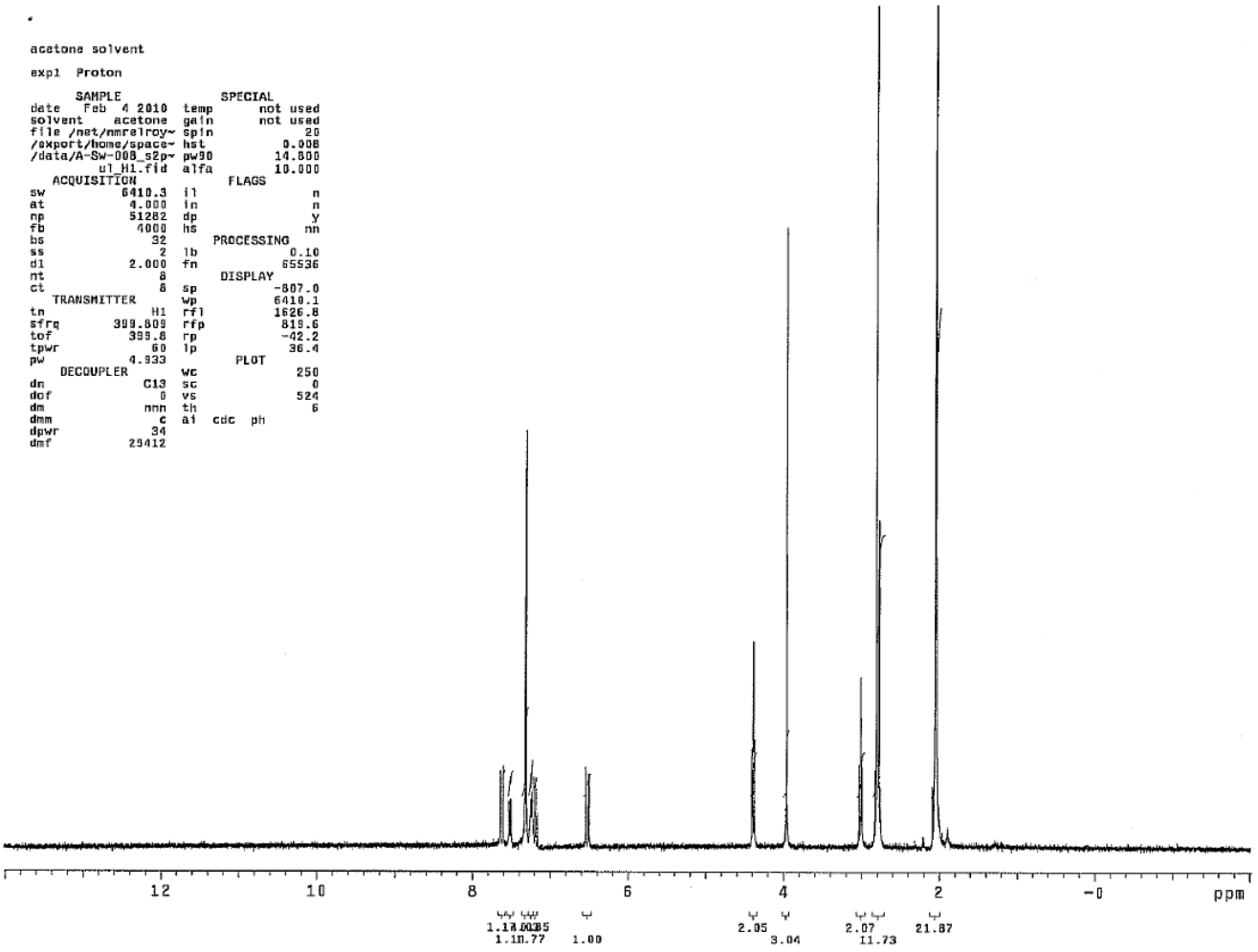
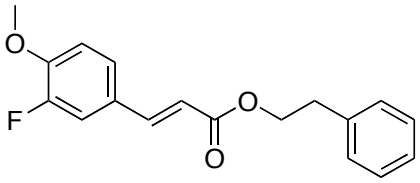
np 32000
sw 4186.4
fb 2400
bs 16
tpwr 60
pw 3.0
d1 1.000
tof 152.3
nt 32
ct 32
alock n
gain not used
FLAGS
il n
in n
dp y
hs nn
DISPLAY
sp -126.8
wp 3221.5
vs 173
sc 0
wc 250
hzmm 12.89
is 500.00
rfl 451.6
rfp 0
th 20
ins 18.868
nm cdc ph
DEC. & VT
dfrq 300.141
dn H1
dpwr 30
dof 0
dm nnn
dmm c
dmf 200
dseq
dres 1.0
homo n
PROCESSING
lb 0.10
wtfile
proc ft
fn not used
math f
werr
wexp
wbs
wnt
10
9
8
7
6
5
4
3
2
1
ppm
1.11
7.57
1.08
1.00
1.00
2.94
2.14
2.06

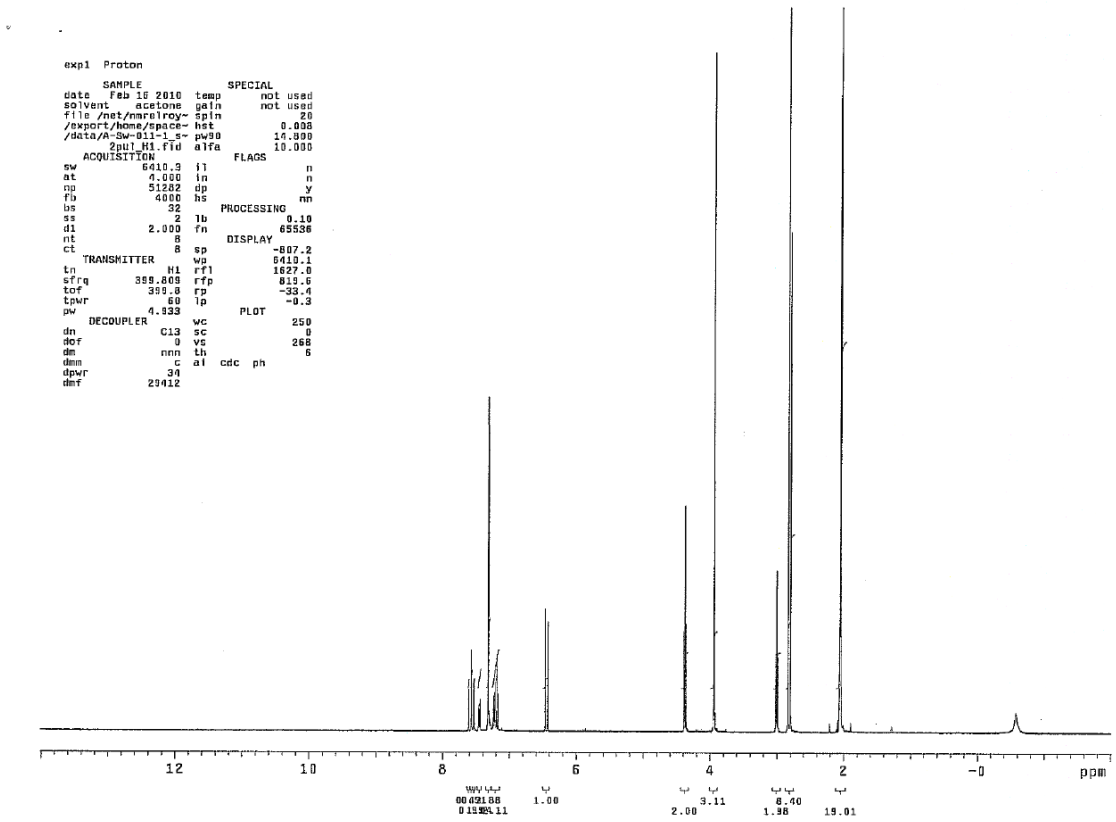

F
O
O
O

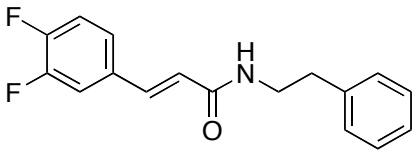
Mis-108


acetone solvent
exp1 Proton
SAMPLE
date Feb 4 2010
solvent acetone
file /net/nmrelroy~
/export/home/space~
/data/A-Sw-008_s2p~
u1_H1.fid
ACQUISITION
sw 6410.3
at 4.000
np 51282
fb 4000
bs 32
ss 2
d1 2.000
nt 8
ct 8
TRANSMITTER
tn H1
sfrq 399.805
tof 399.8
tpwr 60
pw 4.933
DECOUPLER
dn C13
dof 0
dm nnn
dmm c
dpwr 34
dmf 29412
SPECIAL
temp not used
gain not used
spin 20
hst 0.008
pw90 14.800
alfa 10.000
FLAGS
il n
in n
dp y
hs nn
PROCESSING
lb 0.10
fn 65536
DISPLAY
sp -807.0
wp 6410.1
rfl 1626.8
rfp 819.6
rp -42.2
lp 36.4
PLOT
wc 250
sc 0
vs 524
th 6
al cdc ph
12
10
8
6
4
2
-0
ppm
1.17
1.10
1.77
1.00
2.05
3.04
2.07
11.73
21.87

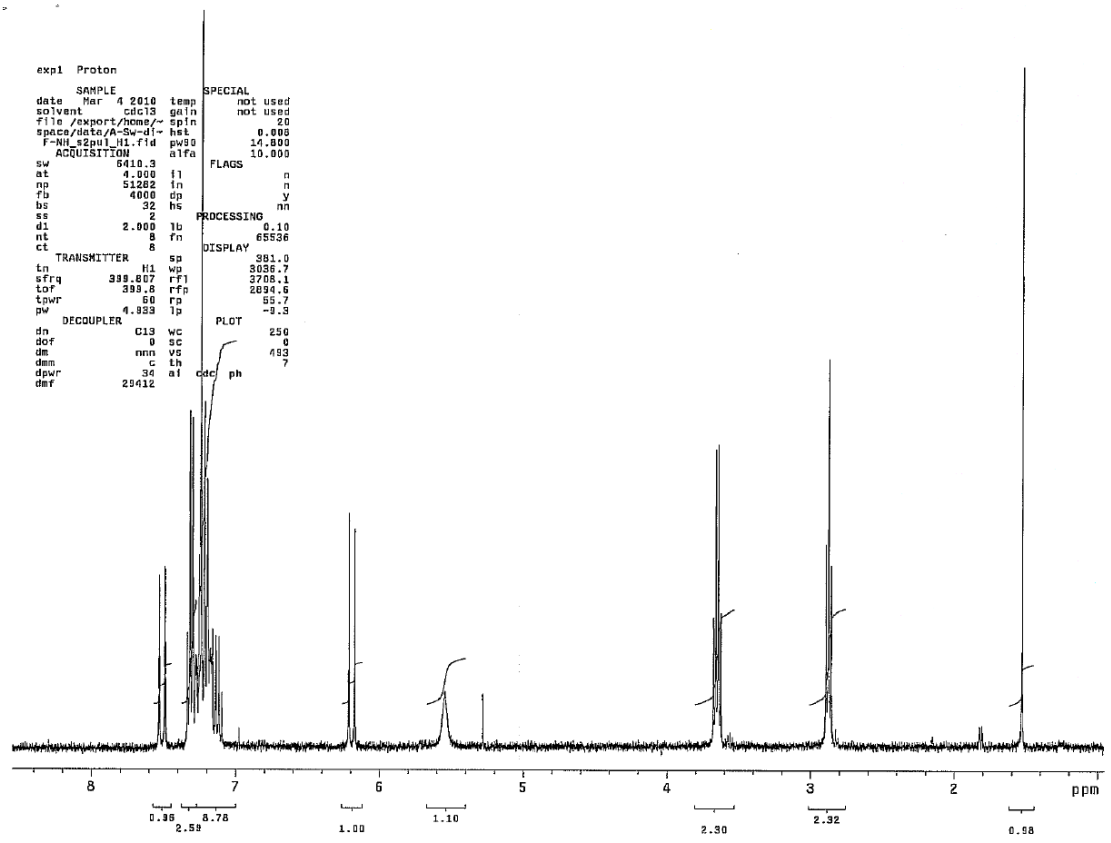

O
F
O
O

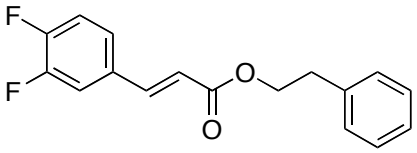
Mis-109


expl Proton
SAMPLE
date Feb 16 2010
solvent acetone
file /net/marelroy~
/export/home/space~
/data/A-Sw-011-1_s~
2pul_H1.fid
ACQUISITION
sw 6410.9
at 4.000
np 51282
fb 4000
bs 32
ss 2
d1 2.000
nt 8
ct 8
TRANSMITTER
tn H1
sfrq 399.809
tof 399.8
tpwr 60
pw 4.933
DECOUPLER
dn C13
dof 0
dm nnn
dmm c
dpwr 34
dmf 29412
SPECIAL
temp not used
gain not used
spin 20
hst 0.006
pw90 14.800
alfa 10.000
FLAGS
il n
in n
dp y
hs nn
PROCESSING
lb 0.10
fn 65536
DISPLAY
sp -807.2
wp 5410.1
rf1 1627.0
rfp 819.6
rp -33.4
lp -0.3
PLOT
wc 250
sc 0
vs 268
th 6
al cdc ph
12
10
8
6
4
2
-0
ppm
1.00
3.11
8.40
2.00
1.98
19.01

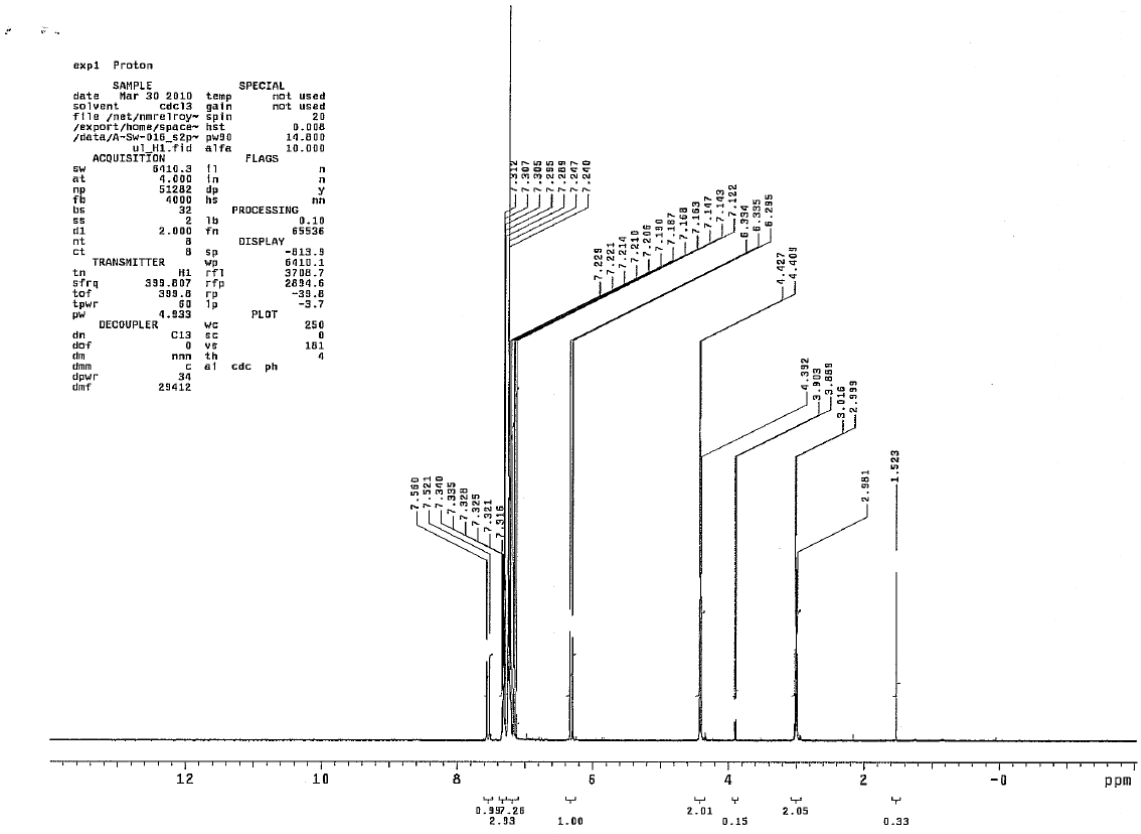

F
F
H
N
O

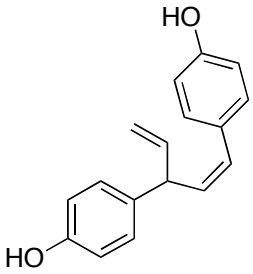
Mis-112A


exp1 Proton
SAMPLE
date Mar 4 2010
solvent cdcl3
file /export/home/v
space/data/A-Sw-dl
F-NH_s2pul_H1.fid
ACQUISITION
sw 5410.3
at 4.000
np 51282
fb 4000
bs 32
ss 2
di 2.000
nt 8
ct 8
TRANSMITTER
tn H1
sfrq 399.807
tof 399.8
tpwr 60
pw 4.933
DECOUPLER
dn C13
def 0
dm nnn
dmm c
dpwr 34
dmf 29412
temp not used
gain not used
spin 20
hst 0.000
pw90 14.800
alfa 10.000
FLAGS
fl n
fn n
dp y
hs nn
PROCESSING
lb 0.10
fn 65536
DISPLAY
sp 881.0
wp 3036.7
rfl 3708.1
rfp 2894.6
rp 55.7
lp -9.3
PLOT
wc 250
sc 0
vs 493
th 7
al cdc ph
8
7
6
5
4
3
2
ppm
0.98
8.78
2.59
1.00
1.10
2.30
2.32
0.98

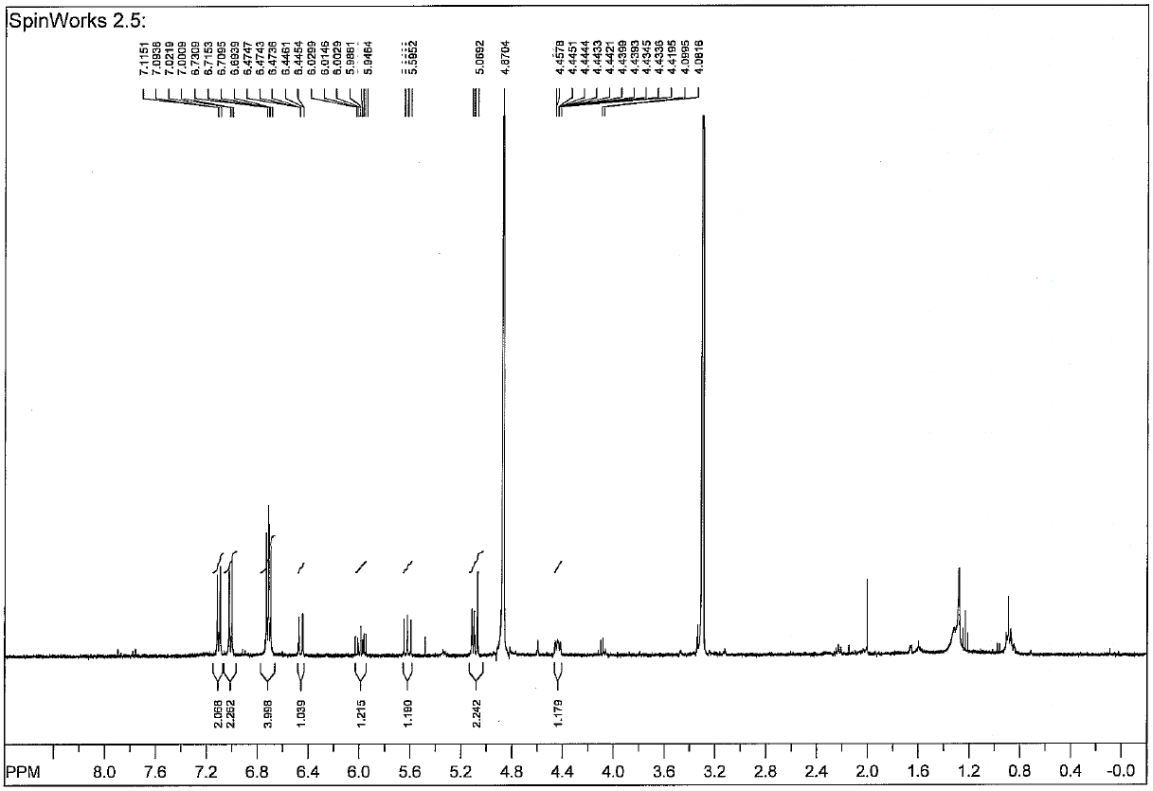

F
F
O
O

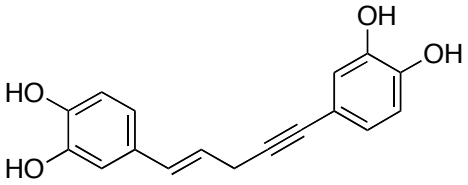
Mis-113A


exp1 Proton
SAMPLE
date Mar 30 2010
solvent cdcl3
file /net/nmrelroy~
/export/home/space~
/data/A-SW-916_s2p~
u1_H1.fid
ACQUISITION
sw 6410.3
at 4.000
np 51282
fb 4000
bs 32
ss 2
d1 2.000
nt 8
ct 8
TRANSMITTER
tn H1
sfrq 399.807
tof 399.8
tpwr 50
pw 4.933
DECOUPLER
dn C13
dof 0
dm nnn
dmm c
dpwr 34
dmf 29412
SPECIAL
temp not used
gain not used
spin 20
hst 9.008
pw90 14.000
alfa 10.000
FLAGS
fl n
in n
dp y
hs nn
PROCESSING
lb 0.10
fn 65536
DISPLAY
sp -813.9
wp 6410.1
rfl 3708.7
rfp 2694.6
rp -39.8
lp -3.7
PLOT
wc 250
sc 0
vs 181
th 4
al cdc ph
7.312
7.307
7.305
7.285
7.269
7.267
7.240
7.226
7.221
7.214
7.210
7.206
7.190
7.187
7.168
7.163
7.147
7.143
7.122
6.334
6.295
4.407
4.409
4.332
3.903
3.889
3.015
2.999
2.681
1.523
7.560
7.521
7.340
7.335
7.328
7.325
7.321
7.316
12
10
8
6
4
2
-0
ppm
0.997.26
2.93
1.00
2.01
0.15
2.05
0.33

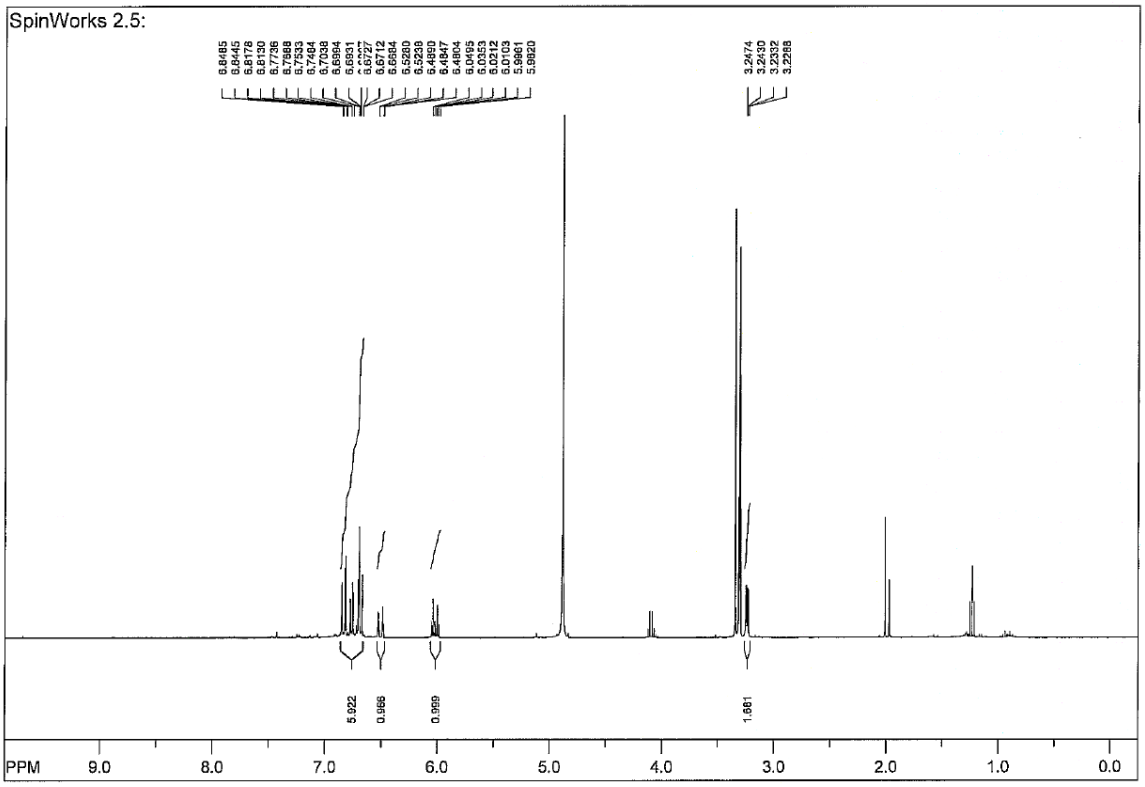

HO
HO

nyasol


SpinWorks 2.5:
7.1151
7.0938
7.0219
7.0009
6.7309
6.7153
6.7095
6.6939
6.4747
6.4743
6.4728
6.4461
6.4454
6.0299
6.0145
6.0029
5.9861
5.9464
5.5652
5.0682
4.6704
4.4573
4.4451
4.4444
4.4433
4.4427
4.4389
4.4383
4.4345
4.4338
4.4195
4.0995
4.0818
2.058
2.222
3.958
1.039
1.215
1.180
2.242
1.179
PPM
8.0
7.6
7.2
6.8
6.4
6.0
5.6
5.2
4.8
4.4
4.0
3.6
3.2
2.8
2.4
2.0
1.6
1.2
0.8
0.4
-0.0


OH
OH
HO
HO

rooperol


SpinWorks 2.5:
8.8485
8.8445
8.8178
8.8130
8.7736
8.7888
8.7353
8.7044
8.7038
8.6994
8.6931
8.6727
8.6712
8.6684
8.5280
8.5238
8.4990
8.4847
8.4804
8.0495
8.0353
8.0212
8.0103
5.9861
5.9820
3.2474
3.2430
3.2332
3.2288
5.922
0.966
0.999
1.861
PPM
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0

References

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