

SUPPORTING INFORMATION

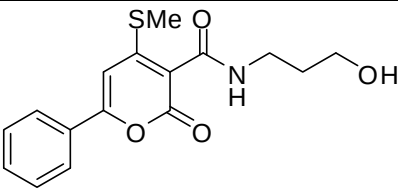
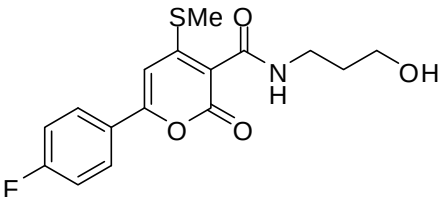
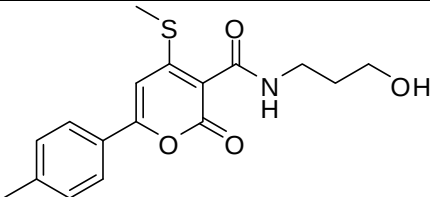
Anti-HSV activity and mode of action study of α -pyrone carboxamides

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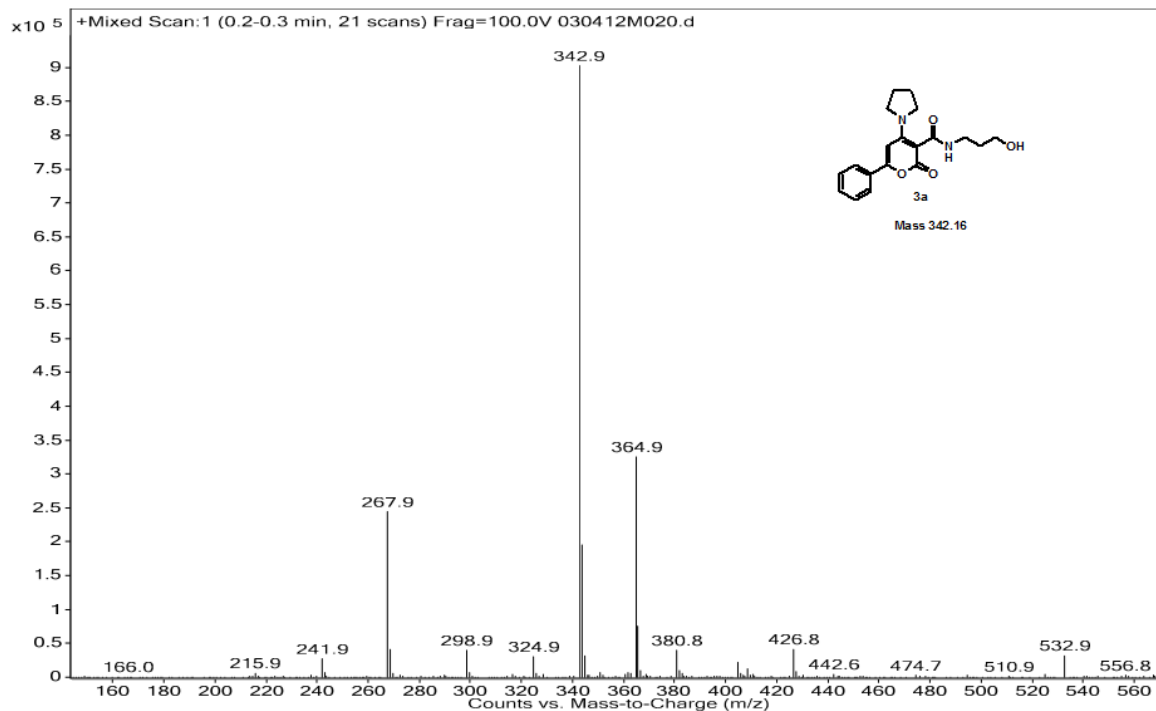
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Table 1 Spectroscopic and analytical data of synthesized compounds

S.No.	Compound	Spectral data
2a	 Chemical Formula: C₁₆H₁₇NO₄S Molecular Weight: 319.38	Yellow crystalline solid, yield: 92%; mp: 117-118 °C; MS-ESI (m/z): [M ⁺ +1]. 320.02; IR: (KBr) (v, cm ⁻¹) 3425.58 (NH), 3371.57 (OH), 1685.79 and 1606.63.(C=O); ¹ H NMR: (400 MHz, DMSO-d ₆) δ 1.59-1.62 (t, J =6.8 Hz, 2H), 2.57 (s, 3H), 3.16-3.19(t, J=6Hz, 2H), 3.44-3.47(t, J =6Hz, 2H), 4.42-4.45 (t, J=5.2Hz, 1H OH), 6.69 (s, 1H), 7.49-7.51(m, 3H), 7.89-7.90(m, 2H), 8.06-8.09(t, J=5.6Hz, 1H NH)
2b	 Chemical Formula: C₁₆H₁₆FNO₄S Molecular Weight: 337.37	Yellow crystalline solid, yield: 94%; mp: 134-135 °C; MS-ESI (m/z): [M ⁺ +1]. 337.8; IR: (KBr) (v, cm ⁻¹) 3448.14 (NH), 3362.524 (OH), 1681.53 and 1596.42.(C=O); ¹ H NMR: (400 MHz, DMSO-d ₆) δ 1.61-1.64(t, J=6.4Hz, 2H), 2.59(s, 3H-SMe), 3.26-3.29(t, J=6 Hz, 2H), 3.44-3.46(t, J=6Hz, 2H), 4.49-4.51(t, J=4.8Hz, 1H-OH), 7.12(s, 1H), 7.40-7.44(m, 2H), 8.06-8.09(m, 2H), 8.76(s, 1H-NH).
2c	 Chemical Formula: C₁₇H₁₉NO₄S Molecular Weight: 333.40	Light yellow crystalline solid, yield: 92%; mp: 150-151°C; MS-ESI (m/z): [M ⁺ +1]. 334.0; ¹ H NMR: (400 MHz, DMSO-d ₆) δ 1.61-1.64 (t, J =6.4 Hz, 2H), 2.39 (s, 3H), 2.58(s, 3H), 3.12-3.15(q, J=4.4Hz, 2H), 3.44-3.48(t, J =5.6Hz, 2H), 4.47-4.50 (t, J=5.2Hz, 1H OH), 7.09 (s, 1H), 7.37-7.39 (d, J=8.4Hz, 2H), 7.89-7.91(d, J=8Hz, 2H), 8.75-8.78(t, J=5.6Hz, 1H NH)

Sample Name	SK-III-6-24	Position	Vial 7	Instrument Name	Instrument 1	User Name	
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Data Filename	030412M020.d	ACQ Method	ILS-UNL.m	Comment		Acquired Time	4/3/2012 1:11:23 PM



SK-III-6-24 in DMSO-d6
File No: 20120405_45

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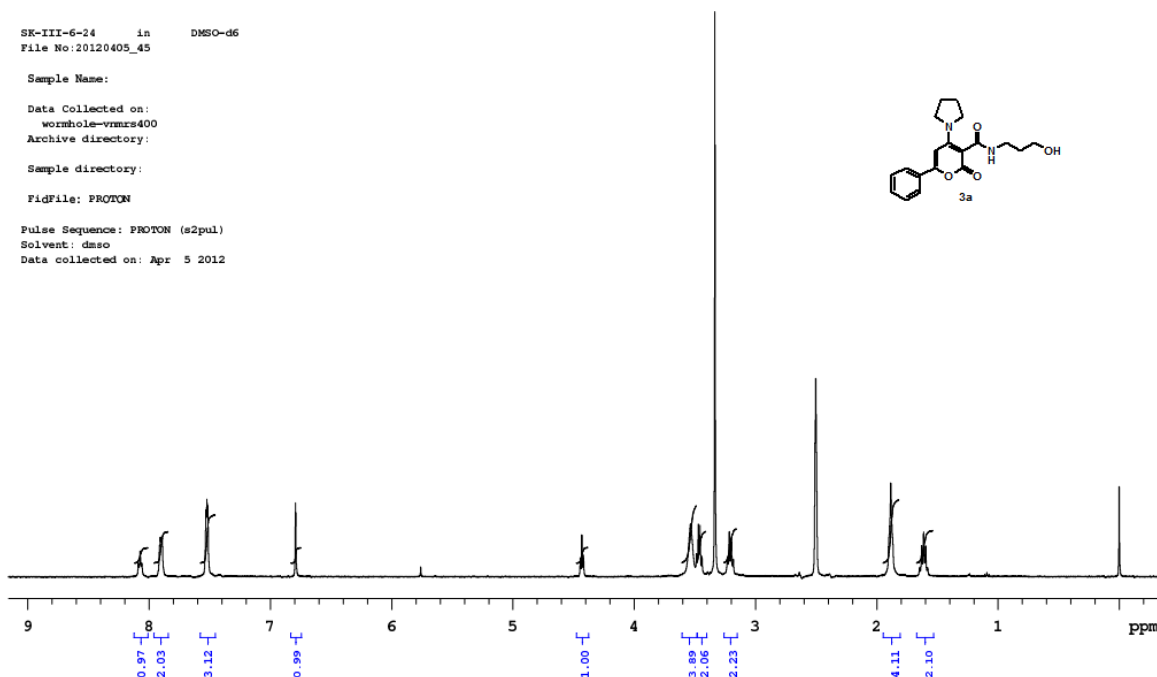
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Archive directory:

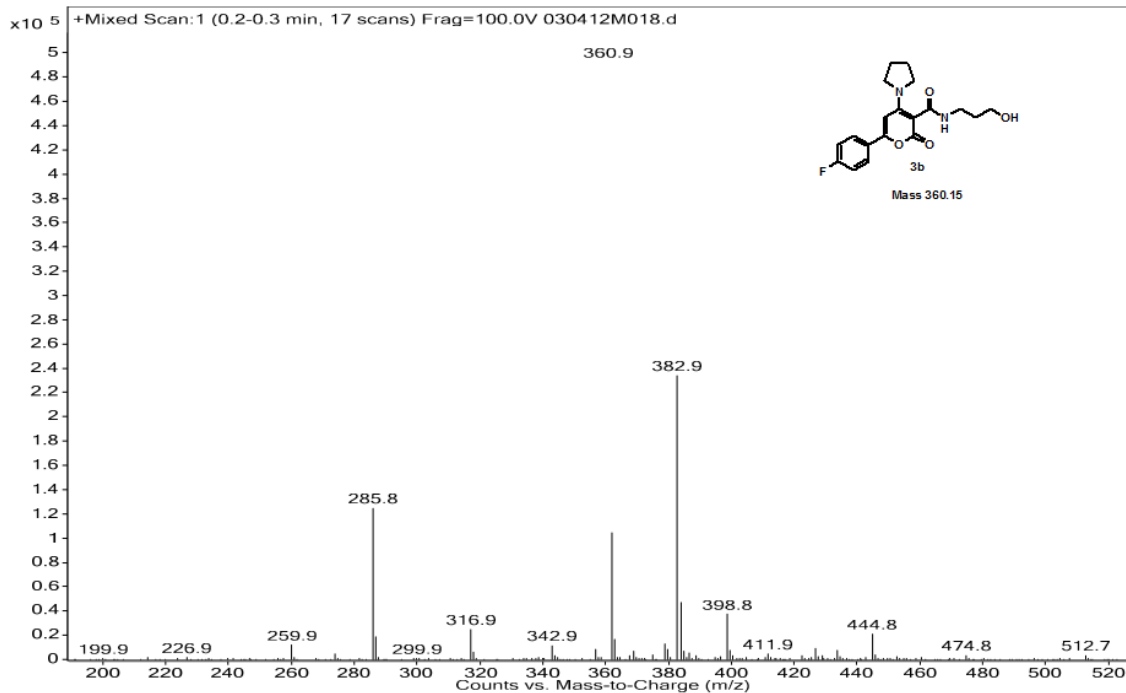
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Pulse Sequence: PROTON (s2pul)
Solvent: dms
Data collected on: Apr 5 2012



Sample Name	SK-III-10-25	Position	Vial 5	Instrument Name	Instrument 1	User Name	
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Data Filename	030412M018.d	ACQ Method	ILS-UNI.m	Comment		Acquired Time	4/3/2012 1:08:31 PM



SK-III-10-25 in DMSO-d6
File No:20120405_44

Sample Name:

Data Collected on:

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Archive directory:

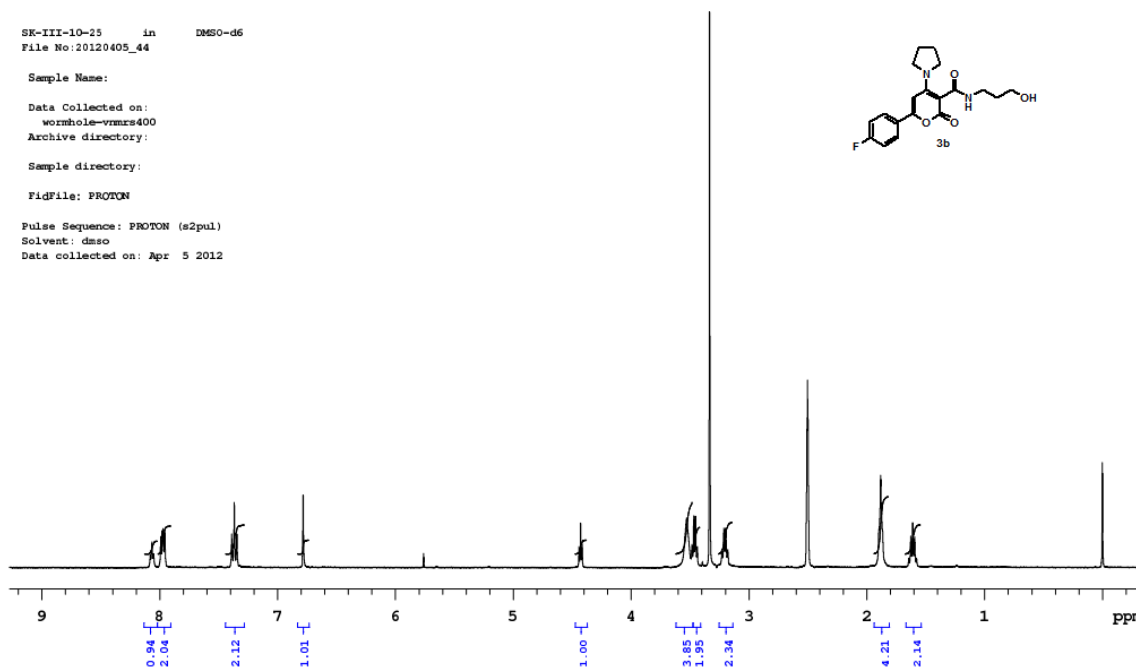
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Pulse Sequence: PROTON (s2pul)

Solvent: dmsd

Data collected on: Apr 5 2012

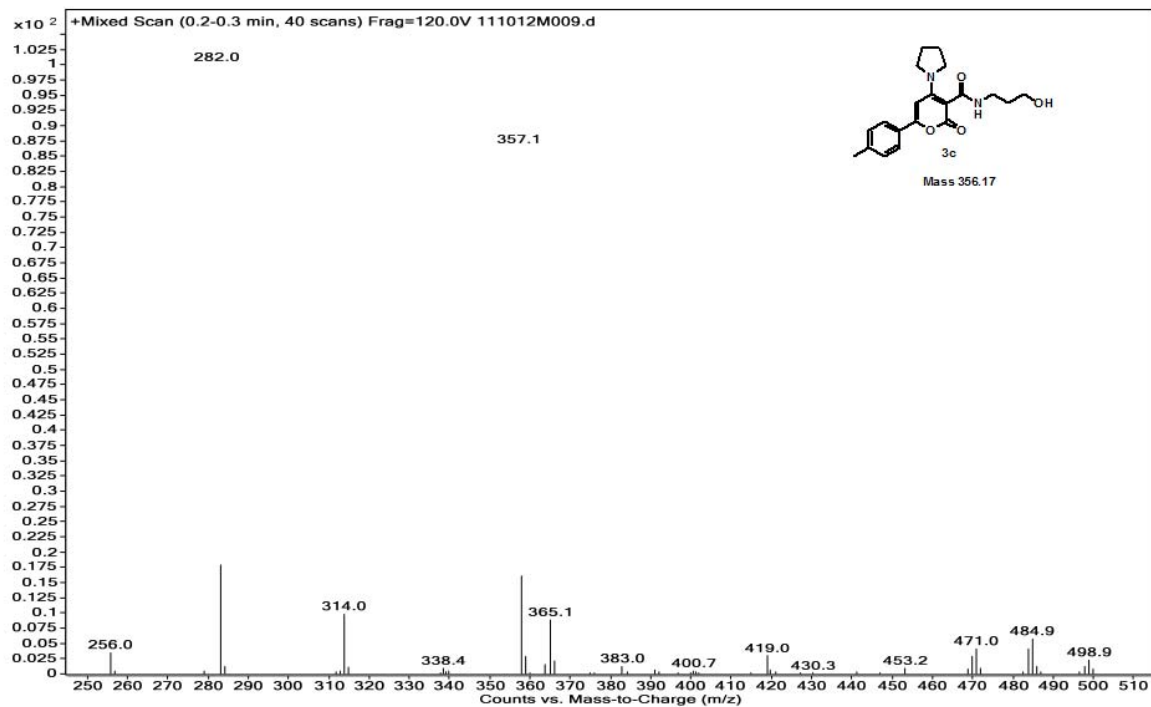


Sample Name SK-III-39-25
Inj Vol 0.5
Data Filename 111012M009.d

Position Vial 15
InjPosition
ACQ Method ILS.m

Instrument Name Instrument 1
SampleType Sample
Comment

User Name
IRM Calibration Status Not Applicable
Acquired Time 10/11/2012 11:22:57 AM



SK-III-39-25 in DMSO-d6
File No: 20120831_62

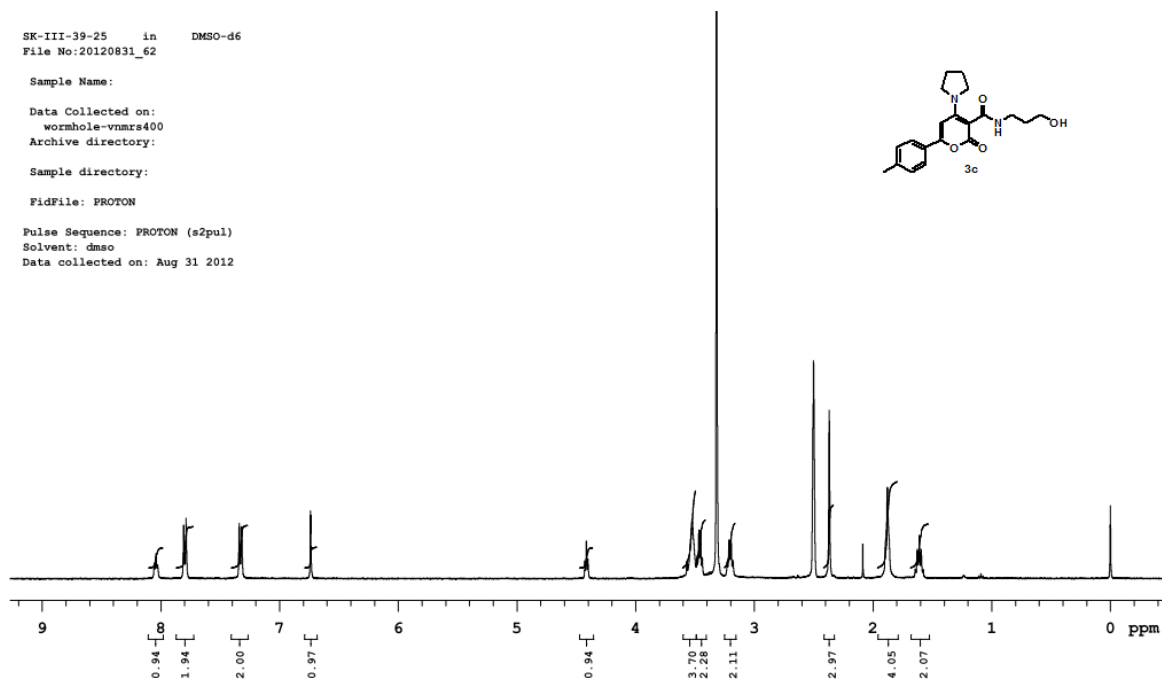
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Data Collected on:
wormhole-vnmrs400
Archive directory:

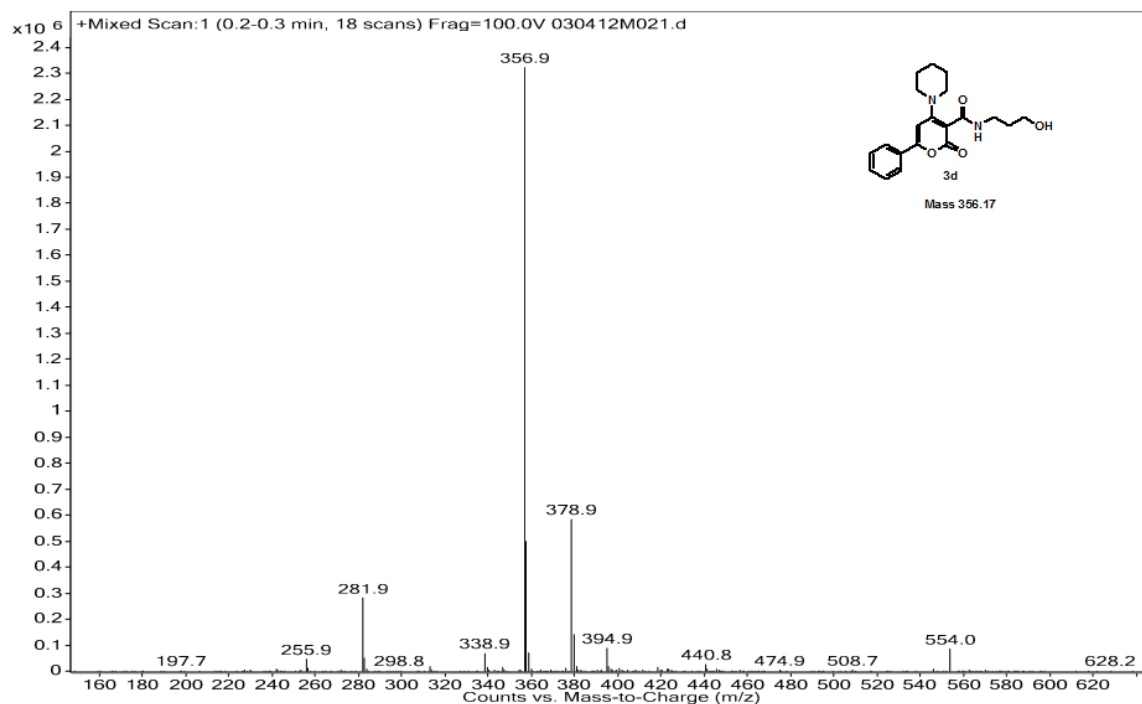
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FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: dmsd
Data collected on: Aug 31 2012



Sample Name	SK-III-7-25	Position	Vial 8	Instrument Name	Instrument 1	User Name	
Inj Vol	0.3	InjPosition		SampleType	Sample	IRM Calibration Status	Not Applicable
Data Filename	030412M021.d	ACQ Method	ILS-UNI.m	Comment		Acquired Time	4/3/2012 1:12:49 PM



SK-III-7-25 in DMSO-d6
File No:20120405_46

Sample Name:

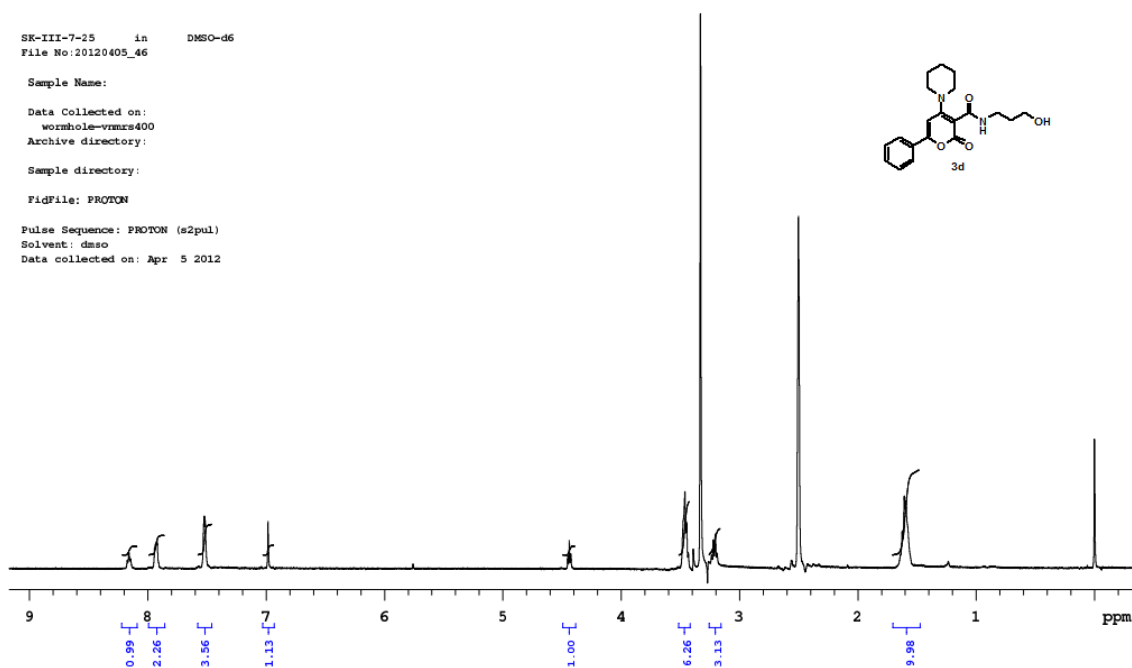
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Archive directory:

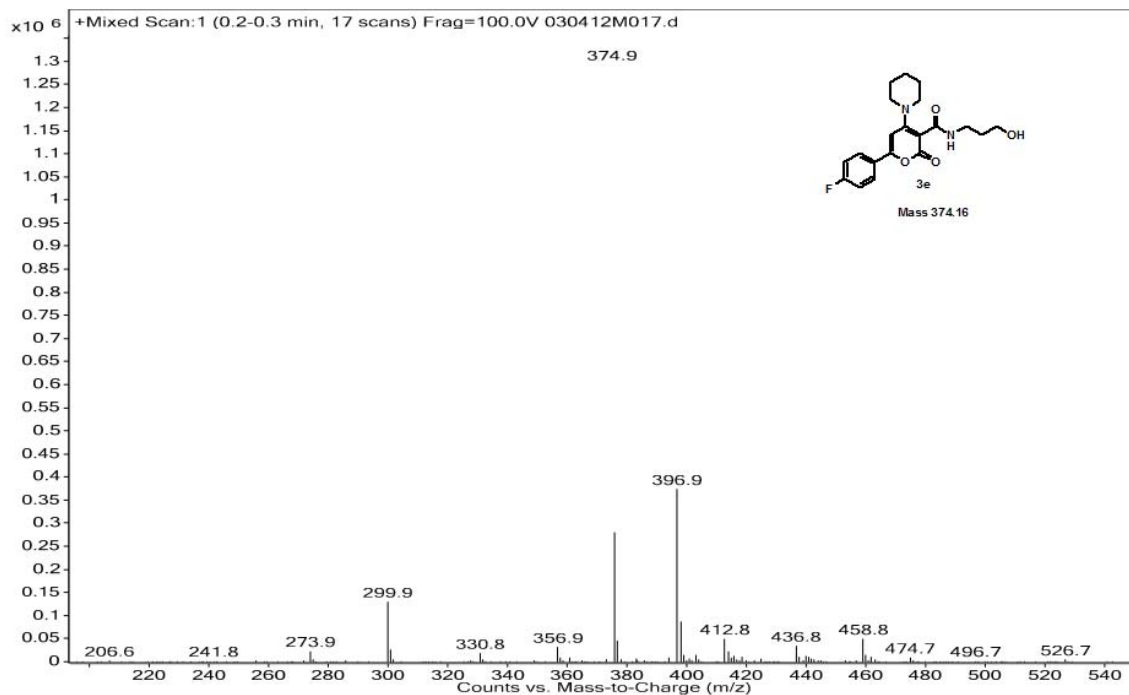
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FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: dms
Data collected on: Apr 5 2012



Sample Name	SK-III-11-25	Position	Vial 4	Instrument Name	Instrument 1	User Name	
Inj Vol	0.3	InjPosition		SampleType	Sample	IRM Calibration Status	Not Applicable
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SK-III-11-25
File No: 20120405_15

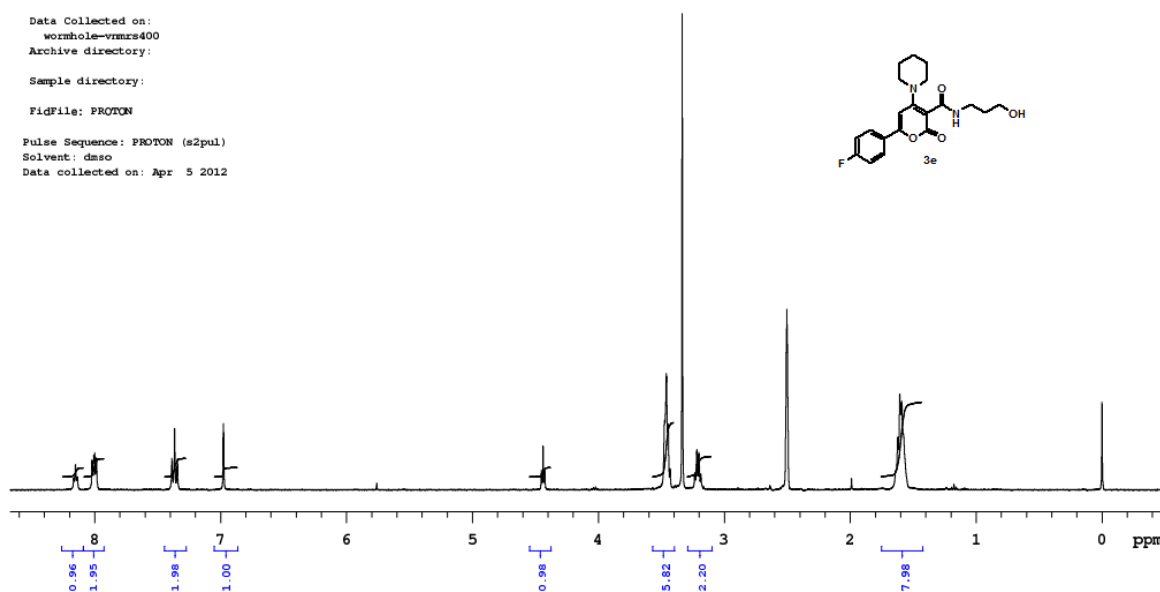
Sample Name:

Data Collected on:
wormhole-vmrms400
Archive directory:

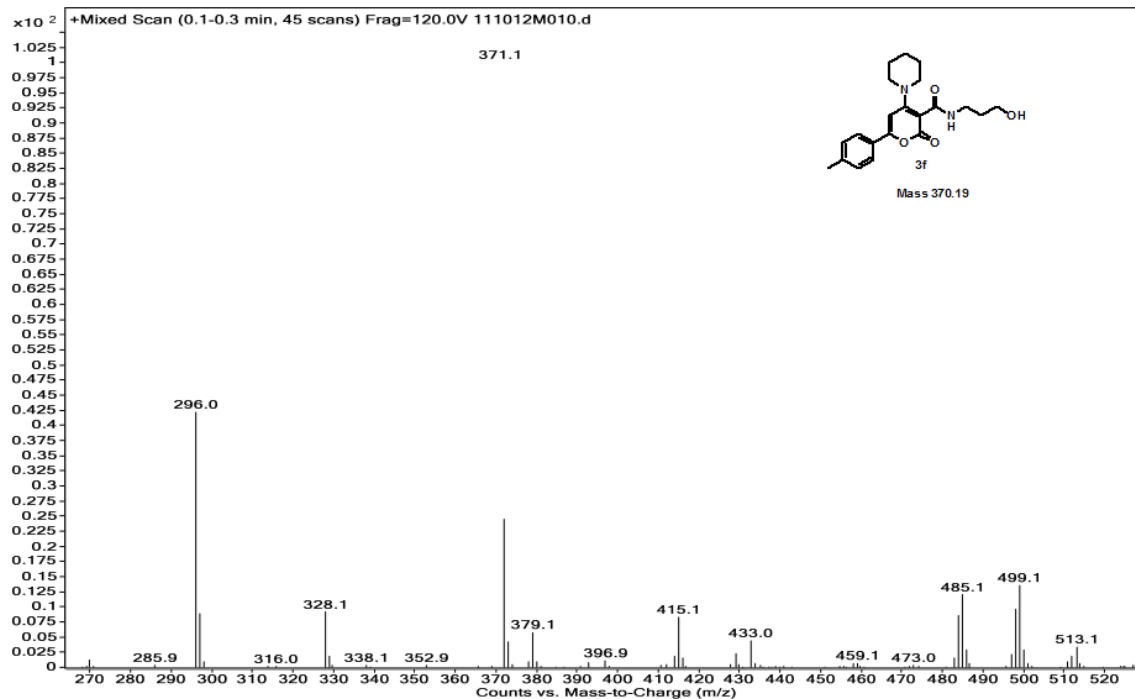
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FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: dmsd
Data collected on: Apr 5 2012



Sample Name	SK-III-40-25	Position	Vial 16	Instrument Name	Instrument 1	User Name	
Inj Vol	0.5	InjPosition		SampleType	Sample	IRM Calibration Status	Not Applicable
Data Filename	111012M010.d	ACQ Method	ILS.m	Comment		Acquired Time	10/11/2012 11:24:11 AM



SK-III-40-25 in DMSO-d6
File No: 20120831_60

Sample Name:

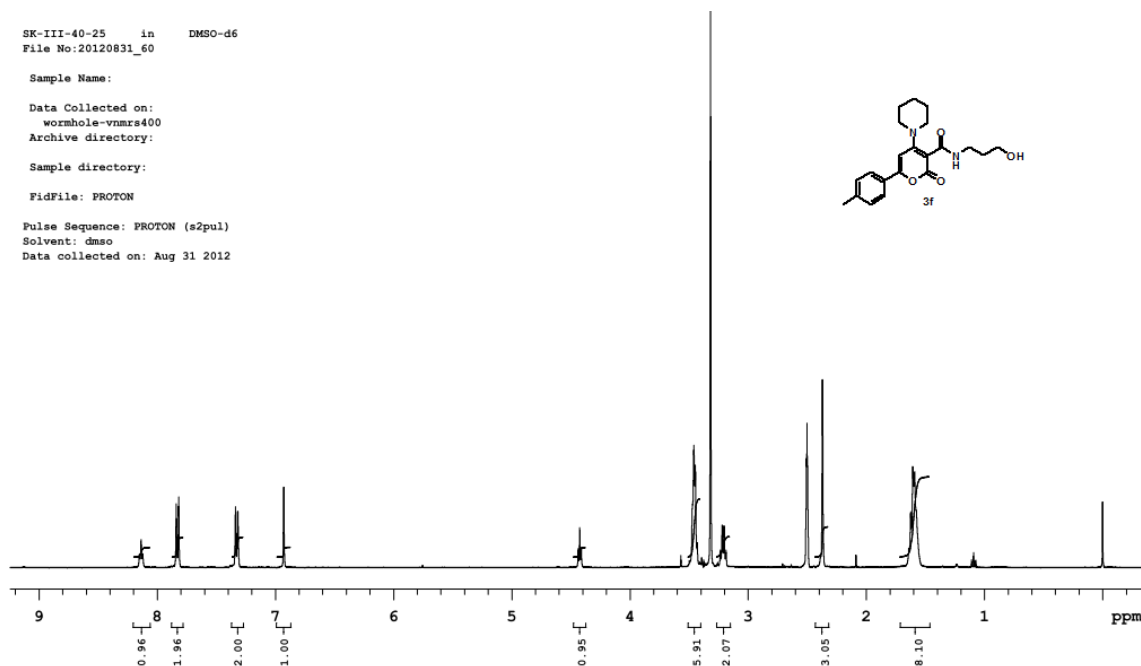
Data Collected on:
wormhole-vmmrs400

Archive directory:

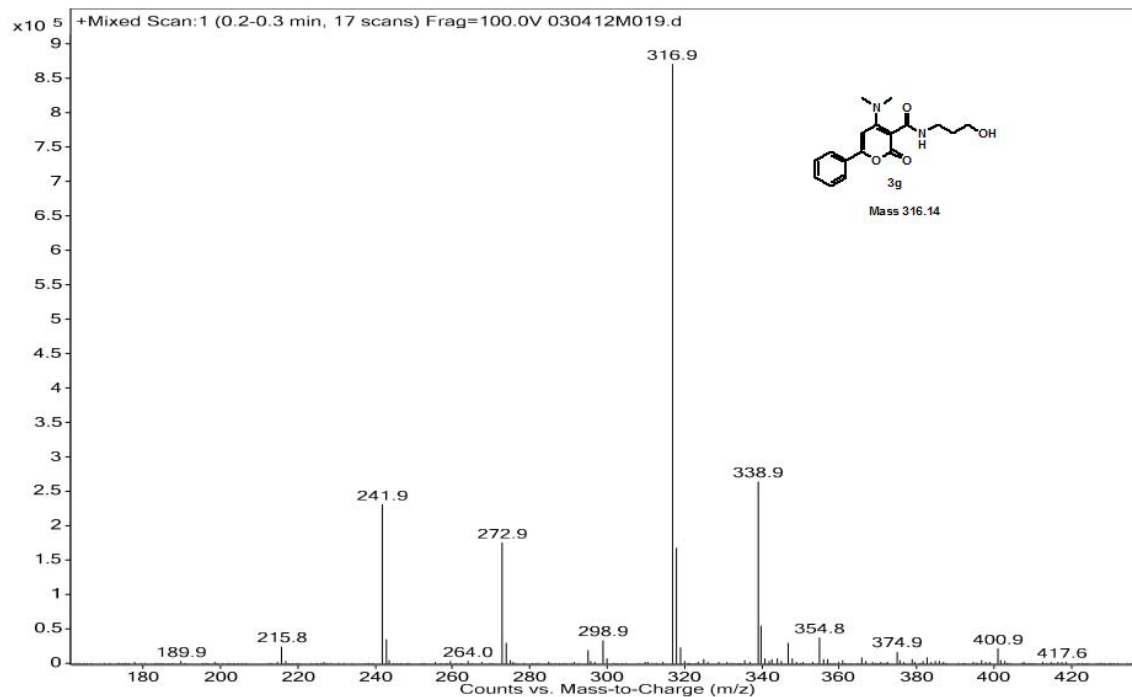
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FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: dmsd
Data collected on: Aug 31 2012



Sample Name	SK-III-8-25	Position	Vial 6	Instrument Name	Instrument 1	User Name	
Inj Vol	0.3	InjPosition		SampleType	Sample	IRM Calibration Status	Not Applicable
Data Filename	030412M019.d	ACQ Method	ILS-UNI.m	Comment		Acquired Time	4/3/2012 1:09:55 PM



SK-III-8-25
File No:20120405_14

Sample Name:

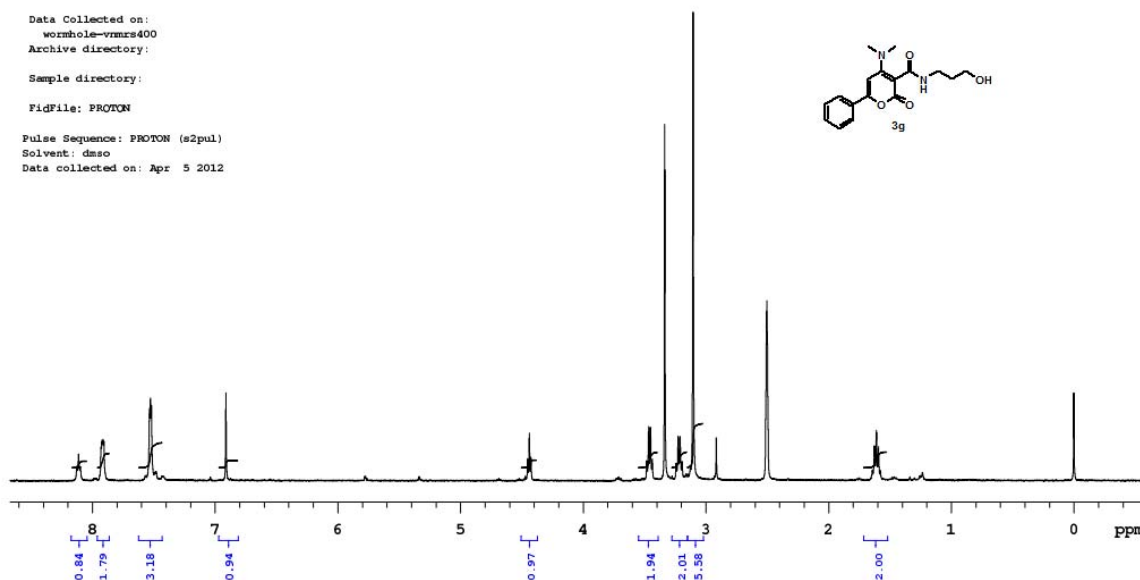
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wormhole-vmmrs400

Archive directory:

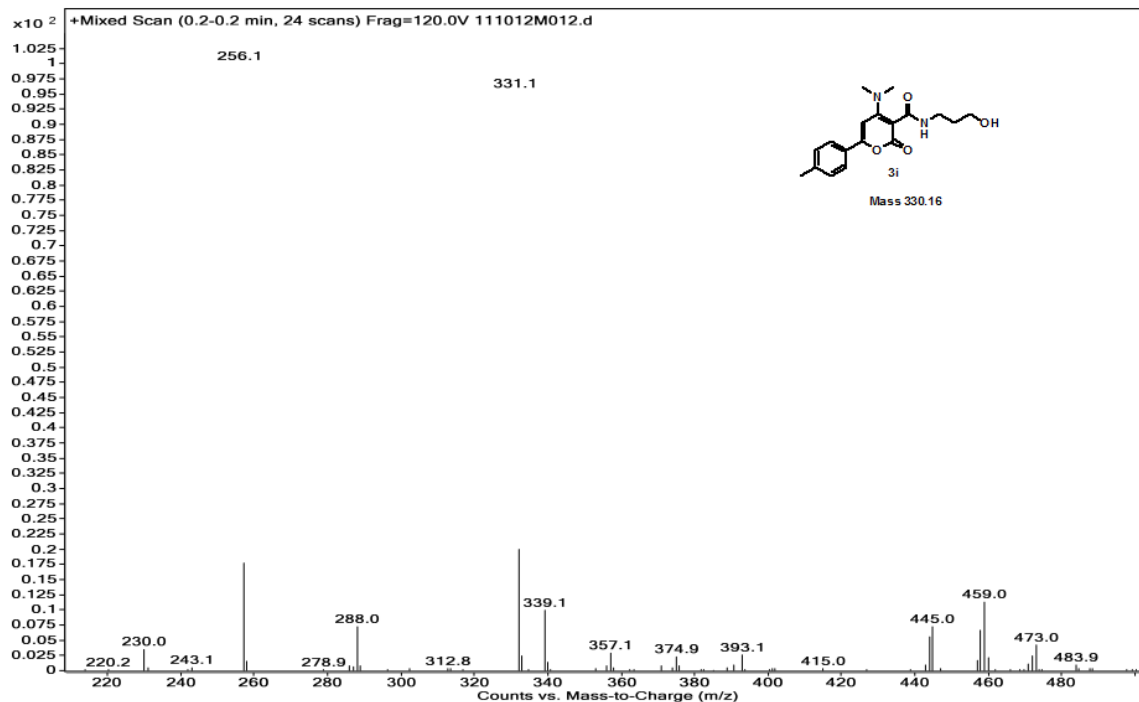
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Pulse Sequence: PROTON (s2pul)
Solvent: dmsd
Data collected on: Apr 5 2012



Sample Name	SK-III-42-25	Position	Vial 18	Instrument Name	Instrument 1	User Name	
Inj Vol	0.5	InjPosition		SampleType	Sample	IRM Calibration Status	Not Applicable
Data Filename	111012M012.d	ACQ Method	ILS.m	Comment		Acquired Time	10/11/2012 11:26:46 AM



SK-III-42-25
File No:20120907_36

Sample Name:

Data Collected on:
wormhole-vnmrs400

Archive directory:

Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: dmsd
Data collected on: Sep 7 2012

