

Supporting Information

Small Molecule Receptor Protein Tyrosine Phosphatase γ (RPTP γ)

Ligands That Inhibit Phosphatase Activity via Perturbation of the Tryptophan-Proline-Aspartate (WPD)-Loop

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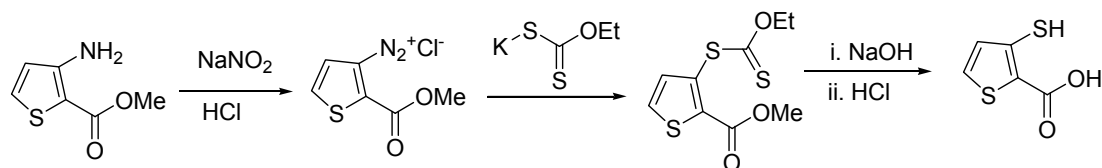
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Procedure for the synthesis of 3-mercaptothiophene-2-carboxylic acid:

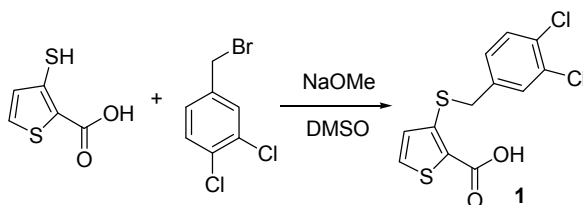
3-Mercaptothiophene-2-carboxylic acid was prepared according to the literature procedure (Corral, C.; Lissavetzky, J.; Alvarez-Insua, A. S.; Valdeolmillos, A. M. *Org. Prep. Proc. Int.* **1985**, *17*, 163) as shown below:



To 14 mL of 6 M HCl solution was added 3-amino-2-methoxycarbonylthiophene (2.5 g, 16 mmol, 1.0 eq.) gradually at room temperature. The resulting mixture was stirred at room temperature for 30 min, cooled to 0 °C, then diazotized with NaNO₂ (1.1 g, 16 mmol, 1.0 eq.) in 8 mL of water. After the resulting mixture was stirred at 0 °C for an additional 1 h, the mixture was slowly poured into a well-stirred solution of Na₂CO₃ (2.2 g, 19 mmol) and potassium ethylxanthogenate in 25 mL of water. The resulting mixture was warmed and maintained at 60-70 °C until the evolution of nitrogen ceased. After cooling to room temperature, the mixture was extracted with EtOAc (3x). The combined organic layer was washed with 10% sodium hydroxide (20 mL) and water (2 x 20 mL), dried (anh. sodium sulfate) and evaporated under reduced pressure to afford an oil, which was dissolved in ethanol (15 mL), then 125 mL of 4M sodium hydroxide was added. The resulting mixture was heated to reflux for 2 h. It was then cooled to room temperature and ethanol was removed by evaporation. Water was added and the mixture was extracted with ether (2x) to remove impurities. The aqueous layer was acidified with 6N HCl to pH = 3, then extracted with EtOAc (3x). The combined organic layer was dried and evaporated to leave 2.29 g of solid as the product. ¹H NMR (DMSO-d₆)

δ : 1.15 (1H, s), 7.2 (1H, d, $J = 5$ Hz), 7.95 (1H, d, $J = 5$ Hz). LC/MS (ESI) m/z ($M+H$)⁺: 319.05, $t_R = 0.840$ min.

General procedure for preparation of compound 1:



To a solution of 3-mercaptothiophene-2-carboxylic acid (1.07 g, 6.69 mM, 1.0 eq.) and 3,4-dichlorobenzyl bromide (1.6 g, 6.69 mmol, 1.0 eq.) in DMSO (15 mL) was added NaOMe (25 wt. % in methanol, 3.06 mL, 13.375 mM, 2.0 eq.) dropwise at room temperature. The resulting mixture was stirred at room temperature for 6 h, then poured into water (10 mL), acidified with 6M HCl to pH = 4, then extracted with EtOAc (3x). The combined organic layer was washed with water (3x), brine, dried over Na₂SO₄ and evaporated under reduced pressure to afford 1.81 g (85% yield) of 3-(3,4-dichlorobenzylthio)thiophene-2-carboxylic acid **1** as off-white solid. ¹H NMR (DMSO-d₆) δ : 7.90 (1H, d, $J = 5.2$ Hz), 7.84 (1H, s), 7.70 (1H, d, $J = 8$ Hz), 7.61 (1H, d, $J = 8.2$ Hz), 7.34 (1H, d, $J = 5.2$ Hz), 4.53 (2H, s). LC/MS (ESI) m/z ($M+H$)⁺: 318.0, $t_R = 0.915$ min.

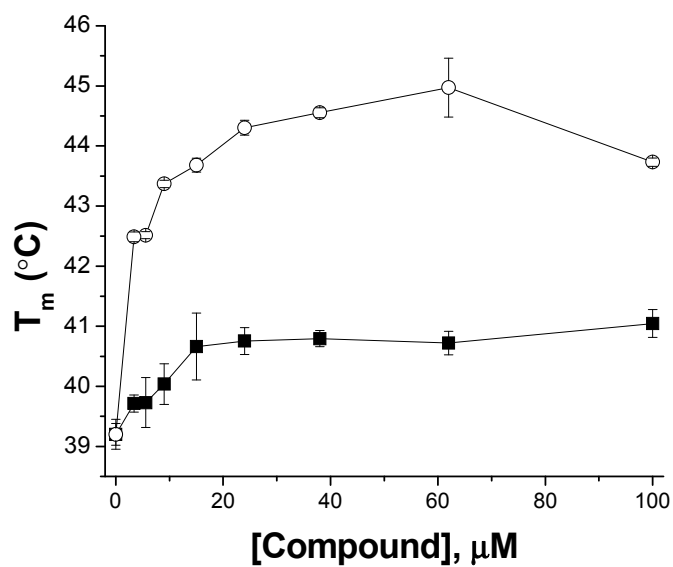


Figure S1. Effect of compounds **1** (■) and **15** (○) on the thermal stability of PTP γ . Error bars represent standard deviation from multiple replicates. Reactions contained 2.6 μM PTP γ , 25 mM MOPS, pH 7, 100 mM NaCl, 1 mM DTT, 0.2 mM EDTA, 200 μM 1,8-ANS, and 5% (v/v) DMSO.

Table S1. Refinement statistics**(a) “open” forms**

	apo, orthorhombic	apo, trigonal
Resolution, Å	23.5-2.1	49.5-2.41
R-work	0.254	0.198
R-free	0.305	0.234
r.m.s.d. bond distances, Å	0.005	0.010
r.m.s.d. bond angles, °	0.8	1.1
Ramachandran favored and allowed, %*	99.0	98.5
Ramachandran disallowed, %*	0	0
PDB ID	3QCB	3QCN

(b) “closed” forms

	Vanadate, orthorhombic	Vanadate, trigonal
Resolution, Å	40.7-2.1	26.4-1.8
R-work	0.224	0.241
R-free	0.266	0.258
r.m.s.d. bond distances, Å	0.006	0.006
r.m.s.d. bond angles, °	0.9	0.9
Ramachandran favored and allowed, %*	99.2	99.6
Ramachandran disallowed, %*	0	0
PDB ID	3QCC	3QCD

(c) “super-open” forms

	Compound 1 , co-crystal	Compound 1 , soak	Compound S1 , soak
Resolution, Å	25.4-2.5	31.4-2.1	27.6-2.05
R-work	0.264	0.233	0.218
R-free	0.324	0.261	0.254
r.m.s.d. bond distances, Å	0.007	0.006	0.006
r.m.s.d. bond angles, °	1.4	1.3	1.3
Ramachandran favored and allowed, %*	99.0	99.2	99.6
Ramachandran disallowed, %*	0.0	0.0	0.0
PDB ID	3QCF	3QCE	3QCG

	Compound 12 , soak	Compound 14 , soak	Compound 15 , soak
Resolution, Å	33.9-2.4	40.1-2.26	40.2-2.26
R-work	0.240	0.241	0.217
R-free	0.271	0.289	0.245
r.m.s.d. bond distances, Å	0.007	0.007	0.006
r.m.s.d. bond angles, °	1.4	1.0	1.3
Ramachandran favored and allowed, %*	99.2	98.8	99.2
Ramachandran disallowed, %*	0.0	0.4	0.0
PDB ID	3QCH	3QCI	3QCJ

	Compound 17 , soak	Compound 20 , soak	Compound S2 , co-crystal
Resolution, Å	30.1-2.05	33.8-2.4	39.4-2.4
R-work	0.245	0.217	0.201
R-free	0.262	0.258	0.246
r.m.s.d. bond distances, Å	0.006	0.010	0.010
r.m.s.d. bond angles, °	0.8	1.1	1.1
Ramachandran favored and allowed, %*	98.8	99.2	98.8
Ramachandran disallowed, %*	0.0	0.4	0.2
PDB ID	3QCK	3QCL	3QCM

* Laskowski, R. A.; MacArthur, M. W.; Moss, D. S.; Thornton, J. M. *J. Appl. Crystallogr.* **1993**, *26*, 283-291.

All structures except the trigonal apo and compounds **20** and **S2** were refined with CNX (Brünger *et al.*, 1998). The apo trigonal structures and compounds **20** and **S2** were refined with autoBUSTER (Blanc *et al.*, 2004).

Figures showing X-ray co-crystal structures of RPTPy with compound 1 analogs:

Although the structure of **1** in the trigonal crystal form was not determined, the structure of the closely related 3-(3-bromo-4-chlorobenzylthio)thiophene-2-carboxylic acid (**S1**) in the trigonal crystal form was determined to show that the same binding pattern occurs in the trigonal crystal form. Moreover, the higher resolution of this structure clarified the nature of the disorder observed in one of the two molecules in the orthorhombic crystal form, namely that the site was only partially occupied by **1** when bound to chain A and the remainder of the molecules were in the “open” conformation.

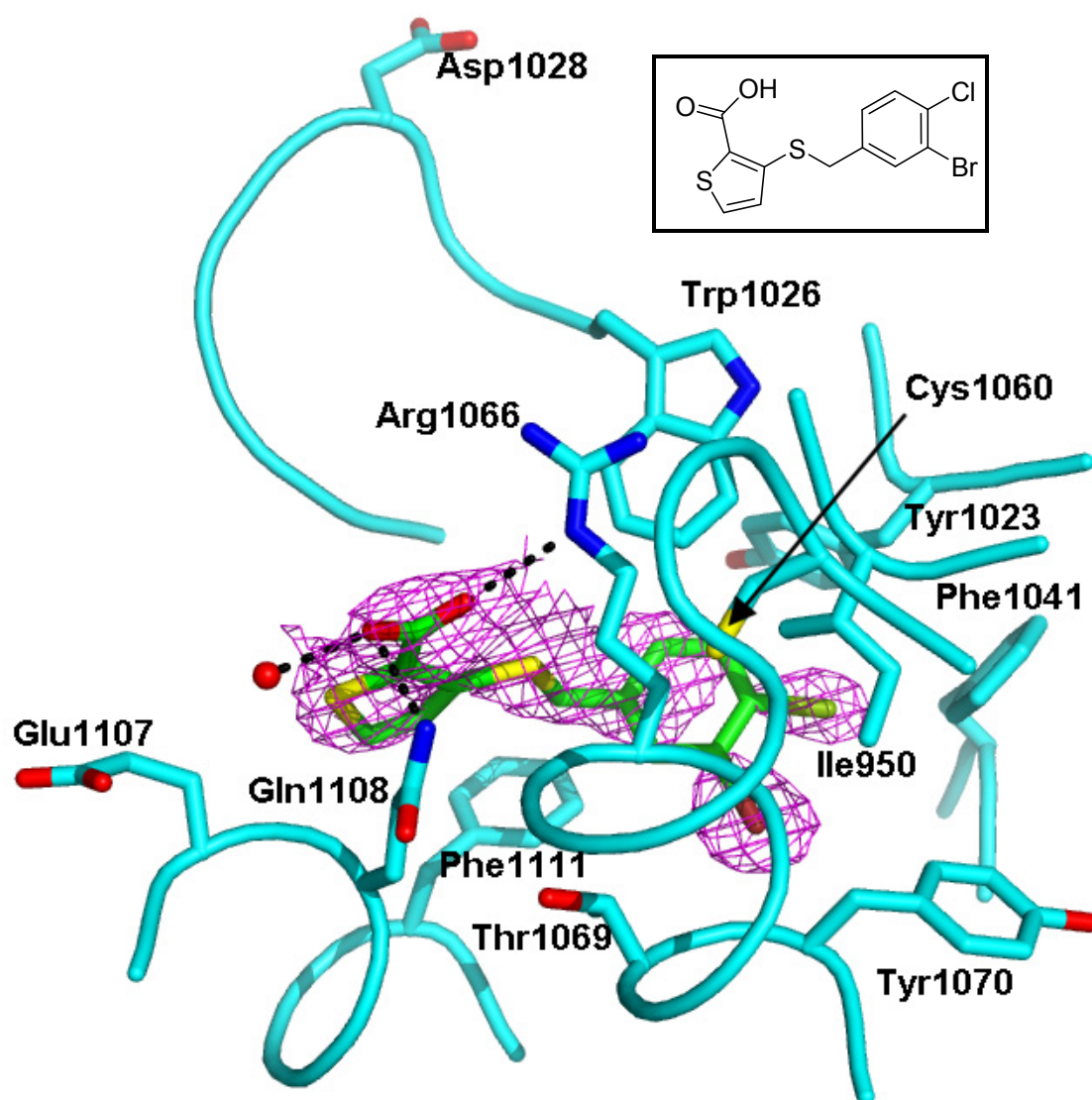


Figure S2. Compound S1 (3-(3-bromo-4-chlorobenzylthio)thiophene-2-carboxylic acid) bound to RPTP γ . Selected portions of PTP γ are shown either as a worm representing the backbone or with side chain atoms represented by sticks. RPTP γ carbon atoms are shown in cyan. Compound S1 carbon atoms are shown in green. Nitrogen atoms are shown in blue, oxygen atoms in red, sulfur atoms in yellow, chlorine atoms in

light green, and bromine atoms in magenta. Initial (i.e. prior to fitting **S1**) 2Fo-Fc electron density is shown as magenta caged contours at 1 σ . Image created with PyMOL.

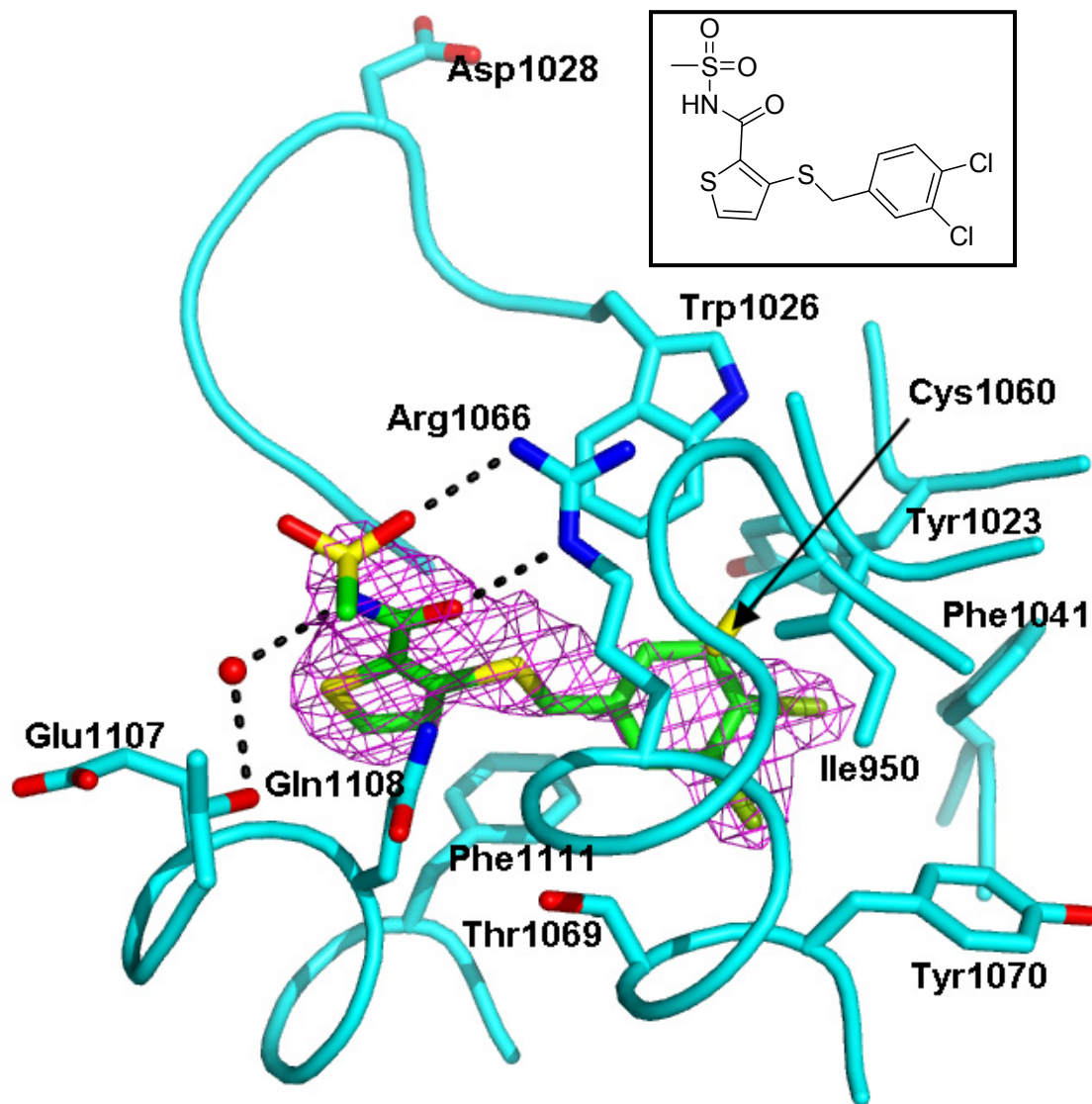


Figure S3. Compound **12** bound to RPTPy. Selected portions of RPTPy are shown either as a worm representing the backbone or with side chain atoms represented by

sticks. RPTPy carbon atoms are shown in cyan. Compound **12** carbon atoms are shown in green. Nitrogen atoms are shown in blue, oxygen atoms in red, sulfur atoms in yellow, and chlorine atoms in light green. Initial (i.e. prior to fitting **12**) 2Fo-Fc electron density is shown as magenta caged contours at 1 σ . Image created with PyMOL.

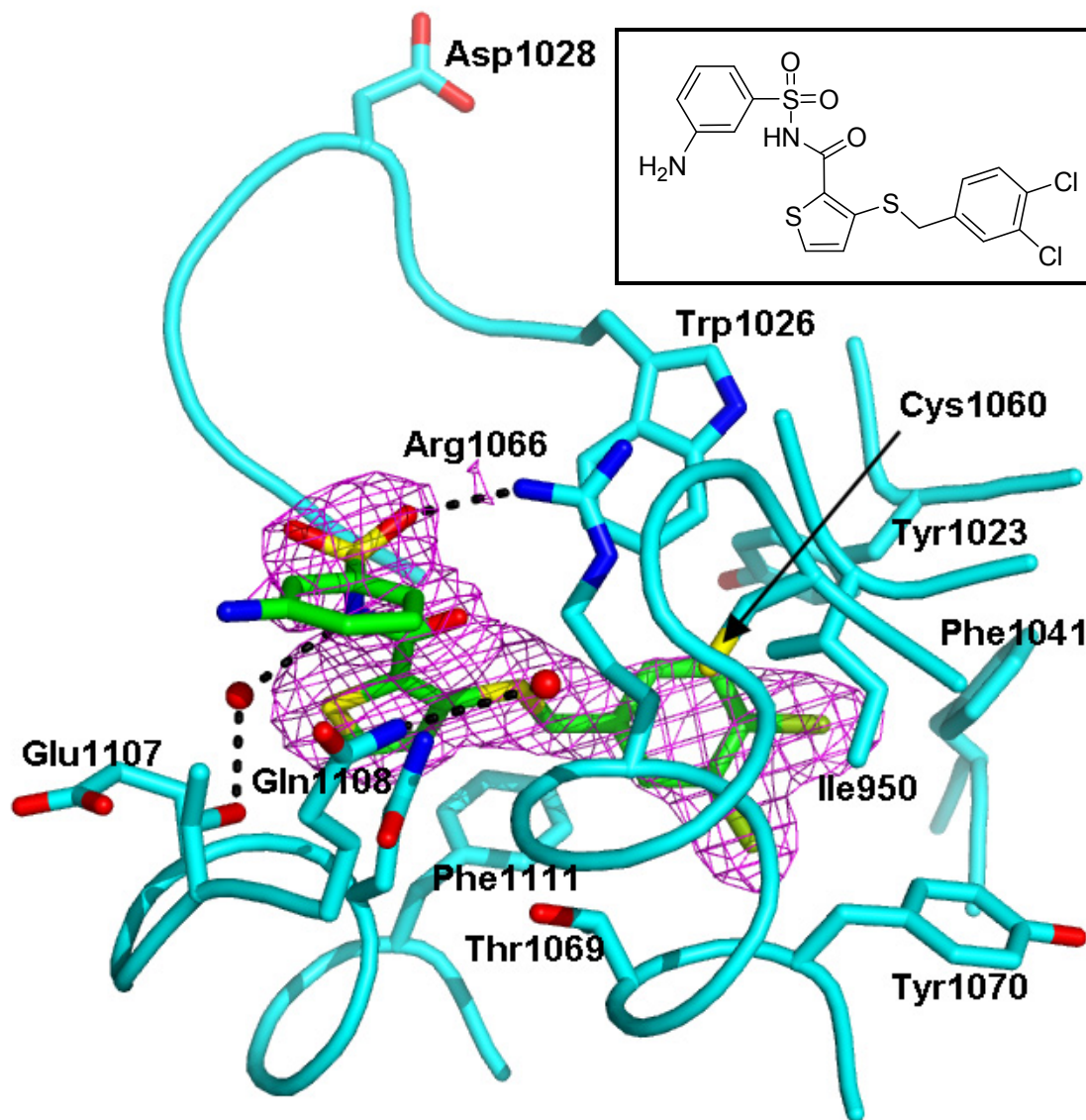


Figure S4. Compound **14** bound to RPTPy. Selected portions of RPTPy are shown either as a worm representing the backbone or with side chain atoms represented by

sticks. RPTPy carbon atoms are shown in cyan. Compound **14** carbon atoms are shown in green. Nitrogen atoms are shown in blue, oxygen atoms in red, sulfur atoms in yellow, and chlorine atoms in light green. Initial (i.e. prior to fitting **14**) 2Fo-Fc electron density is shown as magenta caged contours at 1σ . Image created with PyMOL.

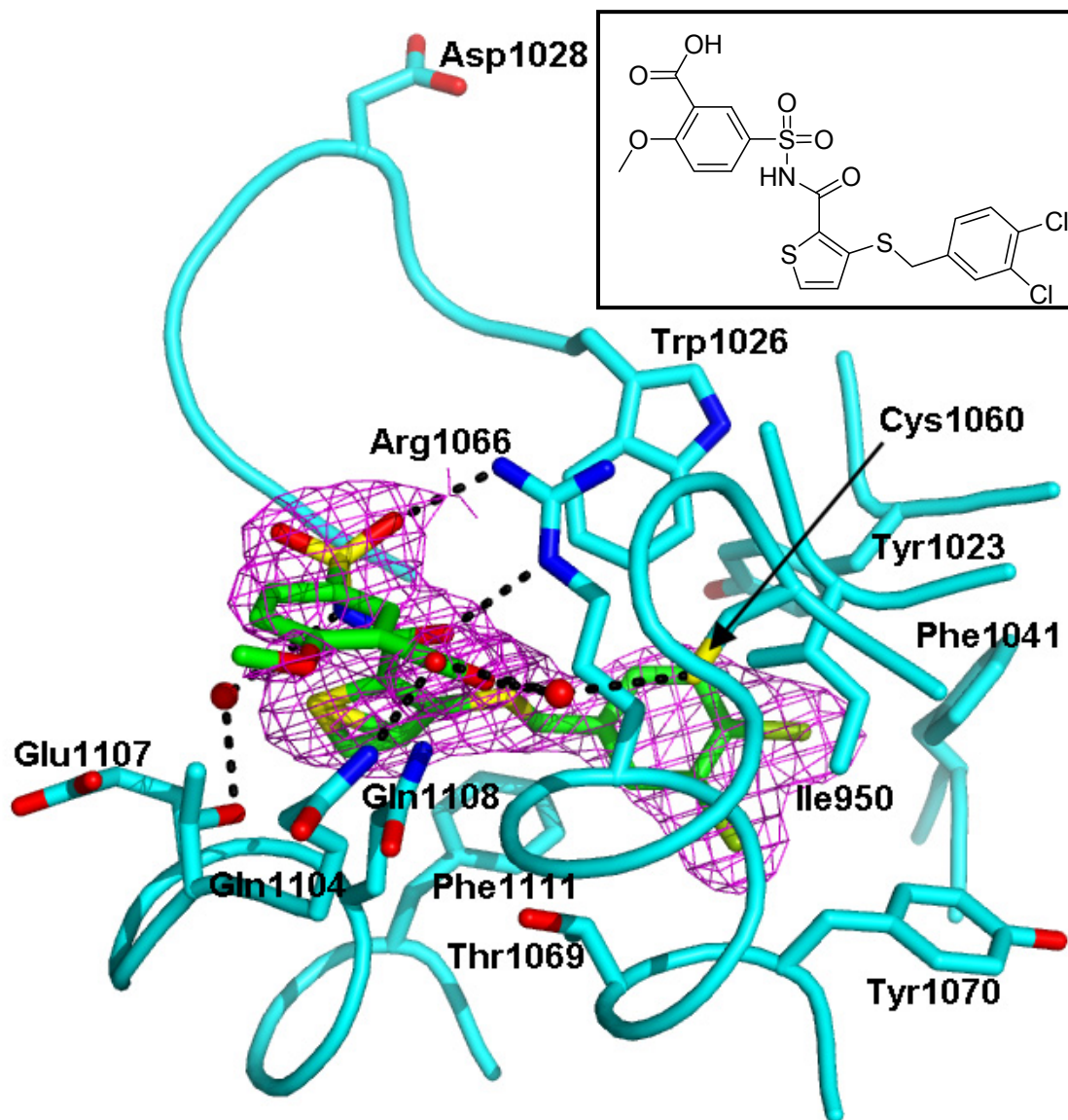


Figure S5. Compound **15** bound to RPTPy. Selected portions of RPTPy are shown either as a worm representing the backbone or with side chain atoms represented by

sticks. RPTPy carbon atoms are shown in cyan. Compound **15** carbon atoms are shown in green. Nitrogen atoms are shown in blue, oxygen atoms in red, sulfur atoms in yellow, and chlorine atoms in light green. Initial (i.e. prior to fitting **15**) 2Fo-Fc electron density is shown as magenta caged contours at 1σ . Image created with PyMOL.

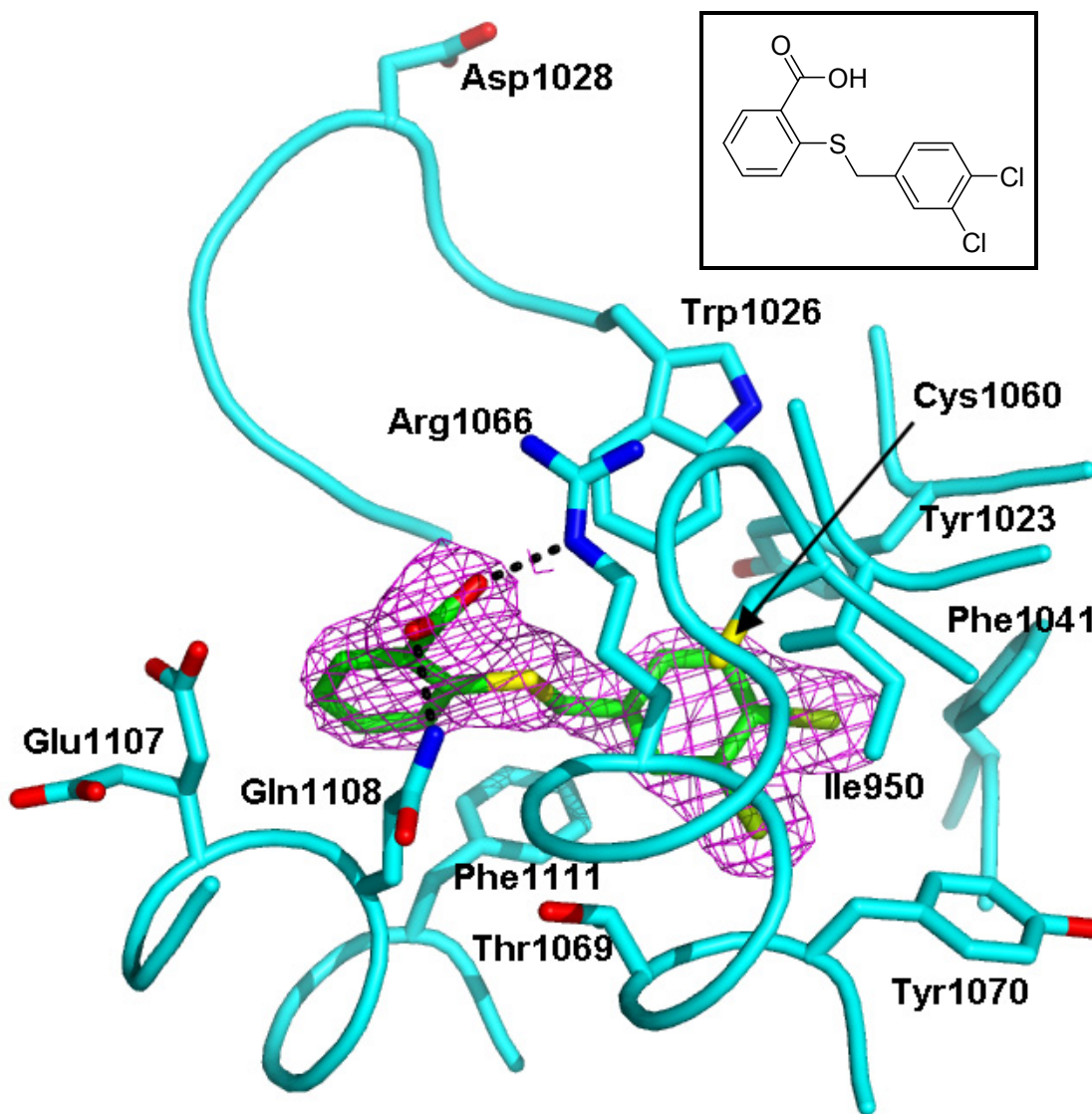


Figure S6. Compound **17** bound to RPTPy. Selected portions of RPTPy are shown either as a worm representing the backbone or with side chain atoms represented by

sticks. RPTPy carbon atoms are shown in cyan. Compound **17** carbon atoms are shown in green. Nitrogen atoms are shown in blue, oxygen atoms in red, sulfur atoms in yellow, and chlorine atoms in light green. Initial (i.e. prior to fitting **17**) 2Fo-Fc electron density is shown as magenta caged contours at 1σ . Image created with PyMOL.

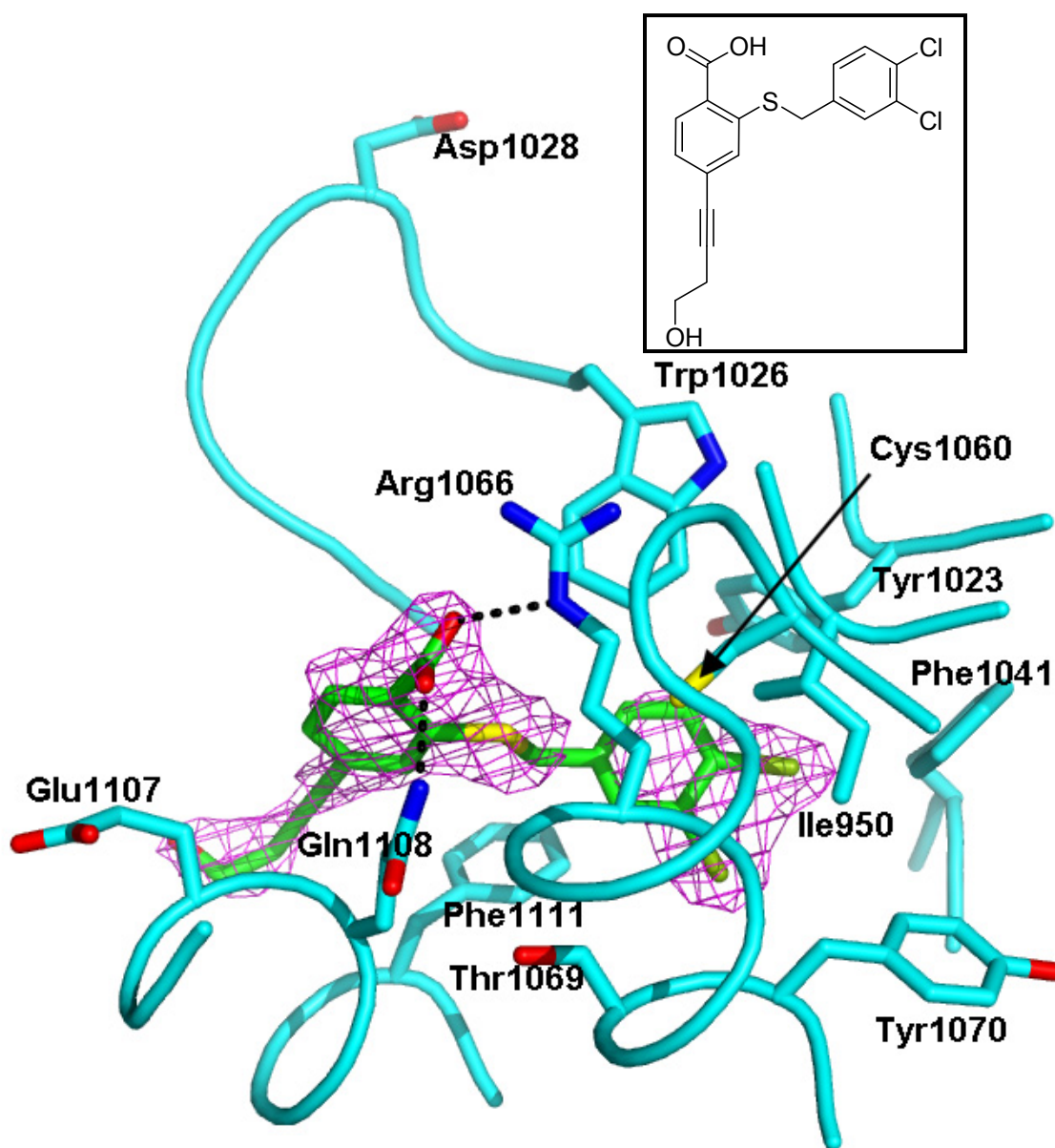


Figure S7. Compound **20** bound to RPTPy. Selected portions of RPTPy are shown either as a worm representing the backbone or with side chain atoms represented by

sticks. RPTPy carbon atoms are shown in cyan. Compound **20** carbon atoms are shown in green. Nitrogen atoms are shown in blue, oxygen atoms in red, sulfur atoms in yellow, and chlorine atoms in light green. Initial (i.e. prior to fitting **20**) 2Fo-Fc electron density is shown as magenta caged contours at 1σ . Image created with PyMOL.

Modeling suggested that a rather elaborated molecule would form interactions with the side chains of Glu1106 and Glu1107. However, no improvement in binding potency was observed so the structure was determined to ascertain if the binding mode was different than predicted. This compound required co-crystallization (Kish et al., 2011). Although the initial electron density was not very good for the ethynyl linker (Figure S8), it was clear that this molecule bound more or less as expected. Although the electron density improved during refinement for the ethynyl linker, the electron density for the 2-(methylamino)ethylamino moiety remained poor, the electron density that was present was relatively near the side chains of glutamate residues 1106 and 1107.

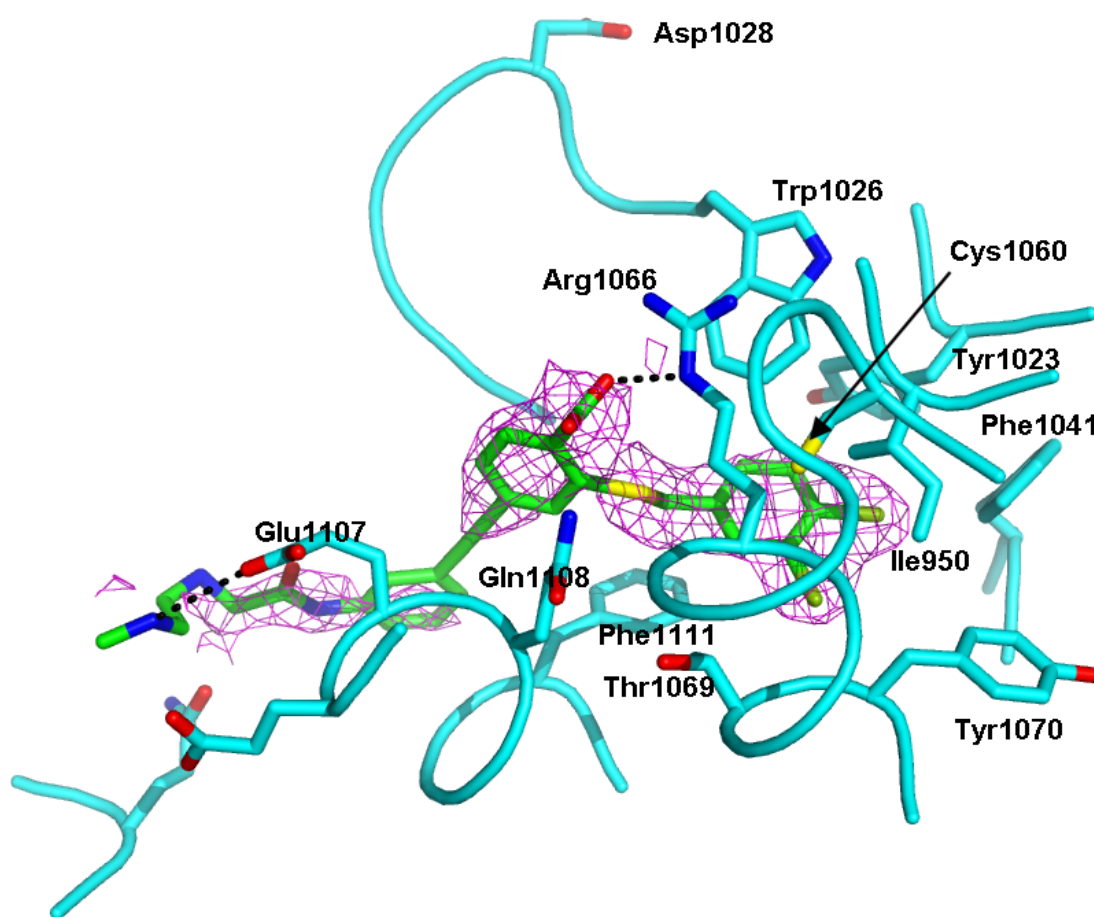
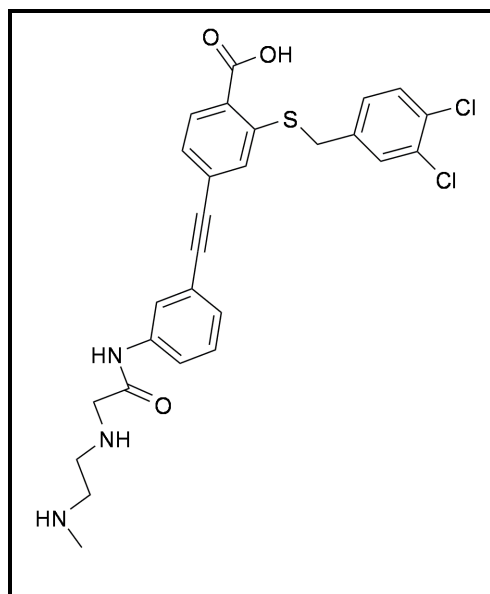
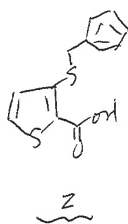
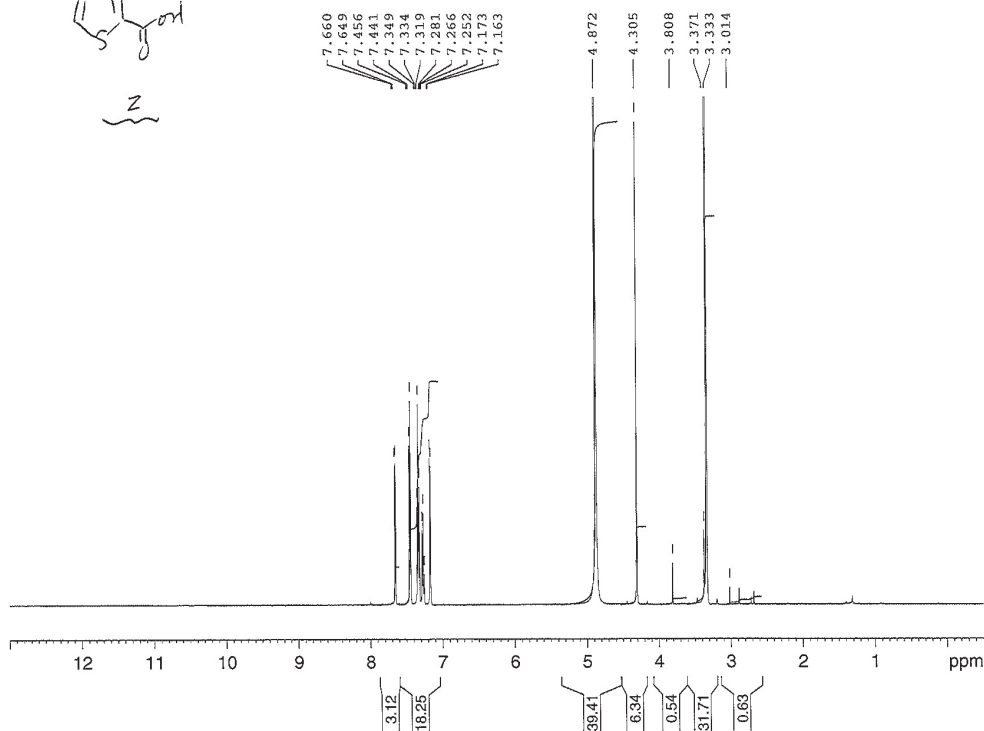


Figure S8. Compound **S2** bound to RPTP γ . Selected portions of RPTP γ are shown either as a worm representing the backbone or with side chain atoms represented by sticks. RPTP γ carbon atoms are shown in cyan. Compound **S2** carbon atoms are shown in green. Nitrogen atoms are shown in blue, oxygen atoms in red, sulfur atoms in yellow, and chlorine atoms in light green. Initial (i.e. prior to fitting **S2**) 2Fo-Fc electron density is shown as magenta caged contours at 1 σ . Image created with PyMOL.

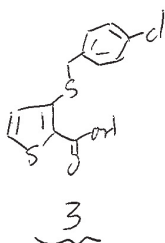
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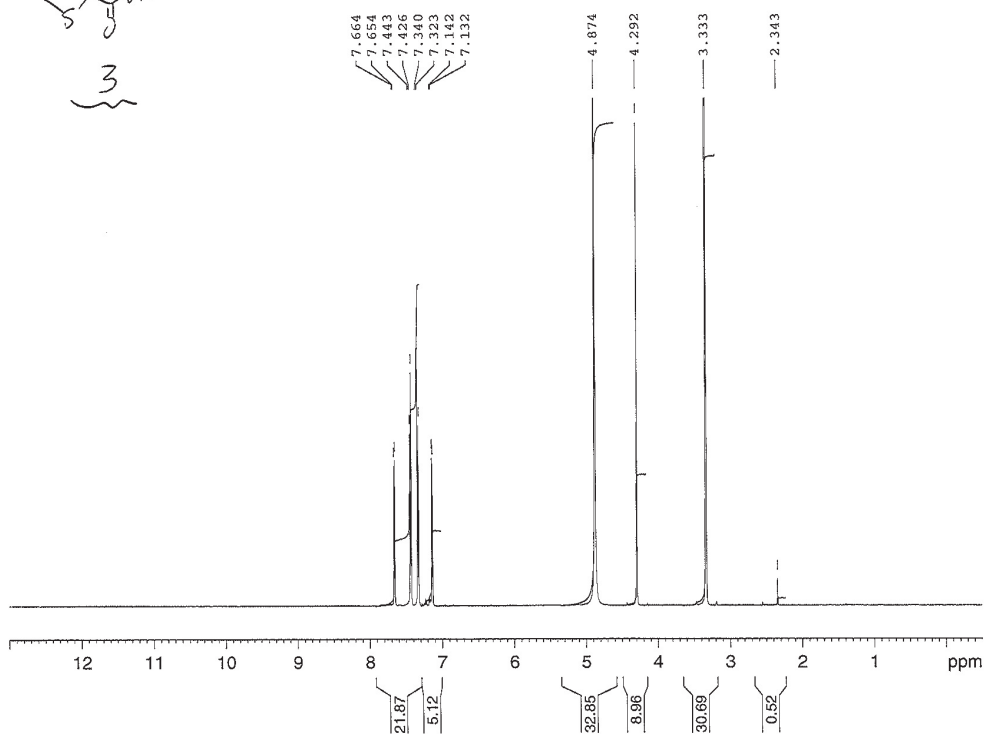
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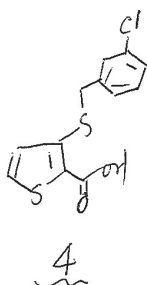
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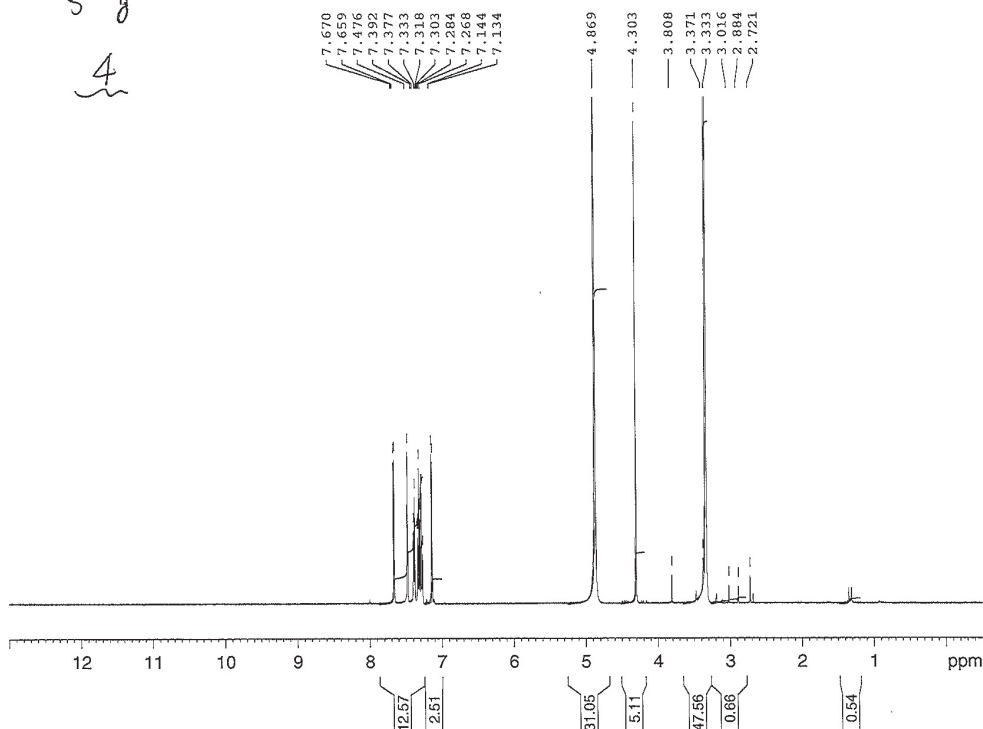
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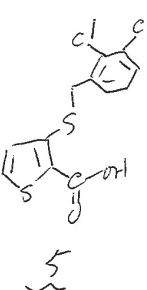
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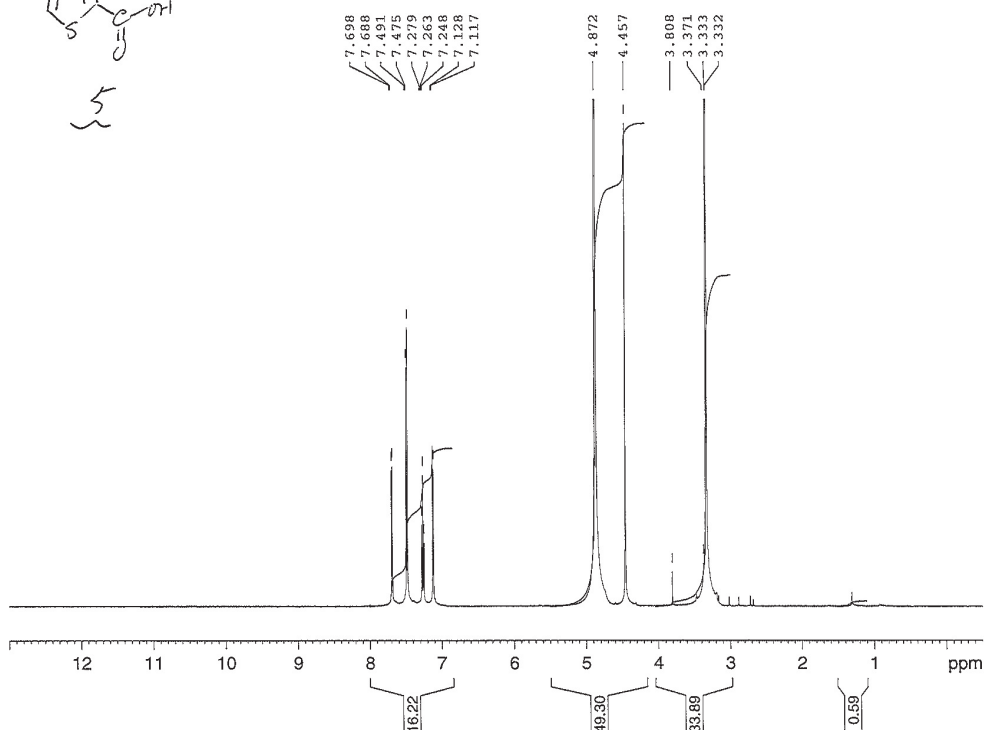
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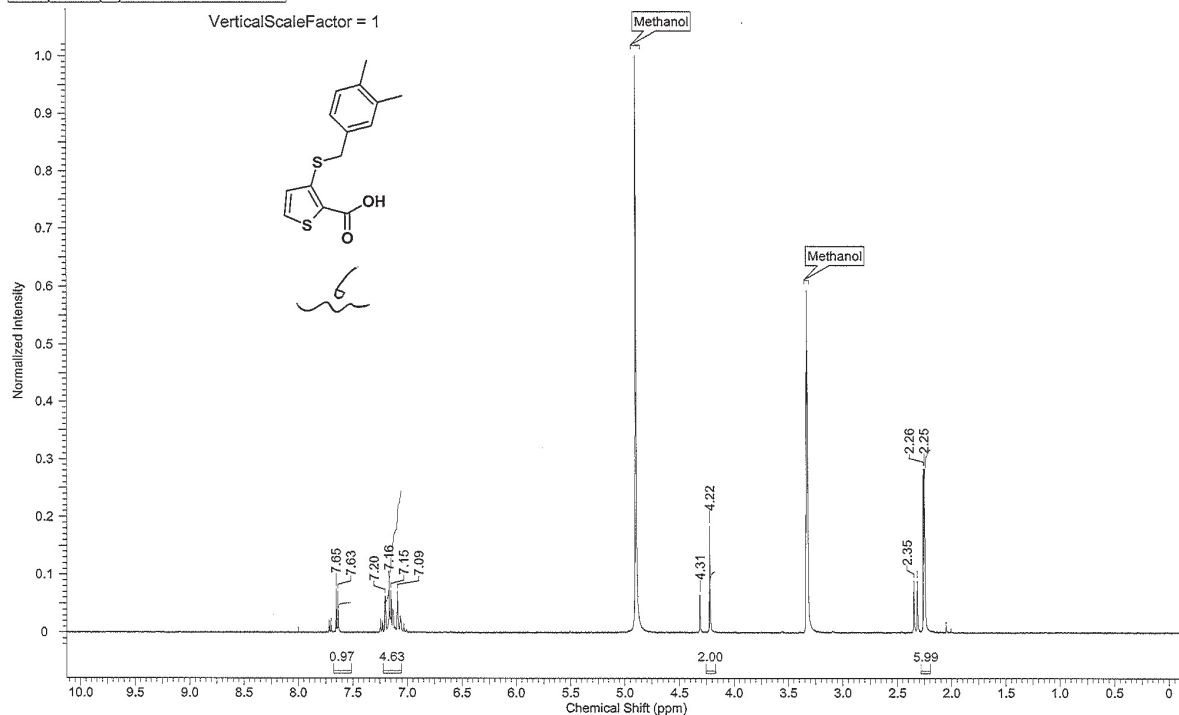
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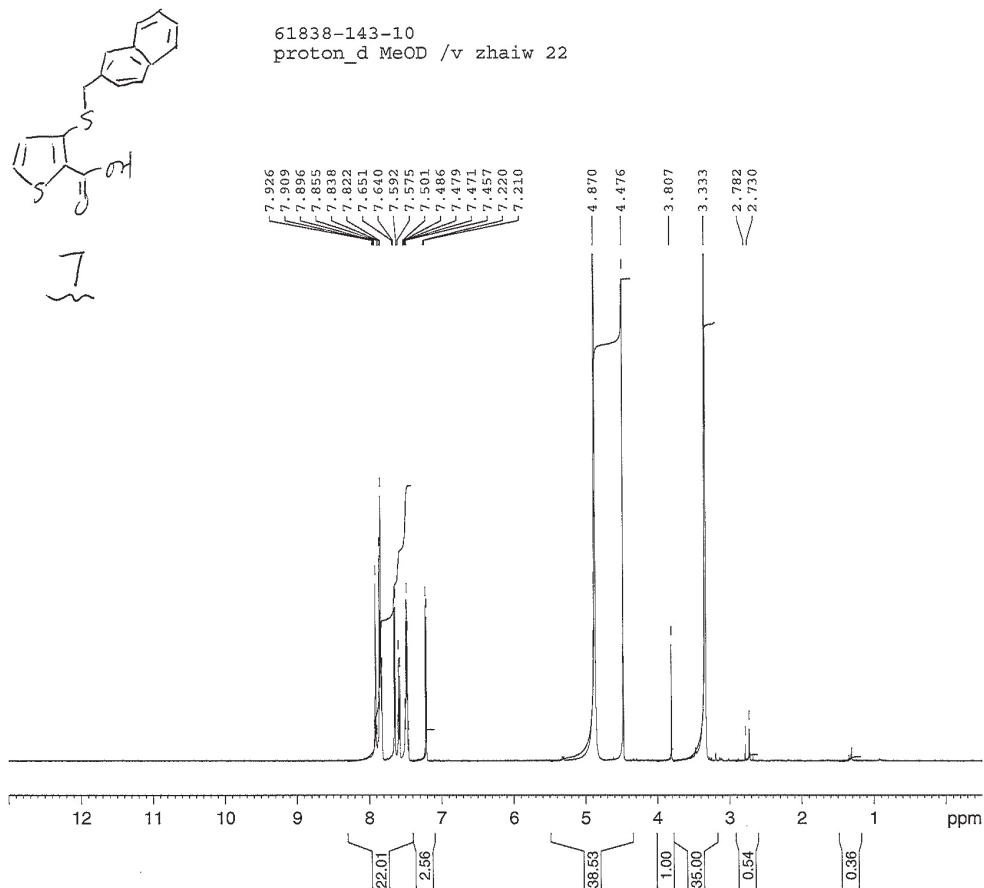
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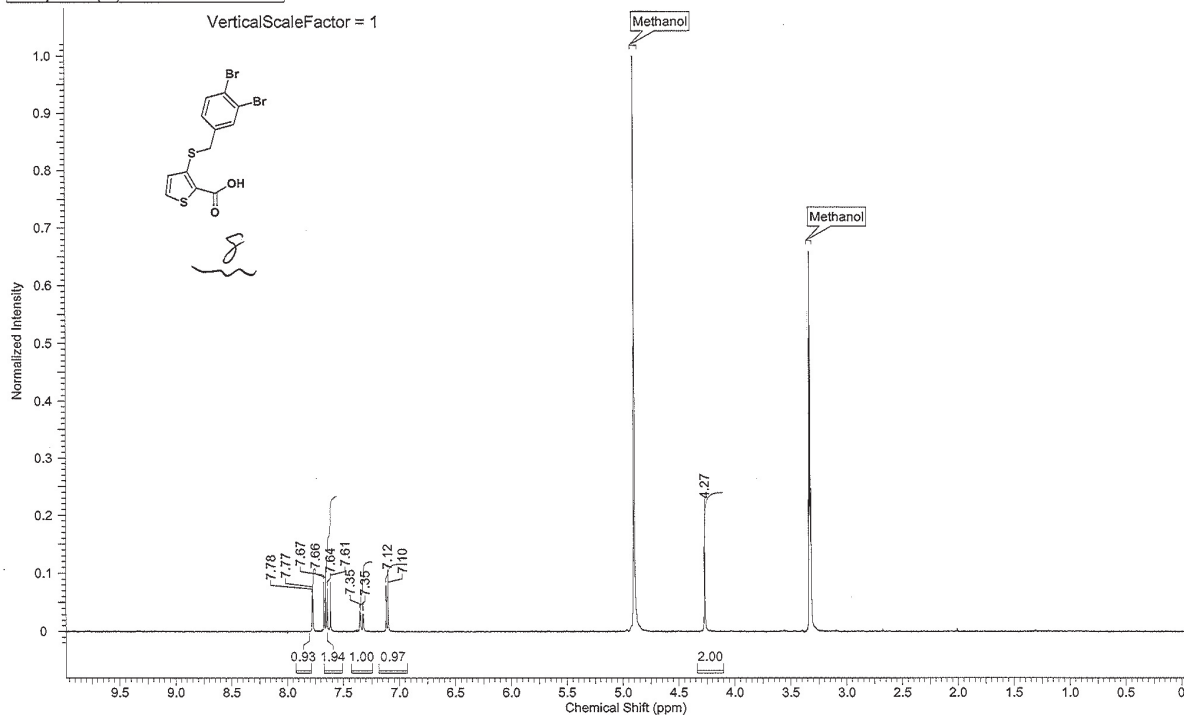
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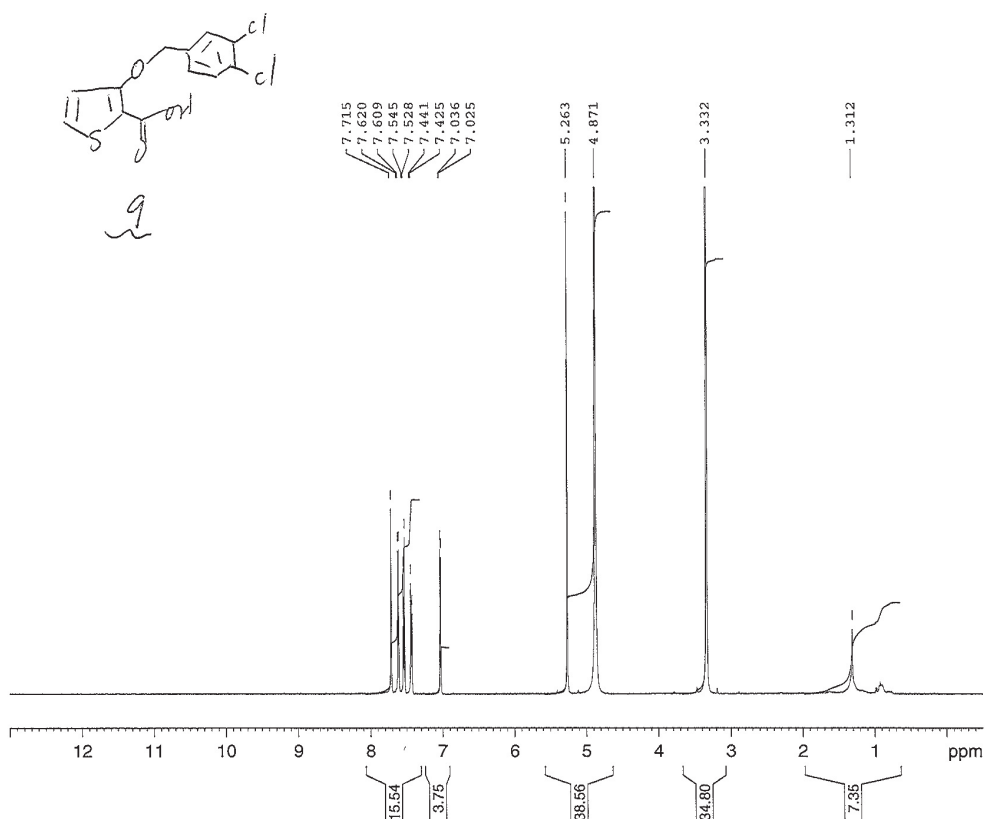
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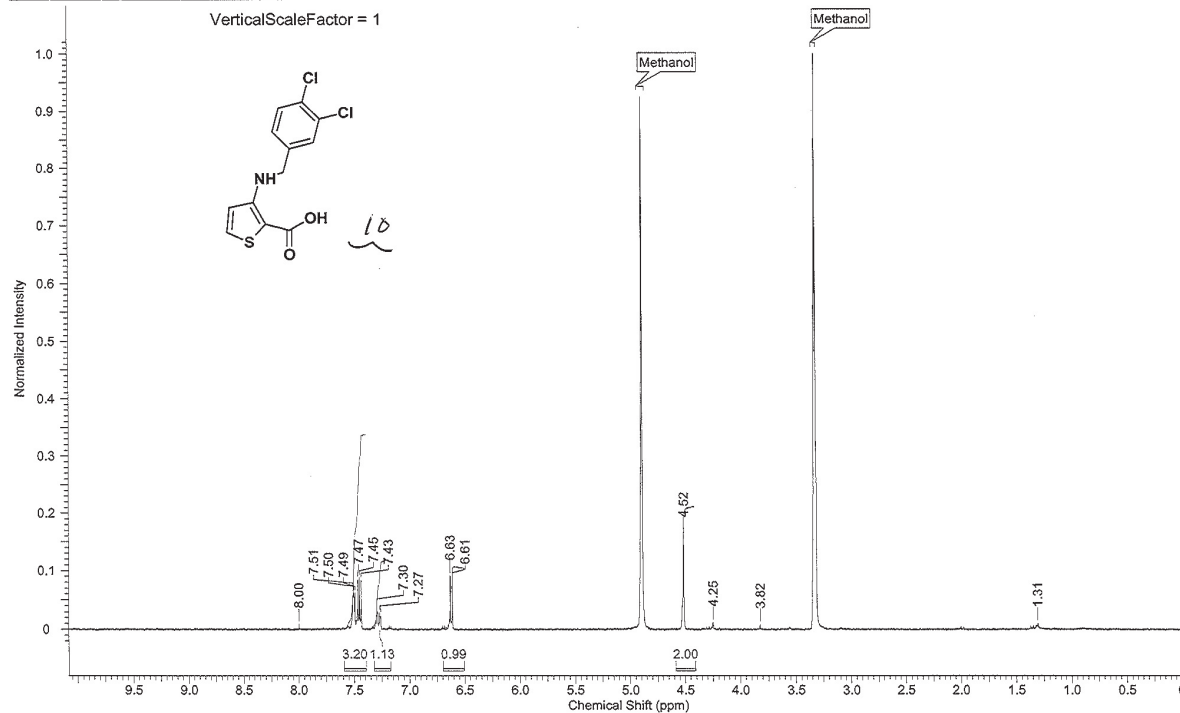
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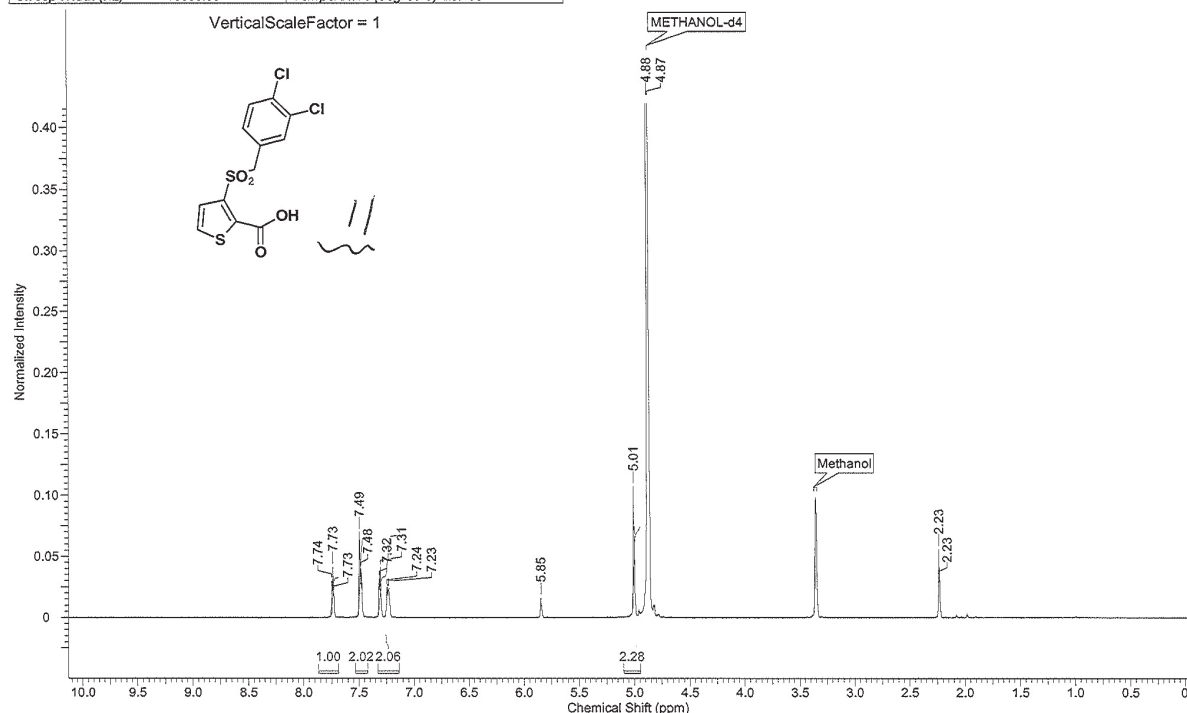
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61838-196

7/11/2011 10:49:55 AM

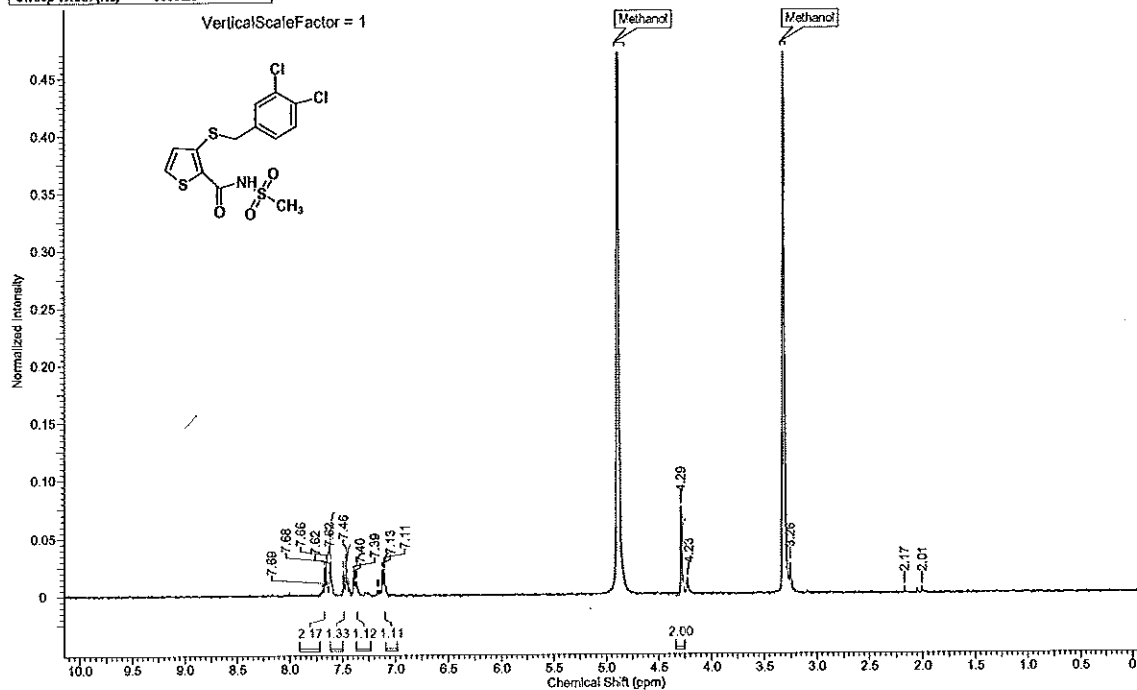
Acquisition Time (sec)	3.2768	Comment	61838-196 proton. d MeOD v zhaiw 43	Date	07 Mar 2006 16:18:35
Date Stamp	07 Mar 2006 16:18:35				
File Name	\\cruncher.wfd.pri.bms.com\nmread1\JDX2005-2007\ZHAIW\61838-196_10_DRX500A.JDX			Frequency (MHz)	500.13
Nucleus	1H	Number of Transients	16	Origin	61838-196
Owner	zhaiw	Points Count	32768	Solvent	METHANOL-d4
Sweep Width (Hz)	10000.00	Temperature (degree C)	28.160	Spectrum Offset (Hz)	4012.6965



H-NMR of Compound 12

1/13/2011 2:41:13 PM

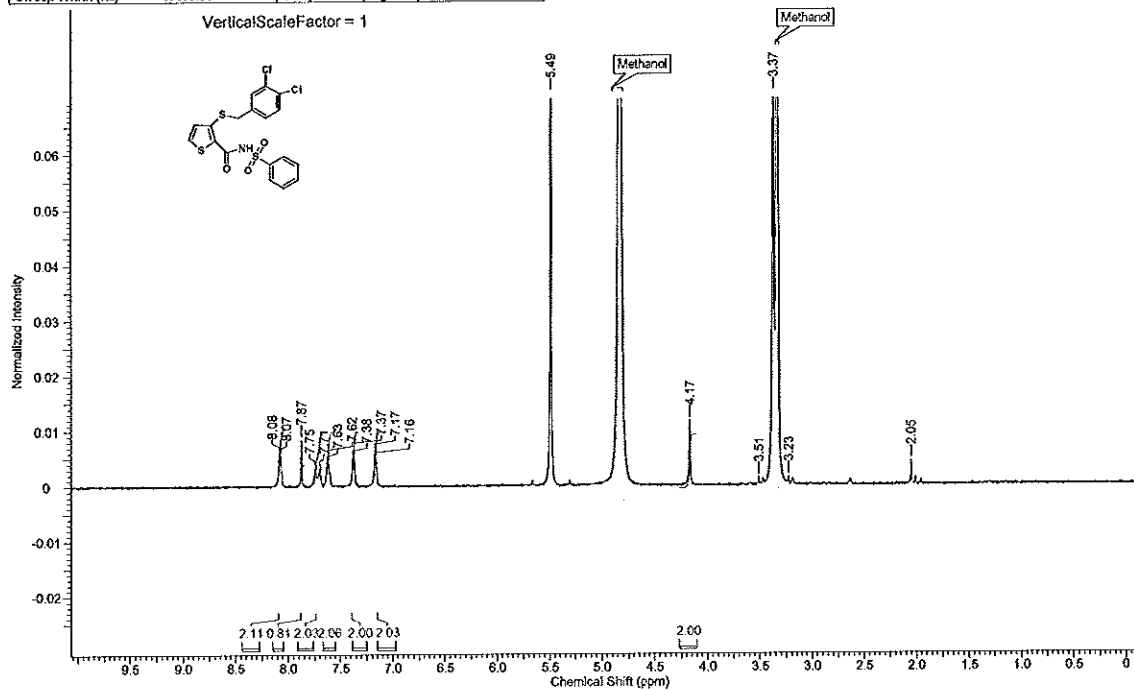
Acquisition Time (sec)	2.7329	Comment	61838-184 proton, d MeOD v zha1w 13	Date	27 Feb 2006 09:57:04
Date Stamp	27 Feb 2006 09:57:04				
File Name	Verucher.wfd pri.bms.com/nmrread1UDX2005-2007/ZHAWW/61838-184_10_DPX-3008.JDX			Frequency (MHz)	300.13
Nucleus	¹ H	Number of Transients	16	Original Points Count	16384
Owner	zha1w	Points Count	16384	Solvent	METHANOL-d4
Sweep Width (Hz)	6995.20			Spectrum Offset (Hz)	2401.8840



H-NMR of Compound 13

1/13/2011 2:52:42 PM

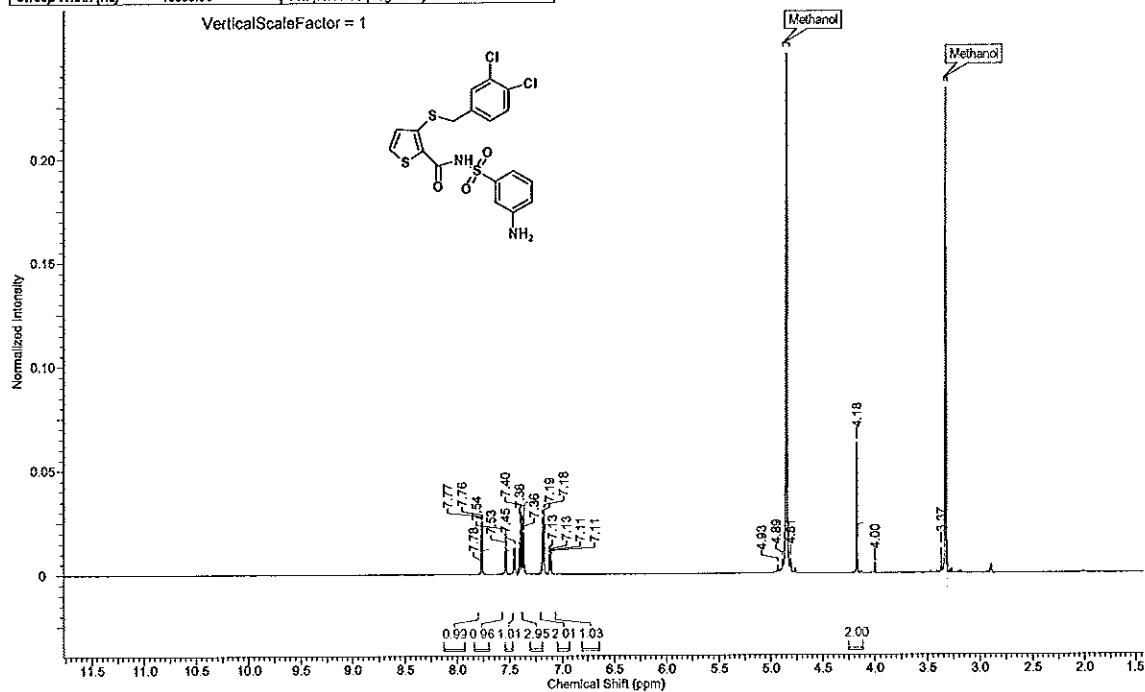
Acquisition Time (sec)	3.2768	Comment	65859-038 proton_d MeOD y zha'w 116	Date	11 Apr 2006 15:57:05
Date Stamp	11 Apr 2006 15:57:05				
File Name	Venucher.wfd pr.bms.com/nmrread1/UDX2005-2007/ZHA'W/65859-038_10_DRX500A.JDX			Frequency (MHz)	500.13
Nucleus	¹ H	Number of Transients	64	Origin	65859-038
Owner	zha'w	Points Count	32768	Solvent	METHANOL-d4
Sweep Width (Hz)	10000.00	Temperature (degree C)	28.160	Spectrum Offset (Hz)	4001.1123



H-NMR of Compound 14

1/13/2011 2:30:52 PM

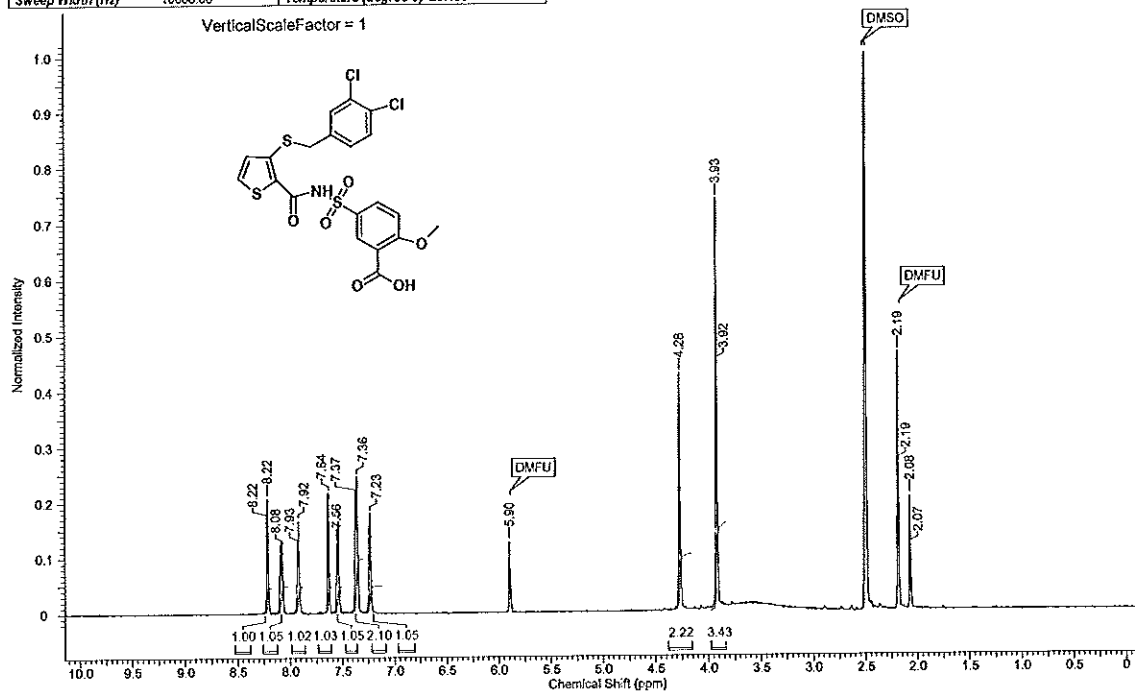
Acquisition Time (sec)	3 2768	Comment	65859-047-02-6 proton, d MeOD v zha'w 63	Date	21 Apr 2006 15:56:44
Data Stamp	21 Apr 2006 15:56:44				
File Name	Voruncher.wfd pri bms com\nmread1\VDX2005-2007\ZHAW\65859-047-2-6_20_DRX500A.JDX			Frequency (MHz)	500.13
Nucleus	¹ H	Number of Transients	16	Origin	65859-047-2-6
Owner	zha'w	Points Count	32768	Solvent	METHANOL-d4
Sweep Width (Hz)	10000.00	Temperature (degree C)	28.160	Original Points Count	32768
				Spectrum Offset (Hz)	4001.1123



H-NMR of Compound 15

1/13/2011 3:33:35 PM

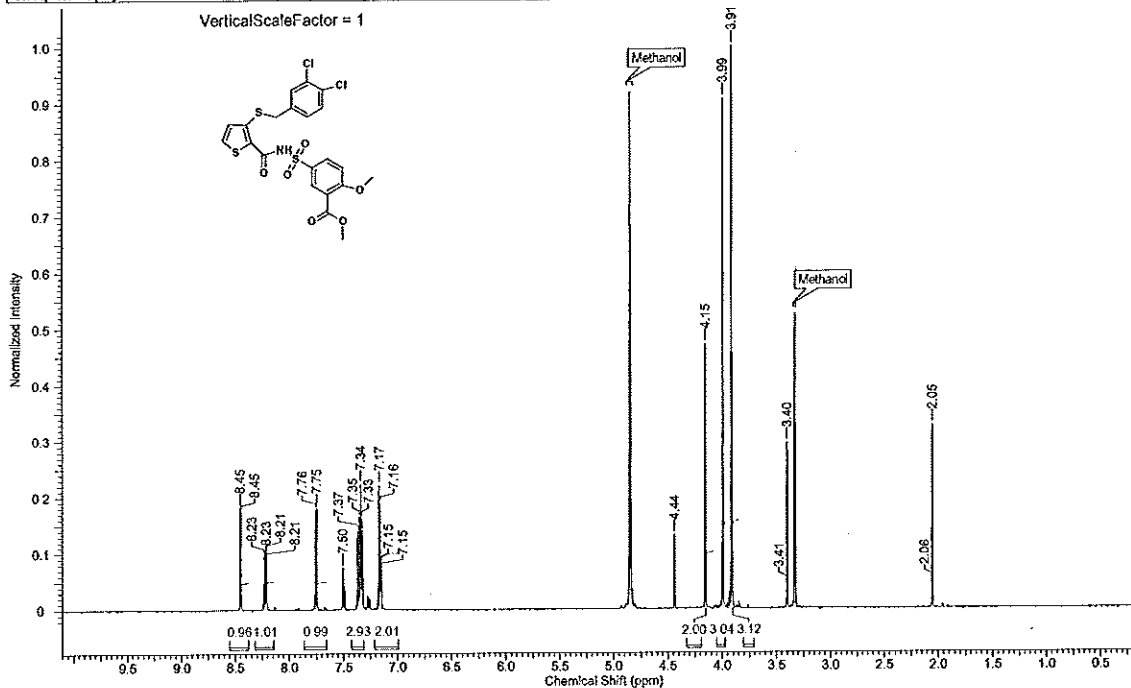
Acquisition Time (sec)	3.2768	Comment	65859-070-02 proton, d DMSO v zha/w 62	Date	19 May 2008 12:37:47
Date Stamp	19 May 2008 12:37:47				
File Name	\\cruncher.wfd.prl.bms.com\innread1\DX2005-2007\ZHA\W\65859-070-02_10_DRX500A.JDX				
Nucleus	¹ H	Number of Transients	16	Origin	65859-070-02
Owner	zha/w	Points Count	32768	Solvent	DMSO-d6
Sweep Width (Hz)	10000.00	Temperature (degree C)	28.160	Frequency (MHz)	500.13
				Original Points Count	32768
				Spectrum Offset (Hz)	3998.6709



H-NMR of Compound 16

1/13/2011 3:38:08 PM

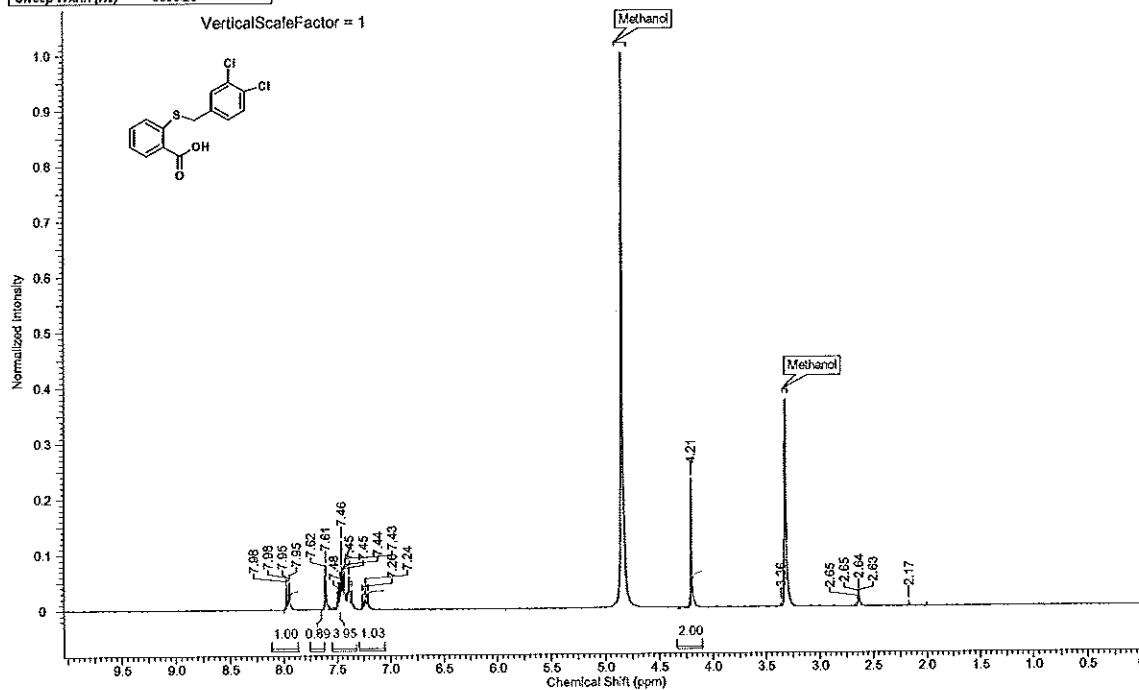
Acquisition Time (sec)	3.2768	Comment	65859-066-03 proton d MeOD v zha1w 20	Date	17 May 2006 09:54:15
Date Stamp	17 May 2006 09:54:15				
File Name	Vcruncher.wfd prbms.com/nmrread1UDX2005-2007ZHAJW65859-066-03_20_DRX500A.JDX			Frequency (MHz)	500.13
Nucleus	¹ H	Number of Transients	16	Origin	65859-066-03
Owner	zha1w	Points Count	32768	Solvent	METHANOL-d4
Sweep Width (Hz)	10000.00	Temperature (degree C)	28.160	Spectrum Offset (Hz)	4001.1123



H-NMR of Compound 17

1/13/2011 3:43:06 PM

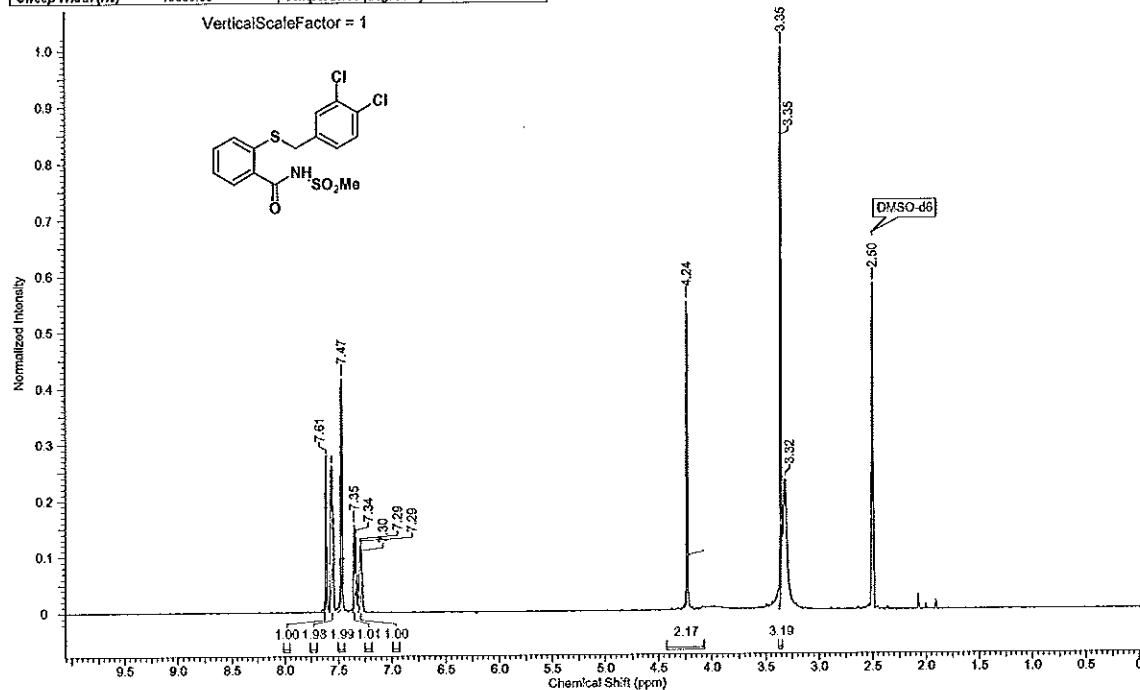
Acquisition Time (sec)	2.7329	Comment	61839-183 proton_d MeOD v zha1w 16	Date	27 Feb 2006 10:25:23
Date Stamp	27 Feb 2006 10:25:23				
File Name	\\cruncher.wfd.prl.bms.com\nmrread\1UDX2005-2007\ZHAI\WV61839-183_10_DPX-300B.JDX			Frequency (MHz)	300.13
Nucleus	1H	Number of Transients	16	Origin	61839-183
Owner	zha1w	Points Count	16384	Solvent	METHANOL-d4
Sweep Width (Hz)	5995.20			Spectrum Offset (Hz)	2401.0340



H-NMR of Compound 18

1/13/2011 3:57:46 PM

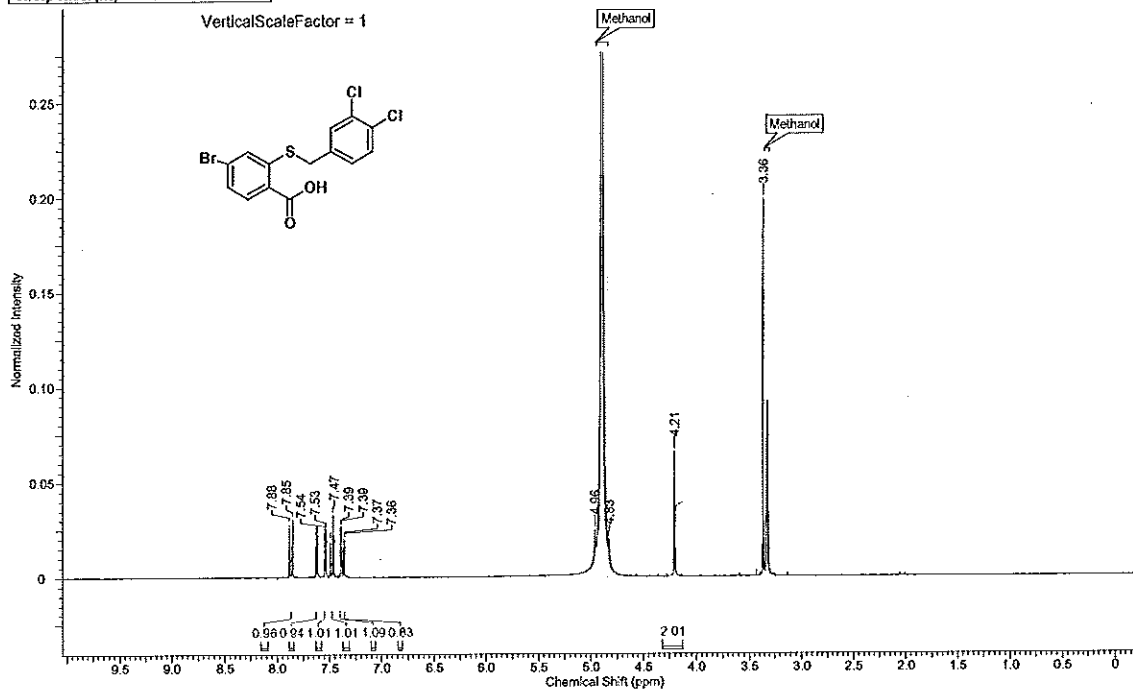
Acquisition Time (sec)	3.2768	Comment	65859-061-01 proton_d DMSO v zha1w80	Date	11 May 2008 14:42:08
Date Stamp	11 May 2008 14:42:08				
File Name	voruncher.wfd.pr.bms.com/tomread1UDX2005-2007VZHA1W155859-061-01_10.DRX500A.JDX			Frequency (MHz)	500.13
Nucleus	¹ H	Number of Transients	16	Origin	65859-061-01
Owner	zha1w	Points Count	32768	Solvent	DMSO-d6
Sweep Width (Hz)	10000.00	Temperature (degree C)	28.160	Spectrum Offset (Hz)	3927.7639



H-NMR of Compound 19

1/13/2011 4:16:08 PM

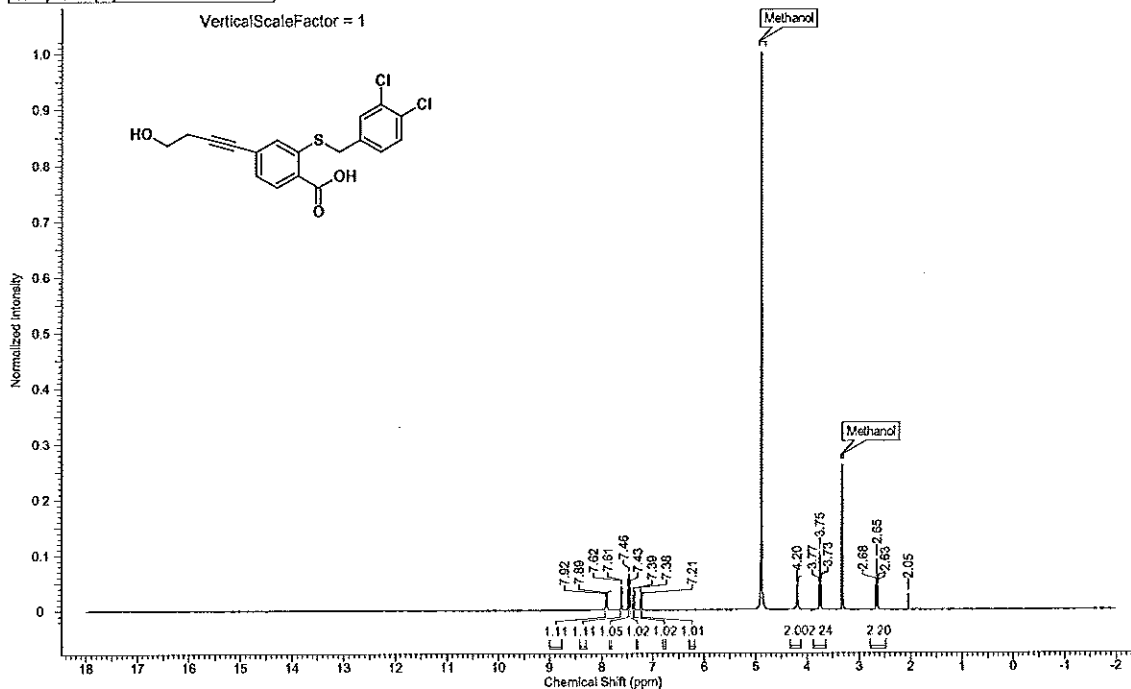
Acquisition Time (sec)	2.7329	Comment	65859-119 proton_d MeOD v zhaW 78	Date	14 Jul 2006 11:24:15
Date Stamp	14 Jul 2006 11:24:15	File Name	Venricher.wfd pri bms.com\rmread\1\NDX2005-2007\ZHA\W\65859-119_19_DPX-300B.JDX	Frequency (MHz)	300.13
Nucleus	¹ H	Number of Transients	16	Origin	65859-119
Owner	zhaW	Points Count	16384	Solvent	METHANOL-d4
Sweep Width (Hz)	6995.20			Spectrum Offset (Hz)	2401.0840



H-NMR of Compound 20

1/13/2011 4:20:24 PM

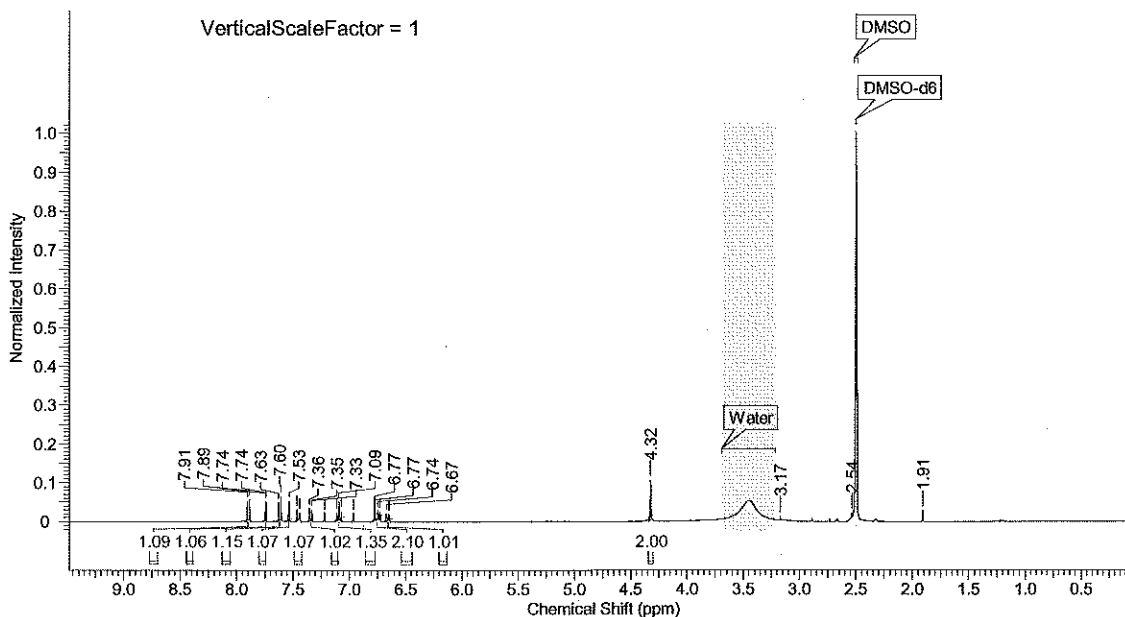
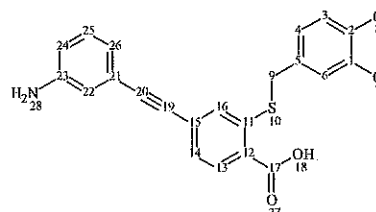
Acquisition Time (sec)	2.7329	Comment	65859-187-02 proton d MeOD v zha'w 78	Date	05 Oct 2006 13:13:39
Date Stamp	05 Oct 2006 13:13:30				
File Name	W:\nchrer.wfd.pri.bms.com\rmread\UDX2005-2007\ZHAI\W\65859-187-02_10_DPX-300B.JDX			Frequency (MHz)	300.13
Nucleus	¹ H	Number of Transients	80	Origin	65859-187-02
Owner	zha'w	Points Count	16384	Solvent	METHANOL-d4
Sweep Width (Hz)	5995.20			Original Points Count	16384
				Spectrum Offset (Hz)	2491.0840



1H-NMR of Compound 21

1/11/2011 4:44:10 PM

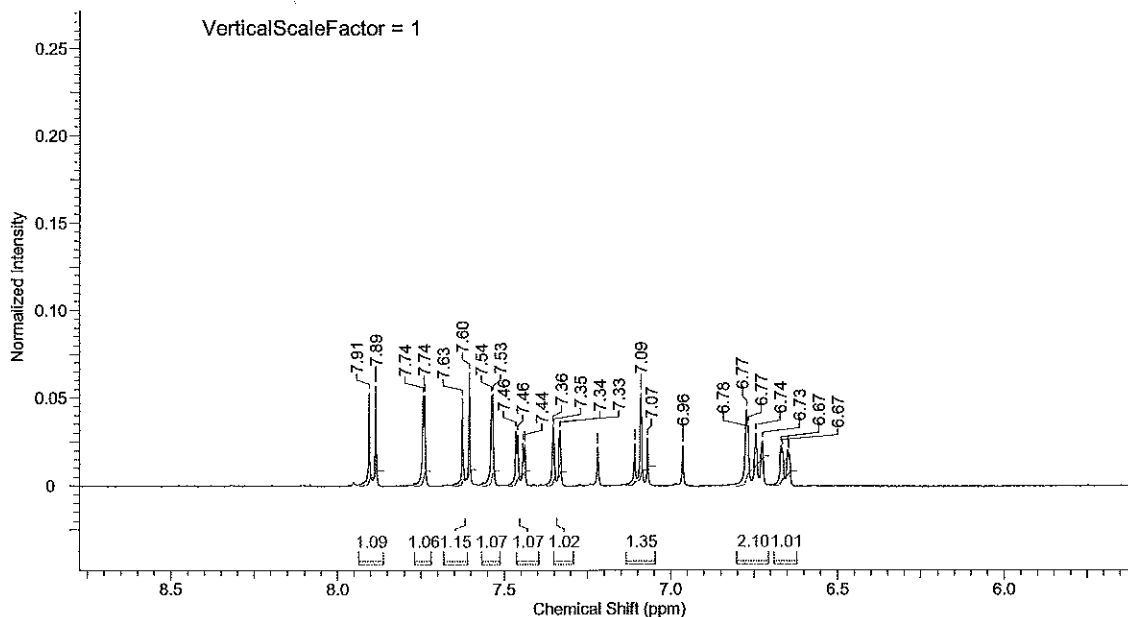
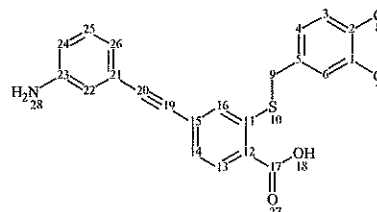
Formula	C ₂₂ H ₁₈ Cl ₂ NO ₂ S	FW	428.3310
Acquisition Time (sec)	3.9847	Comment	86453-003 proton_d np DMSO /v zhus 57
Date	06 Apr 2010 16:48:17	Date Stamp	06 Apr 2010 16:48:17
File Name	\\CRUNCHER.WFD.PRJ.BMS.COM\NMR\READ1\JDX2008-2010\zhus\86453-003_10_AV400.jdx		
Frequency (MHz)	400.13	Nucleus	1H
Origin	86453-003	Original Points Count	32768
Points Count	32768	Solvent	DMSO-d6
Sweep Width (Hz)	8223.43	Temperature (degree C)	27.000
		Number of Transients	64
		Owner	zhus
		Spectrum Offset (Hz)	3197.9250



1H-NMR of Compound 21

1/11/2011 4:47:18 PM

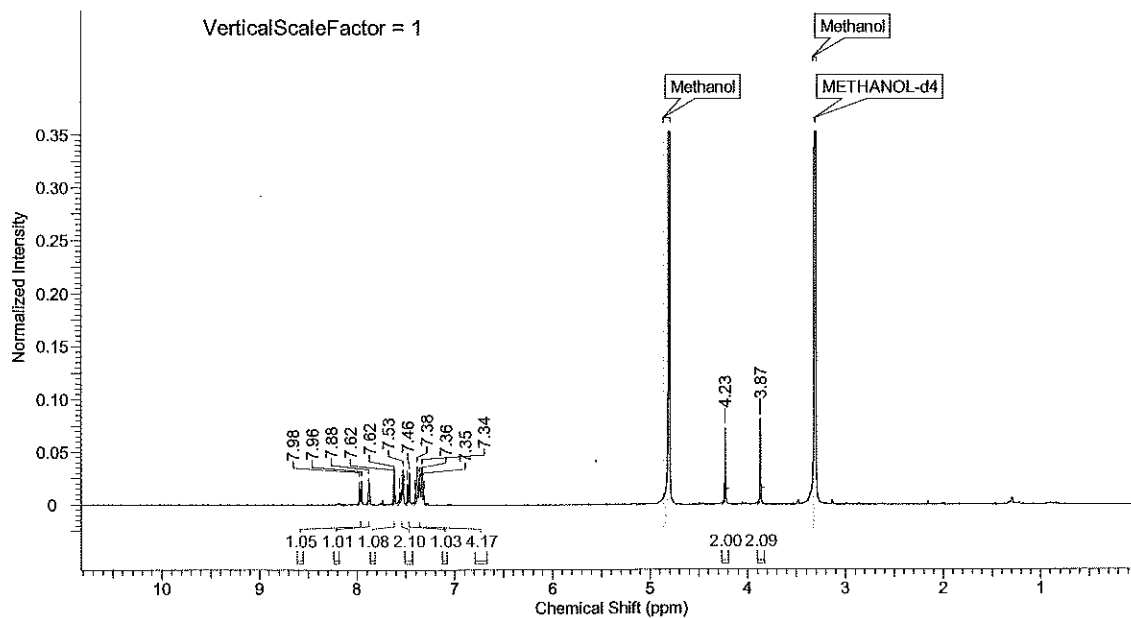
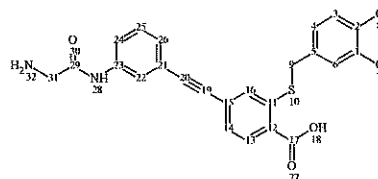
Formula	C ₂₂ H ₁₆ Cl ₂ NO ₂ S	FW	428.3310
Acquisition Time (sec)	3.9847	Comment	86453-003 proton_d_np DMSO /v zhus 57
Date	06 Apr 2010 16:48:17	Date Stamp	06 Apr 2010 16:48:17
File Name	\\CRUNCHER.WFD.PRI.BMS.COM\NMR\READ1\JDX2008-2010\zhus\86453-003_10_AV400.jdx		
Frequency (MHz)	400.13	Nucleus	1H
Origin	86453-003	Original Points Count	32768
Points Count	32768	Solvent	DMSO-d6
Sweep Width (Hz)	8223.43	Temperature (degree C)	27.000
		Number of Transients	64
		Owner	zhus
		Spectrum Offset (Hz)	3197.9250



1H-NMR of Compound 22

1/11/2011 11:40:48 AM

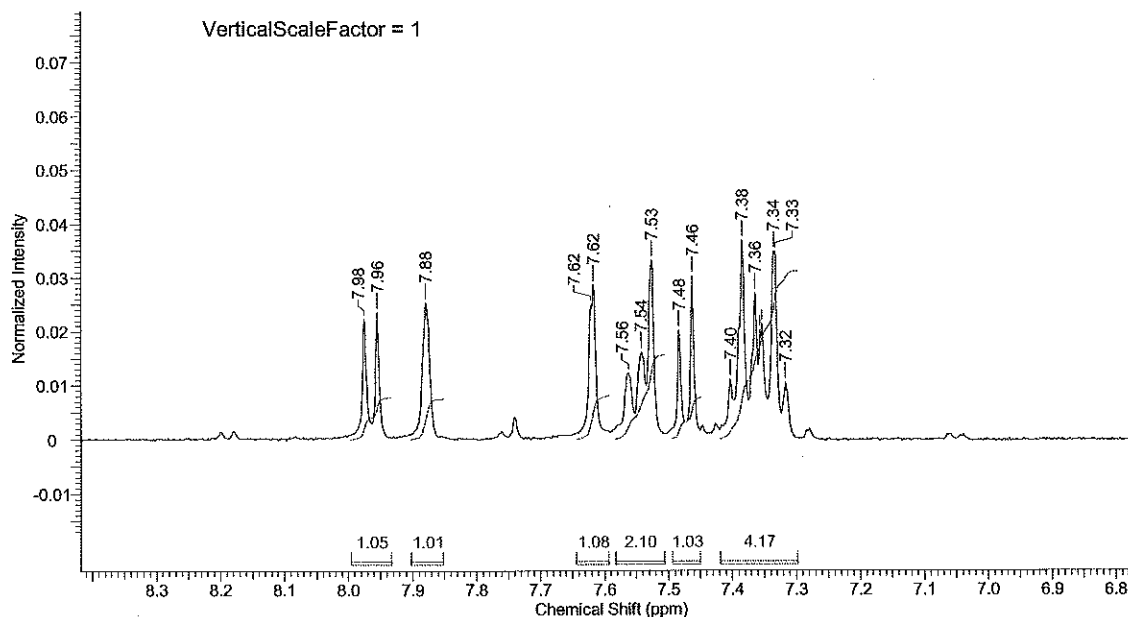
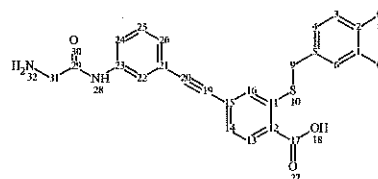
Formula C ₂₄ H ₁₈ Cl ₂ N ₂ O ₃ S		FW 485.3823	
Acquisition Time (sec)	3.9847	Comment	
Date	17 Apr 2010 13:30:58	Date Stamp	17 Apr 2010 13:30:58
File Name			
Frequency (MHz)	400.13	Nucleus	1H
Origin		Original Points Count	32768
Points Count	32768	Solvent	METHANOL-d4
Sweep Width (Hz)	8223.43	Temperature (degree C)	27.000
		Number of Transients	128
		Owner	zhush
		Spectrum Offset (Hz)	3193.2664



1H-NMR of Compound 22

1/11/2011 11:46:32 AM

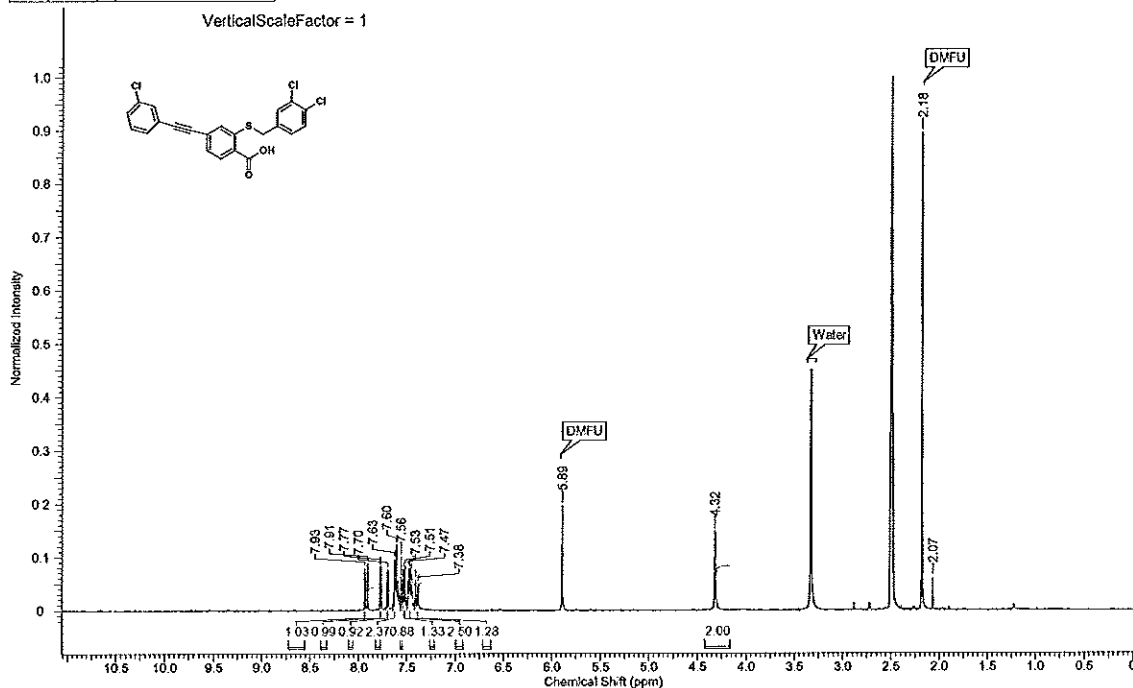
Formula C ₂₄ H ₁₅ Cl ₂ N ₂ O ₃ S		FW 485.3823	
Acquisition Time (sec)	3.9847	Comment	
Date	17 Apr 2010 13:30:58	Date Stamp	17 Apr 2010 13:30:58
File Name			
Frequency (MHz)	400.13	Nucleus	1H
Origin		Original Points Count	32768
Points Count	32768	Solvent	METHANOL-d4
Sweep Width (Hz)	8223.43	Temperature (degree C)	27.000
		Number of Transients	128
		Owner	zhus
		Spectrum Offset (Hz)	3193.2664



H-NMR of Compound 23

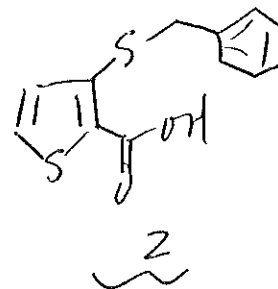
1/13/2011 4:31:48 PM

Acquisition Time (sec)	2.7329	Comment	66596-031-05 proton, d DMSO v zha'w 38	Date	12 Jan 2007 14:36:37
Date Stamp	12 Jan 2007 14:36:37				
File Name	Voruncher.wfd.prl.bms.com\rmread1\UDX2005-2007\ZHA\W\66596-031-05_10_DPX-3008.JDX			Frequency (MHz)	300.13
Nucleus	¹ H	Number of Transients	80	Origin	66596-031-05
Owner	zha'w	Points Count	16384	Solvent	DMSO-d6
Sweep Width (Hz)	6995.20			Spectrum Offset (Hz)	2398.6438

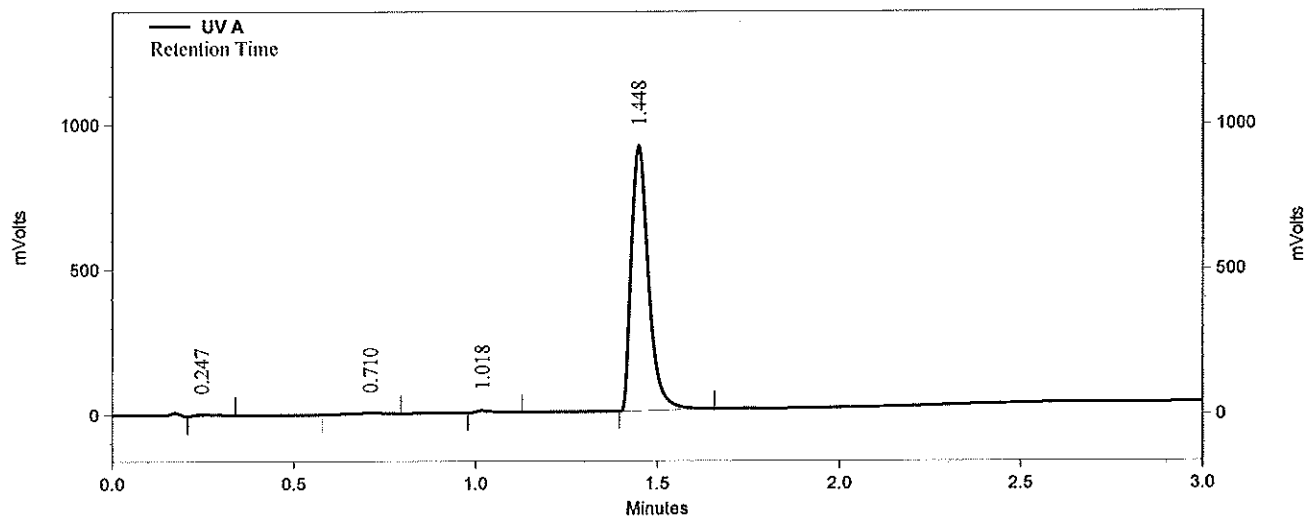


Analytical HPLC Report

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 Sample ID: = 61838-143-01
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 File = 2011_0713_1602.047
 User = weixu.zhai
 Instrument = WFD-409D-LCMS3
 Well = 188 Inj. Vol. = 3 uL
 Start % B = 0
 Final % B = 100
 Gradient Time = 2 min
 Flow Rate = 1 ml/min
 Wavelength = 220
 Solvent Pair = Water/ Acetonitrile/ 0.1%TFA
 Solvent A = 90% Water/ 10% Acetonitrile/ 0.1%TFA
 Solvent B = 10% Water/ 90% Acetonitrile/ 0.1%TFA
 Column 1 = 1.) Phenomenex LUNA C18, 30x2, 3u
 MW1 = 132+
 Oven Temp. = 40



61838-143-01



UV A Results

Pk #	RT	Area	Area %	Height (uV)	Plates
1	0.247	22096	0.726	5815	94
2	0.710	20783	0.682	2891	239
3	1.018	22402	0.736	7747	3082
4	1.448	2980064	97.856	911696	4774

Totals		3045345	100.000	928149	
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Sample: 1

Vial: 1:A, 1

ID: 61838-143-01

File: 2011_0713_1602-047

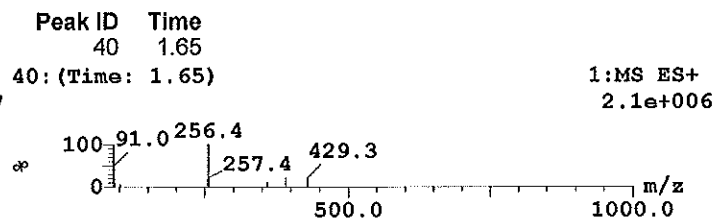
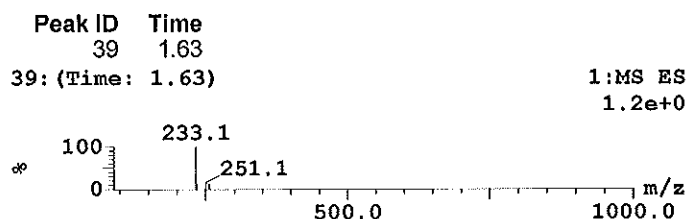
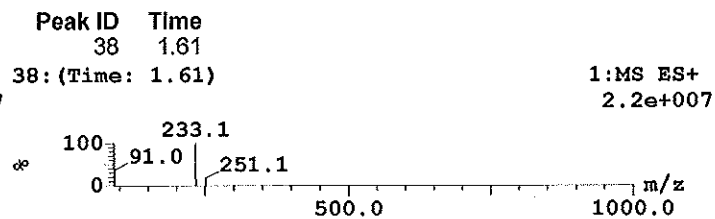
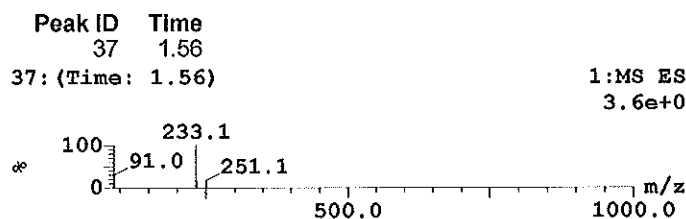
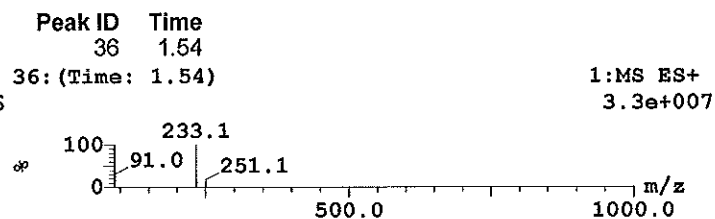
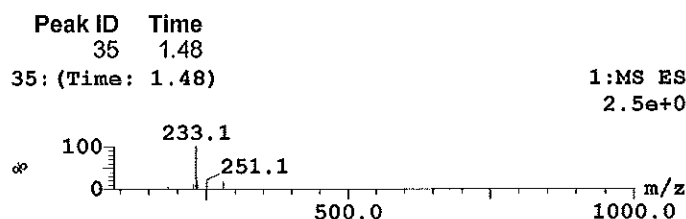
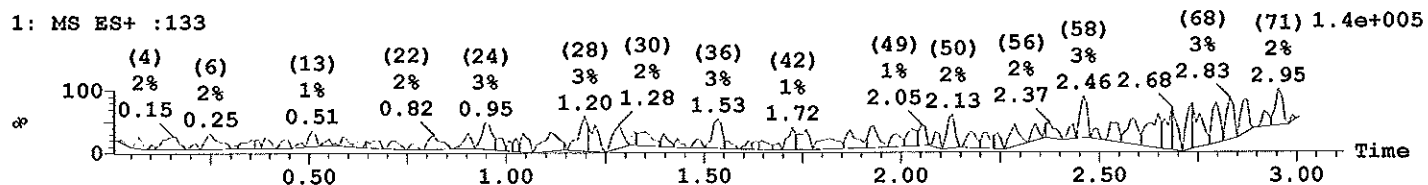
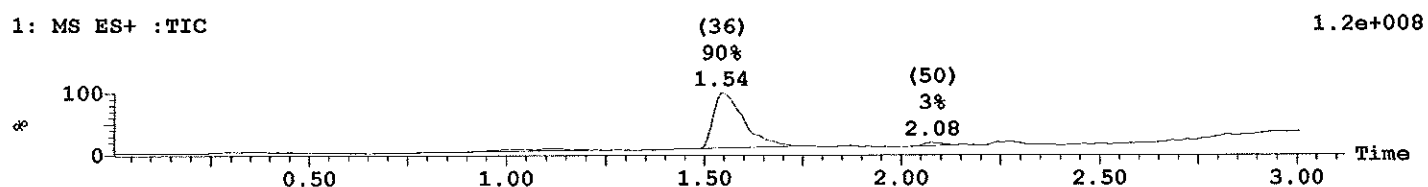
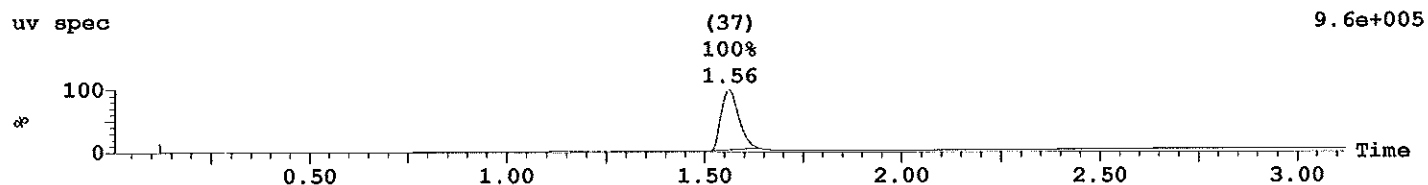
Date: 13-Jul-2011

Time: 16:04:04

Description:

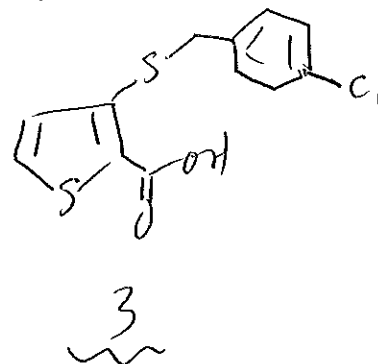
Printed: Wed Jul 13 16:11:13 2011

Sample Report:

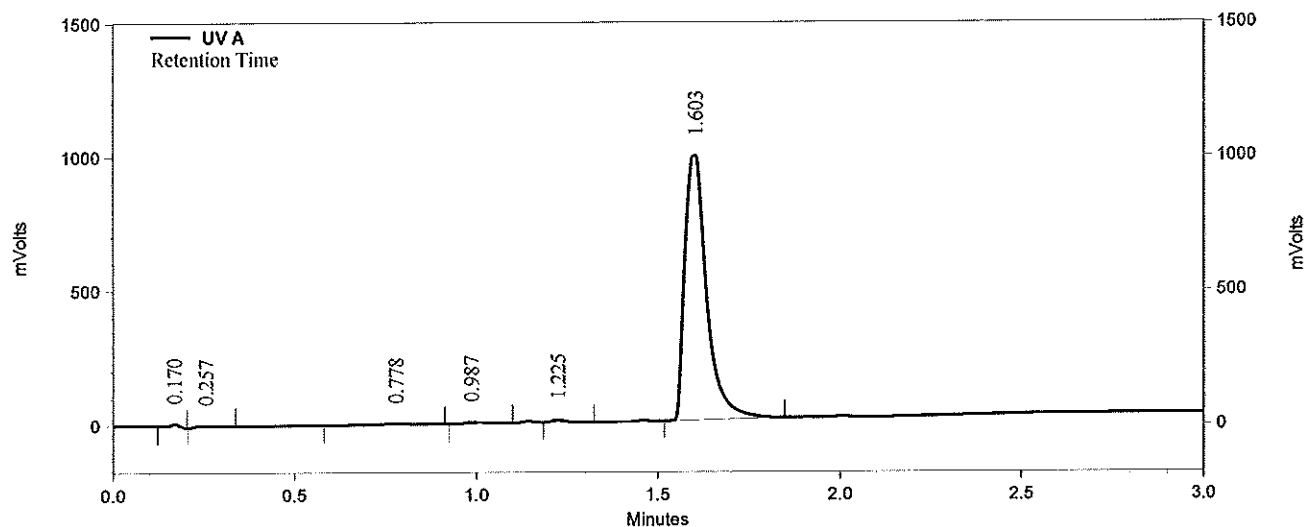


Analytical HPLC Report

File: =
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 File = 2011_0713_1611.048
 User = weixu.zhai
 Instrument = WFD-409D-LCMS3
 Well = 189 Inj. Vol. = 3 uL
 Start % B = 0
 Final % B = 100
 Gradient Time = 2 min
 Flow Rate = 1 ml/min
 Wavelength = 220
 Solvent Pair = Water/ Acetonitrile/ 0.1%TFA
 Solvent A = 90% Water/ 10% Acetonitrile/ 0.1%TFA
 Solvent B = 10% Water/ 90% Acetonitrile/ 0.1%TFA
 Column 1 = 1.) Phenomenex LUNA C18, 30x2, 3u
 MWl = 132+
 Oven Temp. = 40



61838-143-13



UV A Results

Pk #	RT	Area	Area %	Height (uV)	Plates
1	0.170	21287	0.505	10984	191
2	0.257	23439	0.556	5135	72
3	0.778	31205	0.741	3015	132
4	0.987	24962	0.593	5516	886
5	1.225	23775	0.564	8112	4519
6	1.603	4087587	97.040	982329	4147

Totals		4212255	100.000	1015091	
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Sample: 1

Vial: 1:A,1

ID: 61838-143-13

File: 2011_0713_1611-048

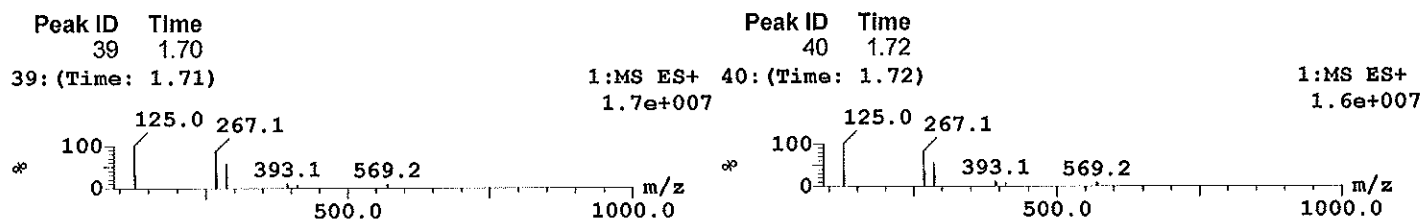
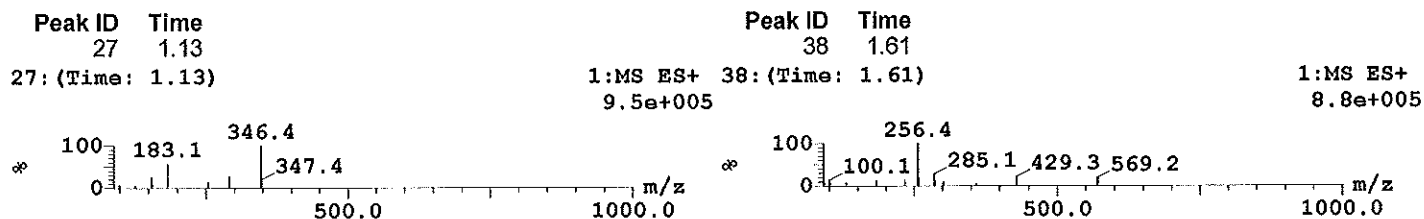
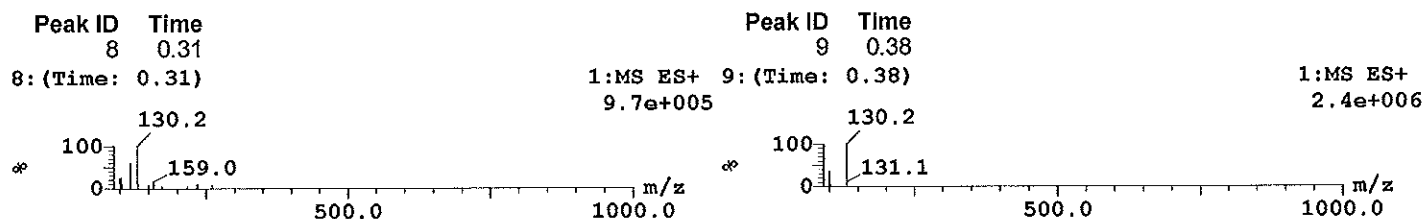
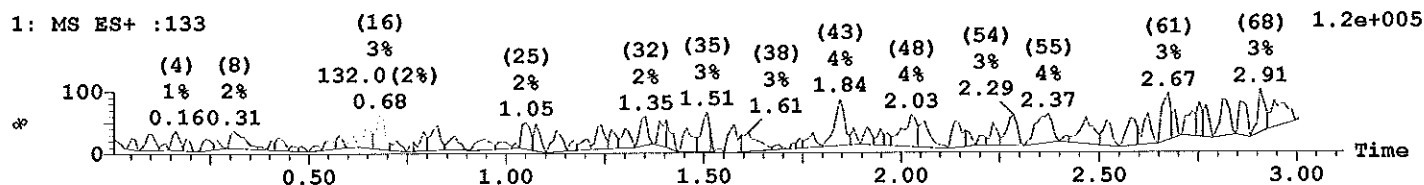
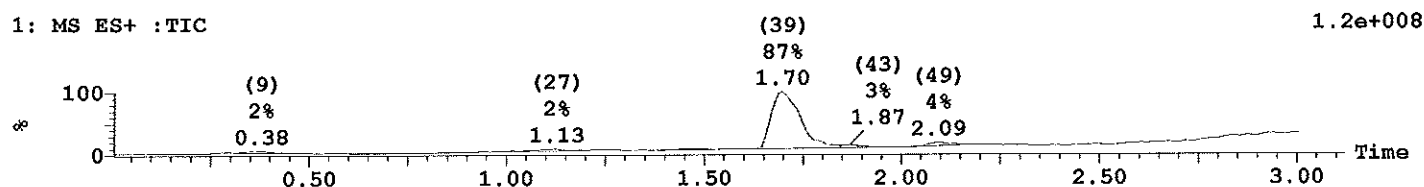
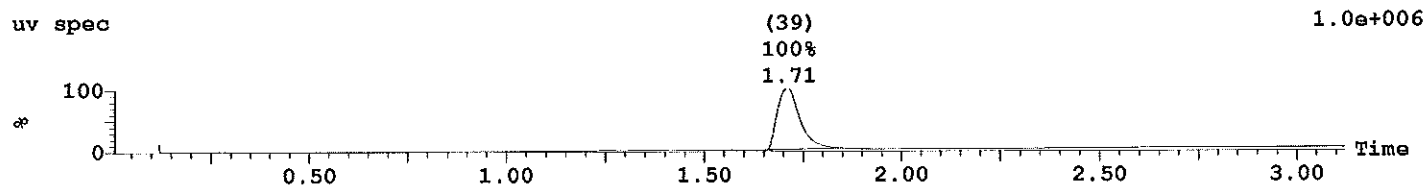
Date: 13-Jul-2011

Time: 16:12:01

Description:

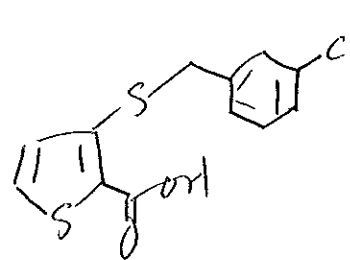
Printed: Wed Jul 13 16:18:56 2011

Sample Report:



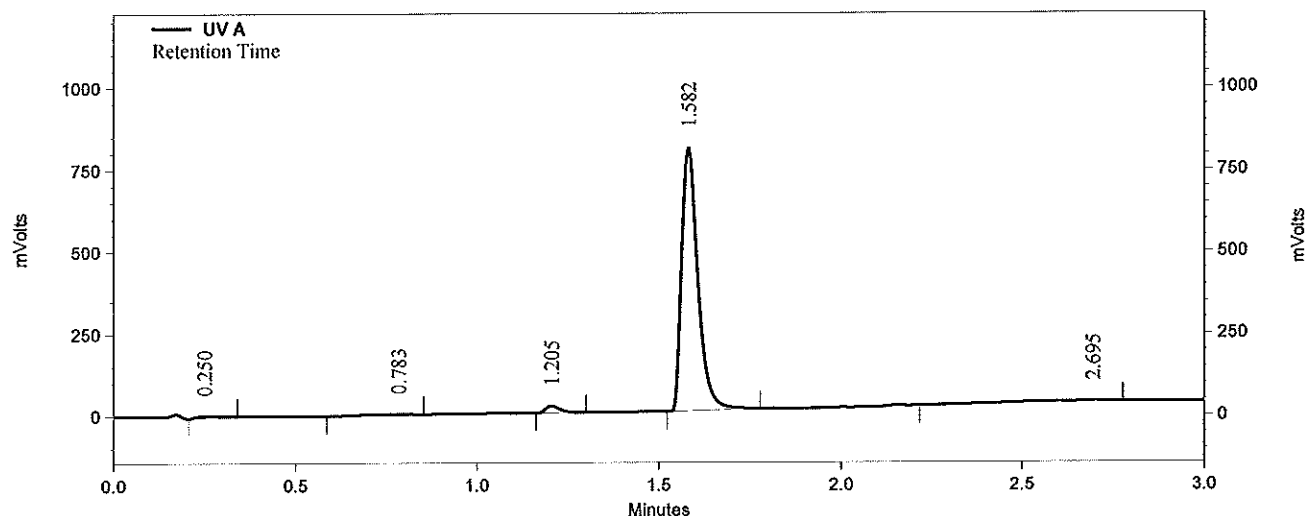
Analytical HPLC Report

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 File = 2011_0713_1619.049
 User = weixu.zhai
 Instrument = WFD-409D-LCMS3
 Well = 190 Inj. Vol. = 3 uL
 Start % B = 0
 Final % B = 100
 Gradient Time = 2 min
 Flow Rate = 1 ml/min
 Wavelength = 220
 Solvent Pair = Water/ Acetonitrile/ 0.1%TFA
 Solvent A = 90% Water/ 10% Acetonitrile/ 0.1%TFA
 Solvent B = 10% Water/ 90% Acetonitrile/ 0.1%TFA
 Column 1 = 1.) Phenomenex LUNA C18, 30x2, 3u
 MW1 = 132+
 Oven Temp. = 40



4

61838-143-08



UV A Results

PK #	RT	Area	Area %	Height (uV)	Plates
1	0.250	22941	0.862	5516	82
2	0.783	22672	0.852	2193	164
3	1.205	57716	2.169	20589	4292
4	1.582	2489563	93.570	800701	6227
5	2.695	67750	2.546	3754	0
Totals		2660642	100.000	832753	

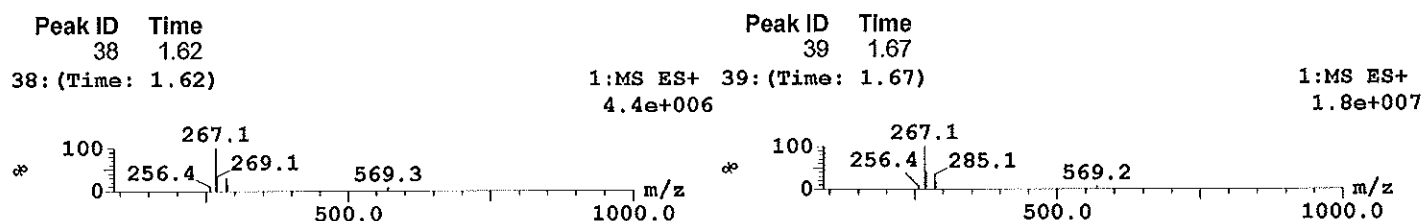
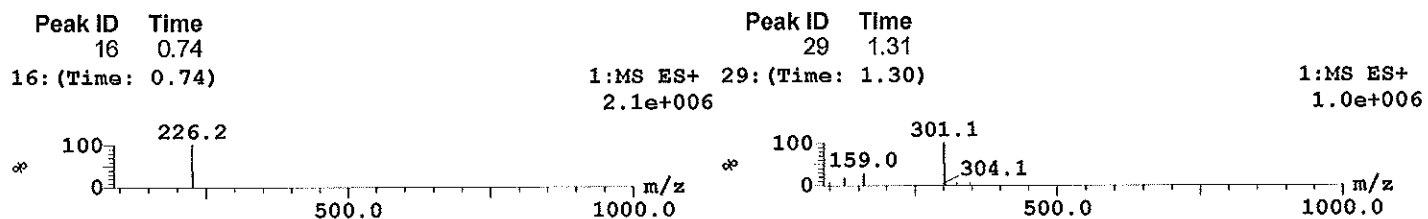
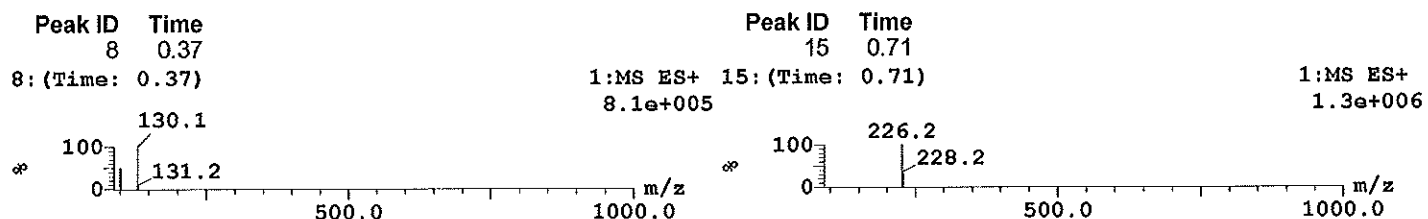
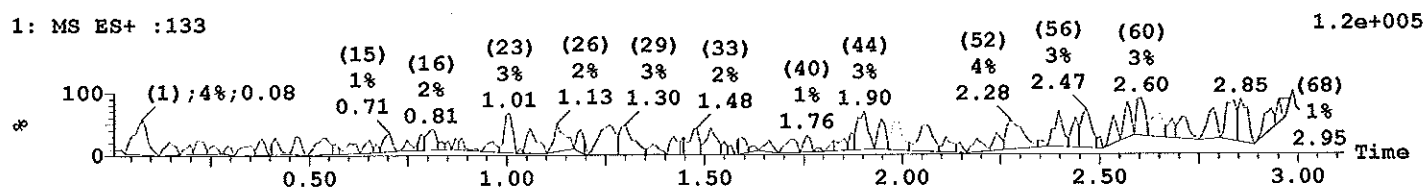
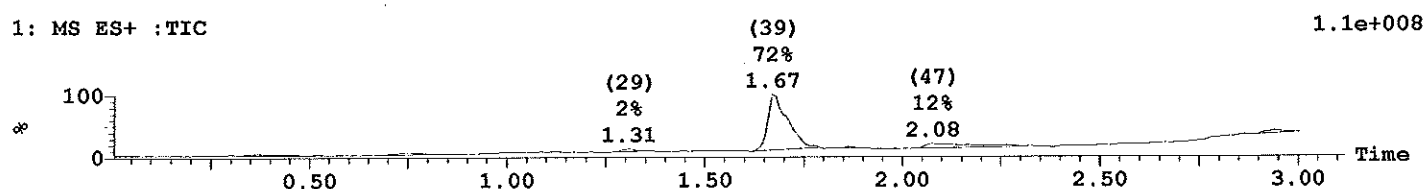
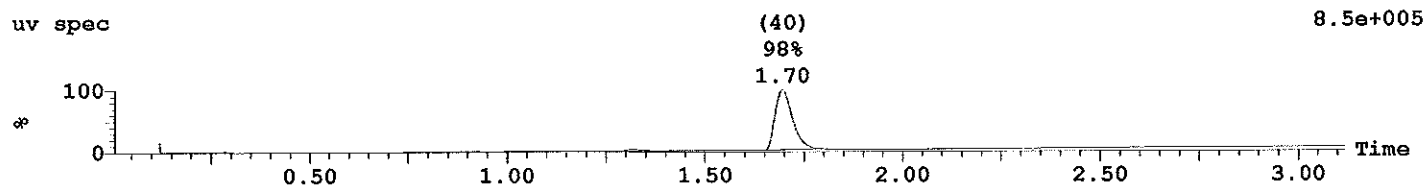
Sample: 1
File:2011_0713_1619-049
Description:

Vial:1:A,1
Date:13-Jul-2011

ID:61838-143-08
Time:16:19:41

Printed: Wed Jul 13 16:26:41 2011

Sample Report:



Sample: 1
File:2011_0713_1619-049
Description:

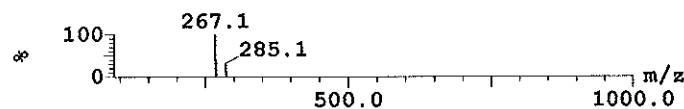
Vial:1:A,1
Date:13-Jul-2011

ID:61838-143-08
Time:16:19:41

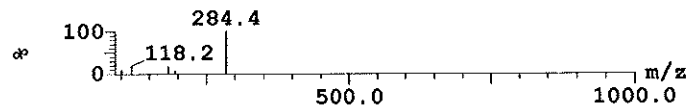
Printed: Wed Jul 13 16:26:41 2011

Sample Report (continued):

Peak ID Time
40 1.72
40: (Time: 1.70)

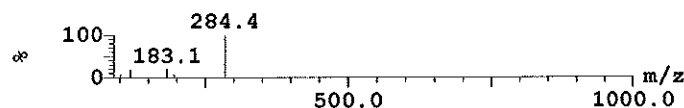


Peak ID Time
42 1.86
1:MS ES+ 42: (Time: 1.86)
2.0e+007

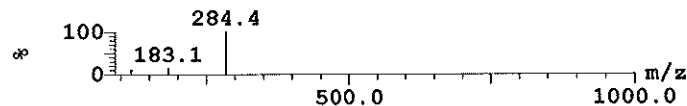


1:MS ES+
1.1e+006

Peak ID Time
43 1.87
43: (Time: 1.87)

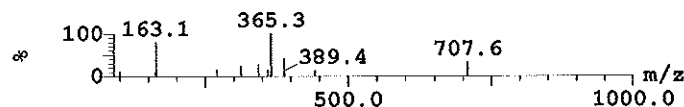


Peak ID Time
44 1.90
1:MS ES+ 44: (Time: 1.90)
1.1e+006

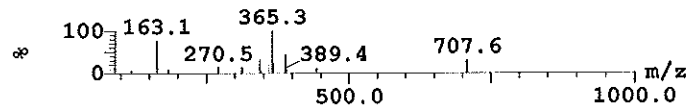


1:MS ES+
1.1e+006

Peak ID Time
47 2.08
47: (Time: 2.08)

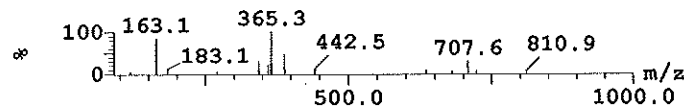


Peak ID Time
48 2.11
1:MS ES+ 48: (Time: 2.11)
1.1e+006

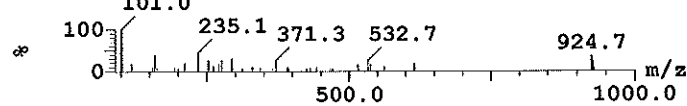


1:MS ES+
1.3e+006

Peak ID Time
49 2.15
49: (Time: 2.15)

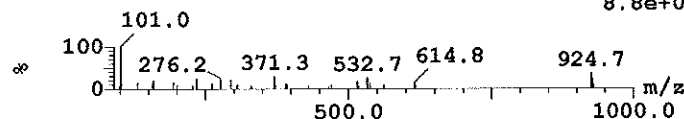


Peak ID Time
67 2.94
1:MS ES+ 67: (Time: 2.94)
9.0e+005



1:MS ES+
1.0e+006

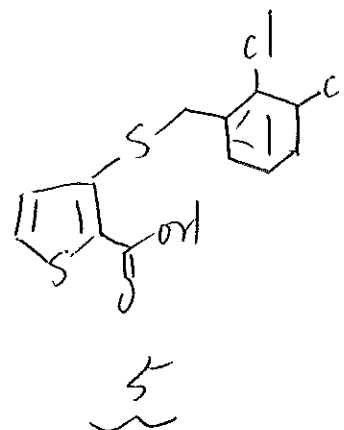
Peak ID Time
68 2.95
68: (Time: 2.95)



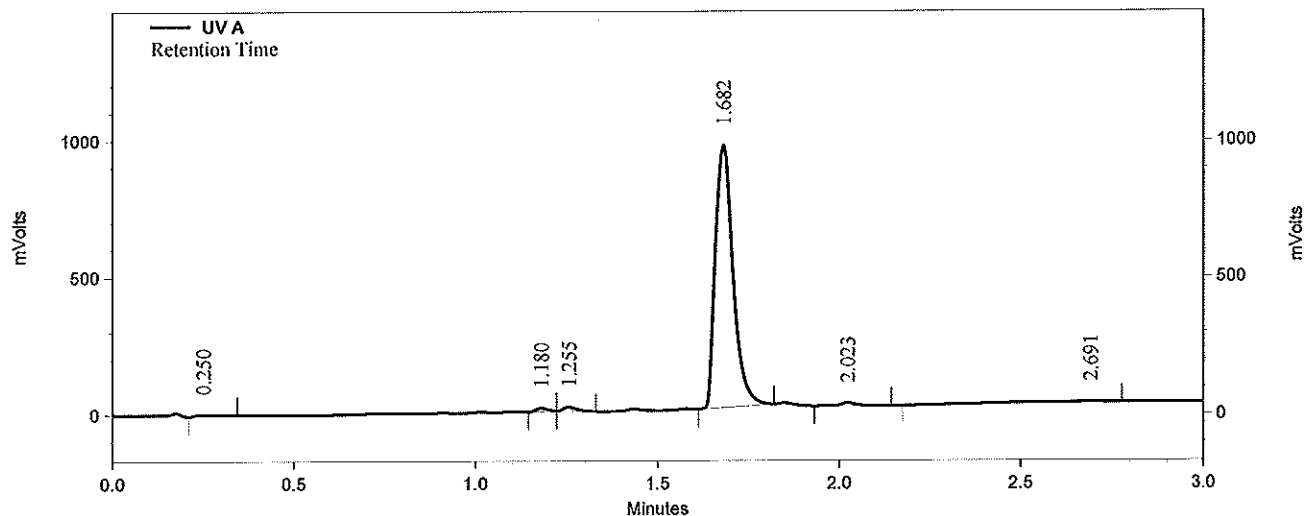
1:MS ES+
8.8e+005

Analytical HPLC Report

File: =
 c:\shimadzu\data\public\weixu.zhai\20110713\2011_0713_1627-050.dat
 Sample ID: = 61838-144-25
 Acquired: = 7/13/2011 4:30:32 PM
 File = 2011_0713_1627.050
 User = weixu.zhai
 Instrument = WFD-409D-LCMS3
 Well = 191 Inj. Vol. = 3 uL
 Start % B = 0
 Final % B = 100
 Gradient Time = 2 min
 Flow Rate = 1 ml/min
 Wavelength = 220
 Solvent Pair = Water/ Acetonitrile/ 0.1%TFA
 Solvent A = 90% Water/ 10% Acetonitrile/ 0.1%TFA
 Solvent B = 10% Water/ 90% Acetonitrile/ 0.1%TFA
 Column 1 = 1.) Phenomenex LUNA C18, 30x2, 3u
 MW1 = 132+
 Oven Temp. = 40



61838-144-25



UV A Results

Pk #	RT	Area	Area %	Height (uV)	Plates
1	0.250	21720	0.630	5352	85
2	1.180	26752	0.775	11947	5848
3	1.255	36299	1.052	14190	5310
4	1.682	3260108	94.489	956042	5863
5	2.023	29600	0.858	10673	14205
6	2.691	75787	2.197	3555	366

Totals		3450266	100.000	1001759	
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Sample: 1

Vial: 1:A, 1

ID: 61838-144-25

File: 2011_0713_1627-050

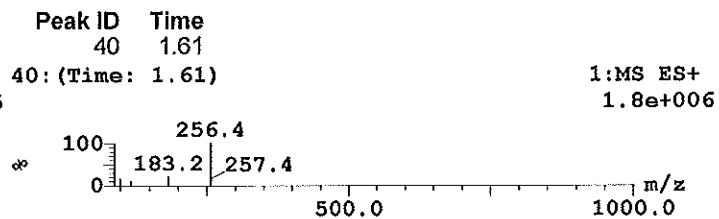
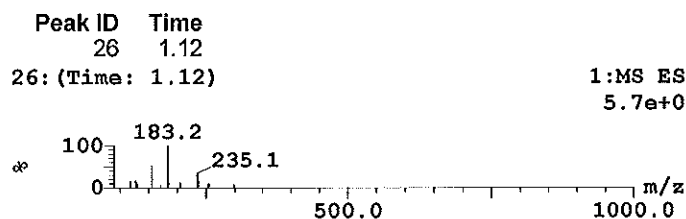
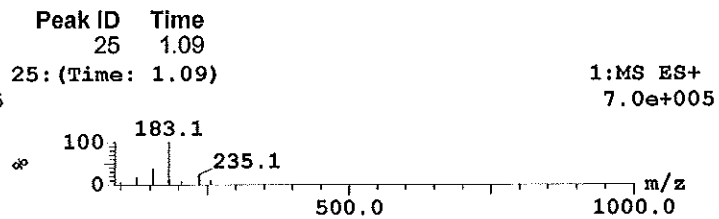
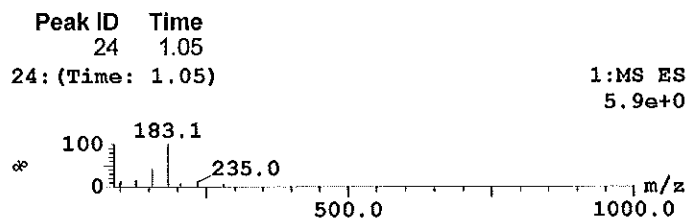
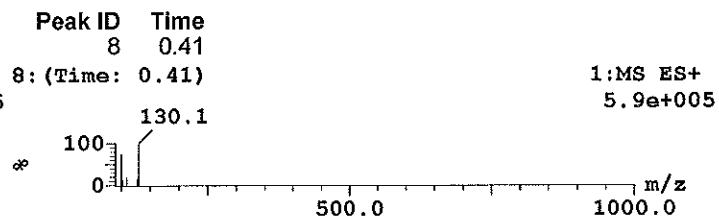
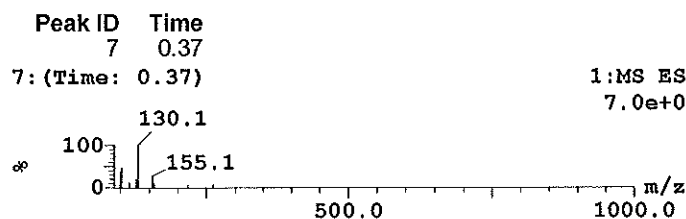
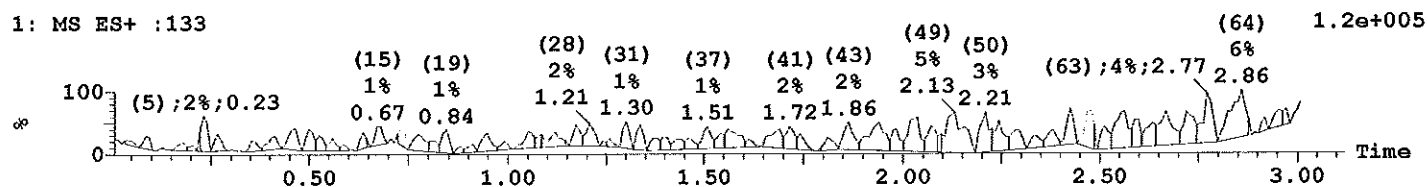
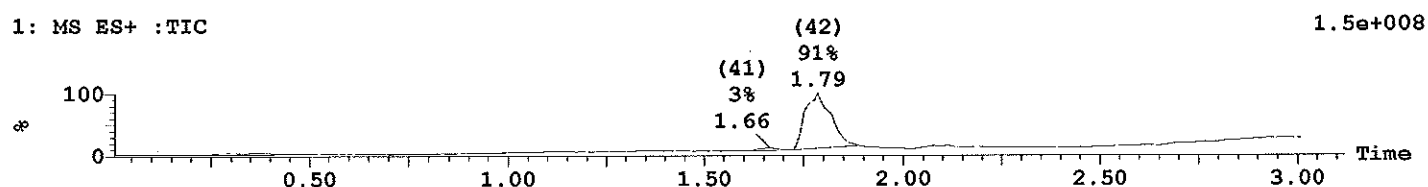
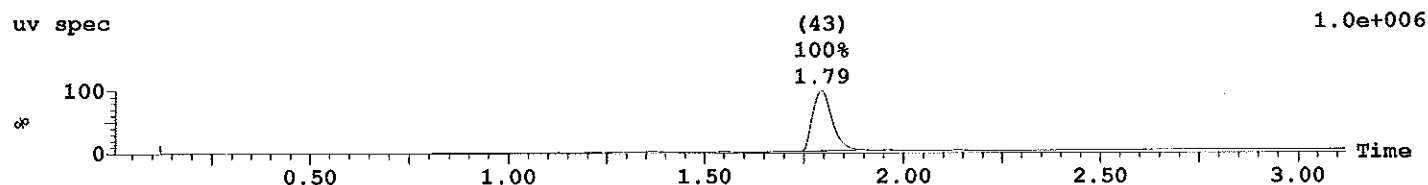
Date: 13-Jul-2011

Time: 16:27:27

Description:

Printed: Wed Jul 13 16:34:24 2011

Sample Report:



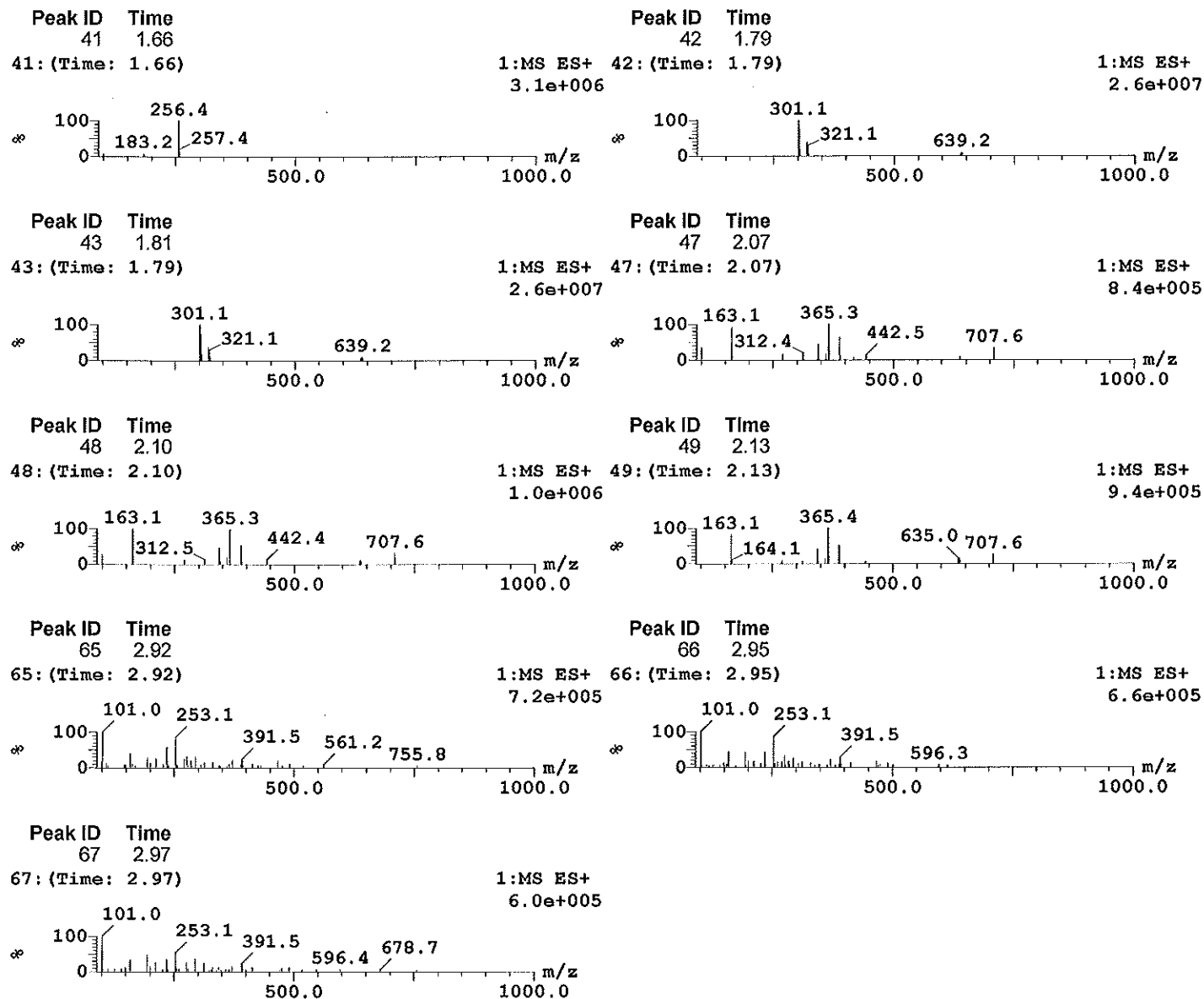
Sample: 1
File:2011_0713_1627-050
Description:

Vial:1:A,1
Date:13-Jul-2011

ID:61838-144-25
Time:16:27:27

Printed: Wed Jul 13 16:34:24 2011

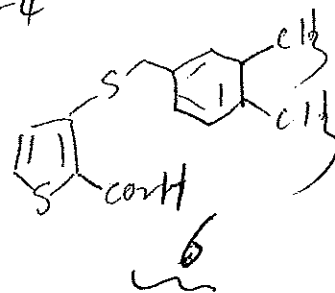
Sample Report (continued):



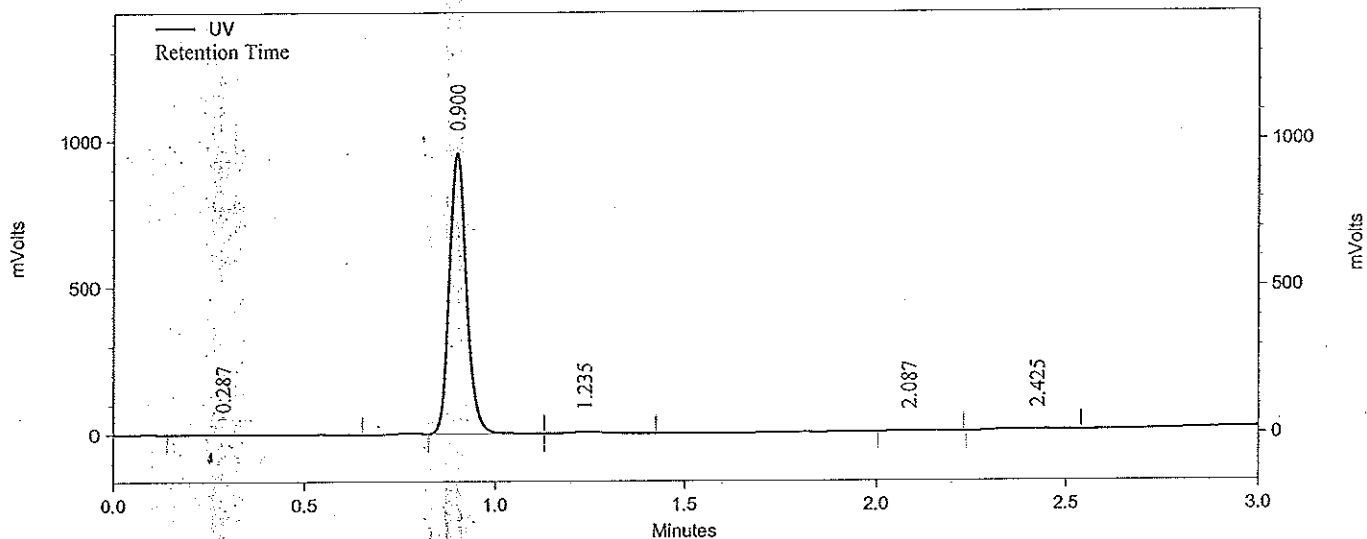
Analytical HPLC Report

File: = C:\CLASS-VP\CHROM\0206R.014
 Sample ID: = 4-24 MW 278
 Acquired: = 2/7/2006 10:02:36 AM
 User = weixu.zhai
 Instrument = WFD-409D-LCMS2
 Well = 192 Inj. Vol. = 10 uL
 Start % B = 0
 Final % B = 100
 Gradient Time = 2 min
 Flow Rate = 5 ml/min
 Wavelength = 220
 Solvent A = H2O : ACN 95% : 5% 10 mm Ammonium Acetate
 Solvent B = H2O : ACN 5% : 95% 10 mm Ammonium Acetate
 Column 2 = LUNA 3.0 x 50MM S10

61838-172-4



4-24



UV Results

Pk #	RT	Area	Area %	Height (uV)	Plates
1	0.287	29125	0.933	1744	6
2	0.900	3002558	96.218	955525	1920
3	1.235	26825	0.860	5018	1505
4	2.087	20501	0.657	2461	1609
5	2.425	41571	1.332	3512	1210

Totals		3120580	100.000	968260	
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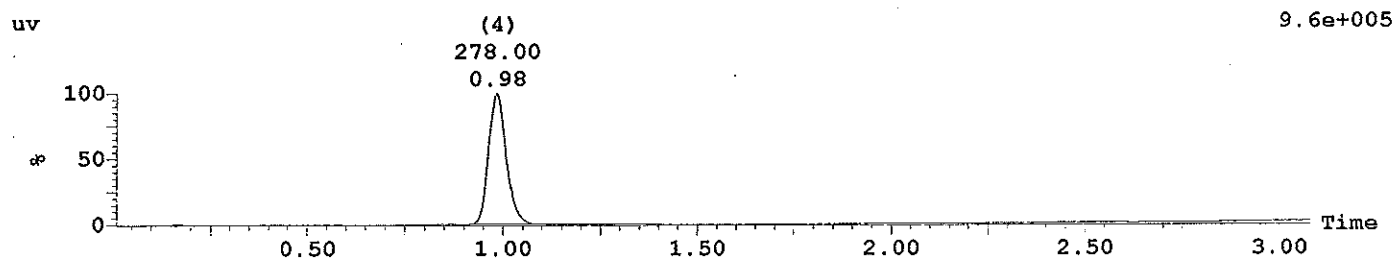
Sample: 1
File:0206R014
Description:

Vial:1:A,1
Date:07-Feb-2006

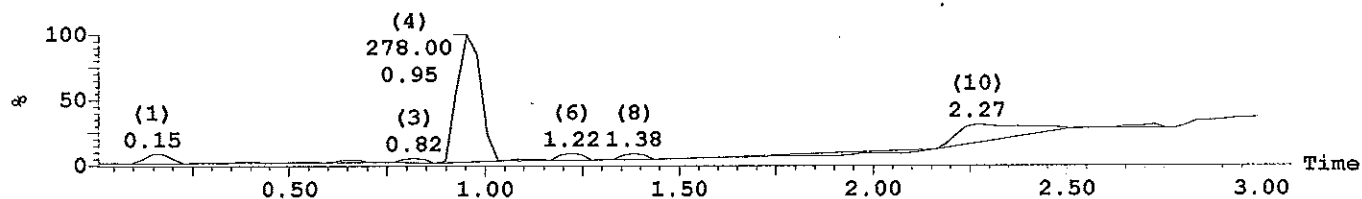
ID:4-24
Time:09:56:27

Printed: Tue Feb 07 10:02:20 2006

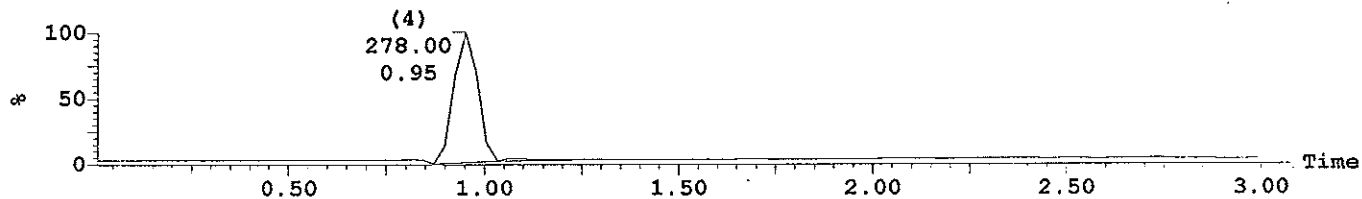
Sample Report:



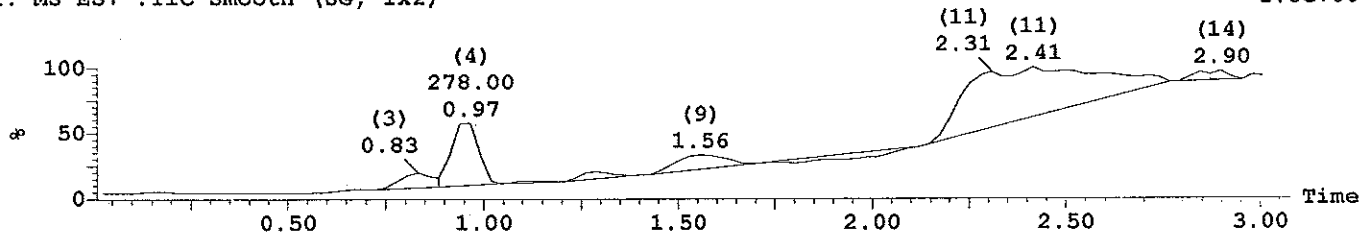
1: MS ES- :TIC Smooth (SG, 1x2) 4.8e+007



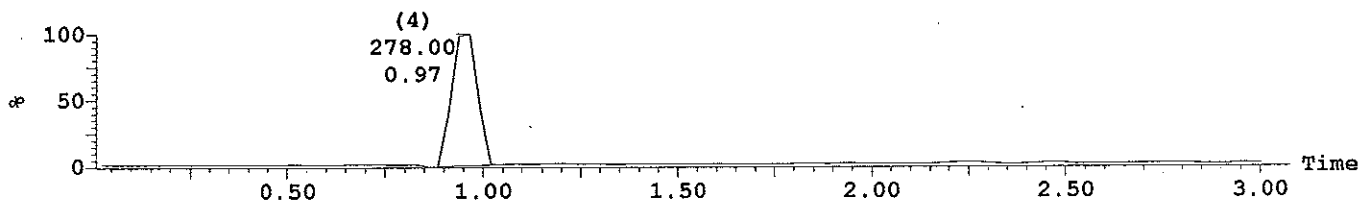
1: MS ES- :277 Smooth (SG, 1x2) 5.5e+006



2: MS ES+ :TIC Smooth (SG, 1x2) 1.8e+008



2: MS ES+ :279 Smooth (SG, 1x2) 1.5e+007



Sample: 1
File:0206R014
Description:

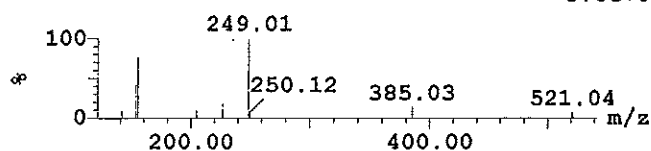
Vial:1:A,1
Date:07-Feb-2006

ID:4-24
Time:09:56:27

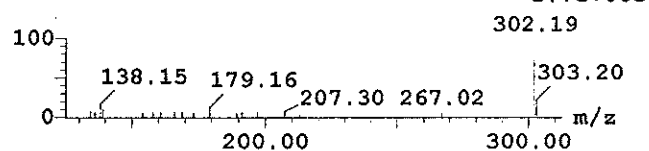
Printed: Tue Feb 07 10:02:20 2006

Sample Report (continued):

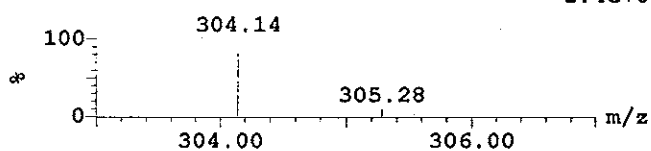
Peak ID Time
1 0.15
Combine (4:8-15:16)



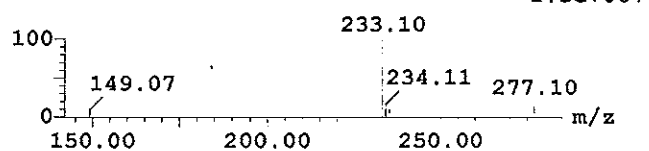
Peak ID Time
3 0.82
Combine (29:33-(22:23+39:40))



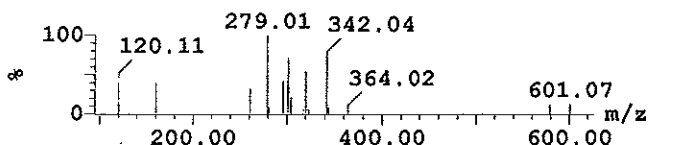
Peak ID Time
3 0.82
Combine (29:33-(20:21+39:40))



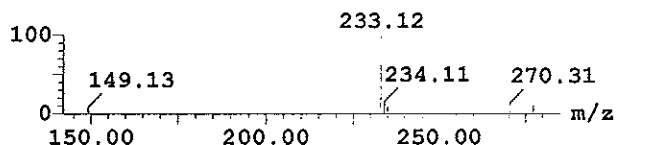
Peak ID Time
4 0.95
Combine (35:39-(27:29+46:48))



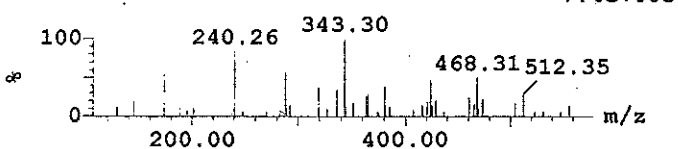
Peak ID Time
4 0.95
Combine (34:38-(26:27+45:46))



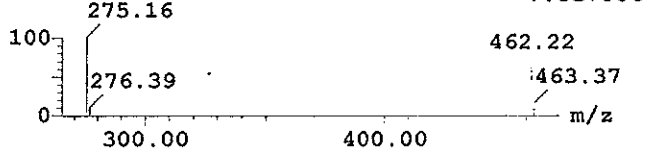
Peak ID Time
5 1.06
Combine (38:42-(32:33+57:58))



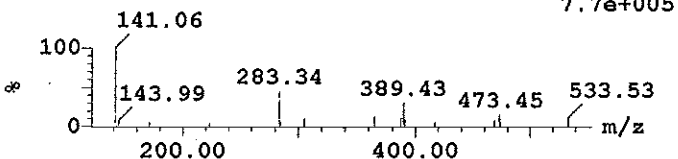
Peak ID Time
7 1.29
Combine (46:50-(38:39+58:59))



Peak ID Time
9 1.56
Combine (56:60-(46:47+69:70))

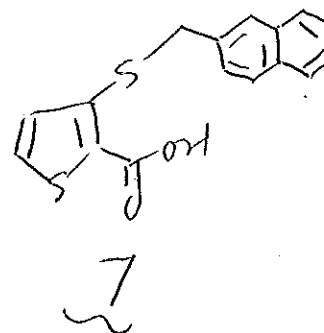


Peak ID Time
10 2.27
Combine (83:87-(74:75+100:101))

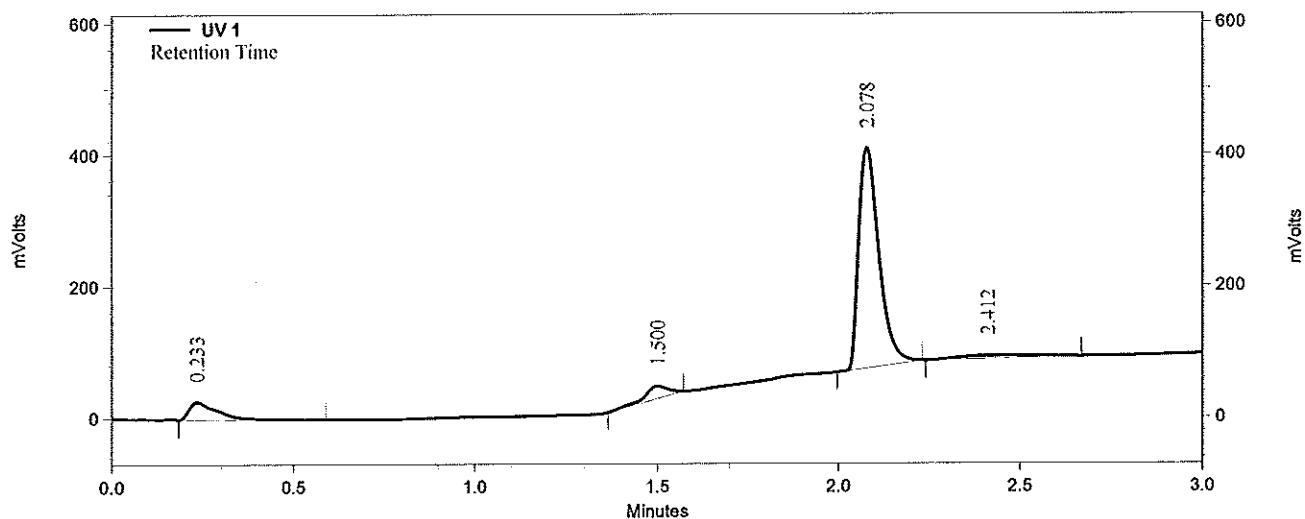


Analytical HPLC Report

File: =
 C:\shimadzu\data\public\weixu.zhai\20110714\2011_0714_1030-007.dat
 Sample ID: = 61838-143-10
 Acquired: = 7/14/2011 10:32:49 AM
 File = 2011_0714_1030.007
 User = weixu.zhai
 Instrument = WFD-409D-LCMS
 Well = 192 Inj. Vol. = 3 uL
 Start % B = 0
 Final % B = 100
 Gradient Time = 2 min
 Flow Rate = 1 ml/min
 Wavelength = 220
 Solvent Pair = Water :Methanol: 0.1% TFA
 Solvent A = 90% Water :10% Methanol: 0.1% TFA
 Solvent B = 10% Water :90% Methanol: 0.1% TFA
 Column 1 = (1)PHENOMENEX-LUNA 2.0 x 30mm 3um
 MWl = 132+
 Oven Temp. = 40



61838-143-10



UV 1 Results

Pk #	RT	Area	Area %	Height (uV)	Plates
1	0.233	144462	9.092	26695	47
2	1.500	85528	5.383	18485	2756
3	2.078	1295833	81.556	333595	6769
4	2.412	63062	3.969	4524	568

Totals		1588885	100.000	383299	
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Sample: 1

Vial: 1:A, 1

ID: 61838-143-10

File: 2011_0714_1030-007

Date: 14-Jul-2011

Time: 10:30:58

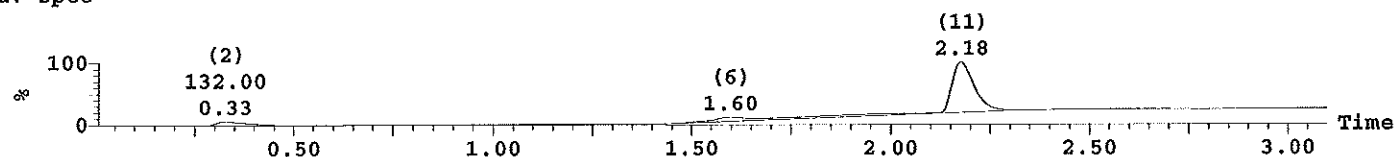
Description:

Printed: Thu Jul 14 10:35:55 2011

Sample Report:

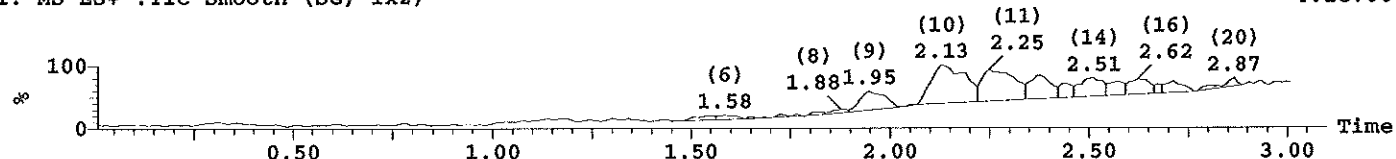
uv spec

4.1e+005



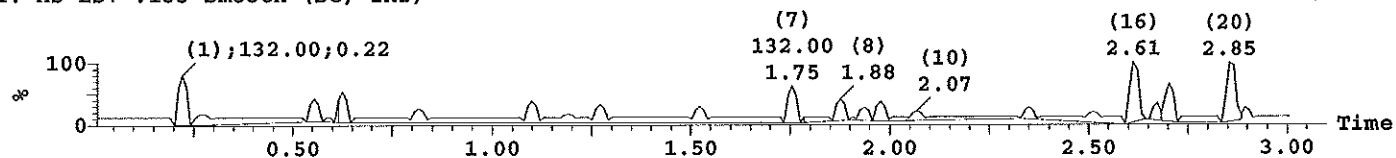
1: MS ES+ :TIC Smooth (SG, 1x2)

4.1e+006



1: MS ES+ :133 Smooth (SG, 1x2)

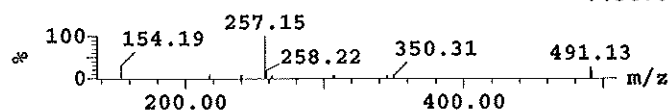
1.4e+004



Peak ID Time
5 1.54

Combine (148:158-(126:131+170:175))

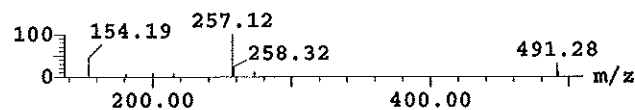
1:MS ES+
7.3e+004



Peak ID Time
6 1.58

Combine (154:163-(124:129+180:185))

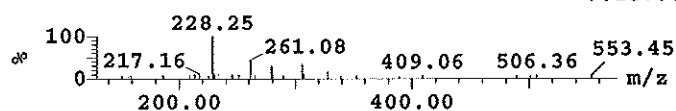
1:MS ES+
7.4e+004



Peak ID Time
8 1.88

Combine (181:191-(164:169+203:208))

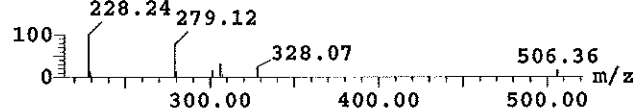
1:MS ES+
7.1e+004



Peak ID Time
9 1.95

Combine (188:198-(168:173+217:222))

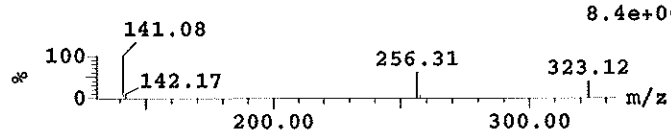
1:MS ES+
2.7e+005



Peak ID Time
10 2.13

Combine (206:216-(185:190+235:240))

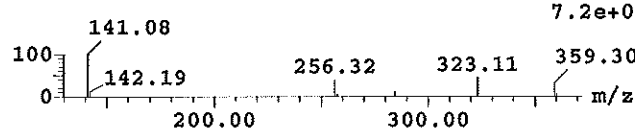
1:MS ES+
8.4e+005



Peak ID Time
11 2.25

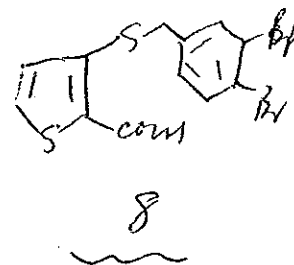
Combine (211:221-(145:150+245:250))

1:MS ES+
7.2e+005

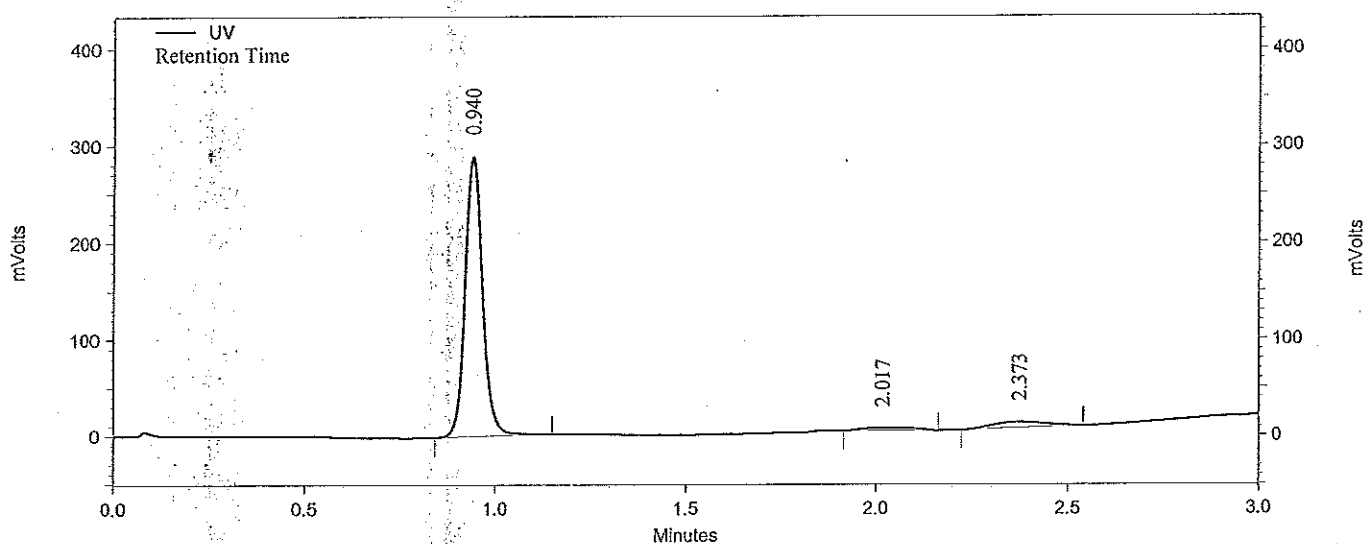


Analytical HPLC Report

File: = C:\CLASS-VP\CHROM\0206R.001
 Sample ID: = 172-01-20 MW 408
 Acquired: = 2/6/2006 4:37:10 PM
 User = weixu.zhai
 Instrument = WFD-409D-LCMS2
 Well = 192 Inj. Vol. = 10 uL
 Start % B = 0
 Final % B = 100
 Gradient Time = 2 min
 Flow Rate = 5 ml/min
 Wavelength = 220
 Solvent A = H2O : ACN 95% : 5% 10 mM Ammonium Acetate
 Solvent B = H2O : ACN 5% : 95% 10 mM Ammonium Acetate
 Column 2 = LUNA 3.0 x 50MM S10



172-01-20



UV Results						
Pk #	RT	Area	Area %	Height (uV)	Plates	
1	0.940	918306	91.496	288930	2158	
2	2.017	27541	2.744	2768	1234	
3	2.373	57813	5.760	5964	1235	
Totals		1003660	100.000	297662		

Sample: 1
File:0206R001
Description:

Vial:1:A,1
Date:06-Feb-2006

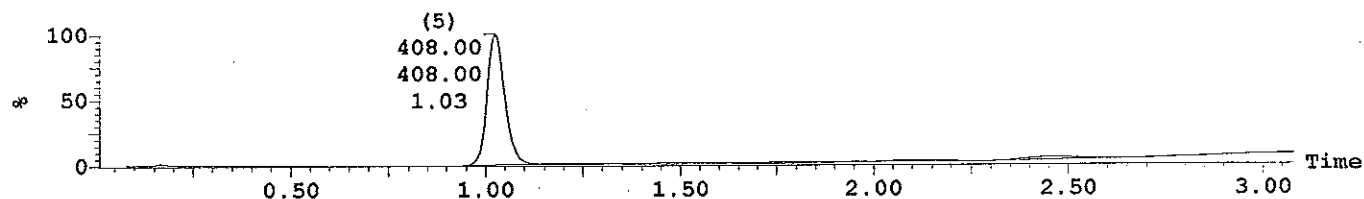
ID:172-01-20
Time:16:30:24

Printed: Mon Feb 06 16:36:57 2006

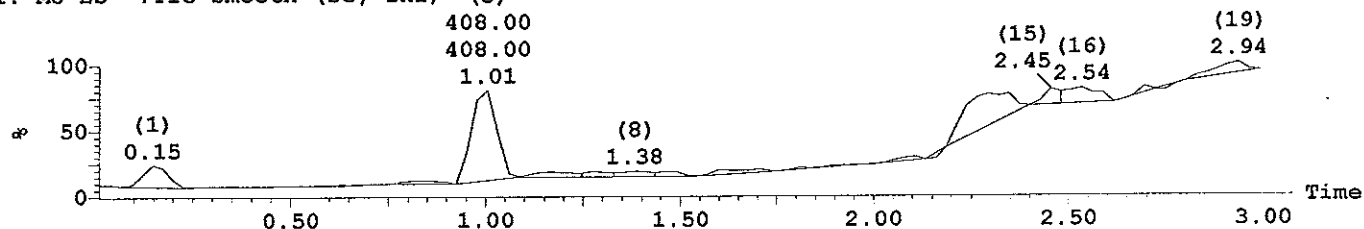
Sample Report:

uv

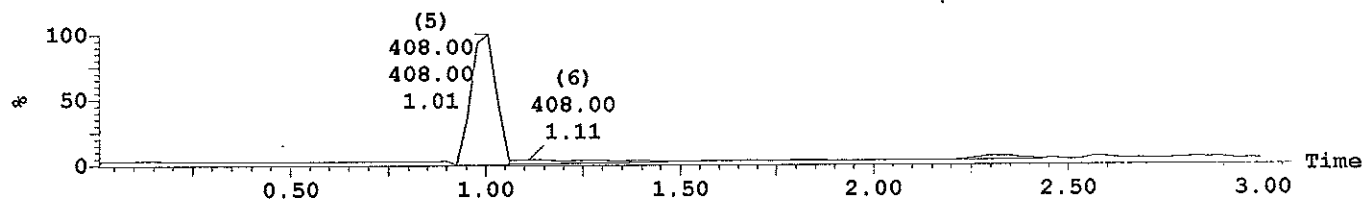
2.9e+005



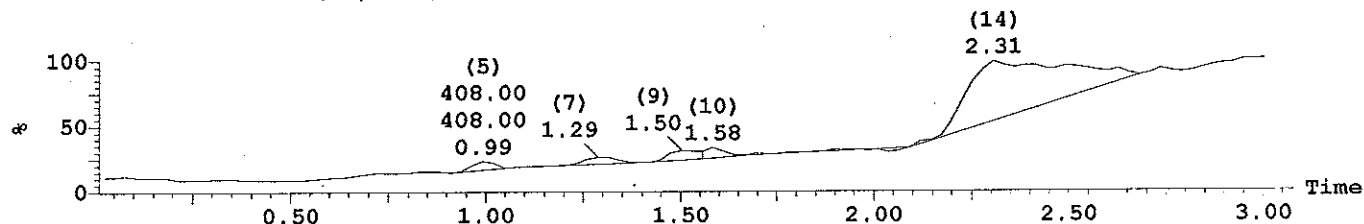
1: MS ES- :TIC Smooth (SG, 1x2) (5) 2.8e+007



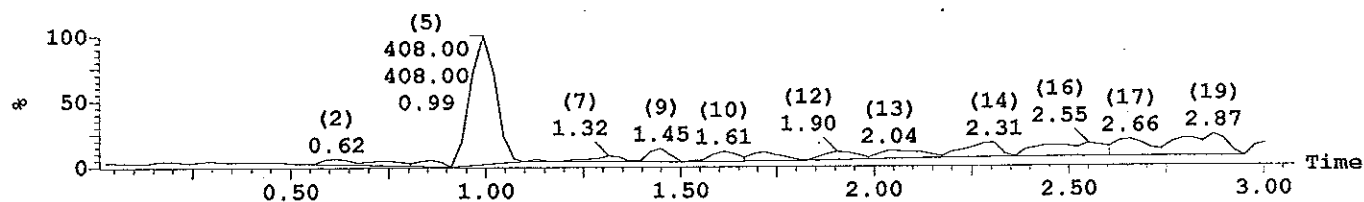
1: MS ES- :407 Smooth (SG, 1x2) 2.6e+006



2: MS ES+ :TIC Smooth (SG, 1x2) 2.1e+008



2: MS ES+ :409 Smooth (SG, 1x2) 1.1e+006



Sample: 1
File: 0206R001
Description:

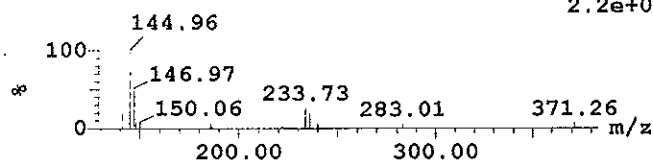
Vial: 1:A,1
Date: 06-Feb-2006

ID: 172-01-20
Time: 16:30:24

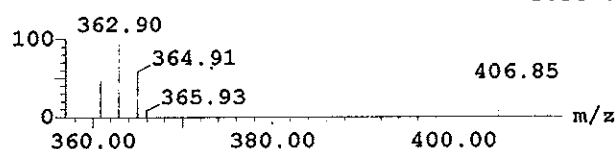
Printed: Mon Feb 06 16:36:57 2006

Sample Report (continued):

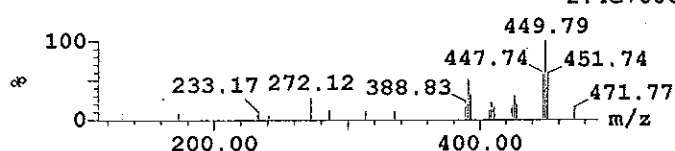
Peak ID Time
3 0.75
Combine (26:30-(18:19+36:37)) 2:MS ES+
2.2e+006



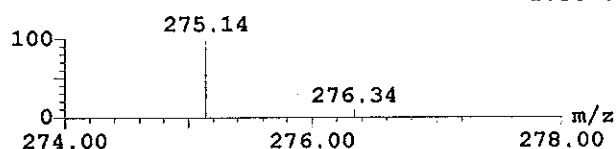
Peak ID Time
5 1.01
Combine (37:41-(28:30+49:51)) 1:MS ES-
3.3e+006



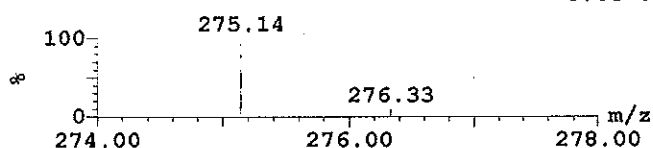
Peak ID Time
5 1.01
Combine (36:40-(28:30+48:50)) 2:MS ES+
2.4e+006



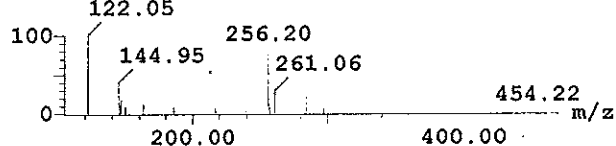
Peak ID Time
9 1.49
Combine (54:58-(46:47+64:65)) 2:MS ES+
1.3e+007



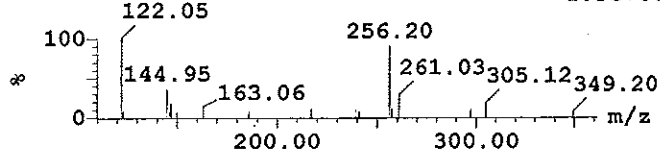
Peak ID Time
10 1.60
Combine (58:62-(49:50+68:69)) 2:MS ES+
8.6e+006



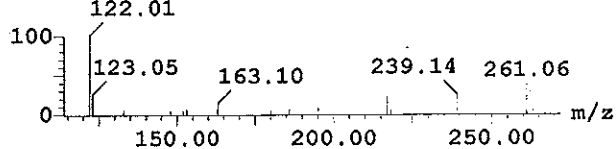
Peak ID Time
14 2.35
Combine (84:88-(71:72+106:107)) 2:MS ES+
1.3e+007



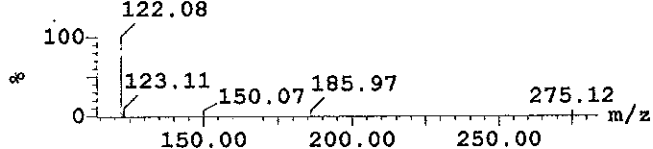
Peak ID Time
15 2.45
Combine (90:93-(78:80+103:105)) 2:MS ES+
1.3e+007



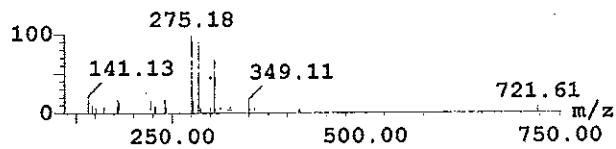
Peak ID Time
16 2.54
Combine (93:97-(87:88+103:104)) 2:MS ES+
3.6e+006



Peak ID Time
17 2.70
Combine (97:101-(90:91+108:109)) 2:MS ES+
1.0e+007

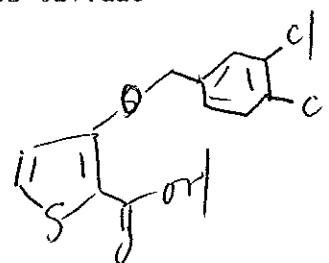


Peak ID Time
18 2.82
Combine (103:107-(95:96+112)) 2:MS ES+
2.5e+006



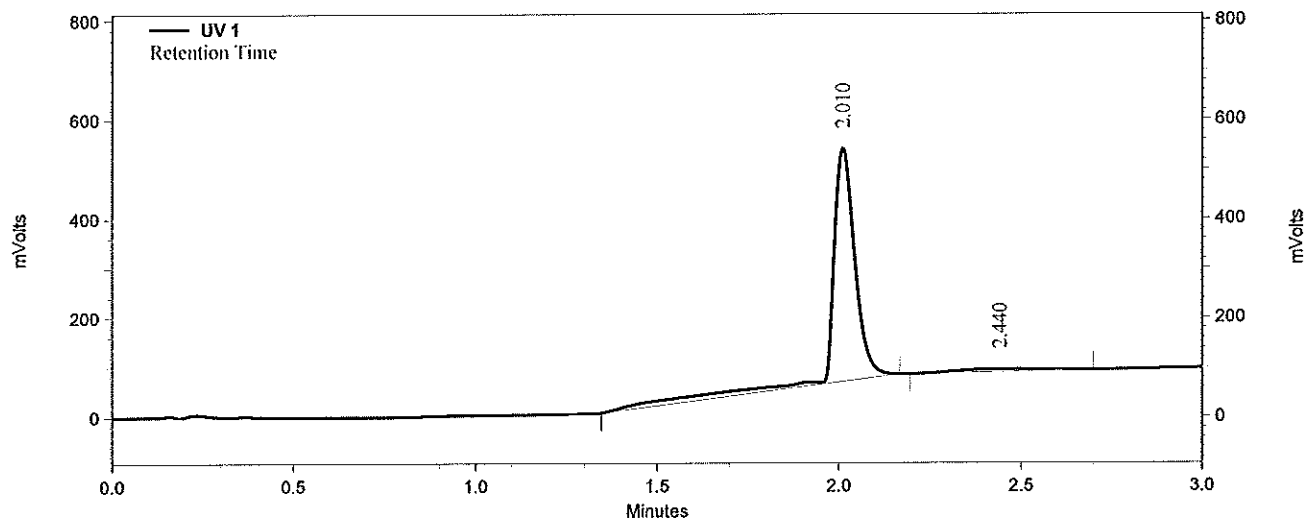
Analytical HPLC Report

File: =
 C:\shimadzu\data\public\weixu.zhai\20110713\2011_0713_1552-027.dat
 Sample ID: = 61838-193
 Acquired: = 7/13/2011 3:54:56 PM
 File = 2011_0713_1552.027
 User = weixu.zhai
 Instrument = WFD-409D-LCMS
 Well = 192 Inj. Vol. = 3 uL
 Start % B = 0
 Final % B = 100
 Gradient Time = 2 min
 Flow Rate = 1 ml/min
 Wavelength = 220
 Solvent Pair = Water :Methanol: 0.1% TFA
 Solvent A = 90% Water :10% Methanol: 0.1% TFA
 Solvent B = 10% Water :90% Methanol: 0.1% TFA
 Column 1 = (1) PHENOMENEX-LUNA 2.0 x 30mm 3um
 MW1 = 132+
 Oven Temp. = 40



9

61838-193



UV 1 Results

Pk #	RT	Area	Area %	Height (uV)	Plates
1	2.010	2082311	95.866	469483	6475
2	2.440	89785	4.134	5705	481
Totals		2172096	100.000	475188	

Sample: 1
File:2011_0713_1552-027
Description:

Vial:1:A,1
Date:13-Jul-2011

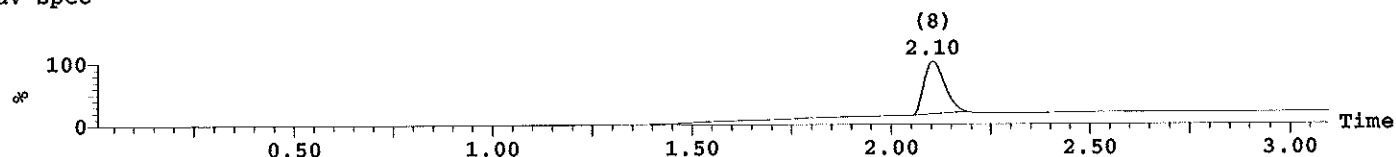
ID:61838-193
Time:15:52:52

Printed: Wed Jul 13 15:58:03 2011

Sample Report:

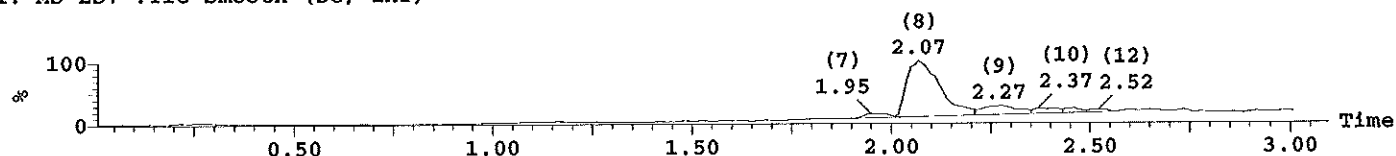
uv spec

5.4e+005



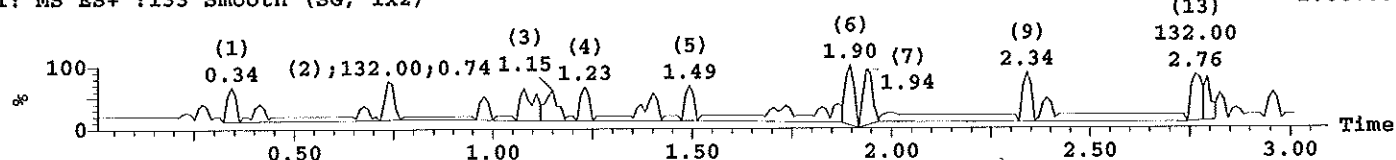
1: MS ES+ :TIC Smooth (SG, 1x2)

1.6e+007



1: MS ES+ :133 Smooth (SG, 1x2)

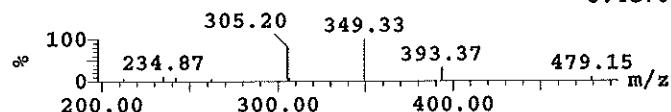
1.6e+004



Peak ID Time
3 1.15

Combine (109:119-(91:96+132:137))

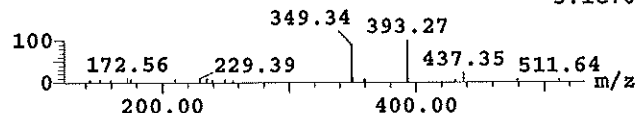
1:MS ES+
8.4e+004



Peak ID Time
4 1.23

Combine (117:127-(100:105+139:144))

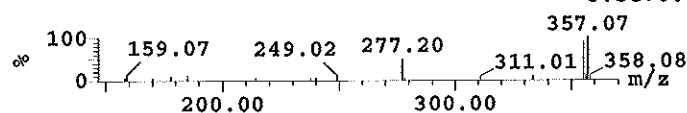
1:MS ES+
5.1e+004



Peak ID Time
5 1.49

Combine (143:153-(126:131+165:170))

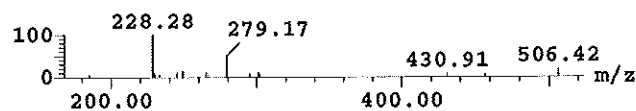
1:MS ES+
5.5e+004



Peak ID Time
6 1.90

Combine (183:193-(166:171+205:210))

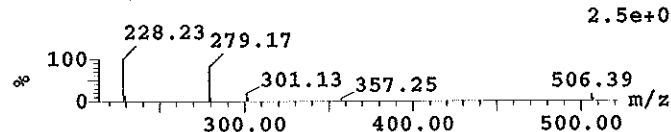
1:MS ES+
1.4e+005



Peak ID Time
7 1.95

Combine (187:197-(170:175+210:215))

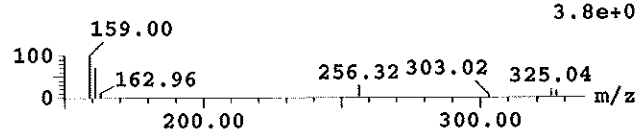
1:MS ES+
2.5e+005



Peak ID Time
8 2.07

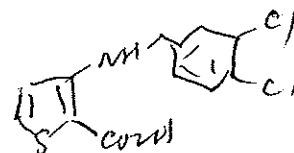
Combine (203:213-(184:189+232:237))

1:MS ES+
3.8e+006



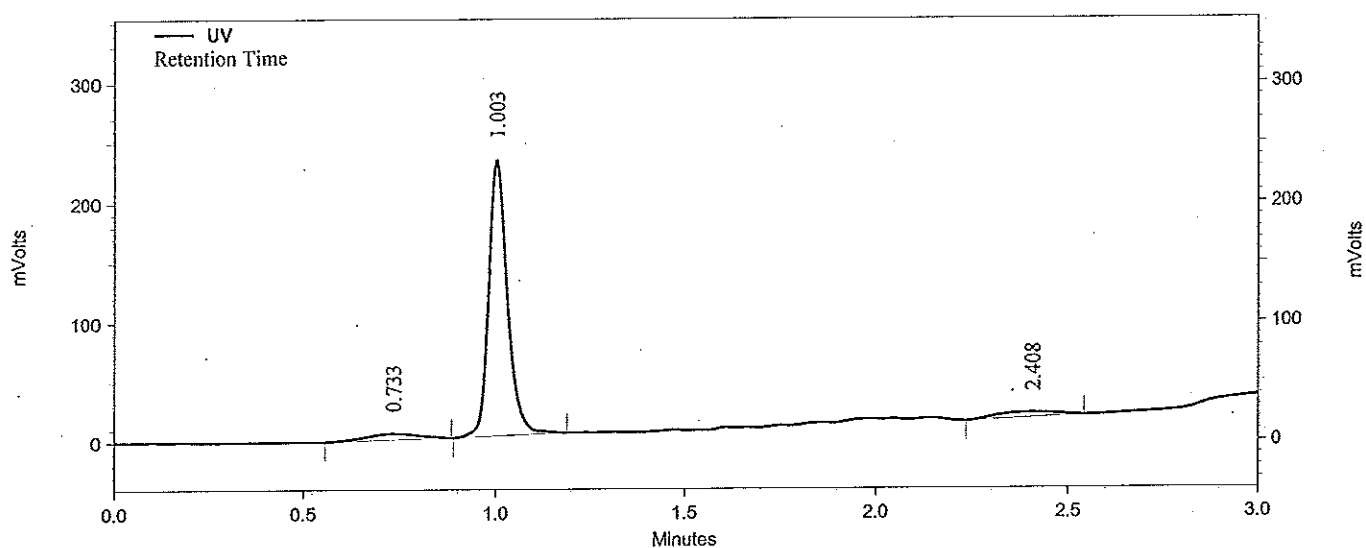
Analytical HPLC Report

File: = C:\CLASS-VP\CHROM\0320I.015
 Sample ID: = 65859-015 MW 302
 Acquired: = 3/20/2006 2:18:31 PM
 User = weixu.zhai
 Instrument = WFD-409D-LCMS2
 Well = 192 Inj. Vol. = 10 uL
 Start % B = 0
 Final % B = 100
 Gradient Time = 2 min
 Flow Rate = 5 ml/min
 Wavelength = 220
 Solvent A = H2O : ACN 95% : 5% 10 mM Ammonium Acetate
 Solvent B = H2O : ACN 5% : 95% 10 mM Ammonium Acetate
 Column 2 = LUNA 3.0 x 50MM S10



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65859-015



UV Results					
Pk #	RT	Area	Area %	Height (uV)	Plates
1	0.733	49824	5.595	5111	127
2	1.003	794773	89.247	230522	2083
3	2.408	45939	5.159	4042	1177
Totals		890536	100.000	239675	

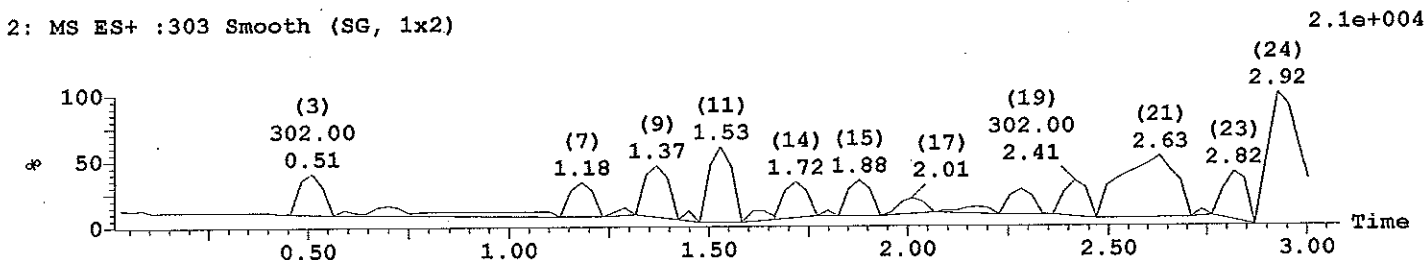
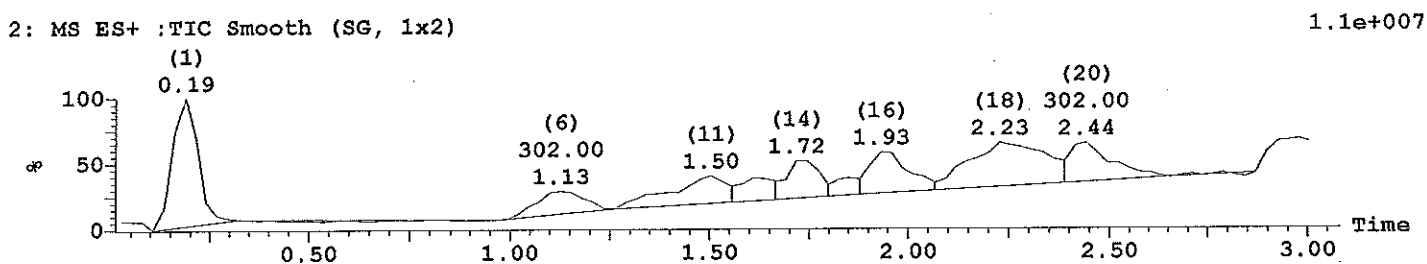
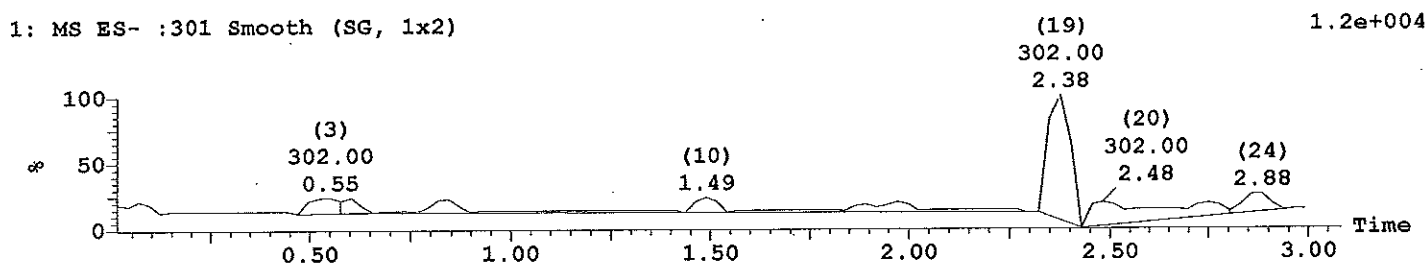
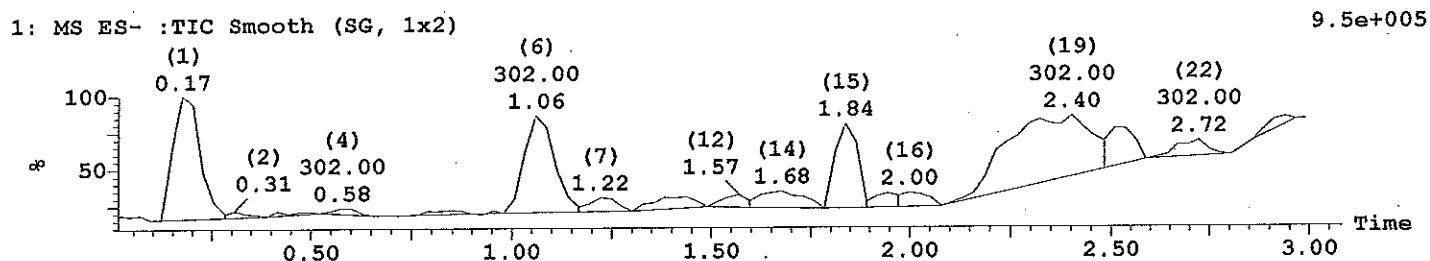
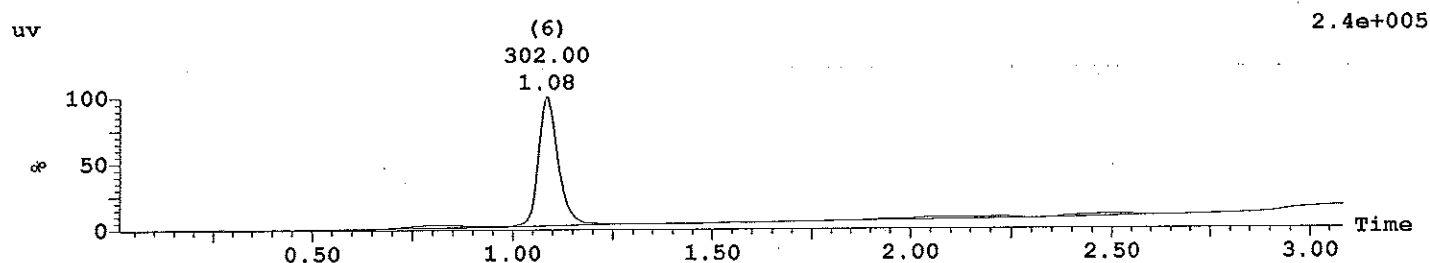
Sample: 1
File:03201015
Description:

Vial:1:A,1
Date:20-Mar-2006

ID:65859-015
Time:14:11:38

Printed: Mon Mar 20 14:17:36 2006

Sample Report:



Sample: 1
File:03201015
Description:

Vial:1:A,1
Date:20-Mar-2006

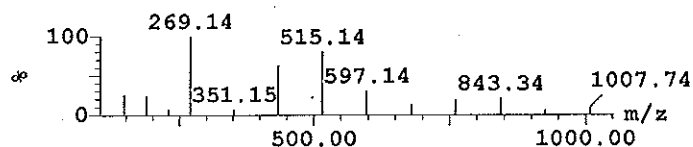
ID:65859-015
Time:14:11:38

Printed: Mon Mar 20 14:17:36 2006

Sample Report (continued):

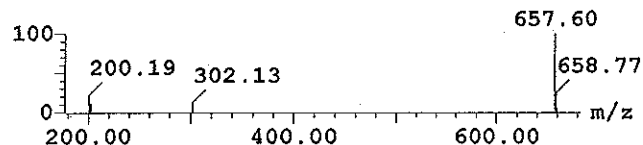
Peak ID Time
1 0.17
Combine (5:9-18:19)

2:MS ES+
1.0e+006



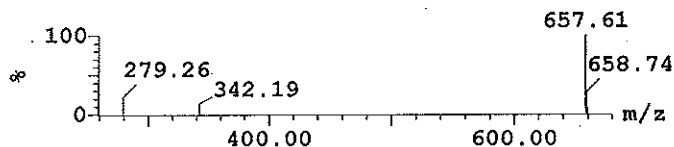
Peak ID Time
6 1.06
Combine (39:42-(29:31+52:54))

2:MS ES+
5.8e+005



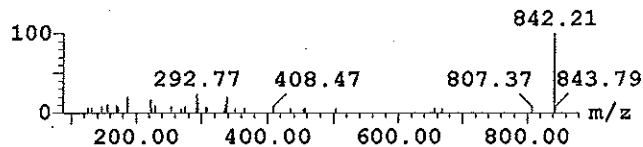
Peak ID Time
7 1.22
Combine (42:46-(35:36+52:53))

2:MS ES+
5.6e+005



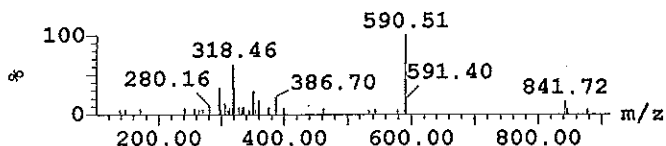
Peak ID Time
9 1.37
Combine (49:53-(42:43+59:60))

2:MS ES+
1.3e+005



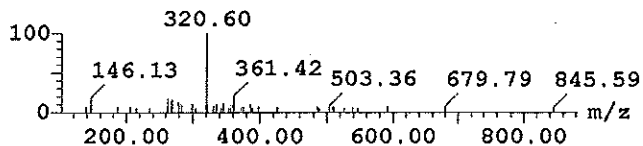
Peak ID Time
11 1.50
Combine (55:59-(48:49+65:66))

2:MS ES+
1.4e+005



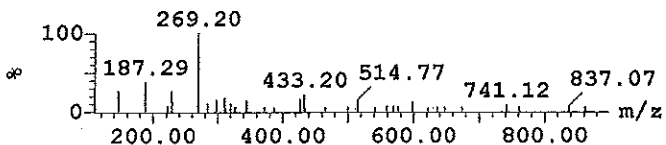
Peak ID Time
13 1.61
Combine (58:62-(51:52+68:69))

2:MS ES+
1.5e+005



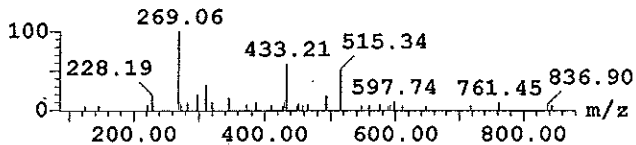
Peak ID Time
15 1.84
Combine (68:72-(61:62+78:79))

2:MS ES+
1.8e+005



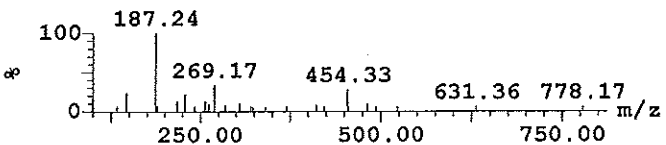
Peak ID Time
16 1.95
Combine (70:74-(63:64+83:84))

2:MS ES+
1.7e+005



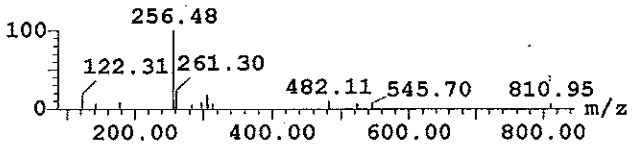
Peak ID Time
18 2.23
Combine (81:85-(70:71+95:96))

2:MS ES+
3.2e+005



Peak ID Time
20 2.51
Combine (89:93-(82:83+105:106))

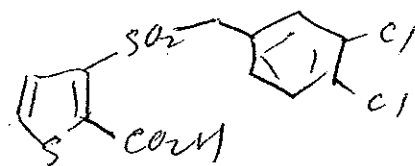
2:MS ES+
3.1e+005



Analytical HPLC Report

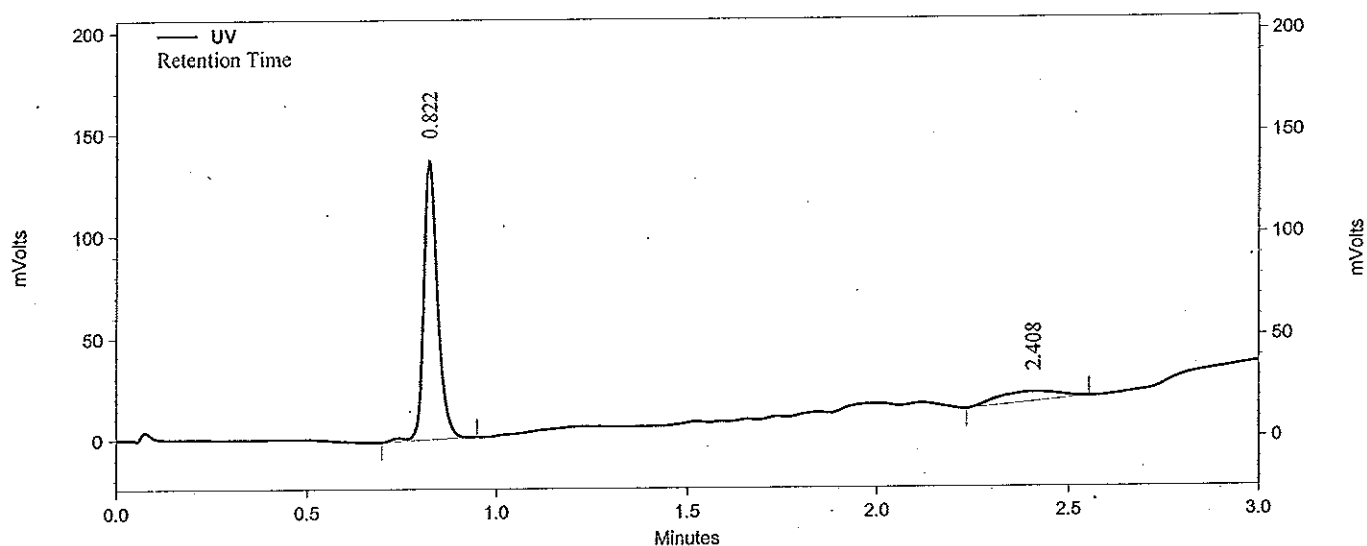
File: = C:\CLASS-VP\CHROM\0307U.008
 Sample ID: = 196-7 MW 351
 Acquired: = 3/7/2006 9:40:19 AM
 User = weixu.zhai
 Instrument = WFD-409D-LCMS2
 Well = 192 Inj. Vol. = 10 uL
 Start % B = 0
 Final % B = 100
 Gradient Time = 2 min
 Flow Rate = 5 ml/min
 Wavelength = 220
 Solvent A = H2O : ACN 95% : 5% 10 mM Ammonium Acetate
 Solvent B = H2O : ACN 5% : 95% 10 mM Ammonium Acetate
 Column 2 = LUNA 3.0 x 50MM S10

61838-196



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196-7



UV Results

Pk #	RT	Area	Area %	Height (uV)	Plates
1	0.822	351201	86.734	136965	2546
2	2.408	53715	13.266	4706	1149
Totals		404916	100.000	141671	

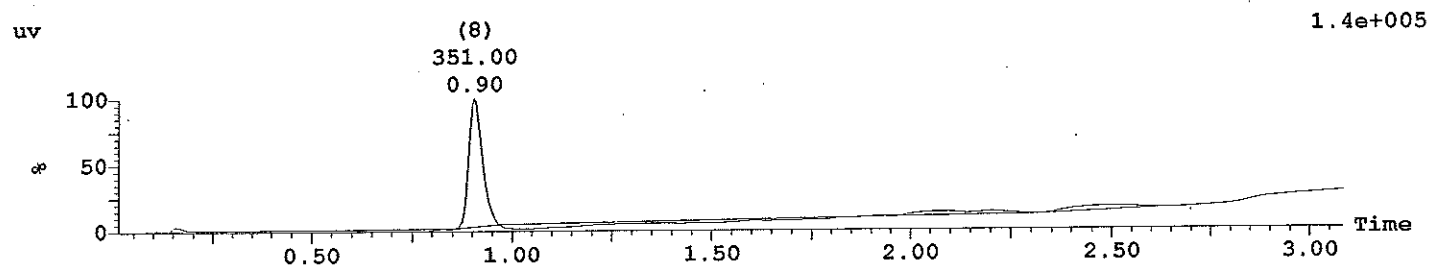
Sample: 1
File:0307U008
Description:

Vial:1:A,1
Date:07-Mar-2006

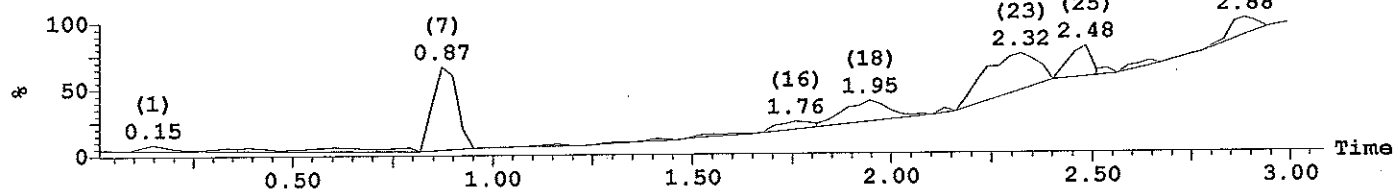
ID:196-7
Time:09:35:30

Printed: Tue Mar 07 09:39:38 2006

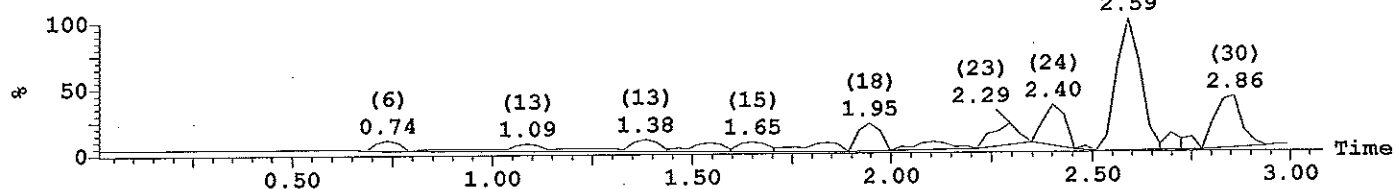
Sample Report:



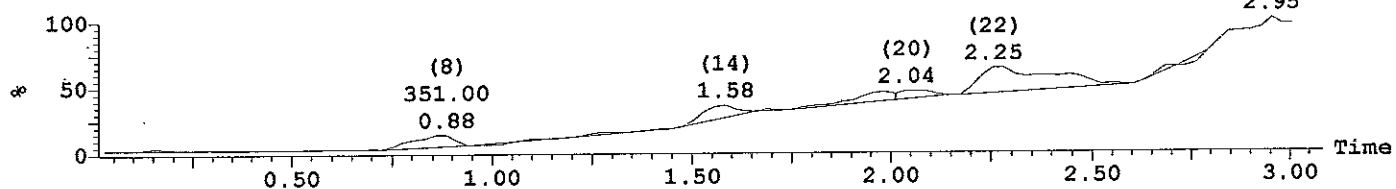
1: MS ES- :TIC Smooth (SG, 1x2)



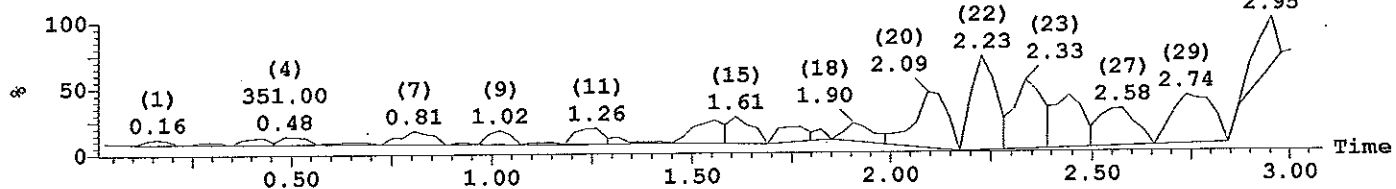
1: MS ES- :350 Smooth (SG, 1x2)



2: MS ES+ :TIC Smooth (SG, 1x2)



2: MS ES+ :352 Smooth (SG, 1x2)



Sample: 1
File:0307U008
Description:

Vial:1:A,1
Date:07-Mar-2006

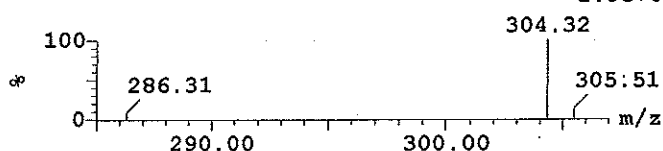
ID:196-7
Time:09:35:30

Printed: Tue Mar 07 09:39:38 2006

Sample Report (continued):

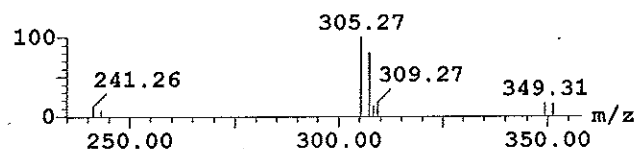
Peak ID Time
7 0.87
Combine (28:32-(20:21+39:40))

2:MS ES+
1.9e+006



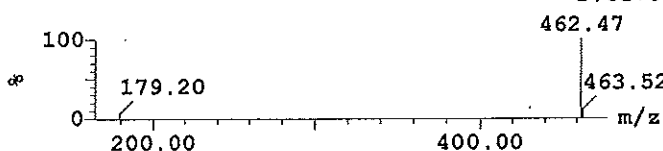
Peak ID Time
8 0.89
Combine (32:36-(25:27+42:44))

1:MS ES-
7.5e+005



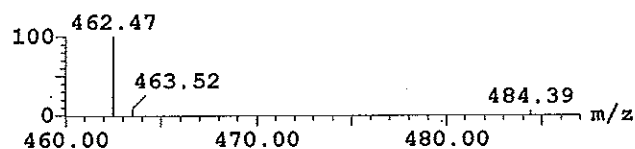
Peak ID Time
14 1.54
Combine (57:61-(47:48+68:69))

2:MS ES+
3.6e+006



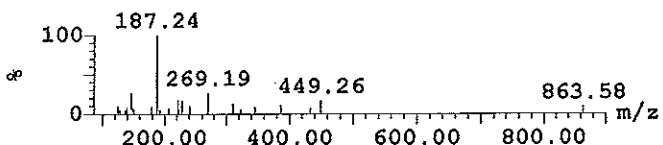
Peak ID Time
15 1.62
Combine (58:62-(52:53+69:70))

2:MS ES+
3.2e+006



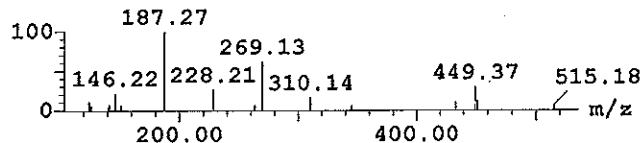
Peak ID Time
18 1.95
Combine (69:73-(62:63+80:81))

2:MS ES+
8.7e+005



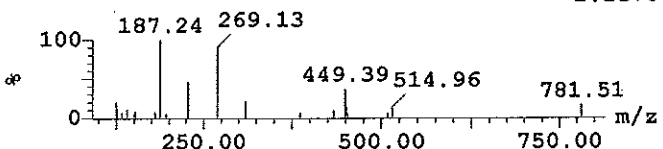
Peak ID Time
19 1.99
Combine (72:76-(58:59+81:82))

2:MS ES+
1.4e+006



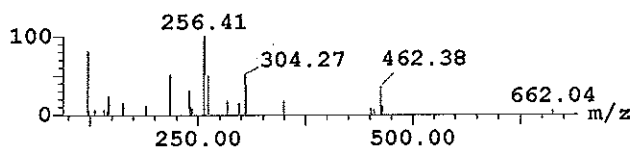
Peak ID Time
20 2.04
Combine (76:80-(67:68+87:88))

2:MS ES+
1.1e+006



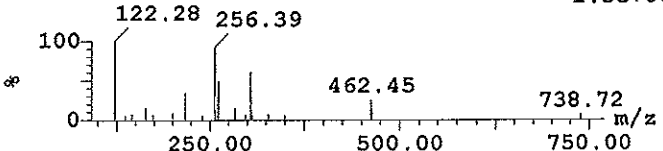
Peak ID Time
23 2.32
Combine (85:89-(78:79+95:96))

2:MS ES+
1.2e+006



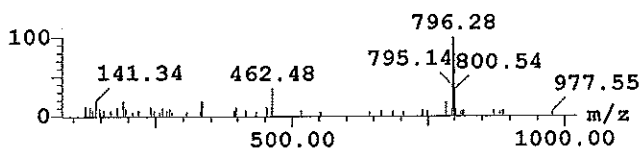
Peak ID Time
25 2.48
Combine (91:94-(79:81+104:106))

2:MS ES+
1.5e+006



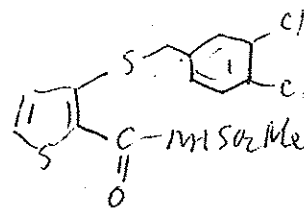
Peak ID Time
29 2.75
Combine (100:104-(92:93+112))

2:MS ES+
6.7e+005



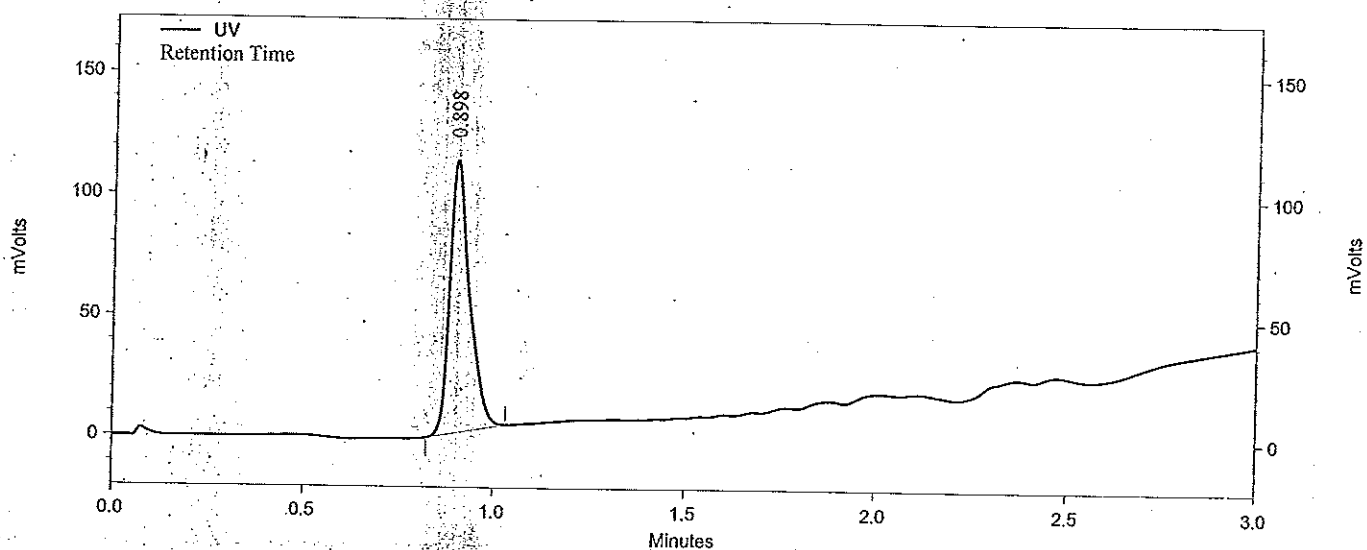
Analytical HPLC Report

File: = C:\CLASS-VP\CHROM\0224I.016
 Sample ID: = 184-12 MW 396
 Acquired: = 2/24/2006 9:50:11 AM
 User = weixu.zhai
 Instrument = WFD-409D-LCMS2
 Well = 191 Inj. Vol. = 10 uL
 Start % B = 0
 Final % B = 100
 Gradient Time = 2 min
 Flow Rate = 5 ml/min
 Wavelength = 220
 Solvent A = H2O : ACN 95% : 5% 10 mm Ammonium Acetate
 Solvent B = H2O : ACN 5% : 95% 10 mm Ammonium Acetate
 Column 2 = LUNA 3.0 x 50MM S10



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184-12



UV Results					
PK #	RT	Area	Area %	Height (uV)	Plates
1	0.898	410405	100.000	112774	1492
Totals		410405	100.000	112774	

Sample: 1
File:0224I016
Description:

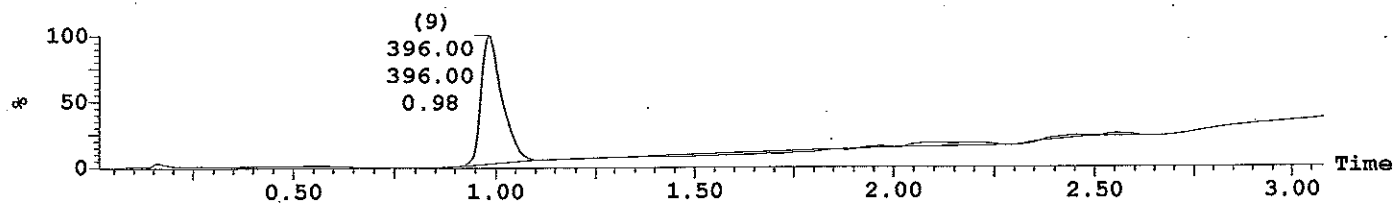
Vial:1:A,1
Date:24-Feb-2006

ID:184-12
Time:09:45:38

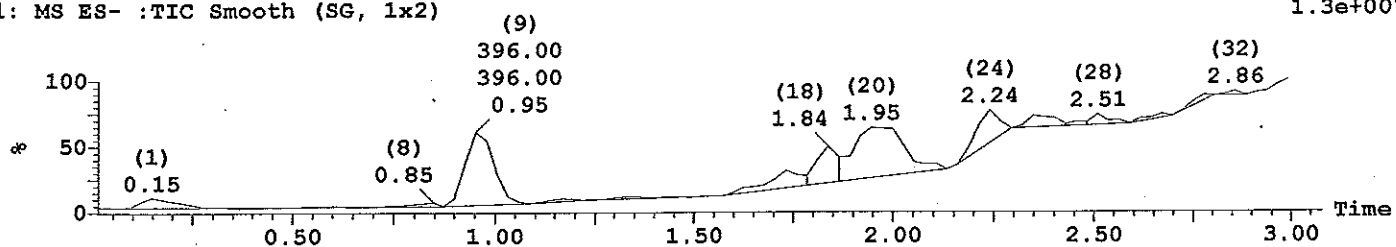
Printed: Fri Feb 24 09:51:47 2006

Sample Report:

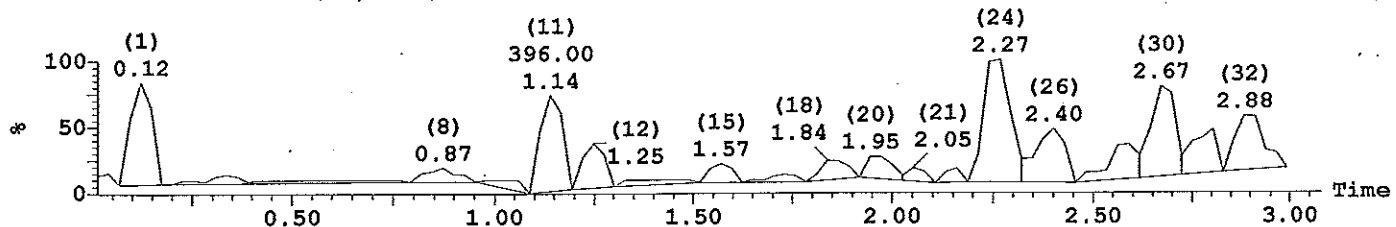
uv 1.2e+005



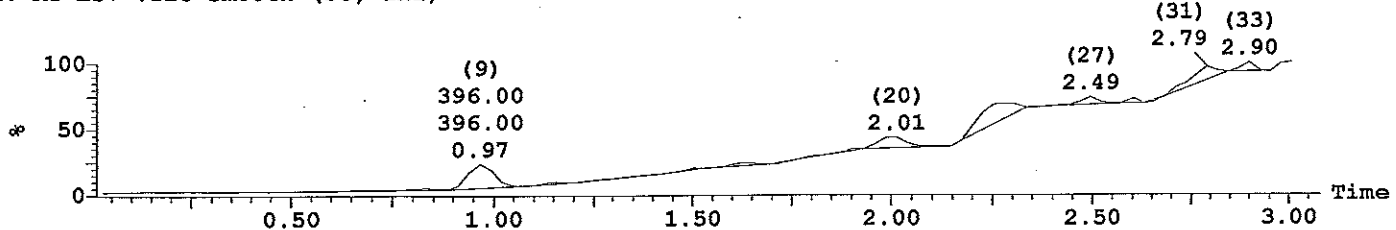
1: MS ES- :TIC Smooth (SG, 1x2) 1.3e+007



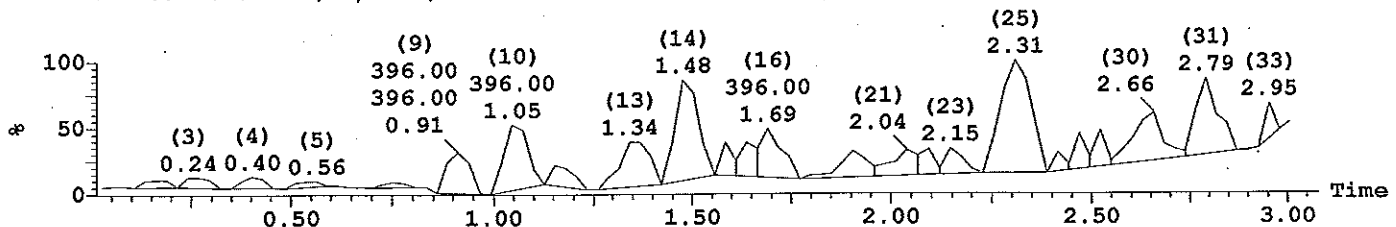
1: MS ES- :395 Smooth (SG, 1x2) 1.3e+004



2: MS ES+ :TIC Smooth (SG, 1x2) 1.3e+008



2: MS ES+ :397 Smooth (SG, 1x2) 7.7e+004



Sample: 1
File:02241016
Description:

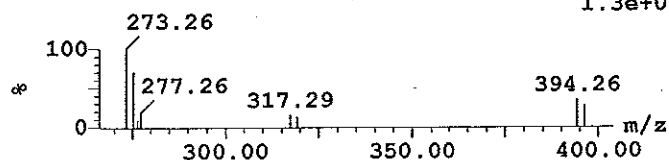
Vial:1:A,1
Date:24-Feb-2006

ID:184-12
Time:09:45:38

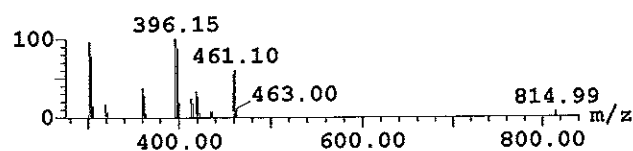
Printed: Fri Feb 24 09:51:47 2006

Sample Report (continued):

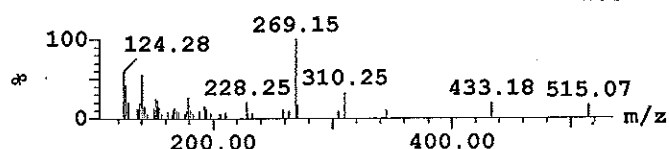
Peak ID Time
9 0.95
Combine (35:39-(27:29+47:49)) 1:MS ES-
1.3e+006



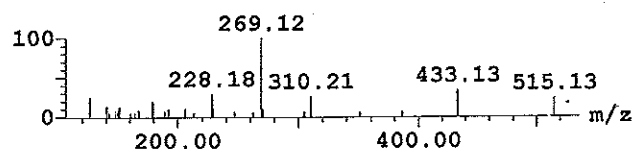
Peak ID Time
9 0.95
Combine (35:38-(26:28+47:49)) 2:MS ES+
1.8e+006



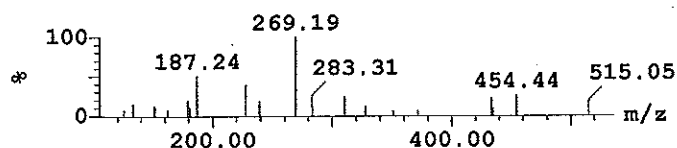
Peak ID Time
20 1.95
Combine (73:77-(65:66+86:87)) 2:MS ES+
1.3e+006



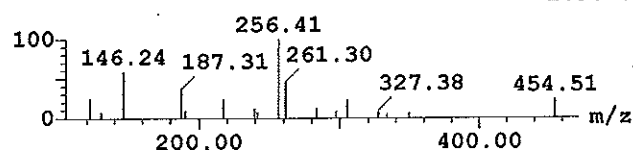
Peak ID Time
22 2.09
Combine (76:80-(70:71+85:86)) 2:MS ES+
1.0e+006



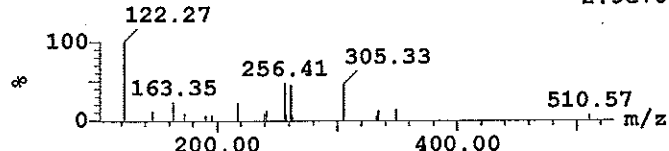
Peak ID Time
23 2.16
Combine (80:83-(68:69+91:93)) 2:MS ES+
1.7e+006



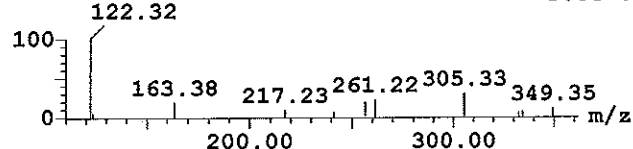
Peak ID Time
24 2.24
Combine (83:87-(74:75+93:94)) 2:MS ES+
2.9e+006



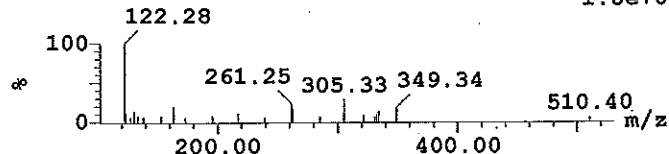
Peak ID Time
26 2.45
Combine (90:93-(81:82+98:100)) 2:MS ES+
2.9e+006



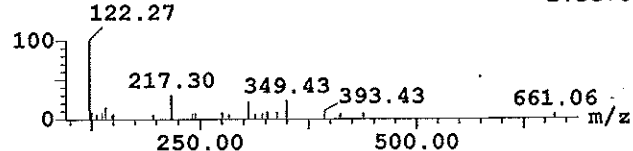
Peak ID Time
27 2.50
Combine (91:95-(82:83+101:102)) 2:MS ES+
3.8e+006



Peak ID Time
28 2.51
Combine (92:96-(86:87+101:102)) 2:MS ES+
1.8e+006

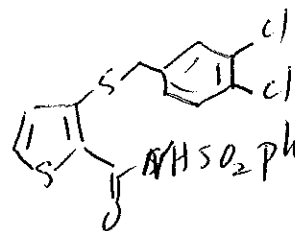


Peak ID Time
29 2.59
Combine (95:99-(88:89+104:105)) 2:MS ES+
1.3e+006



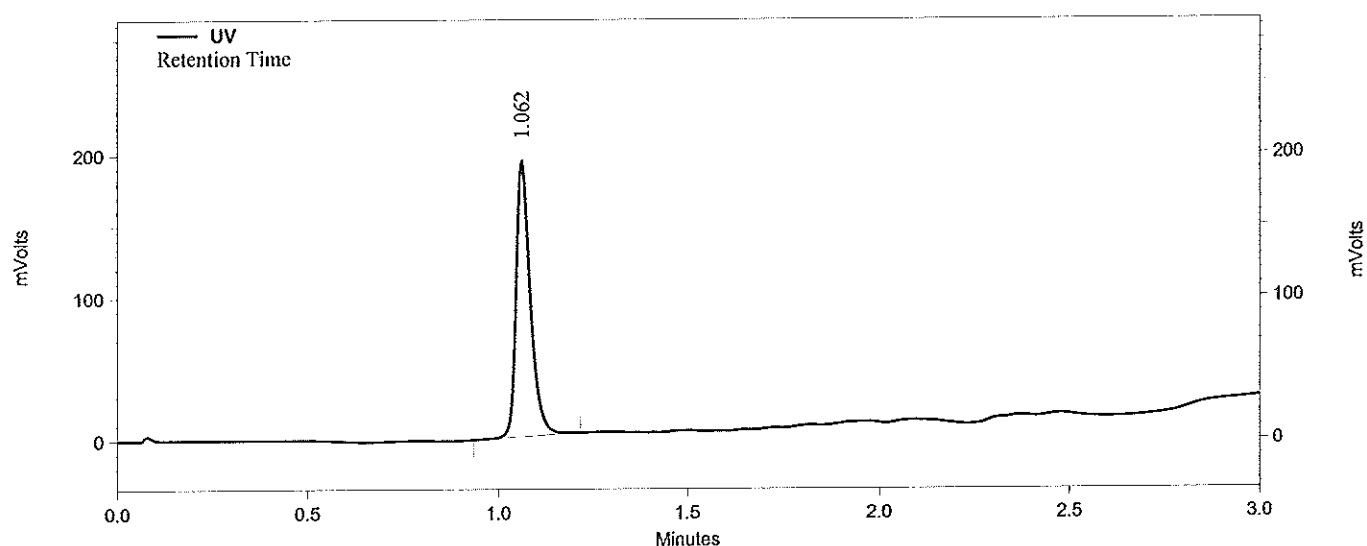
Analytical HPLC Report

File: = C:\CLASS-VP\CHROM\0410Z.024
 Sample ID: = 65859-038-19 MW 458
 Acquired: = 4/10/2006 11:44:37 AM
 User = weixu.zhai
 Instrument = WFD-409D-LCMS2
 Well = 190 Inj. Vol. = 10 uL
 Start % B = 0
 Final % B = 100
 Gradient Time = 2 min
 Flow Rate = 5 ml/min
 Wavelength = 220
 Solvent A = H2O : ACN 95% : 5% 10 mm Ammonium Acetate
 Solvent B = H2O : ACN 5% : 95% 10 mm Ammonium Acetate
 Column 2 = LUNA 3.0 x 50MM S10



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65859-038-19



UV Results					
Pk #	RT	Area	Area %	Height (uV)	Plates
1	1.062	502787	100.000	193267	4050
Totals					
		502787	100.000	193267	

Sample: 1

Vial:1:A,1

ID:65859-038-19

File:0410Z024

Date:10-Apr-2006

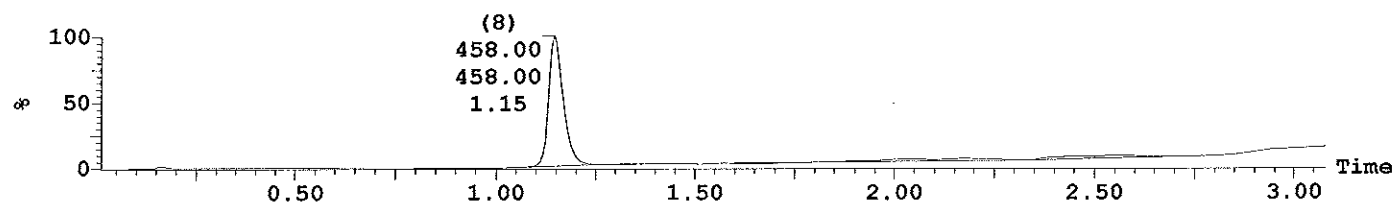
Time:11:41:04

Description:

Printed: Mon Apr 10 11:47:13 2006

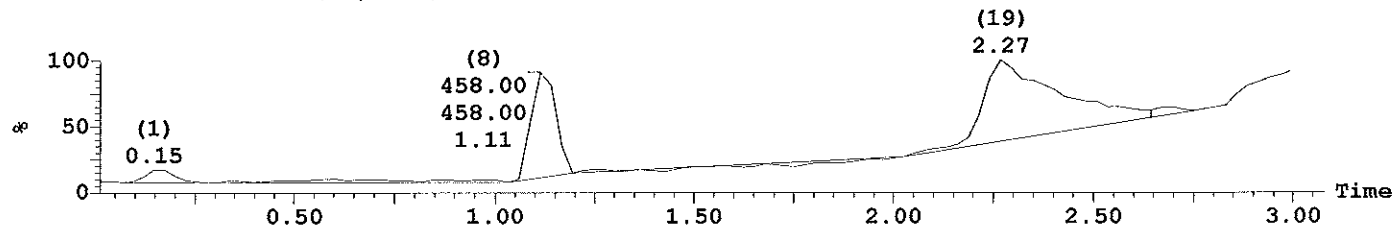
Sample Report:

uv 2.0e+005



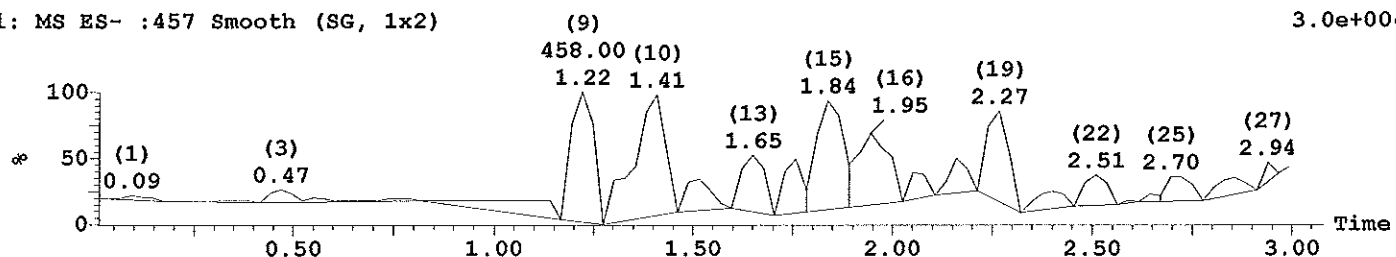
1: MS ES- :TIC Smooth (SG, 1x2)

6.9e+006



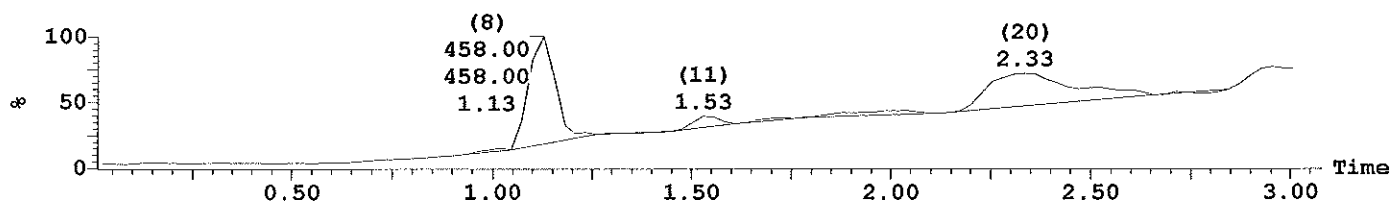
1: MS ES- :457 Smooth (SG, 1x2)

3.0e+004



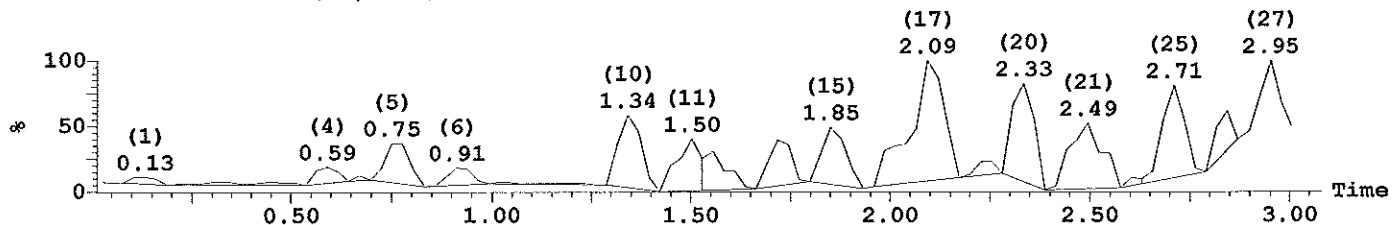
2: MS ES+ :TIC Smooth (SG, 1x2)

6.6e+007



2: MS ES+ :459 Smooth (SG, 1x2)

5.5e+004



Sample: 1
File:0410Z024
Description:

Vial:1:A,1
Date:10-Apr-2006

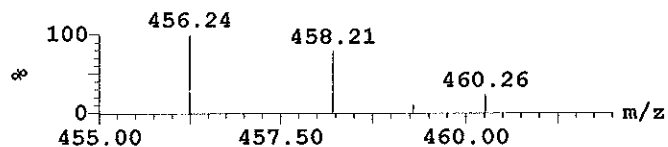
ID:65859-038-19
Time:11:41:04

Printed: Mon Apr 10 11:47:13 2006

Sample Report (continued):

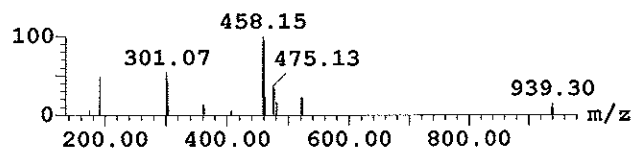
Peak ID Time
8 1.11
Combine (41:45-(31:33+53:55))

1:MS ES-
1.3e+006



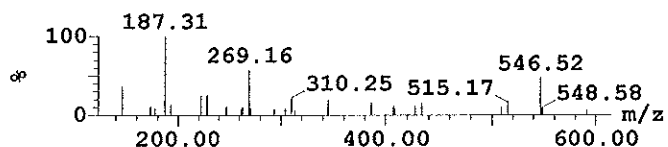
Peak ID Time
8 1.11
Combine (41:45-(30:32+53:55))

2:MS ES+
4.9e+006



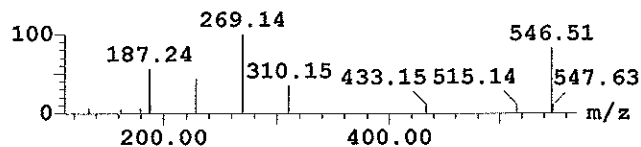
Peak ID Time
15 1.84
Combine (67:71-(60:61+78:79))

2:MS ES+
6.3e+005



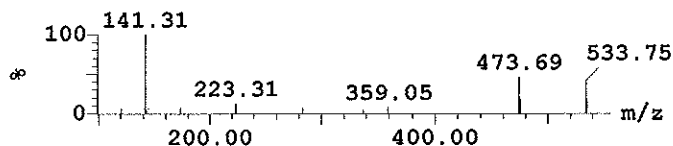
Peak ID Time
17 2.05
Combine (76:80-(66:67+87:88))

2:MS ES+
1.0e+006



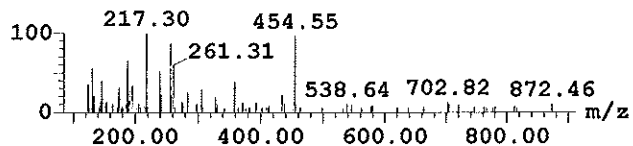
Peak ID Time
19 2.27
Combine (83:87-(69:70+105:106))

1:MS ES-
4.8e+005



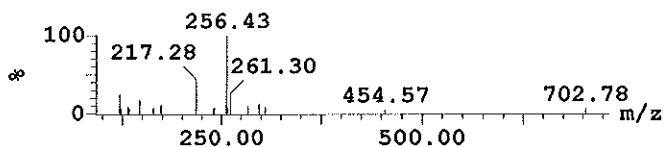
Peak ID Time
19 2.27
Combine (82:86-(74:75+91:92))

2:MS ES+
4.6e+005



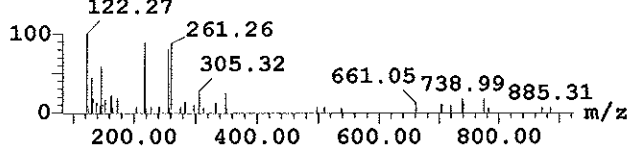
Peak ID Time
20 2.40
Combine (85:89-(73:74+105:106))

2:MS ES+
2.7e+006



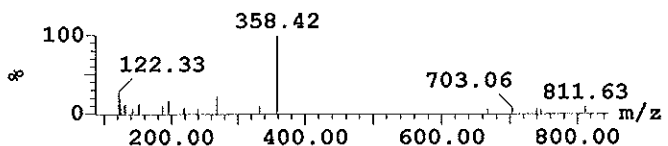
Peak ID Time
21 2.50
Combine (91:95-(82:83+102:103))

2:MS ES+
7.0e+005



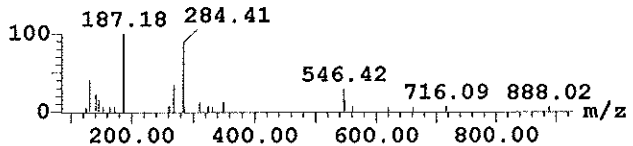
Peak ID Time
25 2.70
Combine (99:103-(91:92+110:111))

2:MS ES+
7.6e+005



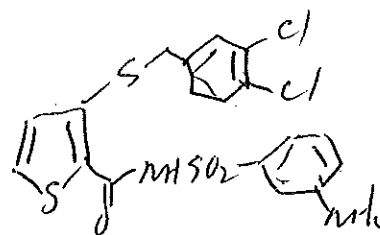
Peak ID Time
26 2.86
Combine (104:108-97:98)

2:MS ES+
8.7e+005



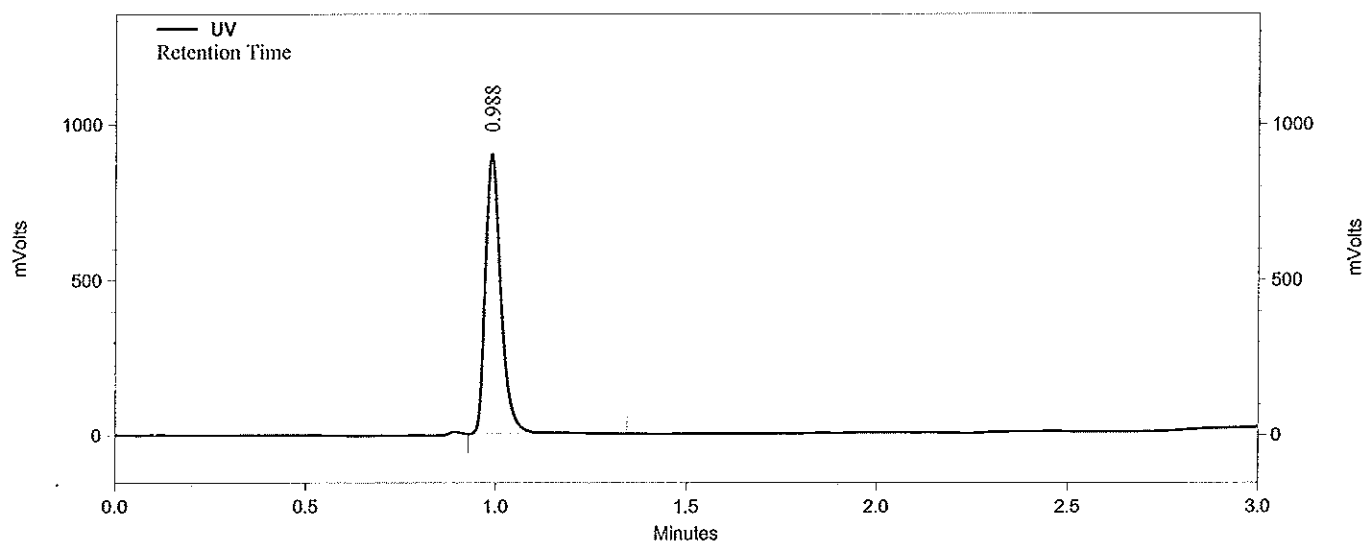
Analytical HPLC Report

File: = C:\CLASS-VP\CHROM\0420H.023
 Sample ID: = 47-2-6 MW 50
 Acquired: = 4/20/2006 1:42:20 PM
 User = weixu.zhai
 Instrument = WFD-409D-LCMS2
 Well = 188 Inj. Vol. = 10 uL
 Start % B = 0
 Final % B = 100
 Gradient Time = 2 min
 Flow Rate = 5 ml/min
 Wavelength = 220
 Solvent A = H2O : ACN 95% : 5% 10 mM Ammonium Acetate
 Solvent B = H2O : ACN 5% : 95% 10 mM Ammonium Acetate
 Column 2 = LUNA 3.0 x 50MM S10



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47-2-6



UV Results

PK #	RT	Area	Area %	Height (uV)	Plates
1	0.988	2579045	100.000	900288	2869
Totals					
		2579045	100.000	900288	

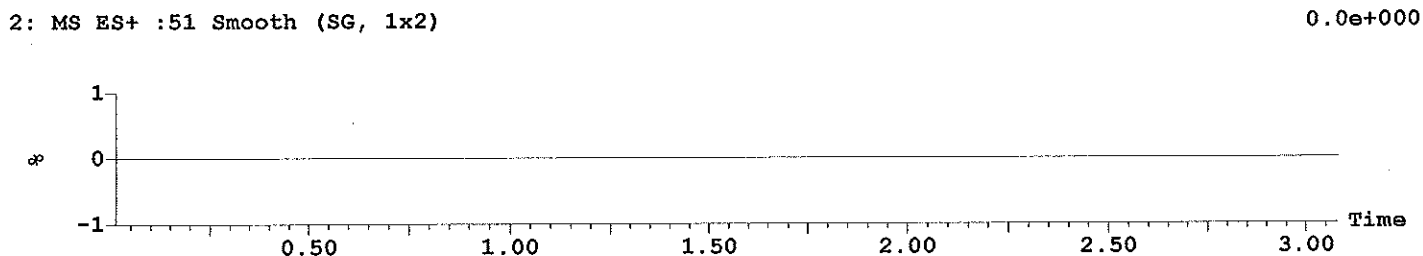
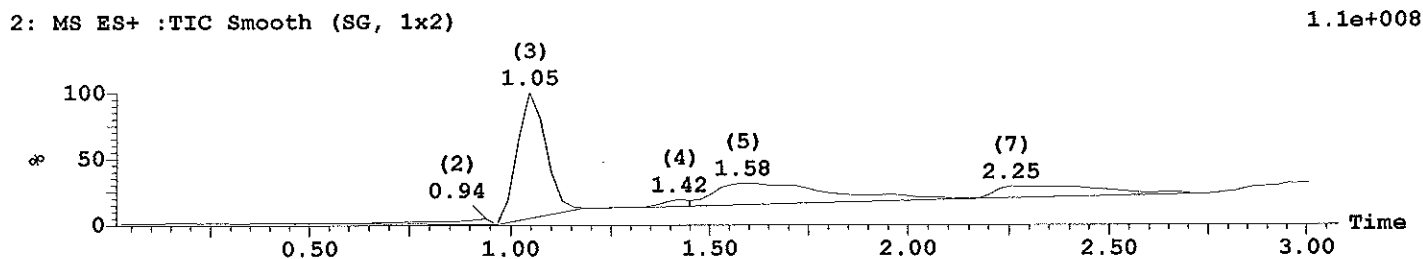
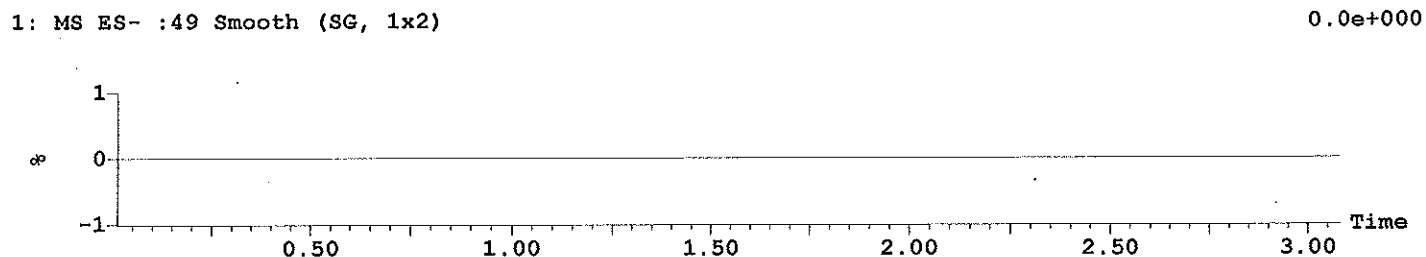
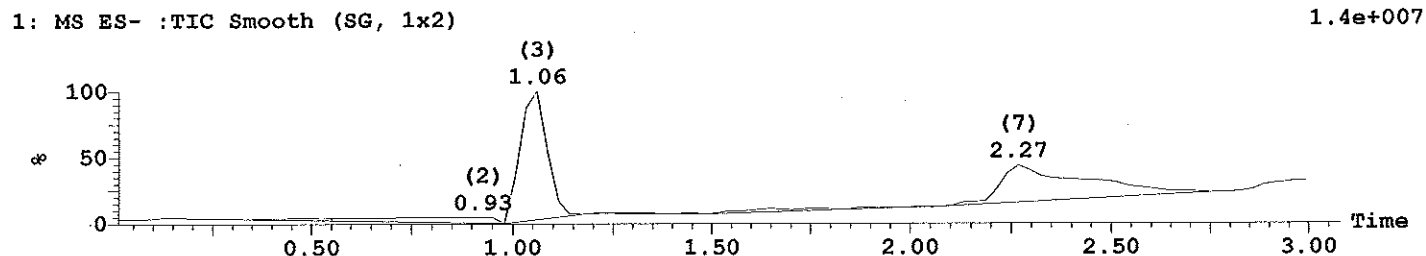
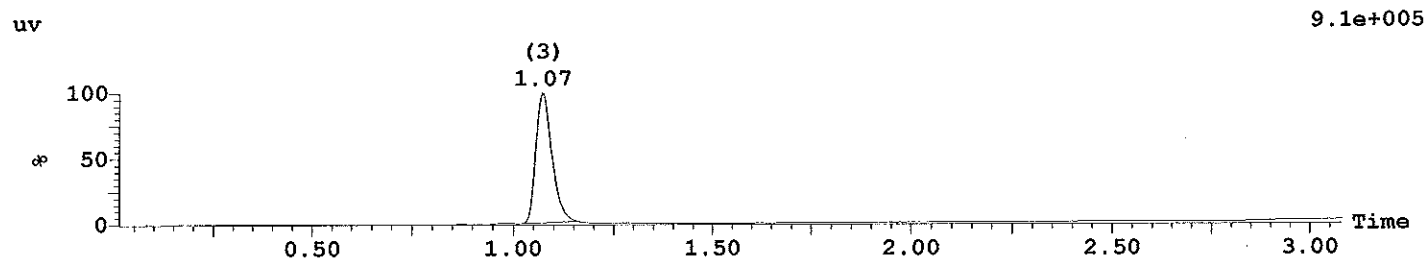
Sample: 1
File:0420H023
Description:

Vial:1:A,1
Date:20-Apr-2006

ID:47-2-6
Time:13:38:37

Printed: Thu Apr 20 13:44:45 2006

Sample Report:



Sample: 1
File:0420H023
Description:

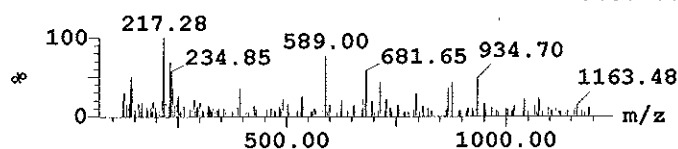
Vial:1:A,1
Date:20-Apr-2006

ID:47-2-6
Time:13:38:37

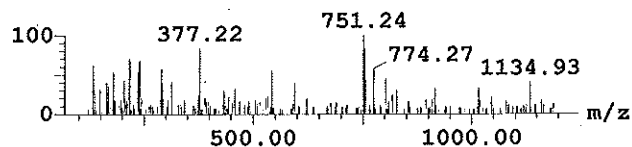
Printed: Thu Apr 20 13:44:45 2006

Sample Report (continued):

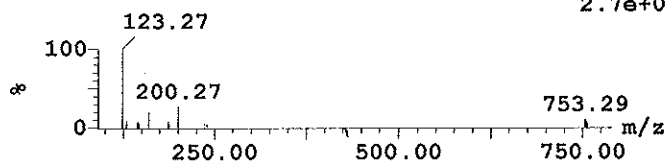
Peak ID Time
1 0.50
Combine (17:21-(6:7+27:28)) 1:MS ES-
9.3e+003



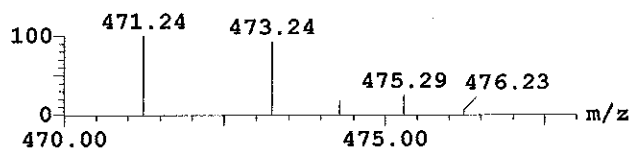
Peak ID Time
2 0.93
Combine (33:37-(14:15+43:44)) 1:MS ES-
8.9e+003



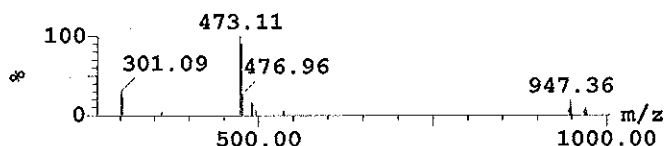
Peak ID Time
2 0.93
Combine (33:37-(10:11+42:43)) 2:MS ES+
2.7e+005



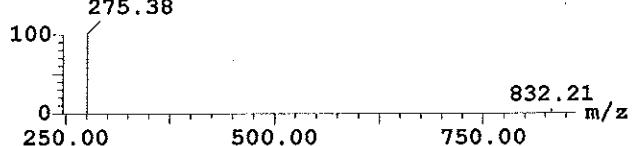
Peak ID Time
3 1.06
Combine (39:42-(31:33+49:51)) 1:MS ES-
3.5e+006



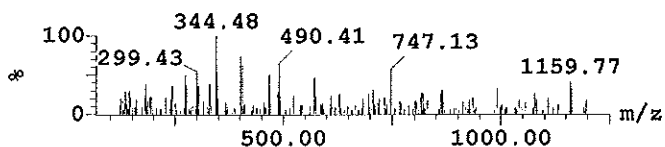
Peak ID Time
3 1.06
Combine (38:42-(30:32+49:51)) 2:MS ES+
1.3e+007



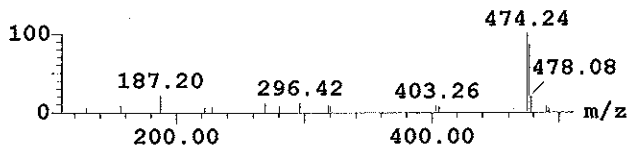
Peak ID Time
4 1.42
Combine (51:55-(42:43+60:61)) 2:MS ES+
2.3e+006



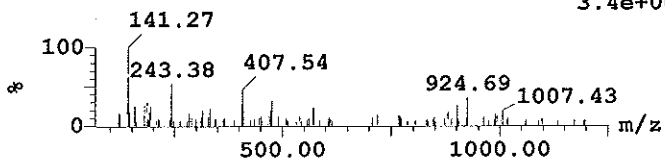
Peak ID Time
5 1.65
Combine (60:64-(49:50+70:71)) 1:MS ES-
1.6e+004



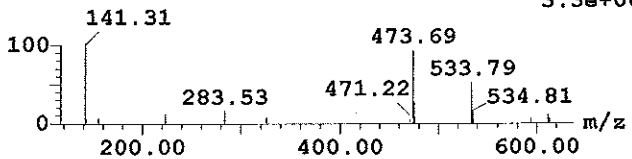
Peak ID Time
5 1.65
Combine (57:61-(47:48+87:88)) 2:MS ES+
3.9e+006



Peak ID Time
6 1.76
Combine (64:68-(57:58+75:76)) 1:MS ES-
3.4e+004

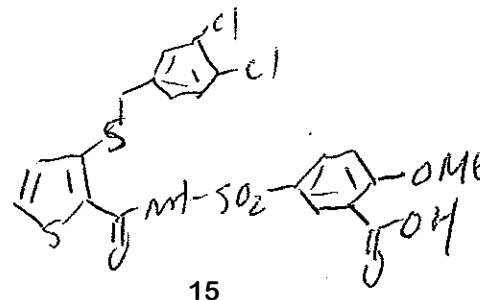


Peak ID Time
7 2.27
Combine (83:87-(71:72+109:110)) 1:MS ES-
3.3e+005

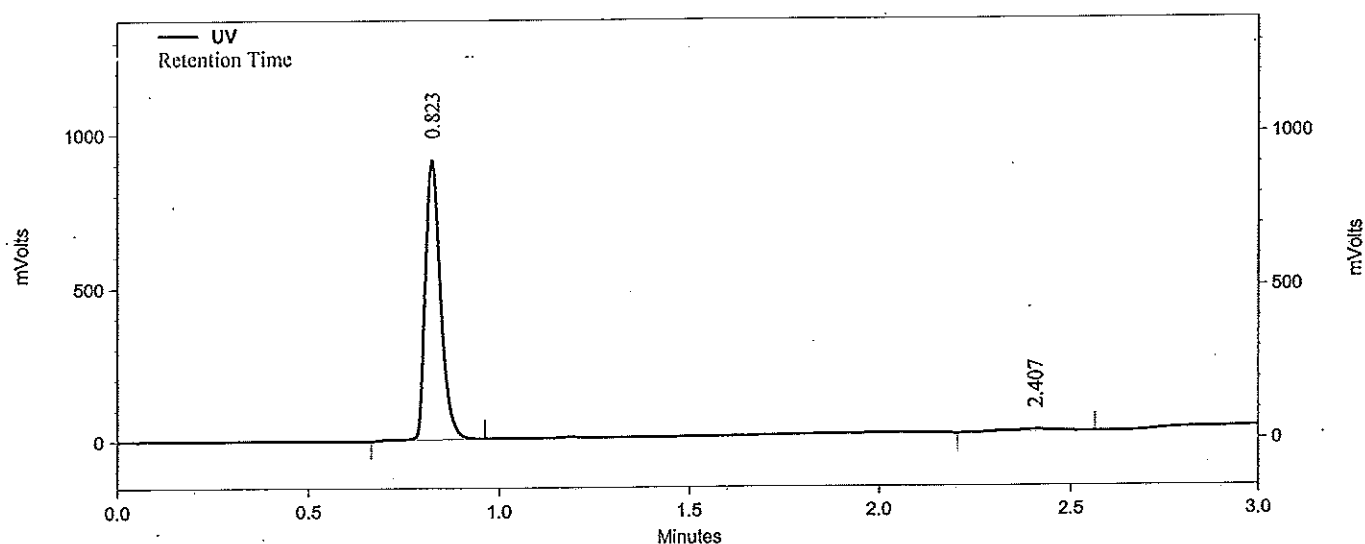


Analytical HPLC Report

File: = C:\CLASS-VP\CHROM\05180.010
 Sample ID: = 70-2-9 MW 532
 Acquired: = 5/18/2006 10:53:42 AM
 User = weixu.zhai
 Instrument = WFD-409D-LCMS2
 Well = 184 Inj. Vol. = 10 uL
 Start % B = 0
 Final % B = 100
 Gradient Time = 2 min
 Flow Rate = 5 ml/min
 Wavelength = 220
 Solvent A = H2O : ACN 95% : 5% 10 mM Ammonium Acetate
 Solvent B = H2O : ACN 5% : 95% 10 mM Ammonium Acetate
 Column 2 = LUNA 3.0 x 50MM S10



70-2-9



UV Results

Pk #	RT	Area	Area %	Height (uV)	Plates
1	0.823	2618509	96.942	910912	1899
2	2.407	82596	3.058	7994	1184
Totals		2701105	100.000	918906	

Sample: 1
File:05180010
Description:

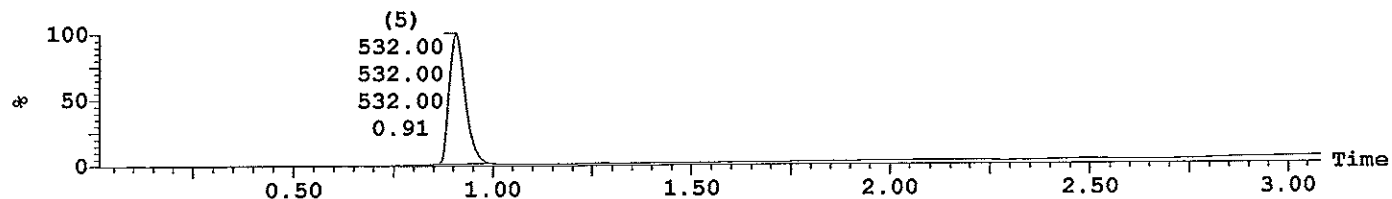
Vial:1:A,1
Date:18-May-2006

ID:70-2-9
Time:10:51:16

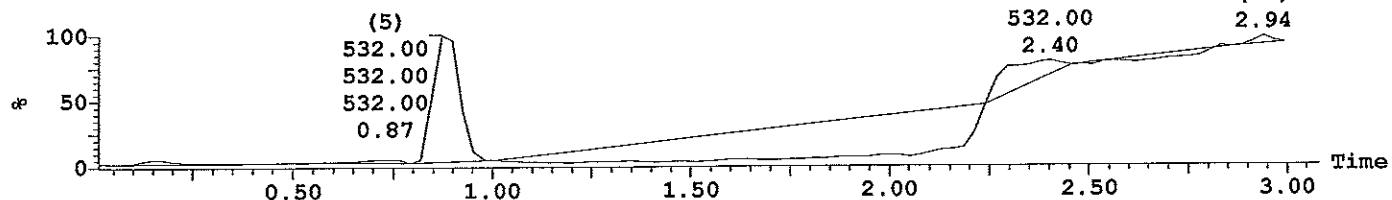
Printed: Thu May 18 10:55:37 2006

Sample Report:

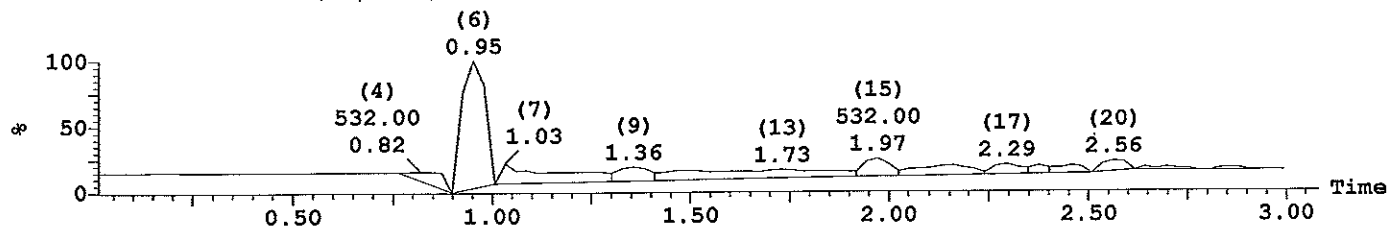
uv 9.2e+005



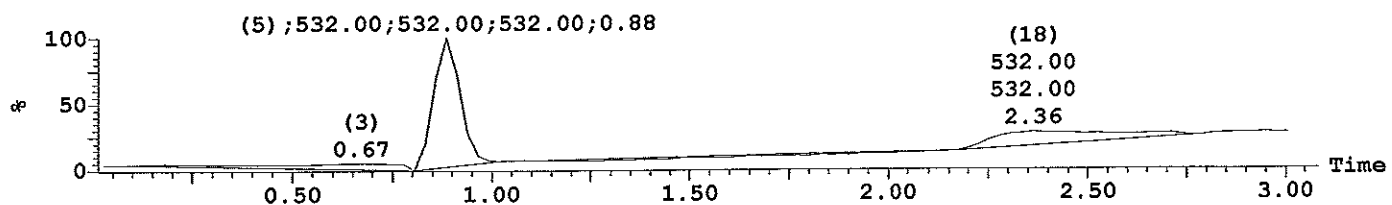
1: MS ES- :TIC Smooth (SG, 1x2) 1.2e+007



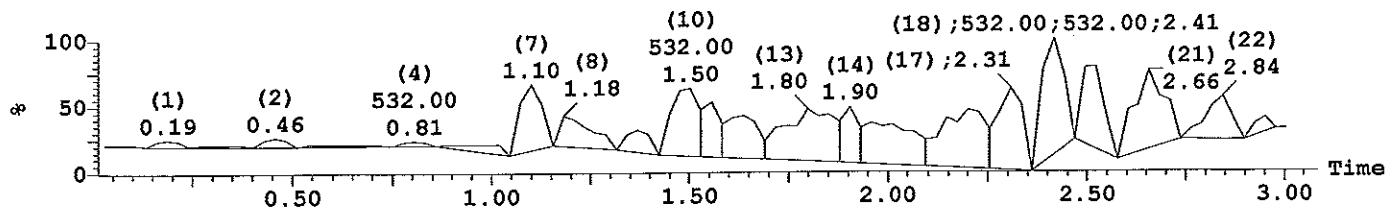
1: MS ES- :531 Smooth (SG, 1x2) 8.5e+004



2: MS ES+ :TIC Smooth (SG, 1x2) 1.0e+008



2: MS ES+ :533 Smooth (SG, 1x2) 8.2e+004



Sample: 1
File:05180010
Description:

Vial:1:A,1
Date:18-May-2006

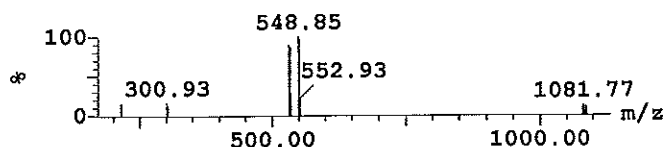
ID:70-2-9
Time:10:51:16

Printed: Thu May 18 10:55:37 2006

Sample Report (continued):

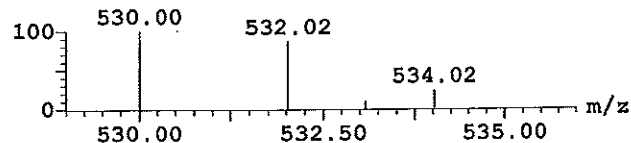
Peak ID Time
4 0.82
Combine (28:32-(21:22+38:39))

2:MS ES+
2.4e+006



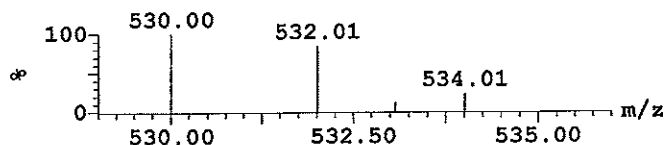
Peak ID Time
5 0.87
Combine (31:35-(23:24+44:45))

1:MS ES-
2.5e+006



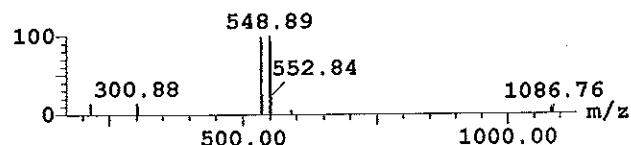
Peak ID Time
5 0.87
Combine (33:36-(24:26+43:45))

1:MS ES-
2.9e+006



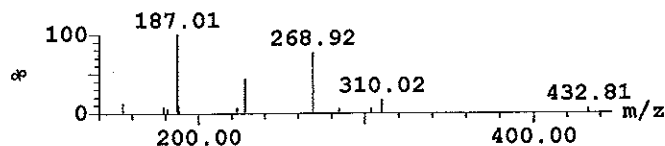
Peak ID Time
5 0.87
Combine (32:36-(24:26+43:44))

2:MS ES+
9.4e+006



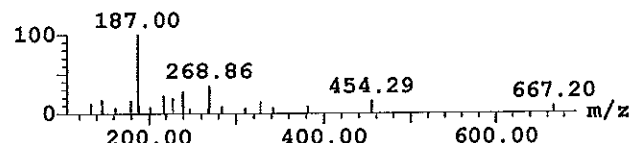
Peak ID Time
15 1.97
Combine (71:75-(65:66+84:85))

2:MS ES+
4.1e+005



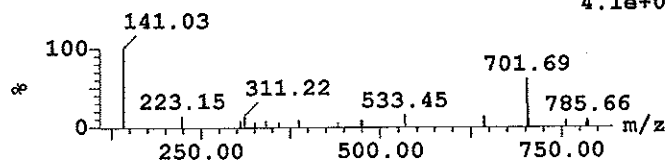
Peak ID Time
16 2.16
Combine (80:84-(71:72+90:91))

2:MS ES+
4.1e+005



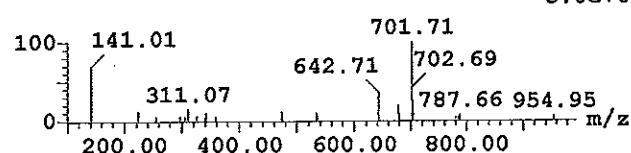
Peak ID Time
17 2.29
Combine (84:88-(77:78+94:95))

1:MS ES-
4.1e+005



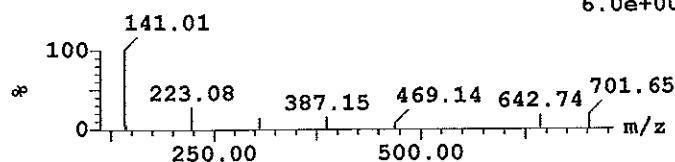
Peak ID Time
18 2.40
Combine (88:92-(77:78+98:99))

1:MS ES-
5.0e+005



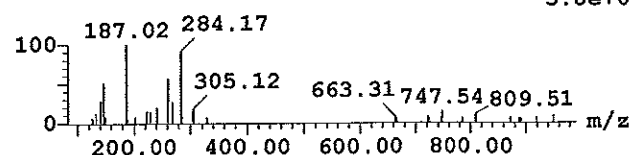
Peak ID Time
22 2.86
Combine (105:109-98:99)

1:MS ES-
6.0e+005



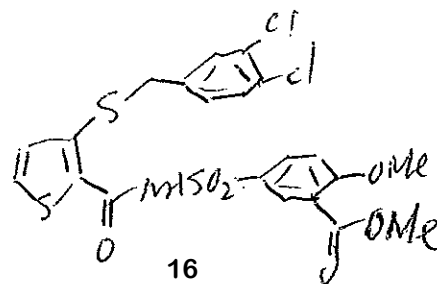
Peak ID Time
22 2.86
Combine (104:108-95:96)

2:MS ES+
5.8e+005

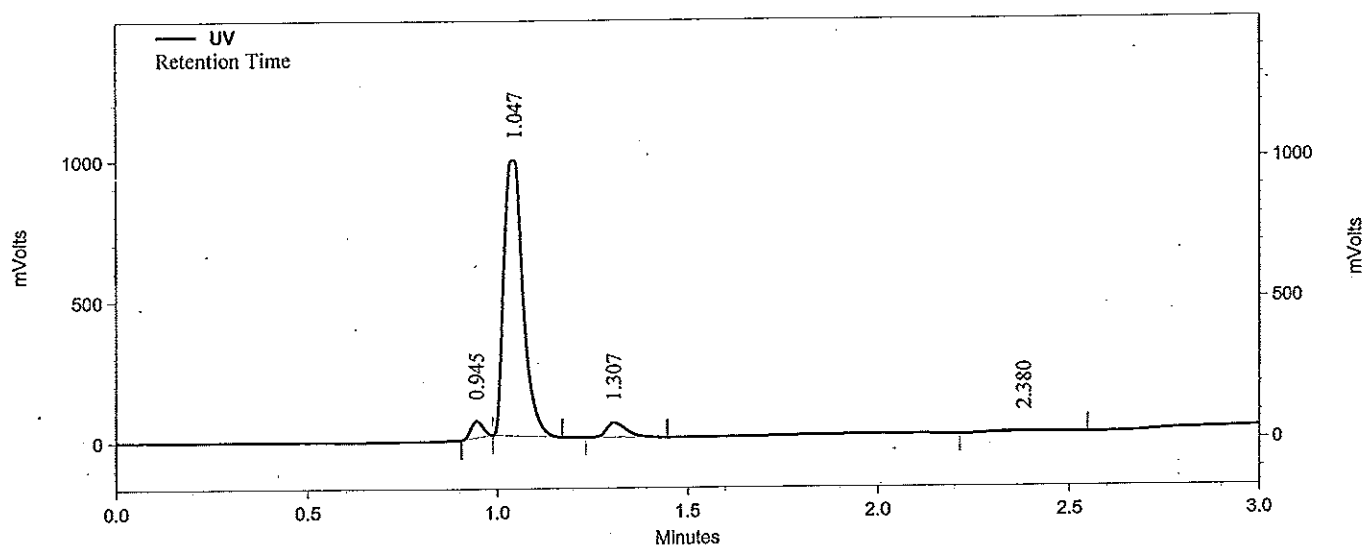


Analytical HPLC Report

File: = C:\CLASS-VP\CHROM\0515I.012
 Sample ID: = 66-3-29 MW 50
 Acquired: = 5/15/2006 11:10:43 AM
 User = weixu.zhai
 Instrument = WFD-409D-LCMS2
 Well = 192 Inj. Vol. = 10 uL
 Start % B = 0
 Final % B = 100
 Gradient Time = 2 min
 Flow Rate = 5 ml/min
 Wavelength = 220
 Solvent A = H2O : ACN 95% : 5% 10 mm Ammonium Acetate
 Solvent B = H2O : ACN 5% : 95% 10 mm Ammonium Acetate
 Column 2 = LUNA 3.0 x 50MM S10



66-3-29



UV Results						
Pk #	RT	Area	Area %	Height (uV)	Plates	
1	0.945	134641	3.536	59253	3652	
2	1.047	3408325	89.523	977312	2424	
3	1.307	195240	5.128	52268	2832	
4	2.380	68995	1.812	6531	1089	
Totals		3807201	100.000	1095364		

Open
Sample
File: 12
Des: 1

Vial: 1:A,1
Date: 15-May-2006

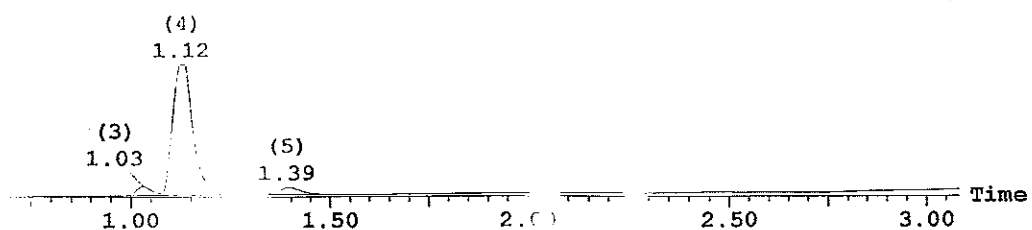
ID: 13-29
Time: 11:08:47

Page 1

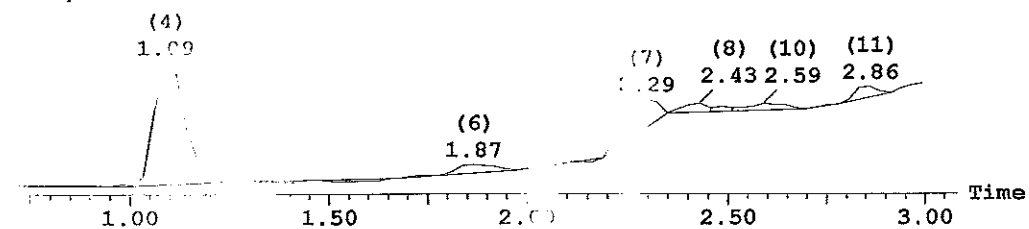
Print: 1x1

Sample Type

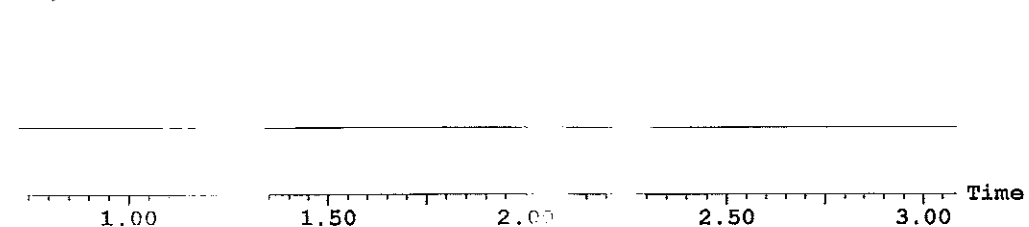
uv 1.0e+006



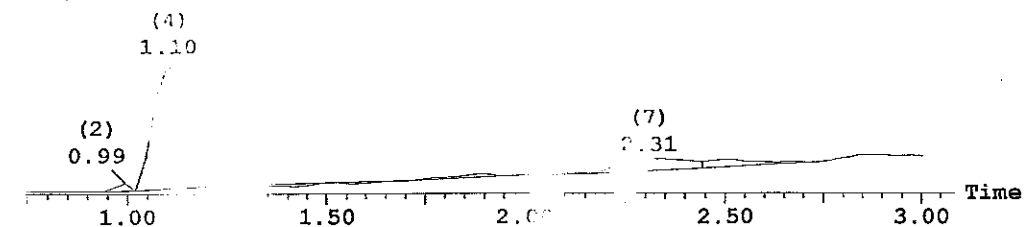
1: 1x2) 3.2e+006



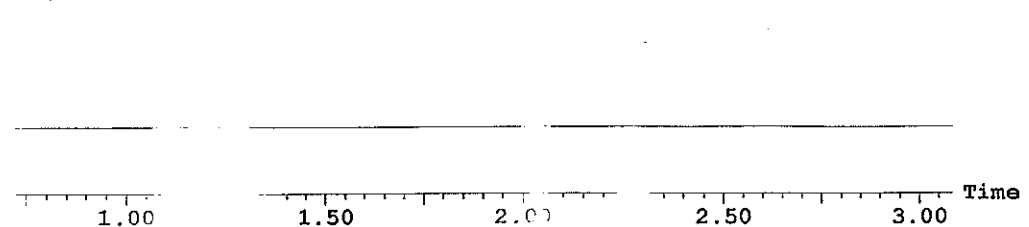
1: 1x2) 0.0e+000



2: 1x2) 4.9e+007



2: 1x2) 0.0e+000



Op: _____
 Sar: _____
 File: _____
 Des: _____

Vial:1:3:1
Date:10-11-2016

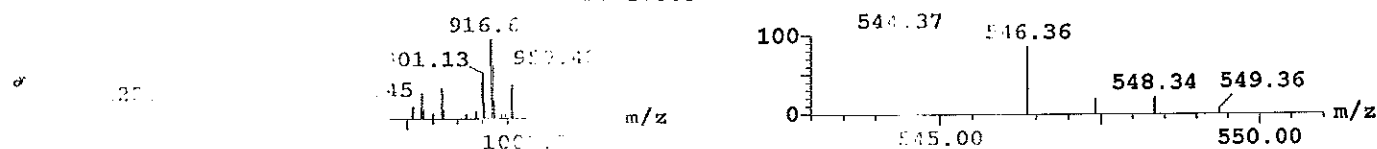
ID:66-3-29
Time:11:08:47

Primer

San

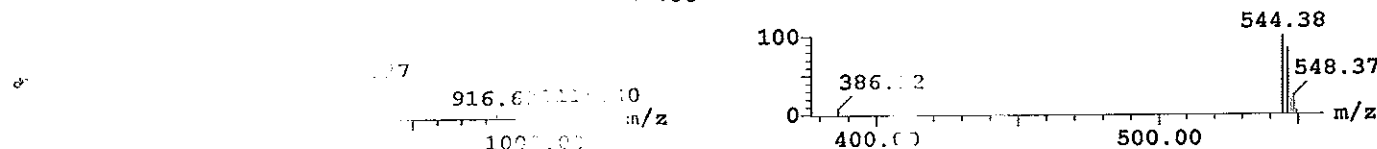
Peak ID	Time
3	1.0

Combine (37: 1-(27:29+46:48)) 1:MS ES-
4.1e+005



Peak ID	Time
4	1.1

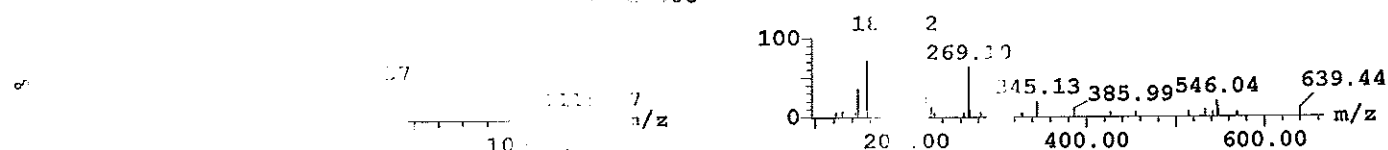
Combine (41:33:35+54:56)) 1:MS ES-
7.4e+005



Peak ID	Time
6	1.8

Combine (61:79)-(57:58+79:80))

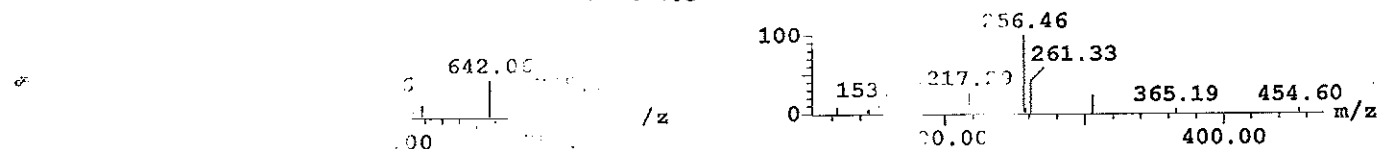
2:MS ES+
2.0e+005



Peak ID	Time
7	2.2

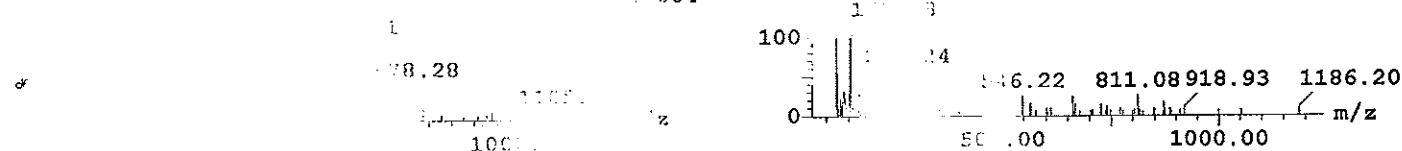
Combine (84) = (74:75+97:98)

2:MS ES+
7.2e+005



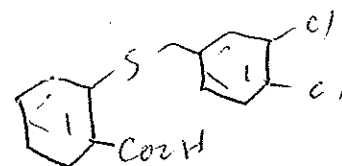
Peak ID	Time
10	2.9

Combine (93:7)-(84:95+107:108)) 2:MS ES+
1.7e+005



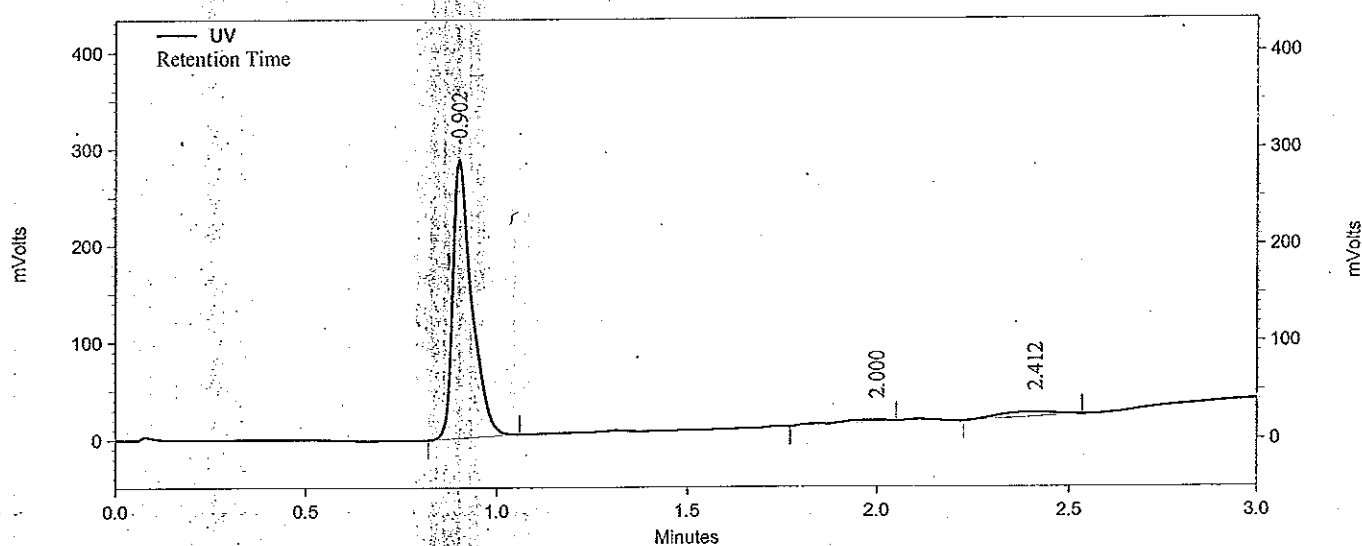
Analytical HPLC Report

File: = C:\CLASS-VP\CHROM\0224I.015
 Sample ID: = 183-19 MW 313
 Acquired: = 2/24/2006 9:43:29 AM
 User = weixu.zhai
 Instrument = WFD-409D-LCMS2
 Well = 104 Inj. Vol. = 10 uL
 Start % B = 0
 Final % B = 100
 Gradient Time = 2 min
 Flow Rate = 5 ml/min
 Wavelength = 220
 Solvent A = H2O : ACN 95% : 5% 10 mM Ammonium Acetate
 Solvent B = H2O : ACN 5% : 95% 10 mM Ammonium Acetate
 Column 2 = LUNA 3.0 x 50MM S10



17

183-19



UV Results						
Pk #	RT	Area	Area %	Height (uV)	Plates	
1	0.902	969904	92.960	286863	1880	
2	2.000	20758	1.990	1768	2024	
3	2.412	52696	5.051	4737	1211	
Totals		1043358	100.000	293368		

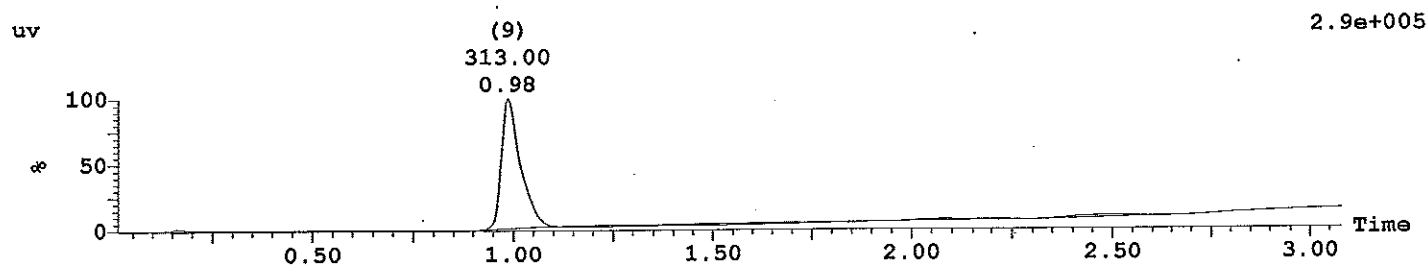
Sample: 1
File:0224I015
Description:

Vial:1:A,1
Date:24-Feb-2006

ID:183-19
Time:09:40:48

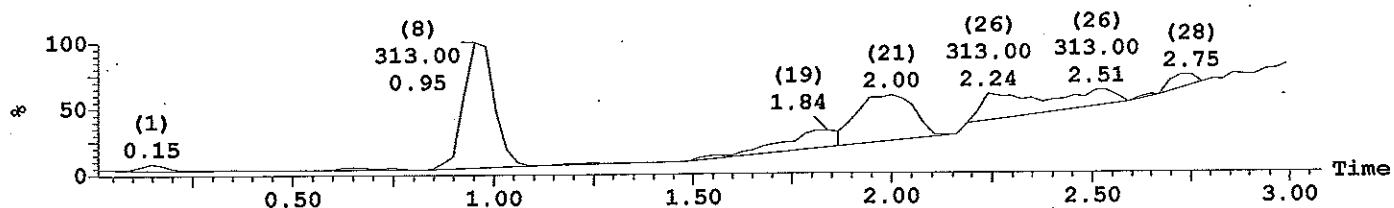
Printed: Fri Feb 24 09:45:04 2006

Sample Report:



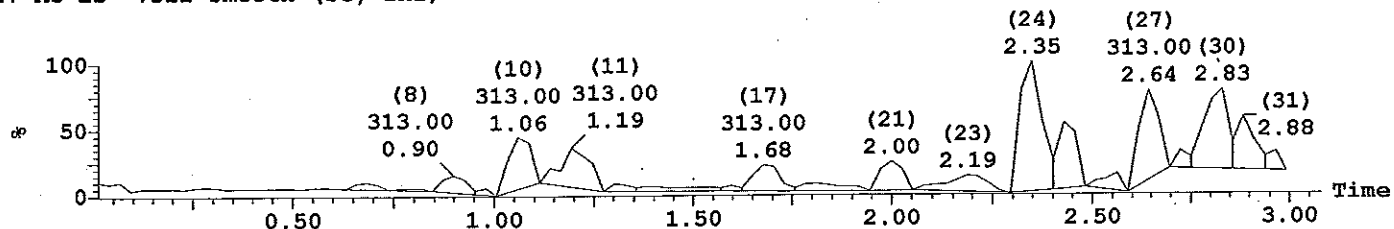
1: MS ES- :TIC Smooth (SG, 1x2)

1.5e+007



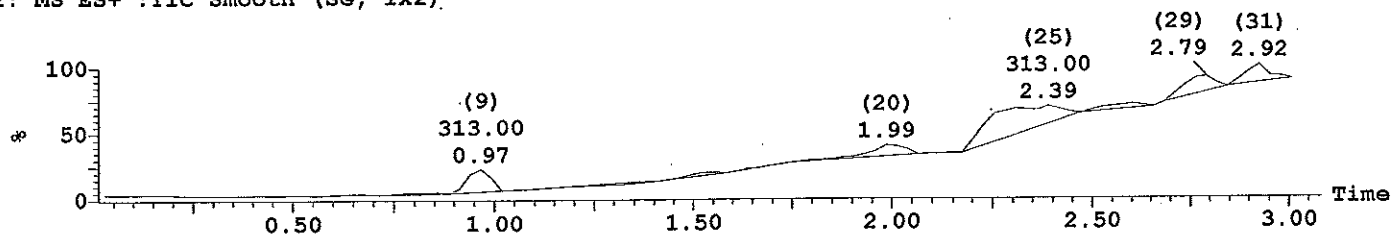
1: MS ES- :312 Smooth (SG, 1x2)

8.8e+004



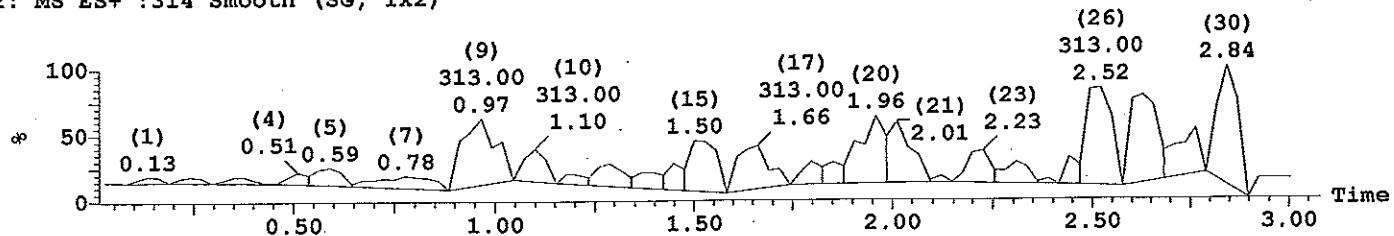
2: MS ES+ :TIC Smooth (SG, 1x2)

1.3e+008



2: MS ES+ :314 Smooth (SG, 1x2)

1.7e+005



Sample: 1
File:02241015
Description:

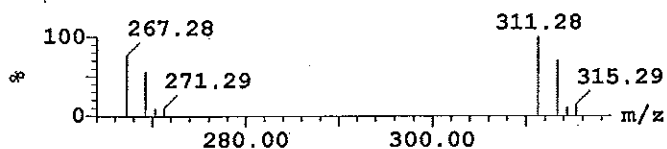
Vial:1:A,1
Date:24-Feb-2006

ID:183-19
Time:09:40:48

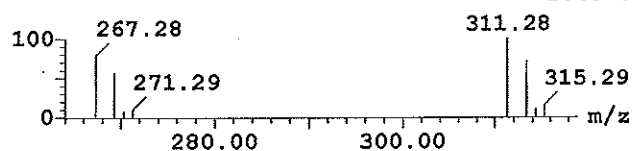
Printed: Fri Feb 24 09:45:04 2006

Sample Report (continued):

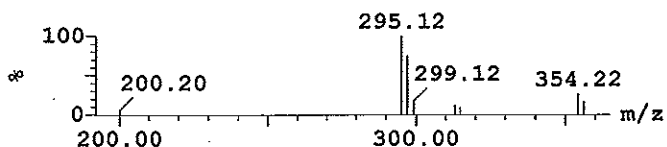
Peak ID Time
8 0.95
Combine (34:38-(24:25+48:49)) 1:MS ES-
2.3e+006



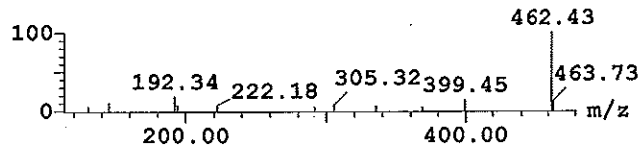
Peak ID Time
9 0.98
Combine (35:39-(27:29+47:49)) 1:MS ES-
2.4e+006



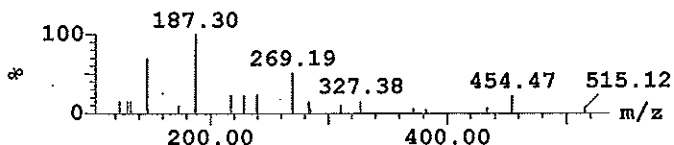
Peak ID Time
9 0.98
Combine (35:39-(26:28+46:48)) 2:MS ES+
3.5e+006



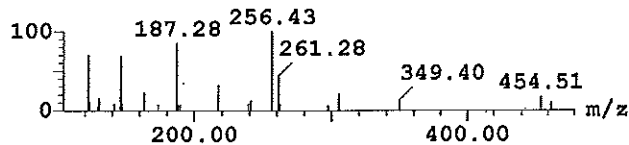
Peak ID Time
15 1.54
Combine (54:58-(48:49+65:66)) 2:MS ES+
1.1e+006



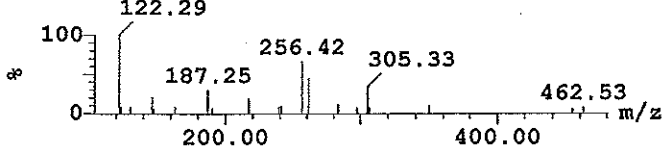
Peak ID Time
23 2.19
Combine (81:85-(73:74+90:91)) 2:MS ES+
1.7e+006



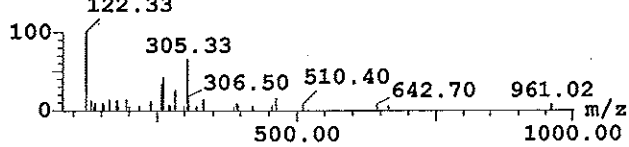
Peak ID Time
24 2.35
Combine (84:88-(77:78+94:95)) 2:MS ES+
2.6e+006



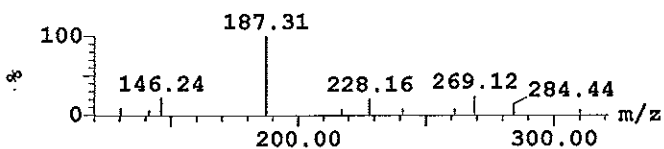
Peak ID Time
25 2.43
Combine (87:91-(74:75+98:99)) 2:MS ES+
3.8e+006



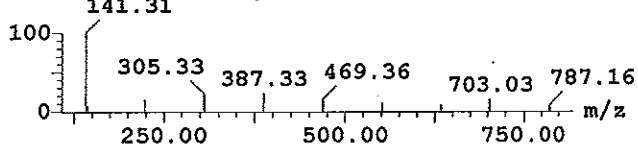
Peak ID Time
26 2.51
Combine (92:96-(85:86+102:103)) 2:MS ES+
8.6e+005



Peak ID Time
29 2.79
Combine (102:106-(93:94+112)) 2:MS ES+
5.4e+006

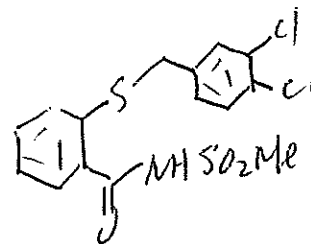


Peak ID Time
30 2.83
Combine (104:108-96:97) 1:MS ES-
9.3e+005



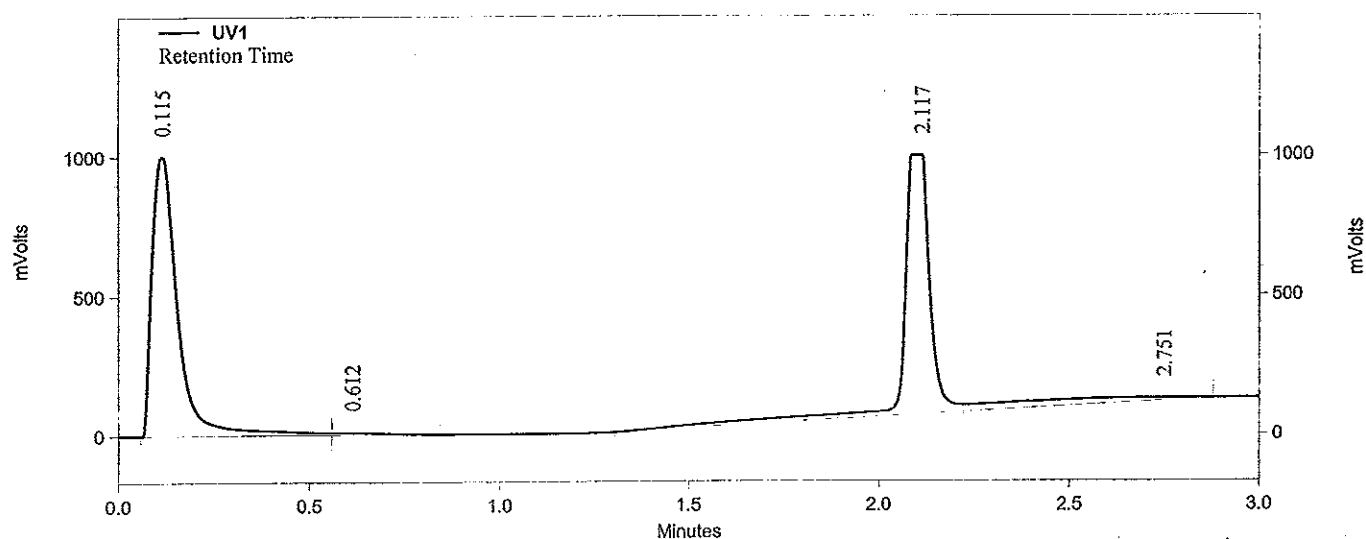
Analytical HPLC Report

File: = C:\CLASS-VP\CHROM\0511M.042
 Sample ID: = 65859-061-01 MW 390
 Acquired: = 5/11/2006 4:37:26 PM
 User = weixu.zhai
 Instrument = WFD-409D-LCMS
 Well = 192 Inj. Vol. = 5 uL
 Start % B = 0
 Final % B = 100
 Gradient Time = 2 min
 Flow Rate = 5 ml/min
 Wavelength = 220
 Solvent A = 10% MeOH - 90% H2O - 0.1% TFA
 Solvent B = 90% MeOH - 10% H2O - 0.1% TFA
 Column 1 = (1) Phenomenex 10u C18 3.0X50mm



18

65859-061-01



UV1 Results						
Pk #	RT	Area	Area %	Height (uV)	Plates	
1	0.115	4759938	48.029	999026	17	
2	0.612	63322	0.639	7333	0	
3	2.117	4403798	44.436	928873	8831	
4	2.751	683426	6.896	10099	0	
Totals		9910484	100.000	1945331		

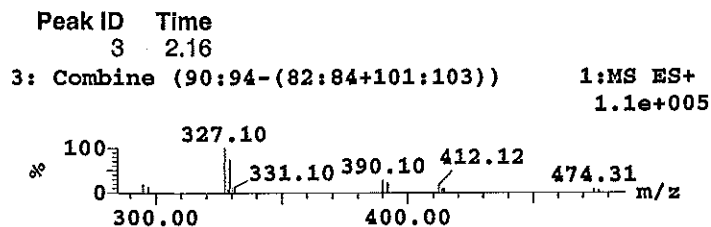
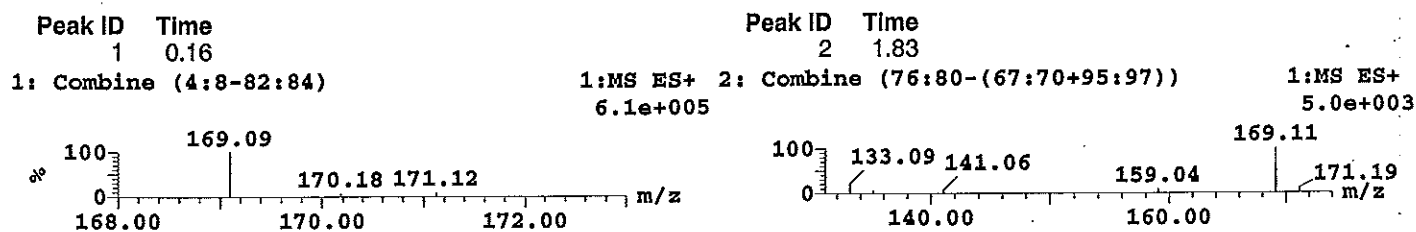
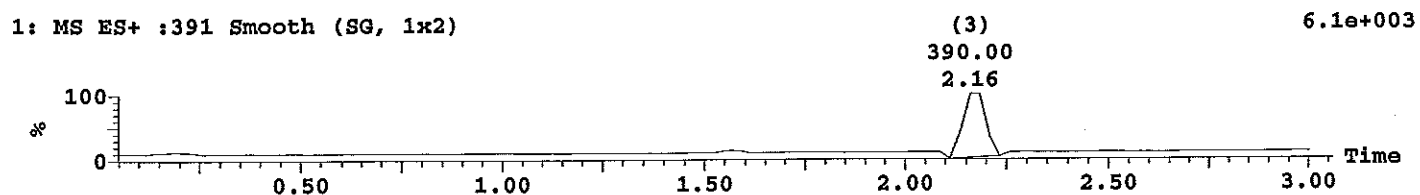
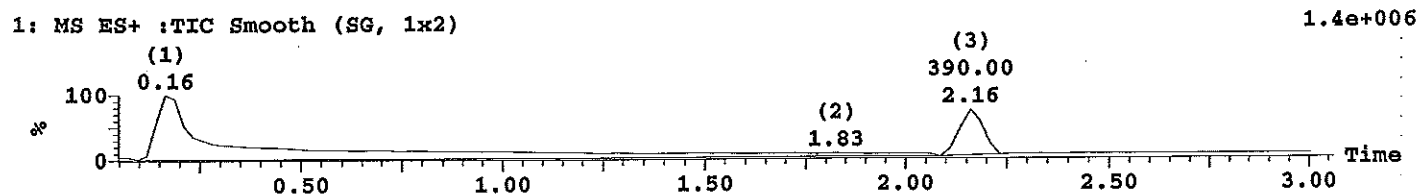
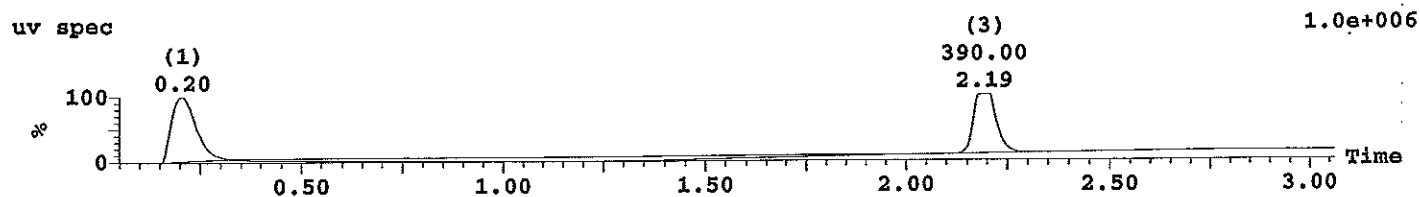
Sample: 1
File:0511M042
Description:

Vial:1:A,1
Date:11-May-2006

ID:65859-061-01
Time:16:33:52

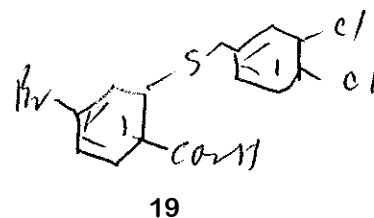
Printed: Thu May 11 16:39:13 2006

Sample Report:

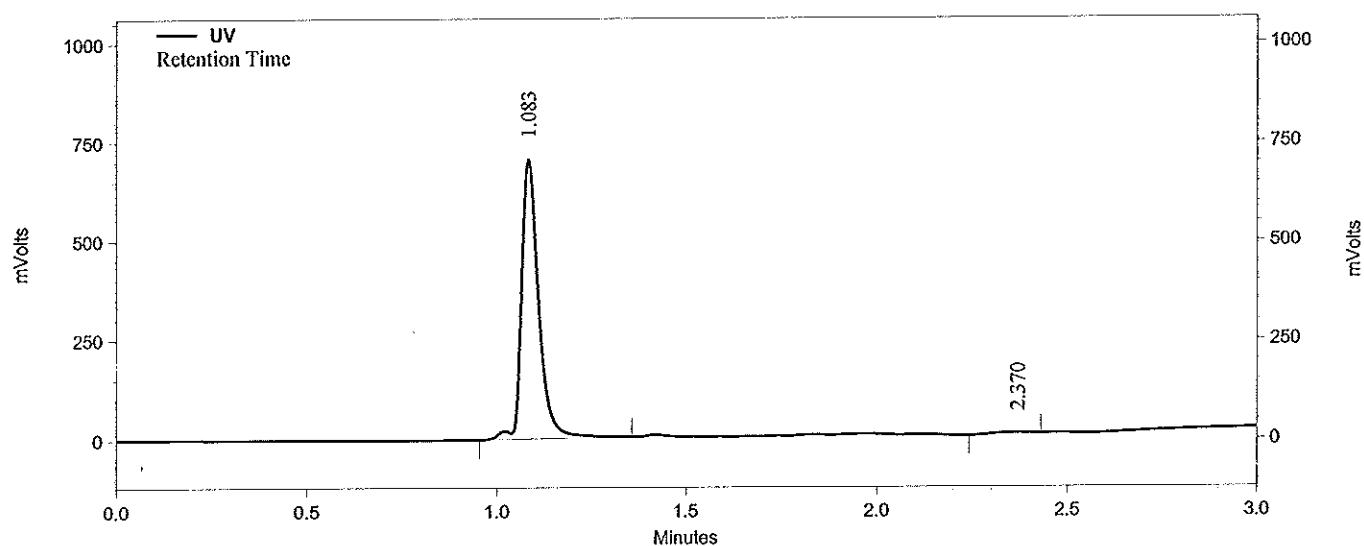


Analytical HPLC Report

File: = C:\CLASS-VP\CHROM\0713R.035
 Sample ID: = 119-53 MW 392
 Acquired: = 7/13/2006 2:41:03 PM
 User = weixu.zhai
 Instrument = WFD-409D-LCMS2
 Well = 191 Inj. Vol. = 10 uL
 Start % B = 0
 Final % B = 100
 Gradient Time = 2 min
 Flow Rate = 5 ml/min
 Wavelength = 220
 Solvent A = H2O : ACN 95% : 5% 10 mM Ammonium Acetate
 Solvent B = H2O : ACN 5% : 95% 10 mM Ammonium Acetate
 Column 2 = LUNA 3.0 x 50MM S10



119-53



UV Results

Pk #	RT	Area	Area %	Height (uV)	Plates
1	1.083	2272724	99.121	705259	2916
2	2.370	20160	0.879	3138	3688
Totals		2292884	100.000	708397	

Sample: 1
File:0713R035
Description:

Vial:1:A,1
Date:13-Jul-2006

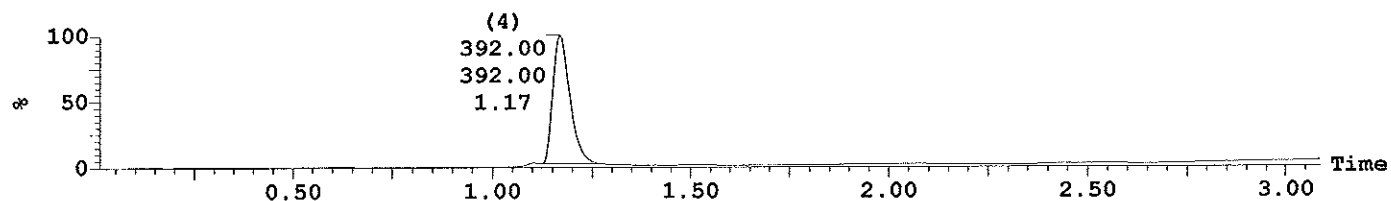
ID:119-53
Time:14:35:38

Printed: Thu Jul 13 14:41:49 2006

Sample Report:

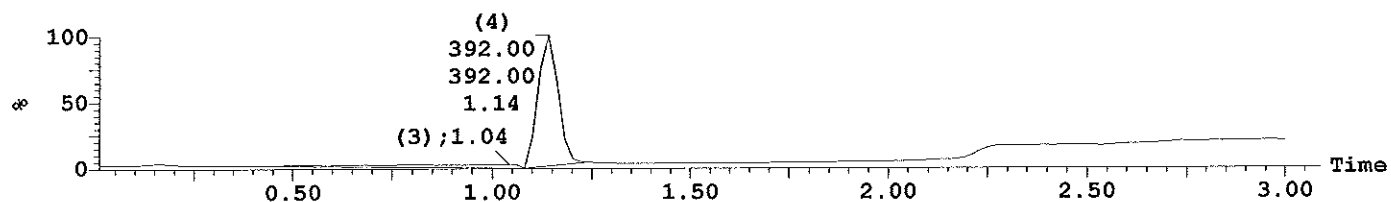
Channel 1

7.1e+005



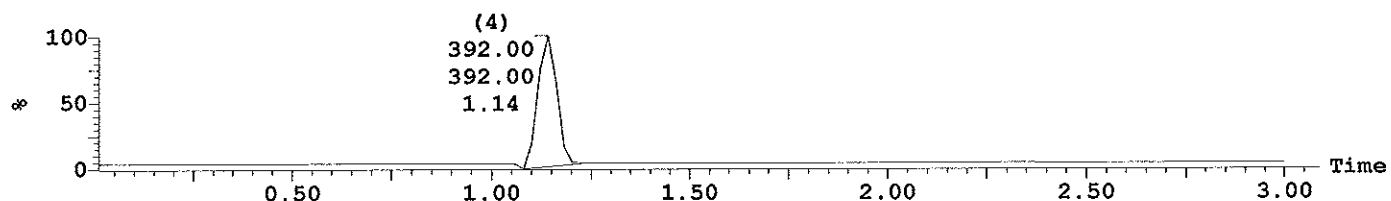
1: MS ES- :TIC Smooth (SG, 1x2)

5.2e+007



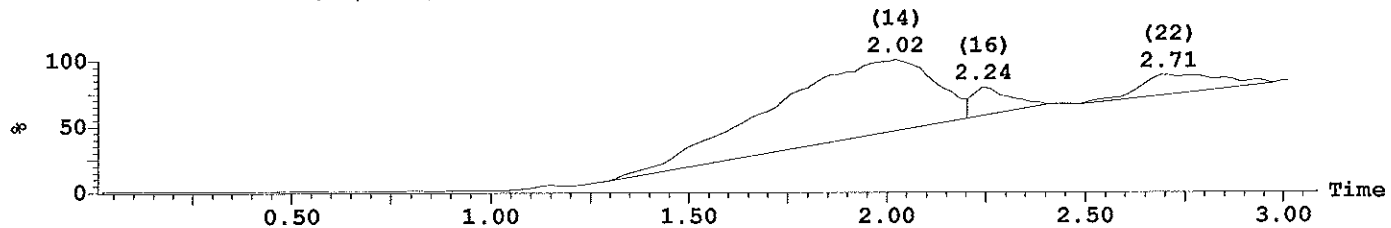
1: MS ES- :391 Smooth (SG, 1x2)

1.1e+007



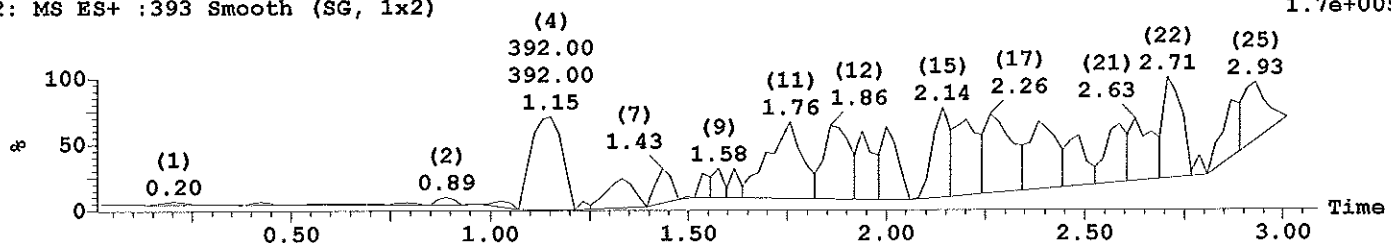
2: MS ES+ :TIC Smooth (SG, 1x2)

1.3e+008



2: MS ES+ :393 Smooth (SG, 1x2)

1.7e+005



Sample: 1
File:0713R035
Description:

Vial:1:A,1
Date:13-Jul-2006

ID:119-53
Time:14:35:38

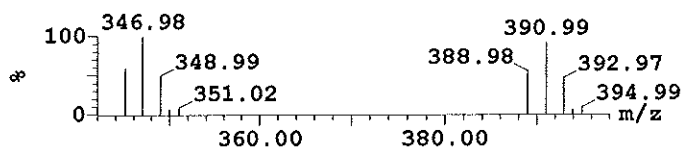
Printed: Thu Jul 13 14:41:49 2006

Sample Report (continued):

Peak ID Time
4 1.14

Combine (55:59-(44:47+69:72))

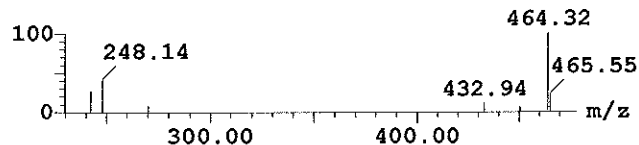
1:MS ES-
5.8e+006



Peak ID Time
9 1.58

Combine (76:80-(67:70+86:89))

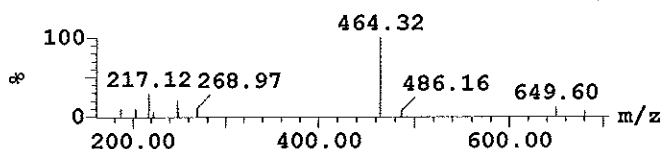
2:MS ES+
1.9e+006



Peak ID Time
11 1.76

Combine (85:89-(71:74+97:100))

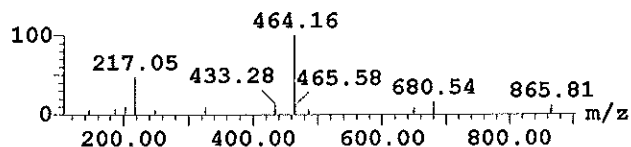
2:MS ES+
5.7e+006



Peak ID Time
12 1.86

Combine (90:94-(80:83+102:105))

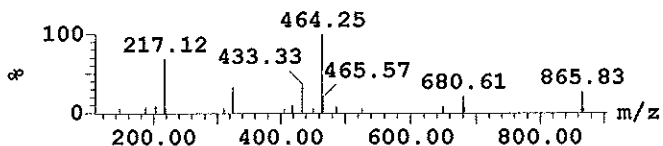
2:MS ES+
5.4e+006



Peak ID Time
13 1.94

Combine (94:98-(85:88+105:108))

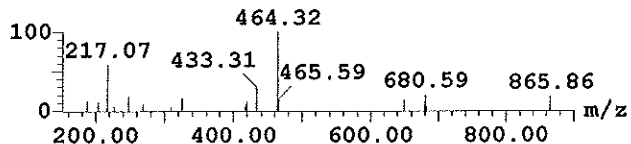
2:MS ES+
4.5e+006



Peak ID Time
14 2.02

Combine (98:102-(54:57+116:119))

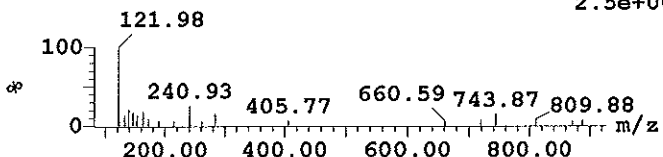
2:MS ES+
1.7e+007



Peak ID Time
18 2.38

Combine (116:120-(106:109+128:131))

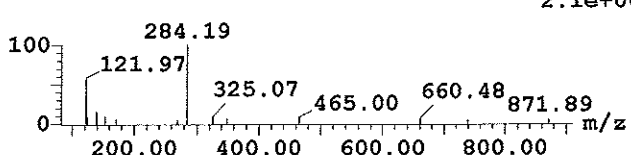
2:MS ES+
2.5e+006



Peak ID Time
20 2.59

Combine (126:130-(115:118+136:139))

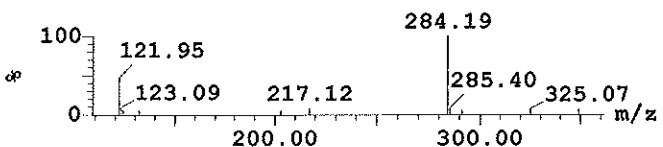
2:MS ES+
2.1e+006



Peak ID Time
21 2.63

Combine (128:132-(119:122+140:143))

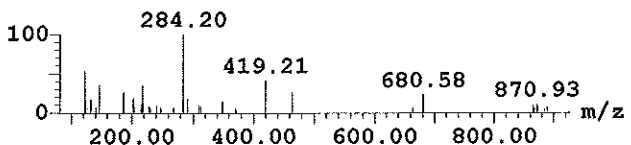
2:MS ES+
3.6e+006



Peak ID Time
22 2.71

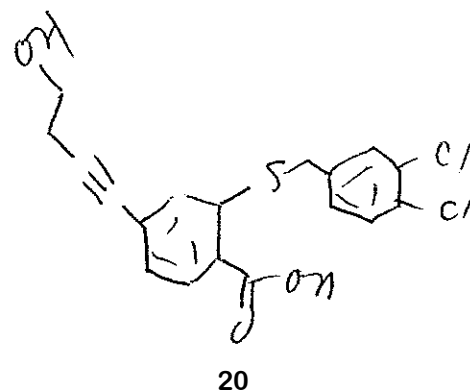
Combine (132:136-113:116)

2:MS ES+
3.0e+006

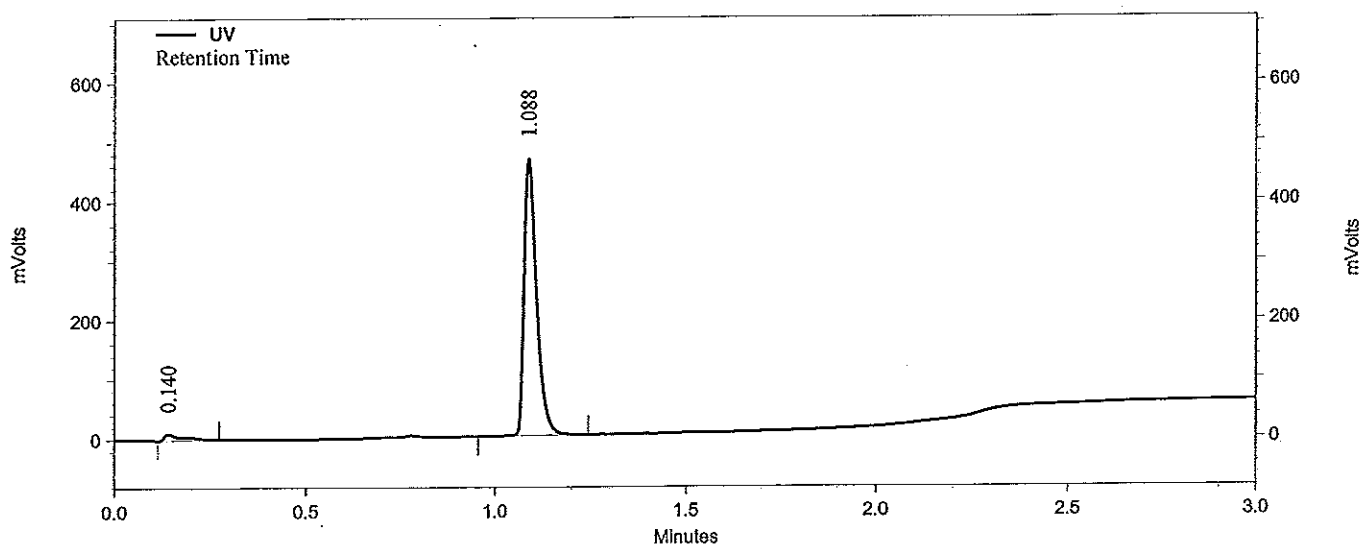


Analytical HPLC Report

File: = C:\CLASS-VP\CHROM\1004F.021
 Sample ID: = 187-02-09 MW 381
 Acquired: = 10/4/2006 12:23:46 PM
 User = weixu.zhai
 Instrument = WFD-409D-LCMS2
 Well = 192 Inj. Vol. = 10 uL
 Start % B = 0
 Final % B = 100
 Gradient Time = 2 min
 Flow Rate = 5 ml/min
 Wavelength = 220
 Solvent A = H2O : ACN 95% : 5% 10 mM Ammonium Acetate
 Solvent B = H2O : ACN 5% : 95% 10 mM Ammonium Acetate
 Column 2 = Xbridge C18 4.6 x 50MM S5



187-02-09



UV Results					
Pk #	RT	Area	Area %	Height (uV)	Plates
1	0.140	37380	3.432	10966	68
2	1.088	1051869	96.568	466617	5588
Totals		1089249	100.000	477583	

Sample: 1

Vial:1:A,1

ID:187-02-09

File:1004F021

Date:04-Oct-2006

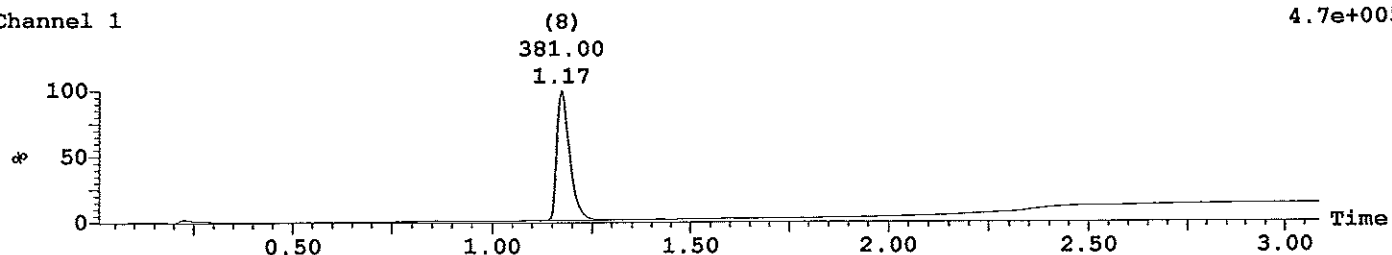
Time:12:19:55

Description:

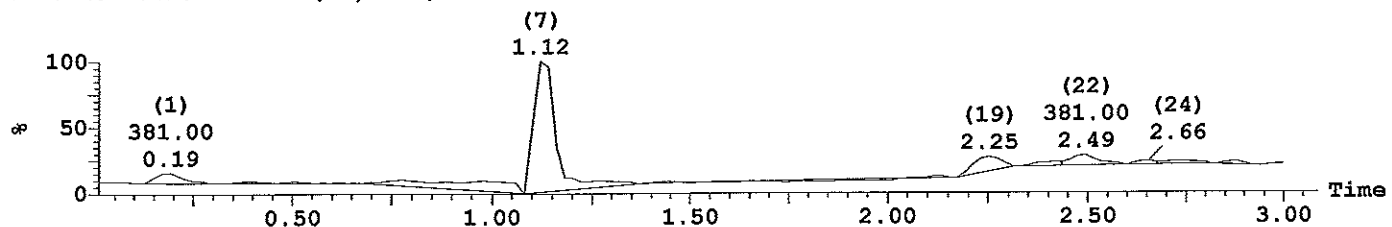
Printed: Wed Oct 04 12:24:58 2006

Sample Report:

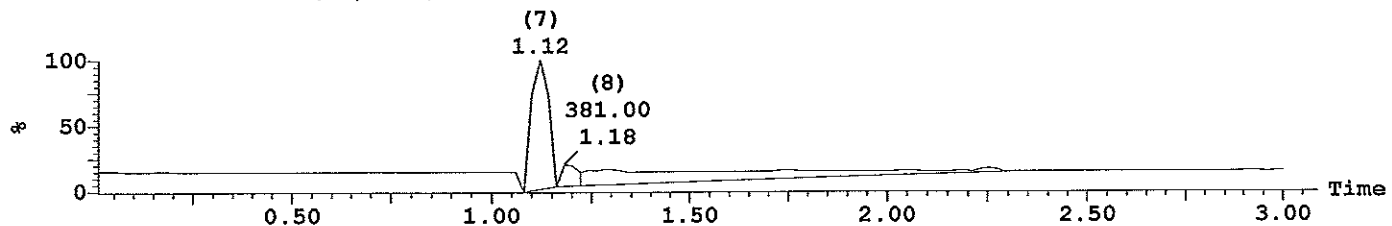
Channel 1 4.7e+005



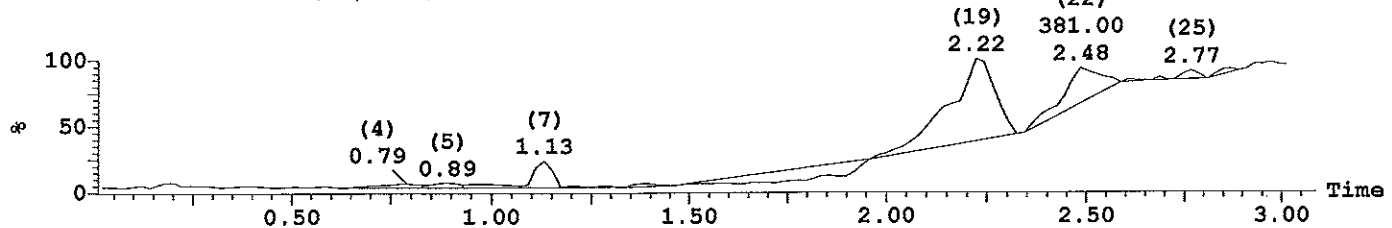
1: MS ES- :TIC Smooth (SG, 1x2) 5.1e+006



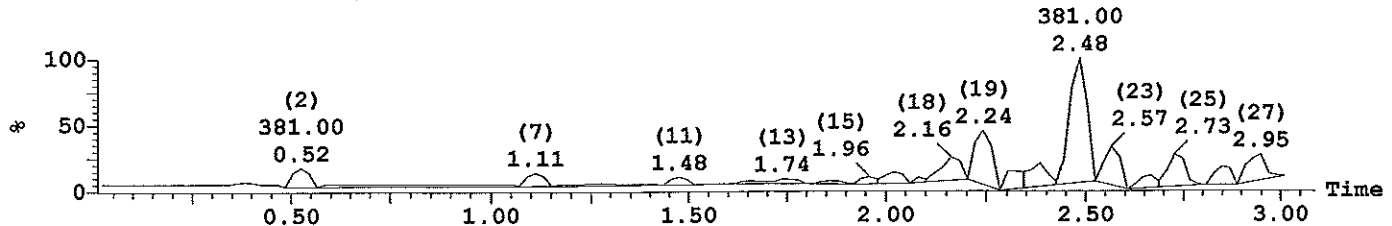
1: MS ES- :380 Smooth (SG, 1x2) 1.6e+005



2: MS ES+ :TIC Smooth (SG, 1x2) 2.2e+007



2: MS ES+ :382 Smooth (SG, 1x2) 1.1e+005



Sample: 1

Vial:1:A,1

ID:187-02-09

File:1004F021

Date:04-Oct-2006

Time:12:19:55

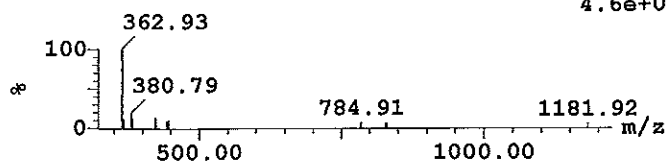
Description:

Printed: Wed Oct 04 12:24:58 2006

Sample Report (continued):

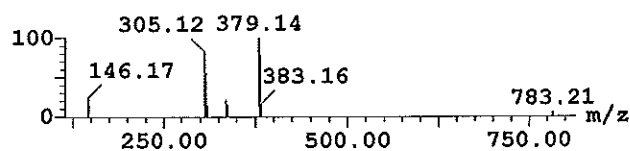
Peak ID Time
7 1.12
Combine (54:58-(43:46+65:68))

2:MS ES+
4.6e+005



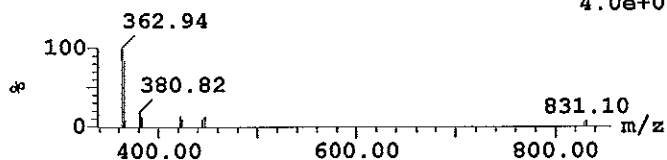
Peak ID Time
8 1.18
Combine (56:61-(42:44+73:76))

1:MS ES-
3.9e+005



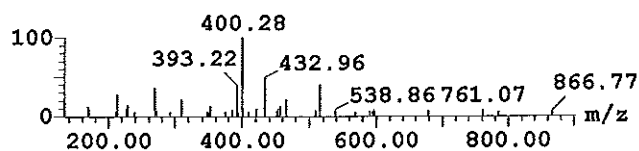
Peak ID Time
8 1.18
Combine (56:60-(42:44+73:75))

2:MS ES+
4.0e+005



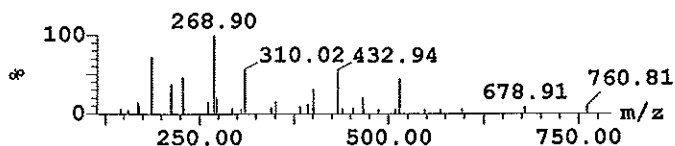
Peak ID Time
17 2.08
Combine (101:105-(92:95+111:114))

2:MS ES+
3.1e+005



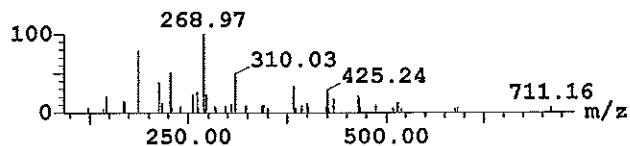
Peak ID Time
18 2.16
Combine (105:109-(94:97+116:119))

2:MS ES+
6.8e+005



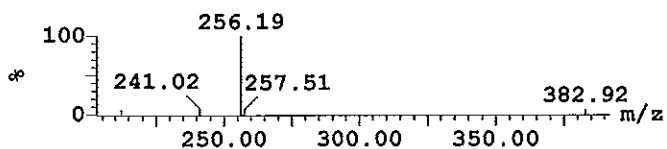
Peak ID Time
19 2.25
Combine (108:112-(87:90+122:125))

2:MS ES+
6.5e+005



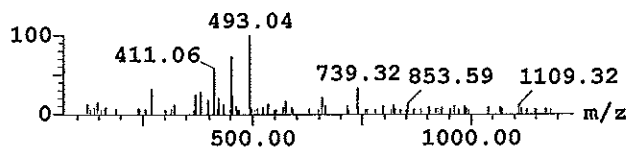
Peak ID Time
20 2.30
Combine (112:116-(103:106+123:126))

2:MS ES+
5.7e+005



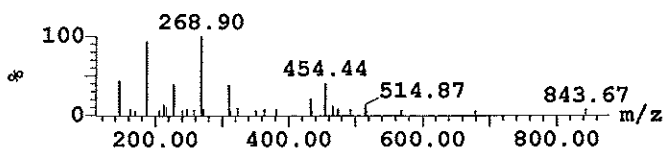
Peak ID Time
22 2.49
Combine (121:125-(110:113+132:135))

2:MS ES+
2.0e+005



Peak ID Time
23 2.57
Combine (125:129-(115:118+136:139))

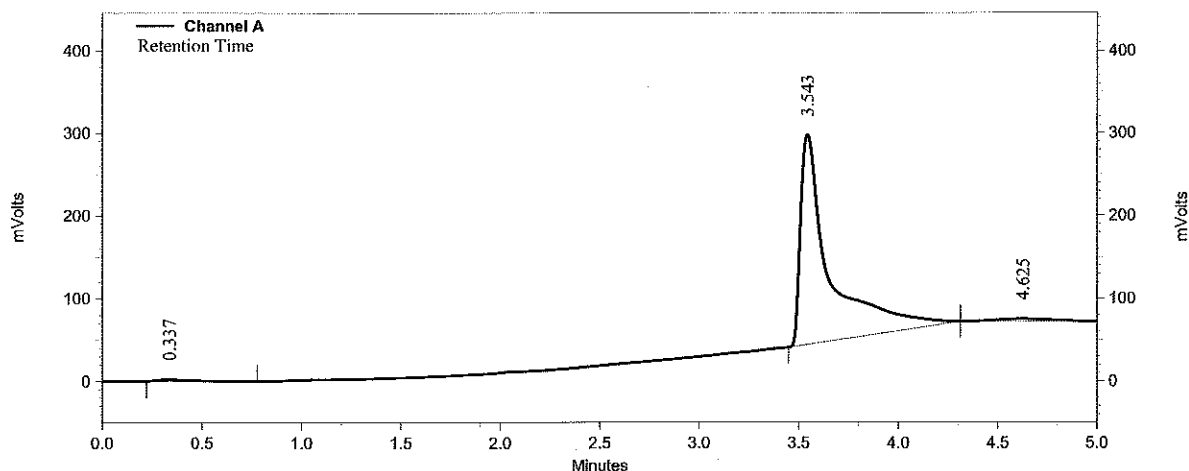
2:MS ES+
4.6e+005



Analytical HPLC Report

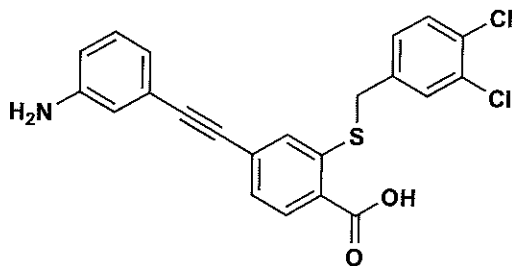
File: =
 c:\shimadzu\data\public\shirong.zhu\20100405\2010_0405_1624-027.dat
 Sample ID: = 86453-003T3
 Acquired: = 4/5/2010 4:28:35 PM
 File = 2010_0405_1624.027
 User = shirong.zhu
 Instrument = WFD-409D-LCMS2
 Well = 177 Inj. Vol. = 10 uL
 Start % B = 0
 Final % B = 100
 Gradient Time = 4 min
 Flow Rate = .8 ml/min
 Wavelength = 220
 Solvent Pair = Water/Methanol/Ammonium Acetate
 Solvent A = 95% Water/ 5% Methanol/10 mM Ammonium Acetate
 Solvent B = 5% Water/ 95% Methanol/10 mM Ammonium Acetate
 Column 2 = (2) PHENOMENEX-LUNA 2.0 x 50 mm 3um
 MW1 = 132+/-

86453-003T3



Channel A Results

Pk #	RT	Area	Area %	Height (uV)	Plates
1	0.337	29983	1.111	2606	27
2	3.543	2612521	96.787	253206	4607
3	4.625	56750	2.102	2950	1203
Totals		2699254	100.000	258762	



Exact Mass: 427.02

Compound 21

Openlynx Report BMS LCMS Report- shirong.zhu

Page 1

Sample: 1
 File: 2010_0405_1624-027
 Description:

Vial: 1:A,1
 Date: 05-Apr-2010

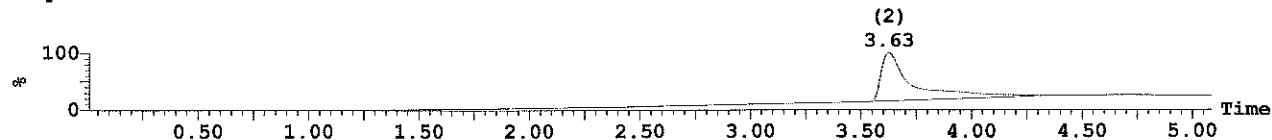
ID: 86453-003T3
 Time: 16:25:59

Printed: Mon Apr 05 16:33:38 2010

Sample Report:

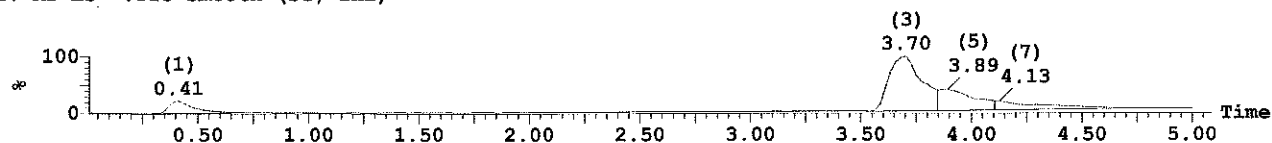
uv spec

3.0e+005



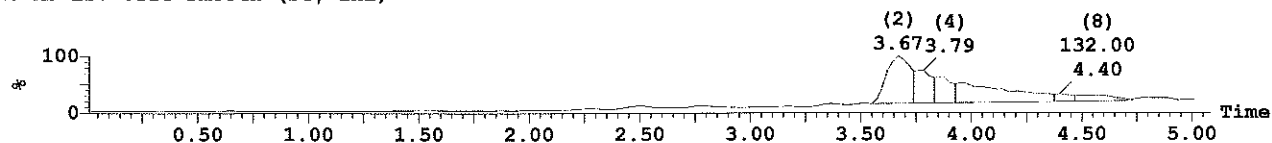
1: MS ES- :TIC Smooth (SG, 1x2)

2.2e+007



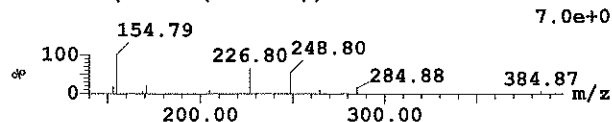
2: MS ES+ :TIC Smooth (SG, 1x2)

4.7e+007



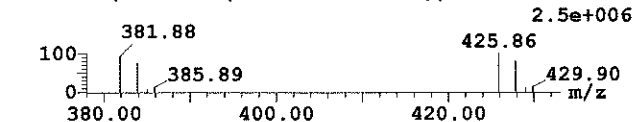
Peak ID Time
 1 0.41

Combine (14:22-(1+44:46))



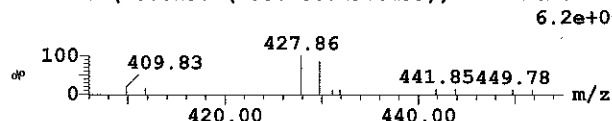
Peak ID Time
 2 3.67

Combine (150:159-(136:138+197:200))



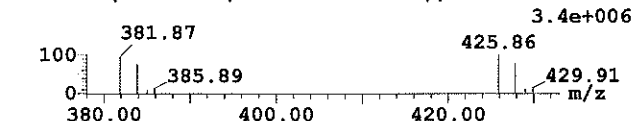
Peak ID Time
 2 3.67

Combine (150:158-(135:138+197:199))



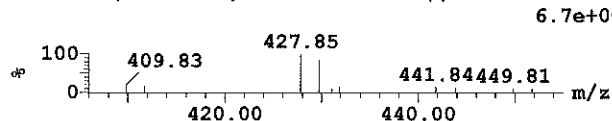
Peak ID Time
 3 3.71

Combine (154:162-(136:138+177:179))



Peak ID Time
 4 3.79

Combine (157:165-(144:146+176:178))



Openlynx Report BMS LCMS Report- shirong.zhu

Page 2

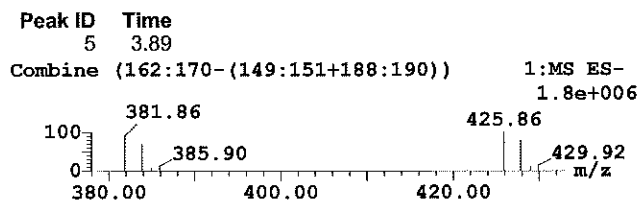
Sample: 1
File: 2010_0405_1624-027
Description:

Vial: 1:A,1
Date: 05-Apr-2010

ID: 86453-003T3
Time: 16:25:59

Printed: Mon Apr 05 16:33:38 2010

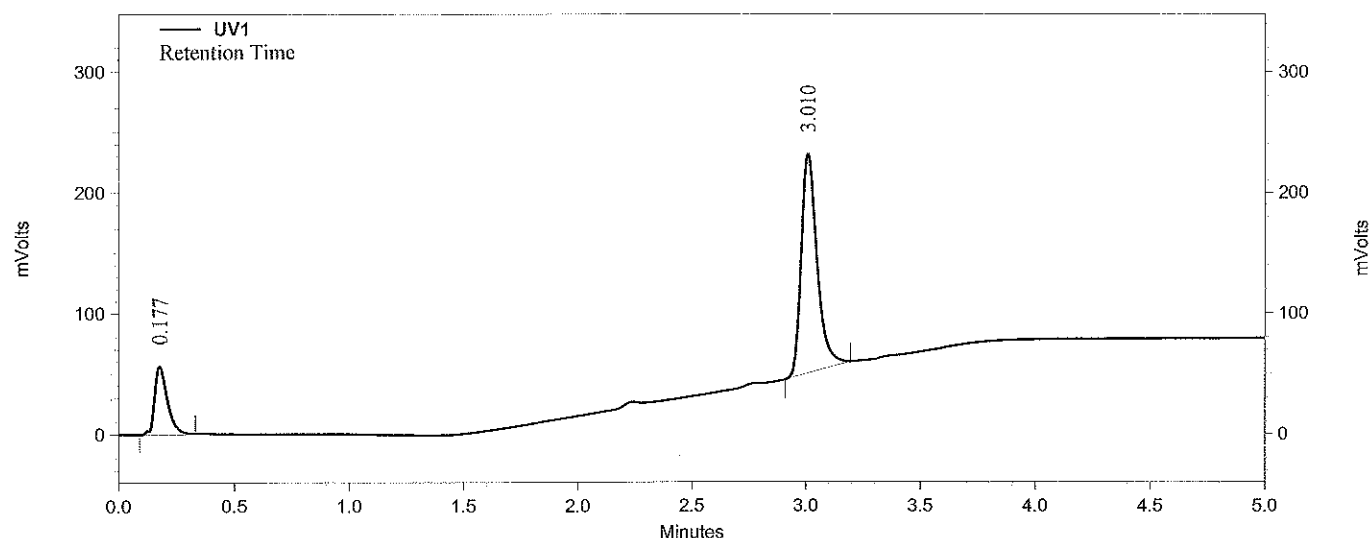
Sample Report (continued):



Analytical HPLC Report

File: = C:\CLASS-VP\CHROM\0126G.025
 Sample ID: = 62464-130-1 MW 50
 Acquired: = 1/26/2007 11:06:45 AM
 User = shirong.zhu
 Instrument = WFD-409D-LCMS
 Well = 121 Inj. Vol. = 5 uL
 Start % B = 0
 Final % B = 100
 Gradient Time = 3 min
 Flow Rate = 4 ml/min
 Wavelength = 220
 Solvent A = 10% MeOH - 90% H2O - 0.1% TFA
 Solvent B = 90% MeOH - 10% H2O - 0.1% TFA
 Column 6 = (6) XTERRA 4.6 X 30mm S5

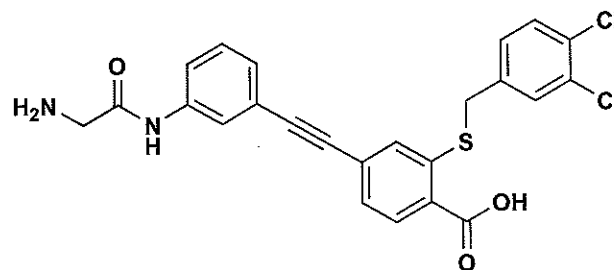
62464-130-1



UV1 Results

Pk #	RT	Area	Area %	Height (uV)	Plates
1	0.177	219326	20.032	56441	52
2	3.010	875565	79.968	181570	9405

Totals		1094891	100.000	238011	
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Exact Mass: 484.04

Compound 22

Sample: 1
File:0126G025
Description:

Vial:1:A,1
Date:26-Jan-2007

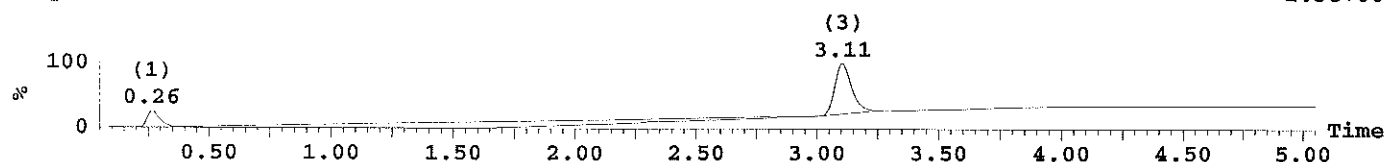
ID:62464-130-1
Time:11:03:50

Printed: Fri Jan 26 11:10:05 2007

Sample Report:

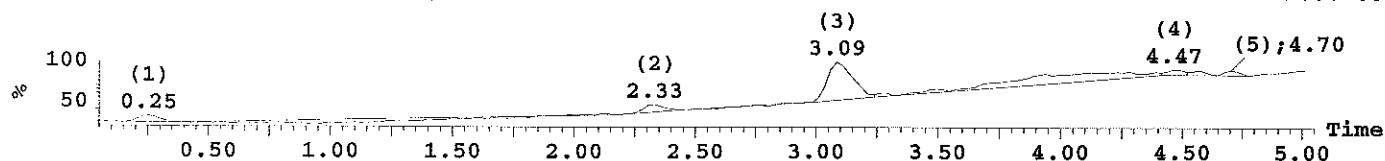
uv spec

2.3e+005



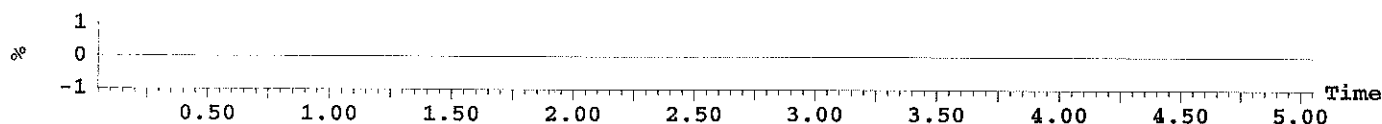
1: MS ES+ :TIC Smooth (SG, 1x2)

2.3e+005



1: MS ES+ :51 Smooth (SG, 1x2)

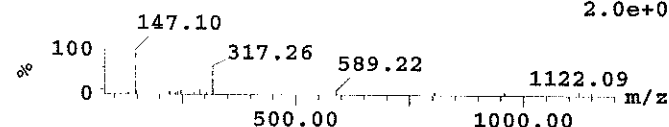
0.0e+000



Peak ID Time
1 0.25

Combine (6:15-29:31)

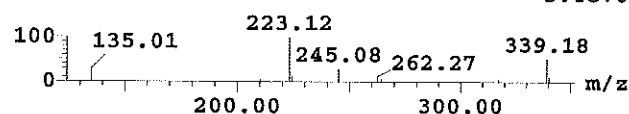
1:MS ES+
2.0e+003



Peak ID Time
2 2.33

Combine (96:104-(80:82+116:118))

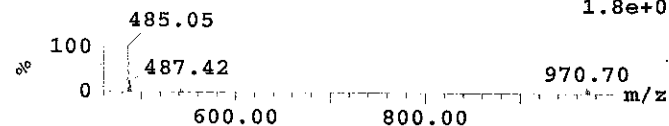
1:MS ES+
3.4e+003



Peak ID Time
3 3.09

Combine (127:135-(113:115+148:150))

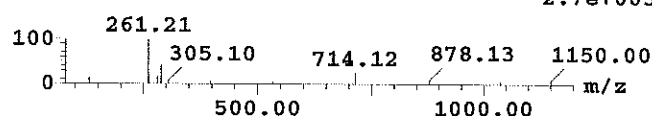
1:MS ES+
1.8e+004



Peak ID Time
4 4.47

Combine (179:187-(168:170+196:198))

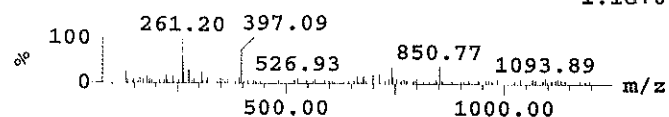
1:MS ES+
2.7e+003



Peak ID Time
5 4.70

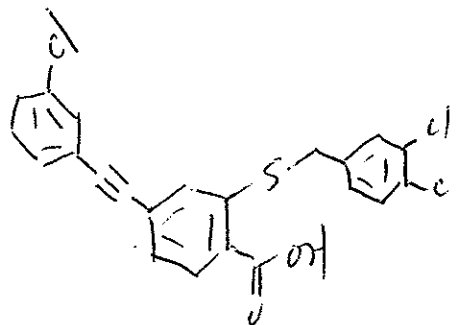
Combine (188:196-177:179)

1:MS ES+
1.1e+003



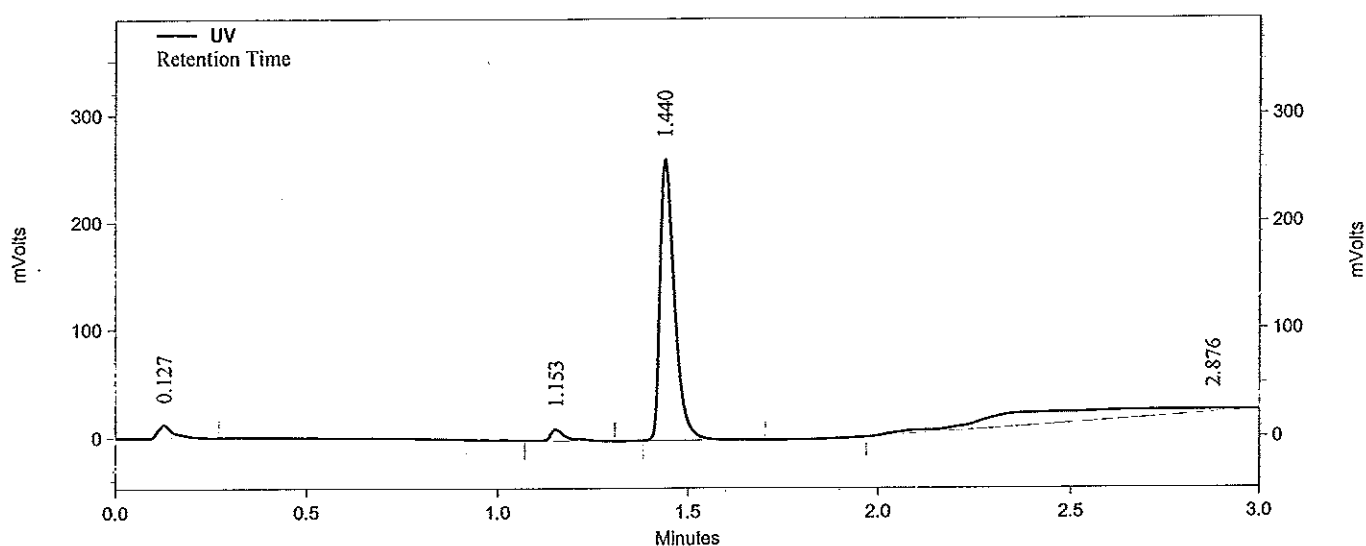
Analytical HPLC Report

File: = C:\CLASS-VP\CHROM\0111S.023
 Sample ID: = 31-6-12 MW 447
 Acquired: = 1/11/2007 3:06:01 PM
 User = weixu.zhai
 Instrument = WFD-409D-LCMS2
 Well = 192 Inj. Vol. = 10 uL
 Start % B = 0
 Final % B = 100
 Gradient Time = 2 min
 Flow Rate = 5 ml/min
 Wavelength = 220
 Solvent A = H2O : ACN 95% : 5% 10 mM Ammonium Acetate
 Solvent B = H2O : ACN 5% : 95% 10 mM Ammonium Acetate
 Column 2 = Xbridge C18 4.6 x 50MM S5



23

31-6-12



UV Results

Pk #	RT	Area	Area %	Height (uV)	Plates
1	0.127	37034	3.303	12606	54
2	1.153	29774	2.655	10423	5130
3	1.440	681928	60.820	261146	7544
4	2.876	372496	33.222	2985	165

Totals		1121232	100.000	287160	
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Sample: 1

Vial:1:A,1

ID:31-6-12

File:0111S023

Date:11-Jan-2007

Time:14:58:08

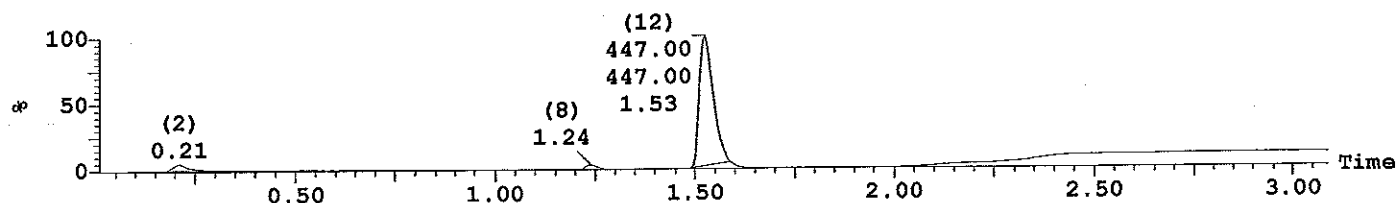
Description:

Printed: Thu Jan 11 15:03:11 2007

Sample Report:

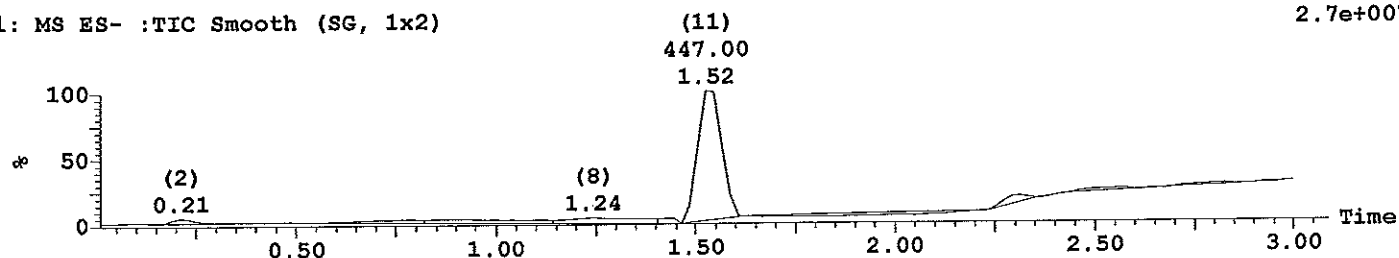
Channel 1

2.6e+005



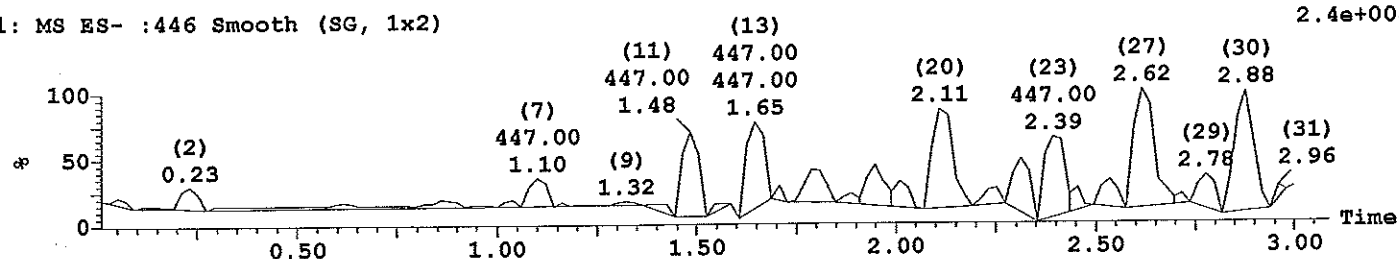
1: MS ES- :TIC Smooth (SG, 1x2)

2.7e+007



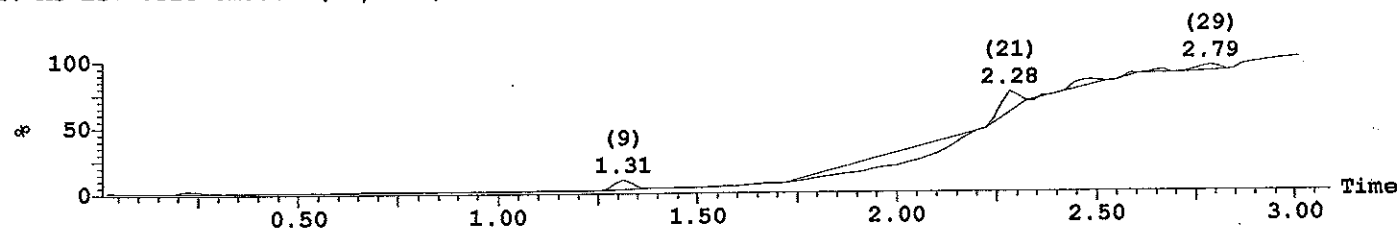
1: MS ES- :446 Smooth (SG, 1x2)

2.4e+004



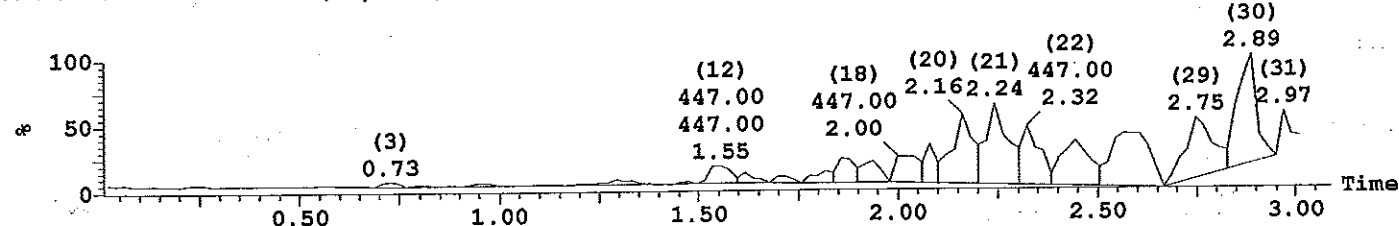
2: MS ES+ :TIC Smooth (SG, 1x2)

1.5e+008



2: MS ES+ :448 Smooth (SG, 1x2)

3.1e+005



Sample: 1
File:0111S023
Description:

Vial:1:A,1
Date:11-Jan-2007

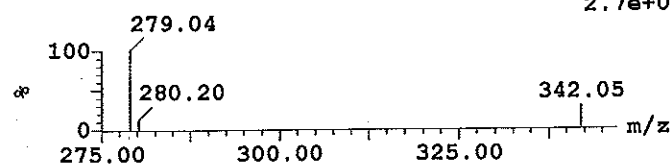
ID:31-6-12
Time:14:58:08

Printed: Thu Jan 11 15:03:11 2007

Sample Report (continued):

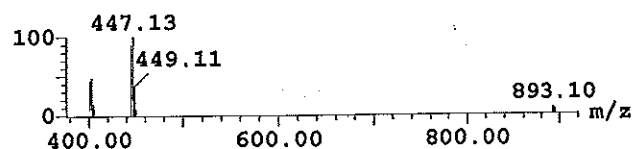
Peak ID Time
9 1.32
Combine (63:67-(52:55+75:78))

2:MS ES+
2.7e+006



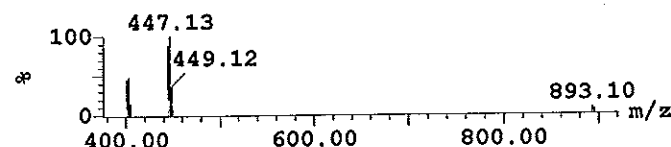
Peak ID Time
11 1.52
Combine (74:78-(63:66+88:91))

1:MS ES-
4.0e+006



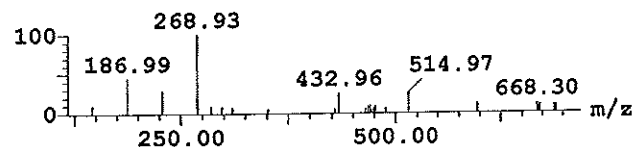
Peak ID Time
12 1.54
Combine (74:79-(64:67+87:89))

1:MS ES-
3.4e+006



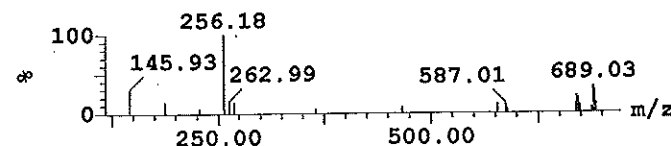
Peak ID Time
20 2.11
Combine (105:109-(94:97+116:119))

2:MS ES+
2.8e+006



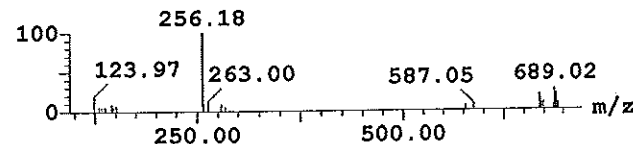
Peak ID Time
21 2.25
Combine (111:115-(100:103+122:125))

2:MS ES+
4.3e+006



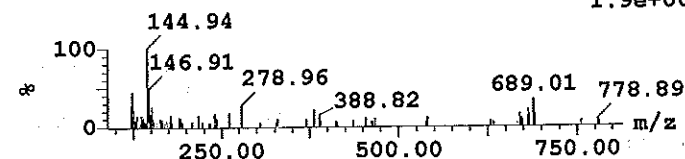
Peak ID Time
22 2.31
Combine (113:117-(104:107+125:128))

2:MS ES+
4.1e+006



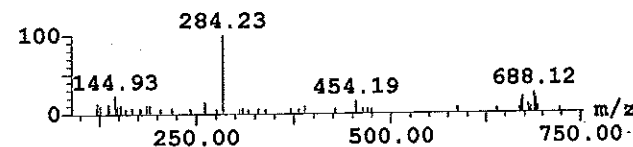
Peak ID Time
24 2.45
Combine (121:125-(109:112+132:135))

2:MS ES+
1.9e+006



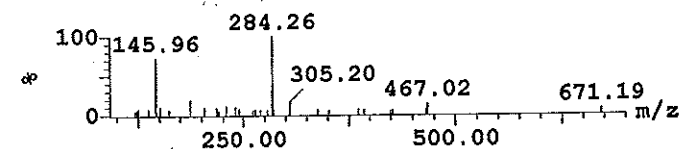
Peak ID Time
25 2.57
Combine (125:129-(114:117+139:142))

2:MS ES+
1.7e+006



Peak ID Time
27 2.62
Combine (130:134-(119:122+140:143))

2:MS ES+
1.9e+006



Peak ID Time
29 2.82
Combine (136:140-(124:127+147:149))

2:MS ES+
1.4e+006

