

Synthesis and biological properties of conjugates between fluoroquinolones and a N3"-functionalized pyochelin

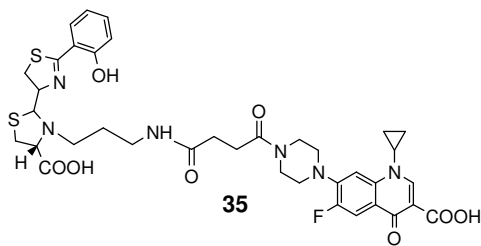
Sabrina Noël,[†] Véronique Gasser,[†] Bénédicte Pesset,[†] Françoise Hoegy,[†] Didier Rognan,[‡]
Isabelle J. Schalk,[†] Gaëtan L. A. Mislin^{†,*}

Team "Transports Membranaires Bactériens". UMR 7242-Université de Strasbourg/CNRS. Boulevard Sébastien Brant, 67400 Illkirch-Graffenstaden, France. Team "Chémogénomique Structurale" Laboratoire d'Innovation Thérapeutique (LIT). UMR 7200-CNRS/Université de Strasbourg. Faculté de Pharmacie, 74 route du Rhin, 67400 Illkirch-Graffenstaden, France.

mislin@unistra.fr

SUPPORTING INFORMATION

LC-HRMS Spectrum of conjugate 35	S1
HPLC-MS Spectrum of conjugate 35	S2
¹ H-NMR Spectrum of conjugate 35	S3
LC-HRMS Spectrum of conjugate 36	S4
HPLC-MS Spectrum of conjugate 36	S5
¹ H-NMR Spectrum of conjugate 36	S6
LC-HRMS Spectrum of conjugate 37	S7
HPLC-MS Spectrum of conjugate 37	S8
¹ H-NMR Spectrum of conjugate 37	S9
LC-HRMS Spectrum of conjugate 38	S10
HPLC-MS Spectrum of conjugate 38	S11
¹ H-NMR Spectrum of conjugate 38	S12
LC-HRMS Spectrum of conjugate 39	S13
HPLC-MS Spectrum of conjugate 39	S14
¹ H-NMR Spectrum of conjugate 39	S15
LC-HRMS Spectrum of conjugate 40	S16
HPLC-MS Spectrum of conjugate 40	S17
¹ H-NMR Spectrum of conjugate 40	S18

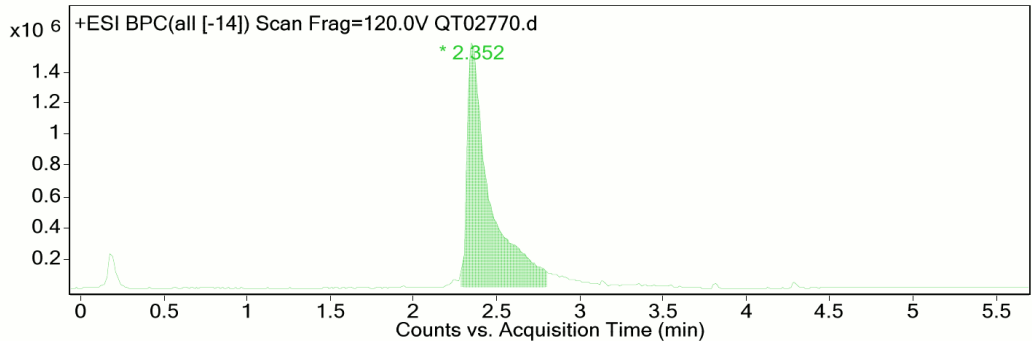


Qualitative Analysis Report

Data Filename	QT02770.d	Sample Name	C1
Sample Type	Sample	Position	P1-A4
Instrument Name	SCA Pharma Stbg QToF	User Name	PW
Acq Method	C18 1x3x1,9Fast.m	Acquired Time	2/3/2011 12:01:32 PM
IRM Calibration Status	Success	DA Method	C18 1x3x1,9Fast.m
Comment			

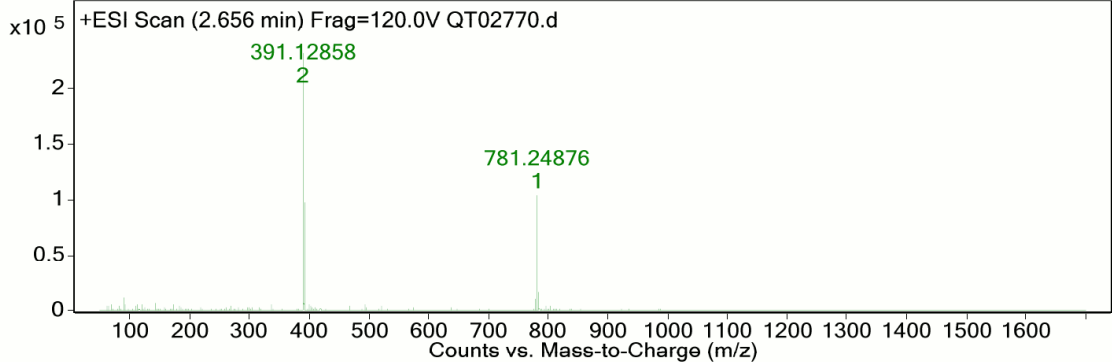
User Chromatograms

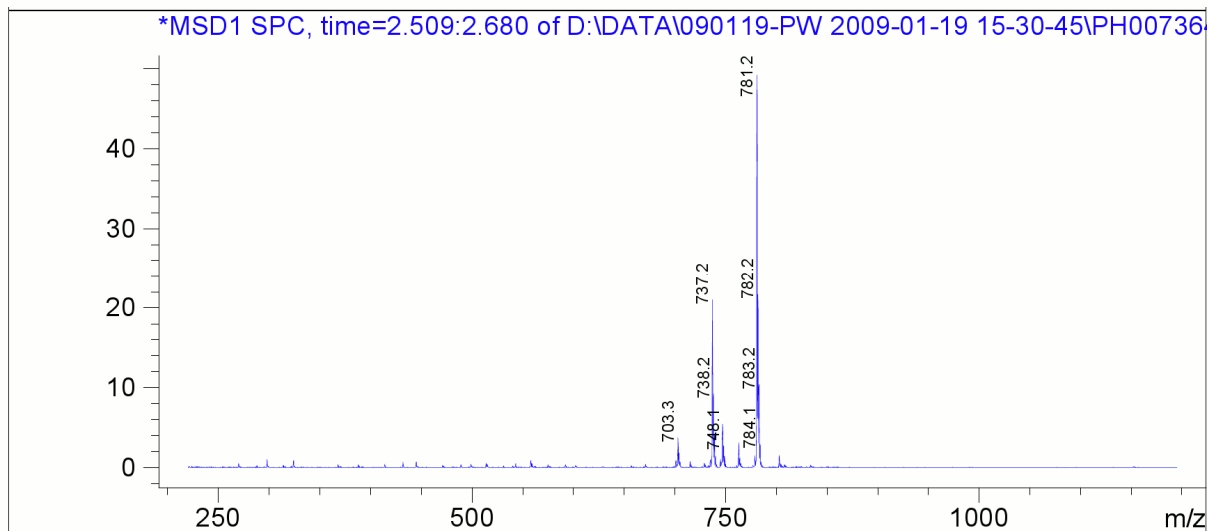
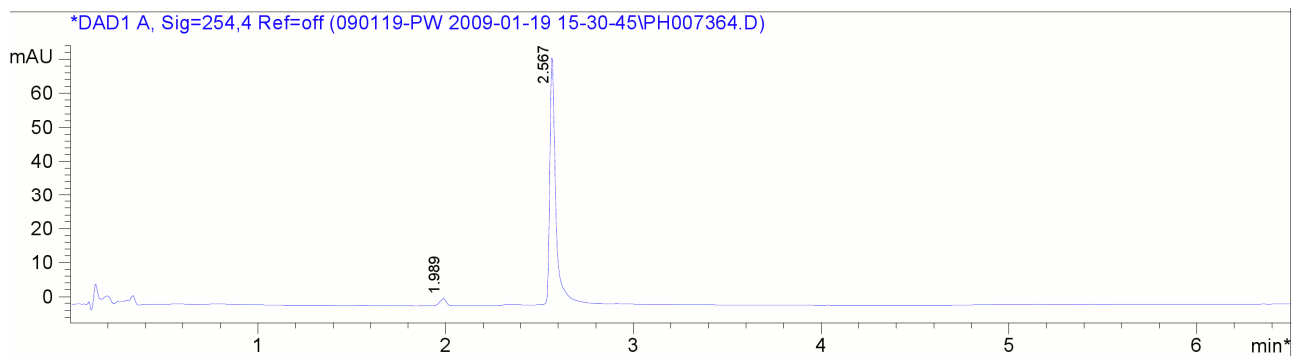
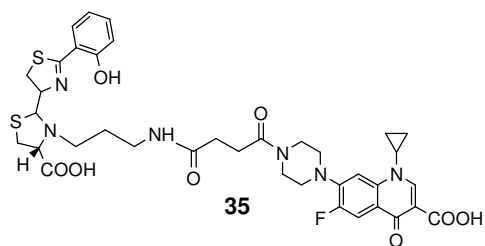
Fragmentor Voltage 120 Collision Energy 0 Ionization Mode ESI

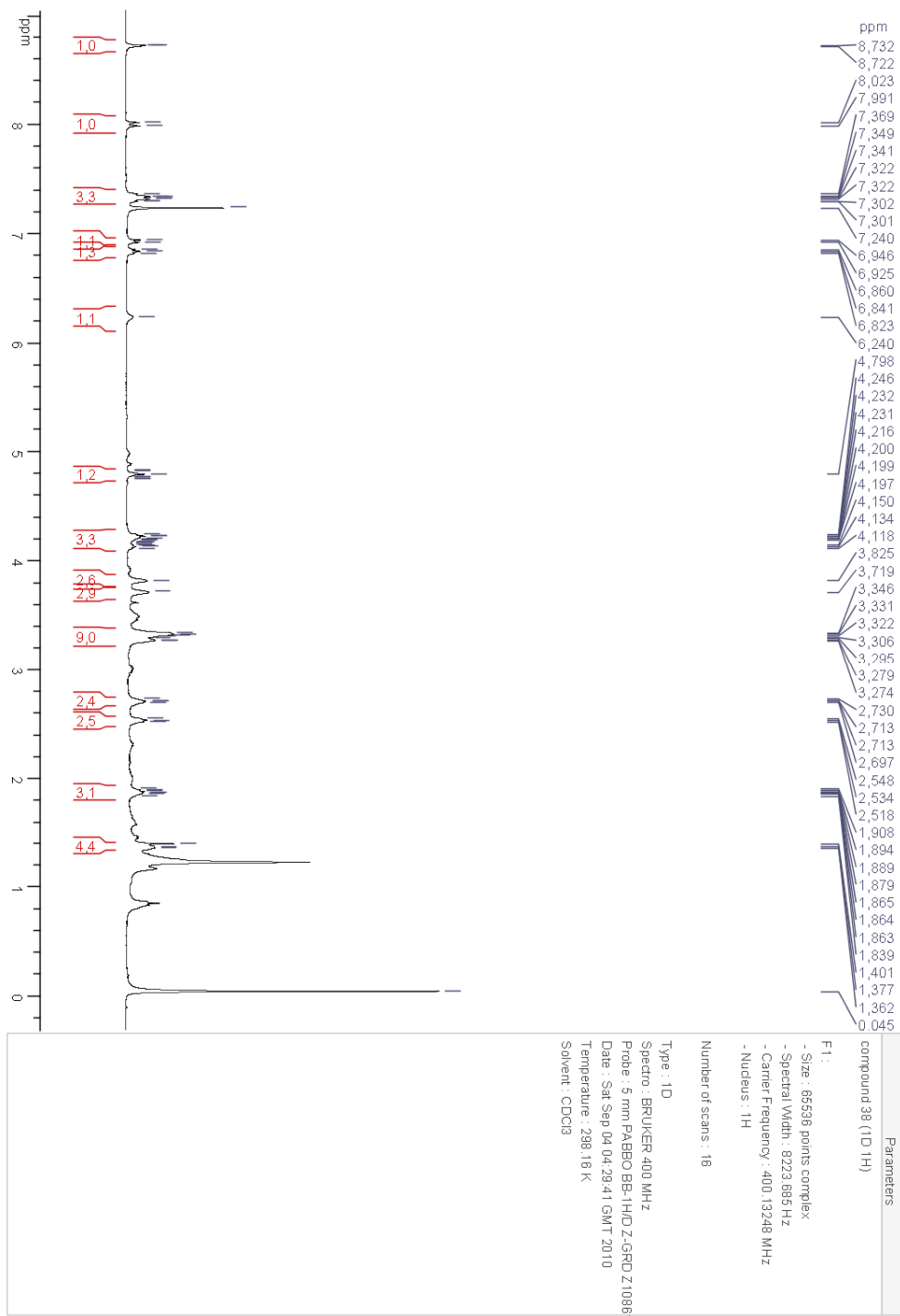
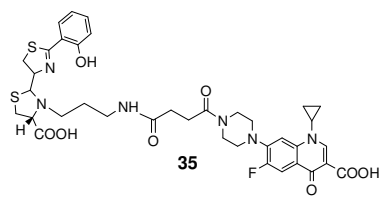


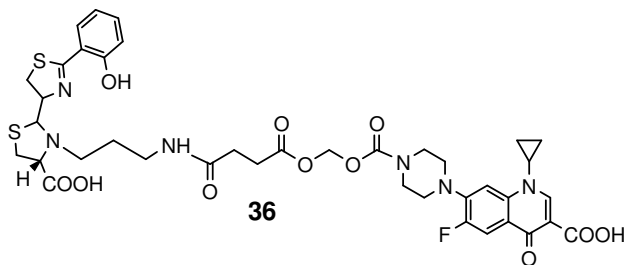
User Spectra

Fragmentor Voltage 120 Collision Energy 0 Ionization Mode ESI



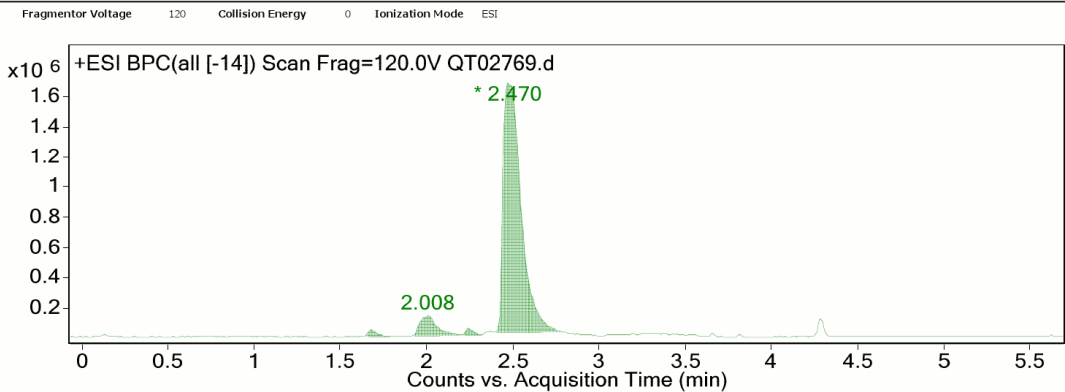






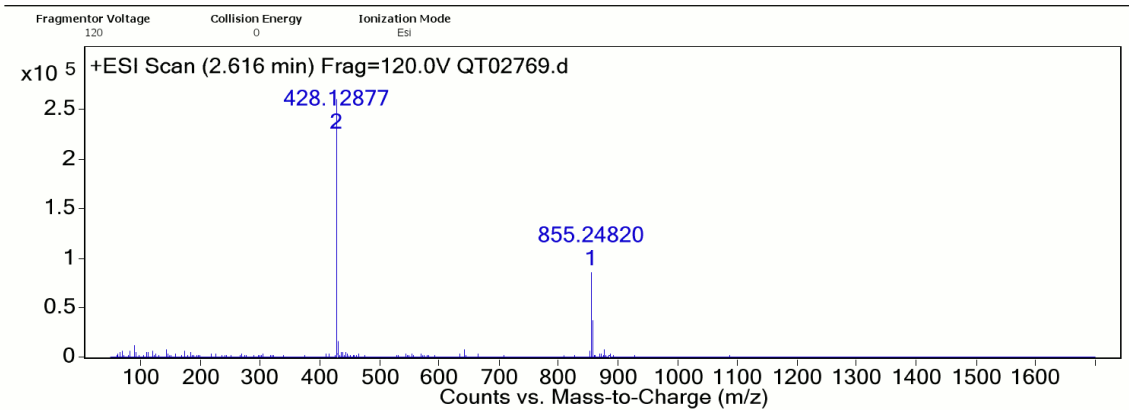
Qualitative Analysis Report

Data Filename	QT02769.d	Sample Name	C1'
Sample Type	Sample	Position	P1-A3
Instrument Name	SCA Pharma S1bg QToF	User Name	PW
Acq Method	C18 1x3x1,9Fast.m	Acquired Time	2/3/2011 11:51:59 AM
IRM Calibration Status	Success	DA Method	C18 1x3x1,9Fast.m
Comment			
User Chromatograms			



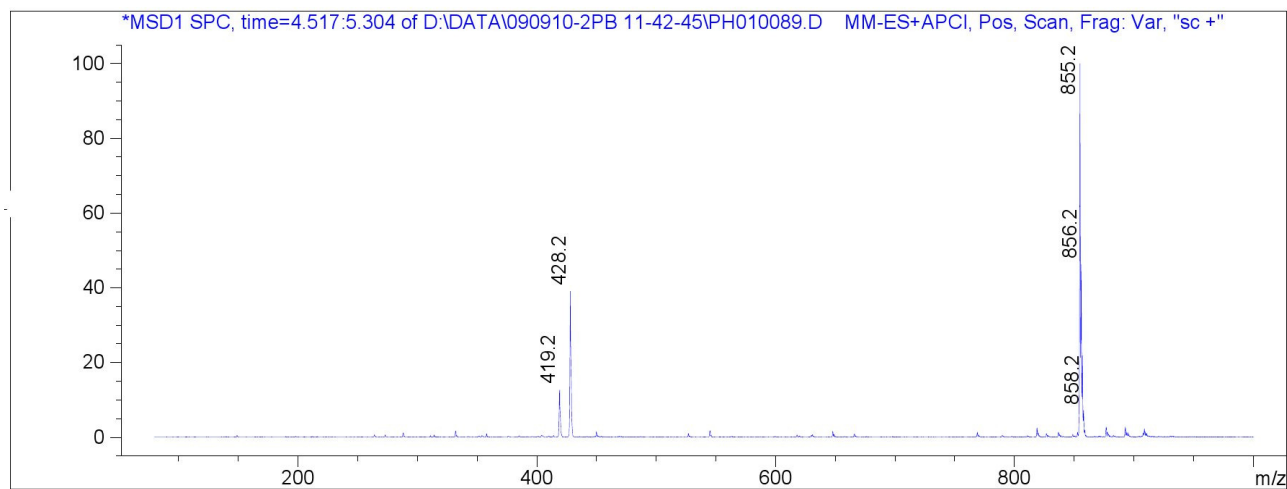
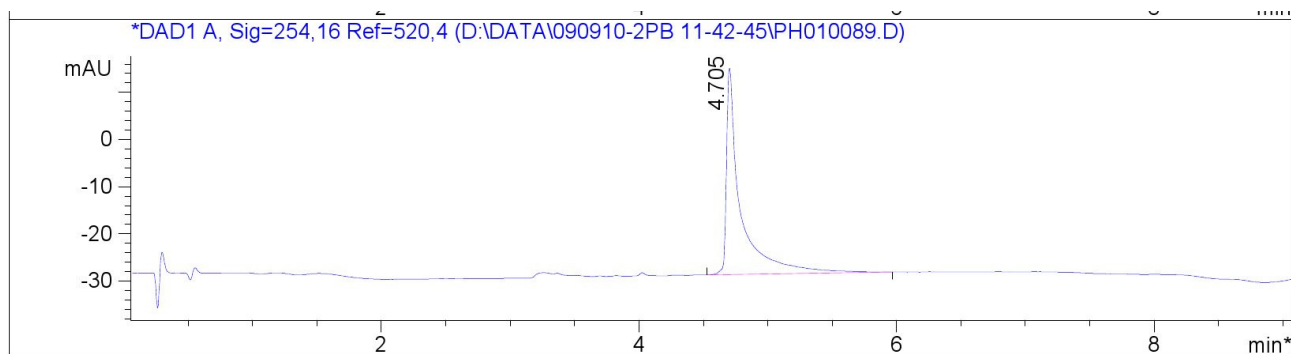
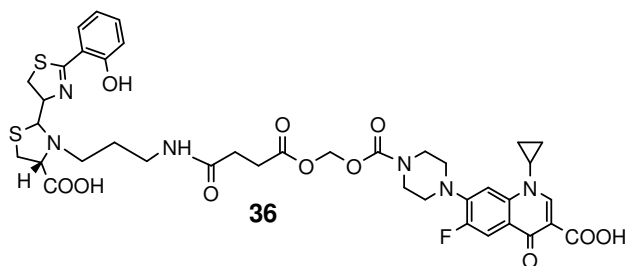
Integration Peak List

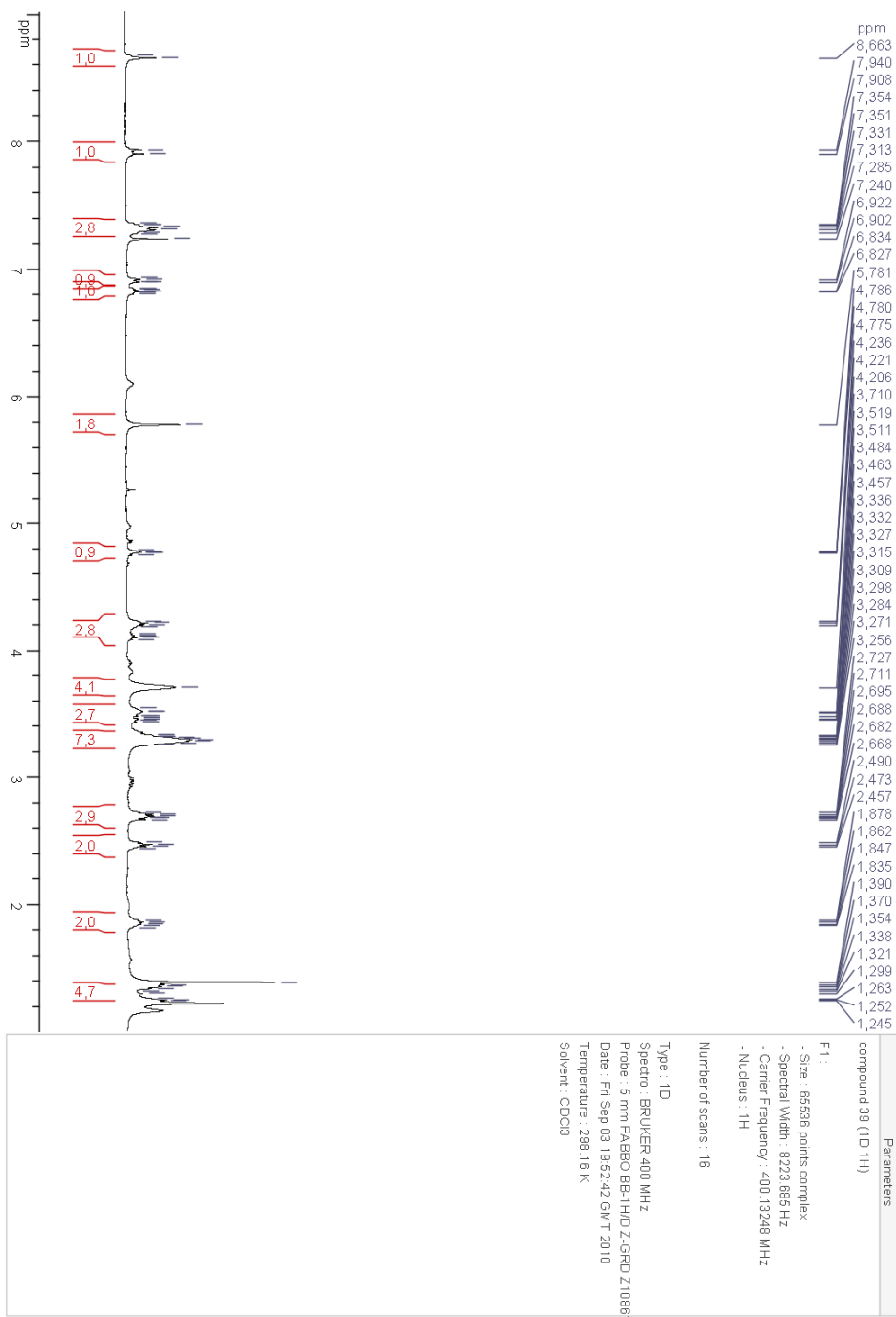
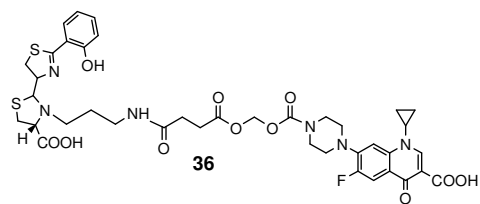
Peak	Start	RT	End	Height	Area	Area %	AreaSum%
1	1.648	1.681	1.794	45729	146841	1.22	1.11
2	1.918	2.008	2.211	134686	920538	7.64	6.94
3	2.211	2.245	2.323	46724	139869	1.16	1.05
4	2.402	2.47	2.796	1650779	12051810	100	90.89

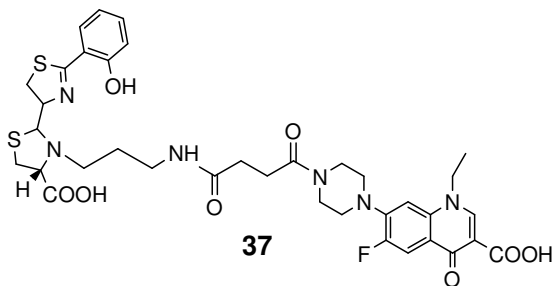


Peak List

m/z	z	Abund	Formula	Ion
427.11968		16949		
428.12877	2	259694	C39 H45 F N6 O11 S2	(M+2H)+2
428.62971	2	116160	C39 H45 F N6 O11 S2	(M+2H)+2
429.12848	2	49794	C39 H45 F N6 O11 S2	(M+2H)+2
429.63033	2	15066	C39 H45 F N6 O11 S2	(M+2H)+2
855.2482	1	85506	C39 H44 F N6 O11 S2	(M+H)+
856.25173	1	37490	C39 H44 F N6 O11 S2	(M+H)+
857.25025	1	16570	C39 H44 F N6 O11 S2	(M+H)+

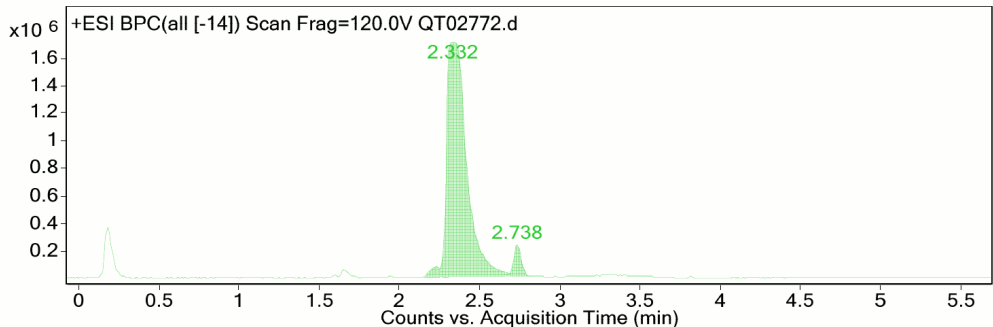




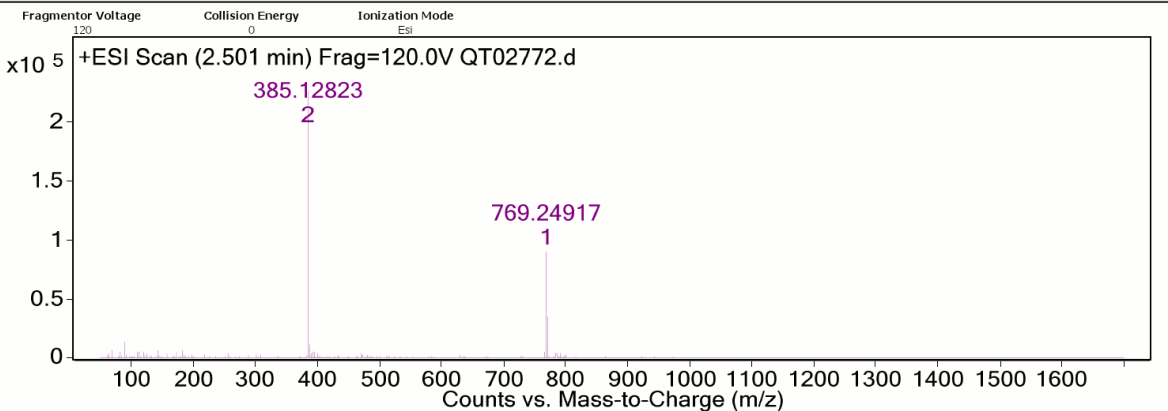


Qualitative Analysis Report

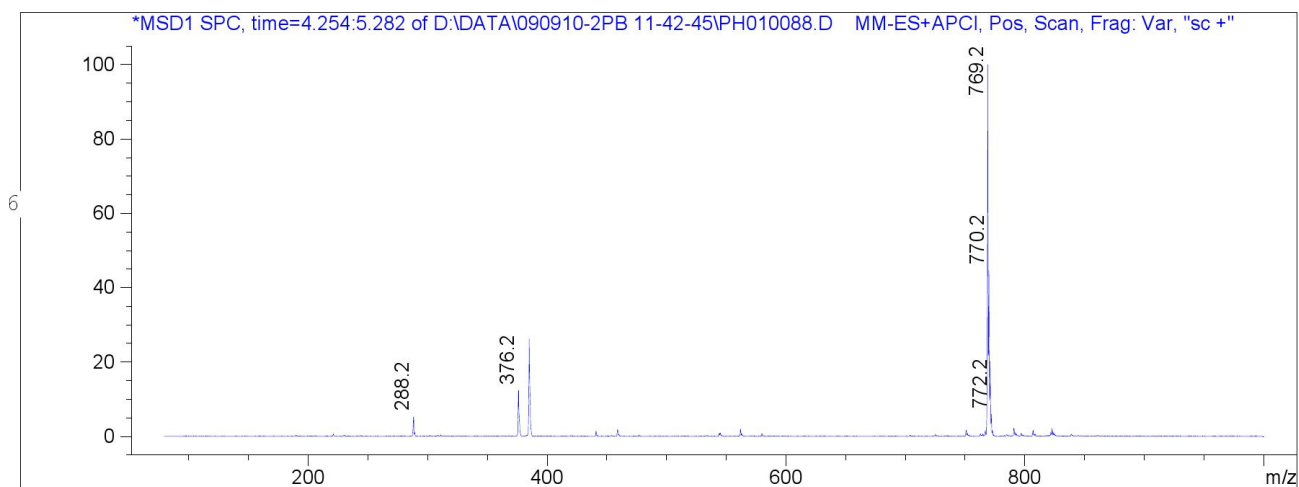
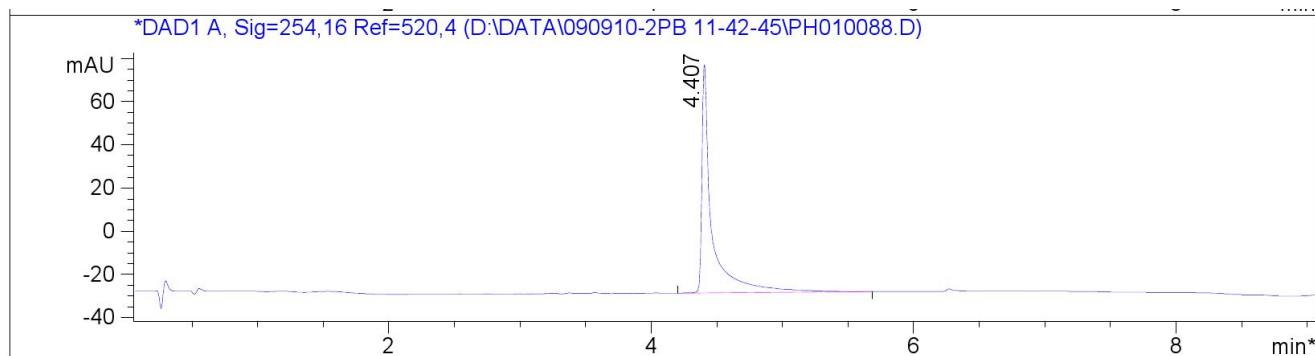
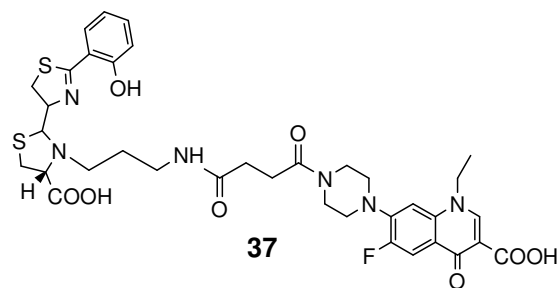
Data Filename	QT02772.d	Sample Name	N1
Sample Type	Sample	Position	P1-A6
Instrument Name	SCA Pharma Stbg QToF	User Name	PW
Acq Method	C18 1x3x1,9Fast.m	Acquired Time	2/3/2011 12:20:29 PM
IRM Calibration Status	Success	DA Method	C18 1x3x1,9Fast.m
Comment			
User Chromatograms			
Fragmentor Voltage	120	Collision Energy	0
		Ionization Mode	ESI

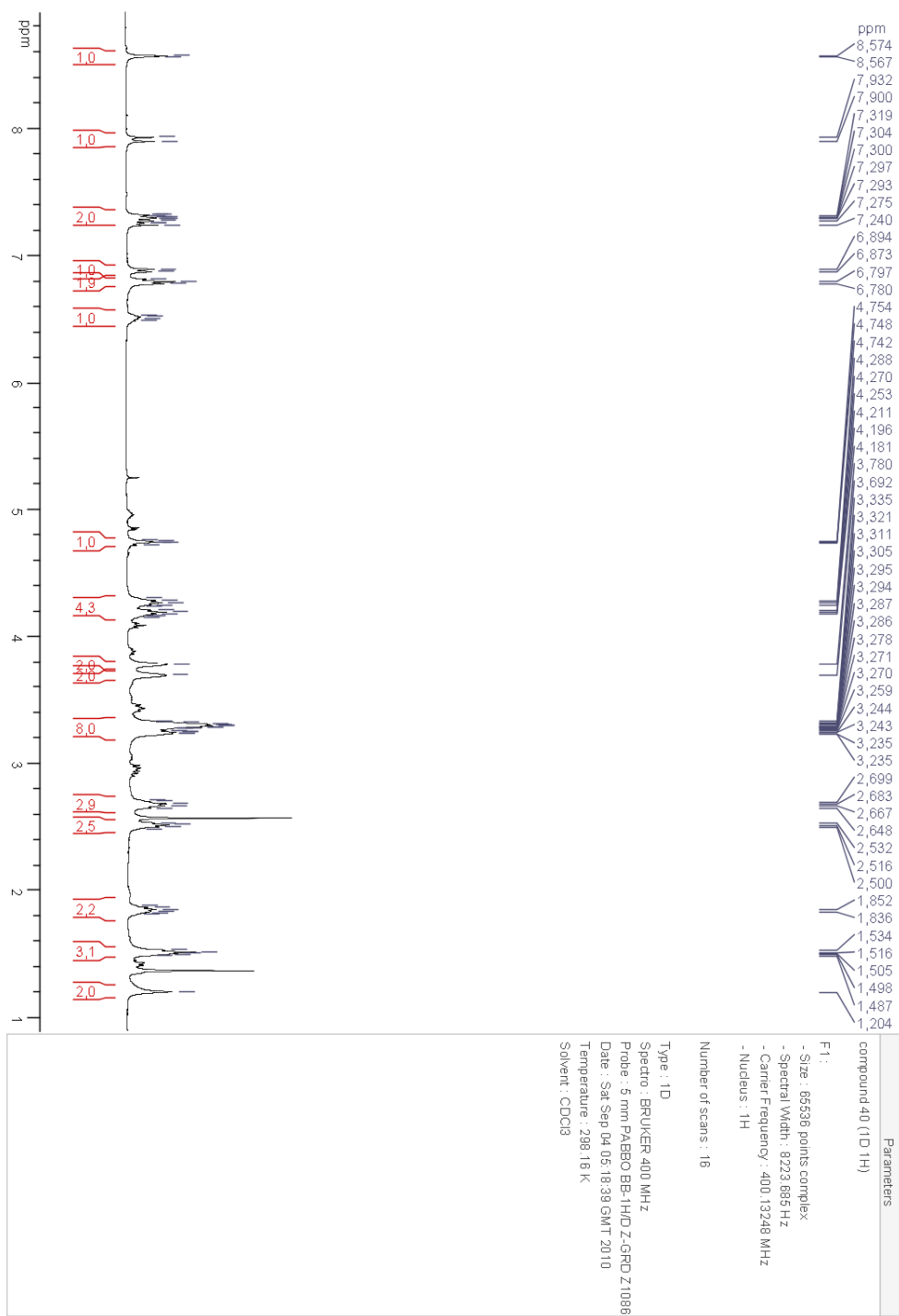
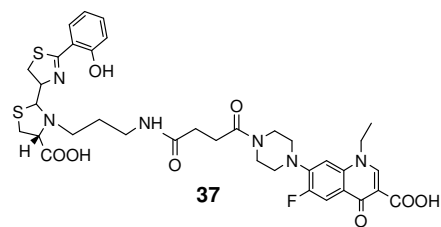


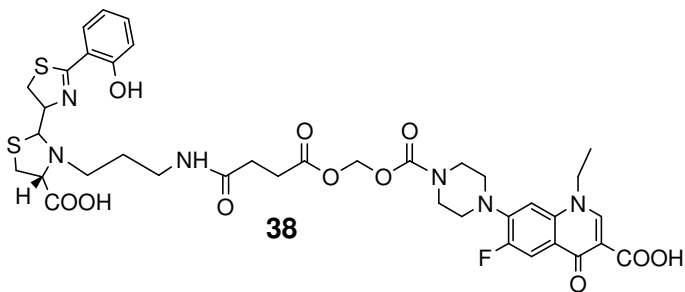
Peak	Start	RT	End	Height	Area	Area %	AreaSum%
1	2.141	2.231	2.253	79914	331089	2.25	2.1
2	2.253	2.332	2.693	1690951	14747595	100	93.38
3	2.693	2.738	2.817	221160	714450	4.84	4.52



Peak List				
m/z	z	Abund	Formula	Ion
89.50716		14018		
384.11959		12726		
385.12823	2	232782	C36 H43 F N6 O8 S2	(M+2H)+2
385.62925	2	99640	C36 H43 F N6 O8 S2	(M+2H)+2
386.12881	2	41176	C36 H43 F N6 O8 S2	(M+2H)+2
769.24917	1	90953	C36 H42 F N6 O8 S2	(M+H)+
770.25059	1	35749	C36 H42 F N6 O8 S2	(M+H)+
771.24892	1	15326	C36 H42 F N6 O8 S2	(M+H)+

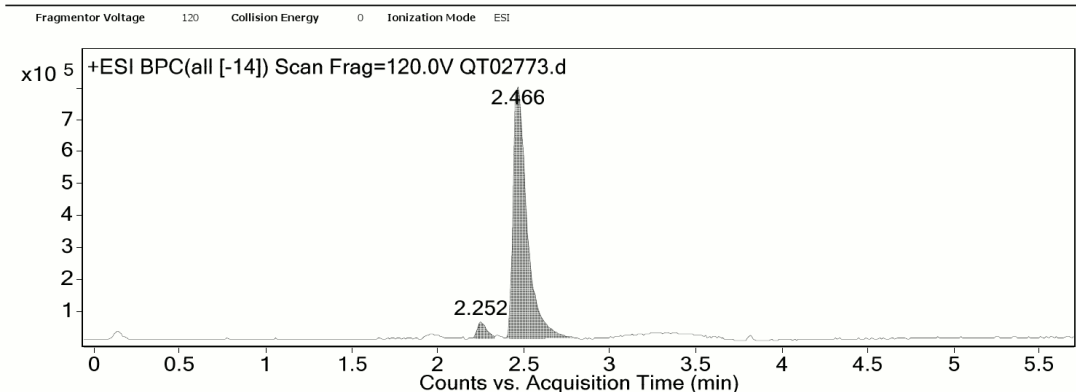






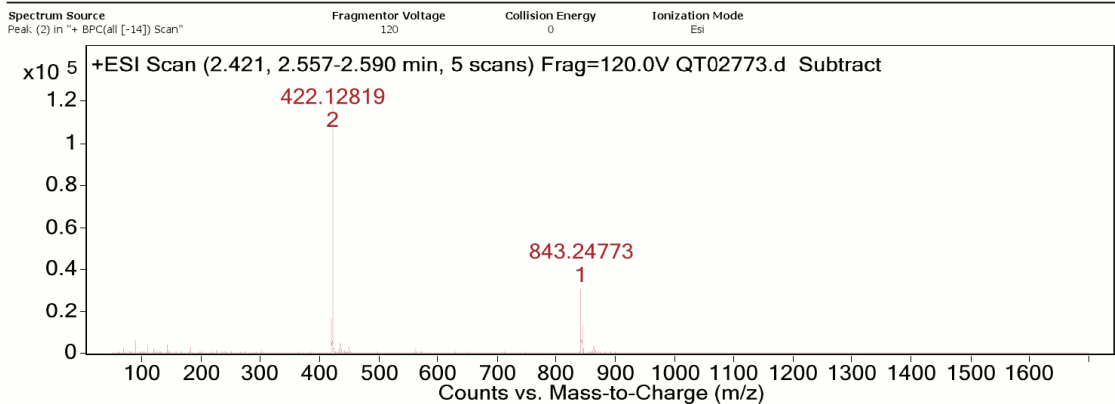
Qualitative Analysis Report

Data Filename	QT02773.d	Sample Name	N1'
Sample Type	Sample	Position	P1-A7
Instrument Name	SCA Pharma Stbg QToF	User Name	PW
Acq Method	C18 1x3x1,9Fast.m	Acquired Time	2/3/2011 12:30:03 PM
IRM Calibration Status	Success	DA Method	C18 1x3x1,9Fast.m
Comment			
User Chromatograms			



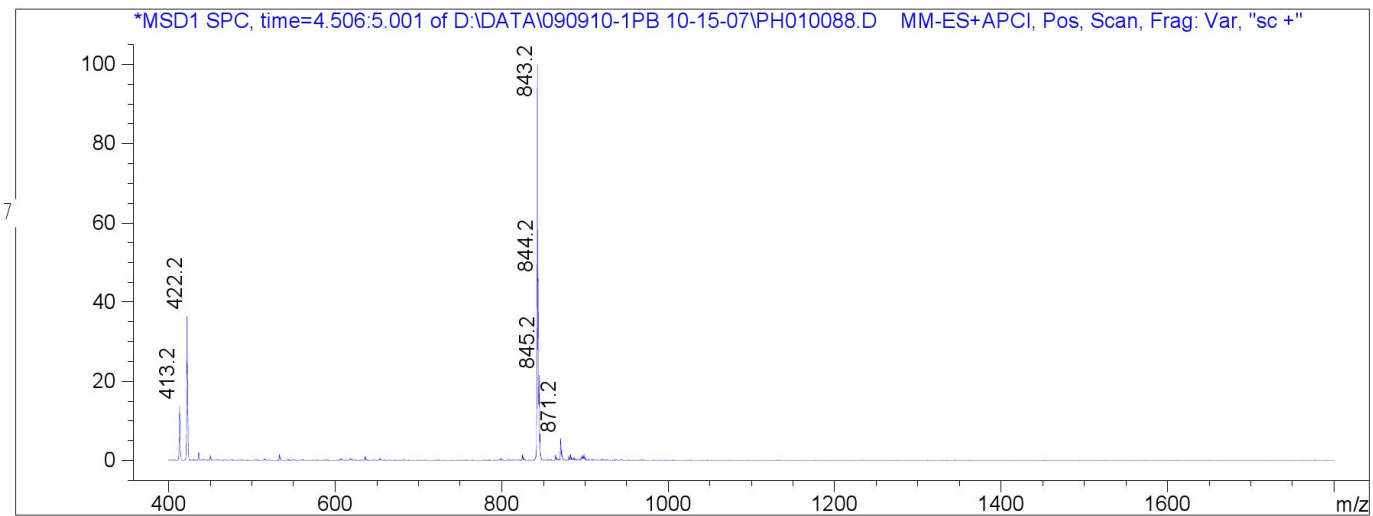
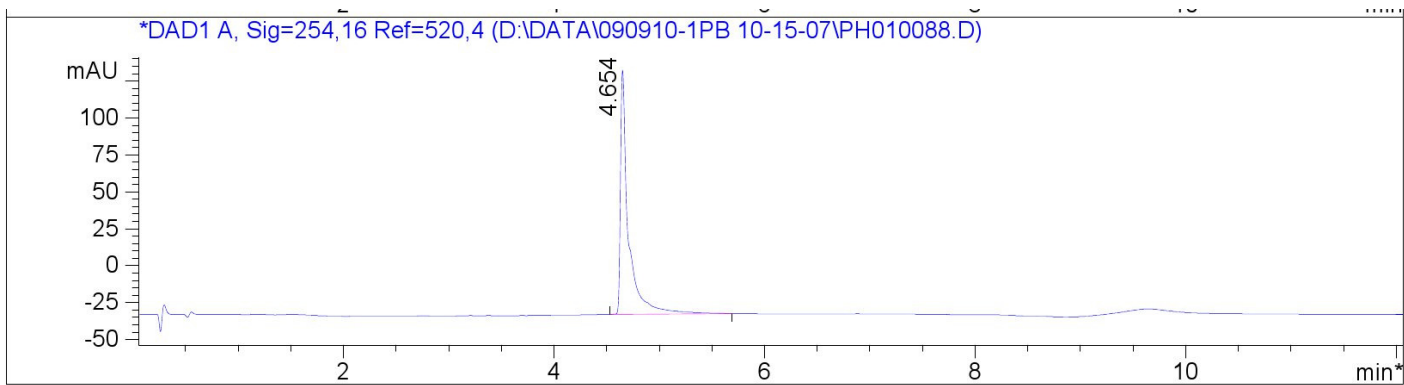
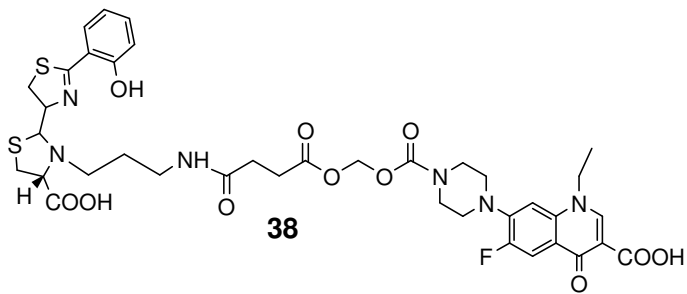
Integration Peak List

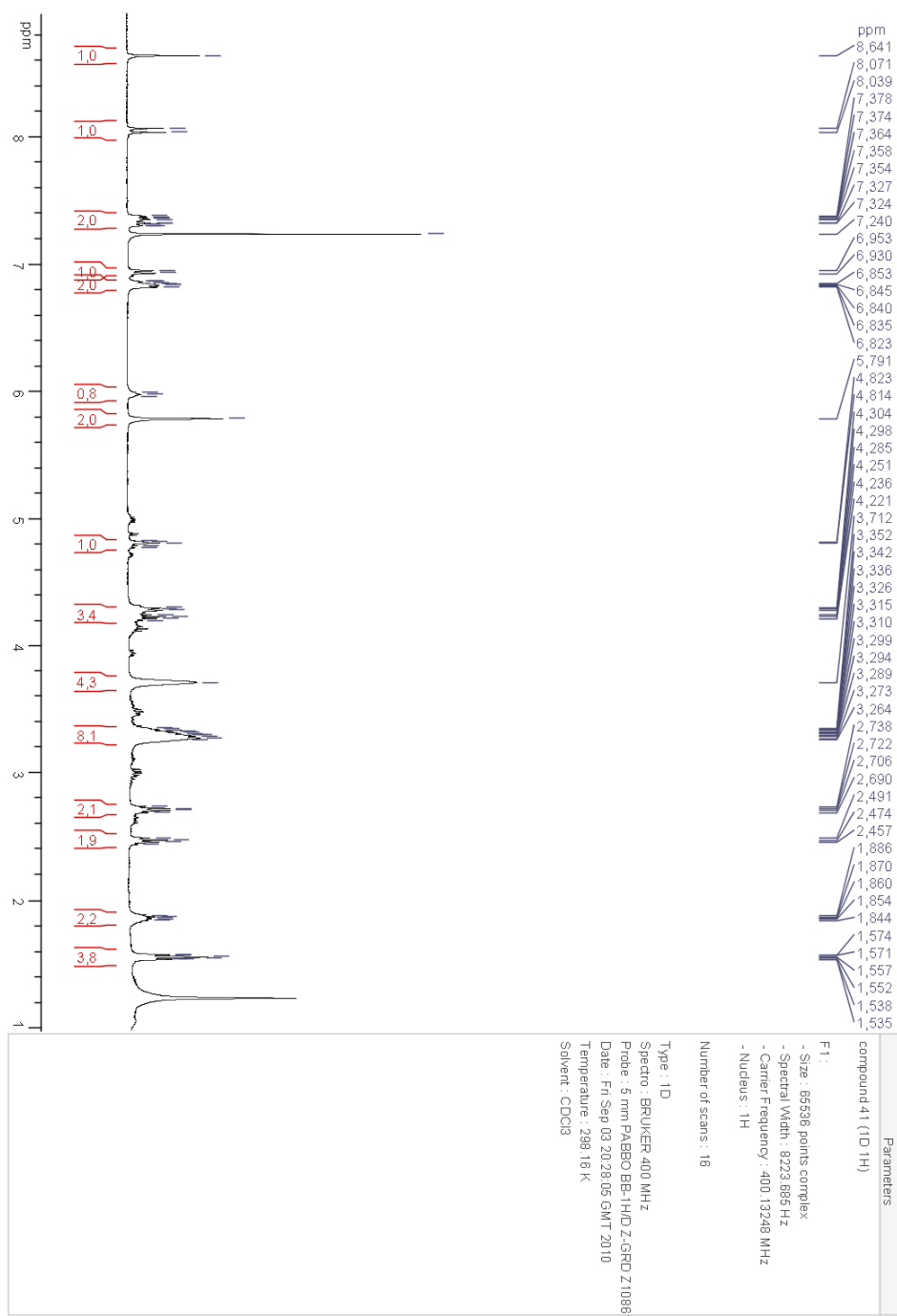
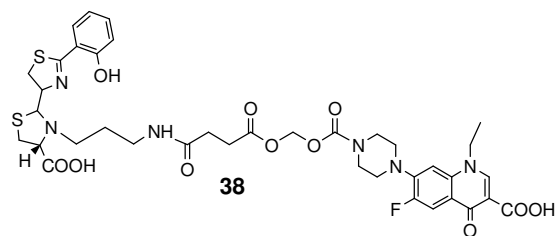
Peak	Start	RT	End	Height	Area	Area %	AreaSum%
1	2.207	2.252	2.331	51609	204360	4.55	4.35
2	2.399	2.466	2.793	790475	4492987	100	95.65

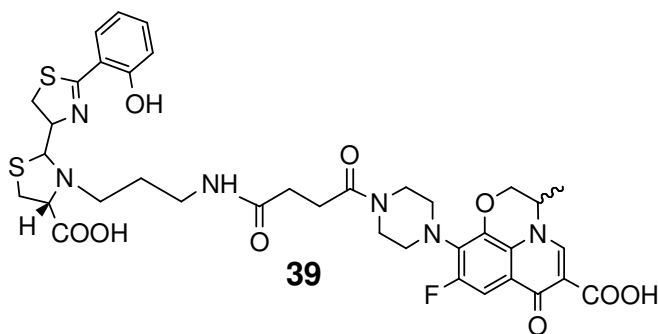


Peak List

m/z	z	Abund	Formula	Ion
421.11971	2	16393		
421.62181	2	7999		
422.12819	2	124476	C38 H45 F N6 O11 S2	(M+2H)+2
422.62957	2	54313	C38 H45 F N6 O11 S2	(M+2H)+2
423.12873	2	23723	C38 H45 F N6 O11 S2	(M+2H)+2
423.62892	2	7139	C38 H45 F N6 O11 S2	(M+2H)+2
843.24773	1	31123	C38 H44 F N6 O11 S2	(M+H)+
844.25115	1	12910	C38 H44 F N6 O11 S2	(M+H)+



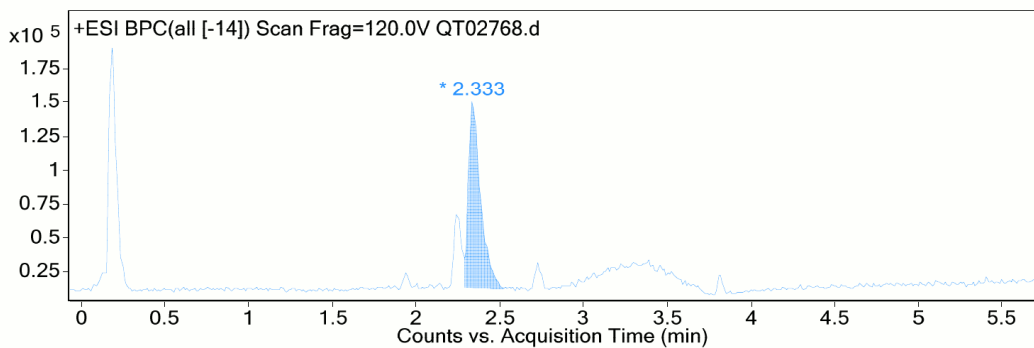




Qualitative Analysis Report

Data Filename	QT02768.d	Sample Name	O1
Sample Type	Sample	Position	P1-A2
Instrument Name	SCA Pharma Stbg QToF	User Name	PW
Acq Method	C18 1x3x1,9Fast.m	Acquired Time	2/3/2011 11:42:26 AM
IRM Calibration Status	Success	DA Method	C18 1x3x1,9Fast.m
Comment			
User Chromatograms			

Fragmentor Voltage 120 Collision Energy 0 Ionization Mode ESI

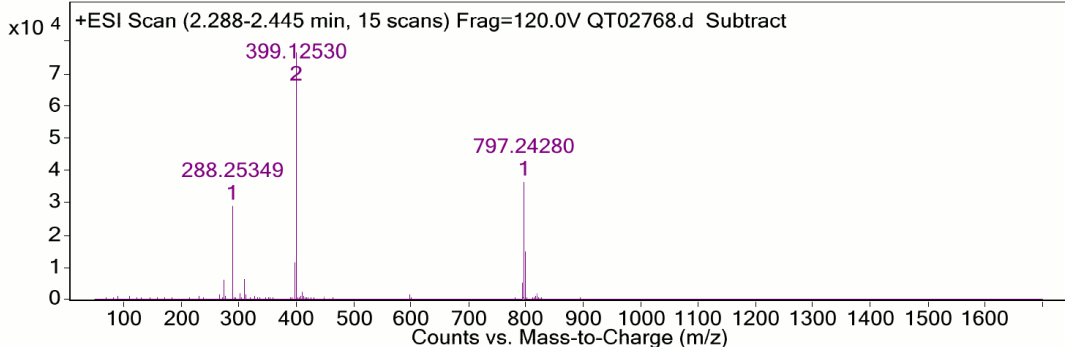


Integration Peak List

Peak	Start	RT	End	Height	Area	Area %	AreaSum%
1	2.288	2.333	2.524	138184	698352	100	100

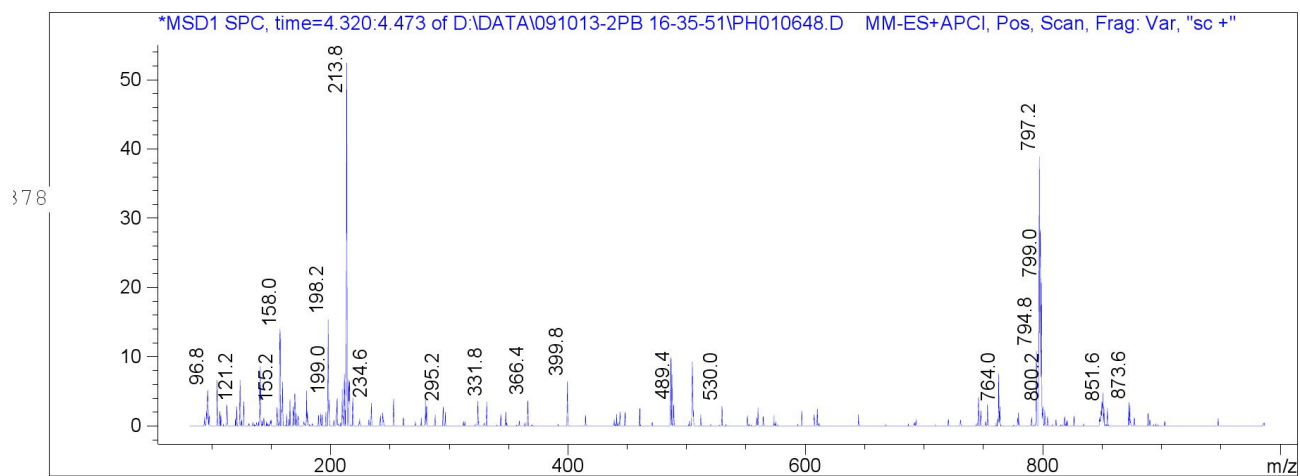
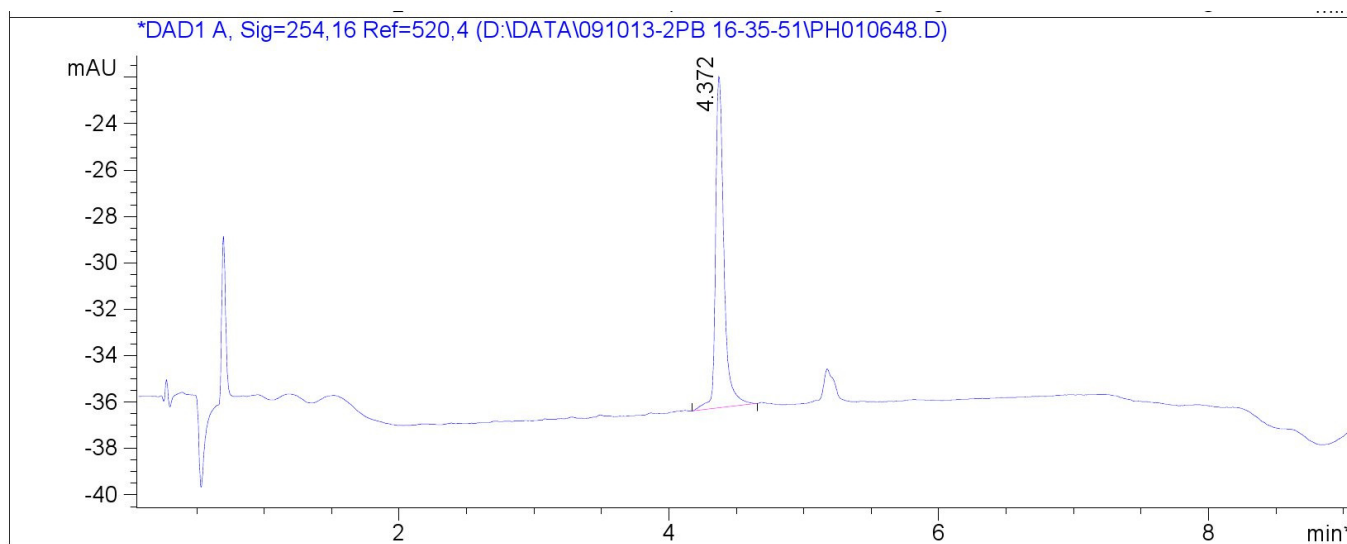
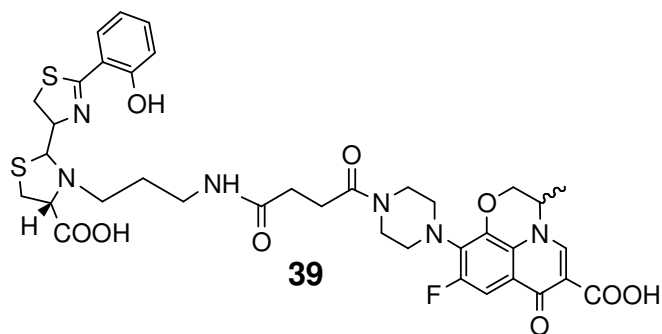
User Spectra

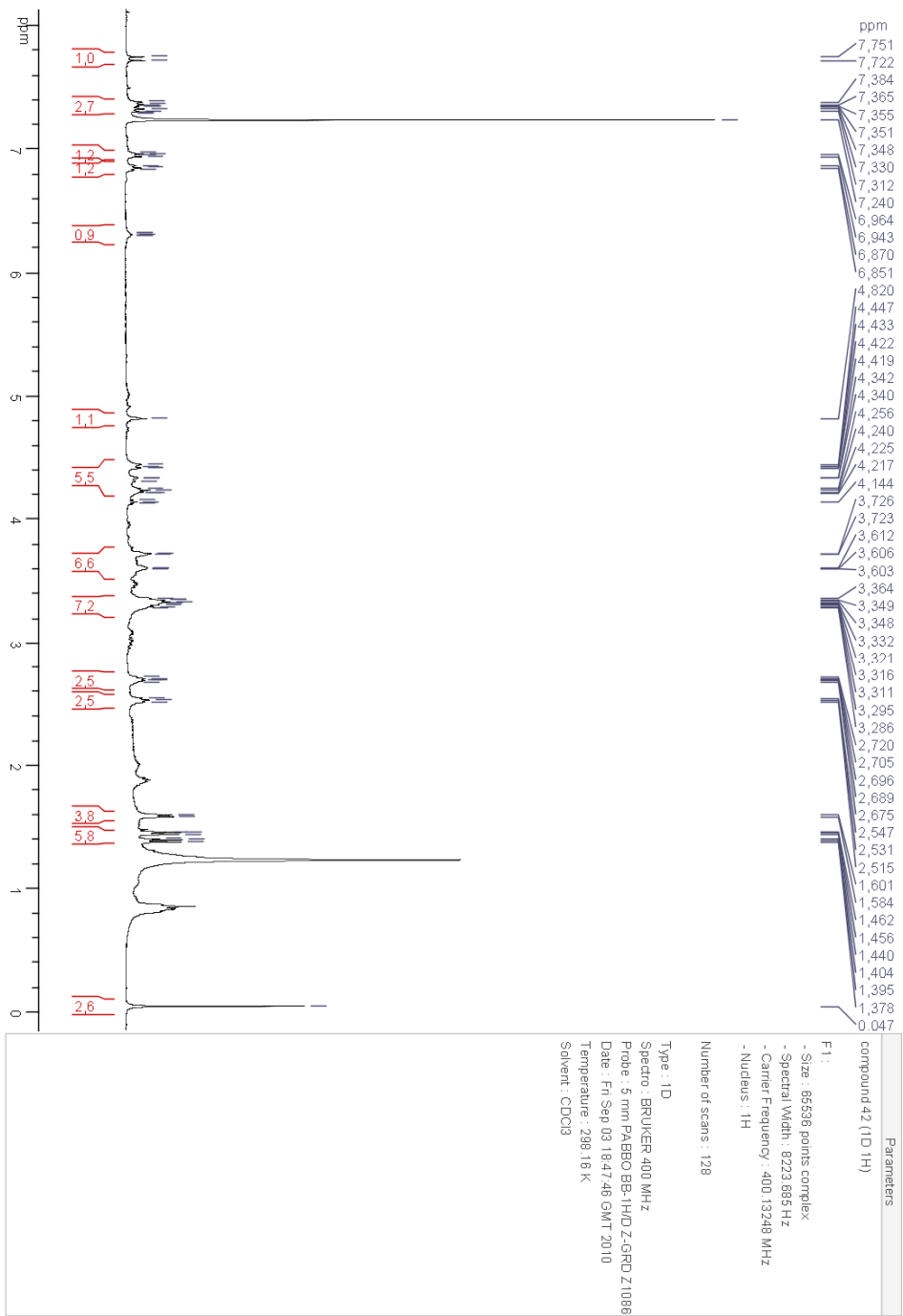
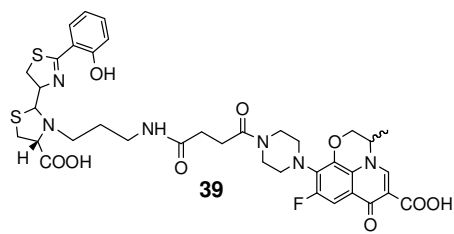
Spectrum Source Peak: (1) in "+ BPC(all [-14]) Scan" Fragmentor Voltage 120 Collision Energy 0 Ionization Mode ESI

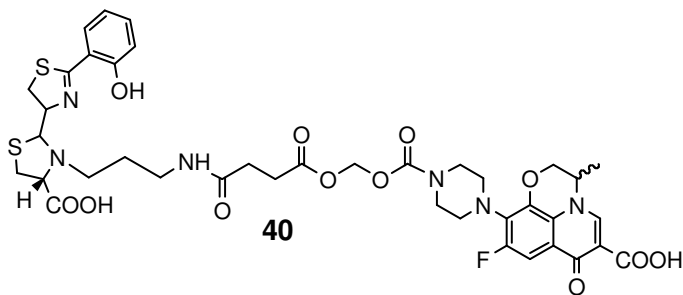


Peak List

m/z	z	Abund	Formula	Ion
274.2744		5674		
288.25349	1	29119		
310.23485		6538		
398.117	2	11644		
399.1253	2	77781	C40 H42 N6 O8 S2	(M+2H)+2
399.62647	2	33453	C40 H42 N6 O8 S2	(M+2H)+2
400.12572	2	14366	C40 H42 N6 O8 S2	(M+2H)+2
797.2428	1	36970	C40 H41 N6 O8 S2	(M+H)+
798.24536	1	15120	C40 H41 N6 O8 S2	(M+H)+
799.24344	1	6546	C40 H41 N6 O8 S2	(M+H)+



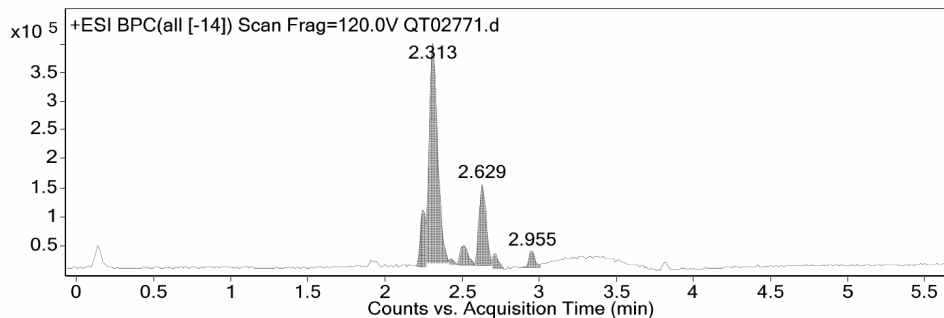




Qualitative Analysis Report

Data Filename	QT02771.d	Sample Name	O1'
Sample Type	Sample	Position	P1-A5
Instrument Name	SCA Pharma Sitbg QToF	User Name	PW
Acq Method	C18 1x31,9Fast.m	Acquired Time	2/3/2011 12:11:08 PM
IRM Calibration Status	Success	DA Method	C18 1x31,9Fast.m
Comment			
User Chromatograms			

Fragmentor Voltage 120 Collision Energy 0 Ionization Mode ESI



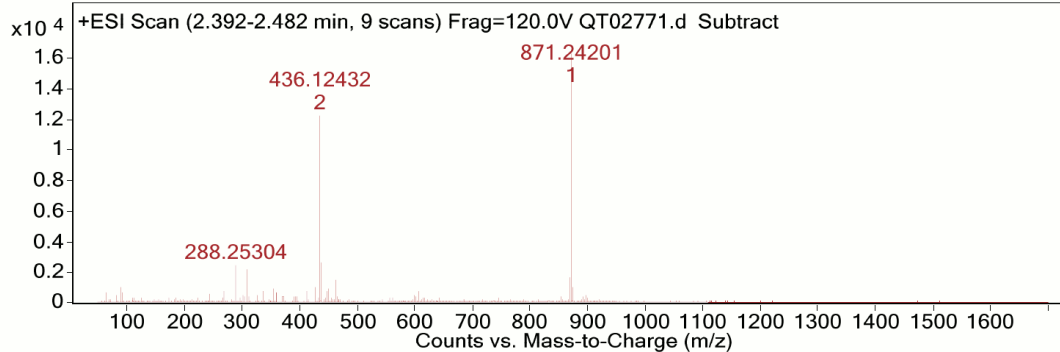
Peak	Start	RT	End	Height	Area	Area %	AreaSum%
1	2.201	2.246	2.268	98232	258099	17.98	10.56
2	2.268	2.313	2.415	381041	1435246	100	58.72
3	2.415	2.426	2.471	9097	16698	1.16	0.68
4	2.471	2.516	2.584	34633	126856	8.84	5.19
5	2.584	2.629	2.696	139873	460797	32.11	18.85
6	2.696	2.719	2.786	25461	59660	4.16	2.44
7	2.877	2.955	3.012	28445	86710	6.04	3.55

Spectrum Source
Peak: (1) in "+" EIC(871.24372) Scan"

Fragmentor Voltage 120

Collision Energy 0

Ionization Mode ESI



Peak List

m/z	z	Abund	Formula	Ion
288.25304		2514		
310.23475		2263		
435.11766		1928		
436.12432	2	12433	C42 H44 N6 O11 S2	(M+2H)+2
436.62623	2	5736	C42 H44 N6 O11 S2	(M+2H)+2
437.12537	2	2694	C42 H44 N6 O11 S2	(M+2H)+2
869.22499		1659		
871.24201	1	16245	C39 H44 F N6 O12 S2	(M+H)+
872.24531	1	7137	C39 H44 F N6 O12 S2	(M+H)+
873.24161	1	3239	C39 H44 F N6 O12 S2	(M+H)+

