

# Synthesis and evaluation of 7-substituted 4-aminoquinoline analogs for antimalarial activity

Jong Yeon Hwang,<sup>1</sup> Takashi Kawasuji,<sup>1,2</sup> David J. Lowes,<sup>1</sup> Julie A. Clark,<sup>1</sup> Michele C. Connelly,<sup>1</sup> Fangyi Zhu,<sup>1</sup> W. Armand Guiguemde<sup>1</sup> Martina S. Sigal,<sup>1</sup> Emily B. Wilson,<sup>3</sup> Joseph L. DeRisi,<sup>3</sup> and R. Kiplin Guy<sup>1,\*</sup>

R. Kiplin Guy, St Jude Children's Research Hospital, Department of Chemical Biology and Therapeutics, 262 Danny Thomas Place, Memphis TN, 38105-3678, USA. Tel (901) 595-5714; Fax (901) 595-5715 e-mail: kip.guy@stjude.org

<sup>1</sup>Department of Chemical Biology and Therapeutics, St. Jude Children's Research Hospital, 262 Danny Thomas Place, Memphis, TN 38105, USA

<sup>2</sup>Medicinal Research Laboratories, Shionogi & CO., LTD. 12-4, Sagisu 5-chome, Fukushima-ku, Osaka, Japan

<sup>3</sup>Department of Biochemistry and Biophysics, University of California at San Francisco, 600 16<sup>th</sup> Street, San Francisco, CA 94143, USA

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**SI-Table 1. Biological and pharmacological evaluation for diarylethers.**

SAMPLE	No. 3{x,y,z}	R <sub>1</sub>	R <sub>2</sub>	3D7 <sup>a</sup> EC <sub>50</sub> , μM	K1 <sup>a</sup> EC <sub>50</sub> , μM	K1/3D7	HepG2 <sup>b</sup> EC <sub>50</sub> , μM	HEK293 <sup>b</sup> EC <sub>50</sub> , μM	Raji <sup>b</sup> EC <sub>50</sub> , μM	BJ <sup>b</sup> EC <sub>50</sub> , μM	HepG2 /3D7	HepG2 /K1	Avg. Sol <sup>b</sup> μM	Avg. Pe <sup>b</sup> X 10 <sup>6</sup> cm/s	ALogP <sup>b</sup>	pKa1 <sup>b</sup> (ring)	pKa2 <sup>b</sup> (chain)
SJ000311206-1	3{1,1,1}	PhO	Furfuryl	0.314±0.013	6.0±0.1	19.0	>16	>16	>16	>16	50.9	2.5	37.8±2.4	1016±223	3.81	8.6	9.28
SJ000311207-1	3{1,1,2}	PhO	2-HO-3-MeO-Bn	0.015±0.002	1.8±2.0	122.0	9.0±0.9	>16	>16	>16	595.1	3.7	39.5±1.3	1002±107	4.38	7.83	9.28
SJ000311208-1	3{1,1,3}	PhO	Piperonyl	0.018±0.002	0.078±0.109	4.3	1.3±0.2	>16	7.8±1.3	4.8±2.9	71.7	34.2	41.0±0.7	1376±155	4.4	8.15	9.28
SJ000311209-1	3{1,1,4}	PhO	3-F-6-MeO-Bn	0.162±0.016	0.138±0.014	0.9	0.8±0.2	4.6±1.6	2.8±0.3	3.1±3.1	5.2	11.1	42.7±0.9	1228±245	4.82	8.11	9.28
SJ000311210-1	3{1,2,1}	2-MeO-PhO	Furfuryl	0.001±0.003	0.087±0.867	66.9	2.9±0.5	>16	8.8±1.3	13.7±5.6	2218.8	74.9	38.8±0.6	521±146	3.8	8.6	9.28
SJ000311211-1	3{1,2,2}	2-MeO-PhO	2-HO-3-MeO-Bn	0.009±0.085	5.7±7.4	626.4	15.4±1.6	>16	>16	>16	1694.7	2.0	42.9±2.7	318±68	4.36	7.83	9.28
SJ000311212-1	3{1,2,3}	2-MeO-PhO	Piperonyl	0.014±0.015	0.517±0.583	37.7	6.1±0.8	>16	>16	15.3±3.5	448.7	11.3	43.4±0.9	1031±72	4.38	8.15	9.28
SJ000311213-1	3{1,2,4}	2-MeO-PhO	3-F-6-MeO-Bn	0.022±0.024	0.960±1.882	44.0	8.4±4.4	>16	>16	>16	385.9	6.7	44.5±1.9	696±102	4.81	8.11	9.28
SJ000311214-1	3{1,3,1}	3-MeO-PhO	Furfuryl	0.009±0.021	0.153±0.279	17.4	8.2±1.4	>16	>16	>16	929.9	101.6	40.6±0.2	698±68	3.8	8.6	9.28
SJ000311215-1	3{1,3,2}	3-MeO-PhO	2-HO-3-MeO-Bn	0.018±0.002	3.0±3.1	42.0	>16	>16	>16	>16	888.9	1.8	44.0±1.0	329±134	4.36	7.83	9.28
SJ000311216-1	3{1,3,3}	3-MeO-PhO	Piperonyl	0.162±0.016	0.600±0.800	50.0	>16	>16	>16	>16	98.8	23.6	42.6±0.3	1012±33	4.38	8.15	9.28
SJ000311217-1	3{1,3,4}	3-MeO-PhO	3-F-6-MeO-Bn	2.4±0.1	0.296±0.678	0.1	6.9±1.1	>16	12.1±0.7	14.9±2.4	2.9	24.0	46.0±1.1	943±83	4.81	8.11	9.28
SJ000311218-1	3{1,4,1}	4-MeO-PhO	Furfuryl	0.004±0.001	0.020±0.026	5.6	2.8±1.0	>16	9.2±1.5	9.6±5.0	776.5	264.9	38.3±0.4	588±70	3.8	8.6	9.28
SJ000311219-1	3{1,4,2}	4-MeO-PhO	2-HO-3-MeO-Bn	0.004±0.002	0.375±0.404	91.5	4.3±0.8	>16	9.3±0.7	15.5±7.2	1044.3	14.7	42.3±1.2	612±225	4.36	7.83	9.28
SJ000311220-1	3{1,4,3}	4-MeO-PhO	Piperonyl	0.046±0.226	1.4±2.8	30.9	8.6±1.3	>16	>16	15.9±0.4	187.2	5.6	43.3±2.8	989±193	4.38	8.15	9.28
SJ000311221-1	3{1,4,4}	4-MeO-PhO	3-F-6-MeO-Bn	0.054±0.005	0.660±1.793	12.2	9.1±3.0	>16	>16	15.6±4.7	169.1	10.6	42.6±1.6	566±88	4.81	8.11	9.28
SJ000311222-1	3{1,5,1}	4-F-PhO	Furfuryl	0.026±0.075	0.096±0.01	3.6	>16	>16	>16	>16	610.7	167.4	37.1±0.8	1177±173	4.02	8.6	9.28
SJ000311223-1	3{1,5,2}	4-F-PhO	2-HO-3-MeO-Bn	0.011±0.002	3.1±3.4	282.2	13.9±2.8	>16	>16	>16	1254.5	3.5	40.9±0.4	1016±165	4.58	7.83	9.28
SJ000311224-1	3{1,5,3}	4-F-PhO	Piperonyl	0.015±0.002	0.667±0.760	44.5	>16	>16	>16	>16	1066.7	24.0	40.6±0.6	702±189	4.61	8.15	9.28
SJ000311225-1	3{1,5,4}	4-F-PhO	3-F-6-MeO-Bn	0.297±1.065	0.135±0.014	0.5	8.6±3.4	>16	>16	>16	28.8	48.8	42.2±1.1	1310±205	5.03	8.11	9.28
SJ000311226-1	3{1,6,1}	4-Cl-PhO	Furfuryl	0.040±0.049	0.793±1.115	19.8	10.1±1.4	>16	>16	>16	252.6	9.8	35.7±1.1	1032±121	4.48	8.6	9.28
SJ000311227-1	3{1,6,2}	4-Cl-PhO	Furfuryl	0.011±0.003	0.785±0.849	70.7	6.8±1.1	>16	15.0±0.5	15.4±2.5	612.6	7.3	42.8±1.5	777±156	5.04	7.83	9.28
SJ000311228-1	3{1,6,3}	4-Cl-PhO	Piperonyl	0.038±0.040	0.320±0.650	8.4	8.8±2.4	>16	>16	>16	231.4	22.5	40.8±2.1	1102±153	5.07	8.15	9.28
SJ000311229-1	3{1,6,4}	4-Cl-PhO	3-F-6-MeO-Bn	0.031±0.060	0.109±0.196	3.5	6.1±0.3	>16	>16	>16	193.4	41.2	41.8±2.5	1284±65	5.49	8.11	9.28
SJ000311230-1	3{1,7,1}	3-Me2N-PhO	Furfuryl	0.027±0.341	0.155±0.242	5.7	>16	>16	>16	>16	588.2	103.0	33.7±0.8	906±51	3.98	8.6	9.28
SJ000311231-1	3{1,7,2}	3-Me2N-PhO	2-HO-3-MeO-Bn	0.010±0.241	2.0±2.1	215.1	10.9±0.8	>16	>16	>16	1144.4	3.6	40.0±2.1	347±56	4.54	7.83	9.28
SJ000311232-1	3{1,7,3}	3-Me2N-PhO	Piperonyl	1.4±0.7	3.9±7.8	2.9	>16	>16	>16	5.9±5.1	11.7	4.1	39.2±0.5	584±74	4.56	8.15	9.28
SJ000311233-1	3{1,7,4}	3-Me2N-PhO	3-F-6-MeO-Bn	0.007±0.005	0.031±0.326	4.7	2.0±0.1	>16	3.4±0.3	5.1±0.5	305.0	109.6	39.1±1.1	579±16	4.99	8.11	9.28
SJ000311234-1	3{1,8,1}	4-tertBu-PhO	Furfuryl	1.1±0.2	4.8±8.4	4.3	3.9±0.8	>16	10.7±0.7	>16	3.5	0.6	30.6±1.5	1049±44	5.22	8.6	9.28
SJ000311235-1	3{1,8,2}	4-tertBu-PhO	2-HO-3-MeO-Bn	0.054±0.021	0.249±0.277	4.6	1.2±0.3	>16	3.0±0.8	4.8±1.5	22.9	6.1	27.4±0.2	644±135	5.78	7.83	9.28
SJ000311236-1	3{1,8,3}	4-tertBu-PhO	Piperonyl	0.137±0.031	2.5±3.1	17.9	1.2±0.4	15.3±0.5	8.9±3.1	>16	8.9	0.4	14.5±0.4	1054±380	5.8	8.15	9.28
SJ000311237-1	3{1,8,4}	4-tertBu-PhO	3-F-6-MeO-Bn	0.106±0.046	2.8±4.0	26.2	8.8±0.4	>16	10.1±1.9	>16	83.0	2.6	23.1±1.1	917±240	6.22	8.11	9.28

<sup>a</sup>Values are the mean of three independent experiments in triplicate. <sup>b</sup>Values are means of an experiment in triplicate. <sup>c</sup>pKa and Alog P was calculated by

Pipeline pilot of Accelrys Software Inc.

**SI-Table 2 Biological and pharmacological evaluation for biaryls.**

SAMPLE	No. 3{x,y,z}	R <sub>1</sub>	R <sub>2</sub>	3D7 <sup>a</sup>	K1 <sup>a</sup>	K1/3D7	HepG2 <sup>b</sup>	HEK293 <sup>b</sup>	Raji <sup>b</sup>	BJ <sup>b</sup>	HepG2	HepG2	Avg. Sol <sup>b</sup>	Avg. Pe <sup>b</sup>	AlogP <sup>b</sup>	pKa1 <sup>b</sup>	pKa2 <sup>b</sup>
				EC <sub>50</sub> , μM	EC <sub>50</sub> , μM		EC <sub>50</sub> , μM	EC <sub>50</sub> , μM	EC <sub>50</sub> , μM	EC <sub>50</sub> , μM	EC <sub>50</sub> , μM	EC <sub>50</sub> , μM	/3D7	/K1		μM	X 10 <sup>6</sup> cm/s
SJ000311238-1	3{2,1,1}	4-F-Ph	Furfuryl	0.032±0.043	0.069±0.098	2.1	9.7±1.1	>16	>16	>16	299.4	113.2	35.9±0.3	340±35	3.98	8.6	9.47
SJ000311239-1	3{2,1,2}	4-F-Ph	2-HO-3-MeO-Bn	0.009±0.084	0.85±1.23	92.8	9.4±2.5	>16	>16	>16	1020.6	8.0	40.7±2.1	269±59	4.54	7.83	9.47
SJ000311240-1	3{2,1,3}	4-F-Ph	Piperonyl	0.018±0.009	0.035±0.004	2.0	12.0±5.5	>16	>16	>16	678.6	252.0	41.5±1.8	1130±89	4.57	8.15	9.47
SJ000311241-1	3{2,1,4}	4-F-Ph	3-F-6-MeO-Bn	0.018±0.0112	0.097±0.107	5.5	1.0±0.2	>16	>16	15.5±2.8	56.9	7.9	40.1±1.5	997±66	4.99	8.11	9.47
SJ000311270-1	3{2,2,1}	3,5-CF3-Ph	Furfuryl	0.285±0.164	0.972±1.41	3.4	3.0±0.2	15.3±0.3	8.6±0.4	5.3±1.2	10.7	2.5	40.1±1.0	818±121	5.66	8.6	9.47
SJ000311271-1	3{2,2,2}	3,5-CF3-Ph	2-HO-3-MeO-Bn	0.029±0.008	0.209±1.74	7.2	1.2±0.4	12.1±2.9	3.6±0.8	5.5±1.7	42.8	4.5	37.2±1.0	237±173	6.22	7.83	9.47
SJ000311272-1	3{2,2,3}	3,5-CF3-Ph	Piperonyl	0.284±0.170	0.604±0.68	2.1	1.4±0.5	6.4±1.3	1.8±0.3	4.8±1.1	4.9	1.9	39.2±1.2	1477±127	6.24	8.15	9.47
SJ000311273-1	3{2,2,4}	3,5-CF3-Ph	3-F-6-MeO-Bn	0.092±0.105	0.81±0.98	8.8	1.0±0.1	>16	2.2±0.2	7.2±5.8	10.5	1.1	37.7±0.4	1380±47	6.67	8.11	9.47
SJ000311274-1	3{2,3,1}	1-Naphtyl	Furfuryl	0.031±0.006	1.3±1.3	41.2	8.1±1.8	>16	>16	>16	258.5	4.3	37.6±0.5	1400±214	4.68	8.6	9.47
SJ000311275-1	3{2,3,2}	1-Naphtyl	2-HO-3-MeO-Bn	0.033±0.004	1.1±1.1	33.9	3.7±0.7	>16	10.6±0.4	>16	112.0	2.3	42.4±0.4	476±130	5.24	7.83	9.47
SJ000311276-1	3{2,3,3}	1-Naphtyl	Piperonyl	0.598±2.558	0.54±0.79	0.9	6.9±0.7	>16	11.7±0.3	>16	11.5	12.2	41.7±0.7	1228±47	5.27	8.15	9.47
SJ000311277-1	3{2,3,4}	1-Naphtyl	3-F-6-MeO-Bn	1.2±0.2	1.0±2.2	0.9	>16	>16	>16	>16	13.9	15.5	41.0±1.1	1056±238	5.69	8.11	9.47
SJ000311278-1	3{2,4,1}	4-CF3-Ph	Furfuryl	0.020±0.002	0.22±1.01	11.0	6.8±4.8	>16	12.9±1.2	15.3±5.3	332.9	15.5	34.4±0.3	1917±203	4.72	8.6	9.47
SJ000311279-1	3{2,4,2}	4-CF3-Ph	2-HO-3-MeO-Bn	0.013±0.014	0.024±0.041	1.8	4.2±3.2	11.8±0.6	4.2±1.2	>16	312.4	91.0	38.6±0.6	822±286	5.28	7.83	9.47
SJ000311280-1	3{2,4,3}	4-CF3-Ph	Piperonyl	0.025±0.003	0.098±0.131	3.9	3.3±0.3	>16	8.3±0.5	15.6±3.9	132.4	19.2	37.7±1.3	1389±212	5.3	8.15	9.47
SJ000311281-1	3{2,4,4}	4-CF3-Ph	3-F-6-MeO-Bn	0.054±0.004	0.089±0.098	1.7	8.1±1.3	>16	11.4±0.7	>16	150.5	58.4	39.9±1.8	1266±129	5.72	8.11	9.47
SJ000311282-1	3{2,5,1}	Ph	Furfuryl	0.020±0.001	0.13±0.14	6.3	8.1±2.9	>16	>16	>16	398.9	46.4	36.2±2.4	1795±215	3.77	8.6	9.47
SJ000311283-1	3{2,5,2}	Ph	2-HO-3-MeO-Bn	0.009±0.061	1.9±2.1	212.7	3.9±0.5	>16	15.3±0.8	13.6±6.8	429.7	1.7	42.1±0.7	445±164	4.33	7.83	9.47
SJ000311284-1	3{2,5,3}	Ph	Piperonyl	0.017±0.002	0.029±0.208	1.7	4.7±0.4	>16	9.1±0.3	5.9±1.5	269.9	138.9	41.8±1.5	1606±493	4.36	8.15	9.47
SJ000311285-1	3{2,5,4}	Ph	3-F-6-MeO-Bn	0.011±0.004	0.045±0.082	4.2	3.5±0.2	>16	11.7±0.3	14.9±2.2	327.4	66.3	40.7±0.4	1204±251	4.78	8.11	9.47
SJ000311286-1	3{2,6,1}	4-tertBu-Ph	Furfuryl	0.704±0.363	0.33±0.57	0.5	3.9±1.3	>16	8.9±1.5	15.9±5.6	5.5	9.7	37.8±0.9	2059±532	5.17	8.6	9.47

SJ000311287-1	3{2,6,2}	4-tertBu-Ph	2-HO-3-MeO-Bn	0.251±0.027	0.42±0.50	1.7	0.7±0.2	>16	2.1±0.9	18.0±16.2	3.0	1.7	41.5±1.9	579±536	5.73	7.83	9.47
SJ000311288-1	3{2,6,3}	4-tertBu-Ph	Piperonyl	0.223±0.084	0.49±0.60	2.2	1.6±0.3	>16	2.5±0.6	13.4±12.7	6.9	2.8	32.3±0.3	1196±148	5.76	8.15	9.47
SJ000311289-1	3{2,6,4}	4-tertBu-Ph	3-F-6-MeO-Bn	0.144±0.060	1.6±9.9	11.0	1.0±0.1	13.6±1.5	3.3±2.8	15.2±13.6	6.6	0.4	38.6±0.7	1104±203	6.18	8.11	9.47
SJ000311290-1	3{2,7,1}	Piperonyl	Furfuryl	0.019±0.005	0.046±0.071	2.4	8.4±0.8	>16	>16	>16	437.3	142.2	36.5±1.0	1266±88	3.54	8.6	9.47
SJ000311291-1	3{2,7,2}	Piperonyl	2-HO-3-MeO-Bn	0.008±0.007	0.050±0.531	6.0	1.9±1.6	15.8±0.4	8.7±1.7	7.7±6.1	226.0	22.7	39.8±1.7	317±41	4.1	7.83	9.47
SJ000311292-1	3{2,7,3}	Piperonyl	Piperonyl	0.026±0.041	0.027±0.003	1.0	7.6±3.3	>16	13.4±1.2	14.7±3.3	295.2	178.8	36.0±1.4	1234±42	4.13	8.15	9.47
SJ000311293-1	3{2,7,4}	Piperonyl	3-F-6-MeO-Bn	0.031±0.003	0.024±0.106	0.8	9.0±1.1	>16	14.7±1.2	12.1±7.6	289.3	255.8	39.3±0.9	1031±82	4.55	8.11	9.47
SJ000311294-1	3{2,8,1}	4-MeO-Ph	Furfuryl	0.011±0.028	0.023±0.032	2.2	7.6±2.3	>16	>16	>16	720.8	261.9	39.4±1.7	906±119	3.76	8.6	9.47
SJ000311295-1	3{2,8,2}	4-MeO-Ph	2-HO-3-MeO-Bn	0.013±0.006	0.078±0.146	6.0	2.5±0.3	>16	11.6±0.7	14.9±14.1	194.9	20.6	42.4±0.2	282±130	4.32	7.83	9.47
SJ000311296-1	3{2,8,3}	4-MeO-Ph	Piperonyl	0.029±0.025	0.026±0.628	0.9	6.5±0.9	>16	11.4±0.7	14.9±2.6	222.5	218.3	39.1±0.6	1663±454	4.34	8.15	9.47

<sup>a</sup>Values are the mean of three independent experiments in triplicate. <sup>b</sup>Values are means of an experiment in triplicate. <sup>c</sup>pKa and Alog P was calculated by

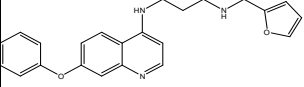
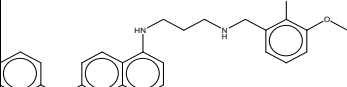
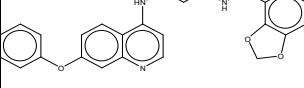
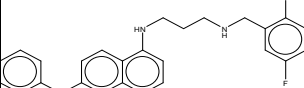
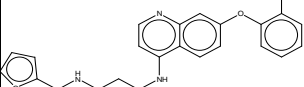
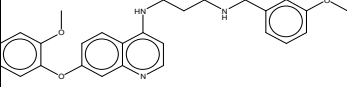
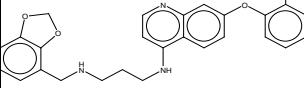
Pipeline pilot of Accelrys Software Inc.

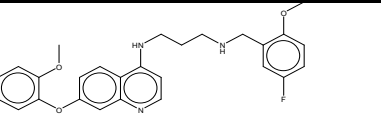
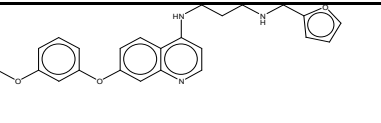
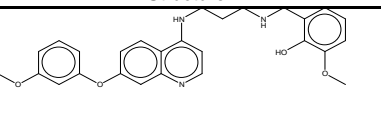
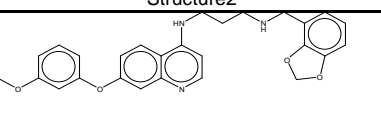
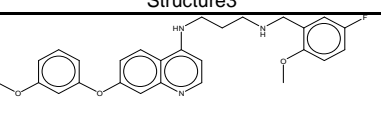
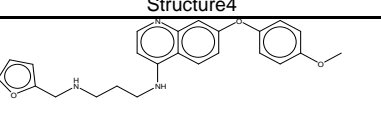
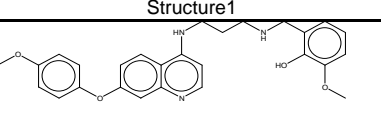
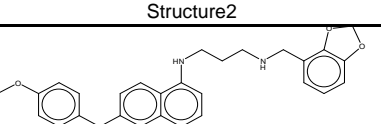
### SI-Table 3. Biological and pharmacological evaluation for akylaryls.

SAMPLE	No. 3{x,y,z}	R <sub>1</sub>	R <sub>2</sub>	3D7 <sup>a</sup> EC <sub>50</sub> , μM	K1 <sup>a</sup> EC <sub>50</sub> , μM	K1/3D7	HepG2 <sup>b</sup> EC <sub>50</sub> , μM	HEK293 <sup>b</sup> EC <sub>50</sub> , μM	Raji <sup>b</sup> EC <sub>50</sub> , μM	BJ <sup>b</sup> EC <sub>50</sub> , μM	HepG2 /3D7	HepG2 /K1	Avg. Sol <sup>b</sup> μM	Avg. Pe <sup>b</sup> X 10 <sup>6</sup> cm/s	AlogP <sup>b</sup>	pKa1 <sup>b</sup> (ring)	pKa2 <sup>b</sup> (chain)
SJ000311297-1	3{2,8,4}	4-MeO-Ph	3-F-6-MeO-Bn	0.096±0.010	0.029±1.437	0.3	9.1±1.2	>16	>16	15.1±1.3	94.6	205.5	40.2±2.8	2101±616	4.76	8.11	9.47
SJ000311242-1	3{3,1,1}	4-F-Bn	Furfuryl	0.057±0.004	1.7±1.9	28.9	6.1±0.3	>16	>16	>16	106.5	3.4	33.8±0.9	776±141	4.43	8.6	9.47
SJ000311243-1	3{3,1,2}	4-F-Bn	2-HO-3-MeO-Bn	0.015±0.004	7.2±24.5	473.5	9.4±7.5	>16	>16	15.4±2.5	624.7	0.7	38.0±0.6	199±48	5	7.83	9.47
SJ000311244-1	3{3,1,3}	4-F-Bn	Piperonyl	0.127±0.196	0.26±0.29	2.0	7.0±0.4	>16	>16	15.9±7.3	55.2	21.7	39.2±0.7	909±117	5.02	8.15	9.47
SJ000311245-1	3{3,1,4}	4-F-Bn	3-F-6-MeO-Bn	0.075±0.206	0.58±0.67	7.8	2.9±1.7	>16	8.2±0.4	5.0±0.6	38.5	6.1	40.1±1.1	838±204	5.44	8.11	9.47
SJ000311258-1	3{3,10,1}	iso-butyl	Furfuryl	0.581±0.024	4.5±4.7	7.7	>16	>16	>16	>16	27.5	3.6	31.6±2.8	715±101	3.9	8.6	9.47
SJ000311259-1	3{3,10,2}	iso-butyl	2-HO-3-MeO-Bn	0.020±0.001	8.100	402.5	3.9±0.9	>16	>16	>16	195.4	0.4	37.8±0.5	220±37	4.46	7.83	9.47
SJ000311260-1	3{3,10,3}	iso-butyl	Piperonyl	0.066±0.002	1.8±2.0	27.7	2.7±0.6	>16	12.1±0.5	>16	41.5	1.3	33.2±0.4	1494±52	4.49	8.15	9.47
SJ000311261-1	3{3,10,4}	iso-butyl	3-F-6-MeO-Bn	0.089±0.045	2.1±2.3	23.9	3.6±0.6	>16	>16	15.5±3.8	40.0	1.4	37.4±0.9	1061±487	4.91	8.11	9.47
SJ000311262-1	3{3,11,1}	cHex	Furfuryl	0.118±0.071	3.9±4.4	33.1	6.6±1.0	>16	>16	15.4±2.9	55.6	1.2	37.1±2.1	1178±201	4.45	8.6	9.47
SJ000311263-1	3{3,11,2}	cHex	2-HO-3-MeO-Bn	0.019±0.003	16.000	864.9	1.7±0.3	>16	>16	15.9±1.9	90.8	0.1	38.4±0.4	241±12	5.01	7.83	9.47
SJ000311264-1	3{3,11,3}	cHex	Piperonyl	0.128±0.079	4.7±8.8	36.7	5.4±0.5	>16	>16	15.0±2.4	41.8	0.6	36.9±0.3	1298±387	5.03	8.15	9.47
SJ000311265-1	3{3,11,4}	cHex	3-F-6-MeO-Bn	0.090±0.195	1.6±1.8	17.7	3.2±0.5	>16	>16	14.9±3.0	35.1	1.4	42.4±0.8	1050±406	5.45	8.11	9.47

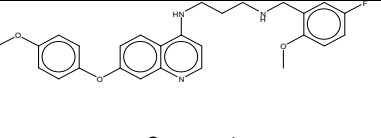
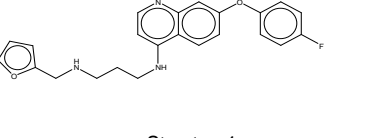
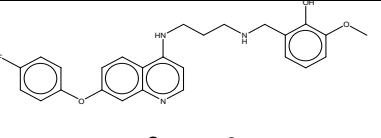
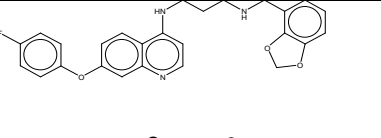
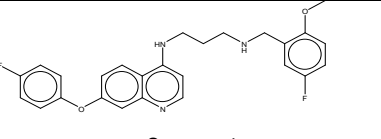
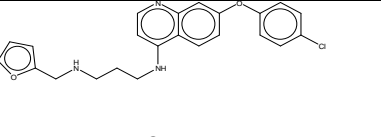
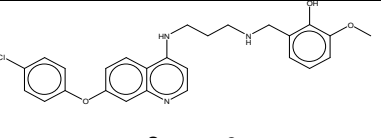
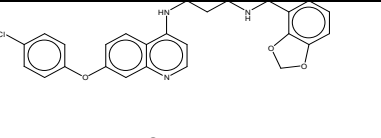
SJ000311266-1	3{3,12,1}	1-Et-Pr	Furfuryl	0.086±0.047	4.3±6.0	50.1	10.3±1.4	>16	>16	>16	119.7	1.6	39.0±1.0	482±132	4.36	8.6	9.47
SJ000311267-1	3{3,12,2}	1-Et-Pr	2-HO-3-MeO-Bn	0.004±0.001	0.27±0.32	68.3	0.11±0.05	1.3±0.4	1.1±0.2	0.2±0.2	28.3	1.5	41.0±1.9	23±1	4.92	7.83	9.47
SJ000311268-1	3{3,12,3}	1-Et-Pr	Piperonyl	0.027±0.080	1.1±1.2	39.5	7.4±1.9	>16	>16	15.5±3.0	275.9	6.0	37.2±1.2	404±119	4.95	8.15	9.47
SJ000311269-1	3{3,12,4}	1-Et-Pr	3-F-6-MeO-Bn	0.040±0.115	1.9±2.1	48.0	9.3±1.6	>16	>16	>16	230.5	4.1	39.2±1.3	120±21	5.37	8.11	9.47
SJ000311298-1	3{3,2,1}	3-CF3-Bn	Furfuryl	0.056±0.008	0.74±0.81	13.2	3.9±0.3	>16	10.5±0.4	15.7±3.5	69.8	4.3	29.2±1.7	1052±28	5.17	8.6	9.47
SJ000311299-1	3{3,2,2}	3-CF3-Bn	2-HO-3-MeO-Bn	0.025±0.005	2.2±3.4	87.9	2.1±0.4	13.7±0.2	9.6±0.5	15.7±10.1	85.8	0.8	36.1±1.7	226±80	5.73	7.83	9.47
SJ000311300-1	3{3,2,3}	3-CF3-Bn	Piperonyl	0.039±0.036	1.3±2.0	33.5	2.5±0.6	>16	9.1±0.5	15.7±3.8	64.2	1.7	35.5±1.3	1819±266	5.76	8.15	9.47
SJ000311301-1	3{3,2,4}	3-CF3-Bn	3-F-6-MeO-Bn	0.040±0.037	0.32±0.77	8.1	0.4±0.1	>16	9.3±1.0	12.1±1.8	10.2	1.3	35.5±2.0	1544±307	6.18	8.11	9.47
SJ000311302-1	3{3,3,1}	4-CN-Bn	Furfuryl	0.039±0.013	0.38±0.76	9.7	11.4±1.4	>16	>16	>16	290.7	20.7	33.0±0.2	908±72	4.11	8.6	9.47
SJ000311303-1	3{3,3,2}	4-CN-Bn	2-HO-3-MeO-Bn	0.011±0.003	5.4±5.8	513.5	8.6±1.7	>16	>16	14.1±4.8	815.3	1.3	36.8±0.2	95±64	4.67	7.83	9.47
SJ000311304-1	3{3,3,3}	4-CN-Bn	Piperonyl	0.023±0.013	3.1±3.2	136.4	8.6±3.6	>16	>16	15.2±5.2	380.2	2.0	36.0±0.3	1647±177	4.7	8.15	9.47
SJ000311305-1	3{3,3,4}	4-CN-Bn	3-F-6-MeO-Bn	0.028±0.037	0.77±1.42	27.5	7.6±2.4	>16	>16	15.7±5.5	270.4	7.9	37.0±1.8	1521±182	5.12	8.11	9.47
SJ000311306-1	3{3,4,1}	Bn	Furfuryl	0.040±0.037	3.6±3.9	89.9	>16	>16	>16	>16	405.1	4.5	32.3±0.3	1179±316	4.23	8.6	9.47
SJ000311307-1	3{3,4,2}	Bn	2-HO-3-MeO-Bn	0.017±0.001	7.0±0.70	400.6	8.1±1.4	>16	>16	>16	467.1	0.8	32.3±0.6	174±9	4.79	7.83	9.47
SJ000311308-1	3{3,4,3}	Bn	Piperonyl	0.720±3.504	1.2±1.4	1.7	8.2±3.3	>16	>16	15.6±7.0	11.4	5.1	36.0±0.6	1664±108	4.82	8.15	9.47
SJ000311309-1	3{3,4,4}	Bn	3-F-6-MeO-Bn	0.011±0.001	1.4±1.5	129.5	8.3±1.2	>16	>16	15.2±2.6	752.8	5.6	36.3±0.4	1718±794	5.24	8.11	9.47
SJ000311318-1	3{3,5,1}	3,5-Me-Bn	Furfuryl	0.009±0.001	0.68±0.74	77.0	7.2±1.7	>16	>16	>16	804.8	9.2	34.6±1.3	953±96	5.2	8.6	9.47
SJ000311319-1	3{3,5,2}	3,5-Me-Bn	2-HO-3-MeO-Bn	0.009±0.008	1.4±1.4	160.0	2.5±0.7	14.6±0.5	8.7±0.7	5.7±0.8	296.8	2.0	30.6±1.6	174±98	5.76	7.83	9.47
SJ000311320-1	3{3,5,3}	3,5-Me-Bn	Piperonyl	0.041±0.028	1.0±1.1	25.6	3.0±0.7	>16	>16	>16	73.2	2.2	20.6±0.4	756±70	5.79	8.15	9.47
SJ000311321-1	3{3,5,4}	3,5-Me-Bn	3-F-6-MeO-Bn	0.034±0.098	0.79±0.95	23.1	0.9±0.2	>16	9.3±1.5	>16	26.7	1.2	25.0±2.1	885±58	6.21	8.11	9.47
SJ000311322-1	3{3,6,1}	2-Cl-4-F-Bn	Furfuryl	0.020±0.003	1.2±1.4	62.1	8.7±2.3	>16	>16	>16	441.4	4.7	31.6±1.1	1312±14	5.1	8.6	9.47
SJ000311323-1	3{3,6,2}	2-Cl-4-F-Bn	2-HO-3-MeO-Bn	0.013±0.067	5.1±5.4	404.4	2.9±0.5	>16	>16	>16	228.5	0.5	36.1±3.3	611±182	5.66	7.83	9.47
SJ000311324-1	3{3,6,3}	2-Cl-4-F-Bn	Piperonyl	0.027±0.067	1.0±1.0	35.9	5.3±0.7	>16	>16	>16	201.3	16.8	39.9±2.0	1438±73	5.69	8.15	9.47
SJ000311325-1	3{3,6,4}	2-Cl-4-F-Bn	3-F-6-MeO-Bn	0.208±0.356	1.1±2.8	5.4	3.2±0.5	>16	>16	>16	15.6	2.2	38.6±1.9	1337±28	6.11	8.11	9.47
SJ000311246-1	3{3,7,1}	iso-pentyl	Furfuryl	0.176±0.019	4.6±1.7	26.1	>16	>16	>16	>16	90.7	2.4	31.8±1.8	861±102	4.36	8.6	9.47
SJ000311247-1	3{3,7,2}	iso-pentyl	2-HO-3-MeO-Bn	0.022±0.007	8.0±9.6	365.3	6.4±0.3	>16	>16	>16	294.2	0.7	35.9±1.4	230±53	4.92	7.83	9.47
SJ000311248-1	3{3,7,3}	iso-pentyl	Piperonyl	0.027±0.246	0.21±0.54	7.6	2.9±1.3	>16	>16	>16	105.6	13.5	36.5±0.7	2110.1	4.95	8.15	9.47
SJ000311249-1	3{3,7,4}	iso-pentyl	3-F-6-MeO-Bn	0.116±0.007	0.36±0.51	3.1	1.0±0.1	>16	>16	>16	8.8	2.5	35.4±1.3	1447±107	5.37	8.11	9.47
SJ000311250-1	3{3,8,1}	cHexmethyl	Furfuryl	0.055±0.015	0.62±1.72	11.2	2.2±0.3	>16	>16	>16	40.3	2.7	31.5±0.4	1165±110	4.9	8.6	9.47
SJ000311251-1	3{3,8,2}	cHexmethyl	2-HO-3-MeO-Bn	0.050±0.105	2.6±2.8	52.7	1.2±0.2	>16	12.2±0.8	13.9±1.0	24.8	0.4	38.0±0.7	327±21	5.46	7.83	9.47
SJ000311252-1	3{3,8,3}	cHexmethyl	Piperonyl	0.041±0.010	0.70±0.77	17.3	9.4±4.6	>16	>16	>16	231.1	9.0	35.5±1.0	2035±335	5.49	8.15	9.47
SJ000311253-1	3{3,8,4}	cHexmethyl	3-F-6-MeO-Bn	0.138±0.076	0.69±0.80	5.0	2.8±1.5	>16	>16	>16	20.6	2.7	37.5±1.4	1654±455	5.91	8.11	9.47
SJ000311254-1	3{3,9,1}	PhEt	Furfuryl	0.046±0.019	2.9±3.1	63.7	>16	>16	>16	>16	347.8	5.5	22.5±2.5	459±58	4.69	8.6	9.47
SJ000311255-1	3{3,9,2}	PhEt	2-HO-3-MeO-Bn	0.017±0.002	5.5±14.0	324.5	7.6±0.7	>16	>16	15.4±3.8	445.5	1.2	14.4±0.6	159±41	5.25	7.83	9.47
SJ000311256-1	3{3,9,3}	PhEt	Piperonyl	0.013±0.002	1.5±1.9	117.1	5.9±0.3	>16	>16	15.0±5.3	449.5	3.2	4.2±0.3	685±149	5.69	8.15	9.47
SJ000311257-1	3{3,9,4}	PhEt	3-F-6-MeO-Bn	0.132±0.110	2.1±2.2	16.2	5.6±0.3	>16	>16	16.0±4.4	42.7	2.0	11.3±1.5	783±268	5.27	8.11	9.47

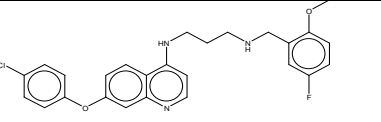
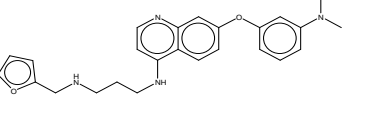
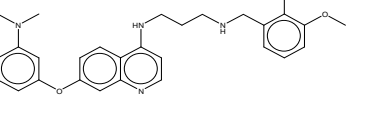
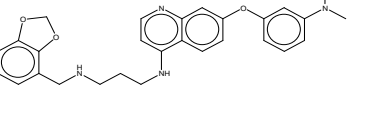
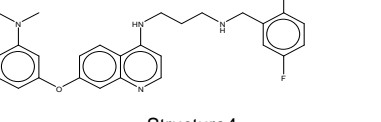
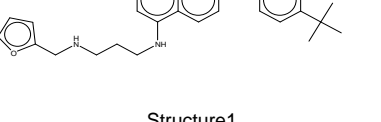
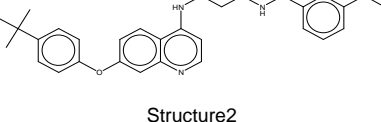
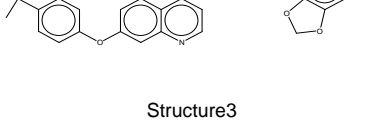
<sup>a</sup>Values are the mean of three independent experiments in triplicate. <sup>b</sup>Values are means of an experiment in triplicate. <sup>c</sup>pKa and Alog P was calculated by Pipeline pilot of Accelrys Software Inc.

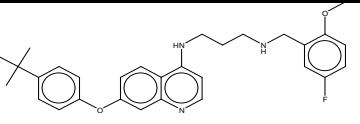
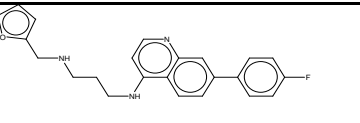
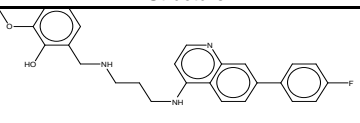
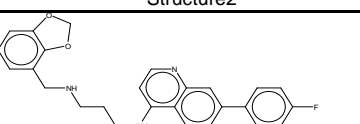
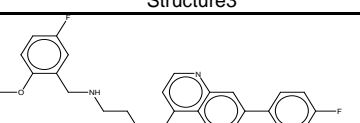
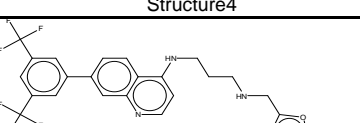
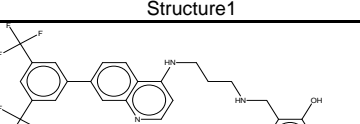
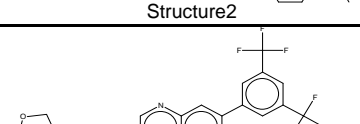
Structure	No. 3{x,y,z}	SJ-number	<sup>1</sup> H NMR (DMSO-d <sub>6</sub> )	MW	MW+2HCl	Yield (%)	Purity (UV)	Purity (ELSD)	Purity (UV- ELSD, Avg.)
	3{1,1,1}	SJ000311206-1	13.63 (s, 1H), 9.50 (s, 1H), 9.38 (s, 1H), 8.66 (d, J = 9.2 Hz, 1H), 8.48 (d, J = 6.4 Hz, 1H), 7.76 (dd, J = 2.0, 0.8 Hz, 1H), 7.55 (dd, J = 9.2, 8.0 Hz, 2H), 7.47 (dd, J = 9.2, 2.4 Hz, 1H), 7.35 (t, J = 7.2 Hz, 1H), 7.25 (d, J = 7.6 Hz, 2H), 7.21 (d, J = 2.4 Hz, 1H), 6.8 (d, J = 7.2 Hz, 1H), 6.65 (d, J = 3.2 Hz, 1H), 6.52 (dd, J = 3.2, 1.6 Hz, 1H), 4.24 (s, 2H), 3.63 (brs, 2H), 3.03 (brs, 2H), 2.10-1.99 (m, 2H)	373.45	446.37	59.7	54.48	64.06	59.27
	3{1,1,2}	SJ000311207-1	13.63 (brs, 1H), 9.45 (brs, 1H), 9.35 (brs, 1H), 9.07 (brs, 1H), 8.99 (brs, 1H), 8.63 (d, J = 9.2 Hz, 1H), 8.47 (d, J = 7.2 Hz, 1H), 7.55 (dd, J = 8.4, 7.6 Hz, 2H), 7.47 (dd, J = 9.2, 2.8 Hz, 1H), 7.35 (t, J = 7.2 Hz, 1H), 7.25 (d, J = 7.6 Hz, 2H), 7.20 (d, J = 2.4 Hz, 1H), 7.01 (dd, J = 1.6, 8.0 Hz, 2H), 6.82 (q, J = 8.0 Hz, 2H), 4.09 (s, 2H), 3.81 (s, 3H), 3.62 (s, 2H), 3.03 (brs, 2H), 2.06 (brs, 2H)	429.51	502.43	55.9	97.14	100	98.57
	3{1,1,3}	SJ000311208-1	13.63 (brs, 1H), 9.52 (brs, 1H), 9.37 (brs, 1H), 8.66 (d, J = 9.2 Hz, 1H), 8.48 (t, J = 4.8 Hz, 1H), 7.55 (dd, J = 8.4, 7.6 Hz, 2H), 7.47 (dd, J = 9.6, 2.4 Hz, 1H), 7.35 (t, J = 7.6 Hz, 1H), 7.25 (d, J = 7.2 Hz, 2H), 7.21 (d, J = 2.4 Hz, 1H), 7.09 (d, J = 7.6 Hz, 1H), 6.96 (dd, J = 6.4, 1.2 Hz, 1H), 6.89 (t, J = 7.6 Hz, 1H), 6.85 (d, J = 7.2 Hz, 1H), 6.06 (s, 2H), 4.10 (t, J = 5.0 Hz, 2H), 3.64 (q, J = 6.4 Hz, 2H), 3.07 (brs, 2H), 2.12-2.02 (m, 2H)	427.5	500.42	63.3	100	100	100
	3{1,1,4}	SJ000311209-1	13.77 (d, J = 5.8 Hz, 1H), 9.63 (t, J = 4.8 Hz, 1H), 9.35 (brs, 2H), 8.73 (d, J = 9.3 Hz, 1H), 8.47 (t, J = 6.7 Hz, 1H), 7.54 (t, J = 8.0 Hz, 2H), 7.47 (dd, J = 5.3, 3.2 Hz, 1H), 7.44 (dd, J = 4.4, 2.4 Hz, 1H), 7.35 (t, J = 7.4 Hz, 1H), 7.27-7.20 (m, 4H), 7.08 (dd, J = 4.4, 9.1 Hz, 1H), 6.86 (d, J = 6.9 Hz, 1H), 4.10 (t, J = 5.4 Hz, 2H), 3.81 (s, 3H), 3.65 (q, J = 6.2 Hz, 2H), 3.08-2.99 (brs, 2H), 2.15-2.05 (m, 2H)	431.5	504.42	68.5	100	100	100
	3{1,2,1}	SJ000311210-1	13.55 (brs, 1H), 9.46 (brs, 1H), 9.39 (brs, 2H), 8.62 (d, J = 9.6 Hz, 1H), 8.44 (d, J = 7.2 Hz, 1H), 7.76-7.75 (m, 1H), 7.40 (dd, J = 2.8, 9.6 Hz, 1H), 7.37 (dt, J = 1.6, 7.7 Hz, 1H), 7.29 (dd, J = 1.2, 7.2 Hz, 1H), 7.26 (dd, J = 1.6, 6.0 Hz, 1H), 7.09 (dt, J = 1.2, 7.6 Hz, 1H), 7.05 (d, J = 2.4 Hz, 1H), 6.82 (d, J = 7.6 Hz, 1H), 6.65 (d, J = 3.2 Hz, 1H), 6.51 (dd, J = 2.0, 3.2 Hz, 1H), 4.23 (s, 2H), 3.74 (s, 3H), 3.62 (brs, 2H), 3.02 (brs, 2H), 2.10-1.99 (m, 2H)	403.48	476.4	53.5	87.35	100	93.675
	3{1,2,2}	SJ000311211-1	13.59 (brs, 1H), 9.48 (brs, 1H), 9.34 (brs, 1H), 9.06 (brs, 1H), 8.61 (brs, 1H), 8.44 (brs, 1H), 7.43-7.34 (m, 2H), 7.30 (dd, J = 1.6, 8.4 Hz, 1H), 7.26 (dd, J = 1.6, 7.6 Hz, 1H), 7.09 (dt, J = 1.6, 8.0 Hz, 2H), 7.08-6.98 (m, 2H), 6.82 (d, J = 7.2 Hz, 1H), 6.79 (d, J = 8.0 Hz, 1H), 4.09 (brs, 2H), 3.81 (s, 3H), 3.74 (s, 3H), 3.62 (brs, 2H), 3.03 (brs, 2H), 2.06 (brs, 2H)	459.54	532.46	50.2	90.33	100	95.165
	3{1,2,3}	SJ000311212-1	13.36 (brs, 1H), 9.57 (brs, 1H), 9.50 (brs, 2H), 8.66 (d, J = 9.6 Hz, 1H), 8.44 (t, J = 6.6 Hz, 1H), 7.41-7.34 (m, 2H), 7.29 (dd, J = 8.2, 1.4 Hz, 1H), 7.26 (dd, J = 8.0, 1.6 Hz, 1H), 7.14-7.05 (m, 3H), 6.95 (dd, J = 7.6, 1.2 Hz, 1H), 6.88 (t, J = 8.0 Hz, 1H), 6.83 (d, J = 6.8 Hz, 1H), 6.06 (s, 2H), 4.08 (t, J = 5.6 Hz, 2H), 3.74 (s, 3H), 3.64 (q, J = 6.4 Hz, 2H), 3.06 (brs, 2H), 2.13-2.03 (m, 2H)	457.53	530.45	59.5	95.77	100	97.885

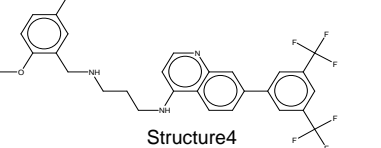
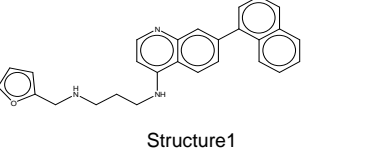
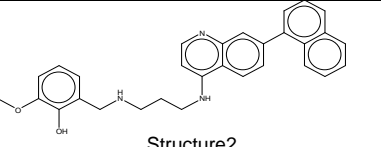
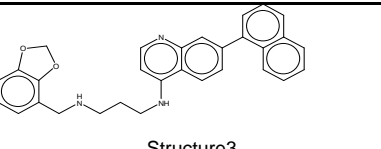
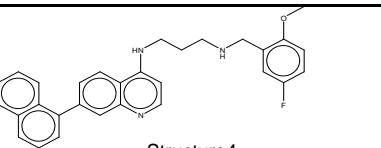
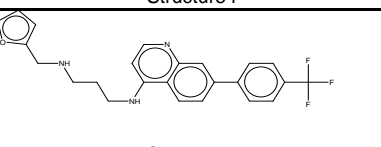
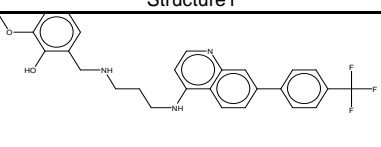
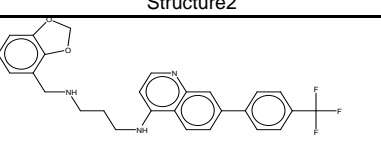
 Structure4	3{1,2,4}	SJ000311213-1	13.55 (brs, 1H), 9.47 (brs, 1H), 9.22 (brs, 2H), 8.63 (d, J = 9.2 Hz, 1H), 8.44 (t, J = 6.8 Hz, 1H), 7.45-7.34 (m, 3H), 7.31-7.20 (m, 3H), 7.12-7.06 (m, 2H), 7.05 (d, J = 2.4 Hz, 1H), 6.83 (d, J = 7.2 Hz, 1H), 4.11 (s, 2H), 3.81 (s, 3H), 3.74 (s, 3H), 3.63 (brs, 2H), 3.04 (brs, 2H), 2.13-2.03 (m, 2H)	461.53	534.45	51.1	95.67	100	97.835
 Structure1	3{1,3,1}	SJ000311214-1	13.77 (brs, 1H), 9.61 (brs, 1H), 9.51 (brs, 2H), 8.72 (d, J = 9.2 Hz, 1H), 8.49 (d, J = 6.4 Hz, 1H), 7.78-7.74 (m, 1H), 7.48-7.41 (m, 2H), 7.29 (d, J = 2.4 Hz, 1H), 6.92 (dd, J = 8.4, 2.4 Hz, 1H), 6.86 (d, J = 7.2 Hz, 1H), 6.84 (t, J = 2.2 Hz, 1H), 6.80 (dd, J = 8.0, 2.4 Hz, 1H), 6.66 (d, J = 3.2 Hz, 1H), 6.52 (dd, J = 2.0, 2.8 Hz, 1H), 4.23 (s, 2H), 3.79 (s, 3H), 3.70-3.60 (m, 2H), 3.03 (brs, 2H), 2.13-2.03 (m, 2H)	403.48	476.4	55.3	71.78	85.48	78.63
 Structure2	3{1,3,2}	SJ000311215-1	13.72 (d, J = 6.0 Hz, 1H), 9.45 (t, J = 5.6 Hz, 1H), 9.36 (s, 1H), 9.09 (brs, 2H), 8.67 (d, J = 9.2 Hz, 1H), 8.48 (t, J = 6.6 Hz, 1H), 7.48-7.42 (m, 2H), 7.28 (d, J = 2.4 Hz, 1H), 7.02 (t, J = 6.6 Hz, 2H), 6.93 (dd, J = 8.0, 2.8 Hz, 1H), 6.88-6.77 (m, 4H), 4.10 (t, J = 5.4 Hz, 2H), 3.82 (s, 3H), 3.79 (s, 3H), 3.67-3.60 (m, 2H), 3.04 (brs, 2H), 2.13-2.02 (m, 2H)	459.54	532.46	64.0	94.43	100	97.215
 Structure3	3{1,3,3}	SJ000311216-1	13.66 (s, 1H), 9.54 (brs, 1H), 9.41 (brs, 2H), 8.67 (d, J = 9.2 Hz, 1H), 8.49 (t, J = 6.6 Hz, 1H), 7.47 (dd, J = 8.8, 2.4 Hz, 1H), 7.45 (t, J = 8.4 Hz, 1H), 7.26 (d, J = 2.4 Hz, 1H), 7.11 (d, J = 8.0 Hz, 1H), 6.99-6.78 (m, 6H), 6.07 (s, 2H), 4.10 (brs, 2H), 3.79 (s, 3H), 3.65 (brs, 2H), 3.08 (brs, 2H), 2.13-2.02 (m, 2H)	457.53	530.45	62.8	97.54	100	98.77
 Structure4	3{1,3,4}	SJ000311217-1	13.55 (brs, 1H), 9.40 (brs, 1H), 9.10 (brs, 2H), 8.60 (brs, 1H), 8.50 (d, J = 6.8 Hz, 1H), 7.52-7.36 (m, 3H), 7.28-7.22 (m, 2H), 7.11 (dd, J = 9.2, 4.4 Hz, 1H), 6.93 (dd, J = 8.4, 2.4 Hz, 1H), 6.88-6.78 (m, 3H), 4.12 (s, 2H), 3.83 (s, 3H), 3.79 (s, 3H), 3.64 (brs, 2H), 3.06 (brs, 2H), 2.07 (brs, 2H)	461.53	534.45	50.7	100	100	100
 Structure1	3{1,4,1}	SJ000311218-1	13.54 (brs, 1H), 9.44 (brs, 1H), 9.36 (brs, 2H), 8.63 (d, J = 9.2 Hz, 1H), 8.47 (d, J = 7.2 Hz, 1H), 7.78-7.77 (m, 1H), 7.45 (dd, J = 9.2, 2.4 Hz, 1H), 7.23-7.18 (m, 2H), 7.13-7.07 (m, 3H), 6.83 (d, J = 7.6 Hz, 1H), 6.65 (d, J = 3.2 Hz, 1H), 6.53 (dd, J = 3.2, 1.8 Hz, 1H), 4.24 (s, 2H), 3.81 (s, 3H), 3.63 (brs, 2H), 3.03 (brs, 2H), 2.09-1.99 (m, 2H)	403.48	476.4	65.8	92.29	100	96.145
 Structure2	3{1,4,2}	SJ000311219-1	13.69 (brs, 1H), 9.57 (brs, 1H), 9.34 (s, 1H), 9.15 (brs, 2H), 8.68 (d, J = 9.6 Hz, 1H), 8.46 (d, J = 6.8 Hz, 1H), 7.42 (dd, J = 9.6, 2.4 Hz, 1H), 7.23-7.18 (m, 2H), 7.16 (d, J = 2.8 Hz, 1H), 7.12-7.06 (m, 2H), 7.02 (dd, J = 12.0, 8.4 Hz, 2H), 6.83 (d, J = 7.2 Hz, 1H), 6.81 (t, J = 8.0 Hz, 1H), 4.09 (brs, 2H), 3.82 (s, 3H), 3.81 (s, 3H), 3.63 (brs, 2H), 3.03 (brs, 2H), 2.14-2.02 (m, 2H)	459.54	532.46	69.9	96.71	100	98.355
 Structure3	3{1,4,3}	SJ000311220-1	13.50 (brs, 1H), 9.43 (brs, 1H), 9.33 (brs, 2H), 8.65 (brs, 1H), 8.39 (d, J = 7.2 Hz, 1H), 7.37 (dd, J = 9.6, 2.4 Hz, 1H), 7.16-7.10 (m, 2H), 7.07-6.99 (m, 4H), 6.89 (dd, J = 8.0, 1.2 Hz, 1H), 8.62 (t, J = 8.0 Hz, 1H), 6.76 (d, J = 7.2 Hz, 1H), 5.99 (s, 2H), 4.02 (s, 2H), 3.74 (s, 3H), 3.56 (brs, 2H), 2.99 (brs, 2H), 2.05-1.95 (m, 2H)	457.53	530.45	61.6	100	100	100

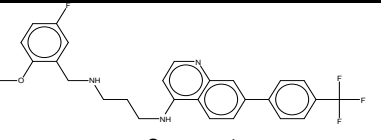
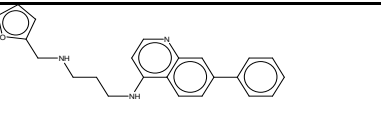
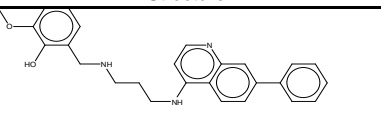
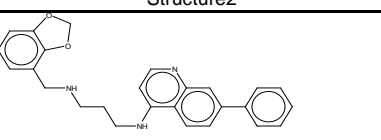
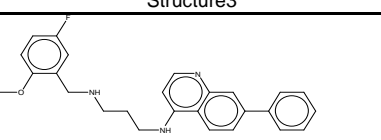
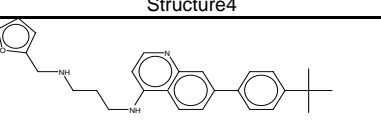
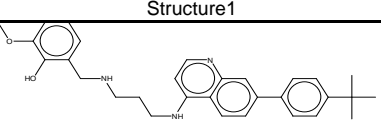
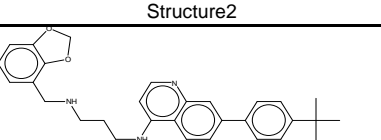


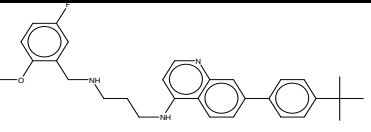
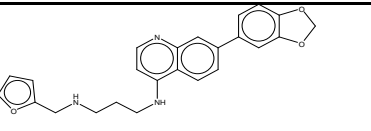
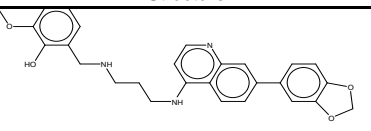
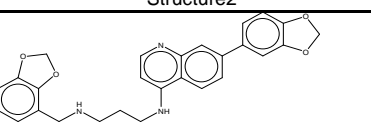
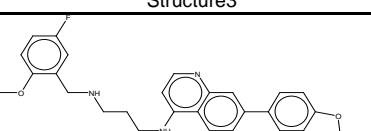
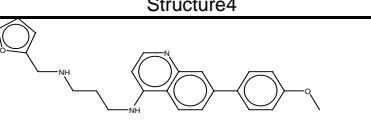
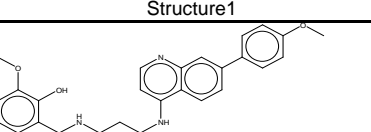
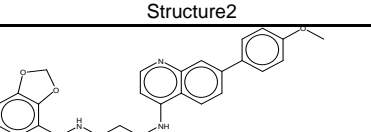
	3{1,4,4}	SJ000311221-1	13.61 (brs, 1H), 9.55 (brs, 1H), 9.31 (brs, 2H), 8.67 (brs, 1H), 8.47 (d, J = 7.2 Hz, 1H), 7.48-7.40 (m, 2H), 7.28-7.18 (m, 3H), 7.17-7.07 (m, 4H), 6.45 (d, J = 7.6 Hz, 1H), 4.11 (s, 2H), 3.82 (s, 3H), 3.81 (s, 3H), 3.64 (brs, 2H), 3.05 (brs, 2H), 2.09 (brs, 2H)	461.53	534.45	63.6	100	100	100
<b>Structure4</b>									
	3{1,5,1}	SJ000311222-1	13.69 (brs, 1H), 9.55 (brs, 1H), 9.45 (brs, 2H), 8.69 (d, J = 9.6 Hz, 1H), 8.49 (d, J = 7.2 Hz, 1H), 7.78-7.76 (m, 1H), 7.47 (dd, J = 9.2, 2.4 Hz, 1H), 7.42-7.30 (m, 4H), 7.20 (d, J = 2.8 Hz, 1H), 6.85 (d, J = 7.6 Hz, 1H), 6.66 (d, J = 3.2 Hz, 1H), 6.52 (dd, J = 3.2, 2.0 Hz, 1H), 4.24 (s, 2H), 3.64 (brs, 2H), 3.03 (brs, 2H), 2.10-2.00 (m, 2H)	391.44	464.36	54.3	93.43	100	96.715
<b>Structure1</b>									
	3{1,5,2}	SJ000311223-1	13.58 (brs, 1H), 9.39 (brs, 2H), 8.94 (brs, 2H), 8.61 (d, J = 9.2 Hz, 1H), 8.49 (d, J = 7.2 Hz, 1H), 7.48 (dd, J = 9.2, 2.8 Hz, 1H), 7.43-7.36 (m, 2H), 7.35-7.29 (m, 2H), 7.19-7.16 (m, 1H), 7.01 (t, J = 8.0 Hz, 2H), 6.87-6.79 (m, 2H), 4.10 (s, 2H), 3.82 (s, 3H), 3.62 (brs, 2H), 3.04 (brs, 2H), 2.12-2.00 (m, 2H)	447.5	520.42	53.6	97.28	100	98.64
<b>Structure2</b>									
	3{1,5,3}	SJ000311224-1	13.56 (brs, 1H), 9.42 (brs, 1H), 9.26 (brs, 2H), 8.62 (d, J = 9.6 Hz, 1H), 8.50 (d, J = 7.2 Hz, 1H), 7.48 (dd, J = 9.2, 2.4 Hz, 1H), 7.43-7.36 (m, 2H), 7.35-7.29 (m, 2H), 7.17 (d, J = 2.4 Hz, 1H), 7.07 (d, J = 8.0 Hz, 1H), 6.98 (d, J = 7.2 Hz, 1H), 6.90 (t, J = 7.8 Hz, 1H), 8.65 (d, J = 7.6 Hz, 1H), 6.07 (s, 2H), 4.11 (s, 2H), 3.63 (brs, 2H), 3.07 (brs, 2H), 2.12-2.00 (m, 2H)	445.49	518.41	45.6	100	100	100
<b>Structure3</b>									
	3{1,5,4}	SJ000311225-1	13.61 (brs, 1H), 9.50 (brs, 1H), 9.18 (brs, 2H), 8.66 (d, J = 9.2 Hz, 1H), 8.50 (d, J = 7.2 Hz, 1H), 7.48 (dd, J = 9.2, 2.8 Hz, 1H), 7.45-7.36 (m, 3H), 7.35-7.29 (m, 2H), 7.25 (dt, J = 3.2, 8.6 Hz, 1H), 7.18 (d, J = 2.4 Hz, 1H), 7.10 (dd, J = 7.2, 4.4 Hz, 1H), 6.86 (d, J = 7.2 Hz, 1H), 4.12 (s, 2H), 3.82 (s, 3H), 3.64 (brs, 2H), 3.05 (brs, 2H), 2.12-2.00 (m, 2H)	449.49	522.41	44.2	100	100	100
<b>Structure4</b>									
	3{1,6,1}	SJ000311226-1	13.66 (brs, 1H), 9.55 (brs, 1H), 9.40 (brs, 2H), 8.68 (brs, 1H), 8.51 (d, J = 7.2 Hz, 1H), 7.79-7.76 (m, 1H), 7.63-7.58 (m, 2H), 7.50 (dd, J = 9.6, 2.4 Hz, 1H), 7.33-7.23 (m, 3H), 6.86 (d, J = 7.2 Hz, 1H), 6.65 (t, J = 2.4 Hz, 1H), 6.53 (dd, J = 3.2, 1.8 Hz, 1H), 4.25 (s, 2H), 3.64 (brs, 2H), 3.03 (brs, 2H), 2.05 (brs, 2H)	407.9	480.82	48.9	84.35	100	92.175
<b>Structure1</b>									
	3{1,6,2}	SJ000311227-1	13.62 (brs, 1H), 9.46 (brs, 1H), 9.39 (brs, 1H), 8.96 (brs, 2H), 8.63 (d, J = 9.2 Hz, 1H), 8.51 (d, J = 7.2 Hz, 1H), 7.64-7.58 (m, 2H), 7.50 (dd, J = 9.6, 2.4 Hz, 1H), 7.33-7.27 (m, 2H), 7.24 (d, J = 2.4 Hz, 1H), 7.01 (t, J = 7.2 Hz, 2H), 6.86 (d, J = 7.2 Hz, 1H), 6.82 (t, J = 8.0 Hz, 1H), 4.10 (s, 2H), 3.82 (s, 3H), 3.62 (brs, 2H), 3.04 (brs, 2H), 2.12-2.01 (m, 2H)	463.96	536.88	47.8	96.44	100	98.22
<b>Structure2</b>									
	3{1,6,3}	SJ000311228-1	13.66 (brs, 1H), 9.53 (brs, 1H), 9.38 (brs, 2H), 8.67 (d, J = 9.6 Hz, 1H), 8.51 (d, J = 7.2 Hz, 1H), 7.63-7.58 (m, 2H), 7.50 (dd, J = 9.6, 2.8 Hz, 1H), 7.33-7.27 (m, 2H), 7.25 (d, J = 2.0 Hz, 1H), 7.10 (d, J = 6.0 Hz, 1H), 6.97 (d, J = 7.6 Hz, 1H), 6.93-6.84 (m, 2H), 6.07 (s, 2H), 4.10 (s, 2H), 3.65 (brs, 2H), 3.07 (brs, 2H), 2.12-2.01 (m, 2H)	461.95	534.87	53.3	100	100	100
<b>Structure3</b>									

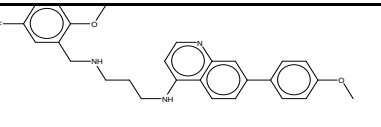
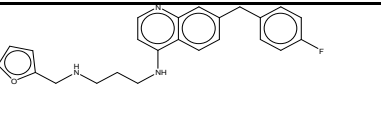
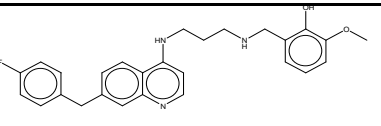
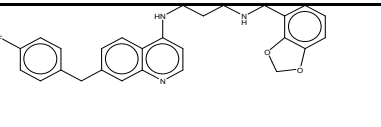
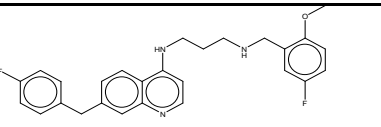
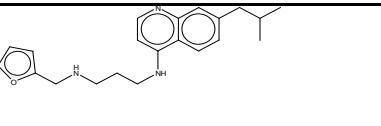
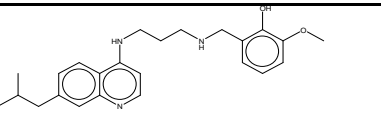
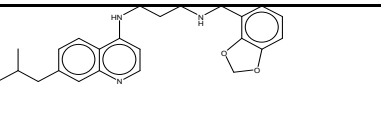
 Structure4	3{1,6,4}	SJ000311229-1	13.65 (brs, 1H), 9.54 (brs, 1H), 9.22 (brs, 2H), 8.68 (brs, 1H), 8.51 (d, J = 6.8 Hz, 1H), 7.64-7.58 (m, 2H), 7.50 (dd, J = 9.2, 2.0 Hz, 1H), 7.47-7.40 (m, 1H), 7.33-7.22 (m, 4H), 7.10 (dd, J = 9.2, 4.8 Hz, 1H), 6.87 (d, J = 7.2 Hz, 1H), 4.12 (s, 2H), 3.82 (s, 3H), 3.65 (brs, 2H), 3.05 (brs, 2H), 2.15-2.03 (m, 2H)	465.95	538.87	47.6	100	100	100
 Structure1	3{1,7,1}	SJ000311230-1	13.68 (brs, 1H), 9.56 (brs, 1H), 9.49 (brs, 2H), 8.71-8.64 (m, 1H), 8.47 (t, J = 6.6 Hz, 1H), 7.78-7.76 (m, 1H), 7.44 (dd, J = 9.2, 4.4 Hz, 1H), 7.33 (t, J = 8.0 Hz, 1H), 7.25 (brs, 1H), 6.84 (d, J = 6.8 Hz, 1H), 6.77-6.69 (m, 1H), 6.66 (d, J = 3.2 Hz, 1H), 6.58 (brs, 1H), 6.55-6.45 (m, 2H), 4.24 (t, J = 5.2 Hz, 2H), 3.68-3.60 (m, 2H), 3.02 (brs, 2H), 2.94 (s, 6H), 2.11-2.01 (m, 2H)	416.52	489.44	43.3	92.48	100	96.24
 Structure2	3{1,7,2}	SJ000311231-1	13.71 (brs, 1H), 9.55 (brs, 1H), 9.35 (brs, 1H), 9.13 (brs, 2H), 8.67 (brs, 1H), 8.46 (t, J = 6.6 Hz, 1H), 7.44 (d, J = 9.2 Hz, 1H), 7.33 (t, J = 4.4 Hz, 1H), 7.26 (brs, 1H), 7.06-6.99 (m, 2H), 6.84 (d, J = 7.2 Hz, 1H), 6.81 (t, J = 7.8 Hz, 1H), 6.73 (brs, 1H), 6.59 (brs, 1H), 6.49 (brs, 1H), 4.09 (brs, 2H), 3.82 (s, 3H), 3.69-3.59 (m, 2H), 3.03 (brs, 2H), 2.94 (s, 6H), 2.13-2.03 (m, 2H)	472.58	545.5	38.8	77.01	100	88.505
 Structure3	3{1,7,3}	SJ000311232-1	13.64 (brs, 1H), 9.53 (brs, 1H), 9.45 (brs, 2H), 8.67 (d, J = 9.6 Hz, 1H), 8.47 (t, J = 6.6 Hz, 1H), 7.45 (dd, J = 9.2, 2.4 Hz, 1H), 7.33 (t, J = 8.2 Hz, 1H), 7.26-7.22 (m, 1H), 7.12 (d, J = 8.0 Hz, 1H), 6.97 (dd, J = 7.6, 1.2 Hz, 1H), 6.90 (t, J = 8.0 Hz, 1H), 6.84 (d, J = 7.2 Hz, 1H), 6.71 (d, J = 8.0 Hz, 1H), 6.57 (brs, 1H), 6.48 (d, J = 8.0 Hz, 1H), 6.07 (s, 2H), 4.10 (t, J = 5.6 Hz, 2H), 3.69-3.60 (m, 2H), 3.07 (brs, 2H), 2.94 (s, 6H), 2.13-2.03 (m, 2H)	470.57	543.49	41.7	100	100	100
 Structure4	3{1,7,4}	SJ000311233-1	13.68 (brs, 1H), 9.58 (brs, 1H), 9.32 (brs, 2H), 8.69 (dd, J = 9.2, 4.0 Hz, 1H), 8.46 (t, J = 6.6 Hz, 1H), 7.48-7.41 (m, 2H), 7.32 (t, J = 8.0 Hz, 1H), 7.27-7.20 (m, 2H), 7.08 (dd, J = 9.2, 4.8 Hz, 1H), 6.84 (d, J = 7.2 Hz, 1H), 6.73 (brs, 1H), 6.59 (brs, 1H), 6.48 (brs, 1H), 4.10 (t, J = 5.6 Hz, 2H), 3.81 (s, 3H), 3.69-3.60 (m, 2H), 3.04 (brs, 2H), 2.93 (s, 6H), 2.13-2.03 (m, 2H)	474.57	547.49	42.8	94.12	100	97.06
 Structure1	3{1,8,1}	SJ000311234-1	13.63 (brs, 1H), 9.53 (brs, 3H), 8.73-8.63 (m, 1H), 8.47 (d, J = 7.2 Hz, 1H), 7.76 (dd, J = 1.7, 0.8 Hz, 1H), 7.57-7.51 (m, 2H), 7.50-7.43 (m, 1H), 7.22-7.14 (m, 3H), 6.64 (d, J = 7.2 Hz, 1H), 6.65 (d, J = 2.8 Hz, 1H), 6.52 (dd, J = 3.2, 2.0 Hz, 1H), 4.10 (s, 2H), 3.63 (brs, 2H), 3.02 (brs, 2H), 2.10-1.99 (m, 2H), 1.33 (s, 9H).	429.56	502.48	58.2	58.8	67.55	63.175
 Structure2	3{1,8,2}	SJ000311235-1	13.63 (brs, 1H), 9.51 (brs, 1H), 9.36 (s, 1H), 9.05 (brs, 2H), 8.66 (d, J = 9.6 Hz, 1H), 8.47 (d, J = 6.8 Hz, 1H), 7.57-7.52 (m, 2H), 7.47 (dd, J = 9.2, 2.8 Hz, 1H), 7.21-7.14 (m, 3H), 7.04-6.99 (m, 2H), 6.86-6.78 (m, 2H), 4.09 (brs, 2H), 3.81 (s, 3H), 3.63 (brs, 2H), 3.03 (brs, 2H), 2.12-2.02 (m, 2H), 1.33 (s, 9H).	485.62	558.54	60.0	96.86	100	98.43
 Structure3	3{1,8,3}	SJ000311236-1	13.59 (brs, 1H), 9.52 (brs, 1H), 9.38 (s, 2H), 8.66 (d, J = 9.6 Hz, 1H), 8.47 (d, J = 7.2 Hz, 1H), 7.57-7.52 (m, 2H), 7.47 (dd, J = 9.6, 2.4 Hz, 1H), 7.21-7.14 (m, 3H), 7.09 (d, J = 7.6 Hz, 1H), 6.96 (d, J = 7.2 Hz, 1H), 6.89 (t, J = 7.8 Hz, 1H), 6.85 (d, J = 9.2 Hz, 1H), 6.06 (s, 2H), 4.10 (s, 2H), 3.64 (brs, 2H), 3.07 (brs, 2H), 2.12-2.00 (m, 2H), 1.33 (s, 9H).	483.61	556.53	57.7	100	100	100

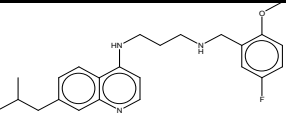
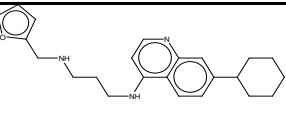
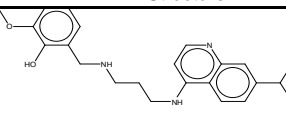
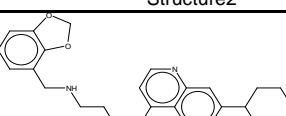
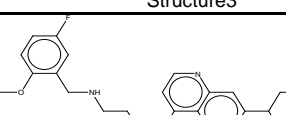
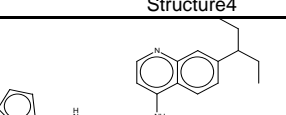
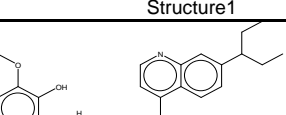
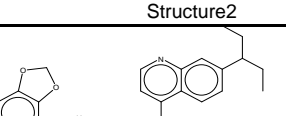
 Structure4	3{1,8,4}	SJ000311237-1	13.54 (brs, 1H), 9.44 (brs, 1H), 9.10 (brs, 2H), 8.63 (brs, 1H), 8.48 (d, J = 7.2 Hz, 1H), 7.57-7.52 (m, 2H), 7.48 (dd, J = 9.6, 2.4 Hz, 1H), 7.44-7.38 (m, 1H), 7.25 (dt, J = 8.8, 2.8 Hz, 1H), 7.20-7.14 (m, 3H), 7.10 (dd, J = 9.2, 4.8 Hz, 1H), 6.85 (d, J = 6.8 Hz, 1H), 4.12 (s, 2H), 3.82 (s, 3H), 3.63 (brs, 2H), 3.05 (brs, 2H), 2.07 (brs, 2H), 1.33 (s, 9H).	487.61	560.53	61.1	98.02	100	99.01
 Structure1	3{2,1,1}	SJ000311238-1	14.07 (brs, 1H), 9.57 (brs, 1H), 9.38 (brs, 2H), 8.71 (d, J = 8.8 Hz, 1H), 8.61 (d, J = 7.2 Hz, 1H), 8.16 (s, 1H), 8.07 (dd, J = 8.8, 2.0 Hz, 1H), 7.93-7.87 (m, 2H), 7.77 (dd, J = 1.8, 0.7 Hz, 1H), 7.47-7.40 (m, 2H), 6.93 (d, J = 7.2 Hz, 1H), 6.65 (d, J = 3.2 Hz, 1H), 6.52 (dd, J = 3.2, 2.0 Hz, 1H), 4.25 (s, 2H), 3.67 (brs, 2H), 3.05 (brs, 2H), 2.12-2.02 (m, 2H).	375.44	448.36	65.9	88.94	100	94.47
 Structure2	3{2,1,2}	SJ000311239-1	14.04 (brs, 1H), 9.51 (brs, 1H), 9.38 (brs, 1H), 8.97 (brs, 2H), 8.68 (d, J = 8.8 Hz, 1H), 8.60 (d, J = 7.2 Hz, 1H), 8.15 (d, J = 1.6 Hz, 1H), 8.06 (dd, J = 8.8, 2.0 Hz, 1H), 7.93-7.87 (m, 2H), 7.47-7.40 (m, 2H), 7.03-6.98 (m, 2H), 6.92 (d, J = 7.2 Hz, 1H), 6.81 (t, J = 7.8 Hz, 1H), 4.11 (s, 2H), 3.81 (s, 3H), 3.66 (brs, 2H), 3.06 (brs, 2H), 2.12-2.02 (m, 2H).	431.5	504.42	61.9	100	100	100
 Structure3	3{2,1,3}	SJ000311240-1	14.04 (brs, 1H), 9.57 (brs, 1H), 9.35 (brs, 2H), 8.70 (d, J = 8.8 Hz, 1H), 8.61 (d, J = 7.2 Hz, 1H), 8.16 (s, 1H), 8.07 (dd, J = 8.8, 1.8 Hz, 1H), 7.93-7.87 (m, 2H), 7.47-7.40 (m, 2H), 7.09 (d, J = 8.0 Hz, 1H), 6.97 (dd, J = 8.0, 1.2 Hz, 1H), 6.93 (d, J = 7.2 Hz, 1H), 6.90 (t, J = 8.0 Hz, 1H), 6.07 (s, 2H), 4.11 (s, 2H), 3.68 (brs, 2H), 3.09 (brs, 2H), 2.15-2.04 (m, 2H).	429.49	502.41	55.4	100	100	100
 Structure4	3{2,1,4}	SJ000311241-1	14.04 (brs, 1H), 9.57 (brs, 1H), 9.18 (brs, 2H), 8.71 (d, J = 8.8 Hz, 1H), 8.61 (d, J = 7.2 Hz, 1H), 8.16 (s, 1H), 8.06 (dd, J = 8.8, 1.2 Hz, 1H), 7.93-7.87 (m, 2H), 7.47-7.40 (m, 3H), 7.24 (dt, J = 3.2, 8.6 Hz, 1H), 7.09 (dd, J = 10.8, 2.4 Hz, 1H), 6.93 (d, J = 7.2 Hz, 1H), 4.12 (brs, 2H), 3.82 (s, 3H), 3.68 (brs, 2H), 3.07 (brs, 2H), 2.15-2.04 (m, 2H).	433.49	506.41	63.3	100	100	100
 Structure1	3{2,2,1}	SJ000311270-1	13.98 (brs, 1H), 9.66 (brs, 1H), 9.35 (brs, 2H), 8.78 (d, J = 8.8 Hz, 1H), 8.66 (d, J = 7.2 Hz, 1H), 8.52 (s, 2H), 8.35-8.26 (m, 3H), 7.77-7.76 (m, 1H), 6.70 (d, J = 7.6 Hz, 1H), 6.65 (d, J = 3.2 Hz, 1H), 6.52 (dd, J = 3.2, 2.0 Hz, 1H), 4.25 (brs, 2H), 3.68 (brs, 2H), 3.05 (brs, 2H), 2.15-2.04 (m, 2H).	493.45	566.37	79.1	65.58	76.56	71.07
 Structure2	3{2,2,2}	SJ000311271-1	14.06 (brs, 1H), 9.70 (brs, 1H), 9.37 (brs, 1H), 9.06 (brs, 2H), 8.79 (d, J = 8.8 Hz, 1H), 8.64 (d, J = 7.2 Hz, 1H), 8.52 (s, 2H), 8.35 (d, J = 1.8 Hz, 1H), 8.30-8.25 (m, 2H), 7.04-6.99 (m, 2H), 6.97 (d, J = 7.2 Hz, 1H), 6.81 (t, J = 8.0 Hz, 1H), 4.11 (brs, 2H), 3.81 (s, 3H), 3.68 (brs, 2H), 3.06 (brs, 2H), 2.16-2.06 (m, 2H).	549.51	622.43	79.6	100	100	100
 Structure3	3{2,2,3}	SJ000311272-1	14.05 (brs, 1H), 9.76 (brs, 1H), 9.44 (brs, 2H), 8.82 (d, J = 8.8 Hz, 1H), 8.65 (d, J = 7.2 Hz, 1H), 8.52 (s, 2H), 8.35 (d, J = 1.6 Hz, 1H), 8.30-8.25 (m, 2H), 7.11 (d, J = 8.0 Hz, 1H), 7.00-6.94 (m, 2H), 6.89 (t, J = 7.8 Hz, 1H), 6.07 (s, 2H), 4.11 (brs, 2H), 3.70 (brs, 2H), 3.10 (brs, 2H), 2.17-2.07 (m, 2H).	547.5	620.42	79.1	96.37	100	98.185

	3{2,2,4}	SJ000311273-1	13.93 (brs, 1H), 9.62 (brs, 1H), 9.10 (brs, 2H), 8.76 (d, J = 8.8 Hz, 1H), 8.66 (d, J = 7.2 Hz, 1H), 8.52 (s, 2H), 8.32 (d, J = 1.6 Hz, 1H), 8.30-8.25 (m, 2H), 7.41 (dd, J = 8.8, 3.2 Hz, 1H), 7.25 (dt, J = 8.8, 3.2 Hz, 1H), 7.10 (dd, J = 8.8, 4.4 Hz, 1H), 6.97 (d, J = 7.2 Hz, 1H), 4.13 (brs, 2H), 3.82 (s, 3H), 3.68 (brs, 2H), 3.08 (brs, 2H), 2.16-2.06 (m, 2H).	551.5	624.42	64.1	97.66	100	98.83
	3{2,3,1}	SJ000311274-1	14.04 (brs, 1H), 9.55 (brs, 1H), 9.29 (brs, 2H), 8.73 (d, J = 8.8 Hz, 1H), 8.66 (d, J = 7.2 Hz, 1H), 8.09 (d, J = 8.0 Hz, 2H), 8.03 (d, J = 1.5 Hz, 1H), 7.88 (dd, J = 8.4, 1.6 Hz, 1H), 7.83-7.78 (m, 2H), 7.68 (t, J = 7.2 Hz, 1H), 7.65-7.53 (m, 3H), 6.92 (d, J = 7.2 Hz, 1H), 6.65 (d, J = 3.2 Hz, 1H), 6.54 (dd, J = 3.2, 2.0 Hz, 1H), 4.27 (brs, 2H), 3.70 (brs, 2H), 3.07 (brs, 2H), 2.13-2.03 (m, 2H).	407.51	480.43	76.8	76.6	89.78	83.19
	3{2,3,2}	SJ000311275-1	14.09 (brs, 1H), 9.58 (brs, 1H), 9.40 (brs, 1H), 8.98 (brs, 2H), 8.74 (d, J = 8.8 Hz, 1H), 8.65 (d, J = 7.2 Hz, 1H), 8.09 (d, J = 8.0 Hz, 2H), 8.04 (d, J = 1.5 Hz, 1H), 7.87 (dd, J = 8.8, 1.6 Hz, 1H), 7.81 (d, J = 8.4 Hz, 1H), 7.81 (d, J = 8.4 Hz, 1H), 7.68 (t, J = 7.6 Hz, 1H), 7.65-7.53 (m, 3H), 7.04-6.96 (m, 3H), 6.83 (t, J = 8.0 Hz, 1H), 4.12 (brs, 2H), 3.82 (s, 3H), 3.69 (brs, 2H), 3.08 (brs, 2H), 2.17-2.06 (m, 2H).	463.57	536.49	75.5	100	100	100
	3{2,3,3}	SJ000311276-1	14.13 (brs, 1H), 9.65 (brs, 1H), 9.40 (brs, 2H), 8.78 (d, J = 8.8 Hz, 1H), 8.65 (d, J = 7.2 Hz, 1H), 8.09 (d, J = 8.0 Hz, 2H), 8.05 (d, J = 1.6 Hz, 1H), 7.87 (dd, J = 8.8, 1.6 Hz, 1H), 7.81 (d, J = 8.4 Hz, 1H), 7.68 (t, J = 7.6 Hz, 1H), 7.65-7.53 (m, 3H), 7.11 (dd, J = 8.0, 0.8 Hz, 1H), 7.01-6.95 (m, 2H), 6.90 (t, J = 7.8 Hz, 1H), 6.08 (s, 2H), 4.12 (brs, 2H), 3.72 (brs, 2H), 3.11 (brs, 2H), 2.17-2.06 (m, 2H).	461.56	534.48	73.1	100	100	100
	3{2,3,4}	SJ000311277-1	14.04 (brs, 1H), 9.58 (brs, 1H), 9.12 (brs, 2H), 8.75 (d, J = 8.8 Hz, 1H), 8.66 (d, J = 7.2 Hz, 1H), 8.09 (d, J = 8.0 Hz, 2H), 8.03 (d, J = 1.5 Hz, 1H), 7.88 (dd, J = 8.8, 1.5 Hz, 1H), 7.81 (d, J = 8.4 Hz, 1H), 7.68 (t, J = 7.6 Hz, 1H), 7.65-7.53 (m, 3H), 7.42 (dd, J = 9.2, 3.2 Hz, 1H), 7.26 (dt, J = 8.8, 3.2 Hz, 1H), 7.11 (dd, J = 9.2, 4.4 Hz, 1H), 6.99 (d, J = 7.2 Hz, 1H), 4.14 (brs, 2H), 3.83 (s, 3H), 3.71 (brs, 2H), 3.10 (brs, 2H), 2.17-2.06 (m, 2H).	465.56	538.48	77.9	100	100	100
	3{2,4,1}	SJ000311278-1	14.12 (brs, 1H), 9.61 (brs, 1H), 9.35 (brs, 2H), 8.76 (d, J = 9.2 Hz, 1H), 8.64 (d, J = 7.2 Hz, 1H), 8.25 (d, J = 1.6 Hz, 1H), 8.13 (dd, J = 8.8, 1.6 Hz, 1H), 8.07 (d, J = 8.0 Hz, 2H), 7.96 (d, J = 8.0 Hz, 2H), 7.78-7.76 (m, 1H), 6.95 (d, J = 7.2 Hz, 1H), 6.65 (d, J = 3.2 Hz, 1H), 6.52 (dd, J = 3.2, 2.0 Hz, 1H), 4.25 (brs, 2H), 3.68 (brs, 2H), 3.05 (brs, 2H), 2.12-2.03 (m, 2H).	425.45	498.37	57.1	77.14	88.8	82.97
	3{2,4,2}	SJ000311279-1	14.11 (brs, 1H), 9.57 (brs, 1H), 9.38 (brs, 1H), 8.98 (brs, 2H), 8.74 (d, J = 9.2 Hz, 1H), 8.63 (d, J = 7.2 Hz, 1H), 8.25 (d, J = 1.6 Hz, 1H), 8.13 (dd, J = 8.8, 1.6 Hz, 1H), 8.07 (d, J = 8.0 Hz, 2H), 7.96 (d, J = 8.0 Hz, 2H), 7.05-6.93 (m, 2H), 6.95 (d, J = 7.2 Hz, 1H), 6.81 (t, J = 8.0 Hz, 1H), 4.11 (brs, 2H), 3.81 (s, 3H), 3.67 (brs, 2H), 3.06 (brs, 2H), 2.15-2.04 (m, 2H).	481.51	554.43	77.5	97.23	100	98.615
	3{2,4,3}	SJ000311280-1	14.00 (brs, 1H), 9.50 (brs, 1H), 9.20 (brs, 2H), 8.71 (d, J = 9.2 Hz, 1H), 8.64 (d, J = 7.2 Hz, 1H), 8.22 (d, J = 1.6 Hz, 1H), 8.14 (dd, J = 8.8, 1.6 Hz, 1H), 8.07 (d, J = 8.0 Hz, 2H), 7.96 (d, J = 8.0 Hz, 2H), 7.05 (d, J = 8.0 Hz, 1H), 7.00-6.87 (m, 3H), 6.07 (s, 2H), 4.12 (brs, 2H), 3.67 (brs, 2H), 3.10 (brs, 2H), 2.15-2.02 (m, 2H).	479.5	552.42	76.7	100	100	100

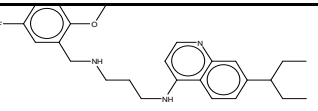
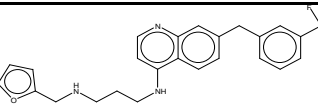
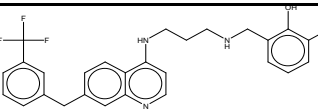
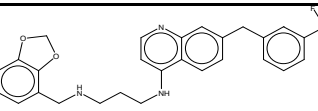
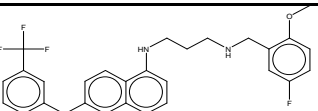
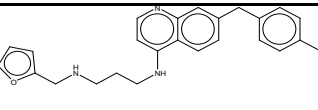
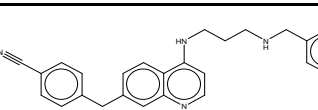
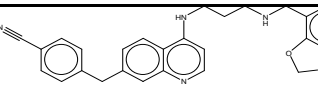
 Structure4	3{2,4,4}	SJ000311281-1	14.09 (brs, 1H), 9.60 (brs, 1H), 9.15 (brs, 2H), 8.76 (d, J = 9.2 Hz, 1H), 8.64 (d, J = 7.2 Hz, 1H), 8.25 (d, J = 1.6 Hz, 1H), 8.13 (dd, J = 8.8, 1.6 Hz, 1H), 8.06 (d, J = 8.0 Hz, 2H), 7.97 (d, J = 8.0 Hz, 2H), 7.42 (dd, J = 9.0, 3.2 Hz, 1H), 7.24 (dt, J = 8.6, 2.8 Hz, 1H), 7.09 (dd, J = 8.8, 4.4 Hz, 1H), 6.96 (d, J = 7.2 Hz, 1H), 4.13 (brs, 2H), 3.82 (s, 3H), 3.69 (brs, 2H), 3.07 (brs, 2H), 2.16-2.06 (m, 2H).	483.5	556.42	77.2	100	100	100
 Structure1	3{2,5,1}	SJ000311282-1	14.06 (brs, 1H), 9.54 (brs, 1H), 9.35 (brs, 2H), 8.70 (d, J = 8.8 Hz, 1H), 8.61 (d, J = 7.2 Hz, 1H), 8.19 (d, J = 1.6 Hz, 1H), 8.08 (dd, J = 8.8, 1.6 Hz, 1H), 7.87-7.82 (m, 2H), 7.78-7.76 (m, 1H), 7.63-7.56 (m, 2H), 7.55-7.50 (m, 1H), 6.93 (d, J = 6.8 Hz, 1H), 6.65 (d, J = 3.2 Hz, 1H), 6.52 (dd, J = 3.2, 2.0 Hz, 1H), 4.25 (s, 2H), 3.67 (brs, 2H), 3.05 (brs, 2H), 2.13-2.02 (m, 2H).	357.45	430.37	53.6	82.69	93.48	88.085
 Structure2	3{2,5,2}	SJ000311283-1	13.99 (brs, 1H), 9.41 (brs, 2H), 8.91 (brs, 2H), 8.70 (d, J = 8.8 Hz, 1H), 8.62 (d, J = 7.2 Hz, 1H), 8.17 (d, J = 1.6 Hz, 1H), 8.09 (dd, J = 8.8, 1.6 Hz, 1H), 7.88-7.83 (m, 2H), 7.63-7.57 (m, 2H), 7.56-7.51 (m, 1H), 7.04-6.97 (m, 2H), 6.93 (d, J = 7.2 Hz, 1H), 6.82 (t, J = 8.0 Hz, 1H), 4.12 (s, 2H), 3.82 (s, 3H), 3.66 (brs, 2H), 3.07 (brs, 2H), 2.15-2.04 (m, 2H).	413.51	486.43	62.1	100	100	100
 Structure3	3{2,5,3}	SJ000311284-1	14.06 (brs, 1H), 9.55 (brs, 1H), 9.35 (brs, 2H), 8.71 (d, J = 8.8 Hz, 1H), 8.62 (d, J = 7.1 Hz, 1H), 8.19 (d, J = 1.6 Hz, 1H), 8.09 (dd, J = 8.8, 1.6 Hz, 1H), 7.88-7.83 (m, 2H), 7.63-7.57 (m, 2H), 7.56-7.51 (m, 1H), 7.10 (d, J = 7.6 Hz, 1H), 6.97 (dd, J = 8.0, 1.2 Hz, 1H), 6.94 (d, J = 7.6 Hz, 1H), 6.90 (t, J = 6.8 Hz, 1H), 6.07 (s, 2H), 4.12 (s, 2H), 3.69 (brs, 2H), 3.10 (brs, 2H), 2.15-2.05 (m, 2H).	411.5	484.42	79.4	100	100	100
 Structure4	3{2,5,4}	SJ000311285-1	13.99 (brs, 1H), 9.50 (brs, 1H), 9.10 (brs, 2H), 8.69 (d, J = 8.8 Hz, 1H), 8.61 (d, J = 7.2 Hz, 1H), 8.17 (d, J = 1.6 Hz, 1H), 8.08 (dd, J = 8.8, 1.6 Hz, 1H), 7.85 (d, J = 7.2 Hz, 2H), 7.63-7.56 (m, 2H), 7.56-7.51 (m, 1H), 7.41 (dd, J = 9.2, 3.2 Hz, 1H), 7.25 (dt, J = 8.8, 3.2 Hz, 1H), 7.10 (dd, J = 8.8, 4.0 Hz, 1H), 6.93 (d, J = 7.2 Hz, 1H), 4.12 (s, 2H), 3.82 (s, 3H), 3.68 (brs, 2H), 3.07 (brs, 2H), 2.15-2.05 (m, 2H).	415.5	488.42	83.2	100	100	100
 Structure1	3{2,6,1}	SJ000311286-1	14.01 (brs, 1H), 9.51 (brs, 1H), 9.33 (brs, 2H), 8.68 (d, J = 8.8 Hz, 1H), 8.60 (d, J = 7.2 Hz, 1H), 8.16 (d, J = 1.6 Hz, 1H), 8.07 (dd, J = 8.8, 1.6 Hz, 1H), 7.81-7.75 (m, 3H), 7.61 (d, J = 8.4 Hz, 2H), 6.92 (d, J = 7.2 Hz, 1H), 6.65 (d, J = 3.2 Hz, 1H), 6.52 (dd, J = 4.0, 2.0 Hz, 1H), 4.25 (s, 2H), 3.66 (brs, 2H), 3.05 (brs, 2H), 2.12-2.00 (m, 2H), 1.34 (s, 9H).	413.56	486.48	46.4	71.11	83.1	77.105
 Structure2	3{2,6,2}	SJ000311287-1	14.00 (brs, 1H), 9.48 (brs, 1H), 9.38 (brs, 1H), 8.95 (brs, 2H), 8.66 (d, J = 8.8 Hz, 1H), 8.59 (d, J = 7.2 Hz, 1H), 8.12 (d, J = 1.6 Hz, 1H), 8.06 (dd, J = 8.8, 1.6 Hz, 1H), 7.78 (d, J = 8.4 Hz, 2H), 7.61 (d, J = 8.4 Hz, 2H), 7.03-6.98 (m, 2H), 6.91 (d, J = 7.2 Hz, 1H), 6.81 (t, J = 8.0 Hz, 1H), 4.11 (s, 2H), 3.81 (s, 3H), 3.65 (brs, 2H), 3.05 (brs, 2H), 2.13-2.03 (m, 2H), 1.34 (s, 9H).	469.62	542.54	48.7	97.91	100	98.955
 Structure3	3{2,6,3}	SJ000311288-1	13.96 (brs, 1H), 9.49 (brs, 1H), 9.26 (brs, 2H), 8.66 (d, J = 8.8 Hz, 1H), 8.60 (d, J = 7.2 Hz, 1H), 8.15 (d, J = 1.6 Hz, 1H), 8.07 (dd, J = 8.8, 1.6 Hz, 1H), 7.78 (d, J = 8.4 Hz, 2H), 7.61 (d, J = 8.4 Hz, 2H), 7.07 (dd, J = 7.2, 0.8 Hz, 1H), 6.97 (dd, J = 8.0, 0.8 Hz, 1H), 6.94-6.87 (m, 2H), 6.07 (s, 2H), 4.11 (s, 2H), 3.67 (brs, 2H), 3.09 (brs, 2H), 2.13-2.03 (m, 2H), 1.35 (s, 9H).	467.61	540.53	74.1	100	100	100

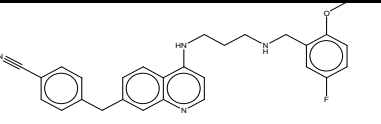
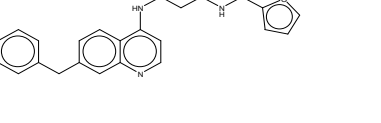
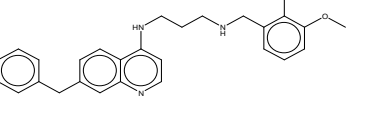
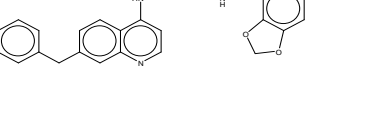
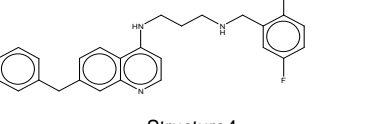
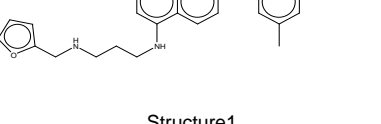
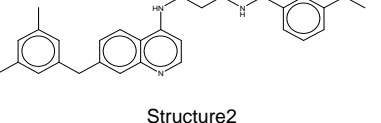
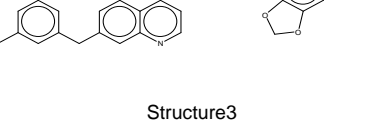
 Structure4	3{2,6,4}	SJ000311289-1	14.01 (brs, 1H), 9.53 (brs, 1H), 9.14 (brs, 2H), 8.69 (d, J = 8.8 Hz, 1H), 8.60 (d, J = 7.2 Hz, 1H), 8.16 (d, J = 1.6 Hz, 1H), 8.06 (dd, J = 8.8, 1.6 Hz, 1H), 7.78 (d, J = 8.4 Hz, 2H), 7.61 (d, J = 8.4 Hz, 2H), 7.42 (dd, J = 8.8, 3.2 Hz, 1H), 7.24 (dt, J = 8.6, 3.2 Hz, 1H), 7.09 (dd, J = 9.2, 4.4 Hz, 1H), 6.92 (d, J = 7.2, 1H), 4.12 (s, 2H), 3.82 (s, 3H), 3.68 (brs, 2H), 3.07 (brs, 2H), 2.15-2.05 (m, 2H), 1.35 (s, 9H).	471.61	544.53	65.7	100	100	100
 Structure1	3{2,7,1}	SJ000311290-1	13.97 (brs, 1H), 9.42 (brs, 1H), 9.25 (brs, 2H), 8.63-8.57 (m, 2H), 8.07 (d, J = 1.6 Hz, 1H), 8.03 (dd, J = 8.8, 1.6 Hz, 1H), 7.78-7.76 (m, 1H), 7.44 (d, J = 2.0 Hz, 1H), 7.35 (dd, J = 8.0, 2.0 Hz, 1H), 7.13 (d, J = 8.0 Hz, 1H), 6.90 (d, J = 7.6 Hz, 1H), 6.64 (d, J = 3.2 Hz, 1H), 6.52 (dd, J = 3.2, 2.0 Hz, 1H), 6.14 (s, 2H), 4.25 (s, 2H), 3.65 (brs, 2H), 3.06 (brs, 2H), 2.10-2.00 (m, 2H).	401.66	474.58	72.6	73.73	86.18	79.955
 Structure2	3{2,7,2}	SJ000311291-1	14.00 (brs, 1H), 9.49 (brs, 1H), 9.37 (brs, 1H), 9.00 (brs, 2H), 8.64 (d, J = 8.8 Hz, 1H), 8.57 (d, J = 7.2 Hz, 1H), 8.10 (d, J = 1.6 Hz, 1H), 8.02 (dd, J = 8.8, 1.6 Hz, 1H), 7.44 (d, J = 1.8 Hz, 1H), 7.35 (dd, J = 8.0, 2.0 Hz, 1H), 7.13 (d, J = 8.0 Hz, 1H), 7.00 (d, J = 8.0, 8.0 Hz, 2H), 6.90 (d, J = 7.2 Hz, 1H), 6.81 (t, J = 8.0 Hz, 1H), 6.13 (s, 2H), 4.10 (s, 2H), 3.81 (s, 3H), 3.65 (brs, 2H), 3.05 (brs, 2H), 2.14-2.04 (m, 2H).	457.72	530.64	72.3	100	100	100
 Structure3	3{2,7,3}	SJ000311292-1	13.85 (brs, 1H), 9.40 (brs, 1H), 9.18 (brs, 2H), 8.62-8.57 (m, 2H), 8.06 (d, J = 1.6 Hz, 1H), 8.03 (dd, J = 8.8, 1.6 Hz, 1H), 7.44 (d, J = 1.8 Hz, 1H), 7.36 (dd, J = 8.0, 2.0 Hz, 1H), 7.13 (d, J = 8.0 Hz, 1H), 7.05 (d, J = 7.6 Hz, 1H), 6.97 (dd, J = 7.6, 0.8 Hz, 1H), 6.93-6.86 (m, 2H), 6.14 (s, 2H), 6.07 (s, 2H), 4.11 (s, 2H), 3.66 (brs, 2H), 3.09 (brs, 2H), 2.12-2.02 (m, 2H).	455.71	528.63	78.4	100	100	100
 Structure4	3{2,7,4}	SJ000311293-1	13.97 (brs, 1H), 9.52 (brs, 1H), 9.16 (brs, 2H), 8.65 (d, J = 8.8 Hz, 1H), 8.58 (d, J = 7.2 Hz, 1H), 8.10 (d, J = 1.6 Hz, 1H), 8.03 (dd, J = 8.8, 1.6 Hz, 1H), 7.44 (d, J = 4.2 Hz, 1H), 7.42 (dd, J = 8.8, 3.2 Hz, 1H), 7.35 (dd, J = 8.0, 2.0 Hz, 1H), 7.23 (dd, J = 8.8, 3.2 Hz, 1H), 7.13 (d, J = 8.0 Hz, 1H), 7.09 (dd, J = 9.2, 4.4 Hz, 1H), 6.91 (d, J = 7.2 Hz, 1H), 6.14 (s, 2H), 4.12 (s, 2H), 3.82 (s, 3H), 3.67 (brs, 2H), 3.06 (brs, 2H), 2.15-2.04 (m, 2H).	459.71	532.63	75.3	100	100	100
 Structure1	3{2,8,1}	SJ000311294-1	14.01 (brs, 1H), 9.52 (brs, 1H), 9.38 (brs, 2H), 8.67 (d, J = 8.8 Hz, 1H), 8.59 (d, J = 7.2 Hz, 1H), 8.14 (d, J = 1.6 Hz, 1H), 8.06 (dd, J = 8.8, 1.6 Hz, 1H), 7.82 (d, J = 8.8 Hz, 2H), 7.78-7.76 (m, 1H), 7.15 (d, J = 8.8 Hz, 2H), 6.90 (d, J = 7.2 Hz, 1H), 6.66 (d, J = 3.2 Hz, 1H), 6.53 (dd, J = 3.2, 2.0 Hz, 1H), 4.25 (s, 2H), 3.85 (s, 3H), 3.67 (brs, 2H), 3.05 (brs, 2H), 2.13-2.00 (m, 2H).	387.48	460.4	69.4	80.43	92.14	86.285
 Structure2	3{2,8,2}	SJ000311295-1	13.92 (brs, 1H), 9.40 (brs, 2H), 8.93 (brs, 2H), 8.63 (d, J = 8.8 Hz, 1H), 8.58 (d, J = 7.2 Hz, 1H), 8.11 (d, J = 1.6 Hz, 1H), 8.06 (dd, J = 8.8, 1.6 Hz, 1H), 7.82 (d, J = 8.8 Hz, 2H), 7.15 (d, J = 8.8 Hz, 2H), 7.00 (t, J = 7.6 Hz, 2H), 6.90 (d, J = 7.2 Hz, 1H), 6.82 (t, J = 8.0 Hz, 1H), 4.11 (s, 2H), 3.85 (s, 3H), 3.82 (s, 3H), 3.66 (brs, 2H), 3.06 (brs, 2H), 2.13-2.00 (m, 2H).	443.54	516.46	67.5	100	100	100
 Structure3	3{2,8,3}	SJ000311296-1	13.90 (brs, 1H), 9.45 (brs, 1H), 9.28 (brs, 2H), 8.64 (d, J = 8.8 Hz, 1H), 8.58 (d, J = 7.2 Hz, 1H), 8.11 (d, J = 1.6 Hz, 1H), 8.05 (dd, J = 8.8, 1.6 Hz, 1H), 7.81 (d, J = 8.8 Hz, 2H), 7.15 (d, J = 8.8 Hz, 2H), 7.07 (dd, J = 8.0, 0.8 Hz, 1H), 6.97 (dd, J = 8.0, 1.0 Hz, 1H), 6.90-6.87 (m, 2H), 6.07 (s, 2H), 4.11 (s, 2H), 3.85 (s, 3H), 3.66 (brs, 2H), 3.09 (brs, 2H), 2.15-2.00 (m, 2H).	441.53	514.45	70.6	100	100	100

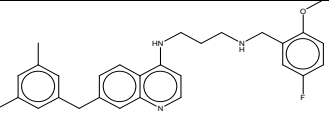
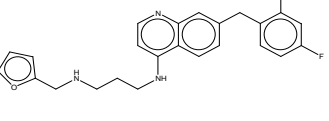
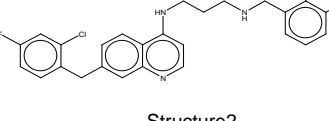
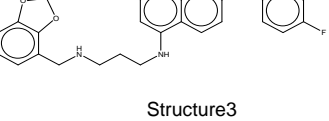
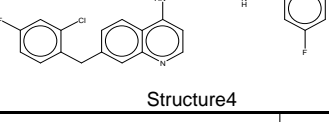
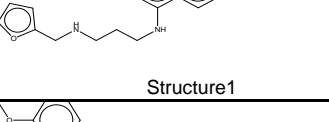
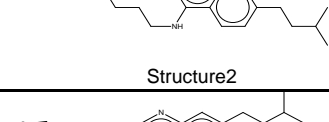
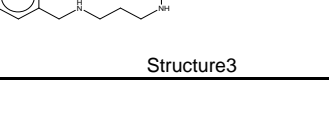
 Structure4	3{2,8,4}	SJ000311297-1	13.94 (brs, 1H), 9.48 (brs, 1H), 9.13 (brs, 2H), 8.66 (d, J = 8.8 Hz, 1H), 8.59 (d, J = 7.2 Hz, 1H), 8.12 (d, J = 1.6 Hz, 1H), 8.05 (dd, J = 8.8, 1.6 Hz, 1H), 7.82 (d, J = 8.8 Hz, 2H), 7.43 (dd, J = 8.8, 3.2, Hz, 1H), 7.25 (td, J = 8.8, 3.2 Hz, 1H), 7.15 (d, J = 8.8 Hz, 2H), 7.10 (dd, J = 8.8, 4.4, 1H), 6.91 (d, J = 7.2 Hz, 1H), 4.13 (s, 2H), 3.85 (s, 3H), 3.83 (s, 3H), 3.68 (brs, 2H), 3.07 (brs, 2H), 2.15-2.00 (m, 2H).	445.53	518.45	71.9	100	100	100
 Structure1	3{3,1,1}	SJ000311242-1	13.91 (brs, 1H), 9.49 (brs, 1H), 9.41 (brs, 2H), 8.58 (d, J = 8.0 Hz, 1H), 8.52 (d, J = 7.2 Hz, 1H), 7.76 (d, J = 1.6 Hz, 1H), 7.70 (s, 1H), 7.61 (dd, J = 8.8, 1.2 Hz, 1H), 7.34 (dd, J = 8.8, 4.8 Hz, 2H), 7.17 (t, J = 8.8 Hz, 2H), 6.88 (d, J = 7.2, Hz, 1H), 6.64 (d, J = 3.2 Hz, 1H), 6.51 (dd, J = 3.2, 1.8 Hz, 1H), 4.23 (s, 2H), 4.20 (s, 2H), 3.64 (s, 2H), 3.02 (brs, 2H), 2.10-2.00 (m, 2H).	389.47	462.39	85.9	56.63	70.44	63.535
 Structure2	3{3,1,2}	SJ000311243-1	13.89 (brs, 1H), 9.46 (brs, 1H), 9.36 (brs, 1H), 9.01 (brs, 2H), 8.55 (d, J = 8.8 Hz, 1H), 8.51 (d, J = 7.2 Hz, 1H), 7.69 (s, 1H), 7.61 (dd, J = 8.8, 1.2 Hz, 1H), 7.34 (dd, J = 8.8, 4.8 Hz, 2H), 7.18 (t, J = 8.8 Hz, 2H), 7.00 (d, J = 8.8, Hz, 2H), 6.87 (d, J = 7.2 Hz, 1H), 6.80 (t, J = 8.0 Hz, 1H), 4.20 (s, 2H), 4.09 (s, 2H), 3.81 (s, 3H), 3.63 (s, 2H), 3.02 (brs, 2H), 2.12-2.00 (m, 2H).	445.53	518.45	87.7	96.35	100	98.175
 Structure3	3{3,1,3}	SJ000311244-1	13.90 (brs, 1H), 9.52 (brs, 1H), 9.41 (brs, 2H), 8.58 (d, J = 8.8 Hz, 1H), 8.51 (d, J = 7.2 Hz, 1H), 7.70 (s, 1H), 7.61 (dd, J = 8.8, 1.2 Hz, 1H), 7.34 (dd, J = 8.8, 4.8 Hz, 2H), 7.18 (t, J = 8.8 Hz, 2H), 7.10 (d, J = 8.0, Hz, 1H), 6.95 (d, J = 7.2 Hz, 1H), 6.91-6.85 (m, 2H), 6.06 (s, 2H), 4.20 (s, 2H), 4.09 (brs, 2H), 3.63 (brs, 2H), 3.07 (brs, 2H), 2.12-2.00 (m, 2H).	443.52	516.44	86.9	96.85	100	98.425
 Structure4	3{3,1,4}	SJ000311245-1	13.92 (brs, 1H), 9.54 (brs, 1H), 9.26 (brs, 2H), 8.63-8.56 (m, 1H), 8.54-8.49 (m, 1H), 7.70 (s, 1H), 7.61 (d, J = 8.8 Hz, 1H), 7.47-7.41 (m, 1H), 7.34(dd, J = 8.8, 4.8 Hz, 2H), 7.23 (dt, J = 8.8, 3.2 Hz, 1H), 7.18 (t, J = 8.8 Hz, 2H), 7.08 (dd, J = 9.2, 4.4 Hz, 1H), 6.89 (d, J = 7.2 Hz, 1H), 4.20 (s, 2H), 4.09 (brs, 2H), 3.81 (s, 3H), 3.65 (brs, 2H), 3.05 (brs, 2H), 2.14-2.04 (m, 2H).	447.52	520.44	87.4	97.4	100	98.7
 Structure1	3{3,10,1}	SJ000311258-1	14.02 (brs, 1H), 9.48 (brs, 3H), 8.57 (d, J = 8.0 Hz, 1H), 8.53 (d, J = 7.2 Hz, 1H), 7.76 (s, 1H), 7.71 (s, 1H), 7.57 (d, J = 8.4 Hz, 1H), 6.88 (d, J = 7.2 Hz, 1H), 6.65 (d, J = 3.2 Hz, 1H), 6.52 (dd, J = 3.2, 2.0 Hz, 1H), 4.24 (brs, 2H), 3.65 (brs, 2H), 3.03 (brs, 2H), 2.69 (d, J = 7.2 Hz, 2H), 2.12-2.02 (m, 2H), 2.01-1.92 (m, 1H), 0.91 (d, J = 6.8 Hz, 6H).	337.46	410.38	51.7	87.52	100	93.76
 Structure2	3{3,10,2}	SJ000311259-1	13.92 (brs, 1H), 9.38 (brs, 2H), 8.98 (brs, 2H), 8.55-8.50 (m, 2H), 7.69 (brs, 1H), 7.59-7.57(m, 1H), 7.02-6.99 (m, 2H), 6.87 (d, J = 8.0 Hz, 1H), 6.81 (t, J = 8.0 Hz, 1H), 4.10 (brs, 2H), 3.82 (s, 3H), 3.63 (brs, 2H), 3.05 (brs, 2H), 2.69 (d, J = 7.2Hz, 2H), 2.12-2.02 (m, 2H), 2.02-1.92 (m, 1H), 0.91 (d, J = 6.8Hz, 6H).	393.52	466.44	53.8	96.35	100	98.175
 Structure3	3{3,10,3}	SJ000311260-1	13.92 (brs, 1H), 9.45 (brs, 1H), 9.36 (brs, 2H), 8.56-8.52 (m, 2H), 7.69 (s, 1H), 7.58(dd, J = 8.8, 1.6Hz, 1H), 7.09 (d, J = 8.0 Hz, 1H), 6.97 (d, J = 8.4 Hz, 1H), 6.92-6.86 (m, 2H), 6.08 (s, 2H), 4.10 (brs, 2H), 3.65 (brs, 2H), 3.08 (brs, 2H), 2.69 (d, J = 7.2Hz, 2H), 2.12-2.02 (m, 2H), 2.02-1.92 (m, 1H), 0.91 (d, J = 6.8Hz, 6H).	391.51	464.43	69.3	94.96	100	97.48

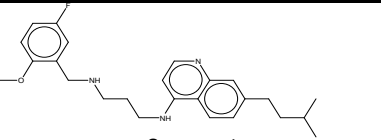
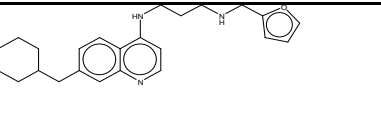
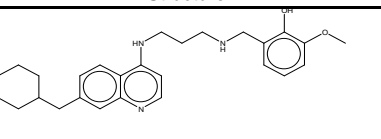
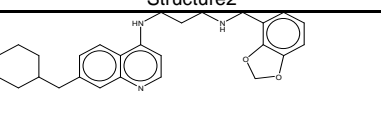
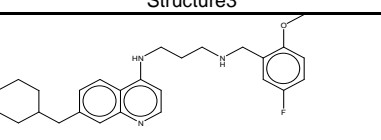
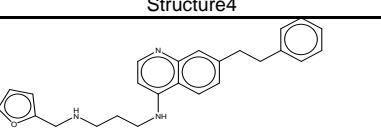
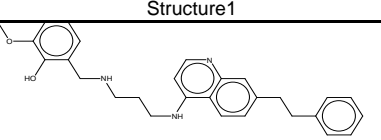
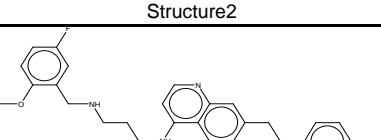
 <p>Structure4</p>	3{3,10,4}	SJ000311261-1	13.90 (brs, 1H), 9.45 (brs, 1H), 9.16 (brs, 2H), 8.56-8.51 (m, 2H), 7.69 (s, 1H), 7.58 (d, J = 8.4 Hz, 1H), 7.42 (dd, J = 8.8, 3.2 Hz, 1H), 7.24 (dt, J = 8.4, 3.2 Hz, 1H), 7.09 (dd, J = 9.2, 4.4 Hz, 1H), 6.89 (d, J = 7.2, 1H), 4.12 (s, 2H), 3.82 (s, 3H), 3.66 (brs, 2H), 3.06 (brs, 2H), 2.69 (d, J = 7.2Hz, 2H), 2.12-2.02 (m, 2H), 2.02-1.92 (m, 1H), 0.91 (d, J = 6.8Hz, 6H).	395.51	468.43	82.4	94.89	100	97.445
 <p>Structure1</p>	3{3,11,1}	SJ000311262-1	13.89 (brs, 1H), 9.30(brs, 3H), 8.54 (d, J = 7.2 Hz, 1H), 8.50 (d, J = 8.8Hz, 1H), 7.77-7.76 (m, 1H), 7.71 (brs, 1H), 7.66 (d, J = 8.4 Hz, 1H), 6.86 (d, J = 7.2 Hz, 1H), 6.65 (d, J = 3.2 Hz, 1H), 6.52 (dd, J = 3.2, 2.0 Hz, 1H), 4.23 (brs, 2H), 3.63 (brs, 2H), 3.03 (brs, 2H), 2.80-2.72 (m, 1H), 2.12-2.02 (m, 2H), 1.94-1.81 (m, 4H), 1.78-1.73 (m, 1H), 1.54-1.37 (m, 4H), 1.35-1.24 (m, 1H).	363.5	436.42	45.7	82.21	100	91.105
 <p>Structure2</p>	3{3,11,2}	SJ000311263-1	14.00 (brs, 1H), 9.42 (brs, 1H), 9.36 (brs, 1H), 9.02 (brs, 2H), 8.55-8.50 (m, 2H), 7.75 (brs, 1H), 7.66-7.58 (m, 1H), 7.01 (d, J = 7.2 Hz, 2H), 6.87 (d, J = 8.0 Hz, 1H), 6.81 (t, J = 8.0 Hz, 1H), 4.09 (brs, 2H), 3.01 (s,3H), 3.63 (brs, 2H), 3.04 (brs, 2H), 2.80-2.72 (m, 1H), 2.12-2.02 (m, 2H), 1.94-1.81 (m, 4H), 1.78-1.73 (m, 1H), 1.54-1.37 (m, 4H), 1.35-1.24 (m, 1H).	419.56	492.48	45.1	94.64	100	97.32
 <p>Structure3</p>	3{3,11,3}	SJ000311264-1	13.98 (brs, 1H), 9.43 (brs, 1H), 9.35 (brs, 2H), 8.56-8.52 (m, 2H), 7.74 (s, 1H), 7.66 (dd, J = 8.8, 1.2 Hz, 1H), 7.09 (d, J = 8.0 Hz, 1H), 7.00-6.87 (m, 3H), 6.06 (s, 2H), 4.10 (brs, 2H), 3.65 (brs, 2H), 3.07 (brs, 2H), 2.81-2.72 (m, 1H), 2.12-2.02 (m, 2H), 1.94-1.81 (m, 4H), 1.78-1.72 (m, 1H), 1.54-1.37 (m, 4H), 1.35-1.24 (m, 1H).	417.55	490.47	70.8	92.64	100	96.32
 <p>Structure4</p>	3{3,11,4}	SJ000311265-1	13.87 (brs, 1H), 9.36 (brs, 1H), 9.09 (brs, 2H), 8.56-8.51 (m, 2H), 7.72 (s, 1H), 7.66 (d, J = 8.4 Hz, 1H), 7.41 (dd, J = 8.8, 3.2 Hz, 1H), 7.24 (dt, J = 8.4, 3.2 Hz, 1H), 7.09 (dd, J = 9.2, 4.4 Hz, 1H), 6.88 (d, J = 7.2, 1H), 4.11 (s, 2H), 3.82 (s, 3H), 3.65 (brs, 2H), 3.05 (brs, 2H), 2.81-2.72 (m, 1H), 2.12-2.02 (m, 2H), 1.94-1.81 (m, 4H), 1.78-1.72 (m, 1H), 1.54-1.37 (m, 4H), 1.35-1.24 (m, 1H).	421.55	494.47	73.7	93.15	100	96.575
 <p>Structure1</p>	3{3,12,1}	SJ000311266-1	14.12 (brs, 1H), 9.48 (brs, 3H), 8.76 (d, J = 9.2 Hz, 1H), 8.64-8.52 (m, 1H), 7.75 (d, J = 8.0 Hz, 2H), 7.66-7.58 (m, 1H), 6.87 (d, J = 7.2 Hz, 1H), 6.65 (d, J = 3.2 Hz, 1H), 6.52 (dd, J = 3.2, 2.0 Hz, 1H), 4.24 (brs, 2H), 3.65 (brs, 2H), 3.03 (brs, 2H), 2.81 (m, 1H), 2.08-2.02 (m, 2H), 1.72-1.57 (m, 2H), 1.33-1.27 (m, 5H), 0.90-0.84 (m, 3H).	351.49	424.41	36.5	99.01	100	99.505
 <p>Structure2</p>	3{3,12,2}	SJ000311267-1	14.00 (brs, 1H), 9.42 (brs, 1H), 9.37 (brs, 1H), 9.01 (brs, 2H), 8.55-8.50 (m, 2H), 7.73 (brs, 1H), 7.66-7.58 (m, 1H), 7.01 (d, J = 7.2 Hz, 2H), 6.87 (d, J = 8.0 Hz, 1H), 6.81 (t, J = 8.0 Hz, 1H), 4.10 (brs, 2H), 3.02 (s, 3H), 3.63 (brs, 2H), 3.04 (brs, 2H), 2.82-2.78 (m, 1H), 2.12-2.02 (m, 2H), 1.72-1.57 (m, 2H), 1.38-1.10 (m, 5H), 0.90-0.84 (m, 3H).	407.55	480.47	43.0	98.27	100	99.135
 <p>Structure3</p>	3{3,12,3}	SJ000311268-1	13.82 (brs, 1H), 9.37 (brs, 1H), 9.25 (brs, 2H), 8.56-8.48 (m, 2H), 7.70 (s, 1H), 7.67-7.59 (m, 1H), 7.06 (d, J = 8.0 Hz, 1H), 6.97 (d, J = 8.4Hz, 1H), 6.92-6.86 (m, 2H), 6.07 (s, 2H), 4.11 (brs, 2H), 3.65 (brs, 2H), 3.08 (brs, 2H), 2.82-2.78 (m, 1H), 2.12-2.02 (m, 2H), 1.72-1.57 (m, 2H), 1.38-1.10 (m, 5H), 0.90-0.84 (m, 3H).	405.54	478.46	70.2	97.22	100	98.61

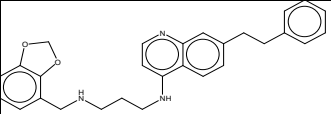


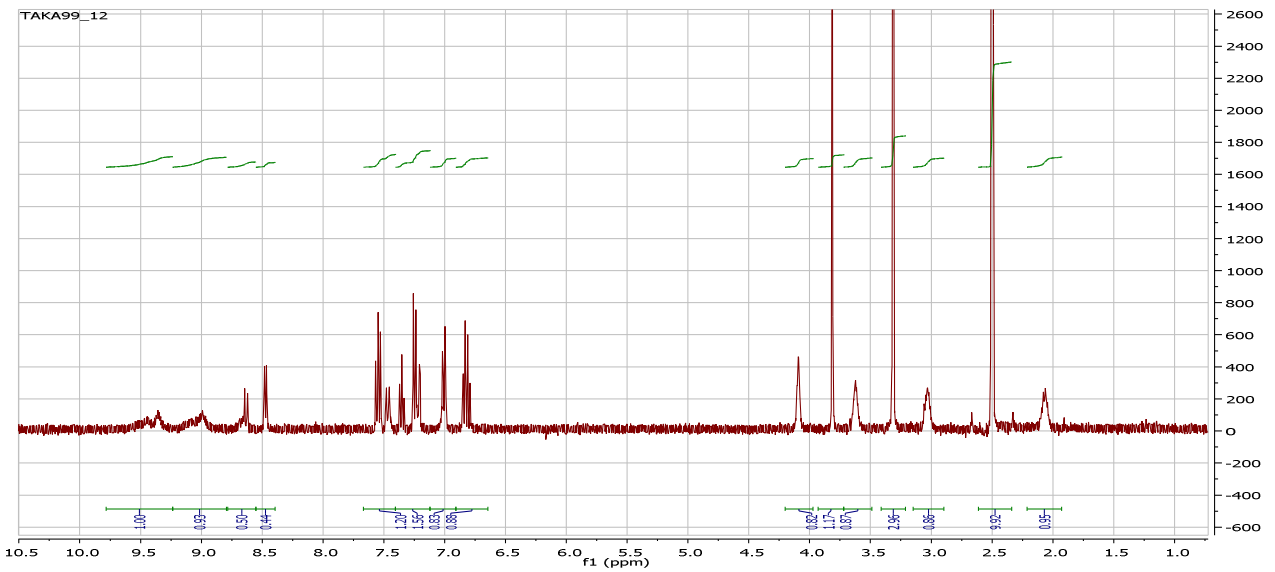
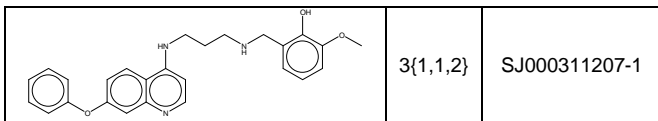
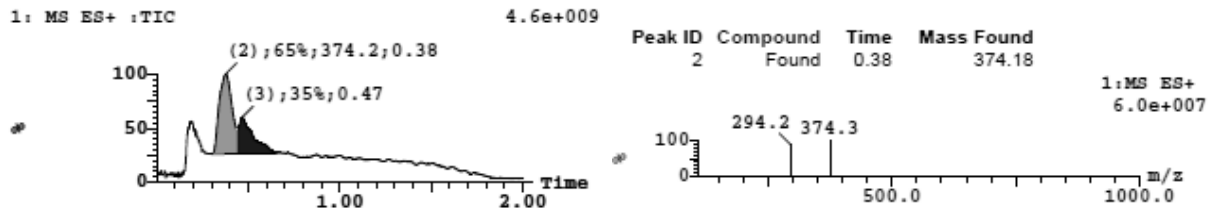
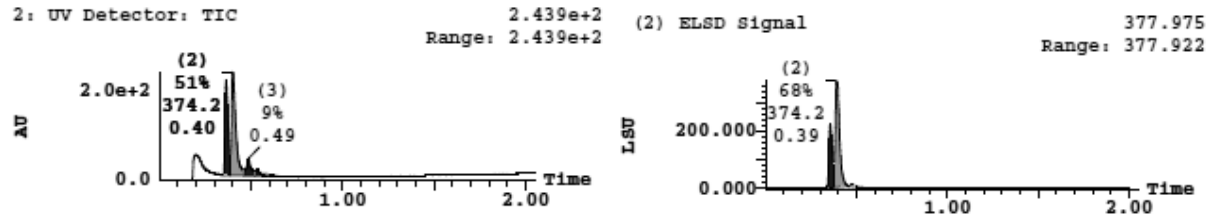
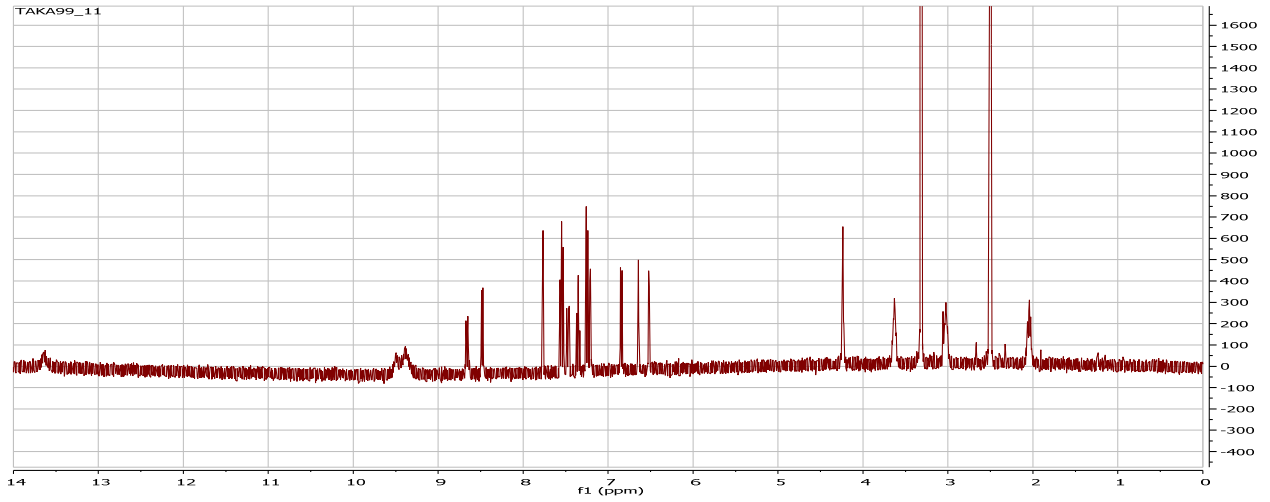
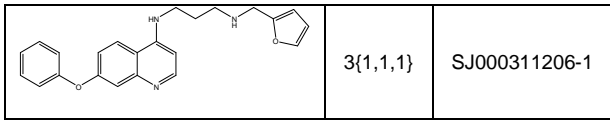
 Structure4	3{3,12,4}	SJ000311269-1	13.91 (brs, 1H), 9.46 (brs, 1H), 9.20 (brs, 2H), 8.56-8.51 (m, 2H), 7.69 (s, 1H), 7.62 (d, J = 8.4 Hz, 1H), 7.43 (dd, J = 8.8, 3.2 Hz, 1H), 7.24 (dt, J = 8.4, 3.2 Hz, 1H), 7.09 (dd, J = 9.2, 4.4 Hz, 1H), 6.88 (d, J = 7.2, 1H), 4.11 (s, 2H), 3.82 (s, 3H), 3.66 (brs, 2H), 3.05 (brs, 2H), 2.82-2.78 (m, 1H), 2.12-2.02 (m, 2H), 1.72-1.57 (m, 2H), 1.38-1.10 (m, 5H), 0.90-0.84 (m, 3H).	409.54	482.46	72.3	97.75	100	98.875
 Structure1	3{3,2,1}	SJ000311298-1	13.87 (brs, 1H), 9.48 (brs, 1H), 9.36 (brs, 2H), 8.58 (d, J = 8.8 Hz, 1H), 8.52 (d, J = 7.2 Hz, 1H), 7.76-7.75 (m, 1H), 7.73 (brs, 1H), 7.71 (brs, 1H), 7.68-7.56(m, 4H), 6.88 (d, J = 7.2 Hz, 1H), 6.64 (d, J = 3.2 Hz, 1H), 6.51 (dd, J = 3.2, 1.8 Hz, 1H), 4.33 (s, 2H), 4.23 (s, 2H), 3.63 (brs, 2H), 3.02 (brs, 2H), 2.10-1.99 (m, 2H).	439.48	512.4	81.0	92.01	100	96.005
 Structure2	3{3,2,2}	SJ000311299-1	13.80 (brs, 1H), 9.38 (brs, 2H), 8.90 (brs, 2H), 8.52 (s, 1H), 8.50 (s, 1H), 7.71 (s, 2H), 7.68-7.56 (m, 4H), 6.98 (t, J = 7.2 Hz, 2H), 6.87 (d, J = 7.2 Hz, 1H), 6.80 (t, J = 8.0 Hz, 1H), 4.33 (s, 2H), 4.09 (s, 2H), 3.62 (brs, 2H), 3.03 (brs, 2H), 2.10-2.00 (m, 2H).	495.54	568.46	76.2	100	100	100
 Structure3	3{3,2,3}	SJ000311300-1	13.78 (brs, 1H), 9.38 (brs, 1H), 9.22 (brs, 2H), 8.54 (d, J = 2.8Hz, 1H), 8.51 (s, 1H), 7.71 (s, 2H), 7.68-7.56 (m, 4H), 7.05 (d, J = 8.0 Hz, 1H), 6.96 (dd, J = 8.0, 0.8 Hz, 1H), 6.91-6.86 (m, 2H), 6.06 (s, 2H), 4.33 (s, 2H), 4.10 (s, 2H), 3.64 (brs, 2H), 3.07 (brs, 2H), 2.10-2.00 (m, 2H).	493.53	566.45	80.7	97.9	100	98.95
 Structure4	3{3,2,4}	SJ000311301-1	13.82 (brs, 1H), 9.43 (brs, 1H), 9.10 (brs, 2H), 8.55 (d, J = 8.8 Hz, 1H), 8.52 (d, J = 6.8 Hz, 1H), 7.71 (s, 2H), 7.68-7.56 (m, 4H), 7.40 (dd, J = 8.8, 3.2 Hz, 1H), 7.23 (dt, J = 9.0, 3.2 Hz, 1H), 7.08 (dd, J = 8.8, 4.4 Hz, 1H), 6.88 (d, J = 7.2 Hz, 1H), 4.33 (s, 2H), 4.11 (s, 2H), 3.01 (brs, 3H), 3.64 (brs, 2H), 3.05 (brs, 2H), 2.10-2.00 (m, 2H).	497.53	570.45	74.9	100	100	100
 Structure1	3{3,3,1}	SJ000311302-1	13.89 (brs, 1H), 9.46 (brs, 1H), 9.34 (brs, 2H), 8.56 (d, J = 8.8 Hz, 1H), 8.53 (d, J = 7.2 Hz, 1H), 7.83 (d, J = 8.0 Hz, 2H), 7.70-7.75 (m, 1H), 7.71 (s, 1H), 7.63 (dd, J = 8.8, 1.2 Hz, 1H), 7.52 (d, J = 8.8 Hz, 2H), 6.88 (d, J = 7.2, Hz, 1H), 6.64 (d, J = 3.2 Hz, 1H), 6.52 (dd, J = 3.2, 1.8 Hz, 1H), 4.32 (s, 2H), 4.23 (s, 2H), 3.63 (s, 2H), 3.02 (brs, 2H), 2.10-2.00 (m, 2H).	396.49	469.41	79.6	94.81	100	97.405
 Structure2	3{3,3,2}	SJ000311303-1	13.80 (brs, 1H), 9.39 (brs, 2H), 8.88 (brs, 2H), 8.52 (d, J = 7.2 Hz, 1H), 8.51 (d, J = 8.8 Hz, 1H), 7.83 (d, J = 8.0 Hz, 2H), 7.70 (s, 1H), 7.63 (d, J = 8.0 Hz, 1H), 7.52 (d, J = 8.0 Hz, 2H), 6.98 (dd, J = 8.0, 10.0, Hz, 2H), 6.87 (d, J = 7.2 Hz, 1H), 6.80 (t, J = 7.6 Hz, 1H), 4.32 (s, 2H), 4.09 (s, 2H), 3.81 (s, 3H), 3.62 (s, 2H), 3.03 (brs, 2H), 2.10-2.00 (m, 2H).	452.55	525.47	76.4	87.72	95.72	91.72
 Structure3	3{3,3,3}	SJ000311304-1	13.84 (brs, 1H), 9.45 (brs, 1H), 9.28 (brs, 2H), 8.55 (d, J = 8.8 Hz, 1H), 8.53 (d, J = 7.2 Hz, 1H), 7.83 (d, J = 8.0 Hz, 2H), 7.70 (s, 1H), 7.63 (dd, J = 8.8, 1.2 Hz, 1H), 7.52 (d, J = 8.0 Hz, 2H), 7.07 (d, J = 8.0, Hz, 1H), 6.96 (d, J = 7.6 Hz, 1H), 6.91-6.86 (m, 2H), 6.06 (s, 2H), 4.32 (s, 2H), 4.10 (s, 2H), 3.64 (s, 2H), 3.07 (brs, 2H), 2.10-2.00 (m, 2H).	450.54	523.46	61.8	91.83	100	95.915

 Structure4	3{3,3,4}	SJ000311305-1	13.79 (brs, 1H), 9.39 (brs, 1H), 9.04 (brs, 2H), 8.53 (d, J = 8.0 Hz, 2H), 7.83 (d, J = 8.0 Hz, 2H), 7.70 (s, 1H), 7.64 (dd, J = 8.8, 1.2 Hz, 1H), 7.52 (d, J = 8.0 Hz, 2H), 7.39 (dd, J = 8.8, 2.8 Hz, 1H), 7.24 (dt, J = 8.6, 2.8 Hz, 1H), 7.09 (dd, J = 8.8, 4.4, 1H), 6.88 (d, J = 6.8 Hz, 1H), 4.32 (s, 2H), 4.11 (s, 2H), 3.81 (s, 3H), 3.63 (s, 2H), 3.05 (brs, 2H), 2.10-2.00 (m, 2H).	454.54	527.46	52.9	81.69	91.5	86.595
 Structure1	3{3,4,1}	SJ000311306-1	13.82 (brs, 1H), 9.40 (brs, 1H), 9.30 (brs, 2H), 8.53 (d, J = 8.8 Hz, 1H), 8.52 (d, J = 6.8 Hz, 1H), 7.77-7.75 (m, 1H), 7.70 (s, 1H), 7.62 (dd, J = 8.8, 1.2 Hz, 1H), 7.38-7.22 (m, 5H), 6.87 (d, J = 7.2 Hz, 1H), 6.63 (d, J = 3.2 Hz, 1H), 6.51 (dd, J = 3.2, 1.8 Hz, 1H), 4.23 (s, 2H), 4.20 (s, 2H), 3.63 (brs, 2H), 3.02 (brs, 2H), 2.10-1.98 (m, 2H).	371.48	444.4	55.9	97.13	100	98.565
 Structure2	3{3,4,2}	SJ000311307-1	13.82 (brs, 1H), 9.38 (brs, 2H), 8.93 (brs, 2H), 8.51 (d, J = 8.0 Hz, 2H), 7.70 (s, 1H), 7.62 (dd, J = 8.8, 1.2 Hz, 1H), 7.38-7.22 (m, 5H), 7.01-6.96 (m, 2H), 6.87 (d, J = 7.2 Hz, 1H), 6.80 (t, J = 8.0 Hz, 1H), 4.20 (s, 2H), 4.09 (s, 2H), 3.81 (s, 3H), 3.62 (brs, 2H), 3.03 (brs, 2H), 2.10-2.00 (m, 2H).	427.54	500.46	74.4	100	100	100
 Structure3	3{3,4,3}	SJ000311308-1	13.85 (brs, 1H), 9.42 (brs, 1H), 9.31 (brs, 2H), 8.53 (d, J = 8.8 Hz, 1H), 8.51 (d, J = 7.2 Hz, 1H), 7.70 (s, 1H), 7.62 (dd, J = 8.8, 1.2 Hz, 1H), 7.38-7.22 (m, 5H), 7.07 (d, J = 7.6 Hz, 1H), 6.95 (d, J = 7.2 Hz, 1H), 6.88 (t, J = 7.2 Hz, 2H), 6.06 (s, 2H), 4.20 (s, 2H), 4.09 (s, 2H), 3.64 (brs, 2H), 3.06 (brs, 2H), 2.10-2.00 (m, 2H).	425.53	498.45	35.7	100	100	100
 Structure4	3{3,4,4}	SJ000311309-1	13.84 (brs, 1H), 9.44 (brs, 1H), 9.14 (brs, 2H), 8.55 (d, J = 8.8 Hz, 1H), 8.51 (d, J = 7.2 Hz, 1H), 7.70 (s, 1H), 7.62 (dd, J = 8.8, 1.2 Hz, 1H), 7.41 (dd, J = 8.8, 3.2 Hz, 1H), 7.38-7.19 (m, 6H), 7.08 (dd, J = 9.2, 4.4 Hz, 1H), 6.88 (d, J = 7.2 Hz, 1H), 4.20 (s, 2H), 4.11 (s, 2H), 3.81 (s, 3H), 3.65 (brs, 2H), 3.04 (brs, 2H), 2.10-2.00 (m, 2H).	429.53	502.45	30.1	100	100	100
 Structure1	3{3,5,1}	SJ000311318-1	13.83 (brs, 1H), 9.32 (brs, 3H), 8.53 (d, J = 8.8 Hz, 1H), 8.52 (d, J = 7.2 Hz, 1H), 7.76 (brs, 1H), 7.69 (brs, 1H), 7.60 (dd, J = 8.8, 1.2 Hz, 1H), 6.89-6.86 (m, 3H), 6.63 (d, J = 3.2 Hz, 1H), 6.52 (dd, J = 3.2, 2.0 Hz, 1H), 4.23 (s, 2H), 4.11 (brs, 2H), 3.63 (brs, 2H), 3.02 (brs, 2H), 2.24 (s, 6H), 2.08-2.00 (m, 2H).	399.53	472.45	80.7	96.16	100	98.08
 Structure2	3{3,5,2}	SJ000311319-1	13.82 (brs, 1H), 9.38 (brs, 2H), 8.96 (brs, 2H), 8.52-8.49 (m, 2H), 7.69 (s, 1H), 7.60 (d, J = 8.8 Hz, 1H), 6.99 (d, J = 8.0 Hz, 2H), 6.89-6.85 (m, 4H), 6.80 (t, J = 8.0 Hz, 1H), 4.11 (s, 2H), 4.09 (brs, 2H), 3.81 (s, 3H), 3.62 (brs, 2H), 3.03 (brs, 2H), 2.24 (s, 6H), 2.11-2.02 (m, 2H).	455.59	528.51	40.3	100	100	100
 Structure3	3{3,5,3}	SJ000311320-1	13.81 (brs, 1H), 9.42 (brs, 1H), 9.30 (brs, 2H), 8.53 (d, J = 8.8 Hz, 1H), 8.51 (d, J = 7.2 Hz, 1H), 7.69 (s, 1H), 7.60 (d, J = 8.4 Hz, 1H), 7.07 (d, J = 8.0 Hz, 1H), 6.96 (d, J = 7.6 Hz, 1H), 6.90-6.86 (m, 5H), 6.91-6.87 (m, 2H), 6.06 (s, 2H), 4.11 (s, 2H), 4.10 (brs, 2H), 3.64 (brs, 2H), 3.07 (brs, 2H), 2.24 (s, 6H), 2.10-2.02 (m, 2H).	453.58	526.5	80.9	100	100	100

 Structure4	3{3,5,4}	SJ000311321-1	13.79 (brs, 1H), 9.43 (brs, 1H), 9.10 (brs, 2H), 8.54-8.50 (m, 2H), 7.69 (s, 1H), 7.61 (dd, J = 8.8, 1.2 Hz, 1H), 7.40 (dd, J = 9.2, 3.6 Hz, 1H), 7.24 (dt, J = 8.8, 3.2 Hz, 1H), 7.09 (dd, J = 9.2, 4.4 Hz, 1H), 6.90-6.87 (m, 4H), 4.11 (brs, 4H), 3.81 (s, 3H), 3.65 (brs, 2H), 3.04 (brs, 2H), 2.24 (s, 3H), 2.11-2.04 (m, 2H).	457.58	530.5	29.6	100	100	100
 Structure1	3{3,6,1}	SJ000311322-1	13.81 (brs, 1H), 9.46 (brs, 1H), 9.33 (brs, 2H), 8.56 (d, J = 8.8 Hz, 1H), 8.52 (d, J = 7.2 Hz, 1H), 7.76 (brs, 1H), 7.61-7.50 (m, 5H), 7.29 (dt, J = 8.4, 2.8 Hz, 1H), 6.87 (d, J = 7.2 Hz, 1H), 6.65 (d, J = 3.2 Hz, 1H), 6.52 (dd, J = 3.2, 2.0 Hz, 1H), 4.32 (s, 2H), 4.23 (brs, 2H), 3.63 (brs, 2H), 3.03 (brs, 2H), 2.09-2.00 (m, 2H).	423.91	496.83	80.5	95.3	100	97.65
 Structure2	3{3,6,2}	SJ000311323-1	13.75 (brs, 1H), 9.39 (brs, 2H), 8.88 (brs, 2H), 8.52-8.49 (m, 2H), 7.61-7.51 (m, 4H), 7.29 (dt, J = 8.0, 2.8 Hz, 1H), 7.01-6.96 (m, 2H), 6.87 (d, J = 8.0 Hz, 1H), 6.80 (t, J = 8.0 Hz, 1H), 4.32 (s, 2H), 4.09 (brs, 2H), 3.81 (s, 3H), 3.62 (brs, 2H), 3.03 (brs, 2H), 2.09-2.02 (m, 2H).	479.97	552.89	77.5	100	100	100
 Structure3	3{3,6,3}	SJ000311324-1	13.77 (brs, 1H), 9.43 (brs, 1H), 9.27 (brs, 2H), 8.55 (d, J = 8.8 Hz, 1H), 8.52 (d, J = 7.2 Hz, 1H), 7.61-7.50 (m, 5H), 7.29 (dt, J = 8.4, 2.8 Hz, 1H), 7.06 (d, J = 8.0 Hz, 1H), 6.96 (dd, J = 8.4, 1.2 Hz, 1H), 6.91-6.87 (m, 2H), 6.06 (s, 2H), 4.32 (s, 2H), 4.10 (brs, 2H), 3.64 (brs, 2H), 3.07 (brs, 2H), 2.10-2.02 (m, 2H).	477.96	550.88	79.8	100	100	100
 Structure4	3{3,6,4}	SJ000311325-1	13.78 (brs, 1H), 9.44 (brs, 1H), 9.11 (brs, 2H), 8.55 (d, J = 8.8 Hz, 1H), 8.52 (d, J = 7.2 Hz, 1H), 7.61-7.50 (m, 4H), 7.40 (dd, J = 8.8, 3.2 Hz, 1H), 7.29 (dt, J = 8.4, 2.8 Hz, 1H), 7.24 (dt, J = 8.4, 3.2 Hz, 1H), 7.09 (dd, J = 8.8, 4.4 Hz, 1H), 6.88 (d, J = 7.2, 1H), 4.32 (s, 2H), 4.11 (s, 2H), 3.81 (s, 3H), 3.64 (brs, 2H), 3.05 (brs, 2H), 2.11-2.04 (m, 2H).	481.96	554.88	21.3	100	100	100
 Structure1	3{3,7,1}	SJ000311246-1	14.01 (brs, 1H), 9.48 (brs, 3H), 8.57 (d, J = 9.2 Hz, 1H), 8.53 (d, J = 7.2 Hz, 1H), 7.76 (d, J = 1.2 Hz, 1H), 7.75 (s, 1H), 7.61 (d, J = 8.4 Hz, 1H), 6.87 (d, J = 7.2 Hz, 1H), 6.65 (d, J = 3.2 Hz, 1H), 6.52 (dd, J = 3.2, 2.0 Hz, 1H), 4.24 (brs, 2H), 3.64 (brs, 2H), 3.03 (brs, 2H), 2.84-2.80 (m, 2H), 2.12-2.02 (m, 2H), 1.62-1.53 (m, 3H), 0.94 (d, J = 6.0 Hz, 6H).	351.49	424.41	79.4	66.96	85.03	75.995
 Structure2	3{3,7,2}	SJ000311247-1	13.99 (brs, 1H), 9.44 (brs, 1H), 9.37 (brs, 1H), 9.05 (brs, 2H), 8.55-8.50 (m, 2H), 7.71 (brs, 1H), 7.61 (d, J = 8.8 Hz, 1H), 7.03-7.00 (m, 2H), 6.87 (d, J = 8.0 Hz, 1H), 6.81 (t, J = 8.0 Hz, 1H), 4.10 (brs, 2H), 3.82 (s, 3H), 3.63 (brs, 2H), 3.04 (brs, 2H), 2.84-2.80 (m, 2H), 2.12-2.02 (m, 2H), 1.62-1.53 (m, 3H), 0.95 (d, J = 6.0 Hz, 6H).	407.55	480.47	76.4	89.95	100	94.975
 Structure3	3{3,7,3}	SJ000311248-1	13.95 (brs, 1H), 9.45 (brs, 3H), 8.59-8.51 (m, 2H), 7.73 (s, 1H), 7.60 (d, J = 8.8 Hz, 1H), 7.10 (d, J = 8.0 Hz, 1H), 6.95 (dd, J = 8.4, 1.2 Hz, 1H), 6.90-6.86 (m, 2H), 6.06 (s, 2H), 4.09 (brs, 2H), 3.65 (brs, 2H), 3.06 (brs, 2H), 2.83-2.79 (m, 2H), 2.12-2.02 (m, 2H), 1.61-1.52 (m, 3H), 0.95 (d, J = 6.0 Hz, 6H).	405.54	478.46	78.2	96.46	100	98.23

 Structure4	3{3,7,4}	SJ000311249-1	13.94 (brs, 1H), 9.46 (brs, 1H), 9.22 (brs, 2H), 8.56-8.51 (m, 2H), 7.73 (s, 1H), 7.60 (d, J = 8.4 Hz, 1H), 7.43 (dd, J = 8.8, 3.2 Hz, 1H), 7.24 (dt, J = 8.4, 3.2 Hz, 1H), 7.09 (dd, J = 9.2, 4.4 Hz, 1H), 6.88 (d, J = 7.2, 1H), 4.11 (s, 2H), 3.81 (s, 3H), 3.65 (brs, 2H), 3.04 (brs, 2H), 2.83-2.79 (m, 2H), 2.12-2.02 (m, 2H), 1.61-1.52 (m, 3H), 0.94 (d, J = 6.0 Hz, 6H).	409.54	482.46	79.1	96.75	100	98.375
 Structure1	3{3,8,1}	SJ000311250-1	13.97 (brs, 1H), 9.47 (brs, 1H), 9.40 (brs, 2H), 8.55 (d, J = 9.2 Hz, 1H), 8.53 (d, J = 7.2 Hz, 1H), 7.76 (s, 1H), 7.68 (s, 1H), 7.56 (d, J = 8.4 Hz, 1H), 6.87 (d, J = 7.2 Hz, 1H), 6.64 (d, J = 3.2 Hz, 1H), 6.51 (dd, J = 3.2, 2.0 Hz, 1H), 4.23 (brs, 2H), 3.64 (brs, 2H), 3.02 (brs, 2H), 2.69 (d, J = 7.2 Hz, 2H), 2.12-2.02 (m, 2H), 1.70-1.55 (m, 6H), 1.24-1.10 (m, 3H), 1.3-0.93 (m, 2H).	377.53	450.45	76.5	77.78	95.93	86.855
 Structure2	3{3,8,2}	SJ000311251-1	13.97 (brs, 1H), 9.44 (brs, 1H), 9.27 (brs, 1H), 9.03 (brs, 2H), 8.55-8.50 (m, 2H), 7.69 (brs, 1H), 7.56 (d, J = 8.8 Hz, 1H), 7.02-6.99 (m, 2H), 6.87 (d, J = 8.0 Hz, 1H), 6.81 (t, J = 8.0 Hz, 1H), 4.10 (brs, 2H), 3.82 (s, 3H), 3.63 (brs, 2H), 3.04 (brs, 2H), 2.70 (d, J = 7.2 Hz, 2H), 2.12-2.02 (m, 2H), 1.70-1.55 (m, 6H), 1.24-1.10 (m, 3H), 1.3-0.93 (m, 2H).	433.59	506.51	75.4	90.63	100	95.315
 Structure3	3{3,8,3}	SJ000311252-1	14.02 (brs, 1H), 9.51 (brs, 3H), 8.61-8.52 (m, 2H), 7.70 (s, 1H), 7.57 (d, J = 8.8 Hz, 1H), 7.12 (dd, J = 8.0, 3.2 Hz, 1H), 6.97 (dd, J = 8.4, 1.2 Hz, 1H), 6.92-6.86 (m, 2H), 6.08 (s, 2H), 4.11 (brs, 2H), 3.66 (brs, 2H), 3.08 (brs, 2H), 2.70 (d, J = 7.2 Hz, 2H), 2.12-2.02 (m, 2H), 1.70-1.55 (m, 6H), 1.24-1.10 (m, 3H), 1.3-0.93 (m, 2H).	431.58	504.5	78.2	91.37	100	95.685
 Structure4	3{3,8,4}	SJ000311253-1	13.91 (brs, 1H), 9.45 (brs, 1H), 9.19 (brs, 2H), 8.59-8.51 (m, 2H), 7.67 (s, 1H), 7.56 (d, J = 8.4 Hz, 1H), 7.42 (dd, J = 8.8, 3.2 Hz, 1H), 7.24 (dt, J = 8.4, 3.2 Hz, 1H), 7.09 (dd, J = 9.2, 4.4 Hz, 1H), 6.88 (d, J = 7.2, 1H), 4.11 (s, 2H), 3.81 (s, 3H), 3.65 (brs, 2H), 3.05 (brs, 2H), 2.69 (d, J = 7.2 Hz, 2H), 2.12-2.02 (m, 2H), 1.70-1.55 (m, 6H), 1.24-1.10 (m, 3H), 1.3-0.93 (m, 2H).	435.58	508.5	78.8	80.2	98.62	89.41
 Structure1	3{3,9,1}	SJ000311254-1	13.88 (brs, 1H), 9.42 (brs, 3H), 8.53 (d, J = 8.4 Hz, 1H), 8.50 (d, J = 6.8 Hz, 1H), 7.76 (d, J = 1.6 Hz, 1H), 7.69 (s, 1H), 7.63 (dd, J = 8.8, 1.2 Hz, 1H), 7.33-7.23 (m, 5H), 7.20-7.16 (m, 1H), 6.86 (d, J = 7.2 Hz, 1H), 6.63 (d, J = 3.2 Hz, 1H), 6.51 (dd, J = 3.2, 2.0 Hz, 1H), 4.23 (brs, 2H), 3.63 (brs, 2H), 3.15-3.11 (m, 2H), 3.05-2.97 (m, 4H), 2.07-2.00 (m, 2H).	385.51	458.43	55.5	66.53	78.46	72.495
 Structure2	3{3,9,2}	SJ000311255-1	13.83 (brs, 1H), 9.36 (brs, 2H), 8.94 (brs, 2H), 8.51 (d, J = 7.2 Hz, 1H), 8.49 (d, J = 9.2 Hz, 1H), 7.69 (d, J = 1.6 Hz, 1H), 7.64 (dd, J = 9.2, 1.6 Hz, 1H), 7.33-7.24 (m, 5H), 7.21-7.17 (m, 1H), 7.02-6.98 (m, 2H), 6.86 (d, J = 7.2 Hz, 1H), 6.82 (t, J = 8.0 Hz, 1H), 4.12 (s, 2H), 3.82 (s, 3H), 3.63 (brs, 2H), 3.16-3.12 (m, 2H), 3.08-2.98 (m, 4H), 2.09-2.02 (m, 2H).	441.57	514.49	63.3	90.63	100	95.315
 Structure3	3{3,9,3}	SJ000311256-1	13.86 (brs, 1H), 9.42 (brs, 1H), 9.14 (brs, 2H), 8.53 (d, J = 9.6 Hz, 1H), 8.52 (d, J = 6.8 Hz, 1H), 7.69 (d, J = 1.6 Hz, 1H), 7.64 (dd, J = 8.8, 1.6 Hz, 1H), 7.42 (dd, J = 8.8, 3.2 Hz, 1H), 7.33-7.24 (m, 5H), 7.22-7.17 (m, 1H), 7.09 (dd, J = 9.2, 4.4 Hz, 1H), 6.88 (d, J = 7.2 Hz, 1H), 4.12 (s, 2H), 3.82 (s, 3H), 3.65 (brs, 2H), 3.16-3.12 (m, 2H), 3.08-2.98 (m, 4H), 2.12-2.04 (m, 2H).	439.56	512.48	67.5	96.89	100	98.445

 <p>Structure4</p>	3{3,9,4}	SJ000311257-1	<p>13.92 (brs, 1H), 9.48 (brs, 1H), 9.71 (brs, 2H), 8.56-8.50 (m, 2H), 7.70 (d, J = 1.6 Hz, 1H), 7.63 (dd, J = 8.8, 1.6 Hz, 1H), 7.33-7.23 (m, 5H), 7.20-7.16 (m, 1H), 7.10 (d, J = 7.6 Hz, 1H), 6.95 (d, J = 7.6 Hz, 1H), 6.88 (t, J = 7.6 Hz, 1H), 6.05 (s, 2H), 4.09 (s, 2H), 3.65 (brs, 2H), 3.16-2.97 (m, 6H), 2.15-2.05 (m, 2H).</p>	443.56	516.48	67.0	97.98	100	98.99
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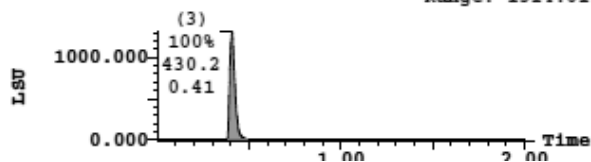
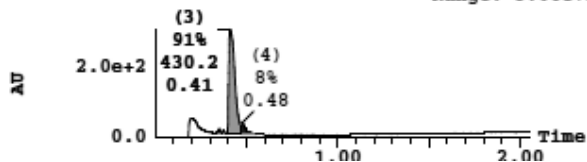


2: UV Detector: TIC

3.081e+2  
Range: 3.08e+2

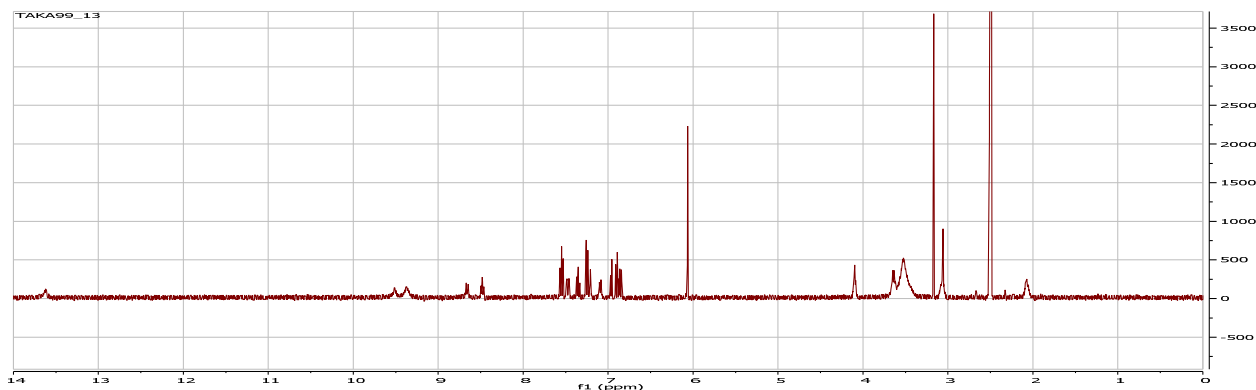
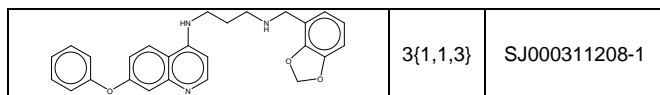
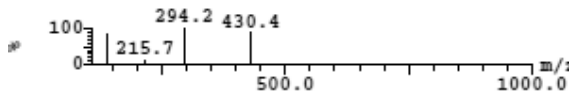
(2) ELSD signal

1314.627  
Range: 1314.614



Peak ID	Compound	Time	Mass Found
3	Found	0.40	430.21

1:MS ES+  
8.4e+007

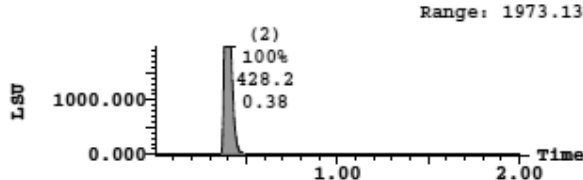
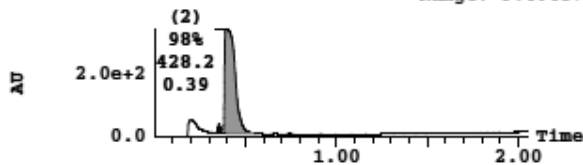


2: UV Detector: TIC

3.404e+2  
Range: 3.404e+2

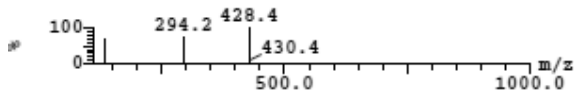
(2) ELSD signal

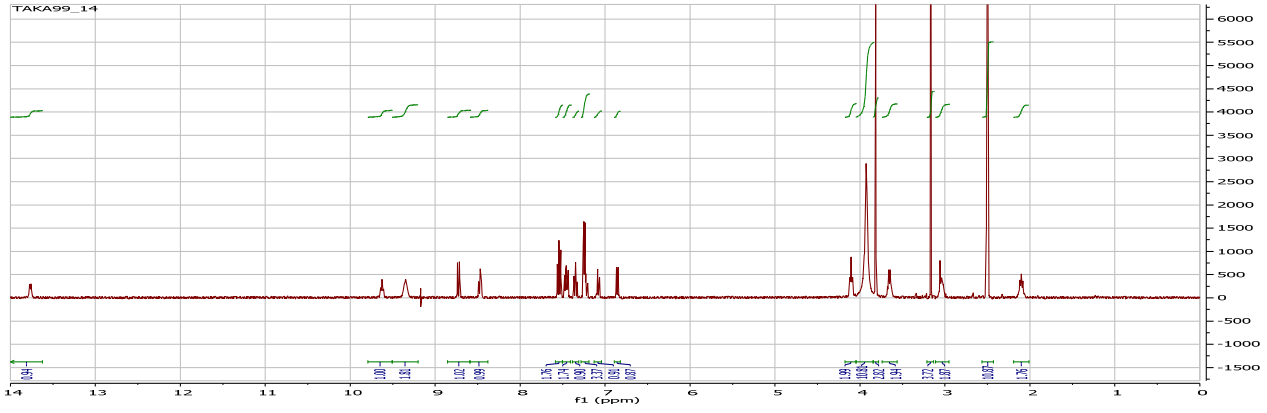
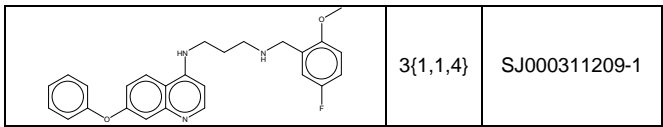
1973.276  
Range: 1973.138



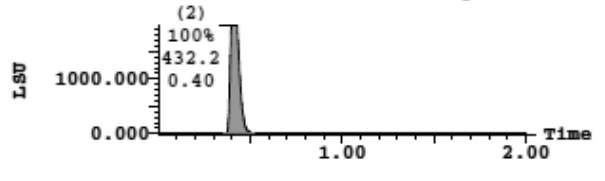
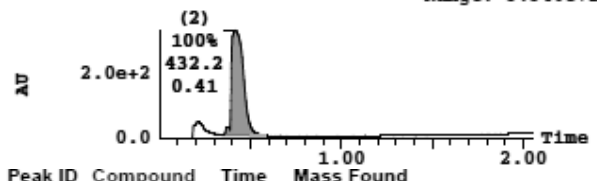
Peak ID	Compound	Time	Mass Found
2	Found	0.38	428.19

1:MS ES+  
9.9e+007



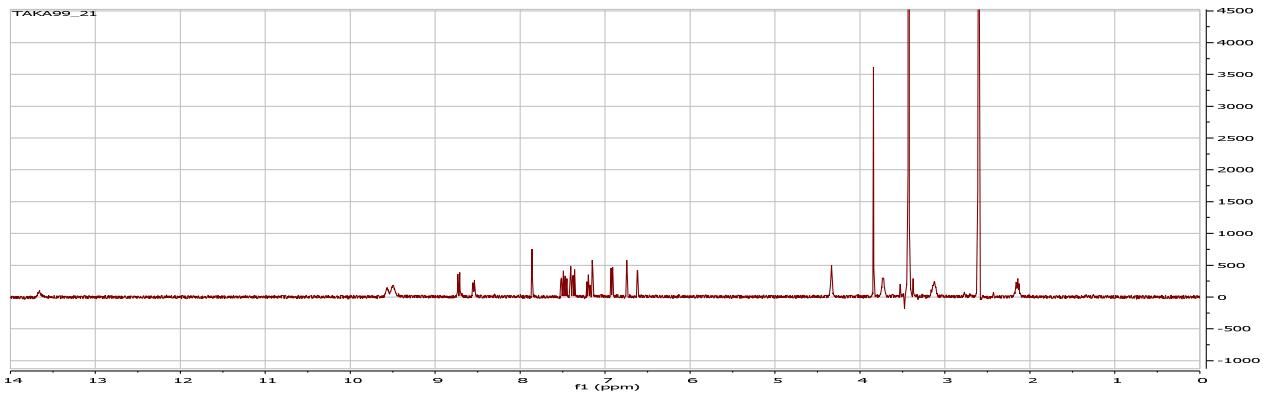
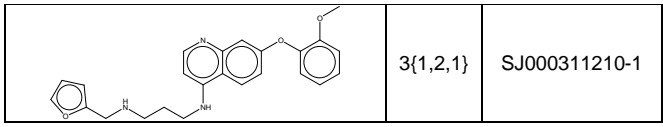
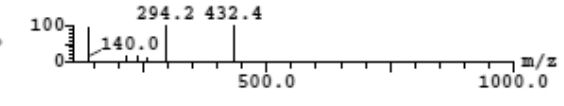


2: UV Detector: TIC 3.347e+2 (2) ELSD Signal 1973.105  
 Range: 3.346e+2 Range: 1973.046



Peak ID	Compound Found	Time	Mass Found
2	Found	0.40	432.20

1:MS ES+  
1.0e+008



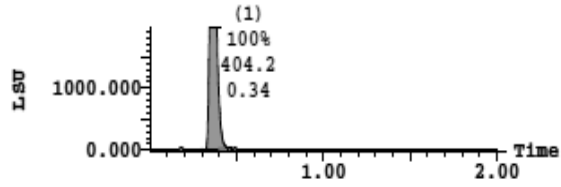
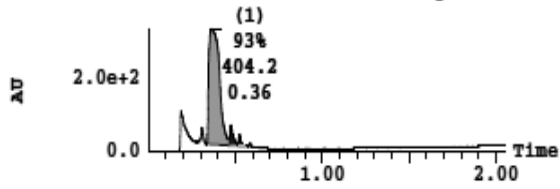


2: UV Detector: TIC

3.369e+2  
Range: 3.369e+2

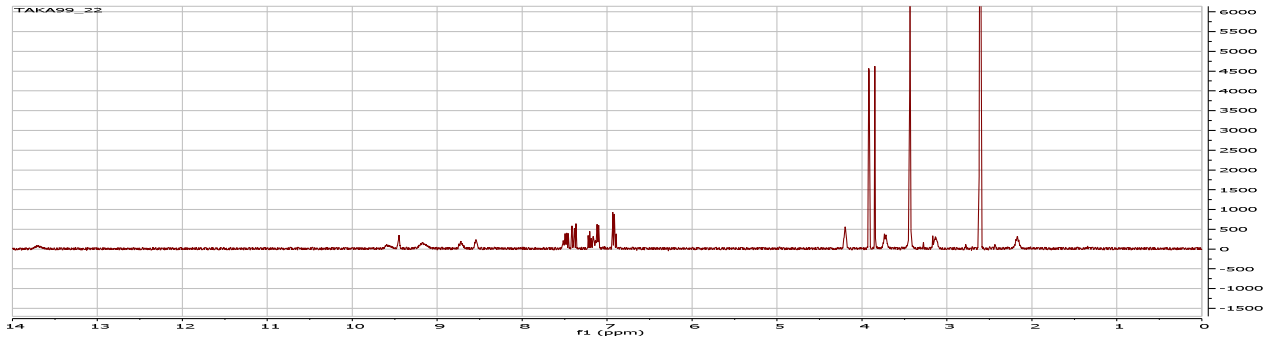
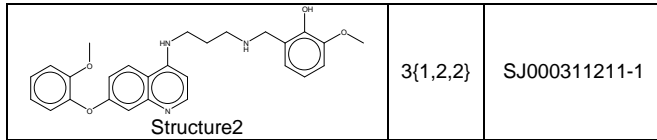
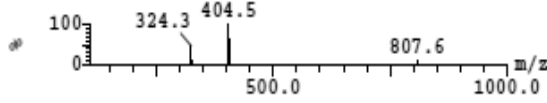
(2) ELSD signal

1973.365  
Range: 1973.325



Peak ID	Compound	Time	Mass Found
1	Found	0.34	404.19

1:MS ES+  
7.6e+007

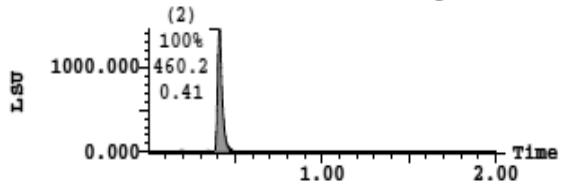
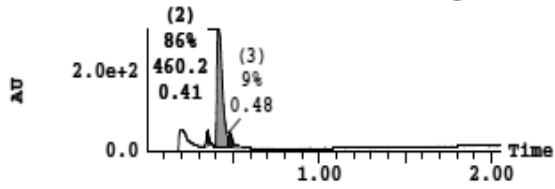


2: UV Detector: TIC

3.1e+2  
Range: 3.1e+2

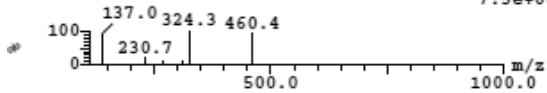
(2) ELSD signal

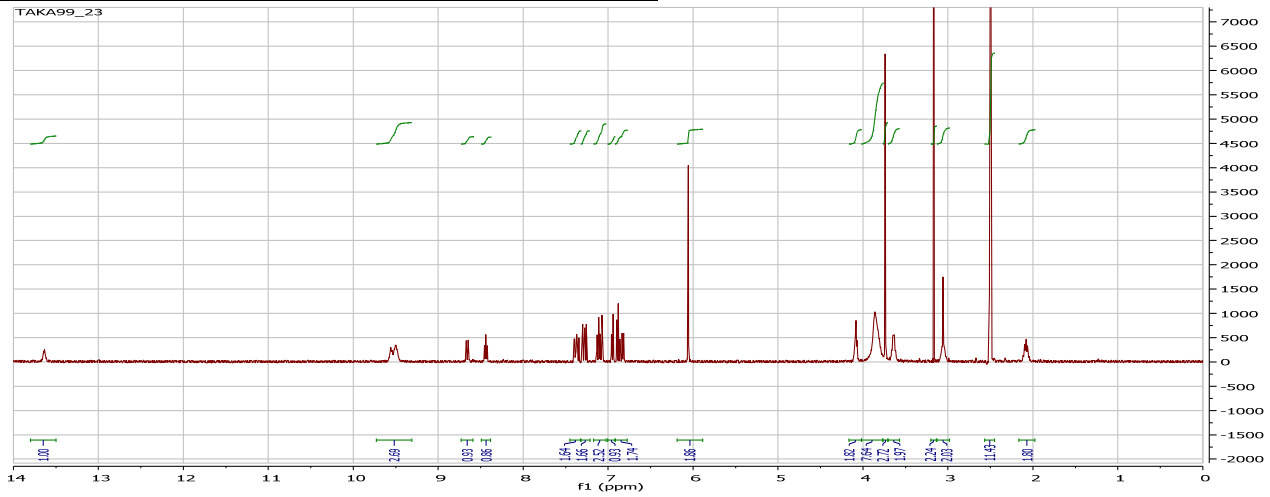
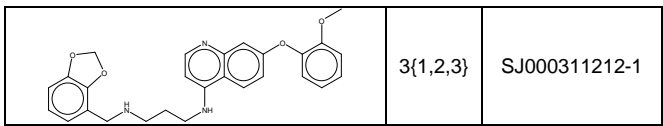
1447.316  
Range: 1447.287



Peak ID	Compound	Time	Mass Found
2	Found	0.40	460.22

1:MS ES+  
7.3e+007

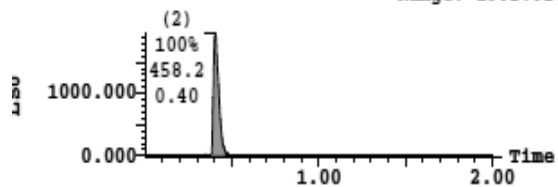
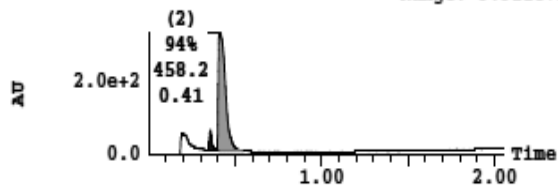




2: UV Detector: TIC

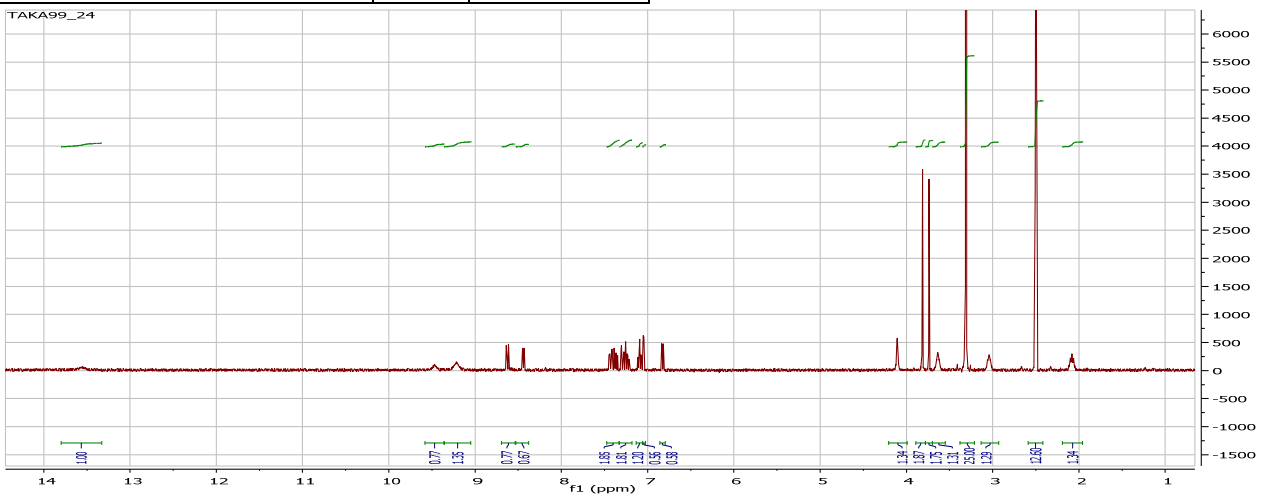
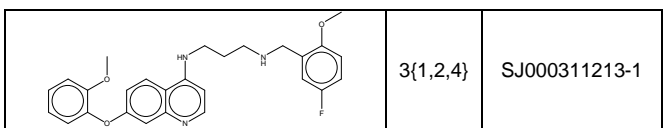
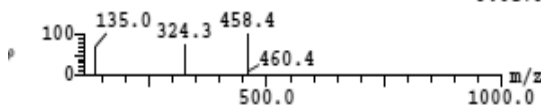
3.311e+2 (2) ELSD signal  
Range: 3.311e+2

1962.653  
Range: 1962.614



Peak ID	Compound	Time	Mass Found
2	Found	0.40	458.20

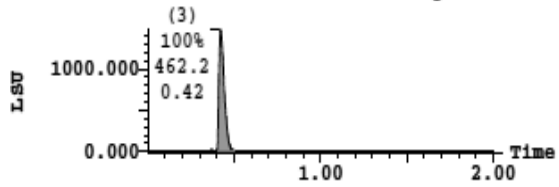
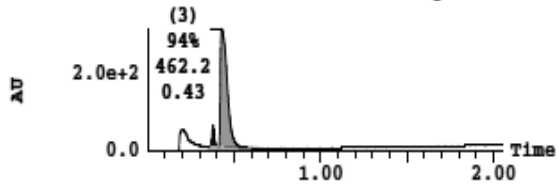
1:MS ES+  
9.0e+007



2: UV Detector: TIC

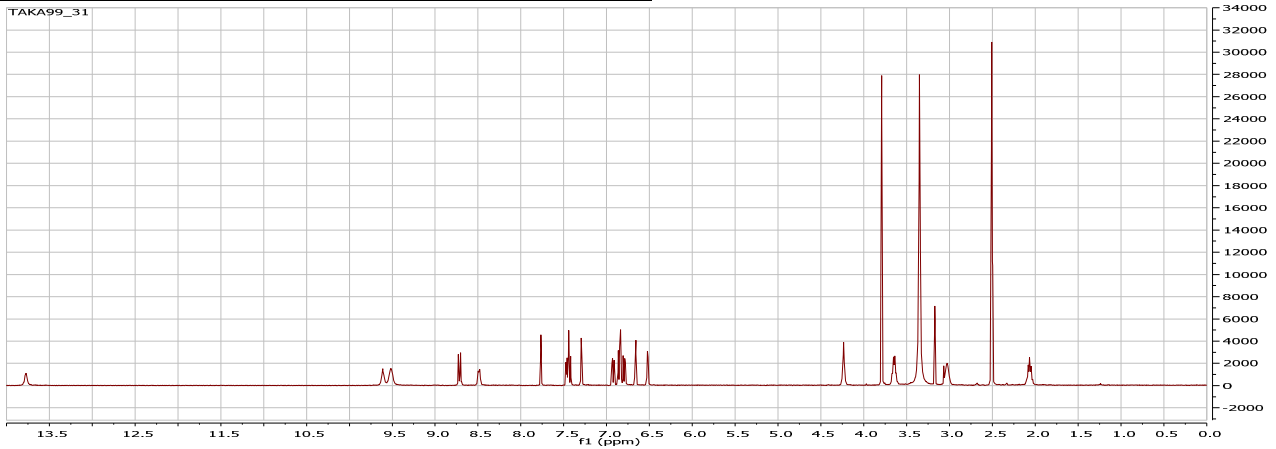
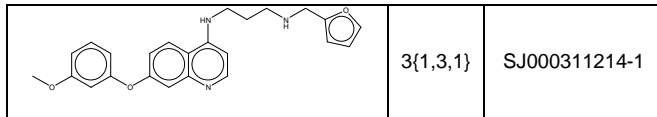
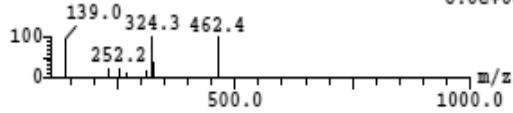
3.155e+2 (2) ELSD signal  
Range: 3.155e+2

1474.565  
Range: 1474.477



Peak ID	Compound	Time	Mass Found
3	Found	0.41	462.21

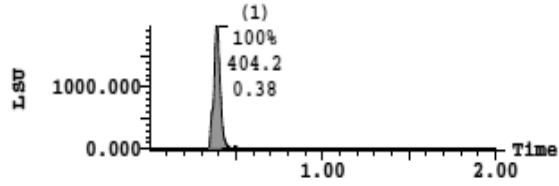
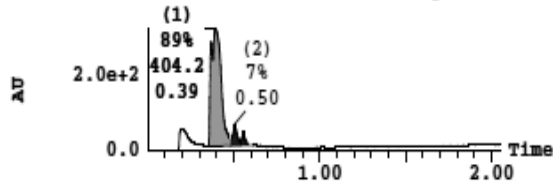
1:MS ES+  
8.0e+007



2: UV Detector: TIC

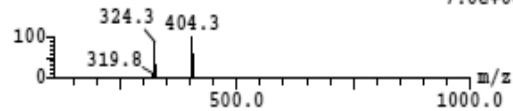
3.271e+2 (2) ELSD signal  
Range: 3.271e+2

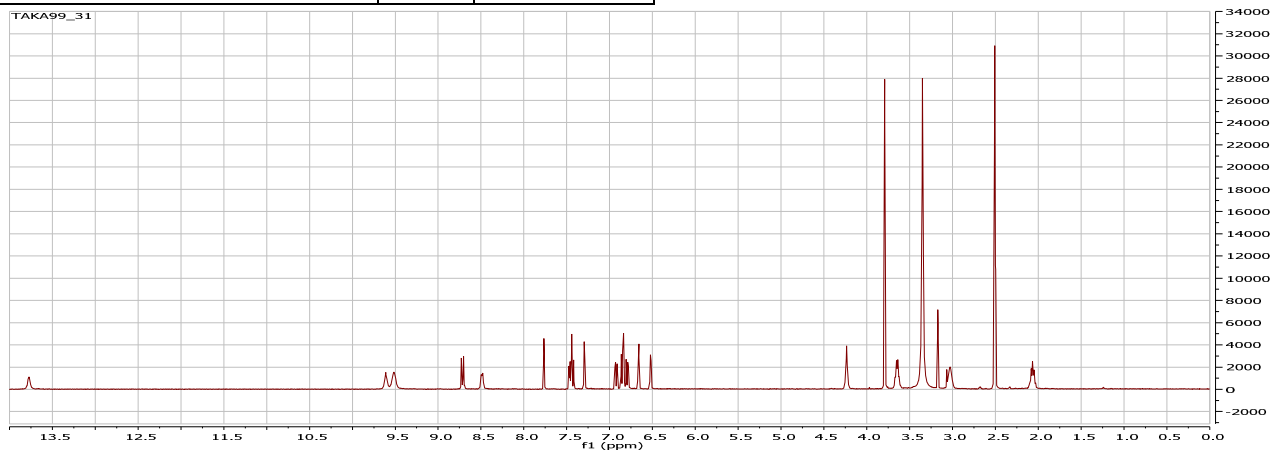
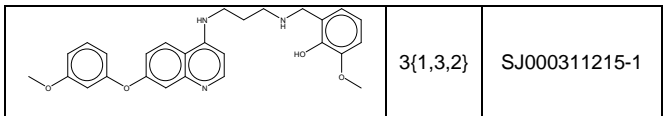
1972.963  
Range: 1972.904



Peak ID	Compound	Time	Mass Found
1	Found	0.37	404.19

1:MS ES+  
7.0e+007

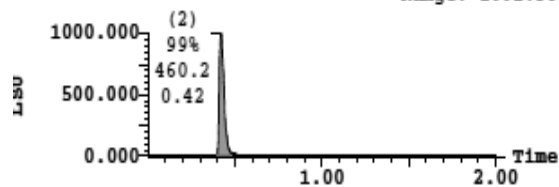
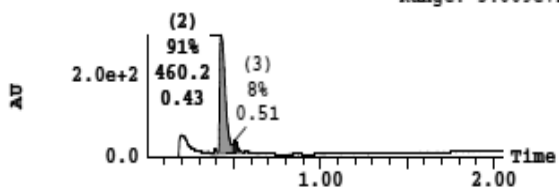




2: UV Detector: TIC

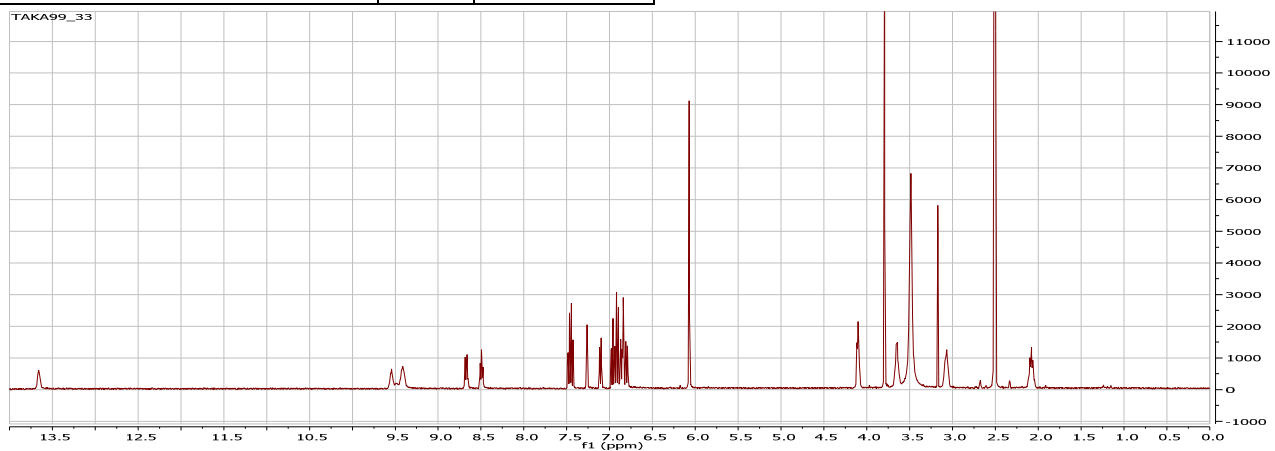
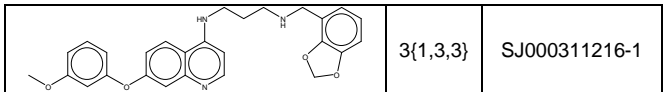
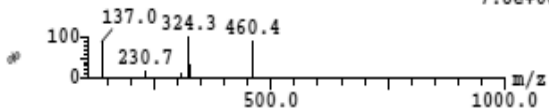
3.009e+2 (2) ELSD Signal  
Range: 3.009e+2

1001.676  
Range: 1001.585



Peak ID	Compound	Time	Mass Found
2	Found	0.41	460.22

1:MS ES+  
7.8e+007

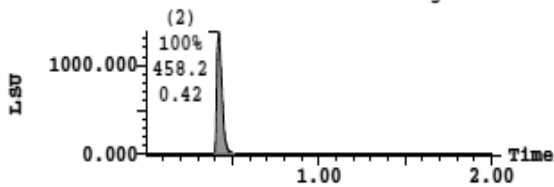
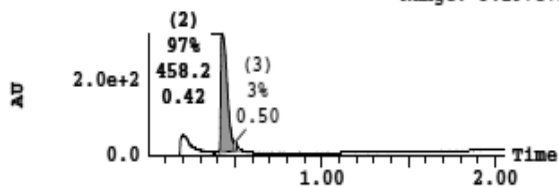


2: UV Detector: TIC

3.197e+2  
Range: 3.197e+2

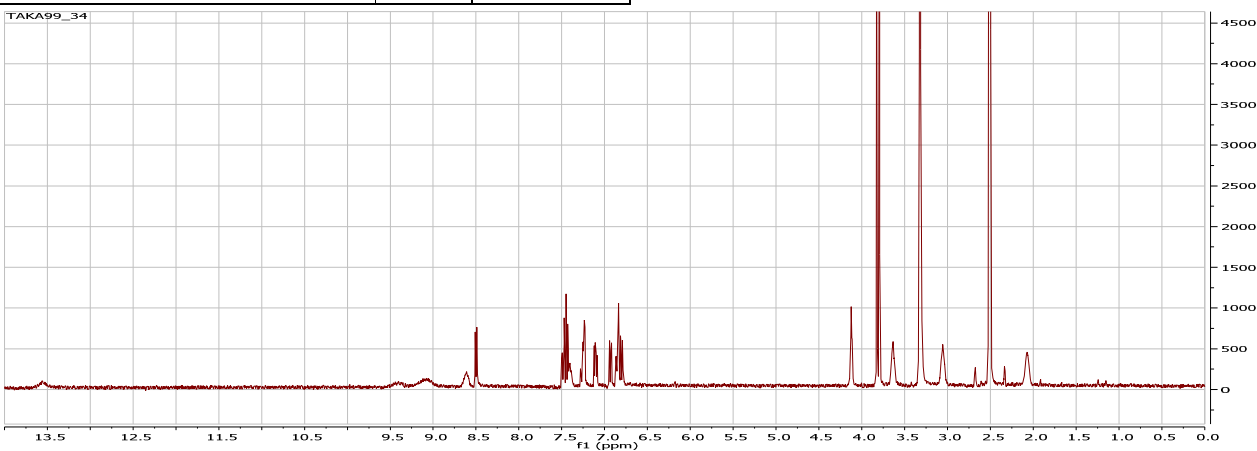
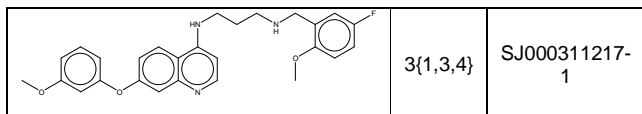
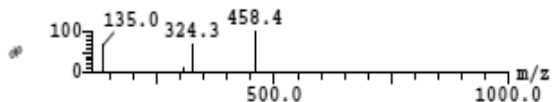
(2) ELSD Signal

1378.798  
Range: 1378.743



Peak ID	Compound	Time	Mass Found
2	Found	0.41	458.20

1:MS ES+  
9.0e+007

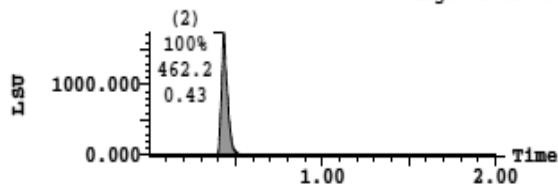
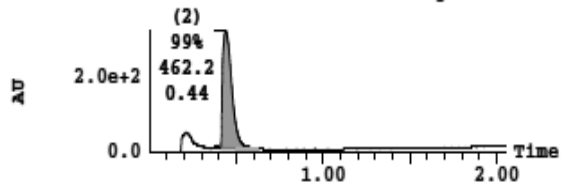


2: UV Detector: TIC

3.213e+2  
Range: 3.213e+2

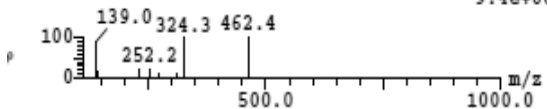
(2) ELSD Signal

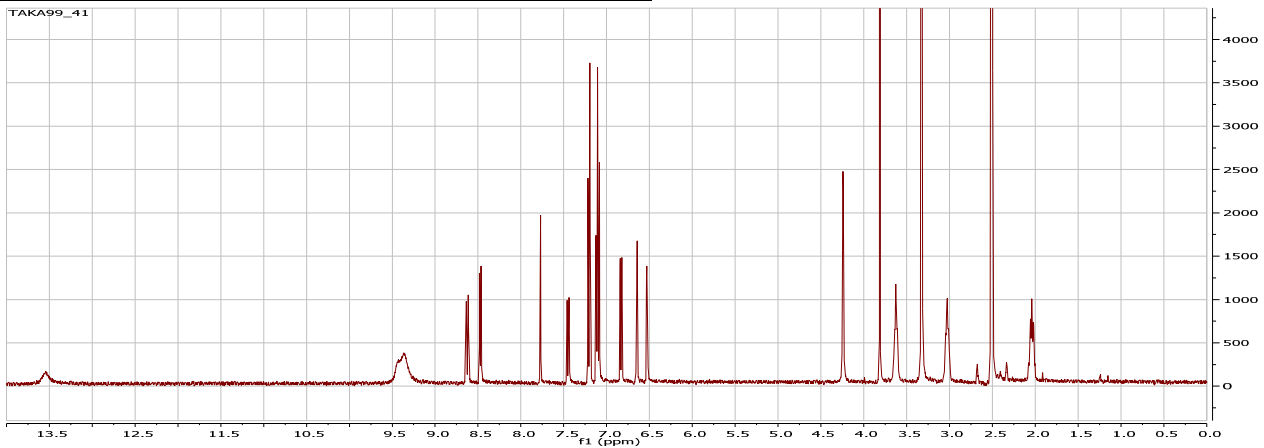
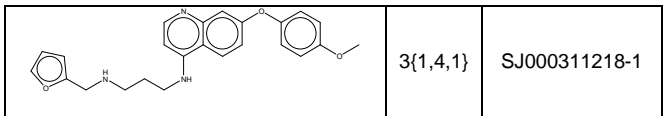
1742.850  
Range: 1742.815



Peak ID	Compound	Time	Mass Found
2	Found	0.42	462.21

1:MS ES+  
9.4e+007

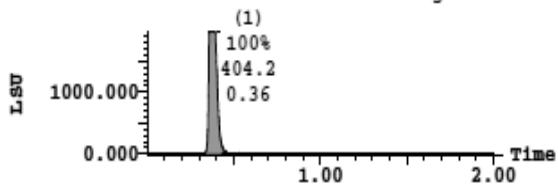
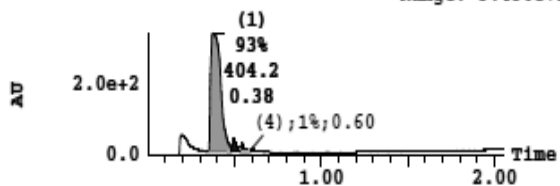




2: UV Detector: TIC

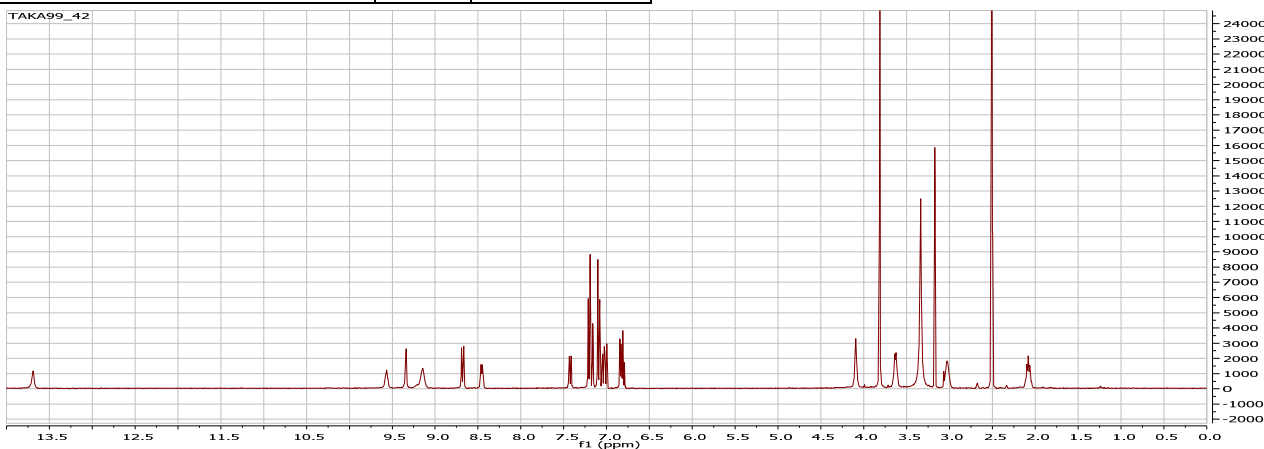
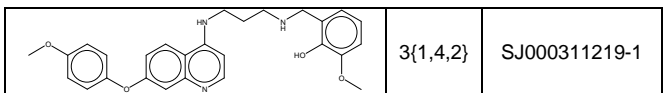
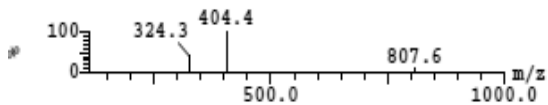
3.436e+2 (2) ELSD signal  
Range: 3.436e+2

1973.094  
Range: 1973.054



Peak ID	Compound	Time	Mass Found
1	Found	0.38	404.19

1:MS ES+  
8.5e+007

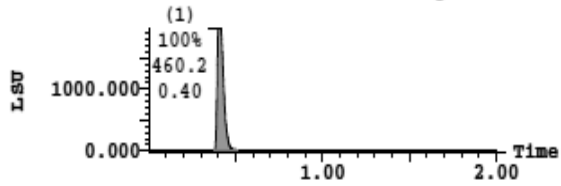
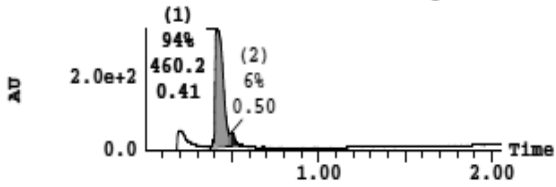


2: UV Detector: TIC

3.336e+2  
Range: 3.336e+2

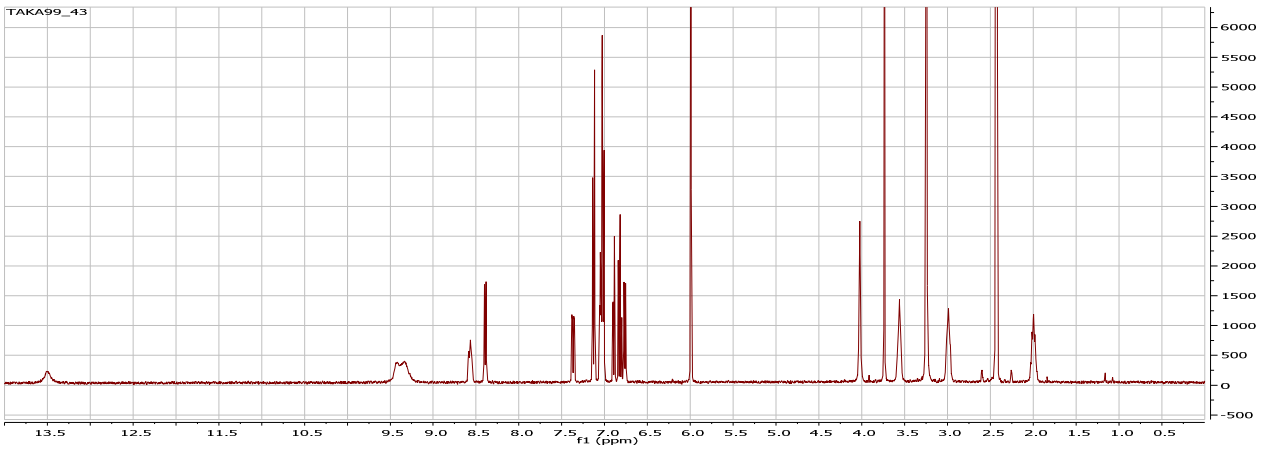
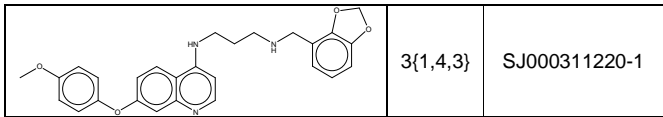
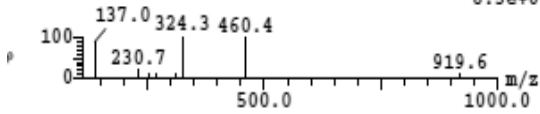
(2) ELSD Signal

1973.198  
Range: 1973.139



Peak ID	Compound	Time	Mass Found
1	Found	0.40	460.22

1:MS ES+  
8.3e+007

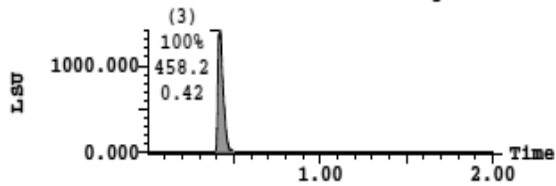
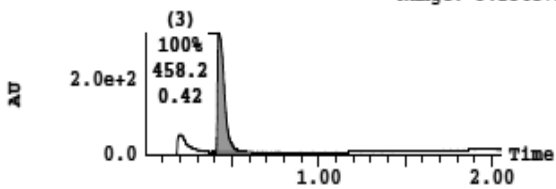


2: UV Detector: TIC

3.254e+2  
Range: 3.254e+2

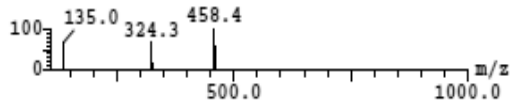
(2) ELSD Signal

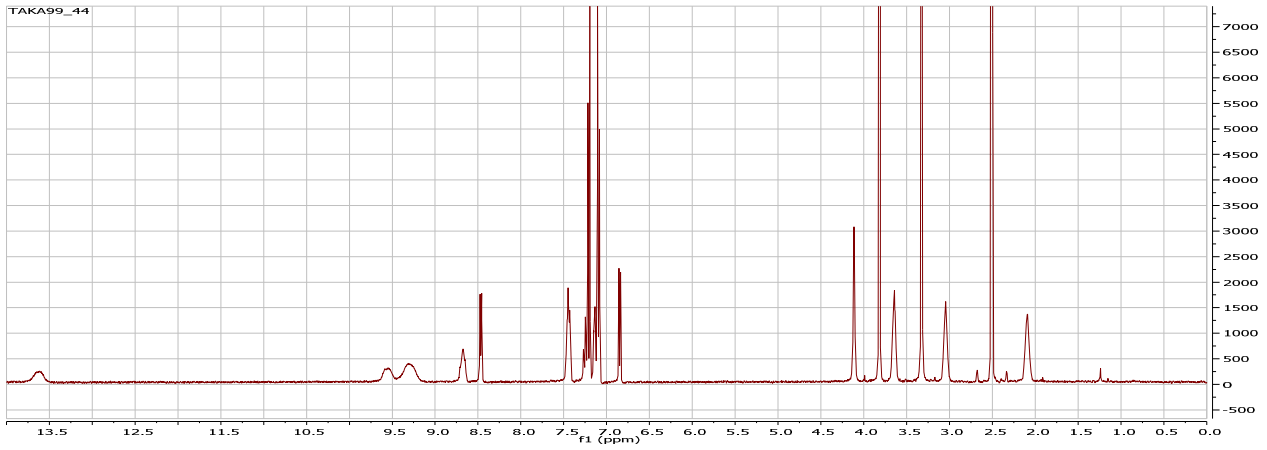
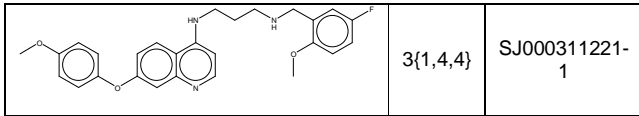
1402.075  
Range: 1401.893



Peak ID	Compound	Time	Mass Found
3	Found	0.41	458.20

1:MS ES+  
8.7e+007

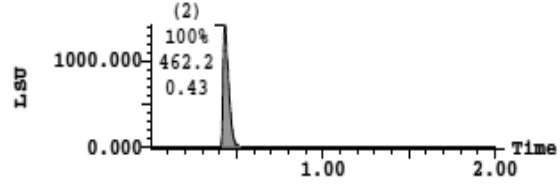
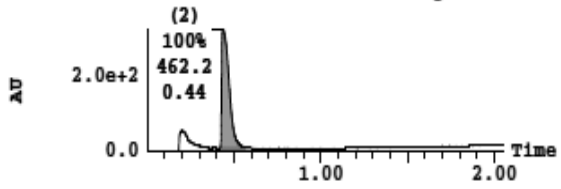




2: UV Detector: TIC

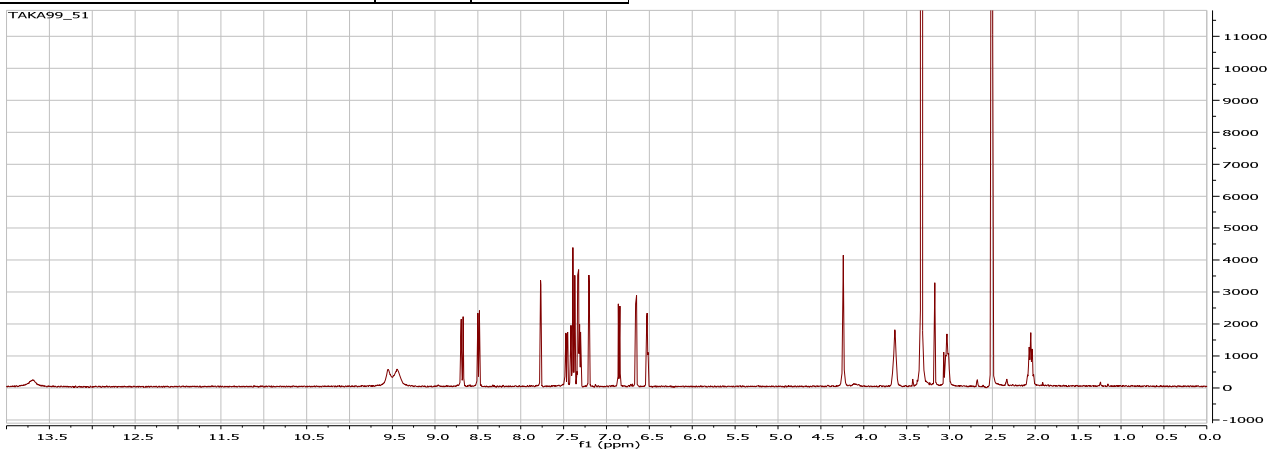
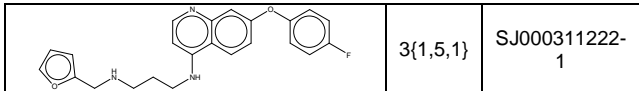
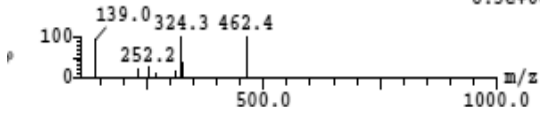
3.201e+2 (2) ELSD signal  
Range: 3.201e+2

1416.251  
Range: 1416.166



Peak ID	Compound	Time	Mass Found
2	Found	0.42	462.21

1:MS ES+  
8.3e+007





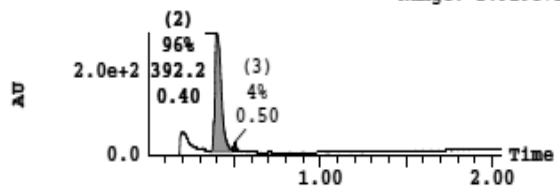
2: UV Detector: TIC

2.919e+2 (2) ELSD Signal

1049.791

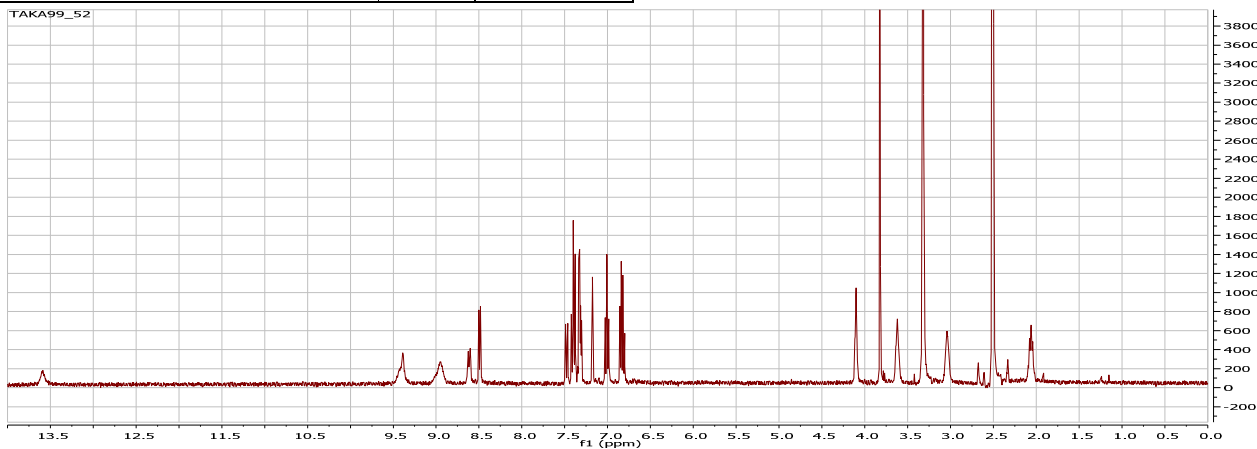
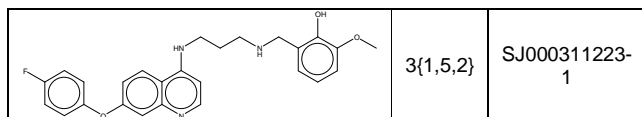
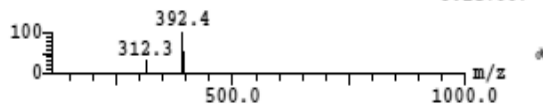
Range: 2.919e+2

Range: 1049.717



Peak ID	Compound	Time	Mass Found
2	Found	0.38	392.17

1:MS ES+  
8.1e+007



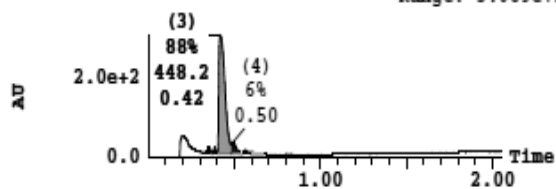
2: UV Detector: TIC

3.089e+2 (2) ELSD Signal

1457.820

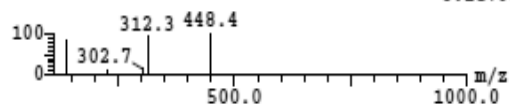
Range: 3.089e+2

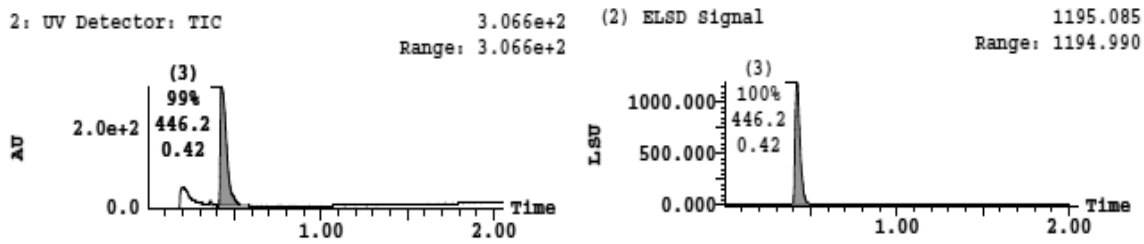
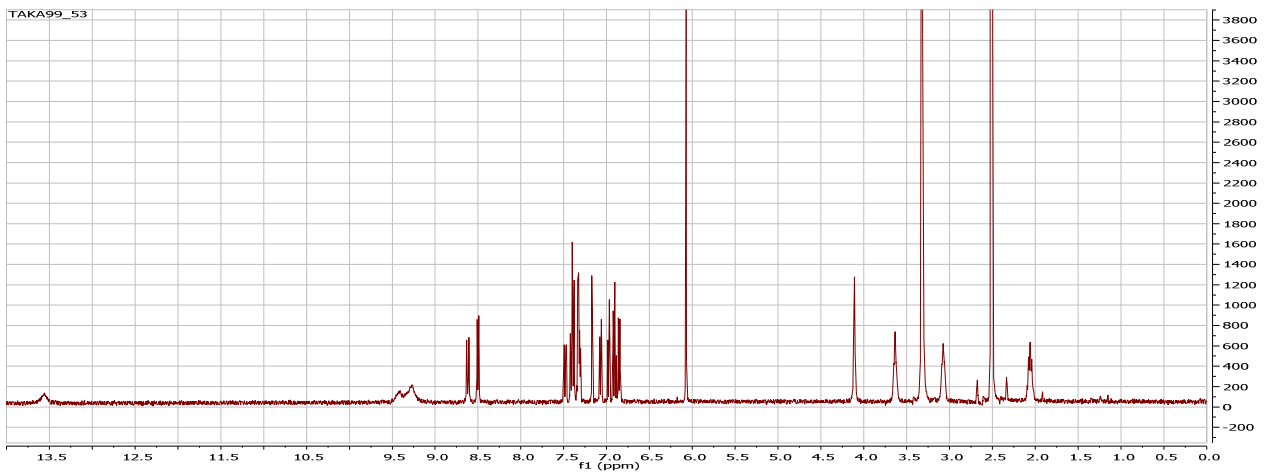
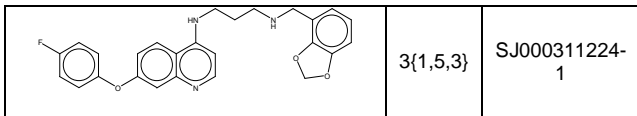
Range: 1457.776



Peak ID	Compound	Time	Mass Found
3	Found	0.40	448.20

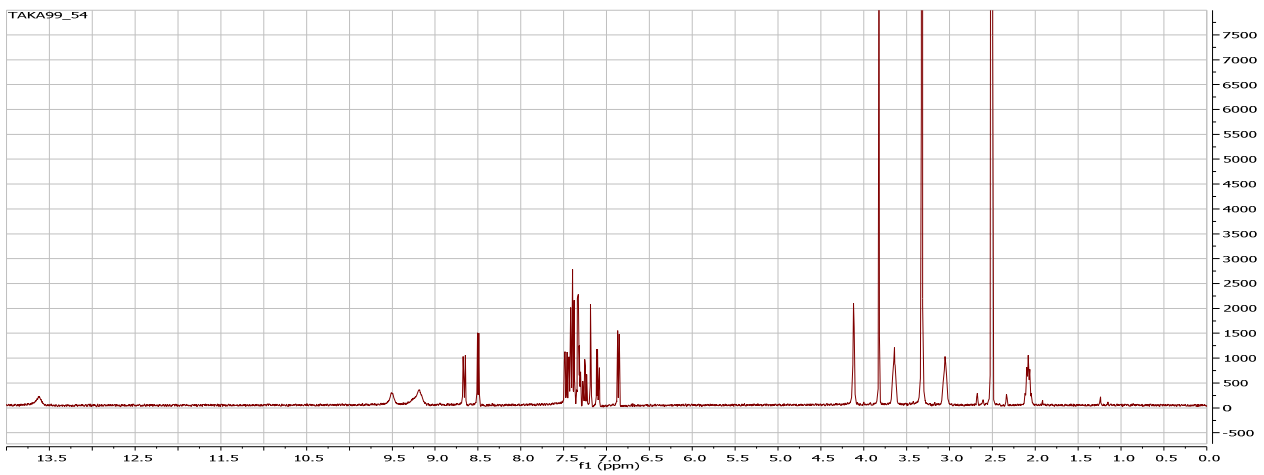
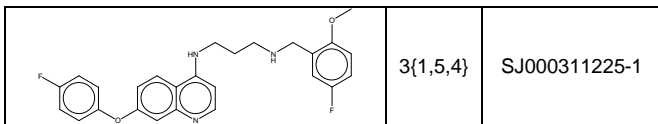
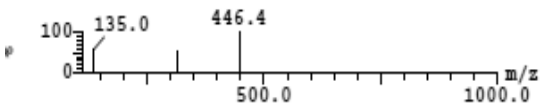
1:MS ES+  
8.1e+007





Peak ID	Compound	Time	Mass Found
3	Found	0.41	446.18

1:MS ES+  
9.2e+007

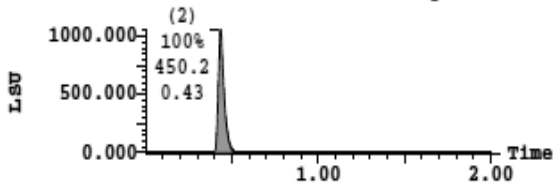
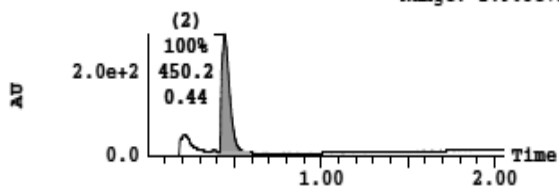


2: UV Detector: TIC

2.903e+2  
Range: 2.903e+2

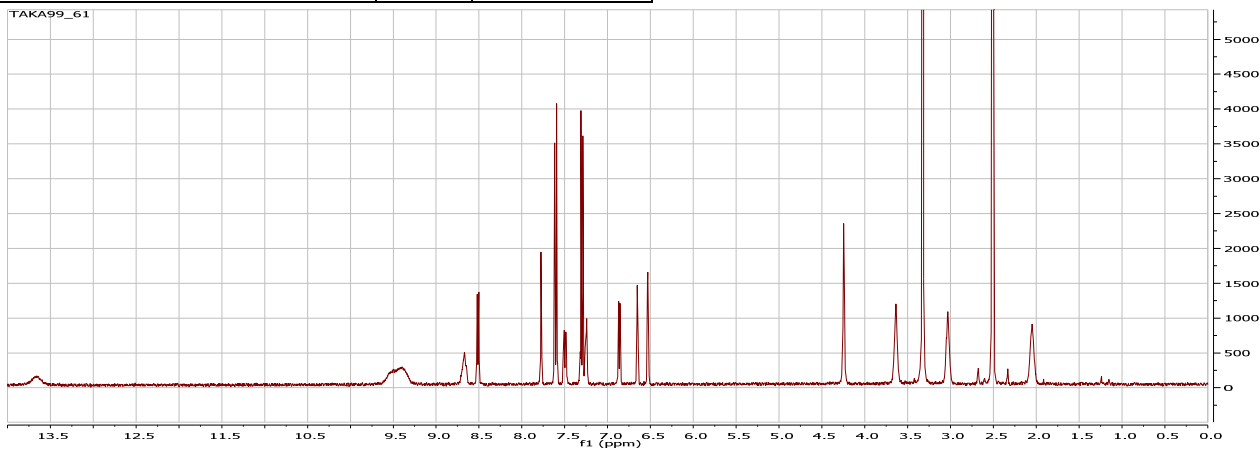
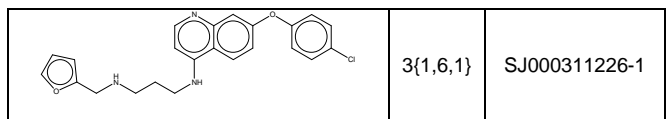
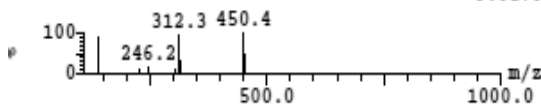
(2) ELSD signal

1056.806  
Range: 1056.774



Peak ID	Compound	Time	Mass Found
2	Found	0.43	450.19

1:MS ES+  
9.0e+007

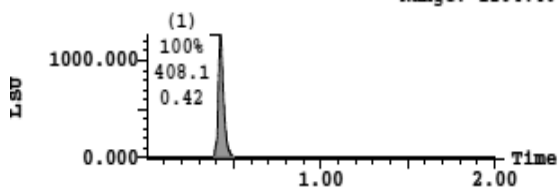
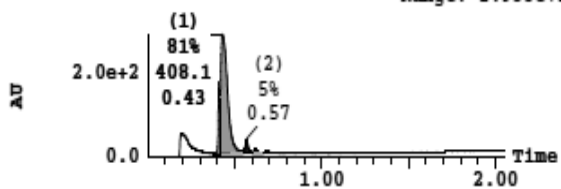


2: UV Detector: TIC

2.933e+2  
Range: 2.933e+2

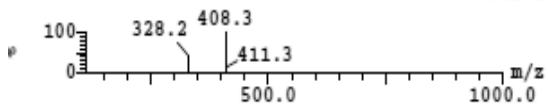
(2) ELSD signal

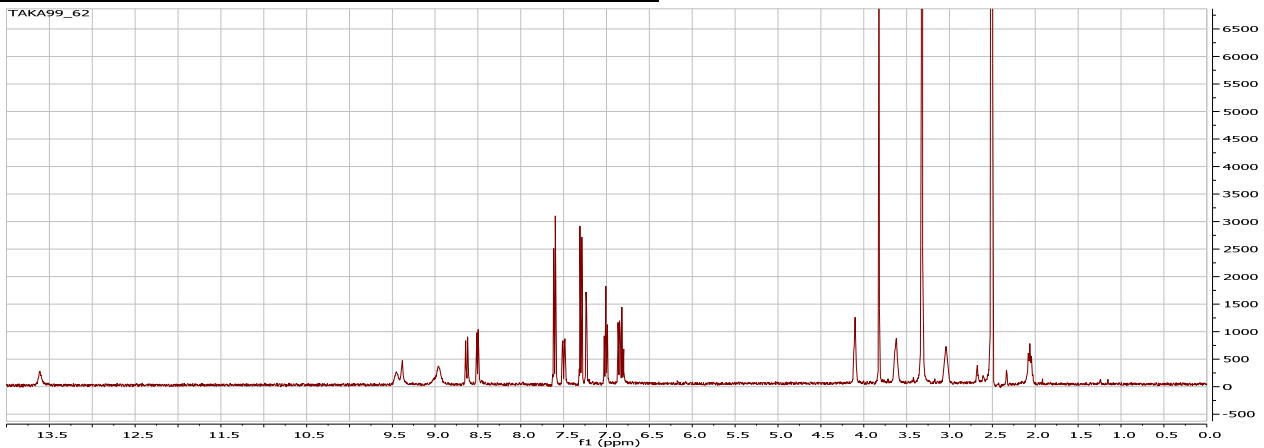
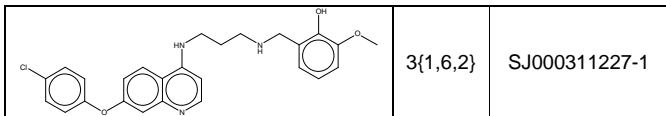
1264.564  
Range: 1264.400



Peak ID	Compound	Time	Mass Found
1	Found	0.41	408.14

1:MS ES+  
7.0e+007

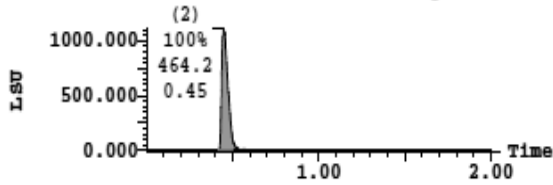
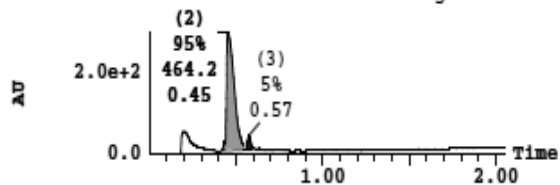




2: UV Detector: TIC

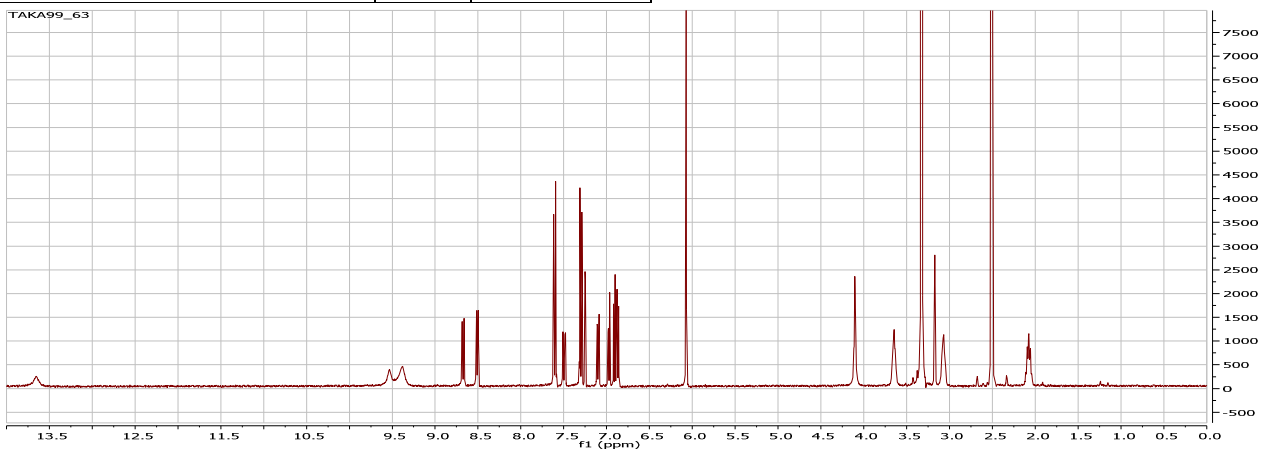
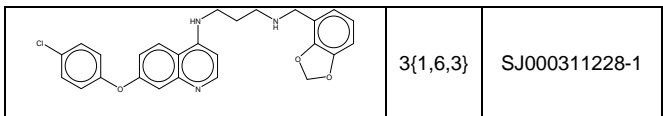
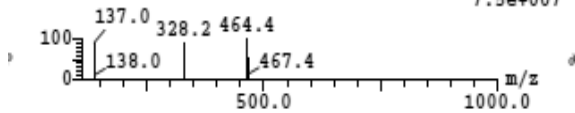
2.953e+2 (2) ELSD signal  
Range: 2.953e+2

1110.261  
Range: 1110.172



Peak ID	Compound	Time	Mass Found
2	Found	0.44	464.17

1:MS ES+  
7.5e+007

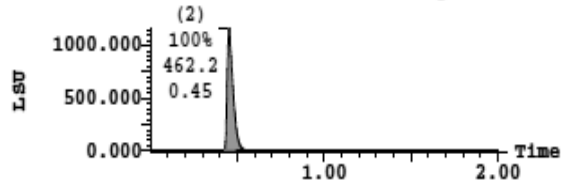
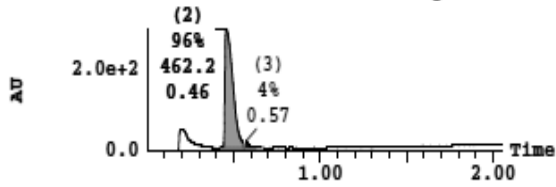


2: UV Detector: TIC

2.996e+2  
Range: 2.996e+2

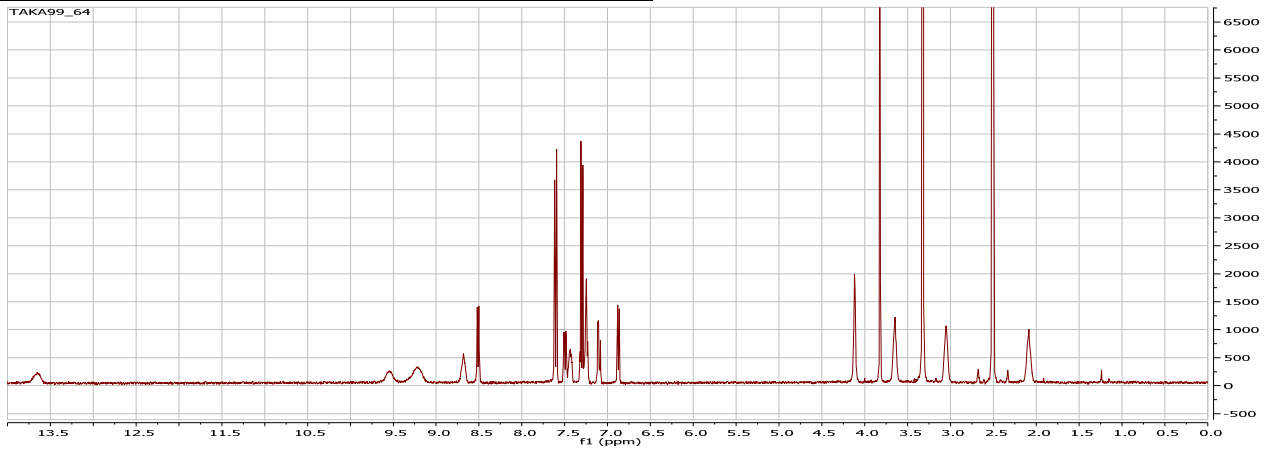
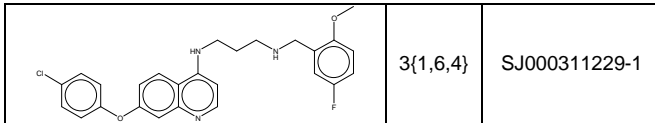
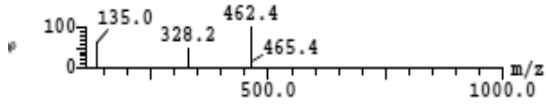
(2) ELSD Signal

1162.589  
Range: 1162.543



Peak ID	Compound	Time	Mass Found
2	Found	0.45	462.15

1:MS ES+  
8.5e+007

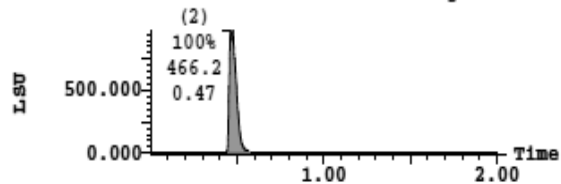
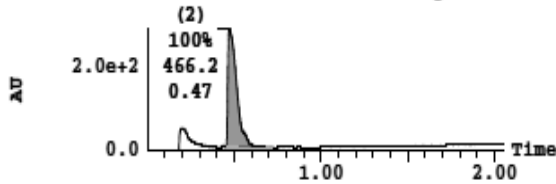


2: UV Detector: TIC

2.908e+2  
Range: 2.908e+2

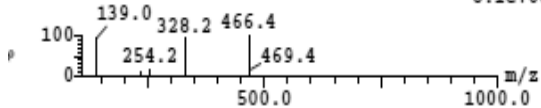
(2) ELSD signal

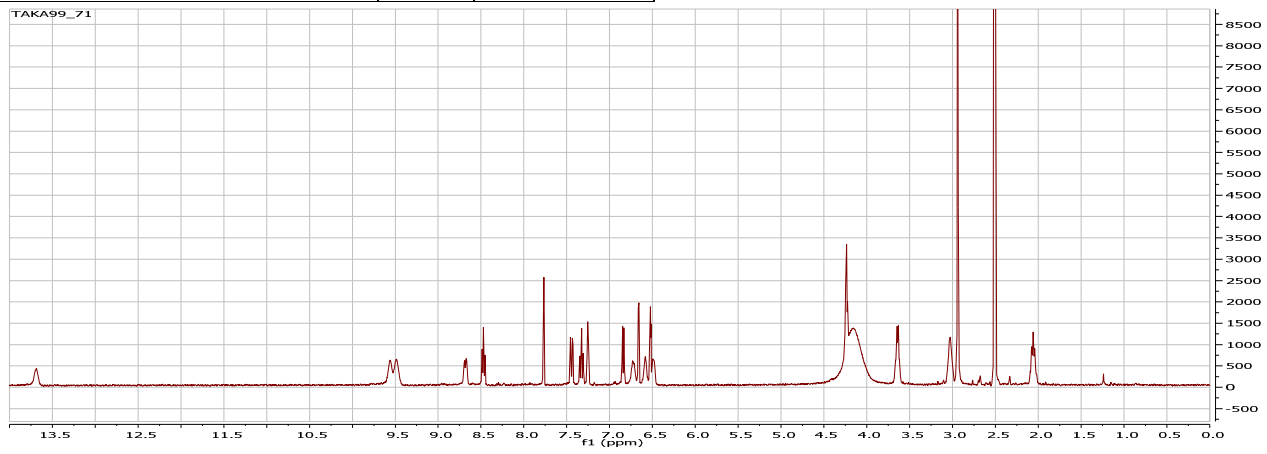
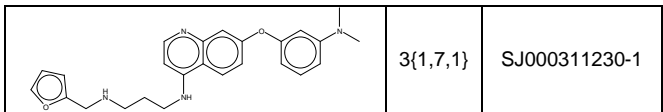
975.362  
Range: 975.216



Peak ID	Compound	Time	Mass Found
2	Found	0.48	466.16

1:MS ES+  
8.1e+007



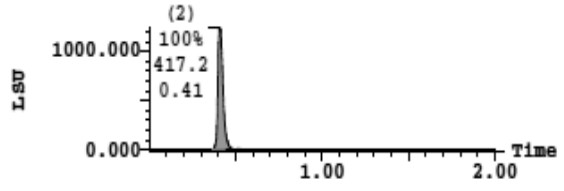
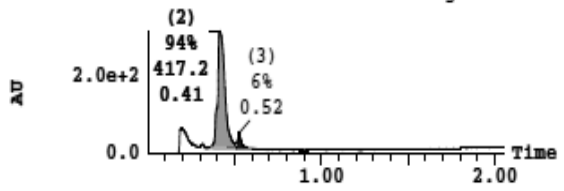


2: UV Detector: TIC

3.11e+2  
Range: 3.11e+2

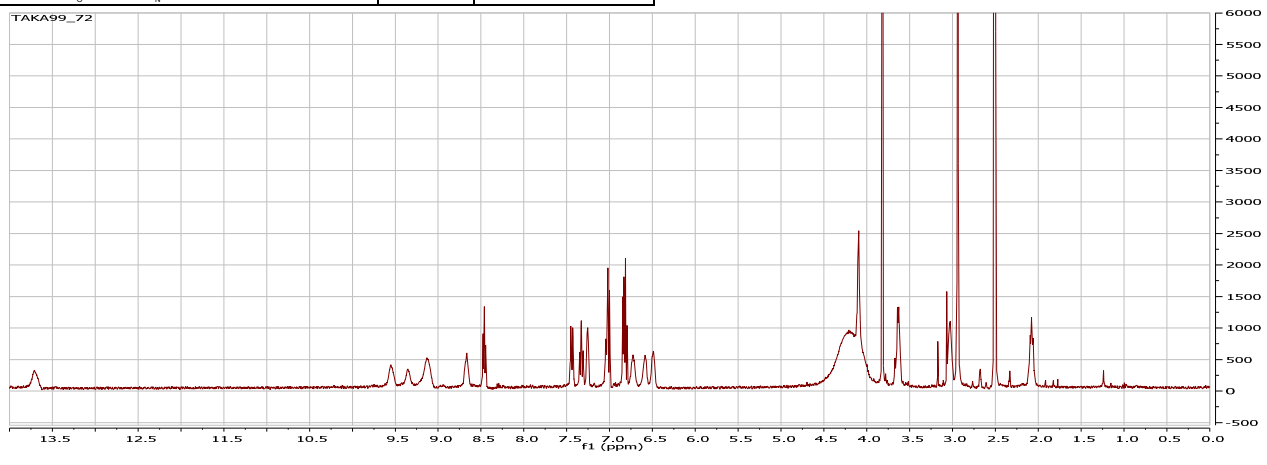
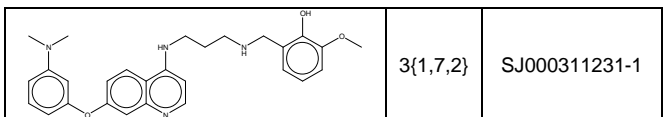
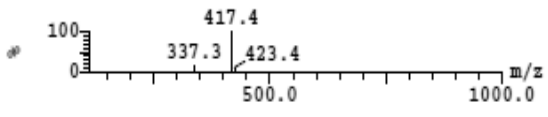
(2) ELSD signal

1241.109  
Range: 1241.084



Peak ID	Compound	Time	Mass Found
2	Found	0.39	417.22

1:MS ES+  
7.3e+007

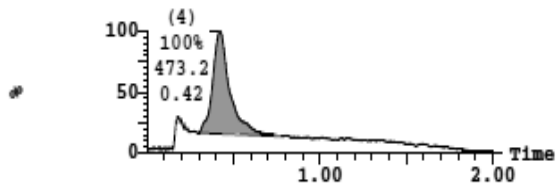
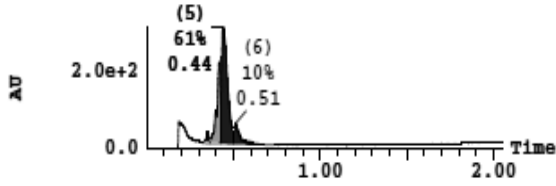


2: UV Detector: TIC

3.132e+2  
Range: 3.132e+2

1: MS ES+ :TIC

9.2e+00

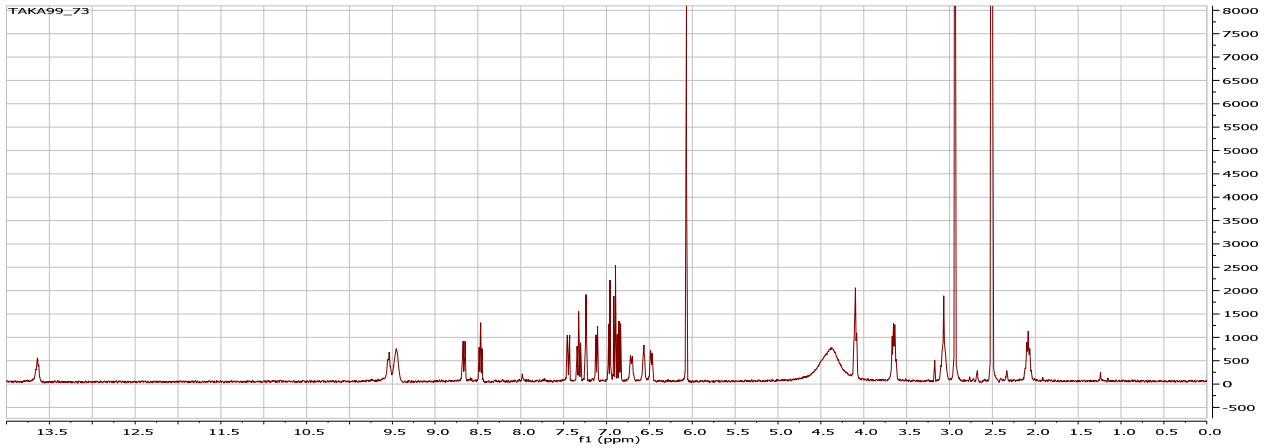
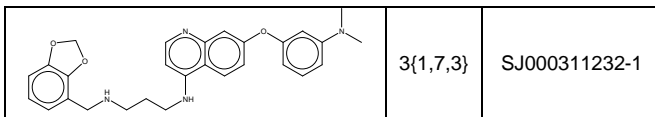
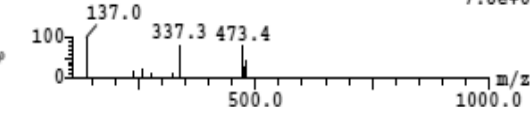
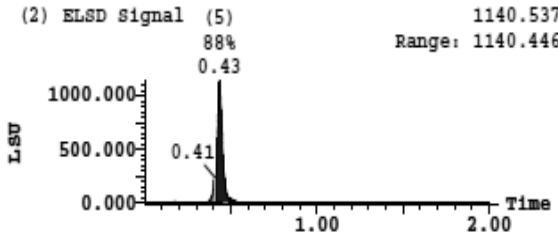


(2) ELSD Signal

1140.537  
Range: 1140.446

Peak ID	Compound	Time	Mass Found
4	Found	0.42	473.25

1:MS ES+  
7.8e+007

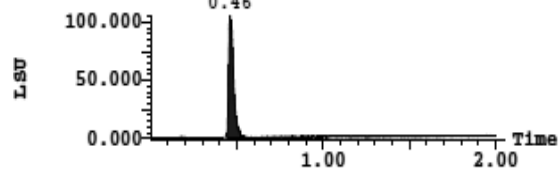
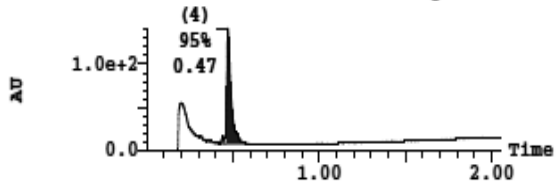


2: UV Detector: TIC

1.408e+2  
Range: 1.408e+2

(2) ELSD signal

105.344  
Range: 105.324

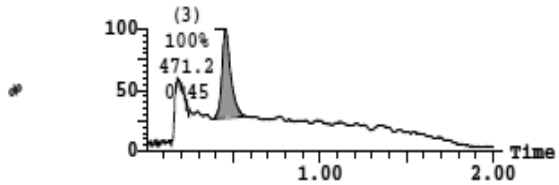
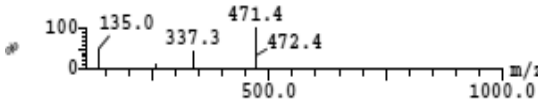


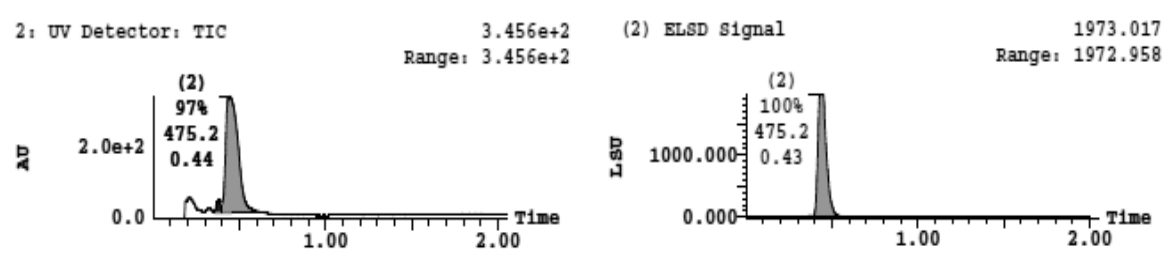
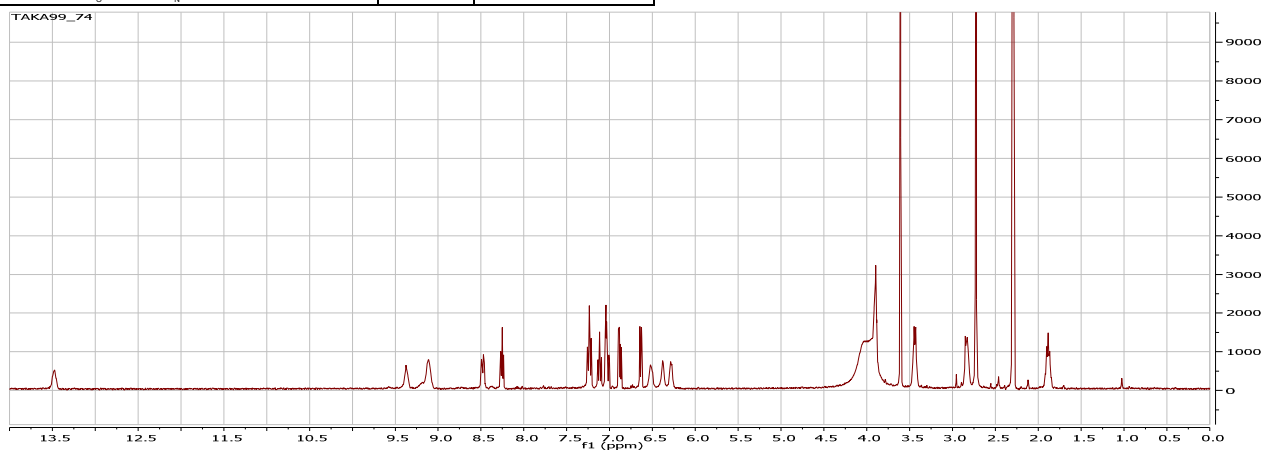
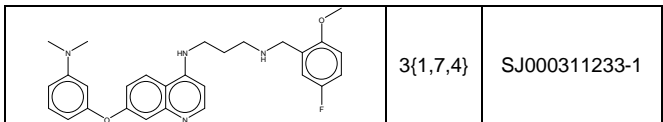
Peak ID	Compound	Time	Mass Found
3	Found	0.45	471.23

1:MS ES+  
4.5e+007

1: MS ES+ :TIC

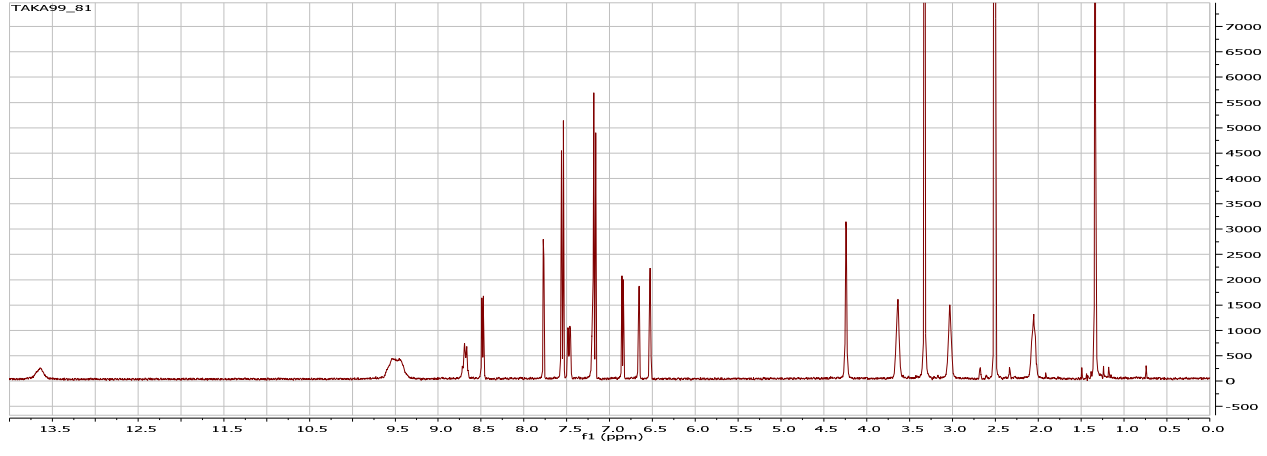
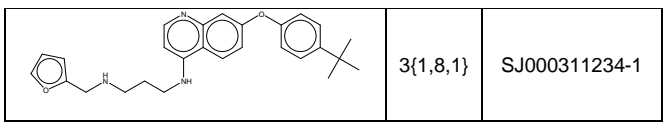
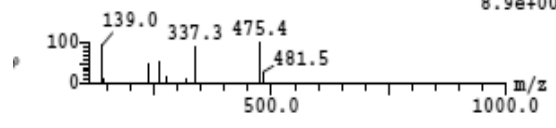
4.6e+009





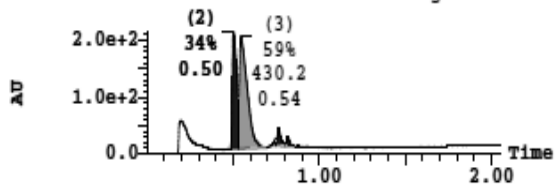
Peak ID	Compound	Time	Mass Found
2	Found	0.42	475.24

1:MS ES+  
8.9e+007

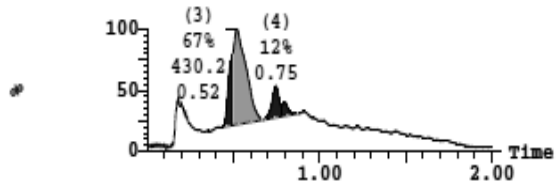




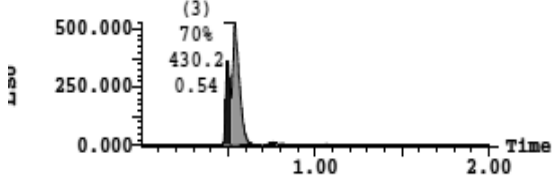
2: UV Detector: TIC 2.157e+2  
Range: 2.157e+2



1: MS ES+ :TIC 5.6e+009

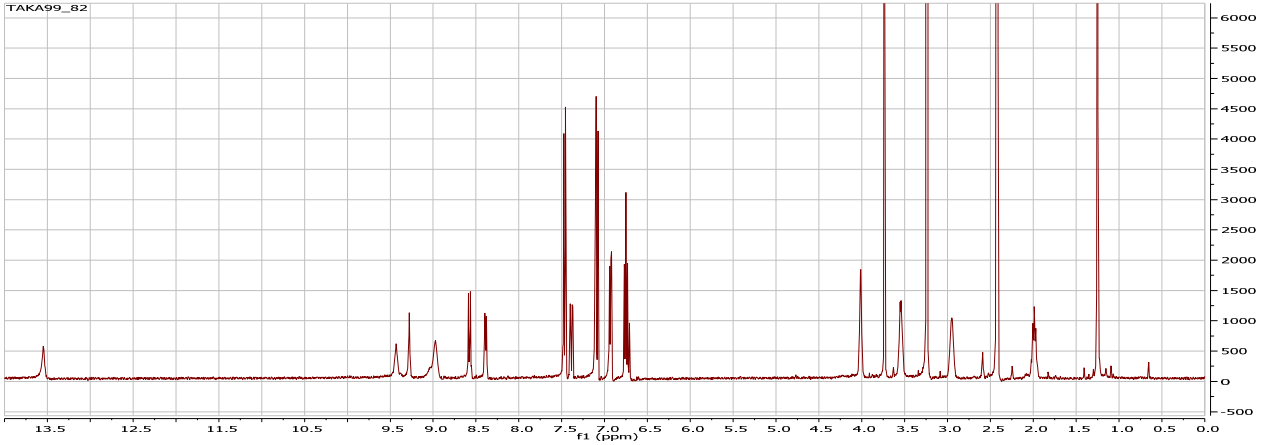
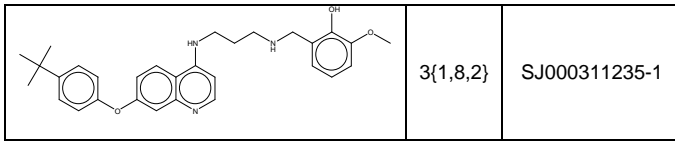
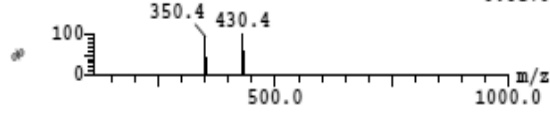


(2) ELSD signal 526.063  
Range: 525.984

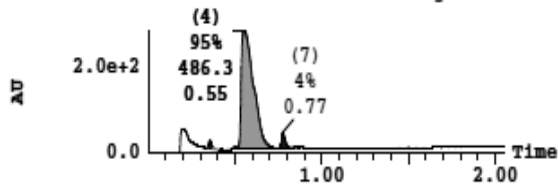


Peak ID	Compound	Time	Mass Found
3	Found	0.52	430.24

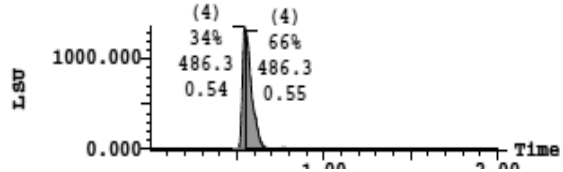
1:MS ES+  
6.8e+007



2: UV Detector: TIC 2.827e+2  
Range: 2.827e+2

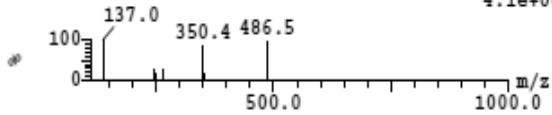


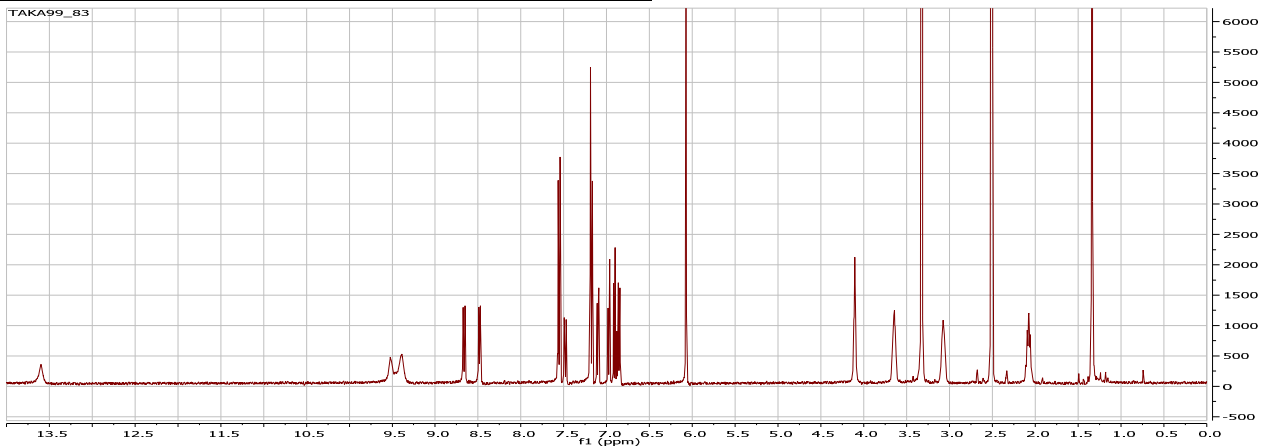
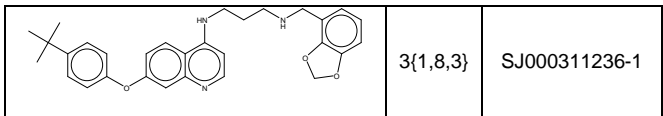
(2) ELSD Signal 1360.029  
Range: 1360.002



Peak ID	Compound	Time	Mass Found
5	Found	0.59	486.27

1:MS ES+  
4.1e+007



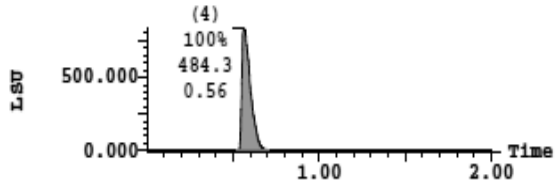
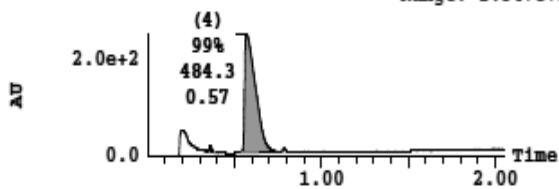


2: UV Detector: TIC

2.547e+2  
Range: 2.547e+2

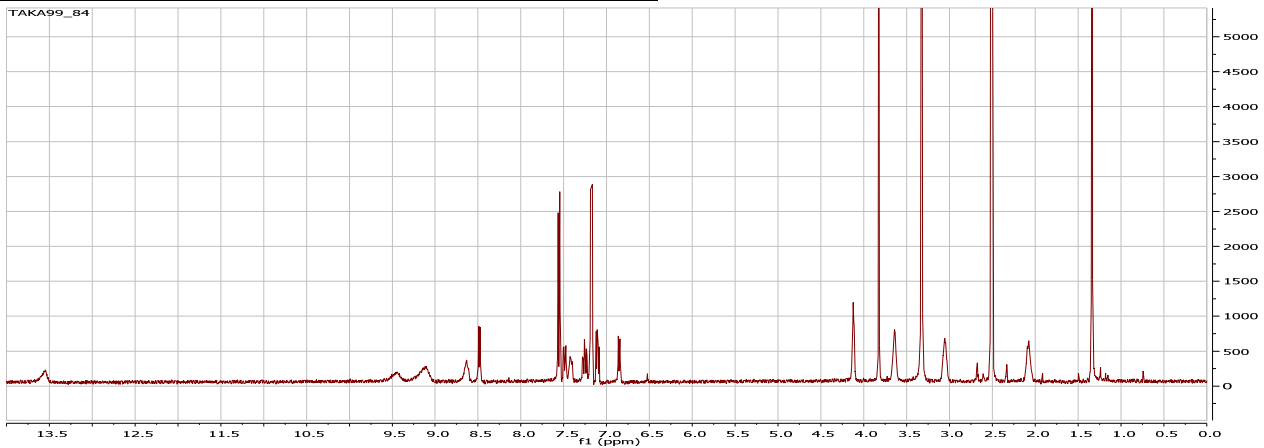
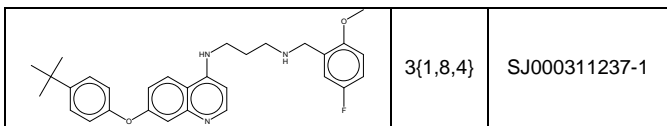
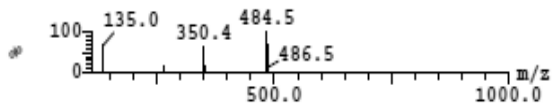
(2) ELSD Signal

834.972  
Range: 834.947

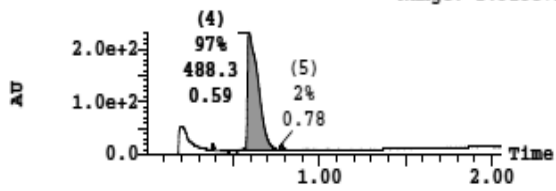


Peak ID	Compound	Time	Mass Found
4	Found	0.56	484.25

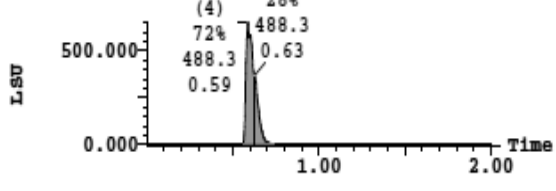
1:MS ES+  
1.1e+008



2: UV Detector: TIC 2.315e+2  
 Range: 2.315e+2

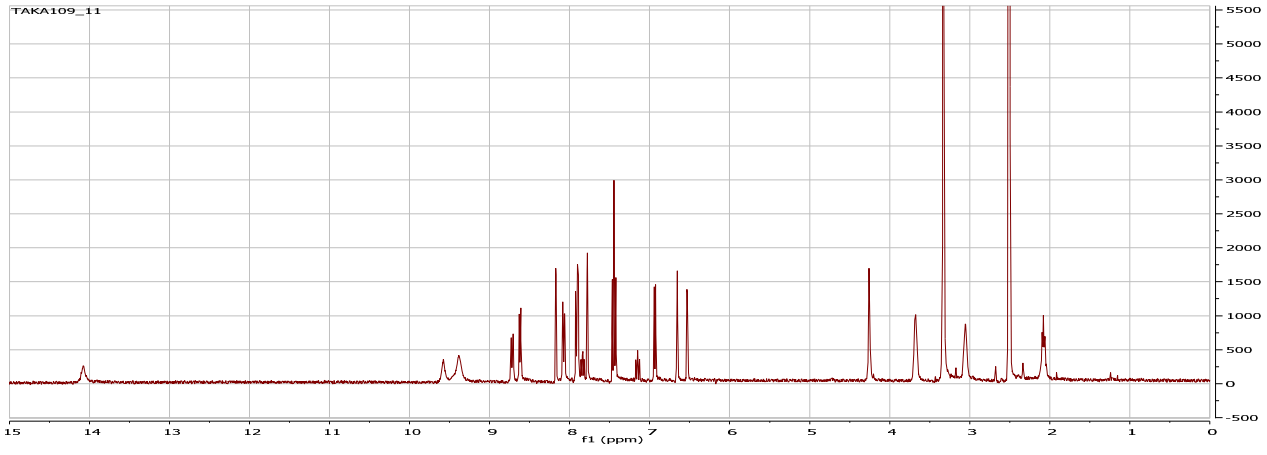
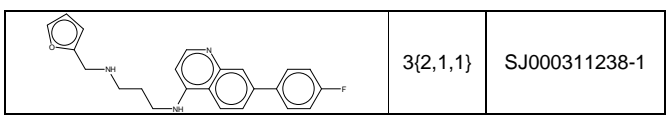
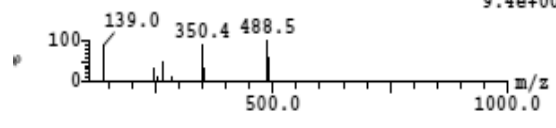


(2) ELSD Signal 651.556  
 Range: 651.530

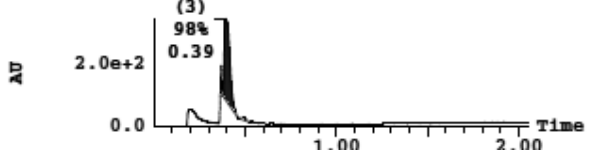


Peak ID	Compound	Time	Mass Found
4	Found	0.58	488.28

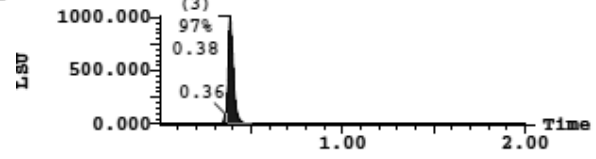
1:MS ES+  
 9.4e+007



2: UV Detector: TIC 3.471e+2  
 Range: 3.471e+2

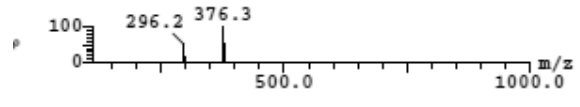


(2) ELSD Signal 1016.209  
 Range: 1016.169

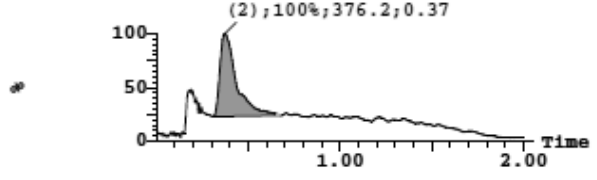


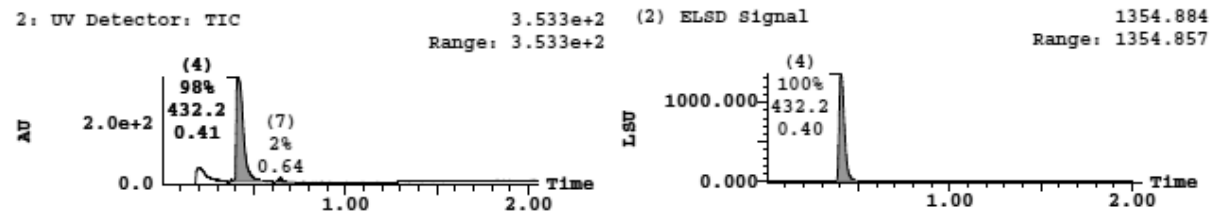
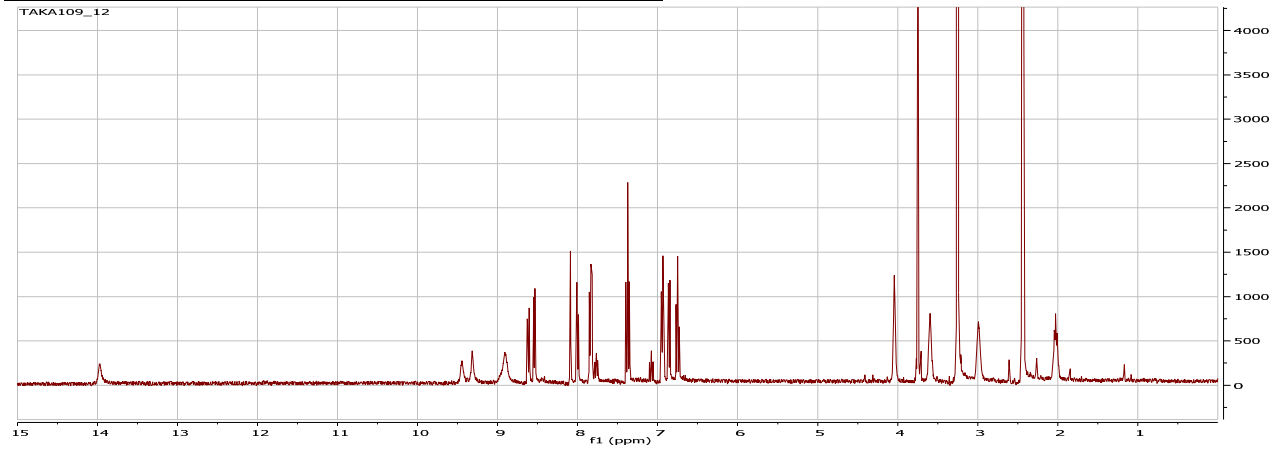
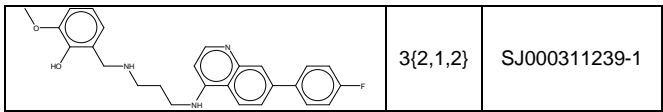
Peak ID	Compound	Time	Mass Found
2	Found	0.37	376.17

1:MS ES+  
 7.8e+007

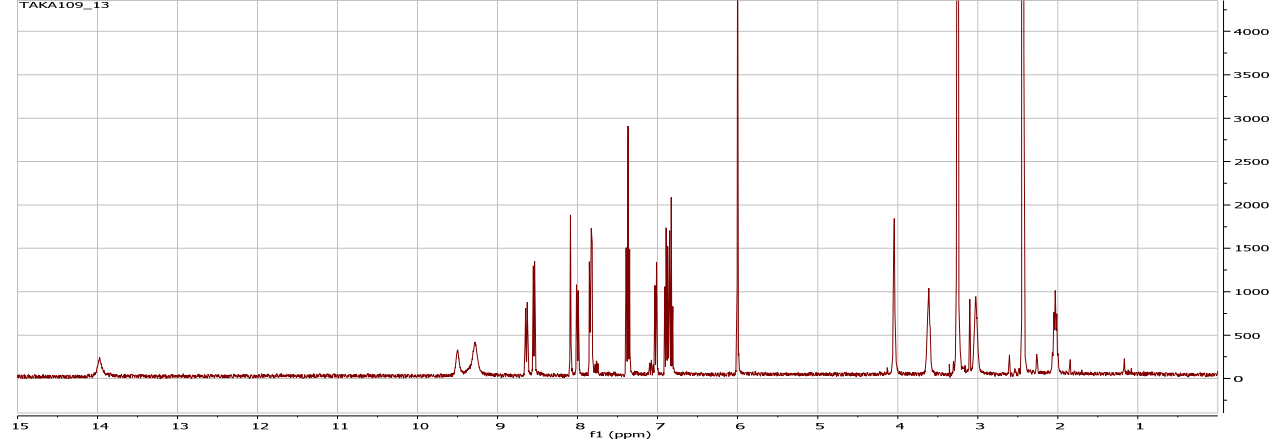
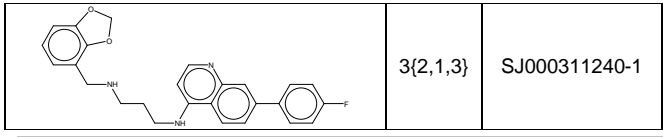
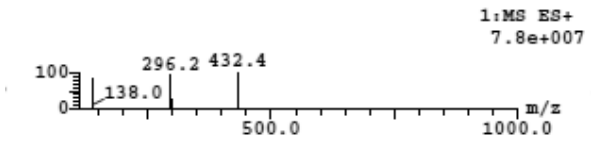


1: MS ES+ :TIC 4.8e+009 1:



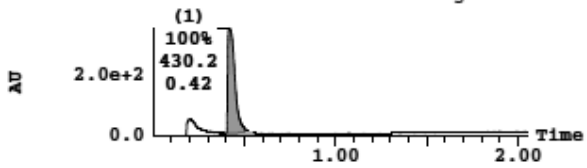


Peak ID	Compound	Time	Mass Found
4	Found	0.40	432.20



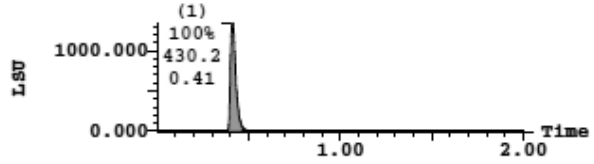
2: UV Detector: TIC

3.514e+2  
Range: 3.514e+2



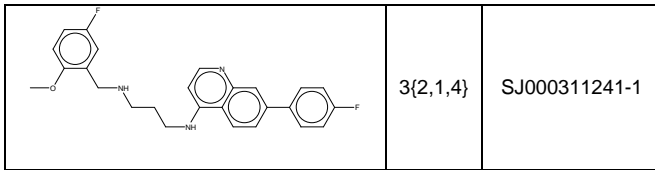
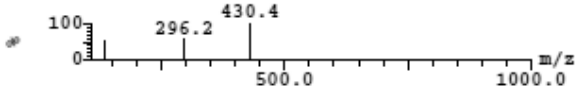
(2) ELSD Signal

1342.332  
Range: 1342.292

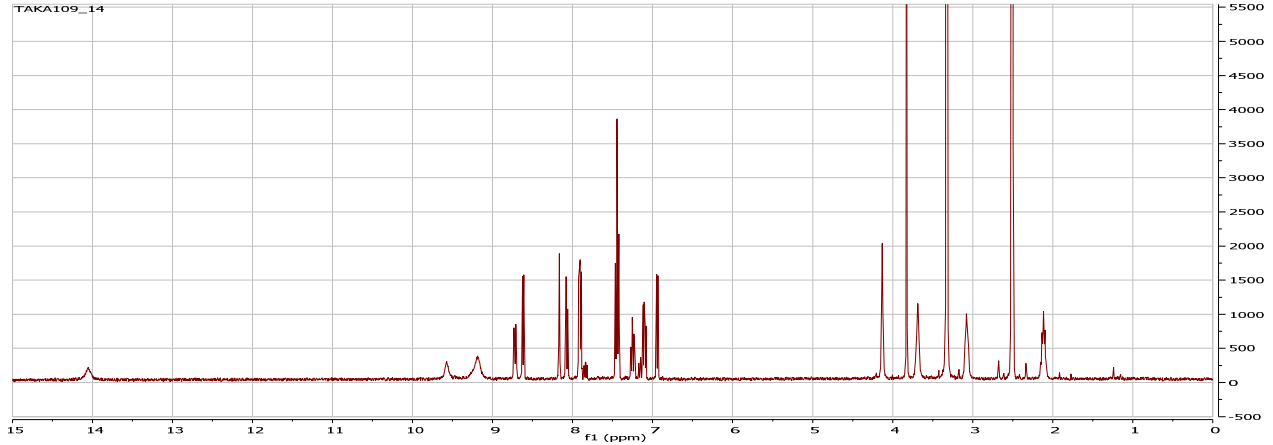


Peak ID	Compound	Time	Mass Found
1	Found	0.40	430.19

1:MS ES+  
8.6e+007

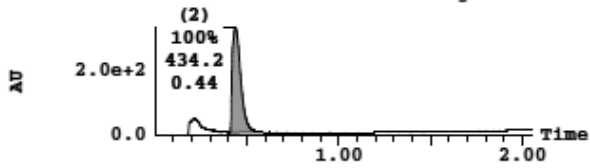


TAKA109\_14



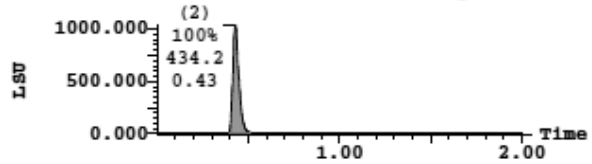
2: UV Detector: TIC

3.368e+2  
Range: 3.368e+2



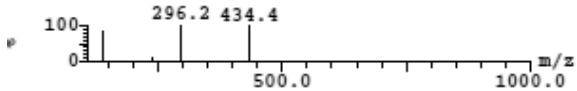
(2) ELSD Signal

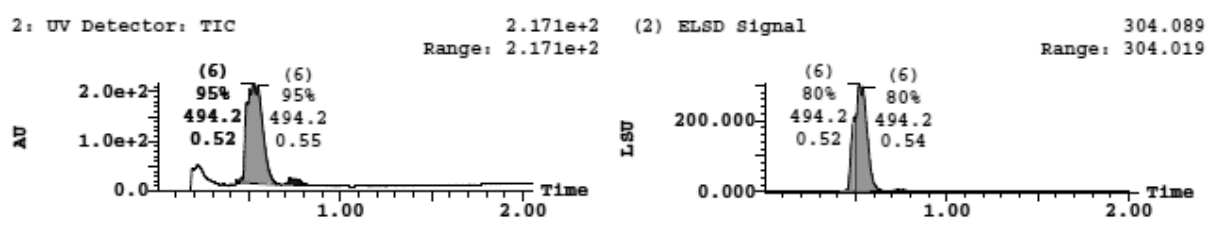
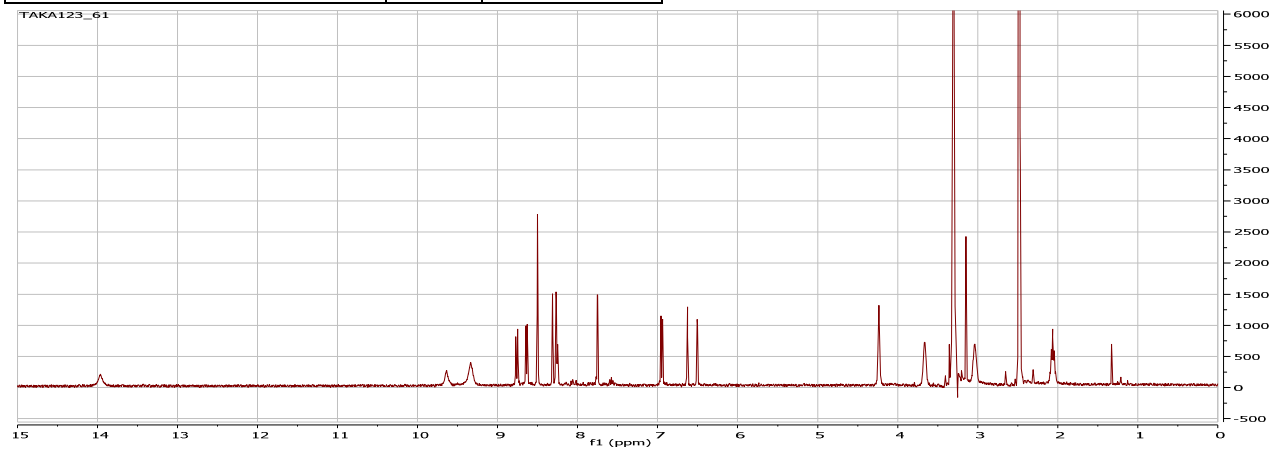
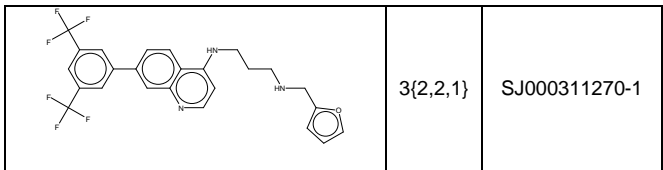
1039.268  
Range: 1039.247



Peak ID	Compound	Time	Mass Found
2	Found	0.42	434.20

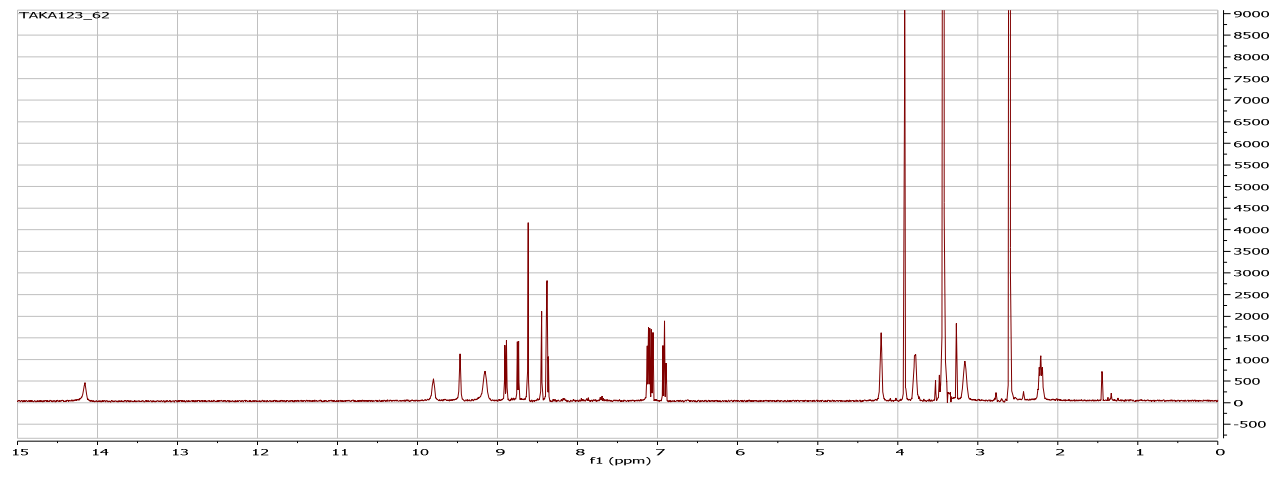
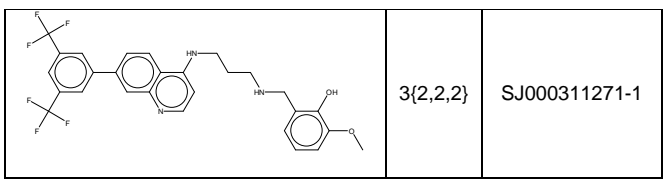
1:MS ES+  
9.3e+007





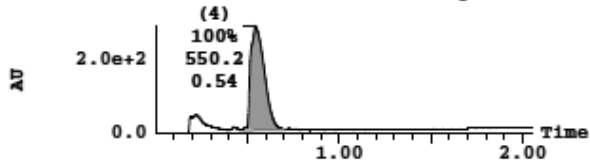
Peak ID	Compound	Time	Mass Found
6	Found	0.50	494.16

1:MS ES+  
8.0e+007



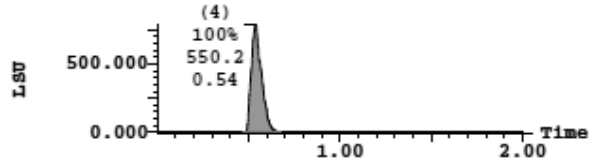
2: UV Detector: TIC

2.933e+2  
Range: 2.933e+2



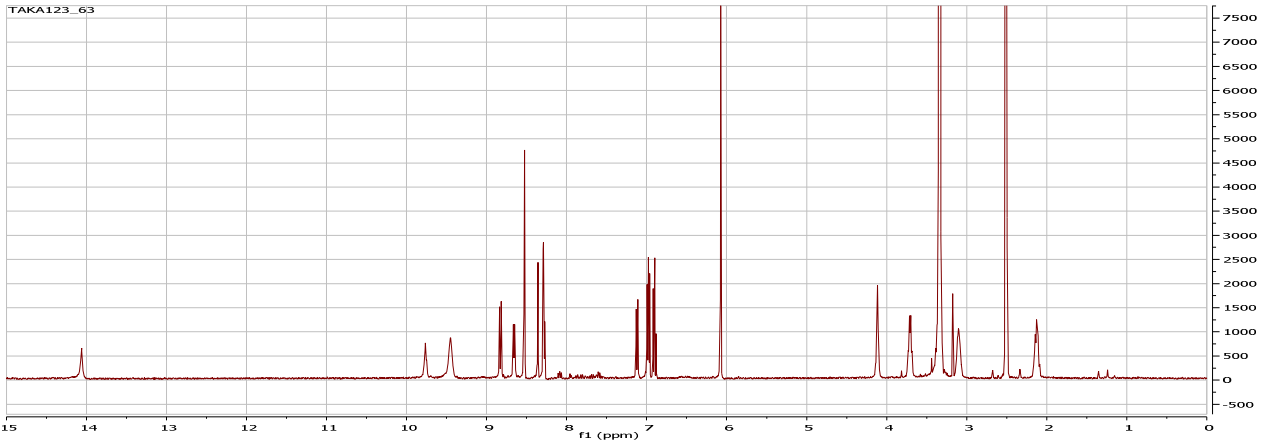
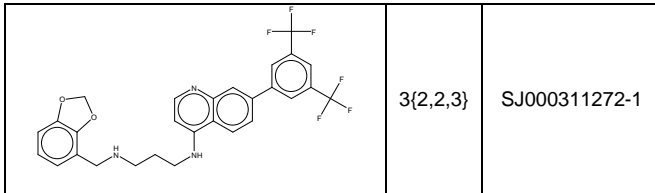
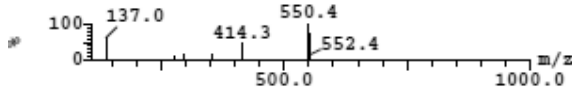
(2) ELSD Signal

785.831  
Range: 785.634



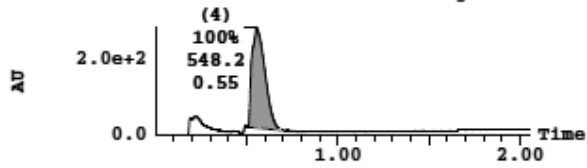
Peak ID	Compound	Time	Mass Found
4	Found	0.53	550.19

1:MS ES+  
1.2e+008



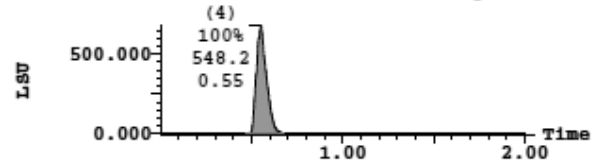
2: UV Detector: TIC

2.858e+2  
Range: 2.858e+2



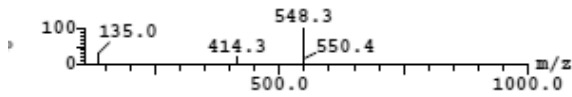
(2) ELSD Signal

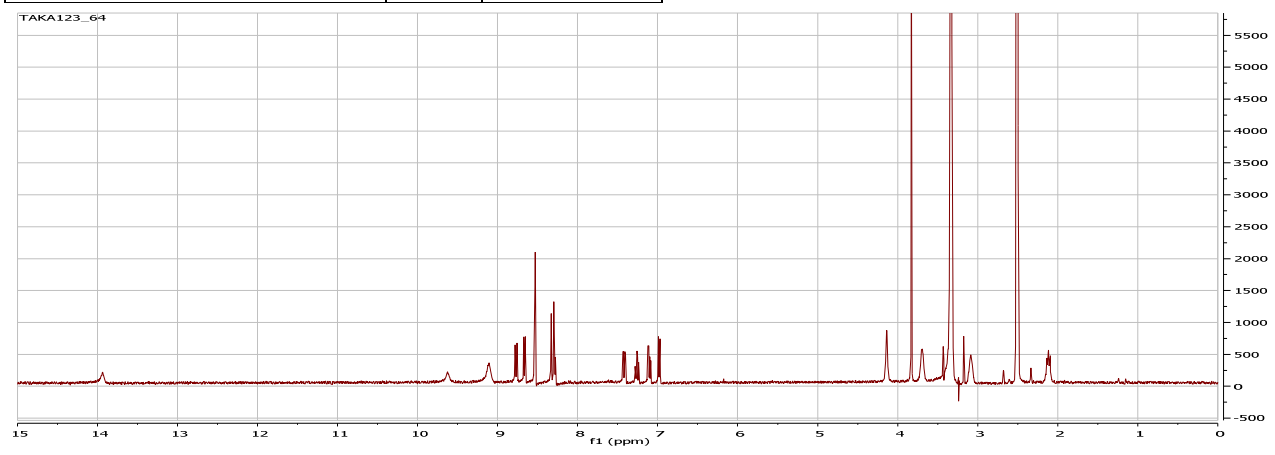
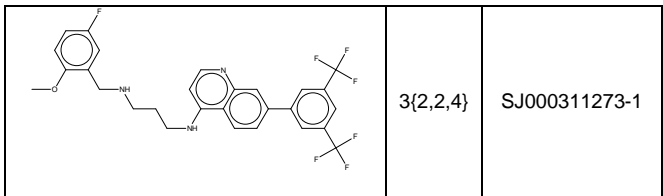
681.303  
Range: 681.248



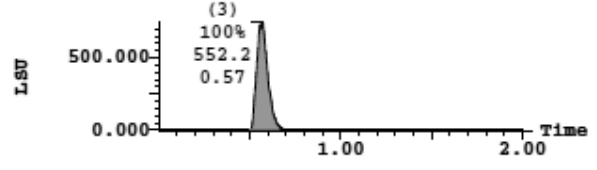
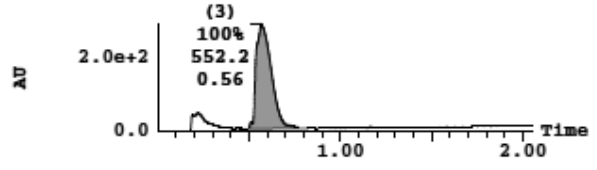
Peak ID	Compound	Time	Mass Found
4	Found	0.54	548.17

1:MS ES+  
1.3e+008



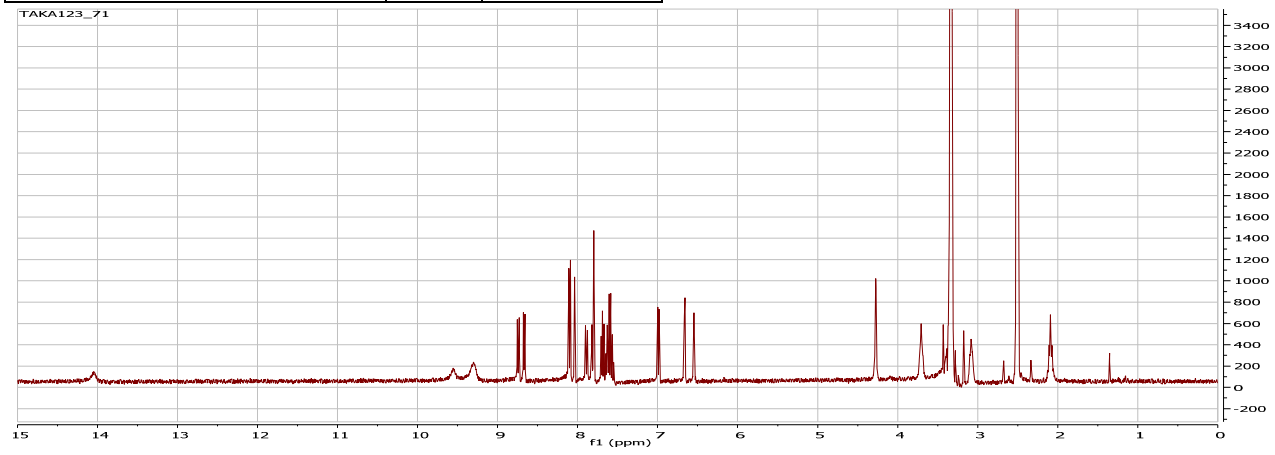
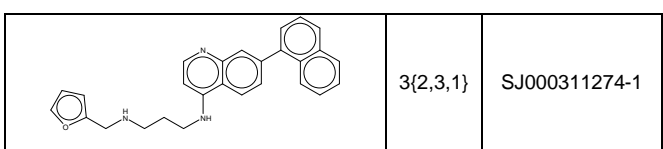
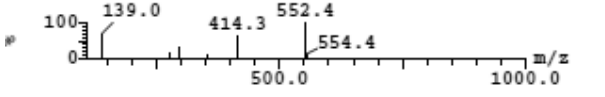


2: UV Detector: TIC 2.932e+2 (2) ELSD Signal 747.933  
 Range: 2.932e+2 Range: 747.850



Peak ID	Compound	Time	Mass Found
3	Found	0.56	552.18

1: MS ES+  
1.2e+008



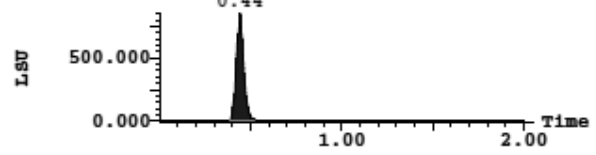
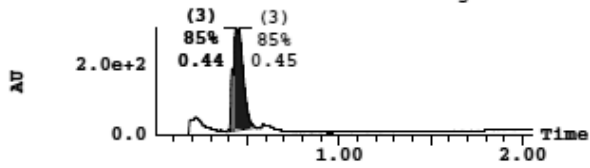


2: UV Detector: TIC

3.092e+2  
Range: 3.092e+2

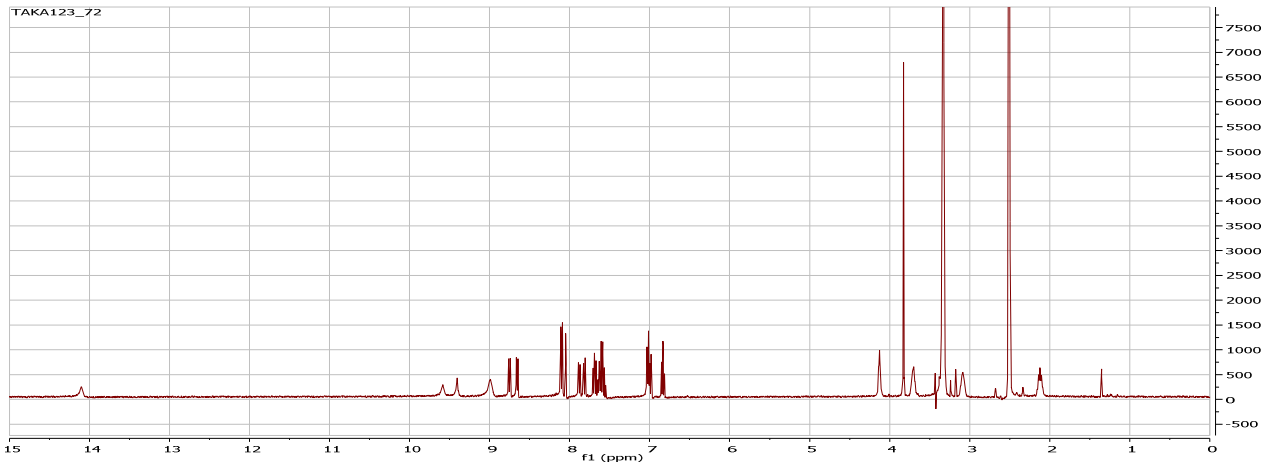
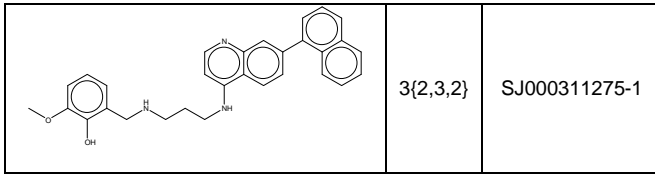
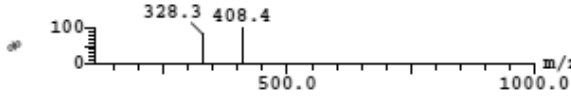
(2) ELSD signal (3)

852.270  
Range: 852.211



Peak ID	Compound	Time	Mass Found
2	Found	0.42	408.20

1:MS ES+  
7.9e+007

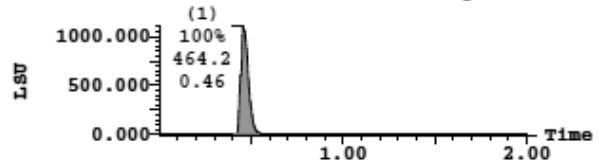
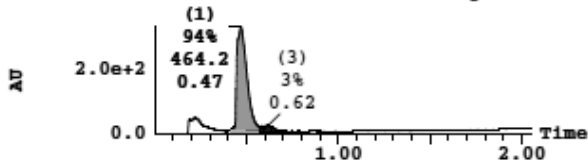


2: UV Detector: TIC

3.291e+2  
Range: 3.291e+2

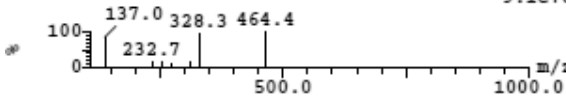
(2) ELSD signal

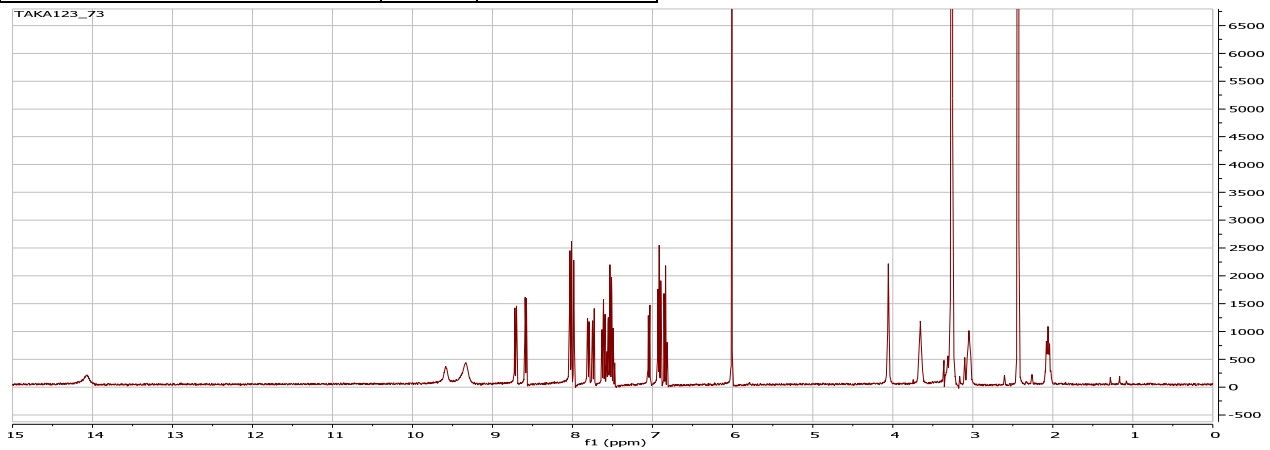
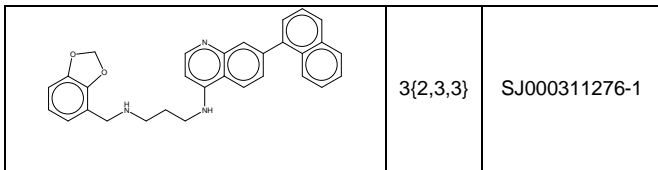
1108.180  
Range: 1108.003



Peak ID	Compound	Time	Mass Found
1	Found	0.45	464.23

1:MS ES+  
9.1e+007



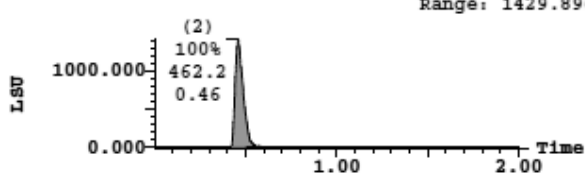
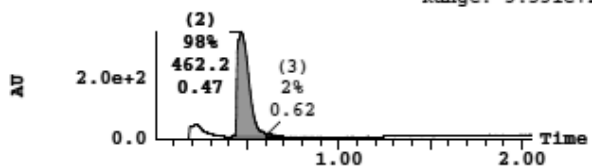


2: UV Detector: TIC

3.531e+2  
Range: 3.531e+2

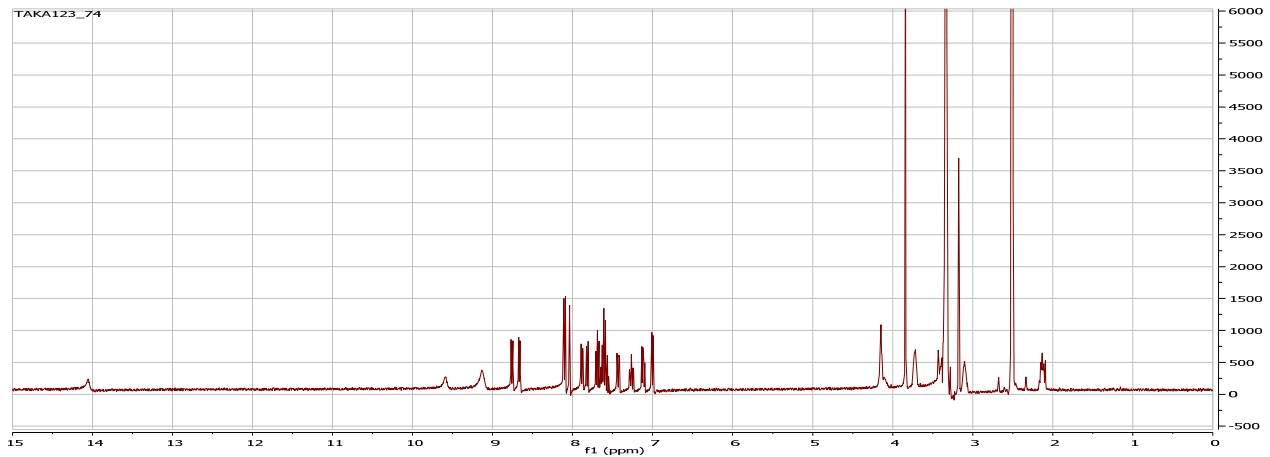
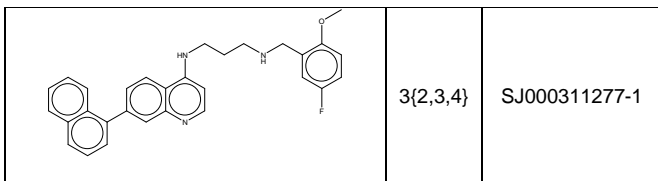
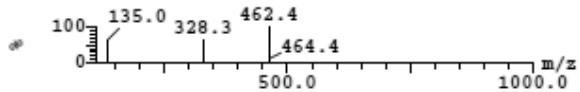
(2) ELSD Signal

1429.924  
Range: 1429.896



Peak ID	Compound	Time	Mass Found
2	Found	0.45	462.21

1:MS ES+  
1.1e+008

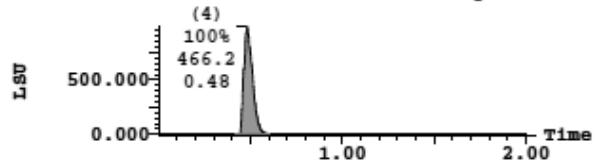
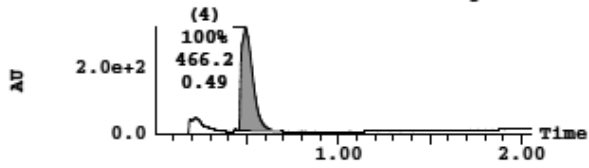


2: UV Detector: TIC

3.28e+2  
Range: 3.28e+2

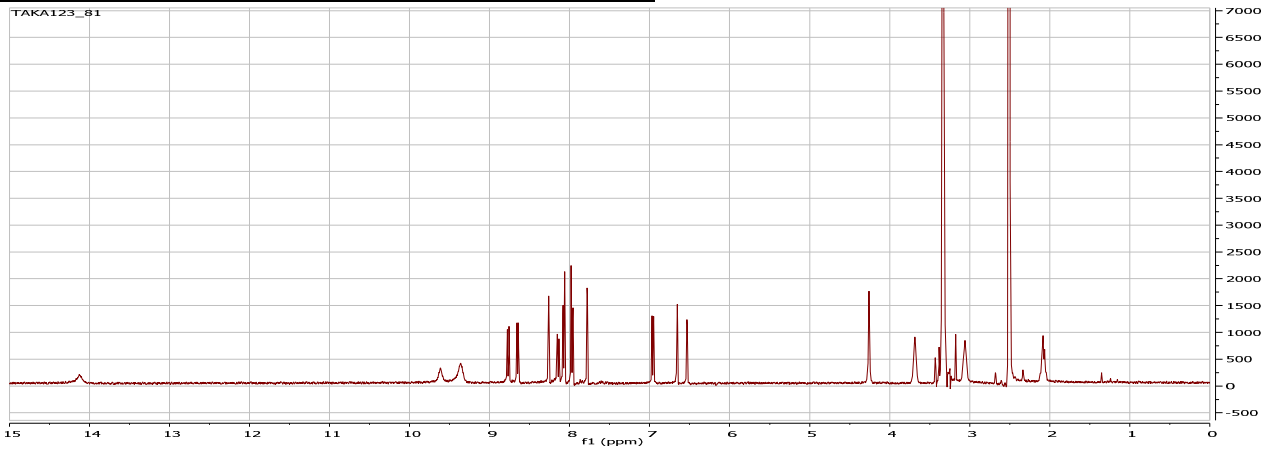
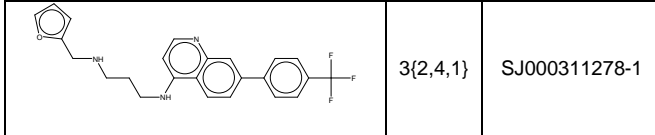
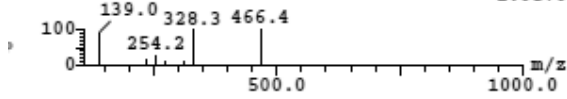
(2) ELSD Signal

989.378  
Range: 989.348



Peak ID	Compound	Time	Mass Found
4	Found	0.47	466.22

1:MS ES+  
1.0e+008

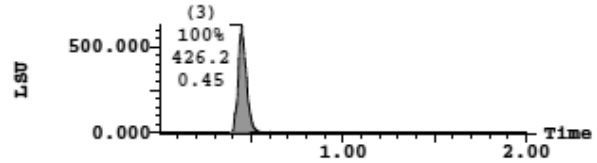
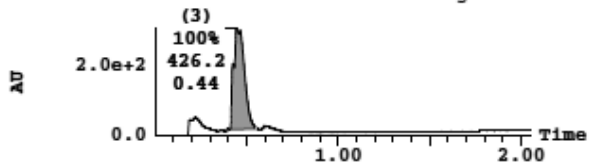


2: UV Detector: TIC

3.077e+2  
Range: 3.077e+2

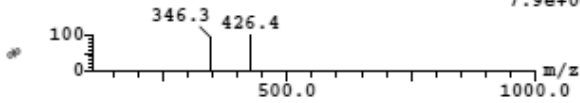
(2) ELSD Signal

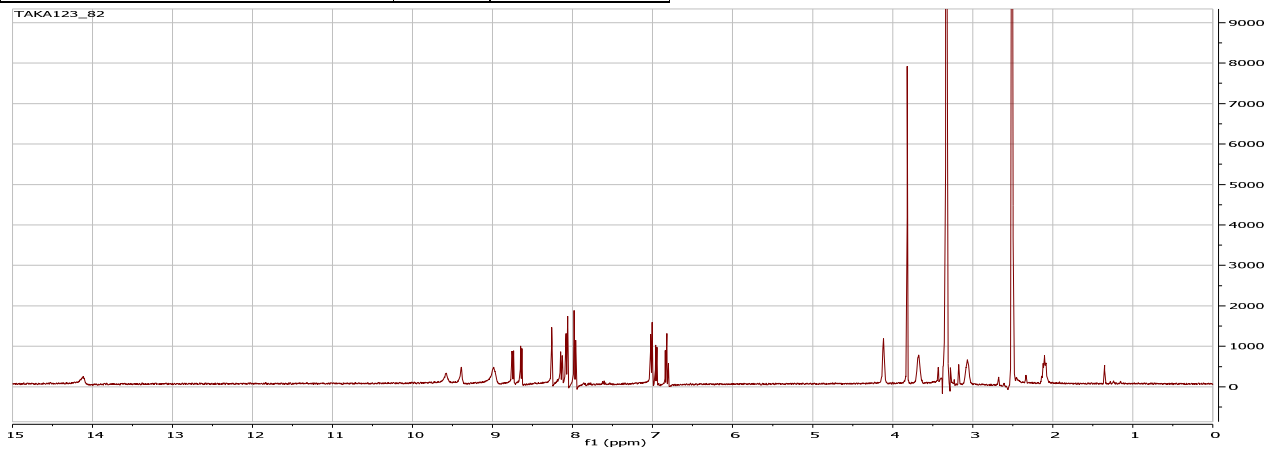
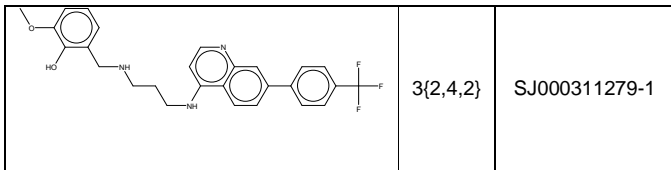
627.190  
Range: 627.102



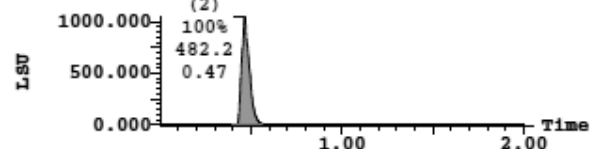
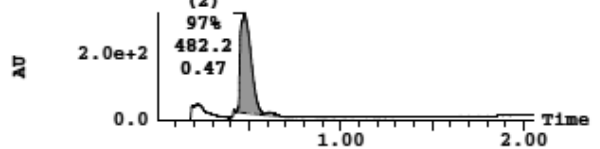
Peak ID	Compound	Time	Mass Found
3	Found	0.43	426.17

1:MS ES+  
7.9e+007



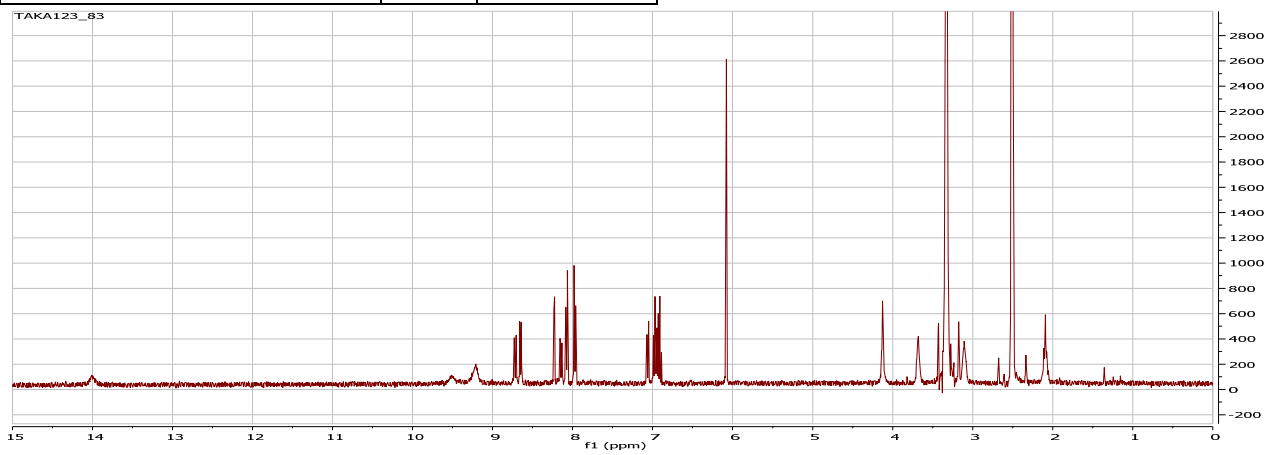
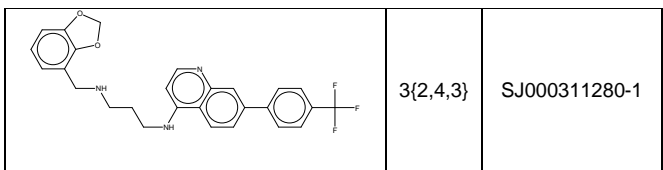
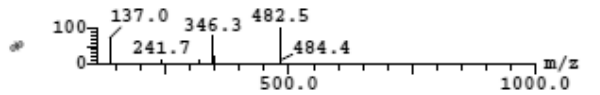


2: UV Detector: TIC 3.229e+2 (2) ELSD signal 1046.748  
Range: 3.229e+2 Range: 1046.727



Peak ID	Compound	Time	Mass Found
2	Found	0.45	482.20

1: MS ES+  
9.8e+007

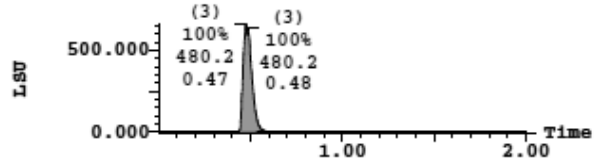
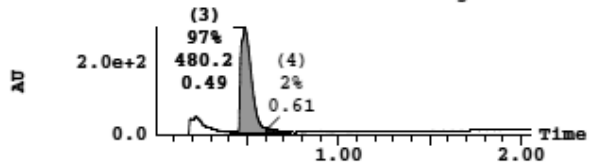


2: UV Detector: TIC

3.014e+2  
Range: 3.014e+2

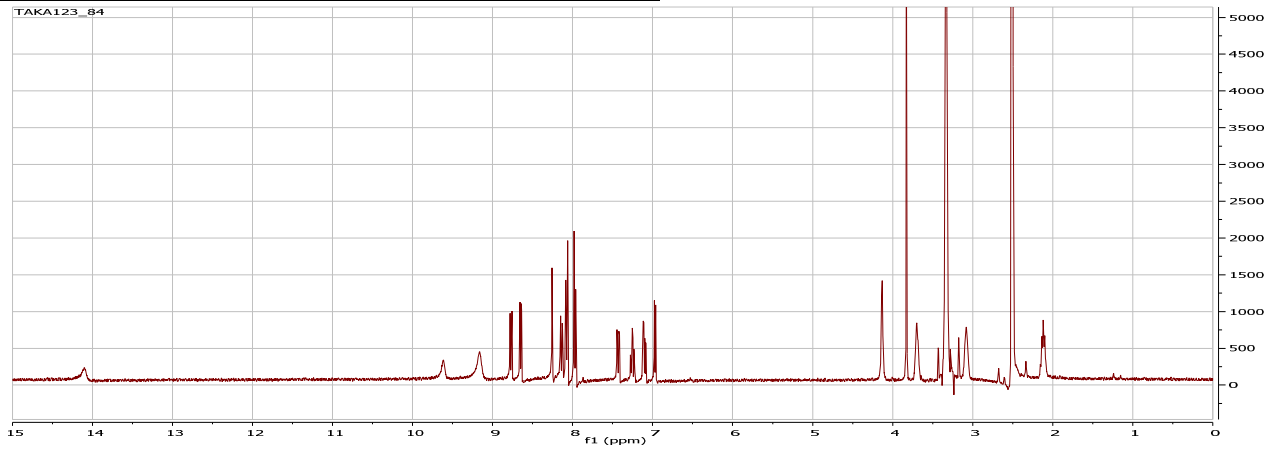
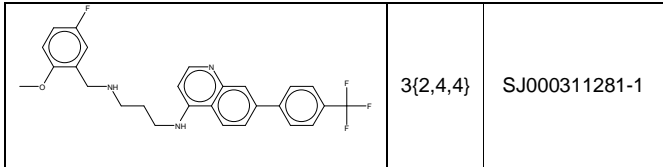
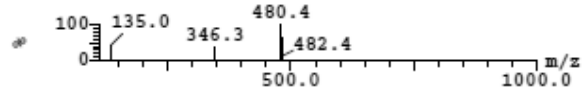
(2) ELSD Signal

660.448  
Range: 660.421



Peak ID	Compound	Time	Mass Found
3	Found	0.46	480.18

1:MS ES+  
1.1e+008

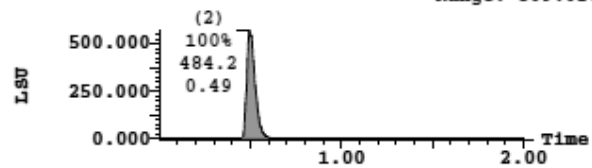
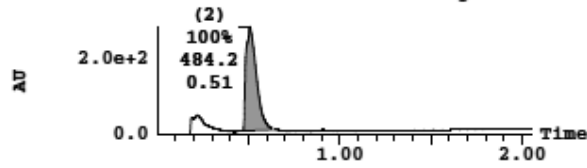


2: UV Detector: TIC

2.818e+2  
Range: 2.818e+2

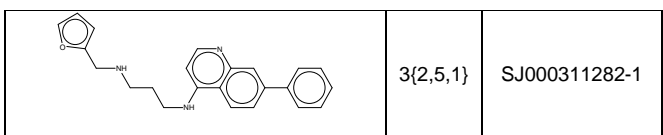
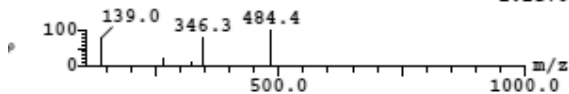
(2) ELSD Signal

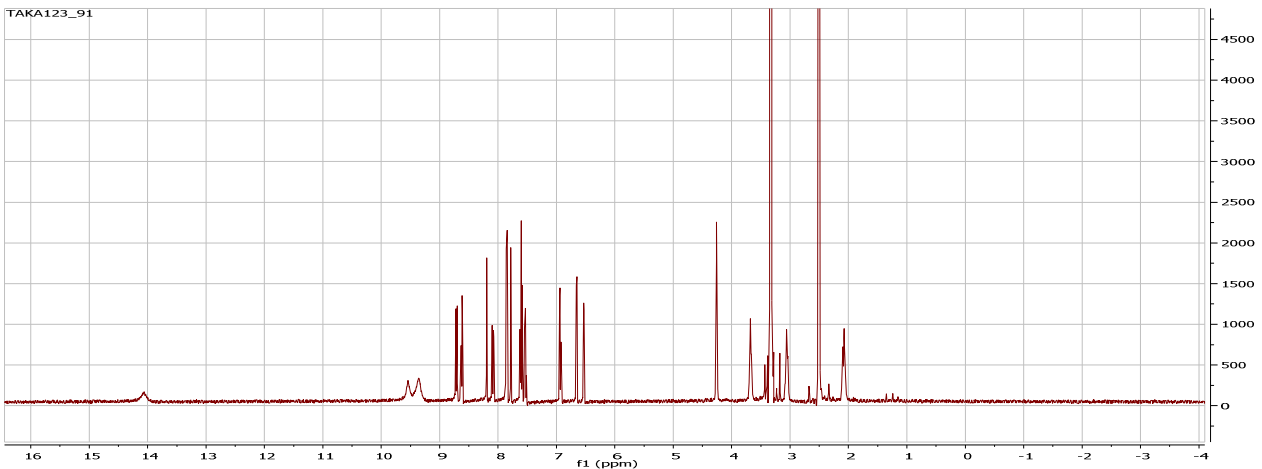
569.739  
Range: 569.620



Peak ID	Compound	Time	Mass Found
2	Found	0.49	484.19

1:MS ES+  
1.1e+008



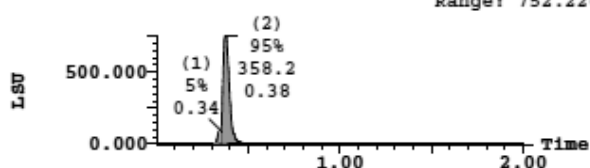
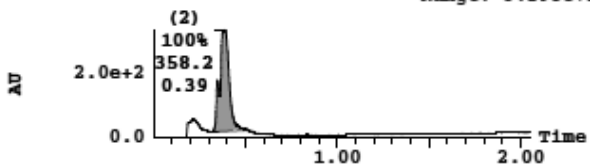


2: UV Detector: TIC

3.295e+2  
Range: 3.295e+2

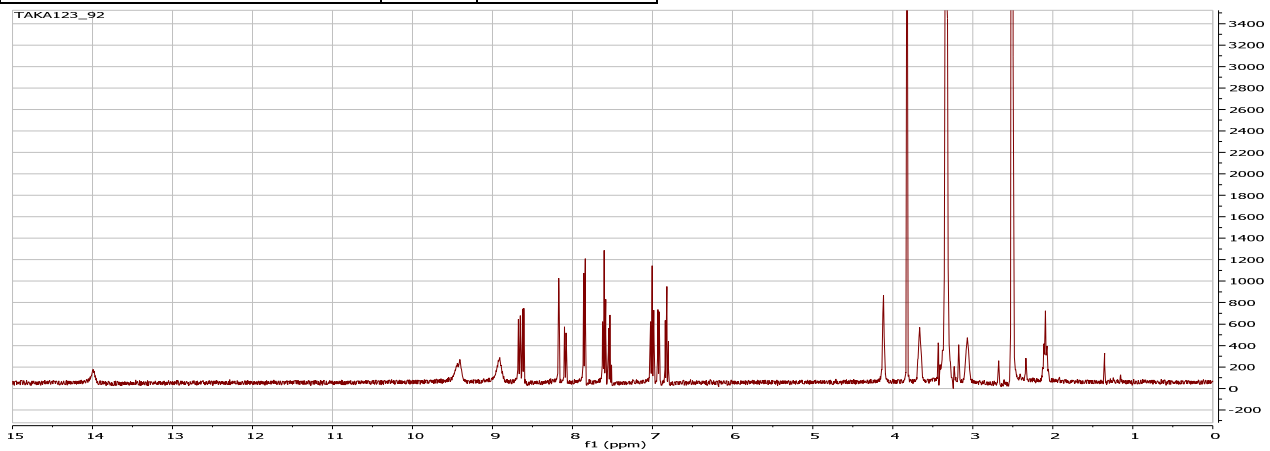
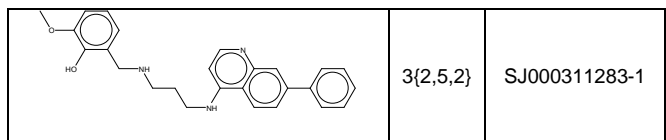
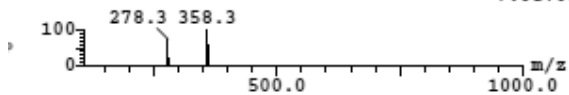
(2) ELSD signal

752.256  
Range: 752.226



Peak ID	Compound	Time	Mass Found
2	Found	0.38	358.18

1: MS ES+  
7.6e+007

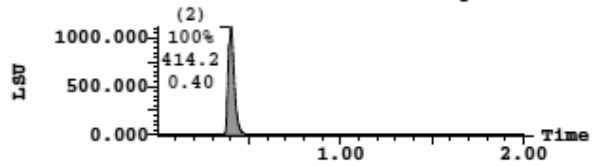
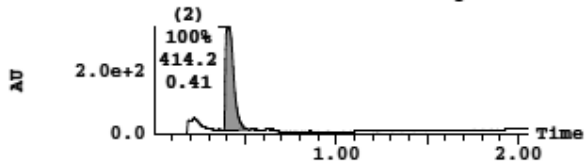


2: UV Detector: TIC

3.419e+2  
Range: 3.419e+2

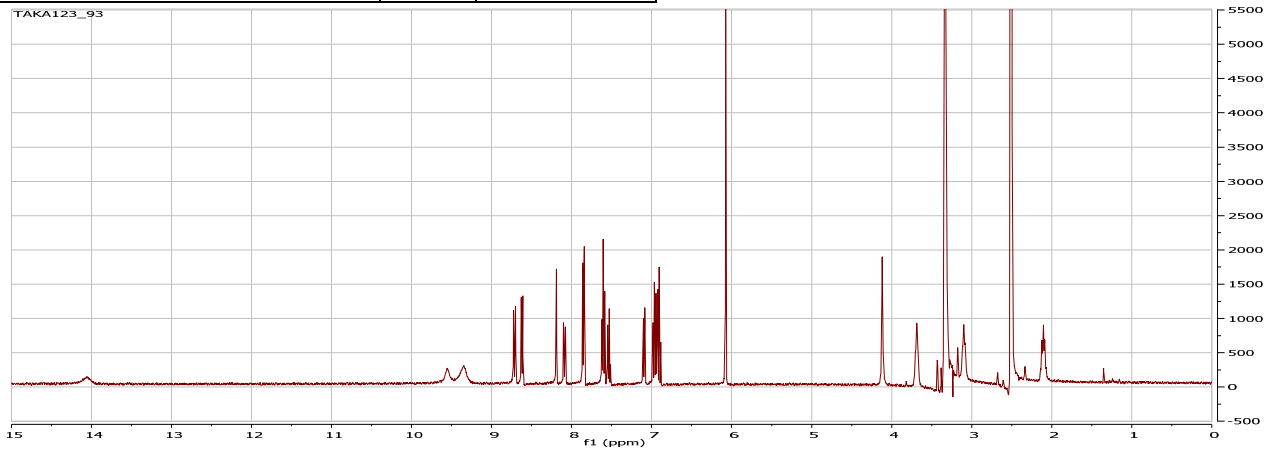
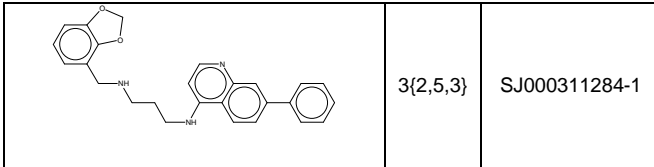
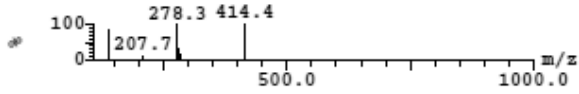
(2) ELSD Signal

1111.511  
Range: 1111.445



Peak ID	Compound	Time	Mass Found
2	Found	0.39	414.21

1:MS ES+  
8.1e+007

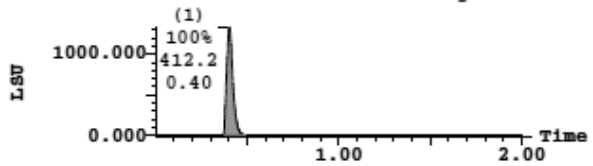
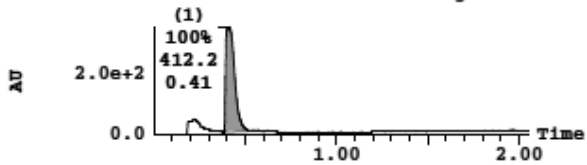


2: UV Detector: TIC

3.529e+2  
Range: 3.529e+2

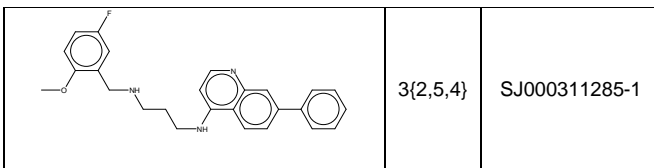
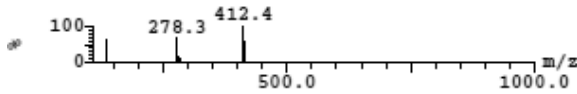
(2) ELSD Signal

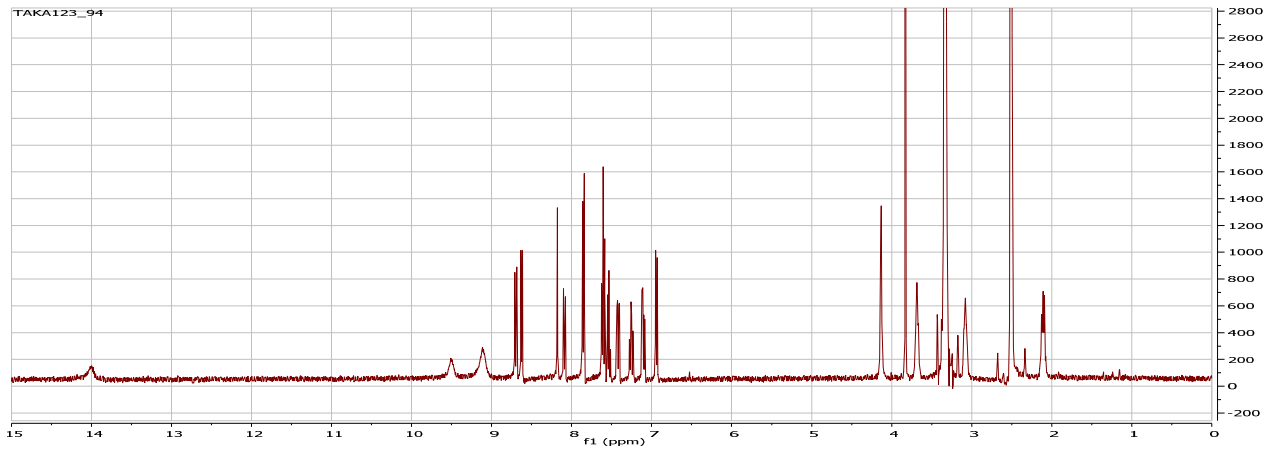
1330.226  
Range: 1330.159



Peak ID	Compound	Time	Mass Found
1	Found	0.39	412.19

1:MS ES+  
9.1e+007



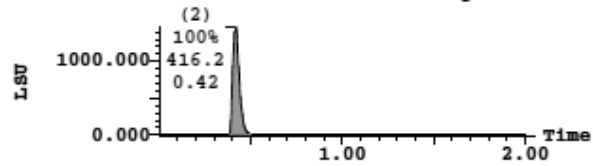
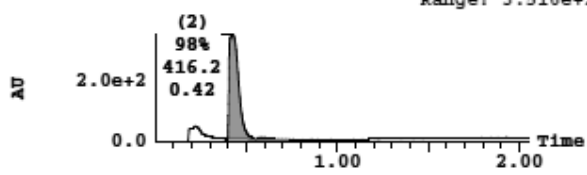


2: UV Detector: TIC

3.516e+2  
Range: 3.516e+2

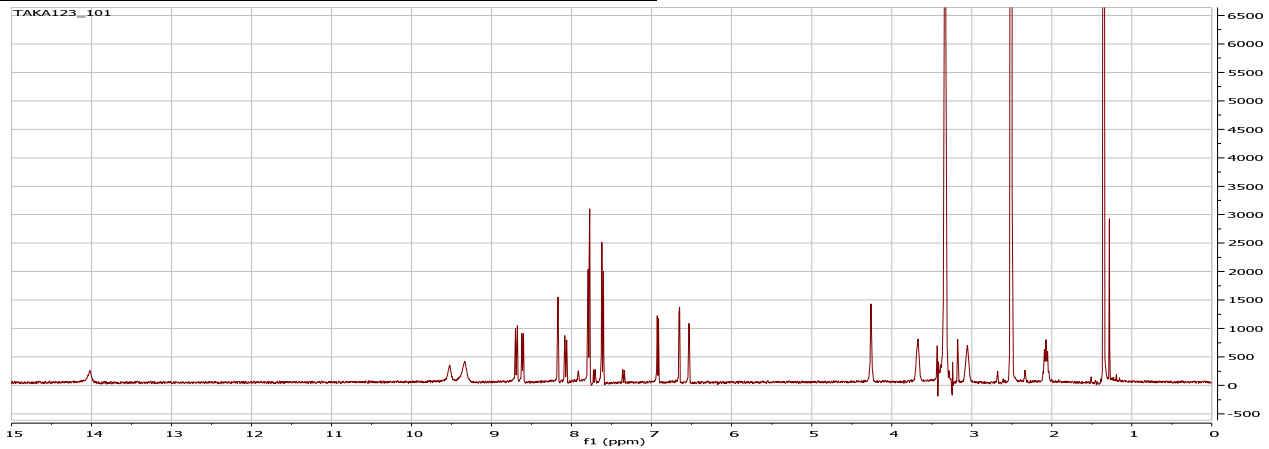
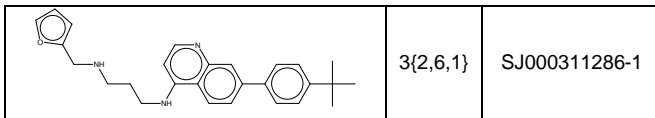
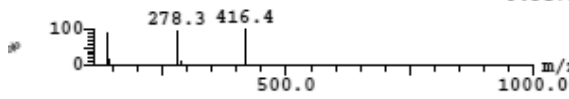
(2) ELSD Signal

1463.979  
Range: 1463.906



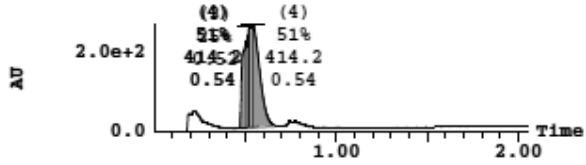
Peak ID	Compound	Time	Mass Found
2	Found	0.41	416.21

1:MS ES+  
9.3e+007

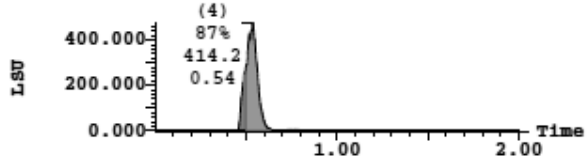




2: UV Detector: TIC 2.687e+2  
Range: 2.687e+2

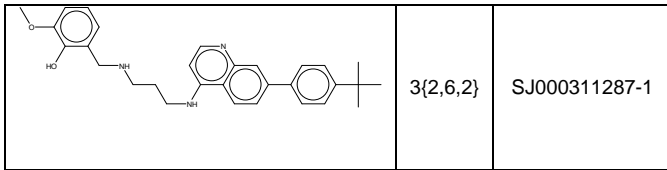
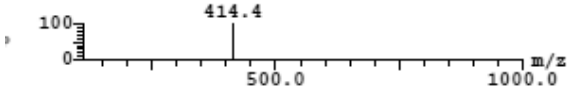


(2) ELSD Signal 474.544  
Range: 474.516

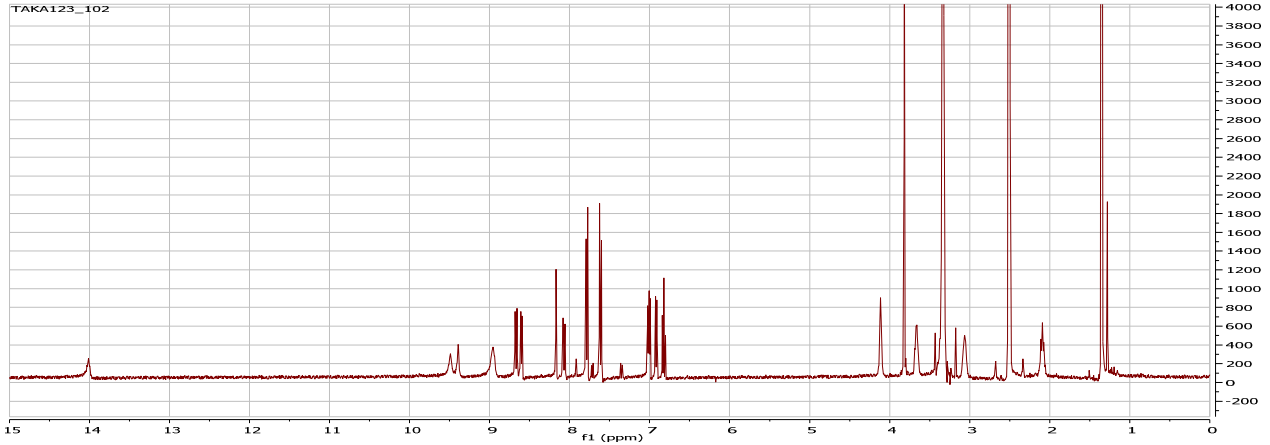


Peak ID	Compound Found	Time	Mass Found
4	Found	0.58	414.25

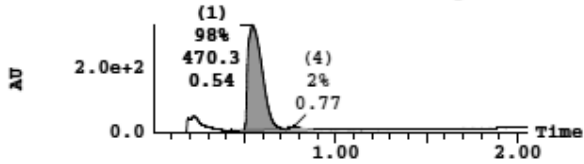
1:MS ES+  
8.0e+007



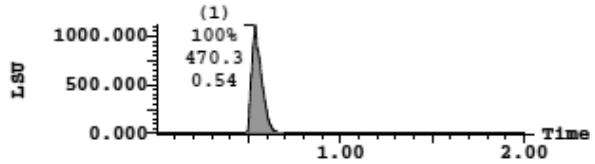
TAKA123\_102



2: UV Detector: TIC 3.321e+2  
Range: 3.321e+2

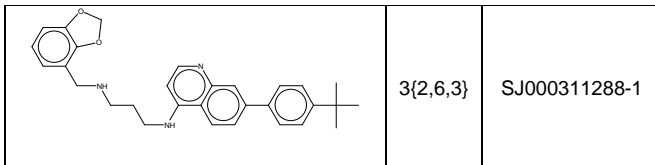
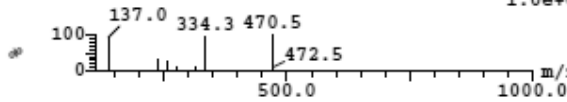


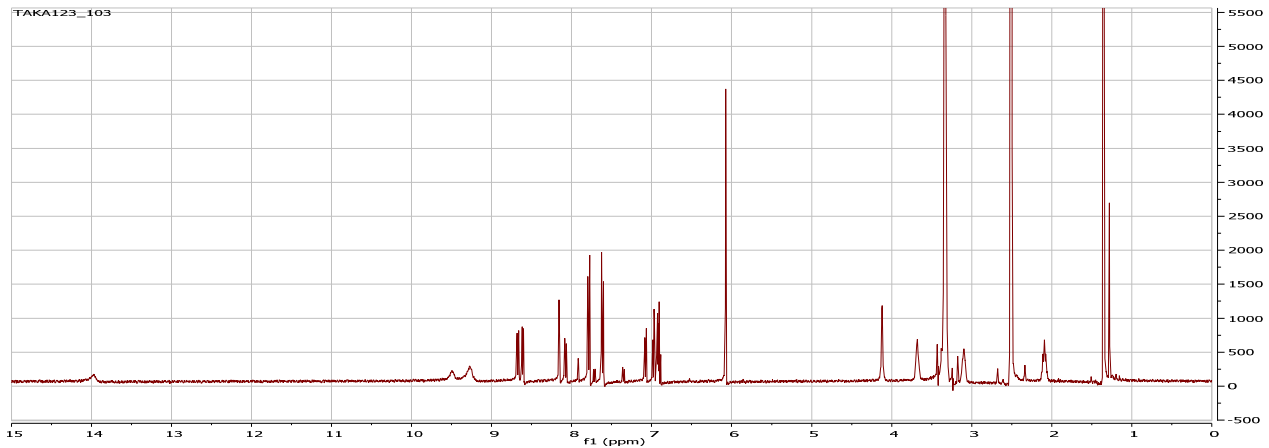
(2) ELSD Signal 1114.774  
Range: 1114.741



Peak ID	Compound Found	Time	Mass Found
1	Found	0.53	470.27

1:MS ES+  
1.0e+008



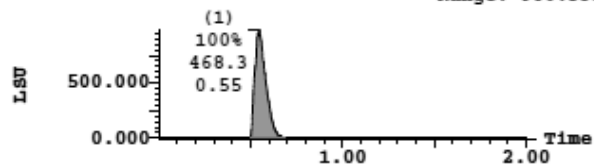
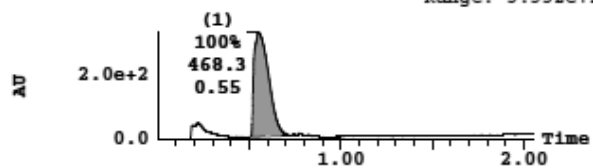


2: UV Detector: TIC

3.332e+2  
Range: 3.332e+2

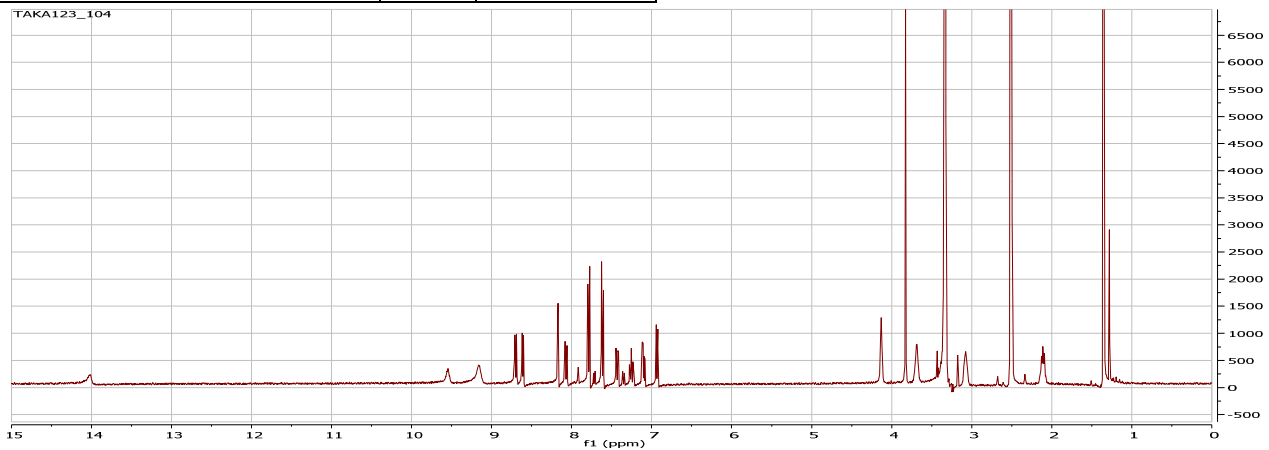
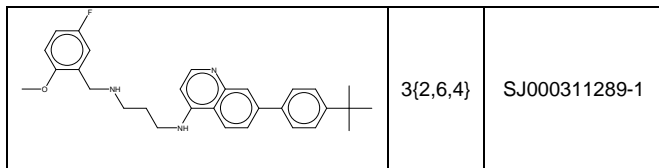
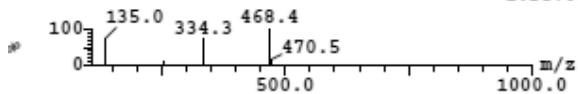
(2) ELSD signal

980.542  
Range: 980.533



Peak ID	Compound	Time	Mass Found
1	Found	0.54	468.26

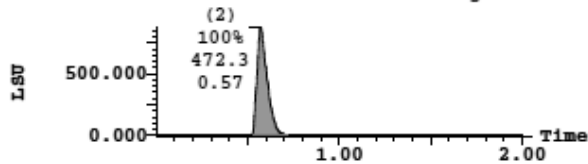
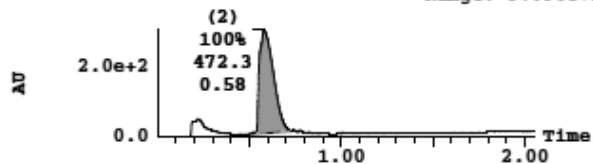
1:MS ES+  
1.2e+008



2: UV Detector: TIC 3.098e+2  
Range: 3.098e+2

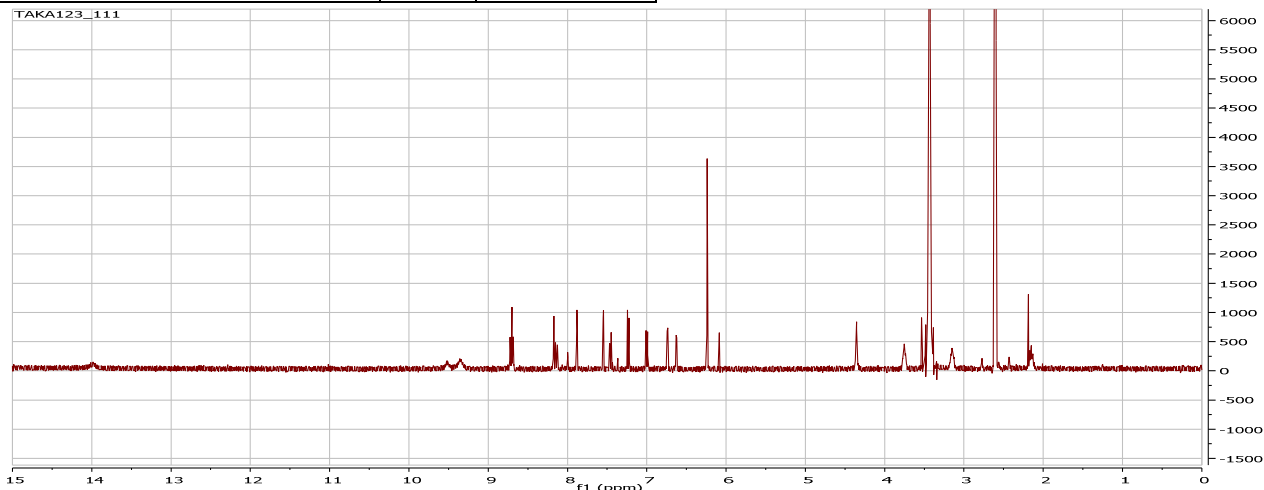
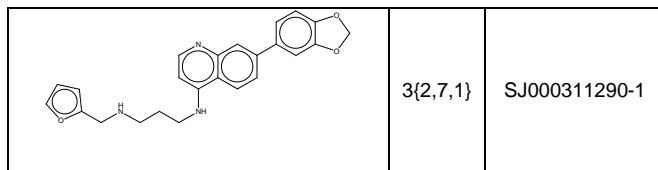
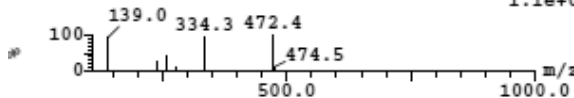
(2) ELSD Signal

876.415  
Range: 876.301



Peak ID	Compound	Time	Mass Found
2	Found	0.58	472.27

1:MS ES+  
1.1e+008

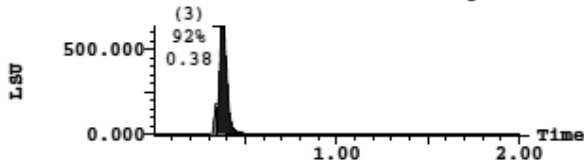
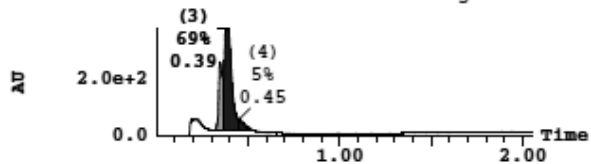


2: UV Detector: TIC

3.721e+2  
Range: 3.721e+2

(2) ELSD Signal

635.899  
Range: 635.702

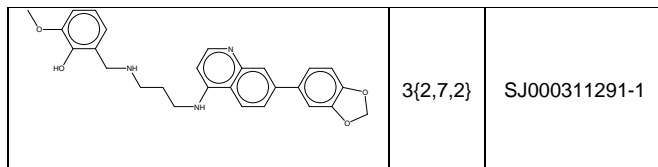
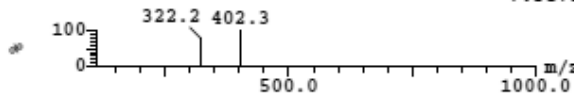
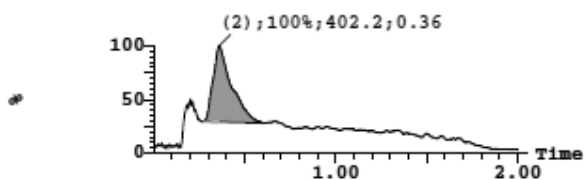


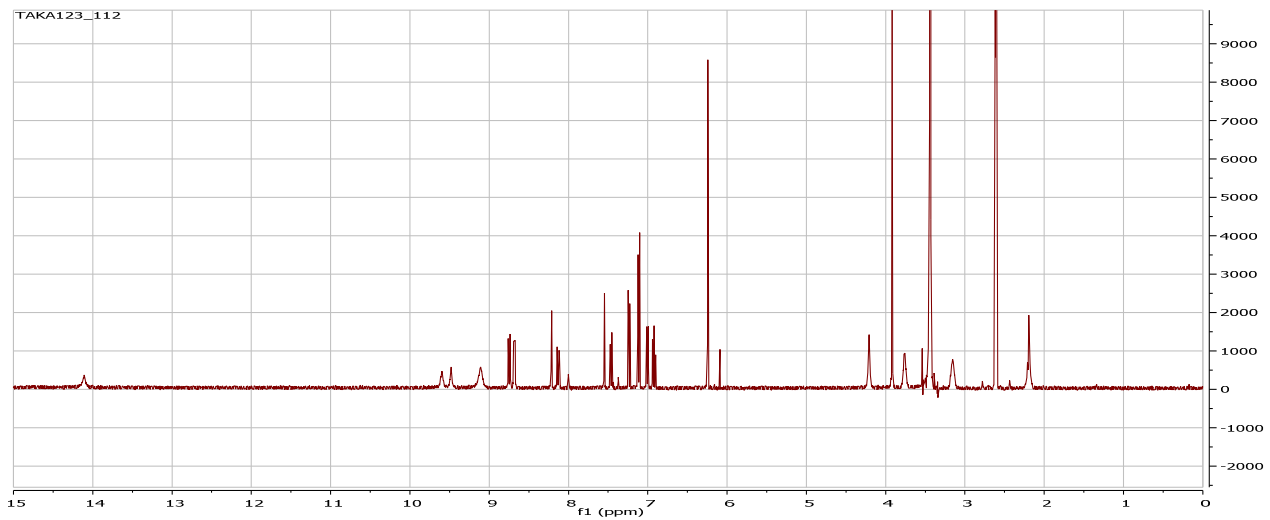
1: MS ES+ :TIC

5.1e+009

Peak ID	Compound	Time	Mass Found
2	Found	0.36	402.17

1:MS ES+  
7.5e+007



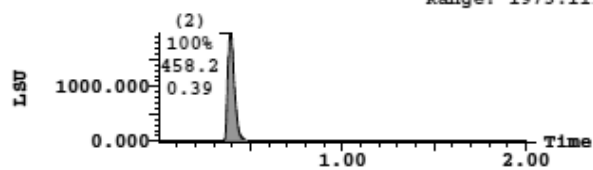
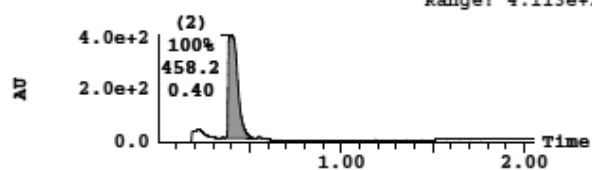


2: UV Detector: TIC

4.113e+2  
Range: 4.113e+2

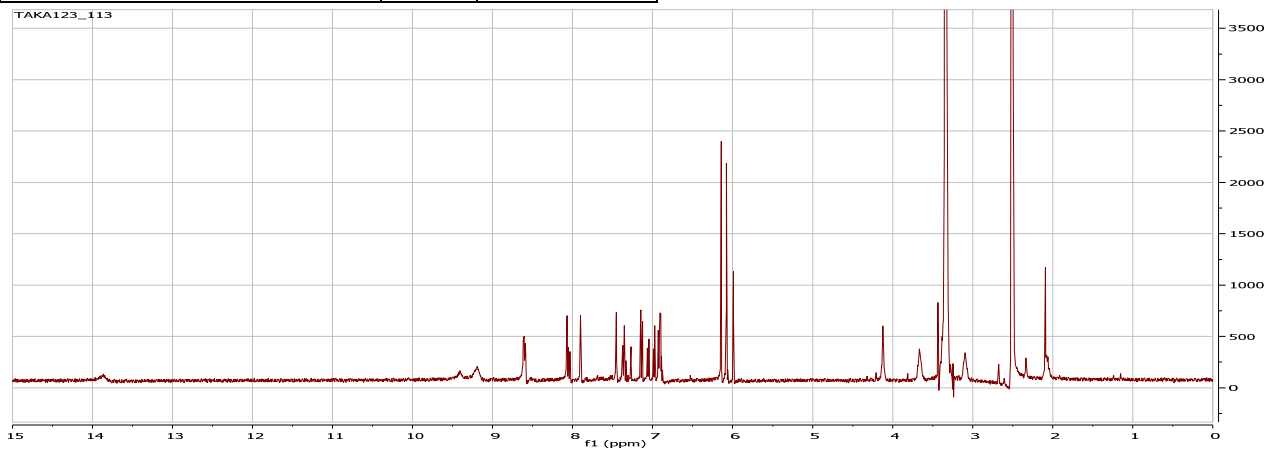
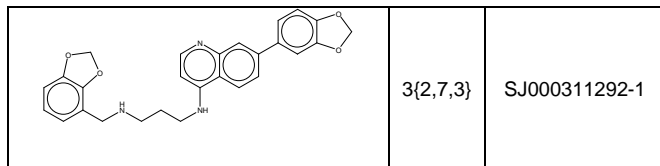
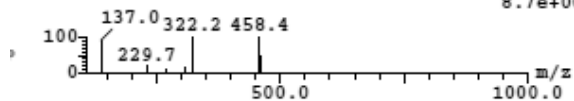
(2) ELSD Signal

1973.171  
Range: 1973.111



Peak ID	Compound	Time	Mass Found
2	Found	0.38	458.20

1:MS ES+  
8.7e+007

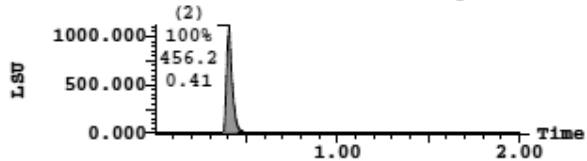
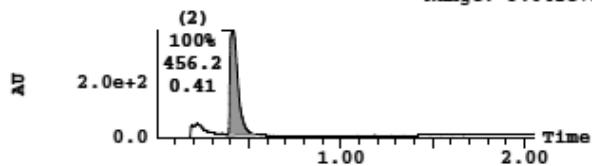


2: UV Detector: TIC

3.842e+2  
Range: 3.842e+2

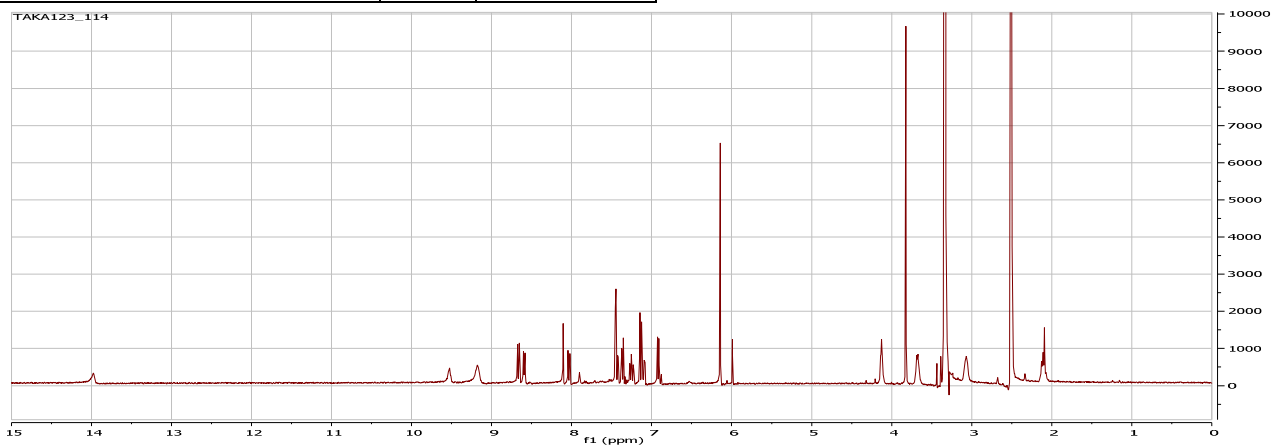
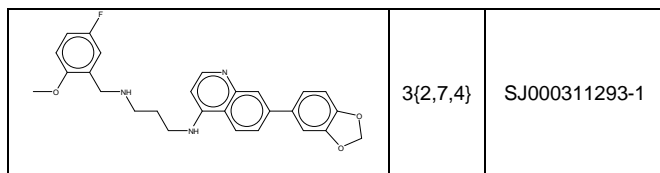
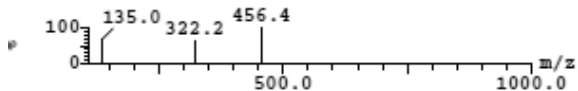
(2) ELSD Signal

1113.967  
Range: 1113.956



Peak ID	Compound	Time	Mass Found
2	Found	0.39	456.18

1:MS ES+  
8.7e+007

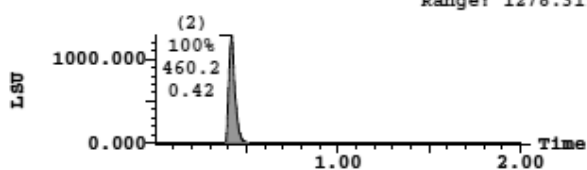
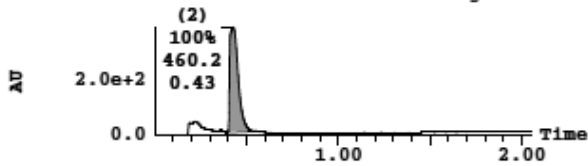


2: UV Detector: TIC

3.93e+2  
Range: 3.93e+2

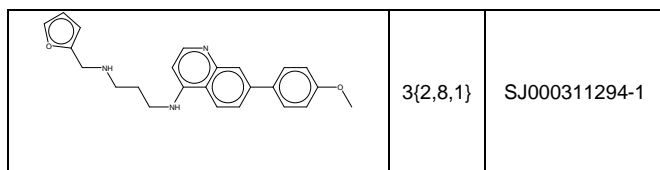
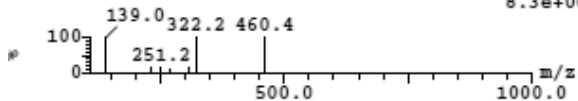
(2) ELSD signal

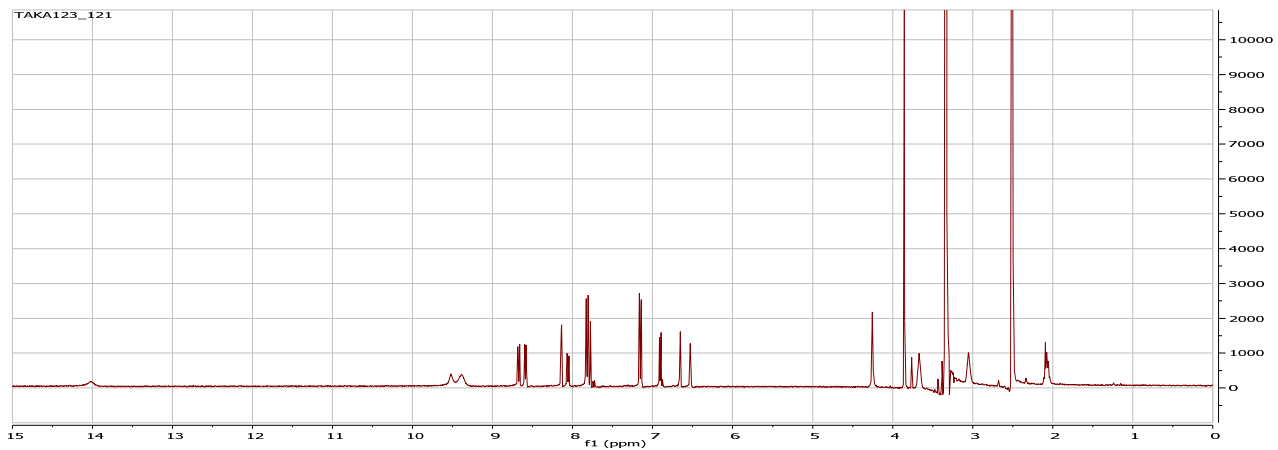
1278.421  
Range: 1278.319



Peak ID	Compound	Time	Mass Found
2	Found	0.41	460.20

1:MS ES+  
8.3e+007



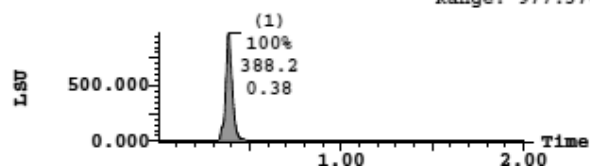
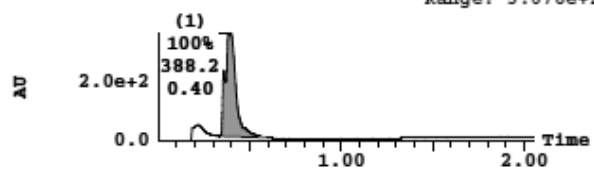


2: UV Detector: TIC

3.678e+2  
Range: 3.678e+2

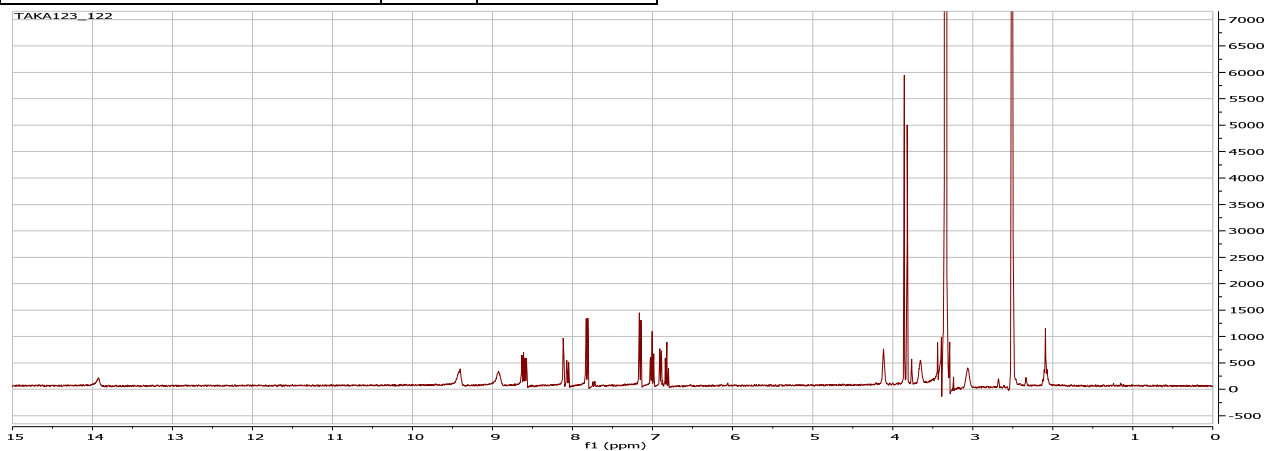
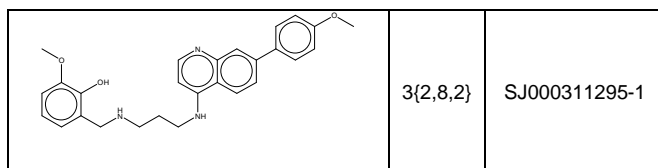
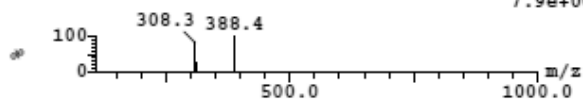
(2) ELSD Signal

977.543  
Range: 977.376



Peak ID	Compound	Time	Mass Found
1	Found	0.37	388.19

1:MS ES+  
7.9e+007

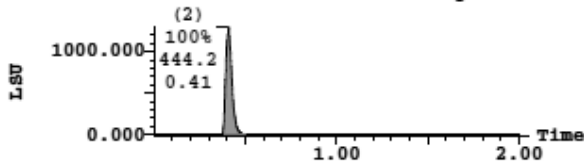
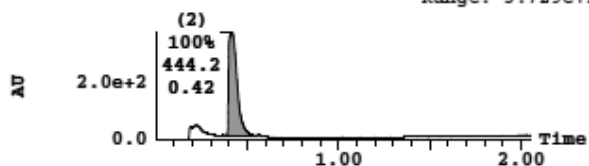


2: UV Detector: TIC

3.729e+2  
Range: 3.729e+2

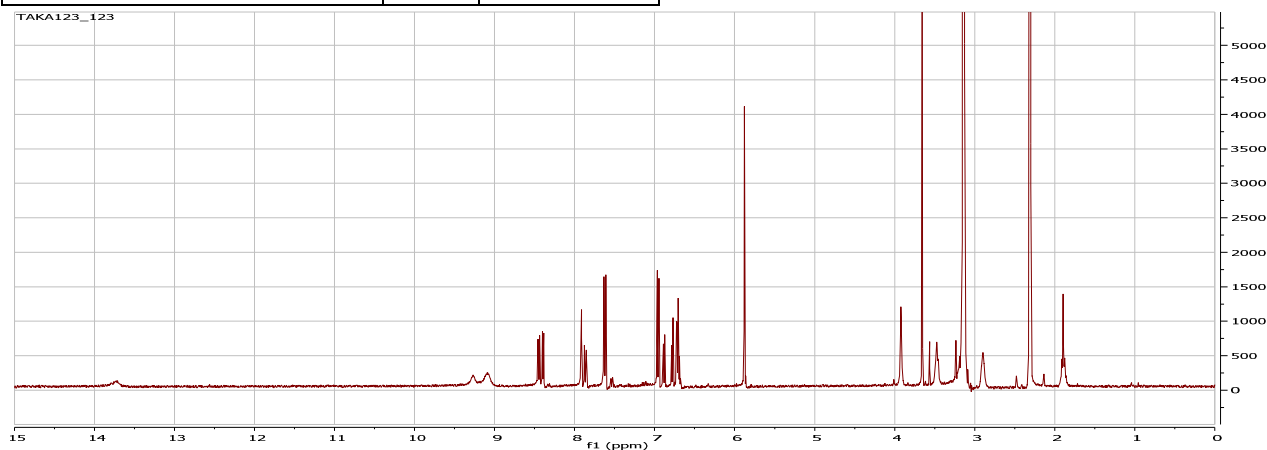
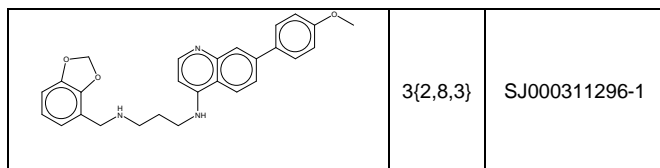
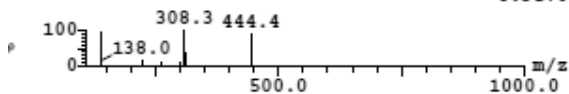
(2) ELSD Signal

1295.556  
Range: 1295.491



Peak ID	Compound Found	Time	Mass Found
2	Found	0.39	444.22

1:MS ES+  
8.3e+007

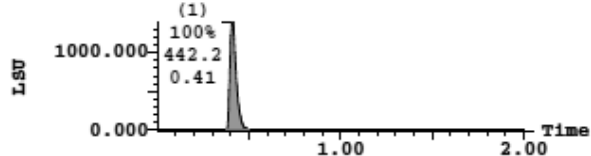
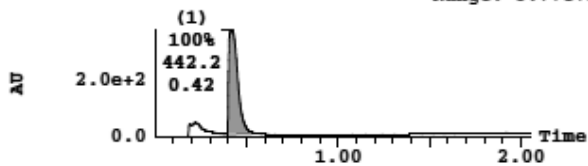


2: UV Detector: TIC

3.77e+2  
Range: 3.77e+2

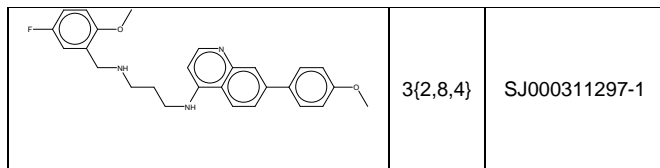
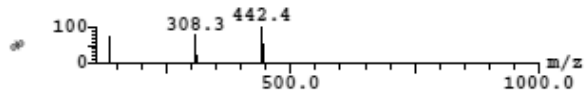
(2) ELSD Signal

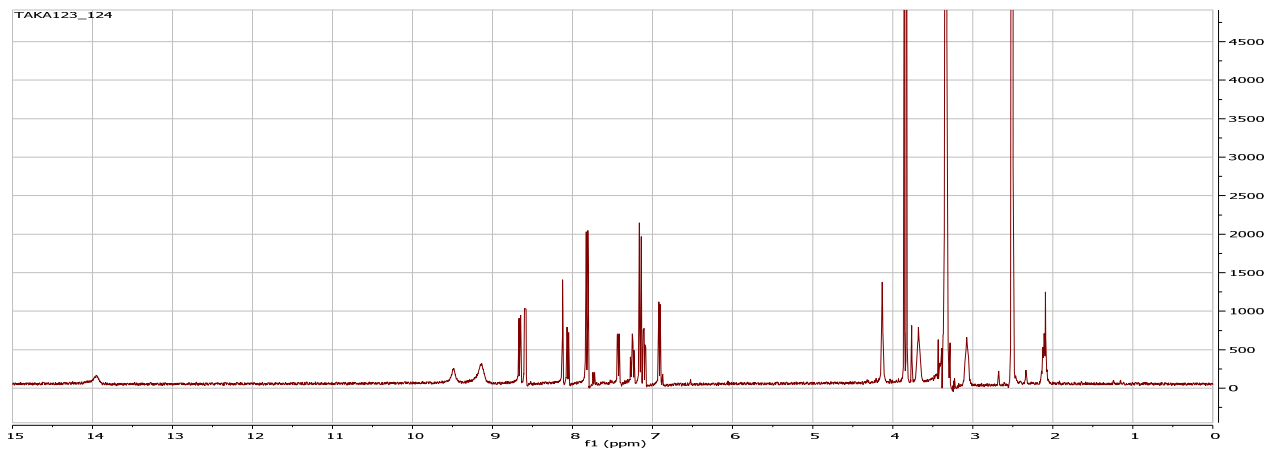
1388.959  
Range: 1388.931



Peak ID	Compound Found	Time	Mass Found
1	Found	0.40	442.21

1:MS ES+  
9.5e+007

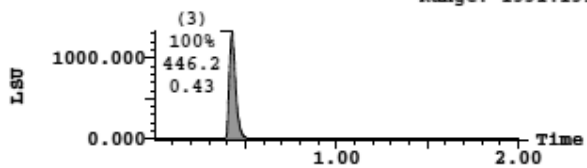
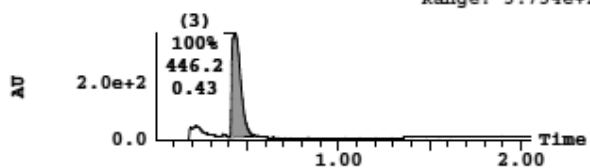




2: UV Detector: TIC

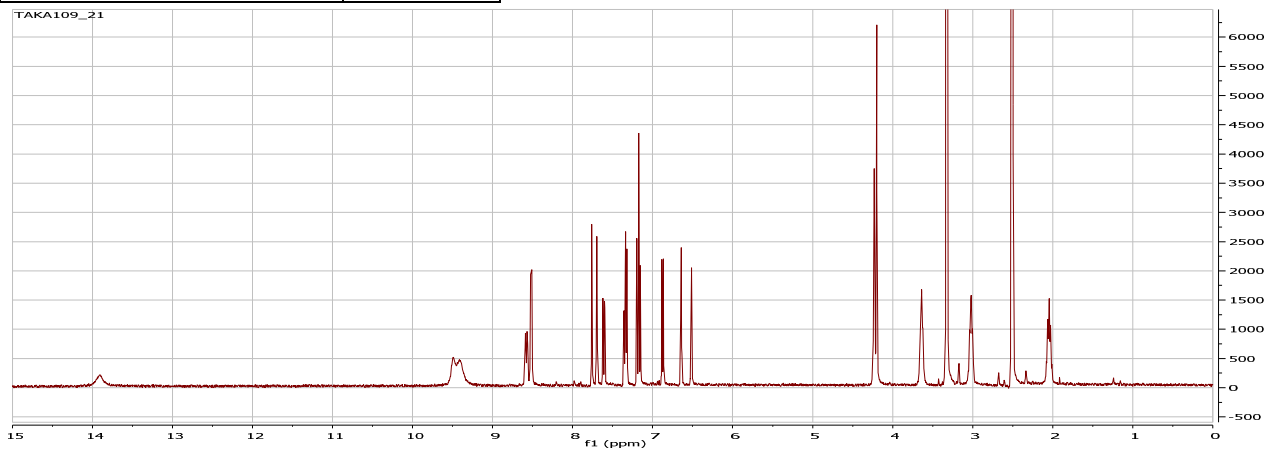
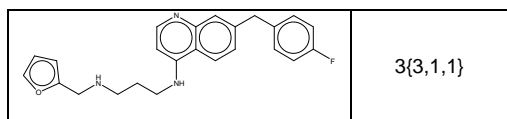
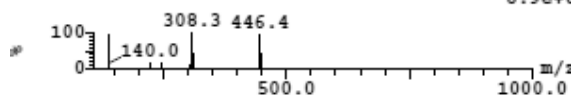
3.734e+2 (2) ELSD Signal  
Range: 3.734e+2

1331.206  
Range: 1331.139



Peak ID	Compound	Time	Mass Found
3	Found	0.41	446.22

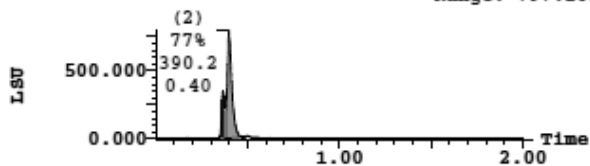
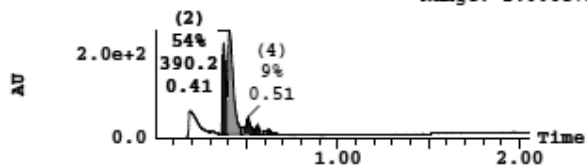
1:MS ES+  
8.9e+007





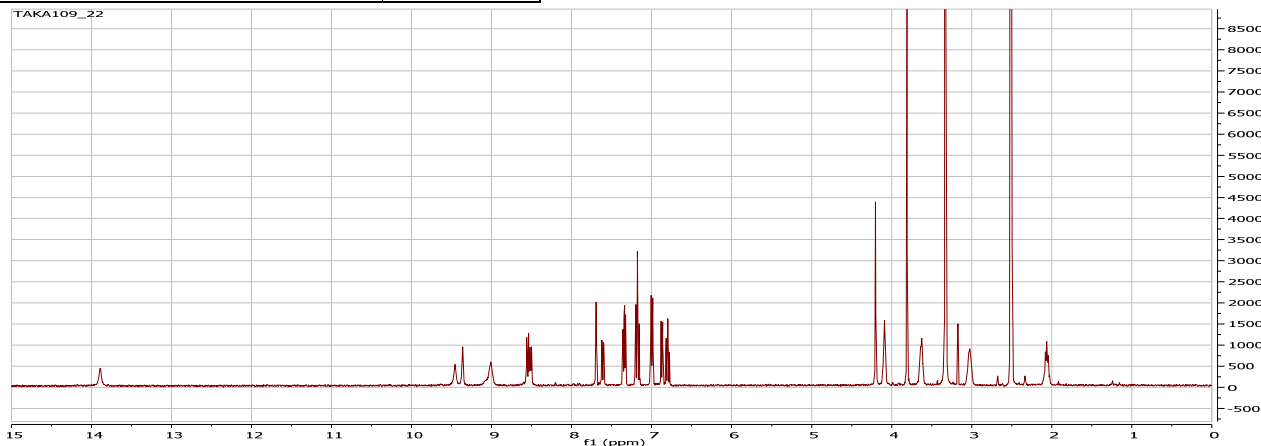
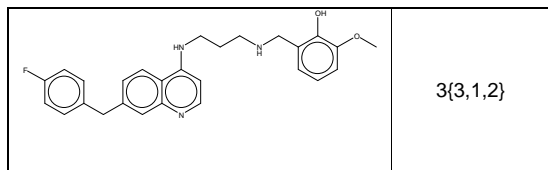
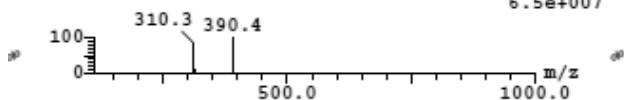
2: UV Detector: TIC Range: 2.608e+2

(2) ELSD Signal Range: 797.244  
797.189



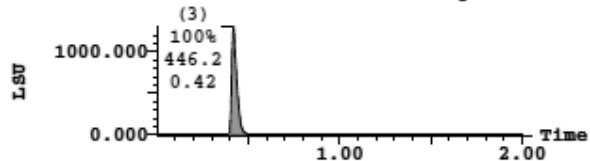
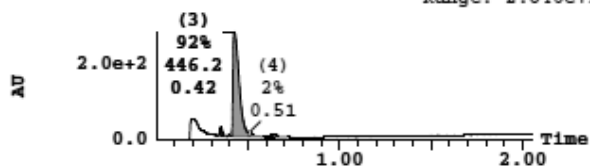
Peak ID	Compound	Time	Mass Found
2	Found	0.38	390.19

1:MS ES+  
6.5e+007



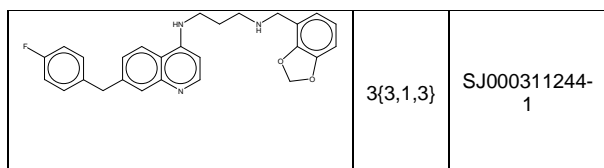
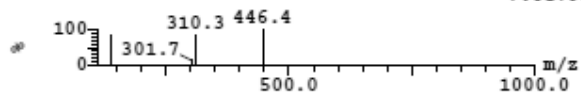
2: UV Detector: TIC Range: 2.846e+2

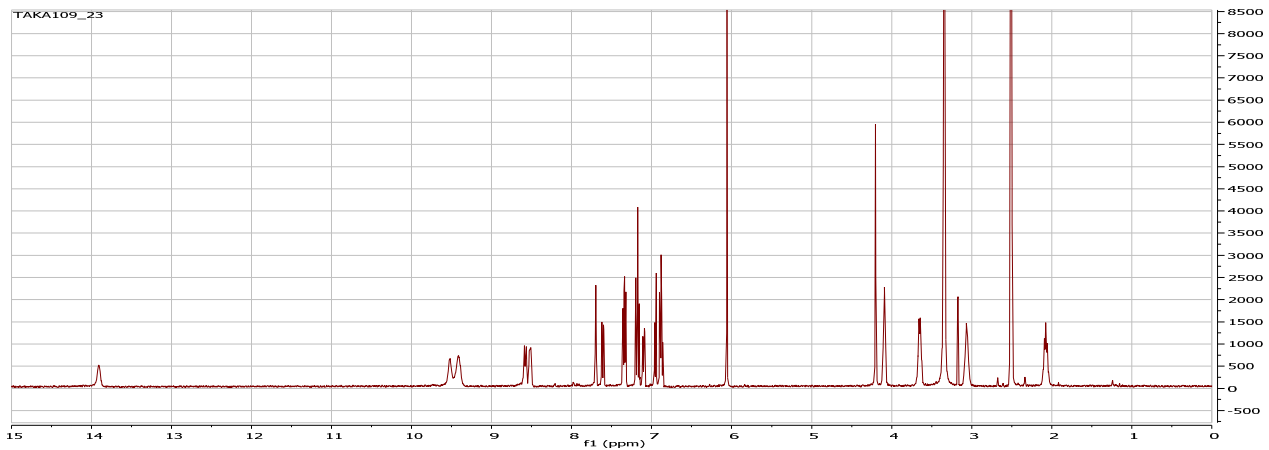
(2) ELSD Signal Range: 1299.995  
1299.930



Peak ID	Compound	Time	Mass Found
3	Found	0.41	446.22

1:MS ES+  
7.6e+007





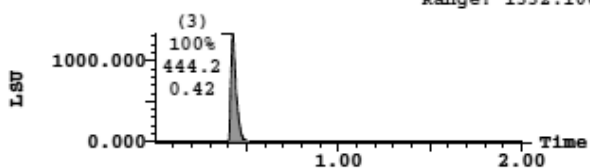
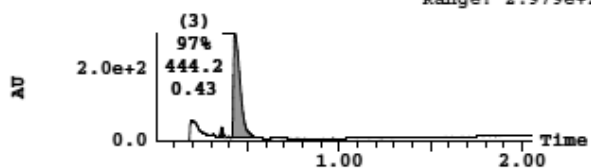
2: UV Detector: TIC

2.979e+2 (2) ELSD Signal

1332.146

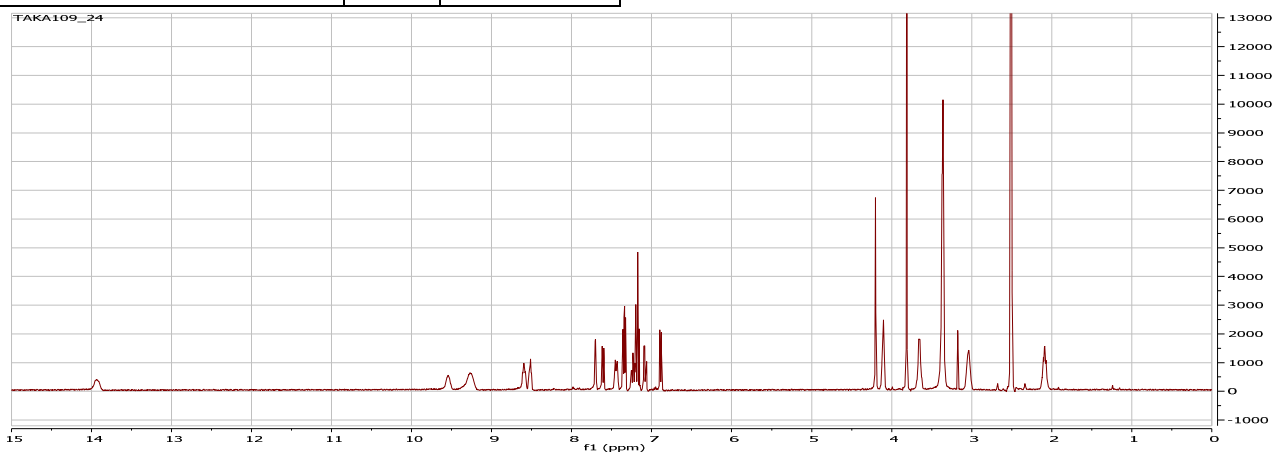
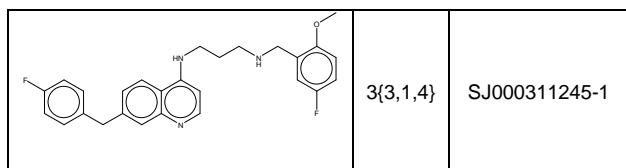
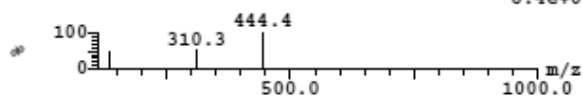
Range: 2.979e+2

Range: 1332.106



Peak ID	Compound	Time	Mass Found
3	Found	0.41	444.20

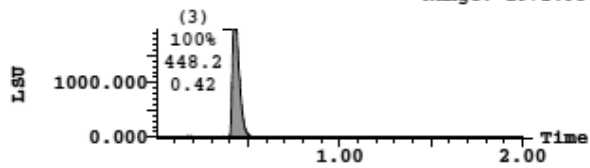
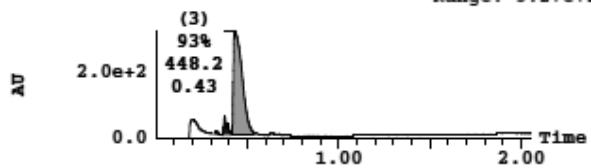
1:MS ES+  
8.4e+007



2: UV Detector: TIC

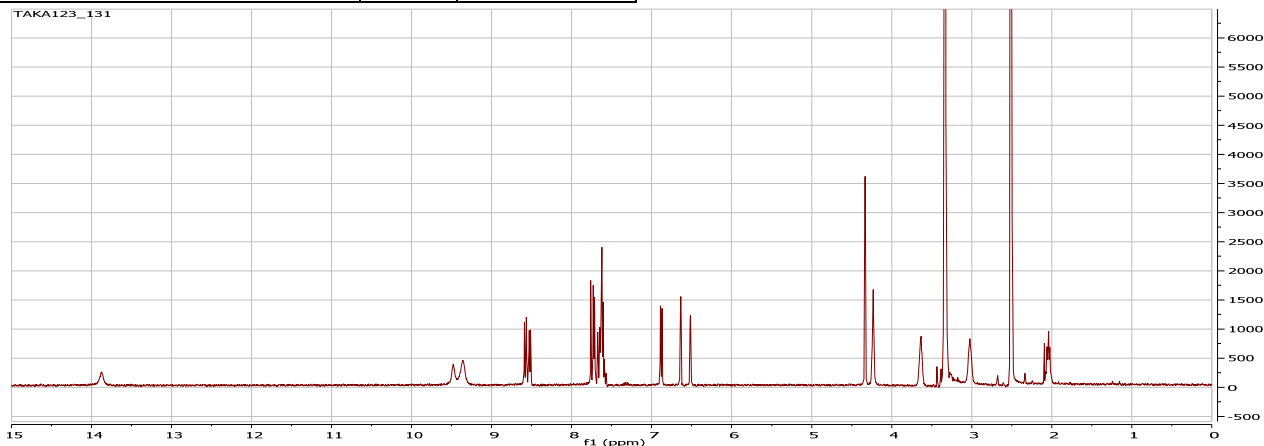
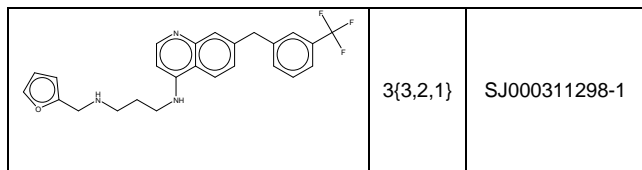
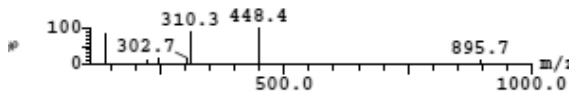
3.27e+2 (2) ELSD Signal  
Range: 3.27e+2

1973.116  
Range: 1972.938



Peak ID	Compound	Time	Mass Found
3	Found	0.42	448.21

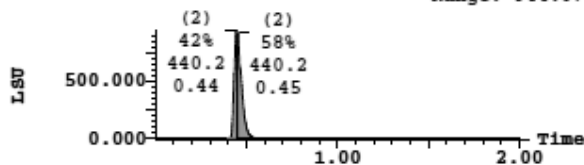
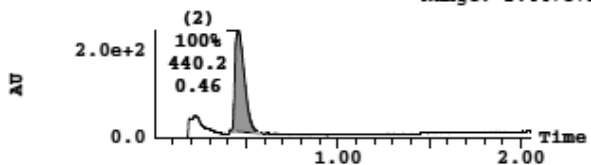
1:MS ES+  
8.9e+007



2: UV Detector: TIC

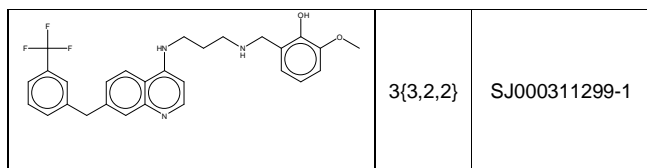
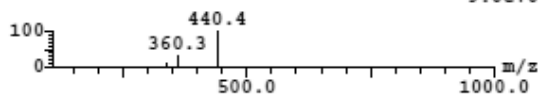
2.447e+2 (2) ELSD Signal  
Range: 2.447e+2

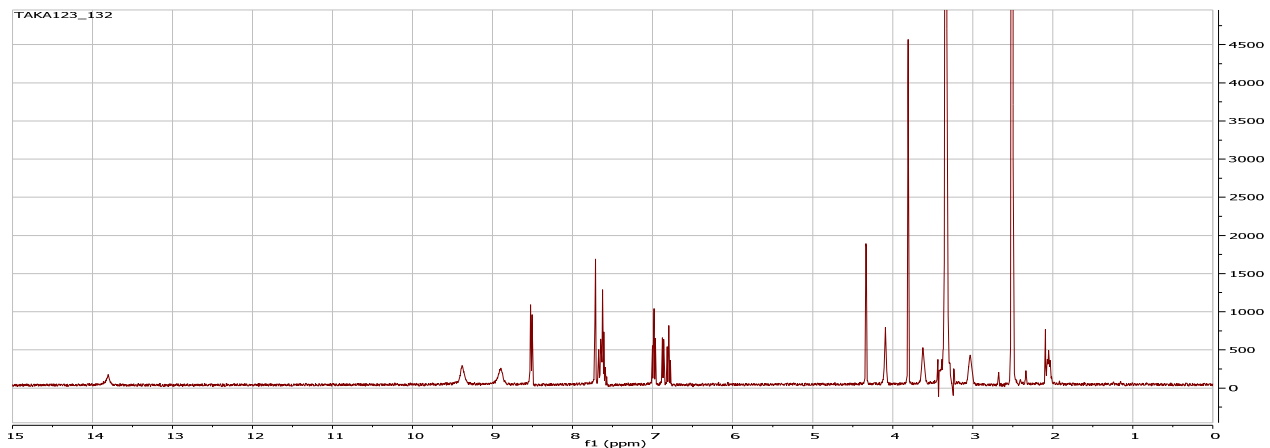
944.683  
Range: 944.674



Peak ID	Compound	Time	Mass Found
2	Found	0.43	440.19

1:MS ES+  
9.0e+007



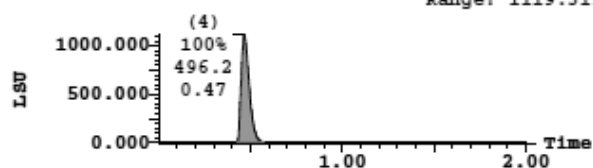
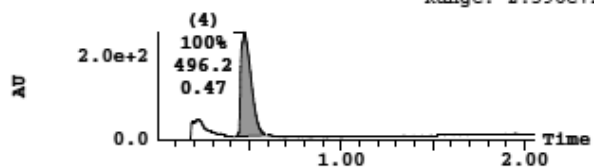


2: UV Detector: TIC

2.598e+2  
Range: 2.598e+2

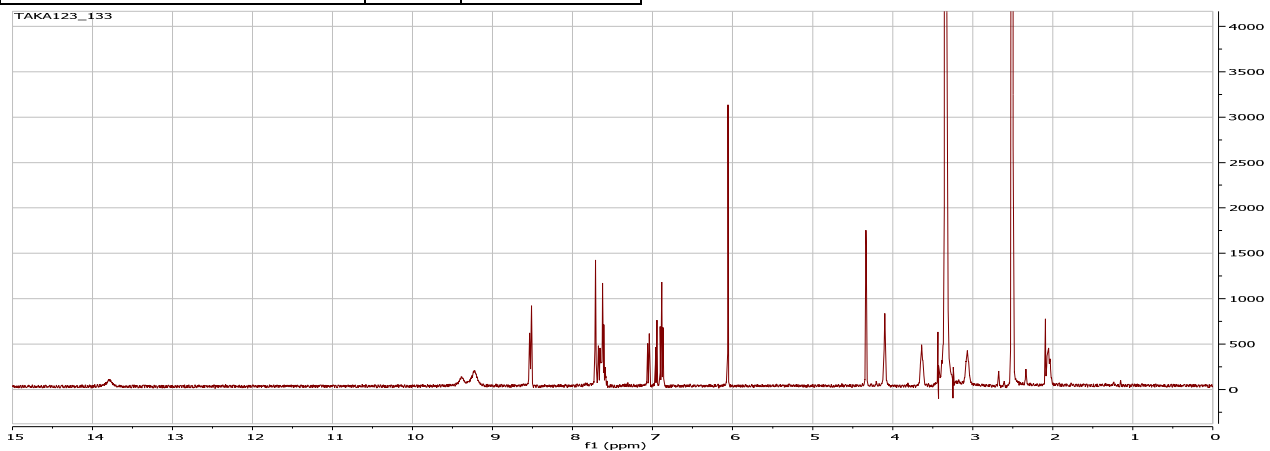
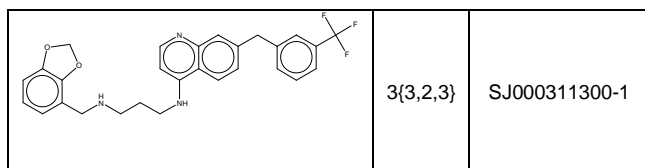
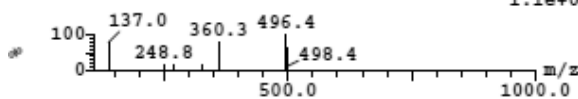
(2) ELSD Signal

1119.397  
Range: 1119.319



Peak ID	Compound	Time	Mass Found
4	Found	0.46	496.21

1:MS ES+  
1.1e+008

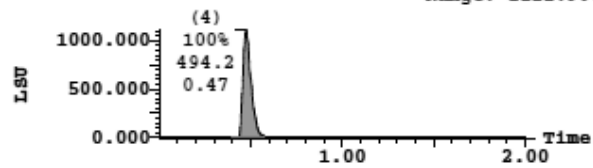
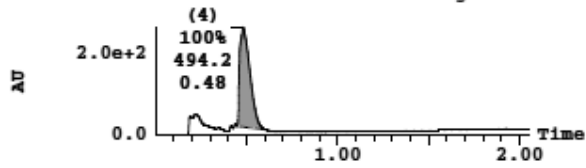


2: UV Detector: TIC

2.618e+2  
Range: 2.618e+2

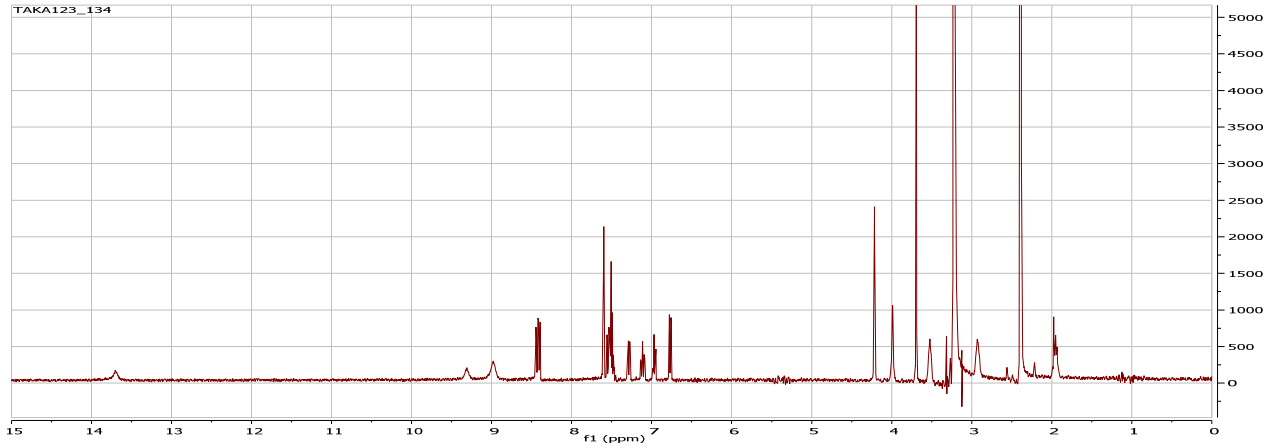
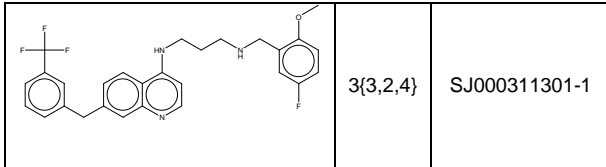
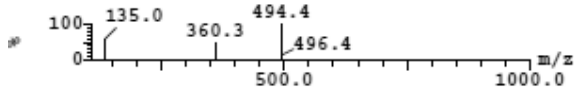
(2) ELSD signal

1112.085  
Range: 1111.907



Peak ID	Compound	Time	Mass Found
4	Found	0.48	494.20

1:MS ES+  
1.0e+008

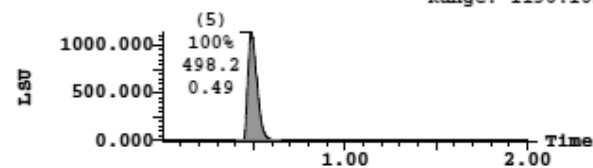
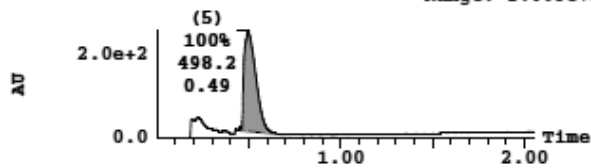


2: UV Detector: TIC

2.603e+2  
Range: 2.603e+2

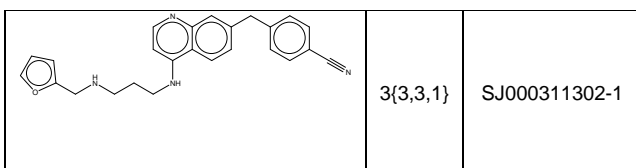
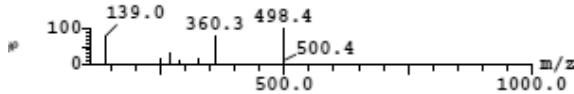
(2) ELSD signal

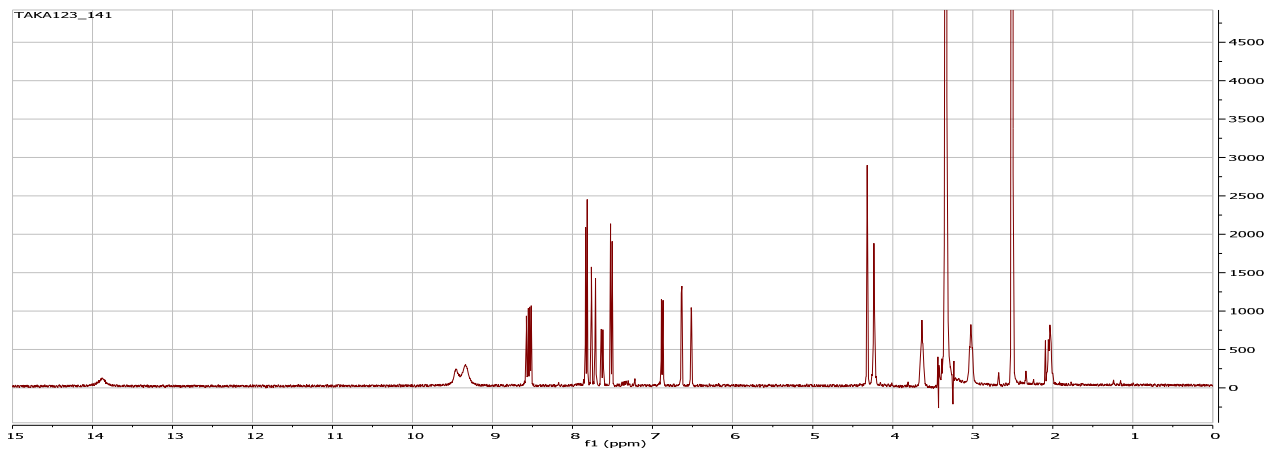
1136.186  
Range: 1136.163



Peak ID	Compound	Time	Mass Found
5	Found	0.47	498.21

1:MS ES+  
1.1e+008



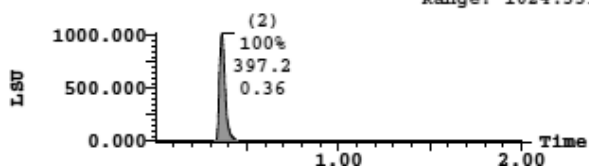
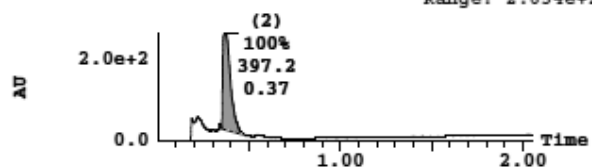


2: UV Detector: TIC

2.634e+2  
Range: 2.634e+2

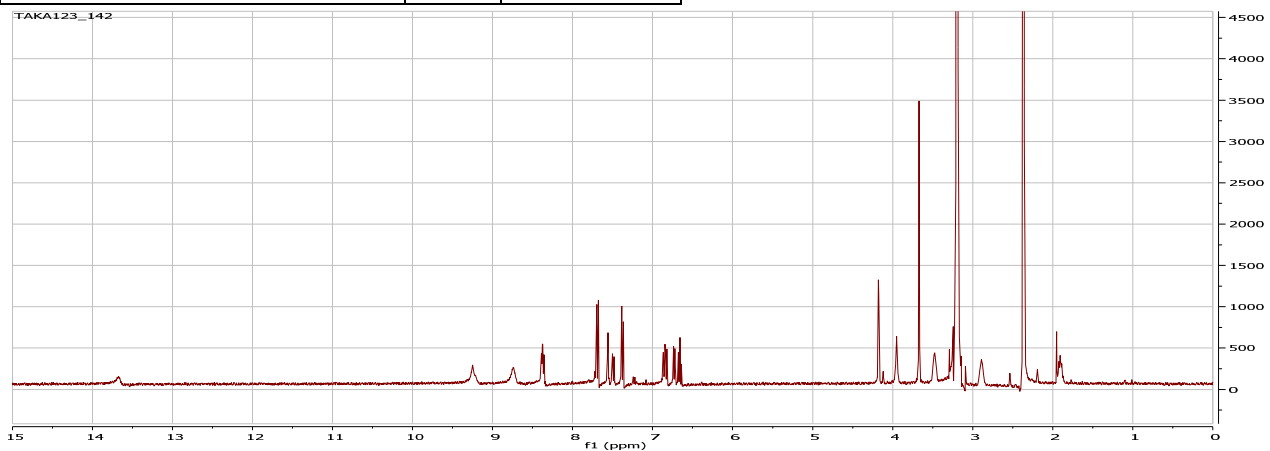
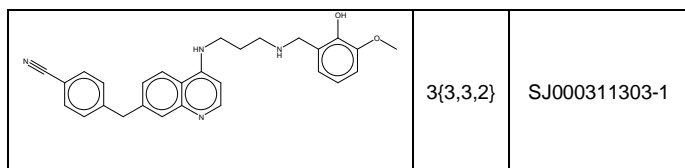
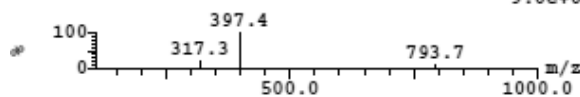
(2) ELSD Signal

1024.433  
Range: 1024.331



Peak ID	Compound	Time	Mass Found
2	Found	0.35	397.20

1:MS ES+  
9.0e+007

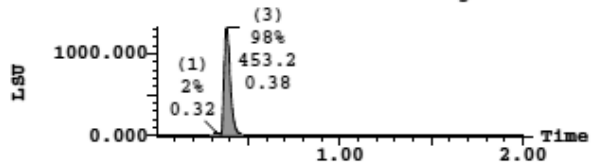
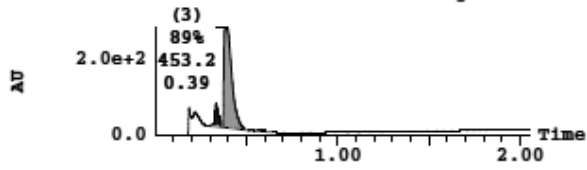


2: UV Detector: TIC

2.829e+2  
Range: 2.829e+2

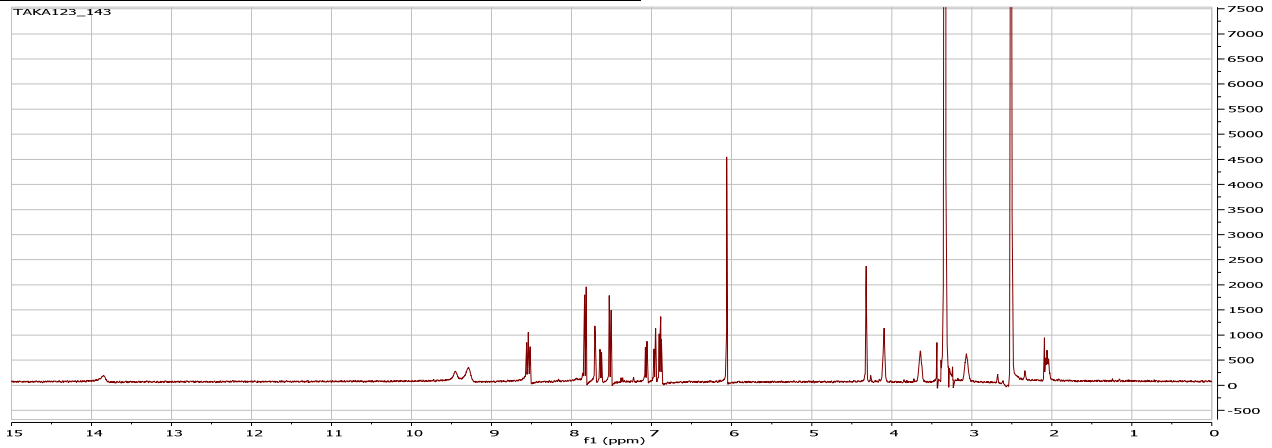
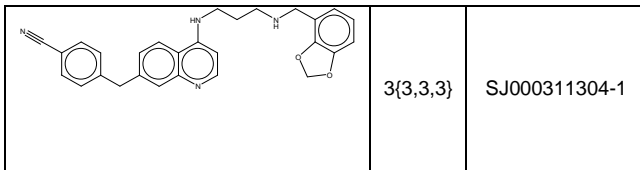
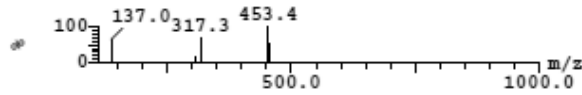
(2) ELSD Signal

1320.579  
Range: 1320.487



Peak ID	Compound Found	Time	Mass Found
3	Found	0.37	453.22

1:MS ES+  
8.6e+007

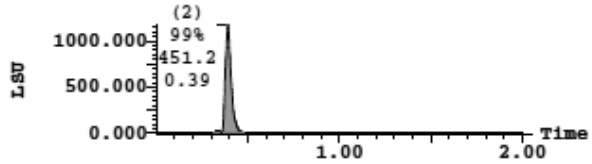
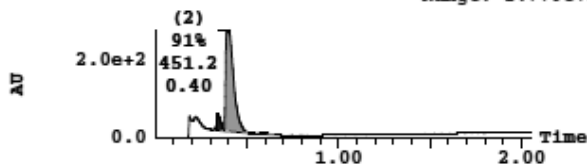


2: UV Detector: TIC

2.779e+2  
Range: 2.779e+2

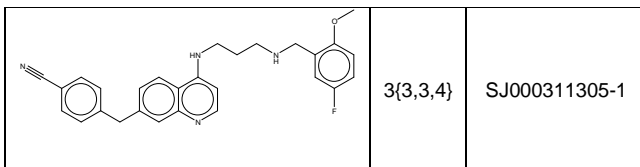
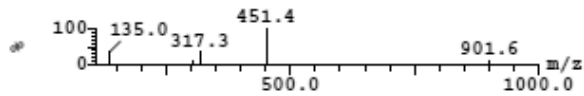
(2) ELSD Signal

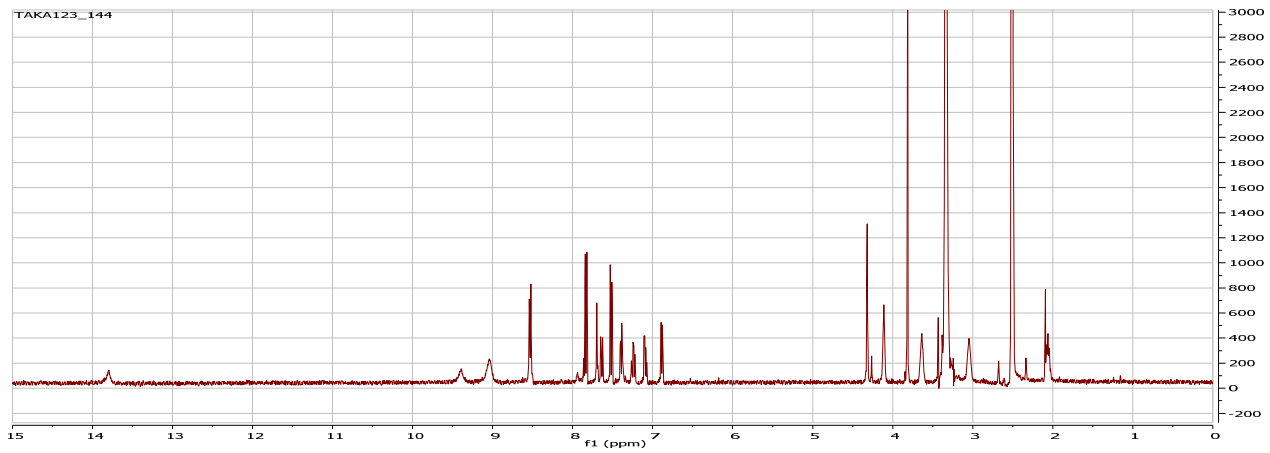
1173.306  
Range: 1173.271



Peak ID	Compound Found	Time	Mass Found
2	Found	0.38	451.21

1:MS ES+  
9.0e+007



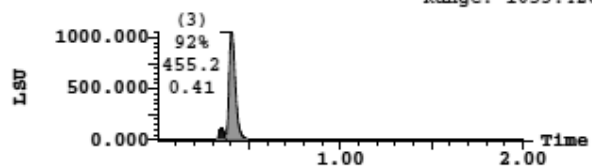
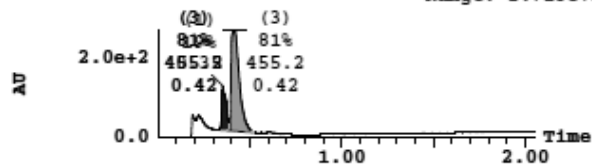


2: UV Detector: TIC

2.713e+2  
Range: 2.713e+2

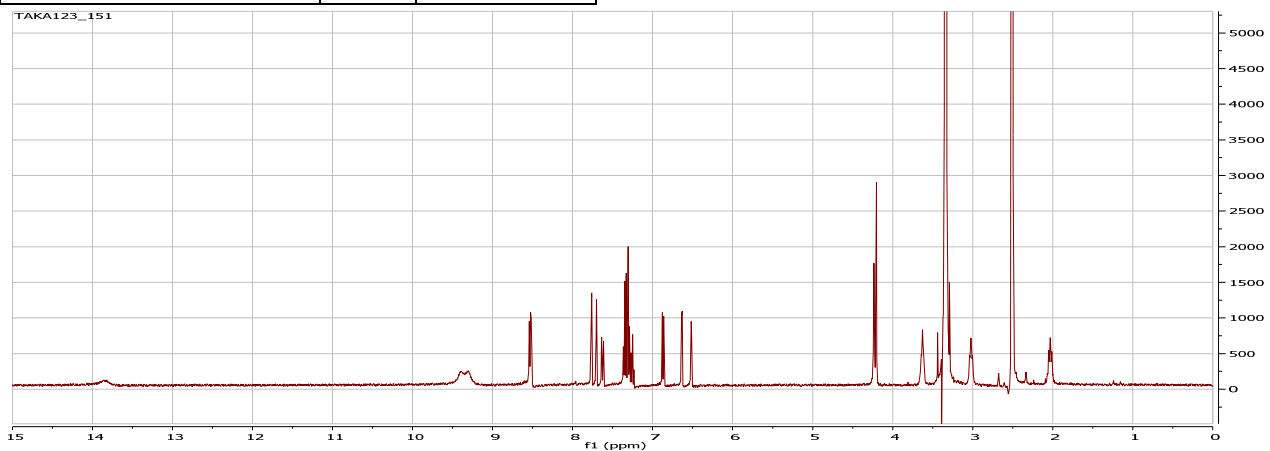
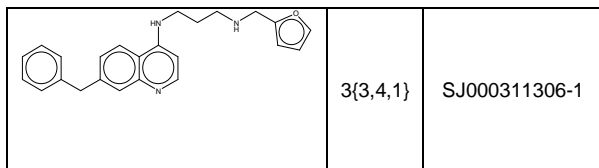
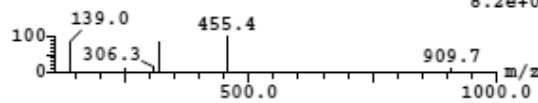
(2) ELSD Signal

1053.533  
Range: 1053.428



Peak ID	Compound	Time	Mass Found
3	Found	0.39	455.22

1:MS ES+  
8.2e+007



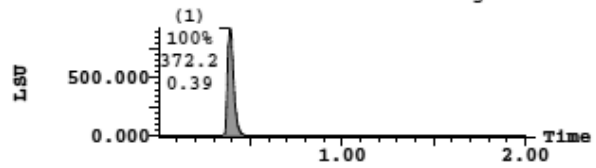
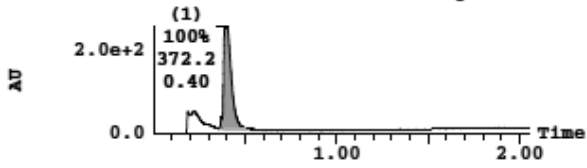


2: UV Detector: TIC

2.562e+2  
Range: 2.562e+2

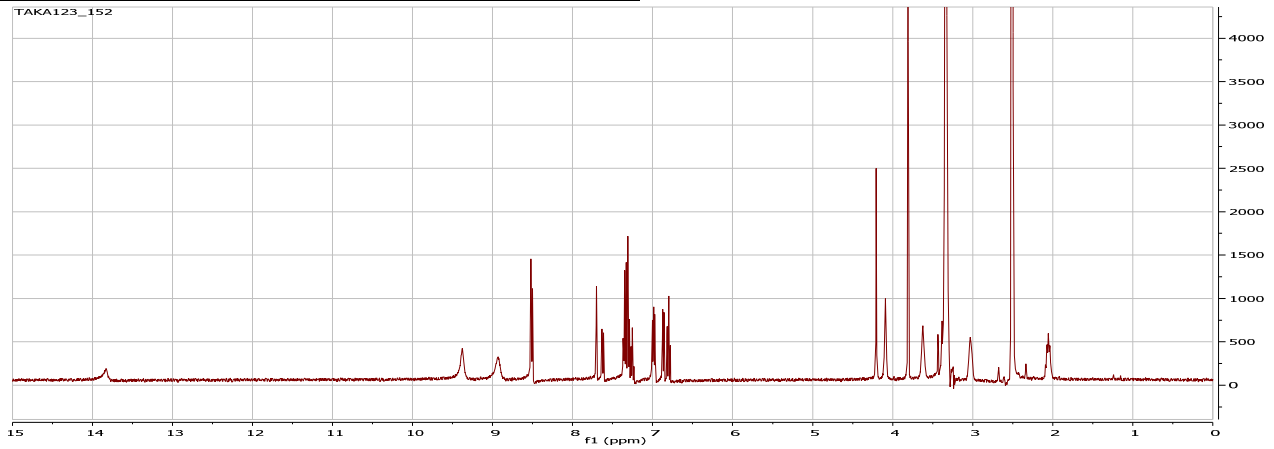
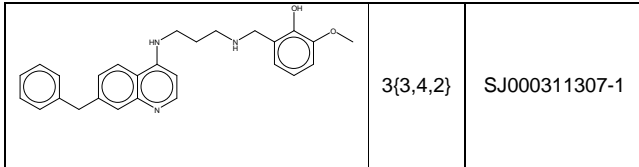
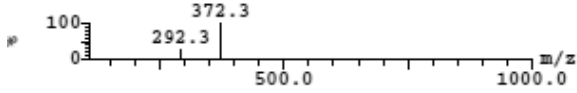
(2) ELSD Signal

923.104  
Range: 923.030



Peak ID	Compound Found	Time	Mass Found
1	Found	0.38	372.20

1:MS ES+  
9.0e+007

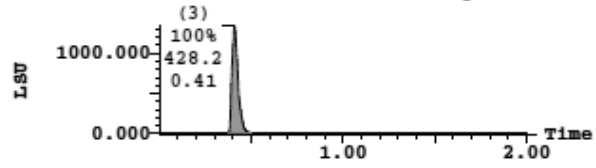
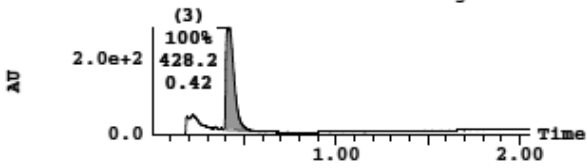


2: UV Detector: TIC

2.804e+2  
Range: 2.804e+2

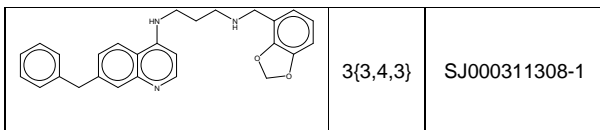
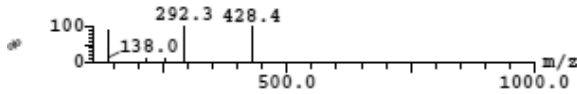
(2) ELSD Signal

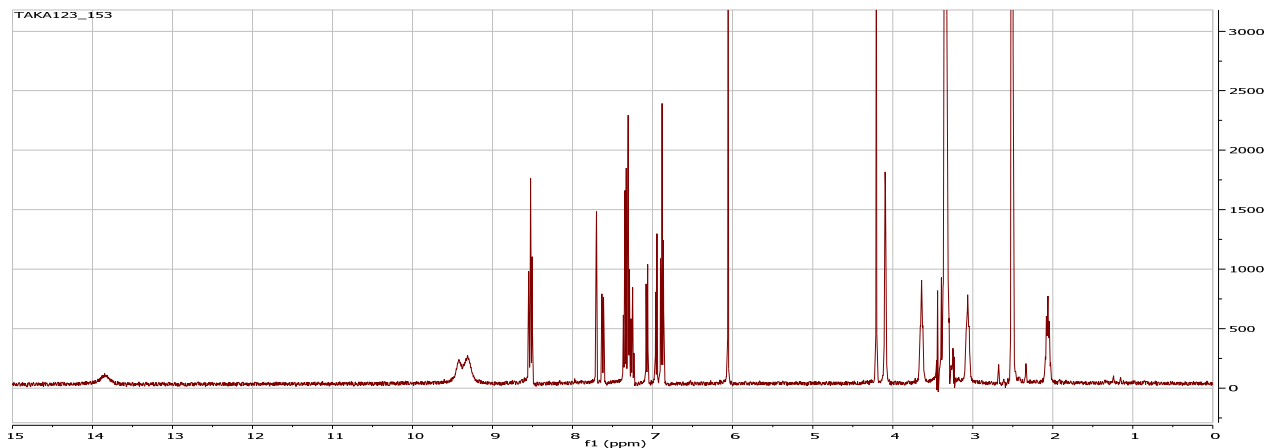
1344.506  
Range: 1344.493



Peak ID	Compound Found	Time	Mass Found
3	Found	0.40	428.23

1:MS ES+  
8.7e+007



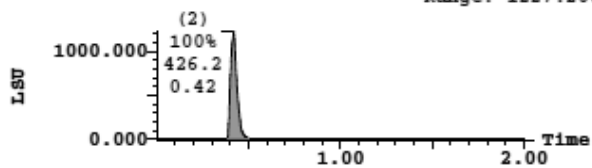
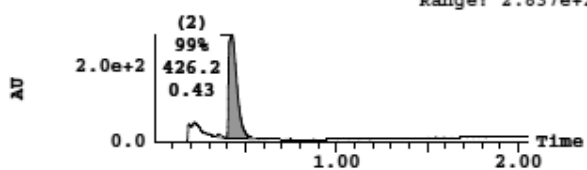


2: UV Detector: TIC

2.838e+2  
Range: 2.837e+2

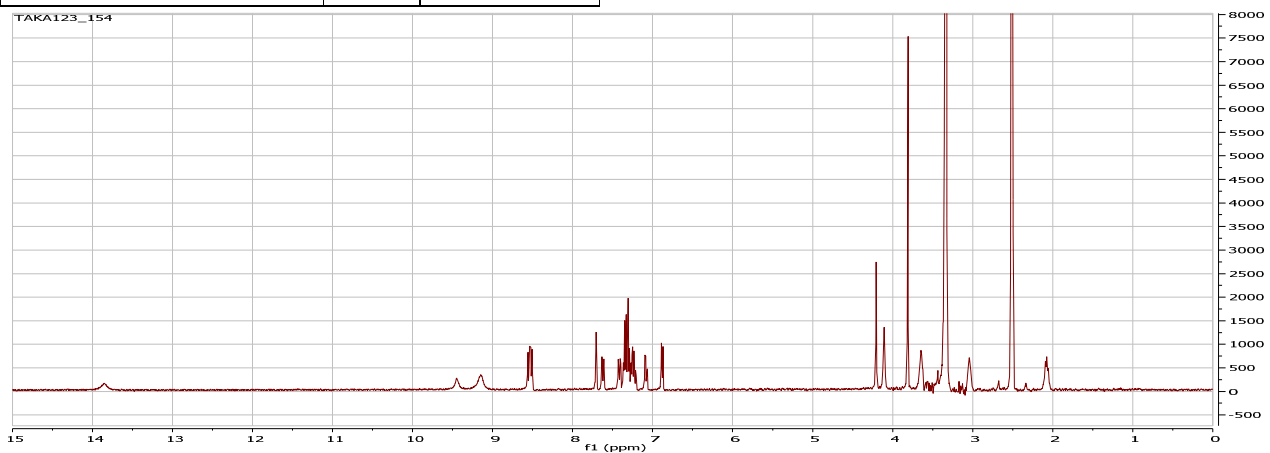
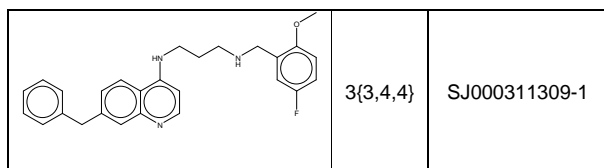
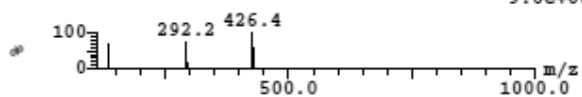
(2) ELSD Signal

1227.290  
Range: 1227.266



Peak ID	Compound	Time	Mass Found
2	Found	0.41	426.21

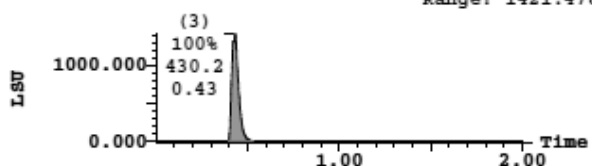
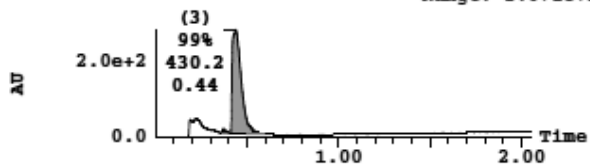
1:MS ES+  
9.6e+007



2: UV Detector: TIC

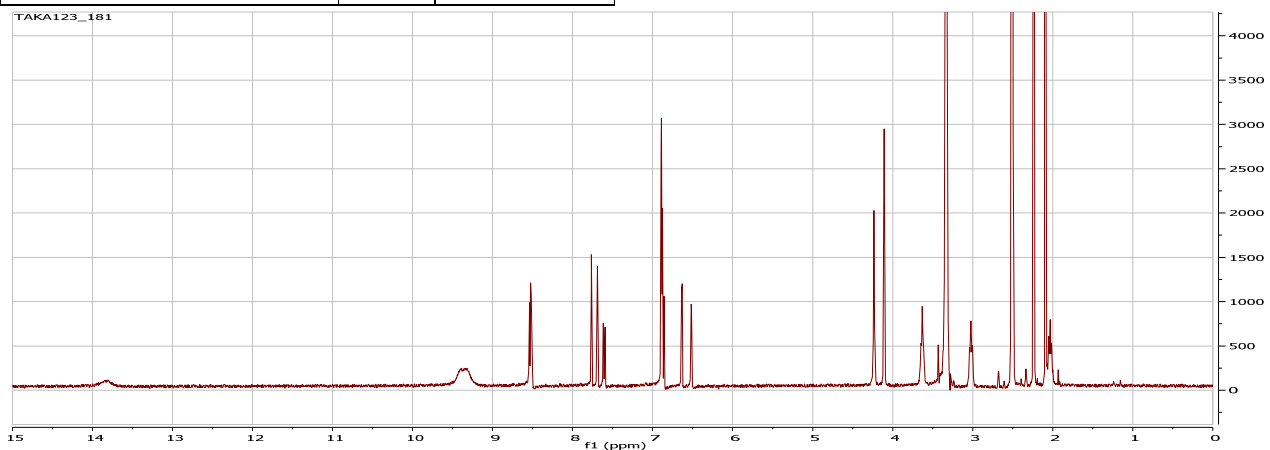
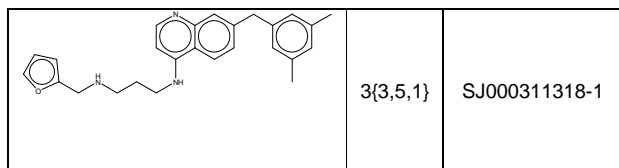
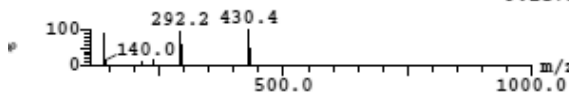
2.871e+2 (2) ELSD signal  
Range: 2.871e+2

1421.634  
Range: 1421.478



Peak ID	Compound	Time	Mass Found
3	Found	0.42	430.22

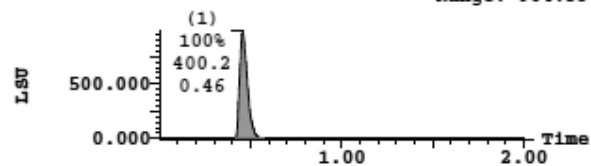
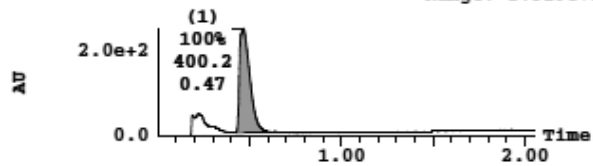
1:MS ES+  
9.1e+007



2: UV Detector: TIC

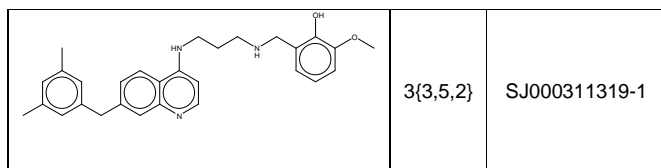
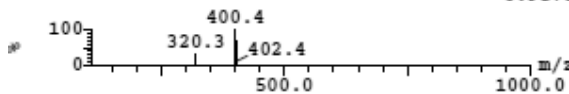
2.519e+2 (2) ELSD signal  
Range: 2.519e+2

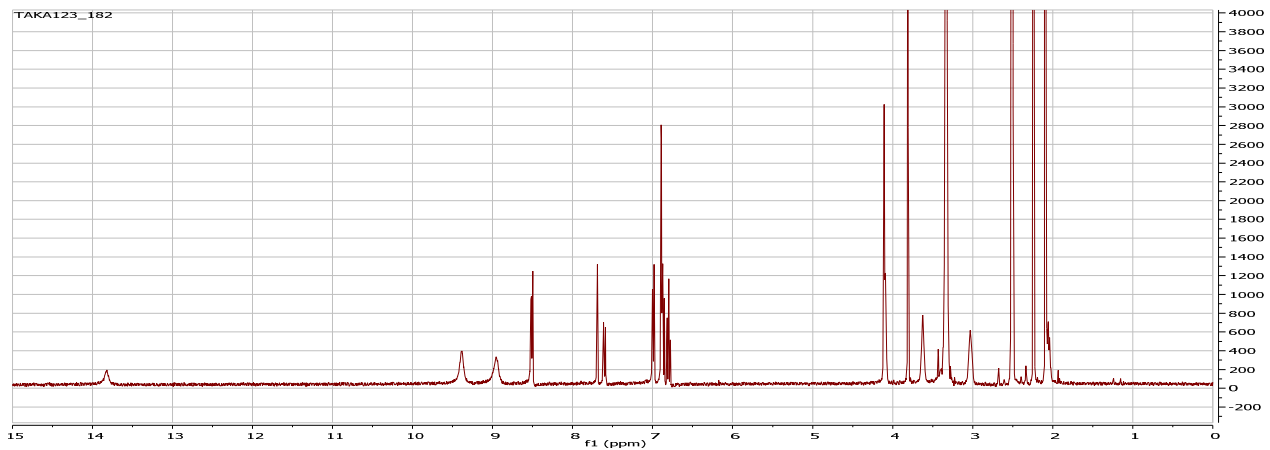
984.691  
Range: 984.534



Peak ID	Compound	Time	Mass Found
1	Found	0.44	400.23

1:MS ES+  
8.9e+007

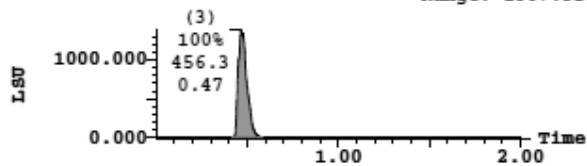
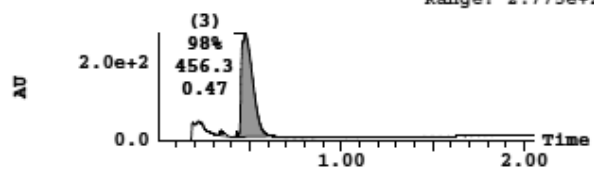




2: UV Detector: TIC

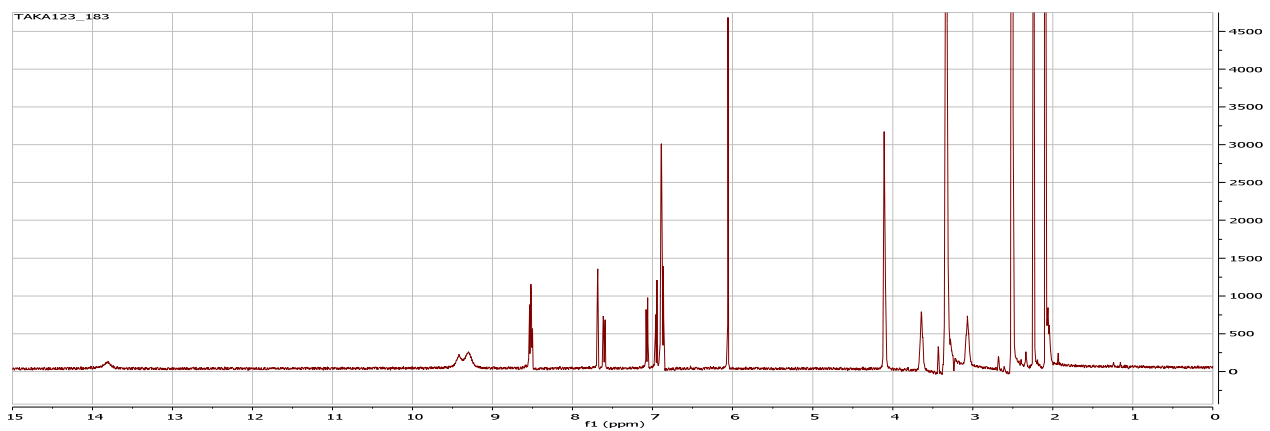
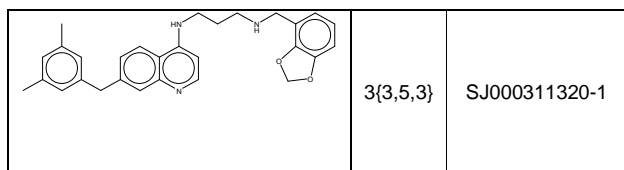
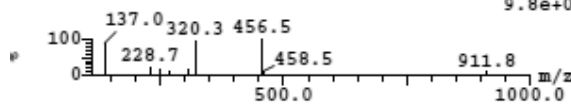
2.775e+2 (2) ELSD Signal  
Range: 2.775e+2

1387.543  
Range: 1387.529



Peak ID	Compound	Time	Mass Found
3	Found	0.48	456.28

1: MS ES+  
9.8e+007

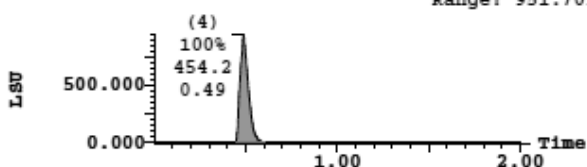
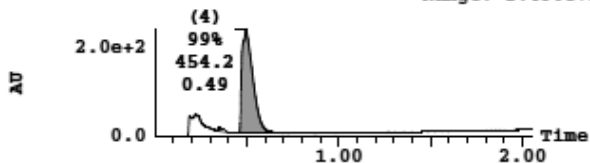


2: UV Detector: TIC

2.436e+2  
Range: 2.436e+2

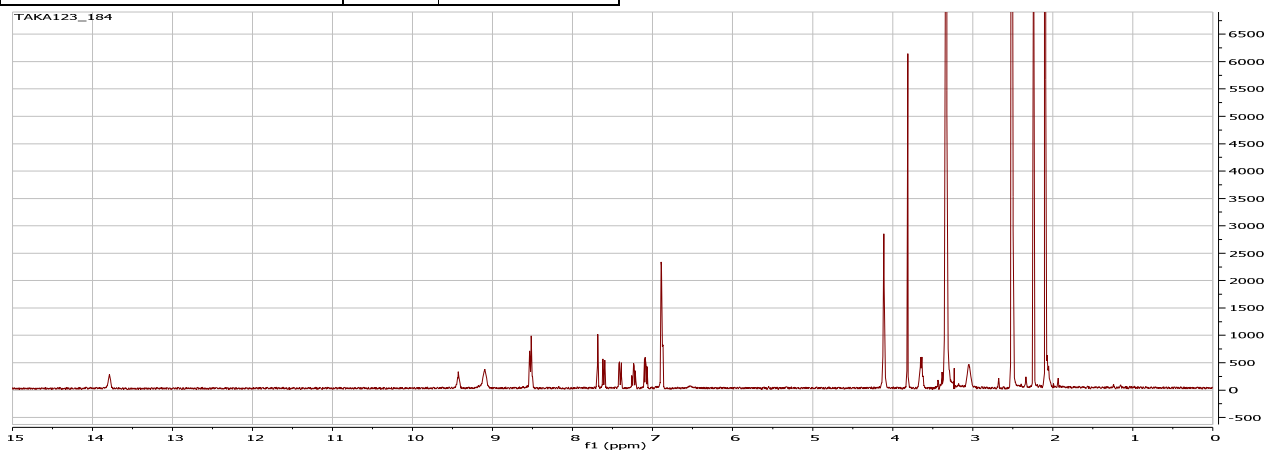
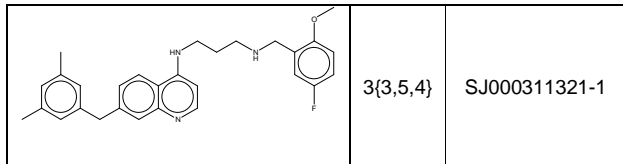
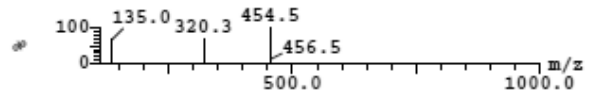
(2) ELSD signal

951.739  
Range: 951.701



Peak ID	Compound	Time	Mass Found
4	Found	0.47	454.24

1:MS ES+  
1.0e+008

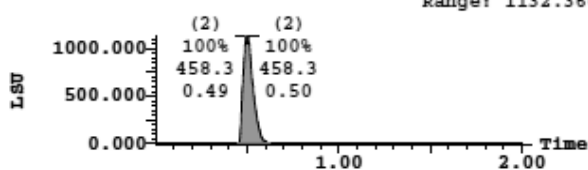
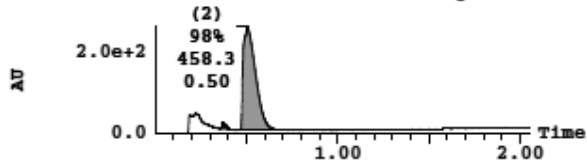


2: UV Detector: TIC

2.657e+2  
Range: 2.657e+2

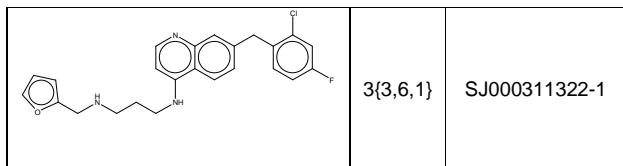
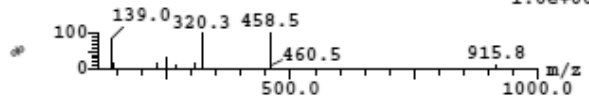
(2) ELSD signal

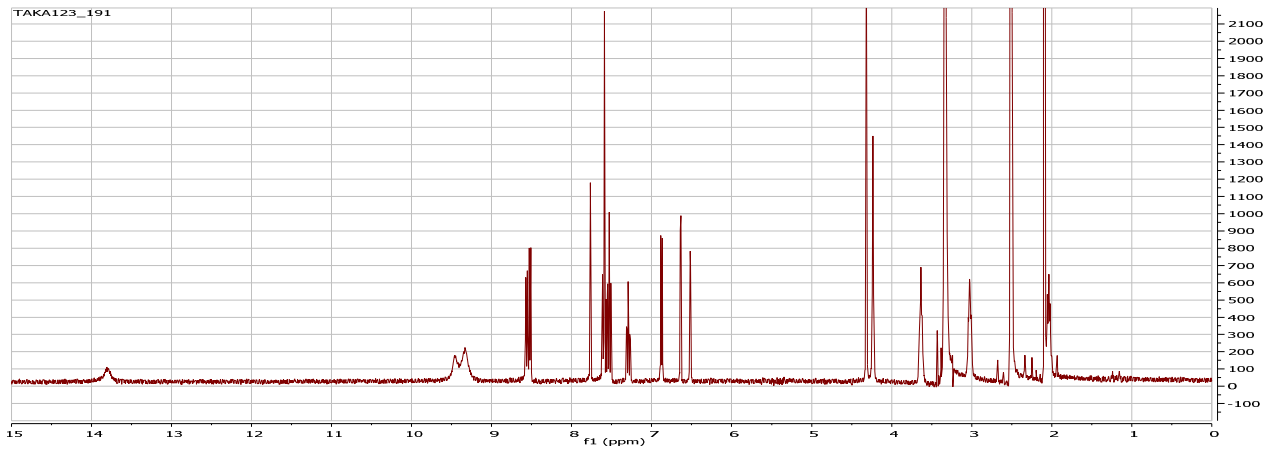
1132.513  
Range: 1132.366



Peak ID	Compound	Time	Mass Found
2	Found	0.48	458.25

1:MS ES+  
1.0e+008





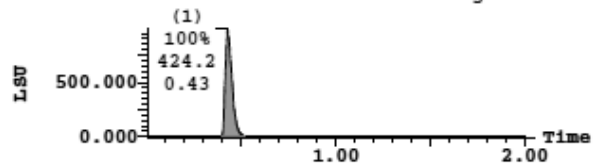
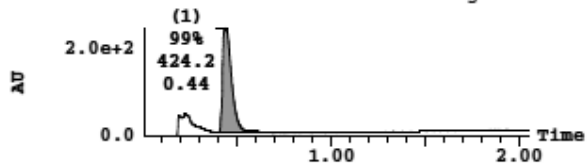
2: UV Detector: TIC

2.47e+2 (2) ELSD Signal

994.057

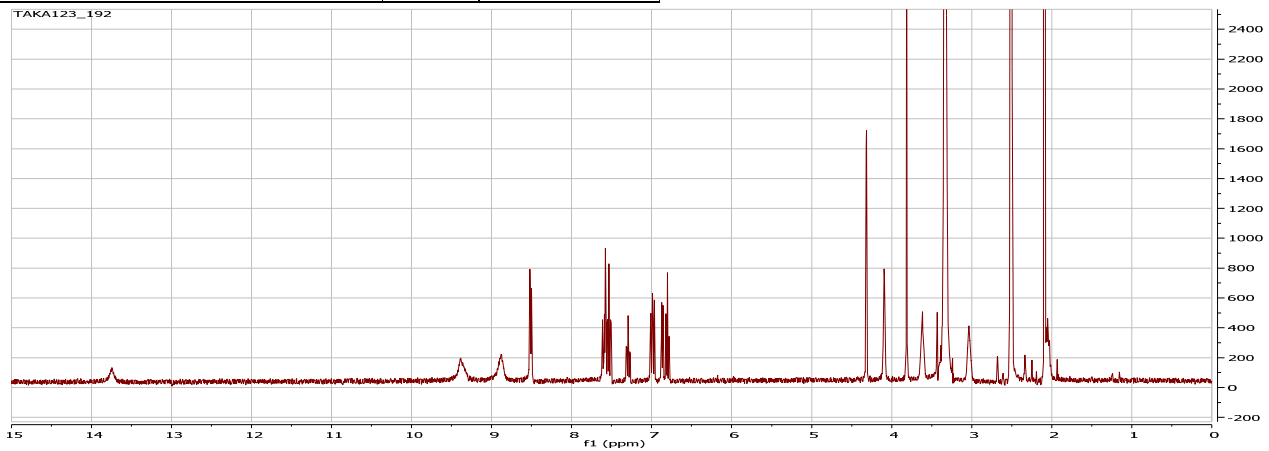
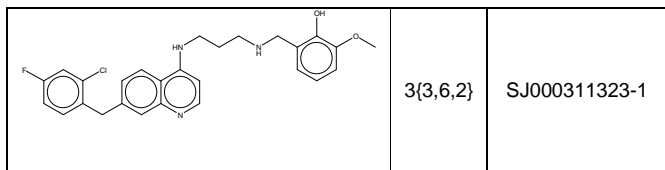
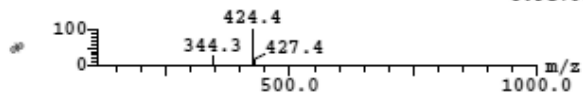
Range: 2.47e+2

Range: 994.007



Peak ID	Compound	Time	Mass Found
1	Found	0.41	424.15

1:MS ES+  
8.9e+007

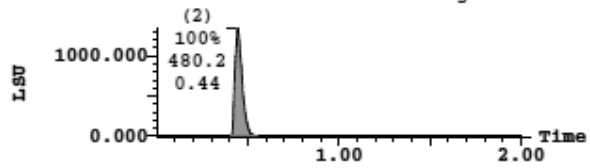
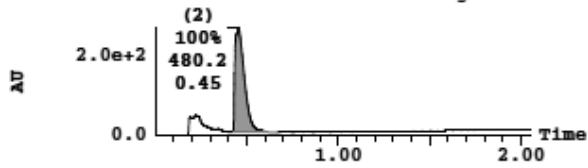


2: UV Detector: TIC

2.687e+2  
Range: 2.687e+2

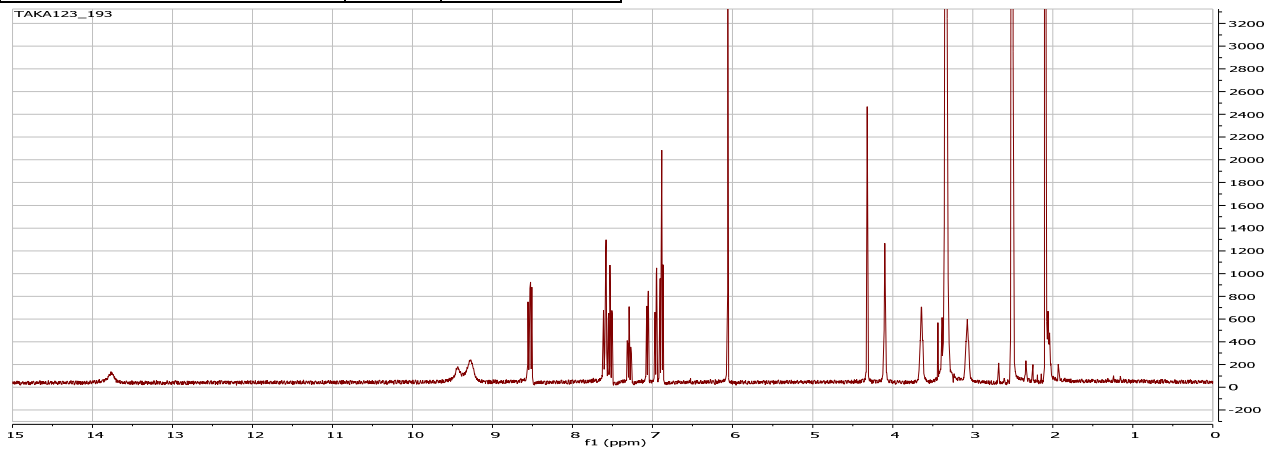
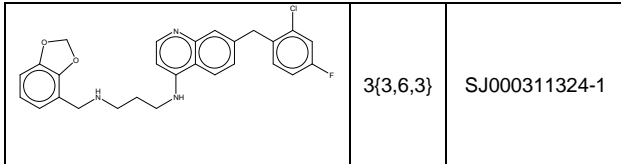
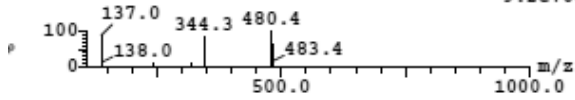
(2) ELSD Signal

1343.382  
Range: 1343.073



Peak ID	Compound	Time	Mass Found
2	Found	0.44	480.18

1:MS ES+  
9.2e+007

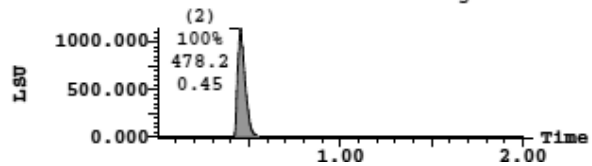
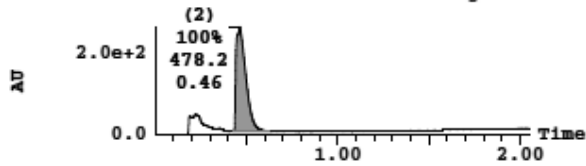


2: UV Detector: TIC

2.66e+2  
Range: 2.66e+2

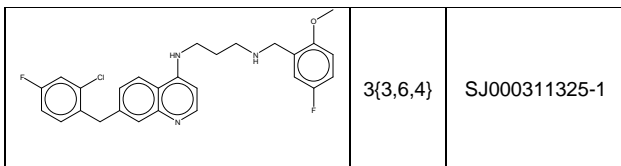
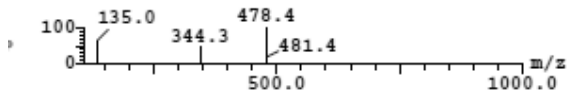
(2) ELSD Signal

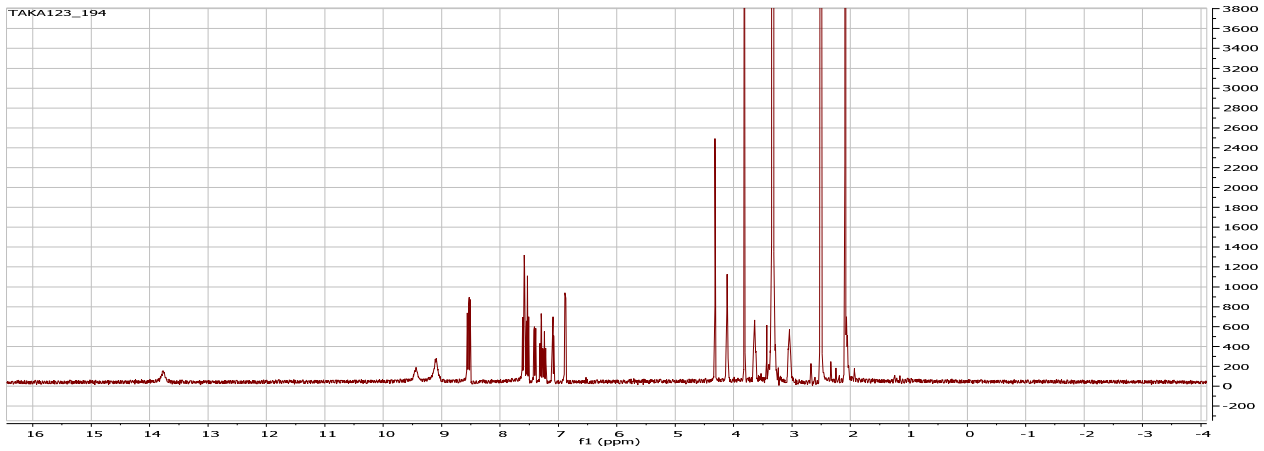
1140.233  
Range: 1140.187



Peak ID	Compound	Time	Mass Found
2	Found	0.44	478.16

1:MS ES+  
1.0e+008



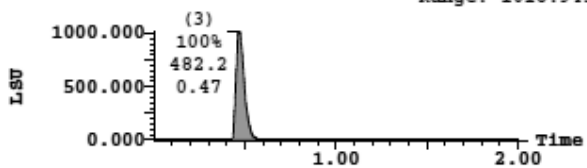
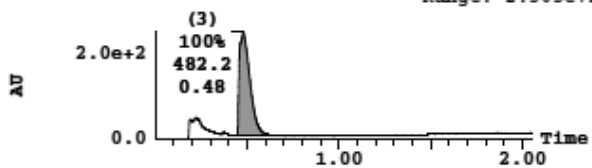


2: UV Detector: TIC

2.505e+2  
Range: 2.505e+2

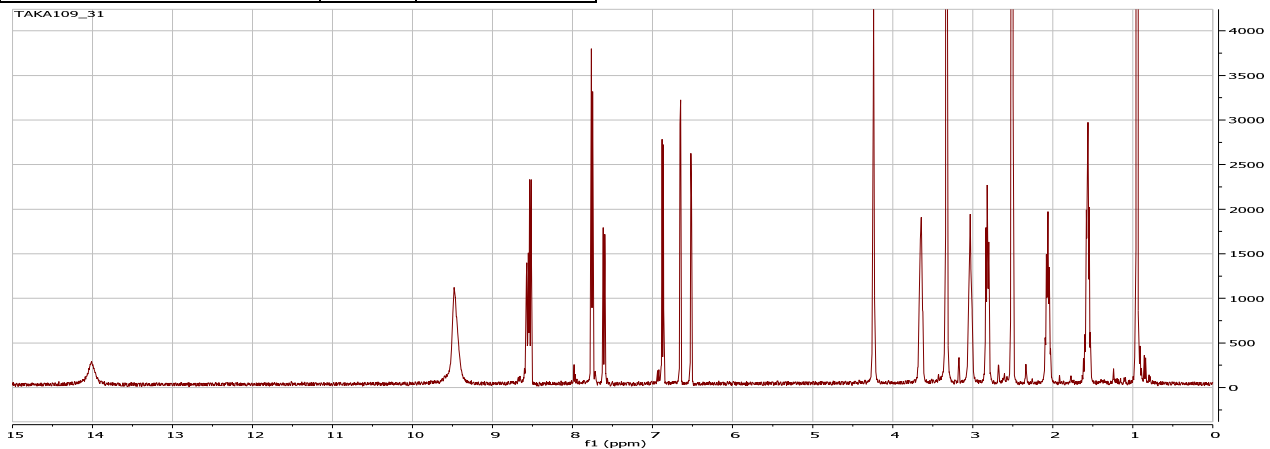
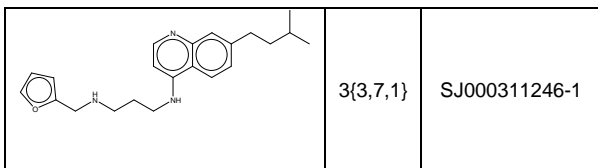
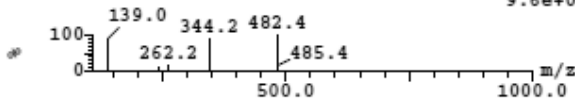
(2) ELSD Signal

1018.996  
Range: 1018.945



Peak ID	Compound	Time	Mass Found
3	Found	0.48	482.17

1:MS ES+  
9.6e+007



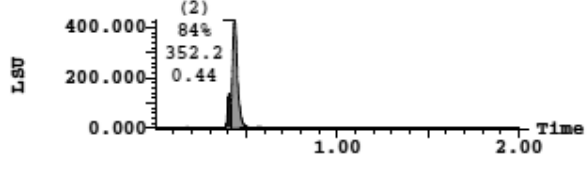
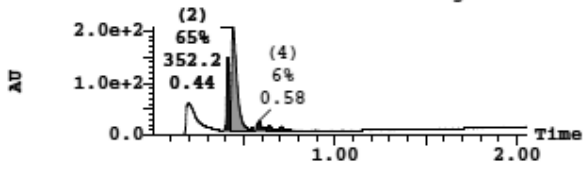


2: UV Detector: TIC

2.073e+2  
Range: 2.073e+2

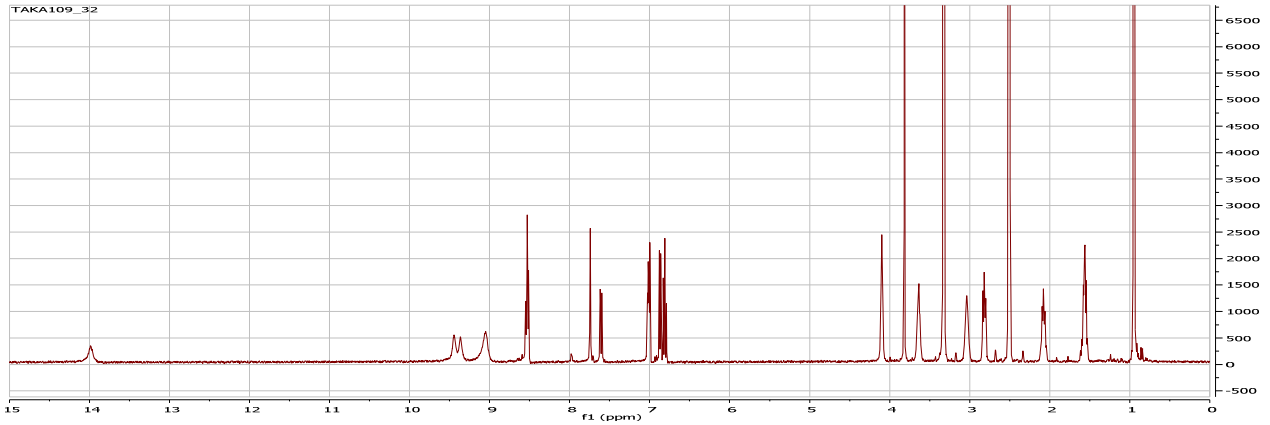
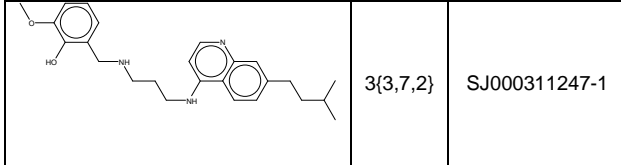
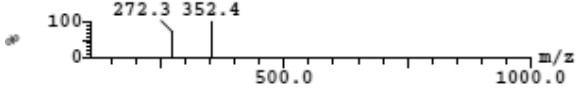
(2) ELSD Signal

429.915  
Range: 429.760



Peak ID	Compound	Time	Mass Found
2	Found	0.42	352.23

1:MS ES+  
7.3e+007

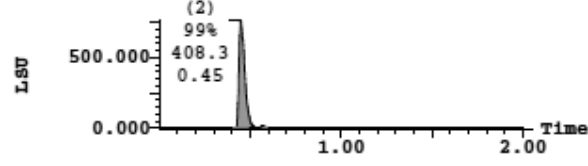
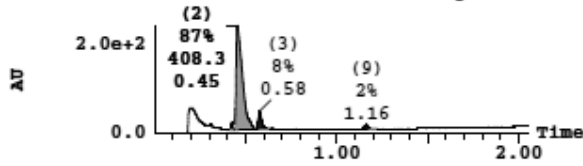


2: UV Detector: TIC

2.432e+2  
Range: 2.432e+2

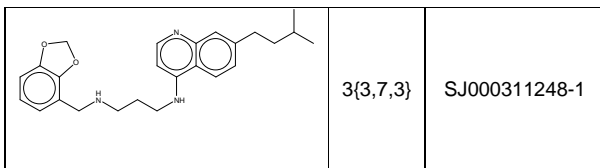
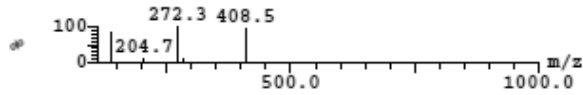
(2) ELSD Signal

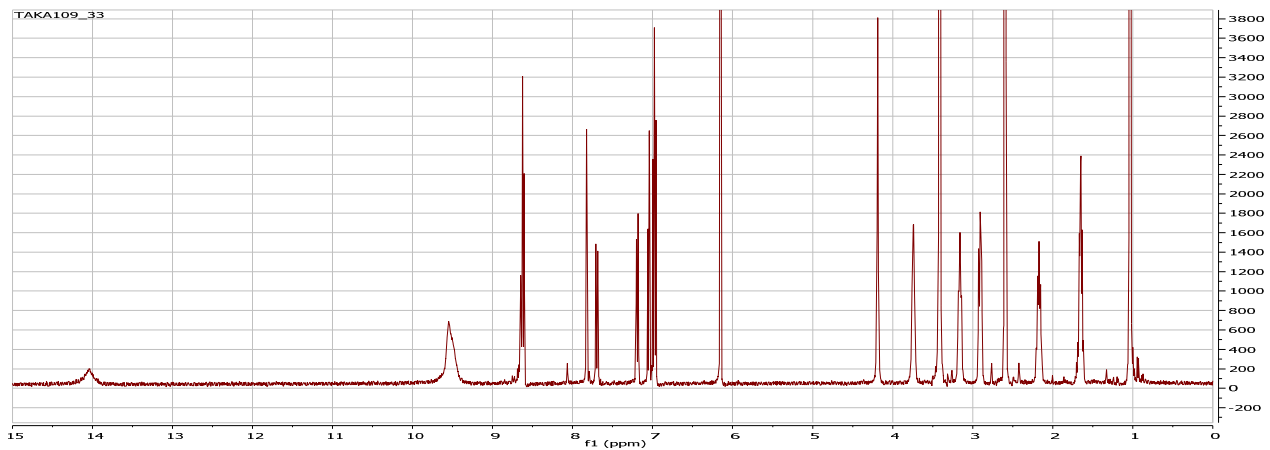
765.502  
Range: 765.464



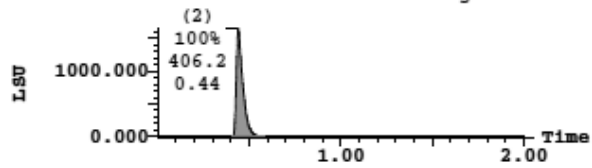
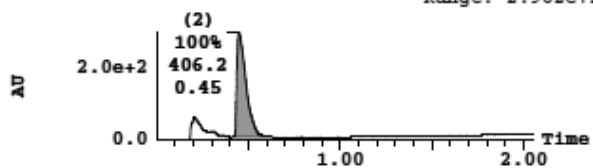
Peak ID	Compound	Time	Mass Found
2	Found	0.44	408.26

1:MS ES+  
8.0e+007



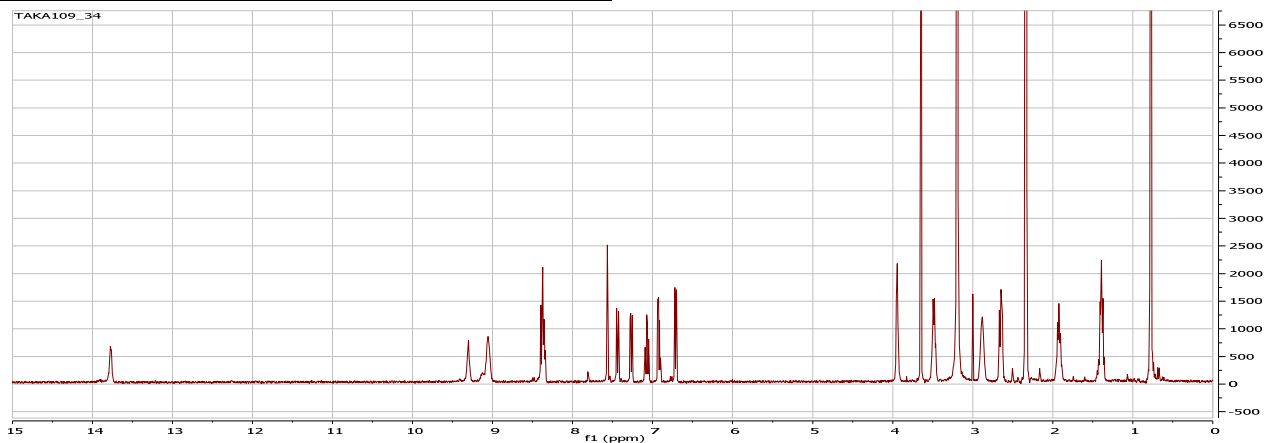
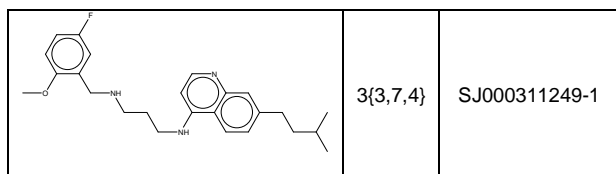
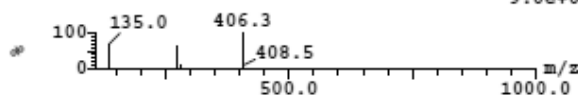


2: UV Detector: TIC 2.982e+2 (2) ELSD signal 1651.719  
 Range: 2.982e+2 Range: 1651.488



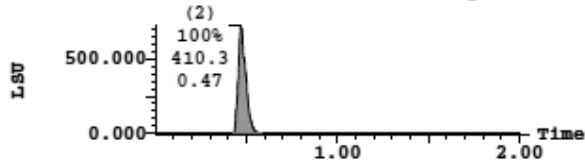
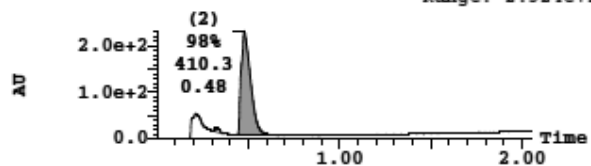
Peak ID	Compound	Time	Mass Found
2	Found	0.44	406.24

1:MS ES+  
9.0e+007



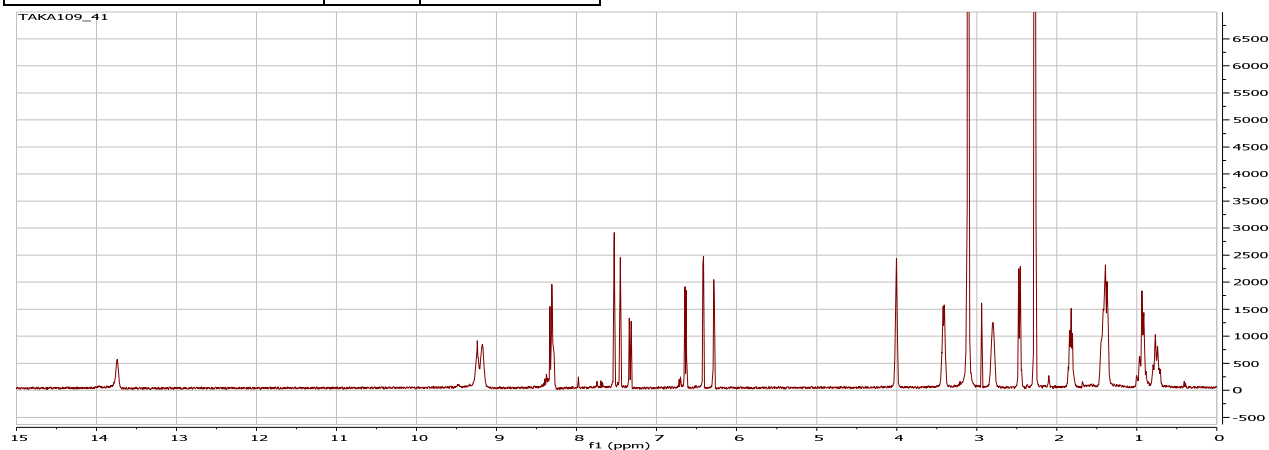
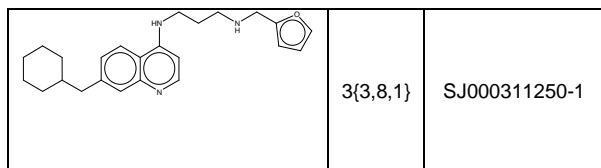
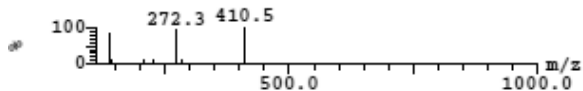
2: UV Detector: TIC 2.324e+2  
Range: 2.324e+2

(2) ELSD Signal 720.869  
Range: 720.826



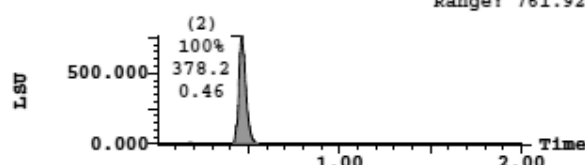
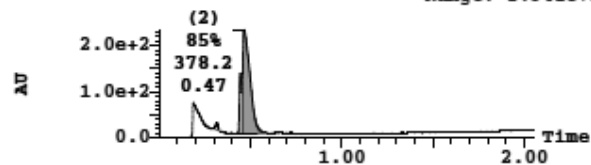
Peak ID	Compound	Time	Mass Found
2	Found	0.48	410.25

1:MS ES+  
9.9e+007



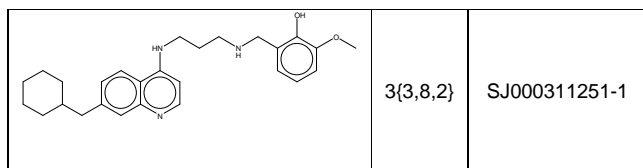
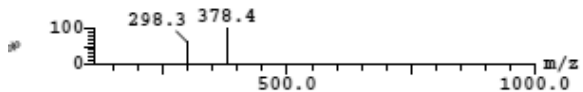
2: UV Detector: TIC 2.341e+2  
Range: 2.341e+2

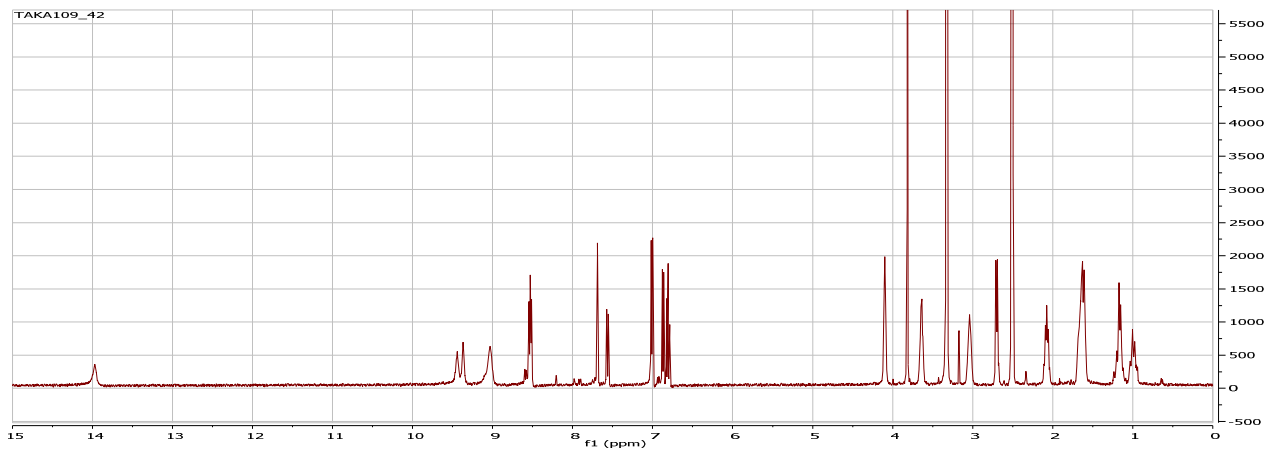
(2) ELSD Signal 761.950  
Range: 761.920



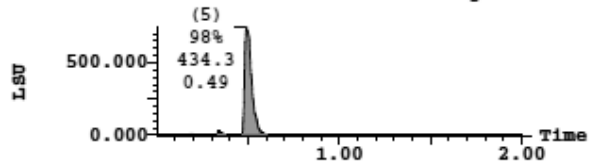
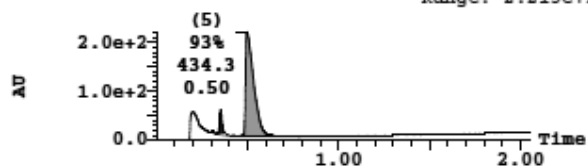
Peak ID	Compound	Time	Mass Found
2	Found	0.44	378.25

1:MS ES+  
7.6e+007



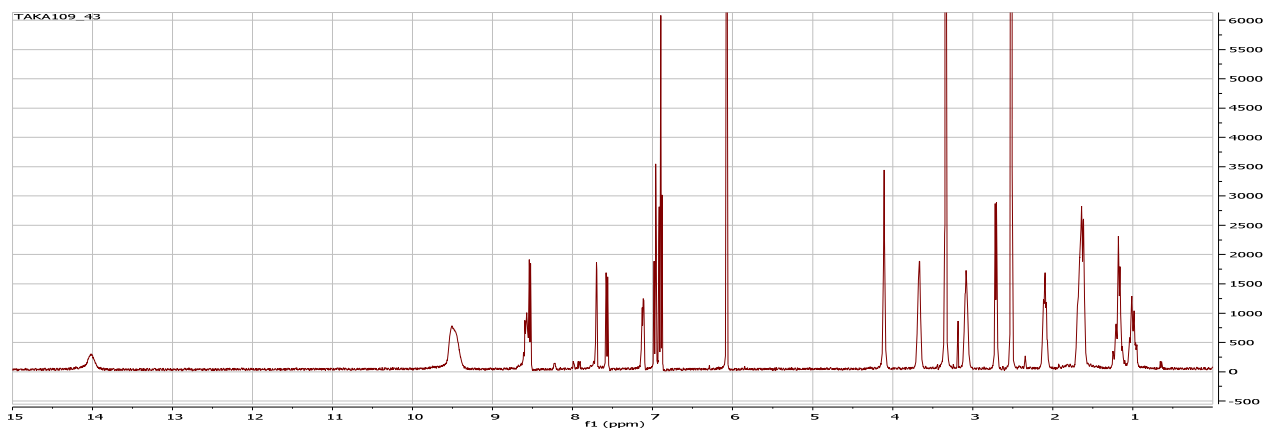
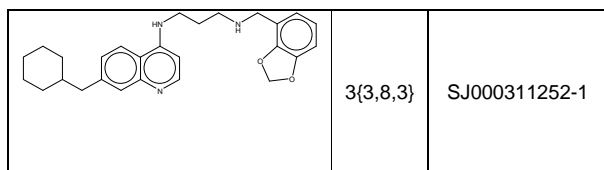
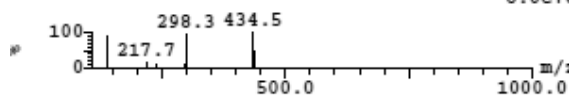


2: UV Detector: TIC 2.213e+2 (2) ELSD Signal 746.412  
 Range: 2.213e+2 Range: 746.382



Peak ID	Compound	Time	Mass Found
5	Found	0.48	434.27

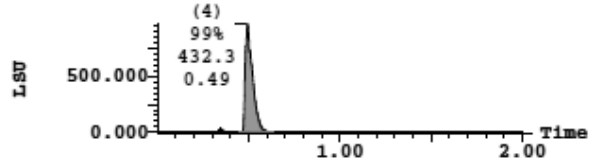
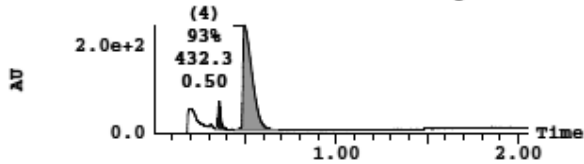
1:MS ES+  
8.0e+007



2: UV Detector: TIC

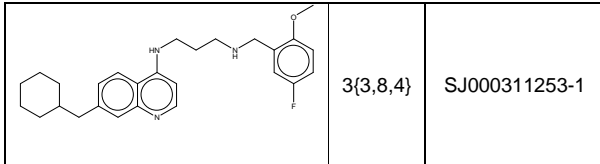
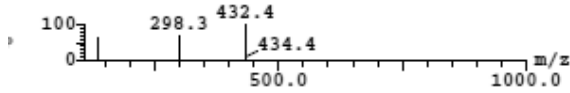
2.479e+2 (2) ELSD Signal  
Range: 2.479e+2

965.782  
Range: 965.695

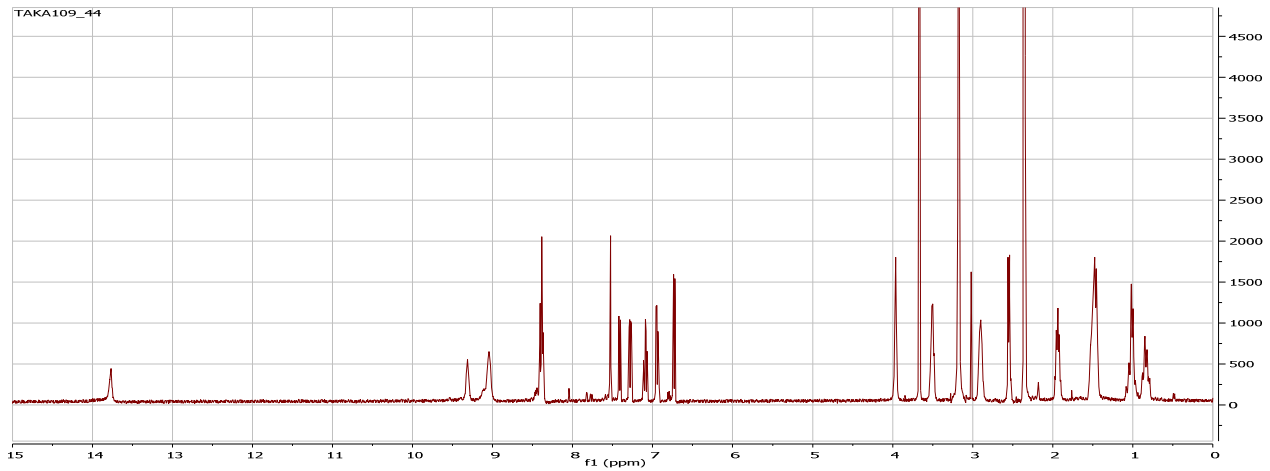


Peak ID	Compound	Time	Mass Found
4	Found	0.49	432.26

1:MS ES+  
9.8e+007



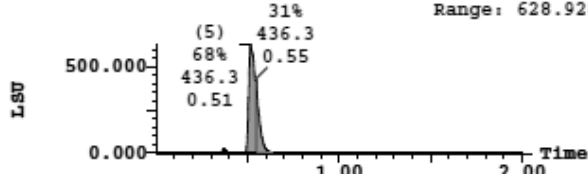
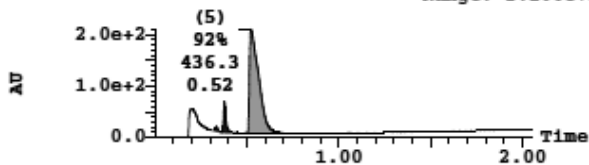
TAKA109\_44



2: UV Detector: TIC

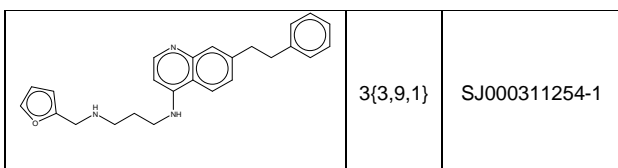
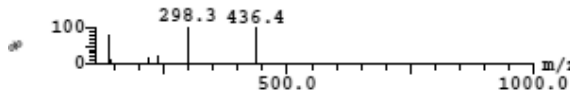
2.106e+2 (2) ELSD Signal  
Range: 2.106e+2

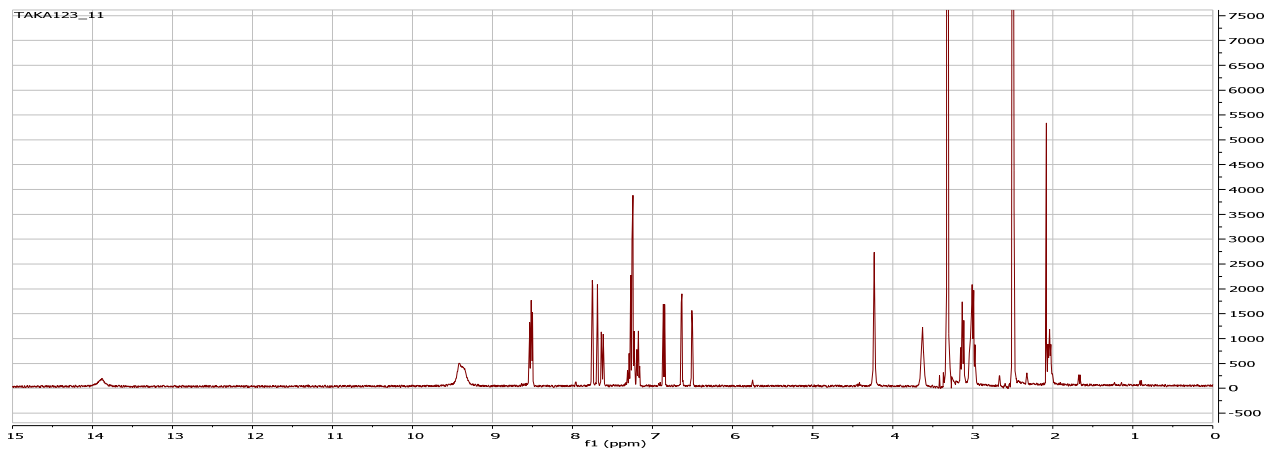
629.029  
Range: 628.928



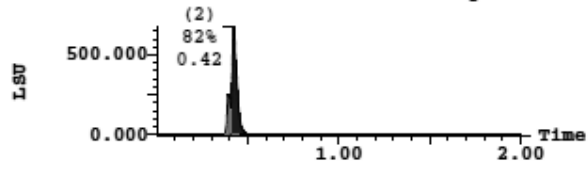
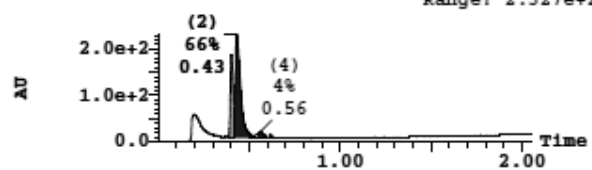
Peak ID	Compound	Time	Mass Found
5	Found	0.51	436.27

1:MS ES+  
8.6e+007



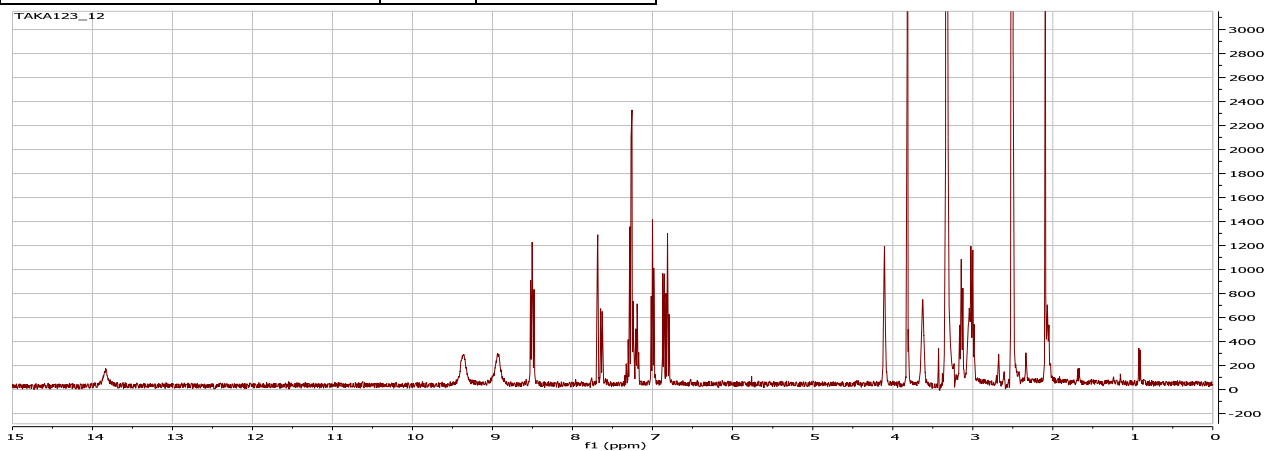
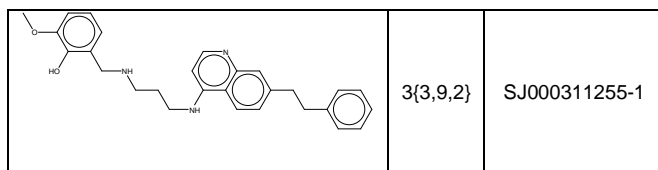
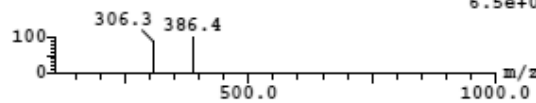


2: UV Detector: TIC 2.327e+2 (2) ELSD signal 676.086  
 Range: 2.327e+2 Range: 676.018



Peak ID	Compound	Time	Mass Found
1	Found	0.40	386.22

1: MS ES+  
6.5e+007

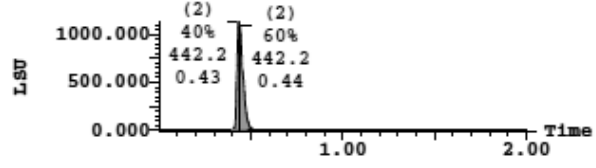
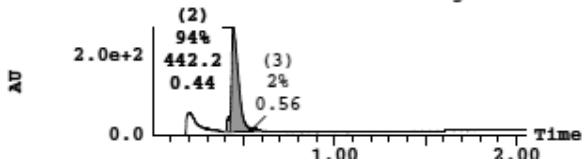


2: UV Detector: TIC

2.734e+2  
Range: 2.733e+2

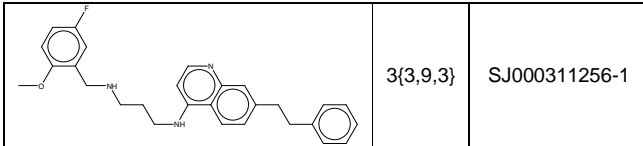
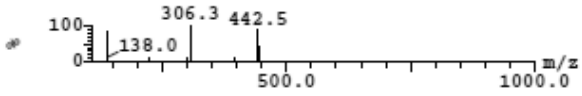
(2) ELSD Signal

1129.778  
Range: 1129.767

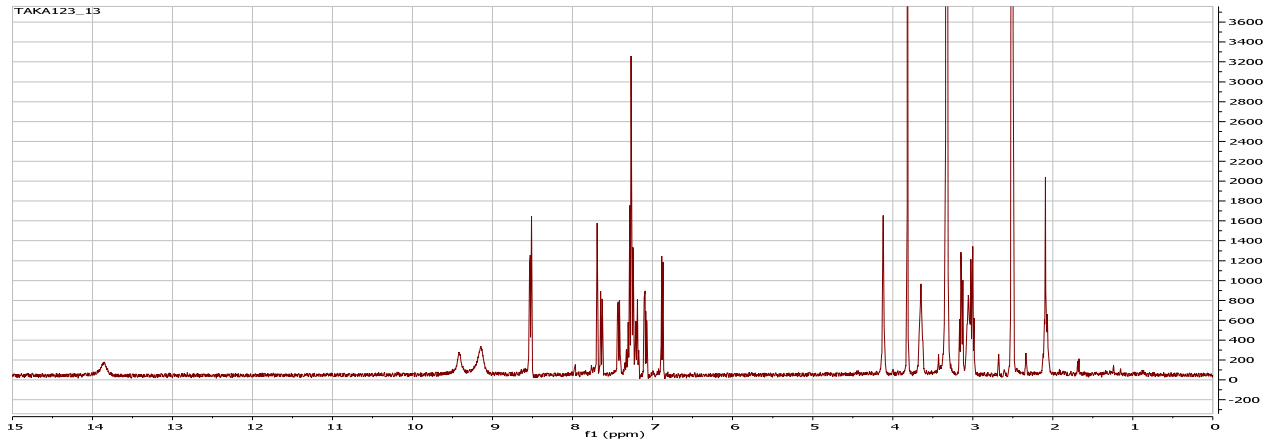


Peak ID	Compound Found	Time	Mass Found
2	Found	0.43	442.24

1:MS ES+  
8.7e+007



TAKA123\_13

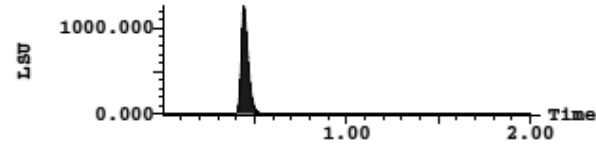
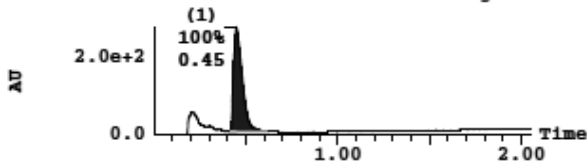


2: UV Detector: TIC

2.8e+2  
Range: 2.8e+2

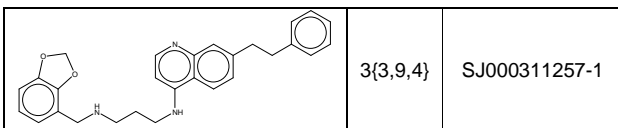
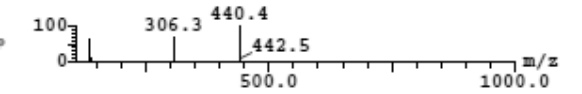
(2) ELSD Signal (1)

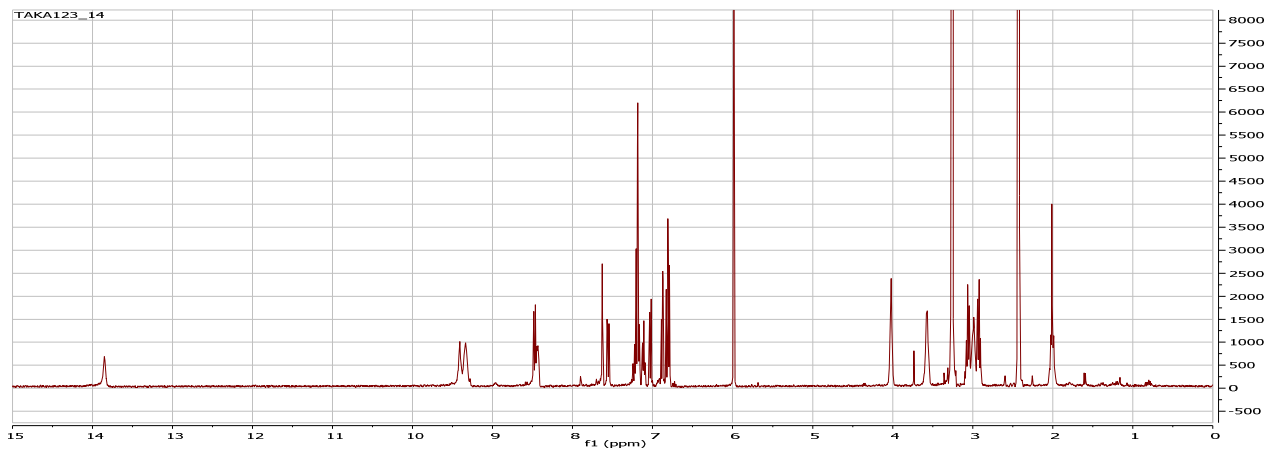
1260.844  
Range: 1260.755



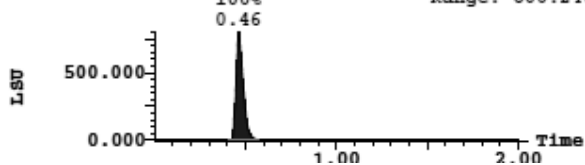
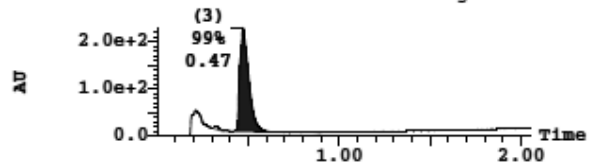
Peak ID	Compound Found	Time	Mass Found
1	Found	0.44	440.4

1:MS ES+  
1.0e+008



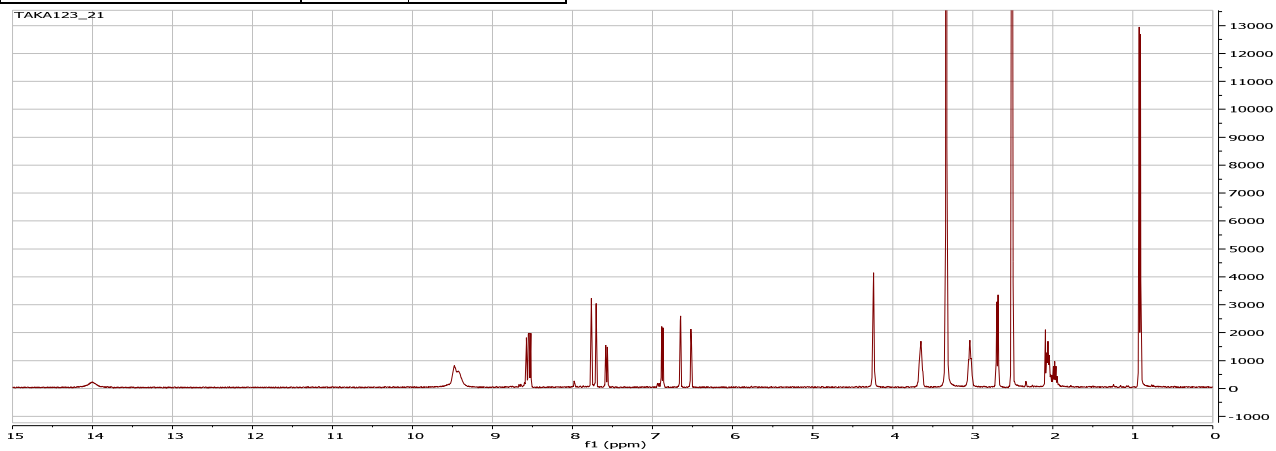
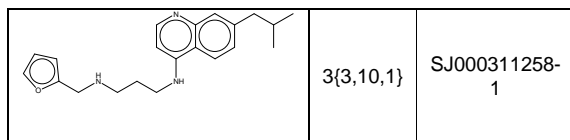
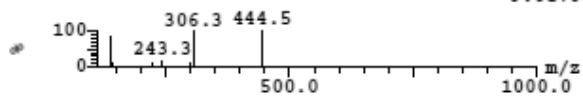


2: UV Detector: TIC 2.294e+2 (2) ELSD Signal (3) 800.374  
 Range: 2.293e+2 100% Range: 800.246  
0.47 0.46



Peak ID	Compound	Time	Mass Found
3		0.45	

1:MS ES+  
9.0e+007





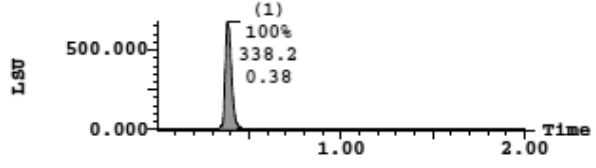
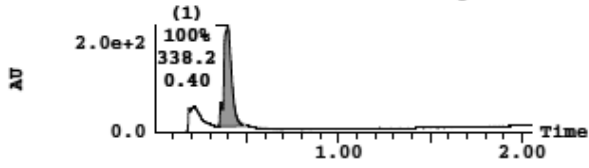
2: UV Detector: TIC

2.435e+2 (2) ELSD Signal

676.609

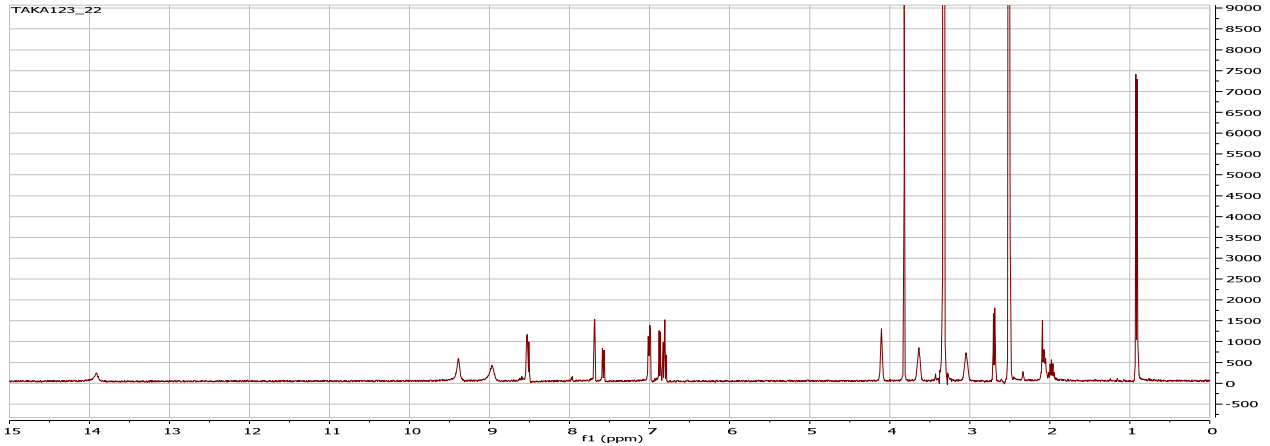
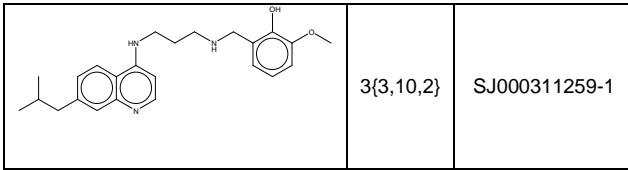
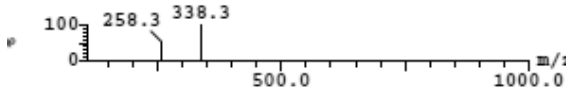
Range: 2.435e+2

Range: 676.514



Peak ID	Compound	Time	Mass Found
1	Found	0.37	338.22

1:MS ES+  
8.6e+007



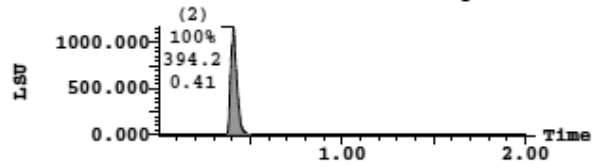
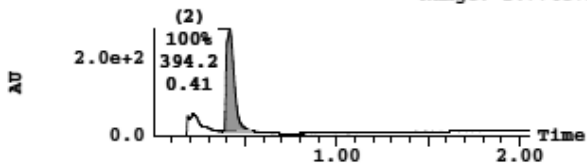
2: UV Detector: TIC

2.774e+2 (2) ELSD Signal

1169.406

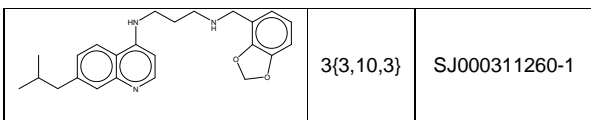
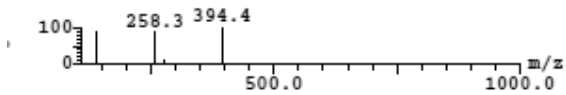
Range: 2.774e+2

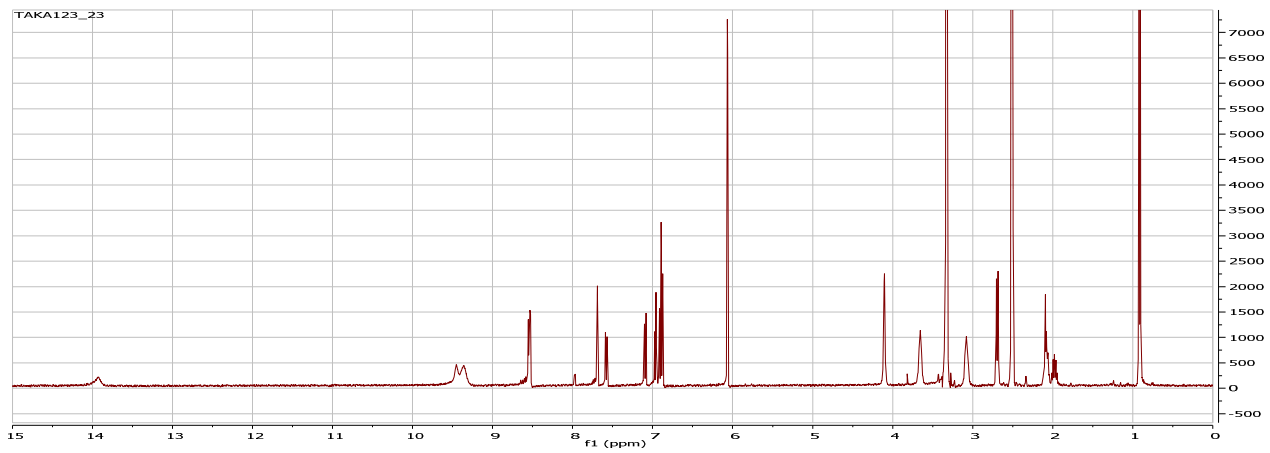
Range: 1169.348



Peak ID	Compound	Time	Mass Found
2	Found	0.39	394.24

1:MS ES+  
9.0e+007



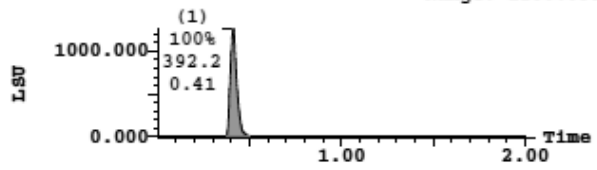
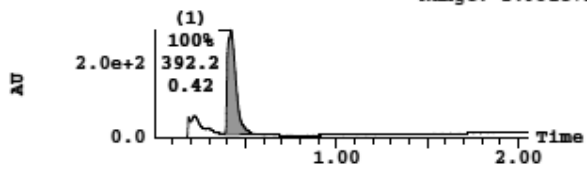


2: UV Detector: TIC

2.931e+2  
Range: 2.931e+2

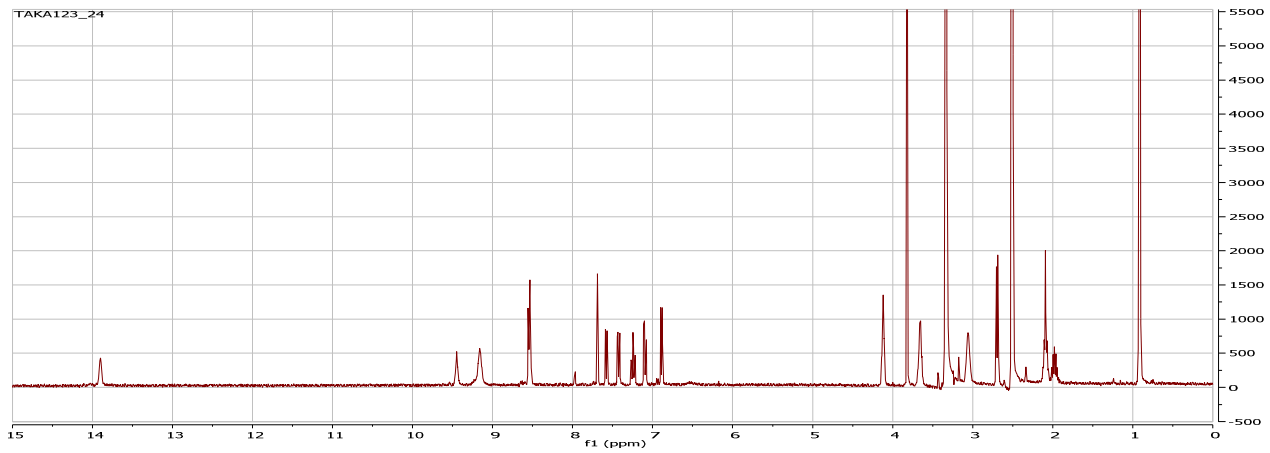
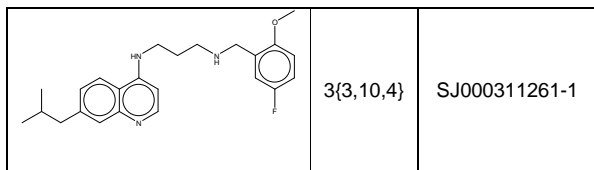
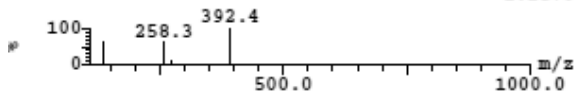
(2) ELSD Signal

1260.165  
Range: 1260.039

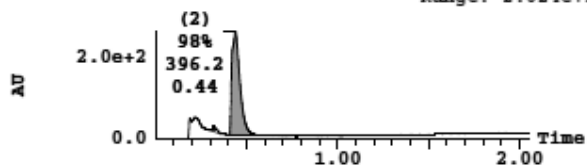


Peak ID	Compound	Time	Mass Found
1	Found	0.40	392.23

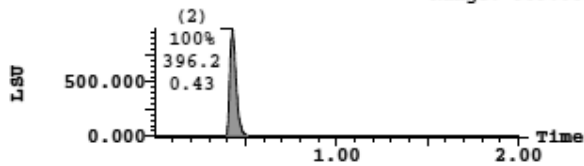
1:MS ES+  
1.1e+008



2: UV Detector: TIC 2.624e+2  
Range: 2.624e+2

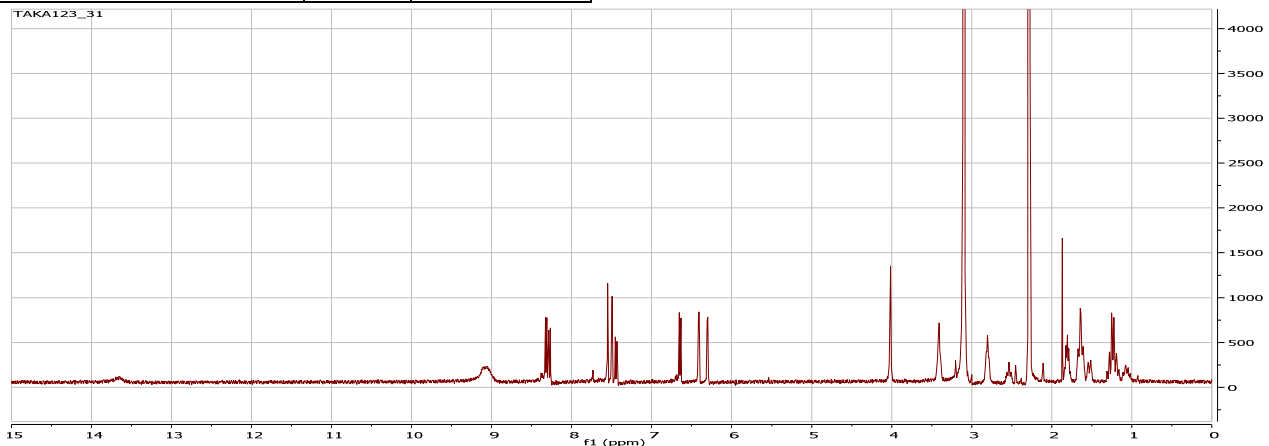
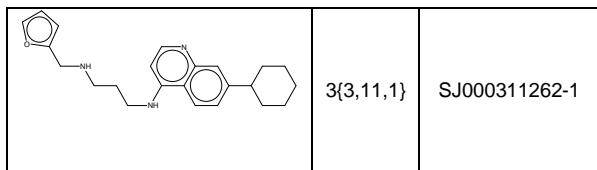
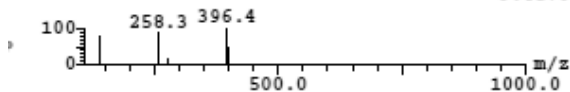


(2) ELSD Signal 989.276  
Range: 989.088

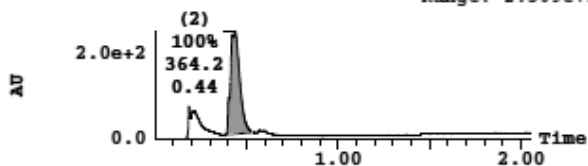


Peak ID	Compound	Time	Mass Found
2	Found	0.42	396.24

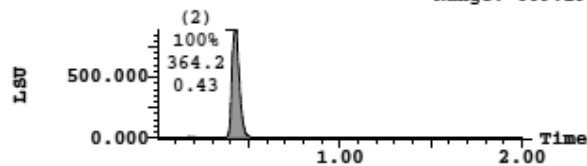
1:MS ES+  
9.4e+007



2: UV Detector: TIC 2.509e+2  
Range: 2.509e+2

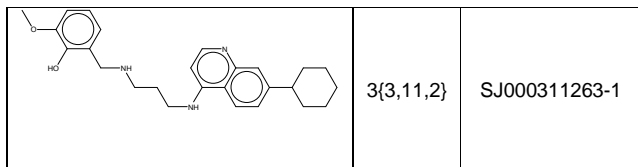
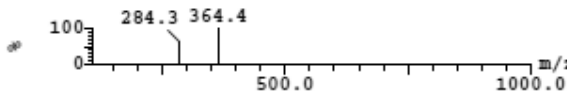


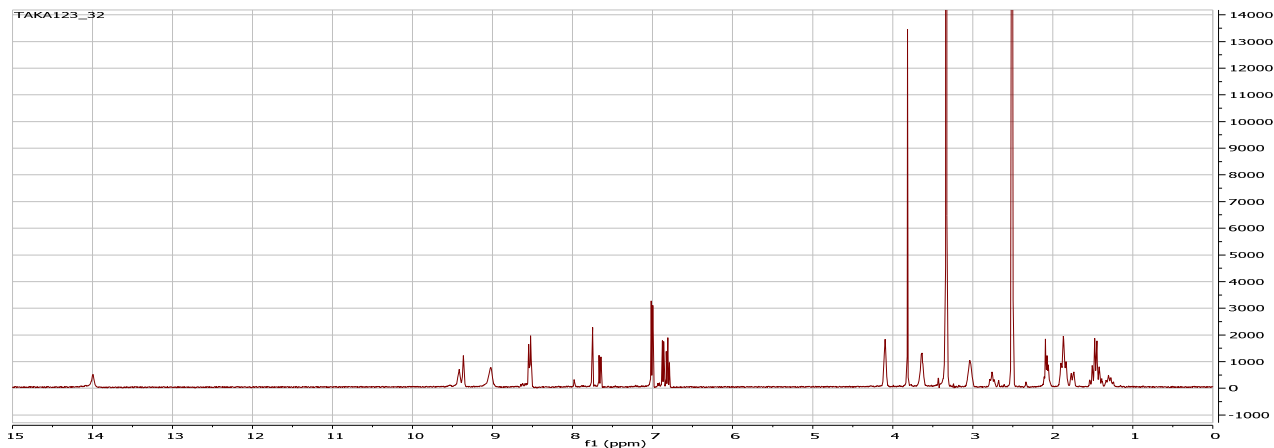
(2) ELSD Signal 889.250  
Range: 889.196



Peak ID	Compound	Time	Mass Found
2	Found	0.40	364.23

1:MS ES+  
8.5e+007



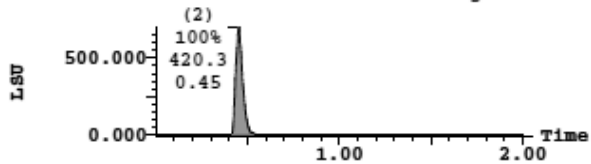
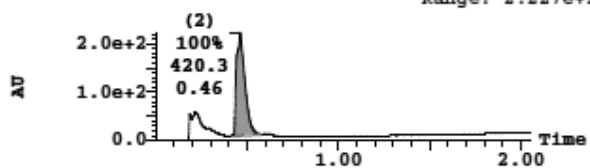


2: UV Detector: TIC

2.227e+2  
Range: 2.227e+2

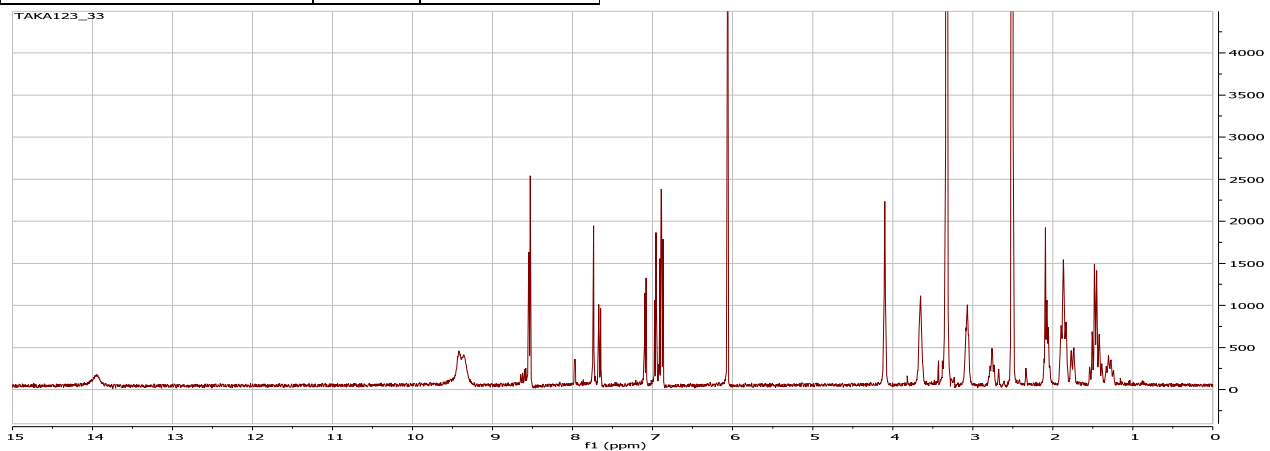
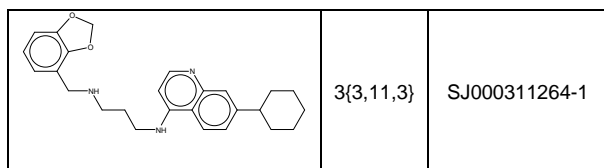
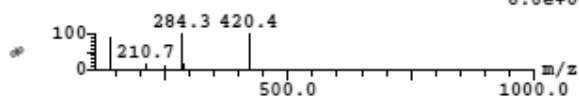
(2) ELSD Signal

699.130  
Range: 699.047



Peak ID	Compound	Time	Mass Found
2	Found	0.44	420.28

1:MS ES+  
8.6e+007

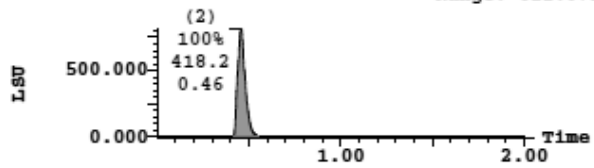
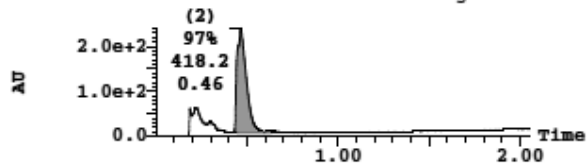


2: UV Detector: TIC

2.412e+2  
Range: 2.412e+2

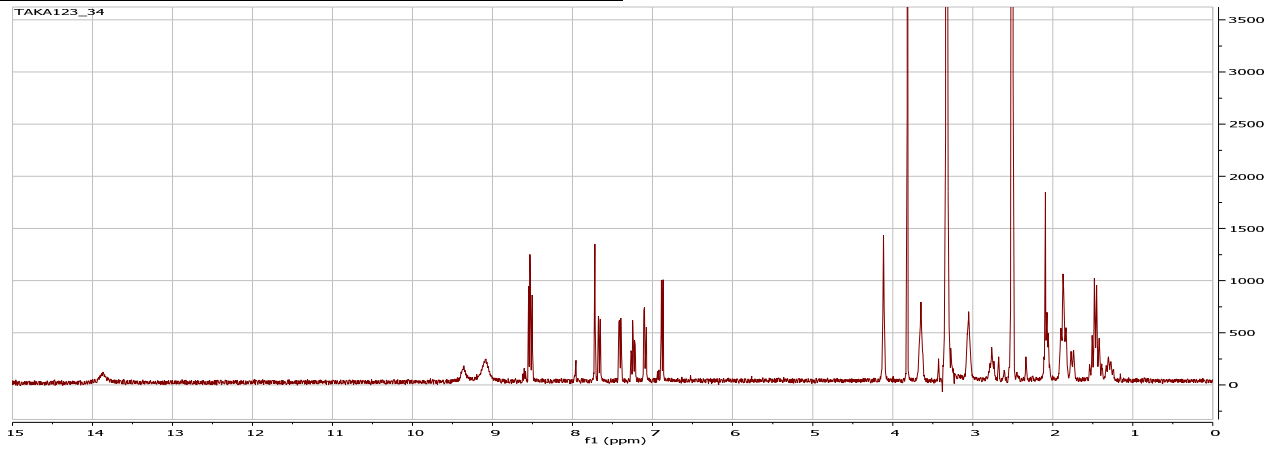
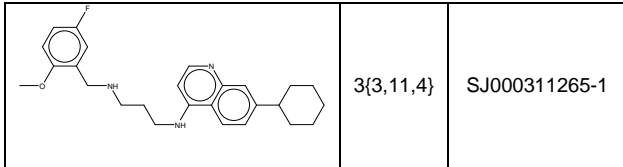
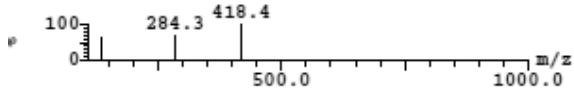
(2) ELSD Signal

811.696  
Range: 811.672



Peak ID	Compound	Time	Mass Found
2	Found	0.45	418.24

1:MS ES+  
1.1e+008

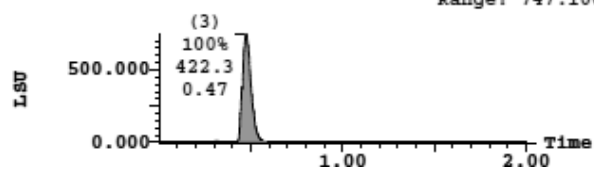
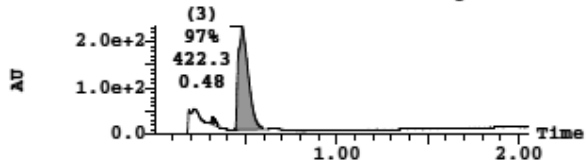


2: UV Detector: TIC

2.342e+2  
Range: 2.342e+2

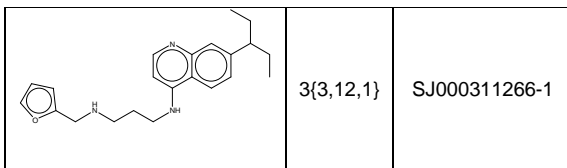
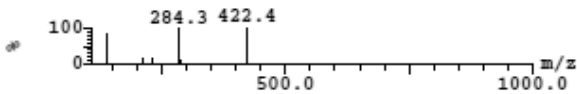
(2) ELSD Signal

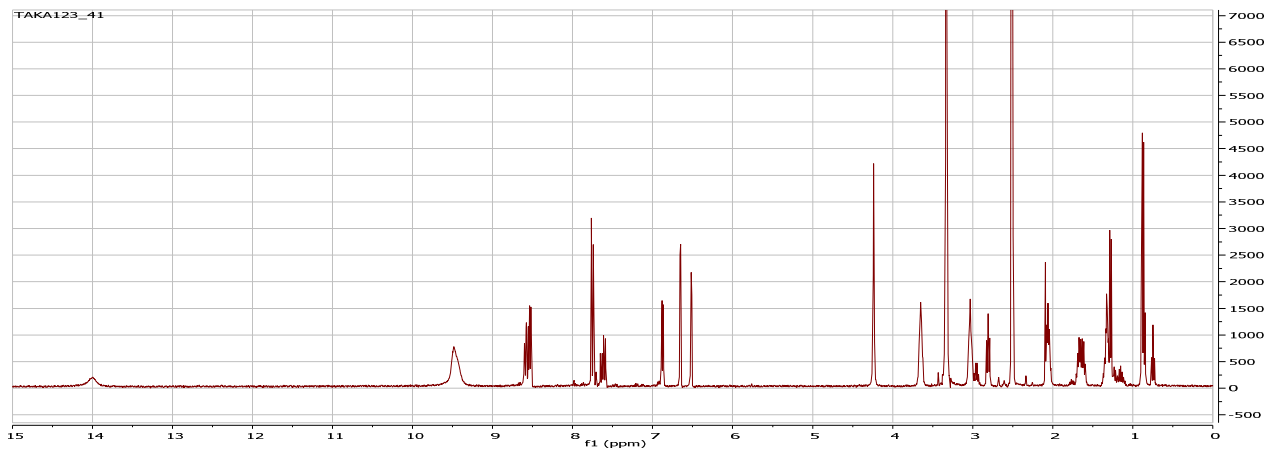
747.114  
Range: 747.106



Peak ID	Compound	Time	Mass Found
3	Found	0.46	422.25

1:MS ES+  
1.0e+008



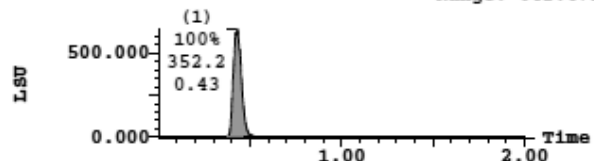
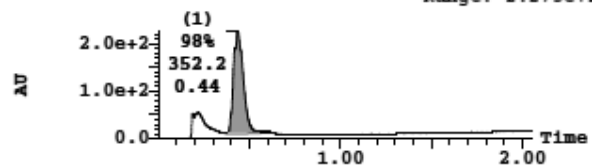


2: UV Detector: TIC

2.275e+2  
Range: 2.275e+2

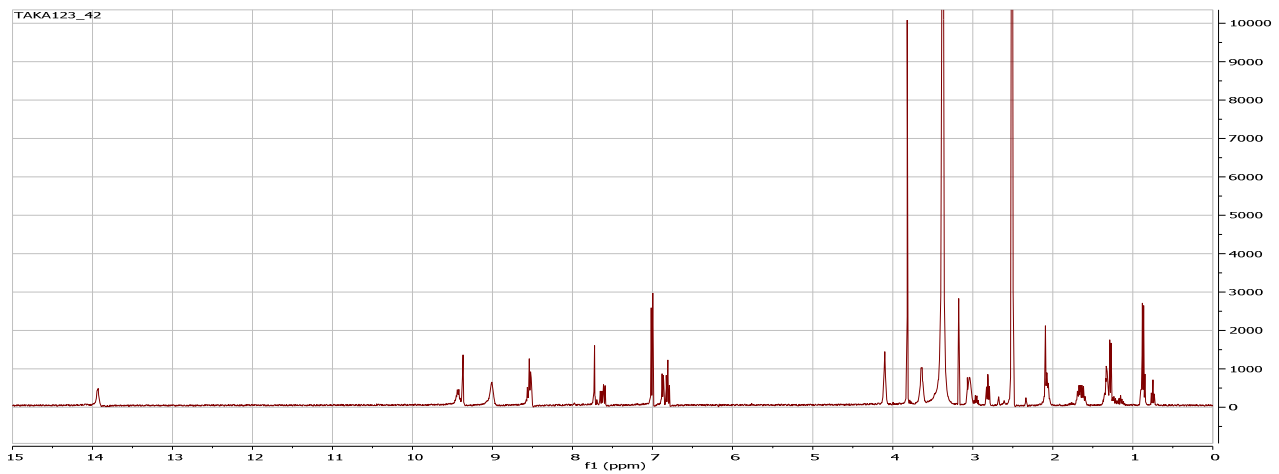
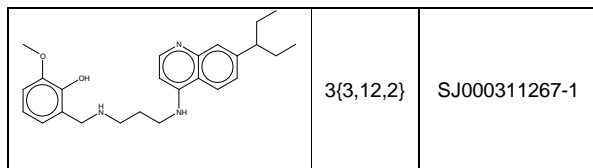
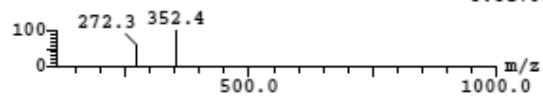
(2) ELSD Signal

642.522  
Range: 642.471

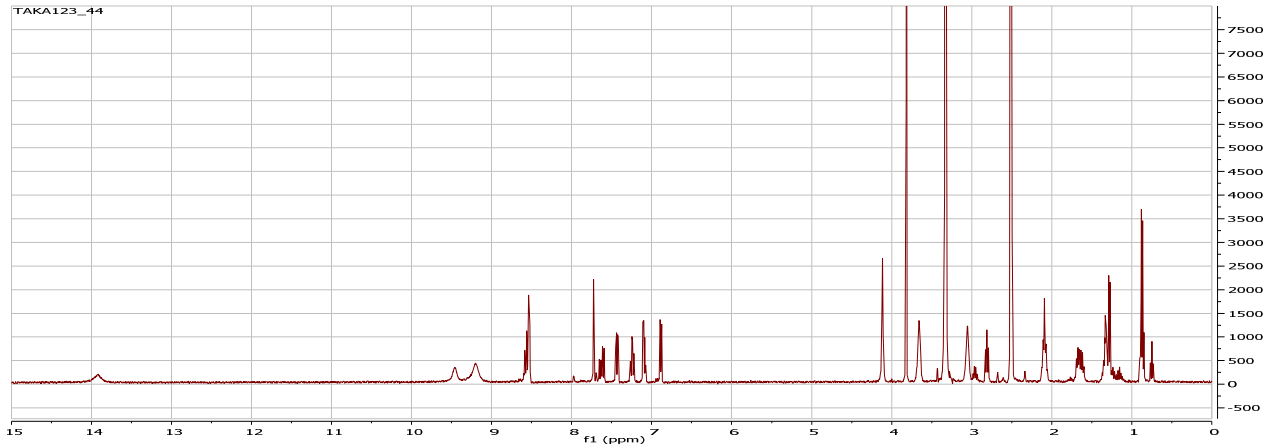


Peak ID	Compound	Time	Mass Found
1	Found	0.40	352.23

1:MS ES+  
8.8e+007

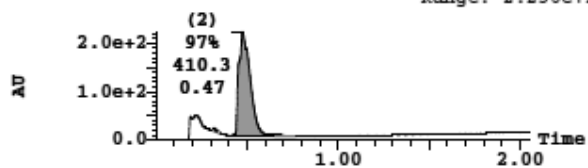






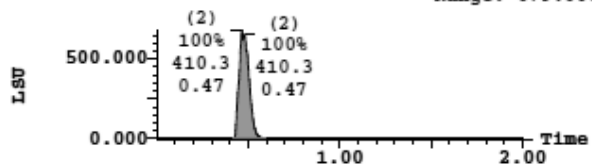
2: UV Detector: TIC

2.236e+2  
Range: 2.236e+2



(2) ELSD signal

679.680  
Range: 679.660



Peak ID	Compound	Time	Mass Found
2	Found	0.46	410.25

1:MS ES+  
1.1e+008

