LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072617\
Data File : BF097104.D
Acq On : 27 Jul 2017 4:38
Operator : SJ/JU
Sample : I4397-01
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T-1A-14.5-15.0-072117

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.657	129	131	150	rBV2	90544	257084	10.40%	1.259%
2	3.234	222	229	238	rVB2	20893	41892	1.69%	0.205%
3	4.646	465	469	483	rBV	162848	256020	10.35%	1.254%
4	5.098	542	546	565	rBV	2292981	2473094	100.00%	12.110%
5	6.163	721	727	741	rBV	2041725	2283791	92.35%	11.183%
6	6.269	741	745	749	rBV	2237688	2123015	85.84%	10.396%
7	6.498	780	784	790	rBV	581594	510471	20.64%	2.500%
8	6.651	806	810	814	rBV	1698633	1560938	63.12%	7.643%
9	7.063	876	880	883	rBV	1318178	1181905	47.79%	5.787%
10	7.204	900	904	910	rVB	26687	28745	1.16%	0.141%
11	7.704	985	989	995	rBV	35499	39704	1.61%	0.194%
12	7.781	998	1002	1006	rBV	770874	622880	25.19%	3.050%
13	8.857	1181	1185	1188	rBV	2037098	1810669	73.21%	8.866%
14	9.257	1249	1253	1256	rBV	330179	253648	10.26%	1.242%
15	9.528	1295	1299	1302	rBV	624053	551066	22.28%	2.698%
16	9.980	1373	1376	1379	rVB	38242	29358	1.19%	0.144%
17	10.310	1429	1432	1441	rBV	988490	930517	37.63%	4.556%
18	10.451	1453	1456	1465	rVB	44452	49637	2.01%	0.243%
19	10.898	1529	1532	1535	rBV	43419	35665	1.44%	0.175%
20	10.998	1546	1549	1552	rBV	562674	515691	20.85%	2.525%
21	11.022	1552	1553	1557	rVV	224949	151235	6.12%	0.741%
22	11.075	1559	1562	1567	rBV	73931	64383	2.60%	0.315%
23	11.251	1586	1592	1598	rBV3	52645	60846	2.46%	0.298%
24	11.504	1628	1635	1637	rBV	22335	25446	1.03%	0.125%
25	11.533	1637	1640	1642	rBV	27005	24735	1.00%	0.121%
26	11.557	1642	1644	1646	rBV	47474	39253	1.59%	0.192%
27	11.610	1650	1653	1656	rBV	32428	33954	1.37%	0.166%
28	12.069	1727	1731	1737	rVB	87827	94112	3.81%	0.461%
29	12.204	1751	1754	1759	rBV	397598	348864	14.11%	1.708%
30	12.339	1774	1777	1784	rVB3	21948	35261	1.43%	0.173%
31	12.433	1788	1793	1796	rVV	301246	329589	13.33%	1.614%
32	12.586	1815	1819	1822	rVB	1603269	1454825	58.83%	7.124%
33	12.657	1826	1831	1834	rBV4	18108	31604	1.28%	0.155%
34	12.763	1846	1849	1854	rVB	43153	42609	1.72%	0.209%

LSC Area Percent Report

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Misc :
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Instrument : BNA_F
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Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
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Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.151	1911	1915	1919	rBV6	22666	50548	2.04%	0.248%
36	13.274	1933	1936	1940	rBV	22183	27727	1.12%	0.136%
37	13.380	1951	1954	1956	rBV	26636	26190	1.06%	0.128%
38	13.480	1968	1971	1972	rBV	32774	29643	1.20%	0.145%
39	13.498	1972	1974	1978	rVB	65274	74594	3.02%	0.365%
40	13.627	1991	1996	1999	rBV2	576268	674014	27.25%	3.300%
41	13.651	1999	2000	2005	rVB	138930	95904	3.88%	0.470%
42	14.198	2091	2093	2094	rBV	40040	31275	1.26%	0.153%
43	14.621	2162	2165	2171	rVB	123091	206993	8.37%	1.014%
44	14.927	2214	2217	2221	rBV	75206	91634	3.71%	0.449%
45	14.980	2222	2226	2229	rBV	311072	339847	13.74%	1.664%
46	16.286	2446	2448	2454	rBV7	34624	48498	1.96%	0.237%
47	16.480	2479	2481	2486	rBV5	38579	74172	3.00%	0.363%
48	16.827	2538	2540	2547	rBV7	49886	97809	3.95%	0.479%
49	17.127	2589	2591	2594	rBV3	33927	31482	1.27%	0.154%
50	17.474	2648	2650	2659	rVB10	30393	38760	1.57%	0.190%
51	18.245	2779	2781	2784	rBV3	29637	40225	1.63%	0.197%
52	18.462	2817	2818	2823	rBV5	29057	26190	1.06%	0.128%
53	18.598	2839	2841	2848	rBV7	36092	60360	2.44%	0.296%
54	18.803	2874	2876	2877	rBV2	32786	26657	1.08%	0.131%
55	19.350	2967	2969	2974	rBV5	24656	36889	1.49%	0.181%

Sum of corrected areas: 20421917

LSC Report - Integrated Chromatogram

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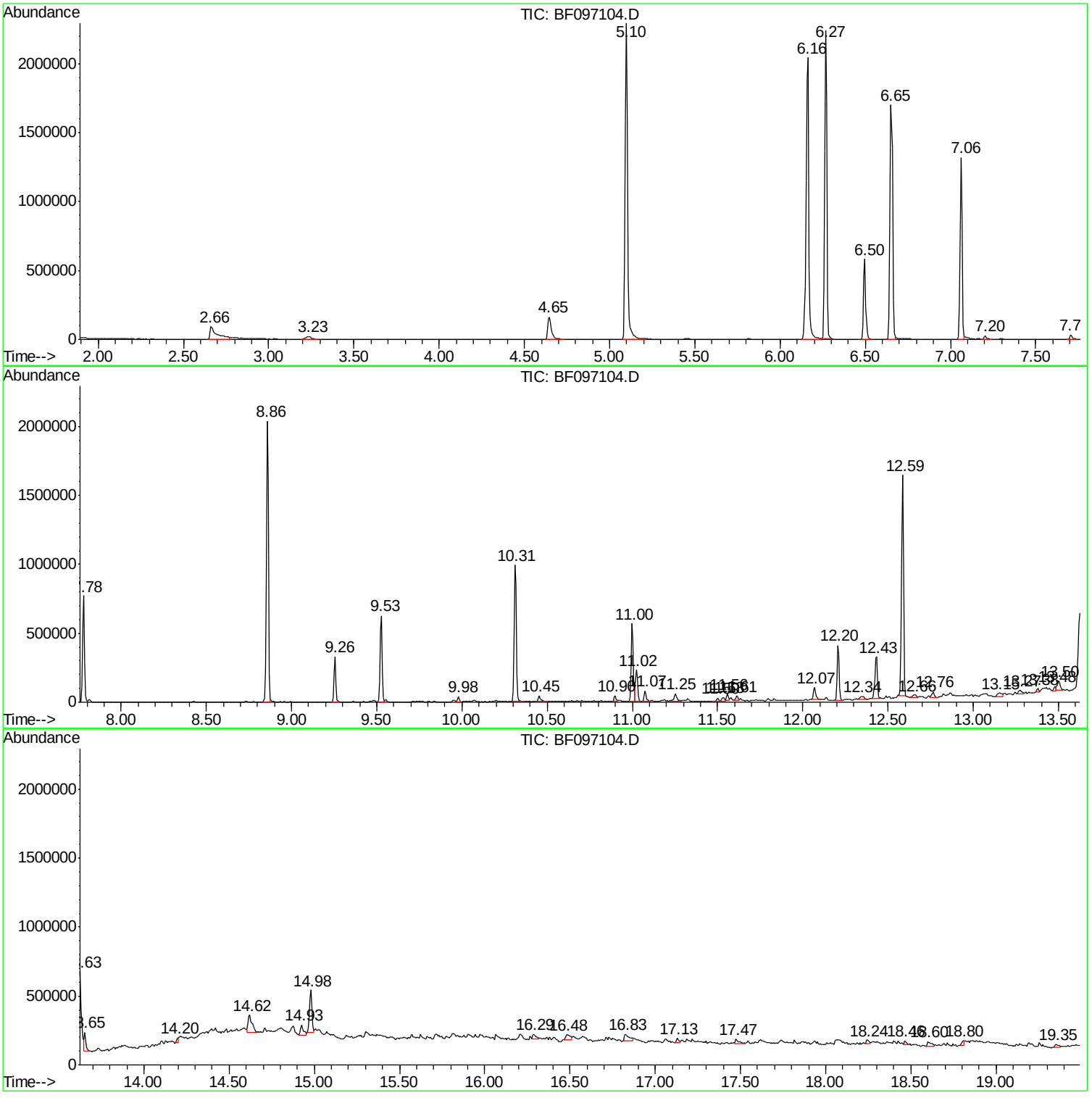
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
T-1A-14.5-15.0-072117

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\HPCHEM1\BNA F\DATA\BF072617\
Data File : BF097104.D
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Instrument : BNA_F
ClientSampleId : T-1A-14.5-15.0-072117

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
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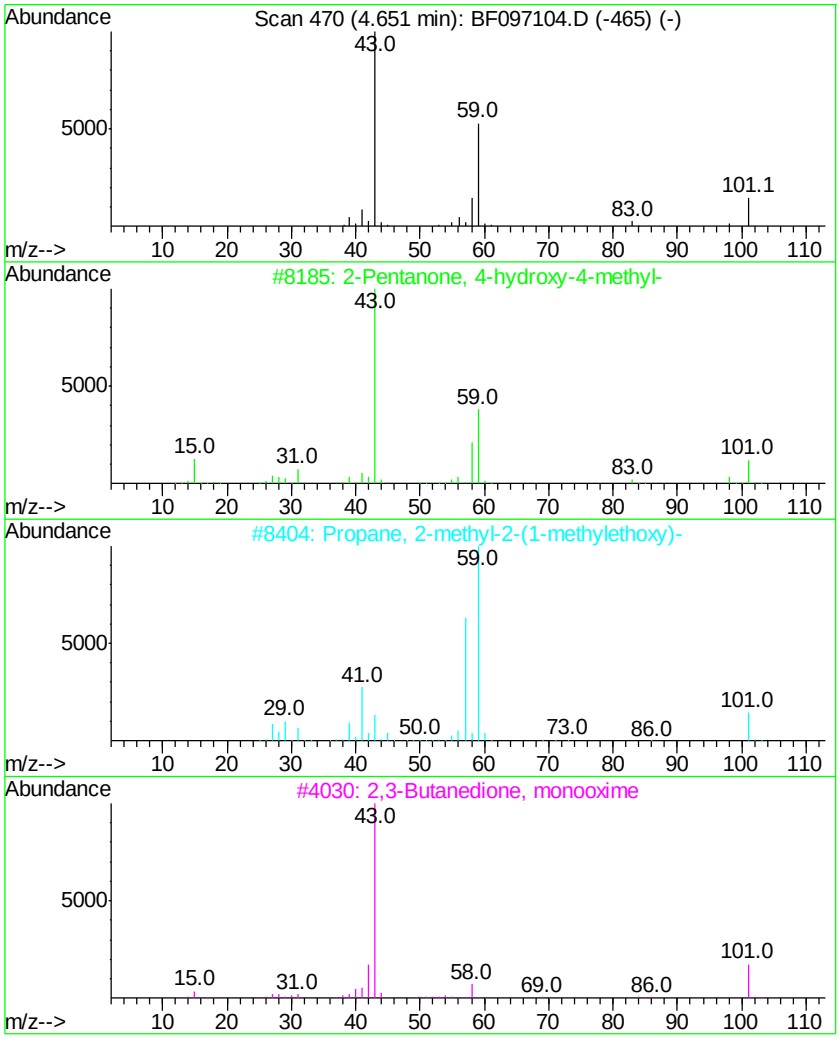
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

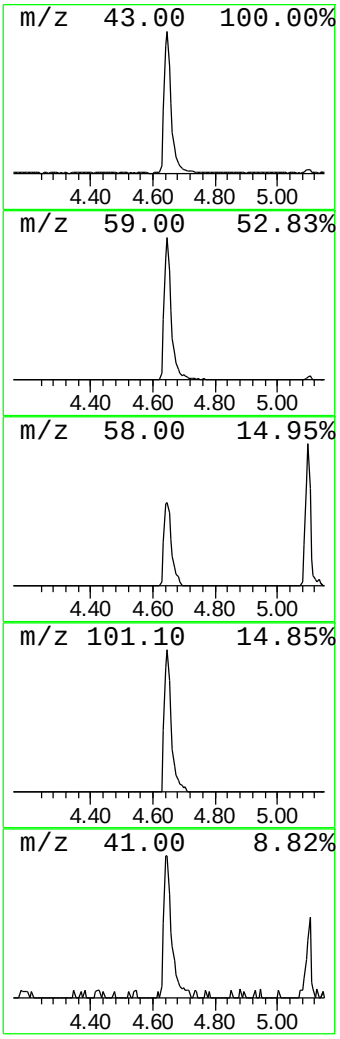
****

Peak Number 2 unknown4.65 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.65	10.03 ng	256020	1,4-Dichlorobenzene-d4	6.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9
5	2-Butanone, 3-ethoxy-3-methyl-	130	C7H14O2	036687-99-7	9





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Data File : BF097104.D
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Operator : SJ/JU
Sample : I4397-01
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T-1A-14.5-15.0-072117

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

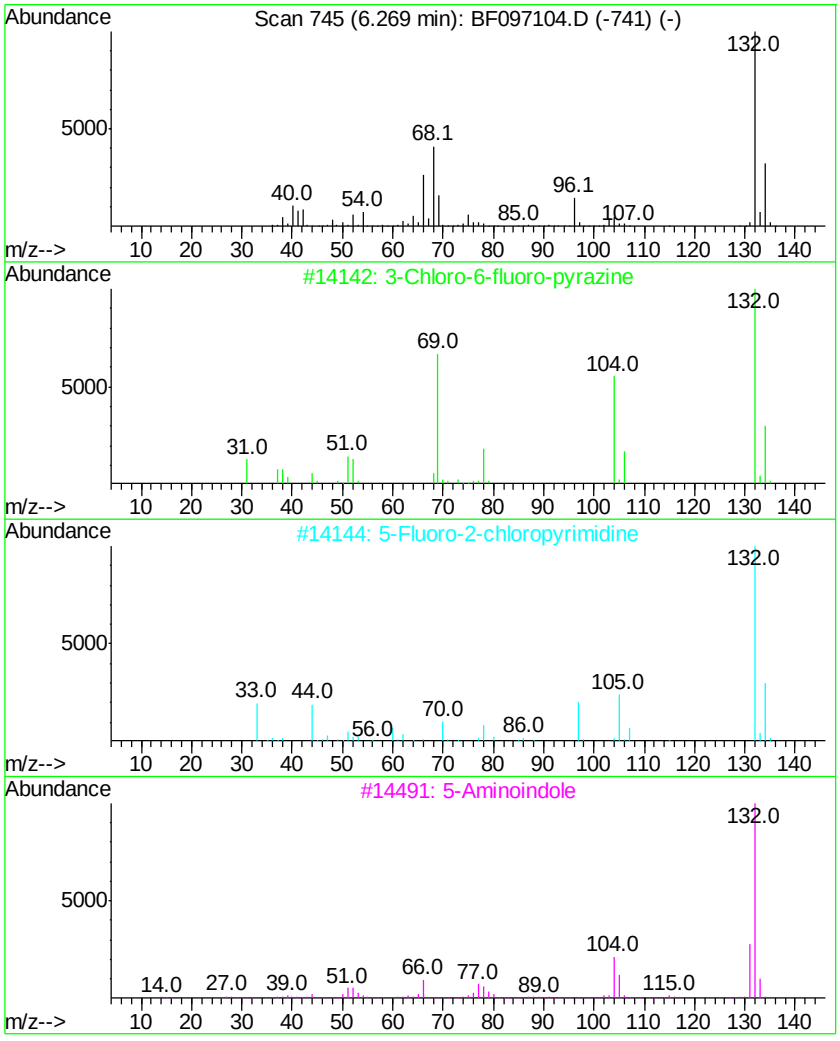
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

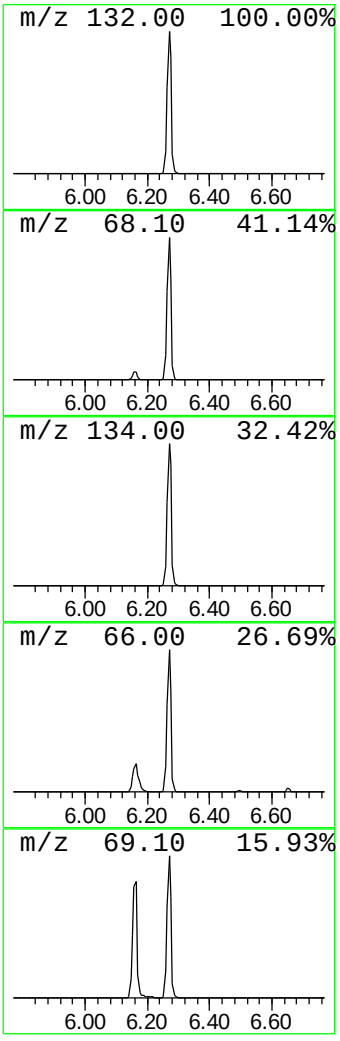
****

Peak Number 3 unknown6.27 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.27	83.18 ng	2123020	1,4-Dichlorobenzene-d4	6.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9





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Sample : I4397-01
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T-1A-14.5-15.0-072117

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
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TIC Library : C:\DATABASE\NIST11.L
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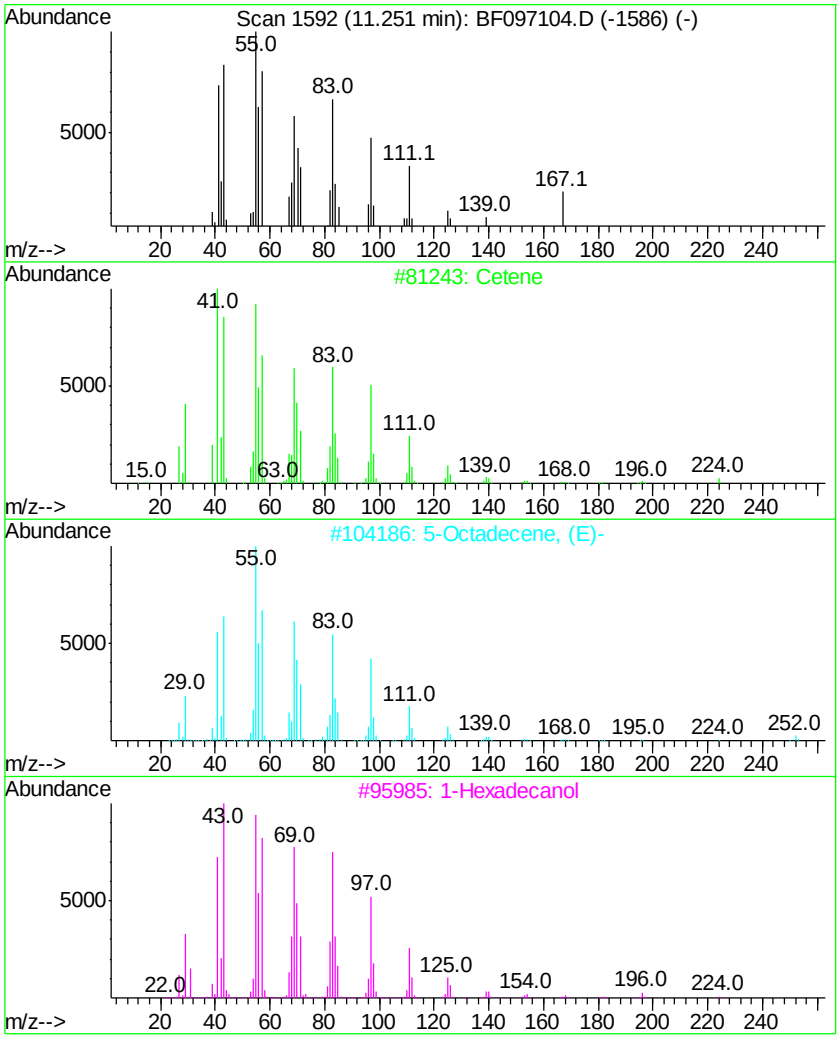
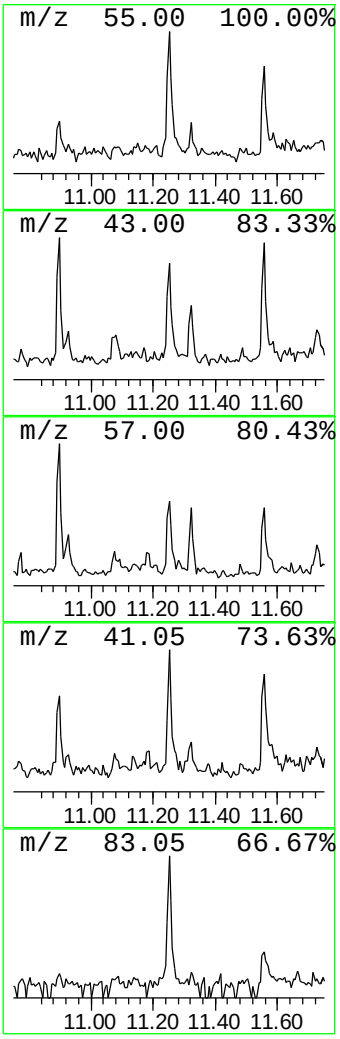
Peak Number 5 Cetene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.25	2.36 ng	60846	Phenanthrene-d10	11.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cetene	224	C16H32	000629-73-2	90
2	5-Octadecene, (E)-	252	C18H36	007206-21-5	87
3	1-Hexadecanol	242	C16H34O	036653-82-4	87
4	n-Heptadecanol-1	256	C17H36O	001454-85-9	87
5	5-Eicosene, (E)-	280	C20H40	074685-30-6	87





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ClientSampleId : T-1A-14.5-15.0-072117

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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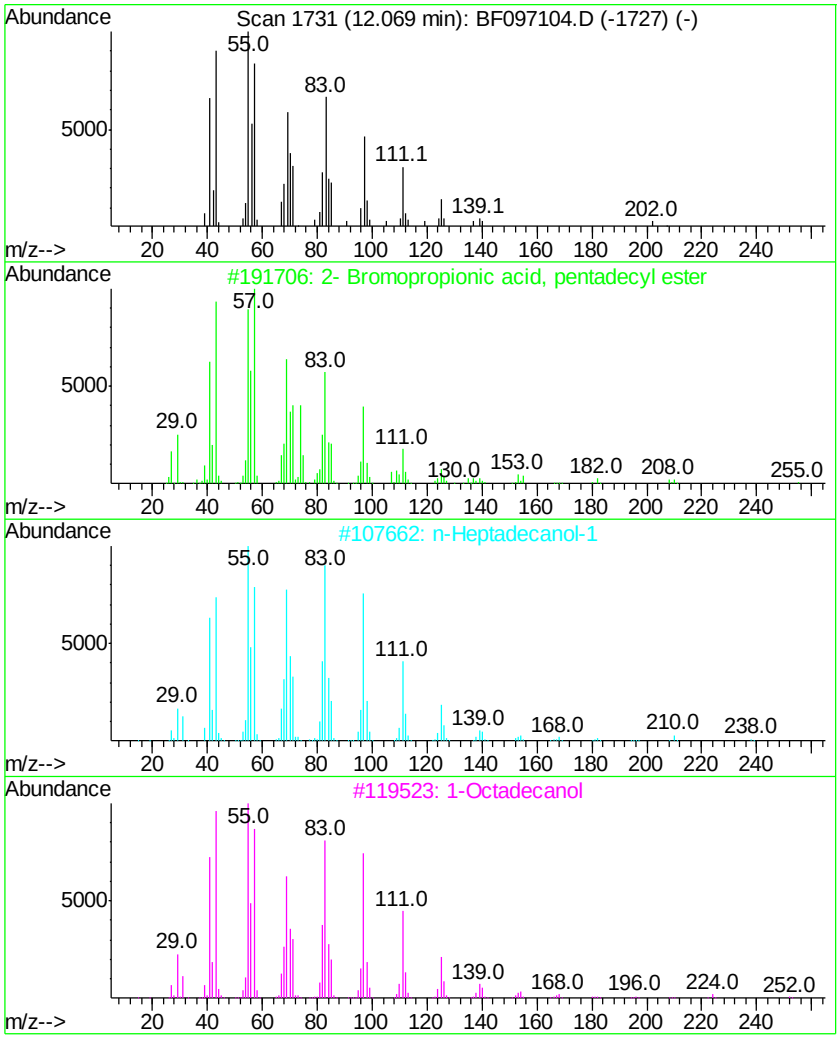
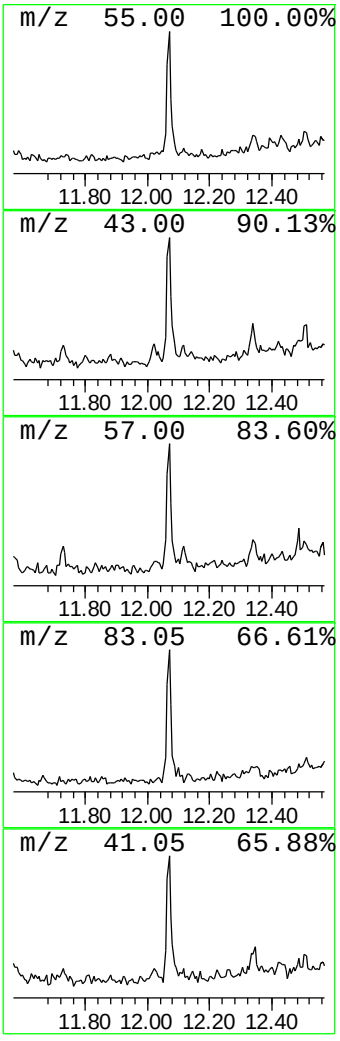
Peak Number 6 2- Bromopropionic acid, pen... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.07	3.65 ng	94112	Phenanthrene-d10	11.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2- Bromopropionic acid, pentadec...	362	C18H35BrO2	1000292-44-2	91
2	n-Heptadecanol-1	256	C17H36O	001454-85-9	91
3	1-Octadecanol	270	C18H38O	000112-92-5	91
4	1-Hexadecanol	242	C16H34O	036653-82-4	90
5	5-Eicosene, (E)-	280	C20H40	074685-30-6	90





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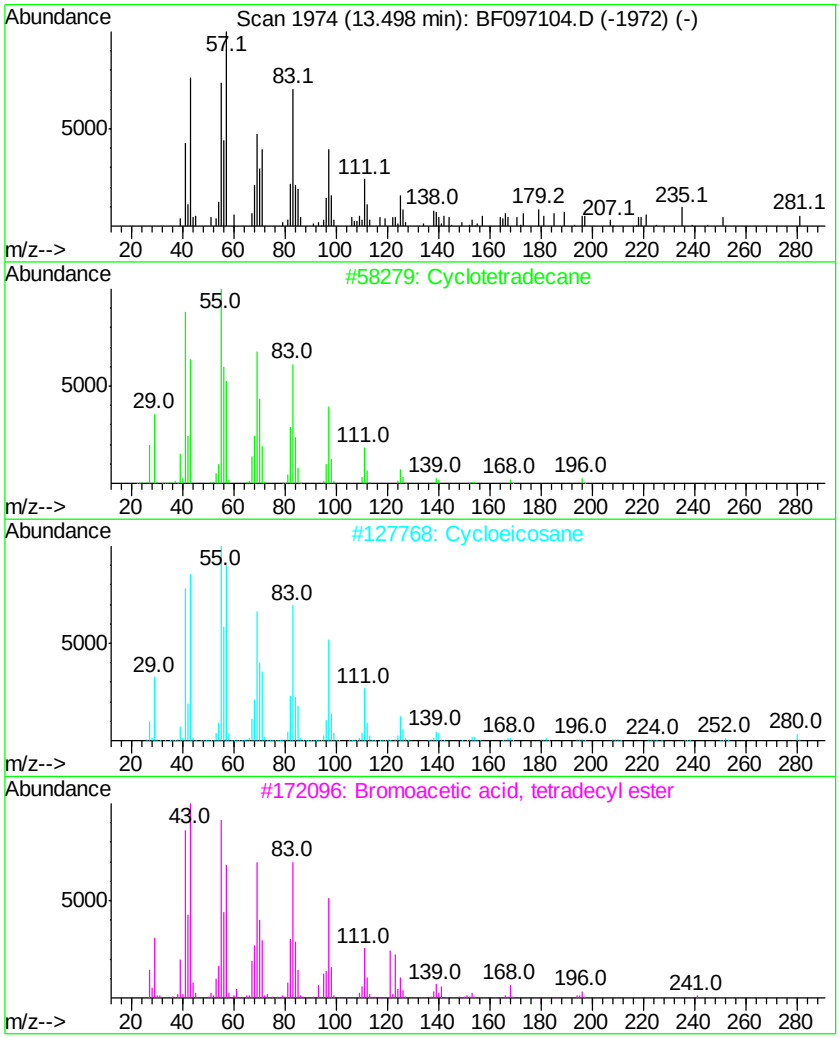
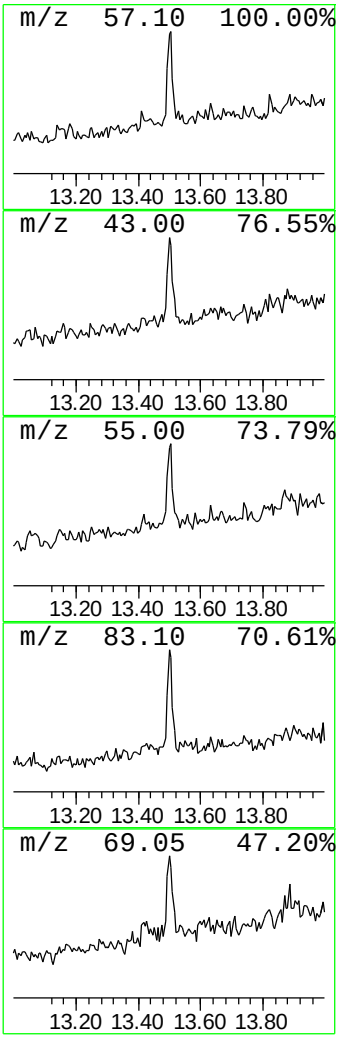
Peak Number 7 Cyclotetradecane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.50	2.21 ng	74594	Chrysene-d12	13.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetradecane	196	C14H28	000295-17-0	96
2	Cycloeicosane	280	C20H40	000296-56-0	87
3	Bromoacetic acid, tetradecyl ester	334	C16H31BrO2	018992-01-3	81
4	Bromoacetic acid, pentadecyl ester	348	C17H33BrO2	131143-01-6	81
5	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	81





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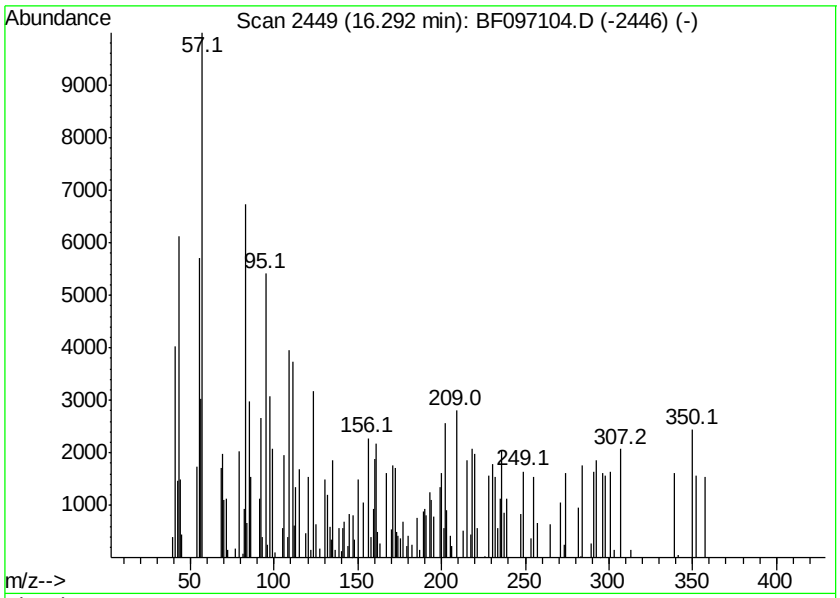
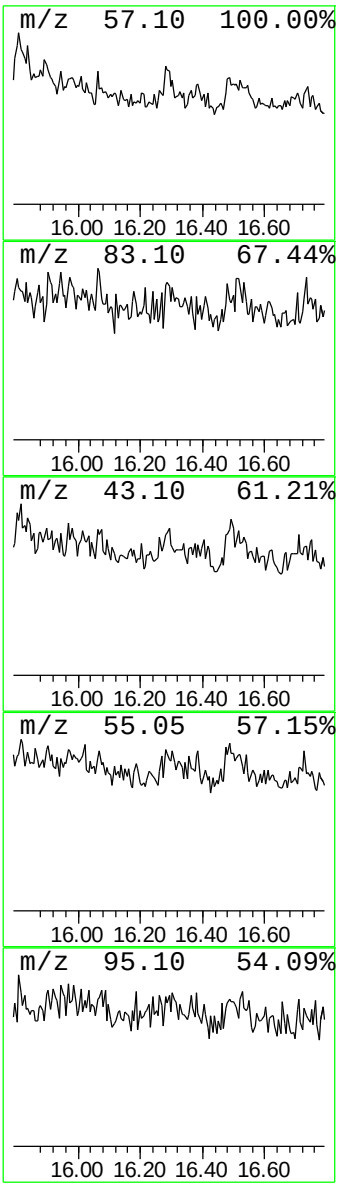
Peak Number 8 unknown16.29 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.29	2.85 ng	48498	Perylene-d12	14.98

Hit# of 1	Tentative ID	MW	MolForm	CAS#	Qual
1	S-(2,5-Dichloro-6-cyano-3-[[(eth...	412	C12H10Cl2N2O2S4	194228-14-3	4





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TIC Library : C:\DATABASE\NIST11.L
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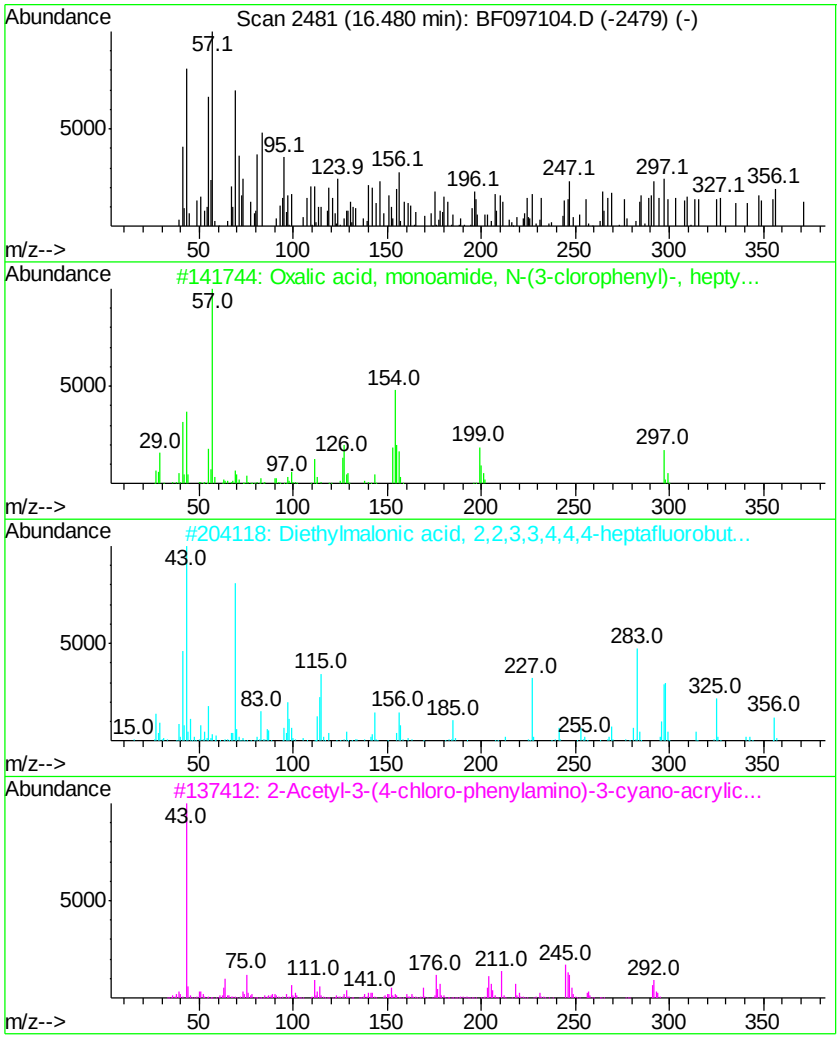
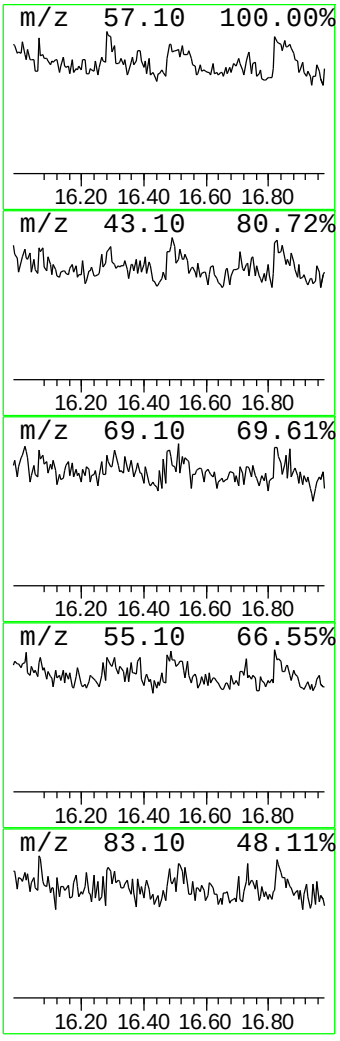
Peak Number 9 unknown16.48 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.48	4.37 ng	74172	Perylene-d12	14.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxalic acid, monoamide, N-(3-clo...	297	C15H20ClNO3	1000309-42-1	10
2	Diethylmalonic acid, 2,2,3,3,4,4...	384	C14H19F7O4	1000368-42-7	7
3	2-Acetyl-3-(4-chloro-phenylamino...	292	C14H13ClN2O3	1000295-99-1	7
4	3.beta.-Acetoxy-16-isothiocyanat...	415	C24H33NO3S	006084-08-8	2
5	1,3-Diethyl-1,1,3-tributoxy-3-ch...	384	C16H37ClO4Si2	1000102-76-3	2





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Instrument : BNA_F
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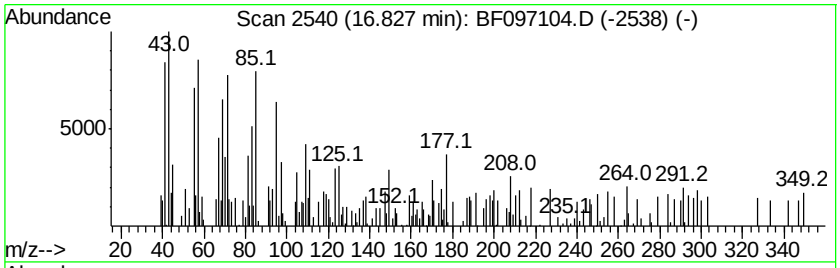
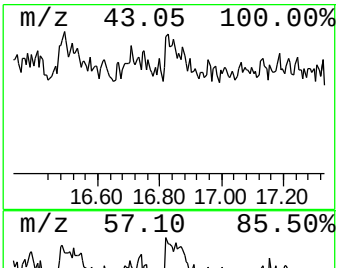
****

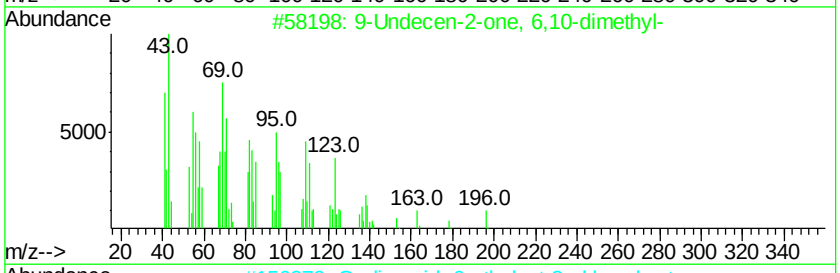
Peak Number 10 9-Undecen-2-one, 6,10-dimet... Concentration Rank 5

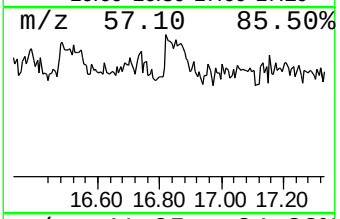
R.T.	EstConc	Area	Relative to ISTD	R.T.
16.83	5.76 ng	97809	Perylene-d12	14.98

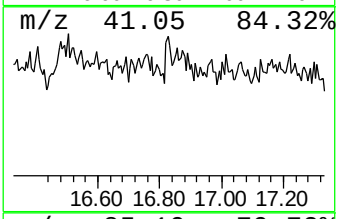
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Undecen-2-one, 6,10-dimethyl-	196	C13H24O	004433-36-7	50
2	Oxalic acid, 6-ethyloct-3-yl hex...	314	C18H34O4	1000309-34-4	35
3	Oxalic acid, 6-ethyloct-3-yl pro...	272	C15H28O4	1000309-34-0	35
4	4-Chloro-2-nitrobenzyl alcohol, ...	299	C9H5Cl2F2NO4	1000376-11-6	25
5	4H-Pyran-4-one, 3,5-diacetyl-2,6...	208	C11H12O4	019396-77-1	25

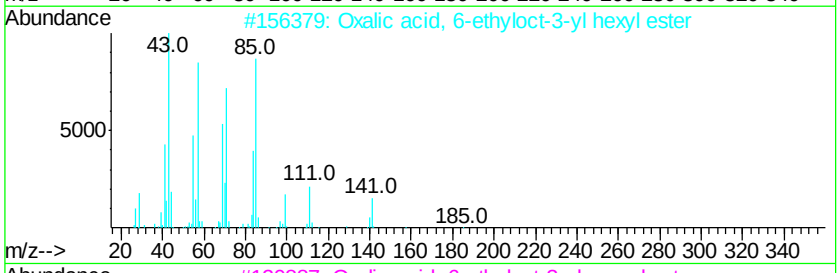


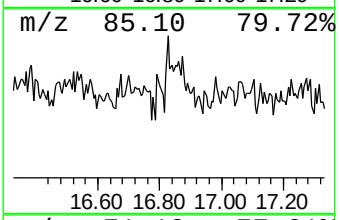


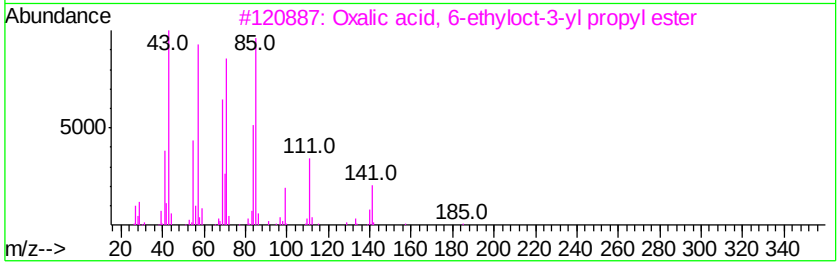


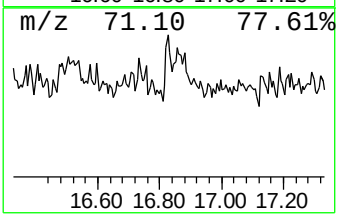












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Data File : BF097104.D
Acq On : 27 Jul 2017 4:38
Operator : SJ/JU
Sample : I4397-01
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T-1A-14.5-15.0-072117

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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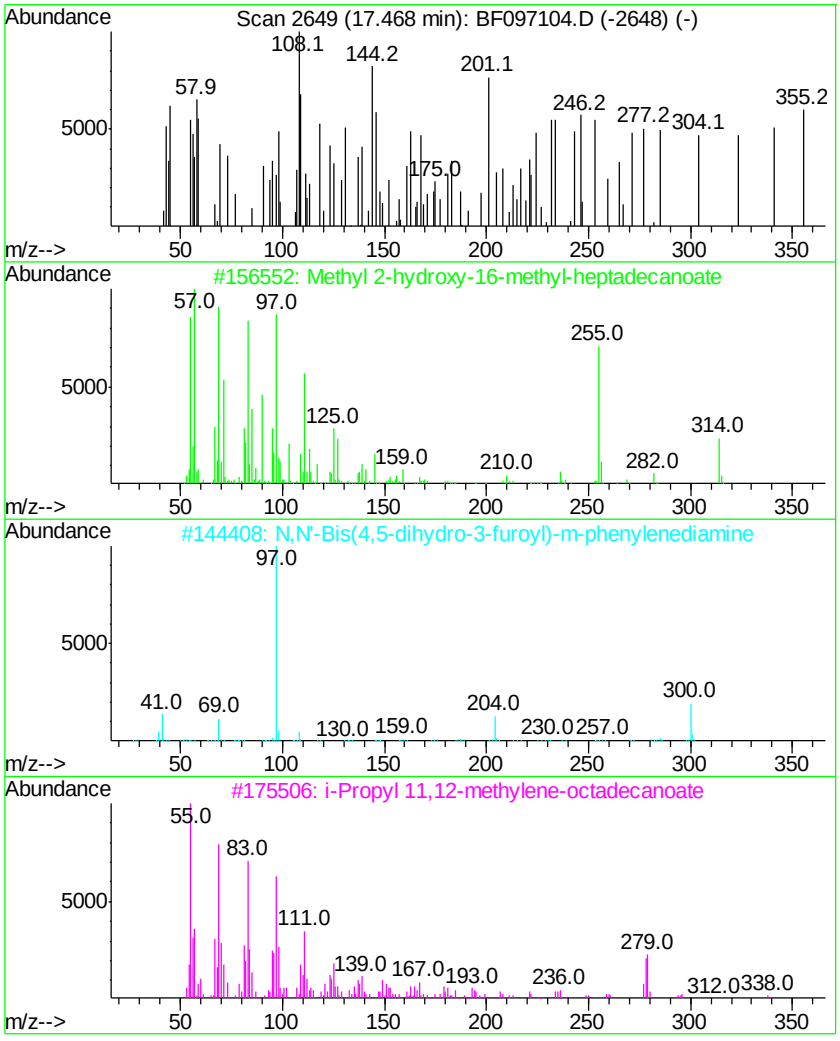
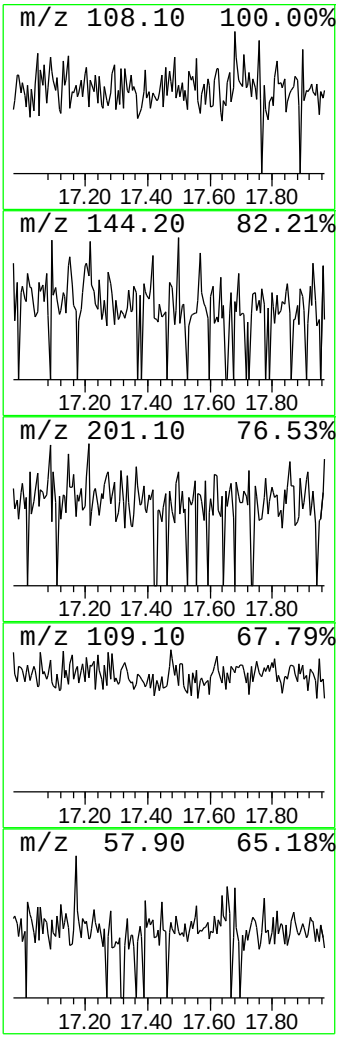
Peak Number 11 unknown17.47 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.47	2.28 ng	38760	Perylene-d12	14.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl 2-hydroxy-16-methyl-hepta...	314	C19H38O3	1000336-40-8	20
2	N,N'-Bis(4,5-dihydro-3-furoyl)-m...	300	C16H16N2O4	1000243-32-6	14
3	i-Propyl 11,12-methylene-octadec...	338	C22H42O2	1000336-77-0	12
4	Cholestan-3,26-diol-22-one	418	C27H46O3	1000252-39-3	12
5	Hexadecanoic acid, 2-hydroxy-, m...	286	C17H34O3	016742-51-1	10





Data Path : Z:\HPCHEM1\BNA F\DATA\BF072617\
Data File : BF097104.D
Acq On : 27 Jul 2017 4:38
Operator : SJ/JU
Sample : I4397-01
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T-1A-14.5-15.0-072117

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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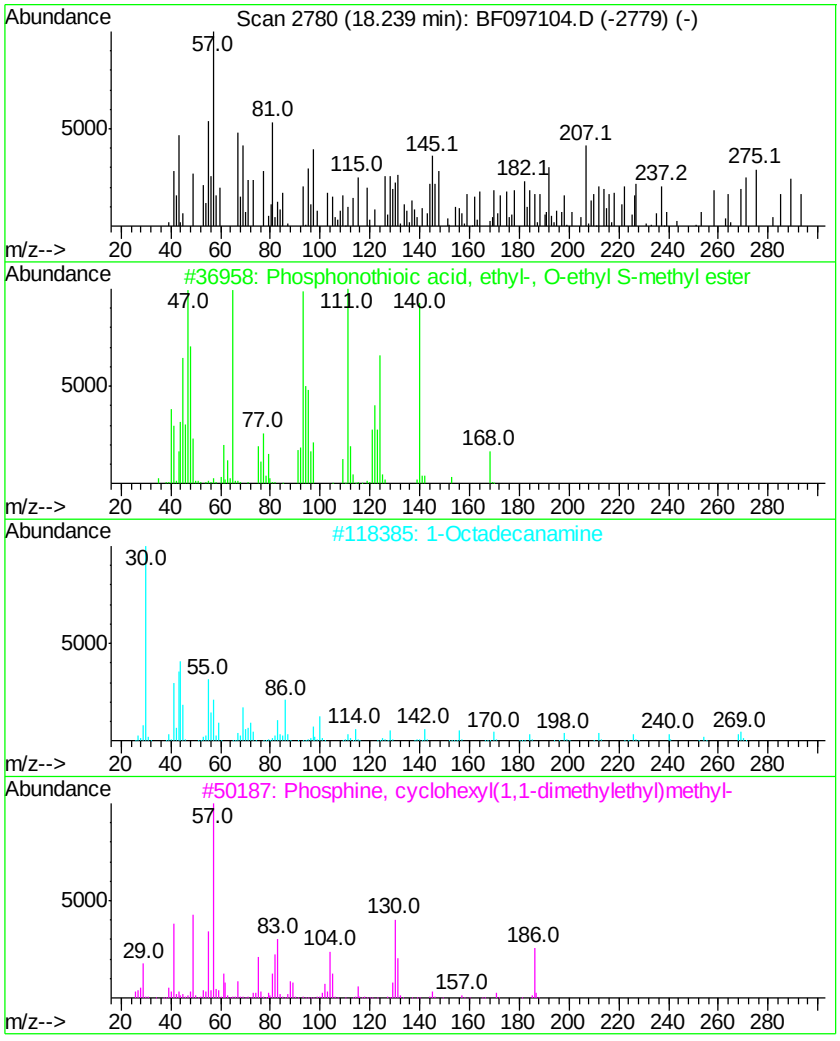
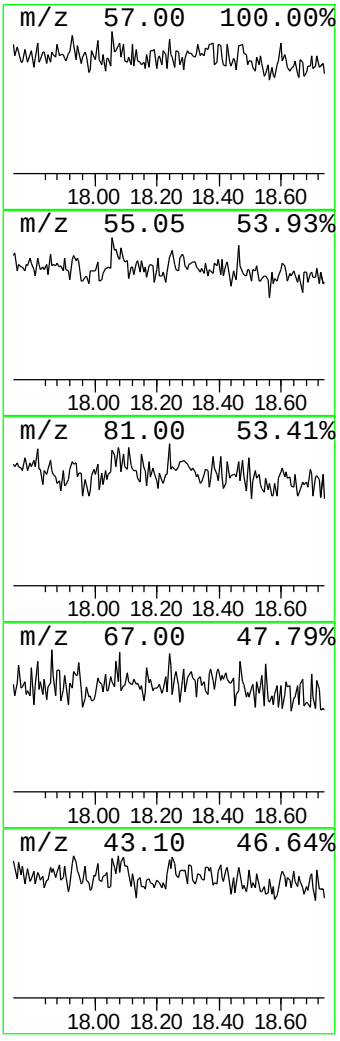
Peak Number 12 unknown18.24 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.24	2.37 ng	40225	Perylene-d12	14.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phosphonothioic acid, ethyl-, O-...	168	C5H13O2PS	002511-12-8	10
2	1-Octadecanamine	269	C18H39N	000124-30-1	10
3	Phosphine, cyclohexyl(1,1-dimeth...	186	C11H23P	074685-81-7	10
4	Chloroacetic acid, hexyl ester	178	C8H15ClO2	005927-57-1	9
5	S-(Isobutoxythiocarbonyl)thiohy...	165	C5H11NOS2	035659-82-6	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF072617\
Data File : BF097104.D
Acq On : 27 Jul 2017 4:38
Operator : SJ/JU
Sample : I4397-01
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T-1A-14.5-15.0-072117

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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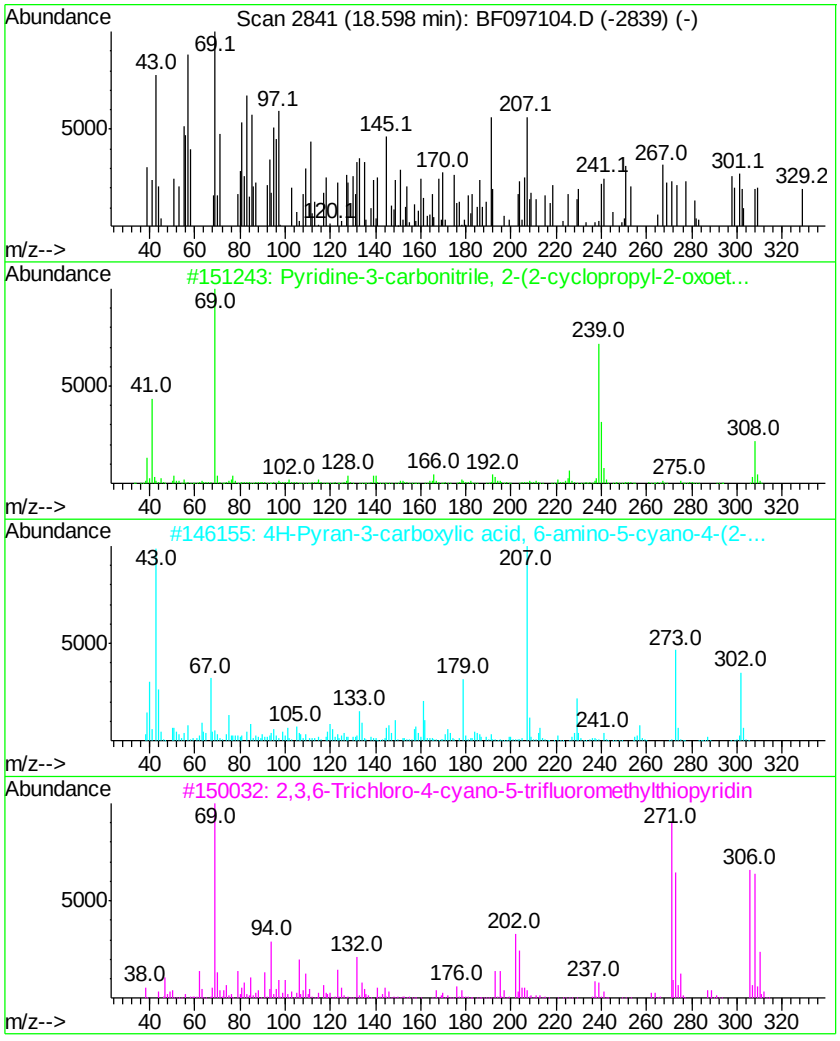
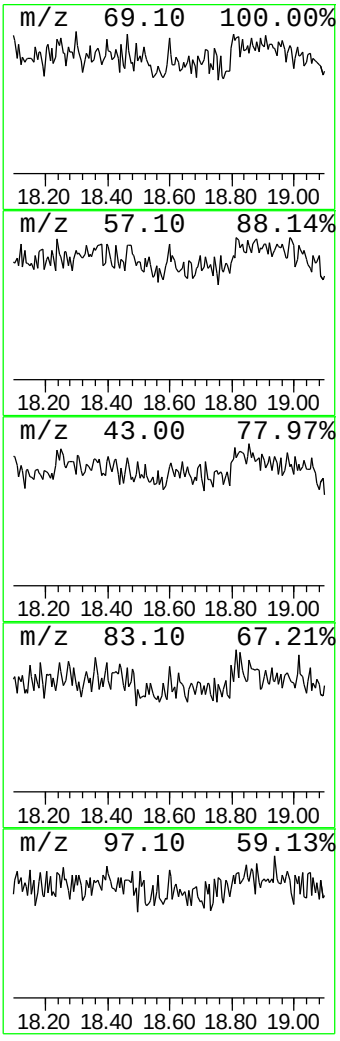
Peak Number 13 unknown18.60 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.60	3.55 ng	60360	Perylene-d12	14.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyridine-3-carbonitrile, 2-(2-cv...	308	C18H16N2OS	1000259-13-4	10
2	4H-Pyran-3-carboxylic acid, 6-am...	302	C16H15FN2O3	339060-50-3	10
3	2,3,6-Trichloro-4-cyano-5-triflu...	306	C7Cl3F3N2S	1000305-24-5	10
4	Docosane, 11-decyl-	451	C32H66	055401-55-3	9
5	Docosane, 9-octyl-	422	C30H62	055319-83-0	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF072617\
Data File : BF097104.D
Acq On : 27 Jul 2017 4:38
Operator : SJ/JU
Sample : I4397-01
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T-1A-14.5-15.0-072117

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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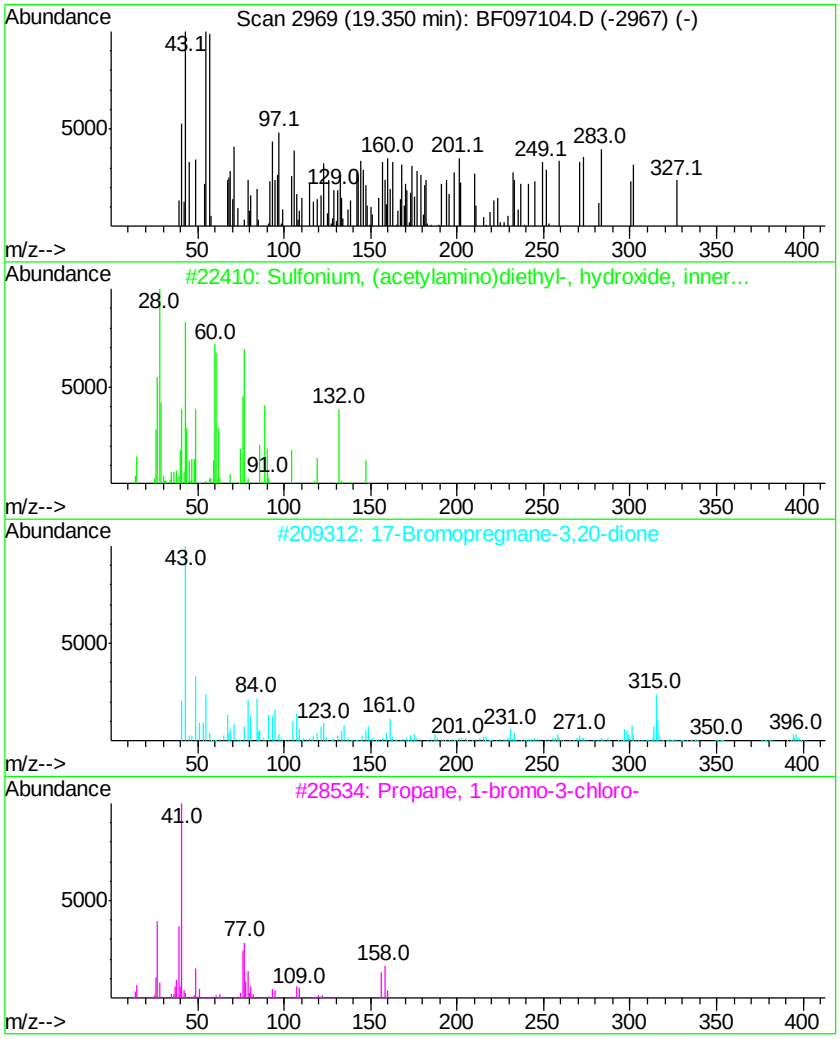
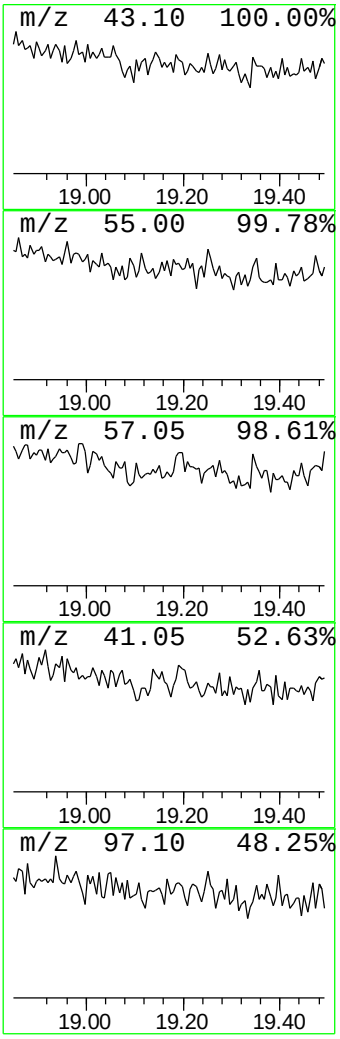
Peak Number 14 unknown19.35 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.35	2.17 ng	36889	Perylene-d12	14.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfonium, (acetylamino)diethyl-...	147	C6H13NOS	032805-46-2	10
2	17-Bromopregnane-3,20-dione	394	C21H31BrO2	062973-42-6	10
3	Propane, 1-bromo-3-chloro-	156	C3H6BrCl	000109-70-6	9
4	Propane, 2-bromo-1-chloro-	156	C3H6BrCl	003017-95-6	9
5	L-Serine, N-(trifluoroacetyl)-, ...	353	C11H13F6NO5	057983-19-4	9





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072617\
Data File : BF097104.D
Acq On : 27 Jul 2017 4:38
Operator : SJ/JU
Sample : I4397-01
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T-1A-14.5-15.0-072117

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown4.65	4.65	10.0	ng	256020	1	6.50	510471	20.0
unknown6.27	6.27	83.2	ng	2123020	1	6.50	510471	20.0
Cetene	11.25	2.4	ng	60846	4	11.00	515691	20.0
2- Bromopropionic...	12.07	3.6	ng	94112	4	11.00	515691	20.0
Cyclotetradecane	13.50	2.2	ng	74594	5	13.63	674014	20.0
unknown16.29	16.29	2.9	ng	48498	6	14.98	339847	20.0
unknown16.48	16.48	4.4	ng	74172	6	14.98	339847	20.0
9-Undecen-2-one, ...	16.83	5.8	ng	97809	6	14.98	339847	20.0
unknown17.47	17.47	2.3	ng	38760	6	14.98	339847	20.0
unknown18.24	18.24	2.4	ng	40225	6	14.98	339847	20.0
unknown18.60	18.60	3.5	ng	60360	6	14.98	339847	20.0
unknown19.35	19.35	2.2	ng	36889	6	14.98	339847	20.0