LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092017\
Data File : BF098669.D
Acq On : 20 Sep 2017 19:28
Operator : SJ/JU
Sample : I5281-05 5X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DUP

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-BF091117.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	4.193	338	358	364	rBV3	24592	106213	4.69%	1.020%
2	4.787	456	459	469	rBV	21145	30444	1.35%	0.292%
3	5.016	479	498	502	rBV2	53596	239766	10.59%	2.303%
4	5.134	506	518	528	rVV2	40187	117449	5.19%	1.128%
5	5.228	531	534	552	rVB	129854	185605	8.20%	1.783%
6	5.434	565	569	579	rBV2	11744	29023	1.28%	0.279%
7	5.716	615	617	623	rBV4	17255	23286	1.03%	0.224%
8	6.051	669	674	680	rBV	25396	41700	1.84%	0.401%
9	6.281	710	713	717	rBV2	101129	152970	6.76%	1.469%
10	6.392	729	732	740	rVB	392428	384169	16.98%	3.690%
11	6.616	767	770	777	rBV	620094	529780	23.41%	5.089%
12	6.775	793	797	805	rBV	364106	364649	16.11%	3.503%
13	7.010	834	837	843	rBV	83137	96514	4.26%	0.927%
14	7.057	843	845	859	rVB	92779	124968	5.52%	1.200%
15	7.186	864	867	877	rBV	309585	292325	12.92%	2.808%
16	7.681	948	951	956	rBV	24386	25168	1.11%	0.242%
17	7.904	985	989	995	rVB	789641	703525	31.09%	6.758%
18	8.204	1036	1040	1051	rVB	109543	134543	5.95%	1.292%
19	8.328	1058	1061	1071	rVB2	37707	53006	2.34%	0.509%
20	8.557	1098	1100	1104	rBV	40362	36138	1.60%	0.347%
21	8.722	1125	1128	1133	rBV	51770	50614	2.24%	0.486%
22	8.845	1146	1149	1151	rBV3	21983	23591	1.04%	0.227%
23	8.975	1168	1171	1175	rBV	665657	535271	23.65%	5.142%
24	9.380	1237	1240	1243	rBV	60584	48024	2.12%	0.461%
25	9.651	1282	1286	1291	rVB2	853418	708308	31.30%	6.804%
26	9.922	1321	1332	1335	rBV	1253449	2263051	100.00%	21.740%
27	10.445	1418	1421	1431	rVB	243986	233183	10.30%	2.240%
28	10.569	1437	1442	1446	rBV2	30364	39928	1.76%	0.384%
29	11.133	1535	1538	1548	rVB	653963	567502	25.08%	5.452%
30	11.369	1573	1578	1583	rBV3	15864	23333	1.03%	0.224%
31	12.716	1803	1807	1811	rVB	352611	280460	12.39%	2.694%
32	13.768	1983	1986	1996	rBV	472234	476745	21.07%	4.580%
33	15.168	2219	2224	2234	rVB	424390	504199	22.28%	4.844%
34	15.562	2286	2291	2295	rBV3	15281	26831	1.19%	0.258%

LSC Area Percent Report

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Data File : BF098669.D
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Operator : SJ/JU
Sample : I5281-05 5X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DUP

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-BF091117.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.657	2302	2307	2310	rVB	20207	28396	1.25%	0.273%
36	15.768	2320	2326	2337	rBV5	73623	159801	7.06%	1.535%
37	15.951	2348	2357	2362	rVV4	304236	673121	29.74%	6.466%
38	15.998	2362	2365	2375	rVB4	49912	96111	4.25%	0.923%

Sum of corrected areas: 10409710

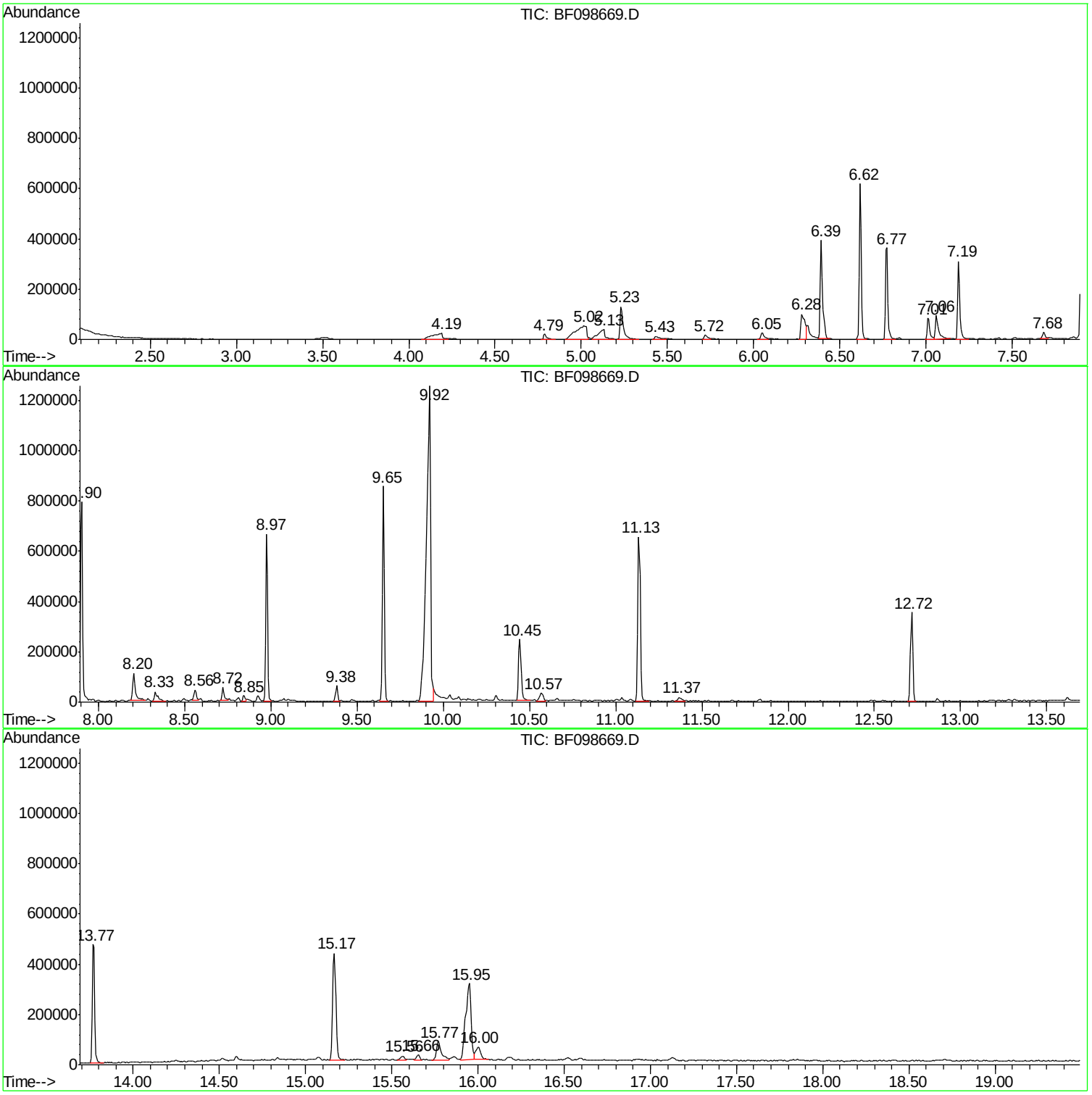
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092017\
Data File : BF098669.D
Acq On : 20 Sep 2017 19:28
Operator : SJ/JU
Sample : I5281-05 5X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DUP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.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\BF092017\
Data File : BF098669.D
Acq On : 20 Sep 2017 19:28
Operator : SJ/JU
Sample : I5281-05 5X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DUP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

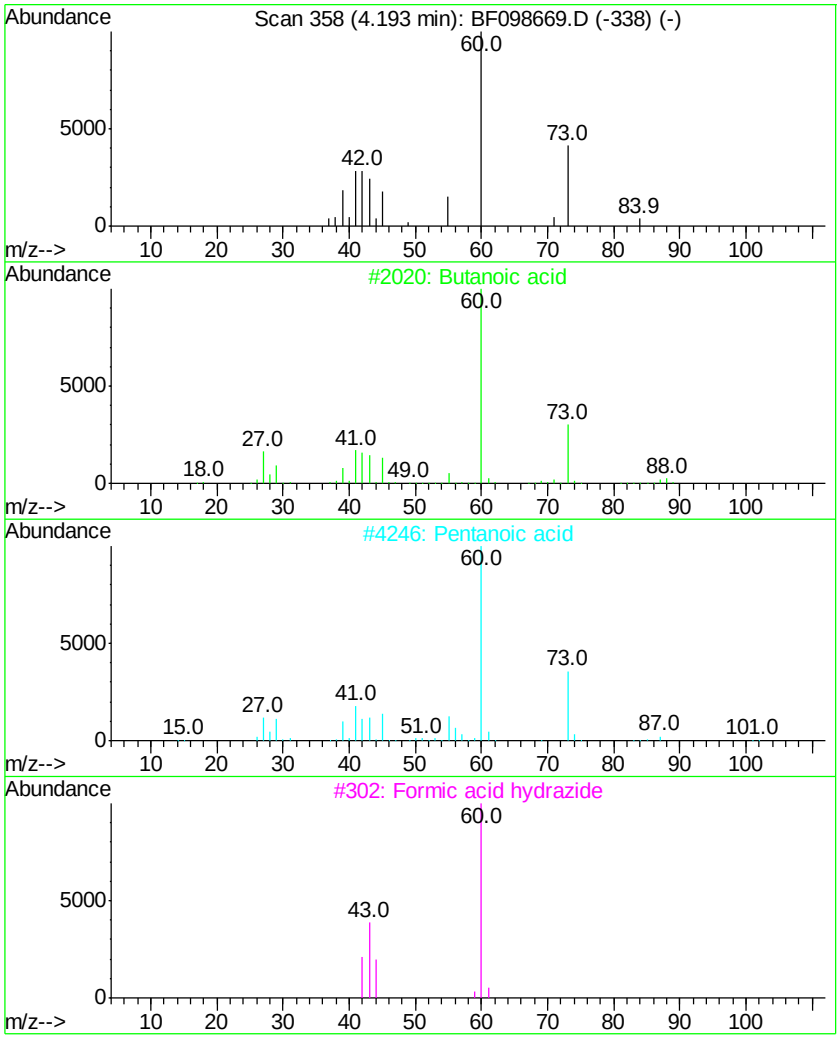
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

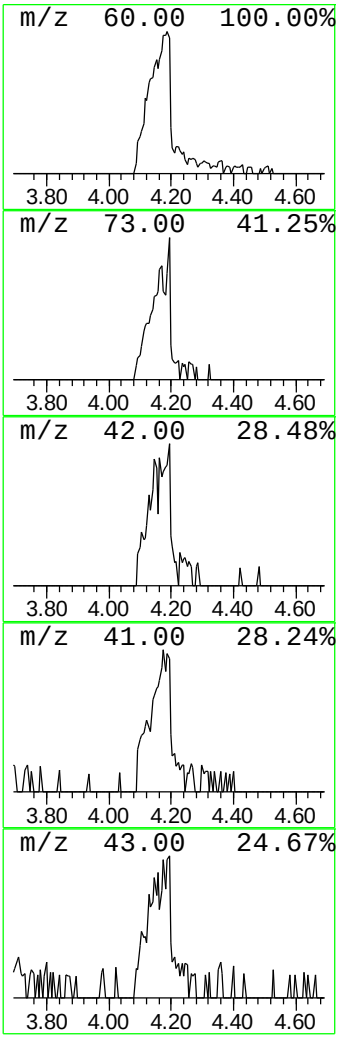
****

Peak Number 1 unknown4.19 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.19	4.01 ng	106213	1,4-Dichlorobenzene-d4	6.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid	88	C4H8O2	000107-92-6	9
2	Pentanoic acid	102	C5H10O2	000109-52-4	9
3	Formic acid hydrazide	60	CH4N2O	000624-84-0	4
4	Hydrazine, 1,1-dimethyl-	60	C2H8N2	000057-14-7	4
5	1-Propanol	60	C3H8O	000071-23-8	4





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Acq On : 20 Sep 2017 19:28
Operator : SJ/JU
Sample : I5281-05 5X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DUP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

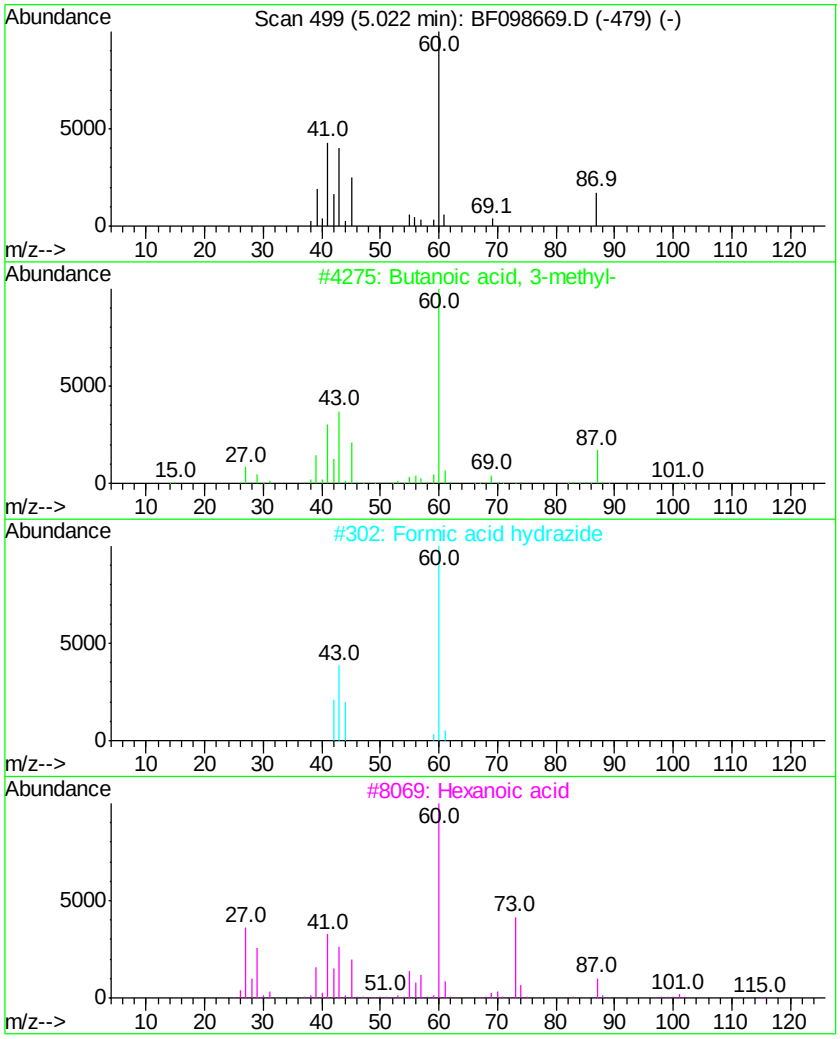
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

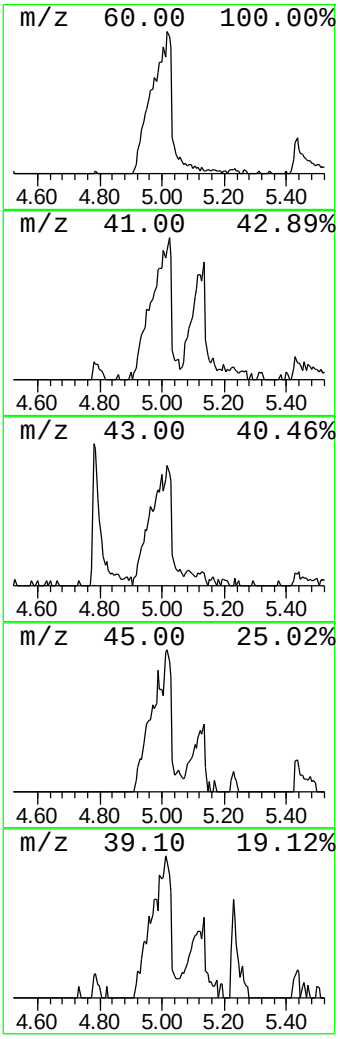
****

Peak Number 2 Butanoic acid, 3-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.02	9.05 ng	239766	1,4-Dichlorobenzene-d4	6.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	78
2	Formic acid hydrazide	60	CH4N2O	000624-84-0	9
3	Hexanoic acid	116	C6H12O2	000142-62-1	9
4	Thiirane	60	C2H4S	000420-12-2	5
5	1-Pentanamine	87	C5H13N	000110-58-7	5





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Acq On : 20 Sep 2017 19:28
Operator : SJ/JU
Sample : I5281-05 5X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DUP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

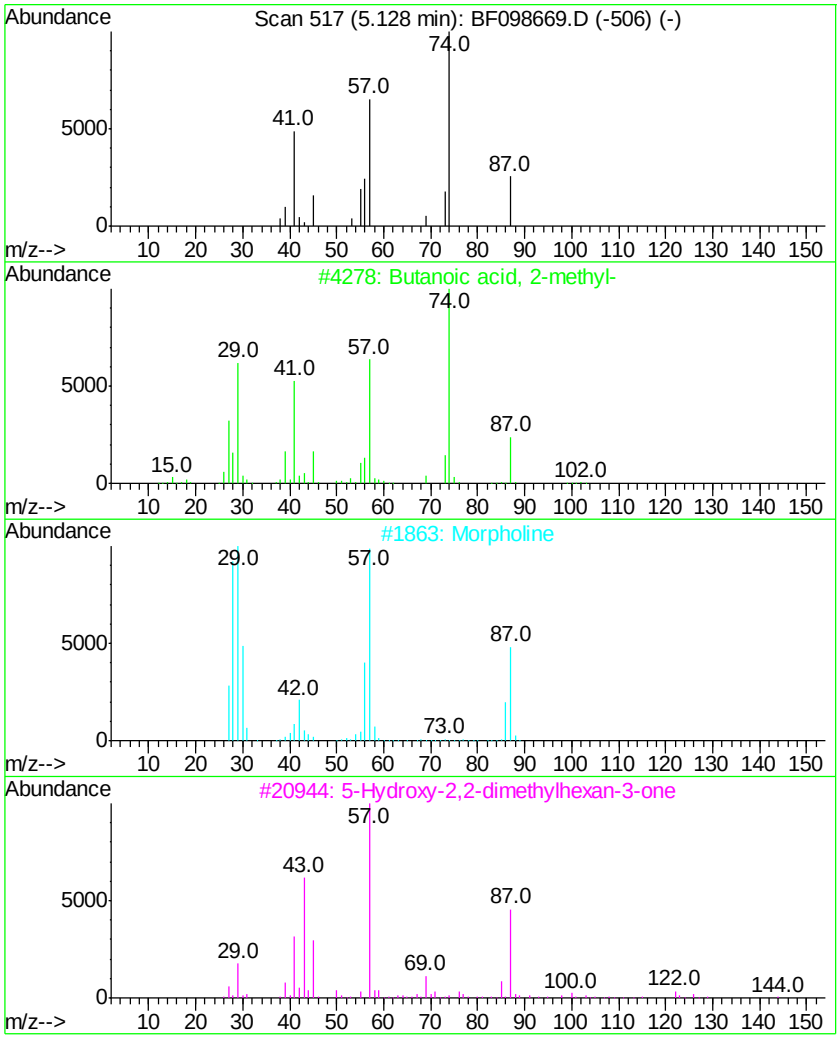
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

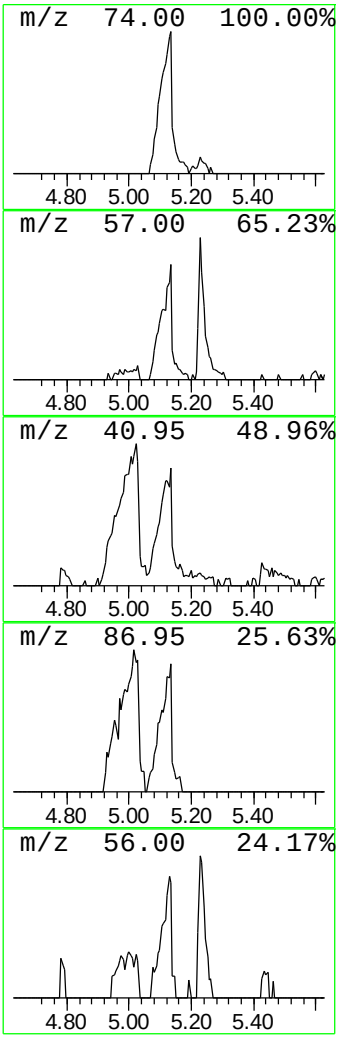
****

Peak Number 3 Butanoic acid, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.13	4.43 ng	117449	1,4-Dichlorobenzene-d4	6.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 2-methyl-	102	C5H10O2	000116-53-0	72
2	Morpholine	87	C4H9NO	000110-91-8	9
3	5-Hydroxy-2,2-dimethylhexan-3-one	144	C8H16O2	173343-33-4	9
4	2-Propenoic acid, 2-methyl-, hex...	170	C10H18O2	000142-09-6	9
5	Oxirane, (butoxymethyl)-	130	C7H14O2	002426-08-6	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092017\
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Acq On : 20 Sep 2017 19:28
Operator : SJ/JU
Sample : I5281-05 5X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DUP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

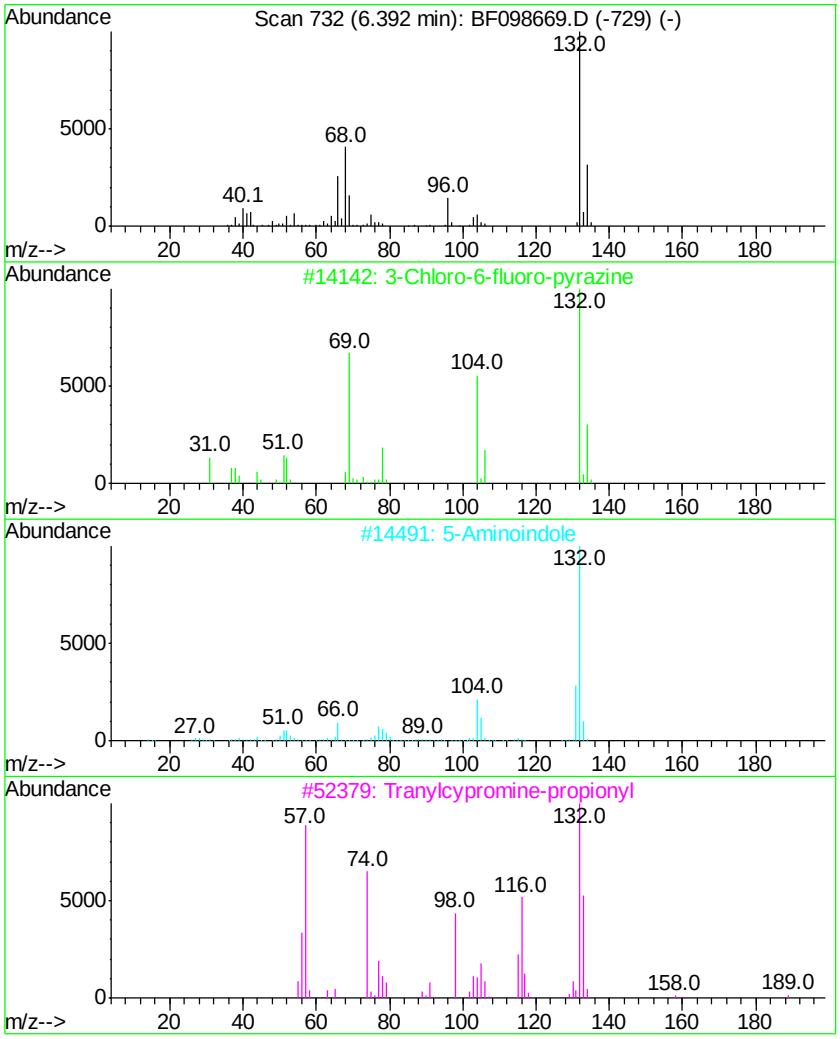
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

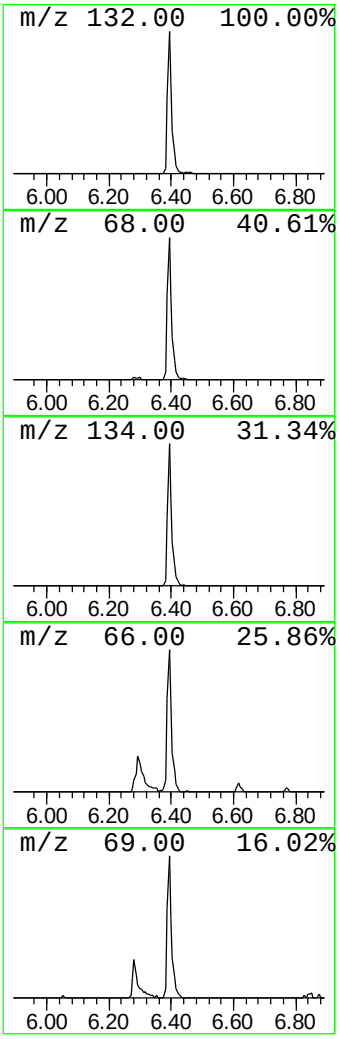
****

Peak Number 4 unknown6.39 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.39	14.50 ng	384169	1,4-Dichlorobenzene-d4	6.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





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Operator : SJ/JU
Sample : I5281-05 5X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DUP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

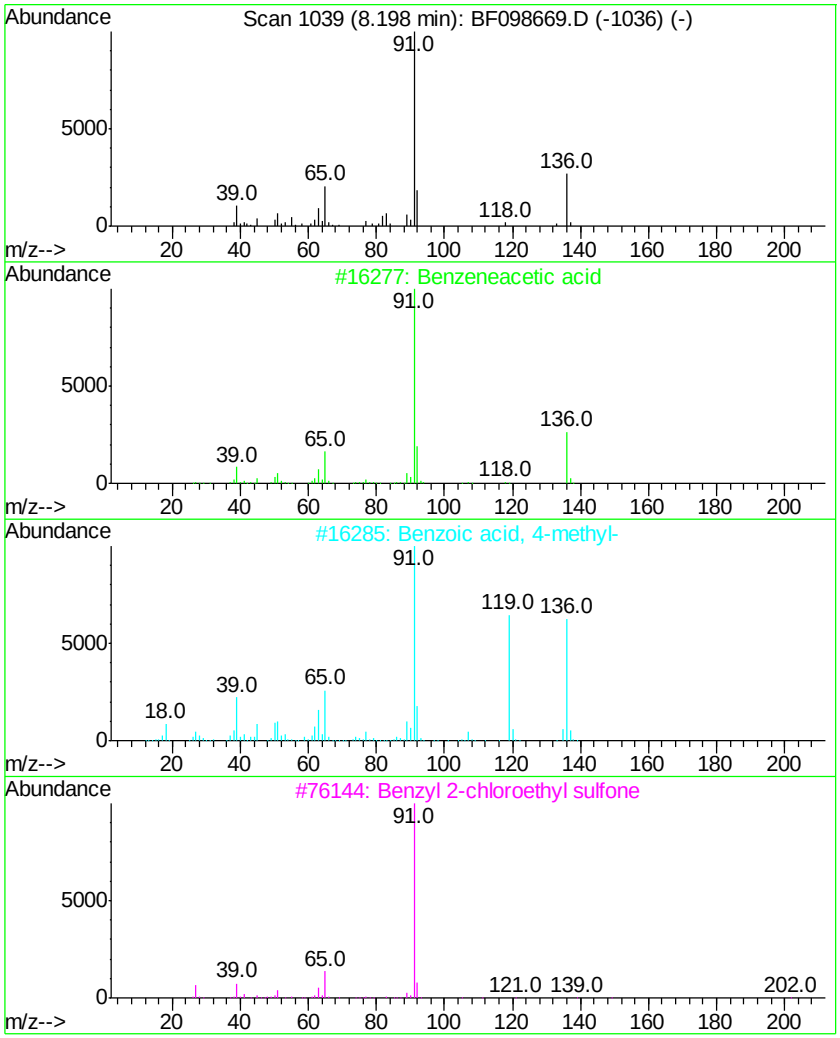
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

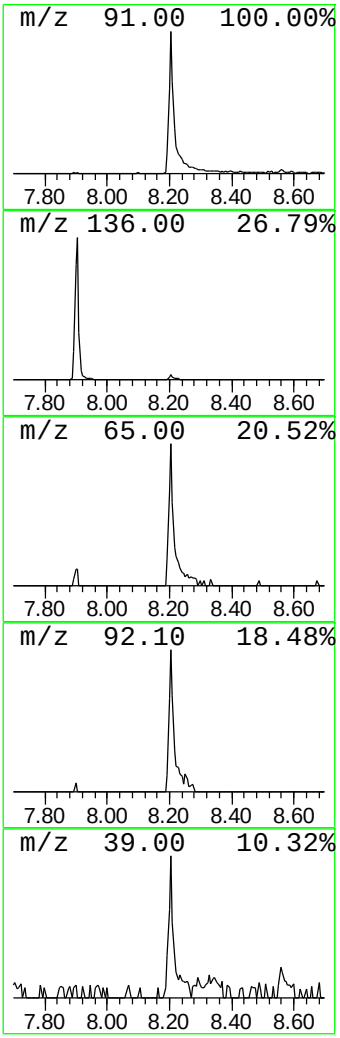
****

Peak Number 6 Benzeneacetic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.20	3.82 ng	134543	Naphthalene-d8	7.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzeneacetic acid	136	C8H8O2	000103-82-2	91
2	Benzoic acid, 4-methyl-	136	C8H8O2	000099-94-5	64
3	Benzyl 2-chloroethyl sulfone	218	C9H11ClO2S	066998-67-2	50
4	3-Oxo-4-phenylbutyronitrile	159	C10H9NO	019212-27-2	50
5	3,3-Bis-benzylsulfanyl-2-fluoro-...	315	C17H14FNS2	1000275-69-6	47





Library Search Compound Report

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Sample : I5281-05 5X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DUP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

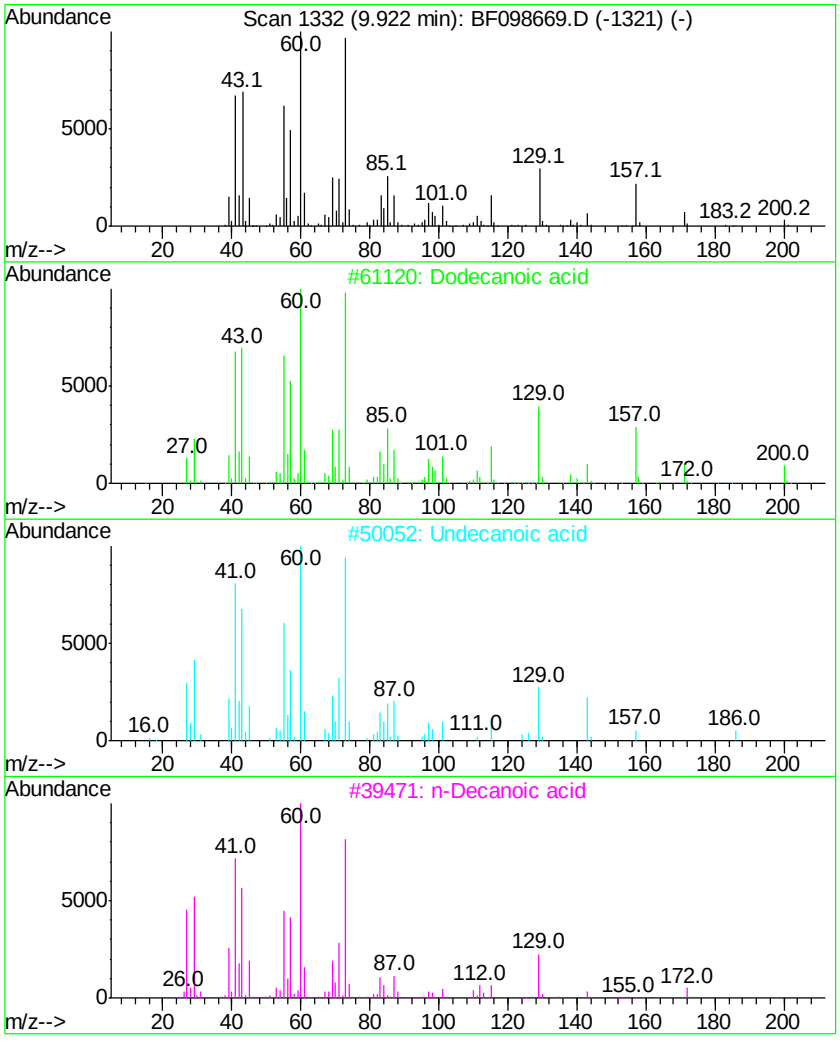
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

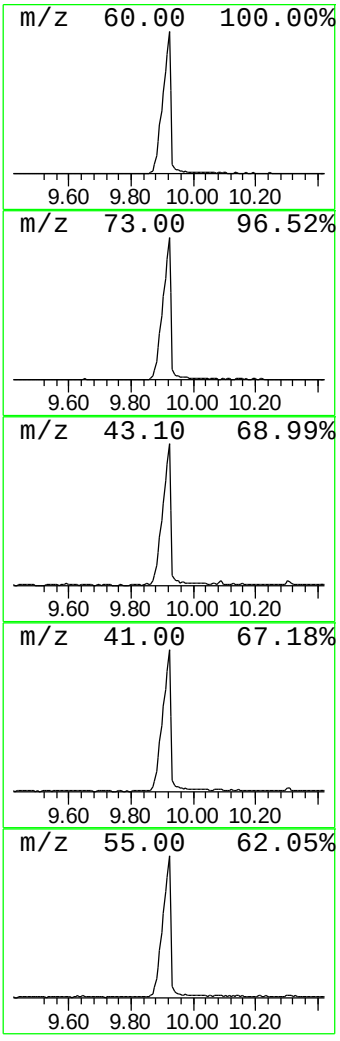
****

Peak Number 7 Dodecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.92	63.90 ng	2263050	Acenaphthene-d10	9.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid	200	C12H24O2	000143-07-7	93
2	Undecanoic acid	186	C11H22O2	000112-37-8	80
3	n-Decanoic acid	172	C10H20O2	000334-48-5	70
4	Nonanoic acid	158	C9H18O2	000112-05-0	49
5	Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NOS	029926-41-8	43





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Misc :
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Instrument : BNA_F
ClientSampleId : DUP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

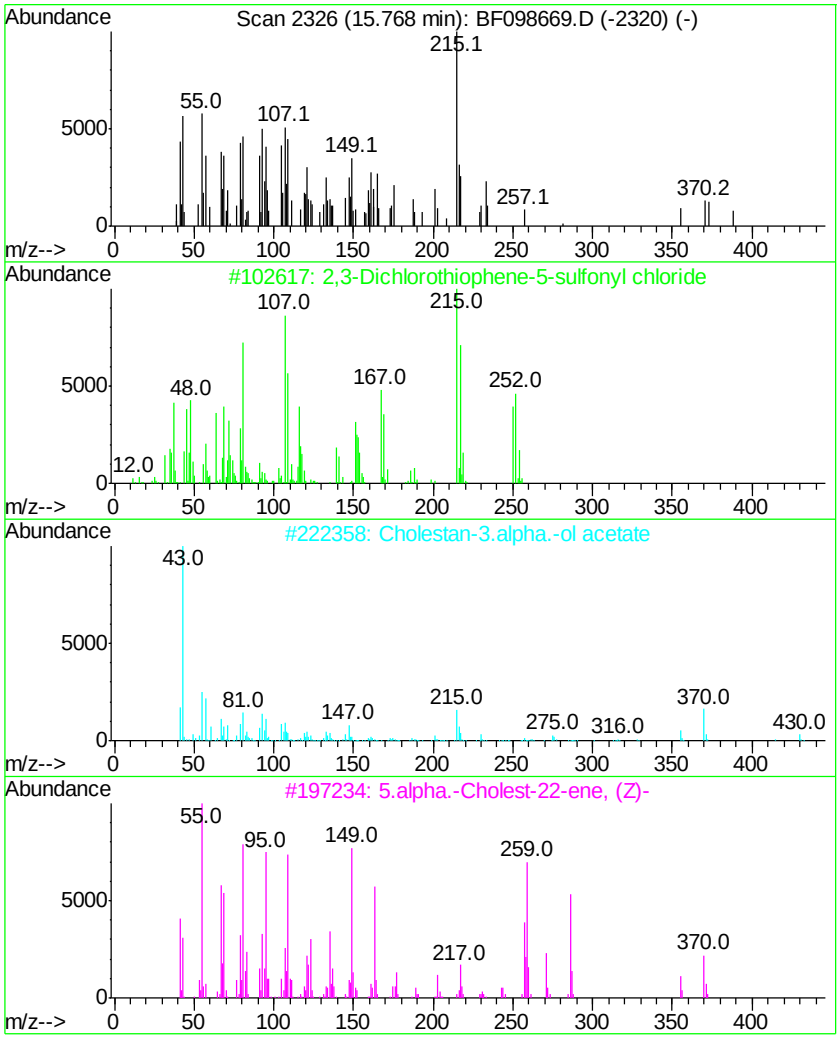
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

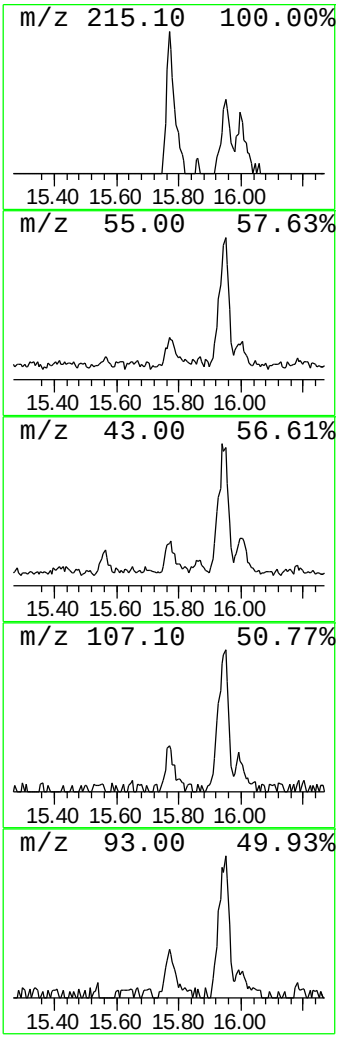
****

Peak Number 8 unknown15.77 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.77	6.34 ng	159801	Perylene-d12	15.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,3-Dichlorothiophene-5-sulfonyl...	250	C4HCl3O2S2	126714-85-0	35
2	Cholestan-3.alpha.-ol acetate	430	C29H50O2	1000214-83-2	35
3	5.alpha.-Cholest-22-ene, (Z)-	370	C27H46	015076-93-4	30
4	4,5-Dichlorophthalimide	215	C8H3Cl2NO2	015997-89-4	27
5	Ethanol, 2-(3,3-dimethylbicyclo[...	166	C11H18O	002226-05-3	25





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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.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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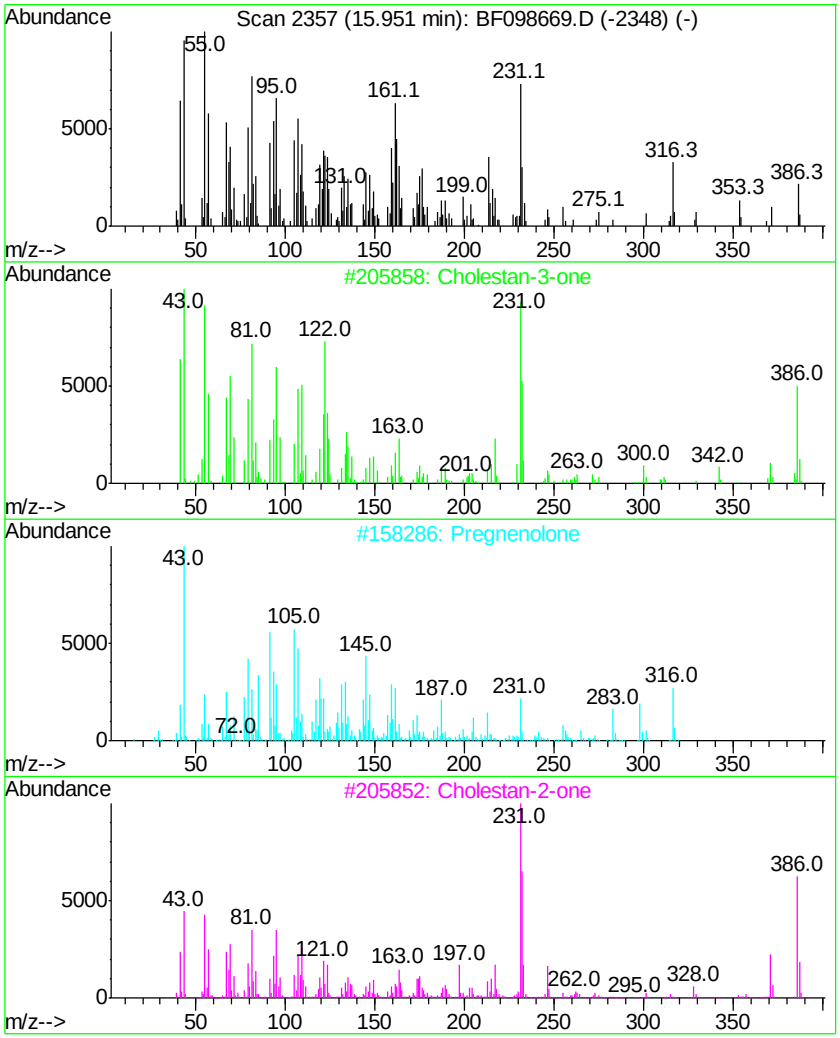
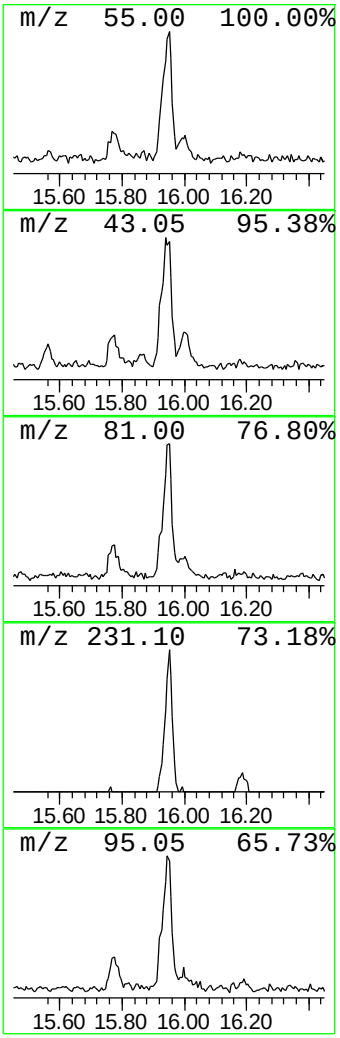
Peak Number 9 Cholestan-3-one Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.95	26.70 ng	673121	Perylene-d12	15.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cholestan-3-one	386	C27H46O	015600-08-5	70
2	Pregnenolone	316	C21H32O2	000145-13-1	52
3	Cholestan-2-one	386	C27H46O	1000210-43-4	52
4	Cholestane, 4,5-epoxy-, (4.alpha...	386	C27H46O	006079-19-2	47
5	Cholest-4-en-3-ol	386	C27H46O	014597-42-3	45





Library Search Compound Report

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Sample : I5281-05 5X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DUP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.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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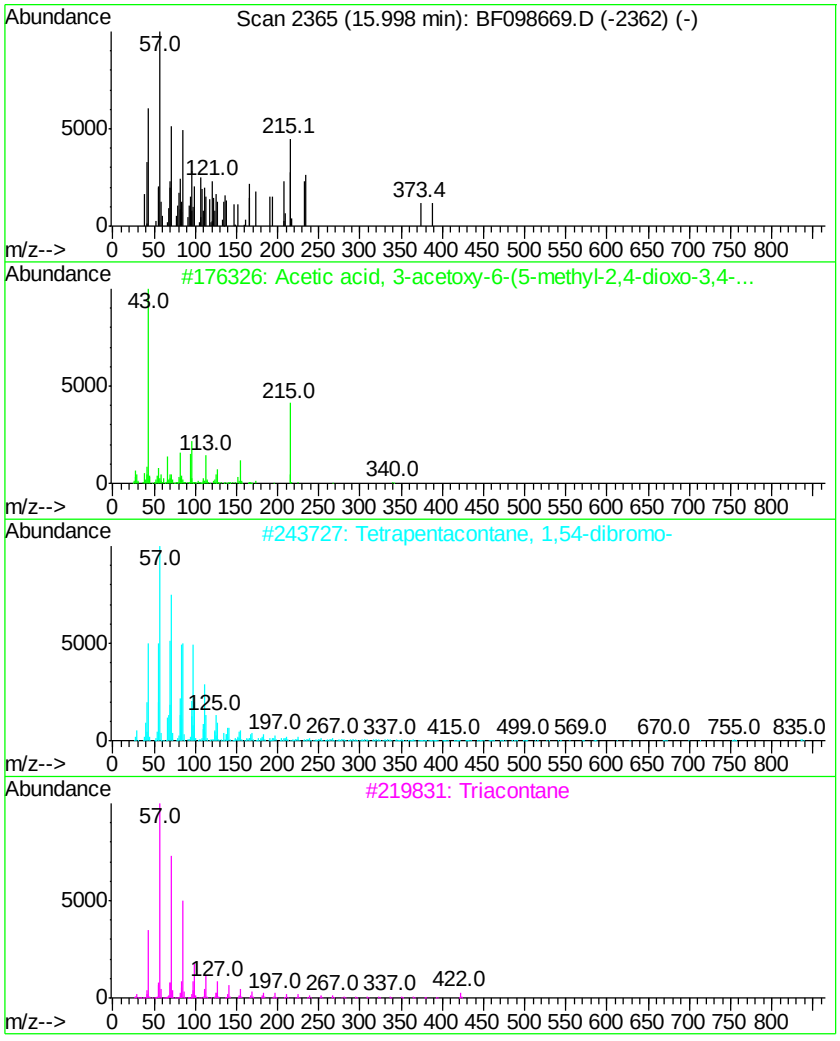
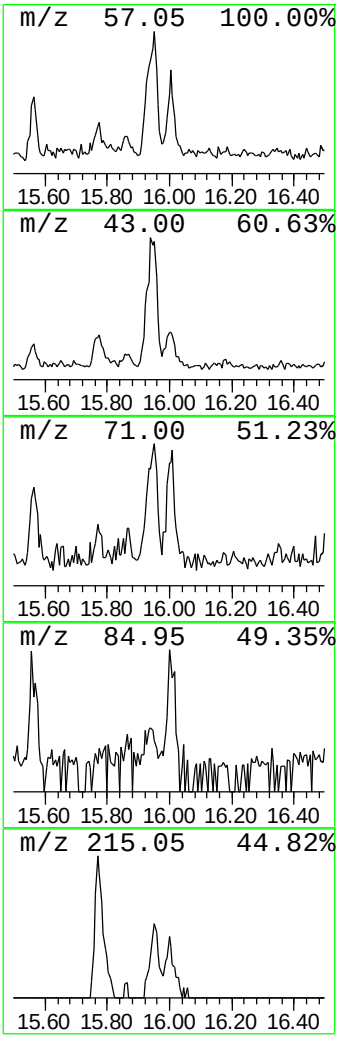
Peak Number 10 unknown16.00 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.00	3.81 ng	96111	Perylene-d12	15.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, 3-acetoxy-6-(5-meth...	340	C15H20N2O7	1000192-89-9	10
2	Tetrapentacontane, 1,54-dibromo-	915	C54H108Br2	1000156-09-4	10
3	Triacontane	422	C30H62	000638-68-6	10
4	Sulfurous acid, butyl pentadecyl...	348	C19H40O3S	1000309-18-2	10
5	Eicosane, 10-methyl-	296	C21H44	054833-23-7	10





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092017\
Data File : BF098669.D
Acq On : 20 Sep 2017 19:28
Operator : SJ/JU
Sample : I5281-05 5X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DUP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.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
unknown4.19	4.19	4.0	ng	106213	1	6.62	529780	20.0
Butanoic acid, 3-...	5.02	9.1	ng	239766	1	6.62	529780	20.0
Butanoic acid, 2-...	5.13	4.4	ng	117449	1	6.62	529780	20.0
unknown6.39	6.39	14.5	ng	384169	1	6.62	529780	20.0
Benzeneacetic acid	8.20	3.8	ng	134543	2	7.90	703525	20.0
Dodecanoic acid	9.92	63.9	ng	2263050	3	9.65	708308	20.0
unknown15.77	15.77	6.3	ng	159801	6	15.17	504199	20.0
Cholestan-3-one	15.95	26.7	ng	673121	6	15.17	504199	20.0
unknown16.00	16.00	3.8	ng	96111	6	15.17	504199	20.0