LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092017\
Data File : BF098668.D
Acq On : 20 Sep 2017 19:00
Operator : SJ/JU
Sample : I5281-04 5X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-8-EW

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	4.787	456	459	471	rBV	16262	28949	2.45%	0.347%
2	4.963	478	489	490	rBV2	33870	80268	6.80%	0.961%
3	5.228	531	534	547	rBV	164138	213665	18.11%	2.558%
4	6.045	669	673	681	rBV	18880	32469	2.75%	0.389%
5	6.281	710	713	727	rBV2	110906	162321	13.76%	1.943%
6	6.392	729	732	749	rVB	445580	442486	37.51%	5.298%
7	6.616	767	770	783	rBV	590152	518073	43.92%	6.203%
8	6.775	793	797	807	rBV	418674	402068	34.08%	4.814%
9	7.186	864	867	879	rBV	328040	325464	27.59%	3.897%
10	7.904	985	989	998	rBV	777774	681299	57.76%	8.157%
11	8.198	1031	1039	1041	rBV3	8950	13676	1.16%	0.164%
12	8.328	1057	1061	1066	rBV	25427	26128	2.21%	0.313%
13	8.633	1109	1113	1121	rBV	25449	39409	3.34%	0.472%
14	8.928	1160	1163	1166	rVB	15295	12467	1.06%	0.149%
15	8.975	1168	1171	1175	rBV	694508	593250	50.29%	7.103%
16	9.380	1237	1240	1243	rBV	50523	38267	3.24%	0.458%
17	9.651	1282	1286	1290	rBV2	810284	686754	58.22%	8.223%
18	10.310	1393	1398	1401	rBV	14379	15156	1.28%	0.181%
19	10.445	1417	1421	1431	rVB	255840	258577	21.92%	3.096%
20	10.575	1438	1443	1449	rVB3	19274	29622	2.51%	0.355%
21	11.133	1535	1538	1546	rBV	623262	544538	46.16%	6.520%
22	11.680	1628	1631	1636	rBV	28848	25472	2.16%	0.305%
23	12.716	1804	1807	1811	rBV	366289	296692	25.15%	3.552%
24	13.621	1957	1961	1965	rBV4	15474	19303	1.64%	0.231%
25	13.774	1983	1987	1992	rVB	474086	442517	37.51%	5.298%
26	14.257	2065	2069	2073	rBV7	10555	15972	1.35%	0.191%
27	14.598	2124	2127	2131	rBV	22940	23350	1.98%	0.280%
28	15.168	2219	2224	2230	rVB	396923	469611	39.81%	5.623%
29	15.562	2288	2291	2295	rVB5	16389	26372	2.24%	0.316%
30	15.651	2302	2306	2311	rBV	19809	31207	2.65%	0.374%
31	15.768	2321	2326	2339	rBV2	178284	333460	28.27%	3.993%
32	15.951	2347	2357	2362	rBV5	496371	1179623	100.00%	14.124%
33	15.998	2362	2365	2377	rVB5	114191	230716	19.56%	2.762%
34	16.186	2393	2397	2403	rVB6	21082	35310	2.99%	0.423%

LSC Area Percent Report

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Misc :
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Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
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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	16.515	2447	2453	2457	rBV6	10048	23791	2.02%	0.285%
36	16.598	2462	2467	2474	rVB6	19044	34728	2.94%	0.416%
37	17.127	2555	2557	2564	rVB7	11682	19034	1.61%	0.228%

Sum of corrected areas: 8352064

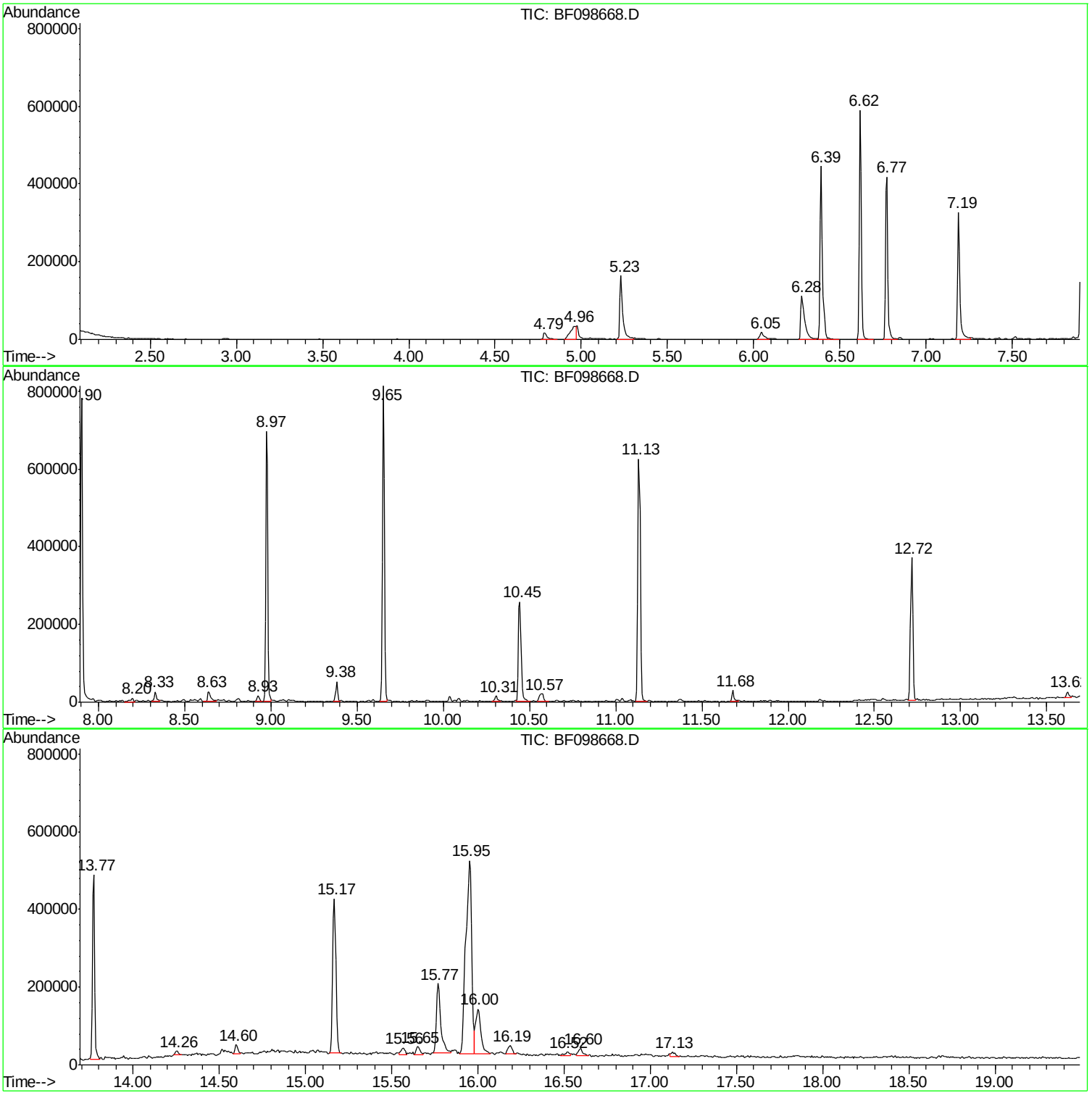
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092017\
Data File : BF098668.D
Acq On : 20 Sep 2017 19:00
Operator : SJ/JU
Sample : I5281-04 5X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-8-EW

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



Library Search Compound Report

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Operator : SJ/JU
Sample : I5281-04 5X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-8-EW

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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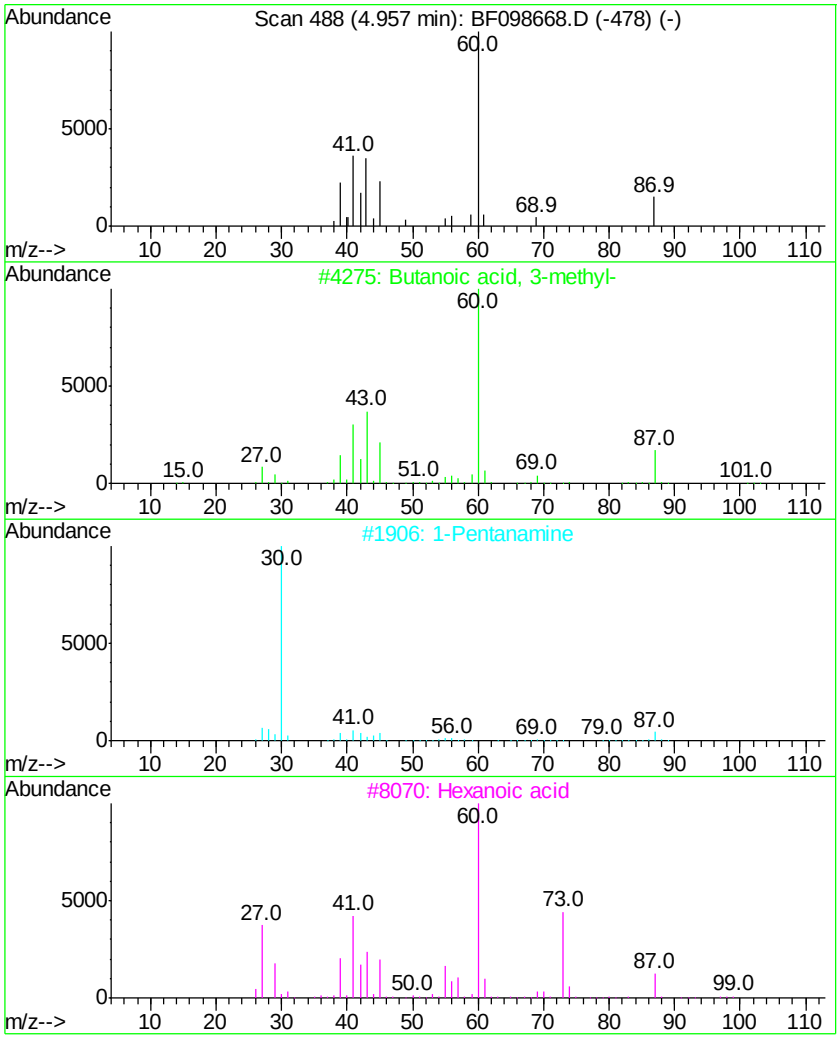
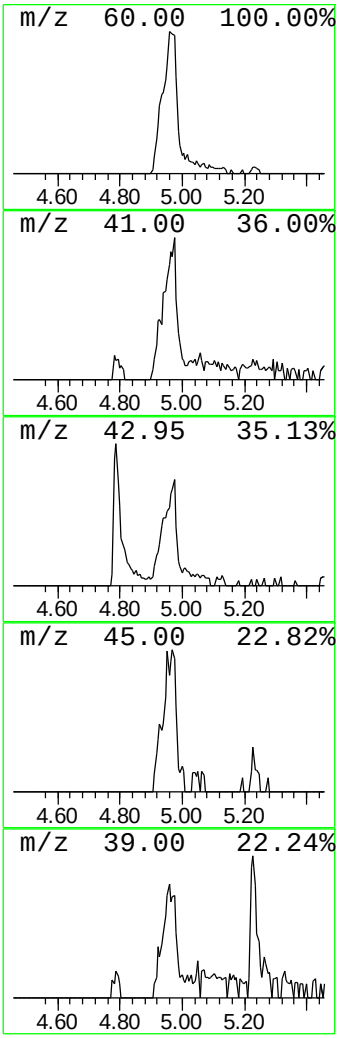
Peak Number 1 Butanoic acid, 3-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.96	3.10 ng	80268	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	83
2	1-Pentanamine	87	C5H13N	000110-58-7	10
3	Hexanoic acid	116	C6H12O2	000142-62-1	9
4	1,5-Pentanediol	104	C5H12O2	000111-29-5	9
5	Pentanoic acid	102	C5H10O2	000109-52-4	9





Library Search Compound Report

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Sample : I5281-04 5X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-8-EW

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

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TIC Integration Parameters: LSCINT.P

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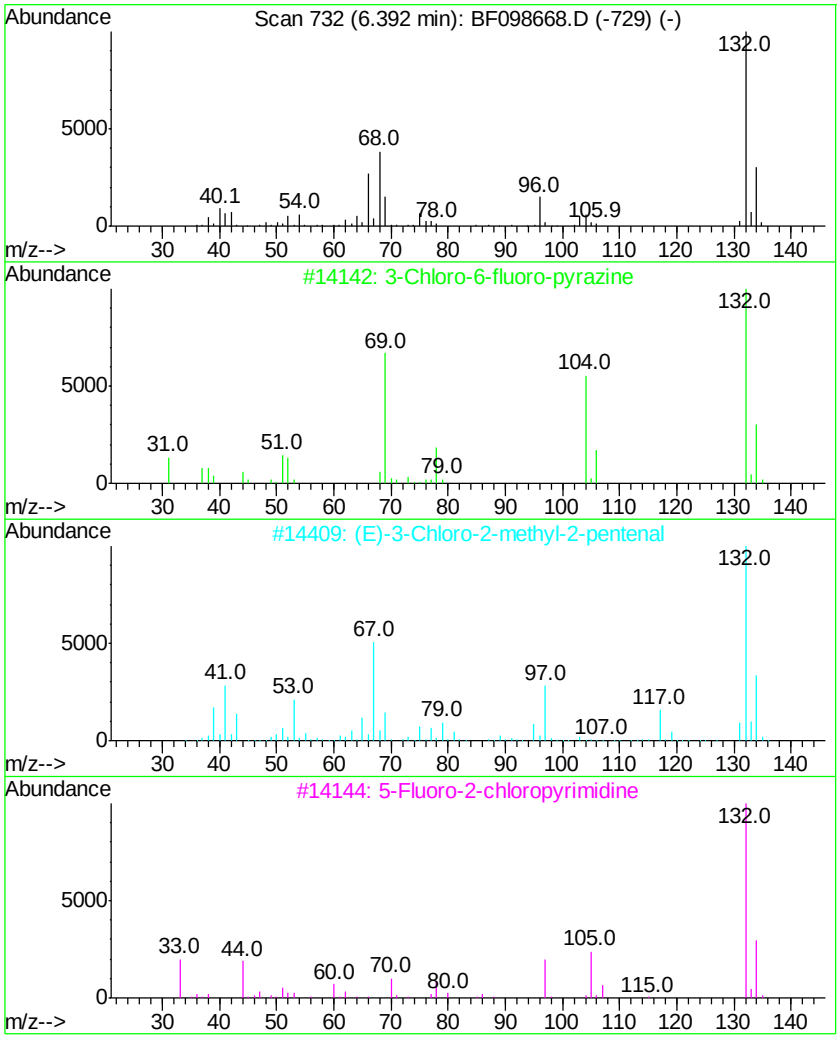
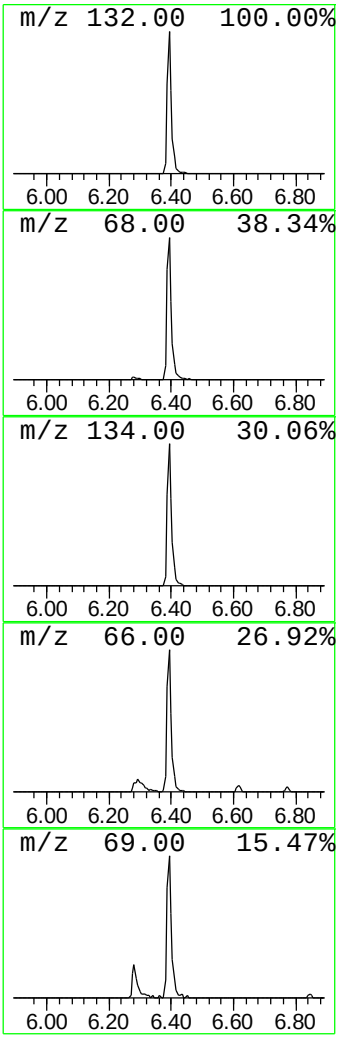
Peak Number 2 unknown6.39 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.39	17.08 ng	442486	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	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092017\
Data File : BF098668.D
Acq On : 20 Sep 2017 19:00
Operator : SJ/JU
Sample : I5281-04 5X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-8-EW

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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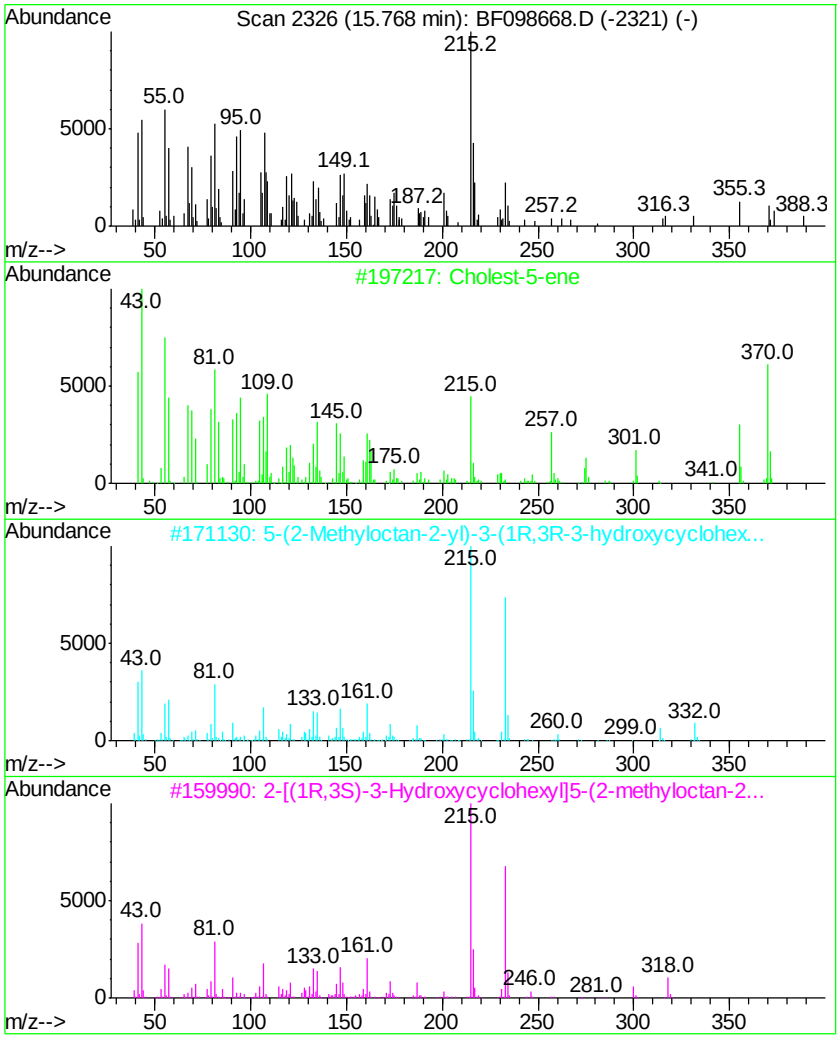
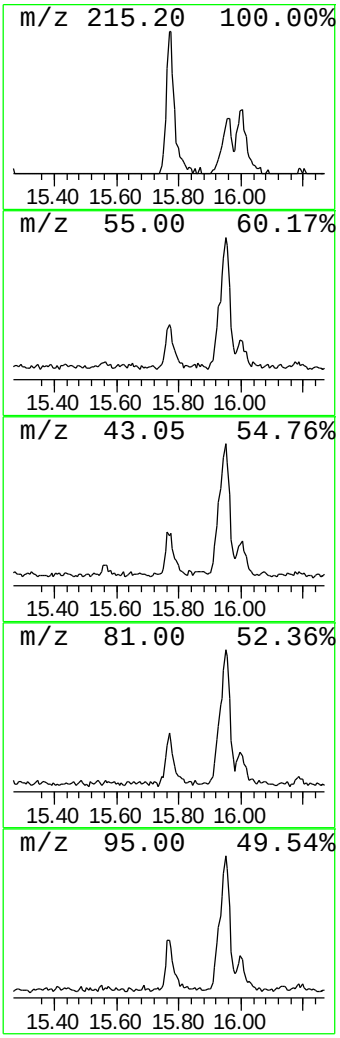
Peak Number 4 unknown15.77 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.77	14.20 ng	333460	Perylene-d12	15.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cholest-5-ene	370	C27H46	000570-74-1	38
2	5-(2-Methyloctan-2-yl)-3-(1R,3R-...	332	C22H36O2	070434-92-3	32
3	2-[(1R,3S)-3-Hydroxycyclohexyl]5...	318	C21H34O2	070434-82-1	25
4	Acetic acid, 2-acetoxymethyl-6-(...	326	C14H18N2O7	1000193-93-8	25
5	2,2,2-Trifluoro-N-[[4-[[(2,2,2-t...	328	C12H10F6N2O2	1000372-96-8	22





Library Search Compound Report

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Sample : I5281-04 5X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-8-EW

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
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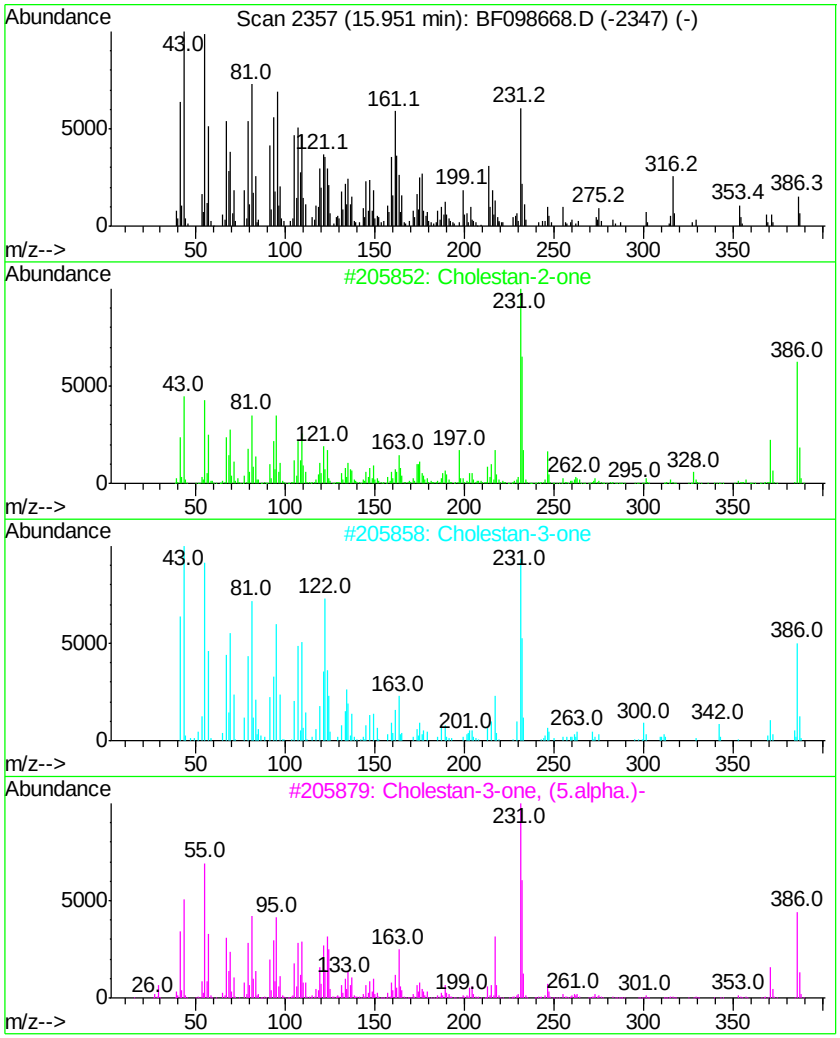
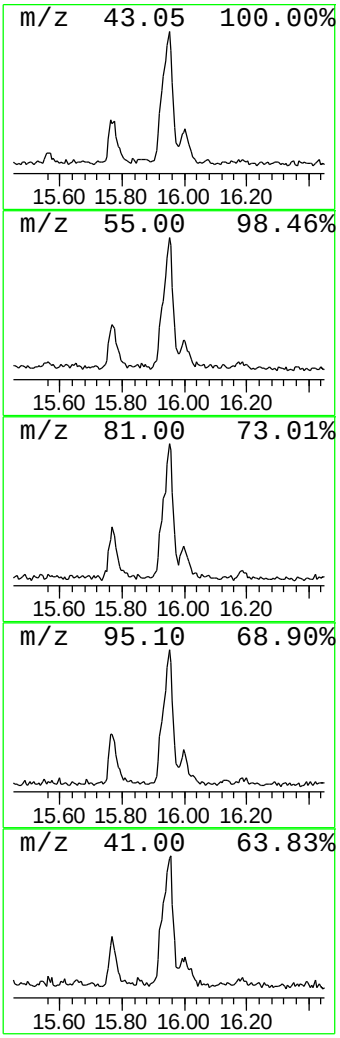
****

Peak Number 5 Cholestan-2-one Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.95	50.24 ng	1179620	Perylene-d12	15.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cholestan-2-one	386	C27H46O	1000210-43-4	78
2	Cholestan-3-one	386	C27H46O	015600-08-5	60
3	Cholestan-3-one, (5.alpha.)-	386	C27H46O	000566-88-1	58
4	Cholest-4-en-3-ol	386	C27H46O	014597-42-3	55
5	Cholestane, 4,5-epoxy-, (4.alpha...	386	C27H46O	006079-19-2	53





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Misc :
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Instrument : BNA_F
ClientSampleId : MW-8-EW

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

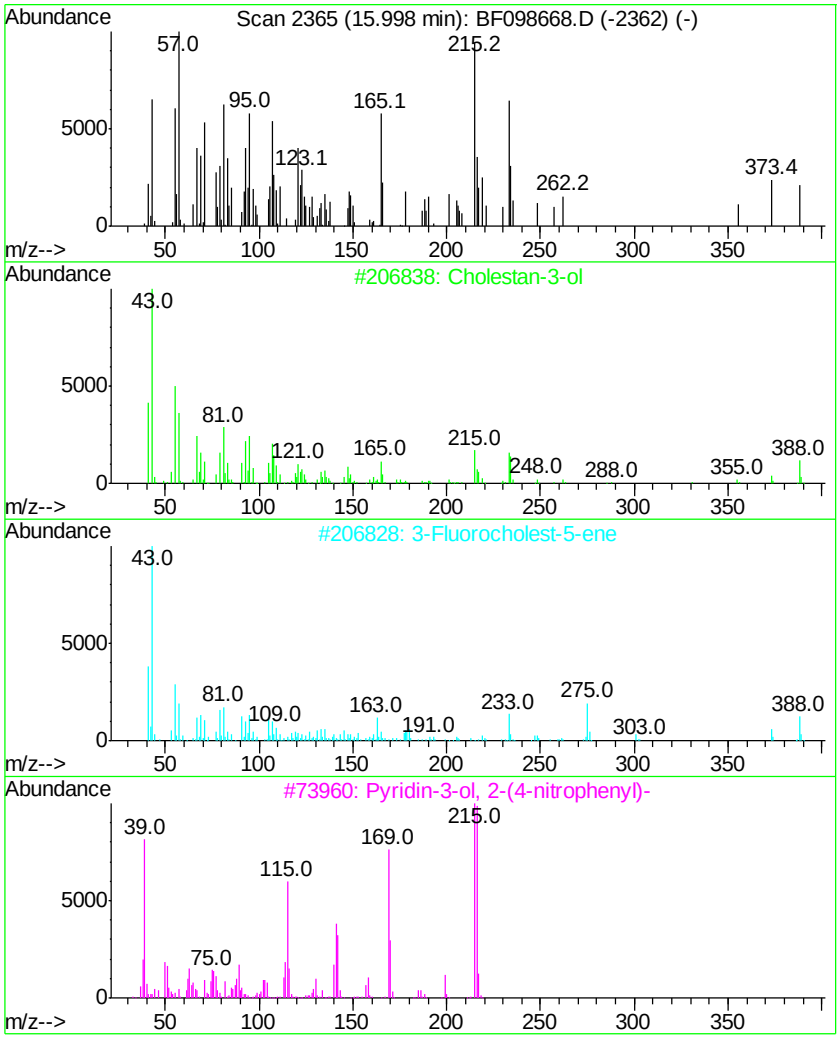
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

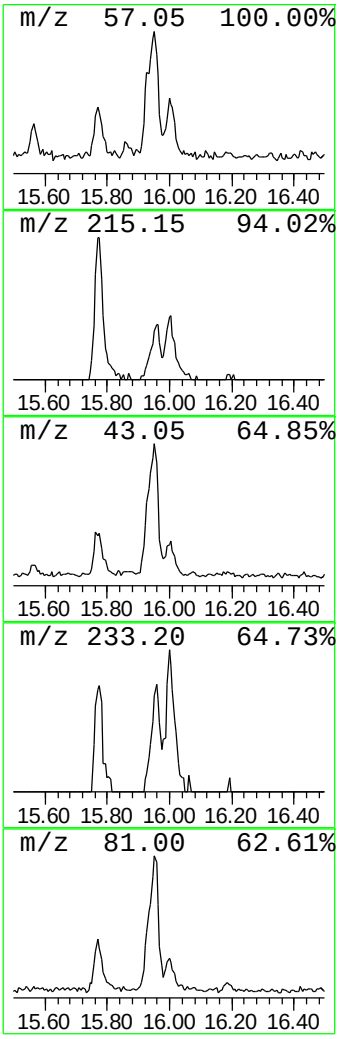
****

Peak Number 6 unknown16.00 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.00	9.83 ng	230716	Perylene-d12	15.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cholestan-3-ol	388	C27H48O	027409-41-2	43
2	3-Fluorocholest-5-ene	388	C27H45F	059331-45-2	25
3	Pyridin-3-ol, 2-(4-nitrophenyl)-	216	C11H8N2O3	030820-89-4	18
4	Cyclopent[e]-1,3-oxazine, octahy...	216	C13H16N2O	1000138-92-2	14
5	3-Buten-2-one, 4-(3-hydroxy-6,6-...	208	C13H20O2	1000142-31-3	14





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butanoic acid, 3-...	4.96	3.1	ng	80268	1	6.62	518073	20.0
unknown6.39	6.39	17.1	ng	442486	1	6.62	518073	20.0
unknown15.77	15.77	14.2	ng	333460	6	15.17	469611	20.0
Cholestan-2-one	15.95	50.2	ng	1179620	6	15.17	469611	20.0
unknown16.00	16.00	9.8	ng	230716	6	15.17	469611	20.0