LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011116\
Data File : BF084408.D
Acq On : 12 Jan 2016 5:04
Operator : SJ/UM
Sample : H1067-05
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-03

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-BF123115.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	5.024	255	257	264	rVB	787563	1123631	11.76%	1.517%
2	5.459	293	295	298	rBV	4863331	4692406	49.11%	6.335%
3	6.499	383	386	388	rBV	2308319	3102959	32.48%	4.189%
4	6.624	394	397	399	rBV	8236804	7639609	79.96%	10.314%
5	6.853	414	417	419	rBV	2721484	2243352	23.48%	3.029%
6	7.013	428	431	433	rVB	8330246	7907126	82.76%	10.676%
7	7.425	464	467	469	rBV	6494922	7027016	73.55%	9.487%
8	7.676	487	489	491	rBV	132686	129791	1.36%	0.175%
9	7.882	503	507	511	rBV2	87250	183779	1.92%	0.248%
10	8.145	527	530	532	rBV	2345535	2837846	29.70%	3.831%
11	8.190	532	534	537	rVB	87833	136911	1.43%	0.185%
12	8.259	537	540	542	rBV3	97660	165274	1.73%	0.223%
13	8.385	546	551	552	rBV4	68024	118664	1.24%	0.160%
14	8.419	552	554	557	rBV4	36714	101484	1.06%	0.137%
15	8.522	559	563	565	rBV5	87872	145170	1.52%	0.196%
16	8.579	565	568	570	rBV3	55009	99827	1.04%	0.135%
17	8.625	570	572	575	rVB3	78377	123650	1.29%	0.167%
18	8.670	575	576	577	rBV	114100	102210	1.07%	0.138%
19	8.762	582	584	585	rBV	124427	117483	1.23%	0.159%
20	8.853	590	592	593	rBV	118786	157615	1.65%	0.213%
21	9.036	606	608	609	rBV2	80786	119906	1.26%	0.162%
22	9.139	614	617	619	rVV2	223337	314951	3.30%	0.425%
23	9.173	619	620	621	rVV	222692	176508	1.85%	0.238%
24	9.219	621	624	627	rVV	9774508	9554236	100.00%	12.899%
25	9.310	630	632	634	rVV2	138963	263879	2.76%	0.356%
26	9.379	636	638	639	rVV2	80404	130537	1.37%	0.176%
27	9.402	639	640	642	rVB	275068	255366	2.67%	0.345%
28	9.516	649	650	651	rBV	98099	113347	1.19%	0.153%
29	9.550	651	653	655	rVV2	184317	271220	2.84%	0.366%
30	9.619	655	659	662	rVV6	175342	459055	4.80%	0.620%
31	9.699	664	666	668	rVV3	137350	252689	2.64%	0.341%
32	9.756	669	671	673	rVV2	140029	225759	2.36%	0.305%
33	9.825	675	677	680	rVB4	92171	170563	1.79%	0.230%
34	9.893	681	683	687	rVB	3422494	3112020	32.57%	4.202%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011116\
Data File : BF084408.D
Acq On : 12 Jan 2016 5:04
Operator : SJ/UM
Sample : H1067-05
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-03

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-BF123115.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	10.271	714	716	718	rBV2	176479	299073	3.13%	0.404%
36	10.328	719	721	722	rVV2	193903	216298	2.26%	0.292%
37	10.396	725	727	730	rBV4	321894	437863	4.58%	0.591%
38	10.522	735	738	741	rVV4	227247	562001	5.88%	0.759%
39	10.682	750	752	755	rBV2	3850526	5752080	60.20%	7.766%
40	10.888	768	770	772	rBV2	189930	304769	3.19%	0.411%
41	11.253	801	802	803	rVB	291400	199755	2.09%	0.270%
42	11.379	811	813	815	rBV	2843984	2406002	25.18%	3.248%
43	11.425	815	817	819	rVV2	470280	564243	5.91%	0.762%
44	11.573	828	830	831	rBV	247681	260998	2.73%	0.352%
45	11.928	859	861	863	rBV3	213712	220791	2.31%	0.298%
46	12.968	949	952	954	rBV	6354586	5988107	62.67%	8.085%
47	14.019	1041	1044	1046	rBV	1369234	1769659	18.52%	2.389%
48	15.437	1166	1168	1171	rBV	1082146	1509473	15.80%	2.038%

Sum of corrected areas: 74066951

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Misc :
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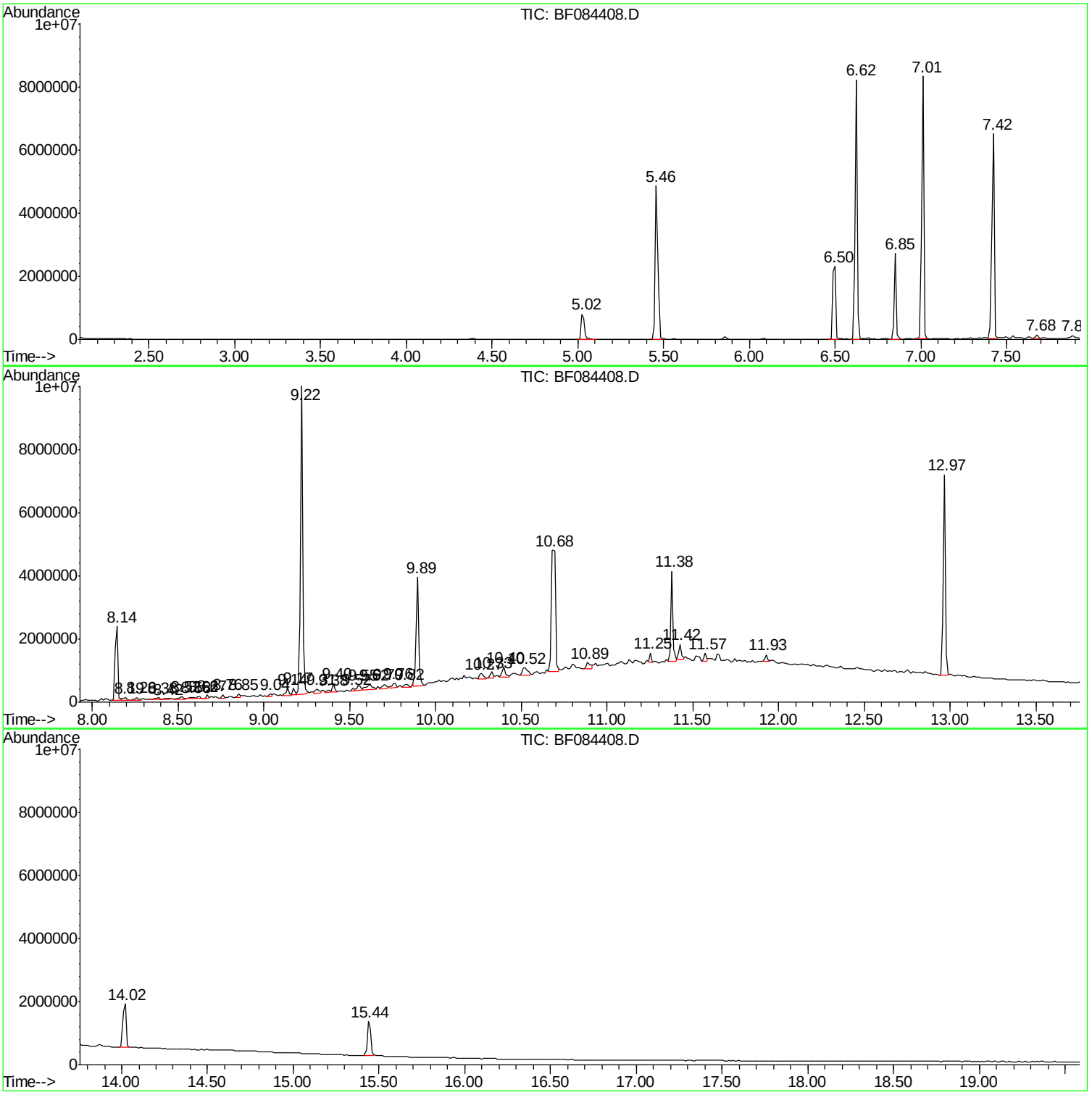
Instrument :
BNA_F
ClientSampleId :
MW-03

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011116\
Data File : BF084408.D
Acq On : 12 Jan 2016 5:04
Operator : SJ/UM
Sample : H1067-05
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-03

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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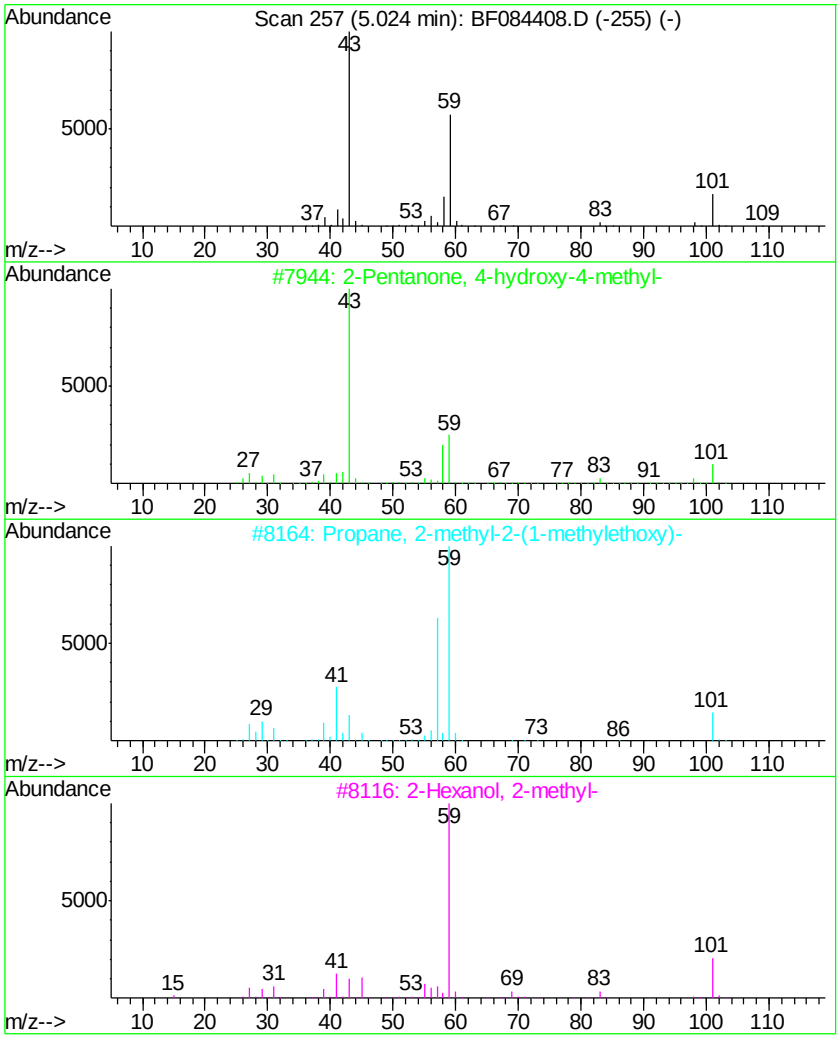
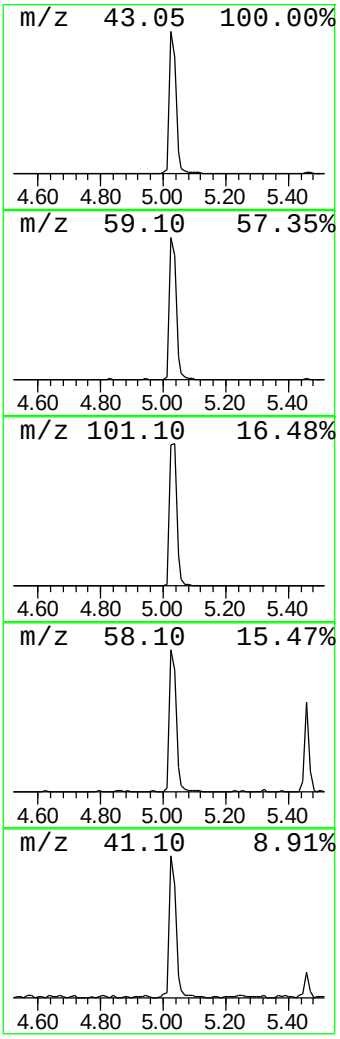
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.02	10.02 ng	1123630	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





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Data File : BF084408.D
Acq On : 12 Jan 2016 5:04
Operator : SJ/UM
Sample : H1067-05
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-03

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

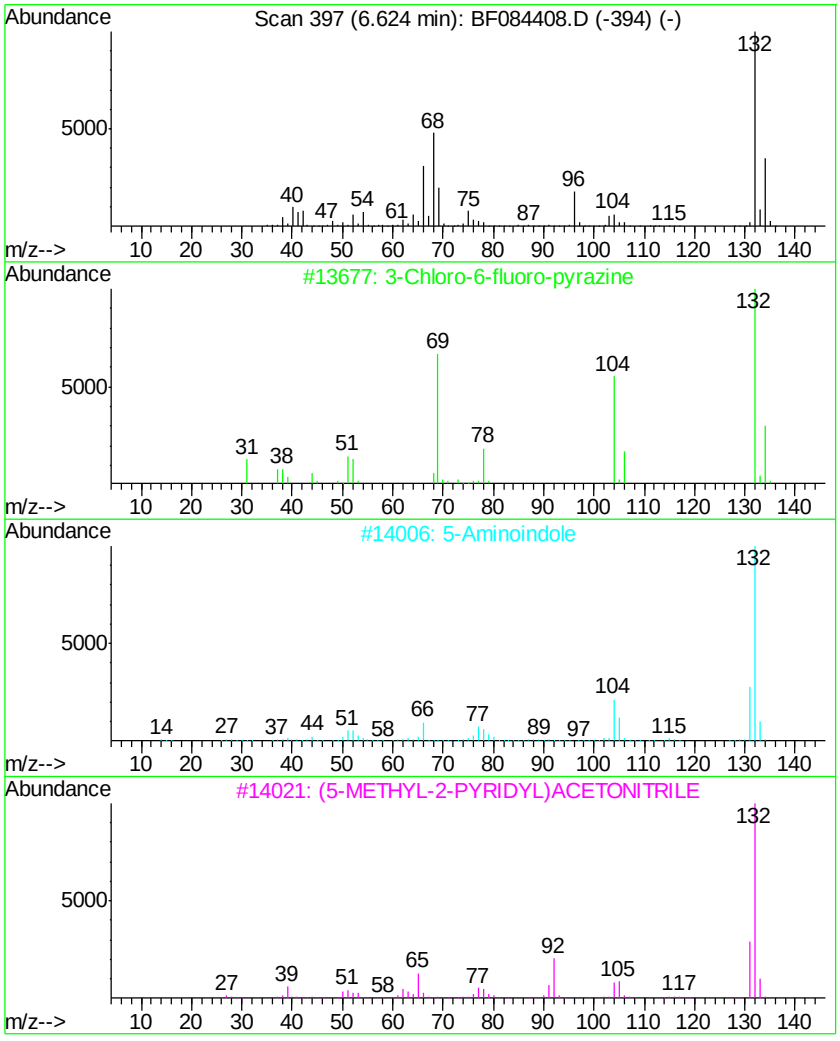
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

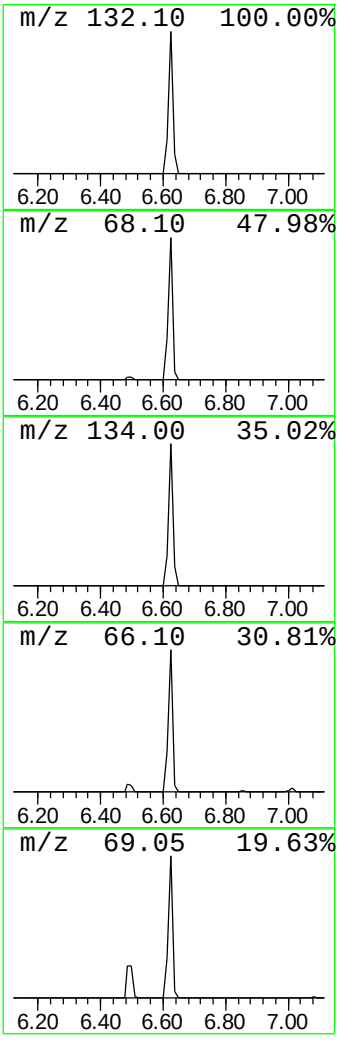
****

Peak Number 2 unknown6.62 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	68.11 ng	7639610	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
4	1,2,3-Trifluorobenzene	132	C6H3F3	001489-53-8	9
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011116\
Data File : BF084408.D
Acq On : 12 Jan 2016 5:04
Operator : SJ/UM
Sample : H1067-05
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-03

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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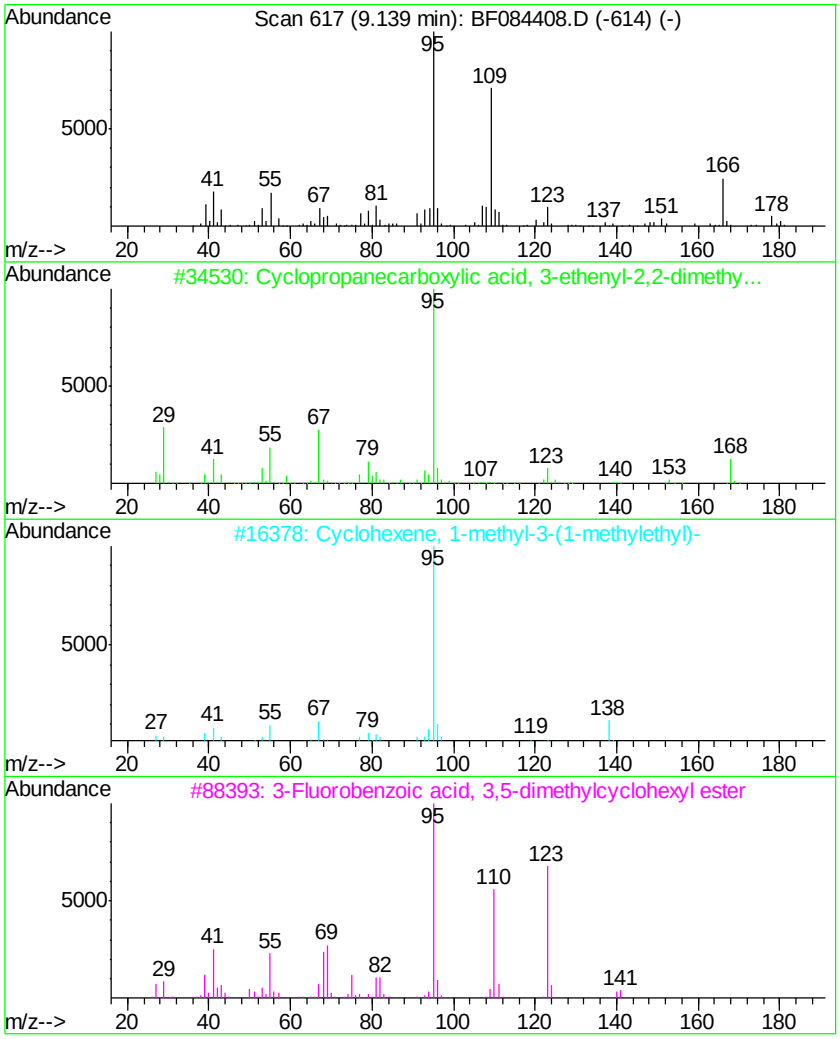
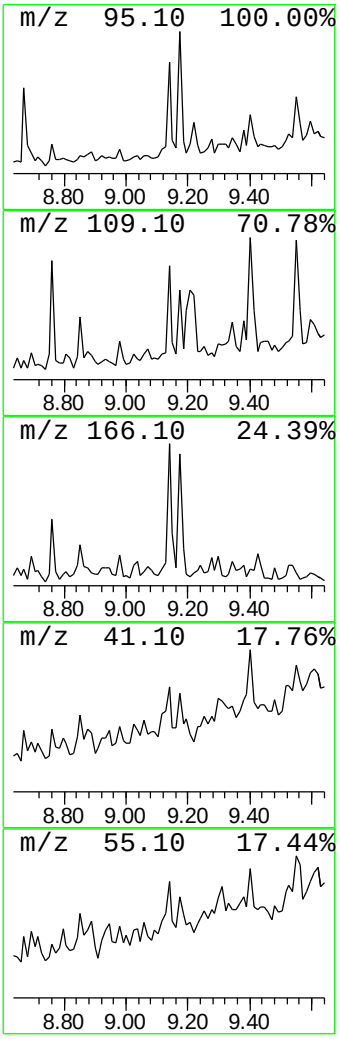
Peak Number 4 unknown9.14 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.14	2.02 ng	314951	Acenaphthene-d10	9.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopropanecarboxylic acid, 3-e...	168	C10H16O2	060066-50-4	43
2	Cyclohexene, 1-methyl-3-(1-methy...	138	C10H18	013828-31-4	38
3	3-Fluorobenzoic acid, 3,5-dimeth...	250	C15H19FO2	1000279-01-8	38
4	2-Furancarbonyl chloride	130	C5H3ClO2	000527-69-5	38
5	Cyclohexene, 3-(iodomethyl)-	222	C7H11I	034825-94-0	35





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011116\
Data File : BF084408.D
Acq On : 12 Jan 2016 5:04
Operator : SJ/UM
Sample : H1067-05
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-03

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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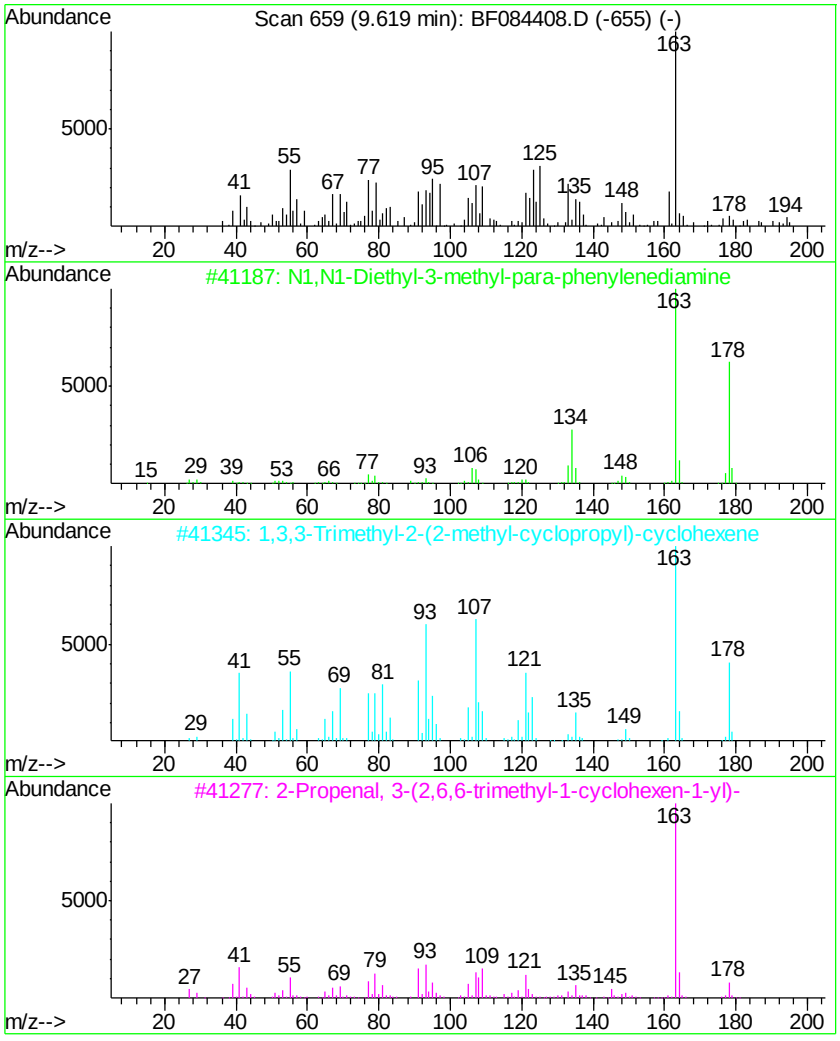
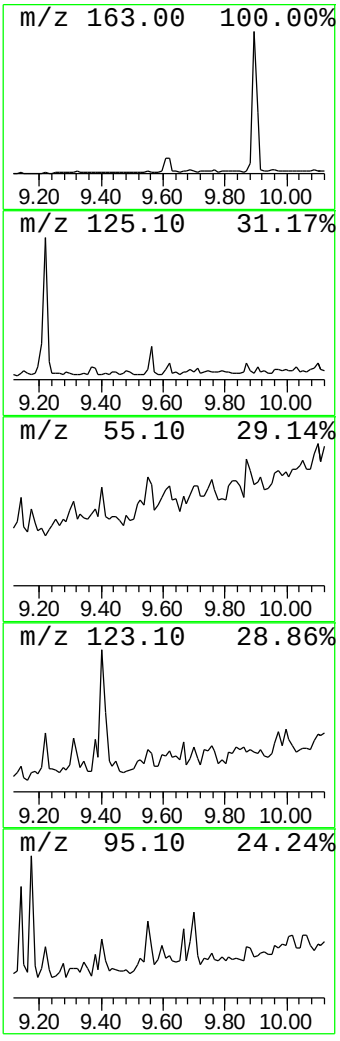
Peak Number 5 unknown9.62 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.62	2.95 ng	459055	Acenaphthene-d10	9.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	N1,N1-Diethyl-3-methyl-para-phen...	178	C11H18N2	002051-79-8	43
2	1,3,3-Trimethyl-2-(2-methyl-cycl...	178	C13H22	285129-06-8	38
3	2-Propenal, 3-(2,6,6-trimethyl-1...	178	C12H18O	004951-40-0	37
4	Benzenamine, 2,3,4,5,6-pentamethyl-	163	C11H17N	002243-30-3	32
5	4H-1,3,2-Dioxaborin, 4,6-diethen...	178	C10H15BO2	074630-03-8	27





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Acq On : 12 Jan 2016 5:04
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Sample : H1067-05
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-03

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

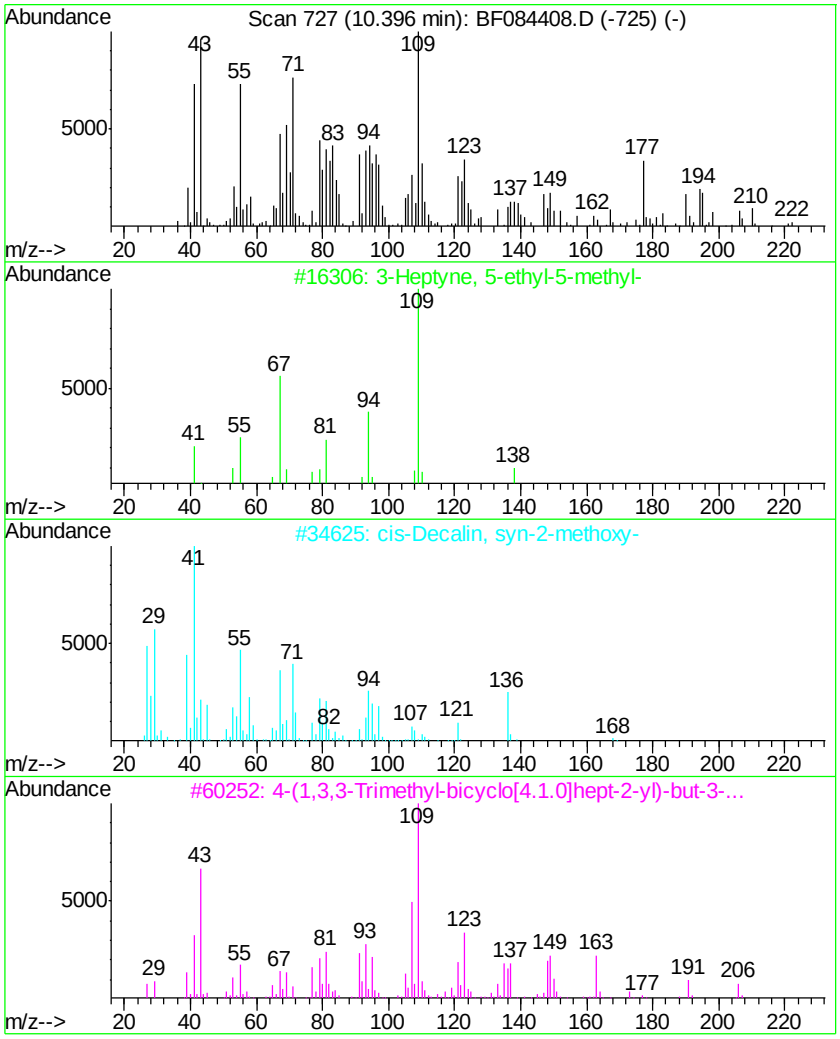
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

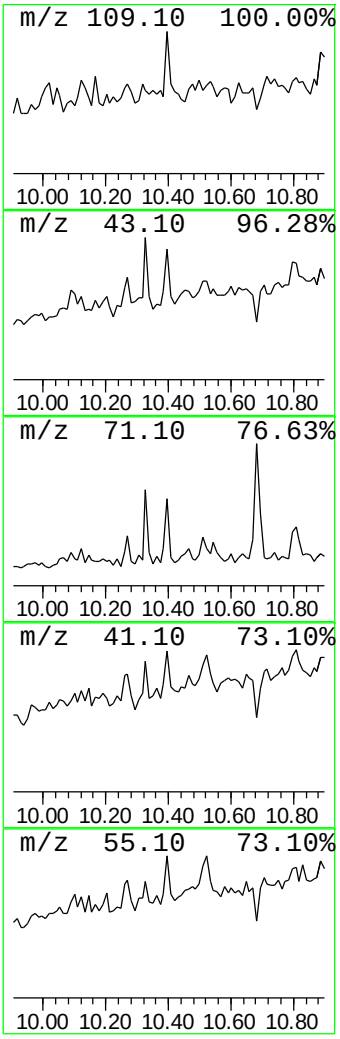
****

Peak Number 6 unknown10.40 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.40	2.81 ng	437863	Acenaphthene-d10	9.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Heptyne, 5-ethyl-5-methyl-	138	C10H18	061228-10-2	25
2	cis-Decalin, syn-2-methoxy-	168	C11H20O	1000158-93-6	22
3	4-(1,3,3-Trimethyl-bicyclo[4.1.0...	206	C14H22O	077143-31-8	20
4	Ketone, isopropylidenecyclopropy...	124	C8H12O	029765-67-1	18
5	Ledol	222	C15H26O	000577-27-5	15





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011116\
Data File : BF084408.D
Acq On : 12 Jan 2016 5:04
Operator : SJ/UM
Sample : H1067-05
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-03

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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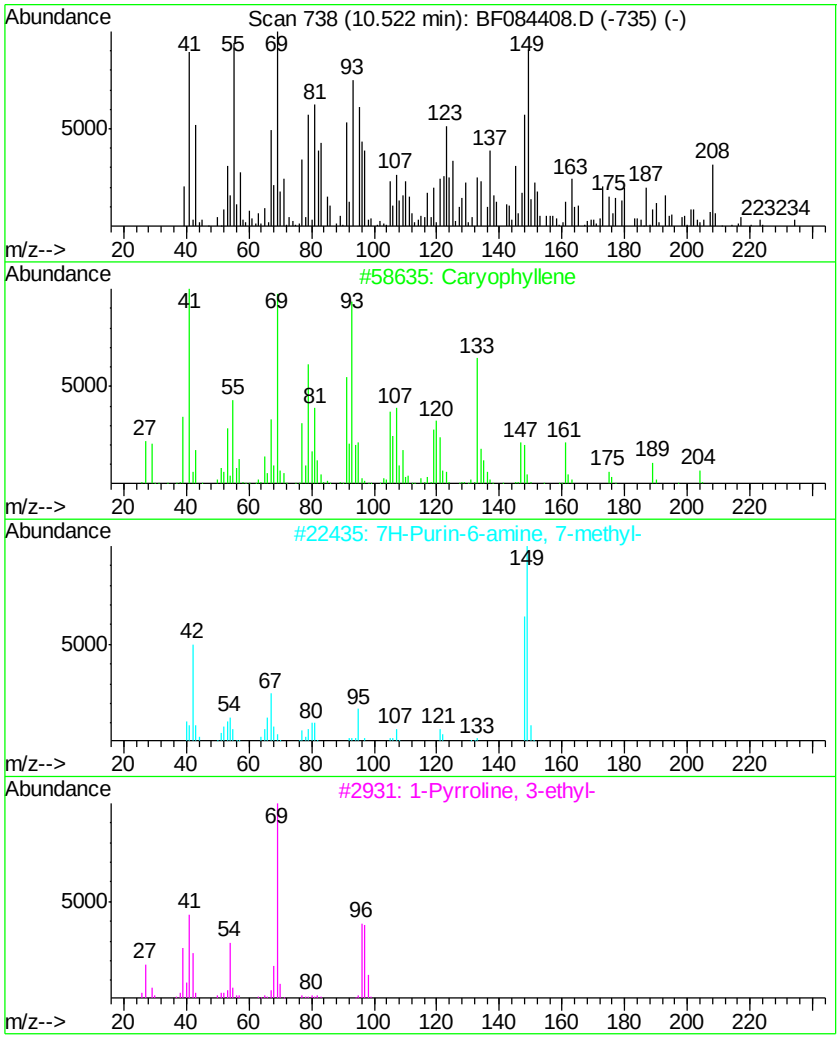
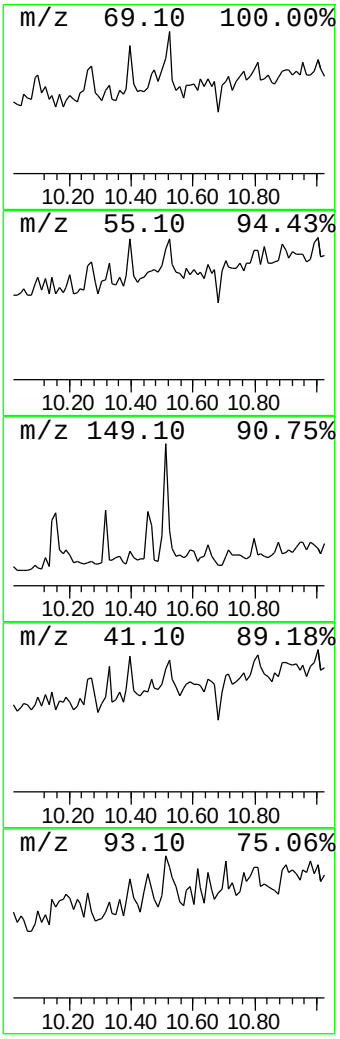
Peak Number 7 unknown10.52 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.52	3.61 ng	562001	Acenaphthene-d10	9.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Caryophyllene	204	C15H24	000087-44-5	22
2	7H-Purin-6-amine, 7-methyl-	149	C6H7N5	000935-69-3	20
3	1-Pyrroline, 3-ethyl-	97	C6H11N	1000073-06-0	18
4	10-Methyltricyclo[4.3.1.1(2,5)]u...	180	C12H20O	1000187-06-1	15
5	1,6,10-Dodecatriene, 7,11-dimeth...	204	C15H24	018794-84-8	14





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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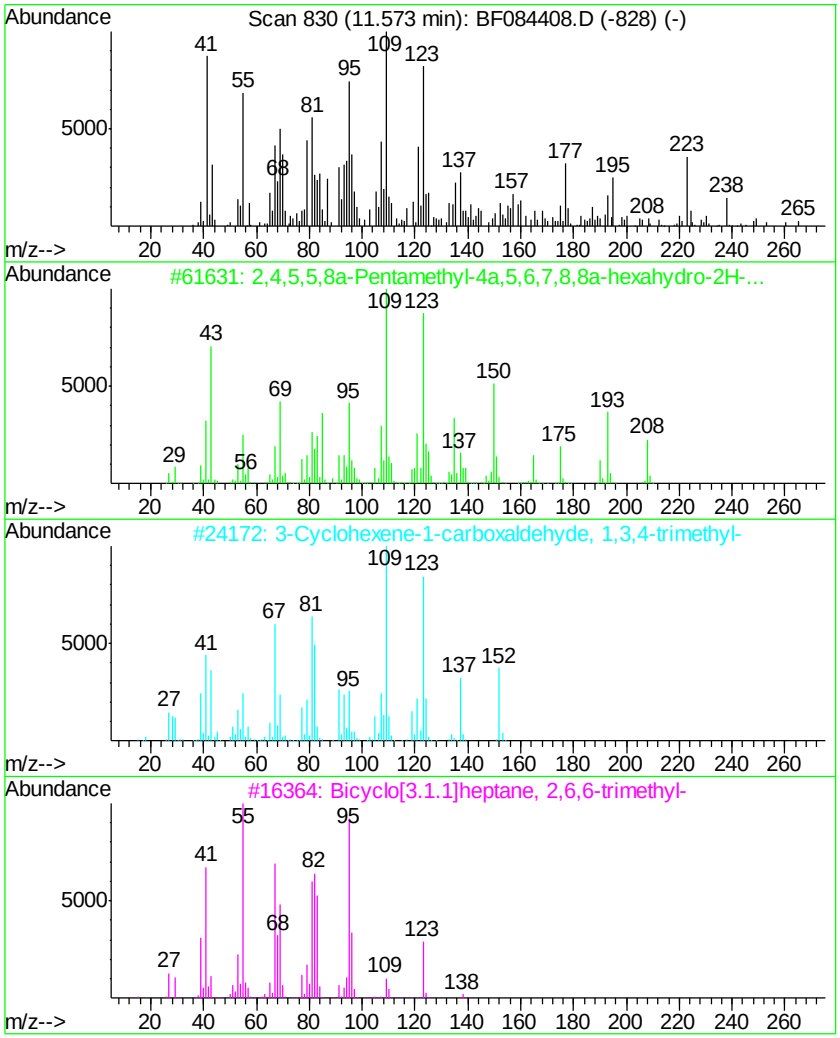
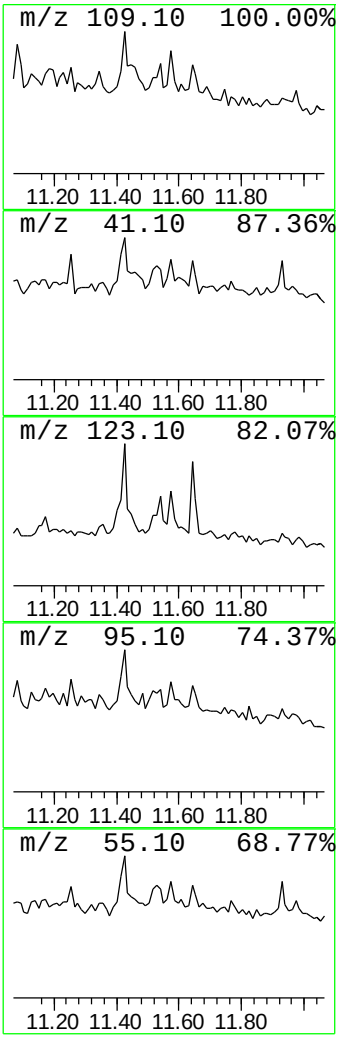
Peak Number 9 2,4,5,5,8a-Pentamethyl-4a,5... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.57	2.17 ng	260998	Phenanthrene-d10	11.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,5,5,8a-Pentamethyl-4a,5,6,7,...	208	C14H24O	1000195-30-1	53
2	3-Cyclohexene-1-carboxaldehyde, ...	152	C10H16O	040702-26-9	46
3	Bicyclo[3.1.1]heptane, 2,6,6-tri...	138	C10H18	000473-55-2	41
4	Cyclopropanemethanol, .alpha.,2-...	182	C12H22O	121959-70-4	38
5	1-Hydroxymethyl-3,3-dimethyl-2-(...	224	C14H24O2	1000190-51-5	30





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011116\
Data File : BF084408.D
Acq On : 12 Jan 2016 5:04
Operator : SJ/UM
Sample : H1067-05
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-03

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.02	10.0	ng	1123630	1	6.85	2243350	20.0
unknown6.62	6.62	68.1	ng	7639610	1	6.85	2243350	20.0
unknown9.14	9.14	2.0	ng	314951	3	9.89	3112020	20.0
unknown9.62	9.62	3.0	ng	459055	3	9.89	3112020	20.0
unknown10.40	10.40	2.8	ng	437863	3	9.89	3112020	20.0
unknown10.52	10.52	3.6	ng	562001	3	9.89	3112020	20.0
2,4,5,5,8a-Pentam...	11.57	2.2	ng	260998	4	11.38	2406000	20.0