LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070216\
Data File : BF088618.D
Acq On : 2 Jul 2016 15:42
Operator : UM/SJ
Sample : H3871-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : R5-B6(0-11)C

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-BF063016.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	1.724	10	12	21	rVB	70618	123006	4.76%	0.499%
2	1.861	21	24	35	rVB	386193	756795	29.27%	3.069%
3	3.004	122	124	136	rBV	15870	42440	1.64%	0.172%
4	4.959	292	295	299	rBB	142563	183161	7.08%	0.743%
5	5.382	329	332	335	rBV	1771723	2341993	90.58%	9.499%
6	6.422	420	423	426	rBV	1799858	2585492	100.00%	10.486%
7	6.559	432	435	437	rBV	2602103	2383977	92.21%	9.669%
8	6.787	453	455	458	rVB	628562	681751	26.37%	2.765%
9	6.947	467	469	472	rVB	2064893	1836067	71.01%	7.447%
10	7.359	502	505	507	rBV	1784306	1830349	70.79%	7.424%
11	8.079	565	568	570	rBV	1175417	988500	38.23%	4.009%
12	9.153	660	662	665	rVB	2610028	2385493	92.26%	9.675%
13	9.496	689	692	694	rBV	185400	184698	7.14%	0.749%
14	9.553	694	697	699	rVB	400048	464601	17.97%	1.884%
15	9.771	715	716	718	rBV	36573	30418	1.18%	0.123%
16	9.828	718	721	723	rVB	1225945	1077548	41.68%	4.370%
17	10.274	758	760	761	rVB	51326	40900	1.58%	0.166%
18	10.342	764	766	768	rVV	40737	38100	1.47%	0.155%
19	10.616	787	790	792	rBV	1225864	1445758	55.92%	5.864%
20	10.742	800	801	805	rVB	59376	60013	2.32%	0.243%
21	11.188	838	840	842	rBV	125581	115467	4.47%	0.468%
22	11.302	848	850	854	rVB	922384	877884	33.95%	3.561%
23	11.371	854	856	860	rVB2	31799	64092	2.48%	0.260%
24	11.531	869	870	875	rVB3	18527	35200	1.36%	0.143%
25	11.611	875	877	880	rVB	68690	76336	2.95%	0.310%
26	11.839	895	897	899	rVB	34007	31936	1.24%	0.130%
27	12.514	953	956	958	rBV	67447	80620	3.12%	0.327%
28	12.731	972	975	978	rBV	65393	83600	3.23%	0.339%
29	12.891	987	989	991	rVB	1834883	1675335	64.80%	6.795%
30	13.645	1053	1055	1057	rBV	117150	135534	5.24%	0.550%
31	13.794	1065	1068	1077	rBV2	113317	158670	6.14%	0.644%
32	13.931	1077	1080	1082	rBV	748767	742339	28.71%	3.011%
33	14.434	1120	1124	1128	rBV4	17173	39249	1.52%	0.159%
34	14.788	1153	1155	1157	rVB	32970	33190	1.28%	0.135%

LSC Area Percent Report

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Acq On : 2 Jul 2016 15:42
Operator : UM/SJ
Sample : H3871-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : R5-B6(0-11)C

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-BF063016.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.937	1165	1168	1172	rBV	50296	120804	4.67%	0.490%
36	15.028	1174	1176	1182	rVV2	17193	39388	1.52%	0.160%
37	15.211	1190	1192	1195	rVB	31031	34563	1.34%	0.140%
38	15.268	1195	1197	1199	rBV	35982	42798	1.66%	0.174%
39	15.325	1199	1202	1205	rBV	577396	689296	26.66%	2.796%
40	15.657	1229	1231	1235	rVB4	12092	26648	1.03%	0.108%
41	15.828	1244	1246	1253	rVB6	15639	38230	1.48%	0.155%
42	16.663	1316	1319	1324	rVB2	14937	33755	1.31%	0.137%

Sum of corrected areas: 24655994

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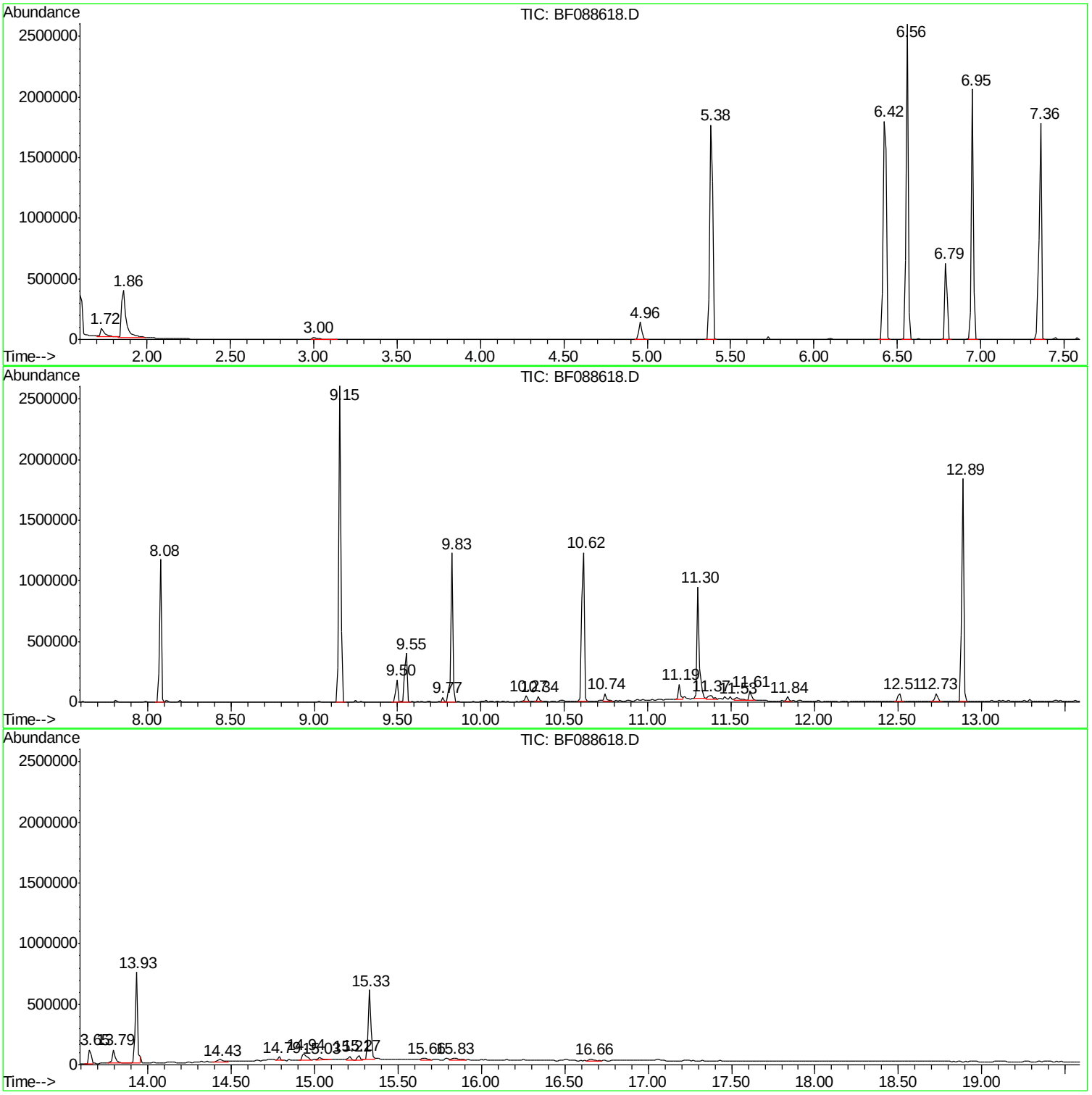
Instrument : BNA_F
ClientSampleId : R5-B6(0-11)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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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Data File : BF088618.D
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Operator : UM/SJ
Sample : H3871-05
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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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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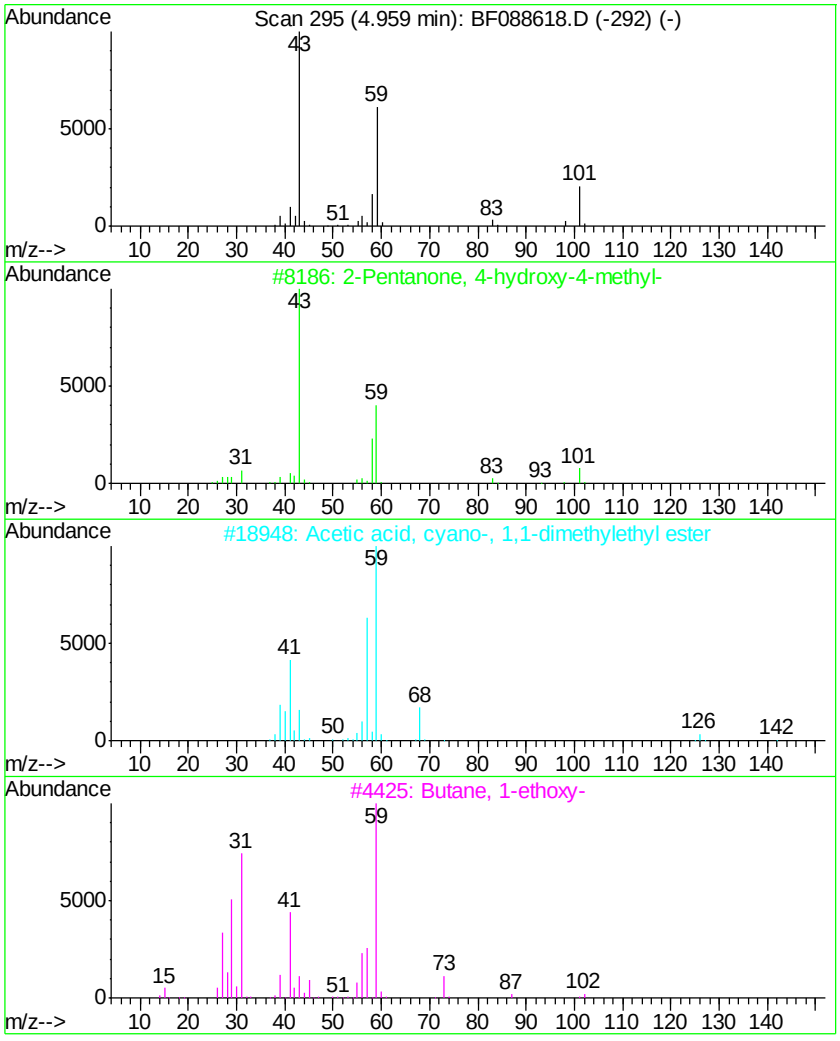
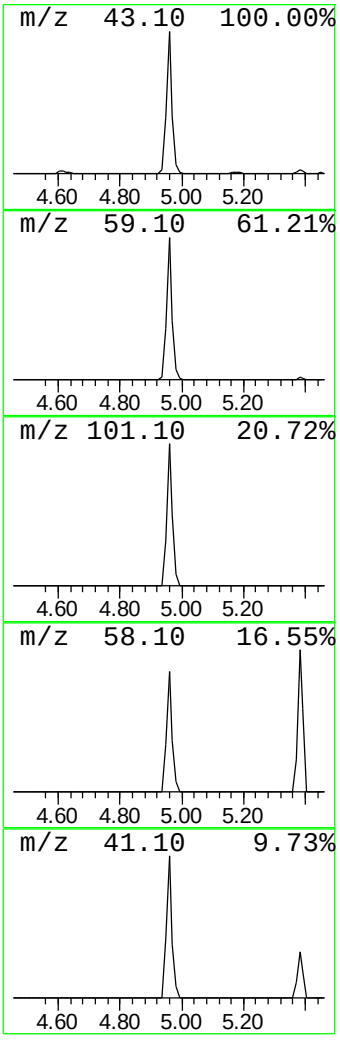
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.96	5.37 ng	183161	1,4-Dichlorobenzene-d4	6.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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Data File : BF088618.D
Acq On : 2 Jul 2016 15:42
Operator : UM/SJ
Sample : H3871-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : R5-B6(0-11)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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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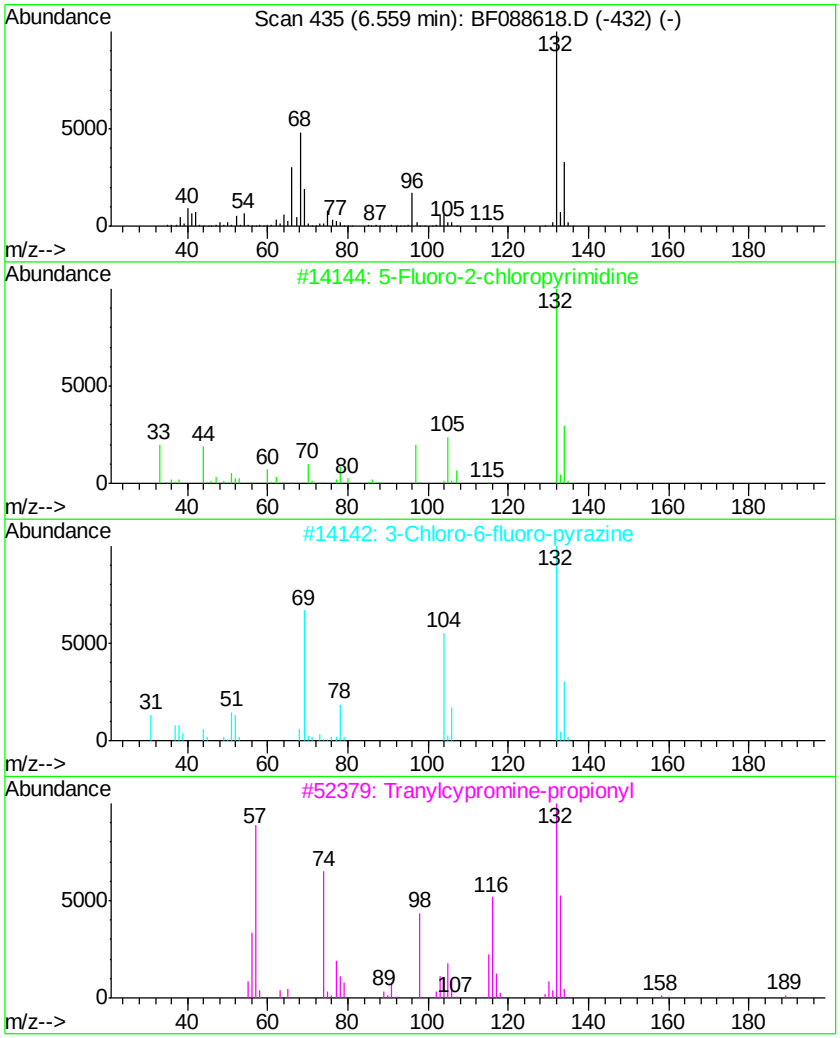
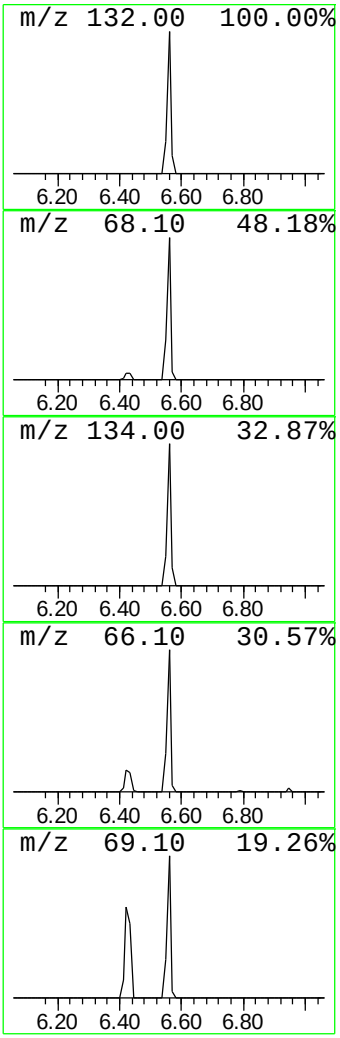
Peak Number 4 unknown6.56 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	69.94 ng	2383980	1,4-Dichlorobenzene-d4	6.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	27
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





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Sample : H3871-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : R5-B6(0-11)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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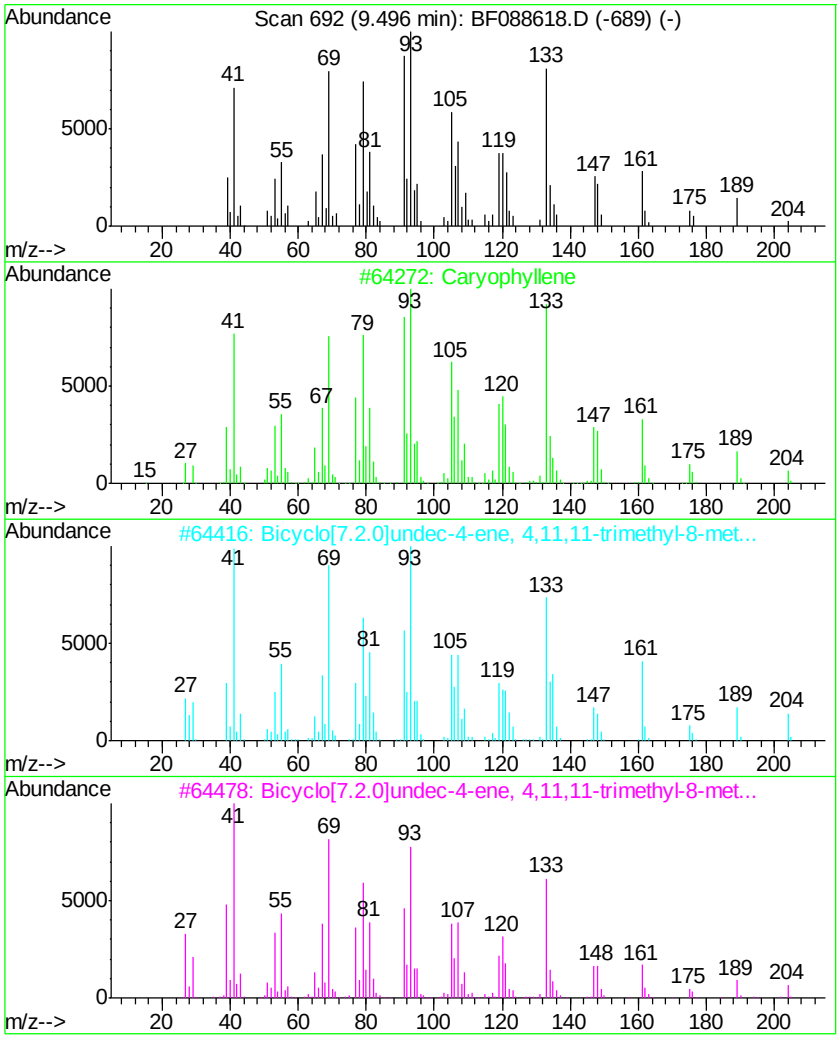
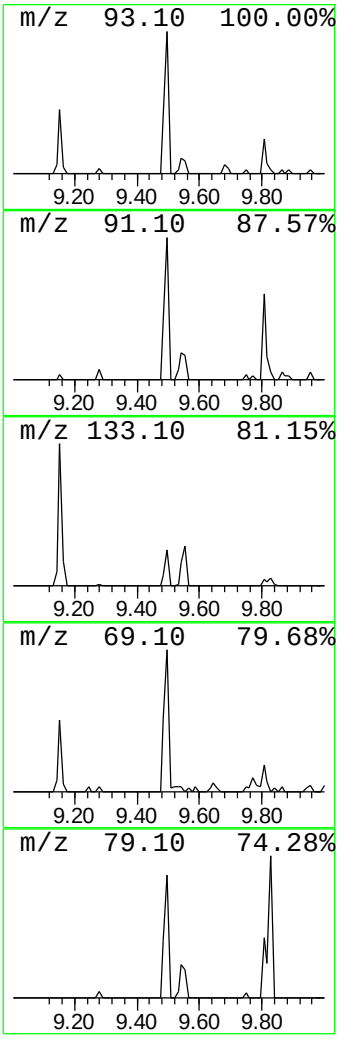
Peak Number 6 Caryophyllene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.50	3.43 ng	184698	Acenaphthene-d10	9.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Caryophyllene	204	C15H24	000087-44-5	94
2	Bicyclo[7.2.0]undec-4-ene, 4,11,...	204	C15H24	013877-93-5	93
3	Bicyclo[7.2.0]undec-4-ene, 4,11,...	204	C15H24	000118-65-0	91
4	6-(1'-Oxo-2'-propenyl)-1,3-cis,c...	162	C11H14O	138146-05-1	35
5	Spiro[4.4]nona-1,3-diene, 1,2-di...	148	C11H16	1000163-57-6	35





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Sample : H3871-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : R5-B6(0-11)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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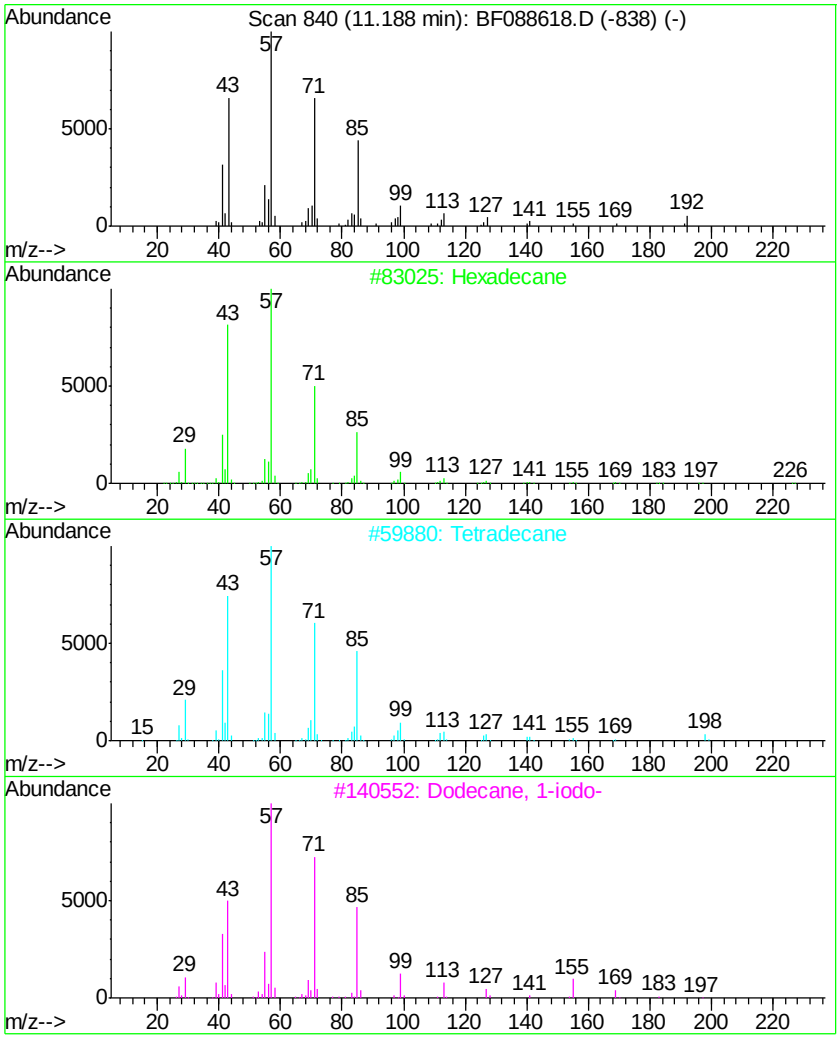
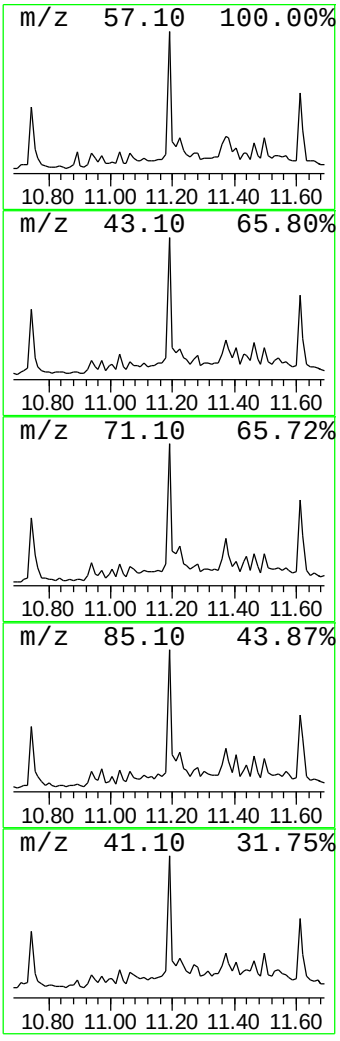
Peak Number 7 Hexadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.19	2.63 ng	115467	Phenanthrene-d10	11.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	90
2	Tetradecane	198	C14H30	000629-59-4	86
3	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	86
4	Heneicosane	296	C21H44	000629-94-7	86
5	Tridecane	184	C13H28	000629-50-5	86





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Sample : H3871-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : R5-B6(0-11)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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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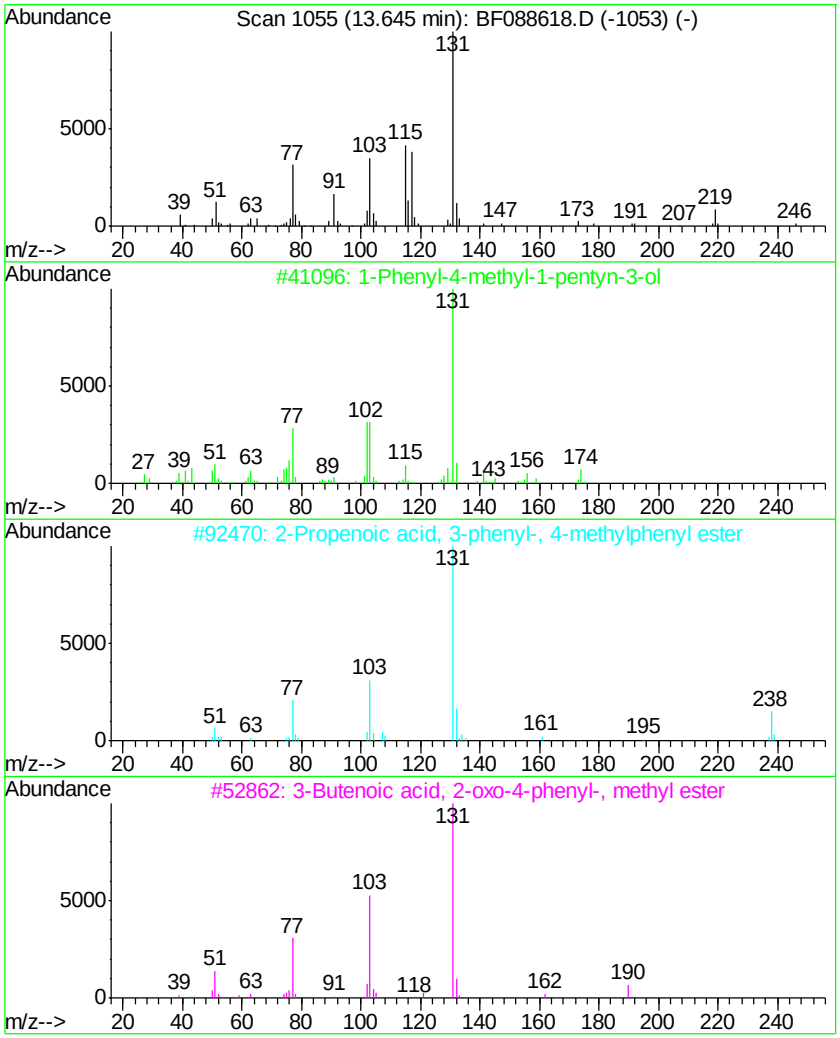
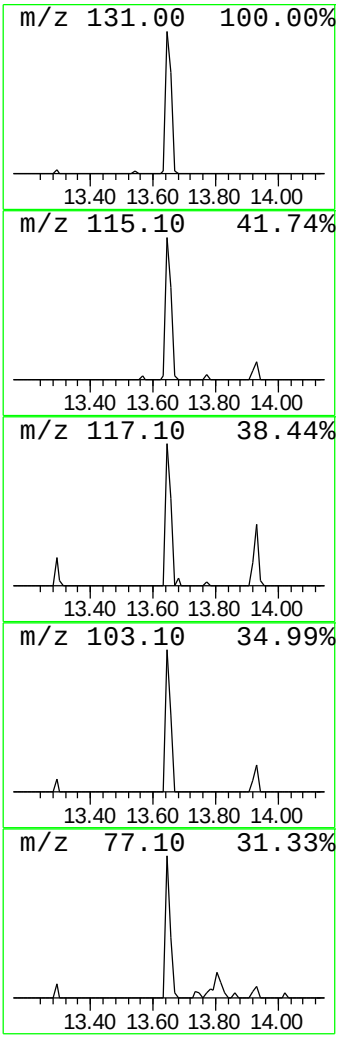
Peak Number 9 unknown13.65 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.65	3.65 ng	135534	Chrysene-d12	13.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenyl-4-methyl-1-pentyn-3-ol	174	C12H14O	005923-02-4	47
2	2-Propenoic acid, 3-phenyl-, 4-m...	238	C16H14O2	010519-07-0	43
3	3-Butenoic acid, 2-oxo-4-phenyl-...	190	C11H10O3	1000142-22-4	43
4	N-(p-Vinylbenzoyl)-l-alanine	219	C12H13NO3	139184-60-4	43
5	2-Iodo-benzoic acid N'-(3-phenyl...	392	C16H13IN2O2	315672-62-9	43





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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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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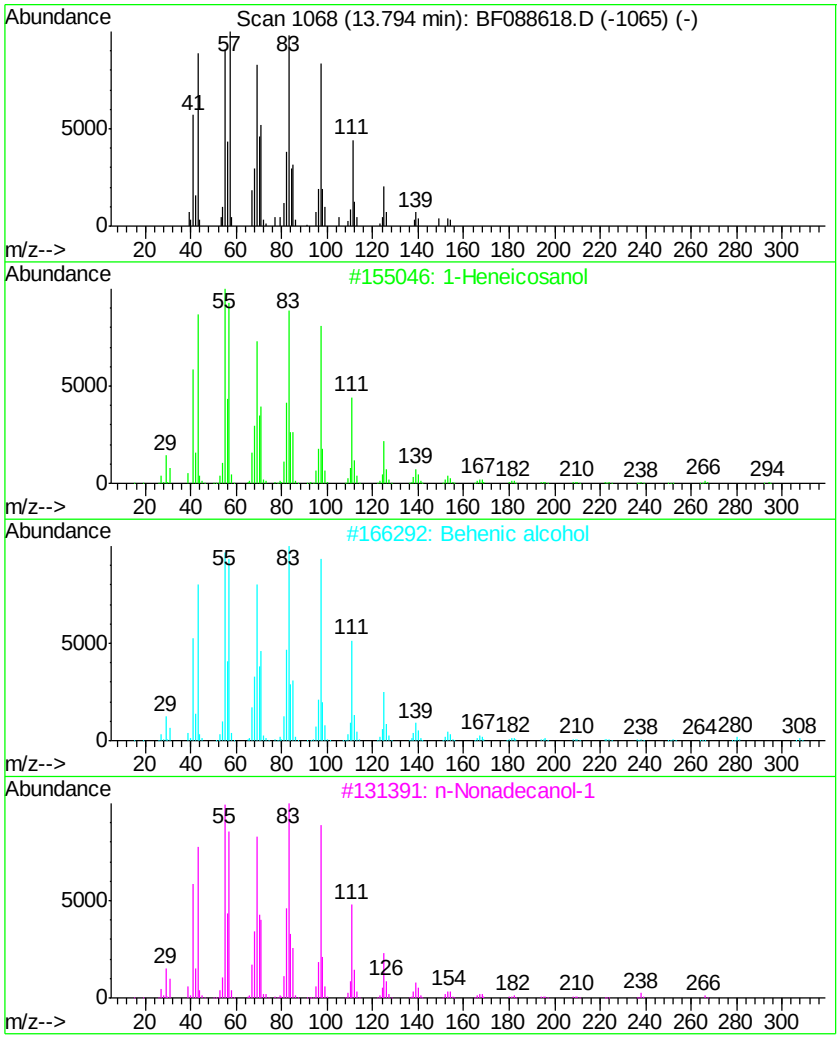
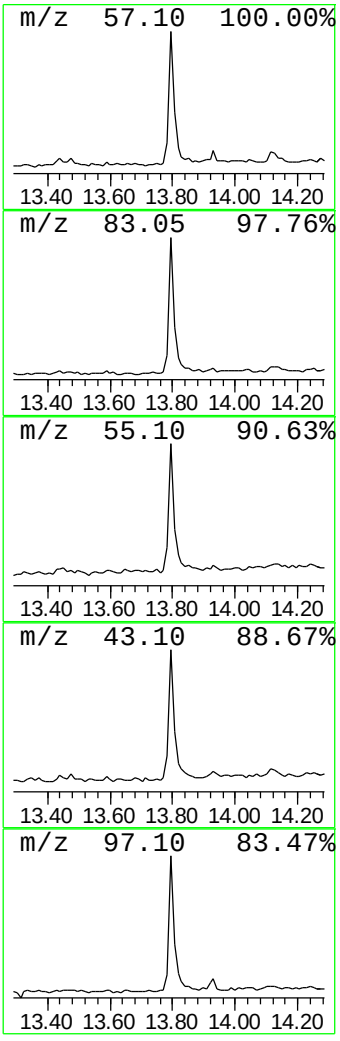
Peak Number 10 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.79	4.27 ng	158670	Chrysene-d12	13.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	Behenic alcohol	326	C22H46O	000661-19-8	95
3	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
5	1-Nonadecene	266	C19H38	018435-45-5	91





Tentatively Identified Compound (LSC) summary

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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
2-Pentanone, 4-hy...	4.96	5.4	ng	183161	1	6.79	681751	20.0
unknown6.56	6.56	69.9	ng	2383980	1	6.79	681751	20.0
Caryophyllene	9.50	3.4	ng	184698	3	9.83	1077550	20.0
Hexadecane	11.19	2.6	ng	115467	4	11.30	877884	20.0
unknown13.65	13.65	3.6	ng	135534	5	13.93	742339	20.0
1-Heneicosanol	13.79	4.3	ng	158670	5	13.93	742339	20.0