LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012120\
Data File : BF118633.D
Acq On : 21 Jan 2020 14:00
Operator : CG/JU
Sample : PB126152BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB126152BL

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012020.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	2.187	11	17	26	rVB	1534983	2061437	20.06%	2.516%
2	5.098	504	512	521	rBV	1288191	1531262	14.90%	1.869%
3	5.504	575	581	584	rBV	6686737	6686334	65.06%	8.160%
4	6.504	745	751	754	rBV	6886884	7289426	70.93%	8.896%
5	6.651	771	776	779	rBV	7713526	7451364	72.51%	9.093%
6	6.881	811	815	818	rBV	2694492	2207965	21.48%	2.694%
7	7.039	837	842	845	rBV	6491289	5931572	57.72%	7.238%
8	7.434	904	909	913	rBV	4300067	4515384	43.94%	5.510%
9	8.163	1028	1033	1036	rBV	3059322	2860208	27.83%	3.490%
10	9.239	1210	1216	1219	rBV	9225639	9289885	90.40%	11.337%
11	9.363	1234	1237	1248	rVB	87578	109442	1.06%	0.134%
12	9.628	1278	1282	1285	rBV	381594	326250	3.17%	0.398%
13	9.916	1324	1331	1335	rBV	4185640	3547210	34.52%	4.329%
14	10.704	1460	1465	1468	rBV	6705709	6102337	59.38%	7.447%
15	11.398	1579	1583	1587	rBV	3804745	3629614	35.32%	4.429%
16	12.986	1848	1853	1856	rBV	10701355	10276932	100.00%	12.541%
17	13.874	2001	2004	2019	rBV	1008863	1178495	11.47%	1.438%
18	14.033	2027	2031	2035	rBV	3154009	3007625	29.27%	3.670%
19	14.510	2107	2112	2118	rBV	177290	231704	2.25%	0.283%
20	14.821	2161	2165	2170	rBV	212316	234446	2.28%	0.286%
21	15.162	2219	2223	2230	rBV	248842	302501	2.94%	0.369%
22	15.510	2276	2282	2286	rBV	1933055	2372897	23.09%	2.896%
23	15.545	2286	2288	2293	rVB	229014	277339	2.70%	0.338%
24	15.992	2359	2364	2368	rBV	172614	264398	2.57%	0.323%
25	16.039	2369	2372	2380	rVB7	70682	123669	1.20%	0.151%
26	16.504	2448	2451	2456	rVB	83779	135135	1.31%	0.165%

Sum of corrected areas: 81944831

LSC Report - Integrated Chromatogram

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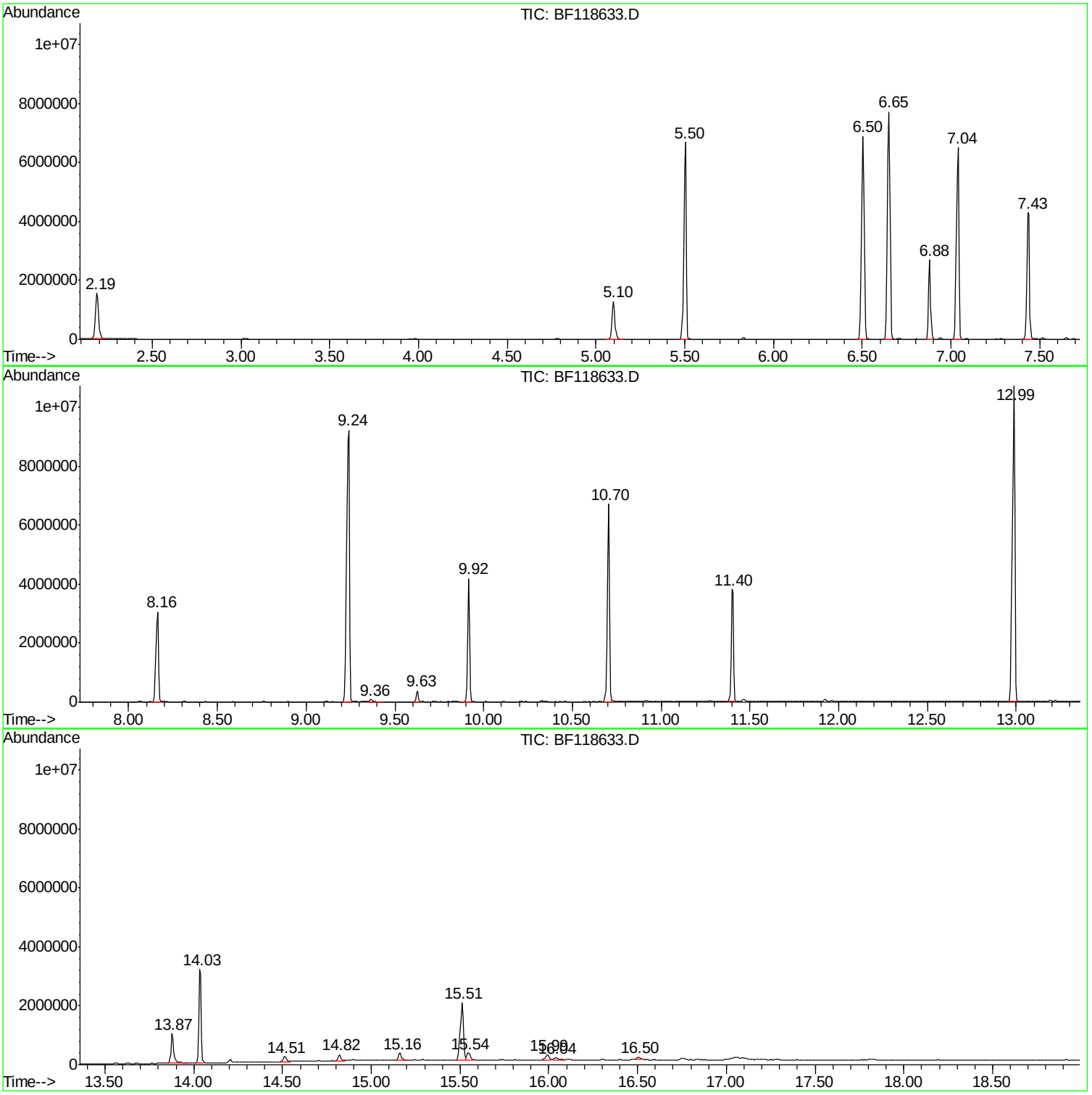
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB126152BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012020.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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Instrument : BNA_F
ClientSampleId : PB126152BL

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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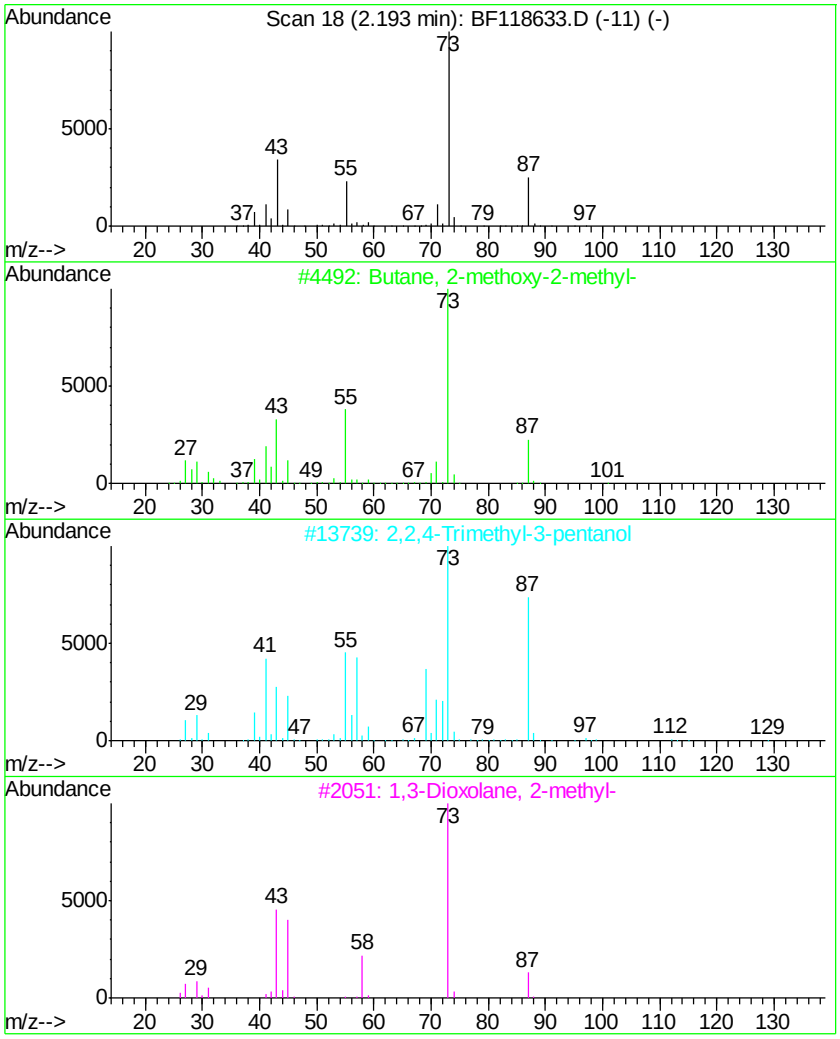
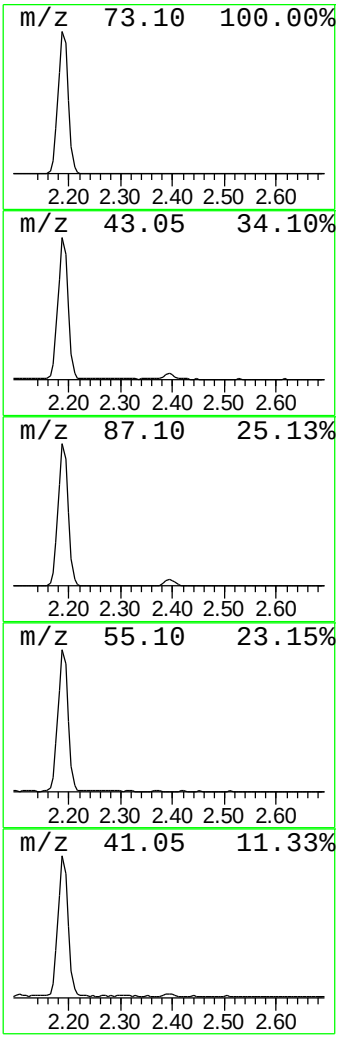
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.19	18.67 ng	2061440	1,4-Dichlorobenzene-d4	6.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22





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Operator : CG/JU
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Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB126152BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012020.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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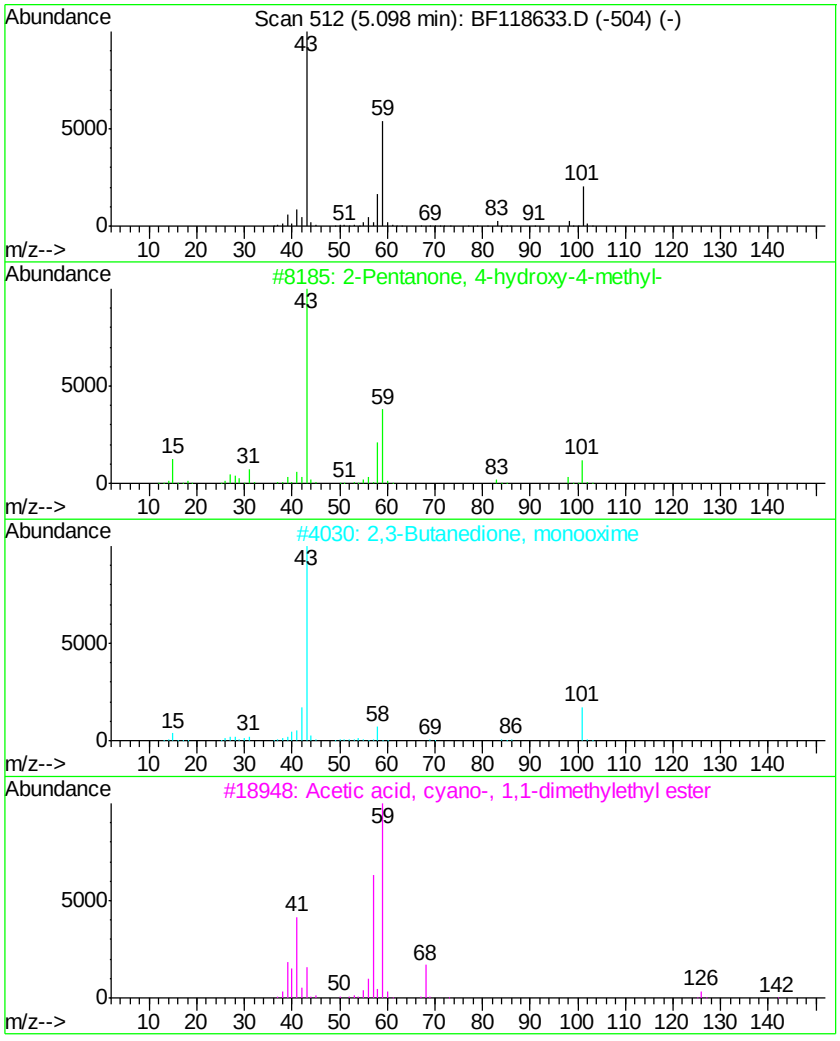
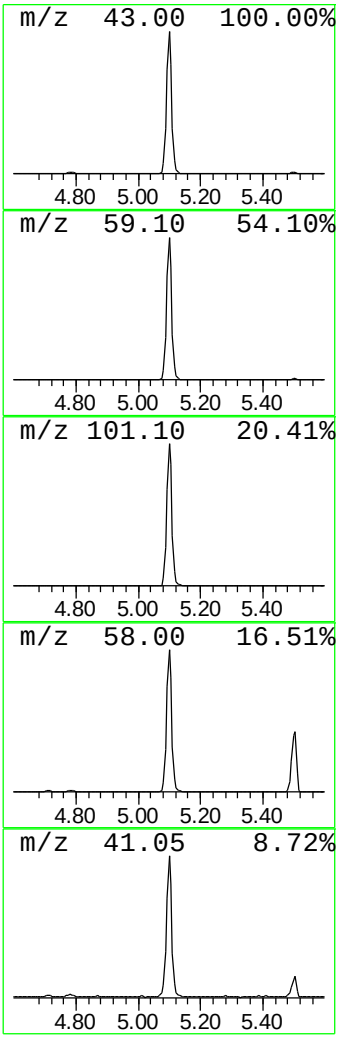
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.10	13.87 ng	1531260	1,4-Dichlorobenzene-d4	6.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012120\
Data File : BF118633.D
Acq On : 21 Jan 2020 14:00
Operator : CG/JU
Sample : PB126152BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB126152BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012020.M
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TIC Library : C:\DATABASE\NIST11.L
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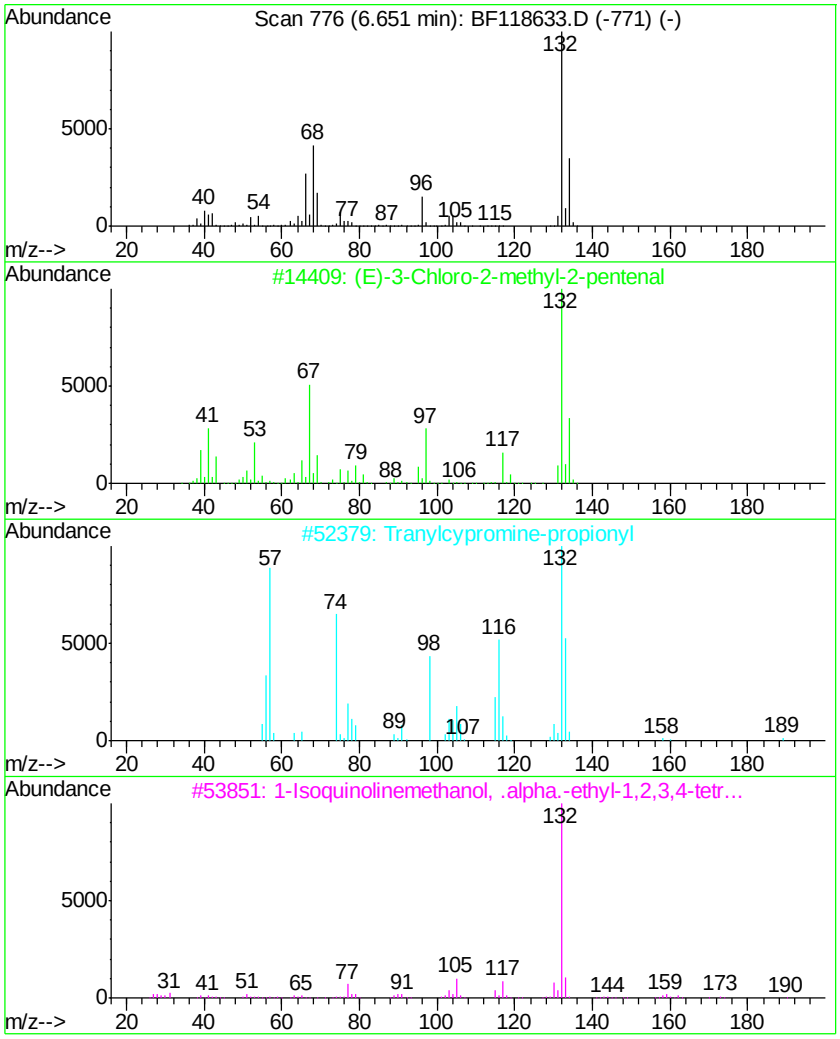
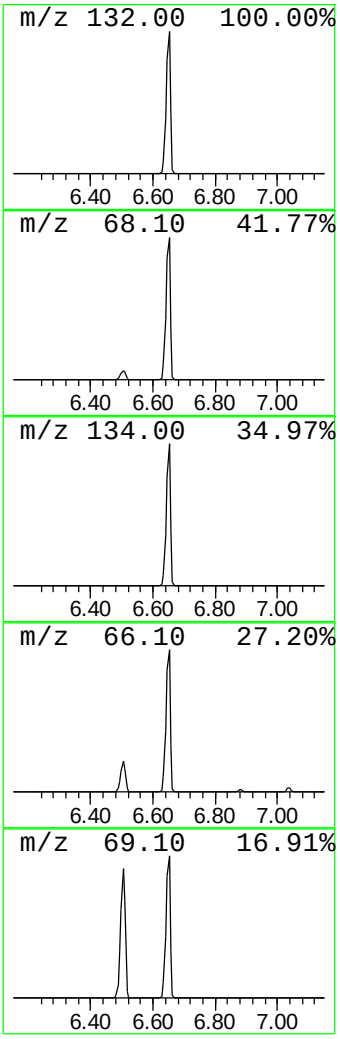
Peak Number 3 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	67.50 ng	7451360	1,4-Dichlorobenzene-d4	6.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	27
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3	1-Isoquinolinemethanol, .alpha.-...	191	C12H17NO	114608-92-3	12
4	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	12
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





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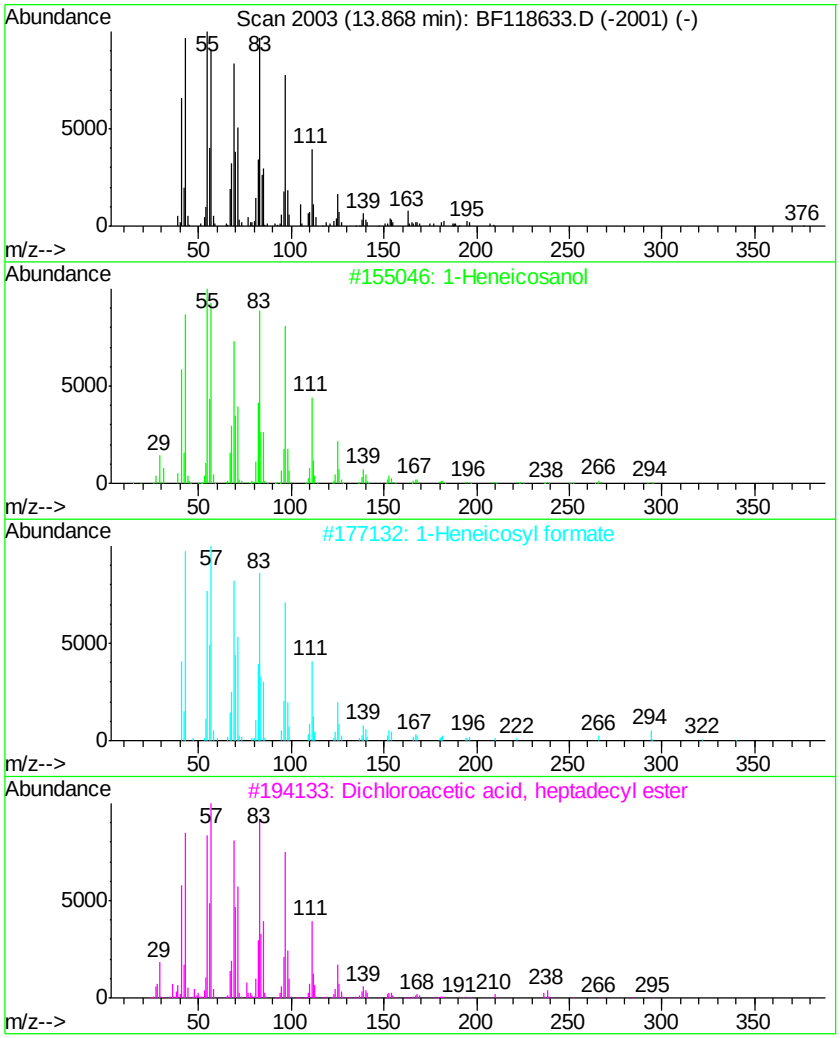
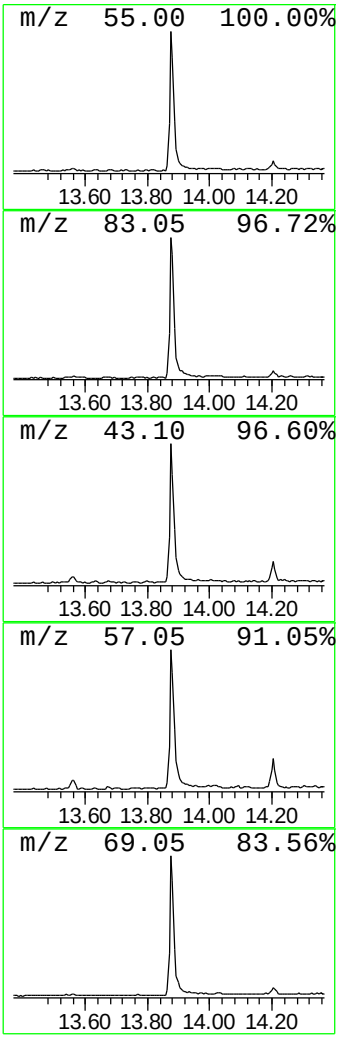
Peak Number 5 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	7.84 ng	1178500	Chrysene-d12	14.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
3	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	94





Library Search Compound Report

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Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB126152BL

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TIC Library : C:\DATABASE\NIST11.L
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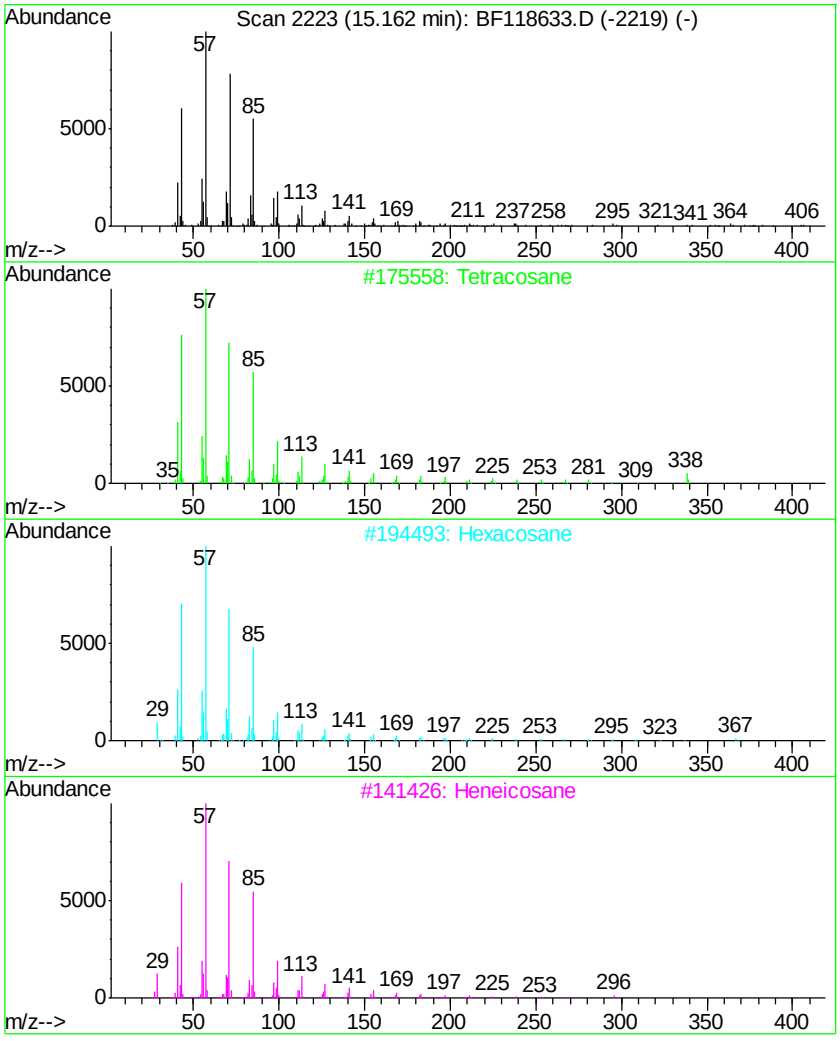
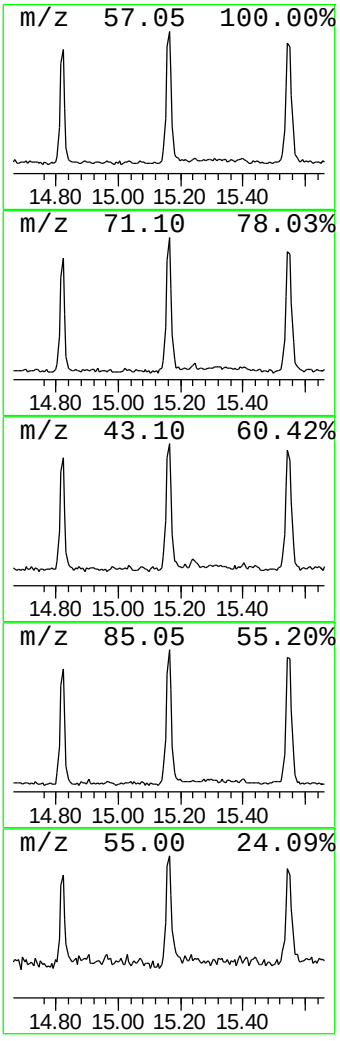
****

Peak Number 6 Tetracosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.16	2.55 ng	302501	Perylene-d12	15.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	97
2	Hexacosane	366	C26H54	000630-01-3	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	Hentriacontane	437	C31H64	000630-04-6	91
5	Tetracosane, 11-decyl-	479	C34H70	055429-84-0	91





Library Search Compound Report

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Sample : PB126152BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB126152BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012020.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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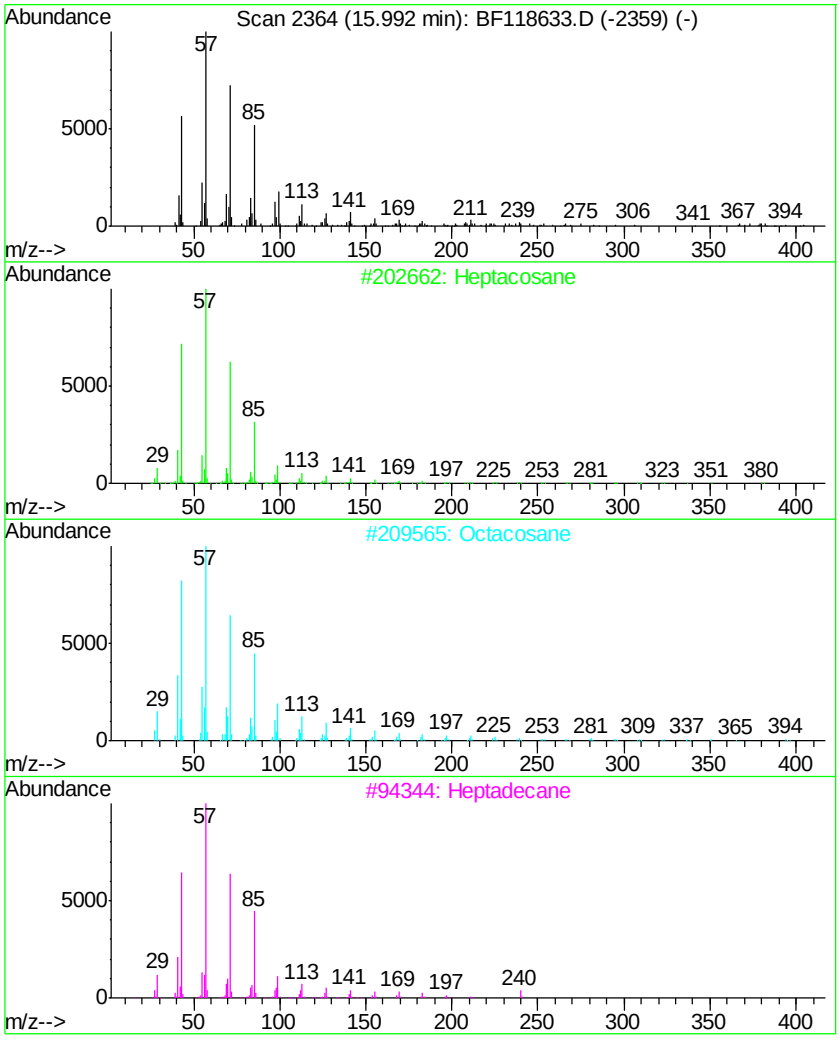
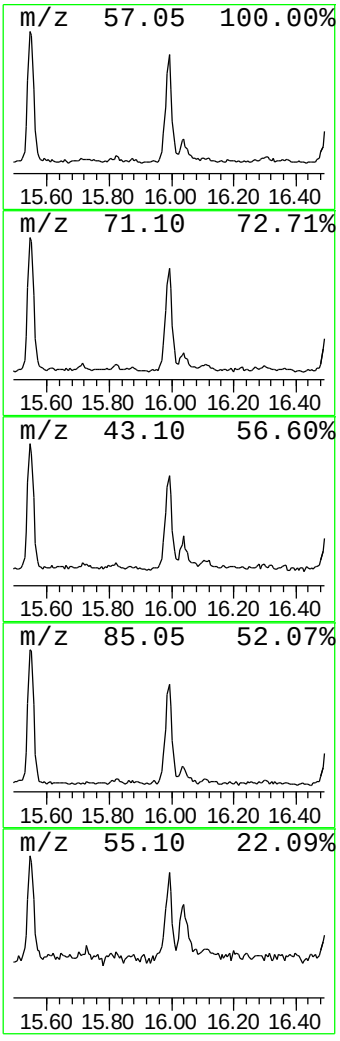
Peak Number 7 Heptacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.99	2.23 ng	264398	Perylene-d12	15.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	96
2	Octacosane	394	C28H58	000630-02-4	93
3	Heptadecane	240	C17H36	000629-78-7	93
4	Tetradecane, 2,6,10-trimethyl-	240	C17H36	014905-56-7	93
5	Triacontane	422	C30H62	000638-68-6	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF012120\
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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
Butane, 2-methoxy...	2.19	18.7	ng	2061440	1	6.88	2207970	20.0
2-Pentanone, 4-hy...	5.10	13.9	ng	1531260	1	6.88	2207970	20.0
unknown6.65	6.65	67.5	ng	7451360	1	6.88	2207970	20.0
1-Heneicosanol	13.87	7.8	ng	1178500	5	14.03	3007630	20.0
Tetracosane	15.16	2.5	ng	302501	6	15.51	2372900	20.0
Heptacosane	15.99	2.2	ng	264398	6	15.51	2372900	20.0