LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031821\
Data File : BF123380.D
Acq On : 18 Mar 2021 12:00
Operator : JU/CG
Sample : PB135194BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB135194BL

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-BF031721.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF123380.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.210	16	21	34	rVB	115413	171113	2.74%	0.384%
2	5.028	495	500	509	rBV	268753	385177	6.16%	0.865%
3	5.428	563	568	583	rBV	5169516	6022560	96.37%	13.524%
4	6.440	734	740	743	rBV	5022548	5960954	95.38%	13.386%
5	6.793	796	800	803	rBV	1498790	1399696	22.40%	3.143%
6	7.357	890	896	899	rBV	3682518	4153380	66.46%	9.327%
7	8.075	1013	1018	1021	rBV	2017628	1979009	31.67%	4.444%
8	9.151	1195	1201	1204	rBV	5381157	6249657	100.00%	14.034%
9	9.828	1311	1316	1320	rBV	2265237	2130333	34.09%	4.784%
10	10.622	1445	1451	1455	rBV	2984930	3341290	53.46%	7.503%
11	10.763	1471	1475	1485	rVB	121563	186489	2.98%	0.419%
12	10.969	1506	1510	1521	rVV5	58804	155080	2.48%	0.348%
13	11.045	1521	1523	1531	rVB	45447	65850	1.05%	0.148%
14	11.316	1565	1569	1573	rBV	2182536	1979231	31.67%	4.444%
15	11.839	1654	1658	1667	rBV	220468	406641	6.51%	0.913%
16	11.992	1676	1684	1688	rBV	246475	400711	6.41%	0.900%
17	12.027	1688	1690	1705	rVB2	160936	386612	6.19%	0.868%
18	12.633	1788	1793	1805	rBV2	102493	201036	3.22%	0.451%
19	12.916	1835	1841	1844	rBV	4539908	5322268	85.16%	11.951%
20	13.451	1927	1932	1939	rVB3	58619	70056	1.12%	0.157%
21	13.963	2015	2019	2023	rBV	1864852	1672198	26.76%	3.755%
22	15.410	2260	2265	2275	rVB2	1262005	1661320	26.58%	3.731%
23	15.857	2337	2341	2347	rVB	64536	96214	1.54%	0.216%
24	16.351	2420	2425	2434	rVB2	70700	135380	2.17%	0.304%

Sum of corrected areas: 44532255

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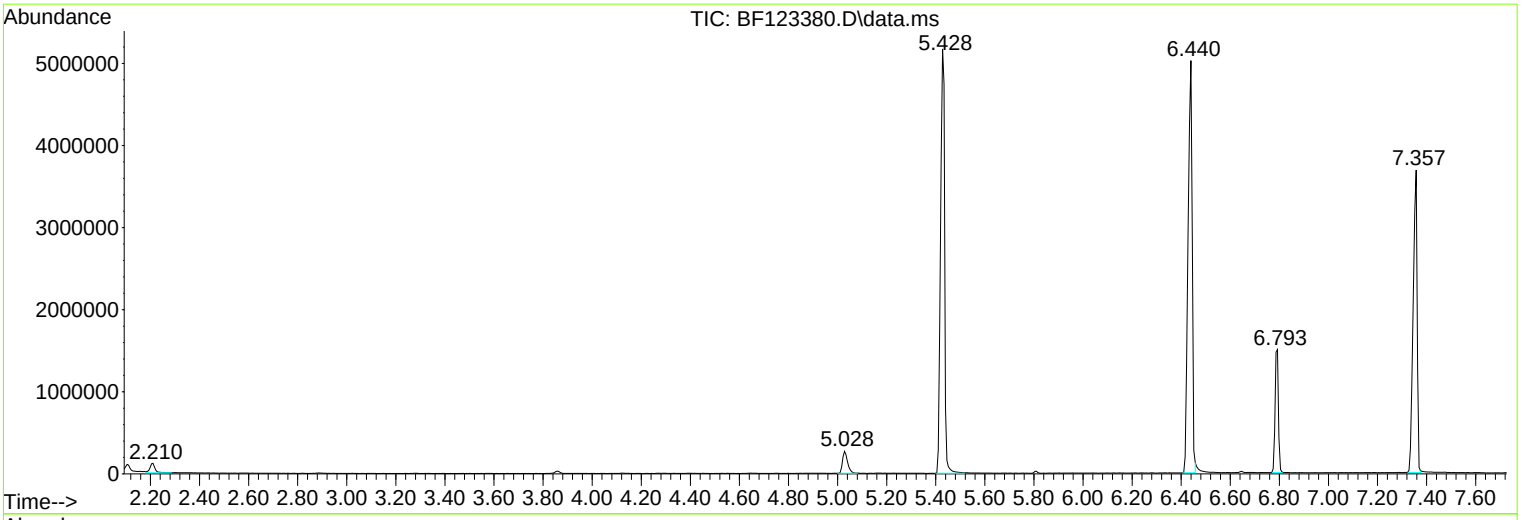
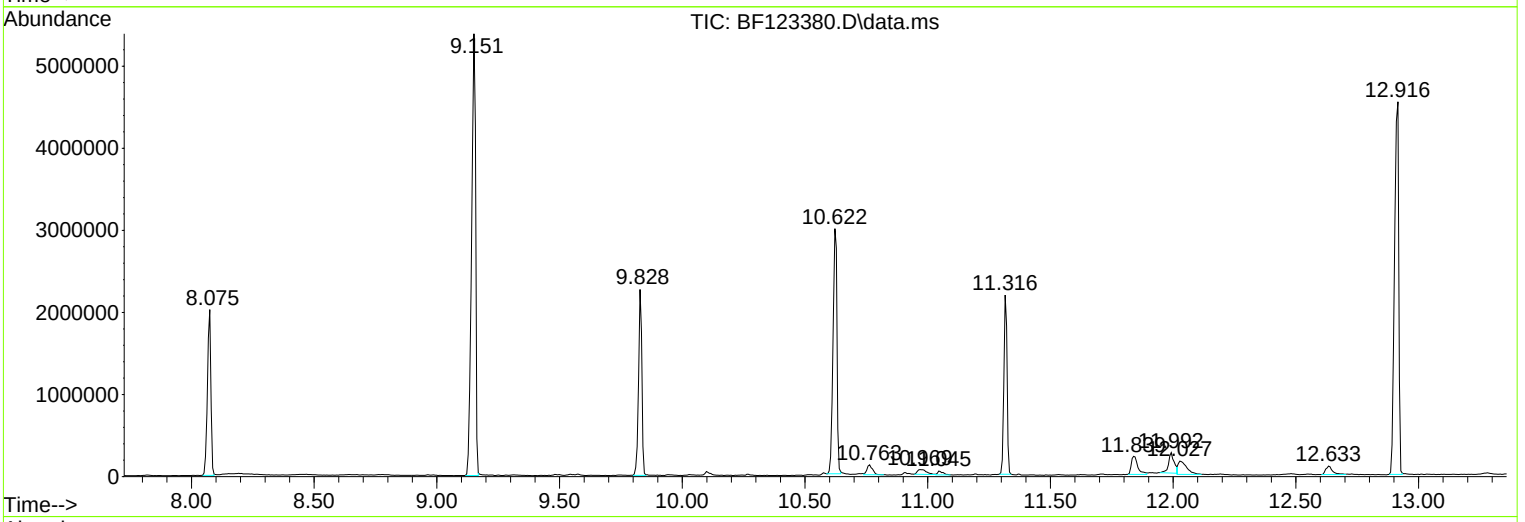
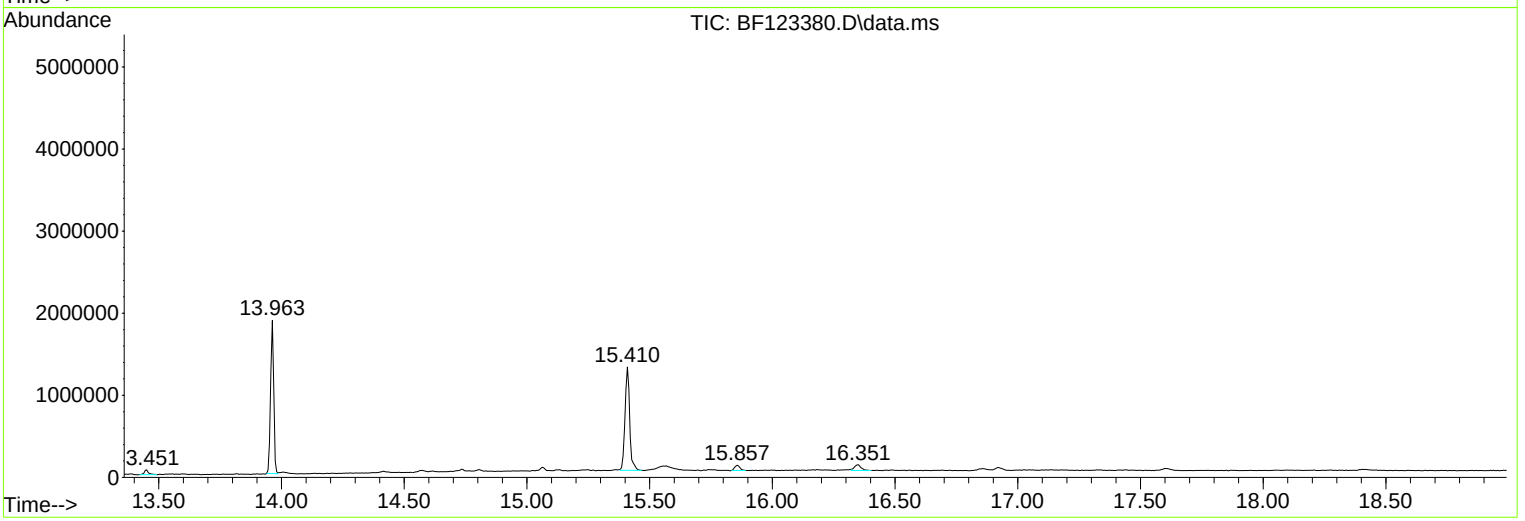
BNA_F
ClientSampleId :
PB135194BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF031721.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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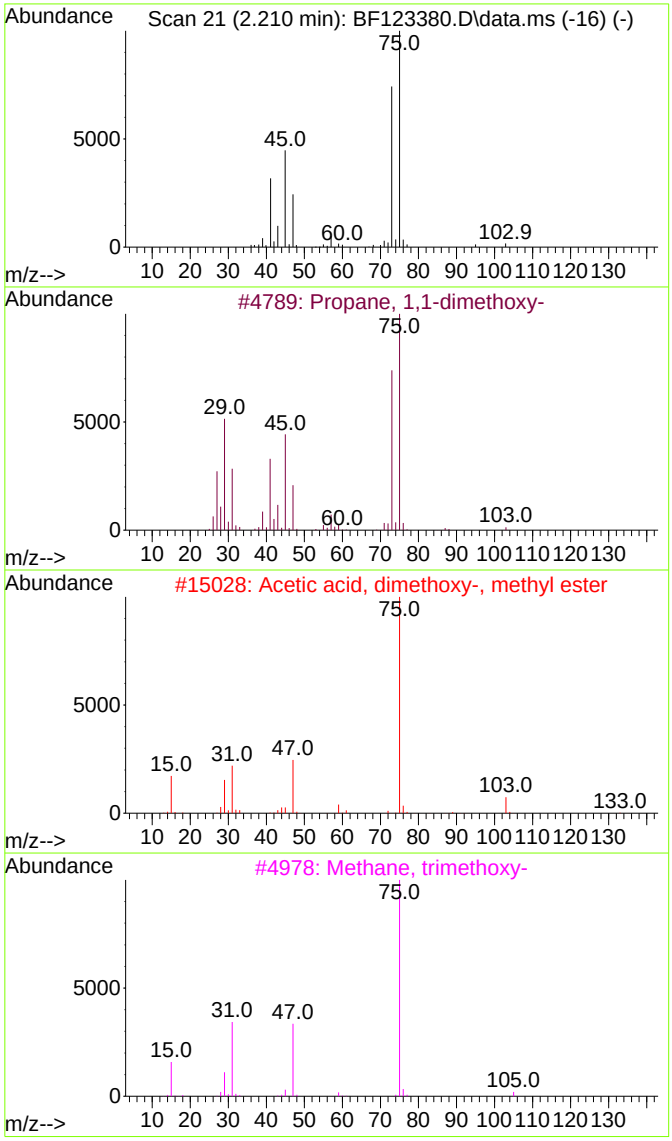
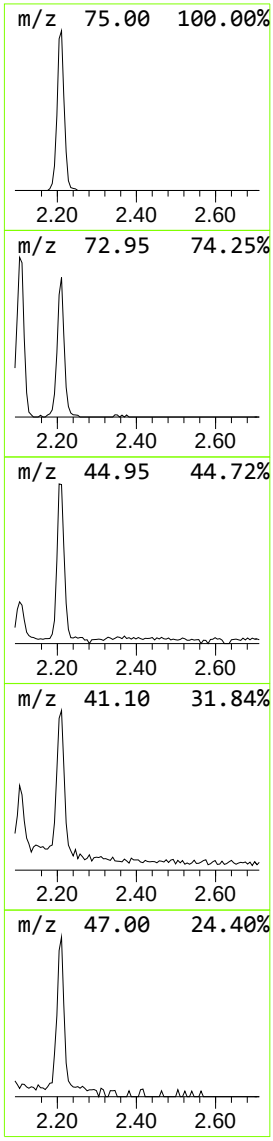
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Propane, 1,1-dimethoxy- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.210	2.44 ng	171113	1,4-Dichlorobenzene-d4	6.793

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	74
2	Acetic acid, dimethoxy-, methyl ...	134	C5H10O4	000089-91-8	28
3	Methane, trimethoxy-	106	C4H10O3	000149-73-5	28
4	Aminoacetaldehyde dimethyl acetal	105	C4H11NO2	022483-09-6	28
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	22





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Sample : PB135194BL
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ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB135194BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF031721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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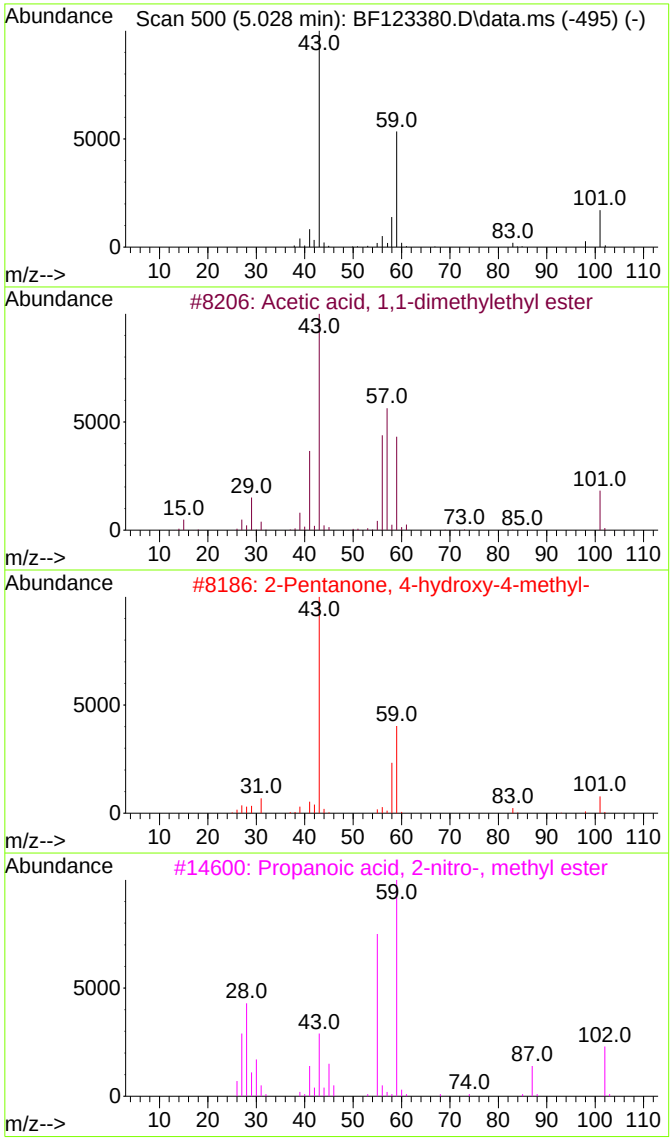
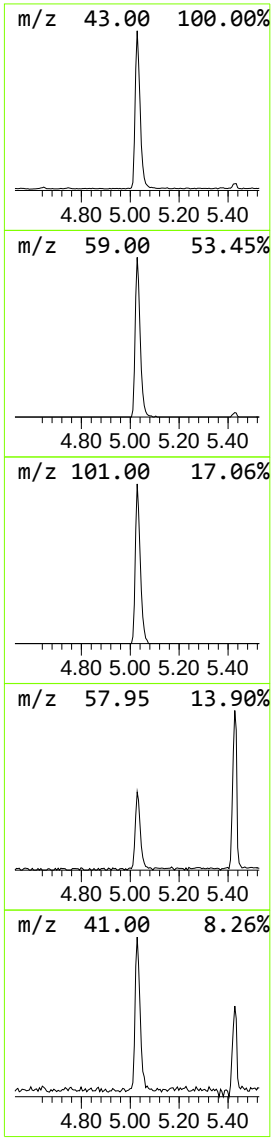
****

Peak Number 2 unknown5.02 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.028	5.50 ng	385177	1,4-Dichlorobenzene-d4	6.793

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
2	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	38
3	Propanoic acid, 2-nitro-, methyl...	133	C4H7NO4	006118-50-9	9
4	3-Pentanol, 2-methyl-	102	C6H14O	000565-67-3	9
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9





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Operator : JU/CG
Sample : PB135194BL
Misc :
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Instrument :
BNA_F
ClientSampleId :
PB135194BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF031721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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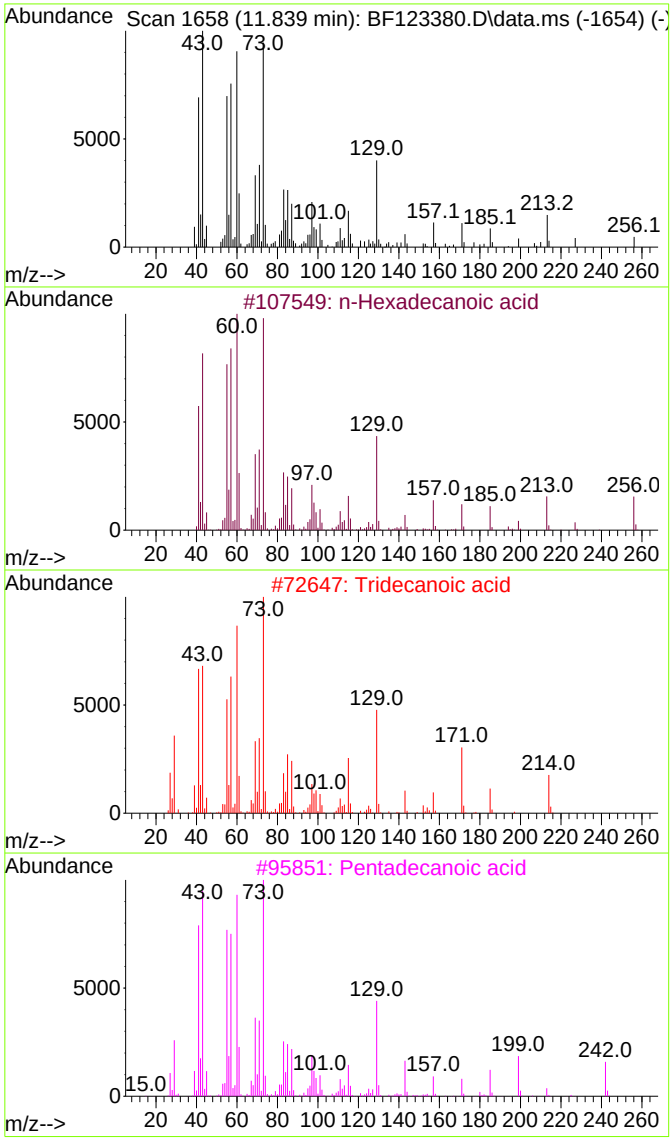
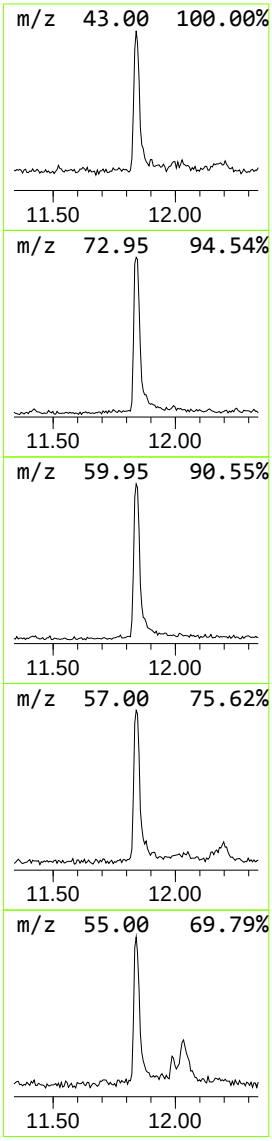
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.839	4.11 ng	406641	Phenanthrene-d10	11.316

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	n-Decanoic acid	172	C10H20O2	000334-48-5	70





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Sample : PB135194BL
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Instrument :
BNA_F
ClientSampleId :
PB135194BL

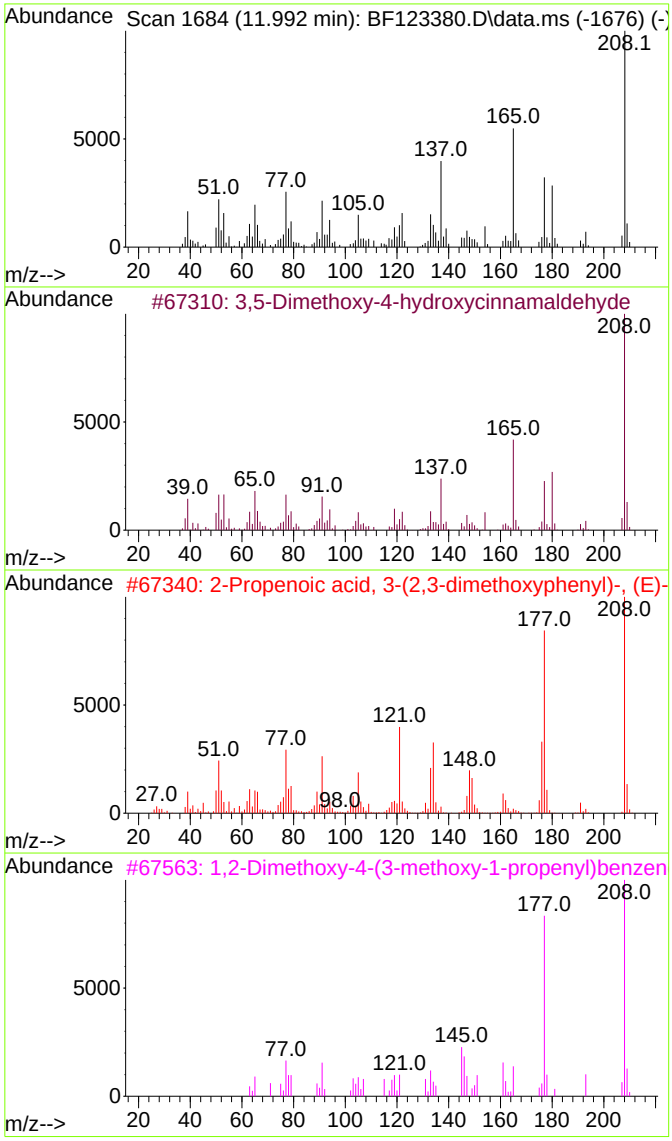
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF031721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

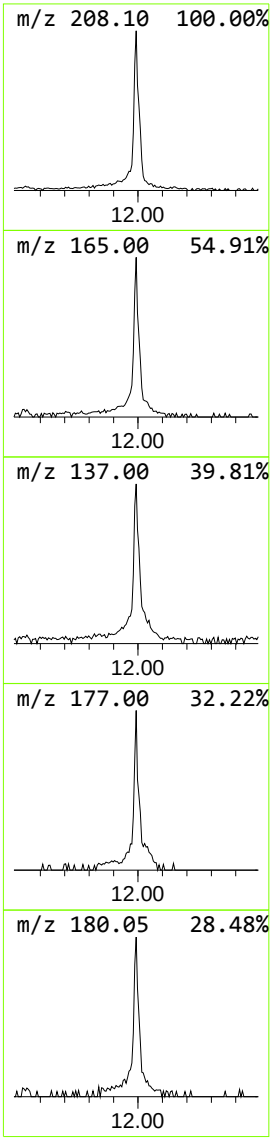
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 3,5-Dimethoxy-4-hydroxycinn... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.992	4.05 ng	400711	Phenanthrene-d10	11.316

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,5-Dimethoxy-4-hydroxycinnamald...	208	C11H12O4	087345-53-7	95
2	2-Propenoic acid, 3-(2,3-dimetho...	208	C11H12O4	007345-82-6	62
3	1,2-Dimethoxy-4-(3-methoxy-1-pro...	208	C12H16O3	1000313-35-0	43
4	Benzenamide, N-cyano-3,4,5-trime...	208	C10H12N2O3	055305-77-6	43
5	3-tert-Butyl-4-hydroxyanisole	180	C11H16O2	000121-00-6	42





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ALS Vial : 3 Sample Multiplier: 1

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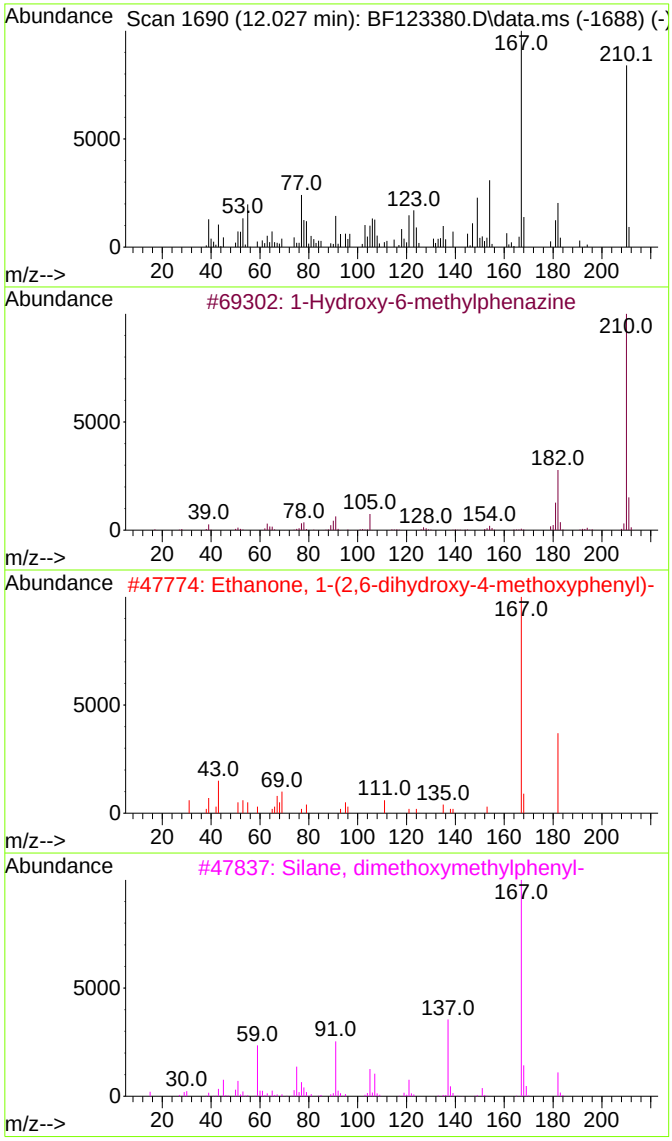
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

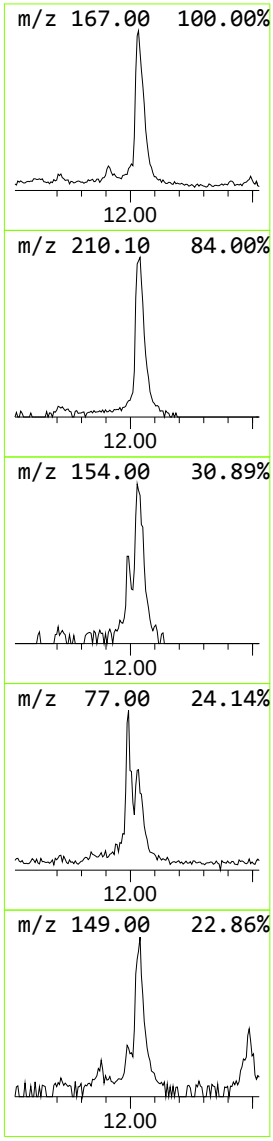
****

Peak Number 5 unknown12.02 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.028	3.91 ng	386612	Phenanthrene-d10	11.316

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hydroxy-6-methylphenazine	210	C13H10N2O	014031-08-4	38
2	Ethanone, 1-(2,6-dihydroxy-4-met...	182	C9H10O4	007507-89-3	35
3	Silane, dimethoxymethylphenyl-	182	C9H14O2Si	003027-21-2	27
4	2,2'-Dimethylbiphenyl	182	C14H14	000605-39-0	27
5	Ethanol, 2-(6-amino-1H-purin-8-y...	211	C7H9N5OS	057654-58-7	27





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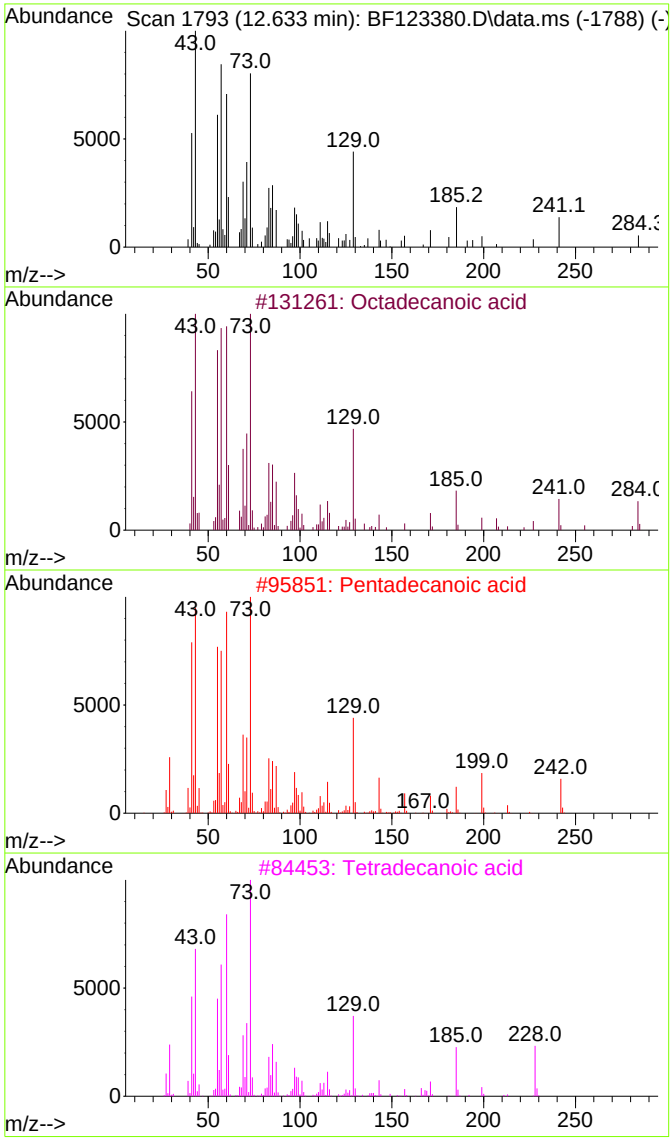
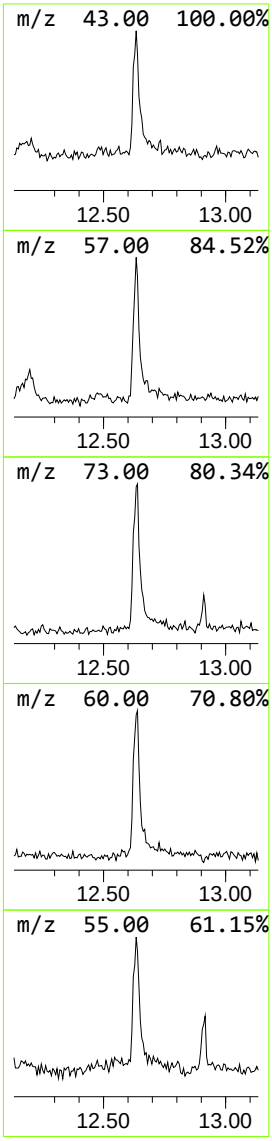
****

Peak Number 6 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.633	2.03 ng	201036	Phenanthrene-d10	11.316

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	97
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4	n-Decanoic acid	172	C10H20O2	000334-48-5	46
5	Oxalic acid, propyl tetradecyl e...	328	C19H36O4	1000309-26-7	25





Tentatively Identified Compound (LSC) summary

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ClientSampleId : PB135194BL

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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
Propane, 1,1-di...	2.210	2.4	ng	171113	1	6.793	1399700	20.0
unknown5.02	5.028	5.5	ng	385177	1	6.793	1399700	20.0
n-Hexadecanoic ...	11.839	4.1	ng	406641	4	11.316	1979230	20.0
3,5-Dimethoxy-4...	11.992	4.0	ng	400711	4	11.316	1979230	20.0
unknown12.02	12.028	3.9	ng	386612	4	11.316	1979230	20.0
Octadecanoic acid	12.633	2.0	ng	201036	4	11.316	1979230	20.0