LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022221\
Data File : BF123262.D
Acq On : 22 Feb 2021 17:03
Operator : JU/CG
Sample : M1425-12
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-3

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-BF021921.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF123262.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.810	117	123	130	rVB	222057	303575	6.74%	1.092%
2	4.657	433	437	442	rBV	521062	525559	11.66%	1.890%
3	4.728	445	449	454	rVB	61357	65897	1.46%	0.237%
4	5.075	505	508	510	rBV	110680	126023	2.80%	0.453%
5	5.099	510	512	516	rVB	323975	292018	6.48%	1.050%
6	5.487	574	578	581	rBV	3783922	3396611	75.39%	12.213%
7	6.493	744	749	761	rBV	2631057	2590459	57.49%	9.314%
8	6.857	807	811	814	rBV	890625	689893	15.31%	2.481%
9	7.416	901	906	909	rBV	1999574	1880963	41.75%	6.763%
10	8.140	1025	1029	1032	rBV	1170780	918966	20.40%	3.304%
11	9.216	1207	1212	1215	rBV	3674617	3312524	73.52%	11.910%
12	9.898	1324	1328	1331	rBV	1288342	1053401	23.38%	3.788%
13	10.692	1458	1463	1466	rBV	2741806	2573590	57.12%	9.253%
14	11.386	1577	1581	1584	rBV	1345065	1139379	25.29%	4.097%
15	11.922	1668	1672	1685	rBV	777775	891421	19.78%	3.205%
16	12.210	1718	1721	1725	rBV	68478	70744	1.57%	0.254%
17	12.369	1744	1748	1751	rVB	389484	313809	6.96%	1.128%
18	12.427	1755	1758	1762	rBV	99724	88410	1.96%	0.318%
19	12.710	1803	1806	1814	rBV	379064	469465	10.42%	1.688%
20	12.986	1847	1853	1856	rBV	4645075	4505600	100.00%	16.200%
21	13.910	2002	2010	2028	rBV3	132665	527822	11.71%	1.898%
22	14.039	2028	2032	2035	rVB	1228315	1071081	23.77%	3.851%
23	15.510	2276	2282	2295	rBV	749206	1005071	22.31%	3.614%

Sum of corrected areas: 27812281

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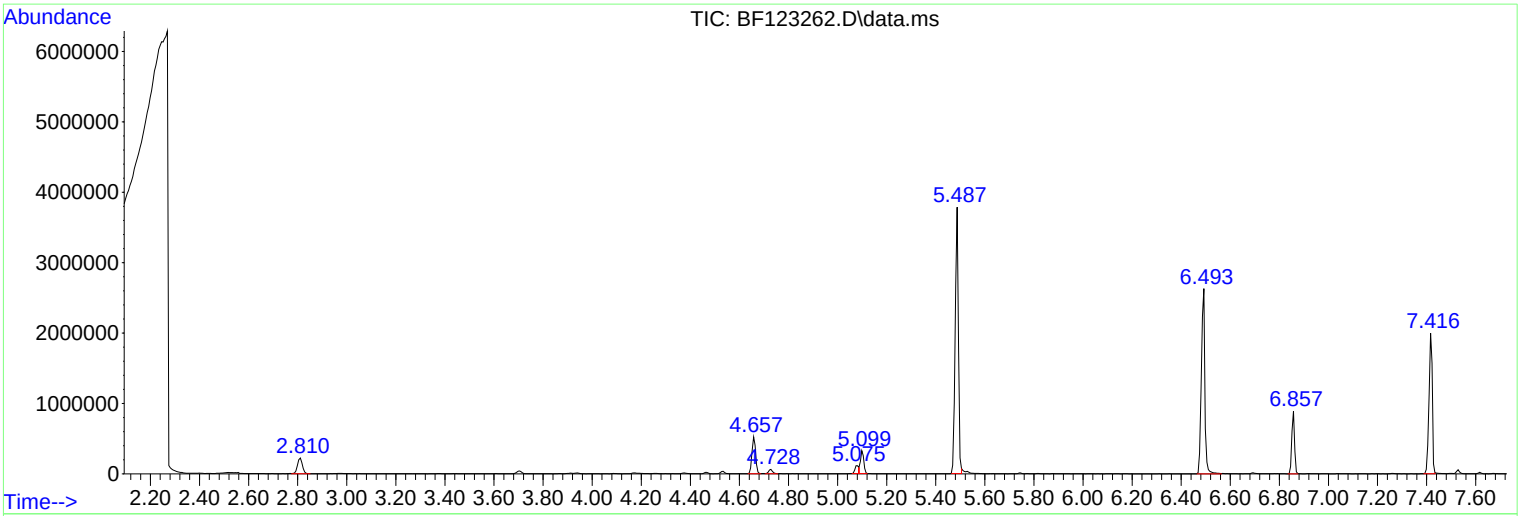
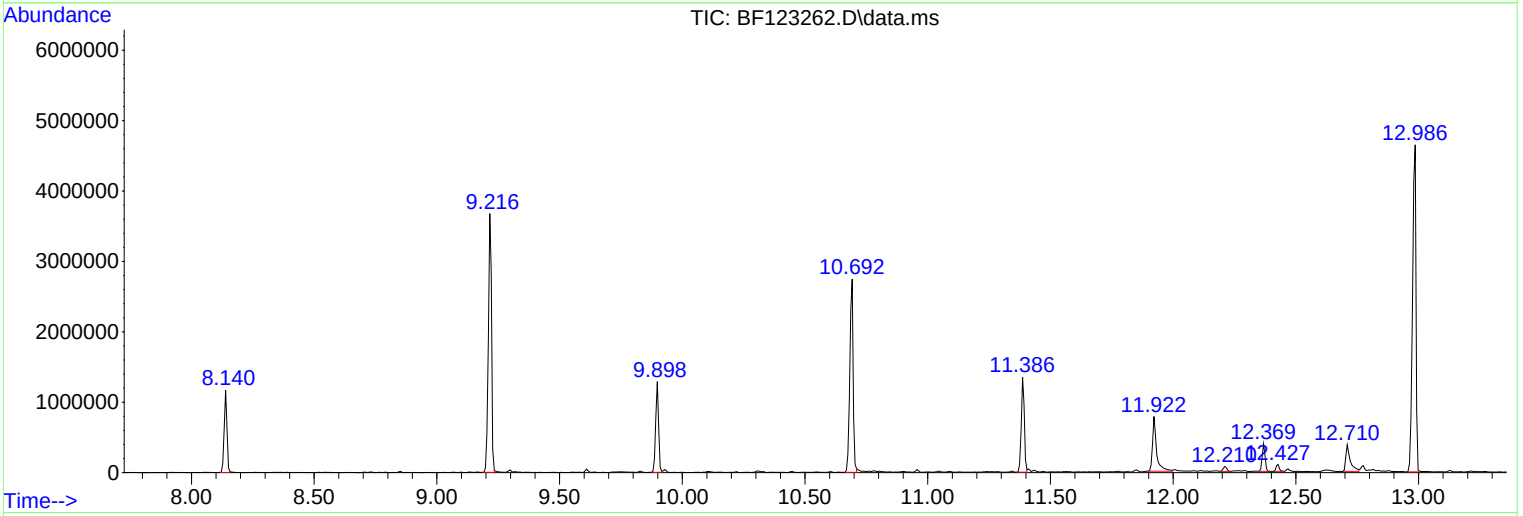
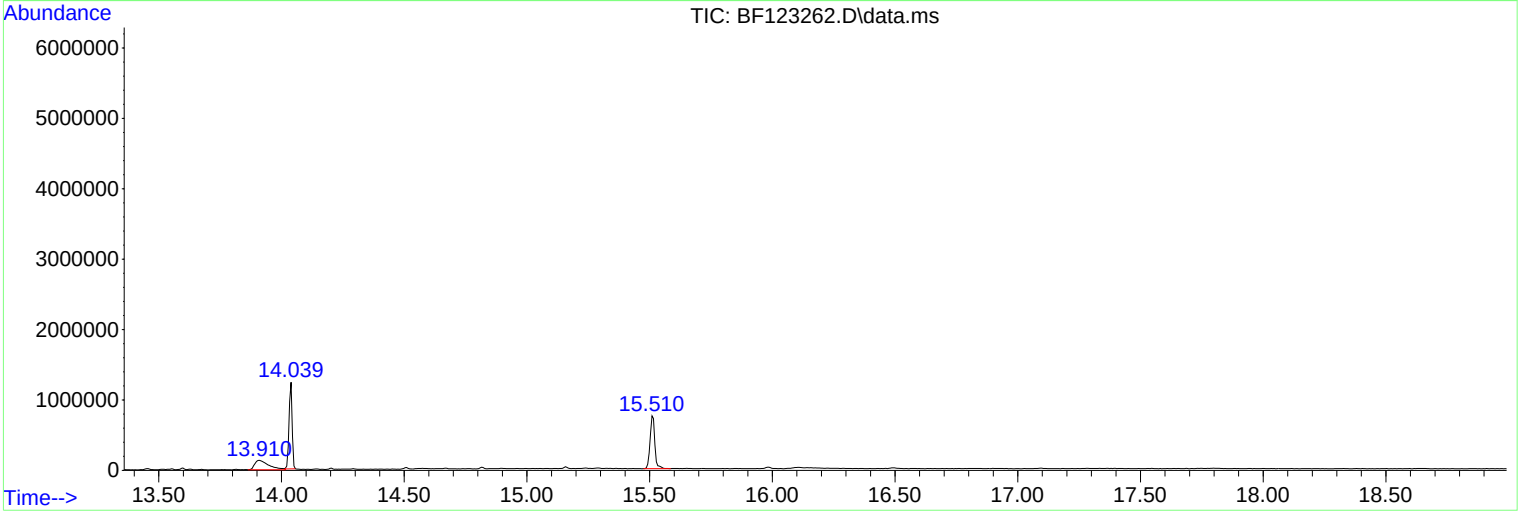
Instrument :
BNA_F
ClientSampleId :
TP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF021921.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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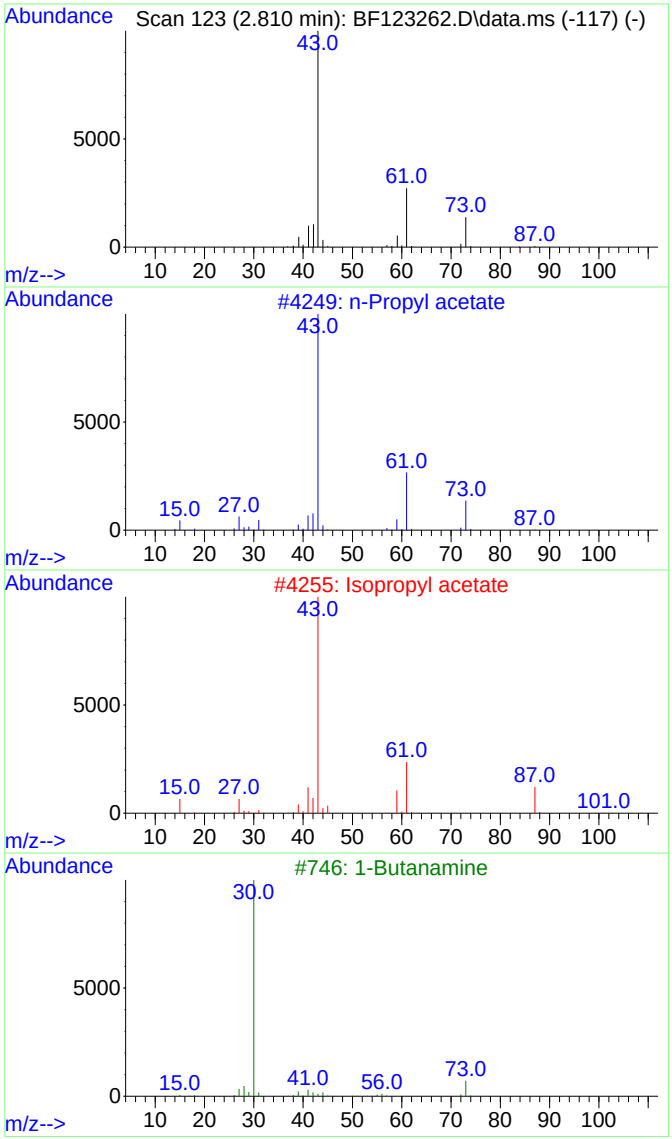
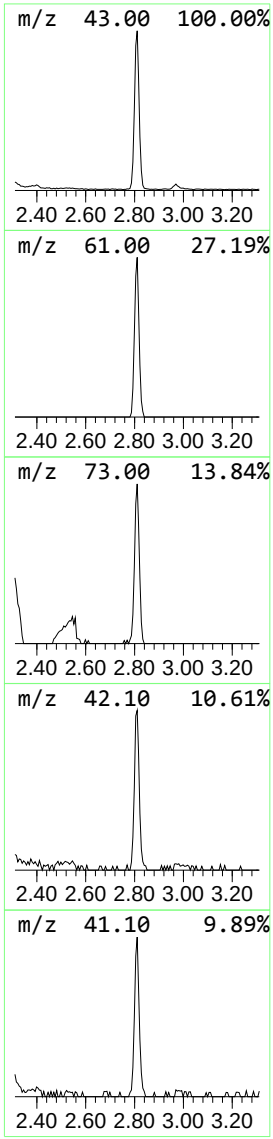
****

Peak Number 1 n-Propyl acetate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.810	8.80 ng	303575	1,4-Dichlorobenzene-d4	6.857

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Propyl acetate	102	C5H10O2	000109-60-4	83
2	Isopropyl acetate	102	C5H10O2	000108-21-4	38
3	1-Butanamine	73	C4H11N	000109-73-9	7
4	Isobutylamine	73	C4H11N	000078-81-9	5
5	Butane, 2-methyl-	72	C5H12	000078-78-4	4





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Sample : M1425-12
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-3

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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TIC Integration Parameters: LSCINT.P

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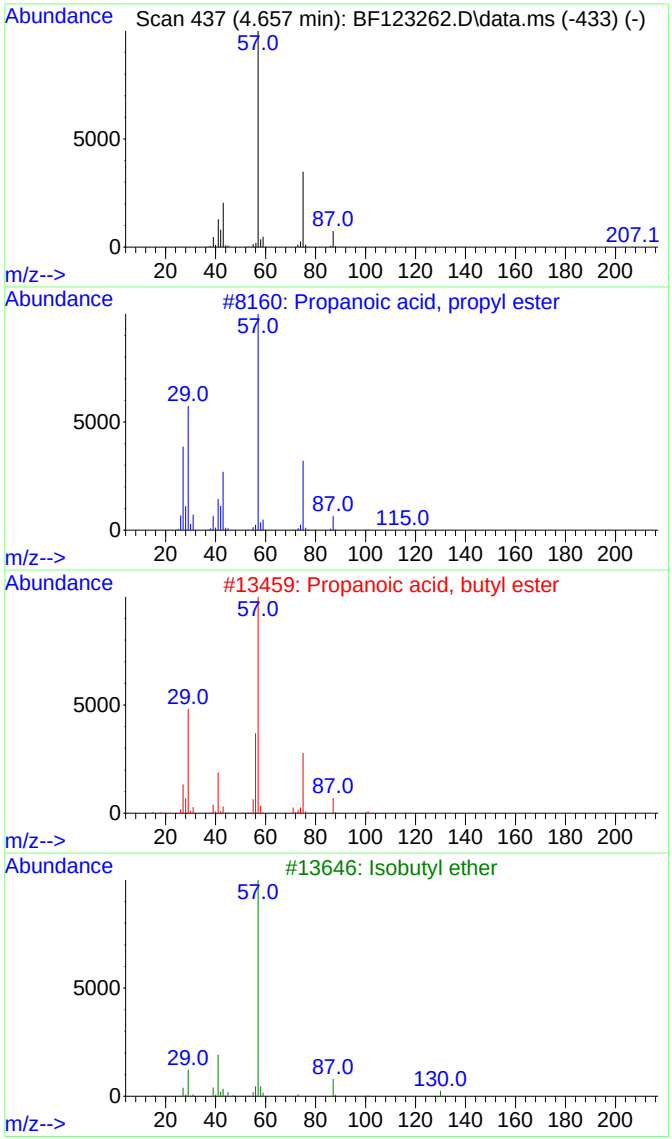
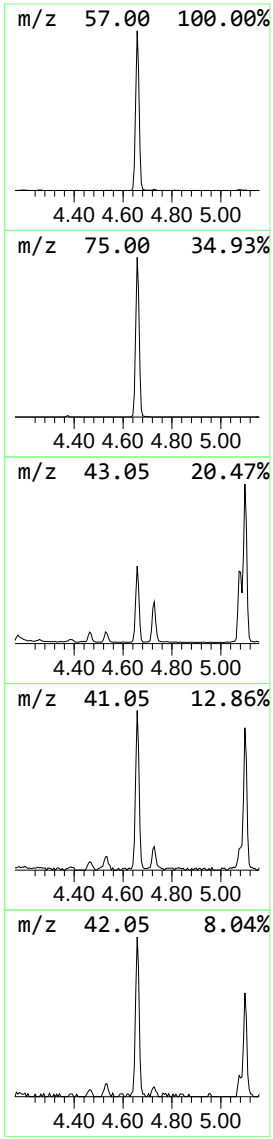
Peak Number 2 Propanoic acid, propyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.657	15.24 ng	525559	1,4-Dichlorobenzene-d4	6.857

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	83
2	Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	38
3	Isobutyl ether	130	C8H18O	000628-55-7	9
4	di-tert-Butyl dicarbonate	218	C10H18O5	024424-99-5	9
5	1-Butanamine, 2-methyl-	87	C5H13N	000096-15-1	7





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Sample : M1425-12
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-3

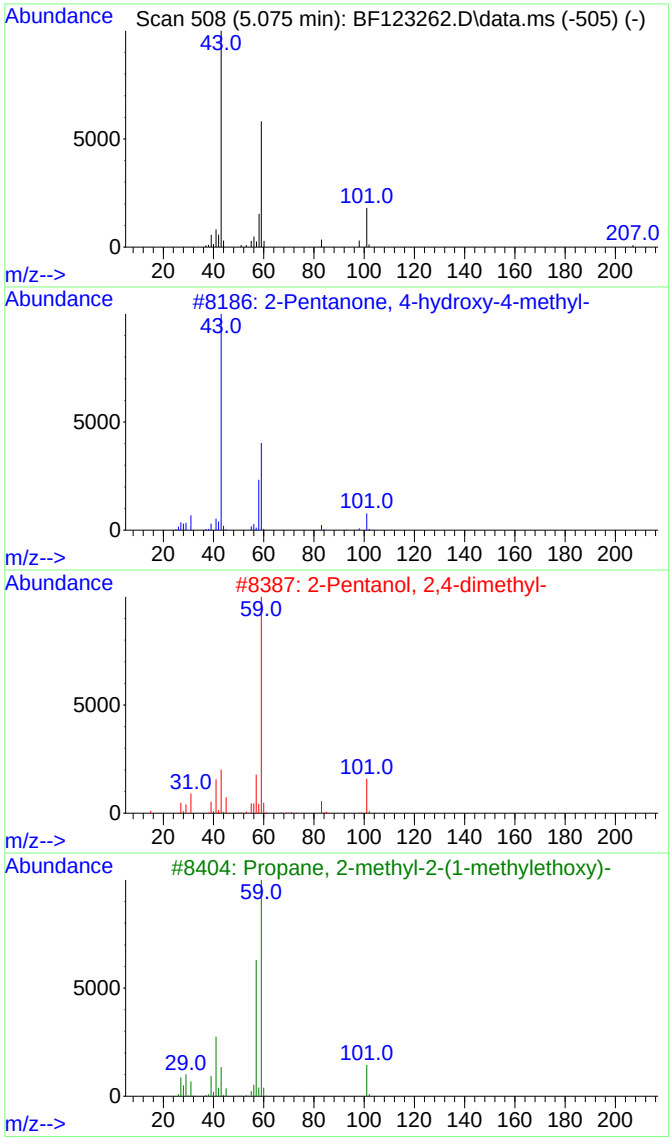
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF021921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

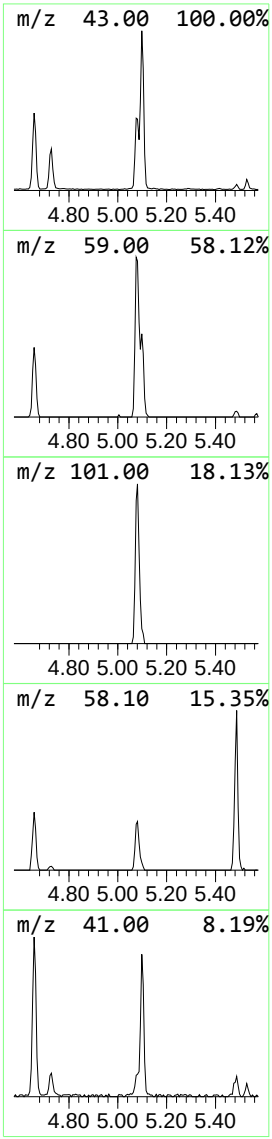
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.075	3.65 ng	126023	1,4-Dichlorobenzene-d4	6.857

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	33
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
4	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	28
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27





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Instrument : BNA_F
ClientSampleId : TP-3

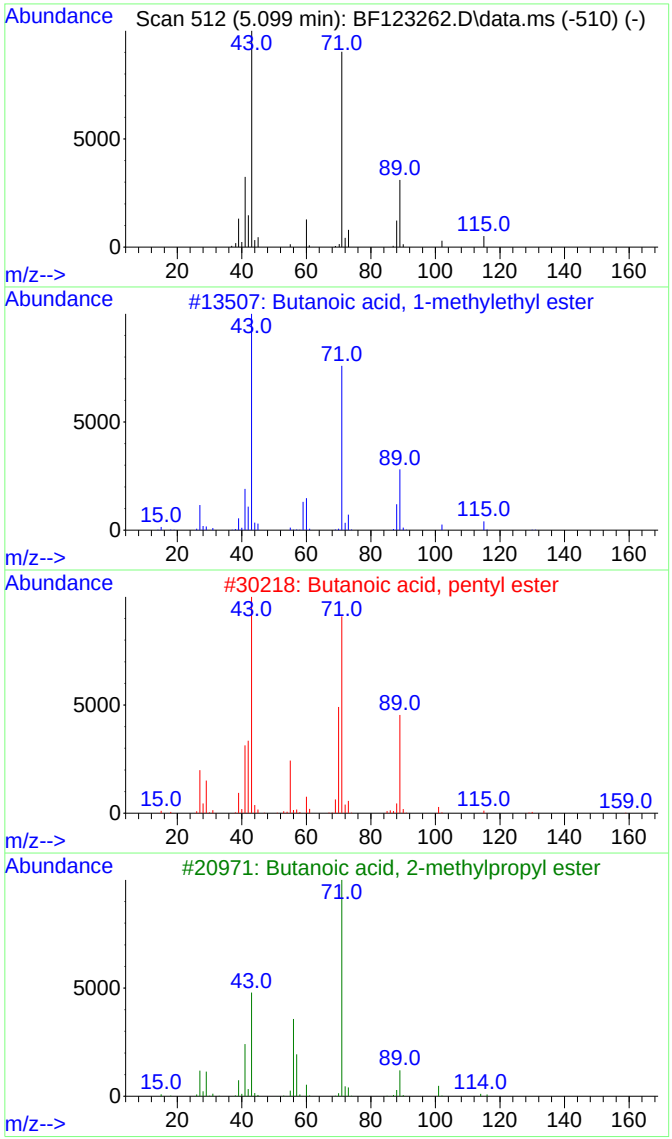
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF021921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

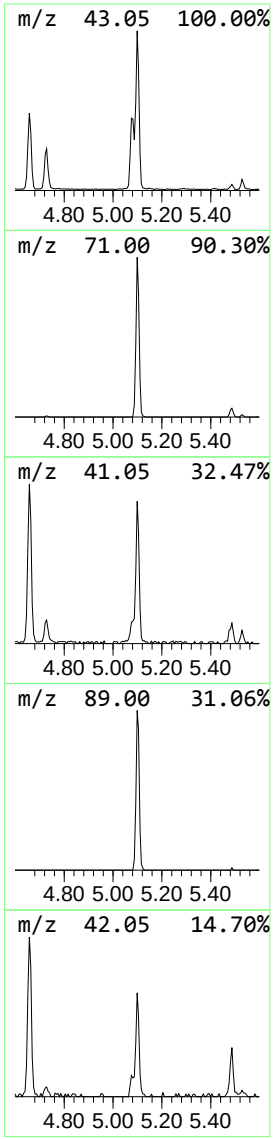
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Butanoic acid, 1-methylethy... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.099	8.47 ng	292018	1,4-Dichlorobenzene-d4	6.857

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	83
2	Butanoic acid, pentyl ester	158	C9H18O2	000540-18-1	72
3	Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	64
4	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	64
5	Butanoic acid, 1-methylpropyl ester	144	C8H16O2	000819-97-6	64





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

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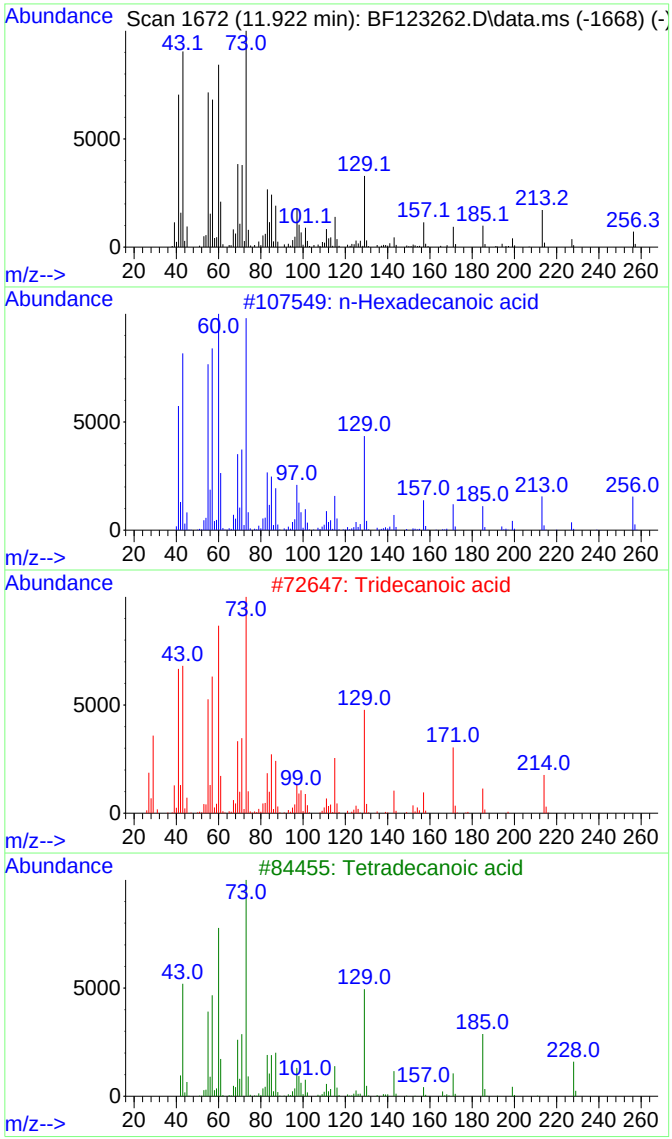
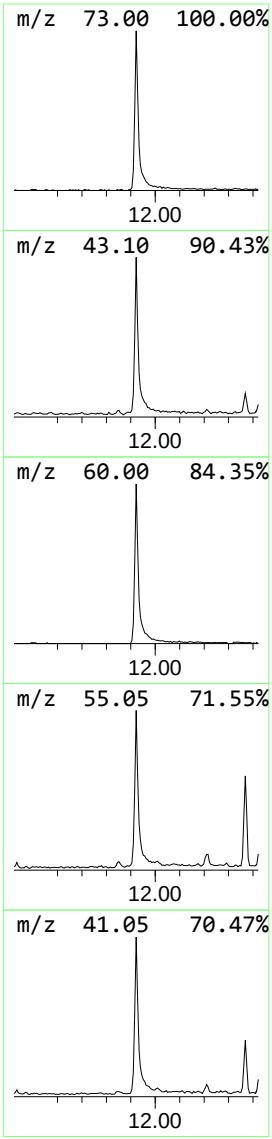
Peak Number 5 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.922	15.65 ng	891421	Phenanthrene-d10	11.386

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	96
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
5	n-Decanoic acid	172	C10H20O2	000334-48-5	53





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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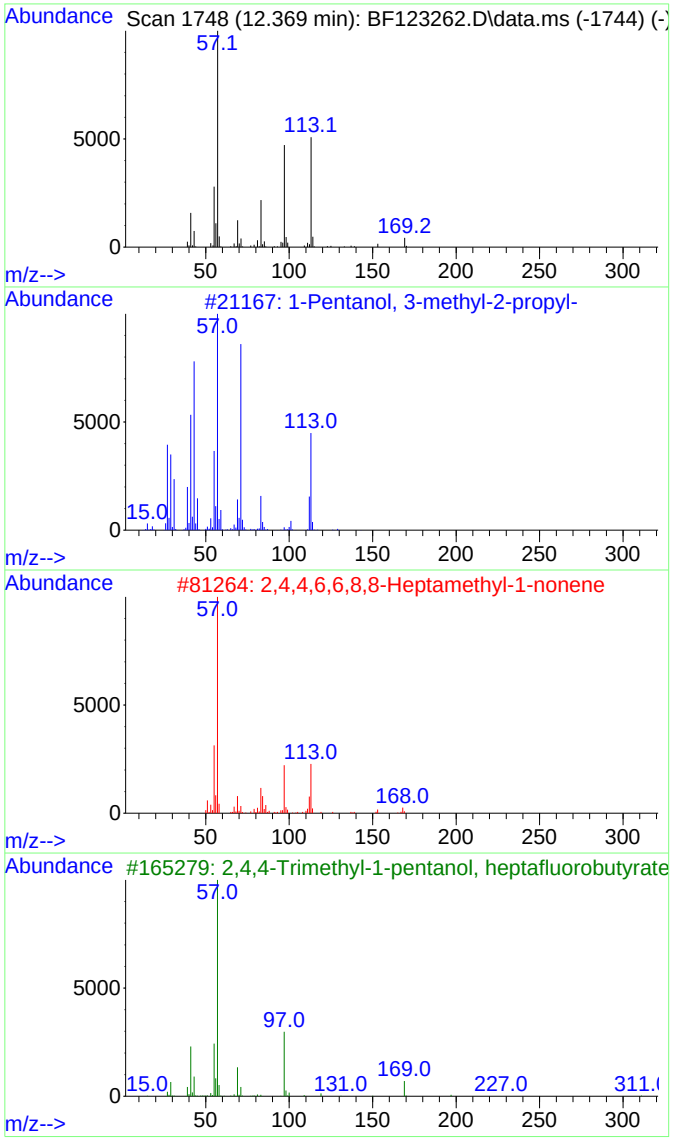
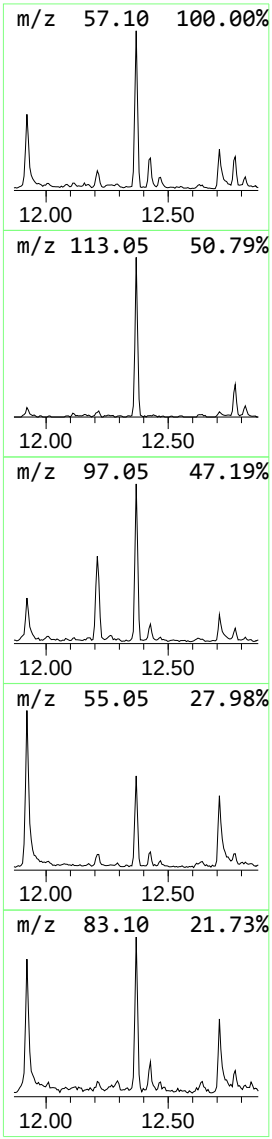
Peak Number 6 unknown12.36 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.369	5.51 ng	313809	Phenanthrene-d10	11.386

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentanol, 3-methyl-2-propyl-	144	C9H20O	054004-40-9	40
2	2,4,4,6,6,8,8-Heptamethyl-1-nonene	224	C16H32	015796-04-0	37
3	2,4,4-Trimethyl-1-pentanol, hept...	326	C12H17F7O2	1000365-01-4	35
4	2,4,4-Trimethyl-1-pentanol, pent...	276	C11H17F5O2	1000365-51-0	32
5	Formic acid, 2,4,4-trimethylpent...	158	C9H18O2	1000368-95-2	25





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Sample : M1425-12
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Instrument : BNA_F
ClientSampleId : TP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF021921.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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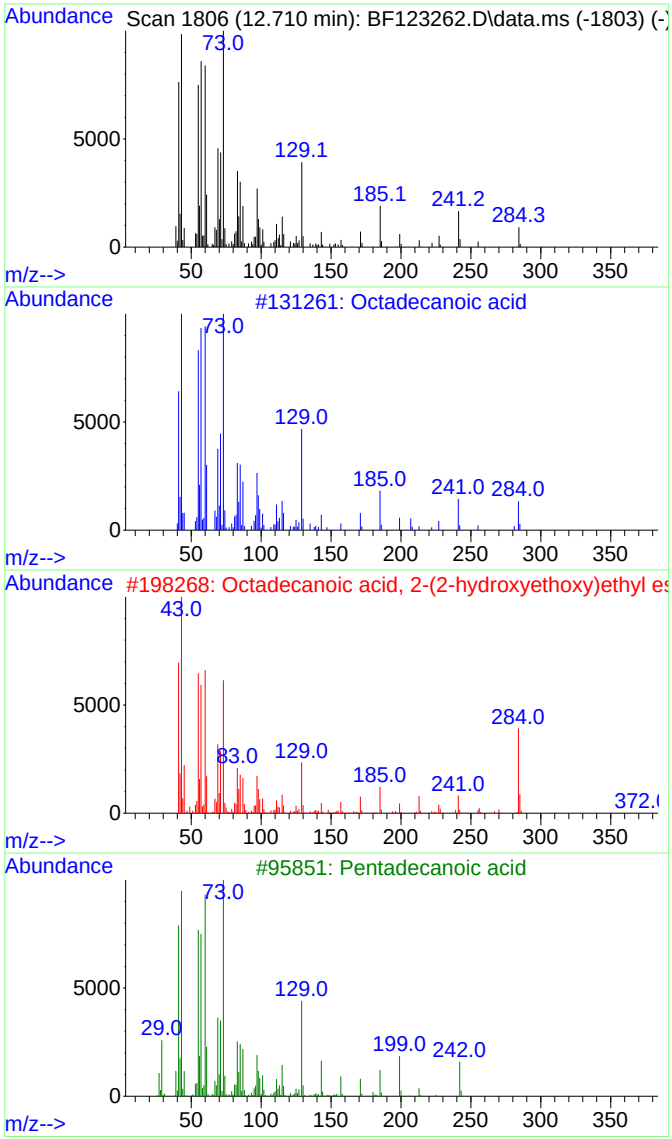
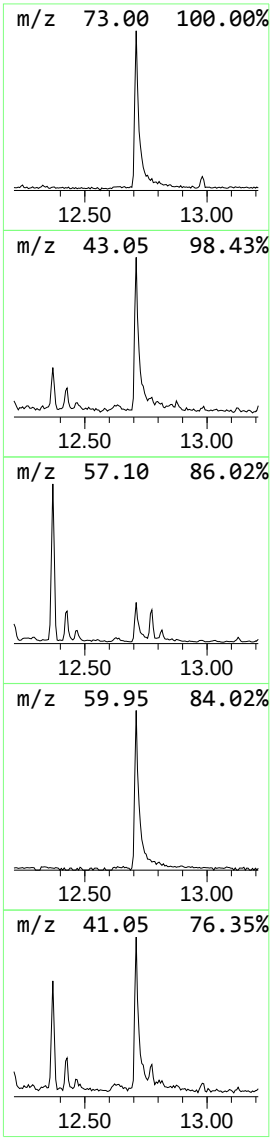
Peak Number 7 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.710	8.24 ng	469465	Phenanthrene-d10	11.386

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	n-Decanoic acid	172	C10H20O2	000334-48-5	70
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	70





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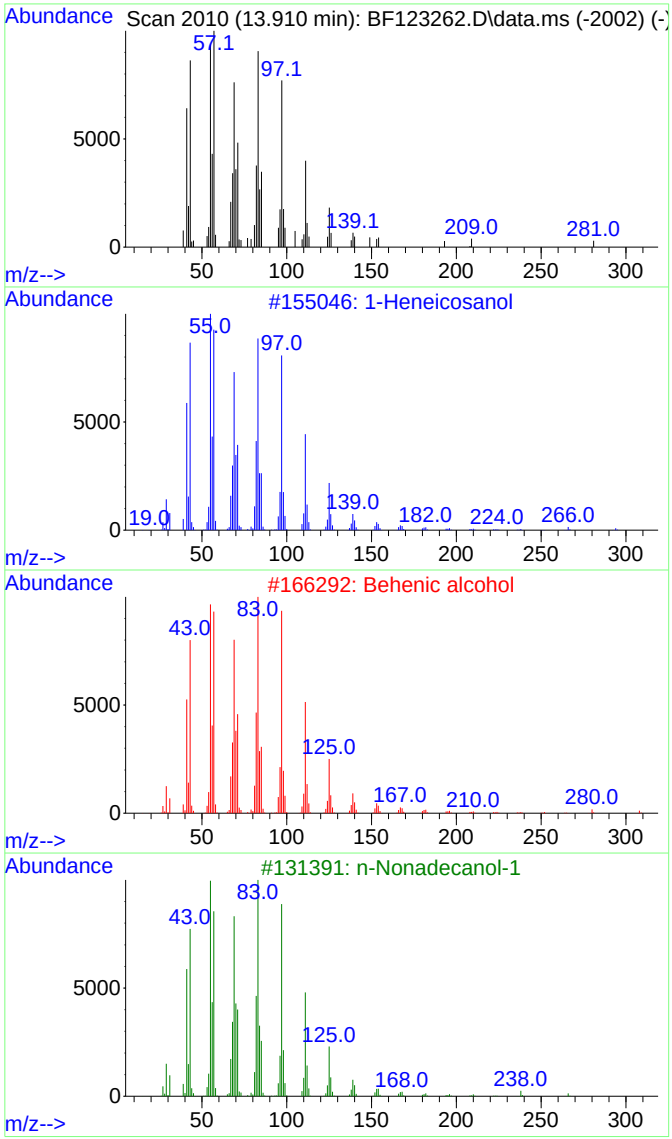
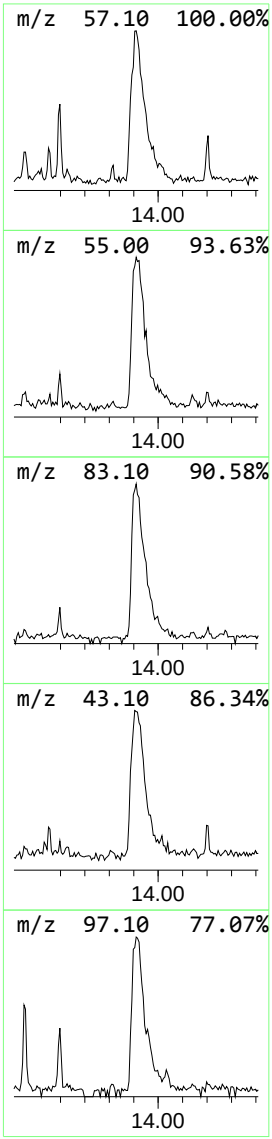
Peak Number 8 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.910	9.86 ng	527822	Chrysene-d12	14.039

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	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	95
5	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	94





Tentatively Identified Compound (LSC) summary

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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF021921.M
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
n-Propyl acetate	2.810	8.8	ng	303575	1	6.857	689893	20.0
Propanoic acid,...	4.657	15.2	ng	525559	1	6.857	689893	20.0
2-Pentanone, 4-...	5.075	3.6	ng	126023	1	6.857	689893	20.0
Butanoic acid, ...	5.099	8.5	ng	292018	1	6.857	689893	20.0
n-Hexadecanoic ...	11.922	15.7	ng	891421	4	11.386	1139380	20.0
unknown12.36	12.369	5.5	ng	313809	4	11.386	1139380	20.0
Octadecanoic acid	12.710	8.2	ng	469465	4	11.386	1139380	20.0
1-Heneicosanol	13.910	9.9	ng	527822	5	14.039	1071080	20.0