LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032421\
Data File : BF123439.D
Acq On : 24 Mar 2021 15:08
Operator : JU/CG
Sample : M1770-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-105I

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-BF032321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF123439.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.252	20	28	33	rBV	4004551	5166258	63.90%	10.370%
2	2.358	41	46	52	rVB	191307	233795	2.89%	0.469%
3	5.140	512	519	525	rVB	115356	152518	1.89%	0.306%
4	5.528	581	585	589	rBV	3841726	3807935	47.10%	7.643%
5	6.528	750	755	760	rBV	2758594	2593057	32.07%	5.205%
6	6.910	817	820	824	rBV	1680469	1405176	17.38%	2.821%
7	7.475	910	916	919	rBV	4586944	4959709	61.35%	9.955%
8	8.198	1034	1039	1042	rBV	2127280	1843707	22.81%	3.701%
9	9.281	1217	1223	1226	rBV	8402596	8084640	100.00%	16.228%
10	9.669	1285	1289	1293	rBV	124089	127789	1.58%	0.257%
11	9.957	1334	1338	1341	rBV	2495887	2000549	24.75%	4.016%
12	10.163	1365	1373	1379	rBV	430728	437248	5.41%	0.878%
13	10.751	1467	1473	1476	rBV	5563486	5224776	64.63%	10.487%
14	11.022	1516	1519	1523	rVB	103336	81698	1.01%	0.164%
15	11.104	1529	1533	1538	rBV	141104	137876	1.71%	0.277%
16	11.304	1562	1567	1573	rBV4	69737	144339	1.79%	0.290%
17	11.445	1588	1591	1595	rBV	2073616	1815408	22.46%	3.644%
18	11.975	1675	1681	1691	rBV	826941	911393	11.27%	1.829%
19	12.433	1756	1759	1762	rBV	117511	99952	1.24%	0.201%
20	12.686	1796	1802	1811	rBV	286937	374122	4.63%	0.751%
21	12.763	1812	1815	1822	rVB	202848	211419	2.62%	0.424%
22	13.045	1858	1863	1866	rBV	6543088	6080673	75.21%	12.205%
23	13.322	1907	1910	1917	rBV	363436	358183	4.43%	0.719%
24	13.939	2012	2015	2027	rVB	954134	1071358	13.25%	2.150%
25	14.098	2038	2042	2045	rBV	1183140	1072976	13.27%	2.154%
26	15.604	2292	2298	2302	rBV	916053	1165308	14.41%	2.339%
27	16.168	2389	2394	2402	rBV2	133451	258012	3.19%	0.518%

Sum of corrected areas: 49819874

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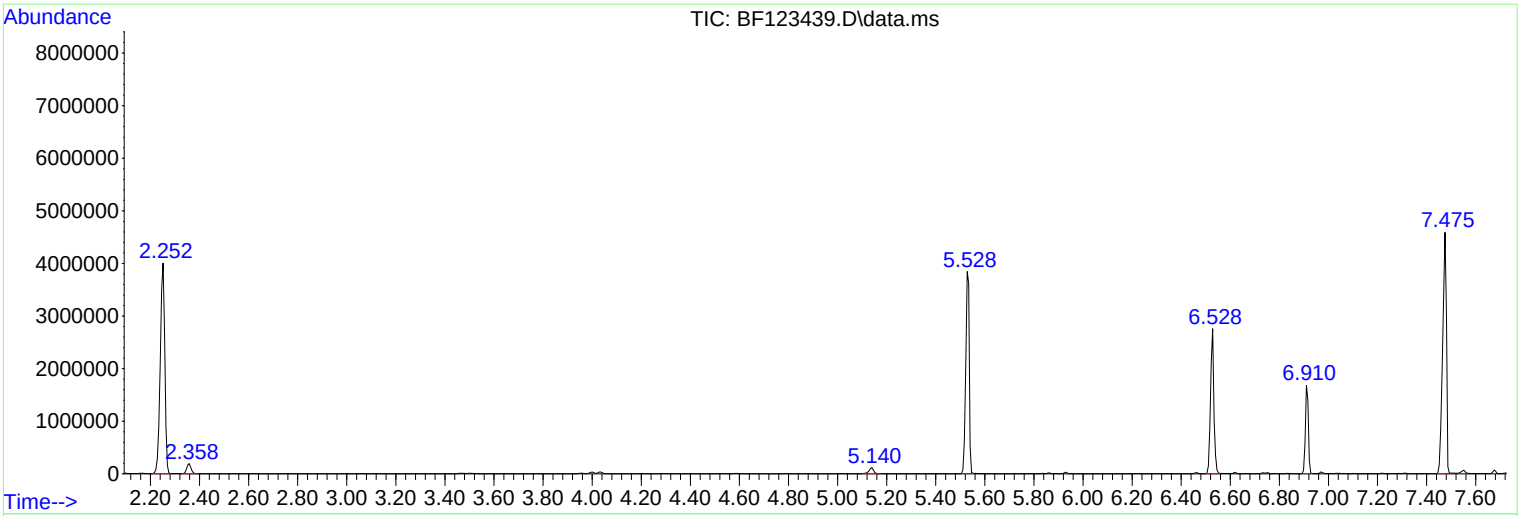
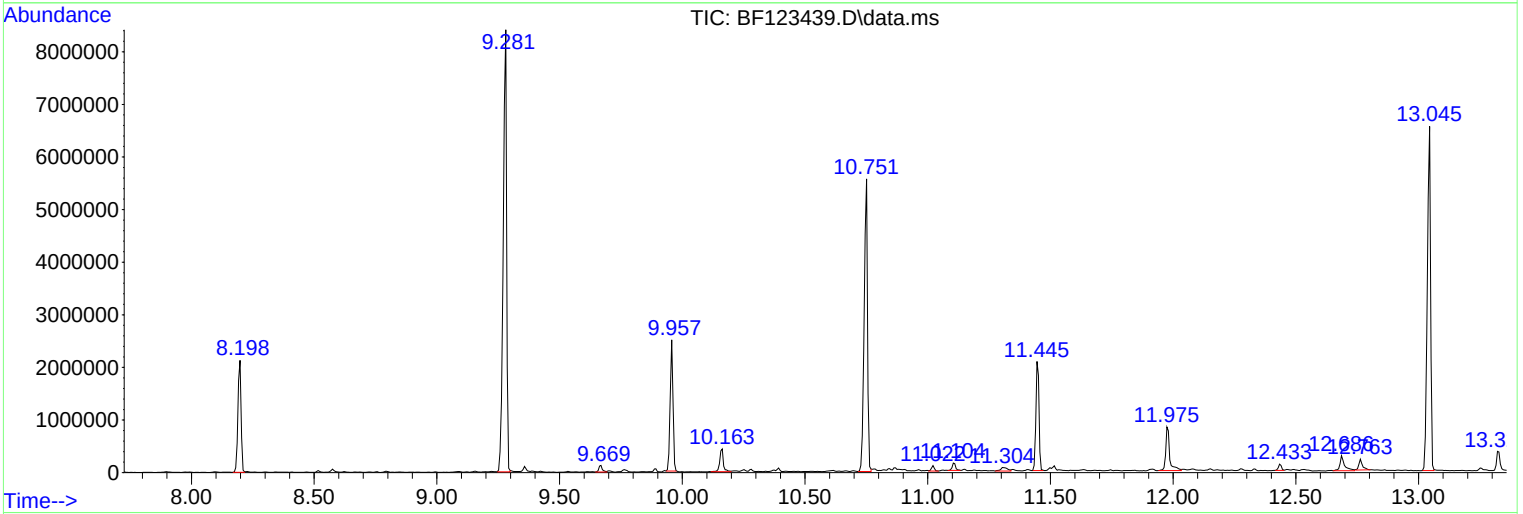
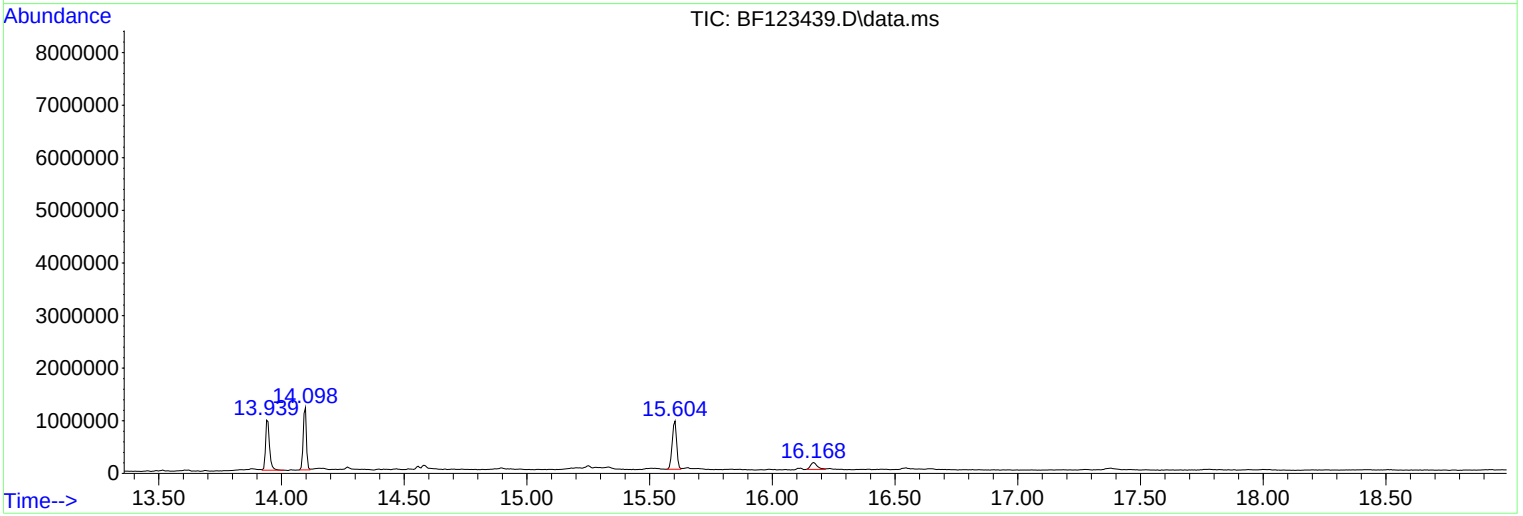
ClientSampleId :
MW-105I

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.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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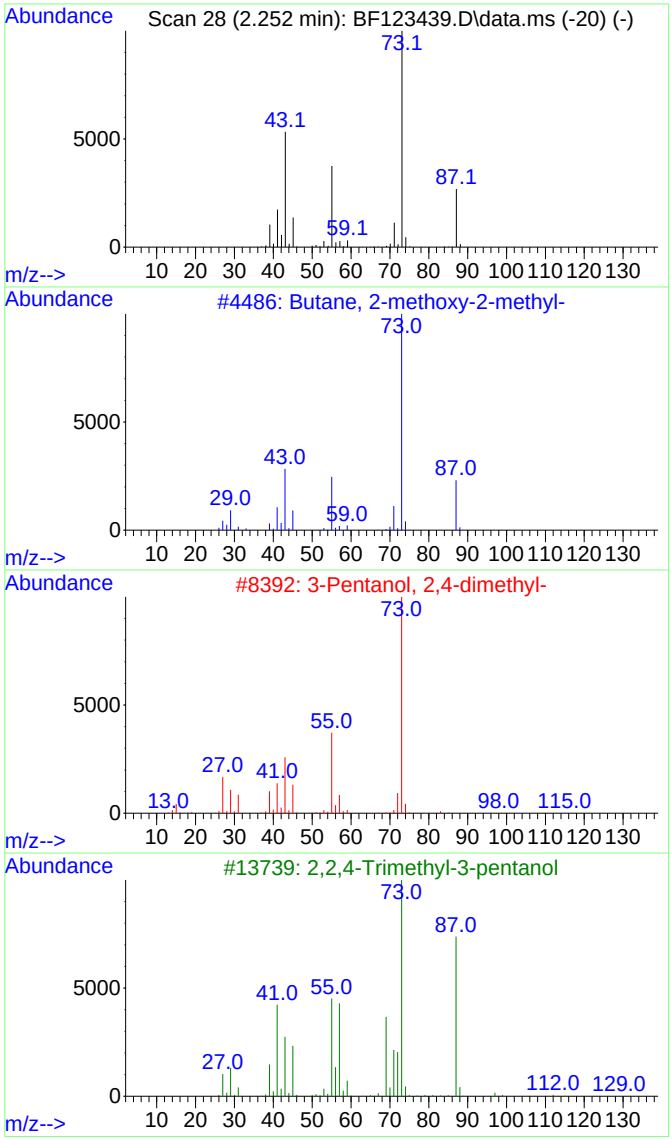
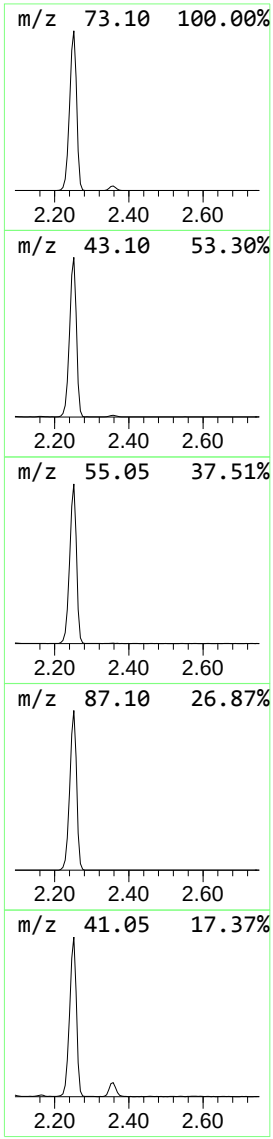
****
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.252	73.53 ng	5166260	1,4-Dichlorobenzene-d4	6.910

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	43
3	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
5	Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9





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Operator : JU/CG
Sample : M1770-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-105I

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.M
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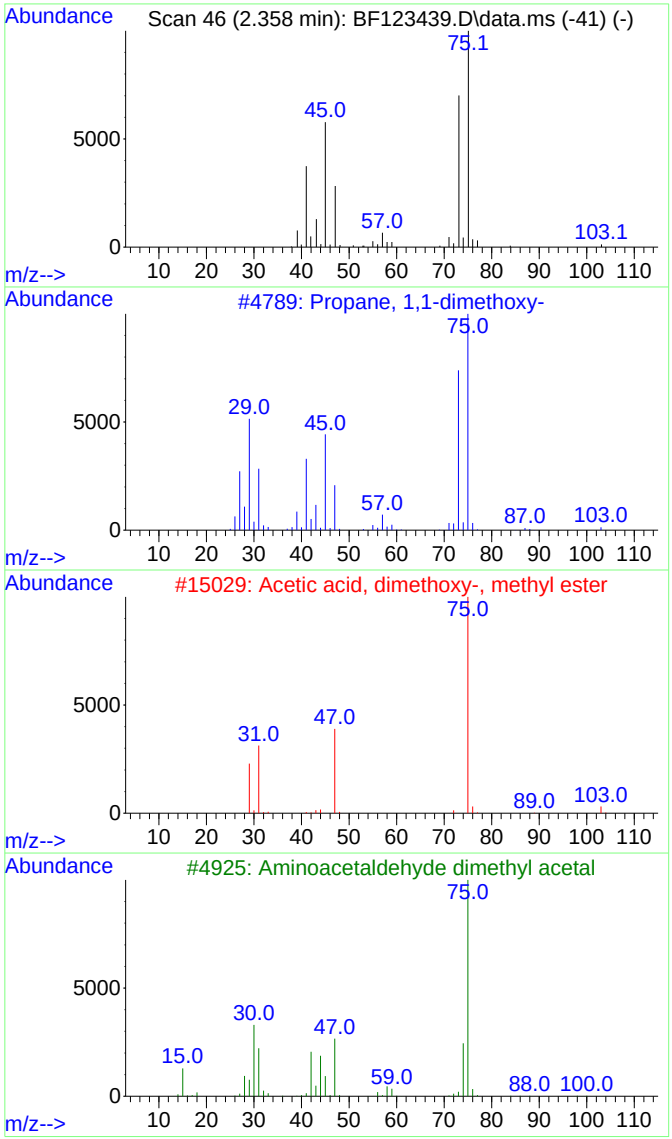
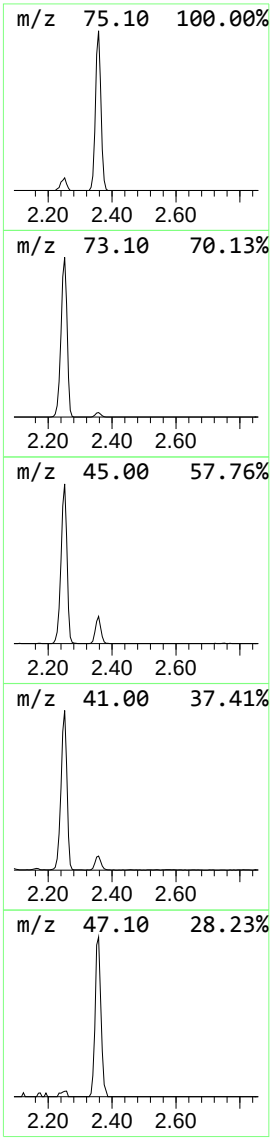
Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.358	3.33 ng	233795	1,4-Dichlorobenzene-d4	6.910

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	83
2	Acetic acid, dimethoxy-, methyl ...	134	C5H10O4	000089-91-8	40
3	Aminoacetaldehyde dimethyl acetal	105	C4H11NO2	022483-09-6	36
4	2-Propanol, 1,1-dimethoxy-	120	C5H12O3	042919-42-6	36
5	Methane, trimethoxy-	106	C4H10O3	000149-73-5	33





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Sample : M1770-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-105I

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.M
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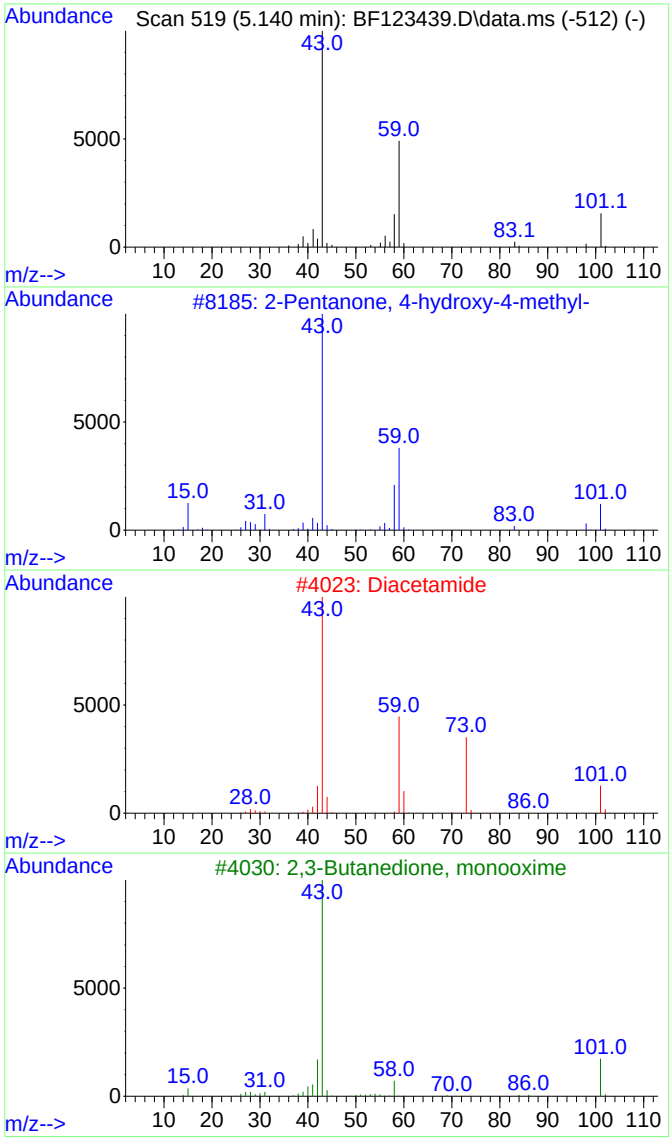
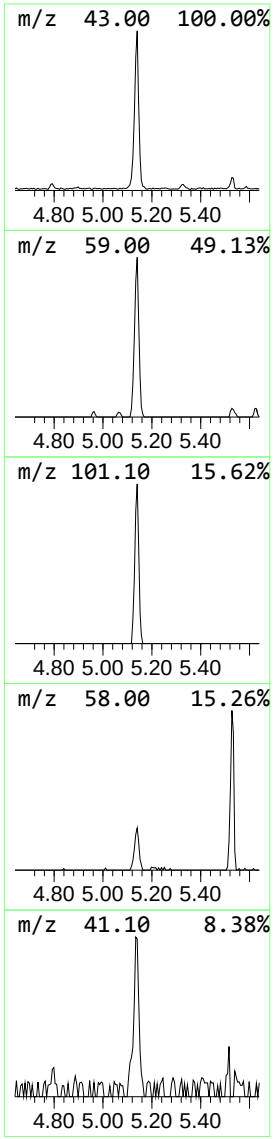
****
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.140	2.17 ng	152518	1,4-Dichlorobenzene-d4	6.910

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Diacetamide	101	C4H7NO2	000625-77-4	9
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
5	Propylamine	59	C3H9N	000107-10-8	7





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Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-105I

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.M
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TIC Library : C:\DATABASE\NIST11.L
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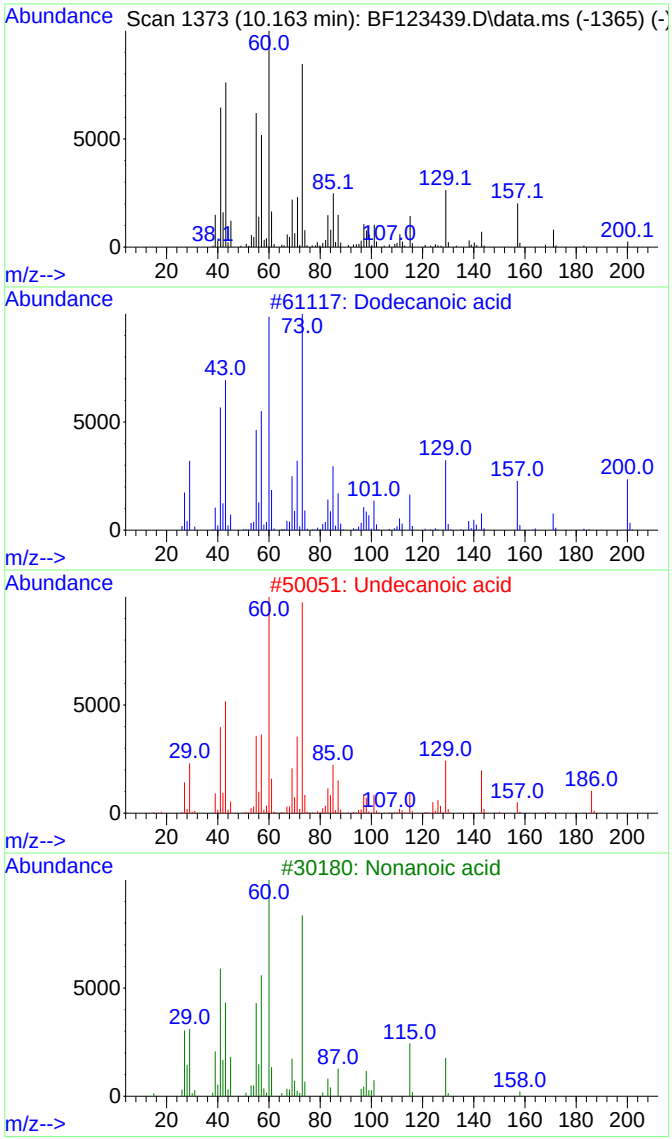
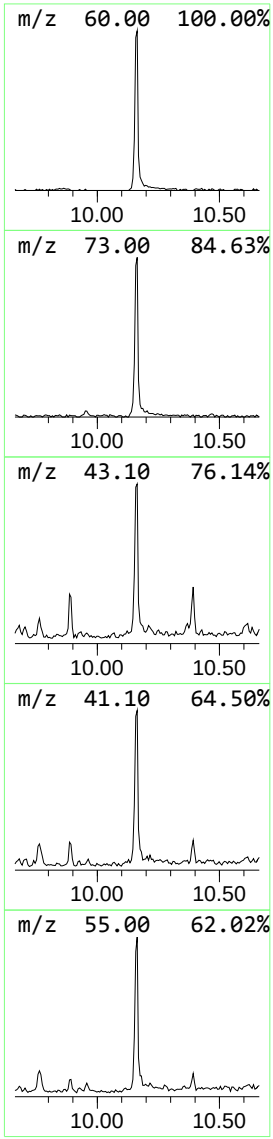
Peak Number 4 Dodecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.163	4.37 ng	437248	Acenaphthene-d10	9.957

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid	200	C12H24O2	000143-07-7	91
2	Undecanoic acid	186	C11H22O2	000112-37-8	80
3	Nonanoic acid	158	C9H18O2	000112-05-0	64
4	n-Decanoic acid	172	C10H20O2	000334-48-5	53
5	Octanoic acid, silver(1+) salt	250	C8H15AgO2	024927-67-1	50





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Sample : M1770-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-105I

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.M
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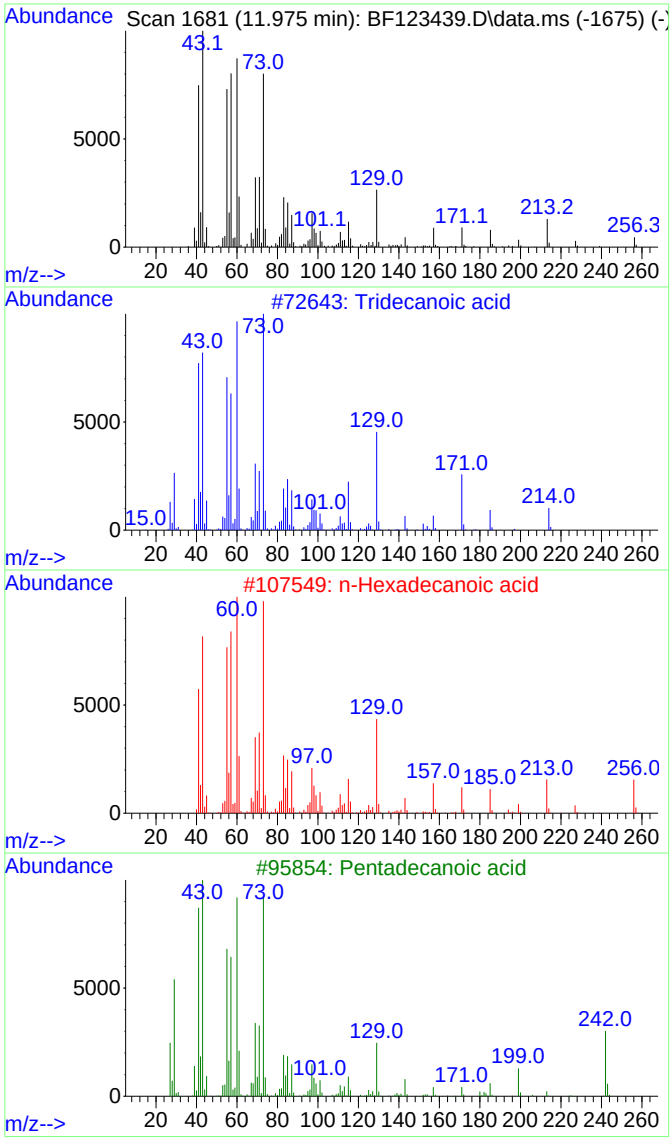
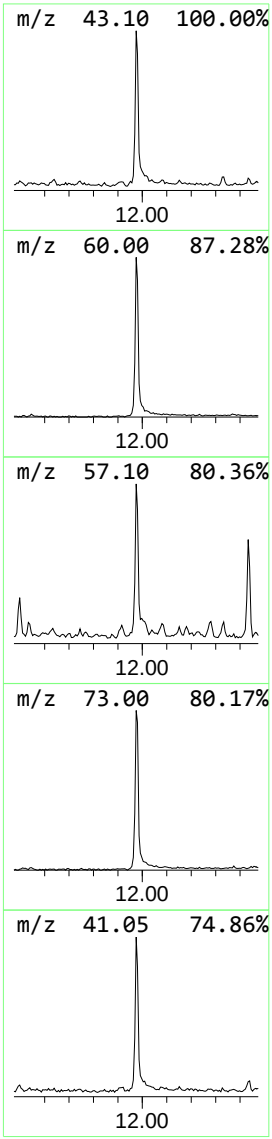
Peak Number 5 Tridecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.975	10.04 ng	911393	Phenanthrene-d10	11.445

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	95
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Dodecanoic acid	200	C12H24O2	000143-07-7	81
5	Undecanoic acid	186	C11H22O2	000112-37-8	80





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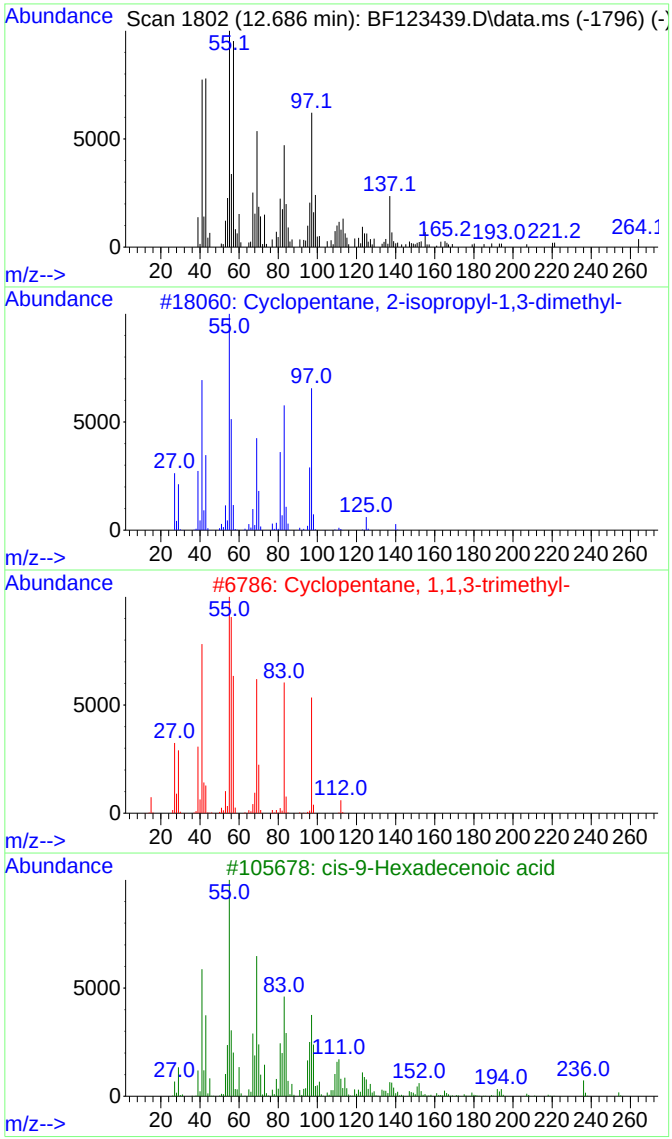
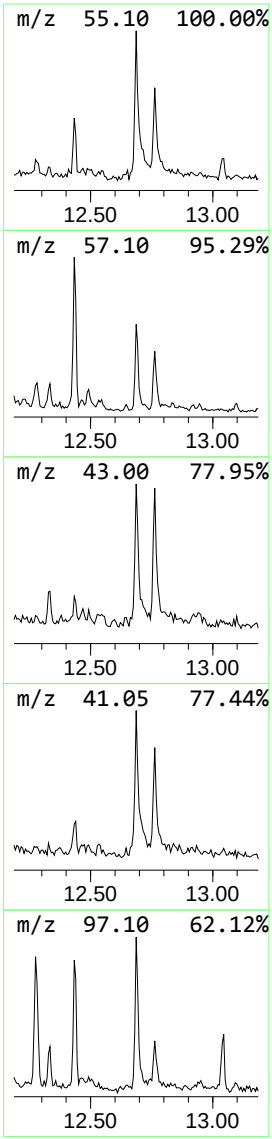
Peak Number 6 unknown12.686 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.686	4.12 ng	374122	Phenanthrene-d10	11.445

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, 2-isopropyl-1,3-di...	140	C10H20	032281-85-9	46
2	Cyclopentane, 1,1,3-trimethyl-	112	C8H16	004516-69-2	46
3	cis-9-Hexadecenoic acid	254	C16H30O2	1000333-19-5	45
4	9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	43
5	Z-11-Tetradecenoic acid	226	C14H26O2	1000130-83-3	38





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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.M
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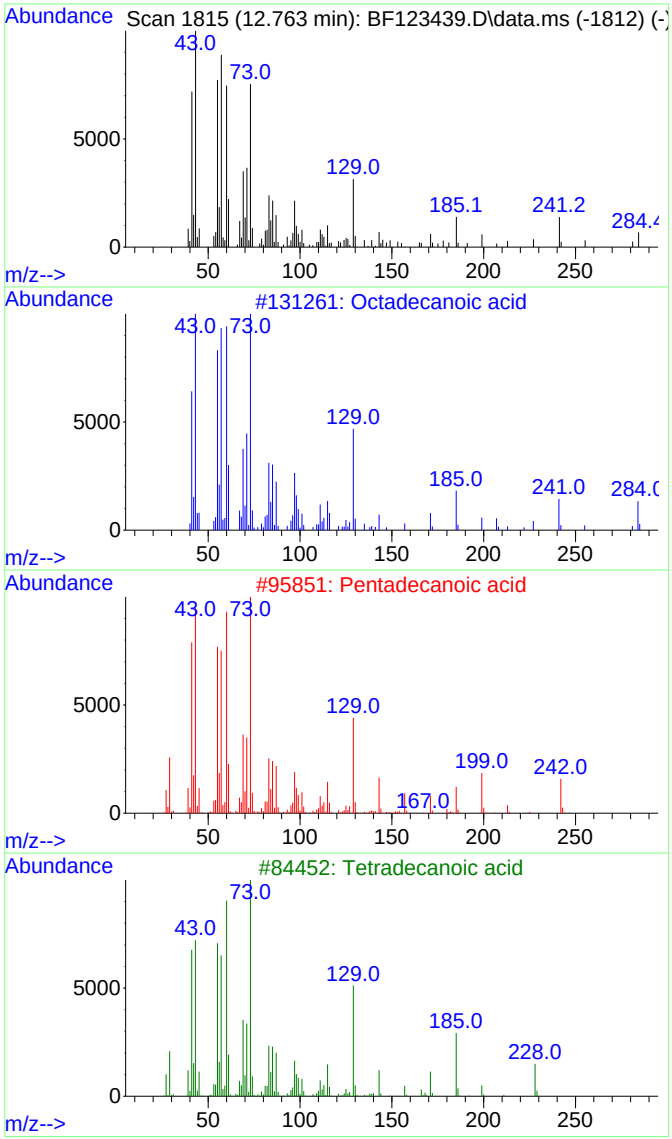
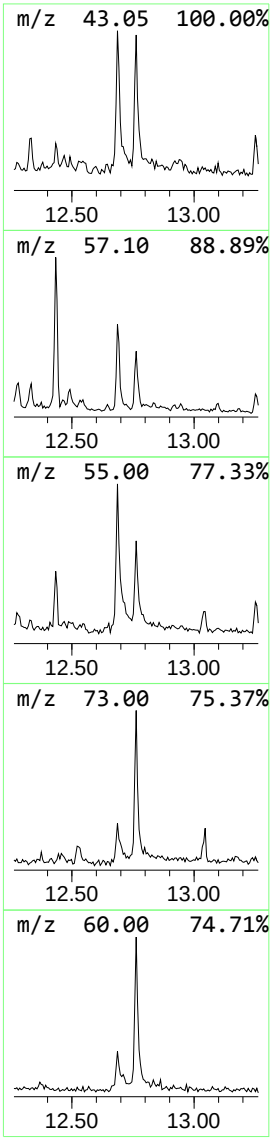
Peak Number 7 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.763	2.33 ng	211419	Phenanthrene-d10	11.445

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	95
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	58
5	n-Decanoic acid	172	C10H20O2	000334-48-5	53





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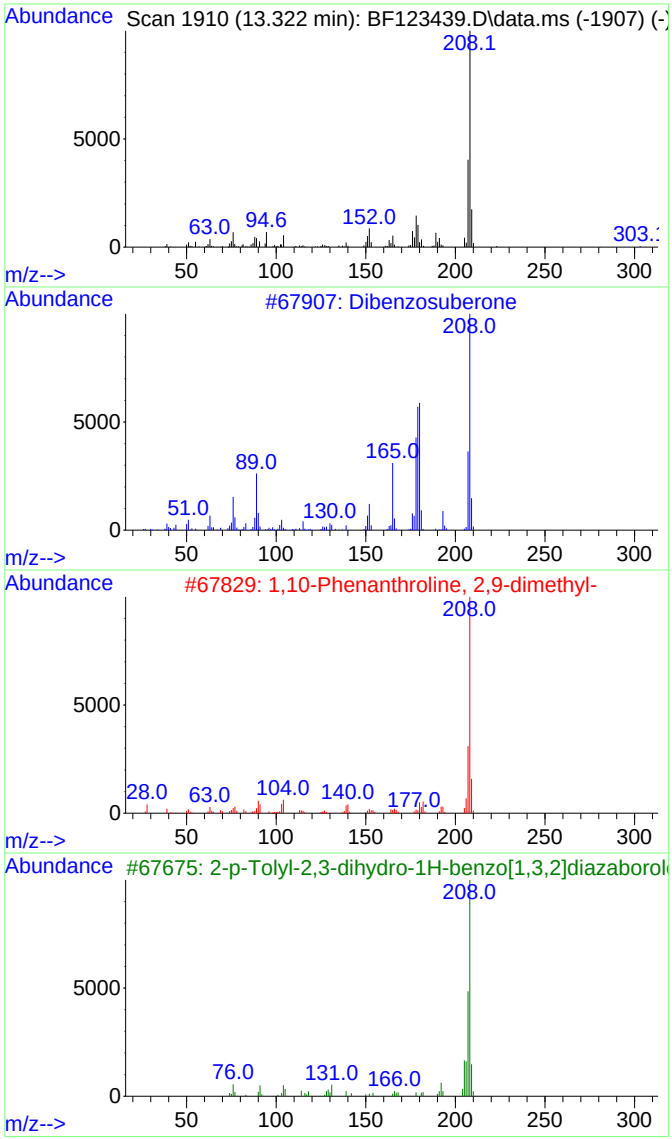
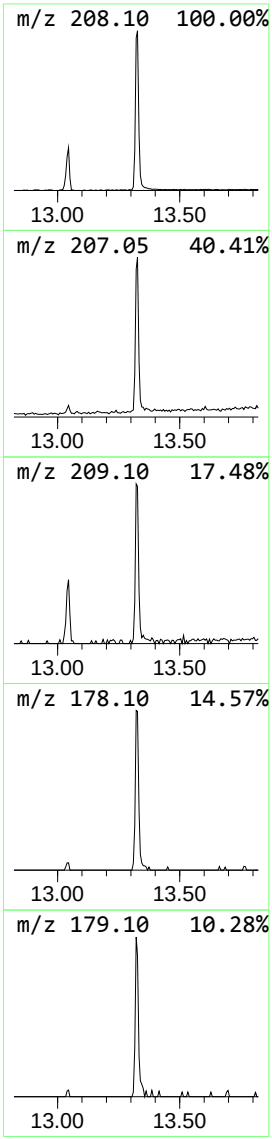
Peak Number 8 Dibenzosuberone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.322	6.68 ng	358183	Chrysene-d12	14.098

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dibenzosuberone	208	C15H12O	001210-35-1	86
2	1,10-Phenanthroline, 2,9-dimethyl-	208	C14H12N2	000484-11-7	72
3	2-p-Tolyl-2,3-dihydro-1H-benzo[1...	208	C13H13BN2	1000296-11-8	72
4	3-Phenyl-1-indanone	208	C15H12O	016618-72-7	72
5	Benzeneacetonitrile, 4-amino-.al...	208	C14H12N2	004760-58-1	72





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Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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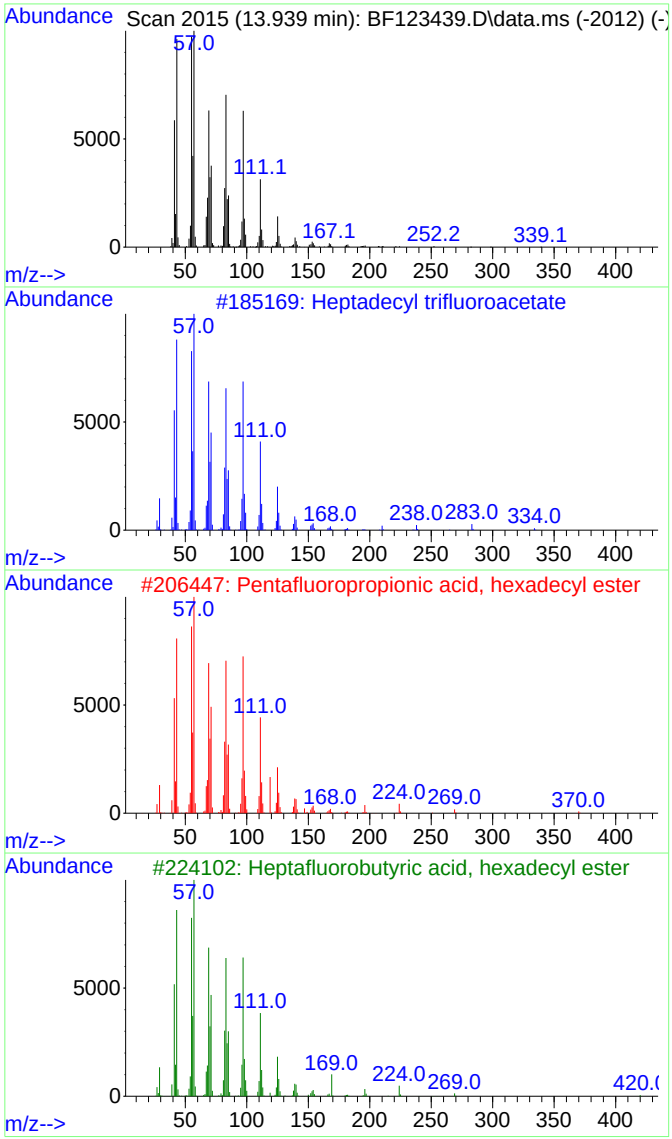
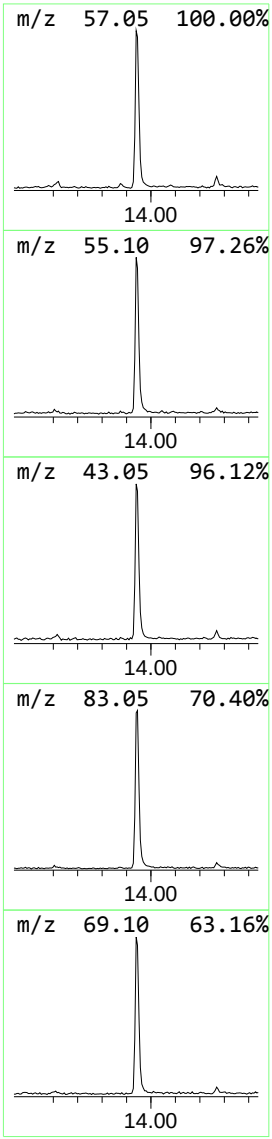
Peak Number 9 Heptadecyl trifluoroacetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.939	19.97 ng	1071360	Chrysene-d12	14.098

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	94
2	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	94
3	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	94
4	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
5	1-Nonadecene	266	C19H38	018435-45-5	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032421\
Data File : BF123439.D
Acq On : 24 Mar 2021 15:08
Operator : JU/CG
Sample : M1770-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-105I

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

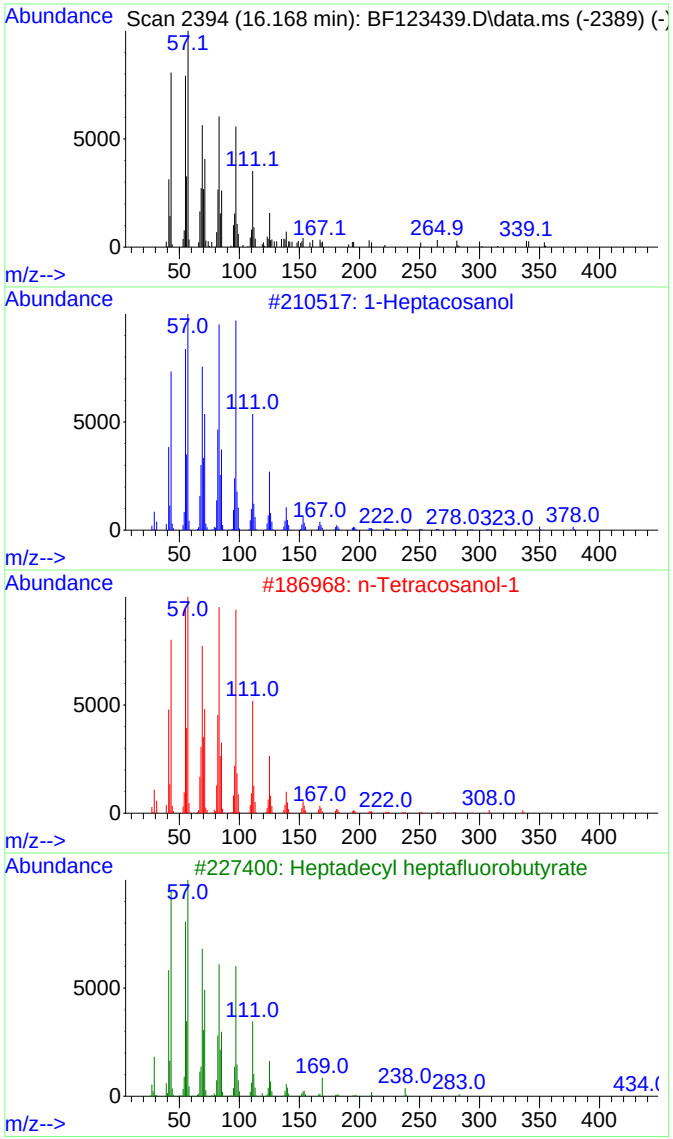
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

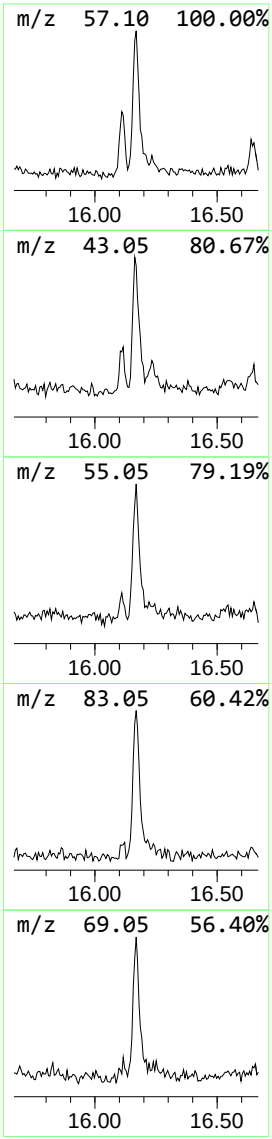
****

Peak Number 10 1-Heptacosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.168	4.43 ng	258012	Perylene-d12	15.604

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	95
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	95
3	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
4	Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	94
5	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032421\
Data File : BF123439.D
Acq On : 24 Mar 2021 15:08
Operator : JU/CG
Sample : M1770-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-105I

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.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
Butane, 2-metho...	2.252	73.5	ng	5166260	1	6.910	1405180	20.0
Propane, 1,1-di...	2.358	3.3	ng	233795	1	6.910	1405180	20.0
2-Pentanone, 4-...	5.140	2.2	ng	152518	1	6.910	1405180	20.0
Dodecanoic acid	10.163	4.4	ng	437248	3	9.957	2000550	20.0
Tridecanoic acid	11.975	10.0	ng	911393	4	11.445	1815410	20.0
unknown12.686	12.686	4.1	ng	374122	4	11.445	1815410	20.0
Octadecanoic acid	12.763	2.3	ng	211419	4	11.445	1815410	20.0
Dibenzosuberone	13.322	6.7	ng	358183	5	14.098	1072980	20.0
Heptadecyl trif...	13.939	20.0	ng	1071360	5	14.098	1072980	20.0
1-Heptacosanol	16.168	4.4	ng	258012	6	15.604	1165310	20.0