LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030321\
Data File : BF123363.D
Acq On : 3 Mar 2021 19:14
Operator : JU/CG
Sample : M1545-08
Misc :
ALS Vial : 12 Sample Multiplier: 4

Instrument : BNA_F
ClientSampleId : MH-G

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: BF123363.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.857	126	131	134	rVB	4839014	6088077	37.09%	5.274%
2	5.575	587	593	596	rBV	6716481	7327664	44.64%	6.348%
3	6.516	747	753	770	rBV	3116722	5358817	32.64%	4.642%
4	6.634	770	773	776	rVB	483172	376636	2.29%	0.326%
5	6.857	806	811	818	rBV	2910575	2878449	17.53%	2.494%
6	7.428	897	908	911	rBV2	5626668	11135298	67.83%	9.646%
7	8.128	1019	1027	1031	rBV	2466704	3868921	23.57%	3.352%
8	8.445	1079	1081	1095	rVB4	77424	181656	1.11%	0.157%
9	8.845	1143	1149	1156	rBV	169530	212166	1.29%	0.184%
10	8.963	1162	1169	1177	rBV2	96220	227779	1.39%	0.197%
11	9.216	1201	1212	1215	rVB	8361376	16413401	99.98%	14.219%
12	9.604	1272	1278	1281	rBV	167938	229118	1.40%	0.198%
13	9.816	1310	1314	1317	rVV3	147583	212897	1.30%	0.184%
14	9.892	1317	1327	1330	rVB	2861890	4565992	27.81%	3.955%
15	10.316	1392	1399	1402	rVB4	77996	166992	1.02%	0.145%
16	10.698	1448	1464	1467	rBV	6312004	11545667	70.33%	10.002%
17	11.239	1553	1556	1561	rBV5	106768	175842	1.07%	0.152%
18	11.386	1570	1581	1584	rBV	3753484	4377615	26.67%	3.792%
19	11.886	1662	1666	1667	rBV3	165068	217572	1.33%	0.188%
20	11.933	1668	1674	1677	rVB	3258027	4188504	25.51%	3.628%
21	12.198	1716	1719	1723	rVB	212365	246388	1.50%	0.213%
22	12.357	1743	1746	1749	rVV	985218	872399	5.31%	0.756%
23	12.415	1753	1756	1761	rVB	187606	209104	1.27%	0.181%
24	12.715	1803	1807	1812	rBV	2444684	2470114	15.05%	2.140%
25	12.998	1841	1855	1858	rBV	9583672	16416326	100.00%	14.221%
26	13.186	1884	1887	1892	rBV	164867	205696	1.25%	0.178%
27	13.874	2001	2004	2013	rVB	3300383	3538297	21.55%	3.065%
28	14.045	2028	2033	2035	rVB	3925596	3930181	23.94%	3.405%
29	14.145	2048	2050	2056	rVB2	273537	322390	1.96%	0.279%
30	14.515	2110	2113	2116	rVB	263351	293126	1.79%	0.254%
31	15.145	2217	2220	2223	rVB	175520	178586	1.09%	0.155%
32	15.527	2277	2285	2288	rBV	2920401	4301774	26.20%	3.727%
33	15.962	2355	2359	2364	rBV	223873	318709	1.94%	0.276%
34	16.027	2365	2370	2377	rBV	535852	1033112	6.29%	0.895%
35	16.468	2441	2445	2449	rBV	196986	317964	1.94%	0.275%
36	17.068	2543	2547	2555	rVB2	159561	323965	1.97%	0.281%

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Misc :
ALS Vial : 12 Sample Multiplier: 4

Instrument : BNA_F
ClientSampleId : MH-G

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

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Peak separation: 5

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

37	17.180	2560	2566	2576	rVV3	137140	405541	2.47%	0.351%
38	17.774	2663	2667	2676	rVB	142421	302829	1.84%	0.262%

Sum of corrected areas: 115435564

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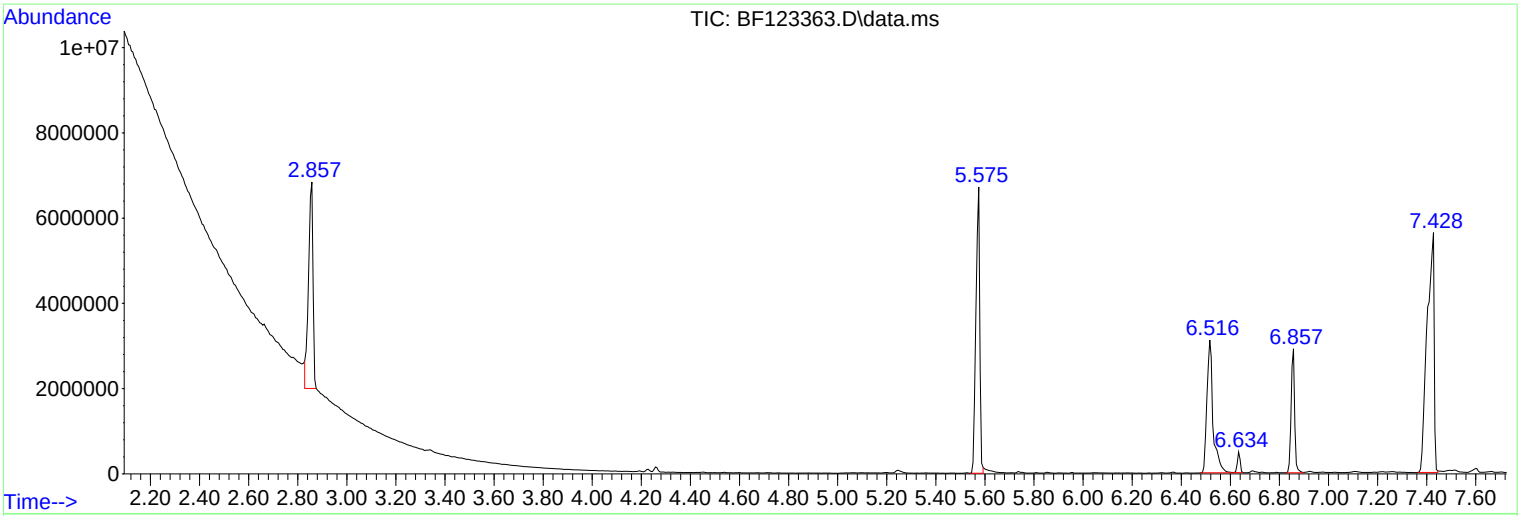
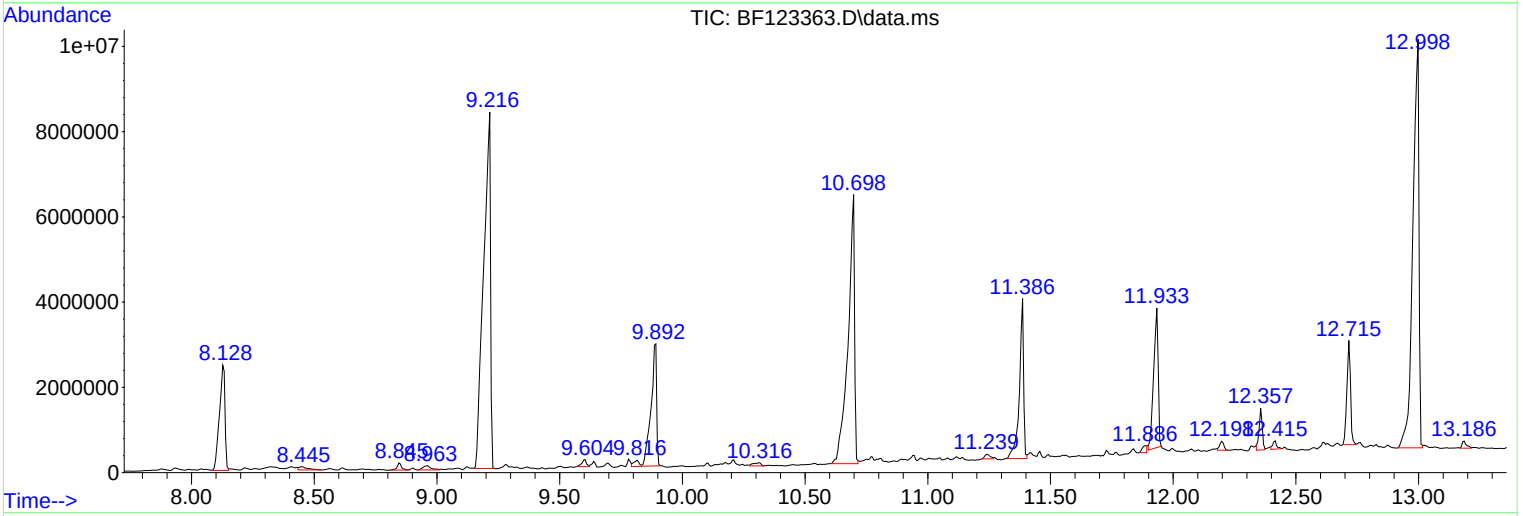
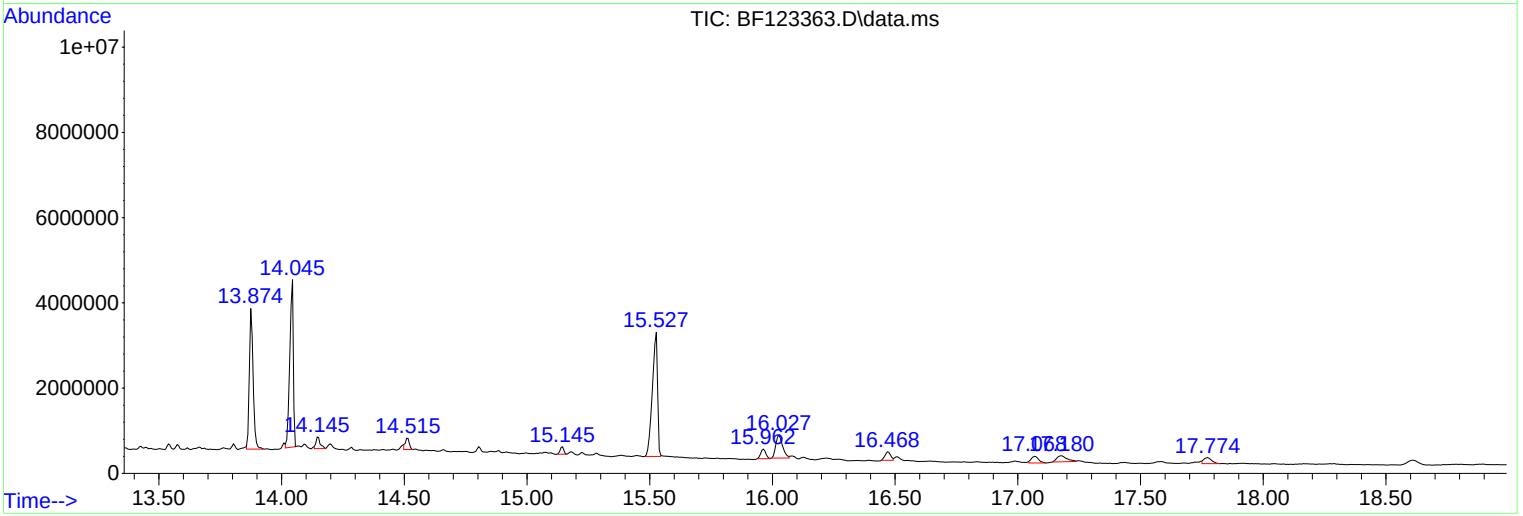
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF021921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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Data File : BF123363.D
Acq On : 3 Mar 2021 19:14
Operator : JU/CG
Sample : M1545-08
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ALS Vial : 12 Sample Multiplier: 4

Instrument : BNA_F
ClientSampleId : MH-G

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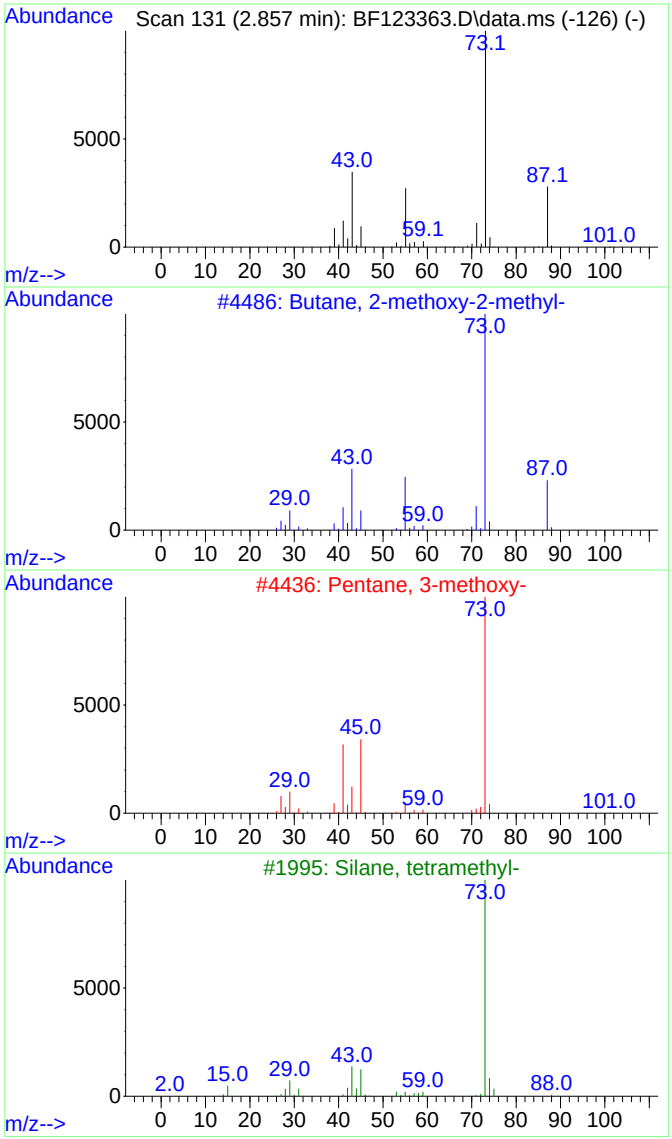
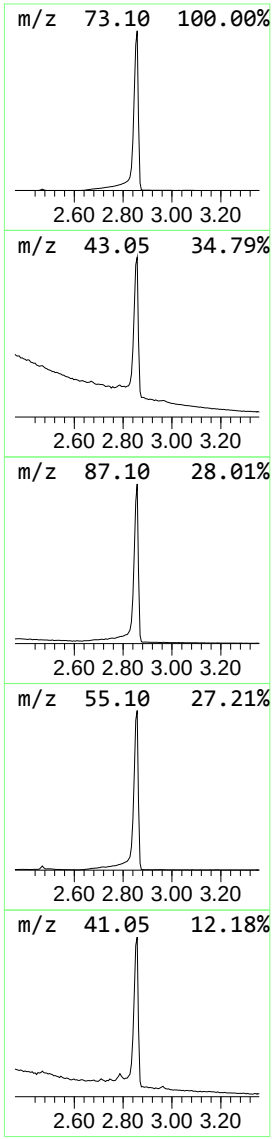
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.857	42.30 ng	6088080	1,4-Dichlorobenzene-d4	6.857

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
3	Silane, tetramethyl-	88	C4H12Si	000075-76-3	16
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	10
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





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Instrument : BNA_F
ClientSampleId : MH-G

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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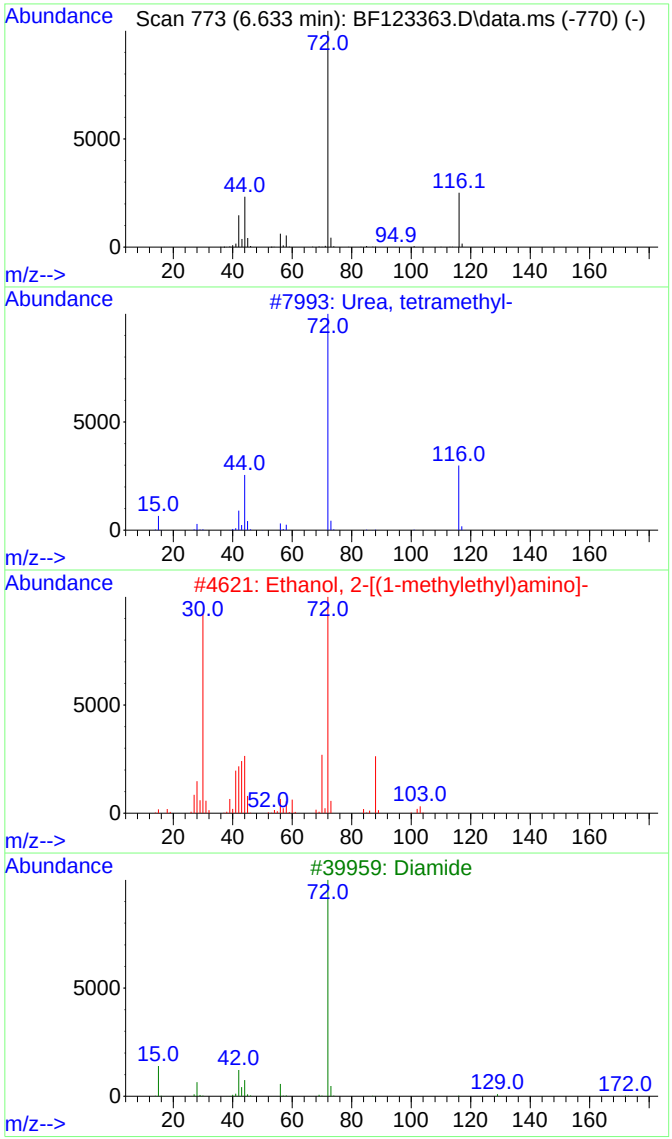
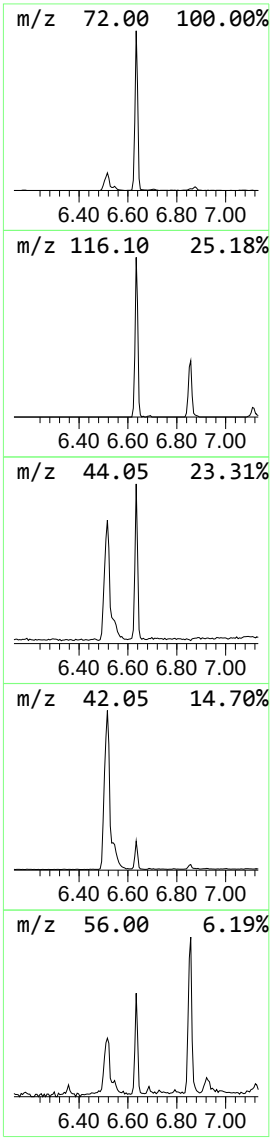
Peak Number 2 Urea, tetramethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.633	2.62 ng	376636	1,4-Dichlorobenzene-d4	6.857

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Urea, tetramethyl-	116	C5H12N2O	000632-22-4	91
2	Ethanol, 2-[(1-methylethyl)amino]-	103	C5H13NO	000109-56-8	50
3	Diamide	172	C6H12N4O2	010465-78-8	42
4	[2-(N,N-Dimethyl)]-1,2-propanedi...	102	C5H14N2	1000133-38-7	38
5	DL-Norvaline	117	C5H11NO2	000760-78-1	36





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030321\
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Acq On : 3 Mar 2021 19:14
Operator : JU/CG
Sample : M1545-08
Misc :
ALS Vial : 12 Sample Multiplier: 4

Instrument : BNA_F
ClientSampleId : MH-G

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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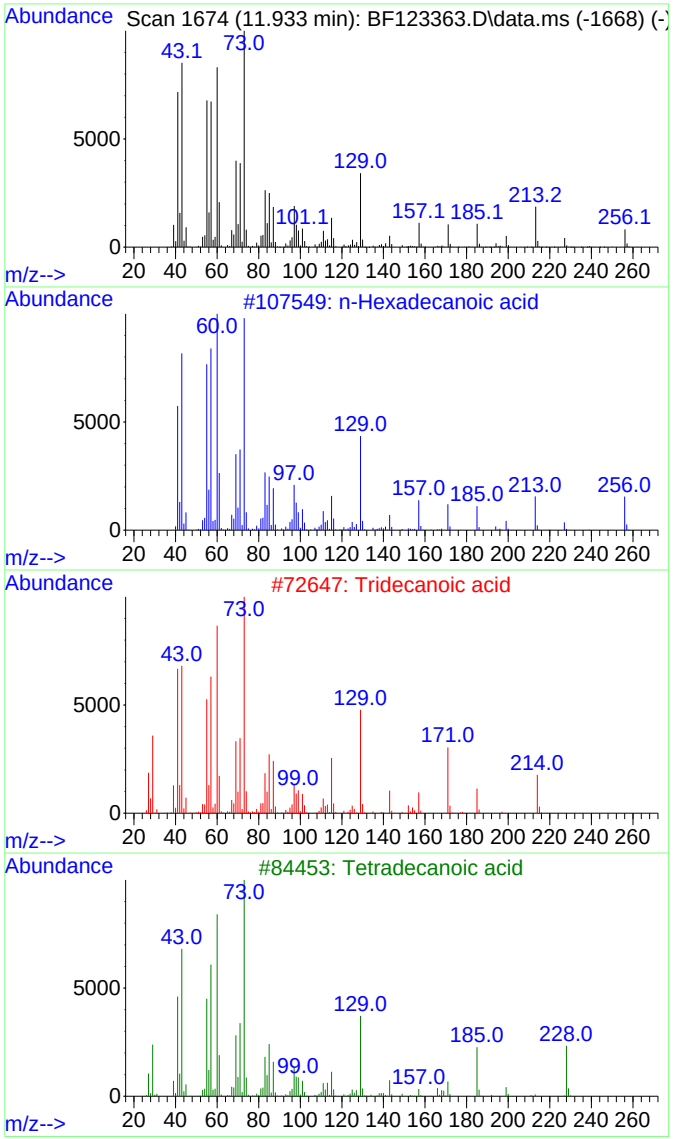
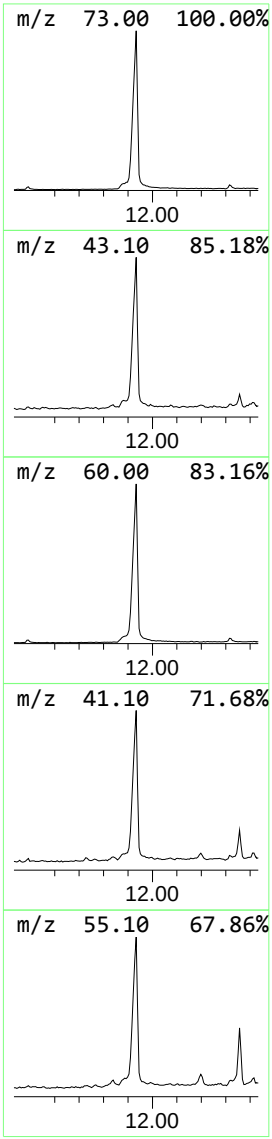
Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.933	19.14 ng	4188500	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	93
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
5	Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030321\
Data File : BF123363.D
Acq On : 3 Mar 2021 19:14
Operator : JU/CG
Sample : M1545-08
Misc :
ALS Vial : 12 Sample Multiplier: 4

Instrument : BNA_F
ClientSampleId : MH-G

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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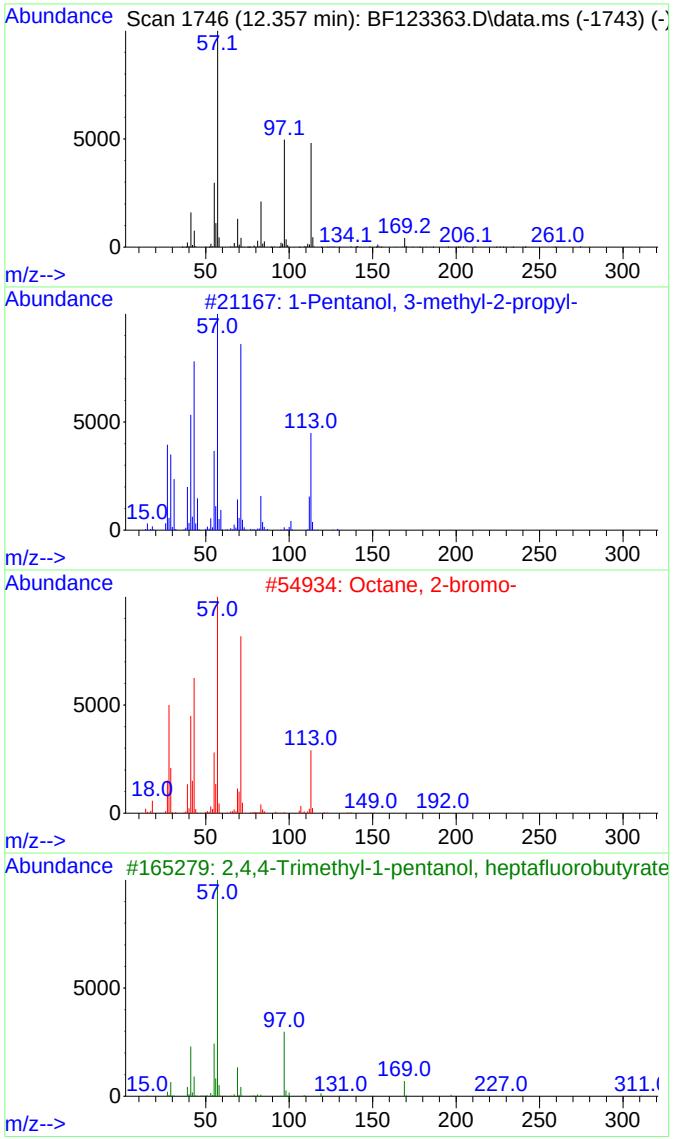
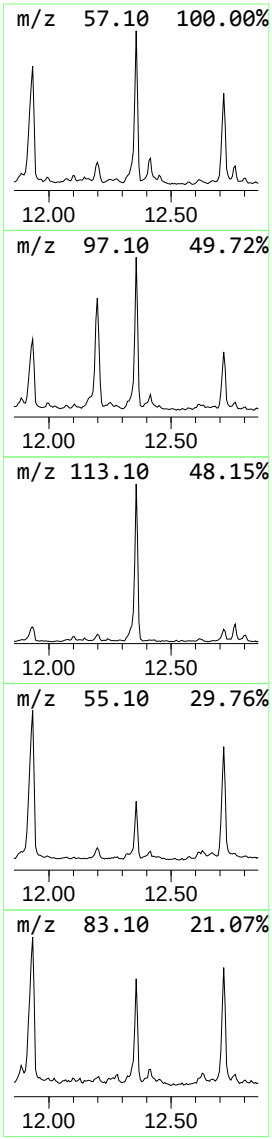
Peak Number 4 unknown12.357 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.357	3.99 ng	872399	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	Octane, 2-bromo-	192	C8H17Br	000557-35-7	38
3	2,4,4-Trimethyl-1-pentanol, hept...	326	C12H17F7O2	1000365-01-4	37
4	2,4,4-Trimethyl-1-pentanol, pent...	276	C11H17F5O2	1000365-51-0	32
5	Octane, 2-iodo-	240	C8H17I	000557-36-8	25





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Sample : M1545-08
Misc :
ALS Vial : 12 Sample Multiplier: 4

Instrument : BNA_F
ClientSampleId : MH-G

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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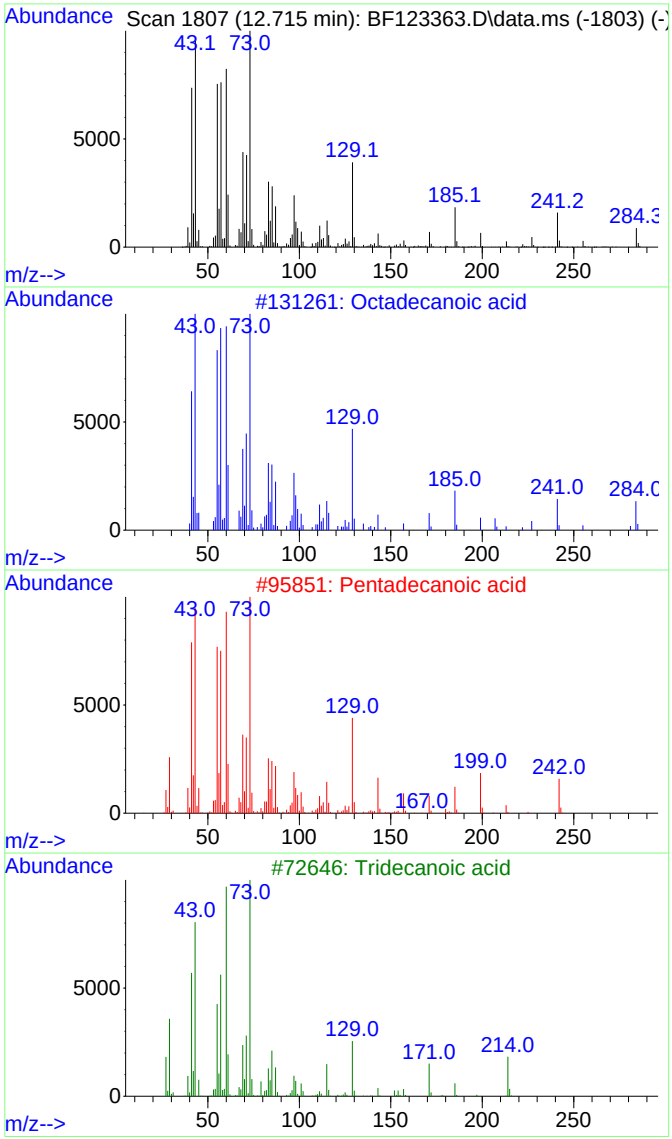
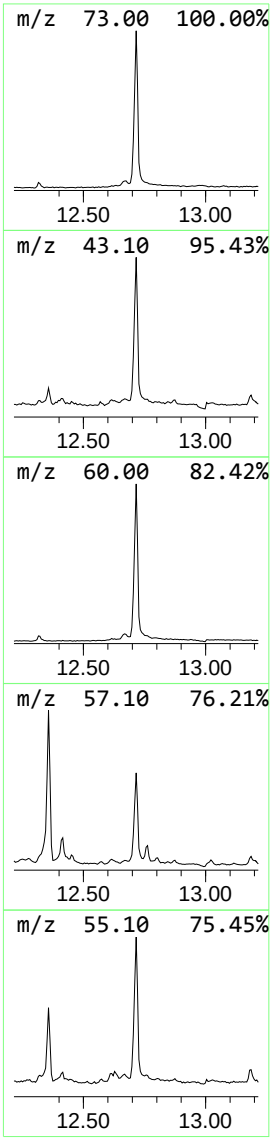
Peak Number 5 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.716	12.57 ng	2470110	Chrysene-d12	14.045

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	Tridecanoic acid	214	C13H26O2	000638-53-9	76
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5	n-Decanoic acid	172	C10H20O2	000334-48-5	62





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Misc :
ALS Vial : 12 Sample Multiplier: 4

Instrument : BNA_F
ClientSampleId : MH-G

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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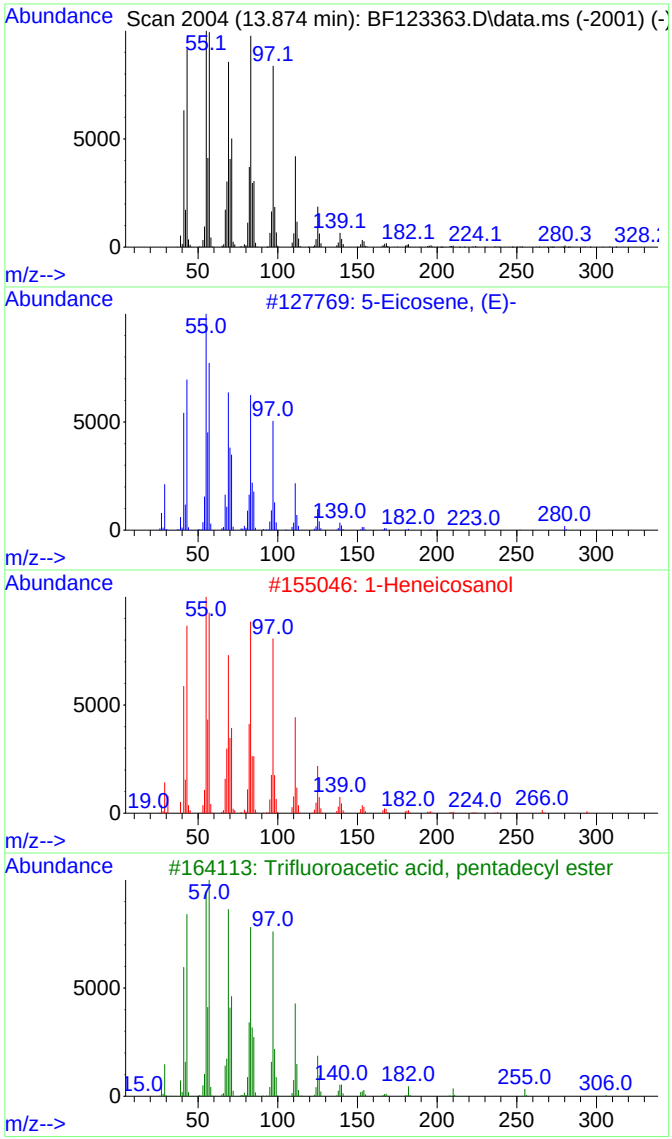
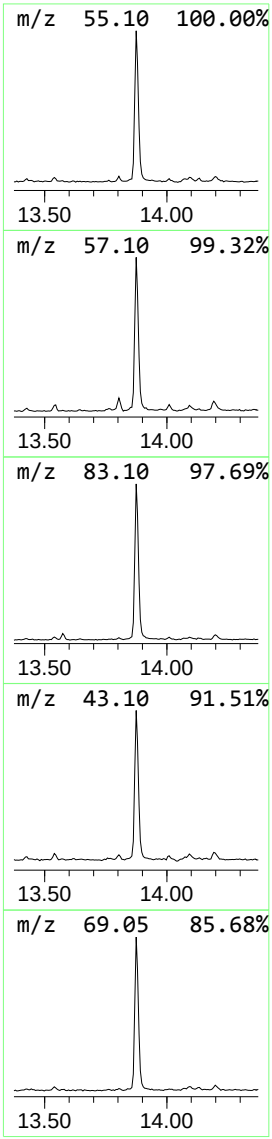
Peak Number 6 5-Eicosene, (E)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	18.01 ng	3538300	Chrysene-d12	14.045

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	99
2	1-Heneicosanol	312	C21H44O	015594-90-8	95
3	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94
4	n-Nonadecanol-1	284	C19H40O	001454-84-8	94
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	94





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

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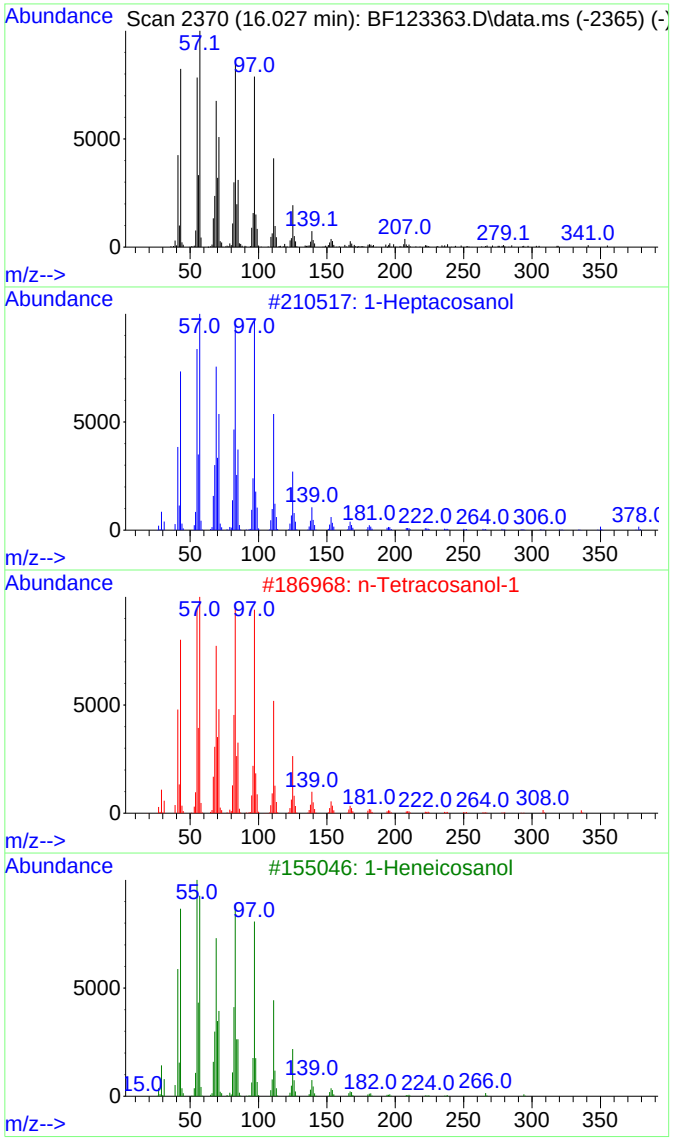
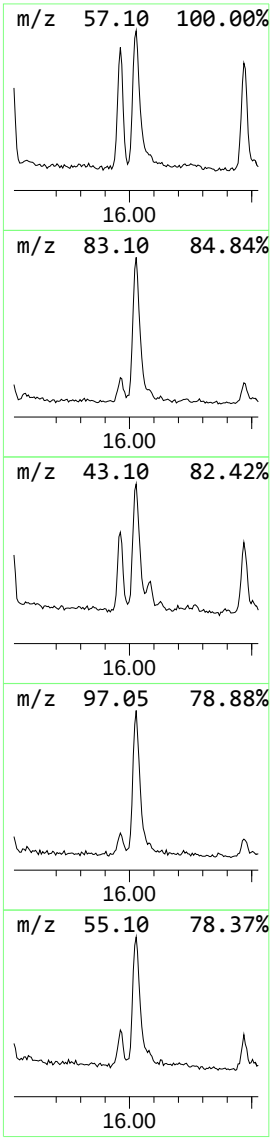
Peak Number 7 1-Heptacosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.027	4.80 ng	1033110	Perylene-d12	15.527

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	93
3	1-Heneicosanol	312	C21H44O	015594-90-8	93
4	Octacosanol	410	C28H58O	000557-61-9	91
5	Behenic alcohol	326	C22H46O	000661-19-8	90





Tentatively Identified Compound (LSC) summary

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Instrument : BNA_F
ClientSampleId : MH-G

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
Butane, 2-metho...	2.857	42.3	ng	6088080	1	6.857	2878450	20.0
Urea, tetramethyl-	6.633	2.6	ng	376636	1	6.857	2878450	20.0
n-Hexadecanoic ...	11.933	19.1	ng	4188500	4	11.386	4377620	20.0
unknown12.357	12.357	4.0	ng	872399	4	11.386	4377620	20.0
Octadecanoic acid	12.716	12.6	ng	2470110	5	14.045	3930180	20.0
5-Eicosene, (E)-	13.874	18.0	ng	3538300	5	14.045	3930180	20.0
1-Heptacosanol	16.027	4.8	ng	1033110	6	15.527	4301770	20.0