LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012821\
Data File : BF123061.D
Acq On : 28 Jan 2021 16:02
Operator : JU/CG
Sample : M1236-08
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PS1419LN

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-BF012721.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF123061.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.181	9	16	22	rBV	663803	834435	12.88%	1.508%
2	5.110	503	514	521	rBV	340572	421232	6.50%	0.761%
3	5.510	576	582	585	rBV	4496856	4535176	70.00%	8.195%
4	6.510	747	752	755	rBV	4672818	4676768	72.18%	8.450%
5	6.892	813	817	820	rBV	1918171	1503542	23.21%	2.717%
6	7.451	907	912	915	rBV	3276573	2988008	46.12%	5.399%
7	8.175	1031	1035	1038	rBV	2381264	1994437	30.78%	3.604%
8	9.251	1213	1218	1222	rBV	5548883	5420173	83.66%	9.794%
9	9.645	1282	1285	1288	rBV	114577	95872	1.48%	0.173%
10	9.933	1330	1334	1338	rBV	2717876	2396298	36.99%	4.330%
11	10.722	1463	1468	1472	rBV	3923105	3688144	56.93%	6.664%
12	11.086	1526	1530	1534	rBV	227142	194682	3.00%	0.352%
13	11.427	1582	1588	1591	rBV	2795576	2529760	39.05%	4.571%
14	11.527	1601	1605	1608	rBV2	132786	119228	1.84%	0.215%
15	11.874	1661	1664	1671	rBV2	189126	245610	3.79%	0.444%
16	11.957	1672	1678	1690	rVV2	1710783	1837536	28.36%	3.320%
17	12.251	1725	1728	1732	rBV	108387	135845	2.10%	0.245%
18	12.410	1752	1755	1759	rBV	747097	662277	10.22%	1.197%
19	12.468	1762	1765	1769	rVV	233551	195731	3.02%	0.354%
20	12.510	1769	1772	1779	rVB2	80455	87134	1.34%	0.157%
21	12.663	1793	1798	1807	rBV3	160269	251358	3.88%	0.454%
22	12.739	1808	1811	1816	rBV	333745	359412	5.55%	0.649%
23	12.815	1821	1824	1827	rBV	202770	158900	2.45%	0.287%
24	13.021	1854	1859	1862	rBV	6902609	6478928	100.00%	11.707%
25	13.168	1880	1884	1888	rBV	102225	113609	1.75%	0.205%
26	13.251	1894	1898	1906	rVB3	54564	83792	1.29%	0.151%
27	13.498	1936	1940	1944	rVB	205674	199067	3.07%	0.360%
28	13.639	1961	1964	1967	rBV	701970	609447	9.41%	1.101%
29	13.674	1967	1970	1973	rVB2	171208	142422	2.20%	0.257%
30	13.927	2009	2013	2022	rBV	730647	1269796	19.60%	2.294%
31	13.992	2022	2024	2029	rVB	91779	89378	1.38%	0.161%
32	14.074	2034	2038	2042	rBV	3000140	2714945	41.90%	4.906%
33	14.551	2114	2119	2121	rBV2	60439	68193	1.05%	0.123%
34	14.945	2181	2186	2190	rBV	4896407	4886435	75.42%	8.829%
35	15.209	2228	2231	2235	rBV	69666	73547	1.14%	0.133%
36	15.562	2285	2291	2295	rBV	2036336	2558273	39.49%	4.623%

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Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PS1419LN

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-BF012721.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.604	2295	2298	2311	rVB2	72237	125361	1.93%	0.227%
38	16.051	2370	2374	2379	rBV	60440	89407	1.38%	0.162%
39	16.133	2380	2388	2410	rVV6	65939	319132	4.93%	0.577%
40	16.492	2443	2449	2459	rBV8	64695	190536	2.94%	0.344%

Sum of corrected areas: 55343826

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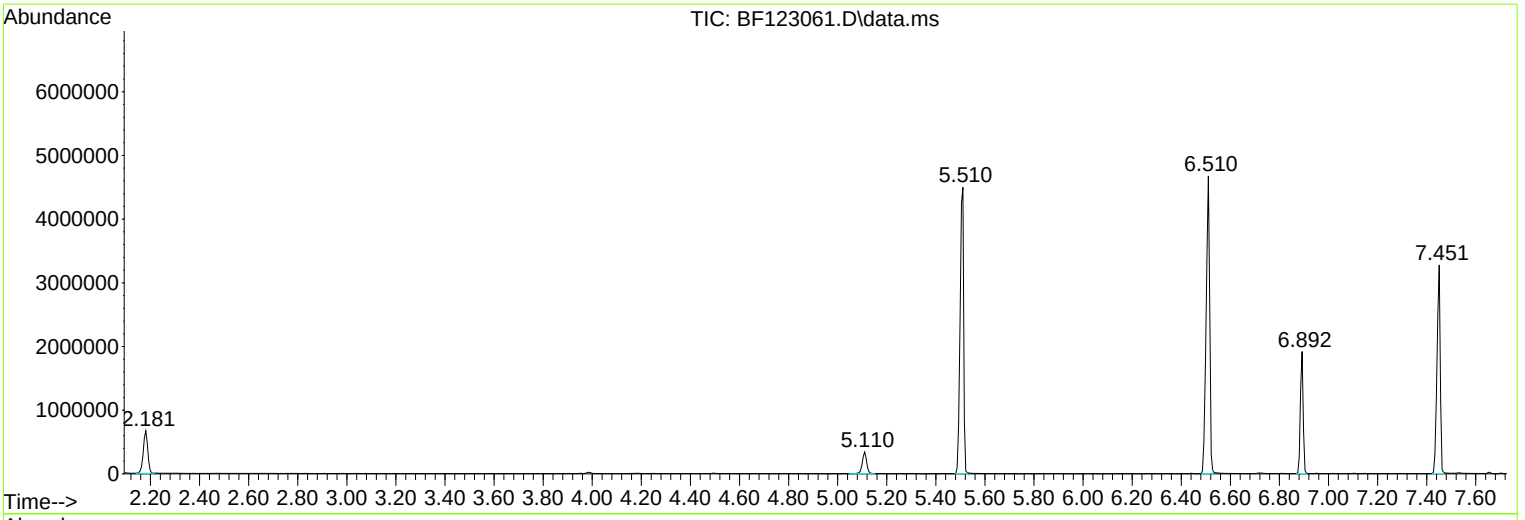
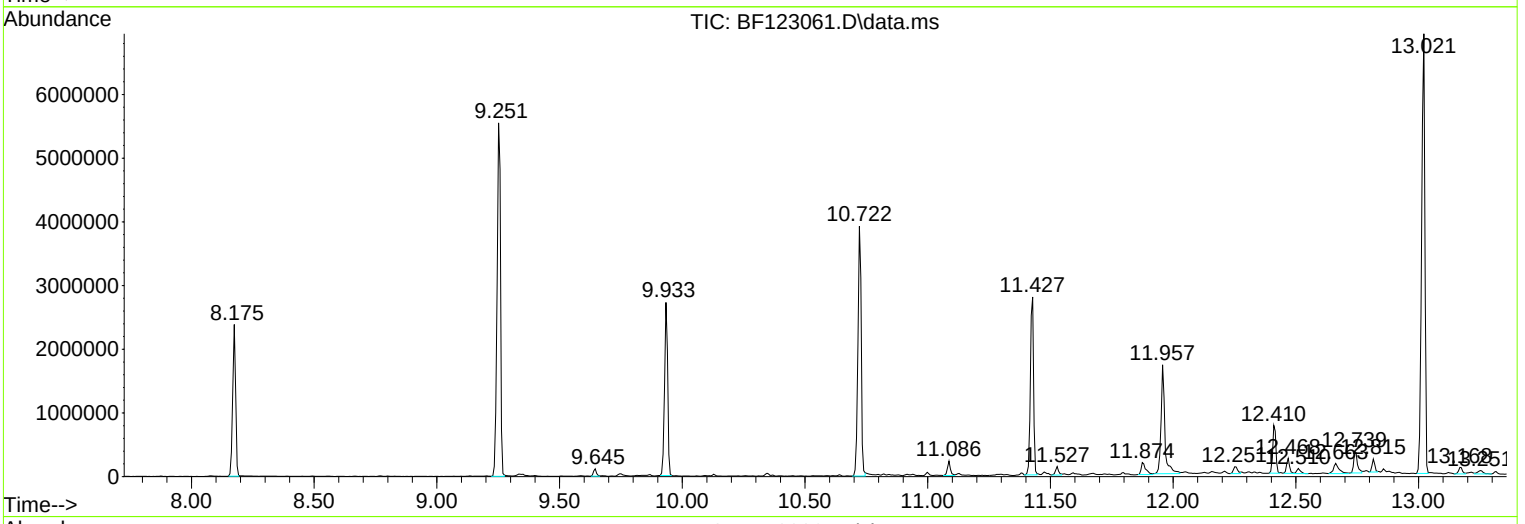
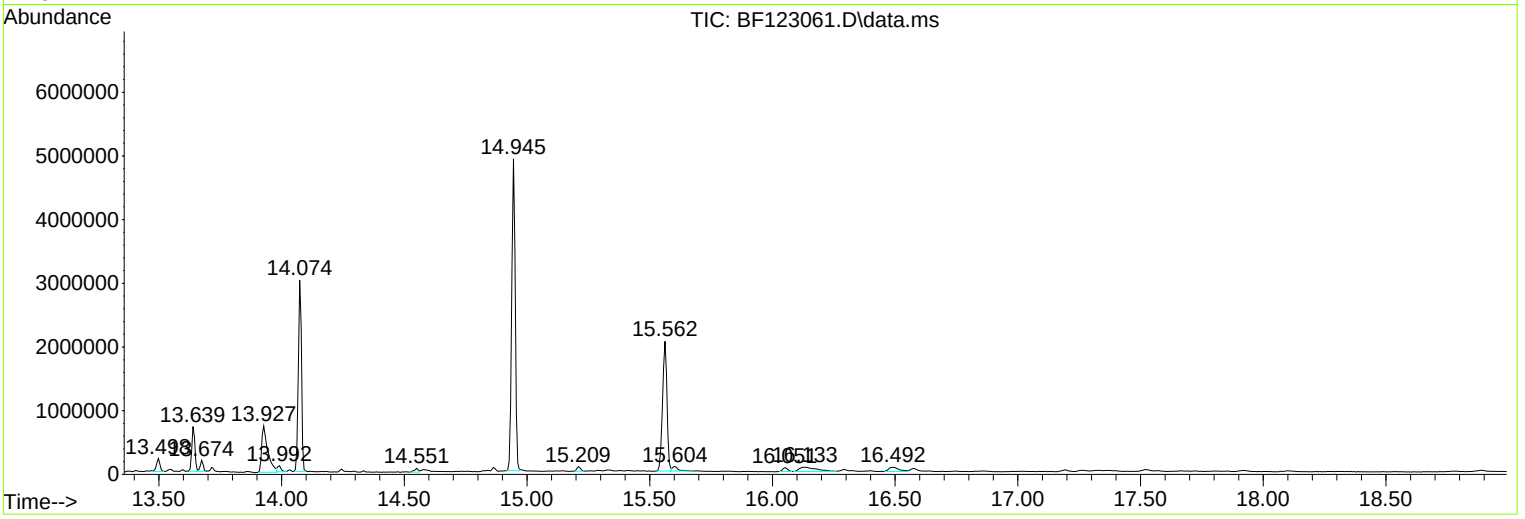
Instrument :
BNA_F
ClientSampleId :
PS1419LN

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012721.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 : BF123061.D
Acq On : 28 Jan 2021 16:02
Operator : JU/CG
Sample : M1236-08
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PS1419LN

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

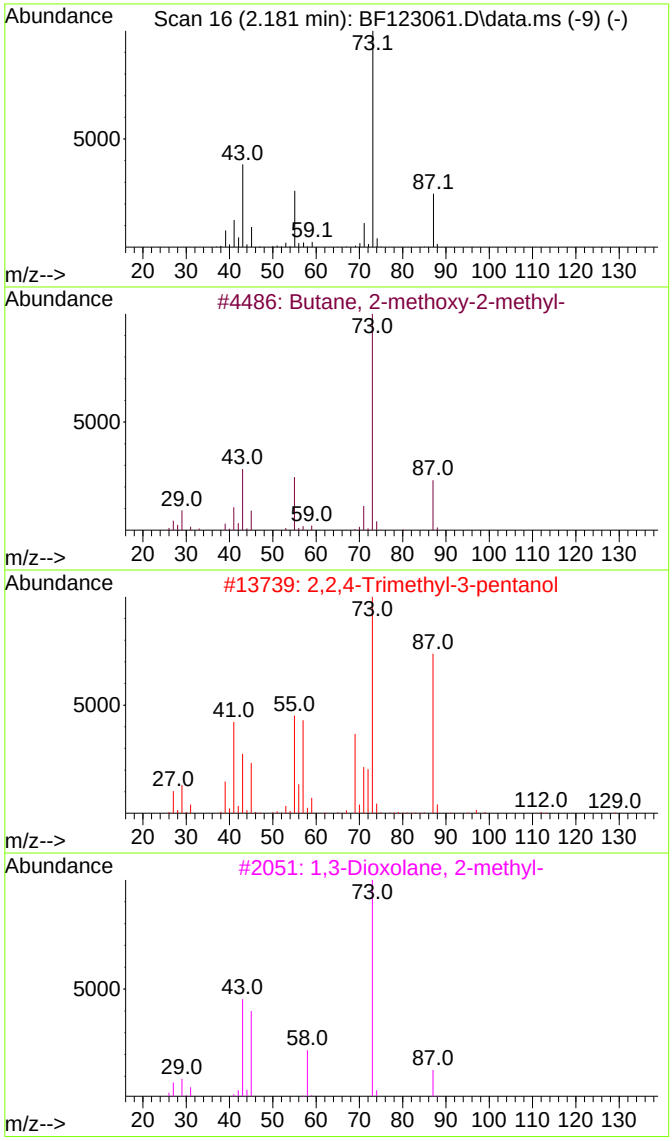
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

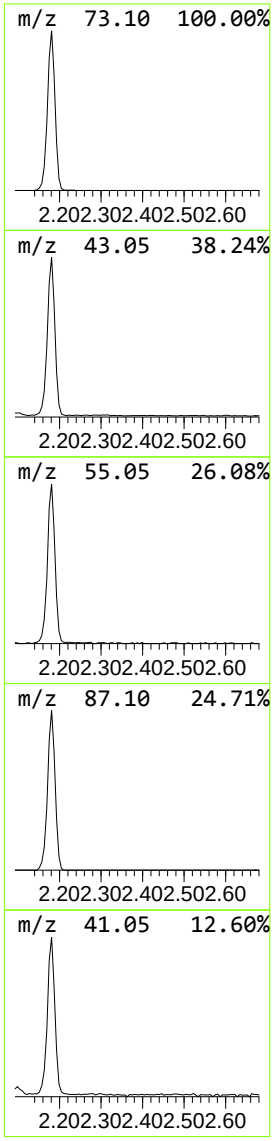
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.181	11.10 ng	834435	1,4-Dichlorobenzene-d4	6.892

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	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	16
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





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Operator : JU/CG
Sample : M1236-08
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PS1419LN

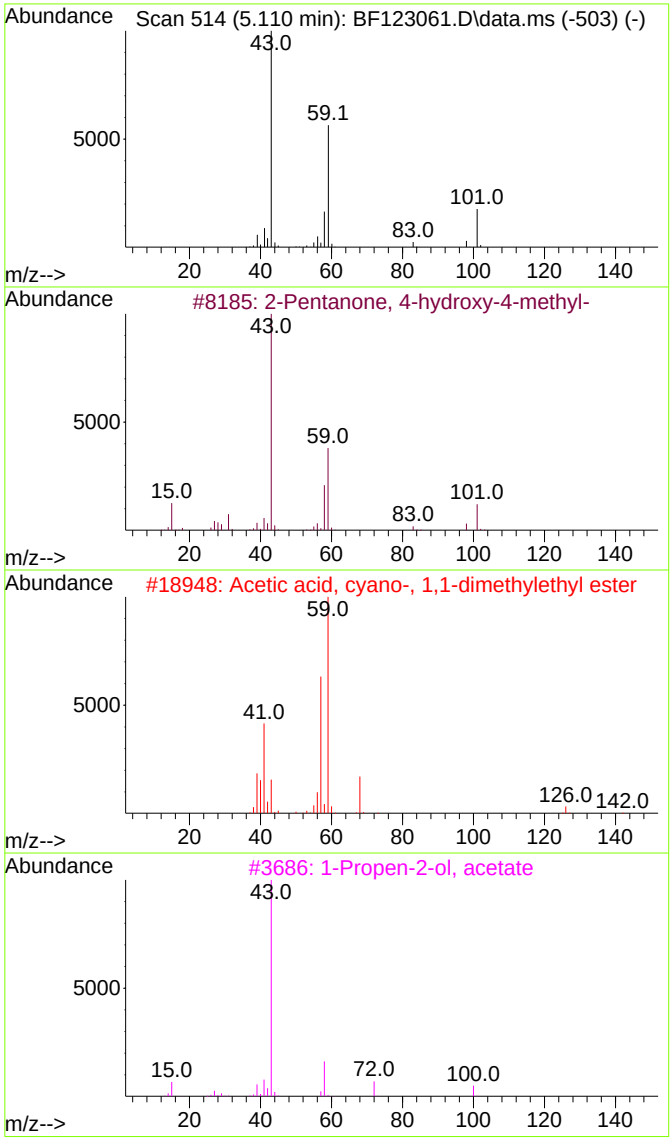
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

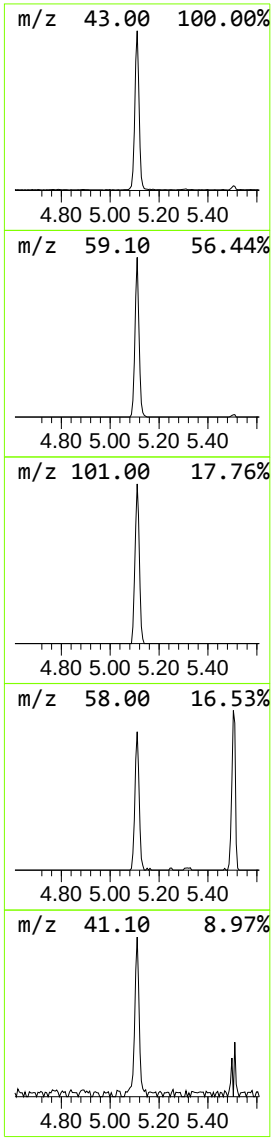
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.110	5.60 ng	421232	1,4-Dichlorobenzene-d4	6.892

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	Butane	58	C4H10	000106-97-8	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





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Data File : BF123061.D
Acq On : 28 Jan 2021 16:02
Operator : JU/CG
Sample : M1236-08
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PS1419LN

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

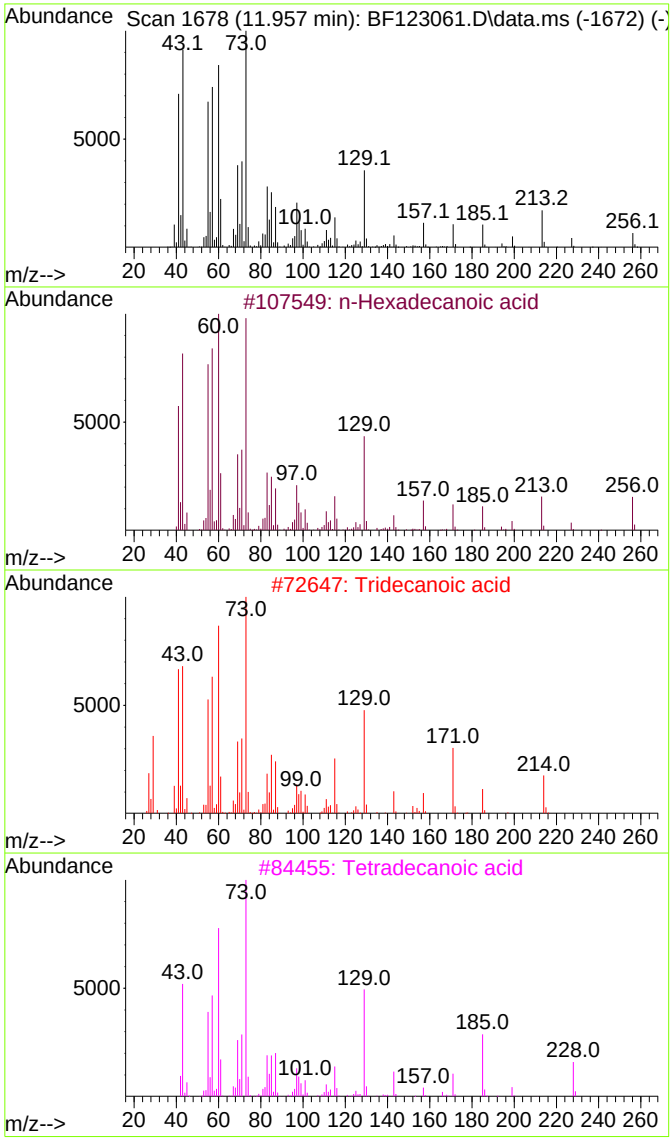
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

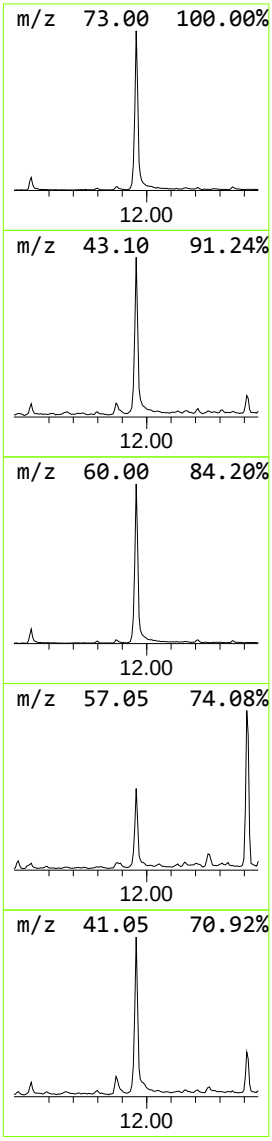
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.957	14.53 ng	1837540	Phenanthrene-d10	11.427

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	Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	20





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Operator : JU/CG
Sample : M1236-08
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PS1419LN

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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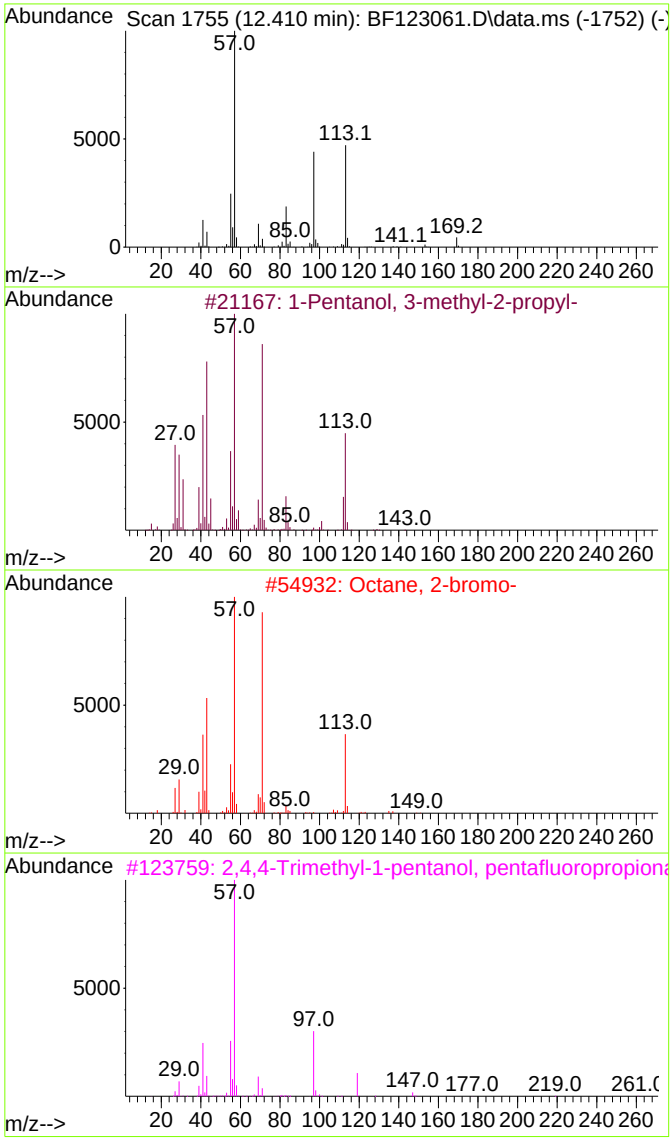
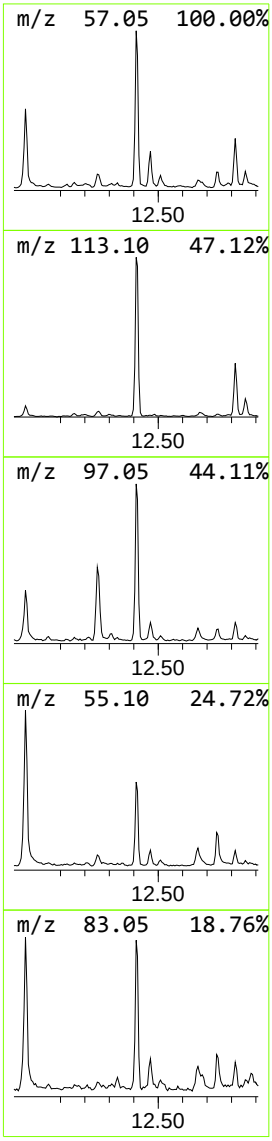
Peak Number 4 unknown12.41 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.410	5.24 ng	662277	Phenanthrene-d10	11.427

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, pent...	276	C11H17F5O2	1000365-51-0	37
4	2,4,4-Trimethyl-1-pentanol, trif...	226	C10H17F3O2	1000365-19-5	32
5	2,4,4,6,6,8,8-Heptamethyl-1-nonene	224	C16H32	015796-04-0	28





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Sample : M1236-08
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PS1419LN

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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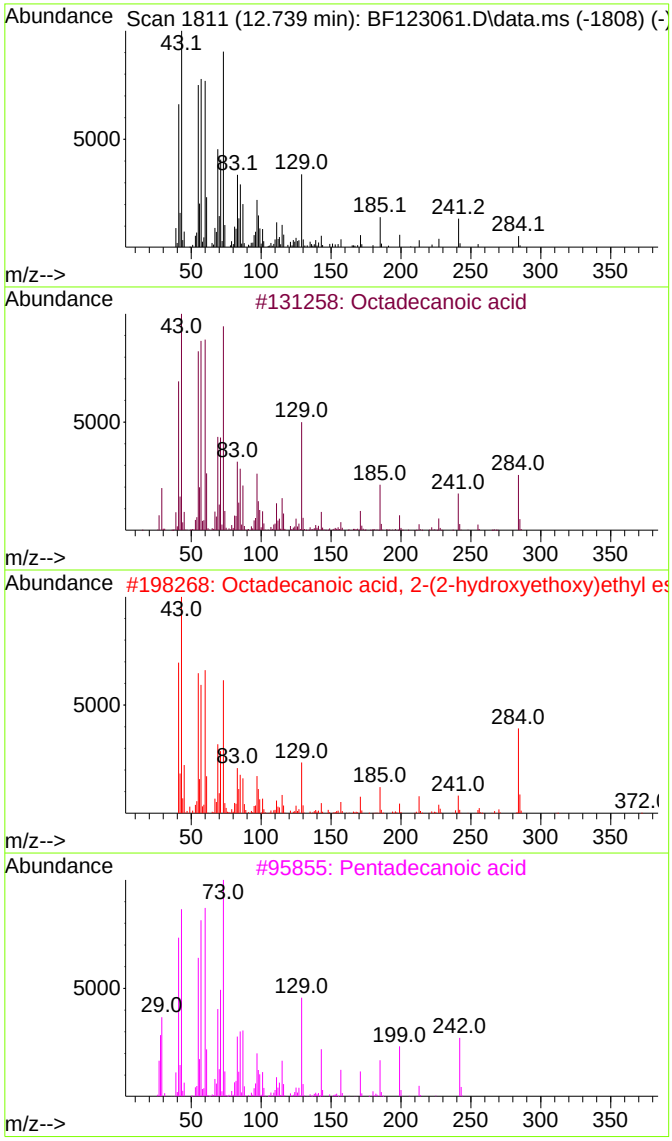
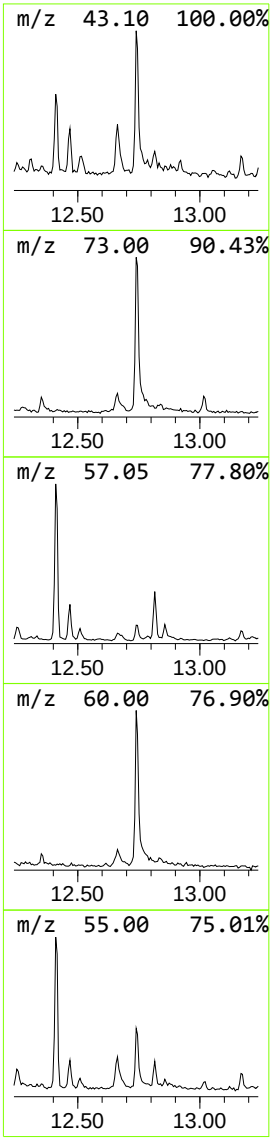
Peak Number 5 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.739	2.84 ng	359412	Phenanthrene-d10	11.427

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-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
5	Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	35





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Sample : M1236-08
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PS1419LN

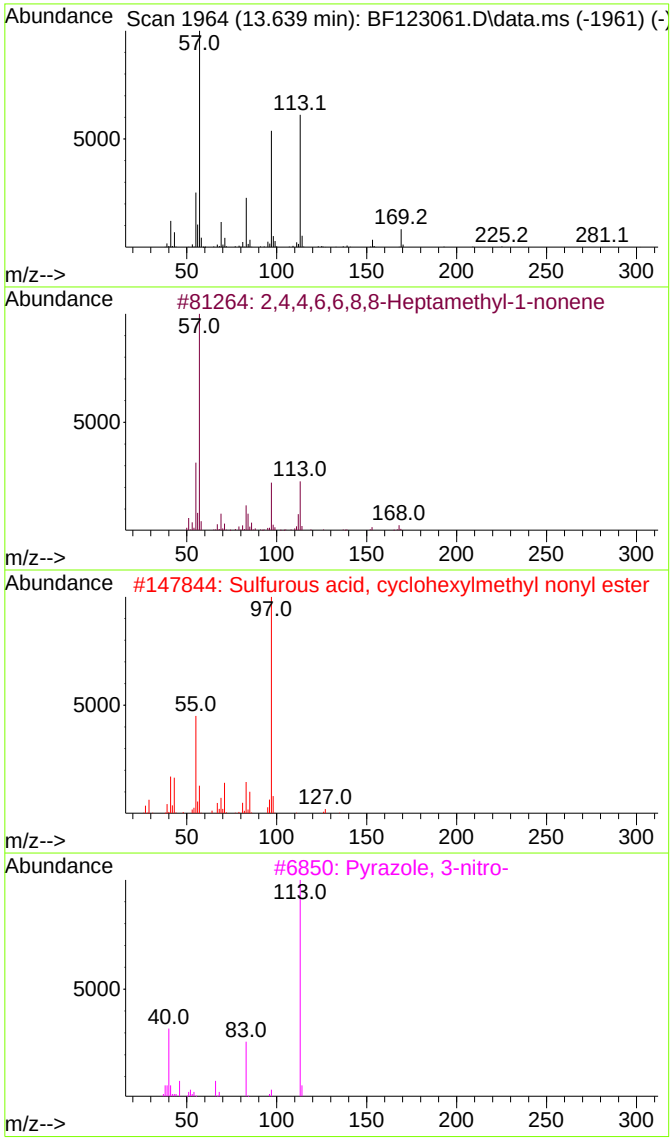
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

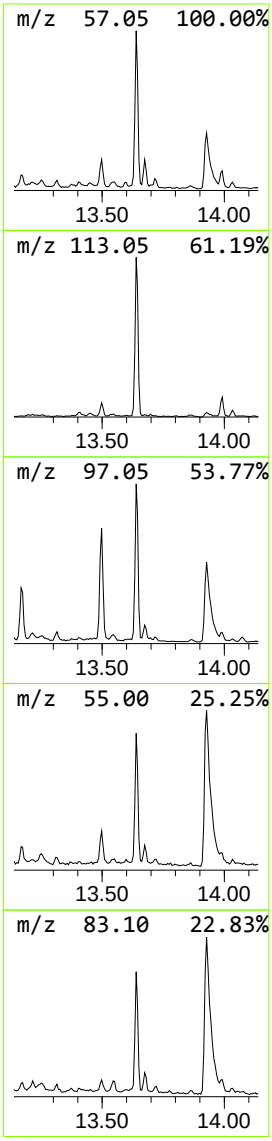
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 2,4,4,6,6,8,8-Heptamethyl-1... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.639	4.49 ng	609447	Chrysene-d12	14.074

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,4,6,6,8,8-Heptamethyl-1-nonene	224	C16H32	015796-04-0	83
2	Sulfurous acid, cyclohexylmethyl...	304	C16H32O3S	1000309-21-8	43
3	Pyrazole, 3-nitro-	113	C3H3N3O2	026621-44-3	38
4	Cyclohexane, (bromomethyl)-	176	C7H13Br	002550-36-9	35
5	Cyclopentanecarboxylic acid, 4-h...	338	C22H42O2	1000282-77-5	25





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Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012721.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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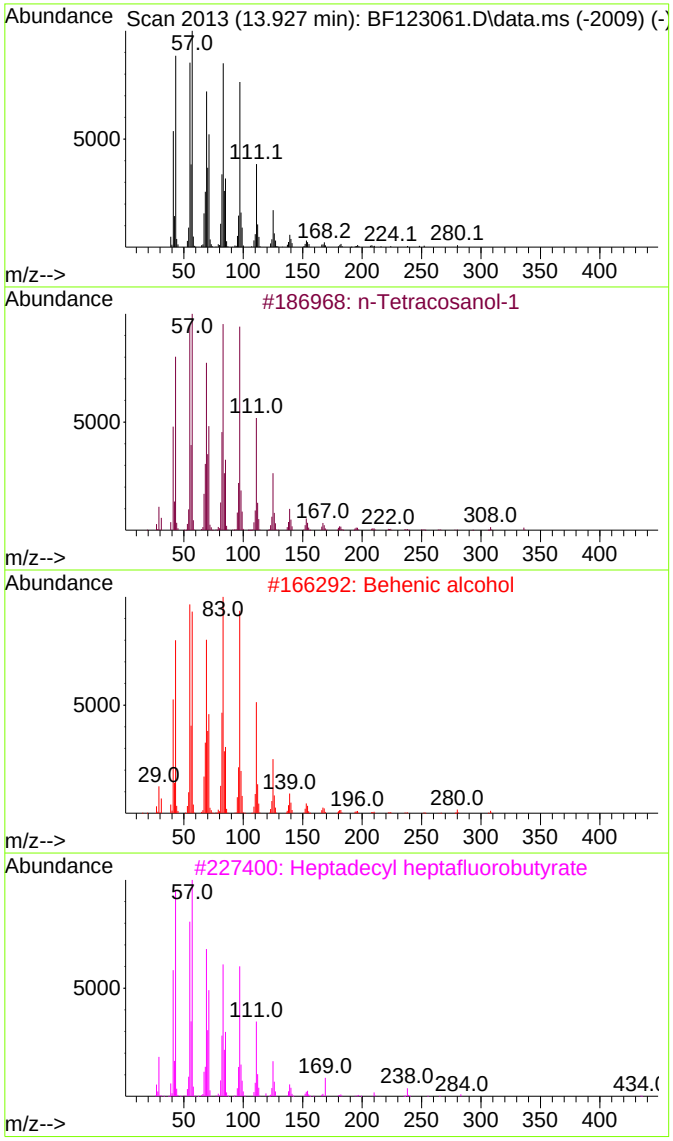
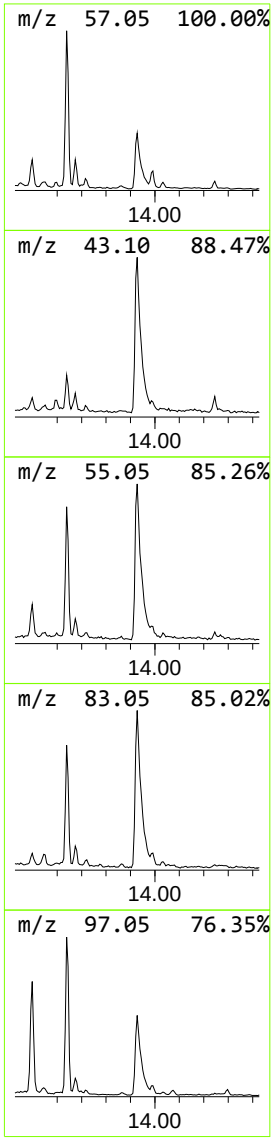
Peak Number 7 n-Tetracosanol-1 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.927	9.35 ng	1269800	Chrysene-d12	14.074

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
2	Behenic alcohol	326	C22H46O	000661-19-8	94
3	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
4	1-Heneicosanol	312	C21H44O	015594-90-8	93
5	Cyclopentadecane	210	C15H30	000295-48-7	93





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012821\
Data File : BF123061.D
Acq On : 28 Jan 2021 16:02
Operator : JU/CG
Sample : M1236-08
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PS1419LN

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012721.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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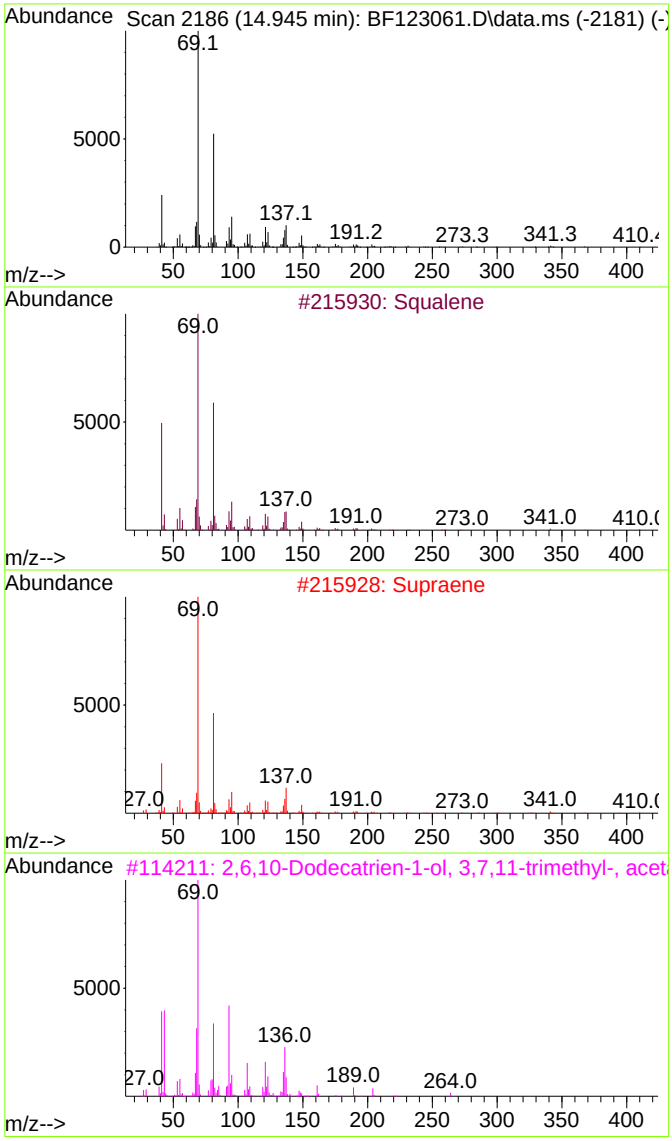
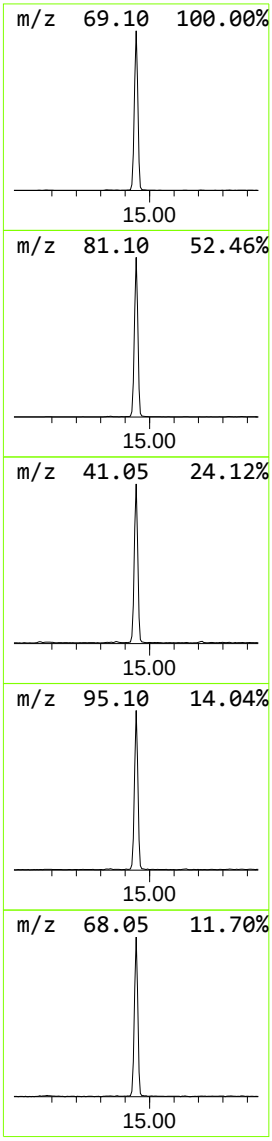
Peak Number 8 Squalene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.945	38.20 ng	4886440	Perylene-d12	15.562

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	91
2	Supraene	410	C30H50	007683-64-9	91
3	2,6,10-Dodecatrien-1-ol, 3,7,11-...	264	C17H28O2	004128-17-0	64
4	2,3,5-Trimethyl-2,3,5-hexanetric...	203	C12H17N3	003974-79-6	50
5	2,6-Octadiene, 4-methyl-	124	C9H16	074498-94-5	50





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Data File : BF123061.D
Acq On : 28 Jan 2021 16:02
Operator : JU/CG
Sample : M1236-08
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PS1419LN

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

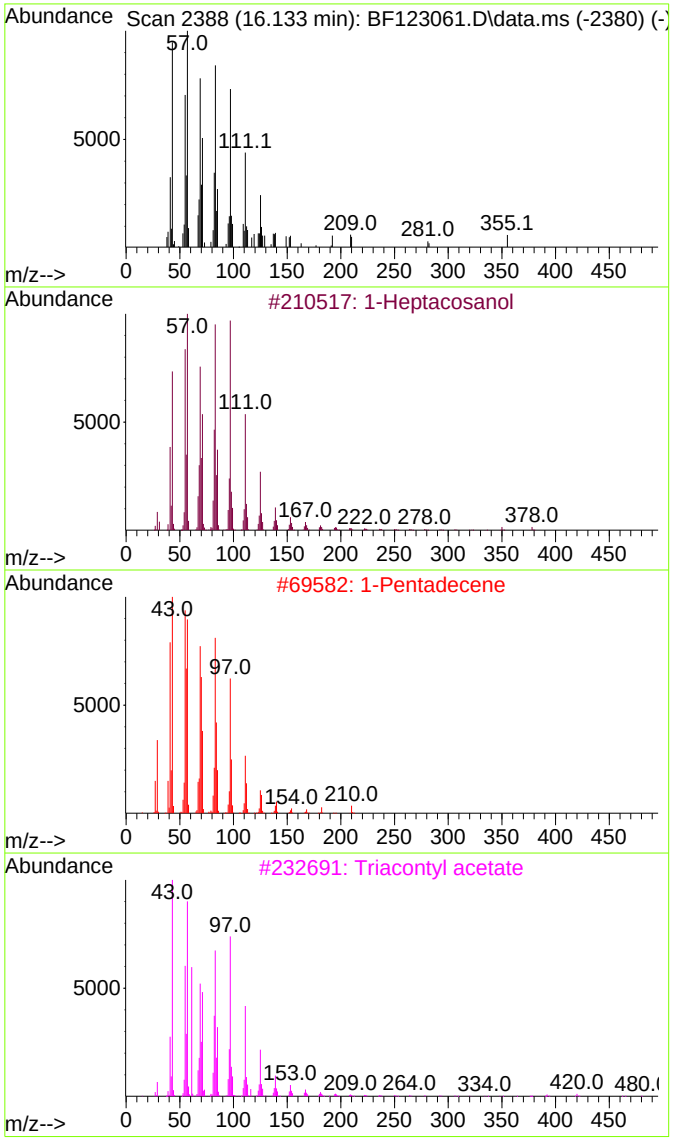
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

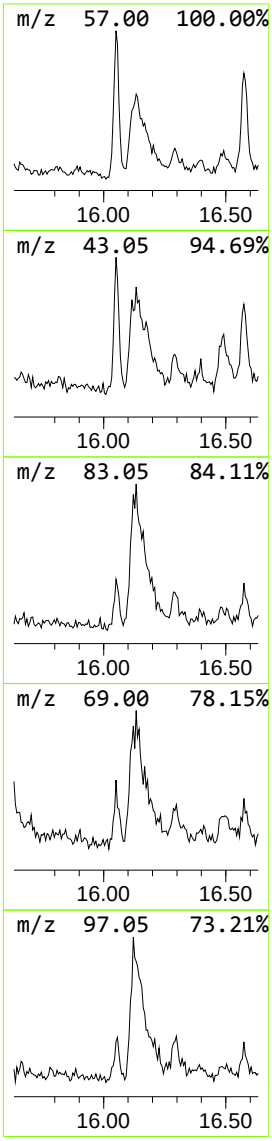
****

Peak Number 9 1-Heptacosanol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.133	2.49 ng	319132	Perylene-d12	15.562

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	92
2	1-Pentadecene	210	C15H30	013360-61-7	90
3	Triacontyl acetate	480	C32H64O2	041755-58-2	89
4	Behenic alcohol	326	C22H46O	000661-19-8	70
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	70





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012821\
Data File : BF123061.D
Acq On : 28 Jan 2021 16:02
Operator : JU/CG
Sample : M1236-08
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PS1419LN

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012721.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...	2.181	11.1	ng	834435	1	6.892	1503540	20.0
2-Pentanone, 4-...	5.110	5.6	ng	421232	1	6.892	1503540	20.0
n-Hexadecanoic ...	11.957	14.5	ng	1837540	4	11.427	2529760	20.0
unknown12.41	12.410	5.2	ng	662277	4	11.427	2529760	20.0
Octadecanoic acid	12.739	2.8	ng	359412	4	11.427	2529760	20.0
2,4,4,6,6,8,8-H...	13.639	4.5	ng	609447	5	14.074	2714950	20.0
n-Tetracosanol-1	13.927	9.3	ng	1269800	5	14.074	2714950	20.0
Squalene	14.945	38.2	ng	4886440	6	15.562	2558270	20.0
1-Heptacosanol	16.133	2.5	ng	319132	6	15.562	2558270	20.0