LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF092419\
Data File : BF117218.D
Acq On : 24 Sep 2019 16:27
Operator : JU
Sample : PB123339BL
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB123339BL

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-BF091319.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.116	3	5	15	rVB	291851	316497	22.77%	3.103%
2	5.445	567	571	574	rBV	995744	897715	64.58%	8.801%
3	6.457	738	743	746	rBV	984593	1005079	72.30%	9.853%
4	6.586	761	765	768	rBV	1167130	1077285	77.50%	10.561%
5	6.810	800	803	815	rBB	216736	203615	14.65%	1.996%
6	6.969	826	830	834	rBV	898855	791115	56.91%	7.756%
7	7.375	895	899	917	rBV	575066	641823	46.17%	6.292%
8	8.092	1017	1021	1036	rBV	238985	257410	18.52%	2.523%
9	9.169	1199	1204	1207	rBV	1474818	1244302	89.51%	12.198%
10	9.563	1267	1271	1280	rBV	79929	76292	5.49%	0.748%
11	9.845	1315	1319	1332	rBB	331510	302655	21.77%	2.967%
12	10.639	1450	1454	1464	rBV	850604	801192	57.64%	7.854%
13	11.333	1568	1572	1581	rBV	293596	285246	20.52%	2.796%
14	11.857	1658	1661	1669	rBV2	30216	35858	2.58%	0.352%
15	12.416	1751	1756	1764	rBV5	17030	42885	3.09%	0.420%
16	12.921	1837	1842	1845	rBV	1468876	1390104	100.00%	13.628%
17	13.798	1988	1991	1994	rBV2	12249	16408	1.18%	0.161%
18	13.833	1994	1997	2014	rVV3	57899	142190	10.23%	1.394%
19	13.974	2017	2021	2031	rVB	204166	205074	14.75%	2.010%
20	14.427	2094	2098	2105	rBV	20683	21252	1.53%	0.208%
21	14.727	2143	2149	2157	rVB	37904	41178	2.96%	0.404%
22	15.057	2201	2205	2213	rVB	48233	55983	4.03%	0.549%
23	15.427	2262	2268	2279	rBV	154697	217059	15.61%	2.128%
24	15.851	2330	2340	2346	rBV2	42160	66619	4.79%	0.653%
25	16.333	2414	2422	2430	rBV3	26159	50889	3.66%	0.499%
26	16.909	2515	2520	2526	rVB3	8106	14829	1.07%	0.145%

Sum of corrected areas: 10200554

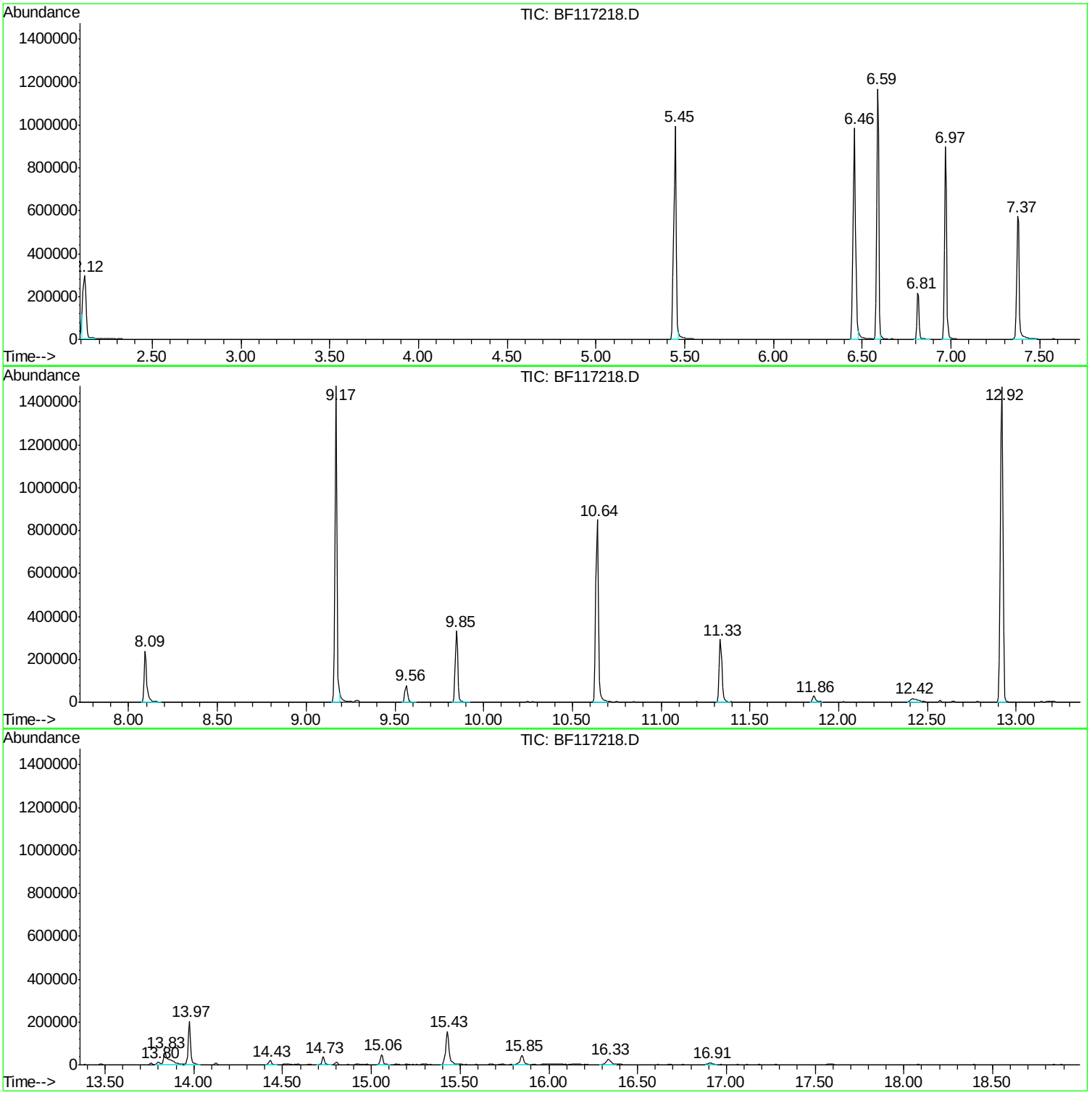
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF092419\
Data File : BF117218.D
Acq On : 24 Sep 2019 16:27
Operator : JU
Sample : PB123339BL
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB123339BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

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Data File : BF117218.D
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Instrument : BNA_F
ClientSampleId : PB123339BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

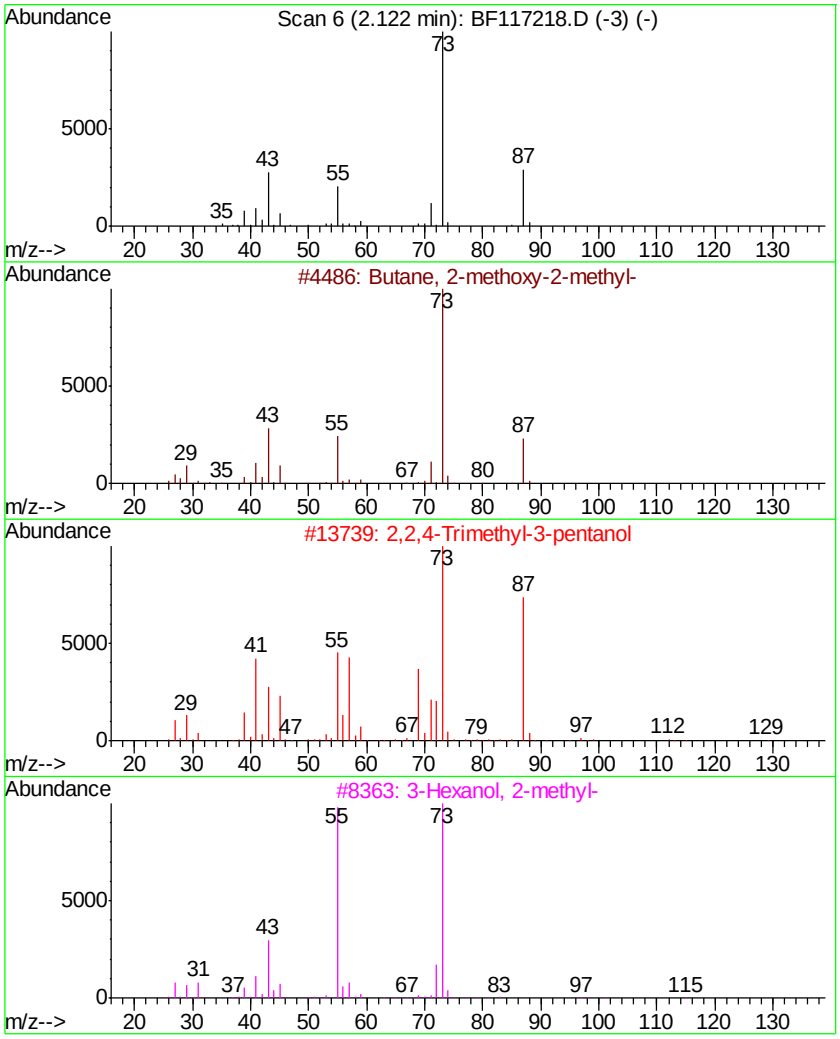
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

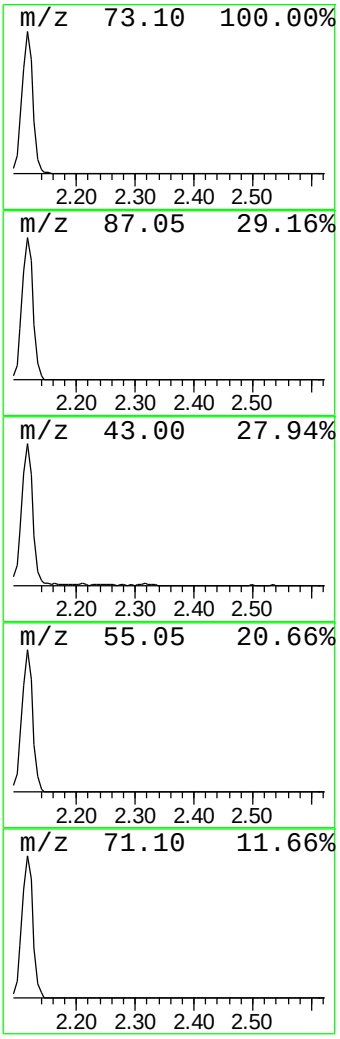
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.12	31.09 ng	316497	1,4-Dichlorobenzene-d4	6.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	17
4	1,4-Butanediamine	88	C4H12N2	000110-60-1	9
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





Library Search Compound Report

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Data File : BF117218.D
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Operator : JU
Sample : PB123339BL
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB123339BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.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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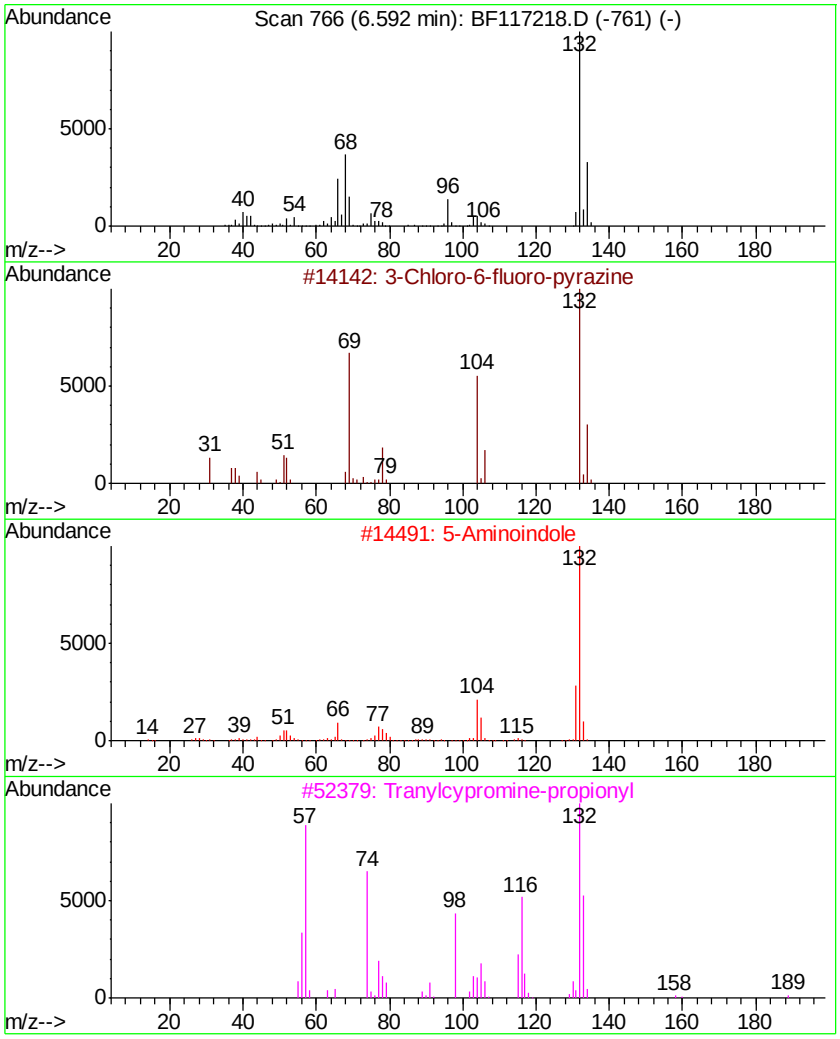
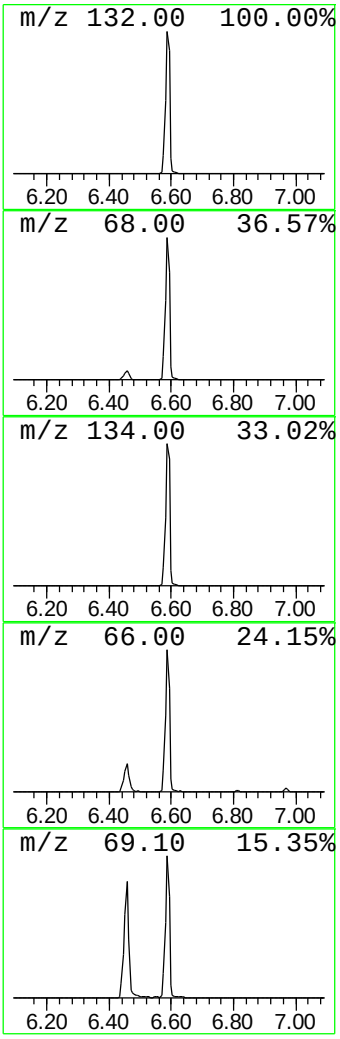
Peak Number 2 unknown6.59 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.59	105.82 ng	1077290	1,4-Dichlorobenzene-d4	6.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	1,2,4-Trifluorobenzene	132	C6H3F3	000367-23-7	9





Library Search Compound Report

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Data File : BF117218.D
Acq On : 24 Sep 2019 16:27
Operator : JU
Sample : PB123339BL
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB123339BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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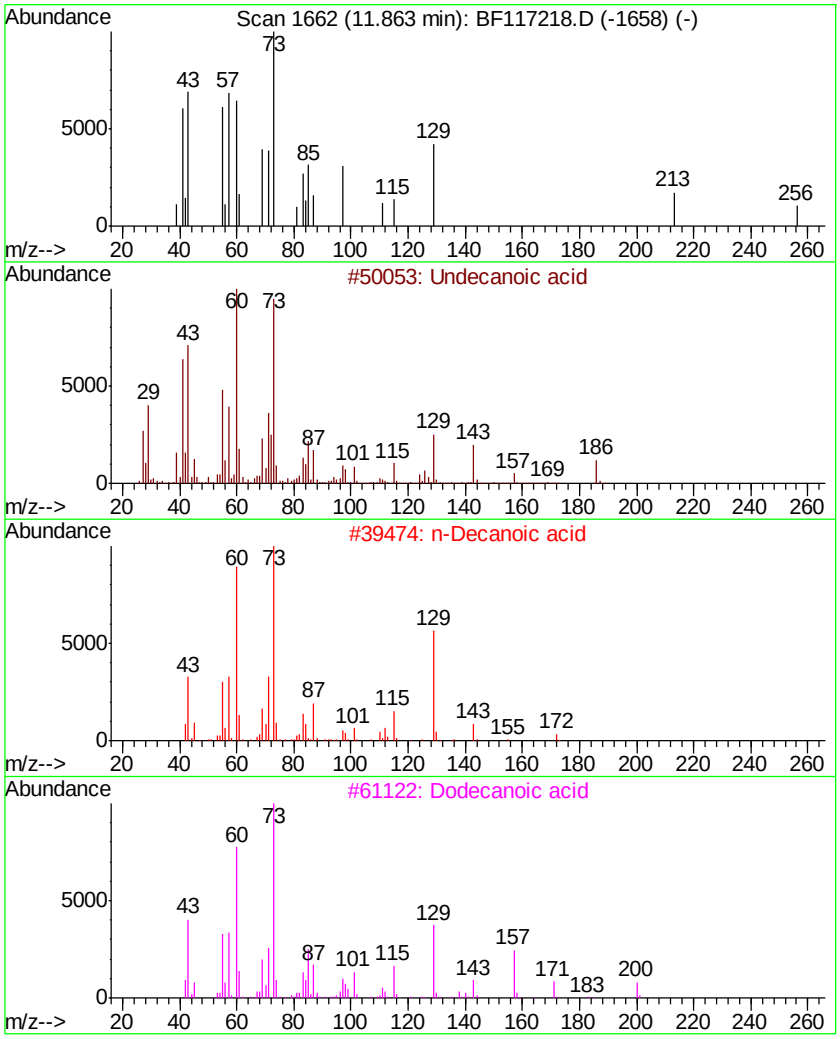
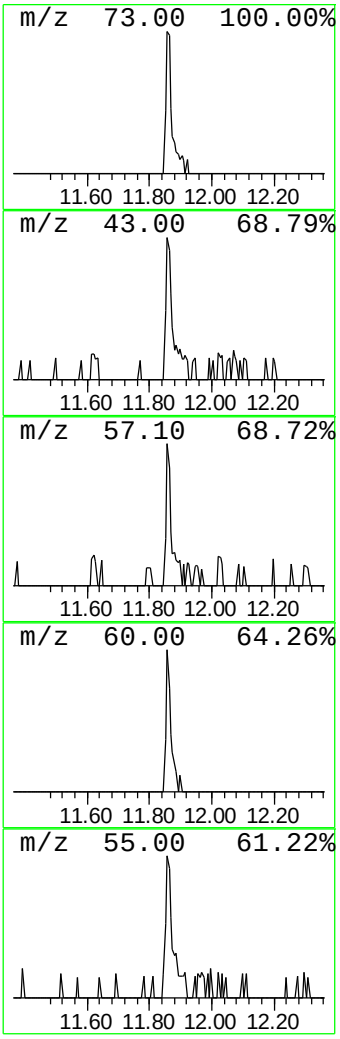
Peak Number 4 Undecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.86	2.51 ng	35858	Phenanthrene-d10	11.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecanoic acid	186	C11H22O2	000112-37-8	64
2	n-Decanoic acid	172	C10H20O2	000334-48-5	53
3	Dodecanoic acid	200	C12H24O2	000143-07-7	53
4	Maltose	342	C12H22O11	000069-79-4	38
5	.beta.-D-Mannofuranoside, 1-O-(1...	332	C17H32O6	1000155-29-9	22





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF092419\
Data File : BF117218.D
Acq On : 24 Sep 2019 16:27
Operator : JU
Sample : PB123339BL
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB123339BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

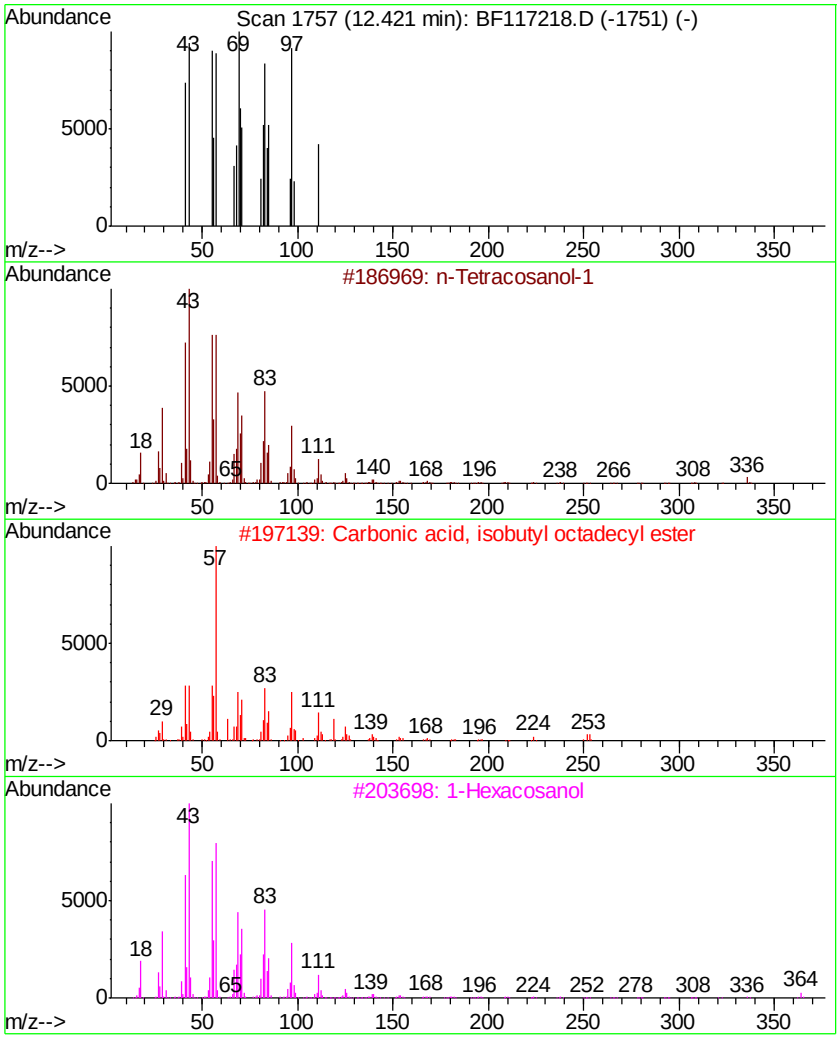
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

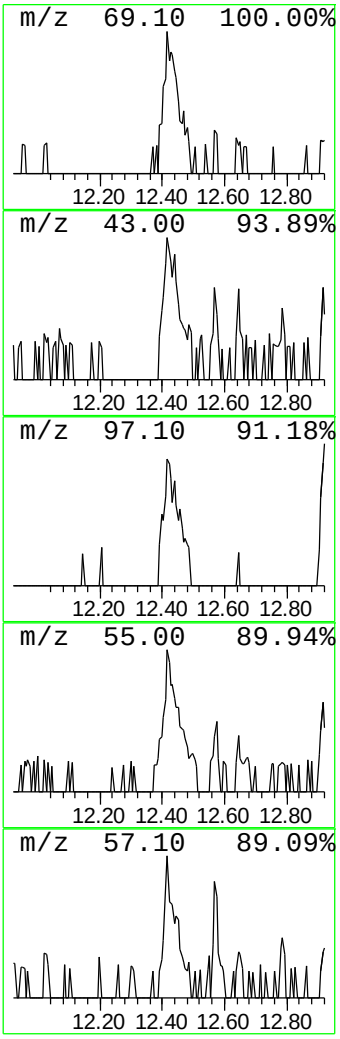
****

Peak Number 5 n-Tetracosanol-1 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.42	3.01 ng	42885	Phenanthrene-d10	11.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	59
2	Carbonic acid, isobutyl octadecy...	370	C23H46O3	1000314-61-5	53
3	1-Hexacosanol	382	C26H54O	000506-52-5	50
4	Cyclopentane, (2-methylbutyl)-	140	C10H20	053366-38-4	47
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	47





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF092419\
Data File : BF117218.D
Acq On : 24 Sep 2019 16:27
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Sample : PB123339BL
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB123339BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

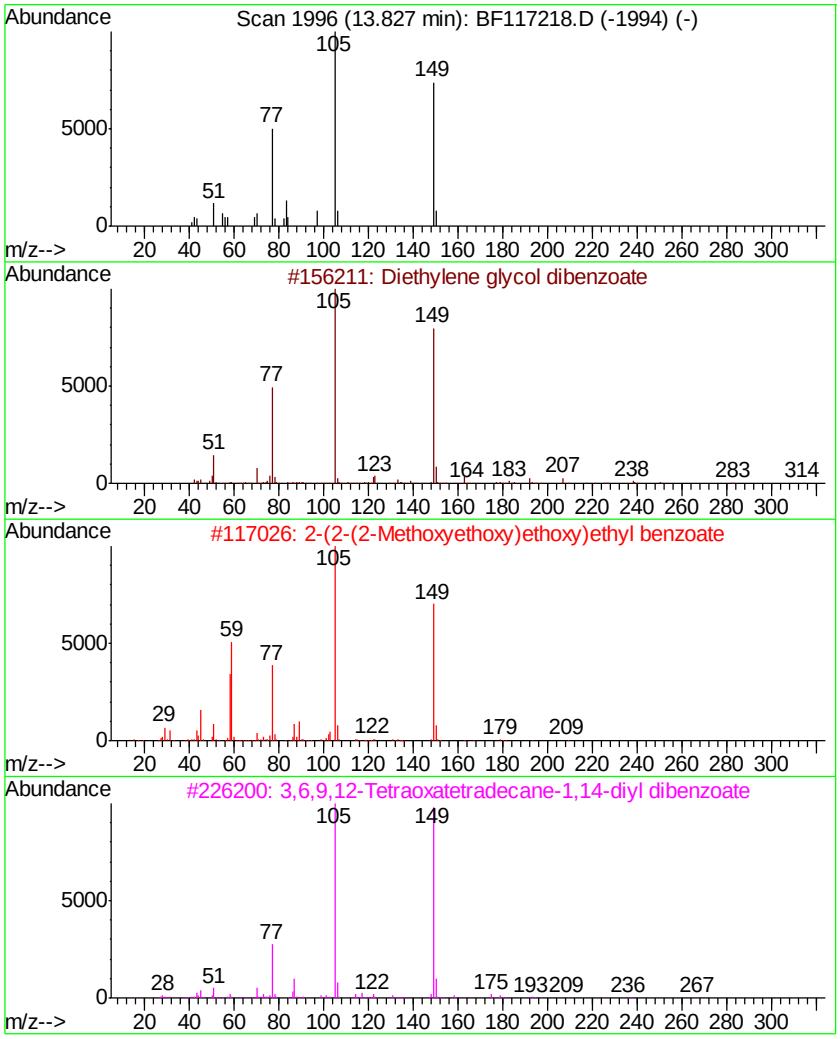
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

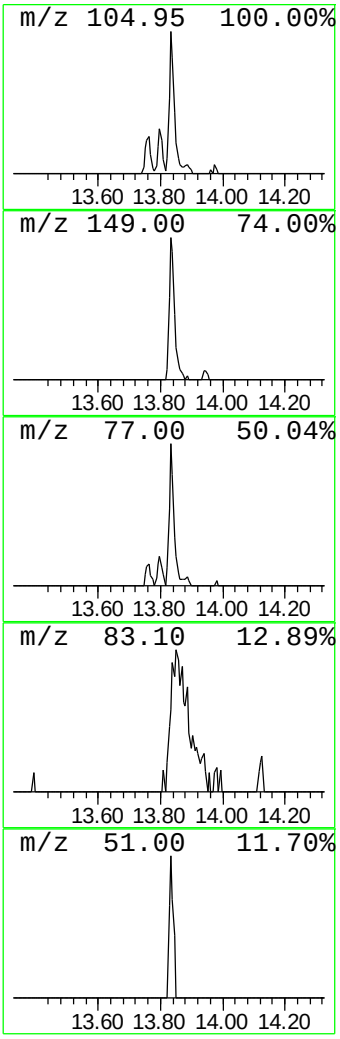
****

Peak Number 6 Diethylene glycol dibenzoate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	13.87 ng	142190	Chrysene-d12	13.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	72
2	2-(2-(2-Methoxyethoxy)ethoxy)eth...	268	C14H20O5	1000366-99-1	72
3	3,6,9,12-Tetraoxatetradecane-1,1...	446	C24H30O8	1000366-97-0	64
4	1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	64
5	2,2'-(Ethane-1,2-diylbis(oxy))bi...	358	C20H22O6	1000366-99-4	59





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF092419\
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Sample : PB123339BL
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB123339BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

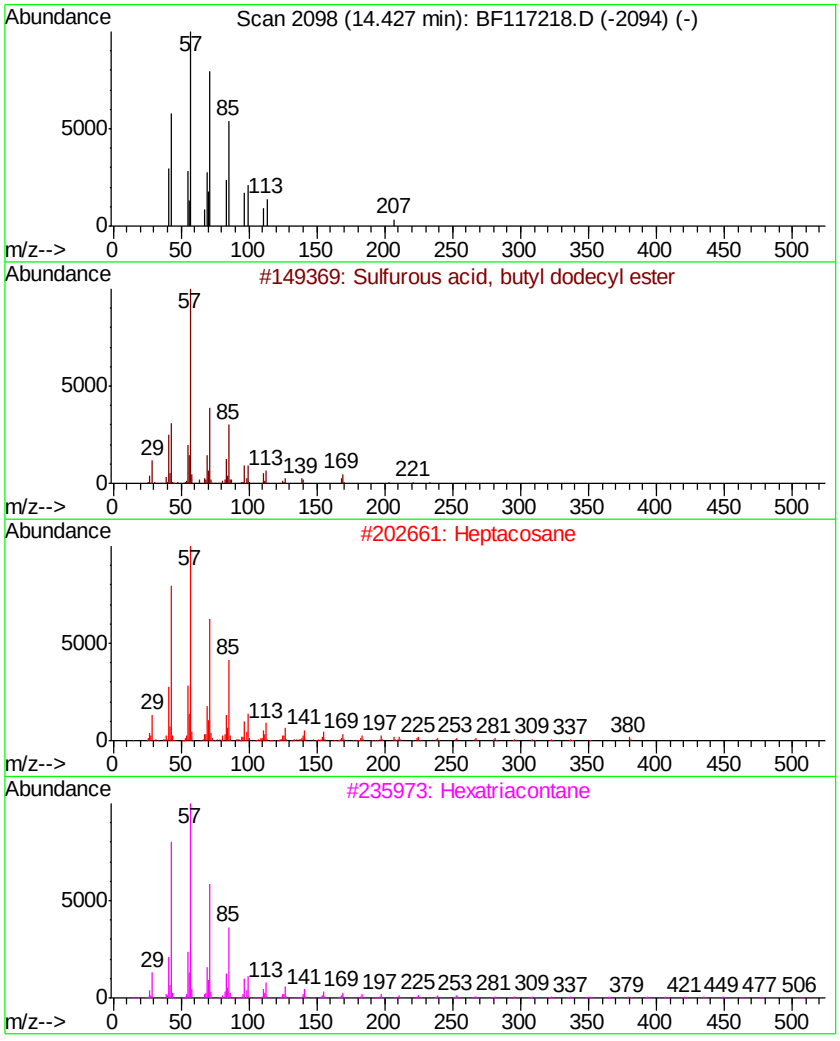
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

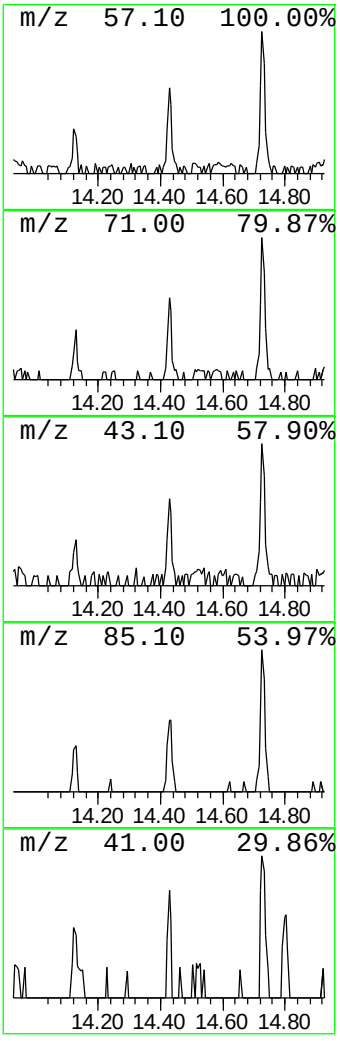
****

Peak Number 7 Sulfurous acid, butyl dodec... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.43	2.07 ng	21252	Chrysene-d12	13.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	86
2	Heptacosane	380	C27H56	000593-49-7	83
3	Hexatriacontane	507	C36H74	000630-06-8	83
4	Sulfurous acid, butyl tridecyl e...	320	C17H36O3S	1000309-18-0	78
5	Triacontane	422	C30H62	000638-68-6	72





Library Search Compound Report

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Data File : BF117218.D
Acq On : 24 Sep 2019 16:27
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Sample : PB123339BL
Misc :
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Instrument : BNA_F
ClientSampleId : PB123339BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

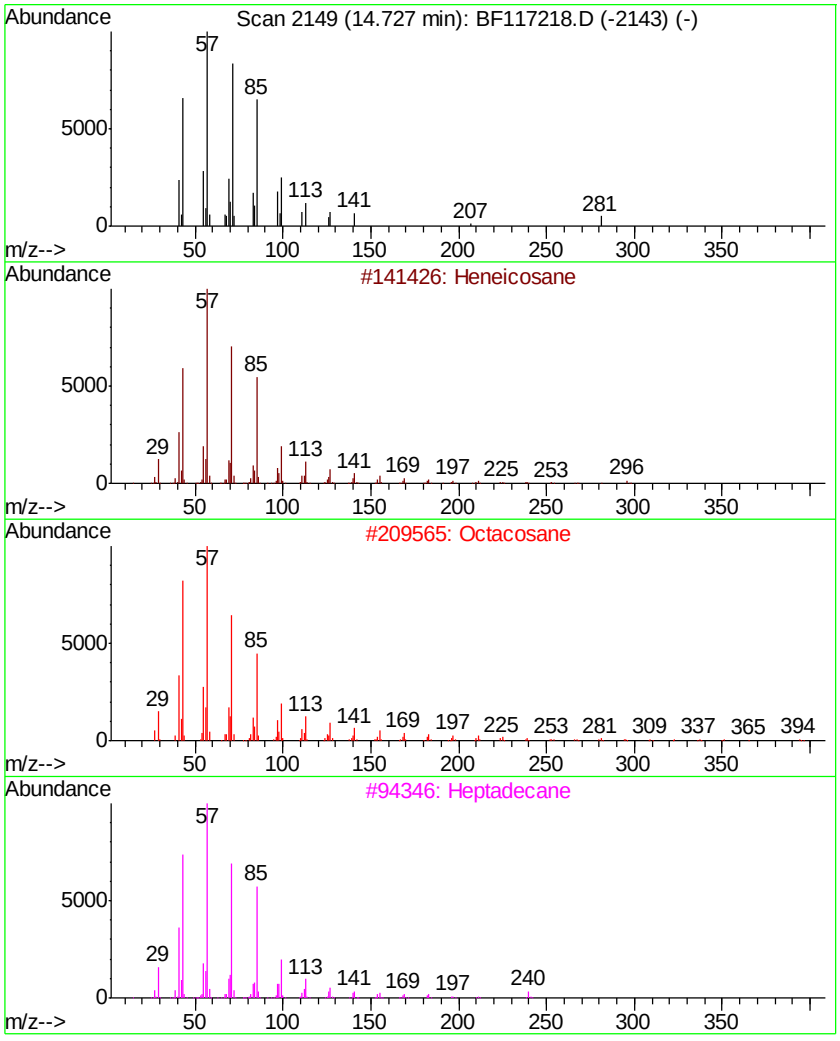
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

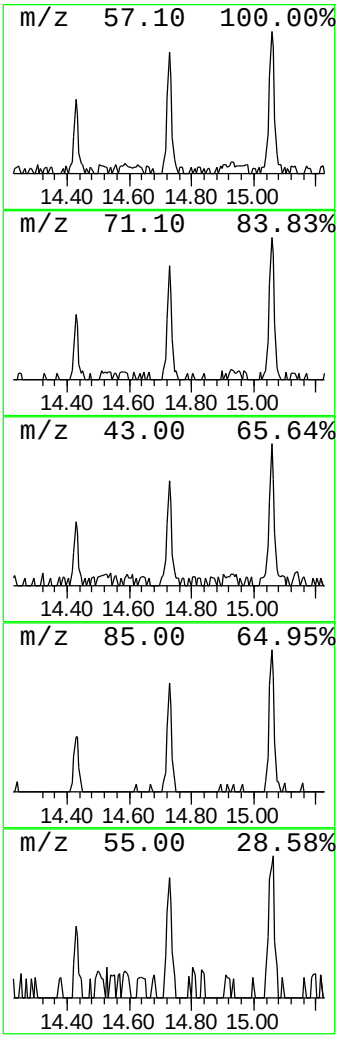
****

Peak Number 8 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.73	3.79 ng	41178	Perylene-d12	15.43

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	90
2	Octacosane	394	C28H58	000630-02-4	90
3	Heptadecane	240	C17H36	000629-78-7	90
4	2-methyloctacosane	408	C29H60	1000376-72-8	90
5	Hexacosane	366	C26H54	000630-01-3	86





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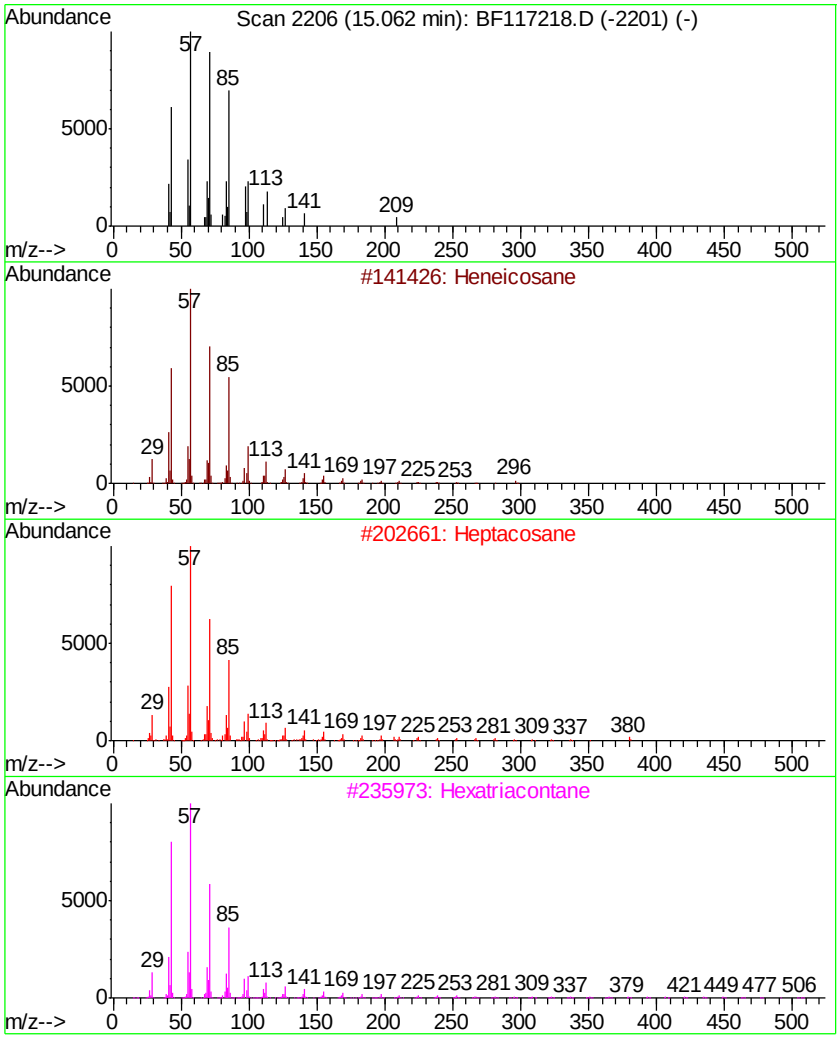
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

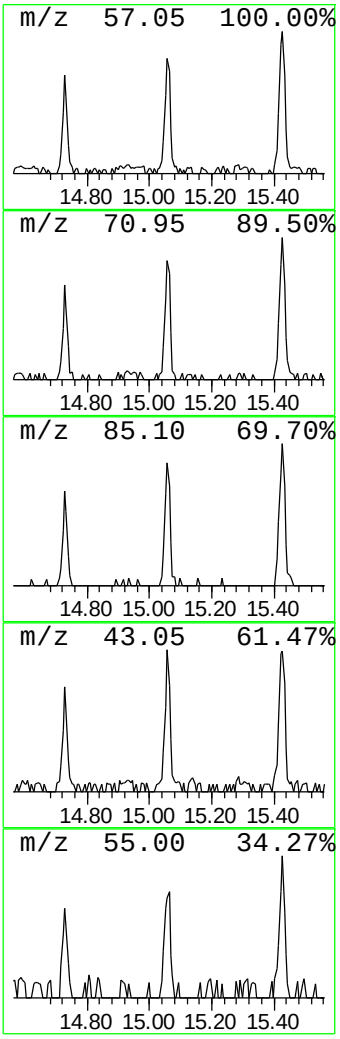
****

Peak Number 9 Heptacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.06	5.16 ng	55983	Perylene-d12	15.43

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Heptacosane	380	C27H56	000593-49-7	87
3	Hexatriacontane	507	C36H74	000630-06-8	86
4	2-methyloctacosane	408	C29H60	1000376-72-8	86
5	Hexacosane	366	C26H54	000630-01-3	86





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Instrument : BNA_F
ClientSampleId : PB123339BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.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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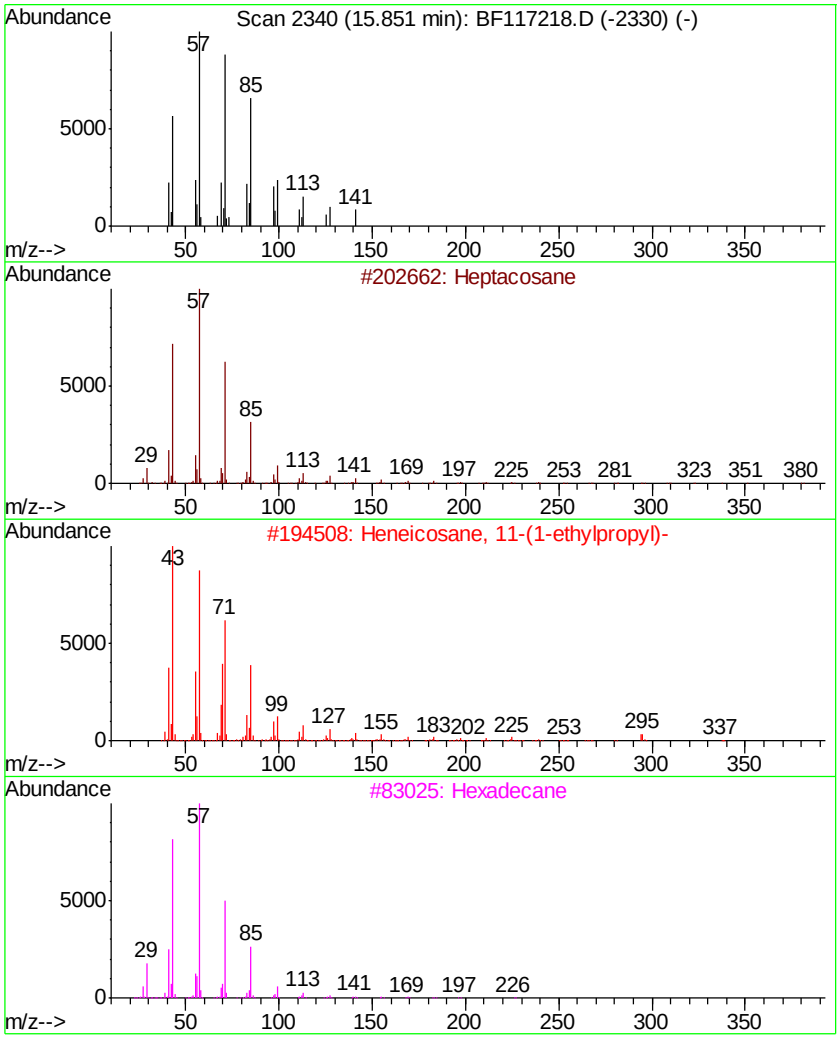
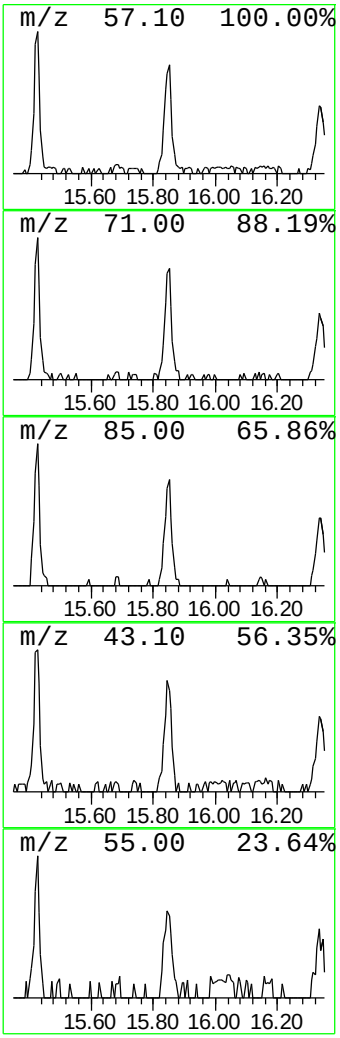
Peak Number 10 Hexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.85	6.14 ng	66619	Perylene-d12	15.43

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	78
2	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	78
3	Hexadecane	226	C16H34	000544-76-3	72
4	Hexacosane	366	C26H54	000630-01-3	72
5	Tetracosane	338	C24H50	000646-31-1	64





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF092419\
Data File : BF117218.D
Acq On : 24 Sep 2019 16:27
Operator : JU
Sample : PB123339BL
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB123339BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.M
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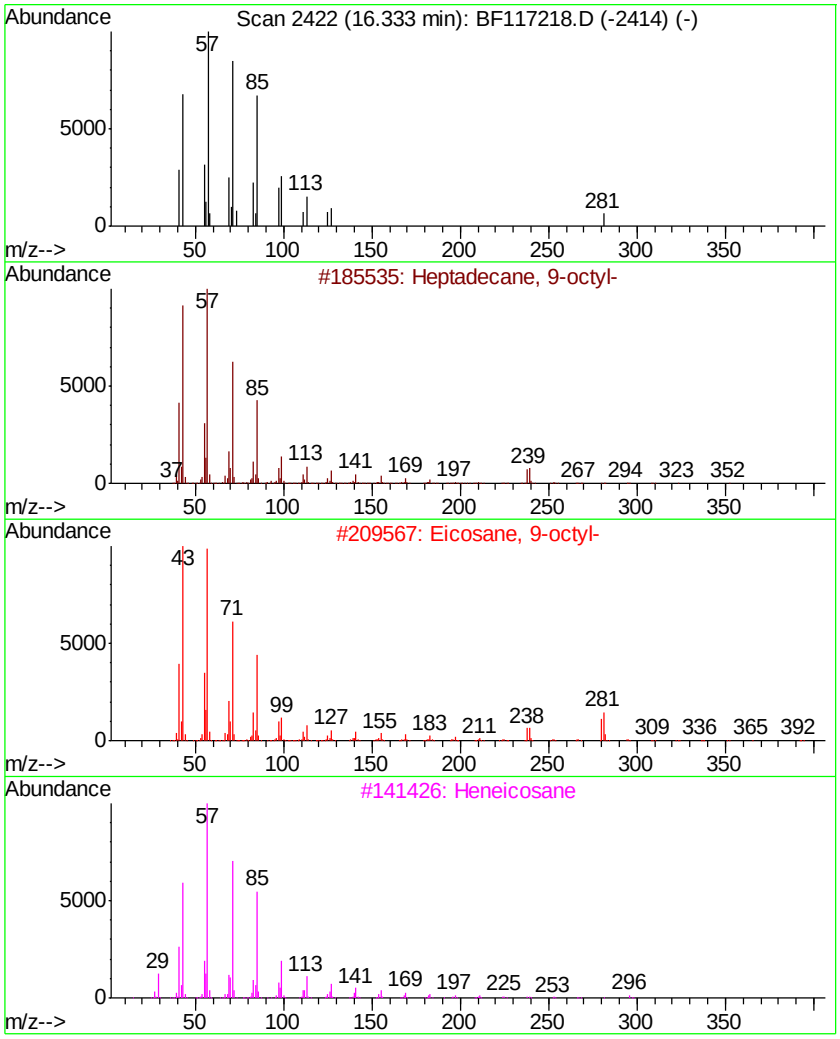
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

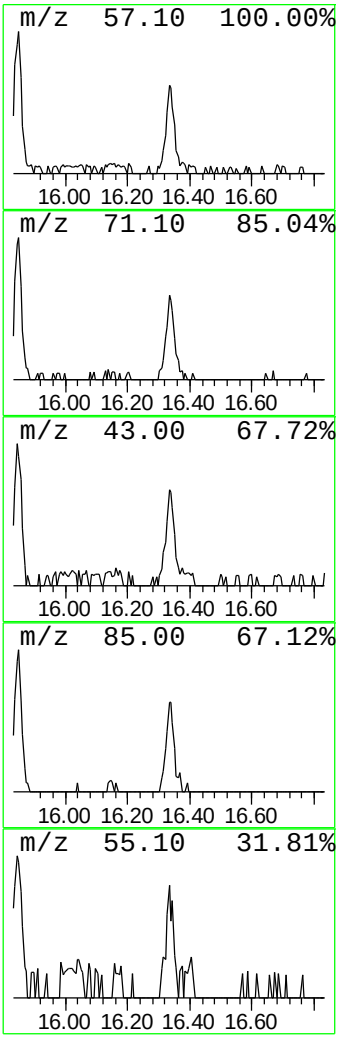
****

Peak Number 11 Heptadecane, 9-octyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.33	4.69 ng	50889	Perylene-d12	15.43

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	72
2	Eicosane, 9-octyl-	394	C28H58	013475-77-9	72
3	Heneicosane	296	C21H44	000629-94-7	72
4	Triacontane	422	C30H62	000638-68-6	64
5	Sulfurous acid, butyl undecyl ester	292	C15H32O3S	1000309-17-8	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF092419\
Data File : BF117218.D
Acq On : 24 Sep 2019 16:27
Operator : JU
Sample : PB123339BL
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB123339BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.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-methoxy...	2.12	31.1	ng	316497	1	6.81	203615	20.0
unknown6.59	6.59	105.8	ng	1077290	1	6.81	203615	20.0
Undecanoic acid	11.86	2.5	ng	35858	4	11.33	285246	20.0
n-Tetracosanol-1	12.42	3.0	ng	42885	4	11.33	285246	20.0
Diethylene glycol...	13.83	13.9	ng	142190	5	13.97	205074	20.0
Sulfurous acid, b...	14.43	2.1	ng	21252	5	13.97	205074	20.0
Heneicosane	14.73	3.8	ng	41178	6	15.43	217059	20.0
Heptacosane	15.06	5.2	ng	55983	6	15.43	217059	20.0
Hexadecane	15.85	6.1	ng	66619	6	15.43	217059	20.0
Heptadecane, 9-oc...	16.33	4.7	ng	50889	6	15.43	217059	20.0