LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100319\
Data File : BF117317.D
Acq On : 3 Oct 2019 15:40
Operator : JU
Sample : PB123339BL
Misc :
ALS Vial : 3 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	5.434	565	569	591	rBV	1032829	1133537	65.82%	8.326%
2	6.451	737	742	759	rBV	1066579	1334172	77.47%	9.799%
3	6.581	759	764	773	rVV	1427512	1352519	78.54%	9.934%
4	6.804	798	802	812	rVB	311987	301417	17.50%	2.214%
5	6.957	824	828	837	rBV	1044935	1022530	59.38%	7.510%
6	7.369	893	898	916	rBV	659123	830179	48.21%	6.098%
7	8.086	1015	1020	1043	rBV	311548	404768	23.50%	2.973%
8	9.157	1197	1202	1219	rBV	1671827	1722094	100.00%	12.649%
9	9.551	1265	1269	1281	rBB	70531	69014	4.01%	0.507%
10	9.839	1313	1318	1331	rBV	455636	489334	28.42%	3.594%
11	10.627	1448	1452	1468	rBV	835435	936801	54.40%	6.881%
12	11.321	1567	1570	1589	rBV	410288	465189	27.01%	3.417%
13	12.904	1835	1839	1850	rBV	1582836	1599762	92.90%	11.750%
14	13.468	1928	1935	1938	rBV2	25053	23803	1.38%	0.175%
15	13.798	1985	1991	1993	rBV3	62283	74682	4.34%	0.549%
16	13.968	2016	2020	2027	rBV	312411	338003	19.63%	2.483%
17	14.110	2039	2044	2048	rBV	63498	65751	3.82%	0.483%
18	14.415	2091	2096	2100	rBV	124874	113736	6.60%	0.835%
19	14.715	2142	2147	2155	rBV	179190	193143	11.22%	1.419%
20	14.786	2155	2159	2163	rBV2	17830	17466	1.01%	0.128%
21	15.045	2197	2203	2209	rBV	203937	240433	13.96%	1.766%
22	15.415	2260	2266	2280	rBV2	293879	517849	30.07%	3.804%
23	15.833	2329	2337	2344	rBV	124291	199131	11.56%	1.463%
24	16.315	2408	2419	2428	rBV2	63748	134677	7.82%	0.989%
25	16.880	2510	2515	2522	rVB6	16977	34786	2.02%	0.256%

Sum of corrected areas: 13614776

LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100319\
Data File : BF117317.D
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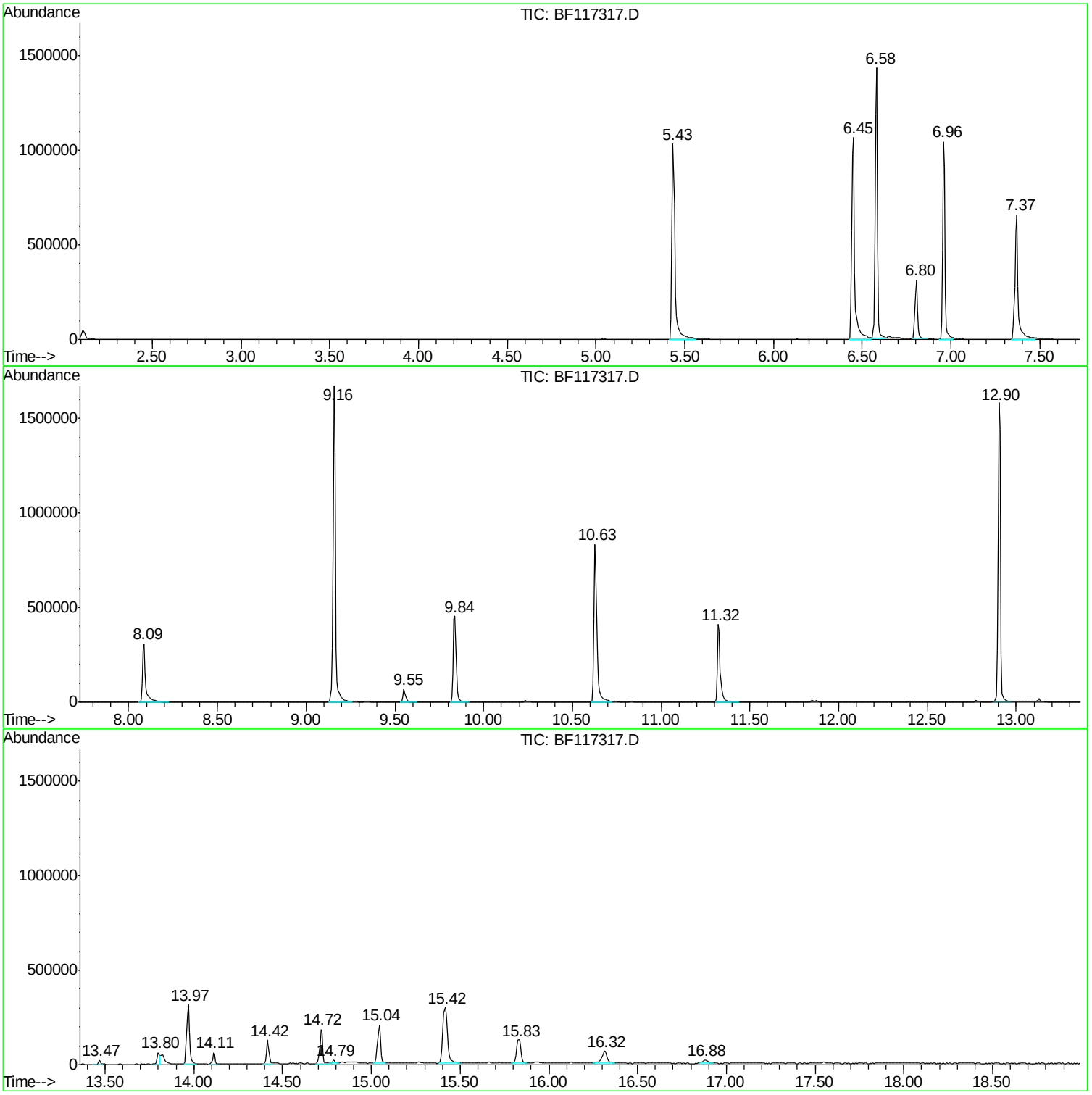
Operator : JU
Sample : PB123339BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100319\
Data File : BF117317.D
Acq On : 3 Oct 2019 15:40
Operator : JU
Sample : PB123339BL
Misc :
ALS Vial : 3 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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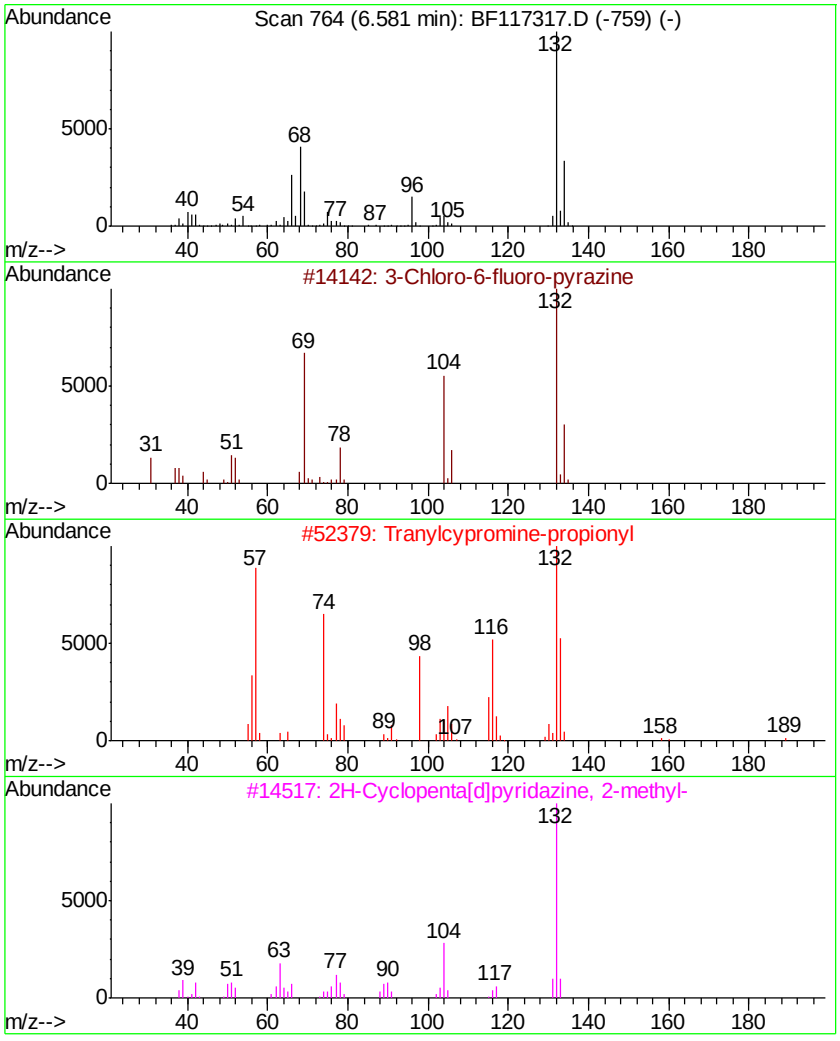
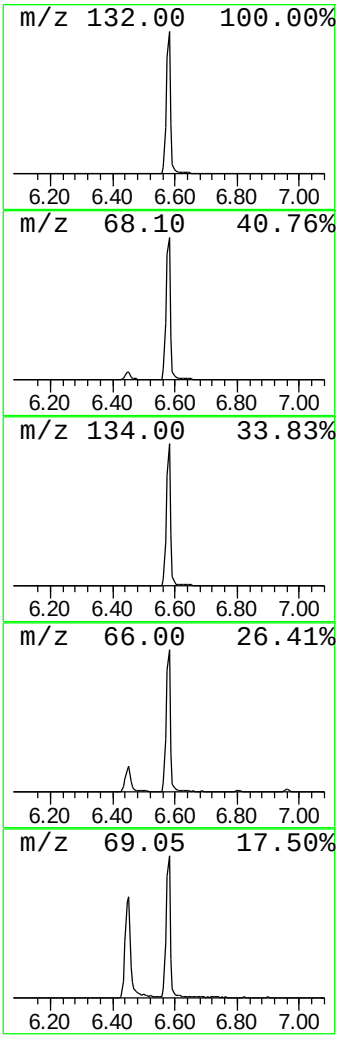
Peak Number 1 unknown6.58 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.58	89.74 ng	1352520	1,4-Dichlorobenzene-d4	6.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
4	Xenon	132	Xe	007440-63-3	9
5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9





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Data File : BF117317.D
Acq On : 3 Oct 2019 15:40
Operator : JU
Sample : PB123339BL
Misc :
ALS Vial : 3 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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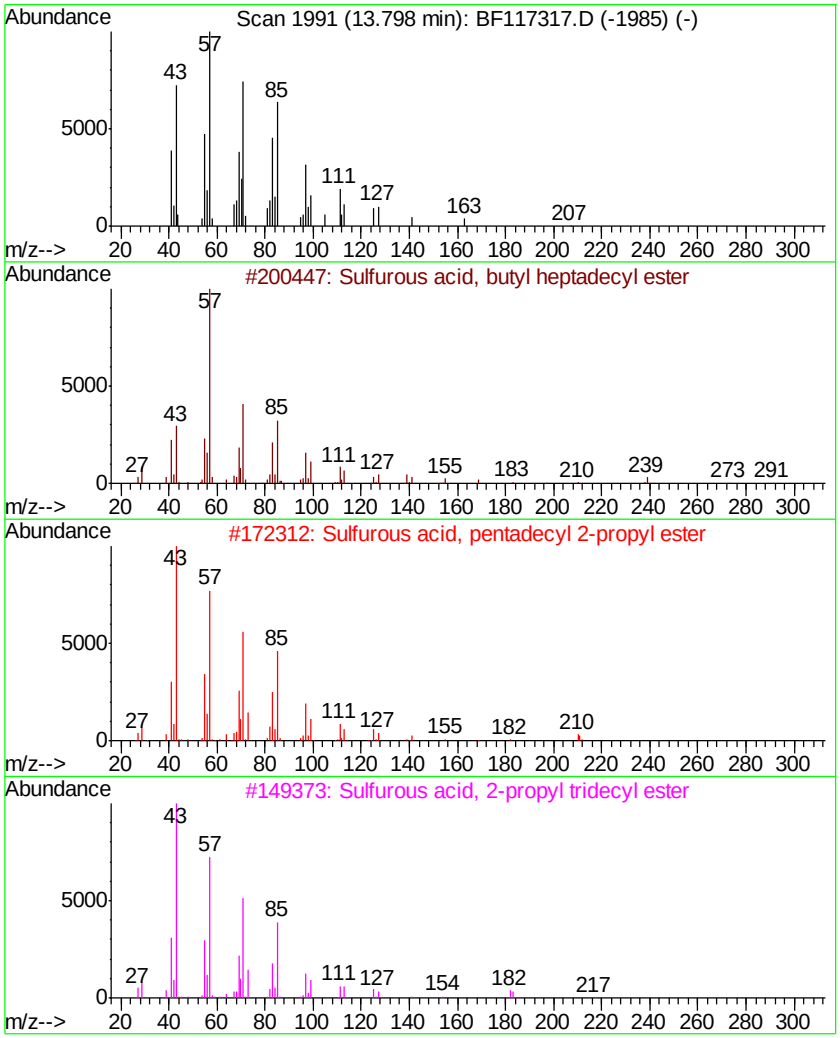
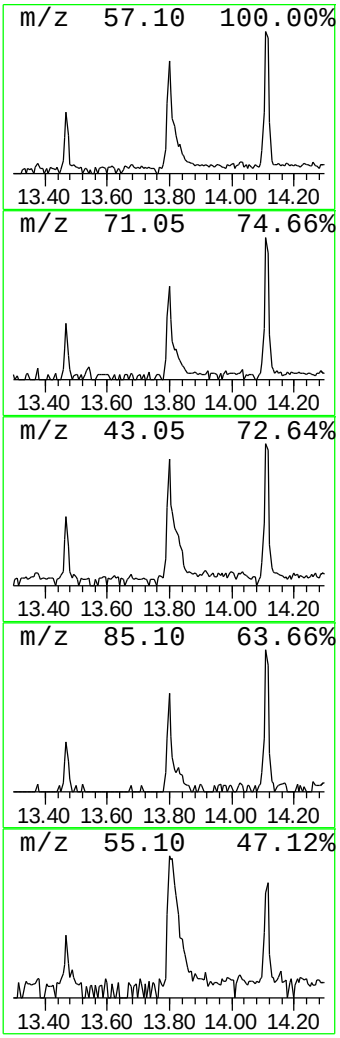
Peak Number 3 Sulfurous acid, butyl hepta... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.80	4.42 ng	74682	Chrysene-d12	13.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, butyl heptadecyl...	376	C21H44O3S	1000309-18-4	90
2	Sulfurous acid, pentadecyl 2-pro...	334	C18H38O3S	1000309-12-6	86
3	Sulfurous acid, 2-propyl tridecy...	306	C16H34O3S	1000309-12-4	83
4	Hexacosane	366	C26H54	000630-01-3	58
5	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	43





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100319\
Data File : BF117317.D
Acq On : 3 Oct 2019 15:40
Operator : JU
Sample : PB123339BL
Misc :
ALS Vial : 3 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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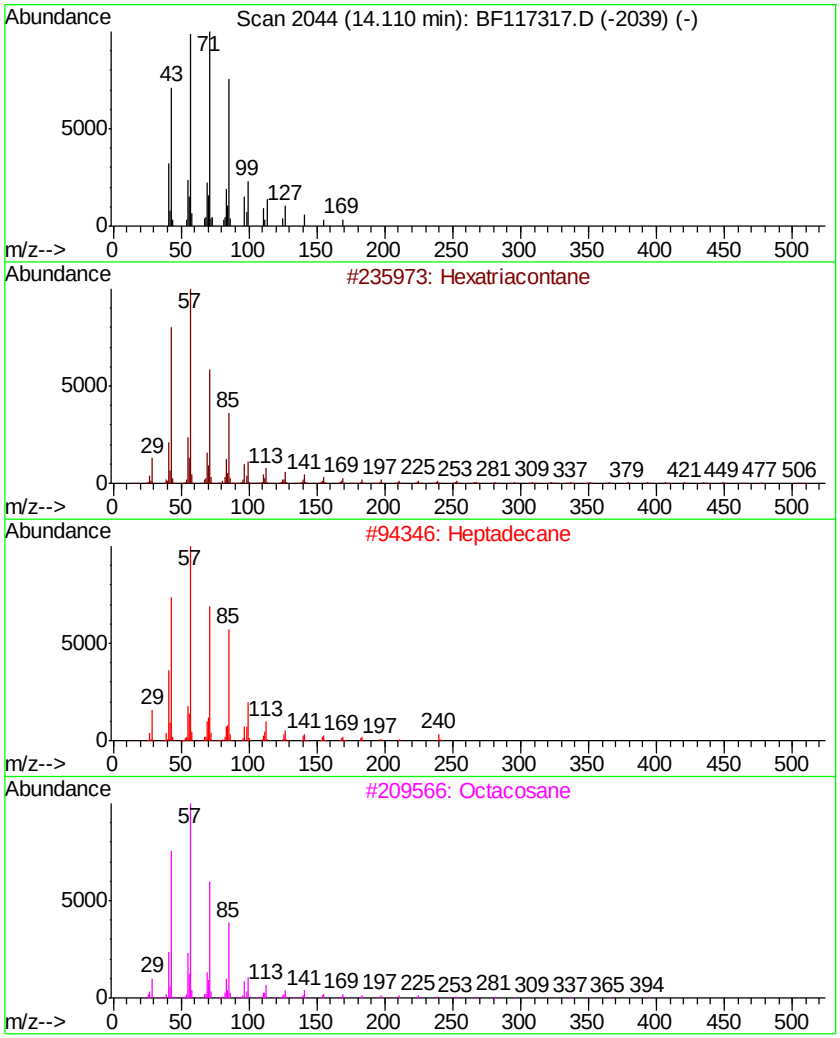
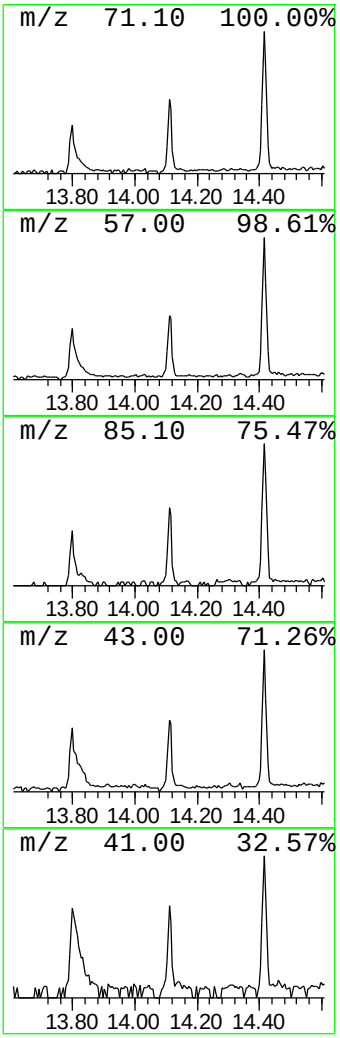
Peak Number 4 Hexatriacontane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.11	3.89 ng	65751	Chrysene-d12	13.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexatriacontane	507	C36H74	000630-06-8	86
2	Heptadecane	240	C17H36	000629-78-7	83
3	Octacosane	394	C28H58	000630-02-4	80
4	Heneicosane	296	C21H44	000629-94-7	72
5	Sulfurous acid, butyl nonyl ester	264	C13H28O3S	1000309-17-6	72





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100319\
Data File : BF117317.D
Acq On : 3 Oct 2019 15:40
Operator : JU
Sample : PB123339BL
Misc :
ALS Vial : 3 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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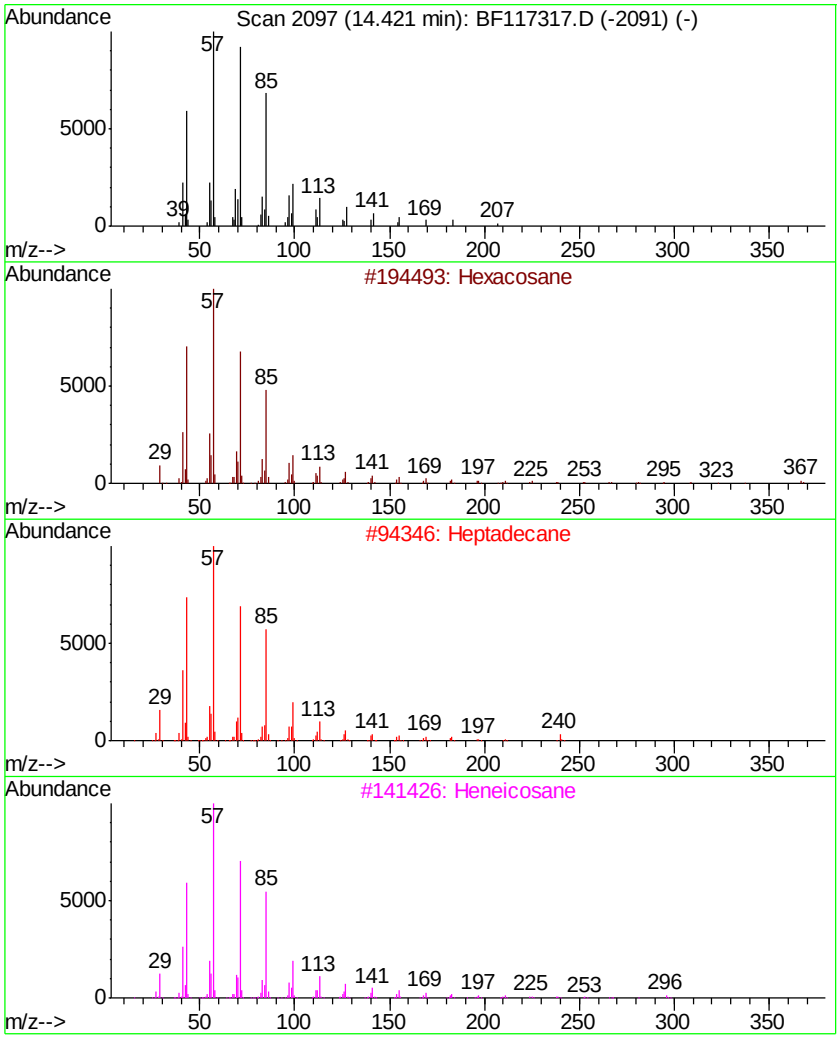
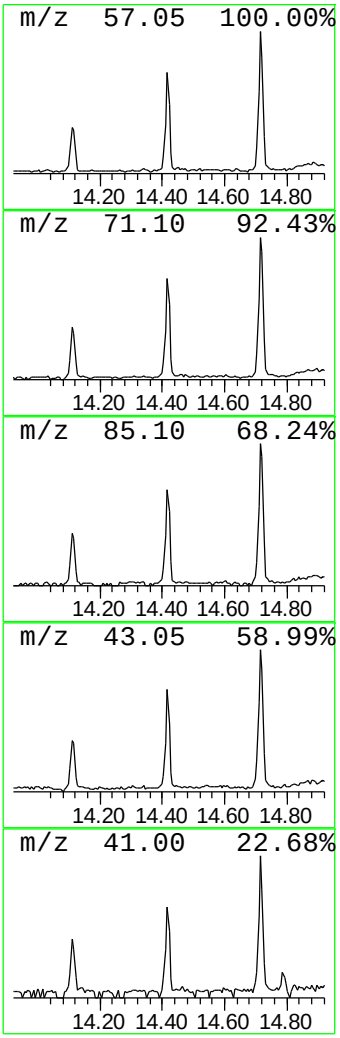
Peak Number 5 Hexacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.42	6.73 ng	113736	Chrysene-d12	13.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	Heptadecane	240	C17H36	000629-78-7	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	Tetracosane	338	C24H50	000646-31-1	86
5	Hexadecane	226	C16H34	000544-76-3	80





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100319\
Data File : BF117317.D
Acq On : 3 Oct 2019 15:40
Operator : JU
Sample : PB123339BL
Misc :
ALS Vial : 3 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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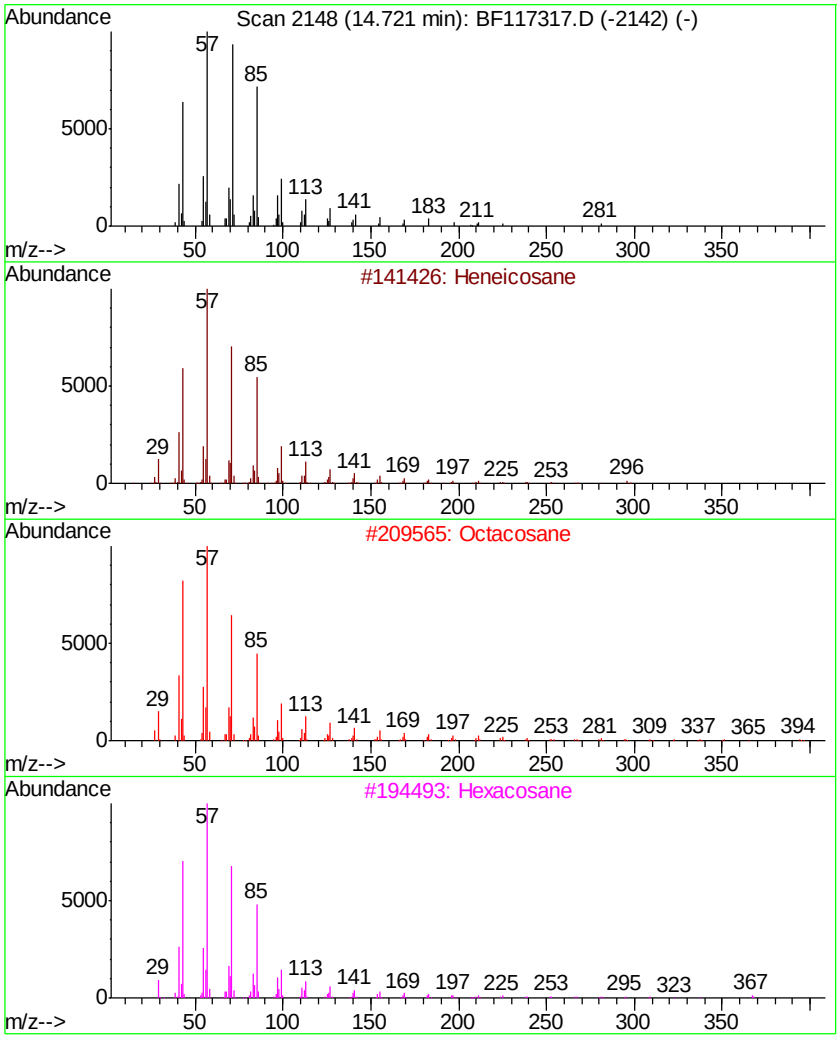
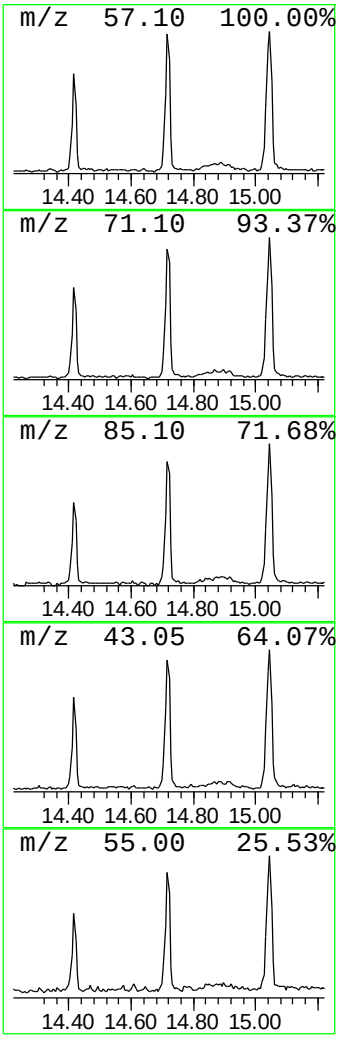
Peak Number 6 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.72	7.46 ng	193143	Perylene-d12	15.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Octacosane	394	C28H58	000630-02-4	91
3	Hexacosane	366	C26H54	000630-01-3	90
4	Eicosane, 10-methyl-	296	C21H44	054833-23-7	86
5	Nonadecane	268	C19H40	000629-92-5	86





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100319\
Data File : BF117317.D
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Sample : PB123339BL
Misc :
ALS Vial : 3 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

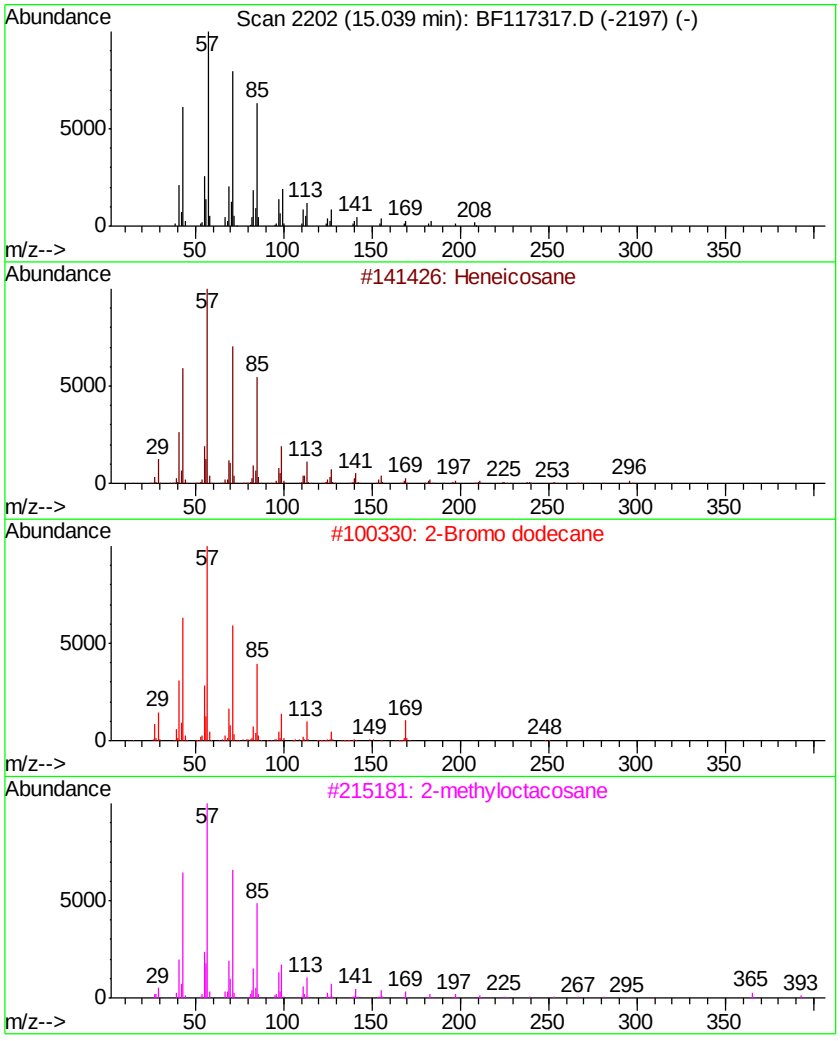
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

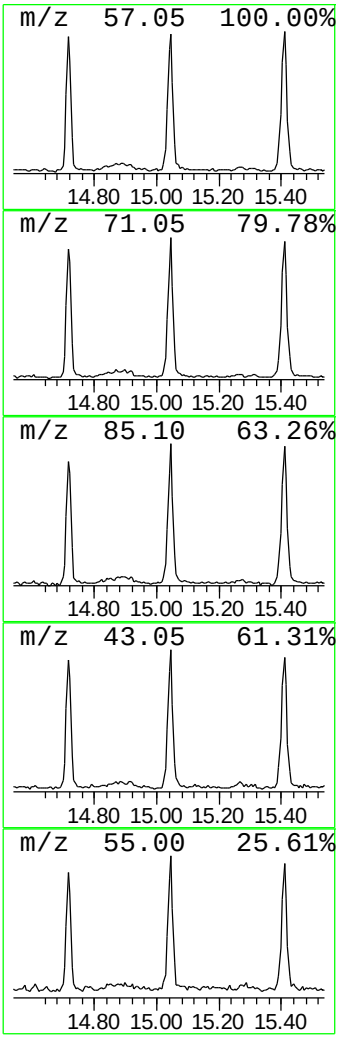
****

Peak Number 7 2-Bromo dodecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.04	9.29 ng	240433	Perylene-d12	15.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	2-Bromo dodecane	248	C12H25Br	013187-99-0	90
3	2-methyloctacosane	408	C29H60	1000376-72-8	87
4	Hentriacontane	437	C31H64	000630-04-6	87
5	Octadecane	254	C18H38	000593-45-3	86





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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

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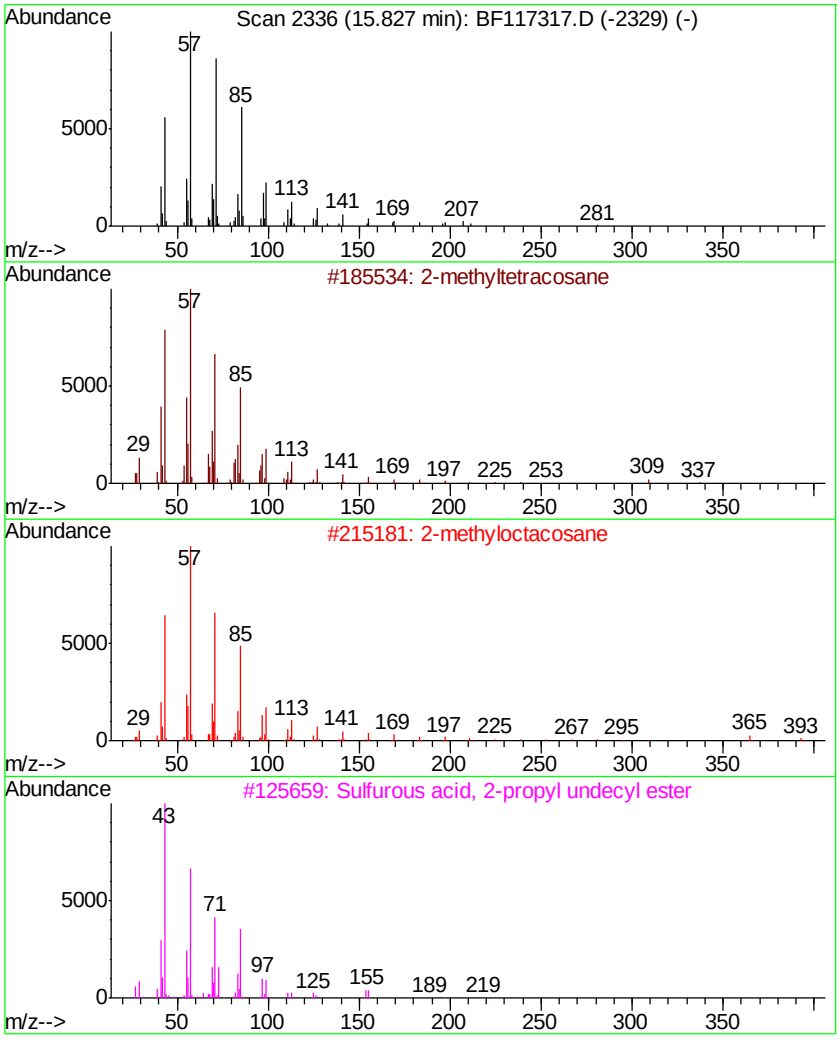
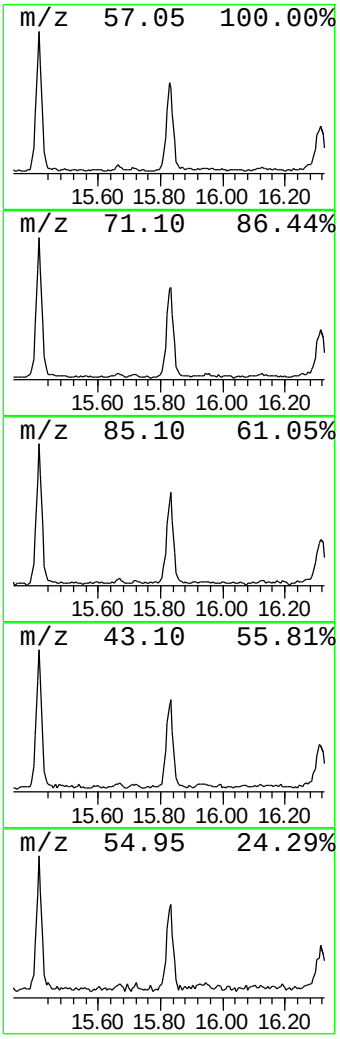
Peak Number 8 2-methyltetracosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.83	7.69 ng	199131	Perylene-d12	15.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyltetracosane	352	C25H52	1000376-72-6	90
2	2-methyloctacosane	408	C29H60	1000376-72-8	87
3	Sulfurous acid, 2-propyl undecyl...	278	C14H30O3S	1000309-12-2	86
4	Heneicosane	296	C21H44	000629-94-7	83
5	Tetratetracontane	619	C44H90	007098-22-8	83





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Misc :
ALS Vial : 3 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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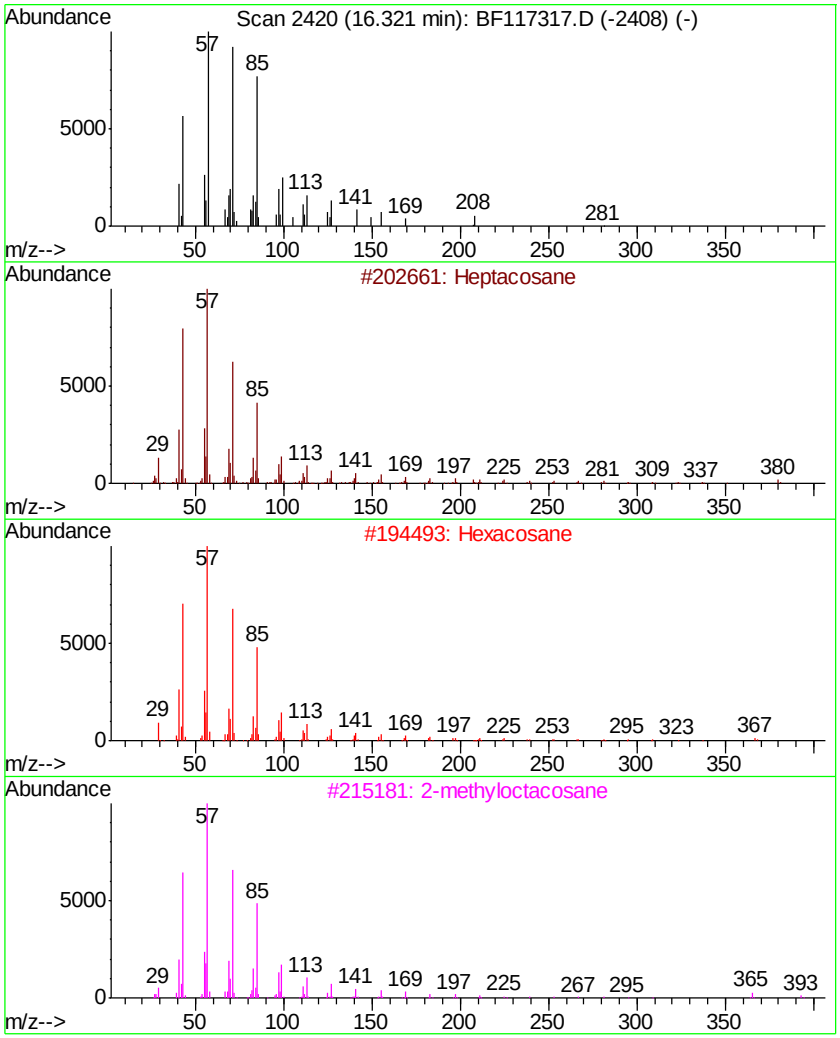
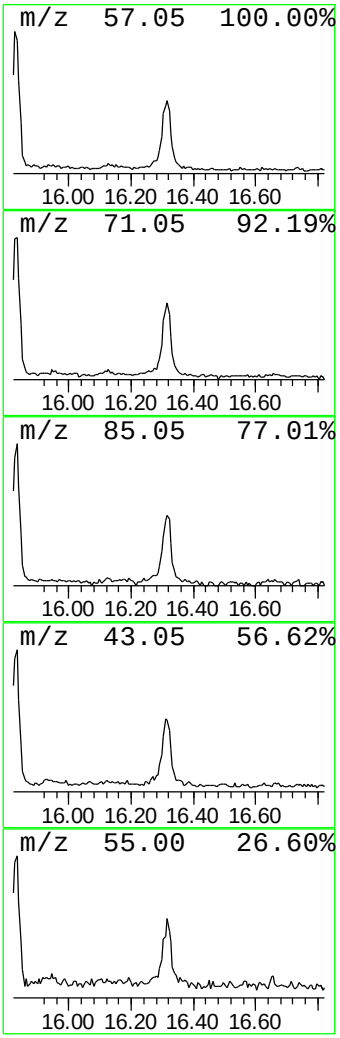
Peak Number 9 Heptacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.32	5.20 ng	134677	Perylene-d12	15.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	90
2	Hexacosane	366	C26H54	000630-01-3	90
3	2-methyloctacosane	408	C29H60	1000376-72-8	90
4	Hentriacontane	437	C31H64	000630-04-6	90
5	2-methyltetracosane	352	C25H52	1000376-72-6	90





Tentatively Identified Compound (LSC) summary

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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
unknown6.58	6.58	89.7	ng	1352520	1	6.80	301417	20.0
Sulfurous acid, b...	13.80	4.4	ng	74682	5	13.97	338003	20.0
Hexatriacontane	14.11	3.9	ng	65751	5	13.97	338003	20.0
Hexacosane	14.42	6.7	ng	113736	5	13.97	338003	20.0
Heneicosane	14.72	7.5	ng	193143	6	15.42	517849	20.0
2-Bromo dodecane	15.04	9.3	ng	240433	6	15.42	517849	20.0
2-methyltetracosane	15.83	7.7	ng	199131	6	15.42	517849	20.0
Heptacosane	16.32	5.2	ng	134677	6	15.42	517849	20.0