LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100319\
Data File : BF117320.D
Acq On : 3 Oct 2019 17:07
Operator : JU
Sample : PB123594BL
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB123594BL

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	5.439	566	570	585	rBV	1119756	1207514	65.45%	8.748%
2	6.451	737	742	760	rBV	1222800	1417953	76.86%	10.272%
3	6.581	760	764	775	rVV	1529896	1459037	79.08%	10.570%
4	6.804	799	802	813	rBV	309645	297285	16.11%	2.154%
5	6.963	825	829	845	rBV	1219557	1127609	61.12%	8.169%
6	7.369	894	898	927	rBV	748592	909598	49.30%	6.590%
7	8.086	1016	1020	1039	rBV	302691	381008	20.65%	2.760%
8	9.163	1198	1203	1219	rBV	1806090	1805143	97.84%	13.077%
9	9.557	1266	1270	1279	rBV	73593	82170	4.45%	0.595%
10	9.839	1314	1318	1330	rBV	467655	450264	24.41%	3.262%
11	10.633	1448	1453	1469	rBV	953579	1055156	57.19%	7.644%
12	11.327	1567	1571	1588	rBV	391744	434185	23.53%	3.145%
13	11.851	1656	1660	1664	rBV3	15295	22538	1.22%	0.163%
14	12.910	1835	1840	1843	rBV	1945923	1844954	100.00%	13.366%
15	13.821	1986	1995	2006	rBV5	55178	156431	8.48%	1.133%
16	13.968	2016	2020	2029	rBV	353764	364818	19.77%	2.643%
17	14.115	2038	2045	2048	rBV2	18654	21337	1.16%	0.155%
18	14.415	2092	2096	2101	rBV	37120	39686	2.15%	0.288%
19	14.715	2142	2147	2155	rBV	62148	65482	3.55%	0.474%
20	15.045	2198	2203	2209	rVB	77287	86234	4.67%	0.625%
21	15.421	2260	2267	2276	rBV2	232765	402707	21.83%	2.917%
22	15.827	2331	2336	2343	rBV2	60592	88281	4.78%	0.640%
23	16.315	2411	2419	2425	rBV2	34194	59967	3.25%	0.434%
24	16.886	2510	2516	2524	rVB6	11344	24112	1.31%	0.175%

Sum of corrected areas: 13803469

LSC Report - Integrated Chromatogram

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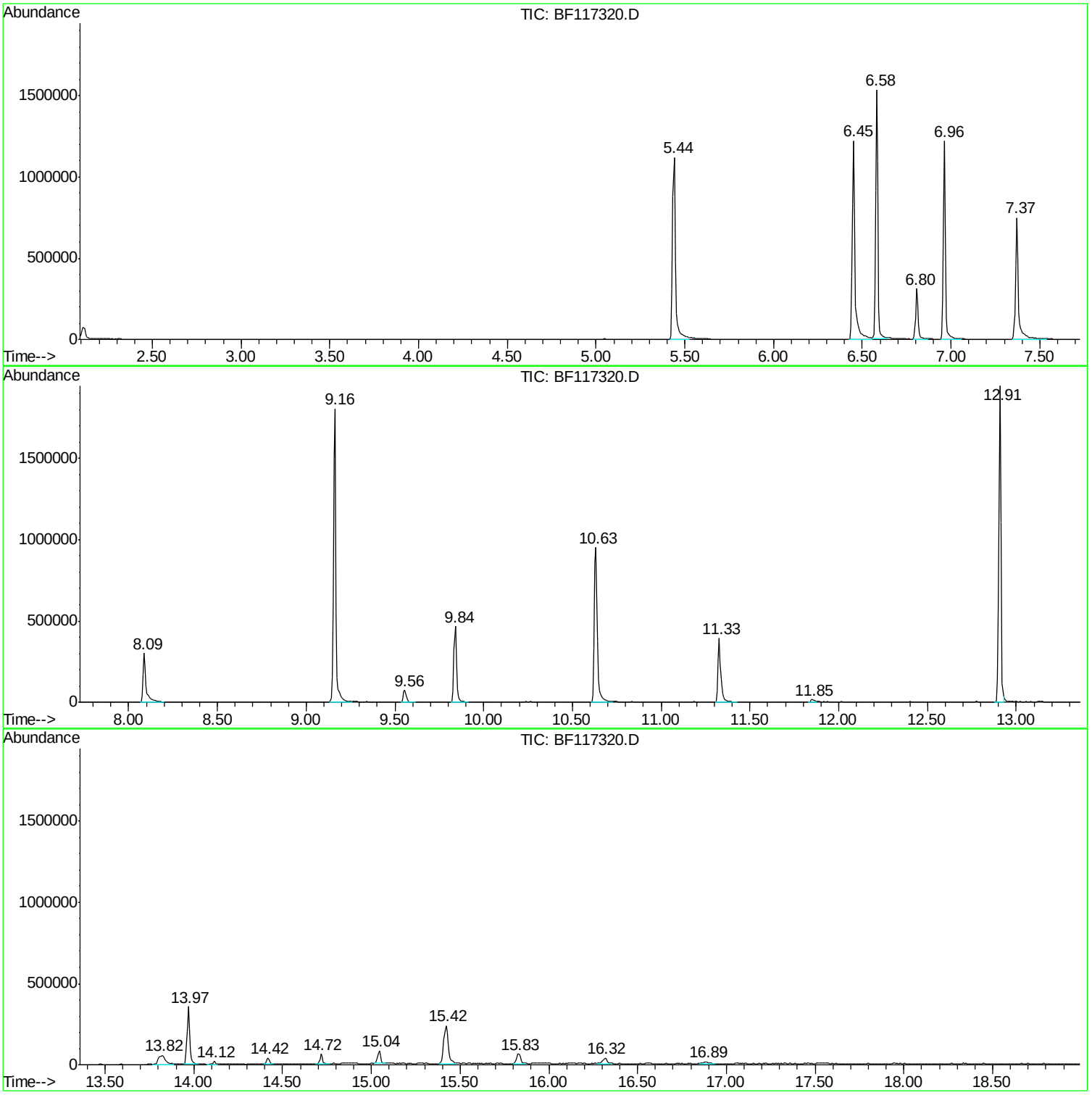
Sample : PB123594BL
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB123594BL

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 : BF117320.D
Acq On : 3 Oct 2019 17:07
Operator : JU
Sample : PB123594BL
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB123594BL

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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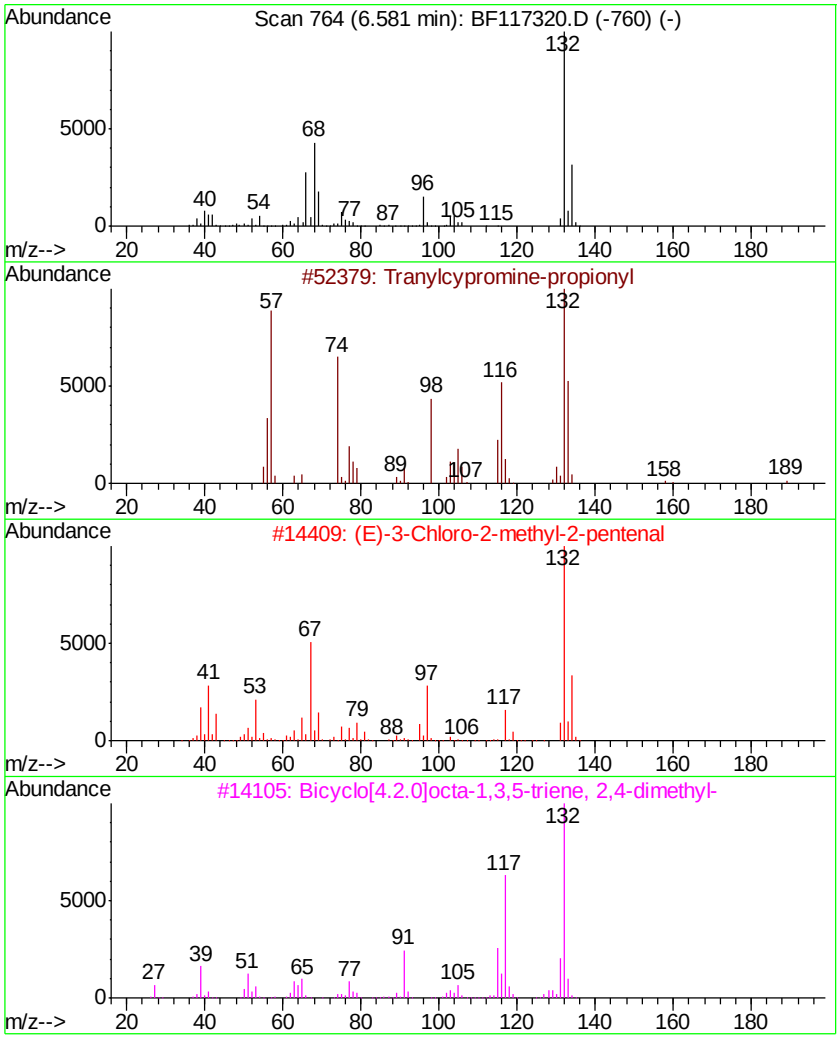
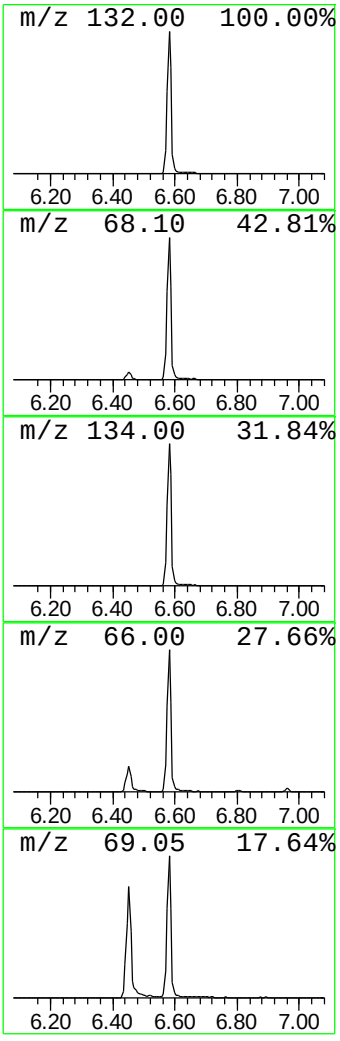
Peak Number 1 unknown6.58 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.58	98.16 ng	1459040	1,4-Dichlorobenzene-d4	6.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100319\
Data File : BF117320.D
Acq On : 3 Oct 2019 17:07
Operator : JU
Sample : PB123594BL
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB123594BL

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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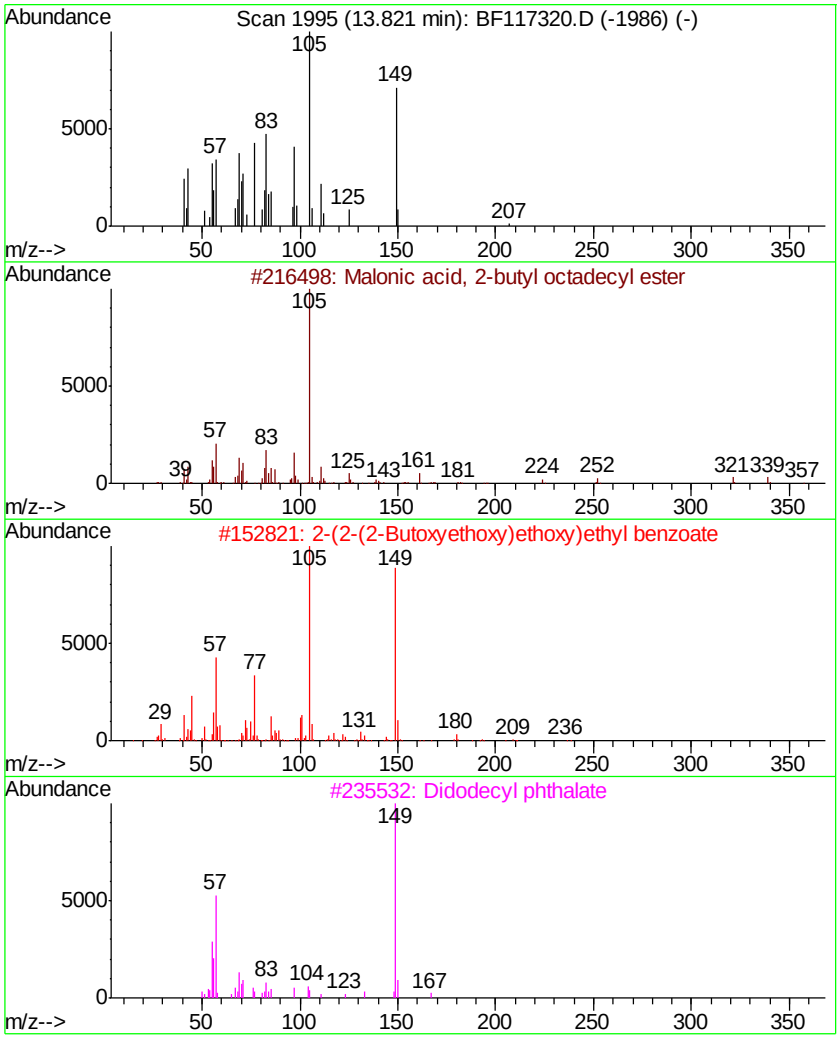
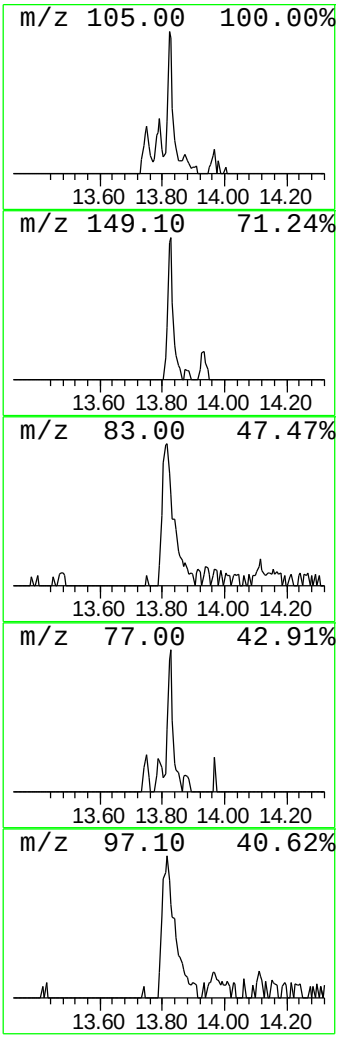
Peak Number 3 unknown13.82 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.82	8.58 ng	156431	Chrysene-d12	13.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Malonic acid, 2-butyl octadecyl ...	412	C25H48O4	1000349-08-4	37
2	2-(2-(2-Butoxyethoxy)ethoxy)ethy...	310	C17H26O5	1000366-97-2	35
3	Didodecyl phthalate	502	C32H54O4	002432-90-8	35
4	2-(2-(2-Methoxyethoxy)ethoxy)eth...	268	C14H20O5	1000366-99-1	16
5	3,6,9,12-Tetraoxatetradecane-1,1...	446	C24H30O8	1000366-97-0	16





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100319\
Data File : BF117320.D
Acq On : 3 Oct 2019 17:07
Operator : JU
Sample : PB123594BL
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB123594BL

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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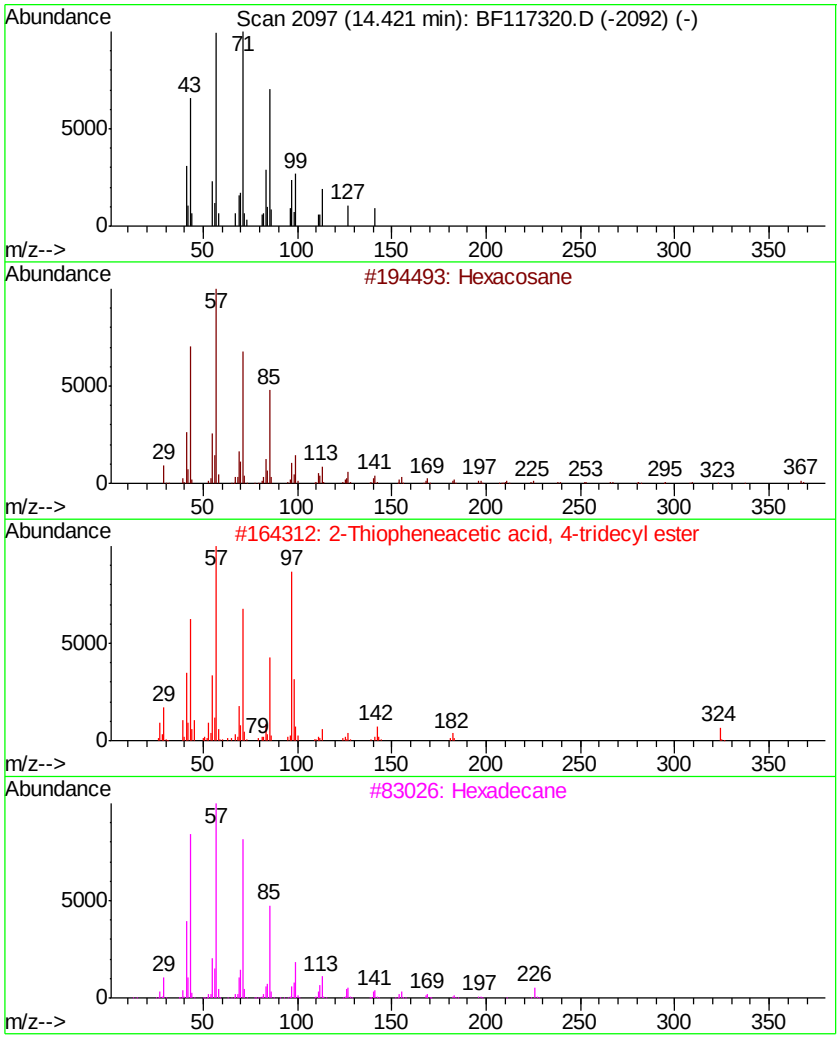
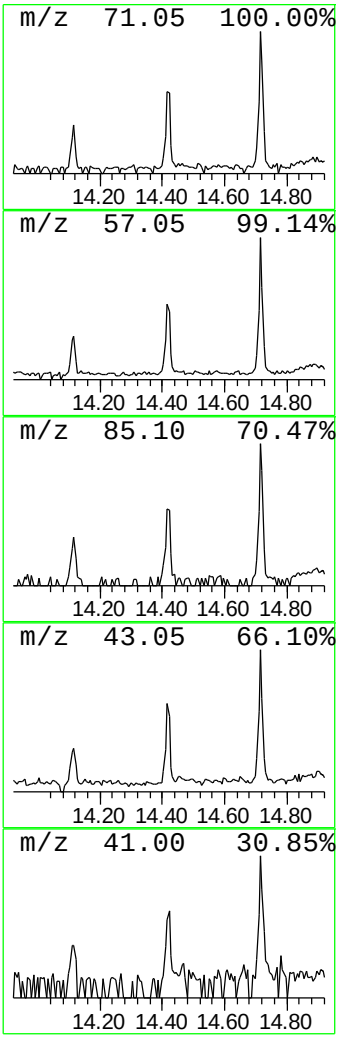
Peak Number 4 Hexacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.42	2.18 ng	39686	Chrysene-d12	13.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	72
2	2-Thiopheneacetic acid, 4-tridec...	324	C19H32O2S	1000280-66-8	70
3	Hexadecane	226	C16H34	000544-76-3	64
4	Heptadecane	240	C17H36	000629-78-7	64
5	Sulfurous acid, butyl nonyl ester	264	C13H28O3S	1000309-17-6	64





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100319\
Data File : BF117320.D
Acq On : 3 Oct 2019 17:07
Operator : JU
Sample : PB123594BL
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB123594BL

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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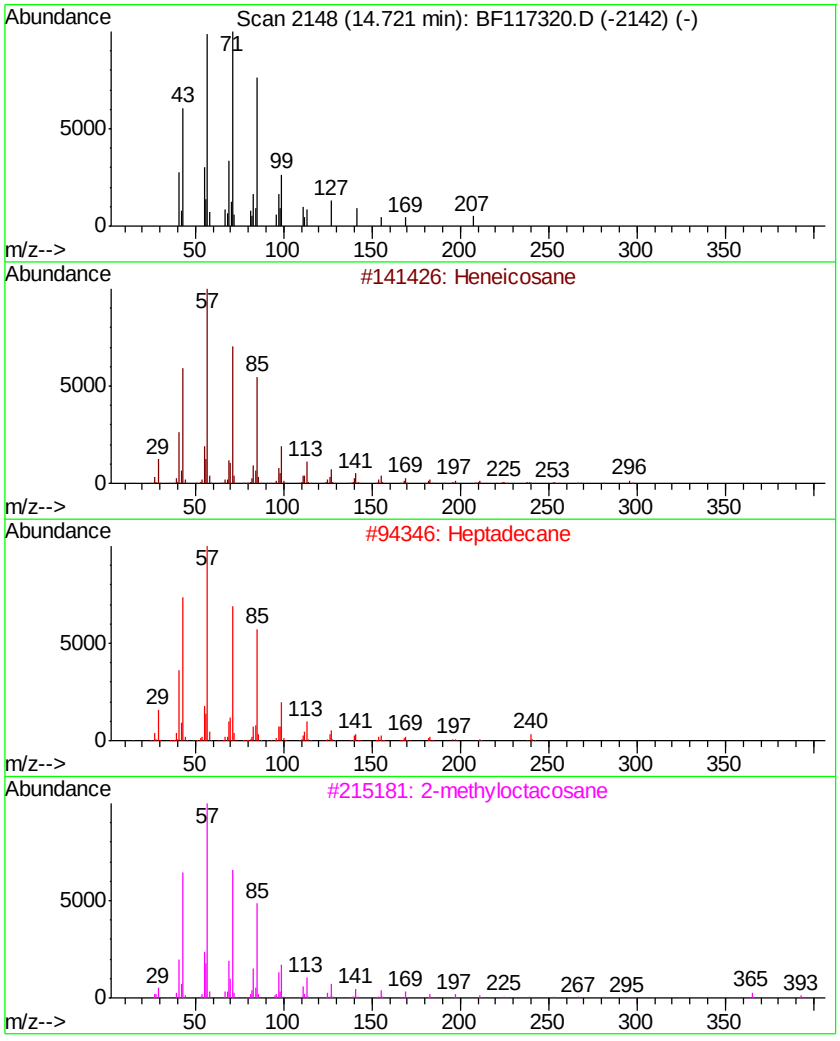
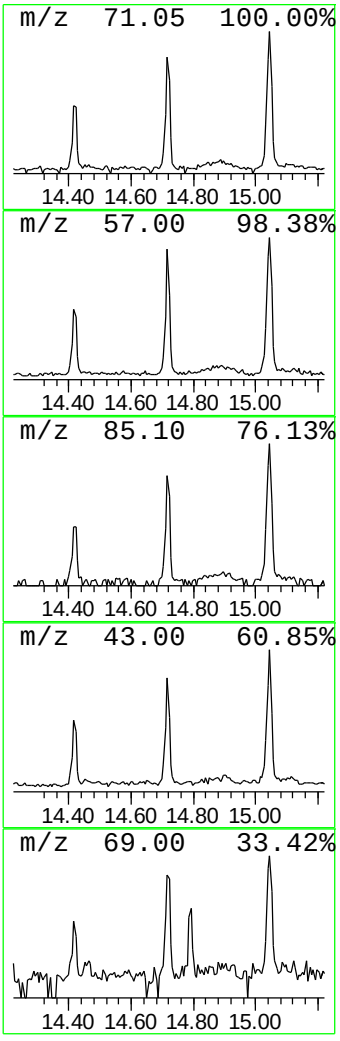
Peak Number 5 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.72	3.25 ng	65482	Perylene-d12	15.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Heptadecane	240	C17H36	000629-78-7	90
3	2-methyloctacosane	408	C29H60	1000376-72-8	90
4	2-methyltetracosane	352	C25H52	1000376-72-6	90
5	10-Methylnonadecane	282	C20H42	056862-62-5	86





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100319\
Data File : BF117320.D
Acq On : 3 Oct 2019 17:07
Operator : JU
Sample : PB123594BL
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB123594BL

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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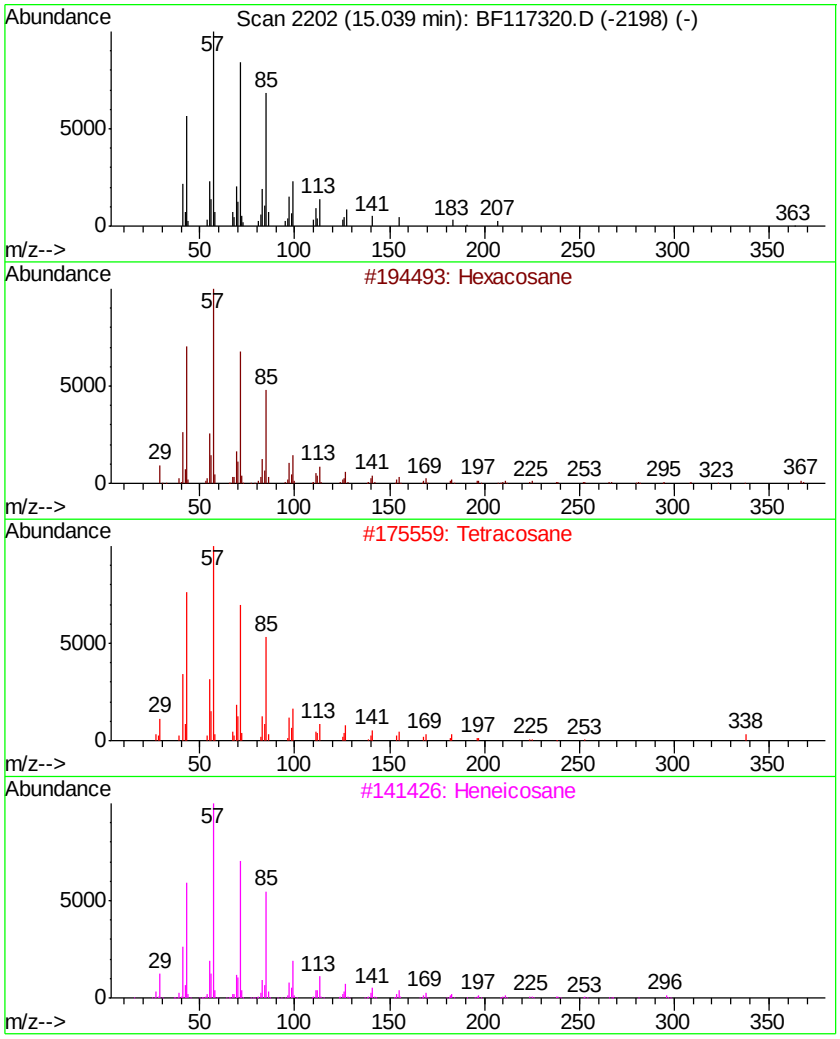
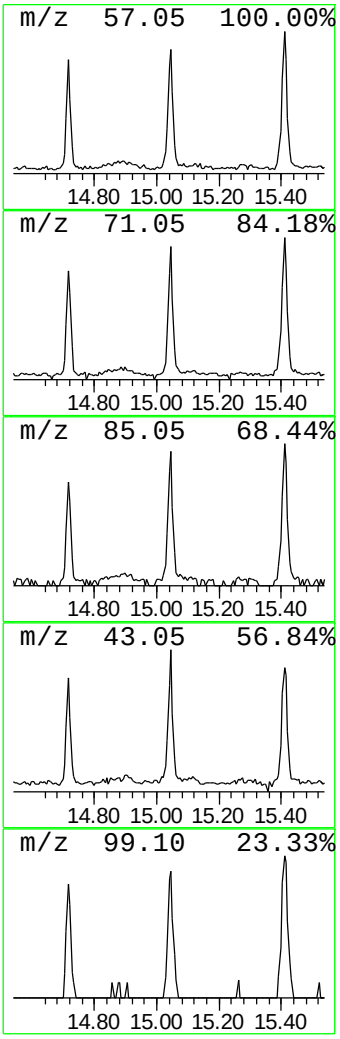
Peak Number 6 Tetracosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.04	4.28 ng	86234	Perylene-d12	15.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	Tetracosane	338	C24H50	000646-31-1	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	Hentriacontane	437	C31H64	000630-04-6	91
5	Triacontane	422	C30H62	000638-68-6	91





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Sample : PB123594BL
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB123594BL

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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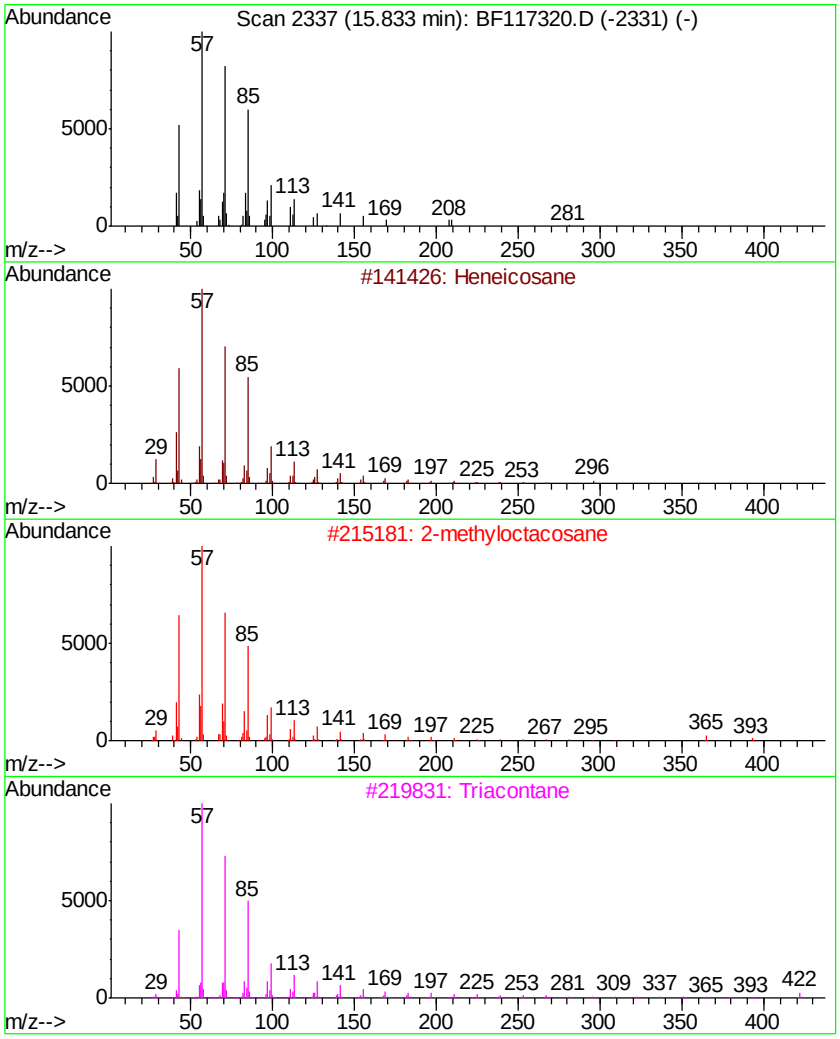
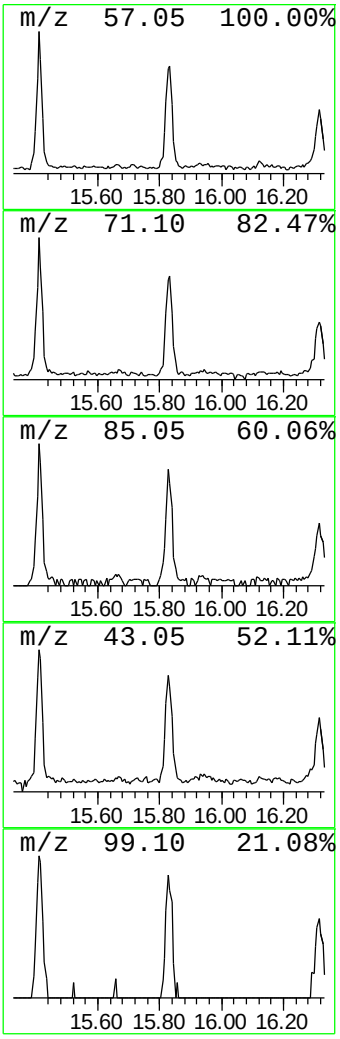
Peak Number 7 2-methyloctacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.83	4.38 ng	88281	Perylene-d12	15.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	2-methyloctacosane	408	C29H60	1000376-72-8	91
3	Triacontane	422	C30H62	000638-68-6	90
4	Hexacosane	366	C26H54	000630-01-3	86
5	Heptadecane	240	C17H36	000629-78-7	86





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Instrument : BNA_F
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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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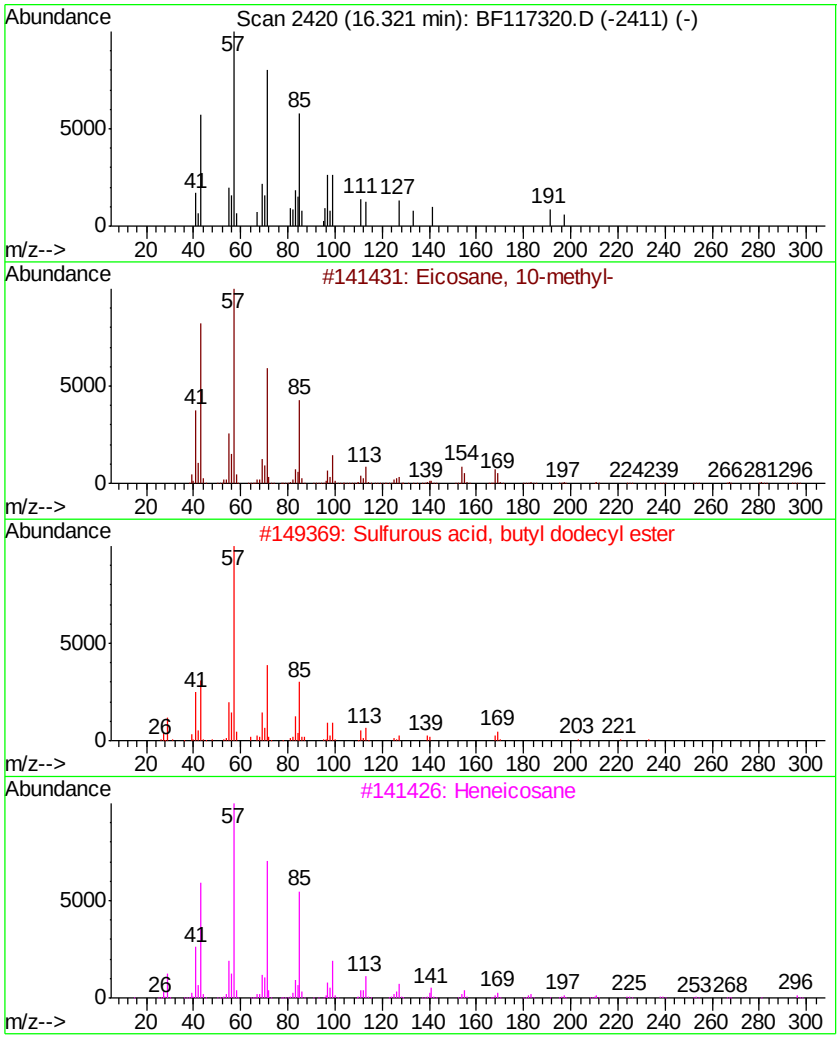
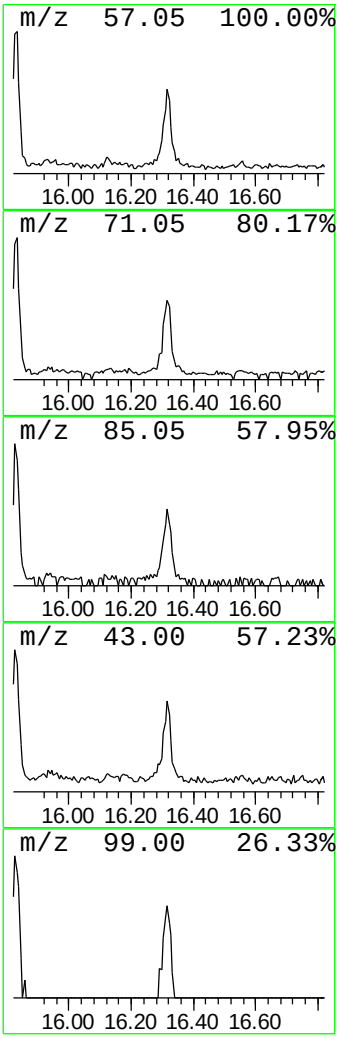
Peak Number 8 Eicosane, 10-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.32	2.98 ng	59967	Perylene-d12	15.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane, 10-methyl-	296	C21H44	054833-23-7	90
2	Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	90
3	Heneicosane	296	C21H44	000629-94-7	86
4	10-Methylnonadecane	282	C20H42	056862-62-5	86
5	Sulfurous acid, 2-propyl tridecy...	306	C16H34O3S	1000309-12-4	86





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF100319\
Data File : BF117320.D
Acq On : 3 Oct 2019 17:07
Operator : JU
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Instrument : BNA_F
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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	98.2	ng	1459040	1	6.80	297285	20.0
unknown13.82	13.82	8.6	ng	156431	5	13.97	364818	20.0
Hexacosane	14.42	2.2	ng	39686	5	13.97	364818	20.0
Heneicosane	14.72	3.3	ng	65482	6	15.42	402707	20.0
Tetracosane	15.04	4.3	ng	86234	6	15.42	402707	20.0
2-methyloctacosane	15.83	4.4	ng	88281	6	15.42	402707	20.0
Eicosane, 10-methyl-	16.32	3.0	ng	59967	6	15.42	402707	20.0