LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100319\
Data File : BF117318.D
Acq On : 3 Oct 2019 16:07
Operator : JU
Sample : K5168-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 20190763-SS-COMPOSITE-3

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	586	rBV	719279	821643	68.39%	7.843%
2	6.445	737	741	759	rBV	851877	1018230	84.76%	9.720%
3	6.575	759	763	778	rVB	1038189	1037861	86.39%	9.907%
4	6.804	798	802	816	rVB	311653	301413	25.09%	2.877%
5	6.957	824	828	847	rBV	790248	771556	64.23%	7.365%
6	7.363	893	897	916	rBV	434996	607242	50.55%	5.797%
7	8.086	1016	1020	1038	rBV	290489	392667	32.69%	3.748%
8	9.157	1197	1202	1219	rBV	1228944	1201329	100.00%	11.468%
9	9.551	1265	1269	1280	rBV	127094	129052	10.74%	1.232%
10	9.833	1313	1317	1330	rBV	469670	475198	39.56%	4.536%
11	10.627	1448	1452	1469	rBV	582311	664831	55.34%	6.346%
12	11.322	1567	1570	1580	rBV	369634	444743	37.02%	4.245%
13	11.851	1658	1660	1669	rBV3	8339	16360	1.36%	0.156%
14	12.904	1835	1839	1849	rBV	1144337	1068280	88.92%	10.198%
15	13.804	1986	1992	2005	rBV3	64217	164660	13.71%	1.572%
16	13.968	2016	2020	2033	rBV	284177	319631	26.61%	3.051%
17	14.115	2041	2045	2049	rBV	25443	27215	2.27%	0.260%
18	14.415	2092	2096	2100	rBV	68079	64554	5.37%	0.616%
19	14.715	2141	2147	2154	rBV	121266	124210	10.34%	1.186%
20	15.045	2198	2203	2210	rBV	134183	158281	13.18%	1.511%
21	15.415	2259	2266	2274	rBV2	229184	420307	34.99%	4.012%
22	15.827	2330	2336	2343	rBV	95509	143721	11.96%	1.372%
23	16.315	2412	2419	2424	rBV2	44413	77976	6.49%	0.744%
24	16.874	2510	2514	2521	rBV5	12734	24752	2.06%	0.236%

Sum of corrected areas: 10475712

LSC Report - Integrated Chromatogram

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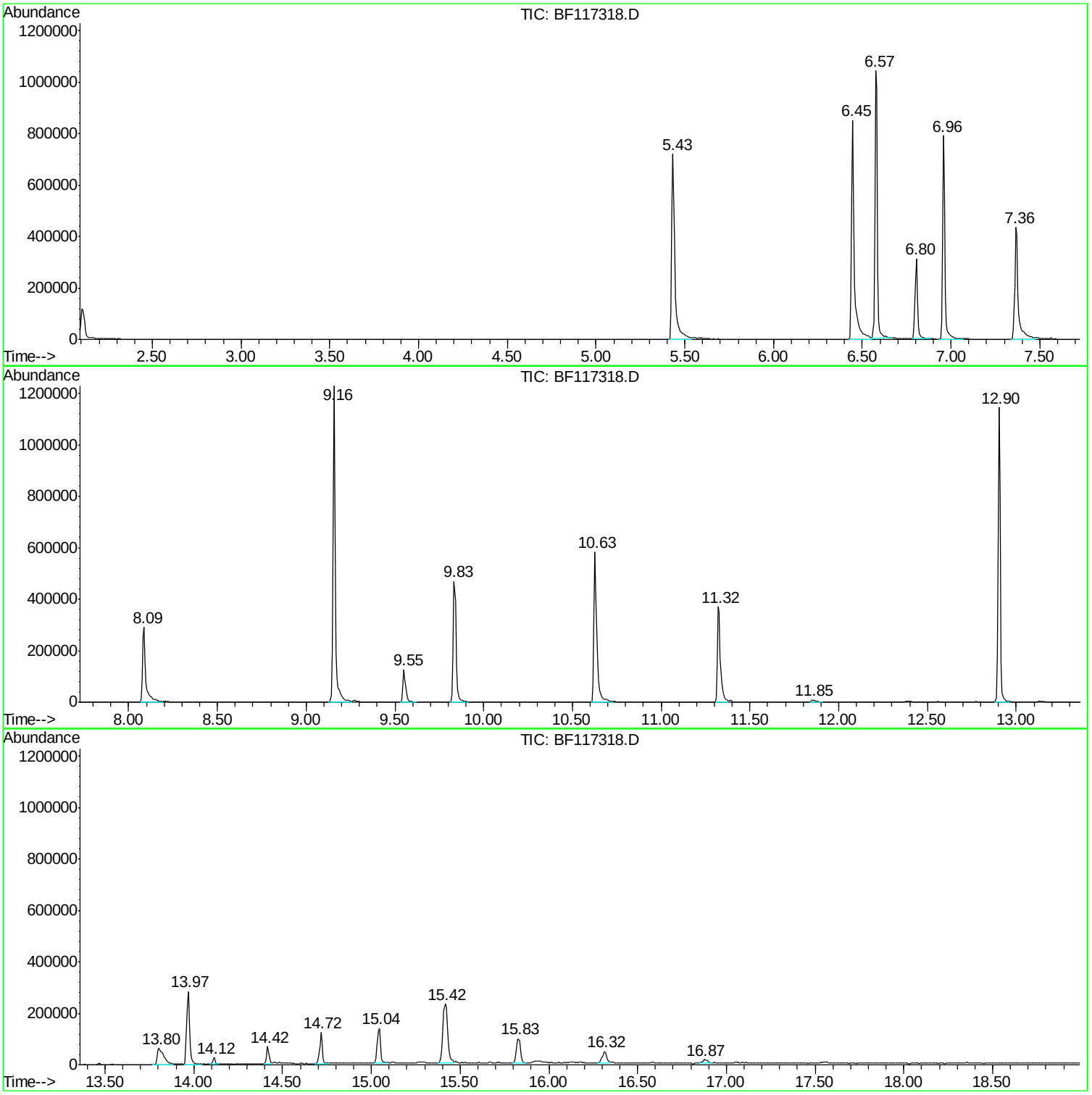
Operator : JU
Sample : K5168-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20190763-SS-COMPOSITE-3

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

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100319\
Data File : BF117318.D
Acq On : 3 Oct 2019 16:07
Operator : JU
Sample : K5168-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 20190763-SS-COMPOSITE-3

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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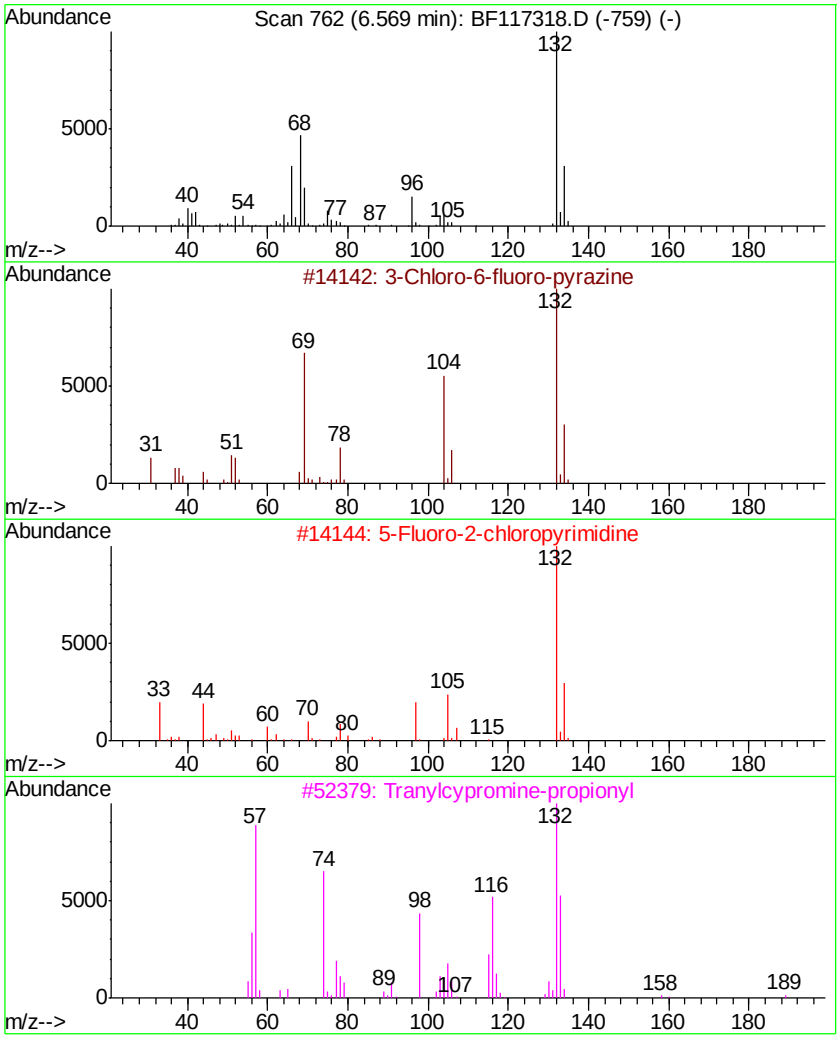
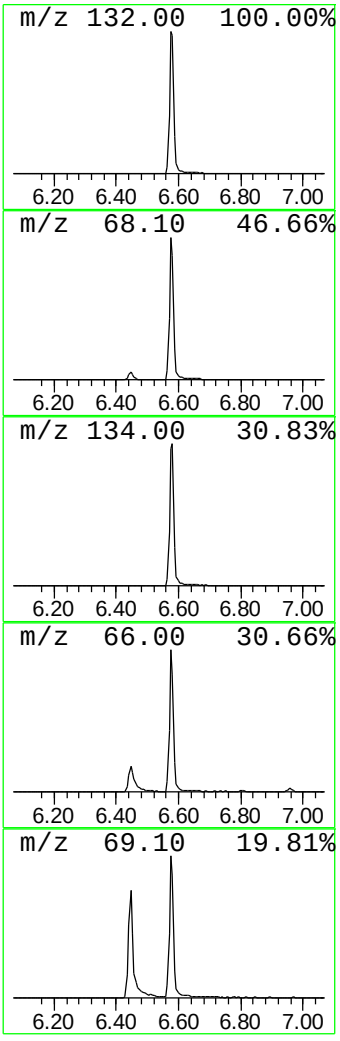
Peak Number 1 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	68.87 ng	1037860	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	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Xenon	132	Xe	007440-63-3	9
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





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Acq On : 3 Oct 2019 16:07
Operator : JU
Sample : K5168-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 20190763-SS-COMPOSITE-3

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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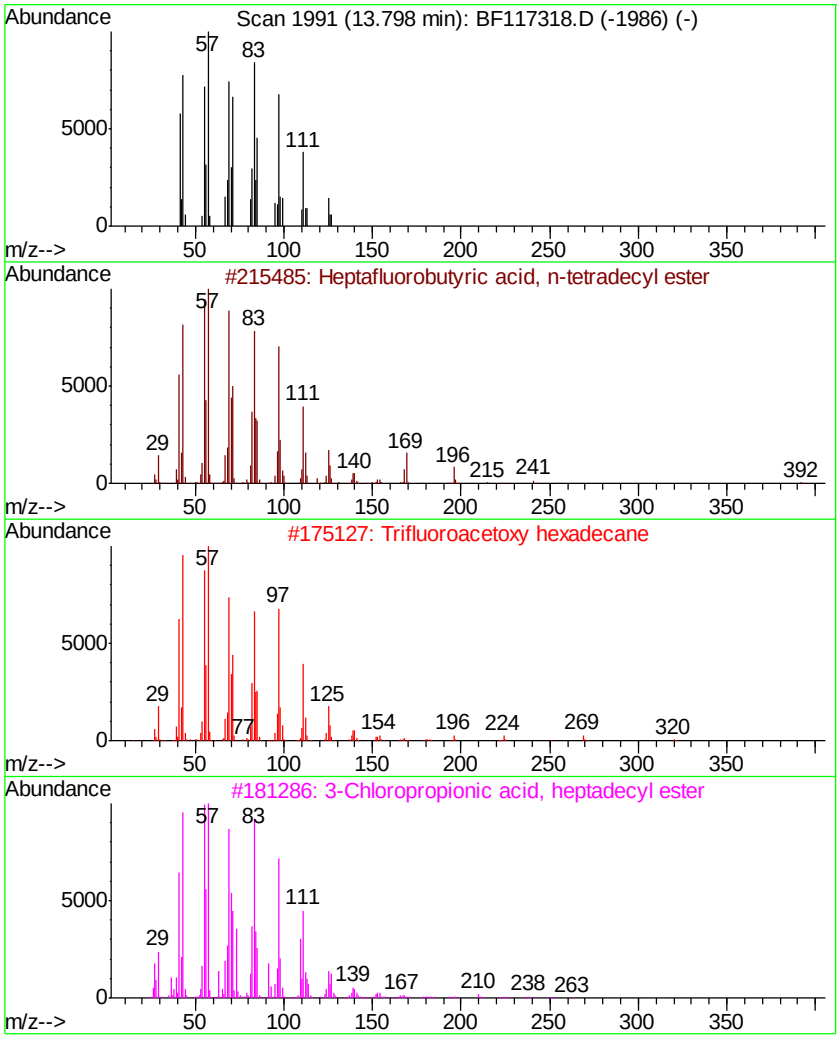
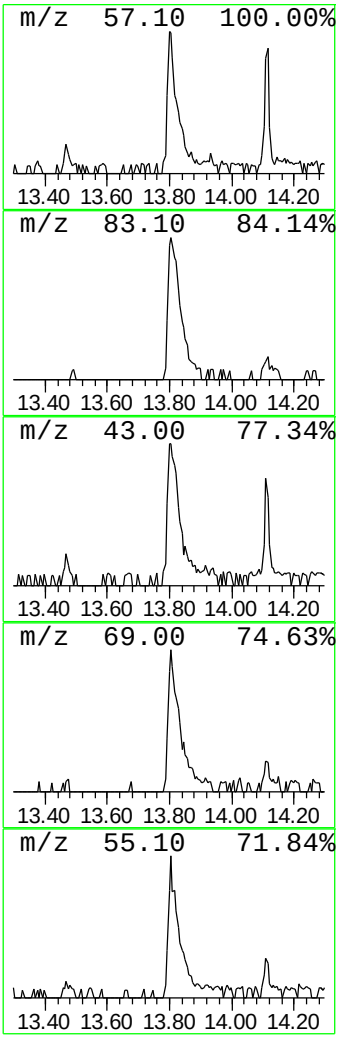
Peak Number 3 Heptafluorobutyric acid, n-... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.80	10.30 ng	164660	Chrysene-d12	13.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	91
2	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
3	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	90
4	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	90
5	n-Heptadecanol-1	256	C17H36O	001454-85-9	90





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100319\
Data File : BF117318.D
Acq On : 3 Oct 2019 16:07
Operator : JU
Sample : K5168-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 20190763-SS-COMPOSITE-3

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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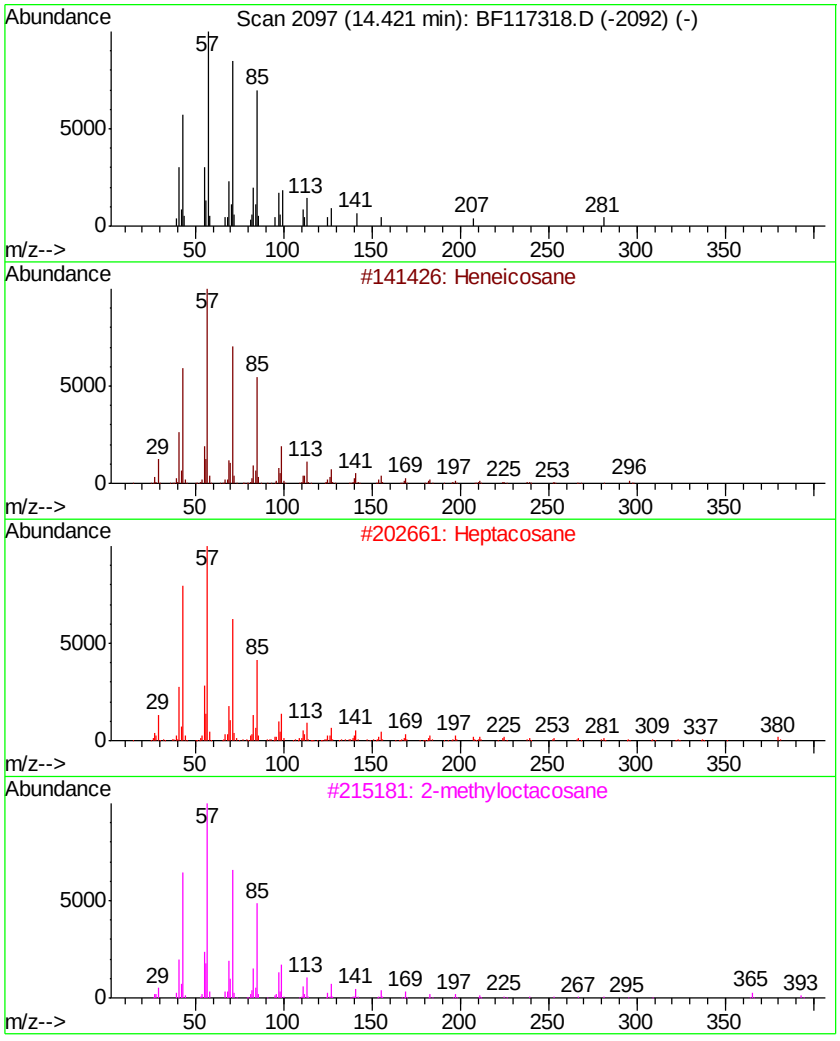
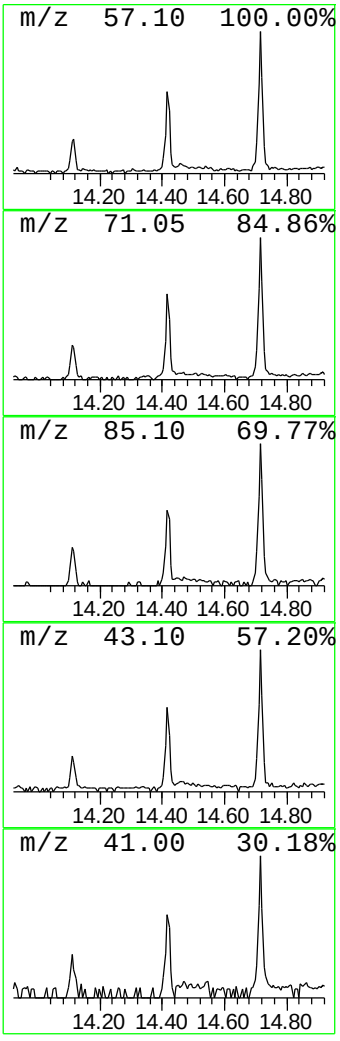
Peak Number 4 Heneicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.42	4.04 ng	64554	Chrysene-d12	13.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	90
2	Heptacosane	380	C27H56	000593-49-7	87
3	2-methyloctacosane	408	C29H60	1000376-72-8	87
4	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	86
5	Triacontane	422	C30H62	000638-68-6	86





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100319\
Data File : BF117318.D
Acq On : 3 Oct 2019 16:07
Operator : JU
Sample : K5168-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 20190763-SS-COMPOSITE-3

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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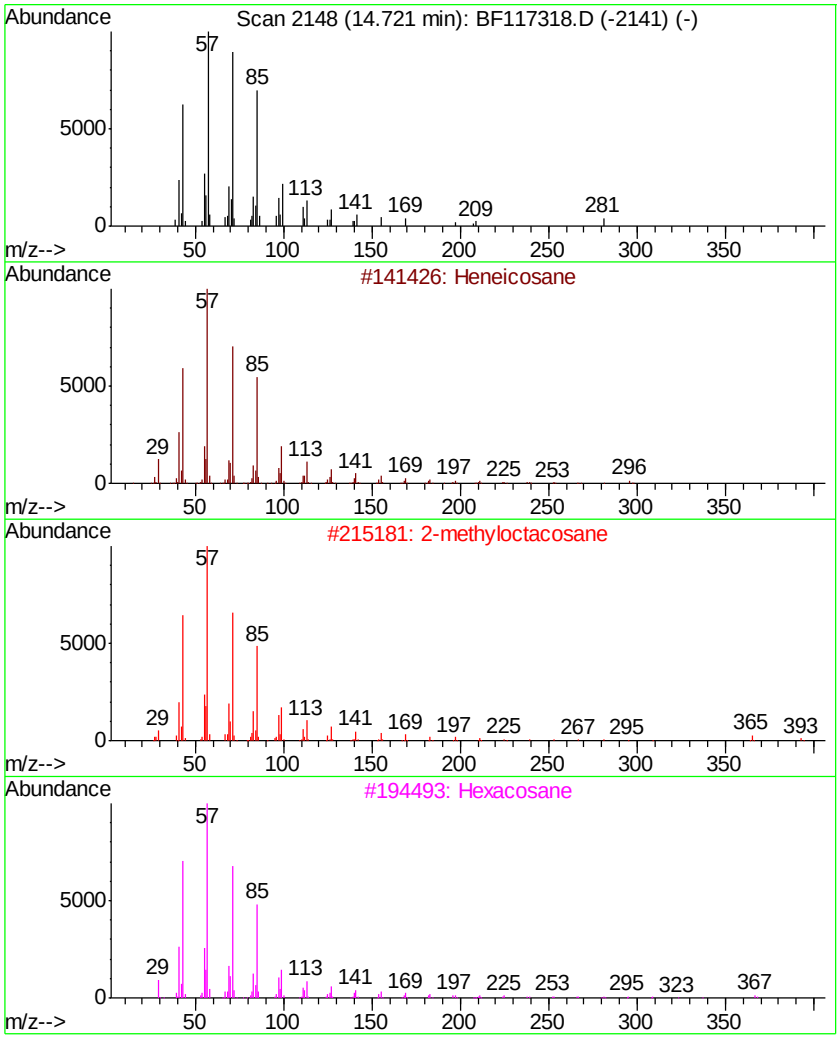
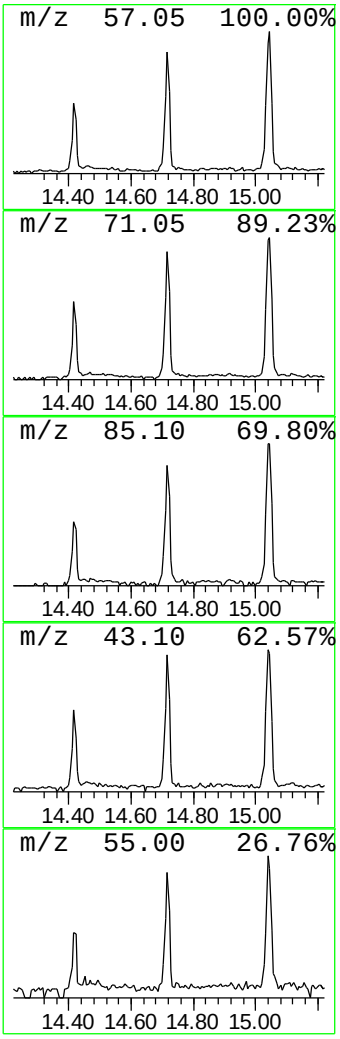
Peak Number 5 2-methyloctacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.72	5.91 ng	124210	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	Hexacosane	366	C26H54	000630-01-3	90
4	Heptadecane	240	C17H36	000629-78-7	86
5	10-Methylnonadecane	282	C20H42	056862-62-5	86





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100319\
Data File : BF117318.D
Acq On : 3 Oct 2019 16:07
Operator : JU
Sample : K5168-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 20190763-SS-COMPOSITE-3

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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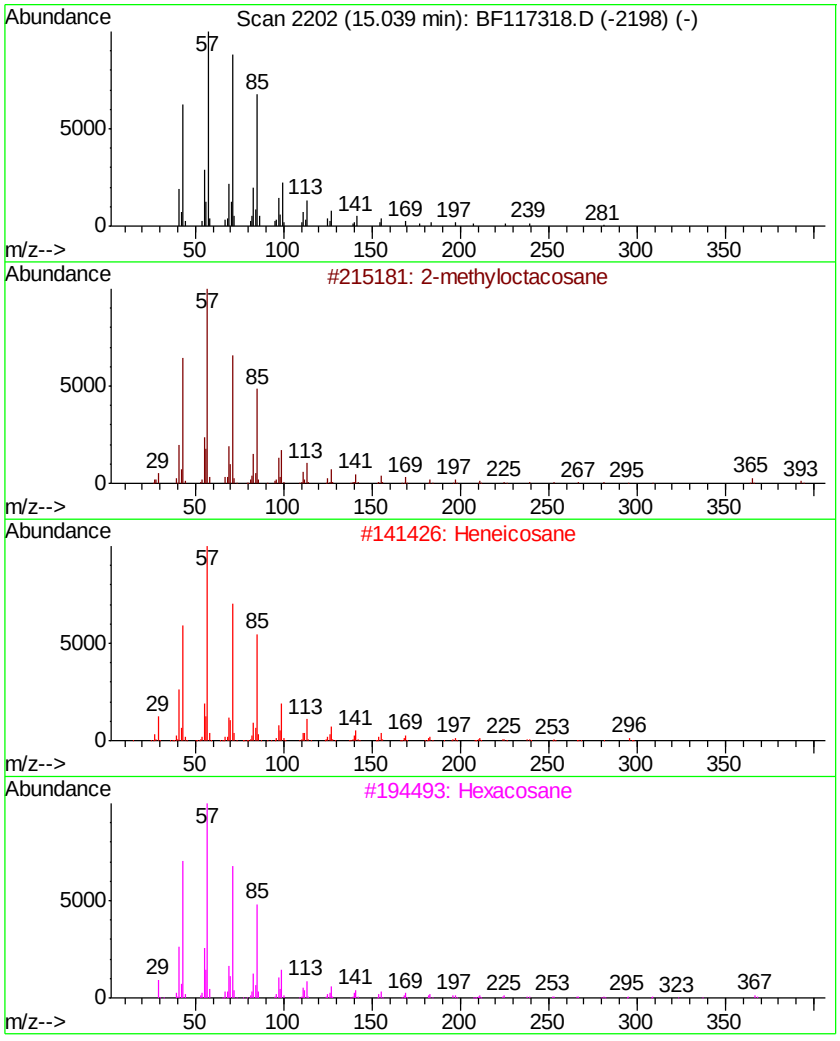
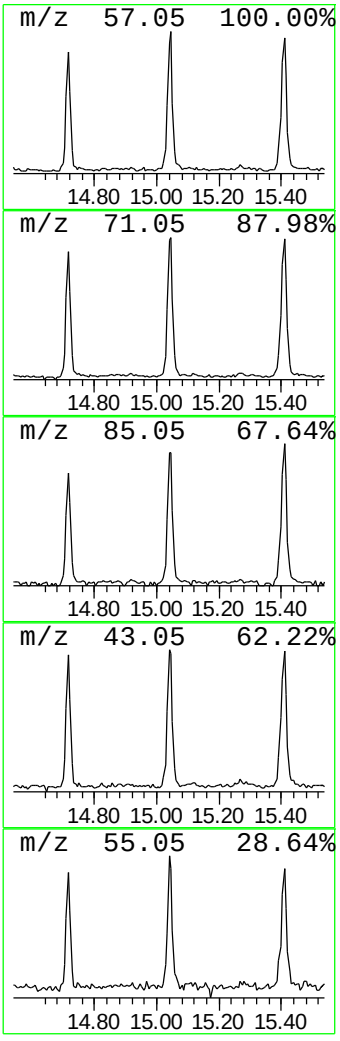
Peak Number 6 Hexacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.04	7.53 ng	158281	Perylene-d12	15.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane	408	C29H60	1000376-72-8	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Hexacosane	366	C26H54	000630-01-3	90
4	Octacosane	394	C28H58	000630-02-4	90
5	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	90





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100319\
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Acq On : 3 Oct 2019 16:07
Operator : JU
Sample : K5168-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 20190763-SS-COMPOSITE-3

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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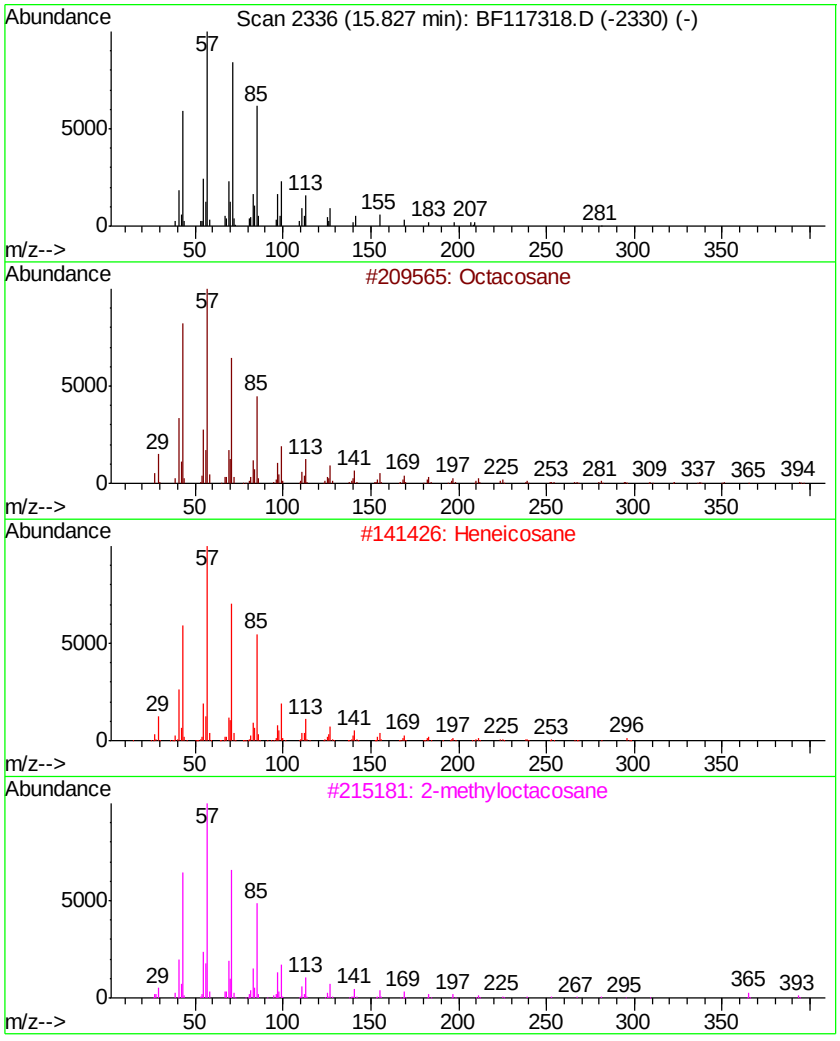
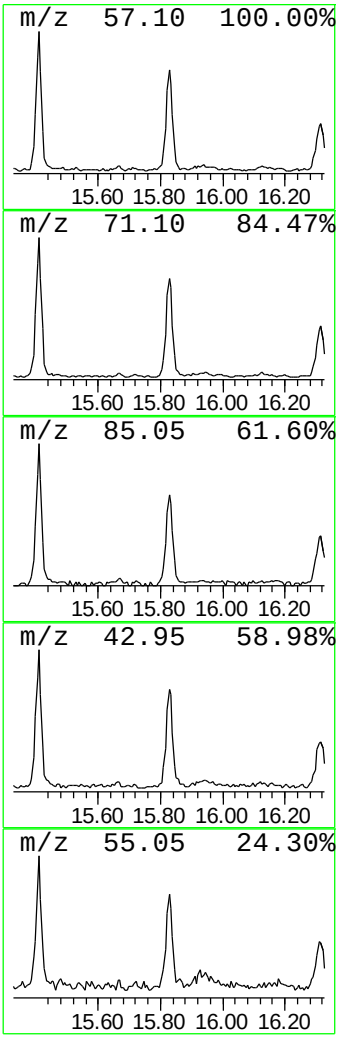
Peak Number 7 Octacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.83	6.84 ng	143721	Perylene-d12	15.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	2-methyloctacosane	408	C29H60	1000376-72-8	91
4	2-methyltetracosane	352	C25H52	1000376-72-6	90
5	Pentacosane	352	C25H52	000629-99-2	90





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Operator : JU
Sample : K5168-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 20190763-SS-COMPOSITE-3

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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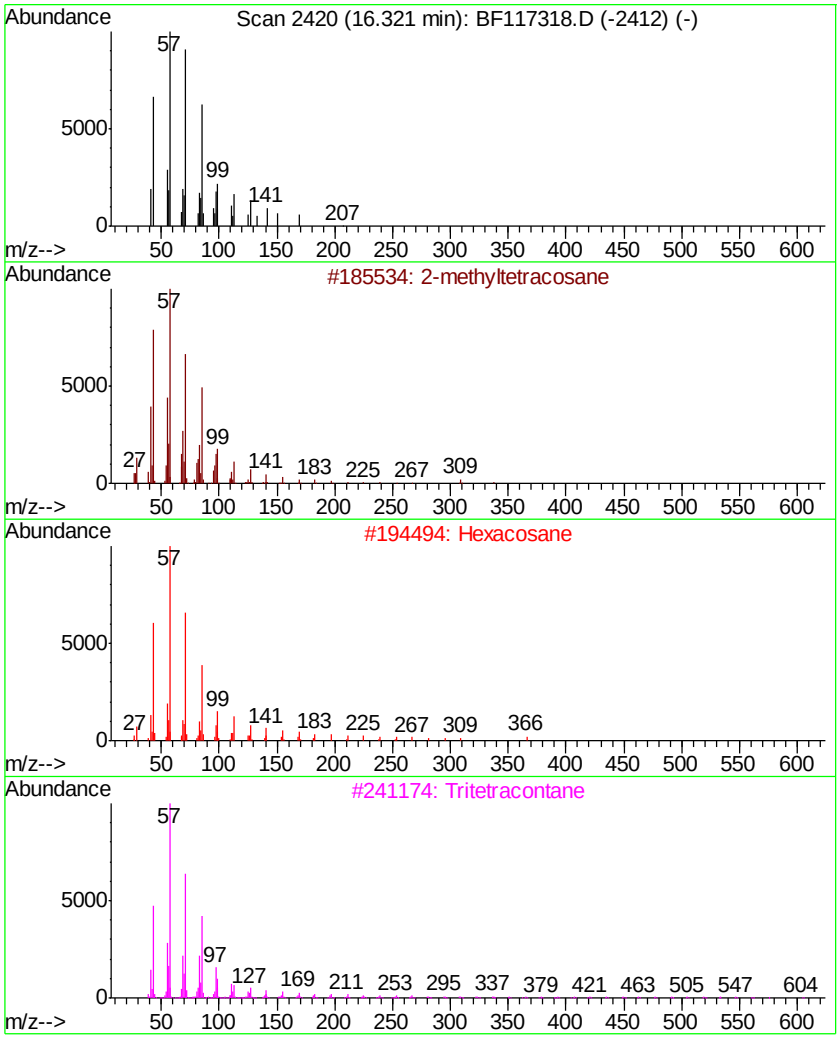
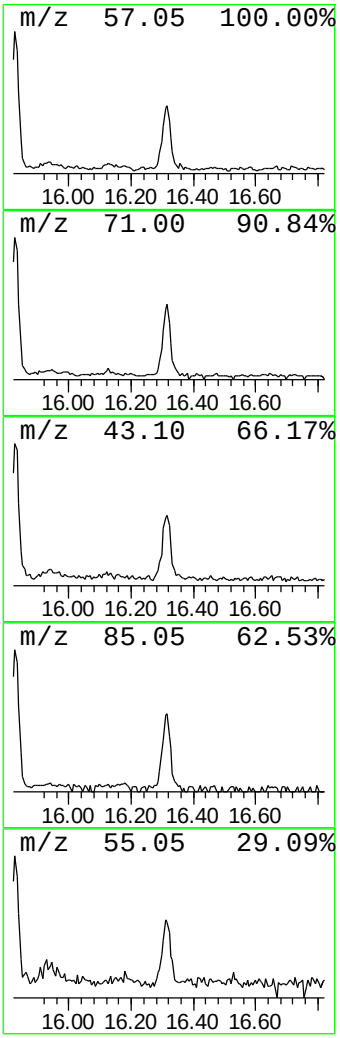
Peak Number 8 Tritetracontane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.32	3.71 ng	77976	Perylene-d12	15.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyltetracosane	352	C25H52	1000376-72-6	87
2	Hexacosane	366	C26H54	000630-01-3	86
3	Tritetracontane	605	C43H88	007098-21-7	86
4	Octacosane	394	C28H58	000630-02-4	86
5	Heptadecane	240	C17H36	000629-78-7	83





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF100319\
Data File : BF117318.D
Acq On : 3 Oct 2019 16:07
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Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 20190763-SS-COMPOSITE-3

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
unknown6.57	6.57	68.9	ng	1037860	1	6.80	301413	20.0
Heptafluorobutyri...	13.80	10.3	ng	164660	5	13.97	319631	20.0
Heneicosane	14.42	4.0	ng	64554	5	13.97	319631	20.0
2-methyloctacosane	14.72	5.9	ng	124210	6	15.42	420307	20.0
Hexacosane	15.04	7.5	ng	158281	6	15.42	420307	20.0
Octacosane	15.83	6.8	ng	143721	6	15.42	420307	20.0
Tritetracontane	16.32	3.7	ng	77976	6	15.42	420307	20.0