LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102119\
Data File : BF117463.D
Acq On : 21 Oct 2019 22:28
Operator : JU
Sample : K5448-01
Misc :
ALS Vial : 16 Sample Multiplier: 2

Instrument : BNA_F
ClientSampleId : SP

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-BF101819.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	5.345	551	554	581	rBV	674372	810090	72.50%	7.193%
2	6.375	726	729	747	rBV	915381	912980	81.70%	8.107%
3	6.504	747	751	758	rBV	1075714	926123	82.88%	8.224%
4	6.734	787	790	803	rBV	350486	366834	32.83%	3.257%
5	6.887	812	816	831	rBV	763234	679926	60.85%	6.038%
6	7.298	882	886	912	rBV	492079	548187	49.06%	4.868%
7	8.010	1004	1007	1028	rBV	515143	502590	44.98%	4.463%
8	9.086	1186	1190	1205	rBV	1180796	1032973	92.44%	9.172%
9	9.480	1254	1257	1267	rBV	175141	146406	13.10%	1.300%
10	9.763	1301	1305	1321	rBB	729994	608509	54.46%	5.403%
11	10.551	1436	1439	1453	rBV	675402	628515	56.25%	5.581%
12	11.245	1554	1557	1567	rBV	583271	601042	53.79%	5.337%
13	11.780	1645	1648	1655	rBV	60542	62653	5.61%	0.556%
14	12.563	1778	1781	1791	rBV2	10545	15128	1.35%	0.134%
15	12.827	1822	1826	1830	rBV	1178043	1117412	100.00%	9.922%
16	13.398	1920	1923	1927	rBV2	15771	14999	1.34%	0.133%
17	13.727	1975	1979	1994	rBV	117261	199262	17.83%	1.769%
18	13.892	2003	2007	2018	rBV	551462	579932	51.90%	5.150%
19	14.045	2029	2033	2041	rBV	82240	73618	6.59%	0.654%
20	14.345	2081	2084	2088	rBV	122211	120223	10.76%	1.068%
21	14.645	2130	2135	2141	rBV	165199	153852	13.77%	1.366%
22	14.715	2143	2147	2154	rVB2	14170	15176	1.36%	0.135%
23	14.963	2182	2189	2193	rBV	147061	165488	14.81%	1.469%
24	15.315	2243	2249	2264	rBV2	533471	699393	62.59%	6.210%
25	15.715	2312	2317	2323	rBV	84119	121473	10.87%	1.079%
26	15.786	2323	2329	2343	rVB5	11969	42119	3.77%	0.374%
27	16.186	2390	2397	2407	rBV2	47846	79882	7.15%	0.709%
28	16.733	2482	2490	2497	rBV2	17988	36899	3.30%	0.328%

Sum of corrected areas: 11261684

LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102119\
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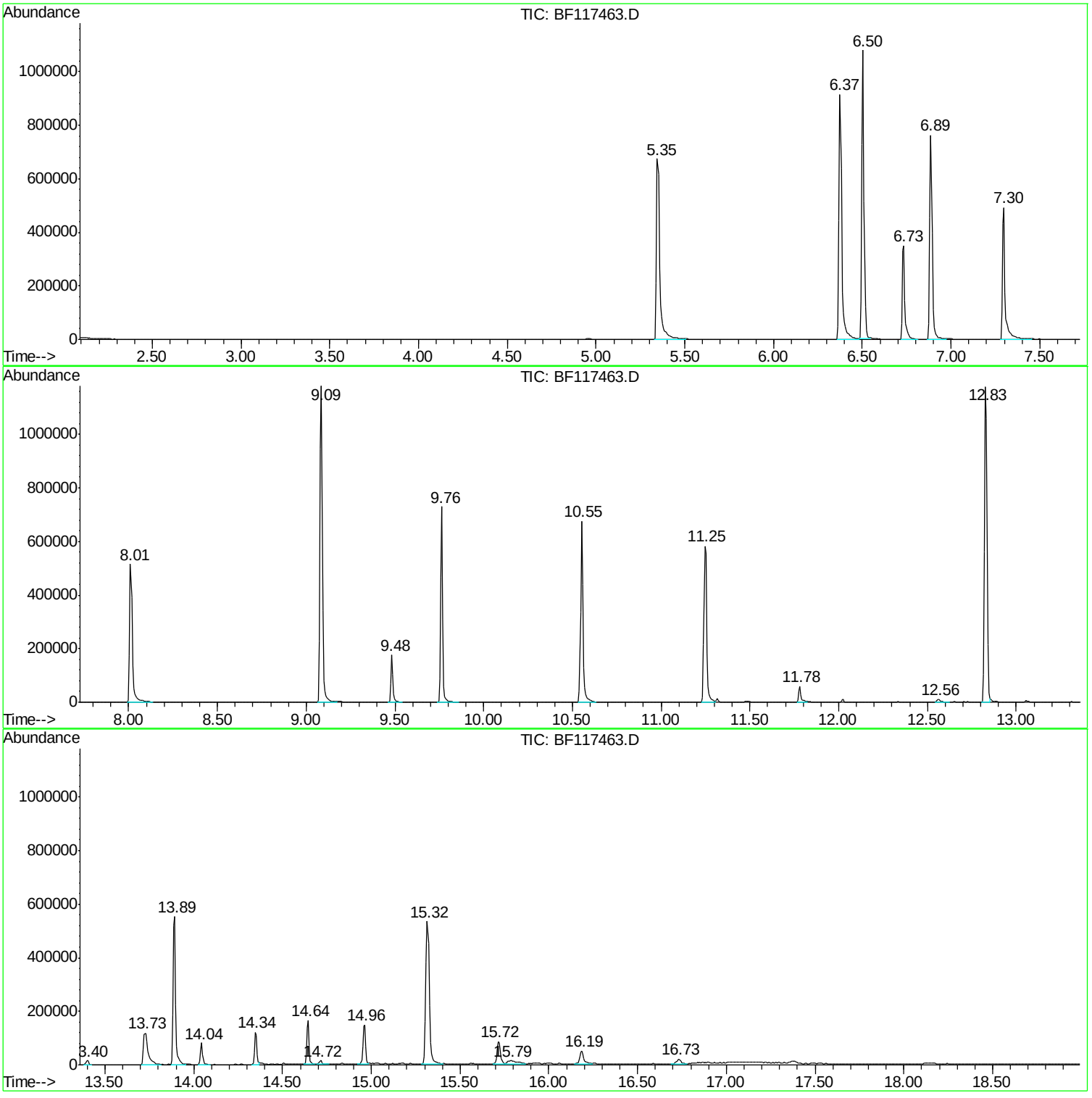
Operator : JU
Sample : K5448-01
Misc :
ALS Vial : 16 Sample Multiplier: 2

Instrument :
BNA_F
ClientSampleId :
SP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.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 : BF117463.D
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Operator : JU
Sample : K5448-01
Misc :
ALS Vial : 16 Sample Multiplier: 2

Instrument : BNA_F
ClientSampleId : SP

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

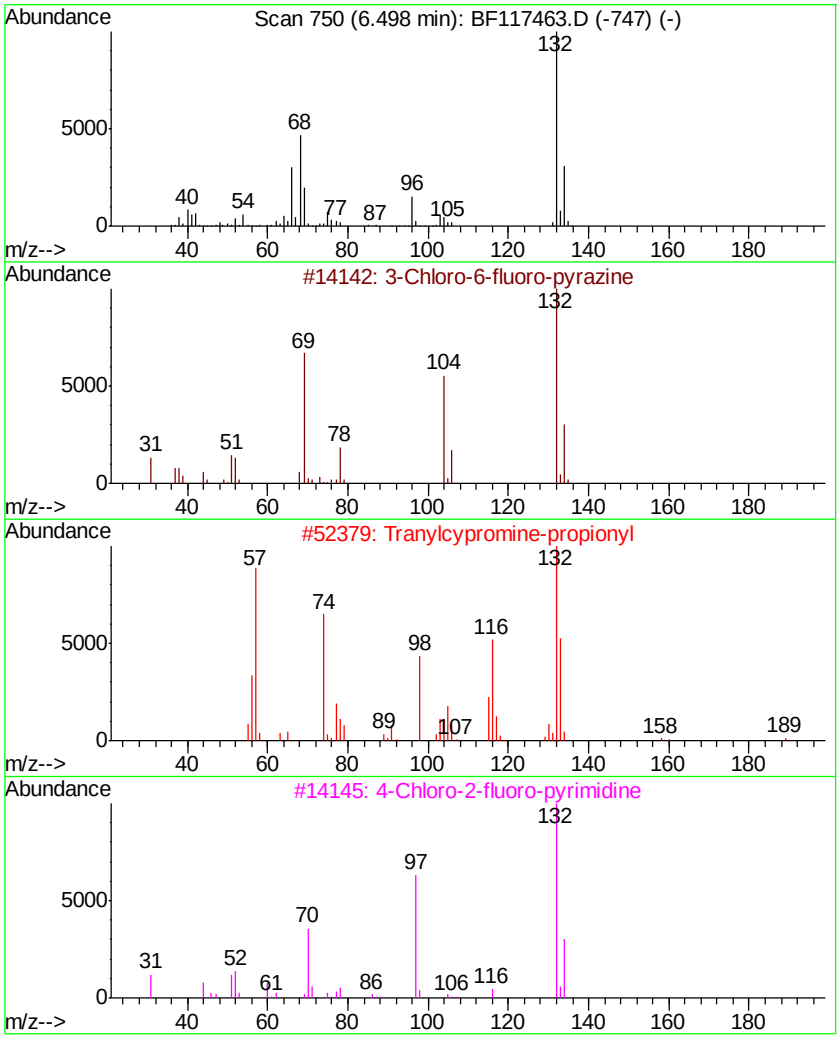
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

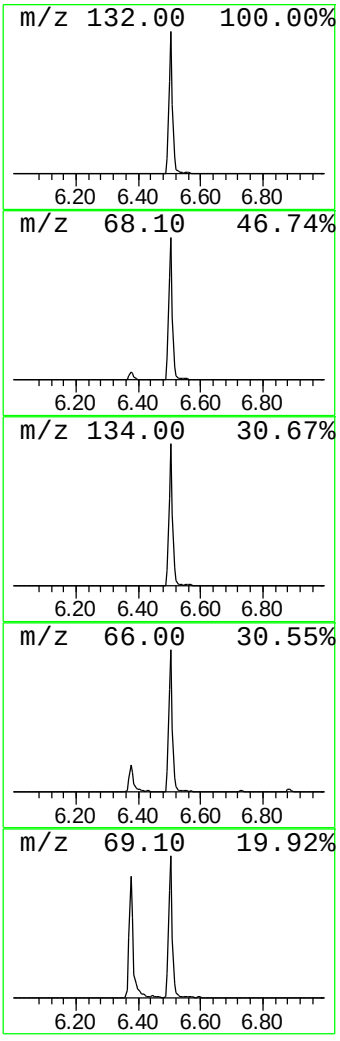
****

Peak Number 1 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	50.49 ng	926123	1,4-Dichlorobenzene-d4	6.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9





Library Search Compound Report

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Operator : JU
Sample : K5448-01
Misc :
ALS Vial : 16 Sample Multiplier: 2

Instrument : BNA_F
ClientSampleId : SP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.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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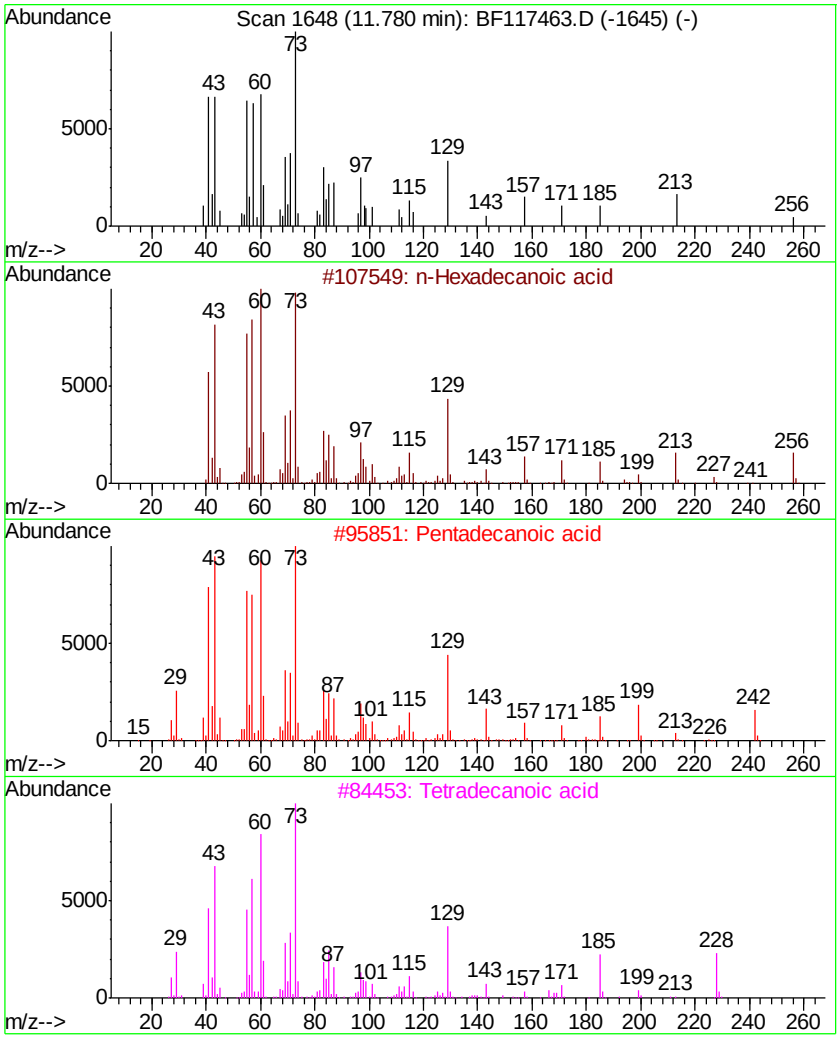
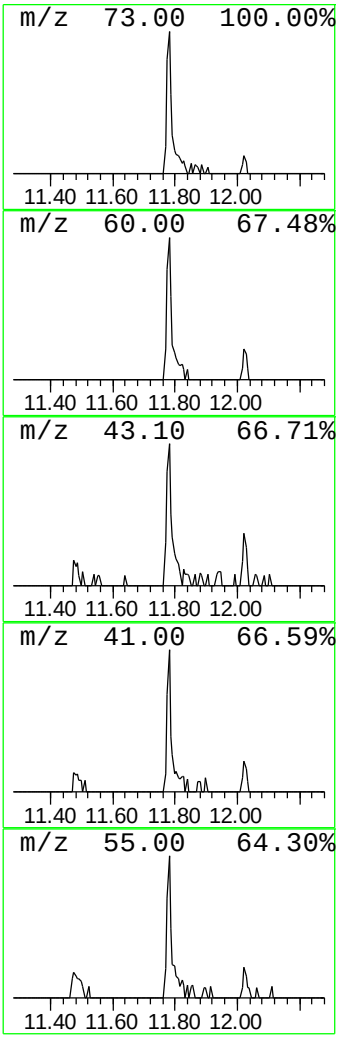
Peak Number 3 n-Hexadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.78	2.08 ng	62653	Phenanthrene-d10	11.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	53
4	Tridecanoic acid	214	C13H26O2	000638-53-9	53
5	Dodecanoic acid	200	C12H24O2	000143-07-7	53





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102119\
Data File : BF117463.D
Acq On : 21 Oct 2019 22:28
Operator : JU
Sample : K5448-01
Misc :
ALS Vial : 16 Sample Multiplier: 2

Instrument : BNA_F
ClientSampleId : SP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

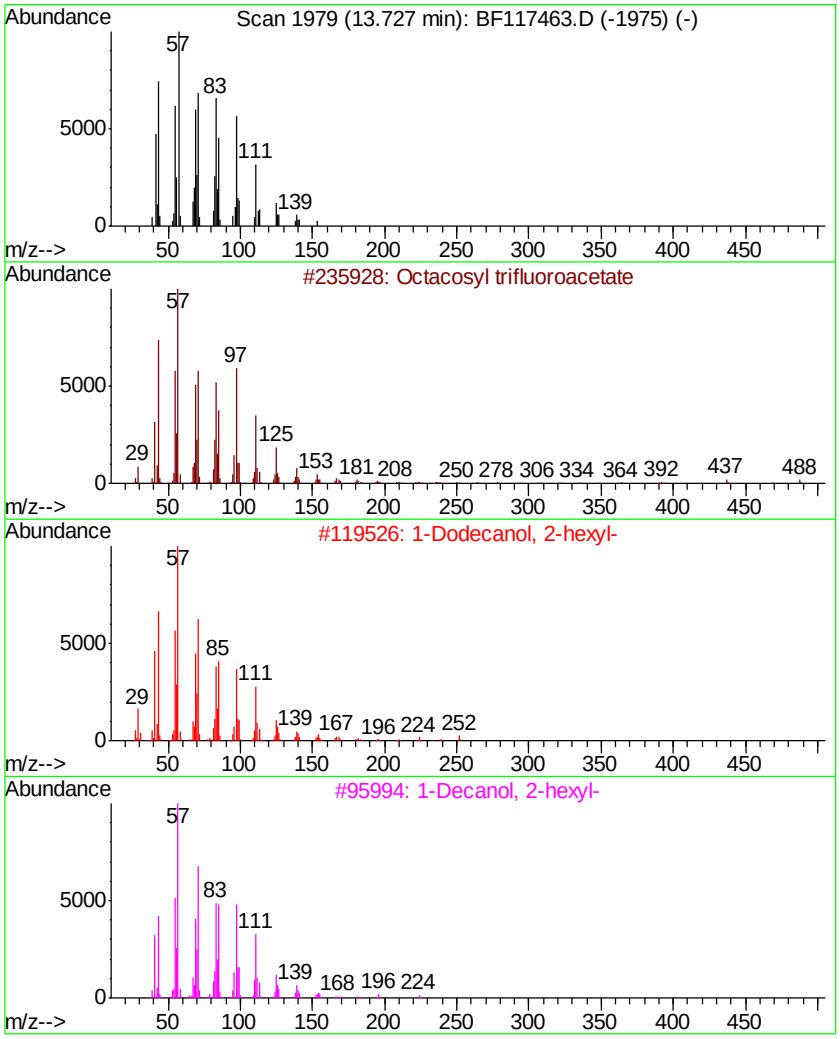
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

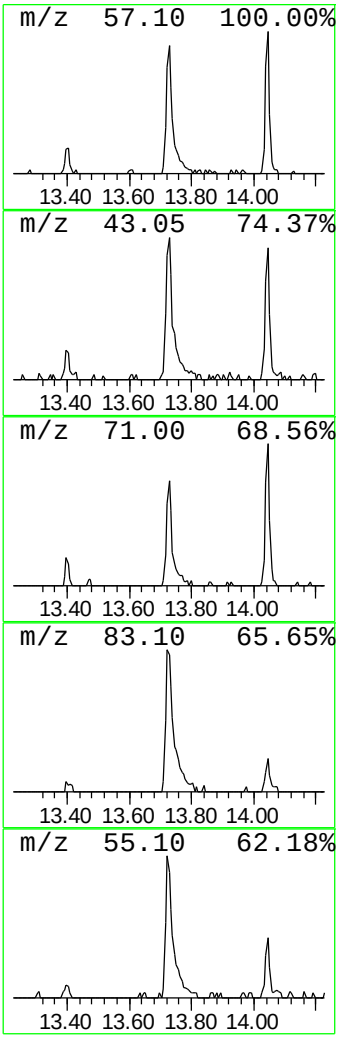
****

Peak Number 4 Octacosyl trifluoroacetate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.73	6.87 ng	199262	Chrysene-d12	13.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	86
2	1-Dodecanol, 2-hexyl-	270	C18H38O	110225-00-8	76
3	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	74
4	17-Pentatriacontene	491	C35H70	006971-40-0	72
5	1-Heneicosanol	312	C21H44O	015594-90-8	70





Library Search Compound Report

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Data File : BF117463.D
Acq On : 21 Oct 2019 22:28
Operator : JU
Sample : K5448-01
Misc :
ALS Vial : 16 Sample Multiplier: 2

Instrument : BNA_F
ClientSampleId : SP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

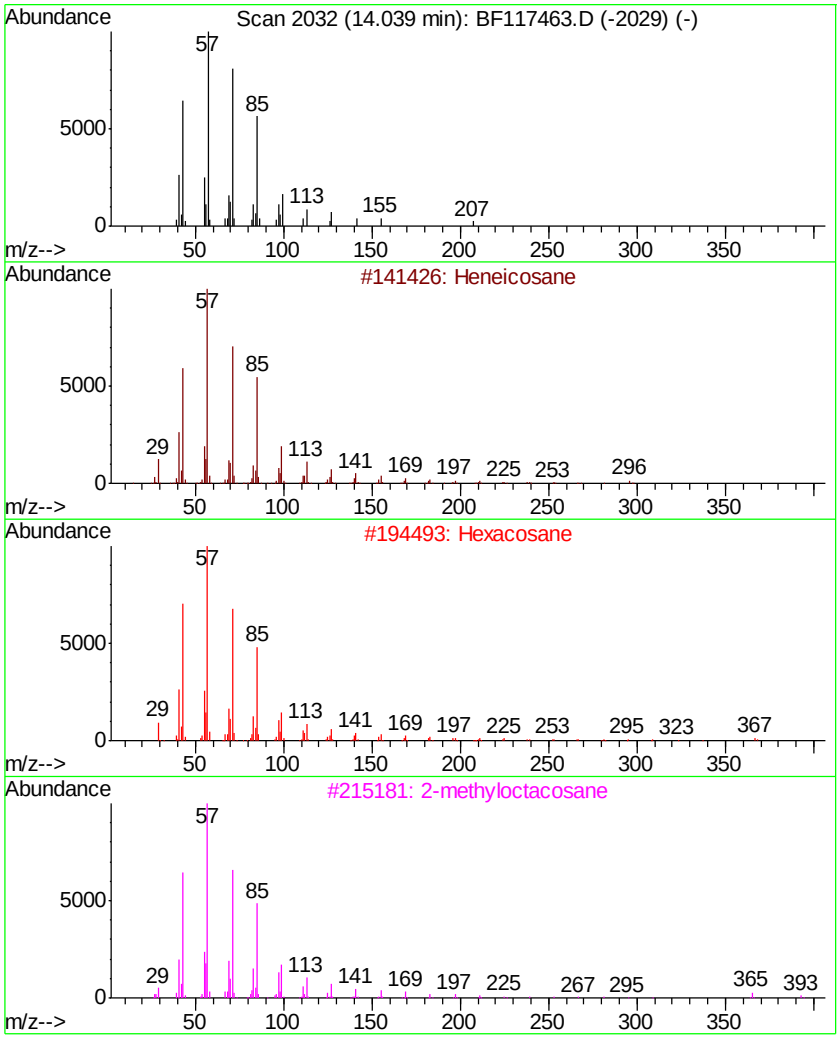
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

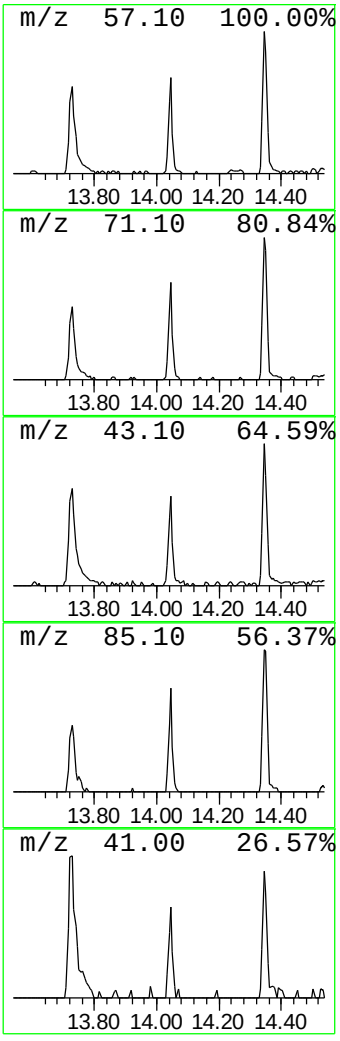
****

Peak Number 5 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.04	2.54 ng	73618	Chrysene-d12	13.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Hexacosane	366	C26H54	000630-01-3	91
3	2-methyloctacosane	408	C29H60	1000376-72-8	90
4	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	86
5	Octacosane	394	C28H58	000630-02-4	83





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102119\
Data File : BF117463.D
Acq On : 21 Oct 2019 22:28
Operator : JU
Sample : K5448-01
Misc :
ALS Vial : 16 Sample Multiplier: 2

Instrument : BNA_F
ClientSampleId : SP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

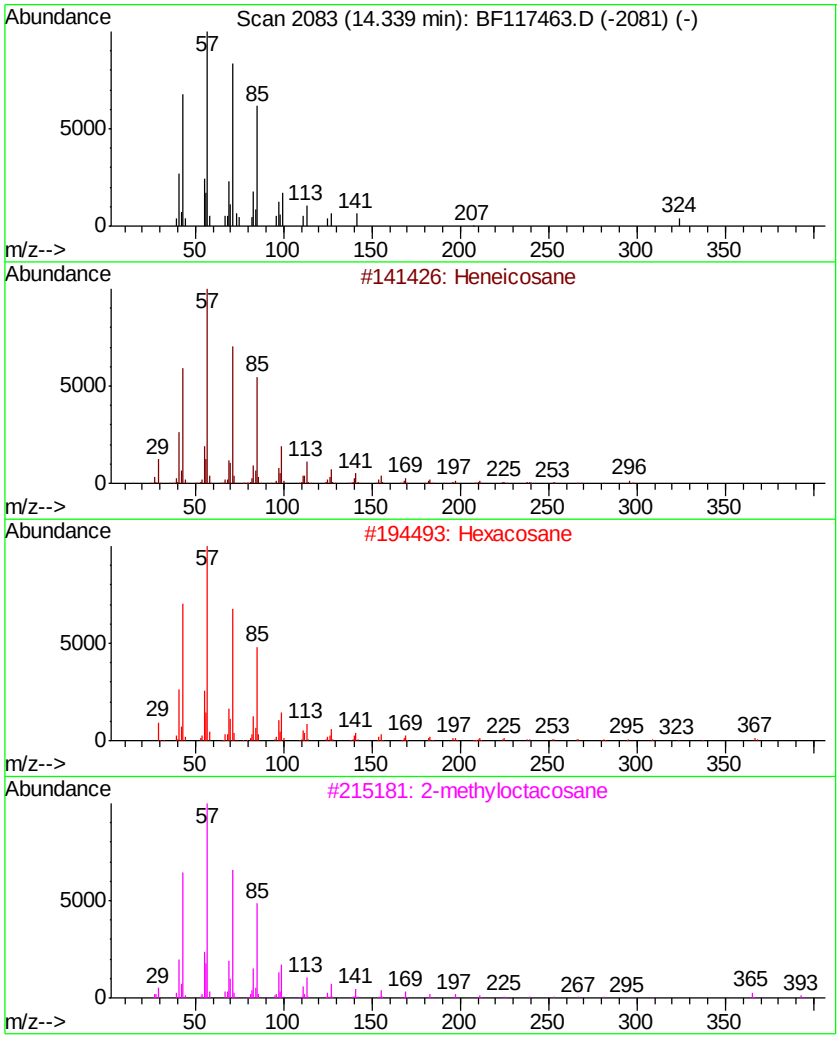
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

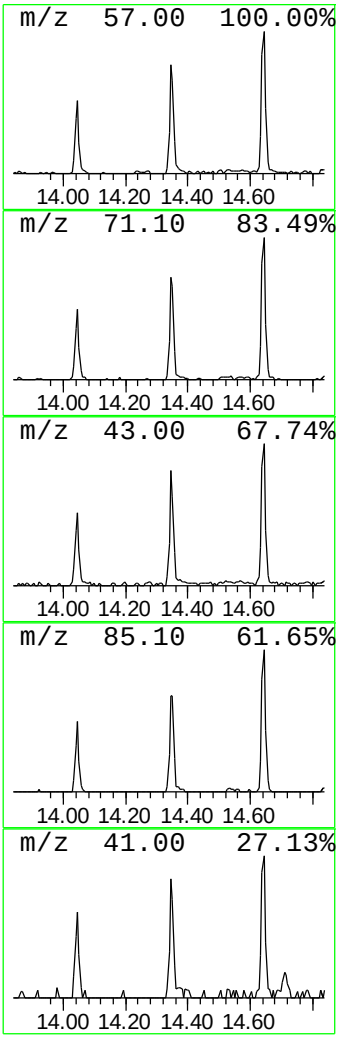
****

Peak Number 6 Hexacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.34	4.15 ng	120223	Chrysene-d12	13.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Hexacosane	366	C26H54	000630-01-3	91
3	2-methyloctacosane	408	C29H60	1000376-72-8	90
4	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	86
5	Pentacosane	352	C25H52	000629-99-2	86





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102119\
Data File : BF117463.D
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Operator : JU
Sample : K5448-01
Misc :
ALS Vial : 16 Sample Multiplier: 2

Instrument : BNA_F
ClientSampleId : SP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

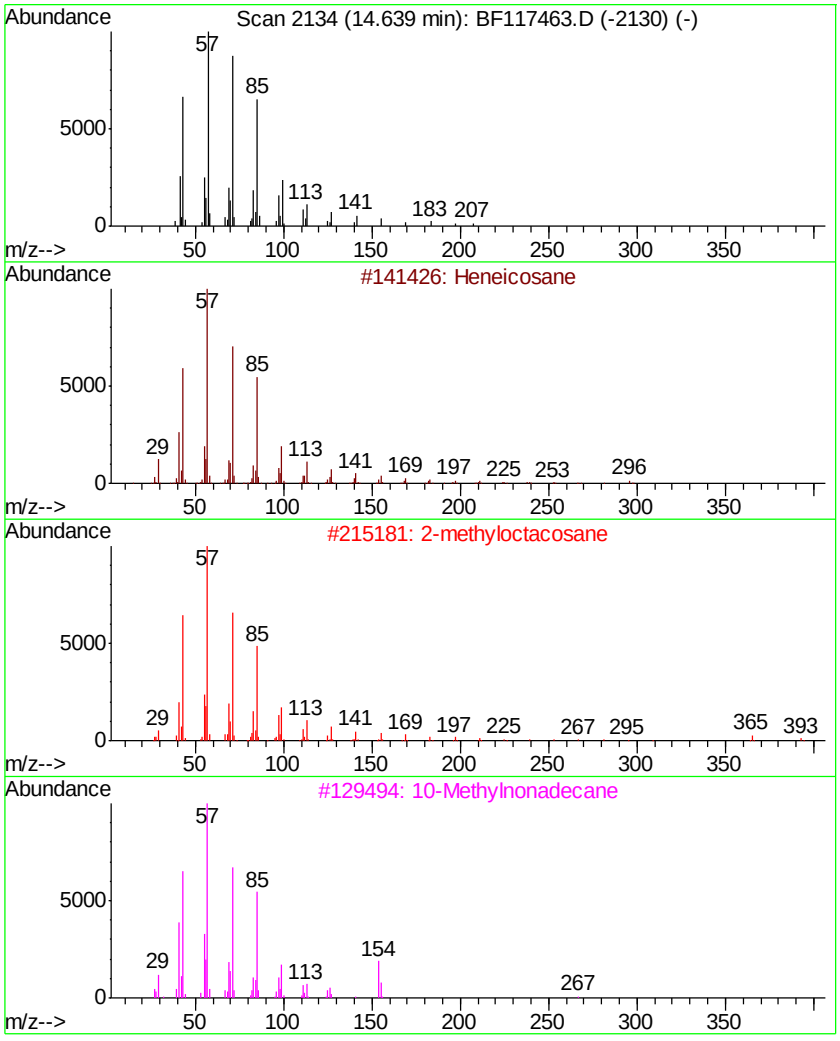
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

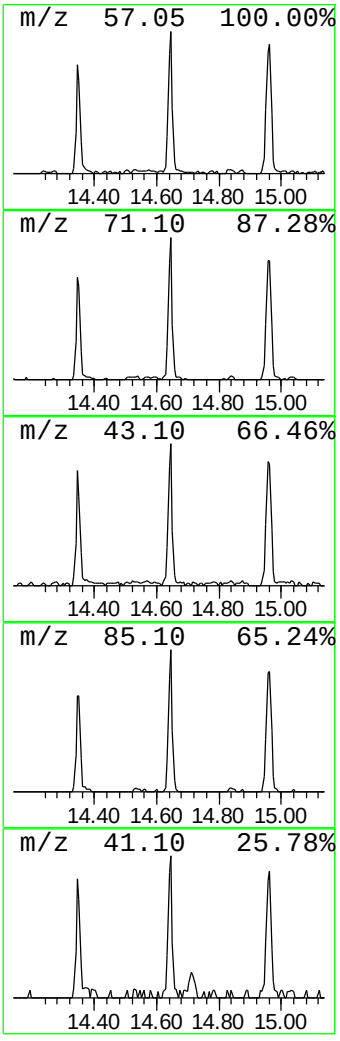
****

Peak Number 7 2-methyloctacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.64	4.40 ng	153852	Perylene-d12	15.32

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	90
3	10-Methylnonadecane	282	C20H42	056862-62-5	87
4	Hexacosane	366	C26H54	000630-01-3	87
5	Heptacosane	380	C27H56	000593-49-7	87





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Misc :
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Instrument : BNA_F
ClientSampleId : SP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

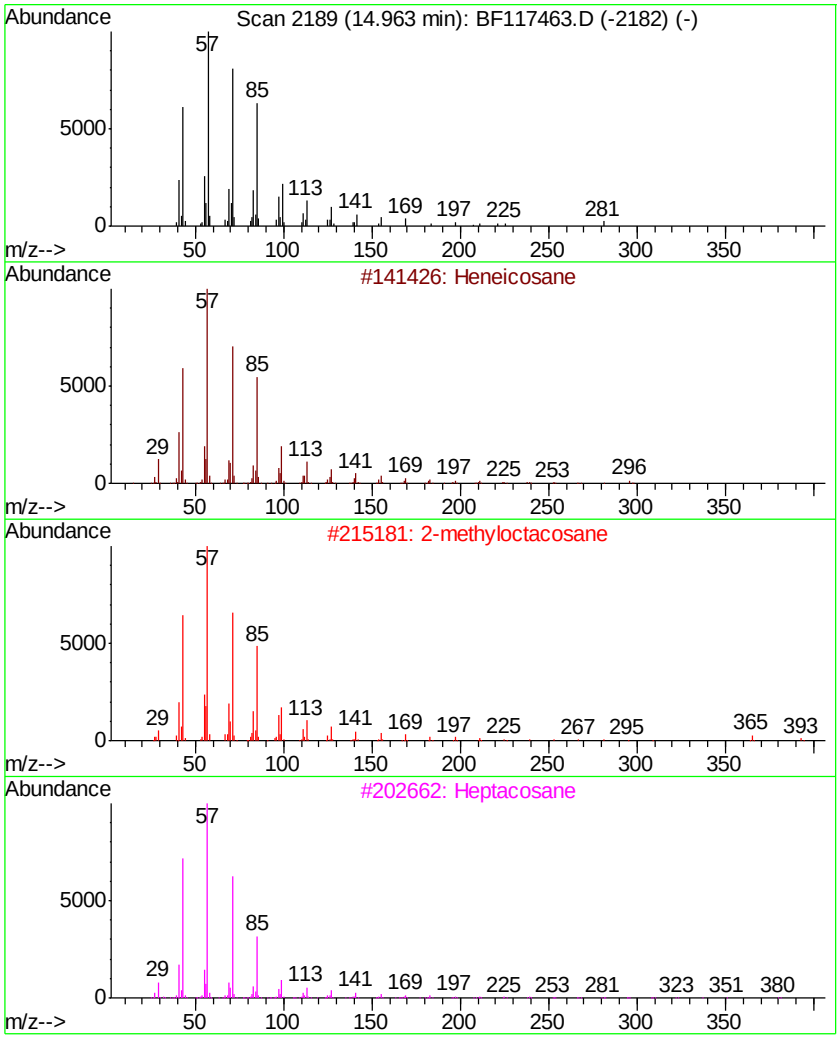
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

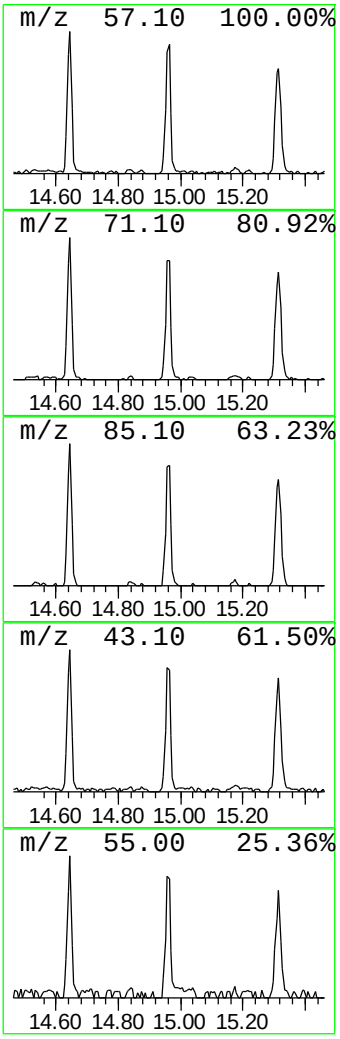
****

Peak Number 8 Heptacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.96	4.73 ng	165488	Perylene-d12	15.32

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	Heptacosane	380	C27H56	000593-49-7	91
4	Triacontane	422	C30H62	000638-68-6	91
5	Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	90





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Sample : K5448-01
Misc :
ALS Vial : 16 Sample Multiplier: 2

Instrument : BNA_F
ClientSampleId : SP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

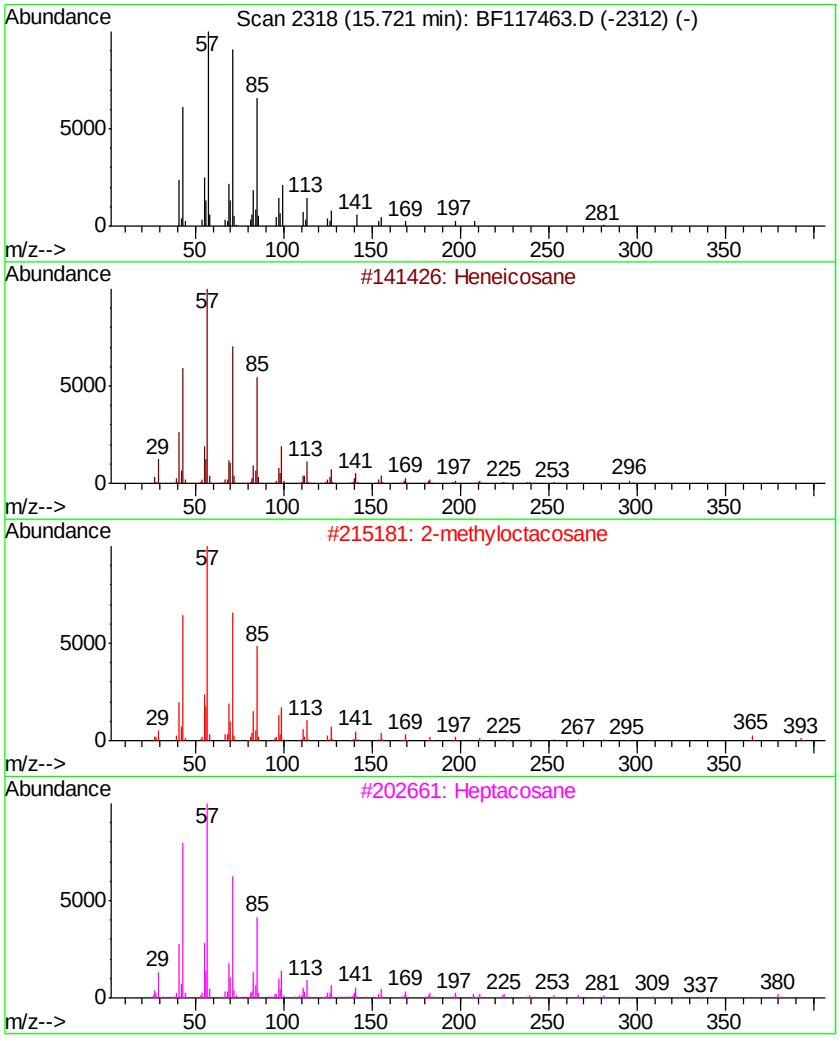
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

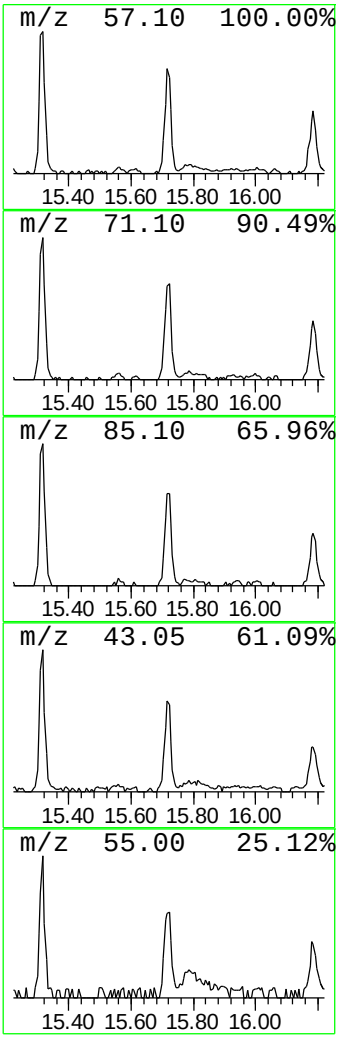
****

Peak Number 9 Heneicosane, 11-(1-ethylpro... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.72	3.47 ng	121473	Perylene-d12	15.32

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	Heptacosane	380	C27H56	000593-49-7	91
4	Hexacosane	366	C26H54	000630-01-3	91
5	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91





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ClientSampleId : SP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

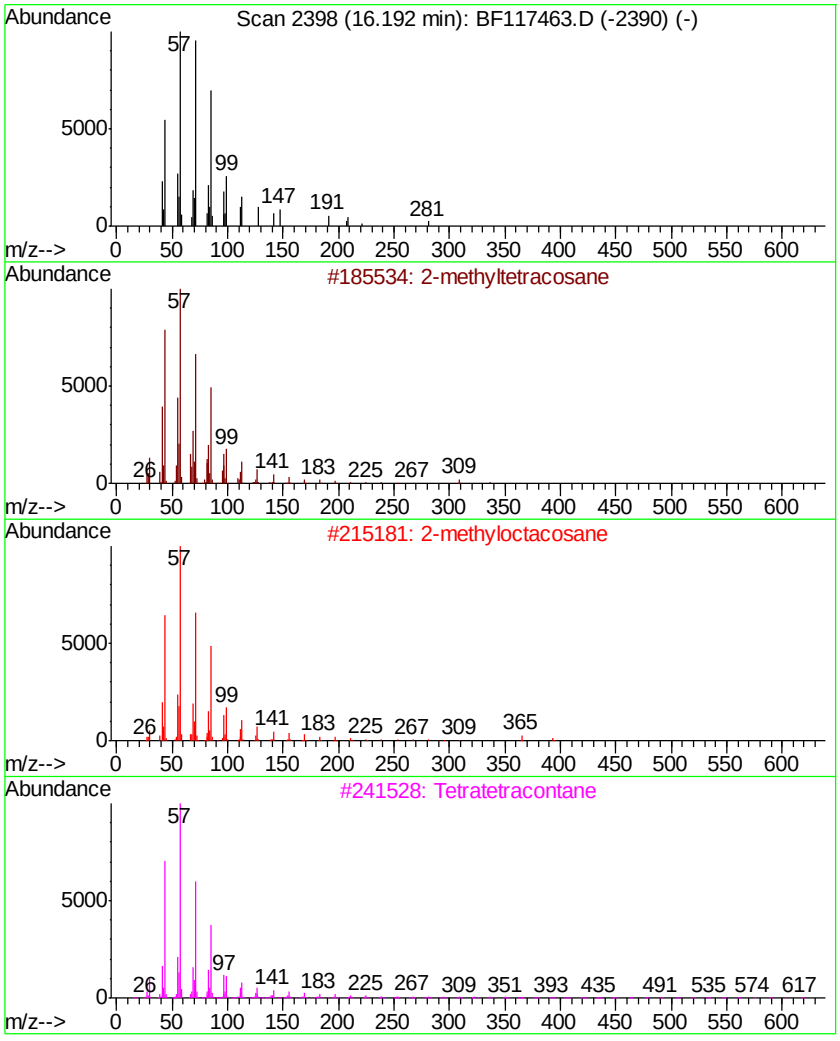
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

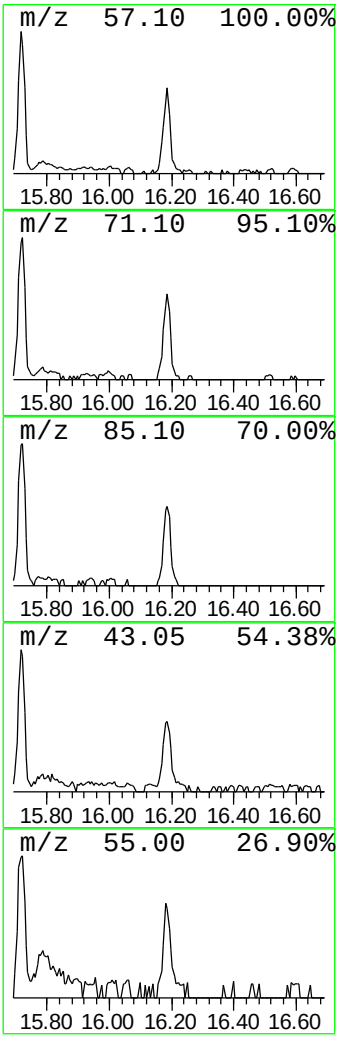
****

Peak Number 10 2-methyltetracosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.19	2.28 ng	79882	Perylene-d12	15.32

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	90
3	Tetratetracontane	619	C44H90	007098-22-8	86
4	Heneicosane	296	C21H44	000629-94-7	80
5	Tritetracontane	605	C43H88	007098-21-7	80





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF102119\
Data File : BF117463.D
Acq On : 21 Oct 2019 22:28
Operator : JU
Sample : K5448-01
Misc :
ALS Vial : 16 Sample Multiplier: 2

Instrument : BNA_F
ClientSampleId : SP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.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
unknown6.50	6.50	50.5	ng	926123	1	6.73	366834	20.0
n-Hexadecanoic acid	11.78	2.1	ng	62653	4	11.25	601042	20.0
Octacosyl trifluo...	13.73	6.9	ng	199262	5	13.89	579932	20.0
Heneicosane	14.04	2.5	ng	73618	5	13.89	579932	20.0
Hexacosane	14.34	4.2	ng	120223	5	13.89	579932	20.0
2-methyloctacosane	14.64	4.4	ng	153852	6	15.32	699393	20.0
Heptacosane	14.96	4.7	ng	165488	6	15.32	699393	20.0
Heneicosane, 11-(...	15.72	3.5	ng	121473	6	15.32	699393	20.0
2-methyltetracosane	16.19	2.3	ng	79882	6	15.32	699393	20.0