LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF042319\
Data File : BF113917.D
Acq On : 23 Apr 2019 13:54
Operator : JU/SJ
Sample : K2532-07
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-2

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-BF042219.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	2.210	18	21	29	rVB	49332	76637	2.02%	0.218%
2	5.128	512	517	522	rVB	33551	41674	1.10%	0.119%
3	5.528	580	585	588	rBV	2755882	2760354	72.78%	7.864%
4	6.528	749	755	758	rBV	2836734	2869080	75.65%	8.174%
5	6.669	774	779	782	rBV	3217441	3032922	79.97%	8.641%
6	6.898	814	818	821	rBV	979153	776429	20.47%	2.212%
7	7.057	840	845	848	rBV	2724663	2415934	63.70%	6.883%
8	7.451	907	912	916	rBV	1812293	1891009	49.86%	5.388%
9	8.175	1031	1035	1039	rBV	1055879	990976	26.13%	2.823%
10	9.251	1213	1218	1222	rBV	3784998	3556626	93.77%	10.133%
11	9.639	1280	1284	1289	rBV	471181	390698	10.30%	1.113%
12	9.933	1329	1334	1340	rVB	1411320	1236442	32.60%	3.523%
13	10.721	1463	1468	1481	rBV	2469211	2448017	64.54%	6.974%
14	11.416	1582	1586	1590	rBV	1542074	1367008	36.04%	3.895%
15	11.945	1666	1676	1686	rBV	603955	908980	23.97%	2.590%
16	12.627	1789	1792	1794	rBV2	60903	71836	1.89%	0.205%
17	12.727	1804	1809	1822	rVB	964812	1359996	35.86%	3.875%
18	12.951	1841	1847	1848	rBV2	62980	113848	3.00%	0.324%
19	13.004	1851	1856	1859	rVB	4166076	3792811	100.00%	10.806%
20	13.233	1892	1895	1902	rBV	91299	100945	2.66%	0.288%
21	13.580	1951	1954	1957	rVB	133749	118426	3.12%	0.337%
22	13.909	2006	2010	2013	rBV	178265	156851	4.14%	0.447%
23	14.021	2025	2029	2031	rBV4	60003	95377	2.51%	0.272%
24	14.062	2032	2036	2039	rVB	1362370	1199275	31.62%	3.417%
25	14.233	2062	2065	2068	rBV	156129	133788	3.53%	0.381%
26	14.357	2080	2086	2102	rVB2	152660	423179	11.16%	1.206%
27	14.551	2116	2119	2124	rVB	181617	168100	4.43%	0.479%
28	14.868	2169	2173	2177	rVB	218656	228079	6.01%	0.650%
29	15.215	2227	2232	2237	rBV	250445	322104	8.49%	0.918%
30	15.292	2241	2245	2253	rVB3	71233	161884	4.27%	0.461%
31	15.562	2286	2291	2295	rBV	773631	1012450	26.69%	2.884%
32	15.604	2295	2298	2307	rVB	247744	336566	8.87%	0.959%
33	16.051	2369	2374	2380	rBV	202569	319608	8.43%	0.911%
34	16.568	2458	2462	2473	rVB	119950	221823	5.85%	0.632%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF042319\
Data File : BF113917.D
Acq On : 23 Apr 2019 13:54
Operator : JU/SJ
Sample : K2532-07
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-2

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-BF042219.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

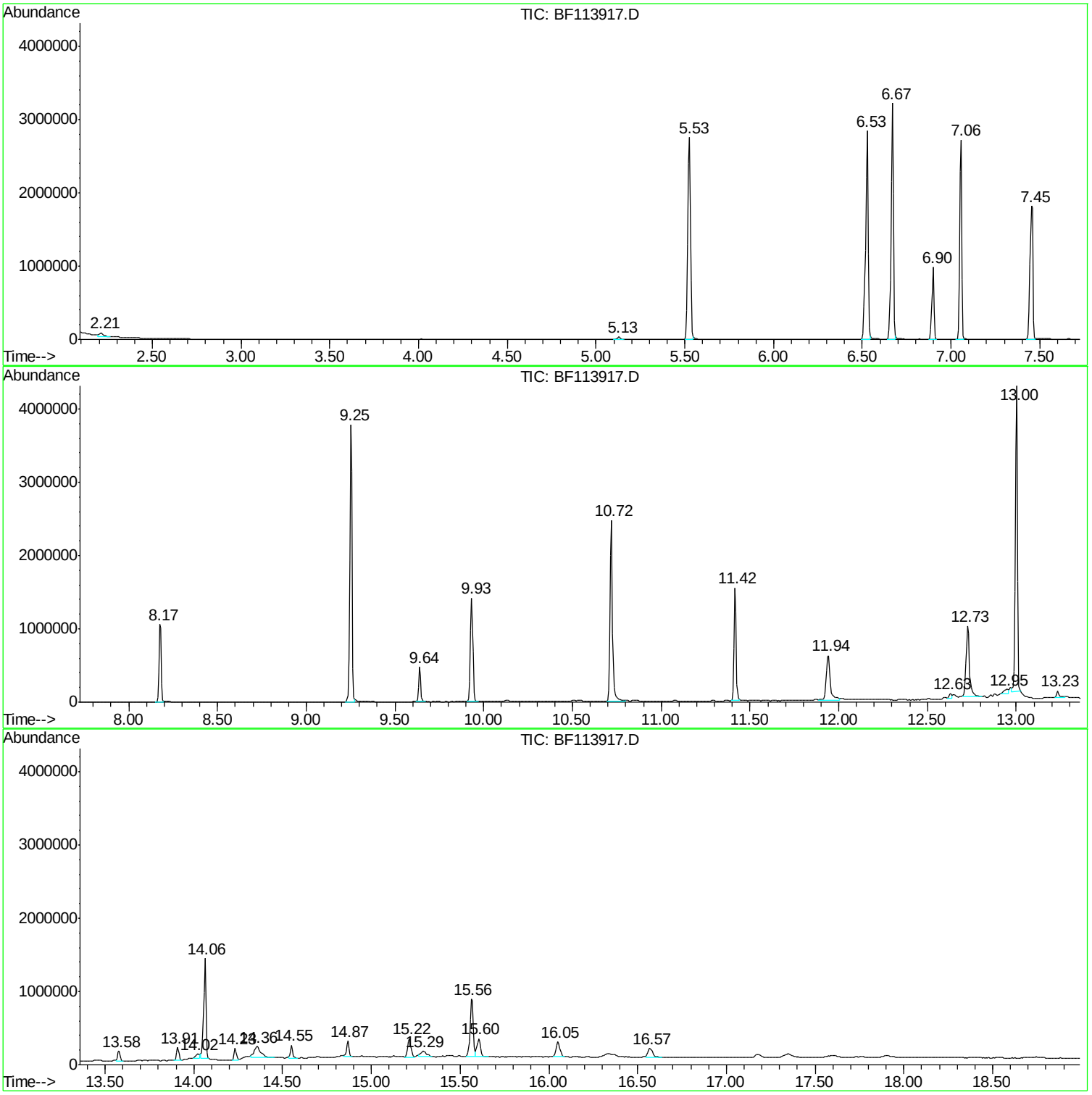
Sum of corrected areas: 35099732

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF042319\
Data File : BF113917.D
Acq On : 23 Apr 2019 13:54
Operator : JU/SJ
Sample : K2532-07
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042219.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\BF042319\
Data File : BF113917.D
Acq On : 23 Apr 2019 13:54
Operator : JU/SJ
Sample : K2532-07
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

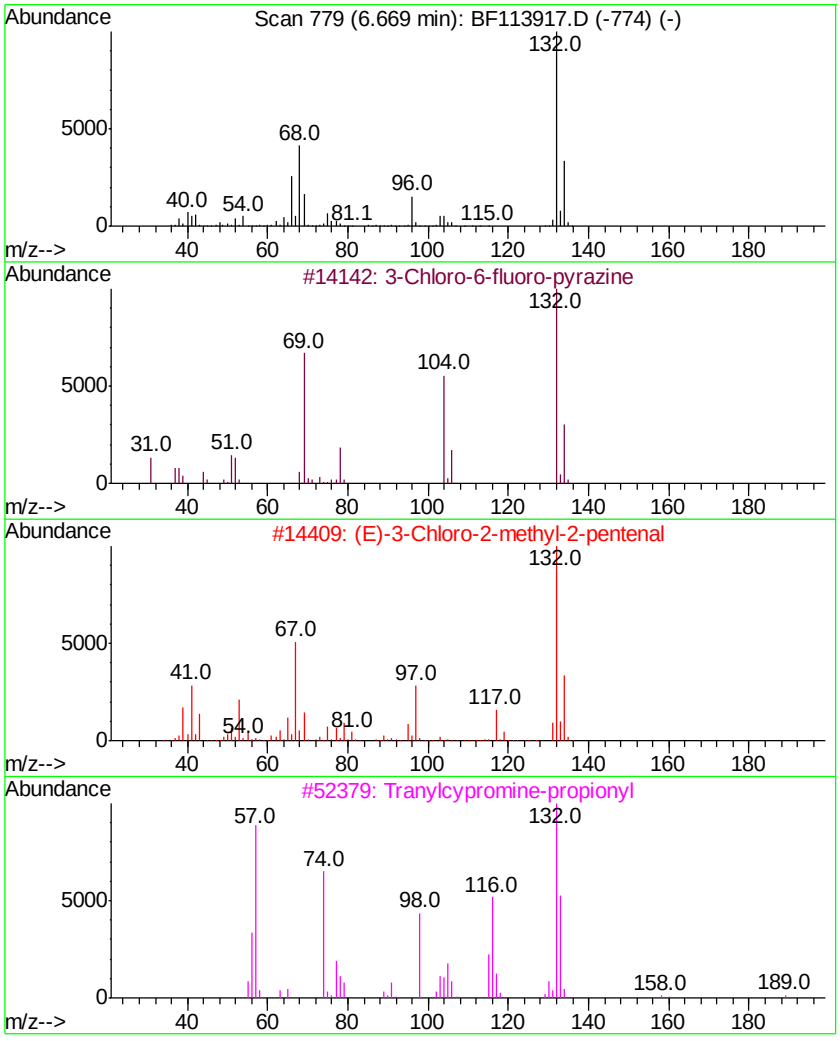
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

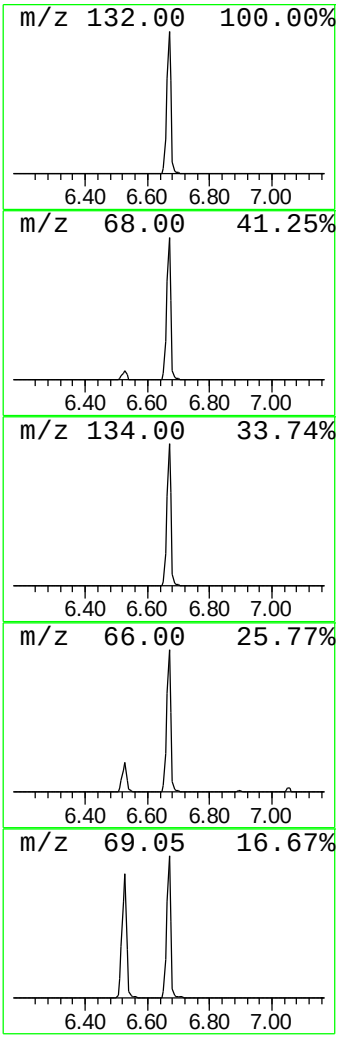
****

Peak Number 1 unknown6.67 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.67	78.12 ng	3032920	1,4-Dichlorobenzene-d4	6.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF042319\
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Sample : K2532-07
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

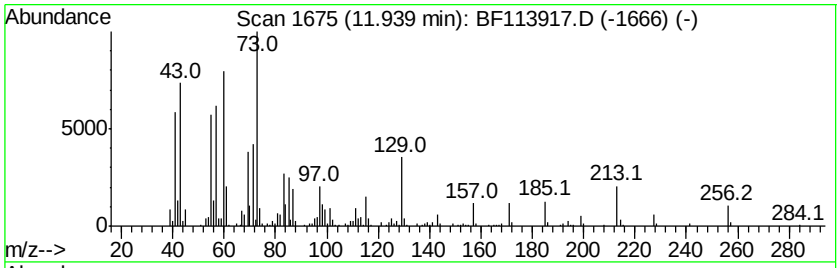
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

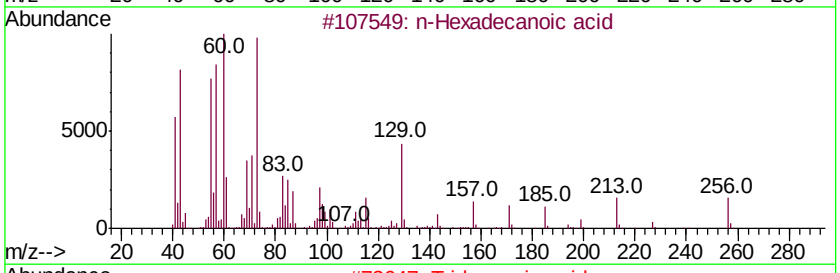
****

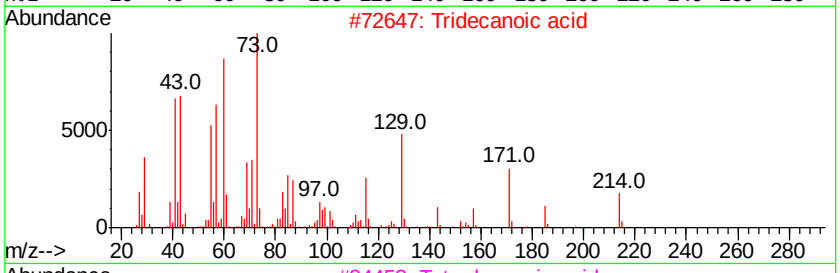
Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

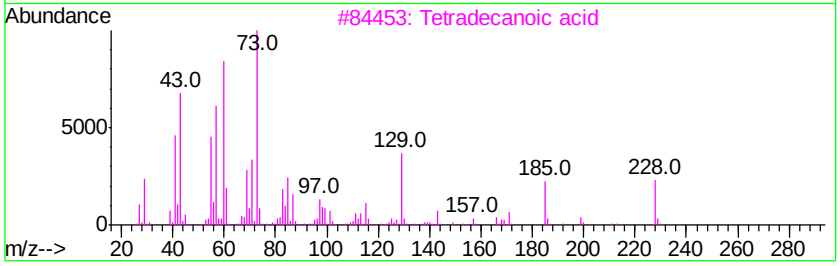
R.T.	EstConc	Area	Relative to ISTD	R.T.
11.94	13.30 ng	908980	Phenanthrene-d10	11.42

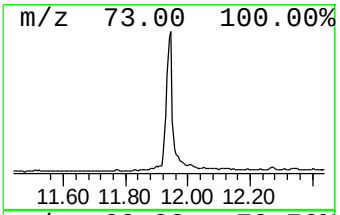
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	94
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	89
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	68
5	n-Decanoic acid	172	C10H20O2	000334-48-5	60

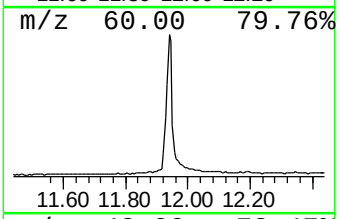


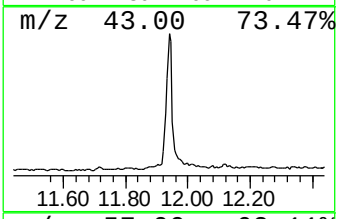


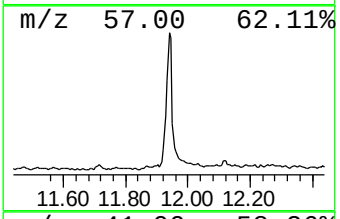


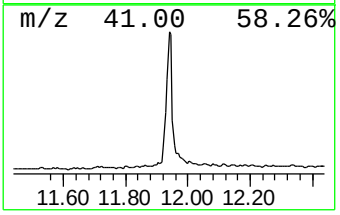












Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF042319\
Data File : BF113917.D
Acq On : 23 Apr 2019 13:54
Operator : JU/SJ
Sample : K2532-07
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

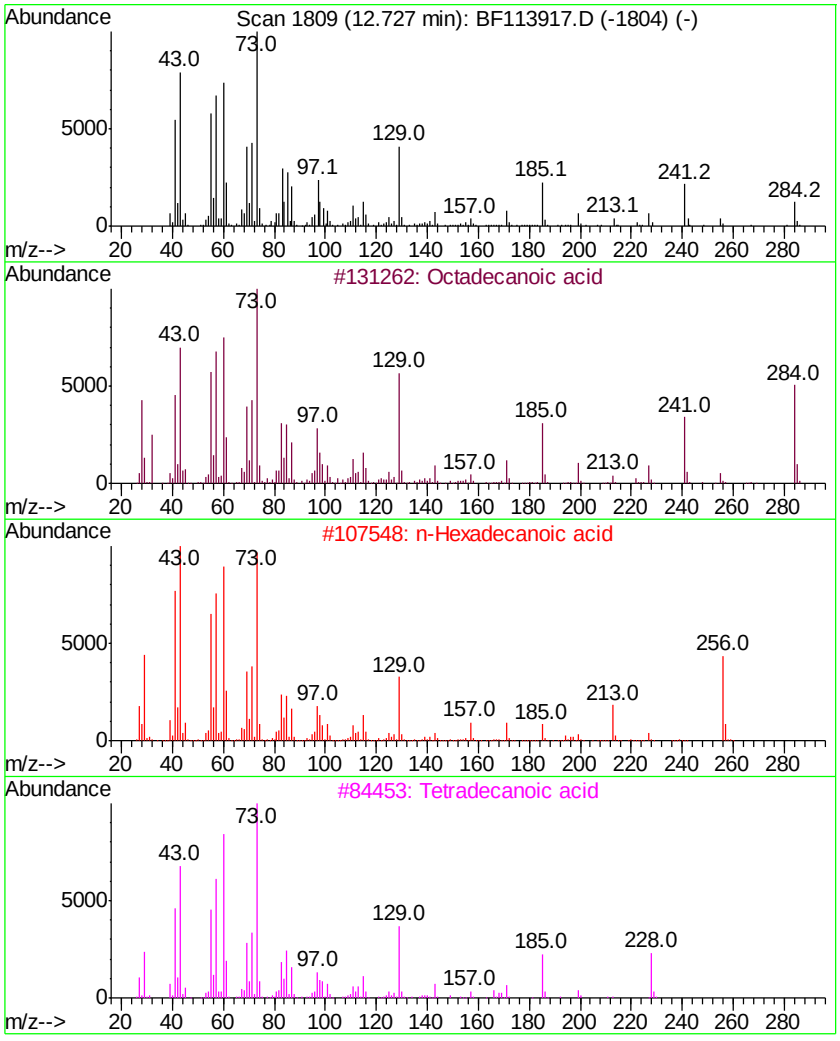
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

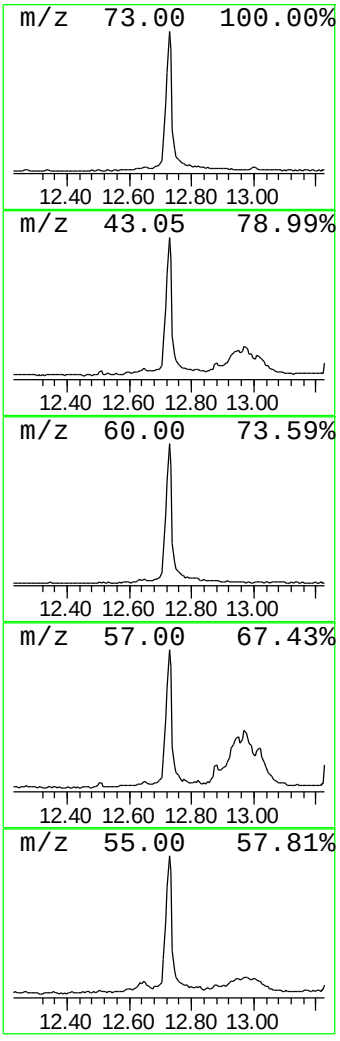
****

Peak Number 4 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.73	19.90 ng	1360000	Phenanthrene-d10	11.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5	Tridecanoic acid	214	C13H26O2	000638-53-9	76





Library Search Compound Report

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Misc :
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Instrument : BNA_F
ClientSampleId : TP-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

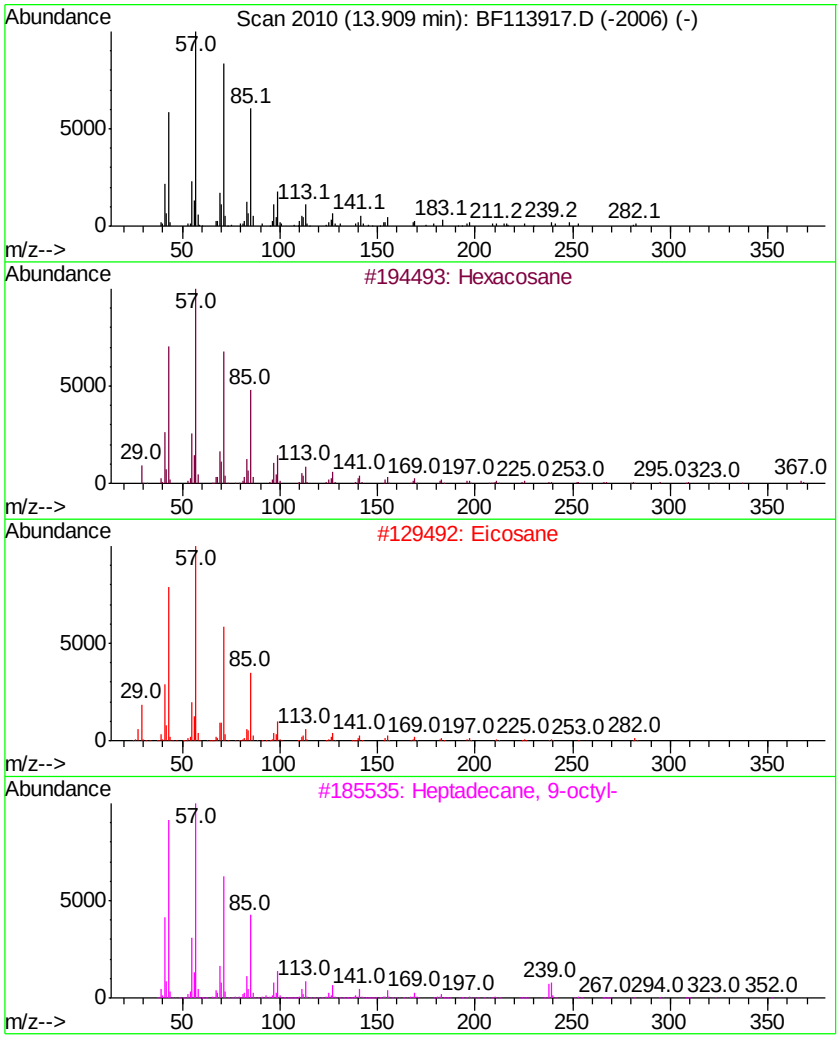
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

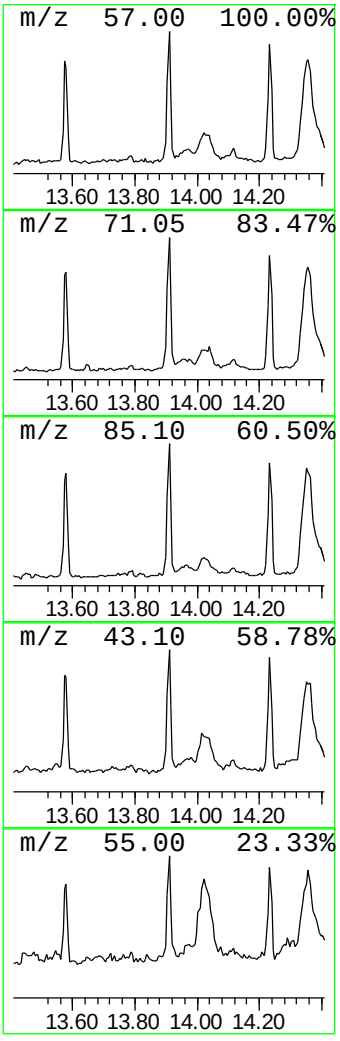
****

Peak Number 5 Hexacosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.91	2.62 ng	156851	Chrysene-d12	14.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	94
2	Eicosane	282	C20H42	000112-95-8	94
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4	Octacosane	394	C28H58	000630-02-4	91
5	Heneicosane	296	C21H44	000629-94-7	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF042319\
Data File : BF113917.D
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Operator : JU/SJ
Sample : K2532-07
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

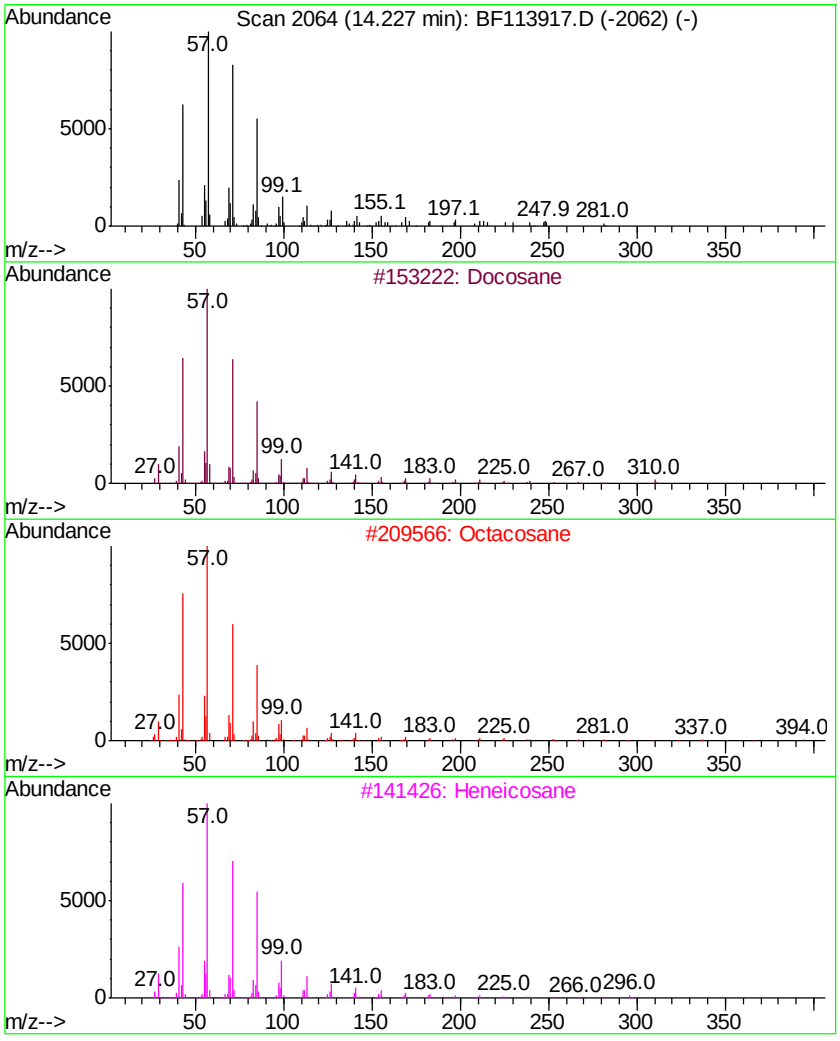
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

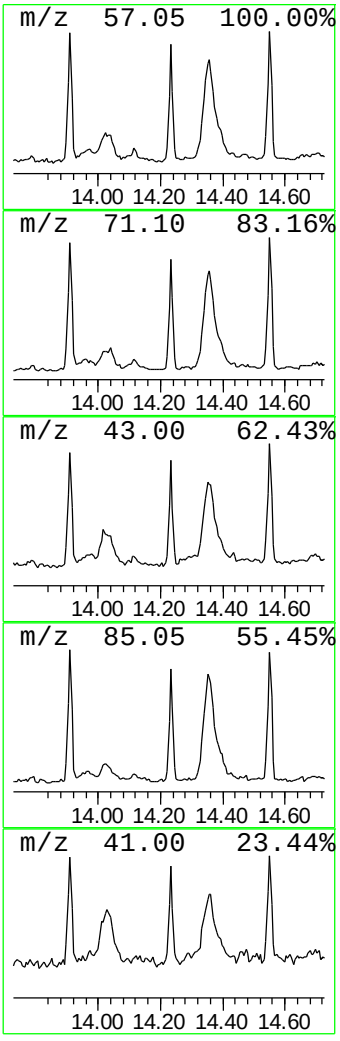
****

Peak Number 6 Docosane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.23	2.23 ng	133788	Chrysene-d12	14.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosane	310	C22H46	000629-97-0	91
2	Octacosane	394	C28H58	000630-02-4	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	2-methyloctacosane	408	C29H60	1000376-72-8	91
5	Heptacosane	380	C27H56	000593-49-7	91





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF042319\
Data File : BF113917.D
Acq On : 23 Apr 2019 13:54
Operator : JU/SJ
Sample : K2532-07
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042219.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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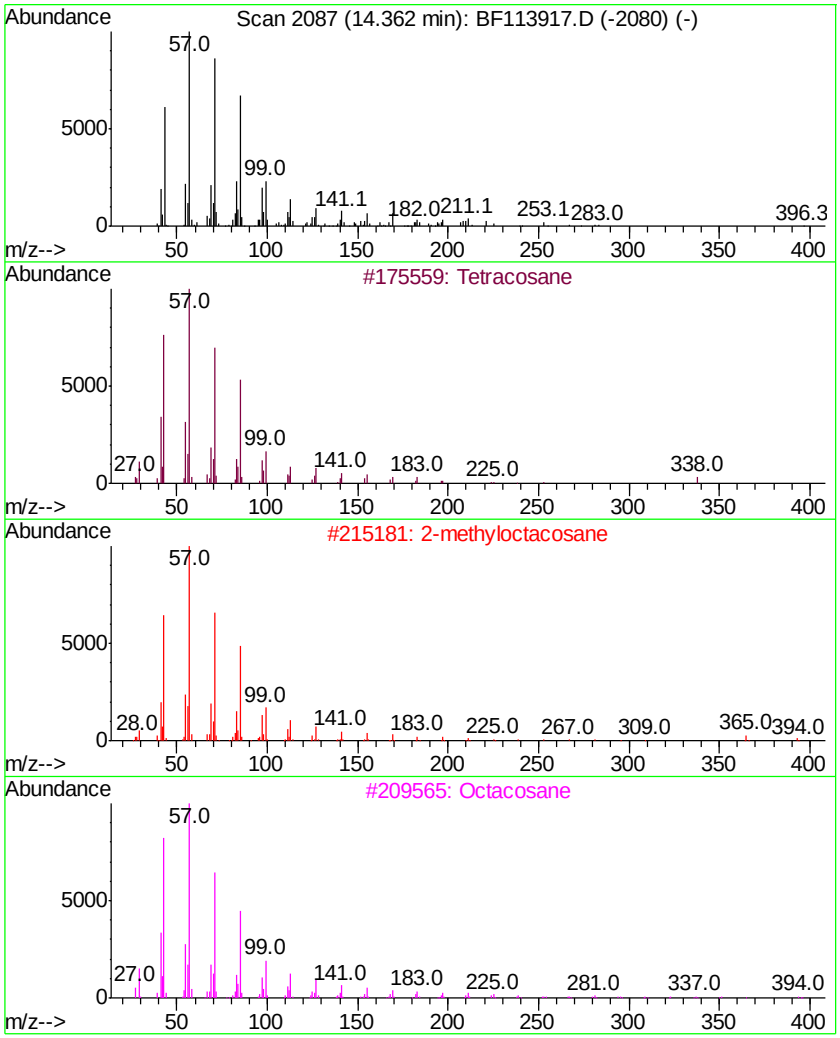
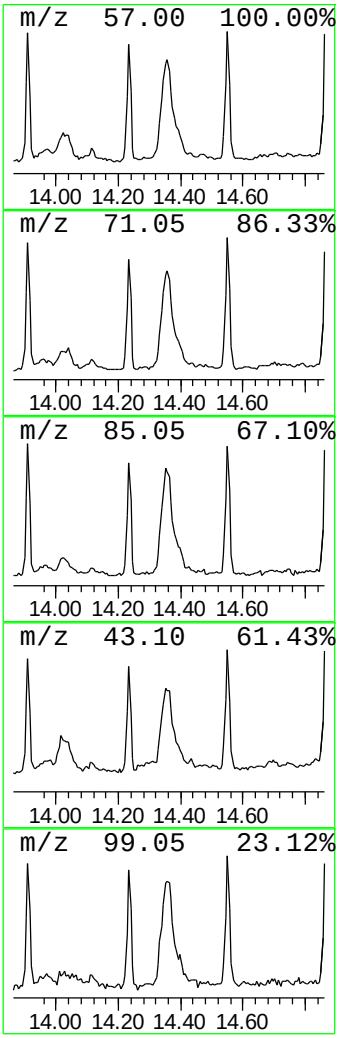
Peak Number 7 Tetracosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.36	7.06 ng	423179	Chrysene-d12	14.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	91
2	2-methyloctacosane	408	C29H60	1000376-72-8	91
3	Octacosane	394	C28H58	000630-02-4	91
4	Hexacosane	366	C26H54	000630-01-3	91
5	Triacontane	422	C30H62	000638-68-6	91





Library Search Compound Report

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Data File : BF113917.D
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Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

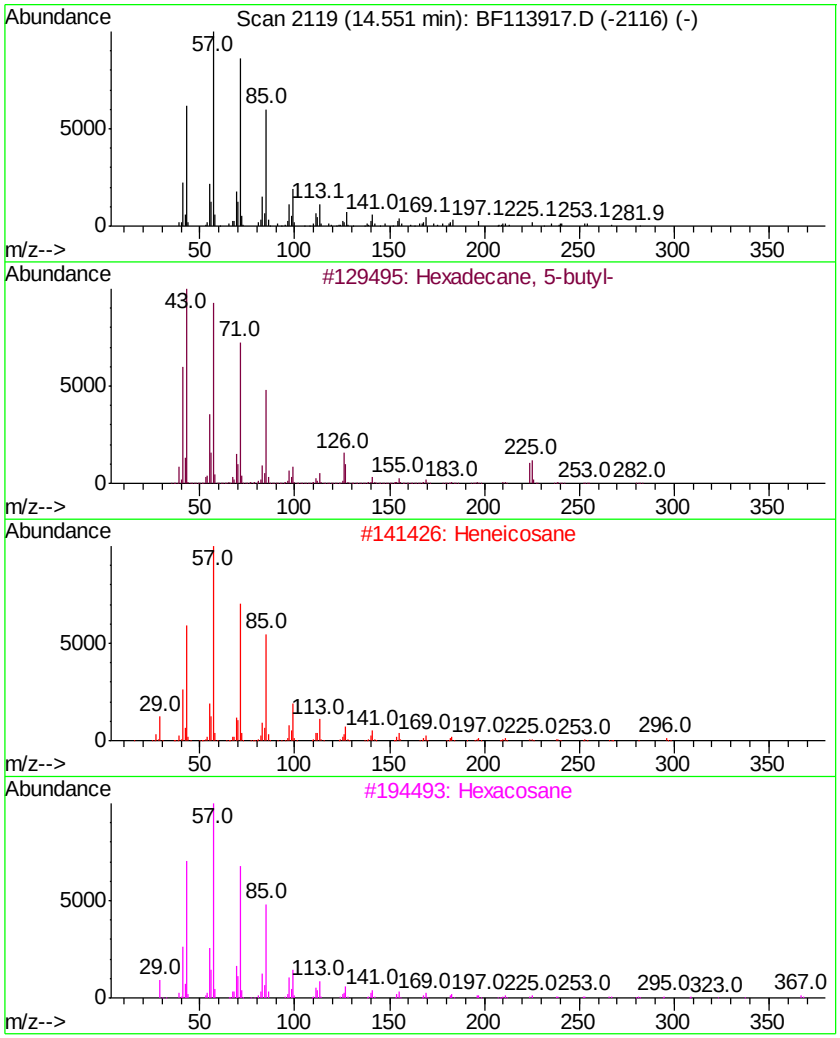
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

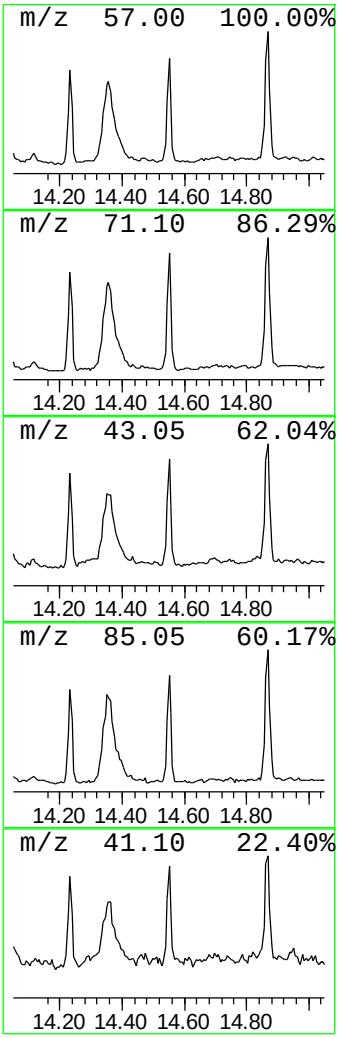
****

Peak Number 8 Hexadecane, 5-butyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.55	2.80 ng	168100	Chrysene-d12	14.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane, 5-butyl-	282	C20H42	006912-07-8	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Hexacosane	366	C26H54	000630-01-3	91
4	2-methyloctacosane	408	C29H60	1000376-72-8	91
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF042319\
Data File : BF113917.D
Acq On : 23 Apr 2019 13:54
Operator : JU/SJ
Sample : K2532-07
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042219.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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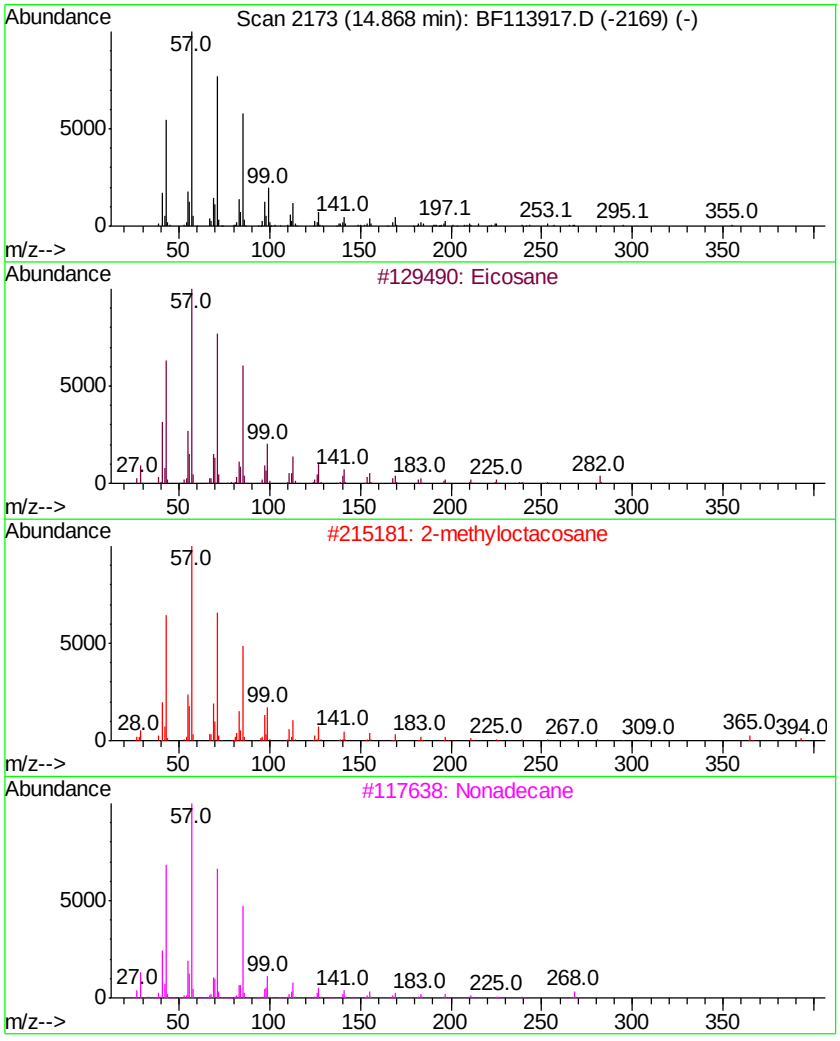
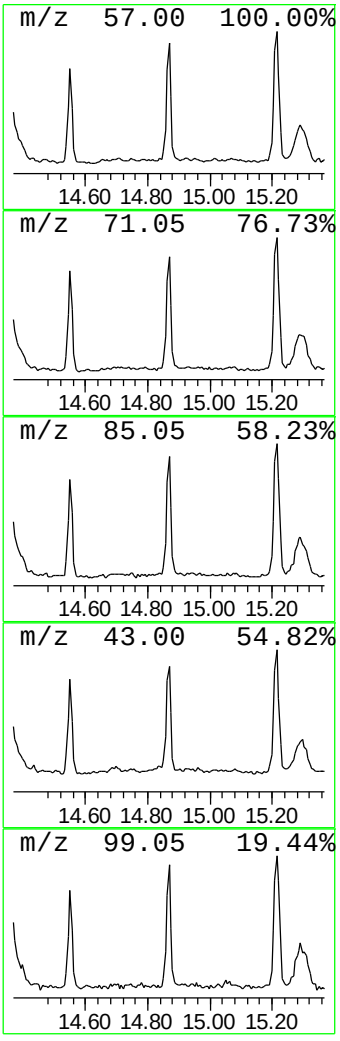
Peak Number 9 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.87	4.51 ng	228079	Perylene-d12	15.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	94
2	2-methyloctacosane	408	C29H60	1000376-72-8	91
3	Nonadecane	268	C19H40	000629-92-5	91
4	Heneicosane	296	C21H44	000629-94-7	91
5	Hexacosane	366	C26H54	000630-01-3	90





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF042319\
Data File : BF113917.D
Acq On : 23 Apr 2019 13:54
Operator : JU/SJ
Sample : K2532-07
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042219.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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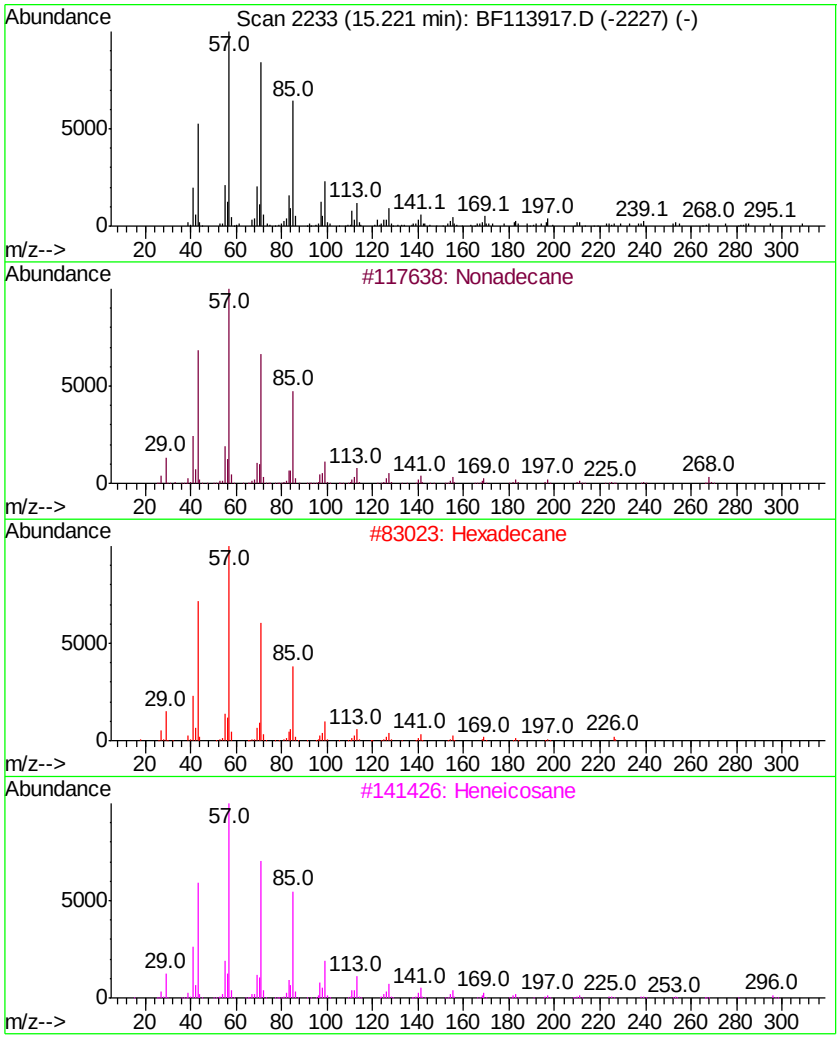
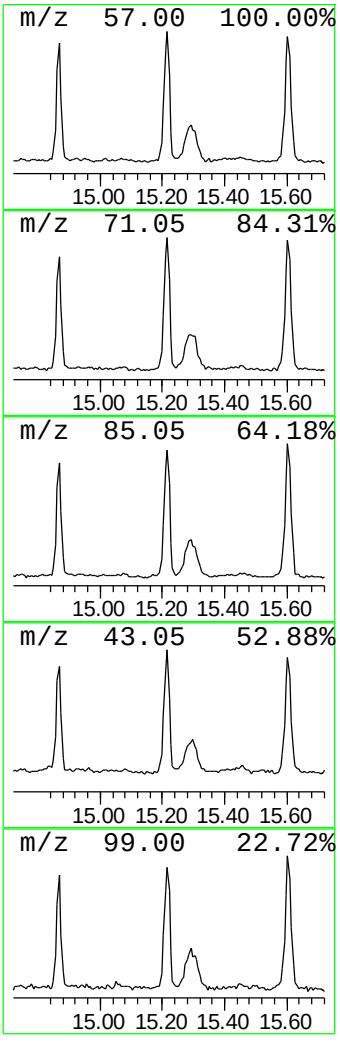
Peak Number 10 Nonadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.22	6.36 ng	322104	Perylene-d12	15.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	93
2	Hexadecane	226	C16H34	000544-76-3	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	Hexacosane	366	C26H54	000630-01-3	91
5	Tetradecane	198	C14H30	000629-59-4	90





Library Search Compound Report

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Data File : BF113917.D
Acq On : 23 Apr 2019 13:54
Operator : JU/SJ
Sample : K2532-07
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042219.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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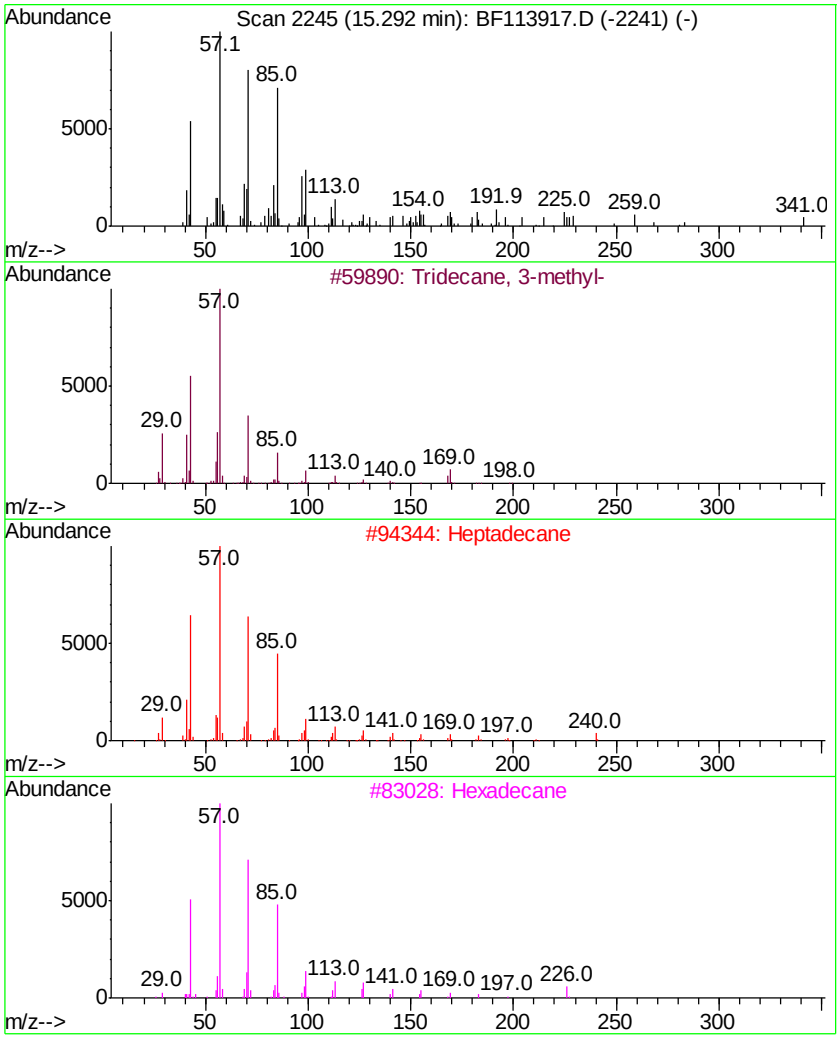
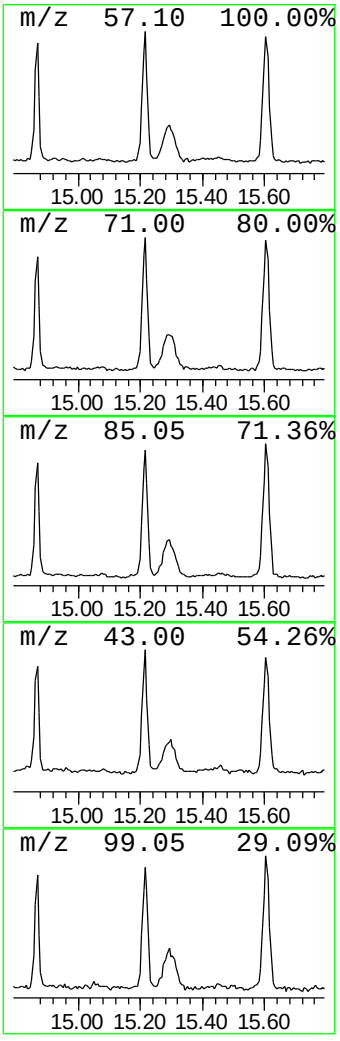
Peak Number 11 Tridecane, 3-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.29	3.20 ng	161884	Perylene-d12	15.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane, 3-methyl-	198	C14H30	006418-41-3	72
2	Heptadecane	240	C17H36	000629-78-7	64
3	Hexadecane	226	C16H34	000544-76-3	60
4	Sulfurous acid, 2-propyl undecyl...	278	C14H30O3S	1000309-12-2	59
5	Hexacosane	366	C26H54	000630-01-3	59





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Data File : BF113917.D
Acq On : 23 Apr 2019 13:54
Operator : JU/SJ
Sample : K2532-07
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042219.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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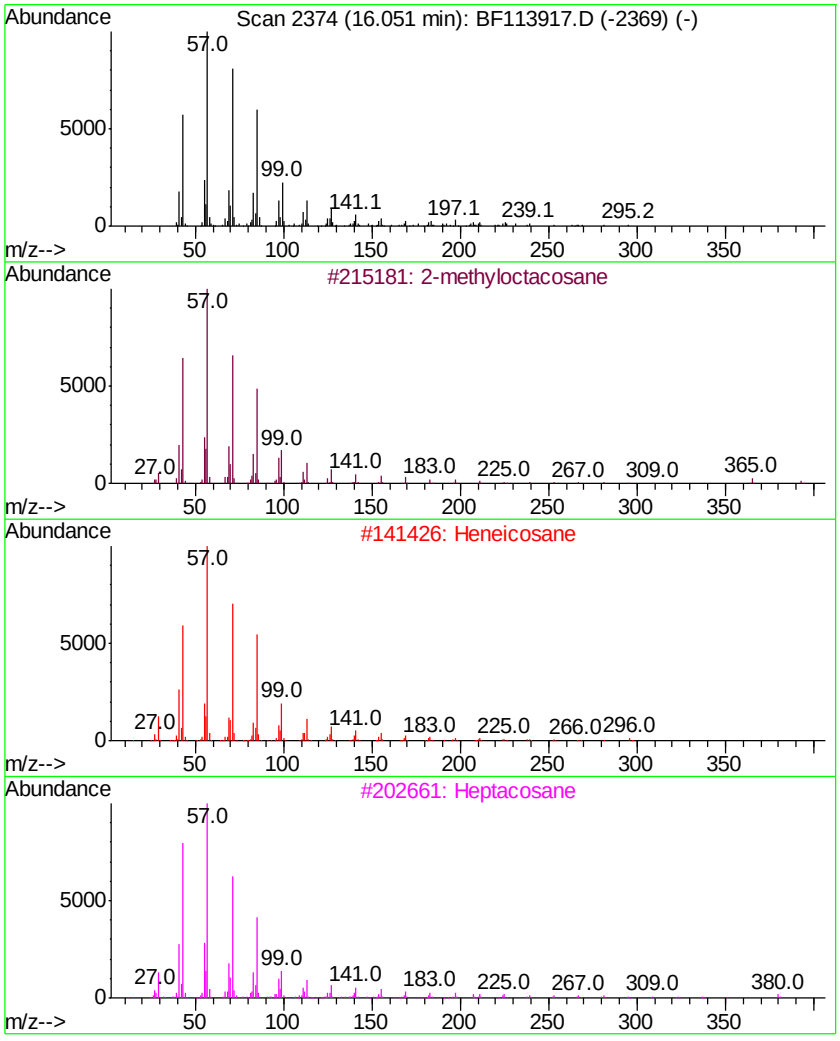
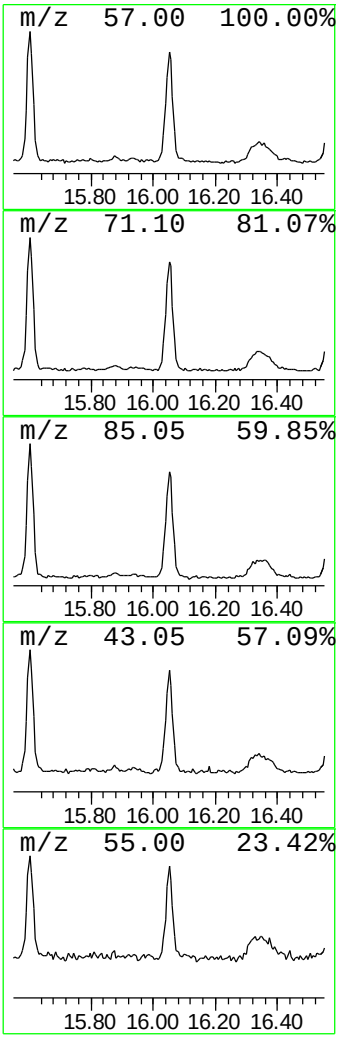
Peak Number 12 Heptacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.05	6.31 ng	319608	Perylene-d12	15.57

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	Heptacosane	380	C27H56	000593-49-7	90
4	Pentacosane	352	C25H52	000629-99-2	90
5	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	90





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF042319\
Data File : BF113917.D
Acq On : 23 Apr 2019 13:54
Operator : JU/SJ
Sample : K2532-07
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042219.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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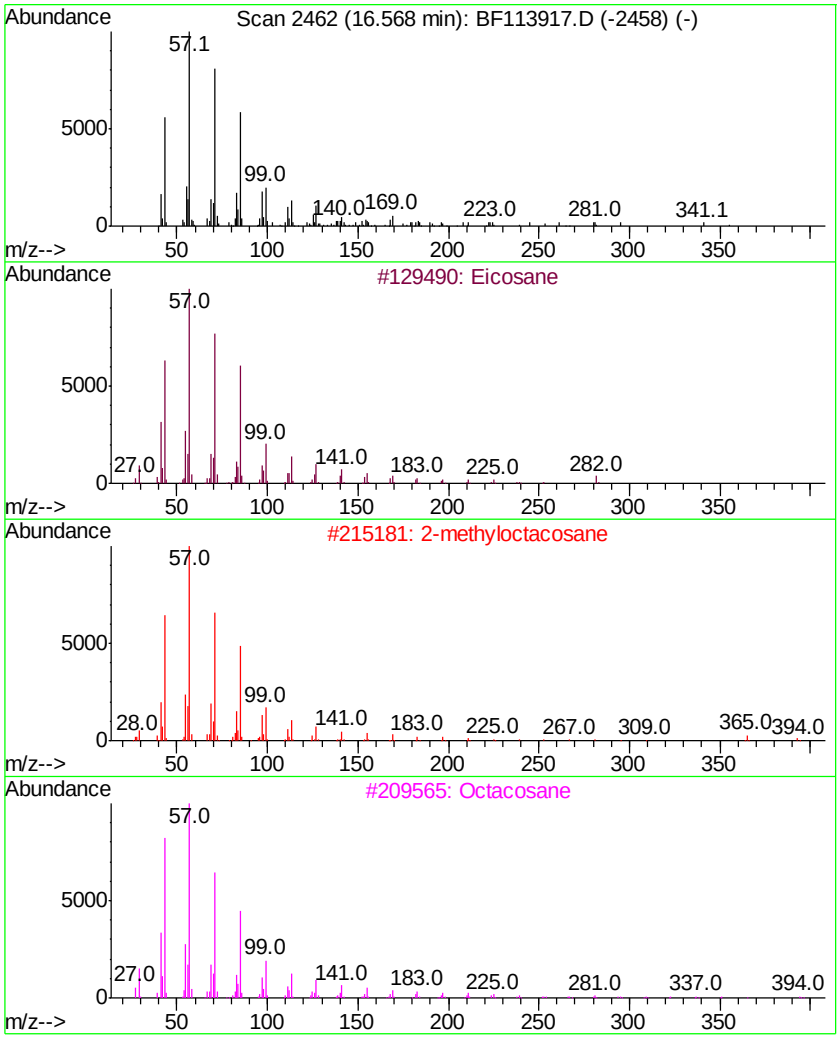
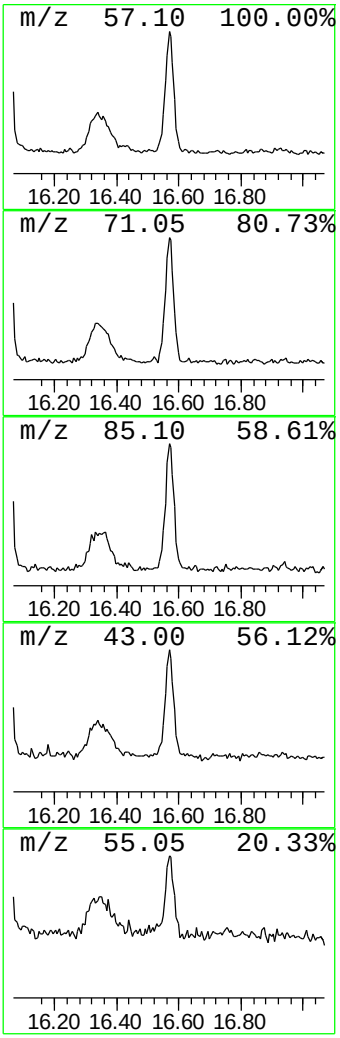
Peak Number 13 2-methyloctacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.57	4.38 ng	221823	Perylene-d12	15.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	94
2	2-methyloctacosane	408	C29H60	1000376-72-8	91
3	Octacosane	394	C28H58	000630-02-4	91
4	Pentacosane	352	C25H52	000629-99-2	91
5	Hentriacontane	437	C31H64	000630-04-6	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF042319\
Data File : BF113917.D
Acq On : 23 Apr 2019 13:54
Operator : JU/SJ
Sample : K2532-07
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042219.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
unknown6.67	6.67	78.1	ng	3032920	1	6.90	776429	20.0
n-Hexadecanoic acid	11.94	13.3	ng	908980	4	11.42	1367010	20.0
Octadecanoic acid	12.73	19.9	ng	1360000	4	11.42	1367010	20.0
Hexacosane	13.91	2.6	ng	156851	5	14.06	1199280	20.0
Docosane	14.23	2.2	ng	133788	5	14.06	1199280	20.0
Tetracosane	14.36	7.1	ng	423179	5	14.06	1199280	20.0
Hexadecane, 5-butyl-	14.55	2.8	ng	168100	5	14.06	1199280	20.0
Eicosane	14.87	4.5	ng	228079	6	15.57	1012450	20.0
Nonadecane	15.22	6.4	ng	322104	6	15.57	1012450	20.0
Tridecane, 3-methyl-	15.29	3.2	ng	161884	6	15.57	1012450	20.0
Heptacosane	16.05	6.3	ng	319608	6	15.57	1012450	20.0
2-methyloctacosane	16.57	4.4	ng	221823	6	15.57	1012450	20.0