LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF040320\
Data File : BF119744.D
Acq On : 4 Apr 2020 4:53
Operator : MA/SJ
Sample : L2129-26
Misc :
ALS Vial : 33 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-BF031820.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	5.040	498	502	509	rVB	115546	169894	2.24%	0.306%
2	5.428	562	568	571	rBV	6274939	6948180	91.56%	12.499%
3	6.440	733	740	743	rBV	5399483	7014580	92.43%	12.618%
4	6.628	770	772	778	rBV	199325	172667	2.28%	0.311%
5	6.804	798	802	805	rBV	1375552	1063854	14.02%	1.914%
6	6.963	824	829	832	rBV	6043577	5458404	71.93%	9.819%
7	7.369	892	898	901	rBV	4086406	4624302	60.93%	8.318%
8	8.087	1015	1020	1023	rBV	1630094	1350938	17.80%	2.430%
9	9.169	1198	1204	1207	rBV	7534215	7588922	100.00%	13.651%
10	9.557	1267	1270	1274	rBV	883381	740209	9.75%	1.332%
11	9.845	1312	1319	1322	rBV	1720840	1438486	18.96%	2.588%
12	10.633	1447	1453	1457	rBV	4160480	4359087	57.44%	7.841%
13	11.333	1567	1572	1574	rBV	1388016	1348977	17.78%	2.427%
14	11.351	1574	1575	1579	rVB	329908	248675	3.28%	0.447%
15	11.863	1659	1662	1668	rBV	1020958	909856	11.99%	1.637%
16	12.545	1774	1778	1781	rBV	457806	397877	5.24%	0.716%
17	12.645	1792	1795	1802	rBV2	274892	322337	4.25%	0.580%
18	12.769	1810	1816	1819	rBV	354975	400115	5.27%	0.720%
19	12.922	1837	1842	1845	rBV	5766778	5605458	73.86%	10.083%
20	12.992	1849	1854	1858	rBV3	44491	78308	1.03%	0.141%
21	13.204	1887	1890	1894	rVB2	73542	81726	1.08%	0.147%
22	13.398	1920	1923	1927	rBV2	117264	108116	1.42%	0.194%
23	13.498	1934	1940	1943	rBV5	72919	135031	1.78%	0.243%
24	13.816	1991	1994	2002	rVB	704998	834059	10.99%	1.500%
25	13.968	2015	2020	2023	rBV2	1113436	1176281	15.50%	2.116%
26	13.998	2023	2025	2030	rVB	171115	165830	2.19%	0.298%
27	14.145	2047	2050	2055	rVB2	108416	113632	1.50%	0.204%
28	14.451	2098	2102	2105	rBV3	218439	288346	3.80%	0.519%
29	14.751	2150	2153	2156	rBV	136588	133385	1.76%	0.240%
30	14.998	2191	2195	2203	rBV	155600	301219	3.97%	0.542%
31	15.086	2206	2210	2212	rBV3	139832	165930	2.19%	0.298%
32	15.298	2243	2246	2252	rVB	103371	121699	1.60%	0.219%
33	15.357	2252	2256	2260	rBV	139703	178400	2.35%	0.321%
34	15.421	2263	2267	2271	rVV	795956	953000	12.56%	1.714%

LSC Area Percent Report

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Operator : MA/SJ
Sample : L2129-26
Misc :
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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-BF031820.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.463	2271	2274	2279	rVB2	100232	146030	1.92%	0.263%
36	15.898	2343	2348	2352	rBV2	93933	154548	2.04%	0.278%
37	15.951	2352	2357	2361	rBV5	80649	171879	2.26%	0.309%
38	16.857	2507	2511	2520	rVB2	60353	121580	1.60%	0.219%

Sum of corrected areas: 55591817

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF040320\
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Sample : L2129-26
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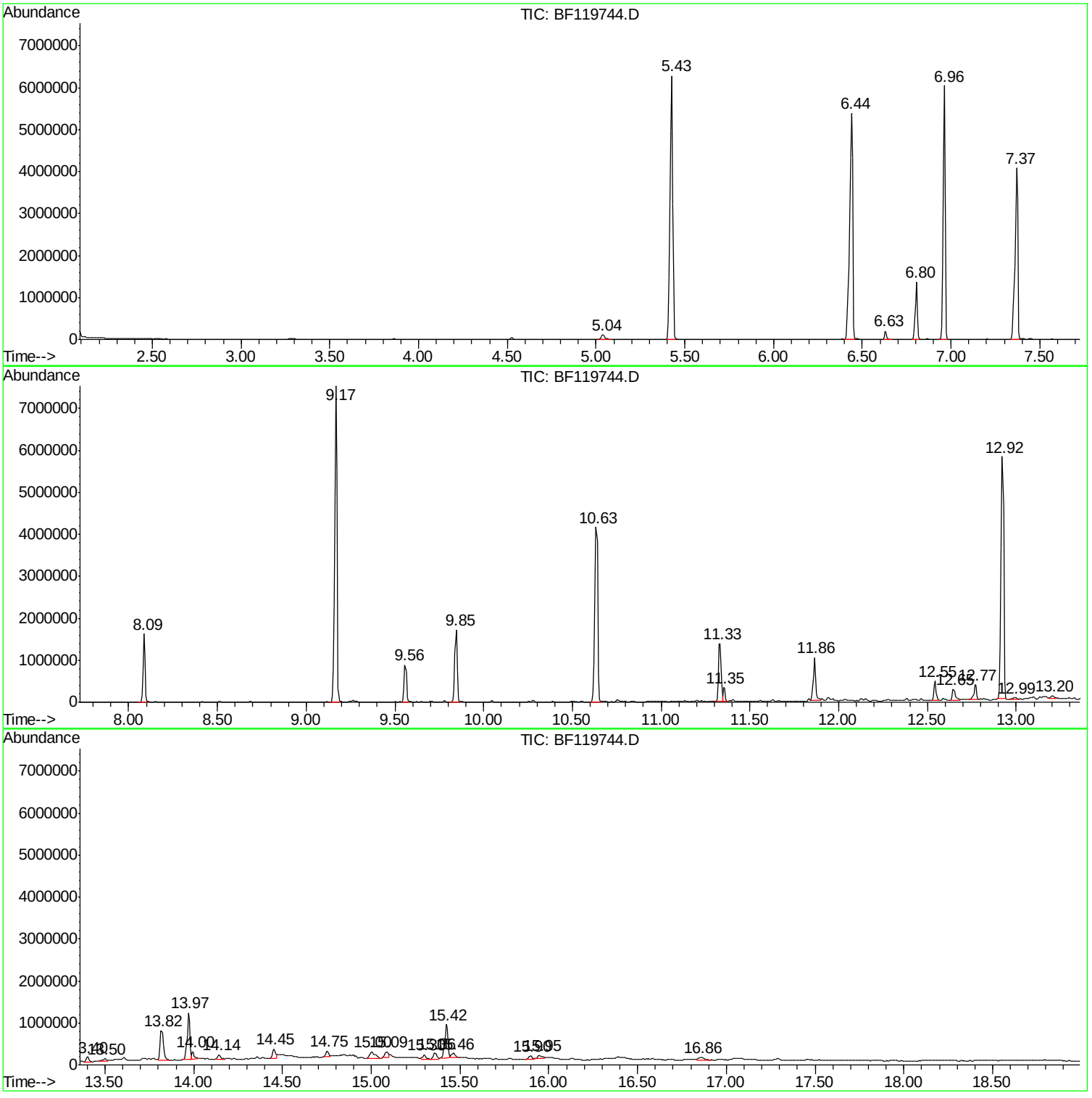
Instrument :
BNA_F
ClientSampleId :
TP-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF031820.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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Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF031820.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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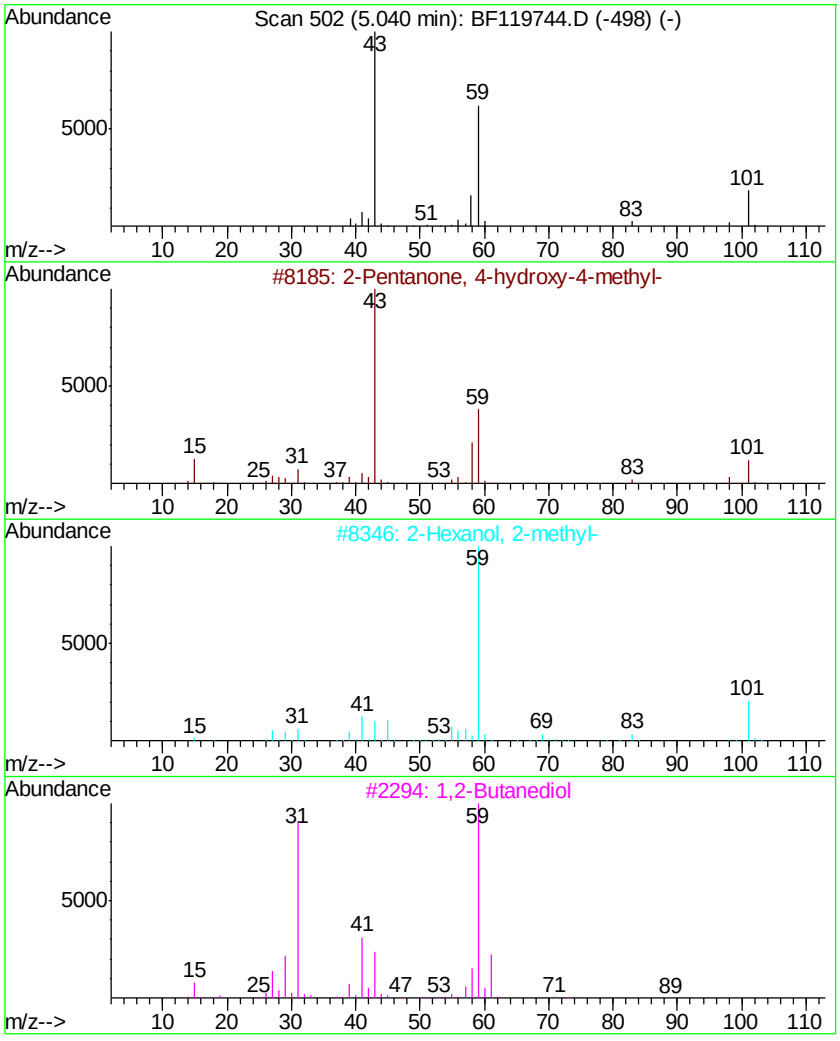
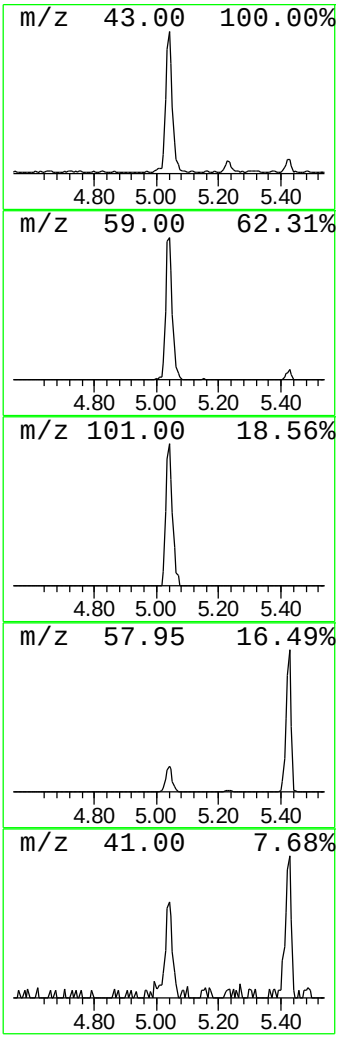
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.04	3.19 ng	169894	1,4-Dichlorobenzene-d4	6.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	38
3	1,2-Butanediol	90	C4H10O2	000584-03-2	28
4	Guanidine	59	CH5N3	000113-00-8	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





Library Search Compound Report

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Data File : BF119744.D
Acq On : 4 Apr 2020 4:53
Operator : MA/SJ
Sample : L2129-26
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF031820.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

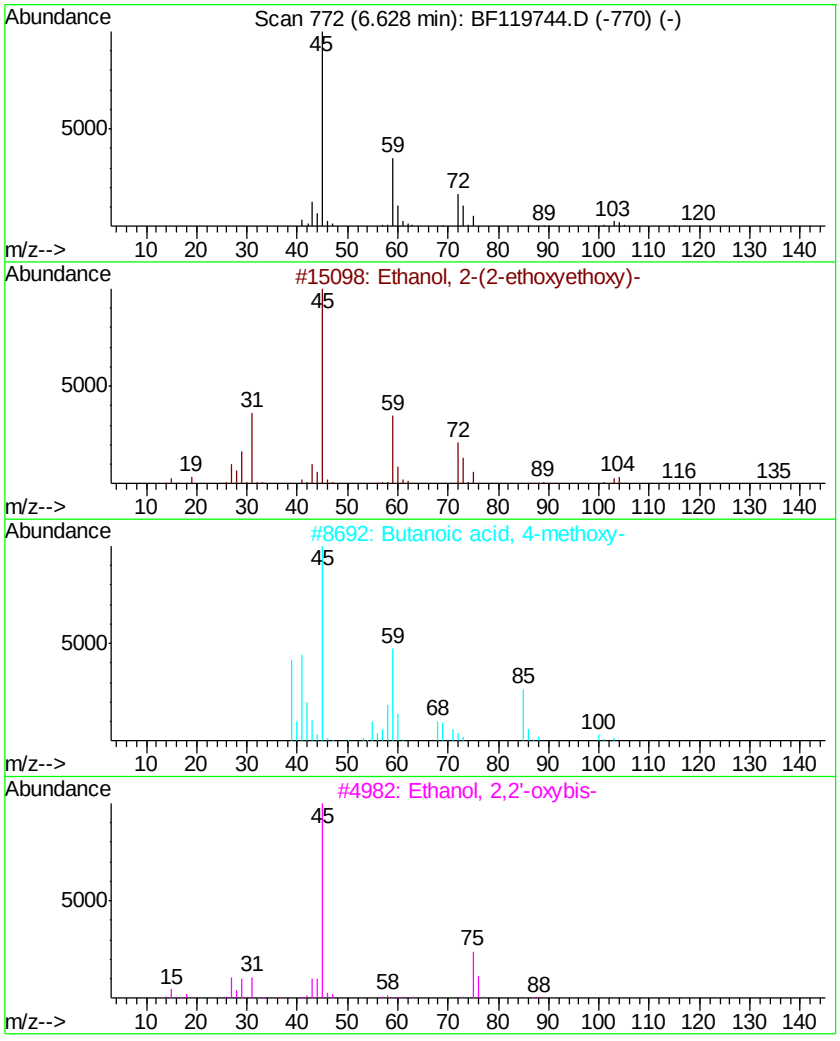
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

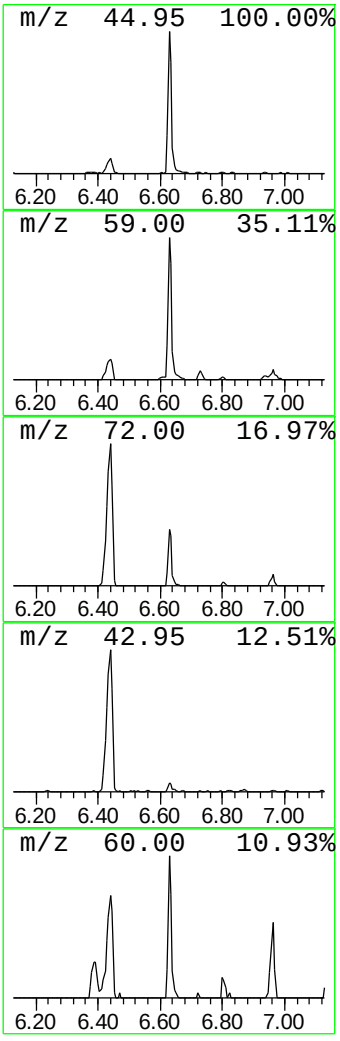
****

Peak Number 2 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	3.25 ng	172667	1,4-Dichlorobenzene-d4	6.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	74
2	Butanoic acid, 4-methoxy-	118	C5H10O3	029006-02-8	39
3	Ethanol, 2,2'-oxybis-	106	C4H10O3	000111-46-6	38
4	2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	38
5	Ethanol, 2-[2-(2-propenyloxy)eth...	146	C7H14O3	015075-50-0	36





Library Search Compound Report

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Data File : BF119744.D
Acq On : 4 Apr 2020 4:53
Operator : MA/SJ
Sample : L2129-26
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF031820.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

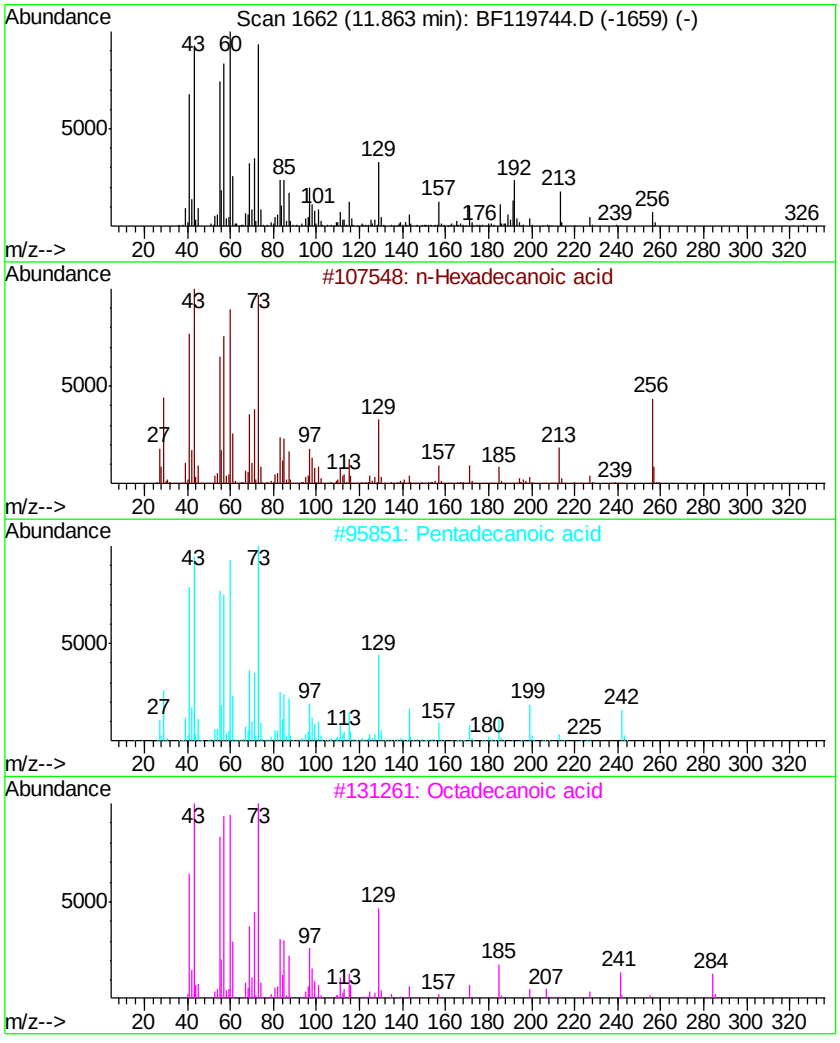
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

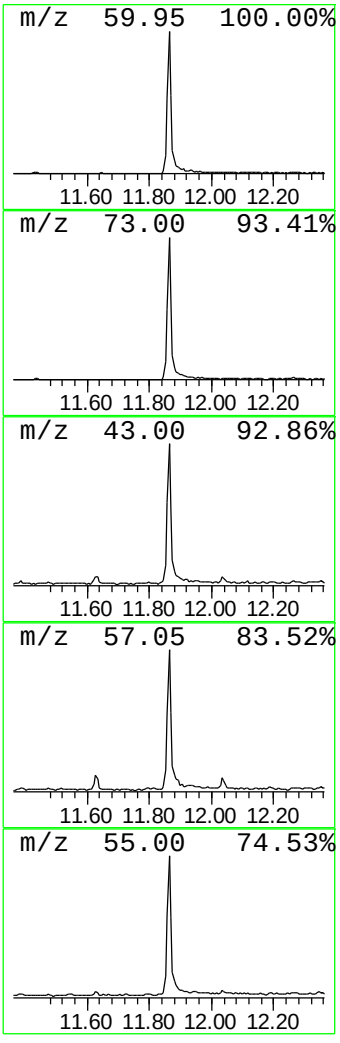
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.86	13.49 ng	909856	Phenanthrene-d10	11.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
3	Octadecanoic acid	284	C18H36O2	000057-11-4	81
4	Tridecanoic acid	214	C13H26O2	000638-53-9	64
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	64





Library Search Compound Report

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Data File : BF119744.D
Acq On : 4 Apr 2020 4:53
Operator : MA/SJ
Sample : L2129-26
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF031820.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

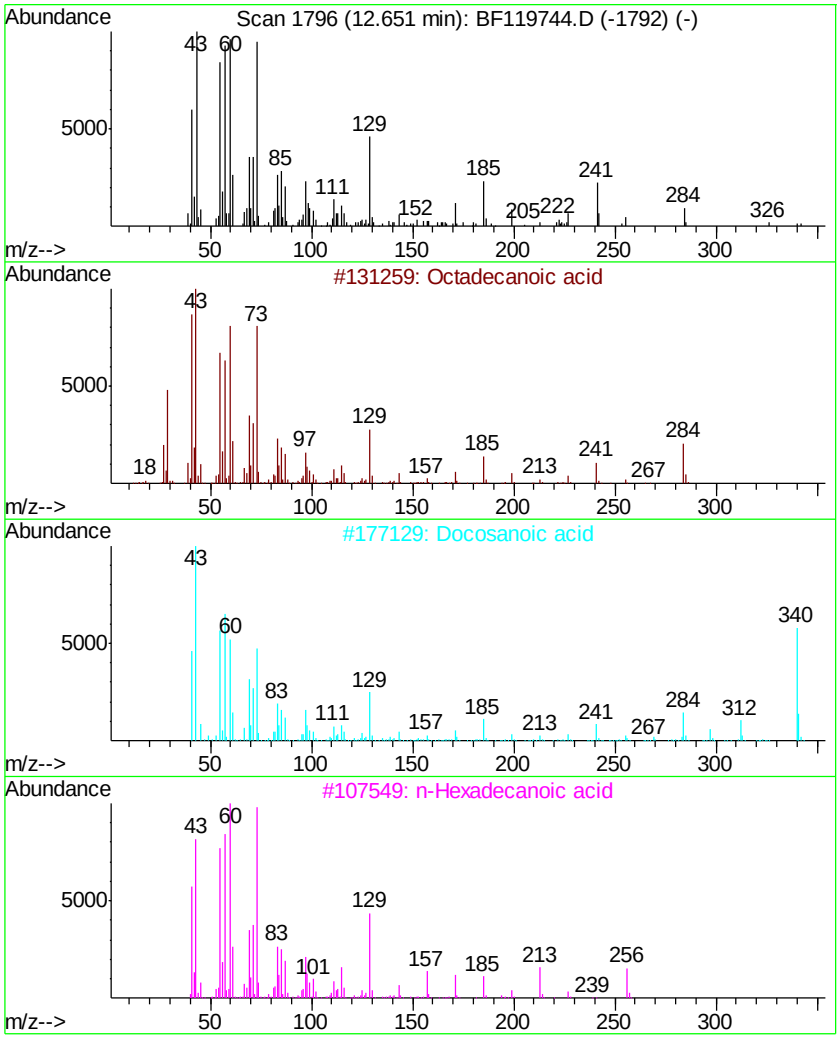
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

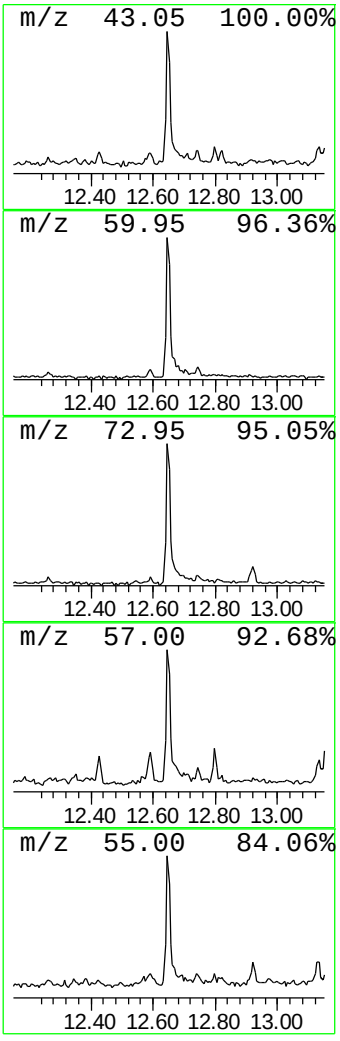
****

Peak Number 5 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.65	4.78 ng	322337	Phenanthrene-d10	11.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	Docosanoic acid	340	C22H44O2	000112-85-6	87
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	68





Library Search Compound Report

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Sample : L2129-26
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF031820.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

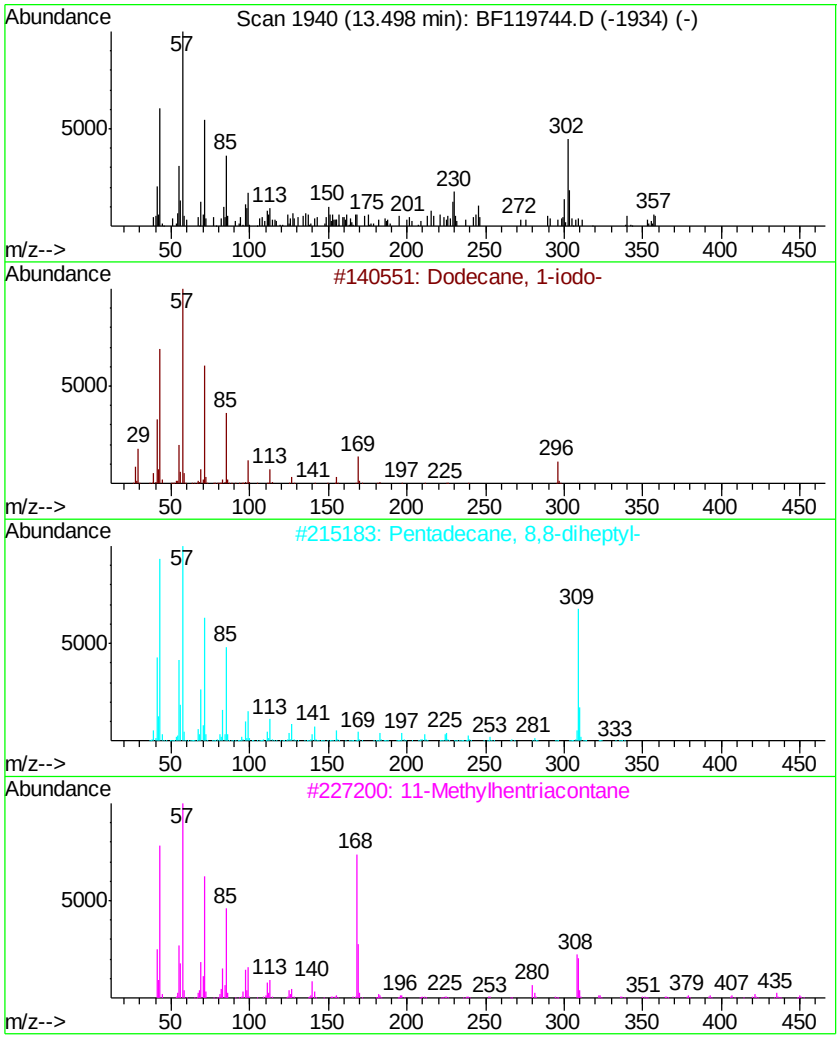
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

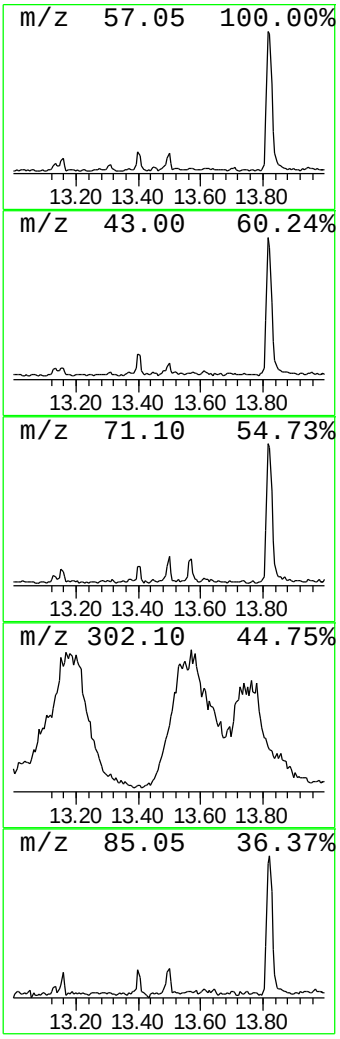
****

Peak Number 6 unknown13.50 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.50	2.30 ng	135031	Chrysene-d12	13.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	22
2	Pentadecane, 8,8-diheptyl-	408	C29H60	055268-72-9	22
3	11-Methylhentriacontane	451	C32H66	035799-05-4	12
4	1-[5-(3-Acetyl-4-hydroxyphenylth...	302	C16H14O4S	028992-32-7	10
5	Docosane, 9-butyl-	366	C26H54	055282-14-9	10





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Instrument : BNA_F
ClientSampleId : TP-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF031820.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

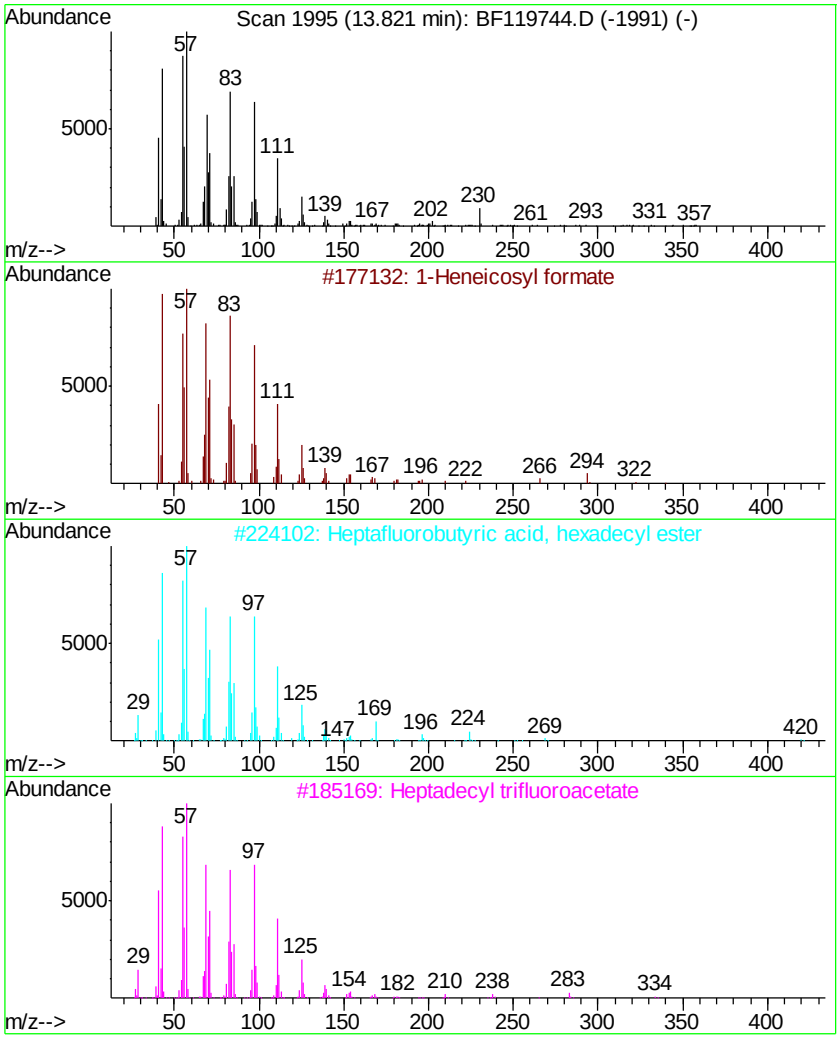
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

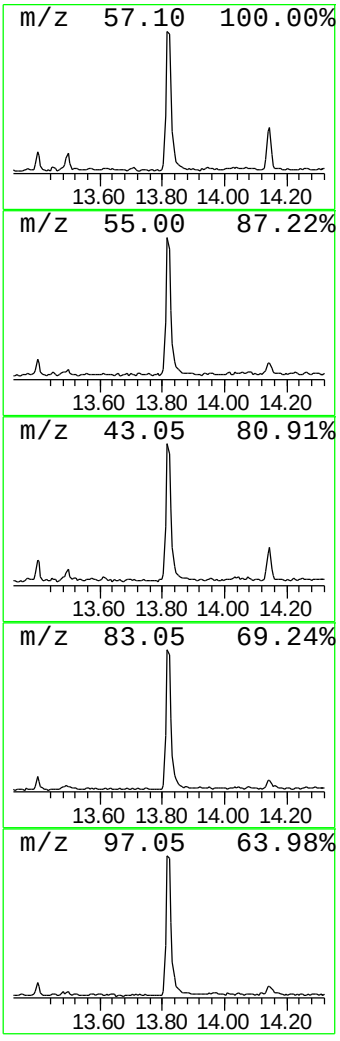
****

Peak Number 7 1-Heneicosyl formate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.82	14.18 ng	834059	Chrysene-d12	13.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosyl formate	340	C22H44O2	077899-03-7	93
2	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	93
3	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	93
4	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	93
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	90





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

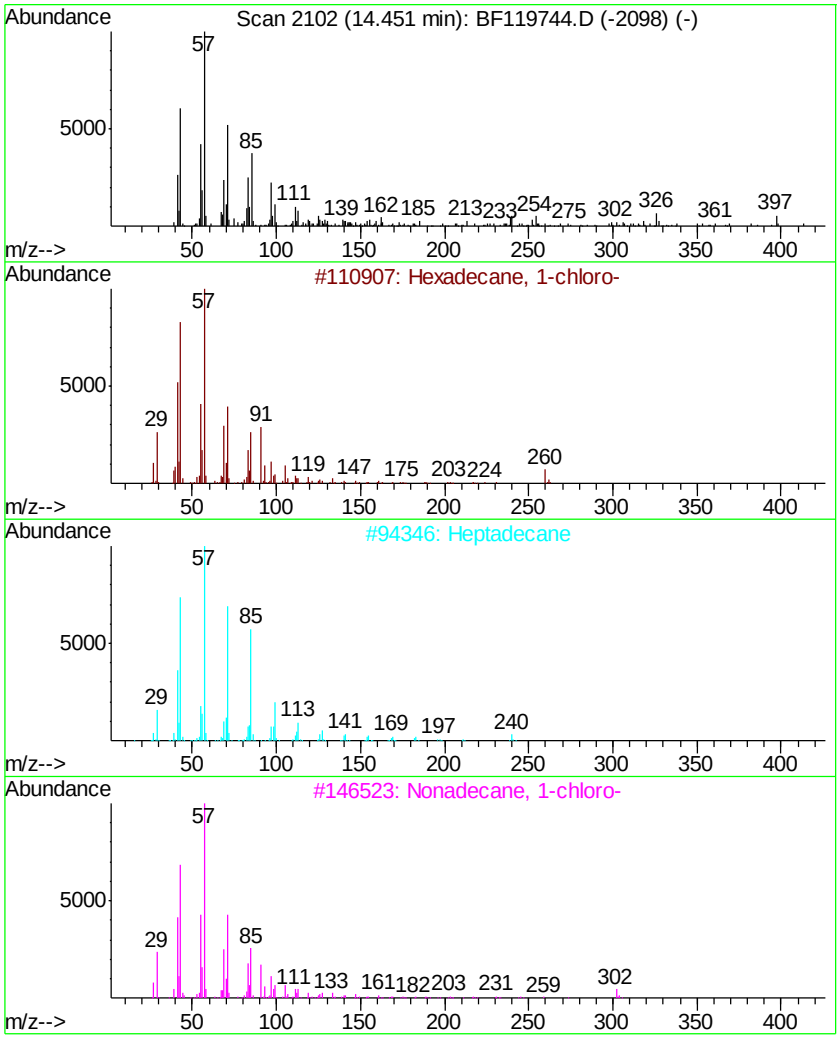
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

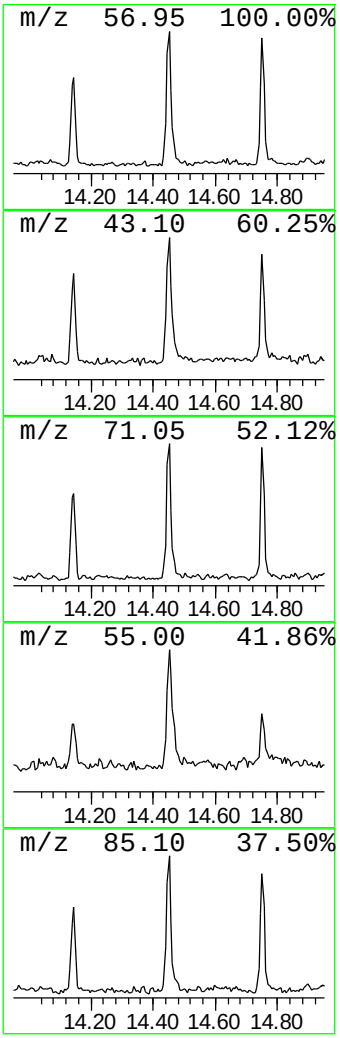
****

Peak Number 8 Hexadecane, 1-chloro- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.45	4.90 ng	288346	Chrysene-d12	13.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane, 1-chloro-	260	C16H33Cl	004860-03-1	93
2	Heptadecane	240	C17H36	000629-78-7	91
3	Nonadecane, 1-chloro-	302	C19H39Cl	062016-76-6	90
4	Octacosane	394	C28H58	000630-02-4	83
5	Sulfurous acid, butyl octadecyl ...	390	C22H46O3S	1000309-18-5	74





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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF031820.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

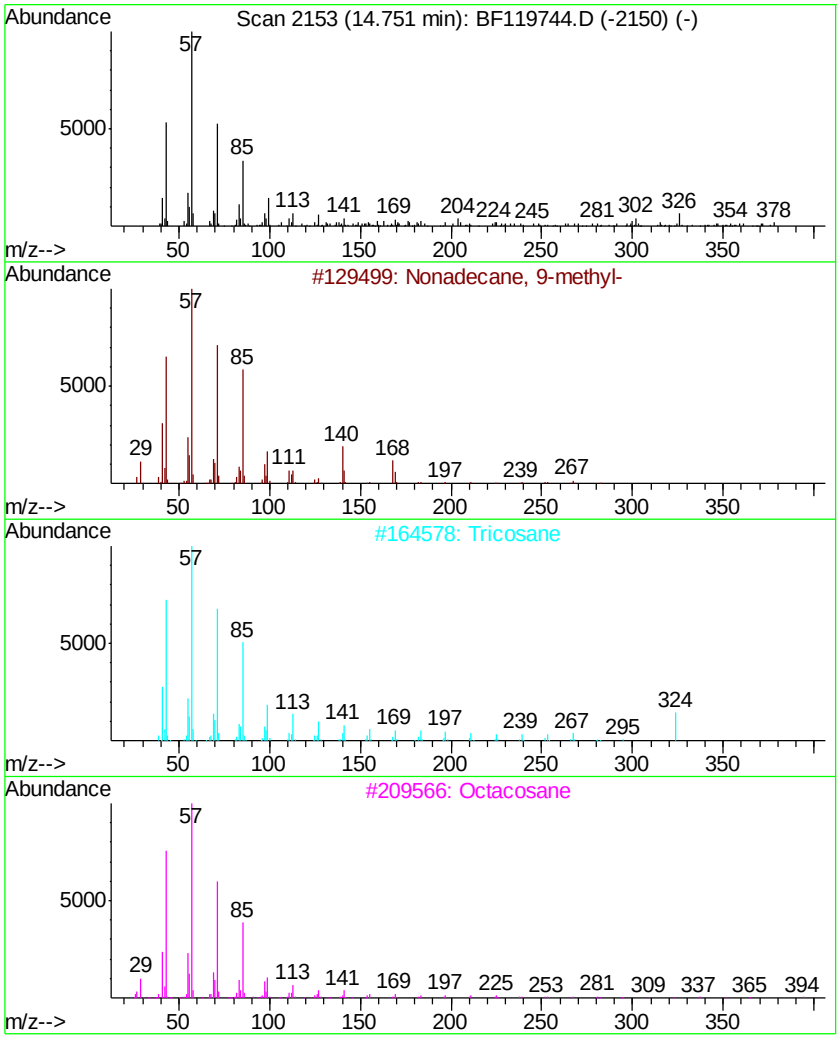
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

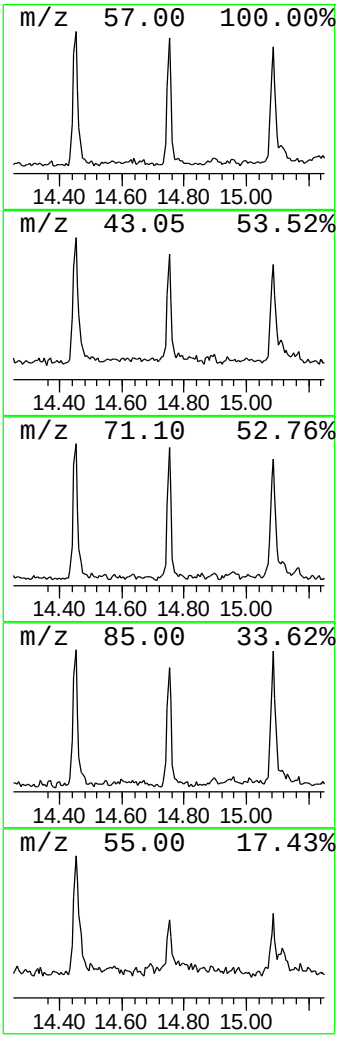
****

Peak Number 9 Nonadecane, 9-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.75	2.80 ng	133385	Perylene-d12	15.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	93
2	Tricosane	324	C23H48	000638-67-5	90
3	Octacosane	394	C28H58	000630-02-4	74
4	Hexacosane	366	C26H54	000630-01-3	72
5	Tetratetracontane	619	C44H90	007098-22-8	72





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF040320\
Data File : BF119744.D
Acq On : 4 Apr 2020 4:53
Operator : MA/SJ
Sample : L2129-26
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF031820.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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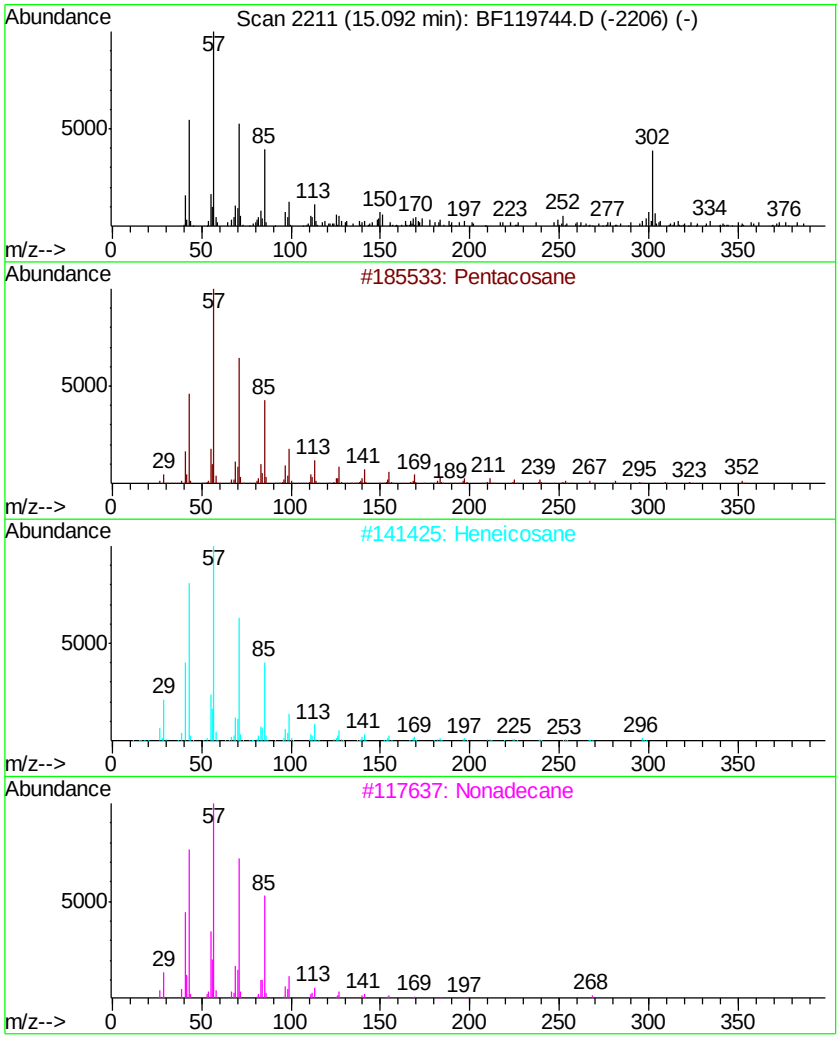
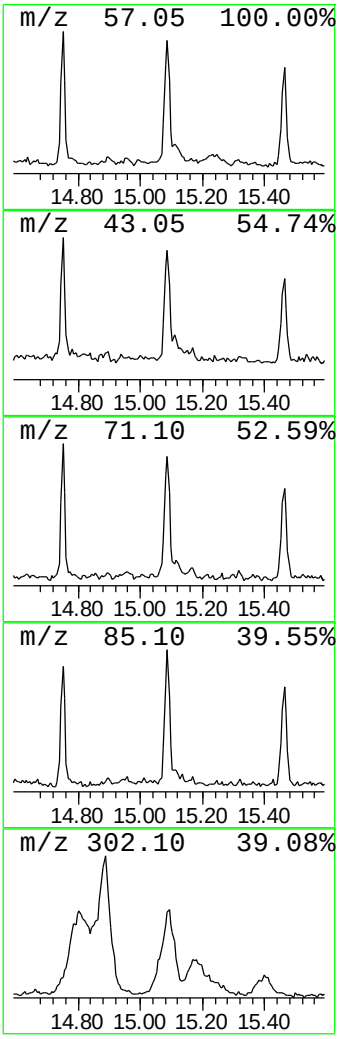
Peak Number 10 Pentacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.09	3.48 ng	165930	Perylene-d12	15.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane	352	C25H52	000629-99-2	90
2	Heneicosane	296	C21H44	000629-94-7	78
3	Nonadecane	268	C19H40	000629-92-5	58
4	Dodecane	170	C12H26	000112-40-3	58
5	Hexacosane	366	C26H54	000630-01-3	53





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF040320\
Data File : BF119744.D
Acq On : 4 Apr 2020 4:53
Operator : MA/SJ
Sample : L2129-26
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF031820.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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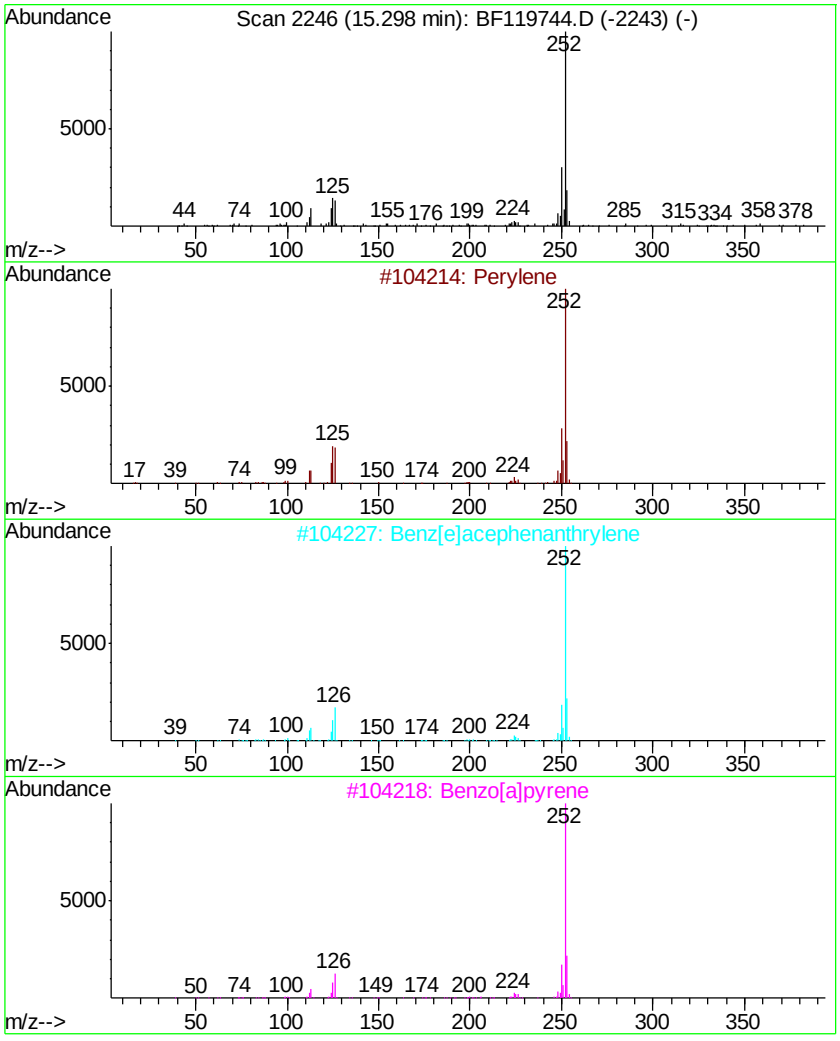
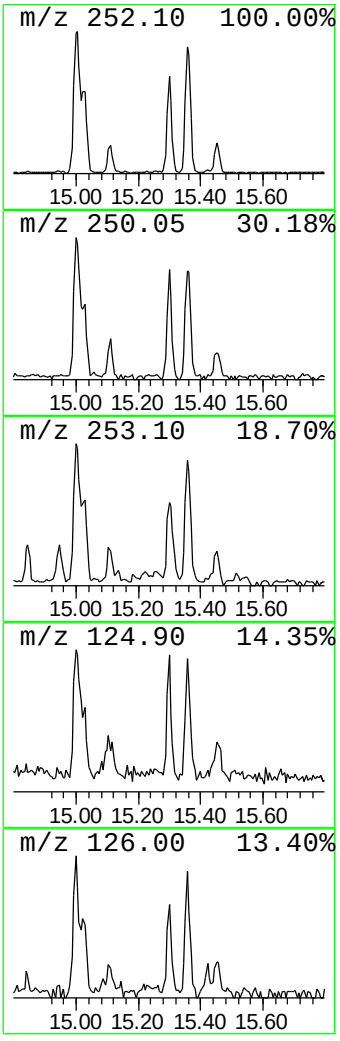
Peak Number 11 Perylene Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.30	2.55 ng	121699	Perylene-d12	15.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Perylene	252	C20H12	000198-55-0	98
2	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	95
3	Benzo[a]pyrene	252	C20H12	000050-32-8	94
4	Benzo[e]pyrene	252	C20H12	000192-97-2	93
5	Benzo[k]fluoranthene	252	C20H12	000207-08-9	91





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF040320\
Data File : BF119744.D
Acq On : 4 Apr 2020 4:53
Operator : MA/SJ
Sample : L2129-26
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF031820.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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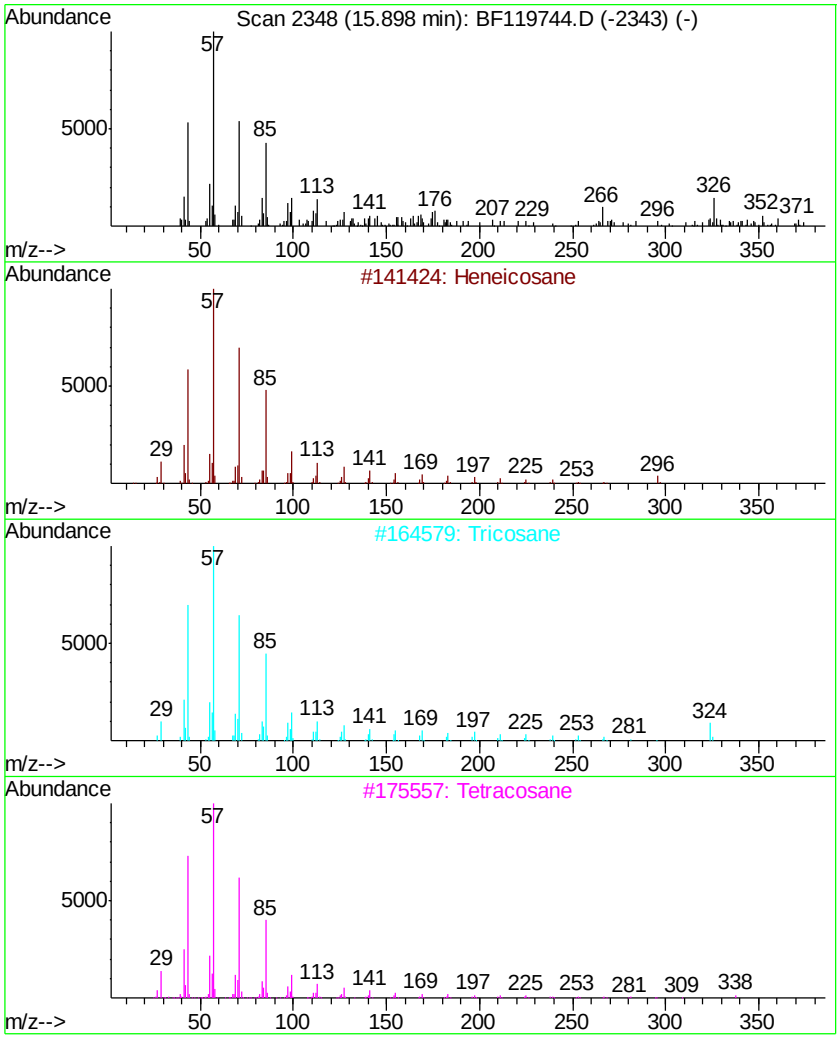
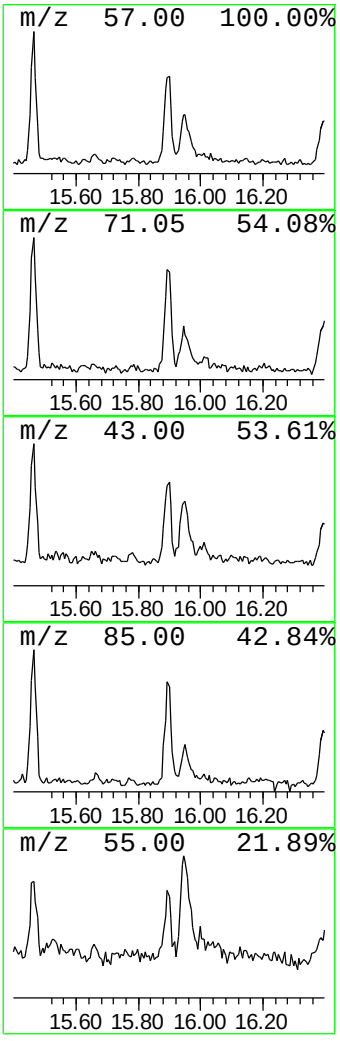
Peak Number 12 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.90	3.24 ng	154548	Perylene-d12	15.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	95
2	Tricosane	324	C23H48	000638-67-5	93
3	Tetracosane	338	C24H50	000646-31-1	90
4	Pentacosane	352	C25H52	000629-99-2	83
5	Tricosane, 2-methyl-	338	C24H50	001928-30-9	78





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF040320\
Data File : BF119744.D
Acq On : 4 Apr 2020 4:53
Operator : MA/SJ
Sample : L2129-26
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF031820.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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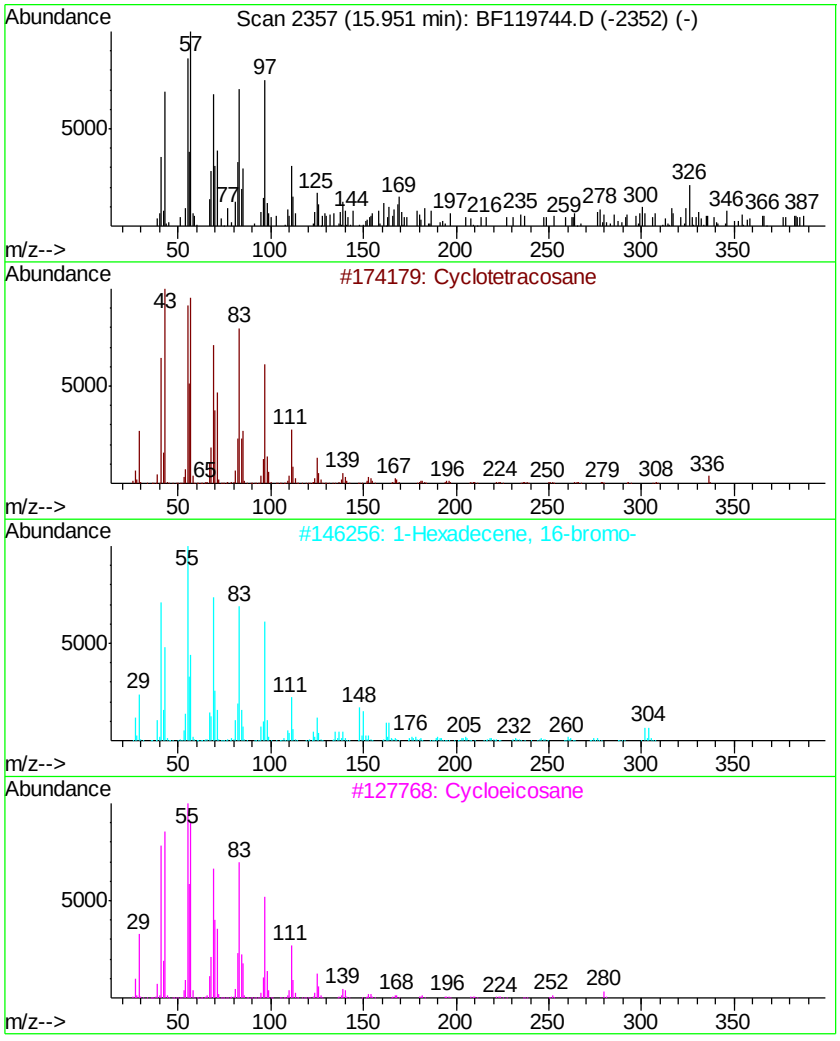
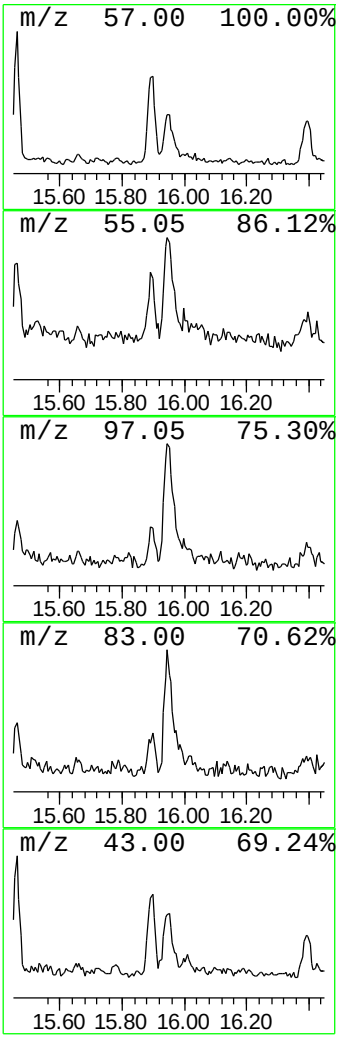
Peak Number 13 Cyclotetracosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.95	3.61 ng	171879	Perylene-d12	15.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetracosane	336	C24H48	000297-03-0	98
2	1-Hexadecene, 16-bromo-	302	C16H31Br	118625-56-2	91
3	Cycloeicosane	280	C20H40	000296-56-0	89
4	5-Eicosene, (E)-	280	C20H40	074685-30-6	89
5	1-Eicosene	280	C20H40	003452-07-1	83





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF040320\
Data File : BF119744.D
Acq On : 4 Apr 2020 4:53
Operator : MA/SJ
Sample : L2129-26
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF031820.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
2-Pentanone, 4-hy...	5.04	3.2	ng	169894	1	6.80	1063850	20.0
Ethanol, 2-(2-eth...	6.63	3.3	ng	172667	1	6.80	1063850	20.0
n-Hexadecanoic acid	11.86	13.5	ng	909856	4	11.33	1348980	20.0
Octadecanoic acid	12.65	4.8	ng	322337	4	11.33	1348980	20.0
unknown13.50	13.50	2.3	ng	135031	5	13.97	1176280	20.0
1-Heneicosyl formate	13.82	14.2	ng	834059	5	13.97	1176280	20.0
Hexadecane, 1-chl...	14.45	4.9	ng	288346	5	13.97	1176280	20.0
Nonadecane, 9-met...	14.75	2.8	ng	133385	6	15.42	953000	20.0
Pentacosane	15.09	3.5	ng	165930	6	15.42	953000	20.0
Perylene	15.30	2.5	ng	121699	6	15.42	953000	20.0
Heneicosane	15.90	3.2	ng	154548	6	15.42	953000	20.0
Cyclotetracosane	15.95	3.6	ng	171879	6	15.42	953000	20.0