LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF062917\
Data File : BF096289.D
Acq On : 29 Jun 2017 14:02
Operator : SJ/MA
Sample : I3897-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 72-11931

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:\HPCHEM1\BNA_F\METHODS\8270-BF062717.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	4.975	486	491	499	rVB	711284	865193	21.27%	2.503%
2	5.393	556	562	565	rBV	4006927	4068007	100.00%	11.770%
3	6.404	729	734	737	rVB	3717596	3901273	95.90%	11.288%
4	6.539	753	757	761	rBV	3763395	3758380	92.39%	10.874%
5	6.598	764	767	770	rBV	65912	49906	1.23%	0.144%
6	6.769	791	796	800	rBV	1154704	1098503	27.00%	3.178%
7	6.898	815	818	820	rBV	81896	78886	1.94%	0.228%
8	6.928	820	823	827	rVB	2759447	2428605	59.70%	7.027%
9	7.328	886	891	894	rBV	2399550	2318722	57.00%	6.709%
10	7.428	903	908	912	rBV	84555	99270	2.44%	0.287%
11	7.763	959	965	967	rBV	88888	116388	2.86%	0.337%
12	8.051	1010	1014	1017	rBV	1464722	1309200	32.18%	3.788%
13	9.128	1192	1197	1202	rVB	2730900	2524754	62.06%	7.305%
14	9.251	1215	1218	1222	rVB	91934	78760	1.94%	0.228%
15	9.522	1259	1264	1267	rBV	1633543	1354093	33.29%	3.918%
16	9.804	1307	1312	1316	rBV2	1322419	1165503	28.65%	3.372%
17	10.251	1385	1388	1391	rVB	81110	68948	1.69%	0.199%
18	10.469	1419	1425	1428	rBV2	31313	46727	1.15%	0.135%
19	10.586	1441	1445	1449	rBV	1717637	1619497	39.81%	4.686%
20	10.722	1464	1468	1475	rBV	109139	121670	2.99%	0.352%
21	11.169	1540	1544	1547	rBV2	67728	58975	1.45%	0.171%
22	11.286	1560	1564	1567	rBV	1081285	940102	23.11%	2.720%
23	11.357	1570	1576	1579	rBV2	37326	42286	1.04%	0.122%
24	11.522	1600	1604	1607	rBV	467418	430740	10.59%	1.246%
25	11.821	1651	1655	1658	rBV	293424	277843	6.83%	0.804%
26	12.339	1739	1743	1746	rBV	1518427	1319774	32.44%	3.819%
27	12.492	1766	1769	1772	rBV	73153	76884	1.89%	0.222%
28	12.604	1785	1788	1793	rVB3	61525	52247	1.28%	0.151%
29	12.868	1829	1833	1837	rBV	1969360	1774886	43.63%	5.135%
30	13.086	1867	1870	1873	rBV2	60228	66945	1.65%	0.194%
31	13.327	1908	1911	1914	rBV	123444	119678	2.94%	0.346%
32	13.421	1924	1927	1931	rBV2	65903	66112	1.63%	0.191%
33	13.568	1950	1952	1955	rBV	107571	99038	2.43%	0.287%
34	13.768	1984	1986	1993	rVB	289584	329434	8.10%	0.953%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF062917\
Data File : BF096289.D
Acq On : 29 Jun 2017 14:02
Operator : SJ/MA
Sample : I3897-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 72-11931

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:\HPCHEM1\BNA_F\METHODS\8270-BF062717.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.915	2007	2011	2015	rBV2	1096328	1055531	25.95%	3.054%
36	14.215	2060	2062	2065	rBV	113865	113300	2.79%	0.328%
37	15.339	2250	2253	2262	rVB	522402	666318	16.38%	1.928%

Sum of corrected areas: 34562378

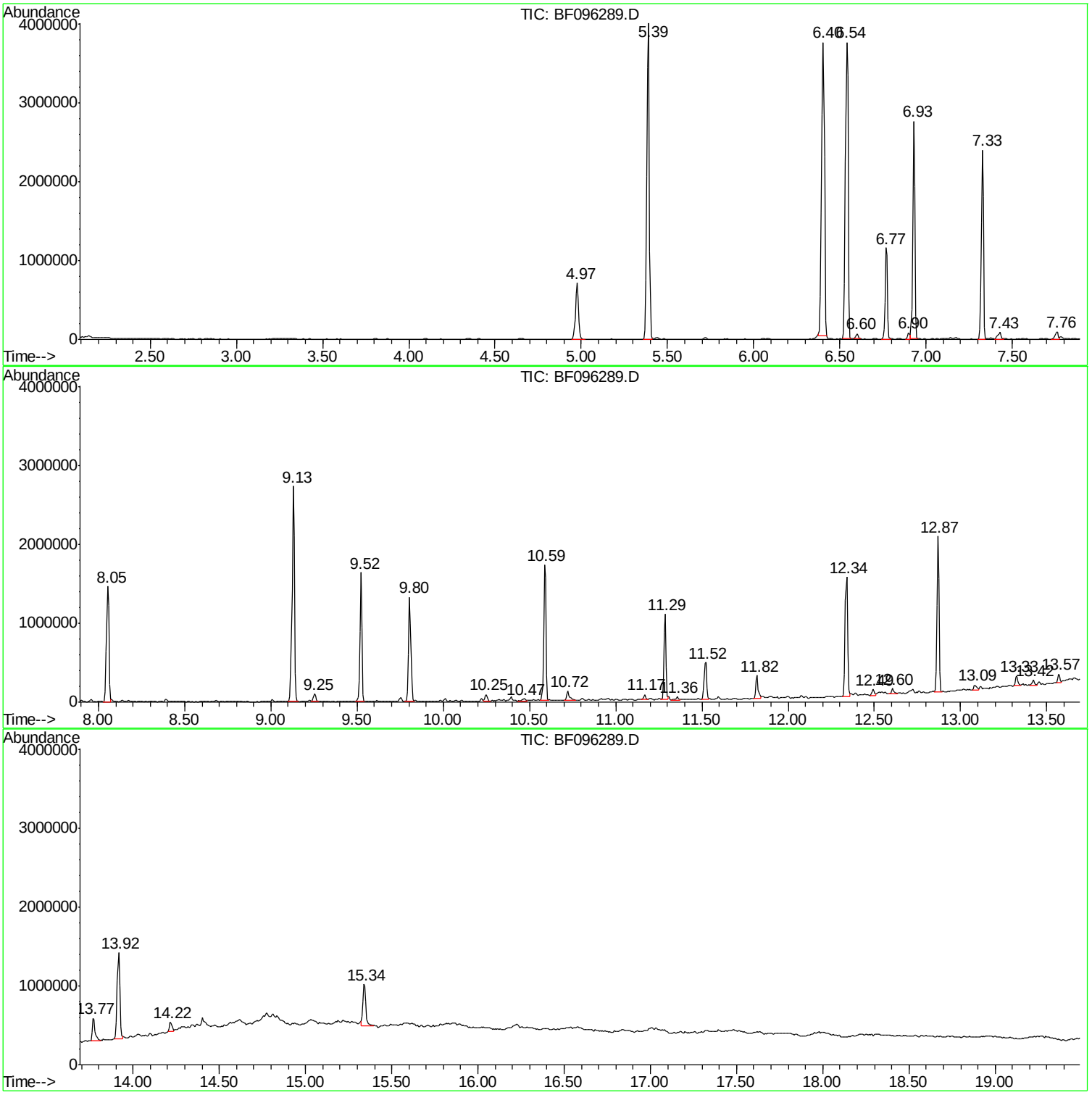
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF062917\
Data File : BF096289.D
Acq On : 29 Jun 2017 14:02
Operator : SJ/MA
Sample : I3897-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 72-11931

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF062717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF062917\
Data File : BF096289.D
Acq On : 29 Jun 2017 14:02
Operator : SJ/MA
Sample : I3897-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 72-11931

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF062717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

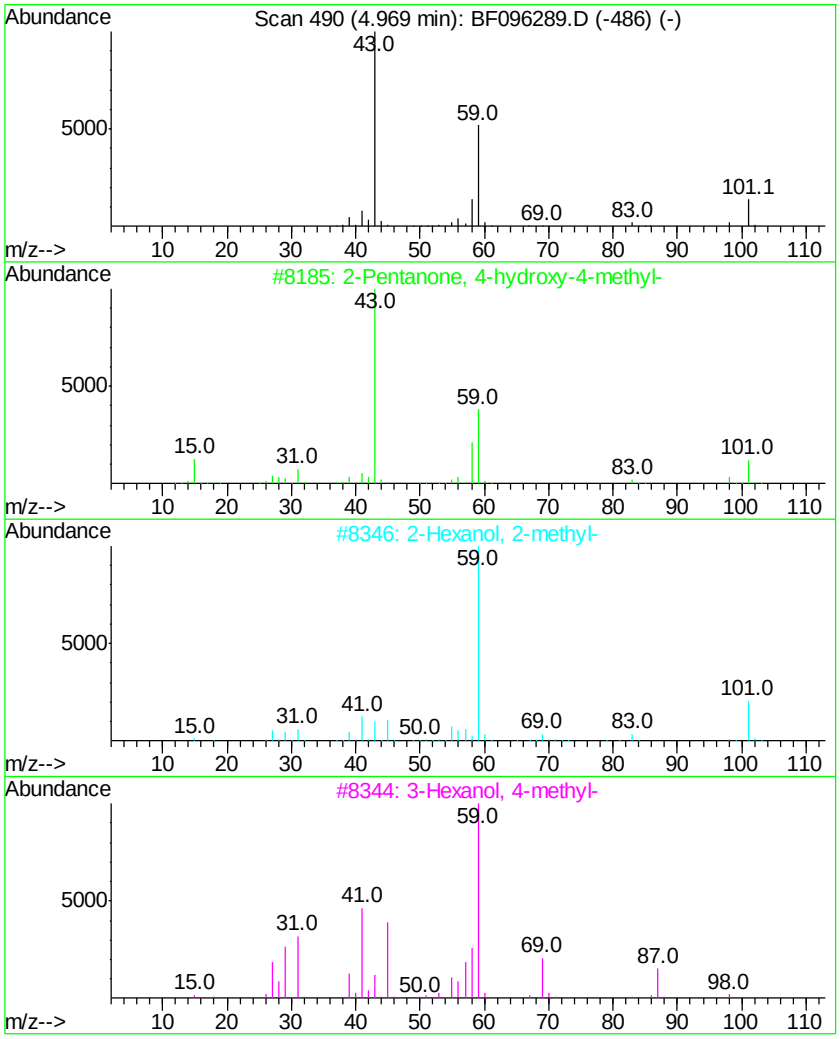
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

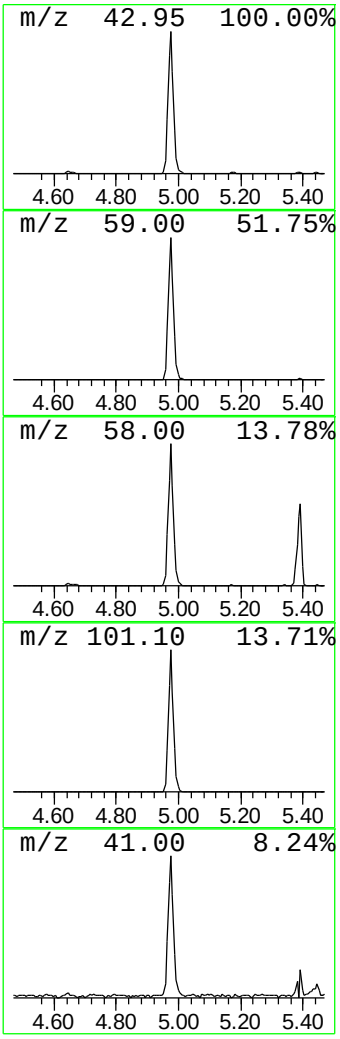
****

Peak Number 1 unknown4.97 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.97	15.75 ng	865193	1,4-Dichlorobenzene-d4	6.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	38
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF062917\
Data File : BF096289.D
Acq On : 29 Jun 2017 14:02
Operator : SJ/MA
Sample : I3897-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 72-11931

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF062717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

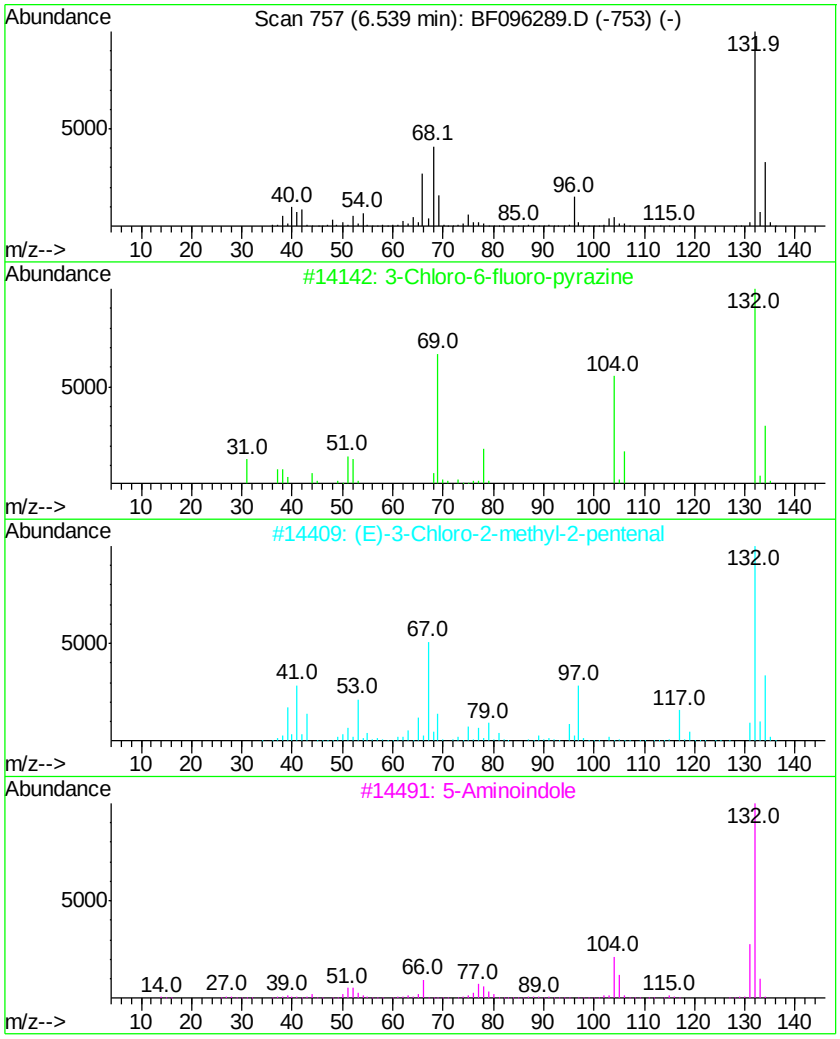
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

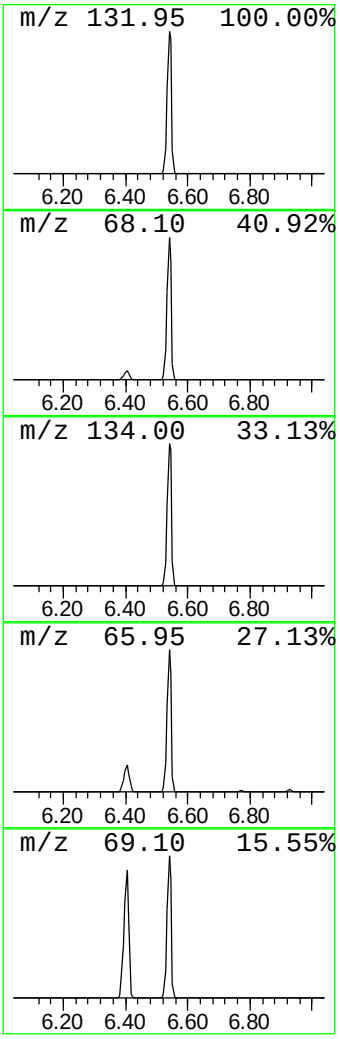
****

Peak Number 2 unknown6.54 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.54	68.43 ng	3758380	1,4-Dichlorobenzene-d4	6.77

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	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF062917\
Data File : BF096289.D
Acq On : 29 Jun 2017 14:02
Operator : SJ/MA
Sample : I3897-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 72-11931

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF062717.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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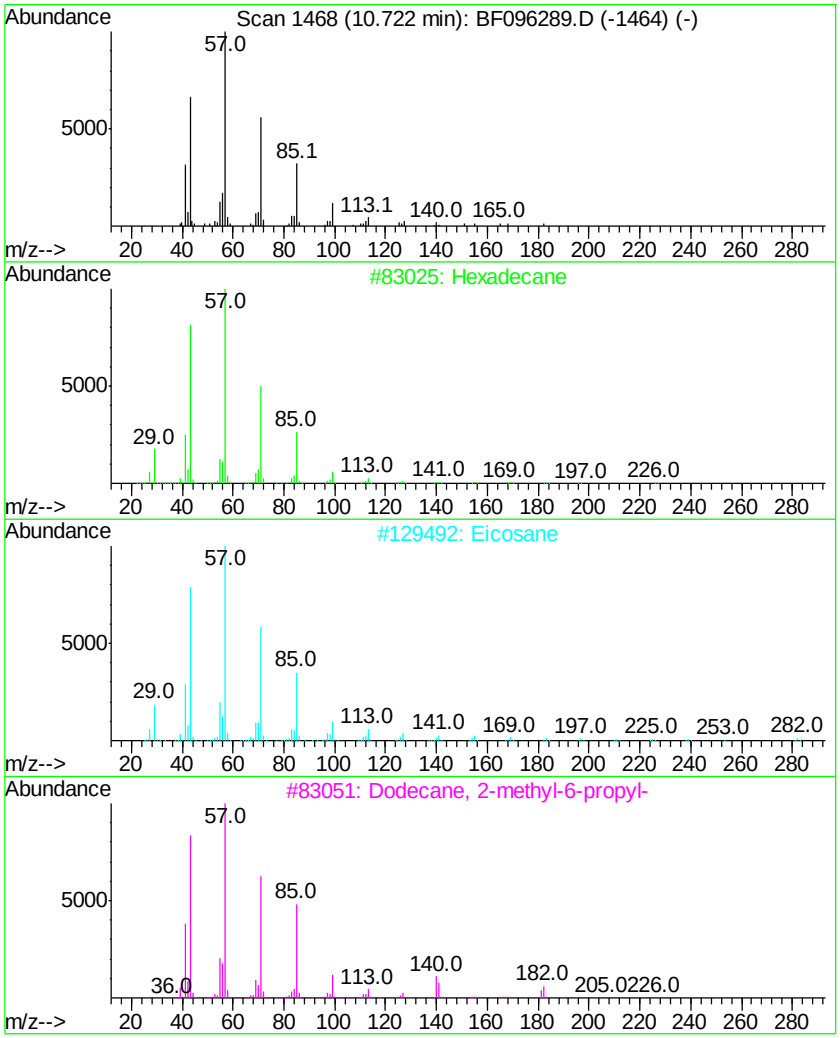
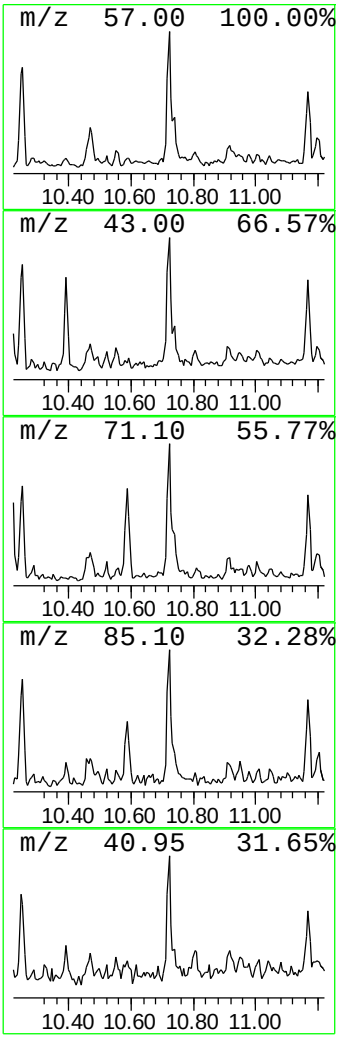
Peak Number 4 Hexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.72	2.59 ng	121670	Phenanthrene-d10	11.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	86
2	Eicosane	282	C20H42	000112-95-8	86
3	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	86
4	Pentadecane	212	C15H32	000629-62-9	80
5	Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	78





Data Path : Z:\HPCHEM1\BNA F\DATA\BF062917\
Data File : BF096289.D
Acq On : 29 Jun 2017 14:02
Operator : SJ/MA
Sample : I3897-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 72-11931

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF062717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

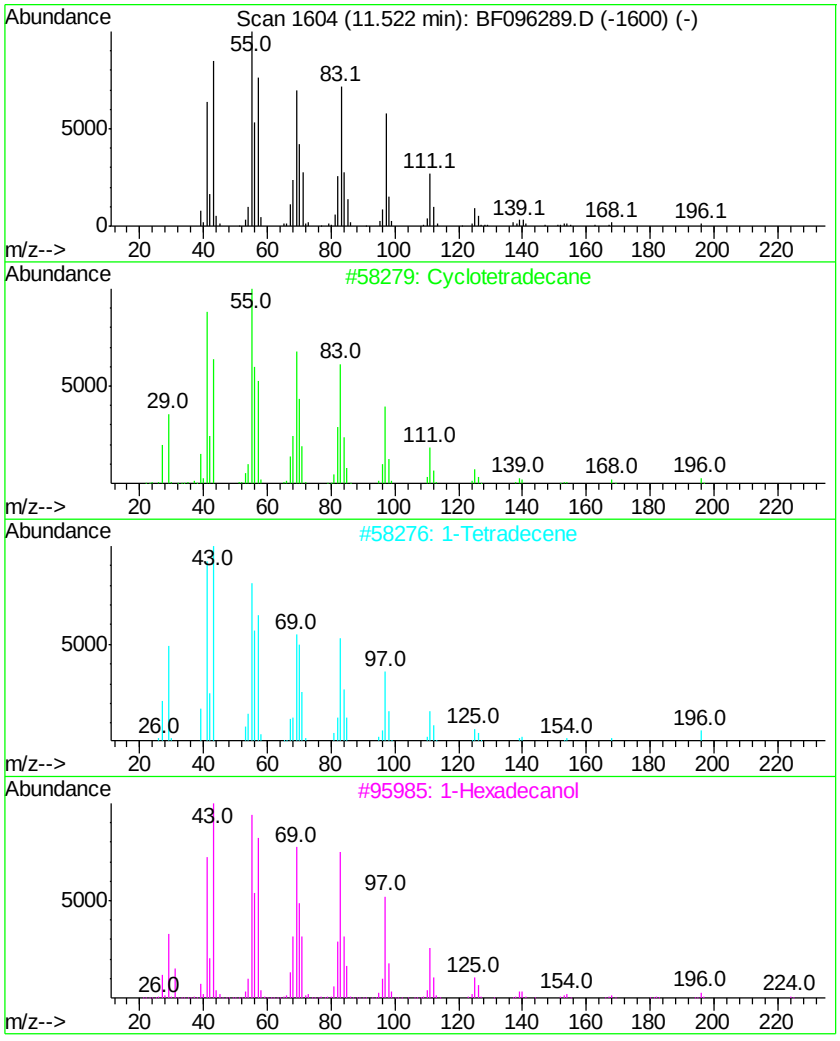
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

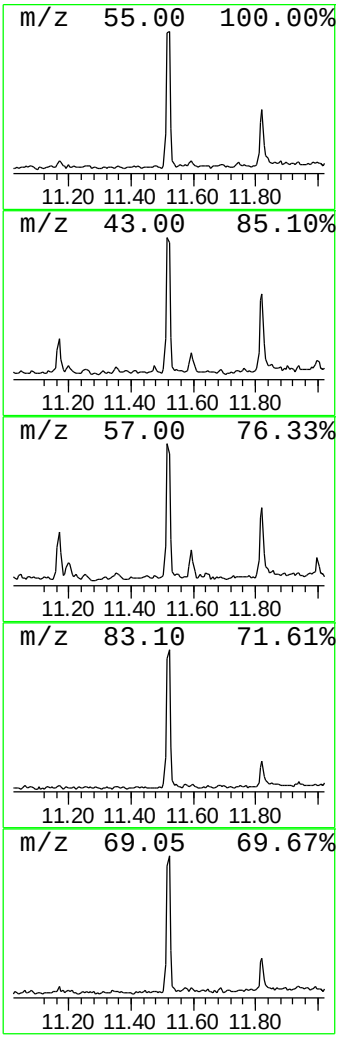
****

Peak Number 5 Cyclotetradecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.52	9.16 ng	430740	Phenanthrene-d10	11.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetradecane	196	C14H28	000295-17-0	95
2	1-Tetradecene	196	C14H28	001120-36-1	95
3	1-Hexadecanol	242	C16H34O	036653-82-4	94
4	n-Heptadecanol-1	256	C17H36O	001454-85-9	91
5	n-Pentadecanol	228	C15H32O	000629-76-5	91





Data Path : Z:\HPCHEM1\BNA F\DATA\BF062917\
Data File : BF096289.D
Acq On : 29 Jun 2017 14:02
Operator : SJ/MA
Sample : I3897-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 72-11931

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF062717.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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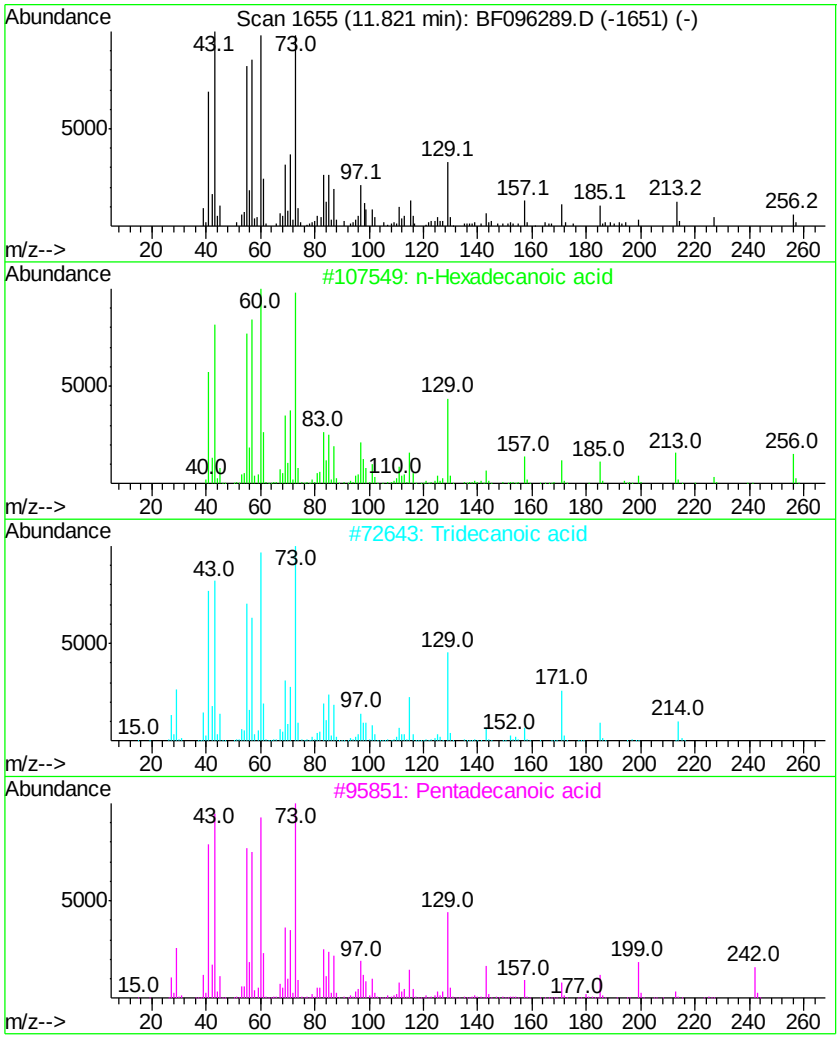
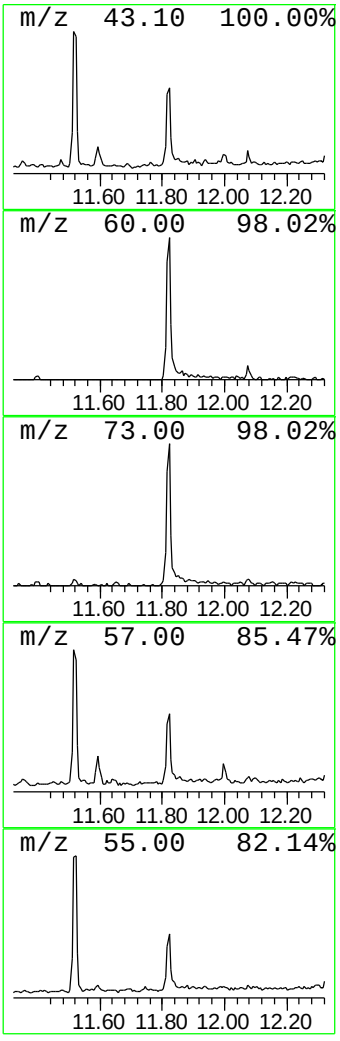
Peak Number 6 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.82	5.91 ng	277843	Phenanthrene-d10	11.29

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	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
5	Dodecanoic acid	200	C12H24O2	000143-07-7	80





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Data File : BF096289.D
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Operator : SJ/MA
Sample : I3897-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 72-11931

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF062717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

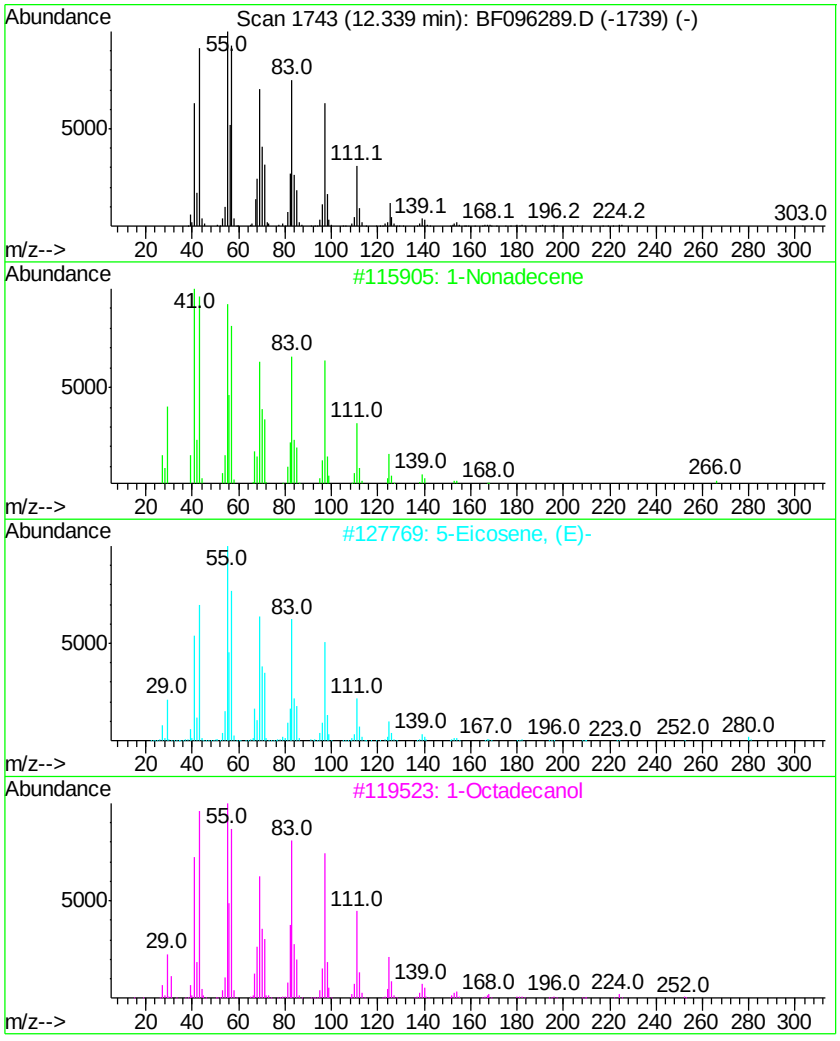
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

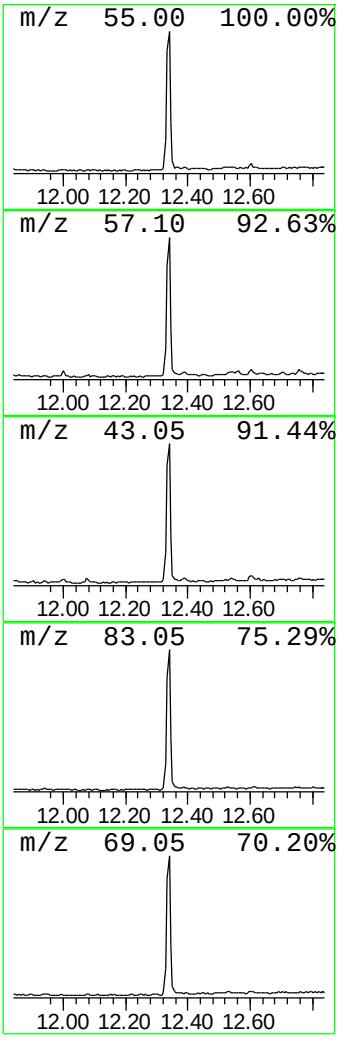
****

Peak Number 7 1-Nonadecene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.34	28.08 ng	1319770	Phenanthrene-d10	11.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene	266	C19H38	018435-45-5	91
2	5-Eicosene, (E)-	280	C20H40	074685-30-6	91
3	1-Octadecanol	270	C18H38O	000112-92-5	91
4	9-Eicosene, (E)-	280	C20H40	074685-29-3	91
5	Cyclohexadecane	224	C16H32	000295-65-8	91





Data Path : Z:\HPCHEM1\BNA F\DATA\BF062917\
Data File : BF096289.D
Acq On : 29 Jun 2017 14:02
Operator : SJ/MA
Sample : I3897-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 72-11931

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF062717.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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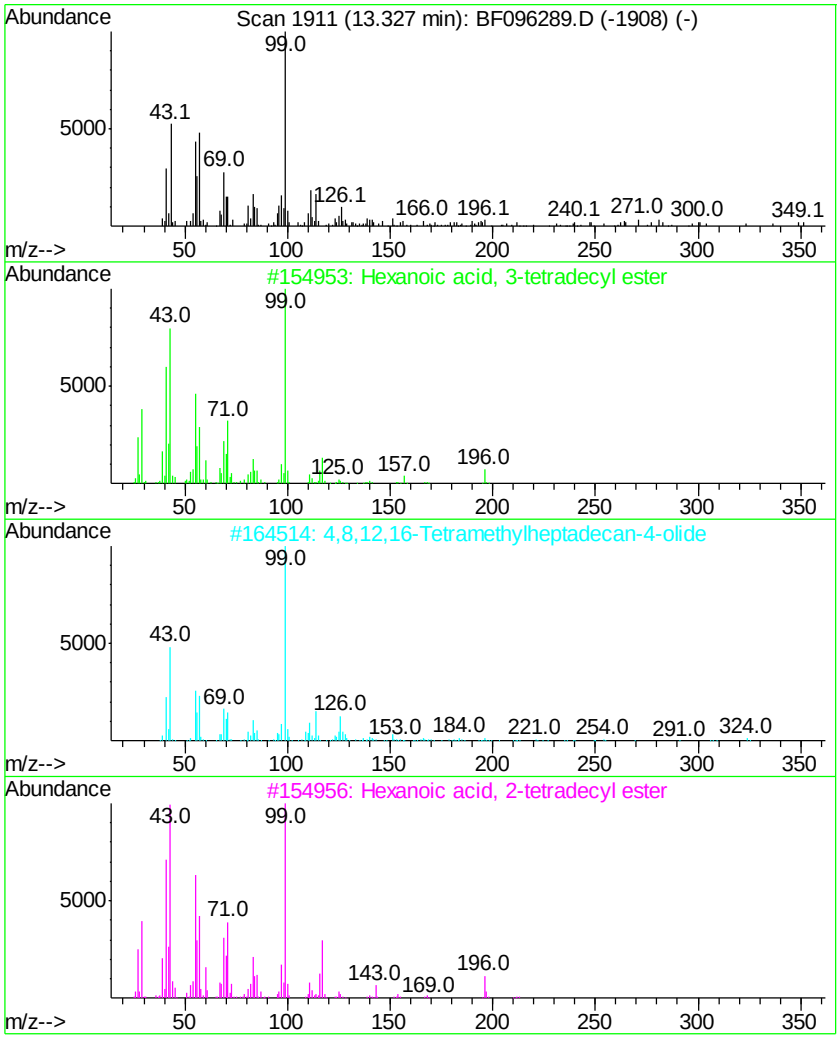
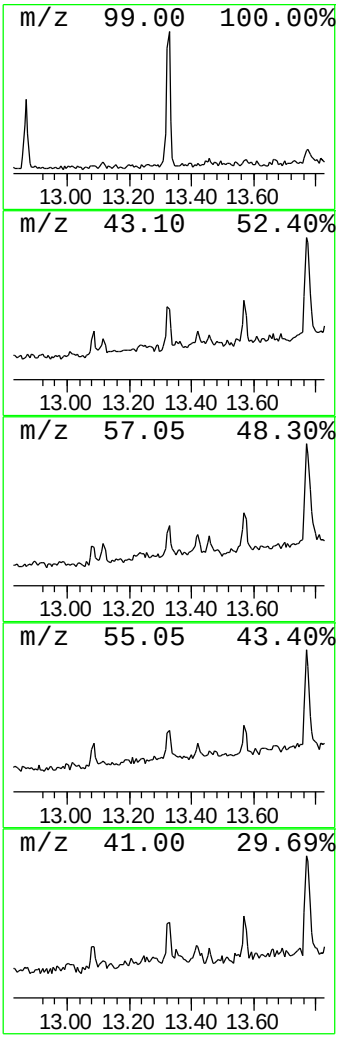
Peak Number 8 Hexanoic acid, 3-tetradecyl... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.33	2.27 ng	119678	Chrysene-d12	13.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 3-tetradecyl ester	312	C20H40O2	1000279-29-7	64
2	4,8,12,16-Tetramethylheptadecan-...	324	C21H40O2	096168-15-9	53
3	Hexanoic acid, 2-tetradecyl ester	312	C20H40O2	055193-21-0	53
4	N-Ethylpiperazine-2,3-dione	142	C6H10N2O2	059702-31-7	49
5	Ethanedicarboxamide, N-(3,5-dime...	304	C16H24N4O2	346596-53-0	47





Data Path : Z:\HPCHEM1\BNA F\DATA\BF062917\
Data File : BF096289.D
Acq On : 29 Jun 2017 14:02
Operator : SJ/MA
Sample : I3897-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 72-11931

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF062717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

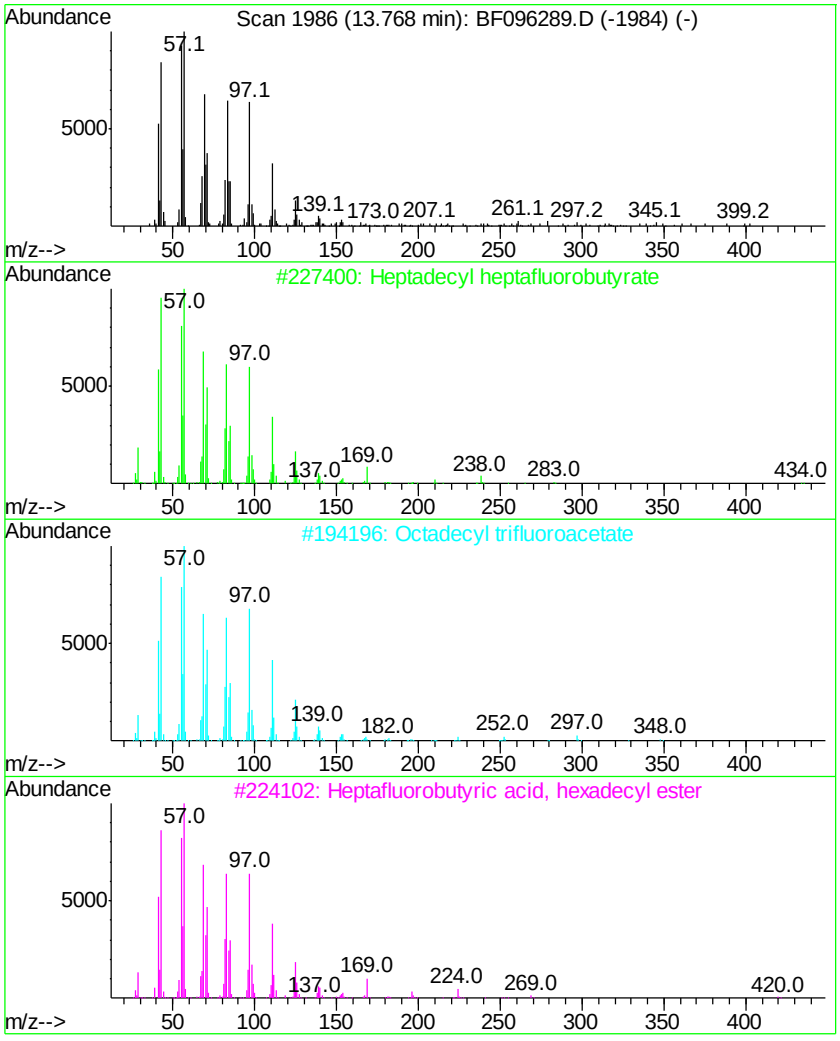
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

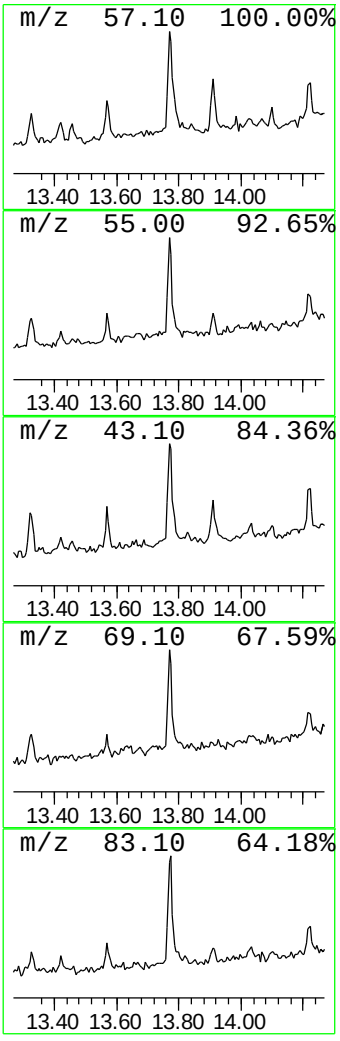
****

Peak Number 9 Heptadecyl heptafluorobutyrate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.77	6.24 ng	329434	Chrysene-d12	13.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	94
3	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	94
4	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	94
5	Cyclotetracosane	336	C24H48	000297-03-0	94





Data Path : Z:\HPCHEM1\BNA F\DATA\BF062917\
Data File : BF096289.D
Acq On : 29 Jun 2017 14:02
Operator : SJ/MA
Sample : I3897-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 72-11931

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF062717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

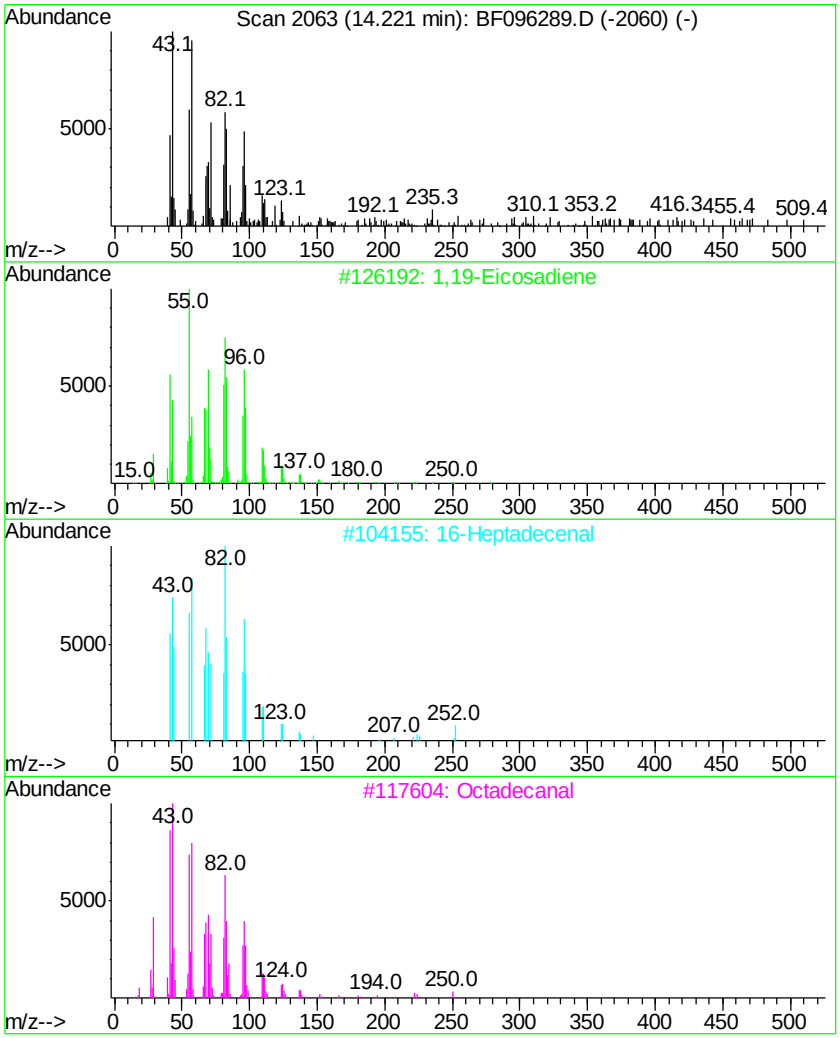
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

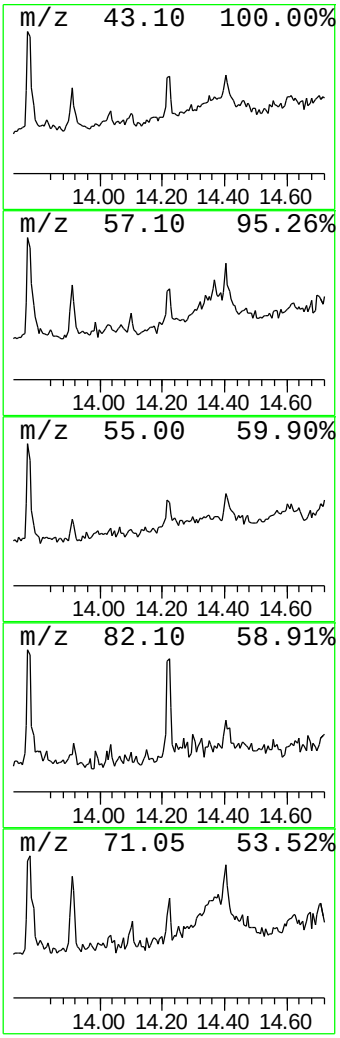
****

Peak Number 10 1,19-Eicosadiene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.22	2.15 ng	113300	Chrysene-d12	13.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,19-Eicosadiene	278	C20H38	014811-95-1	83
2	16-Heptadecenal	252	C17H32O	1000144-57-9	80
3	Octadecanal	268	C18H36O	000638-66-4	64
4	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	64
5	Bicyclo[10.8.0]eicosane, cis-	278	C20H38	1000155-82-2	59





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062917\
Data File : BF096289.D
Acq On : 29 Jun 2017 14:02
Operator : SJ/MA
Sample : I3897-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 72-11931

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF062717.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
unknown4.97	4.97	15.8	ng	865193	1	6.77	1098500	20.0
unknown6.54	6.54	68.4	ng	3758380	1	6.77	1098500	20.0
Hexadecane	10.72	2.6	ng	121670	4	11.29	940102	20.0
Cyclotetradecane	11.52	9.2	ng	430740	4	11.29	940102	20.0
n-Hexadecanoic acid	11.82	5.9	ng	277843	4	11.29	940102	20.0
1-Nonadecene	12.34	28.1	ng	1319770	4	11.29	940102	20.0
Hexanoic acid, 3-...	13.33	2.3	ng	119678	5	13.92	1055530	20.0
Heptadecyl heptaf...	13.77	6.2	ng	329434	5	13.92	1055530	20.0
1,19-Eicosadiene	14.22	2.1	ng	113300	5	13.92	1055530	20.0