LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091718\
Data File : BF109070.D
Acq On : 18 Sep 2018 2:10
Operator : JU/SJ
Sample : J4936-07
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PHASE-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-BF091418.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	4.266	324	328	337	rBV	92639	113143	3.48%	0.404%
2	4.919	434	439	448	rVB	140377	189926	5.85%	0.678%
3	5.331	504	509	512	rBV	2827045	3008036	92.63%	10.742%
4	6.360	678	684	687	rBV	3079171	3072131	94.60%	10.971%
5	6.490	701	706	709	rBV	3204872	3069074	94.51%	10.960%
6	6.719	742	745	749	rBV	896989	753246	23.20%	2.690%
7	6.878	768	772	775	rBV	3029715	2493129	76.77%	8.903%
8	7.284	836	841	844	rBV	2008424	1911472	58.86%	6.826%
9	8.001	959	963	966	rBV	1093154	849757	26.17%	3.035%
10	9.078	1142	1146	1149	rBV	3685829	3247401	100.00%	11.597%
11	9.466	1209	1212	1216	rBV	183807	160531	4.94%	0.573%
12	9.748	1257	1260	1264	rBV	961775	856025	26.36%	3.057%
13	10.536	1390	1394	1397	rBV	2071372	1827675	56.28%	6.527%
14	11.225	1508	1511	1515	rBV	973009	884250	27.23%	3.158%
15	12.813	1777	1781	1784	rBV	3114084	2999691	92.37%	10.712%
16	13.724	1932	1936	1942	rVB	186599	250620	7.72%	0.895%
17	13.854	1954	1958	1965	rVB	1048572	960997	29.59%	3.432%
18	14.042	1987	1990	1995	rBV	115713	98886	3.05%	0.353%
19	14.342	2038	2041	2044	rBV	107873	87203	2.69%	0.311%
20	14.636	2088	2091	2101	rVB	129300	145980	4.50%	0.521%
21	14.954	2142	2145	2150	rVB	115721	123355	3.80%	0.441%
22	15.254	2192	2196	2201	rVB	579284	672824	20.72%	2.403%
23	15.307	2202	2205	2213	rVB	98436	140123	4.31%	0.500%
24	15.713	2270	2274	2279	rBV2	62596	87298	2.69%	0.312%

Sum of corrected areas: 28002773

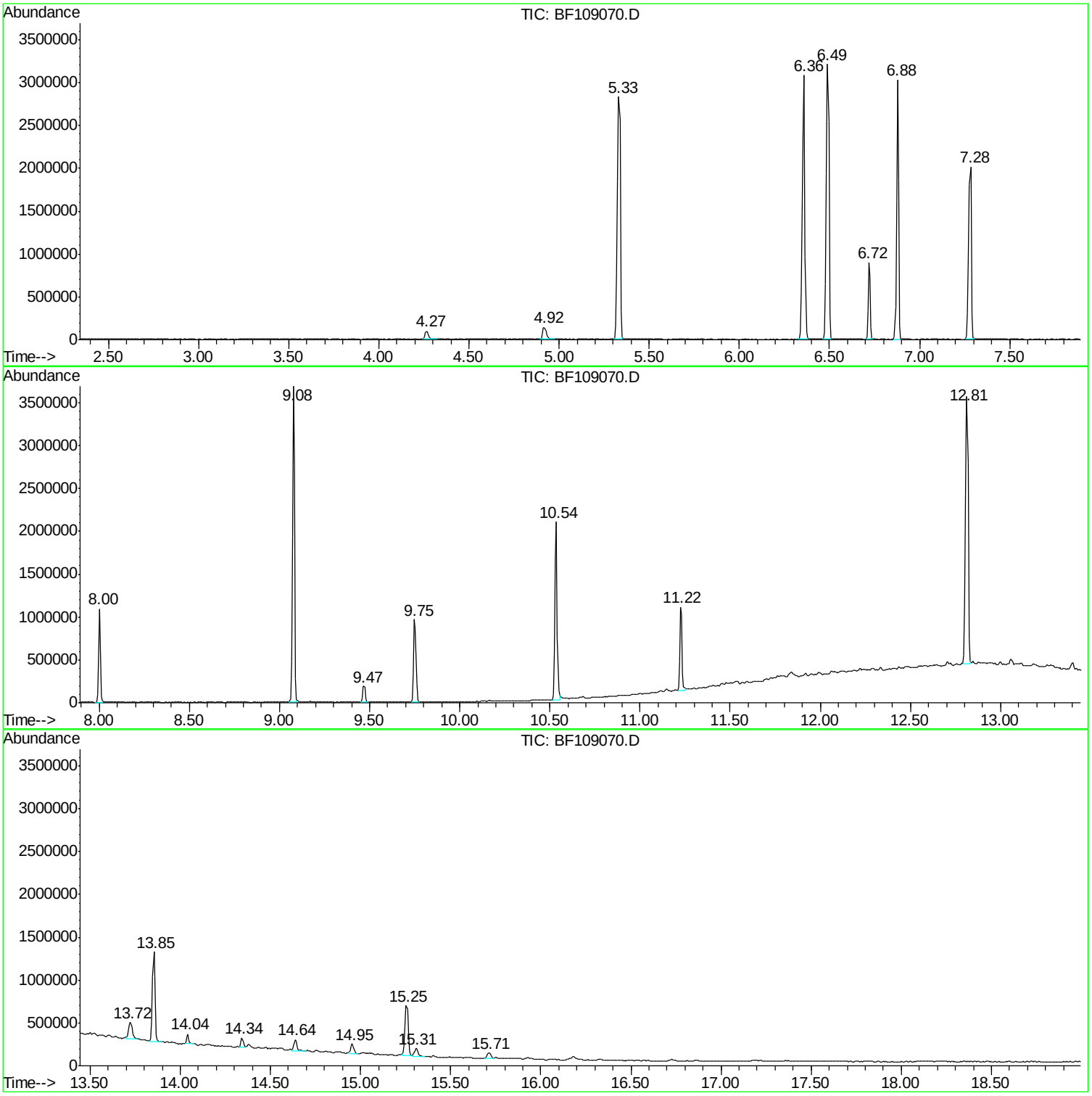
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091718\
Data File : BF109070.D
Acq On : 18 Sep 2018 2:10
Operator : JU/SJ
Sample : J4936-07
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PHASE-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.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\BF091718\
Data File : BF109070.D
Acq On : 18 Sep 2018 2:10
Operator : JU/SJ
Sample : J4936-07
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PHASE-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

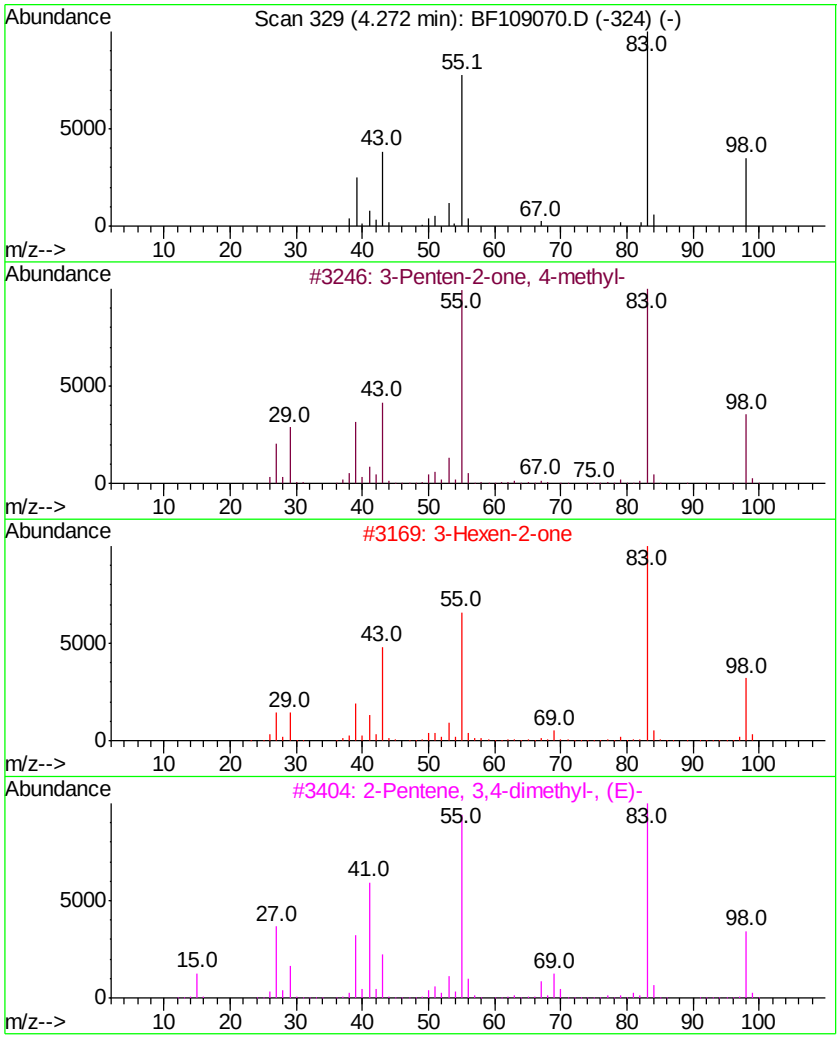
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

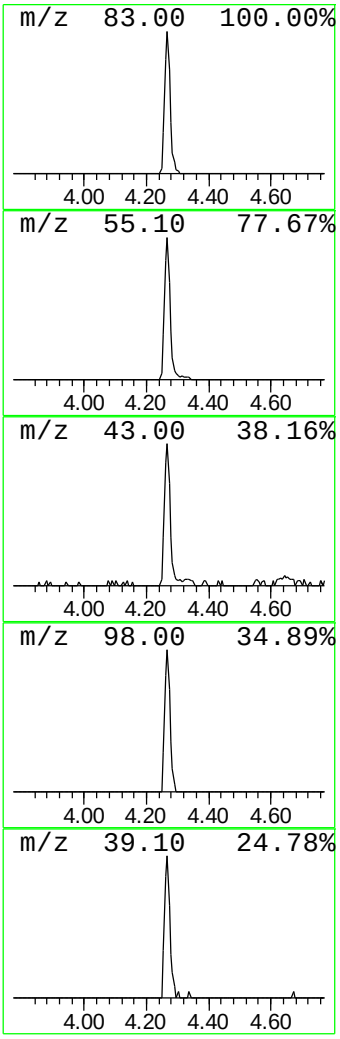
****

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.27	3.00 ng	113143	1,4-Dichlorobenzene-d4	6.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	95
2	3-Hexen-2-one	98	C6H10O	000763-93-9	90
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091718\
Data File : BF109070.D
Acq On : 18 Sep 2018 2:10
Operator : JU/SJ
Sample : J4936-07
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PHASE-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.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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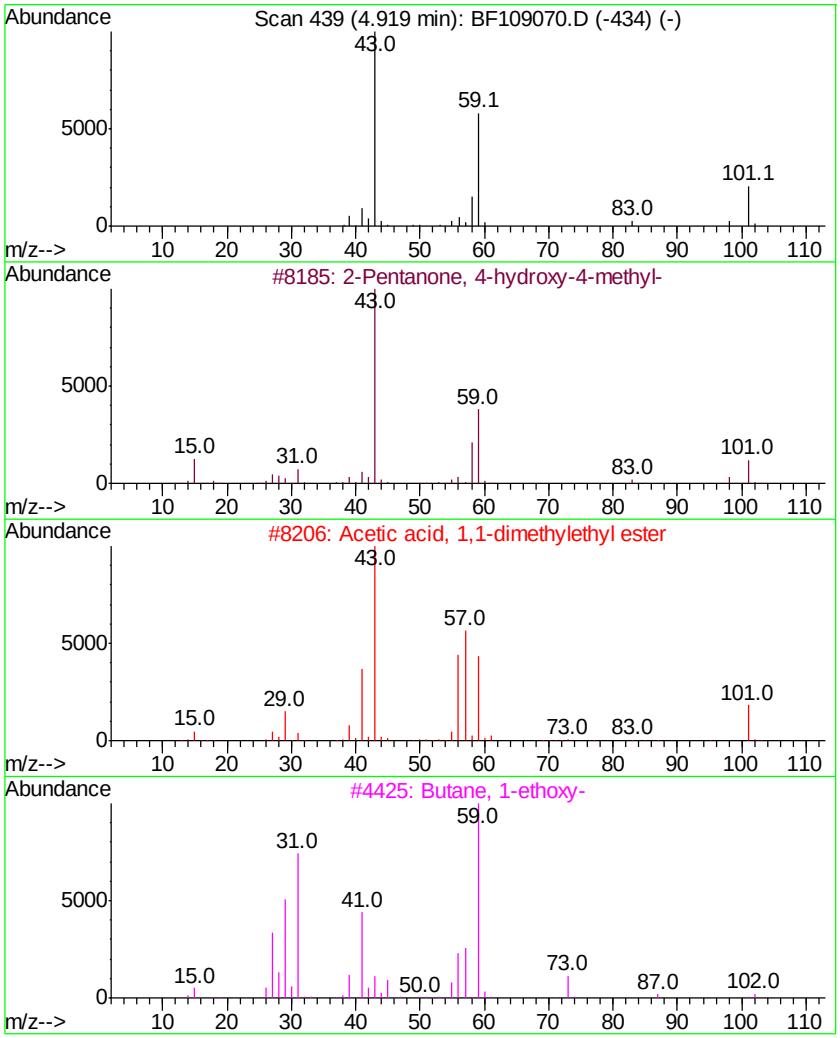
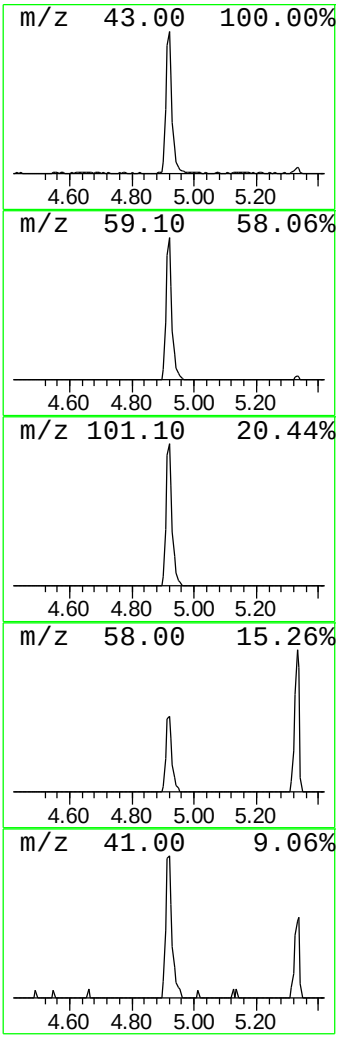
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.92	5.04 ng	189926	1,4-Dichlorobenzene-d4	6.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091718\
Data File : BF109070.D
Acq On : 18 Sep 2018 2:10
Operator : JU/SJ
Sample : J4936-07
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PHASE-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.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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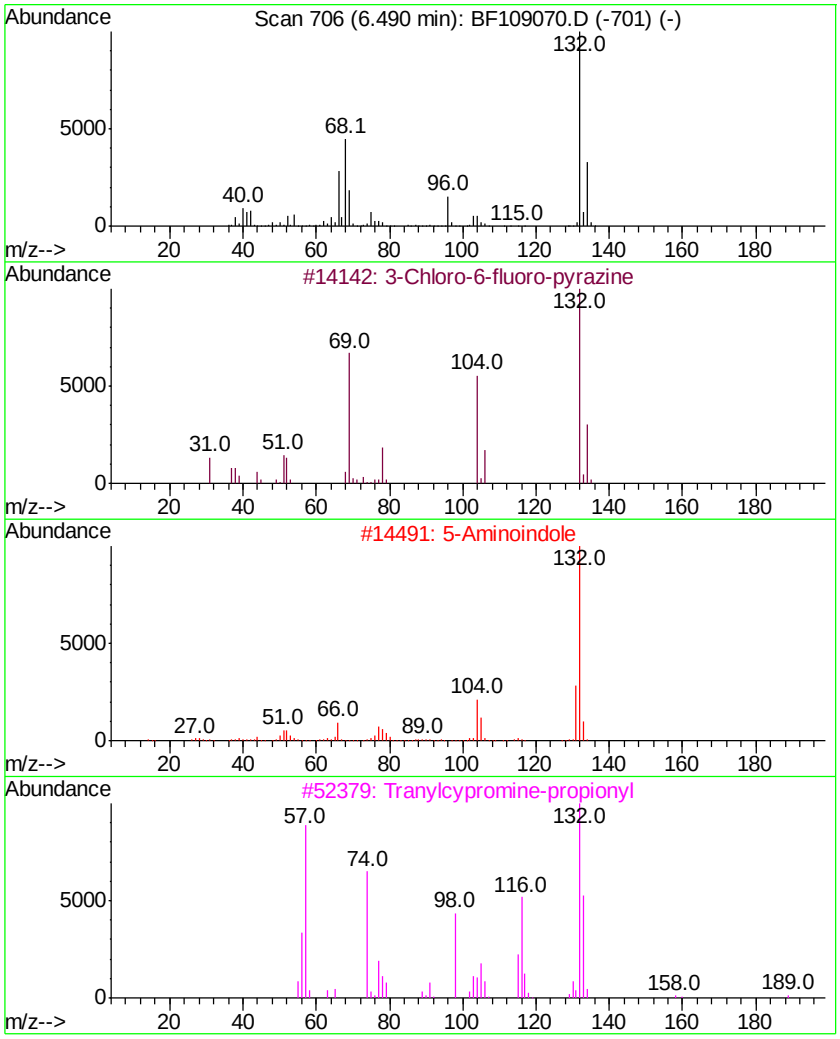
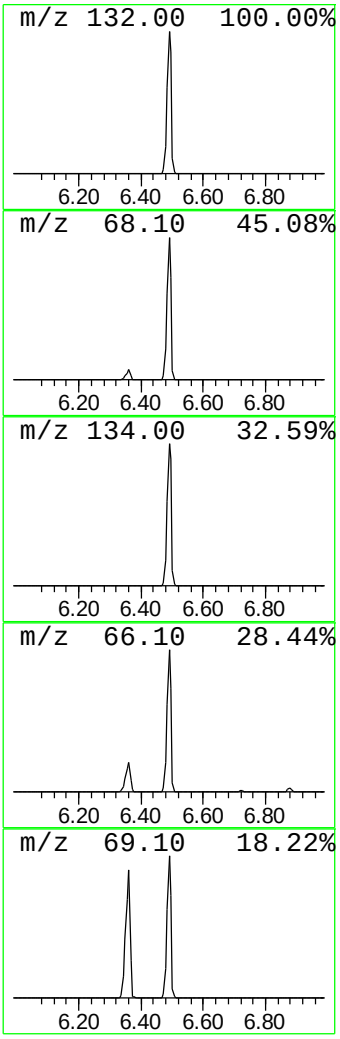
Peak Number 3 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	81.49 ng	3069070	1,4-Dichlorobenzene-d4	6.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091718\
Data File : BF109070.D
Acq On : 18 Sep 2018 2:10
Operator : JU/SJ
Sample : J4936-07
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PHASE-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

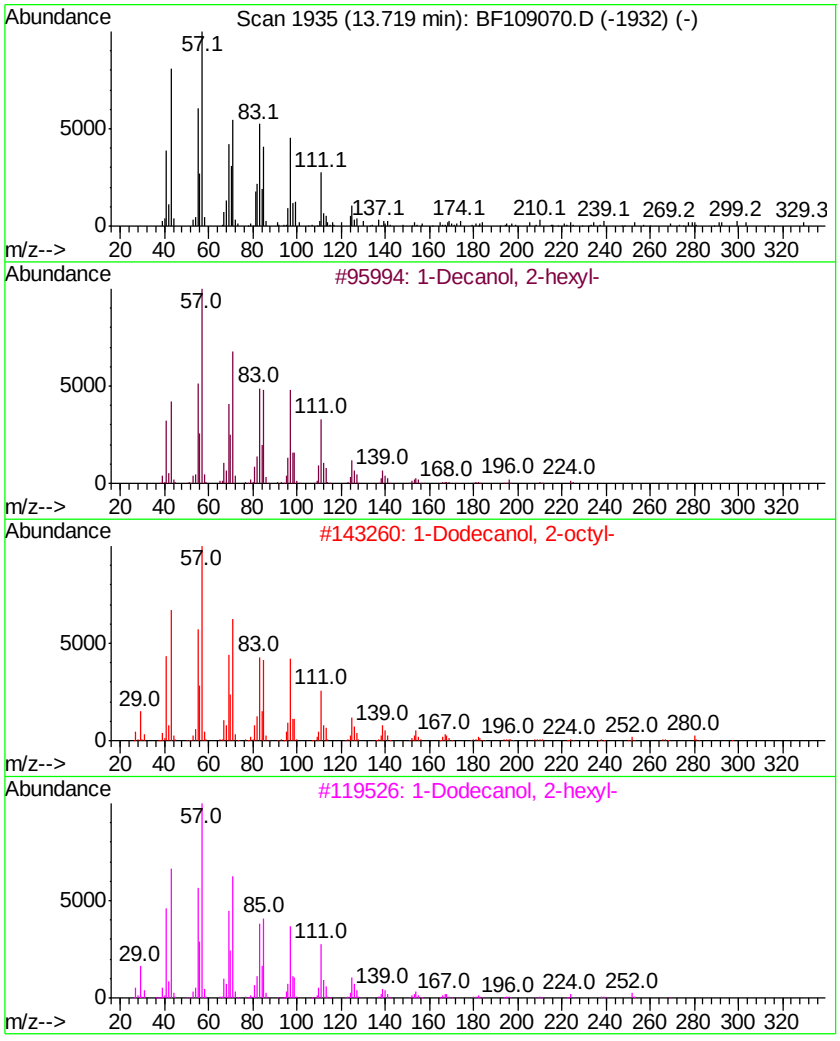
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

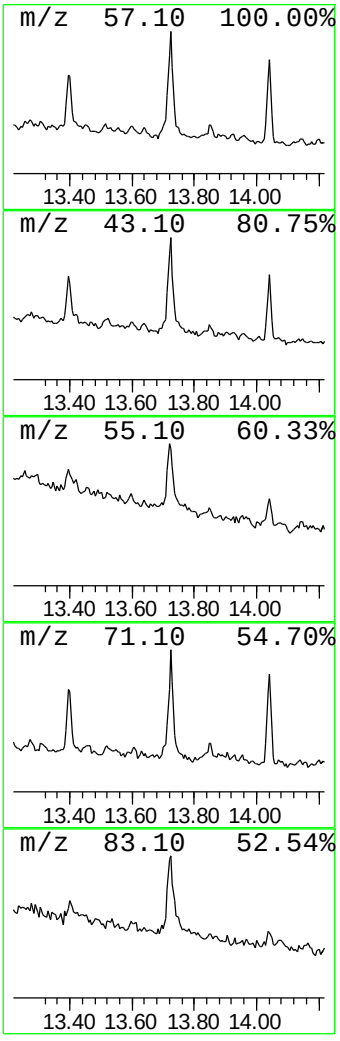
****

Peak Number 5 1-Decanol, 2-hexyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.72	5.22 ng	250620	Chrysene-d12	13.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	90
2	1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	87
3	1-Dodecanol, 2-hexyl-	270	C18H38O	110225-00-8	87
4	Decane, 1,1'-oxybis-	298	C20H42O	002456-28-2	87
5	Oxalic acid, isobutyl tetradecyl...	342	C20H38O4	1000309-37-9	80





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091718\
Data File : BF109070.D
Acq On : 18 Sep 2018 2:10
Operator : JU/SJ
Sample : J4936-07
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PHASE-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

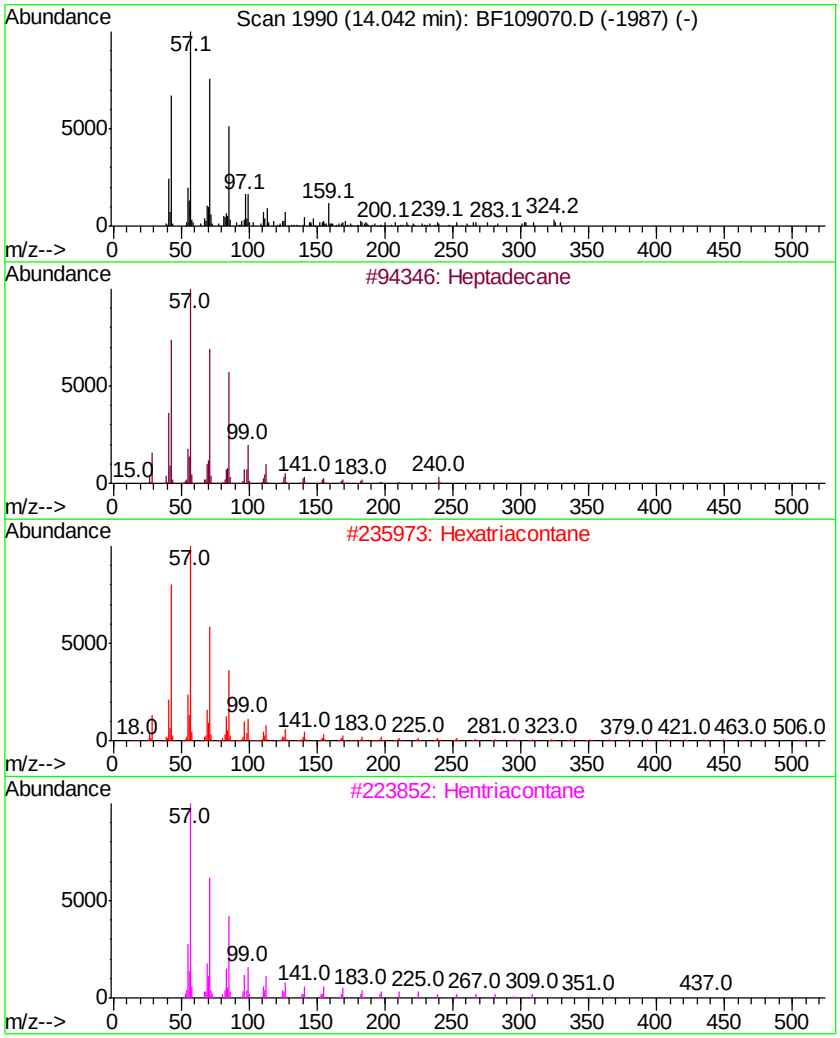
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

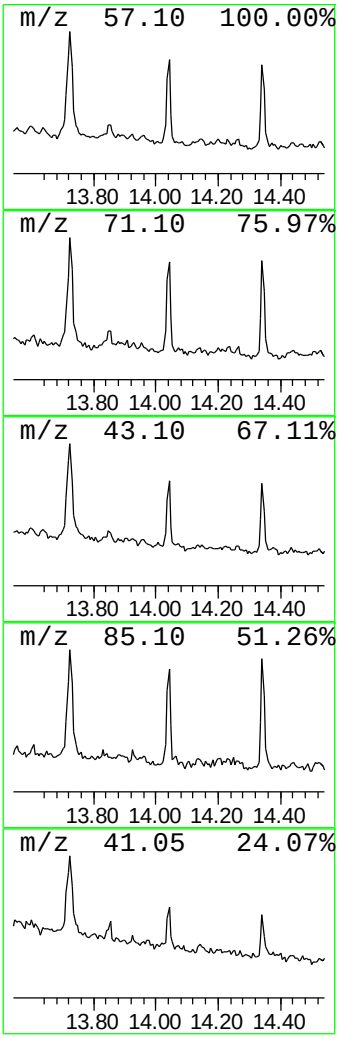
****

Peak Number 6 Heptadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.04	2.06 ng	98886	Chrysene-d12	13.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	91
2	Hexatriacontane	507	C36H74	000630-06-8	86
3	Hentriacontane	437	C31H64	000630-04-6	86
4	2-methyltetracosane	352	C25H52	1000376-72-6	86
5	Hexacosane	366	C26H54	000630-01-3	86





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091718\
Data File : BF109070.D
Acq On : 18 Sep 2018 2:10
Operator : JU/SJ
Sample : J4936-07
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PHASE-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

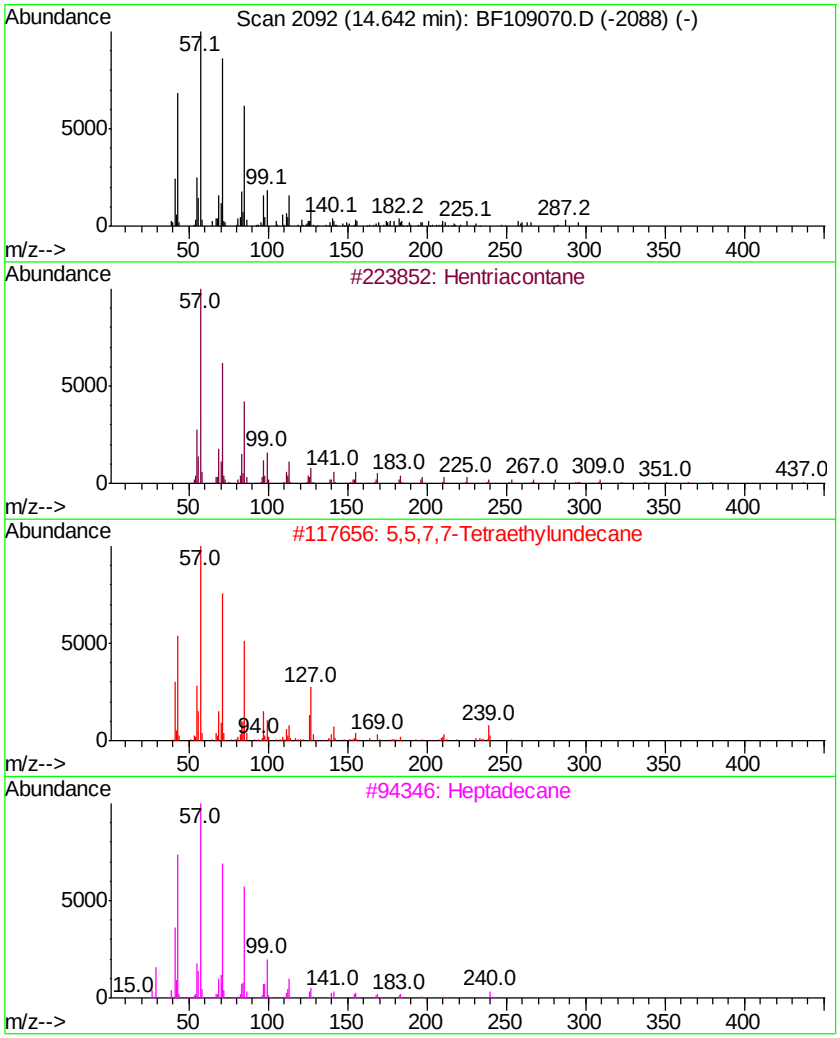
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

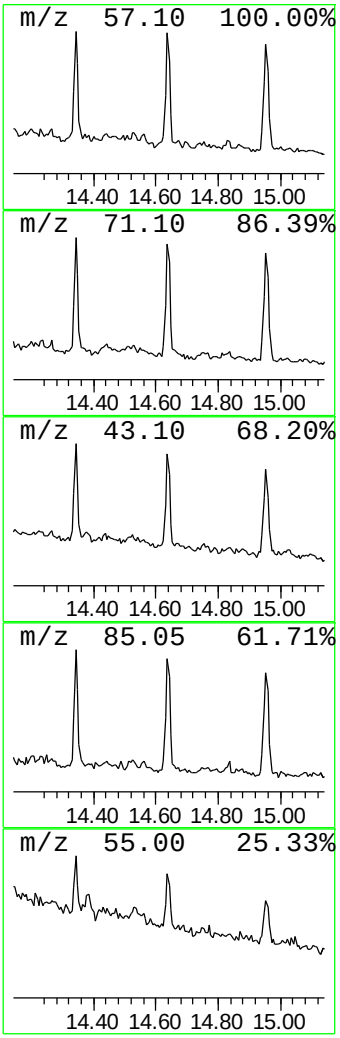
****

Peak Number 7 Hentriacontane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.64	4.34 ng	145980	Perylene-d12	15.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane	437	C31H64	000630-04-6	91
2	5,5,7,7-Tetraethylundecane	268	C19H40	1000360-42-0	90
3	Heptadecane	240	C17H36	000629-78-7	86
4	Octadecane	254	C18H38	000593-45-3	80
5	Tetratetracontane	619	C44H90	007098-22-8	74





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091718\
Data File : BF109070.D
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Misc :
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Instrument : BNA_F
ClientSampleId : PHASE-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.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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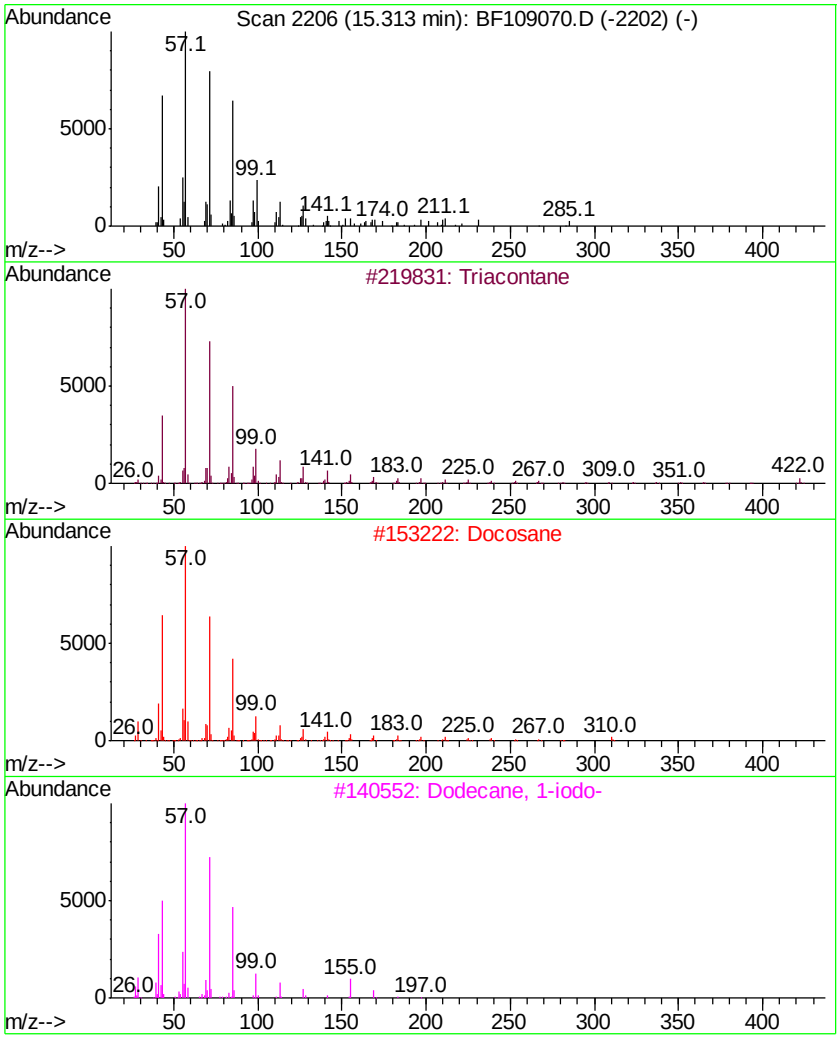
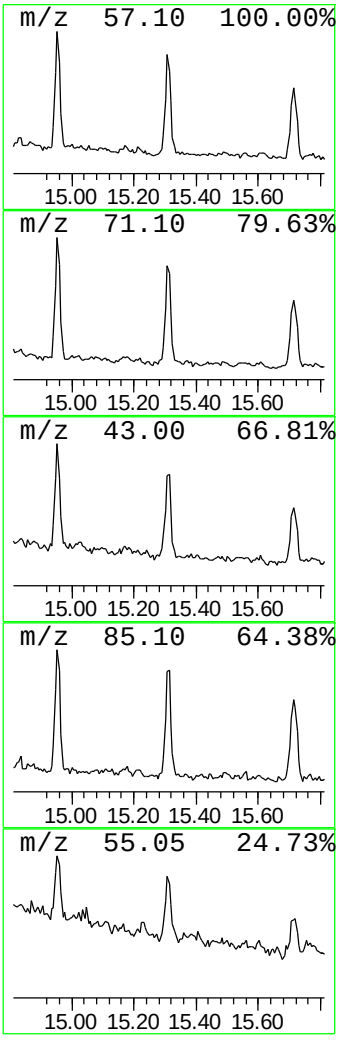
Peak Number 9 Triacontane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.31	4.17 ng	140123	Perylene-d12	15.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triacontane	422	C30H62	000638-68-6	87
2	Docosane	310	C22H46	000629-97-0	87
3	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	86
4	Octadecane	254	C18H38	000593-45-3	86
5	Hexadecane	226	C16H34	000544-76-3	86





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091718\
Data File : BF109070.D
Acq On : 18 Sep 2018 2:10
Operator : JU/SJ
Sample : J4936-07
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PHASE-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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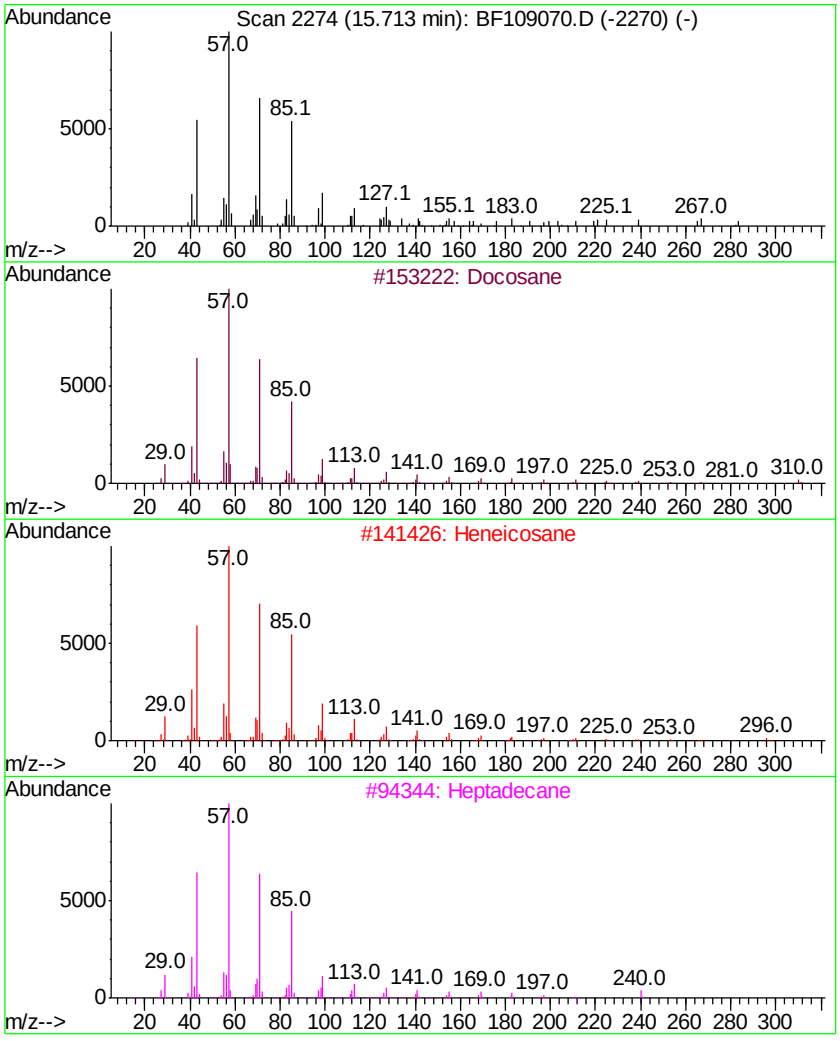
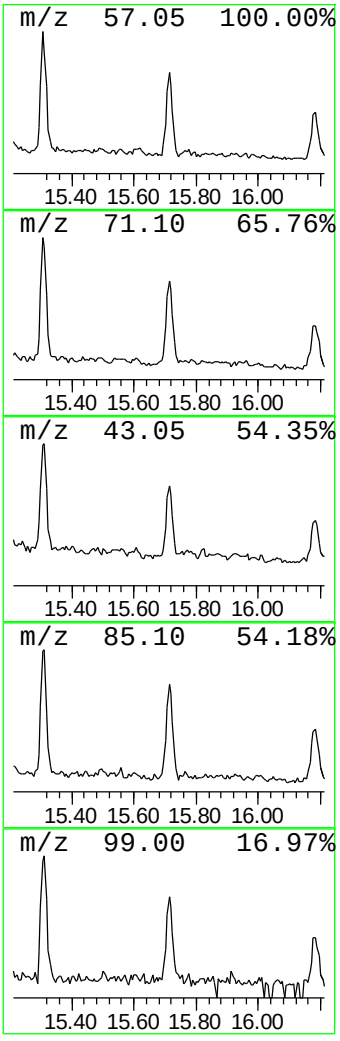
Peak Number 10 Docosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.71	2.59 ng	87298	Perylene-d12	15.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosane	310	C22H46	000629-97-0	90
2	Heneicosane	296	C21H44	000629-94-7	87
3	Heptadecane	240	C17H36	000629-78-7	86
4	Eicosane	282	C20H42	000112-95-8	86
5	Hexadecane	226	C16H34	000544-76-3	80





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF091718\
Data File : BF109070.D
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Operator : JU/SJ
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Misc :
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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
3-Penten-2-one, 4...	4.27	3.0	ng	113143	1	6.72	753246	20.0
2-Pentanone, 4-hy...	4.92	5.0	ng	189926	1	6.72	753246	20.0
unknown6.49	6.49	81.5	ng	3069070	1	6.72	753246	20.0
1-Decanol, 2-hexyl-	13.72	5.2	ng	250620	5	13.85	960997	20.0
Heptadecane	14.04	2.1	ng	98886	5	13.85	960997	20.0
Hentriacontane	14.64	4.3	ng	145980	6	15.25	672824	20.0
Triacontane	15.31	4.2	ng	140123	6	15.25	672824	20.0
Docosane	15.71	2.6	ng	87298	6	15.25	672824	20.0