LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101718\
Data File : BF109934.D
Acq On : 17 Oct 2018 21:42
Operator : JU/SJ
Sample : J5539-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DUP

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-BF101518.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	2.316	34	39	49	rVB	594246	781686	14.58%	1.559%
2	5.216	528	532	539	rVB	201847	236776	4.42%	0.472%
3	5.598	591	597	600	rBV	5076386	4979215	92.87%	9.932%
4	6.598	760	767	771	rBV	4713611	5361711	100.00%	10.695%
5	6.745	787	792	795	rBV	5502965	5139729	95.86%	10.252%
6	6.975	828	831	835	rBV	1687366	1384217	25.82%	2.761%
7	7.133	854	858	861	rBV	4844091	4055980	75.65%	8.090%
8	7.539	922	927	930	rBV	3535483	3202185	59.72%	6.387%
9	8.257	1045	1049	1053	rBV	1944972	1668601	31.12%	3.328%
10	9.333	1228	1232	1235	rBV	6119116	5258484	98.07%	10.489%
11	9.721	1295	1298	1301	rBV	772612	559439	10.43%	1.116%
12	10.016	1345	1348	1352	rBV	1819553	1596807	29.78%	3.185%
13	10.804	1478	1482	1486	rBV	2670465	2590966	48.32%	5.168%
14	11.510	1598	1602	1604	rBV	1634784	1351544	25.21%	2.696%
15	11.533	1604	1606	1610	rVB	111851	91287	1.70%	0.182%
16	12.015	1684	1688	1691	rBV2	170608	158738	2.96%	0.317%
17	12.727	1805	1809	1812	rBV	176410	152192	2.84%	0.304%
18	12.951	1842	1847	1850	rBV	151010	164977	3.08%	0.329%
19	13.092	1867	1871	1875	rBV	4366399	3988584	74.39%	7.956%
20	13.974	2018	2021	2033	rVB	512324	540726	10.08%	1.079%
21	14.151	2047	2051	2054	rBV	1645439	1541156	28.74%	3.074%
22	14.180	2054	2056	2060	rVB	73908	63340	1.18%	0.126%
23	14.298	2073	2076	2081	rBV	203851	185990	3.47%	0.371%
24	14.604	2125	2128	2137	rVB2	419701	517545	9.65%	1.032%
25	14.927	2179	2183	2192	rVB	384836	471086	8.79%	0.940%
26	15.003	2194	2196	2200	rVB	71449	70057	1.31%	0.140%
27	15.080	2206	2209	2212	rVB	86902	87455	1.63%	0.174%
28	15.221	2230	2233	2236	rBV	60639	83174	1.55%	0.166%
29	15.280	2239	2243	2246	rBV	470623	551425	10.28%	1.100%
30	15.680	2306	2311	2320	rBV2	1460027	2062546	38.47%	4.114%
31	16.150	2386	2391	2396	rBV	401085	580550	10.83%	1.158%
32	16.203	2397	2400	2409	rVB5	66463	113815	2.12%	0.227%
33	16.692	2478	2483	2490	rVB2	178180	339324	6.33%	0.677%
34	17.327	2587	2591	2599	rVB2	95345	203822	3.80%	0.407%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101718\
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Acq On : 17 Oct 2018 21:42
Operator : JU/SJ
Sample : J5539-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DUP

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-BF101518.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

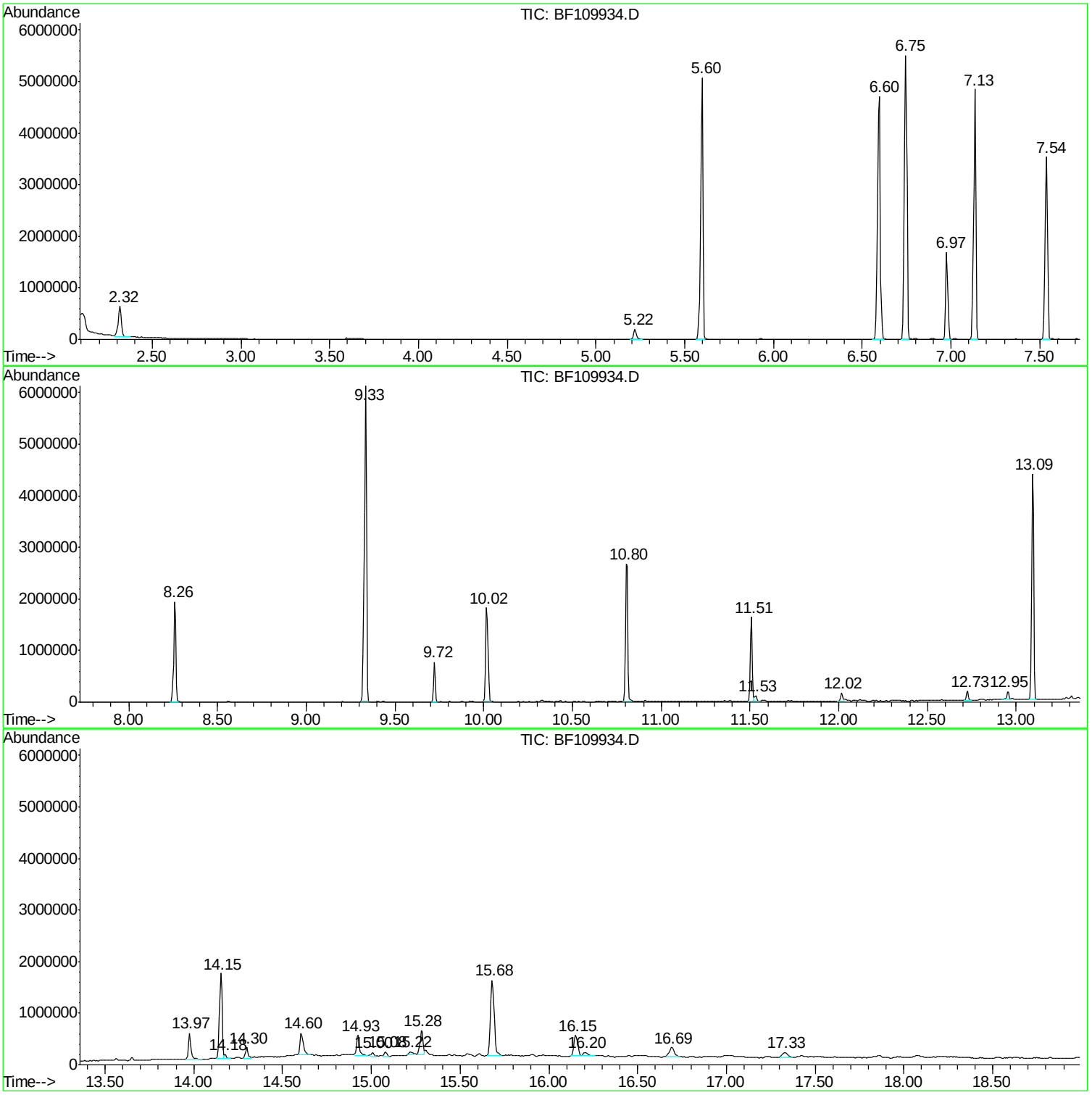
Sum of corrected areas: 50135129

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101718\
Data File : BF109934.D
Acq On : 17 Oct 2018 21:42
Operator : JU/SJ
Sample : J5539-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DUP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101518.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\BF101718\
Data File : BF109934.D
Acq On : 17 Oct 2018 21:42
Operator : JU/SJ
Sample : J5539-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DUP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

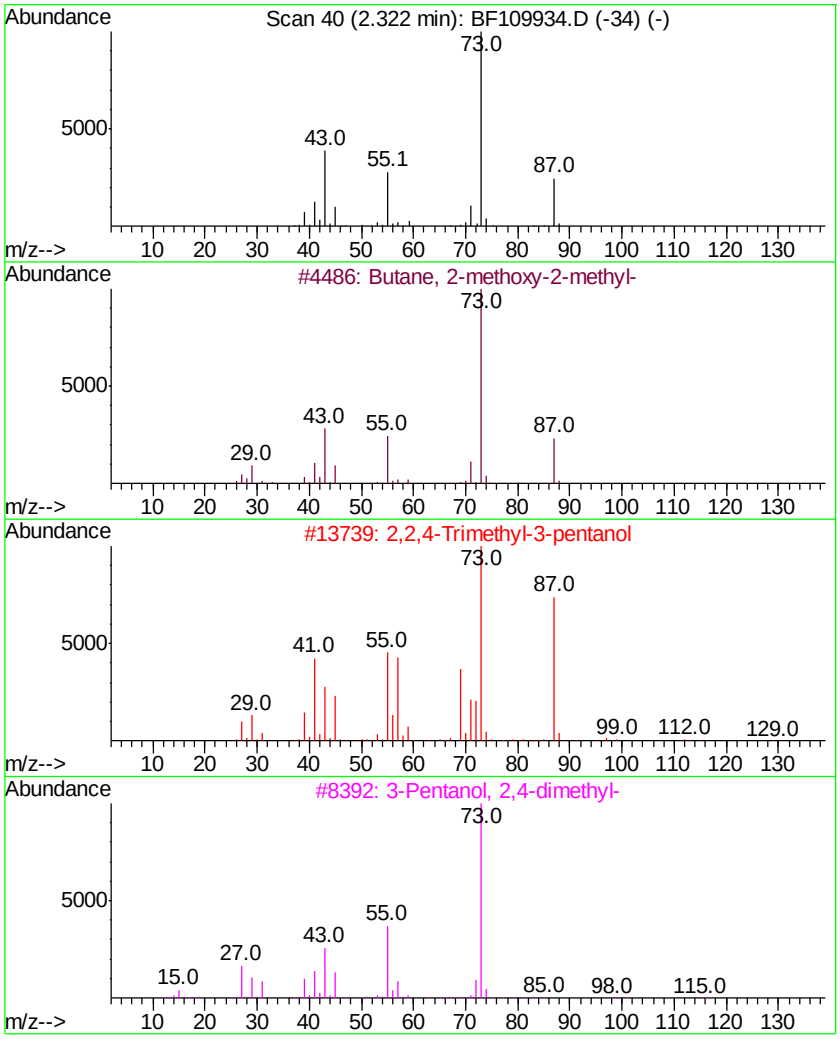
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

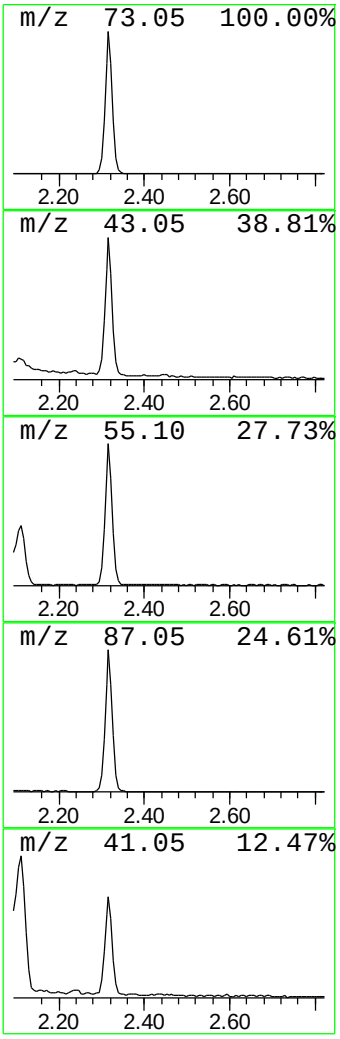
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.32	11.29 ng	781686	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





Library Search Compound Report

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Data File : BF109934.D
Acq On : 17 Oct 2018 21:42
Operator : JU/SJ
Sample : J5539-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DUP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

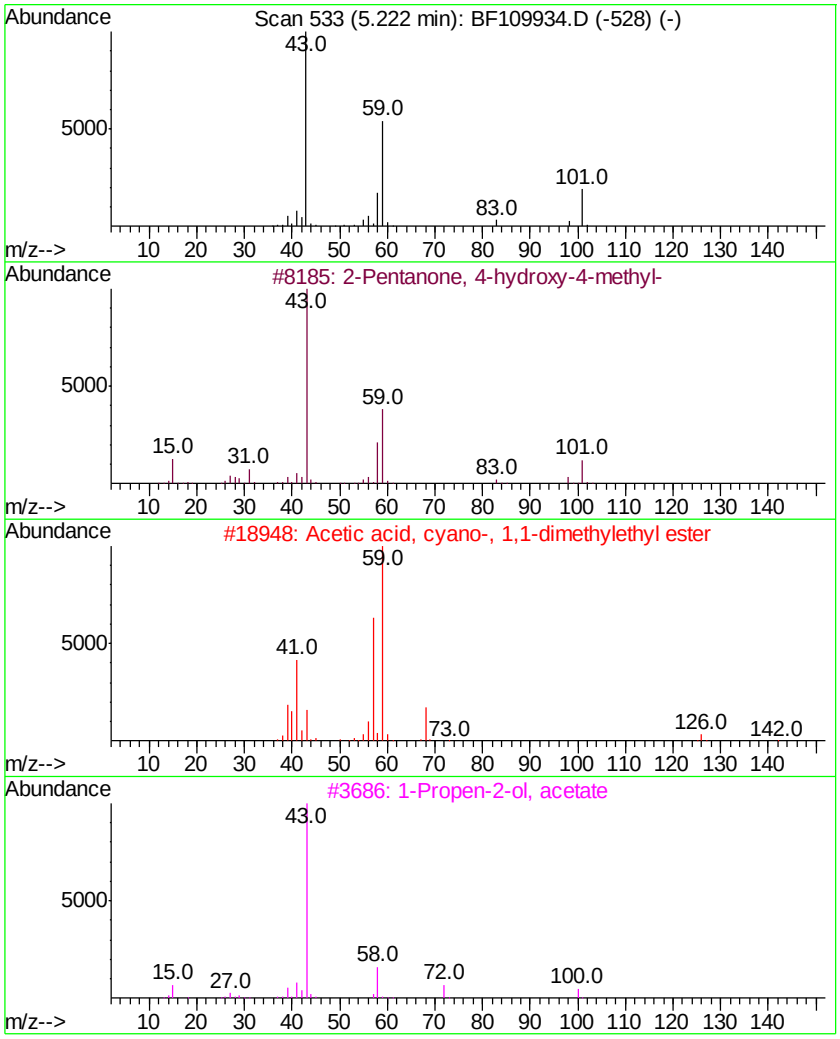
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

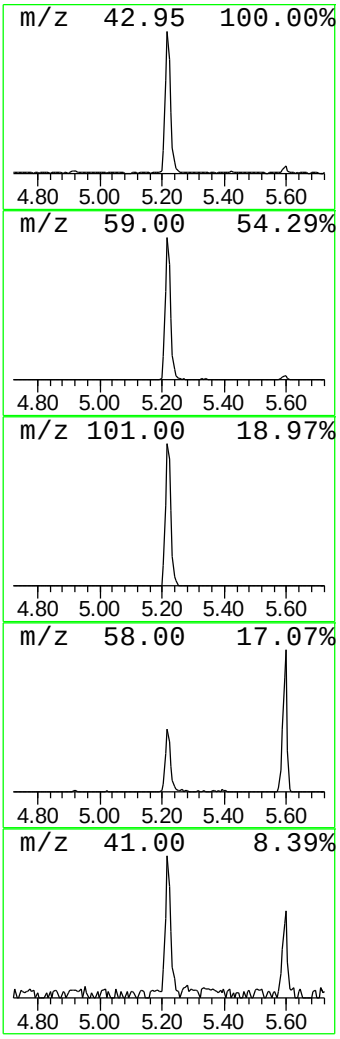
****

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.22	3.42 ng	236776	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101718\
Data File : BF109934.D
Acq On : 17 Oct 2018 21:42
Operator : JU/SJ
Sample : J5539-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DUP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101518.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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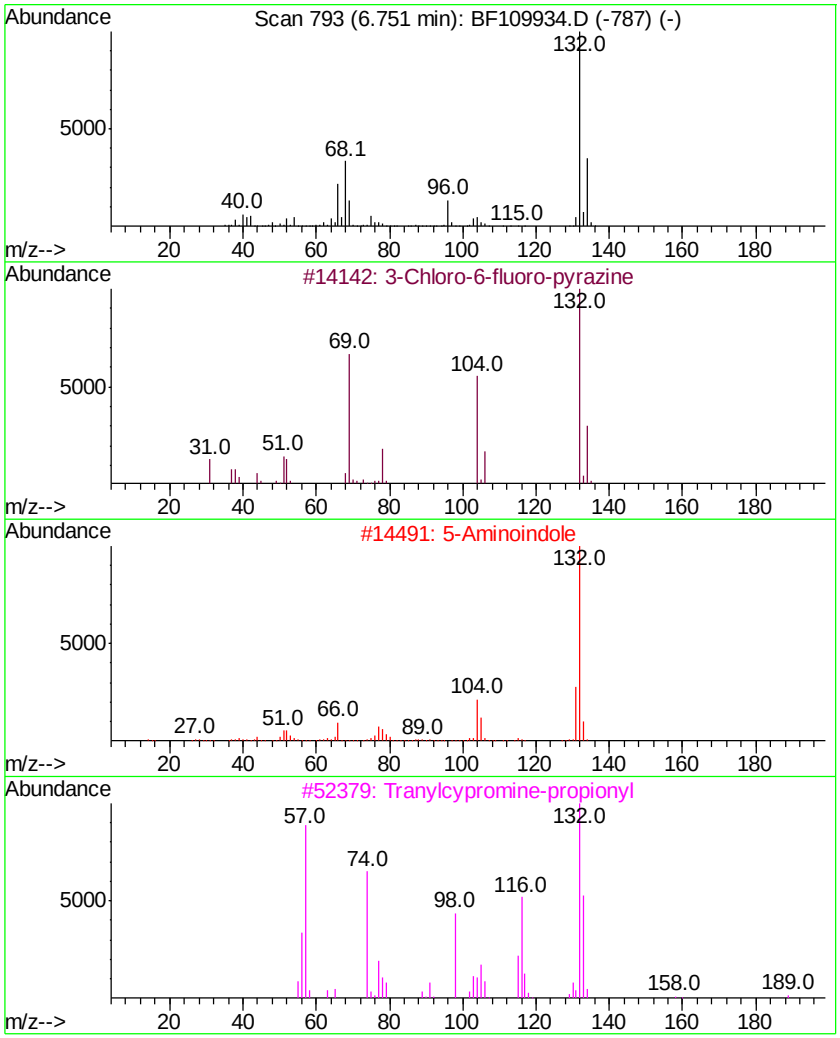
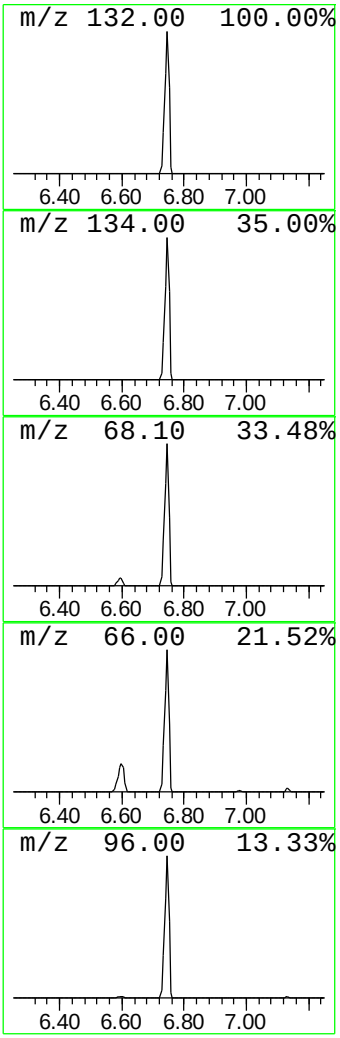
Peak Number 3 unknown6.75 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.75	74.26 ng	5139730	1,4-Dichlorobenzene-d4	6.97

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	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9





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Acq On : 17 Oct 2018 21:42
Operator : JU/SJ
Sample : J5539-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DUP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

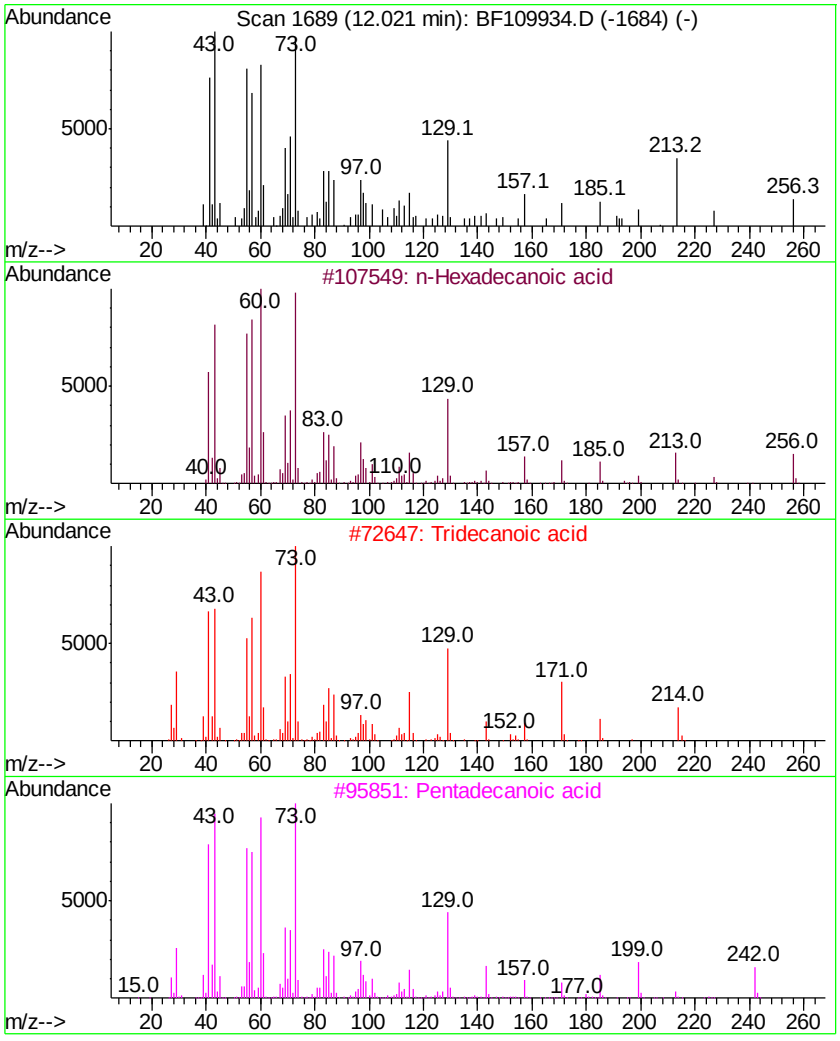
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

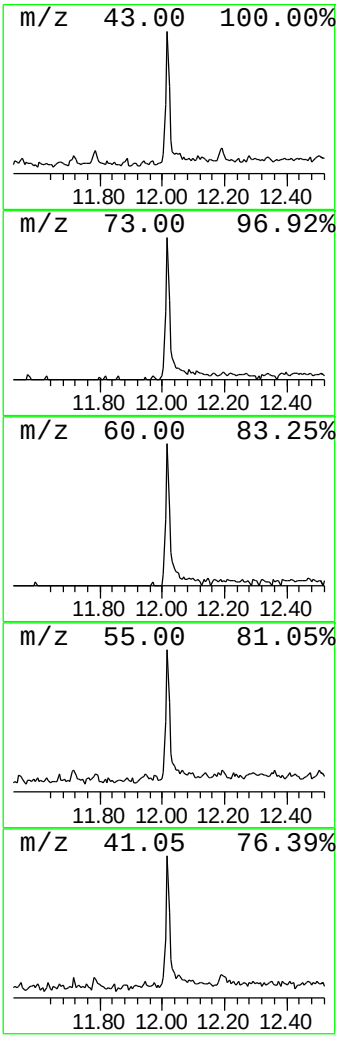
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.02	2.35 ng	158738	Phenanthrene-d10	11.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Tridecanoic acid	214	C13H26O2	000638-53-9	92
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	68
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	n-Decanoic acid	172	C10H20O2	000334-48-5	25





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Misc :
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Instrument : BNA_F
ClientSampleId : DUP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

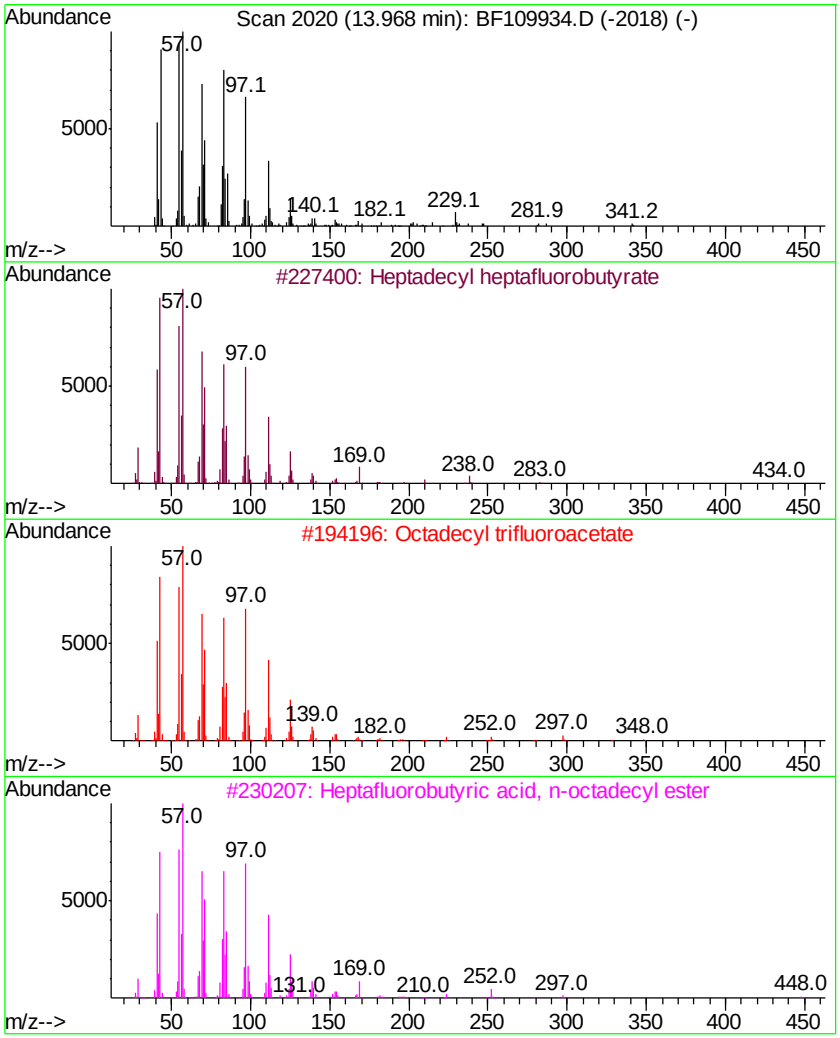
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

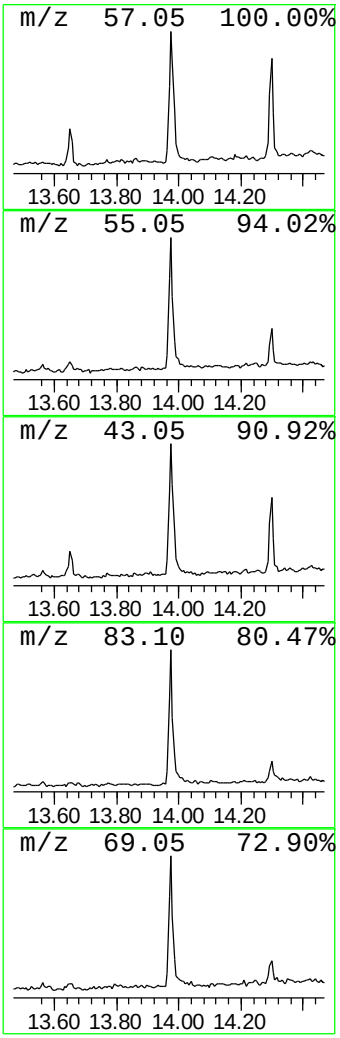
****

Peak Number 7 Heptadecyl heptafluorobutyrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.97	7.02 ng	540726	Chrysene-d12	14.15

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	91
3	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91
4	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	91
5	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91





Library Search Compound Report

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Misc :
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Instrument : BNA_F
ClientSampleId : DUP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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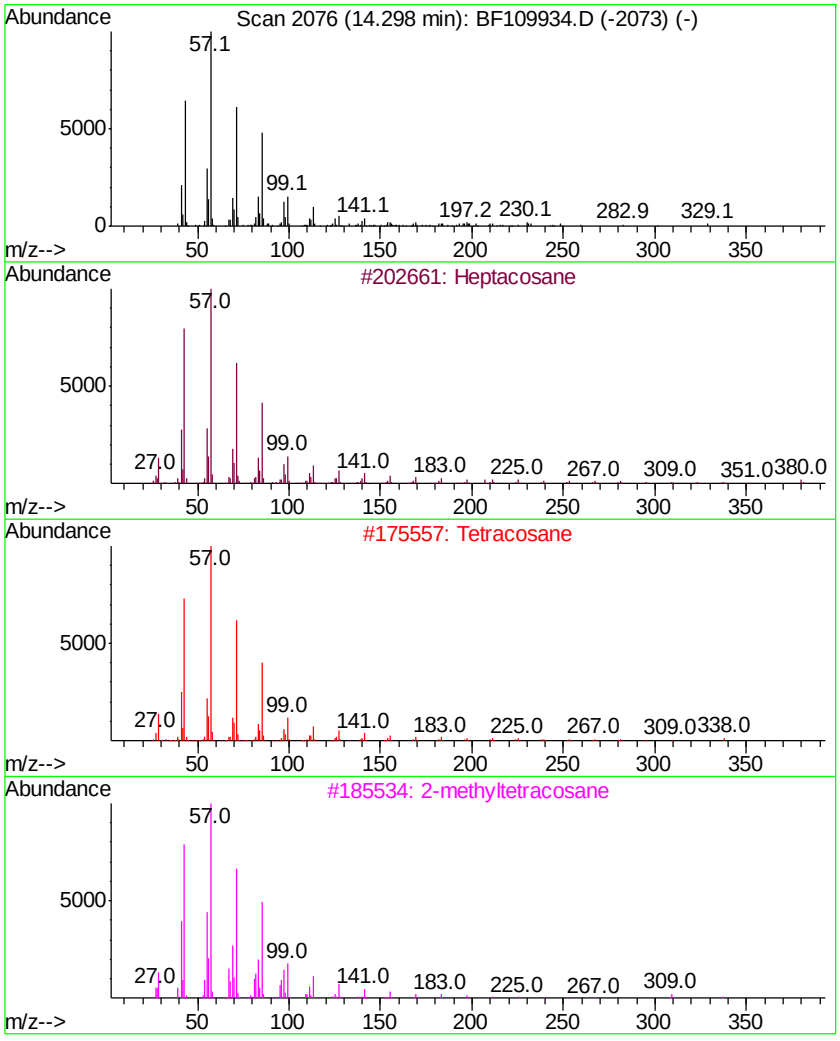
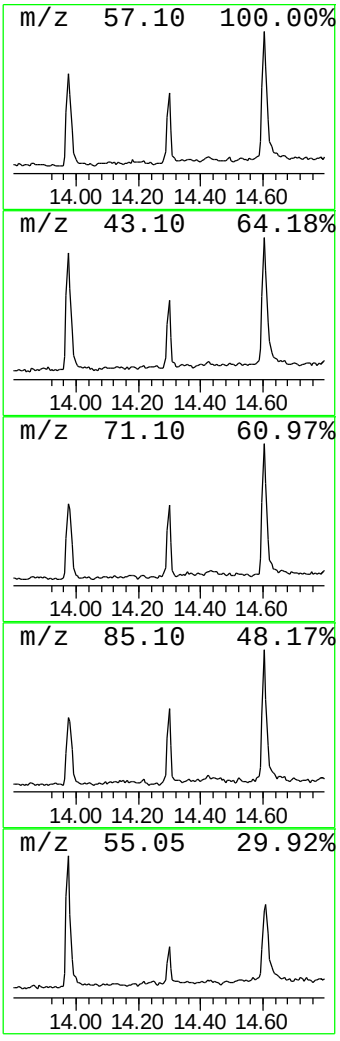
Peak Number 8 Heptacosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.30	2.41 ng	185990	Chrysene-d12	14.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	90
2	Tetracosane	338	C24H50	000646-31-1	87
3	2-methyltetracosane	352	C25H52	1000376-72-6	87
4	2-methyloctacosane	408	C29H60	1000376-72-8	87
5	Heneicosane	296	C21H44	000629-94-7	87





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Operator : JU/SJ
Sample : J5539-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DUP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101518.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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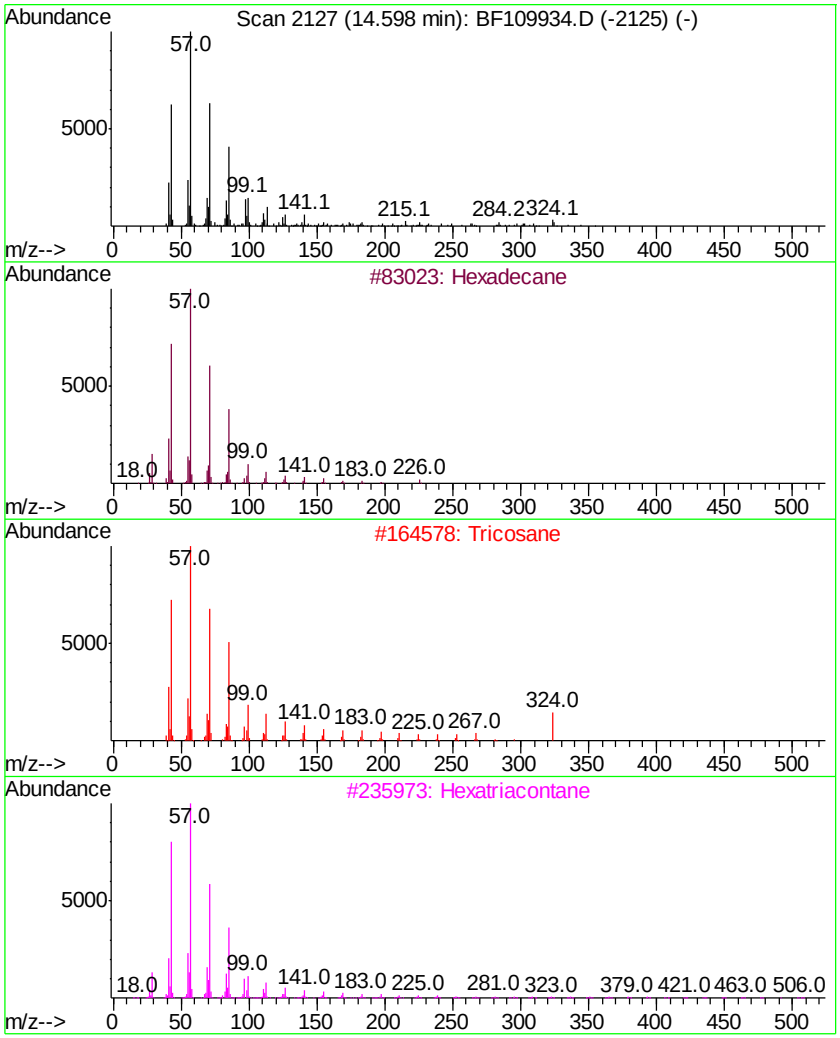
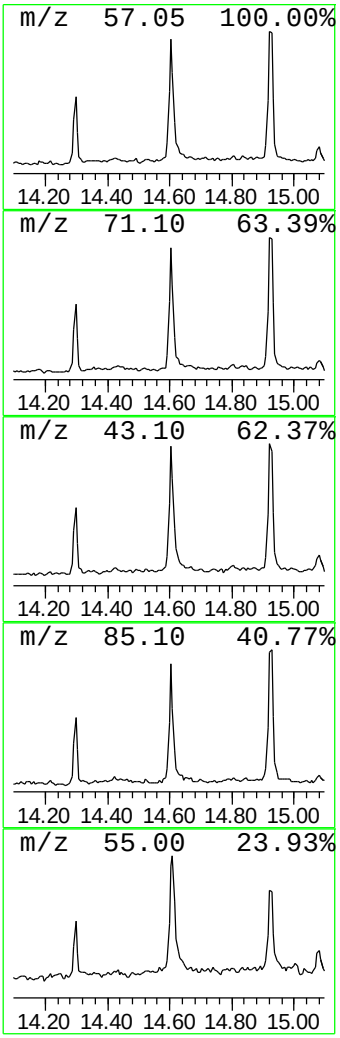
Peak Number 9 Hexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.60	6.72 ng	517545	Chrysene-d12	14.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	92
2	Tricosane	324	C23H48	000638-67-5	91
3	Hexatriacontane	507	C36H74	000630-06-8	91
4	Tetratetracontane	619	C44H90	007098-22-8	91
5	Pentadecane	212	C15H32	000629-62-9	90





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Instrument : BNA_F
ClientSampleId : DUP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101518.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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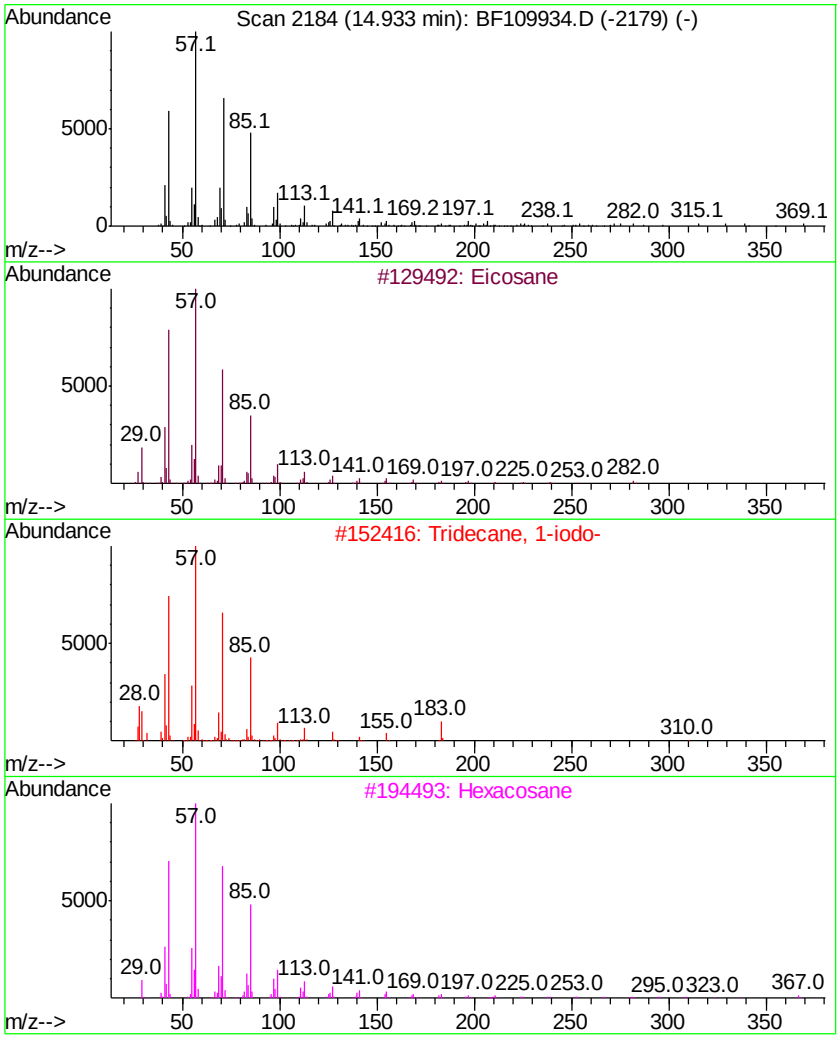
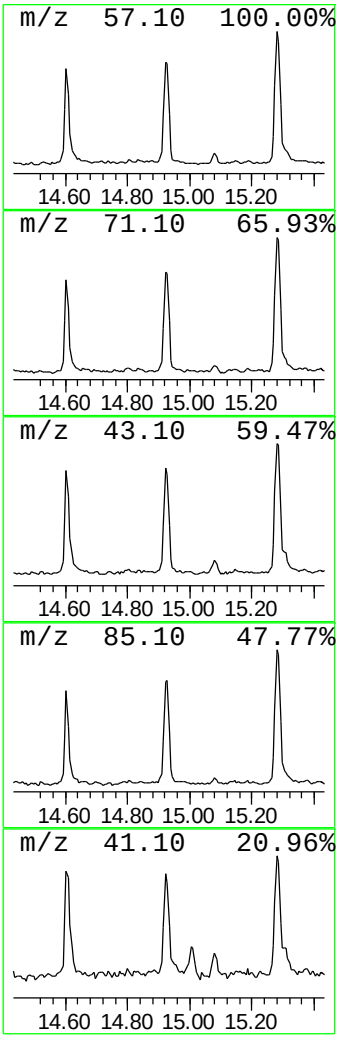
Peak Number 10 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.93	4.57 ng	471086	Perylene-d12	15.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	94
2	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	93
3	Hexacosane	366	C26H54	000630-01-3	91
4	Nonadecane, 2-methyl-	282	C20H42	001560-86-7	90
5	Tetratetracontane	619	C44H90	007098-22-8	87





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Data File : BF109934.D
Acq On : 17 Oct 2018 21:42
Operator : JU/SJ
Sample : J5539-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DUP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101518.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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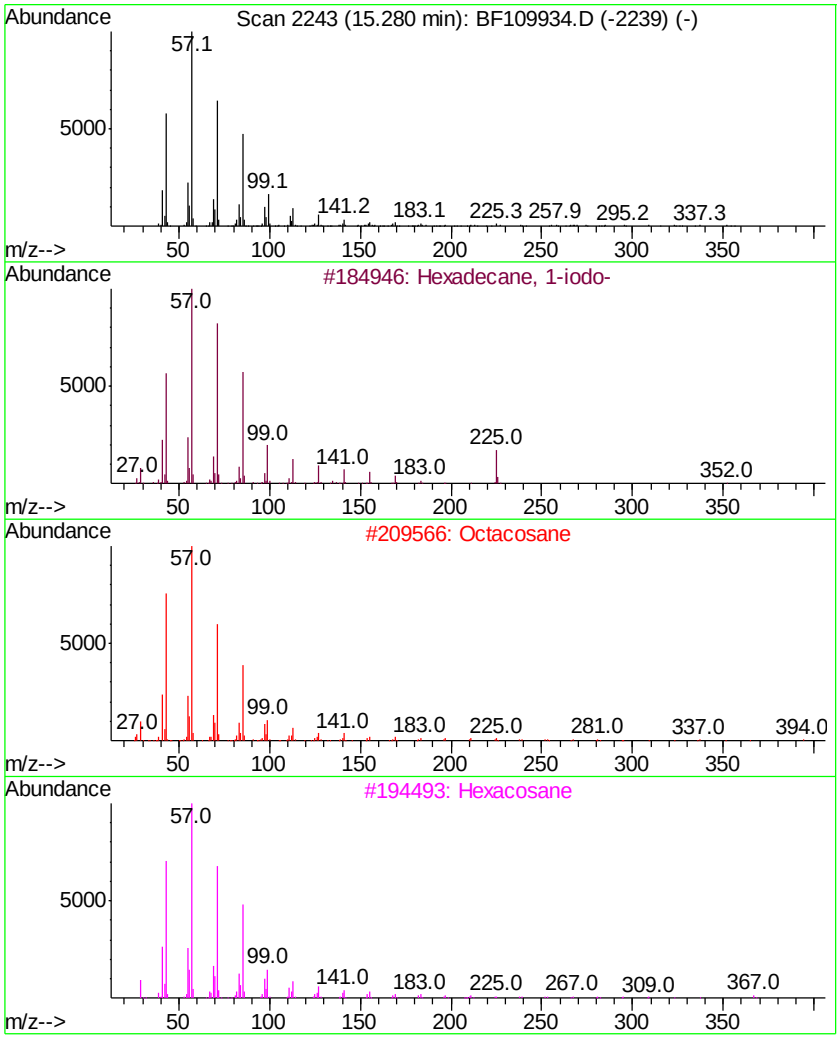
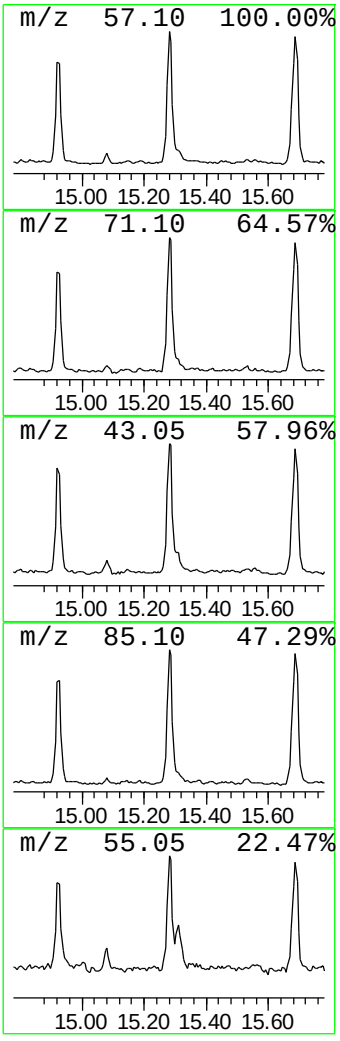
Peak Number 11 Hexadecane, 1-iodo- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.28	5.35 ng	551425	Perylene-d12	15.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	93
2	Octacosane	394	C28H58	000630-02-4	91
3	Hexacosane	366	C26H54	000630-01-3	91
4	Tetracosane	338	C24H50	000646-31-1	91
5	Heptacosane	380	C27H56	000593-49-7	91





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Acq On : 17 Oct 2018 21:42
Operator : JU/SJ
Sample : J5539-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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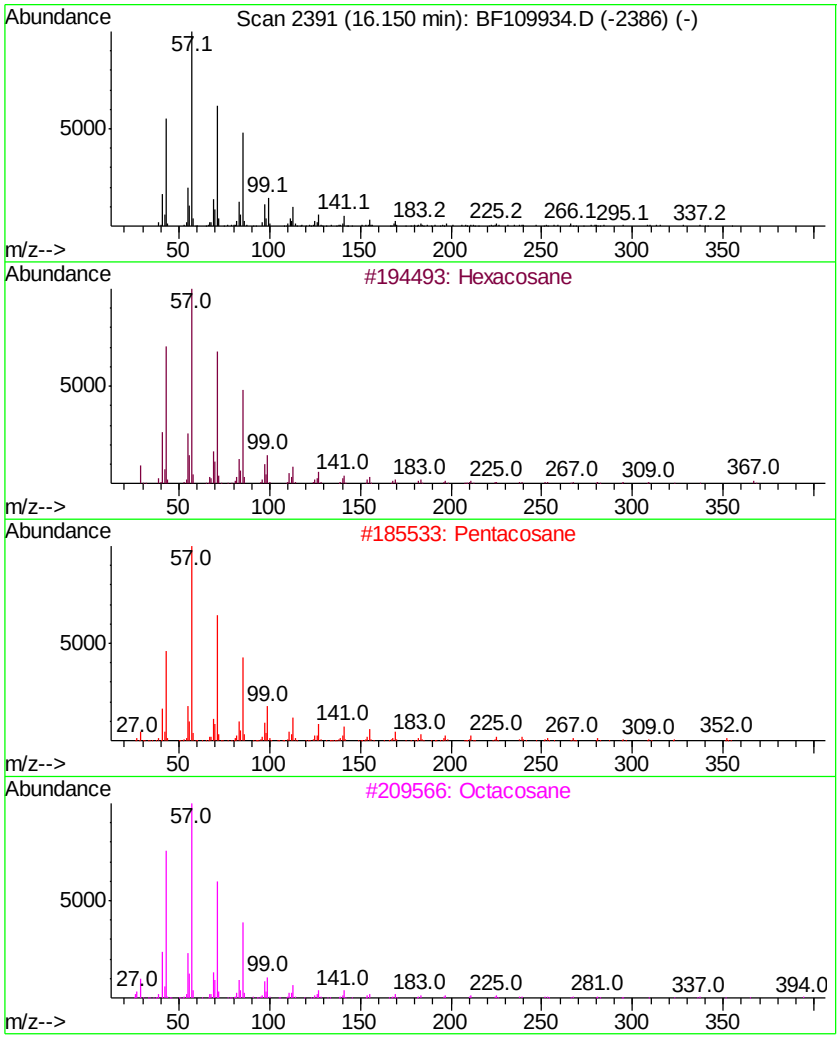
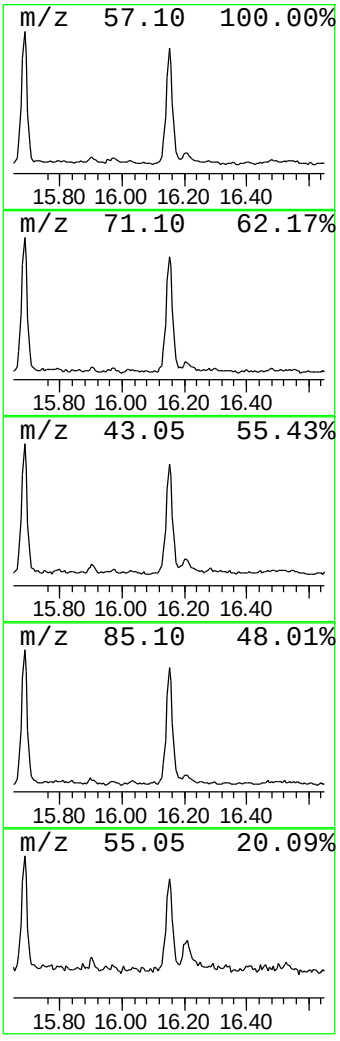
Peak Number 12 Hexacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.15	5.63 ng	580550	Perylene-d12	15.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	Pentacosane	352	C25H52	000629-99-2	91
3	Octacosane	394	C28H58	000630-02-4	91
4	Octadecane	254	C18H38	000593-45-3	91
5	Heneicosane	296	C21H44	000629-94-7	90





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Acq On : 17 Oct 2018 21:42
Operator : JU/SJ
Sample : J5539-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DUP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101518.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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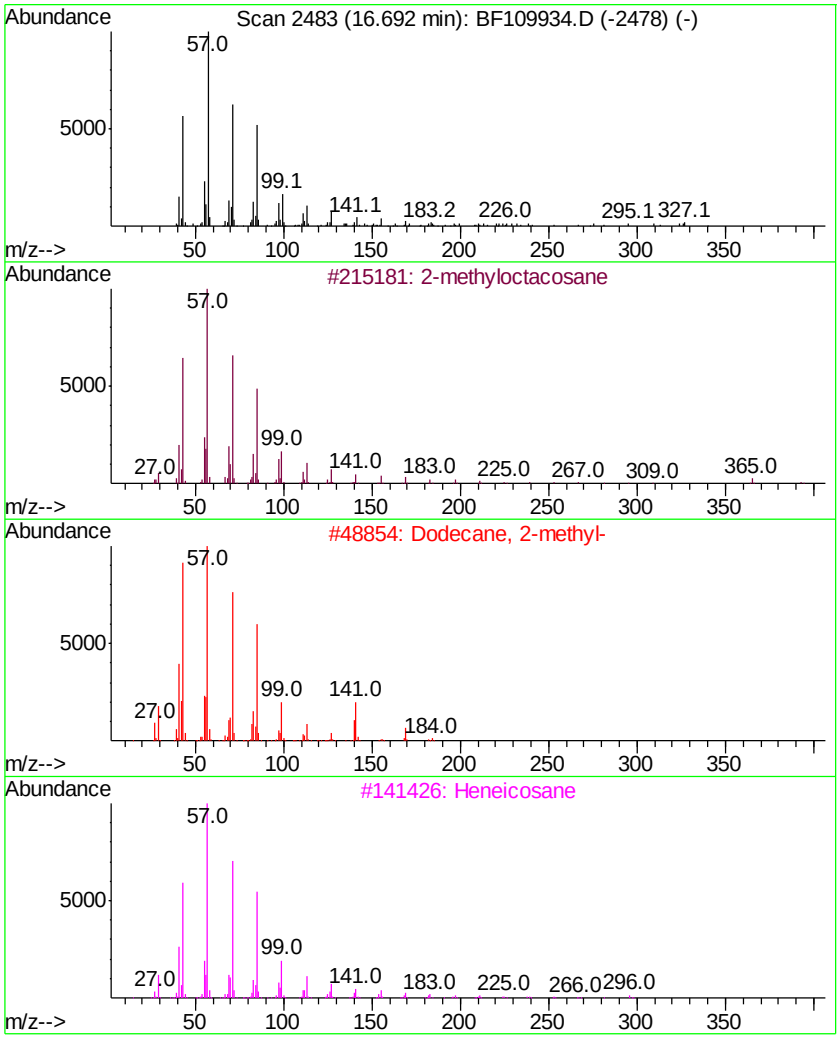
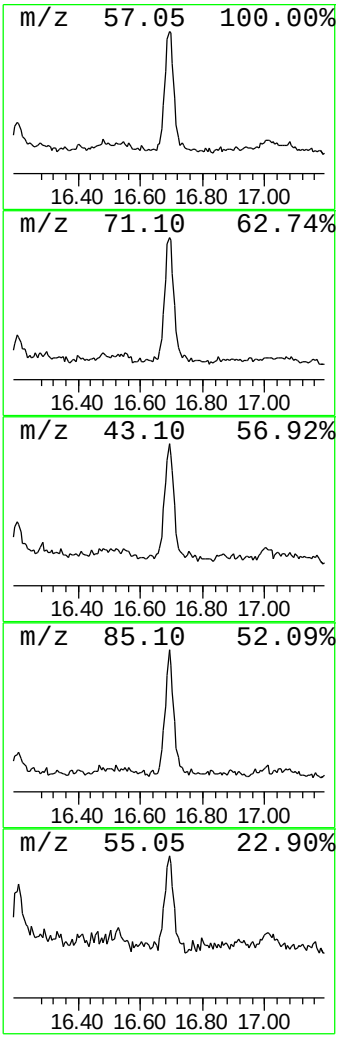
Peak Number 13 2-methyloctacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.69	3.29 ng	339324	Perylene-d12	15.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane	408	C29H60	1000376-72-8	90
2	Dodecane, 2-methyl-	184	C13H28	001560-97-0	90
3	Heneicosane	296	C21H44	000629-94-7	87
4	Octadecane	254	C18H38	000593-45-3	83
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	80





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF101718\
Data File : BF109934.D
Acq On : 17 Oct 2018 21:42
Operator : JU/SJ
Sample : J5539-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DUP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101518.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
Butane, 2-methoxy...	2.32	11.3	ng	781686	1	6.97	1384220	20.0
2-Pentanone, 4-hy...	5.22	3.4	ng	236776	1	6.97	1384220	20.0
unknown6.75	6.75	74.3	ng	5139730	1	6.97	1384220	20.0
n-Hexadecanoic acid	12.02	2.4	ng	158738	4	11.51	1351540	20.0
Heptadecyl heptaf...	13.97	7.0	ng	540726	5	14.15	1541160	20.0
Heptacosane	14.30	2.4	ng	185990	5	14.15	1541160	20.0
Hexadecane	14.60	6.7	ng	517545	5	14.15	1541160	20.0
Eicosane	14.93	4.6	ng	471086	6	15.68	2062550	20.0
Hexadecane, 1-iodo-	15.28	5.3	ng	551425	6	15.68	2062550	20.0
Hexacosane	16.15	5.6	ng	580550	6	15.68	2062550	20.0
2-methyloctacosane	16.69	3.3	ng	339324	6	15.68	2062550	20.0