LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF101717\
Data File : BF099588.D
Acq On : 17 Oct 2017 18:33
Operator : SJ/JU
Sample : I5794-10
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EPE-117-3(10-15)

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-BF092317.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	5.051	501	504	516	rBV	234499	311922	14.19%	1.585%
2	5.451	568	572	591	rBV	1902332	1842773	83.84%	9.366%
3	6.463	739	744	763	rVB	1894833	2015583	91.71%	10.244%
4	6.598	763	767	770	rBV	2154711	1928754	87.76%	9.803%
5	6.828	802	806	814	rVB	640083	601500	27.37%	3.057%
6	6.981	828	832	836	rBV	1783062	1515912	68.97%	7.705%
7	7.392	898	902	905	rBV	1285780	1134737	51.63%	5.767%
8	8.104	1020	1023	1027	rBV	949418	834275	37.96%	4.240%
9	8.563	1098	1101	1107	rBV	30995	26509	1.21%	0.135%
10	8.663	1114	1118	1125	rBB	158530	130593	5.94%	0.664%
11	9.180	1201	1206	1209	rBV	2549844	2197853	100.00%	11.171%
12	9.575	1269	1273	1276	rBV	543898	400325	18.21%	2.035%
13	9.863	1318	1322	1325	rBV	1031220	900922	40.99%	4.579%
14	10.574	1439	1443	1446	rBV	817858	673296	30.63%	3.422%
15	10.651	1452	1456	1464	rVB	960522	797177	36.27%	4.052%
16	11.345	1571	1574	1578	rBV	916670	814216	37.05%	4.138%
17	11.727	1635	1639	1642	rBV	108133	80853	3.68%	0.411%
18	12.410	1752	1755	1757	rBV	191997	166825	7.59%	0.848%
19	12.433	1757	1759	1761	rVB	349528	270225	12.29%	1.373%
20	12.516	1770	1773	1777	rVB	66085	52010	2.37%	0.264%
21	12.927	1839	1843	1846	rBV	1729266	1494227	67.99%	7.595%
22	13.810	1989	1993	1997	rBV2	58247	69556	3.16%	0.354%
23	13.986	2020	2023	2027	rBV	601514	528071	24.03%	2.684%
24	15.062	2202	2206	2212	rBV	253774	262750	11.95%	1.335%
25	15.451	2266	2272	2280	rBV	462184	569097	25.89%	2.893%
26	15.856	2337	2341	2348	rBV	37758	54949	2.50%	0.279%

Sum of corrected areas: 19674910

LSC Report - Integrated Chromatogram

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Data File : BF099588.D
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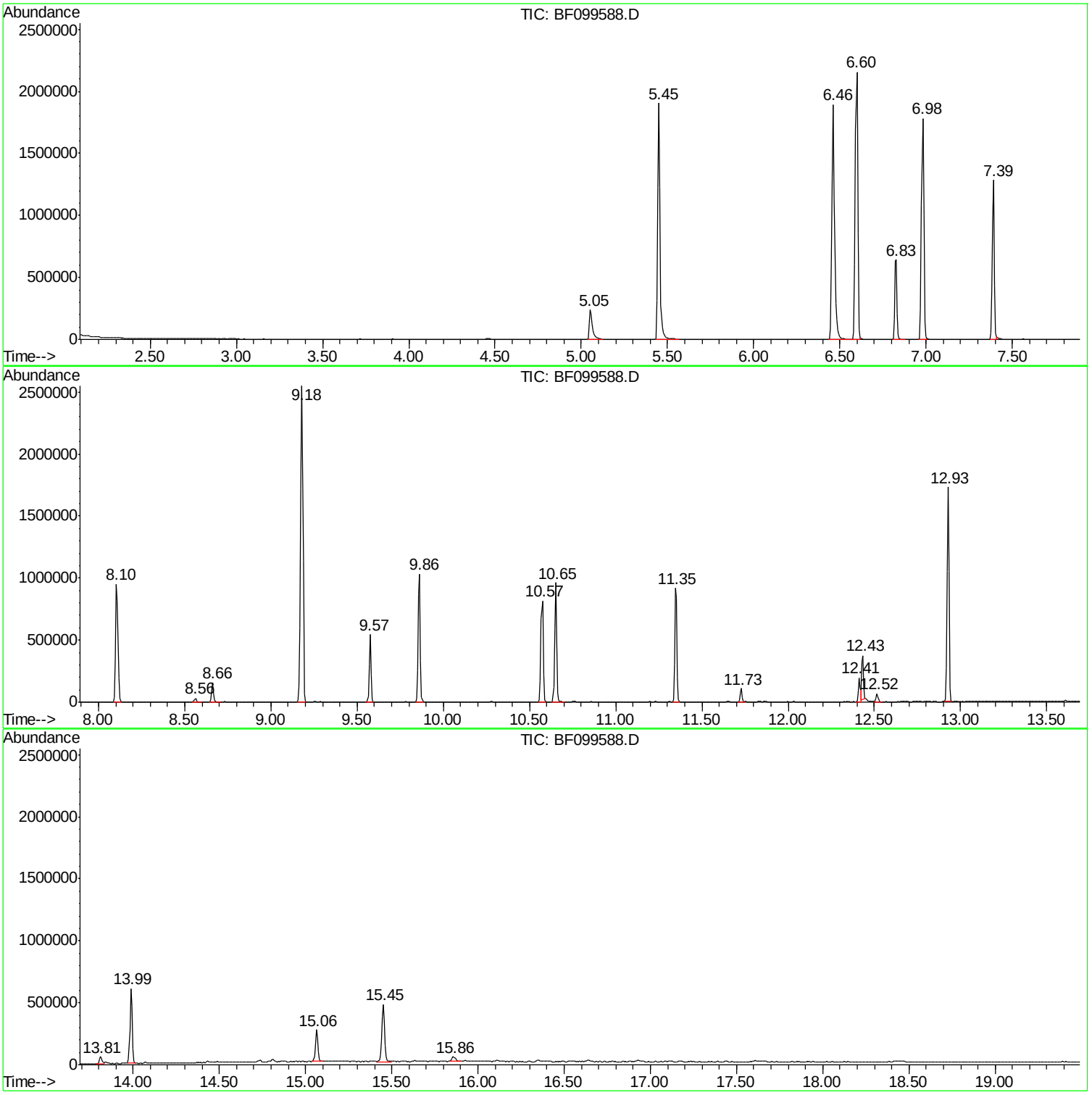
Operator : SJ/JU
Sample : I5794-10
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EPE-117-3(10-15)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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\BF101717\
Data File : BF099588.D
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
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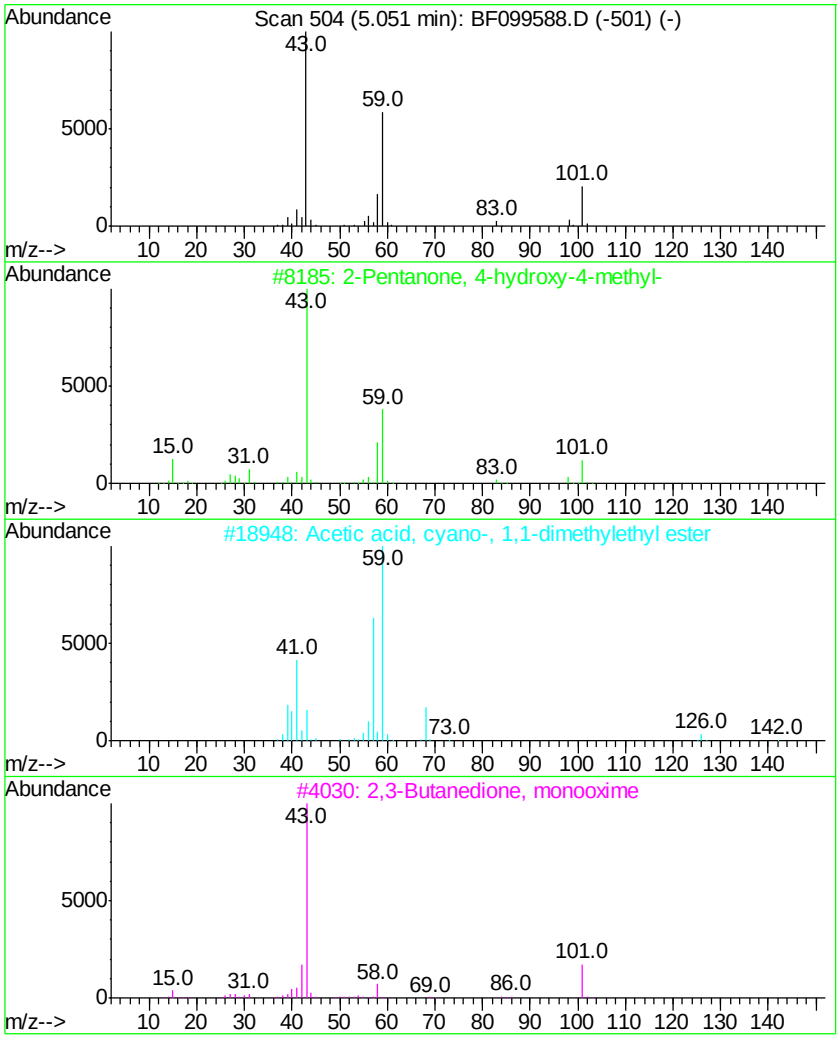
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

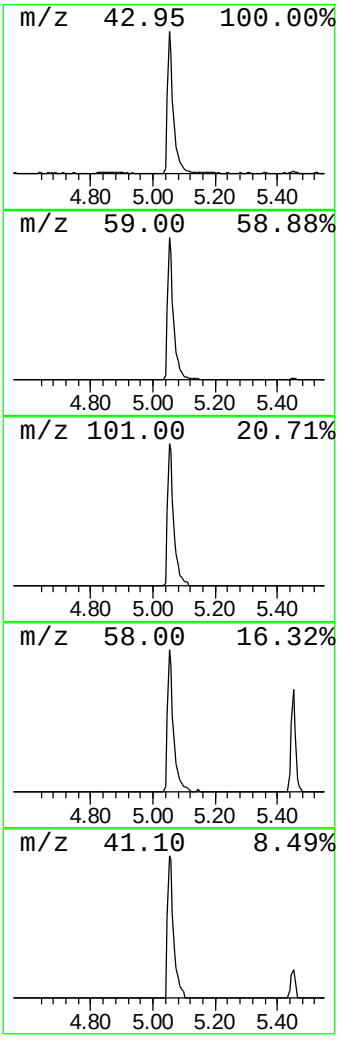
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.05	10.37 ng	311922	1,4-Dichlorobenzene-d4	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF101717\
Data File : BF099588.D
Acq On : 17 Oct 2017 18:33
Operator : SJ/JU
Sample : I5794-10
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EPE-117-3(10-15)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

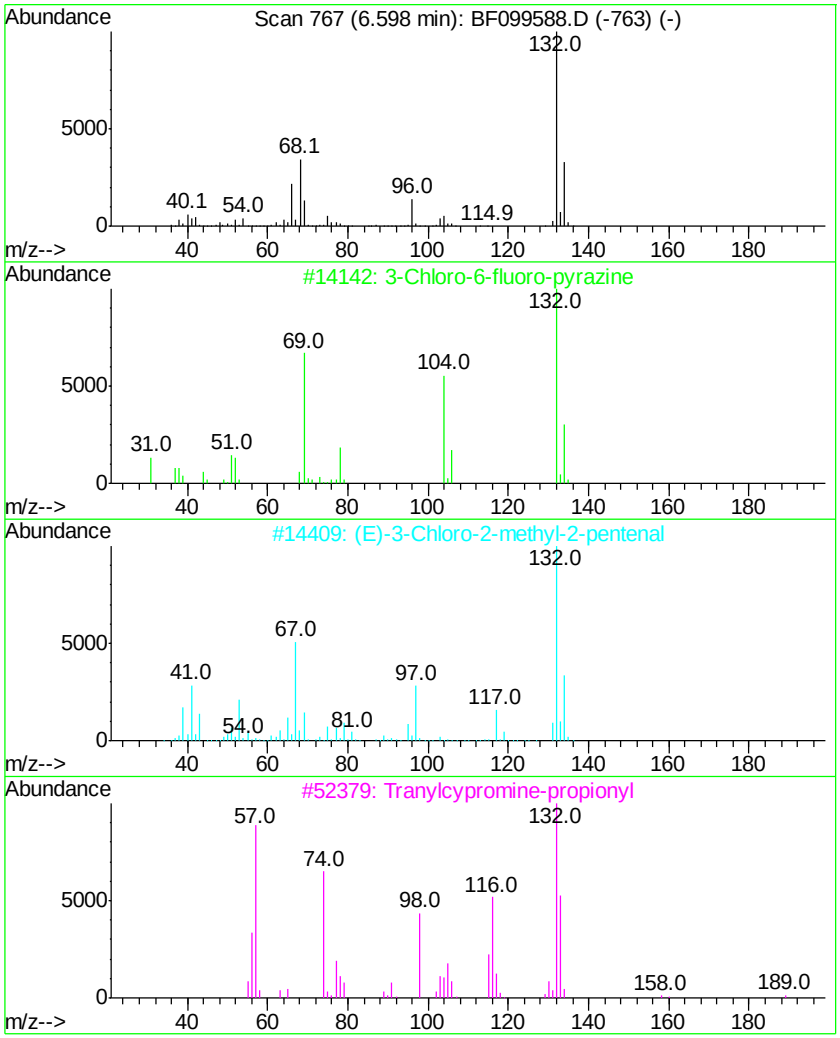
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

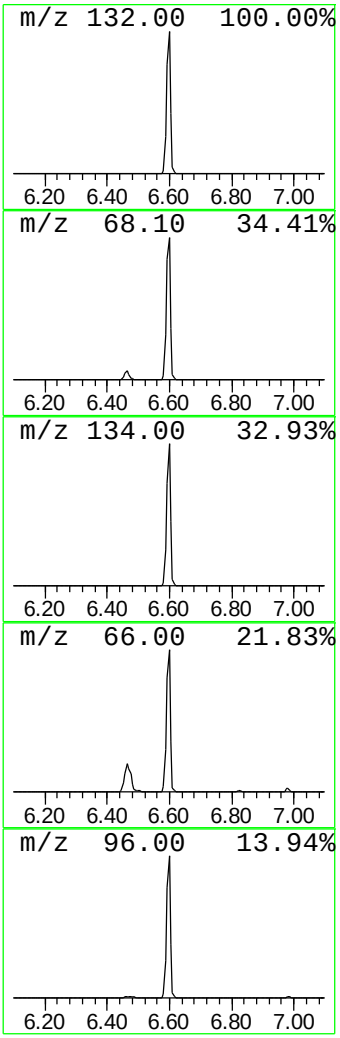
****

Peak Number 2 unknown6.60 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.60	64.13 ng	1928750	1,4-Dichlorobenzene-d4	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF101717\
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Acq On : 17 Oct 2017 18:33
Operator : SJ/JU
Sample : I5794-10
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EPE-117-3(10-15)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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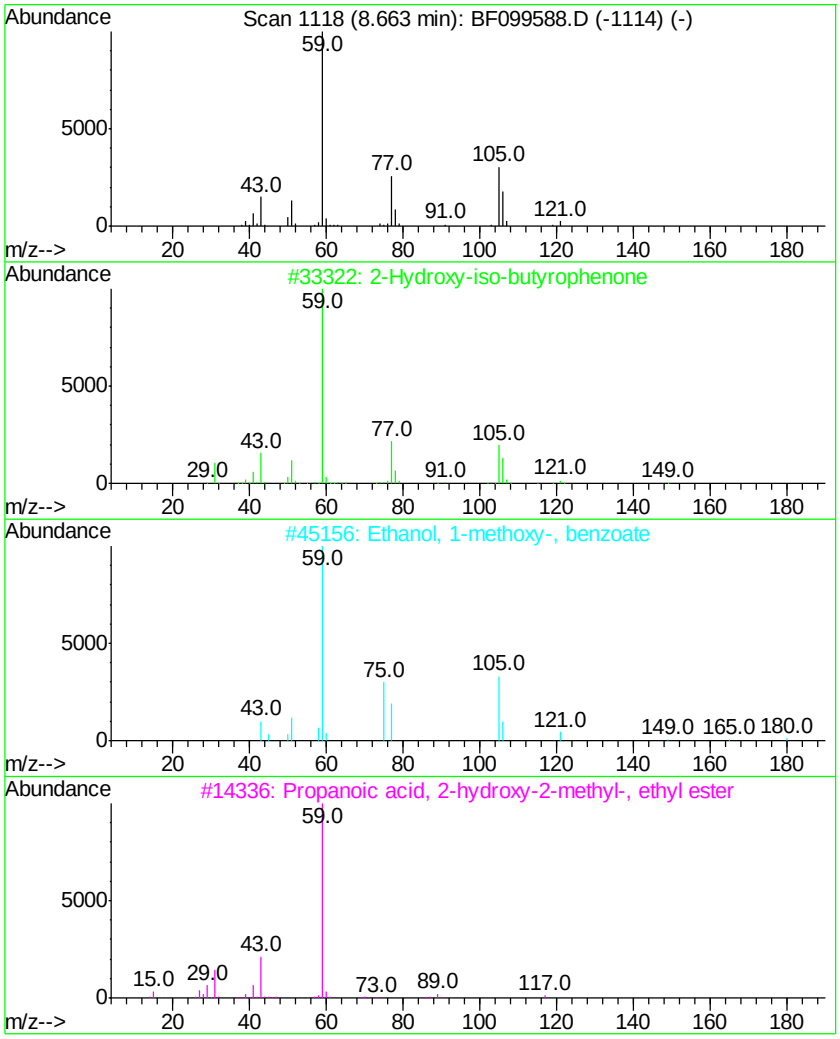
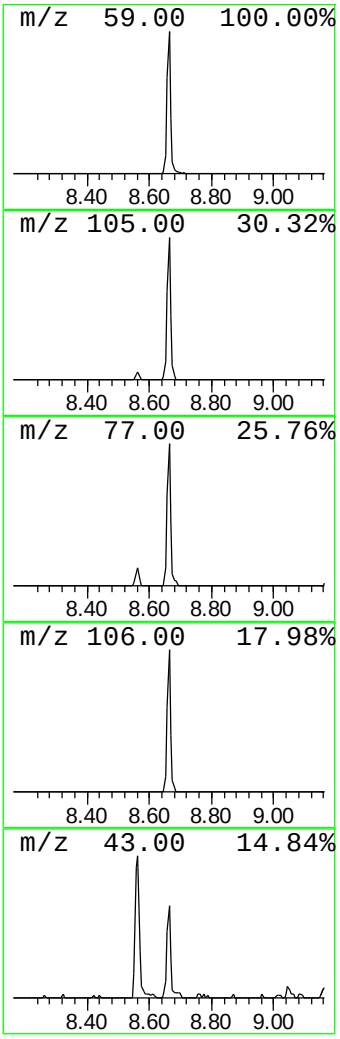
Peak Number 4 2-Hydroxy-iso-butyrophenone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.66	3.13 ng	130593	Naphthalene-d8	8.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hydroxy-iso-butyrophenone	164	C10H12O2	007473-98-5	90
2	Ethanol, 1-methoxy-, benzoate	180	C10H12O3	051835-44-0	50
3	Propanoic acid, 2-hydroxy-2-meth...	132	C6H12O3	000080-55-7	9
4	Propionic acid, 2-isopropoxy-, m...	146	C7H14O3	1000151-15-1	9
5	.alpha.-(Methylthio)acetamide	105	C3H7NOS	022551-24-2	7





Data Path : Z:\HPCHEM1\BNA F\DATA\BF101717\
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Operator : SJ/JU
Sample : I5794-10
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EPE-117-3(10-15)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

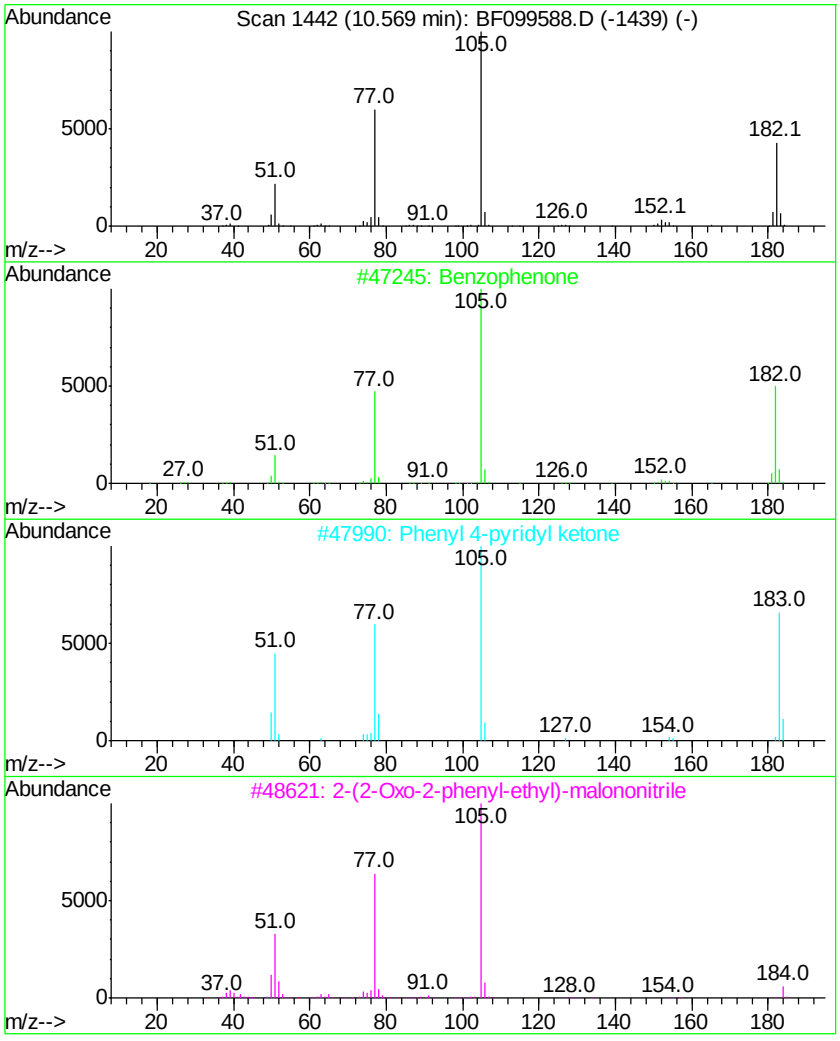
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

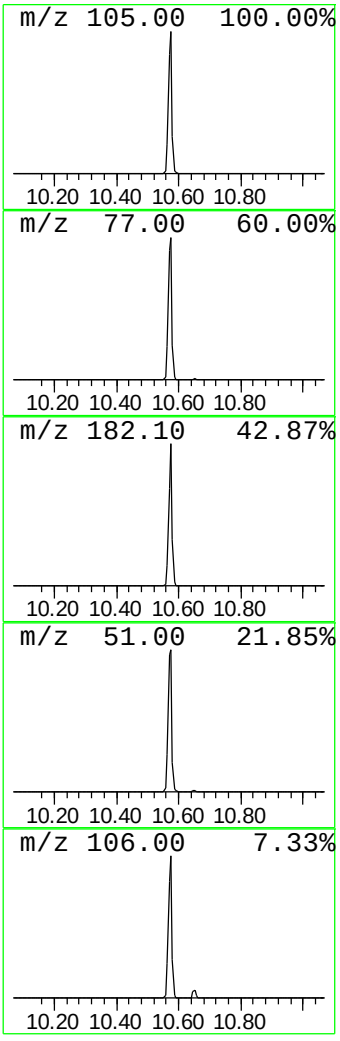
****

Peak Number 5 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.57	14.95 ng	673296	Acenaphthene-d10	9.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	97
2	Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	49
3	2-(2-Oxo-2-phenyl-ethyl)-malonon...	184	C11H8N2O	1000296-76-9	47
4	2-Benzoyloxyacetophenone	240	C15H12O3	004010-33-7	43
5	Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	43





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Misc :
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Instrument : BNA_F
ClientSampleId : EPE-117-3(10-15)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

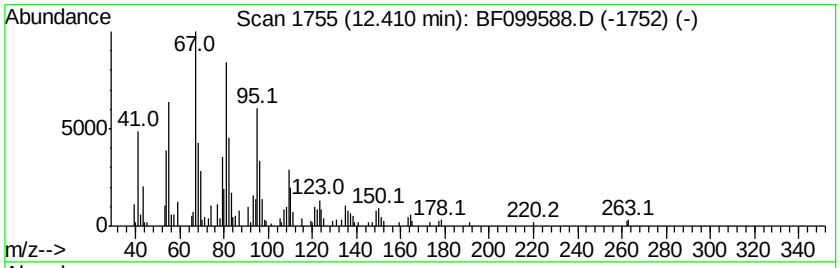
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

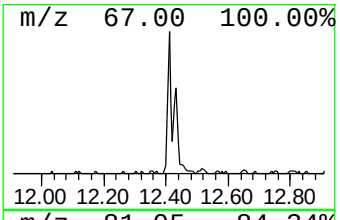
****

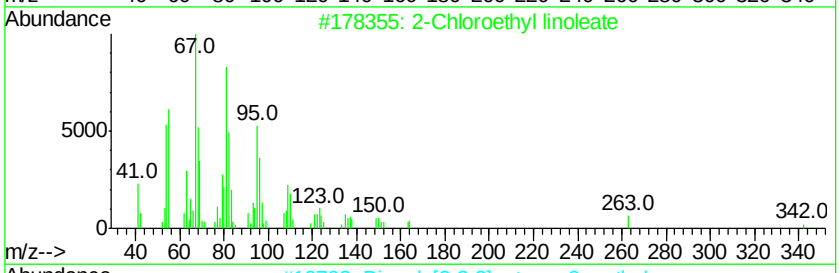
Peak Number 6 2-Chloroethyl linoleate Concentration Rank 7

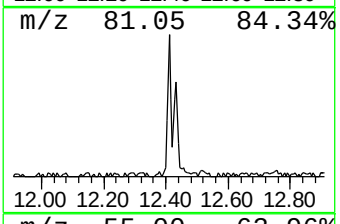
R.T.	EstConc	Area	Relative to ISTD	R.T.
12.41	4.10 ng	166825	Phenanthrene-d10	11.35

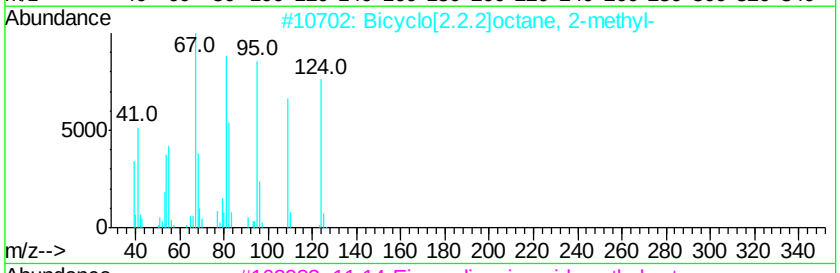
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Chloroethyl linoleate	342	C20H35ClO2	025525-76-2	91
2	Bicyclo[2.2.2]octane, 2-methyl-	124	C9H16	000766-53-0	87
3	11,14-Eicosadienoic acid, methyl...	322	C21H38O2	002463-02-7	81
4	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	76
5	7-Hexadecyne	222	C16H30	074685-28-2	74

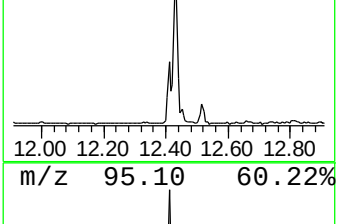


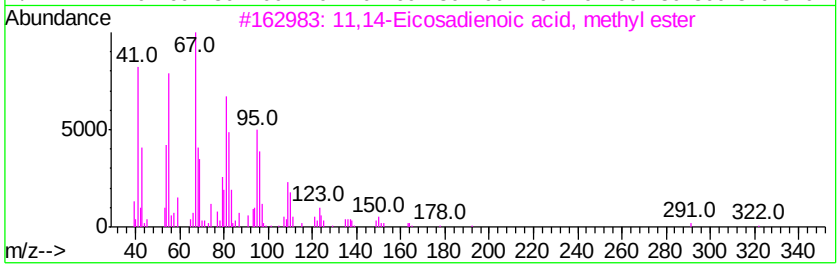


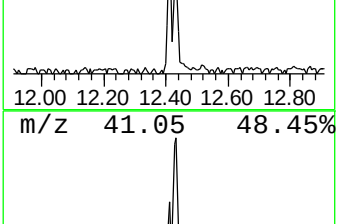


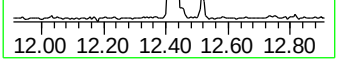












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Instrument : BNA_F
ClientSampleId : EPE-117-3(10-15)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

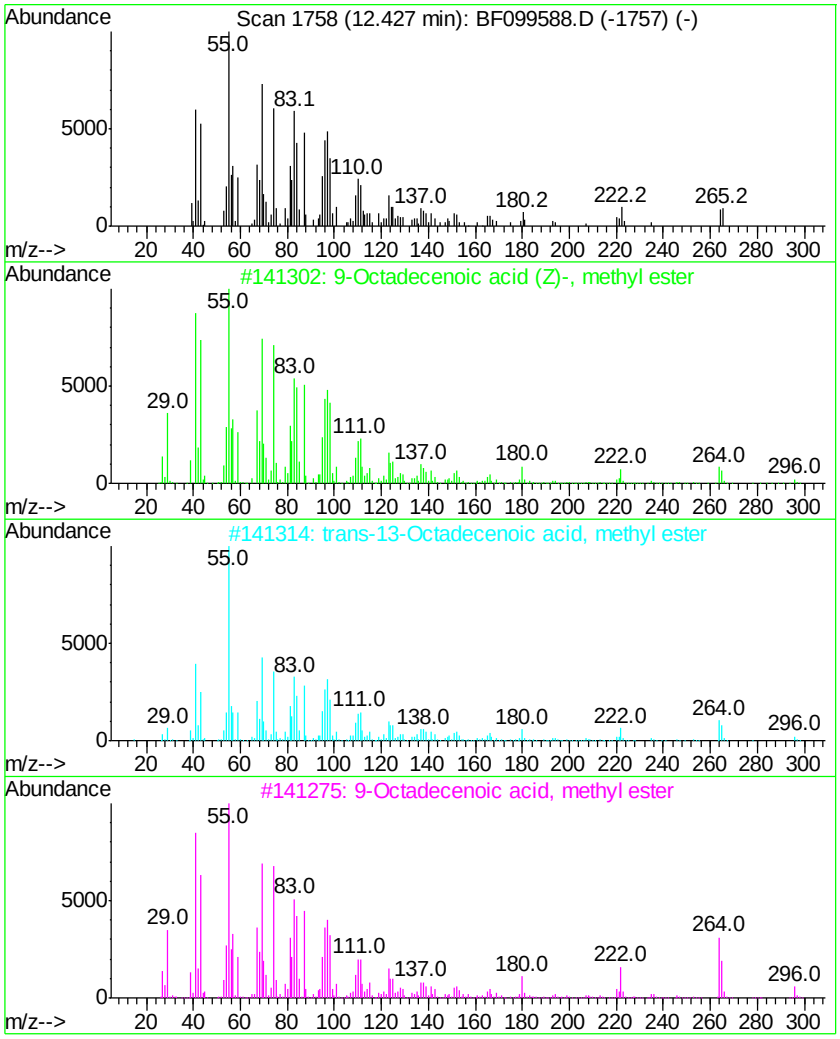
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

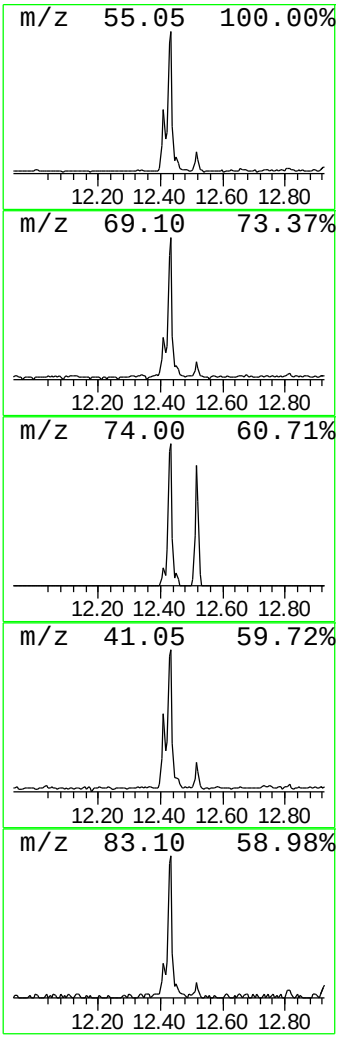
****

Peak Number 7 9-Octadecenoic acid (Z)-, m... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.43	6.64 ng	270225	Phenanthrene-d10	11.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	99
2	trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	99
3	9-Octadecenoic acid, methyl ester	296	C19H36O2	002462-84-2	99
4	8-Octadecenoic acid, methyl ester	296	C19H36O2	002345-29-1	99
5	9-Octadecenoic acid, methyl este...	296	C19H36O2	001937-62-8	99





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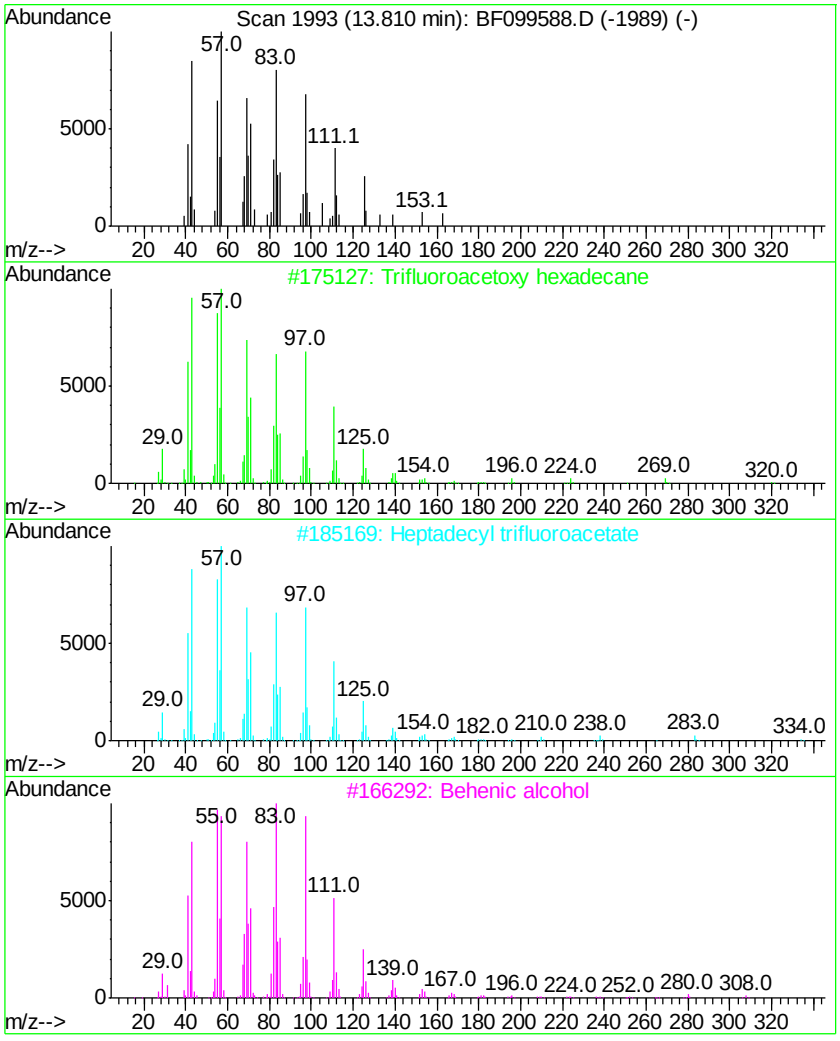
TIC Integration Parameters: LSCINT.P

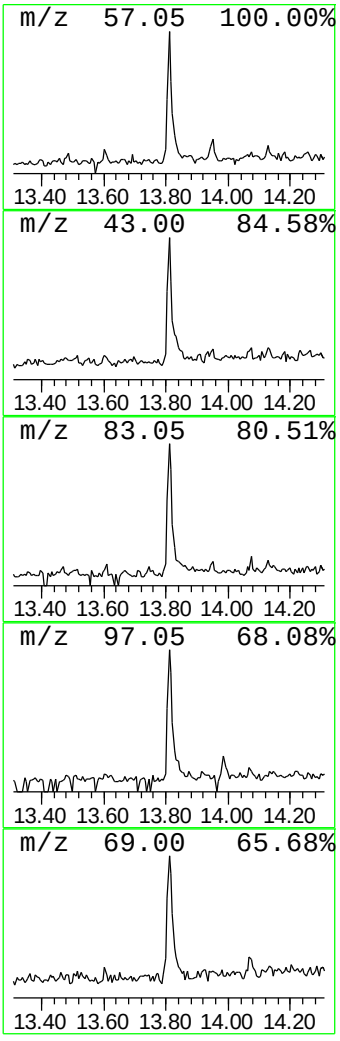
****

Peak Number 8 Trifluoroacetoxy hexadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.81	2.63 ng	69556	Chrysene-d12	13.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
2	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	91
3	Behenic alcohol	326	C22H46O	000661-19-8	90
4	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	87
5	Tricosyl pentafluoropropionate	486	C26H47F5O2	1000351-81-0	86





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TIC Library : C:\DATABASE\NIST11.L
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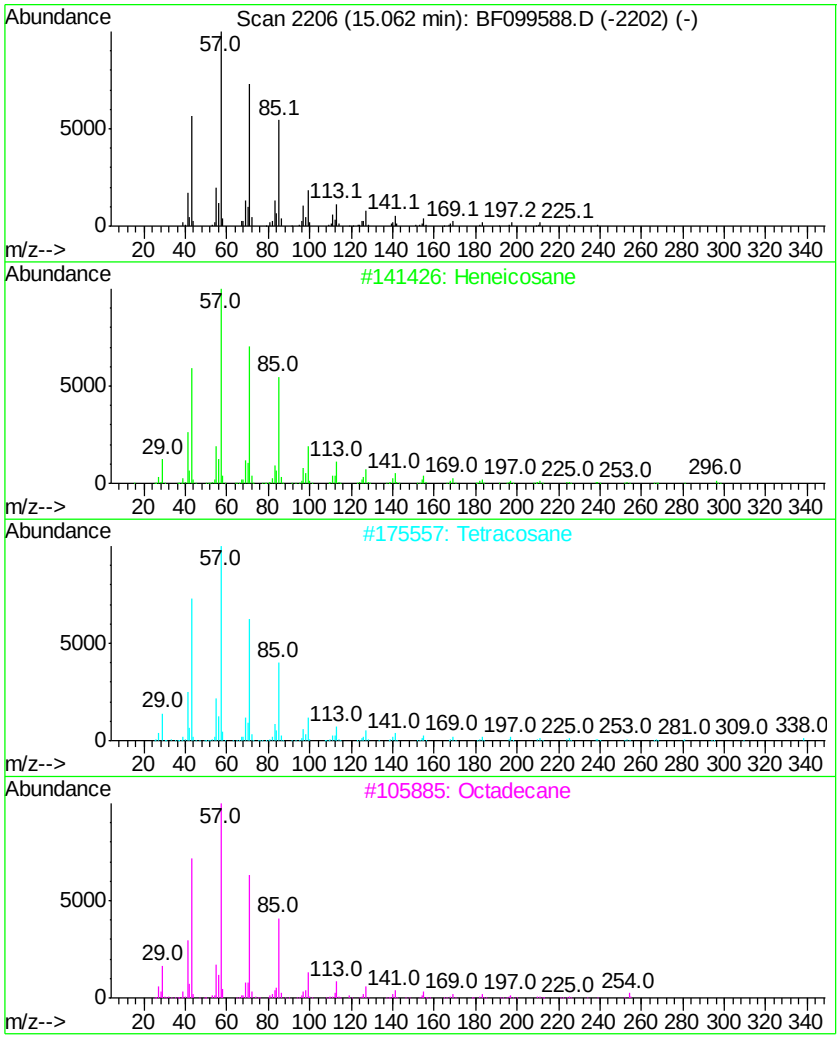
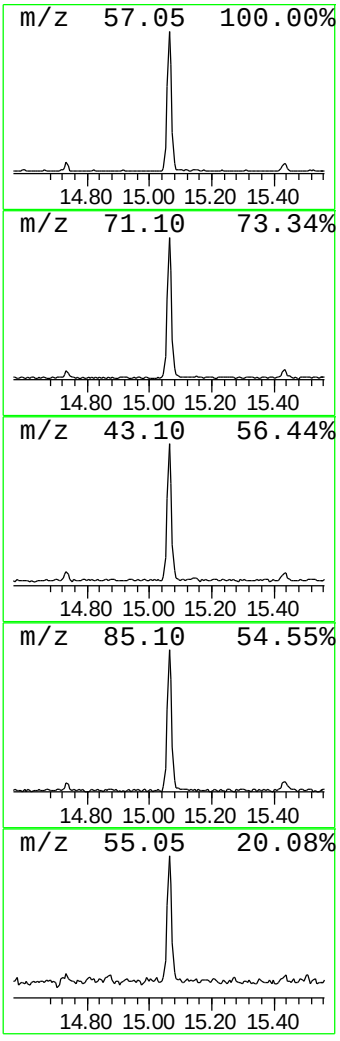
****

Peak Number 9 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.06	9.23 ng	262750	Perylene-d12	15.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Tetracosane	338	C24H50	000646-31-1	91
3	Octadecane	254	C18H38	000593-45-3	90
4	2-Bromotetradecane	276	C14H29Br	074036-95-6	90
5	Hexacosane	366	C26H54	000630-01-3	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101717\
Data File : BF099588.D
Acq On : 17 Oct 2017 18:33
Operator : SJ/JU
Sample : I5794-10
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EPE-117-3(10-15)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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...	5.05	10.4	ng	311922	1	6.83	601500	20.0
unknown6.60	6.60	64.1	ng	1928750	1	6.83	601500	20.0
2-Hydroxy-iso-but...	8.66	3.1	ng	130593	2	8.10	834275	20.0
Benzophenone	10.57	14.9	ng	673296	3	9.86	900922	20.0
2-Chloroethyl lin...	12.41	4.1	ng	166825	4	11.35	814216	20.0
9-Octadecenoic ac...	12.43	6.6	ng	270225	4	11.35	814216	20.0
Trifluoroacetoxy ...	13.81	2.6	ng	69556	5	13.99	528071	20.0
Heneicosane	15.06	9.2	ng	262750	6	15.45	569097	20.0