LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\Data\BF100717\
Data File : BF099209.D
Acq On : 7 Oct 2017 22:14
Operator : SJ/JU
Sample : I5516-01
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-5

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	2.157	7	12	18	rVB	346758	446030	11.33%	2.773%
2	2.987	148	153	160	rBV	38937	59857	1.52%	0.372%
3	3.610	254	259	267	rBV	67572	103494	2.63%	0.644%
4	4.487	401	408	412	rBV	2596103	3936965	100.00%	24.481%
5	5.087	506	510	518	rBV	376682	381560	9.69%	2.373%
6	5.492	575	579	587	rBV	582541	536615	13.63%	3.337%
7	6.492	747	749	760	rVB2	373054	528991	13.44%	3.289%
8	6.634	770	773	777	rBV	1110031	928782	23.59%	5.775%
9	6.863	809	812	816	rBV	696231	614225	15.60%	3.819%
10	7.022	835	839	842	rBV	1304368	1050572	26.68%	6.533%
11	7.428	904	908	911	rBV	901230	733955	18.64%	4.564%
12	8.145	1027	1030	1034	rBV	878674	779585	19.80%	4.848%
13	9.222	1208	1213	1216	rBV	1705062	1399543	35.55%	8.703%
14	9.610	1276	1279	1283	rBV	283367	248024	6.30%	1.542%
15	9.904	1325	1329	1333	rBV	850836	723893	18.39%	4.501%
16	10.322	1397	1400	1403	rVB	100328	76593	1.95%	0.476%
17	10.539	1430	1437	1440	rBV2	35281	56583	1.44%	0.352%
18	10.692	1459	1463	1469	rVB	517537	450160	11.43%	2.799%
19	10.792	1477	1480	1490	rVB	112743	143499	3.64%	0.892%
20	11.245	1553	1557	1559	rBV	64494	57979	1.47%	0.361%
21	11.392	1578	1582	1585	rBV	742367	638101	16.21%	3.968%
22	11.910	1667	1670	1674	rBV	56659	61088	1.55%	0.380%
23	12.851	1827	1830	1837	rVB	74706	83447	2.12%	0.519%
24	12.968	1846	1850	1854	rBV	1110345	1029512	26.15%	6.402%
25	13.857	1999	2001	2007	rBV	72472	83571	2.12%	0.520%
26	14.027	2027	2030	2034	rBV	535180	520142	13.21%	3.234%
27	15.509	2277	2282	2289	rVB	322176	409259	10.40%	2.545%

Sum of corrected areas: 16082025

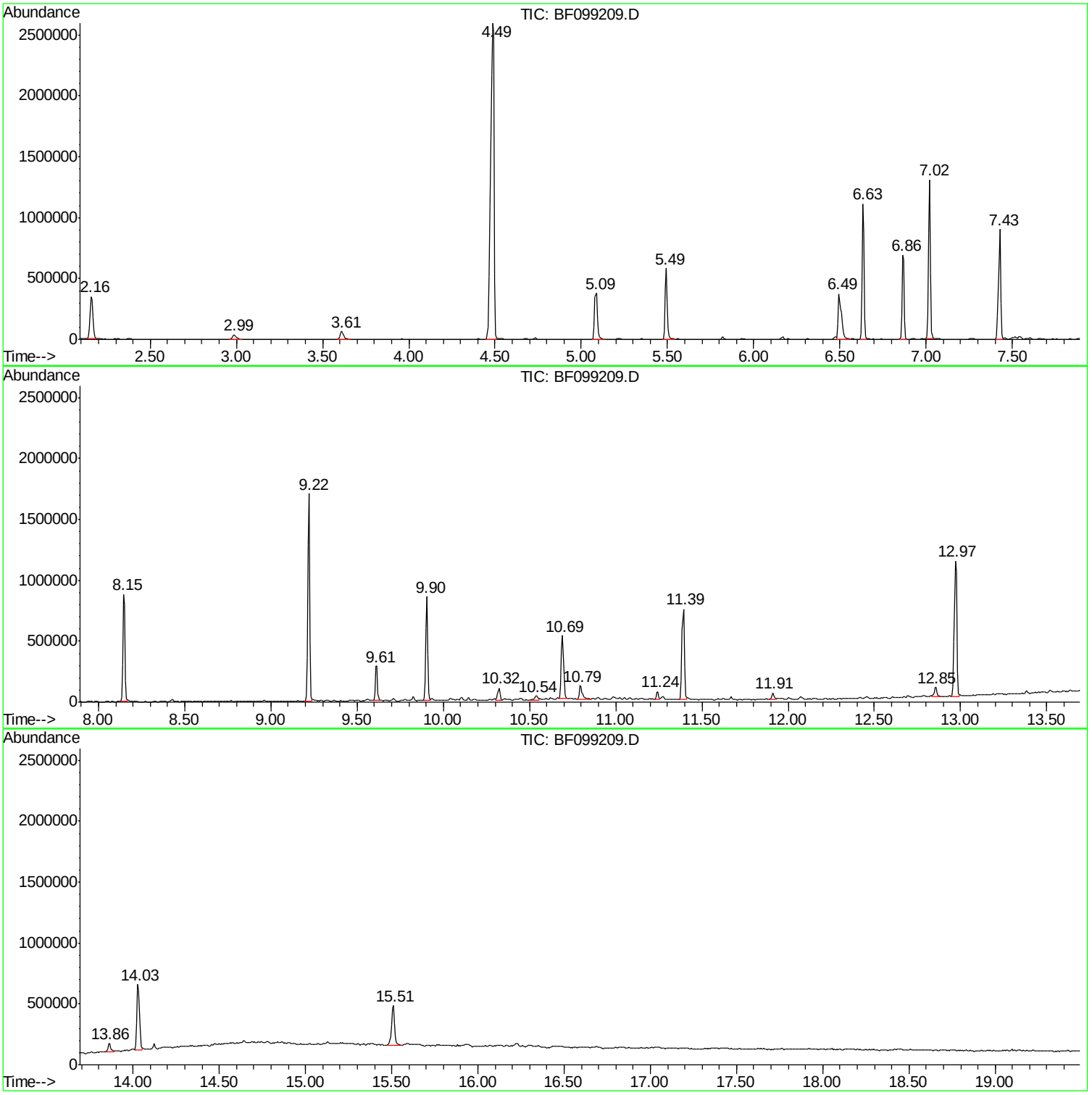
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA_F\Data\BF100717\
Data File : BF099209.D
Acq On : 7 Oct 2017 22:14
Operator : SJ/JU
Sample : I5516-01
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-5

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\BF100717\
Data File : BF099209.D
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Operator : SJ/JU
Sample : I5516-01
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-5

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

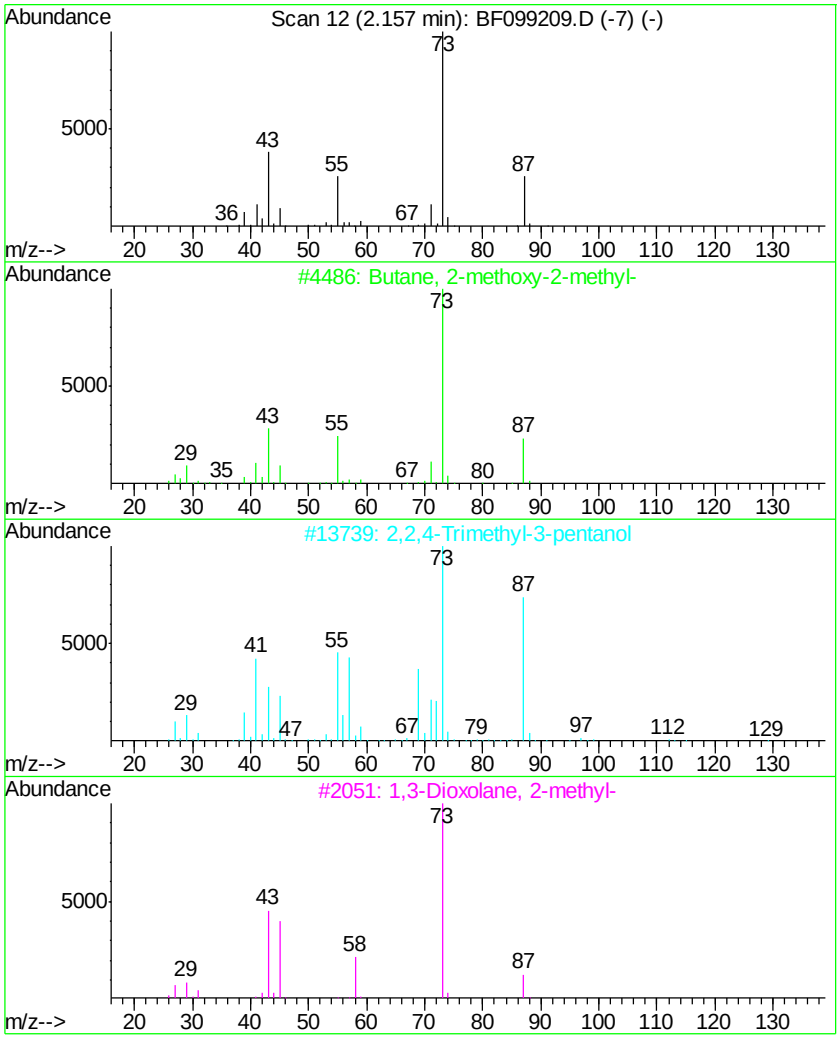
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

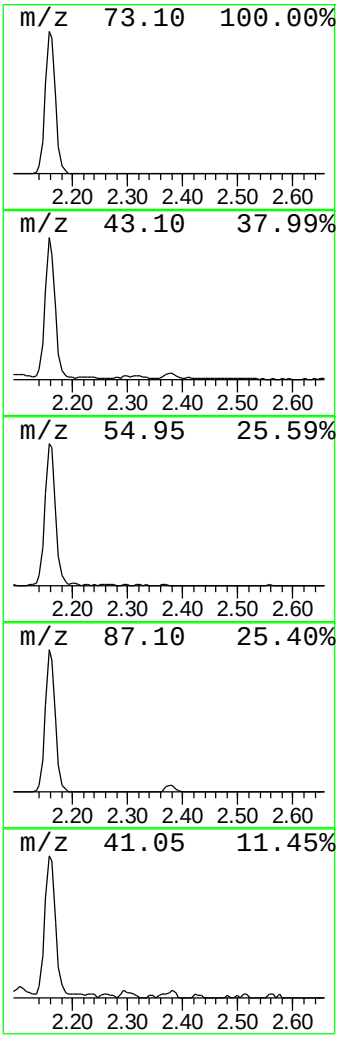
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.16	14.52 ng	446030	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17





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Data File : BF099209.D
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Operator : SJ/JU
Sample : I5516-01
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-5

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

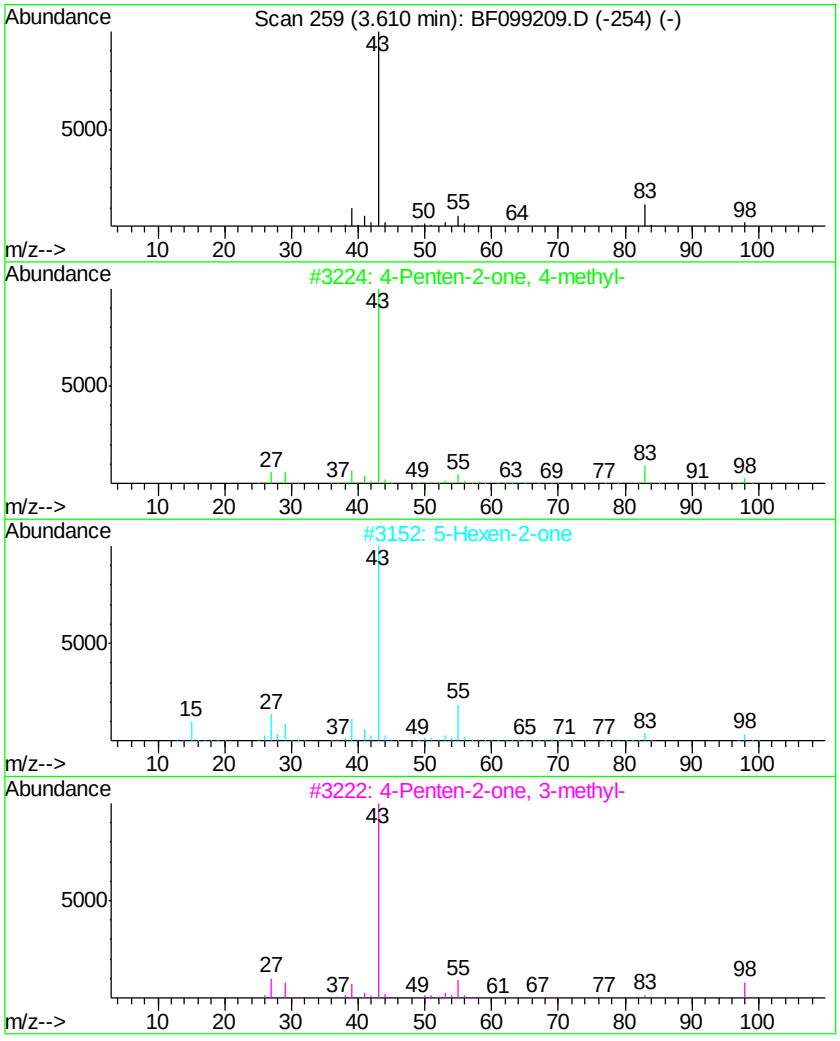
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

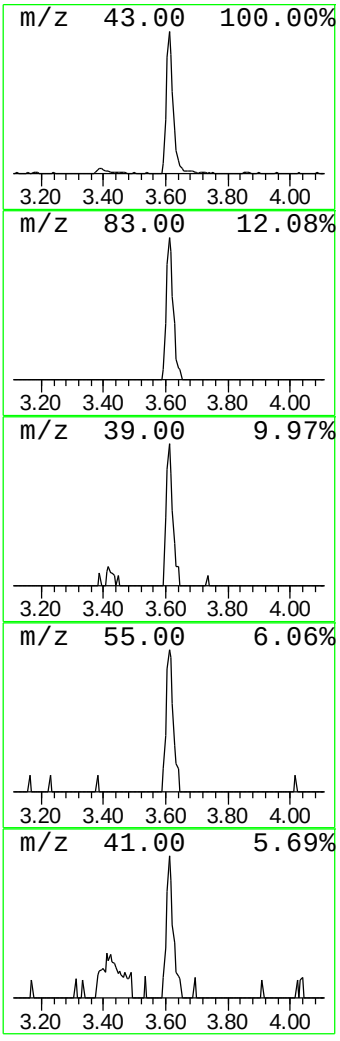
****

Peak Number 2 4-Penten-2-one, 4-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.61	3.37 ng	103494	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	72
2	5-Hexen-2-one	98	C6H10O	000109-49-9	27
3	4-Penten-2-one, 3-methyl-	98	C6H10O	000758-87-2	23
4	2-Pentanone, 3-methylene-	98	C6H10O	004359-77-7	17
5	2-Heptanone, 7,7-dichloro-	182	C7H12Cl2O	066241-43-8	9





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Operator : SJ/JU
Sample : I5516-01
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-5

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

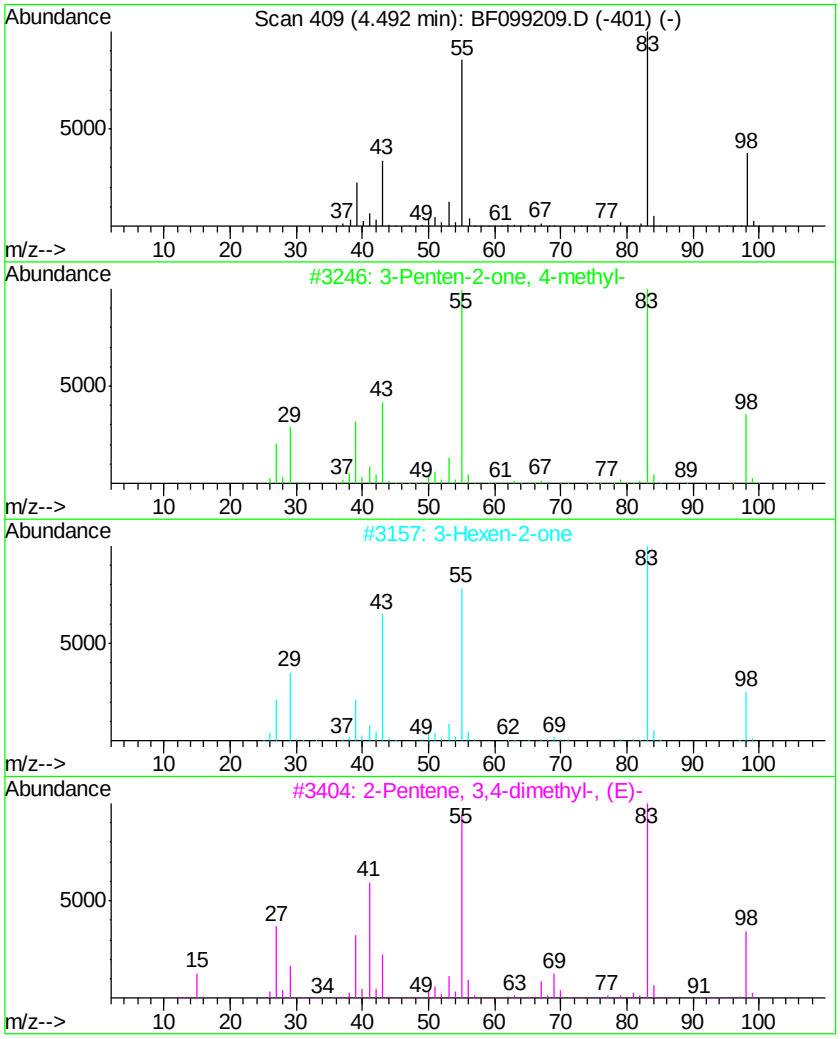
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

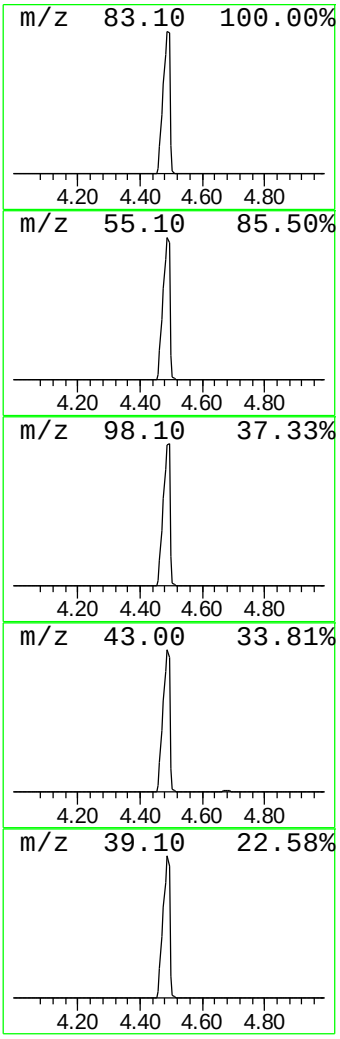
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.49	128.19 ng	3936970	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2	3-Hexen-2-one	98	C6H10O	000763-93-9	91
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, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	78





Data Path : Z:\HPCHEM1\BNA_F\Data\BF100717\
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Sample : I5516-01
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-5

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

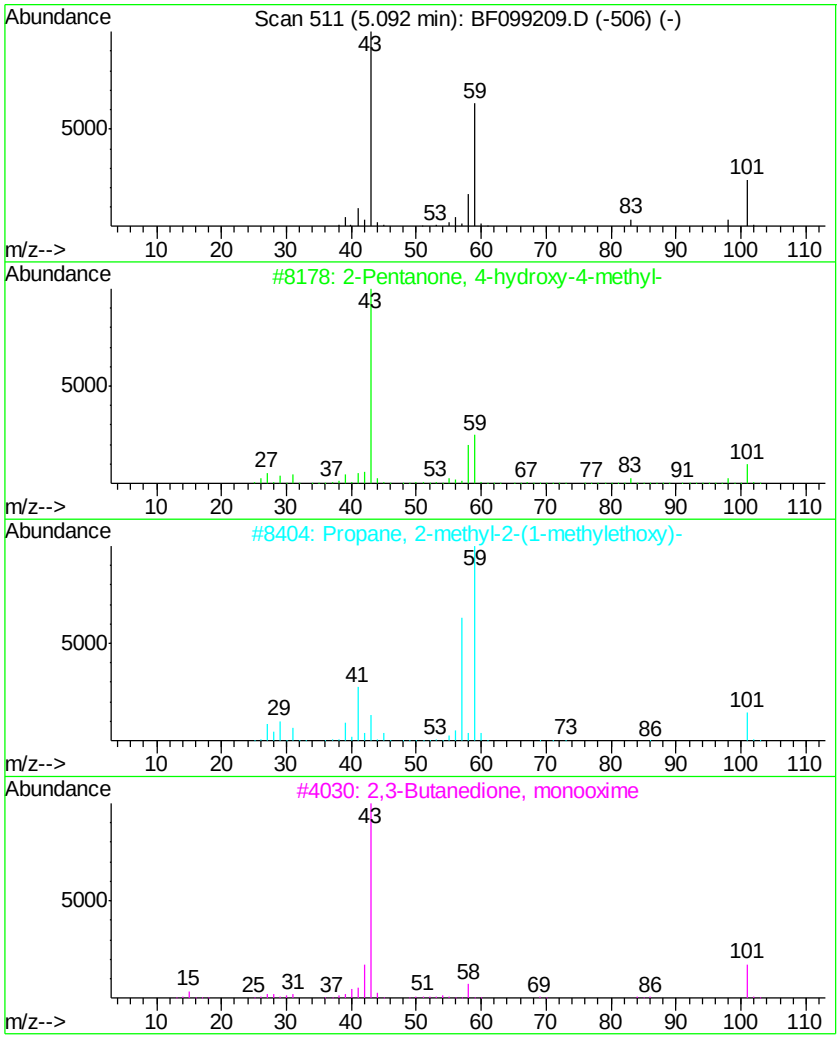
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

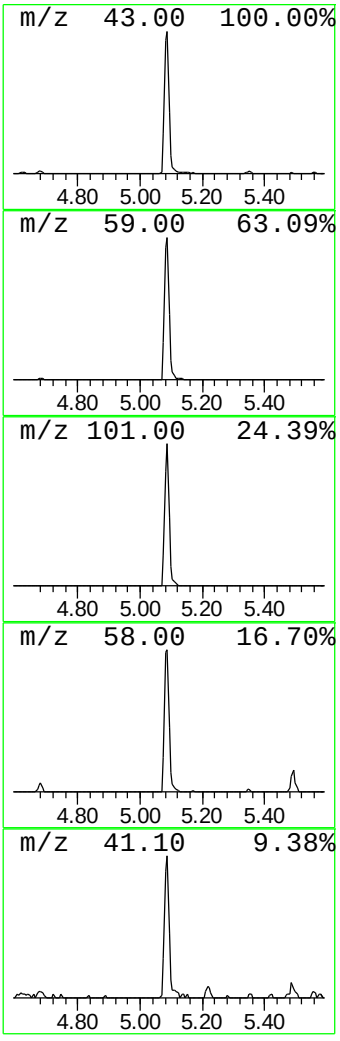
****

Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.09	12.42 ng	381560	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	12
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





Data Path : Z:\HPCHEM1\BNA_F\Data\BF100717\
Data File : BF099209.D
Acq On : 7 Oct 2017 22:14
Operator : SJ/JU
Sample : I5516-01
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-5

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

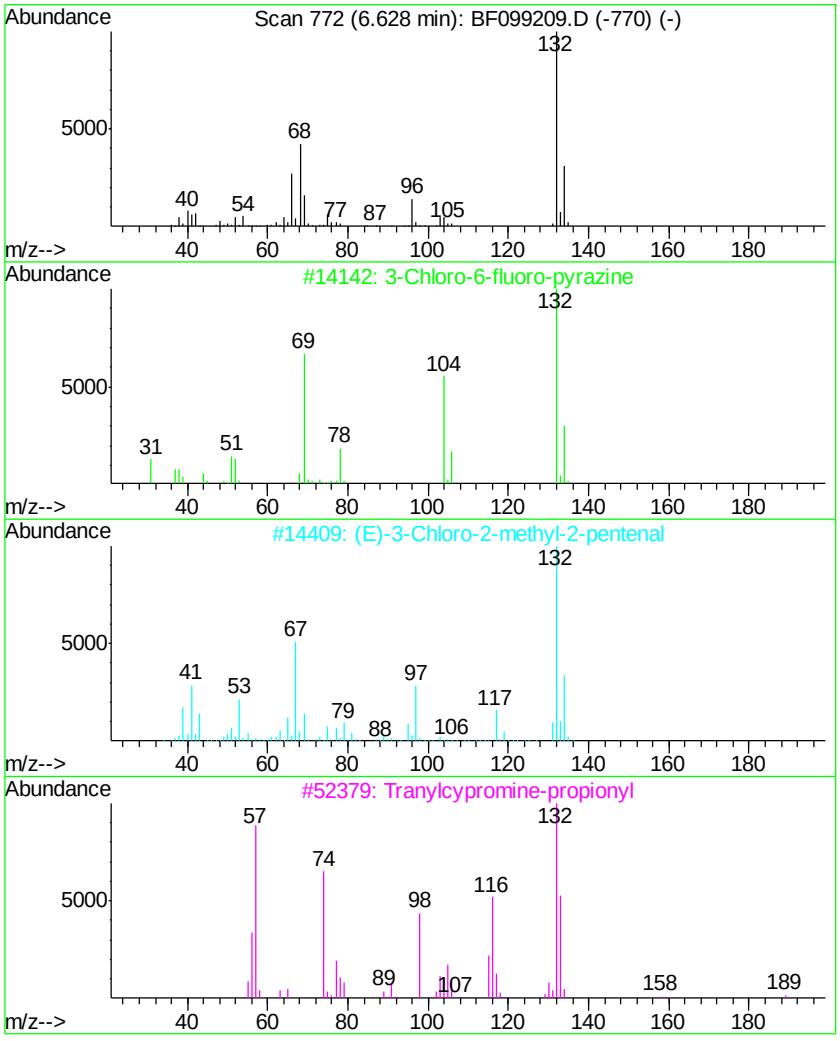
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

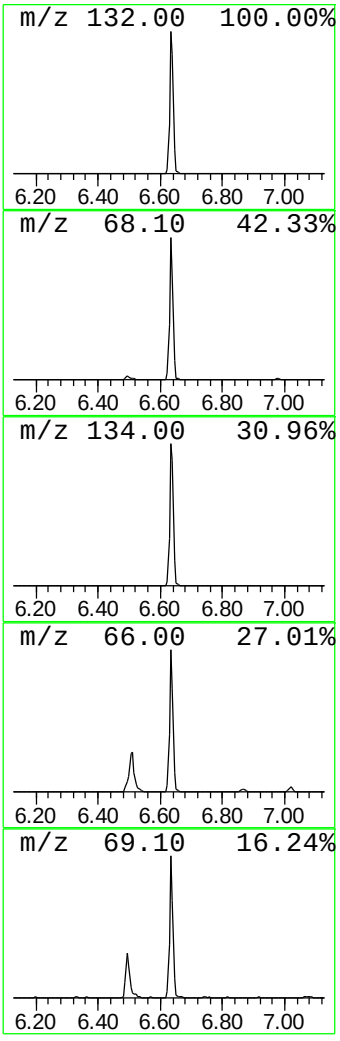
****

Peak Number 5 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	30.24 ng	928782	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





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Operator : SJ/JU
Sample : I5516-01
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-5

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

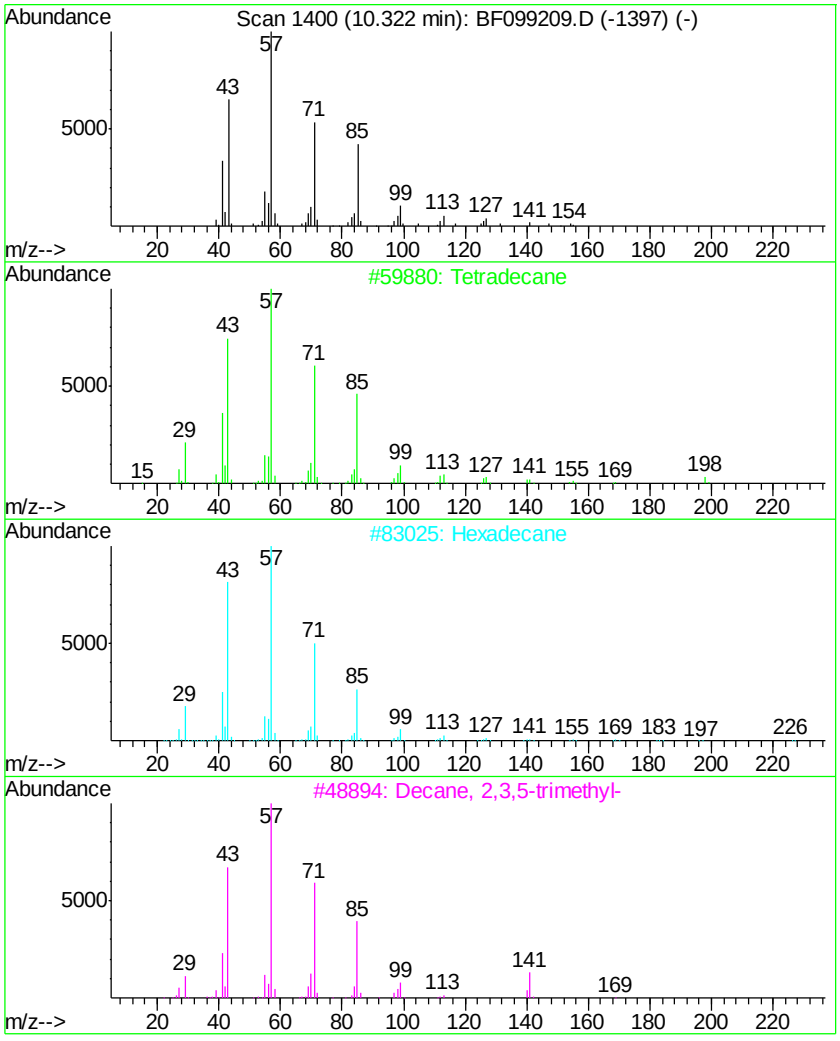
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

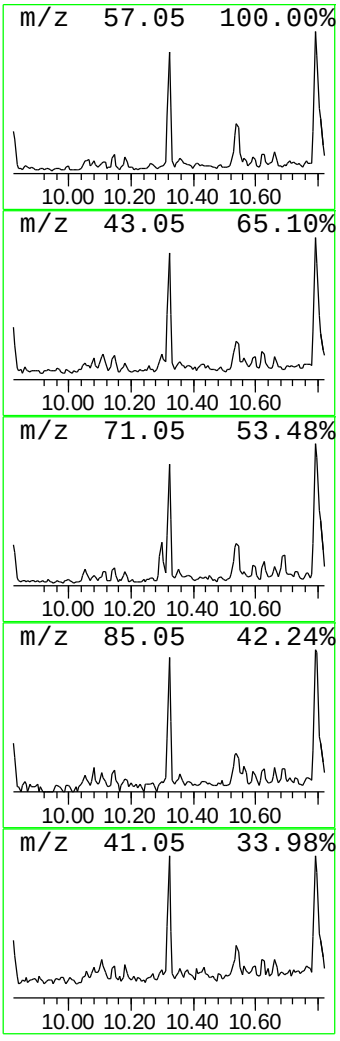
****

Peak Number 7 Tetradecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.32	2.12 ng	76593	Acenaphthene-d10	9.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane	198	C14H30	000629-59-4	91
2	Hexadecane	226	C16H34	000544-76-3	90
3	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	90
4	Pentadecane	212	C15H32	000629-62-9	90
5	Tridecane	184	C13H28	000629-50-5	83





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\Data\BF100717\
Data File : BF099209.D
Acq On : 7 Oct 2017 22:14
Operator : SJ/JU
Sample : I5516-01
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-5

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

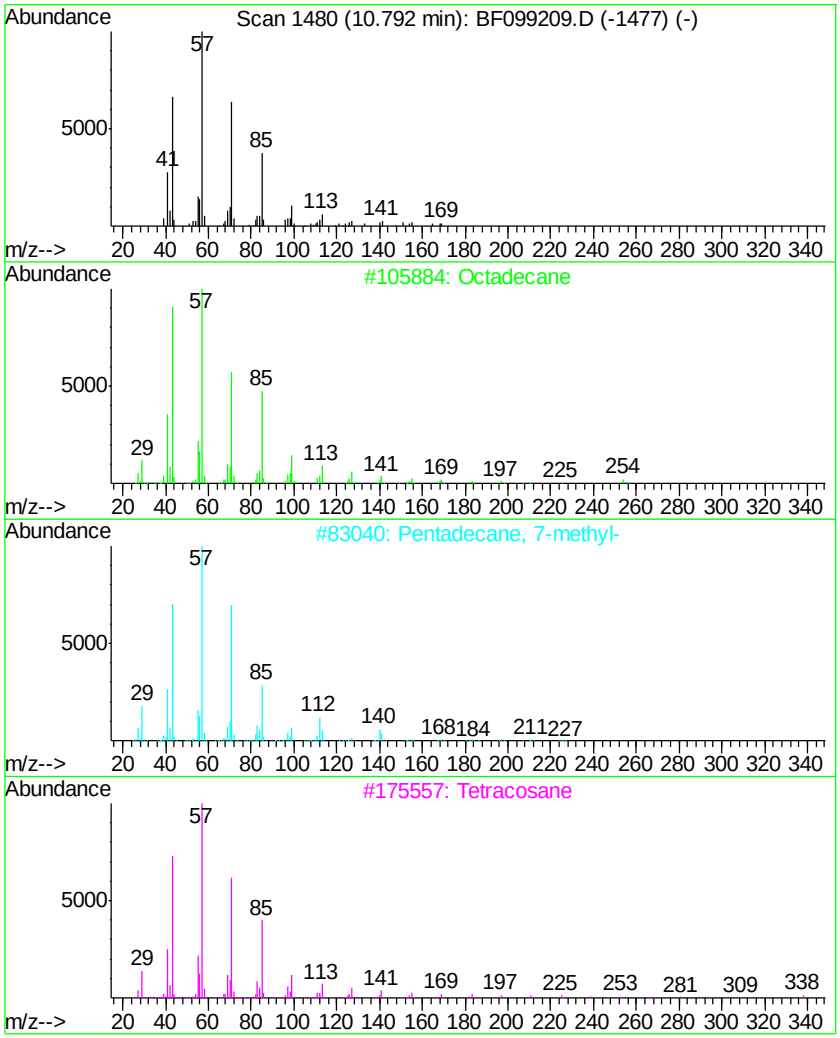
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

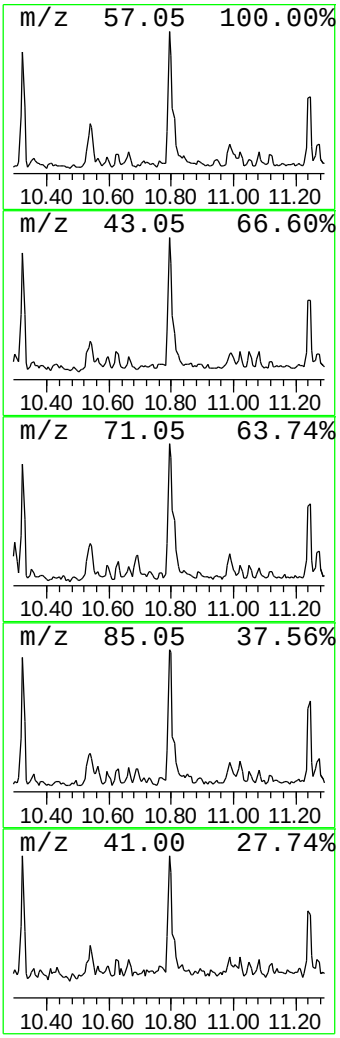
****

Peak Number 8 Octadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.79	4.50 ng	143499	Phenanthrene-d10	11.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	90
2	Pentadecane, 7-methyl-	226	C16H34	006165-40-8	90
3	Tetracosane	338	C24H50	000646-31-1	86
4	Hexadecane	226	C16H34	000544-76-3	86
5	Heptadecane	240	C17H36	000629-78-7	86





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Operator : SJ/JU
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Instrument : BNA_F
ClientSampleId : MW-5

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

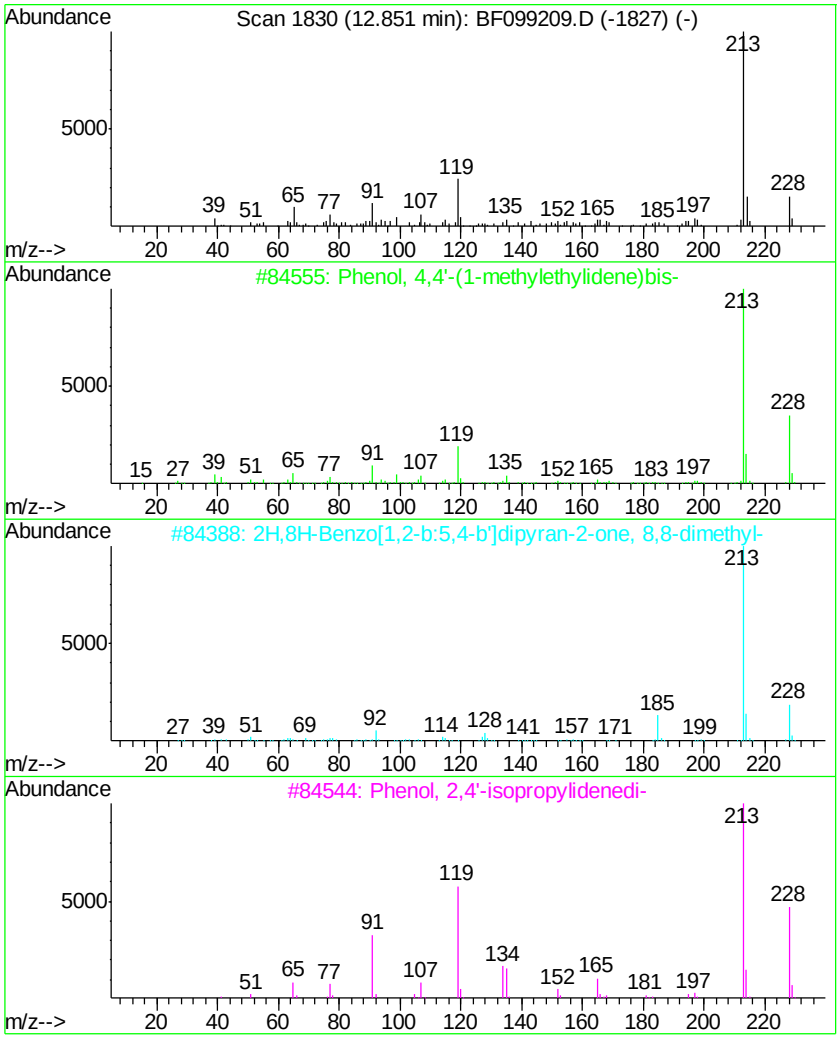
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

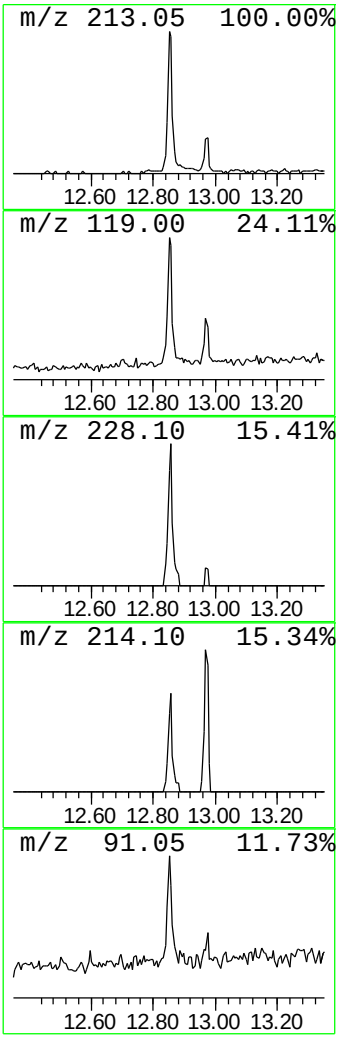
****

Peak Number 9 Phenol, 4,4'-(1-methylethyl... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.85	3.21 ng	83447	Chrysene-d12	14.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	94
2	2H,8H-Benzo[1,2-b:5,4-b']dipyran...	228	C14H12O3	000553-19-5	64
3	Phenol, 2,4'-isopropylidenedi-	228	C15H16O2	000837-08-1	56
4	Carbanilic acid, p-phenyl-	213	C13H11NO2	004474-53-7	52
5	3-Dibenzofuranamine, 2-methoxy-	213	C13H11NO2	005834-17-3	50





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Data File : BF099209.D
Acq On : 7 Oct 2017 22:14
Operator : SJ/JU
Sample : I5516-01
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-5

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

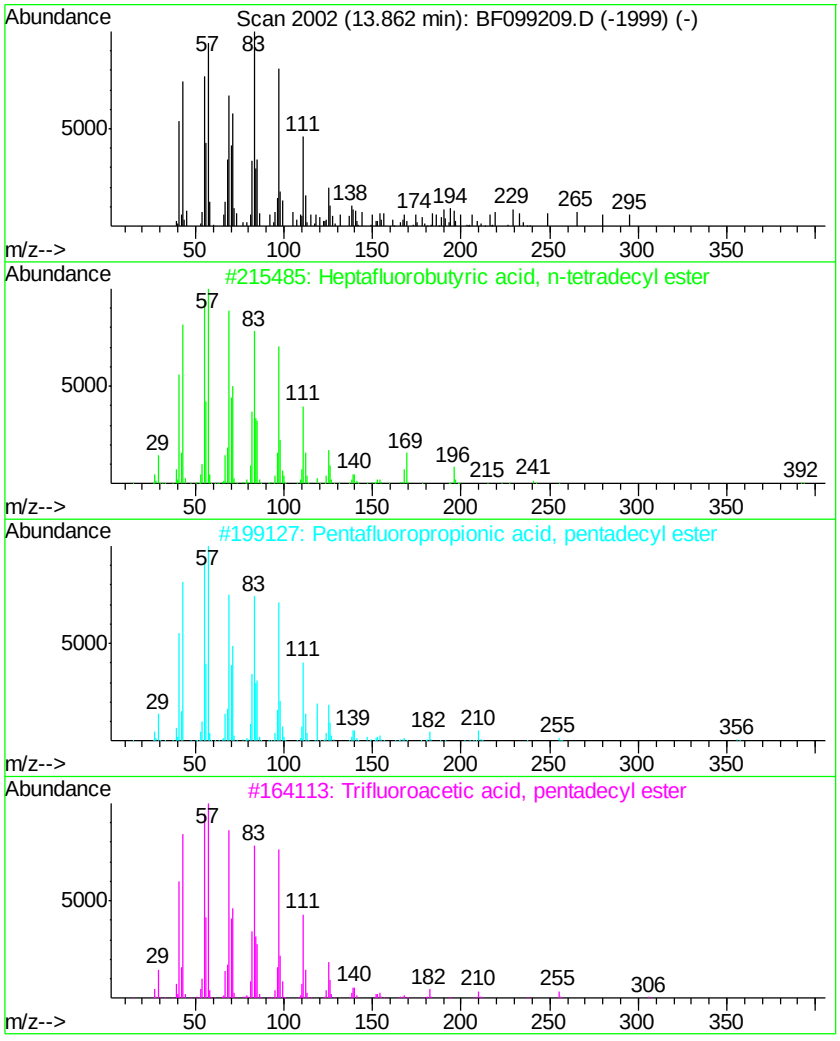
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

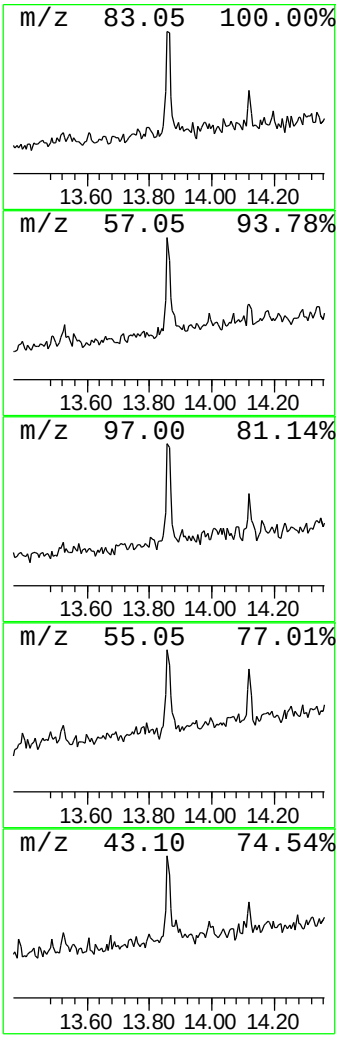
****

Peak Number 10 Heptafluorobutyric acid, n-... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.86	3.21 ng	83571	Chrysene-d12	14.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	95
2	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	95
3	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	95
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\Data\BF100717\
Data File : BF099209.D
Acq On : 7 Oct 2017 22:14
Operator : SJ/JU
Sample : I5516-01
Misc :
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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...	2.16	14.5	ng	446030	1	6.86	614225	20.0
4-Penten-2-one, 4...	3.61	3.4	ng	103494	1	6.86	614225	20.0
3-Penten-2-one, 4...	4.49	128.2	ng	3936970	1	6.86	614225	20.0
2-Pentanone, 4-hy...	5.09	12.4	ng	381560	1	6.86	614225	20.0
unknown-01	6.63	30.2	ng	928782	1	6.86	614225	20.0
Tetradecane	10.32	2.1	ng	76593	3	9.90	723893	20.0
Octadecane	10.79	4.5	ng	143499	4	11.39	638101	20.0
Phenol, 4,4'-(1-m...	12.85	3.2	ng	83447	5	14.03	520142	20.0
Heptafluorobutyri...	13.86	3.2	ng	83571	5	14.03	520142	20.0