LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072517\
Data File : BF097038.D
Acq On : 25 Jul 2017 19:30
Operator : SJ/JU
Sample : I4369-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-4-20170720

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-BF072517.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	4.640	465	468	479	rBV	86111	117402	3.30%	0.498%
2	5.098	542	546	558	rBV	1258802	1386301	38.98%	5.883%
3	6.157	722	726	741	rBV	1074853	1077986	30.31%	4.575%
4	6.269	741	745	749	rBV	2624217	2537999	71.37%	10.771%
5	6.498	780	784	791	rBV	947624	841137	23.65%	3.570%
6	6.651	806	810	814	rBV	2085244	2171979	61.08%	9.217%
7	7.069	875	881	884	rBV	1853946	1925739	54.15%	8.172%
8	7.780	997	1002	1009	rBV	1312573	1144064	32.17%	4.855%
9	8.863	1180	1186	1189	rBV	3347032	3556051	100.00%	15.091%
10	9.257	1249	1253	1256	rBV	172410	130985	3.68%	0.556%
11	9.527	1294	1299	1306	rVB	1224986	1155480	32.49%	4.904%
12	10.316	1428	1433	1436	rBV	1913417	2018976	56.78%	8.568%
13	10.451	1453	1456	1463	rVB	68187	77194	2.17%	0.328%
14	10.898	1527	1532	1534	rBV	51453	46208	1.30%	0.196%
15	10.998	1545	1549	1553	rBV	1201267	1000642	28.14%	4.246%
16	11.321	1598	1604	1607	rBV	27720	36240	1.02%	0.154%
17	11.557	1640	1644	1653	rBV2	198864	210527	5.92%	0.893%
18	12.339	1773	1777	1781	rBV	107744	121631	3.42%	0.516%
19	12.586	1814	1819	1822	rBV2	2488118	2814818	79.16%	11.945%
20	13.492	1970	1973	1980	rBV	60810	90279	2.54%	0.383%
21	13.621	1991	1995	2001	rBV	726928	656138	18.45%	2.784%
22	14.968	2220	2224	2231	rBV	418188	446516	12.56%	1.895%

Sum of corrected areas: 23564292

LSC Report - Integrated Chromatogram

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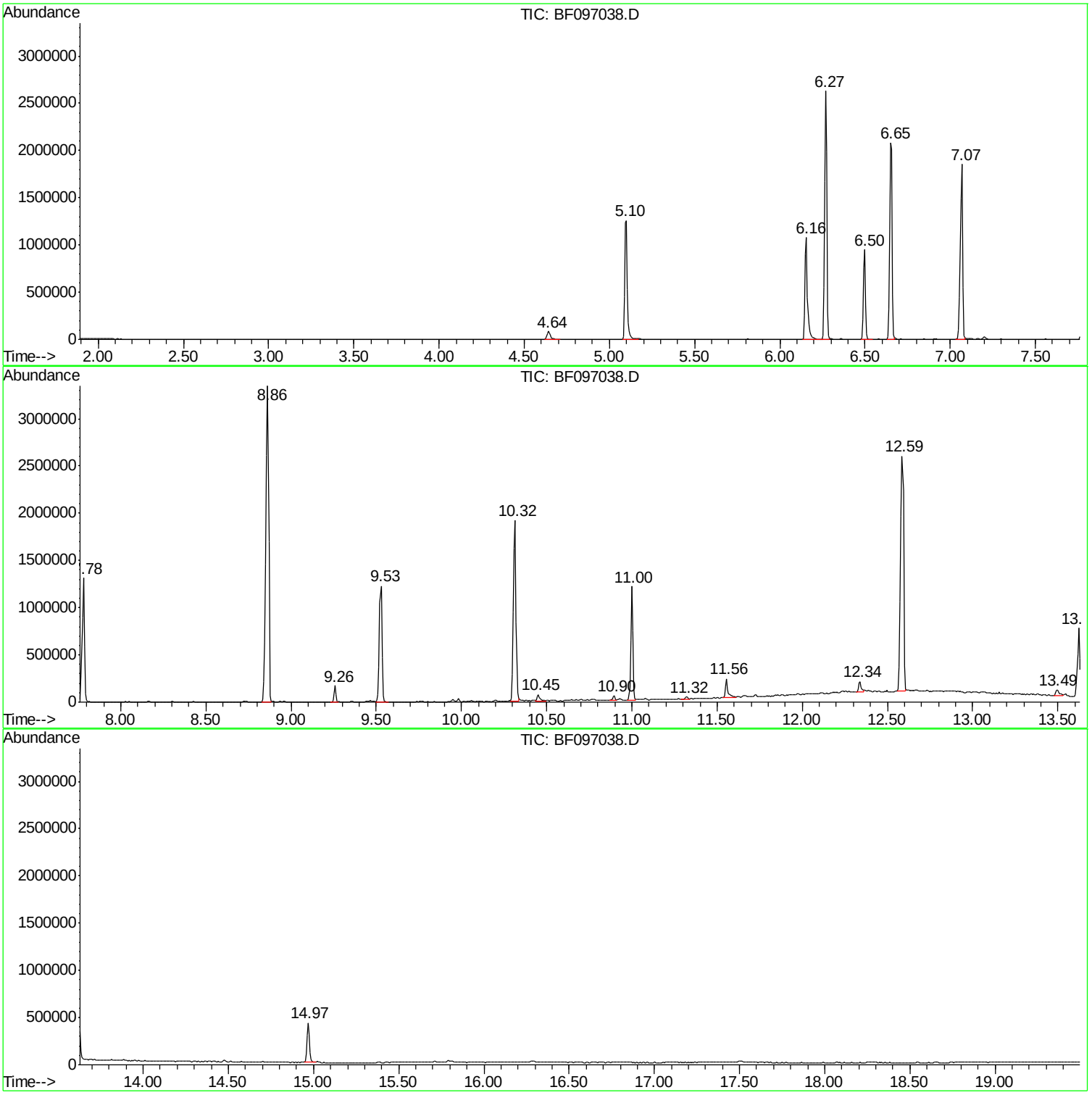
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-4-20170720

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.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:\HPCHEM1\BNA F\DATA\BF072517\
Data File : BF097038.D
Acq On : 25 Jul 2017 19:30
Operator : SJ/JU
Sample : I4369-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-4-20170720

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.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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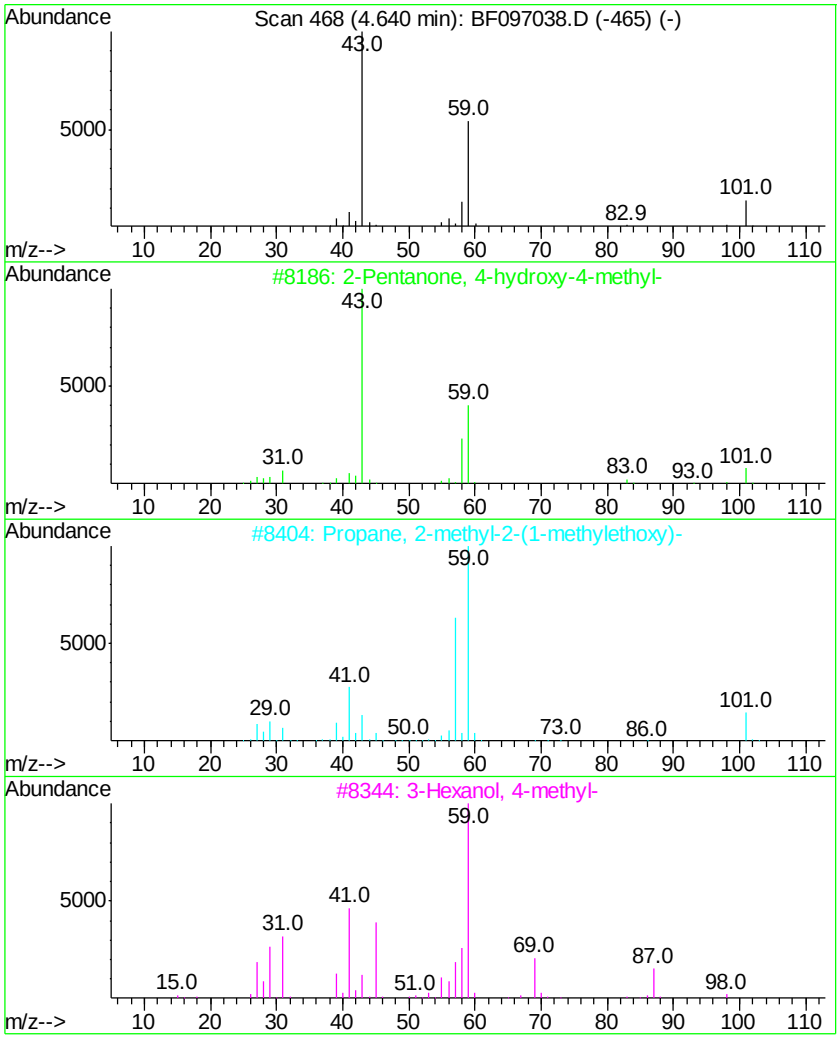
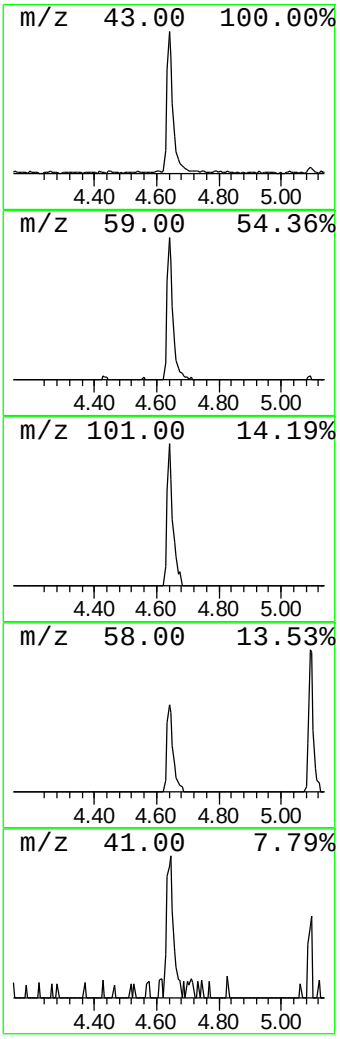
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.64	2.79 ng	117402	1,4-Dichlorobenzene-d4	6.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	3-Hexanol	102	C6H14O	000623-37-0	33
5	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	32





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Instrument : BNA_F
ClientSampleId : MW-4-20170720

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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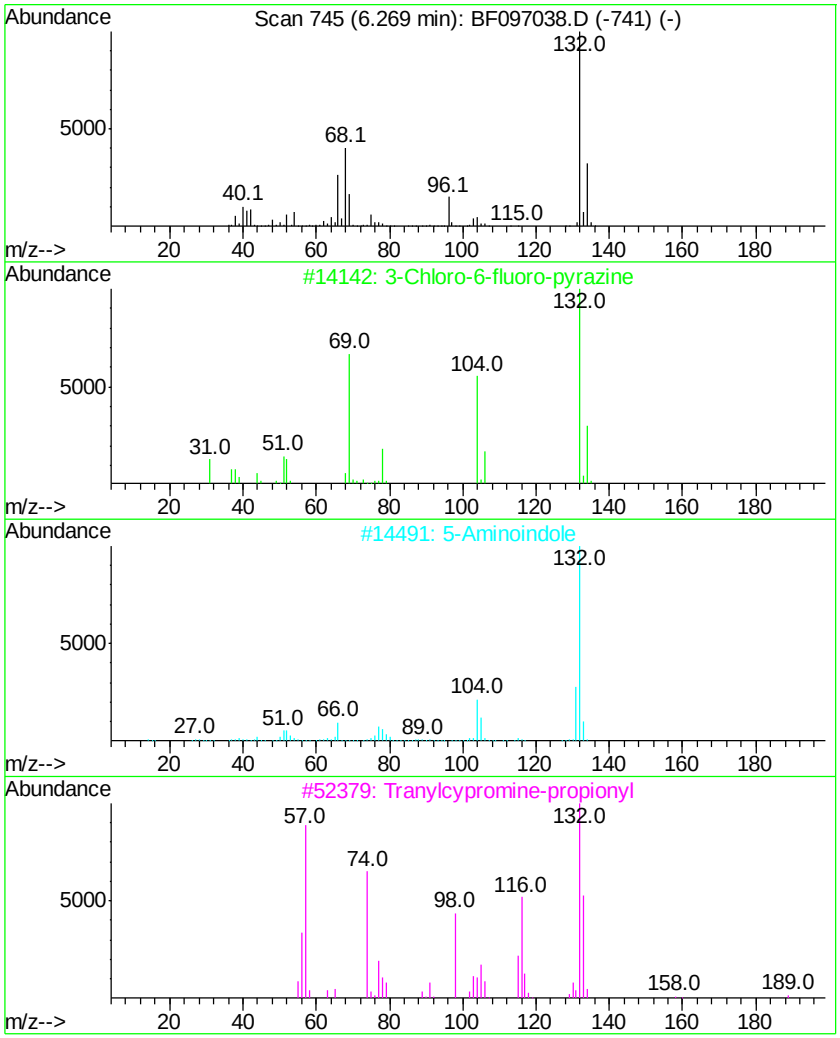
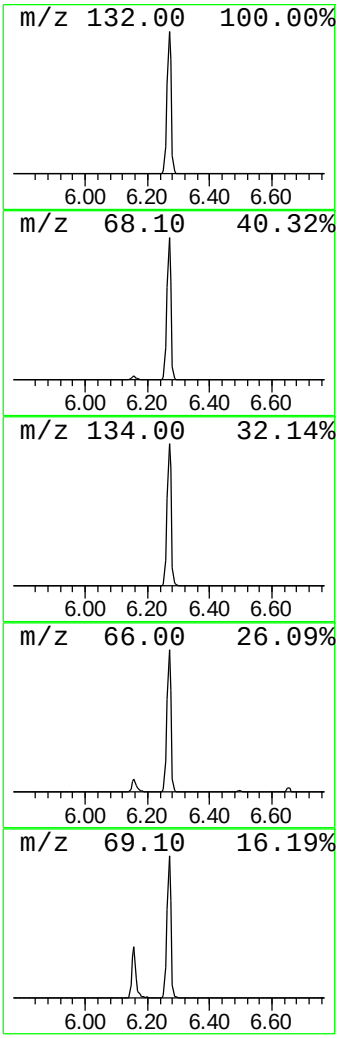
Peak Number 2 unknown6.27 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.27	60.35 ng	2538000	1,4-Dichlorobenzene-d4	6.50

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	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





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Sample : I4369-04
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ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-4-20170720

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
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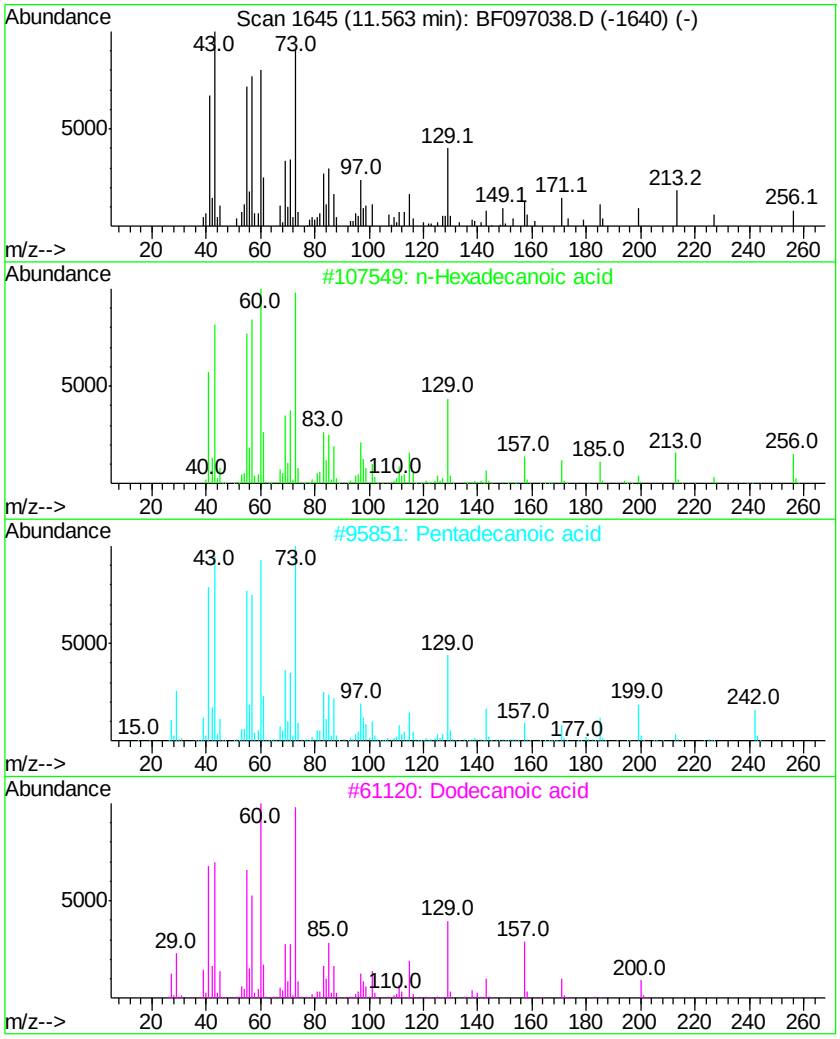
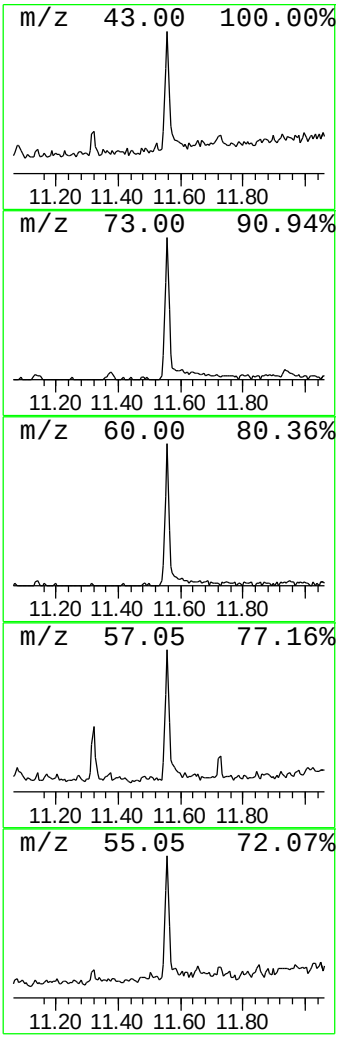
Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.56	4.21 ng	210527	Phenanthrene-d10	11.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Dodecanoic acid	200	C12H24O2	000143-07-7	64
4	Tridecanoic acid	214	C13H26O2	000638-53-9	64
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	64





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Sample : I4369-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-4-20170720

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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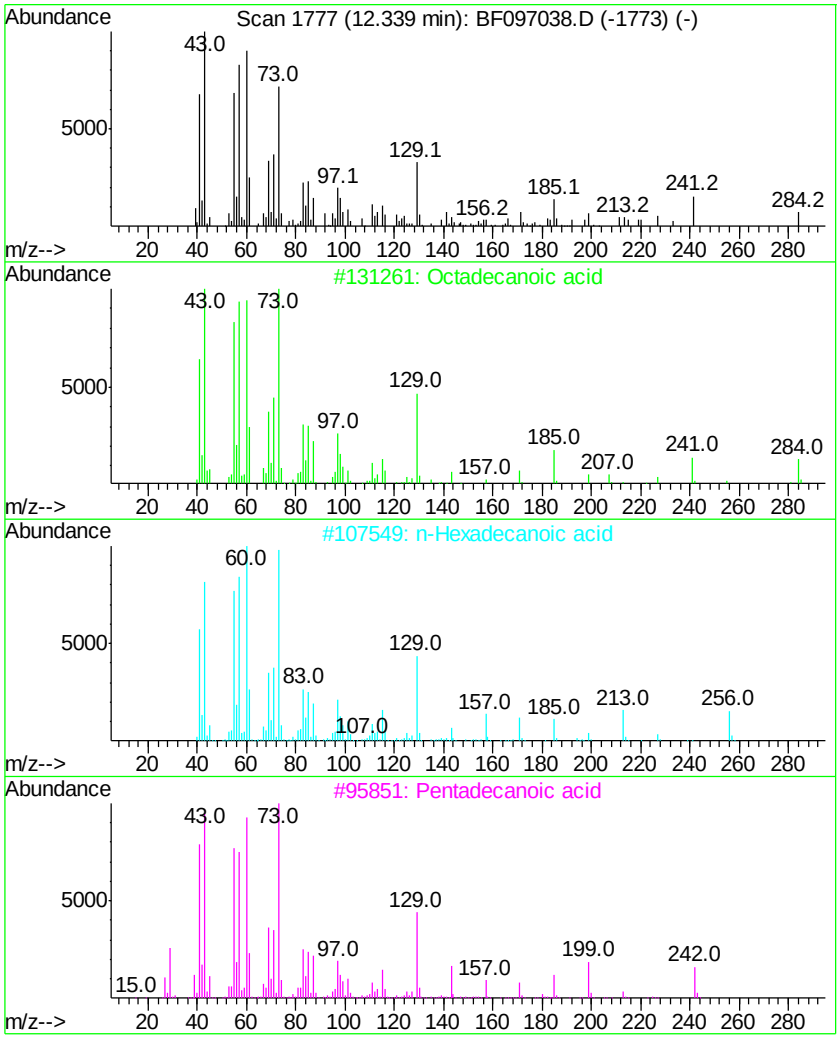
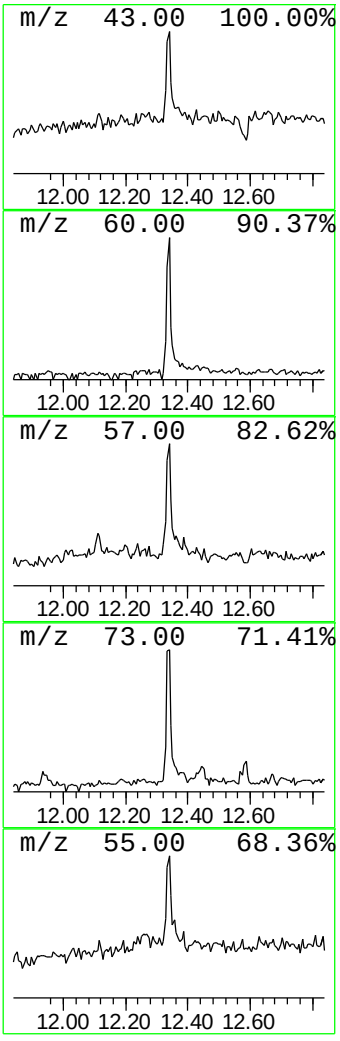
Peak Number 5 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.34	3.71 ng	121631	Chrysene-d12	13.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	72
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	n-Decanoic acid	172	C10H20O2	000334-48-5	55





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Sample : I4369-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-4-20170720

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

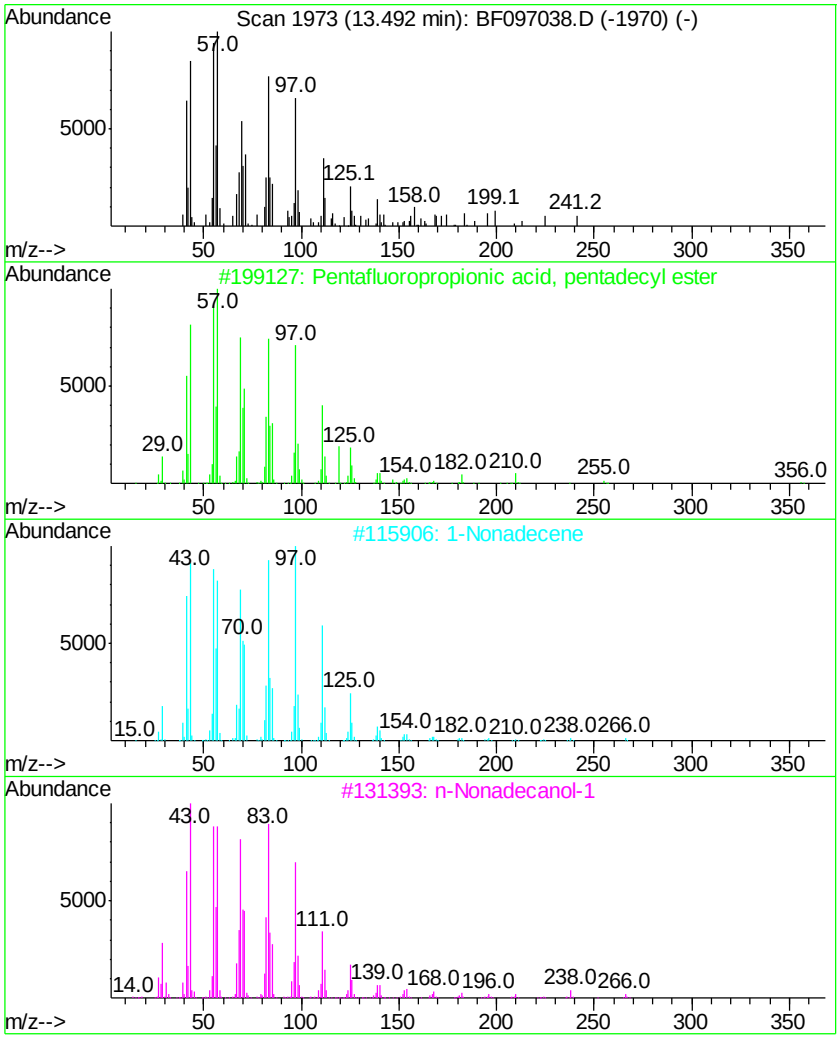
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

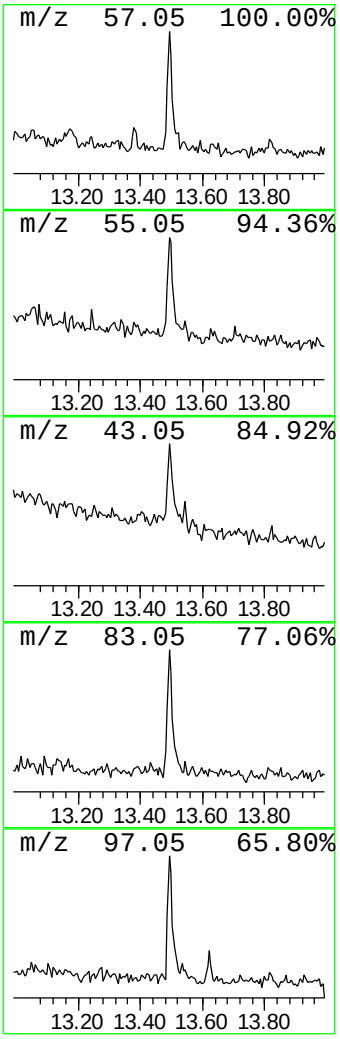
****

Peak Number 6 Pentafluoropropionic acid, ... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.49	2.75 ng	90279	Chrysene-d12	13.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	93
2	1-Nonadecene	266	C19H38	018435-45-5	90
3	n-Nonadecanol-1	284	C19H40O	001454-84-8	87
4	n-Heptadecanol-1	256	C17H36O	001454-85-9	87
5	1-Docosene	308	C22H44	001599-67-3	87





Tentatively Identified Compound (LSC) summary

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Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-4-20170720

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.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...	4.64	2.8	ng	117402	1	6.50	841137	20.0
unknown6.27	6.27	60.4	ng	2538000	1	6.50	841137	20.0
n-Hexadecanoic acid	11.56	4.2	ng	210527	4	11.00	1000640	20.0
Octadecanoic acid	12.34	3.7	ng	121631	5	13.62	656138	20.0
Pentafluoropropio...	13.49	2.8	ng	90279	5	13.62	656138	20.0