LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF051217\
Data File : BF095114.D
Acq On : 12 May 2017 16:21
Operator : SJ/MA
Sample : I3098-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-3

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-BF050217.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	5.007	518	522	533	rBV	39790	92902	2.85%	0.455%
2	5.648	628	631	657	rBV	430428	1093526	33.50%	5.360%
3	7.260	902	905	918	rBV	231312	588348	18.03%	2.884%
4	7.360	918	922	940	rVB	1523642	2402750	73.61%	11.778%
5	7.701	976	980	996	rVB	362103	467799	14.33%	2.293%
6	7.936	1015	1020	1037	rBV	1516479	1880304	57.61%	9.217%
7	8.601	1128	1133	1152	rBV	1139226	1623835	49.75%	7.960%
8	9.725	1319	1324	1347	rVB	403595	674964	20.68%	3.309%
9	11.495	1619	1625	1641	rVB	2630796	3263975	100.00%	16.000%
10	12.195	1737	1744	1752	rBV2	52746	111590	3.42%	0.547%
11	12.548	1799	1804	1815	rBV2	553490	815163	24.97%	3.996%
12	12.966	1867	1875	1879	rBV4	24244	47872	1.47%	0.235%
13	13.436	1951	1955	1961	rBV2	36185	49156	1.51%	0.241%
14	13.848	2019	2025	2035	rBV	1159546	1745681	53.48%	8.557%
15	14.160	2075	2078	2087	rBV3	33355	59398	1.82%	0.291%
16	14.465	2123	2130	2135	rBV6	23097	37082	1.14%	0.182%
17	14.518	2135	2139	2142	rBV3	22965	34203	1.05%	0.168%
18	14.889	2198	2202	2207	rVB3	26273	34263	1.05%	0.168%
19	14.954	2208	2213	2225	rVV	484767	768034	23.53%	3.765%
20	15.918	2373	2377	2389	rBV	131482	197217	6.04%	0.967%
21	17.006	2558	2562	2569	rBV	113988	170032	5.21%	0.833%
22	17.277	2602	2608	2614	rBV2	2238918	2812164	86.16%	13.785%
23	17.512	2642	2648	2649	rBV6	24913	35730	1.09%	0.175%
24	18.524	2816	2820	2827	rBV6	34328	58970	1.81%	0.289%
25	18.624	2833	2837	2844	rBV	517372	720680	22.08%	3.533%
26	19.489	2981	2984	2990	rVB	56733	61106	1.87%	0.300%
27	20.289	3116	3120	3131	rBV	376941	553553	16.96%	2.713%

Sum of corrected areas: 20400297

LSC Report - Integrated Chromatogram

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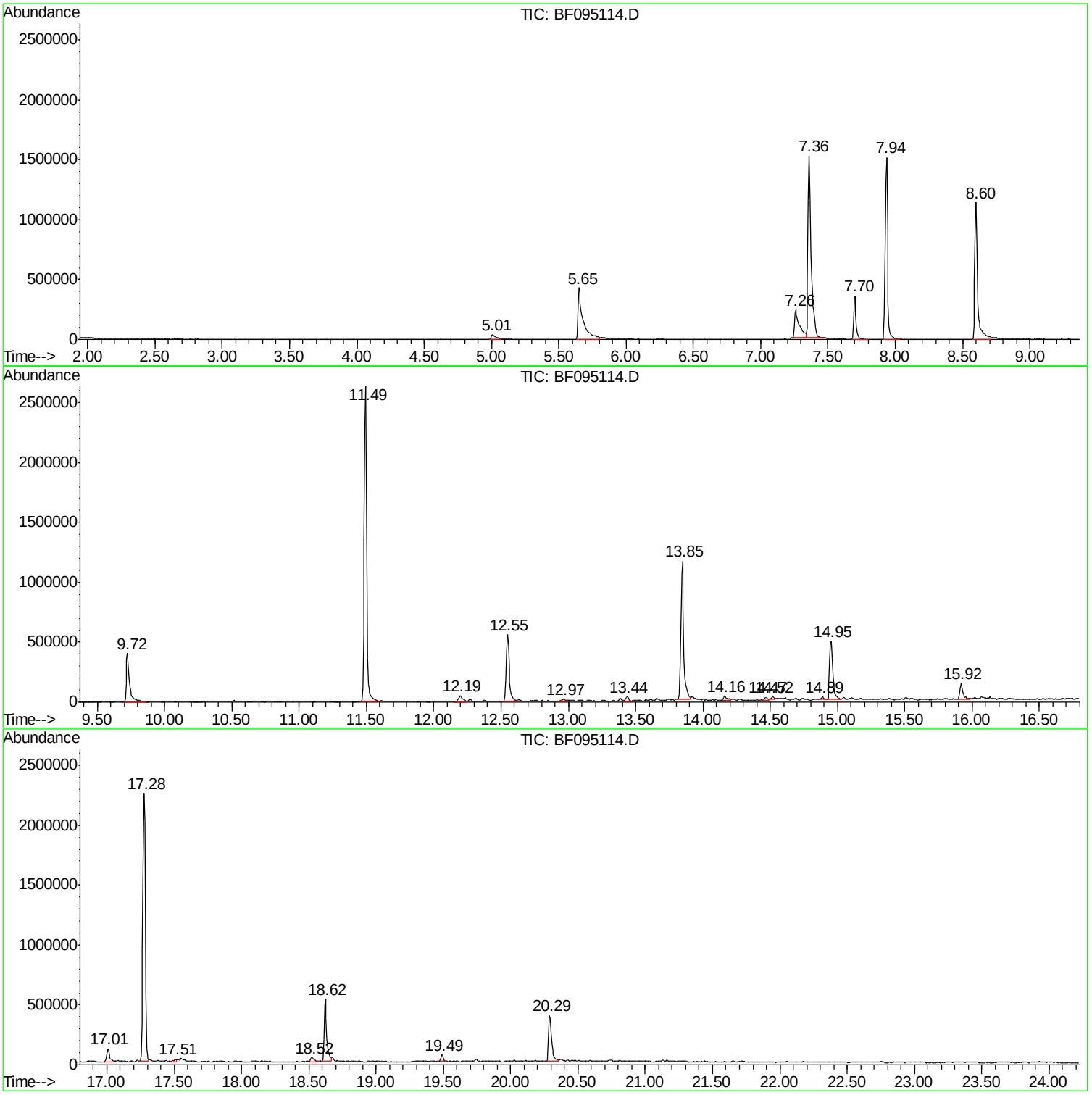
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.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\BF051217\
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Operator : SJ/MA
Sample : I3098-02
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ClientSampleId : MW-3

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

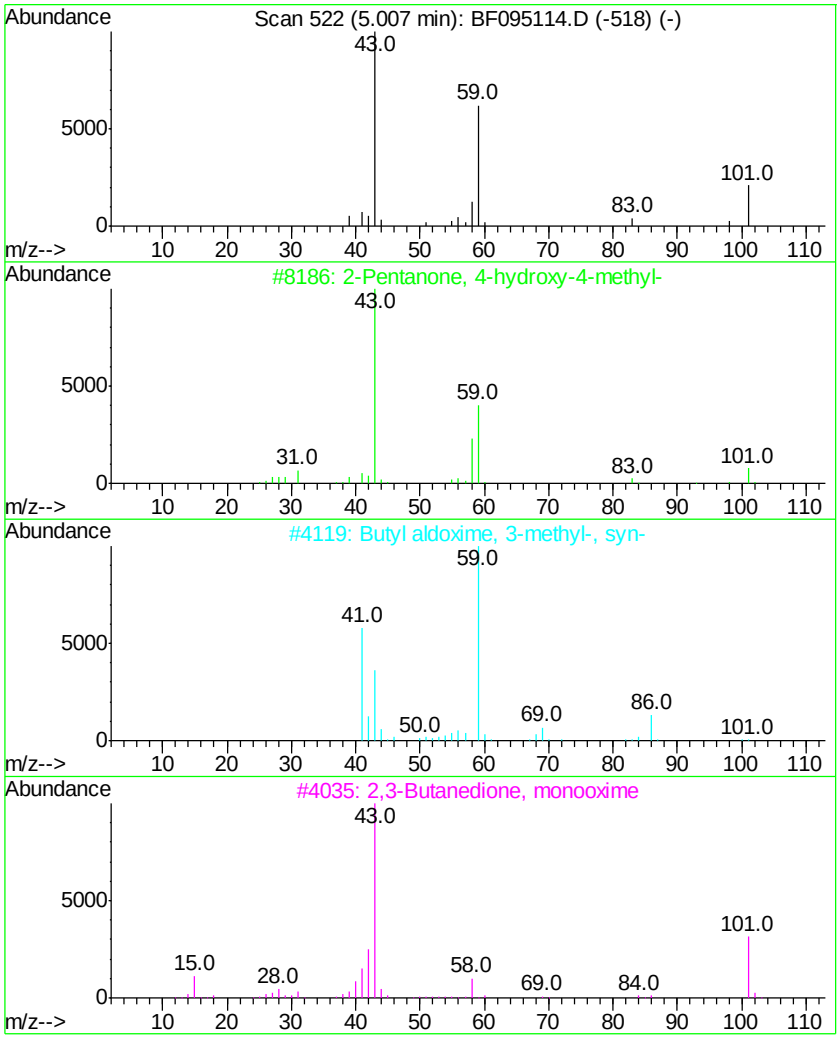
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

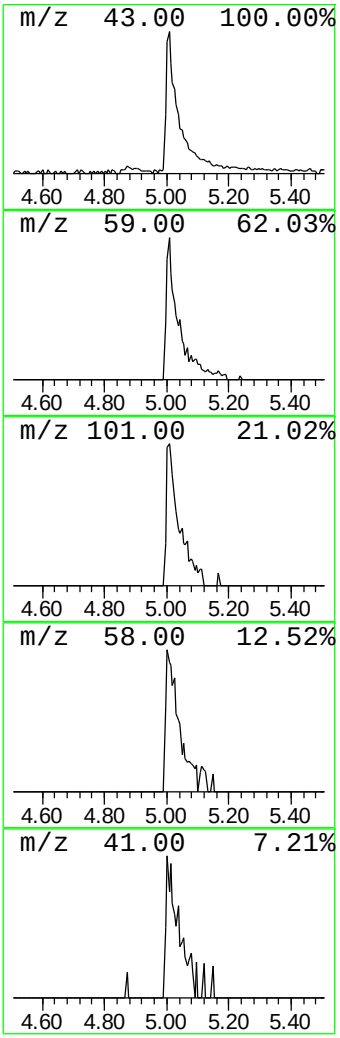
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.01	3.97 ng	92902	1,4-Dichlorobenzene-d4	7.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	23
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	Guanidine	59	CH5N3	000113-00-8	9
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9





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Acq On : 12 May 2017 16:21
Operator : SJ/MA
Sample : I3098-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.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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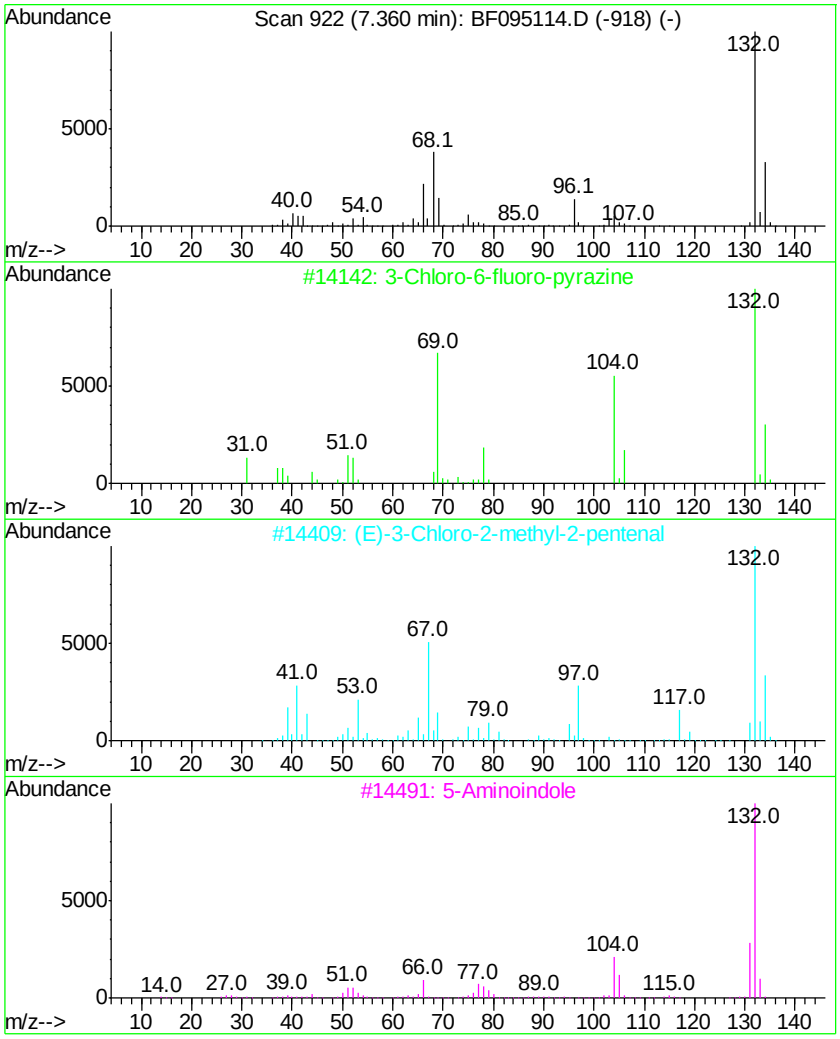
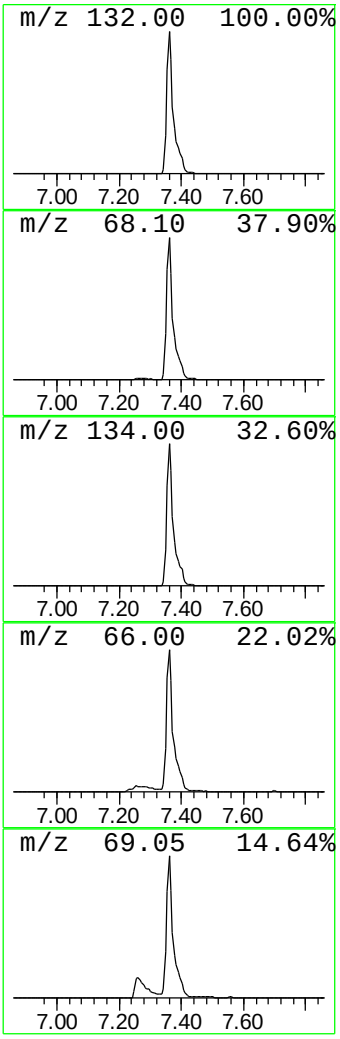
Peak Number 2 unknown7.36 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.36	102.73 ng	2402750	1,4-Dichlorobenzene-d4	7.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





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Instrument : BNA_F
ClientSampleId : MW-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
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TIC Library : C:\DATABASE\NIST11.L
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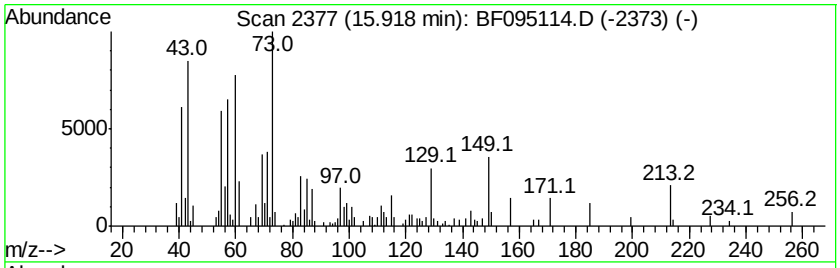
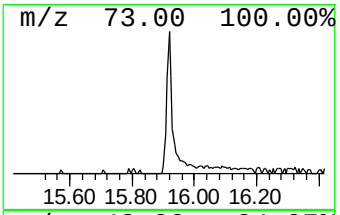
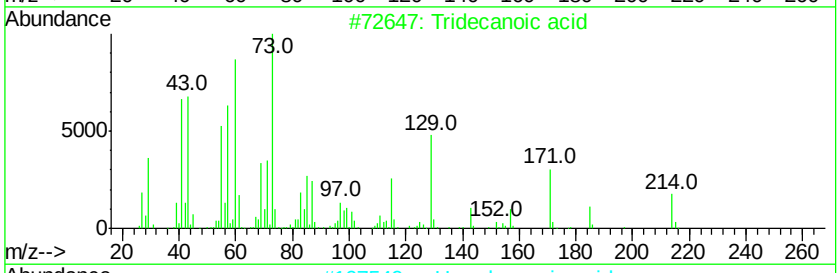
Peak Number 5 Tridecanoic acid Concentration Rank 3

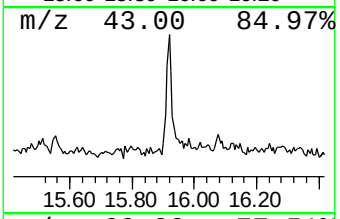
R.T.	EstConc	Area	Relative to ISTD	R.T.
15.92	5.14 ng	197217	Phenanthrene-d10	14.95

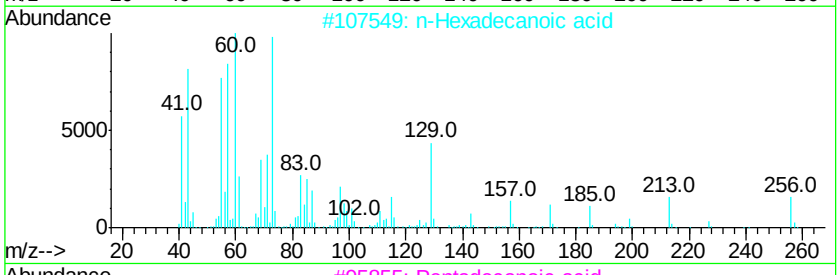
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	95
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	68
4	Dodecanoic acid	200	C12H24O2	000143-07-7	47
5	Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	15

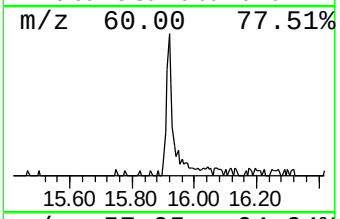


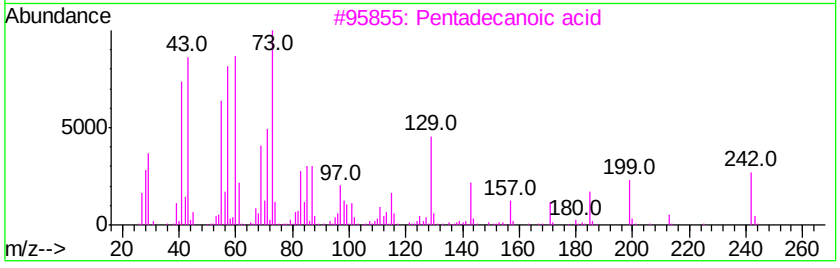


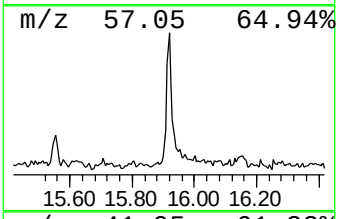


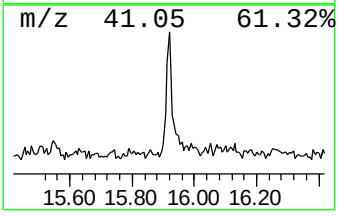












Library Search Compound Report

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ClientSampleId : MW-3

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

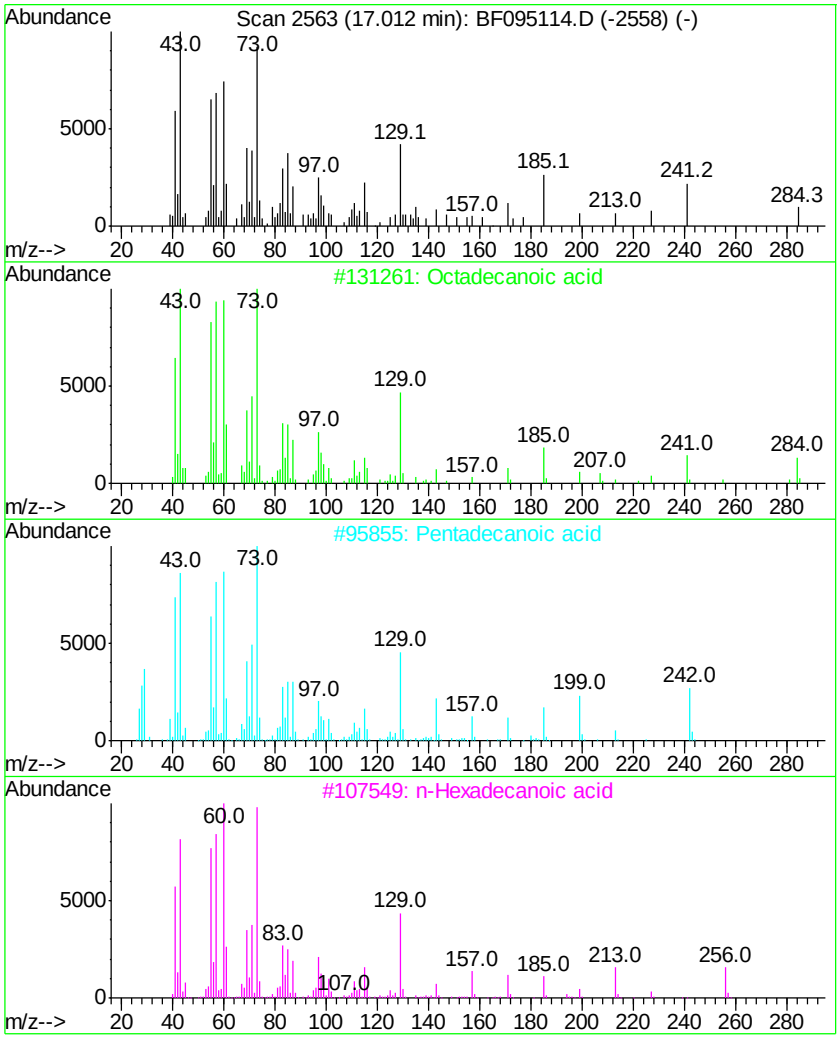
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

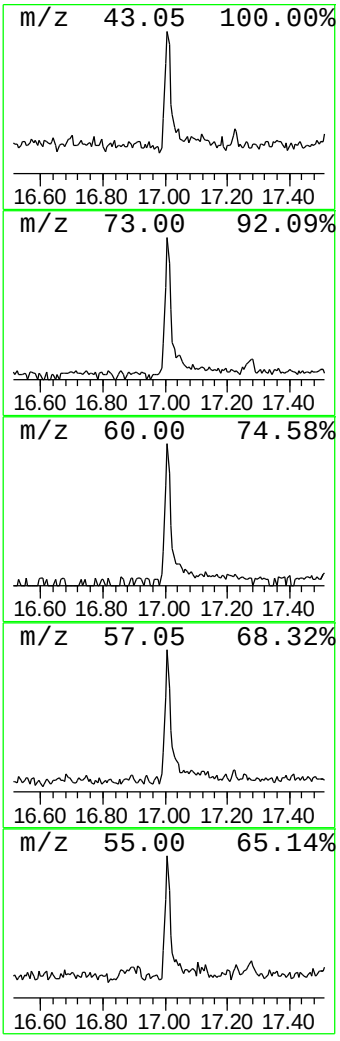
****

Peak Number 6 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.01	4.72 ng	170032	Chrysene-d12	18.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	76
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	74
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	68
5	Undecanoic acid	186	C11H22O2	000112-37-8	58





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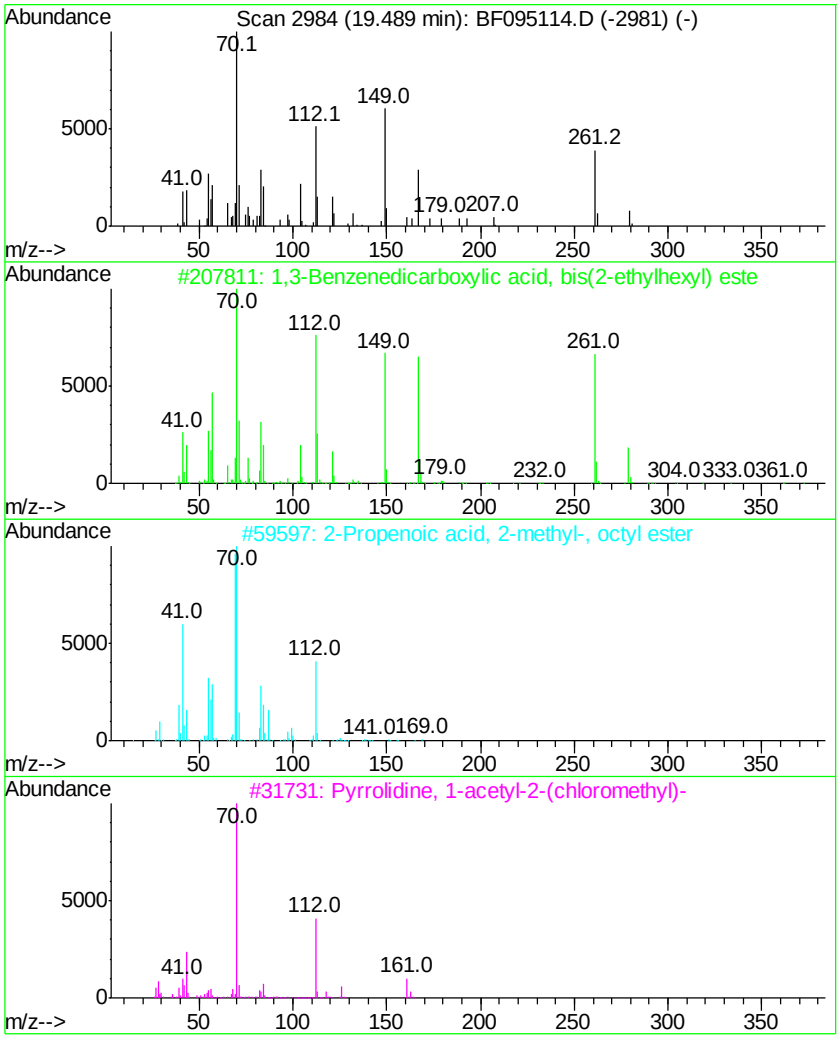
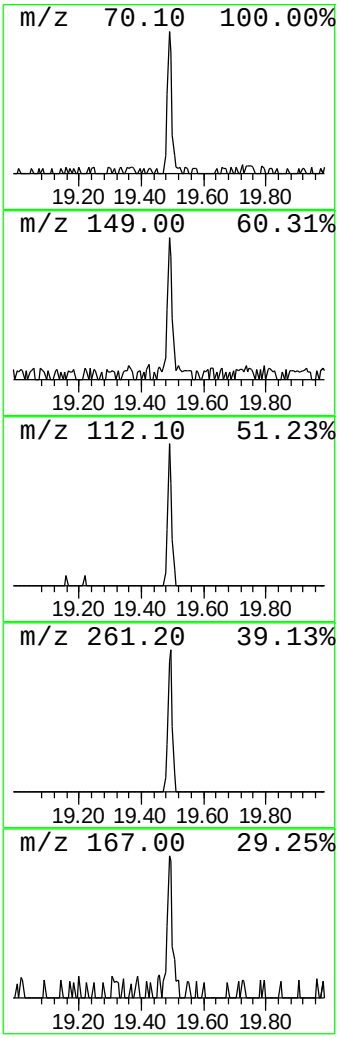
****

Peak Number 7 unknown19.49 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.49	2.21 ng	61106	Perylene-d12	20.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	47
2	2-Propenoic acid, 2-methyl-, oct...	198	C12H22O2	002157-01-9	32
3	Pyrrolidine, 1-acetyl-2-(chlorom...	161	C7H12ClNO	054385-06-7	25
4	Phthalic acid, 3,5-difluorophenyl...	348	C19H18F2O4	1000315-54-1	22
5	Phthalic acid, 3,5-difluorophenyl...	334	C18H16F2O4	1000314-97-0	22





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.01	4.0	ng	92902	1	7.70	467799	20.0
unknown7.36	7.36	102.7	ng	2402750	1	7.70	467799	20.0
Tridecanoic acid	15.92	5.1	ng	197217	4	14.95	768034	20.0
Octadecanoic acid	17.01	4.7	ng	170032	5	18.62	720680	20.0
unknown19.49	19.49	2.2	ng	61106	6	20.29	553553	20.0