LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112316\
Data File : BF091299.D
Acq On : 24 Nov 2016 2:28
Operator : UM/SJ
Sample : H5740-15
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DUP-X

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-BF112316.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	1.767	4	7	9	rBV	4369162	5294920	85.55%	8.774%
2	1.904	17	19	41	rVB	2750265	5136113	82.98%	8.511%
3	2.178	41	43	57	rVB2	84257	234854	3.79%	0.389%
4	5.082	293	297	305	rVB	1487788	2221307	35.89%	3.681%
5	5.493	329	333	335	rBV	5520635	6189441	100.00%	10.257%
6	6.510	419	422	425	rBV	4446496	5680936	91.78%	9.414%
7	6.647	431	434	437	rBV	5025809	5255430	84.91%	8.709%
8	6.876	452	454	457	rBV	1248753	1279600	20.67%	2.120%
9	7.036	465	468	470	rVB	4185987	3992403	64.50%	6.616%
10	7.447	500	504	506	rBV	3354736	3919297	63.32%	6.495%
11	8.168	564	567	569	rBV	1869587	1751943	28.31%	2.903%
12	9.242	658	661	664	rBV	4762275	5253688	84.88%	8.706%
13	9.631	693	695	698	rBV	175933	192326	3.11%	0.319%
14	9.916	718	720	723	rVB	1661247	1621102	26.19%	2.686%
15	10.362	755	759	761	rBV	98591	101786	1.64%	0.169%
16	10.705	786	789	792	rVV	3317801	3168038	51.18%	5.250%
17	10.831	798	800	804	rVB	145232	158838	2.57%	0.263%
18	11.276	837	839	841	rBV	83025	76647	1.24%	0.127%
19	11.402	848	850	852	rBV	1683582	1405671	22.71%	2.329%
20	11.939	894	897	902	rBV2	134700	238629	3.86%	0.395%
21	12.717	963	965	971	rBV	82271	107399	1.74%	0.178%
22	12.991	986	989	991	rBV	4412762	4038995	65.26%	6.693%
23	13.882	1065	1067	1070	rBV	175299	210440	3.40%	0.349%
24	14.031	1078	1080	1083	rBV	1250146	1289144	20.83%	2.136%
25	14.522	1119	1123	1125	rBV2	38335	63545	1.03%	0.105%
26	14.797	1145	1147	1152	rBV	247925	306720	4.96%	0.508%
27	15.471	1203	1206	1209	rBV	787863	1064505	17.20%	1.764%
28	15.997	1250	1252	1259	rBV4	42720	91488	1.48%	0.152%

Sum of corrected areas: 60345205

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Operator : UM/SJ
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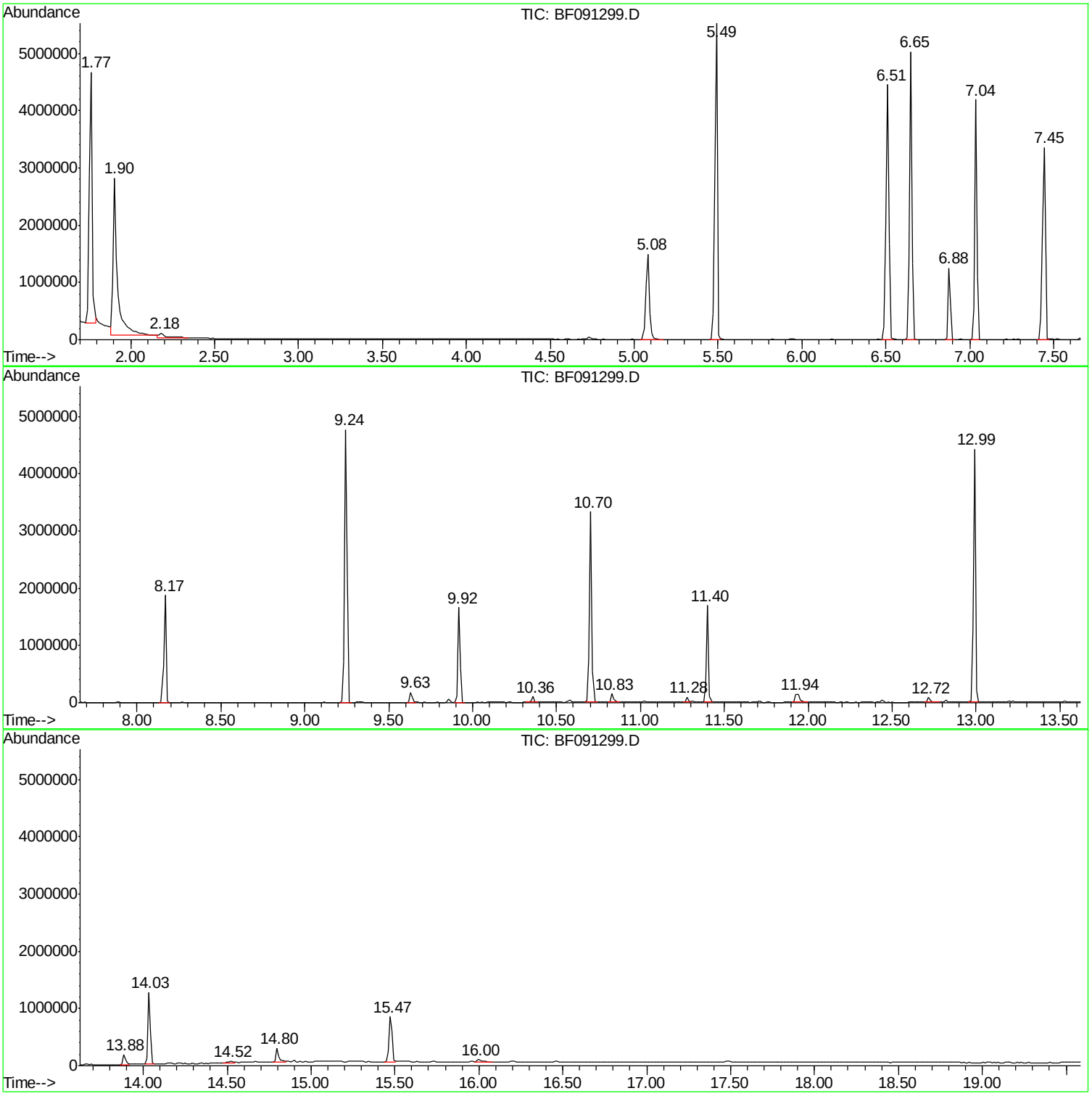
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DUP-X

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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TIC Library : C:\DATABASE\NIST02.L
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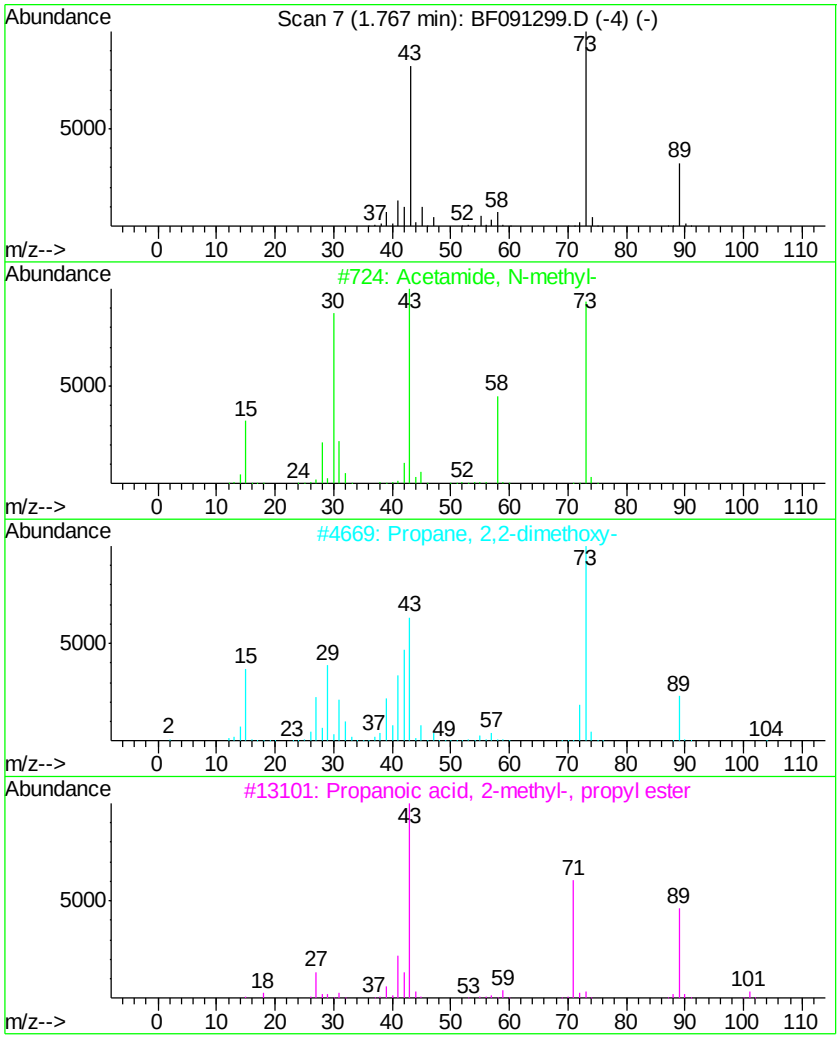
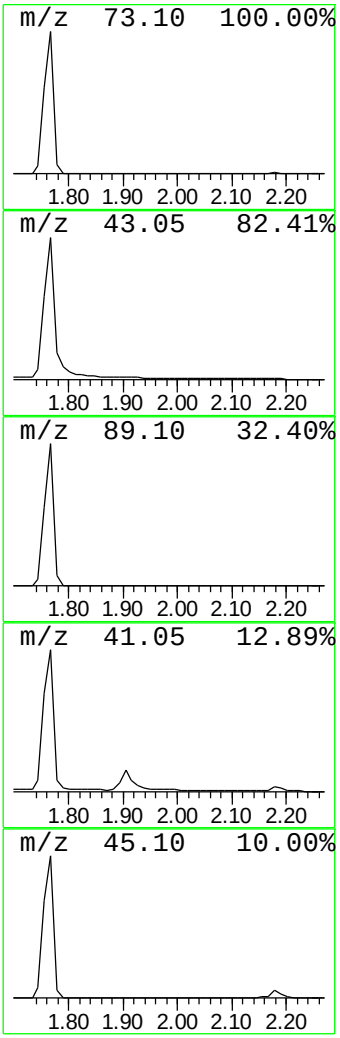
****

Peak Number 1 Acetamide, N-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.77	82.76 ng	5294920	1,4-Dichlorobenzene-d4	6.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	50
2	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	50
3	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	25
4	1-Hexen-4-ol, 1-chloro-3,5-dimet...	162	C8H15ClO	100244-09-5	9
5	Isobutane	58	C4H10	000075-28-5	9





Library Search Compound Report

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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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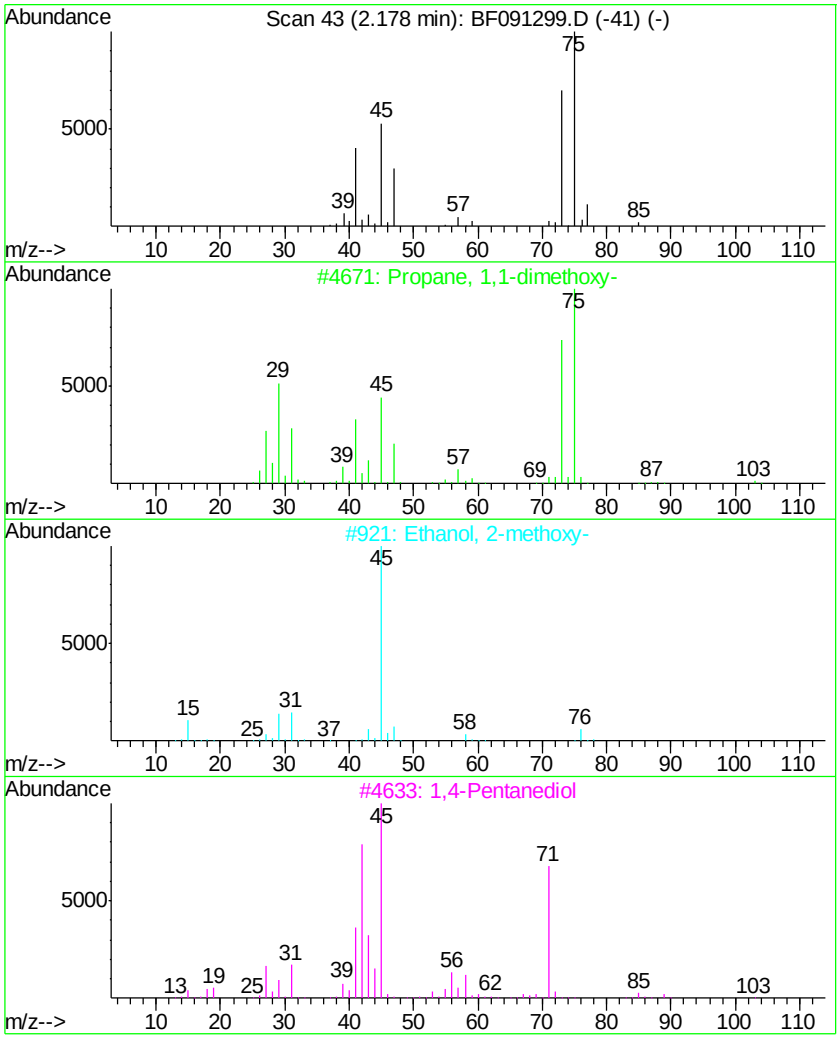
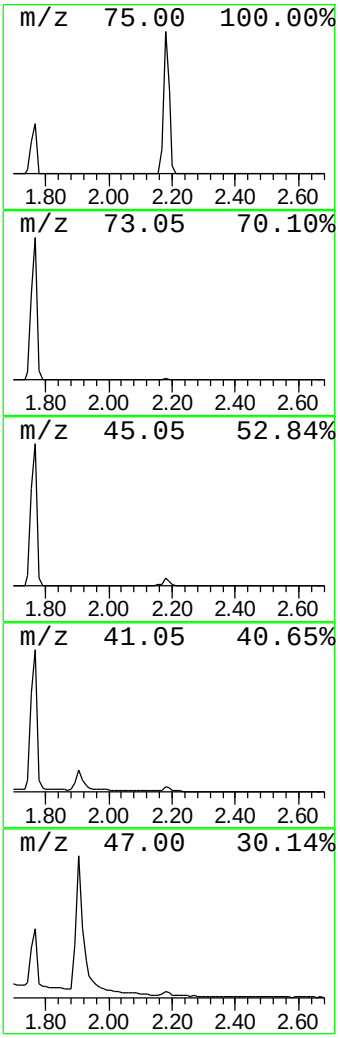
Peak Number 3 Propane, 1,1-dimethoxy- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.18	3.67 ng	234854	1,4-Dichlorobenzene-d4	6.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	64
2	Ethanol, 2-methoxy-	76	C3H8O2	000109-86-4	10
3	1,4-Pentanediol	104	C5H12O2	000626-95-9	9
4	Aminoacetaldehyde dimethyl acetal	105	C4H11NO2	022483-09-6	9
5	Propane, 2-ethoxy-	88	C5H12O	000625-54-7	9





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Instrument : BNA_F
ClientSampleId : DUP-X

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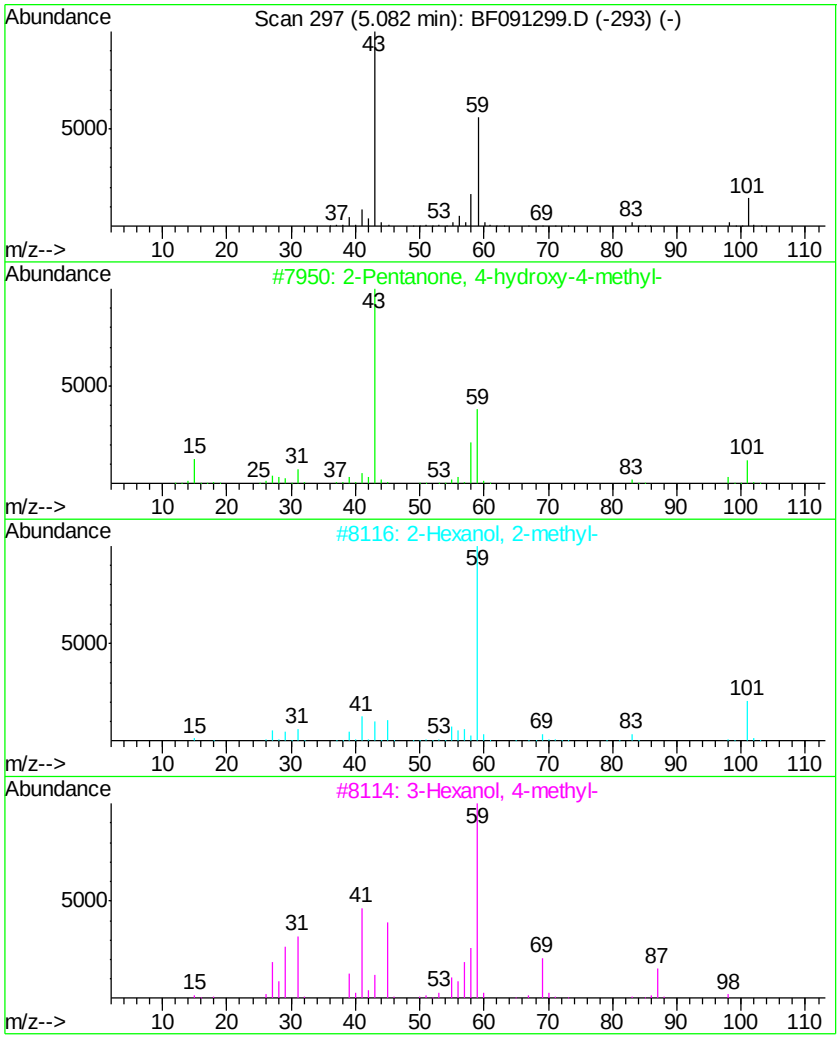
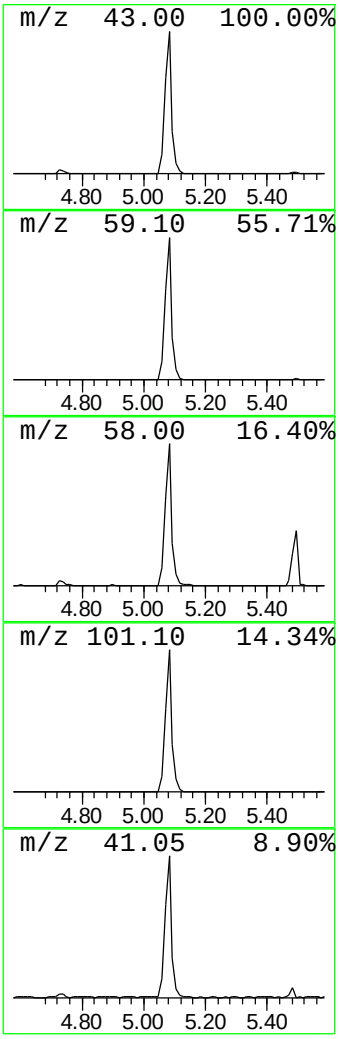
Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.08	34.72 ng	2221310	1,4-Dichlorobenzene-d4	6.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10





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Instrument : BNA_F
ClientSampleId : DUP-X

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112316.M
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TIC Library : C:\DATABASE\NIST02.L
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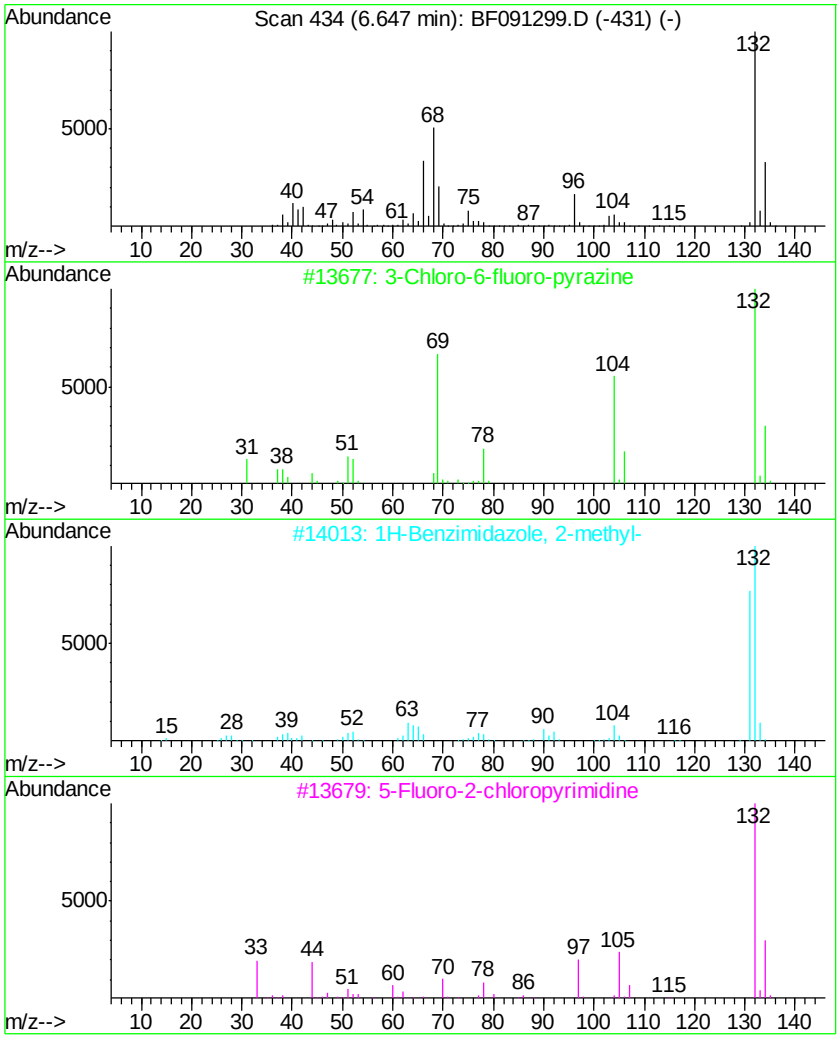
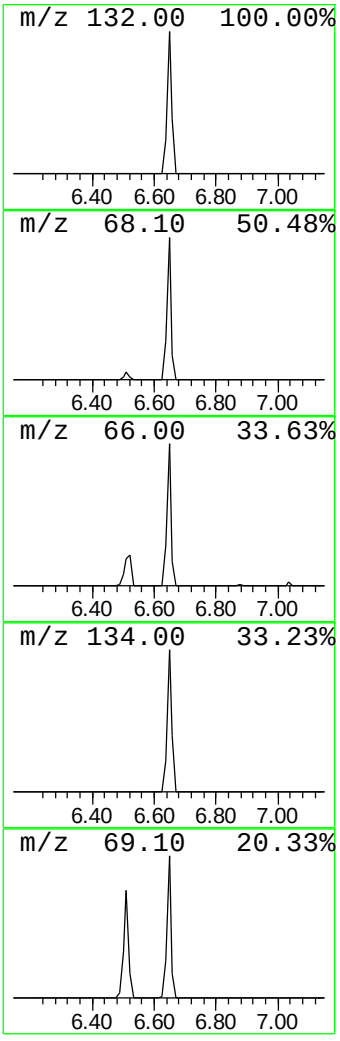
****

Peak Number 5 unknown6.65 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	82.14 ng	5255430	1,4-Dichlorobenzene-d4	6.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4	2-Cyclohexen-1-one	96	C6H8O	000930-68-7	10
5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10





Library Search Compound Report

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Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DUP-X

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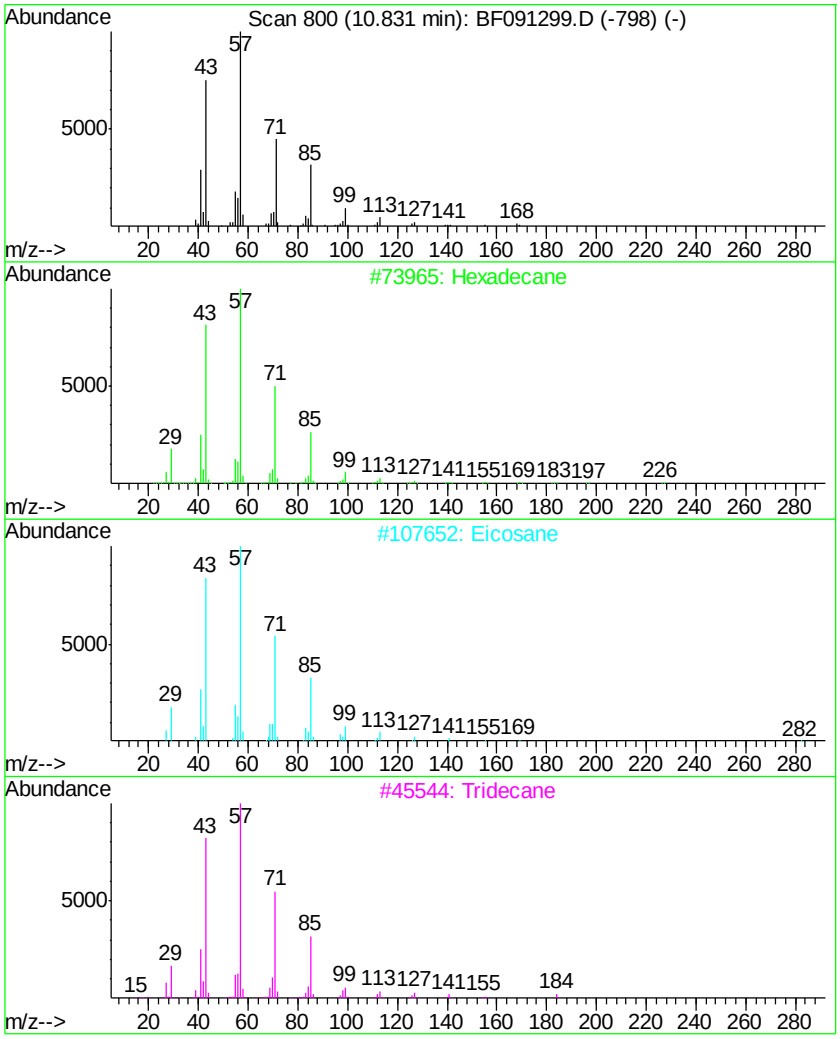
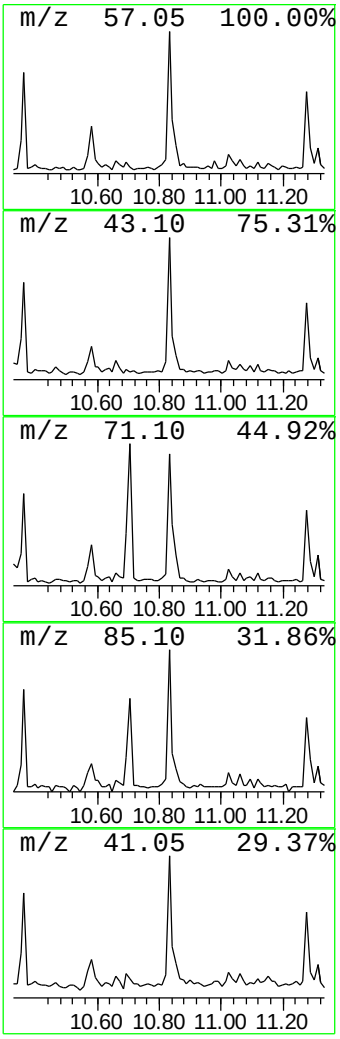
****

Peak Number 7 Hexadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.83	2.26 ng	158838	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	91
2	Eicosane	282	C20H42	000112-95-8	91
3	Tridecane	184	C13H28	000629-50-5	86
4	Dodecane, 3-methyl-	184	C13H28	017312-57-1	72
5	Tetradecane	198	C14H30	000629-59-4	72





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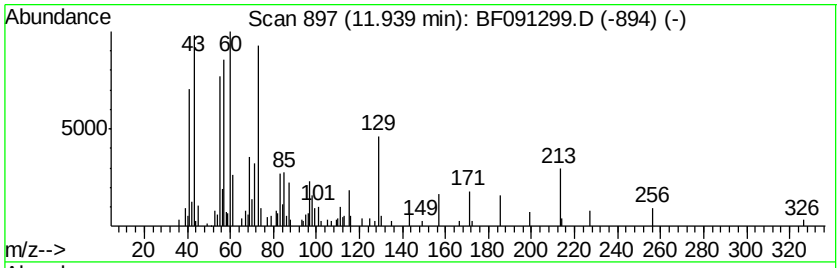
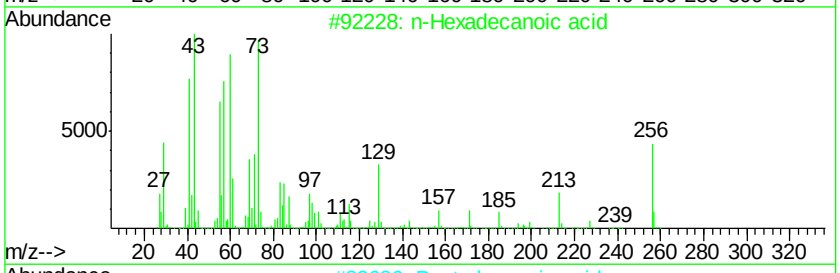
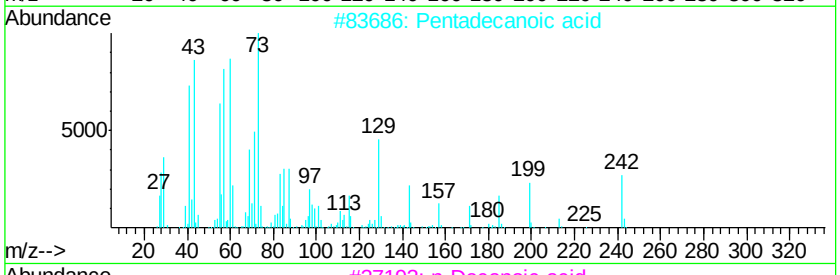
Peak Number 8 n-Hexadecanoic acid Concentration Rank 8

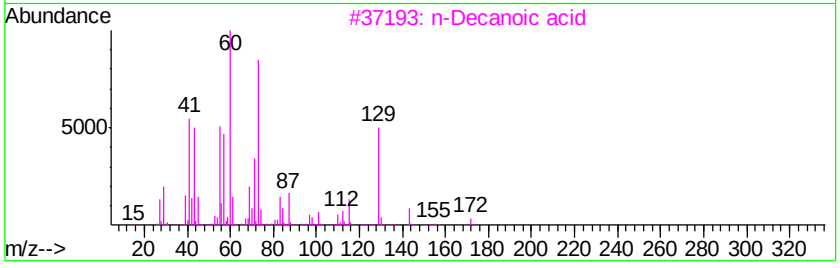
R.T.	EstConc	Area	Relative to ISTD	R.T.
11.94	3.40 ng	238629	Phenanthrene-d10	11.40

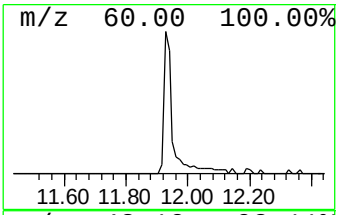
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
3	n-Decanoic acid	172	C10H20O2	000334-48-5	60
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	59
5	Tridecanoic acid	214	C13H26O2	000638-53-9	59

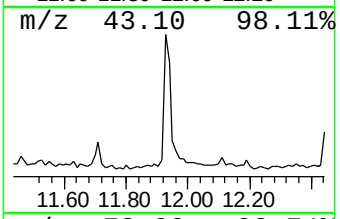


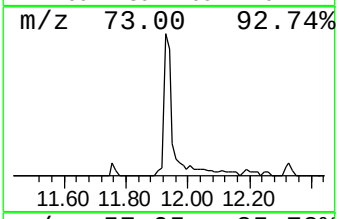


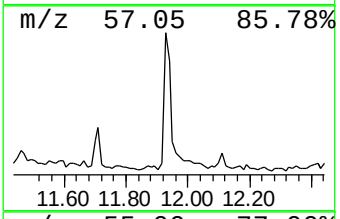


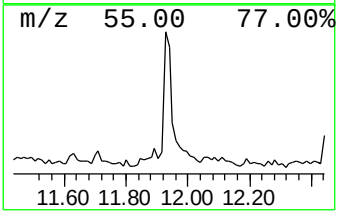












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TIC Library : C:\DATABASE\NIST02.L
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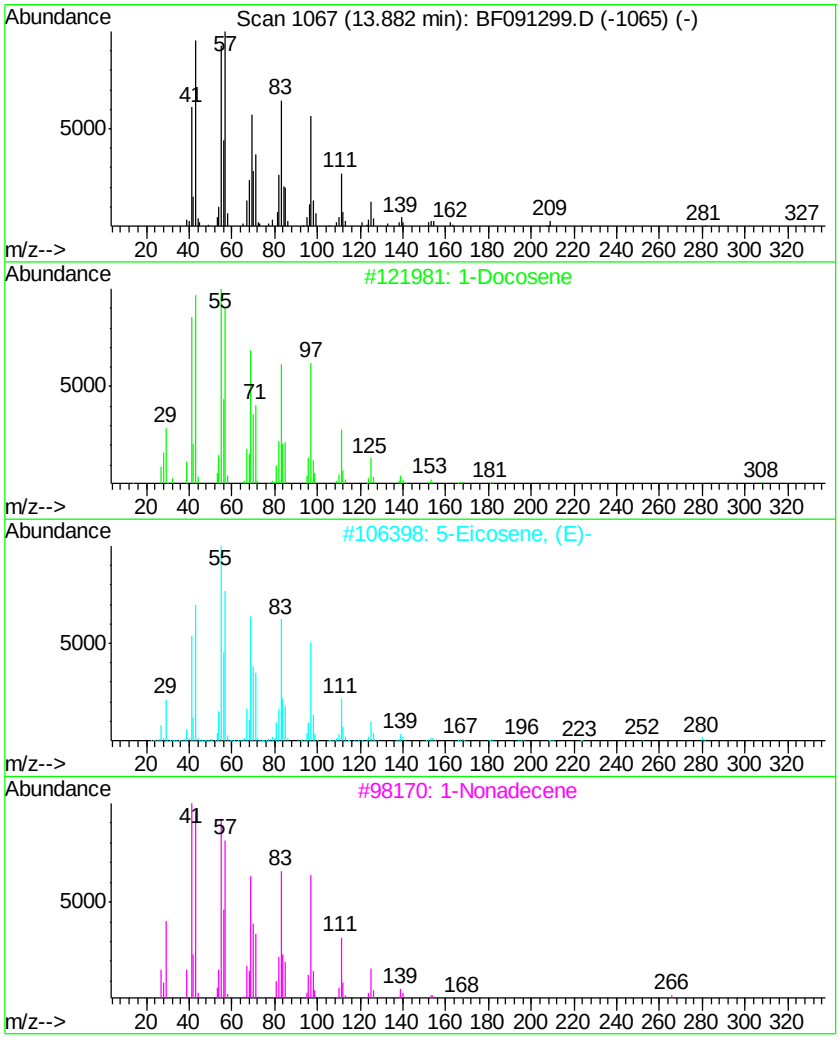
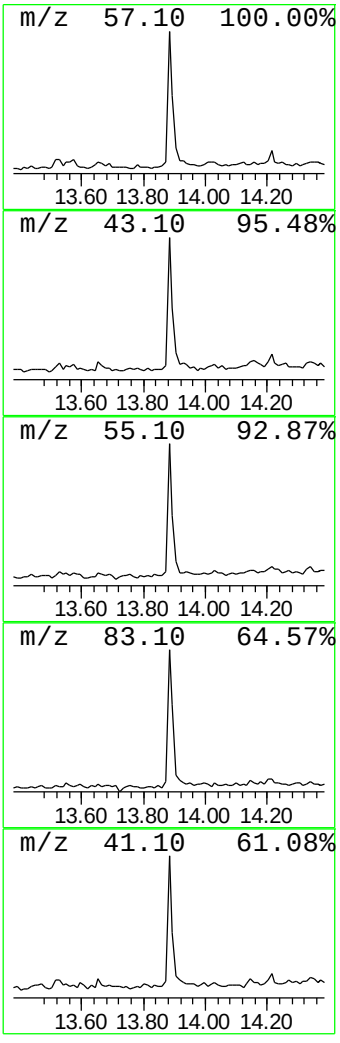
****

Peak Number 9 1-Docosene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.88	3.26 ng	210440	Chrysene-d12	14.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	95
2	5-Eicosene, (E)-	280	C20H40	074685-30-6	90
3	1-Nonadecene	266	C19H38	018435-45-5	90
4	9-Eicosene, (E)-	280	C20H40	074685-29-3	90
5	1-Heptadecanol	256	C17H36O	001454-85-9	87





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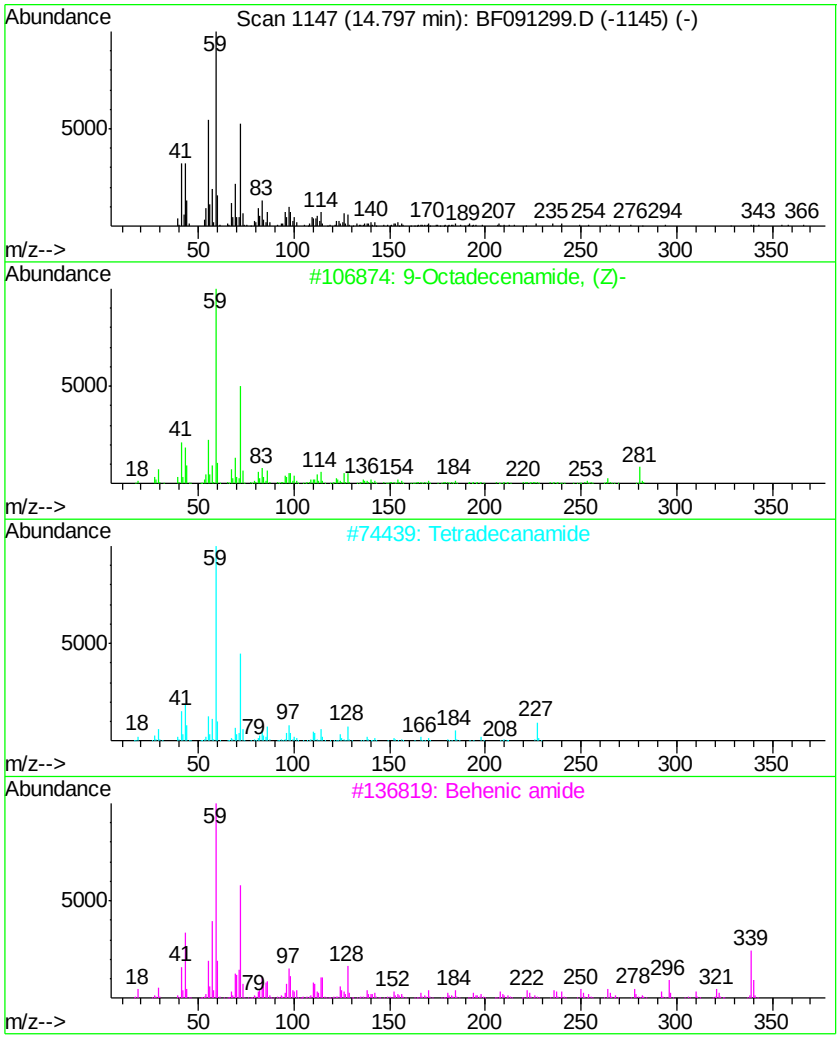
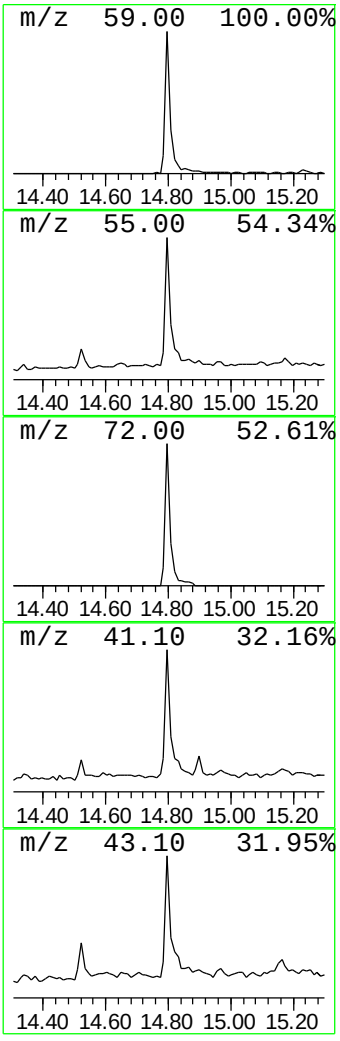
Peak Number 10 9-Octadecenamide, (Z)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.80	5.76 ng	306720	Perylene-d12	15.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	87
2	Tetradecanamide	227	C14H29NO	000638-58-4	86
3	Behenic amide	339	C22H45NO	003061-75-4	86
4	Hexadecanamide	255	C16H33NO	000629-54-9	72
5	Pentadecanamide, 15-bromo-	319	C15H30BrNO	1000163-86-1	59





Tentatively Identified Compound (LSC) summary

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ClientSampleId : DUP-X

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Acetamide, N-methyl-	1.77	82.8	ng	5294920	1	6.88	1279600	20.0
Propane, 1,1-dime...	2.18	3.7	ng	234854	1	6.88	1279600	20.0
2-Pentanone, 4-hy...	5.08	34.7	ng	2221310	1	6.88	1279600	20.0
unknown6.65	6.65	82.1	ng	5255430	1	6.88	1279600	20.0
Hexadecane	10.83	2.3	ng	158838	4	11.40	1405670	20.0
n-Hexadecanoic acid	11.94	3.4	ng	238629	4	11.40	1405670	20.0
1-Docosene	13.88	3.3	ng	210440	5	14.03	1289140	20.0
9-Octadecenamide,...	14.80	5.8	ng	306720	6	15.47	1064510	20.0