LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF021717\
Data File : BF093017.D
Acq On : 17 Feb 2017 18:20
Operator : SJ/MA
Sample : I1879-05
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-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-BF013017.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	4.373	198	200	209	rBV	74731	126993	3.09%	0.329%
2	5.024	255	257	266	rBV	1145362	1697194	41.35%	4.392%
3	5.459	292	295	297	rBV	2932376	3791911	92.37%	9.812%
4	6.499	382	386	388	rBV	2959834	4096548	99.80%	10.601%
5	6.624	394	397	399	rBV	3752122	3707741	90.32%	9.595%
6	6.853	415	417	420	rBV	1297170	1069474	26.05%	2.768%
7	7.013	428	431	433	rBV	3153247	2858453	69.63%	7.397%
8	7.425	464	467	469	rBV	2365579	2484417	60.52%	6.429%
9	8.145	527	530	532	rBV	1213153	1392517	33.92%	3.603%
10	9.219	621	624	626	rBV	3825307	4104933	100.00%	10.622%
11	9.608	656	658	661	rBV	652847	567279	13.82%	1.468%
12	9.825	669	677	680	rBV2	48523	110386	2.69%	0.286%
13	9.893	680	683	685	rVB	1605341	1550306	37.77%	4.012%
14	10.316	719	720	722	rVB	59865	64870	1.58%	0.168%
15	10.533	736	739	743	rBV	25840	47950	1.17%	0.124%
16	10.682	749	752	754	rBV	2083680	2296143	55.94%	5.942%
17	10.796	760	762	766	rVB	99283	132168	3.22%	0.342%
18	11.242	798	801	802	rBV	108219	98118	2.39%	0.254%
19	11.368	810	812	815	rBV	1108556	1519936	37.03%	3.933%
20	11.665	836	838	840	rBV	91228	74217	1.81%	0.192%
21	12.957	948	951	954	rBV	3081616	3506602	85.42%	9.074%
22	13.848	1027	1029	1037	rBV	209603	279688	6.81%	0.724%
23	14.008	1040	1043	1045	rBV	1577098	1461306	35.60%	3.781%
24	14.477	1081	1084	1088	rBV	37771	83006	2.02%	0.215%
25	14.751	1106	1108	1112	rBV2	99886	141415	3.45%	0.366%
26	15.094	1136	1138	1140	rBV	55093	71182	1.73%	0.184%
27	15.437	1165	1168	1174	rBV	913511	1171099	28.53%	3.030%
28	15.871	1203	1206	1209	rBV	63993	93321	2.27%	0.241%
29	16.900	1294	1296	1301	rVB	20200	44668	1.09%	0.116%

Sum of corrected areas: 38643841

LSC Report - Integrated Chromatogram

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Misc :
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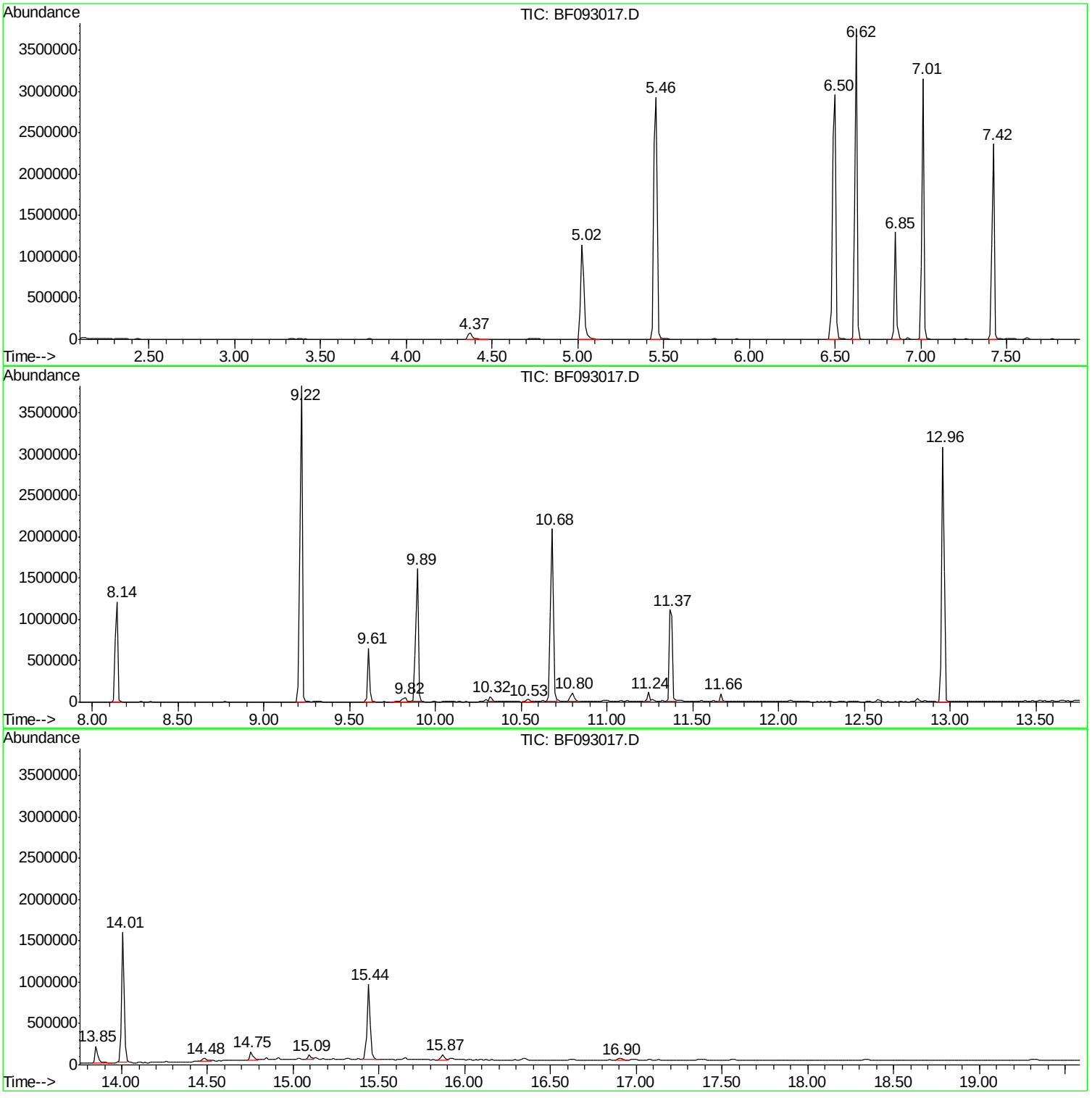
Instrument : BNA_F
ClientSampleId : M-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF021717\
Data File : BF093017.D
Acq On : 17 Feb 2017 18:20
Operator : SJ/MA
Sample : I1879-05
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.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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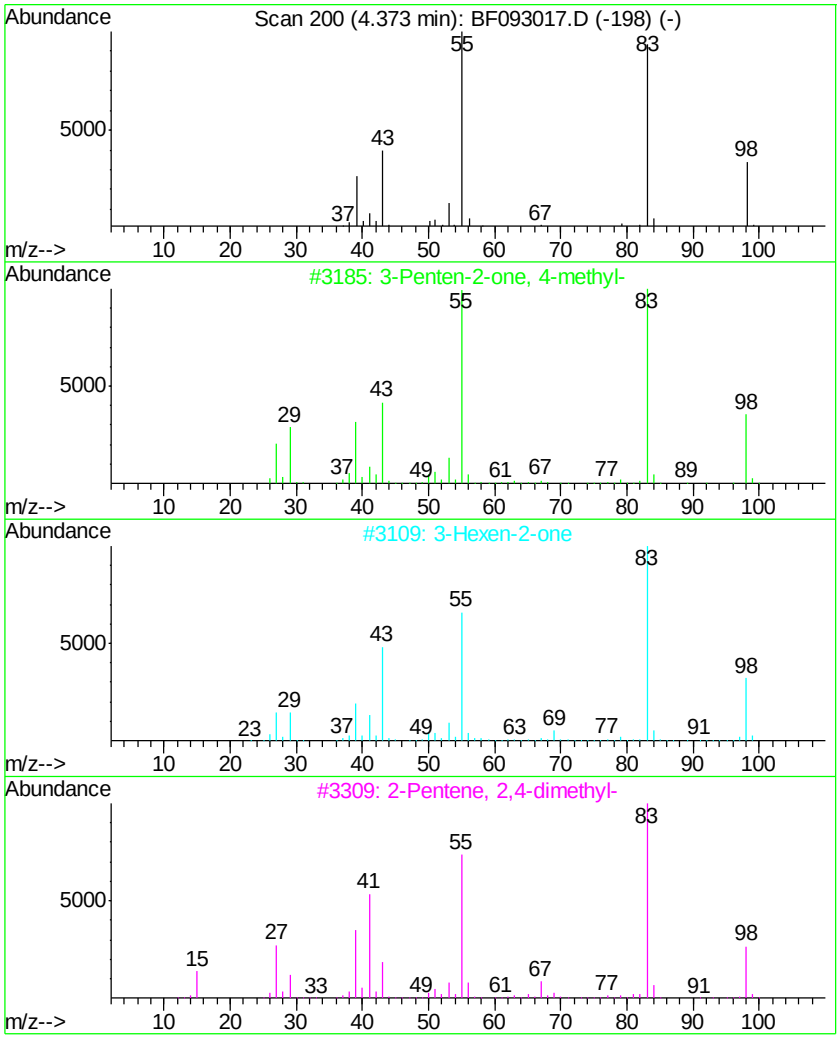
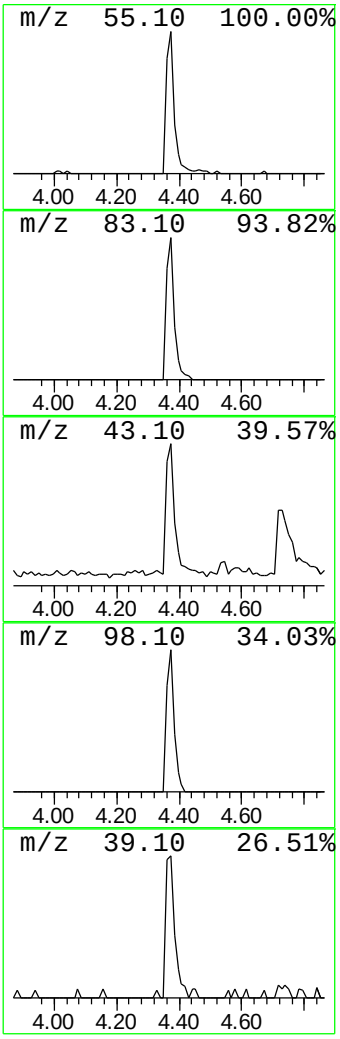
Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.37	2.37 ng	126993	1,4-Dichlorobenzene-d4	6.85

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	87
3	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80
4	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	72
5	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	72





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Sample : I1879-05
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.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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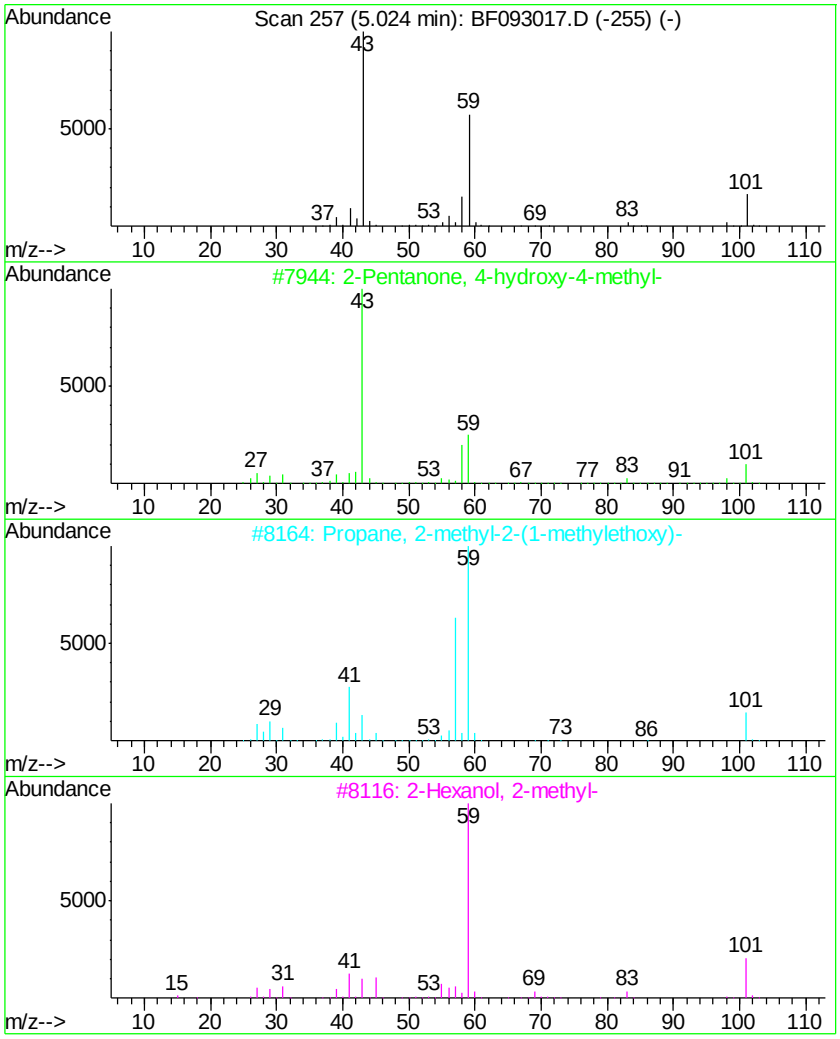
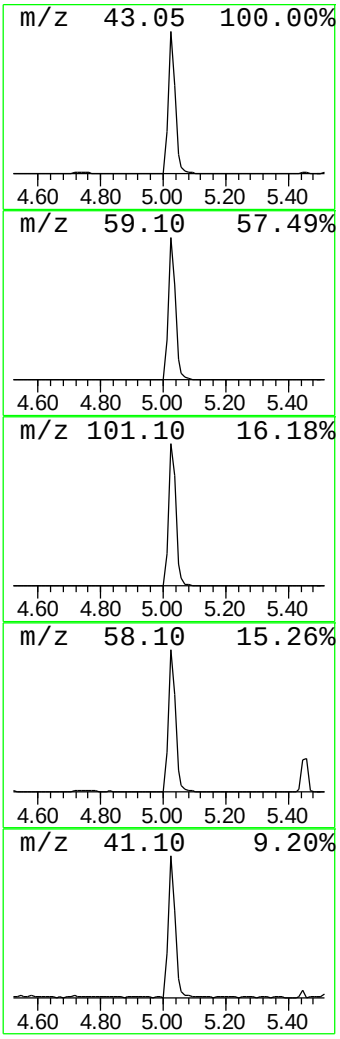
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.02	31.74 ng	1697190	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32





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Sample : I1879-05
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Instrument : BNA_F
ClientSampleId : M-3

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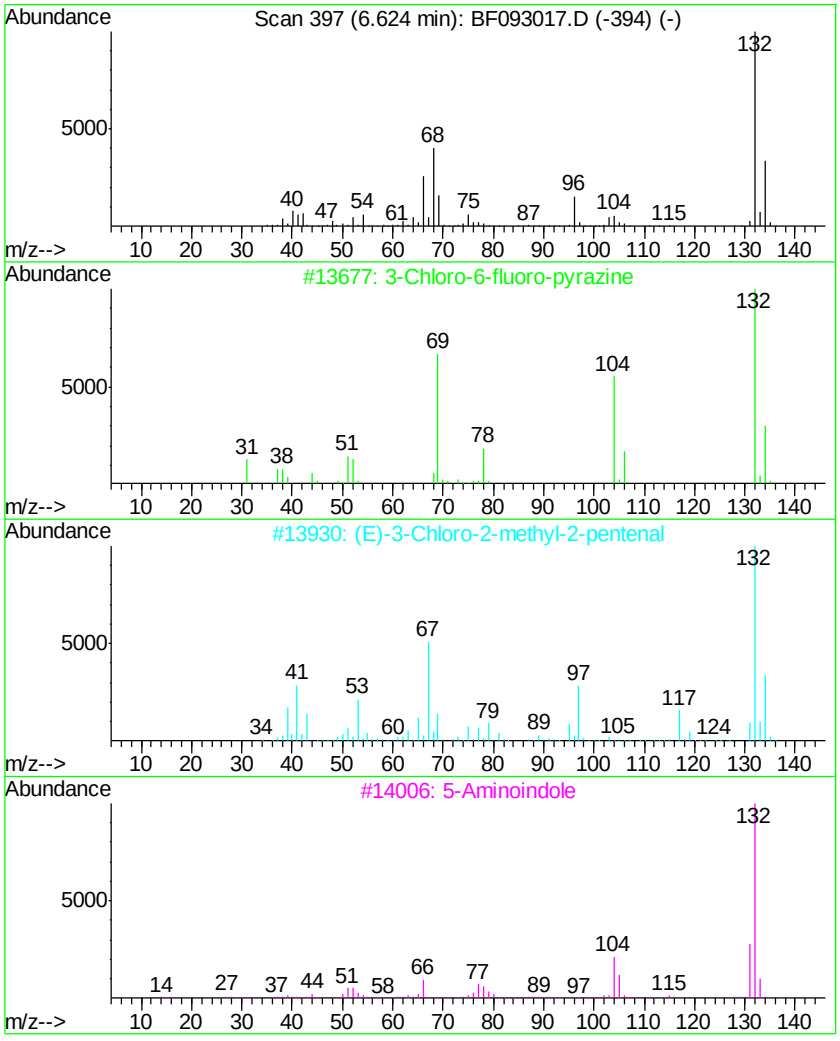
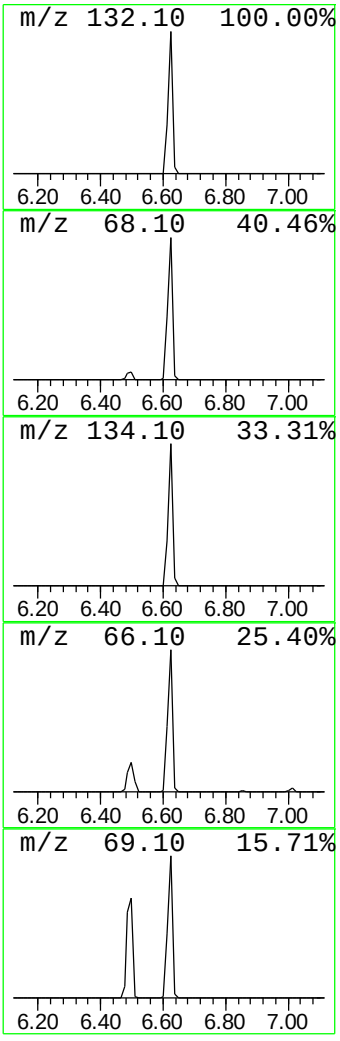
Peak Number 3 unknown6.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	69.34 ng	3707740	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9
5	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9





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ClientSampleId : M-3

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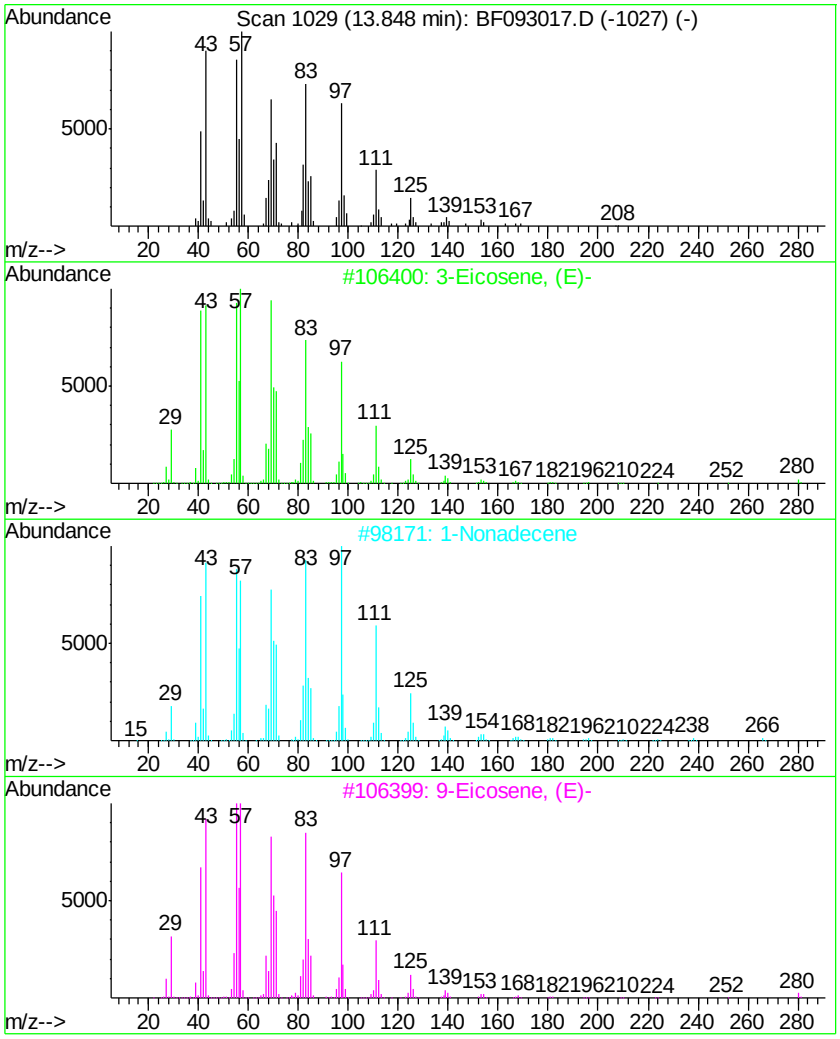
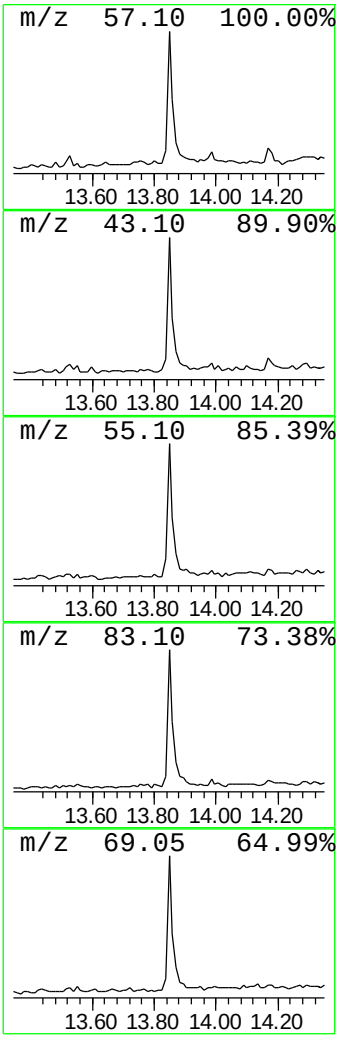
Peak Number 5 3-Eicosene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.85	3.83 ng	279688	Chrysene-d12	14.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
2	1-Nonadecene	266	C19H38	018435-45-5	91
3	9-Eicosene, (E)-	280	C20H40	074685-29-3	91
4	2- Bromopropionic acid, pentadec...	362	C18H35BrO2	1000292-44-2	91
5	1-Docosene	308	C22H44	001599-67-3	91





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Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
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TIC Library : C:\DATABASE\NIST02.L
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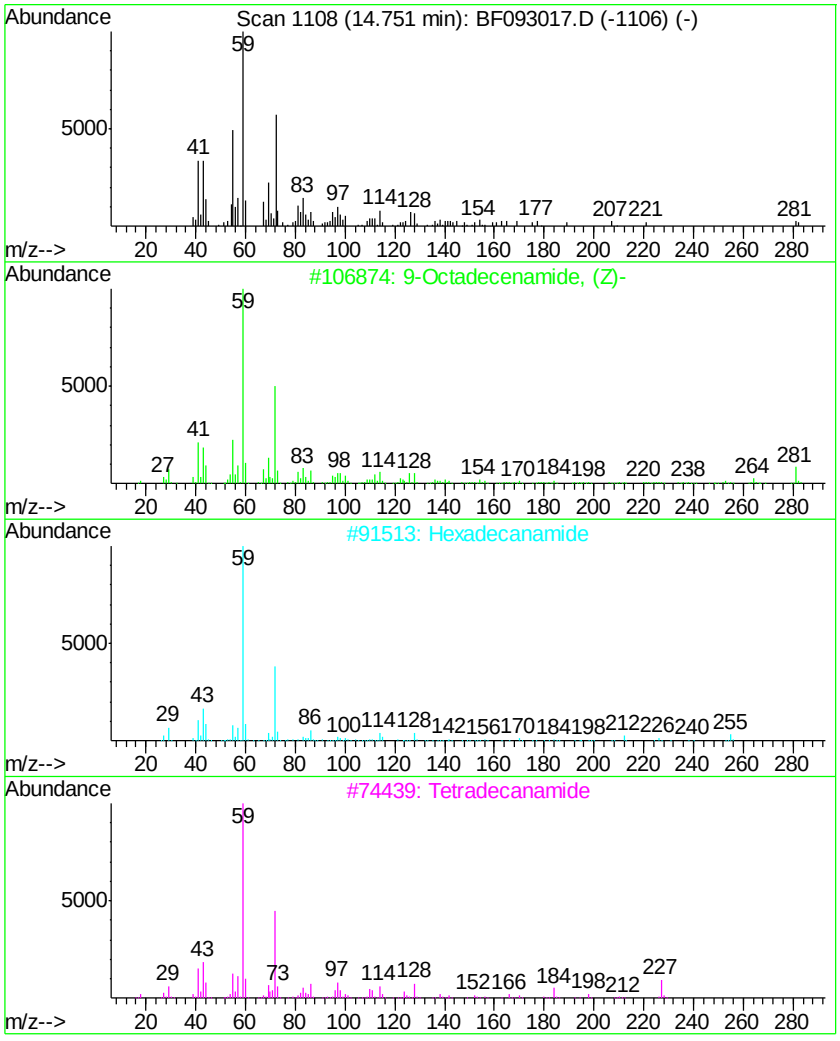
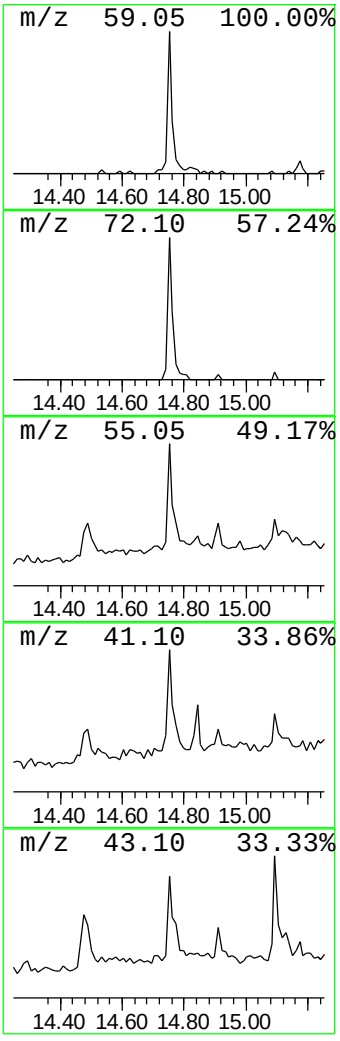
****

Peak Number 6 9-Octadecenamide, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.75	2.42 ng	141415	Perylene-d12	15.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
2	Hexadecanamide	255	C16H33NO	000629-54-9	72
3	Tetradecanamide	227	C14H29NO	000638-58-4	64
4	Decanamide-	171	C10H21NO	002319-29-1	59
5	Pentadecanamide, 15-bromo-	319	C15H30BrNO	1000163-86-1	59





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
3-Penten-2-one, 4...	4.37	2.4	ng	126993	1	6.85	1069470	20.0
2-Pentanone, 4-hy...	5.02	31.7	ng	1697190	1	6.85	1069470	20.0
unknown6.62	6.62	69.3	ng	3707740	1	6.85	1069470	20.0
3-Eicosene, (E)-	13.85	3.8	ng	279688	5	14.01	1461310	20.0
9-Octadecenamide,...	14.75	2.4	ng	141415	6	15.44	1171100	20.0